



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2021 – 06:46 PM EDT

PDB ID : 7RF1
Title : RT XFEL structure of Photosystem II averaged across all S-states at 1.89 Angstrom resolution
Authors : Hussein, R.; Ibrahim, M.; Bhowmick, A.; Simon, P.S.; Chatterjee, R.; Lassalle, L.; Doyle, M.D.; Bogacz, I.; Kim, I.-S.; Cheah, M.H.; Gul, S.; de Lichtenberg, C.; Chernev, P.; Pham, C.C.; Young, I.D.; Carbajo, S.; Fuller, F.D.; Alonso-Mori, R.; Batyuk, A.; Sutherlin, K.D.; Brewster, A.S.; Bolotovskii, R.; Mendez, D.; Holton, J.M.; Moriarty, N.W.; Adams, P.D.; Bergmann, U.; Sauter, N.K.; Dobbek, H.; Messinger, J.; Zouni, A.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on : 2021-07-13
Resolution : 1.89 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

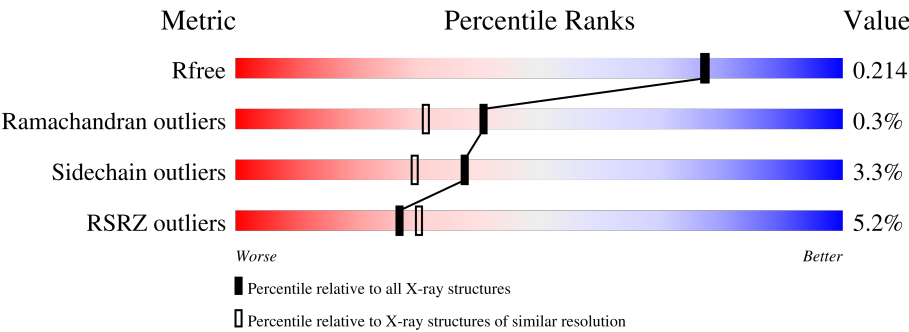
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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.



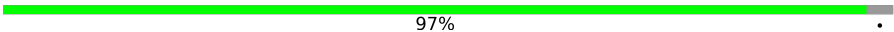
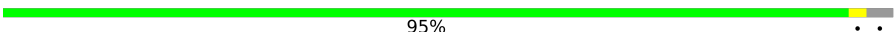










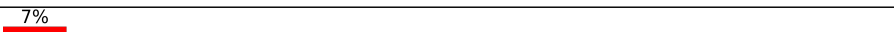

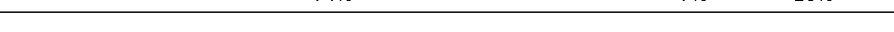
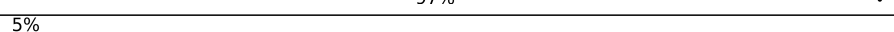
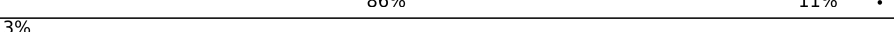








Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	6207 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	344	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>97%</div><div></div></div>
1	a	344	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>93%</div><div></div></div>
2	B	510	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>97%</div><div></div></div>
2	b	510	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>96%</div><div></div></div>
3	C	461	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>95%</div><div></div></div>
3	c	461	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>95%</div><div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	352	 97%
4	d	352	 95%
5	E	84	 94%
5	e	84	 94%
6	F	45	 76% 24%
6	f	45	 76% 24%
7	H	66	 95%
7	h	66	 88% 8% 5%
8	I	38	 84% 11% 5%
8	i	38	 87% 8% 5%
9	J	40	 90% 10%
9	j	40	 85% 5% 10%
10	K	46	 78% 20%
10	k	46	 74% 7% 20%
11	L	37	 97%
11	l	37	 86% 11%
12	M	36	 89% 8%
12	m	36	 86% 11%
13	O	272	 85% 10%
13	o	272	 86% 10%
14	T	32	 88% 6% 6%
14	t	32	 91% 6%
15	U	134	 69% 28%
15	u	134	 70% 28%
16	V	163	 80% 16%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	v	163	
17	Y	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	R	41	
20	r	41	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	404	X	-	-	-
23	CLA	A	407	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	501	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	D	404	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	408	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	c	501	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	h	101	X	-	-	-
27	STE	C	528	-	-	-	X
27	STE	I	102	-	-	-	X
27	STE	i	101	-	-	-	X

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 104284 atoms, of which 51760 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	334	Total	C	H	N	O	S	0	0	0
			5140	1717	2518	431	459	15			
1	a	334	Total	C	H	N	O	S	0	0	0
			5129	1714	2510	431	459	15			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	H	N	O	S	0	5	0
			7878	2631	3873	666	695	13			
2	b	505	Total	C	H	N	O	S	0	1	0
			7824	2614	3840	665	692	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	442	Total	C	H	N	O	S	0	2	0
			6775	2248	3350	571	593	13			
3	c	451	Total	C	H	N	O	S	0	2	0
			6926	2290	3426	587	610	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	341	Total	C	H	N	O	S	0	0	0
			5338	1800	2621	444	461	12			
4	d	341	Total	C	H	N	O	S	0	1	0
			5350	1804	2627	444	463	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	82	Total	C	H	N	O	0	1	0
			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	0	0	0
			598	204	305	43			

Continued on next page...

Continued from previous page...

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	H	N	O	0	1	0
			3700	1168	1830	313	385			
13	o	244	Total	C	H	N	O	0	0	0
			3720	1170	1846	317	383			

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	H	N	O	0	0	0
			1547	491	773	129	154			
15	u	97	Total	C	H	N	O	0	0	0
			1547	491	773	129	154			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	H	N	O	S	0	0
			2137	675	1073	177	208	4		
16	v	137	Total	C	H	N	O	S	0	0
			2137	675	1073	177	208	4		

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

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

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

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

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

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

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

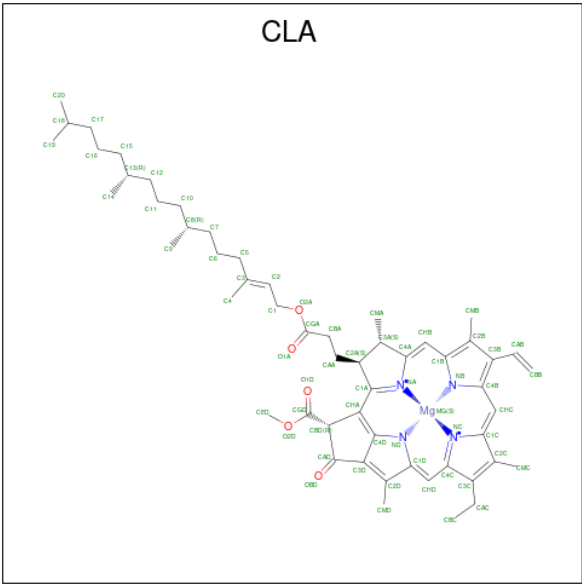
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

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

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

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	C	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

Continued on next page...

Continued from previous page...

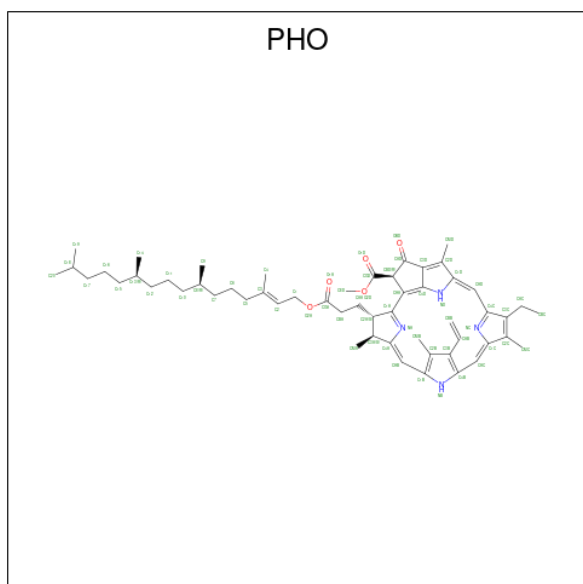
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total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

Continued on next page...

Continued from previous page...

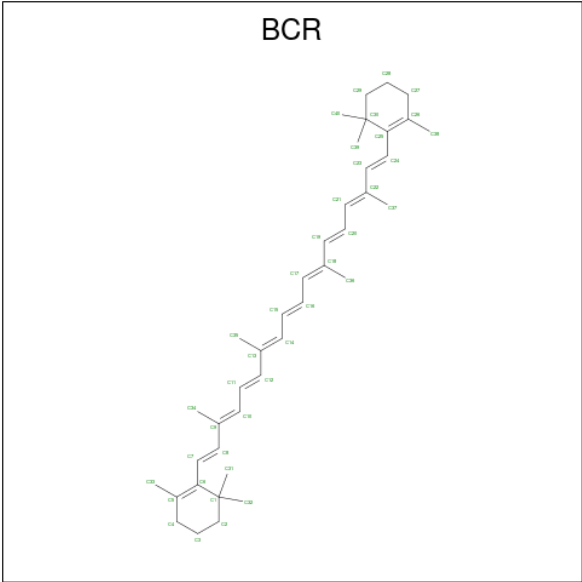
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	h	1	Total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

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



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

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



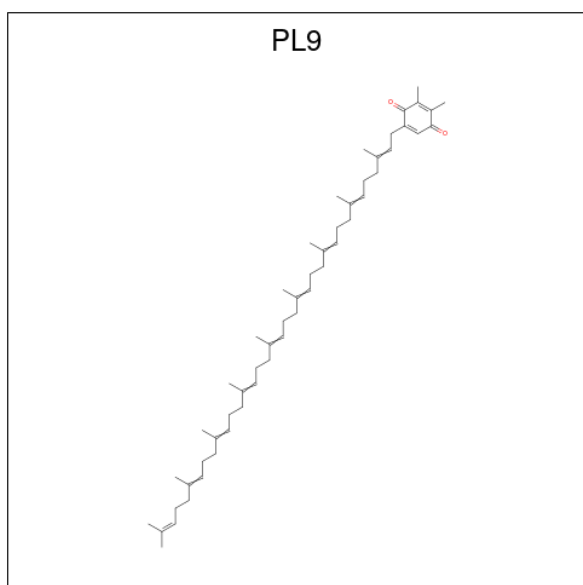
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	C	1	Total	C	H	0	0
			96	40	56		
25	C	1	Total	C	H	0	0
			96	40	56		
25	C	1	Total	C	H	0	0
			96	40	56		
25	D	1	Total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

Continued on next page...

Continued from previous page...

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

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



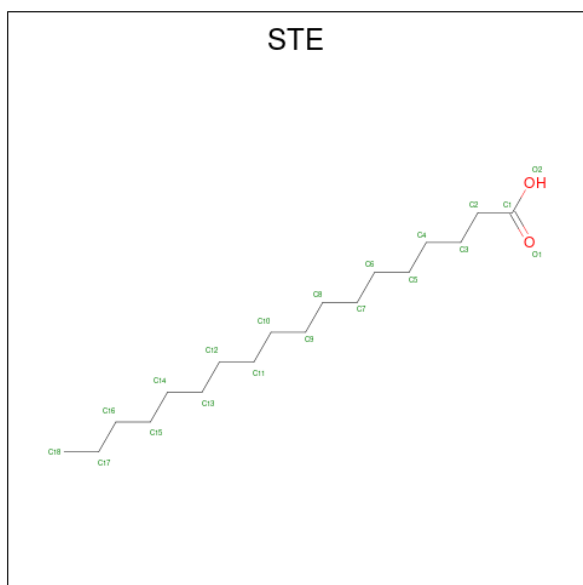
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	H	O	0	0
			135	53	80	2		
26	D	1	Total	C	H	O	0	0
			135	53	80	2		

Continued on next page...

Continued from previous page...

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

- Molecule 27 is STEARIC ACID (three-letter code: STE) (formula: $C_{18}H_{36}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C			0	0
			9	9				
27	A	1	Total	C			0	0
			8	8				
27	A	1	Total	C	H		0	0
			52	17	35			
27	A	1	Total	C			0	0
			11	11				
27	B	1	Total	C	H	O	0	0
			43	15	26	2		
27	B	1	Total	C	H	O	0	0
			28	10	16	2		
27	B	1	Total	C	H		0	0
			41	15	26			
27	C	1	Total	C	H	O	0	0
			35	12	21	2		
27	C	1	Total	C	H		0	0
			15	5	10			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	C	1	Total C 7 7	0	0
27	C	1	Total C H O 28 10 16 2	0	0
27	C	1	Total C H 47 16 31	0	0
27	C	1	Total C 8 8	0	0
27	C	1	Total C 14 14	0	0
27	C	1	Total C H 43 14 29	0	0
27	D	1	Total C H O 55 18 35 2	0	0
27	D	1	Total C 9 9	0	0
27	E	1	Total C H O 28 10 16 2	0	0
27	E	1	Total C 12 12	0	0
27	E	1	Total C H O 55 18 35 2	0	0
27	H	1	Total C H 53 18 35	0	0
27	I	1	Total C H 41 15 26	0	0
27	I	1	Total C H O 45 15 28 2	0	0
27	J	1	Total C H O 28 10 16 2	0	0
27	M	1	Total C H O 37 13 22 2	0	0
27	M	1	Total C H 26 10 16	0	0
27	T	1	Total C H 46 16 30	0	0
27	Z	1	Total C H 52 17 35	0	0
27	a	1	Total C H 26 10 16	0	0
27	a	1	Total C H O 28 10 16 2	0	0

Continued on next page...

Continued from previous page...

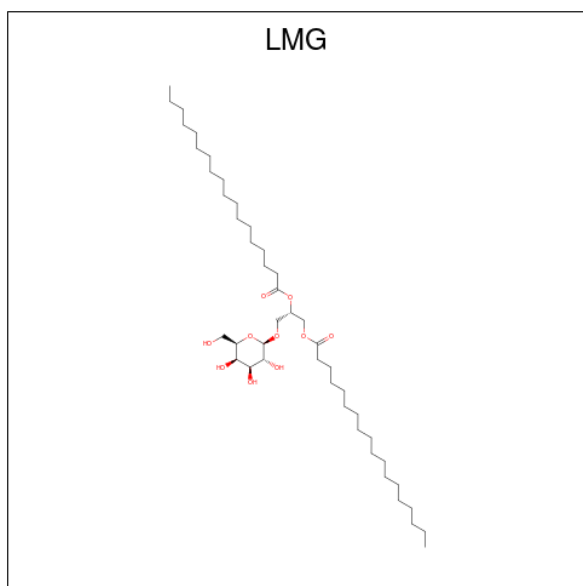
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	b	1	Total C H O 55 18 35 2	0	0
27	b	1	Total C O 20 18 2	0	0
27	b	1	Total C H O 40 14 24 2	0	0
27	b	1	Total C H 26 10 16	0	0
27	b	1	Total C 11 11	0	0
27	c	1	Total C H 37 13 24	0	0
27	c	1	Total C H 53 18 35	0	0
27	d	1	Total C H O 43 15 26 2	0	0
27	d	1	Total C H O 28 10 16 2	0	0
27	d	1	Total C 10 10	0	0
27	e	1	Total C 9 9	0	0
27	e	1	Total C 8 8	0	0
27	e	1	Total C 9 9	0	0
27	e	1	Total C O 13 11 2	0	0
27	i	1	Total C O 12 10 2	0	0
27	i	1	Total C H 18 6 12	0	0
27	j	1	Total C H O 28 10 16 2	0	0
27	j	1	Total C 16 16	0	0
27	l	1	Total C H 53 18 35	0	0
27	m	1	Total C H O 28 10 16 2	0	0
27	m	1	Total C H 44 15 29	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	t	1	Total	C	H	O	0	0
			34	12	20	2		
27	t	1	Total	C	H	O	0	0
			46	16	28	2		
27	x	1	Total	C	H	O	0	0
			55	18	35	2		
27	z	1	Total	C	H		0	0
			24	9	15			

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



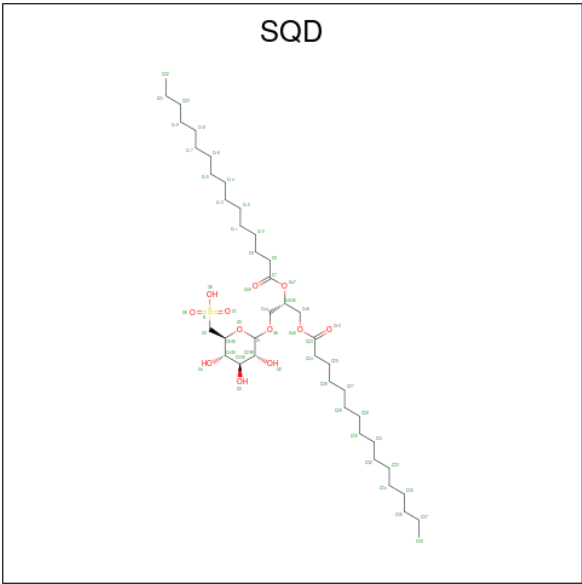
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	H	O	0	0
			114	38	66	10		
28	B	1	Total	C	H	O	0	0
			109	35	64	10		
28	C	1	Total	C	H	O	0	0
			83	26	47	10		
28	C	1	Total	C	H	O	0	0
			114	38	66	10		
28	D	1	Total	C	H	O	0	0
			124	40	74	10		
28	D	1	Total	C	H	O	0	0
			123	41	72	10		
28	M	1	Total	C	H	O	0	0
			123	41	72	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	a	1	Total	C	H	O	0	0
			141	45	86	10		
28	b	1	Total	C	O		0	0
			24	20	4			
28	b	1	Total	C	H	O	0	0
			123	41	72	10		
28	b	1	Total	C	H	O	0	0
			141	45	86	10		
28	c	1	Total	C	H	O	0	0
			75	25	45	5		
28	c	1	Total	C	H	O	0	0
			110	36	64	10		
28	c	1	Total	C	H	O	0	0
			117	38	69	10		
28	c	1	Total	C	H	O	0	0
			117	39	68	10		
28	d	1	Total	C	H	O	0	0
			102	34	58	10		

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



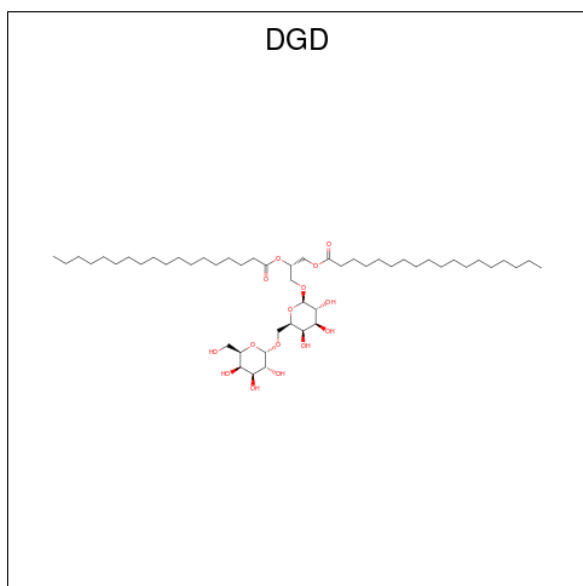
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
29	A	1	Total	C	O	S		0	0
			54	41	12	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	F	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
29	a	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
29	a	1	Total	C	O	S		0	0
			54	41	12	1			
29	b	1	Total	C	H	O	S	0	0
			113	36	64	12	1		
29	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		
29	l	1	Total	C	H	O	S	0	0
			131	41	77	12	1		

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



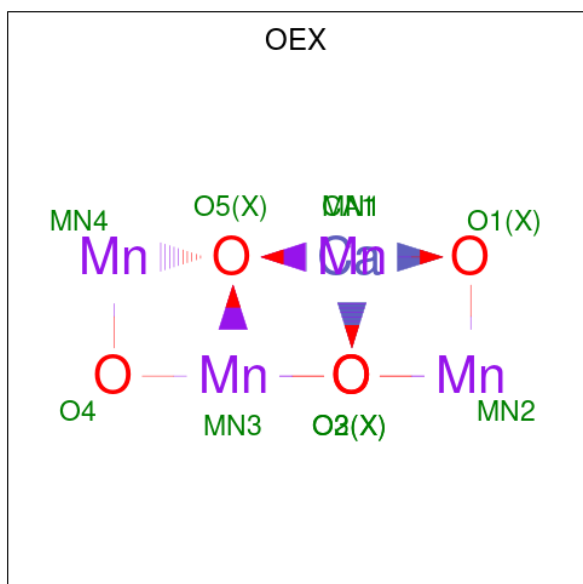
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
30	A	1	Total	C	H	O		0	0
			162	51	96	15			
30	C	1	Total	C	H	O		0	0
			144	47	82	15			
30	C	1	Total	C	H	O		0	0
			144	47	82	15			
30	C	1	Total	C	H	O		0	0
			144	47	82	15			
30	H	1	Total	C	H	O		0	0
			144	47	82	15			

Continued on next page...

Continued from previous page...

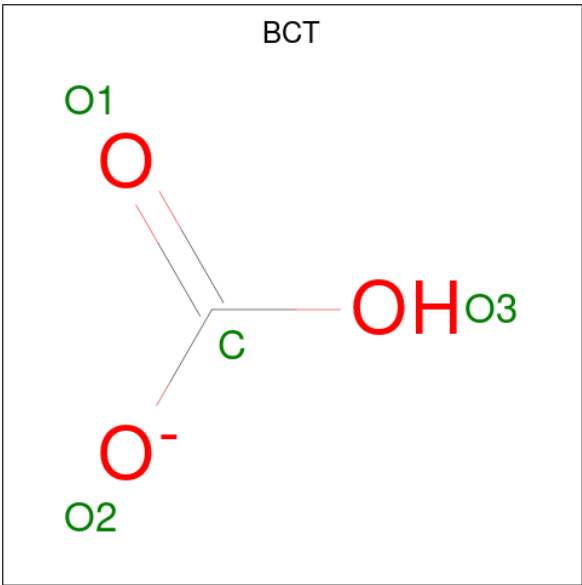
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	h	1	Total	C	H	O	0	0
			144	47	82	15		

- Molecule 31 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



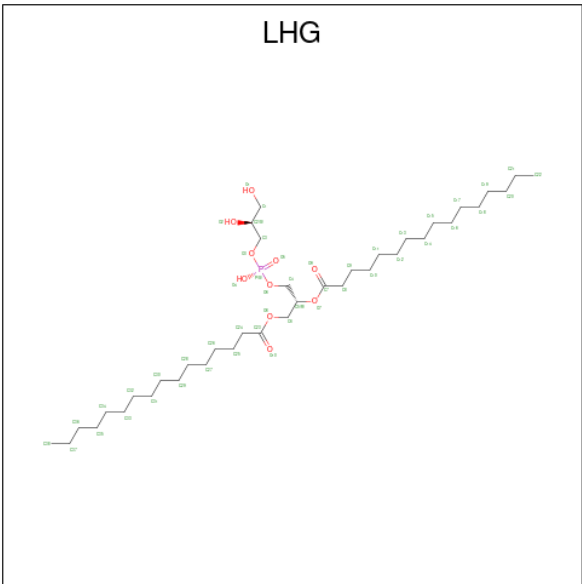
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
31	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

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



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

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



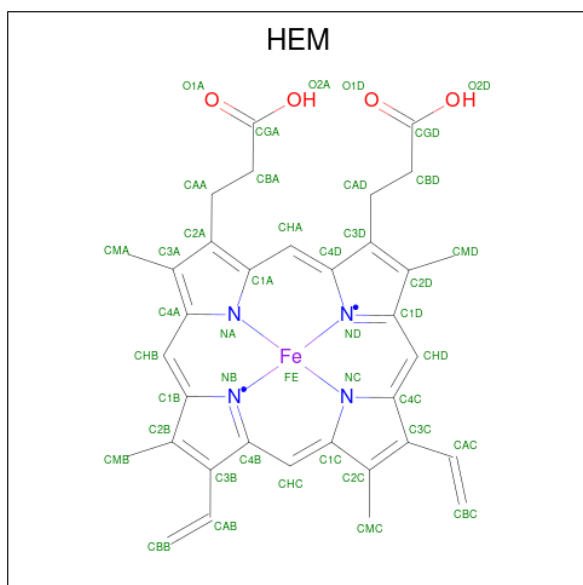
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

Continued on next page...

Continued from previous page...

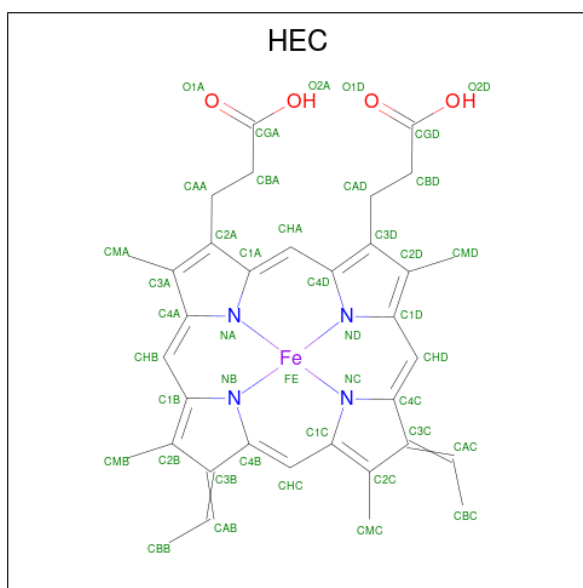
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	D	1	Total 114	C 36	H 67	O 10	P 1	0	0
33	D	1	Total 123	C 38	H 74	O 10	P 1	0	0
33	E	1	Total 123	C 38	H 74	O 10	P 1	0	0
33	L	1	Total 123	C 38	H 74	O 10	P 1	0	0
33	a	1	Total 99	C 31	H 57	O 10	P 1	0	0
33	d	1	Total 123	C 38	H 74	O 10	P 1	0	0
33	d	1	Total 123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

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



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

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



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

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	144	Total	O	0	0
			144	144		
36	B	202	Total	O	0	0
			202	202		
36	C	180	Total	O	0	0
			180	180		
36	D	137	Total	O	0	0
			137	137		
36	E	20	Total	O	0	0
			20	20		
36	F	11	Total	O	0	0
			11	11		
36	H	26	Total	O	0	0
			26	26		
36	I	9	Total	O	0	0
			9	9		
36	J	13	Total	O	0	0
			13	13		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	K	4	Total 4	O 4	0	0
36	L	10	Total 10	O 10	0	0
36	M	7	Total 7	O 7	0	0
36	O	104	Total 104	O 104	0	0
36	T	9	Total 9	O 9	0	0
36	U	45	Total 45	O 45	0	0
36	V	82	Total 82	O 82	0	0
36	Y	1	Total 1	O 1	0	0
36	X	12	Total 12	O 12	0	0
36	a	115	Total 115	O 115	0	0
36	b	200	Total 200	O 200	0	0
36	c	171	Total 171	O 171	0	0
36	d	125	Total 125	O 125	0	0
36	e	10	Total 10	O 10	0	0
36	f	10	Total 10	O 10	0	0
36	h	23	Total 23	O 23	0	0
36	i	5	Total 5	O 5	0	0
36	j	6	Total 6	O 6	0	0
36	k	5	Total 5	O 5	0	0
36	l	15	Total 15	O 15	0	0
36	m	7	Total 7	O 7	0	0

Continued on next page...

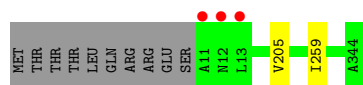
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	o	110	Total 110	O 110	0	0
36	t	12	Total 12	O 12	0	0
36	u	61	Total 61	O 61	0	0
36	v	59	Total 59	O 59	0	0
36	y	2	Total 2	O 2	0	0
36	x	7	Total 7	O 7	0	0
36	z	1	Total 1	O 1	0	0

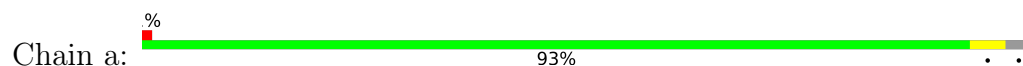
3 Residue-property plots [i](#)

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

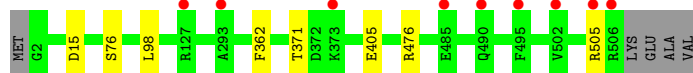
- Molecule 1: Photosystem II protein D1 1



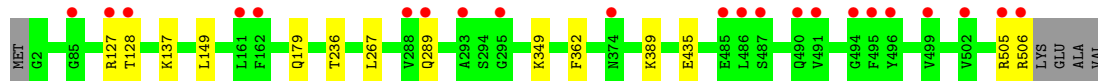
- Molecule 1: Photosystem II protein D1 1



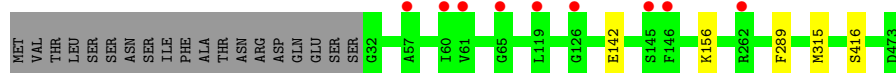
- Molecule 2: Photosystem II CP47 reaction center protein



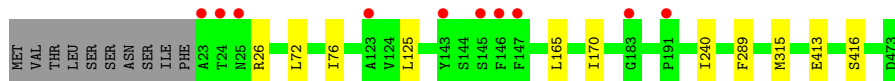
- Molecule 2: Photosystem II CP47 reaction center protein



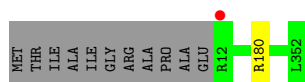
- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein



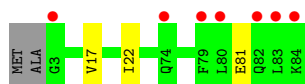
- Molecule 4: Photosystem II D2 protein



- Molecule 4: Photosystem II D2 protein



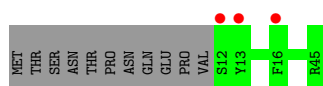
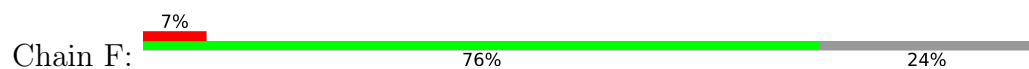
- Molecule 5: Cytochrome b559 subunit alpha



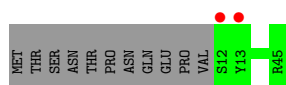
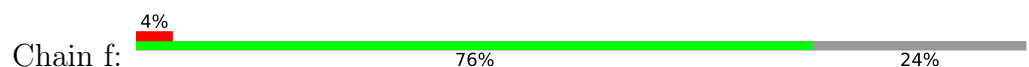
- Molecule 5: Cytochrome b559 subunit alpha



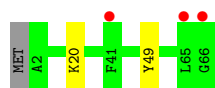
- Molecule 6: Cytochrome b559 subunit beta



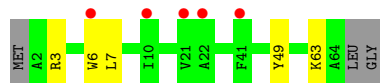
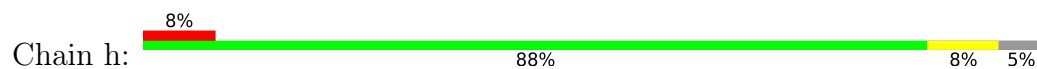
- Molecule 6: Cytochrome b559 subunit beta



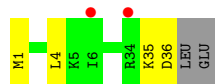
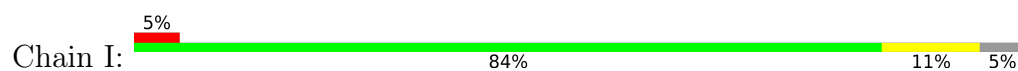
- Molecule 7: Photosystem II reaction center protein H



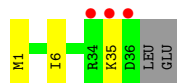
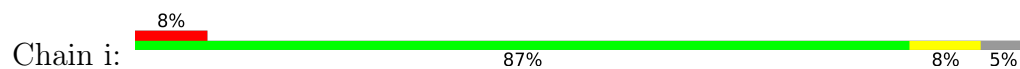
- Molecule 7: Photosystem II reaction center protein H



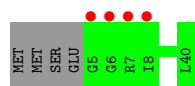
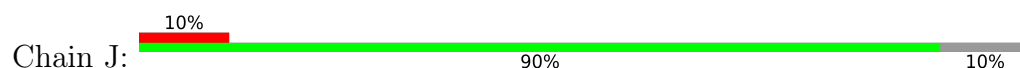
- Molecule 8: Photosystem II reaction center protein I



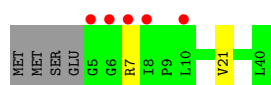
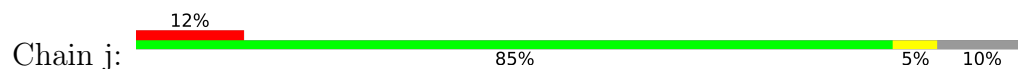
- Molecule 8: Photosystem II reaction center protein I



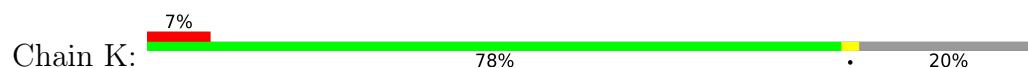
- Molecule 9: Photosystem II reaction center protein J

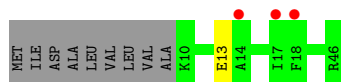


- Molecule 9: Photosystem II reaction center protein J

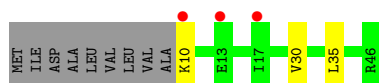
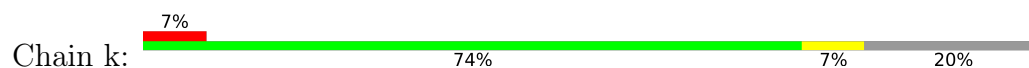


- Molecule 10: Photosystem II reaction center protein K

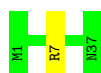




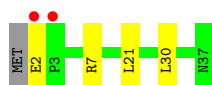
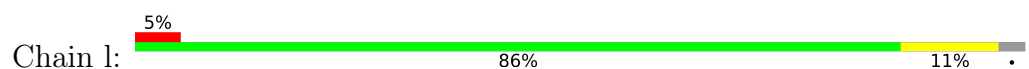
- Molecule 10: Photosystem II reaction center protein K



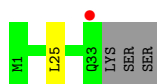
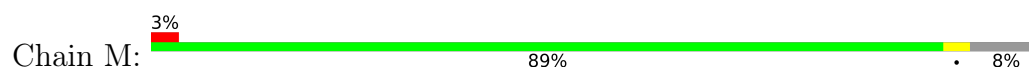
- Molecule 11: Photosystem II reaction center protein L



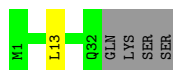
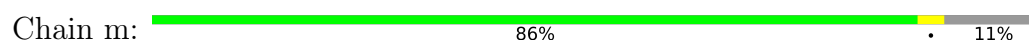
- Molecule 11: Photosystem II reaction center protein L



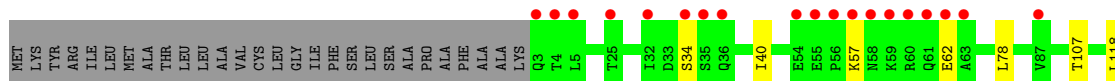
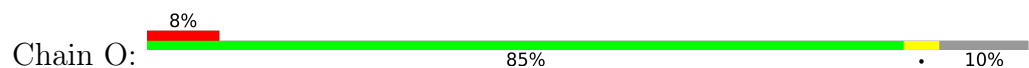
- Molecule 12: Photosystem II reaction center protein M



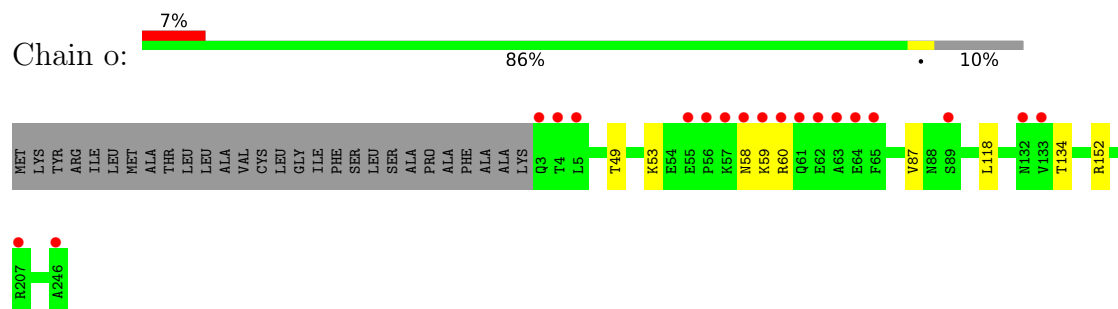
- Molecule 12: Photosystem II reaction center protein M



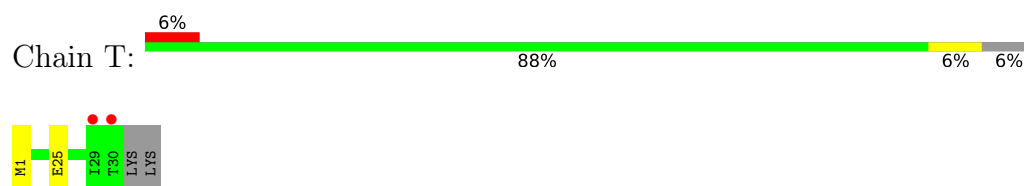
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



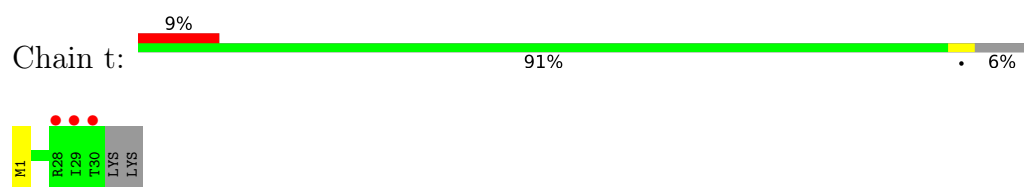
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



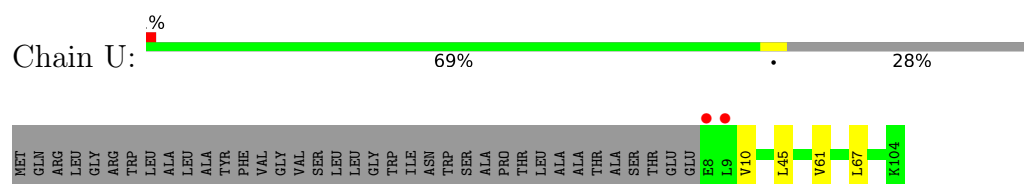
- Molecule 14: Photosystem II reaction center protein T



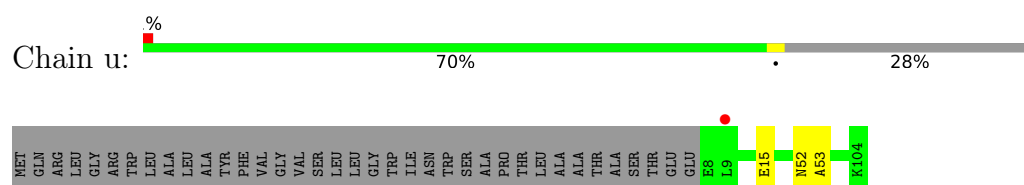
- Molecule 14: Photosystem II reaction center protein T



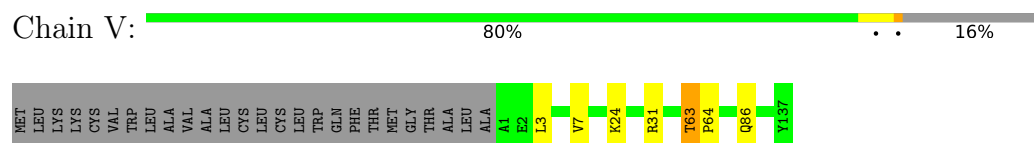
- Molecule 15: Photosystem II 12 kDa extrinsic protein



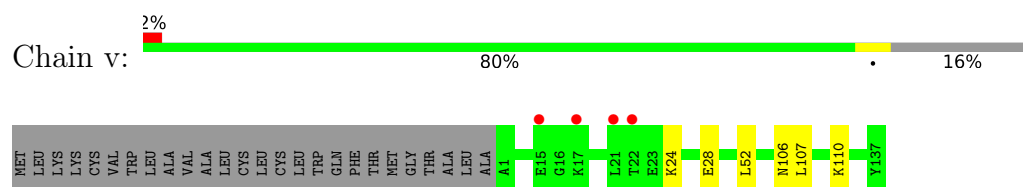
- Molecule 15: Photosystem II 12 kDa extrinsic protein



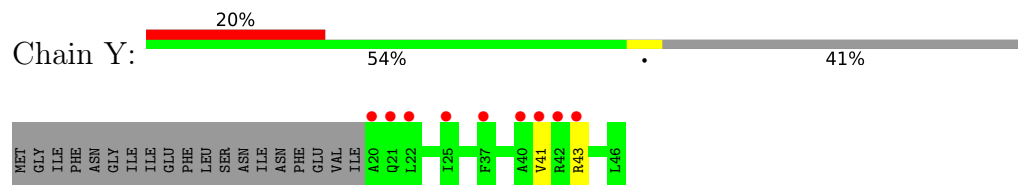
- Molecule 16: Cytochrome c-550



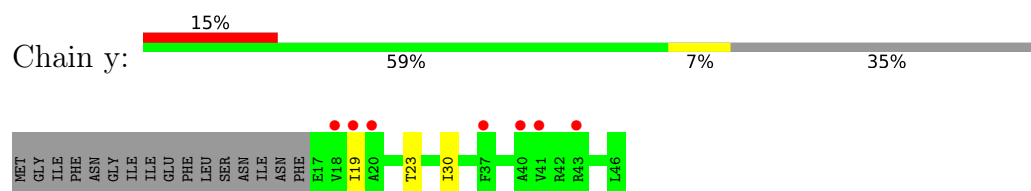
- Molecule 16: Cytochrome c-550



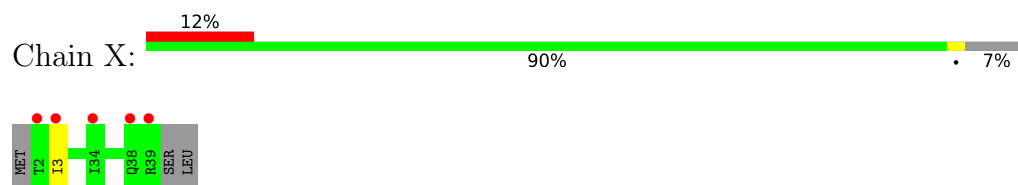
• Molecule 17: Photosystem II reaction center protein Ycf12



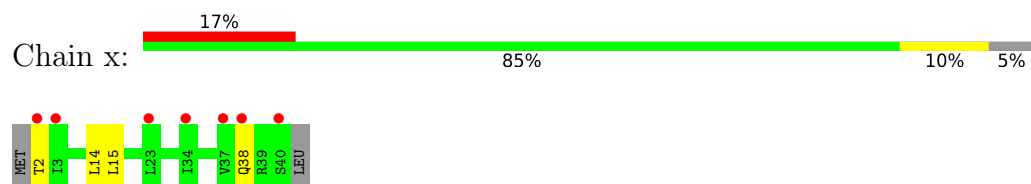
• Molecule 17: Photosystem II reaction center protein Ycf12



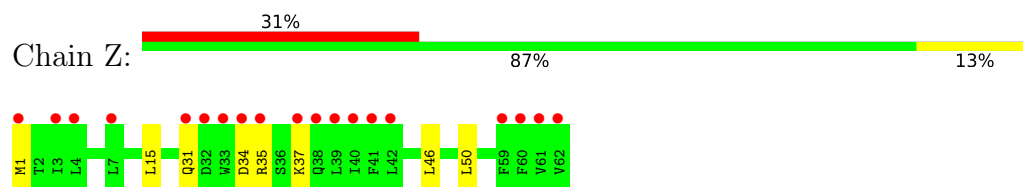
• Molecule 18: Photosystem II reaction center X protein



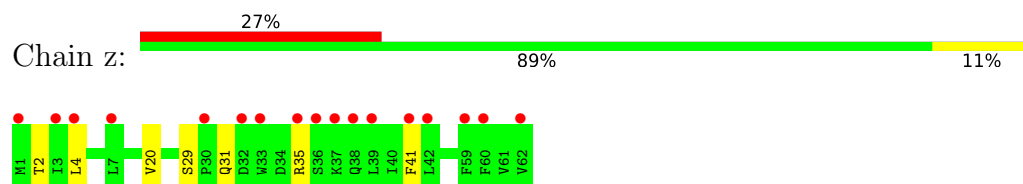
• Molecule 18: Photosystem II reaction center X protein



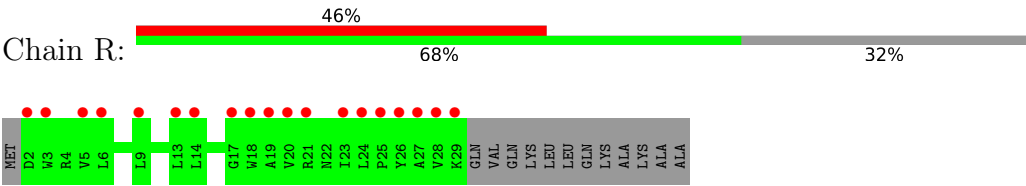
• Molecule 19: Photosystem II reaction center protein Z



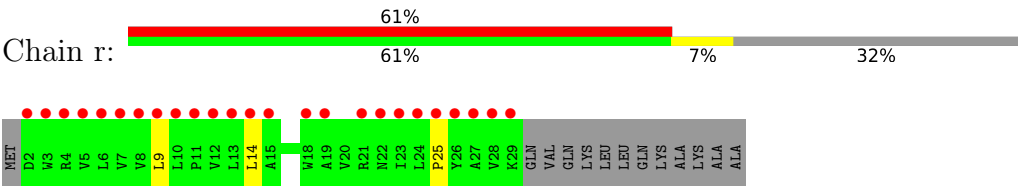
• Molecule 19: Photosystem II reaction center protein Z



● Molecule 20: Photosystem II protein Y



● Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.00Å 221.60Å 307.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.67 – 1.89 33.67 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.4 (33.67-1.89) 89.2 (33.67-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.42 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.171 , 0.214 0.171 , 0.214	Depositor DCC
R_{free} test set	5621 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 67.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	104284	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.61	0/2707	0.67	0/3692
1	a	0.59	0/2704	0.68	1/3688 (0.0%)
2	B	0.59	0/4161	0.68	1/5669 (0.0%)
2	b	0.57	0/4127	0.68	2/5623 (0.0%)
3	C	0.57	0/3546	0.65	0/4828
3	c	0.53	0/3619	0.65	0/4926
4	D	0.63	0/2812	0.67	0/3832
4	d	0.57	0/2821	0.67	0/3844
5	E	0.62	0/688	0.63	0/940
5	e	0.54	0/683	0.63	0/932
6	F	0.64	0/284	0.64	0/387
6	f	0.59	0/284	0.63	0/387
7	H	0.72	0/523	0.74	0/713
7	h	0.60	0/511	0.72	0/697
8	I	0.72	0/293	0.74	0/396
8	i	0.73	0/293	0.76	0/396
9	J	0.55	0/263	0.63	0/356
9	j	0.65	0/263	0.65	0/356
10	K	0.55	0/303	0.72	0/416
10	k	0.54	0/303	0.62	0/416
11	L	0.73	0/311	0.72	0/422
11	l	0.67	0/303	0.72	0/412
12	M	0.67	0/249	0.64	0/341
12	m	0.73	0/244	0.72	0/334
13	O	0.66	0/1904	0.76	1/2585 (0.0%)
13	o	0.64	0/1905	0.77	0/2583
14	T	0.78	0/257	0.76	0/349
14	t	0.81	0/255	0.67	0/346
15	U	0.59	0/785	0.70	0/1064
15	u	0.67	0/785	0.78	0/1064
16	V	0.63	0/1085	0.73	1/1473 (0.1%)
16	v	0.61	0/1085	0.69	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.47	0/197	0.70	0/264
17	y	0.44	0/219	0.60	0/294
18	X	0.52	0/284	0.65	0/384
18	x	0.44	0/289	0.61	0/391
19	Z	0.49	0/490	0.61	0/669
19	z	0.50	0/488	0.61	0/666
20	R	0.41	0/227	0.61	0/313
20	r	0.38	0/227	0.61	0/313
All	All	0.60	0/42777	0.68	6/58234 (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
13	o	0	1
15	u	0	1
16	V	0	1
All	All	0	3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	V	63	THR	C-N-CD	-7.32	104.49	120.60
2	b	267	LEU	CA-CB-CG	-6.88	99.47	115.30
2	B	15	ASP	CB-CG-OD2	-5.60	113.26	118.30
2	b	267	LEU	CB-CG-CD2	5.57	120.47	111.00
1	a	131	TRP	CA-CB-CG	-5.08	104.05	113.70
13	O	158	ASP	CB-CG-OD1	5.07	122.87	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	V	63	THR	Peptide
13	o	152	ARG	Sidechain
15	u	52	ASN	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/344 (96%)	328 (99%)	3 (1%)	1 (0%)	41	31
1	a	332/344 (96%)	327 (98%)	5 (2%)	0	100	100
2	B	508/510 (100%)	500 (98%)	8 (2%)	0	100	100
2	b	504/510 (99%)	493 (98%)	10 (2%)	1 (0%)	47	38
3	C	442/461 (96%)	432 (98%)	9 (2%)	1 (0%)	47	38
3	c	451/461 (98%)	437 (97%)	13 (3%)	1 (0%)	47	38
4	D	339/352 (96%)	330 (97%)	9 (3%)	0	100	100
4	d	340/352 (97%)	332 (98%)	8 (2%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	57 (90%)	6 (10%)	0	100	100
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

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%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	231 (95%)	10 (4%)	2 (1%)	19	9
13	o	242/272 (89%)	233 (96%)	7 (3%)	2 (1%)	19	9
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
15	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
15	u	95/134 (71%)	92 (97%)	2 (2%)	1 (1%)	14	5
16	V	135/163 (83%)	128 (95%)	6 (4%)	1 (1%)	22	12
16	v	135/163 (83%)	132 (98%)	3 (2%)	0	100	100
17	Y	25/46 (54%)	23 (92%)	1 (4%)	1 (4%)	3	0
17	y	28/46 (61%)	27 (96%)	1 (4%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	56 (93%)	3 (5%)	1 (2%)	9	2
19	z	60/62 (97%)	53 (88%)	6 (10%)	1 (2%)	9	2
20	R	26/41 (63%)	26 (100%)	0	0	100	100
20	r	26/41 (63%)	25 (96%)	0	1 (4%)	3	0
All	All	5232/5700 (92%)	5089 (97%)	129 (2%)	14 (0%)	41	31

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
16	V	64	PRO
3	c	416	SER
13	o	58	ASN
15	u	53	ALA
19	z	2	THR
17	Y	43	ARG
13	O	62	GLU
13	o	59	LYS
2	b	505	ARG
19	Z	31	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	r	25	PRO
13	O	133	VAL
1	A	259	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/280 (96%)	269 (100%)	1 (0%)	91	91
1	a	269/280 (96%)	257 (96%)	12 (4%)	27	18
2	B	408/407 (100%)	401 (98%)	7 (2%)	60	57
2	b	403/407 (99%)	391 (97%)	12 (3%)	41	33
3	C	346/362 (96%)	342 (99%)	4 (1%)	71	70
3	c	354/362 (98%)	343 (97%)	11 (3%)	40	32
4	D	276/283 (98%)	275 (100%)	1 (0%)	91	91
4	d	277/283 (98%)	269 (97%)	8 (3%)	42	35
5	E	72/73 (99%)	68 (94%)	4 (6%)	21	11
5	e	71/73 (97%)	68 (96%)	3 (4%)	30	20
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	28 (100%)	0	100	100
7	H	54/55 (98%)	52 (96%)	2 (4%)	34	25
7	h	53/55 (96%)	48 (91%)	5 (9%)	8	3
8	I	32/34 (94%)	29 (91%)	3 (9%)	8	3
8	i	32/34 (94%)	30 (94%)	2 (6%)	18	8
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	22 (92%)	2 (8%)	11	4
10	K	30/37 (81%)	29 (97%)	1 (3%)	38	29
10	k	30/37 (81%)	27 (90%)	3 (10%)	7	3
11	L	35/35 (100%)	34 (97%)	1 (3%)	42	35

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	2
12	M	28/32 (88%)	27 (96%)	1 (4%)	35	26
12	m	28/32 (88%)	27 (96%)	1 (4%)	35	26
13	O	206/228 (90%)	197 (96%)	9 (4%)	28	19
13	o	207/228 (91%)	201 (97%)	6 (3%)	42	35
14	T	26/28 (93%)	25 (96%)	1 (4%)	33	24
14	t	25/28 (89%)	25 (100%)	0	100	100
15	U	84/112 (75%)	80 (95%)	4 (5%)	25	16
15	u	84/112 (75%)	83 (99%)	1 (1%)	71	70
16	V	117/138 (85%)	112 (96%)	5 (4%)	29	19
16	v	117/138 (85%)	111 (95%)	6 (5%)	24	14
17	Y	19/37 (51%)	18 (95%)	1 (5%)	22	13
17	y	22/37 (60%)	19 (86%)	3 (14%)	3	1
18	X	31/34 (91%)	30 (97%)	1 (3%)	39	30
18	x	31/34 (91%)	27 (87%)	4 (13%)	4	1
19	Z	52/52 (100%)	45 (86%)	7 (14%)	4	1
19	z	51/52 (98%)	45 (88%)	6 (12%)	5	2
20	R	22/33 (67%)	22 (100%)	0	100	100
20	r	22/33 (67%)	20 (91%)	2 (9%)	9	3
All	All	4322/4654 (93%)	4178 (97%)	144 (3%)	38	29

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	VAL
2	B	76	SER
2	B	98	LEU
2	B	362	PHE
2	B	371	THR
2	B	405	GLU
2	B	476	ARG
2	B	505	ARG
3	C	142	GLU
3	C	156	LYS
3	C	289	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	315	MET
4	D	180	ARG
5	E	17	VAL
5	E	22[A]	ILE
5	E	22[B]	ILE
5	E	81	GLU
7	H	20	LYS
7	H	49	TYR
8	I	4	LEU
8	I	35	LYS
8	I	36	ASP
10	K	13	GLU
11	L	7	ARG
12	M	25	LEU
13	O	34	SER
13	O	40	ILE
13	O	57	LYS
13	O	78	LEU
13	O	107	THR
13	O	118	LEU
13	O	135	SER
13	O	189	ARG
13	O	214	THR
14	T	25	GLU
15	U	10	VAL
15	U	45	LEU
15	U	61	VAL
15	U	67	LEU
16	V	3	LEU
16	V	7	VAL
16	V	24	LYS
16	V	31	ARG
16	V	86	GLN
17	Y	41	VAL
18	X	3	ILE
19	Z	1	MET
19	Z	15	LEU
19	Z	34	ASP
19	Z	35	ARG
19	Z	37	LYS
19	Z	46	LEU
19	Z	50	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	16	ARG
1	a	28	LEU
1	a	42	LEU
1	a	159	LEU
1	a	200	LEU
1	a	223	LEU
1	a	226	GLU
1	a	230	THR
1	a	231	GLU
1	a	245	THR
1	a	271	LEU
1	a	288	LEU
2	b	127	ARG
2	b	128	THR
2	b	137	LYS
2	b	149	LEU
2	b	179	GLN
2	b	236	THR
2	b	289	GLN
2	b	349	LYS
2	b	362	PHE
2	b	389	LYS
2	b	435	GLU
2	b	506	ARG
3	c	26	ARG
3	c	72	LEU
3	c	76	ILE
3	c	125	LEU
3	c	165	LEU
3	c	170	ILE
3	c	240	ILE
3	c	289	PHE
3	c	315	MET
3	c	413[A]	GLU
3	c	413[B]	GLU
4	d	180	ARG
4	d	182	LEU
4	d	227[A]	GLU
4	d	227[B]	GLU
4	d	259	ILE
4	d	291	LEU
4	d	293	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	d	321	LEU
5	e	4	THR
5	e	75	GLN
5	e	83	LEU
7	h	3	ARG
7	h	6	TRP
7	h	7	LEU
7	h	49	TYR
7	h	63	LYS
8	i	6	ILE
8	i	35	LYS
9	j	7	ARG
9	j	21	VAL
10	k	10	LYS
10	k	30	VAL
10	k	35	LEU
11	l	2	GLU
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
13	o	49	THR
13	o	53	LYS
13	o	60	ARG
13	o	87	VAL
13	o	118	LEU
13	o	134	THR
15	u	15	GLU
16	v	24	LYS
16	v	28	GLU
16	v	52	LEU
16	v	106	ASN
16	v	107	LEU
16	v	110	LYS
17	y	19	ILE
17	y	23	THR
17	y	30	ILE
18	x	2	THR
18	x	14	LEU
18	x	15	LEU
18	x	38	GLN
19	z	4	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	z	20	VAL
19	z	29	SER
19	z	31	GLN
19	z	35	ARG
19	z	41	PHE
20	r	9	LEU
20	r	14	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	ASN
1	A	338	ASN
2	B	409	GLN
2	B	497	GLN
3	C	327	ASN
3	C	385	GLN
13	O	88	ASN
18	X	38	GLN
1	a	19	ASN
1	a	181	ASN
1	a	234	ASN
2	b	179	GLN
3	c	378	ASN
6	f	44	GLN
7	h	59	ASN
13	o	36	GLN
13	o	61	GLN
16	v	106	ASN
18	x	33	GLN
19	z	6	GLN
19	z	58	ASN
20	r	22	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	FME	t	1	14	8,9,10	1.26	1 (12%)	7,9,11	0.96	0
12	FME	m	1	12	8,9,10	1.01	0	7,9,11	0.81	0
8	FME	i	1	8	8,9,10	0.99	0	7,9,11	1.30	1 (14%)
8	FME	I	1	8	8,9,10	0.86	0	7,9,11	1.45	1 (14%)
14	FME	T	1	14	8,9,10	0.90	0	7,9,11	1.48	1 (14%)
12	FME	M	1	12	8,9,10	0.83	0	7,9,11	0.87	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
14	FME	t	1	14	-	3/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
14	FME	T	1	14	-	3/7/9/11	-
12	FME	M	1	12	-	2/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	t	1	FME	CA-N	-2.81	1.42	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1	FME	CA-N-CN	-2.88	118.39	122.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	CA-N-CN	-2.47	119.03	122.82
14	T	1	FME	O1-CN-N	-2.01	119.97	125.27

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 212 ligands modelled in this entry, 6 are monoatomic - leaving 206 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	$\# Z > 2$
26	PL9	D	407	-	55,55,55	1.66	7 (12%)	68,69,69	1.61	16 (23%)
30	DGD	C	521	-	63,63,67	1.22	8 (12%)	77,77,81	1.52	12 (15%)
23	CLA	B	607	36	56,73,73	1.54	9 (16%)	55,113,113	1.72	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	603	-	56,73,73	1.58	5 (8%)	55,113,113	1.86	12 (21%)
23	CLA	C	512	-	56,73,73	1.56	9 (16%)	55,113,113	1.57	13 (23%)
23	CLA	b	614	-	56,73,73	1.64	7 (12%)	55,113,113	1.63	10 (18%)
25	BCR	C	515	-	41,41,41	1.27	3 (7%)	56,56,56	1.36	6 (10%)
27	STE	b	627	-	10,10,19	0.39	0	9,9,19	0.68	0
27	STE	M	102	-	11,14,19	0.44	0	10,14,19	0.67	0
23	CLA	A	404	-	56,73,73	1.47	6 (10%)	55,113,113	1.43	8 (14%)
23	CLA	B	613	-	56,73,73	1.48	7 (12%)	55,113,113	1.34	8 (14%)
27	STE	t	102	-	10,13,19	0.56	0	9,13,19	0.48	0
31	OEX	A	418	1,3,36	0,15,15	-	-	-	-	-
27	STE	d	412	-	9,9,19	0.48	0	8,8,19	0.60	0
23	CLA	c	502	-	56,73,73	1.42	6 (10%)	55,113,113	1.63	8 (14%)
27	STE	E	102	-	8,11,19	0.58	0	7,11,19	0.56	0
33	LHG	E	101	-	48,48,48	1.08	4 (8%)	51,54,54	1.12	2 (3%)
23	CLA	B	616	-	51,68,73	1.70	7 (13%)	49,107,113	1.78	11 (22%)
23	CLA	b	601	-	56,73,73	1.38	8 (14%)	55,113,113	1.85	11 (20%)
27	STE	b	622	-	16,19,19	0.41	0	15,19,19	0.62	0
23	CLA	B	609	-	56,73,73	1.51	7 (12%)	55,113,113	1.59	11 (20%)
23	CLA	a	405	-	56,73,73	1.56	6 (10%)	55,113,113	1.53	8 (14%)
27	STE	d	410	-	13,16,19	0.68	0	12,16,19	0.48	0
23	CLA	a	406	36	56,73,73	1.62	8 (14%)	55,113,113	1.81	11 (20%)
23	CLA	c	511	3	56,73,73	1.76	8 (14%)	55,113,113	1.55	8 (14%)
27	STE	T	102	-	15,15,19	0.50	0	14,14,19	0.55	0
27	STE	x	102	-	16,19,19	0.63	0	15,19,19	0.58	0
34	HEM	F	101	6,5	27,50,50	2.01	6 (22%)	17,82,82	2.60	8 (47%)
27	STE	m	101	-	8,11,19	0.52	0	7,11,19	0.53	0
27	STE	d	411	-	8,11,19	0.47	0	7,11,19	0.47	0
28	LMG	C	517	-	35,35,55	1.39	3 (8%)	43,43,63	1.72	8 (18%)
34	HEM	f	101	6,5	27,50,50	2.08	6 (22%)	17,82,82	2.58	4 (23%)
28	LMG	b	619	-	22,22,55	1.01	2 (9%)	23,23,63	1.06	1 (4%)
27	STE	B	621	-	13,16,19	0.39	0	12,16,19	0.79	0
32	BCT	a	404	21	0,3,3	-	-	0,3,3	-	-
23	CLA	c	509	-	56,73,73	1.57	7 (12%)	55,113,113	1.76	14 (25%)
33	LHG	d	407	-	48,48,48	0.89	2 (4%)	51,54,54	1.13	6 (11%)
28	LMG	c	523	-	48,48,55	1.04	4 (8%)	56,56,63	1.31	8 (14%)
29	SQD	b	620	-	48,49,54	1.57	9 (18%)	57,60,65	2.25	17 (29%)
33	LHG	D	411	-	46,46,48	0.99	2 (4%)	49,52,54	1.27	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	K	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.20	6 (10%)
25	BCR	C	514	-	41,41,41	1.08	2 (4%)	56,56,56	1.21	5 (8%)
25	BCR	H	101	-	41,41,41	0.98	1 (2%)	56,56,56	1.27	7 (12%)
27	STE	C	527	-	7,7,19	0.60	0	6,6,19	0.40	0
23	CLA	B	605	-	56,73,73	1.39	7 (12%)	55,113,113	1.53	11 (20%)
23	CLA	b	604	-	56,73,73	1.43	4 (7%)	55,113,113	1.49	10 (18%)
27	STE	J	101	-	8,11,19	0.24	0	7,11,19	1.22	1 (14%)
29	SQD	l	101	-	53,54,54	1.54	11 (20%)	62,65,65	2.03	8 (12%)
25	BCR	b	616	-	41,41,41	1.14	2 (4%)	56,56,56	1.32	7 (12%)
27	STE	i	101	-	8,11,19	0.38	0	7,11,19	0.98	0
23	CLA	a	411	36	56,73,73	1.56	7 (12%)	55,113,113	1.58	9 (16%)
28	LMG	A	411	-	48,48,55	1.03	2 (4%)	56,56,63	1.34	7 (12%)
23	CLA	C	508	-	56,73,73	1.64	7 (12%)	55,113,113	1.71	13 (23%)
26	PL9	A	409	-	55,55,55	1.29	3 (5%)	68,69,69	1.64	14 (20%)
27	STE	C	528	-	13,13,19	0.46	0	12,12,19	0.63	0
27	STE	j	101	-	8,11,19	0.43	0	7,11,19	0.57	0
27	STE	l	103	-	17,17,19	0.36	0	16,16,19	0.70	0
25	BCR	D	406	-	41,41,41	1.18	2 (4%)	56,56,56	1.15	5 (8%)
23	CLA	C	505	-	56,73,73	1.65	4 (7%)	55,113,113	1.50	7 (12%)
23	CLA	c	501	-	56,73,73	1.59	7 (12%)	55,113,113	1.69	8 (14%)
33	LHG	d	406	-	48,48,48	0.86	2 (4%)	51,54,54	1.35	8 (15%)
23	CLA	c	512	-	56,73,73	1.40	8 (14%)	55,113,113	1.83	13 (23%)
23	CLA	c	513	-	56,73,73	1.71	8 (14%)	55,113,113	1.36	8 (14%)
27	STE	C	525	-	8,11,19	0.33	0	7,11,19	1.43	2 (28%)
25	BCR	c	515	-	41,41,41	1.33	3 (7%)	56,56,56	1.39	10 (17%)
27	STE	a	416	-	9,9,19	0.68	0	8,8,19	0.39	0
27	STE	c	516	-	12,12,19	0.51	0	11,11,19	0.53	0
27	STE	D	414	-	8,8,19	0.38	0	7,7,19	0.99	0
35	HEC	v	201	16	26,50,50	2.41	4 (15%)	18,82,82	1.90	5 (27%)
33	LHG	D	412	-	48,48,48	0.98	2 (4%)	51,54,54	1.32	6 (11%)
23	CLA	B	602	-	56,73,73	1.61	7 (12%)	55,113,113	1.52	10 (18%)
23	CLA	d	402	-	56,73,73	1.69	8 (14%)	55,113,113	1.63	11 (20%)
23	CLA	C	506	-	56,73,73	1.41	4 (7%)	55,113,113	1.40	9 (16%)
27	STE	m	102	-	14,14,19	0.57	0	13,13,19	0.58	0
23	CLA	b	610	-	56,73,73	1.49	6 (10%)	55,113,113	1.50	9 (16%)
27	STE	c	517	-	17,17,19	0.56	0	16,16,19	0.56	0
23	CLA	B	615	-	56,73,73	1.77	11 (19%)	55,113,113	1.28	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	STE	C	519	-	6,6,19	0.45	0	5,5,19	0.79	0
27	STE	e	101	-	8,8,19	0.54	0	7,7,19	0.61	0
26	PL9	a	410	-	55,55,55	0.95	4 (7%)	68,69,69	1.60	13 (19%)
23	CLA	b	613	-	56,73,73	1.69	7 (12%)	55,113,113	1.85	11 (20%)
27	STE	M	103	-	9,9,19	0.47	0	8,8,19	0.43	0
25	BCR	d	404	-	41,41,41	1.11	2 (4%)	56,56,56	1.10	2 (3%)
27	STE	I	101	-	14,14,19	0.51	0	13,13,19	0.53	0
29	SQD	F	102	-	35,36,54	1.64	6 (17%)	42,45,65	2.99	9 (21%)
23	CLA	h	101	36	56,73,73	1.76	10 (17%)	55,113,113	1.76	10 (18%)
29	SQD	a	412	-	53,54,54	1.43	8 (15%)	62,65,65	2.14	18 (29%)
31	OEX	a	418	1,3,36	0,15,15	-	-	-	-	-
23	CLA	D	405	-	56,73,73	1.46	9 (16%)	55,113,113	1.49	9 (16%)
25	BCR	t	101	-	41,41,41	1.23	2 (4%)	56,56,56	1.27	5 (8%)
23	CLA	c	508	-	55,72,73	1.57	8 (14%)	53,111,113	1.57	9 (16%)
23	CLA	C	513	-	56,73,73	1.58	9 (16%)	55,113,113	1.76	11 (20%)
23	CLA	c	506	-	56,73,73	1.58	7 (12%)	55,113,113	1.54	11 (20%)
27	STE	b	625	-	12,15,19	0.46	0	11,15,19	0.63	0
23	CLA	c	507	36	56,73,73	1.56	9 (16%)	55,113,113	1.53	12 (21%)
27	STE	C	516	-	10,13,19	0.42	0	9,13,19	0.76	0
23	CLA	B	601	36	56,73,73	1.84	8 (14%)	55,113,113	1.82	6 (10%)
23	CLA	A	405	36	56,73,73	1.50	6 (10%)	55,113,113	1.41	10 (18%)
23	CLA	B	614	-	56,73,73	1.74	7 (12%)	55,113,113	1.58	13 (23%)
27	STE	z	101	-	8,8,19	0.50	0	7,7,19	0.54	0
23	CLA	b	608	-	56,73,73	1.62	8 (14%)	55,113,113	1.89	15 (27%)
24	PHO	a	407	-	67,69,69	1.07	5 (7%)	85,99,99	1.02	6 (7%)
30	DGD	c	520	-	63,63,67	1.33	10 (15%)	77,77,81	1.55	16 (20%)
33	LHG	a	413	-	41,41,48	1.50	7 (17%)	44,47,54	1.32	4 (9%)
24	PHO	D	402	-	67,69,69	1.07	7 (10%)	85,99,99	1.04	5 (5%)
25	BCR	A	408	-	41,41,41	1.12	3 (7%)	56,56,56	1.37	7 (12%)
23	CLA	A	407	-	45,62,73	1.65	6 (13%)	41,99,113	1.76	10 (24%)
28	LMG	M	101	-	51,51,55	1.05	4 (7%)	59,59,63	1.43	10 (16%)
35	HEC	V	201	16	26,50,50	2.48	4 (15%)	18,82,82	1.89	5 (27%)
25	BCR	b	618	-	41,41,41	1.07	2 (4%)	56,56,56	1.24	7 (12%)
27	STE	Z	101	-	16,16,19	0.49	0	15,15,19	0.50	0
27	STE	e	102	-	7,7,19	0.43	0	6,6,19	0.60	0
23	CLA	C	507	36	56,73,73	1.27	6 (10%)	55,113,113	1.77	12 (21%)
30	DGD	h	102	-	63,63,67	1.17	6 (9%)	77,77,81	1.45	13 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	STE	A	417	-	10,10,19	0.40	0	9,9,19	0.83	0
28	LMG	D	408	-	50,50,55	1.07	3 (6%)	58,58,63	1.27	4 (6%)
29	SQD	a	414	-	53,54,54	1.67	10 (18%)	62,65,65	1.77	9 (14%)
27	STE	e	104	-	9,12,19	0.28	0	8,12,19	0.93	0
33	LHG	D	410	-	48,48,48	0.92	2 (4%)	51,54,54	1.14	5 (9%)
23	CLA	b	612	-	56,73,73	1.63	6 (10%)	55,113,113	1.49	11 (20%)
23	CLA	c	503	-	56,73,73	1.46	8 (14%)	55,113,113	1.63	11 (20%)
23	CLA	B	606	-	56,73,73	1.73	8 (14%)	55,113,113	1.84	10 (18%)
23	CLA	c	504	36	51,68,73	1.61	5 (9%)	49,107,113	1.61	11 (22%)
27	STE	E	104	-	16,19,19	0.48	0	15,19,19	0.67	0
28	LMG	C	524	-	48,48,55	1.02	4 (8%)	56,56,63	1.23	3 (5%)
25	BCR	b	617	-	41,41,41	1.24	2 (4%)	56,56,56	1.16	7 (12%)
27	STE	H	103	-	17,17,19	0.55	0	16,16,19	0.66	0
27	STE	I	102	-	13,16,19	0.57	0	12,16,19	0.54	0
23	CLA	C	501	-	56,73,73	1.89	5 (8%)	55,113,113	1.58	5 (9%)
25	BCR	B	619	-	41,41,41	1.14	3 (7%)	56,56,56	1.27	7 (12%)
27	STE	A	410	-	8,8,19	0.40	0	7,7,19	0.71	0
23	CLA	a	408	-	56,73,73	1.71	7 (12%)	55,113,113	1.71	15 (27%)
27	STE	A	415	-	7,7,19	0.43	0	6,6,19	0.56	0
23	CLA	b	607	-	56,73,73	1.67	7 (12%)	55,113,113	1.51	12 (21%)
27	STE	C	518	-	4,4,19	0.49	0	3,3,19	0.28	0
25	BCR	a	409	-	41,41,41	1.08	3 (7%)	56,56,56	1.15	5 (8%)
28	LMG	a	415	-	55,55,55	1.45	8 (14%)	63,63,63	1.53	8 (12%)
23	CLA	C	511	3	56,73,73	1.80	8 (14%)	55,113,113	1.48	12 (21%)
27	STE	e	103	-	8,8,19	0.39	0	7,7,19	0.69	0
28	LMG	c	518	-	29,29,55	1.11	2 (6%)	31,31,63	1.08	2 (6%)
25	BCR	c	514	-	41,41,41	1.24	3 (7%)	56,56,56	1.28	6 (10%)
33	LHG	l	102	-	48,48,48	0.82	2 (4%)	51,54,54	1.22	4 (7%)
30	DGD	C	523	-	63,63,67	0.93	3 (4%)	77,77,81	1.33	10 (12%)
26	PL9	d	405	-	55,55,55	1.50	9 (16%)	68,69,69	1.59	13 (19%)
27	STE	t	103	-	14,17,19	0.42	0	13,17,19	0.85	0
25	BCR	k	101	-	41,41,41	1.11	3 (7%)	56,56,56	1.12	3 (5%)
27	STE	E	103	-	11,11,19	0.46	0	10,10,19	0.62	0
23	CLA	b	609	36	56,73,73	1.53	7 (12%)	55,113,113	1.63	10 (18%)
27	STE	j	102	-	15,15,19	0.54	0	14,14,19	0.55	0
27	STE	D	413	-	16,19,19	0.44	0	15,19,19	0.97	1 (6%)
30	DGD	H	102	-	63,63,67	1.29	8 (12%)	77,77,81	1.45	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	DGD	c	521	-	63,63,67	0.91	3 (4%)	77,77,81	1.48	11 (14%)
27	STE	b	626	-	9,9,19	0.39	0	8,8,19	0.70	0
25	BCR	B	618	-	41,41,41	1.15	2 (4%)	56,56,56	1.17	6 (10%)
23	CLA	b	606	36	56,73,73	1.40	10 (17%)	55,113,113	1.57	9 (16%)
25	BCR	C	520	-	41,41,41	1.13	4 (9%)	56,56,56	1.13	4 (7%)
28	LMG	B	620	-	45,45,55	1.05	2 (4%)	53,53,63	1.37	4 (7%)
27	STE	C	529	-	13,13,19	0.43	0	12,12,19	0.54	0
23	CLA	B	603	-	56,73,73	1.42	8 (14%)	55,113,113	1.82	13 (23%)
27	STE	i	102	-	5,5,19	0.47	0	4,4,19	0.40	0
27	STE	a	417	-	8,11,19	0.48	0	7,11,19	0.87	1 (14%)
25	BCR	x	101	-	41,41,41	1.19	2 (4%)	56,56,56	1.34	8 (14%)
23	CLA	b	605	-	56,73,73	1.88	9 (16%)	55,113,113	1.58	8 (14%)
30	DGD	c	519	-	63,63,67	1.16	6 (9%)	77,77,81	1.45	11 (14%)
23	CLA	B	610	36	56,73,73	1.67	9 (16%)	55,113,113	1.66	9 (16%)
27	STE	C	526	-	15,15,19	0.56	0	14,14,19	0.46	0
29	SQD	A	413	-	53,54,54	1.64	10 (18%)	62,65,65	1.87	14 (22%)
23	CLA	B	611	-	56,73,73	1.67	9 (16%)	55,113,113	1.80	11 (20%)
23	CLA	C	502	-	56,73,73	1.86	9 (16%)	55,113,113	1.59	9 (16%)
23	CLA	b	611	-	56,73,73	1.45	6 (10%)	55,113,113	1.55	11 (20%)
28	LMG	c	522	-	46,46,55	1.22	5 (10%)	54,54,63	1.27	8 (14%)
23	CLA	B	608	-	56,73,73	1.33	7 (12%)	55,113,113	1.57	9 (16%)
28	LMG	d	409	-	44,44,55	1.09	4 (9%)	52,52,63	1.33	7 (13%)
30	DGD	C	522	-	63,63,67	1.48	10 (15%)	77,77,81	1.29	8 (10%)
30	DGD	A	414	-	67,67,67	1.32	10 (14%)	81,81,81	1.55	17 (20%)
29	SQD	A	412	-	51,52,54	1.54	9 (17%)	60,63,65	2.04	14 (23%)
29	SQD	f	102	-	40,41,54	1.70	10 (25%)	49,52,65	1.78	8 (16%)
24	PHO	A	406	-	67,69,69	1.23	8 (11%)	85,99,99	1.10	8 (9%)
27	STE	B	623	-	14,14,19	0.52	0	13,13,19	0.74	0
28	LMG	D	409	-	51,51,55	1.15	3 (5%)	59,59,63	1.34	5 (8%)
33	LHG	d	408	-	38,38,48	0.97	2 (5%)	41,44,54	1.11	4 (9%)
23	CLA	B	604	-	56,73,73	1.37	10 (17%)	55,113,113	1.88	10 (18%)
23	CLA	C	509	-	56,73,73	1.57	6 (10%)	55,113,113	1.52	9 (16%)
25	BCR	B	617	-	41,41,41	1.08	3 (7%)	56,56,56	1.33	10 (17%)
23	CLA	C	503	-	56,73,73	1.72	7 (12%)	55,113,113	1.65	10 (18%)
23	CLA	C	510	-	56,73,73	1.52	8 (14%)	55,113,113	1.84	12 (21%)
23	CLA	D	404	-	56,73,73	1.35	5 (8%)	55,113,113	1.46	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	STE	b	624	-	16,19,19	0.33	0	15,19,19	1.10	0
23	CLA	b	602	-	56,73,73	1.56	10 (17%)	55,113,113	1.84	15 (27%)
27	STE	A	416	-	16,16,19	0.63	0	15,15,19	0.28	0
23	CLA	C	504	36	50,67,73	1.50	5 (10%)	47,105,113	1.71	13 (27%)
23	CLA	D	403	36	56,73,73	1.63	9 (16%)	55,113,113	1.47	5 (9%)
27	STE	B	622	-	8,11,19	0.45	0	7,11,19	0.67	0
28	LMG	b	621	-	51,51,55	1.00	4 (7%)	59,59,63	1.46	9 (15%)
23	CLA	b	615	-	51,68,73	1.47	8 (15%)	49,107,113	1.80	12 (24%)
33	LHG	L	101	-	48,48,48	0.94	1 (2%)	51,54,54	1.28	8 (15%)
25	BCR	T	101	-	41,41,41	1.28	6 (14%)	56,56,56	1.41	9 (16%)
23	CLA	c	505	-	56,73,73	1.54	7 (12%)	55,113,113	1.49	9 (16%)
23	CLA	B	612	-	56,73,73	1.66	4 (7%)	55,113,113	1.76	13 (23%)
25	BCR	k	102	-	41,41,41	1.04	3 (7%)	56,56,56	1.13	3 (5%)
23	CLA	d	403	-	56,73,73	1.69	9 (16%)	55,113,113	1.28	9 (16%)
24	PHO	d	401	-	67,69,69	1.27	9 (13%)	85,99,99	1.06	7 (8%)
28	LMG	b	623	-	55,55,55	1.01	2 (3%)	63,63,63	1.51	10 (15%)
32	BCT	D	401	21	0,3,3	-	-	0,3,3	-	-
23	CLA	c	510	-	56,73,73	1.69	6 (10%)	55,113,113	1.78	11 (20%)
28	LMG	c	524	-	49,49,55	1.02	4 (8%)	57,57,63	1.30	5 (8%)

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
26	PL9	D	407	-	-	6/53/73/73	0/1/1/1
30	DGD	C	521	-	-	20/51/91/95	0/2/2/2
23	CLA	B	607	36	1/1/20/20	5/37/115/115	-
23	CLA	b	603	-	1/1/20/20	12/37/115/115	-
23	CLA	C	512	-	1/1/20/20	13/37/115/115	-
23	CLA	b	614	-	1/1/20/20	5/37/115/115	-
25	BCR	C	515	-	-	2/29/63/63	0/2/2/2
27	STE	b	627	-	-	6/8/8/17	-
27	STE	M	102	-	-	7/10/12/17	-
23	CLA	A	404	-	1/1/20/20	2/37/115/115	-
23	CLA	B	613	-	1/1/20/20	11/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	STE	t	102	-	-	4/9/11/17	-
27	STE	d	412	-	-	3/7/7/17	-
23	CLA	c	502	-	-	5/37/115/115	-
27	STE	E	102	-	-	5/7/9/17	-
33	LHG	E	101	-	-	28/53/53/53	-
23	CLA	B	616	-	1/1/19/20	6/31/109/115	-
23	CLA	b	601	-	-	4/37/115/115	-
27	STE	b	622	-	-	8/15/17/17	-
23	CLA	B	609	-	-	4/37/115/115	-
23	CLA	a	405	-	1/1/20/20	4/37/115/115	-
27	STE	d	410	-	-	5/12/14/17	-
23	CLA	a	406	36	-	7/37/115/115	-
23	CLA	c	511	3	1/1/20/20	8/37/115/115	-
27	STE	T	102	-	-	8/13/13/17	-
27	STE	x	102	-	-	4/15/17/17	-
34	HEM	F	101	6,5	-	0/6/54/54	-
27	STE	m	101	-	-	4/7/9/17	-
27	STE	d	411	-	-	1/7/9/17	-
28	LMG	C	517	-	-	17/30/50/70	0/1/1/1
34	HEM	f	101	6,5	-	0/6/54/54	-
28	LMG	b	619	-	-	9/21/21/70	-
27	STE	B	621	-	-	7/12/14/17	-
23	CLA	c	509	-	1/1/20/20	11/37/115/115	-
33	LHG	d	407	-	-	13/53/53/53	-
28	LMG	c	523	-	-	22/43/63/70	0/1/1/1
29	SQD	b	620	-	-	17/44/64/69	0/1/1/1
33	LHG	D	411	-	-	13/51/51/53	-
25	BCR	K	101	-	-	7/29/63/63	0/2/2/2
25	BCR	C	514	-	-	8/29/63/63	0/2/2/2
25	BCR	H	101	-	-	3/29/63/63	0/2/2/2
27	STE	C	527	-	-	4/5/5/17	-
23	CLA	B	605	-	1/1/20/20	7/37/115/115	-
23	CLA	b	604	-	1/1/20/20	5/37/115/115	-
27	STE	J	101	-	-	3/7/9/17	-
29	SQD	l	101	-	-	23/49/69/69	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	b	616	-	-	4/29/63/63	0/2/2/2
27	STE	i	101	-	-	6/7/9/17	-
23	CLA	a	411	36	-	3/37/115/115	-
28	LMG	A	411	-	-	16/43/63/70	0/1/1/1
23	CLA	C	508	-	-	11/37/115/115	-
26	PL9	A	409	-	-	16/53/73/73	0/1/1/1
27	STE	C	528	-	-	7/11/11/17	-
27	STE	j	101	-	-	6/7/9/17	-
27	STE	l	103	-	-	9/15/15/17	-
25	BCR	D	406	-	-	4/29/63/63	0/2/2/2
23	CLA	C	505	-	1/1/20/20	10/37/115/115	-
23	CLA	c	501	-	1/1/20/20	5/37/115/115	-
33	LHG	d	406	-	-	18/53/53/53	-
23	CLA	c	512	-	1/1/20/20	16/37/115/115	-
23	CLA	c	513	-	1/1/20/20	18/37/115/115	-
27	STE	C	525	-	-	3/7/9/17	-
25	BCR	c	515	-	-	3/29/63/63	0/2/2/2
27	STE	a	416	-	-	4/7/7/17	-
27	STE	c	516	-	-	3/10/10/17	-
27	STE	D	414	-	-	5/6/6/17	-
35	HEC	v	201	16	-	0/6/54/54	-
33	LHG	D	412	-	-	14/53/53/53	-
23	CLA	B	602	-	1/1/20/20	7/37/115/115	-
23	CLA	d	402	-	1/1/20/20	8/37/115/115	-
23	CLA	C	506	-	1/1/20/20	9/37/115/115	-
27	STE	m	102	-	-	6/12/12/17	-
23	CLA	b	610	-	1/1/20/20	4/37/115/115	-
27	STE	c	517	-	-	4/15/15/17	-
23	CLA	B	615	-	1/1/20/20	8/37/115/115	-
27	STE	C	519	-	-	1/4/4/17	-
27	STE	e	101	-	-	2/6/6/17	-
26	PL9	a	410	-	-	24/53/73/73	0/1/1/1
23	CLA	b	613	-	1/1/20/20	12/37/115/115	-
27	STE	M	103	-	-	1/7/7/17	-
25	BCR	d	404	-	-	5/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	STE	I	101	-	-	5/12/12/17	-
29	SQD	F	102	-	-	12/28/48/69	0/1/1/1
23	CLA	h	101	36	1/1/20/20	24/37/115/115	-
29	SQD	a	412	-	-	20/49/69/69	0/1/1/1
23	CLA	D	405	-	-	13/37/115/115	-
25	BCR	t	101	-	-	1/29/63/63	0/2/2/2
23	CLA	c	508	-	-	8/36/114/115	-
23	CLA	C	513	-	1/1/20/20	13/37/115/115	-
23	CLA	c	506	-	1/1/20/20	15/37/115/115	-
27	STE	b	625	-	-	4/11/13/17	-
23	CLA	c	507	36	1/1/20/20	7/37/115/115	-
27	STE	C	516	-	-	3/9/11/17	-
23	CLA	B	601	36	1/1/20/20	13/37/115/115	-
23	CLA	A	405	36	-	2/37/115/115	-
23	CLA	B	614	-	1/1/20/20	12/37/115/115	-
27	STE	z	101	-	-	3/6/6/17	-
23	CLA	b	608	-	1/1/20/20	4/37/115/115	-
24	PHO	a	407	-	-	2/53/103/103	0/5/6/6
30	DGD	c	520	-	-	19/51/91/95	0/2/2/2
33	LHG	a	413	-	-	19/46/46/53	-
24	PHO	D	402	-	-	1/53/103/103	0/5/6/6
25	BCR	A	408	-	-	7/29/63/63	0/2/2/2
23	CLA	A	407	-	1/1/17/20	2/24/102/115	-
28	LMG	M	101	-	-	21/46/66/70	0/1/1/1
35	HEC	V	201	16	-	0/6/54/54	-
25	BCR	b	618	-	-	2/29/63/63	0/2/2/2
27	STE	Z	101	-	-	9/14/14/17	-
27	STE	e	102	-	-	3/5/5/17	-
23	CLA	C	507	36	1/1/20/20	6/37/115/115	-
30	DGD	h	102	-	-	18/51/91/95	0/2/2/2
27	STE	A	417	-	-	5/8/8/17	-
28	LMG	D	408	-	-	17/45/65/70	0/1/1/1
29	SQD	a	414	-	-	20/49/69/69	0/1/1/1
27	STE	e	104	-	-	5/8/10/17	-
33	LHG	D	410	-	-	22/53/53/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	612	-	1/1/20/20	4/37/115/115	-
23	CLA	c	504	36	1/1/19/20	5/31/109/115	-
23	CLA	B	606	-	1/1/20/20	9/37/115/115	-
23	CLA	c	503	-	-	9/37/115/115	-
27	STE	E	104	-	-	11/15/17/17	-
28	LMG	C	524	-	-	10/43/63/70	0/1/1/1
25	BCR	b	617	-	-	0/29/63/63	0/2/2/2
27	STE	H	103	-	-	8/15/15/17	-
27	STE	I	102	-	-	3/12/14/17	-
23	CLA	C	501	-	1/1/20/20	4/37/115/115	-
25	BCR	B	619	-	-	2/29/63/63	0/2/2/2
27	STE	A	410	-	-	4/6/6/17	-
23	CLA	a	408	-	1/1/20/20	14/37/115/115	-
27	STE	A	415	-	-	4/5/5/17	-
23	CLA	b	607	-	-	1/37/115/115	-
27	STE	C	518	-	-	1/2/2/17	-
25	BCR	a	409	-	-	1/29/63/63	0/2/2/2
28	LMG	a	415	-	-	26/50/70/70	0/1/1/1
23	CLA	C	511	3	-	4/37/115/115	-
27	STE	e	103	-	-	4/6/6/17	-
28	LMG	c	518	-	-	9/31/31/70	-
25	BCR	c	514	-	-	7/29/63/63	0/2/2/2
33	LHG	l	102	-	-	18/53/53/53	-
30	DGD	C	523	-	-	13/51/91/95	0/2/2/2
26	PL9	d	405	-	-	9/53/73/73	0/1/1/1
27	STE	t	103	-	-	9/13/15/17	-
25	BCR	k	101	-	-	11/29/63/63	0/2/2/2
27	STE	E	103	-	-	1/9/9/17	-
23	CLA	b	609	36	1/1/20/20	5/37/115/115	-
27	STE	j	102	-	-	6/13/13/17	-
27	STE	D	413	-	-	5/15/17/17	-
30	DGD	H	102	-	-	21/51/91/95	0/2/2/2
30	DGD	c	521	-	-	18/51/91/95	0/2/2/2
27	STE	b	626	-	-	3/7/7/17	-
25	BCR	B	618	-	-	1/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	606	36	1/1/20/20	12/37/115/115	-
25	BCR	C	520	-	-	3/29/63/63	0/2/2/2
28	LMG	B	620	-	-	13/40/60/70	0/1/1/1
27	STE	C	529	-	-	6/11/11/17	-
23	CLA	B	603	-	1/1/20/20	3/37/115/115	-
27	STE	i	102	-	-	3/3/3/17	-
27	STE	a	417	-	-	4/7/9/17	-
25	BCR	x	101	-	-	7/29/63/63	0/2/2/2
23	CLA	b	605	-	1/1/20/20	7/37/115/115	-
30	DGD	c	519	-	-	26/51/91/95	0/2/2/2
23	CLA	B	610	36	1/1/20/20	4/37/115/115	-
27	STE	C	526	-	-	4/13/13/17	-
29	SQD	A	413	-	-	16/49/69/69	0/1/1/1
23	CLA	B	611	-	-	6/37/115/115	-
23	CLA	C	502	-	-	6/37/115/115	-
23	CLA	b	611	-	1/1/20/20	8/37/115/115	-
28	LMG	c	522	-	-	17/41/61/70	0/1/1/1
23	CLA	B	608	-	-	1/37/115/115	-
28	LMG	d	409	-	-	13/39/59/70	0/1/1/1
30	DGD	C	522	-	-	17/51/91/95	0/2/2/2
30	DGD	A	414	-	-	22/55/95/95	0/2/2/2
29	SQD	A	412	-	-	19/47/67/69	0/1/1/1
29	SQD	f	102	-	-	13/36/56/69	0/1/1/1
24	PHO	A	406	-	-	1/53/103/103	0/5/6/6
27	STE	B	623	-	-	7/12/12/17	-
28	LMG	D	409	-	-	16/46/66/70	0/1/1/1
33	LHG	d	408	-	-	12/43/43/53	-
23	CLA	B	604	-	1/1/20/20	10/37/115/115	-
23	CLA	C	509	-	1/1/20/20	11/37/115/115	-
25	BCR	B	617	-	-	5/29/63/63	0/2/2/2
23	CLA	C	503	-	-	3/37/115/115	-
23	CLA	C	510	-	1/1/20/20	7/37/115/115	-
23	CLA	D	404	-	1/1/20/20	2/37/115/115	-
27	STE	b	624	-	-	7/15/17/17	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	602	-	1/1/20/20	13/37/115/115	-
27	STE	A	416	-	-	9/14/14/17	-
23	CLA	C	504	36	1/1/18/20	5/30/108/115	-
23	CLA	D	403	36	-	6/37/115/115	-
27	STE	B	622	-	-	3/7/9/17	-
28	LMG	b	621	-	-	17/46/66/70	0/1/1/1
23	CLA	b	615	-	1/1/19/20	8/31/109/115	-
33	LHG	L	101	-	-	12/53/53/53	-
25	BCR	T	101	-	-	0/29/63/63	0/2/2/2
23	CLA	c	505	-	1/1/20/20	9/37/115/115	-
23	CLA	B	612	-	1/1/20/20	11/37/115/115	-
25	BCR	k	102	-	-	2/29/63/63	0/2/2/2
23	CLA	d	403	-	-	7/37/115/115	-
24	PHO	d	401	-	-	2/53/103/103	0/5/6/6
28	LMG	b	623	-	-	28/50/70/70	0/1/1/1
23	CLA	c	510	-	1/1/20/20	10/37/115/115	-
28	LMG	c	524	-	-	16/44/64/70	0/1/1/1

All (859) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	612	CLA	C4B-NB	9.02	1.43	1.35
23	C	501	CLA	C4B-NB	8.61	1.42	1.35
35	V	201	HEC	C3C-C2C	-8.38	1.32	1.40
23	b	605	CLA	MG-NA	8.31	2.26	2.06
23	b	613	CLA	C4B-NB	8.28	1.42	1.35
23	d	402	CLA	C4B-NB	8.18	1.42	1.35
23	C	502	CLA	C4B-NB	8.11	1.42	1.35
23	B	614	CLA	C4B-NB	8.07	1.42	1.35
23	d	403	CLA	C4B-NB	8.06	1.42	1.35
23	c	504	CLA	C4B-NB	8.05	1.42	1.35
23	B	601	CLA	C4B-NB	8.01	1.42	1.35
35	v	201	HEC	C3B-C2B	-7.82	1.32	1.40
23	b	603	CLA	C4B-NB	7.80	1.42	1.35
23	h	101	CLA	C4B-NB	7.73	1.42	1.35
23	B	615	CLA	C4B-NB	7.69	1.42	1.35
23	B	602	CLA	C4B-NB	7.60	1.42	1.35
23	D	403	CLA	C4B-NB	7.58	1.42	1.35
23	b	614	CLA	C4B-NB	7.58	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	502	CLA	C4C-NC	7.55	1.41	1.35
23	b	607	CLA	C4C-NC	7.41	1.41	1.35
23	c	513	CLA	C4B-NB	7.40	1.41	1.35
23	c	511	CLA	C4B-NB	7.32	1.41	1.35
23	c	501	CLA	C4B-NB	7.32	1.41	1.35
23	c	505	CLA	C4B-NB	7.32	1.41	1.35
23	B	610	CLA	C4B-NB	7.26	1.41	1.35
23	C	509	CLA	C4B-NB	7.18	1.41	1.35
23	C	505	CLA	C4B-NB	7.17	1.41	1.35
26	D	407	PL9	C7-C3	-7.16	1.44	1.51
23	a	406	CLA	C4B-NB	7.14	1.41	1.35
23	a	408	CLA	C4B-NB	7.13	1.41	1.35
23	b	612	CLA	C4B-NB	7.09	1.41	1.35
35	V	201	HEC	C3B-C2B	-7.03	1.33	1.40
23	B	606	CLA	C4B-NB	7.03	1.41	1.35
23	C	504	CLA	C4B-NB	7.01	1.41	1.35
23	C	511	CLA	C4B-NB	6.80	1.41	1.35
23	B	613	CLA	C4B-NB	6.79	1.41	1.35
23	A	407	CLA	C4B-NB	6.77	1.41	1.35
23	b	612	CLA	C4C-NC	6.77	1.41	1.35
23	c	511	CLA	C4C-NC	6.70	1.41	1.35
23	C	506	CLA	C4B-NB	6.67	1.41	1.35
23	C	503	CLA	C4B-NB	6.60	1.41	1.35
23	B	614	CLA	C4C-NC	6.60	1.41	1.35
23	b	610	CLA	C4C-NC	6.59	1.41	1.35
23	b	605	CLA	C4B-NB	6.59	1.41	1.35
23	C	501	CLA	C4C-NC	6.56	1.41	1.35
23	a	405	CLA	C4B-NB	6.49	1.41	1.35
23	A	404	CLA	C4B-NB	6.48	1.41	1.35
23	c	509	CLA	C4C-NC	6.45	1.41	1.35
23	B	606	CLA	MG-NA	6.43	2.21	2.06
23	B	611	CLA	MG-NA	6.41	2.21	2.06
23	c	506	CLA	C4C-NC	6.40	1.40	1.35
23	c	510	CLA	C4C-NC	6.36	1.40	1.35
23	C	505	CLA	C4C-NC	6.36	1.40	1.35
23	a	408	CLA	C4C-NC	6.36	1.40	1.35
23	C	510	CLA	C4C-NC	6.35	1.40	1.35
23	c	506	CLA	C4B-NB	6.29	1.40	1.35
23	c	507	CLA	C4B-NB	6.28	1.40	1.35
23	B	616	CLA	C4C-NC	6.27	1.40	1.35
23	b	609	CLA	C4B-NB	6.25	1.40	1.35
34	f	101	HEM	C3B-C2B	-6.24	1.31	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	405	CLA	C4B-NB	6.24	1.40	1.35
23	a	405	CLA	C4C-NC	6.24	1.40	1.35
23	B	611	CLA	C4B-NB	6.22	1.40	1.35
23	h	101	CLA	C4C-NC	6.19	1.40	1.35
23	b	602	CLA	C4B-NB	6.19	1.40	1.35
23	C	501	CLA	MG-NA	6.09	2.20	2.06
23	C	512	CLA	C4B-NB	6.09	1.40	1.35
23	B	616	CLA	C4B-NB	6.08	1.40	1.35
23	a	411	CLA	MG-NA	6.03	2.20	2.06
23	C	511	CLA	MG-NA	6.01	2.20	2.06
23	c	509	CLA	C4B-NB	5.99	1.40	1.35
23	B	609	CLA	C4B-NB	5.89	1.40	1.35
23	b	608	CLA	MG-NA	5.88	2.20	2.06
23	B	615	CLA	C4C-NC	5.87	1.40	1.35
23	b	611	CLA	C4C-NC	5.80	1.40	1.35
23	c	501	CLA	C4C-NC	5.78	1.40	1.35
23	b	608	CLA	C4B-NB	5.76	1.40	1.35
23	C	508	CLA	C4C-NC	5.75	1.40	1.35
23	c	503	CLA	C4B-NB	5.75	1.40	1.35
23	b	613	CLA	C4C-NC	5.74	1.40	1.35
23	c	510	CLA	MG-NA	5.71	2.19	2.06
23	b	601	CLA	C4B-NB	5.71	1.40	1.35
23	c	513	CLA	C4C-NC	5.71	1.40	1.35
23	b	604	CLA	C4B-NB	5.69	1.40	1.35
34	F	101	HEM	C3B-C2B	-5.69	1.32	1.40
23	C	503	CLA	MG-NA	5.68	2.19	2.06
23	D	405	CLA	C4B-NB	5.65	1.40	1.35
23	B	601	CLA	MG-NA	5.61	2.19	2.06
23	b	607	CLA	C4B-NB	5.60	1.40	1.35
23	B	605	CLA	C4C-NC	5.58	1.40	1.35
23	b	609	CLA	C4C-NC	5.58	1.40	1.35
23	b	604	CLA	C4C-NC	5.55	1.40	1.35
23	C	503	CLA	C4C-NC	5.54	1.40	1.35
23	C	513	CLA	C4B-NB	5.53	1.40	1.35
23	b	611	CLA	C4B-NB	5.52	1.40	1.35
23	B	601	CLA	C4C-NC	5.46	1.40	1.35
23	c	510	CLA	C4B-NB	5.46	1.40	1.35
23	c	508	CLA	C4B-NB	5.45	1.40	1.35
23	c	508	CLA	MG-NA	5.45	2.19	2.06
23	d	403	CLA	C4C-NC	5.39	1.40	1.35
23	A	405	CLA	C4C-NC	5.37	1.40	1.35
23	c	502	CLA	C4C-NC	5.36	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	610	CLA	C4C-NC	5.35	1.40	1.35
23	C	508	CLA	C4B-NB	5.35	1.40	1.35
23	c	507	CLA	C4C-NC	5.33	1.40	1.35
23	B	612	CLA	C4C-NC	5.31	1.39	1.35
23	B	607	CLA	C4B-NB	5.29	1.39	1.35
23	b	615	CLA	C4B-NB	5.27	1.39	1.35
23	a	406	CLA	C4C-NC	5.27	1.39	1.35
23	c	502	CLA	C4B-NB	5.22	1.39	1.35
28	C	517	LMG	O1-C1	5.22	1.49	1.40
23	b	606	CLA	C4B-NB	5.19	1.39	1.35
23	b	614	CLA	C4C-NC	5.16	1.39	1.35
34	F	101	HEM	C3C-C2C	-5.14	1.33	1.40
23	C	511	CLA	C4C-NC	5.10	1.39	1.35
23	C	510	CLA	C4B-NB	5.07	1.39	1.35
23	b	602	CLA	C4C-NC	5.05	1.39	1.35
26	A	409	PL9	C7-C3	-5.03	1.46	1.51
23	b	610	CLA	C4B-NB	5.02	1.39	1.35
23	c	512	CLA	C4C-NC	5.02	1.39	1.35
23	C	512	CLA	C4C-NC	5.00	1.39	1.35
25	t	101	BCR	C30-C25	-4.98	1.46	1.53
26	d	405	PL9	C6-C1	-4.97	1.39	1.48
23	C	513	CLA	MG-NA	4.94	2.18	2.06
23	B	603	CLA	C4C-NC	4.89	1.39	1.35
35	v	201	HEC	C3D-C2D	4.89	1.52	1.37
23	b	608	CLA	C4C-NC	4.85	1.39	1.35
23	c	503	CLA	C4C-NC	4.80	1.39	1.35
23	a	411	CLA	C4C-NC	4.79	1.39	1.35
29	f	102	SQD	O48-C23	4.79	1.47	1.33
29	A	413	SQD	O48-C23	4.78	1.47	1.33
29	l	101	SQD	O48-C23	4.78	1.47	1.33
23	C	509	CLA	C4C-NC	4.76	1.39	1.35
25	c	515	BCR	C1-C6	-4.75	1.47	1.53
23	c	513	CLA	MG-NA	4.73	2.17	2.06
23	D	404	CLA	C4C-NC	4.73	1.39	1.35
23	c	508	CLA	C4C-NC	4.72	1.39	1.35
23	B	602	CLA	C4C-NC	4.72	1.39	1.35
23	c	505	CLA	C4C-NC	4.67	1.39	1.35
23	B	607	CLA	C4C-NC	4.63	1.39	1.35
34	f	101	HEM	C3C-C2C	-4.59	1.34	1.40
23	B	609	CLA	C4C-NC	4.57	1.39	1.35
25	C	515	BCR	C1-C6	-4.56	1.47	1.53
29	a	414	SQD	O48-C23	4.56	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	615	CLA	C4C-NC	4.56	1.39	1.35
23	C	508	CLA	C1B-NB	4.55	1.39	1.35
23	a	411	CLA	C4B-NB	4.52	1.39	1.35
23	d	402	CLA	MG-NA	4.52	2.17	2.06
23	c	512	CLA	C4B-NB	4.51	1.39	1.35
23	C	502	CLA	MG-NA	4.47	2.16	2.06
23	b	603	CLA	C4C-NC	4.46	1.39	1.35
23	B	608	CLA	C4B-NB	4.42	1.39	1.35
23	C	513	CLA	C4C-NC	4.42	1.39	1.35
29	F	102	SQD	O48-C23	4.41	1.46	1.33
23	c	511	CLA	MG-NA	4.41	2.16	2.06
23	B	603	CLA	C4B-NB	4.39	1.39	1.35
23	B	608	CLA	C4C-NC	4.38	1.39	1.35
23	C	507	CLA	C4B-NB	4.36	1.39	1.35
33	a	413	LHG	O8-C23	4.33	1.46	1.33
25	c	514	BCR	C1-C6	-4.32	1.47	1.53
26	D	407	PL9	C7-C8	-4.31	1.44	1.50
23	a	408	CLA	MG-NA	4.30	2.16	2.06
23	B	604	CLA	C4B-NB	4.30	1.39	1.35
30	C	522	DGD	O5D-C6D	-4.28	1.35	1.43
29	F	102	SQD	O5-C1	4.28	1.52	1.41
35	v	201	HEC	C3C-C2C	-4.27	1.36	1.40
28	a	415	LMG	C4-C5	4.26	1.62	1.53
25	x	101	BCR	C30-C25	-4.25	1.47	1.53
23	C	511	CLA	C1B-NB	4.24	1.39	1.35
23	C	508	CLA	MG-NA	4.24	2.16	2.06
26	d	405	PL9	C3-C4	-4.24	1.42	1.49
23	D	404	CLA	C4B-NB	4.23	1.39	1.35
23	B	605	CLA	C4B-NB	4.22	1.39	1.35
23	D	403	CLA	C4C-NC	4.21	1.39	1.35
23	b	605	CLA	C4C-NC	4.21	1.39	1.35
30	C	521	DGD	C4D-C3D	4.20	1.63	1.52
25	B	618	BCR	C30-C25	-4.20	1.48	1.53
29	A	412	SQD	O48-C23	4.20	1.45	1.33
23	C	506	CLA	C4C-NC	4.19	1.38	1.35
23	c	504	CLA	C4C-NC	4.19	1.38	1.35
23	b	606	CLA	C4C-NC	4.16	1.38	1.35
23	B	609	CLA	MG-NA	4.16	2.16	2.06
23	A	407	CLA	C4C-NC	4.16	1.38	1.35
29	a	414	SQD	O5-C1	4.15	1.52	1.41
23	C	504	CLA	C4C-NC	4.14	1.38	1.35
30	A	414	DGD	C3G-C2G	4.13	1.63	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	606	CLA	C4C-NC	4.10	1.38	1.35
29	b	620	SQD	O48-C23	4.10	1.45	1.33
23	D	405	CLA	C4C-NC	4.09	1.38	1.35
23	B	610	CLA	MG-NA	4.09	2.16	2.06
29	a	414	SQD	O47-C7	4.06	1.45	1.34
29	l	101	SQD	O47-C7	4.05	1.45	1.34
28	a	415	LMG	C4-C3	4.04	1.62	1.52
23	B	611	CLA	C4C-NC	4.03	1.38	1.35
23	b	601	CLA	C4C-NC	4.03	1.38	1.35
25	b	617	BCR	C30-C25	-4.03	1.48	1.53
23	B	616	CLA	MG-NA	4.02	2.15	2.06
23	d	402	CLA	C4C-NC	3.99	1.38	1.35
25	d	404	BCR	C1-C6	-3.99	1.48	1.53
23	C	512	CLA	MG-NA	3.98	2.15	2.06
28	D	408	LMG	C4-C5	3.97	1.61	1.53
25	D	406	BCR	C1-C6	-3.97	1.48	1.53
33	D	411	LHG	P-O6	3.95	1.75	1.59
25	K	101	BCR	C30-C25	-3.94	1.48	1.53
23	B	604	CLA	MG-NA	3.93	2.15	2.06
30	C	522	DGD	C1E-C2E	3.93	1.63	1.52
23	b	603	CLA	MG-NA	3.93	2.15	2.06
23	B	607	CLA	MG-NA	3.91	2.15	2.06
33	D	412	LHG	O7-C5	-3.89	1.36	1.46
30	H	102	DGD	C4D-C5D	3.88	1.61	1.53
29	A	413	SQD	O5-C1	3.87	1.51	1.41
23	A	404	CLA	C4C-NC	3.87	1.38	1.35
23	b	607	CLA	MG-NA	3.85	2.15	2.06
23	a	406	CLA	MG-NA	3.85	2.15	2.06
25	T	101	BCR	C1-C6	-3.84	1.48	1.53
28	c	518	LMG	C7-C8	3.80	1.60	1.51
30	h	102	DGD	O2D-C2D	-3.78	1.34	1.43
23	C	505	CLA	MG-NA	3.75	2.15	2.06
29	A	412	SQD	O47-C45	-3.73	1.37	1.46
26	D	407	PL9	C3-C4	-3.73	1.43	1.49
29	b	620	SQD	O5-C1	3.72	1.51	1.41
23	B	613	CLA	C4C-NC	3.72	1.38	1.35
30	c	520	DGD	C4D-C3D	3.72	1.61	1.52
23	B	607	CLA	C1B-NB	3.71	1.38	1.35
26	d	405	PL9	C7-C8	-3.70	1.45	1.50
23	D	404	CLA	MG-NA	3.69	2.15	2.06
33	E	101	LHG	P-O6	3.67	1.74	1.59
23	B	604	CLA	C4C-NC	3.65	1.38	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	h	102	DGD	C4E-C5E	3.65	1.60	1.53
33	a	413	LHG	C24-C23	3.64	1.61	1.50
33	L	101	LHG	O7-C5	-3.63	1.37	1.46
29	a	412	SQD	O47-C45	-3.62	1.37	1.46
25	b	618	BCR	C30-C25	-3.61	1.48	1.53
29	f	102	SQD	O47-C7	3.60	1.44	1.34
23	h	101	CLA	C1D-C2D	3.59	1.50	1.42
23	c	507	CLA	C3B-C2B	-3.58	1.35	1.40
25	k	101	BCR	C30-C25	-3.57	1.48	1.53
29	a	412	SQD	O48-C23	3.56	1.43	1.33
24	d	401	PHO	CHC-C1C	3.56	1.45	1.38
23	c	510	CLA	CMB-C2B	-3.55	1.44	1.51
33	D	410	LHG	O7-C5	-3.55	1.37	1.46
25	H	101	BCR	C30-C25	-3.54	1.48	1.53
35	V	201	HEC	C3D-C2D	3.53	1.48	1.37
33	a	413	LHG	P-O6	3.52	1.73	1.59
33	d	406	LHG	C24-C23	3.51	1.61	1.50
29	f	102	SQD	O5-C1	3.50	1.50	1.41
25	D	406	BCR	C30-C25	-3.50	1.49	1.53
23	b	605	CLA	C3B-C2B	-3.48	1.35	1.40
29	b	620	SQD	O47-C7	3.47	1.44	1.34
28	M	101	LMG	C9-C8	3.46	1.61	1.50
30	c	519	DGD	C4D-C3D	3.45	1.61	1.52
30	c	520	DGD	C4E-C5E	3.45	1.60	1.53
30	A	414	DGD	C4D-C5D	3.44	1.60	1.53
29	f	102	SQD	O47-C45	-3.44	1.38	1.46
23	C	507	CLA	C4C-NC	3.44	1.38	1.35
30	c	519	DGD	O3E-C3E	-3.43	1.34	1.43
25	a	409	BCR	C1-C6	-3.43	1.49	1.53
23	A	407	CLA	C1B-NB	3.42	1.38	1.35
29	A	413	SQD	O47-C7	3.40	1.43	1.34
23	A	405	CLA	C1B-NB	3.40	1.38	1.35
23	b	606	CLA	C3B-C2B	-3.38	1.35	1.40
30	c	519	DGD	O2E-C2E	-3.37	1.35	1.43
33	a	413	LHG	O8-C6	3.36	1.52	1.45
23	D	405	CLA	MG-NA	3.36	2.14	2.06
23	b	605	CLA	C1B-NB	3.31	1.38	1.35
25	b	616	BCR	C30-C25	-3.30	1.49	1.53
28	c	524	LMG	C4-C5	3.30	1.60	1.53
34	f	101	HEM	C3C-CAC	3.29	1.54	1.47
29	A	413	SQD	C24-C23	3.28	1.60	1.50
34	f	101	HEM	C3B-CAB	3.27	1.54	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	520	DGD	C6E-C5E	3.26	1.62	1.51
26	D	407	PL9	C6-C1	-3.26	1.42	1.48
33	d	408	LHG	P-O6	3.25	1.72	1.59
28	a	415	LMG	C3-C2	3.25	1.60	1.52
23	b	609	CLA	C3B-C2B	-3.22	1.35	1.40
25	B	619	BCR	C30-C25	-3.22	1.49	1.53
23	c	505	CLA	C3B-C2B	-3.21	1.35	1.40
23	B	606	CLA	C3B-C2B	-3.21	1.35	1.40
23	c	509	CLA	C3B-C2B	-3.20	1.35	1.40
30	C	522	DGD	C4D-C3D	3.20	1.60	1.52
28	a	415	LMG	C7-C8	3.18	1.60	1.50
25	b	616	BCR	C1-C6	-3.18	1.49	1.53
25	b	617	BCR	C1-C6	-3.18	1.49	1.53
25	B	617	BCR	C1-C6	-3.18	1.49	1.53
30	C	522	DGD	C6E-C5E	3.17	1.62	1.51
23	A	404	CLA	C1D-C2D	3.17	1.49	1.42
25	k	101	BCR	C1-C6	-3.17	1.49	1.53
28	D	409	LMG	C4-C5	3.16	1.59	1.53
30	C	522	DGD	O3D-C3D	-3.16	1.35	1.43
28	b	619	LMG	C9-C8	3.16	1.58	1.50
28	B	620	LMG	C4-C3	3.14	1.60	1.52
29	A	412	SQD	O5-C1	3.13	1.49	1.41
30	C	521	DGD	C4E-C3E	3.12	1.60	1.52
23	D	403	CLA	C3B-C2B	-3.12	1.36	1.40
28	c	523	LMG	O1-C1	3.12	1.45	1.40
23	b	614	CLA	CMD-C2D	-3.10	1.44	1.51
30	c	520	DGD	O3D-C3D	-3.10	1.35	1.43
28	C	524	LMG	C4-C3	3.10	1.60	1.52
24	d	401	PHO	C1A-NA	3.10	1.43	1.37
28	c	522	LMG	C1-C2	3.09	1.61	1.52
33	a	413	LHG	C6-C5	3.08	1.60	1.50
23	C	510	CLA	CMC-C2C	-3.08	1.44	1.51
23	c	501	CLA	MG-NA	3.08	2.13	2.06
23	b	604	CLA	MG-NA	3.08	2.13	2.06
23	b	601	CLA	CAC-C3C	-3.08	1.44	1.52
25	c	515	BCR	C30-C25	-3.07	1.49	1.53
23	B	608	CLA	C1D-C2D	3.07	1.49	1.42
25	K	101	BCR	C1-C6	-3.07	1.49	1.53
25	c	514	BCR	C30-C25	-3.07	1.49	1.53
23	C	509	CLA	CMB-C2B	-3.07	1.45	1.51
24	d	401	PHO	CMC-C2C	-3.07	1.44	1.50
23	C	513	CLA	C1D-C2D	3.06	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	F	102	SQD	O5-C5	3.05	1.51	1.44
23	a	408	CLA	CMC-C2C	-3.04	1.44	1.51
29	l	101	SQD	O5-C1	3.04	1.49	1.41
23	B	611	CLA	C3B-C2B	-3.03	1.36	1.40
23	B	615	CLA	C3B-C2B	-3.03	1.36	1.40
29	a	412	SQD	O47-C7	3.02	1.42	1.34
23	A	404	CLA	C3B-C2B	-3.02	1.36	1.40
28	d	409	LMG	C4-C5	3.02	1.59	1.53
25	A	408	BCR	C1-C6	-3.01	1.49	1.53
25	B	618	BCR	C1-C6	-3.01	1.49	1.53
28	B	620	LMG	C4-C5	2.99	1.59	1.53
23	B	615	CLA	MG-NA	2.99	2.13	2.06
23	B	602	CLA	MG-NA	2.98	2.13	2.06
28	c	522	LMG	C7-C8	2.98	1.59	1.50
29	l	101	SQD	O47-C45	-2.98	1.39	1.46
25	B	619	BCR	C1-C6	-2.97	1.49	1.53
26	d	405	PL9	C26-C24	-2.97	1.45	1.51
24	a	407	PHO	O2D-CGD	2.97	1.40	1.33
23	B	602	CLA	CMB-C2B	-2.96	1.45	1.51
25	c	515	BCR	C33-C5	-2.95	1.46	1.50
25	T	101	BCR	C30-C25	-2.94	1.49	1.53
23	B	603	CLA	MG-NA	2.94	2.13	2.06
23	a	411	CLA	CMB-C2B	-2.94	1.45	1.51
25	C	520	BCR	C30-C25	-2.94	1.49	1.53
23	B	612	CLA	MG-NA	2.93	2.13	2.06
25	C	514	BCR	C30-C25	-2.93	1.49	1.53
30	A	414	DGD	C3E-C2E	2.93	1.59	1.52
30	c	521	DGD	C1D-C2D	2.92	1.60	1.52
24	d	401	PHO	C3B-C4B	2.92	1.49	1.43
23	D	405	CLA	CMB-C2B	-2.92	1.45	1.51
23	B	608	CLA	MG-NA	2.91	2.13	2.06
29	A	412	SQD	C24-C23	2.91	1.59	1.50
28	c	522	LMG	O1-C1	2.91	1.45	1.40
23	D	403	CLA	C1C-C2C	2.90	1.49	1.42
29	A	412	SQD	O6-C1	-2.90	1.35	1.40
29	a	414	SQD	O47-C45	-2.90	1.39	1.46
25	A	408	BCR	C33-C5	-2.89	1.46	1.50
23	c	511	CLA	C1D-C2D	2.88	1.49	1.42
23	B	613	CLA	MG-NA	2.88	2.13	2.06
23	c	512	CLA	C1D-C2D	2.88	1.49	1.42
28	a	415	LMG	C9-C8	2.88	1.59	1.50
25	B	617	BCR	C30-C25	-2.88	1.49	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	411	CLA	C1D-C2D	2.88	1.49	1.42
28	M	101	LMG	O3-C3	-2.87	1.36	1.43
34	F	101	HEM	C3B-CAB	2.87	1.53	1.47
23	c	503	CLA	C1D-C2D	2.87	1.49	1.42
28	a	415	LMG	O1-C7	2.86	1.49	1.43
23	d	403	CLA	MG-NA	2.86	2.13	2.06
23	b	611	CLA	CMC-C2C	-2.85	1.44	1.51
29	a	414	SQD	C24-C23	2.85	1.59	1.50
26	d	405	PL9	C41-C39	-2.84	1.45	1.51
28	D	408	LMG	C7-C8	2.84	1.59	1.50
23	D	405	CLA	C3B-C2B	-2.84	1.36	1.40
23	d	402	CLA	CMD-C2D	-2.83	1.44	1.51
23	c	512	CLA	CMB-C2B	-2.83	1.45	1.51
23	C	503	CLA	C1D-C2D	2.82	1.49	1.42
23	B	605	CLA	C3B-C2B	-2.82	1.36	1.40
23	d	402	CLA	CMB-C2B	-2.82	1.45	1.51
29	b	620	SQD	O47-C45	-2.82	1.39	1.46
23	b	602	CLA	C3B-C2B	-2.81	1.36	1.40
28	C	524	LMG	O7-C8	-2.81	1.39	1.46
29	a	412	SQD	O6-C1	-2.80	1.35	1.40
28	D	409	LMG	C7-C8	2.80	1.59	1.50
23	B	615	CLA	CMB-C2B	-2.80	1.45	1.51
23	a	405	CLA	C1D-C2D	2.79	1.48	1.42
25	C	514	BCR	C1-C6	-2.78	1.49	1.53
23	C	511	CLA	CMB-C2B	-2.78	1.45	1.51
28	a	415	LMG	C1-C2	2.78	1.60	1.52
23	b	610	CLA	CMC-C2C	-2.78	1.44	1.51
28	b	621	LMG	C1-C2	2.78	1.60	1.52
28	A	411	LMG	C1-C2	2.77	1.60	1.52
29	f	102	SQD	C24-C23	2.77	1.58	1.50
23	B	603	CLA	CMB-C2B	-2.76	1.45	1.51
30	H	102	DGD	O5D-C1E	2.76	1.44	1.40
23	b	601	CLA	C4B-CHC	-2.76	1.33	1.41
23	B	610	CLA	CMB-C2B	-2.76	1.45	1.51
29	a	412	SQD	C6-S	2.76	1.87	1.77
30	c	520	DGD	C3E-C2E	2.76	1.59	1.52
23	b	610	CLA	CMD-C2D	-2.75	1.45	1.51
29	A	413	SQD	O47-C45	-2.75	1.39	1.46
25	A	408	BCR	C30-C25	-2.75	1.50	1.53
23	d	402	CLA	C1D-C2D	2.75	1.48	1.42
23	C	513	CLA	C4B-CHC	-2.75	1.33	1.41
23	B	614	CLA	MG-NA	2.74	2.12	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	618	BCR	C1-C6	-2.74	1.50	1.53
23	b	602	CLA	CMC-C2C	-2.74	1.45	1.51
26	a	410	PL9	C53-C6	-2.73	1.45	1.50
23	h	101	CLA	O2A-CGA	2.73	1.41	1.33
33	l	102	LHG	O8-C6	-2.73	1.38	1.45
23	b	609	CLA	CMB-C2B	-2.73	1.46	1.51
24	A	406	PHO	CHC-C4B	-2.72	1.34	1.40
29	b	620	SQD	C24-C23	2.72	1.58	1.50
29	b	620	SQD	C6-S	2.72	1.87	1.77
29	F	102	SQD	O6-C44	2.71	1.50	1.43
23	B	616	CLA	C3B-C2B	-2.71	1.36	1.40
30	h	102	DGD	C1E-C2E	2.71	1.60	1.52
23	B	615	CLA	C1D-C2D	2.71	1.48	1.42
23	B	604	CLA	C1B-NB	2.71	1.37	1.35
23	c	507	CLA	MG-NA	2.71	2.12	2.06
30	h	102	DGD	C4D-C3D	2.71	1.59	1.52
23	c	509	CLA	CMB-C2B	-2.71	1.46	1.51
23	b	606	CLA	MG-NA	2.70	2.12	2.06
30	H	102	DGD	O2D-C2D	-2.70	1.36	1.43
29	A	412	SQD	O47-C7	2.70	1.41	1.34
30	A	414	DGD	O5D-C1E	2.70	1.44	1.40
30	A	414	DGD	C1E-C2E	2.70	1.60	1.52
23	b	604	CLA	C4B-CHC	-2.69	1.33	1.41
29	F	102	SQD	C24-C23	2.68	1.58	1.50
24	a	407	PHO	C4C-NC	2.67	1.42	1.36
30	C	521	DGD	C6D-C5D	2.67	1.59	1.51
29	a	414	SQD	O7-S	2.67	1.52	1.45
23	C	512	CLA	CMD-C2D	-2.67	1.45	1.51
29	a	414	SQD	C6-S	2.66	1.87	1.77
23	B	601	CLA	CMB-C2B	-2.66	1.46	1.51
23	C	508	CLA	C1D-C2D	2.66	1.48	1.42
23	b	607	CLA	CMB-C2B	-2.65	1.46	1.51
23	C	502	CLA	C1B-NB	2.65	1.37	1.35
34	F	101	HEM	C3C-CAC	2.65	1.53	1.47
23	B	614	CLA	C3B-C2B	-2.65	1.36	1.40
23	B	601	CLA	C1D-C2D	2.64	1.48	1.42
23	B	613	CLA	CMD-C2D	-2.64	1.45	1.51
23	A	407	CLA	C3B-C2B	-2.63	1.36	1.40
25	k	102	BCR	C30-C25	-2.62	1.50	1.53
23	B	609	CLA	C3B-C2B	-2.62	1.36	1.40
23	C	509	CLA	C1B-NB	2.62	1.37	1.35
29	a	414	SQD	O5-C5	2.62	1.50	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	408	CLA	CMD-C2D	-2.62	1.45	1.51
29	l	101	SQD	C24-C23	2.61	1.58	1.50
28	C	517	LMG	C7-C8	2.61	1.58	1.50
23	C	503	CLA	CMD-C2D	-2.61	1.45	1.51
23	C	511	CLA	C1D-C2D	2.61	1.48	1.42
23	a	408	CLA	C4B-CHC	-2.60	1.33	1.41
23	c	504	CLA	CMD-C2D	-2.60	1.45	1.51
23	C	507	CLA	C1B-NB	-2.59	1.32	1.35
29	A	413	SQD	O5-C5	2.59	1.50	1.44
28	C	524	LMG	C4-C5	2.59	1.58	1.53
23	a	406	CLA	CMB-C2B	-2.59	1.46	1.51
23	b	602	CLA	C3B-CAB	-2.59	1.42	1.47
30	A	414	DGD	C4E-C5E	2.59	1.58	1.53
26	A	409	PL9	C21-C19	2.59	1.56	1.51
28	D	408	LMG	O1-C1	2.58	1.44	1.40
23	h	101	CLA	MG-NA	2.58	2.12	2.06
23	B	610	CLA	C1B-NB	2.58	1.37	1.35
28	b	621	LMG	C4-C5	2.57	1.58	1.53
23	c	513	CLA	CMB-C2B	-2.57	1.46	1.51
23	B	607	CLA	CMD-C2D	-2.57	1.45	1.51
30	C	522	DGD	O5D-C1E	2.56	1.44	1.40
23	b	612	CLA	CMB-C2B	-2.56	1.46	1.51
28	c	522	LMG	C4-C3	2.56	1.58	1.52
23	B	616	CLA	C1D-C2D	2.56	1.48	1.42
30	H	102	DGD	C6E-C5E	2.56	1.60	1.51
23	a	405	CLA	C3B-C2B	-2.55	1.36	1.40
23	B	610	CLA	C3B-C2B	-2.55	1.36	1.40
23	c	512	CLA	C3B-CAB	-2.55	1.42	1.47
23	b	610	CLA	C1D-C2D	2.55	1.48	1.42
23	b	614	CLA	C3B-C2B	-2.54	1.36	1.40
23	c	502	CLA	CMD-C2D	-2.54	1.45	1.51
23	B	614	CLA	C1C-C2C	2.54	1.48	1.42
24	D	402	PHO	C4C-NC	2.54	1.42	1.36
24	A	406	PHO	C3B-C4B	2.53	1.48	1.43
23	D	403	CLA	C1D-C2D	2.53	1.48	1.42
23	B	607	CLA	CMB-C2B	-2.53	1.46	1.51
28	D	409	LMG	O3-C3	-2.53	1.37	1.43
23	c	503	CLA	CMC-C2C	-2.53	1.45	1.51
24	A	406	PHO	CMB-C2B	-2.53	1.45	1.50
26	A	409	PL9	C30-C29	-2.52	1.44	1.50
23	D	405	CLA	C4B-CHC	-2.52	1.34	1.41
23	a	406	CLA	CMD-C2D	-2.52	1.45	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	521	DGD	C6D-C5D	2.52	1.59	1.51
25	d	404	BCR	C30-C25	-2.52	1.50	1.53
23	B	601	CLA	CMC-C2C	-2.52	1.45	1.51
23	c	502	CLA	C3B-C2B	-2.52	1.36	1.40
23	B	603	CLA	C3B-C2B	-2.52	1.36	1.40
23	C	509	CLA	O2D-CGD	2.52	1.39	1.33
23	B	613	CLA	C3B-C2B	-2.52	1.36	1.40
23	b	612	CLA	CMD-C2D	-2.51	1.45	1.51
26	d	405	PL9	C31-C29	-2.51	1.46	1.51
33	a	413	LHG	C4-C5	2.51	1.58	1.50
23	b	602	CLA	MG-NA	2.51	2.12	2.06
28	C	517	LMG	O1-C7	-2.51	1.39	1.43
26	d	405	PL9	C46-C44	-2.51	1.46	1.51
28	d	409	LMG	C7-C8	2.50	1.58	1.50
28	c	524	LMG	O6-C5	-2.50	1.38	1.44
24	A	406	PHO	C1A-NA	2.50	1.42	1.37
33	E	101	LHG	O8-C23	2.50	1.40	1.33
25	c	514	BCR	C33-C5	-2.50	1.46	1.50
23	b	608	CLA	C1D-C2D	2.50	1.48	1.42
28	b	621	LMG	O6-C1	2.50	1.48	1.41
24	d	401	PHO	C1C-NC	-2.49	1.33	1.38
23	b	612	CLA	C1D-C2D	2.49	1.48	1.42
25	C	520	BCR	C1-C6	-2.49	1.50	1.53
28	b	621	LMG	C4-C3	2.49	1.58	1.52
23	C	512	CLA	CMB-C2B	-2.48	1.46	1.51
23	B	614	CLA	C3B-CAB	-2.48	1.42	1.47
23	B	603	CLA	C1D-C2D	2.48	1.48	1.42
25	x	101	BCR	C1-C6	-2.48	1.50	1.53
29	F	102	SQD	O9-S	2.48	1.52	1.45
23	b	608	CLA	C3B-CAB	-2.48	1.42	1.47
23	c	512	CLA	C3B-C2B	-2.47	1.36	1.40
23	b	615	CLA	CMC-C2C	-2.47	1.45	1.51
23	b	615	CLA	C1D-C2D	2.47	1.48	1.42
23	C	510	CLA	CMD-C2D	-2.47	1.45	1.51
23	C	512	CLA	C1D-C2D	2.47	1.48	1.42
23	B	610	CLA	C1D-C2D	2.47	1.48	1.42
28	A	411	LMG	C4-C3	2.46	1.58	1.52
25	C	515	BCR	C30-C25	-2.46	1.50	1.53
23	B	605	CLA	C1D-C2D	2.46	1.48	1.42
33	D	412	LHG	C24-C23	2.46	1.57	1.50
23	C	508	CLA	CMB-C2B	-2.45	1.46	1.51
25	C	520	BCR	C33-C5	-2.45	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	606	CLA	CMB-C2B	-2.45	1.46	1.51
23	b	608	CLA	CMB-C2B	-2.45	1.46	1.51
23	c	506	CLA	CAC-C3C	-2.45	1.46	1.52
24	D	402	PHO	C1C-NC	-2.45	1.33	1.38
23	C	501	CLA	CMC-C2C	-2.45	1.45	1.51
23	b	614	CLA	CMB-C2B	-2.45	1.46	1.51
23	d	403	CLA	CMD-C2D	-2.44	1.45	1.51
23	B	608	CLA	CMD-C2D	-2.44	1.45	1.51
30	A	414	DGD	O2G-C1B	2.44	1.41	1.34
23	c	507	CLA	CMC-C2C	-2.44	1.45	1.51
30	C	522	DGD	O3E-C3E	-2.44	1.37	1.43
25	B	617	BCR	C33-C5	-2.43	1.46	1.50
24	A	406	PHO	CHC-C1C	2.43	1.43	1.38
23	B	616	CLA	CAC-C3C	-2.43	1.46	1.52
25	a	409	BCR	C30-C25	-2.43	1.50	1.53
23	B	601	CLA	C3B-C2B	-2.43	1.37	1.40
29	a	414	SQD	O9-S	2.43	1.52	1.45
30	c	520	DGD	O3G-C1D	-2.43	1.36	1.40
23	B	615	CLA	C4B-CHC	-2.43	1.34	1.41
23	A	405	CLA	CMD-C2D	-2.42	1.45	1.51
23	B	616	CLA	CMD-C2D	-2.42	1.45	1.51
26	a	410	PL9	C46-C44	2.42	1.56	1.51
23	c	513	CLA	C1D-C2D	2.42	1.48	1.42
24	D	402	PHO	CHC-C1C	2.42	1.43	1.38
29	A	412	SQD	O9-S	2.41	1.52	1.45
23	C	507	CLA	CMD-C2D	-2.41	1.45	1.51
24	A	406	PHO	CMD-C2D	-2.41	1.45	1.50
29	A	413	SQD	O7-S	2.41	1.52	1.45
23	d	403	CLA	CAC-C3C	-2.41	1.46	1.52
30	h	102	DGD	C4E-C3E	2.41	1.58	1.52
23	b	613	CLA	C1D-C2D	2.40	1.48	1.42
29	a	412	SQD	O5-C1	2.40	1.48	1.41
23	B	608	CLA	C3B-C2B	-2.40	1.37	1.40
23	c	505	CLA	CMB-C2B	-2.40	1.46	1.51
23	C	503	CLA	CAC-C3C	-2.40	1.46	1.52
25	T	101	BCR	C38-C26	-2.40	1.47	1.50
23	b	615	CLA	CMB-C2B	-2.40	1.46	1.51
23	b	605	CLA	CAC-C3C	-2.40	1.46	1.52
23	c	513	CLA	CMC-C2C	-2.40	1.45	1.51
23	B	611	CLA	C1D-C2D	2.39	1.48	1.42
24	a	407	PHO	C3B-C4B	2.39	1.48	1.43
24	a	407	PHO	C1C-NC	-2.39	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	607	CLA	CMC-C2C	-2.39	1.45	1.51
23	D	403	CLA	CMD-C2D	-2.39	1.45	1.51
23	b	611	CLA	MG-NA	2.38	2.11	2.06
23	D	404	CLA	CMD-C2D	-2.38	1.45	1.51
25	C	515	BCR	C33-C5	-2.38	1.47	1.50
23	C	504	CLA	O2D-CGD	2.38	1.39	1.33
28	c	523	LMG	C4-C3	2.37	1.58	1.52
23	c	511	CLA	C1C-C2C	2.37	1.47	1.42
23	b	612	CLA	MG-NA	2.37	2.11	2.06
25	T	101	BCR	C27-C26	-2.37	1.46	1.51
23	C	507	CLA	CMB-C2B	-2.37	1.46	1.51
30	C	521	DGD	O5D-C1E	2.36	1.44	1.40
30	c	519	DGD	C4D-C5D	2.36	1.58	1.53
23	a	408	CLA	CAC-C3C	-2.36	1.46	1.52
26	D	407	PL9	C53-C6	-2.35	1.45	1.50
23	b	601	CLA	CMD-C2D	-2.35	1.46	1.51
23	B	603	CLA	CMD-C2D	-2.35	1.46	1.51
33	E	101	LHG	O7-C5	-2.35	1.40	1.46
29	A	413	SQD	C46-C45	2.34	1.57	1.50
26	D	407	PL9	C52-C5	-2.34	1.45	1.50
30	C	523	DGD	O2G-C2G	-2.34	1.40	1.46
30	c	521	DGD	C2A-C1A	-2.34	1.43	1.50
28	b	623	LMG	O8-C28	2.33	1.40	1.33
24	d	401	PHO	CHD-C4C	-2.33	1.35	1.40
33	d	407	LHG	O7-C5	-2.33	1.40	1.46
30	c	520	DGD	O5E-C6E	-2.32	1.32	1.42
30	C	521	DGD	O1G-C1G	-2.32	1.39	1.45
23	B	605	CLA	MG-NA	2.31	2.11	2.06
23	B	610	CLA	CMC-C2C	-2.31	1.46	1.51
23	A	404	CLA	CAC-C3C	-2.31	1.46	1.52
29	b	620	SQD	O6-C44	2.31	1.48	1.43
30	H	102	DGD	C1E-C2E	2.30	1.59	1.52
25	k	102	BCR	C1-C6	-2.30	1.50	1.53
23	B	611	CLA	CAC-C3C	-2.30	1.46	1.52
30	C	521	DGD	O3D-C3D	-2.30	1.37	1.43
23	C	511	CLA	C4B-CHC	-2.30	1.34	1.41
30	c	520	DGD	O4E-C4E	-2.29	1.37	1.43
23	D	403	CLA	CMB-C2B	-2.29	1.46	1.51
23	B	614	CLA	CMB-C2B	-2.29	1.46	1.51
23	B	611	CLA	CMB-C2B	-2.29	1.46	1.51
23	a	406	CLA	C1D-C2D	2.29	1.47	1.42
24	A	406	PHO	C4C-NC	2.29	1.41	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	503	CLA	CMB-C2B	-2.29	1.46	1.51
30	C	522	DGD	C6D-C5D	2.29	1.58	1.51
30	C	522	DGD	O2D-C2D	-2.28	1.37	1.43
23	c	509	CLA	C3B-CAB	-2.28	1.43	1.47
34	F	101	HEM	C4A-CHB	-2.28	1.34	1.41
23	b	607	CLA	C3B-CAB	-2.28	1.43	1.47
23	a	406	CLA	C3B-C2B	-2.28	1.37	1.40
30	C	523	DGD	O6E-C5E	2.28	1.49	1.44
23	C	510	CLA	CAA-C2A	-2.28	1.49	1.54
23	d	403	CLA	CMC-C2C	-2.28	1.46	1.51
33	d	408	LHG	C6-C5	2.27	1.57	1.50
23	B	602	CLA	C3B-C2B	-2.27	1.37	1.40
23	c	509	CLA	C1D-C2D	2.27	1.47	1.42
33	D	411	LHG	C3-C2	2.26	1.59	1.51
24	A	406	PHO	C1C-NC	-2.26	1.33	1.38
23	C	513	CLA	CMB-C2B	-2.26	1.46	1.51
23	c	505	CLA	C3B-CAB	-2.26	1.43	1.47
23	A	405	CLA	C1D-C2D	2.26	1.47	1.42
23	b	615	CLA	C3B-C2B	-2.26	1.37	1.40
30	A	414	DGD	C6E-C5E	2.26	1.59	1.51
29	l	101	SQD	C6-S	2.25	1.85	1.77
23	b	601	CLA	CMB-C2B	-2.25	1.47	1.51
25	T	101	BCR	C33-C5	-2.25	1.47	1.50
23	C	513	CLA	C1B-NB	2.25	1.37	1.35
23	c	507	CLA	C3B-CAB	-2.25	1.43	1.47
23	b	606	CLA	CMD-C2D	-2.25	1.46	1.51
23	b	613	CLA	C3B-CAB	-2.25	1.43	1.47
23	b	609	CLA	C4B-CHC	-2.25	1.34	1.41
23	D	403	CLA	C1B-NB	2.24	1.37	1.35
28	M	101	LMG	O8-C28	2.24	1.39	1.33
23	C	506	CLA	C1D-C2D	2.24	1.47	1.42
23	c	508	CLA	C1D-C2D	2.24	1.47	1.42
23	d	403	CLA	C3B-CAB	-2.24	1.43	1.47
23	c	505	CLA	CMC-C2C	-2.24	1.46	1.51
23	b	609	CLA	CMD-C2D	-2.24	1.46	1.51
29	a	412	SQD	C24-C23	2.24	1.57	1.50
29	a	412	SQD	O7-S	2.24	1.51	1.45
30	H	102	DGD	C3E-C2E	2.24	1.58	1.52
23	C	510	CLA	C1D-C2D	2.24	1.47	1.42
26	D	407	PL9	C5-C4	-2.24	1.39	1.47
23	a	405	CLA	CMC-C2C	-2.23	1.46	1.51
33	d	406	LHG	O7-C5	-2.23	1.41	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	613	CLA	CMC-C2C	-2.23	1.46	1.51
23	b	605	CLA	C4B-CHC	-2.23	1.34	1.41
23	c	503	CLA	CMD-C2D	-2.23	1.46	1.51
23	b	603	CLA	CMB-C2B	-2.22	1.47	1.51
23	B	602	CLA	C1D-C2D	2.22	1.47	1.42
30	A	414	DGD	O5D-C6D	-2.22	1.39	1.43
29	f	102	SQD	O6-C44	2.22	1.47	1.43
24	d	401	PHO	CAA-C2A	-2.22	1.50	1.54
23	D	404	CLA	C1D-C2D	2.22	1.47	1.42
23	b	614	CLA	MG-NA	2.22	2.11	2.06
23	B	606	CLA	C1D-C2D	2.22	1.47	1.42
33	l	102	LHG	C24-C23	-2.21	1.44	1.50
23	c	507	CLA	C1D-C2D	2.21	1.47	1.42
28	c	518	LMG	O7-C10	2.21	1.40	1.34
23	C	513	CLA	CMC-C2C	-2.21	1.46	1.51
23	b	608	CLA	CAC-C3C	-2.21	1.46	1.52
23	b	605	CLA	C3B-CAB	-2.21	1.43	1.47
25	a	409	BCR	C33-C5	-2.20	1.47	1.50
30	H	102	DGD	O5E-C6E	-2.20	1.33	1.42
30	H	102	DGD	C4E-C3E	2.20	1.57	1.52
24	d	401	PHO	CHC-C4B	-2.20	1.35	1.40
23	C	509	CLA	C3B-C2B	-2.20	1.37	1.40
23	c	508	CLA	CMC-C2C	-2.20	1.46	1.51
28	M	101	LMG	O7-C10	2.20	1.40	1.34
23	d	403	CLA	C4B-CHC	-2.19	1.34	1.41
23	D	405	CLA	CMD-C2D	-2.19	1.46	1.51
23	c	510	CLA	CMC-C2C	-2.19	1.46	1.51
33	E	101	LHG	P-O3	2.19	1.68	1.59
30	c	520	DGD	C4E-C3E	2.19	1.57	1.52
23	a	411	CLA	CMD-C2D	-2.19	1.46	1.51
33	d	407	LHG	O7-C7	2.19	1.40	1.34
23	c	504	CLA	CAC-C3C	-2.19	1.46	1.52
23	C	512	CLA	C3B-C2B	-2.19	1.37	1.40
29	b	620	SQD	C44-C45	2.19	1.57	1.50
23	b	613	CLA	C3B-C2B	-2.18	1.37	1.40
23	D	405	CLA	C1D-C2D	2.18	1.47	1.42
23	c	510	CLA	CAC-C3C	-2.18	1.46	1.52
24	d	401	PHO	C4C-C3C	2.18	1.49	1.45
28	c	524	LMG	O7-C8	-2.18	1.41	1.46
23	A	407	CLA	C1D-C2D	2.17	1.47	1.42
23	B	609	CLA	CMD-C2D	-2.17	1.46	1.51
23	C	513	CLA	C3B-CAB	-2.17	1.43	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	403	CLA	MG-NA	2.17	2.11	2.06
28	d	409	LMG	O1-C7	-2.16	1.39	1.43
23	B	615	CLA	C3B-CAB	-2.16	1.43	1.47
25	T	101	BCR	C4-C5	-2.16	1.46	1.51
29	l	101	SQD	C44-C45	2.16	1.57	1.50
23	c	507	CLA	CMB-C2B	-2.16	1.47	1.51
23	B	609	CLA	C4B-CHC	-2.16	1.35	1.41
23	B	615	CLA	CAC-C3C	-2.16	1.46	1.52
35	V	201	HEC	C1D-CHD	-2.15	1.35	1.41
23	B	606	CLA	C4B-CHC	-2.15	1.35	1.41
23	C	502	CLA	C3B-C2B	-2.15	1.37	1.40
23	B	604	CLA	CMC-C2C	-2.15	1.46	1.51
23	C	504	CLA	CMB-C2B	-2.15	1.47	1.51
23	c	501	CLA	CAC-C3C	-2.15	1.46	1.52
28	C	524	LMG	O1-C1	2.15	1.43	1.40
29	A	412	SQD	C8-C7	2.15	1.57	1.50
23	b	615	CLA	CMD-C2D	-2.15	1.46	1.51
24	a	407	PHO	CHC-C4B	-2.15	1.35	1.40
29	l	101	SQD	C46-C45	2.15	1.57	1.50
23	B	607	CLA	CAC-C3C	-2.15	1.46	1.52
34	f	101	HEM	C4A-CHB	-2.15	1.35	1.41
23	b	611	CLA	C4B-CHC	-2.15	1.35	1.41
29	l	101	SQD	O7-S	2.15	1.51	1.45
23	B	609	CLA	C1D-C2D	2.15	1.47	1.42
23	b	613	CLA	C5-C3	-2.15	1.46	1.51
30	A	414	DGD	C4D-C3D	2.15	1.57	1.52
23	b	607	CLA	C1D-C2D	2.15	1.47	1.42
23	a	406	CLA	CAC-C3C	-2.15	1.46	1.52
23	C	511	CLA	CMC-C2C	-2.14	1.46	1.51
28	c	522	LMG	O2-C2	-2.14	1.37	1.43
23	C	507	CLA	C3B-CAB	-2.14	1.43	1.47
23	b	607	CLA	C3B-C2B	-2.14	1.37	1.40
23	A	404	CLA	CMD-C2D	-2.14	1.46	1.51
23	b	602	CLA	C4B-CHC	-2.14	1.35	1.41
30	C	521	DGD	O4D-C4D	-2.14	1.37	1.43
23	c	503	CLA	C3B-CAB	-2.13	1.43	1.47
30	C	521	DGD	O2E-C2E	-2.13	1.38	1.43
26	d	405	PL9	C41-C42	-2.13	1.46	1.53
30	C	522	DGD	C4E-C3E	2.13	1.57	1.52
23	C	501	CLA	C1D-C2D	2.13	1.47	1.42
30	C	523	DGD	O5D-C1E	2.13	1.43	1.40
23	C	510	CLA	O2A-CGA	2.12	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	602	CLA	C1D-C2D	2.12	1.47	1.42
26	d	405	PL9	C53-C6	-2.12	1.46	1.50
23	B	610	CLA	CAC-C3C	-2.12	1.47	1.52
23	C	506	CLA	C3B-C2B	-2.12	1.37	1.40
28	d	409	LMG	O6-C5	-2.12	1.39	1.44
23	B	604	CLA	CMB-C2B	-2.12	1.47	1.51
23	b	601	CLA	C1D-C2D	2.12	1.47	1.42
28	b	623	LMG	C9-C8	2.12	1.57	1.50
29	b	620	SQD	O9-S	2.12	1.51	1.45
28	c	524	LMG	C3-C2	2.12	1.57	1.52
29	a	414	SQD	C46-C45	2.12	1.57	1.50
23	c	503	CLA	C3B-C2B	-2.12	1.37	1.40
23	b	611	CLA	CMD-C2D	-2.11	1.46	1.51
25	k	102	BCR	C38-C26	-2.11	1.47	1.50
23	B	607	CLA	C1C-C2C	2.11	1.47	1.42
23	c	501	CLA	CMD-C2D	-2.11	1.46	1.51
23	C	505	CLA	C1D-C2D	2.11	1.47	1.42
34	F	101	HEM	CMA-C3A	2.11	1.56	1.51
23	B	608	CLA	CAC-C3C	-2.11	1.47	1.52
23	C	512	CLA	C1A-CHA	-2.11	1.34	1.43
23	h	101	CLA	C3B-CAB	-2.11	1.43	1.47
30	c	519	DGD	C3E-C2E	2.11	1.57	1.52
23	h	101	CLA	CAC-C3C	-2.11	1.47	1.52
26	a	410	PL9	C48-C49	2.11	1.38	1.32
33	D	410	LHG	P-O3	2.11	1.67	1.59
23	h	101	CLA	CMD-C2D	-2.11	1.46	1.51
29	f	102	SQD	O9-S	2.10	1.51	1.45
29	f	102	SQD	C44-C45	2.10	1.57	1.50
23	A	407	CLA	CMB-C2B	-2.10	1.47	1.51
23	C	510	CLA	C1C-C2C	2.10	1.47	1.42
23	b	614	CLA	C3B-CAB	-2.10	1.43	1.47
23	c	506	CLA	CMD-C2D	-2.10	1.46	1.51
23	c	502	CLA	CMC-C2C	-2.10	1.46	1.51
23	c	512	CLA	CAC-C3C	-2.10	1.47	1.52
30	h	102	DGD	O2E-C2E	-2.10	1.38	1.43
24	D	402	PHO	CMB-C2B	-2.10	1.46	1.50
23	B	611	CLA	C1C-C2C	2.10	1.47	1.42
23	c	501	CLA	C1D-C2D	2.10	1.47	1.42
25	k	101	BCR	C33-C5	-2.10	1.47	1.50
23	C	503	CLA	C3B-C2B	-2.10	1.37	1.40
23	B	611	CLA	CMD-C2D	-2.10	1.46	1.51
34	f	101	HEM	C1A-CHA	-2.09	1.35	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	513	CLA	CMD-C2D	-2.09	1.46	1.51
23	b	606	CLA	C1D-C2D	2.09	1.47	1.42
29	l	101	SQD	O9-S	2.09	1.51	1.45
23	b	609	CLA	CAC-C3C	-2.09	1.47	1.52
29	A	413	SQD	O9-S	2.09	1.51	1.45
23	c	505	CLA	O2D-CED	-2.09	1.40	1.45
23	B	613	CLA	C3B-CAB	-2.09	1.43	1.47
29	A	412	SQD	C6-S	2.09	1.85	1.77
23	c	501	CLA	C4B-CHC	-2.09	1.35	1.41
23	a	411	CLA	C3B-C2B	-2.08	1.37	1.40
25	t	101	BCR	C33-C5	-2.08	1.47	1.50
23	b	606	CLA	CMC-C2C	-2.08	1.46	1.51
29	f	102	SQD	C6-S	2.08	1.85	1.77
23	c	506	CLA	CMB-C2B	-2.08	1.47	1.51
23	c	507	CLA	C4B-CHC	-2.08	1.35	1.41
23	c	511	CLA	CAC-C3C	-2.08	1.47	1.52
23	C	502	CLA	C1D-C2D	2.07	1.47	1.42
23	C	504	CLA	CMD-C2D	-2.07	1.46	1.51
23	c	508	CLA	O2D-CED	-2.07	1.40	1.45
23	A	405	CLA	C4B-CHC	-2.07	1.35	1.41
23	D	405	CLA	C3B-CAB	-2.07	1.43	1.47
23	c	506	CLA	C3B-CAB	-2.07	1.43	1.47
23	B	612	CLA	C1D-C2D	2.07	1.47	1.42
28	c	523	LMG	C7-C8	2.07	1.57	1.50
23	h	101	CLA	CMB-C2B	-2.07	1.47	1.51
28	b	619	LMG	O7-C10	2.06	1.40	1.34
28	a	415	LMG	O7-C10	2.06	1.40	1.34
23	c	509	CLA	O2D-CED	-2.06	1.40	1.45
23	c	502	CLA	CMB-C2B	-2.06	1.47	1.51
23	C	502	CLA	C1C-C2C	2.06	1.47	1.42
23	B	613	CLA	CMB-C2B	-2.06	1.47	1.51
23	B	604	CLA	C1D-C2D	2.06	1.47	1.42
23	b	606	CLA	CAC-C3C	-2.06	1.47	1.52
23	B	615	CLA	CMC-C2C	-2.06	1.46	1.51
33	a	413	LHG	P-O3	2.06	1.67	1.59
23	C	502	CLA	CMB-C2B	-2.06	1.47	1.51
23	b	615	CLA	MG-NA	2.05	2.11	2.06
23	b	610	CLA	CAC-C3C	-2.05	1.47	1.52
23	B	601	CLA	C1C-C2C	2.05	1.47	1.42
23	c	512	CLA	CMD-C2D	-2.05	1.46	1.51
29	l	101	SQD	C8-C7	2.05	1.56	1.50
23	d	402	CLA	C4B-CHC	-2.05	1.35	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	c	523	LMG	C9-C8	2.05	1.57	1.50
23	b	602	CLA	CMB-C2B	-2.05	1.47	1.51
23	B	604	CLA	C3B-C2B	-2.05	1.37	1.40
23	B	604	CLA	CAC-C3C	-2.05	1.47	1.52
23	c	511	CLA	C3B-C2B	-2.05	1.37	1.40
23	h	101	CLA	CMC-C2C	-2.05	1.46	1.51
23	c	513	CLA	C3B-C2B	-2.05	1.37	1.40
23	c	506	CLA	CMC-C2C	-2.05	1.46	1.51
24	D	402	PHO	CHC-C4B	-2.05	1.35	1.40
23	c	508	CLA	C3B-C2B	-2.05	1.37	1.40
23	B	604	CLA	CMD-C2D	-2.04	1.46	1.51
30	c	519	DGD	O2D-C2D	-2.04	1.38	1.43
23	b	606	CLA	CMB-C2B	-2.04	1.47	1.51
23	b	606	CLA	C3B-CAB	-2.04	1.43	1.47
29	f	102	SQD	O7-S	2.03	1.51	1.45
23	d	403	CLA	CMB-C2B	-2.03	1.47	1.51
26	a	410	PL9	C30-C29	-2.03	1.45	1.50
23	c	504	CLA	C1C-C2C	2.03	1.47	1.42
23	B	605	CLA	CMC-C2C	-2.03	1.46	1.51
23	d	402	CLA	CAC-C3C	-2.03	1.47	1.52
23	b	605	CLA	C1D-C2D	2.03	1.47	1.42
23	B	602	CLA	CAC-C3C	-2.02	1.47	1.52
23	B	615	CLA	CMD-C2D	-2.02	1.46	1.51
23	B	605	CLA	C3B-CAB	-2.02	1.43	1.47
23	b	608	CLA	C3B-C2B	-2.02	1.37	1.40
23	c	511	CLA	C3B-CAB	-2.02	1.43	1.47
23	B	603	CLA	C3B-CAB	-2.02	1.43	1.47
24	D	402	PHO	CHD-C4C	-2.02	1.35	1.40
25	B	619	BCR	C27-C26	-2.01	1.47	1.51
23	b	603	CLA	C3B-CAB	-2.01	1.43	1.47
35	v	201	HEC	C1B-NB	2.01	1.40	1.36
29	A	413	SQD	C6-S	2.01	1.84	1.77
23	a	405	CLA	CMB-C2B	-2.01	1.47	1.51
23	b	601	CLA	C3B-C2B	-2.01	1.37	1.40
23	C	508	CLA	CMC-C2C	-2.01	1.46	1.51
23	C	512	CLA	O2D-CED	-2.01	1.40	1.45
30	c	520	DGD	O1G-C1A	2.00	1.39	1.33
24	D	402	PHO	C3B-C4B	2.00	1.47	1.43
25	C	520	BCR	C39-C30	-2.00	1.49	1.53
23	b	602	CLA	CAC-C3C	-2.00	1.47	1.52
23	C	502	CLA	CMD-C2D	-2.00	1.46	1.51
23	c	508	CLA	CMD-C2D	-2.00	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	606	CLA	C3B-CAB	-2.00	1.43	1.47

