



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2021 – 04:45 PM EDT

PDB ID : 7RF2
Title : RT XFEL structure of dark-stable state of Photosystem II (0F, S1 rich) at 2.08 Angstrom
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 : 2.08 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

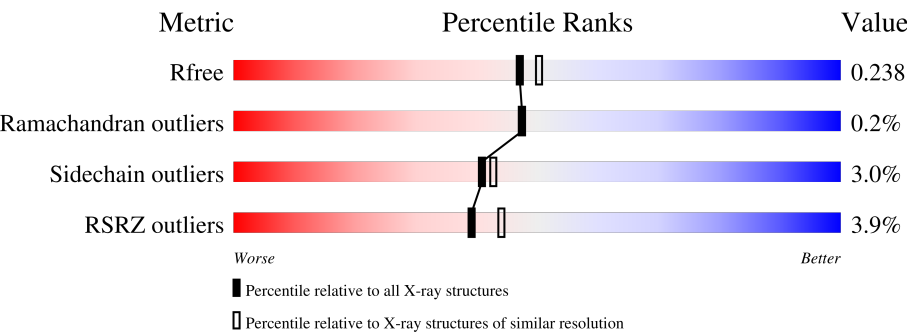
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.08 Å.

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



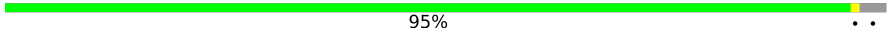
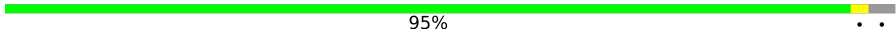
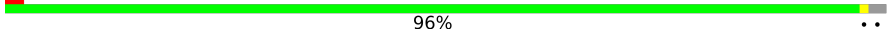
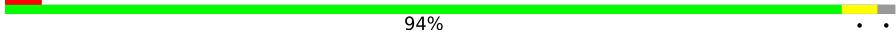


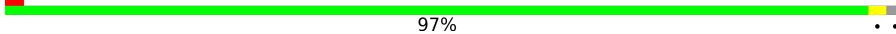







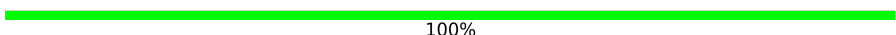

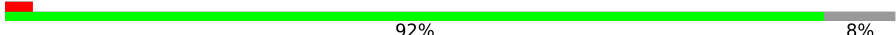








Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	6189 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	
1	a	344	
2	B	510	
2	b	510	
3	C	461	
3	c	461	

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Mol	Chain	Length	Quality of chain
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	R	41	
14	r	41	
15	T	32	
15	t	32	
16	U	134	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	402	X	-	-	-
22	CLA	A	406	X	-	-	-
22	CLA	B	601	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	C	501	X	-	-	-
22	CLA	C	502	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	D	404	X	-	-	-
22	CLA	a	402	X	-	-	-
22	CLA	a	403	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	b	601	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	c	501	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
22	CLA	d	404	X	-	-	-
22	CLA	d	405	X	-	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 103670 atoms, of which 51532 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
			5141	1717	2519	431	459	15			
1	a	334	Total	C	H	N	O	S	0	0	0
			5128	1714	2509	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	0	0
			7814	2610	3836	665	690	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	442	Total	C	H	N	O	S	0	2	0
			6781	2249	3355	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	16	1	0
			1317	436	651	107	123			
5	e	82	Total	C	H	N	O	0	0	0
			1312	434	648	108	122			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	H	N	O	0	0	0
			557	187	282	45	42			
6	f	34	Total	C	H	N	O	0	0	0
			557	187	282	45	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	H	N	O	0	0	0
			1042	341	532	82	85			
7	h	63	Total	C	H	N	O	0	0	0
			1016	333	518	80	83			

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	H	N	O	0	0	0
			593	188	312	45	48			
18	x	39	Total	C	H	N	O	0	0	0
			602	191	316	46	49			

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

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

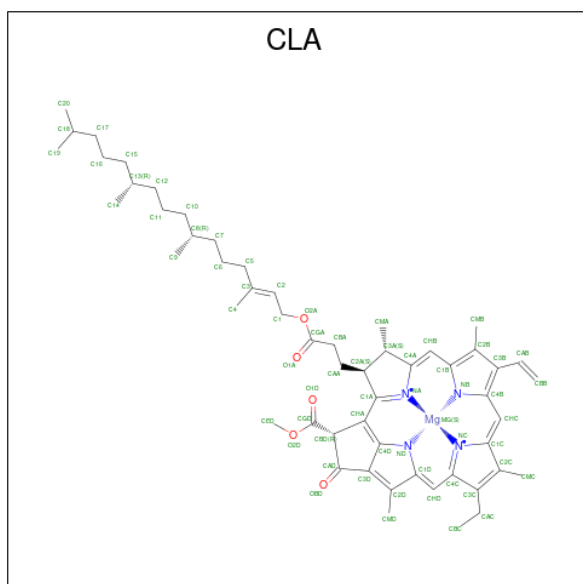
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

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

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

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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

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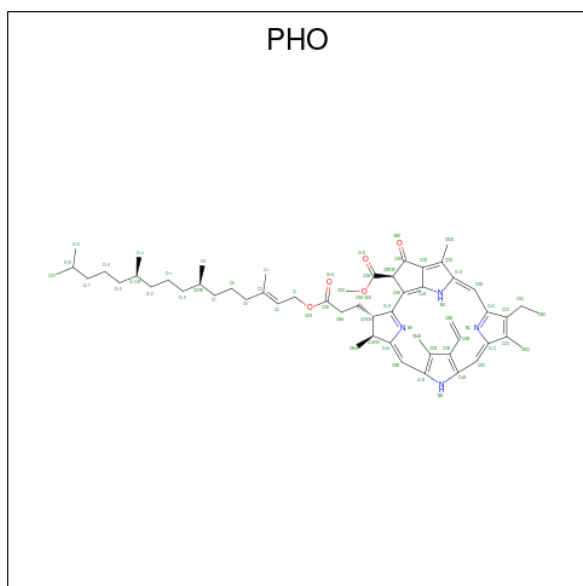
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total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

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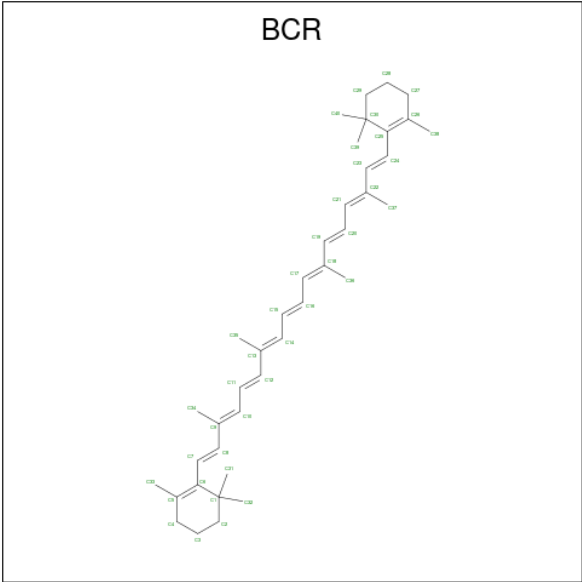
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	d	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	d	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	d	1	Total 137	C 55	H 72	Mg 1	N 4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

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



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

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



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

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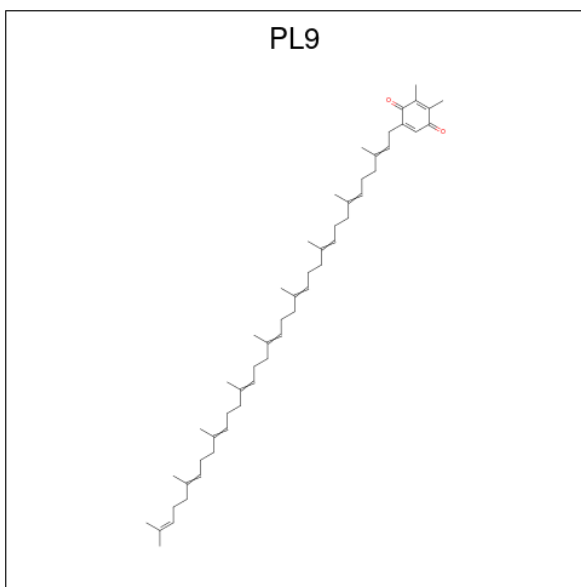
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	b	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	d	1	Total	C	H	0	0
			96	40	56		
24	h	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40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

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

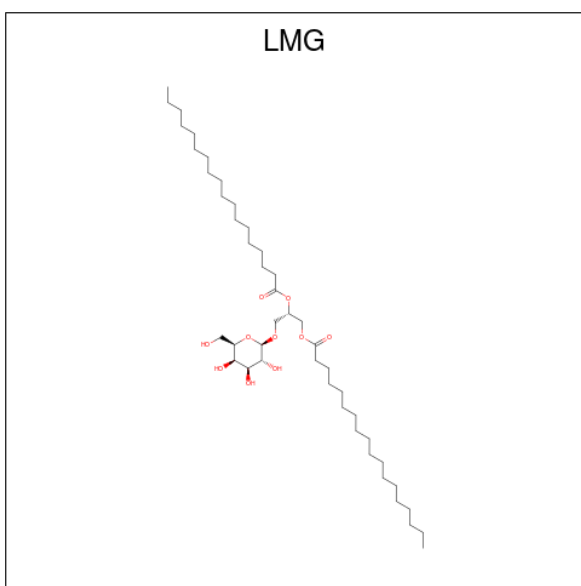
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	2	Total	Cl	0	0
			2	2		
25	a	2	Total	Cl	0	0
			2	2		

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



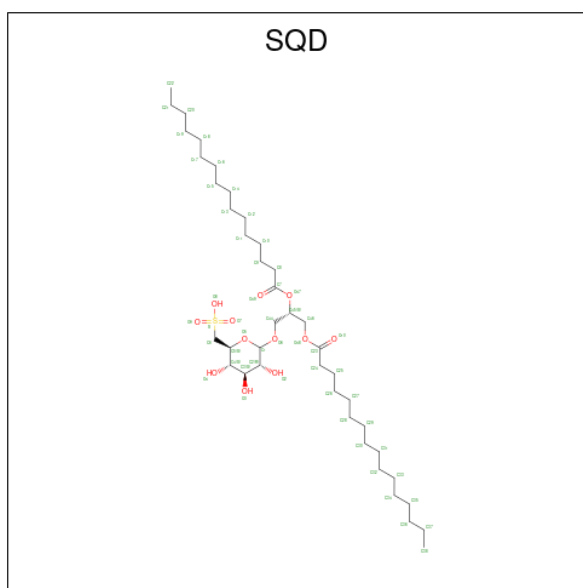
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	H	O	0	0
			135	53	80	2		
26	D	1	Total	C	H	O	0	0
			135	53	80	2		
26	a	1	Total	C	H	O	0	0
			135	53	80	2		
26	d	1	Total	C	H	O	0	0
			135	53	80	2		

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



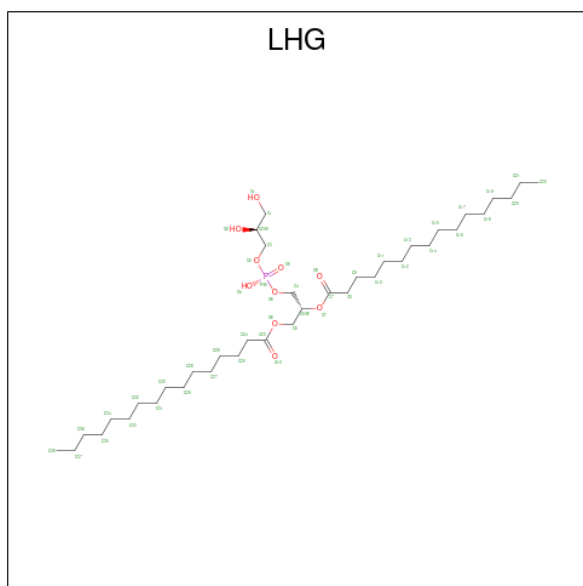
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	H	O	0	0
			114	38	66	10		
27	D	1	Total	C	H	O	0	0
			123	41	72	10		
27	D	1	Total	C	H	O	0	0
			77	27	45	5		
27	M	1	Total	C	H	O	0	0
			123	41	72	10		
27	Y	1	Total	C	H	O	0	0
			114	38	66	10		
27	a	1	Total	C	H	O	0	0
			117	39	68	10		
27	b	1	Total	C	H	O	0	0
			141	45	86	10		
27	c	1	Total	C	H	O	0	0
			81	27	44	10		
27	c	1	Total	C	H	O	0	0
			117	38	69	10		
27	d	1	Total	C	H	O	0	0
			102	34	58	10		
27	h	1	Total	C	H	O	0	0
			57	21	34	2		
27	m	1	Total	C	H	O	0	0
			123	41	72	10		

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



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

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



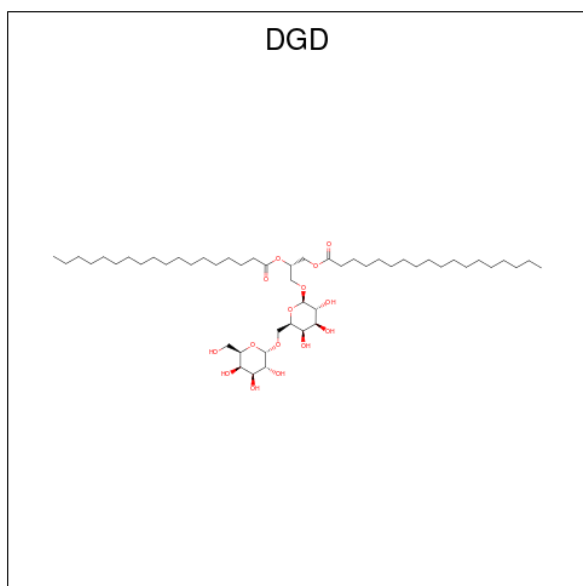
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		

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

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



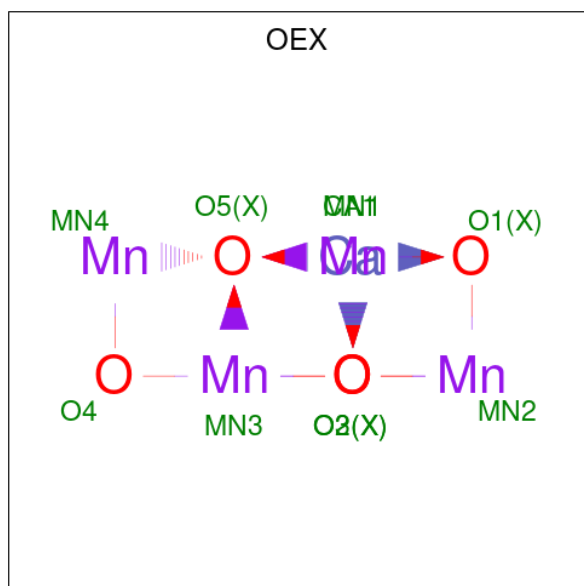
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	H	O	0	0
			162	51	96	15		
30	C	1	Total	C	H	O	0	0
			144	47	82	15		
30	C	1	Total	C	H	O	0	0
			144	47	82	15		
30	C	1	Total	C	H	O	0	0
			144	47	82	15		

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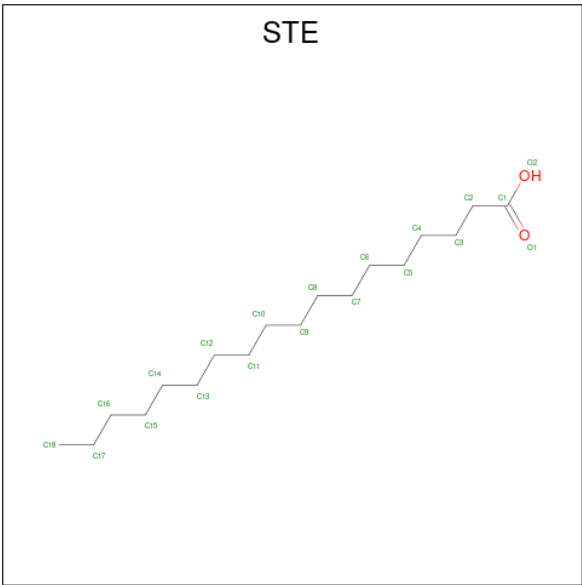
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	H	1	Total	C	H	O	0	0
			144	47	82	15		
30	c	1	Total	C	H	O	0	0
			143	47	81	15		
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	h	1	Total	C	H	O	0	0
			144	47	82	15		
30	o	1	Total	C	H	O	0	0
			119	39	75	5		

- 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 STEARIC ACID (three-letter code: STE) (formula: $\text{C}_{18}\text{H}_{36}\text{O}_2$).



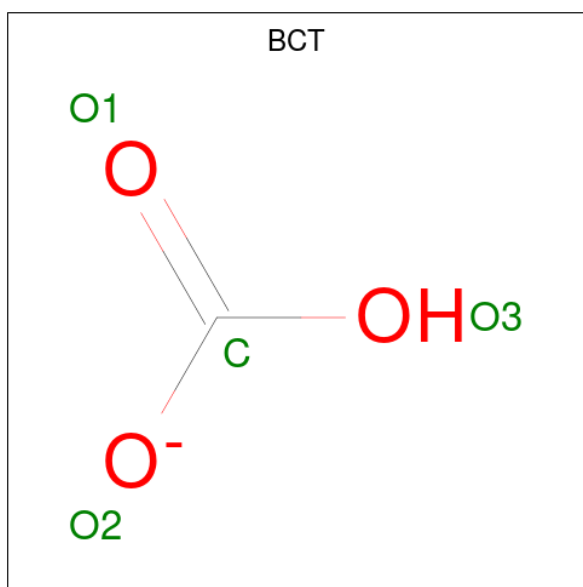
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	H	O	0	0
			43	15	26	2		
32	B	1	Total	C	H	O	0	0
			34	12	20	2		
32	B	1	Total	C	H	O	0	0
			28	10	16	2		
32	B	1	Total	C	H	O	0	0
			46	16	28	2		
32	B	1	Total	C	H		0	0
			47	16	31			
32	B	1	Total	C	H	O	0	0
			28	10	16	2		
32	B	1	Total	C	O		0	0
			16	14	2			
32	C	1	Total	C	H	O	0	0
			28	10	16	2		
32	C	1	Total	C	H		0	0
			47	16	31			
32	C	1	Total	C	H	O	0	0
			28	10	16	2		
32	D	1	Total	C	H	O	0	0
			55	18	35	2		
32	D	1	Total	C	O		0	0
			15	13	2			
32	E	1	Total	C	H	O	0	0
			28	10	16	2		
32	H	1	Total	C	H		0	0
			53	18	35			

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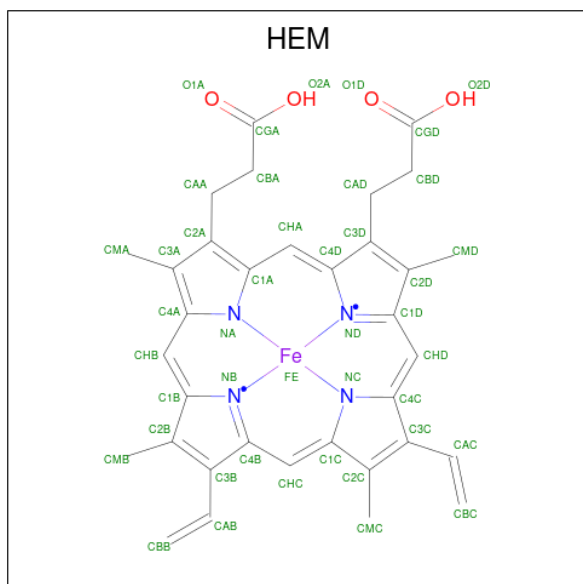
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	I	1	Total C H 41 15 26	0	0
32	J	1	Total C H O 28 10 16 2	0	0
32	M	1	Total C H O 37 13 22 2	0	0
32	M	1	Total C H 26 10 16	0	0
32	M	1	Total C H 53 18 35	0	0
32	T	1	Total C H 44 15 29	0	0
32	a	1	Total C H 26 10 16	0	0
32	a	1	Total C H O 28 10 16 2	0	0
32	b	1	Total C H 47 16 31	0	0
32	b	1	Total C H O 55 18 35 2	0	0
32	b	1	Total C H O 40 14 24 2	0	0
32	b	1	Total C H O 55 18 35 2	0	0
32	b	1	Total C H 26 10 16	0	0
32	c	1	Total C H O 55 18 35 2	0	0
32	c	1	Total C H O 28 10 16 2	0	0
32	d	1	Total C H O 43 15 26 2	0	0
32	d	1	Total C H O 55 18 35 2	0	0
32	j	1	Total C H O 28 10 16 2	0	0
32	m	1	Total C H O 28 10 16 2	0	0

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



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

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



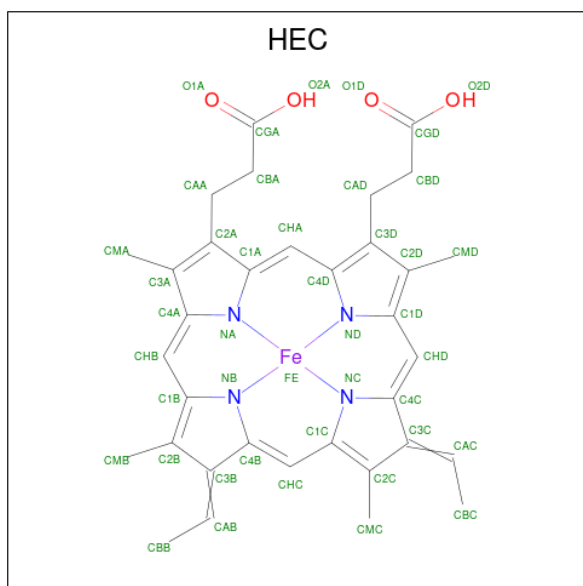
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
34	F	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

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

- 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	204	Total	O	0	0
			204	204		
36	C	182	Total	O	0	0
			182	182		
36	D	136	Total	O	0	0
			136	136		
36	E	30	Total	O	0	0
			30	30		
36	F	7	Total	O	0	0
			7	7		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	H	37	Total O 37 37	0	0
36	I	10	Total O 10 10	0	0
36	J	16	Total O 16 16	0	0
36	K	8	Total O 8 8	0	0
36	L	8	Total O 8 8	0	0
36	M	7	Total O 7 7	0	0
36	O	90	Total O 90 90	0	0
36	T	10	Total O 10 10	0	0
36	U	52	Total O 52 52	0	0
36	V	65	Total O 65 65	0	0
36	X	12	Total O 12 12	0	0
36	Y	6	Total O 6 6	0	0
36	Z	2	Total O 2 2	0	0
36	a	126	Total O 126 126	0	0
36	b	206	Total O 206 206	0	0
36	c	181	Total O 181 181	0	0
36	d	111	Total O 111 111	0	0
36	e	21	Total O 21 21	0	0
36	f	8	Total O 8 8	0	0
36	h	36	Total O 36 36	0	0
36	i	13	Total O 13 13	0	0

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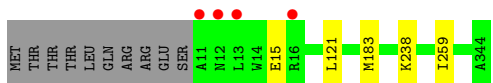
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	j	8	Total 8	O 8	0	0
36	k	6	Total 6	O 6	0	0
36	l	7	Total 7	O 7	0	0
36	m	6	Total 6	O 6	0	0
36	o	102	Total 102	O 102	0	0
36	r	3	Total 3	O 3	0	0
36	t	8	Total 8	O 8	0	0
36	u	58	Total 58	O 58	0	0
36	v	56	Total 56	O 56	0	0
36	x	8	Total 8	O 8	0	0
36	y	3	Total 3	O 3	0	0
36	z	9	Total 9	O 9	0	0

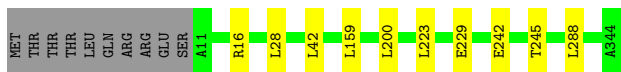
3 Residue-property plots [i](#)

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

- Molecule 1: Photosystem II protein D1 1



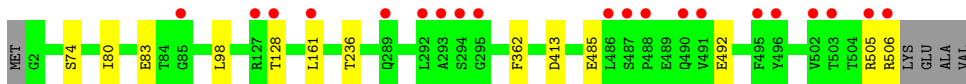
- Molecule 1: Photosystem II protein D1 1



- Molecule 2: Photosystem II CP47 reaction center protein



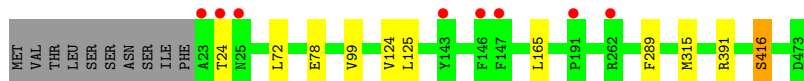
- Molecule 2: Photosystem II CP47 reaction center protein



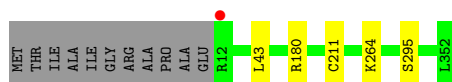
- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein



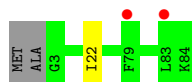
- Molecule 4: Photosystem II D2 protein



- Molecule 4: Photosystem II D2 protein



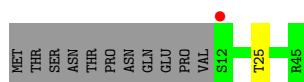
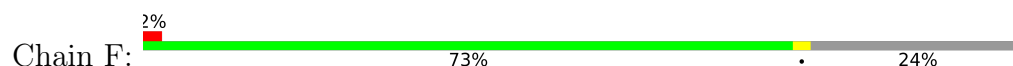
- Molecule 5: Cytochrome b559 subunit alpha



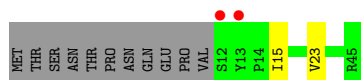
- Molecule 5: Cytochrome b559 subunit alpha



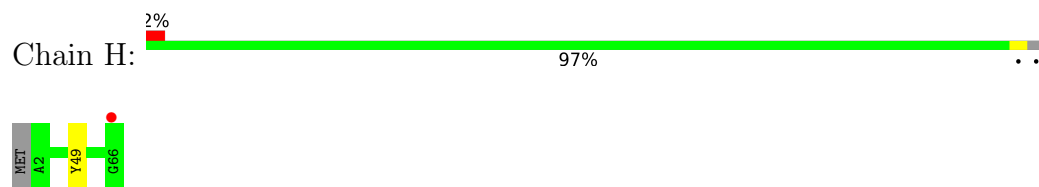
- Molecule 6: Cytochrome b559 subunit beta



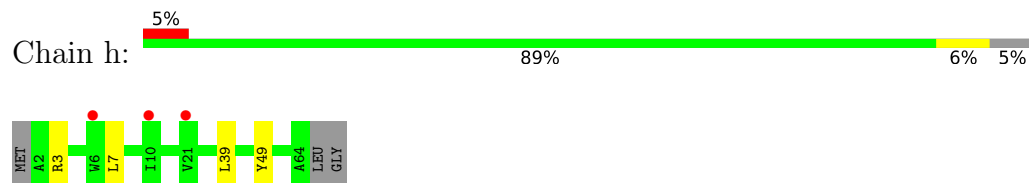
- Molecule 6: Cytochrome b559 subunit beta



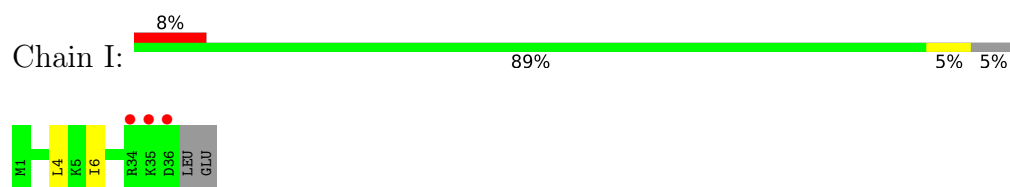
- Molecule 7: Photosystem II reaction center protein H



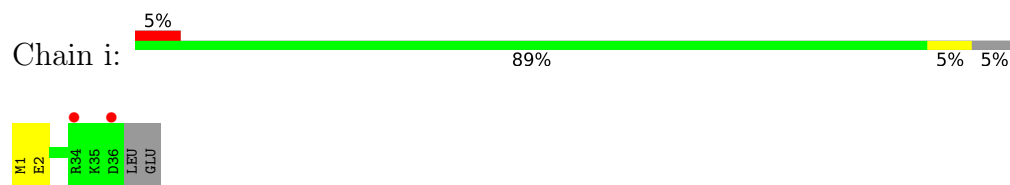
- Molecule 7: Photosystem II reaction center protein H



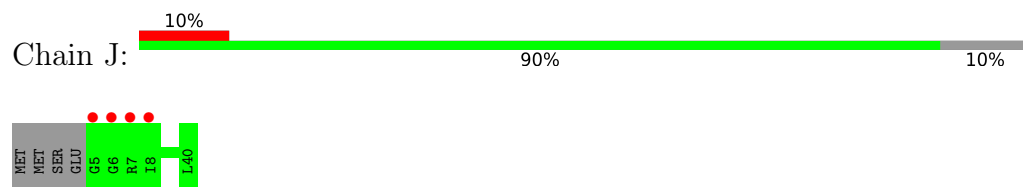
- Molecule 8: Photosystem II reaction center protein I



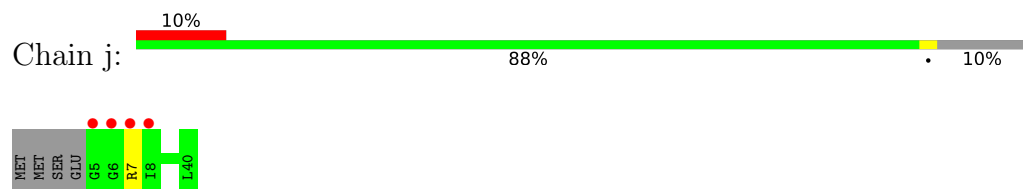
- Molecule 8: Photosystem II reaction center protein I



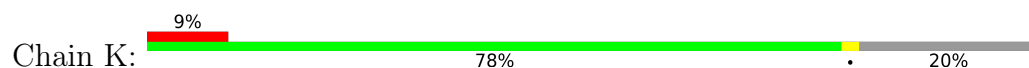
- Molecule 9: Photosystem II reaction center protein J

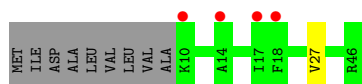


- Molecule 9: Photosystem II reaction center protein J

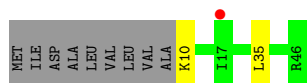
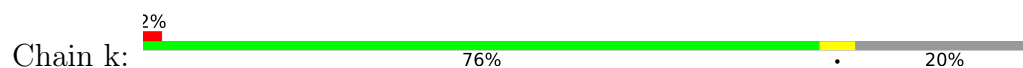


- Molecule 10: Photosystem II reaction center protein K





- Molecule 10: Photosystem II reaction center protein K

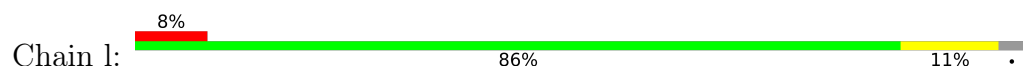


- Molecule 11: Photosystem II reaction center protein L

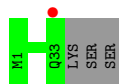


There are no outlier residues recorded for this chain.

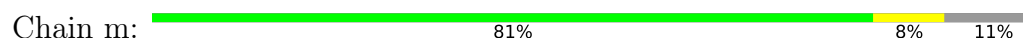
- Molecule 11: Photosystem II reaction center protein L



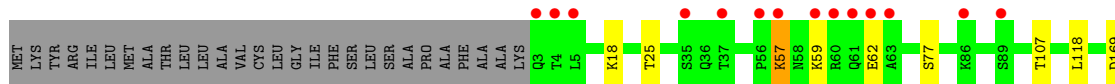
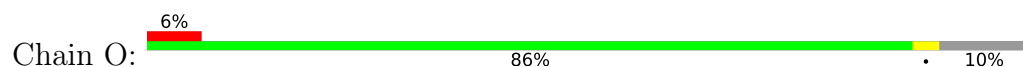
- Molecule 12: Photosystem II reaction center protein M



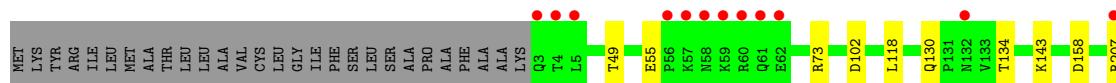
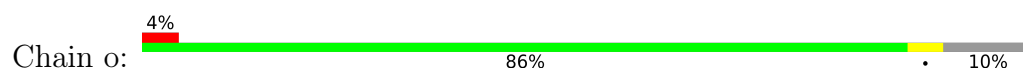
- Molecule 12: Photosystem II reaction center protein M



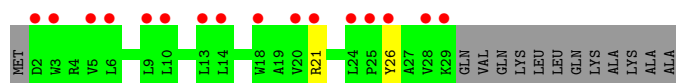
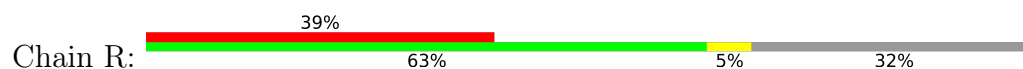
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



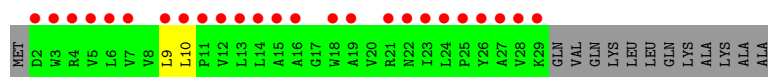
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



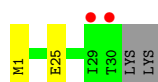
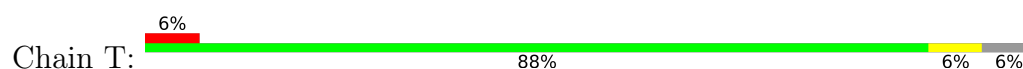
- Molecule 14: Photosystem II protein Y



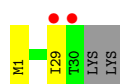
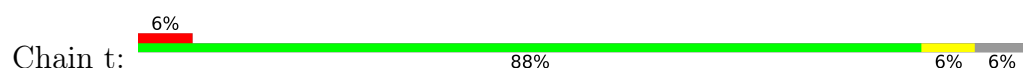
- Molecule 14: Photosystem II protein Y



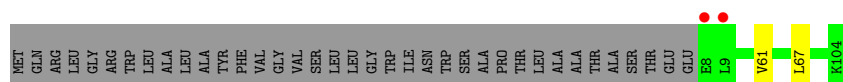
- Molecule 15: Photosystem II reaction center protein T



- Molecule 15: Photosystem II reaction center protein T

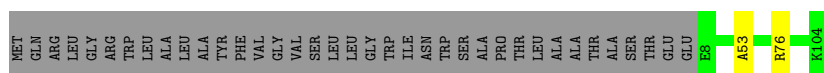


- Molecule 16: Photosystem II 12 kDa extrinsic protein

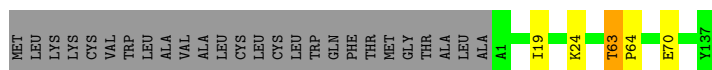
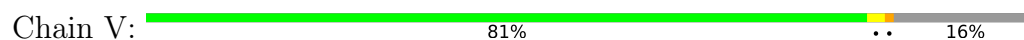


- Molecule 16: Photosystem II 12 kDa extrinsic protein

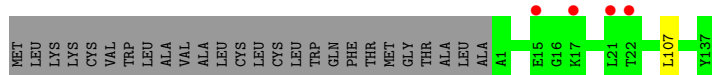
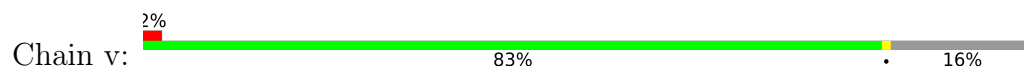




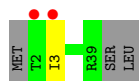
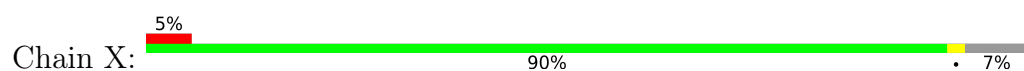
- Molecule 17: Cytochrome c-550



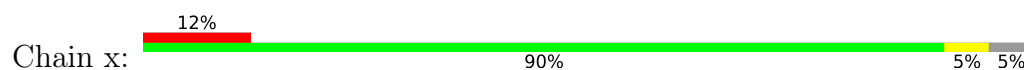
- Molecule 17: Cytochrome c-550



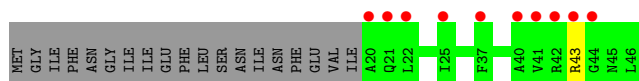
- Molecule 18: Photosystem II reaction center X protein



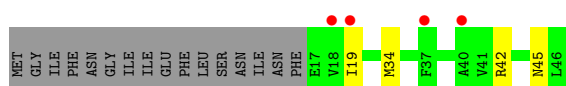
- Molecule 18: Photosystem II reaction center X protein



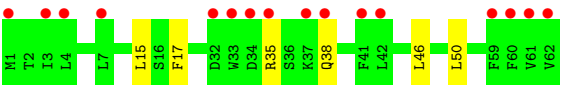
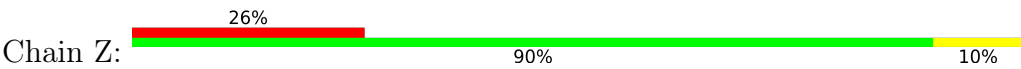
- Molecule 19: Photosystem II reaction center protein Ycf12



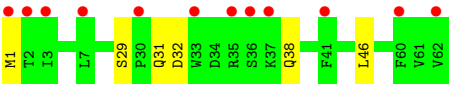
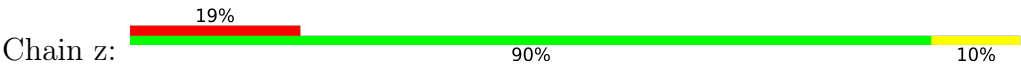
- Molecule 19: Photosystem II reaction center protein Ycf12



- Molecule 20: Photosystem II reaction center protein Z



• Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.92Å 221.63Å 307.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.64 – 2.08 33.64 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.6 (33.64-2.08) 85.1 (33.64-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.55 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.185 , 0.238 0.185 , 0.238	Depositor DCC
R_{free} test set	4226 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	103670	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.62	0/2707	0.66	1/3692 (0.0%)
1	a	0.62	0/2704	0.66	0/3688
2	B	0.61	0/4161	0.66	0/5669
2	b	0.60	0/4118	0.66	0/5611
3	C	0.59	0/3547	0.65	0/4830
3	c	0.57	0/3619	0.64	0/4926
4	D	0.63	1/2812 (0.0%)	0.67	0/3832
4	d	0.59	0/2821	0.65	0/3844
5	E	0.59	0/688	0.67	0/940
5	e	0.54	0/683	0.63	0/932
6	F	0.65	0/284	0.62	0/387
6	f	0.47	0/284	0.66	0/387
7	H	0.72	0/523	0.70	0/713
7	h	0.69	0/511	0.72	0/697
8	I	0.67	0/293	0.70	0/396
8	i	0.75	0/293	0.75	0/396
9	J	0.59	0/263	0.65	0/356
9	j	0.59	0/263	0.70	0/356
10	K	0.53	0/303	0.64	0/416
10	k	0.55	0/303	0.67	0/416
11	L	0.71	0/311	0.72	0/422
11	l	0.76	0/303	0.75	0/412
12	M	0.76	0/249	0.79	0/341
12	m	0.72	0/244	0.72	0/334
13	O	0.69	1/1904 (0.1%)	0.78	1/2585 (0.0%)
13	o	0.65	0/1905	0.79	2/2583 (0.1%)
14	R	0.48	0/227	0.60	0/313
14	r	0.44	0/227	0.59	0/313
15	T	0.78	0/257	0.74	0/349
15	t	0.77	0/255	0.69	0/346
16	U	0.61	0/785	0.70	0/1064
16	u	0.71	0/785	0.76	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	V	0.65	0/1085	0.76	1/1473 (0.1%)
17	v	0.62	0/1085	0.66	0/1473
18	X	0.56	0/284	0.65	0/384
18	x	0.46	0/289	0.59	0/391
19	Y	0.50	0/197	0.67	0/264
19	y	0.45	0/219	0.58	0/294
20	Z	0.51	0/490	0.57	0/669
20	z	0.48	0/488	0.56	0/666
All	All	0.61	2/42769 (0.0%)	0.68	5/58224 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
17	V	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	211	CYS	CB-SG	-5.97	1.72	1.81
13	O	77	SER	CB-OG	-5.16	1.35	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	V	63	THR	C-N-CD	-7.21	104.74	120.60
13	O	169	ASP	CB-CG-OD1	6.47	124.12	118.30
13	o	158	ASP	CB-CG-OD1	5.82	123.54	118.30
1	A	183	MET	CA-CB-CG	5.56	122.75	113.30
13	o	102	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	V	63	THR	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/344 (96%)	326 (98%)	5 (2%)	1 (0%)	41	39
1	a	332/344 (96%)	325 (98%)	7 (2%)	0	100	100
2	B	508/510 (100%)	503 (99%)	5 (1%)	0	100	100
2	b	503/510 (99%)	494 (98%)	9 (2%)	0	100	100
3	C	442/461 (96%)	434 (98%)	7 (2%)	1 (0%)	47	47
3	c	451/461 (98%)	438 (97%)	12 (3%)	1 (0%)	47	47
4	D	339/352 (96%)	331 (98%)	8 (2%)	0	100	100
4	d	340/352 (97%)	331 (97%)	9 (3%)	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%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	31 (91%)	3 (9%)	0	100	100
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	226 (93%)	14 (6%)	3 (1%)	13	7
13	o	242/272 (89%)	233 (96%)	8 (3%)	1 (0%)	34	31
14	R	26/41 (63%)	26 (100%)	0	0	100	100
14	r	26/41 (63%)	25 (96%)	1 (4%)	0	100	100
15	T	28/32 (88%)	28 (100%)	0	0	100	100
15	t	28/32 (88%)	26 (93%)	2 (7%)	0	100	100
16	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
16	u	95/134 (71%)	92 (97%)	2 (2%)	1 (1%)	14	8
17	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	22	17
17	v	135/163 (83%)	132 (98%)	3 (2%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Y	25/46 (54%)	24 (96%)	0	1 (4%)	3	1
19	y	28/46 (61%)	24 (86%)	3 (11%)	1 (4%)	3	1
20	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
20	z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
All	All	5231/5700 (92%)	5092 (97%)	128 (2%)	11 (0%)	47	47

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
13	O	59	LYS
13	O	62	GLU
17	V	64	PRO
3	c	416	SER
16	u	53	ALA
19	Y	43	ARG
19	y	42	ARG
13	O	57	LYS
13	o	73	ARG
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%)	267 (99%)	3 (1%)	73	78
1	a	269/280 (96%)	259 (96%)	10 (4%)	34	34
2	B	408/407 (100%)	401 (98%)	7 (2%)	60	65
2	b	402/407 (99%)	389 (97%)	13 (3%)	39	40
3	C	346/362 (96%)	338 (98%)	8 (2%)	50	53
3	c	354/362 (98%)	342 (97%)	12 (3%)	37	37
4	D	276/283 (98%)	272 (99%)	4 (1%)	67	72
4	d	277/283 (98%)	269 (97%)	8 (3%)	42	44
5	E	72/73 (99%)	70 (97%)	2 (3%)	43	46
5	e	71/73 (97%)	68 (96%)	3 (4%)	30	29
6	F	28/39 (72%)	27 (96%)	1 (4%)	35	35
6	f	28/39 (72%)	26 (93%)	2 (7%)	14	11
7	H	54/55 (98%)	53 (98%)	1 (2%)	57	61
7	h	53/55 (96%)	49 (92%)	4 (8%)	13	9
8	I	32/34 (94%)	30 (94%)	2 (6%)	18	14
8	i	32/34 (94%)	31 (97%)	1 (3%)	40	41
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	23 (96%)	1 (4%)	30	29
10	K	30/37 (81%)	29 (97%)	1 (3%)	38	39
10	k	30/37 (81%)	28 (93%)	2 (7%)	16	12
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	2
12	M	28/32 (88%)	28 (100%)	0	100	100
12	m	28/32 (88%)	26 (93%)	2 (7%)	14	11
13	O	206/228 (90%)	200 (97%)	6 (3%)	42	44
13	o	207/228 (91%)	200 (97%)	7 (3%)	37	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	R	22/33 (67%)	20 (91%)	2 (9%)	9	6
14	r	22/33 (67%)	20 (91%)	2 (9%)	9	6
15	T	26/28 (93%)	25 (96%)	1 (4%)	33	33
15	t	25/28 (89%)	24 (96%)	1 (4%)	31	31
16	U	84/112 (75%)	82 (98%)	2 (2%)	49	52
16	u	84/112 (75%)	84 (100%)	0	100	100
17	V	117/138 (85%)	115 (98%)	2 (2%)	60	65
17	v	117/138 (85%)	116 (99%)	1 (1%)	78	83
18	X	31/34 (91%)	30 (97%)	1 (3%)	39	40
18	x	31/34 (91%)	29 (94%)	2 (6%)	17	13
19	Y	19/37 (51%)	19 (100%)	0	100	100
19	y	22/37 (60%)	19 (86%)	3 (14%)	3	1
20	Z	52/52 (100%)	46 (88%)	6 (12%)	5	3
20	z	51/52 (98%)	45 (88%)	6 (12%)	5	2
All	All	4321/4654 (93%)	4188 (97%)	133 (3%)	41	41

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	121	LEU
1	A	238	LYS
2	B	127	ARG
2	B	240	SER
2	B	362	PHE
2	B	371	THR
2	B	385	ARG
2	B	405	GLU
2	B	476	ARG
3	C	104	GLU
3	C	130	VAL
3	C	141	GLU
3	C	240	ILE
3	C	289	PHE
3	C	315	MET
3	C	416	SER
3	C	418	ASN

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Mol	Chain	Res	Type
4	D	43	LEU
4	D	180	ARG
4	D	264	LYS
4	D	295	SER
5	E	22[A]	ILE
5	E	22[B]	ILE
6	F	25	THR
7	H	49	TYR
8	I	4	LEU
8	I	6	ILE
10	K	27	VAL
13	O	18	LYS
13	O	25	THR
13	O	57	LYS
13	O	107	THR
13	O	118	LEU
13	O	214	THR
14	R	21	ARG
14	R	26	TYR
15	T	25	GLU
16	U	61	VAL
16	U	67	LEU
17	V	19	ILE
17	V	24	LYS
18	X	3	ILE
20	Z	15	LEU
20	Z	17	PHE
20	Z	35	ARG
20	Z	38	GLN
20	Z	46	LEU
20	Z	50	LEU
1	a	16	ARG
1	a	28	LEU
1	a	42	LEU
1	a	159	LEU
1	a	200	LEU
1	a	223	LEU
1	a	229	GLU
1	a	242	GLU
1	a	245	THR
1	a	288	LEU
2	b	74	SER

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Mol	Chain	Res	Type
2	b	80	ILE
2	b	83	GLU
2	b	98	LEU
2	b	128	THR
2	b	161	LEU
2	b	236	THR
2	b	362	PHE
2	b	413	ASP
2	b	485	GLU
2	b	492	GLU
2	b	505	ARG
2	b	506	ARG
3	c	24	THR
3	c	72	LEU
3	c	78	GLU
3	c	99	VAL
3	c	124	VAL
3	c	125	LEU
3	c	165	LEU
3	c	289	PHE
3	c	315	MET
3	c	391[A]	ARG
3	c	391[B]	ARG
3	c	416	SER
4	d	90	LEU
4	d	180	ARG
4	d	230	SER
4	d	259	ILE
4	d	291	LEU
4	d	293	LEU
4	d	307	GLU
4	d	321	LEU
5	e	4	THR
5	e	66	VAL
5	e	83	LEU
6	f	15	ILE
6	f	23	VAL
7	h	3	ARG
7	h	7	LEU
7	h	39	LEU
7	h	49	TYR
8	i	2	GLU

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Mol	Chain	Res	Type
9	j	7	ARG
10	k	10	LYS
10	k	35	LEU
11	l	2	GLU
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
12	m	16	LEU
13	o	49	THR
13	o	55	GLU
13	o	118	LEU
13	o	130	GLN
13	o	134	THR
13	o	143	LYS
13	o	207	ARG
14	r	9	LEU
14	r	10	LEU
15	t	29	ILE
17	v	107	LEU
18	x	2	THR
18	x	15	LEU
19	y	19	ILE
19	y	34	MET
19	y	45	ASN
20	z	1	MET
20	z	29	SER
20	z	31	GLN
20	z	32	ASP
20	z	38	GLN
20	z	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	ASN
1	A	338	ASN
3	C	327	ASN
11	L	8	GLN
14	R	22	ASN
20	Z	6	GLN
20	Z	31	GLN

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Mol	Chain	Res	Type
20	Z	38	GLN
1	a	181	ASN
1	a	234	ASN
2	b	409	GLN
3	c	28	GLN
4	d	338	ASN
5	e	60	GLN
16	u	37	GLN
20	z	58	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	$\# Z > 2$
12	FME	m	1	12	8,9,10	1.13	1 (12%)	7,9,11	0.53	0
8	FME	I	1	8	8,9,10	0.94	0	7,9,11	0.97	0
8	FME	i	1	8	8,9,10	1.27	1 (12%)	7,9,11	1.04	0
15	FME	T	1	15	8,9,10	1.13	1 (12%)	7,9,11	0.77	0
12	FME	M	1	12	8,9,10	1.00	0	7,9,11	0.67	0
15	FME	t	1	15	8,9,10	1.26	2 (25%)	7,9,11	0.99	0

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

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	i	1	FME	CA-N	-2.98	1.42	1.46
12	m	1	FME	CA-N	-2.43	1.42	1.46
15	t	1	FME	CA-N	-2.23	1.43	1.46
15	t	1	FME	CB-CA	2.19	1.57	1.53
15	T	1	FME	CN-N	2.08	1.40	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	T	1	FME	O-C-CA-CB
15	t	1	FME	CB-CG-SD-CE
15	T	1	FME	CB-CG-SD-CE
8	i	1	FME	CA-CB-CG-SD
8	I	1	FME	C-CA-CB-CG
8	i	1	FME	C-CA-CB-CG
8	I	1	FME	CA-CB-CG-SD
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 187 ligands modelled in this entry, 6 are monoatomic - leaving 181 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$
22	CLA	C	510	-	56,73,73	1.52	9 (16%)	55,113,113	1.46	8 (14%)
22	CLA	b	605	-	56,73,73	1.54	7 (12%)	55,113,113	1.76	15 (27%)
22	CLA	A	406	-	45,62,73	1.94	10 (22%)	41,99,113	2.06	11 (26%)
29	LHG	d	409	-	38,38,48	1.00	2 (5%)	41,44,54	1.05	4 (9%)
22	CLA	B	615	-	56,73,73	1.61	10 (17%)	55,113,113	1.47	9 (16%)
32	STE	D	412	-	16,19,19	0.31	0	15,19,19	0.88	0
34	HEM	F	101	5,6	27,50,50	1.96	4 (14%)	17,82,82	2.07	7 (41%)
28	SQD	A	412	-	51,52,54	1.08	5 (9%)	60,63,65	1.68	8 (13%)
29	LHG	d	408	-	48,48,48	0.90	1 (2%)	51,54,54	1.13	2 (3%)
32	STE	b	626	-	9,9,19	0.48	0	8,8,19	0.60	0
29	LHG	l	101	-	48,48,48	0.60	0	51,54,54	1.24	6 (11%)
32	STE	B	623	-	8,11,19	0.40	0	7,11,19	0.89	0
22	CLA	b	612	-	56,73,73	1.40	4 (7%)	55,113,113	1.72	12 (21%)
24	BCR	c	514	-	41,41,41	1.15	2 (4%)	56,56,56	1.11	4 (7%)
22	CLA	b	616	-	51,68,73	1.58	9 (17%)	49,107,113	2.03	11 (22%)
32	STE	B	626	-	8,11,19	0.34	0	7,11,19	0.69	0
22	CLA	b	608	-	56,73,73	1.65	8 (14%)	55,113,113	1.85	13 (23%)
32	STE	b	622	-	16,19,19	0.38	0	15,19,19	0.81	0
22	CLA	b	611	-	56,73,73	1.48	7 (12%)	55,113,113	1.85	7 (12%)
32	STE	T	102	-	14,14,19	0.41	0	13,13,19	0.82	0
24	BCR	t	101	-	41,41,41	1.04	2 (4%)	56,56,56	1.55	11 (19%)
32	STE	M	102	-	11,14,19	0.60	0	10,14,19	0.46	0
32	STE	C	520	-	8,11,19	0.37	0	7,11,19	0.89	0
32	STE	E	101	-	8,11,19	0.57	0	7,11,19	0.32	0
22	CLA	b	615	-	56,73,73	2.01	8 (14%)	55,113,113	1.70	8 (14%)
29	LHG	A	413	-	48,48,48	0.98	3 (6%)	51,54,54	1.18	2 (3%)
28	SQD	f	102	-	40,41,54	1.15	4 (10%)	49,52,65	1.99	11 (22%)
22	CLA	B	601	36	56,73,73	1.93	9 (16%)	55,113,113	1.67	7 (12%)
30	DGD	o	301	-	43,43,67	1.11	2 (4%)	45,45,81	1.48	5 (11%)
22	CLA	c	505	-	56,73,73	1.46	5 (8%)	55,113,113	1.68	10 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	C	514	-	41,41,41	1.21	3 (7%)	56,56,56	1.28	6 (10%)
22	CLA	B	606	-	56,73,73	1.59	8 (14%)	55,113,113	1.75	12 (21%)
32	STE	c	520	-	16,19,19	0.37	0	15,19,19	0.69	0
22	CLA	c	502	-	56,73,73	1.64	10 (17%)	55,113,113	1.64	11 (20%)
24	BCR	b	617	-	41,41,41	1.21	3 (7%)	56,56,56	1.34	8 (14%)
26	PL9	D	406	-	55,55,55	1.46	6 (10%)	68,69,69	1.71	16 (23%)
22	CLA	C	504	36	50,67,73	1.65	8 (16%)	47,105,113	1.68	13 (27%)
30	DGD	C	515	-	63,63,67	1.64	14 (22%)	77,77,81	1.47	12 (15%)
22	CLA	c	509	-	56,73,73	1.47	5 (8%)	55,113,113	1.93	11 (20%)
32	STE	j	101	-	8,11,19	0.56	0	7,11,19	0.55	0
22	CLA	D	403	36	56,73,73	1.59	5 (8%)	55,113,113	1.65	9 (16%)
22	CLA	B	611	-	56,73,73	1.61	10 (17%)	55,113,113	1.68	13 (23%)
22	CLA	A	402	-	56,73,73	1.50	8 (14%)	55,113,113	1.64	10 (18%)
27	LMG	a	414	-	49,49,55	1.00	5 (10%)	57,57,63	1.33	7 (12%)
28	SQD	F	102	-	35,36,54	0.99	3 (8%)	42,45,65	1.96	10 (23%)
24	BCR	K	101	-	41,41,41	1.12	3 (7%)	56,56,56	1.34	6 (10%)
27	LMG	M	101	-	51,51,55	1.10	2 (3%)	59,59,63	1.43	7 (11%)
22	CLA	D	404	-	56,73,73	1.54	8 (14%)	55,113,113	1.35	6 (10%)
22	CLA	D	402	-	56,73,73	1.42	5 (8%)	55,113,113	1.67	11 (20%)
32	STE	c	522	-	8,11,19	0.40	0	7,11,19	0.84	0
24	BCR	B	619	-	41,41,41	1.20	2 (4%)	56,56,56	1.42	7 (12%)
27	LMG	c	521	-	48,48,55	1.24	6 (12%)	56,56,63	1.19	4 (7%)
22	CLA	c	508	-	55,72,73	1.60	7 (12%)	53,111,113	1.61	11 (20%)
27	LMG	m	101	-	51,51,55	1.12	6 (11%)	59,59,63	1.48	11 (18%)
22	CLA	c	507	36	56,73,73	1.57	10 (17%)	55,113,113	1.58	10 (18%)
24	BCR	K	102	-	41,41,41	1.02	2 (4%)	56,56,56	1.16	3 (5%)
33	BCT	D	401	21	0,3,3	-	-	0,3,3	-	-
24	BCR	c	515	-	41,41,41	1.26	4 (9%)	56,56,56	1.28	5 (8%)
22	CLA	B	612	-	56,73,73	1.54	6 (10%)	55,113,113	1.81	11 (20%)
26	PL9	d	407	-	55,55,55	1.54	8 (14%)	68,69,69	1.83	15 (22%)
28	SQD	b	620	-	48,49,54	0.94	2 (4%)	57,60,65	2.39	14 (24%)
22	CLA	C	503	-	56,73,73	1.85	10 (17%)	55,113,113	1.70	11 (20%)
22	CLA	c	506	-	56,73,73	1.63	7 (12%)	55,113,113	1.46	7 (12%)
27	LMG	b	623	-	55,55,55	1.02	4 (7%)	63,63,63	1.74	11 (17%)
22	CLA	a	403	36	56,73,73	1.55	6 (10%)	55,113,113	1.65	11 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	C	502	-	56,73,73	1.73	6 (10%)	55,113,113	1.48	9 (16%)
30	DGD	A	415	-	67,67,67	1.41	10 (14%)	81,81,81	1.50	16 (19%)
26	PL9	a	409	-	55,55,55	1.30	3 (5%)	68,69,69	1.84	16 (23%)
22	CLA	b	601	36	56,73,73	1.79	9 (16%)	55,113,113	1.66	9 (16%)
24	BCR	d	406	-	41,41,41	1.25	2 (4%)	56,56,56	1.22	5 (8%)
23	PHO	a	404	-	67,69,69	1.07	8 (11%)	85,99,99	1.17	8 (9%)
24	BCR	T	101	-	41,41,41	1.22	4 (9%)	56,56,56	1.14	3 (5%)
27	LMG	D	410	-	31,31,55	1.17	3 (9%)	33,33,63	1.13	1 (3%)
22	CLA	C	509	-	56,73,73	1.54	8 (14%)	55,113,113	1.63	7 (12%)
22	CLA	B	603	-	56,73,73	1.49	9 (16%)	55,113,113	1.53	10 (18%)
22	CLA	B	613	-	56,73,73	1.67	8 (14%)	55,113,113	1.78	10 (18%)
22	CLA	a	402	-	56,73,73	1.71	6 (10%)	55,113,113	1.65	10 (18%)
22	CLA	b	613	-	56,73,73	1.71	7 (12%)	55,113,113	1.85	12 (21%)
24	BCR	B	617	-	41,41,41	1.13	3 (7%)	56,56,56	1.21	4 (7%)
22	CLA	b	609	-	56,73,73	1.66	10 (17%)	55,113,113	1.55	10 (18%)
24	BCR	k	102	-	41,41,41	1.03	2 (4%)	56,56,56	1.17	4 (7%)
32	STE	B	624	-	14,17,19	0.43	0	13,17,19	0.82	0
22	CLA	B	608	-	56,73,73	1.78	9 (16%)	55,113,113	1.61	9 (16%)
32	STE	C	519	-	15,15,19	0.67	0	14,14,19	0.27	0
30	DGD	H	102	-	63,63,67	1.32	8 (12%)	77,77,81	1.57	13 (16%)
24	BCR	k	101	-	41,41,41	1.01	3 (7%)	56,56,56	1.07	3 (5%)
32	STE	a	413	-	9,9,19	0.60	0	8,8,19	0.38	0
35	HEC	v	201	17	26,50,50	2.46	7 (26%)	18,82,82	2.14	6 (33%)
30	DGD	c	517	-	63,63,67	1.17	8 (12%)	77,77,81	1.39	10 (12%)
29	LHG	a	410	-	48,48,48	1.01	4 (8%)	51,54,54	1.42	6 (11%)
22	CLA	C	507	36	56,73,73	1.62	7 (12%)	55,113,113	1.92	13 (23%)
32	STE	C	518	-	8,11,19	0.44	0	7,11,19	0.73	0
23	PHO	A	405	-	67,69,69	1.22	8 (11%)	85,99,99	1.14	6 (7%)
22	CLA	C	513	-	56,73,73	1.62	9 (16%)	55,113,113	1.65	9 (16%)
22	CLA	b	606	-	56,73,73	1.83	8 (14%)	55,113,113	1.73	12 (21%)
22	CLA	b	603	-	56,73,73	1.60	7 (12%)	55,113,113	1.72	12 (21%)
30	DGD	C	517	-	63,63,67	1.27	7 (11%)	77,77,81	1.40	10 (12%)
28	SQD	a	411	-	53,54,54	0.99	5 (9%)	62,65,65	2.21	15 (24%)
32	STE	m	102	-	8,11,19	0.48	0	7,11,19	0.80	0
29	LHG	L	101	-	48,48,48	0.88	2 (4%)	51,54,54	1.17	3 (5%)
27	LMG	c	519	-	37,37,55	1.23	5 (13%)	45,45,63	1.38	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	b	618	-	41,41,41	1.20	2 (4%)	56,56,56	1.23	6 (10%)
22	CLA	b	610	36	56,73,73	1.45	8 (14%)	55,113,113	1.59	12 (21%)
32	STE	d	411	-	13,16,19	0.38	0	12,16,19	0.72	0
32	STE	B	627	-	12,15,19	0.40	0	11,15,19	0.88	0
22	CLA	d	405	-	56,73,73	1.57	8 (14%)	55,113,113	1.48	12 (21%)
22	CLA	c	503	-	56,73,73	1.55	8 (14%)	55,113,113	1.75	15 (27%)
32	STE	a	415	-	8,11,19	0.38	0	7,11,19	0.86	0
22	CLA	b	614	-	56,73,73	1.58	9 (16%)	55,113,113	1.38	9 (16%)
27	LMG	Y	101	-	48,48,55	0.95	2 (4%)	56,56,63	1.47	10 (17%)
26	PL9	A	410	-	55,55,55	0.87	2 (3%)	68,69,69	1.53	15 (22%)
22	CLA	B	604	-	56,73,73	1.42	6 (10%)	55,113,113	1.97	14 (25%)
24	BCR	A	407	-	41,41,41	1.18	3 (7%)	56,56,56	1.40	8 (14%)
24	BCR	B	618	-	41,41,41	1.10	2 (4%)	56,56,56	1.37	6 (10%)
28	SQD	a	412	-	35,35,54	1.23	2 (5%)	37,37,65	1.66	6 (16%)
32	STE	b	621	-	15,15,19	0.47	0	14,14,19	0.69	0
22	CLA	B	605	-	56,73,73	1.46	9 (16%)	55,113,113	1.87	15 (27%)
23	PHO	A	404	-	67,69,69	1.24	11 (16%)	85,99,99	1.07	5 (5%)
32	STE	J	101	-	8,11,19	0.31	0	7,11,19	0.88	0
23	PHO	d	401	-	67,69,69	1.26	9 (13%)	85,99,99	1.28	9 (10%)
22	CLA	B	607	36	56,73,73	1.29	9 (16%)	55,113,113	1.63	9 (16%)
32	STE	B	622	-	10,13,19	0.42	0	9,13,19	0.80	0
22	CLA	c	511	3	56,73,73	1.87	7 (12%)	55,113,113	1.71	8 (14%)
24	BCR	H	101	-	41,41,41	0.99	1 (2%)	56,56,56	1.24	7 (12%)
28	SQD	B	621	-	53,54,54	1.00	3 (5%)	62,65,65	1.80	12 (19%)
22	CLA	B	616	-	51,68,73	1.92	9 (17%)	49,107,113	1.93	12 (24%)
34	HEM	f	101	5,6	27,50,50	1.98	4 (14%)	17,82,82	2.34	5 (29%)
22	CLA	C	506	-	56,73,73	1.84	10 (17%)	55,113,113	1.52	9 (16%)
22	CLA	a	405	-	56,73,73	1.68	7 (12%)	55,113,113	1.67	12 (21%)
32	STE	H	103	-	17,17,19	0.39	0	16,16,19	0.84	0
22	CLA	C	511	3	56,73,73	1.60	7 (12%)	55,113,113	1.59	6 (10%)
33	BCT	d	402	21	0,3,3	-	-	0,3,3	-	-
27	LMG	A	411	-	48,48,55	1.02	1 (2%)	56,56,63	1.44	7 (12%)
22	CLA	B	614	-	56,73,73	1.67	7 (12%)	55,113,113	1.56	12 (21%)
24	BCR	b	619	-	41,41,41	1.17	2 (4%)	56,56,56	1.34	9 (16%)
22	CLA	B	610	36	56,73,73	1.69	9 (16%)	55,113,113	1.72	12 (21%)
22	CLA	d	404	36	56,73,73	1.70	6 (10%)	55,113,113	1.85	10 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	c	513	-	56,73,73	1.67	9 (16%)	55,113,113	1.38	8 (14%)
29	LHG	D	411	-	48,48,48	0.85	3 (6%)	51,54,54	1.36	8 (15%)
32	STE	B	620	-	13,16,19	0.52	0	12,16,19	0.61	0
29	LHG	D	409	-	46,46,48	0.95	3 (6%)	49,52,54	1.23	5 (10%)
31	OEX	a	416	36,3,1	0,15,15	-	-	-	-	-
30	DGD	c	516	-	63,63,67	1.38	6 (9%)	77,77,81	1.29	6 (7%)
22	CLA	c	501	-	56,73,73	1.55	6 (10%)	55,113,113	1.90	13 (23%)
27	LMG	d	410	-	44,44,55	1.23	5 (11%)	52,52,63	1.41	5 (9%)
27	LMG	h	102	-	18,21,55	0.70	0	16,20,63	0.92	0
31	OEX	A	416	36,3,1	0,15,15	-	-	-	-	-
30	DGD	C	516	-	63,63,67	1.28	7 (11%)	77,77,81	1.44	9 (11%)
30	DGD	h	103	-	63,63,67	1.23	8 (12%)	77,77,81	1.38	10 (12%)
22	CLA	c	512	-	56,73,73	1.54	7 (12%)	55,113,113	1.52	11 (20%)
32	STE	b	624	-	12,15,19	0.52	0	11,15,19	0.57	0
35	HEC	V	201	17	26,50,50	2.32	3 (11%)	18,82,82	2.04	5 (27%)
22	CLA	A	403	36	56,73,73	1.61	8 (14%)	55,113,113	1.54	10 (18%)
22	CLA	b	602	-	56,73,73	1.67	9 (16%)	55,113,113	1.61	8 (14%)
22	CLA	c	510	-	56,73,73	1.57	8 (14%)	55,113,113	1.80	9 (16%)
29	LHG	D	408	-	48,48,48	0.96	2 (4%)	51,54,54	1.26	7 (13%)
32	STE	D	413	-	11,14,19	0.40	0	10,14,19	0.95	0
24	BCR	K	103	-	41,41,41	1.10	3 (7%)	56,56,56	1.31	10 (17%)
28	SQD	A	414	-	38,38,54	1.07	3 (7%)	40,40,65	1.34	3 (7%)
32	STE	M	104	-	17,17,19	0.36	0	16,16,19	0.86	0
22	CLA	B	609	-	56,73,73	1.44	9 (16%)	55,113,113	1.64	9 (16%)
24	BCR	a	406	-	41,41,41	1.21	4 (9%)	56,56,56	1.19	5 (8%)
24	BCR	h	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.46	8 (14%)
22	CLA	b	607	36	56,73,73	1.59	9 (16%)	55,113,113	1.43	9 (16%)
22	CLA	d	403	-	56,73,73	1.50	7 (12%)	55,113,113	1.37	10 (18%)
22	CLA	b	604	-	56,73,73	1.77	6 (10%)	55,113,113	1.96	12 (21%)
30	DGD	c	518	-	63,63,67	1.21	6 (9%)	77,77,81	1.47	12 (15%)
32	STE	B	625	-	15,15,19	0.47	0	14,14,19	0.70	0
32	STE	d	412	-	16,19,19	0.51	0	15,19,19	0.52	0
32	STE	b	625	-	16,19,19	0.51	0	15,19,19	0.58	0
22	CLA	C	508	-	56,73,73	1.75	6 (10%)	55,113,113	1.69	10 (18%)
32	STE	I	101	-	14,14,19	0.58	0	13,13,19	0.35	0
29	LHG	e	101	-	41,41,48	0.98	3 (7%)	44,47,54	1.22	4 (9%)
22	CLA	C	501	-	56,73,73	1.85	10 (17%)	55,113,113	1.59	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	D	405	-	41,41,41	1.22	2 (4%)	56,56,56	1.18	6 (10%)
32	STE	M	103	-	9,9,19	0.52	0	8,8,19	0.64	0
22	CLA	C	505	-	56,73,73	1.51	6 (10%)	55,113,113	1.83	11 (20%)
22	CLA	C	512	-	56,73,73	1.53	6 (10%)	55,113,113	1.50	11 (20%)
27	LMG	D	407	-	51,51,55	1.00	1 (1%)	59,59,63	1.33	8 (13%)
22	CLA	c	504	36	51,68,73	1.66	7 (13%)	49,107,113	1.72	11 (22%)
22	CLA	B	602	-	56,73,73	1.63	8 (14%)	55,113,113	1.70	9 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	510	-	1/1/20/20	9/37/115/115	-
22	CLA	b	605	-	1/1/20/20	6/37/115/115	-
22	CLA	A	406	-	1/1/17/20	3/24/102/115	-
29	LHG	d	409	-	-	13/43/43/53	-
22	CLA	B	615	-	1/1/20/20	7/37/115/115	-
32	STE	D	412	-	-	7/15/17/17	-
34	HEM	F	101	5,6	-	0/6/54/54	-
28	SQD	A	412	-	-	15/47/67/69	0/1/1/1
29	LHG	d	408	-	-	21/53/53/53	-
32	STE	b	626	-	-	4/7/7/17	-
29	LHG	l	101	-	-	21/53/53/53	-
32	STE	B	623	-	-	3/7/9/17	-
22	CLA	b	612	-	1/1/20/20	7/37/115/115	-
24	BCR	c	514	-	-	7/29/63/63	0/2/2/2
22	CLA	b	616	-	1/1/19/20	13/31/109/115	-
32	STE	B	626	-	-	3/7/9/17	-
22	CLA	b	608	-	-	6/37/115/115	-
32	STE	b	622	-	-	10/15/17/17	-
22	CLA	b	611	-	1/1/20/20	7/37/115/115	-
32	STE	T	102	-	-	7/12/12/17	-
24	BCR	t	101	-	-	2/29/63/63	0/2/2/2
32	STE	M	102	-	-	5/10/12/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	STE	C	520	-	-	3/7/9/17	-
32	STE	E	101	-	-	4/7/9/17	-
22	CLA	b	615	-	1/1/20/20	9/37/115/115	-
29	LHG	A	413	-	-	29/53/53/53	-
28	SQD	f	102	-	-	18/36/56/69	0/1/1/1
22	CLA	B	601	36	1/1/20/20	20/37/115/115	-
30	DGD	o	301	-	-	20/45/45/95	-
22	CLA	c	505	-	1/1/20/20	8/37/115/115	-
24	BCR	C	514	-	-	11/29/63/63	0/2/2/2
22	CLA	B	606	-	1/1/20/20	15/37/115/115	-
32	STE	c	520	-	-	11/15/17/17	-
22	CLA	c	502	-	-	8/37/115/115	-
24	BCR	b	617	-	-	5/29/63/63	0/2/2/2
26	PL9	D	406	-	-	12/53/73/73	0/1/1/1
22	CLA	C	504	36	1/1/18/20	5/30/108/115	-
30	DGD	C	515	-	-	19/51/91/95	0/2/2/2
22	CLA	c	509	-	1/1/20/20	15/37/115/115	-
32	STE	j	101	-	-	3/7/9/17	-
22	CLA	D	403	36	-	9/37/115/115	-
22	CLA	B	611	-	1/1/20/20	6/37/115/115	-
22	CLA	A	402	-	1/1/20/20	3/37/115/115	-
27	LMG	a	414	-	-	23/44/64/70	0/1/1/1
28	SQD	F	102	-	-	12/28/48/69	0/1/1/1
24	BCR	K	101	-	-	9/29/63/63	0/2/2/2
27	LMG	M	101	-	-	24/46/66/70	0/1/1/1
22	CLA	D	404	-	1/1/20/20	14/37/115/115	-
22	CLA	D	402	-	-	6/37/115/115	-
32	STE	c	522	-	-	4/7/9/17	-
24	BCR	B	619	-	-	3/29/63/63	0/2/2/2
27	LMG	c	521	-	-	25/43/63/70	0/1/1/1
22	CLA	c	508	-	-	9/36/114/115	-
27	LMG	m	101	-	-	16/46/66/70	0/1/1/1
22	CLA	c	507	36	1/1/20/20	11/37/115/115	-
24	BCR	K	102	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	c	515	-	-	2/29/63/63	0/2/2/2
22	CLA	B	612	-	1/1/20/20	11/37/115/115	-
26	PL9	d	407	-	-	13/53/73/73	0/1/1/1
28	SQD	b	620	-	-	23/44/64/69	0/1/1/1
22	CLA	C	503	-	1/1/20/20	5/37/115/115	-
22	CLA	c	506	-	1/1/20/20	15/37/115/115	-
27	LMG	b	623	-	-	24/50/70/70	0/1/1/1
22	CLA	a	403	36	1/1/20/20	15/37/115/115	-
22	CLA	C	502	-	1/1/20/20	10/37/115/115	-
30	DGD	A	415	-	-	34/55/95/95	0/2/2/2
26	PL9	a	409	-	-	20/53/73/73	0/1/1/1
22	CLA	b	601	36	1/1/20/20	20/37/115/115	-
24	BCR	d	406	-	-	8/29/63/63	0/2/2/2
23	PHO	a	404	-	-	7/53/103/103	0/5/6/6
24	BCR	T	101	-	-	14/29/63/63	0/2/2/2
27	LMG	D	410	-	-	13/33/33/70	-
22	CLA	C	509	-	1/1/20/20	14/37/115/115	-
22	CLA	B	603	-	1/1/20/20	13/37/115/115	-
22	CLA	B	613	-	1/1/20/20	13/37/115/115	-
22	CLA	a	402	-	1/1/20/20	5/37/115/115	-
22	CLA	b	613	-	1/1/20/20	7/37/115/115	-
24	BCR	B	617	-	-	6/29/63/63	0/2/2/2
22	CLA	b	609	-	-	9/37/115/115	-
24	BCR	k	102	-	-	0/29/63/63	0/2/2/2
32	STE	B	624	-	-	11/13/15/17	-
22	CLA	B	608	-	-	3/37/115/115	-
32	STE	C	519	-	-	5/13/13/17	-
30	DGD	H	102	-	-	19/51/91/95	0/2/2/2
24	BCR	k	101	-	-	13/29/63/63	0/2/2/2
32	STE	a	413	-	-	5/7/7/17	-
35	HEC	v	201	17	-	0/6/54/54	-
30	DGD	c	517	-	-	21/51/91/95	0/2/2/2
29	LHG	a	410	-	-	18/53/53/53	-
22	CLA	C	507	36	1/1/20/20	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	STE	C	518	-	-	4/7/9/17	-
23	PHO	A	405	-	-	1/53/103/103	0/5/6/6
22	CLA	C	513	-	1/1/20/20	15/37/115/115	-
22	CLA	b	606	-	1/1/20/20	8/37/115/115	-
22	CLA	b	603	-	1/1/20/20	10/37/115/115	-
30	DGD	C	517	-	-	14/51/91/95	0/2/2/2
28	SQD	a	411	-	-	21/49/69/69	0/1/1/1
32	STE	m	102	-	-	1/7/9/17	-
29	LHG	L	101	-	-	20/53/53/53	-
27	LMG	c	519	-	-	11/31/51/70	0/1/1/1
24	BCR	b	618	-	-	5/29/63/63	0/2/2/2
22	CLA	b	610	36	1/1/20/20	4/37/115/115	-
32	STE	d	411	-	-	6/12/14/17	-
32	STE	B	627	-	-	6/11/13/17	-
22	CLA	d	405	-	1/1/20/20	5/37/115/115	-
22	CLA	c	503	-	1/1/20/20	9/37/115/115	-
32	STE	a	415	-	-	4/7/9/17	-
22	CLA	b	614	-	1/1/20/20	18/37/115/115	-
27	LMG	Y	101	-	-	23/43/63/70	0/1/1/1
26	PL9	A	410	-	-	23/53/73/73	0/1/1/1
22	CLA	B	604	-	1/1/20/20	12/37/115/115	-
24	BCR	A	407	-	-	8/29/63/63	0/2/2/2
24	BCR	B	618	-	-	10/29/63/63	0/2/2/2
28	SQD	a	412	-	-	16/37/37/69	-
32	STE	b	621	-	-	8/13/13/17	-
22	CLA	B	605	-	1/1/20/20	9/37/115/115	-
23	PHO	A	404	-	-	5/53/103/103	0/5/6/6
32	STE	J	101	-	-	3/7/9/17	-
23	PHO	d	401	-	-	6/53/103/103	0/5/6/6
22	CLA	B	607	36	1/1/20/20	7/37/115/115	-
32	STE	B	622	-	-	2/9/11/17	-
22	CLA	c	511	3	1/1/20/20	11/37/115/115	-
24	BCR	H	101	-	-	6/29/63/63	0/2/2/2
28	SQD	B	621	-	-	19/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	616	-	1/1/19/20	8/31/109/115	-
34	HEM	f	101	5,6	-	1/6/54/54	-
22	CLA	a	405	-	1/1/20/20	7/37/115/115	-
22	CLA	C	506	-	-	10/37/115/115	-
32	STE	H	103	-	-	9/15/15/17	-
22	CLA	C	511	3	1/1/20/20	9/37/115/115	-
27	LMG	A	411	-	-	16/43/63/70	0/1/1/1
22	CLA	B	614	-	1/1/20/20	11/37/115/115	-
24	BCR	b	619	-	-	4/29/63/63	0/2/2/2
22	CLA	B	610	36	1/1/20/20	4/37/115/115	-
22	CLA	d	404	36	1/1/20/20	6/37/115/115	-
22	CLA	c	513	-	1/1/20/20	12/37/115/115	-
29	LHG	D	411	-	-	19/53/53/53	-
32	STE	B	620	-	-	7/12/14/17	-
29	LHG	D	409	-	-	21/51/51/53	-
30	DGD	c	516	-	-	27/51/91/95	0/2/2/2
22	CLA	c	501	-	1/1/20/20	2/37/115/115	-
27	LMG	d	410	-	-	12/39/59/70	0/1/1/1
27	LMG	h	102	-	-	11/15/17/70	-
30	DGD	C	516	-	-	21/51/91/95	0/2/2/2
30	DGD	h	103	-	-	19/51/91/95	0/2/2/2
22	CLA	c	512	-	1/1/20/20	16/37/115/115	-
32	STE	b	624	-	-	5/11/13/17	-
35	HEC	V	201	17	-	0/6/54/54	-
22	CLA	A	403	36	-	12/37/115/115	-
22	CLA	c	510	-	1/1/20/20	7/37/115/115	-
22	CLA	b	602	-	-	11/37/115/115	-
29	LHG	D	408	-	-	24/53/53/53	-
32	STE	D	413	-	-	5/10/12/17	-
24	BCR	K	103	-	-	4/29/63/63	0/2/2/2
28	SQD	A	414	-	-	17/39/39/69	-
32	STE	M	104	-	-	7/15/15/17	-
22	CLA	B	609	-	-	4/37/115/115	-
24	BCR	a	406	-	-	0/29/63/63	0/2/2/2
24	BCR	h	101	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	607	36	1/1/20/20	13/37/115/115	-
22	CLA	d	403	-	-	9/37/115/115	-
22	CLA	b	604	-	1/1/20/20	10/37/115/115	-
30	DGD	c	518	-	-	16/51/91/95	0/2/2/2
32	STE	B	625	-	-	7/13/13/17	-
32	STE	d	412	-	-	11/15/17/17	-
32	STE	b	625	-	-	8/15/17/17	-
22	CLA	C	508	-	-	8/37/115/115	-
32	STE	I	101	-	-	5/12/12/17	-
29	LHG	e	101	-	-	22/46/46/53	-
22	CLA	C	501	-	1/1/20/20	3/37/115/115	-
24	BCR	D	405	-	-	6/29/63/63	0/2/2/2
32	STE	M	103	-	-	4/7/7/17	-
22	CLA	C	505	-	1/1/20/20	15/37/115/115	-
22	CLA	C	512	-	1/1/20/20	14/37/115/115	-
27	LMG	D	407	-	-	14/46/66/70	0/1/1/1
22	CLA	c	504	36	1/1/19/20	10/31/109/115	-
22	CLA	B	602	-	1/1/20/20	8/37/115/115	-

All (836) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	613	CLA	C4B-NB	8.77	1.43	1.35
22	b	604	CLA	C4B-NB	8.75	1.43	1.35
22	b	615	CLA	C4B-NB	8.17	1.42	1.35
22	c	504	CLA	C4B-NB	8.11	1.42	1.35
22	B	601	CLA	C4B-NB	8.04	1.42	1.35
22	B	602	CLA	C4B-NB	7.95	1.42	1.35
22	C	501	CLA	C4B-NB	7.95	1.42	1.35
22	C	506	CLA	C4B-NB	7.85	1.42	1.35
22	b	615	CLA	MG-NA	7.85	2.24	2.06
22	A	406	CLA	C4B-NB	7.85	1.42	1.35
35	V	201	HEC	C3B-C2B	-7.84	1.32	1.40
35	v	201	HEC	C3B-C2B	-7.76	1.32	1.40
22	c	511	CLA	MG-NA	7.71	2.24	2.06
22	C	505	CLA	C4B-NB	7.60	1.42	1.35
22	b	606	CLA	MG-NA	7.48	2.24	2.06
22	a	402	CLA	C4B-NB	7.44	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	506	CLA	C4B-NB	7.40	1.41	1.35
22	B	610	CLA	C4C-NC	7.32	1.41	1.35
22	C	502	CLA	C4C-NC	7.26	1.41	1.35
22	B	606	CLA	C4B-NB	7.25	1.41	1.35
22	b	609	CLA	C4B-NB	7.22	1.41	1.35
22	b	614	CLA	C4B-NB	7.20	1.41	1.35
22	B	616	CLA	MG-NA	7.19	2.23	2.06
22	b	601	CLA	C4B-NB	7.16	1.41	1.35
22	C	512	CLA	C4B-NB	7.11	1.41	1.35
22	c	502	CLA	C4C-NC	7.11	1.41	1.35
22	a	405	CLA	C4C-NC	7.07	1.41	1.35
22	C	511	CLA	C4B-NB	7.05	1.41	1.35
22	b	613	CLA	C4C-NC	7.03	1.41	1.35
22	c	511	CLA	C4B-NB	6.96	1.41	1.35
22	d	405	CLA	C4B-NB	6.94	1.41	1.35
22	c	501	CLA	C4B-NB	6.94	1.41	1.35
22	D	402	CLA	C4B-NB	6.85	1.41	1.35
22	C	503	CLA	C4B-NB	6.83	1.41	1.35
22	c	512	CLA	C4B-NB	6.81	1.41	1.35
22	B	608	CLA	C4C-NC	6.78	1.41	1.35
22	A	403	CLA	C4B-NB	6.78	1.41	1.35
22	a	403	CLA	C4B-NB	6.77	1.41	1.35
22	b	613	CLA	C4B-NB	6.75	1.41	1.35
22	C	513	CLA	C4C-NC	6.73	1.41	1.35
22	B	616	CLA	C4C-NC	6.69	1.41	1.35
22	C	504	CLA	C4B-NB	6.68	1.41	1.35
22	C	502	CLA	C4B-NB	6.67	1.41	1.35
22	A	406	CLA	C4C-NC	6.63	1.41	1.35
22	c	513	CLA	C4B-NB	6.60	1.41	1.35
22	C	508	CLA	C4B-NB	6.59	1.41	1.35
22	b	605	CLA	C4B-NB	6.57	1.41	1.35
22	a	405	CLA	C4B-NB	6.57	1.41	1.35
22	c	503	CLA	C4B-NB	6.54	1.41	1.35
22	C	503	CLA	MG-NA	6.54	2.21	2.06
22	B	614	CLA	C4B-NB	6.53	1.41	1.35
22	b	612	CLA	C4B-NB	6.52	1.41	1.35
22	b	604	CLA	MG-NA	6.51	2.21	2.06
22	c	505	CLA	C4B-NB	6.42	1.40	1.35
22	b	611	CLA	C4C-NC	6.41	1.40	1.35
22	C	507	CLA	MG-NA	6.35	2.21	2.06
22	B	611	CLA	C4B-NB	6.35	1.40	1.35
26	D	406	PL9	C7-C3	-6.30	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	608	CLA	C4B-NB	6.28	1.40	1.35
22	c	507	CLA	C4B-NB	6.28	1.40	1.35
22	C	501	CLA	C4C-NC	6.25	1.40	1.35
22	b	603	CLA	C4B-NB	6.24	1.40	1.35
22	c	509	CLA	C4C-NC	6.24	1.40	1.35
22	b	602	CLA	C4C-NC	6.20	1.40	1.35
22	c	513	CLA	C4C-NC	6.19	1.40	1.35
22	D	403	CLA	C4B-NB	6.18	1.40	1.35
22	b	607	CLA	C4B-NB	6.18	1.40	1.35
22	C	509	CLA	C4B-NB	6.14	1.40	1.35
22	C	513	CLA	C4B-NB	6.13	1.40	1.35
22	d	403	CLA	C4B-NB	6.12	1.40	1.35
22	B	601	CLA	C4C-NC	6.10	1.40	1.35
22	B	612	CLA	C4C-NC	6.08	1.40	1.35
22	b	606	CLA	C4C-NC	6.08	1.40	1.35
34	f	101	HEM	C3B-C2B	-6.02	1.32	1.40
22	b	601	CLA	MG-NA	6.01	2.20	2.06
22	C	508	CLA	MG-NA	5.98	2.20	2.06
22	B	603	CLA	C4C-NC	5.97	1.40	1.35
22	c	511	CLA	C4C-NC	5.97	1.40	1.35
22	C	504	CLA	C4C-NC	5.94	1.40	1.35
22	b	610	CLA	C4C-NC	5.90	1.40	1.35
35	V	201	HEC	C3C-C2C	-5.90	1.34	1.40
22	c	506	CLA	C4C-NC	5.89	1.40	1.35
22	b	616	CLA	C4C-NC	5.86	1.40	1.35
22	B	615	CLA	C4B-NB	5.85	1.40	1.35
22	d	404	CLA	MG-NA	5.84	2.20	2.06
22	B	608	CLA	MG-NA	5.82	2.20	2.06
22	c	501	CLA	C4C-NC	5.79	1.40	1.35
22	B	605	CLA	C4B-NB	5.79	1.40	1.35
22	a	402	CLA	C4C-NC	5.78	1.40	1.35
22	C	510	CLA	C4B-NB	5.77	1.40	1.35
22	B	609	CLA	C4B-NB	5.74	1.40	1.35
22	b	606	CLA	C4B-NB	5.74	1.40	1.35
22	C	506	CLA	MG-NA	5.73	2.19	2.06
22	B	612	CLA	C4B-NB	5.70	1.40	1.35
22	c	509	CLA	C4B-NB	5.68	1.40	1.35
22	C	510	CLA	C4C-NC	5.67	1.40	1.35
22	C	503	CLA	C4C-NC	5.66	1.40	1.35
22	c	502	CLA	C4B-NB	5.66	1.40	1.35
22	c	508	CLA	C4C-NC	5.61	1.40	1.35
22	d	404	CLA	C4C-NC	5.60	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	608	CLA	C4B-NB	5.60	1.40	1.35
22	B	601	CLA	MG-NA	5.58	2.19	2.06
22	D	403	CLA	MG-NA	5.57	2.19	2.06
22	C	506	CLA	C4C-NC	5.57	1.40	1.35
22	D	404	CLA	C4C-NC	5.56	1.40	1.35
22	C	507	CLA	C4B-NB	5.55	1.40	1.35
22	b	601	CLA	C4C-NC	5.54	1.40	1.35
22	b	615	CLA	C4C-NC	5.53	1.40	1.35
22	d	404	CLA	C4B-NB	5.49	1.40	1.35
22	A	402	CLA	C4B-NB	5.43	1.40	1.35
22	B	616	CLA	C4B-NB	5.42	1.40	1.35
34	F	101	HEM	C3C-C2C	-5.41	1.32	1.40
22	C	511	CLA	C4C-NC	5.41	1.40	1.35
22	b	608	CLA	MG-NA	5.40	2.19	2.06
34	F	101	HEM	C3B-C2B	-5.38	1.32	1.40
22	B	614	CLA	C4C-NC	5.36	1.40	1.35
22	B	602	CLA	C4C-NC	5.36	1.40	1.35
22	c	510	CLA	C4C-NC	5.32	1.40	1.35
22	C	509	CLA	C4C-NC	5.31	1.39	1.35
22	A	403	CLA	C4C-NC	5.30	1.39	1.35
22	b	616	CLA	C4B-NB	5.30	1.39	1.35
22	c	507	CLA	C4C-NC	5.29	1.39	1.35
22	C	508	CLA	C4C-NC	5.27	1.39	1.35
22	c	508	CLA	MG-NA	5.25	2.18	2.06
26	a	409	PL9	O1-C4	5.24	1.34	1.23
22	D	404	CLA	C4B-NB	5.22	1.39	1.35
35	v	201	HEC	C3C-C2C	-5.18	1.35	1.40
22	B	610	CLA	C4B-NB	5.17	1.39	1.35
22	c	505	CLA	C4C-NC	5.17	1.39	1.35
22	B	604	CLA	MG-NA	5.16	2.18	2.06
35	v	201	HEC	C3D-C2D	5.15	1.52	1.37
22	a	403	CLA	C4C-NC	5.11	1.39	1.35
22	b	602	CLA	C4B-NB	5.10	1.39	1.35
26	a	409	PL9	C3-C4	5.10	1.58	1.49
22	B	611	CLA	C4C-NC	5.07	1.39	1.35
22	d	405	CLA	C4C-NC	5.04	1.39	1.35
30	C	515	DGD	C6E-C5E	5.02	1.68	1.51
22	C	507	CLA	C4C-NC	5.02	1.39	1.35
22	c	508	CLA	C4B-NB	4.98	1.39	1.35
22	b	605	CLA	C4C-NC	4.97	1.39	1.35
22	b	602	CLA	MG-NA	4.94	2.18	2.06
22	b	608	CLA	C4C-NC	4.91	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	610	CLA	C4B-NB	4.85	1.39	1.35
22	C	512	CLA	C4C-NC	4.83	1.39	1.35
22	d	403	CLA	C4C-NC	4.83	1.39	1.35
22	c	510	CLA	C4B-NB	4.82	1.39	1.35
22	B	606	CLA	MG-NA	4.80	2.17	2.06
30	H	102	DGD	C4E-C5E	4.79	1.63	1.53
22	a	402	CLA	MG-NA	4.78	2.17	2.06
22	A	402	CLA	C4C-NC	4.74	1.39	1.35
26	d	407	PL9	C6-C1	-4.72	1.40	1.48
22	c	510	CLA	MG-NA	4.66	2.17	2.06
22	b	603	CLA	C4C-NC	4.65	1.39	1.35
22	B	605	CLA	C4C-NC	4.63	1.39	1.35
22	b	607	CLA	C4C-NC	4.62	1.39	1.35
22	B	615	CLA	MG-NA	4.61	2.17	2.06
22	b	612	CLA	C4C-NC	4.60	1.39	1.35
22	B	614	CLA	MG-NA	4.53	2.17	2.06
30	C	515	DGD	O5D-C1E	4.53	1.47	1.40
22	c	512	CLA	C4C-NC	4.50	1.39	1.35
30	o	301	DGD	O1G-C1A	4.48	1.46	1.33
22	b	614	CLA	C4C-NC	4.44	1.39	1.35
28	a	412	SQD	O47-C7	4.44	1.46	1.34
24	b	618	BCR	C30-C25	-4.43	1.47	1.53
27	A	411	LMG	O1-C7	-4.42	1.35	1.43
30	c	516	DGD	C3G-C2G	4.42	1.64	1.50
22	c	513	CLA	MG-NA	4.33	2.16	2.06
29	D	408	LHG	O7-C5	-4.32	1.35	1.46
22	D	402	CLA	C4C-NC	4.29	1.39	1.35
30	C	517	DGD	O2G-C2G	-4.28	1.35	1.46
27	D	407	LMG	C4-C5	4.27	1.62	1.53
22	c	503	CLA	C4C-NC	4.26	1.39	1.35
22	B	604	CLA	C4C-NC	4.26	1.39	1.35
24	c	515	BCR	C1-C6	-4.25	1.47	1.53
30	c	516	DGD	O2G-C2G	-4.24	1.36	1.46
22	c	504	CLA	C4C-NC	4.22	1.39	1.35
24	C	514	BCR	C1-C6	-4.21	1.48	1.53
22	b	609	CLA	C4C-NC	4.15	1.38	1.35
30	c	516	DGD	O3E-C3E	-4.14	1.33	1.43
35	V	201	HEC	C3D-C2D	4.12	1.49	1.37
22	C	502	CLA	MG-NA	4.10	2.16	2.06
30	A	415	DGD	C3E-C2E	4.10	1.62	1.52
26	d	407	PL9	C31-C29	-4.09	1.42	1.51
22	b	609	CLA	MG-NA	4.08	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	d	410	LMG	C4-C5	4.05	1.61	1.53
22	B	603	CLA	C4B-NB	4.04	1.38	1.35
28	a	411	SQD	O48-C23	4.03	1.45	1.33
22	b	603	CLA	MG-NA	3.98	2.15	2.06
34	f	101	HEM	C3C-C2C	-3.98	1.34	1.40
22	b	611	CLA	C4B-NB	3.96	1.38	1.35
30	C	515	DGD	C4E-C3E	3.95	1.62	1.52
24	d	406	BCR	C30-C25	-3.93	1.48	1.53
24	T	101	BCR	C1-C6	-3.89	1.48	1.53
22	B	610	CLA	C3B-C2B	-3.87	1.35	1.40
22	C	505	CLA	C4C-NC	3.84	1.38	1.35
22	B	615	CLA	C4C-NC	3.82	1.38	1.35
22	B	613	CLA	C4C-NC	3.81	1.38	1.35
22	C	501	CLA	C3B-C2B	-3.81	1.35	1.40
22	B	609	CLA	MG-NA	3.79	2.15	2.06
27	c	521	LMG	O1-C1	3.79	1.46	1.40
24	d	406	BCR	C1-C6	-3.79	1.48	1.53
22	C	501	CLA	MG-NA	3.76	2.15	2.06
22	B	601	CLA	C3B-C2B	-3.74	1.35	1.40
22	B	609	CLA	C4C-NC	3.73	1.38	1.35
27	m	101	LMG	O7-C8	-3.70	1.37	1.46
22	B	604	CLA	C4B-NB	3.69	1.38	1.35
24	D	405	BCR	C1-C6	-3.69	1.48	1.53
22	B	607	CLA	MG-NA	3.68	2.15	2.06
22	B	607	CLA	C4B-NB	3.67	1.38	1.35
24	B	619	BCR	C1-C6	-3.65	1.48	1.53
22	B	610	CLA	CMB-C2B	-3.65	1.44	1.51
24	K	102	BCR	C30-C25	-3.62	1.48	1.53
30	c	517	DGD	C3E-C2E	3.61	1.61	1.52
22	B	611	CLA	CMB-C2B	-3.60	1.44	1.51
22	D	403	CLA	C4C-NC	3.57	1.38	1.35
24	D	405	BCR	C30-C25	-3.56	1.48	1.53
23	d	401	PHO	C3B-C4B	3.54	1.50	1.43
22	b	611	CLA	MG-NA	3.54	2.14	2.06
29	d	408	LHG	O8-C6	-3.54	1.37	1.45
24	c	514	BCR	C1-C6	-3.53	1.48	1.53
22	c	505	CLA	MG-NA	3.52	2.14	2.06
24	b	619	BCR	C30-C25	-3.51	1.48	1.53
27	D	410	LMG	C9-C8	3.49	1.61	1.50
24	b	617	BCR	C30-C25	-3.48	1.49	1.53
24	b	619	BCR	C1-C6	-3.48	1.49	1.53
24	A	407	BCR	C1-C6	-3.47	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	415	DGD	O3G-C3G	-3.47	1.37	1.43
29	A	413	LHG	C24-C23	3.47	1.60	1.50
22	b	603	CLA	CMD-C2D	-3.45	1.43	1.51
22	b	615	CLA	CMD-C2D	-3.44	1.43	1.51
30	H	102	DGD	C1G-C2G	3.42	1.61	1.50
22	c	510	CLA	CMB-C2B	-3.42	1.44	1.51
28	a	412	SQD	O48-C23	3.41	1.43	1.33
30	o	301	DGD	O2G-C2G	-3.39	1.38	1.46
26	D	406	PL9	C52-C5	-3.39	1.43	1.50
22	b	607	CLA	CMB-C2B	-3.39	1.44	1.51
27	M	101	LMG	O7-C8	-3.38	1.38	1.46
24	B	617	BCR	C30-C25	-3.37	1.49	1.53
28	f	102	SQD	O48-C23	3.37	1.43	1.33
30	c	518	DGD	O2E-C2E	-3.37	1.35	1.43
28	B	621	SQD	O47-C7	3.37	1.43	1.34
30	c	517	DGD	C4D-C3D	3.37	1.60	1.52
22	c	512	CLA	MG-NA	3.36	2.14	2.06
30	h	103	DGD	O3D-C3D	-3.36	1.35	1.43
30	c	518	DGD	O3D-C3D	-3.36	1.35	1.43
22	b	613	CLA	MG-NA	3.35	2.14	2.06
22	b	607	CLA	C3B-C2B	-3.34	1.35	1.40
28	B	621	SQD	O48-C23	3.34	1.43	1.33
30	H	102	DGD	C4D-C5D	3.33	1.60	1.53
24	T	101	BCR	C30-C25	-3.33	1.49	1.53
30	c	516	DGD	C4D-C3D	3.33	1.60	1.52
27	D	410	LMG	C7-C8	3.33	1.59	1.51
28	A	414	SQD	O47-C45	-3.33	1.41	1.47
22	B	611	CLA	MG-NA	3.32	2.14	2.06
22	b	613	CLA	CMB-C2B	-3.32	1.44	1.51
24	B	618	BCR	C30-C25	-3.32	1.49	1.53
30	A	415	DGD	C1E-C2E	3.31	1.62	1.52
26	d	407	PL9	C3-C4	-3.29	1.44	1.49
27	d	410	LMG	O7-C8	-3.28	1.38	1.46
29	a	410	LHG	C24-C23	3.27	1.60	1.50
30	A	415	DGD	C4D-C3D	3.27	1.60	1.52
30	A	415	DGD	O5D-C6D	-3.26	1.37	1.43
22	d	404	CLA	C3B-C2B	-3.26	1.35	1.40
24	c	514	BCR	C30-C25	-3.25	1.49	1.53
22	C	508	CLA	C1D-C2D	3.25	1.49	1.42
26	d	407	PL9	C25-C24	-3.23	1.42	1.50
28	A	414	SQD	O48-C23	3.22	1.42	1.33
30	C	516	DGD	C1E-C2E	3.22	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	C	515	DGD	O2G-C2G	-3.21	1.38	1.46
28	f	102	SQD	O47-C7	3.20	1.43	1.34
22	b	601	CLA	C1D-C2D	3.20	1.49	1.42
30	c	518	DGD	O3G-C3G	-3.20	1.37	1.43
22	C	511	CLA	MG-NA	3.19	2.13	2.06
22	c	506	CLA	CMD-C2D	-3.19	1.44	1.51
27	a	414	LMG	C4-C5	3.19	1.59	1.53
22	C	501	CLA	C1D-C2D	3.17	1.49	1.42
30	A	415	DGD	C4E-C5E	3.17	1.59	1.53
28	A	412	SQD	O48-C23	3.17	1.42	1.33
28	A	414	SQD	O47-C7	3.17	1.43	1.34
28	F	102	SQD	O48-C23	3.16	1.42	1.33
22	c	503	CLA	MG-NA	3.16	2.13	2.06
24	a	406	BCR	C1-C6	-3.16	1.49	1.53
24	h	101	BCR	C30-C25	-3.16	1.49	1.53
24	H	101	BCR	C30-C25	-3.16	1.49	1.53
22	b	609	CLA	CMB-C2B	-3.15	1.45	1.51
24	b	617	BCR	C1-C6	-3.15	1.49	1.53
30	A	415	DGD	O1G-C1G	-3.14	1.38	1.45
30	h	103	DGD	O1G-C1G	-3.14	1.38	1.45
22	B	606	CLA	C3B-CAB	-3.14	1.41	1.47
22	B	615	CLA	CMD-C2D	-3.12	1.44	1.51
22	C	503	CLA	C1D-C2D	3.12	1.49	1.42
27	M	101	LMG	C4-C3	3.12	1.60	1.52
22	c	502	CLA	MG-NA	3.12	2.13	2.06
23	d	401	PHO	CHC-C1C	3.12	1.44	1.38
28	b	620	SQD	O47-C7	3.12	1.43	1.34
24	k	102	BCR	C30-C25	-3.11	1.49	1.53
30	H	102	DGD	C3E-C2E	3.10	1.60	1.52
22	D	404	CLA	CMB-C2B	-3.09	1.45	1.51
30	C	515	DGD	O3E-C3E	-3.08	1.35	1.43
22	b	602	CLA	CMD-C2D	-3.07	1.44	1.51
22	a	403	CLA	CMB-C2B	-3.07	1.45	1.51
22	C	505	CLA	MG-NA	3.07	2.13	2.06
22	a	405	CLA	CMC-C2C	-3.06	1.44	1.51
22	C	509	CLA	MG-NA	3.06	2.13	2.06
24	K	101	BCR	C30-C25	-3.06	1.49	1.53
22	b	605	CLA	MG-NA	3.05	2.13	2.06
22	C	511	CLA	CMB-C2B	-3.05	1.45	1.51
28	A	412	SQD	O2-C2	-3.05	1.35	1.43
22	b	604	CLA	C1D-C2D	3.04	1.49	1.42
28	b	620	SQD	O48-C23	3.04	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	c	521	LMG	C3-C2	3.04	1.60	1.52
22	B	614	CLA	C3B-C2B	-3.03	1.36	1.40
34	f	101	HEM	C3C-CAC	3.03	1.54	1.47
29	D	409	LHG	P-O6	3.03	1.71	1.59
22	b	607	CLA	CMD-C2D	-3.03	1.44	1.51
23	A	405	PHO	CHC-C1C	3.02	1.44	1.38
24	B	617	BCR	C1-C6	-3.01	1.49	1.53
29	A	413	LHG	P-O6	3.01	1.71	1.59
23	A	404	PHO	CHB-C1B	-3.01	1.33	1.38
22	a	405	CLA	C4B-CHC	-3.00	1.32	1.41
22	B	608	CLA	C1D-C2D	3.00	1.49	1.42
23	A	405	PHO	C3B-C4B	2.99	1.49	1.43
24	a	406	BCR	C30-C25	-2.99	1.49	1.53
22	B	601	CLA	C1D-C2D	2.98	1.49	1.42
22	c	507	CLA	MG-NA	2.97	2.13	2.06
22	b	606	CLA	CMB-C2B	-2.96	1.45	1.51
22	B	612	CLA	CMC-C2C	-2.94	1.44	1.51
22	d	403	CLA	CMB-C2B	-2.94	1.45	1.51
22	B	603	CLA	C1D-C2D	2.94	1.49	1.42
22	a	402	CLA	CMB-C2B	-2.94	1.45	1.51
22	D	404	CLA	C3B-C2B	-2.93	1.36	1.40
30	C	516	DGD	C4E-C3E	2.93	1.59	1.52
22	A	403	CLA	C1B-NB	2.93	1.37	1.35
22	C	509	CLA	CMB-C2B	-2.93	1.45	1.51
22	B	615	CLA	CMB-C2B	-2.91	1.45	1.51
30	C	517	DGD	O3G-C1D	2.91	1.45	1.40
22	B	603	CLA	CMD-C2D	-2.90	1.44	1.51
29	d	409	LHG	P-O6	2.90	1.71	1.59
30	c	518	DGD	O4D-C4D	-2.90	1.36	1.43
24	K	101	BCR	C1-C6	-2.89	1.49	1.53
22	D	404	CLA	CMD-C2D	-2.88	1.44	1.51
27	Y	101	LMG	O7-C8	-2.88	1.39	1.46
30	C	515	DGD	O1G-C1G	-2.88	1.38	1.45
22	b	610	CLA	C3B-C2B	-2.88	1.36	1.40
30	h	103	DGD	C4E-C5E	2.88	1.59	1.53
27	c	521	LMG	C1-C2	2.86	1.60	1.52
22	c	503	CLA	CMB-C2B	-2.86	1.45	1.51
24	c	515	BCR	C30-C25	-2.86	1.49	1.53
27	c	519	LMG	O1-C1	2.86	1.45	1.40
30	C	516	DGD	C6E-C5E	2.86	1.61	1.51
22	b	608	CLA	C1D-C2D	2.85	1.49	1.42
22	C	508	CLA	C1B-NB	2.84	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	601	CLA	CMB-C2B	-2.84	1.45	1.51
22	B	614	CLA	C3B-CAB	-2.84	1.42	1.47
24	T	101	BCR	C38-C26	-2.83	1.46	1.50
34	f	101	HEM	C3B-CAB	2.82	1.53	1.47
34	F	101	HEM	C3B-CAB	2.82	1.53	1.47
24	b	617	BCR	C33-C5	-2.81	1.46	1.50
22	C	513	CLA	CMB-C2B	-2.81	1.45	1.51
22	b	606	CLA	C3B-C2B	-2.81	1.36	1.40
22	D	402	CLA	CMB-C2B	-2.80	1.45	1.51
22	c	507	CLA	C3B-C2B	-2.80	1.36	1.40
22	d	404	CLA	CMB-C2B	-2.79	1.45	1.51
34	F	101	HEM	C3C-CAC	2.79	1.53	1.47
27	c	519	LMG	O2-C2	-2.79	1.36	1.43
22	a	405	CLA	CMD-C2D	-2.78	1.44	1.51
22	B	606	CLA	C3B-C2B	-2.77	1.36	1.40
23	a	404	PHO	C3B-C4B	2.77	1.49	1.43
23	A	404	PHO	CMD-C2D	-2.77	1.44	1.50
27	c	521	LMG	C7-C8	2.76	1.59	1.50
22	b	614	CLA	CMB-C2B	-2.75	1.45	1.51
22	B	603	CLA	CMB-C2B	-2.74	1.45	1.51
29	L	101	LHG	O8-C23	2.74	1.41	1.33
24	K	102	BCR	C1-C6	-2.74	1.50	1.53
22	B	606	CLA	CMB-C2B	-2.74	1.45	1.51
30	C	516	DGD	O3G-C3G	-2.74	1.38	1.43
22	b	604	CLA	C4C-NC	2.74	1.37	1.35
22	b	616	CLA	CMB-C2B	-2.73	1.46	1.51
22	B	605	CLA	C3B-C2B	-2.73	1.36	1.40
27	d	410	LMG	O6-C5	-2.73	1.37	1.44
27	m	101	LMG	O1-C7	-2.72	1.38	1.43
29	D	411	LHG	P-O4	-2.72	1.42	1.55
27	a	414	LMG	C1-C2	2.72	1.60	1.52
30	H	102	DGD	O2D-C2D	-2.72	1.36	1.43
22	b	610	CLA	C1D-C2D	2.72	1.48	1.42
30	C	515	DGD	O6D-C5D	-2.72	1.37	1.44
22	b	612	CLA	CMB-C2B	-2.72	1.46	1.51
30	A	415	DGD	O2G-C2G	-2.71	1.39	1.46
22	D	403	CLA	C1D-C2D	2.71	1.48	1.42
22	B	610	CLA	MG-NA	2.71	2.12	2.06
22	C	513	CLA	MG-NA	2.71	2.12	2.06
23	A	404	PHO	C4C-NC	2.71	1.42	1.36
27	b	623	LMG	C4-C5	2.70	1.58	1.53
22	c	503	CLA	C1D-C2D	2.70	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	403	CLA	CMD-C2D	-2.70	1.45	1.51
22	B	615	CLA	C1D-C2D	2.70	1.48	1.42
28	A	412	SQD	O47-C7	2.70	1.41	1.34
22	B	602	CLA	CMB-C2B	-2.69	1.46	1.51
22	b	607	CLA	C1D-C2D	2.69	1.48	1.42
27	c	519	LMG	C7-C8	2.69	1.58	1.50
27	c	519	LMG	O7-C10	2.68	1.41	1.35
24	A	407	BCR	C30-C25	-2.67	1.50	1.53
22	b	603	CLA	CMC-C2C	-2.67	1.45	1.51
22	d	403	CLA	CMD-C2D	-2.66	1.45	1.51
27	m	101	LMG	C4-C5	2.66	1.58	1.53
22	a	403	CLA	CMD-C2D	-2.66	1.45	1.51
22	b	603	CLA	CMB-C2B	-2.66	1.46	1.51
22	B	613	CLA	C1D-C2D	2.66	1.48	1.42
24	C	514	BCR	C30-C25	-2.65	1.50	1.53
29	e	101	LHG	P-O6	2.65	1.70	1.59
23	A	404	PHO	C1C-NC	-2.65	1.32	1.38
22	b	609	CLA	C1D-C2D	2.65	1.48	1.42
22	B	616	CLA	CAC-C3C	-2.64	1.45	1.52
22	D	404	CLA	C4B-CHC	-2.64	1.33	1.41
29	a	410	LHG	O7-C5	-2.64	1.40	1.46
26	D	406	PL9	C31-C29	-2.64	1.45	1.51
22	c	512	CLA	CMD-C2D	-2.64	1.45	1.51
22	b	615	CLA	CAC-C3C	-2.63	1.45	1.52
22	A	406	CLA	C4B-CHC	-2.63	1.33	1.41
22	A	406	CLA	CMD-C2D	-2.63	1.45	1.51
22	C	503	CLA	CMB-C2B	-2.63	1.46	1.51
22	B	614	CLA	CMC-C2C	-2.62	1.45	1.51
22	d	403	CLA	C4B-CHC	-2.62	1.33	1.41
22	d	404	CLA	C1D-C2D	2.61	1.48	1.42
24	A	407	BCR	C33-C5	-2.61	1.46	1.50
22	C	506	CLA	C3B-C2B	-2.61	1.36	1.40
30	C	517	DGD	C3D-C2D	2.61	1.59	1.52
22	B	611	CLA	C3B-C2B	-2.60	1.36	1.40
30	C	517	DGD	C6E-C5E	2.60	1.60	1.51
30	c	517	DGD	O2E-C2E	-2.60	1.36	1.43
22	b	609	CLA	C3B-CAB	-2.60	1.42	1.47
27	b	623	LMG	C4-C3	2.60	1.58	1.52
29	A	413	LHG	O8-C23	2.59	1.40	1.33
22	c	511	CLA	C1D-C2D	2.59	1.48	1.42
24	B	619	BCR	C30-C25	-2.59	1.50	1.53
22	c	510	CLA	C1D-C2D	2.59	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	501	CLA	CMD-C2D	-2.58	1.45	1.51
30	C	515	DGD	C4D-C3D	2.58	1.58	1.52
24	a	406	BCR	C38-C26	-2.58	1.46	1.50
23	A	405	PHO	C4C-NC	2.57	1.42	1.36
22	b	602	CLA	CMB-C2B	-2.57	1.46	1.51
22	b	604	CLA	C1B-NB	2.57	1.37	1.35
22	C	504	CLA	O2D-CGD	2.57	1.39	1.33
22	C	511	CLA	CMC-C2C	-2.56	1.45	1.51
23	A	405	PHO	CMB-C2B	-2.56	1.45	1.50
22	b	615	CLA	CMB-C2B	-2.56	1.46	1.51
22	b	616	CLA	C3B-CAB	-2.55	1.42	1.47
22	b	616	CLA	CAC-C3C	-2.55	1.45	1.52
30	H	102	DGD	C1E-C2E	2.55	1.59	1.52
22	C	503	CLA	C3B-C2B	-2.55	1.36	1.40
22	d	403	CLA	C3B-C2B	-2.55	1.36	1.40
23	A	404	PHO	C1A-NA	2.54	1.42	1.37
22	A	402	CLA	C3D-C2D	-2.54	1.34	1.39
22	B	616	CLA	CMC-C2C	-2.54	1.45	1.51
26	D	406	PL9	C27-C28	-2.53	1.42	1.50
22	c	504	CLA	CMB-C2B	-2.53	1.46	1.51
22	b	603	CLA	C3B-C2B	-2.53	1.36	1.40
22	c	507	CLA	CMD-C2D	-2.53	1.45	1.51
30	C	516	DGD	C4D-C5D	2.52	1.58	1.53
22	C	513	CLA	CMC-C2C	-2.52	1.45	1.51
26	D	406	PL9	C26-C24	-2.52	1.46	1.51
22	b	602	CLA	CAC-C3C	-2.52	1.45	1.52
22	b	613	CLA	CMD-C2D	-2.52	1.45	1.51
30	C	515	DGD	C1G-C2G	2.52	1.58	1.50
22	C	503	CLA	C4B-CHC	-2.52	1.34	1.41
22	C	501	CLA	CMD-C2D	-2.51	1.45	1.51
22	C	506	CLA	CMC-C2C	-2.51	1.45	1.51
22	B	607	CLA	C3B-C2B	-2.51	1.36	1.40
22	a	405	CLA	CMB-C2B	-2.51	1.46	1.51
22	C	503	CLA	C3B-CAB	-2.51	1.42	1.47
22	d	405	CLA	C4B-CHC	-2.51	1.34	1.41
30	C	517	DGD	O1G-C1G	-2.51	1.39	1.45
22	c	504	CLA	CAC-C3C	-2.51	1.46	1.52
30	h	103	DGD	C4D-C3D	2.50	1.58	1.52
22	B	611	CLA	C1D-C2D	2.50	1.48	1.42
23	A	405	PHO	C4C-C3C	2.50	1.49	1.45
22	B	616	CLA	CMB-C2B	-2.50	1.46	1.51
22	b	611	CLA	CMB-C2B	-2.49	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	607	CLA	CAC-C3C	-2.49	1.46	1.52
27	b	623	LMG	C3-C2	2.49	1.58	1.52
27	m	101	LMG	C1-C2	2.48	1.59	1.52
22	c	502	CLA	CMD-C2D	-2.48	1.45	1.51
22	b	616	CLA	C1D-C2D	2.47	1.48	1.42
22	a	405	CLA	CAC-C3C	-2.47	1.46	1.52
24	k	101	BCR	C1-C6	-2.47	1.50	1.53
24	K	103	BCR	C1-C6	-2.47	1.50	1.53
22	B	615	CLA	O2D-CGD	2.46	1.39	1.33
23	A	404	PHO	CHC-C4B	-2.46	1.34	1.40
22	b	606	CLA	C4B-CHC	-2.46	1.34	1.41
22	A	402	CLA	MG-NA	2.46	2.12	2.06
22	B	609	CLA	C3B-C2B	-2.46	1.37	1.40
22	c	505	CLA	CMB-C2B	-2.46	1.46	1.51
22	b	614	CLA	O2D-CGD	2.46	1.39	1.33
22	b	602	CLA	C3B-C2B	-2.46	1.37	1.40
27	m	101	LMG	C9-C8	2.45	1.58	1.50
22	B	616	CLA	C3B-C2B	-2.45	1.37	1.40
22	c	507	CLA	C3B-CAB	-2.45	1.42	1.47
22	B	606	CLA	C4C-NC	2.45	1.37	1.35
22	c	512	CLA	CMB-C2B	-2.45	1.46	1.51
28	B	621	SQD	O2-C2	-2.45	1.37	1.43
22	b	615	CLA	CMC-C2C	-2.45	1.45	1.51
22	C	501	CLA	CMB-C2B	-2.45	1.46	1.51
22	B	607	CLA	CMD-C2D	-2.45	1.45	1.51
23	a	404	PHO	CHC-C4B	-2.45	1.34	1.40
22	B	607	CLA	C4C-NC	2.44	1.37	1.35
27	c	521	LMG	O6-C1	2.44	1.48	1.41
22	b	614	CLA	CMC-C2C	-2.44	1.45	1.51
24	T	101	BCR	C27-C26	-2.44	1.46	1.51
22	c	503	CLA	C3B-C2B	-2.43	1.37	1.40
22	D	404	CLA	C1D-C2D	2.43	1.48	1.42
22	B	607	CLA	C3B-CAB	-2.43	1.43	1.47
22	B	608	CLA	CMB-C2B	-2.43	1.46	1.51
28	A	412	SQD	O3-C3	-2.43	1.37	1.43
28	f	102	SQD	O2-C2	-2.43	1.37	1.43
30	C	515	DGD	O1G-C1A	2.43	1.40	1.33
22	B	613	CLA	CMD-C2D	-2.43	1.45	1.51
30	c	517	DGD	O1G-C1G	-2.42	1.39	1.45
22	c	504	CLA	C1D-C2D	2.42	1.48	1.42
24	C	514	BCR	C33-C5	-2.42	1.47	1.50
22	B	608	CLA	C4B-CHC	-2.42	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	608	CLA	C1B-NB	2.42	1.37	1.35
22	b	601	CLA	O2A-CGA	2.42	1.40	1.33
22	c	512	CLA	C1D-C2D	2.42	1.48	1.42
22	B	603	CLA	MG-NA	2.42	2.12	2.06
26	d	407	PL9	C53-C6	-2.41	1.45	1.50
22	A	406	CLA	CMB-C2B	-2.41	1.46	1.51
22	c	509	CLA	C1D-C2D	2.41	1.48	1.42
22	d	403	CLA	C1D-C2D	2.41	1.48	1.42
22	D	404	CLA	CMC-C2C	-2.41	1.45	1.51
23	d	401	PHO	CMC-C2C	-2.41	1.45	1.50
22	C	502	CLA	C3B-C2B	-2.40	1.37	1.40
22	b	605	CLA	CAC-C3C	-2.40	1.46	1.52
24	c	515	BCR	C33-C5	-2.40	1.47	1.50
22	b	605	CLA	CMD-C2D	-2.40	1.45	1.51
22	B	602	CLA	CAC-C3C	-2.39	1.46	1.52
22	b	602	CLA	C4B-CHC	-2.39	1.34	1.41
24	k	102	BCR	C1-C6	-2.39	1.50	1.53
22	A	406	CLA	CAC-C3C	-2.39	1.46	1.52
22	B	604	CLA	C1D-C2D	2.39	1.48	1.42
23	A	404	PHO	CMC-C2C	-2.39	1.45	1.50
22	B	608	CLA	C3B-C2B	-2.39	1.37	1.40
24	B	617	BCR	C33-C5	-2.39	1.47	1.50
22	b	614	CLA	C3B-CAB	-2.39	1.43	1.47
22	c	512	CLA	CAC-C3C	-2.38	1.46	1.52
22	b	605	CLA	C4B-CHC	-2.38	1.34	1.41
22	C	501	CLA	CMC-C2C	-2.38	1.45	1.51
22	C	510	CLA	CMD-C2D	-2.38	1.45	1.51
24	K	103	BCR	C30-C25	-2.38	1.50	1.53
22	c	501	CLA	CMC-C2C	-2.38	1.45	1.51
30	c	517	DGD	O3D-C3D	-2.37	1.37	1.43
22	B	613	CLA	O2D-CED	-2.37	1.39	1.45
24	k	101	BCR	C30-C25	-2.37	1.50	1.53
30	c	518	DGD	C2A-C1A	-2.37	1.43	1.50
22	b	608	CLA	CMB-C2B	-2.36	1.46	1.51
22	B	615	CLA	C3B-C2B	-2.36	1.37	1.40
27	m	101	LMG	C4-C3	2.36	1.58	1.52
22	c	513	CLA	CMD-C2D	-2.36	1.45	1.51
22	c	501	CLA	CAC-C3C	-2.36	1.46	1.52
22	A	403	CLA	CMB-C2B	-2.36	1.46	1.51
22	C	512	CLA	CMD-C2D	-2.35	1.46	1.51
22	c	513	CLA	C1D-C2D	2.35	1.47	1.42
30	C	516	DGD	O3D-C3D	-2.35	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	402	CLA	CMB-C2B	-2.35	1.46	1.51
22	C	504	CLA	C1D-C2D	2.35	1.47	1.42
29	D	411	LHG	C24-C23	2.35	1.57	1.50
22	B	605	CLA	CMD-C2D	-2.34	1.46	1.51
22	C	507	CLA	CMB-C2B	-2.34	1.46	1.51
23	d	401	PHO	C1C-NC	-2.34	1.33	1.38
26	d	407	PL9	C7-C3	-2.34	1.48	1.51
23	A	405	PHO	CMD-C2D	-2.34	1.45	1.50
22	C	505	CLA	CMB-C2B	-2.34	1.46	1.51
23	A	405	PHO	CHC-C4B	-2.34	1.35	1.40
22	d	405	CLA	CMB-C2B	-2.33	1.46	1.51
22	B	605	CLA	CMC-C2C	-2.33	1.46	1.51
22	c	508	CLA	CMB-C2B	-2.33	1.46	1.51
22	c	507	CLA	CAC-C3C	-2.33	1.46	1.52
23	d	401	PHO	CHC-C4B	-2.33	1.35	1.40
22	B	608	CLA	CMD-C2D	-2.33	1.46	1.51
22	B	607	CLA	CMB-C2B	-2.33	1.46	1.51
22	c	503	CLA	CMD-C2D	-2.33	1.46	1.51
22	C	513	CLA	C1D-C2D	2.33	1.47	1.42
28	A	412	SQD	O47-C45	-2.32	1.40	1.46
22	B	616	CLA	CMD-C2D	-2.32	1.46	1.51
22	C	512	CLA	C1D-C2D	2.32	1.47	1.42
30	c	517	DGD	O6E-C5E	2.32	1.50	1.44
22	c	507	CLA	CMB-C2B	-2.31	1.46	1.51
23	a	404	PHO	C4C-NC	2.30	1.41	1.36
22	C	510	CLA	CMB-C2B	-2.30	1.46	1.51
22	b	604	CLA	CMC-C2C	-2.30	1.46	1.51
22	B	613	CLA	C3B-CAB	-2.30	1.43	1.47
22	c	508	CLA	CMC-C2C	-2.30	1.46	1.51
22	C	504	CLA	CMB-C2B	-2.30	1.46	1.51
28	a	411	SQD	O3-C3	-2.30	1.37	1.43
22	c	508	CLA	CMD-C2D	-2.30	1.46	1.51
22	A	406	CLA	CMA-C3A	-2.30	1.48	1.53
22	B	611	CLA	C3B-CAB	-2.30	1.43	1.47
22	A	403	CLA	C3B-C2B	-2.30	1.37	1.40
22	C	505	CLA	C1D-C2D	2.30	1.47	1.42
22	c	511	CLA	CMB-C2B	-2.29	1.46	1.51
30	H	102	DGD	C4E-C3E	2.29	1.58	1.52
22	c	513	CLA	CMC-C2C	-2.29	1.46	1.51
28	f	102	SQD	O3-C3	-2.29	1.37	1.43
27	Y	101	LMG	O8-C9	-2.29	1.39	1.45
29	D	409	LHG	O3-C3	-2.29	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	609	CLA	O2D-CGD	2.29	1.38	1.33
27	a	414	LMG	O1-C7	-2.29	1.39	1.43
22	B	601	CLA	CMC-C2C	-2.29	1.46	1.51
22	B	614	CLA	CMB-C2B	-2.28	1.46	1.51
22	C	504	CLA	CMD-C2D	-2.28	1.46	1.51
22	b	610	CLA	CMB-C2B	-2.28	1.46	1.51
24	b	618	BCR	C1-C6	-2.28	1.50	1.53
22	c	502	CLA	C3B-CAB	-2.28	1.43	1.47
22	B	606	CLA	CMC-C2C	-2.28	1.46	1.51
22	b	613	CLA	CAA-C2A	-2.27	1.49	1.54
22	B	612	CLA	C1D-C2D	2.27	1.47	1.42
26	d	407	PL9	C30-C29	-2.27	1.44	1.50
22	c	506	CLA	CMC-C2C	-2.27	1.46	1.51
22	C	513	CLA	C4B-CHC	-2.27	1.34	1.41
24	t	101	BCR	C30-C25	-2.26	1.50	1.53
22	B	609	CLA	C3B-CAB	-2.26	1.43	1.47
30	h	103	DGD	O3E-C3E	-2.26	1.37	1.43
22	c	501	CLA	CMB-C2B	-2.26	1.46	1.51
23	A	404	PHO	C3B-C4B	2.26	1.47	1.43
22	c	513	CLA	CMB-C2B	-2.26	1.46	1.51
22	b	616	CLA	CMC-C2C	-2.26	1.46	1.51
22	b	610	CLA	CMD-C2D	-2.26	1.46	1.51
22	B	605	CLA	O2D-CED	-2.26	1.40	1.45
22	B	613	CLA	CMC-C2C	-2.25	1.46	1.51
26	A	410	PL9	C31-C29	-2.25	1.46	1.51
22	b	611	CLA	C1D-C2D	2.25	1.47	1.42
22	b	605	CLA	C1D-C2D	2.25	1.47	1.42
27	c	521	LMG	C4-C3	2.25	1.58	1.52
22	b	606	CLA	CAC-C3C	-2.25	1.46	1.52
22	C	506	CLA	C1D-C2D	2.25	1.47	1.42
22	D	403	CLA	CMD-C2D	-2.25	1.46	1.51
22	B	613	CLA	MG-NA	2.25	2.11	2.06
22	c	505	CLA	CMC-C2C	-2.24	1.46	1.51
22	b	609	CLA	C3B-C2B	-2.24	1.37	1.40
29	e	101	LHG	C3-C2	2.24	1.59	1.51
22	c	513	CLA	C1C-C2C	2.24	1.47	1.42
29	D	408	LHG	O8-C6	-2.24	1.40	1.45
24	k	101	BCR	C33-C5	-2.24	1.47	1.50
22	C	510	CLA	CAC-C3C	-2.23	1.46	1.52
27	b	623	LMG	O6-C1	2.23	1.47	1.41
30	c	518	DGD	O6D-C5D	-2.23	1.38	1.44
22	b	611	CLA	CMD-C2D	-2.23	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	401	PHO	CMD-C2D	-2.23	1.46	1.50
22	b	614	CLA	C1A-CHA	-2.23	1.33	1.43
22	B	610	CLA	C1D-C2D	2.22	1.47	1.42
22	a	403	CLA	C3B-C2B	-2.22	1.37	1.40
22	C	503	CLA	CMC-C2C	-2.22	1.46	1.51
22	C	501	CLA	C1C-C2C	2.22	1.47	1.42
30	h	103	DGD	O2E-C2E	-2.21	1.37	1.43
24	t	101	BCR	C5-C6	2.21	1.38	1.34
29	L	101	LHG	O7-C5	-2.21	1.41	1.46
22	B	603	CLA	C3B-CAB	-2.21	1.43	1.47
22	c	504	CLA	CMD-C2D	-2.21	1.46	1.51
23	d	401	PHO	C4C-C3C	2.21	1.49	1.45
30	C	516	DGD	C4D-C3D	2.21	1.57	1.52
30	C	515	DGD	C3E-C2E	2.20	1.57	1.52
22	b	616	CLA	C3B-C2B	-2.20	1.37	1.40
22	b	611	CLA	C3B-C2B	-2.20	1.37	1.40
22	C	512	CLA	CAC-C3C	-2.20	1.46	1.52
28	F	102	SQD	O4-C4	-2.20	1.37	1.43
22	b	614	CLA	C1D-C2D	2.20	1.47	1.42
22	b	601	CLA	C1B-NB	2.19	1.37	1.35
22	B	615	CLA	C3B-CAB	-2.19	1.43	1.47
22	B	612	CLA	CMB-C2B	-2.19	1.47	1.51
30	c	516	DGD	C4D-C5D	2.19	1.57	1.53
22	C	513	CLA	CMD-C2D	-2.19	1.46	1.51
22	a	402	CLA	C1C-C2C	2.19	1.47	1.42
22	c	502	CLA	C1D-C2D	2.19	1.47	1.42
22	C	507	CLA	C3B-C2B	-2.19	1.37	1.40
22	C	509	CLA	CMC-C2C	-2.19	1.46	1.51
22	B	601	CLA	C3B-CAB	-2.18	1.43	1.47
27	c	519	LMG	C4-C3	2.18	1.57	1.52
30	C	517	DGD	O3D-C3D	-2.18	1.37	1.43
22	c	503	CLA	CMC-C2C	-2.18	1.46	1.51
22	B	609	CLA	C1D-C2D	2.18	1.47	1.42
22	b	601	CLA	C1C-C2C	2.18	1.47	1.42
22	c	508	CLA	C1D-C2D	2.18	1.47	1.42
30	C	517	DGD	C4E-C3E	2.18	1.57	1.52
23	A	404	PHO	CHD-C4C	-2.18	1.35	1.40
22	C	503	CLA	CAC-C3C	-2.18	1.46	1.52
22	c	506	CLA	C1D-C2D	2.18	1.47	1.42
22	c	509	CLA	CMB-C2B	-2.17	1.47	1.51
30	C	515	DGD	O3G-C1D	-2.17	1.36	1.40
30	c	516	DGD	O3D-C3D	-2.17	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	606	CLA	CMD-C2D	-2.17	1.46	1.51
22	B	601	CLA	C4B-CHC	-2.17	1.35	1.41
22	C	509	CLA	O2D-CGD	2.17	1.38	1.33
22	C	504	CLA	CAC-C3C	-2.17	1.46	1.52
30	A	415	DGD	C4D-C5D	2.16	1.57	1.53
22	c	502	CLA	CMC-C2C	-2.16	1.46	1.51
26	D	406	PL9	C53-C6	-2.16	1.46	1.50
22	c	502	CLA	C3B-C2B	-2.16	1.37	1.40
22	b	610	CLA	C4B-CHC	-2.16	1.35	1.41
29	D	411	LHG	O7-C5	-2.16	1.41	1.46
35	v	201	HEC	CMA-C3A	2.15	1.56	1.51
30	A	415	DGD	C3G-C2G	2.15	1.57	1.50
22	B	611	CLA	CMD-C2D	-2.15	1.46	1.51
22	c	507	CLA	CMC-C2C	-2.15	1.46	1.51
23	d	401	PHO	CHD-C4C	-2.15	1.35	1.40
22	c	504	CLA	CMC-C2C	-2.15	1.46	1.51
22	B	609	CLA	CAC-C3C	-2.15	1.46	1.52
24	a	406	BCR	C33-C5	-2.15	1.47	1.50
22	A	402	CLA	C1C-C2C	2.15	1.47	1.42
23	A	404	PHO	CMB-C2B	-2.14	1.46	1.50
35	v	201	HEC	C1D-ND	2.14	1.40	1.36
29	a	410	LHG	P-O4	-2.14	1.45	1.55
28	a	411	SQD	O47-C7	2.14	1.40	1.34
22	b	609	CLA	CAC-C3C	-2.14	1.46	1.52
22	B	609	CLA	CMD-C2D	-2.14	1.46	1.51
22	A	406	CLA	C1D-C2D	2.14	1.47	1.42
22	d	405	CLA	CMC-C2C	-2.14	1.46	1.51
23	a	404	PHO	O2D-CGD	2.14	1.38	1.33
23	A	405	PHO	C1A-NA	2.13	1.41	1.37
22	b	601	CLA	CAC-C3C	-2.13	1.47	1.52
22	c	510	CLA	C5-C3	-2.13	1.46	1.51
22	B	603	CLA	O2D-CED	-2.13	1.40	1.45
22	B	604	CLA	O2A-CGA	2.13	1.39	1.33
22	D	402	CLA	C4B-CHC	-2.13	1.35	1.41
30	h	103	DGD	C1E-C2E	2.13	1.58	1.52
22	B	607	CLA	C1D-C2D	2.13	1.47	1.42
22	c	510	CLA	CAC-C3C	-2.13	1.47	1.52
22	c	506	CLA	CAC-C3C	-2.13	1.47	1.52
22	C	510	CLA	MG-NA	2.13	2.11	2.06
24	B	618	BCR	C33-C5	-2.13	1.47	1.50
22	B	610	CLA	CMC-C2C	-2.12	1.46	1.51
22	b	613	CLA	CMC-C2C	-2.12	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	607	CLA	MG-NA	2.12	2.11	2.06
22	B	602	CLA	C1D-C2D	2.12	1.47	1.42
22	C	506	CLA	C3B-CAB	-2.12	1.43	1.47
22	C	505	CLA	CMC-C2C	-2.12	1.46	1.51
22	C	510	CLA	O2D-CED	-2.12	1.40	1.45
35	v	201	HEC	C1B-NB	2.12	1.40	1.36
22	A	402	CLA	C5-C3	-2.11	1.46	1.51
22	B	615	CLA	CAC-C3C	-2.11	1.47	1.52
29	e	101	LHG	P-O3	2.11	1.67	1.59
22	B	611	CLA	CAC-C3C	-2.11	1.47	1.52
23	d	401	PHO	C1A-NA	2.11	1.41	1.37
22	b	608	CLA	C3B-CAB	-2.11	1.43	1.47
22	C	512	CLA	CMB-C2B	-2.11	1.47	1.51
27	a	414	LMG	O7-C8	-2.11	1.41	1.46
22	A	402	CLA	OBD-CAD	-2.11	1.19	1.22
22	c	502	CLA	C1C-C2C	2.11	1.47	1.42
30	h	103	DGD	O5D-C6D	2.10	1.47	1.43
22	B	604	CLA	CMD-C2D	-2.10	1.46	1.51
35	v	201	HEC	C4D-ND	2.10	1.40	1.36
22	c	502	CLA	O2D-CGD	2.10	1.38	1.33
22	B	602	CLA	MG-NA	2.10	2.11	2.06
26	A	410	PL9	C53-C6	-2.10	1.46	1.50
22	B	603	CLA	C3B-C2B	-2.10	1.37	1.40
22	b	607	CLA	C1A-CHA	-2.10	1.34	1.43
22	b	608	CLA	CMC-C2C	-2.09	1.46	1.51
22	C	502	CLA	CMD-C2D	-2.09	1.46	1.51
30	H	102	DGD	O6D-C5D	-2.09	1.39	1.44
22	c	510	CLA	C3B-C2B	-2.09	1.37	1.40
22	B	611	CLA	C4B-CHC	-2.09	1.35	1.41
22	c	506	CLA	CMB-C2B	-2.09	1.47	1.51
22	C	507	CLA	CMC-C2C	-2.09	1.46	1.51
27	a	414	LMG	O8-C9	-2.08	1.40	1.45
22	C	510	CLA	O2A-CGA	2.08	1.39	1.33
22	c	513	CLA	C3B-C2B	-2.08	1.37	1.40
22	B	602	CLA	CMD-C2D	-2.08	1.46	1.51
22	b	610	CLA	C3B-CAB	-2.08	1.43	1.47
30	c	517	DGD	O6D-C5D	-2.08	1.39	1.44
22	c	511	CLA	C3B-C2B	-2.08	1.37	1.40
22	C	508	CLA	CMC-C2C	-2.08	1.46	1.51
26	a	409	PL9	C53-C6	-2.07	1.46	1.50
24	K	101	BCR	C33-C5	-2.07	1.47	1.50
22	C	501	CLA	CAC-C3C	-2.07	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	517	DGD	C6E-C5E	2.06	1.58	1.51
23	a	404	PHO	C1C-NC	-2.06	1.34	1.38
22	B	612	CLA	MG-NA	2.06	2.11	2.06
22	D	402	CLA	CAC-C3C	-2.06	1.47	1.52
22	B	605	CLA	C1D-C2D	2.06	1.47	1.42
22	c	509	CLA	C4B-CHC	-2.06	1.35	1.41
22	c	511	CLA	C1C-C2C	2.06	1.47	1.42
22	b	616	CLA	C4B-CHC	-2.06	1.35	1.41
22	A	403	CLA	CAA-C2A	-2.05	1.50	1.54
22	B	605	CLA	CAA-C2A	-2.05	1.50	1.54
22	B	605	CLA	C5-C3	-2.05	1.47	1.51
29	D	409	LHG	P-O4	-2.05	1.45	1.55
22	C	509	CLA	CMD-C2D	-2.05	1.46	1.51
22	C	502	CLA	C1C-C2C	2.05	1.47	1.42
22	C	511	CLA	C1D-C2D	2.05	1.47	1.42
22	b	614	CLA	CMD-C2D	-2.05	1.46	1.51
23	a	404	PHO	C4C-C3C	2.04	1.49	1.45
22	C	504	CLA	C3B-C2B	-2.04	1.37	1.40
22	b	601	CLA	C3B-CAB	-2.04	1.43	1.47
22	C	506	CLA	CAC-C3C	-2.04	1.47	1.52
22	C	506	CLA	C1C-C2C	2.04	1.47	1.42
24	c	515	BCR	C36-C18	-2.04	1.46	1.50
22	b	609	CLA	C1A-CHA	-2.04	1.34	1.43
28	F	102	SQD	O2-C2	-2.04	1.38	1.43
27	d	410	LMG	C4-C3	2.03	1.57	1.52
22	A	403	CLA	CAC-C3C	-2.03	1.47	1.52
22	b	615	CLA	C3B-CAB	-2.03	1.43	1.47
23	A	404	PHO	O2D-CGD	2.03	1.38	1.33
22	d	405	CLA	C3B-CAB	-2.03	1.43	1.47
22	B	602	CLA	CMC-C2C	-2.03	1.46	1.51
22	B	616	CLA	C4B-CHC	-2.03	1.35	1.41
22	d	405	CLA	CAC-C3C	-2.03	1.47	1.52
22	b	602	CLA	CMC-C2C	-2.02	1.46	1.51
28	a	411	SQD	O4-C4	-2.02	1.38	1.43
22	C	513	CLA	C3B-C2B	-2.02	1.37	1.40
22	C	510	CLA	C1D-C2D	2.02	1.47	1.42
24	K	103	BCR	C38-C26	-2.02	1.47	1.50
22	d	405	CLA	CMD-C2D	-2.02	1.46	1.51
26	d	407	PL9	C11-C9	-2.02	1.47	1.51
30	C	515	DGD	O2E-C2E	-2.02	1.38	1.43
22	c	507	CLA	C1D-C2D	2.02	1.47	1.42
29	d	409	LHG	C9-C8	2.02	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	406	CLA	C1C-C2C	2.02	1.47	1.42
22	C	511	CLA	C1C-C2C	2.02	1.47	1.42
28	a	411	SQD	O2-C2	-2.02	1.38	1.43
22	b	607	CLA	O2D-CED	-2.02	1.40	1.45
22	b	612	CLA	CMC-C2C	-2.02	1.46	1.51
22	A	406	CLA	C3B-CAB	-2.02	1.43	1.47
22	B	606	CLA	CMD-C2D	-2.02	1.46	1.51
22	C	506	CLA	C1B-NB	-2.02	1.33	1.35
22	a	403	CLA	MG-NA	2.02	2.11	2.06
30	C	515	DGD	C2A-C1A	-2.02	1.44	1.50
22	a	402	CLA	CMD-C2D	-2.02	1.46	1.51
27	d	410	LMG	O1-C7	-2.02	1.40	1.43
27	D	410	LMG	C30-C29	2.01	1.59	1.52
22	B	610	CLA	C3B-CAB	-2.01	1.43	1.47
22	B	609	CLA	O2D-CGD	2.01	1.38	1.33
29	a	410	LHG	C4-C5	2.01	1.56	1.50
22	C	509	CLA	CAC-C3C	-2.01	1.47	1.52
22	C	507	CLA	CAC-C3C	-2.01	1.47	1.52
23	a	404	PHO	C1A-NA	2.01	1.41	1.37
22	B	608	CLA	C3B-CAB	-2.01	1.43	1.47
22	B	610	CLA	CAC-C3C	-2.00	1.47	1.52
23	a	404	PHO	CMD-C2D	-2.00	1.46	1.50