All (1324) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	F	102	SQD	O6-C1-C2	14.95	131.64	108.30
23	B	601	CLA	C4A-NA-C1A	10.21	111.30	106.71
29	l	101	SQD	O7-S-C6	9.75	118.53	106.94
23	B	604	CLA	C4A-NA-C1A	9.51	110.98	106.71
23	B	606	CLA	C4A-NA-C1A	9.23	110.86	106.71
23	B	607	CLA	C4A-NA-C1A	9.20	110.84	106.71
29	b	620	SQD	O6-C1-C2	8.80	122.05	108.30
23	C	510	CLA	C4A-NA-C1A	8.50	110.53	106.71
23	C	513	CLA	C4A-NA-C1A	8.11	110.35	106.71
29	a	414	SQD	O7-S-C6	7.83	116.25	106.94
23	a	406	CLA	C4A-NA-C1A	7.78	110.20	106.71
23	b	613	CLA	C4A-NA-C1A	7.58	110.12	106.71
23	B	611	CLA	C4A-NA-C1A	7.53	110.09	106.71
23	c	510	CLA	C4A-NA-C1A	7.10	109.90	106.71
34	f	101	HEM	CBD-CAD-C3D	-7.04	99.51	112.48
23	c	511	CLA	C4A-NA-C1A	6.92	109.81	106.71
23	B	603	CLA	C4A-NA-C1A	6.88	109.80	106.71
29	a	412	SQD	C1-O5-C5	-6.87	100.20	113.69
23	b	603	CLA	C4A-NA-C1A	6.84	109.78	106.71
23	B	616	CLA	C4A-NA-C1A	6.84	109.78	106.71
23	c	502	CLA	C4A-NA-C1A	6.82	109.77	106.71
26	a	410	PL9	C7-C3-C4	6.77	122.38	116.88
29	F	102	SQD	C1-O5-C5	-6.76	100.41	113.69
23	h	101	CLA	C4A-NA-C1A	6.52	109.64	106.71
23	C	502	CLA	C4A-NA-C1A	6.47	109.62	106.71
23	a	411	CLA	C4A-NA-C1A	6.46	109.61	106.71
23	D	403	CLA	C4A-NA-C1A	6.42	109.59	106.71
23	C	501	CLA	C4A-NA-C1A	6.40	109.58	106.71
23	d	402	CLA	C4A-NA-C1A	6.38	109.58	106.71
23	c	509	CLA	C4A-NA-C1A	6.33	109.55	106.71
23	C	511	CLA	C4A-NA-C1A	6.13	109.46	106.71
23	B	610	CLA	C4A-NA-C1A	6.09	109.44	106.71
23	B	609	CLA	C4A-NA-C1A	6.03	109.42	106.71
23	c	508	CLA	C4A-NA-C1A	5.97	109.39	106.71
23	C	507	CLA	C4A-NA-C1A	5.96	109.39	106.71
34	F	101	HEM	CBD-CAD-C3D	-5.95	101.52	112.48
23	C	503	CLA	C4A-NA-C1A	5.92	109.37	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	f	101	HEM	CBA-CAA-C2A	-5.68	102.01	112.49
23	a	408	CLA	C4A-NA-C1A	5.63	109.24	106.71
28	a	415	LMG	C1-C2-C3	-5.53	98.48	110.00
26	A	409	PL9	C7-C3-C4	5.52	121.36	116.88
29	A	412	SQD	O8-S-C6	5.50	114.50	105.74
29	f	102	SQD	O7-S-C6	5.49	113.47	106.94
23	c	501	CLA	C4A-NA-C1A	5.44	109.15	106.71
23	c	501	CLA	O2D-CGD-O1D	-5.37	113.34	123.84
23	b	608	CLA	CMB-C2B-C1B	-5.36	120.23	128.46
29	a	412	SQD	O6-C1-C2	5.34	116.64	108.30
23	b	605	CLA	C4A-NA-C1A	5.32	109.10	106.71
26	d	405	PL9	C7-C3-C4	5.31	121.19	116.88
29	l	101	SQD	O6-C1-C2	5.30	116.57	108.30
29	A	412	SQD	O6-C44-C45	-5.17	98.43	110.90
23	B	612	CLA	C4A-NA-C1A	5.16	109.03	106.71
23	b	601	CLA	CMB-C2B-C1B	-5.06	120.69	128.46
28	C	517	LMG	O1-C1-C2	-5.04	100.43	108.30
29	A	413	SQD	O5-C5-C4	5.03	118.83	109.69
23	C	508	CLA	C4A-NA-C1A	4.97	108.94	106.71
28	B	620	LMG	C1-C2-C3	-4.97	99.65	110.00
28	a	415	LMG	O1-C1-C2	4.94	116.02	108.30
29	A	413	SQD	O47-C7-C8	4.92	122.09	111.50
29	b	620	SQD	O7-S-C6	4.89	112.75	106.94
23	B	608	CLA	C4A-NA-C1A	4.87	108.90	106.71
29	f	102	SQD	O9-S-O7	-4.86	97.13	113.95
23	b	601	CLA	C4A-NA-C1A	4.84	108.88	106.71
30	C	521	DGD	O3G-C3G-C2G	-4.80	99.32	110.90
29	l	101	SQD	O47-C7-C8	4.79	121.83	111.50
29	a	412	SQD	C3-C4-C5	4.77	118.75	110.24
29	a	412	SQD	C44-O6-C1	-4.77	104.42	113.74
23	b	602	CLA	O2D-CGD-O1D	-4.77	114.51	123.84
23	b	606	CLA	C4A-NA-C1A	4.77	108.85	106.71
23	b	614	CLA	CMB-C2B-C1B	-4.76	121.15	128.46
29	A	412	SQD	O47-C7-C8	4.71	121.65	111.50
29	a	412	SQD	O7-S-C6	4.69	112.51	106.94
23	C	507	CLA	CMB-C2B-C3B	4.68	133.44	124.68
23	C	505	CLA	C4A-NA-C1A	4.66	108.80	106.71
23	b	615	CLA	C4A-NA-C1A	4.66	108.80	106.71
23	c	512	CLA	C1-C2-C3	-4.63	118.04	126.04
23	B	612	CLA	CMB-C2B-C1B	-4.61	121.37	128.46
23	C	501	CLA	O2D-CGD-O1D	-4.60	114.84	123.84
29	a	414	SQD	O9-S-O7	-4.58	98.09	113.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	414	SQD	O47-C7-C8	4.57	121.35	111.50
23	C	507	CLA	CMB-C2B-C1B	-4.52	121.52	128.46
23	b	605	CLA	O2D-CGD-O1D	-4.52	115.01	123.84
29	A	412	SQD	C1-O5-C5	-4.51	104.84	113.69
23	c	512	CLA	C4D-C3D-CAD	-4.51	105.96	108.47
35	v	201	HEC	CMC-C2C-C1C	-4.49	121.56	128.46
23	b	615	CLA	O2D-CGD-O1D	-4.48	115.08	123.84
23	C	512	CLA	CMB-C2B-C1B	-4.48	121.58	128.46
29	f	102	SQD	O9-S-C6	4.46	112.24	106.94
23	A	407	CLA	O2D-CGD-O1D	-4.44	115.16	123.84
23	B	614	CLA	O2D-CGD-O1D	-4.42	115.19	123.84
29	b	620	SQD	O5-C1-C2	-4.40	101.03	110.35
29	l	101	SQD	O48-C23-C24	4.39	125.69	111.91
23	b	614	CLA	C4A-NA-C1A	4.37	108.67	106.71
29	A	413	SQD	O7-S-C6	4.37	112.14	106.94
23	b	602	CLA	CMB-C2B-C1B	-4.34	121.79	128.46
23	C	504	CLA	C4D-C3D-CAD	-4.33	106.06	108.47
23	a	408	CLA	OBD-CAD-CBD	-4.32	119.72	125.89
29	A	413	SQD	O48-C23-C24	4.31	125.45	111.91
23	a	405	CLA	CMB-C2B-C1B	-4.30	121.86	128.46
29	b	620	SQD	O8-S-C6	4.30	112.59	105.74
23	b	601	CLA	O2D-CGD-O1D	-4.29	115.44	123.84
23	h	101	CLA	O2D-CGD-O1D	-4.27	115.49	123.84
23	C	508	CLA	O2D-CGD-O1D	-4.26	115.51	123.84
30	c	519	DGD	O3G-C3G-C2G	-4.24	100.67	110.90
23	D	405	CLA	C4A-NA-C1A	4.24	108.61	106.71
23	C	503	CLA	C7-C6-C5	-4.23	101.86	113.36
28	C	517	LMG	O6-C5-C4	4.23	117.38	109.69
23	b	601	CLA	CMB-C2B-C3B	4.23	132.59	124.68
29	A	412	SQD	O5-C1-C2	-4.20	101.46	110.35
23	b	608	CLA	CMB-C2B-C3B	4.20	132.53	124.68
23	B	611	CLA	O2D-CGD-O1D	-4.19	115.65	123.84
28	b	623	LMG	O1-C1-C2	-4.19	101.77	108.30
23	c	504	CLA	O2D-CGD-O1D	-4.19	115.65	123.84
23	b	612	CLA	CMB-C2B-C1B	-4.18	122.03	128.46
23	b	603	CLA	CMD-C2D-C3D	4.18	132.50	124.68
23	b	615	CLA	CMB-C2B-C1B	-4.18	122.05	128.46
23	c	505	CLA	C4D-C3D-CAD	-4.16	106.15	108.47
26	a	410	PL9	C7-C3-C2	-4.16	117.83	123.30
23	h	101	CLA	O2D-CGD-CBD	4.14	118.62	111.27
34	F	101	HEM	CBA-CAA-C2A	-4.14	104.85	112.49
23	b	608	CLA	O1D-CGD-CBD	4.14	132.95	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	609	CLA	C4A-NA-C1A	4.11	108.55	106.71
23	C	506	CLA	C4A-NA-C1A	4.10	108.55	106.71
23	C	509	CLA	C4A-NA-C1A	4.10	108.55	106.71
23	B	608	CLA	O2D-CGD-O1D	-4.09	115.84	123.84
23	c	504	CLA	CMB-C2B-C1B	-4.08	122.19	128.46
29	a	412	SQD	O8-S-C6	4.08	112.24	105.74
23	B	605	CLA	C4-C3-C5	4.07	122.12	115.27
29	F	102	SQD	O8-S-C6	4.07	112.22	105.74
23	C	503	CLA	O2A-C1-C2	-4.07	97.95	108.64
23	c	509	CLA	CHB-C4A-NA	4.06	130.13	124.51
23	C	504	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
23	c	503	CLA	C4A-NA-C1A	4.02	108.51	106.71
23	C	509	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
33	l	102	LHG	O4-P-O5	4.00	132.04	112.24
33	D	411	LHG	O4-P-O5	3.99	131.99	112.24
23	c	509	CLA	O2A-CGA-O1A	-3.99	113.51	123.59
23	C	508	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
33	a	413	LHG	O4-P-O5	3.99	131.97	112.24
29	b	620	SQD	C3-C4-C5	3.99	117.35	110.24
23	B	602	CLA	CMB-C2B-C1B	-3.99	122.34	128.46
35	V	201	HEC	CMC-C2C-C1C	-3.99	122.34	128.46
23	b	615	CLA	CMB-C2B-C3B	3.98	132.13	124.68
23	b	602	CLA	OBD-CAD-CBD	-3.98	120.21	125.89
23	c	501	CLA	O2D-CGD-CBD	3.98	118.33	111.27
23	B	613	CLA	C1-C2-C3	-3.97	119.18	126.04
23	b	603	CLA	CMB-C2B-C1B	-3.96	122.37	128.46
30	C	522	DGD	O3G-C3G-C2G	-3.95	101.36	110.90
23	a	411	CLA	CMB-C2B-C1B	-3.95	122.40	128.46
33	L	101	LHG	O4-P-O5	3.94	131.71	112.24
23	A	405	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
23	b	603	CLA	C4D-C3D-CAD	-3.93	106.28	108.47
23	c	503	CLA	C4D-C3D-CAD	-3.93	106.28	108.47
29	A	412	SQD	C1-C2-C3	-3.93	101.81	110.00
33	E	101	LHG	O4-P-O5	3.92	131.63	112.24
29	A	413	SQD	C3-C4-C5	3.91	117.22	110.24
23	b	602	CLA	CMB-C2B-C3B	3.91	131.99	124.68
23	c	512	CLA	O2D-CGD-O1D	-3.89	116.23	123.84
23	C	512	CLA	CMB-C2B-C3B	3.88	131.94	124.68
29	F	102	SQD	C44-O6-C1	3.88	120.27	113.84
33	d	406	LHG	O4-P-O5	3.88	131.41	112.24
26	d	405	PL9	C37-C38-C39	-3.88	118.33	127.66
23	D	405	CLA	CMB-C2B-C1B	-3.86	122.53	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	608	CLA	C4D-C3D-CAD	-3.84	106.33	108.47
30	C	523	DGD	O3G-C3G-C2G	-3.83	101.65	110.90
23	c	512	CLA	CHB-C4A-NA	3.83	129.81	124.51
30	H	102	DGD	C1E-O6E-C5E	3.83	121.20	113.69
23	c	507	CLA	C4A-NA-C1A	3.82	108.42	106.71
23	b	614	CLA	CMB-C2B-C3B	3.82	131.82	124.68
29	A	412	SQD	O9-S-C6	3.81	111.47	106.94
23	c	513	CLA	CMB-C2B-C1B	-3.81	122.60	128.46
23	b	608	CLA	C4A-NA-C1A	3.81	108.42	106.71
25	c	514	BCR	C33-C5-C6	-3.81	120.25	124.53
30	A	414	DGD	C3G-O3G-C1D	3.81	121.19	113.74
23	B	614	CLA	C4D-C3D-CAD	-3.81	106.34	108.47
23	c	510	CLA	CMD-C2D-C3D	3.80	131.78	124.68
23	b	606	CLA	CMB-C2B-C1B	-3.79	122.63	128.46
23	C	505	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
23	c	503	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
25	A	408	BCR	C27-C26-C25	3.78	128.22	122.73
23	B	612	CLA	CMB-C2B-C3B	3.77	131.73	124.68
23	c	502	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
23	b	602	CLA	O2D-CGD-CBD	3.75	117.94	111.27
23	C	501	CLA	O2D-CGD-CBD	3.75	117.93	111.27
23	A	404	CLA	C4A-NA-C1A	3.75	108.39	106.71
23	c	506	CLA	C4A-NA-C1A	3.74	108.39	106.71
23	b	613	CLA	C7-C6-C5	-3.73	103.23	113.36
33	D	411	LHG	O8-C23-C24	3.72	123.59	111.91
30	c	520	DGD	O3G-C3G-C2G	-3.70	101.97	110.90
23	B	610	CLA	O2D-CGD-O1D	-3.70	116.61	123.84
23	a	406	CLA	CMD-C2D-C3D	3.69	131.59	124.68
23	c	501	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
23	a	406	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
23	C	502	CLA	C4D-C3D-CAD	-3.68	106.42	108.47
28	C	517	LMG	C6-C5-C4	-3.68	104.38	113.00
29	b	620	SQD	O47-C7-C8	3.68	119.42	111.50
23	b	610	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
29	f	102	SQD	O6-C1-C2	3.67	114.04	108.30
35	V	201	HEC	CBD-CAD-C3D	-3.67	105.71	112.49
23	b	609	CLA	O2D-CGD-O1D	-3.67	116.65	123.84
23	h	101	CLA	CHB-C4A-NA	3.67	129.59	124.51
29	F	102	SQD	C1-C2-C3	-3.67	102.35	110.00
30	H	102	DGD	O3G-C3G-C2G	-3.66	102.06	110.90
23	a	405	CLA	C4A-NA-C1A	3.66	108.35	106.71
28	b	623	LMG	C1-O6-C5	-3.65	106.52	113.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	510	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
35	V	201	HEC	C1D-C2D-C3D	-3.65	104.46	107.00
34	F	101	HEM	C1D-C2D-C3D	3.64	109.53	107.00
33	d	406	LHG	O8-C23-C24	3.63	123.30	111.91
23	b	607	CLA	CMD-C2D-C3D	3.62	131.45	124.68
30	c	519	DGD	O1G-C1A-O1A	-3.61	114.47	123.59
25	b	616	BCR	C2-C1-C6	3.61	116.05	110.48
29	A	413	SQD	O9-S-O7	-3.61	101.44	113.95
23	b	611	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
23	c	506	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
23	B	616	CLA	O2D-CGD-O1D	-3.61	116.78	123.84
23	a	406	CLA	CHB-C4A-NA	3.61	129.50	124.51
23	b	612	CLA	CMC-C2C-C3C	3.61	131.74	124.94
28	C	517	LMG	C7-O1-C1	3.59	120.76	113.74
23	B	614	CLA	O1D-CGD-CBD	3.59	131.83	124.48
23	b	609	CLA	C11-C12-C13	-3.58	104.33	115.92
23	B	612	CLA	C11-C12-C13	-3.58	104.35	115.92
23	b	611	CLA	OBD-CAD-CBD	-3.58	120.79	125.89
23	c	505	CLA	CMD-C2D-C3D	3.57	131.37	124.68
23	C	513	CLA	O2D-CGD-O1D	-3.57	116.85	123.84
33	d	407	LHG	O4-P-O5	3.57	129.88	112.24
23	b	607	CLA	C4A-NA-C1A	3.57	108.31	106.71
26	A	409	PL9	C7-C3-C2	-3.55	118.63	123.30
23	A	407	CLA	C1B-CHB-C4A	-3.55	123.08	130.12
23	b	610	CLA	CMB-C2B-C3B	3.55	131.32	124.68
28	a	415	LMG	O6-C1-C2	-3.55	102.84	110.35
23	C	508	CLA	CMB-C2B-C3B	3.54	131.31	124.68
23	b	607	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
23	b	601	CLA	O2D-CGD-CBD	3.54	117.55	111.27
23	a	405	CLA	CMB-C2B-C3B	3.53	131.29	124.68
23	b	604	CLA	C4A-NA-C1A	3.53	108.29	106.71
25	T	101	BCR	C7-C8-C9	-3.52	120.92	126.23
23	c	504	CLA	CMB-C2B-C3B	3.51	131.25	124.68
23	B	610	CLA	C1B-CHB-C4A	-3.51	123.16	130.12
23	c	508	CLA	O2D-CGD-O1D	-3.51	116.97	123.84
23	b	608	CLA	OBD-CAD-CBD	-3.51	120.88	125.89
29	A	413	SQD	C44-O6-C1	3.51	120.59	113.74
28	D	409	LMG	O3-C3-C2	-3.50	102.26	110.35
33	D	412	LHG	O4-P-O5	3.49	129.50	112.24
33	D	412	LHG	O8-C23-O10	-3.49	114.78	123.59
26	A	409	PL9	C30-C29-C28	-3.48	114.74	123.68
23	A	404	CLA	CHB-C4A-NA	3.48	129.33	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	602	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
23	a	408	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
30	c	521	DGD	O3E-C3E-C2E	-3.48	102.31	110.35
23	B	602	CLA	O2D-CGD-CBD	3.47	117.43	111.27
23	c	502	CLA	CMB-C2B-C3B	3.47	131.16	124.68
25	C	515	BCR	C15-C16-C17	-3.46	116.38	123.47
30	A	414	DGD	C4E-C3E-C2E	-3.45	104.80	110.82
23	b	602	CLA	C1B-CHB-C4A	-3.45	123.28	130.12
25	B	617	BCR	C2-C1-C6	3.45	115.79	110.48
23	A	405	CLA	CMB-C2B-C3B	3.45	131.13	124.68
23	B	601	CLA	O2D-CGD-O1D	-3.45	117.10	123.84
23	C	504	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
23	b	611	CLA	C4D-C3D-CAD	-3.44	106.55	108.47
23	c	507	CLA	C4D-C3D-CAD	-3.44	106.55	108.47
23	d	402	CLA	O2D-CGD-O1D	-3.43	117.14	123.84
29	A	412	SQD	O9-S-O7	-3.43	102.09	113.95
23	c	512	CLA	CMD-C2D-C3D	3.42	131.07	124.68
23	c	503	CLA	OBD-CAD-CBD	-3.40	121.04	125.89
26	D	407	PL9	C20-C19-C21	3.40	120.98	115.27
33	a	413	LHG	O8-C23-C24	3.39	122.55	111.91
25	C	514	BCR	C11-C10-C9	-3.39	122.47	127.31
34	F	101	HEM	C4C-C3C-C2C	3.39	109.26	106.90
30	c	521	DGD	O3G-C3G-C2G	-3.39	102.73	110.90
23	a	405	CLA	C1B-CHB-C4A	-3.38	123.42	130.12
28	b	623	LMG	C8-O7-C10	3.38	126.12	117.79
23	b	605	CLA	C4D-C3D-CAD	-3.37	106.59	108.47
23	b	606	CLA	C4-C3-C5	3.37	120.95	115.27
23	B	603	CLA	CMB-C2B-C3B	3.37	130.98	124.68
28	D	409	LMG	C3-C4-C5	-3.37	104.23	110.24
26	D	407	PL9	C7-C3-C4	3.36	119.61	116.88
23	B	616	CLA	CMB-C2B-C3B	3.36	130.96	124.68
23	b	611	CLA	CMD-C2D-C3D	3.36	130.96	124.68
23	c	513	CLA	CMB-C2B-C3B	3.35	130.94	124.68
23	b	608	CLA	CMD-C2D-C3D	3.35	130.94	124.68
23	A	407	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
23	B	603	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
23	B	610	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
23	B	616	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
33	d	408	LHG	O4-P-O5	3.33	128.71	112.24
23	b	601	CLA	CHB-C4A-NA	3.33	129.12	124.51
23	A	404	CLA	CMB-C2B-C3B	3.33	130.90	124.68
23	b	610	CLA	O2D-CGD-O1D	-3.32	117.34	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	506	CLA	CMD-C2D-C3D	3.32	130.89	124.68
23	B	609	CLA	C4D-C3D-CAD	-3.32	106.62	108.47
23	b	610	CLA	O2D-CGD-CBD	3.32	117.16	111.27
23	a	408	CLA	O2D-CGD-CBD	3.31	117.16	111.27
23	c	513	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
23	b	603	CLA	CMB-C2B-C3B	3.30	130.86	124.68
23	c	503	CLA	C7-C6-C5	-3.30	104.40	113.36
23	B	608	CLA	OBD-CAD-CBD	-3.29	121.19	125.89
23	c	507	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
29	F	102	SQD	O9-S-C6	3.28	110.84	106.94
23	b	604	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
30	h	102	DGD	O6E-C5E-C4E	3.28	115.65	109.69
28	b	623	LMG	O2-C2-C1	-3.28	102.08	110.05
23	A	407	CLA	O2D-CGD-CBD	3.28	117.09	111.27
25	x	101	BCR	C38-C26-C25	-3.27	120.85	124.53
24	A	406	PHO	O2D-CGD-O1D	-3.27	117.44	123.84
30	c	521	DGD	C3D-C4D-C5D	-3.27	104.40	110.24
25	T	101	BCR	C27-C26-C25	3.27	127.48	122.73
25	H	101	BCR	C38-C26-C25	-3.27	120.86	124.53
25	c	515	BCR	C27-C26-C25	3.27	127.48	122.73
23	b	610	CLA	CHB-C4A-NA	3.27	129.03	124.51
23	b	611	CLA	CHB-C4A-NA	3.25	129.01	124.51
23	B	611	CLA	O2D-CGD-CBD	3.25	117.04	111.27
23	B	602	CLA	O2A-CGA-O1A	-3.25	115.39	123.59
23	A	405	CLA	C1B-CHB-C4A	-3.24	123.69	130.12
23	d	402	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
23	d	402	CLA	C4-C3-C5	3.24	120.72	115.27
28	D	408	LMG	O6-C1-O1	-3.24	102.30	109.97
25	A	408	BCR	C37-C22-C21	-3.24	118.39	122.92
28	d	409	LMG	O6-C1-O1	-3.24	102.30	109.97
23	B	604	CLA	CMB-C2B-C1B	-3.23	123.49	128.46
23	B	605	CLA	CMD-C2D-C3D	3.23	130.73	124.68
23	b	611	CLA	CMB-C2B-C3B	3.22	130.71	124.68
25	C	515	BCR	C27-C26-C25	3.22	127.41	122.73
23	B	612	CLA	C4D-C3D-CAD	-3.22	106.67	108.47
30	A	414	DGD	O5D-C1E-C2E	3.22	113.33	108.30
28	C	517	LMG	O7-C10-O9	-3.22	115.92	123.70
35	v	201	HEC	CMA-C3A-C2A	3.22	131.01	124.94
26	d	405	PL9	C22-C23-C24	-3.21	119.92	127.66
26	D	407	PL9	C37-C38-C39	-3.21	119.92	127.66
23	b	606	CLA	CMB-C2B-C3B	3.20	130.67	124.68
23	B	603	CLA	CMD-C2D-C3D	3.19	130.65	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	607	CLA	CMB-C2B-C3B	3.19	130.65	124.68
23	c	510	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
23	b	609	CLA	C1-C2-C3	-3.19	120.53	126.04
23	c	512	CLA	CMB-C2B-C3B	3.18	130.64	124.68
23	D	405	CLA	CMB-C2B-C3B	3.18	130.64	124.68
23	b	613	CLA	CHB-C4A-NA	3.18	128.91	124.51
23	b	613	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
24	d	401	PHO	C1B-NB-C4B	3.18	112.50	106.51
29	a	412	SQD	C1-C2-C3	-3.18	103.38	110.00
23	B	603	CLA	C4D-C3D-CAD	-3.18	106.70	108.47
23	B	612	CLA	CMD-C2D-C3D	3.17	130.62	124.68
28	c	524	LMG	O6-C1-O1	-3.17	102.46	109.97
29	b	620	SQD	O9-S-O7	-3.17	102.99	113.95
23	D	405	CLA	O2D-CGD-O1D	-3.16	117.65	123.84
30	h	102	DGD	C1E-O6E-C5E	3.16	119.90	113.69
23	a	406	CLA	O2D-CGD-CBD	3.16	116.89	111.27
23	b	613	CLA	O2A-CGA-O1A	-3.16	115.61	123.59
23	D	404	CLA	CMD-C2D-C3D	3.16	130.59	124.68
23	c	512	CLA	CMB-C2B-C1B	-3.15	123.61	128.46
23	c	505	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
23	C	506	CLA	C4D-C3D-CAD	-3.14	106.72	108.47
23	B	611	CLA	C1-C2-C3	-3.14	120.61	126.04
28	D	409	LMG	O1-C1-C2	-3.14	103.40	108.30
30	h	102	DGD	O3E-C3E-C2E	-3.14	103.09	110.35
23	A	404	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
25	b	618	BCR	C27-C26-C25	3.13	127.28	122.73
23	c	501	CLA	CMB-C2B-C3B	3.13	130.53	124.68
23	b	614	CLA	C1B-CHB-C4A	-3.12	123.93	130.12
28	b	621	LMG	O3-C3-C2	-3.12	103.13	110.35
23	d	402	CLA	CMD-C2D-C3D	3.12	130.52	124.68
23	C	505	CLA	CMB-C2B-C3B	3.12	130.51	124.68
23	c	504	CLA	C4A-NA-C1A	3.12	108.11	106.71
23	B	613	CLA	CHA-C1A-NA	-3.11	119.27	126.40
23	C	510	CLA	C4D-C3D-CAD	-3.11	106.73	108.47
23	c	506	CLA	OBD-CAD-CBD	-3.11	121.45	125.89
33	D	410	LHG	O4-P-O5	3.11	127.61	112.24
23	B	612	CLA	O2A-CGA-O1A	-3.11	115.75	123.59
23	C	509	CLA	CMB-C2B-C3B	3.11	130.49	124.68
23	c	512	CLA	C4A-NA-C1A	3.11	108.10	106.71
29	l	101	SQD	O9-S-O7	-3.10	103.20	113.95
23	B	604	CLA	CMB-C2B-C3B	3.10	130.48	124.68
30	C	523	DGD	C8B-C7B-C6B	-3.10	98.70	114.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	411	CLA	CMB-C2B-C3B	3.10	130.47	124.68
23	b	609	CLA	C1B-CHB-C4A	-3.10	123.98	130.12
23	D	405	CLA	C1B-CHB-C4A	-3.09	123.99	130.12
30	c	520	DGD	O6D-C1D-O3G	-3.09	102.65	109.97
30	c	520	DGD	C3G-O3G-C1D	3.09	119.78	113.74
23	D	403	CLA	CMD-C2D-C3D	3.09	130.46	124.68
24	A	406	PHO	O1D-CGD-CBD	3.09	130.81	124.48
23	B	606	CLA	OBD-CAD-CBD	-3.09	121.48	125.89
23	D	404	CLA	CMB-C2B-C1B	-3.09	123.72	128.46
23	C	513	CLA	C4D-C3D-CAD	-3.09	106.75	108.47
23	B	616	CLA	C4D-C3D-CAD	-3.08	106.75	108.47
26	A	409	PL9	O1-C4-C3	-3.08	117.32	120.72
23	b	605	CLA	CMC-C2C-C3C	3.08	130.75	124.94
23	c	509	CLA	CMC-C2C-C3C	3.08	130.74	124.94
29	A	412	SQD	C3-C4-C5	3.07	115.72	110.24
23	c	506	CLA	CMB-C2B-C3B	3.07	130.43	124.68
23	b	609	CLA	CHB-C4A-NA	3.07	128.76	124.51
23	C	509	CLA	O2A-CGA-O1A	-3.07	115.84	123.59
23	B	614	CLA	C1B-CHB-C4A	-3.07	124.04	130.12
30	C	521	DGD	O5D-C1E-C2E	-3.07	103.51	108.30
23	d	403	CLA	CMB-C2B-C1B	-3.07	123.75	128.46
23	C	506	CLA	O1D-CGD-CBD	3.06	130.74	124.48
25	c	515	BCR	C33-C5-C6	-3.05	121.10	124.53
30	C	522	DGD	C1D-C2D-C3D	-3.05	103.65	110.00
23	A	405	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
23	C	513	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
23	a	411	CLA	CHB-C4A-NA	3.05	128.73	124.51
33	L	101	LHG	C11-C10-C9	-3.04	98.97	114.42
30	c	521	DGD	O5D-C1E-C2E	3.04	113.05	108.30
23	A	404	CLA	CMD-C2D-C3D	3.03	130.35	124.68
23	a	405	CLA	C7-C6-C5	-3.03	105.14	113.36
23	C	507	CLA	O2A-CGA-O1A	-3.02	115.96	123.59
23	b	602	CLA	OBD-CAD-C3D	3.02	133.00	127.98
29	b	620	SQD	O2-C2-C1	3.02	117.39	110.05
23	c	503	CLA	CMD-C2D-C3D	3.02	130.33	124.68
30	H	102	DGD	C3D-C4D-C5D	-3.02	104.86	110.24
23	c	511	CLA	CMB-C2B-C1B	-3.02	123.83	128.46
25	C	515	BCR	C38-C26-C27	-3.02	107.82	113.62
23	C	508	CLA	CMC-C2C-C3C	3.01	130.62	124.94
26	a	410	PL9	C35-C34-C36	3.01	120.34	115.27
23	c	502	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
23	B	610	CLA	O2A-CGA-O1A	-3.01	115.99	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	x	101	BCR	C35-C13-C14	-3.01	118.70	122.92
25	C	520	BCR	C27-C26-C25	3.01	127.10	122.73
29	f	102	SQD	O47-C7-C8	3.01	119.18	110.80
25	B	619	BCR	C2-C1-C6	3.00	115.10	110.48
23	b	612	CLA	CMB-C2B-C3B	3.00	130.29	124.68
30	h	102	DGD	C3D-C4D-C5D	-3.00	104.89	110.24
25	K	101	BCR	C33-C5-C6	-2.99	121.17	124.53
25	x	101	BCR	C27-C26-C25	2.99	127.07	122.73
23	b	612	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
23	b	611	CLA	C11-C12-C13	-2.99	106.27	115.92
23	B	602	CLA	CMB-C2B-C3B	2.98	130.26	124.68
23	b	613	CLA	C1-C2-C3	-2.98	120.89	126.04
25	B	617	BCR	C29-C30-C25	2.97	115.06	110.48
25	k	101	BCR	C33-C5-C6	-2.97	121.19	124.53
23	C	510	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
23	b	604	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
30	C	521	DGD	C3G-C2G-C1G	-2.97	104.76	111.79
23	B	608	CLA	CMB-C2B-C1B	-2.97	123.90	128.46
23	c	503	CLA	CMB-C2B-C3B	2.97	130.23	124.68
26	d	405	PL9	C7-C3-C2	-2.97	119.40	123.30
33	d	406	LHG	O8-C23-O10	-2.96	116.13	123.59
26	A	409	PL9	O2-C1-C2	-2.96	115.01	121.78
25	T	101	BCR	C38-C26-C27	-2.96	107.94	113.62
33	D	412	LHG	C11-C10-C9	-2.95	99.43	114.42
29	A	412	SQD	O47-C7-O49	-2.95	116.58	123.70
23	b	612	CLA	C4A-NA-C1A	2.94	108.03	106.71
29	A	412	SQD	O8-S-O7	-2.94	104.08	111.27
23	C	502	CLA	CMD-C2D-C3D	2.94	130.18	124.68
34	f	101	HEM	CAD-CBD-CGD	2.94	117.60	112.67
23	b	601	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
23	C	504	CLA	CMD-C2D-C3D	2.94	130.17	124.68
30	c	521	DGD	O6D-C1D-O3G	-2.93	103.03	109.97
26	A	409	PL9	C40-C39-C41	2.93	120.20	115.27
23	B	602	CLA	C4A-NA-C1A	2.93	108.02	106.71
29	b	620	SQD	C1-C2-C3	-2.93	103.90	110.00
23	B	603	CLA	OBD-CAD-CBD	-2.93	121.72	125.89
23	C	510	CLA	C7-C6-C5	-2.92	105.42	113.36
23	C	506	CLA	CHB-C4A-NA	2.92	128.56	124.51
30	c	520	DGD	O3D-C3D-C4D	-2.92	103.59	110.35
23	B	608	CLA	CMB-C2B-C3B	2.92	130.14	124.68
23	b	613	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
23	a	408	CLA	CHB-C4A-NA	2.92	128.54	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	602	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
23	B	614	CLA	CMD-C2D-C3D	2.91	130.12	124.68
23	C	504	CLA	CMB-C2B-C3B	2.90	130.11	124.68
23	A	405	CLA	CED-O2D-CGD	-2.90	109.38	115.94
23	B	615	CLA	CMB-C2B-C1B	-2.90	124.01	128.46
23	b	613	CLA	C4-C3-C5	2.90	120.15	115.27
23	D	403	CLA	CHB-C4A-NA	2.90	128.52	124.51
29	a	412	SQD	C46-C45-C44	-2.90	104.94	111.79
30	C	521	DGD	O5D-C6D-C5D	-2.90	103.69	109.05
25	B	618	BCR	C29-C30-C25	2.89	114.94	110.48
23	c	510	CLA	C4D-C3D-CAD	-2.89	106.86	108.47
23	C	512	CLA	C4A-NA-C1A	2.89	108.01	106.71
23	b	603	CLA	OBD-CAD-CBD	-2.89	121.77	125.89
25	k	102	BCR	C27-C26-C25	2.89	126.92	122.73
23	h	101	CLA	CMB-C2B-C1B	-2.88	124.03	128.46
28	d	409	LMG	C3-C4-C5	-2.88	105.09	110.24
23	c	504	CLA	CMD-C2D-C3D	2.88	130.06	124.68
30	A	414	DGD	O6E-C5E-C4E	2.88	114.92	109.69
28	c	524	LMG	C1-O6-C5	-2.88	108.04	113.69
33	d	406	LHG	C11-C10-C9	-2.87	99.84	114.42
35	v	201	HEC	CMC-C2C-C3C	2.87	129.20	125.82
23	c	504	CLA	CHB-C4A-NA	2.87	128.48	124.51
23	C	508	CLA	C4D-C3D-CAD	-2.87	106.87	108.47
23	C	509	CLA	CHB-C4A-NA	2.87	128.48	124.51
30	C	521	DGD	O6D-C1D-O3G	-2.86	103.19	109.97
30	A	414	DGD	C3G-C2G-C1G	-2.86	105.03	111.79
23	c	509	CLA	CMB-C2B-C3B	2.86	130.02	124.68
30	c	521	DGD	O6E-C5E-C4E	2.86	114.88	109.69
23	a	405	CLA	O1D-CGD-CBD	2.86	130.33	124.48
30	C	521	DGD	CDB-CCB-CBB	-2.85	99.93	114.42
23	b	602	CLA	C4A-NA-C1A	2.85	107.99	106.71
26	a	410	PL9	C22-C23-C24	-2.85	120.80	127.66
23	b	615	CLA	CHB-C4A-NA	2.85	128.45	124.51
23	B	605	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
23	b	612	CLA	CHB-C4A-NA	2.84	128.44	124.51
23	c	507	CLA	O2A-CGA-O1A	-2.84	116.42	123.59
23	B	616	CLA	O2A-CGA-O1A	-2.84	116.42	123.59
30	A	414	DGD	O3G-C3G-C2G	-2.84	104.04	110.90
23	b	614	CLA	CMD-C2D-C3D	2.84	129.99	124.68
23	h	101	CLA	CBA-CAA-C2A	2.84	122.24	113.86
23	B	604	CLA	OBD-CAD-CBD	-2.84	121.84	125.89
23	A	405	CLA	C4A-NA-C1A	2.84	107.98	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	c	523	LMG	O6-C1-O1	-2.84	103.26	109.97
30	H	102	DGD	O5D-C1E-C2E	2.83	112.73	108.30
23	C	513	CLA	CMC-C2C-C3C	2.83	130.28	124.94
23	b	605	CLA	O2D-CGD-CBD	2.83	116.30	111.27
23	b	602	CLA	C4D-C3D-CAD	-2.83	106.89	108.47
23	B	608	CLA	O2D-CGD-CBD	2.83	116.30	111.27
23	a	411	CLA	CMD-C2D-C3D	2.83	129.97	124.68
28	b	619	LMG	C8-O7-C10	2.83	121.52	117.88
30	c	520	DGD	C1E-O6E-C5E	2.83	119.23	113.69
25	c	514	BCR	C24-C23-C22	-2.83	121.97	126.23
23	c	511	CLA	C4D-C3D-CAD	-2.82	106.90	108.47
25	c	514	BCR	C15-C14-C13	-2.82	123.28	127.31
23	c	509	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
25	B	617	BCR	C11-C10-C9	-2.82	123.28	127.31
30	c	519	DGD	O3E-C3E-C2E	-2.82	103.83	110.35
23	B	606	CLA	C4-C3-C5	2.81	120.00	115.27
28	c	523	LMG	O1-C1-C2	-2.81	103.92	108.30
23	C	509	CLA	CMC-C2C-C3C	2.81	130.24	124.94
23	B	603	CLA	C5-C3-C2	-2.80	115.44	121.12
23	B	613	CLA	CMB-C2B-C1B	-2.80	124.16	128.46
25	K	101	BCR	C39-C30-C25	-2.80	105.75	110.30
29	A	412	SQD	C46-C45-C44	-2.80	105.16	111.79
23	C	511	CLA	O2A-CGA-O1A	-2.80	116.53	123.59
23	C	510	CLA	CMD-C2D-C3D	2.80	129.91	124.68
25	K	101	BCR	C27-C26-C25	2.80	126.79	122.73
23	B	602	CLA	CMC-C2C-C3C	2.79	130.21	124.94
23	C	512	CLA	C1-C2-C3	-2.79	121.21	126.04
30	h	102	DGD	O3G-C3G-C2G	-2.79	104.16	110.90
23	c	513	CLA	CHB-C4A-NA	2.79	128.37	124.51
30	C	523	DGD	O6D-C1D-O3G	-2.79	103.36	109.97
23	C	513	CLA	CMB-C2B-C3B	2.79	129.90	124.68
25	k	101	BCR	C27-C26-C25	2.78	126.77	122.73
28	b	623	LMG	O6-C5-C6	2.78	113.35	106.44
28	d	409	LMG	O1-C1-C2	-2.78	103.96	108.30
23	B	611	CLA	OBD-CAD-CBD	-2.78	121.93	125.89
30	c	520	DGD	O2G-C1B-O1B	-2.77	117.00	123.70
28	d	409	LMG	O3-C3-C2	-2.77	103.94	110.35
30	c	520	DGD	C1D-C2D-C3D	-2.77	104.23	110.00
23	b	615	CLA	C4-C3-C5	2.77	119.93	115.27
23	c	511	CLA	OBD-CAD-CBD	-2.77	121.94	125.89
23	D	403	CLA	C1B-CHB-C4A	-2.77	124.64	130.12
25	x	101	BCR	C36-C18-C17	-2.77	119.05	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	H	101	BCR	C2-C1-C6	2.77	114.74	110.48
23	c	507	CLA	CMC-C2C-C3C	2.76	130.15	124.94
26	D	407	PL9	C22-C23-C24	-2.76	121.01	127.66
28	c	524	LMG	C40-C39-C38	-2.76	100.41	114.42
23	b	603	CLA	C6-C7-C8	-2.76	107.01	115.92
29	f	102	SQD	C1-O5-C5	-2.76	108.28	113.69
28	C	524	LMG	O1-C7-C8	-2.75	104.25	110.90
28	A	411	LMG	C1-O6-C5	-2.75	108.28	113.69
23	A	407	CLA	CMB-C2B-C3B	2.75	129.83	124.68
23	c	508	CLA	CHB-C4A-NA	2.75	128.32	124.51
26	D	407	PL9	C12-C13-C14	-2.75	121.04	127.66
23	c	506	CLA	C4-C3-C5	2.75	119.89	115.27
29	A	413	SQD	O48-C23-O10	-2.75	116.66	123.59
23	a	408	CLA	C4D-C3D-CAD	-2.75	106.94	108.47
23	h	101	CLA	O2A-CGA-O1A	-2.74	116.67	123.59
23	d	403	CLA	CMB-C2B-C3B	2.74	129.81	124.68
25	b	618	BCR	C12-C13-C14	-2.74	114.73	118.94
23	C	512	CLA	OBD-CAD-CBD	-2.74	121.98	125.89
23	A	407	CLA	OBD-CAD-C3D	2.73	132.52	127.98
29	a	412	SQD	O47-C7-C8	2.73	117.39	111.50
23	c	513	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
25	b	616	BCR	C15-C16-C17	-2.73	117.89	123.47
23	A	404	CLA	C1B-CHB-C4A	-2.72	124.72	130.12
25	c	515	BCR	C35-C13-C14	-2.72	119.11	122.92
23	C	507	CLA	O2D-CGD-CBD	2.71	116.09	111.27
23	C	508	CLA	O2D-CGD-CBD	2.71	116.09	111.27
29	b	620	SQD	O48-C23-C24	2.71	120.42	111.91
23	b	606	CLA	C6-C7-C8	-2.71	107.15	115.92
25	D	406	BCR	C2-C1-C6	2.71	114.65	110.48
23	a	406	CLA	O2A-CGA-O1A	-2.71	116.76	123.59
23	C	504	CLA	O2A-CGA-O1A	-2.71	116.76	123.59
23	D	404	CLA	CED-O2D-CGD	2.70	122.05	115.94
23	b	615	CLA	O1D-CGD-CBD	2.70	130.01	124.48
33	D	410	LHG	C18-C17-C16	-2.70	100.71	114.42
28	C	517	LMG	O2-C2-C1	-2.70	103.48	110.05
28	M	101	LMG	C1-C2-C3	-2.70	104.37	110.00
29	a	412	SQD	O9-S-O7	-2.70	104.61	113.95
30	C	522	DGD	O5D-C6D-C5D	-2.70	104.06	109.05
28	B	620	LMG	O8-C28-O10	-2.70	116.79	123.59
23	b	613	CLA	CMB-C2B-C3B	2.69	129.72	124.68
26	d	405	PL9	C35-C34-C36	2.69	119.80	115.27
30	c	520	DGD	CDB-CCB-CBB	-2.69	100.77	114.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	C	523	DGD	C6B-C5B-C4B	-2.69	100.79	114.42
23	C	507	CLA	CHB-C4A-NA	2.69	128.22	124.51
26	D	407	PL9	C42-C43-C44	-2.68	121.20	127.66
25	a	409	BCR	C27-C26-C25	2.68	126.62	122.73
23	A	407	CLA	C4A-NA-C1A	2.68	107.91	106.71
26	A	409	PL9	C30-C29-C31	-2.68	110.76	115.27
23	B	601	CLA	C1-O2A-CGA	2.68	123.47	116.44
23	b	601	CLA	CMD-C2D-C3D	2.68	129.68	124.68
23	B	607	CLA	CMB-C2B-C1B	-2.67	124.36	128.46
23	b	602	CLA	C4-C3-C5	2.67	119.77	115.27
23	b	609	CLA	CAA-CBA-CGA	-2.67	105.44	113.25
23	B	609	CLA	CMB-C2B-C1B	-2.67	124.36	128.46
24	D	402	PHO	C1B-NB-C4B	2.67	111.53	106.51
33	d	408	LHG	O8-C23-O10	-2.66	116.87	123.59
26	D	407	PL9	C32-C33-C34	-2.66	121.25	127.66
23	C	511	CLA	C4-C3-C5	2.66	119.75	115.27
25	B	617	BCR	C3-C4-C5	-2.66	109.33	114.08
30	A	414	DGD	O3G-C1D-C2D	-2.66	104.15	108.30
25	t	101	BCR	C7-C8-C9	-2.66	122.22	126.23
24	d	401	PHO	C1-C2-C3	-2.65	121.45	126.04
23	C	510	CLA	CHB-C4A-NA	2.65	128.18	124.51
23	c	513	CLA	CMD-C2D-C3D	2.65	129.64	124.68
30	C	521	DGD	C3D-C4D-C5D	-2.65	105.51	110.24
23	D	404	CLA	C1B-CHB-C4A	-2.65	124.88	130.12
28	C	517	LMG	O1-C7-C8	-2.65	104.52	110.90
23	b	609	CLA	O1D-CGD-CBD	2.64	129.89	124.48
23	C	509	CLA	C2A-C3A-C4A	2.64	106.14	101.87
25	b	616	BCR	C11-C10-C9	-2.64	123.54	127.31
25	C	514	BCR	C2-C1-C6	2.64	114.54	110.48
33	E	101	LHG	O8-C23-C24	2.64	120.18	111.91
23	c	510	CLA	CHB-C4A-NA	2.64	128.16	124.51
26	D	407	PL9	C30-C29-C31	-2.64	110.84	115.27
23	B	601	CLA	O2D-CGD-CBD	2.63	115.95	111.27
23	b	607	CLA	C1B-CHB-C4A	-2.63	124.90	130.12
28	A	411	LMG	O7-C10-O9	-2.63	117.34	123.70
23	B	608	CLA	CMC-C2C-C3C	2.63	129.90	124.94
23	b	611	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
23	d	402	CLA	CMB-C2B-C3B	2.63	129.60	124.68
23	A	405	CLA	CHB-C4A-NA	2.63	128.15	124.51
23	a	408	CLA	OBD-CAD-C3D	2.63	132.34	127.98
30	C	521	DGD	CBB-CAB-C9B	-2.63	101.09	114.42
23	C	501	CLA	O2A-CGA-O1A	-2.63	116.97	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	604	CLA	C1-O2A-CGA	-2.63	109.56	116.44
29	F	102	SQD	C3-C4-C5	2.63	114.92	110.24
23	c	510	CLA	CMB-C2B-C3B	2.62	129.59	124.68
23	B	603	CLA	CHB-C4A-NA	2.62	128.14	124.51
23	C	506	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
34	F	101	HEM	CAD-CBD-CGD	2.62	117.07	112.67
25	b	616	BCR	C33-C5-C6	-2.62	121.59	124.53
25	C	515	BCR	C36-C18-C17	-2.61	119.26	122.92
33	D	412	LHG	O8-C23-C24	2.61	120.11	111.91
23	b	610	CLA	C4A-NA-C1A	2.61	107.88	106.71
35	v	201	HEC	CBD-CAD-C3D	-2.61	107.67	112.49
23	B	609	CLA	OBD-CAD-CBD	-2.61	122.17	125.89
28	A	411	LMG	O7-C10-C11	2.61	117.12	111.50
23	b	613	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
30	H	102	DGD	O6E-C5E-C4E	2.61	114.43	109.69
30	A	414	DGD	C1E-O6E-C5E	2.60	118.80	113.69
23	c	507	CLA	CMB-C2B-C3B	2.60	129.55	124.68
23	c	502	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
23	B	611	CLA	C7-C6-C5	-2.60	106.30	113.36
29	a	412	SQD	O6-C44-C45	-2.60	104.62	110.90
23	a	406	CLA	CMB-C2B-C3B	2.60	129.54	124.68
28	b	623	LMG	O8-C28-O10	-2.60	117.04	123.59
25	H	101	BCR	C34-C9-C10	-2.60	119.29	122.92
23	d	402	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
23	b	608	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
26	A	409	PL9	C20-C19-C21	2.59	119.63	115.27
23	B	615	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
25	b	618	BCR	C38-C26-C25	-2.59	121.62	124.53
23	B	602	CLA	C1-C2-C3	-2.59	121.56	126.04
23	b	615	CLA	CMD-C2D-C3D	2.59	129.53	124.68
23	B	614	CLA	O2A-CGA-O1A	-2.59	117.05	123.59
23	c	502	CLA	CMD-C2D-C3D	2.59	129.52	124.68
28	c	524	LMG	C38-C37-C36	-2.59	101.29	114.42
26	d	405	PL9	C40-C39-C38	-2.59	117.04	123.68
25	C	515	BCR	C35-C13-C14	-2.59	119.30	122.92
23	C	505	CLA	O2A-CGA-O1A	-2.59	117.07	123.59
23	b	608	CLA	CMC-C2C-C3C	2.58	129.81	124.94
23	d	403	CLA	CHA-C1A-NA	-2.58	120.48	126.40
28	c	518	LMG	C9-C8-C7	-2.58	105.75	111.80
25	C	515	BCR	C33-C5-C6	-2.58	121.63	124.53
25	b	616	BCR	C29-C30-C25	2.58	114.45	110.48
30	c	521	DGD	CDB-CCB-CBB	-2.58	101.32	114.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	614	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
23	B	605	CLA	C4D-C3D-CAD	-2.58	107.03	108.47
23	c	507	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
23	B	615	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
26	D	407	PL9	C11-C9-C8	-2.58	115.91	121.12
23	b	601	CLA	CMC-C2C-C3C	2.57	129.80	124.94
23	C	512	CLA	O2A-CGA-O1A	-2.57	117.10	123.59
23	d	403	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
30	c	520	DGD	O6E-C5E-C4E	2.57	114.36	109.69
25	H	101	BCR	C29-C30-C25	2.57	114.44	110.48
23	B	604	CLA	CHB-C4A-NA	2.57	128.07	124.51
23	B	609	CLA	CMB-C2B-C3B	2.57	129.49	124.68
23	C	512	CLA	CHA-C1A-NA	-2.57	120.52	126.40
29	F	102	SQD	C26-C25-C24	-2.57	103.96	113.19
23	c	507	CLA	C4-C3-C5	2.57	119.59	115.27
25	b	617	BCR	C35-C13-C14	-2.56	119.33	122.92
25	B	618	BCR	C2-C1-C6	2.56	114.43	110.48
23	b	607	CLA	O2D-CGD-CBD	2.56	115.82	111.27
28	M	101	LMG	C8-O7-C10	2.56	124.10	117.79
25	t	101	BCR	C2-C1-C6	2.56	114.42	110.48
23	c	511	CLA	CHB-C4A-NA	2.56	128.05	124.51
23	b	607	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
23	c	505	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
27	C	525	STE	C4-C3-C2	-2.56	103.82	113.76
29	A	412	SQD	O5-C1-O6	2.55	116.02	109.97
23	c	505	CLA	OBD-CAD-CBD	-2.55	122.25	125.89
23	b	607	CLA	C4D-C3D-CAD	-2.55	107.05	108.47
23	c	507	CLA	CMD-C2D-C3D	2.55	129.45	124.68
23	D	404	CLA	CMB-C2B-C3B	2.55	129.45	124.68
23	C	510	CLA	OBD-CAD-CBD	-2.55	122.26	125.89
33	a	413	LHG	C20-C19-C18	-2.54	101.51	114.42
30	h	102	DGD	O1G-C1A-O1A	-2.54	117.18	123.59
23	b	609	CLA	O2A-CGA-O1A	-2.54	117.18	123.59
25	b	616	BCR	C27-C26-C25	2.54	126.42	122.73
23	D	404	CLA	C4D-C3D-CAD	-2.54	107.06	108.47
30	c	519	DGD	CDB-CCB-CBB	-2.53	101.56	114.42
23	C	509	CLA	C1-C2-C3	-2.53	121.66	126.04
23	B	610	CLA	O2D-CGD-CBD	2.53	115.77	111.27
23	c	505	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
23	c	509	CLA	CMD-C2D-C3D	2.53	129.41	124.68
25	C	514	BCR	C27-C26-C25	2.53	126.41	122.73
23	B	610	CLA	CHB-C4A-NA	2.53	128.01	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	620	SQD	C1-O5-C5	-2.53	108.72	113.69
33	l	102	LHG	C11-C10-C9	-2.53	101.59	114.42
30	H	102	DGD	O5E-C6E-C5E	-2.53	102.62	111.29
23	c	509	CLA	O1D-CGD-CBD	2.53	129.65	124.48
28	a	415	LMG	C38-C37-C36	-2.53	101.60	114.42
26	A	409	PL9	O2-C1-C6	2.53	124.96	120.59
23	a	408	CLA	CMB-C2B-C1B	-2.53	124.58	128.46
23	B	604	CLA	CMC-C2C-C3C	2.52	129.70	124.94
23	c	504	CLA	O2D-CGD-CBD	2.52	115.75	111.27
25	t	101	BCR	C3-C4-C5	-2.52	109.57	114.08
28	b	621	LMG	O7-C10-O9	-2.52	117.61	123.70
29	b	620	SQD	O5-C5-C4	2.52	114.27	109.69
23	b	610	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
28	b	621	LMG	C40-C39-C38	-2.52	101.63	114.42
26	D	407	PL9	C50-C49-C48	-2.52	115.36	122.65
23	B	614	CLA	C4-C3-C5	2.52	119.51	115.27
29	f	102	SQD	O48-C23-C24	2.51	119.80	111.91
23	c	505	CLA	CMB-C2B-C3B	2.51	129.38	124.68
23	b	608	CLA	CHA-C1A-NA	-2.51	120.65	126.40
23	B	607	CLA	CMD-C2D-C3D	2.51	129.37	124.68
30	C	521	DGD	O3E-C3E-C2E	-2.51	104.56	110.35
28	M	101	LMG	C1-O6-C5	-2.51	108.77	113.69
23	C	507	CLA	OBD-CAD-CBD	-2.51	122.32	125.89
23	c	512	CLA	OBD-CAD-CBD	-2.51	122.32	125.89
23	b	602	CLA	C5-C3-C2	-2.50	116.05	121.12
25	x	101	BCR	C2-C1-C6	2.50	114.33	110.48
33	d	408	LHG	O8-C23-C24	2.50	119.76	111.91
33	L	101	LHG	O8-C23-O10	-2.50	117.28	123.59
23	a	408	CLA	CMD-C2D-C3D	2.50	129.35	124.68
30	c	520	DGD	O2D-C2D-C1D	-2.50	103.97	110.05
23	C	502	CLA	O1D-CGD-CBD	2.50	129.60	124.48
28	d	409	LMG	O1-C7-C8	-2.50	104.87	110.90
23	a	408	CLA	CHA-C1A-NA	-2.50	120.68	126.40
23	C	510	CLA	O2D-CGD-CBD	2.50	115.70	111.27
29	b	620	SQD	C46-C45-C44	-2.50	105.88	111.79
23	C	513	CLA	O2D-CGD-CBD	2.50	115.70	111.27
23	B	613	CLA	CMB-C2B-C3B	2.50	129.35	124.68
29	A	413	SQD	O48-C46-C45	2.50	115.70	108.43
28	M	101	LMG	C38-C37-C36	-2.50	101.76	114.42
30	c	519	DGD	O6D-C1D-O3G	-2.49	104.07	109.97
23	B	609	CLA	CMD-C2D-C3D	2.49	129.34	124.68
23	b	603	CLA	O2D-CGD-O1D	-2.49	118.96	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	l	102	LHG	C20-C19-C18	-2.49	101.77	114.42
24	d	401	PHO	C2B-C1B-NB	-2.49	106.03	109.79
23	B	606	CLA	CMD-C2D-C3D	2.49	129.34	124.68
23	h	101	CLA	O2A-C1-C2	2.49	115.18	108.64
33	d	406	LHG	C27-C26-C25	-2.49	101.78	114.42
23	D	404	CLA	CHB-C4A-NA	2.49	127.95	124.51
28	B	620	LMG	O6-C1-O1	-2.49	104.08	109.97
23	C	508	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
23	B	611	CLA	CHB-C4A-NA	2.49	127.95	124.51
23	C	512	CLA	CHB-C4A-NA	2.49	127.95	124.51
25	b	616	BCR	C8-C7-C6	-2.48	120.22	127.20
25	c	515	BCR	C15-C16-C17	-2.48	118.39	123.47
23	B	613	CLA	C4A-NA-C1A	2.48	107.82	106.71
28	d	409	LMG	O2-C2-C1	-2.48	104.02	110.05
23	c	511	CLA	CMD-C2D-C3D	2.48	129.32	124.68
23	c	512	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
30	c	519	DGD	CBB-CAB-C9B	-2.48	101.84	114.42
25	T	101	BCR	C30-C25-C26	-2.48	119.12	122.61
30	c	519	DGD	O3G-C1D-C2D	-2.48	104.44	108.30
25	D	406	BCR	C27-C26-C25	2.48	126.33	122.73
23	C	504	CLA	C4A-NA-C1A	2.47	107.82	106.71
23	B	614	CLA	CMB-C2B-C1B	-2.47	124.66	128.46
26	D	407	PL9	C35-C34-C36	2.47	119.43	115.27
28	M	101	LMG	C40-C39-C38	-2.47	101.87	114.42
28	c	522	LMG	O8-C28-O10	-2.47	117.36	123.59
23	C	509	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
25	b	617	BCR	C27-C26-C25	2.47	126.32	122.73
27	C	525	STE	C6-C5-C4	-2.47	101.89	114.42
24	a	407	PHO	CBD-CHA-C4D	-2.47	105.76	108.54
23	c	505	CLA	C11-C10-C8	-2.47	107.95	115.92
23	C	504	CLA	OBD-CAD-CBD	-2.47	122.37	125.89
23	a	406	CLA	CMA-C3A-C4A	-2.46	105.16	111.77
30	A	414	DGD	O5E-C6E-C5E	-2.46	102.86	111.29
23	b	601	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
23	C	505	CLA	O1D-CGD-CBD	2.45	129.50	124.48
30	h	102	DGD	C4D-C3D-C2D	-2.45	106.55	110.82
30	C	523	DGD	CBB-CAB-C9B	-2.45	102.00	114.42
24	a	407	PHO	O2A-CGA-O1A	-2.45	117.42	123.59
23	B	607	CLA	C1-C2-C3	-2.45	121.81	126.04
34	F	101	HEM	CMB-C2B-C3B	2.45	129.25	124.68
28	c	523	LMG	O8-C28-O10	-2.44	117.42	123.59
30	c	521	DGD	C3G-C2G-C1G	-2.44	106.01	111.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	612	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
23	c	509	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
23	B	612	CLA	C16-C15-C13	-2.44	108.03	115.92
23	b	607	CLA	OBD-CAD-CBD	-2.44	122.41	125.89
23	b	608	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
29	a	412	SQD	O3-C3-C2	-2.44	104.71	110.35
23	h	101	CLA	CMB-C2B-C3B	2.44	129.24	124.68
23	D	405	CLA	O2D-CGD-CBD	2.44	115.59	111.27
28	A	411	LMG	O8-C28-O10	-2.43	117.45	123.59
30	H	102	DGD	O1G-C1A-O1A	-2.43	117.45	123.59
29	a	414	SQD	C9-C8-C7	-2.43	104.78	113.62
23	B	607	CLA	C4-C3-C5	2.43	119.36	115.27
23	B	610	CLA	CMB-C2B-C3B	2.43	129.23	124.68
23	b	612	CLA	C1-C2-C3	-2.43	121.84	126.04
23	B	616	CLA	CMD-C2D-C3D	2.43	129.23	124.68
23	C	505	CLA	CMD-C2D-C3D	2.43	129.23	124.68
23	B	605	CLA	OBD-CAD-CBD	-2.43	122.42	125.89
23	c	503	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
29	a	412	SQD	O48-C23-C24	2.43	119.53	111.91
24	A	406	PHO	CAC-C3C-C4C	-2.43	122.57	125.22
26	a	410	PL9	C27-C28-C29	-2.43	121.81	127.66
25	H	101	BCR	C16-C15-C14	-2.43	118.50	123.47
28	c	523	LMG	O2-C2-C1	-2.43	104.15	110.05
27	J	101	STE	C6-C5-C4	-2.42	102.12	114.42
28	c	523	LMG	O3-C3-C2	-2.42	104.75	110.35
23	b	608	CLA	OBD-CAD-C3D	2.42	132.00	127.98
23	C	506	CLA	CMB-C2B-C1B	-2.42	124.75	128.46
23	c	508	CLA	CMC-C2C-C3C	2.42	129.50	124.94
23	A	407	CLA	OBD-CAD-CBD	-2.42	122.44	125.89
23	b	614	CLA	CHB-C4A-NA	2.42	127.85	124.51
23	b	614	CLA	C11-C12-C13	-2.41	108.12	115.92
25	a	409	BCR	C33-C5-C6	-2.41	121.82	124.53
26	d	405	PL9	C42-C43-C44	-2.41	121.85	127.66
28	M	101	LMG	O6-C1-O1	-2.41	104.27	109.97
28	c	522	LMG	O6-C1-O1	-2.41	104.27	109.97
23	D	403	CLA	CMB-C2B-C1B	-2.41	124.76	128.46
23	a	406	CLA	C4D-C3D-CAD	-2.41	107.13	108.47
28	c	522	LMG	O7-C10-O9	-2.41	117.88	123.70
23	B	603	CLA	C7-C6-C5	-2.41	106.82	113.36
23	d	403	CLA	CMD-C2D-C3D	2.41	129.18	124.68
23	B	612	CLA	CHB-C4A-NA	2.41	127.84	124.51
25	A	408	BCR	C38-C26-C27	-2.41	108.99	113.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	615	CLA	O2D-CGD-CBD	2.41	115.54	111.27
30	C	522	DGD	O6D-C1D-O3G	-2.40	104.28	109.97
23	B	614	CLA	CHB-C4A-NA	2.40	127.83	124.51
23	C	511	CLA	O2A-C1-C2	-2.40	102.32	108.64
23	c	509	CLA	C1-O2A-CGA	-2.40	110.14	116.44
23	c	512	CLA	O1D-CGD-CBD	2.40	129.39	124.48
23	C	511	CLA	CMC-C2C-C3C	2.40	129.46	124.94
28	b	621	LMG	O6-C1-O1	-2.40	104.30	109.97
23	C	507	CLA	OBD-CAD-C3D	2.40	131.96	127.98
23	b	605	CLA	CMD-C2D-C3D	2.39	129.16	124.68
25	t	101	BCR	C27-C26-C25	2.39	126.21	122.73
29	l	101	SQD	O48-C23-O10	-2.39	117.55	123.59
23	b	604	CLA	CMB-C2B-C3B	2.39	129.15	124.68
25	c	515	BCR	C32-C1-C6	-2.39	106.43	110.30
23	a	405	CLA	CMD-C2D-C3D	2.39	129.14	124.68
23	h	101	CLA	CMC-C2C-C3C	2.39	129.44	124.94
29	b	620	SQD	O9-S-C6	2.39	109.78	106.94
24	d	401	PHO	O2A-CGA-O1A	-2.39	117.57	123.59
30	h	102	DGD	O6D-C1D-O3G	-2.39	104.33	109.97
24	A	406	PHO	C1-C2-C3	-2.38	121.92	126.04
23	b	614	CLA	O2D-CGD-CBD	2.38	115.50	111.27
23	b	615	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
23	C	510	CLA	C11-C10-C8	-2.38	108.22	115.92
30	C	521	DGD	O2D-C2D-C1D	-2.38	104.26	110.05
25	c	515	BCR	C7-C8-C9	-2.38	122.64	126.23
30	A	414	DGD	O2G-C2G-C3G	2.38	117.01	108.40
23	C	502	CLA	CMB-C2B-C1B	-2.38	124.81	128.46
25	c	515	BCR	C2-C1-C6	2.38	114.14	110.48
23	c	507	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
25	b	617	BCR	C7-C8-C9	-2.37	122.65	126.23
26	D	407	PL9	C27-C28-C29	-2.37	121.95	127.66
23	c	504	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
23	B	609	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
26	D	407	PL9	C7-C3-C2	-2.37	120.18	123.30
23	C	504	CLA	C6-C7-C8	-2.37	108.26	115.92
23	C	513	CLA	CMD-C2D-C3D	2.36	129.10	124.68
25	T	101	BCR	C3-C4-C5	-2.36	109.86	114.08
23	b	604	CLA	C1-C2-C3	-2.36	121.95	126.04
23	b	607	CLA	CHB-C4A-NA	2.36	127.78	124.51
23	b	602	CLA	CMA-C3A-C4A	2.36	118.12	111.77
23	B	605	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
25	B	619	BCR	C36-C18-C17	-2.36	119.62	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	V	201	HEC	CMC-C2C-C3C	2.36	128.59	125.82
28	c	523	LMG	C6-C5-C4	-2.36	107.48	113.00
23	c	509	CLA	O2A-CGA-CBA	2.36	119.30	111.91
29	F	102	SQD	O7-S-C6	-2.36	104.14	106.94
23	b	608	CLA	CHB-C4A-NA	2.35	127.77	124.51
30	c	521	DGD	CBB-CAB-C9B	-2.35	102.48	114.42
30	c	520	DGD	CBB-CAB-C9B	-2.35	102.48	114.42
23	C	512	CLA	C6-C5-C3	-2.35	107.29	113.45
25	b	618	BCR	C2-C1-C6	2.35	114.10	110.48
23	b	603	CLA	O1D-CGD-CBD	2.35	129.29	124.48
23	B	606	CLA	CMB-C2B-C1B	-2.35	124.85	128.46
23	C	513	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
23	c	501	CLA	CMC-C2C-C3C	2.35	129.37	124.94
29	a	414	SQD	O9-S-C6	2.35	109.73	106.94
23	c	502	CLA	C1-C2-C3	-2.35	121.98	126.04
23	a	408	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
25	b	617	BCR	C15-C14-C13	-2.35	123.96	127.31
26	d	405	PL9	C7-C8-C9	-2.35	122.88	126.79
23	B	613	CLA	CMD-C2D-C3D	2.35	129.07	124.68
23	b	606	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
25	d	404	BCR	C33-C5-C6	-2.35	121.89	124.53
23	c	503	CLA	O1D-CGD-CBD	2.34	129.28	124.48
23	b	604	CLA	C4-C3-C5	2.34	119.21	115.27
23	B	609	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
24	a	407	PHO	C3A-C4A-CHB	-2.34	117.78	121.83
30	c	520	DGD	C8B-C7B-C6B	-2.34	102.54	114.42
23	c	501	CLA	CED-O2D-CGD	-2.34	110.64	115.94
25	x	101	BCR	C35-C13-C12	2.34	121.76	118.08
23	C	503	CLA	CMC-C2C-C3C	2.34	129.35	124.94
24	d	401	PHO	O2D-CGD-O1D	-2.34	119.27	123.84
25	C	514	BCR	C15-C16-C17	-2.34	118.69	123.47
23	B	608	CLA	C4D-C3D-CAD	-2.34	107.17	108.47
28	c	523	LMG	C9-C8-C7	-2.33	106.27	111.79
29	f	102	SQD	C46-C45-C44	-2.33	106.27	111.79
30	H	102	DGD	C8B-C7B-C6B	-2.33	102.57	114.42
28	b	621	LMG	O1-C1-C2	-2.33	104.66	108.30
25	k	102	BCR	C29-C30-C25	2.33	114.07	110.48
30	C	521	DGD	C4E-C3E-C2E	-2.33	106.75	110.82
35	V	201	HEC	CMB-C2B-C1B	-2.33	124.88	128.46
23	B	604	CLA	OBD-CAD-C3D	2.33	131.85	127.98
23	B	606	CLA	C1-C2-C3	-2.33	122.02	126.04
23	b	608	CLA	C16-C15-C13	-2.33	108.39	115.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	504	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
23	c	513	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
23	c	506	CLA	CED-O2D-CGD	2.33	121.20	115.94
23	b	603	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
23	B	616	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
25	B	618	BCR	C15-C16-C17	-2.32	118.72	123.47
23	b	604	CLA	CHA-C1A-NA	-2.32	121.08	126.40
23	b	601	CLA	C11-C10-C8	-2.32	108.42	115.92
29	A	413	SQD	O6-C44-C45	-2.32	105.30	110.90
23	D	404	CLA	CMC-C2C-C3C	2.32	129.31	124.94
23	B	613	CLA	CHB-C4A-NA	2.32	127.72	124.51
24	a	407	PHO	C2C-C1C-NC	2.32	113.28	109.79
23	b	612	CLA	CHA-C1A-NA	-2.32	121.10	126.40
26	a	410	PL9	C40-C39-C41	2.31	119.17	115.27
23	D	404	CLA	CAA-CBA-CGA	-2.31	106.49	113.25
23	A	407	CLA	CMD-C2D-C3D	2.31	129.01	124.68
26	a	410	PL9	O2-C1-C2	-2.31	116.48	121.78
25	D	406	BCR	C24-C23-C22	-2.31	122.74	126.23
33	D	411	LHG	C11-C10-C9	-2.31	102.69	114.42
26	A	409	PL9	C41-C39-C38	-2.31	116.44	121.12
23	C	507	CLA	CMC-C2C-C3C	2.31	129.30	124.94
30	c	520	DGD	O5D-C1E-C2E	2.31	111.91	108.30
23	B	606	CLA	CHA-C1A-NA	-2.31	121.11	126.40
23	c	510	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
23	b	610	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
30	c	520	DGD	O2E-C2E-C1E	-2.30	104.45	110.05
33	L	101	LHG	C18-C17-C16	-2.30	102.73	114.42
23	c	511	CLA	CMB-C2B-C3B	2.30	128.99	124.68
33	d	408	LHG	C26-C25-C24	2.30	121.47	113.19
24	A	406	PHO	CMB-C2B-C1B	-2.30	121.52	125.06
26	a	410	PL9	C32-C33-C34	-2.30	122.12	127.66
23	c	506	CLA	CHB-C4A-NA	2.30	127.69	124.51
23	B	606	CLA	OBD-CAD-C3D	2.30	131.80	127.98
26	d	405	PL9	C20-C19-C21	2.30	119.14	115.27
25	H	101	BCR	C27-C26-C25	2.30	126.07	122.73
23	B	616	CLA	CMC-C2C-C3C	2.30	129.27	124.94
23	c	507	CLA	CHB-C4A-NA	2.30	127.69	124.51
23	C	508	CLA	OBD-CAD-CBD	-2.30	122.61	125.89
25	K	101	BCR	C30-C25-C26	-2.30	119.38	122.61
23	c	505	CLA	C6-C7-C8	-2.29	108.52	115.92
23	B	614	CLA	O2A-C1-C2	-2.29	102.62	108.64
23	c	509	CLA	CMB-C2B-C1B	-2.29	124.95	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	513	CLA	OBD-CAD-CBD	-2.29	122.63	125.89
25	k	101	BCR	C38-C26-C25	-2.28	121.97	124.53
23	B	601	CLA	CHB-C4A-NA	2.28	127.67	124.51
23	B	616	CLA	O2D-CGD-CBD	2.28	115.32	111.27
30	C	522	DGD	O2D-C2D-C1D	-2.28	104.51	110.05
23	B	614	CLA	C1-C2-C3	-2.28	122.10	126.04
23	b	615	CLA	CAA-CBA-CGA	-2.28	106.59	113.25
23	C	502	CLA	OBD-CAD-CBD	-2.28	122.64	125.89
30	h	102	DGD	O5E-C6E-C5E	-2.28	103.48	111.29
23	b	603	CLA	C11-C10-C8	-2.28	108.56	115.92
26	A	409	PL9	C22-C23-C24	-2.28	122.18	127.66
25	C	520	BCR	C38-C26-C27	-2.27	109.25	113.62
33	D	412	LHG	C18-C17-C16	-2.27	102.88	114.42
23	C	505	CLA	O2D-CGD-O1D	-2.27	119.39	123.84
23	b	612	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
23	a	408	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
23	C	503	CLA	CMB-C2B-C1B	-2.27	124.97	128.46
25	B	619	BCR	C33-C5-C6	-2.27	121.98	124.53
23	b	606	CLA	CED-O2D-CGD	2.27	121.07	115.94
23	B	615	CLA	C5-C3-C2	-2.27	116.53	121.12
25	T	101	BCR	C23-C22-C21	-2.27	115.46	118.94
28	D	409	LMG	O6-C1-O1	-2.27	104.61	109.97
24	A	406	PHO	C3A-C4A-CHB	-2.27	117.91	121.83
25	A	408	BCR	C2-C1-C6	2.27	113.97	110.48
23	B	602	CLA	CMD-C2D-C3D	2.27	128.92	124.68
30	h	102	DGD	CBB-CAB-C9B	-2.27	102.92	114.42
25	c	515	BCR	C34-C9-C10	-2.26	119.75	122.92
23	c	510	CLA	OBD-CAD-CBD	-2.26	122.66	125.89
23	b	611	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
23	b	607	CLA	CHA-C1A-NA	-2.26	121.22	126.40
28	C	524	LMG	O6-C1-O1	-2.26	104.62	109.97
23	b	613	CLA	OBD-CAD-CBD	-2.26	122.67	125.89
23	b	611	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
30	A	414	DGD	O5D-C6D-C5D	-2.26	104.87	109.05
23	a	405	CLA	CHB-C4A-NA	2.26	127.63	124.51
30	h	102	DGD	O6E-C5E-C6E	-2.26	100.82	106.44
23	D	404	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
23	B	615	CLA	C4A-NA-C1A	2.26	107.72	106.71
23	b	611	CLA	CHA-C1A-NA	-2.25	121.23	126.40
23	B	611	CLA	C11-C12-C13	-2.25	108.64	115.92
23	B	612	CLA	C3A-C2A-C1A	2.25	104.71	101.34
23	c	503	CLA	C1B-CHB-C4A	-2.25	125.66	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	C	521	DGD	C3E-C4E-C5E	2.25	114.25	110.24
23	c	509	CLA	C4D-C3D-CAD	-2.25	107.22	108.47
23	D	404	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
23	D	405	CLA	CHA-C1A-NA	-2.25	121.25	126.40
23	c	504	CLA	O1A-CGA-CBA	2.25	132.50	123.73
34	f	101	HEM	CMA-C3A-C4A	-2.25	125.01	128.46
23	B	604	CLA	C11-C10-C8	-2.25	108.66	115.92
24	a	407	PHO	C1B-NB-C4B	2.24	110.74	106.51
23	B	609	CLA	CAA-CBA-CGA	-2.24	106.69	113.25
29	A	412	SQD	C9-C8-C7	-2.24	105.46	113.62
28	D	409	LMG	O2-C2-C1	-2.24	104.59	110.05
23	c	508	CLA	C7-C6-C5	-2.24	107.27	113.36
25	D	406	BCR	C38-C26-C25	-2.24	122.01	124.53
23	B	608	CLA	OBD-CAD-C3D	2.24	131.70	127.98
25	B	617	BCR	C34-C9-C10	-2.24	119.79	122.92
23	B	603	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
29	a	414	SQD	O49-C7-C8	-2.24	115.01	123.73
23	c	501	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
28	C	524	LMG	O2-C2-C1	-2.24	104.62	110.05
30	C	522	DGD	CDB-CCB-CBB	-2.23	103.08	114.42
33	L	101	LHG	C15-C14-C13	-2.23	103.08	114.42
30	h	102	DGD	C7B-C6B-C5B	-2.23	103.09	114.42
34	F	101	HEM	C3C-C4C-NC	-2.23	106.73	110.94
23	a	411	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
26	a	410	PL9	C7-C8-C9	-2.23	123.08	126.79
23	C	503	CLA	C6-C7-C8	-2.23	108.71	115.92
27	D	413	STE	C12-C11-C10	-2.23	103.11	114.42
29	l	101	SQD	C1-O5-C5	-2.23	109.32	113.69
25	B	618	BCR	C27-C26-C25	2.22	125.96	122.73
23	a	411	CLA	O2D-CGD-CBD	2.22	115.22	111.27
23	b	606	CLA	CMD-C2D-C3D	2.22	128.84	124.68
25	B	617	BCR	C15-C16-C17	-2.22	118.92	123.47
23	B	611	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
30	H	102	DGD	C1D-O6D-C5D	-2.22	109.33	113.69
30	c	519	DGD	O1G-C1A-C2A	-2.22	104.94	111.91
23	b	602	CLA	O2A-C1-C2	-2.22	102.80	108.64
26	A	409	PL9	C11-C12-C13	-2.22	104.59	111.88
23	B	612	CLA	O1D-CGD-CBD	2.22	129.02	124.48
24	D	402	PHO	C2B-C1B-NB	-2.22	106.45	109.79
33	D	410	LHG	C20-C19-C18	-2.21	103.18	114.42
23	C	512	CLA	OBD-CAD-C3D	2.21	131.66	127.98
25	A	408	BCR	C33-C5-C6	-2.21	122.04	124.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	C	523	DGD	CDB-CCB-CBB	-2.21	103.19	114.42
25	b	617	BCR	C35-C13-C12	2.21	121.56	118.08
23	b	603	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
23	C	513	CLA	CHB-C4A-NA	2.21	127.57	124.51
28	b	623	LMG	C1-C2-C3	-2.21	105.40	110.00
28	M	101	LMG	O7-C10-O9	-2.21	118.37	123.70
25	c	514	BCR	C2-C1-C6	2.20	113.87	110.48
30	h	102	DGD	O2D-C2D-C1D	-2.20	104.69	110.05
23	c	506	CLA	CHA-C1A-NA	-2.20	121.35	126.40
23	C	503	CLA	CMD-C2D-C3D	2.20	128.79	124.68
23	d	402	CLA	O2D-CGD-CBD	2.20	115.18	111.27
25	A	408	BCR	C36-C18-C17	-2.20	119.84	122.92
29	a	412	SQD	O5-C1-O6	-2.20	104.77	109.97
23	d	402	CLA	C6-C5-C3	2.19	119.21	113.45
23	B	601	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
28	b	623	LMG	C4-C3-C2	-2.19	107.00	110.82
23	b	612	CLA	C7-C6-C5	-2.19	107.41	113.36
28	b	621	LMG	O8-C28-O10	-2.19	118.07	123.59
23	c	506	CLA	OBD-CAD-C3D	2.19	131.62	127.98
25	K	101	BCR	C23-C24-C25	-2.19	121.06	127.20
30	H	102	DGD	O6D-C1D-O3G	-2.19	104.80	109.97
23	B	610	CLA	CMC-C2C-C3C	2.19	129.06	124.94
23	B	611	CLA	CMB-C2B-C1B	-2.19	125.10	128.46
23	C	504	CLA	C4-C3-C5	2.19	118.95	115.27
23	C	510	CLA	CMB-C2B-C3B	2.18	128.77	124.68
23	B	603	CLA	O2A-C1-C2	-2.18	102.89	108.64
23	C	504	CLA	O2D-CGD-CBD	2.18	115.15	111.27
30	C	522	DGD	C6D-O5D-C1E	2.18	118.00	113.74
26	d	405	PL9	C8-C7-C3	2.18	118.15	111.98
30	C	523	DGD	O6D-C5D-C6D	-2.18	102.26	106.67
28	c	522	LMG	C6-C5-C4	-2.18	107.90	113.00
30	C	523	DGD	CAB-C9B-C8B	-2.18	103.36	114.42
23	B	605	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
23	c	510	CLA	O1D-CGD-CBD	2.18	128.94	124.48
25	x	101	BCR	C16-C15-C14	-2.17	119.02	123.47
23	C	512	CLA	CAA-CBA-CGA	-2.17	106.90	113.25
23	d	403	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
23	b	609	CLA	CHA-C1A-NA	-2.17	121.43	126.40
28	a	415	LMG	O8-C28-O10	-2.17	118.12	123.59
25	C	520	BCR	C33-C5-C6	-2.17	122.09	124.53
23	C	503	CLA	CMB-C2B-C3B	2.17	128.74	124.68
23	c	503	CLA	C11-C12-C13	-2.17	108.91	115.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	413	SQD	C11-C10-C9	-2.17	103.43	114.42
23	b	602	CLA	O1A-CGA-CBA	2.17	132.18	123.73
30	c	521	DGD	C7A-C6A-C5A	-2.17	103.43	114.42
23	C	506	CLA	CMB-C2B-C3B	2.17	128.73	124.68
23	C	508	CLA	C5-C3-C2	-2.16	116.74	121.12
30	A	414	DGD	CAB-C9B-C8B	-2.16	103.45	114.42
33	d	407	LHG	C20-C19-C18	-2.16	103.45	114.42
30	A	414	DGD	O1G-C1A-C2A	-2.16	105.13	111.91
24	d	401	PHO	CBD-CHA-C4D	-2.16	106.11	108.54
28	c	518	LMG	C8-O7-C10	2.16	123.11	117.79
25	b	618	BCR	C15-C16-C17	-2.16	119.05	123.47
23	C	504	CLA	CMC-C2C-C3C	2.16	129.01	124.94
23	c	508	CLA	C3B-C4B-NB	-2.16	106.42	109.21
23	C	511	CLA	C1-C2-C3	-2.15	122.32	126.04
23	b	605	CLA	CMB-C2B-C1B	-2.15	125.15	128.46
23	c	512	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
23	B	604	CLA	O2A-C1-C2	2.15	114.29	108.64
33	d	407	LHG	C27-C26-C25	-2.15	103.51	114.42
23	a	406	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
23	C	511	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
23	C	508	CLA	CMD-C2D-C3D	2.15	128.70	124.68
24	D	402	PHO	CAC-C3C-C2C	2.15	131.20	127.53
23	C	508	CLA	C7-C6-C5	-2.15	107.53	113.36
23	C	504	CLA	CHA-C1A-NA	-2.15	121.48	126.40
29	a	414	SQD	C3-C4-C5	2.15	114.07	110.24
33	a	413	LHG	C18-C17-C16	-2.15	103.53	114.42
23	B	615	CLA	CMB-C2B-C3B	2.15	128.69	124.68
23	C	513	CLA	C1-O2A-CGA	-2.14	110.82	116.44
25	a	409	BCR	C8-C7-C6	-2.14	121.18	127.20
26	a	410	PL9	C25-C24-C26	2.14	118.88	115.27
24	D	402	PHO	CMB-C2B-C1B	-2.14	121.77	125.06
25	B	618	BCR	C15-C14-C13	-2.14	124.25	127.31
23	C	503	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
23	B	604	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
23	B	609	CLA	C7-C6-C5	-2.14	107.55	113.36
23	c	511	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
25	B	617	BCR	C27-C26-C25	2.13	125.83	122.73
25	T	101	BCR	C34-C9-C10	-2.13	119.93	122.92
23	a	408	CLA	CMB-C2B-C3B	2.13	128.67	124.68
25	B	619	BCR	C28-C27-C26	-2.13	110.27	114.08
25	D	406	BCR	C16-C15-C14	-2.13	119.11	123.47
28	b	621	LMG	C38-C37-C36	-2.13	103.61	114.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	408	LMG	C14-C13-C12	-2.13	103.61	114.42
23	D	404	CLA	C4A-NA-C1A	2.13	107.66	106.71
29	a	412	SQD	O3-C3-C4	2.13	115.27	110.35
23	c	506	CLA	CBC-CAC-C3C	-2.13	106.85	112.27
25	b	618	BCR	C16-C15-C14	-2.13	119.11	123.47
28	C	517	LMG	O3-C3-C2	-2.13	105.43	110.35
28	c	523	LMG	O7-C10-O9	-2.12	118.57	123.70
23	B	605	CLA	C16-C17-C18	-2.12	105.97	115.98
29	a	412	SQD	C16-C15-C14	-2.12	103.66	114.42
30	H	102	DGD	CAB-C9B-C8B	-2.12	103.66	114.42
30	C	522	DGD	CBB-CAB-C9B	-2.12	103.66	114.42
23	b	605	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
23	C	511	CLA	CMD-C2D-C3D	2.12	128.64	124.68
24	d	401	PHO	O1D-CGD-CBD	2.12	128.82	124.48
28	a	415	LMG	C1-O6-C5	-2.12	109.53	113.69
30	c	519	DGD	O6E-C5E-C4E	2.12	113.54	109.69
28	c	524	LMG	O5-C6-C5	-2.12	104.03	111.29
28	D	408	LMG	O7-C10-O9	-2.12	118.59	123.70
25	C	520	BCR	C11-C10-C9	-2.12	124.29	127.31
23	d	403	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
28	D	408	LMG	O2-C2-C3	-2.11	105.47	110.35
23	B	603	CLA	C6-C5-C3	2.11	118.99	113.45
25	T	101	BCR	C1-C6-C5	-2.11	119.64	122.61
28	a	415	LMG	C9-C8-C7	-2.11	106.80	111.79
25	c	514	BCR	C15-C16-C17	-2.11	119.15	123.47
23	C	508	CLA	CHB-C4A-NA	2.11	127.43	124.51
23	B	606	CLA	O2D-CGD-O1D	-2.11	119.72	123.84
25	B	619	BCR	C3-C4-C5	-2.11	110.31	114.08
23	a	406	CLA	O2D-CGD-O1D	-2.11	119.72	123.84
25	B	617	BCR	C15-C14-C13	-2.11	124.30	127.31
29	a	412	SQD	O4-C4-C5	-2.11	104.07	109.30
23	c	506	CLA	C1B-CHB-C4A	-2.10	125.95	130.12
28	a	415	LMG	C22-C21-C20	-2.10	103.75	114.42
23	A	404	CLA	C17-C16-C15	-2.10	103.58	113.24
25	c	515	BCR	C38-C26-C27	-2.10	109.58	113.62
23	d	403	CLA	OBD-CAD-CBD	-2.10	122.89	125.89
26	A	409	PL9	C12-C13-C14	-2.10	122.60	127.66
33	D	410	LHG	C27-C26-C25	-2.10	103.76	114.42
33	L	101	LHG	C29-C28-C27	-2.10	103.76	114.42
28	c	522	LMG	C9-C8-C7	-2.10	106.82	111.79
23	b	607	CLA	CMC-C2C-C3C	2.10	128.90	124.94
23	B	605	CLA	C16-C15-C13	-2.10	109.13	115.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	410	PL9	C11-C12-C13	-2.10	104.98	111.88
23	C	507	CLA	O2D-CGD-O1D	-2.10	119.74	123.84
30	A	414	DGD	CDB-CCB-CBB	-2.10	103.77	114.42
33	D	412	LHG	O3-P-O5	-2.10	100.88	109.07
25	K	101	BCR	C15-C16-C17	-2.09	119.18	123.47
33	L	101	LHG	C13-C12-C11	-2.09	103.79	114.42
23	d	402	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
23	b	604	CLA	O2A-C1-C2	-2.09	103.13	108.64
23	b	614	CLA	C3B-C4B-NB	-2.09	106.50	109.21
23	c	508	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
23	C	502	CLA	CHA-C1A-NA	-2.09	121.61	126.40
25	b	618	BCR	C7-C8-C9	-2.09	123.07	126.23
23	B	607	CLA	CMB-C2B-C3B	2.09	128.59	124.68
23	C	511	CLA	C11-C10-C8	-2.09	109.16	115.92
30	C	523	DGD	O5D-C6D-C5D	-2.09	105.18	109.05
23	A	405	CLA	O2D-CGD-CBD	2.09	114.98	111.27
23	C	512	CLA	C3B-C4B-NB	-2.09	106.51	109.21
23	c	510	CLA	O2A-C1-C2	-2.09	103.14	108.64
23	B	609	CLA	CMC-C2C-C3C	2.09	128.88	124.94
30	c	520	DGD	C4D-C3D-C2D	2.09	114.47	110.82
23	a	411	CLA	C1-O2A-CGA	2.09	121.92	116.44
26	a	410	PL9	C50-C49-C48	-2.09	116.62	122.65
33	d	407	LHG	C18-C17-C16	-2.08	103.85	114.42
29	A	413	SQD	O9-S-C6	2.08	109.41	106.94
28	b	623	LMG	C40-C39-C38	-2.08	103.86	114.42
23	B	614	CLA	CMB-C2B-C3B	2.08	128.57	124.68
23	a	408	CLA	C2A-C1A-CHA	2.08	127.49	123.86
29	A	413	SQD	O8-S-C6	2.08	109.05	105.74
24	A	406	PHO	O2A-C1-C2	-2.08	103.17	108.64
28	b	621	LMG	C1-C2-C3	-2.08	105.67	110.00
25	t	101	BCR	C1-C6-C5	-2.08	119.69	122.61
25	c	514	BCR	C29-C30-C25	2.08	113.68	110.48
26	A	409	PL9	C50-C49-C48	-2.08	116.65	122.65
24	A	406	PHO	C1B-NB-C4B	2.08	110.42	106.51
25	B	619	BCR	C29-C30-C25	2.07	113.67	110.48
23	c	508	CLA	CMD-C2D-C3D	2.07	128.56	124.68
25	a	409	BCR	C30-C25-C26	-2.07	119.69	122.61
23	C	510	CLA	CHA-C1A-NA	-2.07	121.65	126.40
23	A	405	CLA	CMD-C2D-C3D	2.07	128.56	124.68
29	b	620	SQD	O47-C45-C46	2.07	115.91	108.40
33	d	406	LHG	C20-C19-C18	-2.07	103.91	114.42
26	d	405	PL9	C12-C13-C14	-2.07	122.67	127.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	c	519	DGD	C4E-C3E-C2E	-2.07	107.21	110.82
25	H	101	BCR	C1-C6-C5	-2.07	119.70	122.61
30	A	414	DGD	C4A-C3A-C2A	-2.07	105.75	113.19
23	C	510	CLA	CMB-C2B-C1B	-2.07	125.28	128.46
25	B	619	BCR	C15-C14-C13	-2.07	124.36	127.31
25	x	101	BCR	C11-C10-C9	-2.07	124.36	127.31
23	c	512	CLA	C4-C3-C5	2.07	118.75	115.27
25	T	101	BCR	C4-C5-C6	2.07	125.73	122.73
30	C	523	DGD	O3E-C3E-C2E	-2.06	105.58	110.35
33	d	406	LHG	C18-C17-C16	-2.06	103.94	114.42
33	L	101	LHG	O7-C5-C4	-2.06	100.93	108.40
23	C	507	CLA	CED-O2D-CGD	2.06	120.61	115.94
33	D	410	LHG	O8-C23-C24	2.06	118.38	111.91
27	a	417	STE	C4-C3-C2	-2.06	105.74	113.76
23	c	509	CLA	O2A-C1-C2	2.06	114.05	108.64
28	M	101	LMG	C23-C22-C21	-2.06	103.96	114.42
33	l	102	LHG	C18-C17-C16	-2.06	103.96	114.42
33	d	407	LHG	O8-C6-C5	-2.06	102.44	108.43
23	b	615	CLA	CMC-C2C-C3C	2.06	128.82	124.94
23	b	602	CLA	CMD-C2D-C3D	2.06	128.53	124.68
29	A	413	SQD	C13-C12-C11	-2.06	103.98	114.42
23	d	403	CLA	C1-C2-C3	-2.06	122.49	126.04
28	b	623	LMG	O7-C10-O9	-2.06	118.73	123.70
23	b	610	CLA	CMC-C2C-C3C	2.05	128.81	124.94
35	v	201	HEC	CBA-CAA-C2A	-2.05	108.69	112.48
23	C	506	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
23	B	603	CLA	O2D-CGD-O1D	-2.05	119.82	123.84
28	c	522	LMG	C40-C39-C38	-2.05	104.01	114.42
30	c	520	DGD	O3G-C1D-C2D	-2.05	105.10	108.30
23	C	507	CLA	CMD-C2D-C3D	2.05	128.52	124.68
34	F	101	HEM	CMC-C2C-C3C	2.05	128.52	124.68
23	A	407	CLA	CHA-C1A-NA	-2.05	121.70	126.40
23	B	614	CLA	OBD-CAD-CBD	-2.05	122.97	125.89
28	A	411	LMG	C9-C8-C7	-2.05	106.94	111.79
25	b	617	BCR	C30-C25-C26	-2.05	119.73	122.61
30	c	519	DGD	O2G-C1B-O1B	-2.05	118.76	123.70
29	b	620	SQD	C20-C19-C18	-2.05	104.04	114.42
30	c	521	DGD	CAB-C9B-C8B	-2.04	104.05	114.42
23	D	405	CLA	C4-C3-C5	2.04	118.71	115.27
28	B	620	LMG	C8-O7-C10	2.04	122.82	117.79
28	d	409	LMG	O5-C6-C5	-2.04	104.28	111.29
23	C	511	CLA	O1A-CGA-CBA	2.04	131.70	123.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	411	LMG	O1-C7-C8	-2.04	105.97	110.90
26	a	410	PL9	O2-C1-C6	2.04	124.12	120.59
23	B	613	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
30	H	102	DGD	O2G-C1B-O1B	-2.04	118.77	123.70
28	b	621	LMG	C9-C8-C7	-2.04	106.97	111.79
23	B	605	CLA	C1-C2-C3	-2.04	122.52	126.04
23	C	511	CLA	O1D-CGD-CBD	2.04	128.65	124.48
29	a	412	SQD	O48-C23-O10	-2.04	118.45	123.59
26	D	407	PL9	C31-C32-C33	-2.04	105.19	111.88
26	D	407	PL9	C31-C29-C28	2.03	125.23	121.12
25	B	617	BCR	C33-C5-C6	-2.03	122.24	124.53
25	a	409	BCR	C38-C26-C27	-2.03	109.71	113.62
23	B	606	CLA	C2A-C1A-CHA	2.03	127.41	123.86
25	c	515	BCR	C1-C6-C5	-2.03	119.75	122.61
23	B	607	CLA	CHB-C4A-NA	2.03	127.32	124.51
24	a	407	PHO	O2A-C1-C2	2.03	113.97	108.64
23	C	511	CLA	CHB-C4A-NA	2.03	127.32	124.51
25	C	514	BCR	C33-C5-C6	-2.03	122.25	124.53
33	D	411	LHG	O8-C23-O10	-2.03	118.47	123.59
28	c	522	LMG	C38-C37-C36	-2.03	104.12	114.42
26	D	407	PL9	C8-C7-C3	2.03	117.72	111.98
23	B	615	CLA	CHB-C4A-NA	2.03	127.32	124.51
23	d	402	CLA	C2A-C1A-CHA	2.03	127.40	123.86
23	b	604	CLA	CBC-CAC-C3C	-2.03	107.11	112.27
23	B	612	CLA	C1B-CHB-C4A	-2.03	126.10	130.12
23	c	502	CLA	CHB-C4A-NA	2.03	127.31	124.51
28	M	101	LMG	O2-C2-C1	-2.02	105.13	110.05
23	b	612	CLA	C4D-C3D-CAD	-2.02	107.34	108.47
23	A	404	CLA	CHA-C1A-NA	-2.02	121.76	126.40
23	D	405	CLA	CHB-C4A-NA	2.02	127.31	124.51
28	M	101	LMG	O5-C6-C5	-2.02	104.35	111.29
33	d	406	LHG	O3-P-O5	-2.02	101.17	109.07
25	B	617	BCR	C8-C7-C6	-2.02	121.53	127.20
23	b	615	CLA	O2D-CGD-CBD	2.02	114.86	111.27
25	k	102	BCR	C38-C26-C25	-2.02	122.26	124.53
29	a	414	SQD	O2-C2-C3	-2.02	105.69	110.35
26	d	405	PL9	C32-C33-C34	-2.02	122.80	127.66
23	B	611	CLA	OBD-CAD-C3D	2.02	131.33	127.98
23	D	404	CLA	O2D-CGD-CBD	2.02	114.85	111.27
23	c	507	CLA	O1A-CGA-CBA	2.02	131.60	123.73
23	b	606	CLA	OBD-CAD-CBD	-2.02	123.02	125.89
25	B	618	BCR	C35-C13-C14	-2.01	120.10	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	502	CLA	CMB-C2B-C3B	2.01	128.45	124.68
23	C	512	CLA	C1B-CHB-C4A	-2.01	126.13	130.12
23	B	616	CLA	CHB-C4A-NA	2.01	127.30	124.51
23	a	411	CLA	C2A-C1A-CHA	2.01	127.38	123.86
29	l	101	SQD	O9-S-C6	-2.01	104.55	106.94
23	c	508	CLA	O1D-CGD-CBD	2.01	128.60	124.48
23	b	608	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
23	A	405	CLA	C3D-CAD-CBD	-2.01	104.96	107.61
25	d	404	BCR	C29-C30-C25	2.01	113.57	110.48
23	C	502	CLA	CMC-C2C-C3C	2.01	128.73	124.94
30	A	414	DGD	C3E-C4E-C5E	-2.01	106.66	110.24
25	A	408	BCR	C15-C16-C17	-2.01	119.36	123.47
23	C	501	CLA	CHA-C1A-NA	-2.01	121.80	126.40
29	a	414	SQD	O48-C23-C24	2.01	118.21	111.91
23	c	504	CLA	O1D-CGD-CBD	2.01	128.59	124.48
29	b	620	SQD	O48-C23-O10	-2.00	118.53	123.59
28	c	522	LMG	C3-C4-C5	-2.00	106.66	110.24
25	b	617	BCR	C2-C1-C6	2.00	113.57	110.48
28	A	411	LMG	O6-C1-O1	-2.00	105.23	109.97
23	D	404	CLA	C3B-C4B-NB	-2.00	106.62	109.21
26	d	405	PL9	C11-C12-C13	-2.00	105.30	111.88
23	a	408	CLA	C4-C3-C5	2.00	118.64	115.27
33	d	407	LHG	O7-C7-C8	-2.00	107.18	111.50
24	D	402	PHO	C5-C3-C2	2.00	125.17	121.12
23	B	605	CLA	CHA-C1A-NA	-2.00	121.81	126.40
30	A	414	DGD	O1A-C1A-C2A	2.00	131.54	123.73
23	C	503	CLA	C5-C3-C2	-2.00	117.07	121.12

All (52) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404	CLA	ND
23	A	407	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND
23	B	604	CLA	ND
23	B	605	CLA	ND
23	B	606	CLA	ND
23	B	607	CLA	ND
23	B	610	CLA	ND
23	B	612	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
23	B	613	CLA	ND
23	B	614	CLA	ND
23	B	615	CLA	ND
23	B	616	CLA	ND
23	C	501	CLA	ND
23	C	504	CLA	ND
23	C	505	CLA	ND
23	C	506	CLA	ND
23	C	507	CLA	ND
23	C	509	CLA	ND
23	C	510	CLA	ND
23	C	512	CLA	ND
23	C	513	CLA	ND
23	D	404	CLA	ND
23	a	405	CLA	ND
23	a	408	CLA	ND
23	b	602	CLA	ND
23	b	603	CLA	ND
23	b	604	CLA	ND
23	b	605	CLA	ND
23	b	606	CLA	ND
23	b	608	CLA	ND
23	b	609	CLA	ND
23	b	610	CLA	ND
23	b	611	CLA	ND
23	b	612	CLA	ND
23	b	613	CLA	ND
23	b	614	CLA	ND
23	b	615	CLA	ND
23	c	501	CLA	ND
23	c	504	CLA	ND
23	c	505	CLA	ND
23	c	506	CLA	ND
23	c	507	CLA	ND
23	c	509	CLA	ND
23	c	510	CLA	ND
23	c	511	CLA	ND
23	c	512	CLA	ND
23	c	513	CLA	ND
23	d	402	CLA	ND
23	h	101	CLA	ND