All (1280) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	620	SQD	O6-C1-C2	9.98	123.88	108.30
28	a	411	SQD	O6-C1-C2	9.65	123.37	108.30
22	c	509	CLA	C4A-NA-C1A	8.97	110.74	106.71
22	C	507	CLA	C4A-NA-C1A	8.54	110.55	106.71
22	b	611	CLA	C4A-NA-C1A	8.32	110.45	106.71
22	d	404	CLA	C4A-NA-C1A	8.23	110.41	106.71
22	B	604	CLA	C4A-NA-C1A	8.10	110.35	106.71
22	B	616	CLA	C4A-NA-C1A	8.09	110.34	106.71
22	C	511	CLA	C4A-NA-C1A	7.96	110.28	106.71
26	a	409	PL9	C7-C3-C4	7.70	123.14	116.88
22	b	604	CLA	C4A-NA-C1A	7.67	110.15	106.71
28	b	620	SQD	O7-S-C6	7.63	116.01	106.94
28	f	102	SQD	O9-S-C6	7.59	115.96	106.94
22	c	511	CLA	C4A-NA-C1A	7.58	110.12	106.71
22	D	403	CLA	C4A-NA-C1A	7.38	110.02	106.71
22	c	501	CLA	C4A-NA-C1A	6.98	109.84	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	f	101	HEM	CBD-CAD-C3D	-6.97	99.64	112.48
28	a	411	SQD	O9-S-C6	6.96	115.21	106.94
22	B	601	CLA	C4A-NA-C1A	6.90	109.81	106.71
28	A	412	SQD	O6-C1-C2	6.86	119.01	108.30
22	C	508	CLA	C4A-NA-C1A	6.80	109.76	106.71
22	B	605	CLA	C4A-NA-C1A	6.74	109.73	106.71
22	B	609	CLA	C4A-NA-C1A	6.69	109.71	106.71
22	c	503	CLA	C4A-NA-C1A	6.68	109.71	106.71
22	C	513	CLA	C4A-NA-C1A	6.62	109.68	106.71
22	a	403	CLA	C4A-NA-C1A	6.59	109.67	106.71
22	B	606	CLA	C4A-NA-C1A	6.46	109.61	106.71
22	C	501	CLA	C4A-NA-C1A	6.44	109.60	106.71
22	C	503	CLA	C4A-NA-C1A	6.33	109.55	106.71
22	b	601	CLA	C4A-NA-C1A	6.33	109.55	106.71
26	d	407	PL9	C7-C3-C4	6.26	121.97	116.88
22	c	510	CLA	C4A-NA-C1A	6.26	109.52	106.71
22	B	607	CLA	C4A-NA-C1A	6.23	109.51	106.71
22	c	502	CLA	C4A-NA-C1A	6.20	109.49	106.71
22	b	606	CLA	C4A-NA-C1A	6.09	109.44	106.71
27	b	623	LMG	O1-C1-C2	-6.02	98.90	108.30
22	b	613	CLA	CMB-C2B-C1B	-5.99	119.25	128.46
22	C	505	CLA	C4A-NA-C1A	5.91	109.36	106.71
28	a	412	SQD	O47-C7-C8	5.89	124.19	111.50
22	b	615	CLA	C4A-NA-C1A	5.87	109.35	106.71
22	c	504	CLA	CMB-C2B-C1B	-5.81	119.53	128.46
22	B	612	CLA	CMB-C2B-C1B	-5.80	119.54	128.46
26	a	409	PL9	C7-C3-C2	-5.78	115.70	123.30
22	A	402	CLA	C4A-NA-C1A	5.77	109.30	106.71
28	B	621	SQD	O6-C1-C2	5.76	117.29	108.30
28	F	102	SQD	O9-S-C6	5.73	113.75	106.94
22	B	615	CLA	C4A-NA-C1A	5.70	109.27	106.71
22	C	505	CLA	CMB-C2B-C1B	-5.69	119.72	128.46
22	c	507	CLA	C4A-NA-C1A	5.67	109.25	106.71
22	B	610	CLA	C4A-NA-C1A	5.62	109.23	106.71
22	B	612	CLA	C4A-NA-C1A	5.62	109.23	106.71
22	D	402	CLA	C4A-NA-C1A	5.54	109.19	106.71
22	b	602	CLA	C4A-NA-C1A	5.43	109.14	106.71
22	b	616	CLA	C4A-NA-C1A	5.40	109.13	106.71
22	a	402	CLA	C4A-NA-C1A	5.36	109.12	106.71
22	c	510	CLA	CMB-C2B-C1B	-5.34	120.26	128.46
22	B	602	CLA	CMB-C2B-C1B	-5.33	120.27	128.46
22	B	613	CLA	C4A-NA-C1A	5.30	109.09	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	605	CLA	C4A-NA-C1A	5.30	109.09	106.71
22	A	406	CLA	C4A-NA-C1A	5.29	109.08	106.71
22	A	406	CLA	CMB-C2B-C1B	-5.26	120.37	128.46
30	H	102	DGD	O3G-C3G-C2G	-5.26	98.21	110.90
22	b	604	CLA	CMB-C2B-C1B	-5.24	120.42	128.46
28	F	102	SQD	O6-C1-C2	5.24	116.48	108.30
22	b	613	CLA	C4A-NA-C1A	5.20	109.04	106.71
22	a	405	CLA	C4A-NA-C1A	5.16	109.03	106.71
26	D	406	PL9	C7-C3-C4	5.16	121.07	116.88
22	C	509	CLA	C4A-NA-C1A	5.14	109.02	106.71
22	B	608	CLA	CMB-C2B-C1B	-5.12	120.60	128.46
22	B	612	CLA	CMB-C2B-C3B	5.07	134.17	124.68
22	B	613	CLA	CMB-C2B-C1B	-5.06	120.69	128.46
22	b	616	CLA	CMB-C2B-C3B	5.05	134.13	124.68
26	d	407	PL9	C40-C39-C41	5.01	123.69	115.27
22	c	501	CLA	O2D-CGD-O1D	-4.99	114.08	123.84
22	b	616	CLA	CMB-C2B-C1B	-4.97	120.83	128.46
22	c	512	CLA	C4A-NA-C1A	4.96	108.94	106.71
22	B	602	CLA	C4A-NA-C1A	4.96	108.93	106.71
22	b	608	CLA	CMB-C2B-C1B	-4.95	120.86	128.46
22	C	509	CLA	CMB-C2B-C1B	-4.94	120.86	128.46
22	b	615	CLA	CMB-C2B-C1B	-4.93	120.89	128.46
22	b	603	CLA	C4A-NA-C1A	4.90	108.91	106.71
22	b	612	CLA	CMB-C2B-C1B	-4.88	120.96	128.46
30	o	301	DGD	O3G-C3G-C2G	-4.86	98.89	111.78
22	B	603	CLA	CMB-C2B-C1B	-4.80	121.08	128.46
28	A	414	SQD	C45-O47-C7	4.74	123.97	117.88
22	a	402	CLA	CMB-C2B-C1B	-4.69	121.26	128.46
28	f	102	SQD	O6-C1-C2	4.68	115.61	108.30
28	B	621	SQD	O7-S-C6	4.60	112.40	106.94
22	C	505	CLA	CMB-C2B-C3B	4.57	133.22	124.68
34	F	101	HEM	CBD-CAD-C3D	-4.54	104.11	112.48
28	b	620	SQD	C1-C2-C3	-4.53	100.56	110.00
35	V	201	HEC	CBD-CAD-C3D	-4.52	104.16	112.49
22	b	616	CLA	O2D-CGD-O1D	-4.50	115.03	123.84
27	b	623	LMG	C1-O6-C5	-4.50	104.86	113.69
22	b	604	CLA	CMB-C2B-C3B	4.48	133.06	124.68
22	c	504	CLA	CMB-C2B-C3B	4.46	133.02	124.68
22	B	610	CLA	O2D-CGD-O1D	-4.46	115.12	123.84
28	F	102	SQD	C44-O6-C1	4.44	121.21	113.84
22	c	508	CLA	C4A-NA-C1A	4.44	108.70	106.71
22	b	609	CLA	CMB-C2B-C1B	-4.44	121.64	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	v	201	HEC	CMC-C2C-C1C	-4.44	121.64	128.46
22	B	604	CLA	CMB-C2B-C1B	-4.43	121.65	128.46
22	b	611	CLA	O2D-CGD-O1D	-4.42	115.20	123.84
30	C	516	DGD	O3G-C3G-C2G	-4.41	100.27	110.90
22	d	405	CLA	CMB-C2B-C1B	-4.38	121.73	128.46
22	c	513	CLA	CMB-C2B-C1B	-4.36	121.76	128.46
35	v	201	HEC	CBD-CAD-C3D	-4.35	104.46	112.49
28	F	102	SQD	O8-S-C6	4.35	112.67	105.74
22	b	608	CLA	CMB-C2B-C3B	4.32	132.75	124.68
28	B	621	SQD	O47-C7-C8	4.31	120.79	111.50
24	b	617	BCR	C2-C1-C6	4.30	117.10	110.48
28	a	411	SQD	C1-O5-C5	-4.28	105.28	113.69
22	B	613	CLA	CMB-C2B-C3B	4.28	132.68	124.68
22	c	505	CLA	CMB-C2B-C1B	-4.26	121.91	128.46
22	b	613	CLA	CMB-C2B-C3B	4.24	132.62	124.68
23	A	405	PHO	CMB-C2B-C1B	-4.21	118.58	125.06
29	A	413	LHG	O4-P-O5	4.20	133.00	112.24
30	c	518	DGD	O3G-C3G-C2G	-4.20	100.77	110.90
22	C	509	CLA	CMB-C2B-C3B	4.19	132.52	124.68
29	L	101	LHG	O4-P-O5	4.16	132.82	112.24
22	C	510	CLA	CMB-C2B-C1B	-4.15	122.09	128.46
28	a	411	SQD	O47-C7-O49	-4.14	113.69	123.70
22	c	508	CLA	CMB-C2B-C1B	-4.13	122.11	128.46
22	D	404	CLA	C4A-NA-C1A	4.13	108.56	106.71
22	A	406	CLA	CMB-C2B-C3B	4.13	132.40	124.68
28	b	620	SQD	O48-C23-C24	4.12	124.85	111.91
22	b	602	CLA	CMB-C2B-C1B	-4.12	122.14	128.46
22	B	608	CLA	CMB-C2B-C3B	4.11	132.37	124.68
22	B	613	CLA	C1-C2-C3	-4.11	118.93	126.04
22	c	506	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
22	d	403	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
22	c	509	CLA	CMB-C2B-C1B	-4.10	122.17	128.46
35	V	201	HEC	CMC-C2C-C1C	-4.10	122.17	128.46
22	B	603	CLA	CMB-C2B-C3B	4.10	132.34	124.68
22	b	608	CLA	C4D-C3D-CAD	-4.09	106.19	108.47
22	B	614	CLA	O2D-CGD-O1D	-4.08	115.86	123.84
22	d	405	CLA	CMB-C2B-C3B	4.08	132.31	124.68
22	c	501	CLA	CMB-C2B-C1B	-4.08	122.19	128.46
28	A	412	SQD	C1-C2-C3	-4.07	101.51	110.00
29	e	101	LHG	O4-P-O5	4.07	132.37	112.24
29	D	409	LHG	O4-P-O5	4.06	132.31	112.24
28	B	621	SQD	C1-O5-C5	-4.06	105.72	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	C	515	DGD	O6D-C1D-O3G	-4.06	100.36	109.97
22	B	602	CLA	CMB-C2B-C3B	4.05	132.26	124.68
30	C	517	DGD	O3G-C3G-C2G	-4.05	101.13	110.90
28	f	102	SQD	O9-S-O7	-4.05	99.94	113.95
22	D	402	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
22	c	508	CLA	CMB-C2B-C3B	4.03	132.23	124.68
22	b	608	CLA	OBD-CAD-CBD	-4.03	120.14	125.89
22	b	616	CLA	O1D-CGD-CBD	4.03	132.72	124.48
29	a	410	LHG	O8-C23-C24	4.01	124.50	111.91
22	B	605	CLA	OBD-CAD-CBD	-4.01	120.17	125.89
22	c	502	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
22	C	508	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
28	a	412	SQD	C46-C45-C44	-3.97	102.51	111.80
22	c	505	CLA	O2D-CGD-O1D	-3.97	116.08	123.84
22	C	510	CLA	CMB-C2B-C3B	3.97	132.10	124.68
22	A	406	CLA	O2D-CGD-O1D	-3.97	116.08	123.84
22	b	605	CLA	O2D-CGD-O1D	-3.96	116.09	123.84
24	b	618	BCR	C36-C18-C17	-3.96	117.38	122.92
22	b	605	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
22	b	601	CLA	CHB-C4A-NA	3.95	129.97	124.51
22	C	507	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
28	B	621	SQD	O5-C5-C4	3.94	116.85	109.69
22	c	510	CLA	CMB-C2B-C3B	3.93	132.04	124.68
22	B	605	CLA	O2D-CGD-O1D	-3.93	116.16	123.84
22	C	506	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
29	d	408	LHG	O4-P-O5	3.92	131.63	112.24
22	A	403	CLA	O2D-CGD-O1D	-3.90	116.20	123.84
22	C	502	CLA	CMD-C2D-C3D	3.90	131.97	124.68
22	b	608	CLA	C4A-NA-C1A	3.90	108.46	106.71
22	b	606	CLA	O2D-CGD-O1D	-3.89	116.22	123.84
22	c	505	CLA	CMD-C2D-C3D	3.89	131.96	124.68
22	B	601	CLA	CAA-CBA-CGA	-3.89	101.88	113.25
22	A	406	CLA	C4-C3-C5	3.89	121.81	115.27
28	b	620	SQD	O9-S-O7	-3.88	100.53	113.95
28	A	412	SQD	O47-C7-O49	-3.88	114.33	123.70
28	f	102	SQD	O7-S-C6	3.87	111.54	106.94
28	a	411	SQD	C1-C2-C3	-3.87	101.93	110.00
22	b	603	CLA	O2D-CGD-O1D	-3.87	116.27	123.84
27	d	410	LMG	O1-C1-C2	-3.87	102.26	108.30
22	B	604	CLA	CMB-C2B-C3B	3.87	131.91	124.68
22	B	611	CLA	OBD-CAD-CBD	-3.86	120.38	125.89
29	D	408	LHG	O4-P-O5	3.86	131.33	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	613	CLA	CMD-C2D-C3D	3.86	131.90	124.68
24	T	101	BCR	C7-C8-C9	-3.85	120.41	126.23
22	a	405	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
22	b	602	CLA	O2D-CGD-CBD	3.84	118.10	111.27
22	c	509	CLA	O2A-CGA-O1A	-3.84	113.89	123.59
30	C	516	DGD	O6E-C1E-O5D	-3.83	100.89	109.97
22	c	513	CLA	CMB-C2B-C3B	3.81	131.81	124.68
22	B	601	CLA	O2D-CGD-O1D	-3.80	116.41	123.84
22	C	510	CLA	C4A-NA-C1A	3.79	108.41	106.71
22	c	504	CLA	C4A-NA-C1A	3.79	108.41	106.71
22	b	612	CLA	CMB-C2B-C3B	3.79	131.77	124.68
26	A	410	PL9	C7-C3-C4	3.78	119.95	116.88
22	C	502	CLA	C4A-NA-C1A	3.78	108.41	106.71
29	a	410	LHG	O4-P-O5	3.78	130.91	112.24
22	c	501	CLA	O2D-CGD-CBD	3.77	117.98	111.27
22	b	605	CLA	C1-C2-C3	-3.76	119.53	126.04
22	b	616	CLA	CHB-C4A-NA	3.76	129.71	124.51
30	c	516	DGD	O3G-C3G-C2G	-3.76	101.83	110.90
24	B	619	BCR	C2-C1-C6	3.76	116.27	110.48
29	l	101	LHG	O4-P-O5	3.76	130.81	112.24
22	B	602	CLA	CHB-C4A-NA	3.76	129.71	124.51
22	d	404	CLA	C4D-C3D-CAD	-3.75	106.38	108.47
22	c	509	CLA	CMB-C2B-C3B	3.75	131.69	124.68
30	C	515	DGD	O3G-C3G-C2G	-3.75	101.85	110.90
29	a	410	LHG	O8-C23-O10	-3.75	114.14	123.59
22	D	403	CLA	CHB-C4A-NA	3.74	129.69	124.51
22	c	509	CLA	CHB-C4A-NA	3.74	129.69	124.51
22	c	511	CLA	C4D-C3D-CAD	-3.74	106.39	108.47
22	c	505	CLA	C4A-NA-C1A	3.73	108.38	106.71
22	C	513	CLA	CMB-C2B-C1B	-3.73	122.74	128.46
22	C	504	CLA	C4D-C3D-CAD	-3.72	106.39	108.47
22	d	404	CLA	CHB-C4A-NA	3.72	129.66	124.51
24	B	618	BCR	C37-C22-C21	-3.72	117.71	122.92
24	K	103	BCR	C37-C22-C21	-3.72	117.72	122.92
22	b	611	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
29	D	411	LHG	O4-P-O5	3.70	130.54	112.24
22	B	611	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
22	C	511	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
22	b	612	CLA	CMD-C2D-C3D	3.69	131.59	124.68
22	A	402	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
22	b	606	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
22	B	616	CLA	CMB-C2B-C1B	-3.68	122.81	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	c	517	DGD	C3G-O3G-C1D	3.68	120.92	113.74
28	A	414	SQD	O47-C7-C8	3.68	119.43	111.50
22	B	612	CLA	C11-C12-C13	-3.67	104.04	115.92
22	b	615	CLA	CMB-C2B-C3B	3.67	131.55	124.68
22	B	611	CLA	O2D-CGD-O1D	-3.66	116.68	123.84
22	C	512	CLA	CHB-C4A-NA	3.66	129.57	124.51
22	A	403	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
27	d	410	LMG	O2-C2-C1	-3.65	101.19	110.05
26	D	406	PL9	C40-C39-C41	3.65	121.41	115.27
22	b	606	CLA	O2D-CGD-CBD	3.64	117.74	111.27
24	B	617	BCR	C2-C1-C6	3.64	116.08	110.48
22	c	502	CLA	CMB-C2B-C3B	3.63	131.48	124.68
22	C	502	CLA	C4D-C3D-CAD	-3.63	106.44	108.47
22	b	602	CLA	CMB-C2B-C3B	3.63	131.47	124.68
26	D	406	PL9	C22-C23-C24	-3.62	118.95	127.66
24	h	101	BCR	C37-C22-C21	-3.62	117.86	122.92
22	C	506	CLA	O2D-CGD-O1D	-3.61	116.77	123.84
22	b	607	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
22	b	603	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
27	m	101	LMG	O1-C1-C2	-3.60	102.67	108.30
30	A	415	DGD	O3G-C3G-C2G	-3.60	102.22	110.90
22	B	608	CLA	O2D-CGD-O1D	-3.59	116.82	123.84
30	c	516	DGD	C3D-C4D-C5D	-3.59	103.84	110.24
26	d	407	PL9	C7-C3-C2	-3.58	118.59	123.30
22	a	405	CLA	CMD-C2D-C3D	3.58	131.38	124.68
22	b	604	CLA	OBD-CAD-CBD	-3.58	120.78	125.89
28	A	412	SQD	C1-O5-C5	-3.58	106.66	113.69
22	b	609	CLA	OBD-CAD-CBD	-3.58	120.78	125.89
22	c	506	CLA	CMB-C2B-C3B	3.58	131.38	124.68
22	b	616	CLA	C1B-CHB-C4A	-3.58	123.03	130.12
22	D	402	CLA	CMD-C2D-C3D	3.58	131.37	124.68
22	d	404	CLA	CMB-C2B-C1B	-3.58	122.97	128.46
29	d	409	LHG	O4-P-O5	3.58	129.92	112.24
22	b	608	CLA	O2D-CGD-O1D	-3.57	116.86	123.84
22	A	402	CLA	CHB-C4A-NA	3.56	129.44	124.51
22	C	501	CLA	OBD-CAD-CBD	-3.56	120.81	125.89
22	B	608	CLA	C4A-NA-C1A	3.56	108.31	106.71
27	m	101	LMG	O3-C3-C2	-3.56	102.12	110.35
23	A	405	PHO	C1-C2-C3	-3.55	119.90	126.04
22	B	607	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
22	B	602	CLA	O2D-CGD-CBD	3.55	117.57	111.27
23	d	401	PHO	O2D-CGD-O1D	-3.55	116.90	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	401	PHO	O1D-CGD-CBD	3.55	131.74	124.48
28	b	620	SQD	O2-C2-C1	3.54	118.64	110.05
26	A	410	PL9	C36-C34-C33	-3.54	113.96	121.12
22	B	605	CLA	C4D-C3D-CAD	-3.53	106.50	108.47
27	Y	101	LMG	O1-C7-C8	-3.53	102.38	110.90
22	b	612	CLA	C1B-CHB-C4A	-3.53	123.13	130.12
22	B	606	CLA	C1B-CHB-C4A	-3.53	123.14	130.12
22	B	606	CLA	O2A-CGA-O1A	-3.51	114.73	123.59
22	B	610	CLA	O2A-CGA-O1A	-3.51	114.75	123.59
22	B	606	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
23	a	404	PHO	CMB-C2B-C1B	-3.50	119.68	125.06
28	B	621	SQD	C3-C4-C5	3.49	116.47	110.24
24	h	101	BCR	C38-C26-C25	-3.49	120.61	124.53
22	c	511	CLA	CMD-C2D-C3D	3.49	131.21	124.68
22	B	616	CLA	C4D-C3D-CAD	-3.49	106.53	108.47
22	B	610	CLA	C1B-CHB-C4A	-3.49	123.21	130.12
28	f	102	SQD	O5-C5-C4	3.49	116.02	109.69
22	b	601	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
22	C	507	CLA	CMB-C2B-C3B	3.47	131.17	124.68
22	B	601	CLA	O2D-CGD-CBD	3.47	117.43	111.27
22	a	405	CLA	OBD-CAD-CBD	-3.47	120.94	125.89
22	B	605	CLA	O1D-CGD-CBD	3.46	131.57	124.48
22	B	609	CLA	C4D-C3D-CAD	-3.46	106.54	108.47
22	c	503	CLA	C4D-C3D-CAD	-3.46	106.54	108.47
22	c	502	CLA	C1-C2-C3	-3.45	120.08	126.04
22	C	504	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
22	c	510	CLA	C6-C5-C3	-3.45	104.41	113.45
22	a	403	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
30	C	515	DGD	O5D-C6D-C5D	-3.44	102.67	109.05
22	b	612	CLA	C11-C12-C13	-3.44	104.79	115.92
35	V	201	HEC	CAD-CBD-CGD	-3.44	106.90	112.67
26	D	406	PL9	C42-C43-C44	-3.44	119.39	127.66
26	d	407	PL9	C36-C34-C33	-3.43	114.18	121.12
22	d	403	CLA	CMB-C2B-C3B	3.43	131.09	124.68
34	F	101	HEM	C1D-C2D-C3D	3.42	109.37	107.00
28	a	411	SQD	O2-C2-C1	3.42	118.35	110.05
22	A	403	CLA	CMB-C2B-C3B	3.41	131.07	124.68
27	M	101	LMG	C1-O6-C5	-3.41	106.99	113.69
22	A	403	CLA	C4A-NA-C1A	3.41	108.24	106.71
22	C	503	CLA	O2A-C1-C2	-3.40	99.70	108.64
22	a	402	CLA	CMD-C2D-C3D	3.40	131.03	124.68
24	A	407	BCR	C27-C26-C25	3.40	127.66	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	616	CLA	CMB-C2B-C3B	3.39	131.02	124.68
22	c	505	CLA	CMB-C2B-C3B	3.39	131.01	124.68
22	b	607	CLA	C4-C3-C5	3.38	120.96	115.27
22	c	512	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
22	D	403	CLA	CMB-C2B-C3B	3.37	130.99	124.68
24	K	101	BCR	C2-C1-C6	3.37	115.67	110.48
24	K	101	BCR	C15-C16-C17	-3.36	116.58	123.47
22	b	612	CLA	OBD-CAD-CBD	-3.36	121.09	125.89
24	B	619	BCR	C36-C18-C17	-3.36	118.22	122.92
22	C	508	CLA	CMB-C2B-C3B	3.36	130.96	124.68
22	D	403	CLA	CMB-C2B-C1B	-3.36	123.31	128.46
22	B	610	CLA	CMD-C2D-C3D	3.35	130.95	124.68
22	B	614	CLA	C4-C3-C5	3.35	120.91	115.27
34	F	101	HEM	CBA-CAA-C2A	-3.35	106.31	112.49
22	A	406	CLA	C1B-CHB-C4A	-3.35	123.49	130.12
22	C	507	CLA	O2D-CGD-O1D	-3.34	117.30	123.84
22	C	513	CLA	O2D-CGD-O1D	-3.34	117.30	123.84
22	B	613	CLA	C4-C3-C5	3.34	120.89	115.27
22	b	609	CLA	CMB-C2B-C3B	3.34	130.93	124.68
22	C	504	CLA	C4A-NA-C1A	3.34	108.21	106.71
22	C	504	CLA	O2A-CGA-O1A	-3.33	115.18	123.59
22	C	506	CLA	C4A-NA-C1A	3.33	108.20	106.71
22	C	513	CLA	CMB-C2B-C3B	3.32	130.88	124.68
27	b	623	LMG	C3-C4-C5	-3.32	104.32	110.24
22	B	611	CLA	O2D-CGD-CBD	3.32	117.16	111.27
22	a	402	CLA	CMB-C2B-C3B	3.31	130.88	124.68
22	C	512	CLA	O2D-CGD-CBD	3.31	117.16	111.27
22	B	616	CLA	O1D-CGD-CBD	3.31	131.26	124.48
24	b	619	BCR	C29-C30-C25	3.31	115.58	110.48
22	b	610	CLA	C1B-CHB-C4A	-3.31	123.57	130.12
22	b	614	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
22	D	402	CLA	CMB-C2B-C3B	3.31	130.86	124.68
29	D	411	LHG	O8-C23-C24	3.30	122.28	111.91
30	H	102	DGD	O6E-C5E-C4E	3.30	115.69	109.69
27	c	519	LMG	O3-C3-C2	-3.30	102.73	110.35
22	C	513	CLA	C4-C3-C5	3.30	120.81	115.27
26	a	409	PL9	C35-C34-C36	3.29	120.81	115.27
28	A	412	SQD	O47-C7-C8	3.29	118.59	111.50
27	b	623	LMG	C8-O7-C10	3.29	125.89	117.79
30	c	518	DGD	C1D-C2D-C3D	-3.29	103.15	110.00
30	C	517	DGD	O3E-C3E-C2E	-3.29	102.75	110.35
30	c	518	DGD	C3D-C4D-C5D	-3.28	104.38	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	403	CLA	C1B-CHB-C4A	-3.28	123.62	130.12
22	C	501	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
22	B	609	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
22	a	405	CLA	CMB-C2B-C3B	3.27	130.80	124.68
22	c	501	CLA	CMB-C2B-C3B	3.27	130.79	124.68
26	a	409	PL9	C3-C4-C5	-3.27	114.35	118.60
30	c	517	DGD	O3G-C3G-C2G	-3.26	103.02	110.90
29	D	411	LHG	O8-C23-O10	-3.26	115.36	123.59
22	c	512	CLA	CMD-C2D-C3D	3.26	130.77	124.68
28	B	621	SQD	O8-S-C6	3.25	110.93	105.74
22	B	604	CLA	C1-C2-C3	-3.25	120.42	126.04
24	t	101	BCR	C36-C18-C19	3.25	123.20	118.08
22	d	404	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
27	c	521	LMG	O7-C10-O9	-3.25	115.86	123.70
22	c	508	CLA	CHB-C4A-NA	3.24	129.00	124.51
24	c	515	BCR	C27-C26-C25	3.24	127.44	122.73
22	b	610	CLA	CHB-C4A-NA	3.23	128.98	124.51
30	C	516	DGD	O2D-C2D-C1D	-3.23	102.20	110.05
22	C	504	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
30	A	415	DGD	O5E-C6E-C5E	-3.22	100.23	111.29
26	d	407	PL9	C22-C23-C24	-3.22	119.90	127.66
22	B	608	CLA	O2D-CGD-CBD	3.22	116.99	111.27
22	b	611	CLA	O2D-CGD-CBD	3.22	116.99	111.27
22	C	508	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
22	c	510	CLA	O2D-CGD-O1D	-3.19	117.59	123.84
27	b	623	LMG	O8-C28-O10	-3.19	115.55	123.59
22	C	503	CLA	C7-C6-C5	-3.18	104.71	113.36
28	b	620	SQD	O9-S-C6	3.18	110.72	106.94
35	v	201	HEC	CMB-C2B-C1B	-3.18	123.57	128.46
22	b	613	CLA	C4D-C3D-CAD	-3.18	106.70	108.47
22	b	603	CLA	C1B-CHB-C4A	-3.18	123.82	130.12
27	b	623	LMG	C4-C3-C2	-3.18	105.27	110.82
22	C	501	CLA	OBD-CAD-C3D	3.18	133.25	127.98
22	c	503	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
22	B	610	CLA	CHB-C4A-NA	3.17	128.90	124.51
22	b	602	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
22	D	402	CLA	C1B-CHB-C4A	-3.17	123.84	130.12
24	h	101	BCR	C27-C26-C25	3.17	127.33	122.73
22	C	506	CLA	O1D-CGD-CBD	3.16	130.96	124.48
28	a	412	SQD	O48-C23-O10	-3.15	115.64	123.59
22	B	615	CLA	CHB-C4A-NA	3.15	128.87	124.51
30	A	415	DGD	O6E-C5E-C4E	3.15	115.41	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	h	101	BCR	C36-C18-C17	-3.14	118.52	122.92
28	a	411	SQD	O8-S-O9	-3.14	103.61	111.27
26	d	407	PL9	C7-C8-C9	-3.14	121.57	126.79
22	C	506	CLA	CMB-C2B-C3B	3.13	130.54	124.68
26	d	407	PL9	C30-C29-C31	-3.13	110.00	115.27
30	C	516	DGD	O5D-C6D-C5D	-3.13	103.26	109.05
24	T	101	BCR	C27-C26-C25	3.13	127.27	122.73
22	c	506	CLA	OBD-CAD-CBD	-3.12	121.43	125.89
22	B	611	CLA	OBD-CAD-C3D	3.12	133.17	127.98
22	b	610	CLA	C1-C2-C3	-3.12	120.65	126.04
22	c	507	CLA	CMB-C2B-C1B	-3.11	123.68	128.46
22	b	610	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
22	b	601	CLA	CMB-C2B-C3B	3.11	130.49	124.68
28	a	411	SQD	O7-S-C6	3.10	110.62	106.94
22	a	403	CLA	CHB-C4A-NA	3.10	128.79	124.51
22	B	614	CLA	CMB-C2B-C1B	-3.09	123.72	128.46
24	t	101	BCR	C7-C8-C9	-3.09	121.57	126.23
22	b	604	CLA	CMD-C2D-C3D	3.08	130.44	124.68
22	C	506	CLA	OBD-CAD-CBD	-3.08	121.50	125.89
22	b	610	CLA	CMB-C2B-C3B	3.07	130.43	124.68
22	b	612	CLA	C4D-C3D-CAD	-3.07	106.76	108.47
22	C	509	CLA	CHB-C4A-NA	3.07	128.76	124.51
26	d	407	PL9	C41-C39-C38	-3.07	114.90	121.12
28	a	412	SQD	O48-C23-C24	3.07	121.55	111.91
22	b	608	CLA	CMD-C2D-C3D	3.07	130.42	124.68
22	c	503	CLA	CMD-C2D-C3D	3.07	130.41	124.68
27	Y	101	LMG	O1-C1-C2	-3.06	103.52	108.30
22	b	601	CLA	O2D-CGD-CBD	3.05	116.70	111.27
35	v	201	HEC	C1D-C2D-C3D	-3.05	104.88	107.00
22	b	603	CLA	O2D-CGD-CBD	3.05	116.68	111.27
22	b	614	CLA	CMB-C2B-C3B	3.05	130.38	124.68
22	c	513	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
22	B	612	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
22	B	609	CLA	CMB-C2B-C3B	3.04	130.36	124.68
22	b	614	CLA	O2A-CGA-O1A	-3.04	115.92	123.59
22	B	603	CLA	OBD-CAD-CBD	-3.03	121.57	125.89
22	c	507	CLA	CMB-C2B-C3B	3.03	130.34	124.68
26	d	407	PL9	C35-C34-C36	3.03	120.36	115.27
22	A	402	CLA	CMB-C2B-C3B	3.03	130.34	124.68
22	b	606	CLA	CMD-C2D-C3D	3.02	130.34	124.68
22	B	615	CLA	CMB-C2B-C1B	-3.02	123.82	128.46
28	b	620	SQD	C3-C4-C5	3.02	115.62	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	h	103	DGD	O3G-C3G-C2G	-3.02	103.62	110.90
22	B	605	CLA	OBD-CAD-C3D	3.02	132.99	127.98
27	a	414	LMG	O8-C28-O10	-3.01	115.99	123.59
22	B	604	CLA	C11-C10-C8	-3.01	106.19	115.92
22	b	603	CLA	CMB-C2B-C3B	3.01	130.31	124.68
30	A	415	DGD	C4E-C3E-C2E	-3.01	105.57	110.82
22	b	606	CLA	CHB-C4A-NA	3.01	128.67	124.51
22	b	612	CLA	CHB-C4A-NA	3.01	128.67	124.51
22	B	607	CLA	CMB-C2B-C3B	3.01	130.30	124.68
22	b	605	CLA	CMB-C2B-C3B	3.00	130.30	124.68
24	B	618	BCR	C2-C1-C6	3.00	115.10	110.48
22	b	601	CLA	CMB-C2B-C1B	-3.00	123.85	128.46
26	A	410	PL9	C20-C19-C21	3.00	120.32	115.27
22	c	506	CLA	OBD-CAD-C3D	3.00	132.96	127.98
26	A	410	PL9	C22-C23-C24	-2.99	120.46	127.66
22	b	609	CLA	C4A-NA-C1A	2.99	108.05	106.71
23	d	401	PHO	C1-C2-C3	-2.99	120.87	126.04
22	B	605	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
26	D	406	PL9	C35-C34-C36	2.98	120.29	115.27
26	D	406	PL9	C50-C49-C48	-2.98	114.03	122.65
22	D	404	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
22	b	605	CLA	C4-C3-C5	2.98	120.28	115.27
22	B	607	CLA	O2A-CGA-O1A	-2.97	116.09	123.59
28	a	412	SQD	O49-C7-C8	-2.97	112.15	123.73
22	C	512	CLA	C4A-NA-C1A	2.97	108.04	106.71
22	B	613	CLA	CHB-C4A-NA	2.97	128.61	124.51
28	a	411	SQD	O9-S-O7	-2.96	103.69	113.95
30	h	103	DGD	C3D-C4D-C5D	-2.96	104.95	110.24
24	B	618	BCR	C29-C30-C25	2.96	115.04	110.48
22	d	404	CLA	CMB-C2B-C3B	2.96	130.22	124.68
22	B	606	CLA	CGD-CBD-CAD	-2.96	101.14	110.73
22	B	614	CLA	OBD-CAD-CBD	-2.96	121.67	125.89
30	c	518	DGD	C3G-C2G-C1G	-2.95	104.81	111.79
27	b	623	LMG	O2-C2-C1	-2.95	102.88	110.05
26	D	406	PL9	C7-C3-C2	-2.95	119.42	123.30
22	d	404	CLA	O2D-CGD-CBD	2.95	116.50	111.27
30	H	102	DGD	O2D-C2D-C1D	-2.95	102.89	110.05
24	C	514	BCR	C36-C18-C17	-2.94	118.80	122.92
34	f	101	HEM	CMD-C2D-C1D	-2.94	123.94	128.46
22	c	507	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
24	d	406	BCR	C38-C26-C25	-2.94	121.23	124.53
27	D	407	LMG	O6-C1-O1	-2.94	103.02	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	607	CLA	C4A-NA-C1A	2.93	108.03	106.71
22	B	605	CLA	C16-C15-C13	-2.93	106.44	115.92
24	D	405	BCR	C7-C8-C9	-2.93	121.80	126.23
22	B	609	CLA	OBD-CAD-CBD	-2.93	121.71	125.89
24	b	619	BCR	C37-C22-C21	-2.93	118.82	122.92
22	b	611	CLA	CMB-C2B-C3B	2.92	130.14	124.68
23	d	401	PHO	CMB-C2B-C1B	-2.92	120.57	125.06
22	D	402	CLA	CHB-C4A-NA	2.92	128.55	124.51
22	B	616	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
22	B	615	CLA	O2D-CGD-CBD	2.91	116.44	111.27
22	d	404	CLA	CMD-C2D-C3D	2.91	130.12	124.68
22	C	506	CLA	CMD-C2D-C3D	2.91	130.12	124.68
22	c	511	CLA	OBD-CAD-CBD	-2.90	121.75	125.89
30	A	415	DGD	C1D-C2D-C3D	-2.90	103.95	110.00
28	f	102	SQD	O47-C7-C8	2.90	118.89	110.80
22	b	606	CLA	CMC-C2C-C3C	2.90	130.41	124.94
24	t	101	BCR	C15-C16-C17	-2.90	117.54	123.47
28	b	620	SQD	C45-O47-C7	2.90	124.92	117.79
27	A	411	LMG	C1-O6-C5	-2.90	108.00	113.69
26	a	409	PL9	C22-C23-C24	-2.89	120.69	127.66
24	d	406	BCR	C24-C23-C22	-2.89	121.87	126.23
22	B	602	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
24	B	617	BCR	C37-C22-C23	2.88	122.62	118.08
27	b	623	LMG	O6-C5-C6	2.88	113.59	106.44
23	d	401	PHO	C1B-NB-C4B	2.88	111.93	106.51
30	C	517	DGD	O6D-C1D-O3G	-2.88	103.16	109.97
22	b	614	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
27	a	414	LMG	C1-O6-C5	-2.87	108.05	113.69
22	B	611	CLA	C7-C6-C5	-2.87	105.57	113.36
30	o	301	DGD	CAB-C9B-C8B	-2.87	99.86	114.42
22	c	501	CLA	CED-O2D-CGD	-2.87	109.45	115.94
22	a	405	CLA	O2D-CGD-CBD	2.86	116.35	111.27
22	b	607	CLA	C6-C7-C8	-2.86	106.67	115.92
35	v	201	HEC	CAD-CBD-CGD	-2.86	107.88	112.67
30	H	102	DGD	O6E-C5E-C6E	-2.86	99.33	106.44
22	c	512	CLA	CMB-C2B-C3B	2.85	130.01	124.68
22	b	602	CLA	CHB-C4A-NA	2.85	128.45	124.51
24	A	407	BCR	C37-C22-C21	-2.85	118.94	122.92
22	b	610	CLA	CAA-CBA-CGA	-2.85	104.94	113.25
22	c	501	CLA	CMD-C2D-C3D	2.84	130.00	124.68
24	H	101	BCR	C38-C26-C25	-2.84	121.34	124.53
22	c	508	CLA	C1B-CHB-C4A	-2.83	124.50	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	619	BCR	C38-C26-C25	-2.83	121.35	124.53
22	C	512	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
30	A	415	DGD	O5D-C1E-C2E	2.83	112.72	108.30
22	c	512	CLA	CHB-C4A-NA	2.83	128.42	124.51
27	A	411	LMG	C1-C2-C3	-2.82	104.12	110.00
24	c	515	BCR	C7-C8-C9	-2.82	121.97	126.23
22	B	611	CLA	CMD-C2D-C3D	2.82	129.95	124.68
24	K	101	BCR	C7-C8-C9	-2.82	121.98	126.23
22	b	616	CLA	CMD-C2D-C3D	2.82	129.95	124.68
22	B	607	CLA	CMC-C2C-C3C	2.82	130.25	124.94
28	f	102	SQD	C1-C2-C3	-2.82	104.13	110.00
24	c	514	BCR	C24-C23-C22	-2.81	121.98	126.23
30	C	517	DGD	O6D-C5D-C6D	-2.81	101.00	106.67
30	o	301	DGD	C8B-C7B-C6B	-2.81	100.17	114.42
22	b	614	CLA	CHB-C4A-NA	2.81	128.39	124.51
22	D	404	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
22	A	402	CLA	CAA-CBA-CGA	-2.80	105.07	113.25
24	A	407	BCR	C15-C16-C17	-2.80	117.75	123.47
22	b	603	CLA	OBD-CAD-CBD	-2.80	121.90	125.89
22	b	601	CLA	C1B-CHB-C4A	-2.79	124.58	130.12
28	a	411	SQD	O48-C23-C24	2.79	120.68	111.91
22	B	610	CLA	O2D-CGD-CBD	2.79	116.23	111.27
22	a	403	CLA	CMB-C2B-C3B	2.79	129.90	124.68
26	d	407	PL9	C20-C19-C21	2.79	119.96	115.27
22	b	601	CLA	CMC-C2C-C3C	2.79	130.20	124.94
22	A	402	CLA	C1B-CHB-C4A	-2.79	124.60	130.12
22	a	403	CLA	O2A-CGA-O1A	-2.79	116.56	123.59
22	C	501	CLA	O2A-CGA-O1A	-2.79	116.56	123.59
28	A	412	SQD	O7-S-C6	2.78	110.25	106.94
22	a	405	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
29	e	101	LHG	O8-C23-C24	2.78	120.63	111.91
22	b	605	CLA	CMC-C2C-C3C	2.78	130.18	124.94
22	C	507	CLA	O2D-CGD-CBD	2.78	116.21	111.27
22	a	405	CLA	CHB-C4A-NA	2.78	128.35	124.51
24	H	101	BCR	C2-C1-C6	2.78	114.76	110.48
27	m	101	LMG	O7-C10-O9	-2.78	116.99	123.70
22	b	613	CLA	C1-C2-C3	-2.78	121.24	126.04
30	A	415	DGD	O2D-C2D-C1D	-2.78	103.30	110.05
27	c	519	LMG	O2-C2-C3	-2.78	103.93	110.35
24	D	405	BCR	C24-C23-C22	-2.77	122.04	126.23
22	c	505	CLA	C6-C7-C8	-2.77	106.95	115.92
22	B	612	CLA	C1B-CHB-C4A	-2.77	124.62	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	402	CLA	CHB-C4A-NA	2.77	128.35	124.51
22	c	504	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
22	c	512	CLA	C1-C2-C3	-2.77	121.25	126.04
22	b	604	CLA	C4D-C3D-CAD	-2.77	106.93	108.47
22	c	503	CLA	C7-C6-C5	-2.77	105.84	113.36
22	a	403	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
24	B	619	BCR	C29-C30-C25	2.77	114.74	110.48
22	c	503	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
22	b	611	CLA	CHB-C4A-NA	2.76	128.33	124.51
27	D	407	LMG	O8-C28-O10	-2.76	116.62	123.59
22	c	512	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
22	B	609	CLA	CMD-C2D-C3D	2.76	129.84	124.68
26	A	410	PL9	O1-C4-C3	-2.76	117.69	120.72
29	D	408	LHG	O8-C23-C24	2.75	120.55	111.91
22	b	602	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
27	A	411	LMG	O6-C1-O1	-2.75	103.47	109.97
24	t	101	BCR	C1-C6-C5	-2.74	118.75	122.61
22	b	610	CLA	O2A-CGA-O1A	-2.74	116.67	123.59
22	B	604	CLA	CHB-C4A-NA	2.74	128.30	124.51
22	A	403	CLA	O2D-CGD-CBD	2.74	116.13	111.27
22	b	615	CLA	C1B-CHB-C4A	-2.74	124.70	130.12
22	a	403	CLA	CMD-C2D-C3D	2.73	129.79	124.68
22	C	503	CLA	CMB-C2B-C1B	-2.73	124.26	128.46
24	b	619	BCR	C36-C18-C17	-2.73	119.10	122.92
24	k	102	BCR	C2-C1-C6	2.72	114.67	110.48
22	B	613	CLA	CHA-C1A-NA	-2.72	120.17	126.40
28	F	102	SQD	O9-S-O7	-2.72	104.53	113.95
28	a	412	SQD	O47-C45-C44	2.72	118.12	108.36
26	D	406	PL9	C37-C38-C39	-2.72	121.11	127.66
24	b	619	BCR	C38-C26-C25	-2.72	121.47	124.53
27	b	623	LMG	O7-C10-O9	-2.71	117.14	123.70
22	D	402	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
22	C	502	CLA	OBD-CAD-CBD	-2.71	122.02	125.89
35	V	201	HEC	CMB-C2B-C1B	-2.71	124.30	128.46
22	C	505	CLA	C1-C2-C3	-2.71	121.36	126.04
24	B	618	BCR	C38-C26-C25	-2.71	121.49	124.53
22	b	604	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
22	C	504	CLA	OBD-CAD-CBD	-2.71	122.03	125.89
26	D	406	PL9	C36-C34-C33	-2.71	115.64	121.12
22	b	604	CLA	C1-C2-C3	-2.70	121.37	126.04
22	b	615	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
28	F	102	SQD	O48-C23-O10	-2.70	116.77	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	507	CLA	C4-C3-C5	2.70	119.81	115.27
22	c	501	CLA	OBD-CAD-CBD	-2.70	122.04	125.89
22	B	604	CLA	OBD-CAD-CBD	-2.69	122.05	125.89
22	C	507	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
35	V	201	HEC	CMC-C2C-C3C	2.69	128.98	125.82
27	Y	101	LMG	C1-O6-C5	-2.69	108.42	113.69
23	a	404	PHO	C1-C2-C3	-2.68	121.40	126.04
28	F	102	SQD	C1-O5-C5	-2.68	108.42	113.69
23	A	405	PHO	O2D-CGD-O1D	-2.68	118.60	123.84
22	C	501	CLA	O2D-CGD-CBD	2.68	116.03	111.27
22	a	403	CLA	O2D-CGD-O1D	-2.68	118.61	123.84
22	C	504	CLA	O2D-CGD-CBD	2.67	116.02	111.27
22	A	406	CLA	CHB-C4A-NA	2.67	128.21	124.51
24	H	101	BCR	C29-C30-C25	2.67	114.59	110.48
22	C	504	CLA	C4-C3-C5	2.67	119.77	115.27
27	A	411	LMG	C9-C8-C7	-2.67	105.48	111.79
22	b	609	CLA	OBD-CAD-C3D	2.66	132.41	127.98
24	C	514	BCR	C15-C16-C17	-2.66	118.02	123.47
22	c	511	CLA	CMB-C2B-C1B	-2.66	124.37	128.46
22	B	611	CLA	CMB-C2B-C3B	2.66	129.66	124.68
22	B	612	CLA	CMD-C2D-C3D	2.66	129.66	124.68
22	C	507	CLA	CMC-C2C-C3C	2.66	129.96	124.94
28	b	620	SQD	O47-C7-C8	2.66	117.23	111.50
22	b	613	CLA	CHB-C4A-NA	2.66	128.19	124.51
22	c	513	CLA	CMD-C2D-C3D	2.66	129.65	124.68
30	H	102	DGD	C6D-C5D-C4D	2.66	117.64	112.09
27	d	410	LMG	O6-C1-O1	-2.65	103.69	109.97
26	D	406	PL9	C31-C32-C33	-2.65	103.16	111.88
22	B	605	CLA	C7-C6-C5	-2.65	106.16	113.36
27	m	101	LMG	O6-C1-O1	-2.65	103.70	109.97
22	B	606	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
27	m	101	LMG	C1-O6-C5	-2.65	108.49	113.69
34	f	101	HEM	CBA-CAA-C2A	-2.65	107.61	112.49
30	c	518	DGD	O3D-C3D-C4D	-2.64	104.23	110.35
30	C	515	DGD	C3D-C4D-C5D	-2.64	105.52	110.24
22	C	512	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
24	d	406	BCR	C27-C26-C25	2.64	126.57	122.73
28	B	621	SQD	O3-C3-C2	-2.64	104.24	110.35
22	B	604	CLA	CMC-C2C-C3C	2.64	129.92	124.94
22	a	402	CLA	C4D-C3D-CAD	-2.64	107.00	108.47
22	b	613	CLA	C7-C6-C5	-2.64	106.20	113.36
24	k	102	BCR	C40-C30-C25	2.64	114.58	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	d	405	CLA	C1B-CHB-C4A	-2.64	124.90	130.12
22	C	512	CLA	CMB-C2B-C3B	2.63	129.61	124.68
22	c	508	CLA	C4D-C3D-CAD	-2.63	107.00	108.47
24	b	617	BCR	C15-C16-C17	-2.63	118.08	123.47
30	C	516	DGD	O6D-C1D-O3G	-2.63	103.74	109.97
22	C	508	CLA	CMC-C2C-C3C	2.63	129.90	124.94
27	Y	101	LMG	O2-C2-C1	-2.63	103.67	110.05
28	B	621	SQD	O48-C23-C24	2.63	120.15	111.91
22	B	614	CLA	C1B-CHB-C4A	-2.63	124.92	130.12
22	c	513	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
22	b	610	CLA	CMB-C2B-C1B	-2.62	124.43	128.46
22	A	406	CLA	O2D-CGD-CBD	2.62	115.93	111.27
22	c	503	CLA	C5-C3-C2	-2.62	115.81	121.12
30	h	103	DGD	C4E-C3E-C2E	-2.62	106.25	110.82
34	F	101	HEM	CAD-CBD-CGD	2.62	117.06	112.67
22	B	613	CLA	CMD-C2D-C3D	2.62	129.58	124.68
24	c	515	BCR	C15-C16-C17	-2.62	118.11	123.47
30	c	517	DGD	C3D-C4D-C5D	-2.62	105.57	110.24
24	b	617	BCR	C38-C26-C25	-2.62	121.59	124.53
22	b	607	CLA	CMB-C2B-C3B	2.62	129.57	124.68
22	B	603	CLA	C4A-NA-C1A	2.61	107.88	106.71
30	h	103	DGD	C1D-C2D-C3D	-2.61	104.55	110.00
22	c	504	CLA	O2A-CGA-O1A	-2.61	117.00	123.59
22	B	603	CLA	O2A-CGA-O1A	-2.61	117.00	123.59
22	c	506	CLA	CHB-C4A-NA	2.61	128.12	124.51
23	a	404	PHO	CBD-CHA-C4D	-2.61	105.60	108.54
27	D	410	LMG	O8-C28-O10	-2.61	117.01	123.59
22	a	402	CLA	C7-C6-C5	-2.61	106.28	113.36
22	c	503	CLA	C4-C3-C5	2.60	119.65	115.27
22	c	504	CLA	O2D-CGD-CBD	2.60	115.89	111.27
24	B	618	BCR	C15-C16-C17	-2.60	118.14	123.47
22	C	505	CLA	O2A-CGA-O1A	-2.60	117.03	123.59
22	B	614	CLA	O2A-CGA-O1A	-2.60	117.03	123.59
22	c	502	CLA	OBD-CAD-CBD	-2.59	122.19	125.89
22	C	513	CLA	O2A-CGA-O1A	-2.59	117.05	123.59
22	C	510	CLA	C11-C10-C8	-2.59	107.55	115.92
24	t	101	BCR	C2-C1-C6	2.59	114.47	110.48
22	B	614	CLA	CMB-C2B-C3B	2.59	129.52	124.68
22	B	614	CLA	C4A-NA-C1A	2.59	107.87	106.71
24	a	406	BCR	C8-C7-C6	-2.59	119.94	127.20
22	c	502	CLA	CMD-C2D-C3D	2.58	129.51	124.68
22	C	508	CLA	CHB-C4A-NA	2.58	128.08	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	406	PL9	C7-C8-C9	-2.58	122.49	126.79
22	C	509	CLA	C1-C2-C3	-2.58	121.58	126.04
22	B	604	CLA	OBD-CAD-C3D	2.58	132.26	127.98
22	B	602	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
22	c	509	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
28	b	620	SQD	O48-C23-O10	-2.57	117.10	123.59
23	A	404	PHO	CMB-C2B-C1B	-2.57	121.10	125.06
22	b	603	CLA	C4D-C3D-CAD	-2.57	107.03	108.47
22	C	504	CLA	CMB-C2B-C3B	2.57	129.49	124.68
26	d	407	PL9	C31-C32-C33	-2.57	103.43	111.88
30	H	102	DGD	O5D-C1E-C2E	2.57	112.32	108.30
24	K	103	BCR	C27-C26-C25	2.57	126.46	122.73
22	B	609	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
27	M	101	LMG	O2-C2-C1	-2.57	103.81	110.05
24	t	101	BCR	C37-C22-C23	2.56	122.11	118.08
22	C	503	CLA	CMD-C2D-C3D	2.56	129.47	124.68
22	C	507	CLA	O2A-CGA-O1A	-2.56	117.12	123.59
22	b	610	CLA	C4A-NA-C1A	2.56	107.86	106.71
22	c	508	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
27	M	101	LMG	O6-C1-O1	-2.56	103.91	109.97
22	A	402	CLA	C6-C5-C3	2.56	120.16	113.45
22	B	611	CLA	C14-C13-C15	-2.56	102.04	111.29
30	c	518	DGD	C3E-C4E-C5E	-2.55	105.68	110.24
22	b	606	CLA	CMB-C2B-C3B	2.55	129.45	124.68
30	C	516	DGD	O5D-C1E-C2E	2.55	112.28	108.30
22	d	403	CLA	C4-C3-C5	2.55	119.56	115.27
28	b	620	SQD	O5-C1-C2	-2.55	104.96	110.35
22	B	604	CLA	CGD-CBD-CAD	-2.55	102.49	110.73
22	c	503	CLA	C1B-CHB-C4A	-2.55	125.08	130.12
22	C	507	CLA	CMD-C2D-C3D	2.54	129.44	124.68
22	C	504	CLA	CHB-C4A-NA	2.54	128.03	124.51
28	a	411	SQD	O8-S-C6	2.54	109.79	105.74
22	c	508	CLA	O2A-CGA-O1A	-2.54	117.18	123.59
22	d	405	CLA	CMC-C2C-C3C	2.54	129.73	124.94
22	b	608	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
22	c	507	CLA	C4-C3-C5	2.54	119.54	115.27
30	H	102	DGD	O6D-C1D-O3G	-2.54	103.96	109.97
22	a	403	CLA	O2D-CGD-CBD	2.54	115.77	111.27
22	C	509	CLA	C1B-CHB-C4A	-2.54	125.10	130.12
22	c	508	CLA	C7-C6-C5	-2.53	106.48	113.36
23	A	404	PHO	C5-C3-C2	2.53	126.24	121.12
27	m	101	LMG	O1-C7-C8	-2.53	104.79	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	l	101	LHG	O8-C23-C24	2.53	119.86	111.91
22	D	403	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
22	C	504	CLA	CMC-C2C-C3C	2.53	129.71	124.94
24	K	101	BCR	C11-C10-C9	-2.53	123.70	127.31
22	b	603	CLA	O2A-CGA-O1A	-2.52	117.22	123.59
22	A	406	CLA	CMD-C2D-C3D	2.52	129.40	124.68
22	c	501	CLA	O2A-CGA-O1A	-2.52	117.22	123.59
24	B	619	BCR	C15-C16-C17	-2.52	118.31	123.47
24	D	405	BCR	C2-C1-C6	2.52	114.36	110.48
34	F	101	HEM	CMD-C2D-C1D	-2.52	124.59	128.46
22	C	503	CLA	C4D-C3D-CAD	-2.52	107.06	108.47
27	c	521	LMG	C6-C5-C4	-2.52	107.11	113.00
28	a	411	SQD	O47-C7-C8	2.52	116.93	111.50
22	b	615	CLA	CMD-C2D-C3D	2.52	129.39	124.68
30	A	415	DGD	O5D-C6D-C5D	-2.52	104.39	109.05
24	K	102	BCR	C27-C26-C25	2.52	126.38	122.73
22	A	403	CLA	CHB-C4A-NA	2.52	127.99	124.51
28	F	102	SQD	C1-C2-C3	-2.51	104.76	110.00
22	c	501	CLA	CHB-C4A-NA	2.51	127.99	124.51
22	C	503	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
22	c	502	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
30	h	103	DGD	O6E-C5E-C4E	2.51	114.25	109.69
22	B	605	CLA	CMB-C2B-C3B	2.51	129.37	124.68
30	A	415	DGD	O3G-C1D-C2D	-2.50	104.40	108.30
30	A	415	DGD	C3G-C2G-C1G	-2.50	105.87	111.79
22	b	609	CLA	CHA-C1A-NA	-2.50	120.67	126.40
22	C	509	CLA	CMC-C2C-C3C	2.50	129.66	124.94
22	B	610	CLA	C1-C2-C3	-2.50	121.72	126.04
22	b	607	CLA	CHA-C1A-NA	-2.50	120.68	126.40
24	K	103	BCR	C15-C16-C17	-2.50	118.36	123.47
22	A	406	CLA	O2A-CGA-O1A	-2.50	117.29	123.59
22	B	605	CLA	CMD-C2D-C3D	2.49	129.34	124.68
22	b	602	CLA	CMC-C2C-C3C	2.49	129.64	124.94
24	k	102	BCR	C27-C26-C25	2.49	126.35	122.73
30	o	301	DGD	C6B-C5B-C4B	-2.49	101.78	114.42
22	B	606	CLA	CMB-C2B-C3B	2.49	129.34	124.68
22	D	403	CLA	C3D-CAD-CBD	-2.49	104.33	107.61
22	b	605	CLA	C4D-C3D-CAD	-2.49	107.08	108.47
22	C	502	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
24	K	101	BCR	C27-C26-C25	2.49	126.34	122.73
22	b	612	CLA	OBD-CAD-C3D	2.48	132.10	127.98
27	a	414	LMG	O6-C1-O1	-2.48	104.09	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	507	CLA	O2A-CGA-O1A	-2.48	117.34	123.59
22	D	402	CLA	C4-C3-C5	2.48	119.44	115.27
30	c	517	DGD	C8B-C7B-C6B	-2.48	101.85	114.42
22	D	404	CLA	CMB-C2B-C1B	-2.48	124.66	128.46
22	b	608	CLA	O2A-CGA-O1A	-2.48	117.34	123.59
28	a	411	SQD	O5-C5-C4	2.48	114.19	109.69
22	B	610	CLA	C4D-C3D-CAD	-2.47	107.09	108.47
24	b	617	BCR	C27-C26-C25	2.47	126.32	122.73
22	D	402	CLA	CED-O2D-CGD	2.47	121.53	115.94
27	D	407	LMG	C31-C30-C29	-2.47	104.30	113.19
22	B	606	CLA	CMD-C2D-C3D	2.47	129.30	124.68
22	B	603	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
22	C	511	CLA	CHB-C4A-NA	2.47	127.93	124.51
22	b	615	CLA	CHB-C4A-NA	2.47	127.93	124.51
26	A	410	PL9	C40-C39-C38	-2.47	117.34	123.68
22	B	611	CLA	C4A-NA-C1A	2.47	107.82	106.71
22	b	615	CLA	C3B-C4B-NB	-2.47	106.02	109.21
30	H	102	DGD	C1D-C2D-C3D	-2.47	104.86	110.00
22	B	616	CLA	CMD-C2D-C3D	2.47	129.29	124.68
22	C	512	CLA	CMC-C2C-C3C	2.47	129.59	124.94
23	A	404	PHO	CBD-CHA-C4D	-2.46	105.76	108.54
22	B	608	CLA	C11-C12-C13	-2.46	107.96	115.92
30	c	518	DGD	O6D-C1D-O3G	-2.46	104.15	109.97
30	c	518	DGD	O6E-C5E-C4E	2.46	114.16	109.69
22	d	404	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
22	b	605	CLA	C16-C15-C13	-2.46	107.98	115.92
22	a	405	CLA	OBD-CAD-C3D	2.45	132.06	127.98
27	c	519	LMG	C1-O6-C5	-2.45	108.87	113.69
22	b	609	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
27	Y	101	LMG	O6-C5-C6	2.45	112.53	106.44
26	a	409	PL9	O2-C1-C2	-2.45	116.17	121.78
22	c	505	CLA	O2D-CGD-CBD	2.45	115.62	111.27
30	C	515	DGD	C4E-C3E-C2E	-2.45	106.55	110.82
22	d	405	CLA	CHB-C4A-NA	2.45	127.89	124.51
22	c	502	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
30	c	517	DGD	O4D-C4D-C3D	2.45	116.00	110.35
22	b	608	CLA	CHB-C4A-NA	2.44	127.89	124.51
35	v	201	HEC	CBA-CAA-C2A	-2.44	107.98	112.48
34	f	101	HEM	CAD-CBD-CGD	2.44	116.77	112.67
22	C	502	CLA	CMB-C2B-C1B	-2.44	124.71	128.46
24	K	103	BCR	C7-C8-C9	-2.44	122.55	126.23
22	c	501	CLA	C4D-C3D-CAD	-2.44	107.11	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	k	101	BCR	C27-C26-C25	2.44	126.27	122.73
29	D	408	LHG	O8-C23-O10	-2.44	117.44	123.59
22	C	505	CLA	CMD-C2D-C3D	2.44	129.24	124.68
27	c	519	LMG	O8-C28-O10	-2.44	117.44	123.59
30	C	517	DGD	O2D-C2D-C1D	-2.43	104.13	110.05
22	C	512	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
24	D	405	BCR	C27-C26-C25	2.43	126.26	122.73
29	A	413	LHG	O8-C23-C24	2.43	119.54	111.91
29	l	101	LHG	C27-C26-C25	-2.43	102.09	114.42
22	d	405	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
23	A	405	PHO	C1B-NB-C4B	2.43	111.09	106.51
22	A	403	CLA	C1-C2-C3	-2.43	121.84	126.04
27	a	414	LMG	C9-C8-C7	-2.43	106.05	111.79
30	C	515	DGD	O1G-C1A-C2A	-2.43	104.29	111.91
26	d	407	PL9	C37-C38-C39	-2.43	121.82	127.66
22	c	506	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
22	C	503	CLA	OBD-CAD-CBD	-2.43	122.43	125.89
22	C	506	CLA	O2A-CGA-O1A	-2.42	117.48	123.59
30	C	516	DGD	C1D-C2D-C3D	-2.42	104.95	110.00
30	C	517	DGD	CAB-C9B-C8B	-2.42	102.13	114.42
22	b	608	CLA	OBD-CAD-C3D	2.42	132.00	127.98
29	D	411	LHG	C18-C17-C16	-2.42	102.13	114.42
22	C	507	CLA	C4D-C3D-CAD	-2.42	107.12	108.47
22	a	402	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
24	a	406	BCR	C27-C26-C25	2.41	126.24	122.73
22	c	509	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
30	H	102	DGD	C1E-O6E-C5E	2.41	118.42	113.69
29	a	410	LHG	C11-C10-C9	-2.41	102.18	114.42
22	C	508	CLA	C4D-C3D-CAD	-2.41	107.13	108.47
22	D	404	CLA	CMD-C2D-C3D	2.41	129.19	124.68
26	A	410	PL9	C7-C3-C2	-2.41	120.13	123.30
24	c	514	BCR	C38-C26-C25	-2.41	121.83	124.53
22	b	614	CLA	C4A-NA-C1A	2.41	107.79	106.71
26	D	406	PL9	O2-C1-C2	-2.41	116.27	121.78
22	C	512	CLA	O2A-CGA-O1A	-2.41	117.52	123.59
24	h	101	BCR	C2-C1-C6	2.40	114.18	110.48
29	D	411	LHG	O4-P-O6	-2.40	96.59	107.75
30	C	515	DGD	C5B-C4B-C3B	-2.40	102.24	114.42
28	A	412	SQD	O8-S-C6	2.40	109.56	105.74
22	b	614	CLA	C1-C2-C3	-2.39	121.90	126.04
22	b	616	CLA	C4-C3-C5	2.39	119.30	115.27
22	C	510	CLA	C1B-CHB-C4A	-2.39	125.38	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	618	BCR	C35-C13-C14	-2.39	119.58	122.92
22	B	607	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
22	d	403	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
22	B	607	CLA	CED-O2D-CGD	2.38	121.33	115.94
22	C	505	CLA	C11-C10-C8	-2.38	108.21	115.92
22	c	510	CLA	CHB-C4A-NA	2.38	127.81	124.51
22	C	501	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
24	k	101	BCR	C38-C26-C25	-2.38	121.86	124.53
24	b	619	BCR	C2-C1-C6	2.38	114.14	110.48
22	B	615	CLA	CMB-C2B-C3B	2.38	129.12	124.68
22	B	604	CLA	C6-C5-C3	-2.38	107.22	113.45
22	b	610	CLA	CMC-C2C-C3C	2.38	129.42	124.94
22	C	502	CLA	CHA-C1A-NA	-2.38	120.96	126.40
22	B	610	CLA	O1A-CGA-CBA	2.38	133.00	123.73
30	A	415	DGD	C8B-C7B-C6B	-2.37	102.38	114.42
22	B	605	CLA	C11-C10-C8	-2.37	108.25	115.92
30	c	517	DGD	O2G-C1B-O1B	-2.37	117.97	123.70
22	b	603	CLA	CMA-C3A-C4A	2.37	118.15	111.77
24	C	514	BCR	C27-C26-C25	2.37	126.17	122.73
22	b	607	CLA	O2A-C1-C2	-2.37	102.41	108.64
24	b	618	BCR	C27-C26-C25	2.37	126.17	122.73
22	C	512	CLA	C1-C2-C3	-2.37	121.95	126.04
30	c	516	DGD	O6D-C1D-O3G	-2.37	104.37	109.97
22	B	608	CLA	CHA-C1A-NA	-2.37	120.98	126.40
29	D	408	LHG	C18-C17-C16	-2.37	102.41	114.42
22	B	606	CLA	O2D-CGD-CBD	2.37	115.47	111.27
22	B	611	CLA	CHB-C4A-NA	2.37	127.78	124.51
24	c	515	BCR	C38-C26-C25	-2.37	121.87	124.53
28	a	411	SQD	O5-C1-C2	-2.36	105.34	110.35
22	D	402	CLA	C1-C2-C3	-2.36	121.95	126.04
22	B	614	CLA	O1D-CGD-CBD	2.36	129.32	124.48
22	b	613	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
22	C	501	CLA	CMB-C2B-C1B	-2.36	124.83	128.46
24	A	407	BCR	C36-C18-C17	-2.36	119.61	122.92
22	b	605	CLA	CMD-C2D-C3D	2.36	129.10	124.68
24	H	101	BCR	C37-C22-C23	2.36	121.80	118.08
22	B	615	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
28	f	102	SQD	O5-C1-O6	2.36	115.56	109.97
22	b	605	CLA	CHB-C4A-NA	2.36	127.77	124.51
30	A	415	DGD	CDB-CCB-CBB	-2.36	102.45	114.42
27	m	101	LMG	O8-C28-O10	-2.36	117.64	123.59
28	F	102	SQD	O5-C5-C4	2.36	113.97	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	619	BCR	C16-C15-C14	-2.35	118.65	123.47
22	d	403	CLA	CBA-CAA-C2A	-2.35	106.92	113.86
28	F	102	SQD	O48-C23-C24	2.35	119.29	111.91
29	D	409	LHG	C6-C5-C4	2.35	117.35	111.79
27	m	101	LMG	C38-C37-C36	-2.35	102.49	114.42
28	a	411	SQD	O10-C23-C24	-2.35	114.56	123.73
22	b	612	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
22	C	505	CLA	CAA-CBA-CGA	-2.35	106.39	113.25
27	A	411	LMG	C40-C39-C38	-2.35	102.50	114.42
22	c	507	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
23	a	404	PHO	C1B-NB-C4B	2.34	110.92	106.51
22	C	505	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
22	B	612	CLA	C1-C2-C3	-2.34	122.00	126.04
26	A	410	PL9	C7-C8-C9	-2.33	122.91	126.79
22	B	606	CLA	CHB-C4A-NA	2.33	127.74	124.51
22	C	511	CLA	CMB-C2B-C3B	2.33	129.04	124.68
22	B	601	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
22	b	609	CLA	C4D-C3D-CAD	-2.33	107.17	108.47
22	c	507	CLA	CMD-C2D-C3D	2.33	129.03	124.68
24	b	618	BCR	C15-C16-C17	-2.33	118.71	123.47
22	b	606	CLA	C4-C3-C5	2.33	119.19	115.27
22	B	612	CLA	O2A-CGA-O1A	-2.32	117.72	123.59
23	a	404	PHO	O2A-CGA-O1A	-2.32	117.72	123.59
30	c	516	DGD	C3E-C4E-C5E	-2.32	106.10	110.24
26	a	409	PL9	C46-C47-C48	-2.32	104.25	111.88
24	H	101	BCR	C27-C26-C25	2.32	126.10	122.73
24	t	101	BCR	C27-C26-C25	2.32	126.10	122.73
23	A	405	PHO	C2B-C1B-NB	-2.32	106.29	109.79
24	K	102	BCR	C38-C26-C25	-2.32	121.92	124.53
22	b	614	CLA	CMC-C2C-C3C	2.32	129.31	124.94
34	f	101	HEM	C4C-C3C-C2C	2.32	108.52	106.90
30	H	102	DGD	O5E-C6E-C5E	-2.32	103.35	111.29
27	Y	101	LMG	C40-C39-C38	-2.31	102.70	114.42
22	c	512	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
22	C	502	CLA	CMB-C2B-C3B	2.31	128.99	124.68
30	C	517	DGD	CBB-CAB-C9B	-2.31	102.72	114.42
22	A	403	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
24	H	101	BCR	C37-C22-C21	-2.30	119.70	122.92
22	a	405	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
24	C	514	BCR	C2-C1-C6	2.30	114.02	110.48
22	d	405	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
22	B	613	CLA	C2A-C1A-CHA	2.30	127.88	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	402	CLA	CMD-C2D-C3D	2.30	128.98	124.68
24	D	405	BCR	C38-C26-C25	-2.30	121.95	124.53
22	c	505	CLA	CHB-C4A-NA	2.30	127.69	124.51
30	c	517	DGD	C6D-O5D-C1E	2.29	118.22	113.74
22	c	505	CLA	C11-C10-C8	-2.29	108.51	115.92
26	a	409	PL9	C12-C13-C14	-2.29	122.14	127.66
23	a	404	PHO	C2C-C1C-NC	2.29	113.25	109.79
22	c	503	CLA	OBD-CAD-CBD	-2.29	122.62	125.89
28	b	620	SQD	O47-C45-C46	2.29	116.69	108.40
22	c	503	CLA	CMB-C2B-C3B	2.28	128.95	124.68
23	d	401	PHO	CMC-C2C-C1C	-2.28	121.55	125.06
23	d	401	PHO	C16-C15-C13	-2.28	108.54	115.92
24	b	618	BCR	C38-C26-C25	-2.28	121.97	124.53
22	D	403	CLA	C4D-C3D-CAD	2.28	109.74	108.47
22	c	507	CLA	C4D-C3D-CAD	-2.28	107.20	108.47
26	A	410	PL9	C35-C34-C36	2.28	119.11	115.27
22	c	503	CLA	O1D-CGD-CBD	2.28	129.15	124.48
22	B	603	CLA	OBD-CAD-C3D	2.28	131.76	127.98
24	b	617	BCR	C8-C7-C6	-2.28	120.81	127.20
22	c	511	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
27	A	411	LMG	C38-C37-C36	-2.28	102.87	114.42
22	b	613	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
22	B	616	CLA	CAA-CBA-CGA	-2.27	106.61	113.25
22	B	611	CLA	C1-C2-C3	-2.27	122.11	126.04
22	B	614	CLA	C4D-C3D-CAD	-2.27	107.20	108.47
22	D	404	CLA	CMB-C2B-C3B	2.27	128.93	124.68
22	b	609	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
28	B	621	SQD	C4-C3-C2	2.27	114.79	110.82
22	B	605	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
24	a	406	BCR	C37-C22-C21	-2.27	119.74	122.92
22	b	608	CLA	CHA-C1A-NA	-2.27	121.20	126.40
22	c	512	CLA	O1D-CGD-CBD	2.27	129.13	124.48
22	d	403	CLA	C4A-NA-C1A	2.27	107.73	106.71
22	c	504	CLA	C4-C3-C5	2.27	119.09	115.27
22	C	502	CLA	O1D-CGD-CBD	2.27	129.12	124.48
30	C	515	DGD	O2G-C1B-C2B	-2.27	106.61	111.50
24	b	617	BCR	C36-C18-C17	-2.27	119.75	122.92
24	t	101	BCR	C38-C26-C27	-2.27	109.26	113.62
22	c	501	CLA	CMC-C2C-C3C	2.27	129.21	124.94
27	M	101	LMG	C40-C39-C38	-2.26	102.94	114.42
26	A	410	PL9	C27-C28-C29	-2.26	122.21	127.66
22	b	604	CLA	OBD-CAD-C3D	2.26	131.74	127.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	o	301	DGD	CDB-CCB-CBB	-2.26	102.95	114.42
24	c	515	BCR	C36-C18-C17	-2.26	119.76	122.92
30	c	516	DGD	CBB-CAB-C9B	-2.26	102.95	114.42
29	D	409	LHG	O8-C23-C24	2.26	119.00	111.91
24	K	103	BCR	C16-C15-C14	-2.26	118.85	123.47
22	C	504	CLA	CMD-C2D-C3D	2.26	128.90	124.68
22	B	604	CLA	CHA-C1A-NA	-2.26	121.23	126.40
22	b	609	CLA	CMC-C2C-C3C	2.26	129.19	124.94
24	A	407	BCR	C37-C22-C23	2.25	121.63	118.08
22	c	511	CLA	O2D-CGD-CBD	2.25	115.27	111.27
26	A	410	PL9	C40-C39-C41	2.25	119.06	115.27
22	b	613	CLA	CHA-C1A-NA	-2.25	121.24	126.40
22	B	607	CLA	C3A-C2A-C1A	2.25	104.71	101.34
22	b	613	CLA	C16-C15-C13	-2.25	108.65	115.92
29	l	101	LHG	O8-C23-O10	-2.25	117.92	123.59
22	A	406	CLA	C1-C2-C3	-2.25	122.16	126.04
22	b	604	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
22	C	513	CLA	O2D-CGD-CBD	2.25	115.26	111.27
22	d	403	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
22	b	607	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
22	B	616	CLA	C2A-C3A-C4A	2.24	105.49	101.87
26	a	409	PL9	C7-C8-C9	-2.24	123.06	126.79
26	A	410	PL9	C41-C39-C38	-2.24	116.58	121.12
30	H	102	DGD	C7B-C6B-C5B	-2.24	103.07	114.42
26	A	410	PL9	O2-C1-C2	-2.24	116.66	121.78
26	a	409	PL9	C27-C28-C29	-2.24	122.28	127.66
22	B	602	CLA	CMD-C2D-C3D	2.24	128.86	124.68
26	a	409	PL9	C45-C44-C46	-2.23	111.52	115.27
30	C	515	DGD	C1E-C2E-C3E	-2.23	105.35	110.00
22	a	405	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
22	c	504	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
27	D	407	LMG	O3-C3-C2	-2.23	105.20	110.35
27	b	623	LMG	C40-C39-C38	-2.22	103.14	114.42
22	b	616	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
22	c	510	CLA	CMD-C2D-C3D	2.22	128.84	124.68
22	c	510	CLA	O2A-C1-C2	-2.22	102.80	108.64
26	a	409	PL9	O2-C1-C6	2.22	124.43	120.59
28	f	102	SQD	O5-C1-C2	-2.22	105.65	110.35
30	C	515	DGD	C3B-C2B-C1B	-2.22	105.55	113.62
29	d	409	LHG	C26-C25-C24	2.22	121.16	113.19
30	C	517	DGD	C8B-C7B-C6B	-2.22	103.17	114.42
24	K	103	BCR	C36-C18-C19	2.22	121.57	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	602	CLA	C1-C2-C3	-2.22	122.21	126.04
24	t	101	BCR	C3-C4-C5	-2.21	110.12	114.08
30	c	518	DGD	O6E-C1E-O5D	-2.21	104.74	109.97
22	b	612	CLA	C1-C2-C3	-2.21	122.22	126.04
22	C	510	CLA	OBD-CAD-CBD	-2.21	122.74	125.89
22	c	504	CLA	O2A-C1-C2	-2.21	102.83	108.64
30	H	102	DGD	C1D-O6D-C5D	-2.21	109.36	113.69
24	t	101	BCR	C34-C9-C10	-2.21	119.83	122.92
29	D	408	LHG	O7-C7-C8	-2.20	106.75	111.50
34	F	101	HEM	C3C-C4C-NC	-2.20	106.78	110.94
22	b	601	CLA	CMD-C2D-C3D	2.20	128.79	124.68
22	b	607	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
22	B	605	CLA	CHB-C4A-NA	2.20	127.55	124.51
22	B	611	CLA	C4D-C3D-CAD	-2.20	107.25	108.47
24	b	617	BCR	C37-C22-C21	-2.20	119.85	122.92
22	d	405	CLA	C4A-NA-C1A	2.19	107.69	106.71
22	C	505	CLA	O2A-C1-C2	-2.19	102.88	108.64
22	C	505	CLA	OBD-CAD-CBD	-2.19	122.77	125.89
22	C	506	CLA	CHA-C1A-NA	-2.19	121.38	126.40
22	C	511	CLA	CMD-C2D-C3D	2.19	128.77	124.68
30	c	518	DGD	C4E-C3E-C2E	-2.19	107.00	110.82
26	a	409	PL9	C36-C34-C33	-2.19	116.69	121.12
27	d	410	LMG	C3-C4-C5	-2.18	106.34	110.24
22	C	507	CLA	C1-C2-C3	-2.18	122.27	126.04
22	c	504	CLA	OBD-CAD-CBD	-2.18	122.78	125.89
22	b	611	CLA	CED-O2D-CGD	-2.18	111.01	115.94
22	b	614	CLA	C4-C3-C5	2.18	118.94	115.27
29	d	409	LHG	O8-C6-C5	-2.18	102.09	108.43
29	a	410	LHG	C25-C24-C23	2.18	121.53	113.62
26	D	406	PL9	C30-C29-C31	-2.18	111.61	115.27
22	B	609	CLA	OBD-CAD-C3D	2.17	131.59	127.98
22	b	605	CLA	O1D-CGD-CBD	2.17	128.93	124.48
26	D	406	PL9	C27-C28-C29	-2.17	122.42	127.66
22	B	614	CLA	CMD-C2D-C3D	2.17	128.74	124.68
27	c	521	LMG	O8-C28-O10	-2.17	118.11	123.59
26	d	407	PL9	O1-C4-C3	-2.17	118.33	120.72
27	m	101	LMG	C6-C5-C4	-2.17	107.92	113.00
27	b	623	LMG	C1-C2-C3	-2.17	105.47	110.00
22	a	403	CLA	CED-O2D-CGD	-2.17	111.03	115.94
22	B	616	CLA	CHB-C4A-NA	2.17	127.51	124.51
27	c	519	LMG	O8-C28-C29	2.17	118.70	111.91
30	h	103	DGD	C1D-O6D-C5D	-2.16	109.44	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	c	517	DGD	CDB-CCB-CBB	-2.16	103.45	114.42
24	a	406	BCR	C38-C26-C27	-2.16	109.47	113.62
22	c	507	CLA	CHB-C4A-NA	2.16	127.50	124.51
26	d	407	PL9	C27-C28-C29	-2.16	122.47	127.66
27	a	414	LMG	C4-C3-C2	-2.16	107.06	110.82
22	C	510	CLA	CHA-C1A-NA	-2.15	121.47	126.40
22	B	601	CLA	C4-C3-C5	2.15	118.89	115.27
29	D	411	LHG	O3-P-O5	-2.15	100.66	109.07
27	m	101	LMG	C20-C19-C18	-2.15	103.50	114.42
24	b	617	BCR	C3-C4-C5	-2.15	110.23	114.08
22	B	601	CLA	C2A-C1A-CHA	2.15	127.62	123.86
22	B	612	CLA	CED-O2D-CGD	-2.15	111.08	115.94
24	B	617	BCR	C3-C4-C5	-2.15	110.24	114.08
28	B	621	SQD	O47-C45-C46	2.15	116.18	108.40
29	e	101	LHG	C20-C19-C18	-2.15	103.53	114.42
29	D	409	LHG	O8-C23-O10	-2.15	118.17	123.59
30	C	515	DGD	C2G-O2G-C1B	2.15	123.07	117.79
22	C	507	CLA	CHB-C4A-NA	2.14	127.48	124.51
28	B	621	SQD	O2-C2-C1	2.14	115.25	110.05
22	b	603	CLA	O1A-CGA-CBA	2.14	132.09	123.73
23	a	404	PHO	C3A-C4A-CHB	-2.14	118.13	121.83
22	B	605	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
24	k	101	BCR	C1-C6-C5	-2.14	119.60	122.61
24	T	101	BCR	C38-C26-C27	-2.14	109.50	113.62
27	c	521	LMG	O3-C3-C2	-2.14	105.40	110.35
29	e	101	LHG	C11-C10-C9	-2.14	103.56	114.42
22	c	503	CLA	CHB-C4A-NA	2.14	127.47	124.51
23	a	404	PHO	CMB-C2B-C3B	2.14	133.54	128.30
24	C	514	BCR	C15-C14-C13	-2.14	124.26	127.31
22	B	608	CLA	CMC-C2C-C3C	2.14	128.97	124.94
30	h	103	DGD	C7B-C6B-C5B	-2.14	103.58	114.42
22	B	615	CLA	OBD-CAD-CBD	-2.14	122.84	125.89
22	c	509	CLA	O2A-CGA-CBA	2.14	118.61	111.91
28	f	102	SQD	O47-C7-O49	-2.13	118.55	123.70
27	Y	101	LMG	O8-C28-O10	-2.13	118.21	123.59
30	C	517	DGD	O3D-C3D-C4D	-2.13	105.42	110.35
22	B	614	CLA	CHA-C1A-NA	-2.13	121.52	126.40
27	d	410	LMG	O7-C10-O9	-2.13	118.55	123.70
27	m	101	LMG	C22-C21-C20	-2.13	103.61	114.42
29	d	409	LHG	C27-C26-C25	-2.13	103.61	114.42
22	c	512	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
22	B	604	CLA	C1-O2A-CGA	-2.13	110.86	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	410	PL9	C36-C37-C38	-2.13	104.88	111.88
24	K	103	BCR	C40-C30-C25	2.13	113.75	110.30
24	B	619	BCR	C28-C27-C26	-2.13	110.28	114.08
26	A	410	PL9	C31-C32-C33	-2.13	104.88	111.88
24	B	618	BCR	C40-C30-C25	2.13	113.75	110.30
30	c	518	DGD	CDB-CCB-CBB	-2.13	103.63	114.42
22	B	609	CLA	CHB-C4A-NA	2.13	127.45	124.51
27	D	407	LMG	C3-C4-C5	-2.13	106.45	110.24
22	a	402	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
22	c	508	CLA	C11-C10-C8	-2.12	109.05	115.92
22	a	405	CLA	C4D-C3D-CAD	-2.12	107.29	108.47
30	H	102	DGD	CAB-C9B-C8B	-2.12	103.65	114.42
24	b	619	BCR	C8-C7-C6	-2.12	121.24	127.20
22	b	608	CLA	O2D-CGD-CBD	2.12	115.04	111.27
22	B	613	CLA	OBD-CAD-CBD	-2.12	122.87	125.89
24	d	406	BCR	C16-C15-C14	-2.12	119.14	123.47
24	K	101	BCR	C33-C5-C6	-2.12	122.15	124.53
22	c	505	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
22	C	513	CLA	CMD-C2D-C3D	2.12	128.64	124.68
24	b	619	BCR	C15-C16-C17	-2.12	119.14	123.47
28	f	102	SQD	C45-O47-C7	2.11	122.99	117.79
24	h	101	BCR	C11-C10-C9	-2.11	124.29	127.31
22	d	405	CLA	O1D-CGD-CBD	2.11	128.81	124.48
22	a	403	CLA	CMC-C2C-C3C	2.11	128.92	124.94
22	A	403	CLA	C7-C6-C5	-2.11	107.62	113.36
22	c	502	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
27	a	414	LMG	O5-C6-C5	-2.11	104.05	111.29
22	C	503	CLA	CHA-C1A-NA	-2.11	121.56	126.40
22	C	503	CLA	CMC-C2C-C3C	2.11	128.92	124.94
27	Y	101	LMG	O7-C10-O9	-2.11	118.60	123.70
22	c	513	CLA	CHB-C4A-NA	2.11	127.43	124.51
29	D	409	LHG	O8-C6-C5	-2.11	102.29	108.43
24	h	101	BCR	C16-C17-C18	-2.11	124.30	127.31
22	d	403	CLA	O1D-CGD-CBD	2.11	128.80	124.48
30	C	517	DGD	C3D-C4D-C5D	-2.11	106.48	110.24
30	c	516	DGD	C4A-C3A-C2A	-2.11	105.62	113.19
22	c	508	CLA	CMD-C2D-C3D	2.10	128.62	124.68
26	a	409	PL9	C37-C38-C39	-2.10	122.59	127.66
29	d	408	LHG	O8-C6-C5	-2.10	102.31	108.43
29	L	101	LHG	C12-C11-C10	-2.10	103.75	114.42
22	c	503	CLA	CMC-C2C-C3C	2.10	128.91	124.94
22	b	606	CLA	C5-C3-C2	-2.10	116.86	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	412	SQD	O48-C23-C24	2.10	118.50	111.91
22	C	510	CLA	C7-C6-C5	-2.10	107.66	113.36
27	c	519	LMG	C40-C39-C38	-2.10	103.78	114.42
26	a	409	PL9	C46-C44-C43	2.10	125.36	121.12
27	M	101	LMG	C38-C37-C36	-2.09	103.80	114.42
22	d	403	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
22	b	604	CLA	CMC-C2C-C3C	2.09	128.89	124.94
23	d	401	PHO	CBD-CHA-C4D	-2.09	106.18	108.54
29	D	411	LHG	C11-C10-C9	-2.09	103.81	114.42
24	t	101	BCR	C19-C18-C17	-2.09	115.73	118.94
24	d	406	BCR	C2-C1-C6	2.09	113.70	110.48
22	D	403	CLA	O2D-CGD-CBD	2.09	114.98	111.27
27	M	101	LMG	C17-C16-C15	-2.09	103.82	114.42
30	c	517	DGD	C4E-C3E-C2E	-2.09	107.18	110.82
30	c	517	DGD	O2D-C2D-C1D	-2.09	104.97	110.05
22	a	402	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
22	B	606	CLA	CMC-C2C-C3C	2.09	128.88	124.94
22	b	606	CLA	C6-C5-C3	2.09	118.92	113.45
28	A	414	SQD	O47-C45-C46	2.09	110.96	106.13
22	B	604	CLA	C11-C12-C13	-2.08	109.18	115.92
29	D	411	LHG	C20-C19-C18	-2.08	103.84	114.42
24	C	514	BCR	C7-C8-C9	-2.08	123.08	126.23
22	C	508	CLA	O2D-CGD-CBD	2.08	114.97	111.27
29	l	101	LHG	O10-C23-C24	-2.08	115.60	123.73
22	c	511	CLA	CHB-C4A-NA	2.08	127.39	124.51
23	d	401	PHO	CAA-CBA-CGA	-2.08	107.17	113.25
30	h	103	DGD	O5E-C6E-C5E	-2.08	104.14	111.29
26	D	406	PL9	C20-C19-C21	2.08	118.77	115.27
27	Y	101	LMG	C3-C4-C5	-2.08	106.53	110.24
27	c	519	LMG	C6-C5-C4	-2.08	108.13	113.00
22	b	605	CLA	OBD-CAD-CBD	-2.08	122.92	125.89
29	a	410	LHG	C20-C19-C18	-2.08	103.86	114.42
22	d	404	CLA	C2A-C1A-CHA	2.08	127.50	123.86
24	K	102	BCR	C8-C7-C6	-2.08	121.36	127.20
22	C	513	CLA	C3A-C2A-C1A	2.08	104.45	101.34
22	B	607	CLA	C2A-C1A-CHA	2.08	127.49	123.86
24	a	406	BCR	C37-C22-C23	2.08	121.35	118.08
24	A	407	BCR	C36-C18-C19	2.07	121.35	118.08
22	b	612	CLA	CBC-CAC-C3C	2.07	117.55	112.27
22	d	405	CLA	C4-C3-C5	2.07	118.76	115.27
24	A	407	BCR	C1-C6-C5	-2.07	119.70	122.61
22	B	612	CLA	CHB-C4A-NA	2.07	127.37	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	514	BCR	C2-C1-C6	2.07	113.67	110.48
22	C	508	CLA	CMD-C2D-C3D	2.07	128.54	124.68
22	b	603	CLA	C4-C3-C5	2.06	118.74	115.27
26	D	406	PL9	C12-C13-C14	-2.06	122.69	127.66
22	b	616	CLA	CGD-CBD-CAD	-2.06	104.05	110.73
22	c	509	CLA	CMC-C2C-C3C	2.06	128.83	124.94
27	D	407	LMG	C9-C8-C7	-2.06	106.92	111.79
24	k	102	BCR	C16-C15-C14	-2.06	119.25	123.47
30	A	415	DGD	C6D-O5D-C1E	2.06	117.76	113.74
22	c	501	CLA	C1B-CHB-C4A	-2.06	126.04	130.12
22	D	402	CLA	C6-C5-C3	2.06	118.85	113.45
22	c	506	CLA	O2D-CGD-O1D	-2.05	119.82	123.84
30	c	518	DGD	C6B-C5B-C4B	-2.05	104.00	114.42
24	B	619	BCR	C37-C22-C23	2.05	121.31	118.08
22	b	605	CLA	O2D-CGD-CBD	2.05	114.91	111.27
22	b	610	CLA	C11-C12-C13	-2.05	109.29	115.92
27	Y	101	LMG	O6-C1-O1	-2.05	105.11	109.97
27	D	407	LMG	O2-C2-C1	-2.05	105.06	110.05
22	b	604	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
22	B	610	CLA	OBD-CAD-CBD	-2.05	122.97	125.89
23	A	404	PHO	C1-O2A-CGA	2.05	121.82	116.44
22	d	403	CLA	CMC-C2C-C3C	2.05	128.80	124.94
30	C	516	DGD	O1G-C1A-O1A	-2.05	118.43	123.59
22	B	603	CLA	CHB-C4A-NA	2.05	127.34	124.51
29	l	101	LHG	C20-C19-C18	-2.04	104.05	114.42
30	h	103	DGD	O3E-C3E-C2E	-2.04	105.62	110.35
30	C	516	DGD	C8B-C7B-C6B	-2.04	104.05	114.42
30	A	415	DGD	O1G-C1A-O1A	-2.04	118.44	123.59
22	A	402	CLA	C4D-C3D-CAD	-2.04	107.33	108.47
29	D	408	LHG	C20-C19-C18	-2.04	104.06	114.42
23	A	405	PHO	CBD-CHA-C4D	-2.04	106.24	108.54
29	D	408	LHG	C27-C26-C25	-2.04	104.07	114.42
28	b	620	SQD	O5-C5-C4	2.04	113.40	109.69
22	c	510	CLA	O2D-CGD-CBD	2.04	114.89	111.27
24	K	103	BCR	C3-C4-C5	-2.04	110.44	114.08
22	c	503	CLA	C11-C12-C13	-2.04	109.33	115.92
22	c	502	CLA	C4D-C3D-CAD	-2.04	107.33	108.47
24	B	617	BCR	C15-C16-C17	-2.04	119.31	123.47
22	D	403	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
22	b	606	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
30	A	415	DGD	O4D-C4D-C3D	2.03	115.05	110.35
27	M	101	LMG	O8-C28-O10	-2.03	118.47	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	508	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	B	603	CLA	O1A-CGA-CBA	2.03	131.65	123.73
22	b	610	CLA	C16-C17-C18	-2.03	106.42	115.98
22	B	608	CLA	OBD-CAD-CBD	-2.03	123.00	125.89
26	a	409	PL9	C31-C32-C33	-2.03	105.22	111.88
24	h	101	BCR	C20-C21-C22	-2.03	124.42	127.31
22	B	616	CLA	CHA-C1A-NA	-2.03	121.76	126.40
22	C	511	CLA	CMC-C2C-C3C	2.03	128.76	124.94
22	c	504	CLA	CHB-C4A-NA	2.03	127.31	124.51
22	B	610	CLA	O1D-CGD-CBD	2.03	128.63	124.48
26	d	407	PL9	C8-C7-C3	2.02	117.69	111.98
22	B	615	CLA	C1-O2A-CGA	2.02	121.75	116.44
24	D	405	BCR	C15-C16-C17	-2.02	119.33	123.47
27	D	407	LMG	C38-C37-C36	-2.02	104.17	114.42
29	L	101	LHG	C27-C26-C25	-2.02	104.17	114.42
34	F	101	HEM	C4C-C3C-C2C	2.02	108.31	106.90
22	c	509	CLA	CMD-C2D-C3D	2.02	128.45	124.68
22	B	603	CLA	C1B-CHB-C4A	-2.02	126.12	130.12
24	b	619	BCR	C11-C10-C9	-2.02	124.43	127.31
30	h	103	DGD	O6E-C5E-C6E	-2.02	101.42	106.44
22	C	512	CLA	CMD-C2D-C3D	2.01	128.45	124.68
22	c	512	CLA	C4D-C3D-CAD	-2.01	107.35	108.47
22	A	402	CLA	C16-C15-C13	-2.01	109.41	115.92
22	c	513	CLA	C4A-NA-C1A	2.01	107.61	106.71
23	A	404	PHO	C3A-C4A-CHB	-2.01	118.35	121.83
22	c	513	CLA	O1D-CGD-CBD	2.01	128.60	124.48
22	B	616	CLA	C1B-CHB-C4A	-2.01	126.13	130.12
24	K	103	BCR	C11-C10-C9	-2.01	124.44	127.31
22	B	615	CLA	CMD-C2D-C3D	2.01	128.44	124.68
22	c	502	CLA	CMC-C2C-C3C	2.01	128.73	124.94
24	A	407	BCR	C4-C5-C6	2.01	125.65	122.73
30	C	515	DGD	CDB-CCB-CBB	-2.01	104.23	114.42
22	b	605	CLA	OBD-CAD-C3D	2.01	131.31	127.98
27	a	414	LMG	O2-C2-C3	-2.01	105.71	110.35
22	B	606	CLA	O1A-CGA-CBA	2.01	131.56	123.73
22	c	509	CLA	C1-O2A-CGA	-2.01	111.18	116.44
27	A	411	LMG	C3-C4-C5	-2.01	106.66	110.24
22	C	504	CLA	O1A-CGA-CBA	2.01	131.56	123.73
24	K	103	BCR	C38-C26-C27	-2.01	109.76	113.62
22	d	405	CLA	C1-C2-C3	-2.00	122.58	126.04
22	d	405	CLA	OBD-CAD-CBD	-2.00	123.03	125.89
24	H	101	BCR	C1-C6-C5	-2.00	119.79	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	618	BCR	C15-C14-C13	-2.00	124.45	127.31
22	C	503	CLA	CMB-C2B-C3B	2.00	128.42	124.68
24	c	514	BCR	C7-C8-C9	-2.00	123.21	126.23
30	A	415	DGD	CBB-CAB-C9B	-2.00	104.27	114.42