All (1704) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	407	CLA	C4-C3-C5-C6
23	B	601	CLA	CBA-CGA-O2A-C1
23	B	601	CLA	O1A-CGA-O2A-C1
23	B	606	CLA	CHA-CBD-CGD-O1D
23	B	606	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	B	614	CLA	C2-C3-C5-C6
23	B	614	CLA	C4-C3-C5-C6
23	C	508	CLA	CHA-CBD-CGD-O1D
23	C	512	CLA	O2A-C1-C2-C3
23	a	411	CLA	CHA-CBD-CGD-O1D
23	a	411	CLA	CHA-CBD-CGD-O2D
23	b	604	CLA	C4-C3-C5-C6
23	b	605	CLA	CHA-CBD-CGD-O1D
23	b	605	CLA	CHA-CBD-CGD-O2D
23	b	606	CLA	C2-C3-C5-C6
23	b	606	CLA	C4-C3-C5-C6
23	b	613	CLA	CHA-CBD-CGD-O1D
23	b	613	CLA	CAD-CBD-CGD-O1D
23	b	613	CLA	CAD-CBD-CGD-O2D
23	b	615	CLA	CBD-CGD-O2D-CED
23	c	506	CLA	C4-C3-C5-C6
23	c	507	CLA	C4-C3-C5-C6
23	c	508	CLA	CHA-CBD-CGD-O1D
23	c	510	CLA	C11-C10-C8-C9
23	h	101	CLA	C1A-C2A-CAA-CBA
23	h	101	CLA	C3A-C2A-CAA-CBA
23	h	101	CLA	CHA-CBD-CGD-O1D
23	h	101	CLA	CAD-CBD-CGD-O1D
23	h	101	CLA	CAD-CBD-CGD-O2D
23	h	101	CLA	CBD-CGD-O2D-CED
25	A	408	BCR	C20-C21-C22-C37
25	B	619	BCR	C37-C22-C23-C24
25	C	514	BCR	C10-C11-C12-C13
25	C	514	BCR	C11-C12-C13-C35
25	C	514	BCR	C16-C17-C18-C36
25	C	514	BCR	C20-C21-C22-C37
25	C	520	BCR	C7-C8-C9-C34
25	D	406	BCR	C23-C24-C25-C26
25	D	406	BCR	C23-C24-C25-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	H	101	BCR	C7-C8-C9-C10
25	K	101	BCR	C1-C6-C7-C8
25	K	101	BCR	C5-C6-C7-C8
25	K	101	BCR	C21-C22-C23-C24
25	K	101	BCR	C37-C22-C23-C24
25	c	514	BCR	C7-C8-C9-C34
25	k	101	BCR	C1-C6-C7-C8
25	k	101	BCR	C5-C6-C7-C8
25	k	101	BCR	C21-C22-C23-C24
25	k	101	BCR	C37-C22-C23-C24
26	A	409	PL9	C12-C13-C14-C16
26	A	409	PL9	C27-C28-C29-C30
26	A	409	PL9	C27-C28-C29-C31
26	A	409	PL9	C28-C29-C31-C32
26	A	409	PL9	C37-C38-C39-C41
26	D	407	PL9	C32-C33-C34-C35
26	D	407	PL9	C32-C33-C34-C36
26	a	410	PL9	C22-C23-C24-C26
26	a	410	PL9	C27-C28-C29-C31
26	a	410	PL9	C33-C34-C36-C37
26	a	410	PL9	C44-C46-C47-C48
26	d	405	PL9	C32-C33-C34-C35
26	d	405	PL9	C32-C33-C34-C36
27	B	621	STE	C1-C2-C3-C4
27	E	102	STE	C1-C2-C3-C4
27	E	104	STE	C1-C2-C3-C4
27	i	101	STE	C1-C2-C3-C4
27	j	101	STE	C1-C2-C3-C4
27	m	101	STE	C1-C2-C3-C4
28	A	411	LMG	O6-C1-O1-C7
28	A	411	LMG	O9-C10-O7-C8
28	A	411	LMG	C11-C10-O7-C8
28	C	517	LMG	C2-C1-O1-C7
28	C	517	LMG	O6-C1-O1-C7
28	D	408	LMG	O6-C1-O1-C7
28	D	408	LMG	C11-C10-O7-C8
28	b	619	LMG	O7-C8-C9-O8
28	b	619	LMG	C7-C8-O7-C10
28	b	623	LMG	C2-C1-O1-C7
28	b	623	LMG	O6-C1-O1-C7
28	c	524	LMG	C2-C1-O1-C7
28	c	524	LMG	O6-C1-O1-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	A	413	SQD	O6-C44-C45-O47
29	A	413	SQD	O5-C5-C6-S
29	A	413	SQD	C5-C6-S-O7
29	A	413	SQD	C5-C6-S-O8
29	A	413	SQD	C5-C6-S-O9
29	F	102	SQD	O5-C1-O6-C44
29	a	412	SQD	C5-C6-S-O7
29	a	412	SQD	C5-C6-S-O8
29	a	412	SQD	C5-C6-S-O9
29	a	414	SQD	O6-C44-C45-O47
29	a	414	SQD	O5-C5-C6-S
29	a	414	SQD	C5-C6-S-O7
29	a	414	SQD	C5-C6-S-O8
29	b	620	SQD	C46-C45-O47-C7
29	b	620	SQD	C8-C7-O47-C45
29	f	102	SQD	O5-C1-O6-C44
29	l	101	SQD	C2-C1-O6-C44
29	l	101	SQD	O5-C1-O6-C44
29	l	101	SQD	O6-C44-C45-O47
29	l	101	SQD	O49-C7-O47-C45
29	l	101	SQD	C8-C7-O47-C45
29	l	101	SQD	O5-C5-C6-S
30	A	414	DGD	C2B-C1B-O2G-C2G
30	A	414	DGD	O1B-C1B-O2G-C2G
33	D	410	LHG	O2-C2-C3-O3
33	D	410	LHG	C3-O3-P-O4
33	D	410	LHG	C3-O3-P-O5
33	D	410	LHG	C3-O3-P-O6
33	D	410	LHG	C4-O6-P-O4
33	E	101	LHG	C3-O3-P-O5
33	E	101	LHG	C4-O6-P-O4
33	a	413	LHG	O1-C1-C2-O2
33	a	413	LHG	O1-C1-C2-C3
33	a	413	LHG	C3-O3-P-O4
33	a	413	LHG	C3-O3-P-O5
33	a	413	LHG	C3-O3-P-O6
33	d	406	LHG	O1-C1-C2-C3
33	d	406	LHG	C3-O3-P-O5
33	d	406	LHG	C4-O6-P-O5
33	d	407	LHG	C3-O3-P-O4
33	d	407	LHG	C4-O6-P-O4
33	d	408	LHG	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	l	102	LHG	C4-O6-P-O5
23	c	513	CLA	CBD-CGD-O2D-CED
28	B	620	LMG	O10-C28-O8-C9
23	b	615	CLA	O1D-CGD-O2D-CED
23	h	101	CLA	O1D-CGD-O2D-CED
26	A	409	PL9	C47-C48-C49-C51
26	a	410	PL9	C47-C48-C49-C50
23	B	612	CLA	CBD-CGD-O2D-CED
29	f	102	SQD	O10-C23-O48-C46
29	l	101	SQD	O10-C23-O48-C46
28	D	408	LMG	O9-C10-O7-C8
33	E	101	LHG	O9-C7-O7-C5
28	B	620	LMG	C29-C28-O8-C9
29	f	102	SQD	C24-C23-O48-C46
29	l	101	SQD	C24-C23-O48-C46
26	a	410	PL9	C47-C48-C49-C51
23	D	405	CLA	CBD-CGD-O2D-CED
28	M	101	LMG	O10-C28-O8-C9
26	a	410	PL9	C35-C34-C36-C37
23	b	604	CLA	C2-C3-C5-C6
23	c	506	CLA	C2-C3-C5-C6
23	b	605	CLA	C2A-CAA-CBA-CGA
27	A	417	STE	C13-C14-C15-C16
23	b	601	CLA	C3-C5-C6-C7
23	h	101	CLA	C3-C5-C6-C7
28	C	517	LMG	C29-C28-O8-C9
29	F	102	SQD	C24-C23-O48-C46
26	A	409	PL9	C47-C48-C49-C50
29	A	413	SQD	C16-C17-C18-C19
29	b	620	SQD	O49-C7-O47-C45
29	F	102	SQD	O10-C23-O48-C46
29	F	102	SQD	C44-C45-C46-O48
23	C	511	CLA	CBD-CGD-O2D-CED
23	c	511	CLA	CBD-CGD-O2D-CED
23	c	512	CLA	CBD-CGD-O2D-CED
23	c	513	CLA	O1D-CGD-O2D-CED
28	M	101	LMG	C29-C28-O8-C9
28	d	409	LMG	C10-C11-C12-C13
23	c	501	CLA	CBD-CGD-O2D-CED
30	A	414	DGD	O6E-C5E-C6E-O5E
30	A	414	DGD	C4E-C5E-C6E-O5E
27	b	624	STE	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	d	412	STE	C10-C11-C12-C13
27	i	101	STE	C6-C7-C8-C9
27	j	102	STE	C3-C4-C5-C6
33	d	407	LHG	C28-C29-C30-C31
30	A	414	DGD	C1B-C2B-C3B-C4B
23	C	508	CLA	CBD-CGD-O2D-CED
30	H	102	DGD	O6E-C5E-C6E-O5E
30	h	102	DGD	O6E-C5E-C6E-O5E
23	B	605	CLA	C4-C3-C5-C6
23	b	602	CLA	C4-C3-C5-C6
23	A	407	CLA	C2-C3-C5-C6
23	B	605	CLA	C2-C3-C5-C6
23	b	602	CLA	C2-C3-C5-C6
23	c	507	CLA	C2-C3-C5-C6
29	b	620	SQD	O5-C1-O6-C44
26	A	409	PL9	C24-C26-C27-C28
26	A	409	PL9	C29-C31-C32-C33
26	a	410	PL9	C14-C16-C17-C18
26	a	410	PL9	C19-C21-C22-C23
26	a	410	PL9	C34-C36-C37-C38
29	l	101	SQD	C29-C30-C31-C32
23	c	512	CLA	CBA-CGA-O2A-C1
29	b	620	SQD	C24-C23-O48-C46
23	b	608	CLA	CBD-CGD-O2D-CED
26	a	410	PL9	C27-C28-C29-C30
33	D	410	LHG	C1-C2-C3-O3
33	a	413	LHG	C1-C2-C3-O3
29	a	414	SQD	C17-C18-C19-C20
23	B	616	CLA	CBA-CGA-O2A-C1
23	c	506	CLA	CBA-CGA-O2A-C1
28	c	518	LMG	C29-C28-O8-C9
30	A	414	DGD	C2A-C1A-O1G-C1G
33	a	413	LHG	C27-C28-C29-C30
23	h	101	CLA	C13-C15-C16-C17
27	A	416	STE	C14-C15-C16-C17
23	B	601	CLA	C5-C6-C7-C8
23	c	512	CLA	C8-C10-C11-C12
23	c	513	CLA	C8-C10-C11-C12
33	a	413	LHG	O2-C2-C3-O3
27	b	624	STE	C5-C6-C7-C8
28	C	517	LMG	O10-C28-O8-C9
28	b	623	LMG	O10-C28-O8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	b	620	SQD	O10-C23-O48-C46
23	b	613	CLA	C4-C3-C5-C6
23	b	613	CLA	C2-C3-C5-C6
23	B	613	CLA	C11-C12-C13-C14
23	C	507	CLA	C11-C10-C8-C9
23	C	509	CLA	C11-C10-C8-C9
23	C	512	CLA	C11-C10-C8-C9
23	b	605	CLA	C14-C13-C15-C16
23	c	508	CLA	C14-C13-C15-C16
23	c	512	CLA	C6-C7-C8-C9
33	D	412	LHG	C31-C32-C33-C34
23	b	610	CLA	C13-C15-C16-C17
23	B	606	CLA	C2A-CAA-CBA-CGA
25	C	515	BCR	C11-C12-C13-C35
25	d	404	BCR	C37-C22-C23-C24
25	k	101	BCR	C7-C8-C9-C34
25	k	101	BCR	C36-C18-C19-C20
25	d	404	BCR	C21-C22-C23-C24
28	D	408	LMG	C10-C11-C12-C13
33	E	101	LHG	O10-C23-O8-C6
23	C	505	CLA	C5-C6-C7-C8
33	E	101	LHG	C24-C23-O8-C6
23	B	603	CLA	C5-C6-C7-C8
23	B	614	CLA	C15-C16-C17-C18
23	C	506	CLA	C15-C16-C17-C18
23	b	601	CLA	C13-C15-C16-C17
23	b	602	CLA	C8-C10-C11-C12
23	b	605	CLA	C15-C16-C17-C18
23	b	606	CLA	C10-C11-C12-C13
23	b	610	CLA	C15-C16-C17-C18
23	c	509	CLA	C10-C11-C12-C13
23	h	101	CLA	C10-C11-C12-C13
27	i	101	STE	C3-C4-C5-C6
28	d	409	LMG	C28-C29-C30-C31
33	a	413	LHG	C23-C24-C25-C26
23	A	405	CLA	C15-C16-C17-C18
23	B	608	CLA	C15-C16-C17-C18
23	C	506	CLA	C8-C10-C11-C12
23	a	408	CLA	C13-C15-C16-C17
23	c	503	CLA	C8-C10-C11-C12
23	c	506	CLA	C13-C15-C16-C17
23	c	507	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	a	414	SQD	C30-C31-C32-C33
33	d	406	LHG	O1-C1-C2-O2
28	b	623	LMG	C28-C29-C30-C31
28	c	524	LMG	C28-C29-C30-C31
29	A	412	SQD	C7-C8-C9-C10
29	A	412	SQD	C23-C24-C25-C26
30	c	521	DGD	C1A-C2A-C3A-C4A
27	B	622	STE	C5-C6-C7-C8
23	B	601	CLA	C13-C15-C16-C17
23	D	405	CLA	C5-C6-C7-C8
28	b	623	LMG	O6-C5-C6-O5
23	c	506	CLA	C2-C1-O2A-CGA
23	B	607	CLA	C13-C15-C16-C17
23	C	503	CLA	C5-C6-C7-C8
29	a	412	SQD	C7-C8-C9-C10
30	H	102	DGD	C1A-C2A-C3A-C4A
23	C	501	CLA	CBD-CGD-O2D-CED
23	c	509	CLA	CBD-CGD-O2D-CED
30	h	102	DGD	C4E-C5E-C6E-O5E
23	B	601	CLA	C11-C12-C13-C15
23	C	508	CLA	C11-C10-C8-C7
23	d	402	CLA	C3-C5-C6-C7
23	h	101	CLA	C2A-CAA-CBA-CGA
23	B	612	CLA	O1D-CGD-O2D-CED
23	C	509	CLA	C10-C11-C12-C13
23	b	614	CLA	C5-C6-C7-C8
30	H	102	DGD	C4E-C5E-C6E-O5E
23	c	506	CLA	O1A-CGA-O2A-C1
23	B	606	CLA	C15-C16-C17-C18
23	D	403	CLA	C15-C16-C17-C18
23	b	610	CLA	C8-C10-C11-C12
23	D	405	CLA	O1D-CGD-O2D-CED
26	A	409	PL9	C34-C36-C37-C38
26	a	410	PL9	C24-C26-C27-C28
28	a	415	LMG	C10-C11-C12-C13
28	a	415	LMG	C28-C29-C30-C31
25	c	514	BCR	C18-C19-C20-C21
29	f	102	SQD	O49-C7-O47-C45
23	B	606	CLA	C10-C11-C12-C13
23	b	603	CLA	C10-C11-C12-C13
23	c	512	CLA	O1A-CGA-O2A-C1
28	b	619	LMG	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	611	CLA	C8-C10-C11-C12
23	B	611	CLA	C15-C16-C17-C18
23	b	614	CLA	C8-C10-C11-C12
23	c	503	CLA	C5-C6-C7-C8
23	B	616	CLA	O1A-CGA-O2A-C1
29	f	102	SQD	C8-C7-O47-C45
23	b	615	CLA	C8-C10-C11-C12
23	c	506	CLA	C8-C10-C11-C12
33	E	101	LHG	C3-O3-P-O6
33	L	101	LHG	C4-O6-P-O3
33	d	406	LHG	C3-O3-P-O6
33	d	407	LHG	C3-O3-P-O6
33	d	407	LHG	C4-O6-P-O3
33	l	102	LHG	C4-O6-P-O3
23	B	613	CLA	C8-C10-C11-C12
23	b	603	CLA	C4-C3-C5-C6
29	a	414	SQD	C34-C35-C36-C37
23	d	403	CLA	C8-C10-C11-C12
28	b	621	LMG	C31-C32-C33-C34
29	A	412	SQD	C12-C13-C14-C15
29	a	414	SQD	C9-C10-C11-C12
33	E	101	LHG	C8-C7-O7-C5
25	A	408	BCR	C35-C13-C14-C15
25	A	408	BCR	C16-C17-C18-C36
25	B	617	BCR	C11-C10-C9-C34
25	B	618	BCR	C16-C17-C18-C36
25	B	619	BCR	C11-C10-C9-C34
25	C	514	BCR	C11-C10-C9-C34
25	C	514	BCR	C35-C13-C14-C15
25	C	520	BCR	C11-C10-C9-C34
25	b	616	BCR	C11-C10-C9-C34
25	b	618	BCR	C35-C13-C14-C15
25	b	618	BCR	C20-C21-C22-C37
25	c	514	BCR	C16-C17-C18-C36
25	c	514	BCR	C20-C21-C22-C37
25	d	404	BCR	C11-C10-C9-C34
25	k	101	BCR	C35-C13-C14-C15
25	x	101	BCR	C16-C17-C18-C36
27	A	415	STE	C12-C13-C14-C15
27	I	101	STE	C5-C6-C7-C8
27	c	517	STE	C9-C10-C11-C12
28	C	524	LMG	C17-C18-C19-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	C	524	LMG	C30-C31-C32-C33
28	b	619	LMG	C14-C15-C16-C17
28	c	524	LMG	C17-C18-C19-C20
29	a	412	SQD	C13-C14-C15-C16
30	C	522	DGD	C3A-C4A-C5A-C6A
30	C	522	DGD	CCA-CDA-CEA-CFA
30	c	519	DGD	C2A-C3A-C4A-C5A
33	E	101	LHG	C33-C34-C35-C36
33	L	101	LHG	C17-C18-C19-C20
23	C	509	CLA	C16-C17-C18-C19
23	c	512	CLA	C16-C17-C18-C20
27	B	623	STE	C10-C11-C12-C13
27	b	622	STE	C4-C5-C6-C7
27	b	626	STE	C4-C5-C6-C7
27	c	517	STE	C12-C13-C14-C15
27	t	103	STE	C5-C6-C7-C8
27	x	102	STE	C4-C5-C6-C7
28	B	620	LMG	C31-C32-C33-C34
28	D	408	LMG	C32-C33-C34-C35
29	A	412	SQD	C16-C17-C18-C19
29	A	413	SQD	C34-C35-C36-C37
30	H	102	DGD	C4B-C5B-C6B-C7B
30	c	519	DGD	CBA-CCA-CDA-CEA
30	h	102	DGD	CCA-CDA-CEA-CFA
23	C	507	CLA	C10-C11-C12-C13
28	M	101	LMG	C28-C29-C30-C31
27	E	104	STE	C12-C13-C14-C15
27	t	102	STE	C11-C10-C9-C8
27	x	102	STE	C9-C10-C11-C12
33	E	101	LHG	C11-C12-C13-C14
33	l	102	LHG	C9-C10-C11-C12
27	B	621	STE	C4-C5-C6-C7
27	E	104	STE	C13-C14-C15-C16
27	M	102	STE	C4-C5-C6-C7
28	A	411	LMG	C16-C17-C18-C19
28	A	411	LMG	C36-C37-C38-C39
28	B	620	LMG	C32-C33-C34-C35
28	D	408	LMG	C14-C15-C16-C17
28	D	409	LMG	C12-C13-C14-C15
29	A	413	SQD	C27-C28-C29-C30
29	a	412	SQD	C31-C32-C33-C34
29	b	620	SQD	C13-C14-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	l	101	SQD	C17-C18-C19-C20
33	d	407	LHG	C14-C15-C16-C17
27	E	103	STE	C9-C10-C11-C12
27	M	102	STE	C5-C6-C7-C8
29	A	413	SQD	C28-C29-C30-C31
30	c	521	DGD	C3A-C4A-C5A-C6A
30	h	102	DGD	CAA-CBA-CCA-CDA
30	h	102	DGD	C2B-C3B-C4B-C5B
30	h	102	DGD	C6B-C7B-C8B-C9B
33	d	408	LHG	C30-C31-C32-C33
25	C	514	BCR	C16-C17-C18-C19
25	x	101	BCR	C11-C10-C9-C8
29	F	102	SQD	C2-C1-O6-C44
30	C	522	DGD	C2E-C1E-O5D-C6D
27	C	526	STE	C4-C5-C6-C7
27	b	627	STE	C9-C10-C11-C12
28	b	623	LMG	C15-C16-C17-C18
28	d	409	LMG	C33-C34-C35-C36
29	a	412	SQD	C18-C19-C20-C21
33	l	102	LHG	C14-C15-C16-C17
33	l	102	LHG	C27-C28-C29-C30
23	c	503	CLA	C15-C16-C17-C18
28	a	415	LMG	O10-C28-O8-C9
30	c	521	DGD	O1A-C1A-O1G-C1G
23	B	606	CLA	C16-C17-C18-C19
23	B	611	CLA	C16-C17-C18-C19
23	C	512	CLA	C16-C17-C18-C20
23	C	513	CLA	C16-C17-C18-C20
23	c	512	CLA	O1D-CGD-O2D-CED
23	B	609	CLA	C4-C3-C5-C6
27	C	528	STE	C9-C10-C11-C12
28	C	517	LMG	C14-C15-C16-C17
28	M	101	LMG	C35-C36-C37-C38
29	a	414	SQD	C14-C15-C16-C17
30	A	414	DGD	CCA-CDA-CEA-CFA
30	C	521	DGD	CCA-CDA-CEA-CFA
30	C	523	DGD	CBA-CCA-CDA-CEA
33	l	102	LHG	C13-C14-C15-C16
23	a	408	CLA	C11-C10-C8-C9
23	a	408	CLA	C11-C12-C13-C14
23	b	602	CLA	C6-C7-C8-C9
23	c	505	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	d	406	LHG	C7-C8-C9-C10
27	E	104	STE	C4-C5-C6-C7
27	b	627	STE	C14-C15-C16-C17
27	d	410	STE	C5-C6-C7-C8
28	C	524	LMG	C32-C33-C34-C35
28	D	409	LMG	C14-C15-C16-C17
28	b	621	LMG	C29-C30-C31-C32
28	c	524	LMG	C34-C35-C36-C37
29	a	414	SQD	C32-C33-C34-C35
29	l	101	SQD	C33-C34-C35-C36
30	c	519	DGD	C2B-C3B-C4B-C5B
30	c	521	DGD	C4A-C5A-C6A-C7A
33	d	406	LHG	C27-C28-C29-C30
27	A	417	STE	C12-C13-C14-C15
27	E	104	STE	C3-C4-C5-C6
27	l	103	STE	C6-C7-C8-C9
28	B	620	LMG	C29-C30-C31-C32
28	M	101	LMG	C15-C16-C17-C18
33	d	406	LHG	C29-C30-C31-C32
33	D	411	LHG	O1-C1-C2-C3
30	C	521	DGD	O6E-C5E-C6E-O5E
27	A	415	STE	C15-C16-C17-C18
27	e	101	STE	C12-C13-C14-C15
29	A	412	SQD	C27-C28-C29-C30
30	A	414	DGD	C8B-C9B-CAB-CBB
30	c	519	DGD	C9A-CAA-CBA-CCA
30	h	102	DGD	CAB-CBB-CCB-CDB
33	d	408	LHG	C28-C29-C30-C31
29	a	414	SQD	C23-C24-C25-C26
27	A	410	STE	C2-C3-C4-C5
27	B	621	STE	C7-C8-C9-C10
27	C	527	STE	C12-C13-C14-C15
27	C	529	STE	C14-C15-C16-C17
27	D	413	STE	C7-C8-C9-C10
27	b	624	STE	C12-C13-C14-C15
28	b	623	LMG	C12-C13-C14-C15
28	b	623	LMG	C19-C20-C21-C22
28	b	623	LMG	C31-C32-C33-C34
29	f	102	SQD	C25-C26-C27-C28
30	A	414	DGD	C4B-C5B-C6B-C7B
30	A	414	DGD	C6B-C7B-C8B-C9B
33	D	411	LHG	C29-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	D	412	LHG	C27-C28-C29-C30
23	B	601	CLA	C16-C17-C18-C19
23	B	601	CLA	C16-C17-C18-C20
23	C	509	CLA	C16-C17-C18-C20
23	C	512	CLA	C16-C17-C18-C19
23	a	408	CLA	C16-C17-C18-C19
23	b	606	CLA	C16-C17-C18-C20
23	b	612	CLA	C16-C17-C18-C20
23	c	513	CLA	C16-C17-C18-C19
23	c	513	CLA	C16-C17-C18-C20
23	h	101	CLA	C16-C17-C18-C19
30	C	522	DGD	O6E-C1E-O5D-C6D
23	C	513	CLA	C15-C16-C17-C18
23	c	511	CLA	O1D-CGD-O2D-CED
26	a	410	PL9	C29-C31-C32-C33
27	B	623	STE	C3-C4-C5-C6
27	T	102	STE	C4-C5-C6-C7
27	b	622	STE	C10-C11-C12-C13
27	j	101	STE	C2-C3-C4-C5
27	t	103	STE	C9-C10-C11-C12
28	a	415	LMG	C18-C19-C20-C21
28	c	523	LMG	C38-C39-C40-C41
30	C	523	DGD	C3A-C4A-C5A-C6A
30	C	523	DGD	C8A-C9A-CAA-CBA
30	c	521	DGD	CCB-CDB-CEB-CFB
33	E	101	LHG	C28-C29-C30-C31
27	A	416	STE	C5-C6-C7-C8
27	B	623	STE	C2-C3-C4-C5
27	C	529	STE	C10-C11-C12-C13
27	J	101	STE	C2-C3-C4-C5
27	m	101	STE	C6-C7-C8-C9
27	t	103	STE	C6-C7-C8-C9
27	t	103	STE	C11-C12-C13-C14
29	A	413	SQD	C14-C15-C16-C17
30	c	521	DGD	C6B-C7B-C8B-C9B
30	h	102	DGD	C7A-C8A-C9A-CAA
27	A	416	STE	C11-C10-C9-C8
27	b	624	STE	C11-C12-C13-C14
28	B	620	LMG	C15-C16-C17-C18
28	D	409	LMG	C18-C19-C20-C21
30	C	522	DGD	C8A-C9A-CAA-CBA
30	c	519	DGD	C3A-C4A-C5A-C6A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	d	408	LHG	C31-C32-C33-C34
23	C	511	CLA	O1D-CGD-O2D-CED
27	C	529	STE	C12-C13-C14-C15
27	H	103	STE	C6-C7-C8-C9
29	A	412	SQD	C10-C11-C12-C13
23	B	616	CLA	C5-C6-C7-C8
23	C	506	CLA	C13-C15-C16-C17
23	c	506	CLA	C5-C6-C7-C8
28	B	620	LMG	O6-C5-C6-O5
27	e	104	STE	C5-C6-C7-C8
29	a	412	SQD	C15-C16-C17-C18
33	l	102	LHG	C32-C33-C34-C35
23	B	611	CLA	C16-C17-C18-C20
23	a	408	CLA	C16-C17-C18-C20
27	e	104	STE	C3-C4-C5-C6
27	j	102	STE	C4-C5-C6-C7
27	l	103	STE	C5-C6-C7-C8
30	C	522	DGD	C7B-C8B-C9B-CAB
33	E	101	LHG	C30-C31-C32-C33
28	C	517	LMG	C7-C8-C9-O8
27	b	624	STE	C3-C4-C5-C6
27	b	625	STE	C2-C3-C4-C5
28	M	101	LMG	C30-C31-C32-C33
28	c	524	LMG	C31-C32-C33-C34
30	C	522	DGD	C5A-C6A-C7A-C8A
30	h	102	DGD	C8B-C9B-CAB-CBB
29	l	101	SQD	C23-C24-C25-C26
23	c	510	CLA	C4-C3-C5-C6
23	c	510	CLA	C2-C3-C5-C6
28	B	620	LMG	C14-C15-C16-C17
28	a	415	LMG	C11-C12-C13-C14
27	C	516	STE	C5-C6-C7-C8
27	D	414	STE	C14-C15-C16-C17
28	D	408	LMG	C13-C14-C15-C16
28	b	621	LMG	C14-C15-C16-C17
28	c	523	LMG	C31-C32-C33-C34
30	c	520	DGD	CAB-CBB-CCB-CDB
30	c	521	DGD	C4B-C5B-C6B-C7B
33	d	408	LHG	C27-C28-C29-C30
23	C	513	CLA	C16-C17-C18-C19
23	c	506	CLA	C16-C17-C18-C20
23	c	512	CLA	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	b	620	SQD	C10-C11-C12-C13
30	c	519	DGD	C4B-C5B-C6B-C7B
33	D	412	LHG	O2-C2-C3-O3
23	C	509	CLA	C3-C5-C6-C7
28	b	623	LMG	C39-C40-C41-C42
30	c	520	DGD	C1B-C2B-C3B-C4B
27	B	623	STE	C5-C6-C7-C8
27	H	103	STE	C13-C14-C15-C16
27	I	102	STE	C7-C8-C9-C10
27	t	103	STE	C4-C5-C6-C7
27	a	417	STE	C3-C4-C5-C6
27	d	412	STE	C12-C13-C14-C15
27	j	101	STE	C6-C7-C8-C9
28	a	415	LMG	C13-C14-C15-C16
28	b	623	LMG	C33-C34-C35-C36
33	a	413	LHG	C24-C25-C26-C27
23	b	602	CLA	C13-C15-C16-C17
23	c	505	CLA	C15-C16-C17-C18
30	C	521	DGD	C4B-C5B-C6B-C7B
23	B	606	CLA	C16-C17-C18-C20
25	B	617	BCR	C1-C6-C7-C8
25	B	617	BCR	C5-C6-C7-C8
25	c	514	BCR	C1-C6-C7-C8
25	c	514	BCR	C5-C6-C7-C8
29	A	412	SQD	C26-C27-C28-C29
27	b	622	STE	C3-C4-C5-C6
29	l	101	SQD	C25-C26-C27-C28
33	E	101	LHG	C29-C30-C31-C32
33	L	101	LHG	C27-C28-C29-C30
30	c	520	DGD	O6E-C5E-C6E-O5E
27	C	528	STE	C12-C13-C14-C15
29	b	620	SQD	C30-C31-C32-C33
28	d	409	LMG	O6-C5-C6-O5
27	a	416	STE	C4-C5-C6-C7
27	b	624	STE	C15-C16-C17-C18
27	x	102	STE	C5-C6-C7-C8
28	A	411	LMG	C13-C14-C15-C16
28	D	409	LMG	C30-C31-C32-C33
28	D	409	LMG	C35-C36-C37-C38
28	M	101	LMG	C39-C40-C41-C42
30	c	519	DGD	C5B-C6B-C7B-C8B
33	D	410	LHG	C30-C31-C32-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	D	407	PL9	C45-C44-C46-C47
23	b	608	CLA	O1D-CGD-O2D-CED
23	B	602	CLA	C11-C12-C13-C15
23	B	604	CLA	C11-C10-C8-C7
23	C	509	CLA	C11-C10-C8-C7
23	C	512	CLA	C11-C12-C13-C15
23	a	408	CLA	C11-C10-C8-C7
23	b	601	CLA	C6-C7-C8-C10
23	b	602	CLA	C6-C7-C8-C10
23	h	101	CLA	C11-C12-C13-C15
28	c	518	LMG	O10-C28-O8-C9
27	e	102	STE	C11-C12-C13-C14
28	M	101	LMG	C33-C34-C35-C36
29	A	412	SQD	C32-C33-C34-C35
29	F	102	SQD	C29-C30-C31-C32
23	D	405	CLA	C16-C17-C18-C20
28	M	101	LMG	O9-C10-O7-C8
28	b	623	LMG	O9-C10-O7-C8
28	c	523	LMG	O9-C10-O7-C8
23	C	513	CLA	CBA-CGA-O2A-C1
30	c	519	DGD	C2A-C1A-O1G-C1G
27	A	416	STE	C2-C3-C4-C5
27	e	103	STE	C11-C12-C13-C14
29	a	414	SQD	C33-C34-C35-C36
30	C	522	DGD	C6B-C7B-C8B-C9B
33	d	406	LHG	C10-C11-C12-C13
33	d	407	LHG	C18-C19-C20-C21
23	C	505	CLA	C10-C11-C12-C13
23	C	507	CLA	C13-C15-C16-C17
23	b	612	CLA	C10-C11-C12-C13
28	D	408	LMG	C16-C17-C18-C19
28	M	101	LMG	C16-C17-C18-C19
28	b	621	LMG	C16-C17-C18-C19
29	A	412	SQD	C11-C10-C9-C8
28	c	524	LMG	C10-C11-C12-C13
23	c	509	CLA	C13-C15-C16-C17
28	M	101	LMG	C34-C35-C36-C37
28	c	523	LMG	C30-C31-C32-C33
30	C	522	DGD	C6A-C7A-C8A-C9A
27	Z	101	STE	C10-C11-C12-C13
27	e	102	STE	C14-C15-C16-C17
28	D	409	LMG	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	a	414	SQD	C31-C32-C33-C34
33	a	413	LHG	C11-C12-C13-C14
25	d	404	BCR	C22-C23-C24-C25
23	B	602	CLA	C16-C17-C18-C20
23	c	509	CLA	O1D-CGD-O2D-CED
27	A	416	STE	C7-C8-C9-C10
27	E	104	STE	C9-C10-C11-C12
27	m	102	STE	C11-C10-C9-C8
29	a	414	SQD	C11-C10-C9-C8
29	f	102	SQD	C29-C30-C31-C32
30	C	521	DGD	C4A-C5A-C6A-C7A
30	c	521	DGD	C8A-C9A-CAA-CBA
30	h	102	DGD	CBA-CCA-CDA-CEA
33	E	101	LHG	C23-C24-C25-C26
28	b	621	LMG	C11-C10-O7-C8
25	d	404	BCR	C18-C19-C20-C21
27	B	621	STE	C10-C11-C12-C13
27	C	529	STE	C7-C8-C9-C10
30	A	414	DGD	C9B-CAB-CBB-CCB
33	D	412	LHG	C25-C26-C27-C28
23	B	607	CLA	C15-C16-C17-C18
28	D	409	LMG	C31-C32-C33-C34
28	M	101	LMG	C17-C18-C19-C20
30	A	414	DGD	C4A-C5A-C6A-C7A
33	l	102	LHG	C29-C30-C31-C32
28	b	619	LMG	O9-C10-O7-C8
27	d	410	STE	C2-C3-C4-C5
29	a	414	SQD	C15-C16-C17-C18
33	E	101	LHG	C24-C25-C26-C27
29	f	102	SQD	C2-C1-O6-C44
30	c	520	DGD	C2E-C1E-O5D-C6D
28	a	415	LMG	O7-C8-C9-O8
28	c	523	LMG	O7-C8-C9-O8
28	C	517	LMG	O6-C5-C6-O5
28	A	411	LMG	C33-C34-C35-C36
29	l	101	SQD	C9-C10-C11-C12
33	D	410	LHG	C32-C33-C34-C35
23	B	602	CLA	C13-C15-C16-C17
26	d	405	PL9	C15-C14-C16-C17
23	B	609	CLA	C2-C3-C5-C6
26	a	410	PL9	C18-C19-C21-C22
26	a	410	PL9	C23-C24-C26-C27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	b	627	STE	C13-C14-C15-C16
29	l	101	SQD	C11-C12-C13-C14
23	B	602	CLA	C11-C12-C13-C14
23	B	604	CLA	C11-C10-C8-C9
23	C	508	CLA	C11-C10-C8-C9
23	a	408	CLA	C6-C7-C8-C9
23	b	601	CLA	C6-C7-C8-C9
23	d	403	CLA	C14-C13-C15-C16
23	h	101	CLA	C11-C12-C13-C14
28	D	409	LMG	O6-C5-C6-O5
28	B	620	LMG	C30-C31-C32-C33
30	c	520	DGD	C7B-C8B-C9B-CAB
23	C	512	CLA	C3-C5-C6-C7
29	f	102	SQD	C34-C35-C36-C37
30	C	523	DGD	CAB-CBB-CCB-CDB
33	d	406	LHG	C32-C33-C34-C35
23	B	605	CLA	C8-C10-C11-C12
28	c	523	LMG	C16-C17-C18-C19
28	c	523	LMG	C41-C42-C43-C44
30	C	523	DGD	C9A-CAA-CBA-CCA
30	H	102	DGD	CBA-CCA-CDA-CEA
25	x	101	BCR	C11-C12-C13-C14
23	C	508	CLA	C1A-C2A-CAA-CBA
23	c	513	CLA	C1A-C2A-CAA-CBA
23	B	602	CLA	C16-C17-C18-C19
23	c	506	CLA	C16-C17-C18-C19
33	L	101	LHG	O9-C7-O7-C5
28	C	524	LMG	C18-C19-C20-C21
23	B	612	CLA	C10-C11-C12-C13
33	E	101	LHG	C17-C18-C19-C20
28	b	621	LMG	C28-C29-C30-C31
28	d	409	LMG	C30-C31-C32-C33
33	D	410	LHG	C11-C10-C9-C8
33	L	101	LHG	O6-C4-C5-C6
30	c	520	DGD	C5A-C6A-C7A-C8A
27	c	516	STE	C7-C8-C9-C10
30	C	523	DGD	C5A-C6A-C7A-C8A
28	c	523	LMG	O6-C5-C6-O5
23	C	505	CLA	C15-C16-C17-C18
23	b	603	CLA	C16-C17-C18-C19
23	b	606	CLA	C16-C17-C18-C19
27	E	104	STE	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	m	102	STE	C14-C15-C16-C17
28	a	415	LMG	C30-C31-C32-C33
27	l	103	STE	C11-C10-C9-C8
27	m	101	STE	C2-C3-C4-C5
28	c	522	LMG	C16-C17-C18-C19
28	c	523	LMG	C35-C36-C37-C38
29	A	412	SQD	C11-C12-C13-C14
30	H	102	DGD	CCA-CDA-CEA-CFA
27	A	416	STE	C10-C11-C12-C13
28	b	623	LMG	C29-C30-C31-C32
28	c	522	LMG	C31-C32-C33-C34
33	D	412	LHG	C1-C2-C3-O3
27	d	412	STE	C11-C12-C13-C14
29	F	102	SQD	C32-C33-C34-C35
30	c	519	DGD	C5A-C6A-C7A-C8A
23	b	606	CLA	C8-C10-C11-C12
28	b	623	LMG	C23-C24-C25-C26
30	C	521	DGD	CAB-CBB-CCB-CDB
27	C	528	STE	C7-C8-C9-C10
27	D	414	STE	C10-C11-C12-C13
27	E	104	STE	C10-C11-C12-C13
27	e	104	STE	C4-C5-C6-C7
28	b	621	LMG	C19-C20-C21-C22
29	b	620	SQD	C26-C27-C28-C29
30	c	519	DGD	C7A-C8A-C9A-CAA
33	a	413	LHG	C11-C10-C9-C8
33	l	102	LHG	C17-C18-C19-C20
23	c	511	CLA	C16-C17-C18-C19
27	b	622	STE	C7-C8-C9-C10
28	C	517	LMG	O1-C7-C8-C9
28	a	415	LMG	C7-C8-C9-O8
28	b	623	LMG	O1-C7-C8-C9
28	c	523	LMG	C7-C8-C9-O8
29	a	412	SQD	C44-C45-C46-O48
29	a	414	SQD	O6-C44-C45-C46
29	l	101	SQD	O6-C44-C45-C46
30	A	414	DGD	C1G-C2G-C3G-O3G
33	a	413	LHG	C4-C5-C6-O8
28	a	415	LMG	O6-C5-C6-O5
23	B	606	CLA	C8-C10-C11-C12
23	C	510	CLA	C10-C11-C12-C13
23	c	508	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	B	620	LMG	C33-C34-C35-C36
28	a	415	LMG	C8-C7-O1-C1
30	C	522	DGD	C2G-C3G-O3G-C1D
30	C	522	DGD	C5D-C6D-O5D-C1E
30	c	520	DGD	C2G-C3G-O3G-C1D
30	c	520	DGD	C5D-C6D-O5D-C1E
27	C	527	STE	C15-C16-C17-C18
28	M	101	LMG	C38-C39-C40-C41
29	a	412	SQD	C28-C29-C30-C31
33	d	408	LHG	C25-C26-C27-C28
23	b	603	CLA	C15-C16-C17-C18
27	C	526	STE	C5-C6-C7-C8
27	C	528	STE	C10-C11-C12-C13
27	e	104	STE	C6-C7-C8-C9
28	b	623	LMG	C30-C31-C32-C33
30	C	521	DGD	C5B-C6B-C7B-C8B
33	d	406	LHG	C28-C29-C30-C31
30	H	102	DGD	O2G-C1B-C2B-C3B
28	c	522	LMG	C10-C11-C12-C13
23	b	610	CLA	C10-C11-C12-C13
23	c	507	CLA	C8-C10-C11-C12
27	A	415	STE	C11-C12-C13-C14
27	B	622	STE	C2-C3-C4-C5
27	i	102	STE	C7-C8-C9-C10
33	L	101	LHG	C31-C32-C33-C34
27	A	410	STE	C4-C5-C6-C7
27	D	414	STE	C13-C14-C15-C16
30	H	102	DGD	C3B-C4B-C5B-C6B
27	j	101	STE	C4-C5-C6-C7
30	c	520	DGD	C9A-CAA-CBA-CCA
28	c	523	LMG	C11-C10-O7-C8
27	b	622	STE	C15-C16-C17-C18
27	c	516	STE	C2-C3-C4-C5
25	K	101	BCR	C20-C21-C22-C37
30	c	519	DGD	O6E-C5E-C6E-O5E
30	c	519	DGD	O6D-C5D-C6D-O5D
23	C	510	CLA	C4-C3-C5-C6
26	A	409	PL9	C15-C14-C16-C17
26	d	405	PL9	C45-C44-C46-C47
27	B	621	STE	C2-C3-C4-C5
28	B	620	LMG	C13-C14-C15-C16
23	C	510	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	D	412	LHG	C23-C24-C25-C26
28	b	623	LMG	C29-C28-O8-C9
27	H	103	STE	C2-C3-C4-C5
27	m	102	STE	C4-C5-C6-C7
23	B	616	CLA	C10-C11-C12-C13
23	b	614	CLA	C13-C15-C16-C17
23	b	615	CLA	C10-C11-C12-C13
23	c	513	CLA	C5-C6-C7-C8
27	t	103	STE	C10-C11-C12-C13
28	C	517	LMG	C17-C18-C19-C20
30	C	521	DGD	CDA-CEA-CFA-CGA
28	D	408	LMG	C7-C8-O7-C10
28	b	623	LMG	C9-C8-O7-C10
23	B	616	CLA	C2-C1-O2A-CGA
27	J	101	STE	C6-C7-C8-C9
27	a	416	STE	C1-C2-C3-C4
27	b	627	STE	C11-C12-C13-C14
28	b	623	LMG	C40-C41-C42-C43
33	d	406	LHG	C30-C31-C32-C33
27	I	101	STE	C9-C10-C11-C12
27	I	102	STE	C4-C5-C6-C7
27	a	417	STE	C2-C3-C4-C5
27	b	622	STE	C9-C10-C11-C12
27	d	410	STE	C6-C7-C8-C9
29	b	620	SQD	C11-C10-C9-C8
30	C	521	DGD	C8B-C9B-CAB-CBB
33	E	101	LHG	C14-C15-C16-C17
27	B	621	STE	C12-C13-C14-C15
27	l	103	STE	C3-C4-C5-C6
28	M	101	LMG	C13-C14-C15-C16
23	B	605	CLA	C16-C17-C18-C19
23	D	405	CLA	C16-C17-C18-C19
23	c	511	CLA	C16-C17-C18-C20
27	A	417	STE	C9-C10-C11-C12
27	e	102	STE	C15-C16-C17-C18
30	H	102	DGD	C7A-C8A-C9A-CAA
23	C	513	CLA	O1A-CGA-O2A-C1
28	c	522	LMG	C17-C18-C19-C20
29	a	414	SQD	C25-C26-C27-C28
33	d	407	LHG	C12-C13-C14-C15
23	C	509	CLA	C13-C15-C16-C17
25	x	101	BCR	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	D	408	LMG	C2-C1-O1-C7
28	A	411	LMG	O1-C7-C8-O7
29	a	412	SQD	O47-C45-C46-O48
30	A	414	DGD	O2G-C2G-C3G-O3G
33	E	101	LHG	O7-C5-C6-O8
28	c	523	LMG	C15-C16-C17-C18
28	c	522	LMG	O9-C10-O7-C8
28	c	524	LMG	O9-C10-O7-C8
30	A	414	DGD	O1A-C1A-O1G-C1G
23	c	501	CLA	O1D-CGD-O2D-CED
27	A	416	STE	C12-C13-C14-C15
27	l	103	STE	C1-C2-C3-C4
28	M	101	LMG	C20-C21-C22-C23
23	C	505	CLA	C4-C3-C5-C6
26	a	410	PL9	C22-C23-C24-C25
28	c	518	LMG	C31-C32-C33-C34
23	c	505	CLA	C13-C15-C16-C17
23	C	508	CLA	C12-C13-C15-C16
23	C	513	CLA	C11-C10-C8-C7
23	a	405	CLA	C12-C13-C15-C16
23	a	408	CLA	C6-C7-C8-C10
23	b	603	CLA	C11-C12-C13-C15
23	b	605	CLA	C6-C7-C8-C10
23	b	605	CLA	C12-C13-C15-C16
23	b	606	CLA	C6-C7-C8-C10
23	b	606	CLA	C11-C12-C13-C15
23	b	614	CLA	C11-C12-C13-C15
23	c	505	CLA	C6-C7-C8-C10
23	c	506	CLA	C11-C12-C13-C15
23	c	510	CLA	C11-C10-C8-C7
23	d	402	CLA	C6-C7-C8-C10
23	d	403	CLA	C12-C13-C15-C16
23	C	506	CLA	C3-C5-C6-C7
28	d	409	LMG	C35-C36-C37-C38
23	B	604	CLA	C14-C13-C15-C16
23	B	612	CLA	C14-C13-C15-C16
23	C	506	CLA	C14-C13-C15-C16
23	C	512	CLA	C11-C12-C13-C14
23	D	404	CLA	C11-C12-C13-C14
23	D	405	CLA	C11-C10-C8-C9
23	a	405	CLA	C14-C13-C15-C16
23	b	602	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	603	CLA	C11-C12-C13-C14
23	b	614	CLA	C11-C12-C13-C14
23	c	506	CLA	C11-C12-C13-C14
23	c	513	CLA	C11-C12-C13-C14
23	c	513	CLA	C14-C13-C15-C16
27	x	102	STE	C10-C11-C12-C13
28	D	408	LMG	C31-C32-C33-C34
23	C	513	CLA	C10-C11-C12-C13
27	E	102	STE	C7-C8-C9-C10
28	D	409	LMG	C39-C40-C41-C42
23	b	603	CLA	C16-C17-C18-C20
27	T	102	STE	C10-C11-C12-C13
27	l	103	STE	C15-C16-C17-C18
33	D	412	LHG	C17-C18-C19-C20
27	A	416	STE	C11-C12-C13-C14
33	D	410	LHG	C13-C14-C15-C16
23	D	405	CLA	C10-C11-C12-C13
29	A	413	SQD	C26-C27-C28-C29
29	a	412	SQD	C11-C12-C13-C14
30	H	102	DGD	CDB-CEB-CFB-CGB
27	T	102	STE	C6-C7-C8-C9
28	c	522	LMG	C28-C29-C30-C31
29	a	412	SQD	C23-C24-C25-C26
28	D	408	LMG	C39-C40-C41-C42
28	c	522	LMG	C39-C40-C41-C42
30	c	520	DGD	O6E-C1E-O5D-C6D
33	E	101	LHG	O6-C4-C5-C6
33	l	102	LHG	O6-C4-C5-C6
23	B	615	CLA	C3-C5-C6-C7
30	H	102	DGD	C9B-CAB-CBB-CCB
29	b	620	SQD	C7-C8-C9-C10
27	J	101	STE	C5-C6-C7-C8
29	b	620	SQD	C17-C18-C19-C20
33	L	101	LHG	C11-C10-C9-C8
33	l	102	LHG	C16-C17-C18-C19
23	C	504	CLA	C2-C3-C5-C6
23	C	505	CLA	C2-C3-C5-C6
26	D	407	PL9	C43-C44-C46-C47
33	a	413	LHG	C7-C8-C9-C10
27	M	102	STE	C6-C7-C8-C9
30	c	521	DGD	CBA-CCA-CDA-CEA
23	b	613	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	e	104	STE	C11-C10-C9-C8
27	D	413	STE	C3-C4-C5-C6
28	a	415	LMG	C22-C23-C24-C25
30	H	102	DGD	C4A-C5A-C6A-C7A
28	c	522	LMG	C4-C5-C6-O5
23	a	408	CLA	CBA-CGA-O2A-C1
30	A	414	DGD	O6D-C5D-C6D-O5D
27	Z	101	STE	C11-C12-C13-C14
30	C	521	DGD	CBA-CCA-CDA-CEA
23	C	513	CLA	C8-C10-C11-C12
28	c	523	LMG	C29-C30-C31-C32
28	d	409	LMG	C37-C38-C39-C40
27	b	626	STE	C1-C2-C3-C4
28	b	623	LMG	C37-C38-C39-C40
28	d	409	LMG	C38-C39-C40-C41
29	a	412	SQD	C16-C17-C18-C19
33	d	406	LHG	C17-C18-C19-C20
33	d	407	LHG	C19-C20-C21-C22
23	c	513	CLA	CBA-CGA-O2A-C1
27	D	414	STE	C15-C16-C17-C18
30	c	521	DGD	CAB-CBB-CCB-CDB
23	C	508	CLA	C10-C11-C12-C13
23	b	611	CLA	C10-C11-C12-C13
28	b	619	LMG	C7-C8-C9-O8
33	E	101	LHG	C4-C5-C6-O8
28	C	517	LMG	C16-C17-C18-C19
28	b	623	LMG	C32-C33-C34-C35
28	c	524	LMG	C29-C30-C31-C32
29	a	412	SQD	C27-C28-C29-C30
23	C	513	CLA	O2A-C1-C2-C3
23	c	509	CLA	CAA-CBA-CGA-O2A
27	Z	101	STE	C9-C10-C11-C12
28	a	415	LMG	C35-C36-C37-C38
28	d	409	LMG	C34-C35-C36-C37
27	T	102	STE	C13-C14-C15-C16
29	f	102	SQD	C24-C25-C26-C27
30	c	519	DGD	C8A-C9A-CAA-CBA
23	c	509	CLA	C4-C3-C5-C6
23	B	613	CLA	C16-C17-C18-C20
23	c	503	CLA	C16-C17-C18-C19
23	d	403	CLA	C16-C17-C18-C19
23	d	403	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	B	623	STE	C11-C10-C9-C8
27	E	102	STE	C6-C7-C8-C9
27	c	517	STE	C3-C4-C5-C6
27	b	627	STE	C10-C11-C12-C13
27	t	103	STE	C2-C3-C4-C5
27	t	103	STE	C12-C13-C14-C15
33	E	101	LHG	C16-C17-C18-C19
23	c	507	CLA	O1D-CGD-O2D-CED
27	a	416	STE	C7-C8-C9-C10
30	h	102	DGD	CCB-CDB-CEB-CFB
33	d	408	LHG	O1-C1-C2-O2
23	a	408	CLA	C5-C6-C7-C8
29	A	412	SQD	C9-C10-C11-C12
30	c	521	DGD	C9B-CAB-CBB-CCB
33	a	413	LHG	O6-C4-C5-O7
28	b	621	LMG	O9-C10-O7-C8
27	C	516	STE	C7-C8-C9-C10
27	M	102	STE	C10-C11-C12-C13
29	F	102	SQD	C34-C35-C36-C37
27	Z	101	STE	C6-C7-C8-C9
27	b	622	STE	C14-C15-C16-C17
28	D	408	LMG	C34-C35-C36-C37
28	c	522	LMG	C37-C38-C39-C40
28	c	524	LMG	C38-C39-C40-C41
30	C	522	DGD	C9A-CAA-CBA-CCA
30	c	521	DGD	C5B-C6B-C7B-C8B
33	D	411	LHG	C11-C12-C13-C14
30	c	519	DGD	C4D-C5D-C6D-O5D
28	c	524	LMG	C37-C38-C39-C40
28	C	517	LMG	O1-C7-C8-O7
28	b	623	LMG	O1-C7-C8-O7
28	c	523	LMG	C29-C28-O8-C9
27	A	410	STE	C1-C2-C3-C4
27	C	528	STE	C5-C6-C7-C8
28	A	411	LMG	C35-C36-C37-C38
28	c	524	LMG	C14-C15-C16-C17
29	a	414	SQD	C29-C30-C31-C32
30	c	519	DGD	C6B-C7B-C8B-C9B
30	h	102	DGD	C3B-C4B-C5B-C6B
23	h	101	CLA	C16-C17-C18-C20
28	d	409	LMG	C15-C16-C17-C18
26	a	410	PL9	C9-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	B	622	STE	C7-C8-C9-C10
29	A	412	SQD	C25-C26-C27-C28
30	C	522	DGD	C9B-CAB-CBB-CCB
28	B	620	LMG	O9-C10-O7-C8
23	c	509	CLA	C2-C3-C5-C6
23	B	605	CLA	C6-C7-C8-C9
23	b	612	CLA	C6-C7-C8-C9
23	b	615	CLA	C6-C7-C8-C9
23	c	505	CLA	C6-C7-C8-C9
23	h	101	CLA	C6-C7-C8-C9
23	h	101	CLA	C11-C10-C8-C9
27	D	413	STE	C9-C10-C11-C12
30	A	414	DGD	CAB-CBB-CCB-CDB
33	L	101	LHG	C13-C14-C15-C16
33	l	102	LHG	C19-C20-C21-C22
33	D	411	LHG	C2-C3-O3-P
33	d	408	LHG	C2-C3-O3-P
27	Z	101	STE	C13-C14-C15-C16
27	t	102	STE	C4-C5-C6-C7
28	c	522	LMG	C12-C13-C14-C15
28	c	524	LMG	C19-C20-C21-C22
25	A	408	BCR	C23-C24-C25-C26
25	H	101	BCR	C23-C24-C25-C30
25	b	616	BCR	C1-C6-C7-C8
25	b	616	BCR	C5-C6-C7-C8
25	k	101	BCR	C23-C24-C25-C30
25	k	102	BCR	C1-C6-C7-C8
25	x	101	BCR	C23-C24-C25-C26
23	c	504	CLA	C5-C6-C7-C8
27	m	101	STE	C7-C8-C9-C10
28	b	621	LMG	C22-C23-C24-C25
25	A	408	BCR	C37-C22-C23-C24
25	c	515	BCR	C11-C12-C13-C35
27	z	101	STE	C5-C6-C7-C8
33	E	101	LHG	C34-C35-C36-C37
27	m	102	STE	C9-C10-C11-C12
23	B	615	CLA	C16-C17-C18-C19
23	b	612	CLA	C16-C17-C18-C19
28	M	101	LMG	C19-C20-C21-C22
30	C	521	DGD	C5A-C6A-C7A-C8A
23	B	602	CLA	C15-C16-C17-C18
28	a	415	LMG	C20-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	b	623	LMG	C16-C17-C18-C19
28	c	518	LMG	C16-C17-C18-C19
27	C	528	STE	C11-C10-C9-C8
27	M	102	STE	C7-C8-C9-C10
30	C	523	DGD	C3B-C4B-C5B-C6B
23	B	604	CLA	C11-C12-C13-C15
23	B	604	CLA	C12-C13-C15-C16
23	B	612	CLA	C12-C13-C15-C16
23	B	615	CLA	C12-C13-C15-C16
23	C	502	CLA	C11-C12-C13-C15
23	C	505	CLA	C12-C13-C15-C16
23	C	506	CLA	C12-C13-C15-C16
23	C	507	CLA	C11-C10-C8-C7
23	C	510	CLA	C11-C10-C8-C7
23	C	512	CLA	C11-C10-C8-C7
23	C	513	CLA	C12-C13-C15-C16
23	D	405	CLA	C11-C10-C8-C7
23	b	602	CLA	C11-C10-C8-C7
23	b	603	CLA	C11-C10-C8-C7
23	b	615	CLA	C11-C10-C8-C7
23	c	513	CLA	C11-C10-C8-C7
23	c	513	CLA	C12-C13-C15-C16
25	C	514	BCR	C15-C16-C17-C18
23	B	612	CLA	C16-C17-C18-C20
23	c	510	CLA	C16-C17-C18-C19
27	m	102	STE	C6-C7-C8-C9
30	c	519	DGD	C9B-CAB-CBB-CCB
23	D	405	CLA	C15-C16-C17-C18
28	b	623	LMG	C4-C5-C6-O5
29	A	413	SQD	C24-C25-C26-C27
29	f	102	SQD	C28-C29-C30-C31
29	f	102	SQD	C32-C33-C34-C35
25	B	617	BCR	C20-C21-C22-C37
25	D	406	BCR	C20-C21-C22-C37
25	K	101	BCR	C16-C17-C18-C36
25	b	616	BCR	C20-C21-C22-C37
25	k	101	BCR	C16-C17-C18-C36
25	t	101	BCR	C20-C21-C22-C37
28	A	411	LMG	C11-C12-C13-C14
30	C	522	DGD	CDB-CEB-CFB-CGB
23	B	610	CLA	C16-C17-C18-C19
30	c	521	DGD	C2A-C1A-O1G-C1G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	i	101	STE	C5-C6-C7-C8
27	t	103	STE	C7-C8-C9-C10
28	C	524	LMG	C37-C38-C39-C40
33	D	411	LHG	C26-C27-C28-C29
23	a	408	CLA	C10-C11-C12-C13
23	B	616	CLA	CAD-CBD-CGD-O2D
23	C	501	CLA	CAD-CBD-CGD-O2D
23	C	503	CLA	CAD-CBD-CGD-O2D
23	C	510	CLA	CAD-CBD-CGD-O2D
23	C	513	CLA	CAD-CBD-CGD-O2D
23	b	602	CLA	CAD-CBD-CGD-O2D
23	c	503	CLA	CAD-CBD-CGD-O2D
24	a	407	PHO	CAD-CBD-CGD-O2D
29	l	101	SQD	C46-C45-O47-C7
27	A	410	STE	C3-C4-C5-C6
23	b	602	CLA	C5-C6-C7-C8
23	c	512	CLA	C5-C6-C7-C8
27	E	104	STE	C15-C16-C17-C18
33	D	412	LHG	C11-C12-C13-C14
23	B	613	CLA	C16-C17-C18-C19
23	B	612	CLA	C13-C15-C16-C17
27	t	102	STE	C6-C7-C8-C9
28	M	101	LMG	C7-C8-C9-O8
29	A	413	SQD	O6-C44-C45-C46
30	C	523	DGD	O1A-C1A-O1G-C1G
29	a	412	SQD	C8-C7-O47-C45
23	C	501	CLA	O1D-CGD-O2D-CED
28	D	409	LMG	C20-C21-C22-C23
30	h	102	DGD	C3A-C4A-C5A-C6A
23	c	510	CLA	C8-C10-C11-C12
23	a	408	CLA	O1A-CGA-O2A-C1
23	c	505	CLA	C16-C17-C18-C20
23	C	508	CLA	O1D-CGD-O2D-CED
23	B	601	CLA	CHA-CBD-CGD-O1D
23	B	601	CLA	CHA-CBD-CGD-O2D
23	B	607	CLA	CHA-CBD-CGD-O1D
23	B	610	CLA	CHA-CBD-CGD-O1D
23	C	502	CLA	CHA-CBD-CGD-O1D
23	C	502	CLA	CHA-CBD-CGD-O2D
23	C	508	CLA	CHA-CBD-CGD-O2D
23	b	613	CLA	CHA-CBD-CGD-O2D
23	c	502	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	c	502	CLA	CHA-CBD-CGD-O2D
23	c	504	CLA	CHA-CBD-CGD-O1D
23	c	504	CLA	CHA-CBD-CGD-O2D
23	c	507	CLA	CHA-CBD-CGD-O1D
23	c	507	CLA	CHA-CBD-CGD-O2D
23	c	508	CLA	CHA-CBD-CGD-O2D
23	c	513	CLA	O1A-CGA-O2A-C1
28	C	524	LMG	O10-C28-O8-C9
28	b	621	LMG	O10-C28-O8-C9
27	l	103	STE	C11-C12-C13-C14
33	D	412	LHG	C28-C29-C30-C31
33	d	407	LHG	C30-C31-C32-C33
28	M	101	LMG	O7-C8-C9-O8
27	A	416	STE	C4-C5-C6-C7
30	H	102	DGD	C8B-C9B-CAB-CBB
33	D	410	LHG	C29-C30-C31-C32
33	E	101	LHG	C15-C16-C17-C18
23	c	512	CLA	C13-C15-C16-C17
27	d	410	STE	C4-C5-C6-C7
33	D	411	LHG	C15-C16-C17-C18
33	D	411	LHG	C34-C35-C36-C37
33	E	101	LHG	C9-C10-C11-C12
30	C	521	DGD	C6A-C7A-C8A-C9A
23	C	506	CLA	C4-C3-C5-C6
27	H	103	STE	C5-C6-C7-C8
27	b	626	STE	C3-C4-C5-C6
33	l	102	LHG	C26-C27-C28-C29
27	j	102	STE	C13-C14-C15-C16
29	a	412	SQD	O49-C7-O47-C45
23	B	601	CLA	C11-C12-C13-C14
23	C	502	CLA	C11-C12-C13-C14
23	C	503	CLA	C11-C10-C8-C9
23	C	505	CLA	C14-C13-C15-C16
28	D	409	LMG	C33-C34-C35-C36
30	H	102	DGD	CAB-CBB-CCB-CDB
33	D	410	LHG	C17-C18-C19-C20
33	D	410	LHG	O1-C1-C2-C3
33	D	412	LHG	O1-C1-C2-C3
27	C	518	STE	C3-C4-C5-C6
28	b	623	LMG	C17-C18-C19-C20
30	C	521	DGD	C2B-C3B-C4B-C5B
23	B	614	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	e	101	STE	C13-C14-C15-C16
23	b	615	CLA	C2-C1-O2A-CGA
26	a	410	PL9	C32-C33-C34-C36
33	D	412	LHG	C33-C34-C35-C36
28	M	101	LMG	C22-C23-C24-C25
28	c	522	LMG	C30-C31-C32-C33
29	a	412	SQD	C12-C13-C14-C15
33	E	101	LHG	C10-C11-C12-C13
27	b	624	STE	C9-C10-C11-C12
27	i	101	STE	C7-C8-C9-C10
27	m	102	STE	C13-C14-C15-C16
30	c	520	DGD	CCA-CDA-CEA-CFA
33	D	410	LHG	C25-C26-C27-C28
23	C	504	CLA	C4-C3-C5-C6
23	c	512	CLA	C4-C3-C5-C6
33	E	101	LHG	C3-O3-P-O4
33	L	101	LHG	C4-O6-P-O5
33	d	406	LHG	C3-O3-P-O4
33	d	407	LHG	C4-O6-P-O5
23	B	612	CLA	C16-C17-C18-C19
23	B	615	CLA	C16-C17-C18-C20
23	c	503	CLA	C16-C17-C18-C20
28	b	621	LMG	C18-C19-C20-C21
29	F	102	SQD	C25-C26-C27-C28
30	c	520	DGD	CCB-CDB-CEB-CFB
33	L	101	LHG	O10-C23-O8-C6
24	d	401	PHO	C2C-C3C-CAC-CBC
27	H	103	STE	C7-C8-C9-C10
28	C	517	LMG	C11-C12-C13-C14
30	H	102	DGD	C5A-C6A-C7A-C8A
23	a	405	CLA	C16-C17-C18-C20
30	c	521	DGD	C3B-C4B-C5B-C6B
33	l	102	LHG	C35-C36-C37-C38
23	B	601	CLA	CAD-CBD-CGD-O1D
23	C	502	CLA	CAD-CBD-CGD-O1D
23	C	504	CLA	CAD-CBD-CGD-O1D
23	c	502	CLA	CAD-CBD-CGD-O1D
23	c	504	CLA	CAD-CBD-CGD-O1D
28	c	523	LMG	C10-C11-C12-C13
30	A	414	DGD	C4D-C5D-C6D-O5D
27	a	417	STE	C6-C7-C8-C9
30	C	521	DGD	C7B-C8B-C9B-CAB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	d	406	LHG	C15-C16-C17-C18
27	d	411	STE	C3-C4-C5-C6
33	d	408	LHG	C29-C30-C31-C32
23	B	613	CLA	C11-C12-C13-C15
23	B	613	CLA	C12-C13-C15-C16
23	B	614	CLA	C11-C12-C13-C15
23	C	509	CLA	C12-C13-C15-C16
23	D	405	CLA	C12-C13-C15-C16
23	a	406	CLA	C11-C10-C8-C7
23	c	508	CLA	C12-C13-C15-C16
23	c	512	CLA	C6-C7-C8-C10
23	h	101	CLA	C6-C7-C8-C10
26	d	405	PL9	C13-C14-C16-C17
33	E	101	LHG	O6-C4-C5-O7
33	L	101	LHG	O6-C4-C5-O7
33	l	102	LHG	O6-C4-C5-O7
27	e	103	STE	C10-C11-C12-C13
27	l	103	STE	C10-C11-C12-C13
29	A	412	SQD	C33-C34-C35-C36
29	b	620	SQD	C12-C13-C14-C15
27	M	103	STE	C3-C4-C5-C6
30	h	102	DGD	O2G-C1B-C2B-C3B
27	b	625	STE	C9-C10-C11-C12
28	c	518	LMG	C29-C30-C31-C32
33	D	410	LHG	C33-C34-C35-C36
28	a	415	LMG	C11-C10-O7-C8
33	D	412	LHG	C24-C25-C26-C27
27	I	101	STE	C6-C7-C8-C9
27	T	102	STE	C12-C13-C14-C15
27	c	517	STE	C5-C6-C7-C8
23	B	609	CLA	C13-C15-C16-C17
23	c	509	CLA	C8-C10-C11-C12
28	b	619	LMG	C1-C2-C3-C4
29	l	101	SQD	C44-C45-C46-O48
30	c	519	DGD	CDB-CEB-CFB-CGB
28	C	517	LMG	O7-C8-C9-O8
33	a	413	LHG	O7-C5-C6-O8
30	C	522	DGD	C4A-C5A-C6A-C7A
33	a	413	LHG	C19-C20-C21-C22
23	d	403	CLA	C10-C11-C12-C13
30	h	102	DGD	CBB-CCB-CDB-CEB
28	c	518	LMG	C30-C31-C32-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	H	102	DGD	C7B-C8B-C9B-CAB
28	c	524	LMG	C18-C19-C20-C21
29	A	413	SQD	C11-C12-C13-C14
23	B	604	CLA	C11-C12-C13-C14
23	B	615	CLA	C14-C13-C15-C16
23	C	510	CLA	C11-C10-C8-C9
23	C	513	CLA	C11-C10-C8-C9
23	C	513	CLA	C14-C13-C15-C16
23	D	405	CLA	C11-C12-C13-C14
23	a	406	CLA	C6-C7-C8-C9
23	b	603	CLA	C11-C10-C8-C9
23	b	606	CLA	C11-C12-C13-C14
23	b	615	CLA	C11-C10-C8-C9
23	c	513	CLA	C11-C10-C8-C9
23	d	402	CLA	C6-C7-C8-C9
23	a	405	CLA	C16-C17-C18-C19
29	F	102	SQD	C33-C34-C35-C36
29	b	620	SQD	C27-C28-C29-C30
23	b	613	CLA	C13-C15-C16-C17
29	b	620	SQD	C11-C12-C13-C14
29	A	412	SQD	C14-C15-C16-C17
30	H	102	DGD	C3A-C4A-C5A-C6A
33	d	407	LHG	C34-C35-C36-C37
25	B	617	BCR	C7-C8-C9-C34
23	B	607	CLA	C3-C5-C6-C7
27	E	104	STE	C5-C6-C7-C8
23	B	614	CLA	C16-C17-C18-C19
29	l	101	SQD	C13-C14-C15-C16
27	i	102	STE	C9-C10-C11-C12
28	A	411	LMG	O6-C5-C6-O5
23	c	512	CLA	C2-C3-C5-C6
23	B	605	CLA	C16-C17-C18-C20
23	d	402	CLA	C16-C17-C18-C20
27	C	525	STE	C4-C5-C6-C7
27	j	102	STE	C5-C6-C7-C8
24	d	401	PHO	C4C-C3C-CAC-CBC
28	a	415	LMG	C12-C13-C14-C15
30	C	523	DGD	CDB-CEB-CFB-CGB
27	T	102	STE	C7-C8-C9-C10
28	A	411	LMG	C9-C8-O7-C10
28	a	415	LMG	C7-C8-O7-C10
23	B	613	CLA	C2-C1-O2A-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	D	404	CLA	C2-C1-O2A-CGA
23	d	402	CLA	C2-C1-O2A-CGA
30	C	521	DGD	O6D-C5D-C6D-O5D
27	B	621	STE	C11-C12-C13-C14
33	d	406	LHG	C33-C34-C35-C36
33	E	101	LHG	C2-C3-O3-P
27	Z	101	STE	C4-C5-C6-C7
28	b	619	LMG	C12-C13-C14-C15
28	c	522	LMG	C34-C35-C36-C37
28	c	523	LMG	C14-C15-C16-C17
28	c	522	LMG	C29-C28-O8-C9
28	A	411	LMG	C29-C30-C31-C32
30	c	519	DGD	C4A-C5A-C6A-C7A
23	D	403	CLA	C16-C17-C18-C19
23	b	613	CLA	C16-C17-C18-C19
25	A	408	BCR	C23-C24-C25-C30
25	H	101	BCR	C23-C24-C25-C26
25	k	102	BCR	C5-C6-C7-C8
25	x	101	BCR	C23-C24-C25-C30
23	b	603	CLA	C2-C3-C5-C6
27	E	102	STE	C4-C5-C6-C7
33	D	412	LHG	C16-C17-C18-C19
28	a	415	LMG	C40-C41-C42-C43
23	B	610	CLA	C16-C17-C18-C20
23	c	510	CLA	C16-C17-C18-C20
23	d	402	CLA	C16-C17-C18-C19
30	C	522	DGD	CAB-CBB-CCB-CDB
29	l	101	SQD	O47-C45-C46-O48
28	D	409	LMG	C15-C16-C17-C18
33	d	406	LHG	C25-C26-C27-C28
23	c	508	CLA	C15-C16-C17-C18
28	A	411	LMG	O1-C7-C8-C9
26	a	410	PL9	C45-C44-C46-C47
23	B	606	CLA	C6-C7-C8-C10
23	C	505	CLA	C6-C7-C8-C10
23	C	506	CLA	C2-C3-C5-C6
23	c	502	CLA	C11-C12-C13-C15
23	c	505	CLA	C11-C10-C8-C7
27	E	102	STE	C2-C3-C4-C5
28	a	415	LMG	C14-C15-C16-C17
28	b	621	LMG	C37-C38-C39-C40
23	C	509	CLA	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	a	406	CLA	C11-C10-C8-C9
23	b	606	CLA	C6-C7-C8-C9
30	C	523	DGD	O6D-C5D-C6D-O5D
23	h	101	CLA	C5-C6-C7-C8
27	H	103	STE	C11-C12-C13-C14
28	c	523	LMG	C39-C40-C41-C42
30	c	520	DGD	C8B-C9B-CAB-CBB
28	b	621	LMG	C32-C33-C34-C35
23	B	601	CLA	C10-C11-C12-C13
25	c	515	BCR	C7-C8-C9-C10
27	C	528	STE	C13-C14-C15-C16
27	b	622	STE	C11-C10-C9-C8
28	a	415	LMG	C29-C28-O8-C9
33	D	411	LHG	C25-C26-C27-C28
27	z	101	STE	C6-C7-C8-C9
28	D	409	LMG	C22-C23-C24-C25
27	C	525	STE	C7-C8-C9-C10
27	C	527	STE	C13-C14-C15-C16
29	F	102	SQD	C24-C25-C26-C27
30	c	521	DGD	O6D-C5D-C6D-O5D
28	C	517	LMG	C12-C13-C14-C15
30	c	520	DGD	CAA-CBA-CCA-CDA
29	A	412	SQD	C30-C31-C32-C33
33	a	413	LHG	O6-C4-C5-C6
29	A	413	SQD	C23-C24-C25-C26
23	C	505	CLA	C8-C10-C11-C12
23	c	513	CLA	C15-C16-C17-C18
27	a	416	STE	C2-C3-C4-C5
28	a	415	LMG	C15-C16-C17-C18
26	a	410	PL9	C20-C19-C21-C22
23	c	503	CLA	C10-C11-C12-C13
27	i	101	STE	C2-C3-C4-C5
23	C	509	CLA	C2-C1-O2A-CGA
27	I	101	STE	C12-C13-C14-C15
28	D	409	LMG	C13-C14-C15-C16
28	a	415	LMG	C24-C25-C26-C27
28	c	523	LMG	C42-C43-C44-C45
27	b	625	STE	C7-C8-C9-C10
23	B	603	CLA	C2A-CAA-CBA-CGA
23	c	501	CLA	C2A-CAA-CBA-CGA
28	d	409	LMG	C39-C40-C41-C42
30	C	523	DGD	C7B-C8B-C9B-CAB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	H	102	DGD	CDA-CEA-CFA-CGA
30	h	102	DGD	O1B-C1B-C2B-C3B
28	b	621	LMG	C39-C40-C41-C42
23	C	502	CLA	C16-C17-C18-C20
29	a	414	SQD	C7-C8-C9-C10
30	C	521	DGD	C4D-C5D-C6D-O5D
23	b	603	CLA	C3-C5-C6-C7
26	a	410	PL9	C4-C3-C7-C8
23	c	502	CLA	C11-C12-C13-C14
23	c	510	CLA	C11-C12-C13-C14
23	c	511	CLA	C14-C13-C15-C16
27	c	516	STE	C6-C7-C8-C9
29	f	102	SQD	C33-C34-C35-C36
23	c	504	CLA	C10-C11-C12-C13
27	Z	101	STE	C5-C6-C7-C8
33	a	413	LHG	C12-C13-C14-C15
27	C	526	STE	C11-C10-C9-C8
27	H	103	STE	C11-C10-C9-C8
25	c	515	BCR	C11-C10-C9-C34
23	c	509	CLA	CAA-CBA-CGA-O1A
27	e	103	STE	C13-C14-C15-C16
30	H	102	DGD	CCB-CDB-CEB-CFB
23	c	512	CLA	O2A-C1-C2-C3
24	a	407	PHO	O2A-C1-C2-C3
30	c	519	DGD	O6E-C1E-O5D-C6D
30	C	522	DGD	C4B-C5B-C6B-C7B
25	D	406	BCR	C37-C22-C23-C24
28	D	408	LMG	C17-C18-C19-C20
30	H	102	DGD	C6B-C7B-C8B-C9B
30	c	520	DGD	C4A-C5A-C6A-C7A
23	b	609	CLA	C13-C15-C16-C17
23	c	513	CLA	C13-C15-C16-C17
28	C	517	LMG	C7-C8-O7-C10
23	c	508	CLA	C1A-C2A-CAA-CBA
23	c	511	CLA	C1A-C2A-CAA-CBA
27	D	414	STE	C11-C12-C13-C14
27	T	102	STE	C5-C6-C7-C8
28	B	620	LMG	C34-C35-C36-C37
23	B	613	CLA	C11-C10-C8-C7
23	b	611	CLA	C6-C7-C8-C10
23	b	611	CLA	C11-C10-C8-C7
23	b	607	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	613	CLA	C3-C5-C6-C7
29	b	620	SQD	C29-C30-C31-C32
33	D	410	LHG	C4-O6-P-O3
28	c	518	LMG	O8-C28-C29-C30
27	Z	101	STE	C2-C3-C4-C5
23	B	615	CLA	C8-C10-C11-C12
23	b	604	CLA	C5-C6-C7-C8
23	c	506	CLA	C15-C16-C17-C18
27	M	102	STE	C9-C10-C11-C12
23	B	603	CLA	C15-C16-C17-C18
30	C	521	DGD	C7A-C8A-C9A-CAA
25	k	101	BCR	C11-C10-C9-C8
27	C	526	STE	C6-C7-C8-C9
28	D	408	LMG	C30-C31-C32-C33
28	a	415	LMG	C34-C35-C36-C37
23	b	611	CLA	C3-C5-C6-C7
28	A	411	LMG	C17-C18-C19-C20
28	c	522	LMG	O6-C1-O1-C7
23	h	101	CLA	C4-C3-C5-C6
23	A	404	CLA	C2-C1-O2A-CGA
33	D	411	LHG	C32-C33-C34-C35
23	b	604	CLA	C10-C11-C12-C13
23	b	611	CLA	C11-C10-C8-C9
23	c	508	CLA	C11-C10-C8-C9
30	C	523	DGD	CCA-CDA-CEA-CFA
33	d	408	LHG	C35-C36-C37-C38
23	C	512	CLA	C2A-CAA-CBA-CGA
23	b	609	CLA	C2A-CAA-CBA-CGA
25	A	408	BCR	C1-C6-C7-C8
25	K	101	BCR	C23-C24-C25-C30
27	A	417	STE	C11-C12-C13-C14
27	C	525	STE	C6-C7-C8-C9
23	C	512	CLA	C8-C10-C11-C12
27	Z	101	STE	C3-C4-C5-C6
27	e	103	STE	C14-C15-C16-C17
28	a	415	LMG	C31-C32-C33-C34
27	C	519	STE	C2-C3-C4-C5
23	c	513	CLA	C4-C3-C5-C6
23	C	510	CLA	C15-C16-C17-C18
23	C	512	CLA	C10-C11-C12-C13
30	h	102	DGD	C5B-C6B-C7B-C8B
28	c	524	LMG	C40-C41-C42-C43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	c	520	DGD	CBA-CCA-CDA-CEA
28	b	623	LMG	C8-C7-O1-C1
27	b	625	STE	C6-C7-C8-C9
27	C	529	STE	C11-C12-C13-C14
27	M	102	STE	C3-C4-C5-C6
30	A	414	DGD	C3B-C4B-C5B-C6B
30	c	519	DGD	CDA-CEA-CFA-CGA
23	a	408	CLA	C4-C3-C5-C6
23	a	406	CLA	C6-C7-C8-C10
23	b	602	CLA	C12-C13-C15-C16
23	d	402	CLA	C11-C12-C13-C15
26	A	409	PL9	C18-C19-C21-C22
26	d	405	PL9	C43-C44-C46-C47
23	C	507	CLA	C5-C6-C7-C8
33	D	412	LHG	O1-C1-C2-O2
28	A	411	LMG	C37-C38-C39-C40
30	A	414	DGD	C9A-CAA-CBA-CCA
30	H	102	DGD	C5B-C6B-C7B-C8B
28	b	619	LMG	C9-C8-O7-C10
27	t	102	STE	C2-C3-C4-C5
29	A	412	SQD	C15-C16-C17-C18
29	a	414	SQD	C35-C36-C37-C38
30	C	523	DGD	C6A-C7A-C8A-C9A
30	c	520	DGD	CDA-CEA-CFA-CGA
27	j	101	STE	C5-C6-C7-C8
23	b	613	CLA	C16-C17-C18-C20
23	b	609	CLA	C4C-C3C-CAC-CBC
25	C	515	BCR	C20-C21-C22-C37
25	a	409	BCR	C35-C13-C14-C15
25	x	101	BCR	C11-C10-C9-C34
33	E	101	LHG	C27-C28-C29-C30
28	d	409	LMG	O7-C10-C11-C12
33	D	411	LHG	O8-C23-C24-C25
23	B	611	CLA	C6-C7-C8-C9
23	C	505	CLA	C6-C7-C8-C9
23	C	508	CLA	C14-C13-C15-C16
23	D	405	CLA	C14-C13-C15-C16
23	c	511	CLA	C11-C10-C8-C9
33	D	410	LHG	C34-C35-C36-C37
28	b	623	LMG	C11-C12-C13-C14
23	B	604	CLA	CAD-CBD-CGD-O2D
23	B	610	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	512	CLA	CAD-CBD-CGD-O2D
23	b	603	CLA	CAD-CBD-CGD-O2D
23	b	604	CLA	CAD-CBD-CGD-O2D
23	b	609	CLA	CAD-CBD-CGD-O2D
23	b	611	CLA	CAD-CBD-CGD-O2D
23	c	501	CLA	CAD-CBD-CGD-O2D
23	c	509	CLA	CAD-CBD-CGD-O2D
23	c	512	CLA	CAD-CBD-CGD-O2D
33	D	410	LHG	O9-C7-O7-C5
33	d	407	LHG	C15-C16-C17-C18
27	D	413	STE	C11-C10-C9-C8
27	a	417	STE	C4-C5-C6-C7
28	M	101	LMG	C12-C13-C14-C15
29	l	101	SQD	C11-C10-C9-C8
29	A	412	SQD	O47-C7-C8-C9
27	I	102	STE	C6-C7-C8-C9
28	C	524	LMG	C10-C11-C12-C13
27	A	415	STE	C13-C14-C15-C16
27	C	529	STE	C5-C6-C7-C8
27	j	102	STE	C1-C2-C3-C4
28	C	517	LMG	C15-C16-C17-C18
23	c	513	CLA	C2-C3-C5-C6
26	A	409	PL9	C13-C14-C16-C17
26	a	410	PL9	C43-C44-C46-C47
33	l	102	LHG	C11-C12-C13-C14
25	C	520	BCR	C17-C18-C19-C20
27	z	101	STE	C2-C3-C4-C5
23	A	404	CLA	C2C-C3C-CAC-CBC
23	B	604	CLA	C2C-C3C-CAC-CBC
23	a	411	CLA	C2C-C3C-CAC-CBC
23	b	609	CLA	C2C-C3C-CAC-CBC
23	d	402	CLA	C2C-C3C-CAC-CBC
28	c	522	LMG	O1-C7-C8-C9
30	h	102	DGD	C1G-C2G-C3G-O3G
27	A	417	STE	C11-C10-C9-C8
27	l	103	STE	C4-C5-C6-C7
23	B	604	CLA	O2A-C1-C2-C3
23	C	509	CLA	O2A-C1-C2-C3
23	D	405	CLA	O2A-C1-C2-C3
24	D	402	PHO	O2A-C1-C2-C3
28	c	523	LMG	C34-C35-C36-C37
23	h	101	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	C	527	STE	C11-C12-C13-C14
29	F	102	SQD	C26-C27-C28-C29
28	c	518	LMG	C10-C11-C12-C13
29	l	101	SQD	O48-C23-C24-C25
23	A	405	CLA	CHA-CBD-CGD-O2D
23	C	504	CLA	CHA-CBD-CGD-O1D
23	C	507	CLA	CHA-CBD-CGD-O2D
23	D	403	CLA	CHA-CBD-CGD-O1D
23	D	403	CLA	CHA-CBD-CGD-O2D
23	a	406	CLA	CHA-CBD-CGD-O1D
23	a	406	CLA	CHA-CBD-CGD-O2D
23	b	606	CLA	CHA-CBD-CGD-O1D
23	h	101	CLA	CHA-CBD-CGD-O2D
24	A	406	PHO	CHA-CBD-CGD-O2D
28	C	524	LMG	C12-C13-C14-C15
23	b	613	CLA	C10-C11-C12-C13
23	B	613	CLA	CAA-CBA-CGA-O2A
28	D	409	LMG	O7-C10-C11-C12
29	a	412	SQD	C10-C11-C12-C13
28	b	621	LMG	C12-C13-C14-C15
23	c	510	CLA	CAA-CBA-CGA-O2A
28	c	522	LMG	O6-C5-C6-O5
27	j	101	STE	C3-C4-C5-C6
26	d	405	PL9	C47-C48-C49-C50
33	D	410	LHG	C16-C17-C18-C19
23	B	611	CLA	C6-C7-C8-C10
23	c	501	CLA	C11-C12-C13-C15
23	d	403	CLA	C11-C12-C13-C15
23	h	101	CLA	C2-C3-C5-C6
26	D	407	PL9	C28-C29-C31-C32
26	A	409	PL9	C4-C3-C7-C8
28	c	523	LMG	C33-C34-C35-C36
23	B	612	CLA	C11-C10-C8-C9
23	B	613	CLA	C14-C13-C15-C16
23	B	614	CLA	C11-C12-C13-C14
23	C	511	CLA	C6-C7-C8-C9
23	b	602	CLA	C14-C13-C15-C16
23	c	503	CLA	C11-C10-C8-C9
27	b	627	STE	C15-C16-C17-C18
33	l	102	LHG	C15-C16-C17-C18
30	c	519	DGD	C3B-C4B-C5B-C6B
28	C	517	LMG	C11-C10-O7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	614	CLA	C2A-CAA-CBA-CGA
26	d	405	PL9	C11-C12-C13-C14
30	C	521	DGD	O1B-C1B-C2B-C3B
30	c	520	DGD	O1B-C1B-C2B-C3B
27	B	623	STE	C9-C10-C11-C12
28	b	621	LMG	O8-C28-C29-C30
28	D	408	LMG	C11-C12-C13-C14
27	B	623	STE	C4-C5-C6-C7
28	C	524	LMG	C16-C17-C18-C19
28	c	522	LMG	C29-C30-C31-C32
25	c	514	BCR	C11-C12-C13-C14
33	D	411	LHG	C10-C11-C12-C13
23	B	602	CLA	C1A-C2A-CAA-CBA
27	C	516	STE	C1-C2-C3-C4
27	E	104	STE	C14-C15-C16-C17
33	D	411	LHG	C17-C18-C19-C20
29	l	101	SQD	O10-C23-C24-C25
30	c	519	DGD	O1A-C1A-C2A-C3A
30	c	519	DGD	C6A-C7A-C8A-C9A
23	B	604	CLA	C10-C11-C12-C13
29	A	412	SQD	C35-C36-C37-C38
23	C	501	CLA	C2A-CAA-CBA-CGA
30	c	521	DGD	C2A-C3A-C4A-C5A
23	b	608	CLA	C16-C17-C18-C19
23	c	509	CLA	C16-C17-C18-C19
30	C	521	DGD	C1B-C2B-C3B-C4B
29	a	412	SQD	C24-C25-C26-C27
23	B	612	CLA	CAA-CBA-CGA-O2A
30	C	521	DGD	O1B-C1B-O2G-C2G
27	j	102	STE	C2-C3-C4-C5
33	D	410	LHG	C15-C16-C17-C18
33	D	411	LHG	O10-C23-C24-C25
23	b	602	CLA	C15-C16-C17-C18
33	D	410	LHG	C4-O6-P-O5
23	c	510	CLA	CAA-CBA-CGA-O1A
33	d	408	LHG	O10-C23-C24-C25
23	C	508	CLA	C13-C15-C16-C17
30	c	520	DGD	C3A-C4A-C5A-C6A
25	k	101	BCR	C23-C24-C25-C26
23	C	504	CLA	C11-C12-C13-C14
28	M	101	LMG	C10-C11-C12-C13
30	c	519	DGD	O2G-C1B-C2B-C3B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	c	505	CLA	C16-C17-C18-C19
29	A	412	SQD	O49-C7-C8-C9
23	a	408	CLA	C8-C10-C11-C12
27	H	103	STE	C9-C10-C11-C12
27	I	101	STE	C11-C10-C9-C8
27	D	413	STE	C10-C11-C12-C13
28	c	523	LMG	C36-C37-C38-C39
30	A	414	DGD	CDB-CEB-CFB-CGB
28	D	408	LMG	C28-C29-C30-C31
28	b	621	LMG	O10-C28-C29-C30
28	c	518	LMG	O10-C28-C29-C30
28	d	409	LMG	C29-C30-C31-C32
26	a	410	PL9	C21-C22-C23-C24
23	B	605	CLA	CAD-CBD-CGD-O1D
23	B	607	CLA	CAD-CBD-CGD-O1D
23	B	609	CLA	CAD-CBD-CGD-O1D
23	C	506	CLA	CAD-CBD-CGD-O1D
23	b	606	CLA	CAD-CBD-CGD-O1D
23	b	608	CLA	CAD-CBD-CGD-O1D
23	c	506	CLA	CAD-CBD-CGD-O1D
28	a	415	LMG	C9-C8-O7-C10
23	B	613	CLA	CAA-CBA-CGA-O1A
28	C	524	LMG	C34-C35-C36-C37
30	c	521	DGD	C9A-CAA-CBA-CCA
23	b	611	CLA	CAA-CBA-CGA-O2A
23	D	403	CLA	C14-C13-C15-C16
23	c	511	CLA	C6-C7-C8-C9
33	D	410	LHG	O1-C1-C2-O2
30	c	519	DGD	C7B-C8B-C9B-CAB
33	d	406	LHG	C24-C25-C26-C27
33	L	101	LHG	O9-C7-C8-C9
27	i	102	STE	C11-C10-C9-C8
26	A	409	PL9	C37-C38-C39-C40
27	T	102	STE	C11-C12-C13-C14
28	a	415	LMG	C19-C20-C21-C22
30	A	414	DGD	CFA-CGA-CHA-CIA
26	D	407	PL9	C30-C29-C31-C32
26	a	410	PL9	C30-C29-C31-C32
26	d	405	PL9	C40-C39-C41-C42
23	B	601	CLA	C11-C10-C8-C7
23	B	615	CLA	C6-C7-C8-C10
23	C	511	CLA	C6-C7-C8-C10

Continued on next page...

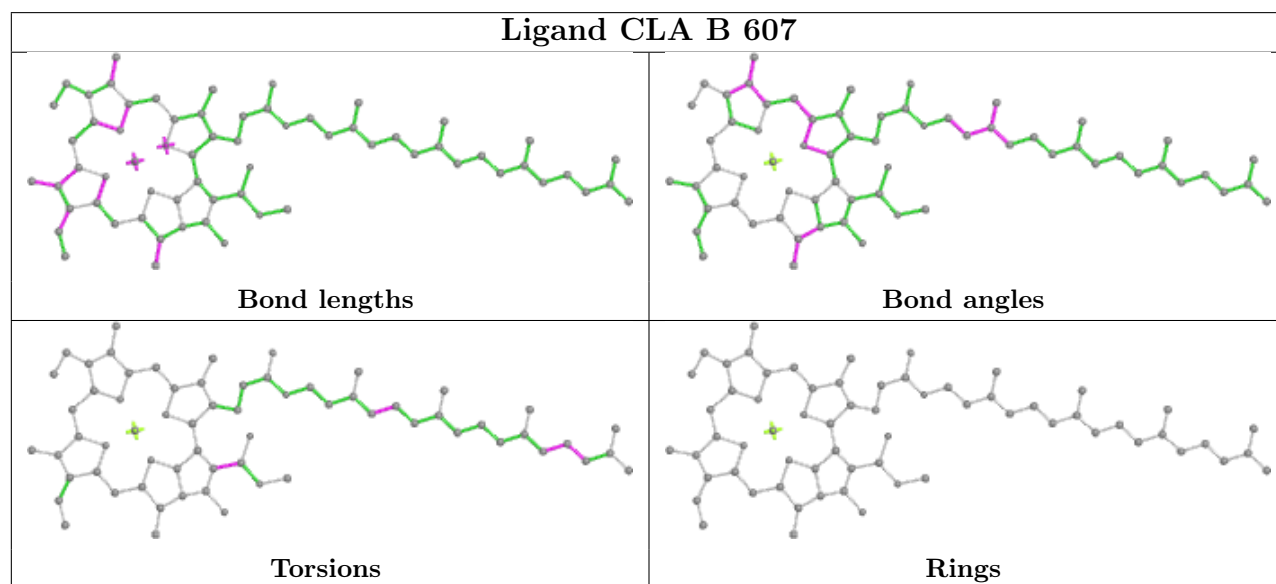
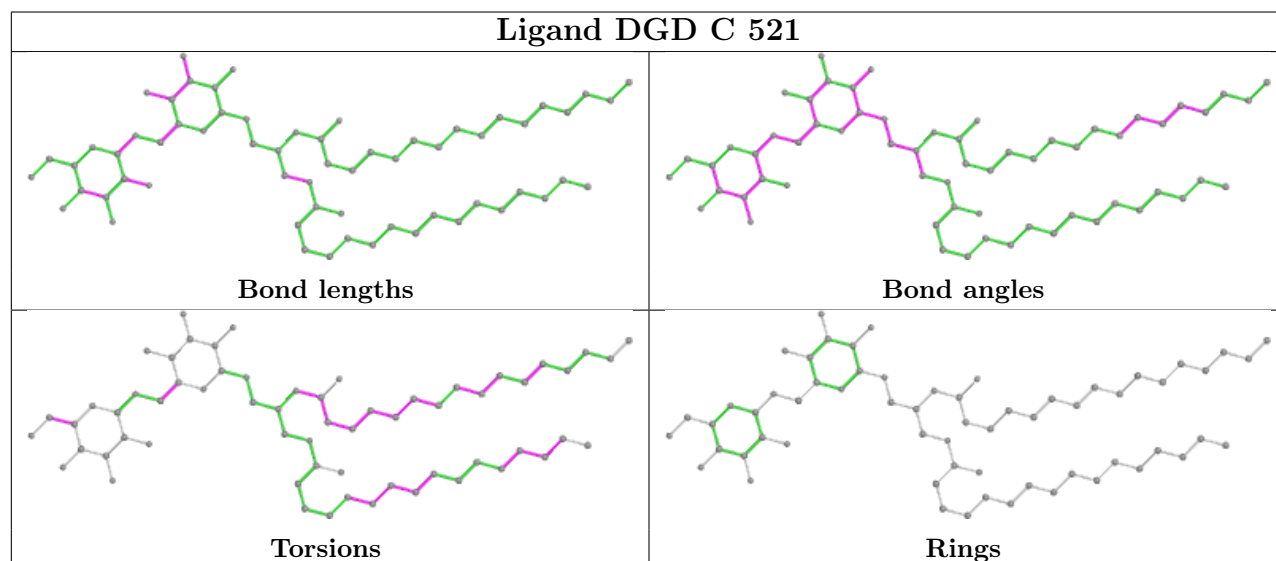
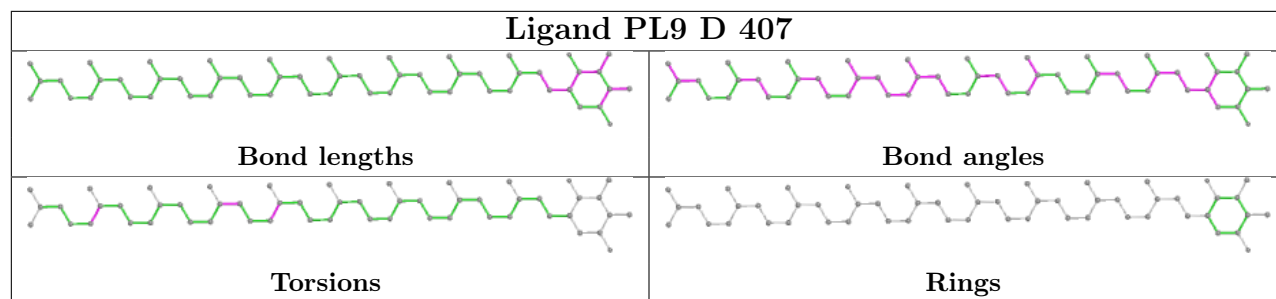
Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	512	CLA	C12-C13-C15-C16
23	D	403	CLA	C12-C13-C15-C16
23	a	406	CLA	C12-C13-C15-C16
23	c	503	CLA	C11-C10-C8-C7
23	c	505	CLA	C11-C12-C13-C15
23	c	512	CLA	C11-C12-C13-C15
23	c	506	CLA	O1D-CGD-O2D-CED
30	c	521	DGD	O1G-C1A-C2A-C3A
28	D	409	LMG	C17-C18-C19-C20
28	c	523	LMG	O10-C28-C29-C30
30	C	521	DGD	C3B-C4B-C5B-C6B
28	c	524	LMG	O8-C28-C29-C30
23	h	101	CLA	O1A-CGA-O2A-C1
28	b	623	LMG	C22-C23-C24-C25
29	A	413	SQD	C19-C20-C21-C22
23	B	615	CLA	C13-C15-C16-C17
27	d	410	STE	C11-C12-C13-C14
23	B	612	CLA	CAA-CBA-CGA-O1A
23	b	611	CLA	CAA-CBA-CGA-O1A
30	c	519	DGD	O1B-C1B-C2B-C3B
26	A	409	PL9	C42-C43-C44-C45
33	d	408	LHG	O8-C23-C24-C25
33	l	102	LHG	O7-C7-C8-C9

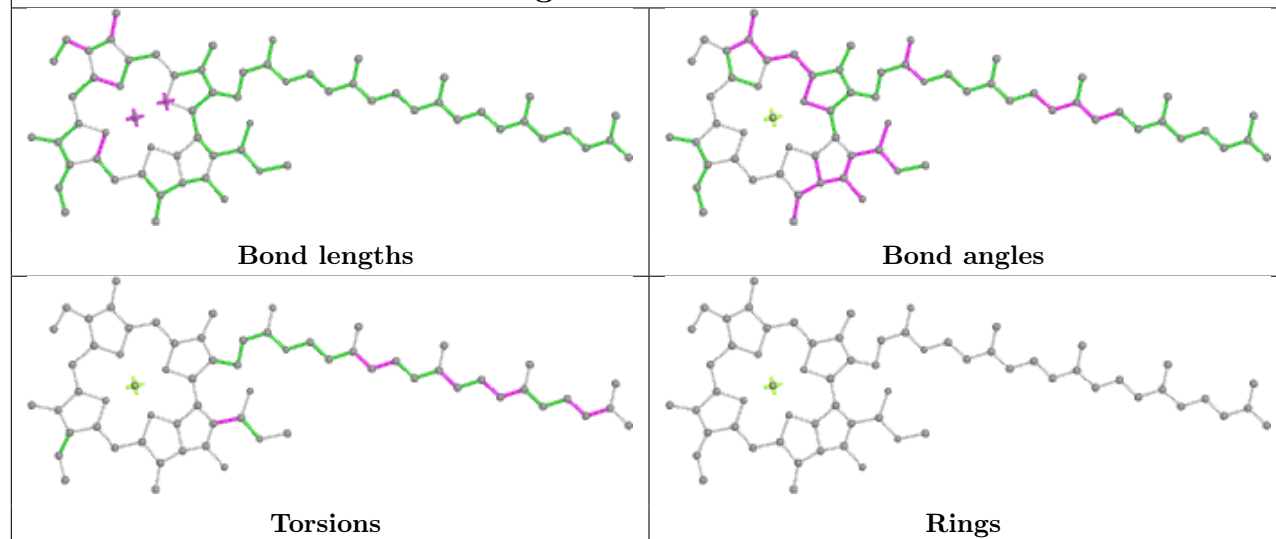
There are no ring outliers.

No monomer is involved in short contacts.

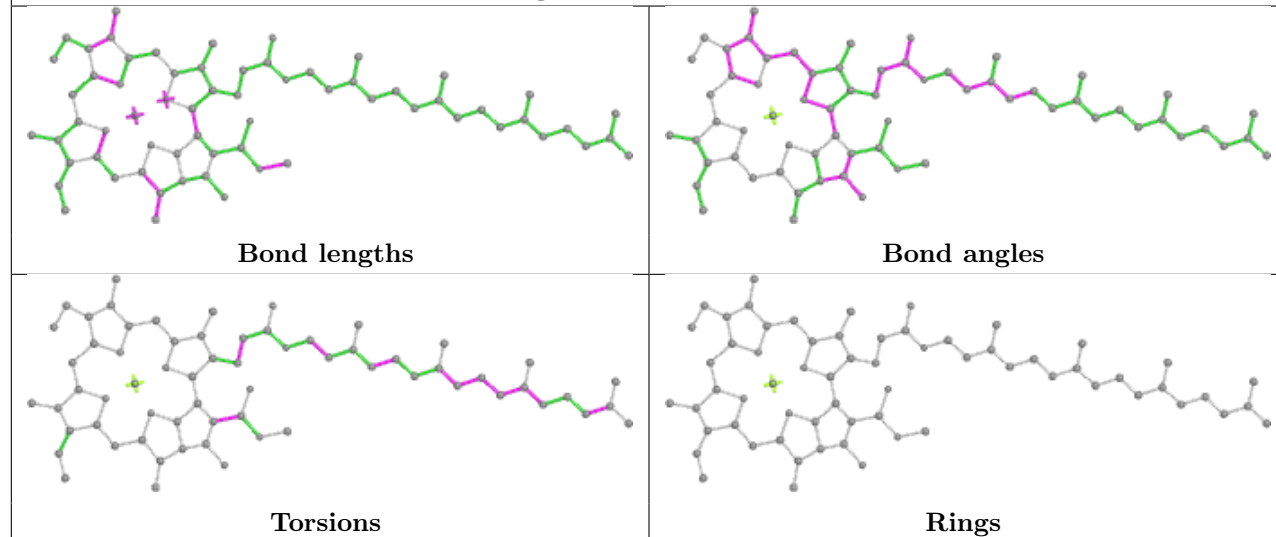
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



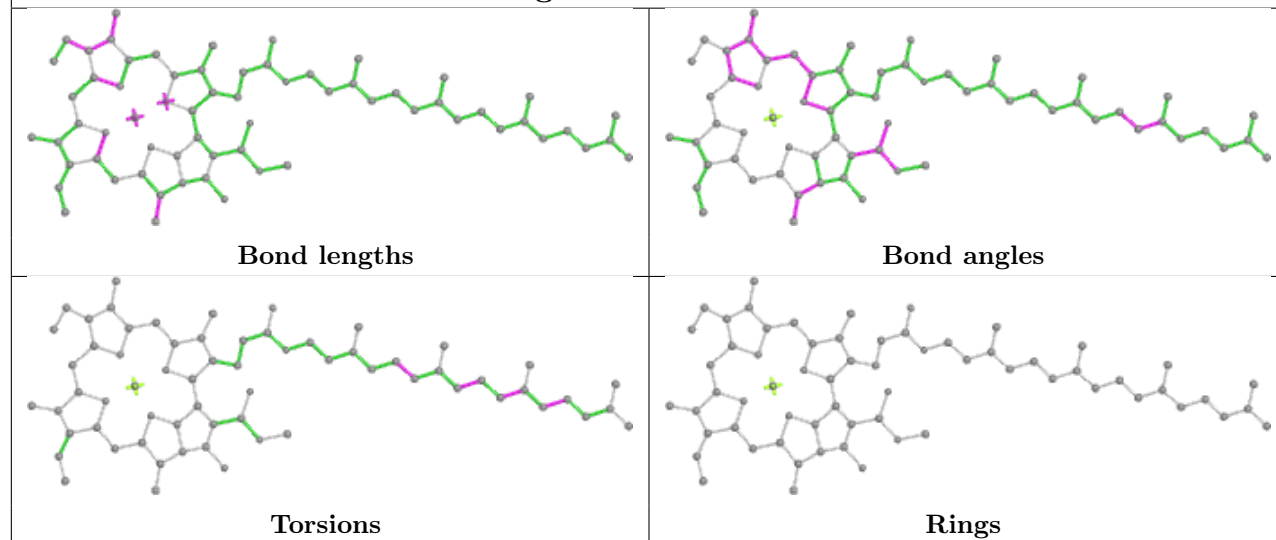
Ligand CLA b 603

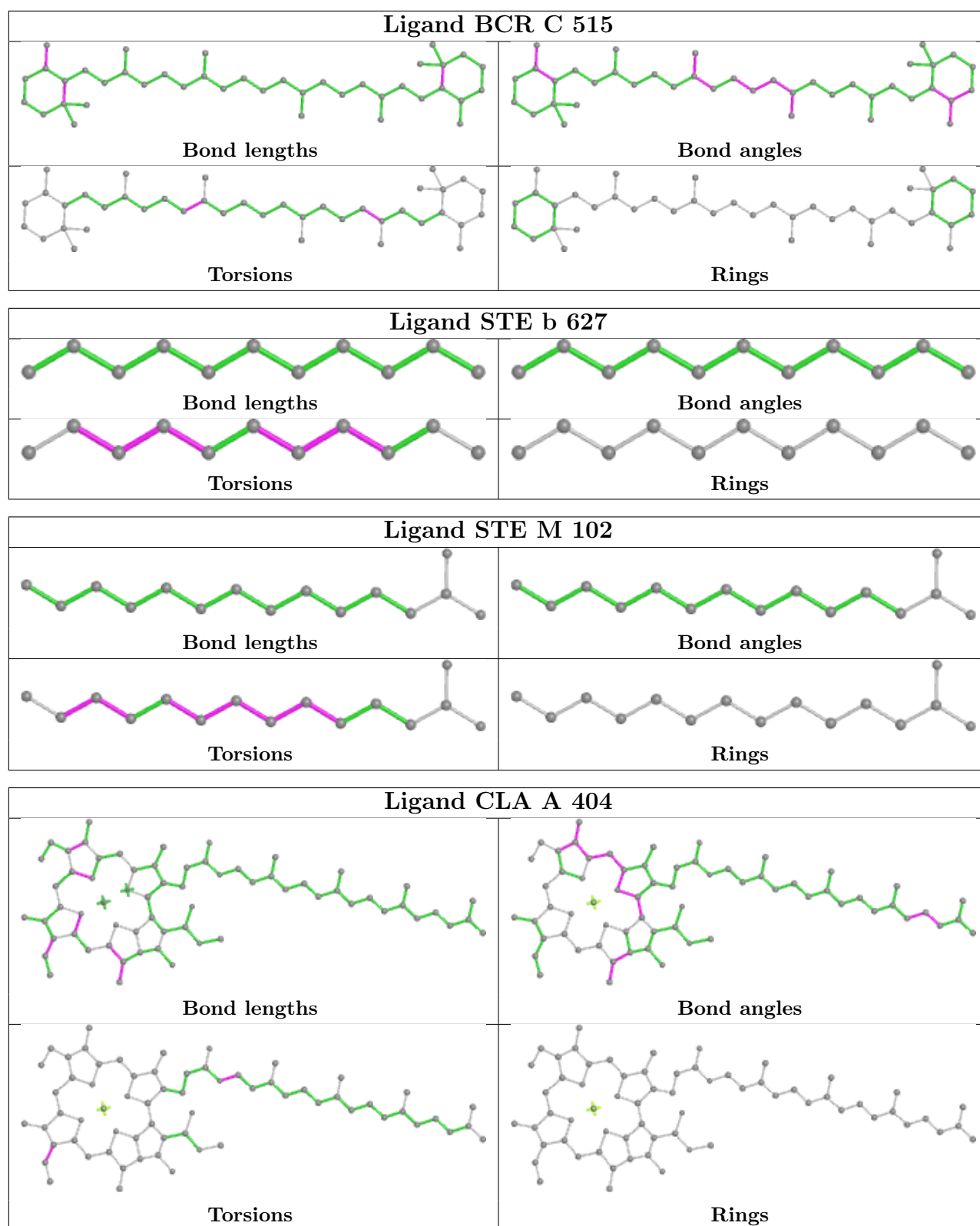


Ligand CLA C 512

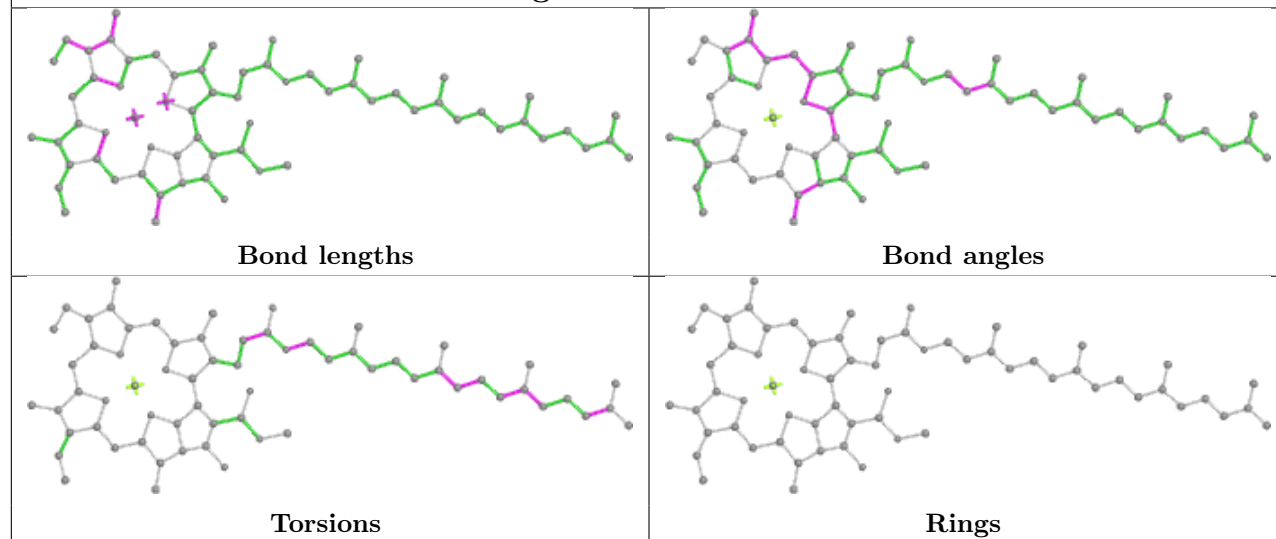


Ligand CLA b 614

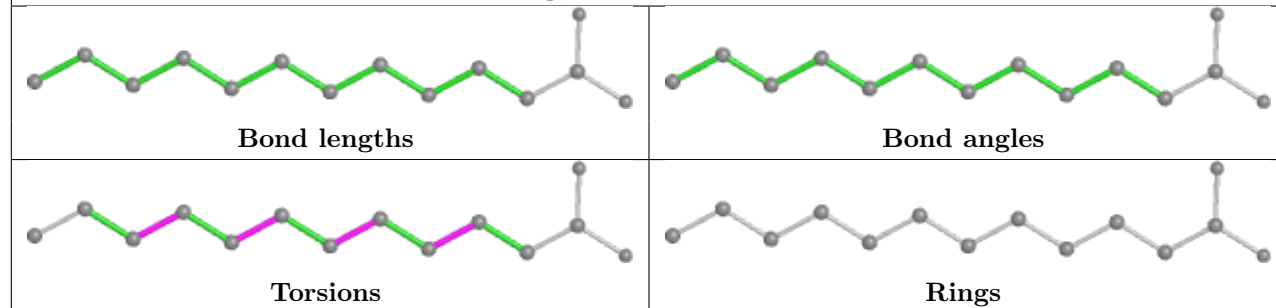




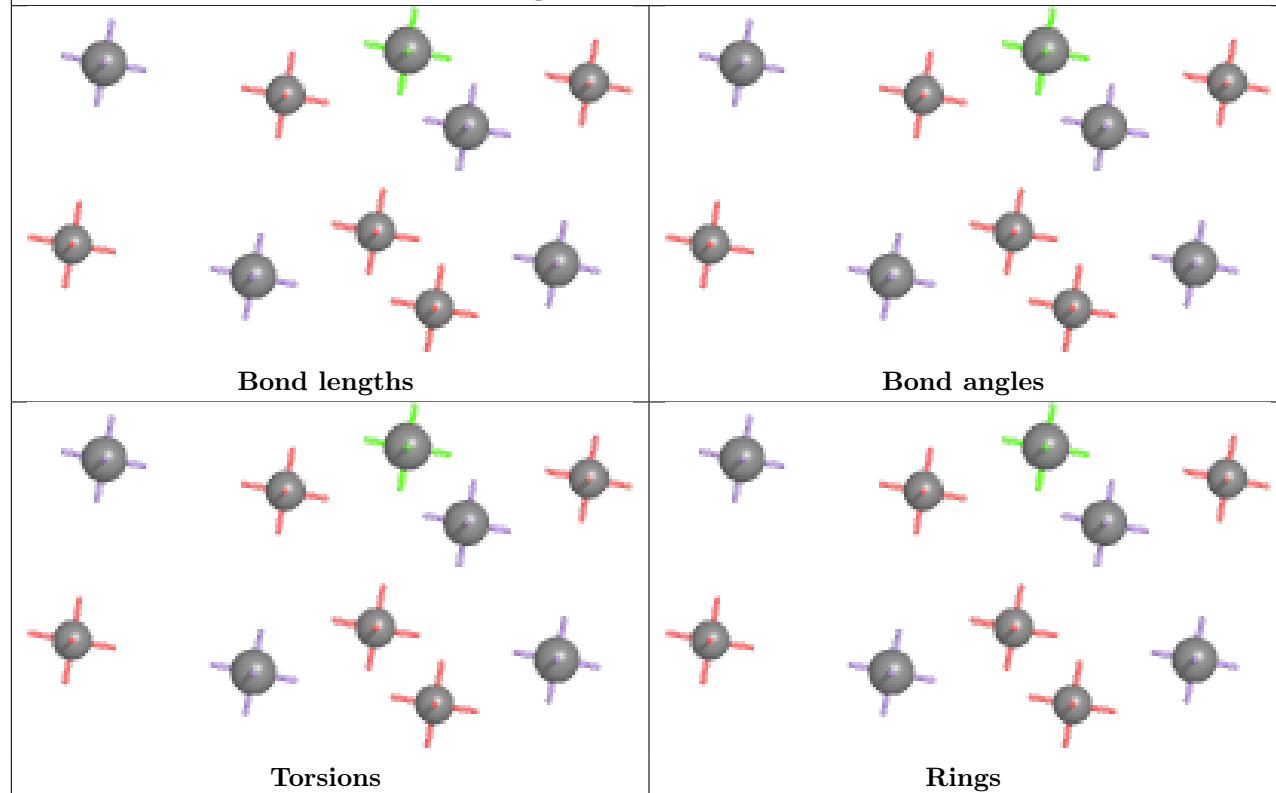
Ligand CLA B 613

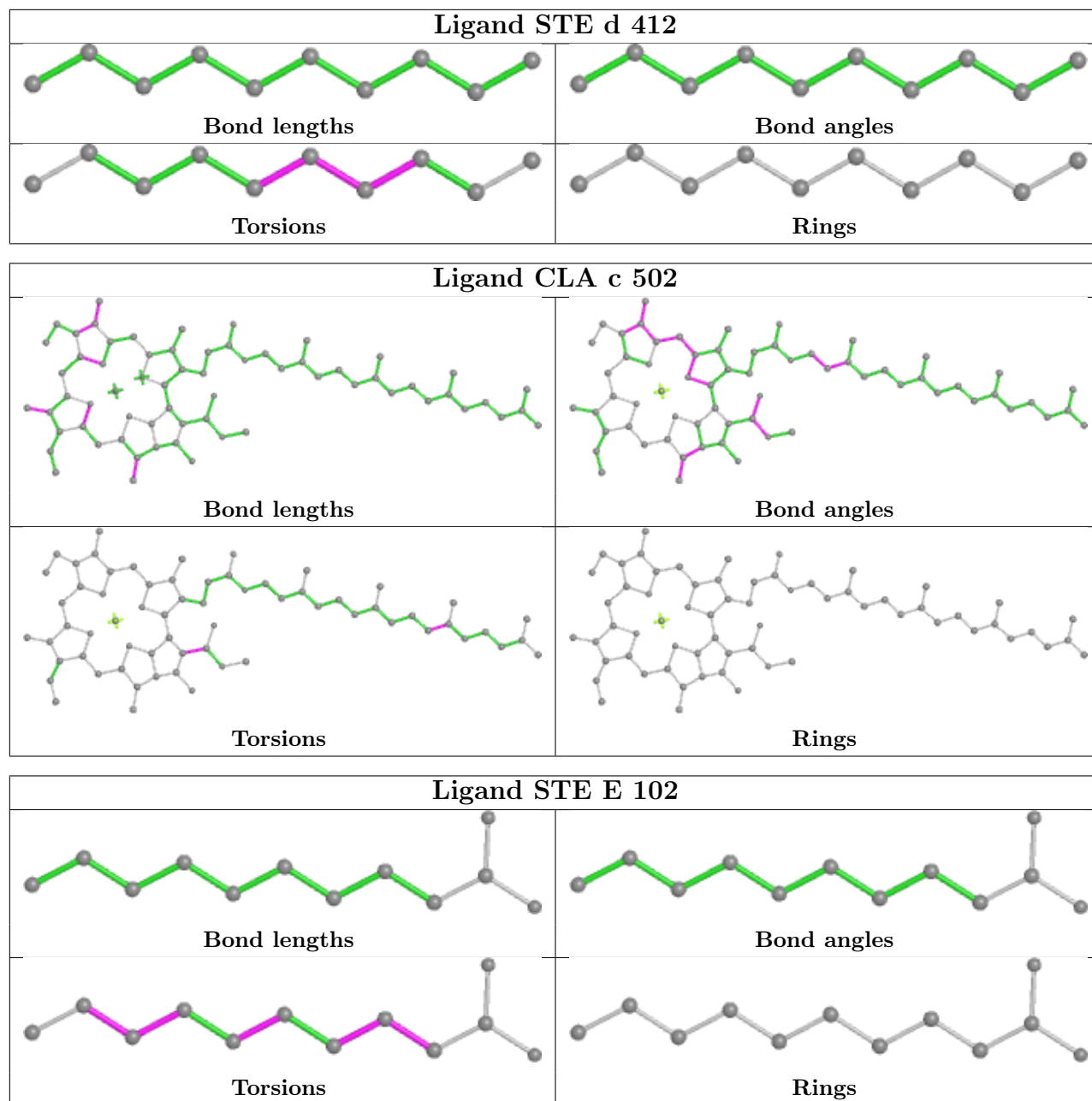


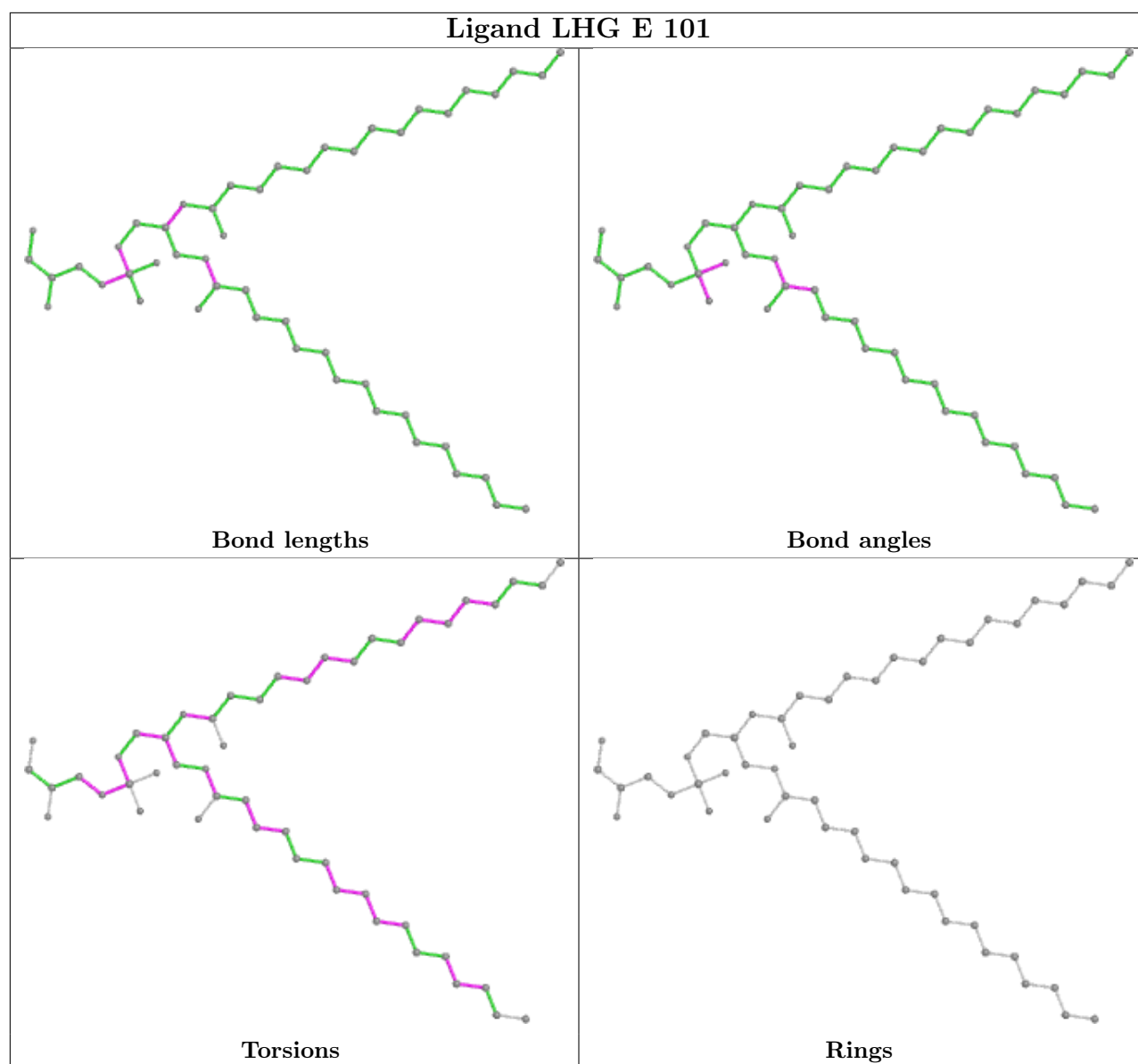
Ligand STE t 102



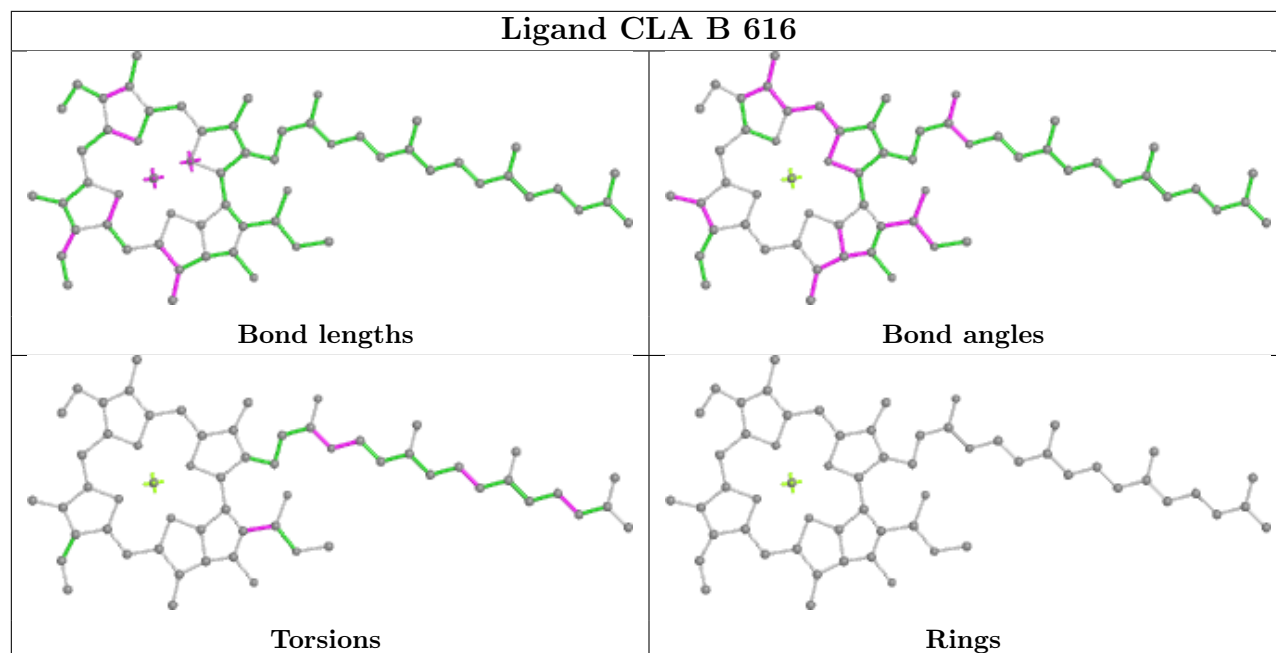
Ligand OEX A 418



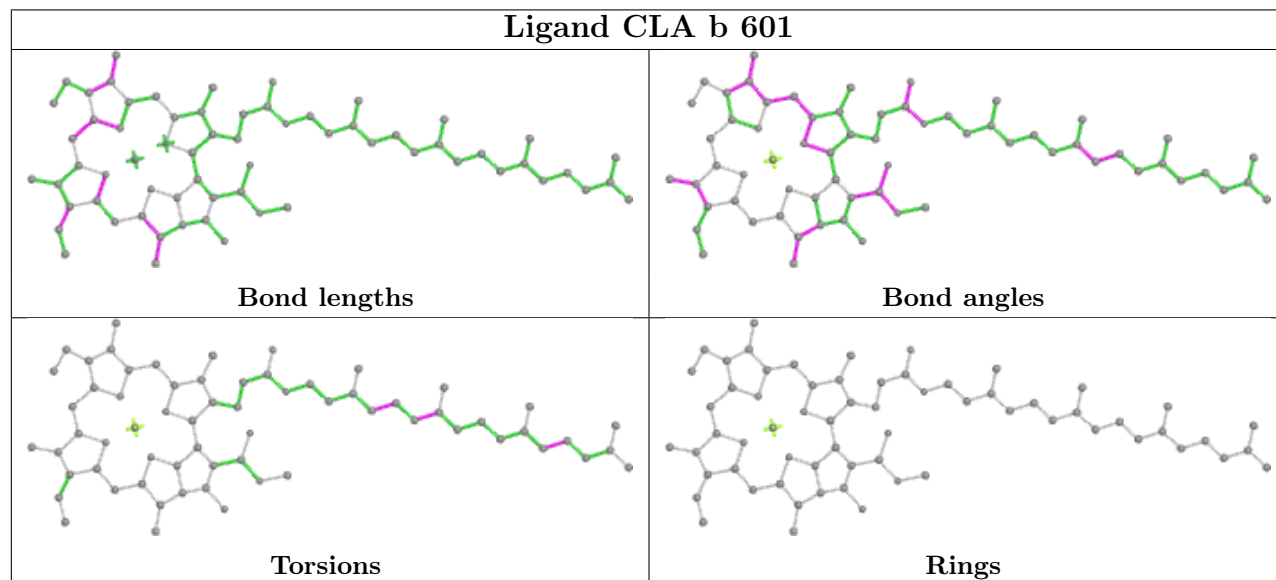




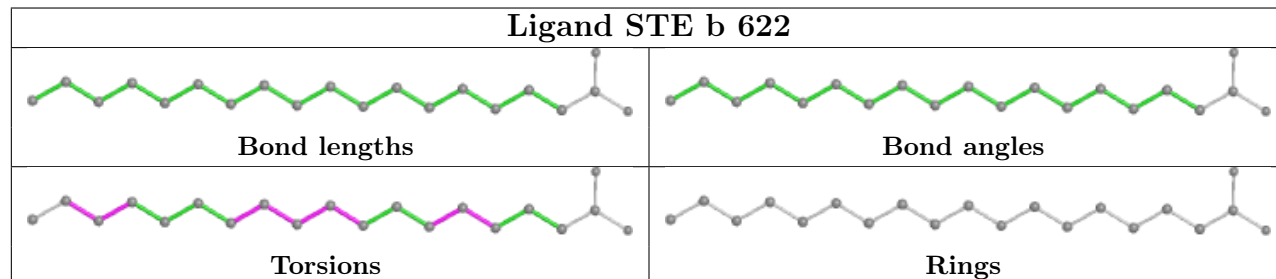
Ligand CLA B 616



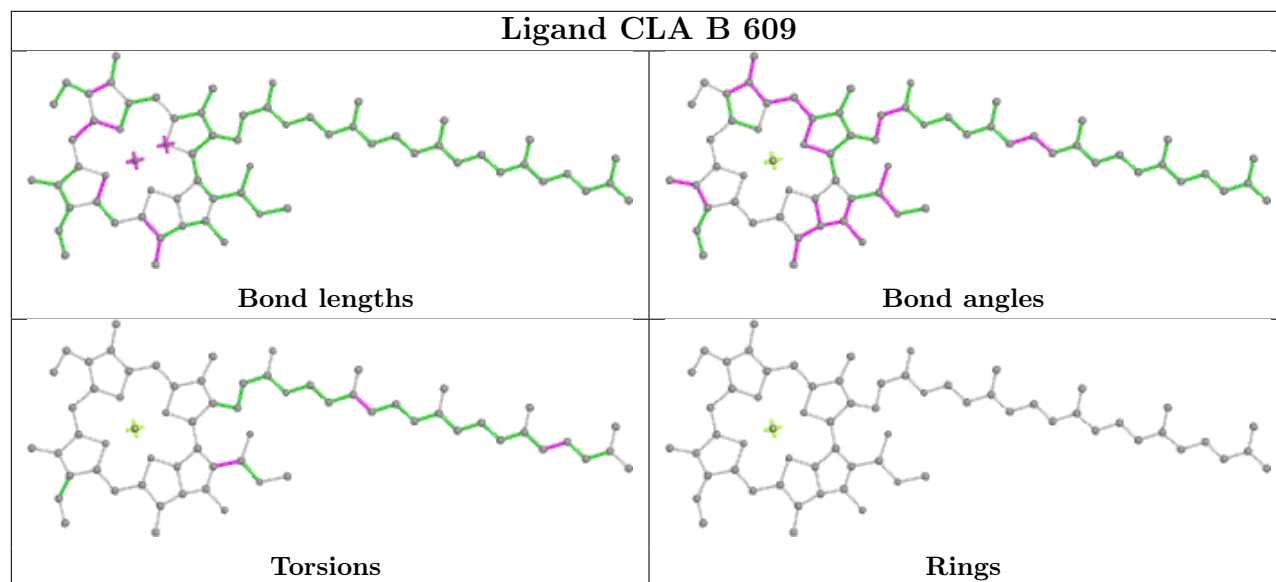
Ligand CLA b 601



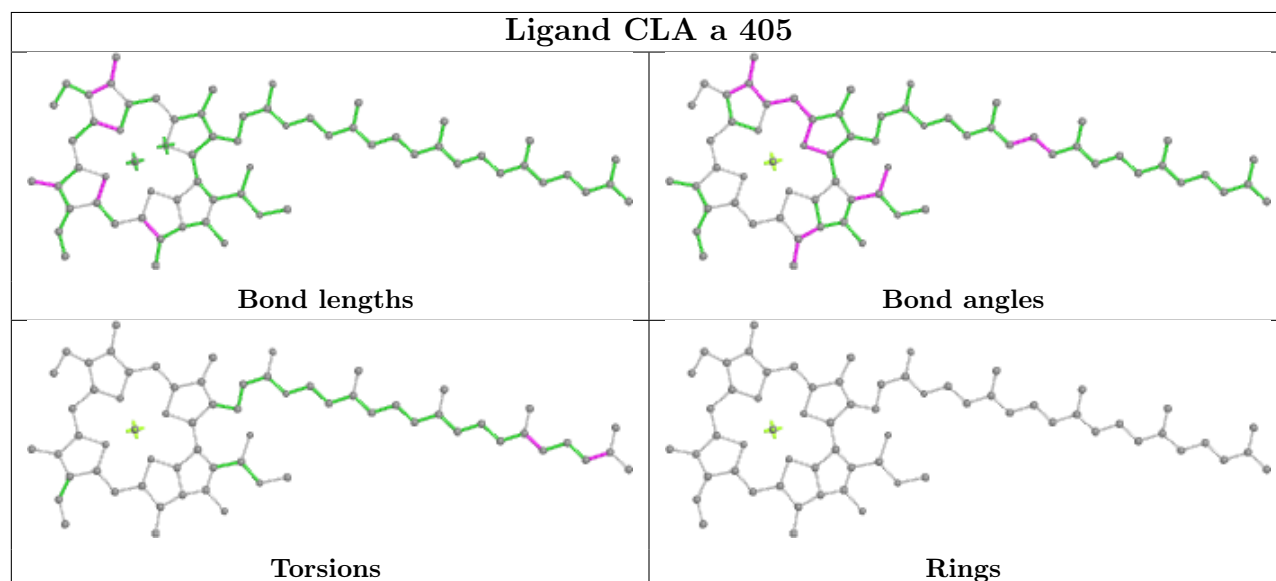
Ligand STE b 622



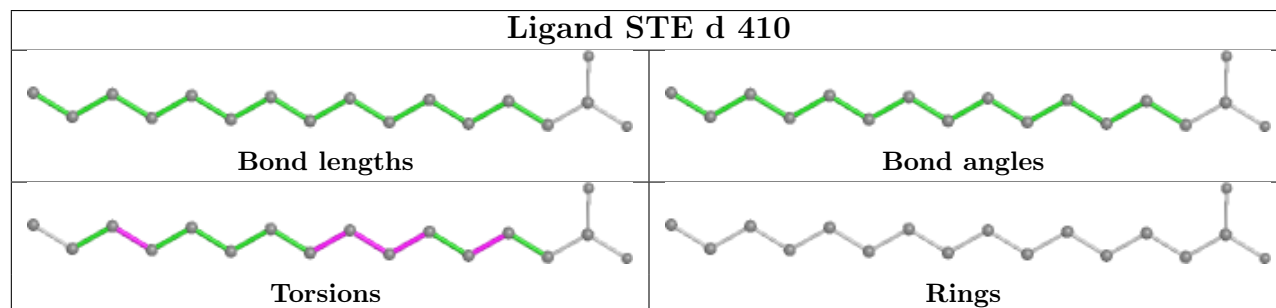
Ligand CLA B 609



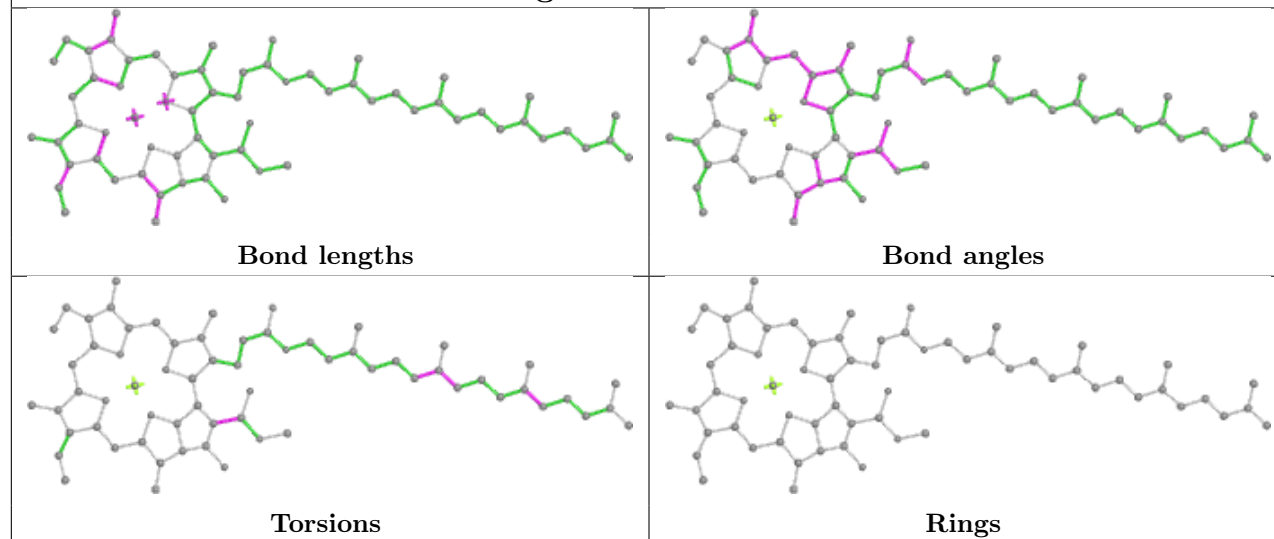
Ligand CLA a 405



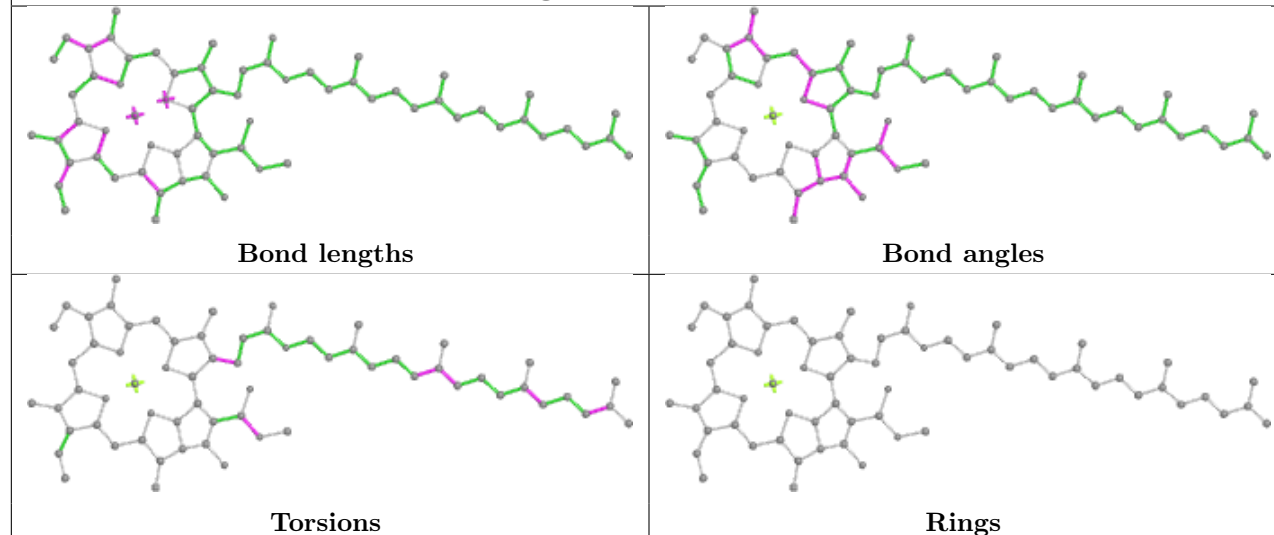
Ligand STE d 410



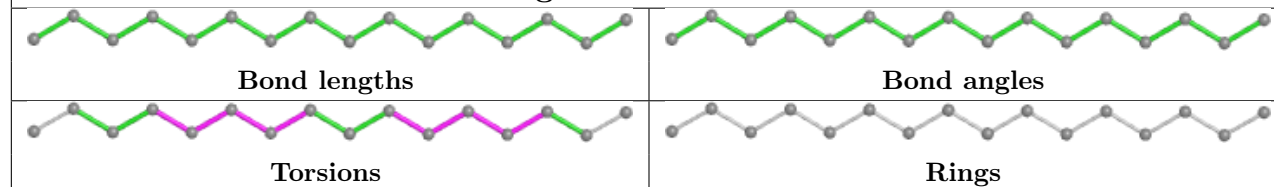
Ligand CLA a 406



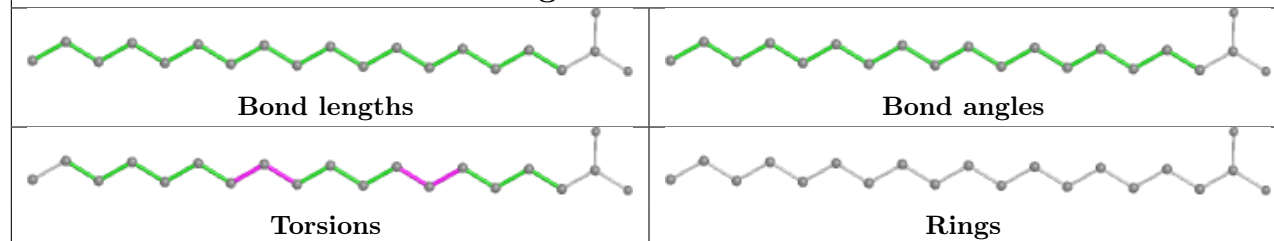
Ligand CLA c 511

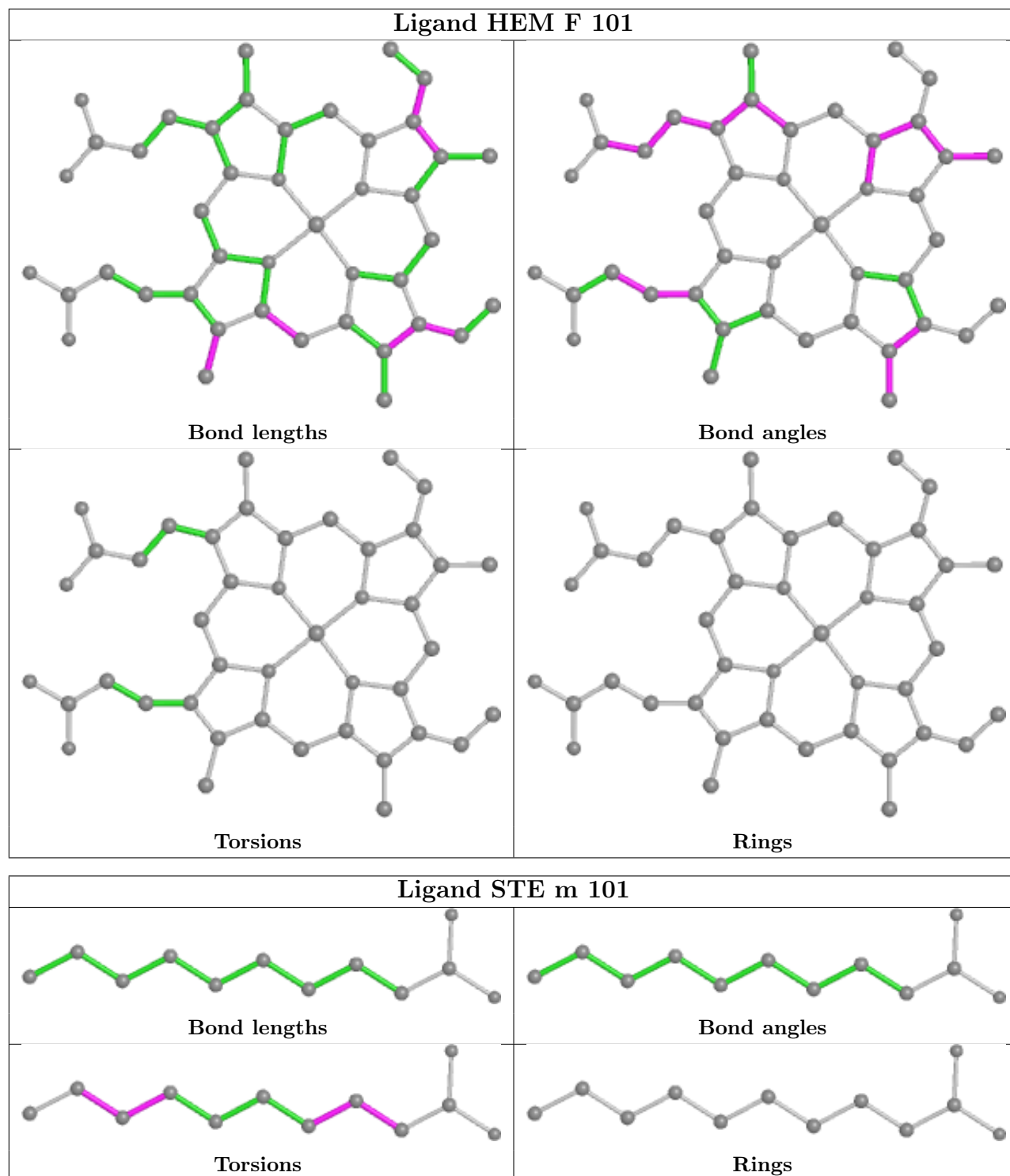


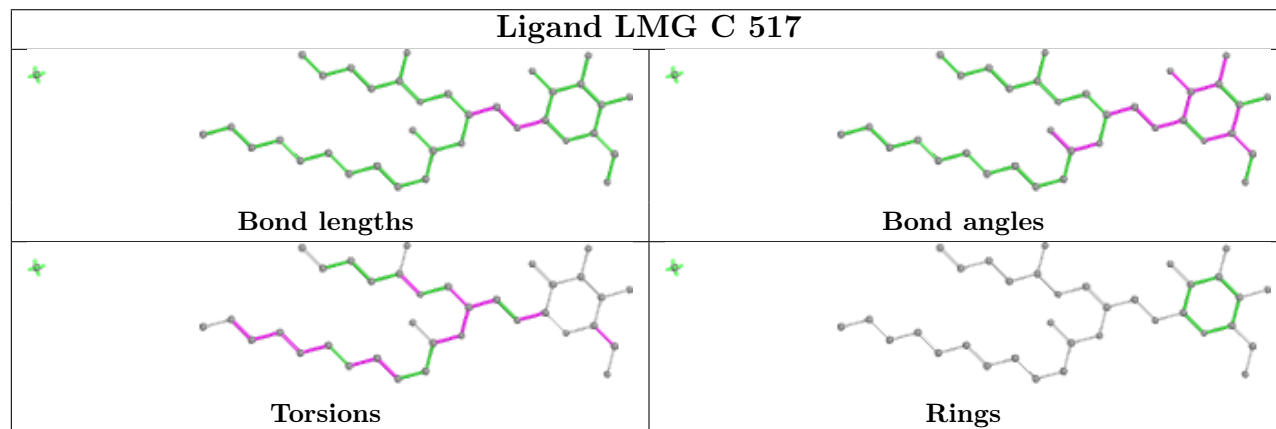
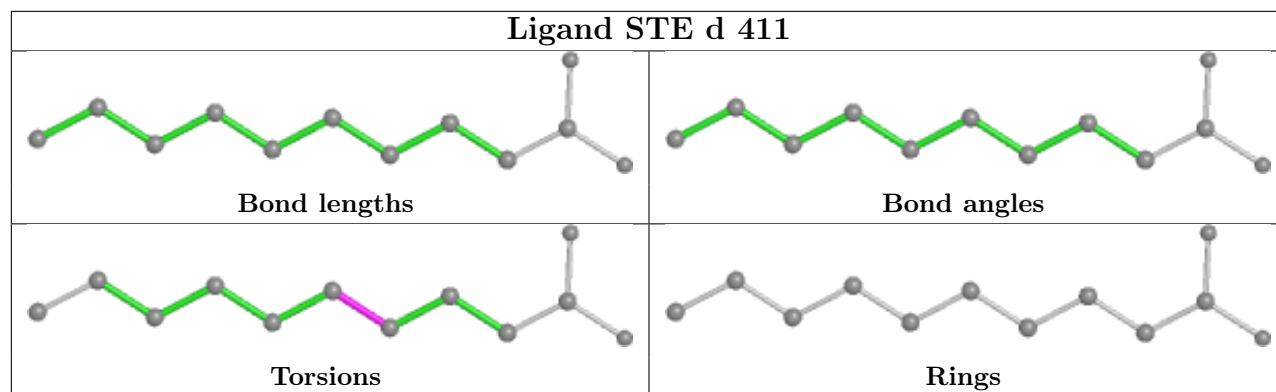
Ligand STE T 102



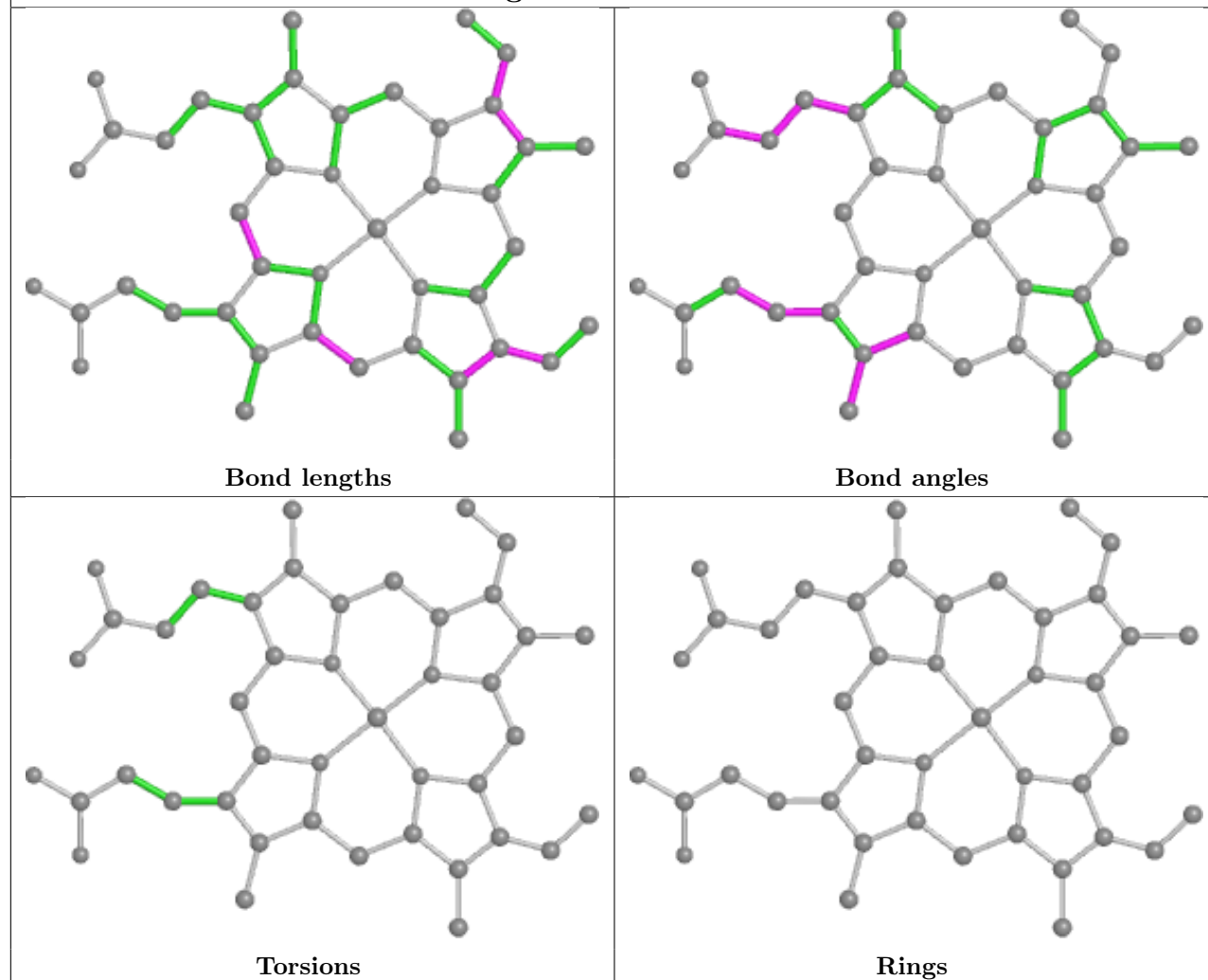
Ligand STE x 102



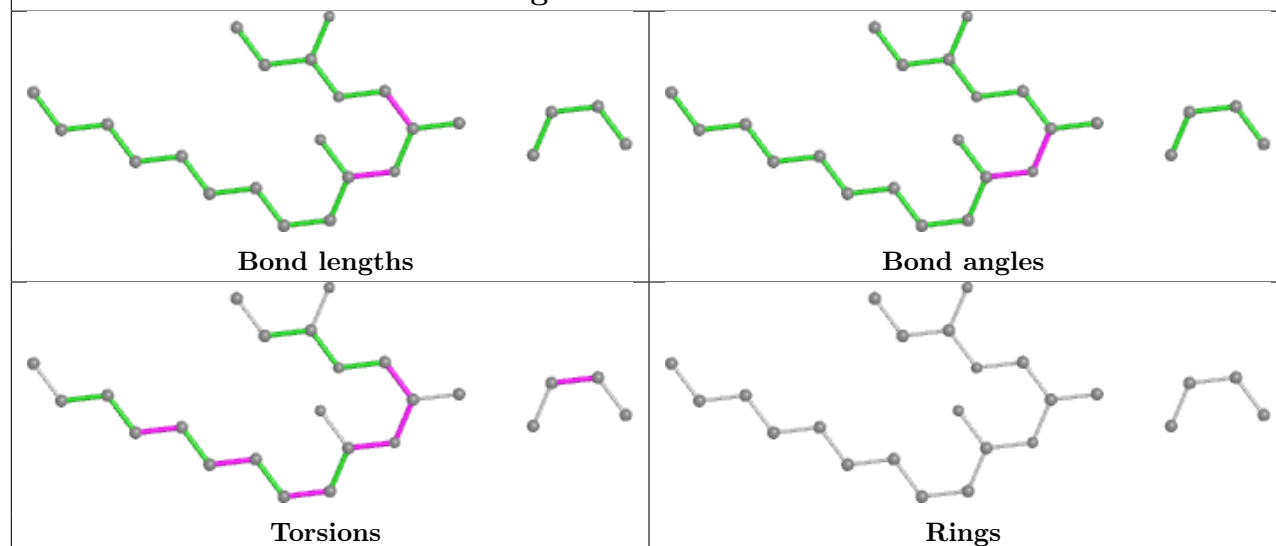


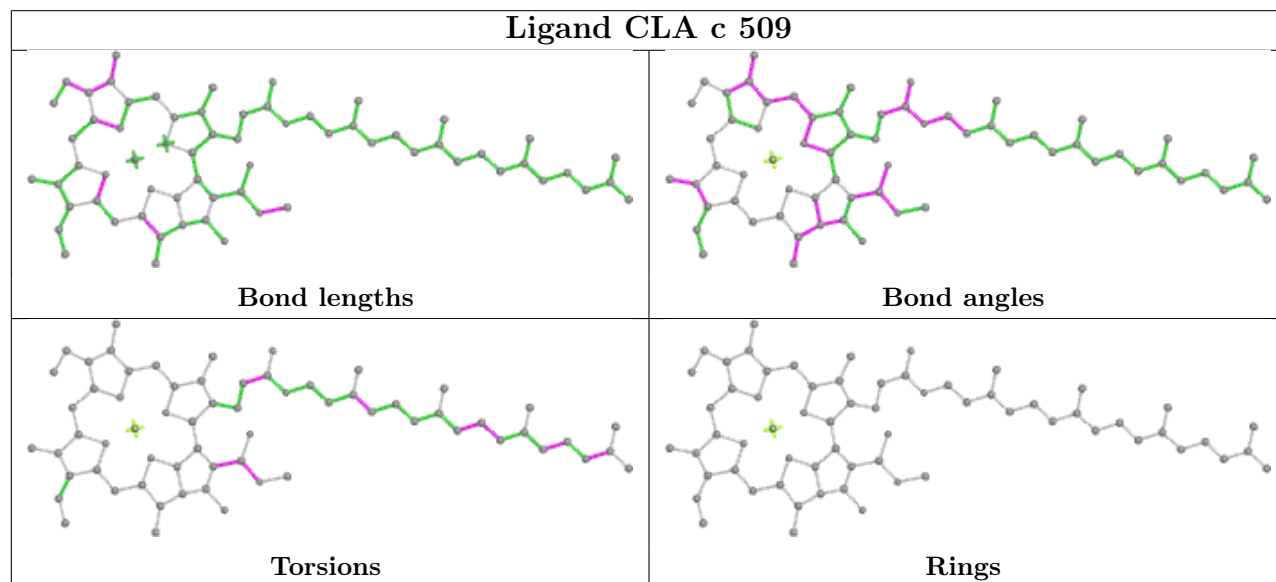
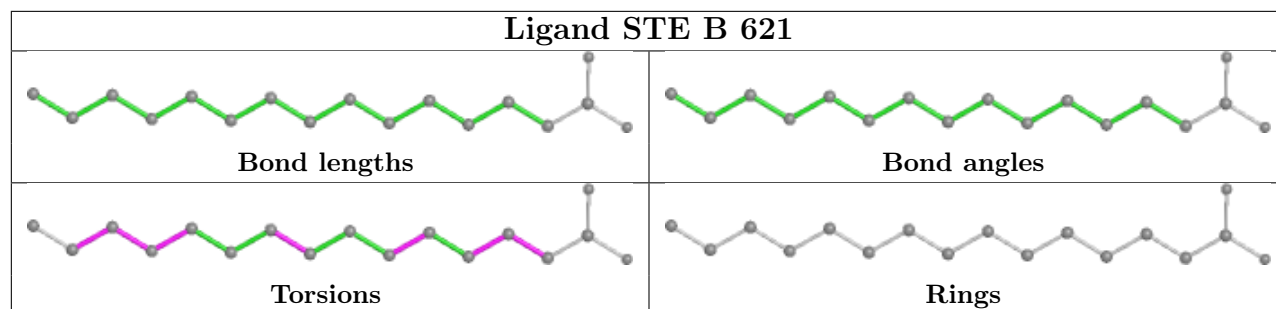


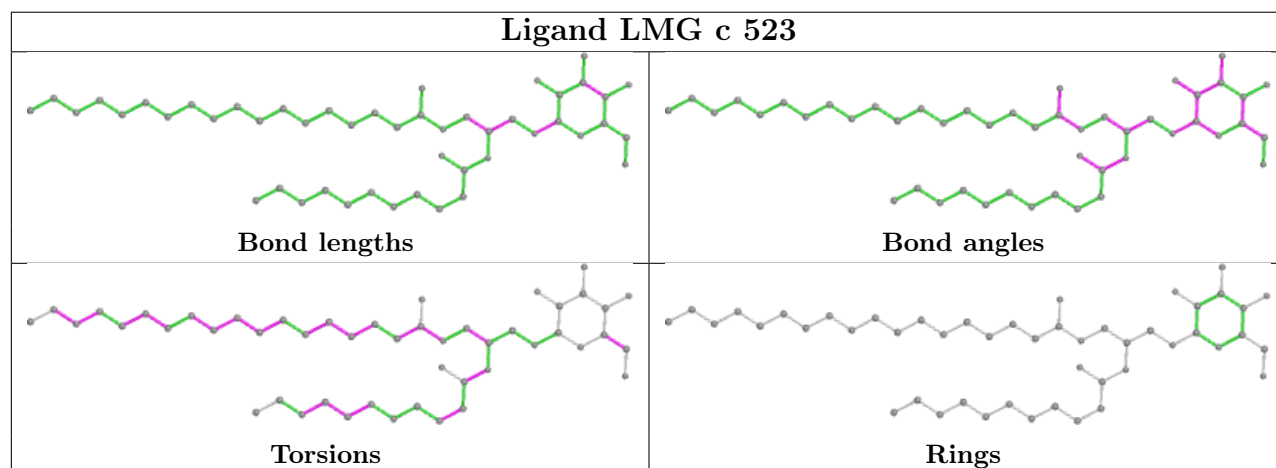
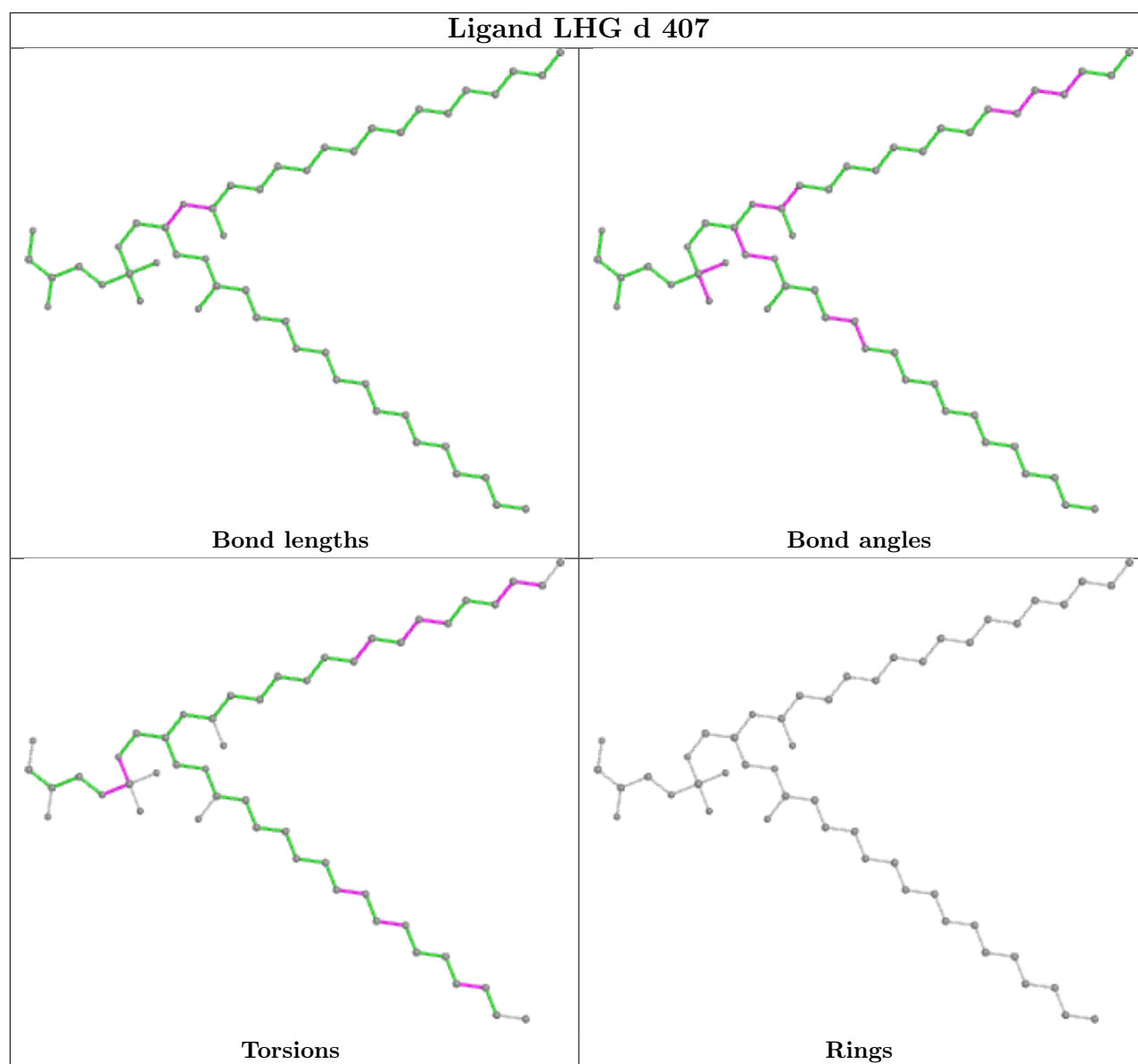
Ligand HEM f 101

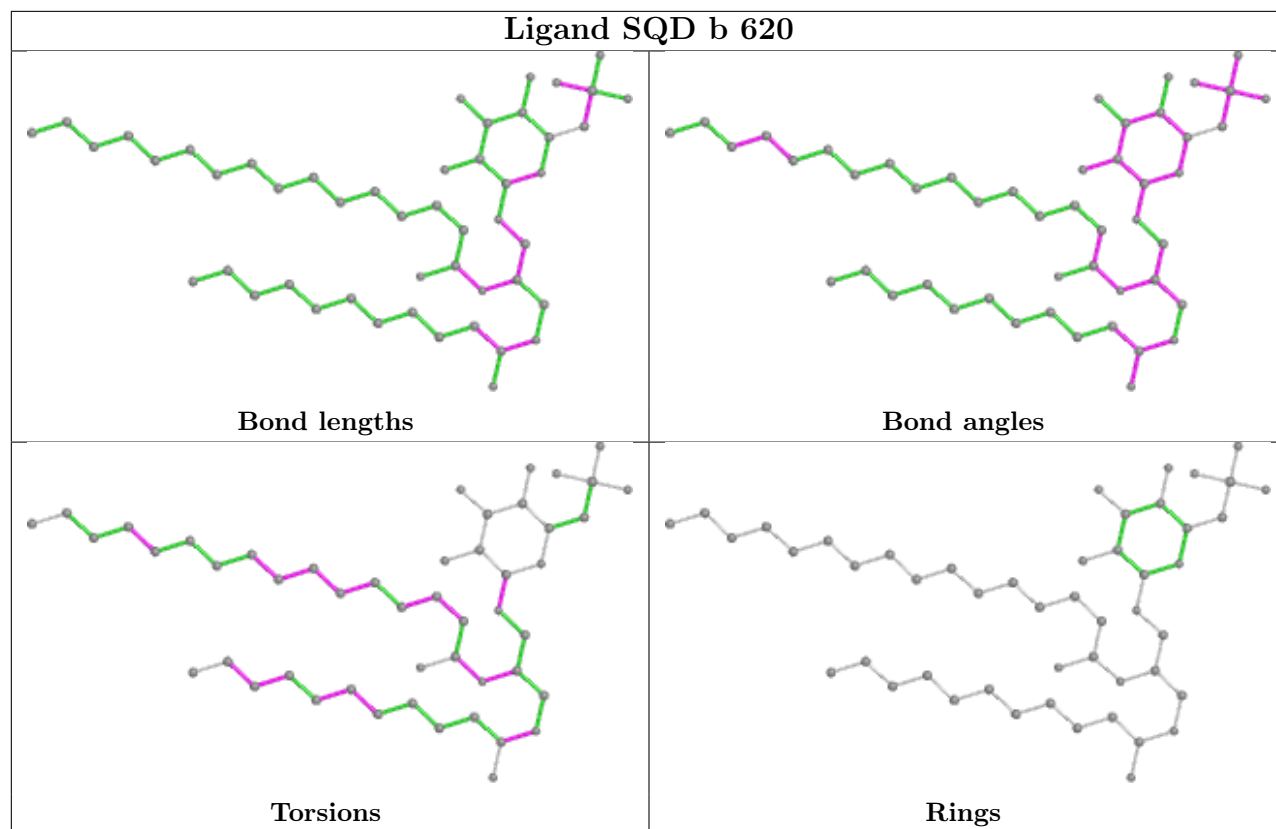


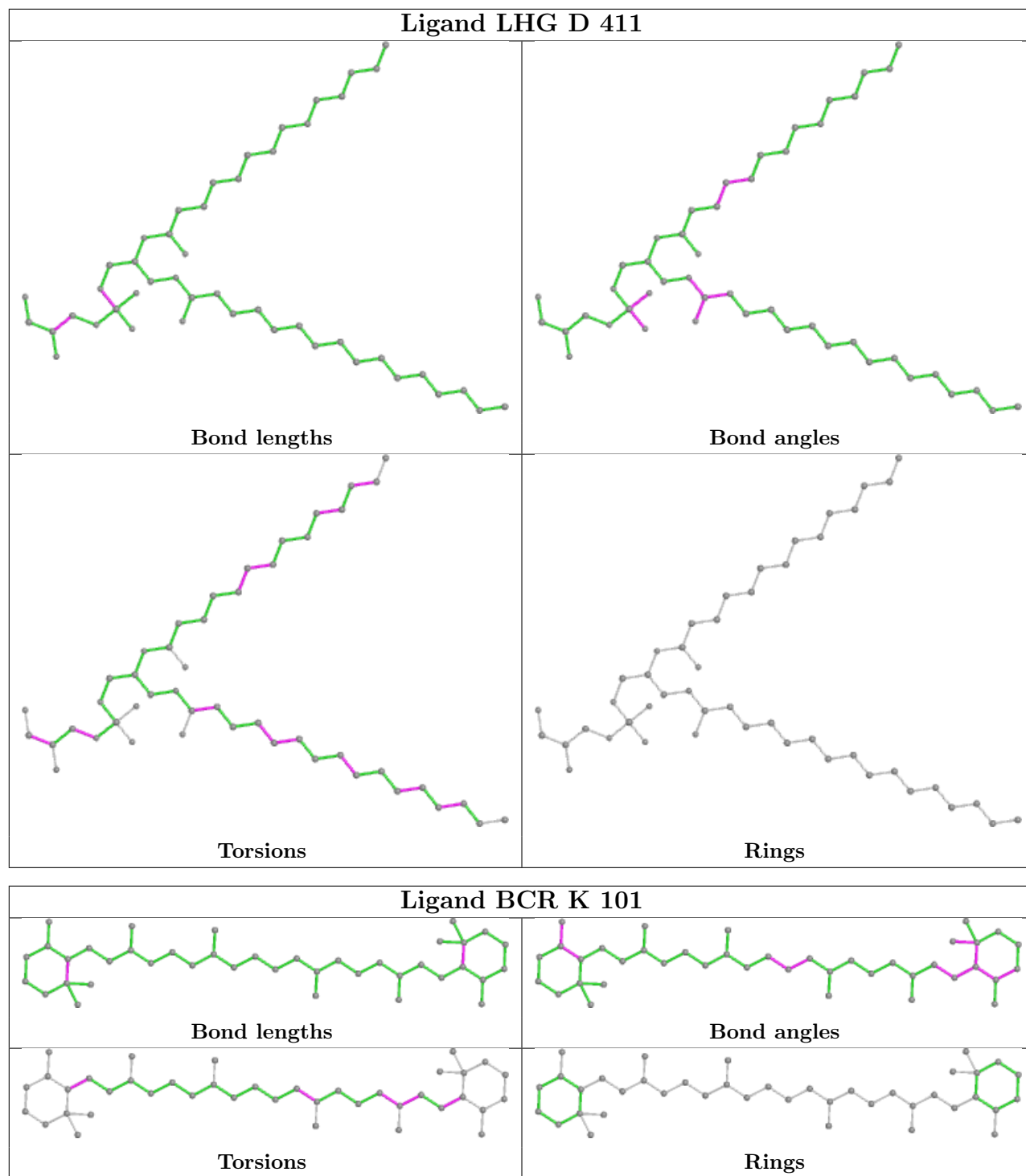
Ligand LMG b 619

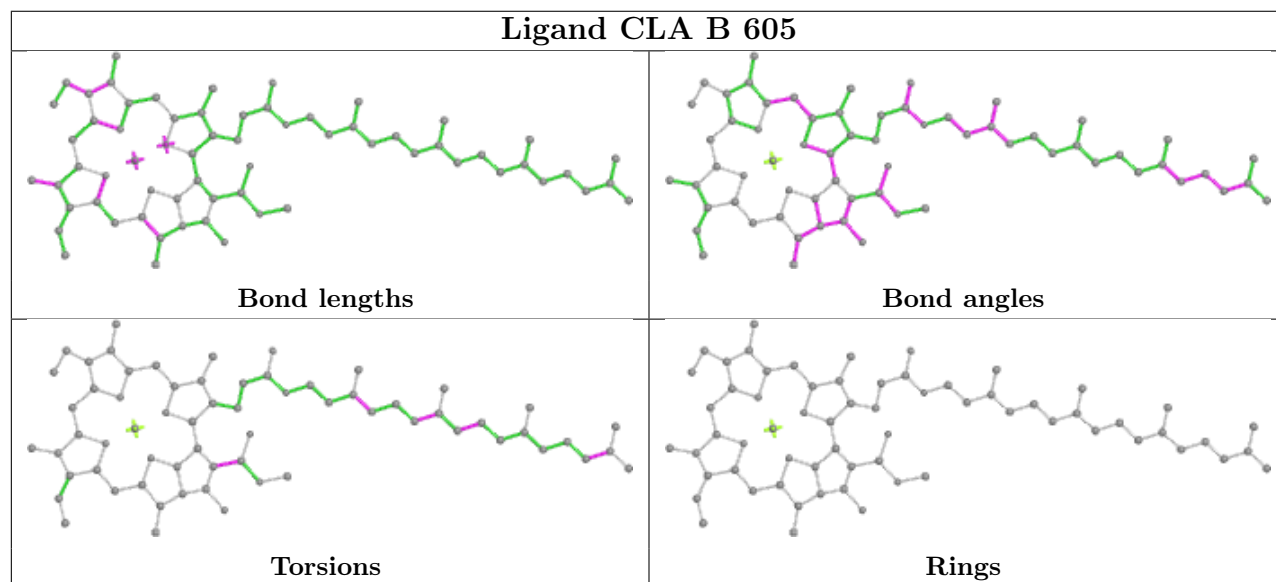
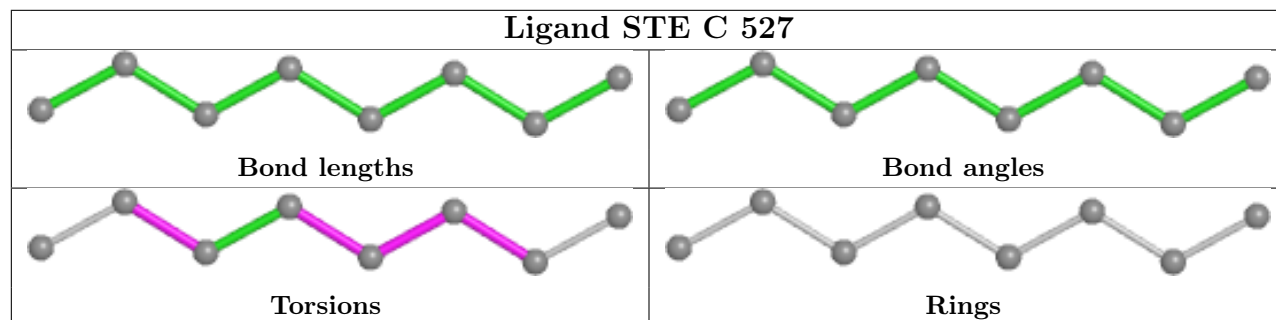
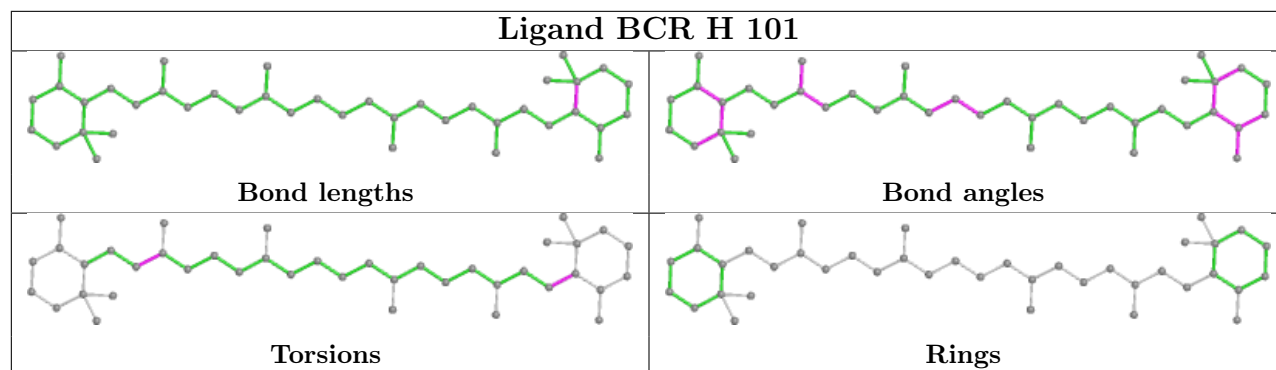
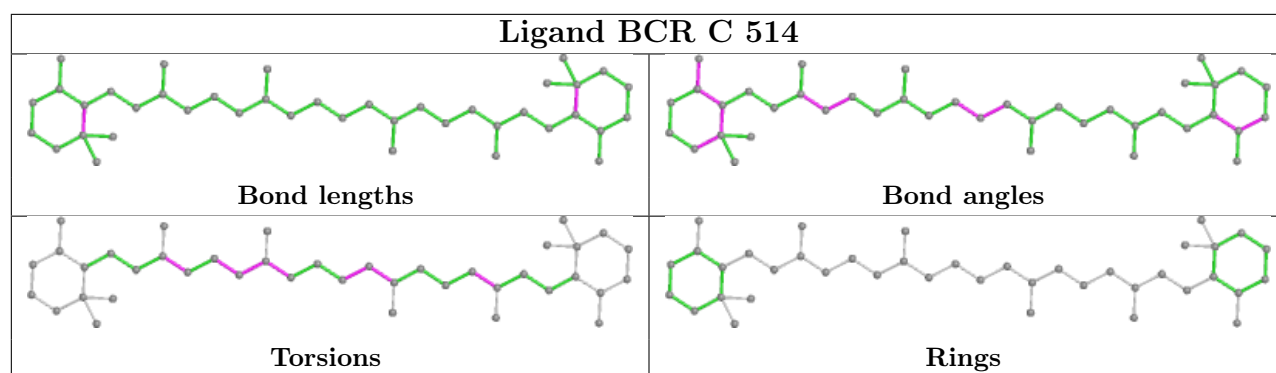