All (57) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	402	CLA	ND
22	A	406	CLA	ND
22	B	601	CLA	ND
22	B	602	CLA	ND
22	B	603	CLA	ND
22	B	604	CLA	ND
22	B	605	CLA	ND
22	B	606	CLA	ND
22	B	607	CLA	ND
22	B	610	CLA	ND
22	B	611	CLA	ND
22	B	612	CLA	ND
22	B	613	CLA	ND
22	B	614	CLA	ND
22	B	615	CLA	ND
22	B	616	CLA	ND
22	C	501	CLA	ND
22	C	502	CLA	ND
22	C	503	CLA	ND
22	C	504	CLA	ND
22	C	505	CLA	ND
22	C	507	CLA	ND
22	C	509	CLA	ND
22	C	510	CLA	ND
22	C	511	CLA	ND
22	C	512	CLA	ND
22	C	513	CLA	ND
22	D	404	CLA	ND
22	a	402	CLA	ND
22	a	403	CLA	ND
22	a	405	CLA	ND
22	b	601	CLA	ND
22	b	603	CLA	ND
22	b	604	CLA	ND

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Mol	Chain	Res	Type	Atom
22	b	605	CLA	ND
22	b	606	CLA	ND
22	b	607	CLA	ND
22	b	610	CLA	ND
22	b	611	CLA	ND
22	b	612	CLA	ND
22	b	613	CLA	ND
22	b	614	CLA	ND
22	b	615	CLA	ND
22	b	616	CLA	ND
22	c	501	CLA	ND
22	c	503	CLA	ND
22	c	504	CLA	ND
22	c	505	CLA	ND
22	c	506	CLA	ND
22	c	507	CLA	ND
22	c	509	CLA	ND
22	c	510	CLA	ND
22	c	511	CLA	ND
22	c	512	CLA	ND
22	c	513	CLA	ND
22	d	404	CLA	ND
22	d	405	CLA	ND

All (1838) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	402	CLA	C2C-C3C-CAC-CBC
22	A	406	CLA	C2-C3-C5-C6
22	A	406	CLA	C4-C3-C5-C6
22	B	601	CLA	C1A-C2A-CAA-CBA
22	B	606	CLA	CHA-CBD-CGD-O1D
22	B	606	CLA	CHA-CBD-CGD-O2D
22	B	614	CLA	CHA-CBD-CGD-O1D
22	B	614	CLA	CAD-CBD-CGD-O1D
22	B	614	CLA	CAD-CBD-CGD-O2D
22	C	509	CLA	C11-C10-C8-C9
22	C	512	CLA	C11-C10-C8-C9
22	C	513	CLA	C6-C7-C8-C9
22	D	403	CLA	CHA-CBD-CGD-O2D
22	a	403	CLA	CHA-CBD-CGD-O1D
22	a	403	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	b	601	CLA	C1A-C2A-CAA-CBA
22	b	606	CLA	CHA-CBD-CGD-O1D
22	b	614	CLA	CAD-CBD-CGD-O1D
22	b	614	CLA	CAD-CBD-CGD-O2D
22	b	616	CLA	C2-C3-C5-C6
22	b	616	CLA	C4-C3-C5-C6
22	c	512	CLA	C1A-C2A-CAA-CBA
22	c	512	CLA	C2A-CAA-CBA-CGA
22	d	404	CLA	CHA-CBD-CGD-O1D
22	d	404	CLA	CHA-CBD-CGD-O2D
24	A	407	BCR	C23-C24-C25-C30
24	B	617	BCR	C35-C13-C14-C15
24	B	618	BCR	C7-C8-C9-C34
24	B	618	BCR	C20-C21-C22-C37
24	B	618	BCR	C23-C24-C25-C30
24	B	619	BCR	C11-C12-C13-C35
24	C	514	BCR	C7-C8-C9-C34
24	C	514	BCR	C16-C17-C18-C19
24	C	514	BCR	C36-C18-C19-C20
24	D	405	BCR	C35-C13-C14-C15
24	D	405	BCR	C23-C24-C25-C26
24	H	101	BCR	C11-C12-C13-C14
24	H	101	BCR	C11-C12-C13-C35
24	K	101	BCR	C10-C11-C12-C13
24	K	101	BCR	C11-C12-C13-C35
24	K	101	BCR	C16-C17-C18-C19
24	K	101	BCR	C16-C17-C18-C36
24	K	102	BCR	C5-C6-C7-C8
24	K	102	BCR	C21-C22-C23-C24
24	K	102	BCR	C37-C22-C23-C24
24	T	101	BCR	C1-C6-C7-C8
24	T	101	BCR	C7-C8-C9-C10
24	T	101	BCR	C12-C13-C14-C15
24	T	101	BCR	C16-C17-C18-C36
24	b	617	BCR	C20-C21-C22-C37
24	b	617	BCR	C21-C22-C23-C24
24	b	618	BCR	C11-C12-C13-C35
24	b	619	BCR	C7-C8-C9-C34
24	b	619	BCR	C11-C12-C13-C35
24	b	619	BCR	C35-C13-C14-C15
24	b	619	BCR	C20-C21-C22-C37
24	c	514	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	c	514	BCR	C11-C12-C13-C14
24	c	514	BCR	C11-C12-C13-C35
24	c	514	BCR	C18-C19-C20-C21
24	d	406	BCR	C7-C8-C9-C34
24	d	406	BCR	C37-C22-C23-C24
24	d	406	BCR	C22-C23-C24-C25
24	k	101	BCR	C5-C6-C7-C8
24	k	101	BCR	C7-C8-C9-C34
24	k	101	BCR	C17-C18-C19-C20
24	k	101	BCR	C36-C18-C19-C20
24	k	101	BCR	C37-C22-C23-C24
26	A	410	PL9	C22-C23-C24-C25
26	A	410	PL9	C23-C24-C26-C27
26	A	410	PL9	C32-C33-C34-C36
26	A	410	PL9	C37-C38-C39-C40
26	A	410	PL9	C37-C38-C39-C41
26	D	406	PL9	C32-C33-C34-C35
26	D	406	PL9	C32-C33-C34-C36
26	D	406	PL9	C47-C48-C49-C51
26	a	409	PL9	C22-C23-C24-C25
26	a	409	PL9	C22-C23-C24-C26
26	a	409	PL9	C24-C26-C27-C28
26	a	409	PL9	C33-C34-C36-C37
26	a	409	PL9	C42-C43-C44-C45
26	a	409	PL9	C47-C48-C49-C51
26	d	407	PL9	C32-C33-C34-C36
26	d	407	PL9	C42-C43-C44-C46
26	d	407	PL9	C47-C48-C49-C51
27	A	411	LMG	O9-C10-O7-C8
27	A	411	LMG	C11-C10-O7-C8
27	a	414	LMG	O6-C1-O1-C7
27	a	414	LMG	O10-C28-O8-C9
27	b	623	LMG	C2-C1-O1-C7
27	b	623	LMG	O6-C1-O1-C7
27	h	102	LMG	C10-C11-C12-C13
28	A	414	SQD	C44-C45-C46-O48
28	B	621	SQD	C2-C1-O6-C44
28	B	621	SQD	O5-C1-O6-C44
28	B	621	SQD	O6-C44-C45-O47
28	B	621	SQD	O49-C7-O47-C45
28	B	621	SQD	C8-C7-O47-C45
28	F	102	SQD	C45-C44-O6-C1

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Mol	Chain	Res	Type	Atoms
28	F	102	SQD	C2-C1-O6-C44
28	a	412	SQD	C8-C7-O47-C45
28	a	412	SQD	O10-C23-O48-C46
28	b	620	SQD	C46-C45-O47-C7
28	b	620	SQD	C8-C7-O47-C45
28	b	620	SQD	O10-C23-O48-C46
28	b	620	SQD	C24-C23-O48-C46
28	f	102	SQD	O5-C1-O6-C44
28	f	102	SQD	O49-C7-O47-C45
29	D	408	LHG	O1-C1-C2-C3
29	D	408	LHG	O2-C2-C3-O3
29	D	408	LHG	C3-O3-P-O4
29	D	408	LHG	C4-O6-P-O4
29	D	409	LHG	C1-C2-C3-O3
29	D	409	LHG	O2-C2-C3-O3
29	D	409	LHG	C3-O3-P-O4
29	D	409	LHG	C3-O3-P-O5
29	D	411	LHG	O1-C1-C2-C3
29	L	101	LHG	C3-O3-P-O4
29	L	101	LHG	C4-O6-P-O4
29	a	410	LHG	C3-O3-P-O4
29	a	410	LHG	C3-O3-P-O5
29	d	408	LHG	C4-O6-P-O4
29	d	408	LHG	C4-O6-P-O5
29	e	101	LHG	C3-O3-P-O5
29	l	101	LHG	C4-O6-P-O3
29	l	101	LHG	C4-O6-P-O4
29	l	101	LHG	C4-O6-P-O5
30	A	415	DGD	C2B-C1B-O2G-C2G
30	A	415	DGD	O1B-C1B-O2G-C2G
30	o	301	DGD	C2B-C1B-O2G-C2G
30	o	301	DGD	O1B-C1B-O2G-C2G
32	B	623	STE	C1-C2-C3-C4
32	B	626	STE	C1-C2-C3-C4
32	B	627	STE	C1-C2-C3-C4
32	C	518	STE	C1-C2-C3-C4
32	J	101	STE	C1-C2-C3-C4
32	b	624	STE	C1-C2-C3-C4
32	b	625	STE	C1-C2-C3-C4
32	c	520	STE	C1-C2-C3-C4
32	d	412	STE	C1-C2-C3-C4
32	j	101	STE	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
34	f	101	HEM	C2A-CAA-CBA-CGA
22	c	509	CLA	O1D-CGD-O2D-CED
22	b	601	CLA	O1D-CGD-O2D-CED
22	b	601	CLA	CBD-CGD-O2D-CED
22	c	509	CLA	CBD-CGD-O2D-CED
22	c	511	CLA	CBD-CGD-O2D-CED
23	d	401	PHO	CBD-CGD-O2D-CED
27	M	101	LMG	O10-C28-O8-C9
29	e	101	LHG	O10-C23-O8-C6
27	a	414	LMG	C29-C28-O8-C9
28	F	102	SQD	C24-C23-O48-C46
28	a	412	SQD	C24-C23-O48-C46
26	a	409	PL9	C47-C48-C49-C50
22	c	513	CLA	CBD-CGD-O2D-CED
28	F	102	SQD	O10-C23-O48-C46
22	C	501	CLA	CBD-CGD-O2D-CED
27	c	521	LMG	O9-C10-O7-C8
28	b	620	SQD	O49-C7-O47-C45
27	c	521	LMG	O10-C28-O8-C9
22	A	403	CLA	C3-C5-C6-C7
22	b	601	CLA	C3-C5-C6-C7
22	b	602	CLA	C3-C5-C6-C7
22	c	513	CLA	C3-C5-C6-C7
27	M	101	LMG	C29-C28-O8-C9
28	f	102	SQD	C24-C23-O48-C46
29	e	101	LHG	C24-C23-O8-C6
28	f	102	SQD	C8-C7-O47-C45
22	C	507	CLA	C4-C3-C5-C6
22	C	513	CLA	C4-C3-C5-C6
22	b	614	CLA	C4-C3-C5-C6
26	a	409	PL9	C35-C34-C36-C37
22	C	507	CLA	C2-C3-C5-C6
26	d	407	PL9	C38-C39-C41-C42
28	f	102	SQD	O10-C23-O48-C46
22	B	608	CLA	C3-C5-C6-C7
22	C	513	CLA	C3-C5-C6-C7
22	b	614	CLA	C3-C5-C6-C7
27	c	521	LMG	C29-C28-O8-C9
30	h	103	DGD	O6E-C5E-C6E-O5E
22	c	511	CLA	O1D-CGD-O2D-CED
26	a	409	PL9	C7-C8-C9-C10
22	C	511	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	c	503	CLA	CBD-CGD-O2D-CED
28	a	412	SQD	O49-C7-O47-C45
26	A	410	PL9	C22-C23-C24-C26
26	a	409	PL9	C42-C43-C44-C46
27	b	623	LMG	O10-C28-O8-C9
30	o	301	DGD	O1A-C1A-O1G-C1G
22	C	513	CLA	CBD-CGD-O2D-CED
23	d	401	PHO	O1D-CGD-O2D-CED
22	B	616	CLA	C3-C5-C6-C7
27	Y	101	LMG	C29-C28-O8-C9
30	c	518	DGD	O1A-C1A-O1G-C1G
27	M	101	LMG	O6-C5-C6-O5
27	Y	101	LMG	C11-C10-O7-C8
29	l	101	LHG	C7-C8-C9-C10
30	C	515	DGD	O6E-C5E-C6E-O5E
22	C	513	CLA	CBA-CGA-O2A-C1
30	H	102	DGD	O6E-C5E-C6E-O5E
30	h	103	DGD	C4E-C5E-C6E-O5E
32	B	625	STE	C11-C12-C13-C14
26	D	406	PL9	C47-C48-C49-C50
22	B	614	CLA	C4-C3-C5-C6
22	c	507	CLA	C4-C3-C5-C6
26	d	407	PL9	C40-C39-C41-C42
27	M	101	LMG	C4-C5-C6-O5
22	B	614	CLA	C2-C3-C5-C6
22	c	507	CLA	C2-C3-C5-C6
26	A	410	PL9	C18-C19-C21-C22
22	b	606	CLA	C2A-CAA-CBA-CGA
30	A	415	DGD	O6E-C5E-C6E-O5E
28	b	620	SQD	O5-C1-O6-C44
26	A	410	PL9	C9-C11-C12-C13
26	A	410	PL9	C14-C16-C17-C18
26	A	410	PL9	C19-C21-C22-C23
26	A	410	PL9	C24-C26-C27-C28
26	a	409	PL9	C19-C21-C22-C23
26	a	409	PL9	C34-C36-C37-C38
30	o	301	DGD	C2A-C1A-O1G-C1G
22	C	513	CLA	O1A-CGA-O2A-C1
26	d	407	PL9	C47-C48-C49-C50
26	A	410	PL9	C12-C13-C14-C15
22	c	502	CLA	CBD-CGD-O2D-CED
27	b	623	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
30	A	415	DGD	C4E-C5E-C6E-O5E
22	c	506	CLA	CBA-CGA-O2A-C1
28	B	621	SQD	C24-C23-O48-C46
30	c	518	DGD	C2A-C1A-O1G-C1G
27	a	414	LMG	C15-C16-C17-C18
29	A	413	LHG	C24-C25-C26-C27
28	A	414	SQD	C44-C45-O47-C7
22	C	505	CLA	C5-C6-C7-C8
22	b	605	CLA	C10-C11-C12-C13
27	D	407	LMG	C10-C11-C12-C13
27	a	414	LMG	C2-C1-O1-C7
28	f	102	SQD	C2-C1-O6-C44
30	A	415	DGD	O2G-C2G-C3G-O3G
22	C	513	CLA	C2-C3-C5-C6
22	b	614	CLA	C2-C3-C5-C6
22	A	403	CLA	C14-C13-C15-C16
22	B	601	CLA	C11-C12-C13-C14
22	B	613	CLA	C11-C12-C13-C14
22	C	503	CLA	C11-C10-C8-C9
22	C	506	CLA	C6-C7-C8-C9
22	b	601	CLA	C11-C10-C8-C9
22	b	604	CLA	C6-C7-C8-C9
22	b	605	CLA	C11-C10-C8-C9
22	b	607	CLA	C11-C10-C8-C9
22	b	616	CLA	C11-C10-C8-C9
22	c	507	CLA	C14-C13-C15-C16
22	c	509	CLA	C6-C7-C8-C9
22	c	509	CLA	C11-C12-C13-C14
22	c	511	CLA	C14-C13-C15-C16
22	c	512	CLA	C6-C7-C8-C9
22	c	513	CLA	C6-C7-C8-C9
22	d	404	CLA	C14-C13-C15-C16
22	c	513	CLA	O1D-CGD-O2D-CED
32	C	520	STE	C4-C5-C6-C7
22	c	507	CLA	C5-C6-C7-C8
22	B	606	CLA	C2A-CAA-CBA-CGA
24	B	618	BCR	C37-C22-C23-C24
24	K	103	BCR	C7-C8-C9-C34
24	T	101	BCR	C7-C8-C9-C34
24	T	101	BCR	C11-C12-C13-C35
24	c	515	BCR	C7-C8-C9-C34
24	h	101	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
24	d	406	BCR	C21-C22-C23-C24
28	b	620	SQD	C23-C24-C25-C26
22	B	614	CLA	C13-C15-C16-C17
22	b	602	CLA	C15-C16-C17-C18
22	b	616	CLA	C8-C10-C11-C12
22	c	509	CLA	C10-C11-C12-C13
22	b	613	CLA	CBD-CGD-O2D-CED
27	m	101	LMG	C29-C28-O8-C9
22	C	512	CLA	C10-C11-C12-C13
22	D	403	CLA	C13-C15-C16-C17
22	b	608	CLA	C13-C15-C16-C17
22	d	404	CLA	C15-C16-C17-C18
27	Y	101	LMG	O6-C5-C6-O5
22	B	603	CLA	C8-C10-C11-C12
22	B	614	CLA	C8-C10-C11-C12
22	C	506	CLA	C13-C15-C16-C17
22	C	509	CLA	C13-C15-C16-C17
22	C	513	CLA	C5-C6-C7-C8
22	b	604	CLA	C10-C11-C12-C13
22	b	611	CLA	C8-C10-C11-C12
22	b	611	CLA	C13-C15-C16-C17
22	b	615	CLA	C8-C10-C11-C12
22	c	505	CLA	C15-C16-C17-C18
22	c	506	CLA	C13-C15-C16-C17
30	C	515	DGD	C4E-C5E-C6E-O5E
27	A	411	LMG	C28-C29-C30-C31
27	D	410	LMG	C10-C11-C12-C13
27	d	410	LMG	C28-C29-C30-C31
28	A	412	SQD	C7-C8-C9-C10
28	B	621	SQD	C23-C24-C25-C26
28	f	102	SQD	C23-C24-C25-C26
29	a	410	LHG	C23-C24-C25-C26
29	e	101	LHG	C23-C24-C25-C26
30	o	301	DGD	C1B-C2B-C3B-C4B
27	c	521	LMG	O6-C5-C6-O5
22	B	602	CLA	C13-C15-C16-C17
22	B	607	CLA	C15-C16-C17-C18
22	C	512	CLA	C13-C15-C16-C17
22	a	405	CLA	C10-C11-C12-C13
22	b	607	CLA	C10-C11-C12-C13
22	c	511	CLA	C15-C16-C17-C18
30	A	415	DGD	C2A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
22	B	616	CLA	C5-C6-C7-C8
22	C	511	CLA	C8-C10-C11-C12
22	c	503	CLA	C8-C10-C11-C12
22	c	505	CLA	C13-C15-C16-C17
22	c	509	CLA	C5-C6-C7-C8
22	B	614	CLA	C15-C16-C17-C18
22	B	615	CLA	C5-C6-C7-C8
22	C	513	CLA	C15-C16-C17-C18
22	b	603	CLA	C5-C6-C7-C8
22	C	508	CLA	C12-C13-C15-C16
22	C	510	CLA	C12-C13-C15-C16
22	C	513	CLA	C11-C10-C8-C7
22	D	404	CLA	C11-C10-C8-C7
22	b	614	CLA	C11-C12-C13-C15
22	c	506	CLA	C12-C13-C15-C16
22	c	506	CLA	O1A-CGA-O2A-C1
22	A	403	CLA	C13-C15-C16-C17
22	B	607	CLA	C13-C15-C16-C17
22	B	613	CLA	C8-C10-C11-C12
22	C	504	CLA	C8-C10-C11-C12
22	a	405	CLA	C15-C16-C17-C18
22	b	614	CLA	C5-C6-C7-C8
22	c	512	CLA	C13-C15-C16-C17
28	A	414	SQD	C46-C45-O47-C7
30	C	516	DGD	O6E-C1E-O5D-C6D
22	C	505	CLA	C10-C11-C12-C13
22	C	506	CLA	C8-C10-C11-C12
22	c	503	CLA	C5-C6-C7-C8
26	A	410	PL9	C34-C36-C37-C38
26	A	410	PL9	C44-C46-C47-C48
24	B	618	BCR	C18-C19-C20-C21
24	B	619	BCR	C10-C11-C12-C13
24	C	514	BCR	C10-C11-C12-C13
24	K	102	BCR	C10-C11-C12-C13
24	K	103	BCR	C18-C19-C20-C21
26	A	410	PL9	C47-C48-C49-C51
29	A	413	LHG	O2-C2-C3-O3
27	D	410	LMG	O9-C10-O7-C8
27	m	101	LMG	O9-C10-O7-C8
22	B	606	CLA	C10-C11-C12-C13
22	C	503	CLA	C5-C6-C7-C8
22	C	510	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	D	404	CLA	C13-C15-C16-C17
22	A	402	CLA	C15-C16-C17-C18
22	C	502	CLA	C13-C15-C16-C17
22	a	403	CLA	C8-C10-C11-C12
22	a	405	CLA	C5-C6-C7-C8
22	b	605	CLA	C5-C6-C7-C8
22	b	616	CLA	C10-C11-C12-C13
22	c	511	CLA	C13-C15-C16-C17
22	B	606	CLA	C15-C16-C17-C18
22	C	512	CLA	C8-C10-C11-C12
22	D	402	CLA	C15-C16-C17-C18
29	D	408	LHG	C3-O3-P-O6
29	D	409	LHG	C3-O3-P-O6
29	a	410	LHG	C3-O3-P-O6
29	d	408	LHG	C4-O6-P-O3
29	e	101	LHG	C3-O3-P-O6
27	c	521	LMG	C10-C11-C12-C13
30	C	515	DGD	C1B-C2B-C3B-C4B
22	B	604	CLA	CBA-CGA-O2A-C1
30	c	516	DGD	CAA-CBA-CCA-CDA
28	F	102	SQD	O6-C44-C45-C46
22	c	503	CLA	O1D-CGD-O2D-CED
30	A	415	DGD	O6D-C5D-C6D-O5D
32	B	624	STE	C11-C12-C13-C14
29	A	413	LHG	C1-C2-C3-O3
27	Y	101	LMG	O9-C10-O7-C8
22	C	509	CLA	C5-C6-C7-C8
22	b	606	CLA	C10-C11-C12-C13
22	B	616	CLA	C11-C12-C13-C15
22	b	611	CLA	C16-C17-C18-C20
27	M	101	LMG	C28-C29-C30-C31
27	M	101	LMG	C36-C37-C38-C39
27	Y	101	LMG	C13-C14-C15-C16
28	A	414	SQD	C13-C14-C15-C16
28	B	621	SQD	C11-C12-C13-C14
30	C	515	DGD	C3B-C4B-C5B-C6B
30	h	103	DGD	C3A-C4A-C5A-C6A
30	o	301	DGD	C2A-C3A-C4A-C5A
32	T	102	STE	C9-C10-C11-C12
32	c	520	STE	C9-C10-C11-C12
22	B	609	CLA	C13-C15-C16-C17
22	b	601	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	b	606	CLA	C15-C16-C17-C18
22	b	612	CLA	C13-C15-C16-C17
24	A	407	BCR	C35-C13-C14-C15
24	B	617	BCR	C11-C10-C9-C34
24	K	103	BCR	C11-C10-C9-C34
24	K	103	BCR	C20-C21-C22-C37
24	T	101	BCR	C35-C13-C14-C15
24	T	101	BCR	C20-C21-C22-C37
24	b	617	BCR	C35-C13-C14-C15
24	b	618	BCR	C35-C13-C14-C15
24	b	618	BCR	C16-C17-C18-C36
24	d	406	BCR	C20-C21-C22-C37
24	k	101	BCR	C35-C13-C14-C15
27	M	101	LMG	C33-C34-C35-C36
27	c	519	LMG	C33-C34-C35-C36
28	A	412	SQD	C34-C35-C36-C37
28	a	411	SQD	C9-C10-C11-C12
28	a	412	SQD	C15-C16-C17-C18
28	a	412	SQD	C24-C25-C26-C27
28	f	102	SQD	C28-C29-C30-C31
28	f	102	SQD	C33-C34-C35-C36
29	A	413	LHG	C10-C11-C12-C13
30	A	415	DGD	CEB-CFB-CGB-CHB
30	c	517	DGD	CBB-CCB-CDB-CEB
30	h	103	DGD	C6A-C7A-C8A-C9A
32	B	626	STE	C5-C6-C7-C8
32	B	627	STE	C5-C6-C7-C8
32	b	624	STE	C3-C4-C5-C6
22	C	501	CLA	O1D-CGD-O2D-CED
22	B	603	CLA	C16-C17-C18-C20
22	B	609	CLA	C16-C17-C18-C20
22	C	502	CLA	C16-C17-C18-C20
22	a	402	CLA	C16-C17-C18-C20
22	b	615	CLA	C16-C17-C18-C19
22	c	503	CLA	C16-C17-C18-C20
22	c	509	CLA	C16-C17-C18-C20
22	B	601	CLA	CBA-CGA-O2A-C1
27	h	102	LMG	C36-C37-C38-C39
29	A	413	LHG	C28-C29-C30-C31
29	D	411	LHG	C16-C17-C18-C19
29	l	101	LHG	C17-C18-C19-C20
30	A	415	DGD	CCB-CDB-CEB-CFB

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Mol	Chain	Res	Type	Atoms
30	C	515	DGD	C5B-C6B-C7B-C8B
30	C	516	DGD	C4A-C5A-C6A-C7A
30	C	516	DGD	C5A-C6A-C7A-C8A
30	h	103	DGD	C6B-C7B-C8B-C9B
32	B	620	STE	C10-C11-C12-C13
32	M	104	STE	C9-C10-C11-C12
27	b	623	LMG	C9-C8-O7-C10
30	c	517	DGD	C1A-C2A-C3A-C4A
27	M	101	LMG	C17-C18-C19-C20
27	a	414	LMG	C29-C30-C31-C32
27	a	414	LMG	C31-C32-C33-C34
30	C	516	DGD	C6A-C7A-C8A-C9A
30	C	517	DGD	CBA-CCA-CDA-CEA
30	c	516	DGD	C4A-C5A-C6A-C7A
30	c	518	DGD	C4A-C5A-C6A-C7A
30	c	518	DGD	C5B-C6B-C7B-C8B
30	o	301	DGD	C6A-C7A-C8A-C9A
30	o	301	DGD	C9A-CAA-CBA-CCA
27	D	407	LMG	C17-C18-C19-C20
28	B	621	SQD	C33-C34-C35-C36
29	A	413	LHG	C30-C31-C32-C33
29	D	409	LHG	C32-C33-C34-C35
29	d	409	LHG	C34-C35-C36-C37
29	e	101	LHG	C16-C17-C18-C19
30	C	515	DGD	C6A-C7A-C8A-C9A
30	C	517	DGD	C4A-C5A-C6A-C7A
30	o	301	DGD	CCA-CDA-CEA-CFA
30	o	301	DGD	C2B-C3B-C4B-C5B
32	D	413	STE	C11-C10-C9-C8
32	b	622	STE	C14-C15-C16-C17
32	b	624	STE	C11-C10-C9-C8
27	a	414	LMG	C17-C18-C19-C20
27	b	623	LMG	C32-C33-C34-C35
27	h	102	LMG	C33-C34-C35-C36
28	A	412	SQD	C16-C17-C18-C19
29	D	408	LHG	C30-C31-C32-C33
29	d	408	LHG	C28-C29-C30-C31
30	c	518	DGD	CCB-CDB-CEB-CFB
32	b	621	STE	C9-C10-C11-C12
32	d	412	STE	C6-C7-C8-C9
24	B	617	BCR	C11-C10-C9-C8
24	B	617	BCR	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
24	B	618	BCR	C11-C10-C9-C8
24	B	619	BCR	C12-C13-C14-C15
24	C	514	BCR	C12-C13-C14-C15
24	T	101	BCR	C16-C17-C18-C19
24	b	617	BCR	C20-C21-C22-C23
24	h	101	BCR	C11-C10-C9-C8
24	k	101	BCR	C12-C13-C14-C15
30	C	516	DGD	C2E-C1E-O5D-C6D
30	c	517	DGD	C2E-C1E-O5D-C6D
27	b	623	LMG	C29-C28-O8-C9
27	c	521	LMG	C30-C31-C32-C33
28	B	621	SQD	C17-C18-C19-C20
29	D	409	LHG	C29-C30-C31-C32
29	L	101	LHG	C14-C15-C16-C17
29	L	101	LHG	C30-C31-C32-C33
32	T	102	STE	C7-C8-C9-C10
32	b	621	STE	C6-C7-C8-C9
32	c	520	STE	C7-C8-C9-C10
22	B	612	CLA	C16-C17-C18-C20
22	c	512	CLA	C16-C17-C18-C20
22	d	403	CLA	C16-C17-C18-C19
22	C	513	CLA	O1D-CGD-O2D-CED
22	b	613	CLA	O1D-CGD-O2D-CED
26	D	406	PL9	C15-C14-C16-C17
27	D	407	LMG	C15-C16-C17-C18
27	a	414	LMG	C11-C12-C13-C14
27	h	102	LMG	C37-C38-C39-C40
28	a	411	SQD	C12-C13-C14-C15
28	a	411	SQD	C34-C35-C36-C37
28	b	620	SQD	C16-C17-C18-C19
29	A	413	LHG	C32-C33-C34-C35
29	a	410	LHG	C28-C29-C30-C31
30	C	517	DGD	C8A-C9A-CAA-CBA
30	c	516	DGD	C3B-C4B-C5B-C6B
30	o	301	DGD	C4A-C5A-C6A-C7A
32	a	415	STE	C4-C5-C6-C7
32	d	412	STE	C3-C4-C5-C6
22	B	606	CLA	C11-C10-C8-C9
22	C	508	CLA	C14-C13-C15-C16
22	C	512	CLA	C11-C12-C13-C14
22	b	601	CLA	C11-C12-C13-C14
22	b	604	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	C	511	CLA	O1D-CGD-O2D-CED
27	Y	101	LMG	C18-C19-C20-C21
27	b	623	LMG	C18-C19-C20-C21
27	b	623	LMG	C40-C41-C42-C43
27	c	519	LMG	O9-C10-O7-C8
27	c	519	LMG	C38-C39-C40-C41
27	c	519	LMG	C39-C40-C41-C42
28	A	412	SQD	C10-C11-C12-C13
28	A	414	SQD	C18-C19-C20-C21
29	A	413	LHG	C12-C13-C14-C15
29	D	408	LHG	C29-C30-C31-C32
29	D	409	LHG	C13-C14-C15-C16
30	c	517	DGD	C8B-C9B-CAB-CBB
30	o	301	DGD	CDB-CEB-CFB-CGB
32	C	519	STE	C4-C5-C6-C7
32	H	103	STE	C6-C7-C8-C9
22	b	616	CLA	C5-C6-C7-C8
22	b	601	CLA	C2A-CAA-CBA-CGA
24	H	101	BCR	C36-C18-C19-C20
28	f	102	SQD	C25-C26-C27-C28
29	d	408	LHG	C26-C27-C28-C29
29	l	101	LHG	C31-C32-C33-C34
32	b	622	STE	C6-C7-C8-C9
29	a	410	LHG	O1-C1-C2-C3
29	d	409	LHG	O1-C1-C2-C3
24	A	407	BCR	C11-C12-C13-C14
24	T	101	BCR	C17-C18-C19-C20
22	C	513	CLA	C8-C10-C11-C12
22	b	607	CLA	C8-C10-C11-C12
27	D	410	LMG	C11-C10-O7-C8
27	c	521	LMG	C11-C10-O7-C8
27	a	414	LMG	C12-C13-C14-C15
27	a	414	LMG	C32-C33-C34-C35
27	b	623	LMG	C19-C20-C21-C22
30	c	516	DGD	C4B-C5B-C6B-C7B
32	B	627	STE	C4-C5-C6-C7
32	M	102	STE	C6-C7-C8-C9
32	d	412	STE	C11-C12-C13-C14
27	M	101	LMG	C10-C11-C12-C13
26	A	410	PL9	C47-C48-C49-C50
27	D	407	LMG	C30-C31-C32-C33
27	M	101	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
27	m	101	LMG	C37-C38-C39-C40
29	d	408	LHG	C13-C14-C15-C16
30	A	415	DGD	C5B-C6B-C7B-C8B
30	C	516	DGD	C7A-C8A-C9A-CAA
30	C	517	DGD	C6B-C7B-C8B-C9B
30	c	518	DGD	CCA-CDA-CEA-CFA
30	h	103	DGD	C5B-C6B-C7B-C8B
32	B	622	STE	C11-C10-C9-C8
32	C	518	STE	C4-C5-C6-C7
32	D	413	STE	C4-C5-C6-C7
32	H	103	STE	C2-C3-C4-C5
32	c	520	STE	C6-C7-C8-C9
32	d	411	STE	C5-C6-C7-C8
22	B	609	CLA	C16-C17-C18-C19
22	B	616	CLA	C11-C12-C13-C14
22	C	506	CLA	C16-C17-C18-C20
22	b	601	CLA	C16-C17-C18-C20
22	b	615	CLA	C16-C17-C18-C20
28	F	102	SQD	O5-C1-O6-C44
30	c	517	DGD	O6E-C1E-O5D-C6D
22	C	507	CLA	C5-C6-C7-C8
27	A	411	LMG	C33-C34-C35-C36
27	D	407	LMG	C37-C38-C39-C40
27	M	101	LMG	C32-C33-C34-C35
27	b	623	LMG	C15-C16-C17-C18
28	a	412	SQD	C14-C15-C16-C17
29	D	409	LHG	C25-C26-C27-C28
29	a	410	LHG	C15-C16-C17-C18
29	d	408	LHG	C29-C30-C31-C32
30	A	415	DGD	CAA-CBA-CCA-CDA
30	A	415	DGD	C2B-C3B-C4B-C5B
30	c	518	DGD	CBA-CCA-CDA-CEA
30	h	103	DGD	C2B-C3B-C4B-C5B
32	D	412	STE	C9-C10-C11-C12
32	M	102	STE	C11-C10-C9-C8
32	M	104	STE	C10-C11-C12-C13
32	T	102	STE	C10-C11-C12-C13
22	c	502	CLA	O1D-CGD-O2D-CED
27	D	410	LMG	C36-C37-C38-C39
27	d	410	LMG	C36-C37-C38-C39
28	a	412	SQD	C11-C12-C13-C14
29	L	101	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
30	C	517	DGD	C5A-C6A-C7A-C8A
30	c	517	DGD	CAA-CBA-CCA-CDA
32	I	101	STE	C7-C8-C9-C10
32	M	102	STE	C7-C8-C9-C10
32	d	411	STE	C3-C4-C5-C6
29	A	413	LHG	C23-C24-C25-C26
22	c	510	CLA	C15-C16-C17-C18
27	b	623	LMG	C38-C39-C40-C41
27	c	521	LMG	C38-C39-C40-C41
29	D	409	LHG	C9-C10-C11-C12
29	D	411	LHG	C18-C19-C20-C21
30	A	415	DGD	C4B-C5B-C6B-C7B
30	H	102	DGD	CCB-CDB-CEB-CFB
30	c	516	DGD	CCB-CDB-CEB-CFB
32	D	412	STE	C5-C6-C7-C8
32	c	520	STE	C3-C4-C5-C6
28	b	620	SQD	C12-C13-C14-C15
28	f	102	SQD	C27-C28-C29-C30
32	M	102	STE	C9-C10-C11-C12
32	b	625	STE	C12-C13-C14-C15
32	d	411	STE	C11-C12-C13-C14
22	b	601	CLA	C3A-C2A-CAA-CBA
22	c	512	CLA	C3A-C2A-CAA-CBA
22	b	604	CLA	C15-C16-C17-C18
27	c	521	LMG	C39-C40-C41-C42
30	C	516	DGD	C8B-C9B-CAB-CBB
22	B	615	CLA	C16-C17-C18-C20
22	C	506	CLA	C16-C17-C18-C19
22	c	512	CLA	C16-C17-C18-C19
27	A	411	LMG	C12-C13-C14-C15
27	D	407	LMG	C35-C36-C37-C38
27	d	410	LMG	C38-C39-C40-C41
27	h	102	LMG	C34-C35-C36-C37
28	a	411	SQD	C24-C25-C26-C27
30	A	415	DGD	C7A-C8A-C9A-CAA
30	C	515	DGD	C4B-C5B-C6B-C7B
27	m	101	LMG	C33-C34-C35-C36
30	c	518	DGD	C9A-CAA-CBA-CCA
24	K	101	BCR	C14-C15-C16-C17
22	b	604	CLA	C3-C5-C6-C7
27	D	410	LMG	C34-C35-C36-C37
29	L	101	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
30	c	516	DGD	C6B-C7B-C8B-C9B
32	B	625	STE	C5-C6-C7-C8
32	b	621	STE	C5-C6-C7-C8
26	A	410	PL9	C40-C39-C41-C42
26	A	410	PL9	C45-C44-C46-C47
22	c	512	CLA	CBA-CGA-O2A-C1
26	A	410	PL9	C33-C34-C36-C37
29	d	409	LHG	C24-C25-C26-C27
22	b	603	CLA	C8-C10-C11-C12
30	c	517	DGD	CCB-CDB-CEB-CFB
30	o	301	DGD	CAB-CBB-CCB-CDB
32	M	104	STE	C14-C15-C16-C17
22	B	604	CLA	O1A-CGA-O2A-C1
22	a	402	CLA	C16-C17-C18-C19
22	b	611	CLA	C16-C17-C18-C19
27	h	102	LMG	C32-C33-C34-C35
32	H	103	STE	C4-C5-C6-C7
27	M	101	LMG	C20-C21-C22-C23
28	b	620	SQD	C13-C14-C15-C16
30	c	517	DGD	C7B-C8B-C9B-CAB
32	H	103	STE	C11-C10-C9-C8
22	B	604	CLA	C10-C11-C12-C13
29	D	408	LHG	C1-C2-C3-O3
27	Y	101	LMG	C17-C18-C19-C20
29	L	101	LHG	C32-C33-C34-C35
30	H	102	DGD	C4B-C5B-C6B-C7B
22	b	616	CLA	C2-C1-O2A-CGA
29	a	410	LHG	C14-C15-C16-C17
29	a	410	LHG	C16-C17-C18-C19
29	l	101	LHG	C27-C28-C29-C30
30	o	301	DGD	C3B-C4B-C5B-C6B
22	B	605	CLA	C15-C16-C17-C18
30	c	517	DGD	C4E-C5E-C6E-O5E
27	Y	101	LMG	C36-C37-C38-C39
28	A	414	SQD	C15-C16-C17-C18
28	A	414	SQD	C24-C25-C26-C27
30	C	516	DGD	C3A-C4A-C5A-C6A
32	B	624	STE	C11-C10-C9-C8
22	B	615	CLA	C16-C17-C18-C19
22	C	502	CLA	C16-C17-C18-C19
22	c	503	CLA	C16-C17-C18-C19
22	d	403	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
24	A	407	BCR	C23-C24-C25-C26
24	B	617	BCR	C1-C6-C7-C8
24	D	405	BCR	C23-C24-C25-C30
24	H	101	BCR	C23-C24-C25-C26
24	K	102	BCR	C1-C6-C7-C8
24	T	101	BCR	C5-C6-C7-C8
24	c	514	BCR	C5-C6-C7-C8
24	k	101	BCR	C1-C6-C7-C8
28	F	102	SQD	C25-C26-C27-C28
28	F	102	SQD	C32-C33-C34-C35
28	a	411	SQD	C24-C23-O48-C46
22	B	601	CLA	C8-C10-C11-C12
22	B	603	CLA	C10-C11-C12-C13
22	C	509	CLA	C10-C11-C12-C13
22	b	615	CLA	C15-C16-C17-C18
27	b	623	LMG	C11-C10-O7-C8
29	d	409	LHG	C27-C28-C29-C30
30	c	518	DGD	C9B-CAB-CBB-CCB
27	Y	101	LMG	O10-C28-O8-C9
27	c	521	LMG	C11-C12-C13-C14
29	e	101	LHG	C14-C15-C16-C17
30	A	415	DGD	C4A-C5A-C6A-C7A
22	B	613	CLA	C5-C6-C7-C8
27	c	521	LMG	C14-C15-C16-C17
28	B	621	SQD	C9-C10-C11-C12
22	C	505	CLA	C4-C3-C5-C6
22	A	403	CLA	C12-C13-C15-C16
22	B	604	CLA	C11-C10-C8-C7
22	C	502	CLA	C11-C12-C13-C15
22	C	505	CLA	C2-C3-C5-C6
22	C	505	CLA	C11-C10-C8-C7
22	C	508	CLA	C11-C10-C8-C7
22	C	511	CLA	C6-C7-C8-C10
22	C	512	CLA	C11-C12-C13-C15
22	b	602	CLA	C11-C12-C13-C15
22	b	604	CLA	C6-C7-C8-C10
22	b	604	CLA	C12-C13-C15-C16
22	b	607	CLA	C11-C10-C8-C7
22	b	608	CLA	C11-C12-C13-C15
22	b	612	CLA	C12-C13-C15-C16
22	c	504	CLA	C11-C10-C8-C7
22	c	506	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	c	508	CLA	C12-C13-C15-C16
22	c	512	CLA	C6-C7-C8-C10
22	c	512	CLA	C12-C13-C15-C16
22	B	601	CLA	O1A-CGA-O2A-C1
22	c	512	CLA	O1A-CGA-O2A-C1
30	C	517	DGD	C4B-C5B-C6B-C7B
30	c	517	DGD	C7A-C8A-C9A-CAA
32	c	520	STE	C11-C12-C13-C14
24	c	514	BCR	C13-C14-C15-C16
22	B	603	CLA	C16-C17-C18-C19
22	B	606	CLA	C16-C17-C18-C20
29	D	408	LHG	C7-C8-C9-C10
22	a	405	CLA	CBA-CGA-O2A-C1
28	A	414	SQD	C24-C23-O48-C46
28	a	411	SQD	C15-C16-C17-C18
29	D	409	LHG	C11-C12-C13-C14
22	B	601	CLA	C5-C6-C7-C8
22	b	605	CLA	C15-C16-C17-C18
22	c	510	CLA	C10-C11-C12-C13
29	d	408	LHG	C11-C12-C13-C14
32	E	101	STE	C6-C7-C8-C9
32	j	101	STE	C3-C4-C5-C6
28	b	620	SQD	C26-C27-C28-C29
27	D	410	LMG	C28-C29-C30-C31
30	H	102	DGD	C1A-C2A-C3A-C4A
27	A	411	LMG	C35-C36-C37-C38
27	D	407	LMG	C12-C13-C14-C15
27	D	407	LMG	C20-C21-C22-C23
28	a	411	SQD	C18-C19-C20-C21
28	b	620	SQD	C24-C25-C26-C27
30	C	516	DGD	CCB-CDB-CEB-CFB
32	C	520	STE	C5-C6-C7-C8
26	d	407	PL9	C42-C43-C44-C45
22	A	406	CLA	C3-C5-C6-C7
29	e	101	LHG	C11-C10-C9-C8
29	e	101	LHG	C27-C28-C29-C30
24	c	514	BCR	C22-C23-C24-C25
30	A	415	DGD	C4D-C5D-C6D-O5D
30	A	415	DGD	C6A-C7A-C8A-C9A
29	D	408	LHG	C8-C7-O7-C5
28	a	411	SQD	C16-C17-C18-C19
28	b	620	SQD	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
28	f	102	SQD	C32-C33-C34-C35
32	b	625	STE	C4-C5-C6-C7
24	k	101	BCR	C14-C15-C16-C17
27	m	101	LMG	C16-C17-C18-C19
29	D	408	LHG	C34-C35-C36-C37
29	D	411	LHG	C29-C30-C31-C32
29	d	408	LHG	C34-C35-C36-C37
30	H	102	DGD	CAB-CBB-CCB-CDB
27	a	414	LMG	O9-C10-O7-C8
28	A	414	SQD	C25-C26-C27-C28
30	C	515	DGD	CCB-CDB-CEB-CFB
30	c	517	DGD	C2A-C3A-C4A-C5A
32	b	622	STE	C5-C6-C7-C8
22	c	503	CLA	C10-C11-C12-C13
28	a	411	SQD	O6-C44-C45-O47
29	l	101	LHG	C26-C27-C28-C29
30	c	516	DGD	CAB-CBB-CCB-CDB
32	b	625	STE	C3-C4-C5-C6
30	H	102	DGD	C4E-C5E-C6E-O5E
27	D	410	LMG	C14-C15-C16-C17
27	c	519	LMG	C36-C37-C38-C39
27	c	521	LMG	C31-C32-C33-C34
28	a	412	SQD	C17-C18-C19-C20
29	D	411	LHG	C32-C33-C34-C35
29	a	410	LHG	C11-C10-C9-C8
32	B	625	STE	C4-C5-C6-C7
32	T	102	STE	C11-C10-C9-C8
32	c	522	STE	C2-C3-C4-C5
27	c	519	LMG	O6-C5-C6-O5
30	c	516	DGD	O6E-C5E-C6E-O5E
26	d	407	PL9	C33-C34-C36-C37
26	d	407	PL9	C43-C44-C46-C47
32	D	412	STE	C4-C5-C6-C7
22	B	604	CLA	C11-C10-C8-C9
22	B	604	CLA	C11-C12-C13-C14
22	C	505	CLA	C11-C10-C8-C9
22	C	508	CLA	C11-C10-C8-C9
22	C	511	CLA	C6-C7-C8-C9
22	b	608	CLA	C11-C12-C13-C14
22	b	612	CLA	C14-C13-C15-C16
22	c	506	CLA	C11-C12-C13-C14
22	c	506	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	c	508	CLA	C14-C13-C15-C16
22	c	512	CLA	C14-C13-C15-C16
22	B	613	CLA	CBD-CGD-O2D-CED
30	H	102	DGD	C7B-C8B-C9B-CAB
22	B	605	CLA	C3-C5-C6-C7
22	b	610	CLA	C2A-CAA-CBA-CGA
24	A	407	BCR	C7-C8-C9-C34
30	c	516	DGD	C1B-C2B-C3B-C4B
22	a	403	CLA	C15-C16-C17-C18
27	D	407	LMG	C38-C39-C40-C41
28	b	620	SQD	C14-C15-C16-C17
22	C	503	CLA	C1A-C2A-CAA-CBA
22	C	513	CLA	C1A-C2A-CAA-CBA
22	c	508	CLA	C1A-C2A-CAA-CBA
22	c	511	CLA	C1A-C2A-CAA-CBA
22	D	403	CLA	C16-C17-C18-C20
29	e	101	LHG	O9-C7-O7-C5
28	A	412	SQD	C26-C27-C28-C29
29	d	409	LHG	C26-C27-C28-C29
30	A	415	DGD	CDB-CEB-CFB-CGB
29	D	408	LHG	C4-O6-P-O3
27	d	410	LMG	C30-C31-C32-C33
28	b	620	SQD	C18-C19-C20-C21
29	a	410	LHG	C18-C19-C20-C21
22	b	616	CLA	CBD-CGD-O2D-CED
27	D	407	LMG	C19-C20-C21-C22
28	B	621	SQD	C16-C17-C18-C19
29	D	411	LHG	C9-C10-C11-C12
29	D	411	LHG	C11-C12-C13-C14
29	L	101	LHG	C13-C14-C15-C16
30	o	301	DGD	C5B-C6B-C7B-C8B
32	b	621	STE	C11-C10-C9-C8
22	C	505	CLA	CBD-CGD-O2D-CED
27	d	410	LMG	C14-C15-C16-C17
29	e	101	LHG	C1-C2-C3-O3
26	D	406	PL9	C30-C29-C31-C32
27	M	101	LMG	C34-C35-C36-C37
27	h	102	LMG	C31-C32-C33-C34
29	l	101	LHG	C14-C15-C16-C17
27	A	411	LMG	C31-C32-C33-C34
29	D	411	LHG	C28-C29-C30-C31
32	H	103	STE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
27	Y	101	LMG	C4-C5-C6-O5
30	c	516	DGD	C7A-C8A-C9A-CAA
32	I	101	STE	C10-C11-C12-C13
27	M	101	LMG	C7-C8-C9-O8
28	B	621	SQD	O6-C44-C45-C46
28	a	411	SQD	O6-C44-C45-C46
27	b	623	LMG	O6-C5-C6-O5
28	a	412	SQD	C31-C32-C33-C34
29	e	101	LHG	C11-C12-C13-C14
30	C	515	DGD	CDA-CEA-CFA-CGA
32	b	621	STE	C12-C13-C14-C15
30	C	516	DGD	C2G-C3G-O3G-C1D
30	c	517	DGD	C2G-C3G-O3G-C1D
30	c	517	DGD	C5D-C6D-O5D-C1E
27	M	101	LMG	C35-C36-C37-C38
27	a	414	LMG	C33-C34-C35-C36
27	h	102	LMG	C35-C36-C37-C38
28	A	412	SQD	C24-C25-C26-C27
29	d	409	LHG	C30-C31-C32-C33
32	B	624	STE	C13-C14-C15-C16
32	M	104	STE	C12-C13-C14-C15
22	B	605	CLA	C10-C11-C12-C13
27	Y	101	LMG	C37-C38-C39-C40
29	e	101	LHG	C28-C29-C30-C31
30	C	516	DGD	CDA-CEA-CFA-CGA
30	C	516	DGD	CDB-CEB-CFB-CGB
30	h	103	DGD	O2G-C1B-C2B-C3B
29	d	409	LHG	C35-C36-C37-C38
22	c	509	CLA	C16-C17-C18-C19
27	a	414	LMG	C20-C21-C22-C23
27	d	410	LMG	C40-C41-C42-C43
29	l	101	LHG	C32-C33-C34-C35
30	C	517	DGD	C9A-CAA-CBA-CCA
32	J	101	STE	C7-C8-C9-C10
23	a	404	PHO	CBD-CGD-O2D-CED
29	D	408	LHG	O1-C1-C2-O2
29	a	410	LHG	O1-C1-C2-O2
28	B	621	SQD	C35-C36-C37-C38
22	c	509	CLA	C8-C10-C11-C12
32	D	412	STE	C6-C7-C8-C9
32	c	522	STE	C5-C6-C7-C8
32	d	412	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	a	414	LMG	C11-C10-O7-C8
29	D	411	LHG	C27-C28-C29-C30
30	H	102	DGD	C6B-C7B-C8B-C9B
30	h	103	DGD	C3B-C4B-C5B-C6B
24	A	407	BCR	C11-C10-C9-C34
27	D	407	LMG	O6-C5-C6-O5
27	d	410	LMG	O6-C5-C6-O5
22	b	609	CLA	C4-C3-C5-C6
26	d	407	PL9	C15-C14-C16-C17
29	l	101	LHG	C34-C35-C36-C37
30	c	517	DGD	C9B-CAB-CBB-CCB
30	o	301	DGD	C7A-C8A-C9A-CAA
22	b	616	CLA	C11-C12-C13-C15
27	Y	101	LMG	C35-C36-C37-C38
29	d	408	LHG	C19-C20-C21-C22
30	h	103	DGD	CAB-CBB-CCB-CDB
32	T	102	STE	C4-C5-C6-C7
22	c	506	CLA	CBD-CGD-O2D-CED
22	c	503	CLA	C15-C16-C17-C18
30	h	103	DGD	CDB-CEB-CFB-CGB
28	A	412	SQD	C17-C18-C19-C20
29	A	413	LHG	C11-C12-C13-C14
32	B	625	STE	C6-C7-C8-C9
29	D	409	LHG	C16-C17-C18-C19
30	o	301	DGD	CBA-CCA-CDA-CEA
28	B	621	SQD	C34-C35-C36-C37
29	D	409	LHG	C24-C25-C26-C27
28	B	621	SQD	C45-C46-O48-C23
27	D	410	LMG	C29-C28-O8-C9
22	B	606	CLA	C16-C17-C18-C19
22	c	511	CLA	C16-C17-C18-C19
30	C	517	DGD	C3B-C4B-C5B-C6B
30	h	103	DGD	C4A-C5A-C6A-C7A
32	B	620	STE	C3-C4-C5-C6
32	b	626	STE	C4-C5-C6-C7
27	c	519	LMG	C34-C35-C36-C37
30	H	102	DGD	CCA-CDA-CEA-CFA
32	a	413	STE	C1-C2-C3-C4
22	a	405	CLA	O1A-CGA-O2A-C1
27	M	101	LMG	C18-C19-C20-C21
28	b	620	SQD	O6-C44-C45-O47
29	D	408	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
29	D	409	LHG	C17-C18-C19-C20
27	M	101	LMG	O9-C10-O7-C8
32	I	101	STE	C12-C13-C14-C15
26	a	409	PL9	C15-C14-C16-C17
29	D	409	LHG	C34-C35-C36-C37
32	M	104	STE	C4-C5-C6-C7
22	b	609	CLA	C15-C16-C17-C18
22	A	403	CLA	C11-C10-C8-C7
22	B	602	CLA	C11-C12-C13-C15
22	B	604	CLA	C11-C12-C13-C15
22	B	604	CLA	C12-C13-C15-C16
22	B	605	CLA	C11-C10-C8-C7
22	B	606	CLA	C6-C7-C8-C10
22	B	606	CLA	C11-C10-C8-C7
22	B	613	CLA	C12-C13-C15-C16
22	B	616	CLA	C6-C7-C8-C10
22	C	504	CLA	C11-C10-C8-C7
22	C	513	CLA	C6-C7-C8-C10
22	a	403	CLA	C11-C10-C8-C7
22	b	608	CLA	C11-C10-C8-C7
22	b	616	CLA	C11-C10-C8-C7
22	c	505	CLA	C6-C7-C8-C10
22	c	505	CLA	C11-C10-C8-C7
22	c	506	CLA	C11-C10-C8-C7
22	c	507	CLA	C11-C10-C8-C7
22	c	511	CLA	C12-C13-C15-C16
22	c	513	CLA	C6-C7-C8-C10
22	c	513	CLA	C11-C10-C8-C7
23	a	404	PHO	C6-C7-C8-C10
22	D	404	CLA	C3-C5-C6-C7
28	a	411	SQD	C17-C18-C19-C20
29	D	411	LHG	C25-C26-C27-C28
30	c	516	DGD	C5B-C6B-C7B-C8B
22	A	403	CLA	C11-C12-C13-C14
22	B	602	CLA	C11-C12-C13-C14
22	B	613	CLA	C14-C13-C15-C16
22	B	615	CLA	C11-C12-C13-C14
22	B	616	CLA	C6-C7-C8-C9
22	C	504	CLA	C11-C10-C8-C9
22	C	505	CLA	C14-C13-C15-C16
22	C	510	CLA	C6-C7-C8-C9
22	C	510	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	C	510	CLA	C14-C13-C15-C16
22	C	511	CLA	C11-C12-C13-C14
22	C	513	CLA	C11-C10-C8-C9
22	D	403	CLA	C11-C12-C13-C14
22	D	404	CLA	C11-C10-C8-C9
22	a	403	CLA	C11-C10-C8-C9
22	b	603	CLA	C11-C12-C13-C14
22	b	615	CLA	C14-C13-C15-C16
22	c	504	CLA	C11-C10-C8-C9
22	c	505	CLA	C6-C7-C8-C9
22	c	506	CLA	C11-C10-C8-C9
22	c	513	CLA	C11-C10-C8-C9
27	c	521	LMG	C28-C29-C30-C31
27	Y	101	LMG	C33-C34-C35-C36
32	m	102	STE	C3-C4-C5-C6
32	B	620	STE	C9-C10-C11-C12
24	T	101	BCR	C36-C18-C19-C20
22	c	511	CLA	C16-C17-C18-C20
24	D	405	BCR	C21-C22-C23-C24
30	h	103	DGD	C2A-C3A-C4A-C5A
22	C	509	CLA	C3-C5-C6-C7
22	C	512	CLA	C3-C5-C6-C7
27	A	411	LMG	C16-C17-C18-C19
27	D	407	LMG	C36-C37-C38-C39
30	H	102	DGD	C3A-C4A-C5A-C6A
32	E	101	STE	C4-C5-C6-C7
27	c	521	LMG	C40-C41-C42-C43
32	b	625	STE	C15-C16-C17-C18
22	B	612	CLA	C10-C11-C12-C13
29	L	101	LHG	C18-C19-C20-C21
30	c	518	DGD	CDA-CEA-CFA-CGA
32	D	413	STE	C6-C7-C8-C9
30	H	102	DGD	O2G-C1B-C2B-C3B
29	A	413	LHG	C13-C14-C15-C16
29	A	413	LHG	C27-C28-C29-C30
30	C	516	DGD	CCA-CDA-CEA-CFA
30	A	415	DGD	O6E-C1E-O5D-C6D
29	A	413	LHG	O6-C4-C5-C6
32	B	627	STE	C6-C7-C8-C9
32	d	411	STE	C2-C3-C4-C5
28	A	412	SQD	C11-C10-C9-C8
32	d	412	STE	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	B	606	CLA	C5-C6-C7-C8
27	Y	101	LMG	C31-C32-C33-C34
29	l	101	LHG	C13-C14-C15-C16
32	c	520	STE	C4-C5-C6-C7
26	d	407	PL9	C45-C44-C46-C47
27	a	414	LMG	C18-C19-C20-C21
28	a	412	SQD	C30-C31-C32-C33
22	B	611	CLA	C8-C10-C11-C12
32	B	624	STE	C4-C5-C6-C7
32	T	102	STE	C11-C12-C13-C14
30	A	415	DGD	C5A-C6A-C7A-C8A
30	h	103	DGD	CCA-CDA-CEA-CFA
22	b	603	CLA	C13-C15-C16-C17
29	D	411	LHG	C26-C27-C28-C29
22	B	607	CLA	O1D-CGD-O2D-CED
22	B	601	CLA	C3A-C2A-CAA-CBA
27	c	521	LMG	C34-C35-C36-C37
27	h	102	LMG	C11-C12-C13-C14
28	F	102	SQD	C28-C29-C30-C31
32	b	622	STE	C12-C13-C14-C15
29	D	409	LHG	C30-C31-C32-C33
27	M	101	LMG	C12-C13-C14-C15
28	a	411	SQD	C29-C30-C31-C32
29	l	101	LHG	C11-C12-C13-C14
30	c	517	DGD	CDB-CEB-CFB-CGB
32	M	104	STE	C13-C14-C15-C16
27	a	414	LMG	O1-C7-C8-C9
27	c	521	LMG	C7-C8-C9-O8
28	a	412	SQD	C44-C45-C46-O48
29	e	101	LHG	C4-C5-C6-O8
30	A	415	DGD	C1G-C2G-C3G-O3G
29	D	409	LHG	C27-C28-C29-C30
29	L	101	LHG	C31-C32-C33-C34
32	B	625	STE	C11-C10-C9-C8
32	D	412	STE	C10-C11-C12-C13
32	J	101	STE	C2-C3-C4-C5
27	Y	101	LMG	C15-C16-C17-C18
28	b	620	SQD	C29-C30-C31-C32
29	A	413	LHG	C19-C20-C21-C22
29	d	408	LHG	C25-C26-C27-C28
32	E	101	STE	C5-C6-C7-C8
30	c	516	DGD	O6D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
27	D	407	LMG	C39-C40-C41-C42
27	c	521	LMG	C32-C33-C34-C35
28	a	411	SQD	C30-C31-C32-C33
27	d	410	LMG	C15-C16-C17-C18
27	m	101	LMG	C39-C40-C41-C42
32	C	518	STE	C2-C3-C4-C5
29	L	101	LHG	O10-C23-O8-C6
28	a	412	SQD	C29-C30-C31-C32
32	a	413	STE	C2-C3-C4-C5
22	B	607	CLA	CBD-CGD-O2D-CED
30	c	516	DGD	C9B-CAB-CBB-CCB
22	B	613	CLA	O1D-CGD-O2D-CED
29	e	101	LHG	C4-O6-P-O3
28	B	621	SQD	O10-C23-O48-C46
30	c	517	DGD	O6E-C5E-C6E-O5E
29	D	411	LHG	C33-C34-C35-C36
29	D	411	LHG	O1-C1-C2-O2
29	d	408	LHG	C10-C11-C12-C13
30	c	518	DGD	C8B-C9B-CAB-CBB
27	A	411	LMG	C14-C15-C16-C17
30	h	103	DGD	O1A-C1A-O1G-C1G
22	B	601	CLA	C16-C17-C18-C19
22	c	509	CLA	CAA-CBA-CGA-O2A
29	D	408	LHG	C35-C36-C37-C38
30	H	102	DGD	C3B-C4B-C5B-C6B
28	A	412	SQD	C35-C36-C37-C38
28	A	414	SQD	O47-C45-C46-O48
30	C	515	DGD	O6D-C5D-C6D-O5D
29	e	101	LHG	O7-C5-C6-O8
22	B	601	CLA	C16-C17-C18-C20
22	B	610	CLA	C16-C17-C18-C19
22	D	403	CLA	C16-C17-C18-C19
27	b	623	LMG	C29-C30-C31-C32
30	H	102	DGD	CBA-CCA-CDA-CEA
30	o	301	DGD	CAA-CBA-CCA-CDA
32	B	624	STE	C12-C13-C14-C15
22	B	613	CLA	C2-C1-O2A-CGA
29	A	413	LHG	C18-C19-C20-C21
32	B	626	STE	C2-C3-C4-C5
22	c	513	CLA	C8-C10-C11-C12
22	B	601	CLA	C11-C10-C8-C9
22	B	604	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	B	605	CLA	C6-C7-C8-C9
22	B	606	CLA	C11-C12-C13-C14
22	b	602	CLA	C14-C13-C15-C16
22	b	609	CLA	C14-C13-C15-C16
22	b	614	CLA	C6-C7-C8-C9
22	c	505	CLA	C11-C10-C8-C9
27	D	410	LMG	C37-C38-C39-C40
29	l	101	LHG	C15-C16-C17-C18
32	D	412	STE	C11-C12-C13-C14
29	d	409	LHG	C2-C3-O3-P
30	c	518	DGD	C3B-C4B-C5B-C6B
32	B	624	STE	C6-C7-C8-C9
32	b	626	STE	C7-C8-C9-C10
22	b	601	CLA	C16-C17-C18-C19
22	b	616	CLA	C11-C12-C13-C14
22	c	504	CLA	C11-C12-C13-C14
24	B	618	BCR	C23-C24-C25-C26
24	H	101	BCR	C23-C24-C25-C30
24	K	101	BCR	C23-C24-C25-C30
24	b	618	BCR	C23-C24-C25-C26
24	b	618	BCR	C23-C24-C25-C30
24	d	406	BCR	C23-C24-C25-C26
24	d	406	BCR	C23-C24-C25-C30
23	d	401	PHO	C2C-C3C-CAC-CBC
30	C	517	DGD	C8B-C9B-CAB-CBB
32	B	624	STE	C7-C8-C9-C10
30	c	517	DGD	C5B-C6B-C7B-C8B
22	b	616	CLA	O1D-CGD-O2D-CED
32	b	621	STE	C3-C4-C5-C6
27	Y	101	LMG	C29-C30-C31-C32
28	b	620	SQD	C15-C16-C17-C18
30	c	518	DGD	C3A-C4A-C5A-C6A
32	B	624	STE	C9-C10-C11-C12
22	B	612	CLA	C16-C17-C18-C19
22	C	508	CLA	C16-C17-C18-C19
32	B	623	STE	C4-C5-C6-C7
32	I	101	STE	C4-C5-C6-C7
22	D	404	CLA	C8-C10-C11-C12
22	b	602	CLA	C8-C10-C11-C12
27	a	414	LMG	C35-C36-C37-C38
28	A	414	SQD	C19-C20-C21-C22
29	l	101	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
27	A	411	LMG	C38-C39-C40-C41
27	c	521	LMG	C33-C34-C35-C36
29	A	413	LHG	C16-C17-C18-C19
22	A	403	CLA	C11-C12-C13-C15
22	B	601	CLA	C11-C10-C8-C7
22	B	608	CLA	C6-C7-C8-C10
22	B	615	CLA	C11-C12-C13-C15
22	C	505	CLA	C12-C13-C15-C16
22	C	509	CLA	C11-C10-C8-C7
22	C	509	CLA	C12-C13-C15-C16
22	C	510	CLA	C6-C7-C8-C10
22	C	510	CLA	C11-C10-C8-C7
22	C	511	CLA	C11-C12-C13-C15
22	C	512	CLA	C11-C10-C8-C7
22	C	512	CLA	C12-C13-C15-C16
22	D	403	CLA	C11-C12-C13-C15
22	a	403	CLA	C12-C13-C15-C16
22	b	602	CLA	C12-C13-C15-C16
22	b	605	CLA	C11-C10-C8-C7
22	b	607	CLA	C11-C12-C13-C15
22	b	609	CLA	C12-C13-C15-C16
22	b	614	CLA	C12-C13-C15-C16
22	b	615	CLA	C12-C13-C15-C16
22	c	505	CLA	C12-C13-C15-C16
22	c	510	CLA	C12-C13-C15-C16
22	c	513	CLA	C11-C12-C13-C15
22	d	403	CLA	C6-C7-C8-C10
22	d	404	CLA	C12-C13-C15-C16
27	c	521	LMG	C15-C16-C17-C18
32	b	624	STE	C9-C10-C11-C12
24	k	101	BCR	C19-C20-C21-C22
22	B	611	CLA	C16-C17-C18-C20
22	b	602	CLA	C16-C17-C18-C19
27	A	411	LMG	C15-C16-C17-C18
32	B	624	STE	C2-C3-C4-C5
32	D	412	STE	C2-C3-C4-C5
26	a	409	PL9	C32-C33-C34-C36
28	A	414	SQD	C35-C36-C37-C38
29	D	408	LHG	C12-C13-C14-C15
32	d	412	STE	C13-C14-C15-C16
27	m	101	LMG	C11-C10-O7-C8
22	B	611	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	D	403	CLA	C15-C16-C17-C18
24	c	515	BCR	C35-C13-C14-C15
24	t	101	BCR	C11-C10-C9-C34
28	b	620	SQD	C19-C20-C21-C22
29	L	101	LHG	C33-C34-C35-C36
30	C	517	DGD	CDA-CEA-CFA-CGA
22	c	506	CLA	O1D-CGD-O2D-CED
30	A	415	DGD	C2A-C3A-C4A-C5A
22	B	603	CLA	CAD-CBD-CGD-O2D
22	B	604	CLA	CAD-CBD-CGD-O2D
22	B	610	CLA	CAD-CBD-CGD-O2D
22	B	616	CLA	CAD-CBD-CGD-O2D
22	C	503	CLA	CAD-CBD-CGD-O2D
22	C	505	CLA	CAD-CBD-CGD-O2D
22	b	603	CLA	CAD-CBD-CGD-O2D
22	b	610	CLA	CAD-CBD-CGD-O2D
22	b	613	CLA	CAD-CBD-CGD-O2D
22	b	616	CLA	CAD-CBD-CGD-O2D
22	c	503	CLA	CAD-CBD-CGD-O2D
22	d	405	CLA	CAD-CBD-CGD-O2D
27	a	414	LMG	C9-C8-O7-C10
23	a	404	PHO	O1D-CGD-O2D-CED
28	A	412	SQD	C11-C12-C13-C14
22	b	613	CLA	C13-C15-C16-C17
24	D	405	BCR	C22-C23-C24-C25
22	c	504	CLA	C11-C12-C13-C15
32	D	413	STE	C7-C8-C9-C10
22	b	609	CLA	C2-C3-C5-C6
30	A	415	DGD	CBB-CCB-CDB-CEB
32	a	413	STE	C7-C8-C9-C10
29	A	413	LHG	O6-C4-C5-O7
29	D	409	LHG	O6-C4-C5-O7
22	b	612	CLA	C10-C11-C12-C13
27	d	410	LMG	C32-C33-C34-C35
30	A	415	DGD	CEA-CFA-CGA-CHA
22	c	508	CLA	C16-C17-C18-C19
22	b	603	CLA	CBD-CGD-O2D-CED
22	B	601	CLA	CHA-CBD-CGD-O1D
22	B	614	CLA	CHA-CBD-CGD-O2D
22	C	502	CLA	CHA-CBD-CGD-O1D
22	C	502	CLA	CHA-CBD-CGD-O2D
22	C	508	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	c	502	CLA	CHA-CBD-CGD-O1D
22	c	502	CLA	CHA-CBD-CGD-O2D
22	c	508	CLA	CHA-CBD-CGD-O1D
22	c	508	CLA	CHA-CBD-CGD-O2D
22	c	509	CLA	CHA-CBD-CGD-O1D
22	c	509	CLA	CHA-CBD-CGD-O2D
30	H	102	DGD	C8B-C9B-CAB-CBB
22	B	606	CLA	C8-C10-C11-C12
28	A	414	SQD	C32-C33-C34-C35
29	d	408	LHG	C12-C13-C14-C15
30	c	517	DGD	CCA-CDA-CEA-CFA
27	a	414	LMG	O1-C7-C8-O7
28	a	411	SQD	O47-C45-C46-O48
30	c	516	DGD	O1G-C1G-C2G-O2G
30	C	517	DGD	CAB-CBB-CCB-CDB
30	C	515	DGD	C9B-CAB-CBB-CCB
22	B	610	CLA	C16-C17-C18-C20
29	d	409	LHG	O1-C1-C2-O2
32	M	103	STE	C3-C4-C5-C6
32	a	415	STE	C6-C7-C8-C9
32	b	624	STE	C7-C8-C9-C10
32	B	620	STE	C4-C5-C6-C7
22	b	611	CLA	C2-C3-C5-C6
26	A	410	PL9	C4-C3-C7-C8
22	B	608	CLA	C6-C7-C8-C9
22	C	502	CLA	C11-C12-C13-C14
22	a	403	CLA	C6-C7-C8-C9
22	b	607	CLA	C11-C12-C13-C14
30	c	516	DGD	C4D-C5D-C6D-O5D
29	A	413	LHG	C31-C32-C33-C34
27	m	101	LMG	C31-C32-C33-C34
29	D	411	LHG	C19-C20-C21-C22
22	b	615	CLA	C5-C6-C7-C8
27	A	411	LMG	C13-C14-C15-C16
29	D	411	LHG	C24-C25-C26-C27
28	a	411	SQD	C32-C33-C34-C35
32	c	520	STE	C15-C16-C17-C18
29	D	408	LHG	C14-C15-C16-C17
24	k	101	BCR	C7-C8-C9-C10
27	c	519	LMG	C32-C33-C34-C35
30	H	102	DGD	CDB-CEB-CFB-CGB
32	b	626	STE	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
32	M	102	STE	C1-C2-C3-C4
32	C	520	STE	C6-C7-C8-C9
32	a	415	STE	C5-C6-C7-C8
29	L	101	LHG	C4-O6-P-O3
29	d	408	LHG	C3-O3-P-O6
30	C	516	DGD	C5B-C6B-C7B-C8B
32	H	103	STE	C9-C10-C11-C12
32	a	413	STE	C6-C7-C8-C9
26	a	409	PL9	C3-C7-C8-C9
29	d	408	LHG	C3-O3-P-O4
29	e	101	LHG	C4-O6-P-O4
22	B	602	CLA	C16-C17-C18-C20
22	C	508	CLA	C16-C17-C18-C20
29	a	410	LHG	C7-C8-C9-C10
29	d	409	LHG	C23-C24-C25-C26
29	D	411	LHG	C24-C23-O8-C6
29	D	409	LHG	O6-C4-C5-C6
29	d	408	LHG	O6-C4-C5-C6
32	M	104	STE	C2-C3-C4-C5
29	e	101	LHG	C12-C13-C14-C15
22	A	403	CLA	C16-C17-C18-C20
29	d	409	LHG	C33-C34-C35-C36
32	B	624	STE	C10-C11-C12-C13
32	b	621	STE	C15-C16-C17-C18
22	B	601	CLA	CAD-CBD-CGD-O1D
22	C	502	CLA	CAD-CBD-CGD-O1D
22	c	502	CLA	CAD-CBD-CGD-O1D
28	a	411	SQD	C5-C6-S-O9
22	d	405	CLA	C5-C6-C7-C8
29	L	101	LHG	C11-C12-C13-C14
29	l	101	LHG	C33-C34-C35-C36
28	B	621	SQD	C13-C14-C15-C16
22	C	506	CLA	C3-C5-C6-C7
30	A	415	DGD	CAB-CBB-CCB-CDB
30	C	517	DGD	O6D-C5D-C6D-O5D
22	D	404	CLA	C10-C11-C12-C13
28	b	620	SQD	C27-C28-C29-C30
30	C	516	DGD	CBB-CCB-CDB-CEB
22	A	403	CLA	C6-C7-C8-C10
22	B	601	CLA	C11-C12-C13-C15
22	B	603	CLA	C12-C13-C15-C16
22	B	612	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	B	613	CLA	C6-C7-C8-C10
22	C	505	CLA	C6-C7-C8-C10
22	D	402	CLA	C11-C12-C13-C15
22	a	403	CLA	C11-C12-C13-C15
22	b	601	CLA	C6-C7-C8-C10
22	b	601	CLA	C11-C10-C8-C7
22	b	603	CLA	C11-C12-C13-C15
22	b	607	CLA	C6-C7-C8-C10
22	b	614	CLA	C11-C10-C8-C7
22	b	615	CLA	C11-C12-C13-C15
22	c	506	CLA	C6-C7-C8-C10
22	c	509	CLA	C6-C7-C8-C10
26	D	406	PL9	C28-C29-C31-C32
28	F	102	SQD	C30-C31-C32-C33
29	D	408	LHG	C31-C32-C33-C34
27	b	623	LMG	C35-C36-C37-C38
29	l	101	LHG	C24-C25-C26-C27
29	A	413	LHG	C9-C10-C11-C12
29	e	101	LHG	O2-C2-C3-O3
30	C	516	DGD	C9A-CAA-CBA-CCA
30	H	102	DGD	CBB-CCB-CDB-CEB
30	c	516	DGD	C5A-C6A-C7A-C8A
32	B	623	STE	C6-C7-C8-C9
30	A	415	DGD	CBA-CCA-CDA-CEA
27	D	407	LMG	C31-C32-C33-C34
27	b	623	LMG	O1-C7-C8-C9
27	d	410	LMG	O9-C10-O7-C8
27	M	101	LMG	O7-C8-C9-O8
27	b	623	LMG	O1-C7-C8-O7
27	c	521	LMG	O7-C8-C9-O8
30	C	516	DGD	O1A-C1A-O1G-C1G
24	t	101	BCR	C14-C15-C16-C17
30	C	516	DGD	C5D-C6D-O5D-C1E
22	C	509	CLA	C16-C17-C18-C19
22	c	510	CLA	C5-C6-C7-C8
27	Y	101	LMG	C14-C15-C16-C17
22	B	601	CLA	C4-C3-C5-C6
27	m	101	LMG	C32-C33-C34-C35
29	A	413	LHG	C29-C30-C31-C32
32	d	412	STE	C12-C13-C14-C15
29	L	101	LHG	C16-C17-C18-C19
22	A	403	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	B	604	CLA	C6-C7-C8-C9
22	B	605	CLA	C11-C10-C8-C9
22	C	509	CLA	C14-C13-C15-C16
22	D	402	CLA	C11-C10-C8-C9
22	D	404	CLA	C11-C12-C13-C14
22	a	403	CLA	C14-C13-C15-C16
22	a	405	CLA	C11-C10-C8-C9
22	b	608	CLA	C11-C10-C8-C9
22	b	614	CLA	C11-C12-C13-C14
22	b	614	CLA	C14-C13-C15-C16
22	c	505	CLA	C14-C13-C15-C16
22	c	510	CLA	C14-C13-C15-C16
22	c	513	CLA	C11-C12-C13-C14
23	A	404	PHO	C14-C13-C15-C16
28	A	412	SQD	O10-C23-O48-C46
26	A	410	PL9	C12-C13-C14-C16
32	H	103	STE	C10-C11-C12-C13
26	d	407	PL9	C44-C46-C47-C48
32	b	621	STE	C10-C11-C12-C13
32	d	411	STE	C10-C11-C12-C13
29	d	408	LHG	O1-C1-C2-O2
24	T	101	BCR	C13-C14-C15-C16
28	f	102	SQD	C30-C31-C32-C33
22	c	504	CLA	C8-C10-C11-C12
22	b	602	CLA	C16-C17-C18-C20
32	I	101	STE	C2-C3-C4-C5
22	a	403	CLA	C13-C15-C16-C17
29	a	410	LHG	C29-C30-C31-C32
27	b	623	LMG	C12-C13-C14-C15
28	A	414	SQD	C11-C10-C9-C8
30	c	517	DGD	C5A-C6A-C7A-C8A
27	M	101	LMG	C11-C12-C13-C14
32	C	519	STE	C9-C10-C11-C12
27	c	519	LMG	C35-C36-C37-C38
32	b	622	STE	C13-C14-C15-C16
22	b	614	CLA	C10-C11-C12-C13
27	D	410	LMG	C9-C8-O7-C10
22	c	501	CLA	C2A-CAA-CBA-CGA
22	c	512	CLA	C8-C10-C11-C12
22	c	507	CLA	C2-C1-O2A-CGA
22	d	403	CLA	C2-C1-O2A-CGA
27	Y	101	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
30	C	515	DGD	O1G-C1A-C2A-C3A
30	c	516	DGD	O1G-C1A-C2A-C3A
22	C	509	CLA	O1D-CGD-O2D-CED
32	d	412	STE	C10-C11-C12-C13
28	F	102	SQD	C27-C28-C29-C30
29	A	413	LHG	C2-C3-O3-P
29	A	413	LHG	C33-C34-C35-C36
30	H	102	DGD	C9B-CAB-CBB-CCB
32	b	625	STE	C9-C10-C11-C12
24	B	617	BCR	C5-C6-C7-C8
22	c	509	CLA	C13-C15-C16-C17
30	c	518	DGD	CBB-CCB-CDB-CEB
32	C	518	STE	C7-C8-C9-C10
32	B	620	STE	C11-C12-C13-C14
32	M	103	STE	C1-C2-C3-C4
22	B	602	CLA	C16-C17-C18-C19
30	C	515	DGD	C4D-C5D-C6D-O5D
27	m	101	LMG	C36-C37-C38-C39
32	B	625	STE	C7-C8-C9-C10
30	A	415	DGD	C2E-C1E-O5D-C6D
29	D	408	LHG	C33-C34-C35-C36
28	a	412	SQD	O47-C45-C46-O48
30	C	515	DGD	O1G-C1G-C2G-O2G
28	A	414	SQD	C27-C28-C29-C30
32	T	102	STE	C12-C13-C14-C15
32	a	413	STE	C4-C5-C6-C7
29	A	413	LHG	C11-C10-C9-C8
32	B	625	STE	C3-C4-C5-C6
30	c	516	DGD	O1G-C1G-C2G-C3G
26	A	410	PL9	C20-C19-C21-C22
22	C	509	CLA	CBD-CGD-O2D-CED
22	B	603	CLA	C6-C7-C8-C10
22	B	606	CLA	C12-C13-C15-C16
22	B	611	CLA	C11-C10-C8-C7
22	C	503	CLA	C11-C10-C8-C7
22	a	405	CLA	C11-C10-C8-C7
22	b	601	CLA	C11-C12-C13-C15
22	b	602	CLA	C6-C7-C8-C10
22	b	603	CLA	C6-C7-C8-C10
22	c	502	CLA	C11-C12-C13-C15
22	d	403	CLA	C11-C12-C13-C15
26	a	409	PL9	C13-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
27	m	101	LMG	O10-C28-O8-C9
22	A	403	CLA	C6-C7-C8-C9
22	B	603	CLA	C14-C13-C15-C16
22	B	612	CLA	C11-C10-C8-C9
22	b	603	CLA	C6-C7-C8-C9
22	b	607	CLA	C6-C7-C8-C9
22	b	613	CLA	C6-C7-C8-C9
22	c	506	CLA	C6-C7-C8-C9
22	c	507	CLA	C11-C10-C8-C9
22	c	511	CLA	C6-C7-C8-C9
23	a	404	PHO	C6-C7-C8-C9
22	d	405	CLA	C8-C10-C11-C12
24	K	101	BCR	C15-C16-C17-C18
27	D	410	LMG	C16-C17-C18-C19
27	m	101	LMG	C17-C18-C19-C20
27	M	101	LMG	C22-C23-C24-C25
29	d	409	LHG	C32-C33-C34-C35
32	B	620	STE	C7-C8-C9-C10
27	c	519	LMG	C30-C31-C32-C33
29	D	408	LHG	C18-C19-C20-C21
22	A	403	CLA	C16-C17-C18-C19
22	B	611	CLA	C16-C17-C18-C19
22	b	609	CLA	C16-C17-C18-C20
30	h	103	DGD	C7A-C8A-C9A-CAA
28	A	412	SQD	C9-C10-C11-C12
30	c	516	DGD	C8B-C9B-CAB-CBB
30	c	516	DGD	CDB-CEB-CFB-CGB
32	c	522	STE	C6-C7-C8-C9
22	c	504	CLA	C4-C3-C5-C6
26	a	409	PL9	C12-C13-C14-C16
22	b	614	CLA	C8-C10-C11-C12
22	B	612	CLA	CBD-CGD-O2D-CED
24	B	618	BCR	C15-C16-C17-C18
24	C	514	BCR	C15-C16-C17-C18
29	d	408	LHG	C30-C31-C32-C33
27	m	101	LMG	C18-C19-C20-C21
24	B	618	BCR	C10-C11-C12-C13
30	C	517	DGD	O1A-C1A-O1G-C1G
22	D	404	CLA	C16-C17-C18-C19
22	b	607	CLA	C4-C3-C5-C6
29	d	408	LHG	C9-C10-C11-C12
22	b	613	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	C	506	CLA	C2-C1-O2A-CGA
22	D	402	CLA	C2-C1-O2A-CGA
22	c	512	CLA	C2-C1-O2A-CGA
22	c	513	CLA	C2-C1-O2A-CGA
29	L	101	LHG	C17-C18-C19-C20
32	C	519	STE	C6-C7-C8-C9
22	b	606	CLA	C3-C5-C6-C7
27	b	623	LMG	C17-C18-C19-C20
32	b	622	STE	C10-C11-C12-C13
22	B	603	CLA	C2A-CAA-CBA-CGA
22	D	402	CLA	C10-C11-C12-C13
29	D	409	LHG	C2-C3-O3-P
27	b	623	LMG	C30-C31-C32-C33
22	C	511	CLA	C16-C17-C18-C19
28	a	412	SQD	C16-C17-C18-C19
22	b	611	CLA	C4-C3-C5-C6
26	a	409	PL9	C4-C3-C7-C8
27	c	521	LMG	C42-C43-C44-C45
32	b	622	STE	C3-C4-C5-C6
22	B	611	CLA	C11-C12-C13-C14
22	B	614	CLA	C14-C13-C15-C16
22	b	601	CLA	C14-C13-C15-C16
22	c	502	CLA	C11-C12-C13-C14
22	C	509	CLA	C16-C17-C18-C20
30	C	516	DGD	C2B-C3B-C4B-C5B
30	c	516	DGD	C7B-C8B-C9B-CAB
32	B	624	STE	C5-C6-C7-C8
24	B	618	BCR	C35-C13-C14-C15
27	Y	101	LMG	O1-C7-C8-C9
27	c	521	LMG	O1-C7-C8-C9
29	D	408	LHG	C4-C5-C6-O8
29	D	411	LHG	C4-C5-C6-O8
28	a	411	SQD	C11-C10-C9-C8
30	C	517	DGD	C6A-C7A-C8A-C9A
23	a	404	PHO	O2A-C1-C2-C3
30	C	516	DGD	O6D-C1D-O3G-C3G
27	D	410	LMG	C31-C32-C33-C34
32	B	627	STE	C2-C3-C4-C5
24	b	617	BCR	C36-C18-C19-C20
30	H	102	DGD	CDA-CEA-CFA-CGA
22	d	403	CLA	C3-C5-C6-C7
32	d	411	STE	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
22	c	512	CLA	C4-C3-C5-C6
30	c	516	DGD	O1B-C1B-O2G-C2G
22	B	601	CLA	C12-C13-C15-C16
22	B	605	CLA	C12-C13-C15-C16
22	C	502	CLA	C12-C13-C15-C16
22	a	403	CLA	C6-C7-C8-C10
22	b	606	CLA	C11-C12-C13-C15
22	c	507	CLA	C11-C12-C13-C15
32	D	413	STE	C10-C11-C12-C13
27	b	623	LMG	C28-C29-C30-C31
32	b	622	STE	C11-C12-C13-C14
27	c	519	LMG	C11-C10-O7-C8
28	A	414	SQD	C16-C17-C18-C19
32	b	622	STE	C15-C16-C17-C18
22	B	613	CLA	C10-C11-C12-C13
27	h	102	LMG	C38-C39-C40-C41
28	f	102	SQD	C31-C32-C33-C34
29	l	101	LHG	O6-C4-C5-O7
32	M	103	STE	C5-C6-C7-C8
22	b	608	CLA	C5-C6-C7-C8
27	h	102	LMG	C40-C41-C42-C43
22	d	405	CLA	O1D-CGD-O2D-CED
32	B	622	STE	C3-C4-C5-C6
22	C	510	CLA	C4-C3-C5-C6
32	d	412	STE	C4-C5-C6-C7
30	c	516	DGD	CBB-CCB-CDB-CEB
22	b	612	CLA	C16-C17-C18-C20
30	c	516	DGD	CBA-CCA-CDA-CEA
24	H	101	BCR	C11-C10-C9-C8
24	k	101	BCR	C11-C10-C9-C8
29	D	408	LHG	O7-C5-C6-O8
24	C	514	BCR	C13-C14-C15-C16
22	B	604	CLA	C13-C15-C16-C17
22	B	612	CLA	O1D-CGD-O2D-CED
22	b	609	CLA	O1D-CGD-O2D-CED
22	C	511	CLA	C16-C17-C18-C20
30	A	415	DGD	C9A-CAA-CBA-CCA
30	A	415	DGD	C3B-C4B-C5B-C6B
22	B	603	CLA	C13-C15-C16-C17
22	B	612	CLA	O1A-CGA-O2A-C1
22	b	610	CLA	C13-C15-C16-C17
22	c	508	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
28	f	102	SQD	C24-C25-C26-C27
29	D	409	LHG	C11-C10-C9-C8
22	b	602	CLA	C6-C7-C8-C9
28	f	102	SQD	C29-C30-C31-C32
27	D	410	LMG	O10-C28-O8-C9
28	a	412	SQD	C18-C19-C20-C21
30	A	415	DGD	C8B-C9B-CAB-CBB
32	b	622	STE	C11-C10-C9-C8
22	c	509	CLA	CAA-CBA-CGA-O1A
24	A	407	BCR	C1-C6-C7-C8
24	C	514	BCR	C1-C6-C7-C8
24	C	514	BCR	C23-C24-C25-C30
24	K	101	BCR	C23-C24-C25-C26
24	K	102	BCR	C23-C24-C25-C30
24	h	101	BCR	C23-C24-C25-C30
24	k	101	BCR	C23-C24-C25-C30
30	C	515	DGD	C1G-C2G-C3G-O3G
22	a	403	CLA	O1D-CGD-O2D-CED
29	A	413	LHG	O1-C1-C2-C3
30	C	515	DGD	CBA-CCA-CDA-CEA
26	D	406	PL9	C40-C39-C41-C42
24	K	101	BCR	C21-C22-C23-C24
22	B	603	CLA	C5-C6-C7-C8
22	b	601	CLA	C15-C16-C17-C18
32	H	103	STE	C13-C14-C15-C16
22	B	601	CLA	C2-C3-C5-C6
22	b	607	CLA	C2-C3-C5-C6
22	c	512	CLA	C2-C3-C5-C6
22	c	510	CLA	C3-C5-C6-C7
30	c	516	DGD	C5D-C6D-O5D-C1E
22	C	504	CLA	C11-C12-C13-C14
32	j	101	STE	C2-C3-C4-C5
29	d	408	LHG	O6-C4-C5-O7
32	c	520	STE	C11-C10-C9-C8
27	d	410	LMG	C34-C35-C36-C37
22	b	605	CLA	C4-C3-C5-C6
29	A	413	LHG	O1-C1-C2-O2
29	l	101	LHG	O10-C23-O8-C6
22	b	613	CLA	C16-C17-C18-C19
22	b	604	CLA	C13-C15-C16-C17
27	A	411	LMG	O1-C7-C8-O7
29	A	413	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
27	Y	101	LMG	C34-C35-C36-C37
27	c	521	LMG	C13-C14-C15-C16
29	a	410	LHG	C10-C11-C12-C13
24	A	407	BCR	C20-C21-C22-C37
22	B	612	CLA	CAA-CBA-CGA-O2A
29	l	101	LHG	O7-C7-C8-C9
26	D	406	PL9	C13-C14-C16-C17
26	a	409	PL9	C28-C29-C31-C32
22	D	404	CLA	C16-C17-C18-C20
22	B	613	CLA	C6-C7-C8-C9
22	B	616	CLA	C11-C10-C8-C9
22	C	505	CLA	C6-C7-C8-C9
22	C	512	CLA	C14-C13-C15-C16
22	a	403	CLA	C11-C12-C13-C14
22	b	602	CLA	C11-C12-C13-C14
22	b	604	CLA	C11-C10-C8-C9
22	b	614	CLA	C11-C10-C8-C9
22	c	507	CLA	C6-C7-C8-C9
22	d	403	CLA	C6-C7-C8-C9
23	A	405	PHO	C6-C7-C8-C9
30	h	103	DGD	CBA-CCA-CDA-CEA
27	M	101	LMG	C13-C14-C15-C16
22	D	404	CLA	C3A-C2A-CAA-CBA
28	a	411	SQD	O47-C7-C8-C9
32	B	627	STE	C7-C8-C9-C10
22	B	605	CLA	CAD-CBD-CGD-O2D
22	B	607	CLA	CAD-CBD-CGD-O2D
22	B	609	CLA	CAD-CBD-CGD-O2D
22	C	506	CLA	CAD-CBD-CGD-O2D
22	C	512	CLA	CAD-CBD-CGD-O2D
22	b	604	CLA	CAD-CBD-CGD-O2D
22	b	609	CLA	CAD-CBD-CGD-O2D
22	b	612	CLA	CAD-CBD-CGD-O2D
22	c	510	CLA	CAD-CBD-CGD-O2D
22	c	513	CLA	CAD-CBD-CGD-O2D
26	D	406	PL9	C16-C17-C18-C19
23	A	404	PHO	C10-C11-C12-C13
30	A	415	DGD	C6B-C7B-C8B-C9B
27	d	410	LMG	O7-C10-C11-C12
30	C	516	DGD	C8A-C9A-CAA-CBA
32	a	415	STE	C7-C8-C9-C10
26	A	410	PL9	C25-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
28	a	411	SQD	C25-C26-C27-C28
22	C	510	CLA	C2-C3-C5-C6
32	c	520	STE	C10-C11-C12-C13
22	D	403	CLA	C2C-C3C-CAC-CBC
22	a	402	CLA	C2C-C3C-CAC-CBC
22	c	502	CLA	C2C-C3C-CAC-CBC
22	d	403	CLA	C2C-C3C-CAC-CBC
22	d	404	CLA	C2C-C3C-CAC-CBC
27	M	101	LMG	O1-C7-C8-C9
30	h	103	DGD	C1G-C2G-C3G-O3G
27	m	101	LMG	O8-C28-C29-C30
22	a	403	CLA	CBD-CGD-O2D-CED
22	C	509	CLA	O2A-C1-C2-C3
22	C	512	CLA	O2A-C1-C2-C3
22	D	404	CLA	O2A-C1-C2-C3
22	b	601	CLA	O2A-C1-C2-C3
22	d	405	CLA	O2A-C1-C2-C3
23	A	404	PHO	O2A-C1-C2-C3
24	T	101	BCR	C14-C15-C16-C17
28	A	414	SQD	C9-C10-C11-C12
32	b	625	STE	C7-C8-C9-C10
22	B	601	CLA	CHA-CBD-CGD-O2D
22	B	602	CLA	CHA-CBD-CGD-O1D
22	B	602	CLA	CHA-CBD-CGD-O2D
22	B	607	CLA	CHA-CBD-CGD-O1D
22	C	505	CLA	CHA-CBD-CGD-O1D
22	C	505	CLA	CHA-CBD-CGD-O2D
22	C	507	CLA	CHA-CBD-CGD-O1D
22	C	507	CLA	CHA-CBD-CGD-O2D
22	C	508	CLA	CHA-CBD-CGD-O2D
22	C	509	CLA	CHA-CBD-CGD-O2D
22	D	403	CLA	CHA-CBD-CGD-O1D
22	b	606	CLA	CHA-CBD-CGD-O2D
22	b	607	CLA	CHA-CBD-CGD-O1D
22	b	607	CLA	CHA-CBD-CGD-O2D
22	b	614	CLA	CHA-CBD-CGD-O1D
22	b	614	CLA	CHA-CBD-CGD-O2D
22	c	504	CLA	CHA-CBD-CGD-O1D
22	c	504	CLA	CHA-CBD-CGD-O2D
22	c	506	CLA	CHA-CBD-CGD-O1D
22	c	507	CLA	CHA-CBD-CGD-O1D
22	c	507	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	A	404	PHO	CHA-CBD-CGD-O1D
23	A	404	PHO	CHA-CBD-CGD-O2D
23	d	401	PHO	CHA-CBD-CGD-O1D
23	d	401	PHO	CHA-CBD-CGD-O2D
27	b	623	LMG	O7-C10-C11-C12
22	c	508	CLA	C2-C3-C5-C6
23	a	404	PHO	C2-C3-C5-C6
27	a	414	LMG	C37-C38-C39-C40
32	C	519	STE	C11-C12-C13-C14
28	A	412	SQD	C12-C13-C14-C15
22	B	613	CLA	CAA-CBA-CGA-O2A
28	A	412	SQD	O47-C7-C8-C9
27	Y	101	LMG	O1-C7-C8-O7
27	c	521	LMG	O1-C7-C8-O7
28	A	412	SQD	O6-C44-C45-O47
28	b	620	SQD	O47-C45-C46-O48
29	D	411	LHG	O7-C5-C6-O8
22	B	603	CLA	C15-C16-C17-C18
29	D	408	LHG	O10-C23-O8-C6
30	C	515	DGD	O2G-C1B-C2B-C3B
30	o	301	DGD	O1G-C1A-C2A-C3A
26	a	409	PL9	C32-C33-C34-C35
32	C	519	STE	C5-C6-C7-C8
32	H	103	STE	C11-C12-C13-C14
22	B	613	CLA	C11-C12-C13-C15
22	B	615	CLA	C6-C7-C8-C10
22	B	615	CLA	C12-C13-C15-C16
22	C	506	CLA	C11-C10-C8-C7
22	C	506	CLA	C12-C13-C15-C16
22	D	404	CLA	C6-C7-C8-C10
22	b	610	CLA	C11-C12-C13-C15
22	b	614	CLA	C6-C7-C8-C10
22	c	504	CLA	C2-C3-C5-C6
22	c	511	CLA	C6-C7-C8-C10
30	c	518	DGD	O6D-C5D-C6D-O5D
22	A	402	CLA	C11-C10-C8-C9
22	B	603	CLA	C6-C7-C8-C9
22	B	606	CLA	C14-C13-C15-C16
22	C	502	CLA	C14-C13-C15-C16
22	D	402	CLA	C11-C12-C13-C14
22	D	404	CLA	C6-C7-C8-C9
22	b	601	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	d	403	CLA	C11-C12-C13-C14
24	d	406	BCR	C19-C20-C21-C22
28	a	411	SQD	C5-C6-S-O8
27	m	101	LMG	C14-C15-C16-C17
30	H	102	DGD	C5A-C6A-C7A-C8A
29	D	411	LHG	C13-C14-C15-C16
22	b	603	CLA	C4-C3-C5-C6
26	D	406	PL9	C45-C44-C46-C47
22	c	501	CLA	CBD-CGD-O2D-CED
27	Y	101	LMG	C39-C40-C41-C42
32	c	520	STE	C14-C15-C16-C17
27	b	623	LMG	O10-C28-C29-C30
28	f	102	SQD	O10-C23-C24-C25
27	A	411	LMG	C18-C19-C20-C21
29	d	409	LHG	C9-C10-C11-C12
22	B	612	CLA	CBA-CGA-O2A-C1
22	B	602	CLA	C1A-C2A-CAA-CBA
22	C	512	CLA	C1A-C2A-CAA-CBA
22	D	404	CLA	C1A-C2A-CAA-CBA
23	d	401	PHO	C1A-C2A-CAA-CBA
32	B	620	STE	C1-C2-C3-C4
32	E	101	STE	C1-C2-C3-C4
28	b	620	SQD	C11-C10-C9-C8
22	C	505	CLA	O1D-CGD-O2D-CED
29	A	413	LHG	C15-C16-C17-C18
27	A	411	LMG	C7-C8-C9-O8
28	b	620	SQD	O6-C44-C45-C46
32	b	625	STE	C2-C3-C4-C5
32	b	626	STE	C1-C2-C3-C4
22	C	501	CLA	C2A-CAA-CBA-CGA
30	c	516	DGD	O1B-C1B-C2B-C3B
30	o	301	DGD	CEB-CFB-CGB-CHB
29	L	101	LHG	C27-C28-C29-C30
30	c	518	DGD	CAA-CBA-CCA-CDA
22	B	612	CLA	CAA-CBA-CGA-O1A
30	A	415	DGD	CCA-CDA-CEA-CFA
32	d	412	STE	C11-C10-C9-C8
29	A	413	LHG	C3-O3-P-O4
29	A	413	LHG	C3-O3-P-O5
29	D	408	LHG	C4-O6-P-O5
29	L	101	LHG	C4-O6-P-O5
29	e	101	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
29	e	101	LHG	C4-O6-P-O5
32	c	522	STE	C7-C8-C9-C10
30	c	517	DGD	O1A-C1A-C2A-C3A
24	C	514	BCR	C5-C6-C7-C8
24	C	514	BCR	C23-C24-C25-C26
24	h	101	BCR	C23-C24-C25-C26
29	e	101	LHG	C17-C18-C19-C20
29	l	101	LHG	C9-C10-C11-C12
30	h	103	DGD	O1B-C1B-C2B-C3B
22	B	601	CLA	C15-C16-C17-C18
27	A	411	LMG	C30-C31-C32-C33
29	a	410	LHG	C25-C26-C27-C28
28	F	102	SQD	C34-C35-C36-C37
29	d	408	LHG	C7-C8-C9-C10
28	B	621	SQD	C11-C10-C9-C8
22	B	607	CLA	CAD-CBD-CGD-O1D
22	C	504	CLA	CAD-CBD-CGD-O1D
22	b	607	CLA	CAD-CBD-CGD-O1D
22	c	504	CLA	CAD-CBD-CGD-O1D
22	c	506	CLA	CAD-CBD-CGD-O1D
22	B	605	CLA	C14-C13-C15-C16
22	B	614	CLA	C6-C7-C8-C9
22	a	402	CLA	C14-C13-C15-C16
22	b	606	CLA	C11-C12-C13-C14
22	b	612	CLA	C11-C10-C8-C9
22	c	508	CLA	C11-C10-C8-C9
22	b	609	CLA	C13-C15-C16-C17
30	A	415	DGD	O2G-C1B-C2B-C3B
32	M	103	STE	C6-C7-C8-C9
27	a	414	LMG	C10-C11-C12-C13
27	Y	101	LMG	C16-C17-C18-C19
27	a	414	LMG	C36-C37-C38-C39
28	a	411	SQD	C14-C15-C16-C17
28	f	102	SQD	O48-C23-C24-C25
30	c	516	DGD	O2G-C1B-C2B-C3B
30	A	415	DGD	O1B-C1B-C2B-C3B
23	a	404	PHO	C4-C3-C5-C6
24	h	101	BCR	C11-C12-C13-C35
22	a	402	CLA	C12-C13-C15-C16
22	b	601	CLA	CAA-CBA-CGA-O2A
29	a	410	LHG	O8-C23-C24-C25
30	c	517	DGD	O2G-C1B-C2B-C3B

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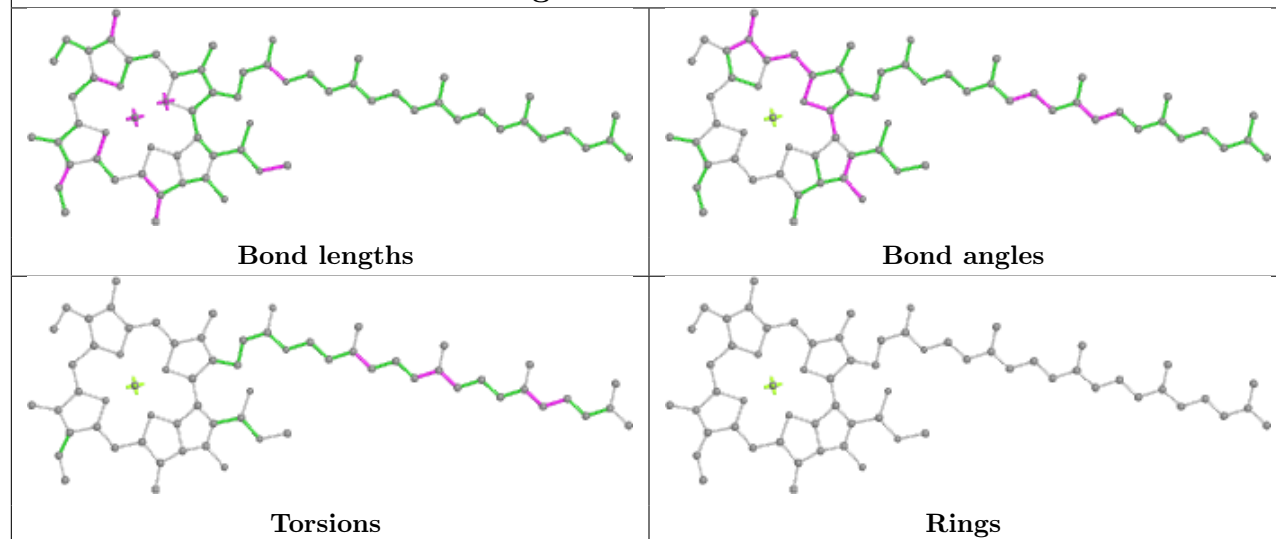
Mol	Chain	Res	Type	Atoms
30	C	515	DGD	CDB-CEB-CFB-CGB
24	D	405	BCR	C11-C12-C13-C14
22	b	601	CLA	CAA-CBA-CGA-O1A
29	L	101	LHG	O7-C7-C8-C9
27	M	101	LMG	C29-C30-C31-C32
30	C	515	DGD	O6E-C1E-O5D-C6D
22	B	601	CLA	C10-C11-C12-C13
22	b	611	CLA	C15-C16-C17-C18
26	D	406	PL9	C44-C46-C47-C48
26	d	407	PL9	C34-C36-C37-C38
27	c	521	LMG	C35-C36-C37-C38
27	m	101	LMG	C40-C41-C42-C43
22	B	610	CLA	C15-C16-C17-C18
29	a	410	LHG	C31-C32-C33-C34
22	C	512	CLA	C15-C16-C17-C18
29	L	101	LHG	C23-C24-C25-C26
22	b	615	CLA	C13-C15-C16-C17

There are no ring outliers.