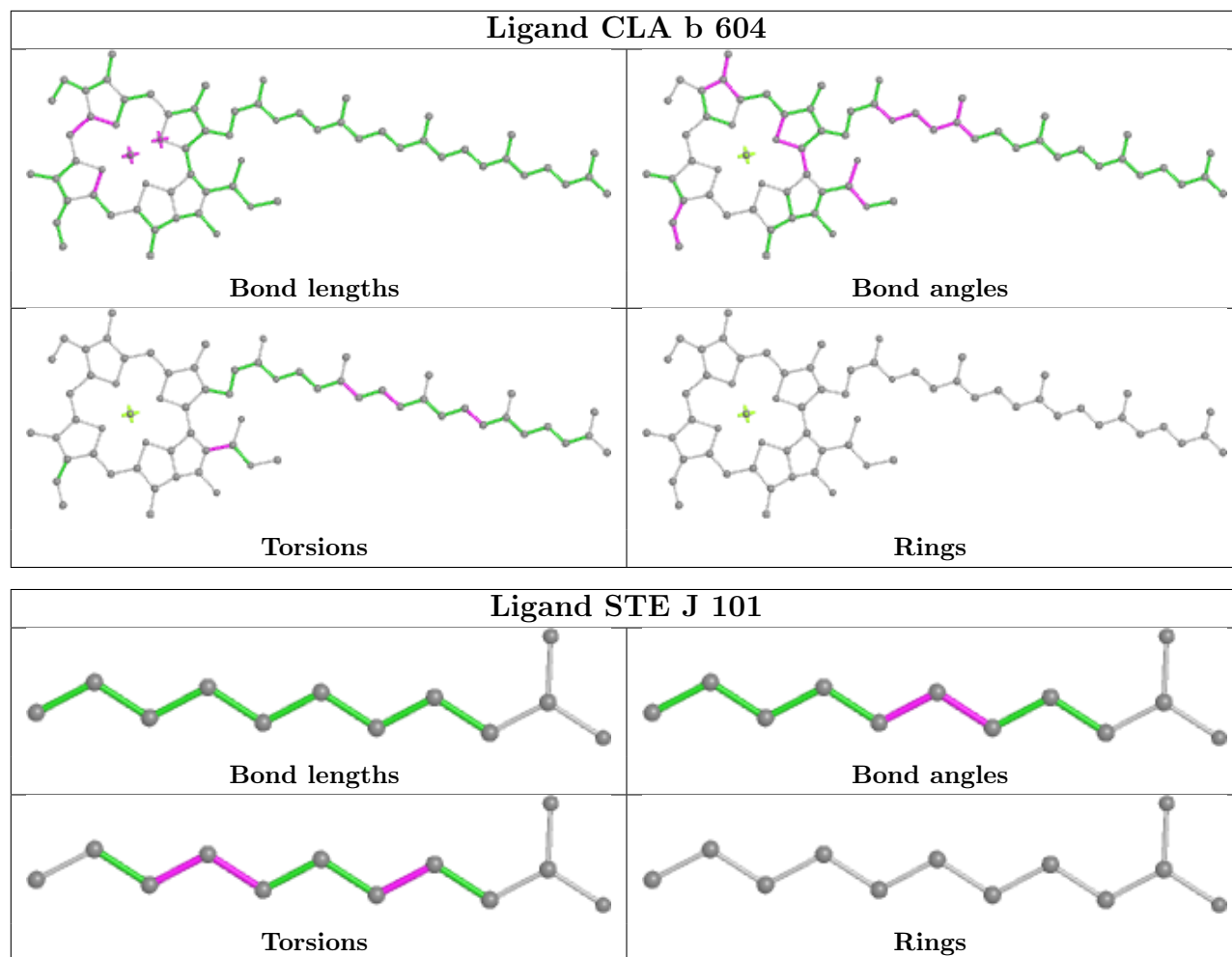


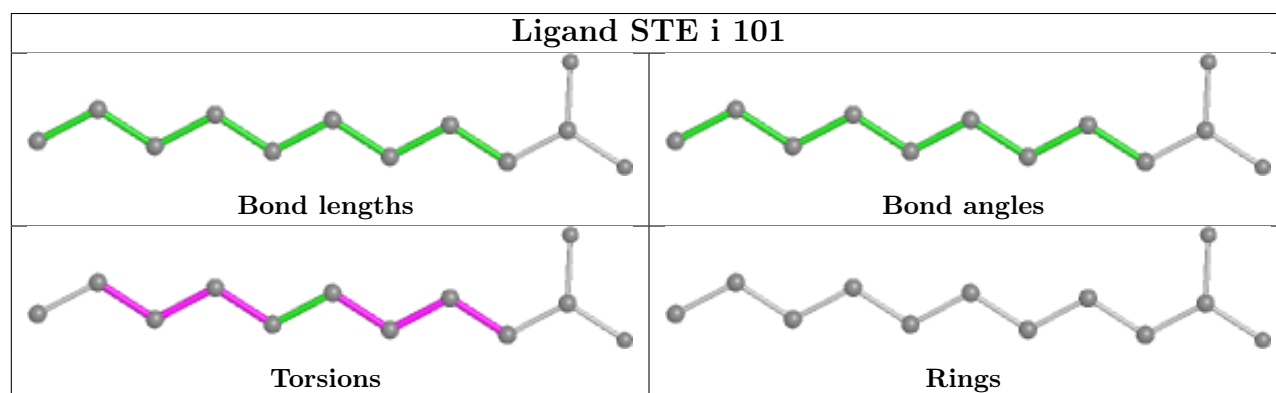
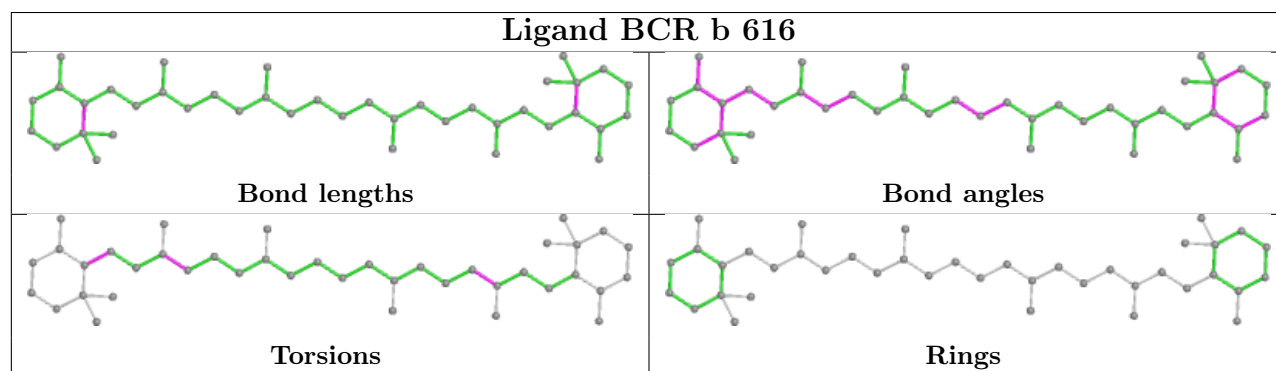
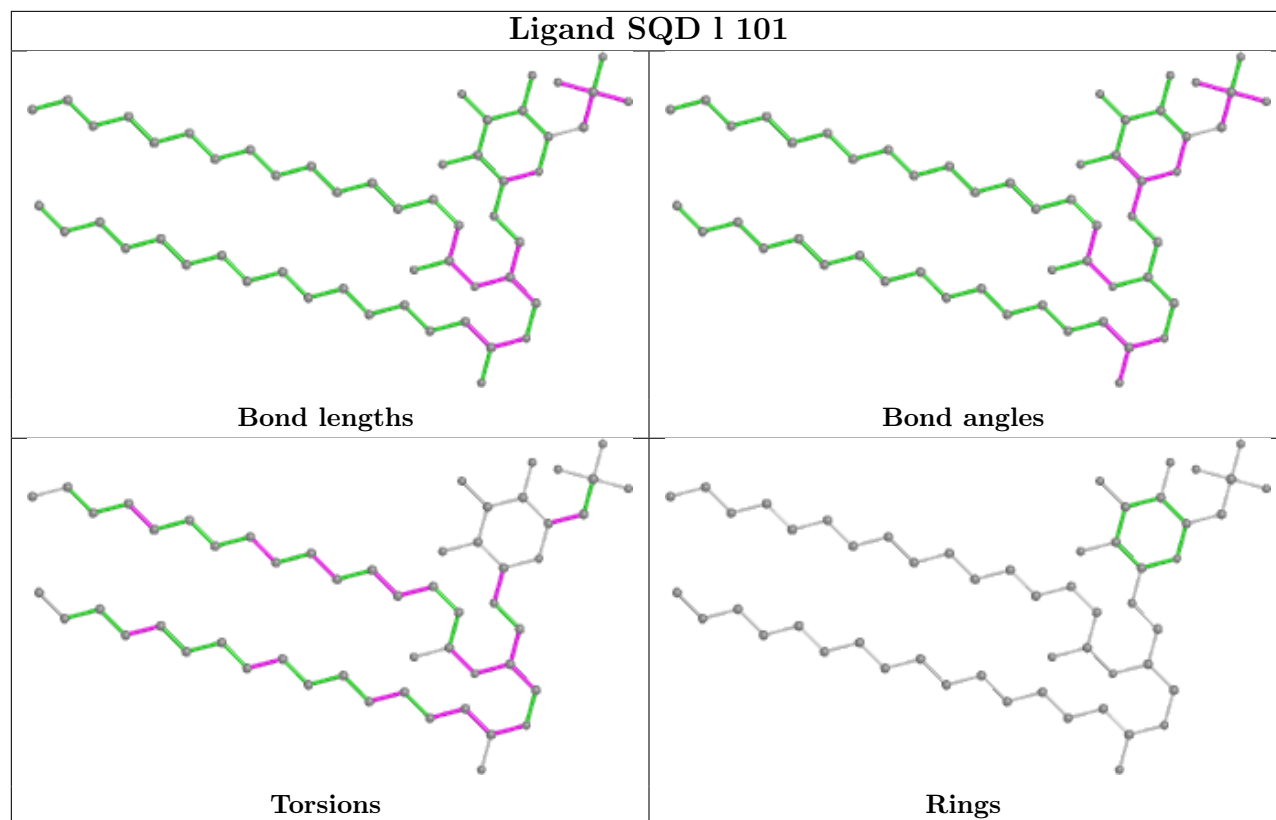




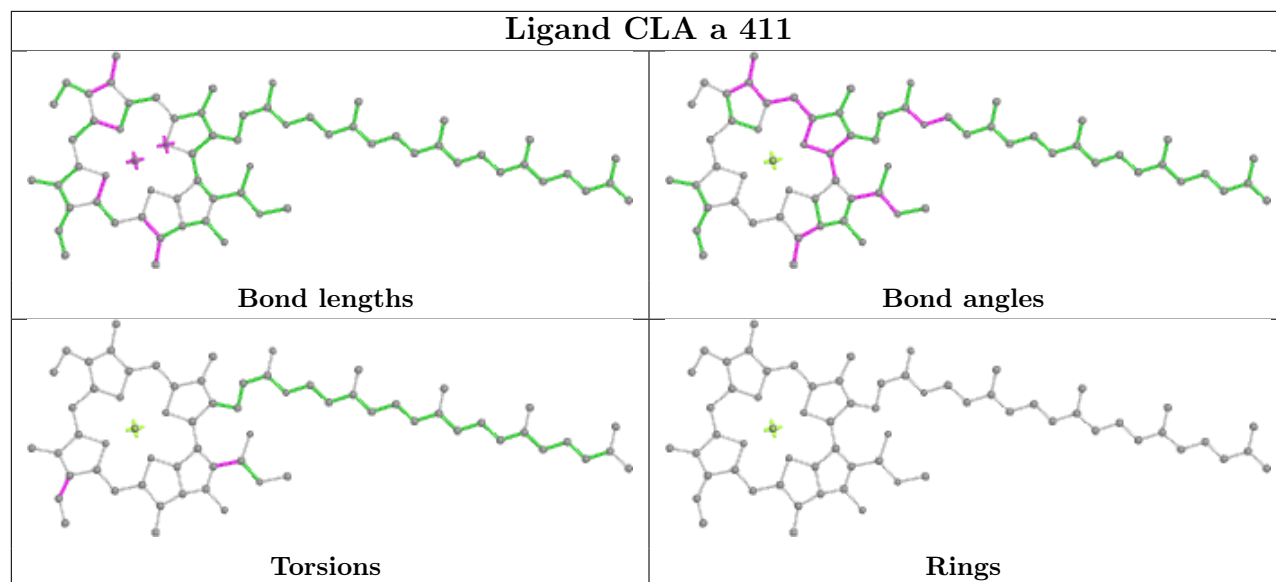




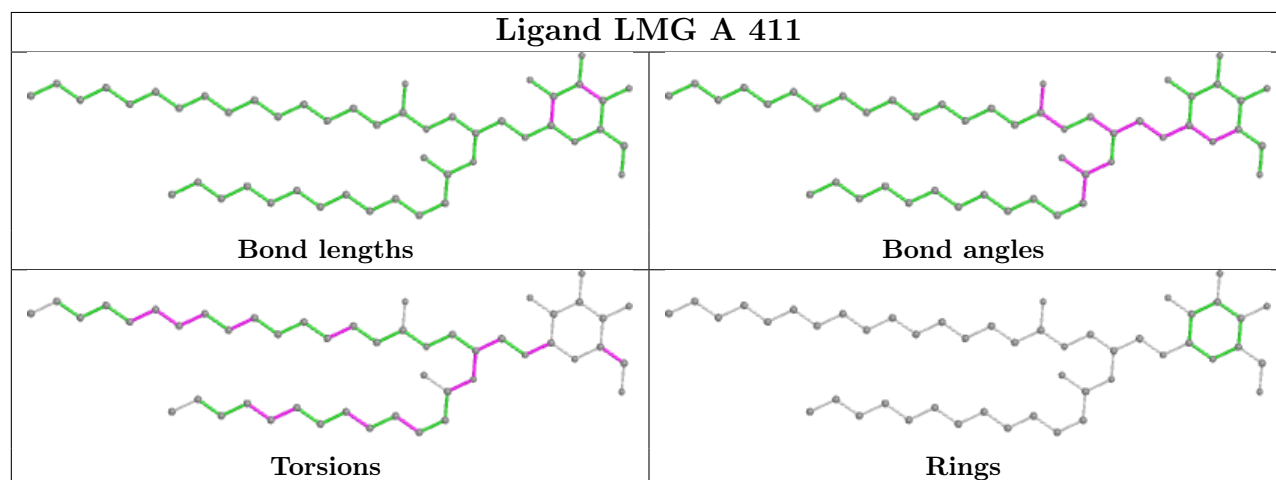




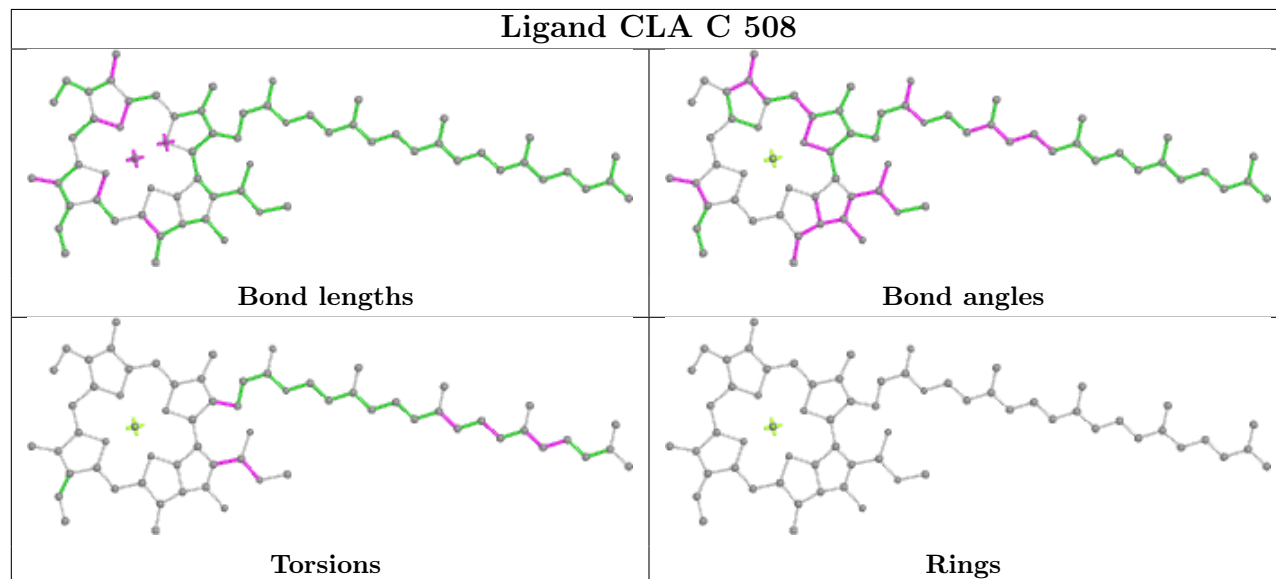
Ligand CLA a 411

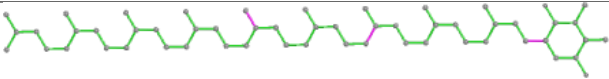
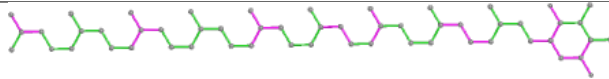
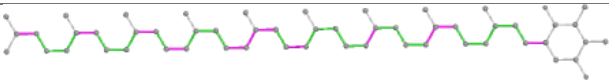
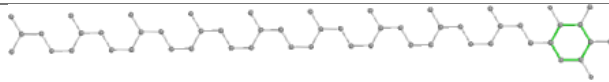


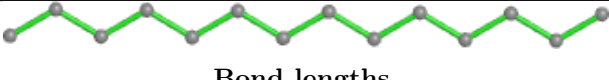
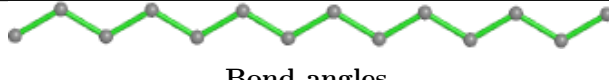


Ligand LMG A 411

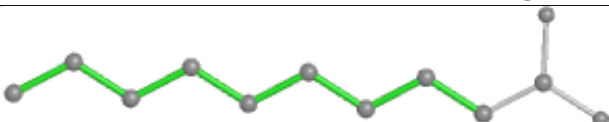
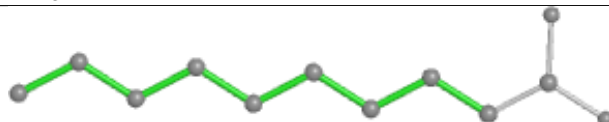
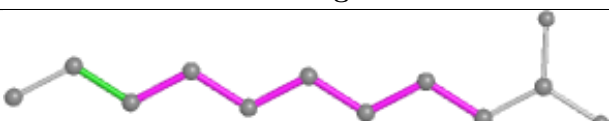
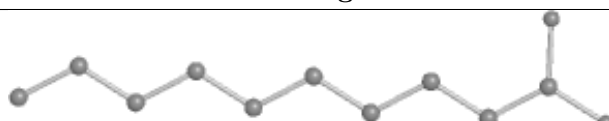



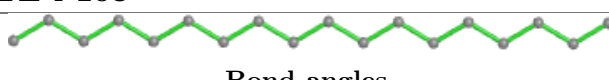


Ligand CLA C 508

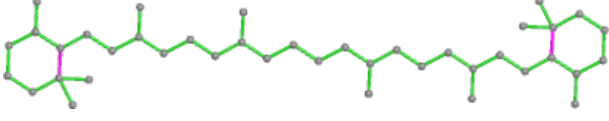
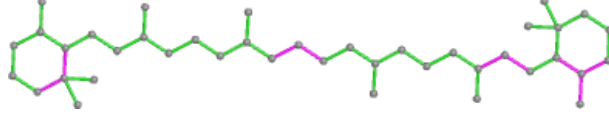
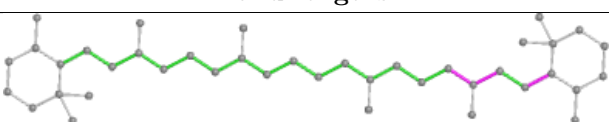
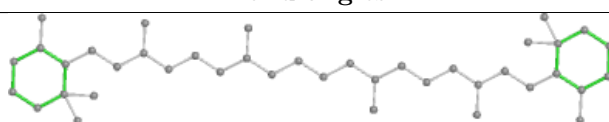


Ligand PL9 A 409	
 Bond lengths	 Bond angles
 Torsions	 Rings

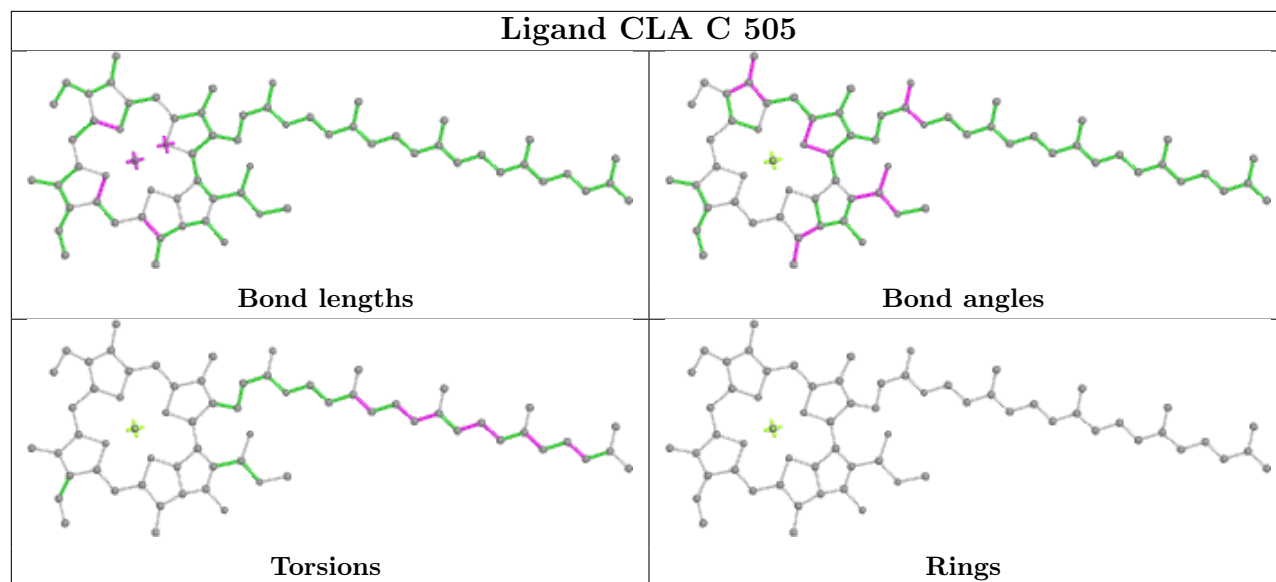
Ligand STE C 528	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand STE j 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

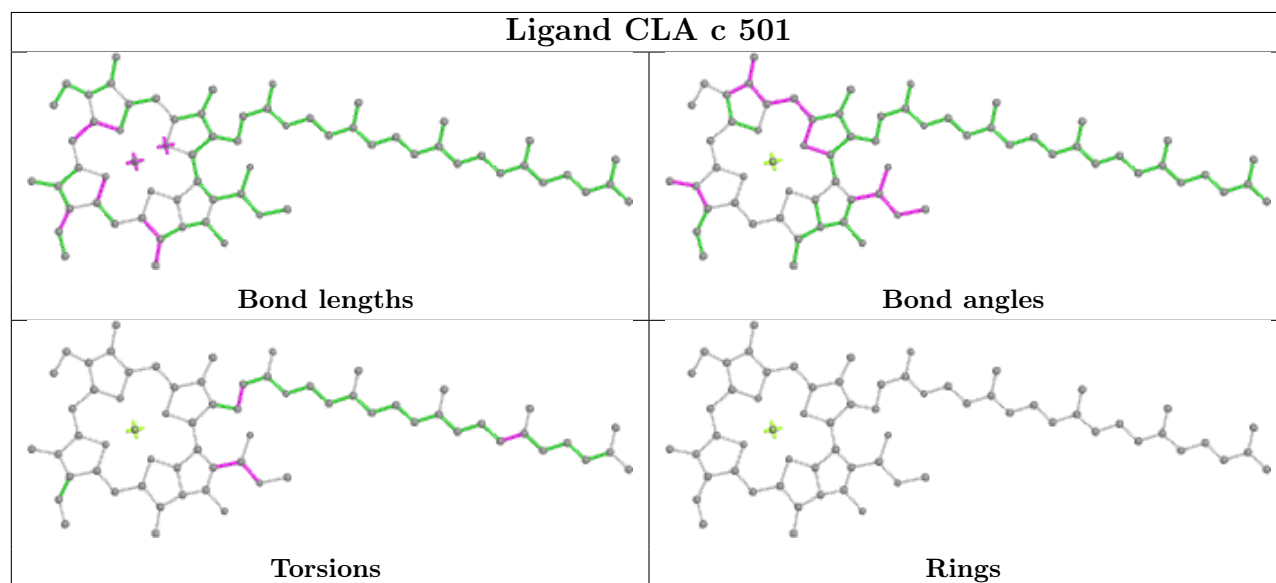
Ligand STE l 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

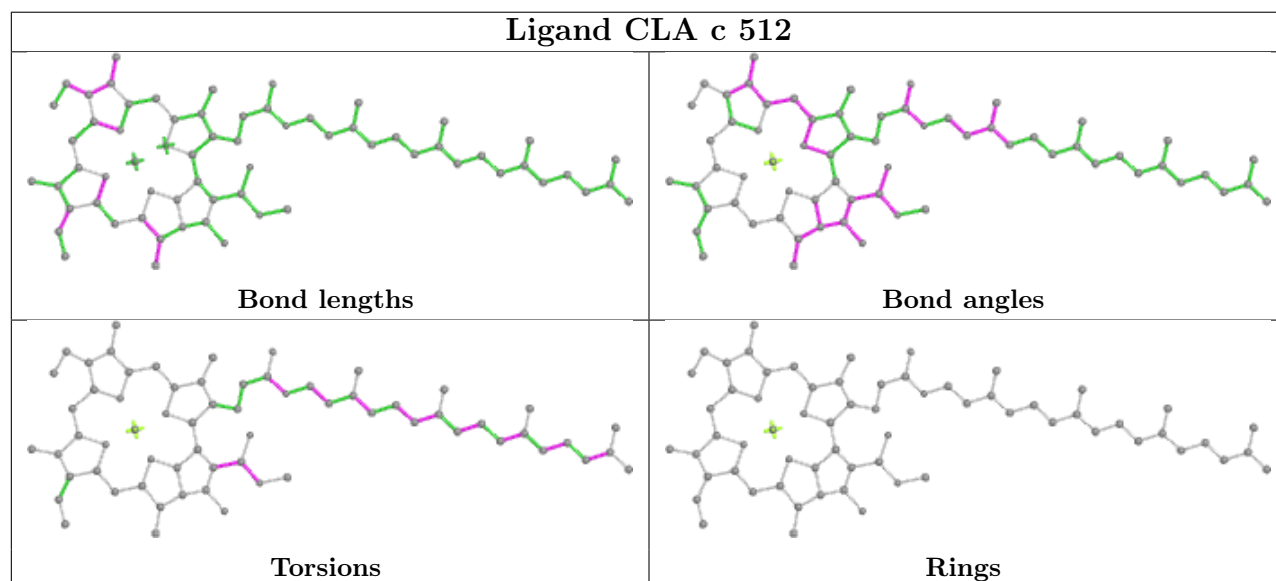
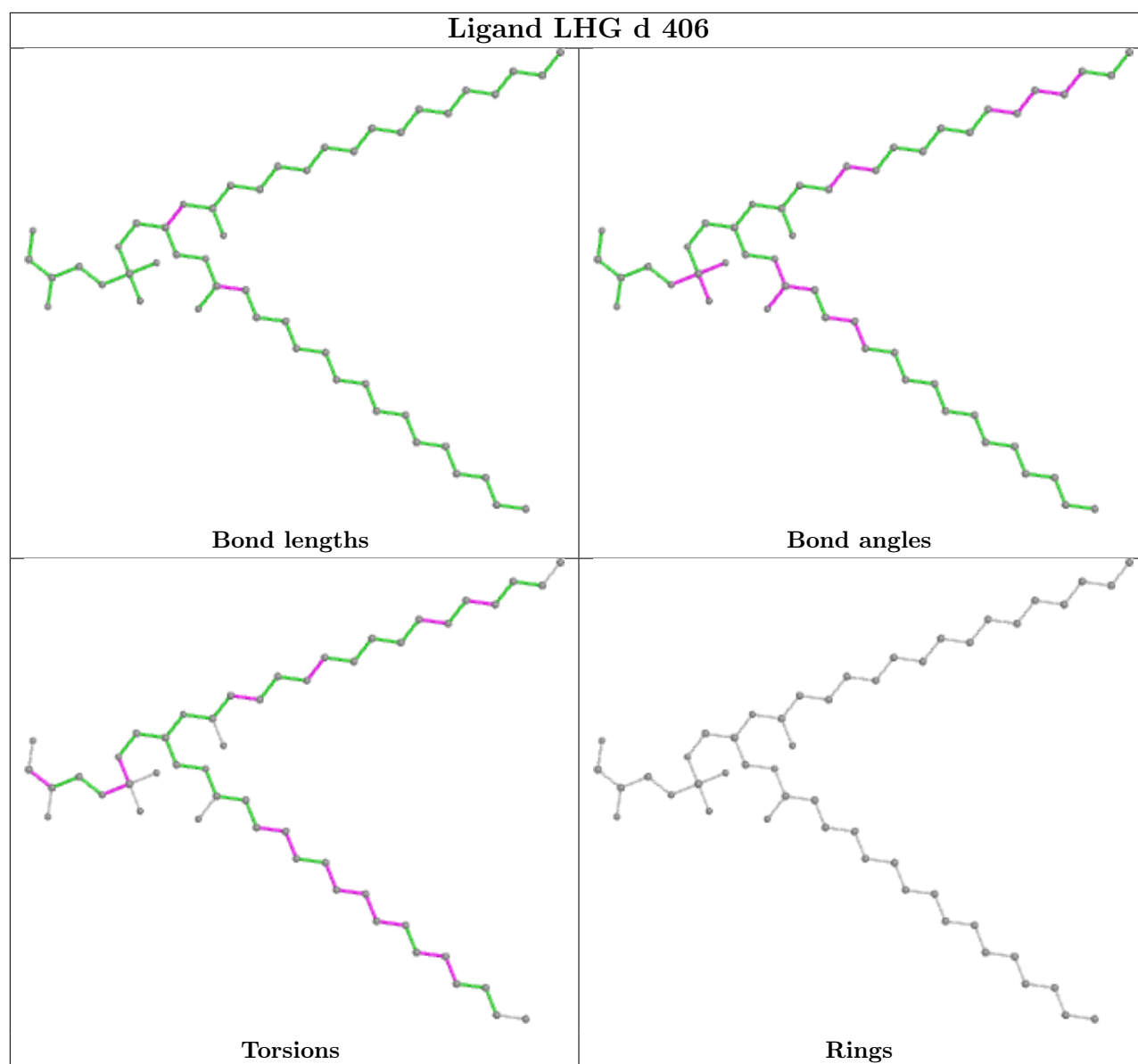
Ligand BCR D 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 505

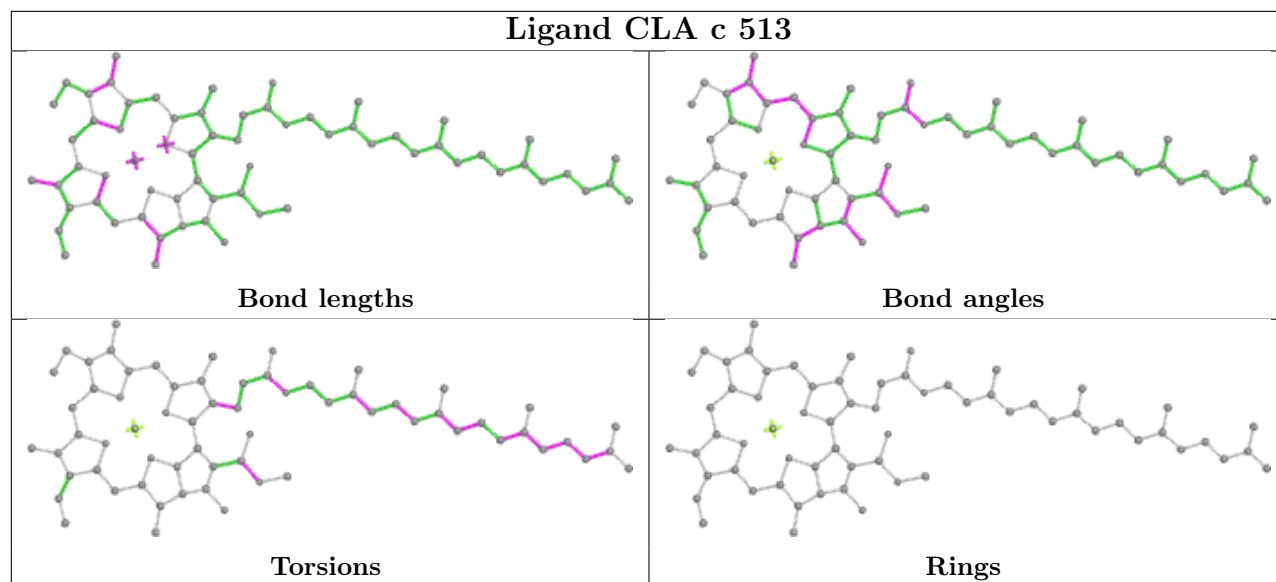


Ligand CLA c 501

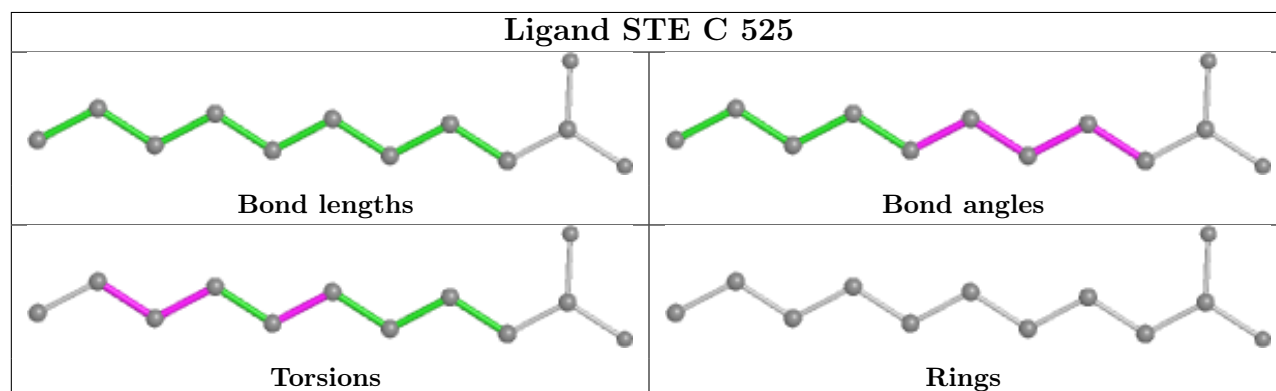




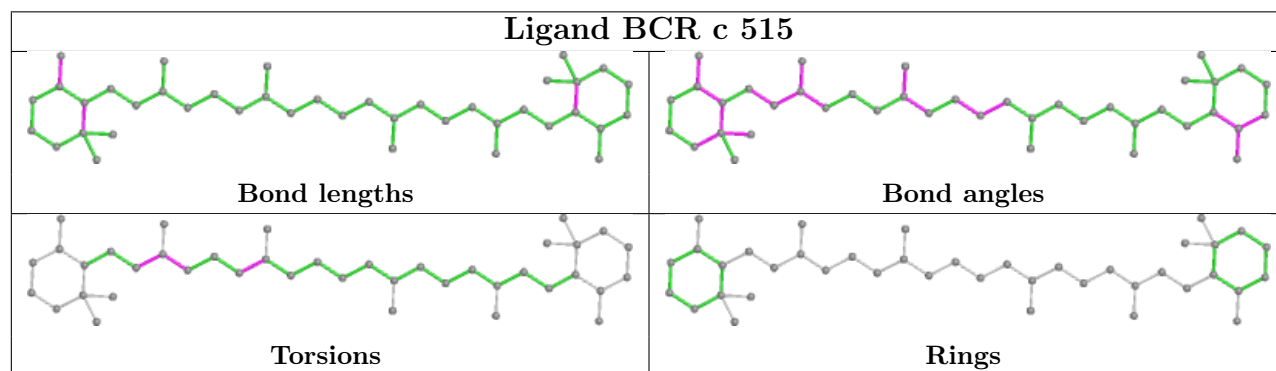
Ligand CLA c 513



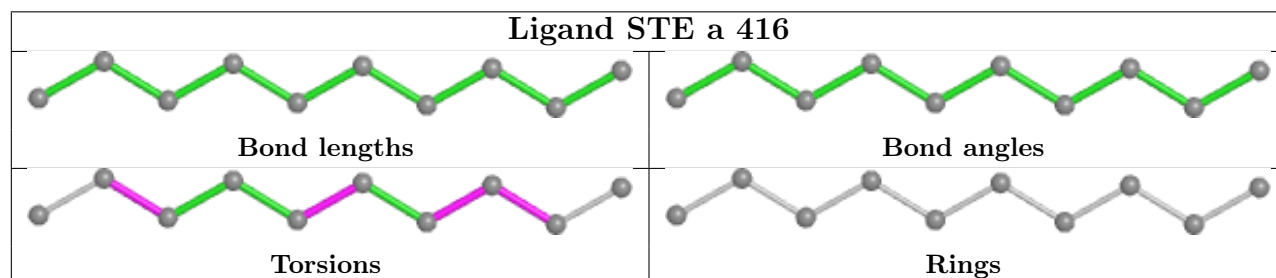
Ligand STE C 525

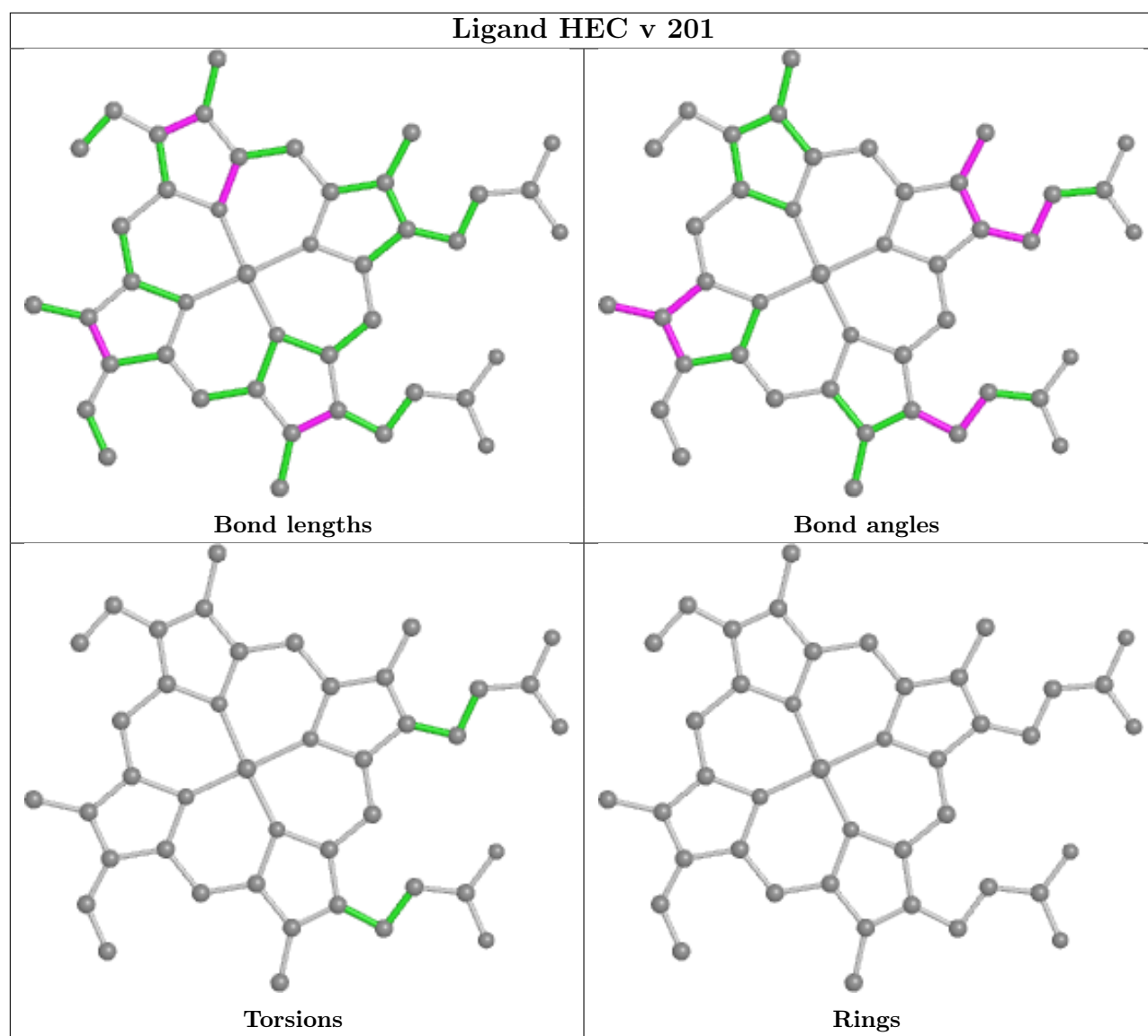
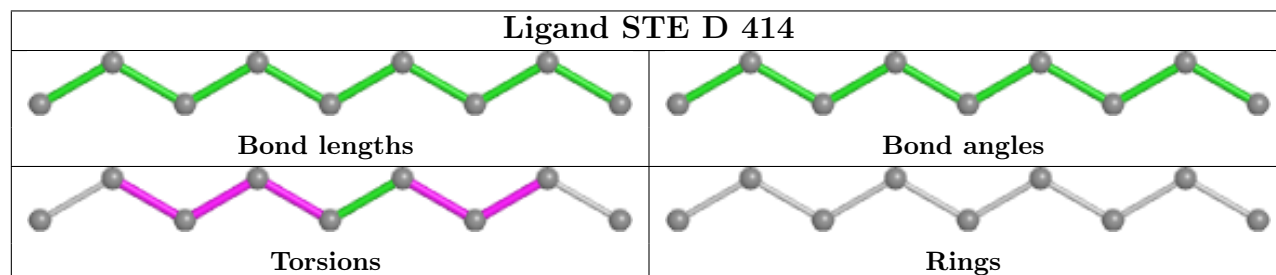
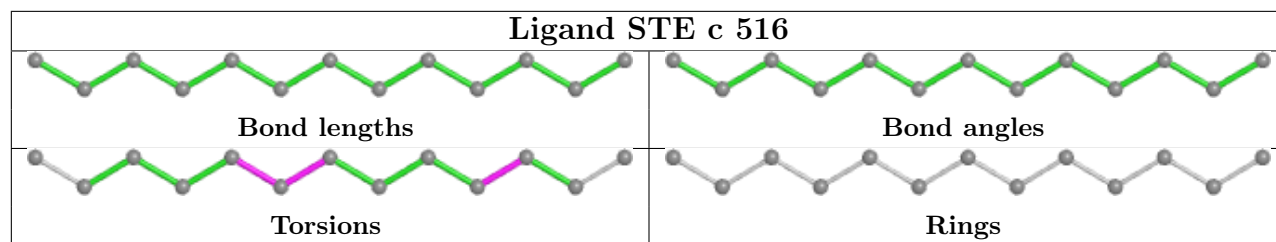


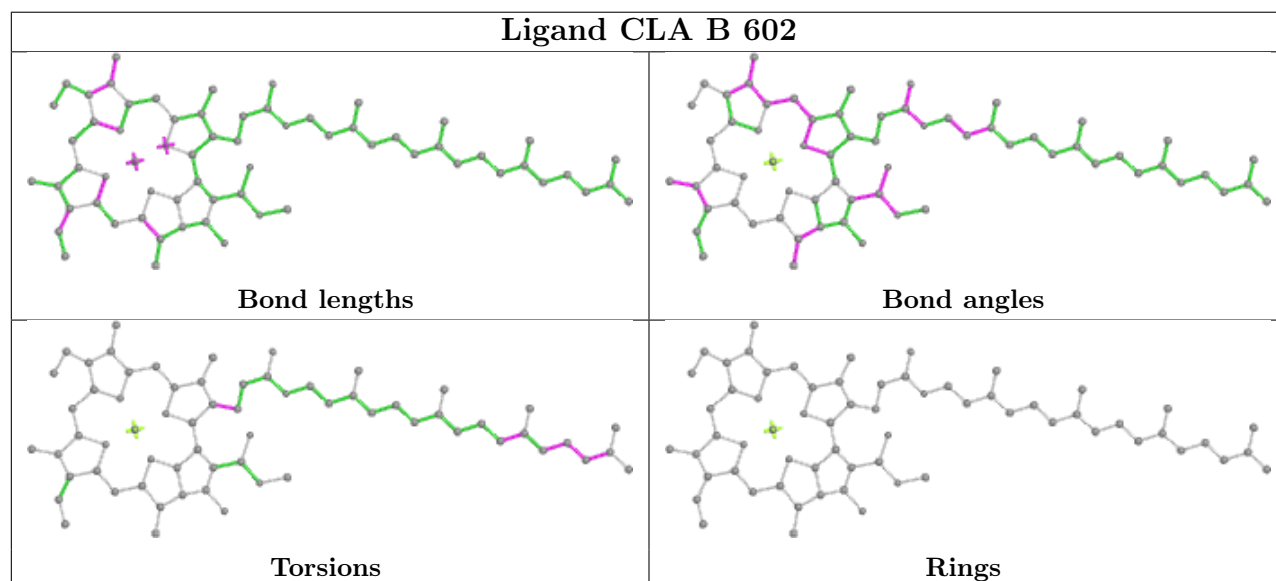
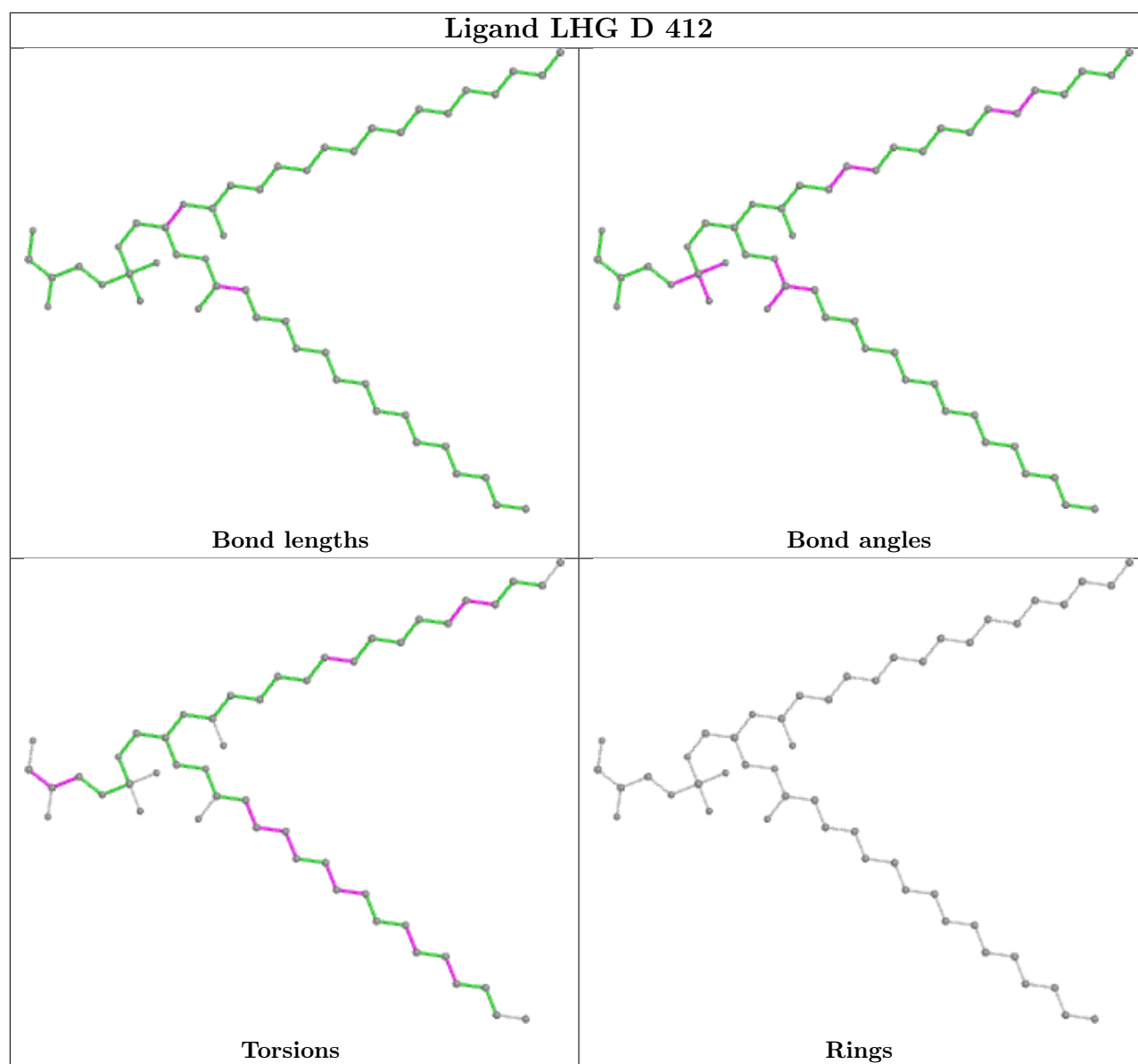
Ligand BCR c 515



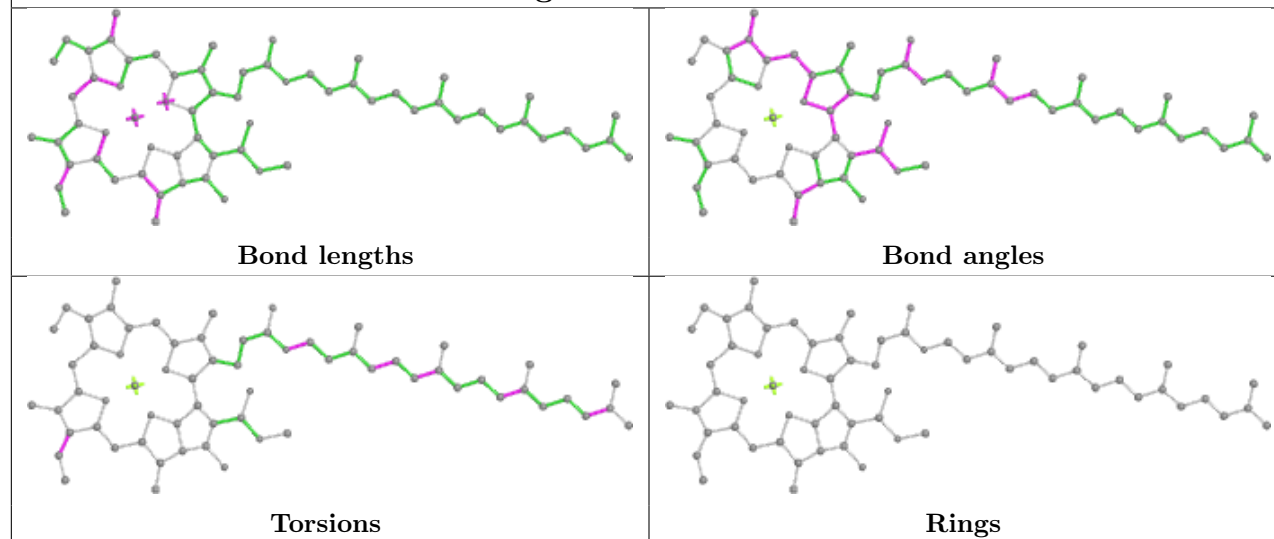
Ligand STE a 416



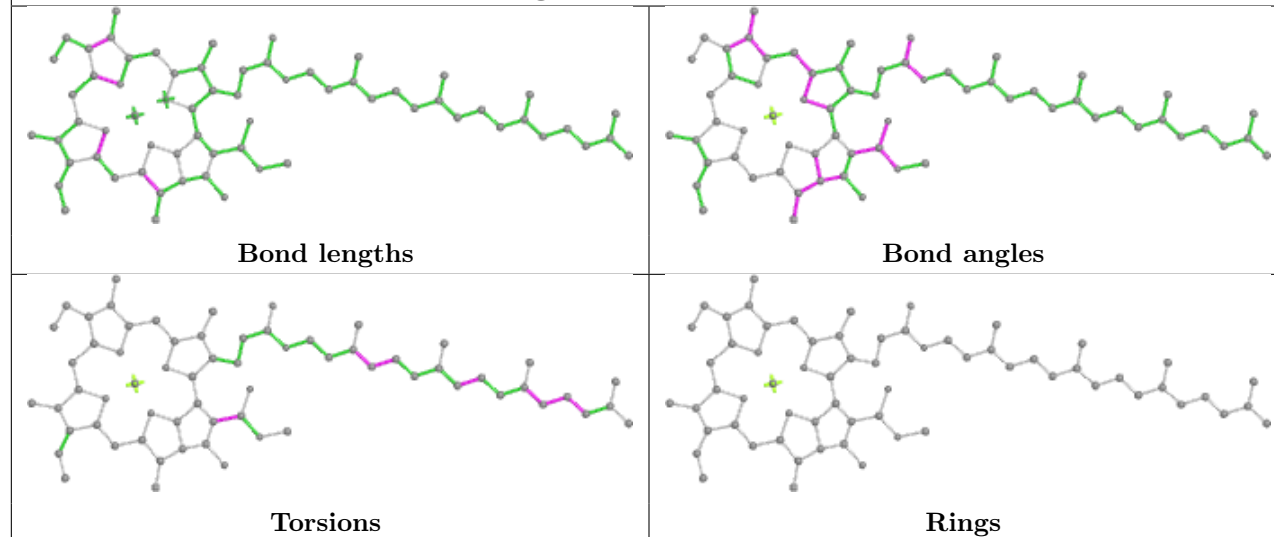




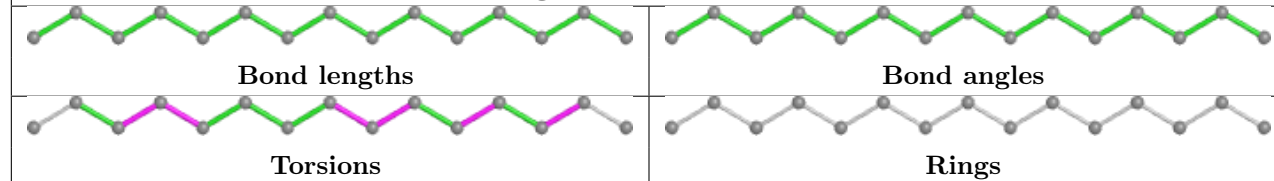
Ligand CLA d 402



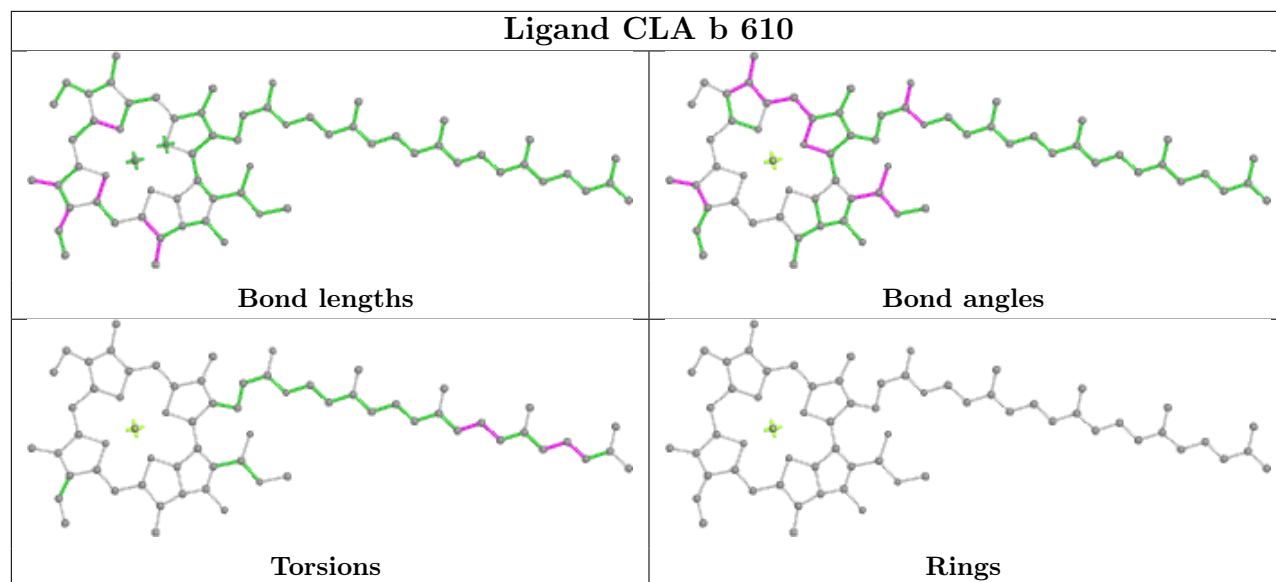
Ligand CLA C 506



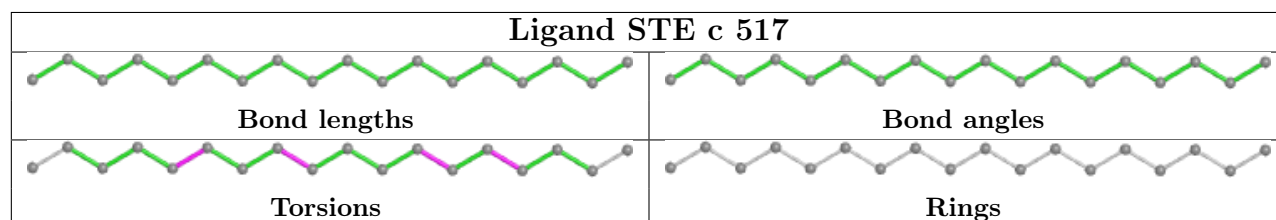
Ligand STE m 102



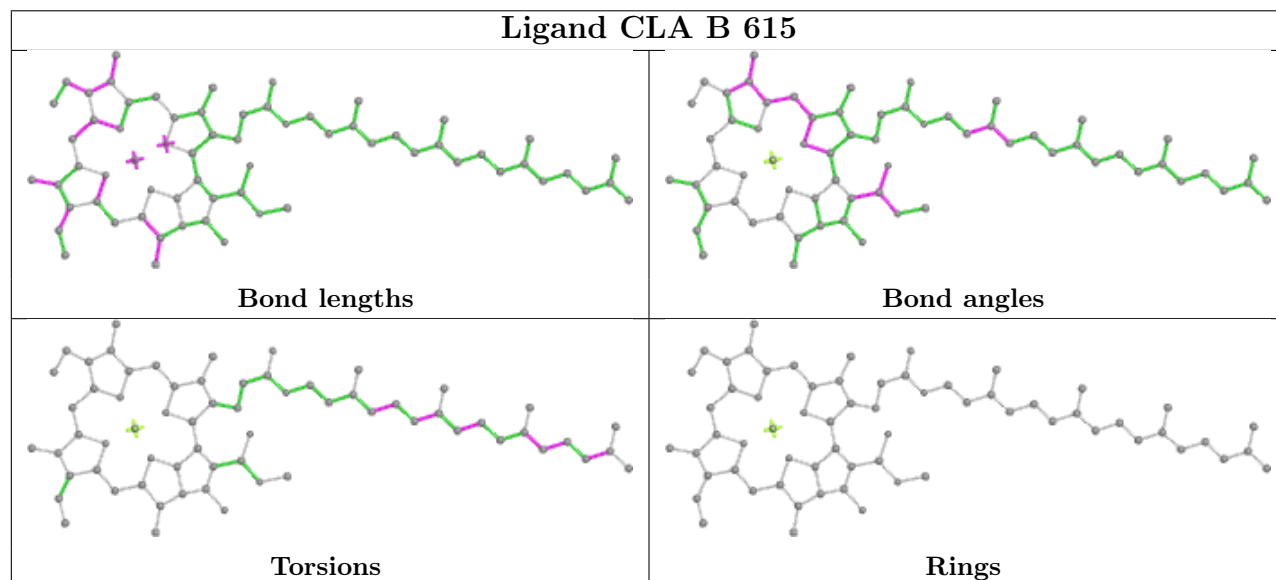
Ligand CLA b 610



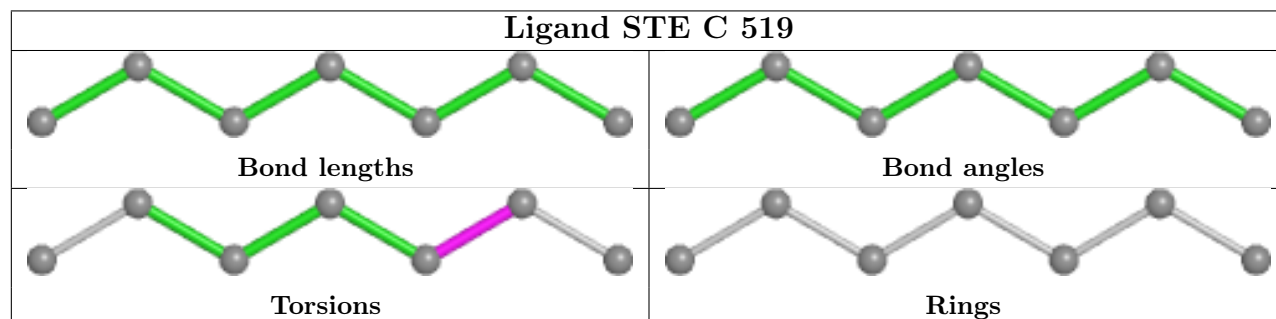
Ligand STE c 517

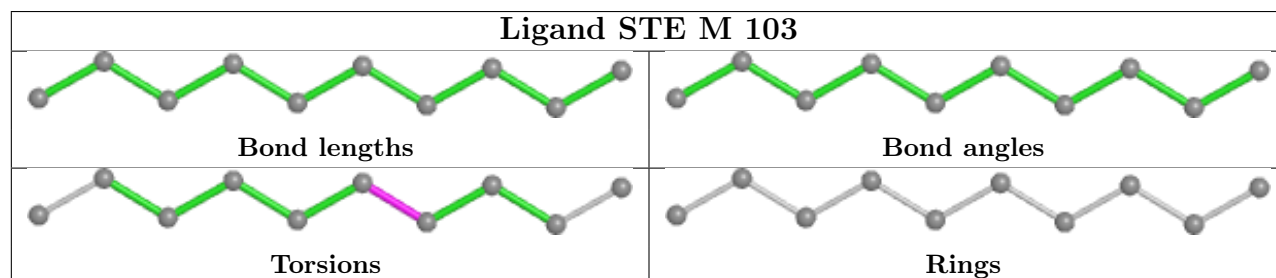
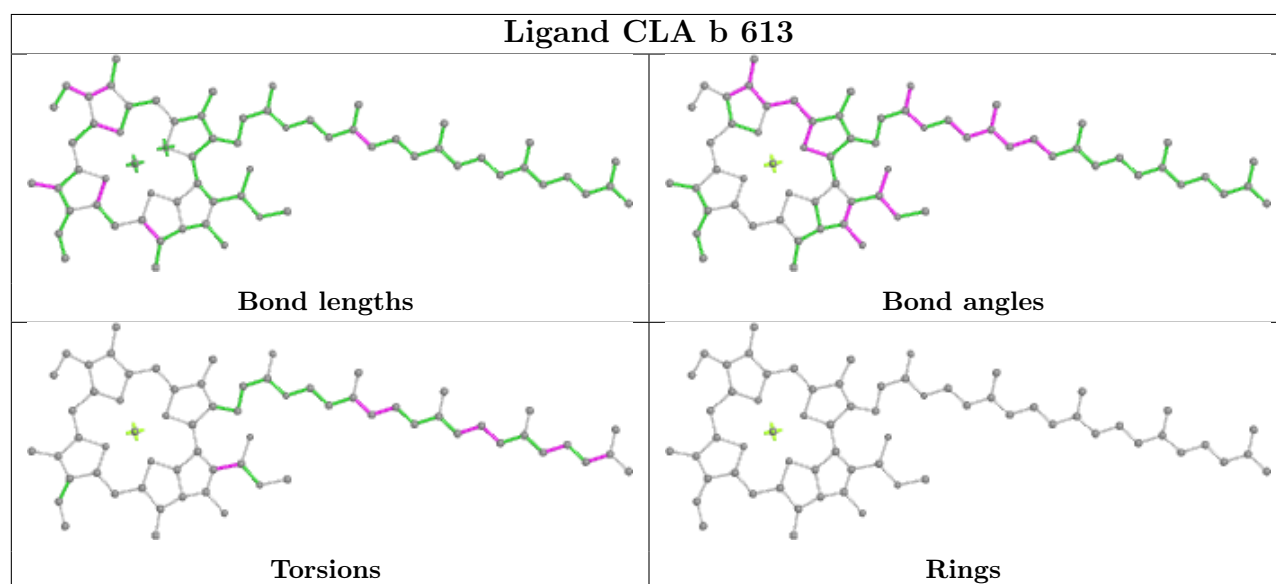
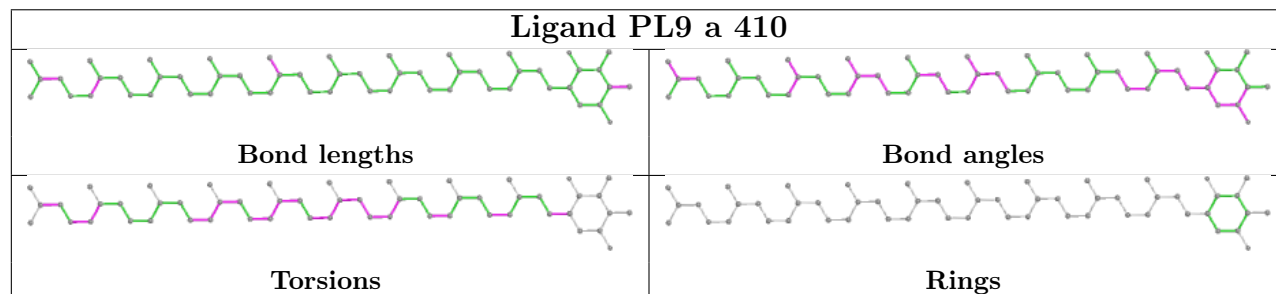
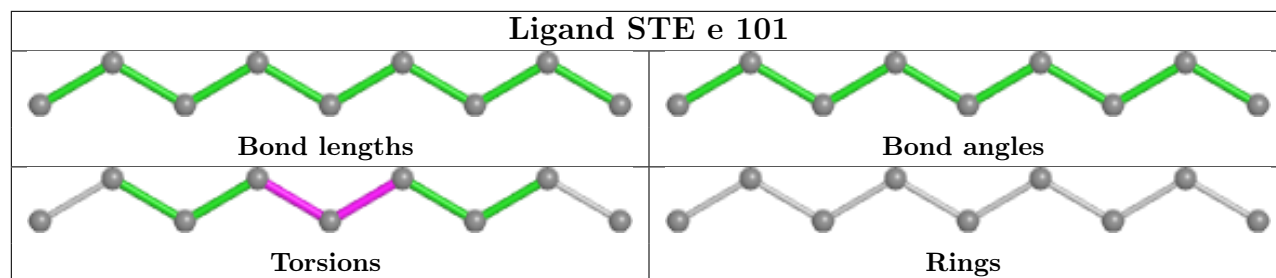


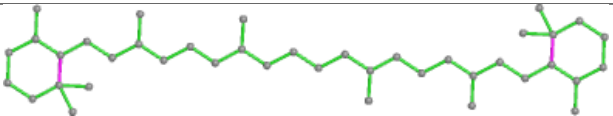
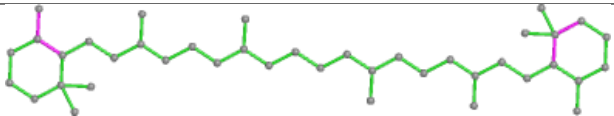
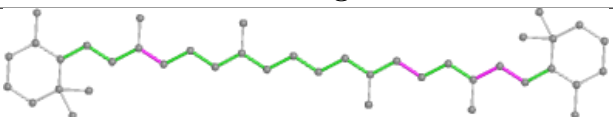
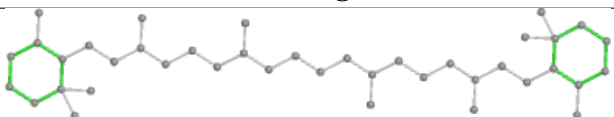
Ligand CLA B 615



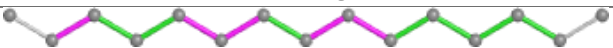



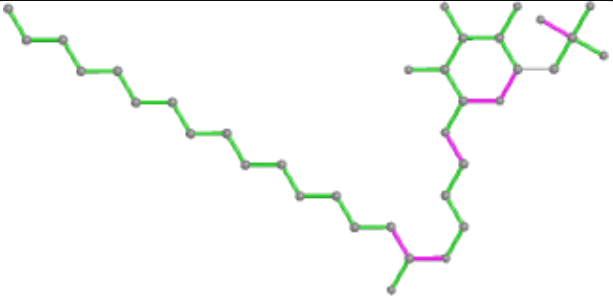
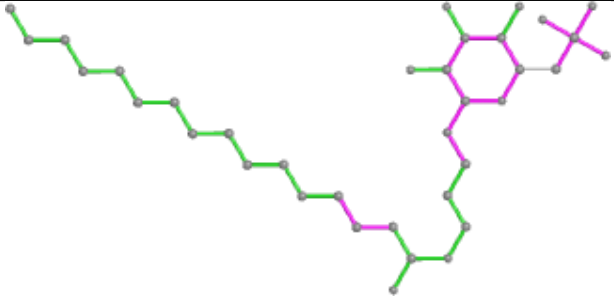
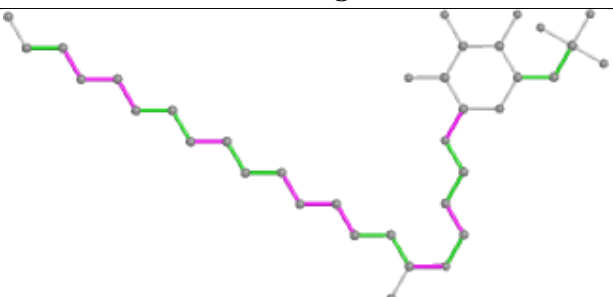
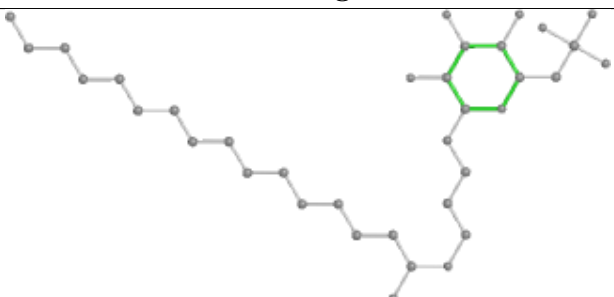
Ligand STE C 519



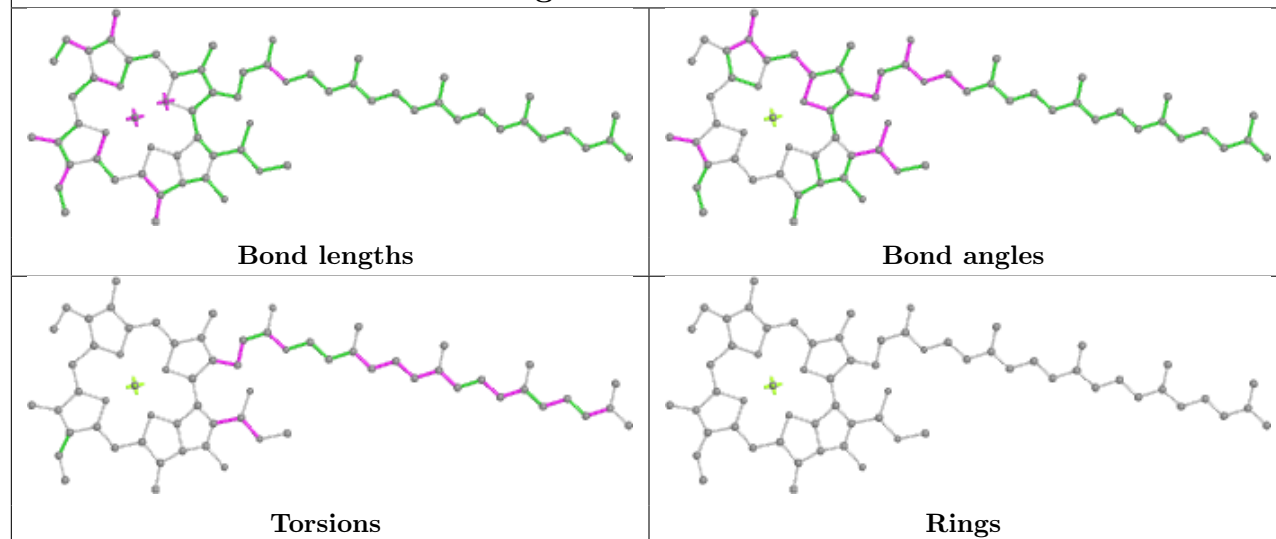


Ligand BCR d 404	
	Bond lengths
	Bond angles
	Torsions
	Rings

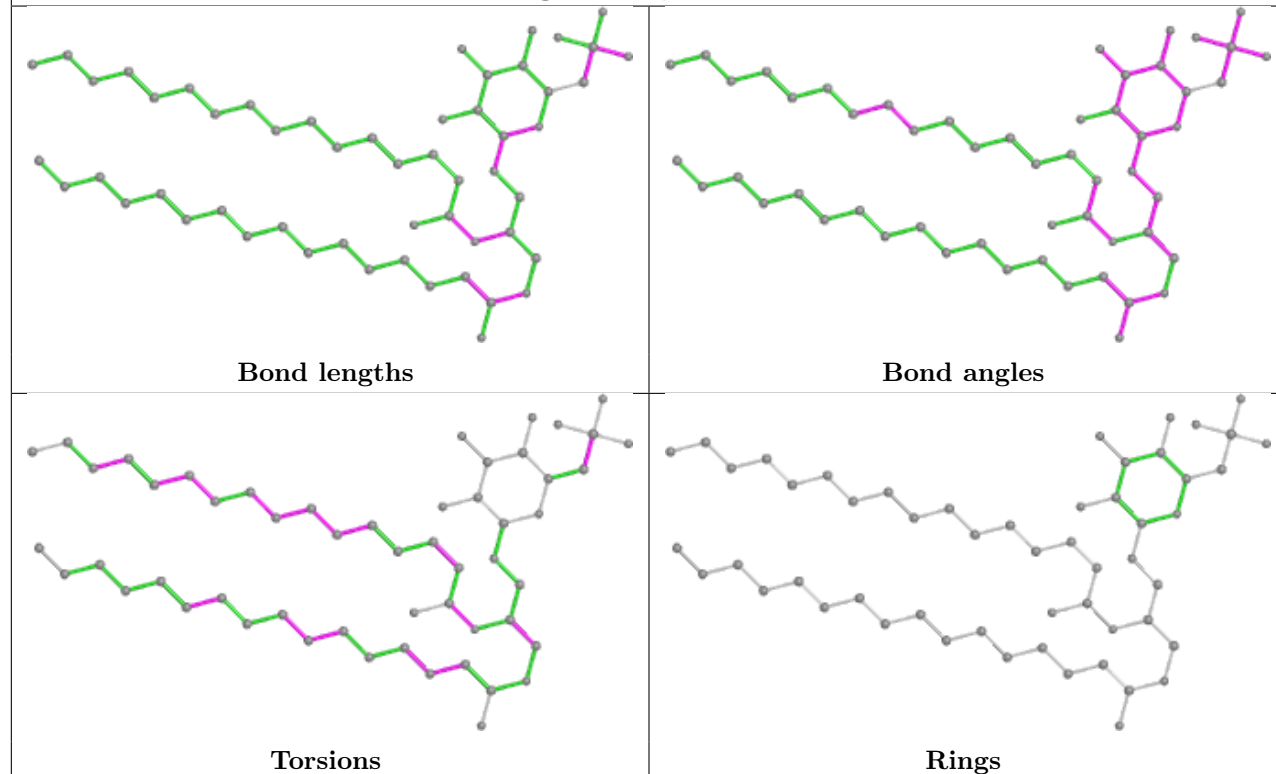
Ligand STE I 101	
	Bond lengths
	Bond angles
	Torsions
	Rings

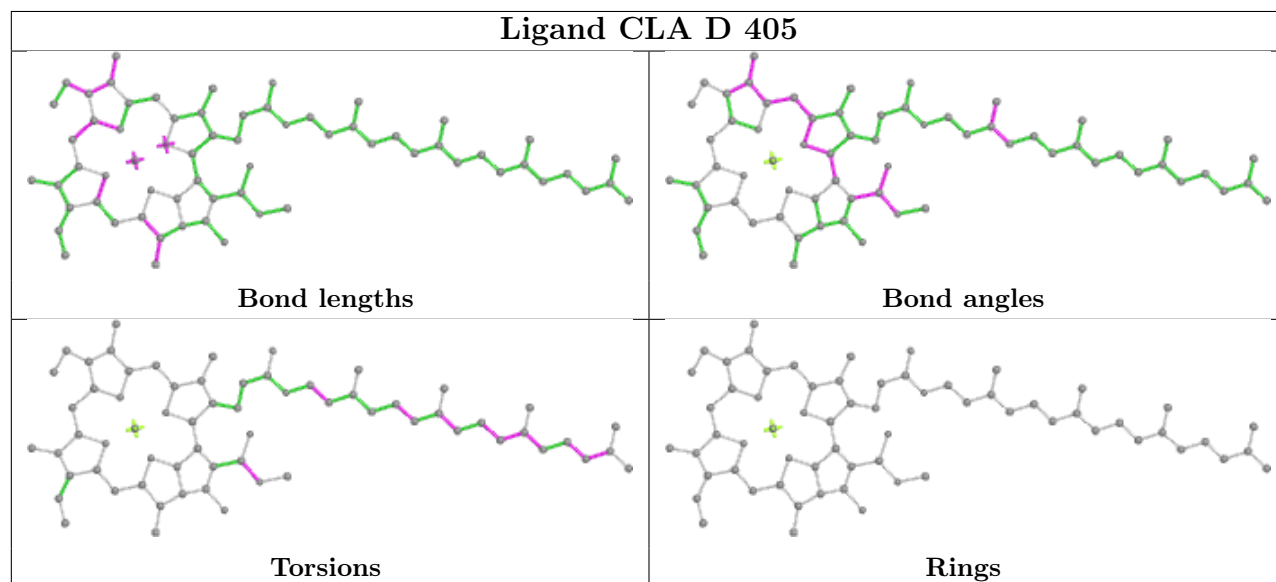
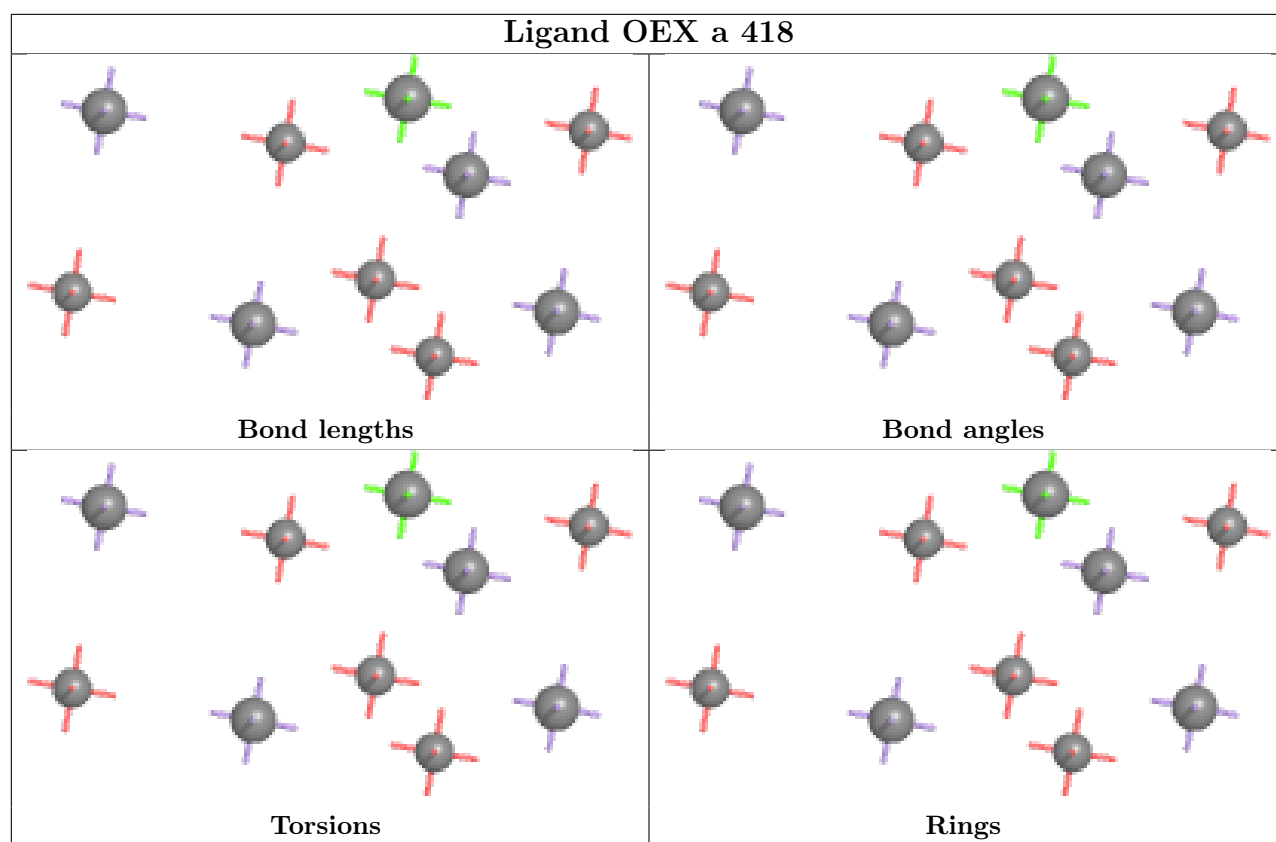
Ligand SQD F 102	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand CLA h 101

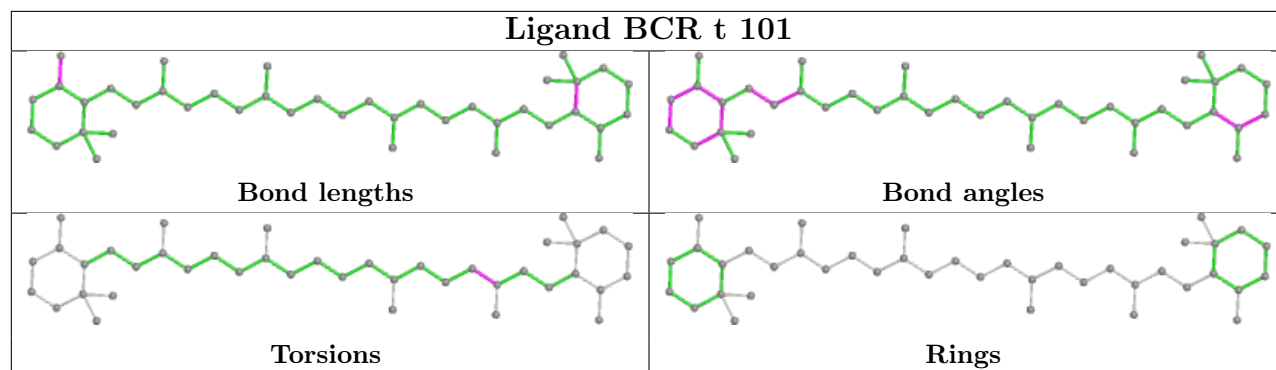


Ligand SQD a 412

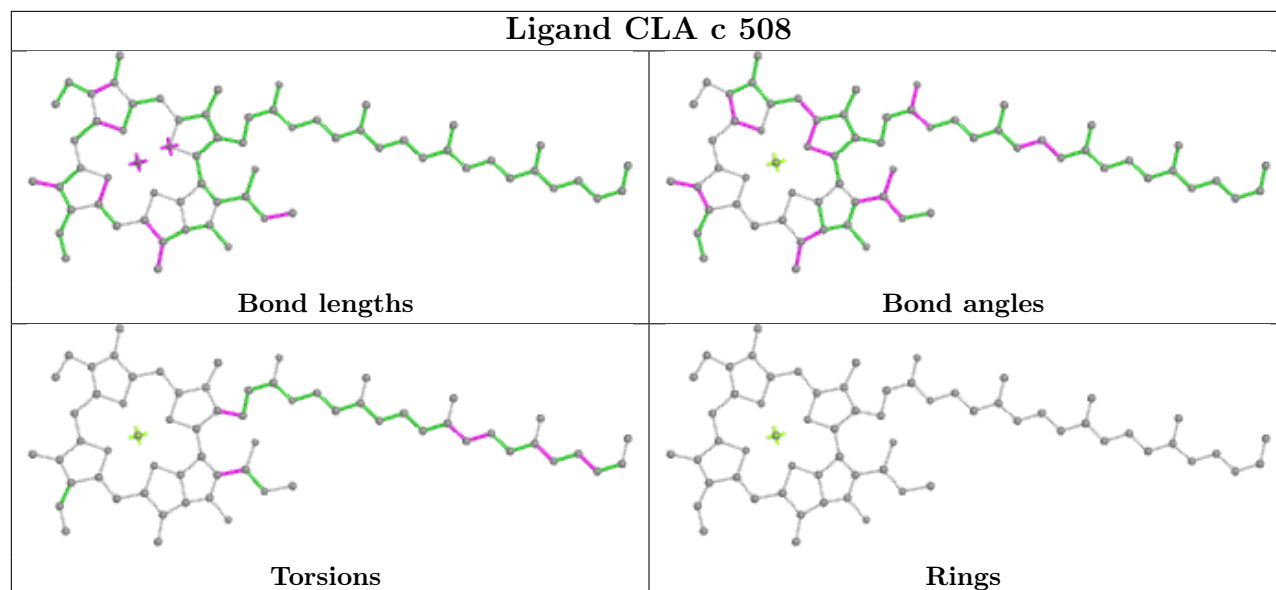




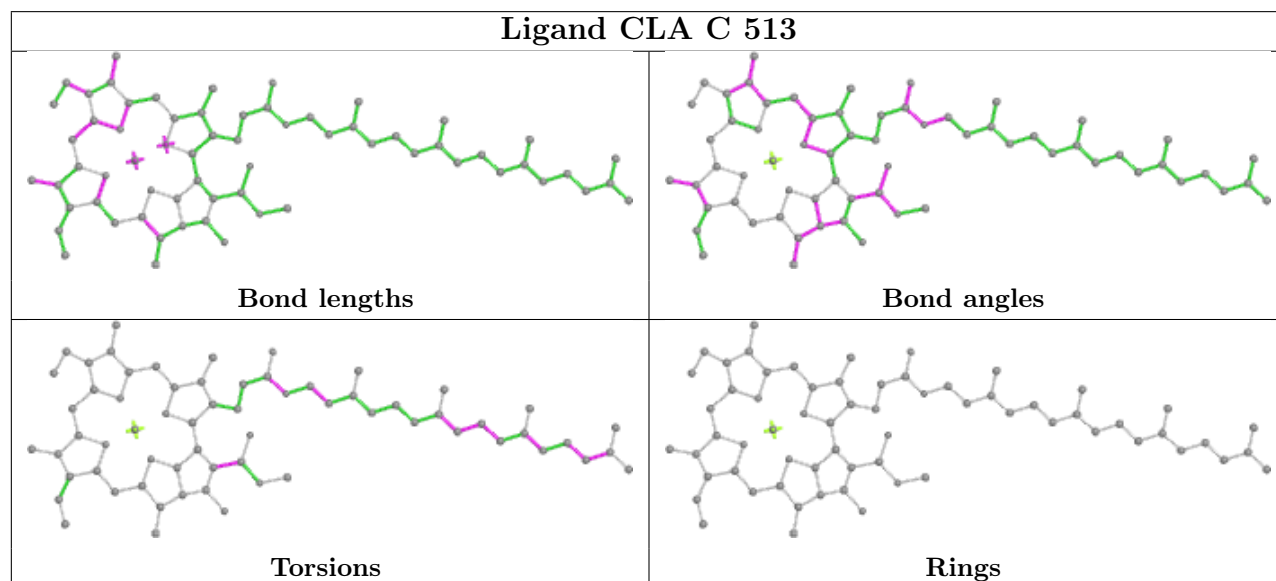
Ligand BCR t 101



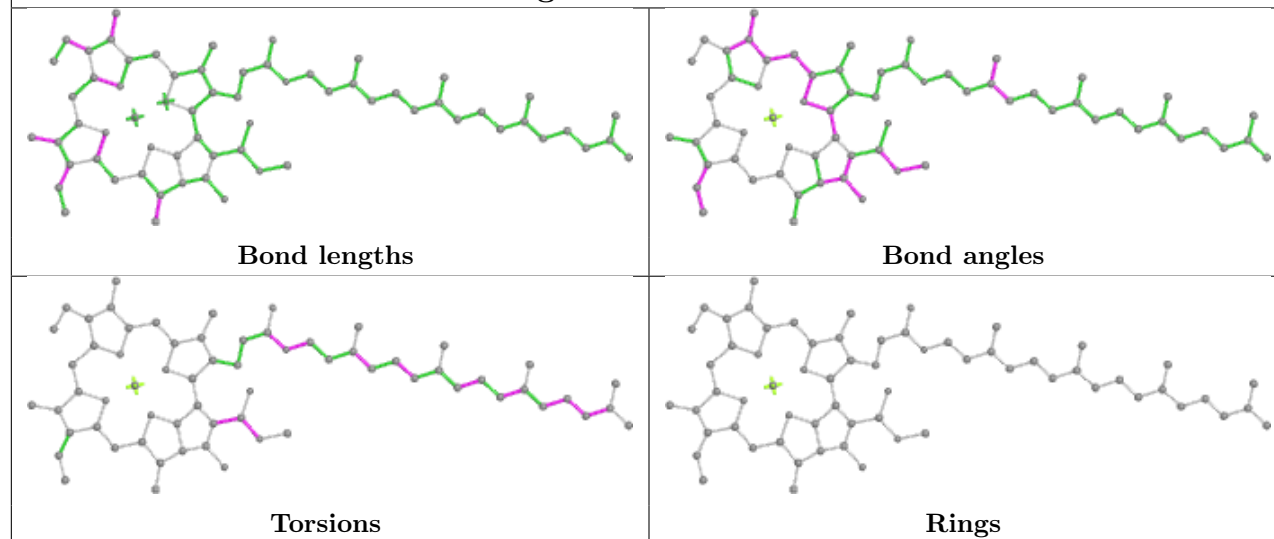
Ligand CLA c 508



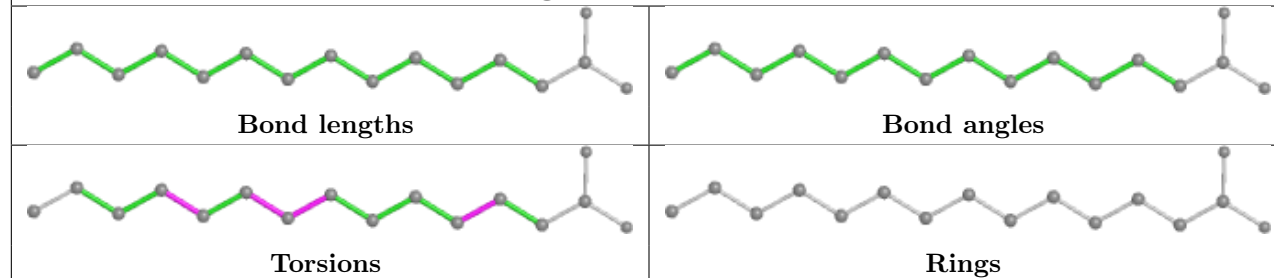
Ligand CLA C 513



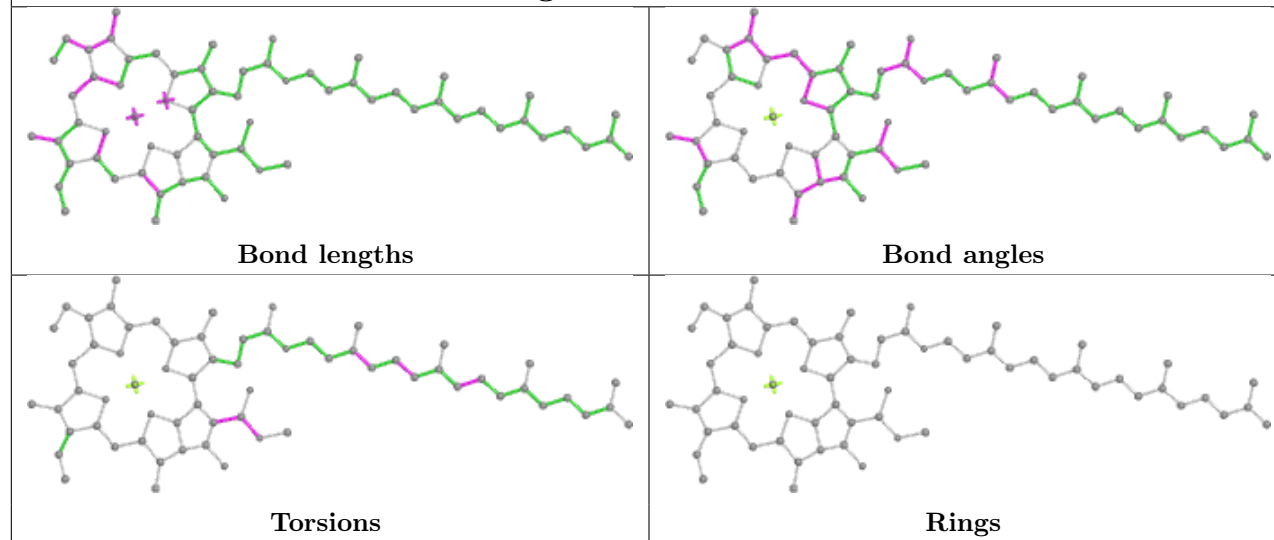
Ligand CLA c 506



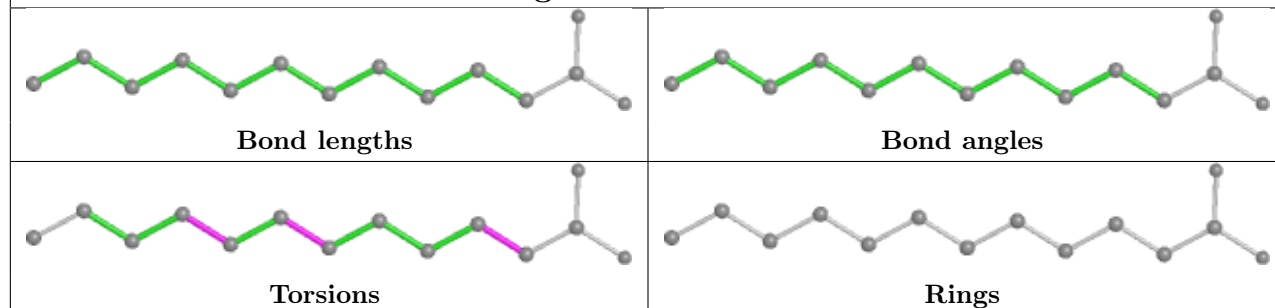
Ligand STE b 625



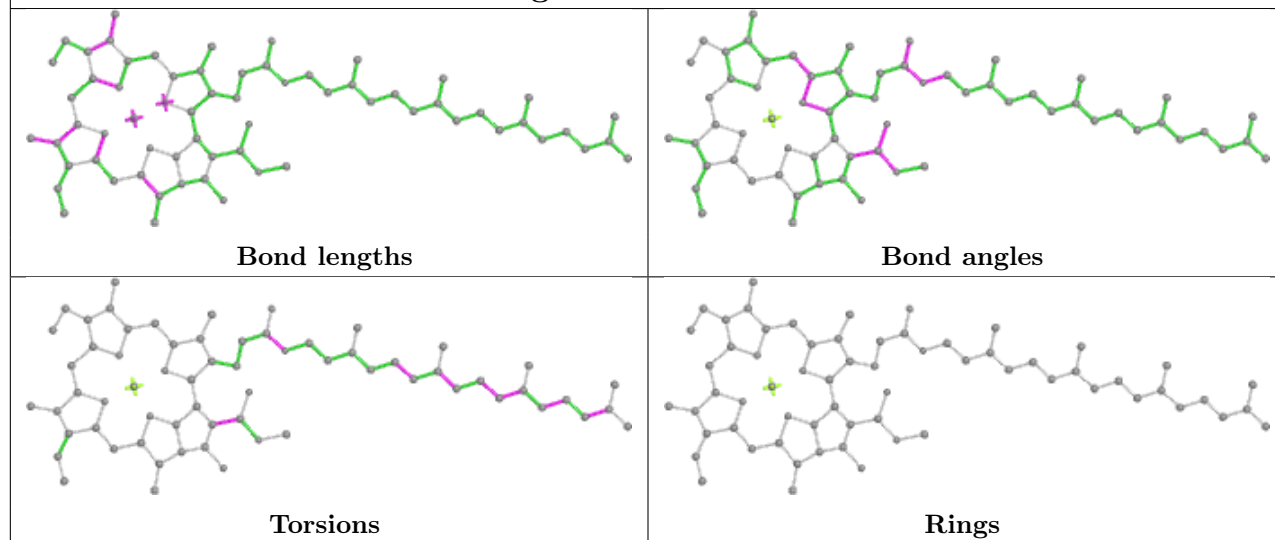
Ligand CLA c 507



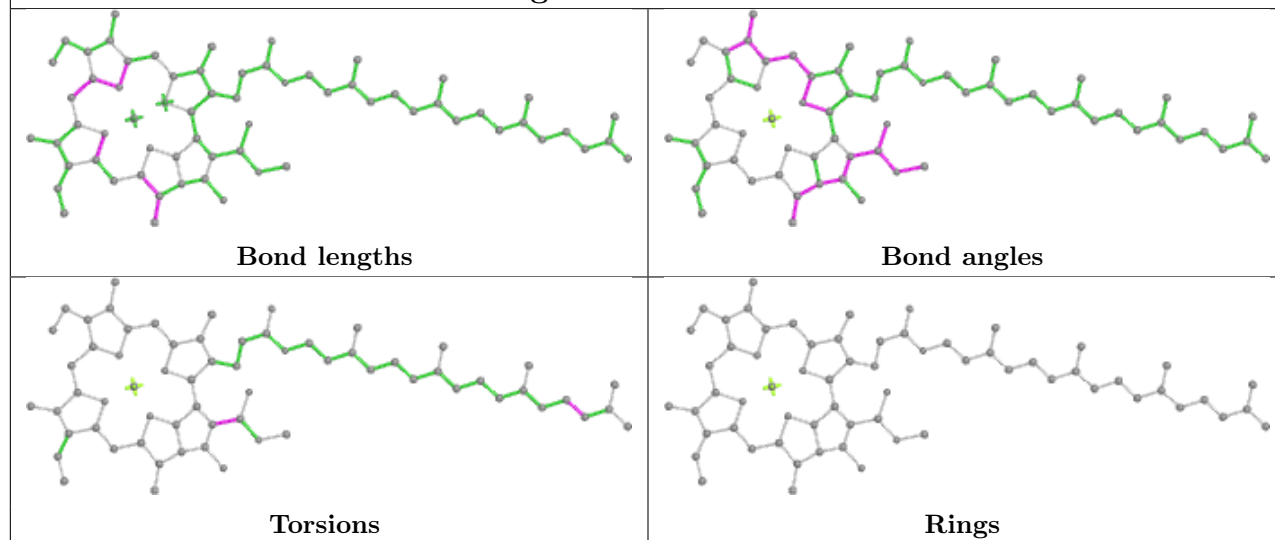
Ligand STE C 516



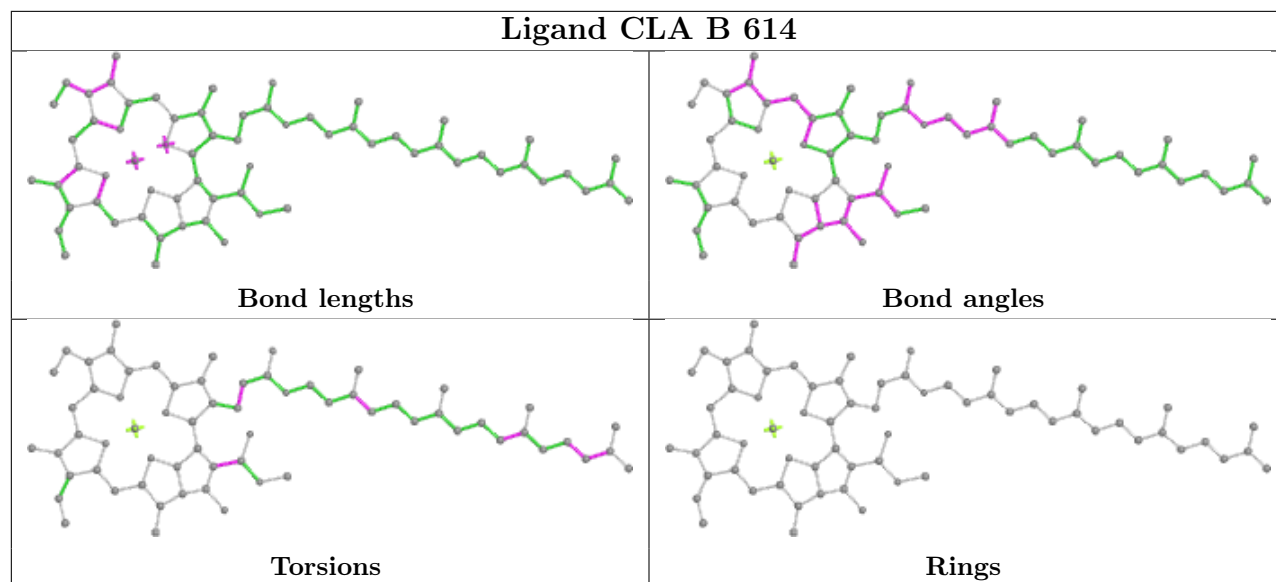
Ligand CLA B 601



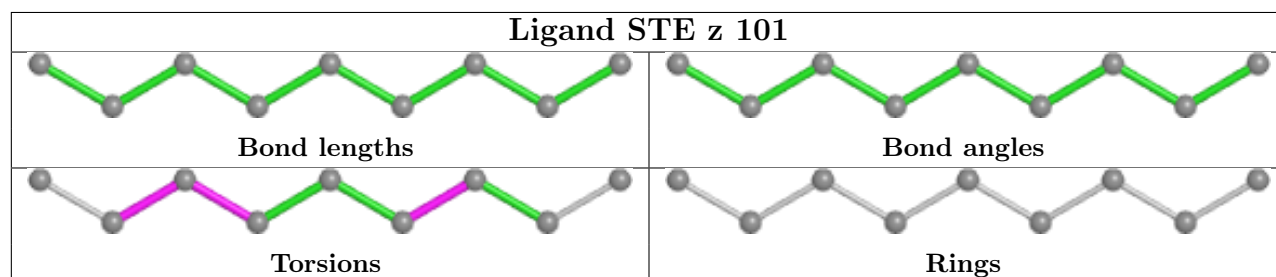
Ligand CLA A 405



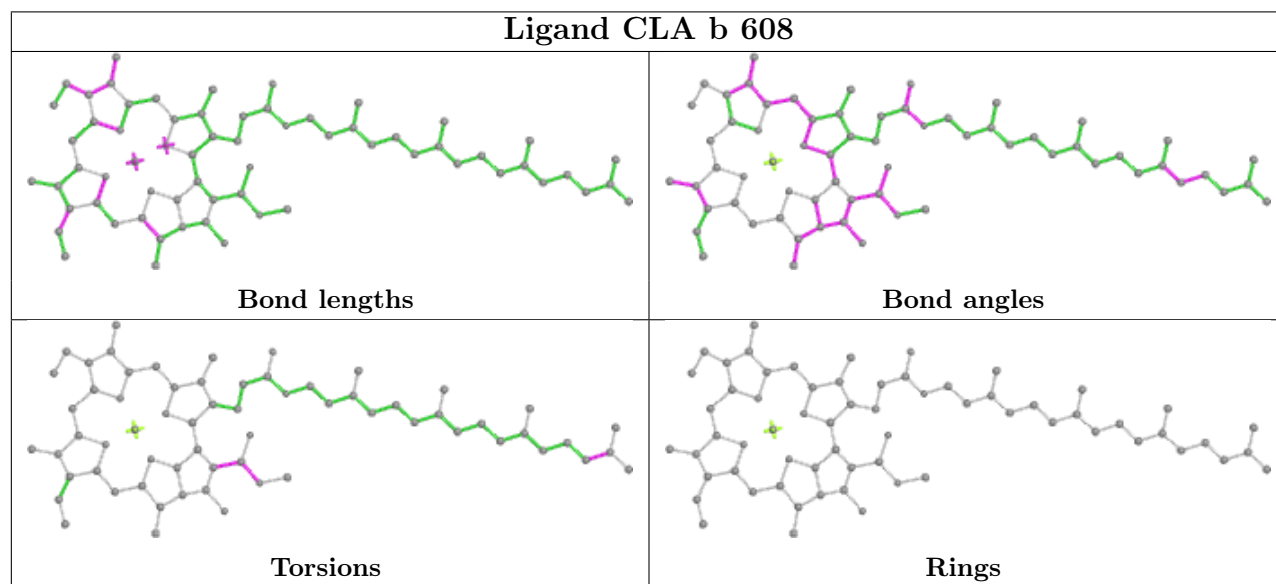
Ligand CLA B 614



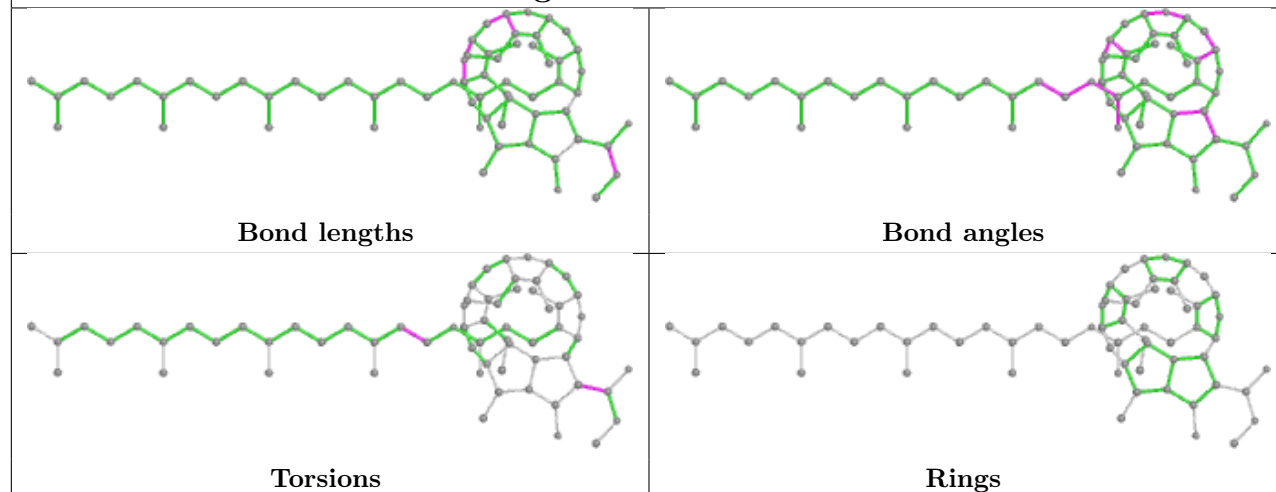
Ligand STE z 101



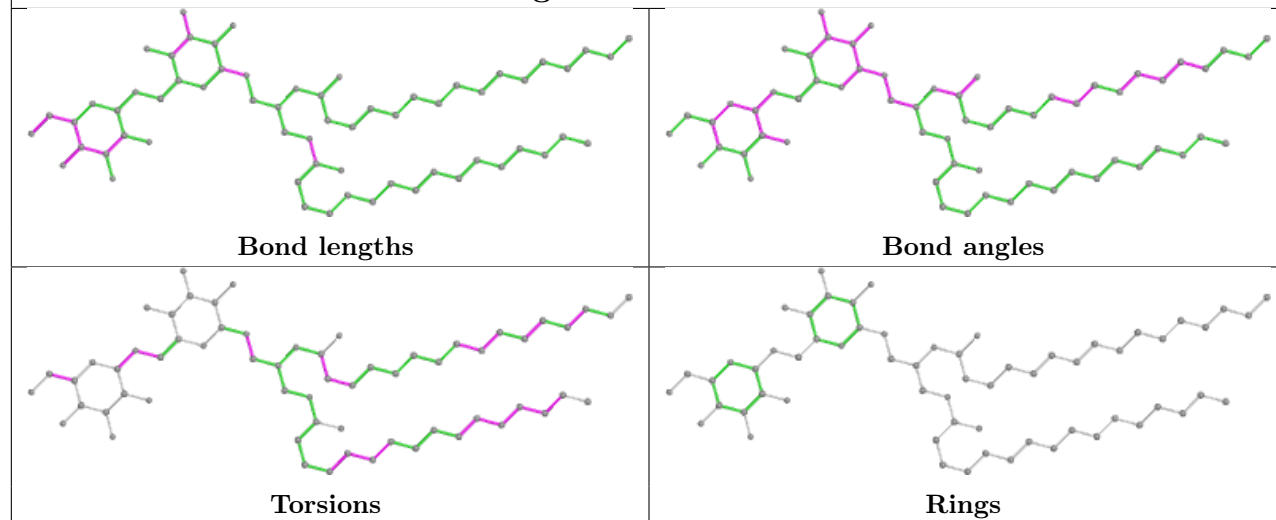
Ligand CLA b 608



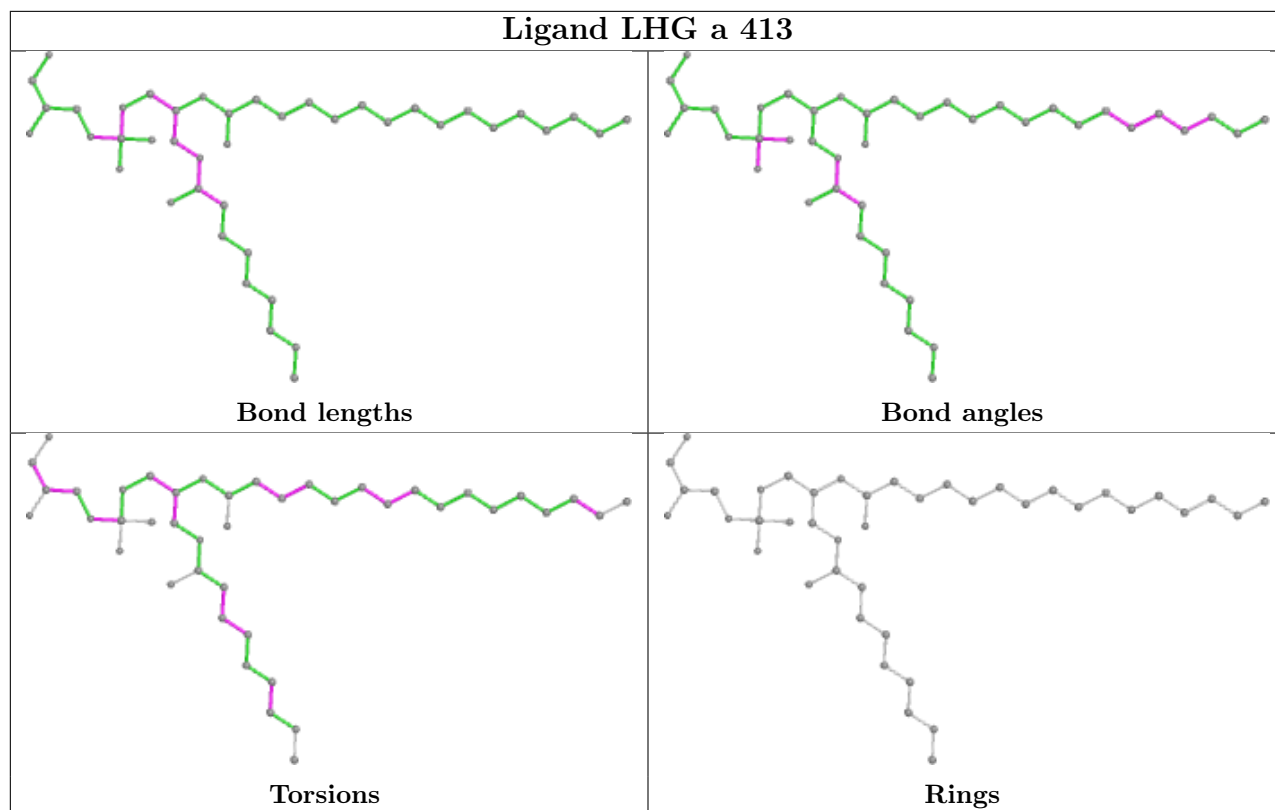
Ligand PHO a 407



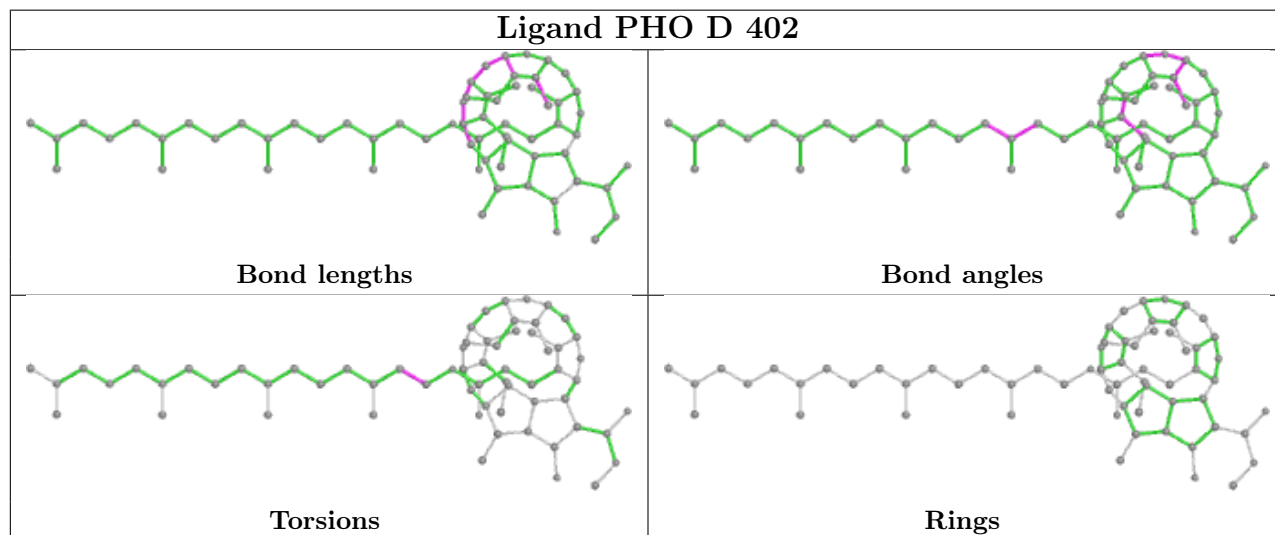
Ligand DGD c 520



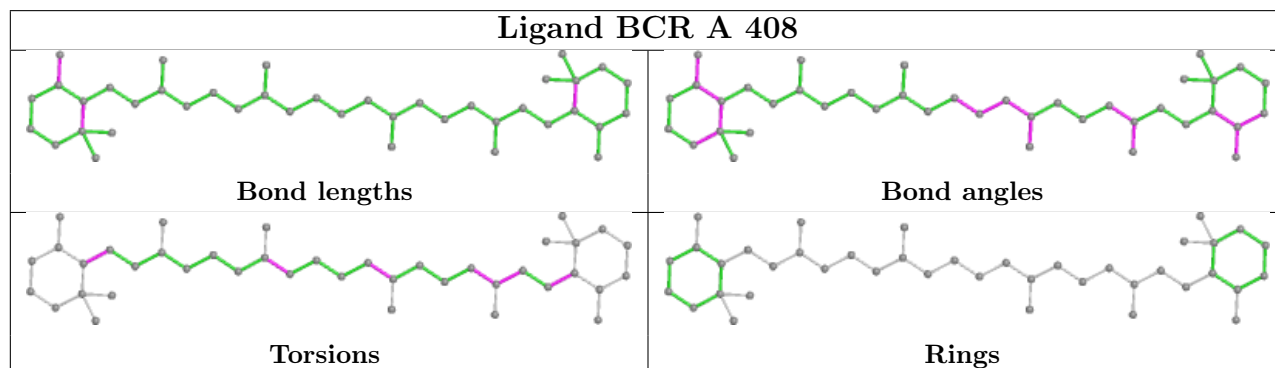
Ligand LHG a 413



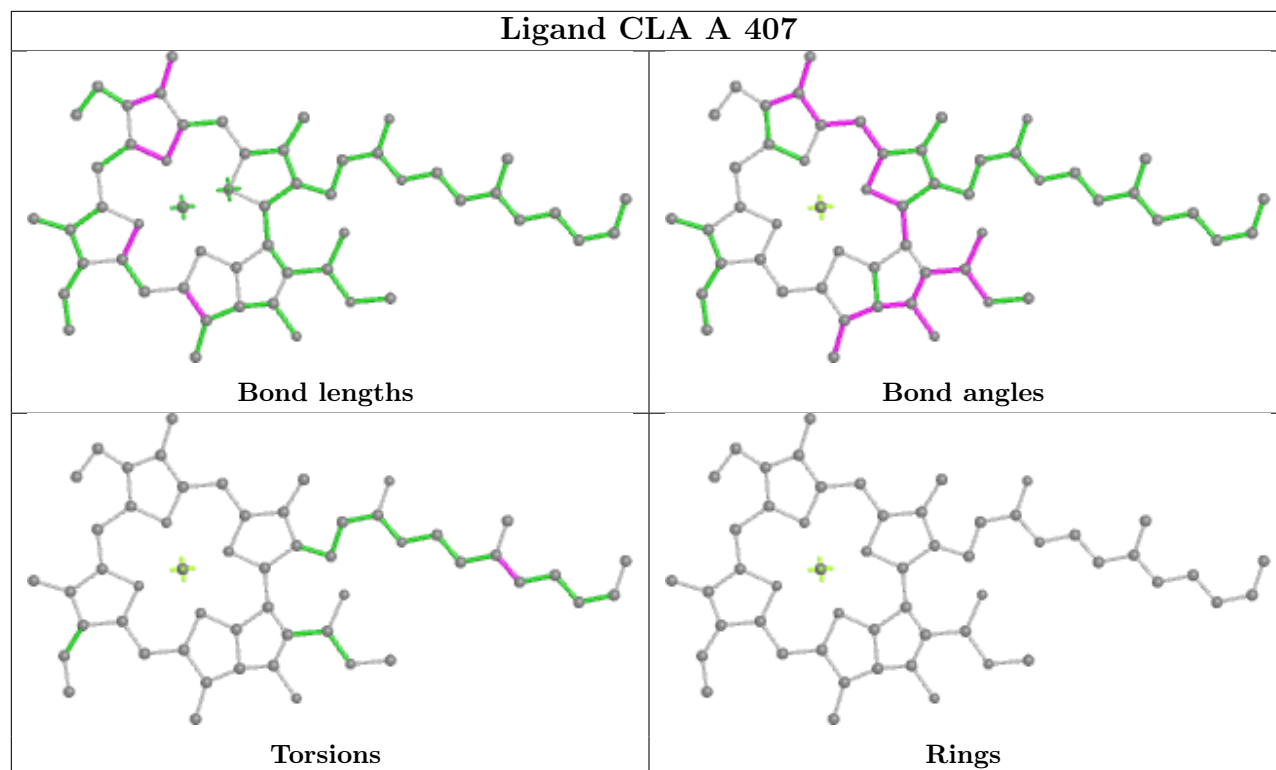
Ligand PHO D 402



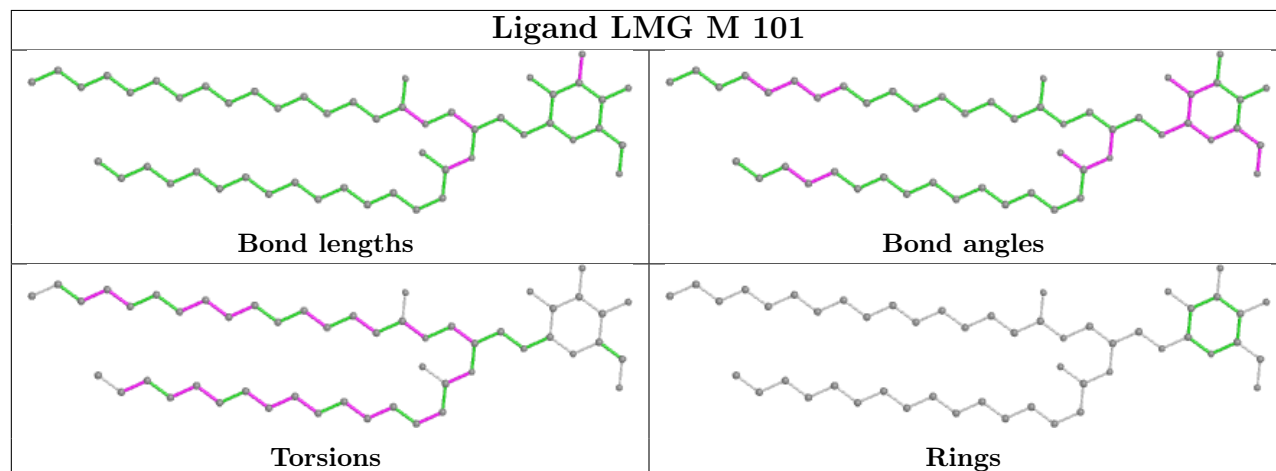
Ligand BCR A 408

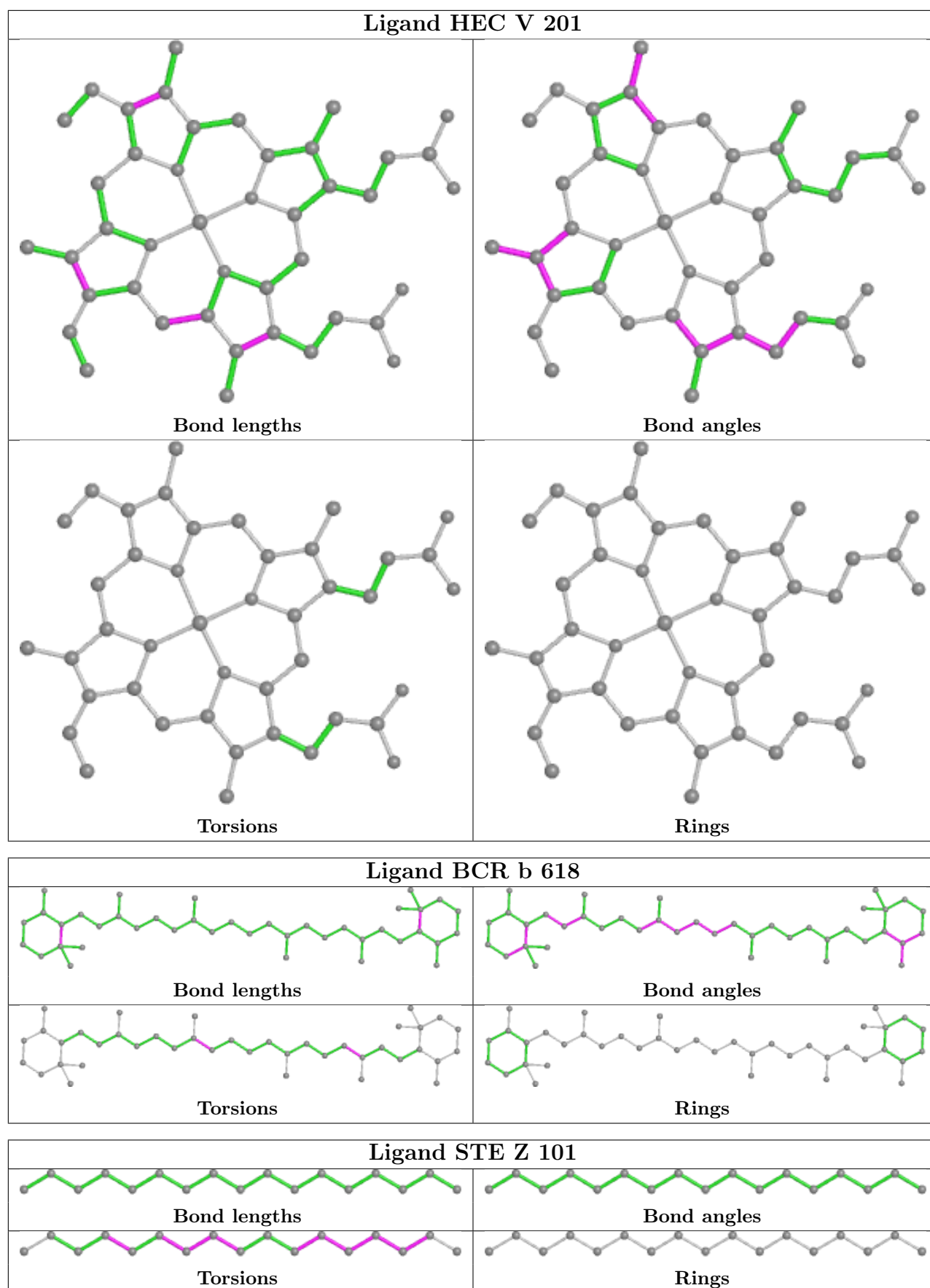


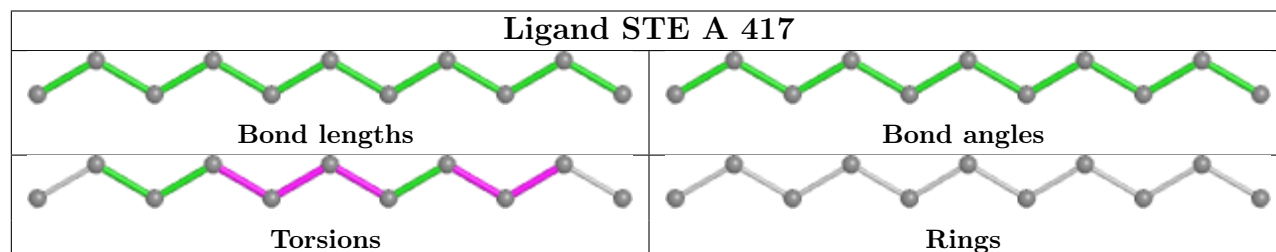
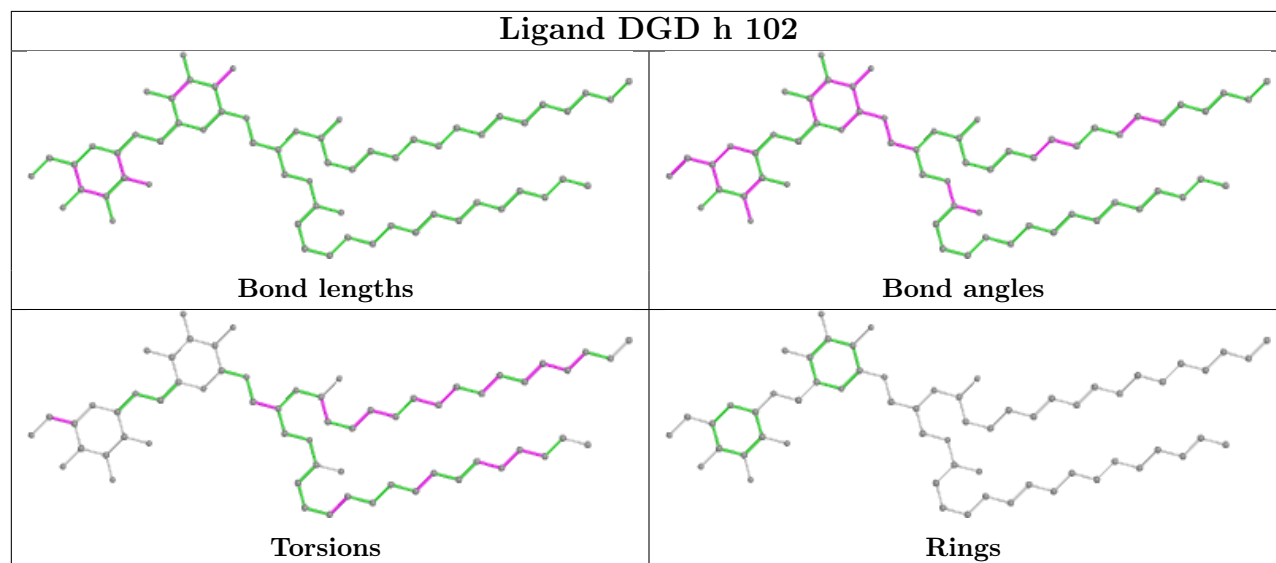
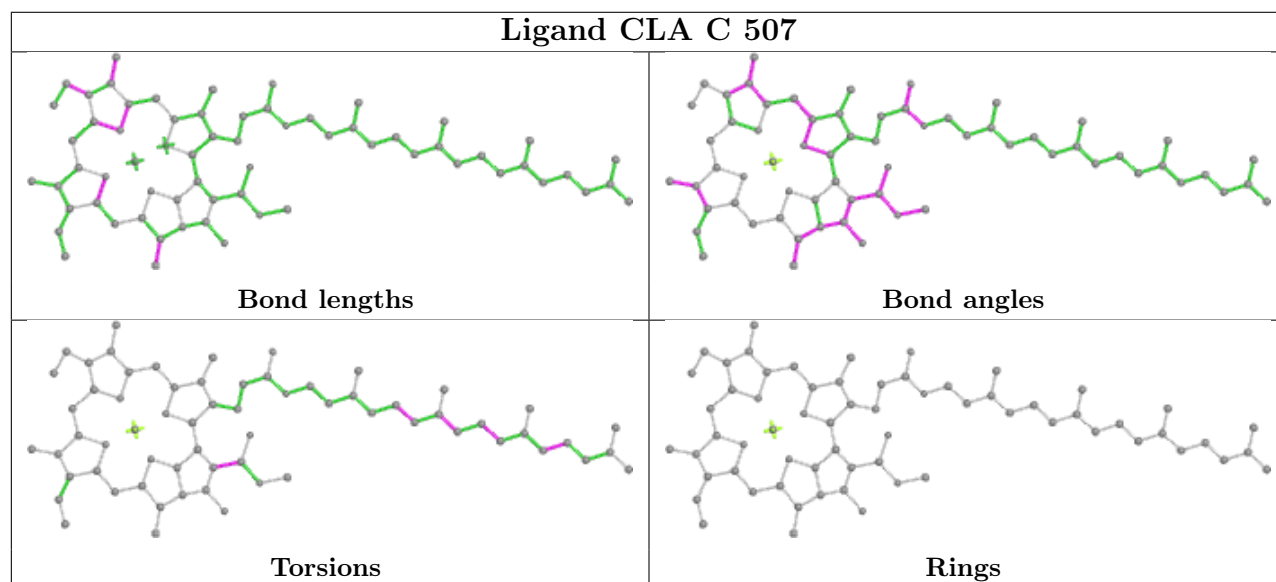
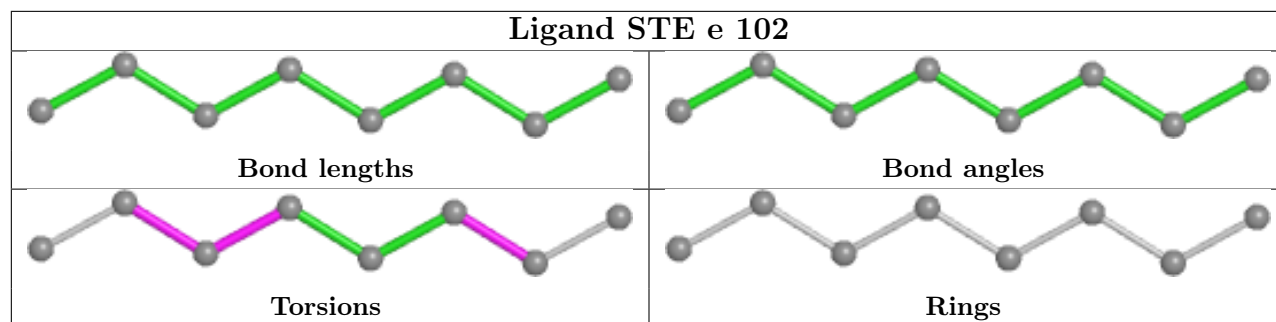
Ligand CLA A 407