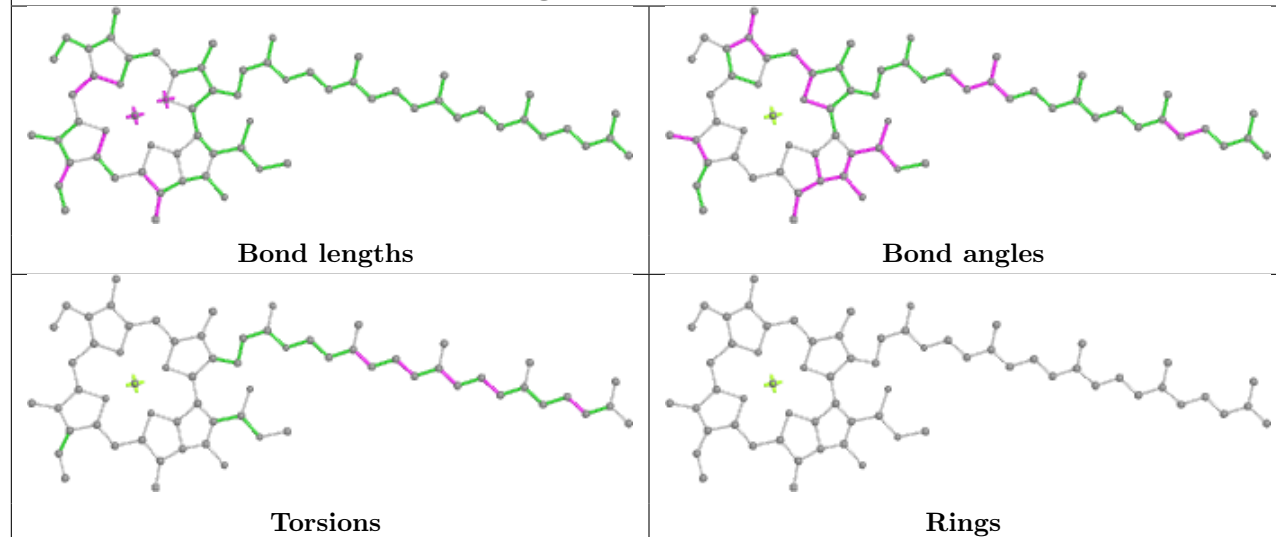
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

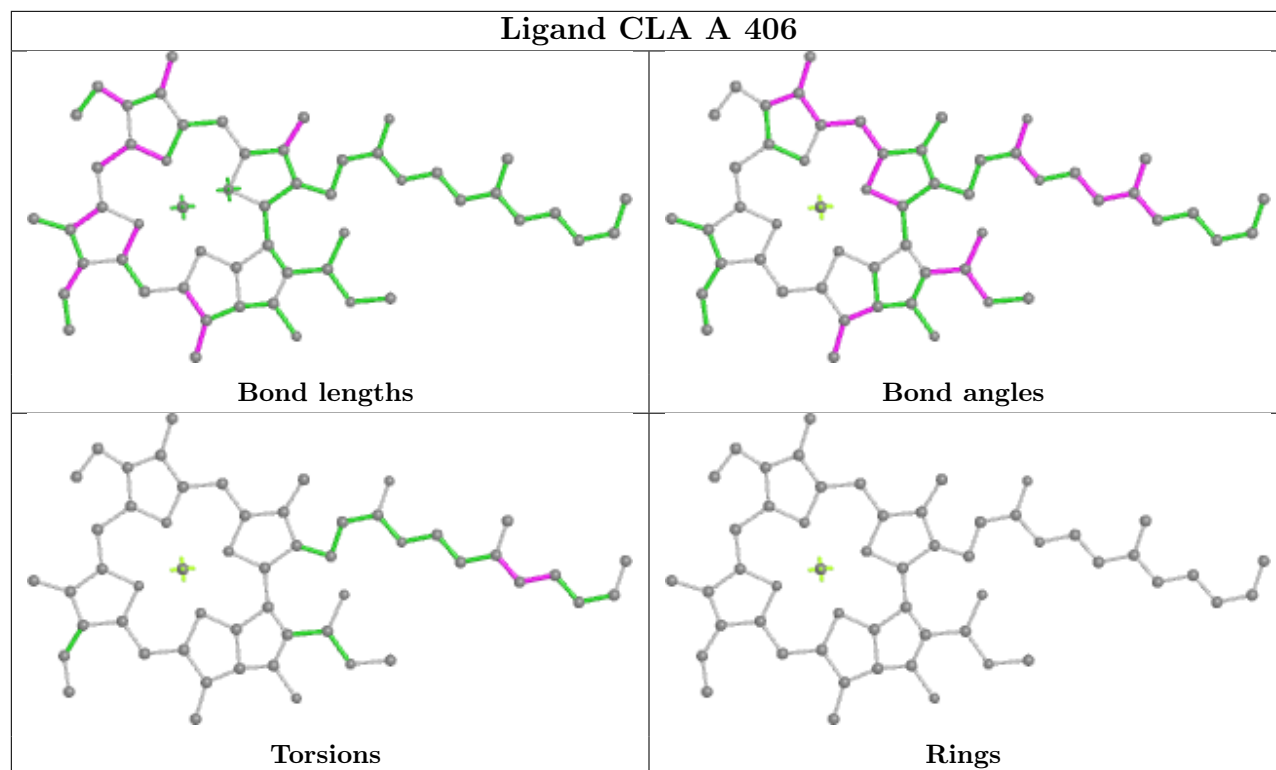
Ligand CLA C 510



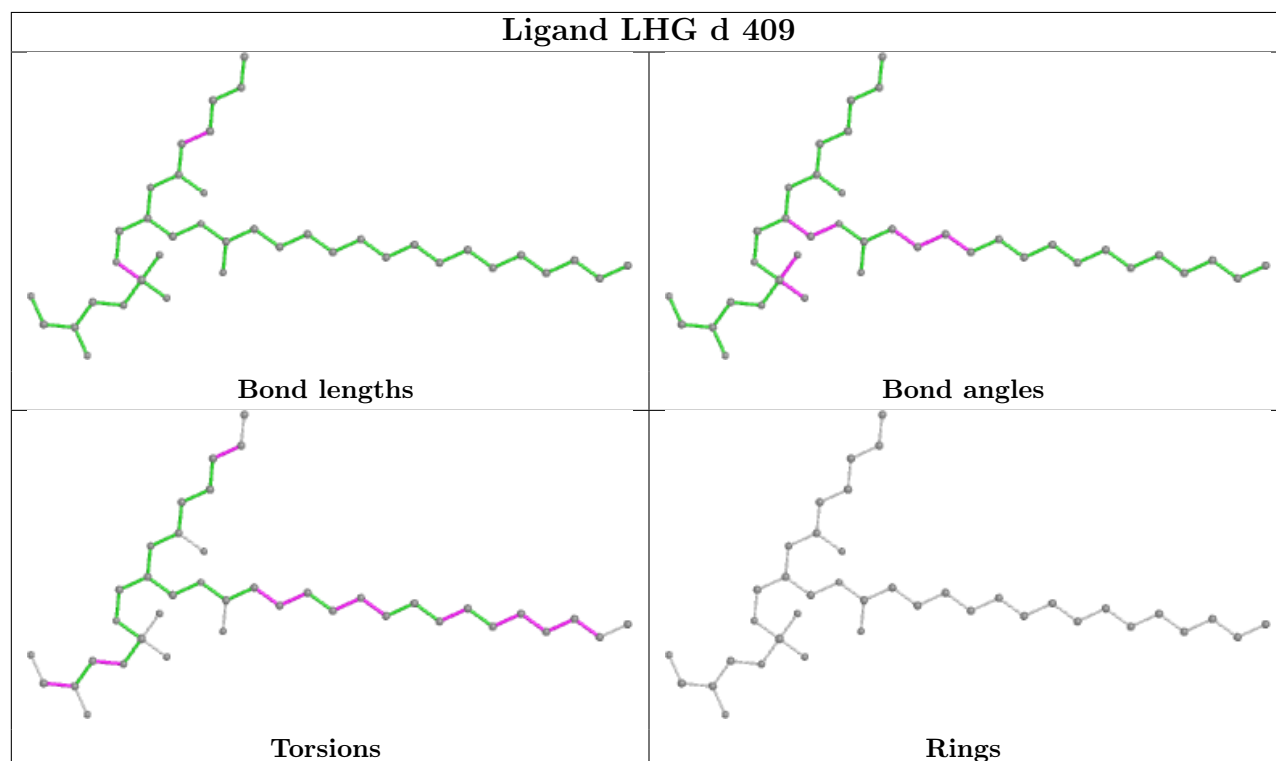
Ligand CLA b 605

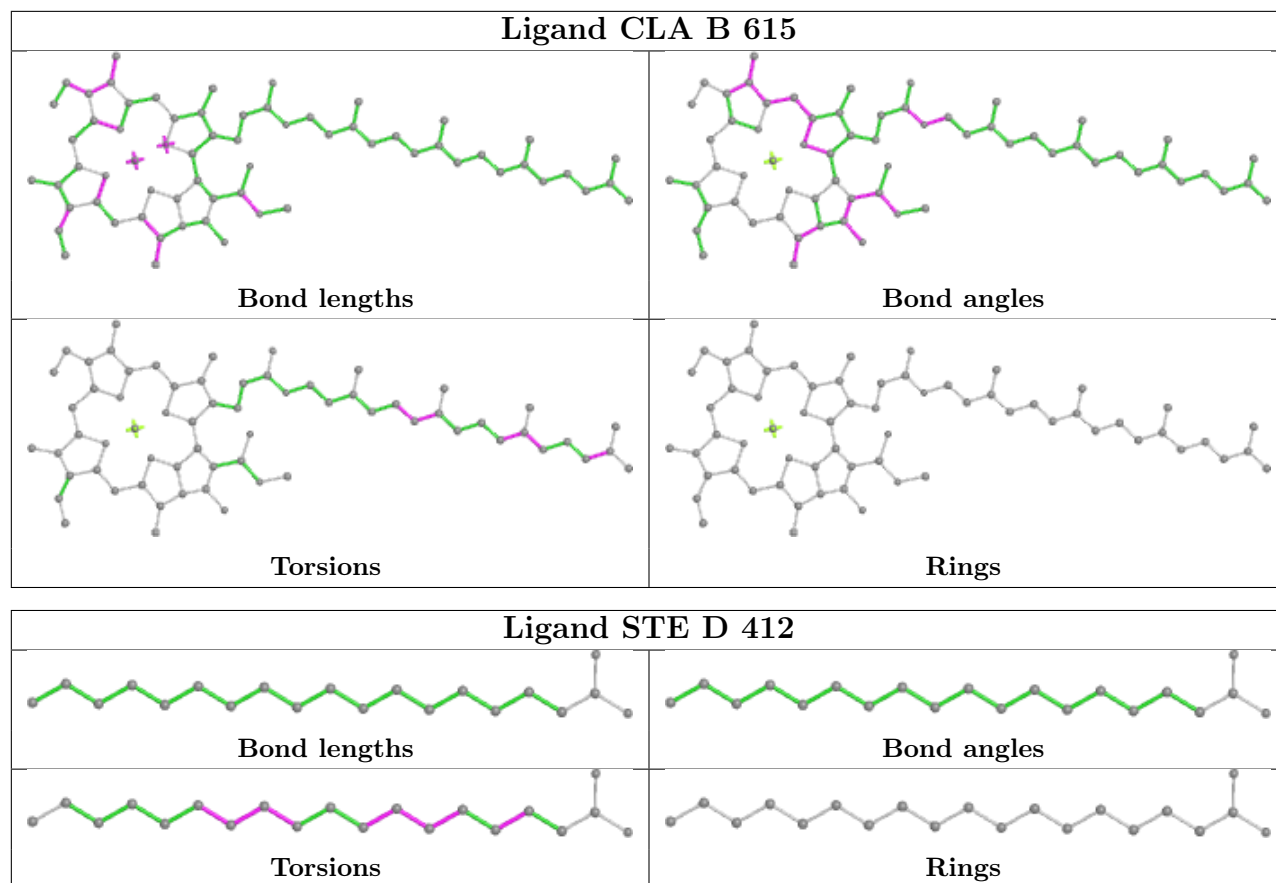


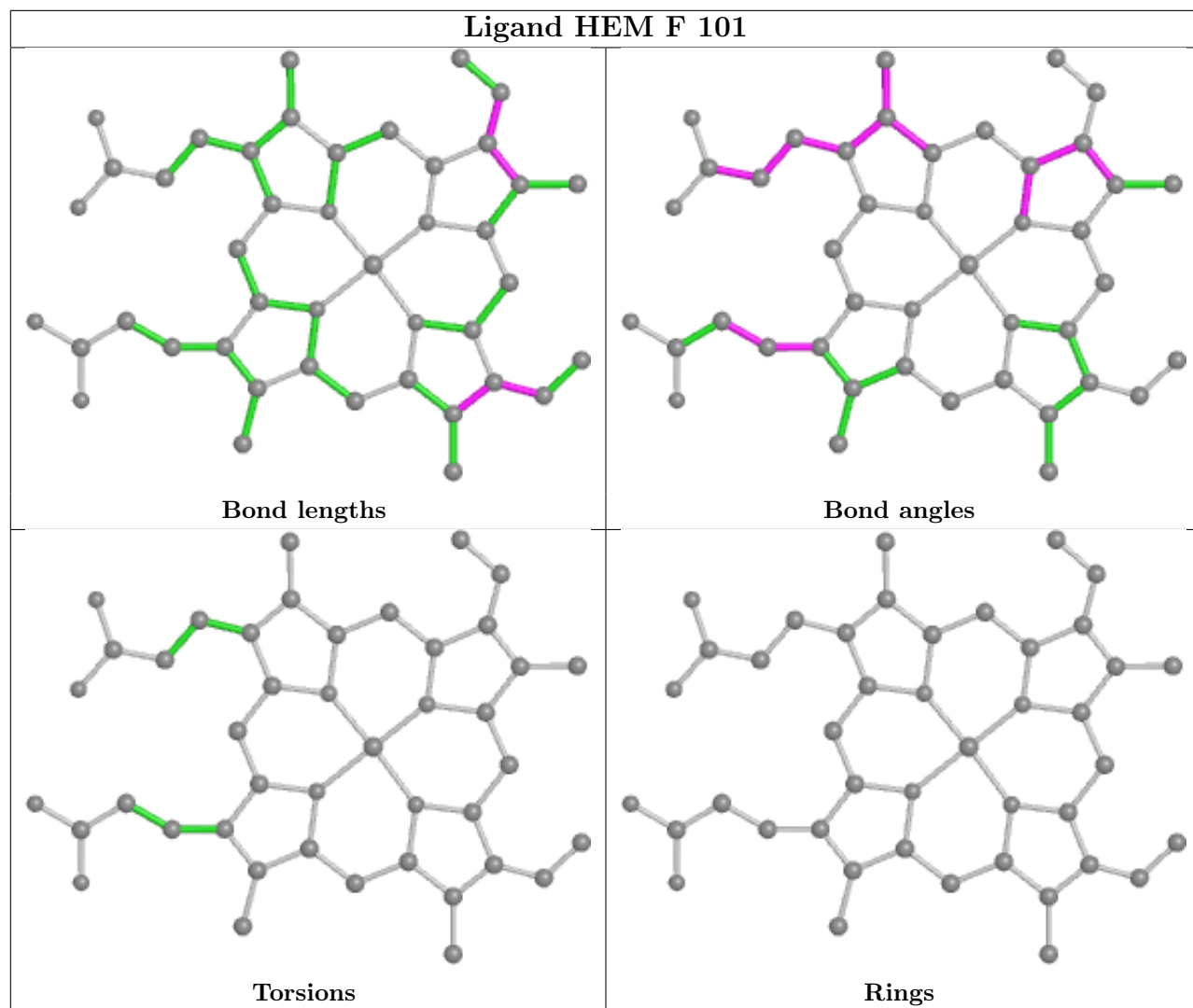
Ligand CLA A 406

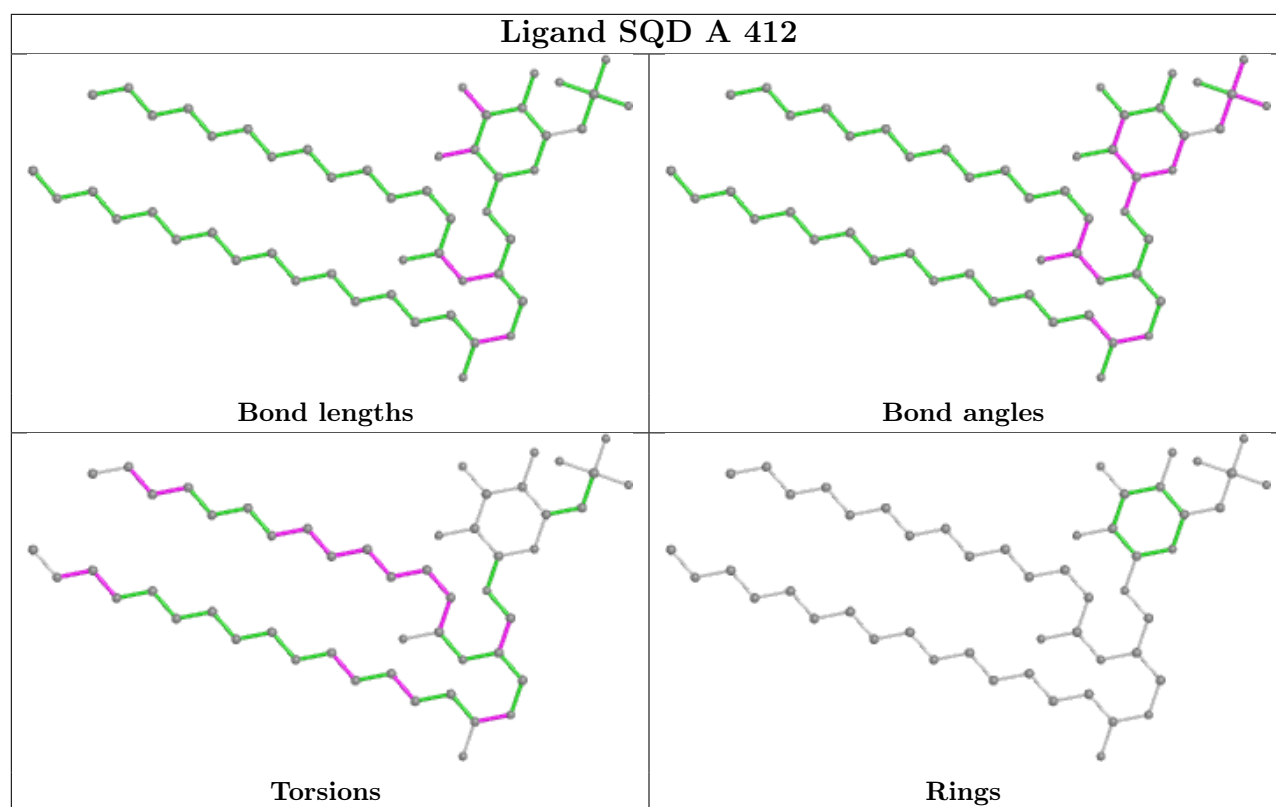


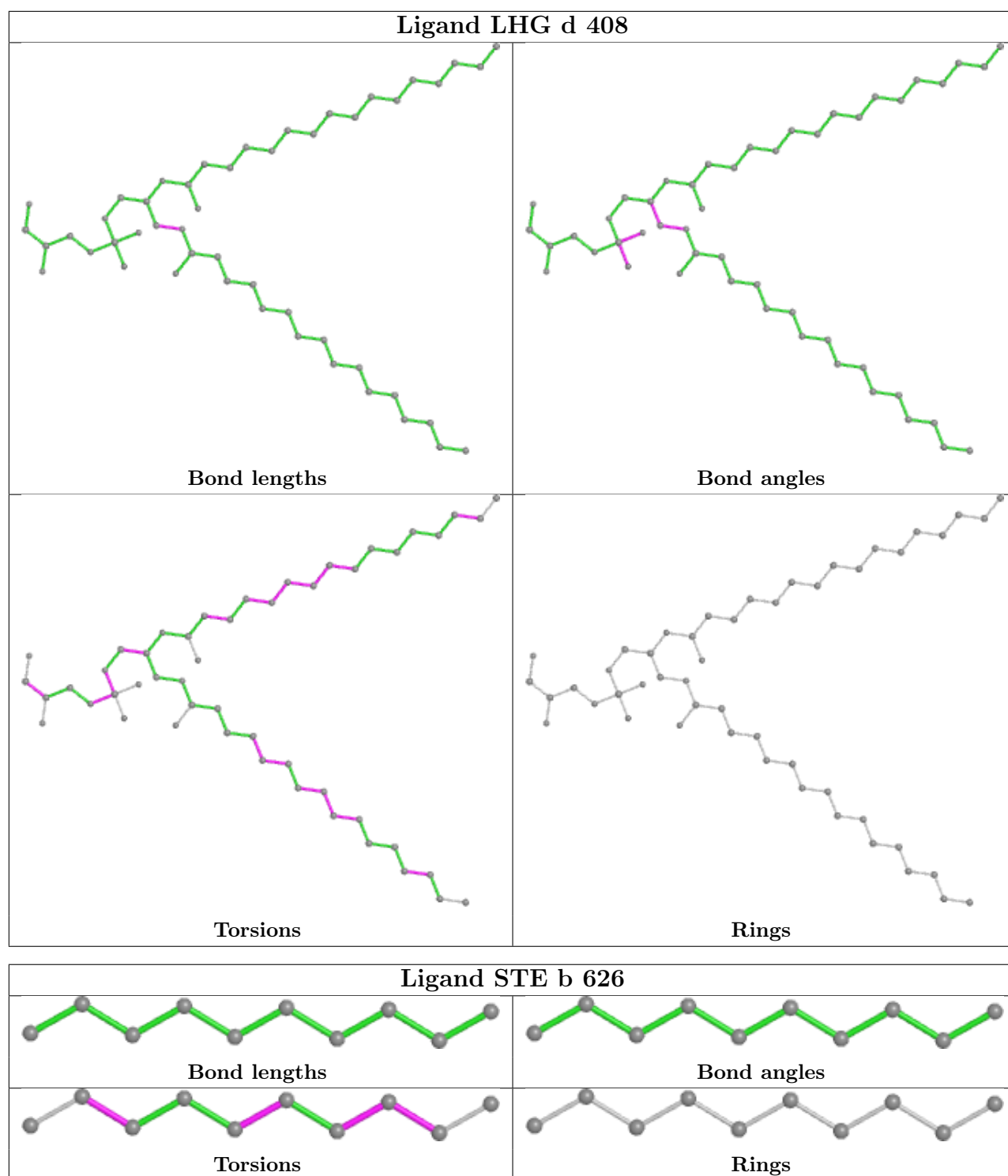
Ligand LHG d 409

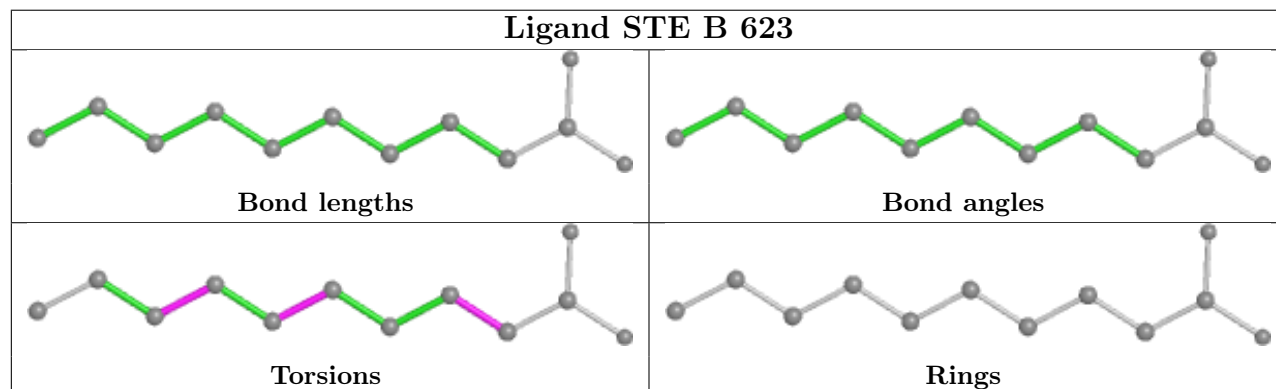
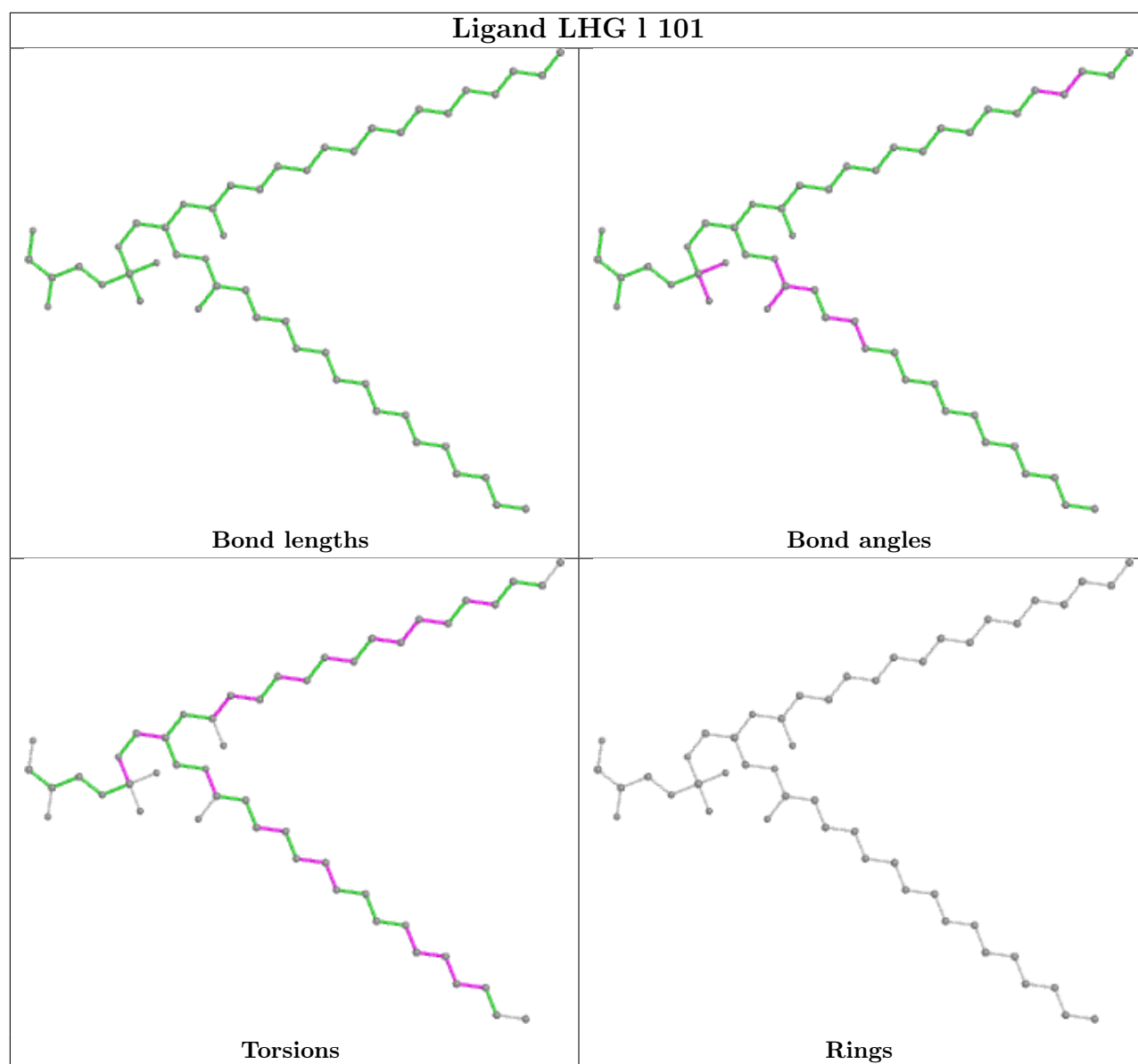




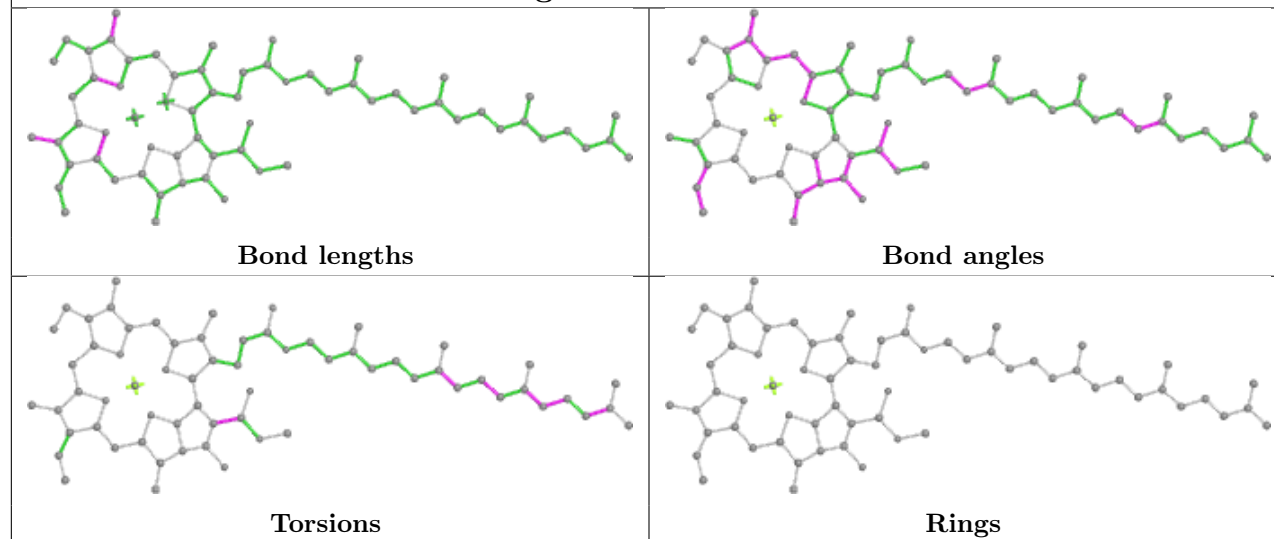




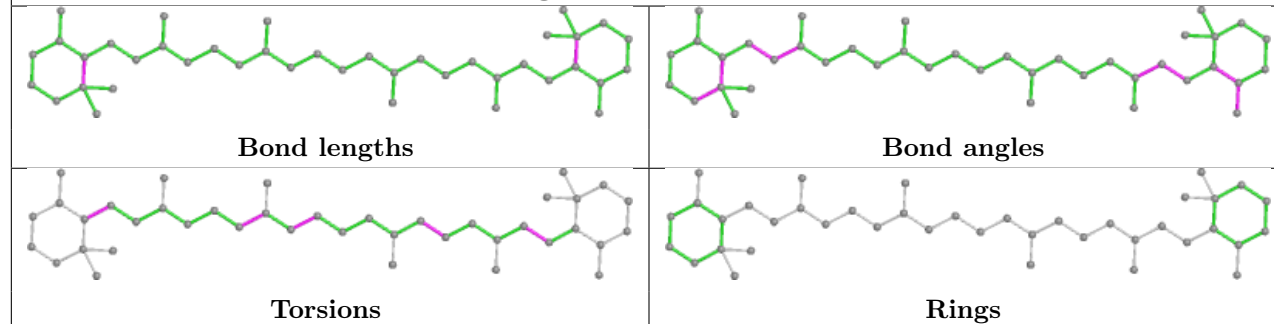




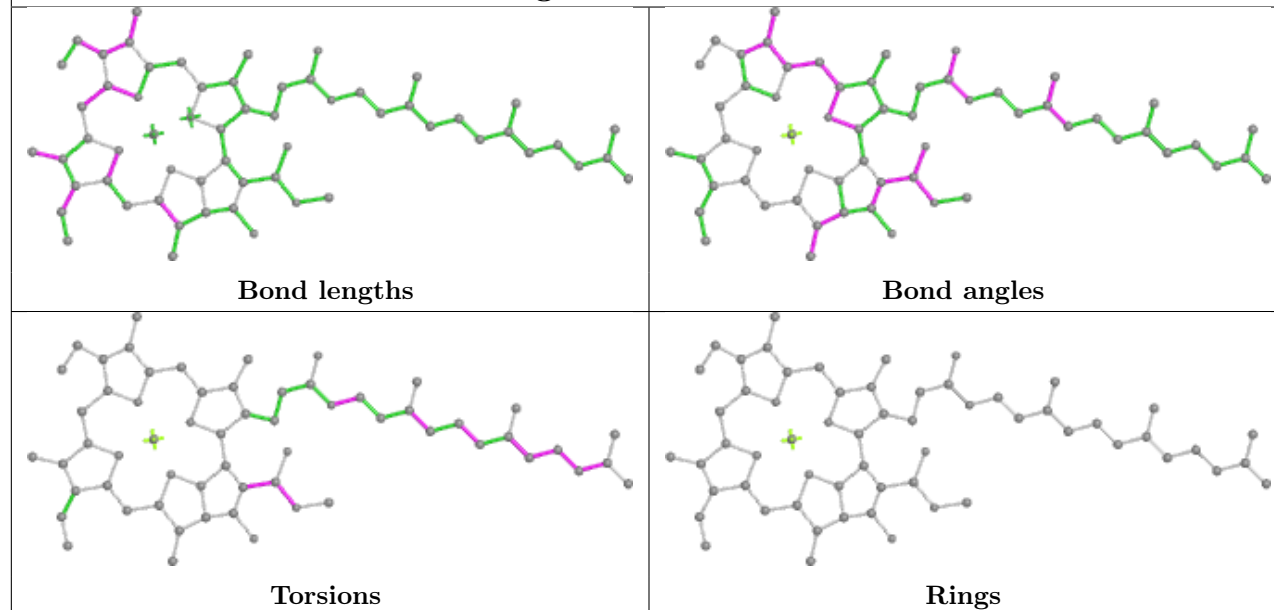
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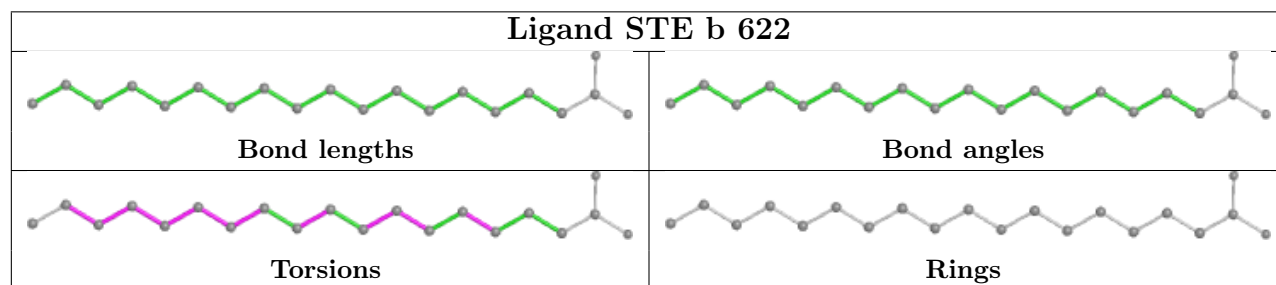
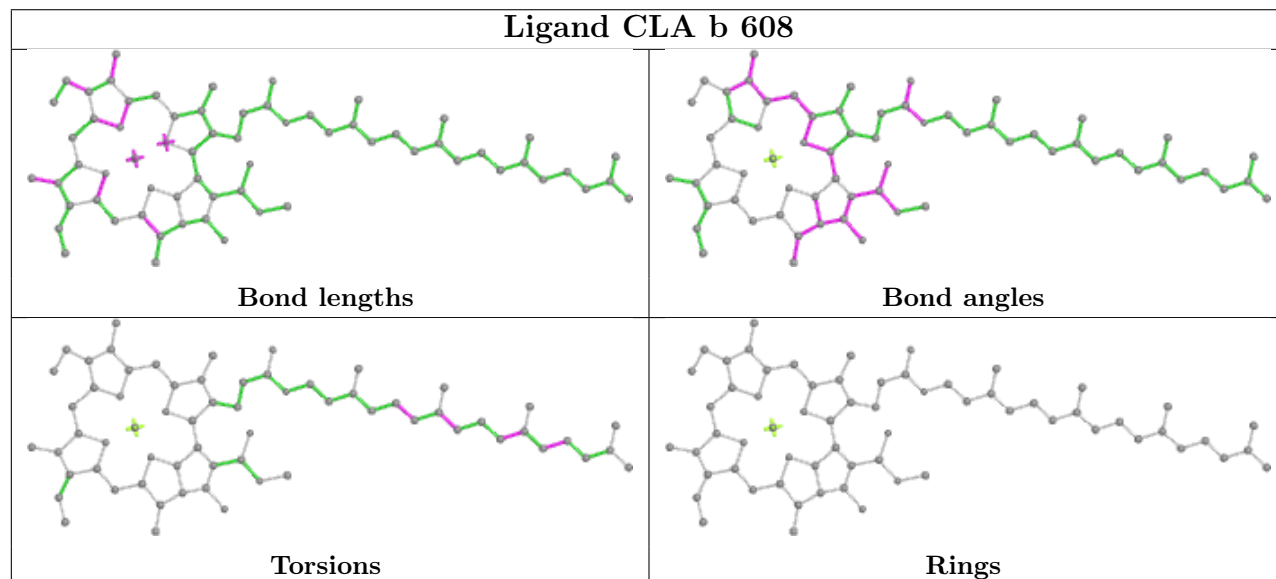
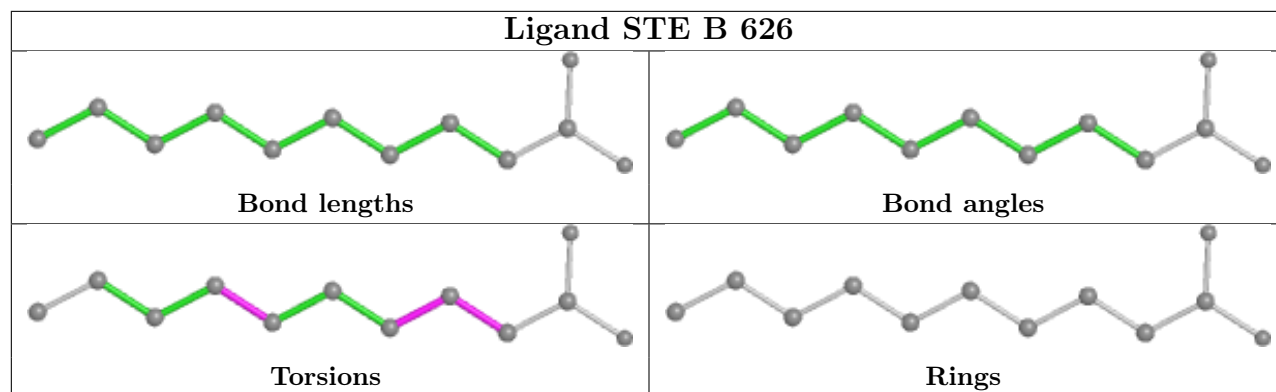


Ligand BCR c 514

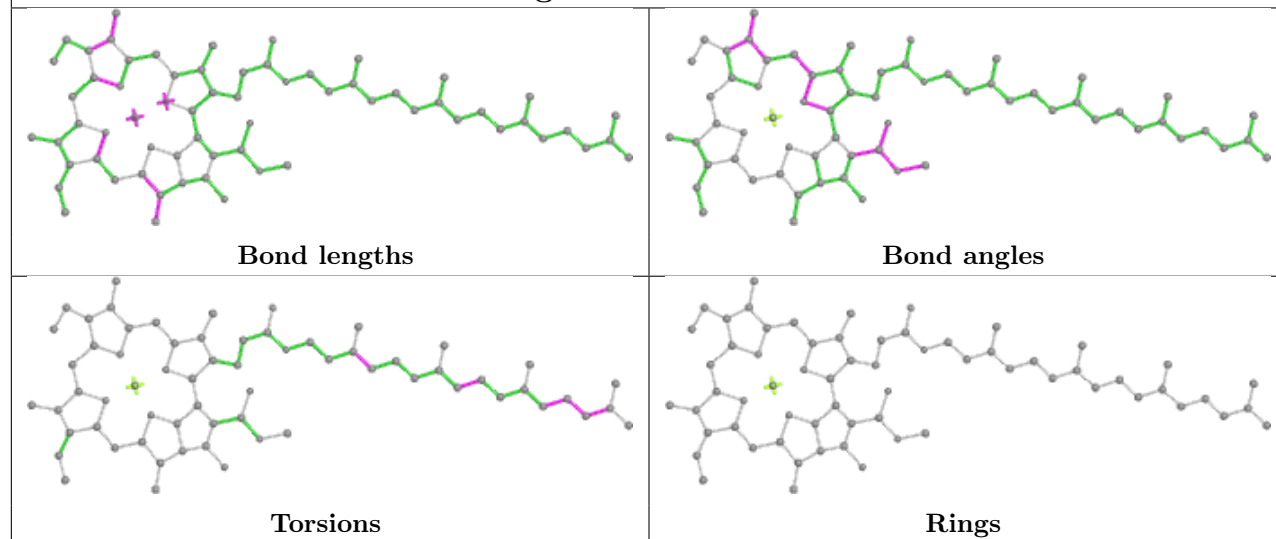


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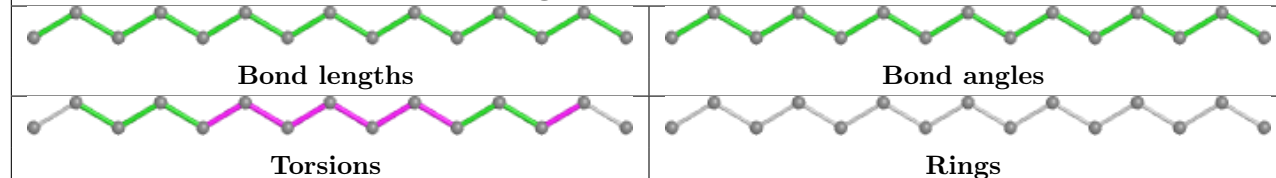




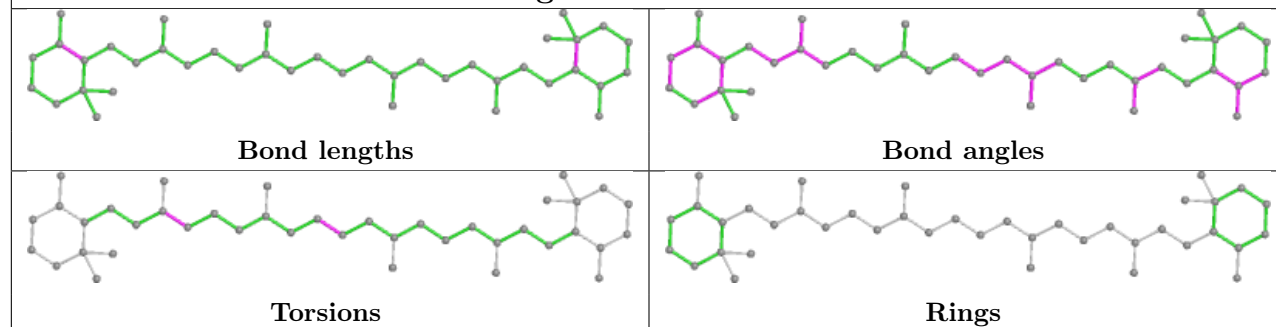
Ligand CLA b 611



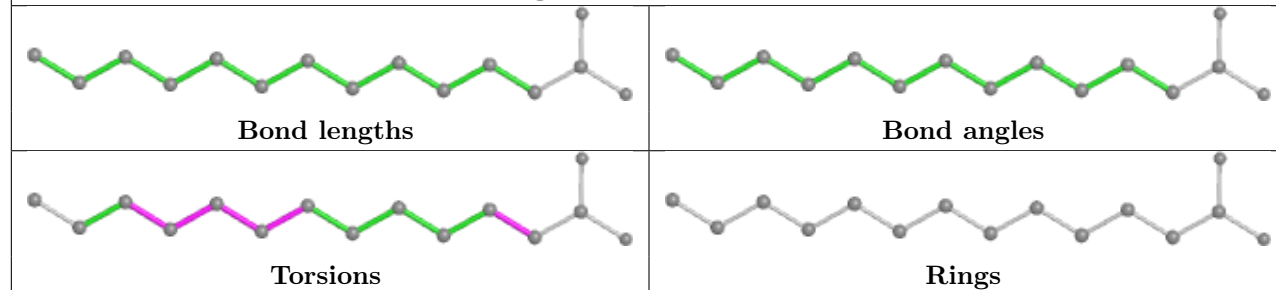
Ligand STE T 102

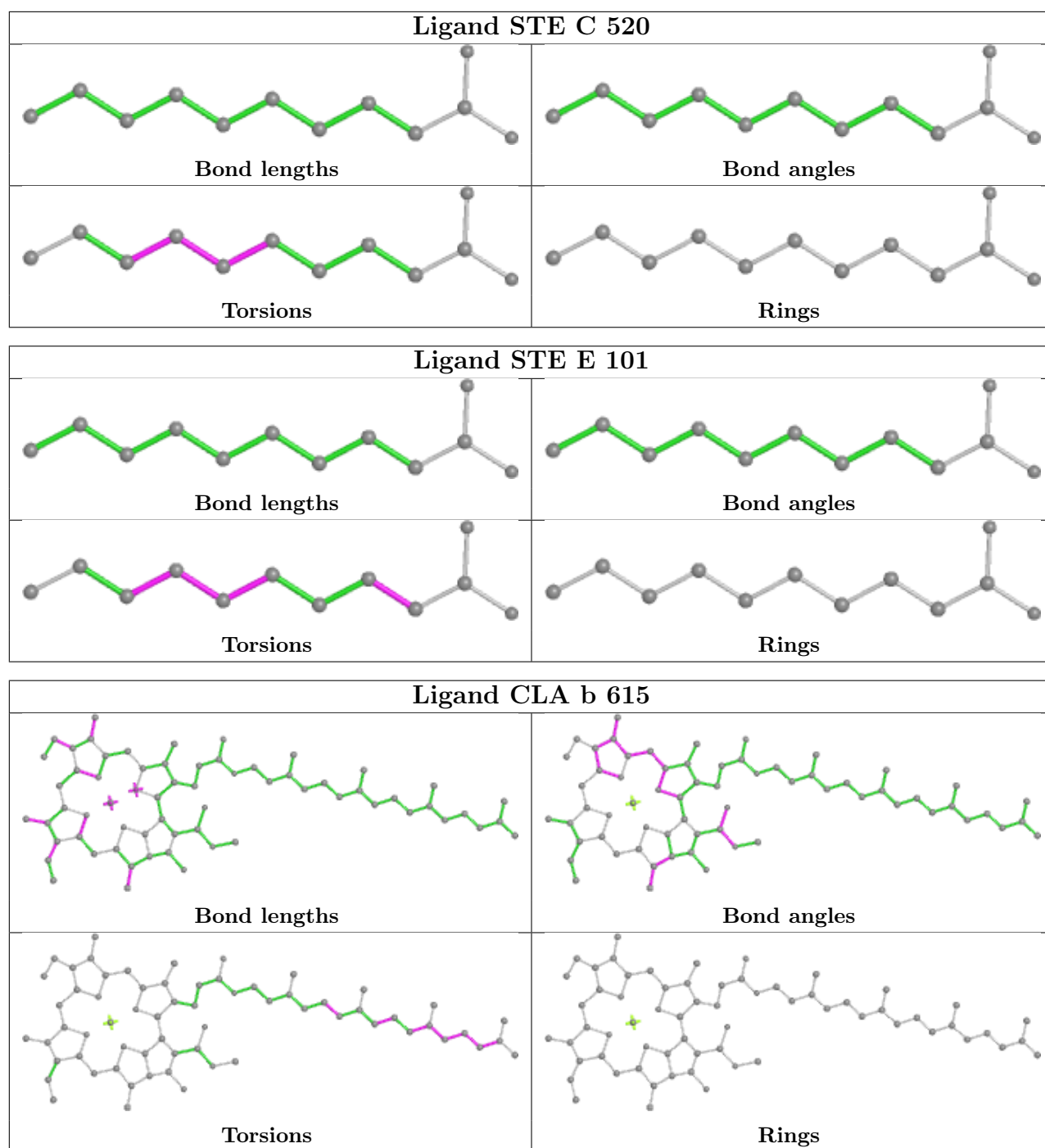


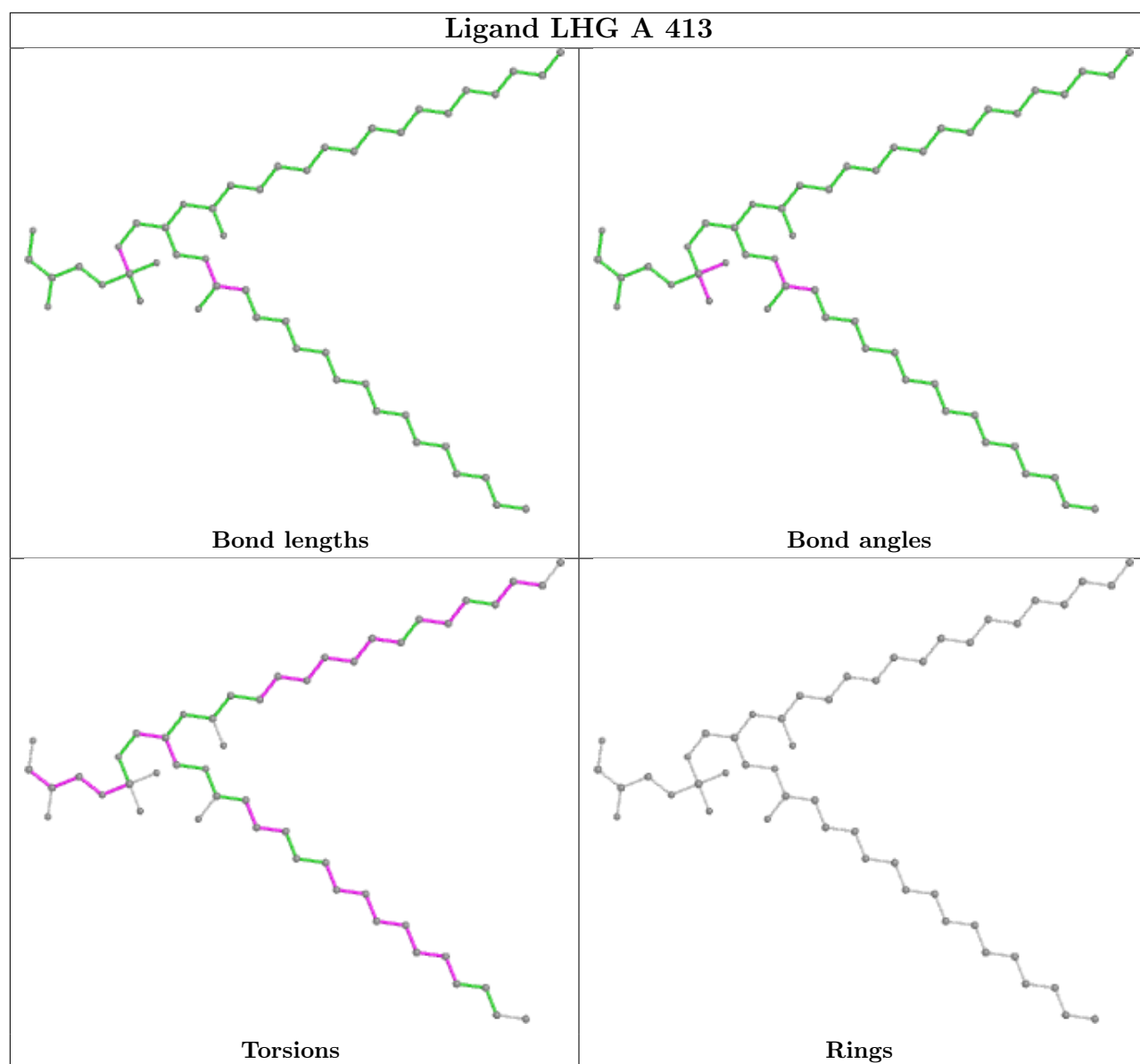
Ligand BCR t 101

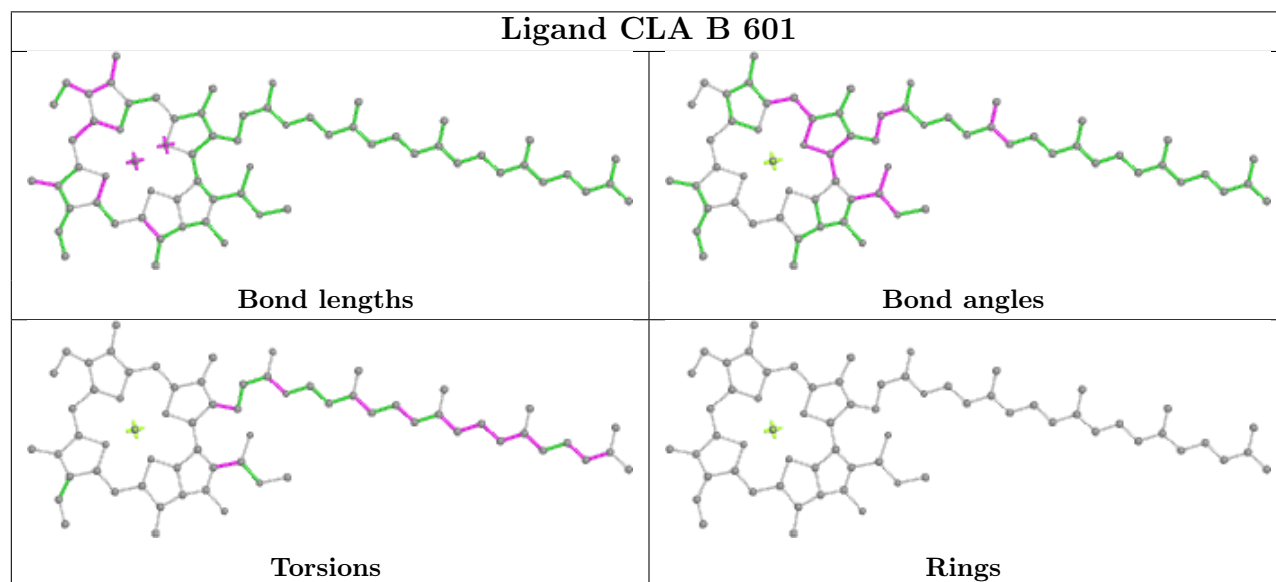
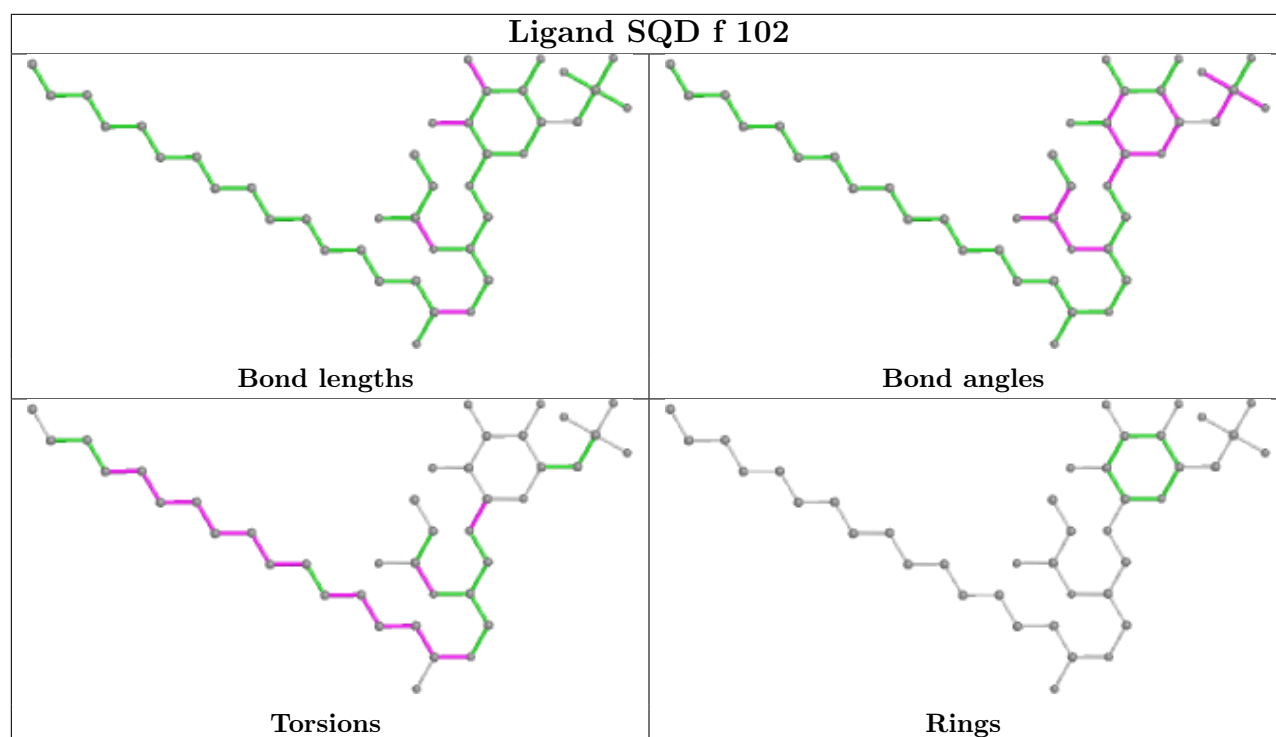


Ligand STE M 102

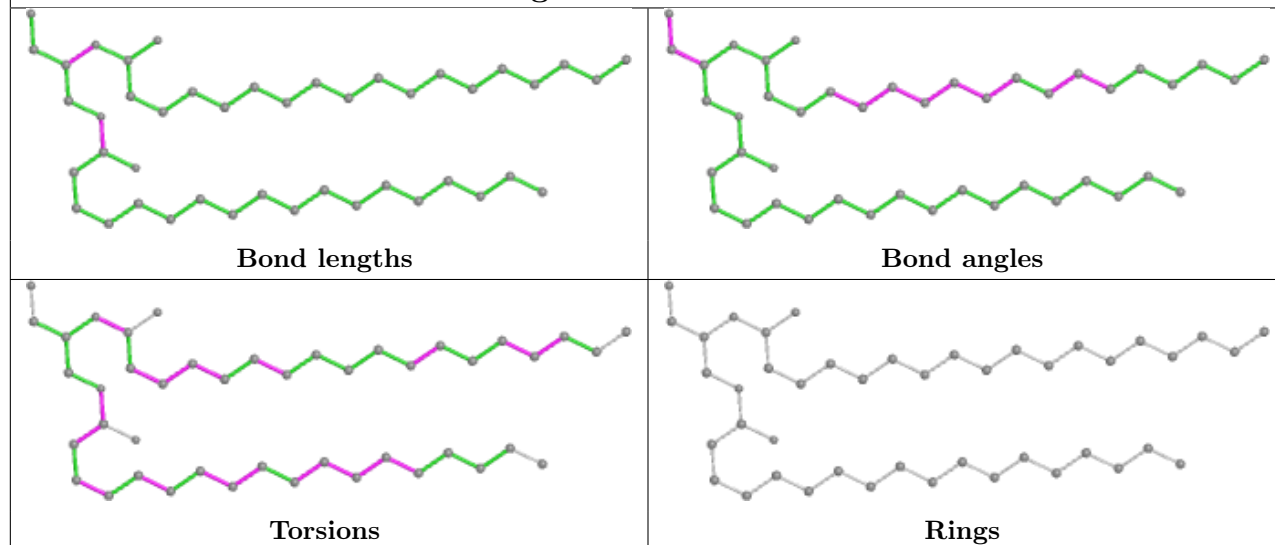




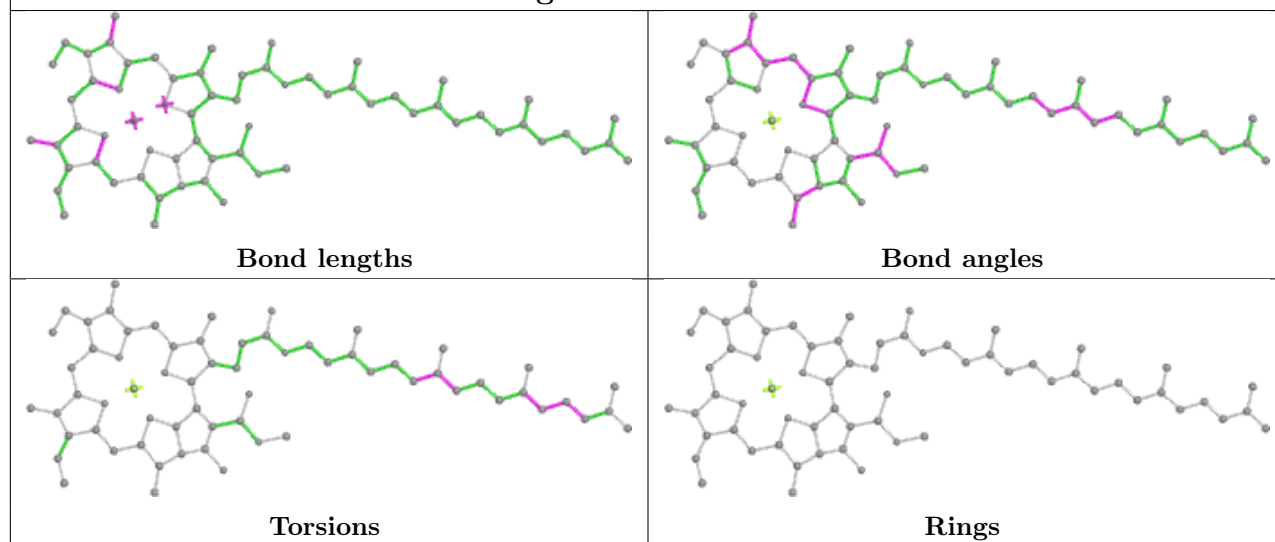




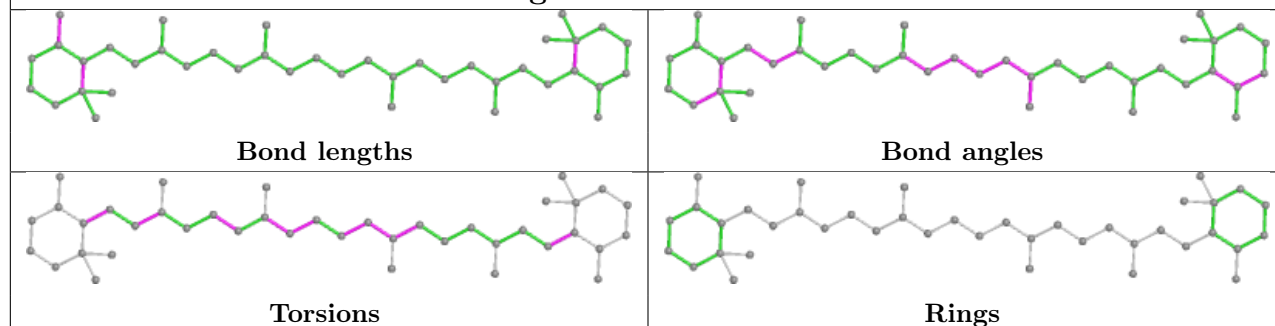
Ligand DGD o 301



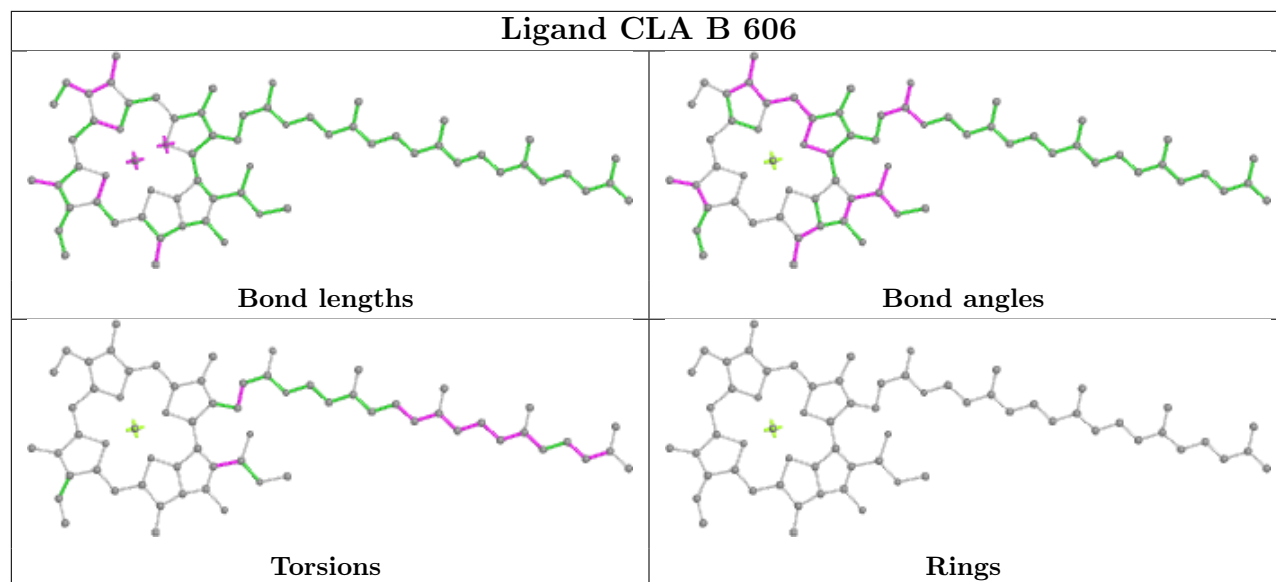
Ligand CLA c 505



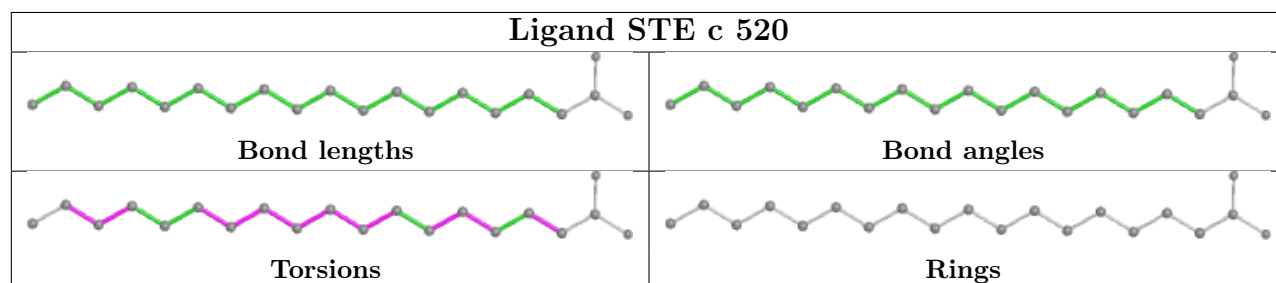
Ligand BCR C 514



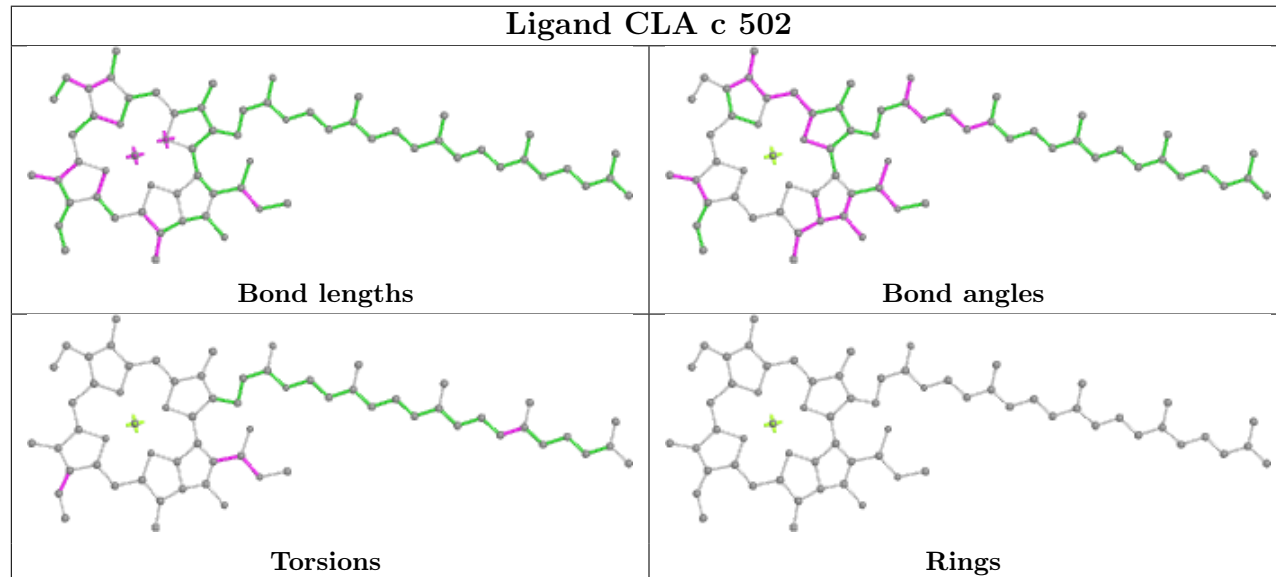
Ligand CLA B 606

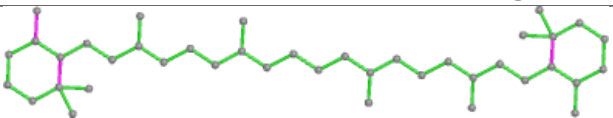
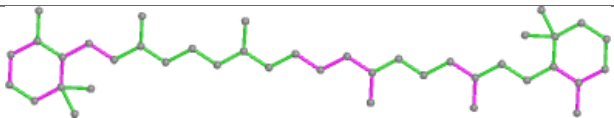
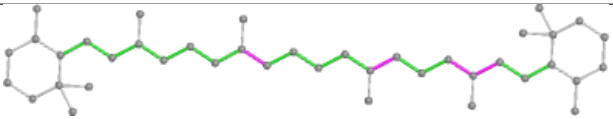
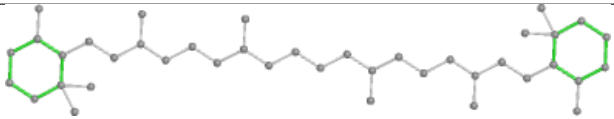


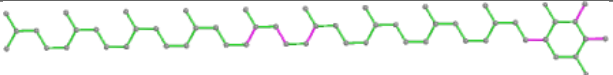
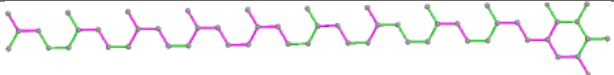
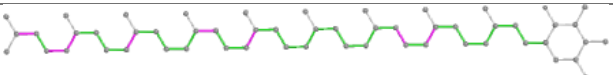
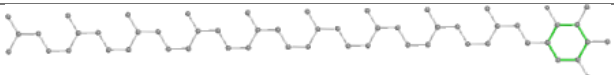
Ligand STE c 520

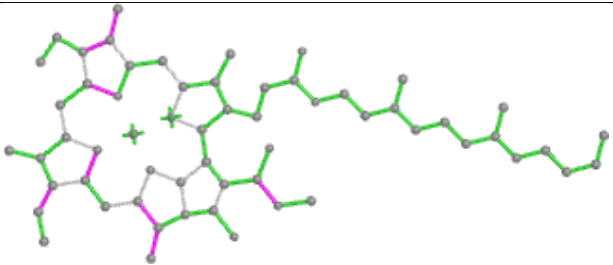
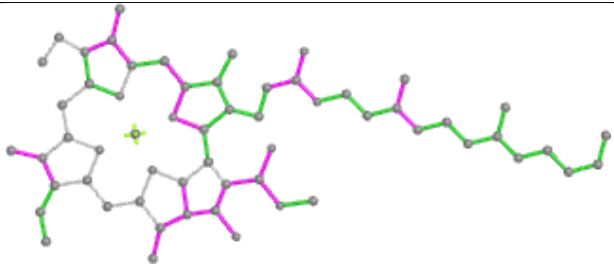
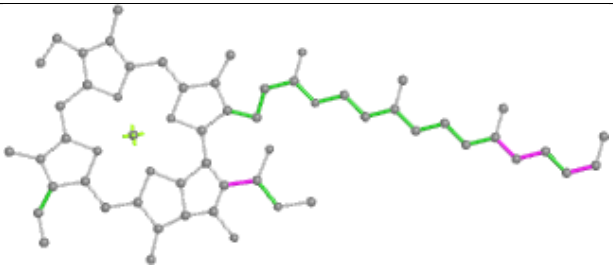
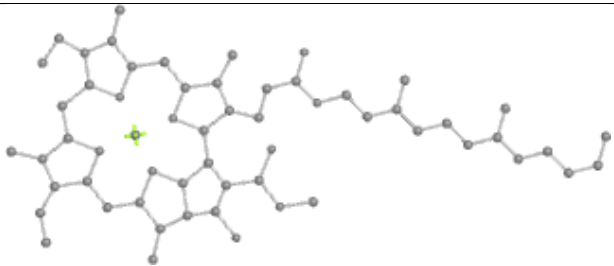


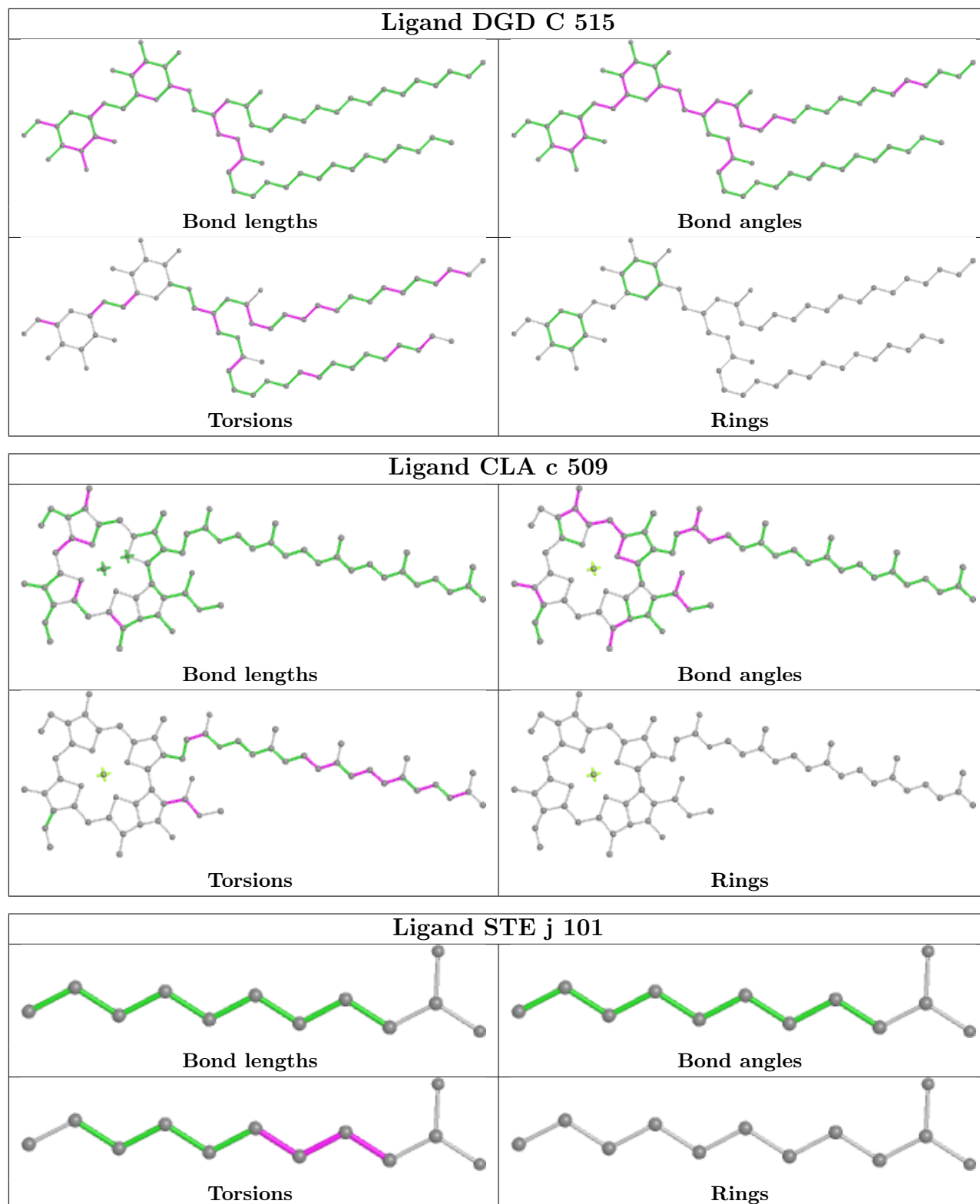
Ligand CLA c 502



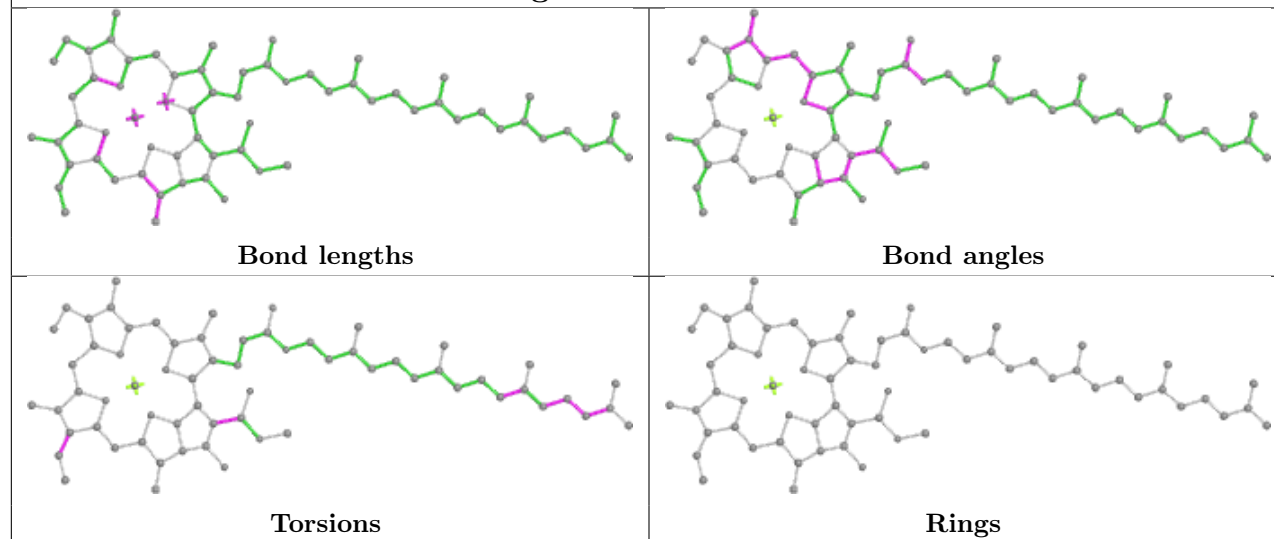
Ligand BCR b 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 D 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

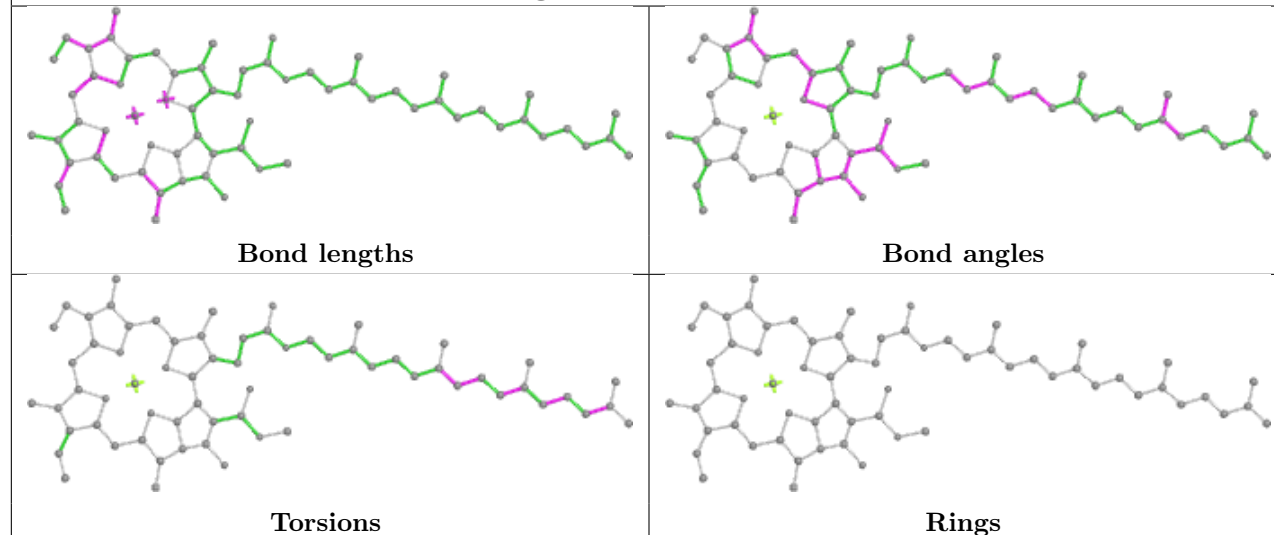
Ligand CLA C 504	
	
Bond lengths	Bond angles
	
Torsions	Rings



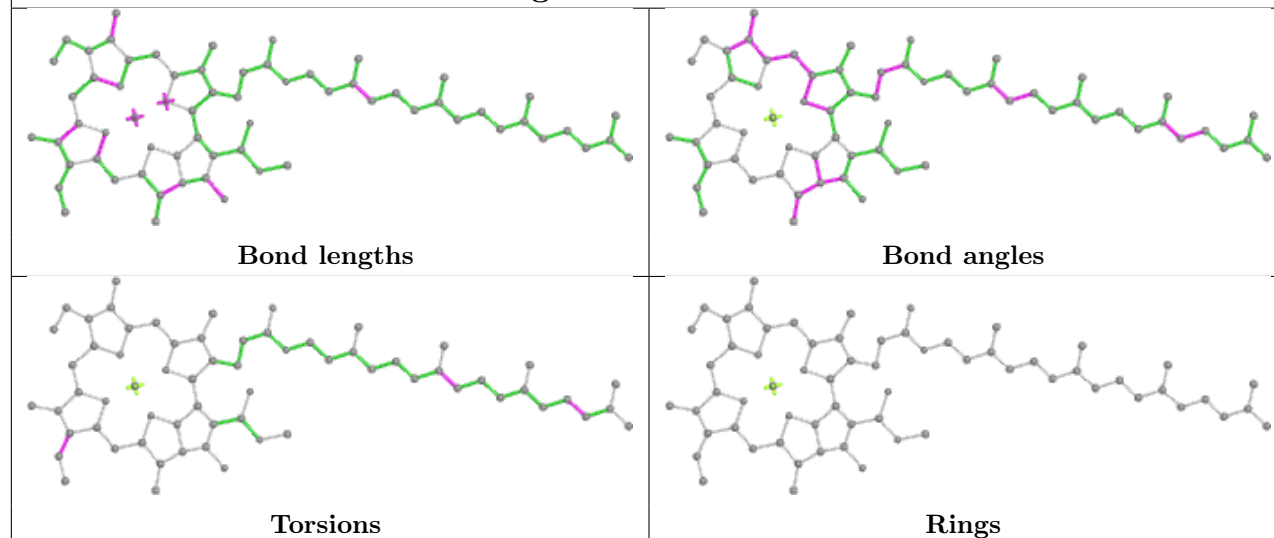
Ligand CLA D 403

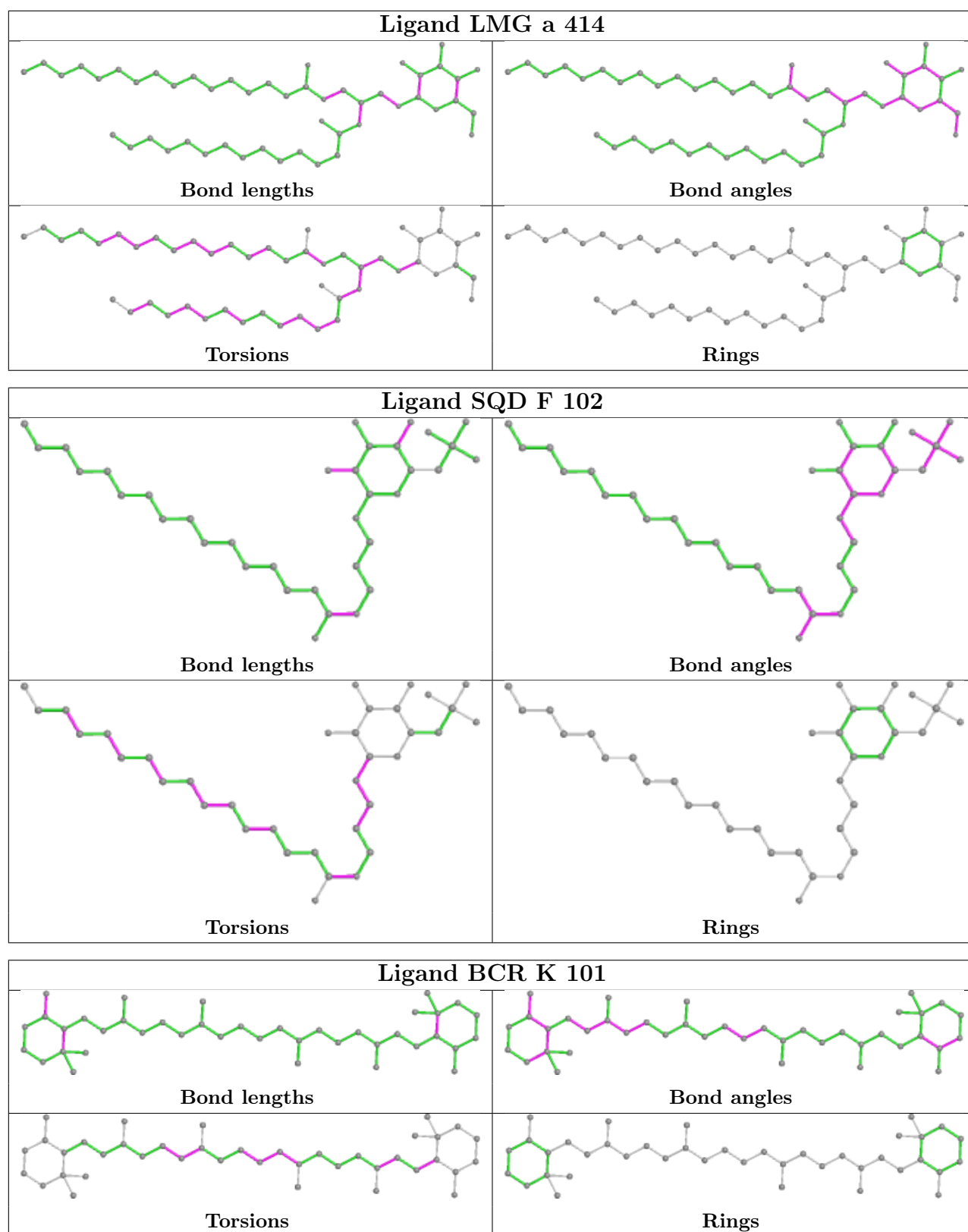


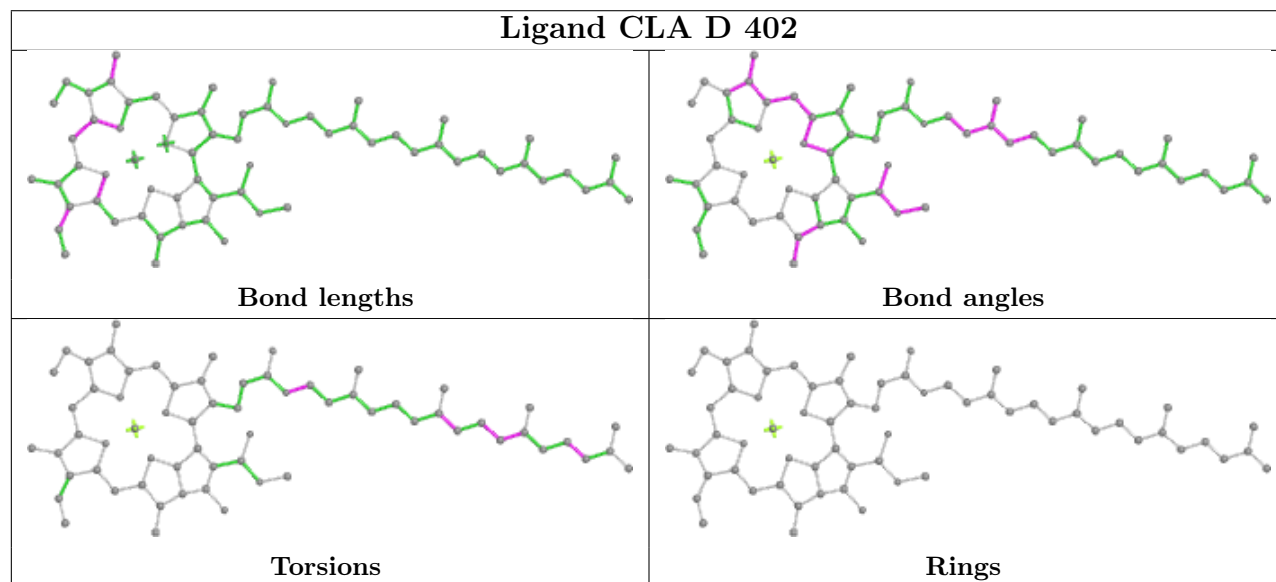
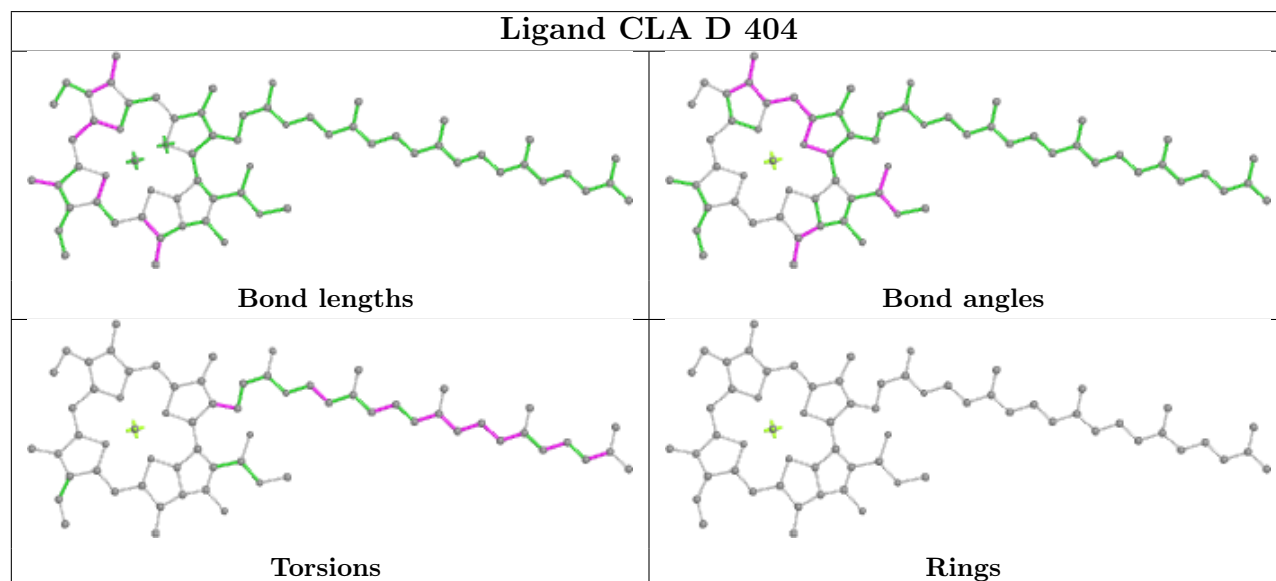
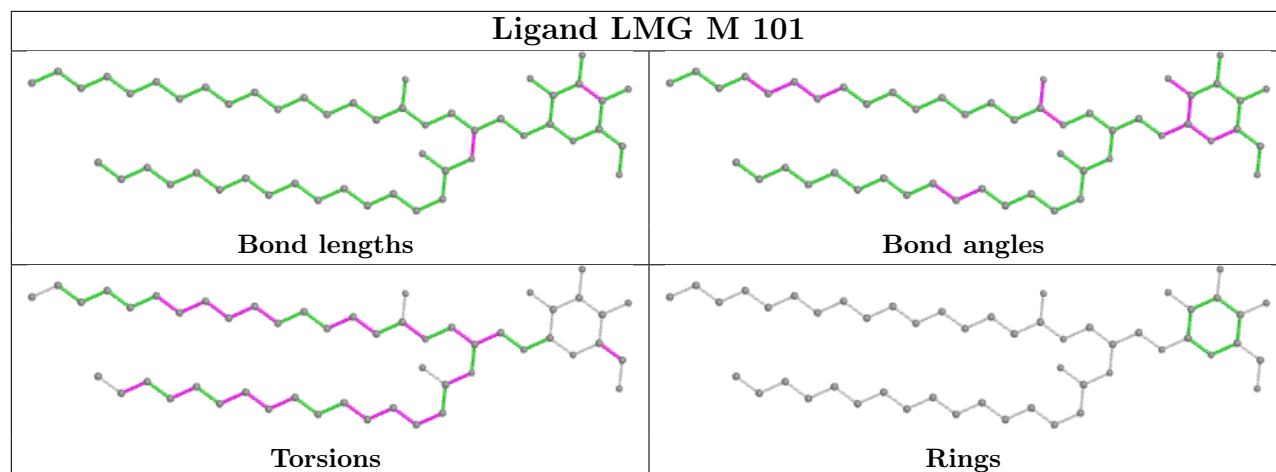
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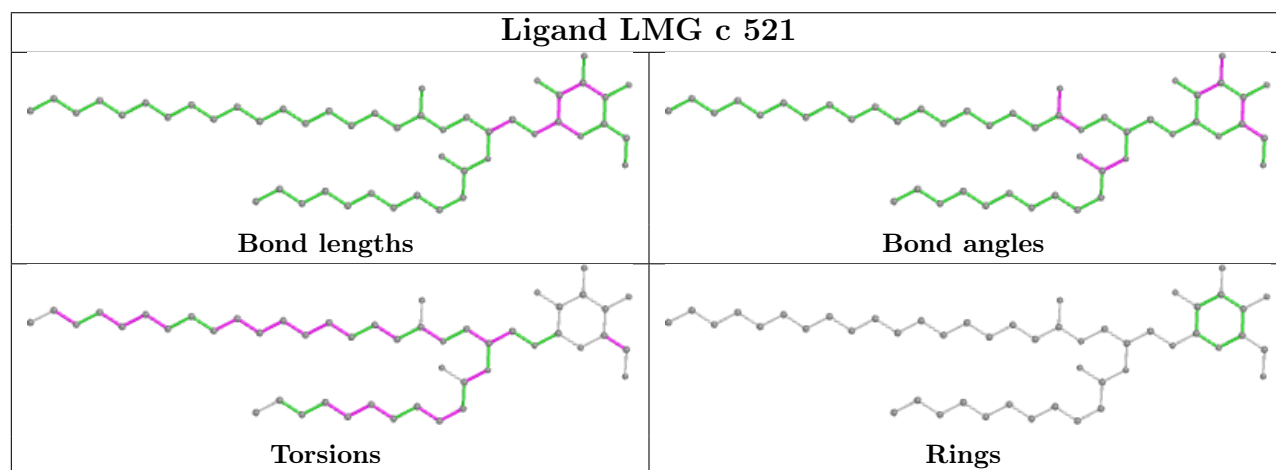
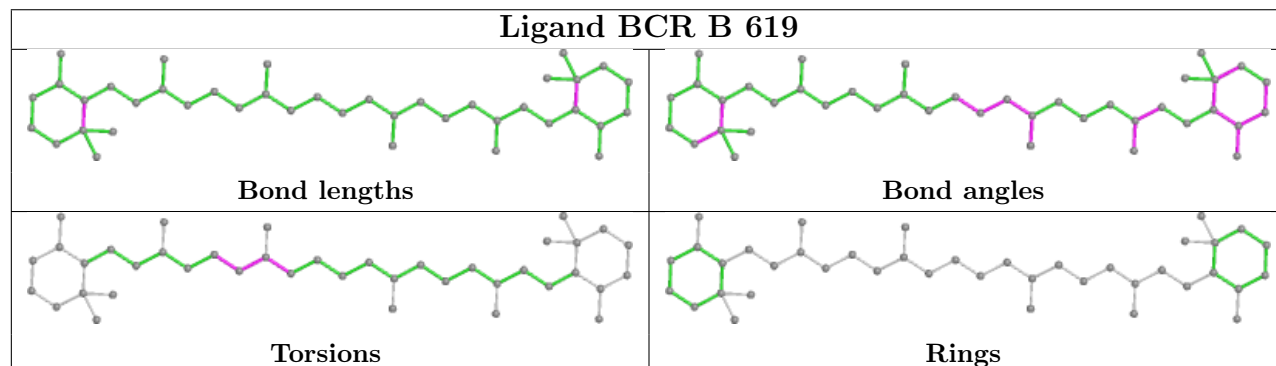
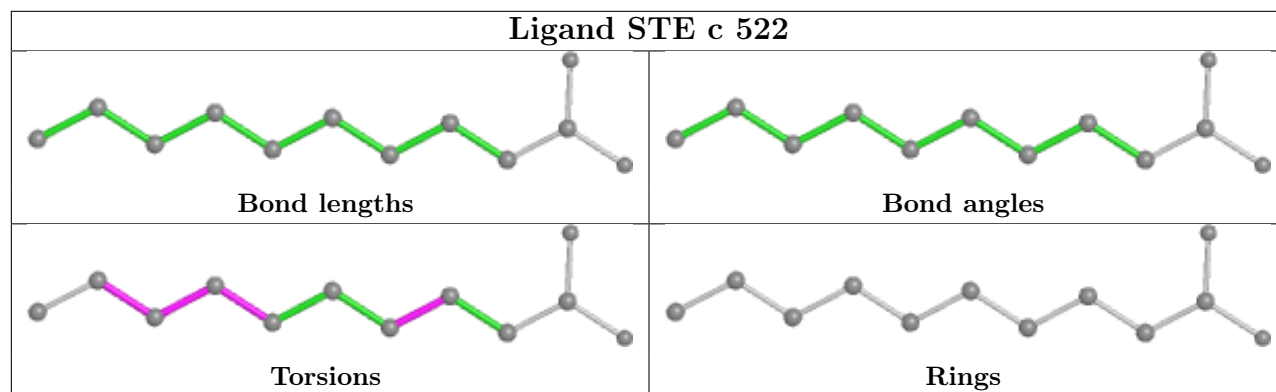


Ligand CLA A 402

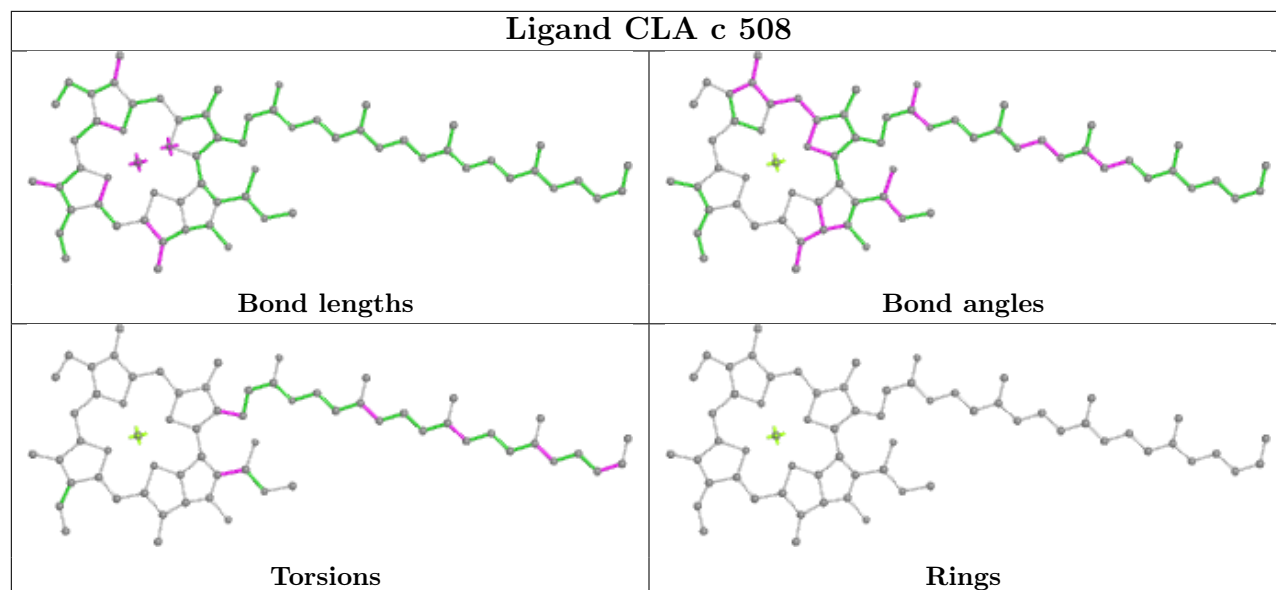




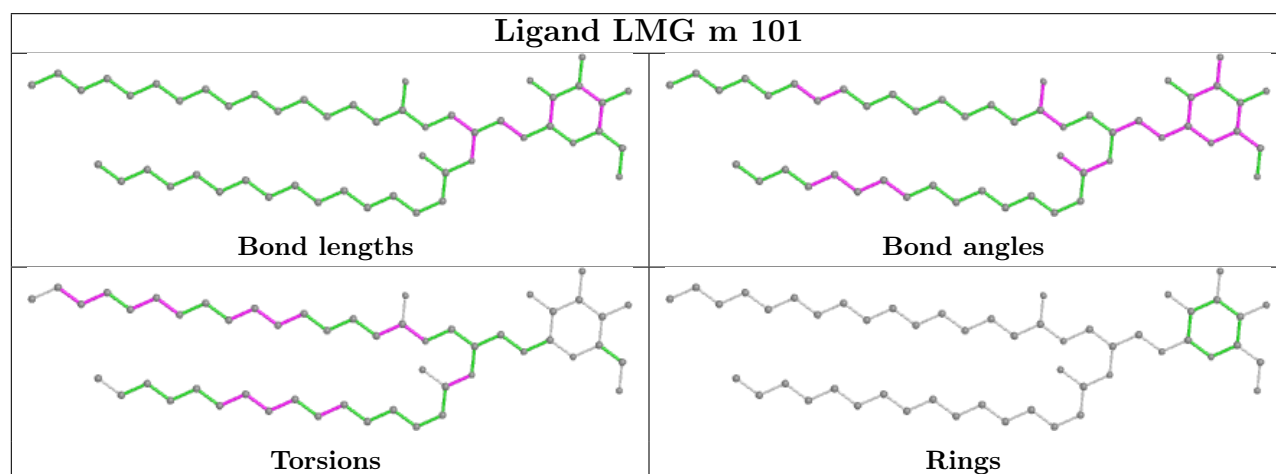




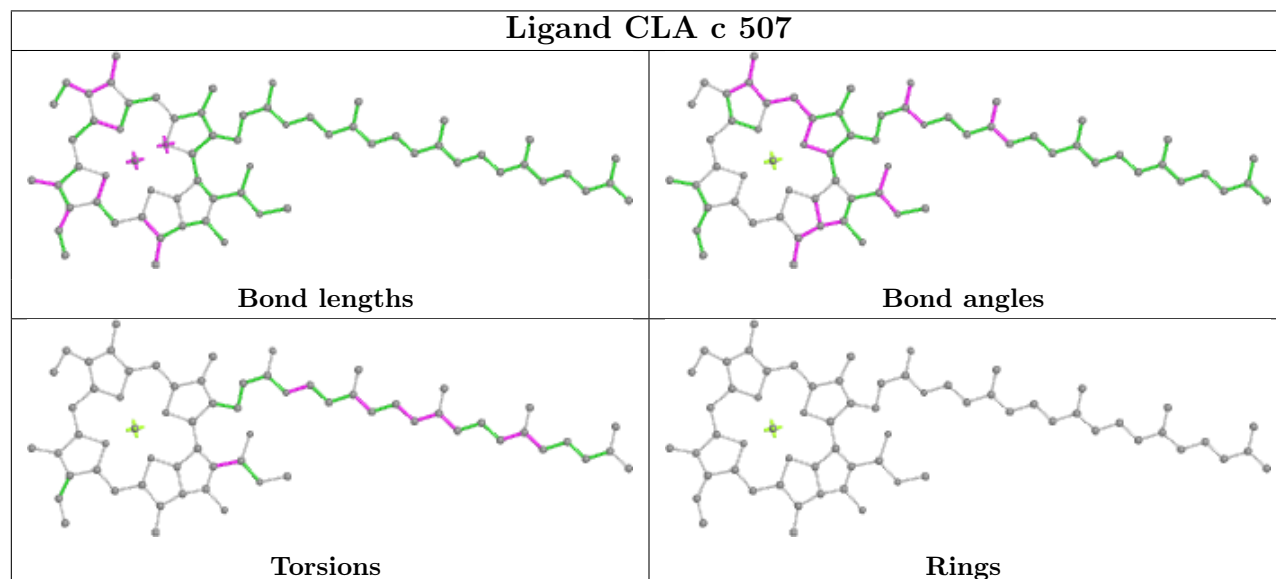
Ligand CLA c 508

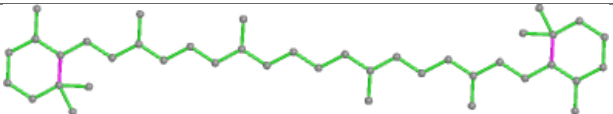
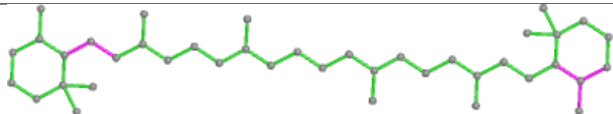
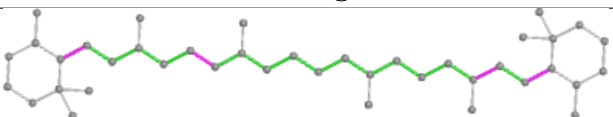
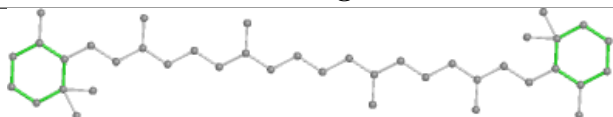


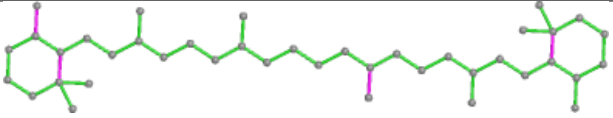
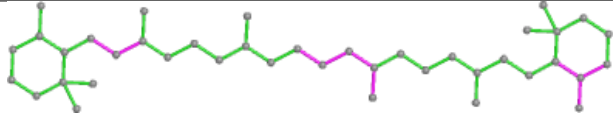
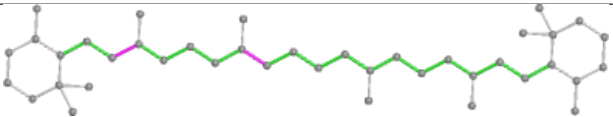
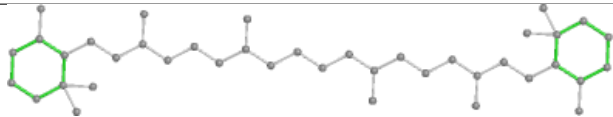
Ligand LMG m 101

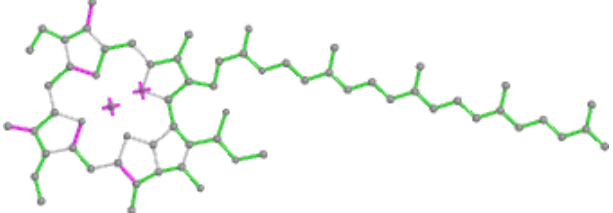
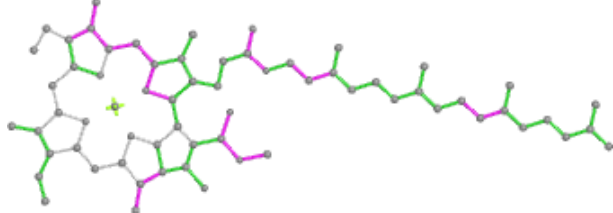
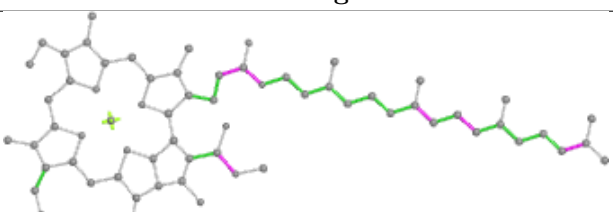
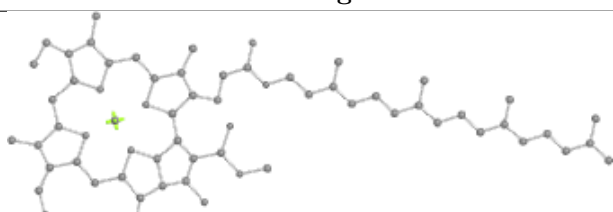


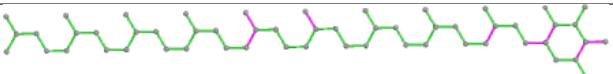
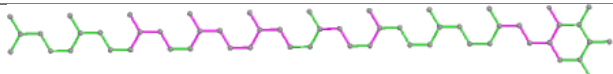
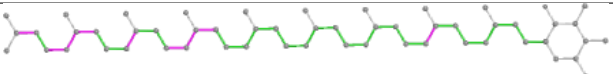
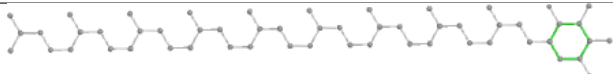
Ligand CLA c 507

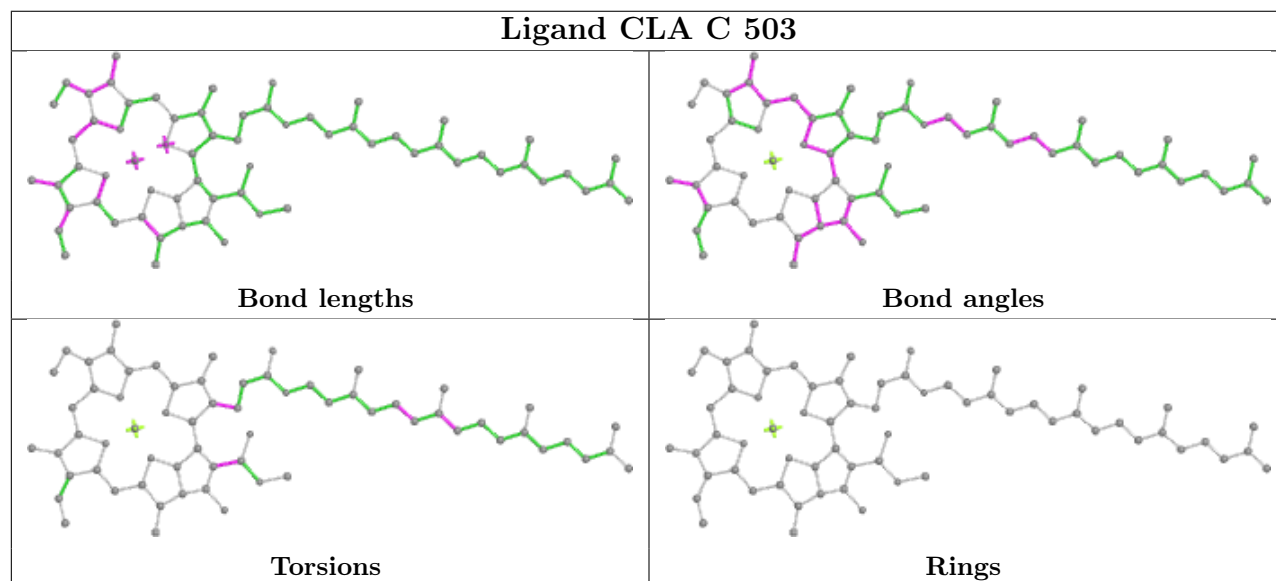
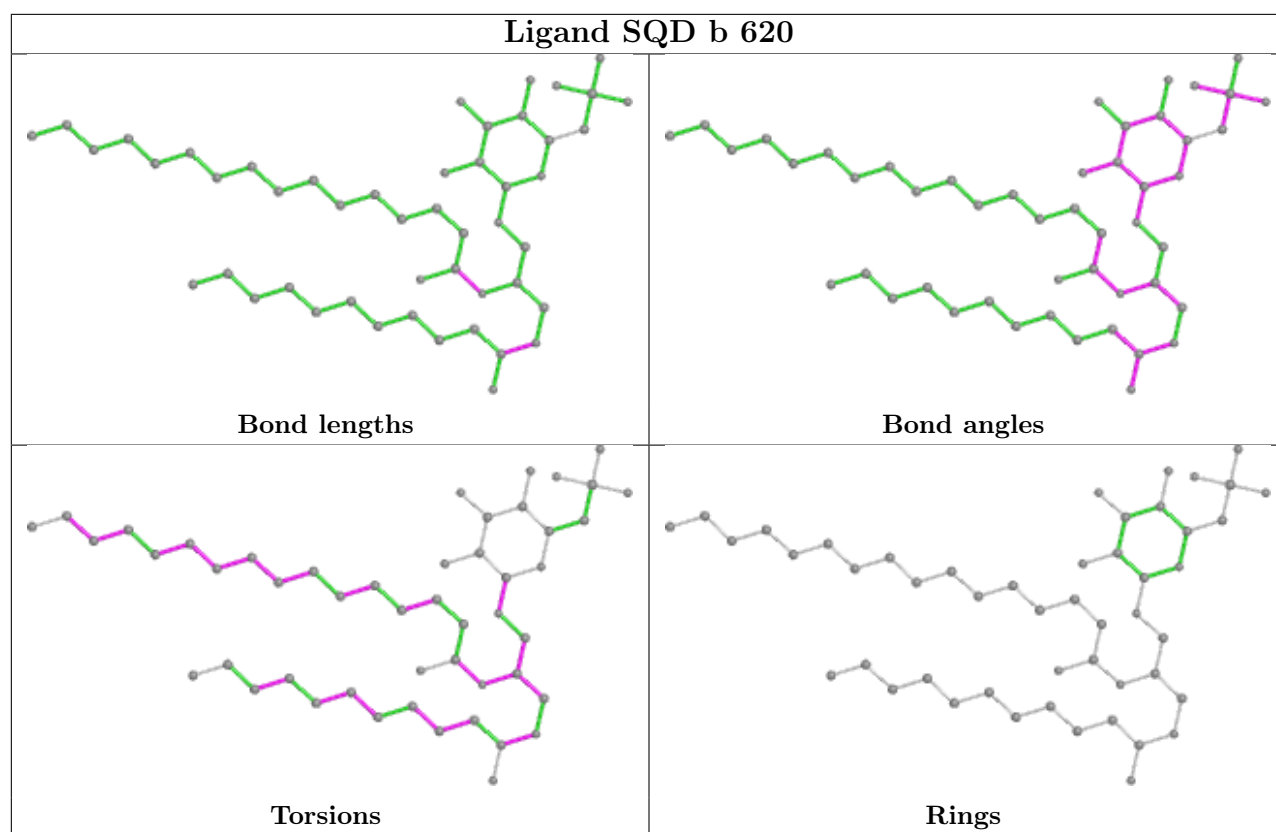


Ligand BCR K 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

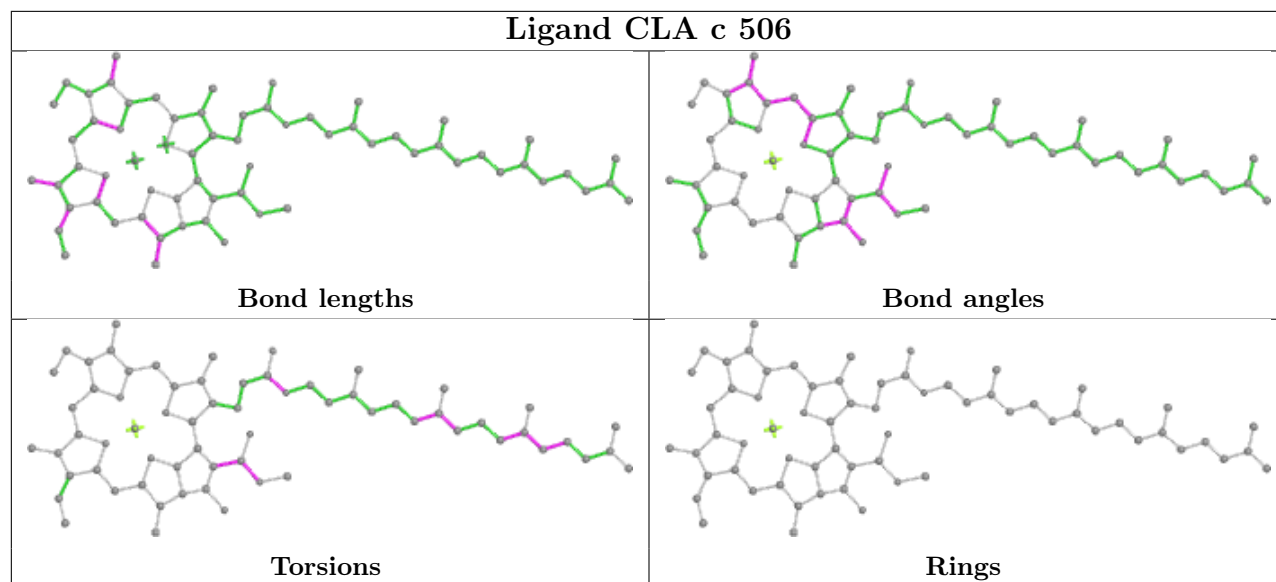
Ligand BCR c 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

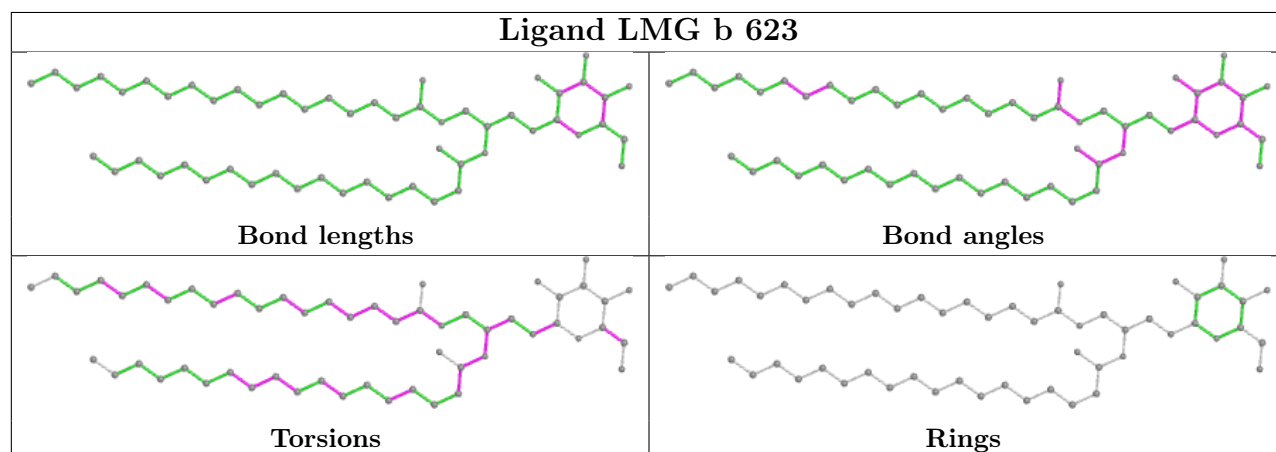
Ligand PL9 d 407	
	
Bond lengths	Bond angles
	
Torsions	Rings



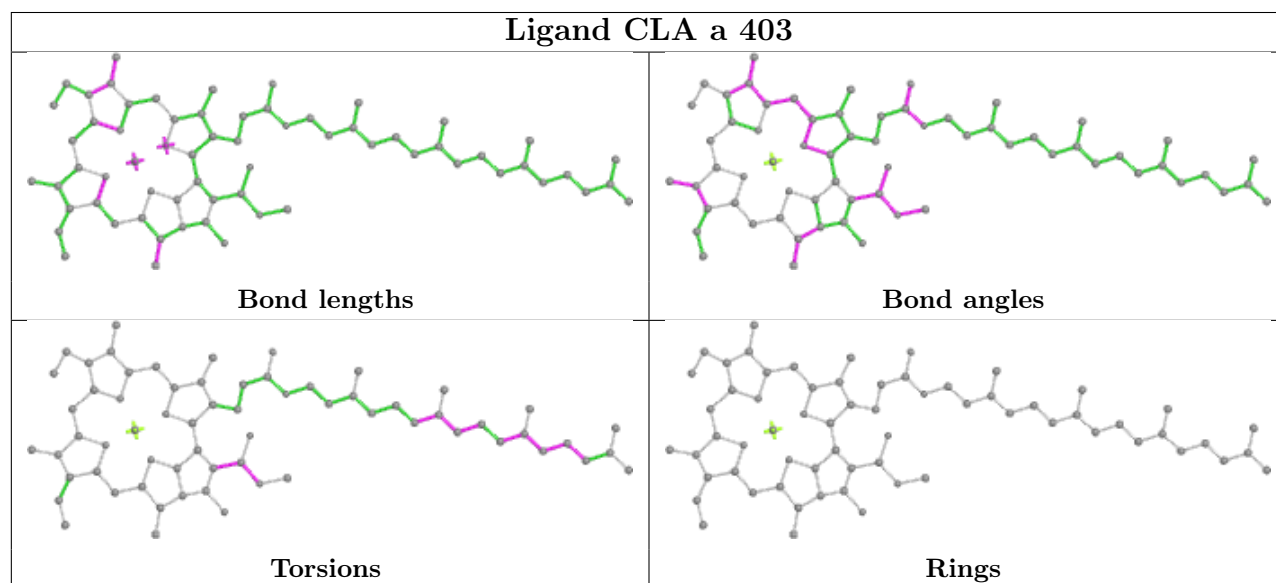
Ligand CLA c 506

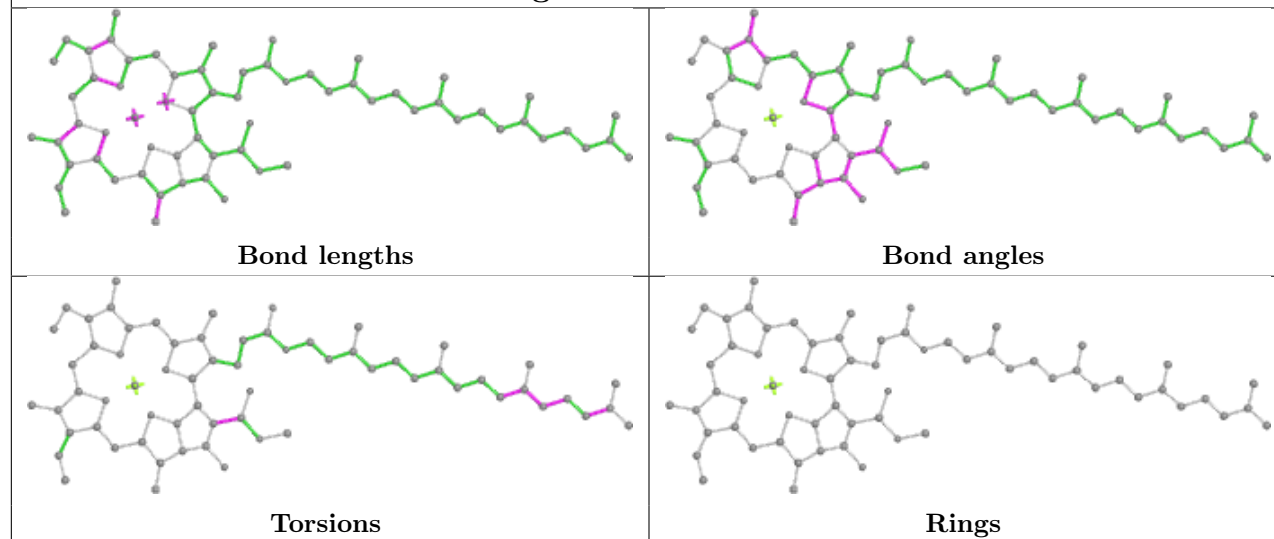
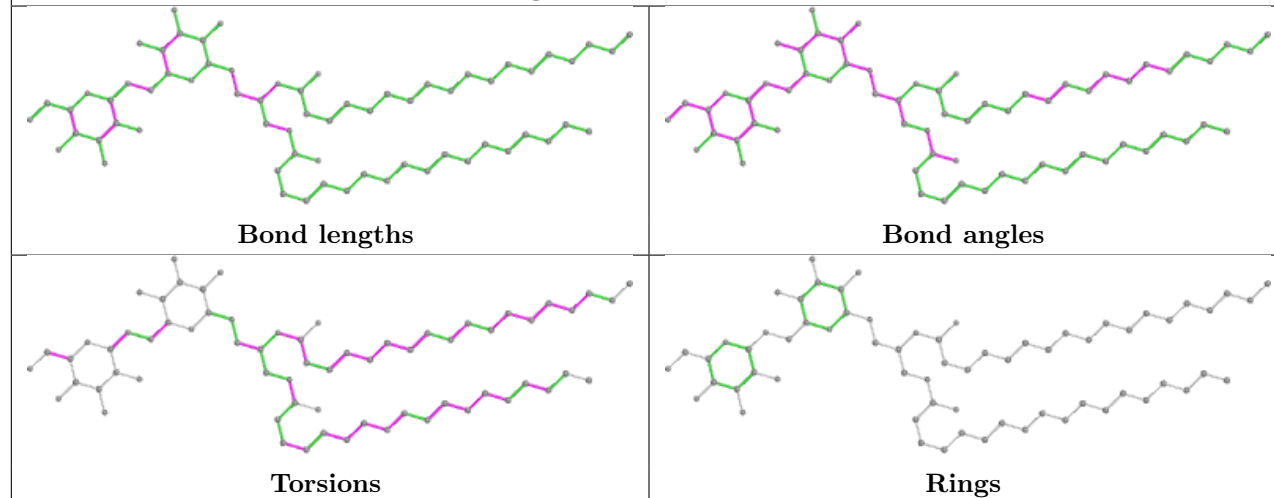
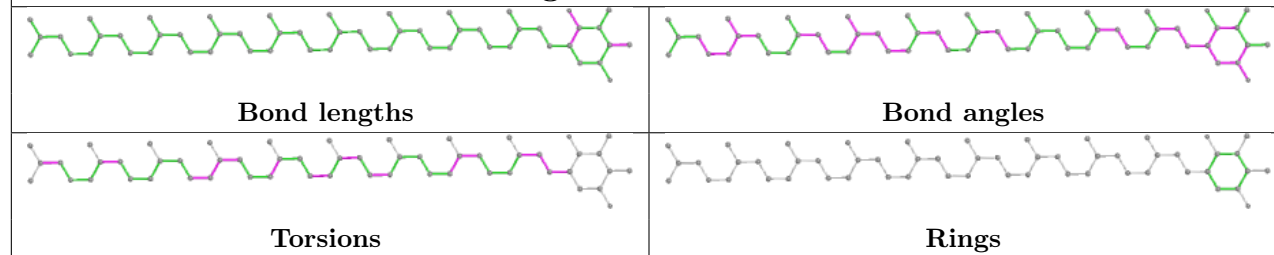