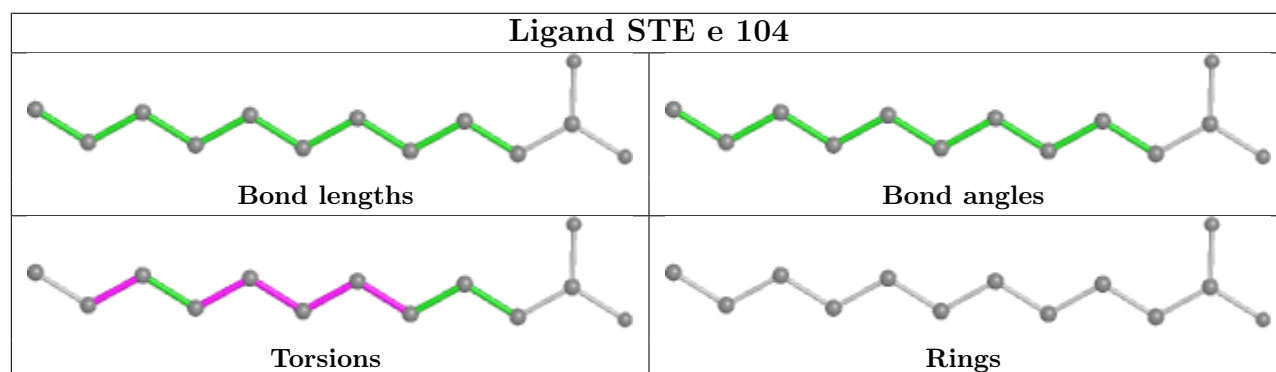
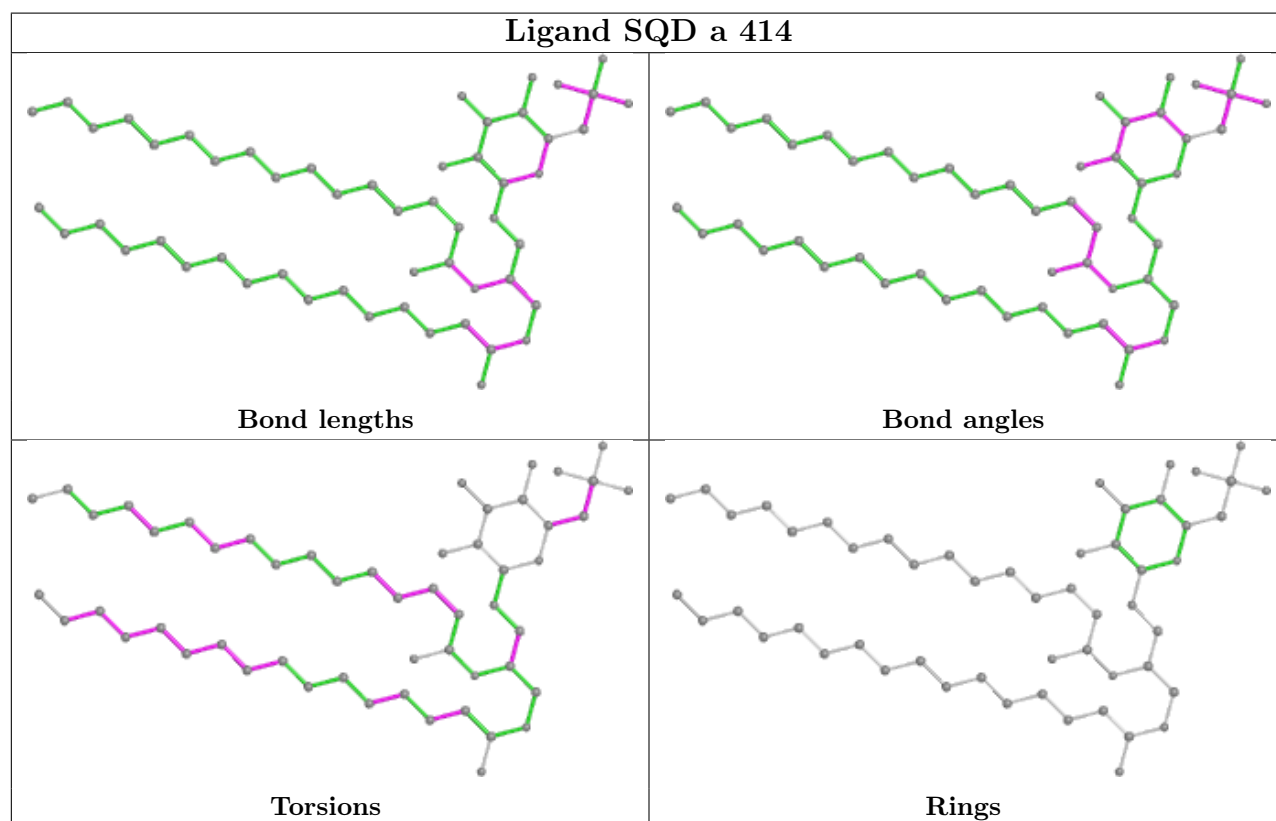
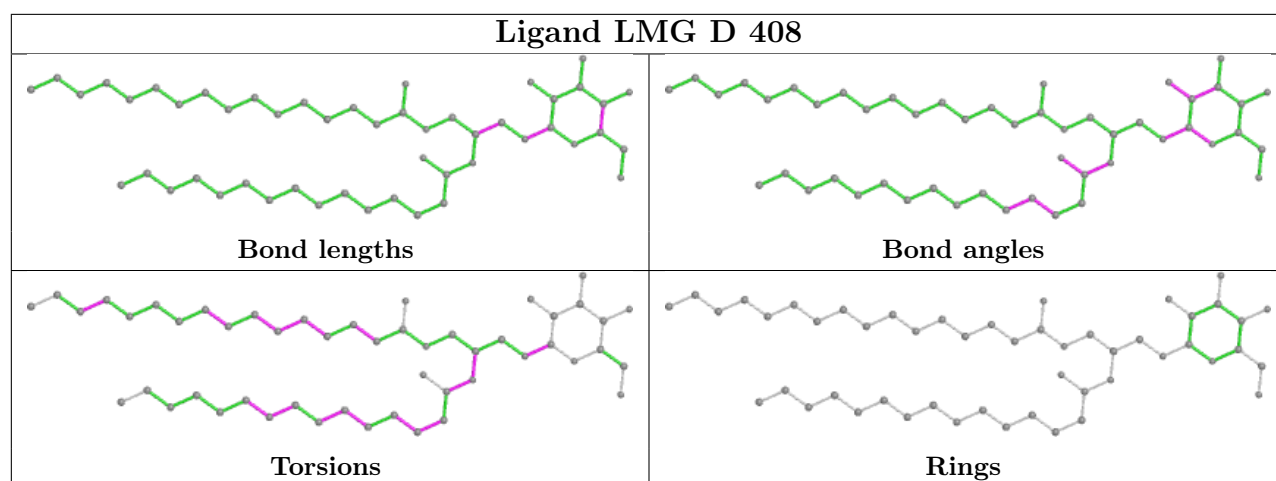


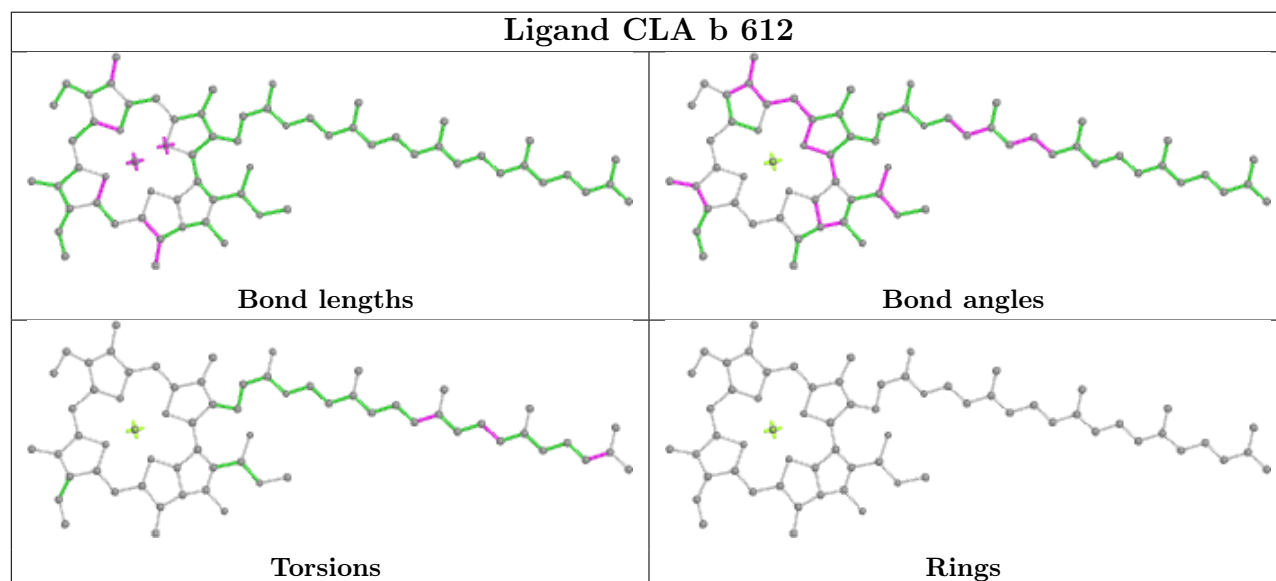
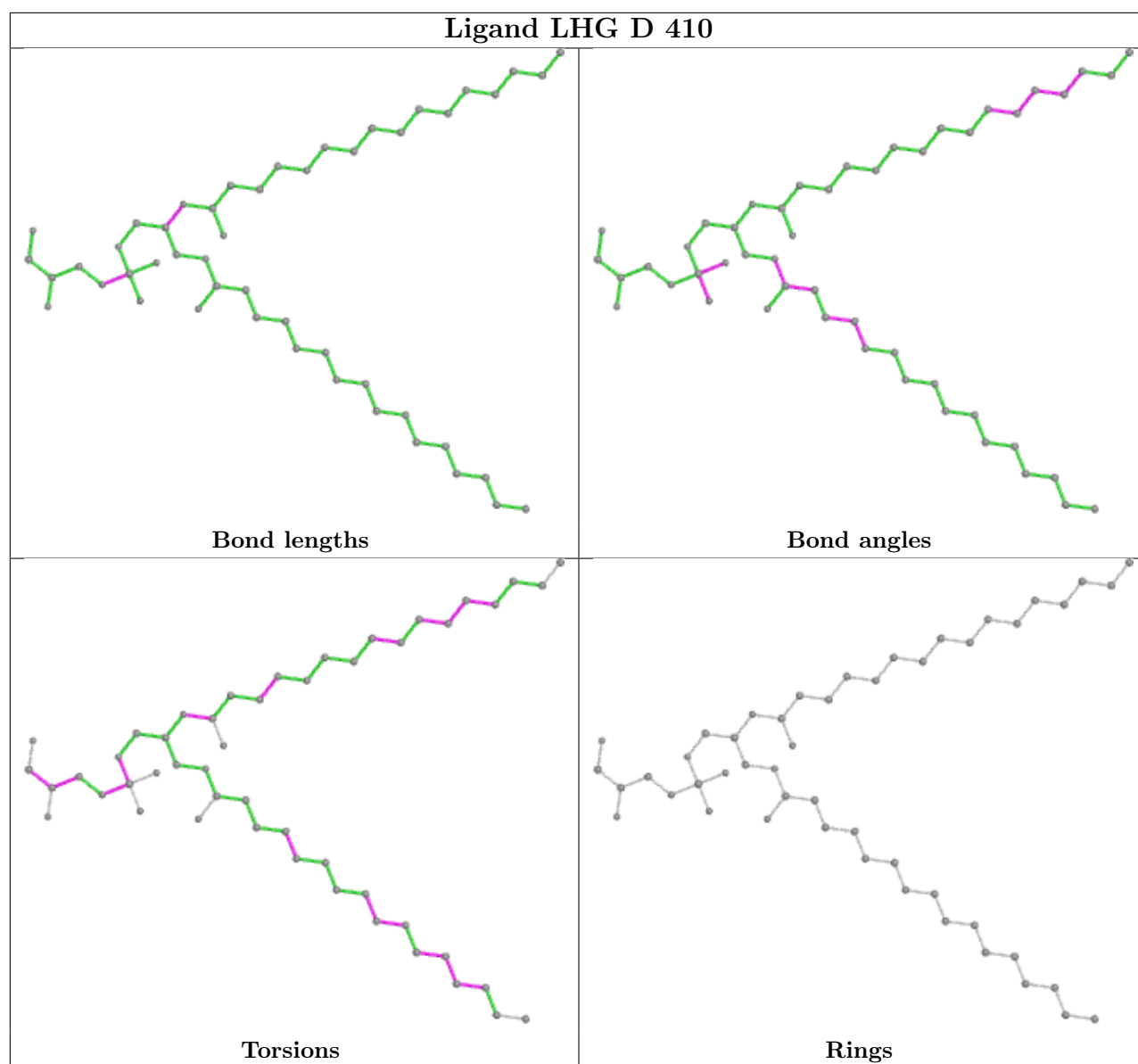
Ligand LMG M 101

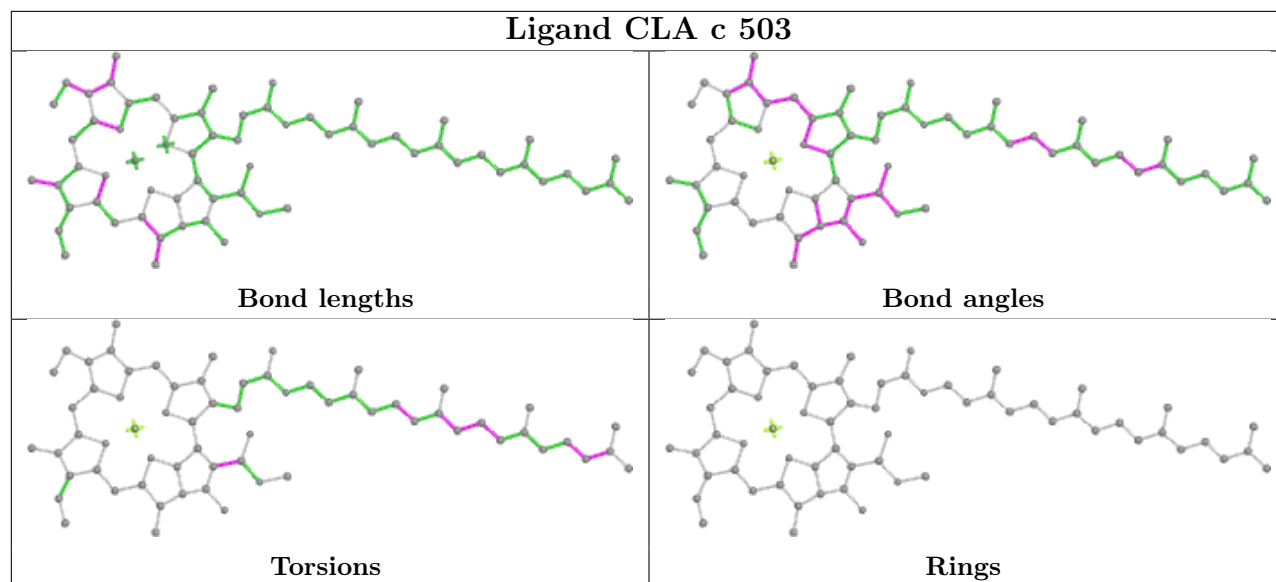
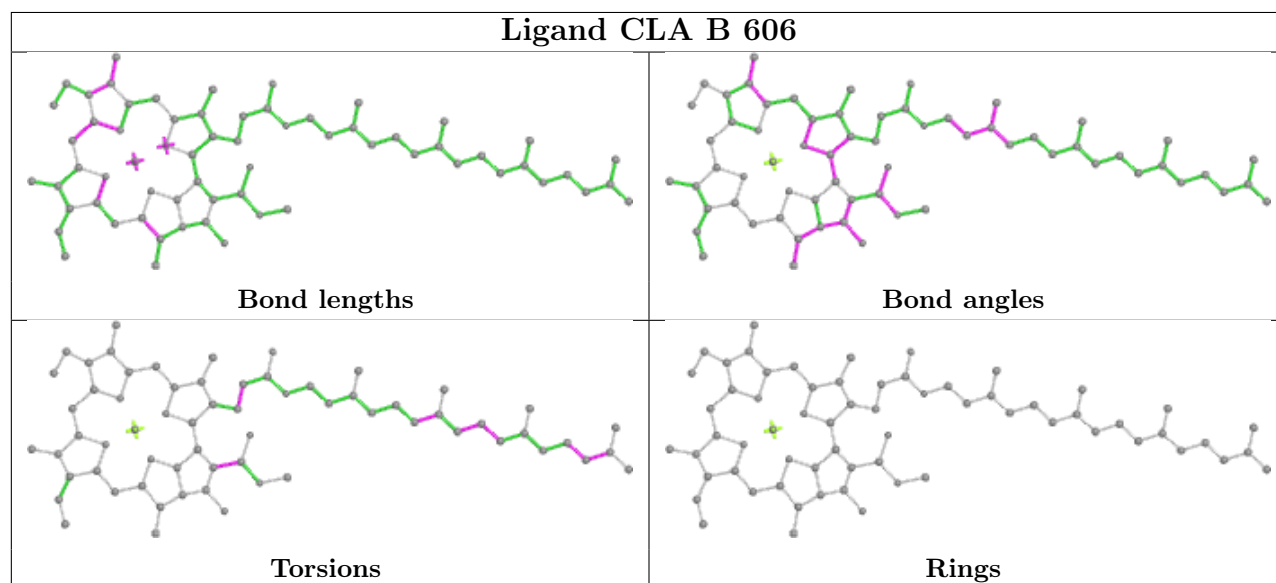


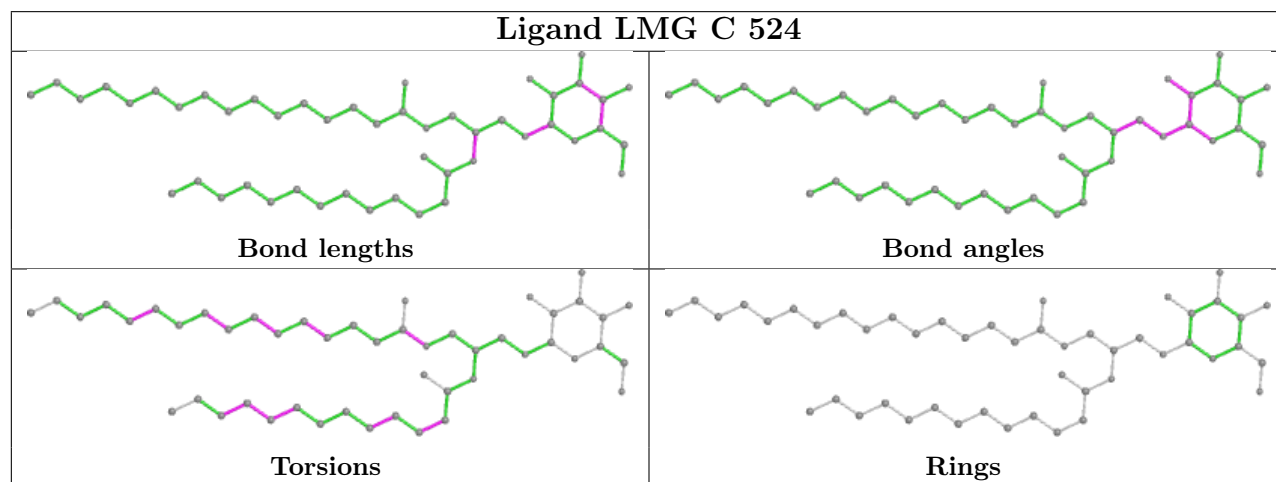
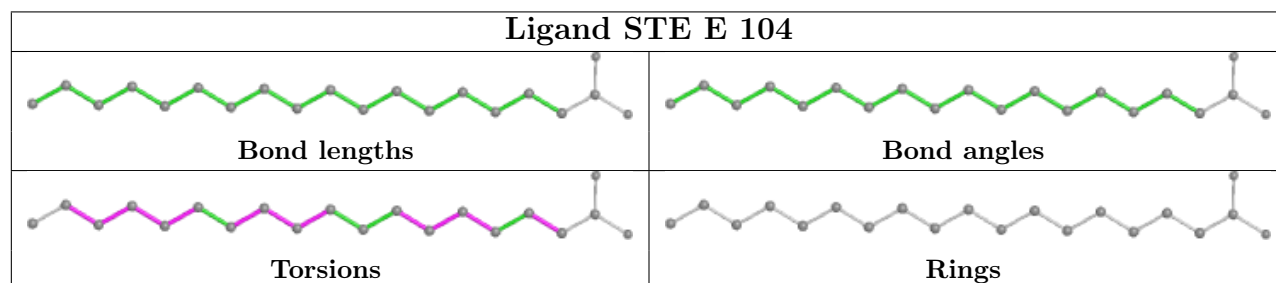
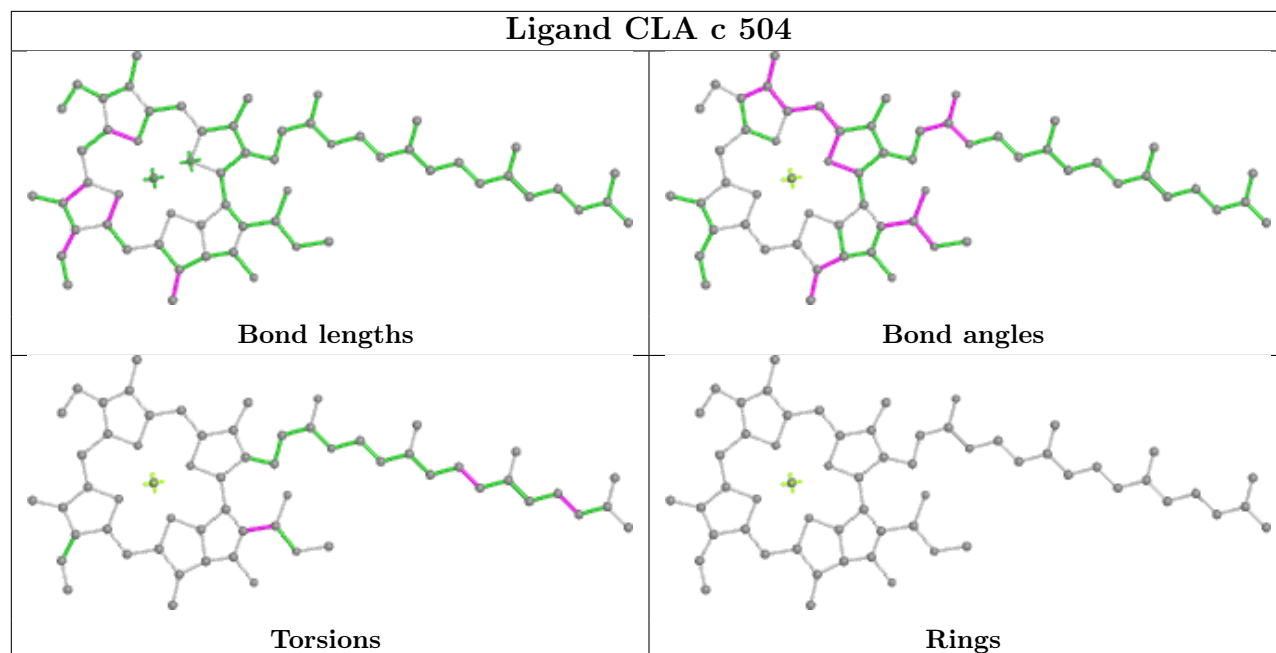


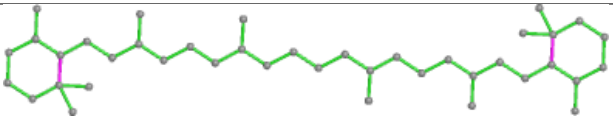
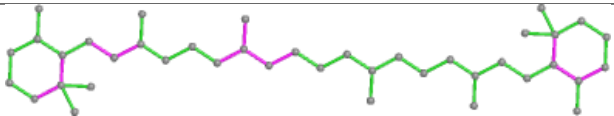
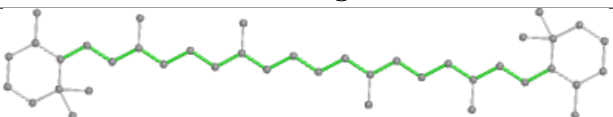
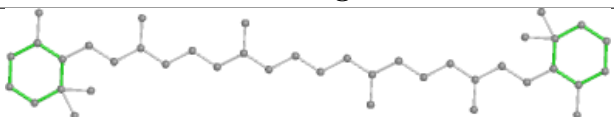




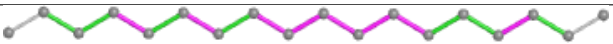



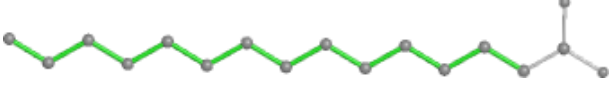
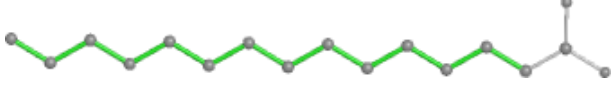
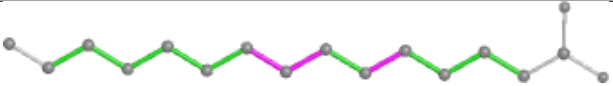
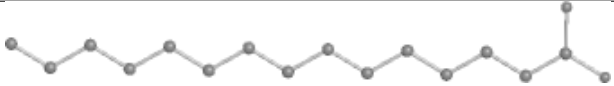


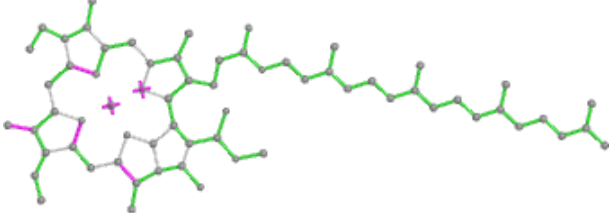
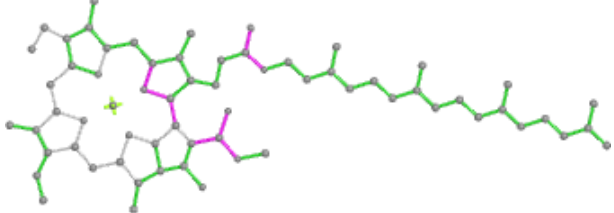
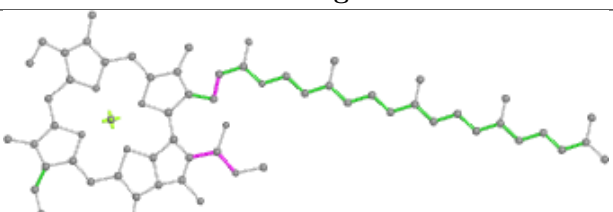
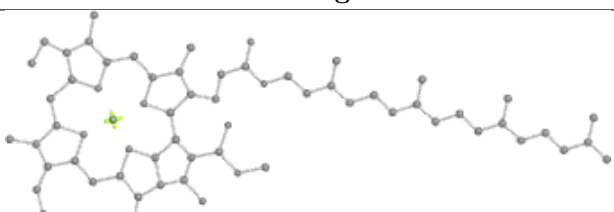
Ligand CLA c 503**Ligand CLA B 606**

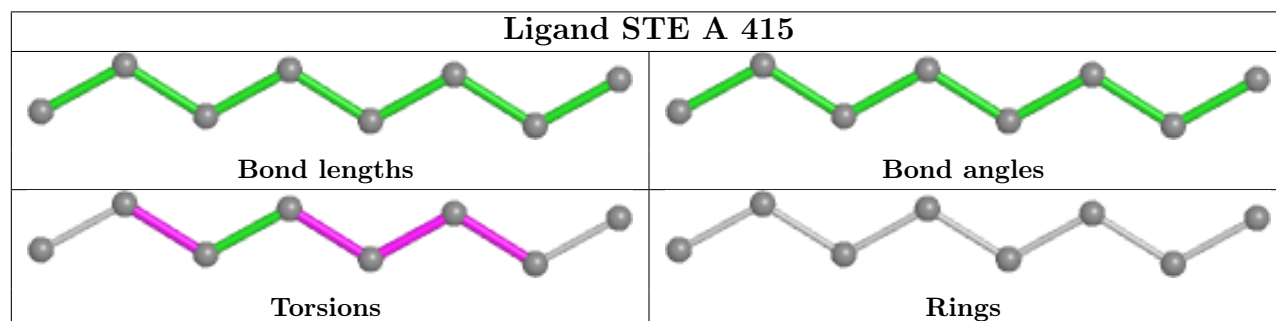
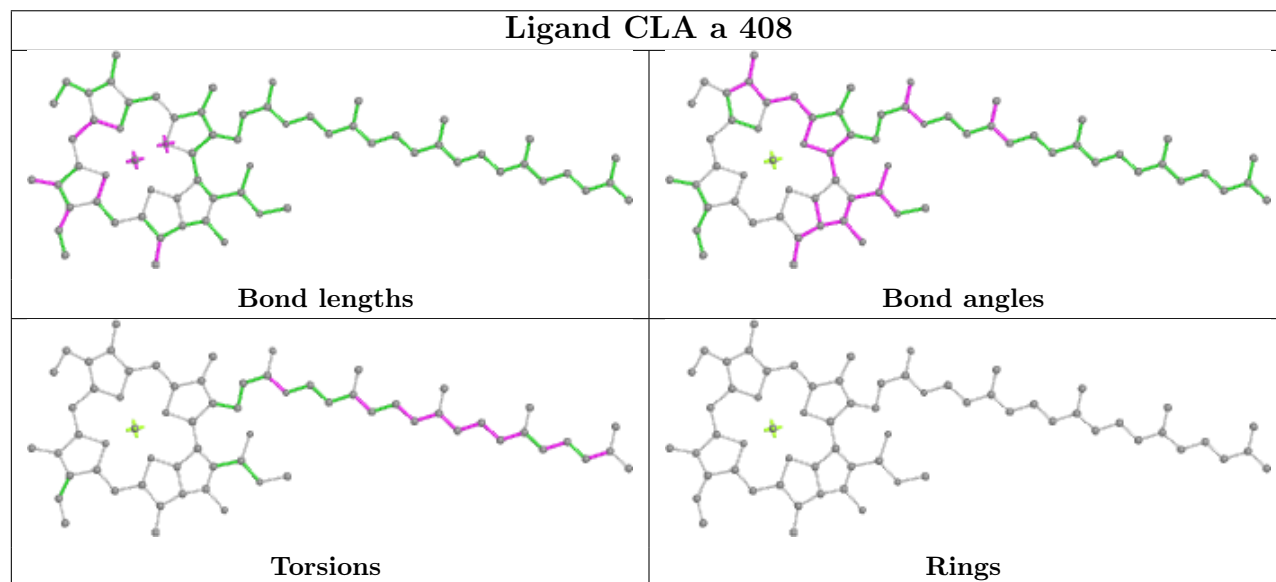
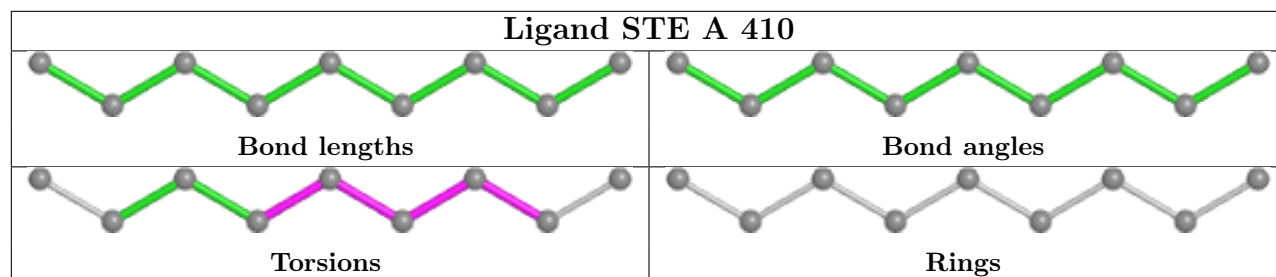
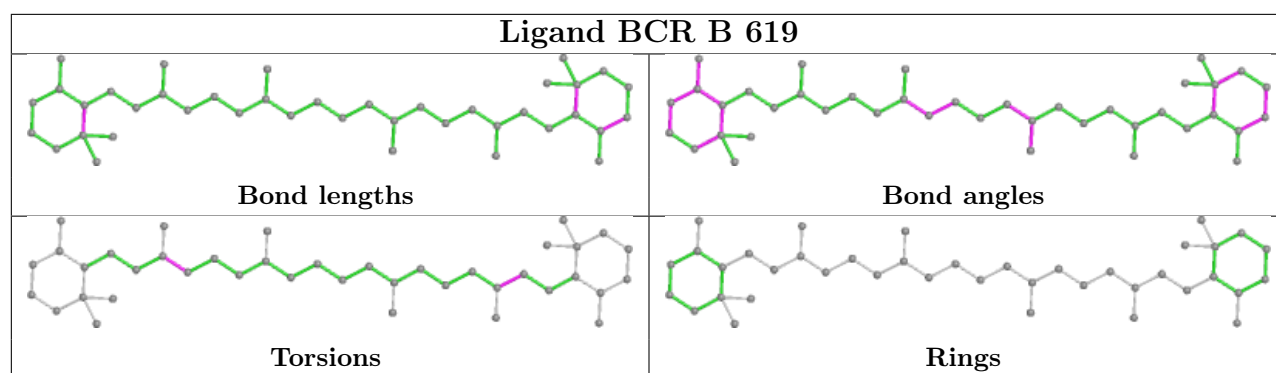


Ligand BCR b 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

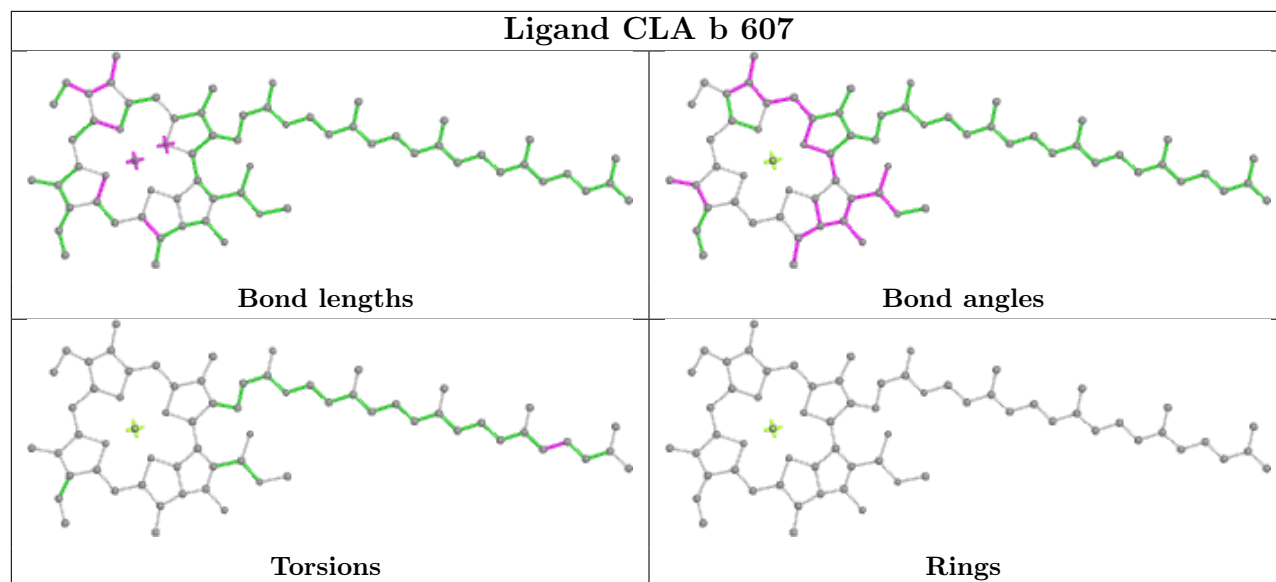
Ligand STE H 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE I 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

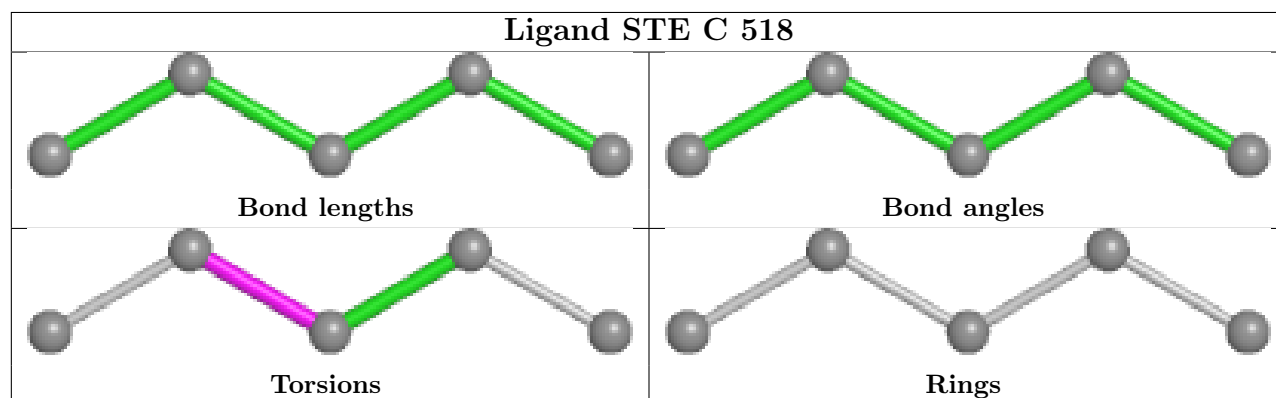
Ligand CLA C 501	
	
Bond lengths	Bond angles
	
Torsions	Rings



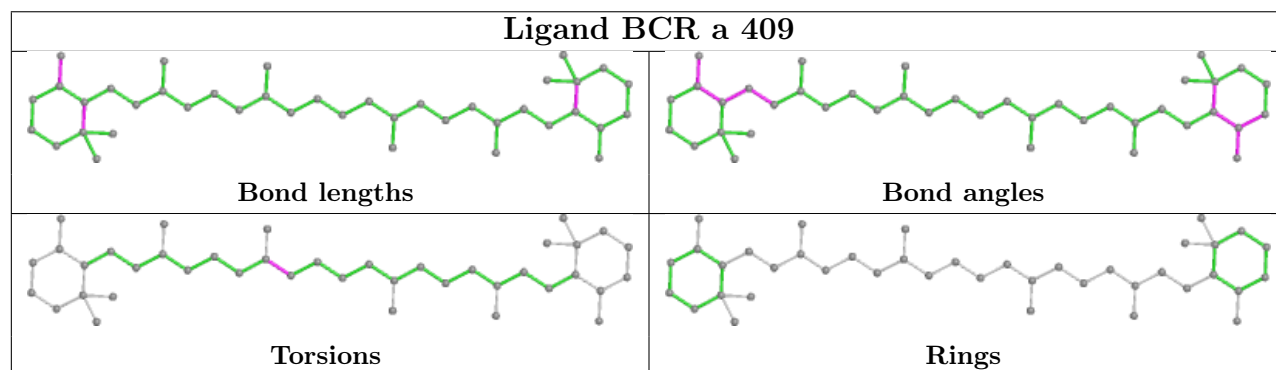
Ligand CLA b 607



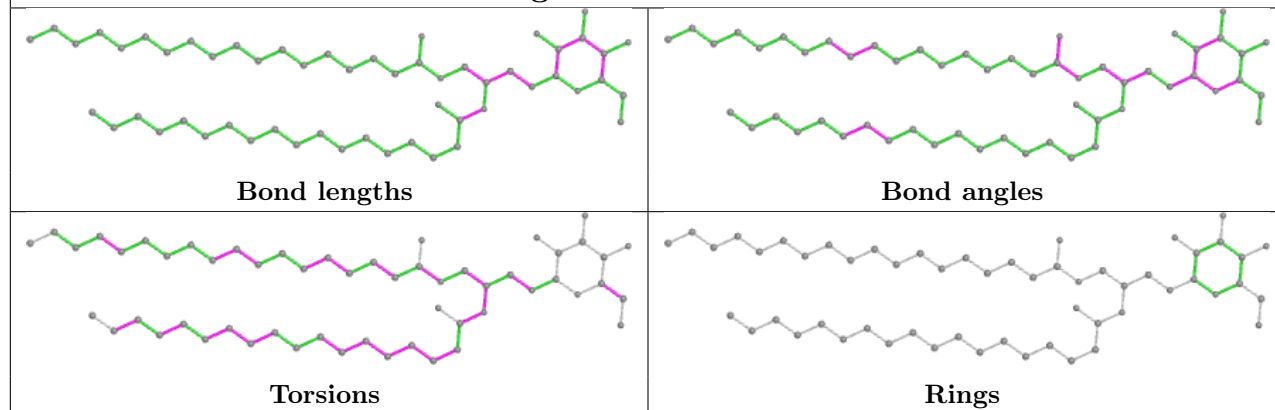
Ligand STE C 518



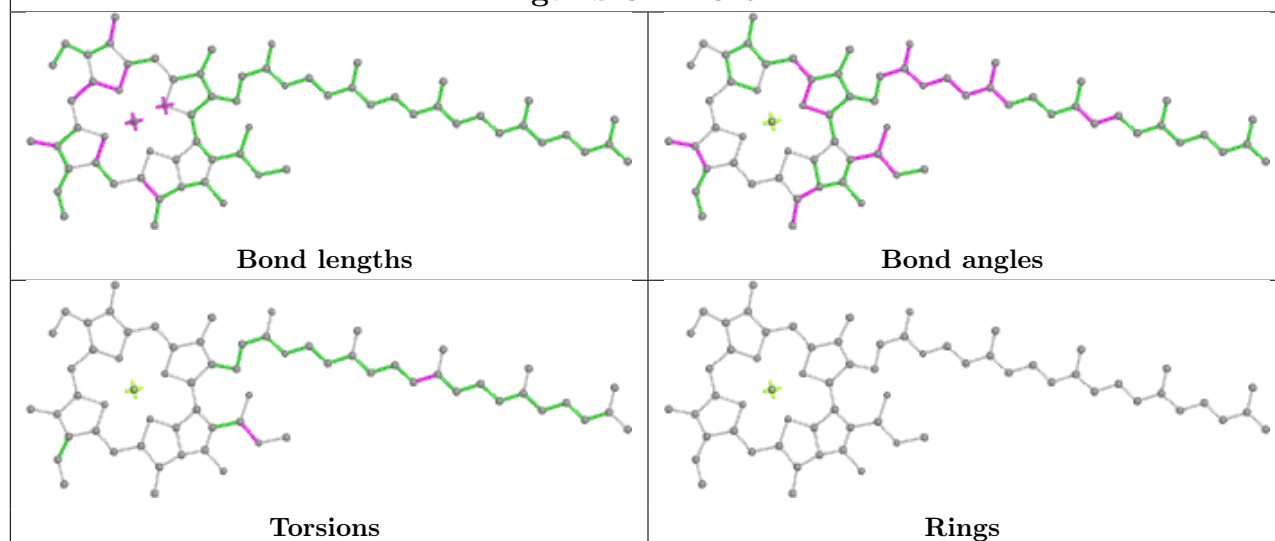
Ligand BCR a 409



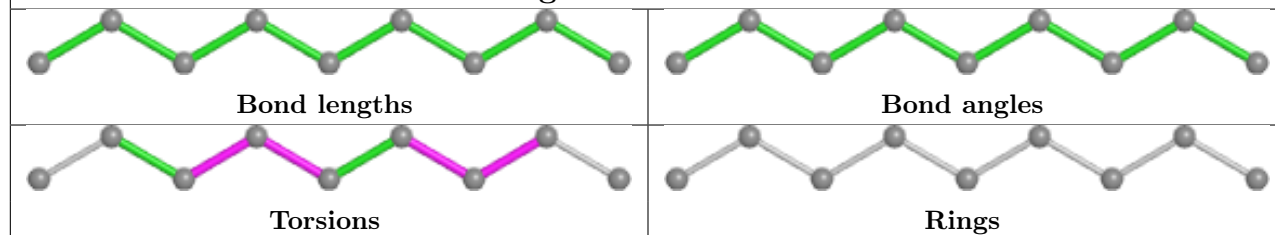
Ligand LMG a 415

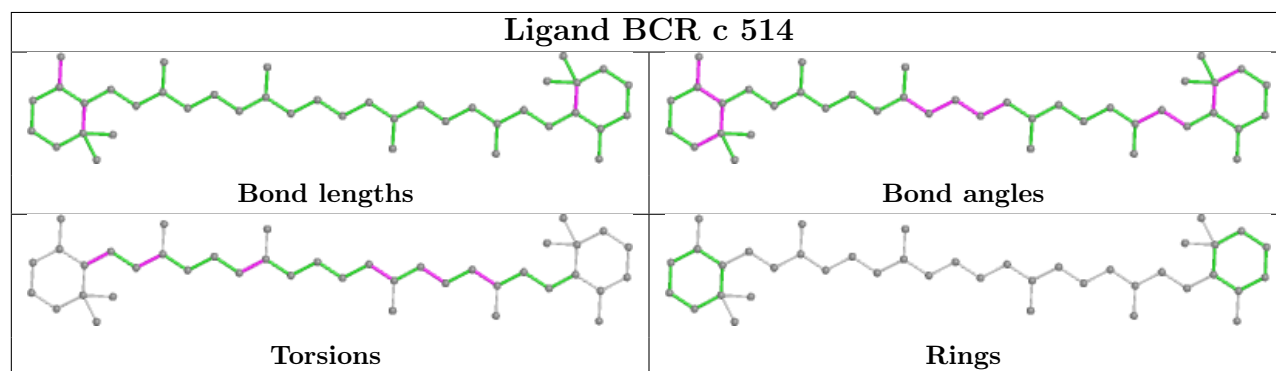
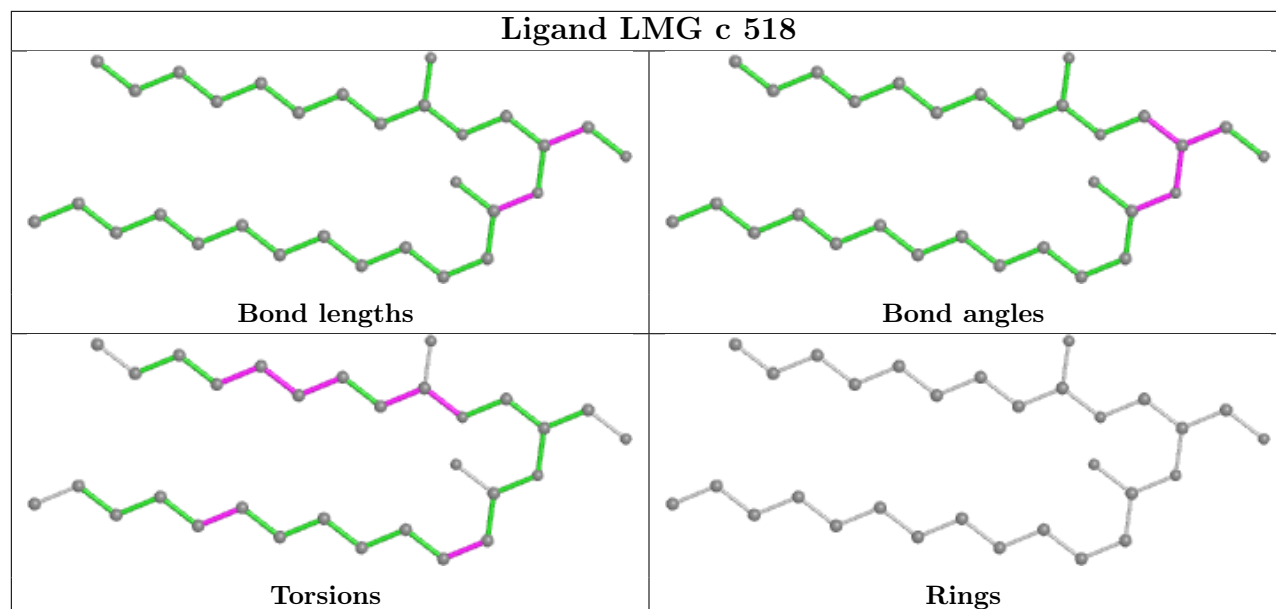


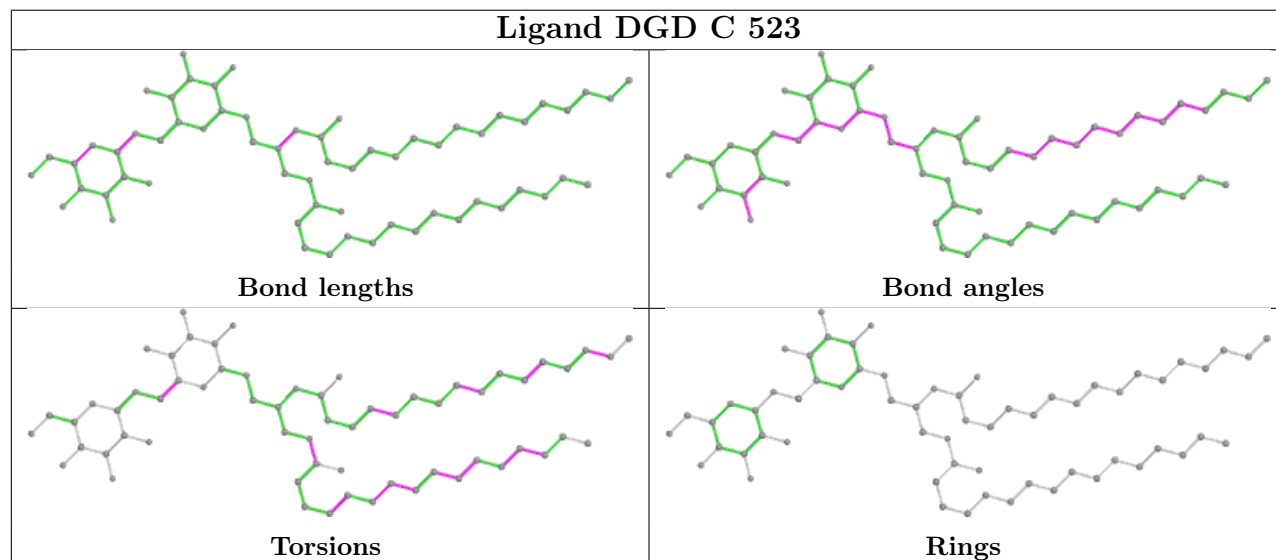
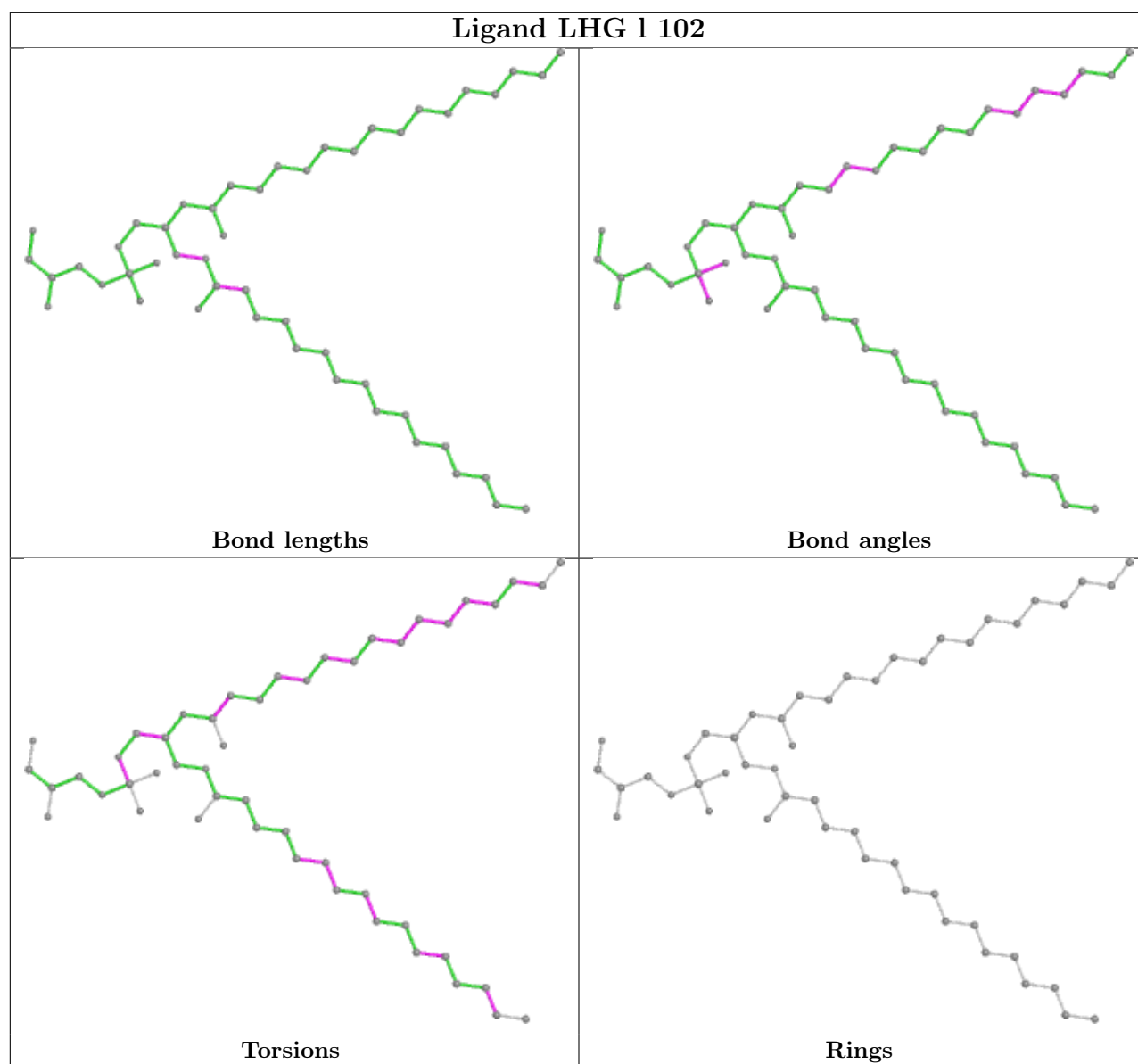
Ligand CLA C 511

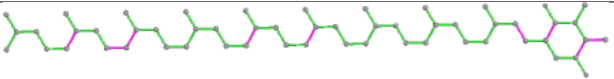
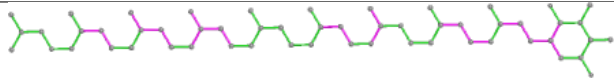
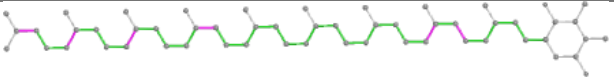
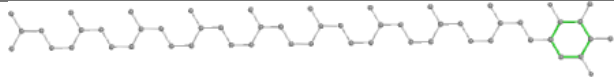



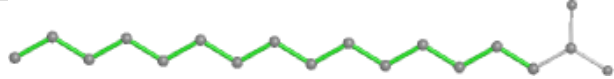

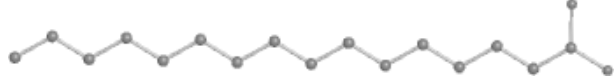
Ligand STE e 103

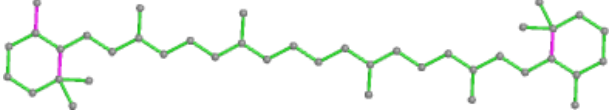
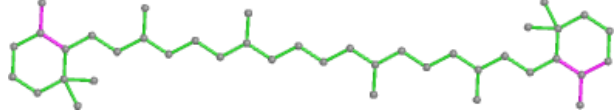
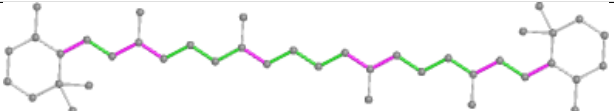
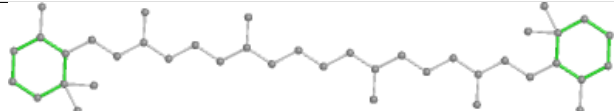



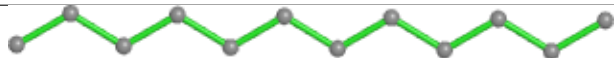




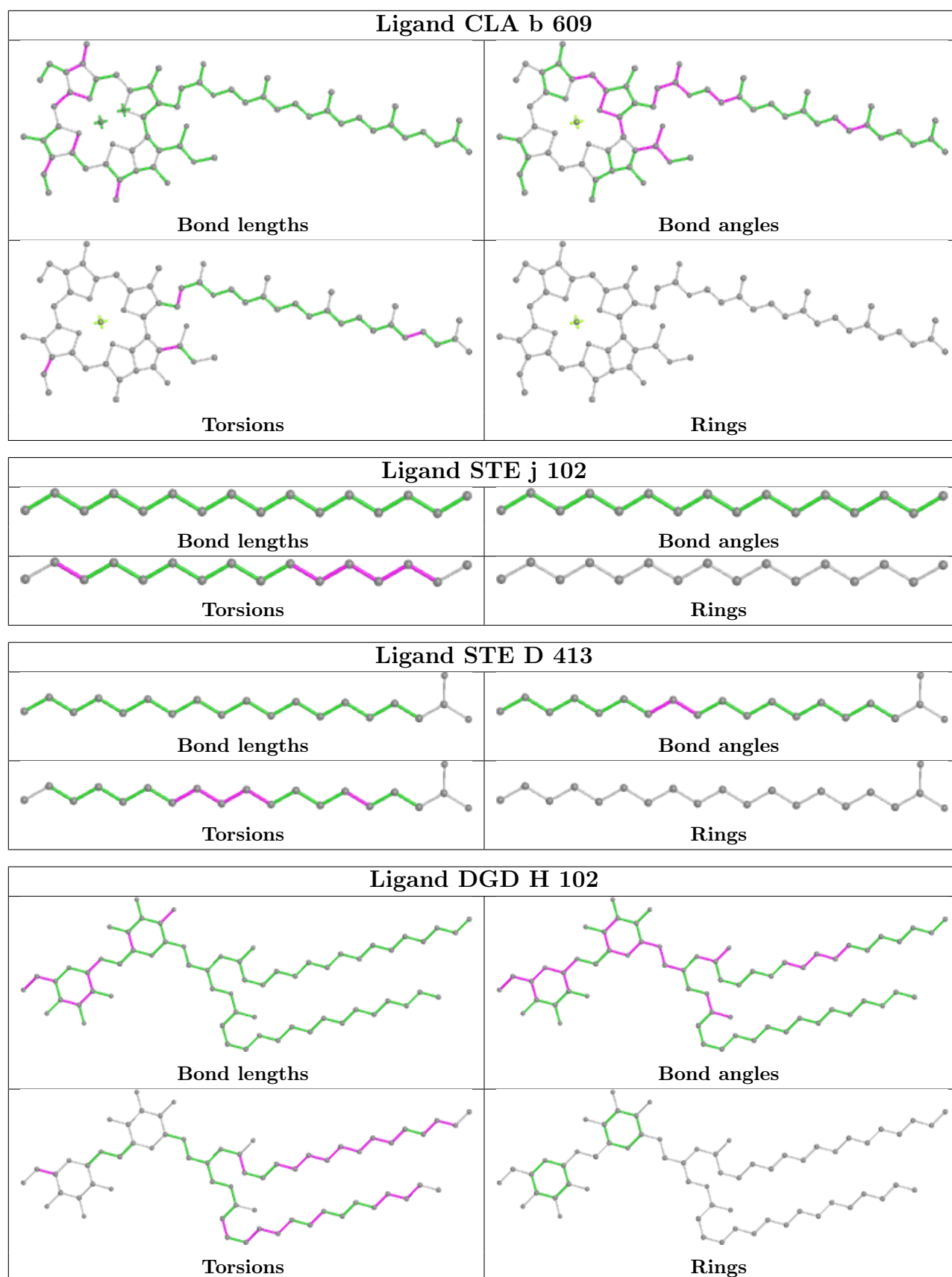


Ligand PL9 d 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

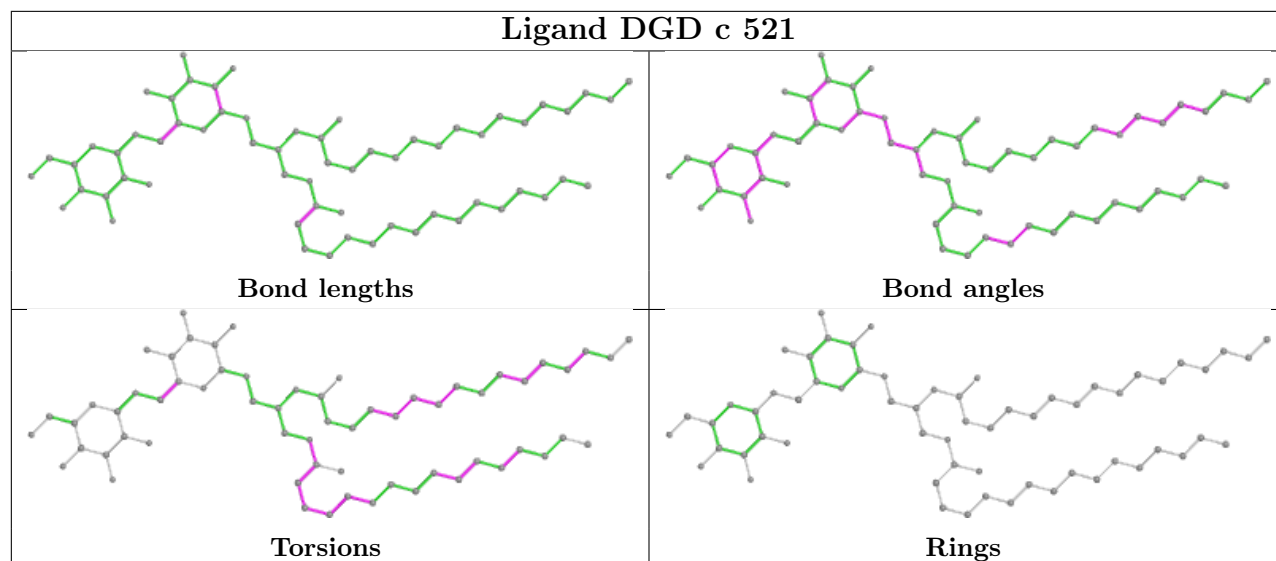
Ligand STE t 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR k 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

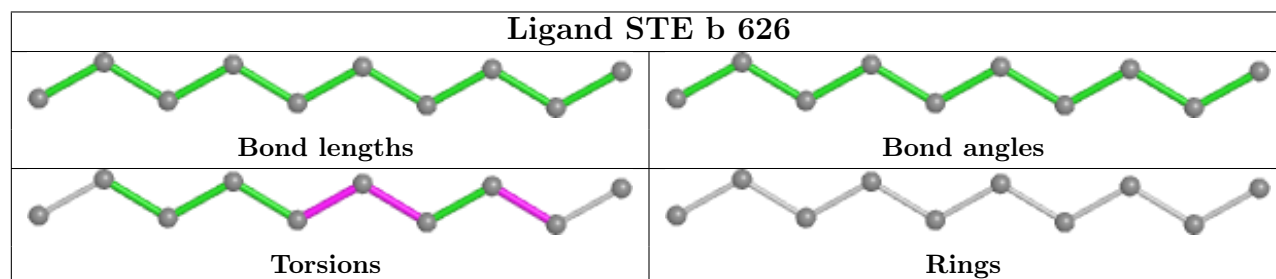
Ligand STE E 103	
 Bond lengths	 Bond angles
 Torsions	 Rings



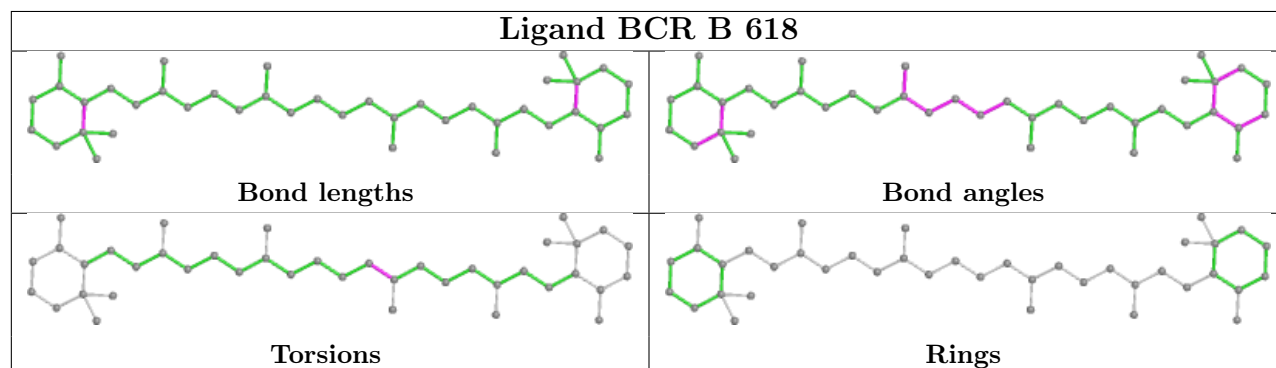
Ligand DGD c 521



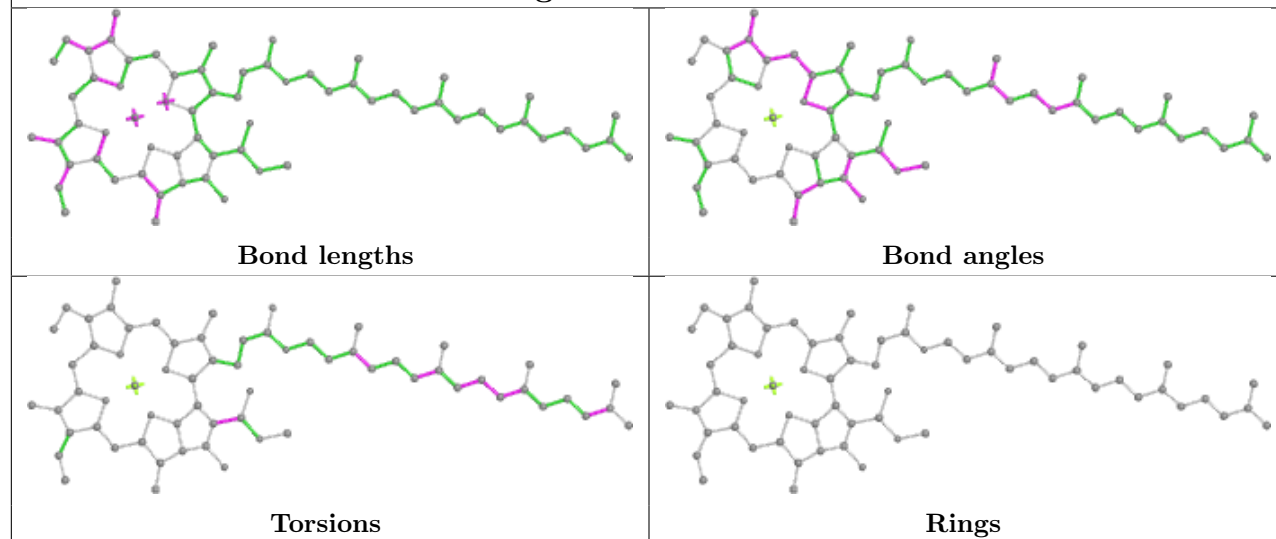
Ligand STE b 626



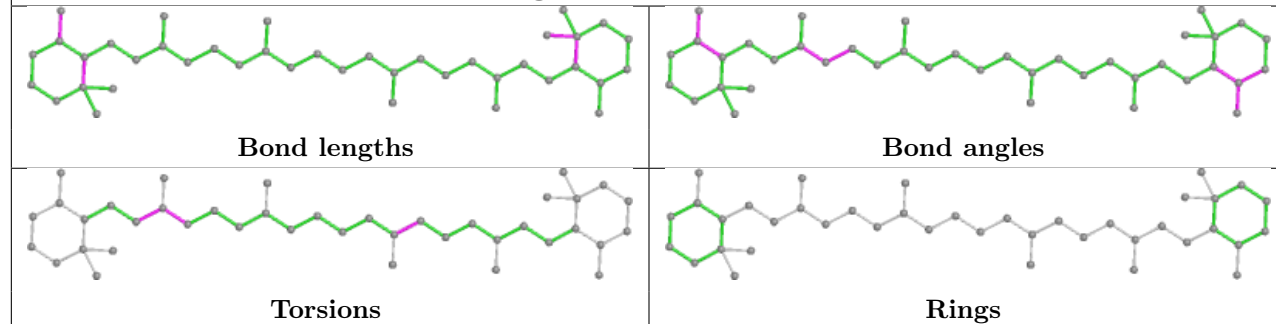
Ligand BCR B 618



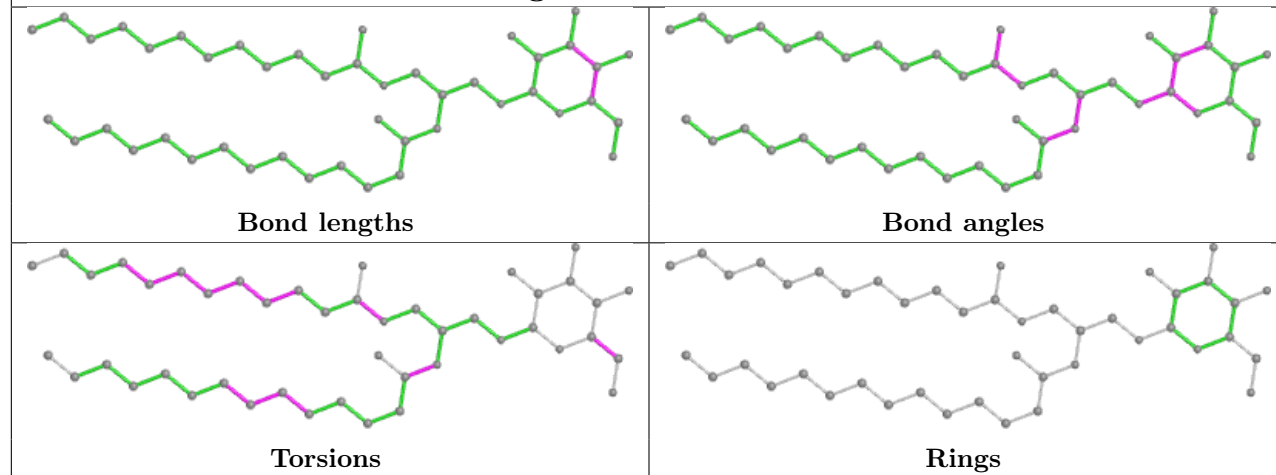
Ligand CLA b 606



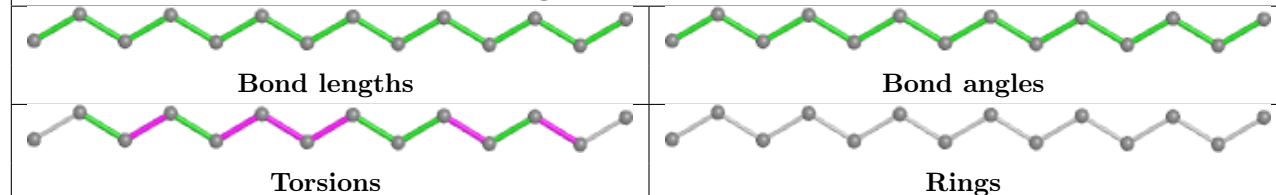
Ligand BCR C 520

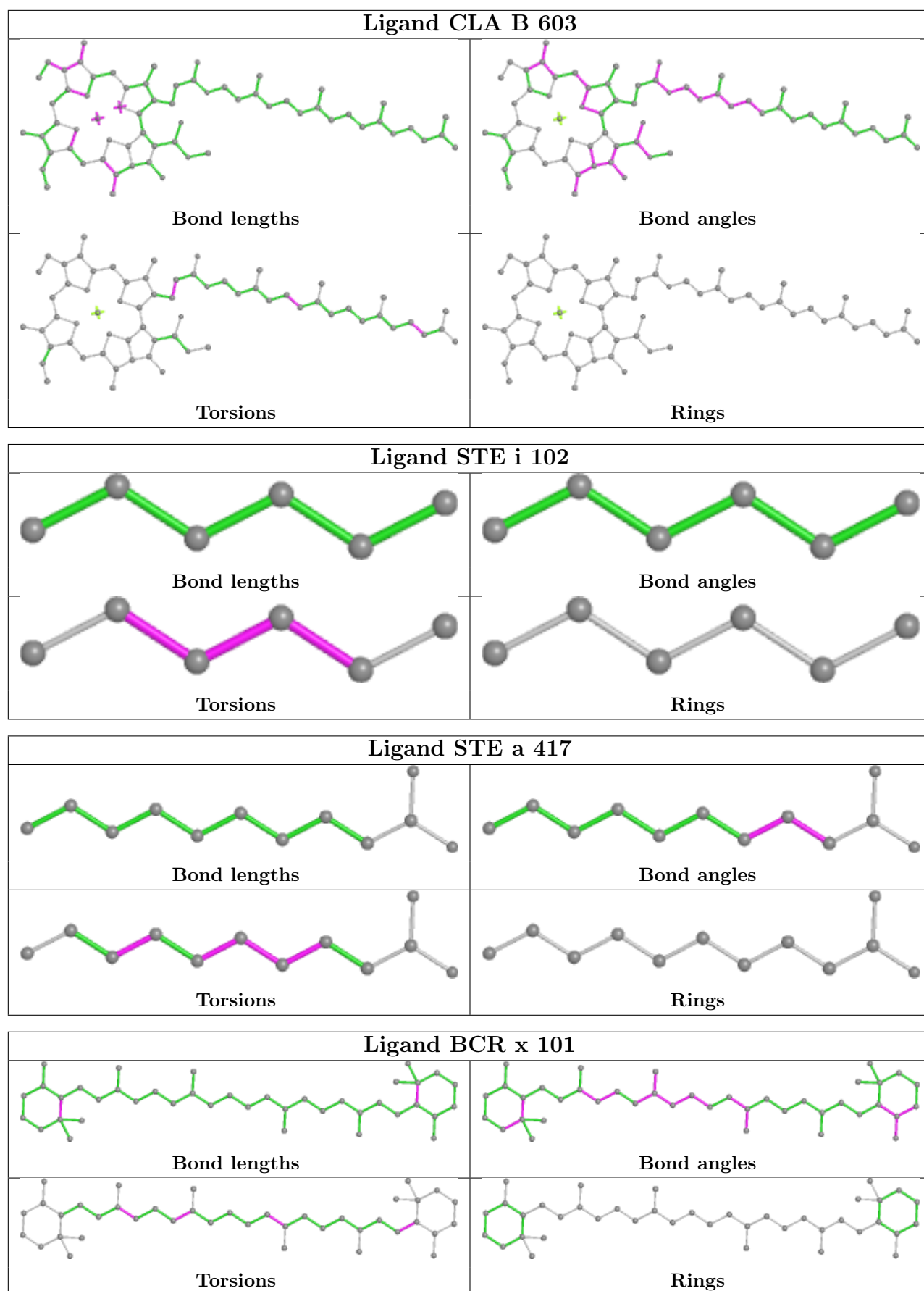


Ligand LMG B 620

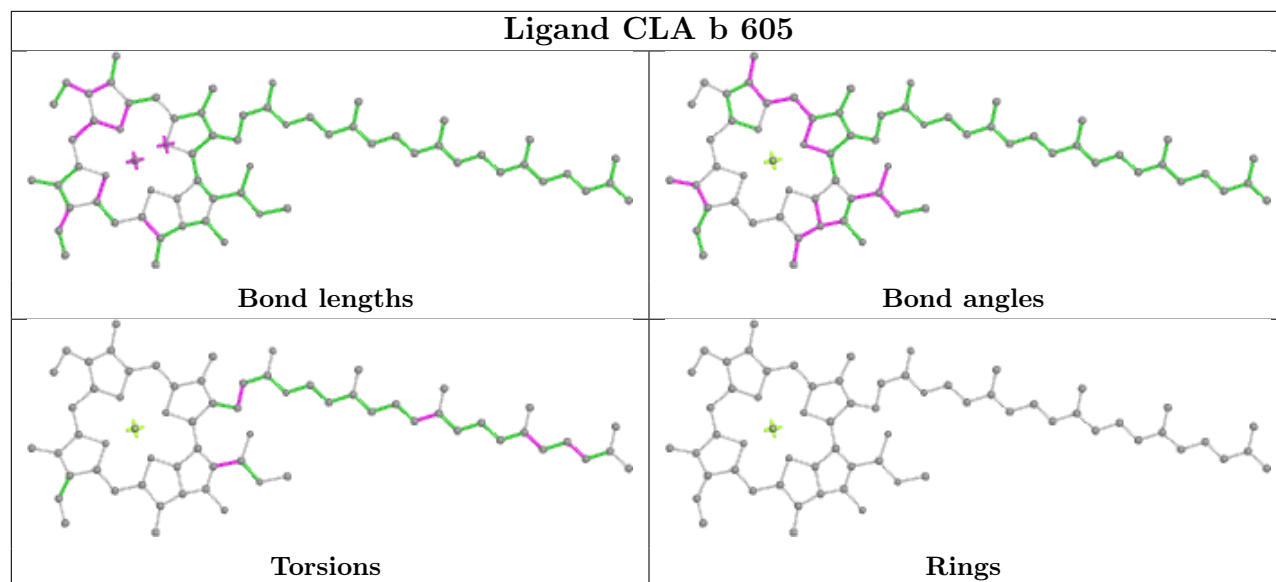


Ligand STE C 529

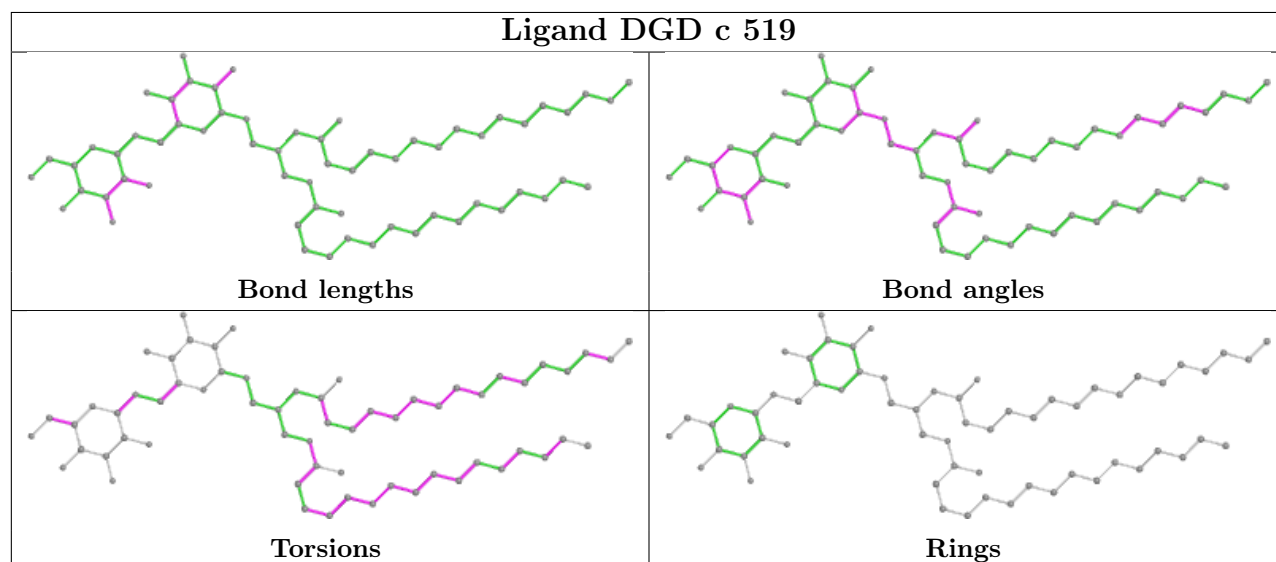




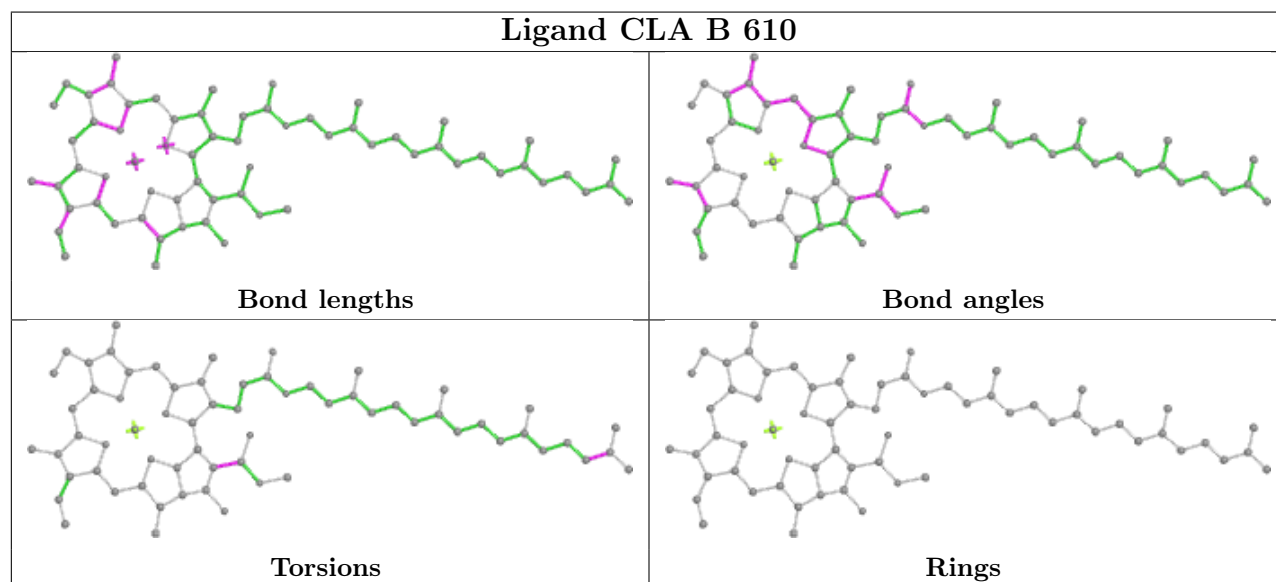
Ligand CLA b 605

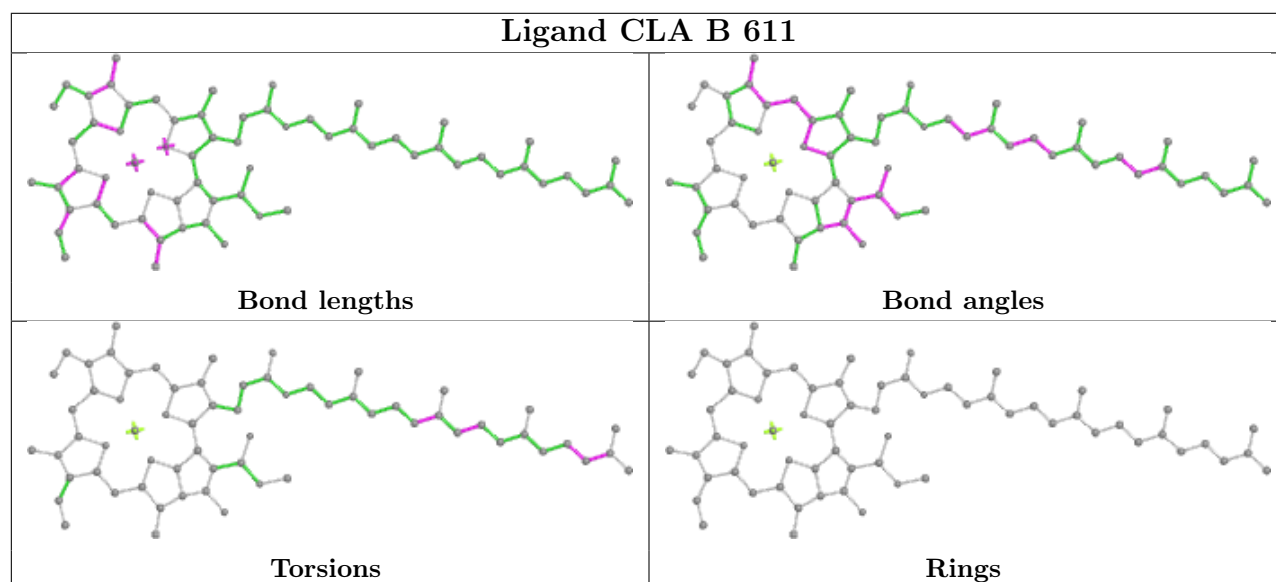
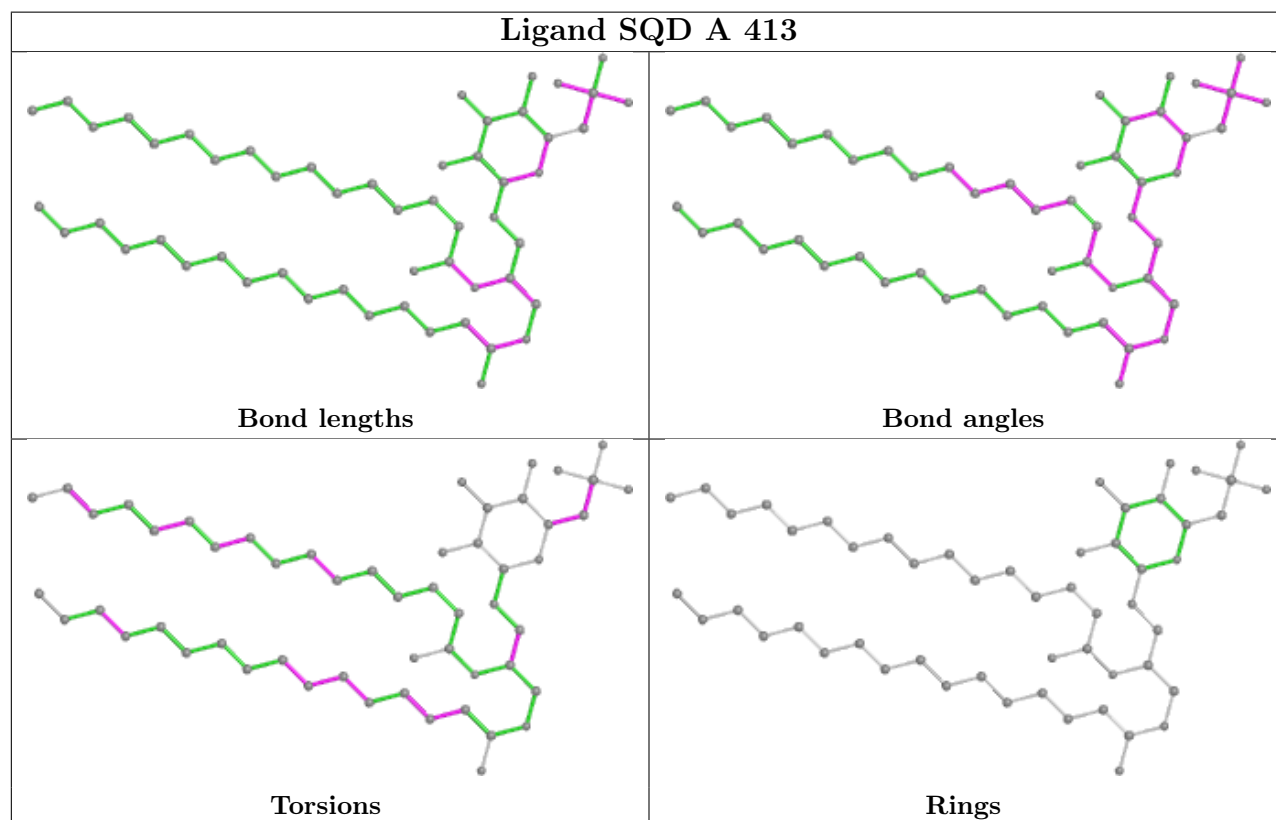
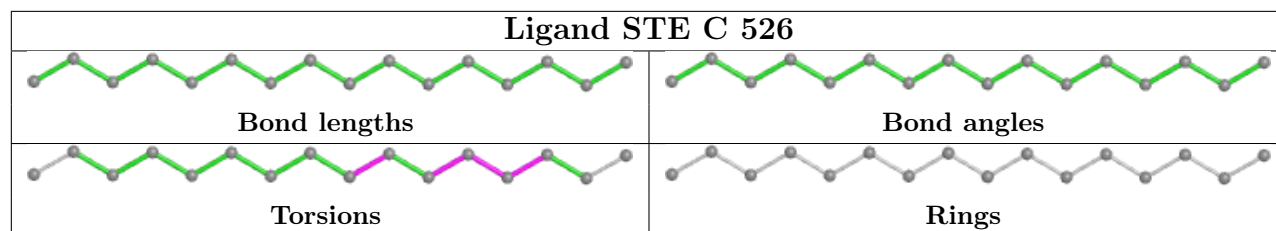


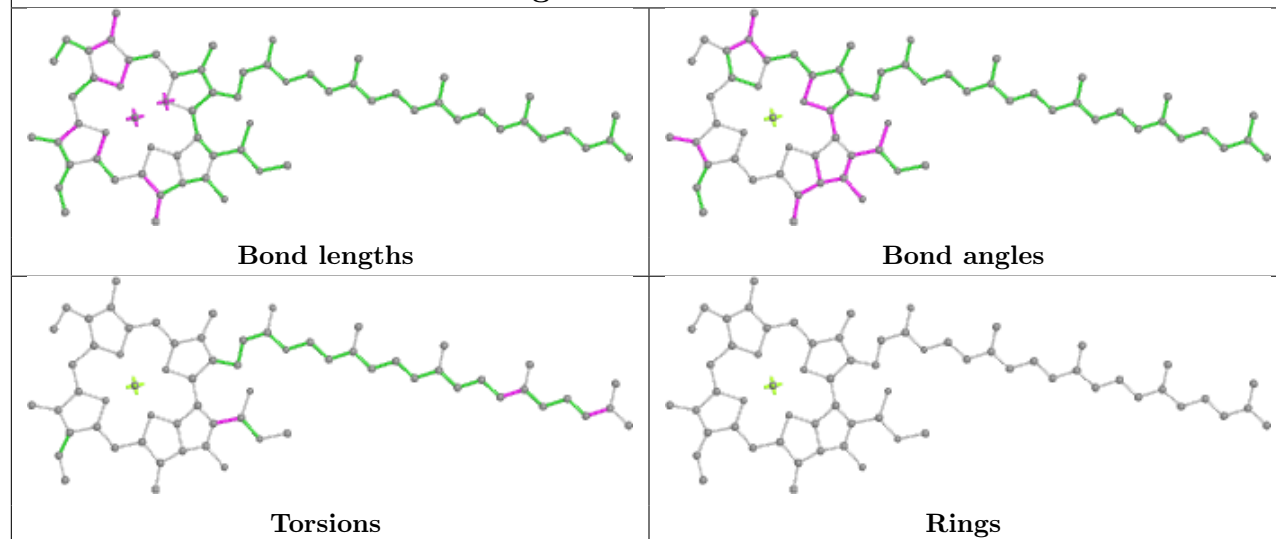
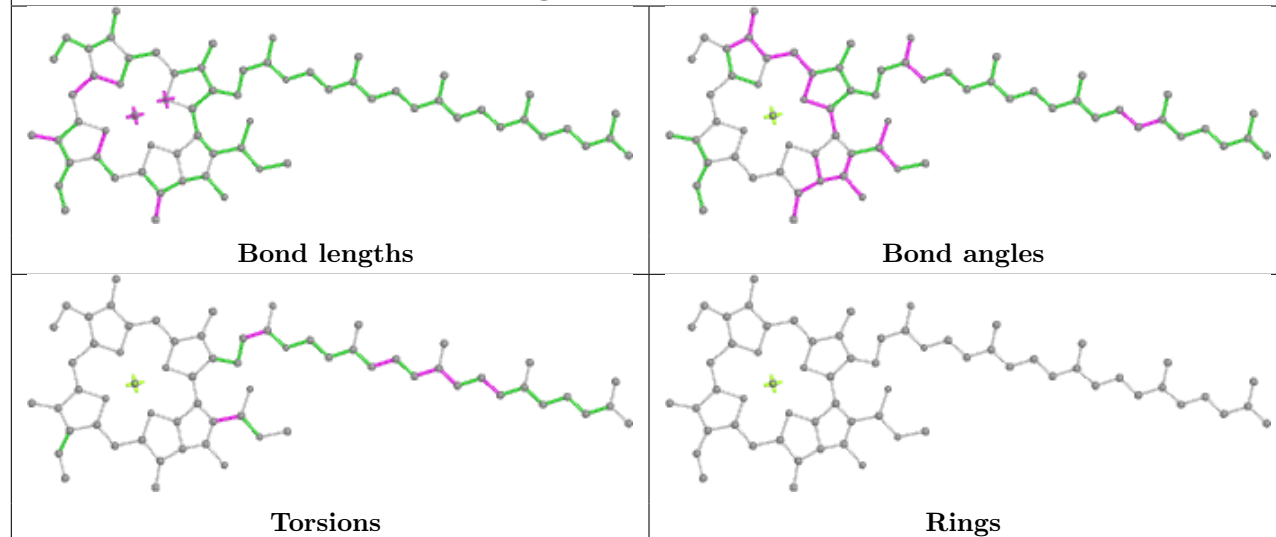
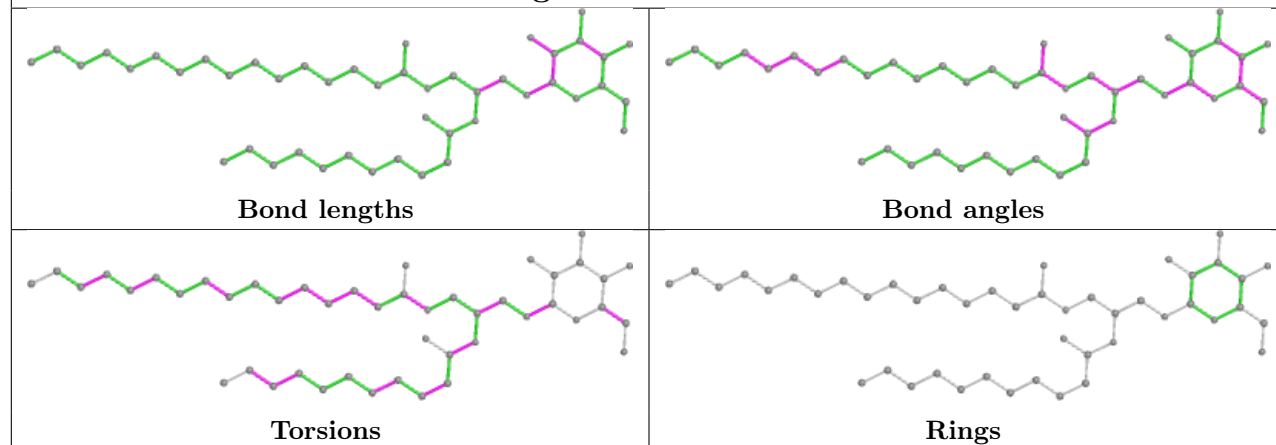
Ligand DGD c 519



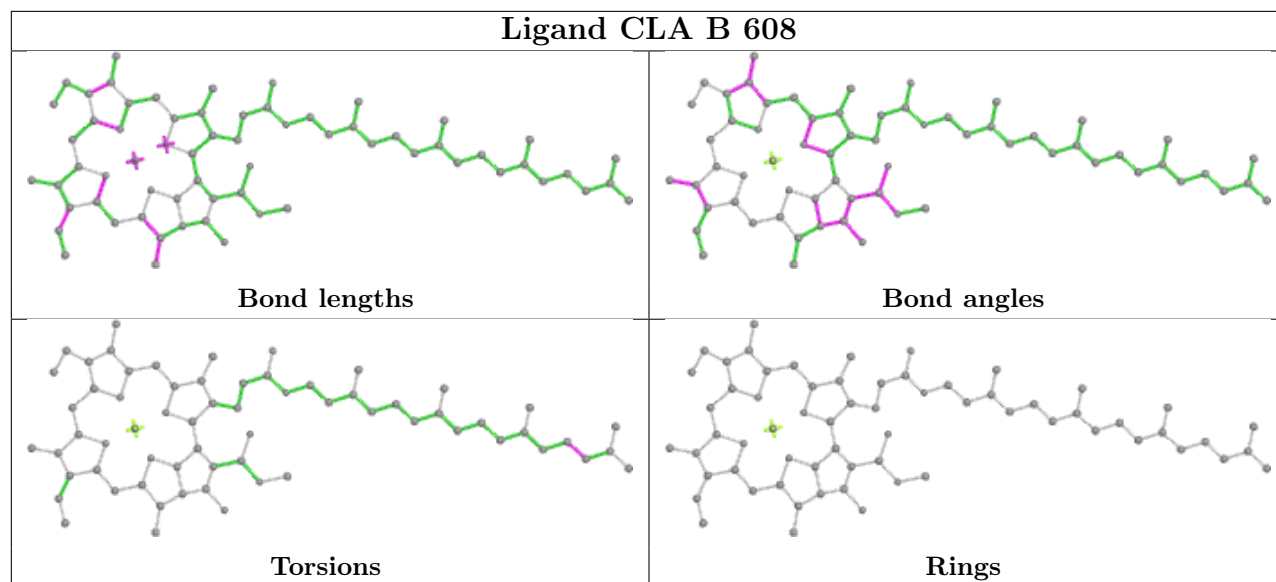
Ligand CLA B 610



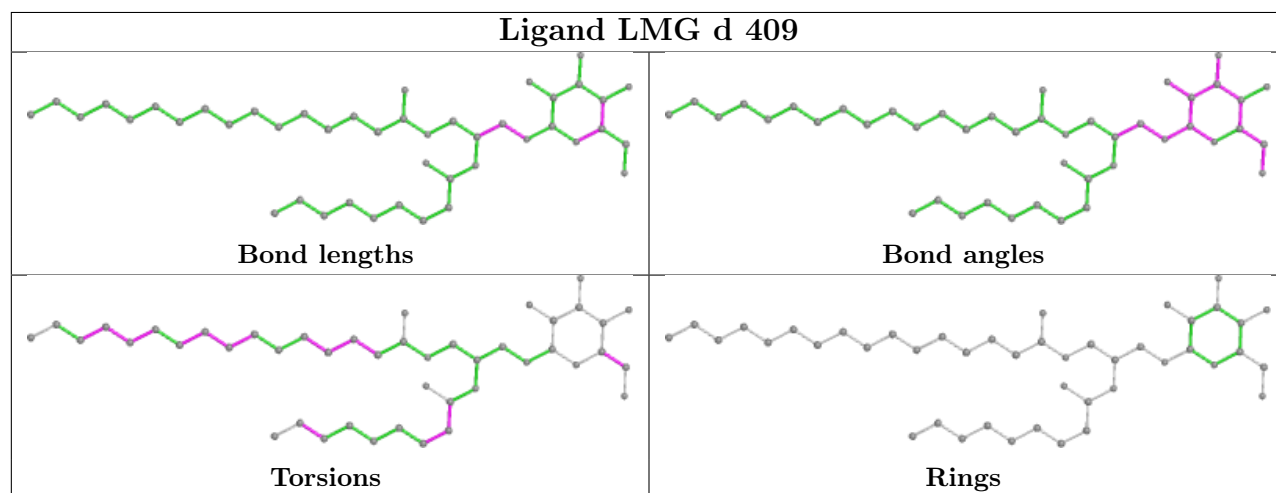


Ligand CLA C 502**Ligand CLA b 611****Ligand LMG c 522**

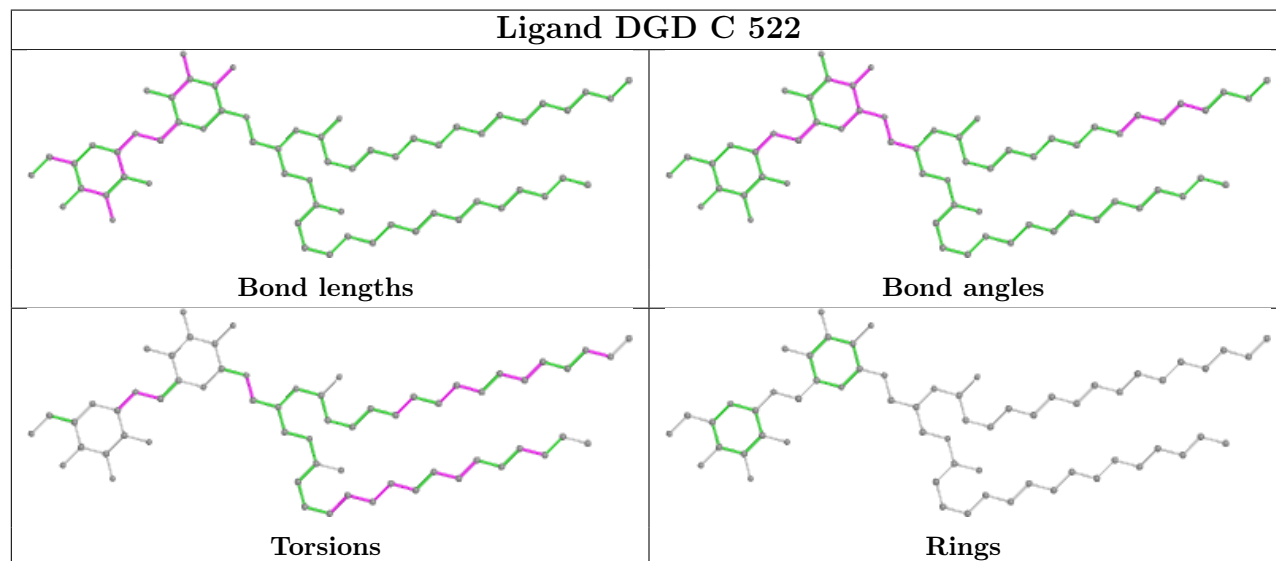
Ligand CLA B 608

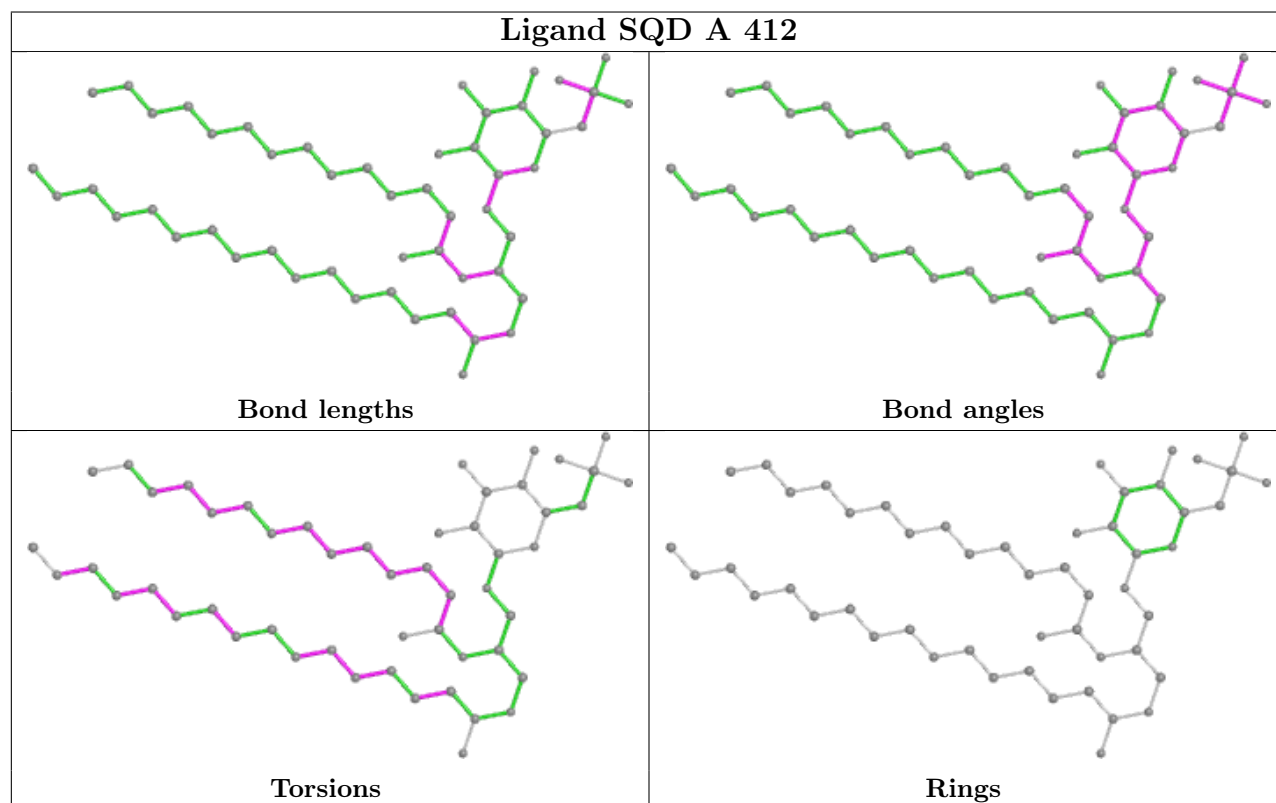
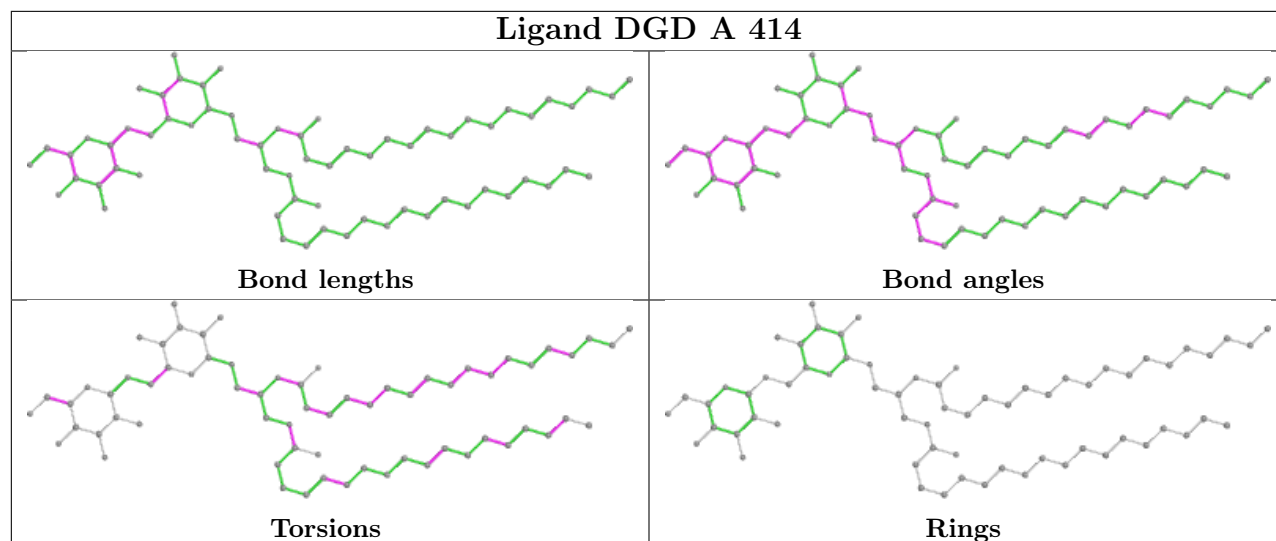


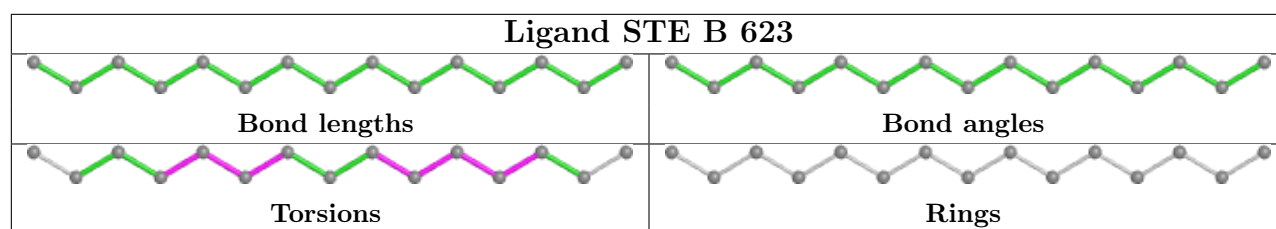
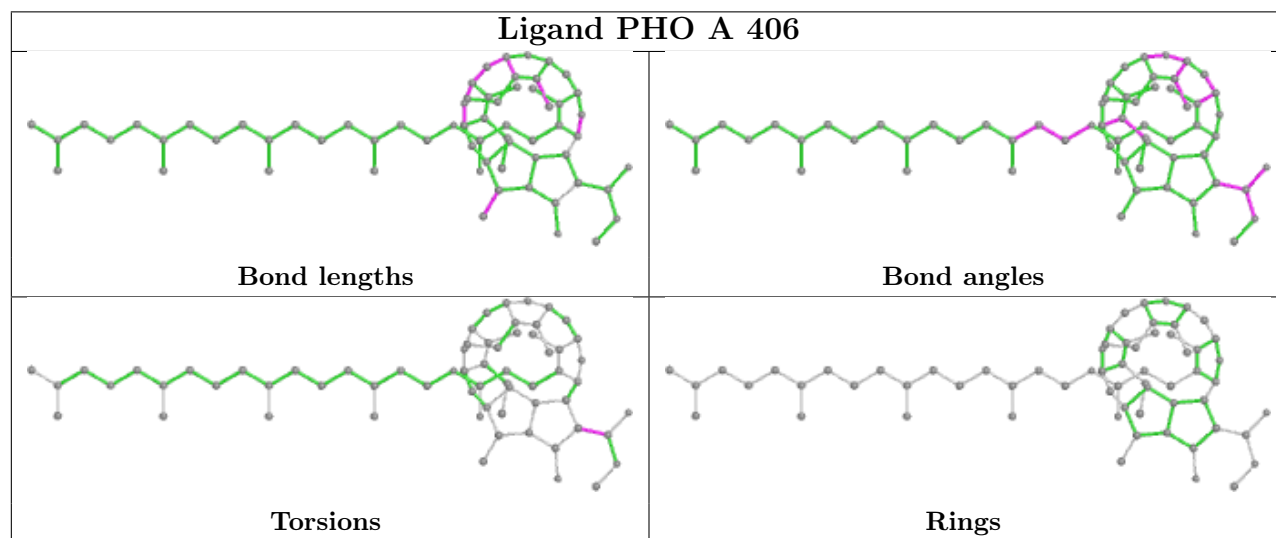
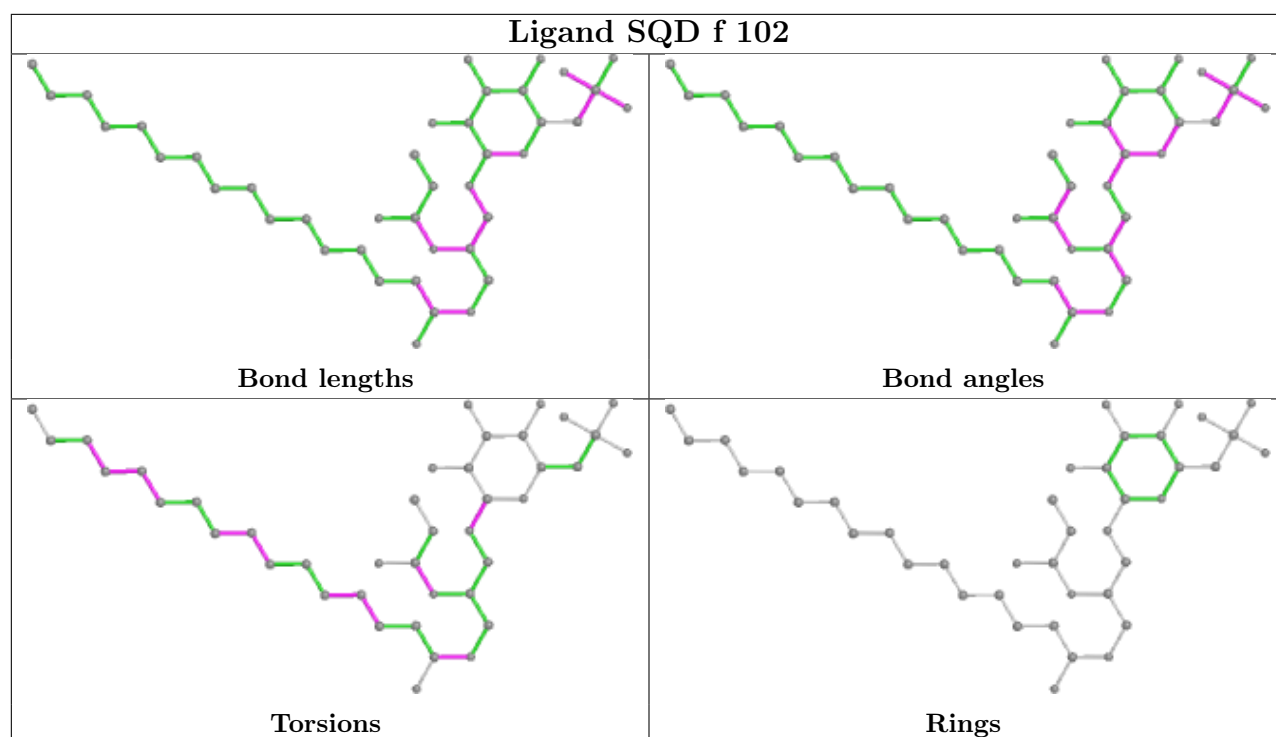
Ligand LMG d 409

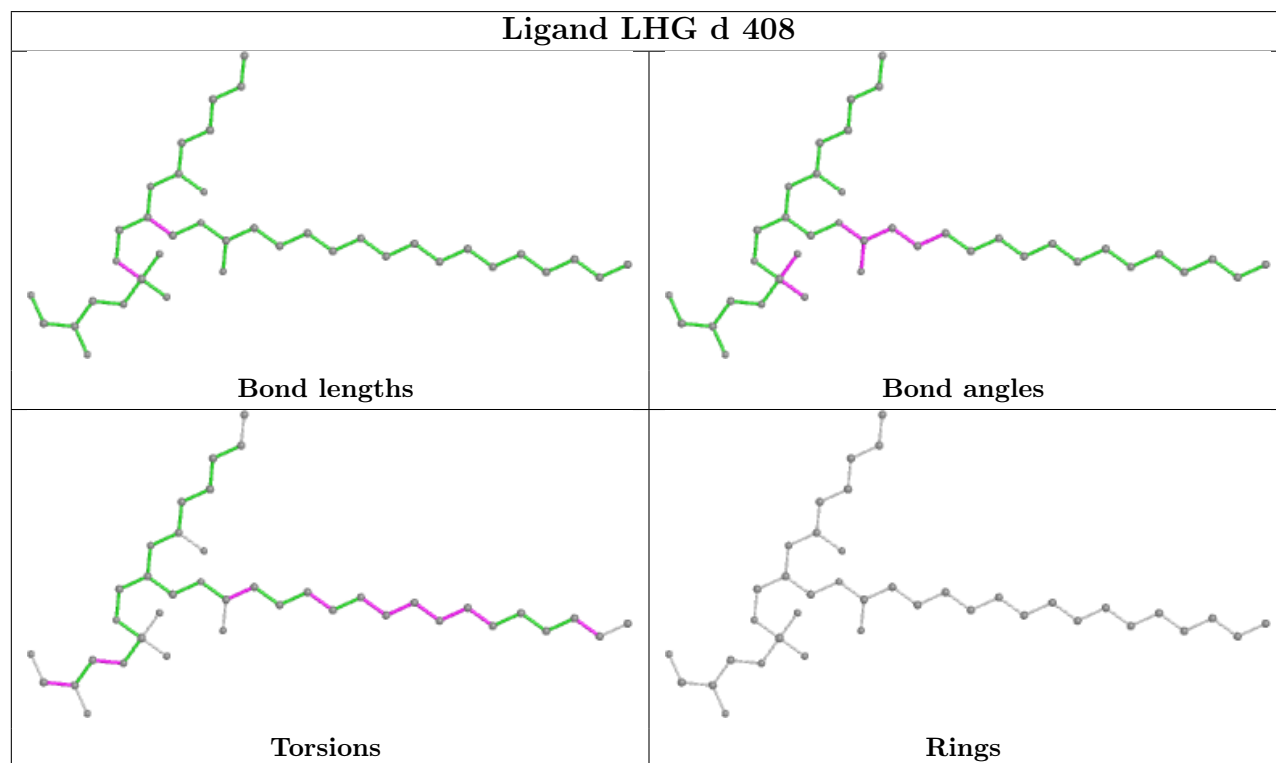
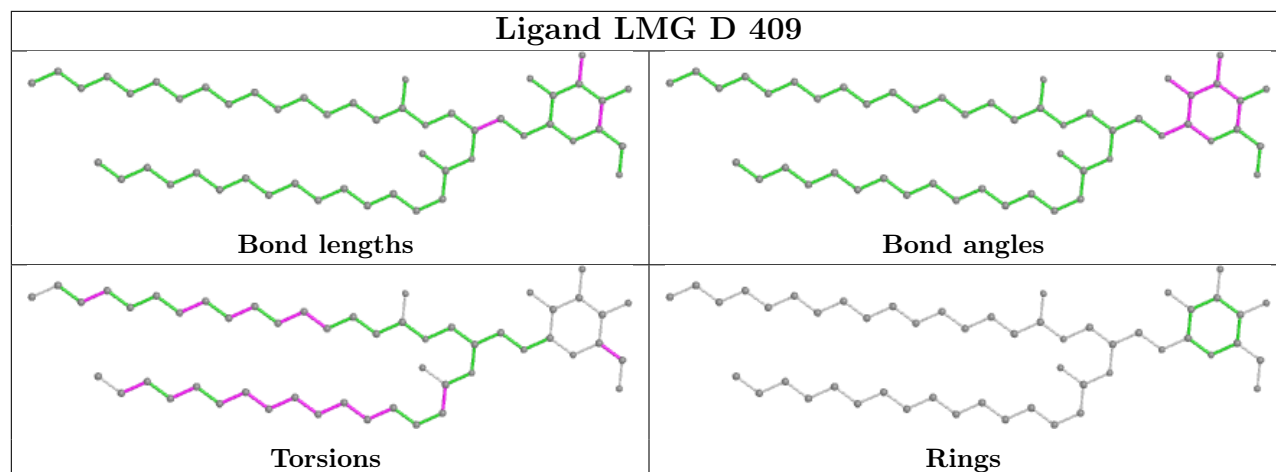


Ligand DGD C 522

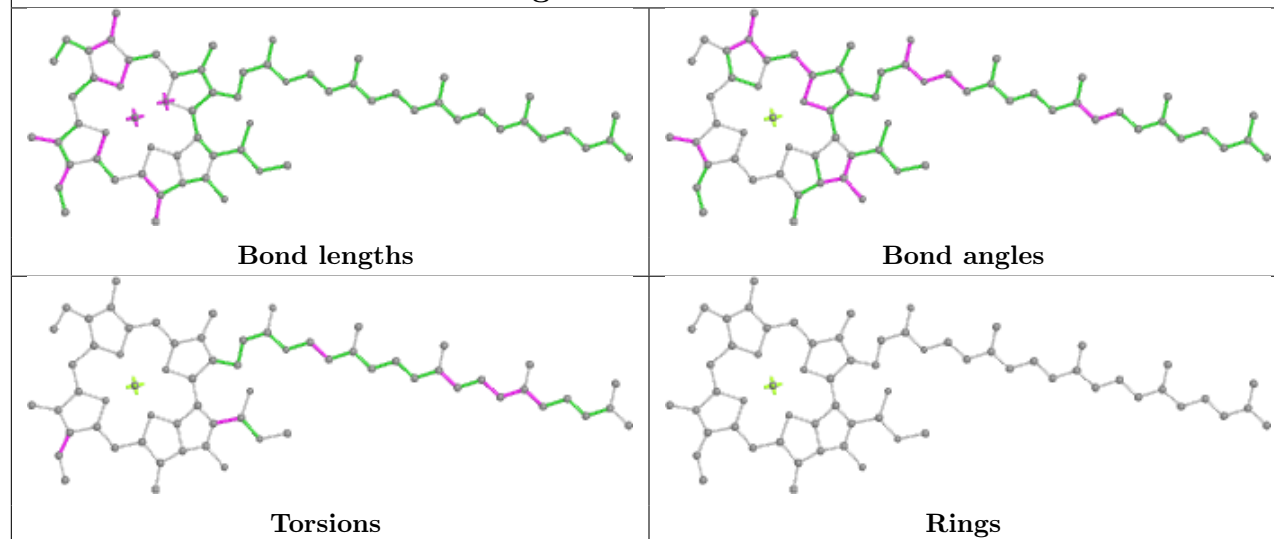




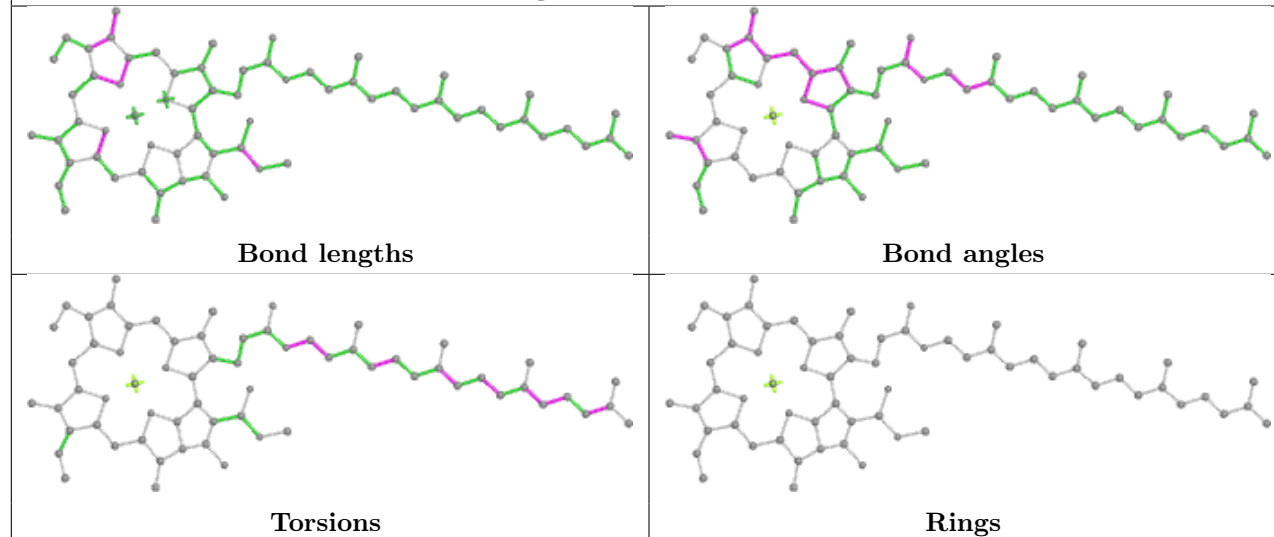




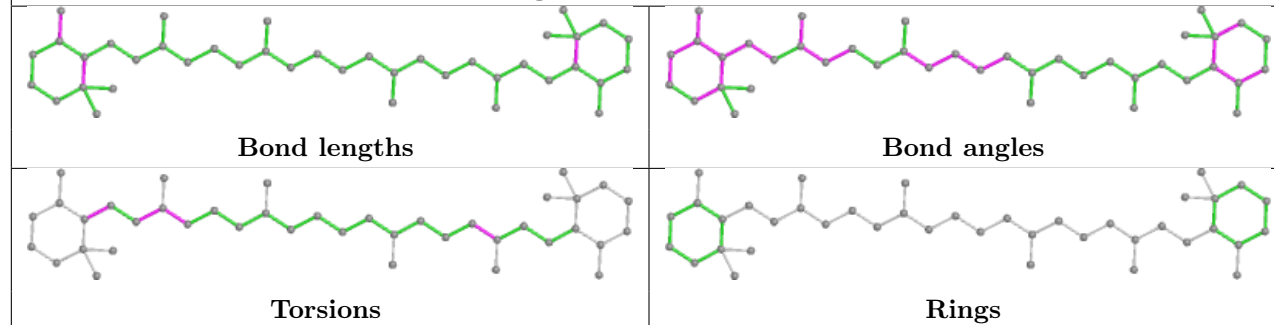
Ligand CLA B 604



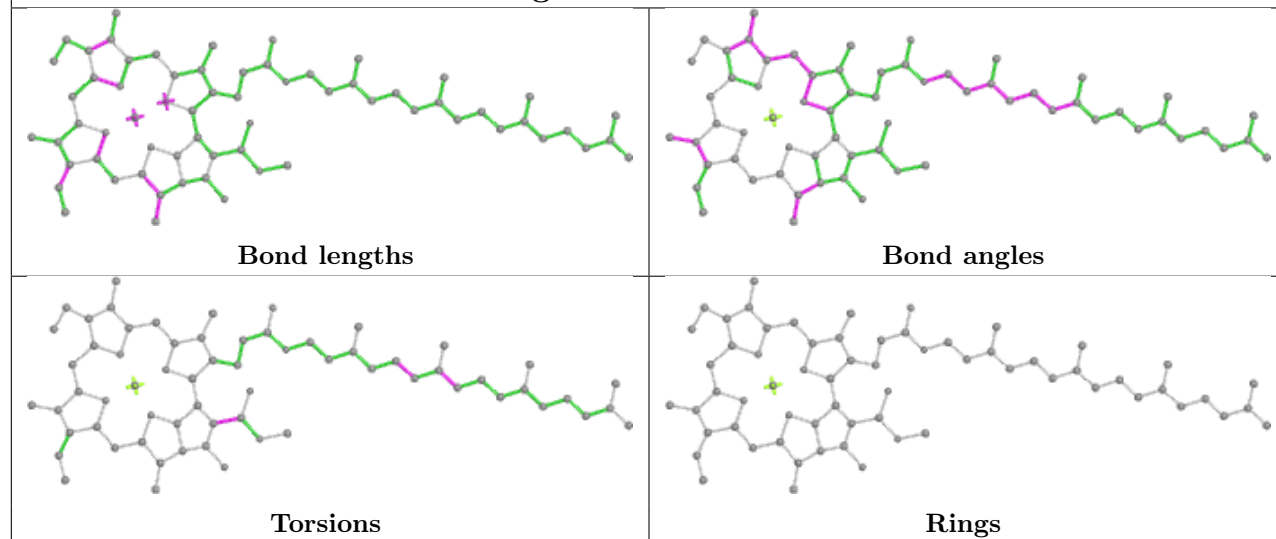
Ligand CLA C 509



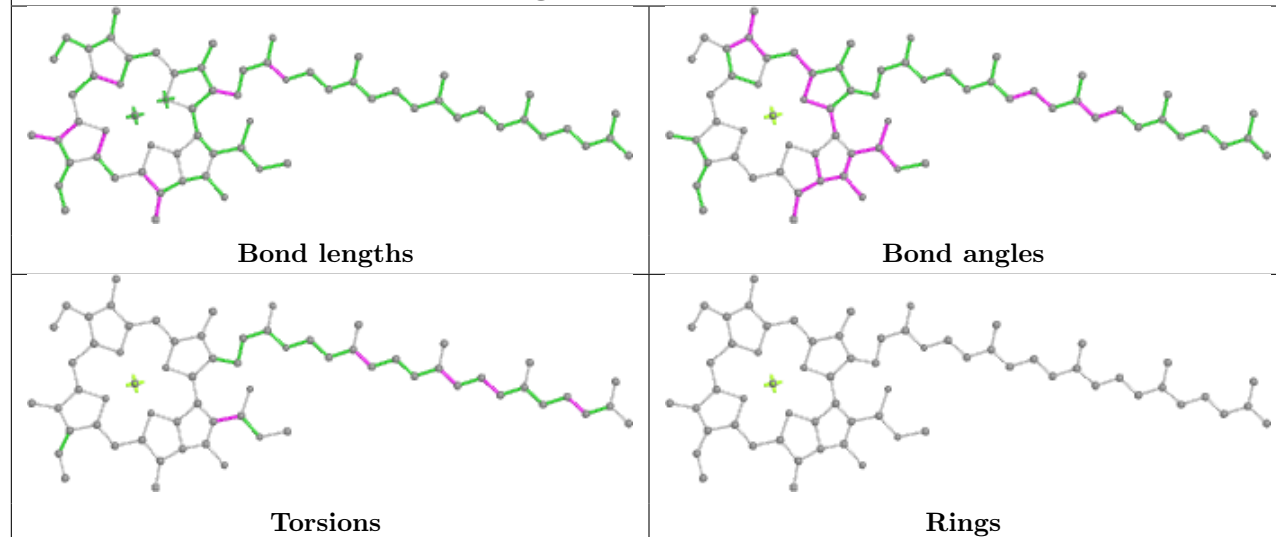
Ligand BCR B 617



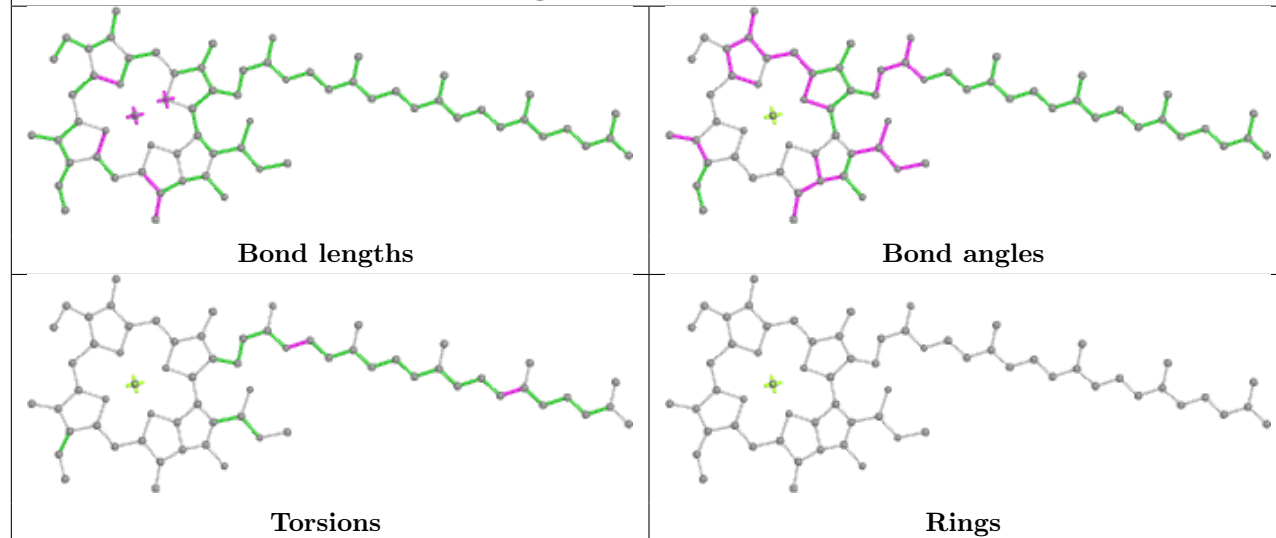
Ligand CLA C 503

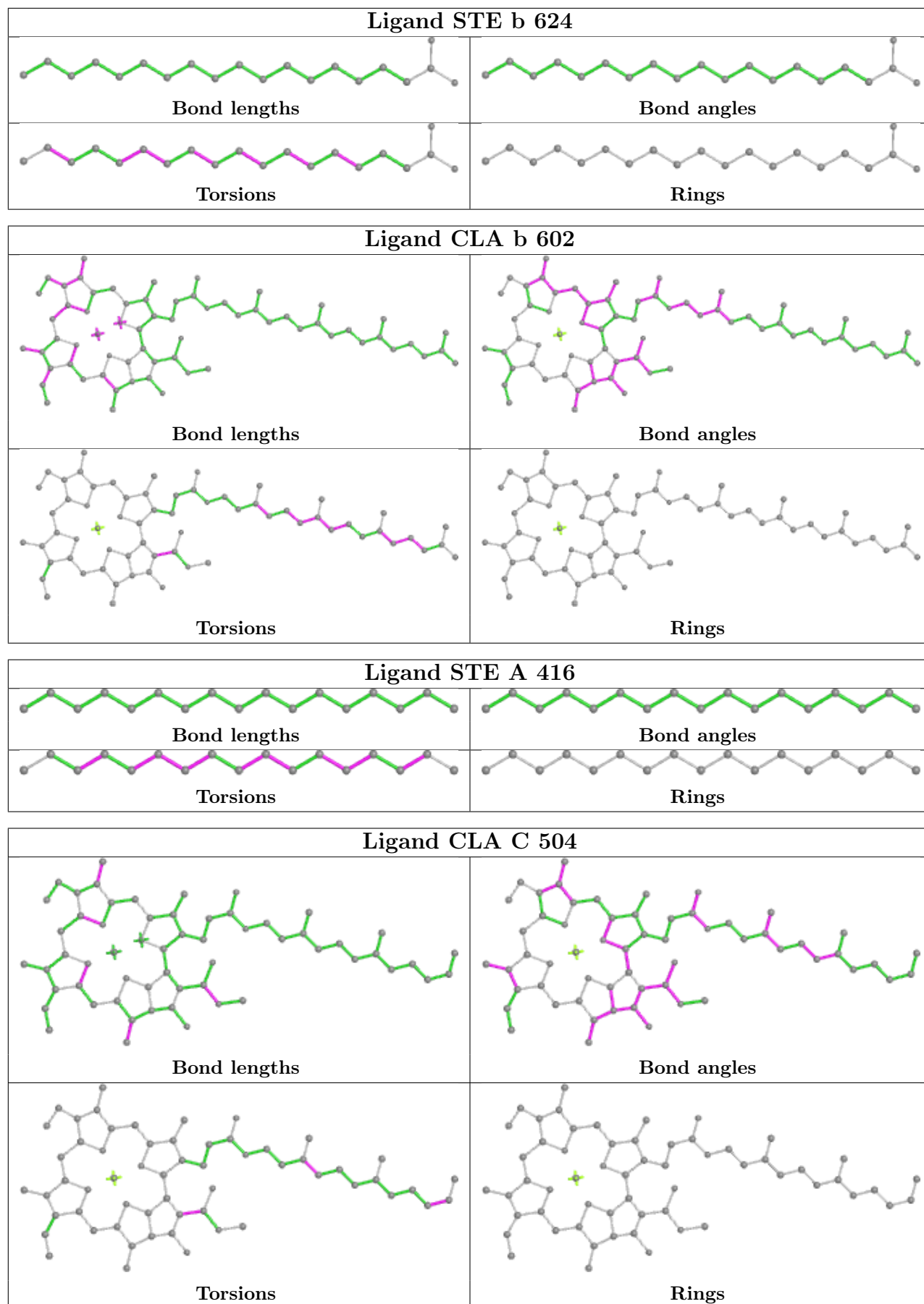


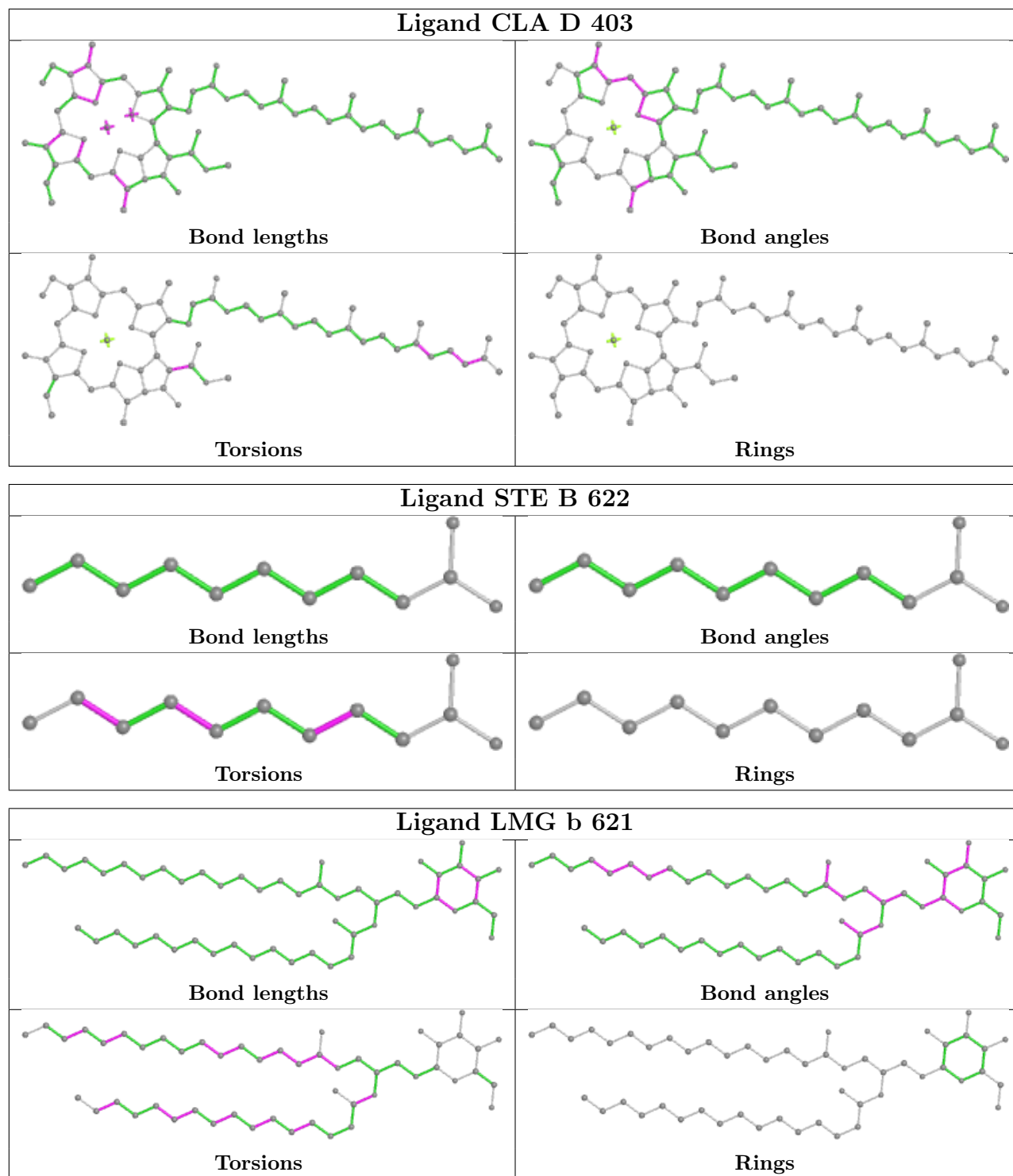
Ligand CLA C 510

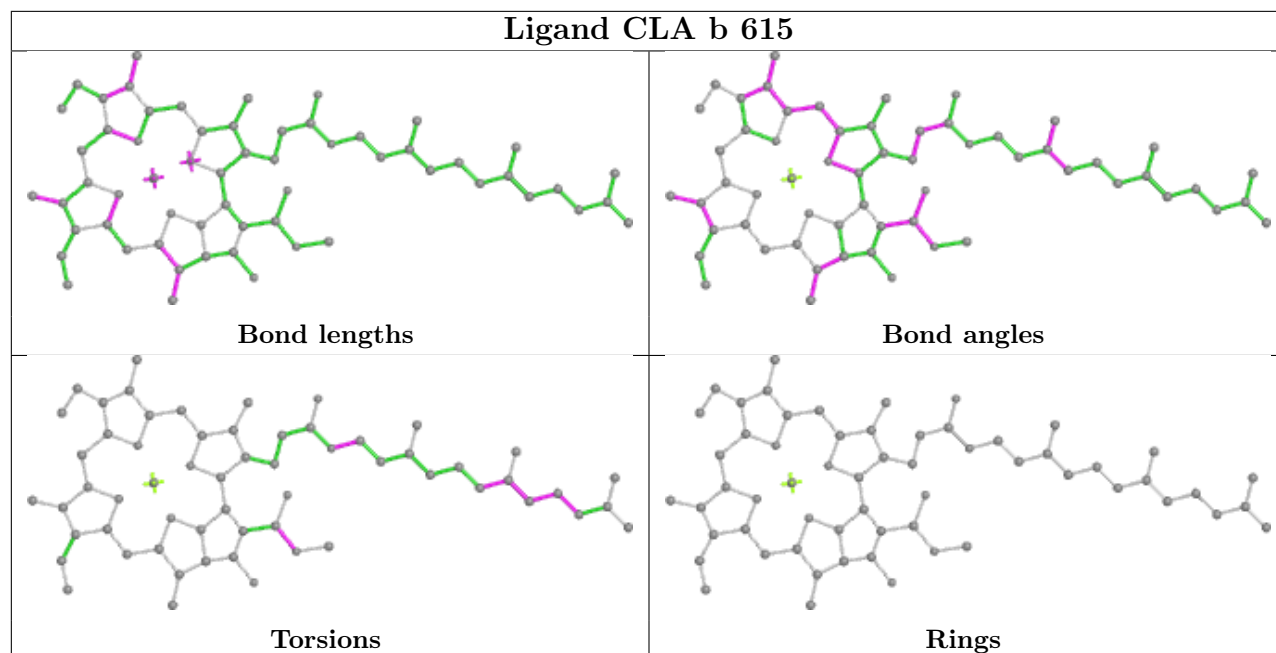


Ligand CLA D 404

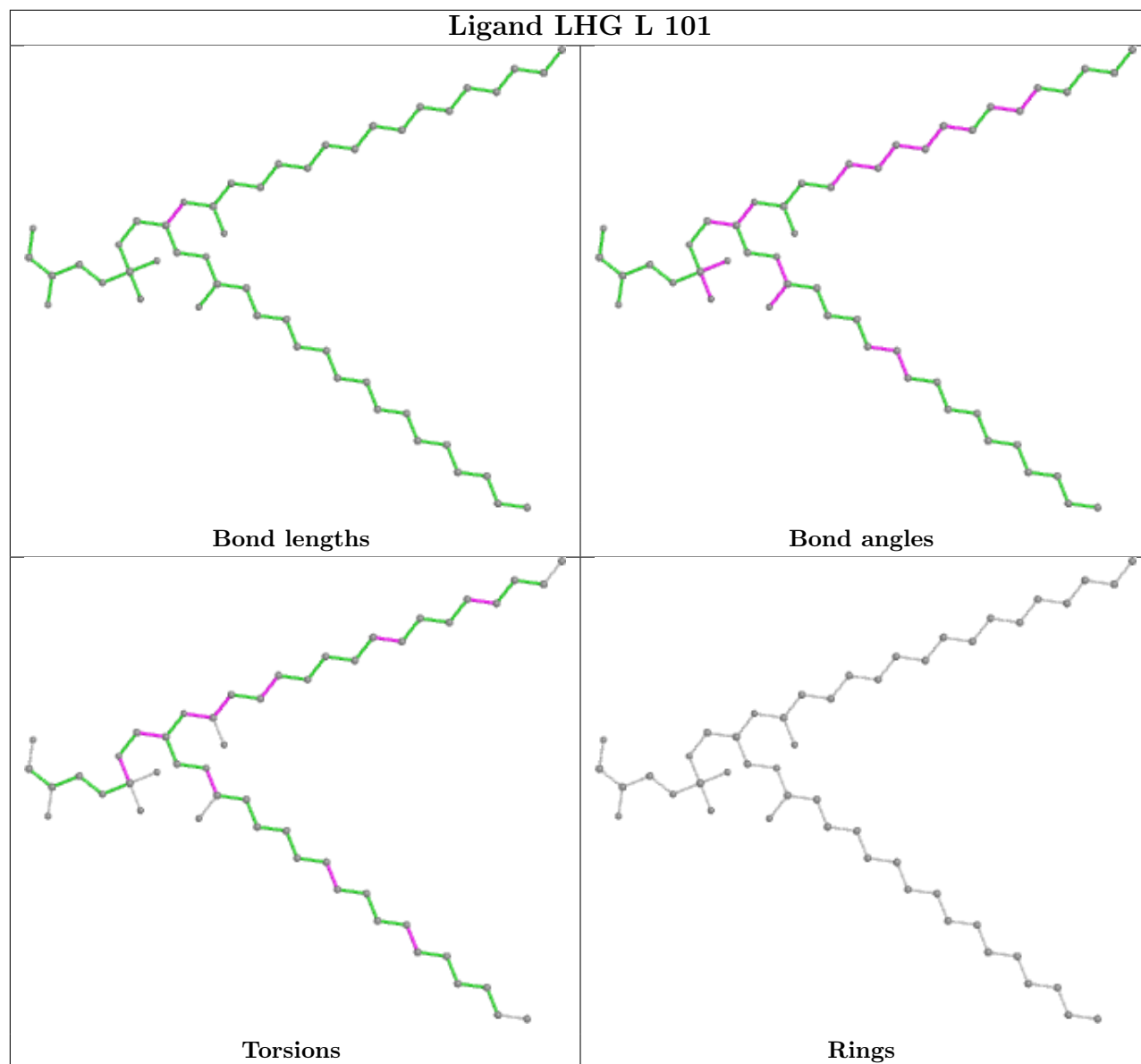




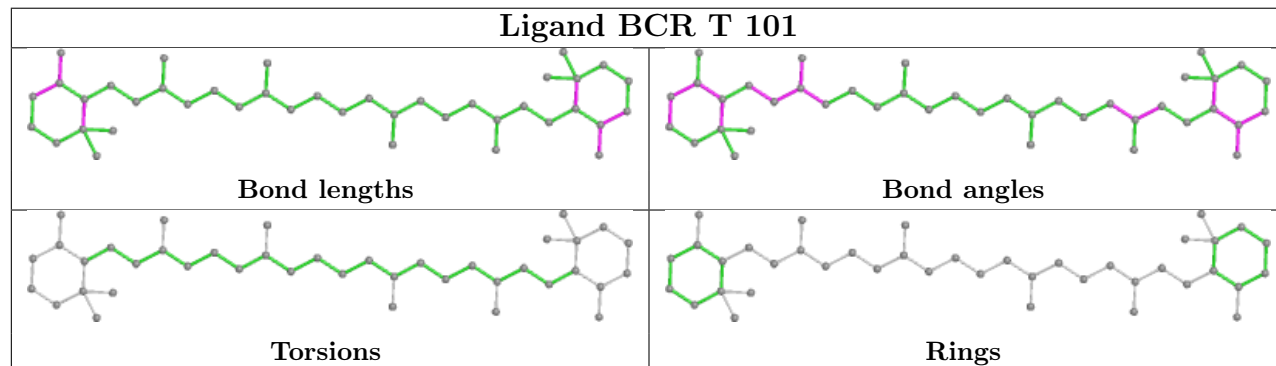




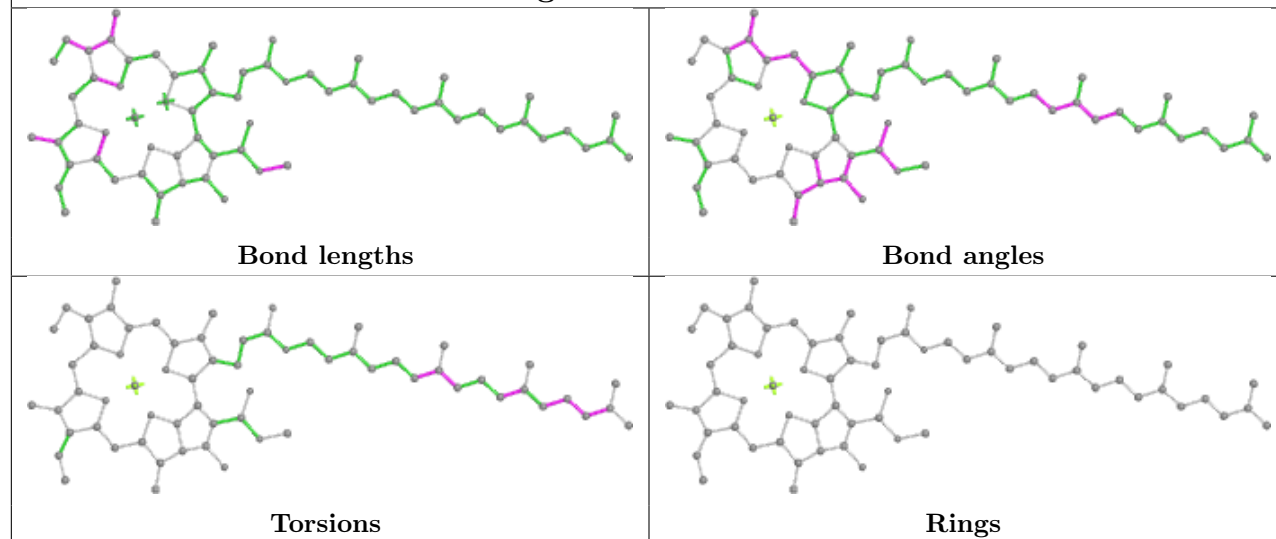
Ligand LHG L 101



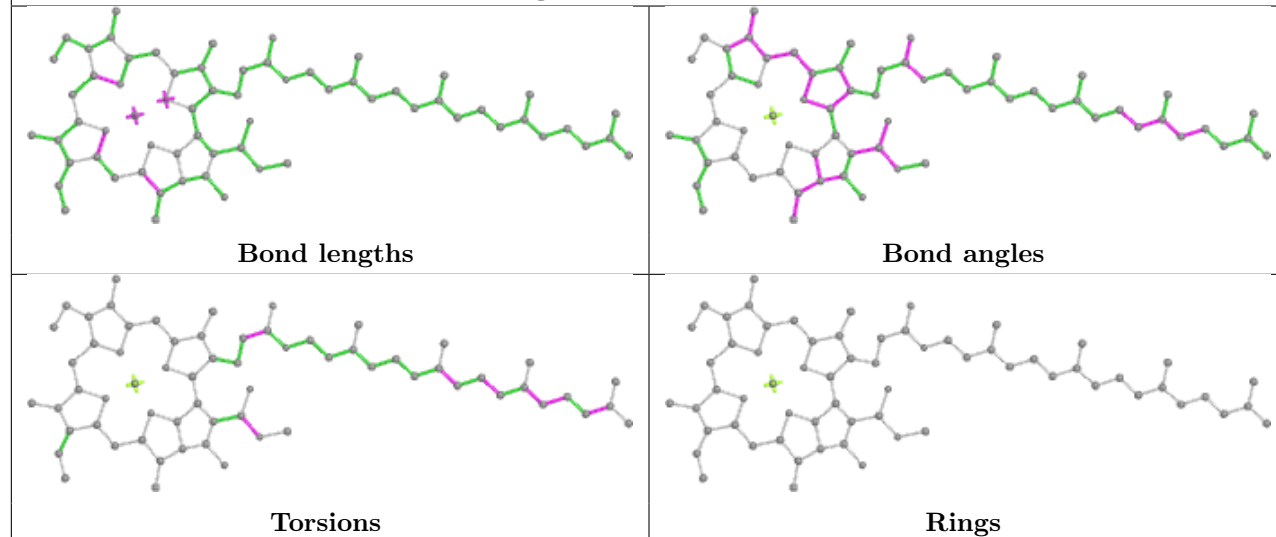
Ligand BCR T 101



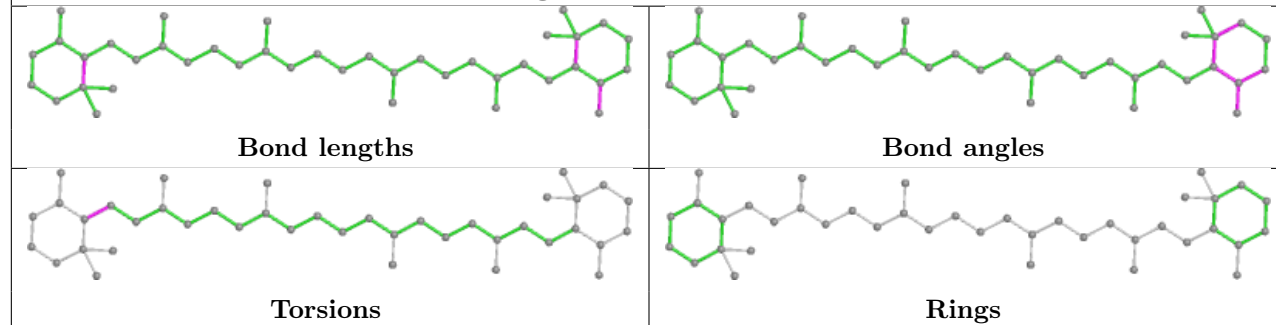
Ligand CLA c 505



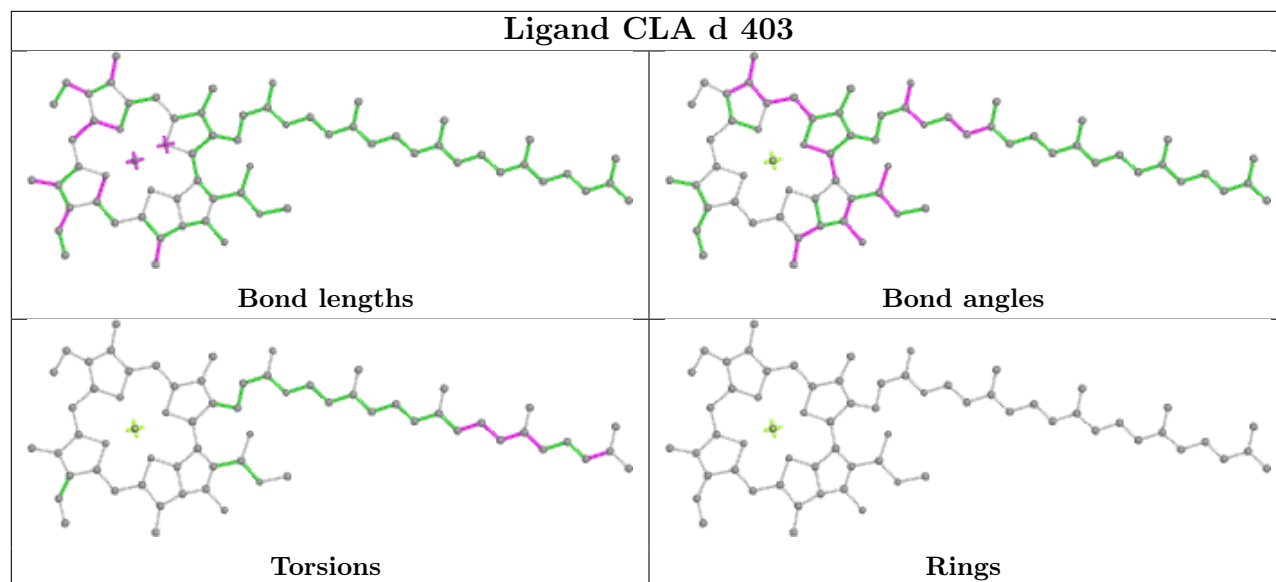
Ligand CLA B 612



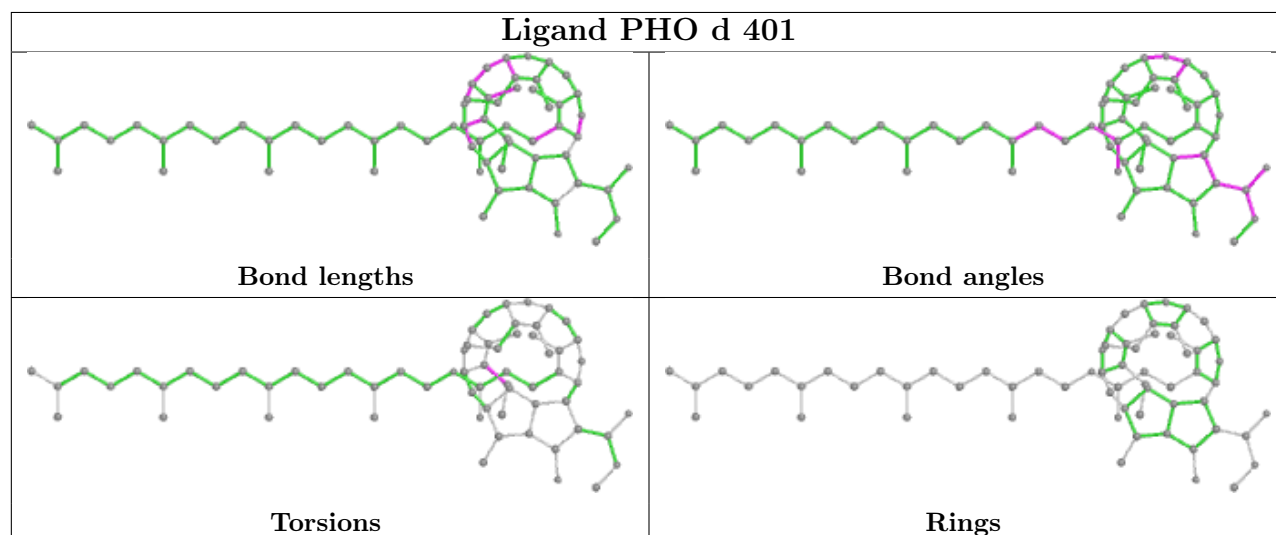
Ligand BCR k 102



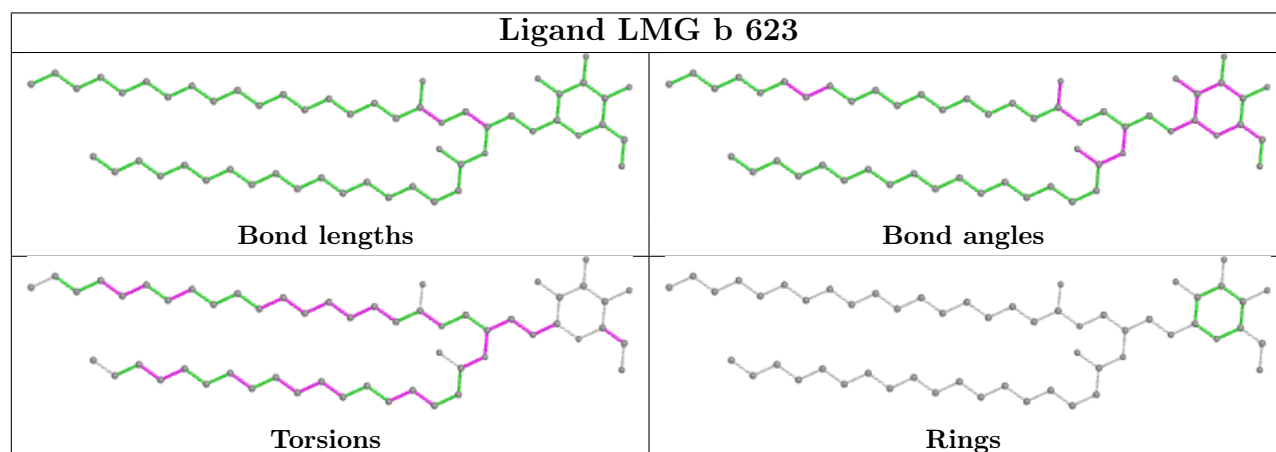
Ligand CLA d 403

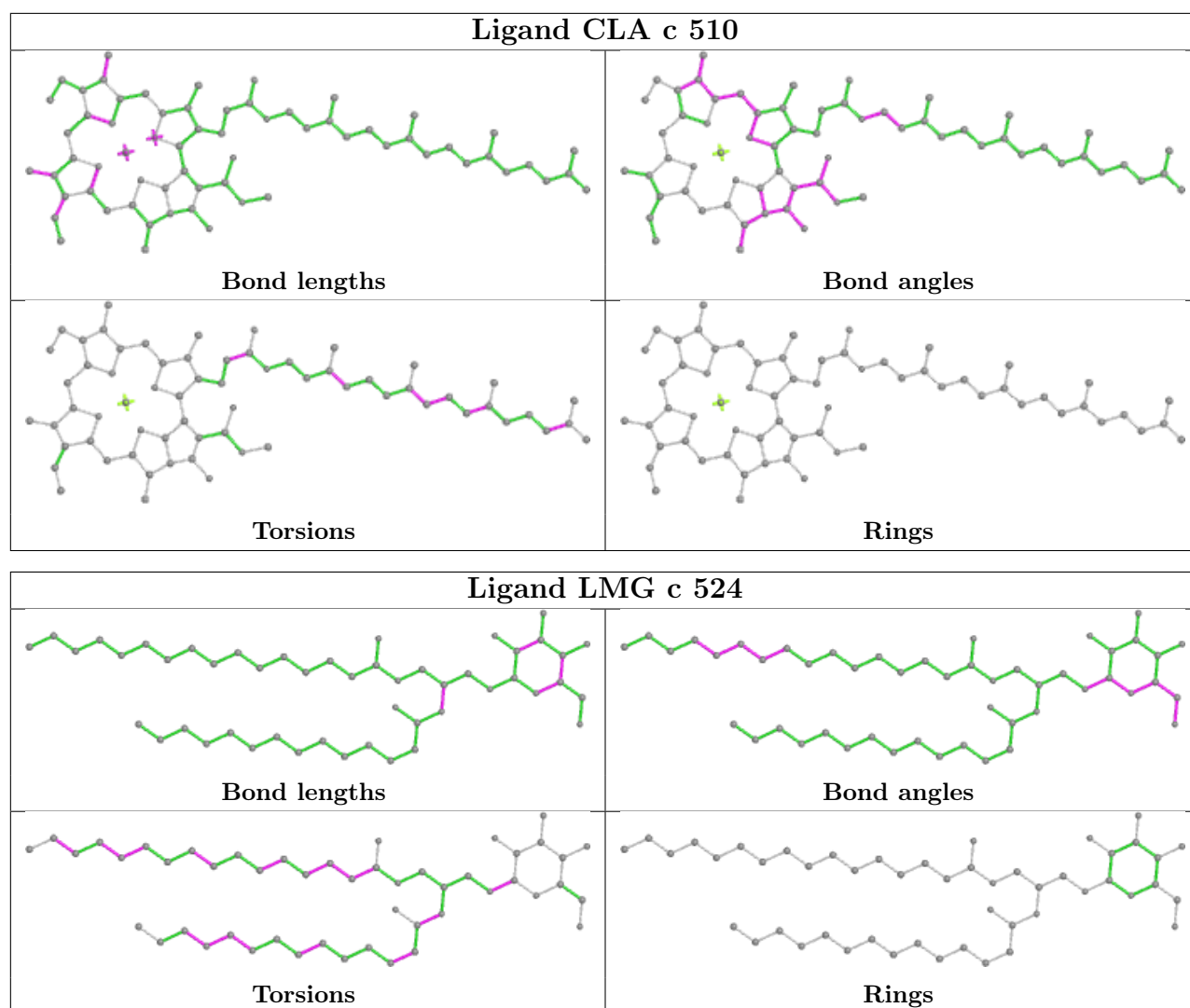


Ligand PHO d 401



Ligand LMG b 623





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.13	3 (0%) 84 85	19, 25, 44, 77	0
1	a	334/344 (97%)	-0.17	4 (1%) 79 81	19, 27, 52, 79	0
2	B	505/510 (99%)	-0.12	9 (1%) 68 71	20, 29, 57, 88	0
2	b	505/510 (99%)	0.07	22 (4%) 34 37	23, 32, 67, 102	0
3	C	442/461 (95%)	-0.05	9 (2%) 65 68	21, 32, 48, 72	0
3	c	451/461 (97%)	0.03	10 (2%) 62 64	23, 35, 57, 92	0
4	D	341/352 (96%)	-0.09	1 (0%) 94 94	18, 26, 43, 76	0
4	d	341/352 (96%)	-0.09	0 100 100	21, 30, 53, 71	0
5	E	82/84 (97%)	0.37	7 (8%) 10 12	30, 45, 64, 75	0
5	e	82/84 (97%)	0.58	12 (14%) 2 2	34, 54, 73, 83	0
6	F	34/45 (75%)	-0.00	3 (8%) 10 11	32, 38, 59, 83	0
6	f	34/45 (75%)	0.11	2 (5%) 22 25	37, 45, 75, 94	0
7	H	65/66 (98%)	0.12	3 (4%) 32 35	27, 37, 56, 75	0
7	h	63/66 (95%)	0.45	5 (7%) 12 14	36, 45, 61, 70	0
8	I	35/38 (92%)	-0.03	2 (5%) 23 26	27, 34, 65, 77	0
8	i	35/38 (92%)	0.09	3 (8%) 10 12	28, 36, 72, 81	0
9	J	36/40 (90%)	0.22	4 (11%) 5 6	29, 45, 69, 87	0
9	j	36/40 (90%)	0.46	5 (13%) 2 3	34, 48, 82, 86	0
10	K	37/46 (80%)	0.38	3 (8%) 12 13	37, 45, 66, 72	0
10	k	37/46 (80%)	0.23	3 (8%) 12 13	43, 49, 61, 74	0
11	L	37/37 (100%)	-0.23	0 100 100	20, 25, 62, 70	0
11	l	36/37 (97%)	-0.13	2 (5%) 24 27	22, 26, 69, 77	0
12	M	32/36 (88%)	0.36	1 (3%) 49 51	24, 29, 56, 68	0
12	m	31/36 (86%)	-0.03	0 100 100	23, 30, 48, 63	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	0.21	23 (9%) 8 9	22, 37, 79, 118	0
13	o	244/272 (89%)	0.13	19 (7%) 13 14	22, 36, 76, 118	0
14	T	29/32 (90%)	-0.26	2 (6%) 16 19	22, 26, 56, 72	0
14	t	29/32 (90%)	0.02	3 (10%) 6 7	24, 27, 77, 90	0
15	U	97/134 (72%)	-0.06	2 (2%) 63 66	27, 39, 63, 82	0
15	u	97/134 (72%)	-0.15	1 (1%) 82 84	25, 36, 52, 80	0
16	V	137/163 (84%)	-0.30	0 100 100	26, 35, 53, 75	0
16	v	137/163 (84%)	0.09	4 (2%) 51 54	29, 42, 62, 84	0
17	Y	27/46 (58%)	1.65	9 (33%) 0 0	49, 68, 85, 94	0
17	y	30/46 (65%)	0.91	7 (23%) 0 0	54, 67, 85, 87	0
18	X	38/41 (92%)	0.46	5 (13%) 3 3	34, 45, 72, 77	0
18	x	39/41 (95%)	0.79	7 (17%) 1 1	45, 53, 81, 91	0
19	Z	62/62 (100%)	1.30	19 (30%) 0 0	51, 63, 103, 113	0
19	z	62/62 (100%)	1.19	17 (27%) 0 0	53, 66, 98, 115	0
20	R	28/41 (68%)	2.69	19 (67%) 0 0	59, 67, 85, 90	0
20	r	28/41 (68%)	4.76	25 (89%) 0 0	73, 97, 104, 110	0
All	All	5293/5700 (92%)	0.09	275 (5%) 27 30	18, 33, 68, 118	0

All (275) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	r	10	LEU	10.3
13	o	58	ASN	9.3
19	z	33	TRP	8.8
20	r	28	VAL	8.7
20	r	6	LEU	8.7
20	r	14	LEU	8.1
20	r	9	LEU	7.9
13	o	3	GLN	7.3
20	r	3	TRP	7.1
13	o	4	THR	6.8
20	r	13	LEU	6.7
13	O	56	PRO	6.5
20	r	25	PRO	6.4
18	X	2	THR	6.4
20	R	3	TRP	6.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
18	x	2	THR	6.2
19	Z	62	VAL	6.2
19	Z	33	TRP	5.8
5	E	79	PHE	5.8
2	b	495	PHE	5.7
20	R	6	LEU	5.7
13	O	3	GLN	5.5
6	f	12	SER	5.5
2	b	502	VAL	5.5
3	c	24	THR	5.5
19	Z	35	ARG	5.5
1	A	13	LEU	5.4
20	r	7	VAL	5.4
3	c	23	ALA	5.4
19	z	3	ILE	5.3
6	F	12	SER	5.2
5	e	79	PHE	5.2
13	O	4	THR	5.1
13	O	61	GLN	5.1
17	Y	40	ALA	5.0
2	b	127	ARG	5.0
3	c	147	PHE	4.9
13	o	57	LYS	4.9
9	j	5	GLY	4.8
20	r	26	TYR	4.8
13	o	59	LYS	4.8
17	Y	21	GLN	4.7
17	y	19	ILE	4.7
20	r	18	TRP	4.7
20	R	24	LEU	4.6
7	H	66	GLY	4.6
20	r	24	LEU	4.6
20	r	29	LYS	4.5
20	r	5	VAL	4.5
17	Y	43	ARG	4.5
9	j	8	ILE	4.5
1	A	11	ALA	4.5
20	r	27	ALA	4.4
9	J	7	ARG	4.4
9	j	6	GLY	4.4
19	Z	4	LEU	4.4
19	Z	1	MET	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	O	55	GLU	4.3
20	R	21	ARG	4.3
19	Z	3	ILE	4.2
13	O	60	ARG	4.2
13	o	60	ARG	4.2
19	Z	7	LEU	4.2
19	Z	61	VAL	4.2
20	R	26	TYR	4.2
14	t	29	ILE	4.0
19	Z	34	ASP	4.0
15	U	8	GLU	4.0
20	r	19	ALA	4.0
19	z	36	SER	4.0
13	O	5	LEU	4.0
10	K	17	ILE	3.9
13	O	59	LYS	3.9
1	a	11	ALA	3.9
11	l	3	PRO	3.9
20	r	2	ASP	3.9
3	c	146	PHE	3.9
13	O	62	GLU	3.8
13	o	61	GLN	3.8
20	r	11	PRO	3.7
14	t	30	THR	3.7
19	z	1	MET	3.7
3	c	143	TYR	3.7
2	B	505	ARG	3.7
13	o	5	LEU	3.7
13	O	36	GLN	3.7
17	Y	20	ALA	3.7
20	r	23	ILE	3.7
2	b	487	SER	3.6
9	J	6	GLY	3.6
2	B	502	VAL	3.6
20	r	4	ARG	3.6
20	R	18	TRP	3.6
5	e	60	GLN	3.6
13	O	63	ALA	3.5
5	e	61	ARG	3.5
17	Y	42	ARG	3.5
20	r	12	VAL	3.5
13	O	57	LYS	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
18	X	3	ILE	3.5
8	i	36	ASP	3.5
19	Z	32	ASP	3.5
2	b	506	ARG	3.5
8	i	34	ARG	3.5
14	T	29	ILE	3.4
20	R	2	ASP	3.4
2	b	505	ARG	3.4
13	o	62	GLU	3.4
13	O	54	GLU	3.4
13	o	56	PRO	3.4
17	Y	25	ILE	3.4
7	h	6	TRP	3.4
9	j	7	ARG	3.4
10	k	17	ILE	3.4
9	J	5	GLY	3.3
8	I	34	ARG	3.3
20	R	25	PRO	3.3
19	z	7	LEU	3.3
20	R	13	LEU	3.3
2	B	495	PHE	3.2
20	R	28	VAL	3.2
19	Z	38	GLN	3.2
2	B	293	ALA	3.2
7	h	10	ILE	3.2
3	C	57	ALA	3.1
19	z	30	PRO	3.1
2	b	485	GLU	3.1
20	r	21	ARG	3.1
20	R	29	LYS	3.1
12	M	33	GLN	3.1
13	O	34	SER	3.1
2	b	85	GLY	3.1
14	T	30	THR	3.1
2	b	161	LEU	3.1
17	Y	22	LEU	3.1
13	o	207	ARG	3.1
19	z	35	ARG	3.1
2	b	499	VAL	3.0
17	y	41	VAL	3.0
19	z	62	VAL	3.0
9	J	8	ILE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
19	Z	41	PHE	3.0
6	F	13	TYR	3.0
2	b	491	VAL	3.0
19	Z	39	LEU	3.0
7	h	21	VAL	3.0
20	R	14	LEU	3.0
17	Y	41	VAL	2.9
19	Z	40	ILE	2.9
13	O	35	SER	2.9
18	x	40	SER	2.9
2	b	490	GLN	2.9
13	O	246	ALA	2.9
2	b	486	LEU	2.9
20	R	20	VAL	2.9
2	b	295	GLY	2.9
3	C	146	PHE	2.9
16	v	15	GLU	2.8
18	x	34	ILE	2.8
5	E	84	LYS	2.8
17	y	37	PHE	2.8
19	Z	42	LEU	2.8
11	l	2	GLU	2.8
5	e	74	GLN	2.8
5	e	84	LYS	2.8
13	O	207	ARG	2.8
19	z	38	GLN	2.8
3	C	65	GLY	2.7
19	z	32	ASP	2.7
19	z	39	LEU	2.7
5	E	3	GLY	2.7
19	Z	59	PHE	2.7
20	R	27	ALA	2.7
2	B	127	ARG	2.7
13	o	64	GLU	2.7
20	r	15	ALA	2.7
5	e	17	VAL	2.7
5	e	76	VAL	2.7
2	b	128	THR	2.7
17	y	20	ALA	2.6
18	X	38	GLN	2.6
7	H	41	PHE	2.6
13	O	58	ASN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
15	U	9	LEU	2.6
16	v	17	LYS	2.6
7	h	41	PHE	2.6
17	y	18	VAL	2.6
13	o	132	ASN	2.6
2	b	289	GLN	2.6
19	z	4	LEU	2.6
3	C	61	VAL	2.6
13	o	133	VAL	2.6
19	Z	60	PHE	2.5
10	k	10	LYS	2.5
3	c	25	ASN	2.5
5	e	82	GLN	2.5
10	k	13	GLU	2.5
20	R	5	VAL	2.5
19	z	41	PHE	2.5
17	y	40	ALA	2.5
5	E	74	GLN	2.5
9	j	10	LEU	2.5
3	C	60	ILE	2.5
13	o	63	ALA	2.5
19	Z	37	LYS	2.5
7	H	65	LEU	2.5
2	B	506	ARG	2.5
18	x	23	LEU	2.4
19	z	42	LEU	2.4
3	c	123	ALA	2.4
20	R	23	ILE	2.4
1	a	14	TRP	2.4
2	b	496	TYR	2.4
8	i	35	LYS	2.4
5	e	80	LEU	2.4
18	x	37	VAL	2.4
20	r	8	VAL	2.4
2	B	490	GLN	2.4
4	D	12	ARG	2.4
13	O	25	THR	2.4
20	r	22	ASN	2.4
5	E	82	GLN	2.4
3	c	145	SER	2.3
5	e	81	GLU	2.3
16	v	21	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
20	R	9	LEU	2.3
10	K	18	PHE	2.3
13	o	89	SER	2.3
3	c	183	GLY	2.3
3	C	119	LEU	2.3
19	z	37	LYS	2.3
20	R	17	GLY	2.3
1	a	13	LEU	2.3
6	F	16	PHE	2.3
19	z	60	PHE	2.3
2	b	293	ALA	2.3
2	B	373	LYS	2.3
1	A	12	ASN	2.2
10	K	14	ALA	2.2
13	O	133	VAL	2.2
17	y	43	ARG	2.2
5	E	80	LEU	2.2
3	C	126	GLY	2.2
6	f	13	TYR	2.2
13	o	65	PHE	2.2
2	b	288	VAL	2.2
5	e	13	ILE	2.2
2	B	485	GLU	2.2
2	b	374	ASN	2.2
2	b	162	PHE	2.2
3	C	145	SER	2.2
19	Z	31	GLN	2.2
16	v	22	THR	2.2
7	h	22	ALA	2.2
5	E	83	LEU	2.1
2	b	494	GLY	2.1
3	C	262	ARG	2.1
1	a	128	GLY	2.1
18	X	34	ILE	2.1
18	x	3	ILE	2.1
5	e	83	LEU	2.1
15	u	9	LEU	2.1
14	t	28	ARG	2.1
17	Y	37	PHE	2.1
18	X	39	ARG	2.1
13	o	246	ALA	2.1
3	c	191	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	O	32	ILE	2.1
13	o	55	GLU	2.0
19	z	59	PHE	2.0
13	O	134	THR	2.0
18	x	38	GLN	2.0
13	O	87	VAL	2.0
20	R	19	ALA	2.0
8	I	6	ILE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	t	1	10/11	0.95	0.10	23,40,71,71	0
14	FME	T	1	10/11	0.96	0.09	27,45,62,62	0
12	FME	M	1	10/11	0.96	0.12	39,50,77,85	0
8	FME	i	1	10/11	0.97	0.12	41,49,59,64	0
8	FME	I	1	10/11	0.97	0.14	37,48,62,65	0
12	FME	m	1	10/11	0.98	0.10	31,44,69,83	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
27	STE	i	102	6/20	0.46	0.34	66,89,108,108	0
27	STE	C	527	8/20	0.54	0.35	38,55,61,70	0
27	STE	d	412	10/20	0.59	0.29	43,55,70,73	0
27	STE	H	103	18/20	0.60	0.32	47,73,92,93	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
27	STE	Z	101	17/20	0.62	0.31	48,69,95,100	0
27	STE	i	101	12/20	0.62	0.51	58,75,94,95	0
27	STE	c	517	18/20	0.62	0.31	50,81,102,102	0
27	STE	E	102	12/20	0.65	0.37	50,74,88,91	0
27	STE	e	101	9/20	0.66	0.29	44,50,58,62	0
27	STE	j	102	16/20	0.67	0.27	42,60,69,70	0
28	LMG	c	518	30/55	0.69	0.28	37,70,100,110	0
28	LMG	D	408	50/55	0.71	0.22	35,67,111,123	0
27	STE	B	623	15/20	0.72	0.23	38,62,88,89	0
28	LMG	b	619	24/55	0.72	0.33	40,54,75,79	0
27	STE	E	103	12/20	0.72	0.27	49,57,79,82	0
27	STE	a	417	12/20	0.73	0.28	47,66,71,71	0
27	STE	I	102	17/20	0.74	0.42	56,72,86,87	0
27	STE	C	529	14/20	0.74	0.32	53,78,105,109	0
27	STE	A	417	11/20	0.74	0.26	45,56,73,77	0
27	STE	x	102	20/20	0.75	0.21	36,55,74,82	0
27	STE	C	528	14/20	0.76	0.47	43,61,87,92	0
27	STE	T	102	16/20	0.76	0.25	38,61,99,102	0
27	STE	d	411	12/20	0.77	0.23	46,73,99,104	0
27	STE	C	526	16/20	0.77	0.16	36,56,73,74	0
27	STE	D	414	9/20	0.77	0.15	39,45,58,58	0
27	STE	m	102	15/20	0.77	0.21	41,58,87,92	0
27	STE	e	102	8/20	0.78	0.27	48,58,60,67	0
27	STE	A	410	9/20	0.78	0.33	46,52,60,64	0
27	STE	z	101	9/20	0.78	0.20	49,64,75,76	0
27	STE	E	104	20/20	0.79	0.32	52,67,80,82	0
27	STE	C	518	5/20	0.79	0.26	47,56,67,67	0
27	STE	a	416	10/20	0.80	0.19	43,64,70,70	0
27	STE	b	626	10/20	0.80	0.26	46,58,66,69	0
33	LHG	E	101	49/49	0.80	0.25	43,80,110,116	0
33	LHG	a	413	42/49	0.80	0.26	61,86,110,123	0
28	LMG	a	415	55/55	0.81	0.17	37,64,89,93	0
27	STE	A	416	17/20	0.81	0.20	51,74,94,96	0
26	PL9	a	410	55/55	0.81	0.20	41,63,83,95	0
30	DGD	A	414	66/66	0.81	0.18	43,68,103,107	0
27	STE	e	104	13/20	0.81	0.30	61,66,79,81	0
27	STE	l	103	18/20	0.81	0.18	35,49,87,89	0
27	STE	B	622	12/20	0.82	0.35	49,66,81,85	0
28	LMG	C	517	36/55	0.82	0.17	36,65,90,102	0
26	PL9	A	409	55/55	0.82	0.26	37,66,87,103	0
29	SQD	a	414	54/54	0.83	0.17	36,53,87,104	0
27	STE	b	625	16/20	0.83	0.18	49,62,85,92	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
27	STE	C	516	14/20	0.84	0.28	54,70,89,93	0
27	STE	e	103	9/20	0.84	0.36	46,49,56,57	0
27	STE	d	410	17/20	0.84	0.13	35,56,72,74	0
28	LMG	c	523	48/55	0.84	0.21	46,78,112,122	0
23	CLA	h	101	65/65	0.84	0.20	39,64,95,103	0
28	LMG	B	620	45/55	0.84	0.18	38,60,103,130	0
27	STE	b	627	11/20	0.84	0.19	45,52,54,58	0
27	STE	c	516	13/20	0.84	0.29	47,75,84,88	0
27	STE	b	624	20/20	0.85	0.17	36,54,73,77	0
23	CLA	C	512	65/65	0.85	0.18	34,52,95,108	0
27	STE	C	519	7/20	0.85	0.22	45,47,51,52	0
29	SQD	A	413	54/54	0.85	0.19	39,60,97,100	0
28	LMG	b	623	55/55	0.86	0.28	48,77,98,104	0
25	BCR	x	101	40/40	0.86	0.14	34,51,70,71	0
25	BCR	K	101	40/40	0.86	0.13	33,51,69,76	0
27	STE	I	101	15/20	0.86	0.21	36,58,84,88	0
25	BCR	H	101	40/40	0.87	0.13	29,43,58,61	0
29	SQD	l	101	54/54	0.87	0.16	38,62,90,105	0
23	CLA	c	513	65/65	0.87	0.18	41,66,99,112	0
27	STE	b	622	20/20	0.87	0.18	38,59,75,77	0
25	BCR	k	101	40/40	0.87	0.14	40,56,69,72	0
27	STE	j	101	12/20	0.88	0.10	45,57,63,64	0
28	LMG	A	411	48/55	0.88	0.14	38,58,77,95	0
28	LMG	c	524	49/55	0.88	0.14	35,59,92,115	0
27	STE	C	525	12/20	0.88	0.12	37,50,60,60	0
27	STE	B	621	17/20	0.88	0.17	35,53,70,73	0
27	STE	m	101	12/20	0.88	0.14	44,57,75,75	0
23	CLA	C	513	65/65	0.88	0.19	38,62,92,99	0
27	STE	t	103	18/20	0.88	0.12	46,61,76,78	0
27	STE	J	101	12/20	0.88	0.13	48,62,68,73	0
28	LMG	C	524	48/55	0.89	0.16	35,69,87,101	0
23	CLA	c	512	65/65	0.90	0.14	37,56,96,103	0
27	STE	t	102	14/20	0.90	0.10	35,51,61,61	0
25	BCR	C	514	40/40	0.90	0.15	41,56,69,74	0
29	SQD	f	102	41/54	0.90	0.21	50,83,102,112	0
25	BCR	D	406	40/40	0.91	0.12	24,42,77,89	0
28	LMG	b	621	51/55	0.91	0.12	38,55,78,90	0
29	SQD	b	620	49/54	0.91	0.13	38,58,89,103	0
23	CLA	B	601	65/65	0.91	0.13	30,63,91,105	0
27	STE	A	415	8/20	0.92	0.16	41,49,54,55	0
25	BCR	d	404	40/40	0.92	0.12	32,48,86,93	0
23	CLA	a	408	65/65	0.92	0.14	18,34,79,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
28	LMG	c	522	46/55	0.92	0.16	40,67,84,89	0
25	BCR	k	102	40/40	0.92	0.16	35,49,64,69	0
23	CLA	b	614	65/65	0.92	0.14	24,38,61,64	0
23	CLA	c	502	65/65	0.92	0.14	26,39,59,63	0
27	STE	M	102	15/20	0.92	0.14	38,47,60,75	0
27	STE	M	103	10/20	0.92	0.14	32,47,57,65	0
27	STE	D	413	20/20	0.92	0.16	30,47,73,81	0
28	LMG	D	409	51/55	0.92	0.17	24,54,83,89	0
28	LMG	M	101	51/55	0.92	0.11	32,51,74,81	0
23	CLA	C	502	65/65	0.92	0.14	23,37,56,61	0
23	CLA	D	405	65/65	0.92	0.13	21,40,105,116	0
23	CLA	c	508	64/65	0.93	0.14	26,41,95,111	0
25	BCR	C	515	40/40	0.93	0.11	24,38,49,58	0
25	BCR	C	520	40/40	0.93	0.16	30,48,65,70	0
23	CLA	d	403	65/65	0.93	0.14	26,46,89,98	0
23	CLA	b	615	60/65	0.93	0.14	25,38,95,99	0
23	CLA	c	505	65/65	0.94	0.17	24,38,69,81	0
23	CLA	c	506	65/65	0.94	0.12	28,45,91,97	0
23	CLA	c	507	65/65	0.94	0.13	25,41,56,72	0
23	CLA	b	601	65/65	0.94	0.14	24,40,60,66	0
23	CLA	c	511	65/65	0.94	0.12	35,49,69,71	0
28	LMG	d	409	44/55	0.94	0.13	29,51,86,99	0
29	SQD	A	412	52/54	0.94	0.16	32,62,92,102	0
25	BCR	b	618	40/40	0.94	0.09	26,42,59,63	0
29	SQD	a	412	54/54	0.94	0.14	38,68,90,94	0
25	BCR	c	514	40/40	0.94	0.12	43,59,73,73	0
23	CLA	b	608	65/65	0.94	0.13	24,42,62,67	0
23	CLA	b	609	65/65	0.94	0.18	23,36,48,51	0
23	CLA	B	614	65/65	0.94	0.17	19,32,82,94	0
23	CLA	C	505	65/65	0.94	0.17	21,36,71,85	0
30	DGD	C	522	62/66	0.94	0.12	28,52,100,111	0
30	DGD	C	523	62/66	0.94	0.12	25,48,79,87	0
30	DGD	H	102	62/66	0.94	0.11	26,45,61,64	0
30	DGD	c	520	62/66	0.94	0.12	29,52,91,99	0
30	DGD	c	521	62/66	0.94	0.13	24,53,88,94	0
25	BCR	B	619	40/40	0.94	0.10	20,39,59,65	0
23	CLA	B	616	60/65	0.94	0.14	20,34,98,116	0
23	CLA	B	615	65/65	0.95	0.11	22,34,62,70	0
23	CLA	B	604	65/65	0.95	0.12	18,28,70,78	0
23	CLA	c	509	65/65	0.95	0.15	27,43,67,72	0
23	CLA	c	510	65/65	0.95	0.13	26,45,63,67	0
23	CLA	B	606	65/65	0.95	0.10	21,32,69,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	a	406	65/65	0.95	0.13	22,35,95,100	0
23	CLA	C	503	65/65	0.95	0.12	25,39,51,54	0
23	CLA	a	411	65/65	0.95	0.12	17,27,49,53	0
23	CLA	C	504	59/65	0.95	0.10	25,37,81,86	0
24	PHO	a	407	64/64	0.95	0.13	17,28,39,40	0
25	BCR	B	618	40/40	0.95	0.09	21,37,53,54	0
23	CLA	b	603	65/65	0.95	0.12	17,32,81,98	0
23	CLA	b	605	65/65	0.95	0.11	21,36,74,84	0
23	CLA	b	607	65/65	0.95	0.14	22,40,58,68	0
23	CLA	B	602	65/65	0.95	0.15	20,33,56,62	0
23	CLA	C	506	65/65	0.95	0.11	20,38,96,105	0
29	SQD	F	102	36/54	0.95	0.17	43,70,88,99	0
23	CLA	b	611	65/65	0.95	0.16	18,33,49,64	0
23	CLA	b	612	65/65	0.95	0.14	16,31,72,80	0
25	BCR	a	409	40/40	0.95	0.08	20,33,44,45	0
25	BCR	b	616	40/40	0.95	0.10	26,38,49,52	0
23	CLA	C	507	65/65	0.95	0.14	21,37,63,67	0
23	CLA	C	508	65/65	0.95	0.11	23,38,101,106	0
25	BCR	c	515	40/40	0.95	0.11	28,42,57,65	0
23	CLA	C	509	65/65	0.95	0.16	22,41,62,69	0
23	CLA	c	503	65/65	0.95	0.13	29,42,52,60	0
23	CLA	c	504	60/65	0.95	0.11	27,44,81,84	0
23	CLA	C	510	65/65	0.95	0.11	25,40,61,63	0
30	DGD	h	102	62/66	0.95	0.11	24,49,60,71	0
23	CLA	C	511	65/65	0.95	0.10	28,46,65,71	0
26	PL9	D	407	55/55	0.95	0.10	18,31,46,50	0
33	LHG	d	406	49/49	0.95	0.13	33,52,73,84	0
24	PHO	d	401	64/64	0.96	0.09	24,35,48,48	0
25	BCR	A	408	40/40	0.96	0.09	21,34,45,48	0
25	BCR	B	617	40/40	0.96	0.11	23,34,54,56	0
23	CLA	A	407	54/65	0.96	0.10	16,30,63,69	0
23	CLA	C	501	65/65	0.96	0.12	19,33,49,58	0
23	CLA	b	613	65/65	0.96	0.12	22,36,74,85	0
23	CLA	D	403	65/65	0.96	0.10	16,26,50,58	0
23	CLA	D	404	65/65	0.96	0.11	16,27,57,62	0
23	CLA	c	501	65/65	0.96	0.12	26,36,50,57	0
23	CLA	A	404	65/65	0.96	0.10	12,26,48,57	0
23	CLA	a	405	65/65	0.96	0.10	16,28,49,59	0
25	BCR	T	101	40/40	0.96	0.08	22,36,49,50	0
23	CLA	B	607	65/65	0.96	0.10	16,31,62,64	0
23	CLA	B	608	65/65	0.96	0.12	18,34,52,61	0
25	BCR	b	617	40/40	0.96	0.09	24,37,54,55	0

Continued on next page...

Continued from previous page...

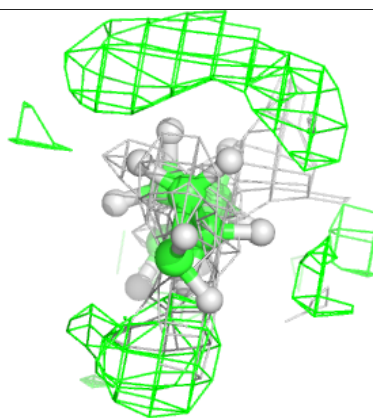
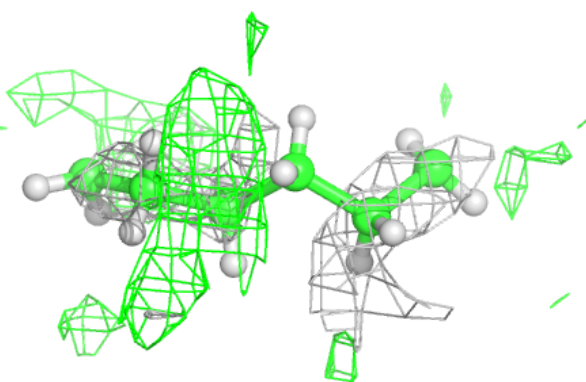
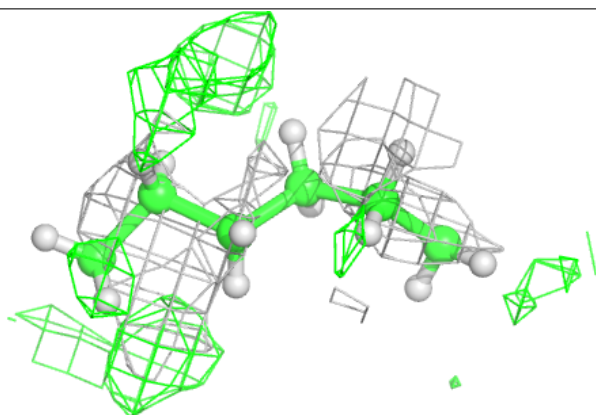
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	B	609	65/65	0.96	0.11	23,34,58,62	0
23	CLA	B	610	65/65	0.96	0.14	19,30,42,46	0
23	CLA	b	602	65/65	0.96	0.14	21,33,69,82	0
23	CLA	B	611	65/65	0.96	0.15	17,29,51,54	0
23	CLA	b	604	65/65	0.96	0.12	19,32,51,55	0
23	CLA	B	612	65/65	0.96	0.12	18,29,47,51	0
25	BCR	t	101	40/40	0.96	0.09	22,36,53,53	0
23	CLA	b	606	65/65	0.96	0.12	17,34,67,70	0
23	CLA	B	613	65/65	0.96	0.14	18,30,69,75	0
23	CLA	d	402	65/65	0.96	0.11	17,31,63,66	0
23	CLA	A	405	65/65	0.96	0.13	18,31,97,104	0
33	LHG	D	411	47/49	0.96	0.11	23,48,78,94	0
33	LHG	D	412	49/49	0.96	0.12	27,44,73,79	0
26	PL9	d	405	55/55	0.96	0.10	20,33,45,50	0
23	CLA	B	603	65/65	0.96	0.16	19,30,61,69	0
23	CLA	b	610	65/65	0.96	0.13	20,30,53,58	0
33	LHG	d	408	39/49	0.96	0.10	30,43,74,86	0
33	LHG	l	102	49/49	0.96	0.09	25,43,59,71	0
34	HEM	f	101	43/43	0.96	0.12	41,55,76,78	0
30	DGD	c	519	62/66	0.97	0.09	18,42,79,86	0
30	DGD	C	521	62/66	0.97	0.10	18,43,81,98	0
33	LHG	L	101	49/49	0.97	0.11	22,42,59,69	0
23	CLA	B	605	65/65	0.97	0.13	17,30,50,54	0
24	PHO	A	406	64/64	0.97	0.13	21,31,41,48	0
33	LHG	d	407	49/49	0.97	0.09	27,42,56,63	0
32	BCT	a	404	4/4	0.97	0.19	30,30,45,54	0
33	LHG	D	410	49/49	0.97	0.09	18,41,53,62	0
34	HEM	F	101	43/43	0.97	0.10	28,45,59,61	0
24	PHO	D	402	64/64	0.97	0.10	16,26,35,39	0
35	HEC	V	201	43/43	0.97	0.11	21,29,38,42	0
32	BCT	D	401	4/4	0.98	0.18	26,28,34,40	0
35	HEC	v	201	43/43	0.98	0.12	23,33,40,43	0
31	OEX	A	418	10/10	0.99	0.14	22,23,26,27	0
31	OEX	a	418	10/10	0.99	0.10	22,23,27,30	0
21	FE2	a	401	1/1	0.99	0.05	29,29,29,29	0
22	CL	A	402	1/1	1.00	0.08	25,25,25,25	0
22	CL	A	403	1/1	1.00	0.03	24,24,24,24	0
22	CL	a	402	1/1	1.00	0.03	25,25,25,25	0
22	CL	a	403	1/1	1.00	0.04	24,24,24,24	0
21	FE2	A	401	1/1	1.00	0.06	23,23,23,23	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.

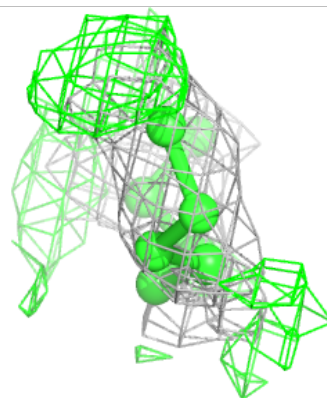
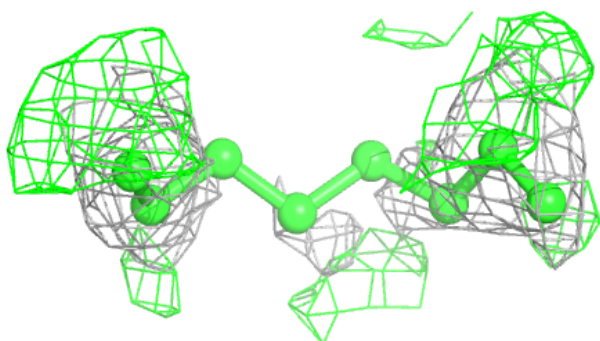
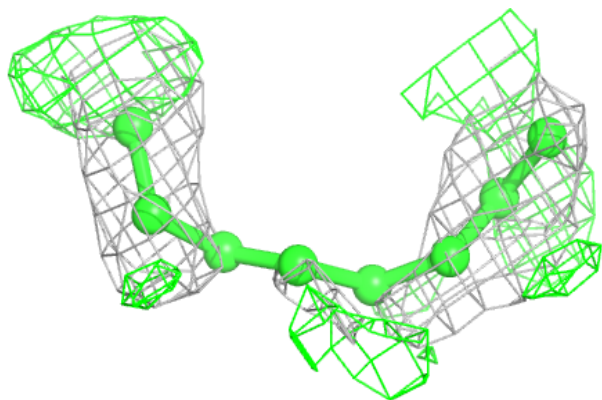
Electron density around STE i 102:

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



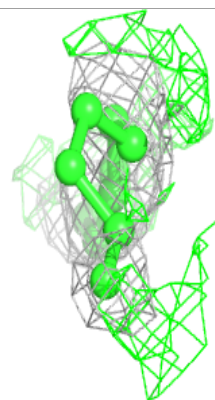
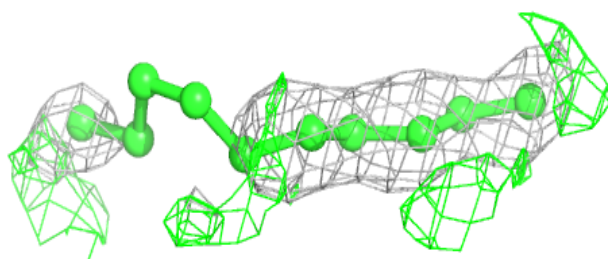
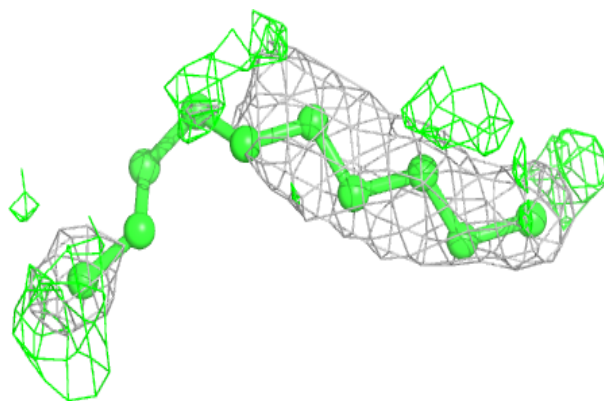
Electron density around STE C 527:

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

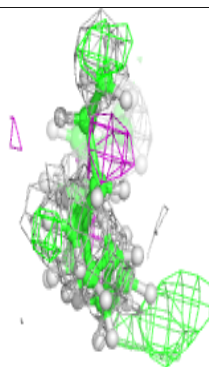
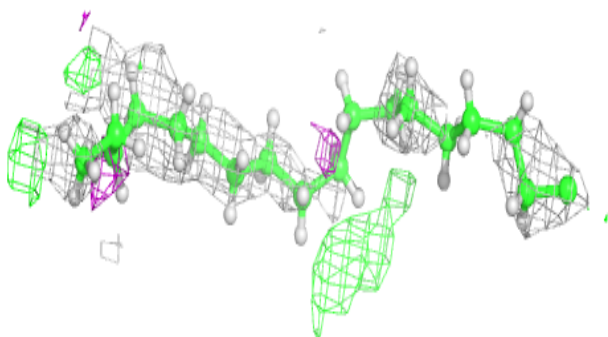
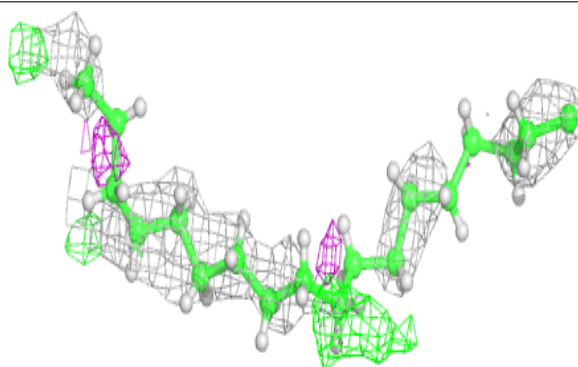


Electron density around STE d 412:

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

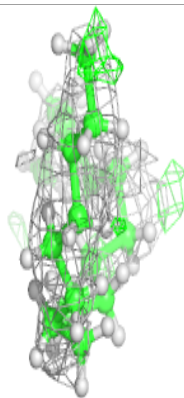
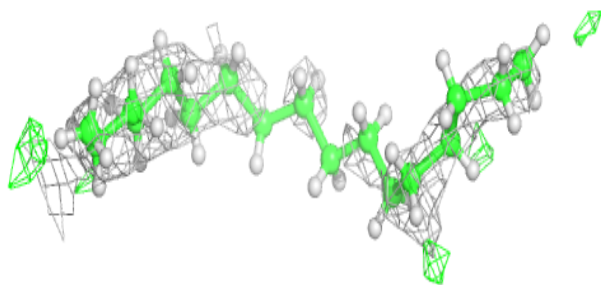
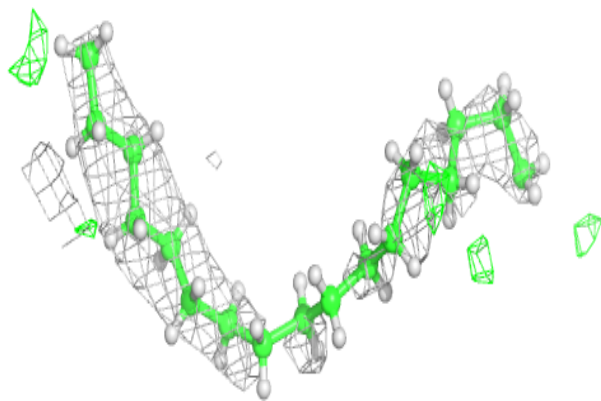
**Electron density around STE H 103:**

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



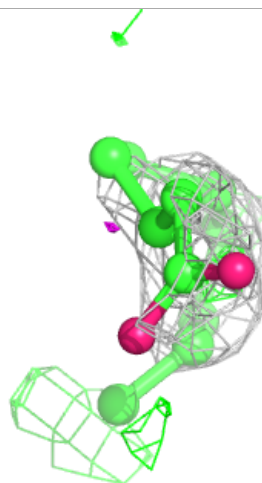
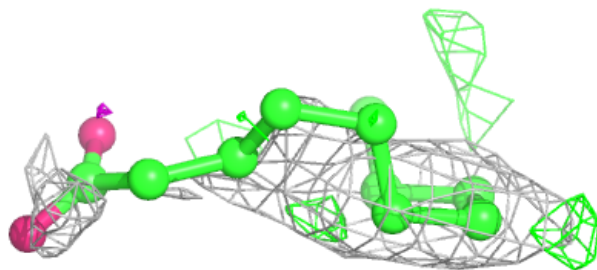
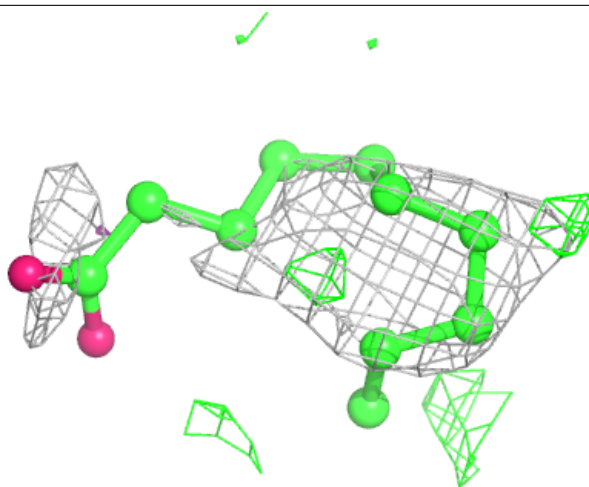
Electron density around STE Z 101:

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



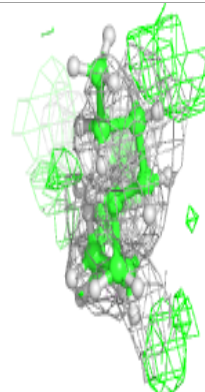
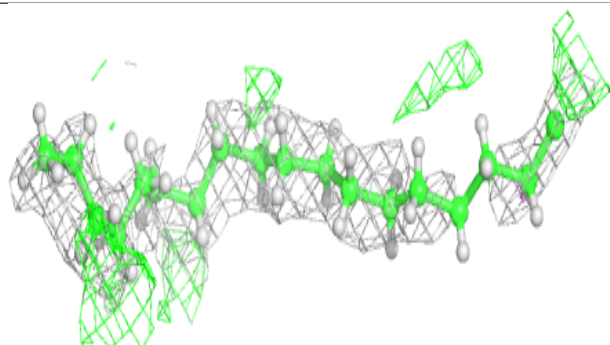
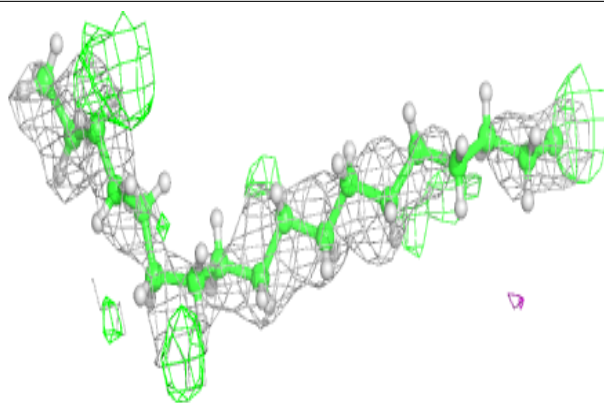
Electron density around STE i 101:

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

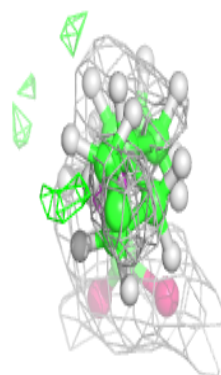
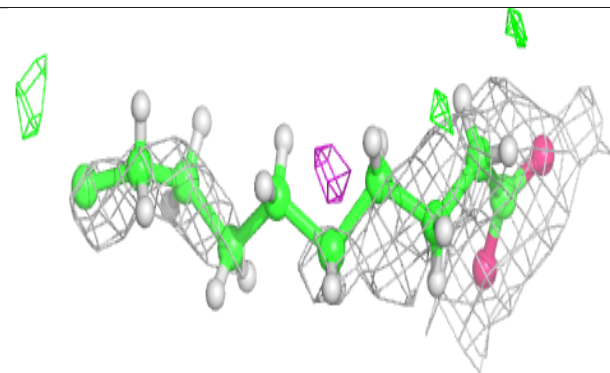
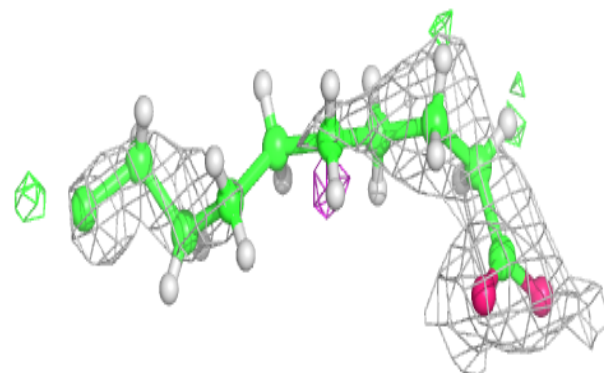


Electron density around STE c 517:

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

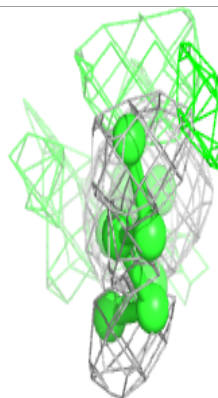
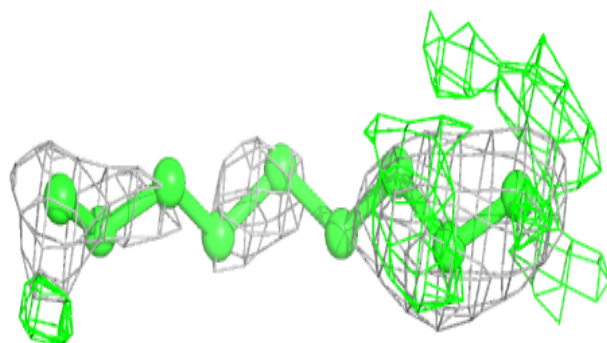
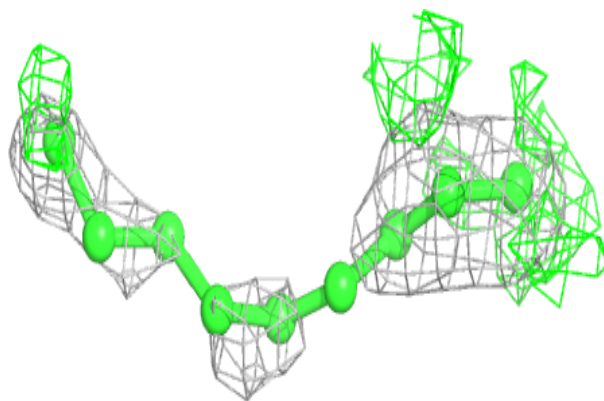
**Electron density around STE E 102:**

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

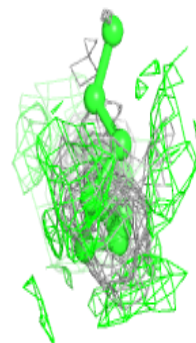
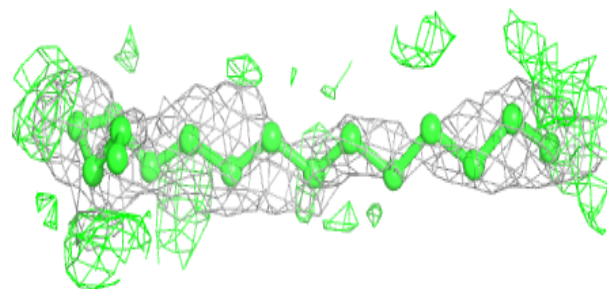
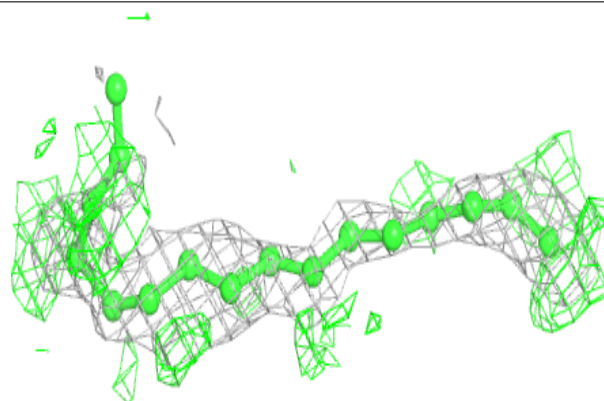


Electron density around STE e 101:

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

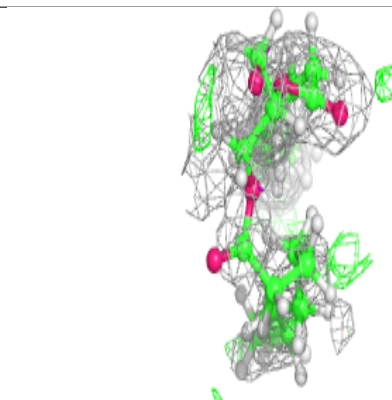
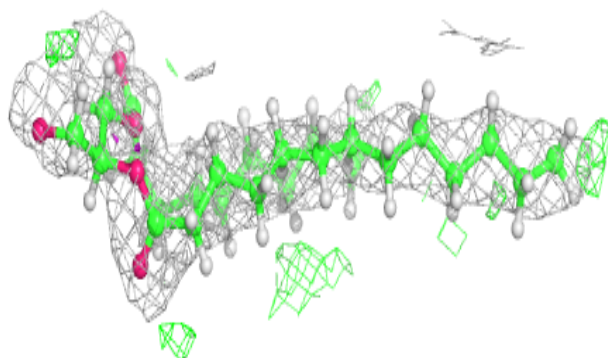
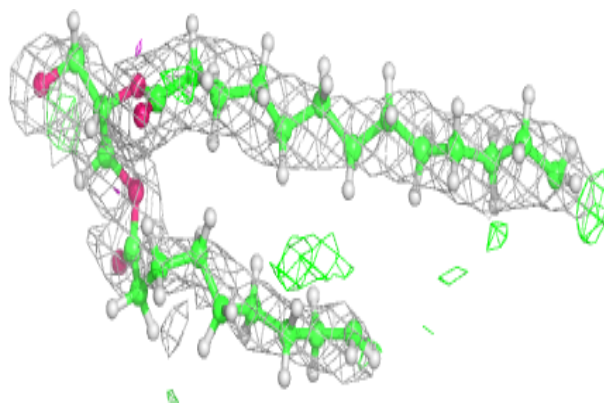
**Electron density around STE j 102:**

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

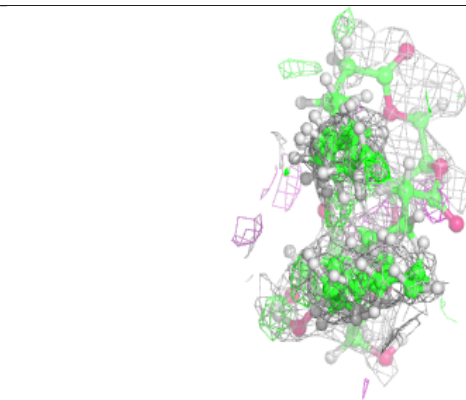
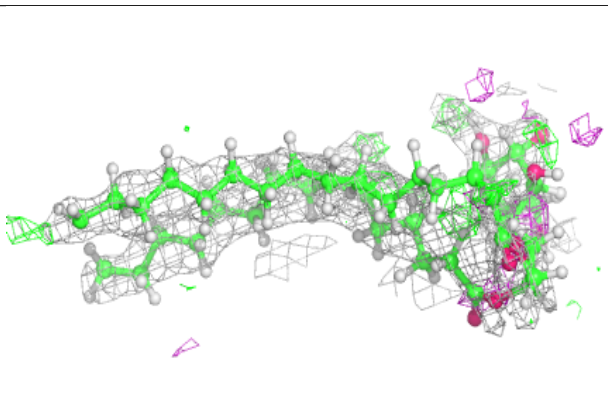
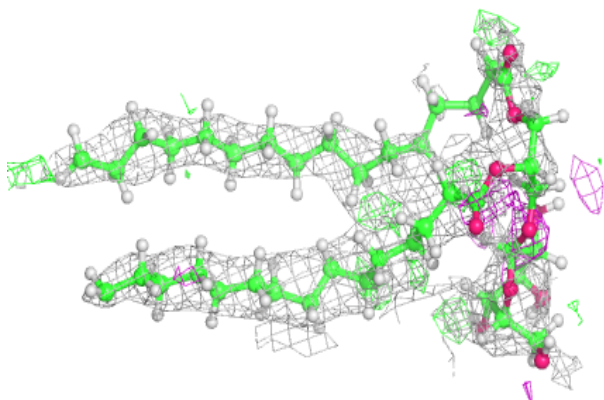


Electron density around LMG c 518:

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

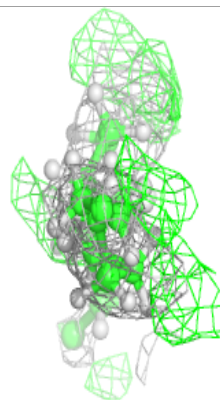
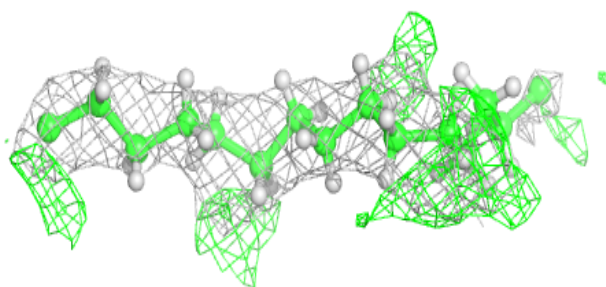
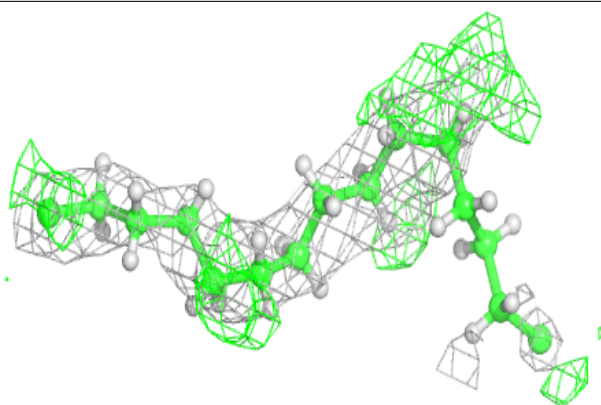
**Electron density around LMG D 408:**

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

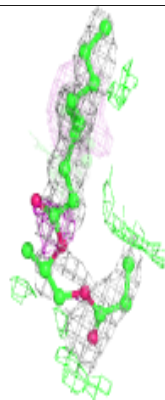
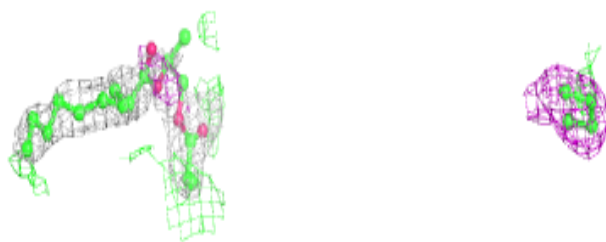
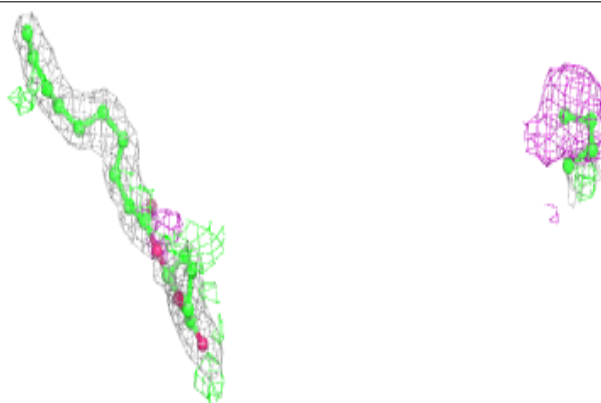


Electron density around STE B 623:

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

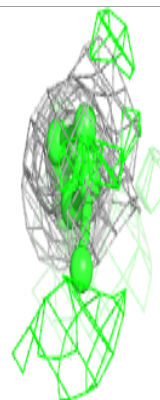
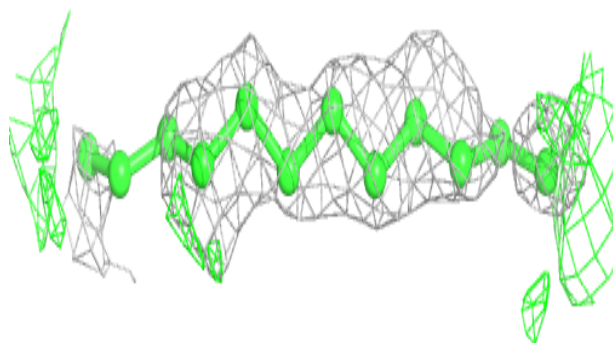
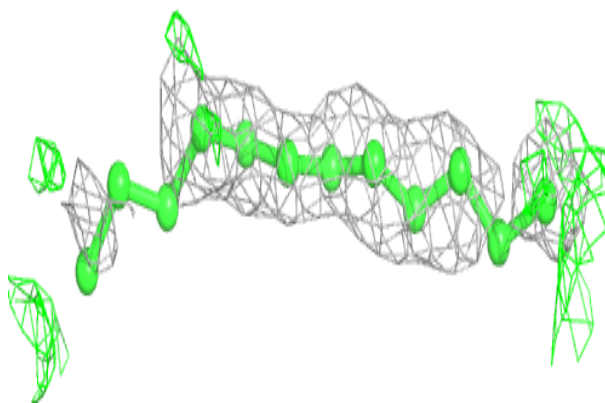
**Electron density around LMG b 619:**

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

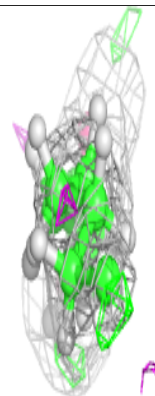
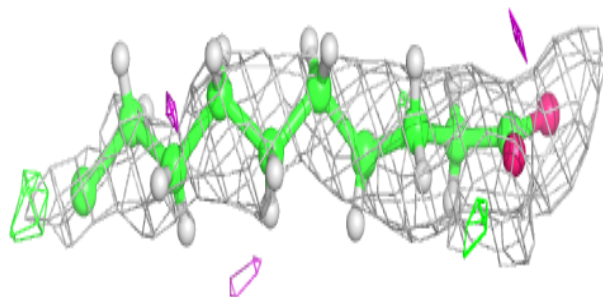
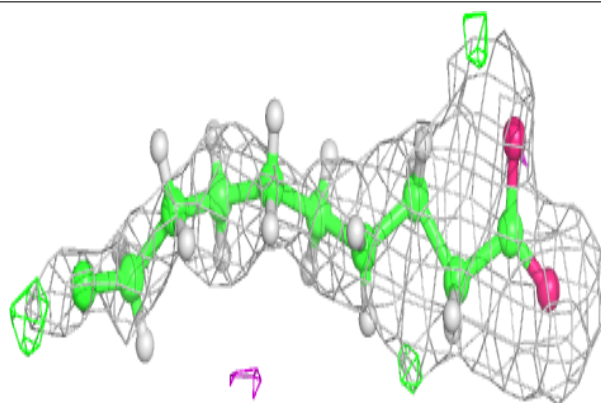


Electron density around STE E 103:

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

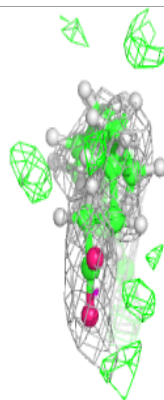
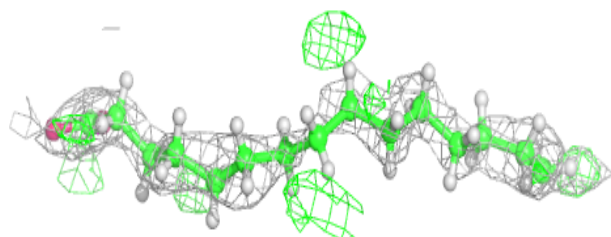
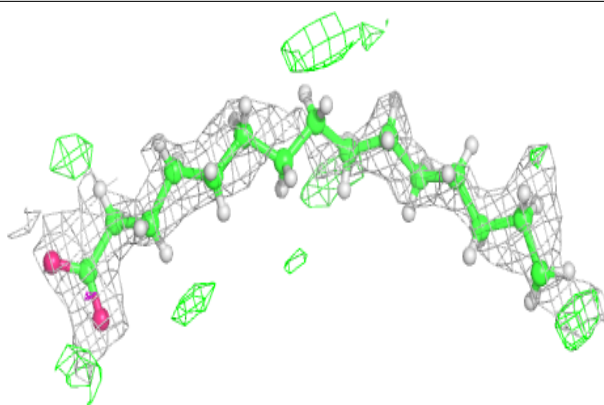
**Electron density around STE a 417:**

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

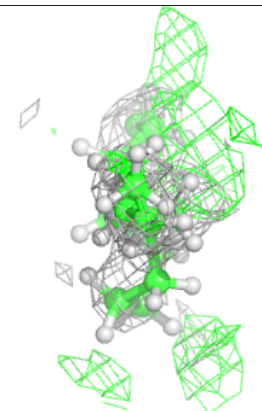
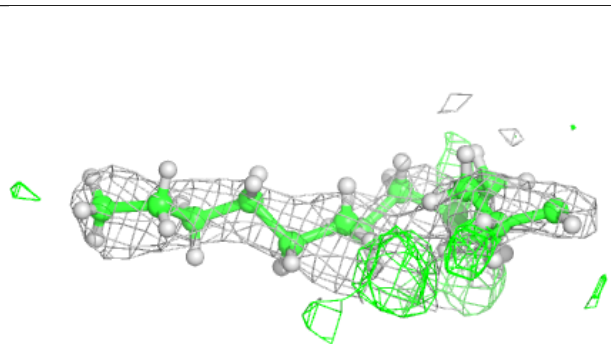
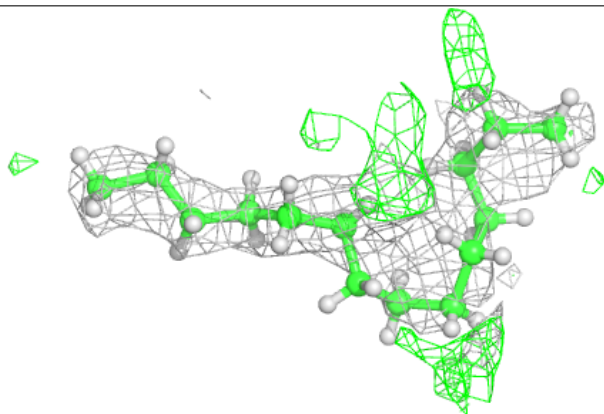


Electron density around STE I 102:

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

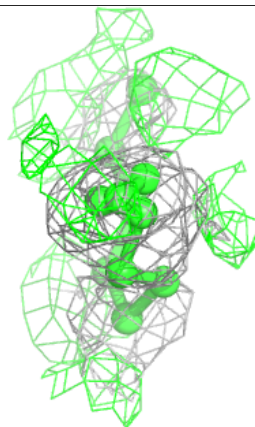
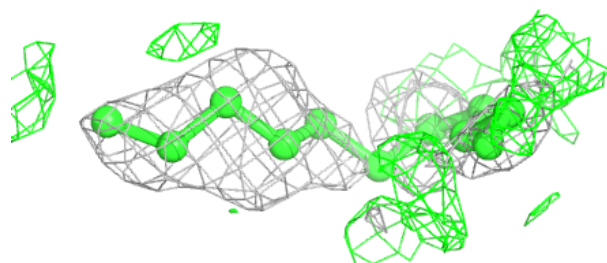
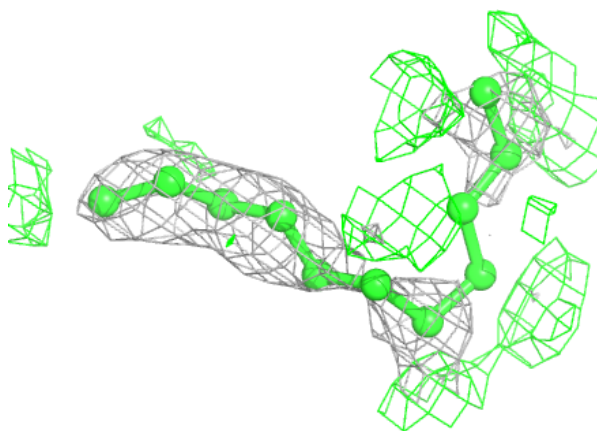
**Electron density around STE C 529:**

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

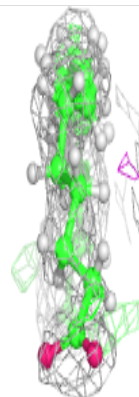
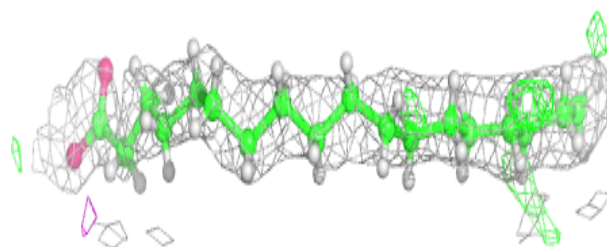
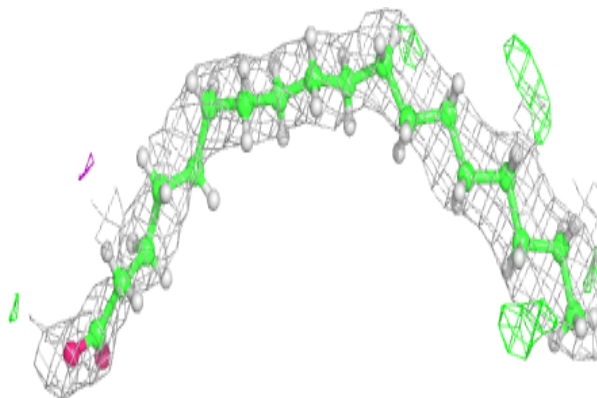


Electron density around STE A 417:

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

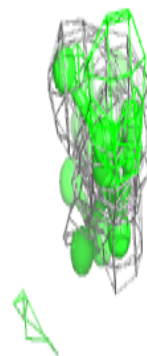
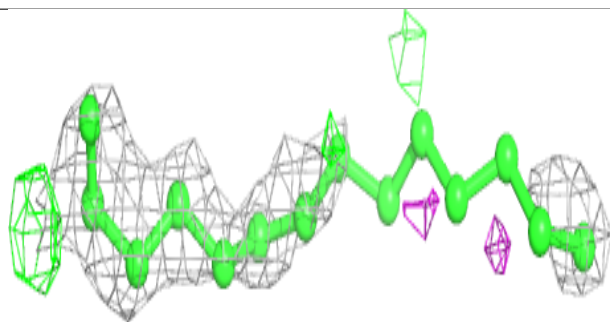
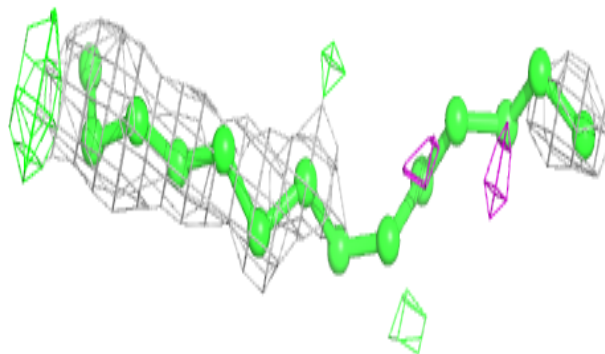
**Electron density around STE x 102:**

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

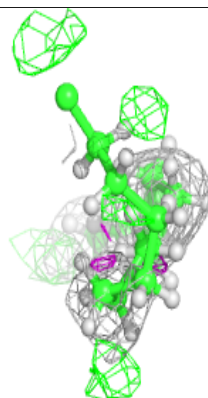
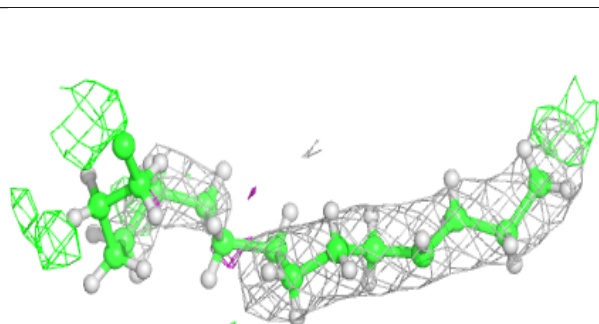
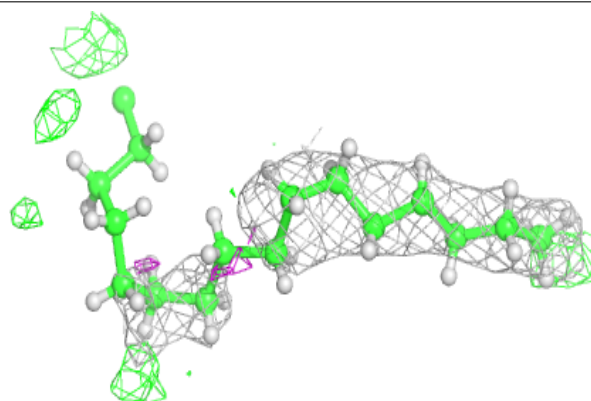


Electron density around STE C 528:

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

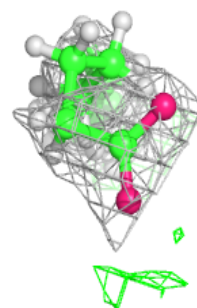
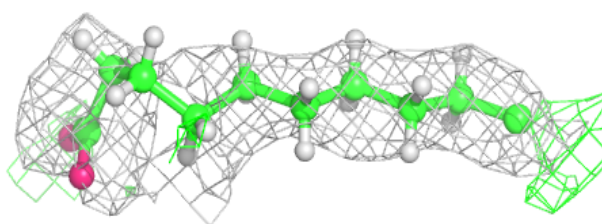
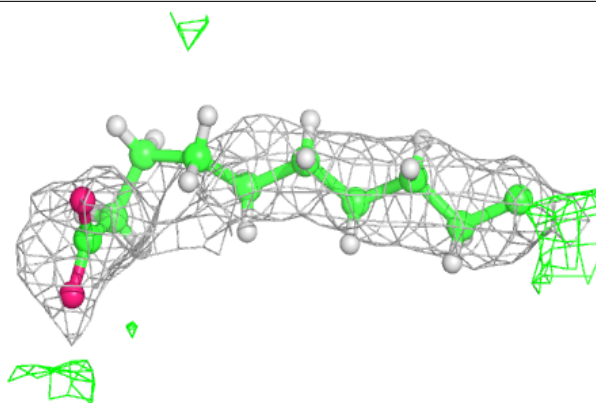
**Electron density around STE T 102:**

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

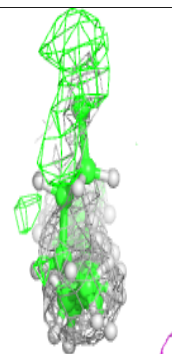
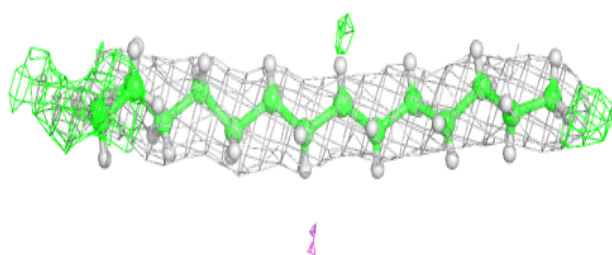
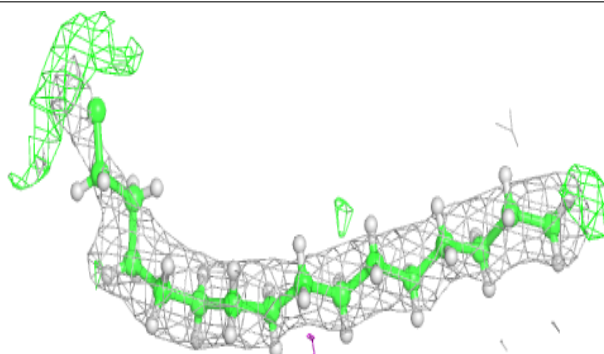


Electron density around STE d 411:

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

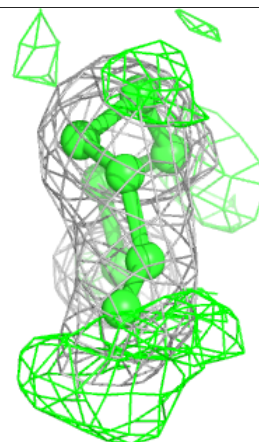
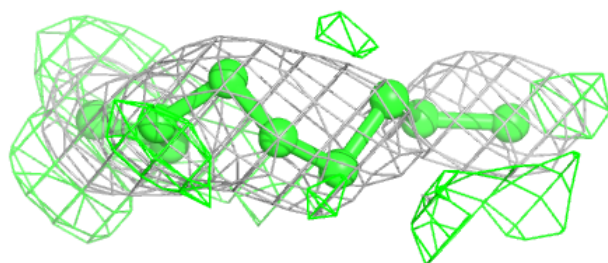
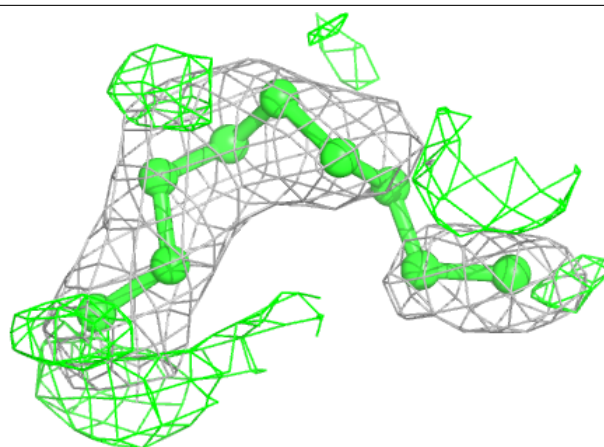
**Electron density around STE C 526:**

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

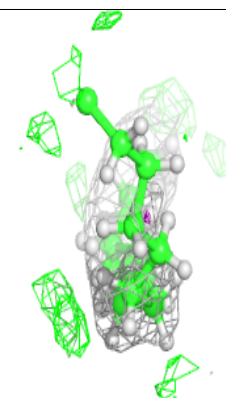
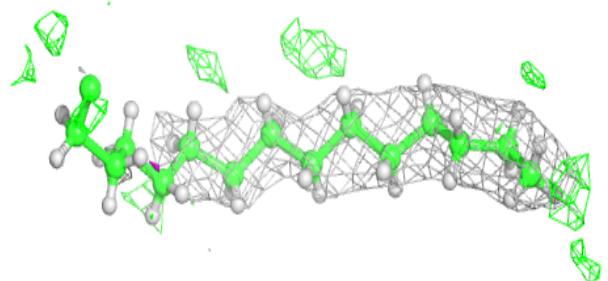
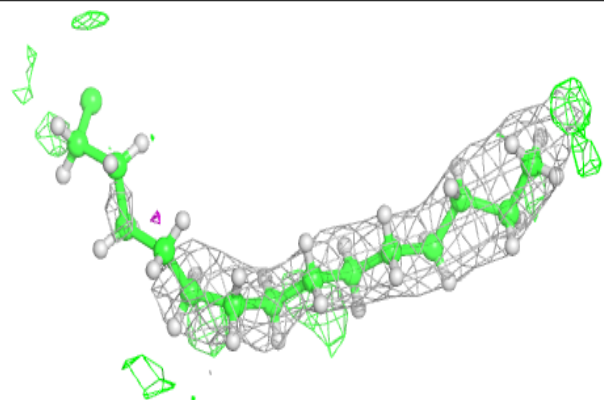


Electron density around STE D 414:

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

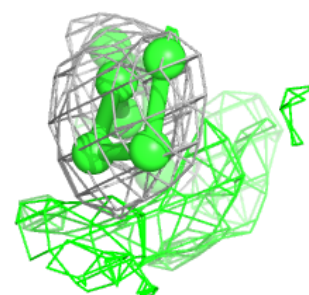
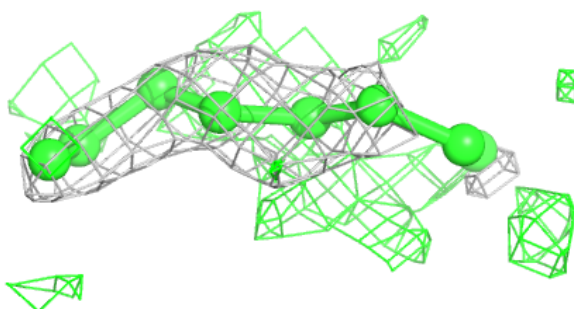
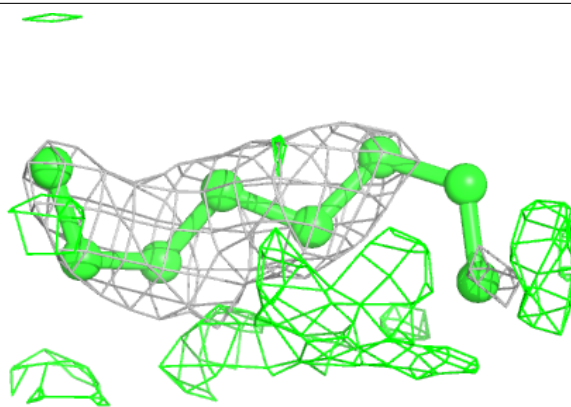
**Electron density around STE m 102:**

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

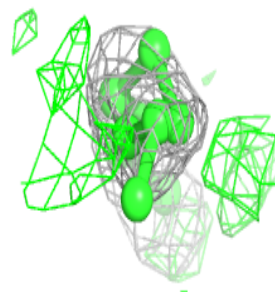
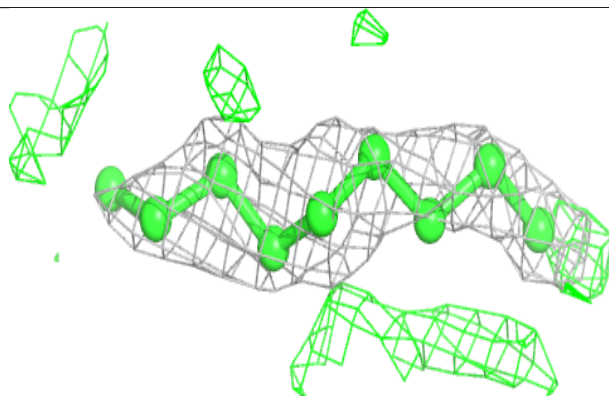
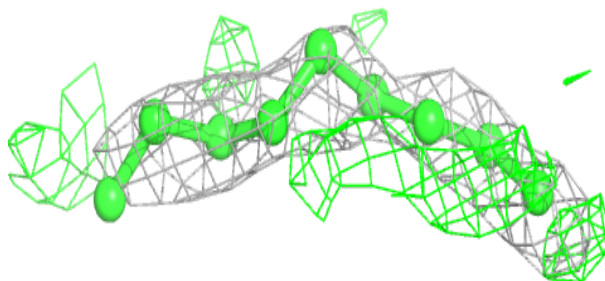


Electron density around STE e 102:

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

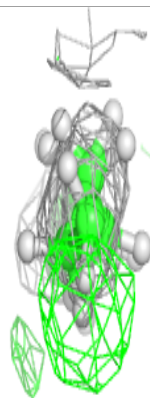
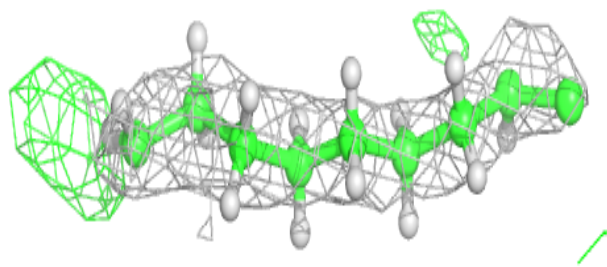
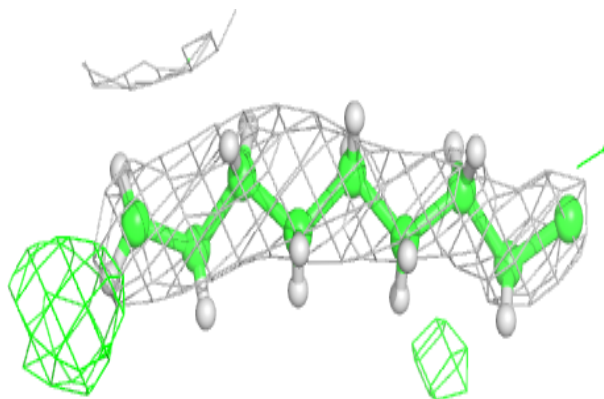
**Electron density around STE A 410:**

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

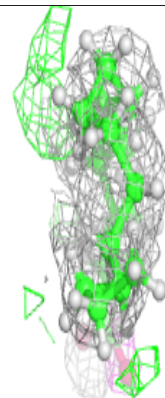
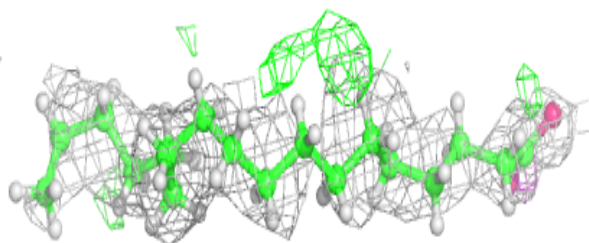
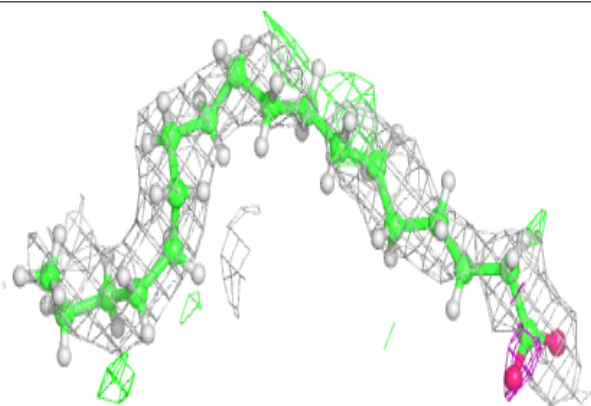


Electron density around STE z 101:

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

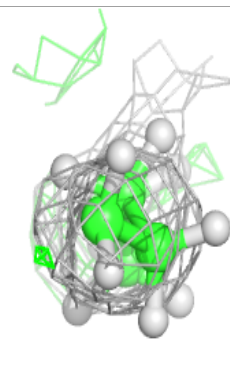
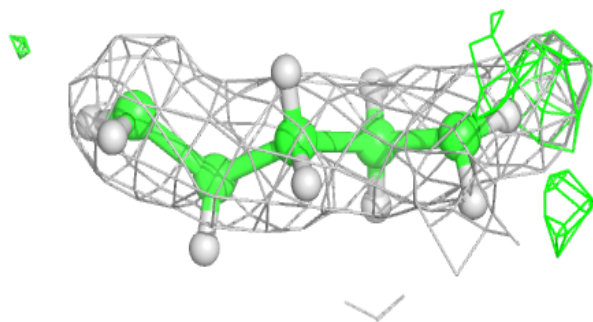
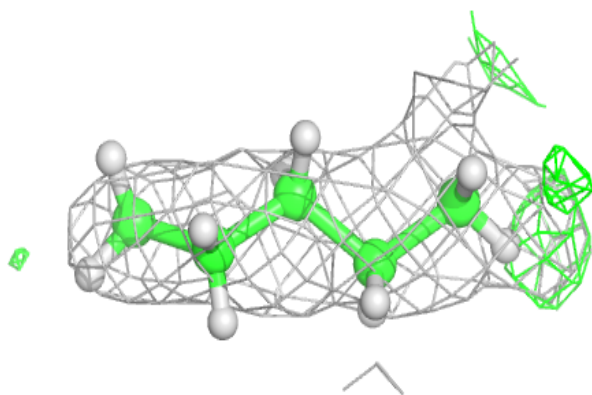
**Electron density around STE E 104:**

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

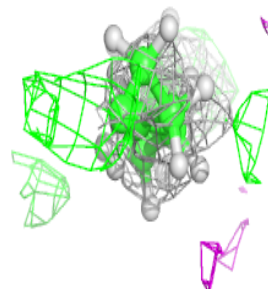
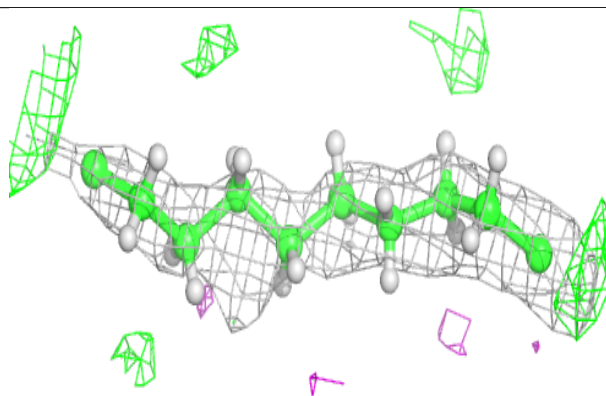
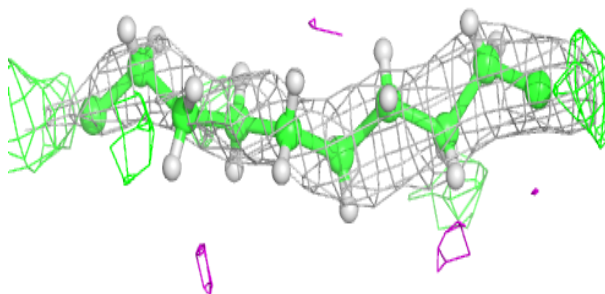


Electron density around STE C 518:

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

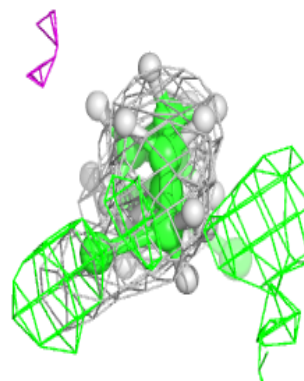
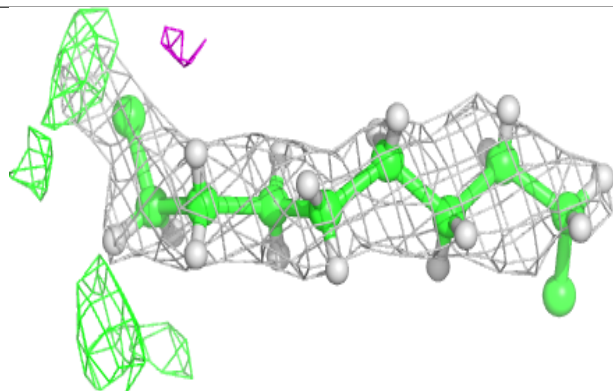
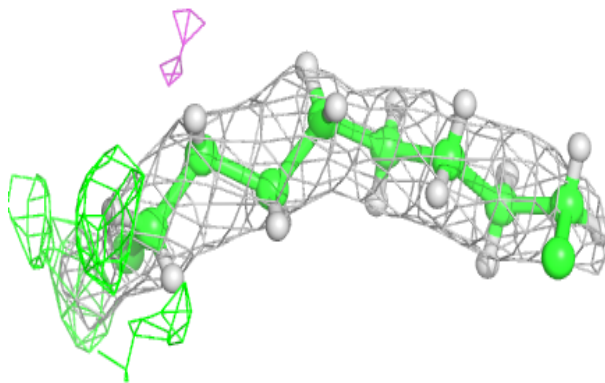
**Electron density around STE a 416:**

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

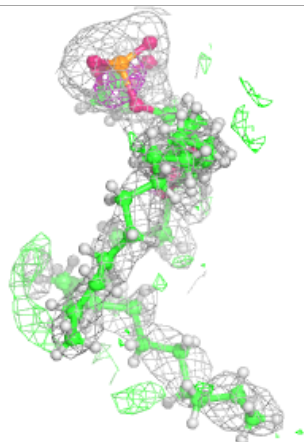
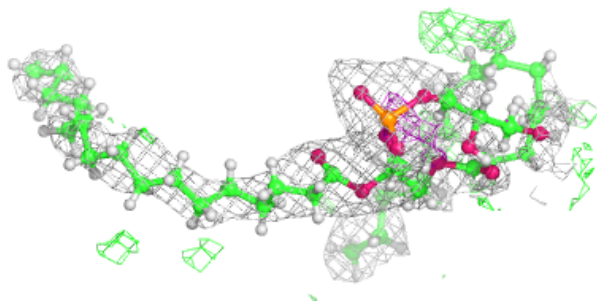
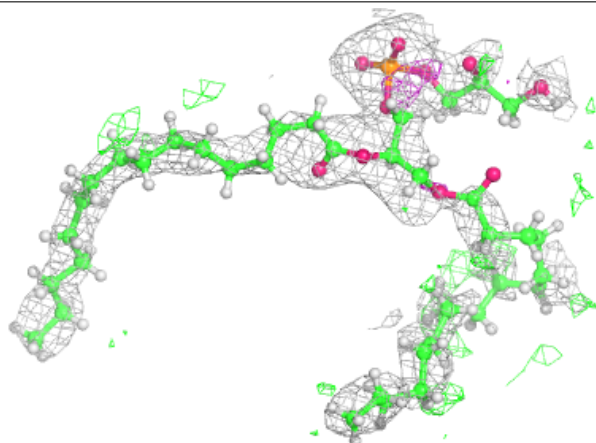


Electron density around STE b 626:

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

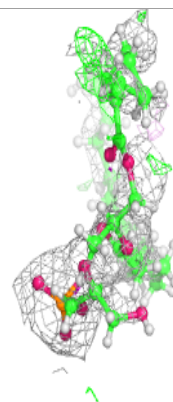
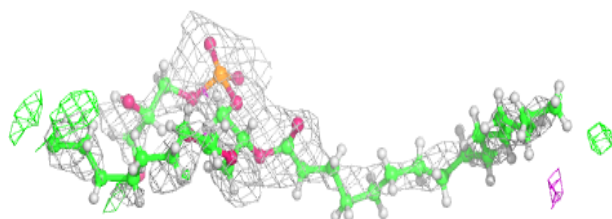
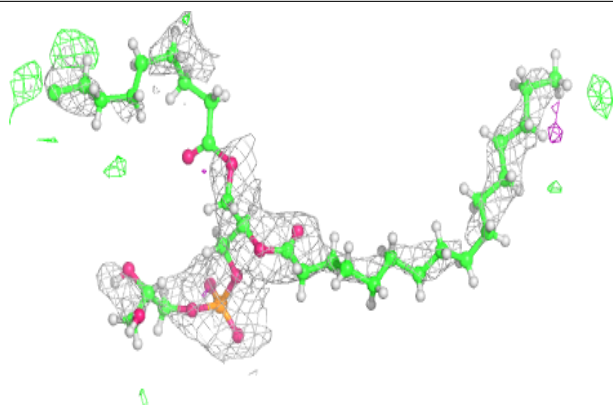
**Electron density around LHG E 101:**

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

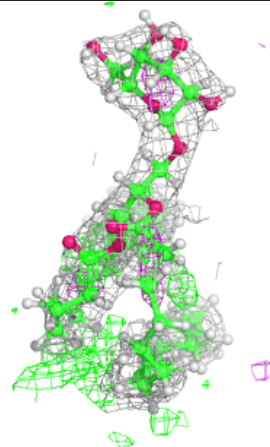
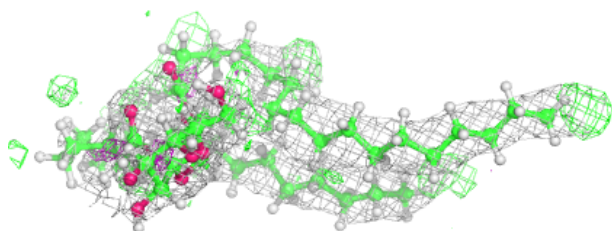
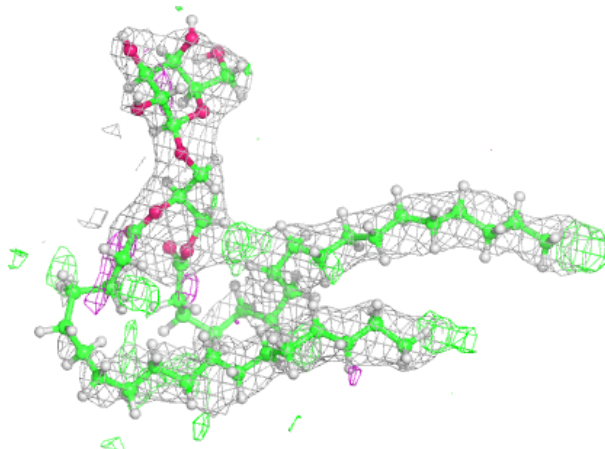


Electron density around LHG a 413:

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

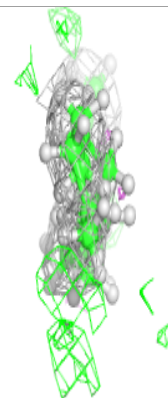
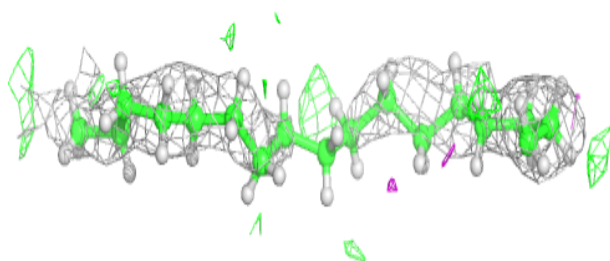
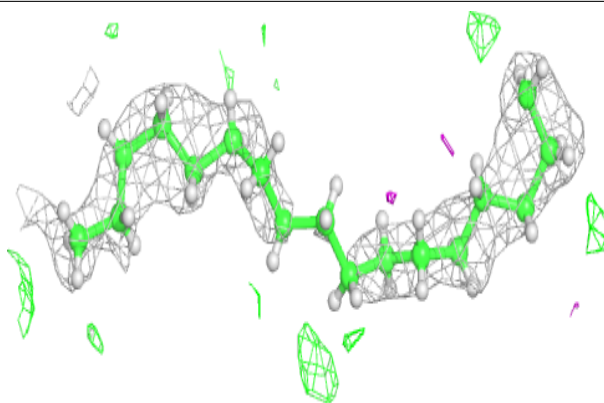
**Electron density around LMG a 415:**

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

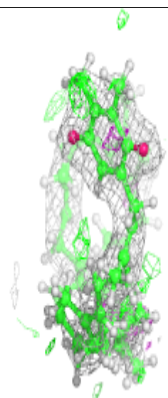
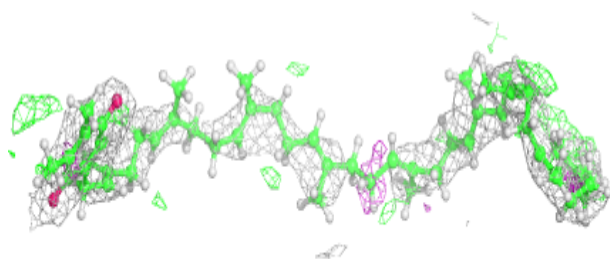
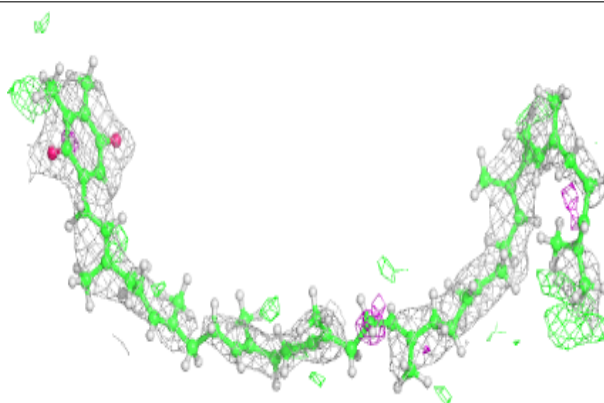


Electron density around STE A 416:

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

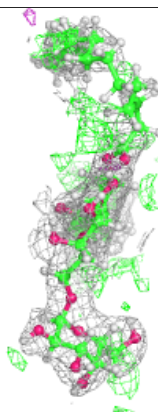
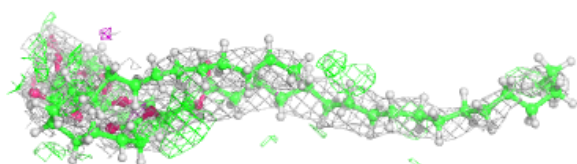
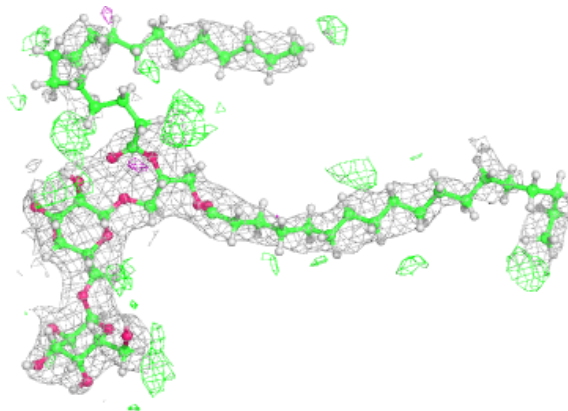
**Electron density around PL9 a 410:**

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

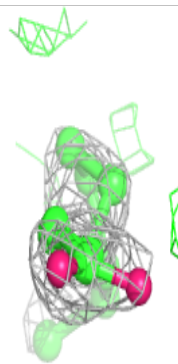
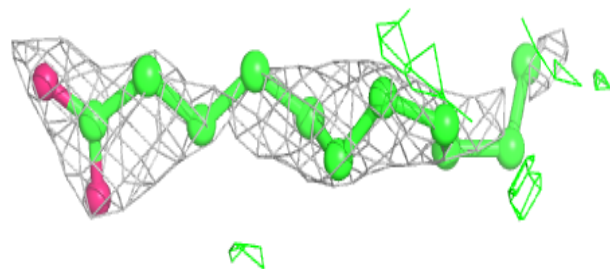
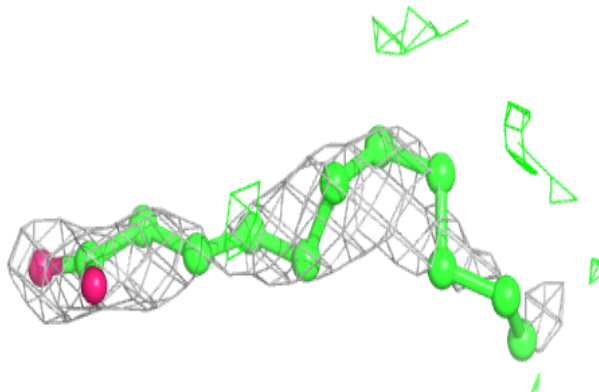


Electron density around DGD A 414:

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

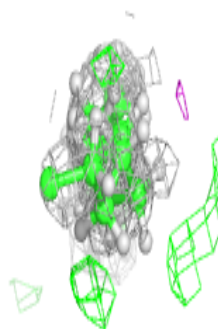
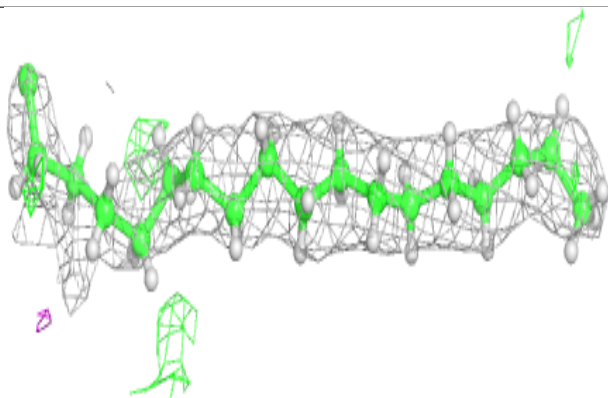
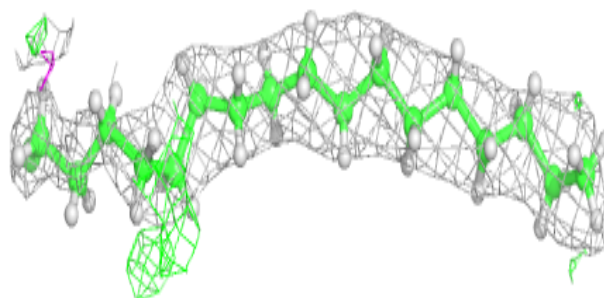
**Electron density around STE e 104:**

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

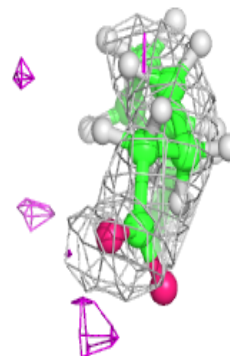
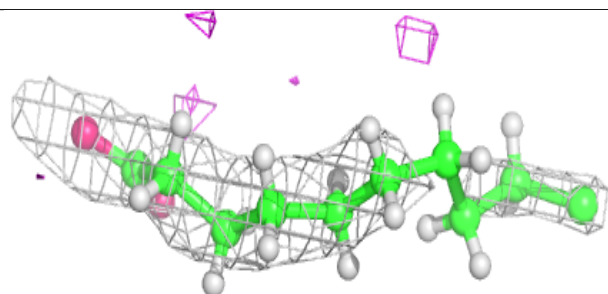
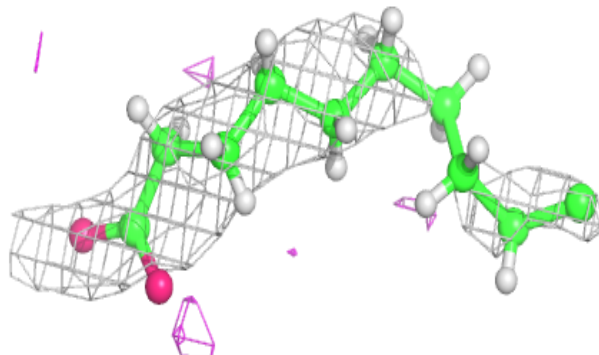


Electron density around STE I 103:

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

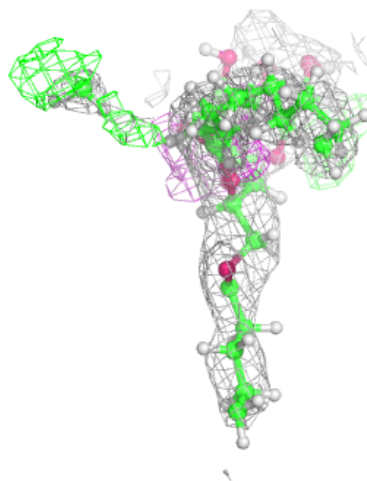
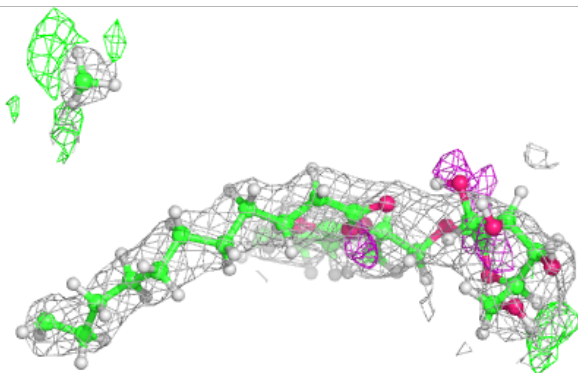
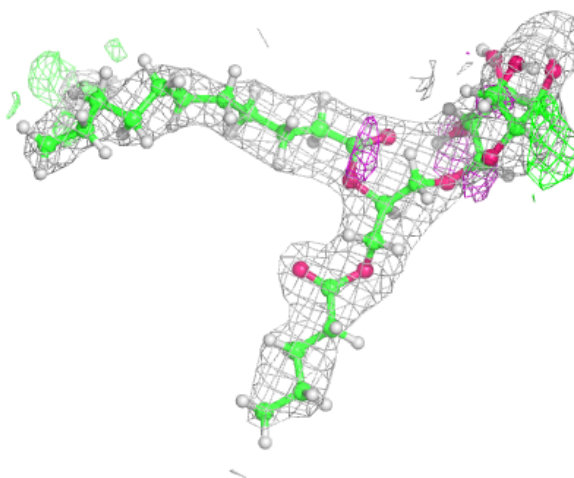
**Electron density around STE B 622:**

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



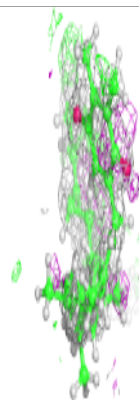
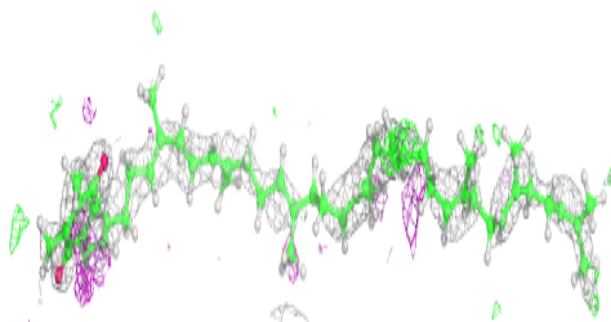
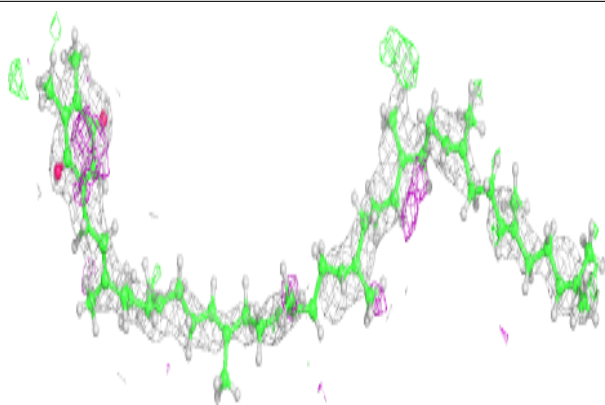
Electron density around LMG C 517:

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

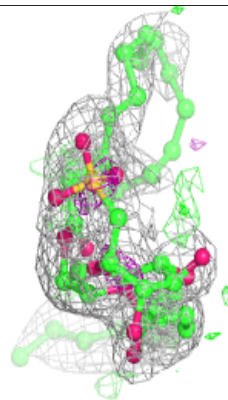
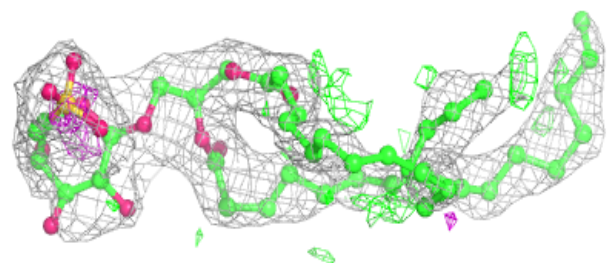
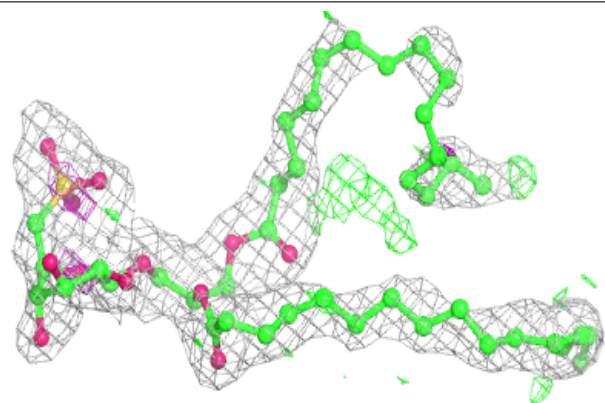


Electron density around PL9 A 409:

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

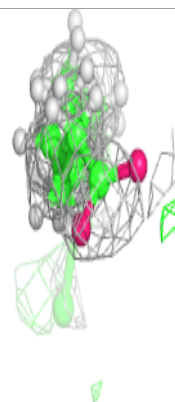
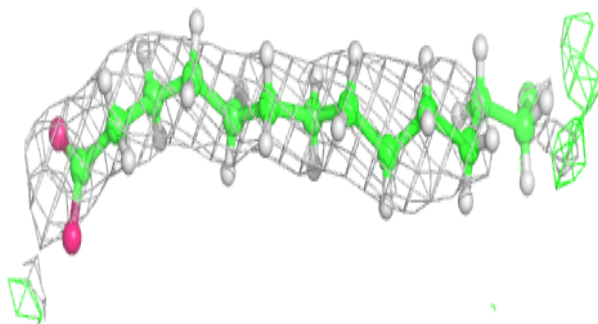
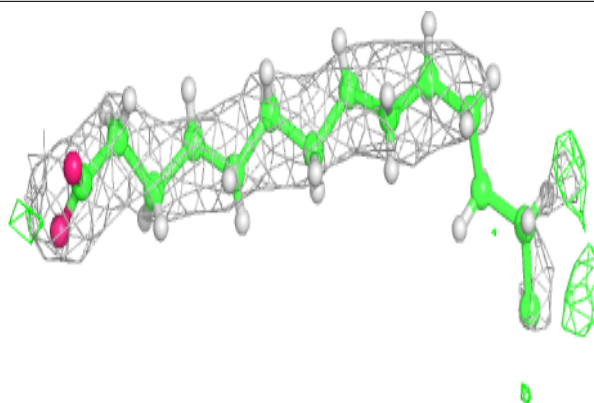
**Electron density around SQD a 414:**

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

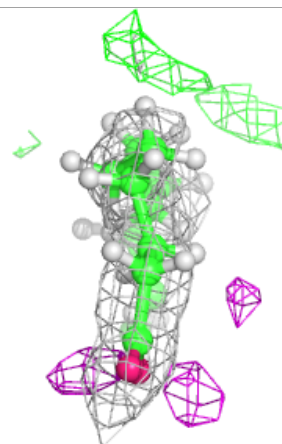
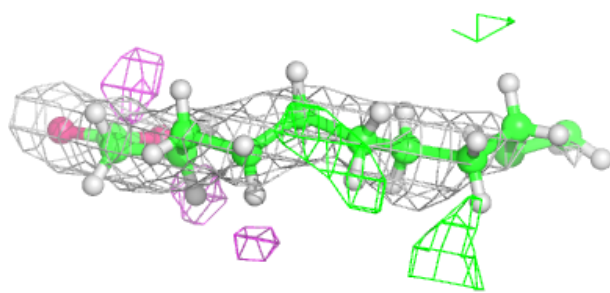
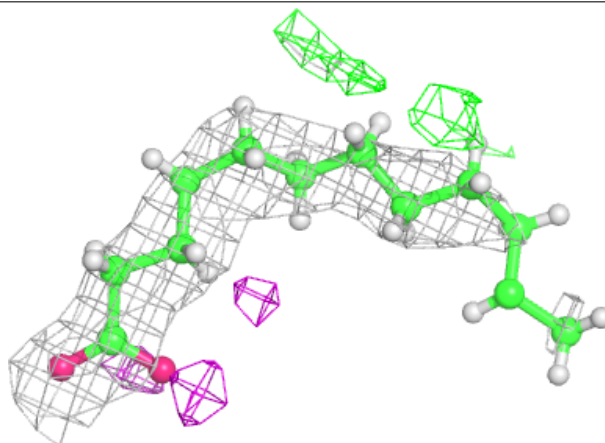


Electron density around STE b 625:

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

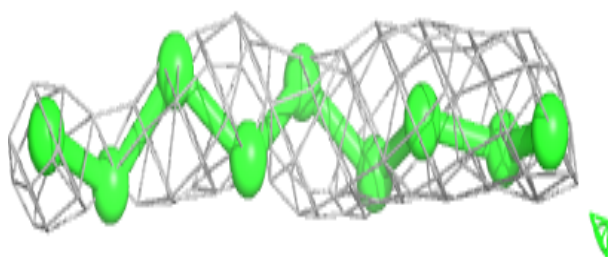
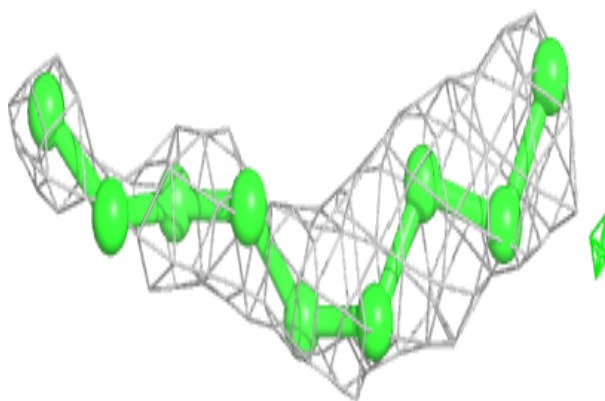
**Electron density around STE C 516:**

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

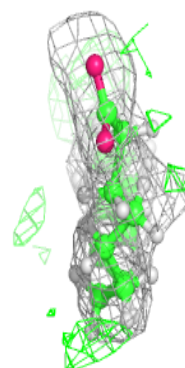
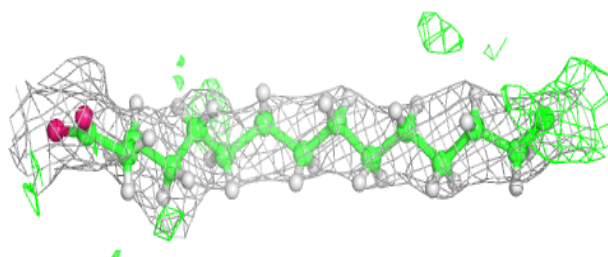
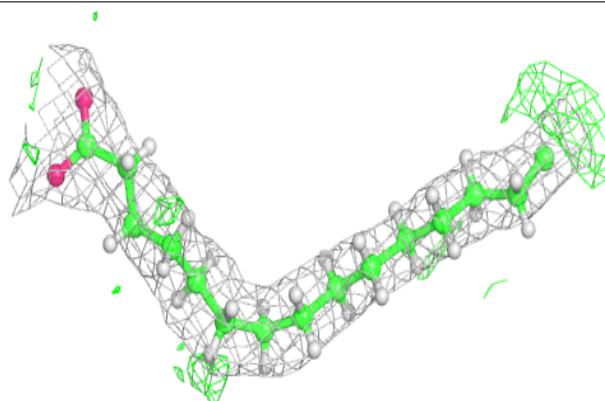


Electron density around STE e 103:

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

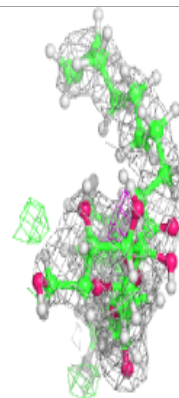
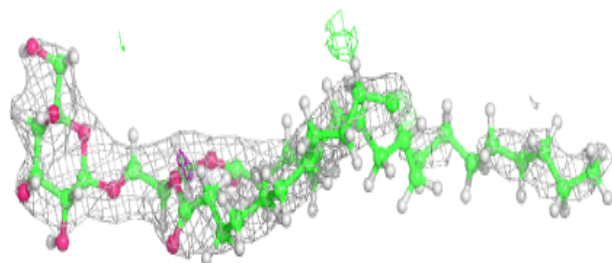
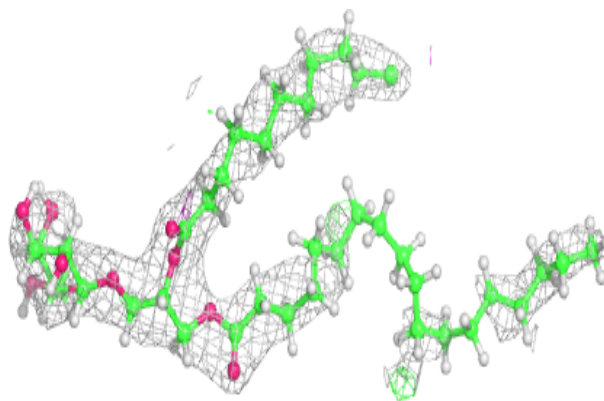
**Electron density around STE d 410:**

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

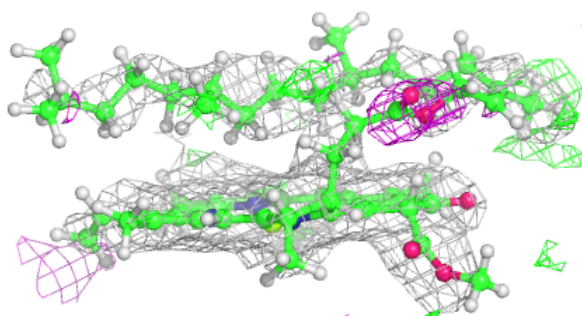
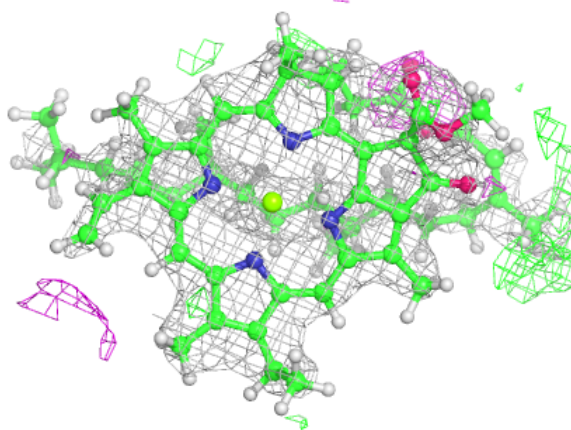


Electron density around LMG c 523:

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

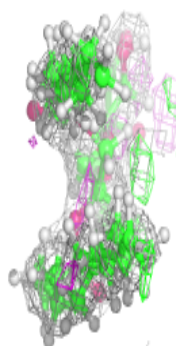
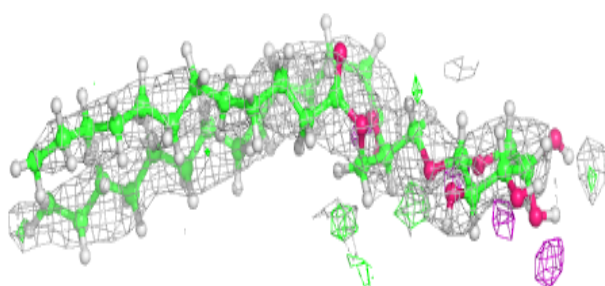
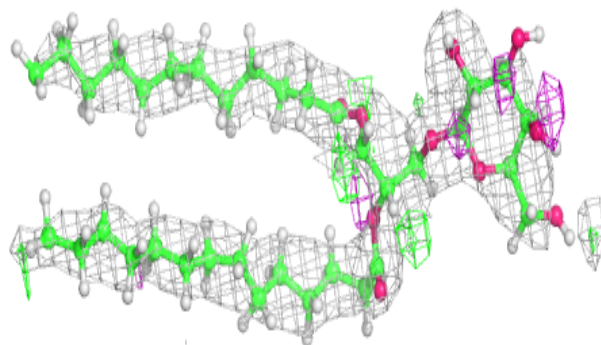
**Electron density around CLA h 101:**

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

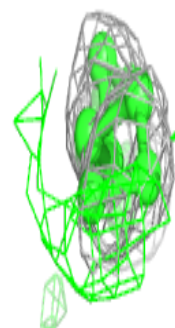
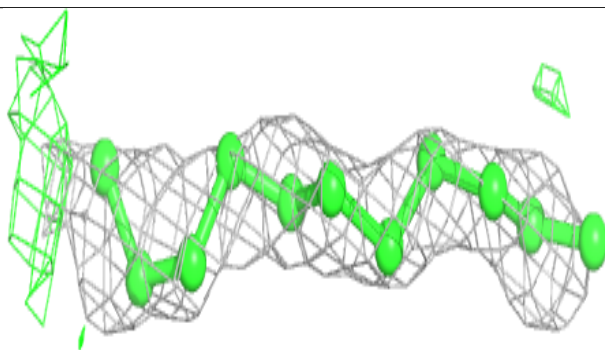
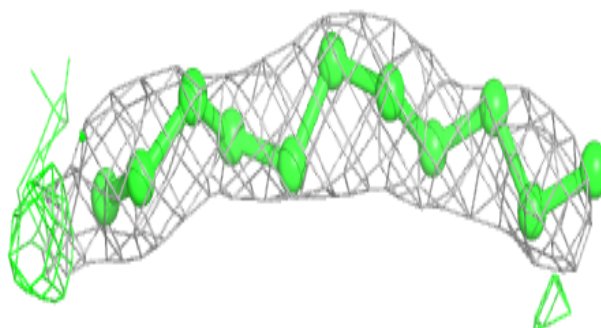


Electron density around LMG B 620:

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

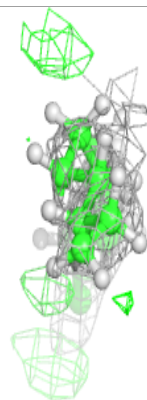
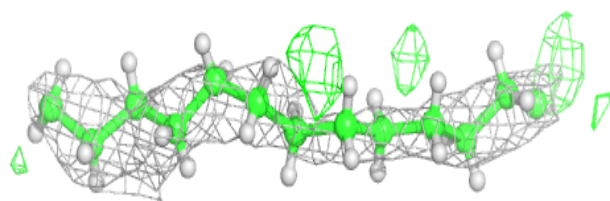
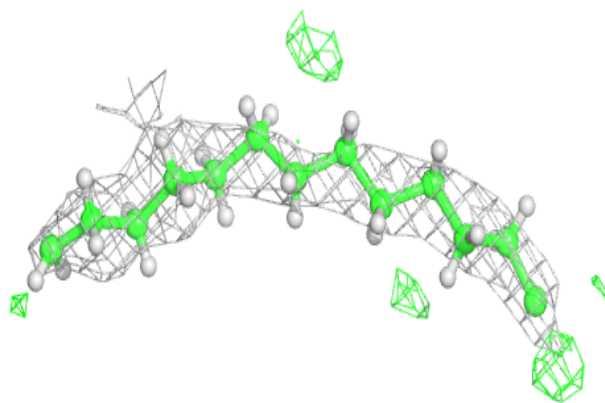
**Electron density around STE b 627:**

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

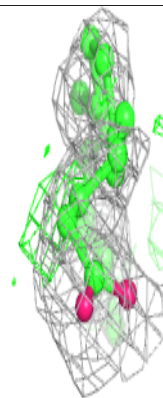
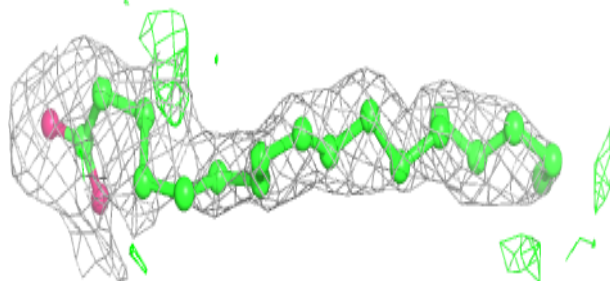
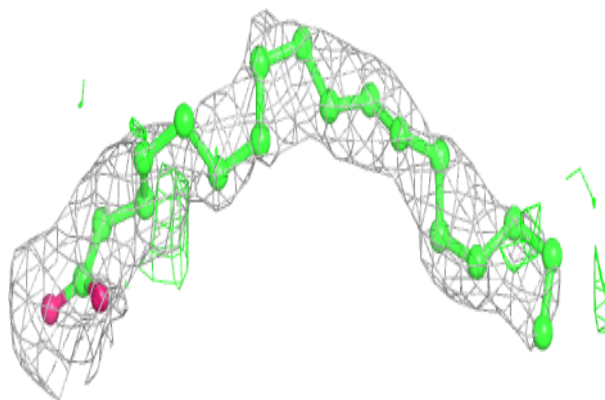


Electron density around STE c 516:

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

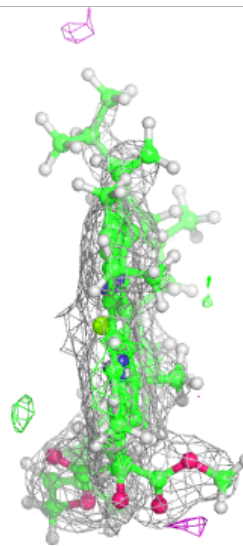
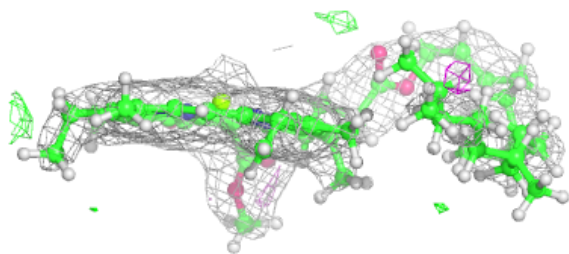
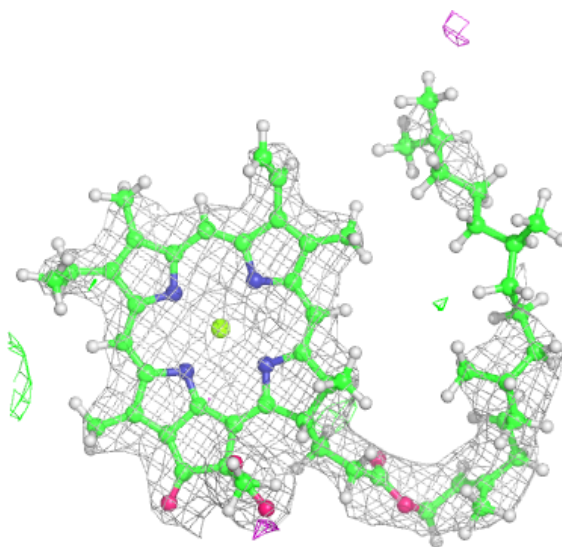
**Electron density around STE b 624:**

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



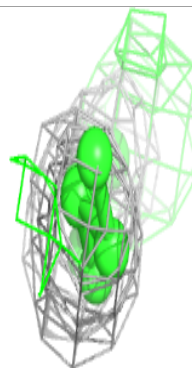
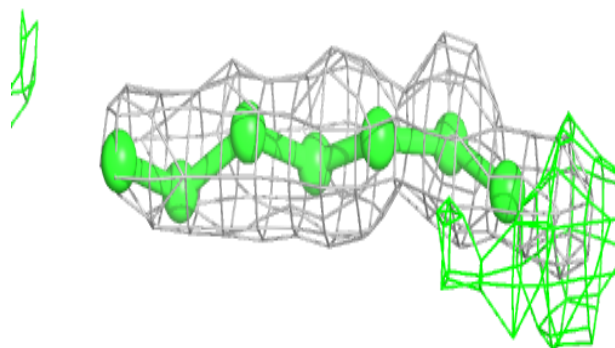
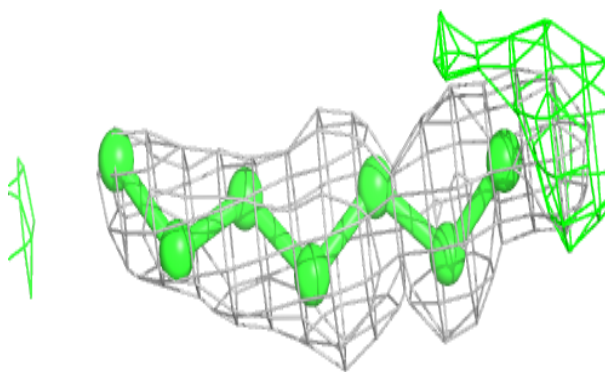
Electron density around CLA C 512:

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

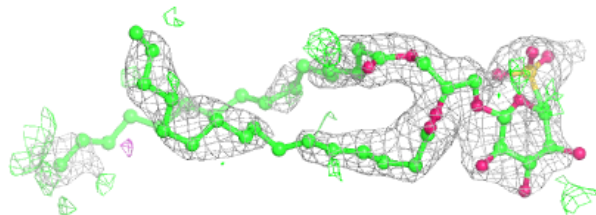
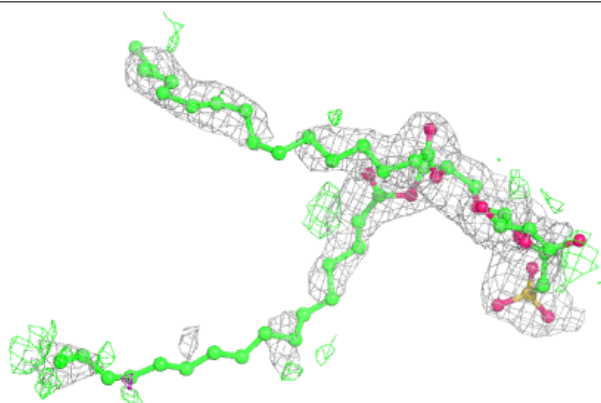


Electron density around STE C 519:

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

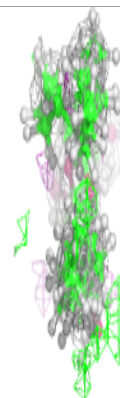
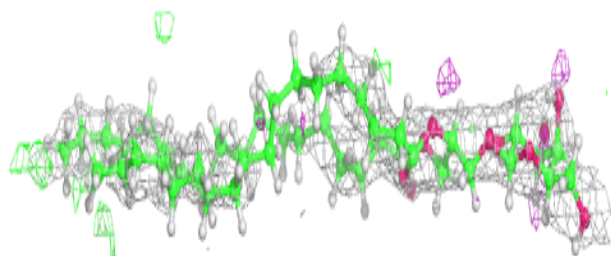
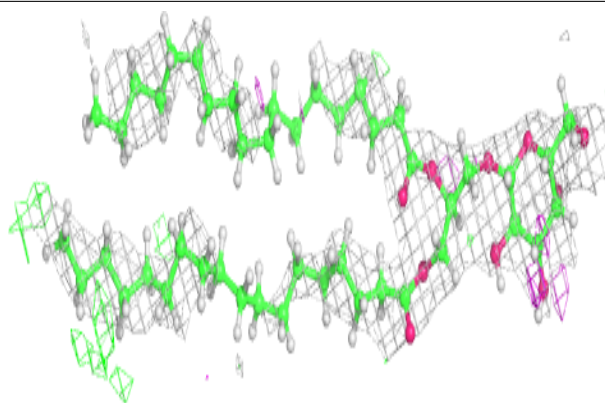
**Electron density around SQD A 413:**

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

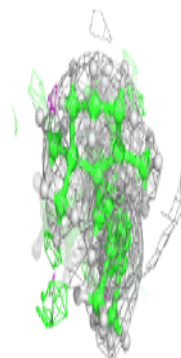
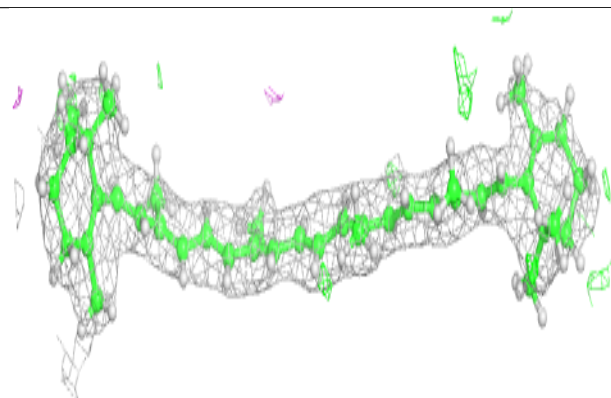
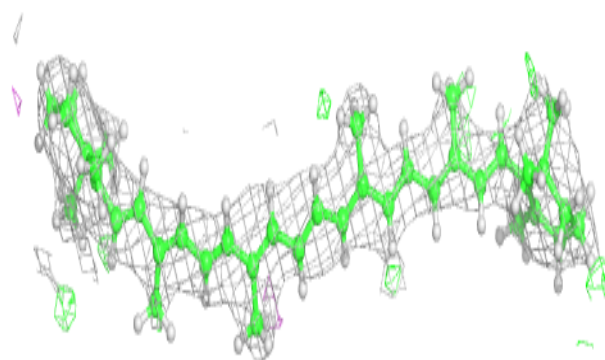


Electron density around LMG b 623:

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

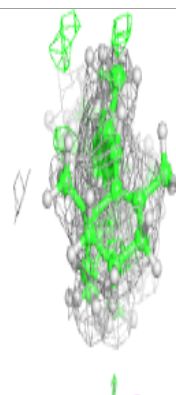
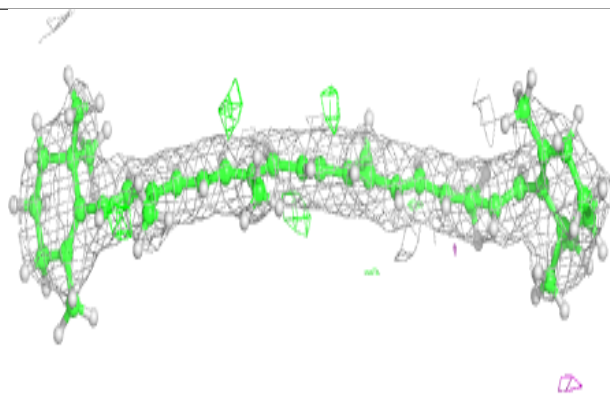
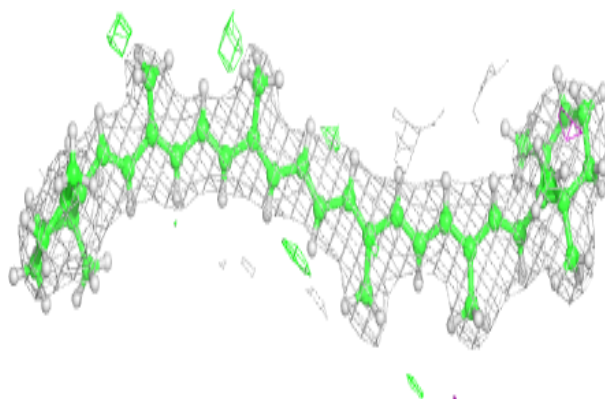
**Electron density around BCR x 101:**

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

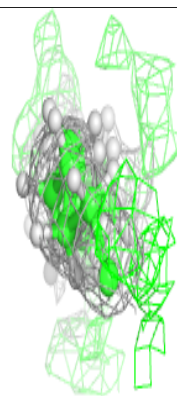
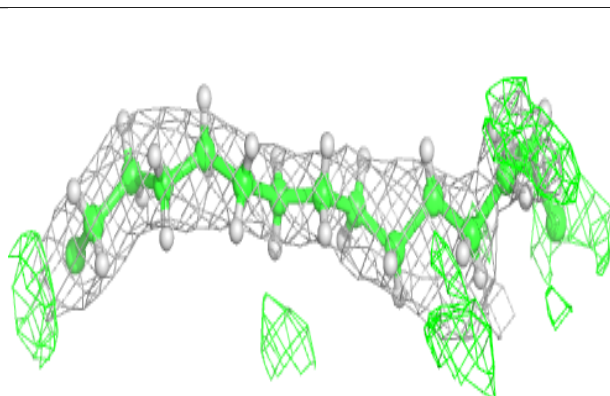
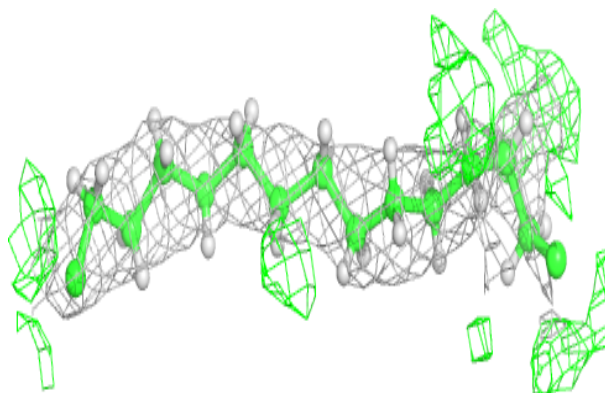


Electron density around BCR K 101:

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

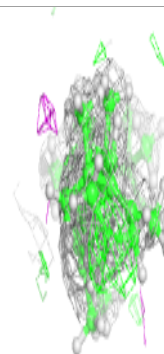
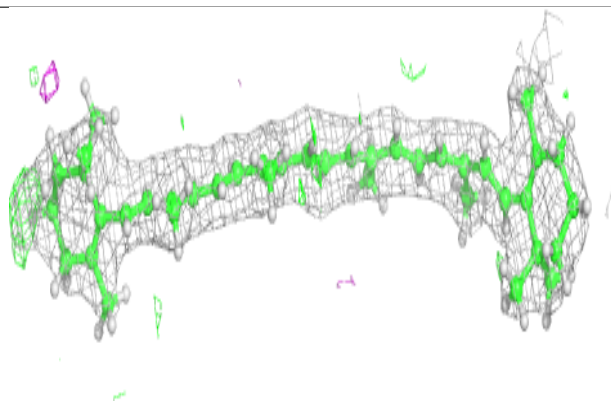
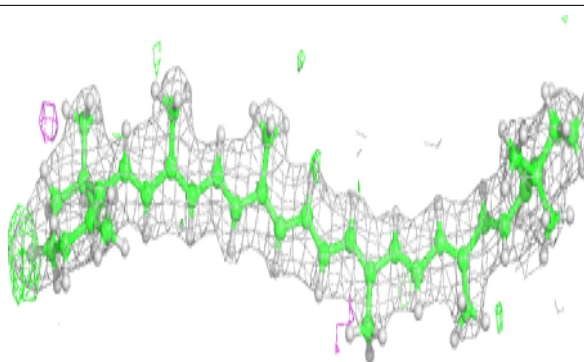
**Electron density around STE I 101:**

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

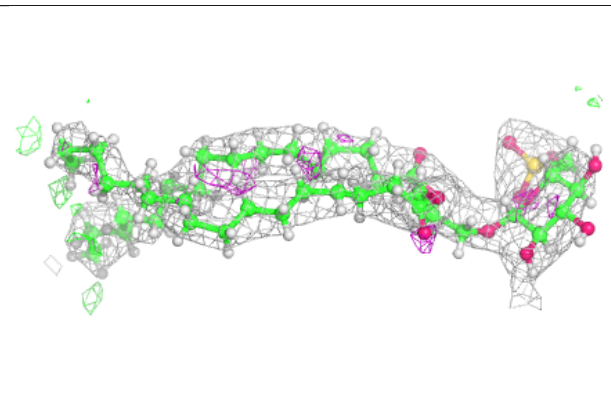
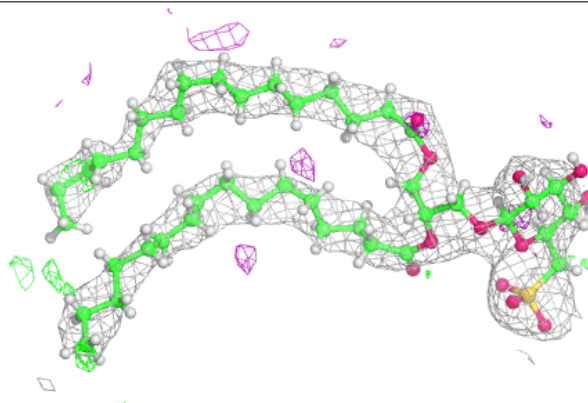


Electron density around BCR H 101:

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

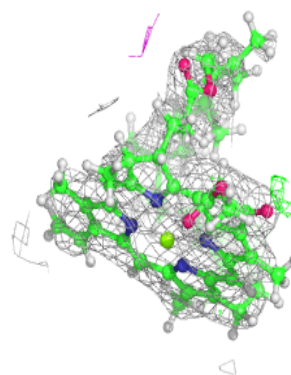
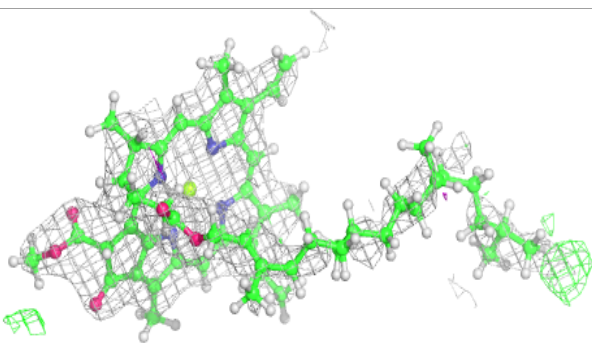
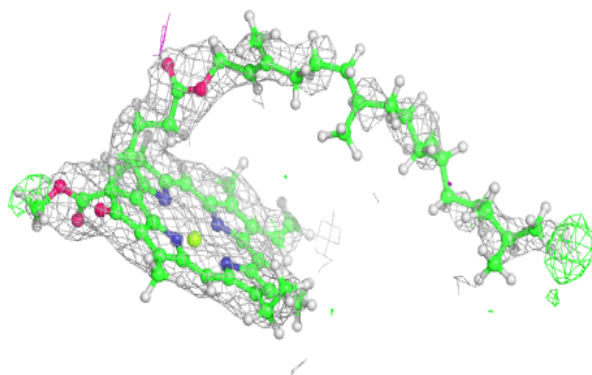
**Electron density around SQD 1 101:**

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

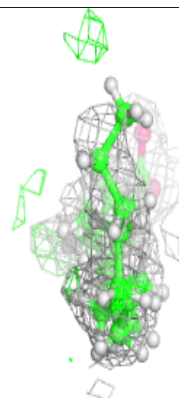
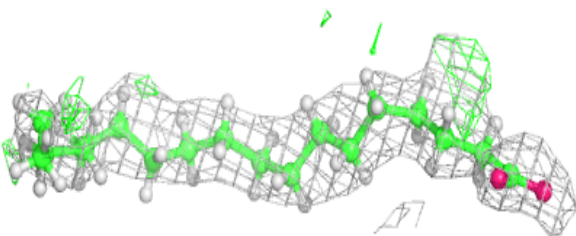
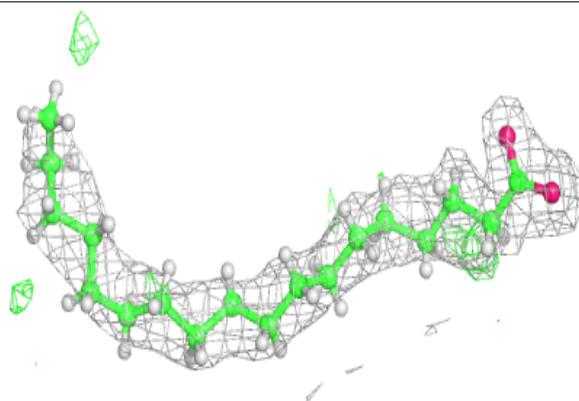


Electron density around CLA c 513:

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

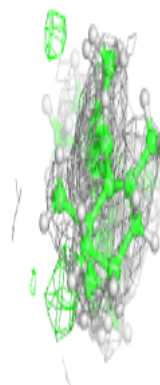
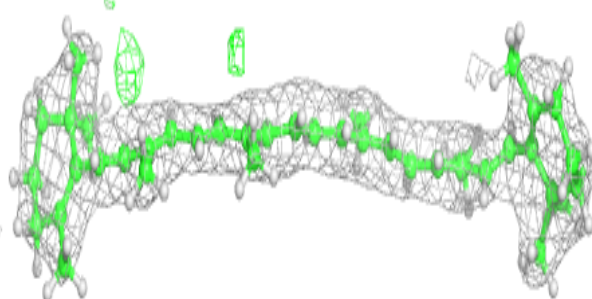
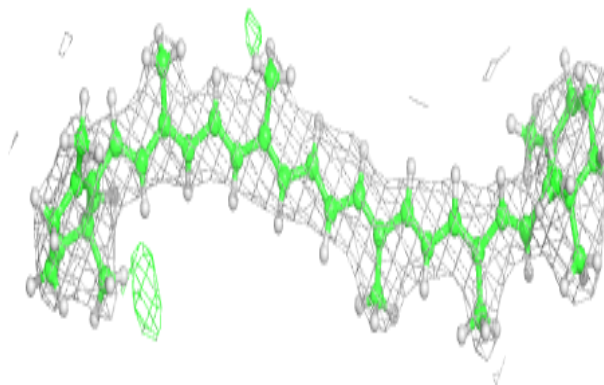
**Electron density around STE b 622:**

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

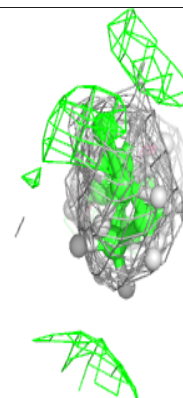
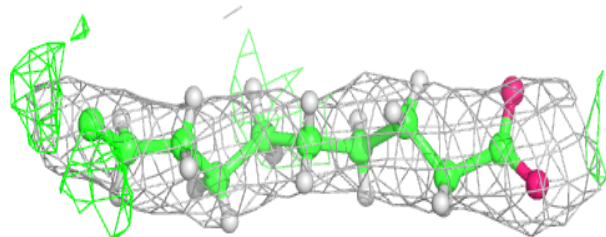
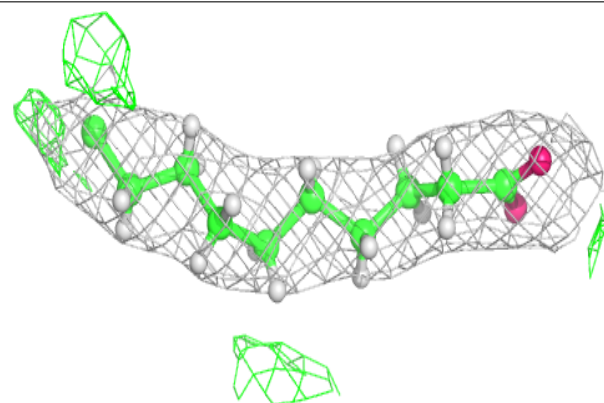


Electron density around BCR k 101:

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

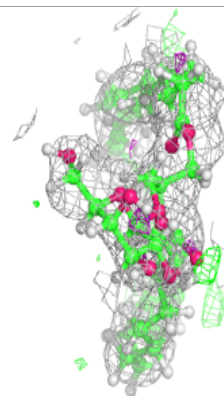
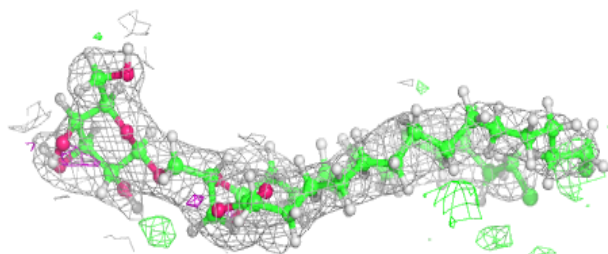
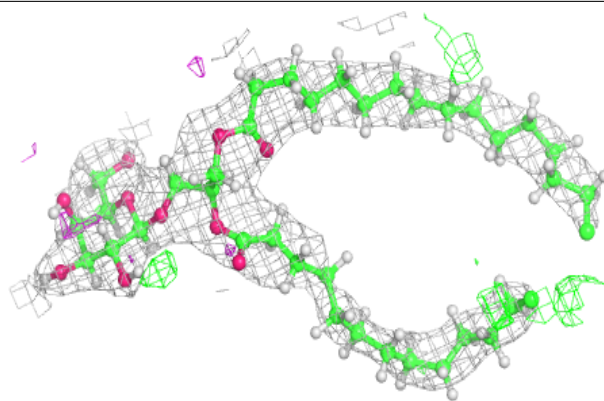
**Electron density around STE j 101:**

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

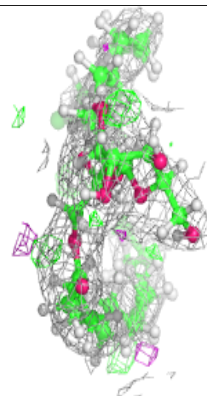
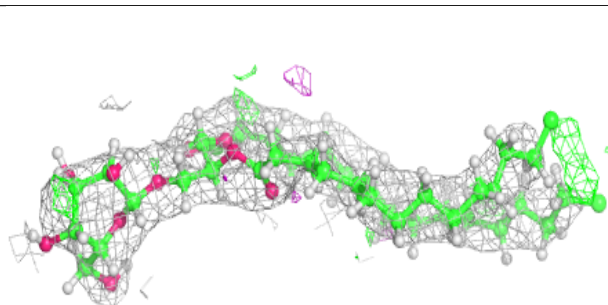
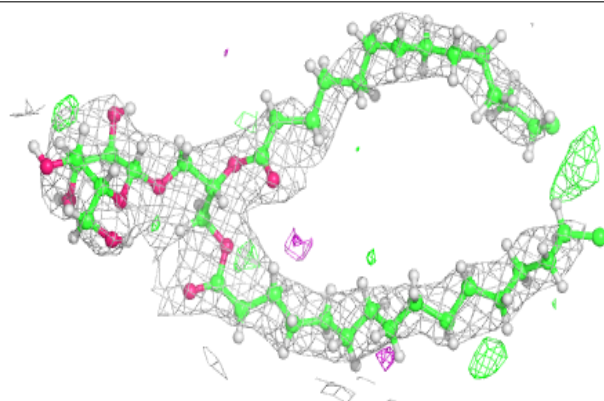


Electron density around LMG A 411:

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

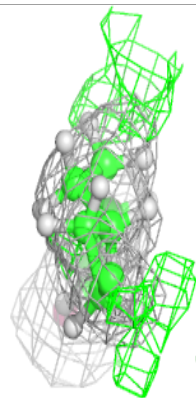
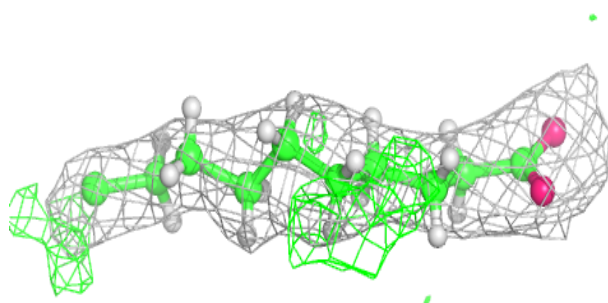
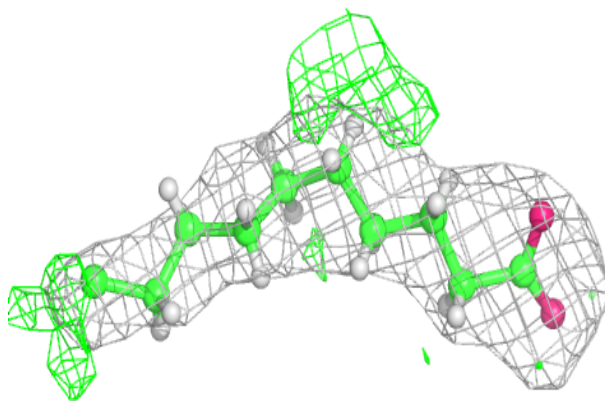
**Electron density around LMG c 524:**

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

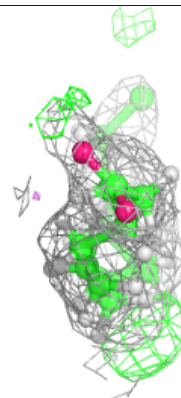
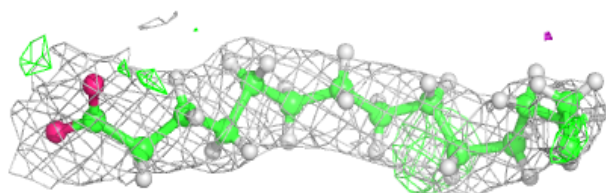
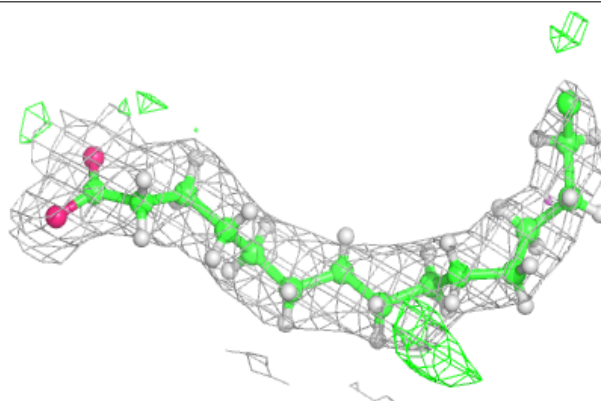


Electron density around STE C 525:

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

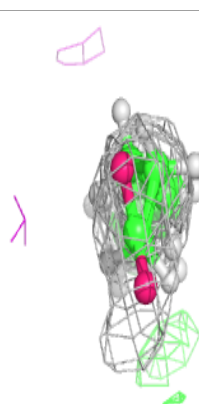
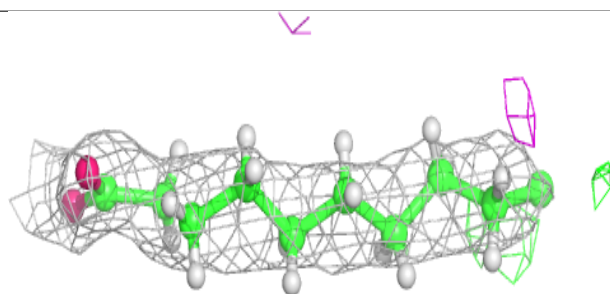
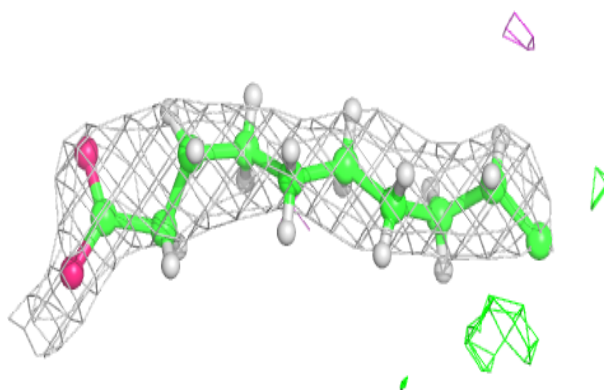
**Electron density around STE B 621:**

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

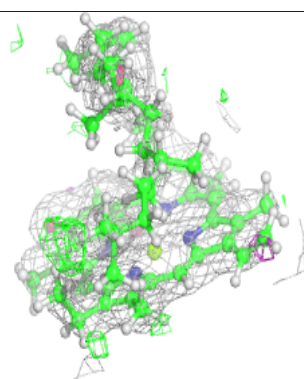
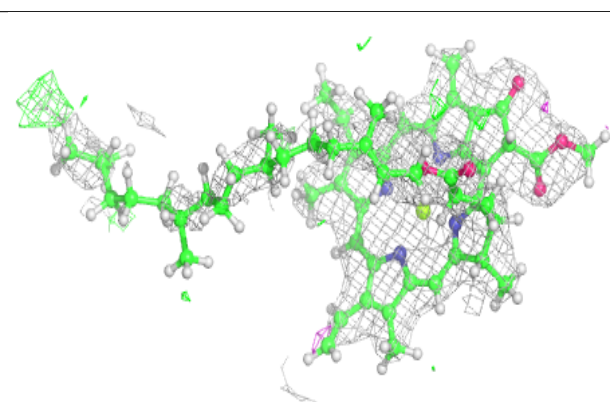
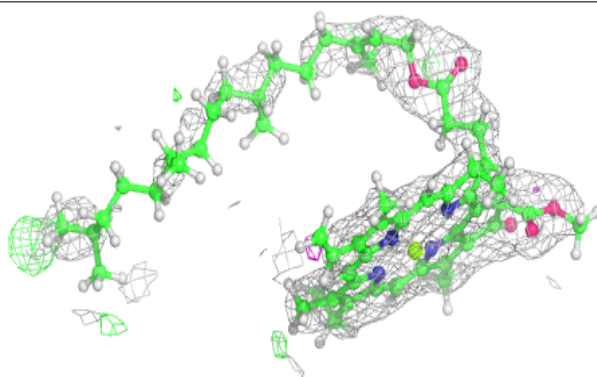


Electron density around STE m 101:

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

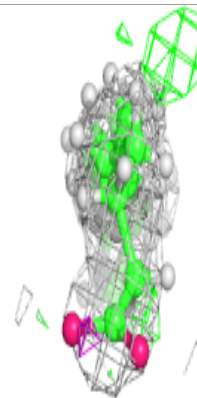
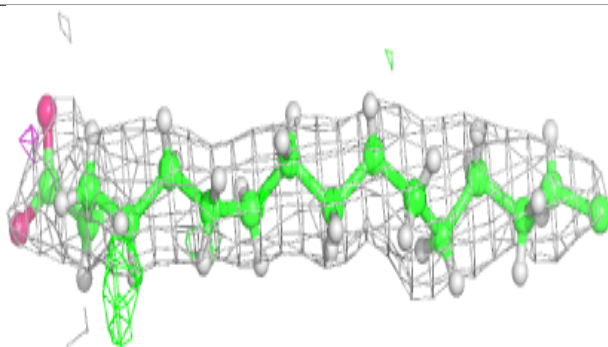
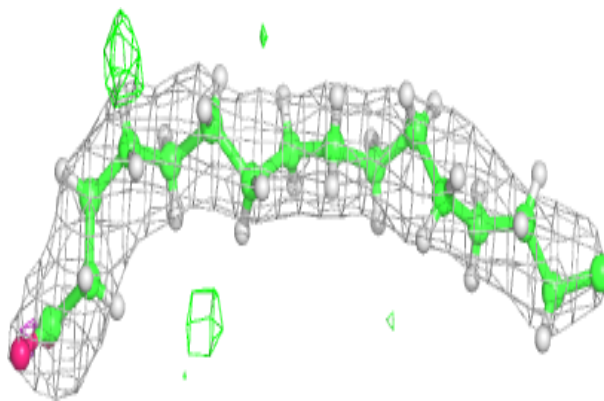
**Electron density around CLA C 513:**

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

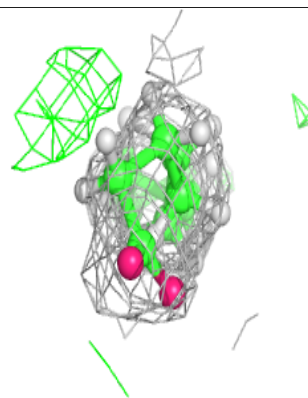
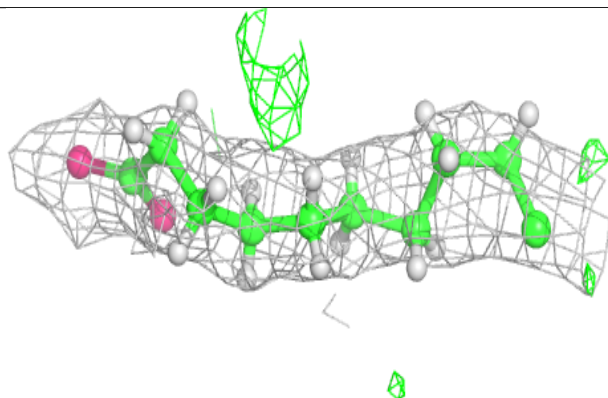
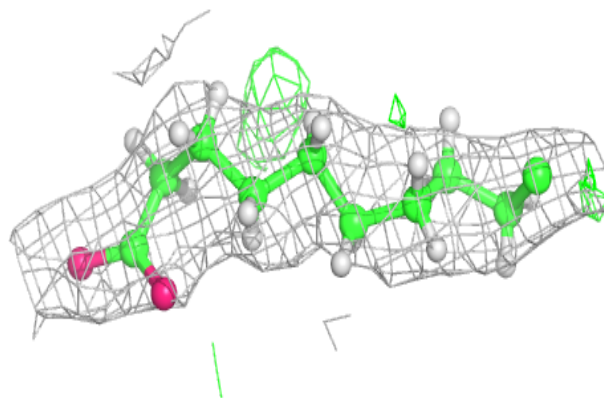


Electron density around STE t 103:

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

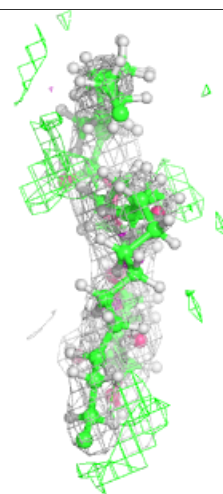
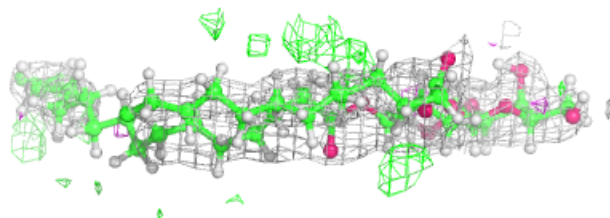
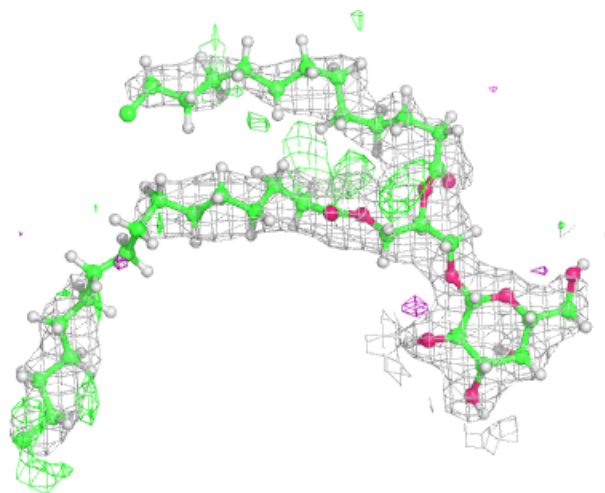
**Electron density around STE J 101:**

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



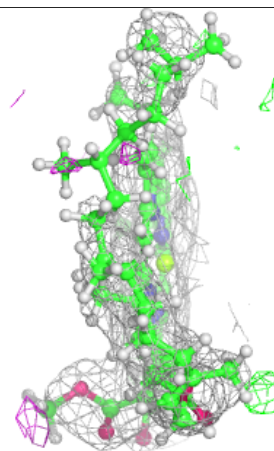
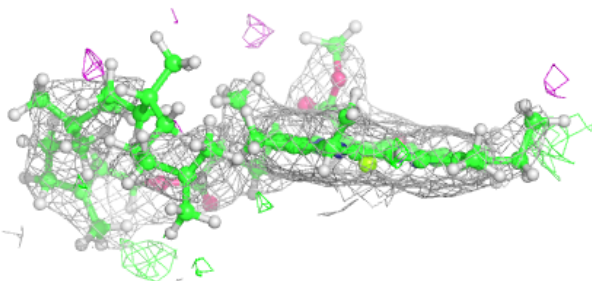
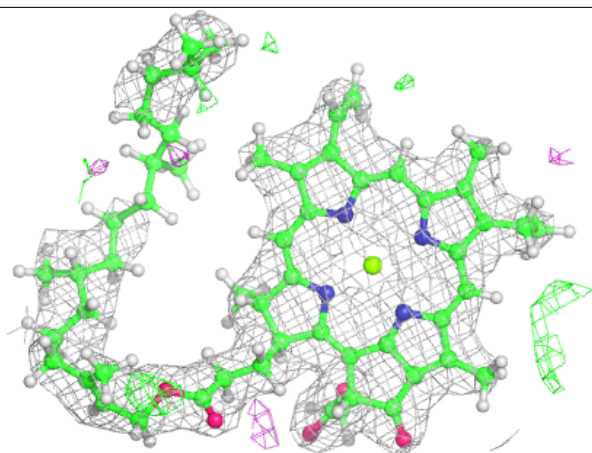
Electron density around LMG C 524:

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

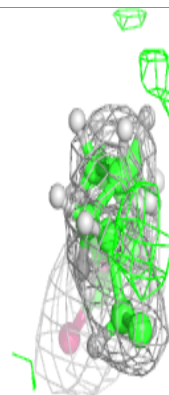
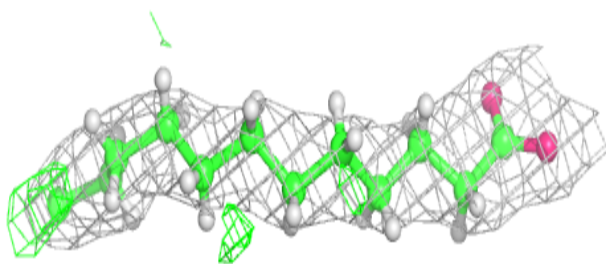
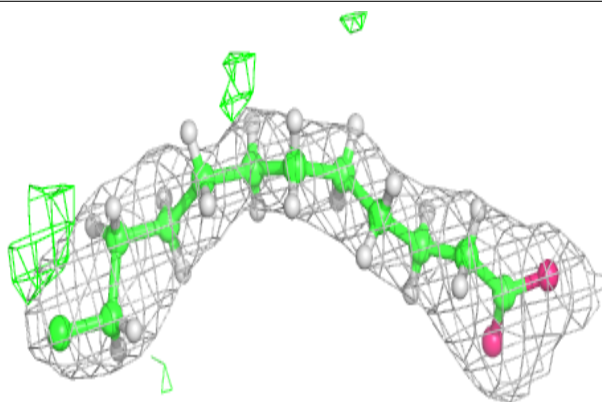


Electron density around CLA c 512:

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

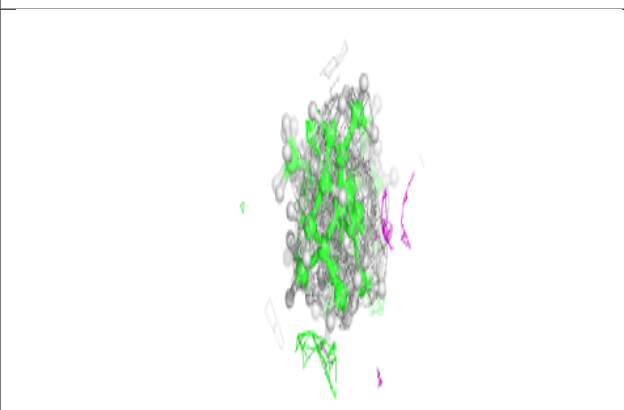
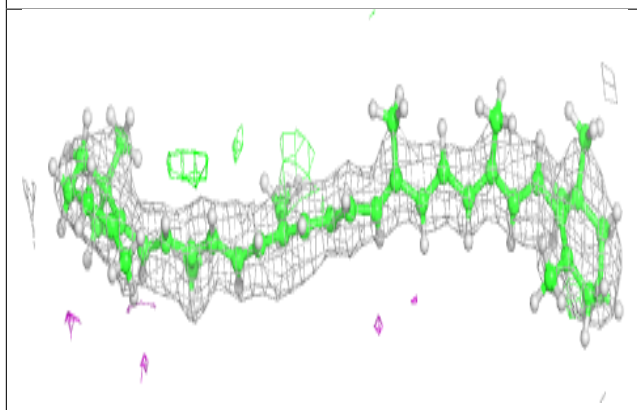
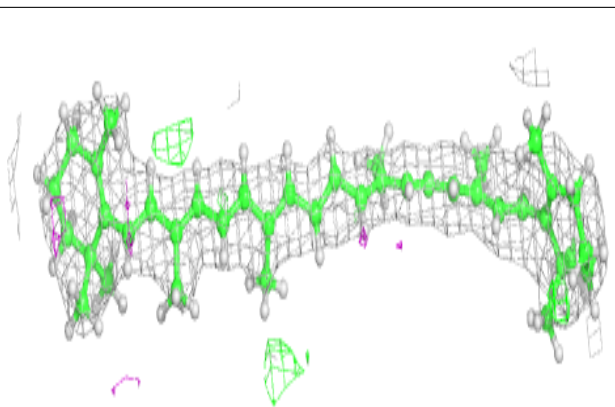
**Electron density around STE t 102:**

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

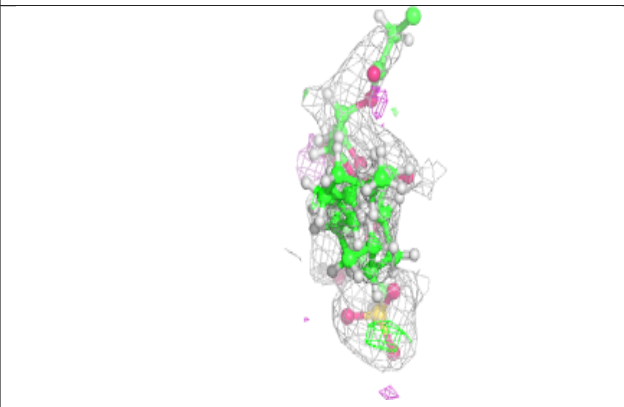
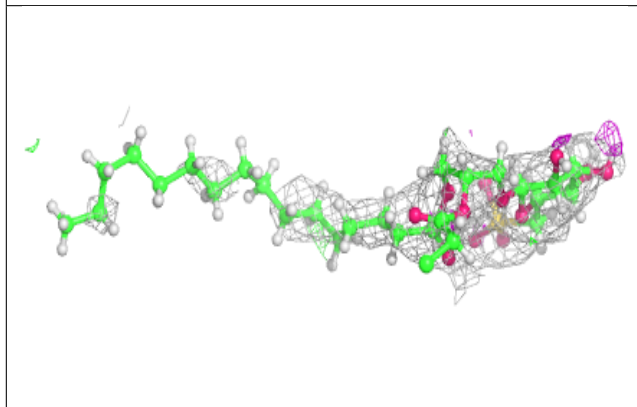
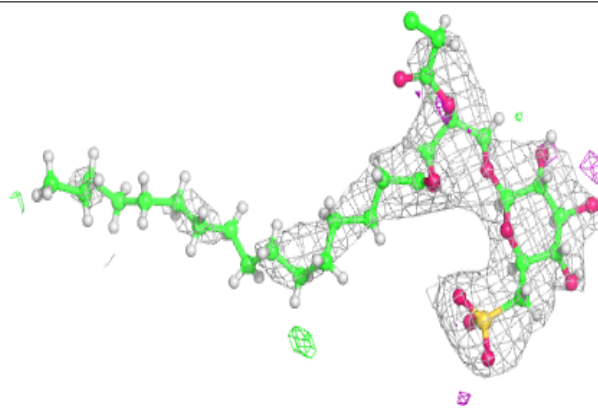


Electron density around BCR C 514:

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

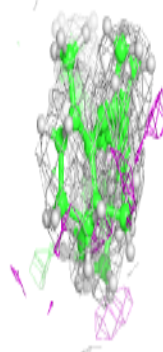
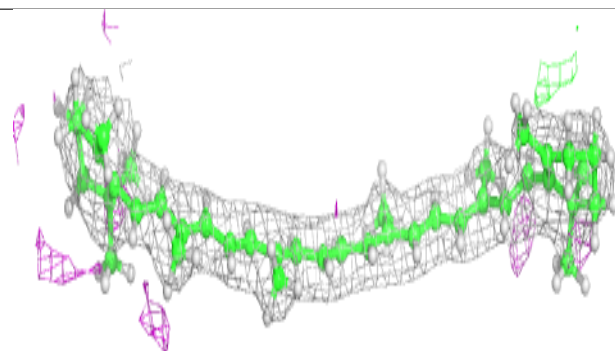
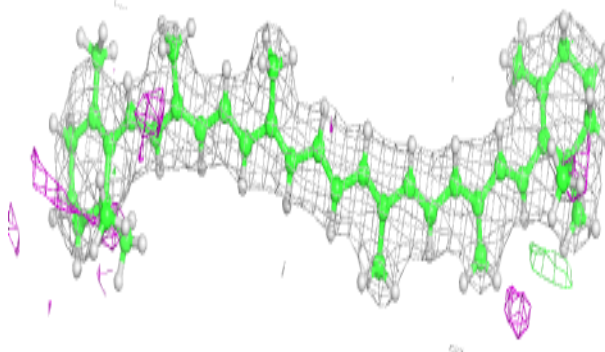
**Electron density around SQD f 102:**

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

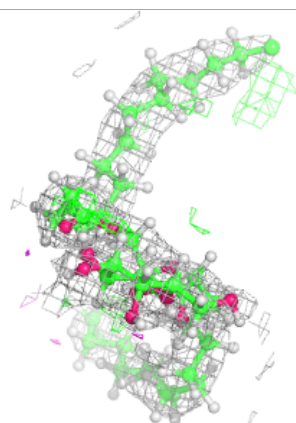
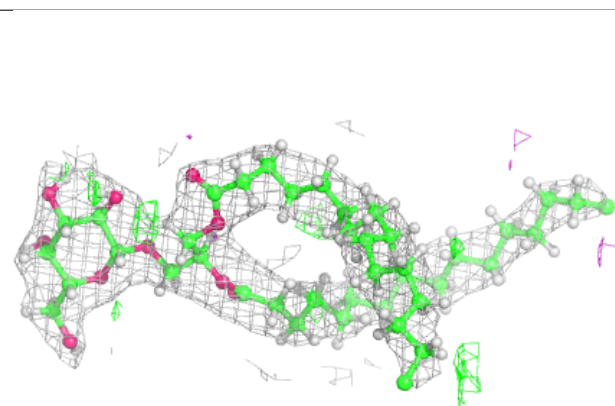
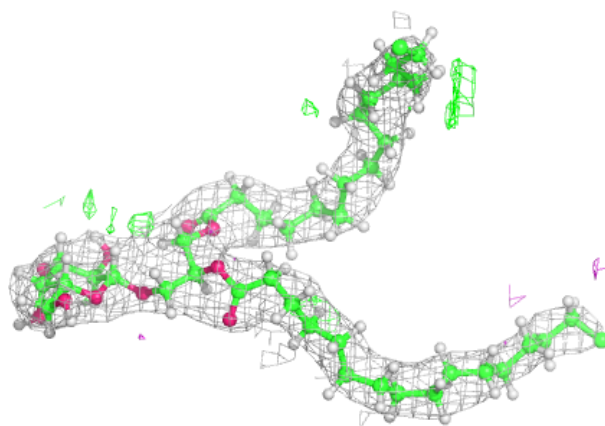


Electron density around BCR D 406:

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

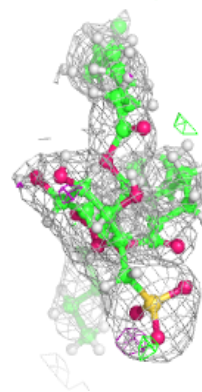
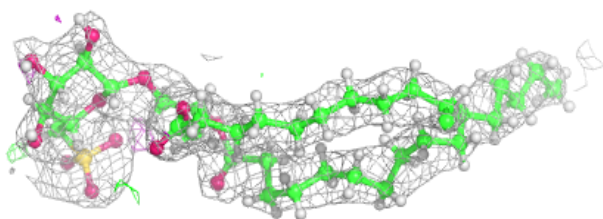
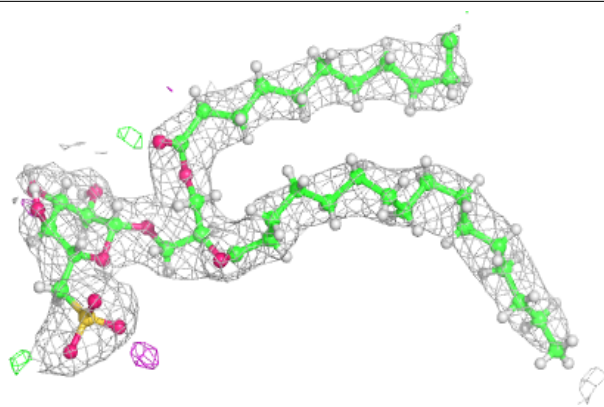
**Electron density around LMG b 621:**

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



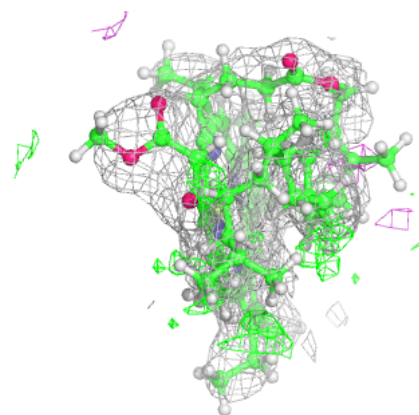
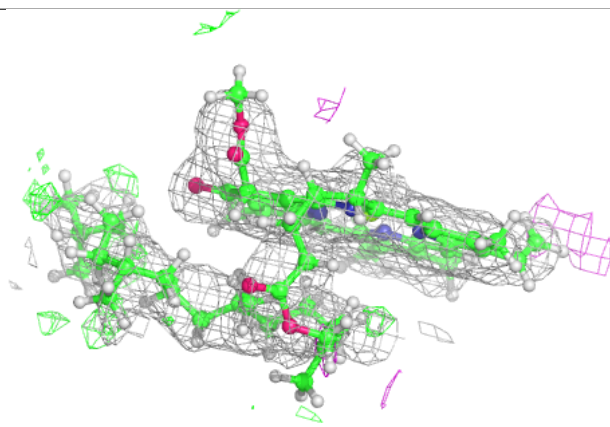
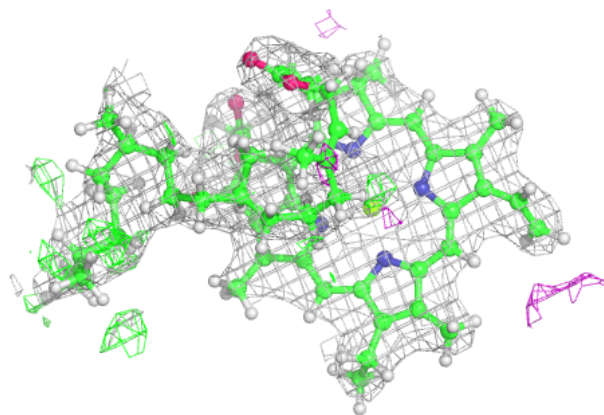
Electron density around SQD b 620:

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



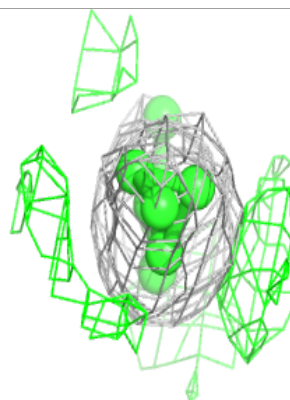
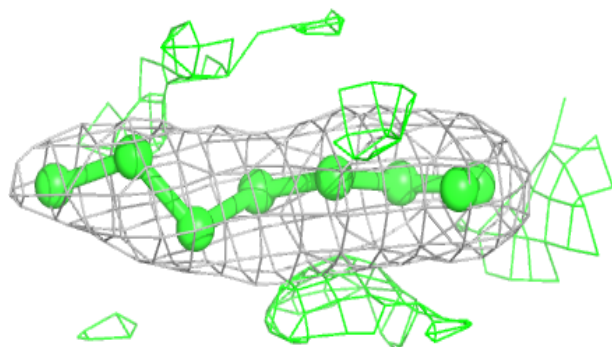
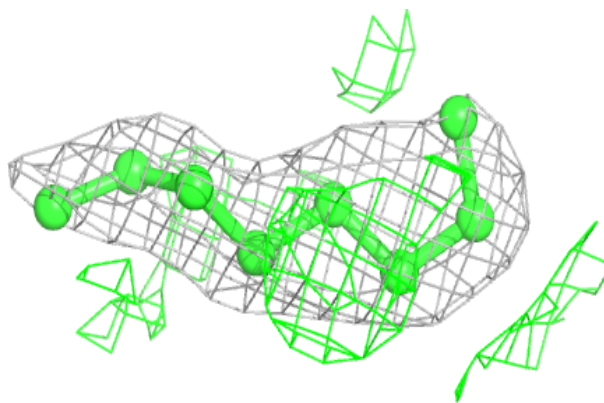
Electron density around CLA B 601:

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

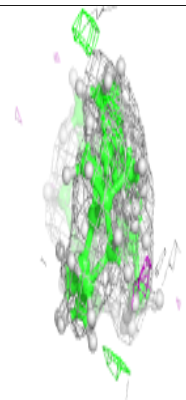
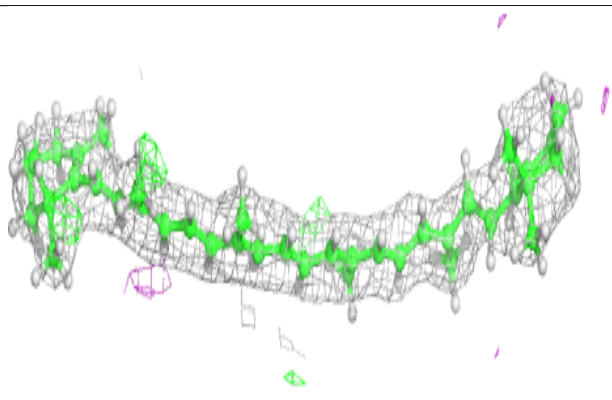
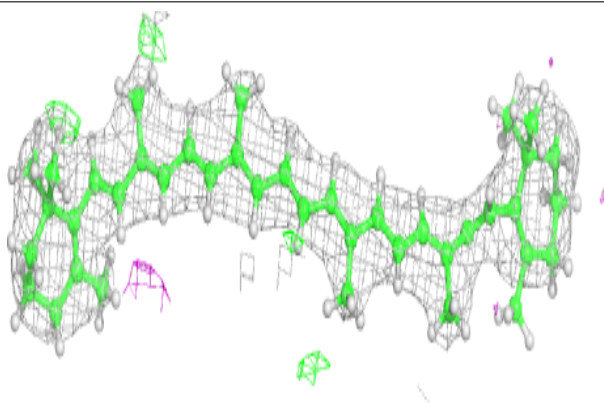


Electron density around STE A 415:

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

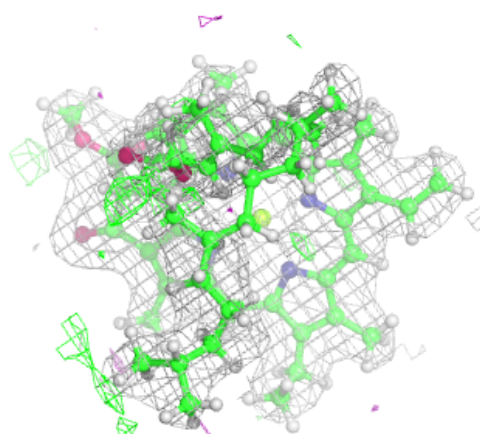
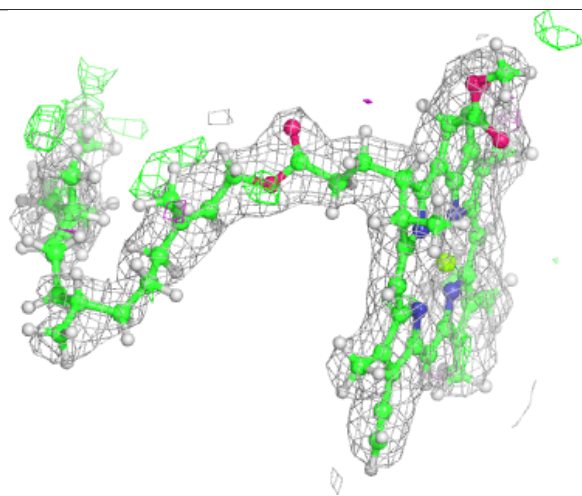
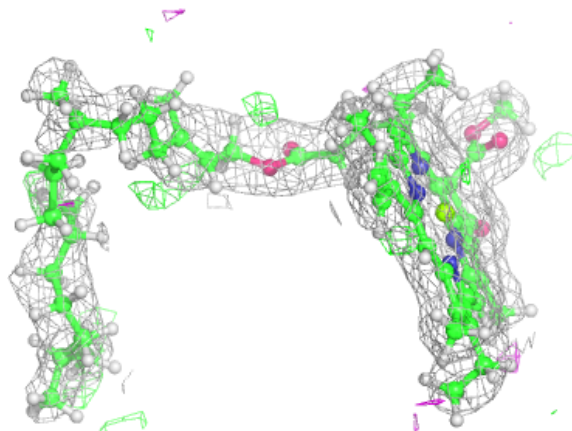
**Electron density around BCR d 404:**

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



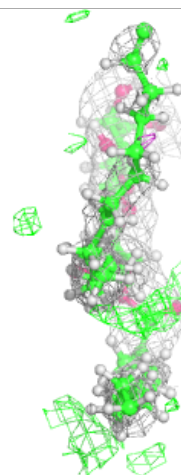
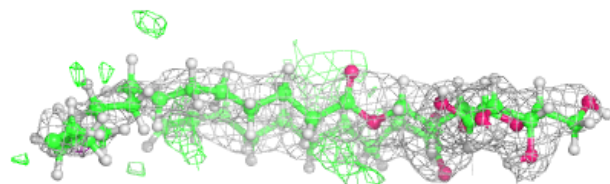
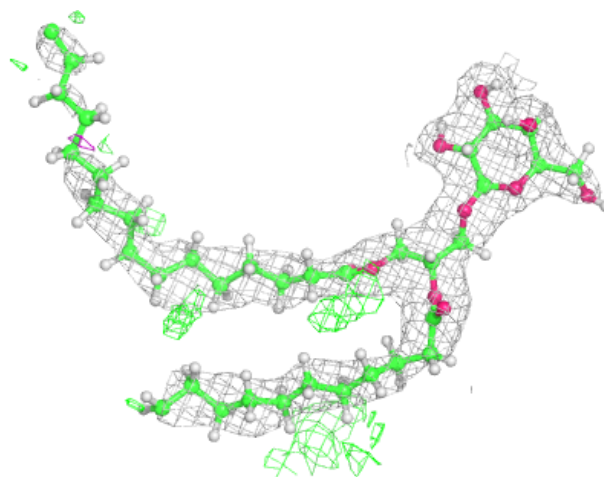
Electron density around CLA a 408:

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



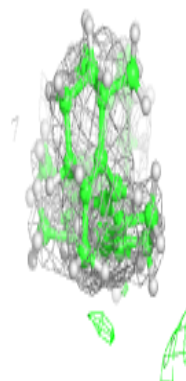
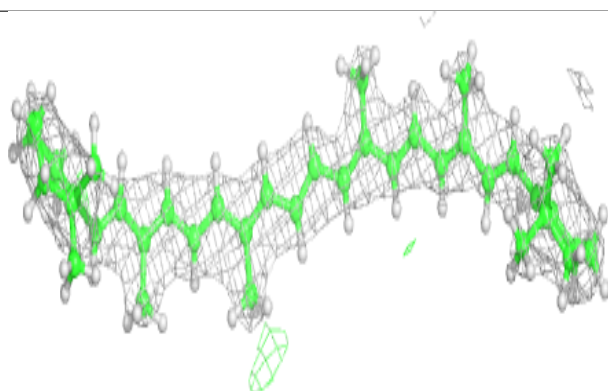
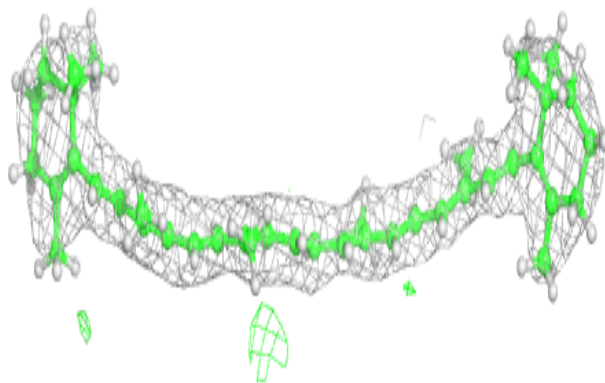
Electron density around LMG c 522:

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



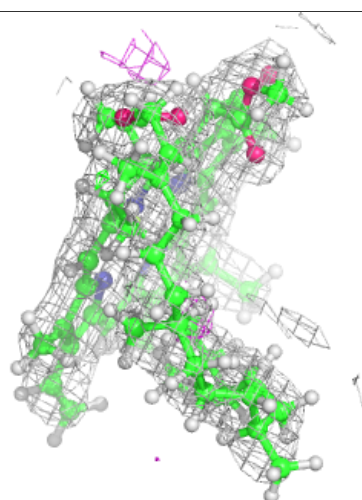
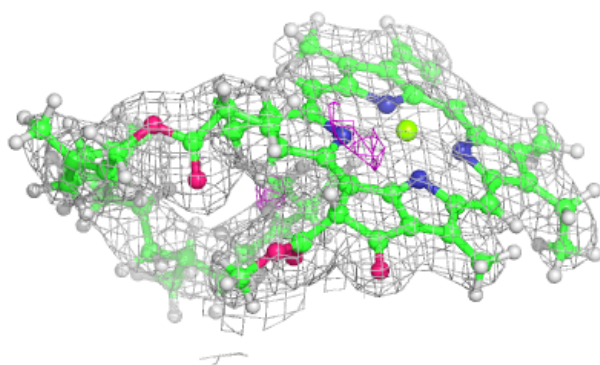
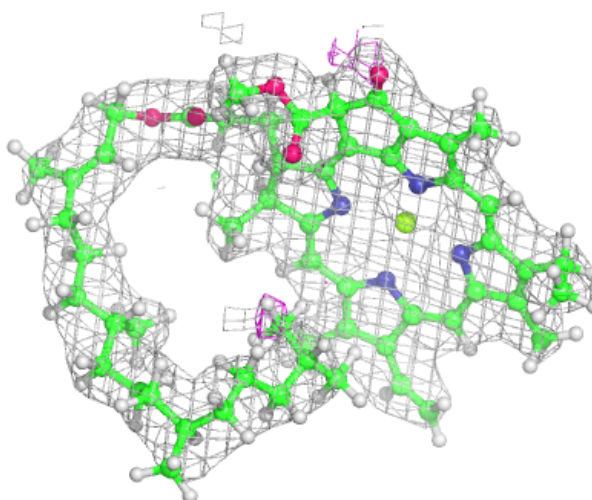
Electron density around BCR k 102:

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



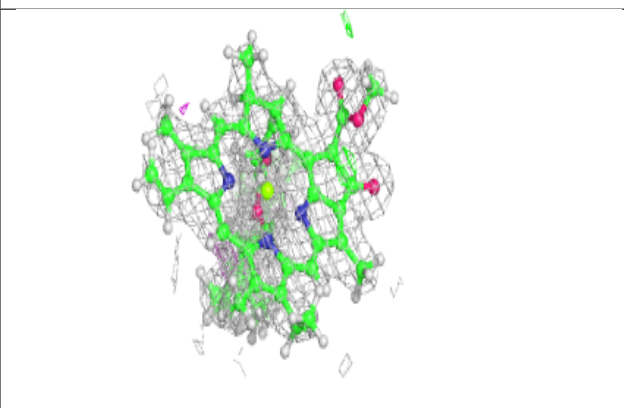
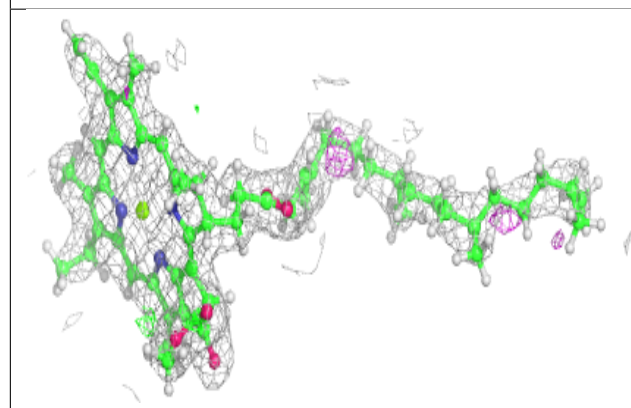
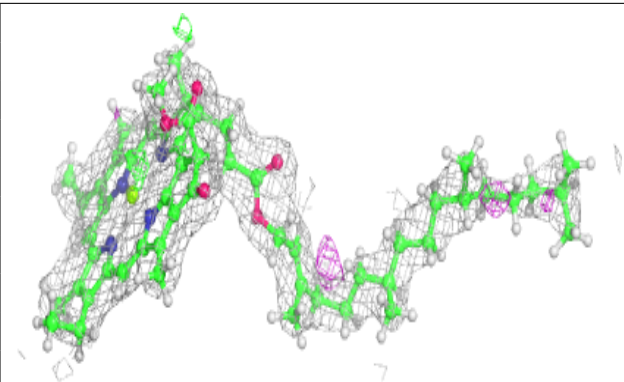
Electron density around CLA b 614:

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

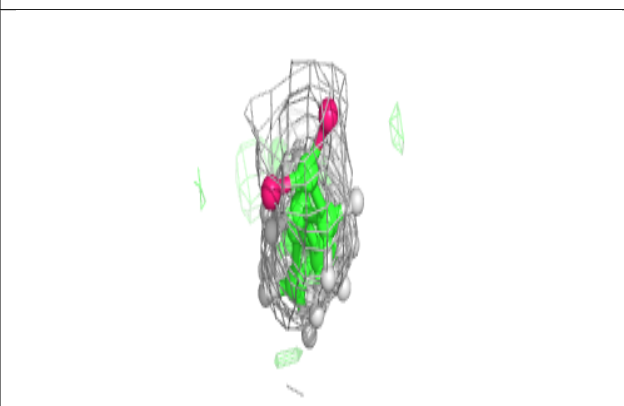
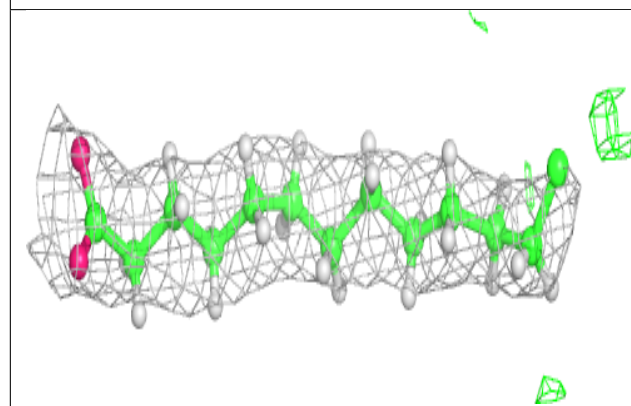
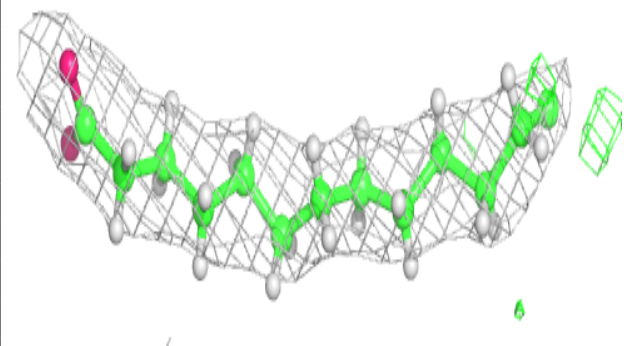


Electron density around CLA c 502:

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

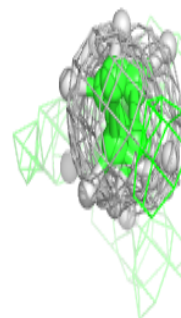
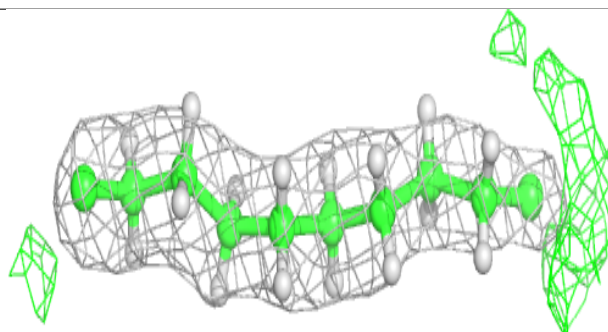
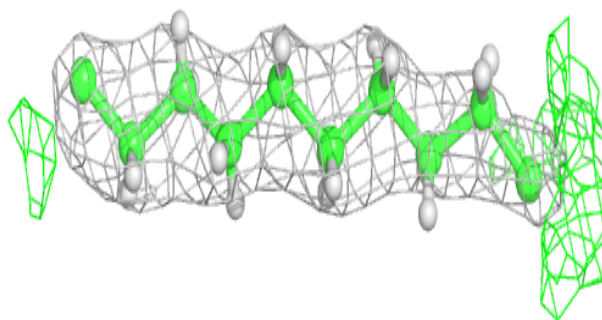
**Electron density around STE M 102:**

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

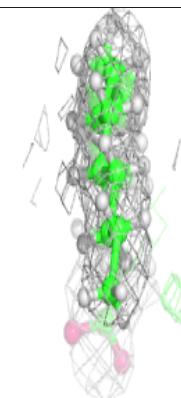
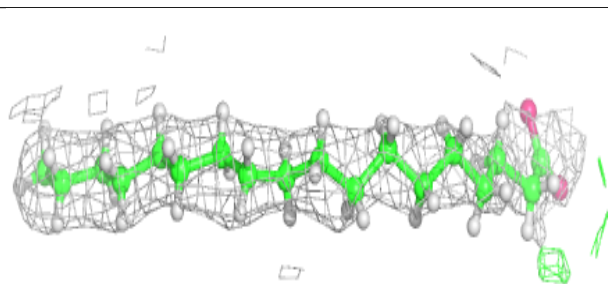
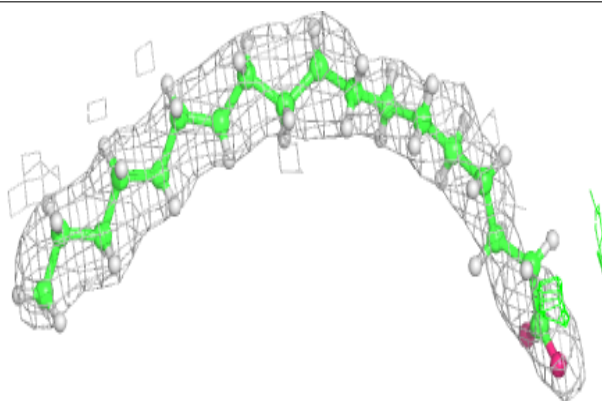


Electron density around STE M 103:

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

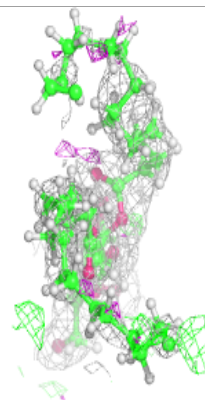
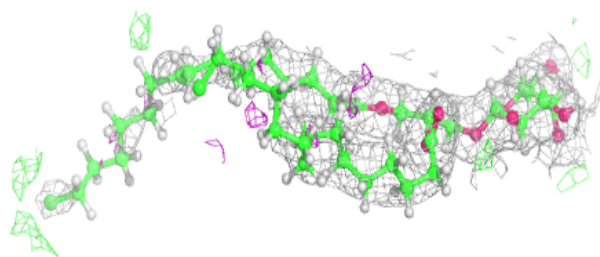
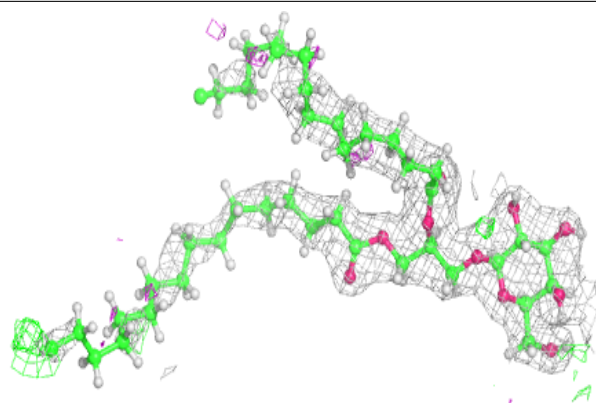
**Electron density around STE D 413:**

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

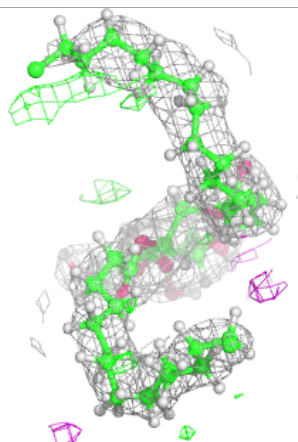
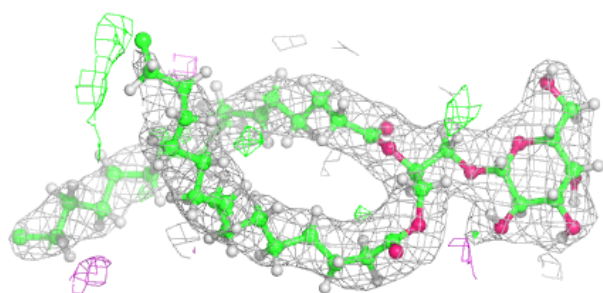
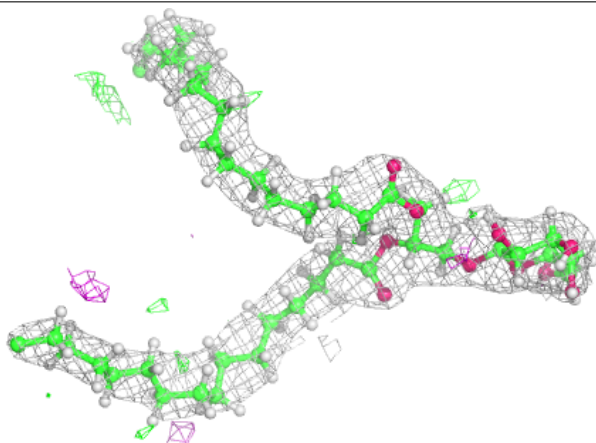


Electron density around LMG D 409:

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

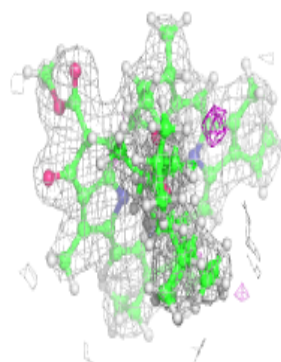
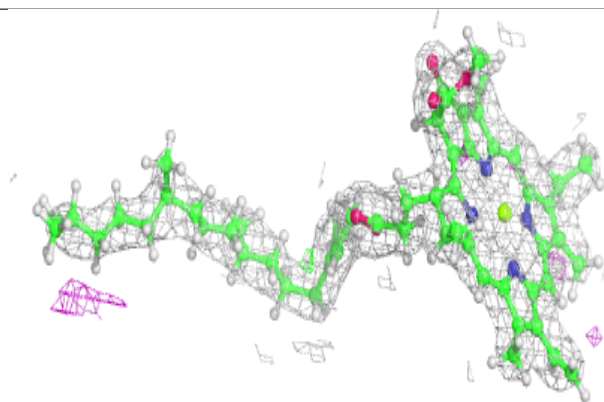
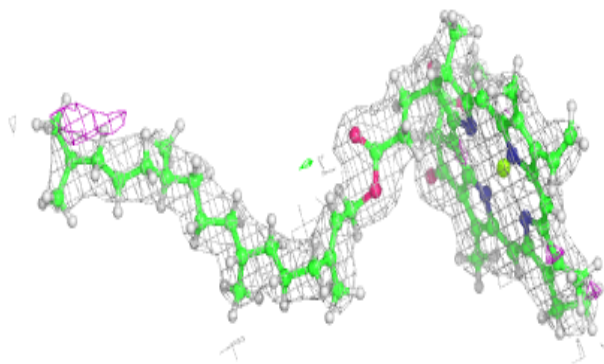
**Electron density around LMG M 101:**

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

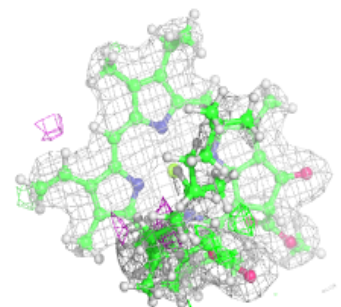
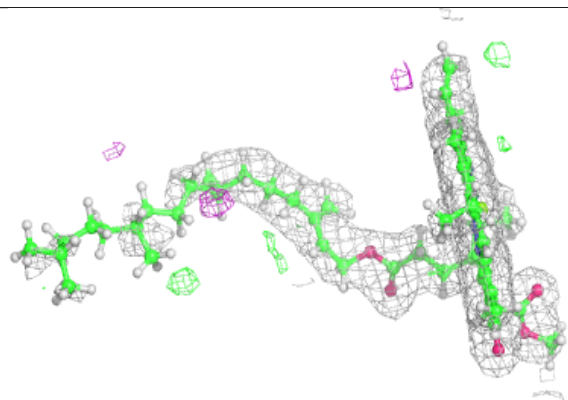
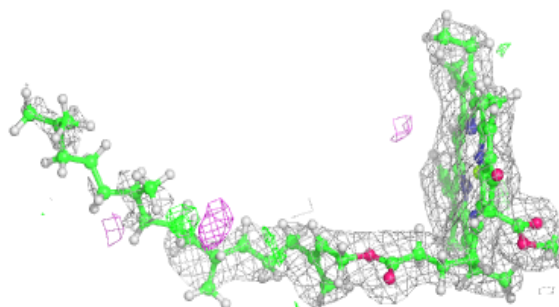


Electron density around CLA C 502:

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

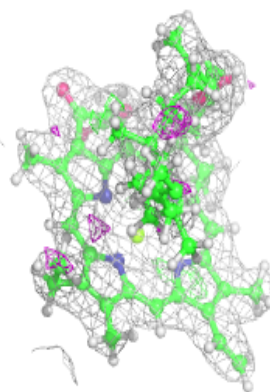
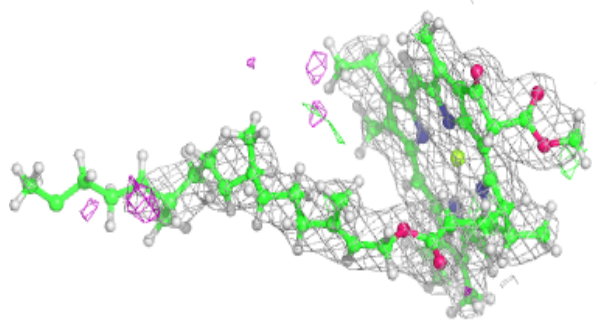
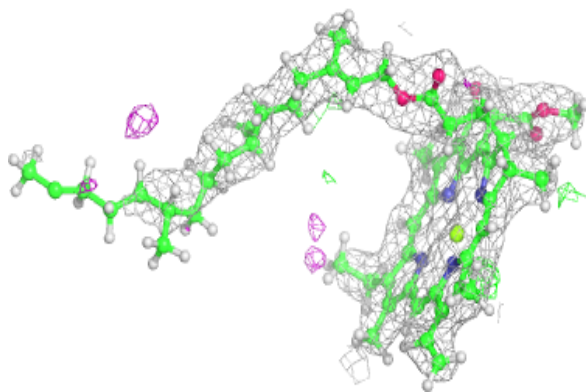
**Electron density around CLA D 405:**

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

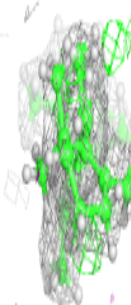
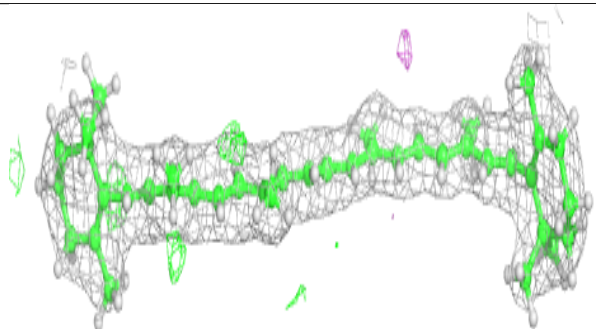
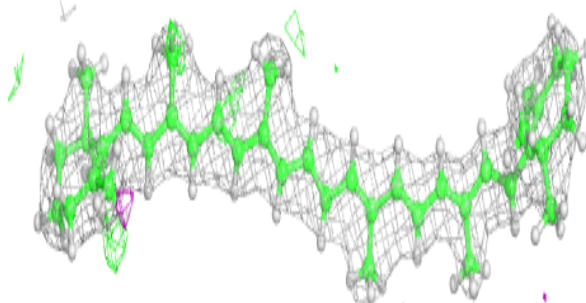


Electron density around CLA c 508:

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

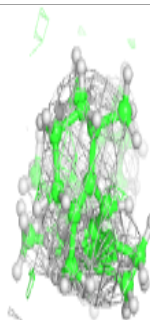
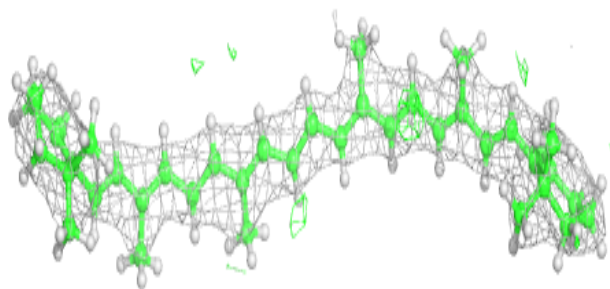
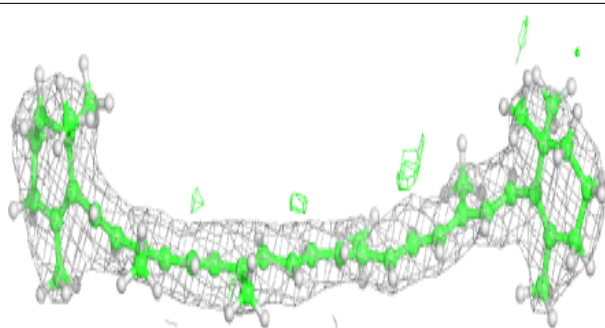
**Electron density around BCR C 515:**

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

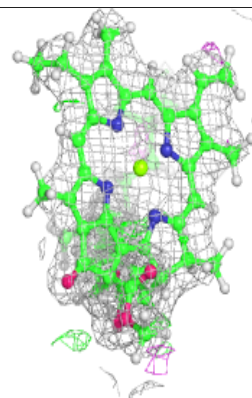
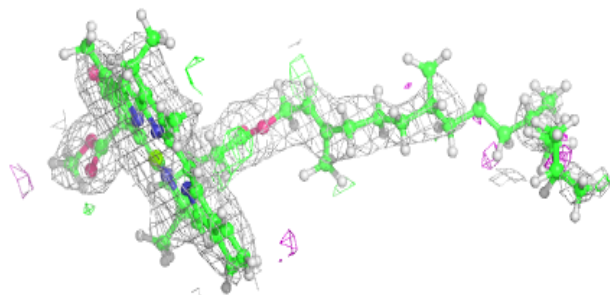
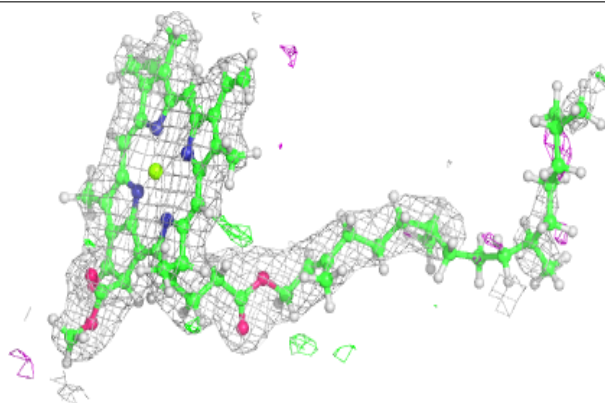


Electron density around BCR C 520:

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

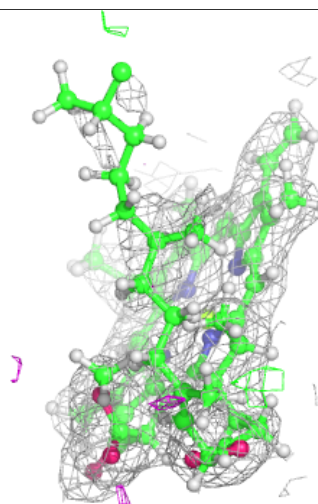
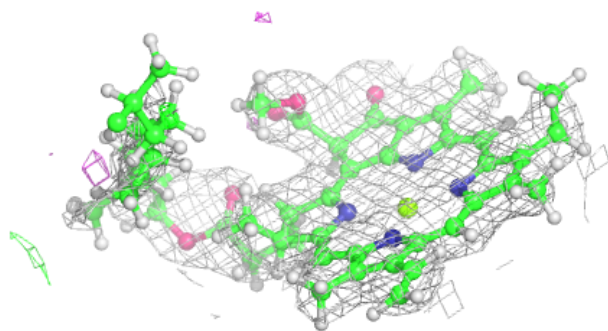
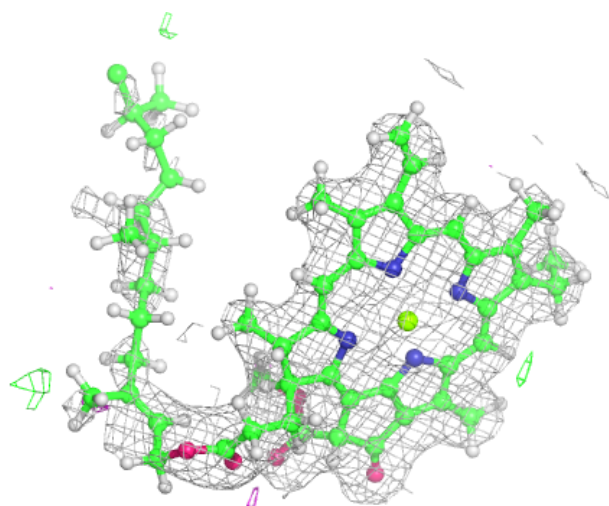
**Electron density around CLA d 403:**

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



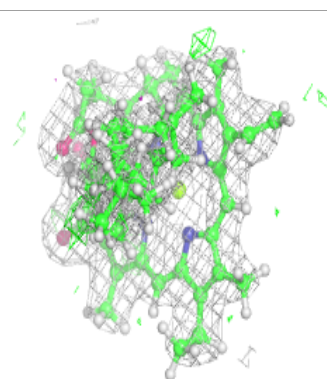
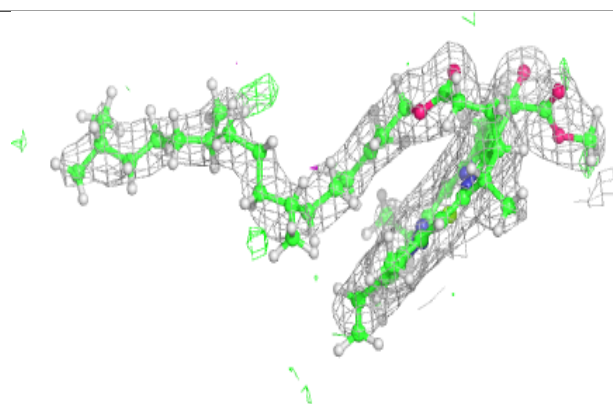
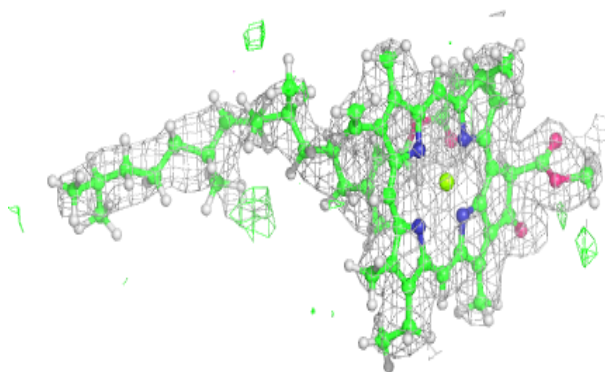
Electron density around CLA b 615:

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

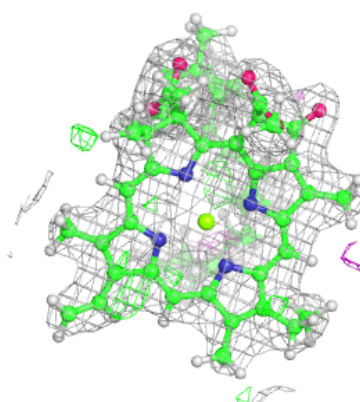
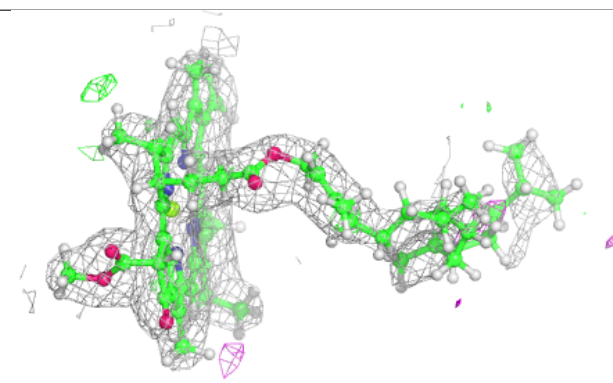
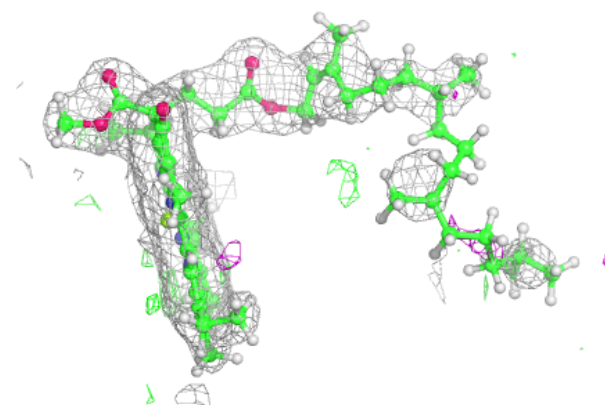


Electron density around CLA c 505:

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

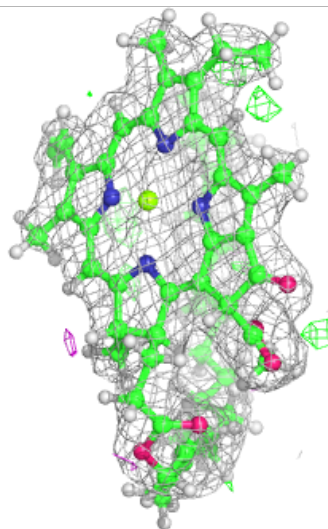
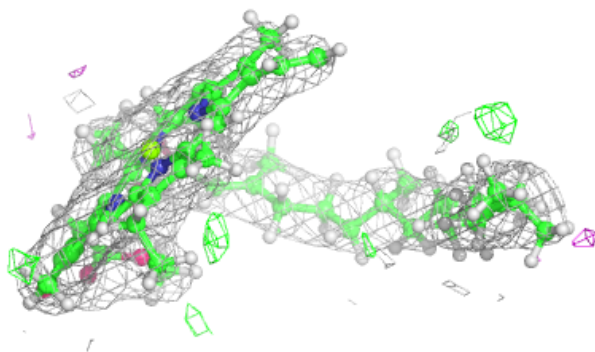
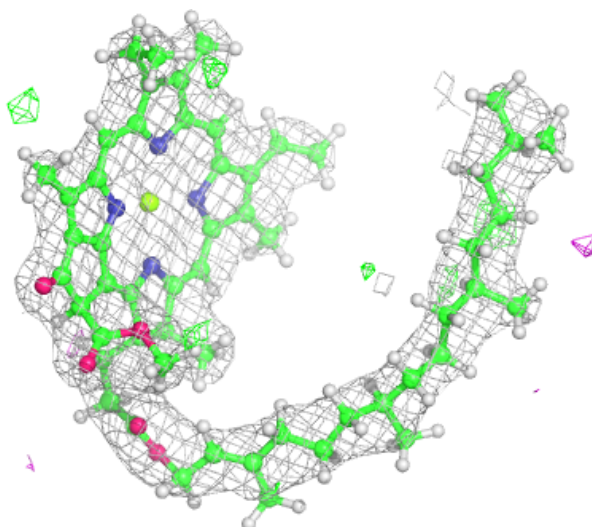
**Electron density around CLA c 506:**

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



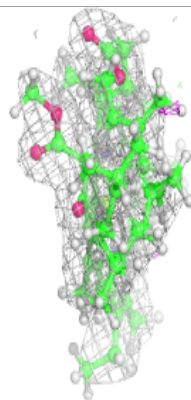
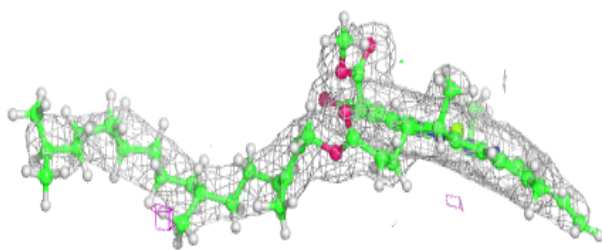
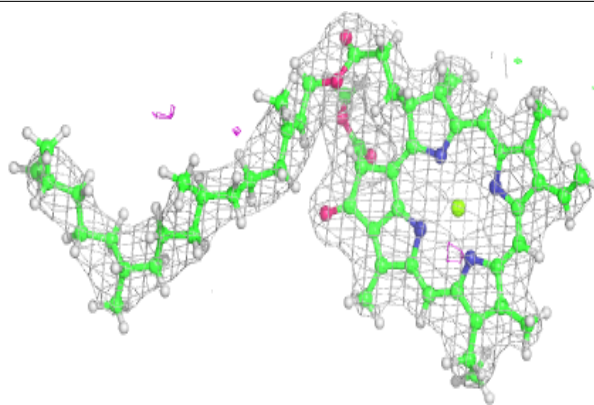
Electron density around CLA c 507:

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

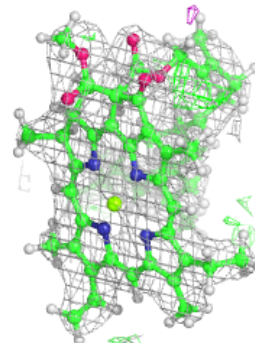
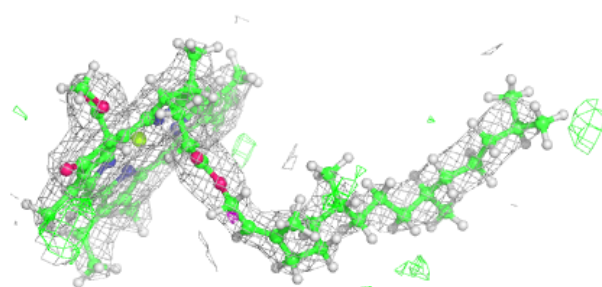
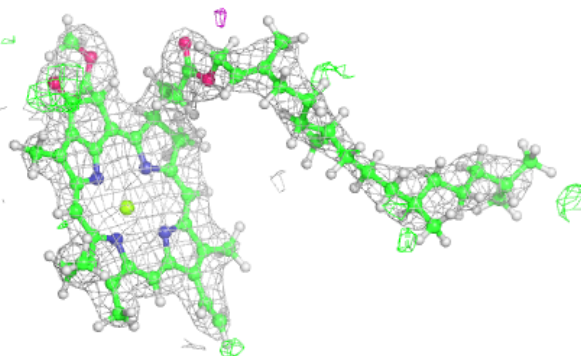


Electron density around CLA b 601:

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

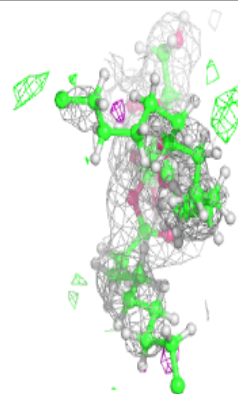
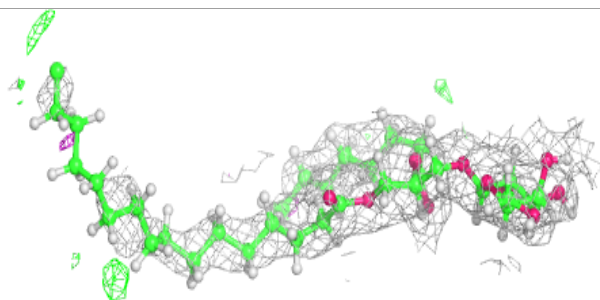
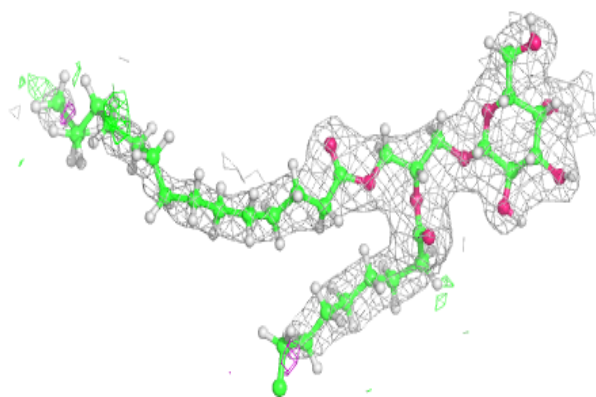
**Electron density around CLA c 511:**

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



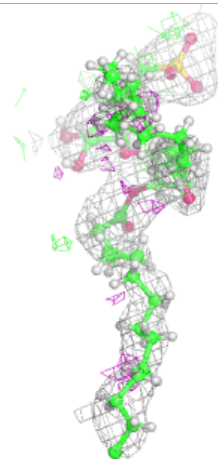
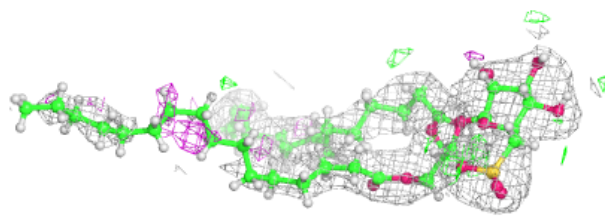
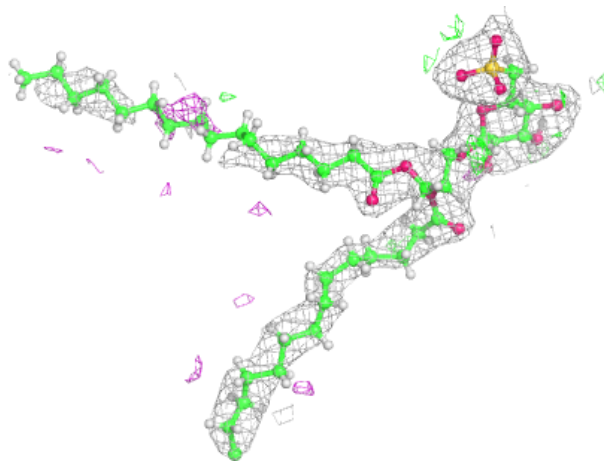
Electron density around LMG d 409:

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



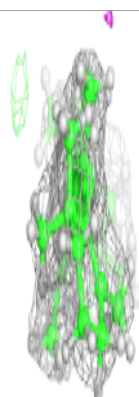
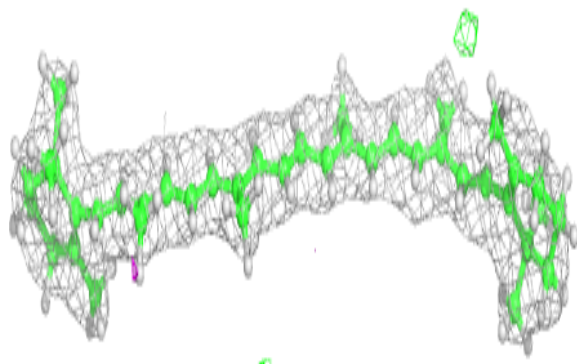
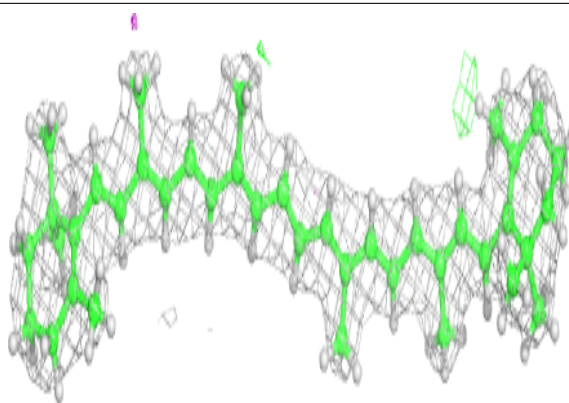
Electron density around SQD A 412:

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



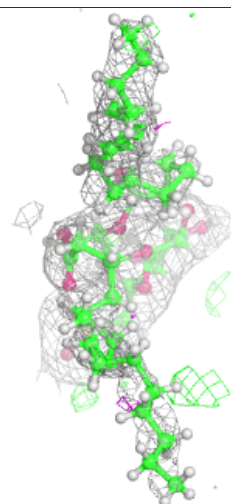
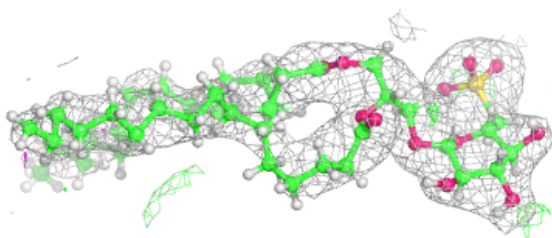
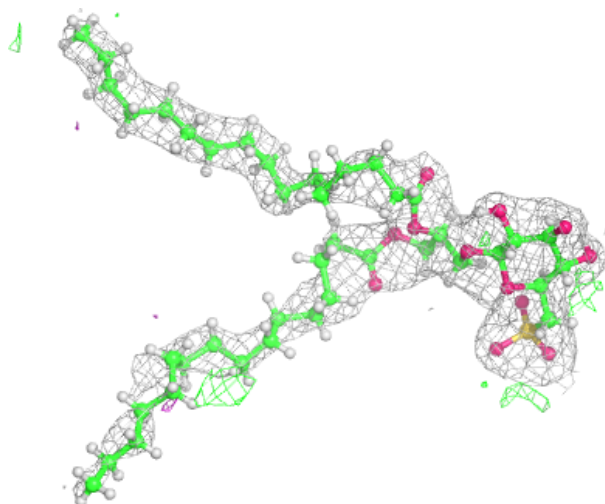
Electron density around BCR b 618:

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



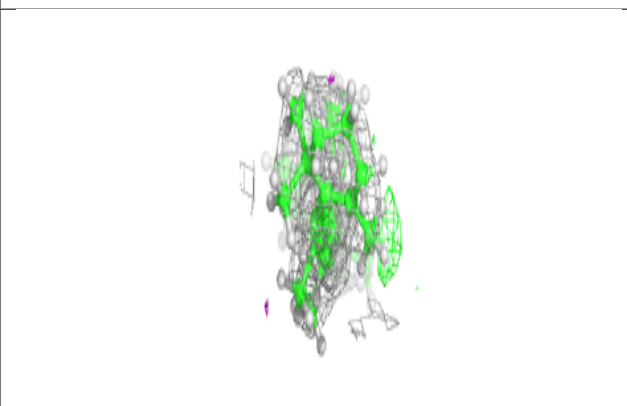
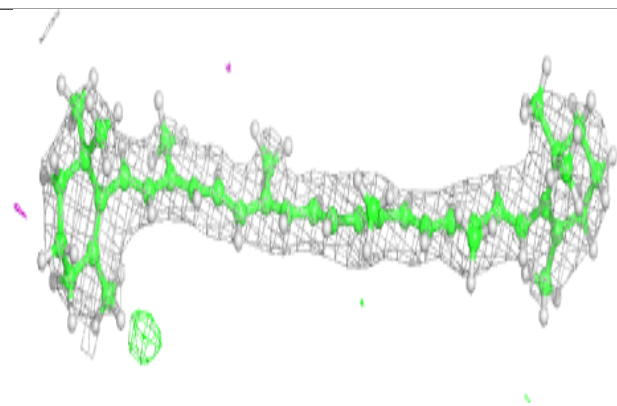
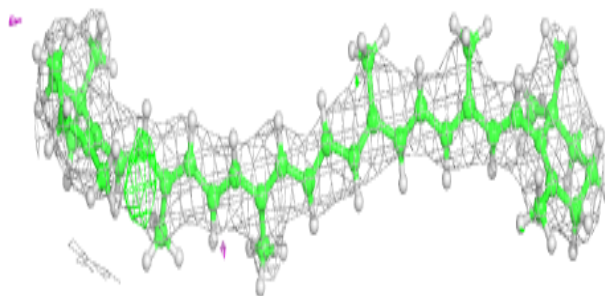
Electron density around SQD a 412:

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

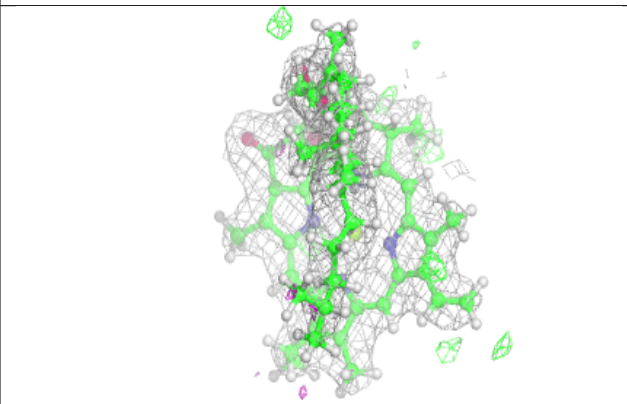
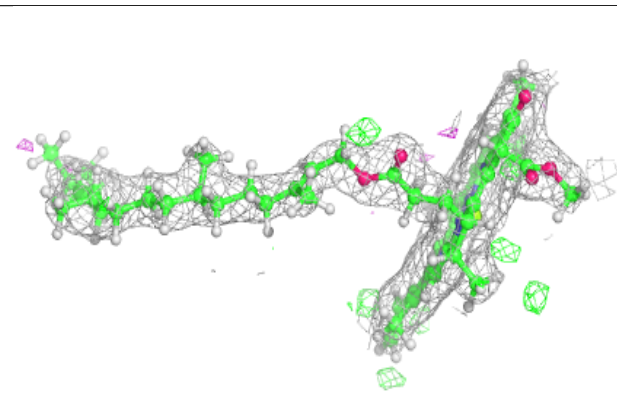
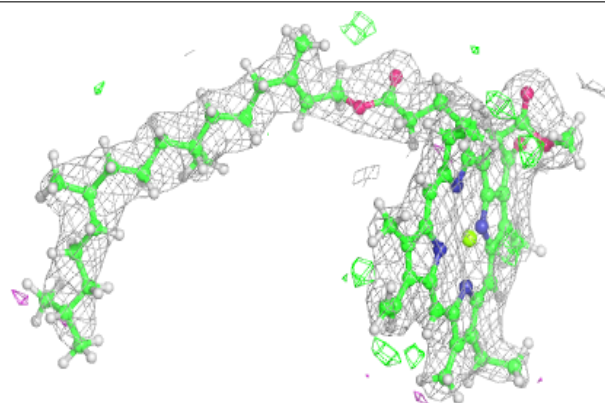


Electron density around BCR c 514:

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

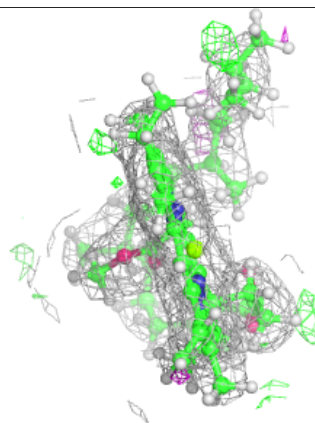
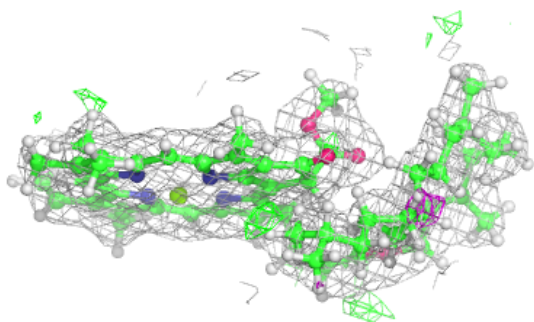
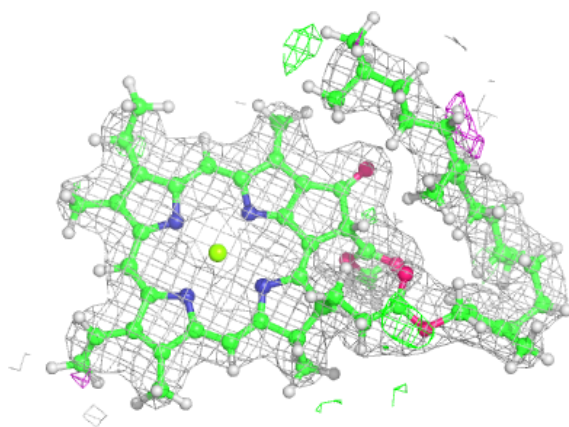
**Electron density around CLA b 608:**

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

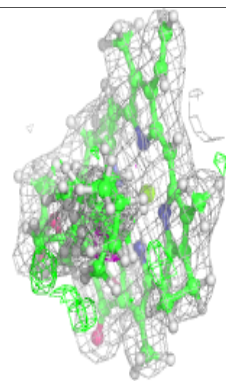
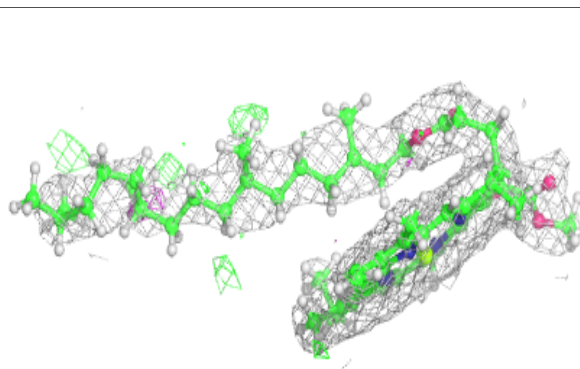
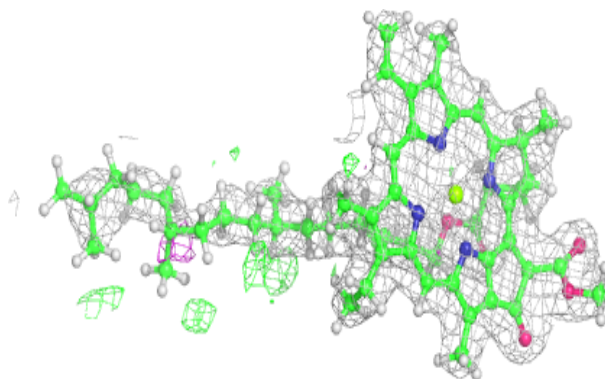


Electron density around CLA b 609:

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

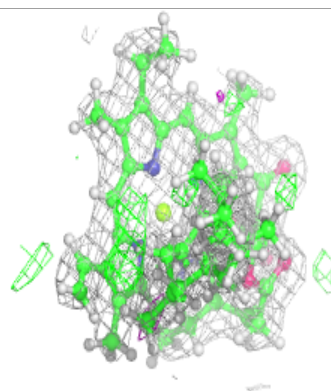
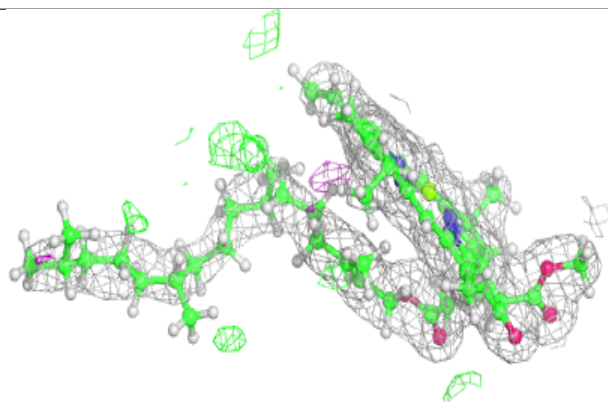
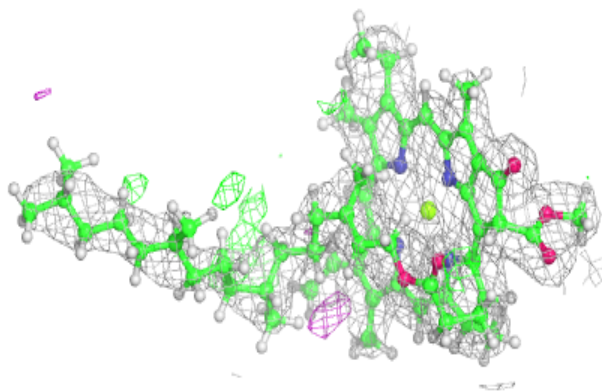
**Electron density around CLA B 614:**

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



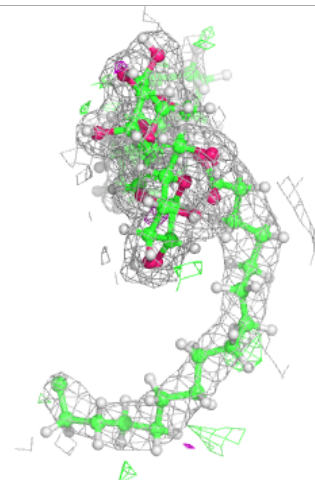
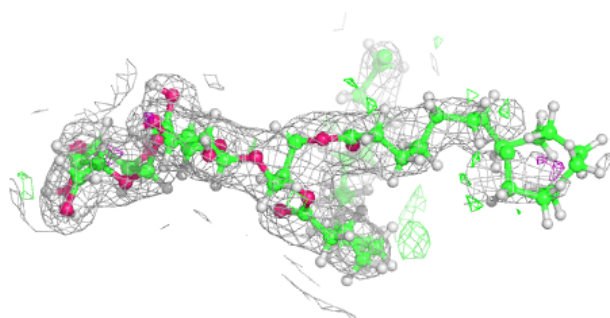
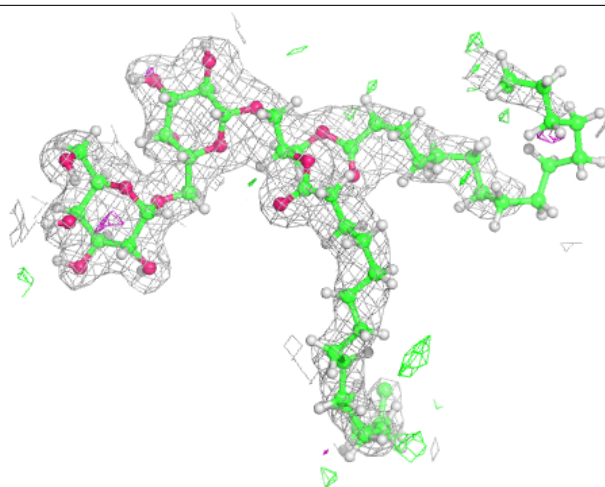
Electron density around CLA C 505:

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



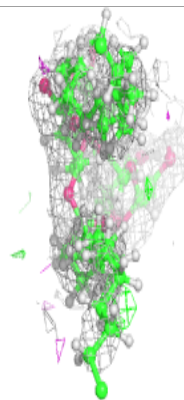
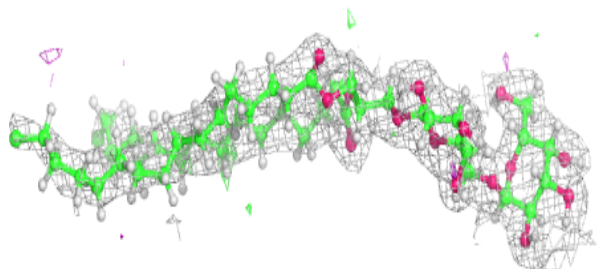
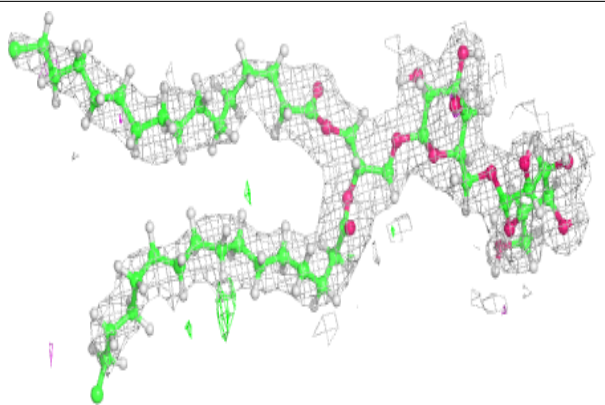
Electron density around DGD C 522:

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

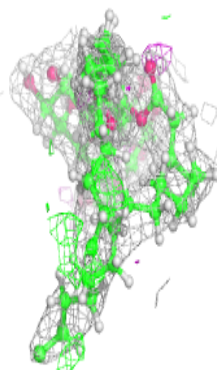
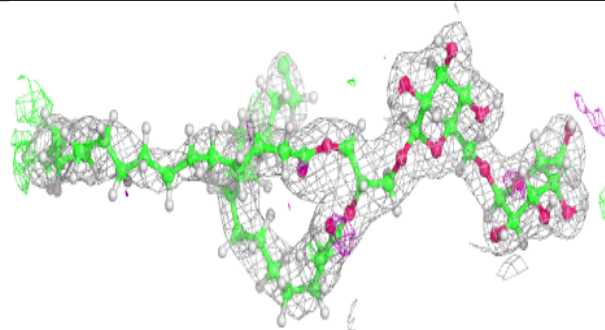
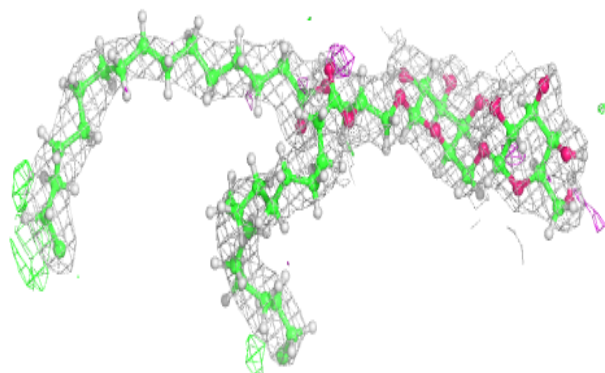


Electron density around DGD C 523:

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

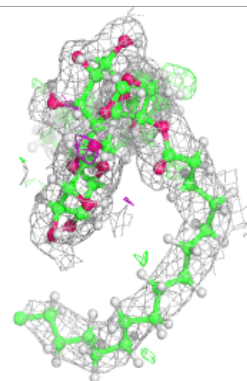
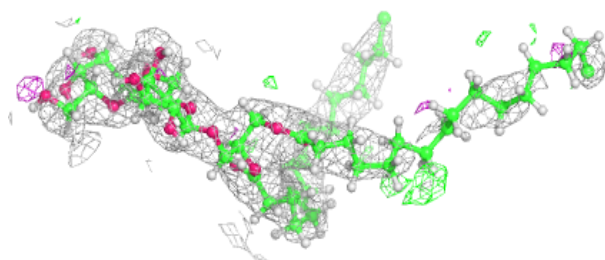
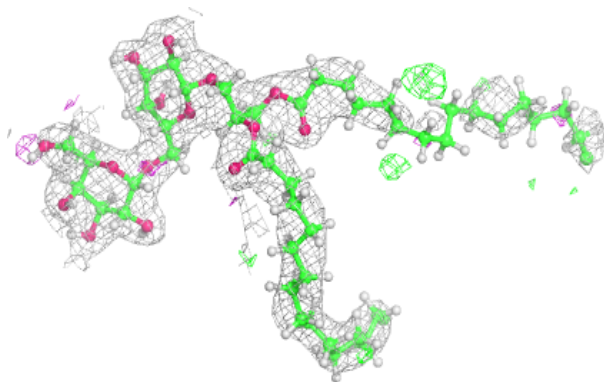
**Electron density around DGD H 102:**

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

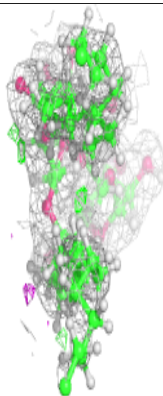
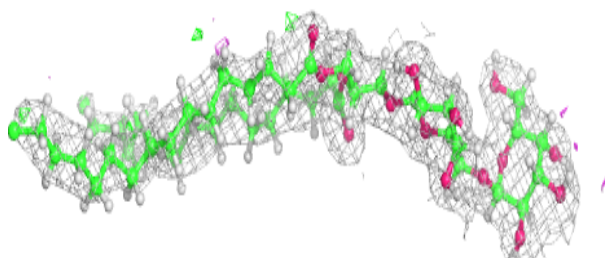
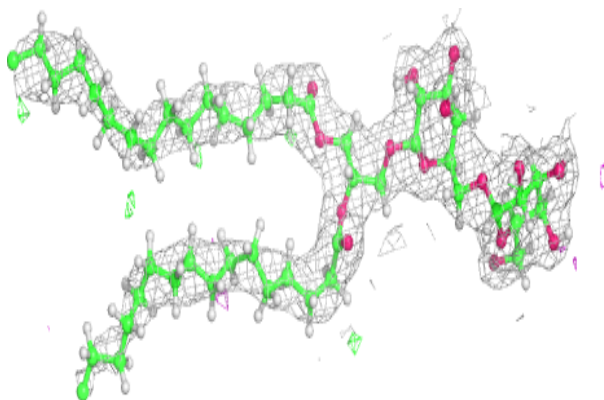


Electron density around DGD c 520:

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

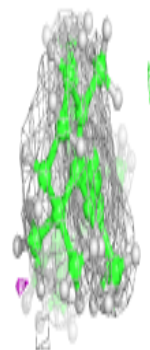
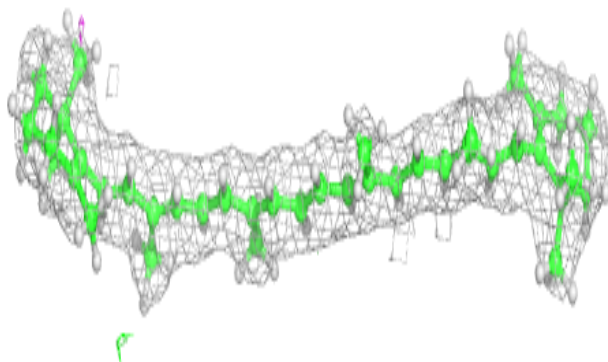
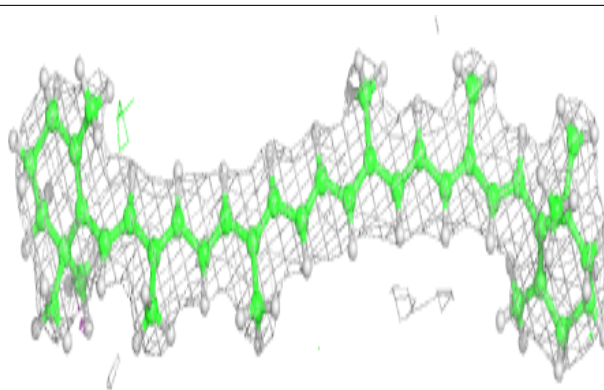
**Electron density around DGD c 521:**

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



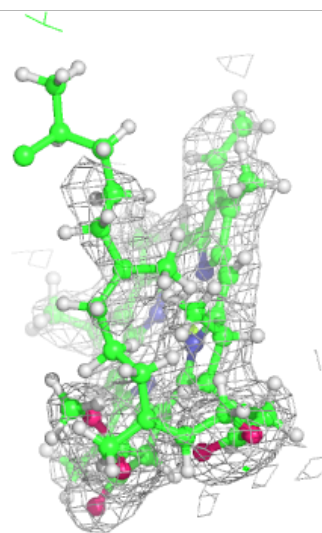
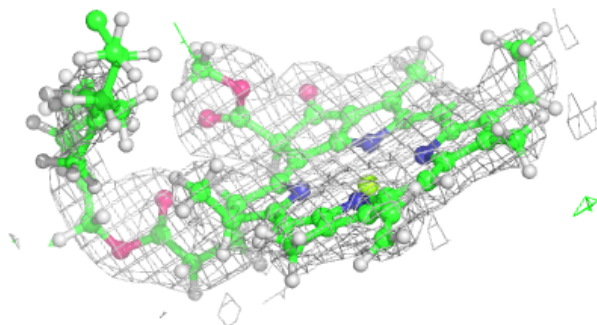
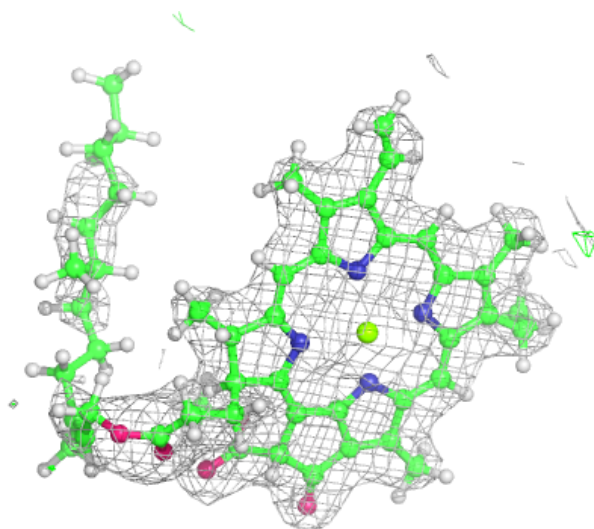
Electron density around BCR B 619:

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



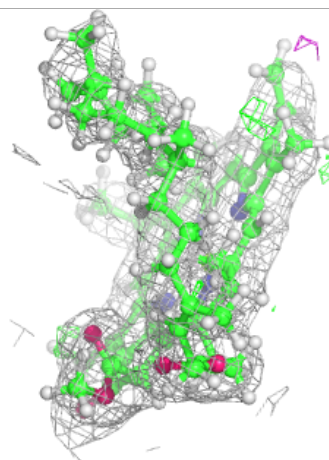
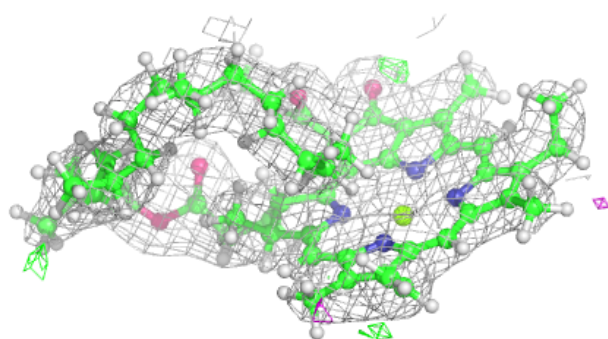
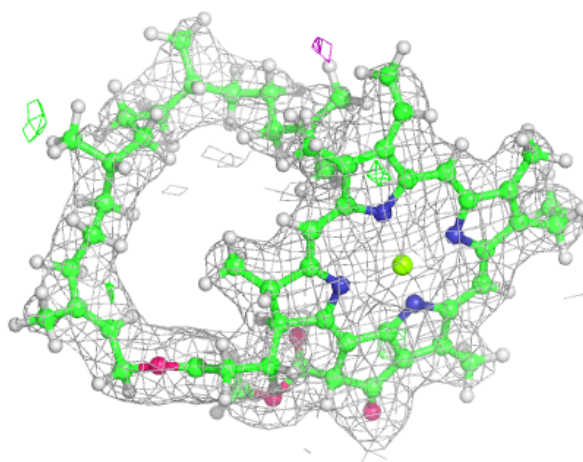
Electron density around CLA B 616:

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



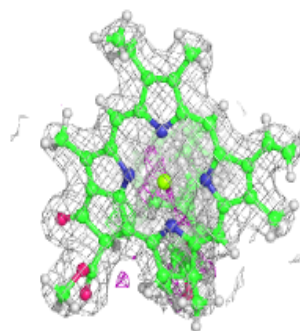
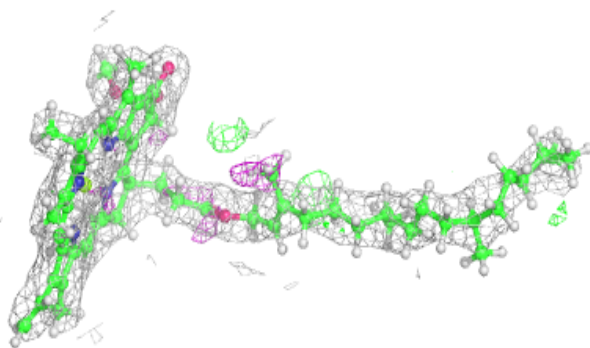
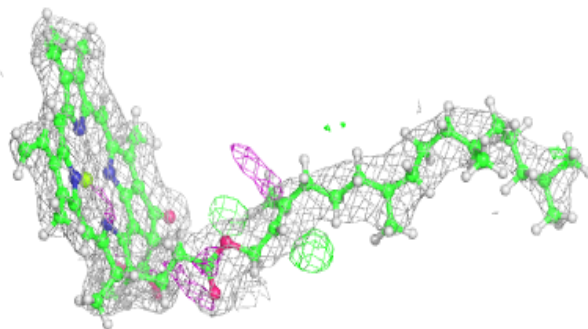
Electron density around CLA B 615:

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



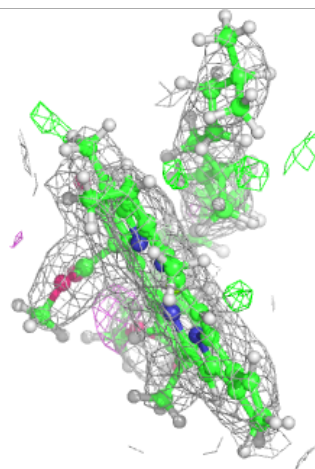
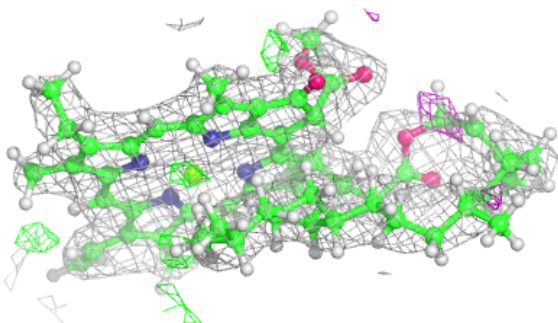
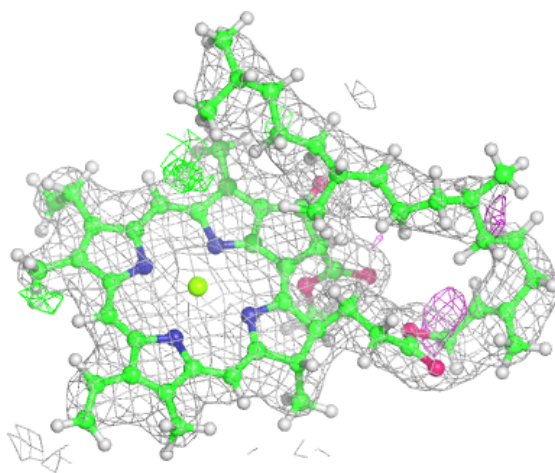
Electron density around CLA B 604:

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



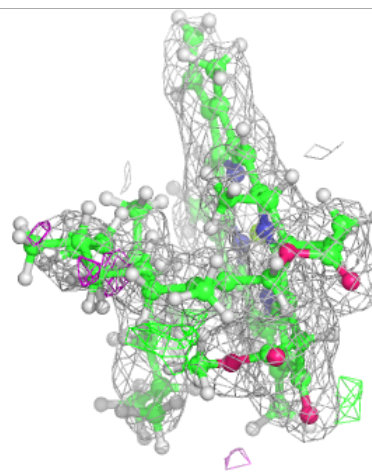
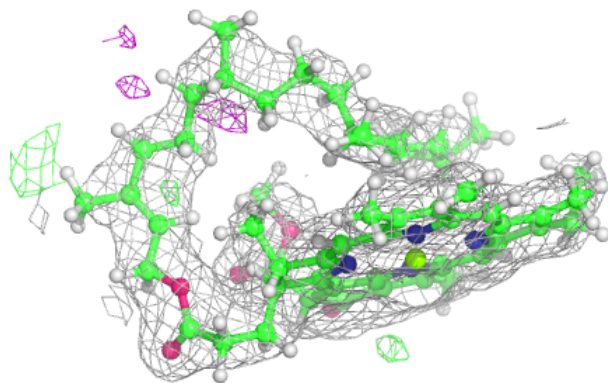
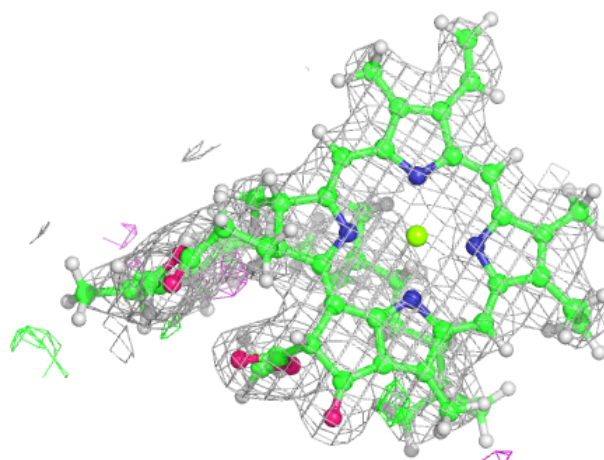
Electron density around CLA c 509:

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



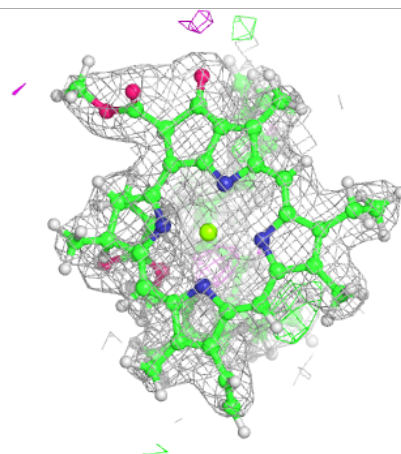
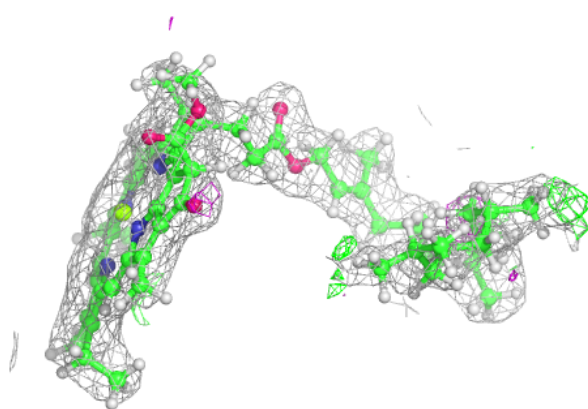
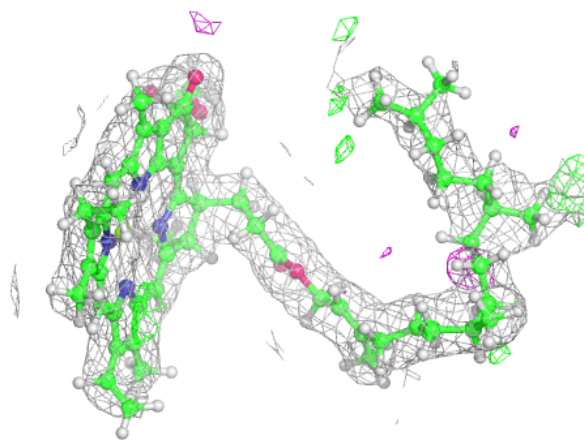
Electron density around CLA c 510:

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



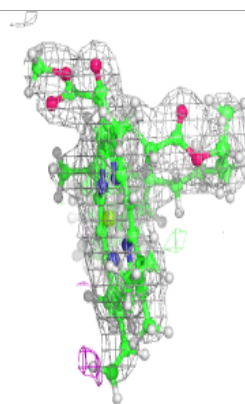
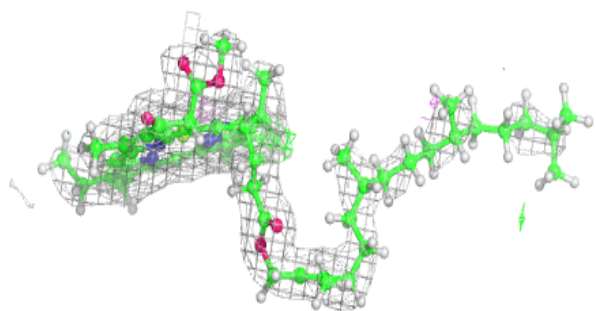
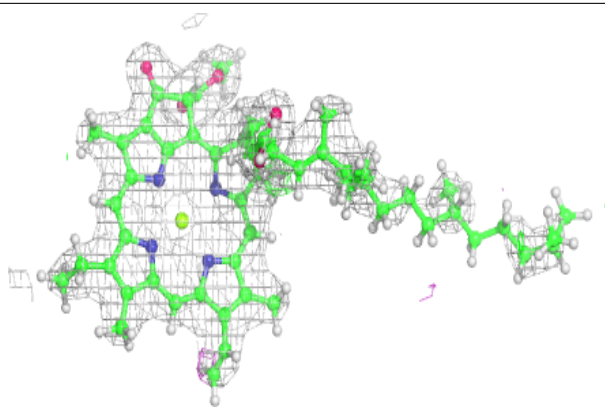
Electron density around CLA B 606:

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



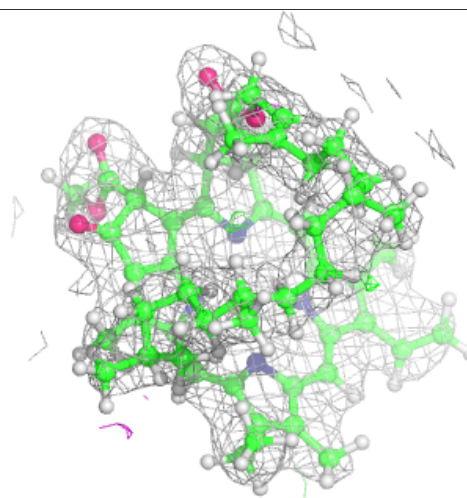
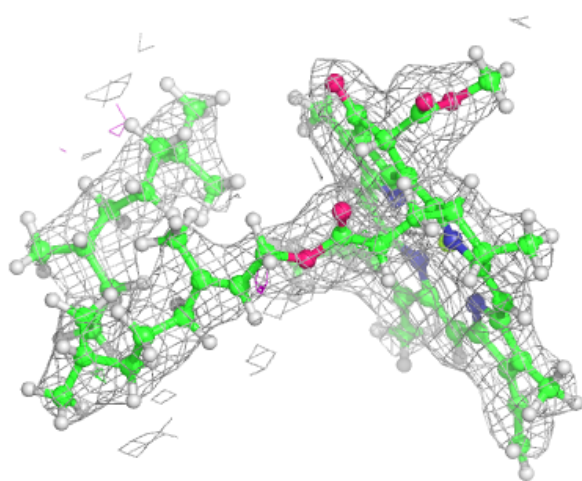
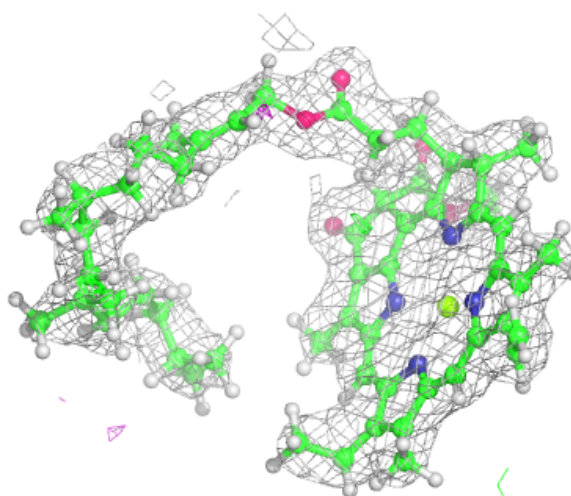
Electron density around CLA a 406:

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



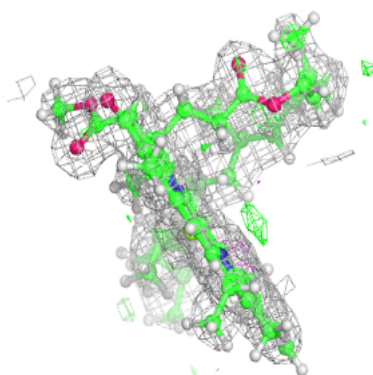
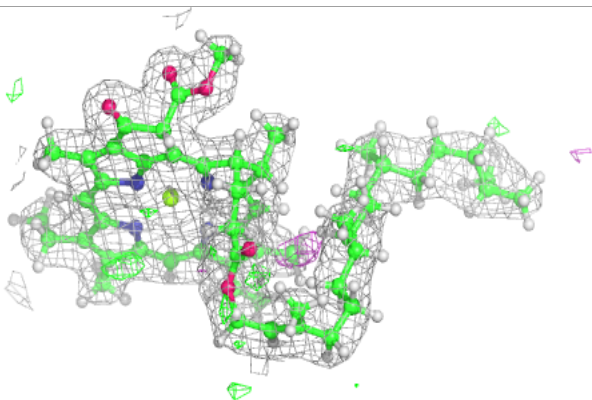
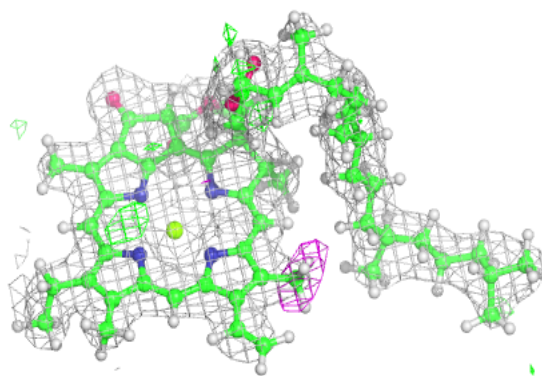
Electron density around CLA C 503:

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

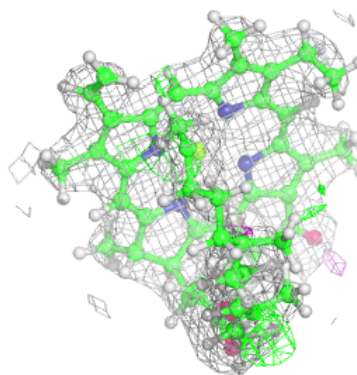
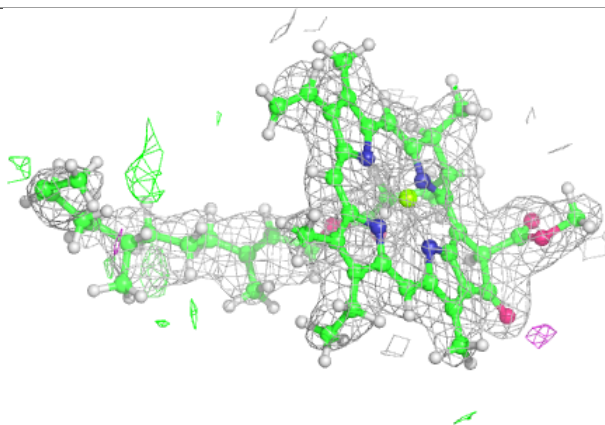
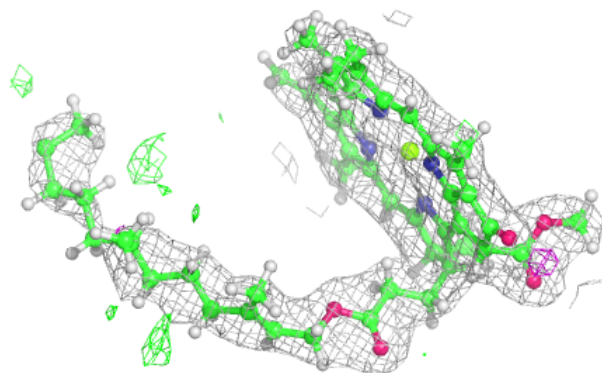


Electron density around CLA a 411:

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

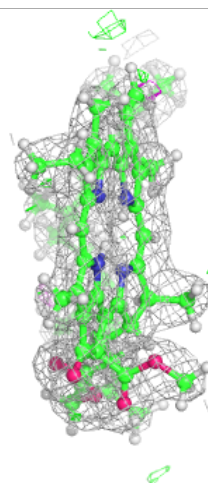
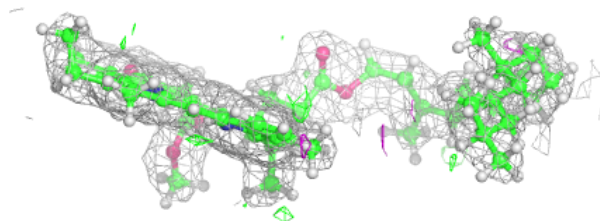
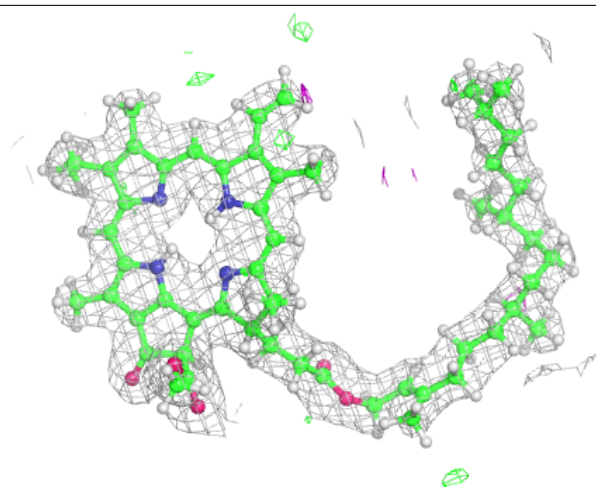
**Electron density around CLA C 504:**

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



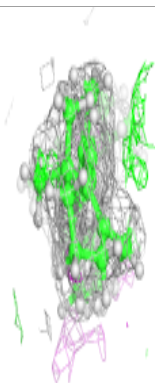
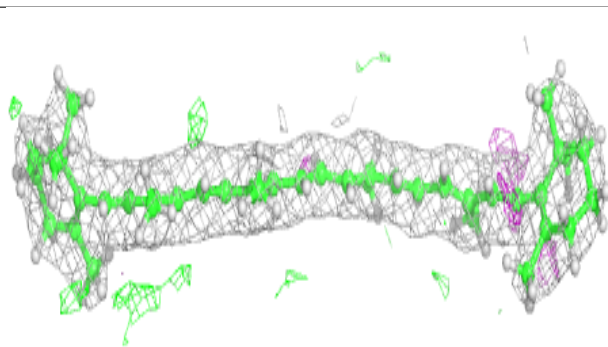
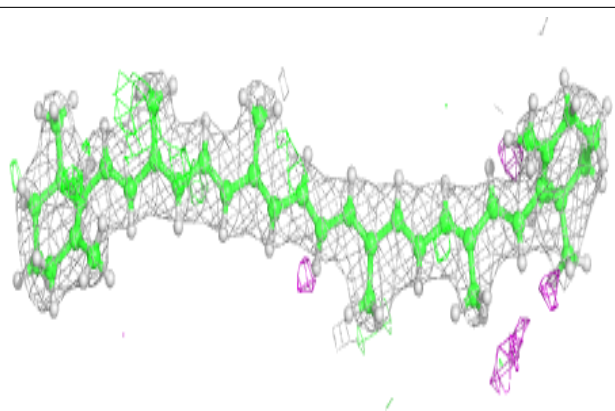
Electron density around PHO a 407:

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

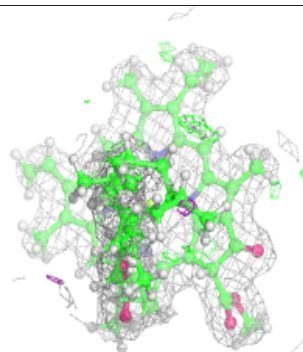
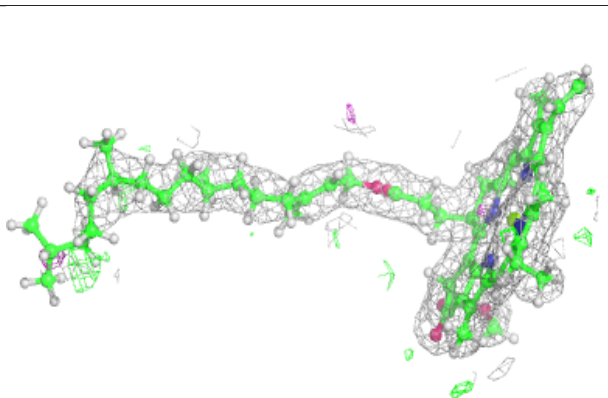
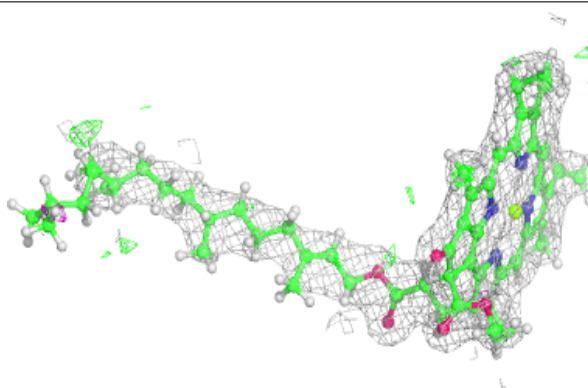


Electron density around BCR B 618:

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

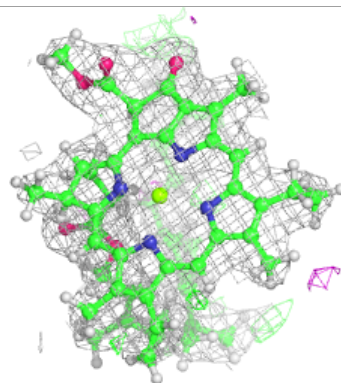
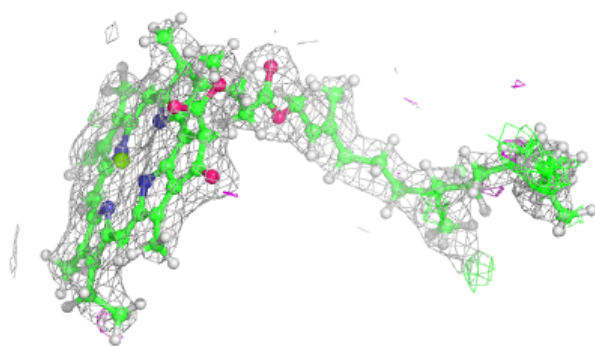
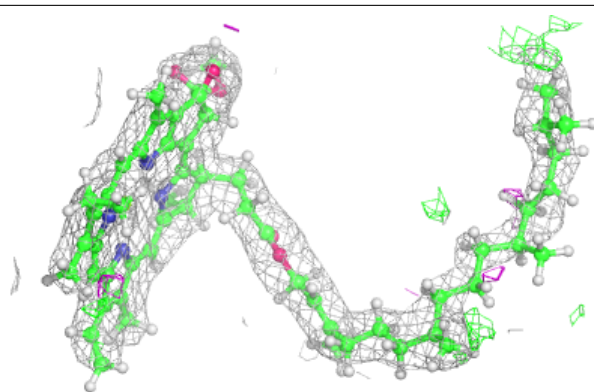
**Electron density around CLA b 603:**

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

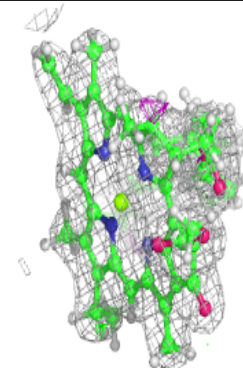
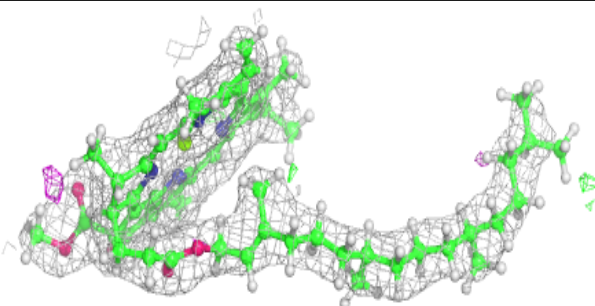
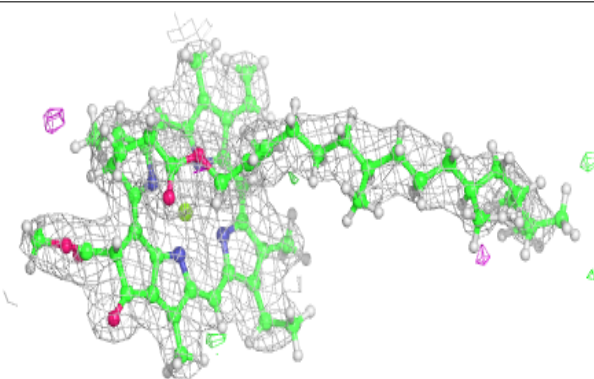


Electron density around CLA b 605:

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

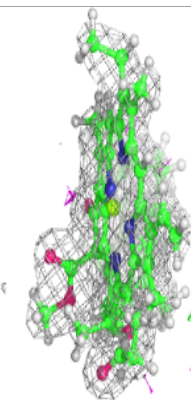
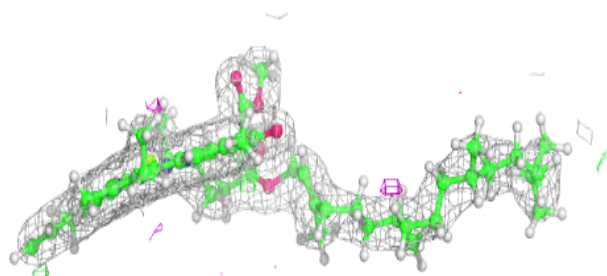
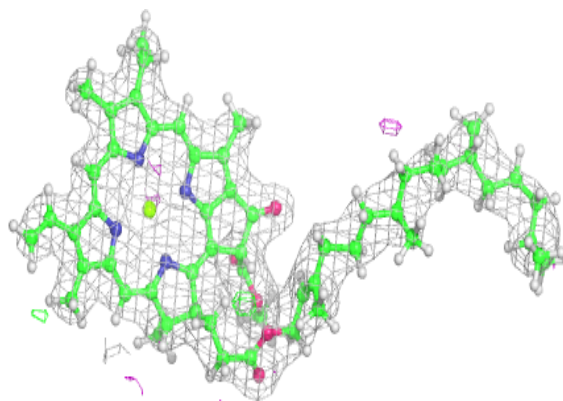
**Electron density around CLA b 607:**

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

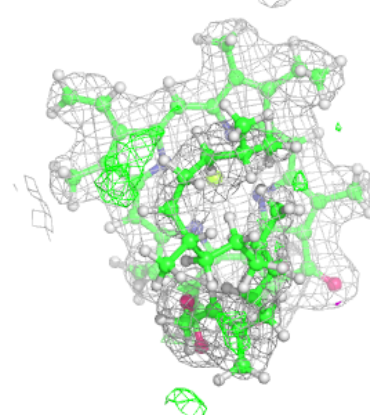
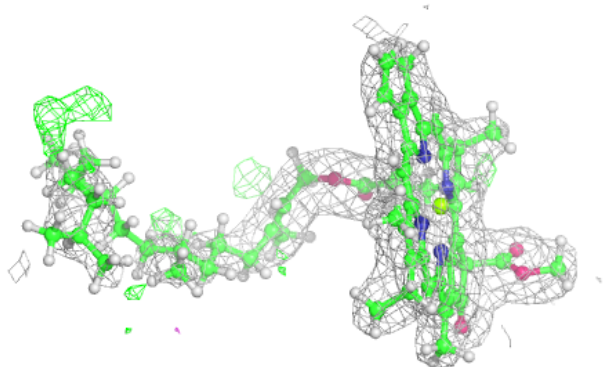
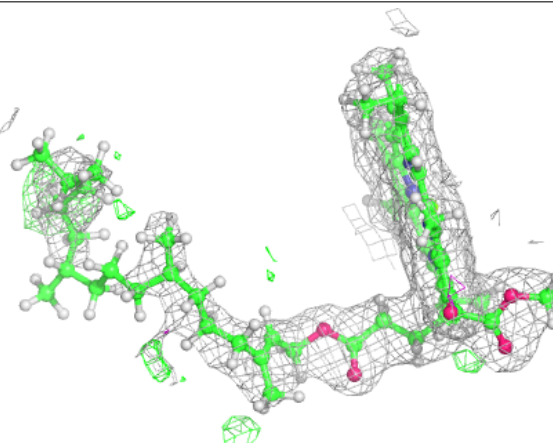


Electron density around CLA B 602:

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

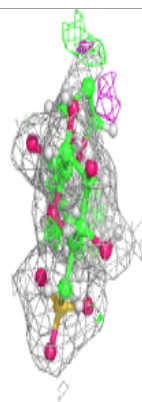
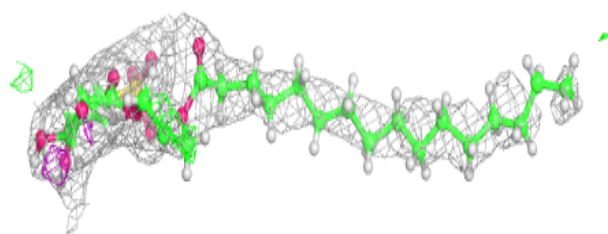
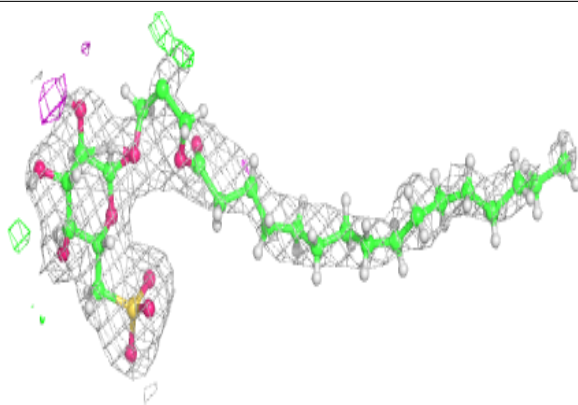
**Electron density around CLA C 506:**

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

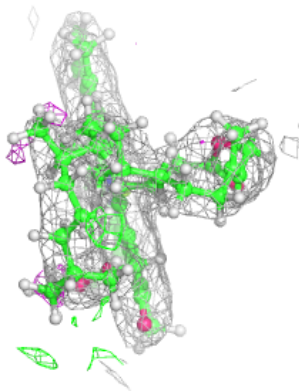
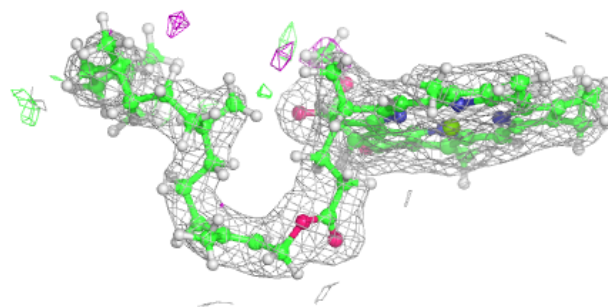
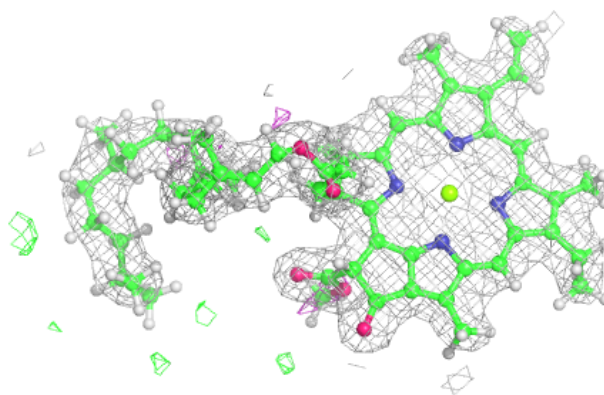


Electron density around SQD F 102:

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

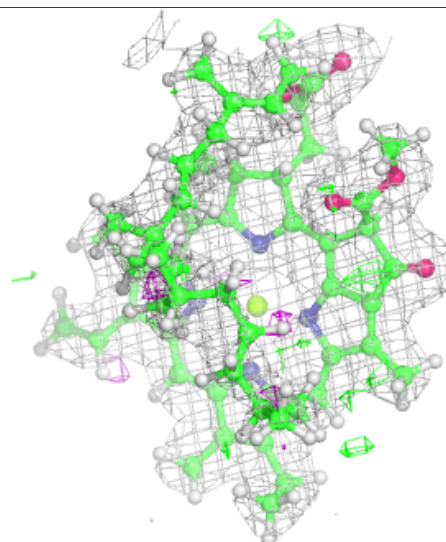
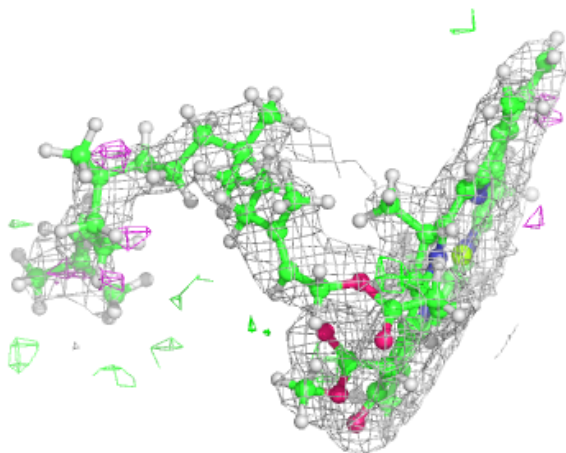
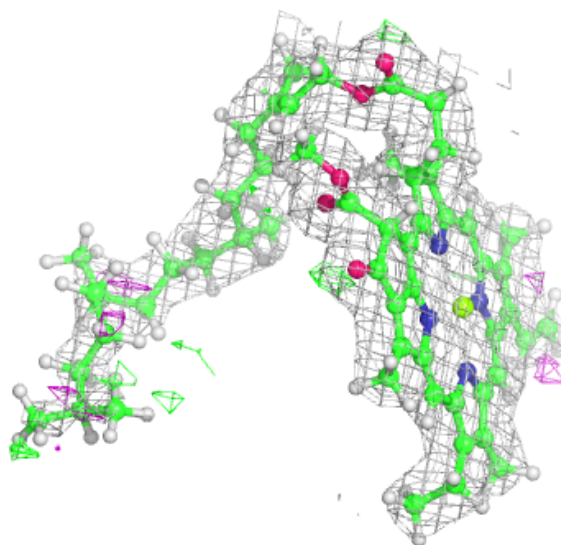
**Electron density around CLA b 611:**

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



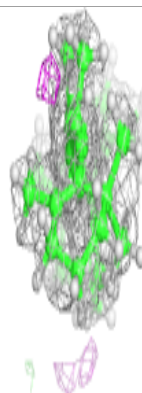
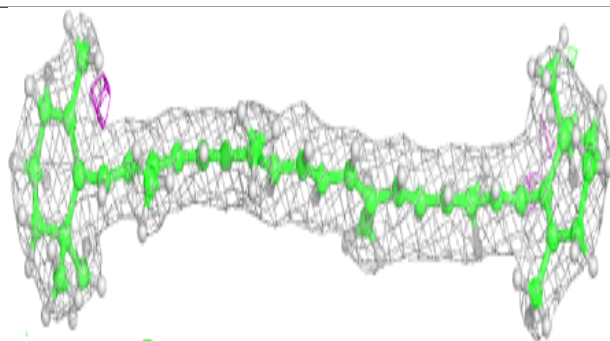
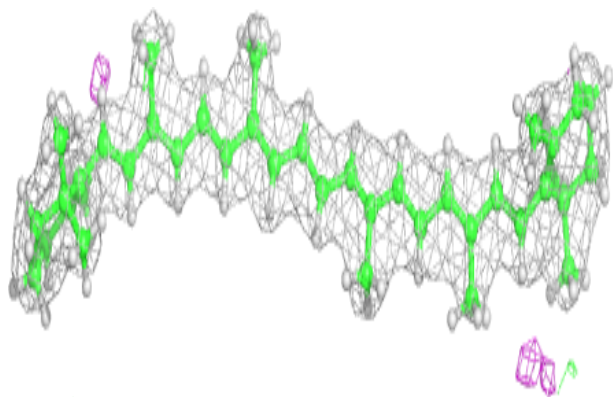
Electron density around CLA b 612:

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

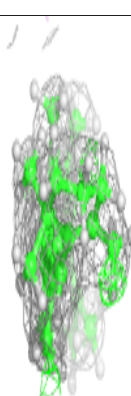
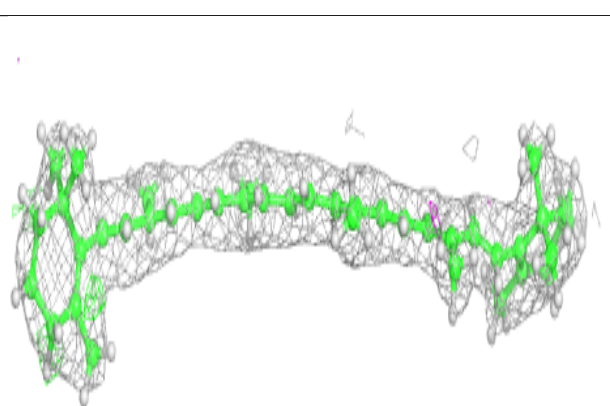
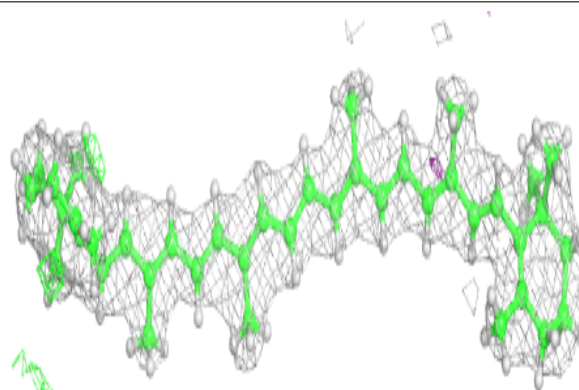


Electron density around BCR a 409:

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

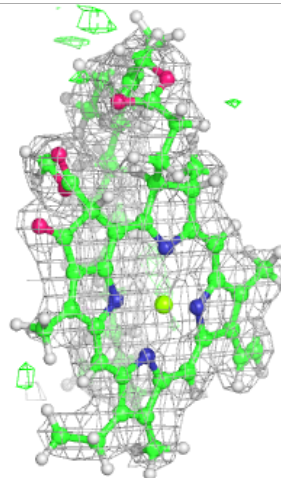
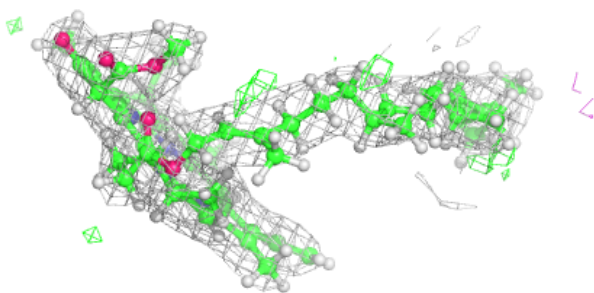
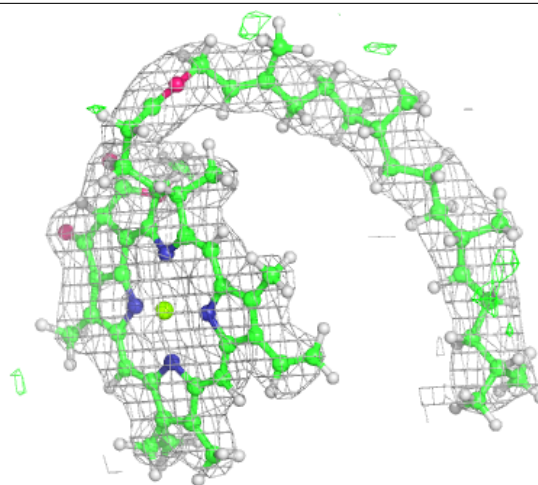
**Electron density around BCR b 616:**

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



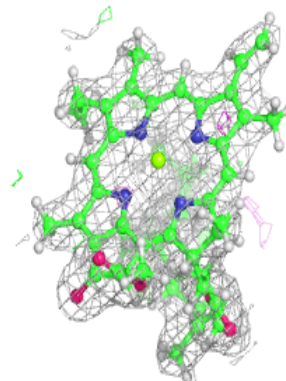
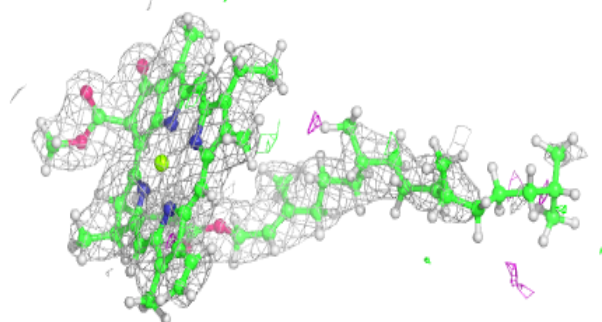
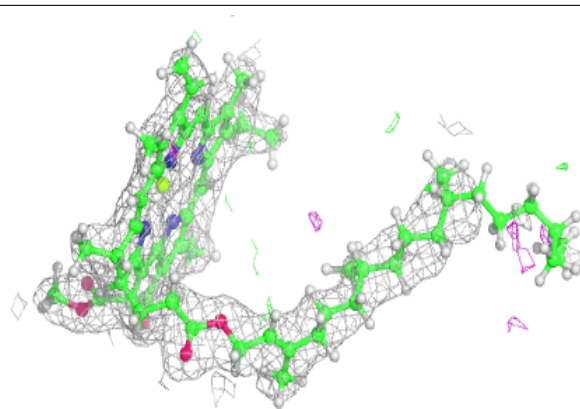
Electron density around CLA C 507:

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

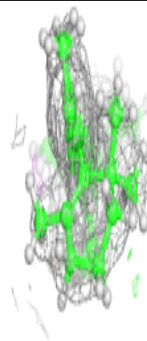
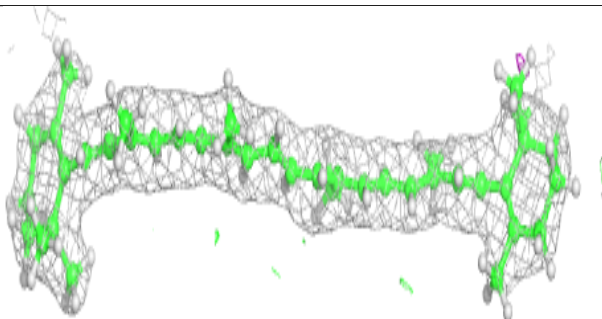
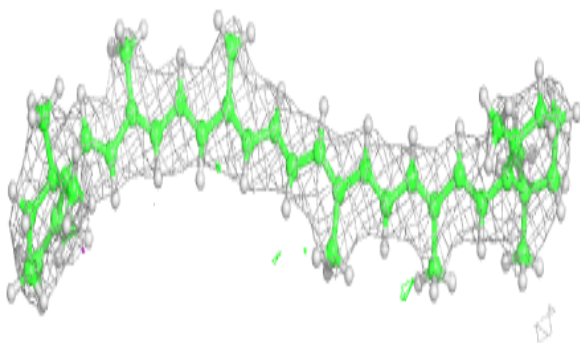


Electron density around CLA C 508:

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

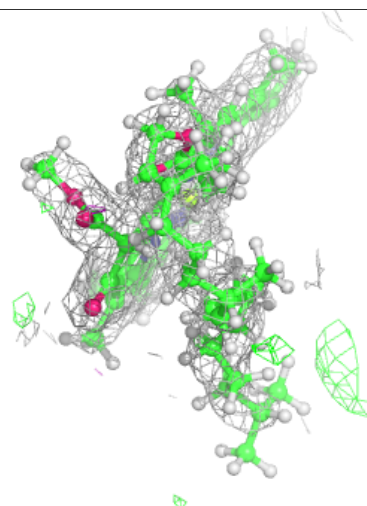
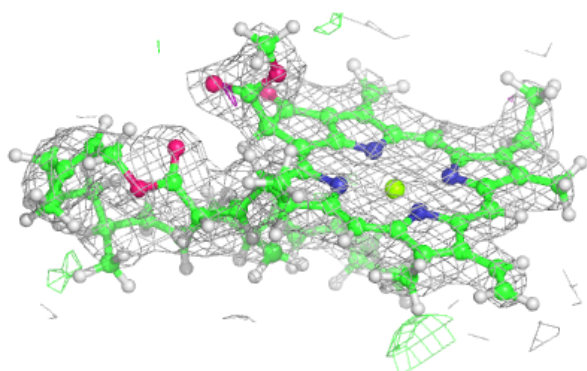
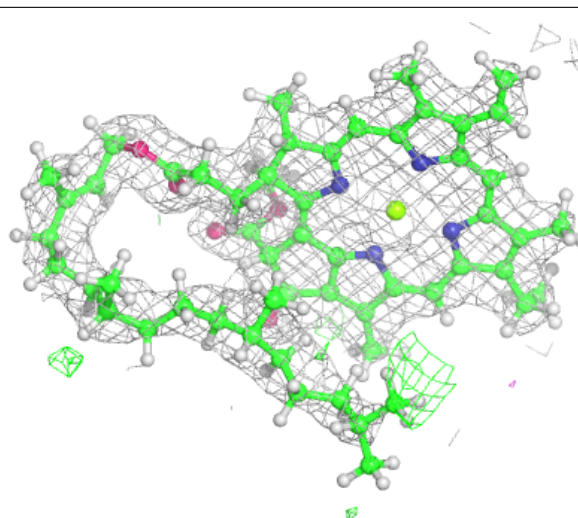
**Electron density around BCR c 515:**

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



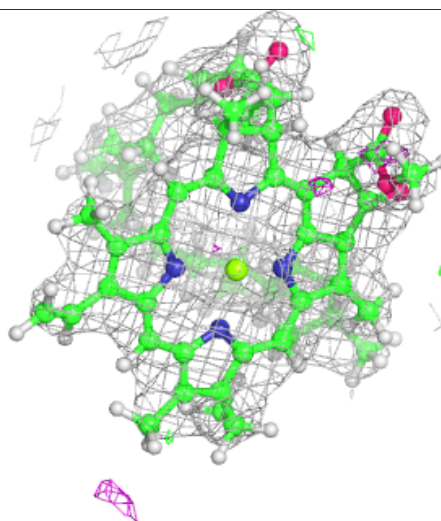
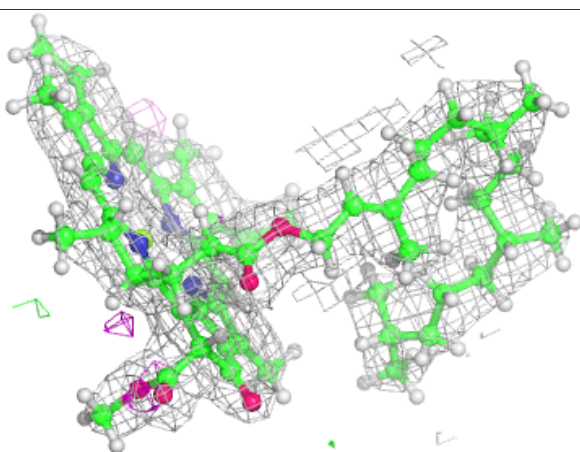
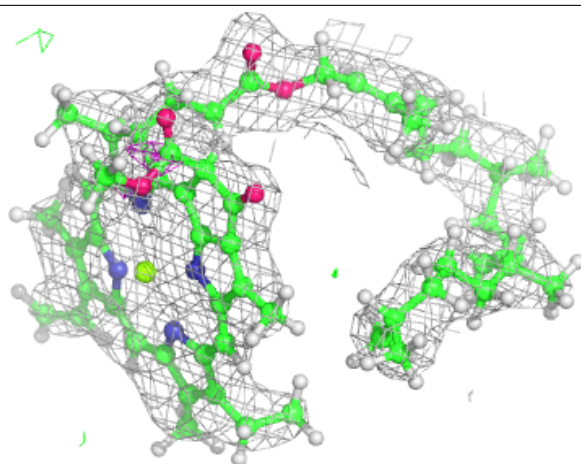
Electron density around CLA C 509:

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



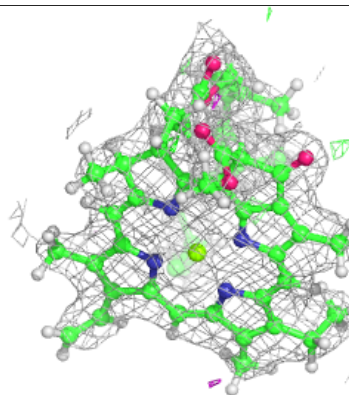
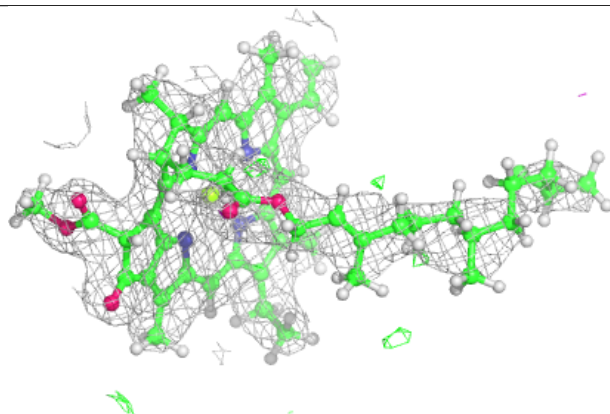
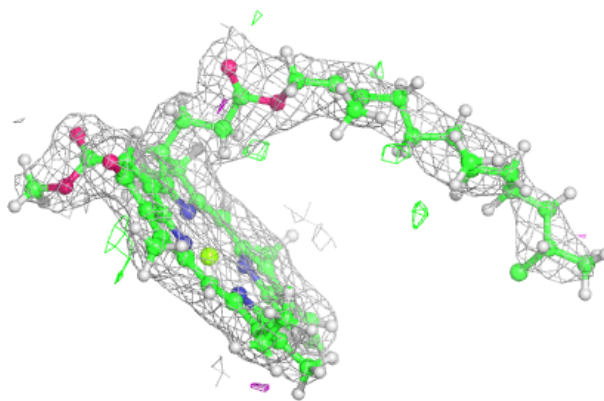
Electron density around CLA c 503:

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

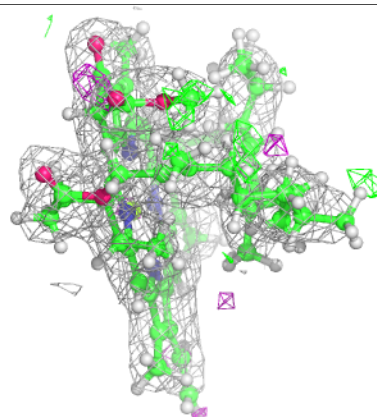
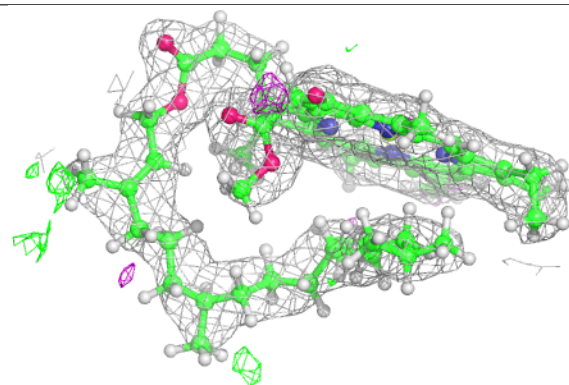
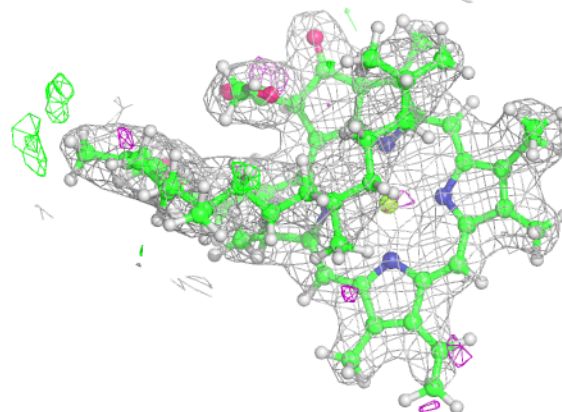


Electron density around CLA c 504:

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

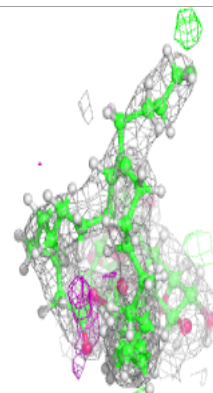
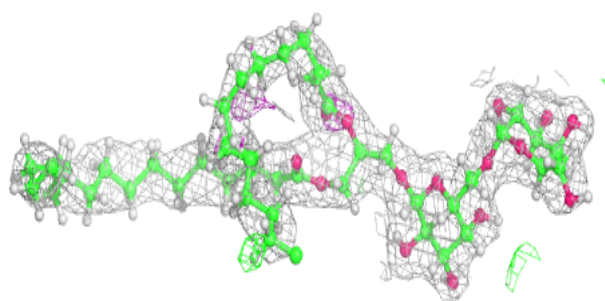
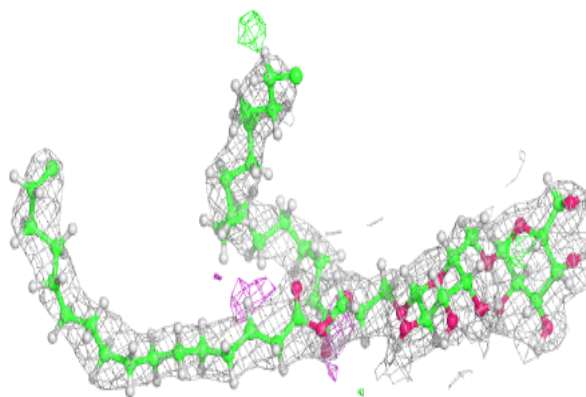
**Electron density around CLA C 510:**

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

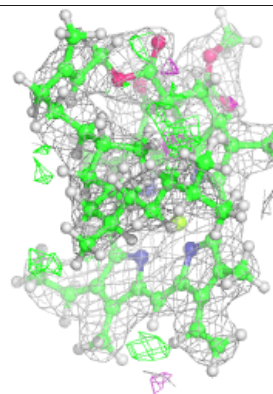
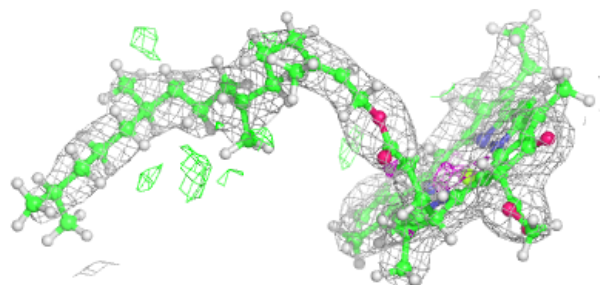
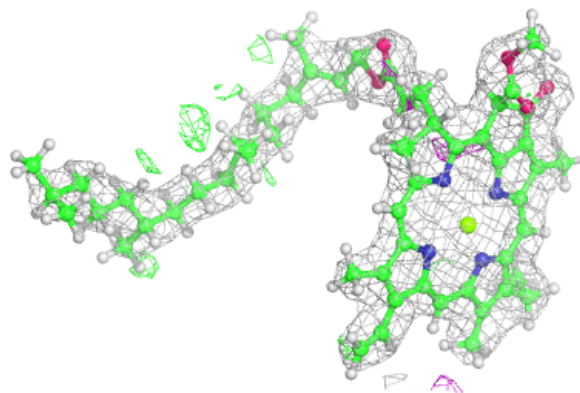


Electron density around DGD h 102:

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

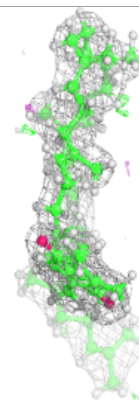
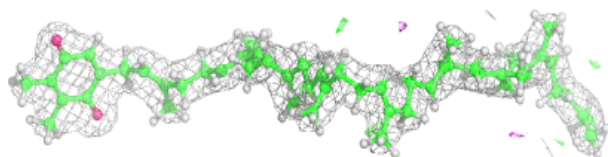
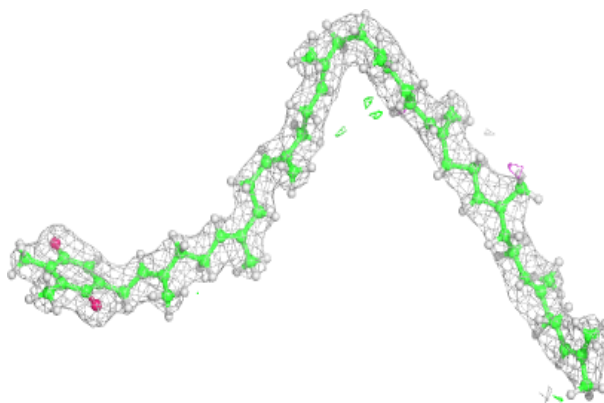
**Electron density around CLA C 511:**

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

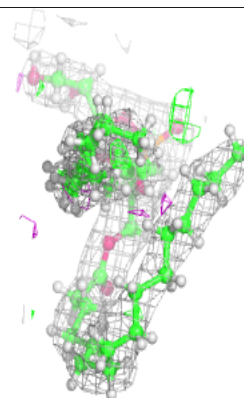
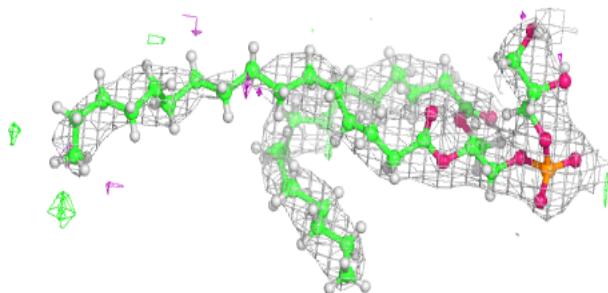
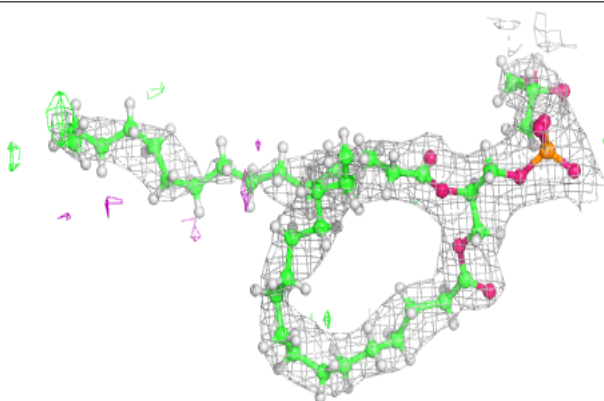


Electron density around PL9 D 407:

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

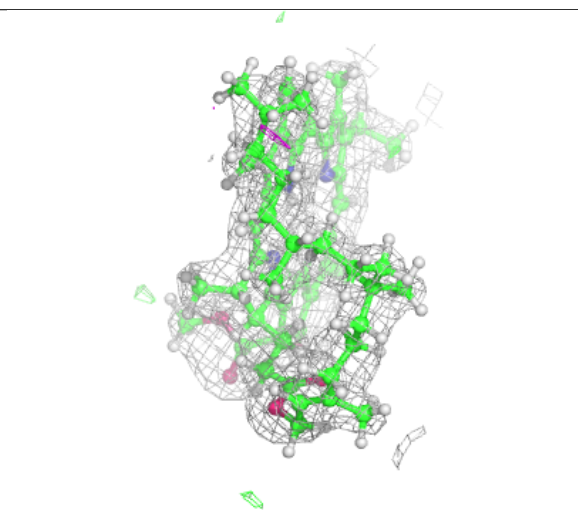
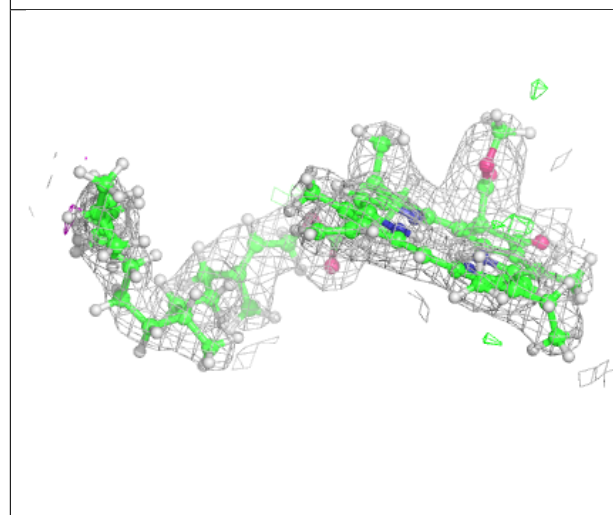
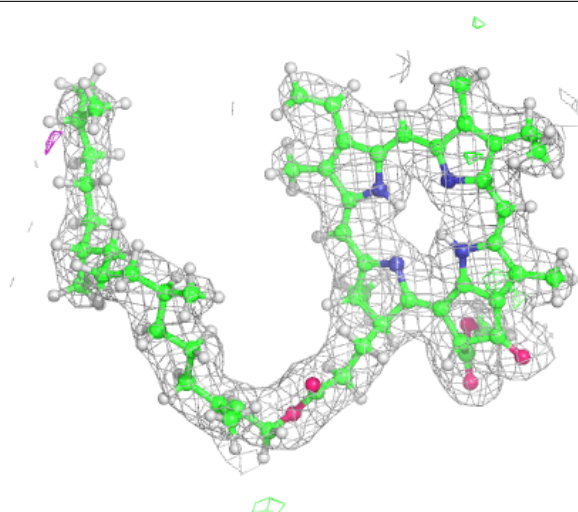
**Electron density around LHG d 406:**

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



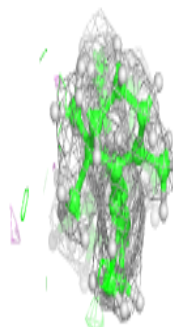
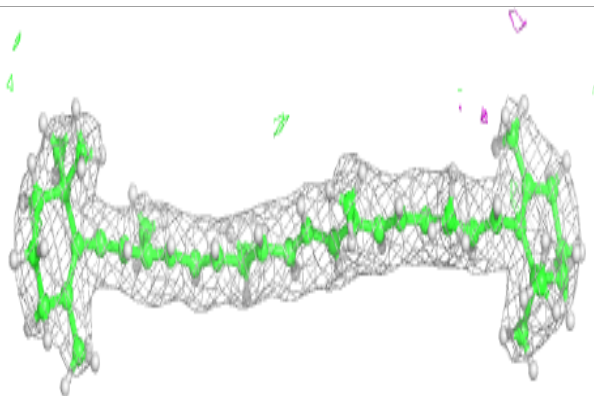
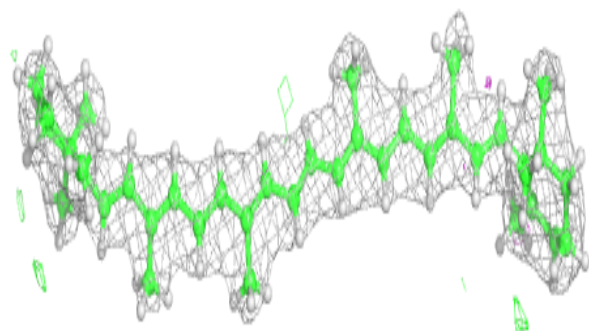
Electron density around PHO d 401:

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

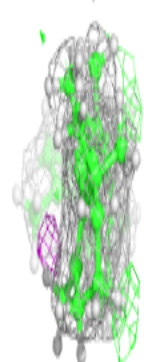
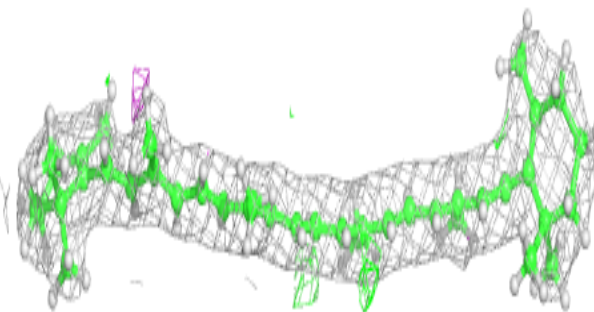
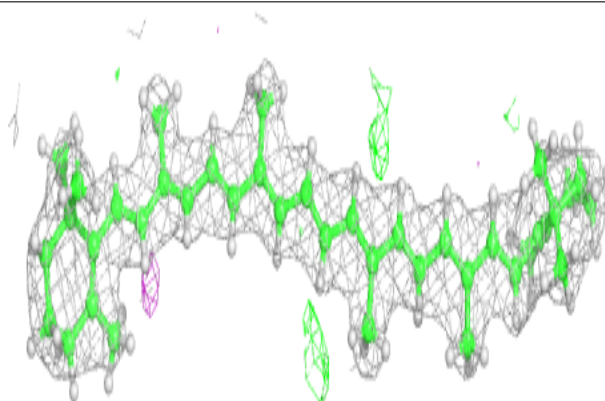


Electron density around BCR A 408:

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

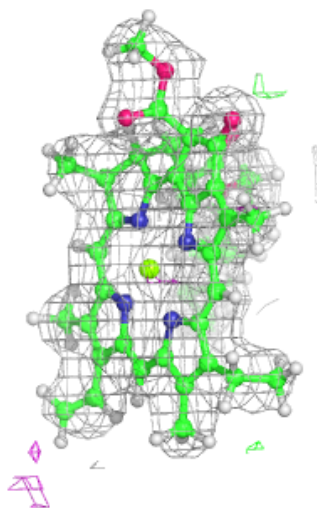
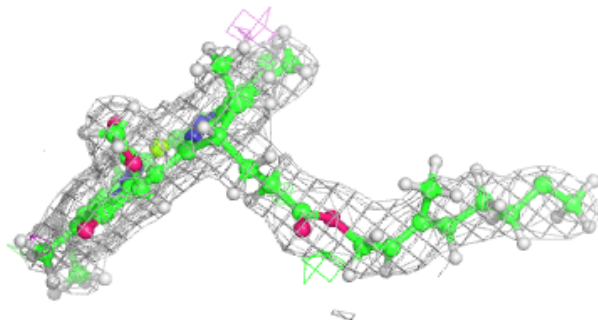
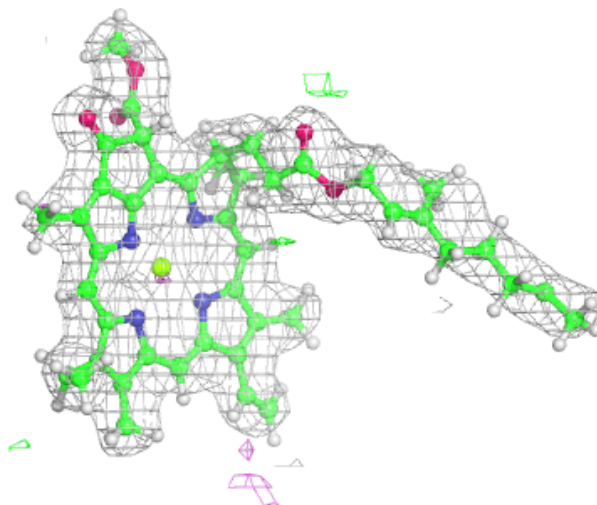
**Electron density around BCR B 617:**

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



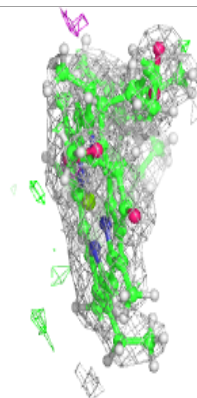
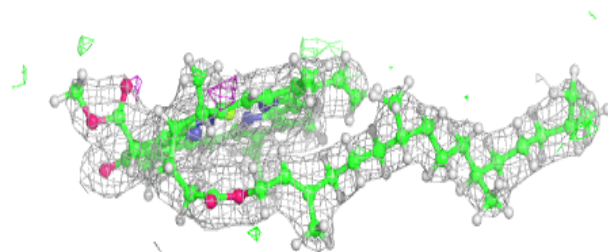
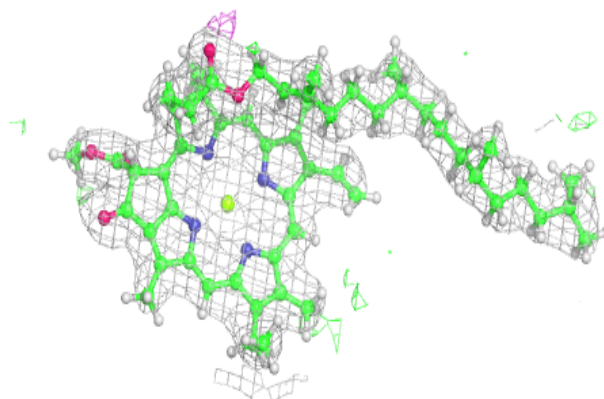
Electron density around CLA A 407:

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

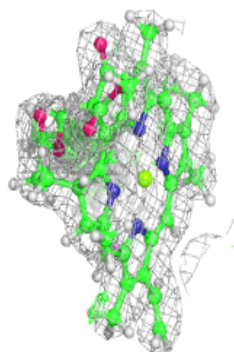
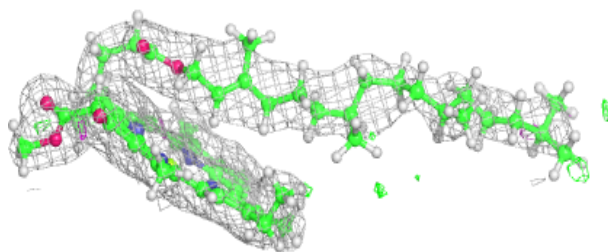
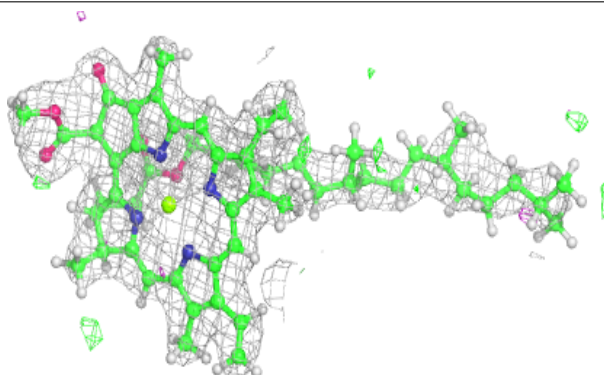


Electron density around CLA C 501:

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

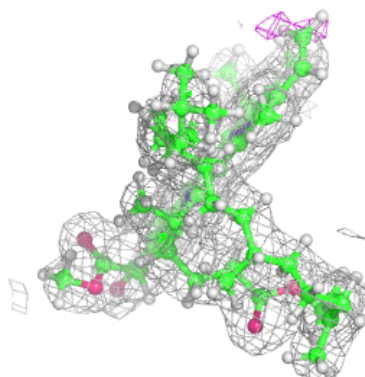
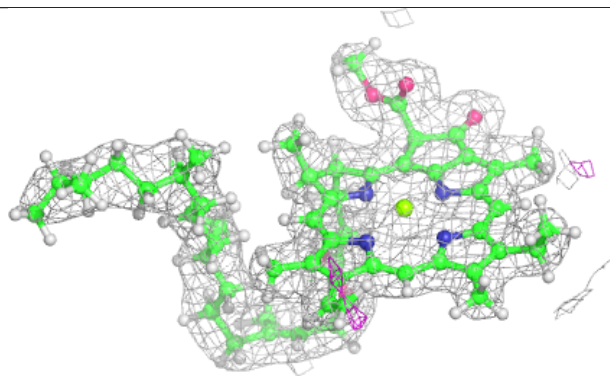
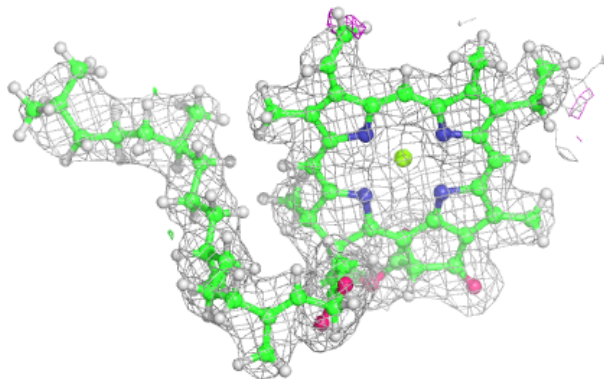
**Electron density around CLA b 613:**

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

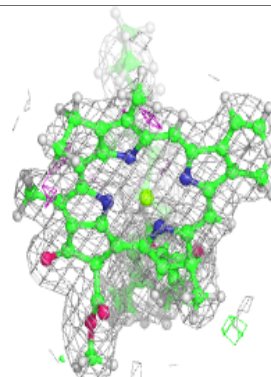
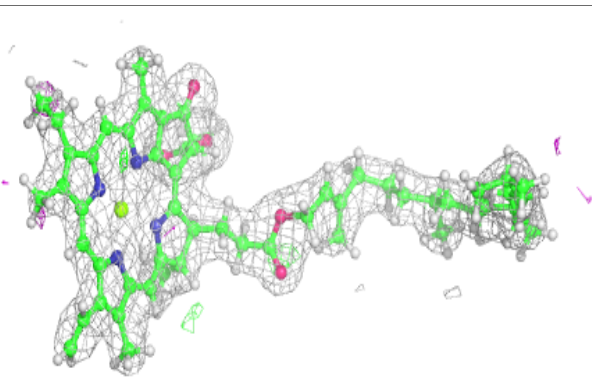
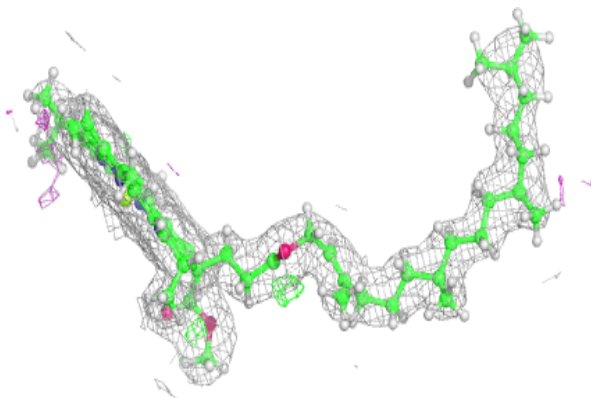


Electron density around CLA D 403:

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

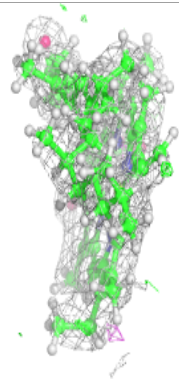
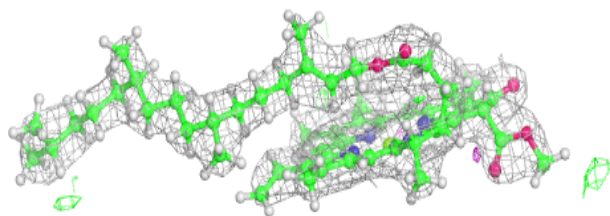
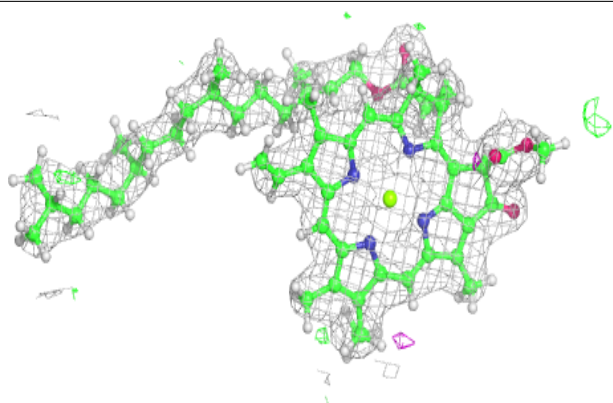
**Electron density around CLA D 404:**

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

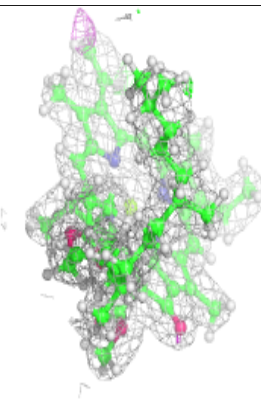
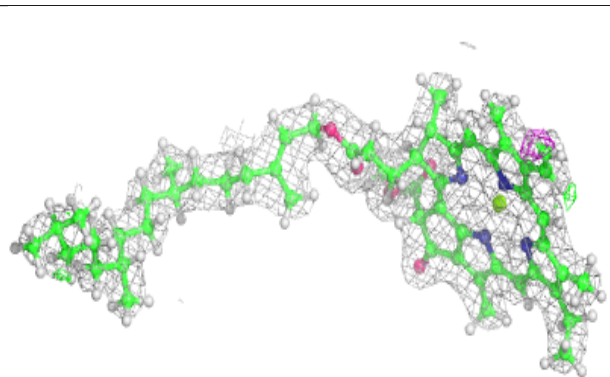
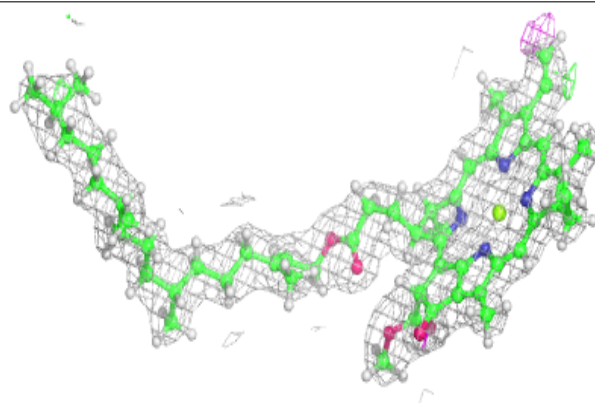


Electron density around CLA c 501:

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

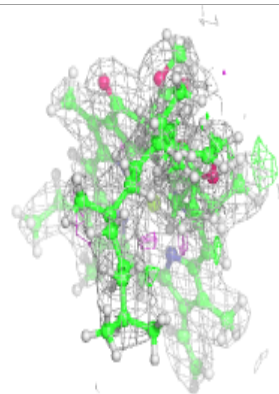
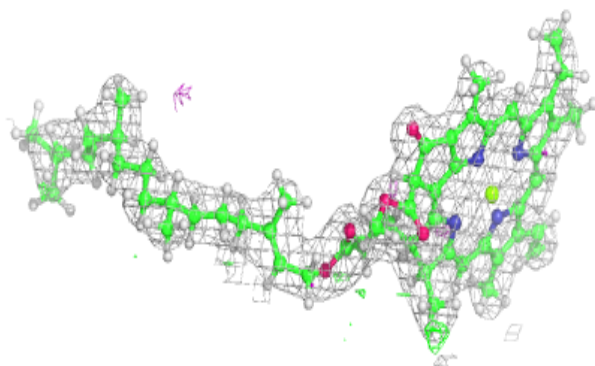
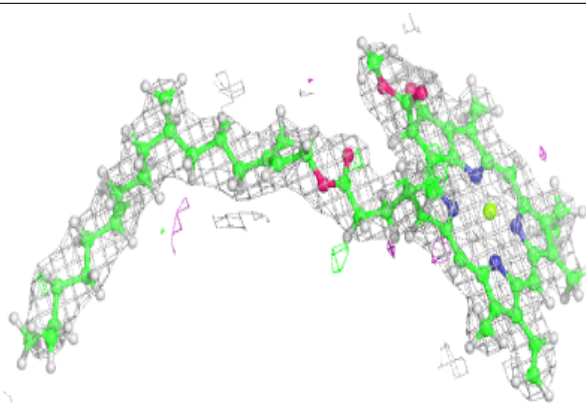
**Electron density around CLA A 404:**

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

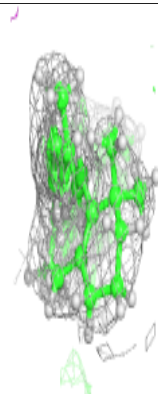
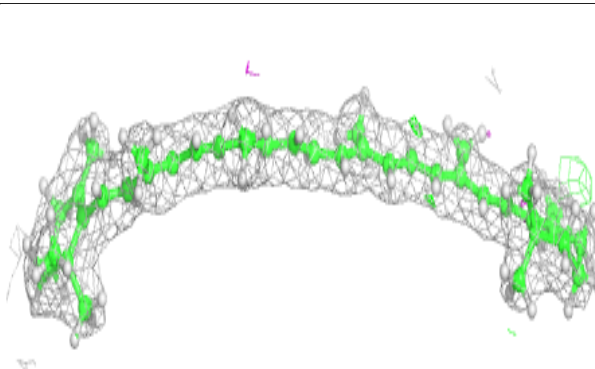
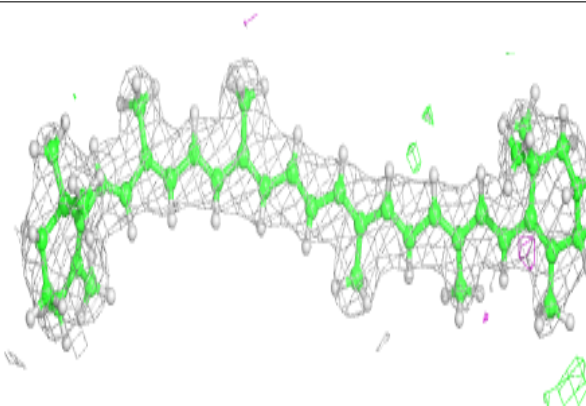


Electron density around CLA a 405:

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

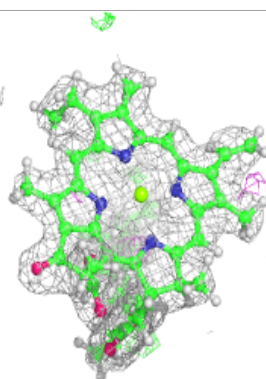
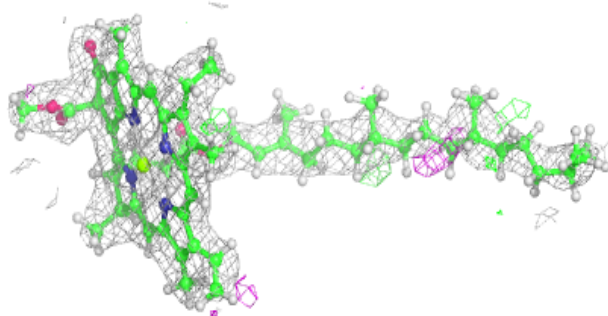
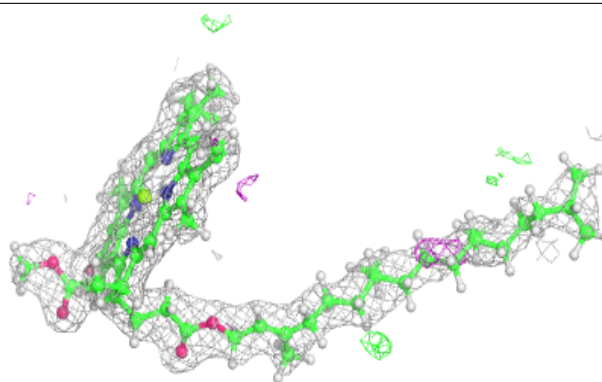
**Electron density around BCR T 101:**

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

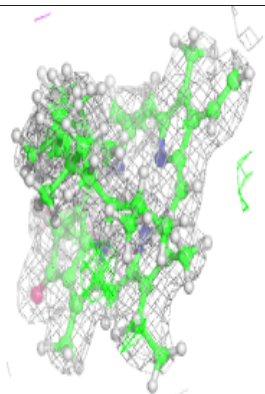
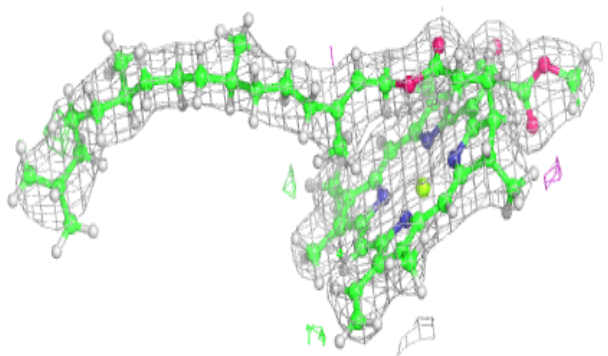
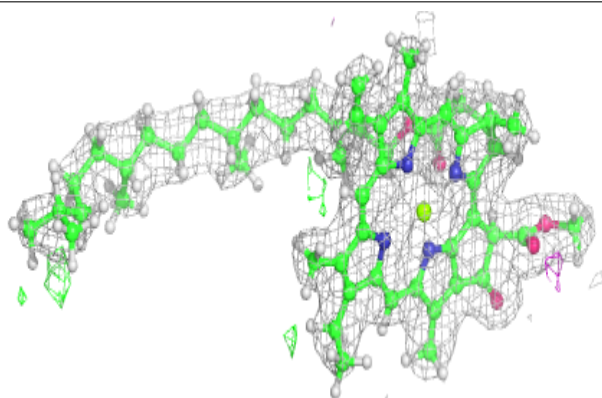


Electron density around CLA B 607:

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

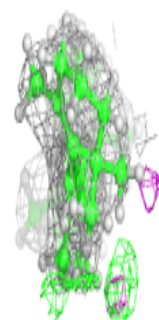
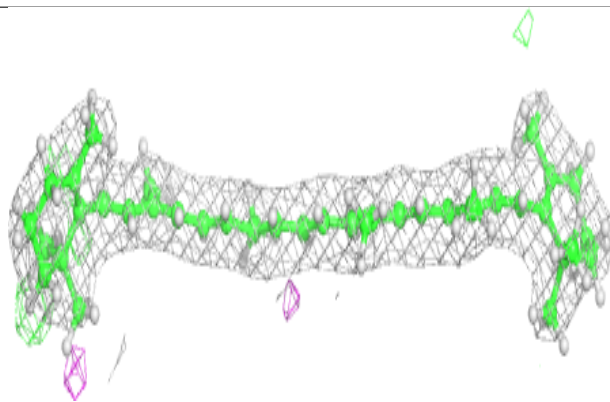
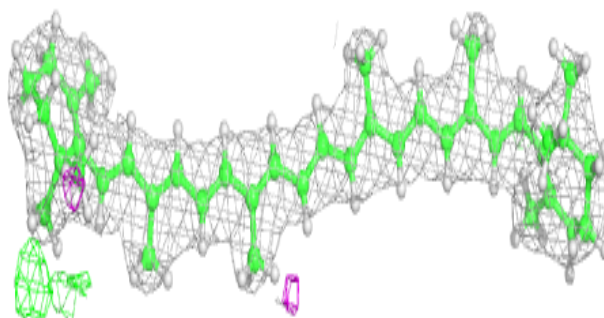
**Electron density around CLA B 608:**

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

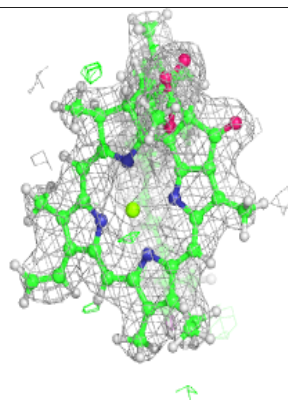
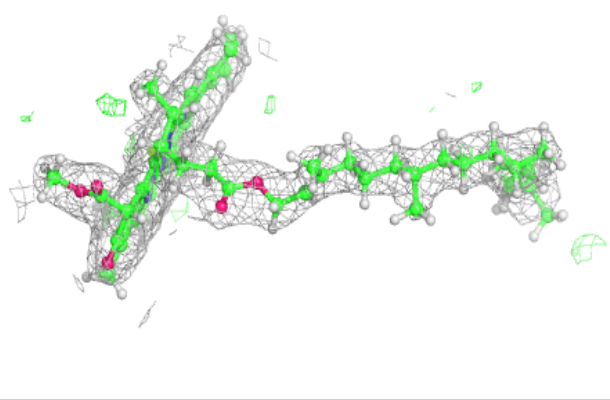
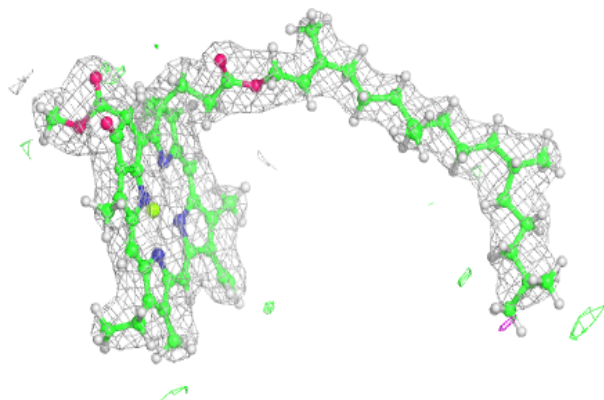


Electron density around BCR b 617:

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

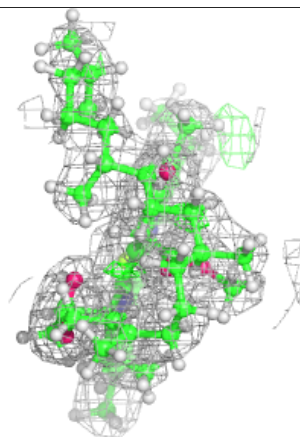
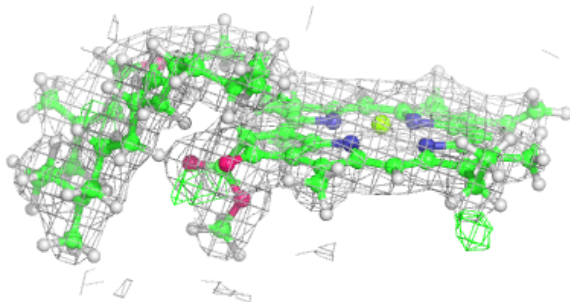
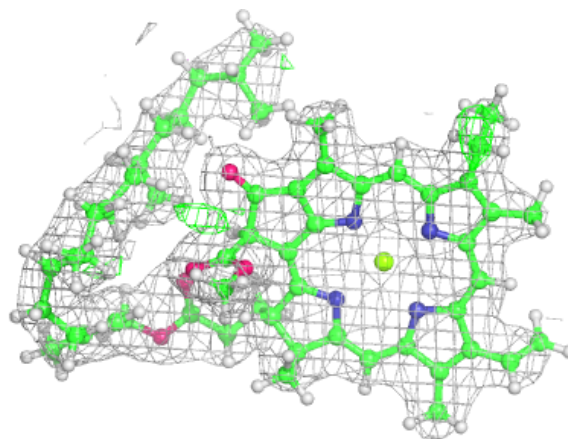
**Electron density around CLA B 609:**

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

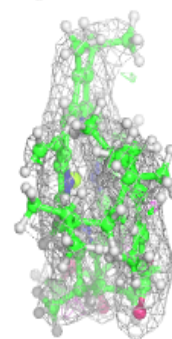
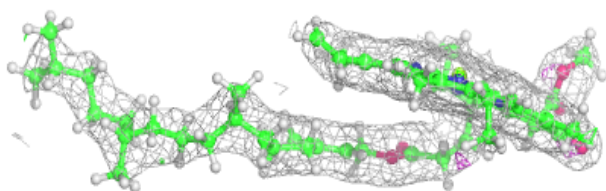
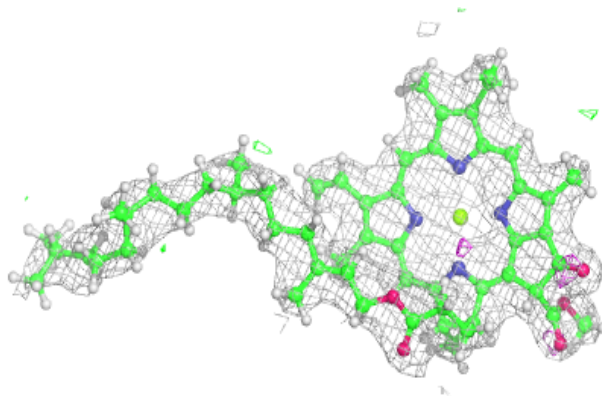


Electron density around CLA B 610:

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

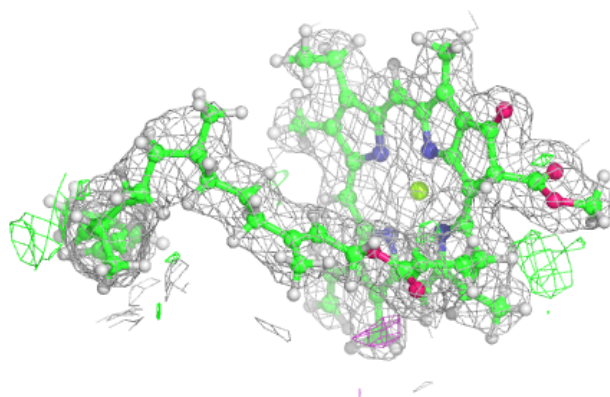
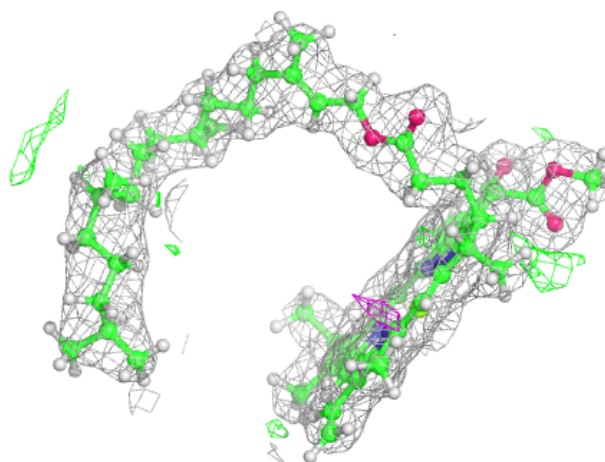
**Electron density around CLA b 602:**

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



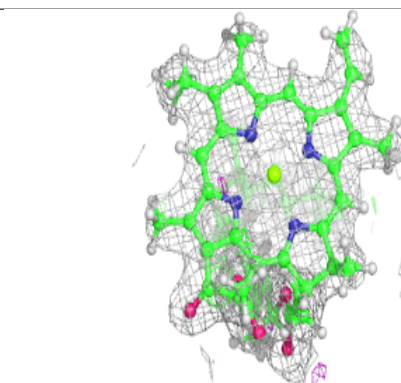
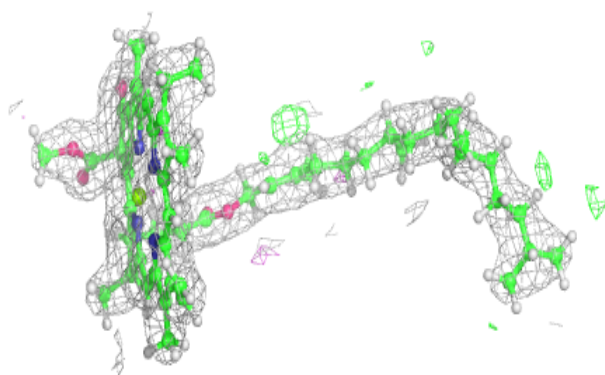
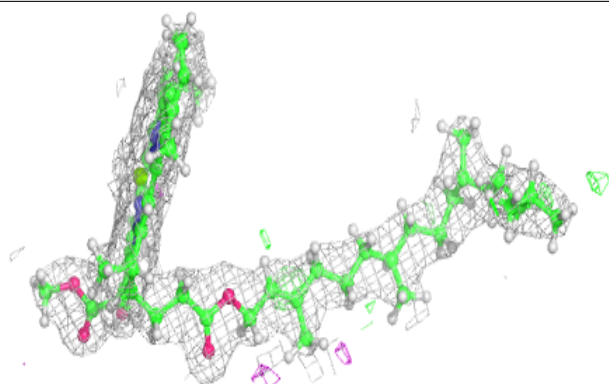
Electron density around CLA B 611:

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

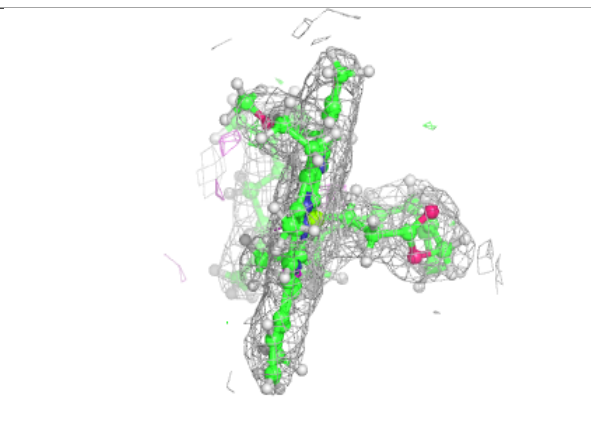
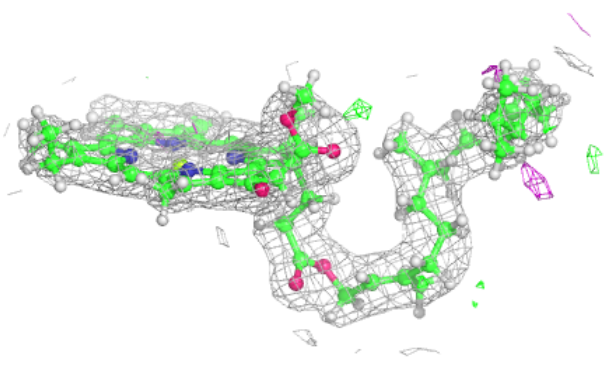
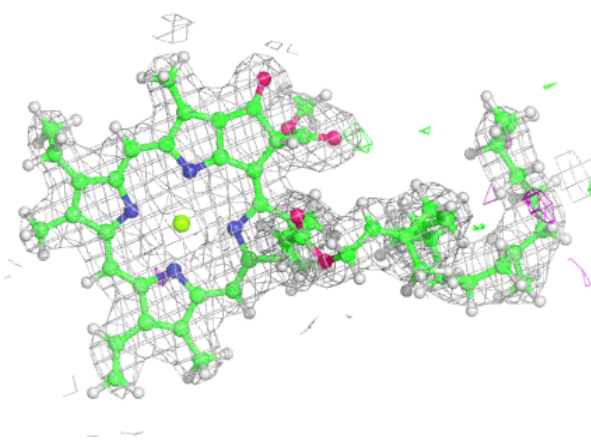


Electron density around CLA b 604:

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

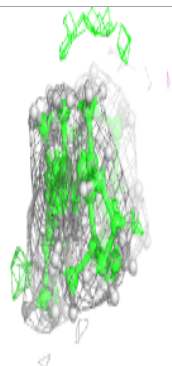
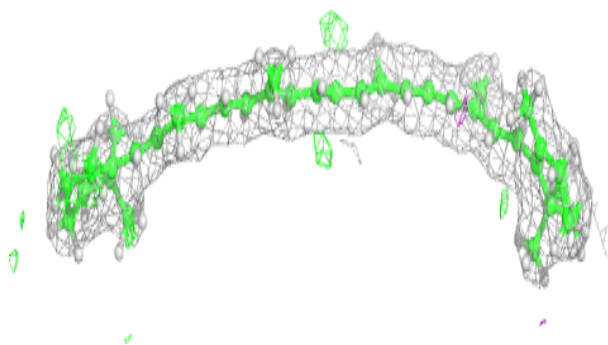
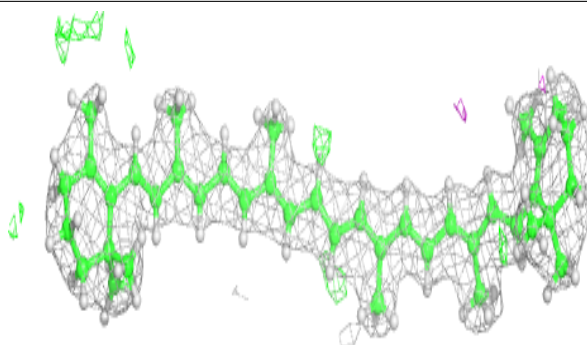
**Electron density around CLA B 612:**

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

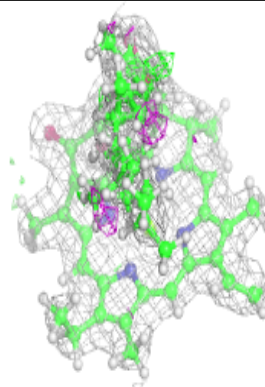
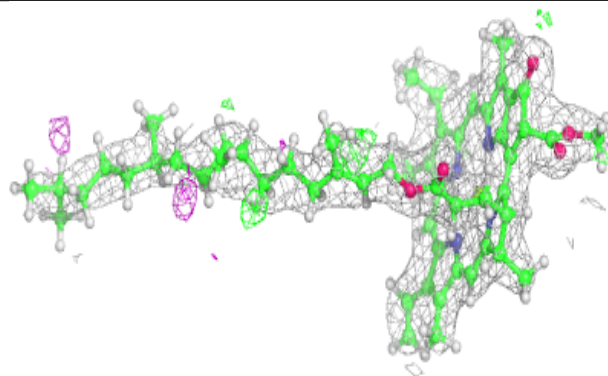
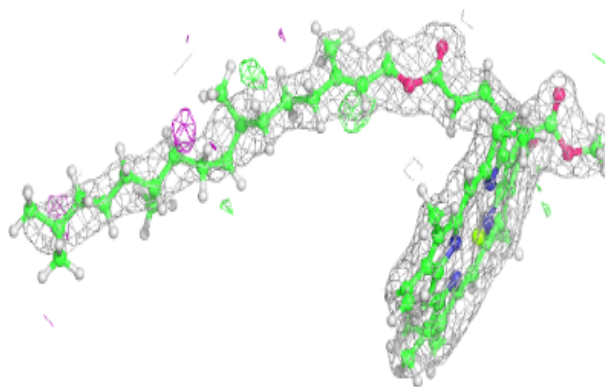


Electron density around BCR t 101:

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

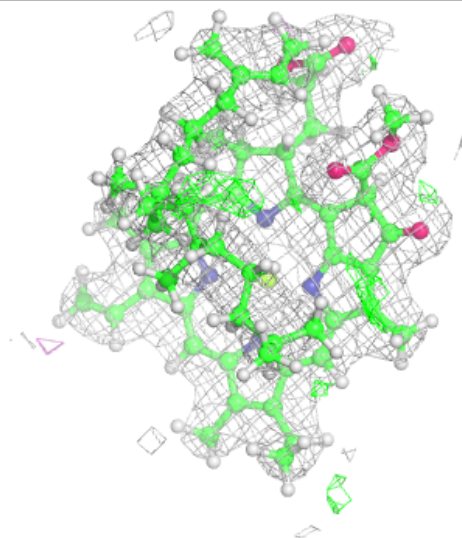
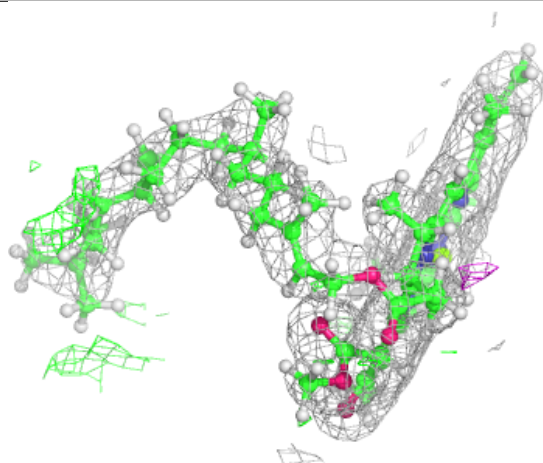
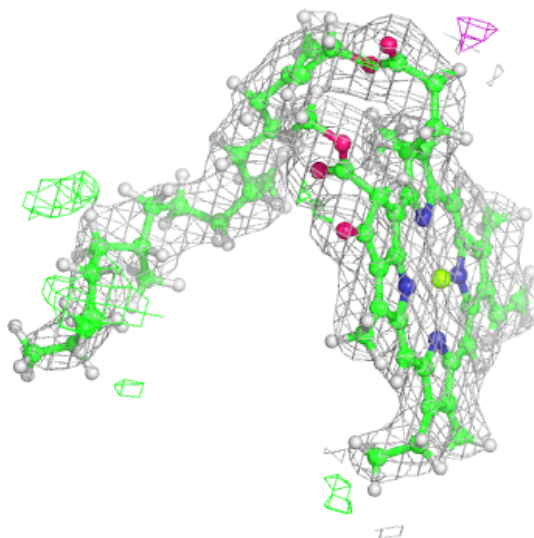
**Electron density around CLA b 606:**

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



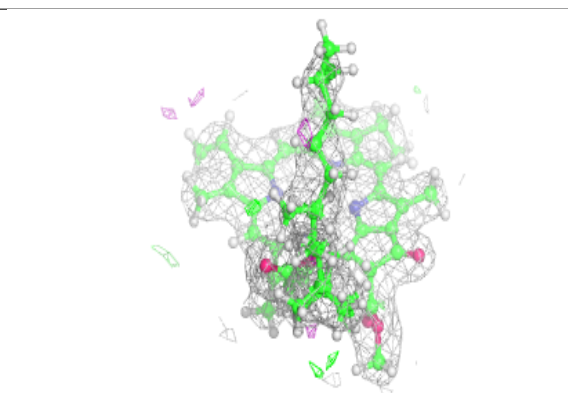
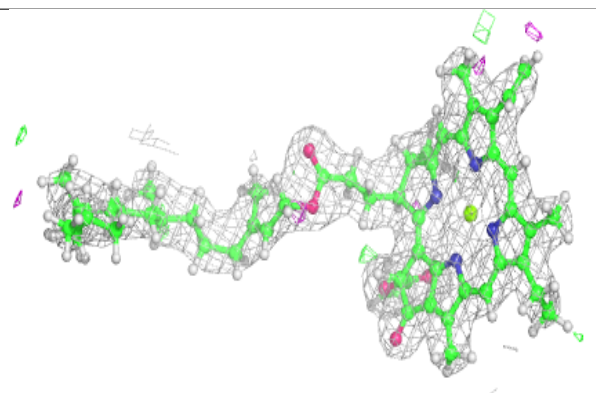
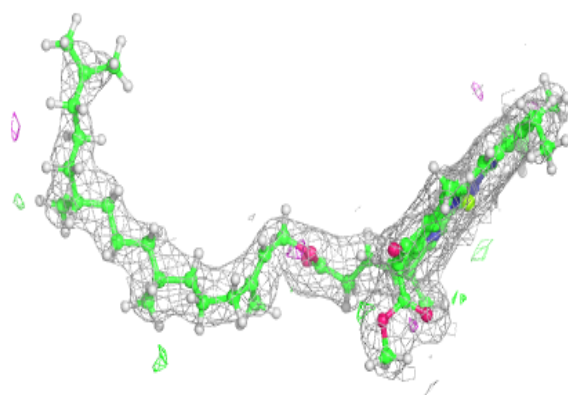
Electron density around CLA B 613:

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

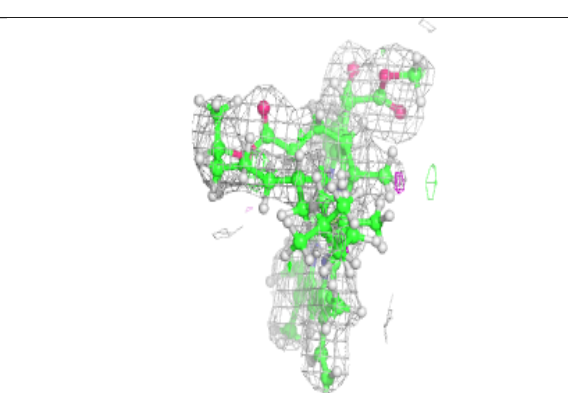
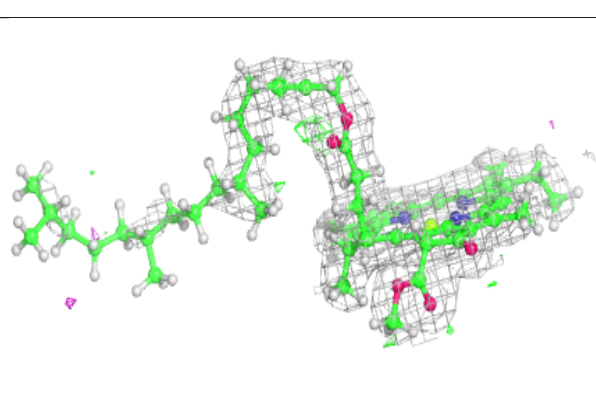
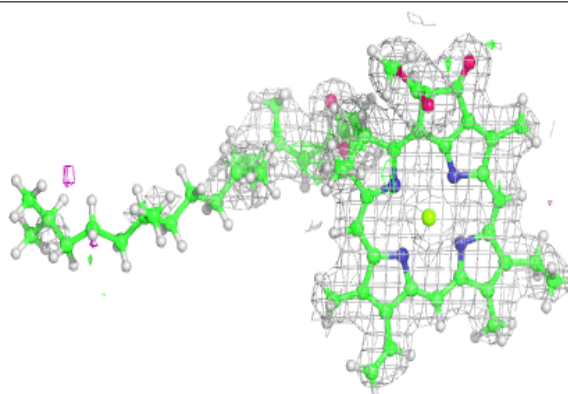


Electron density around CLA d 402:

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

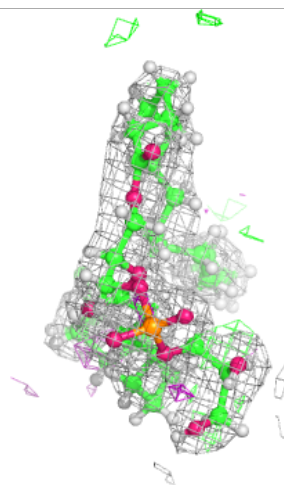
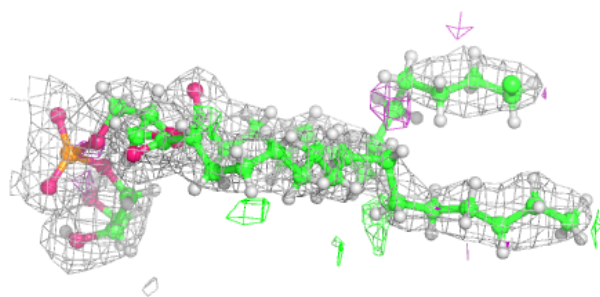
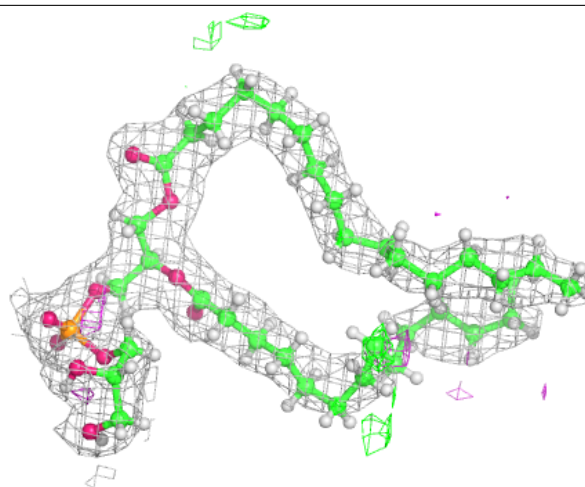
**Electron density around CLA A 405:**

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



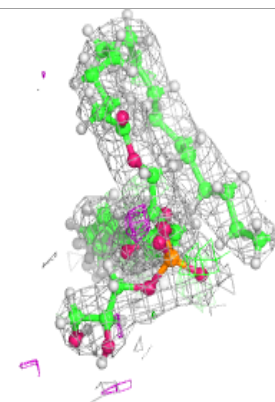
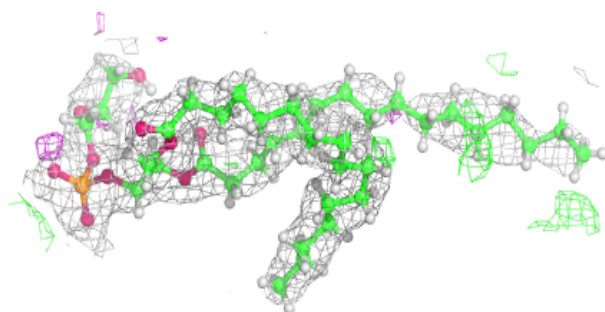
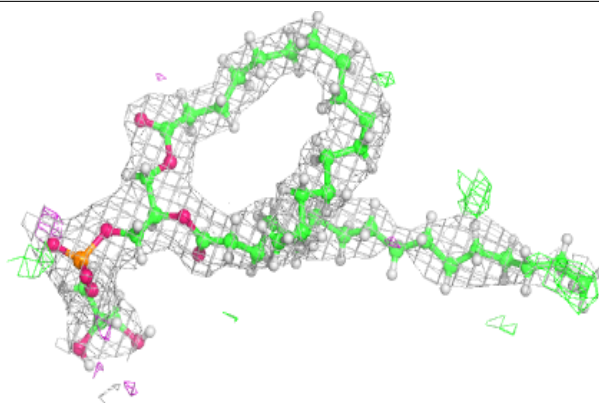
Electron density around LHG D 411:

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

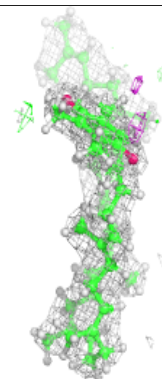
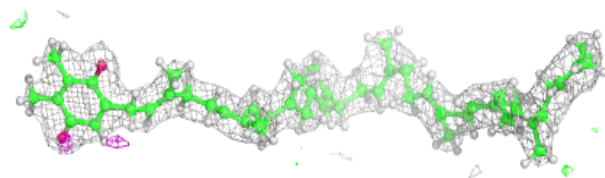
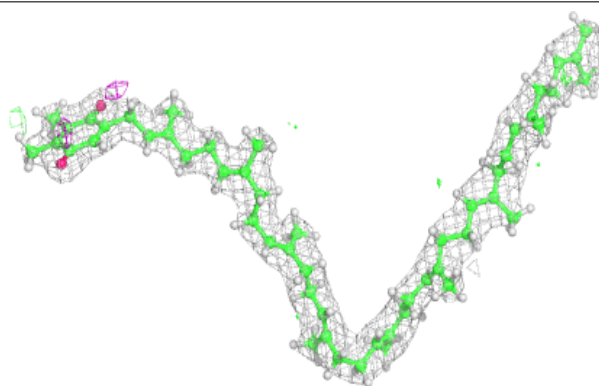


Electron density around LHG D 412:

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

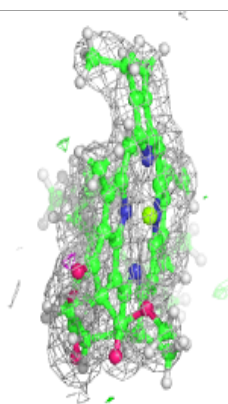
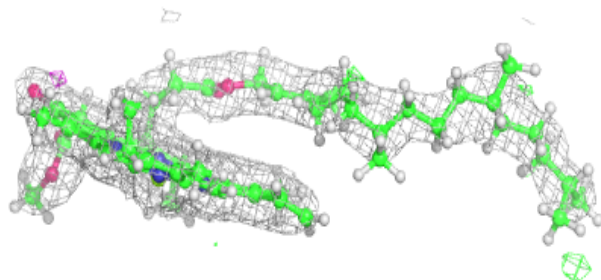
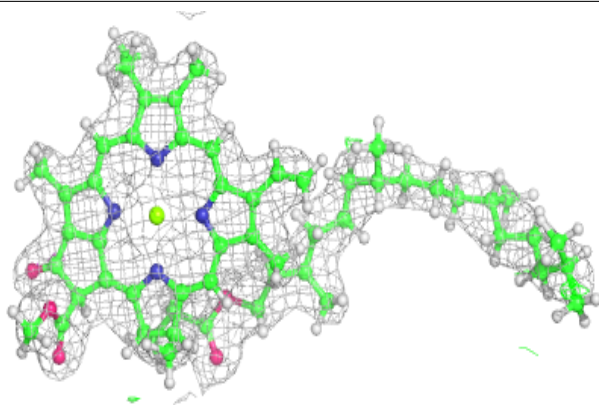
**Electron density around PL9 d 405:**

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



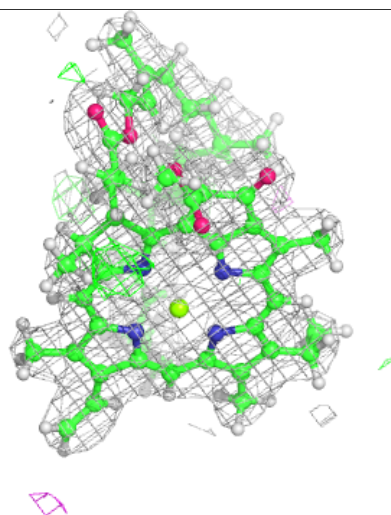
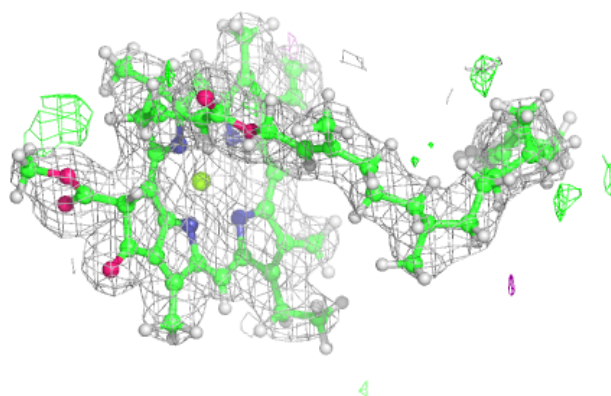
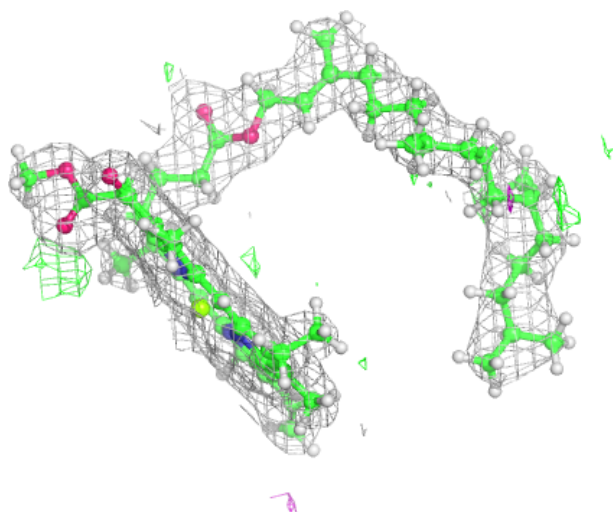
Electron density around CLA B 603:

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



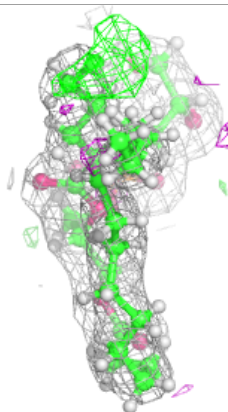
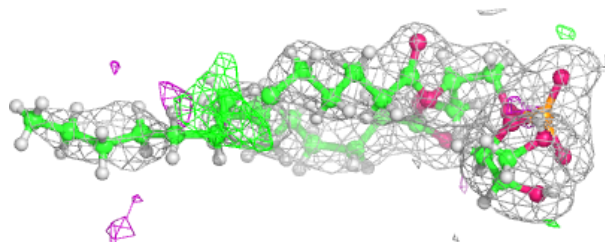
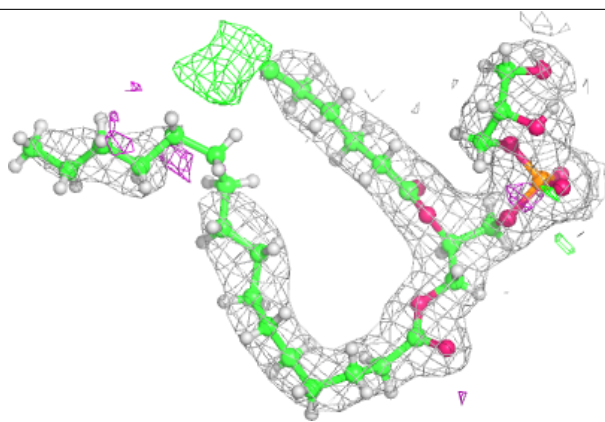
Electron density around CLA b 610:

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



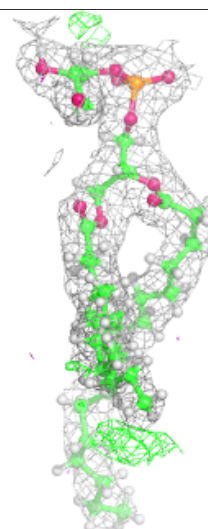
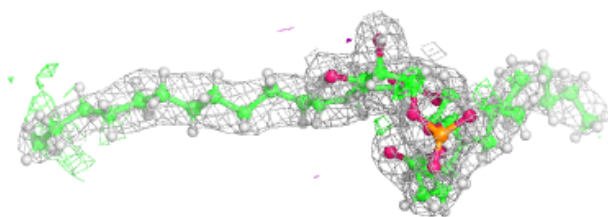
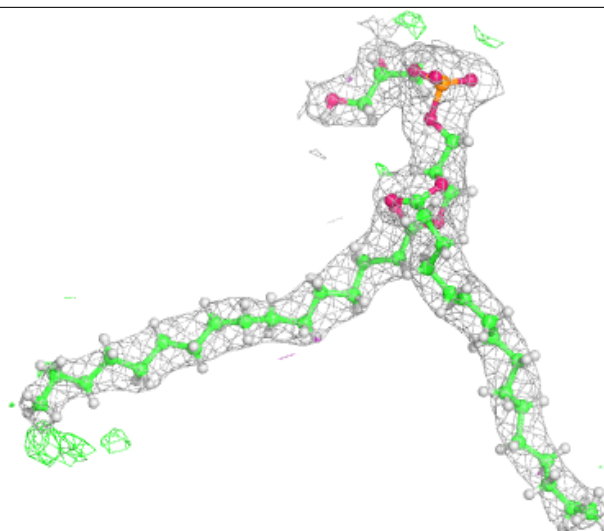
Electron density around LHG d 408:

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



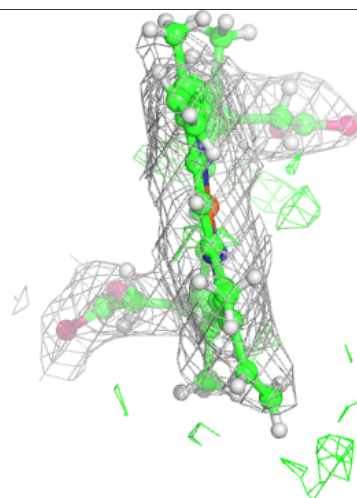
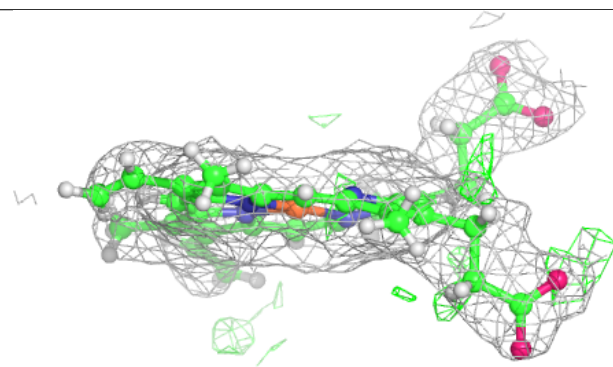
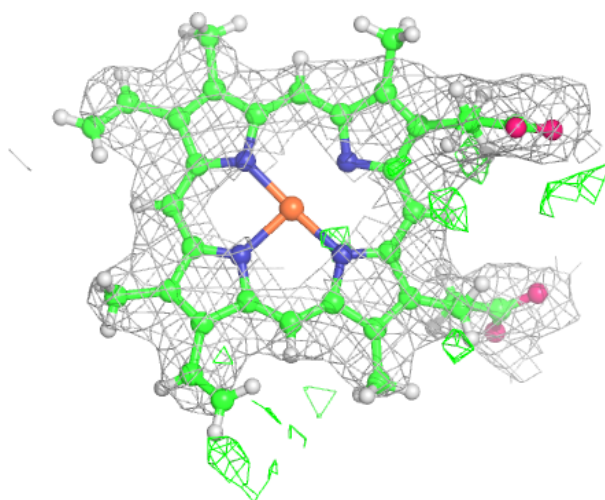
Electron density around LHG 1 102:

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



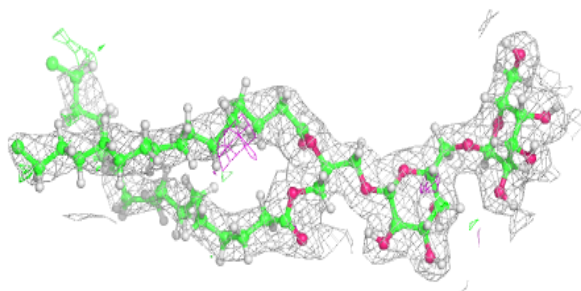
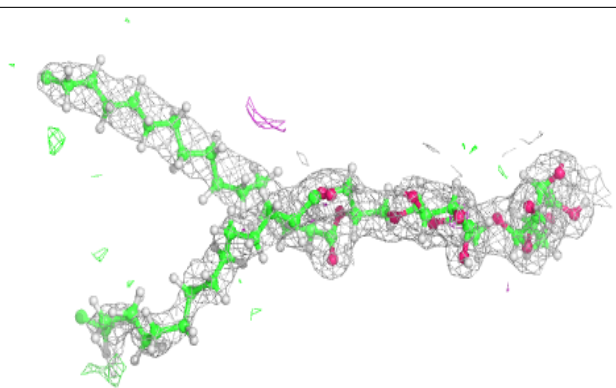
Electron density around HEM f 101:

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

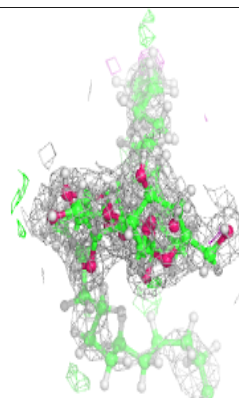
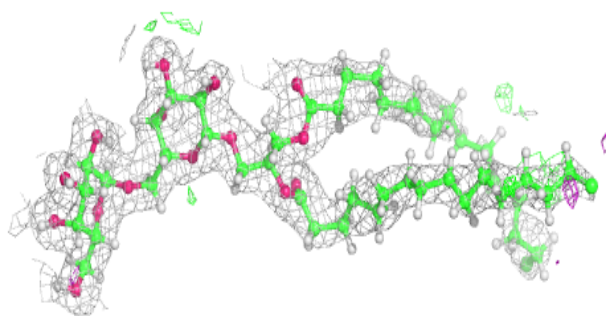
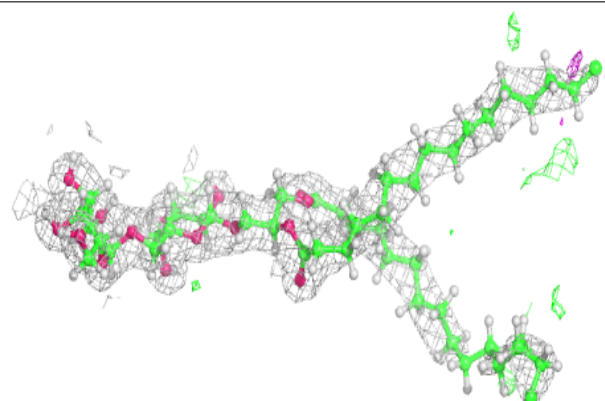


Electron density around DGD c 519:

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

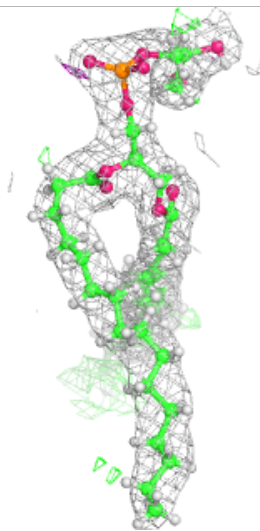
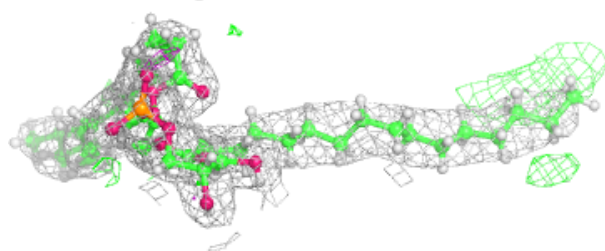
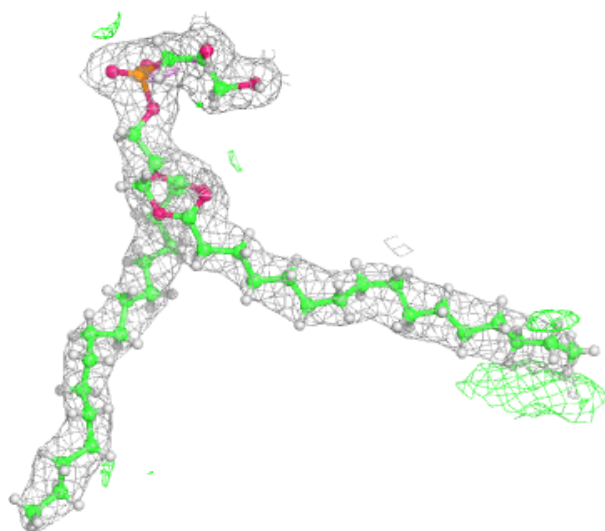
**Electron density around DGD C 521:**

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



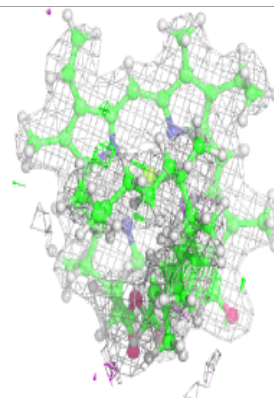
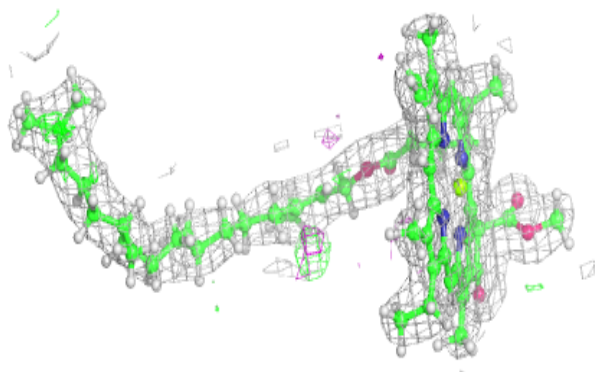
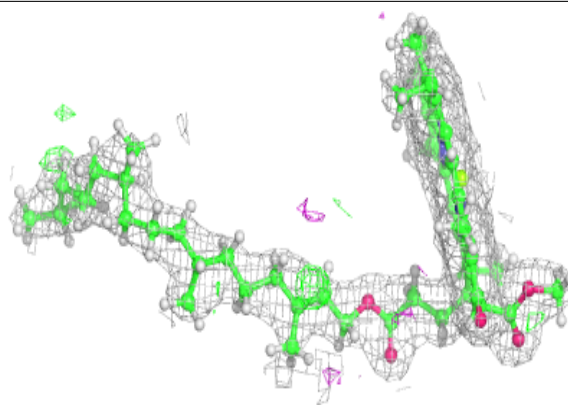
Electron density around LHG L 101:

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



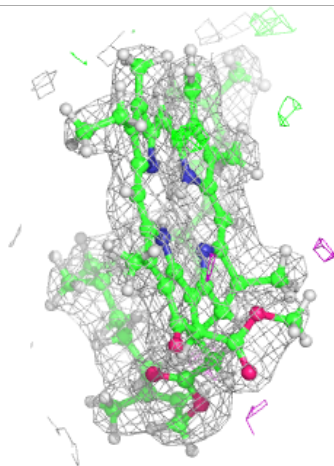
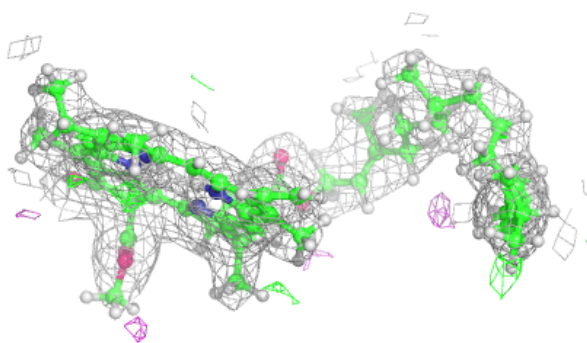
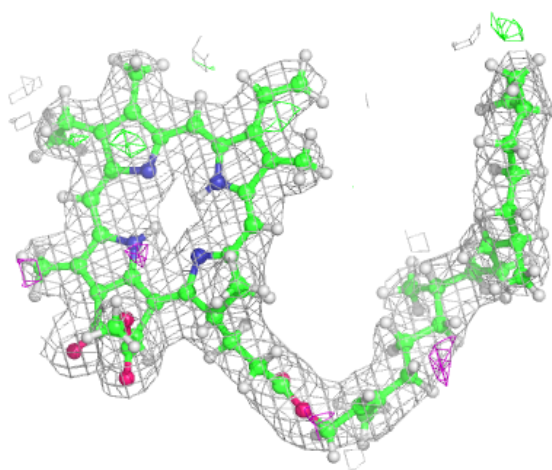
Electron density around CLA B 605:

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



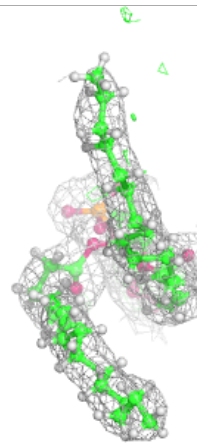
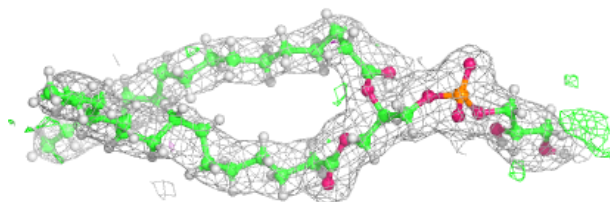
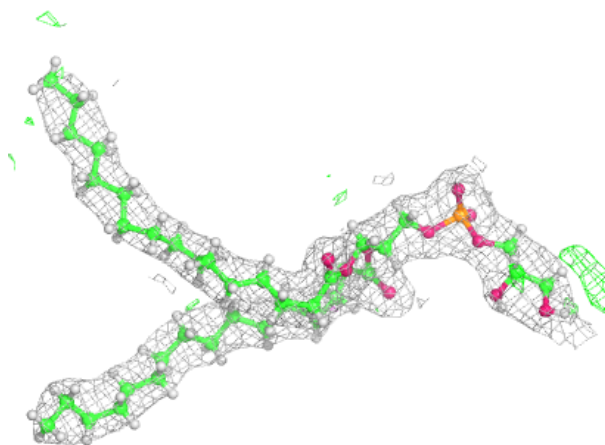
Electron density around PHO A 406:

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



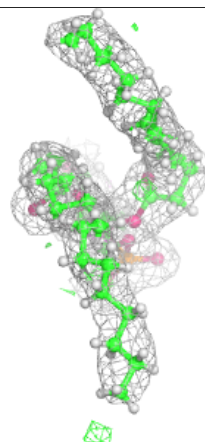
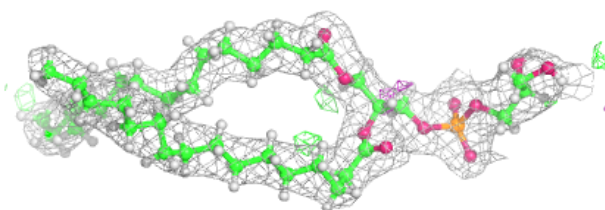
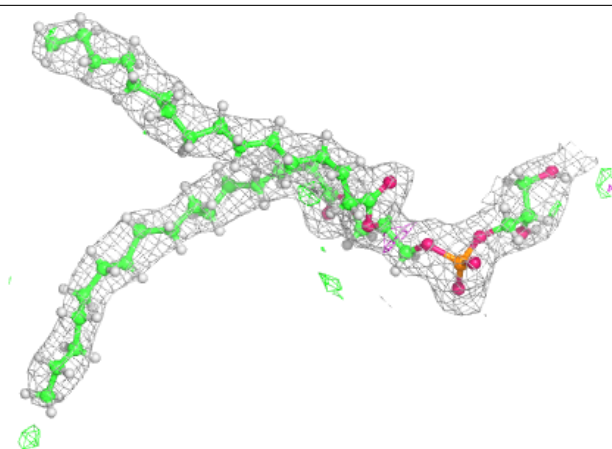
Electron density around LHG d 407:

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



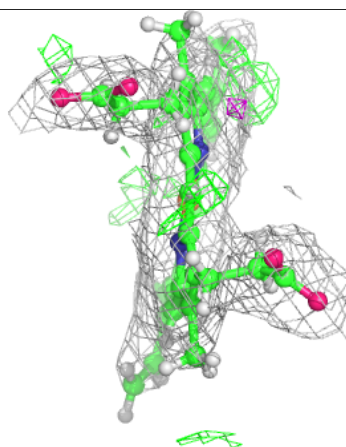
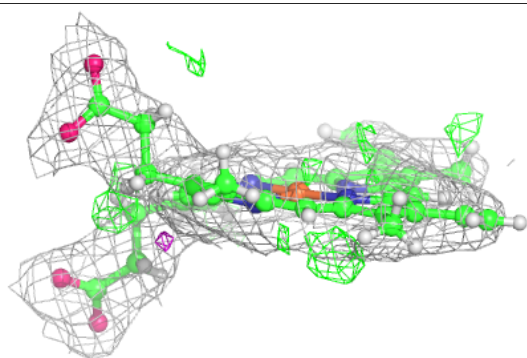
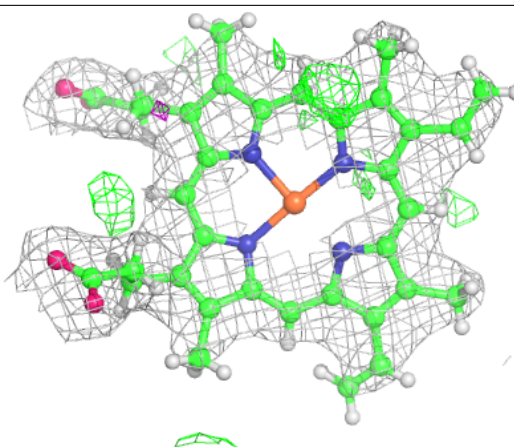
Electron density around LHG D 410:

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



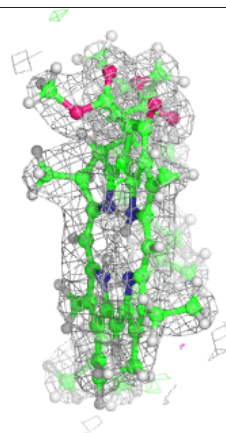
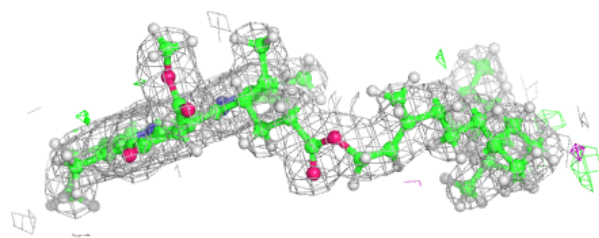
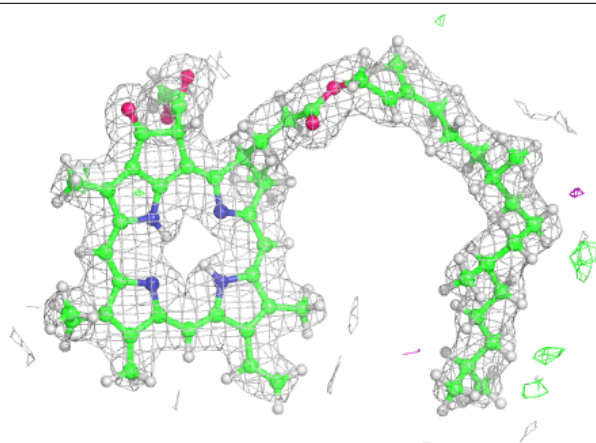
Electron density around HEM F 101:

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



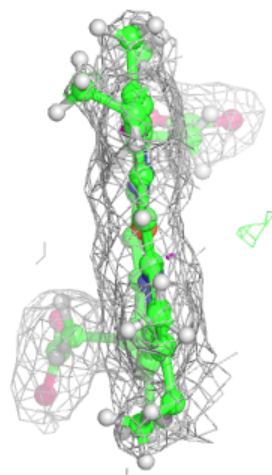
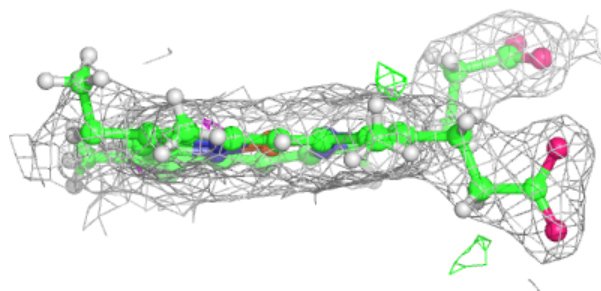
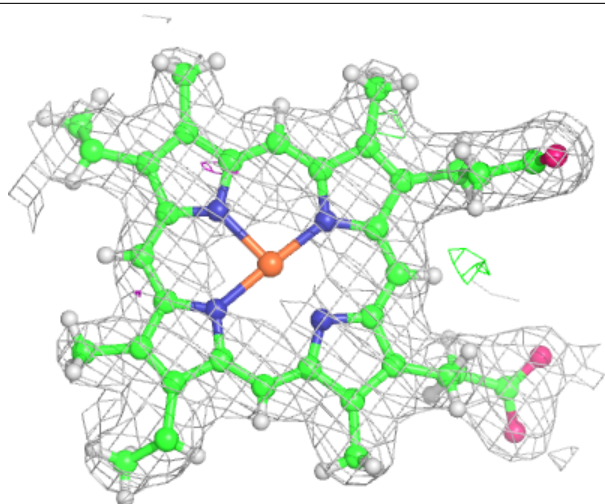
Electron density around PHO D 402:

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



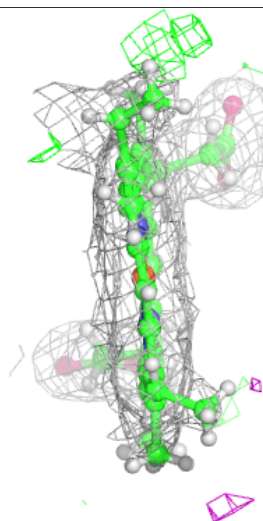
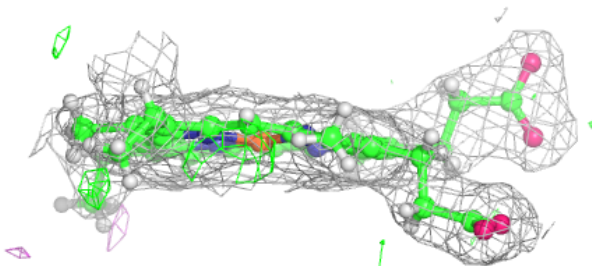
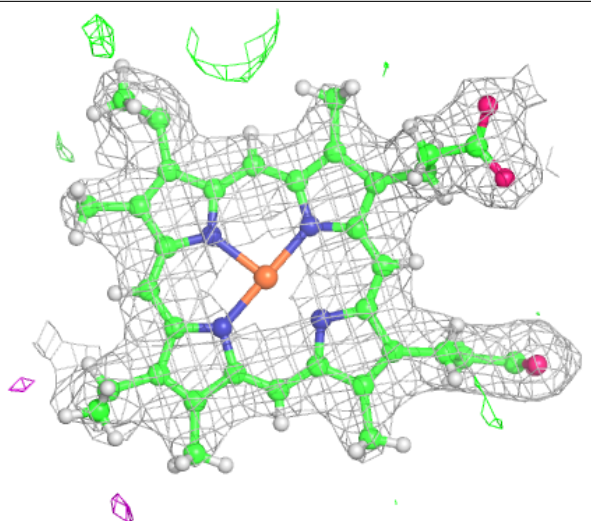
Electron density around HEC V 201:

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



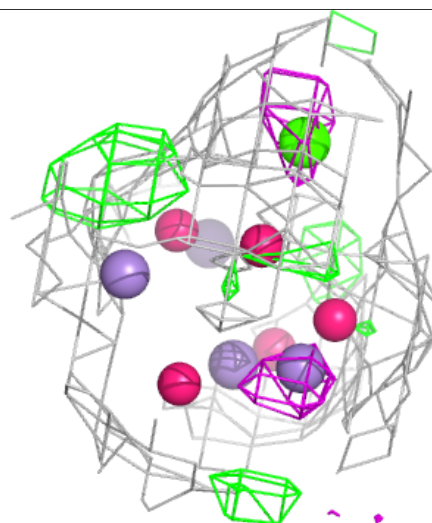
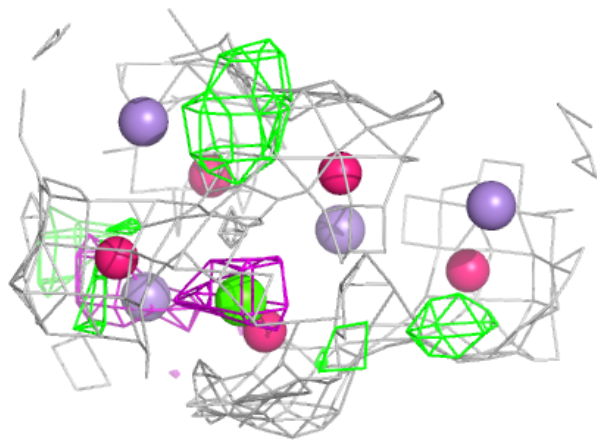
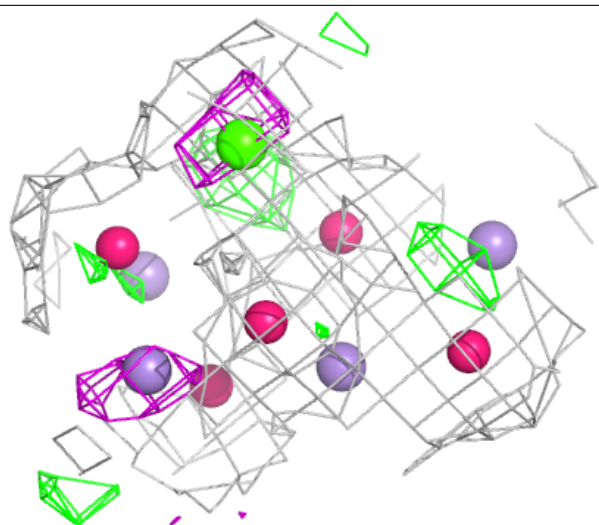
Electron density around HEC v 201:

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



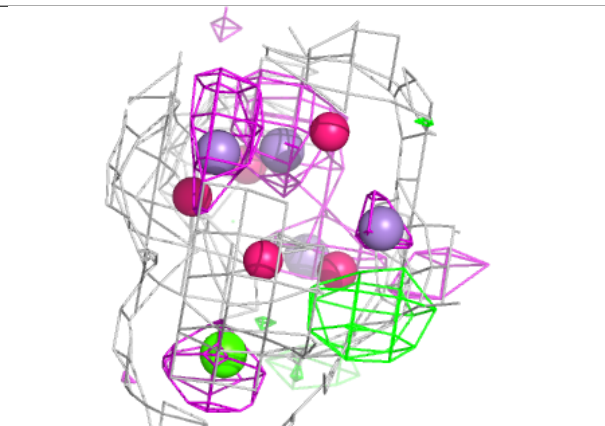
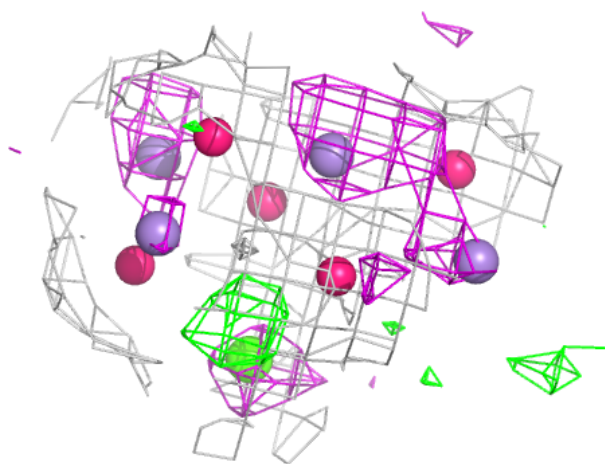
Electron density around OEX A 418:

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



Electron density around OEX a 418:

$2mF_o-DF_c$ (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.