Ligand LMG b 623

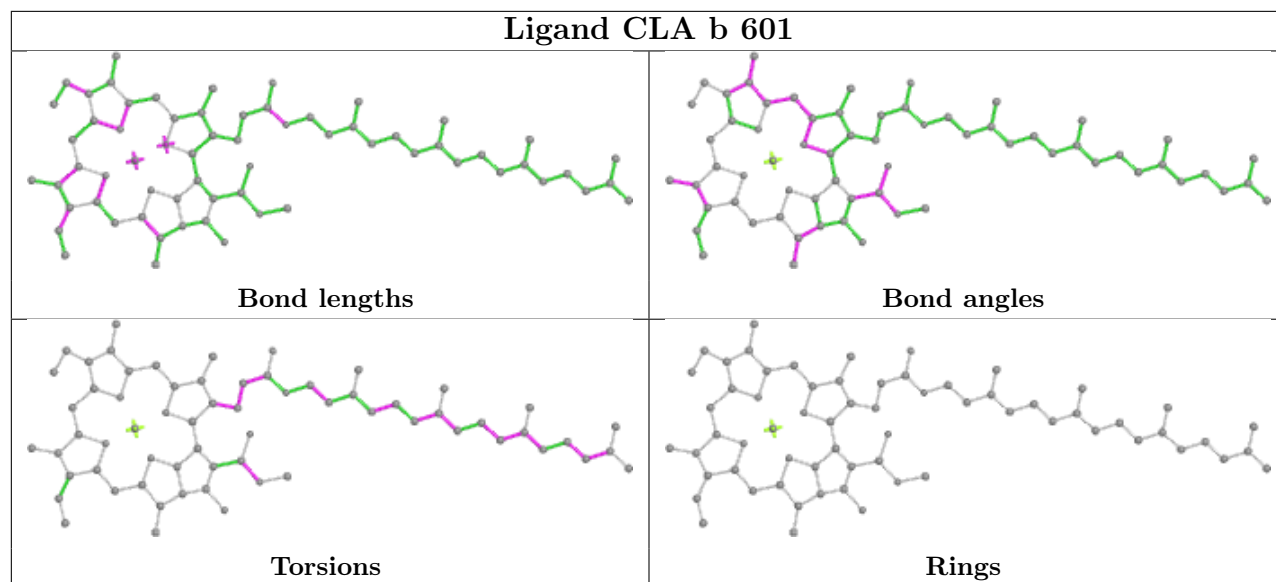


Ligand CLA a 403

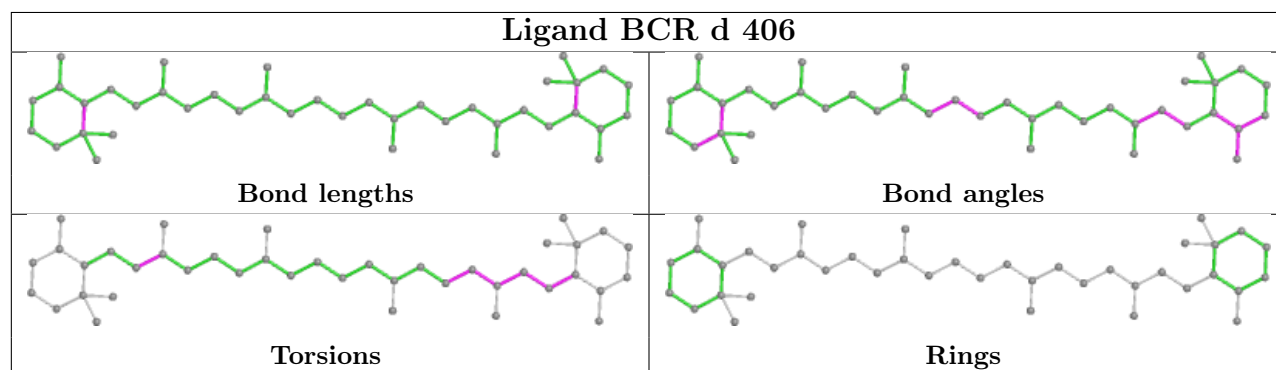


Ligand CLA C 502**Ligand DGD A 415****Ligand PL9 a 409**

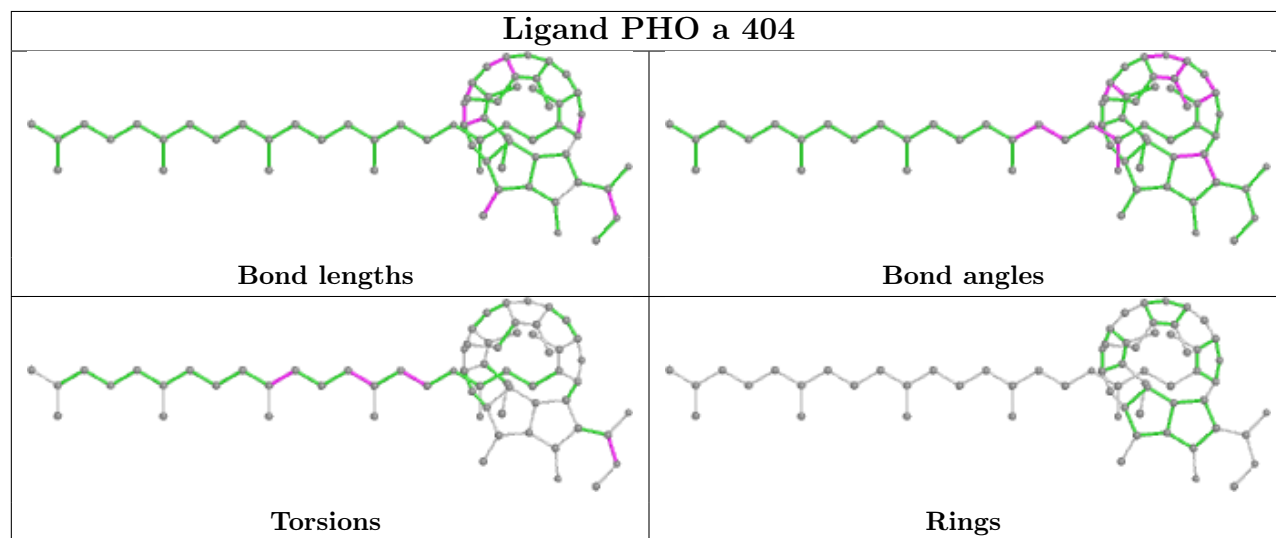
Ligand CLA b 601

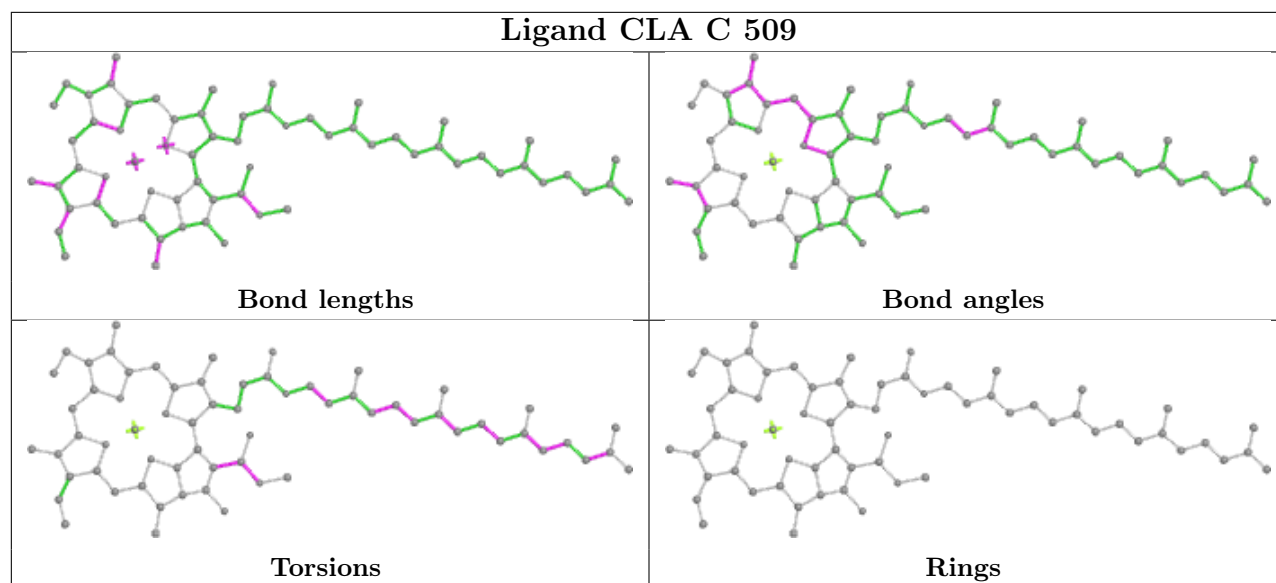
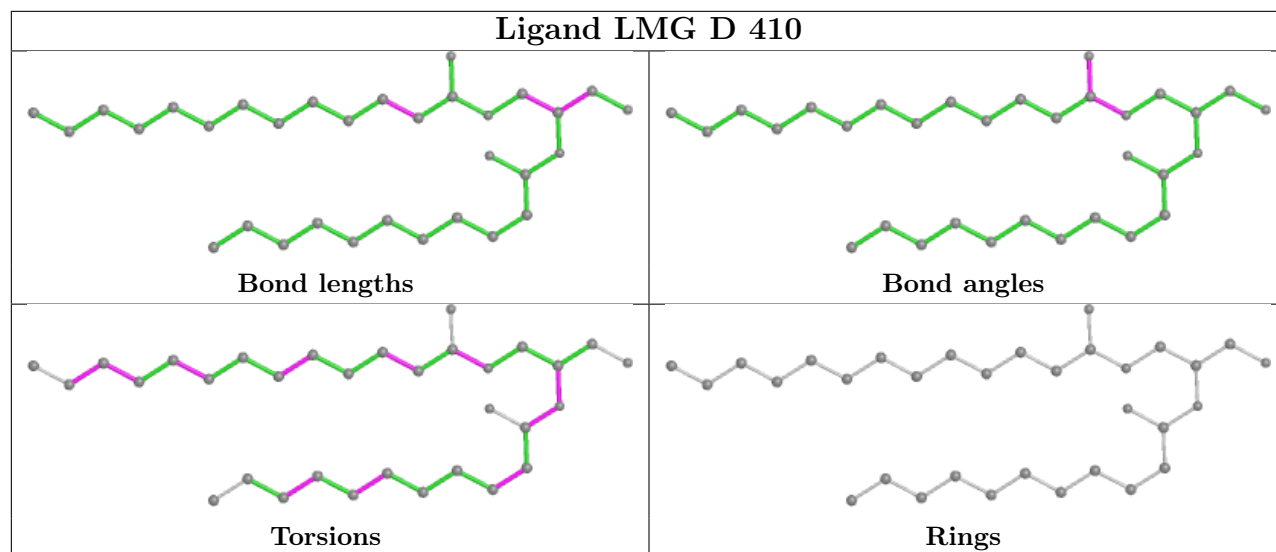
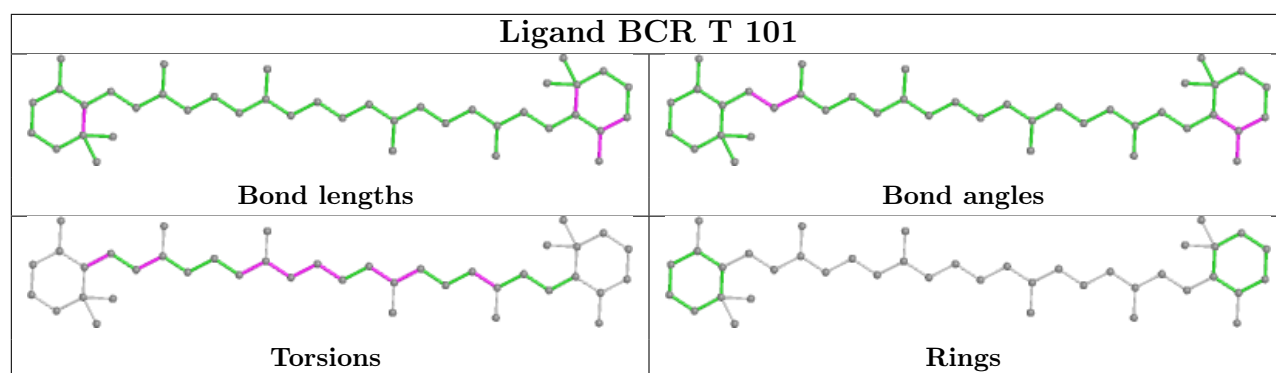


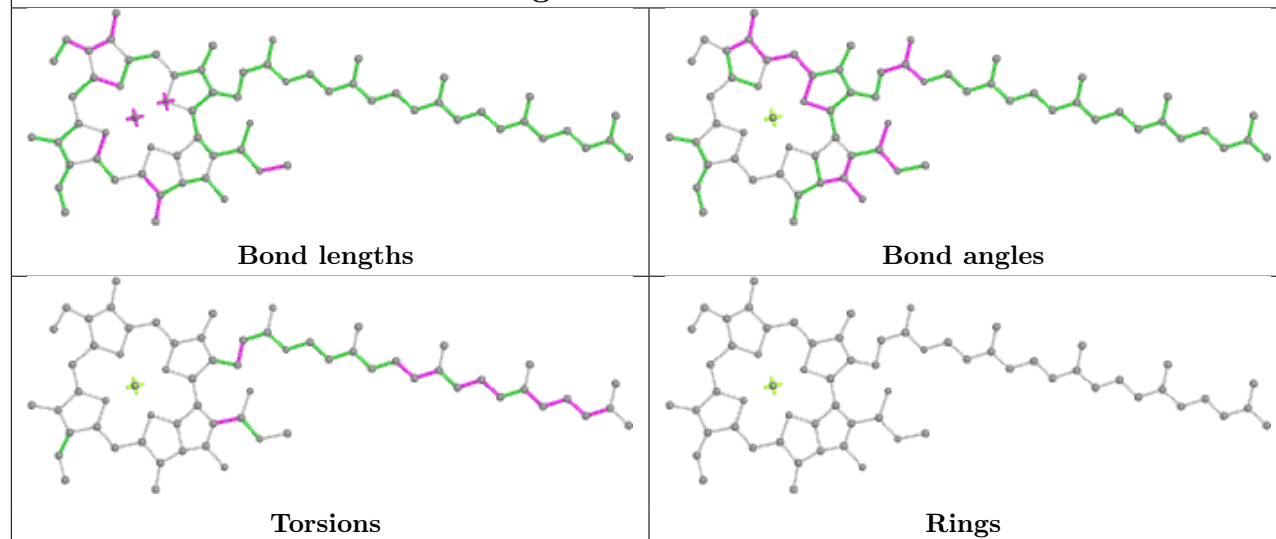
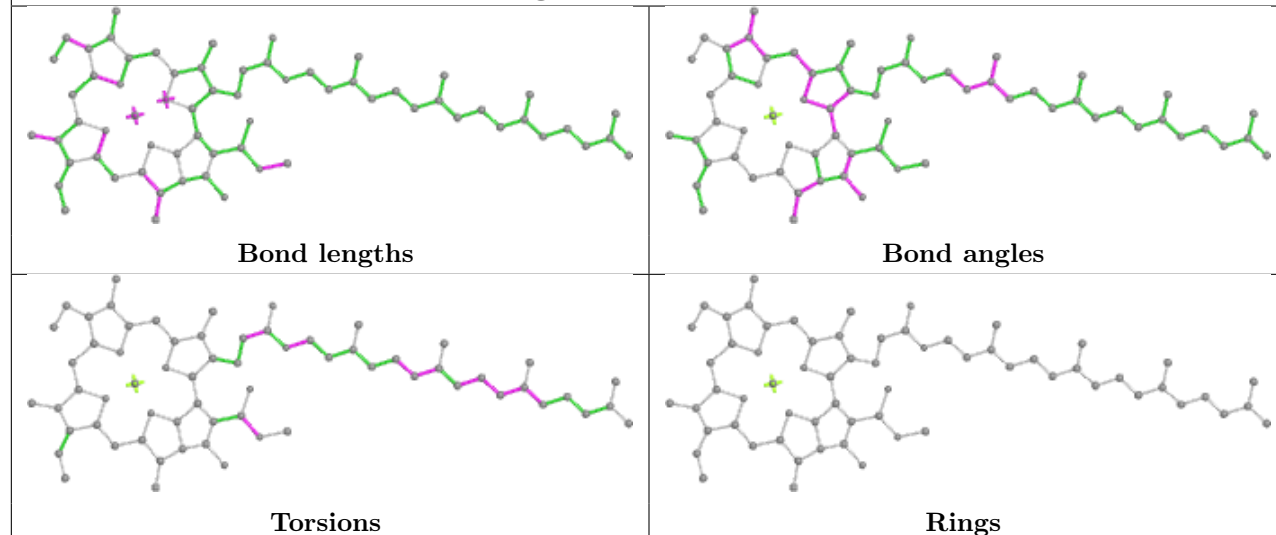
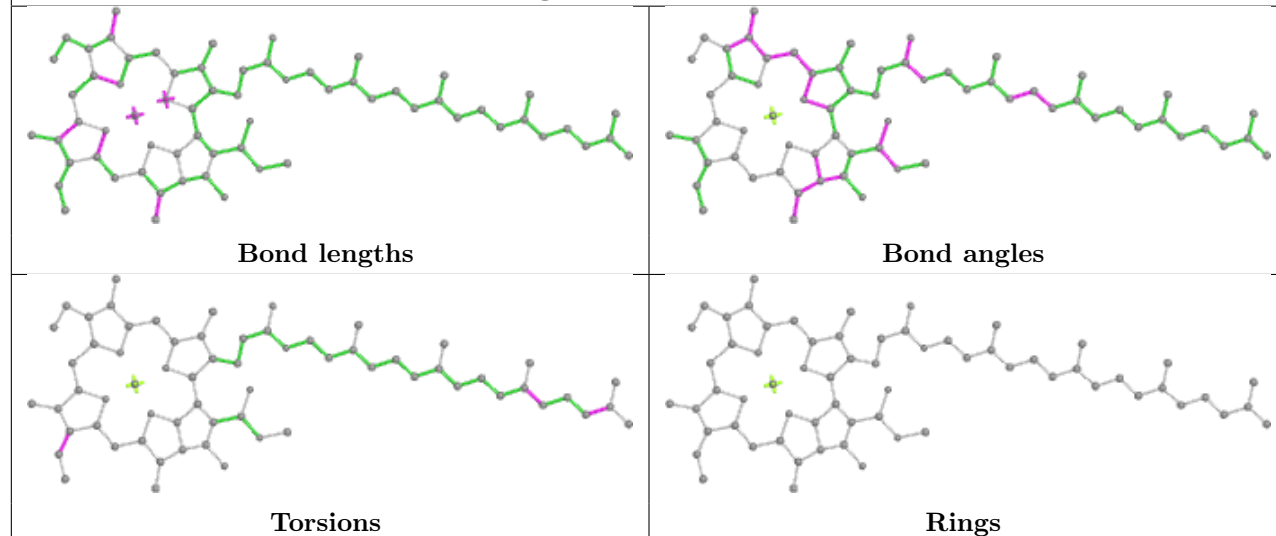
Ligand BCR d 406

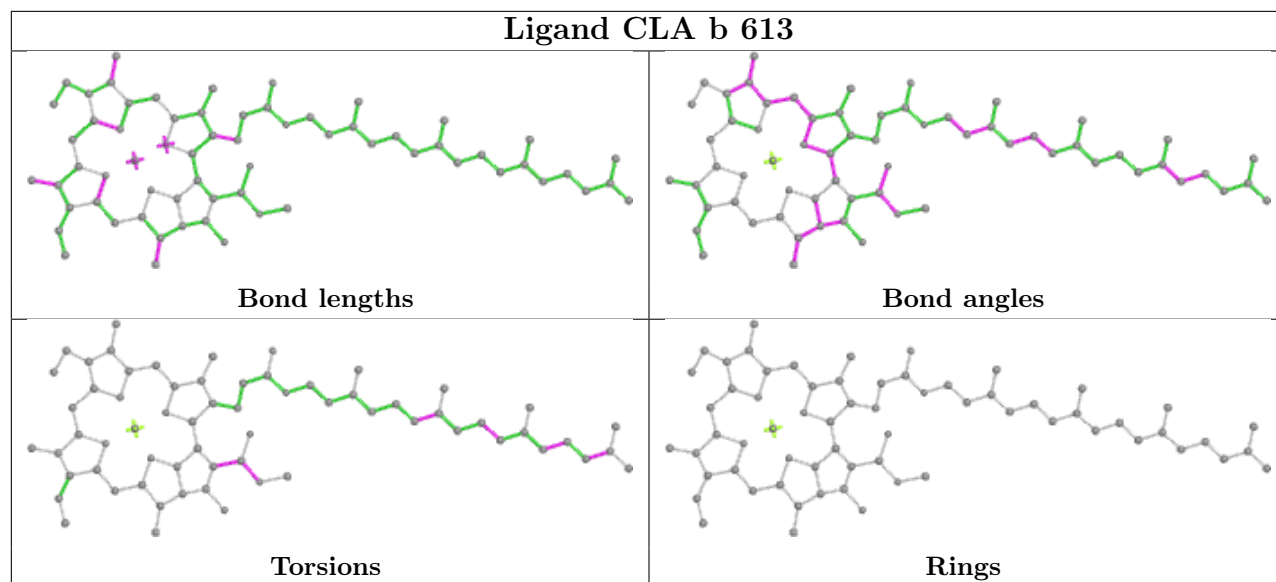
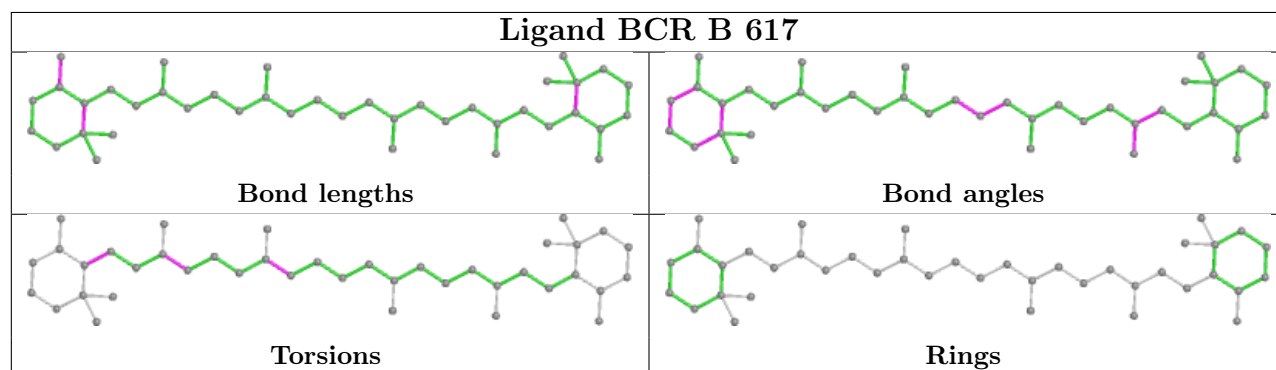
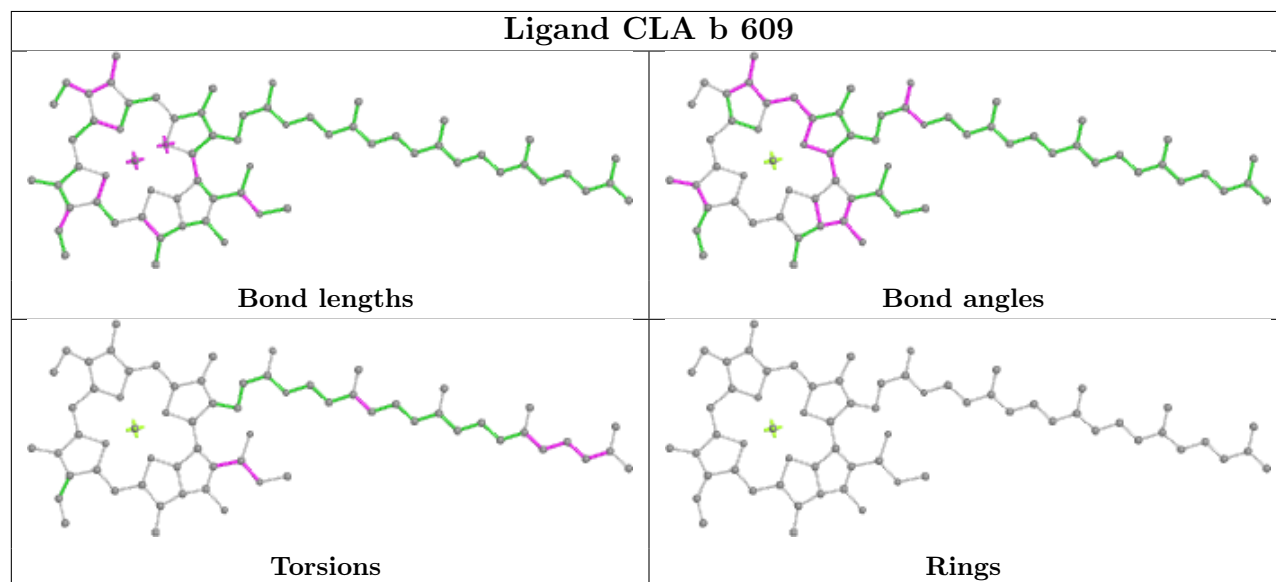


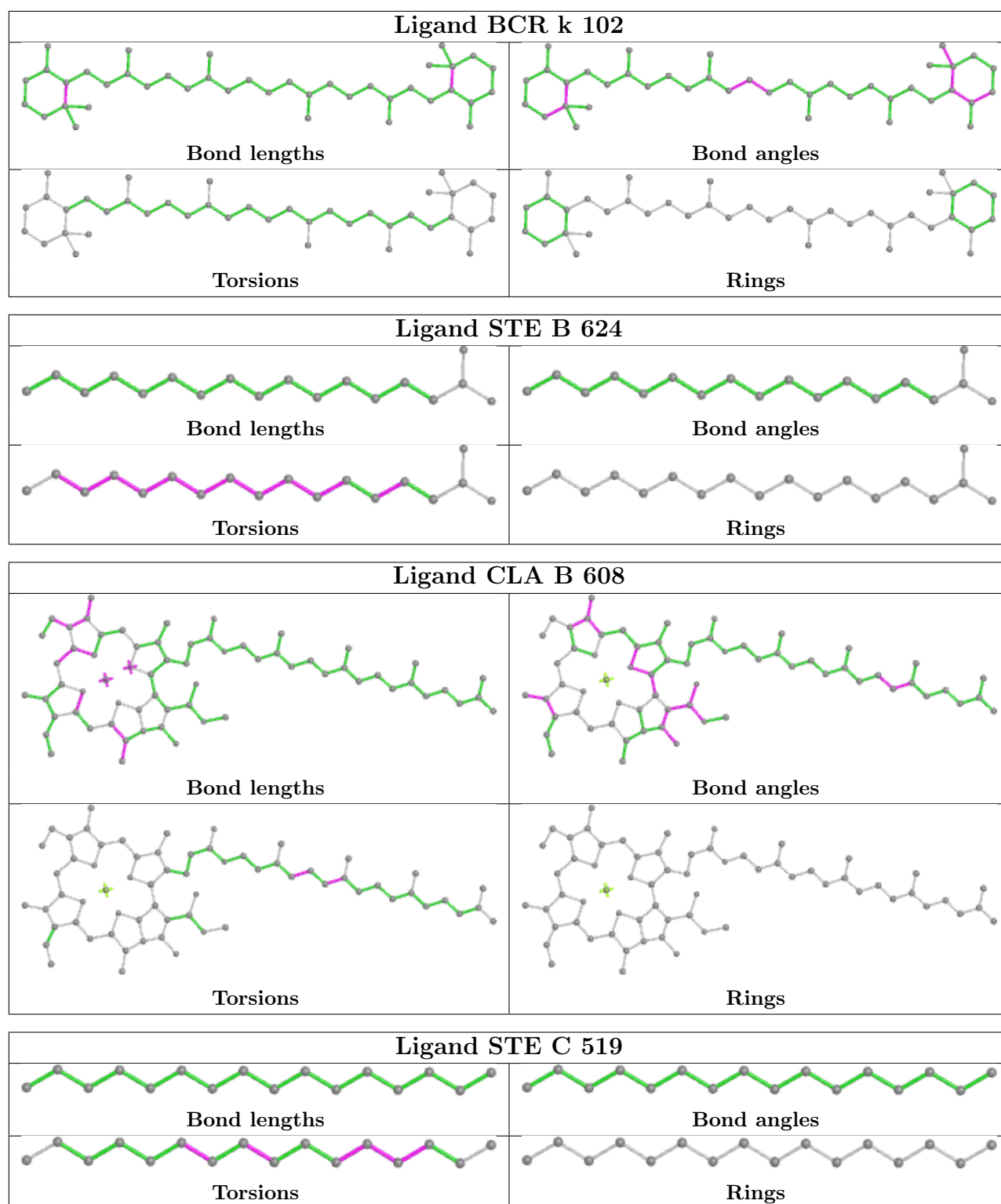
Ligand PHO a 404

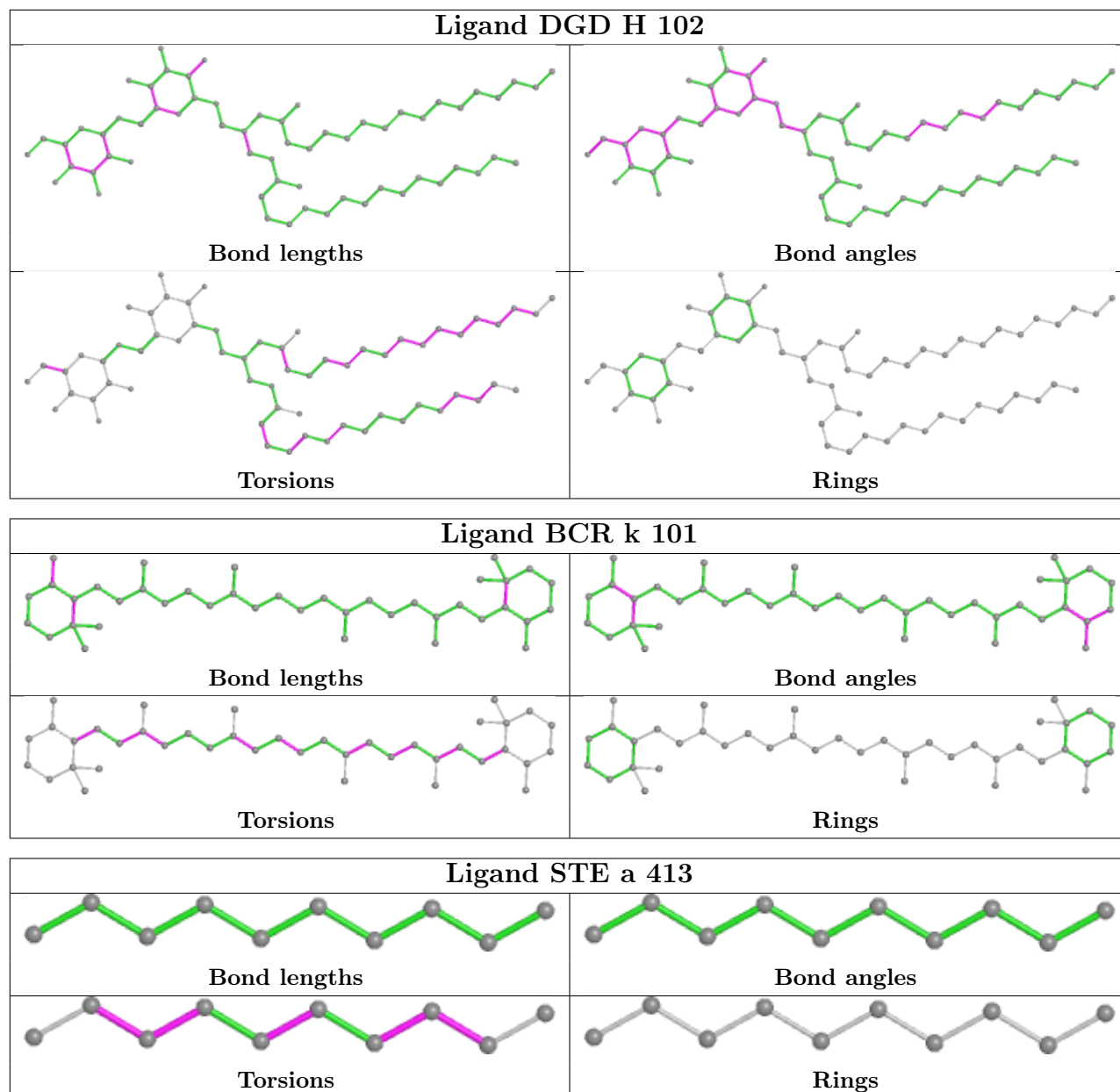




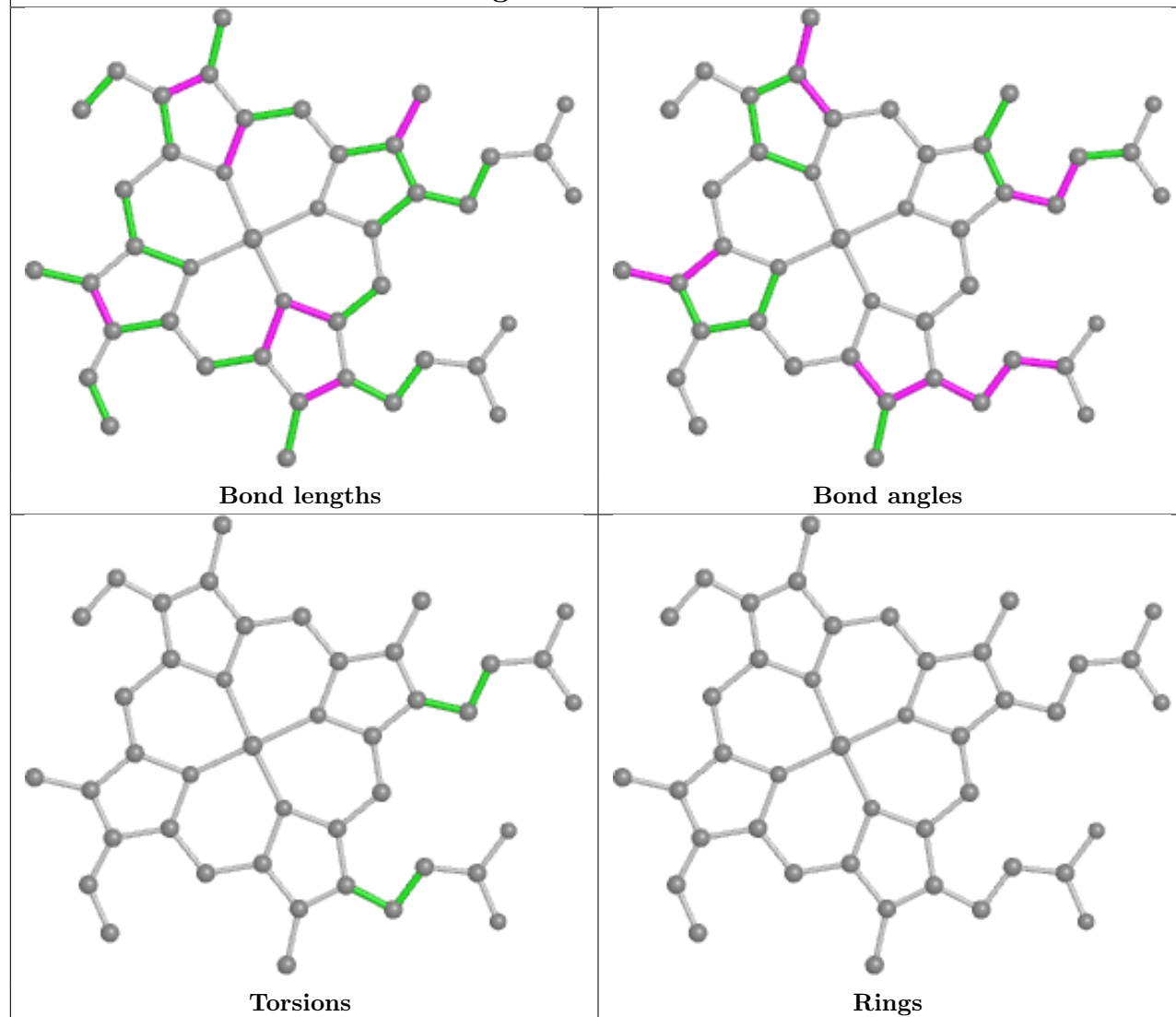
Ligand CLA B 603**Ligand CLA B 613****Ligand CLA a 402**

Ligand CLA b 613**Ligand BCR B 617****Ligand CLA b 609**

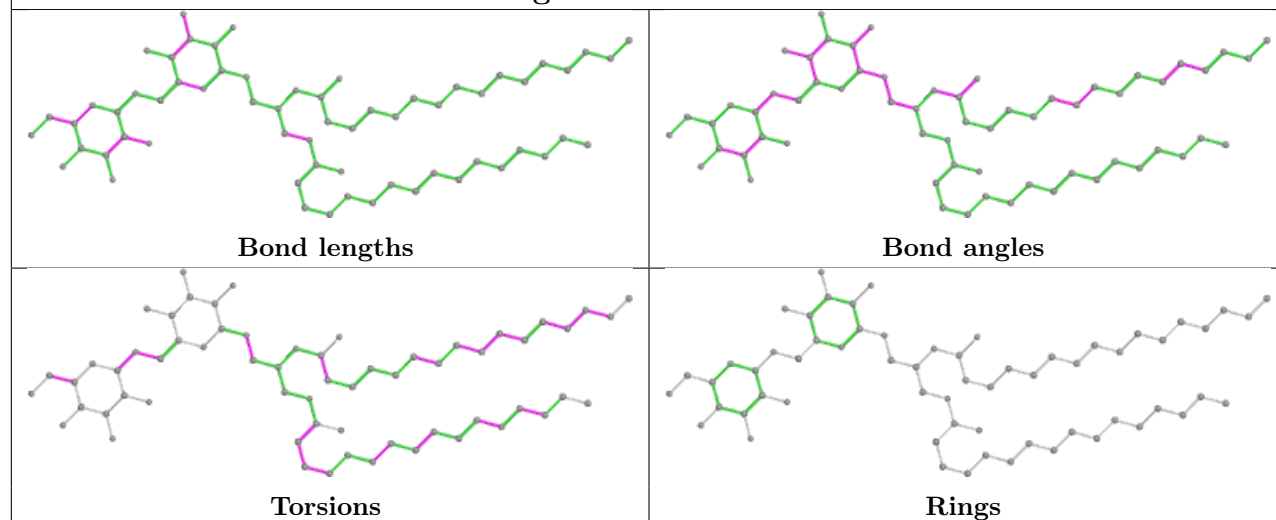


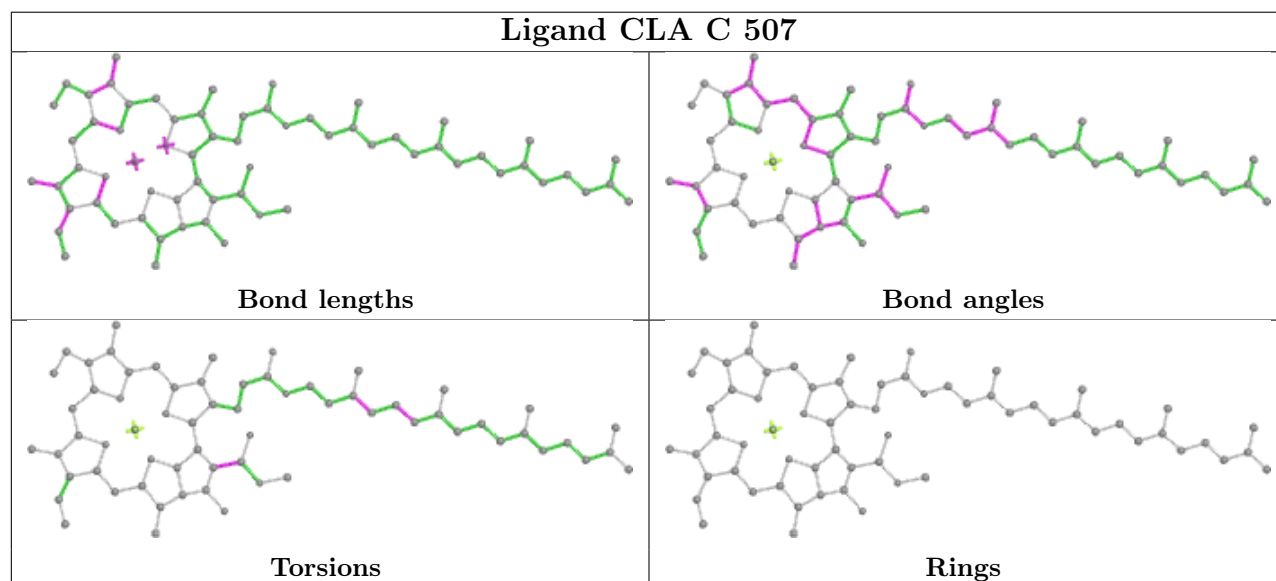
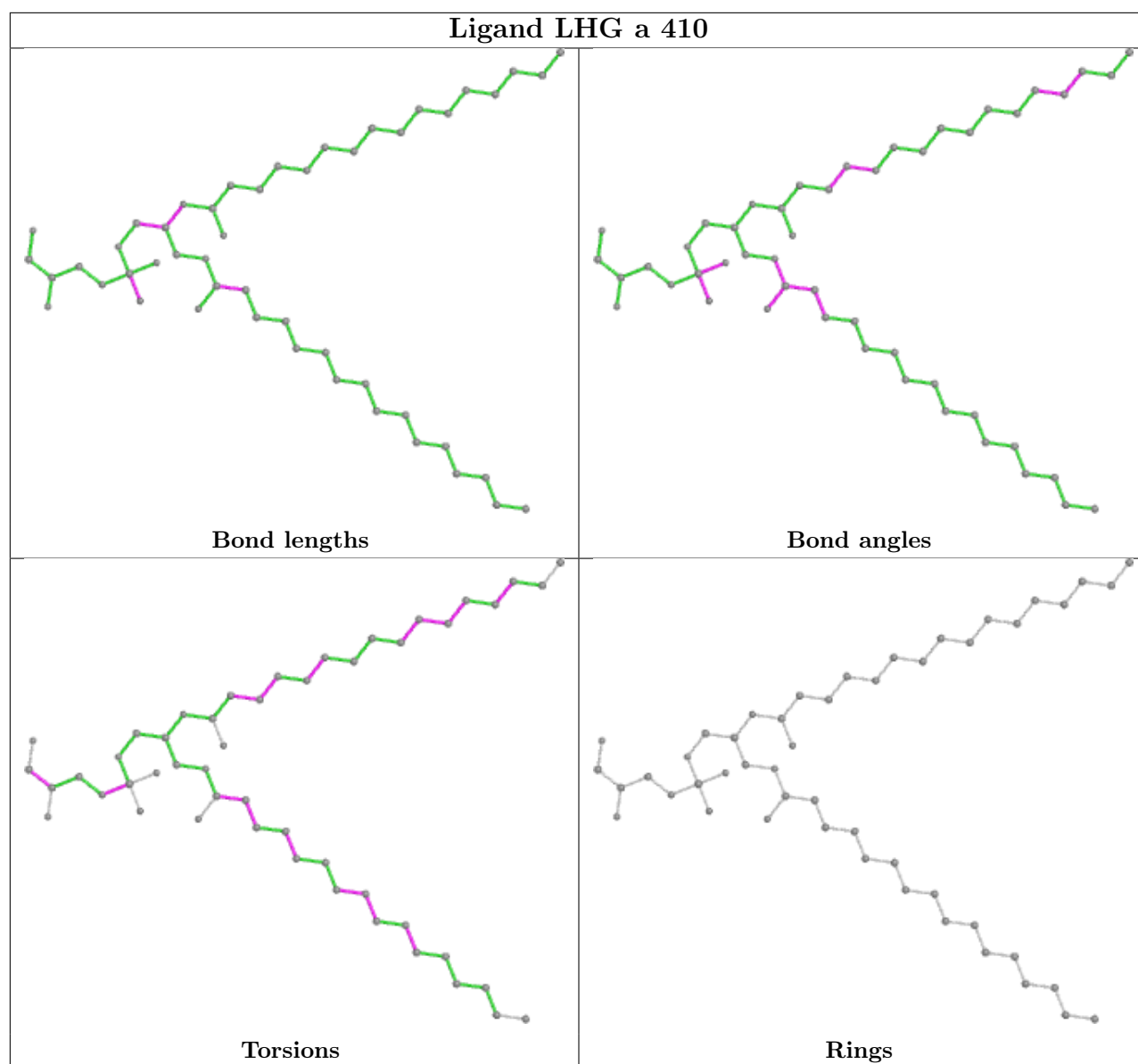


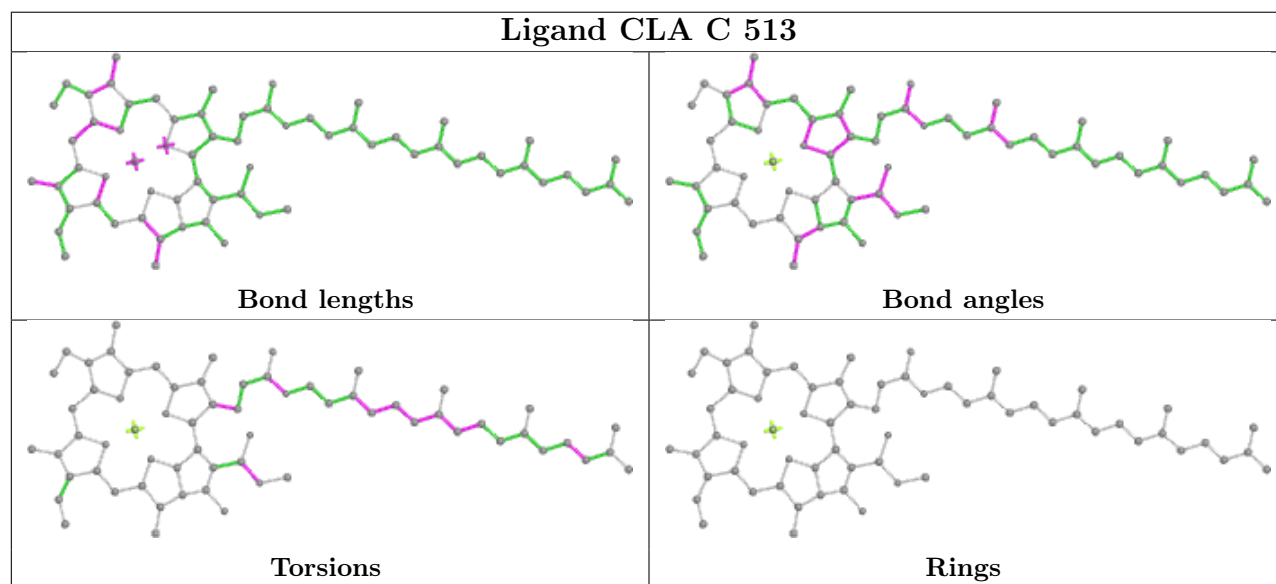
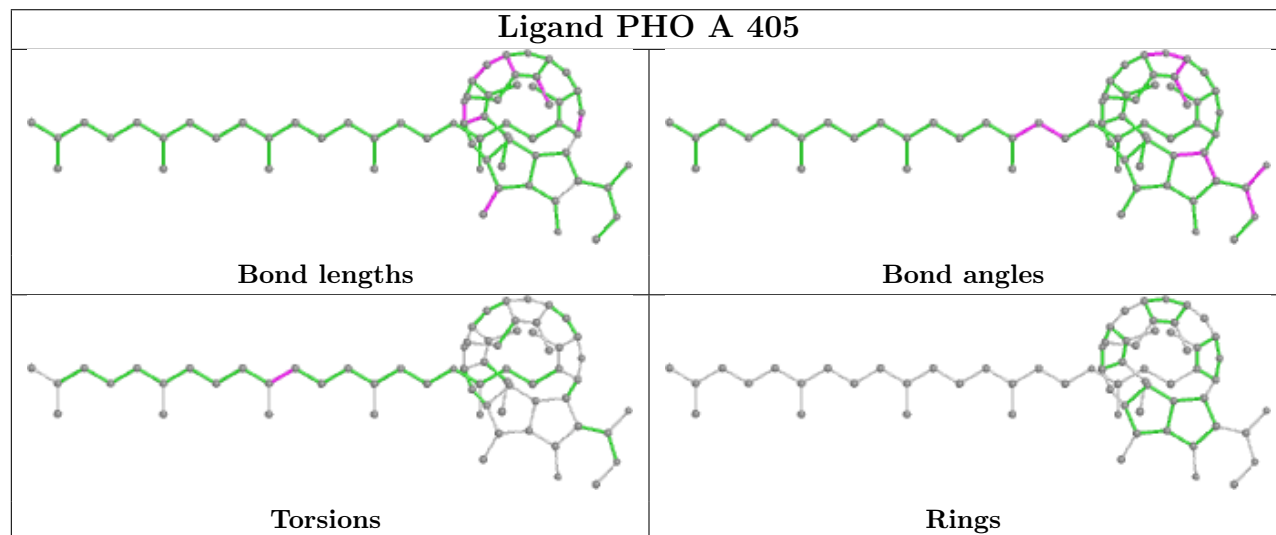
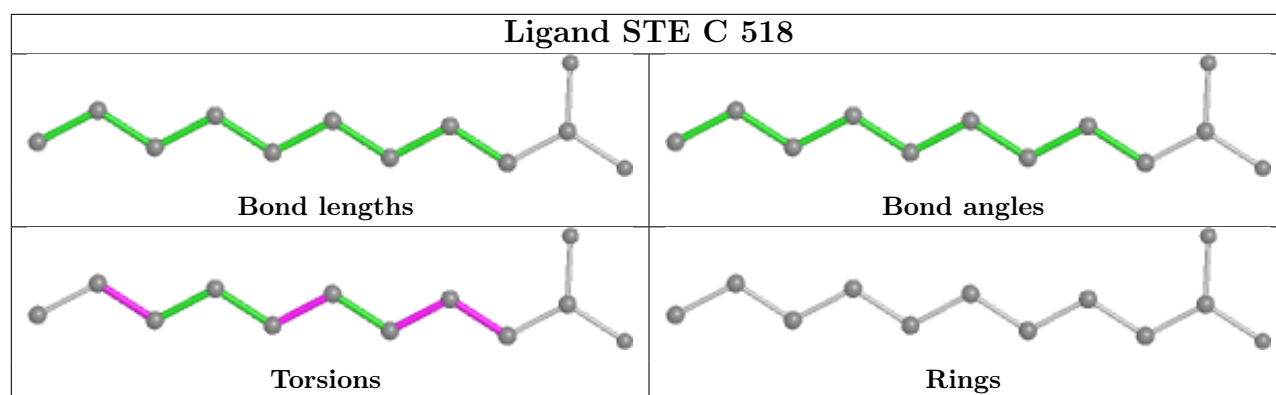
Ligand HEC v 201



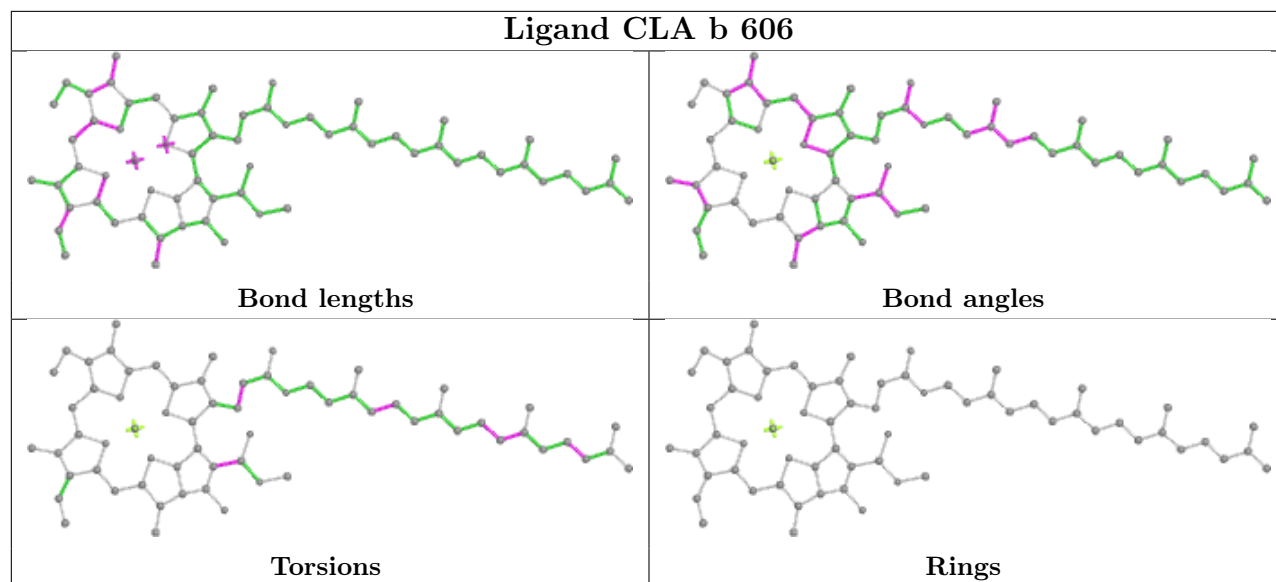
Ligand DGD c 517



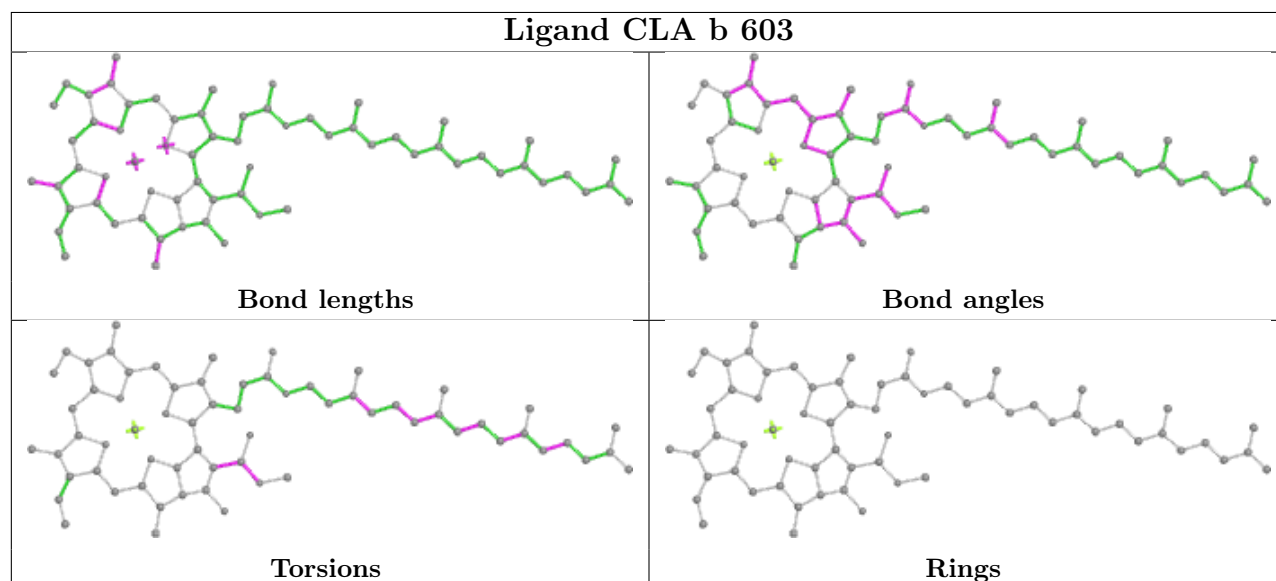




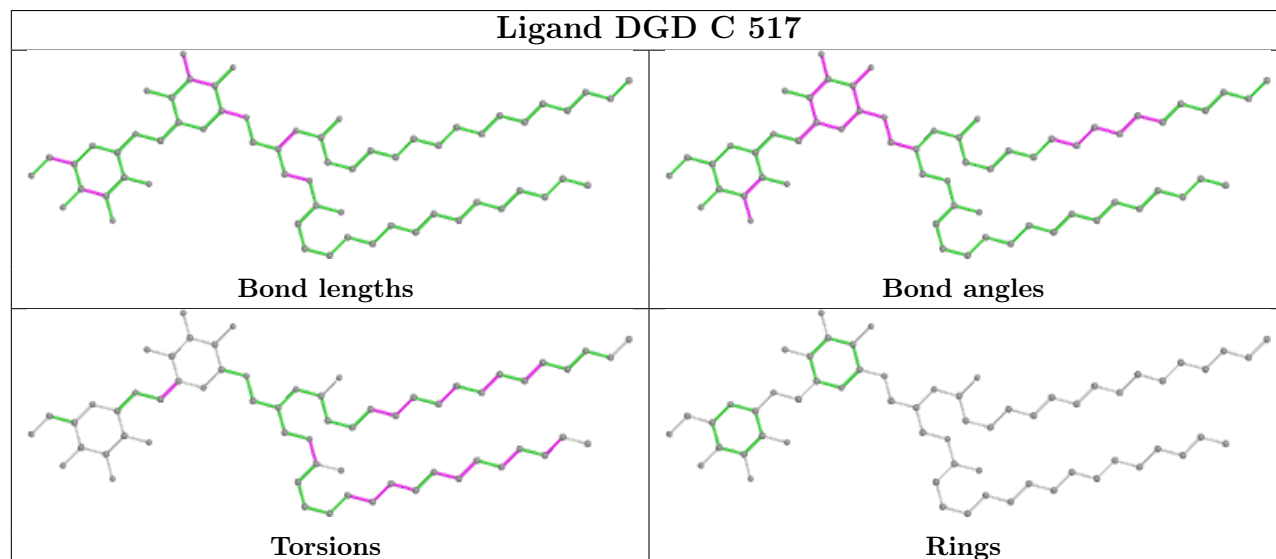
Ligand CLA b 606

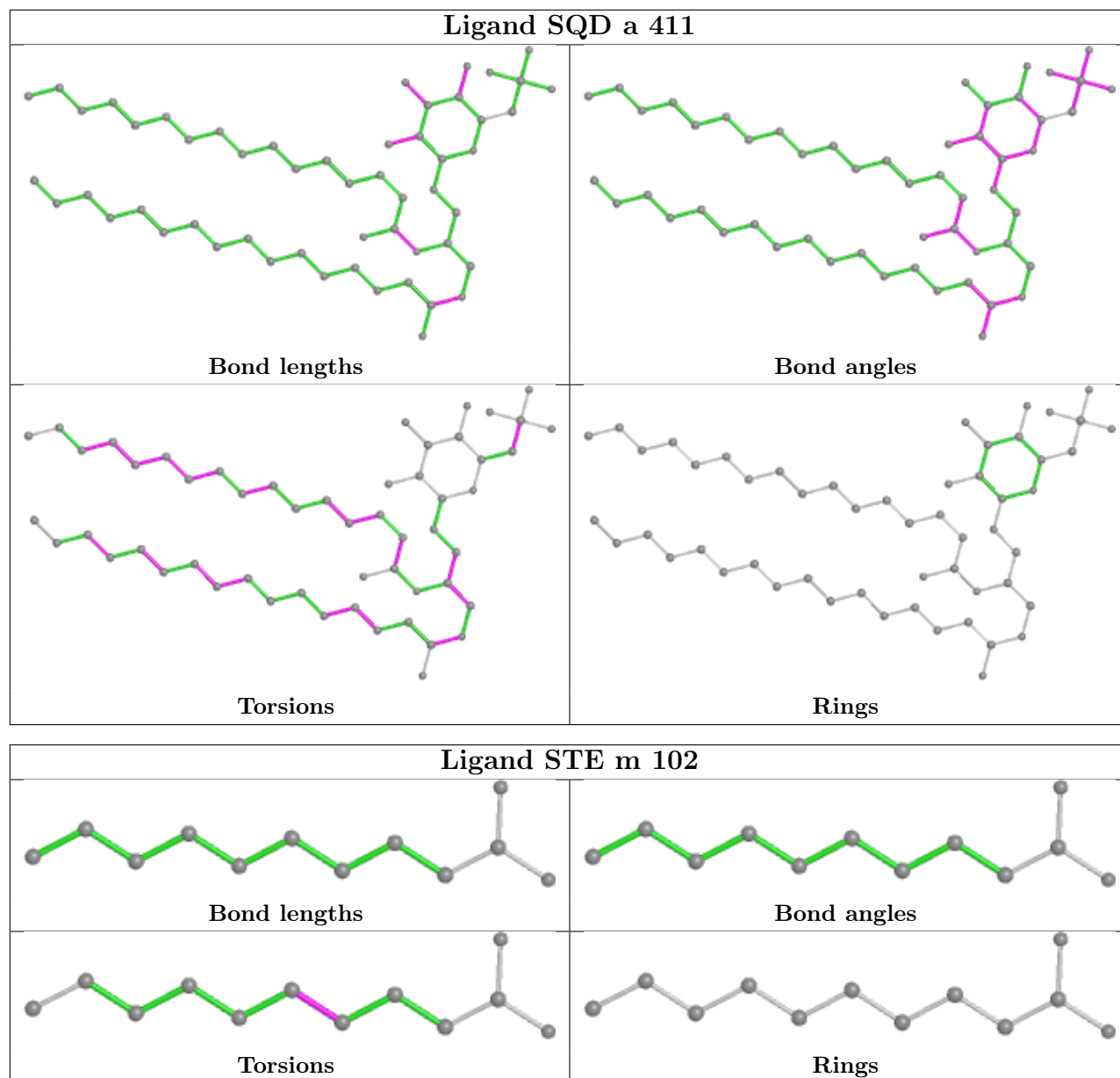


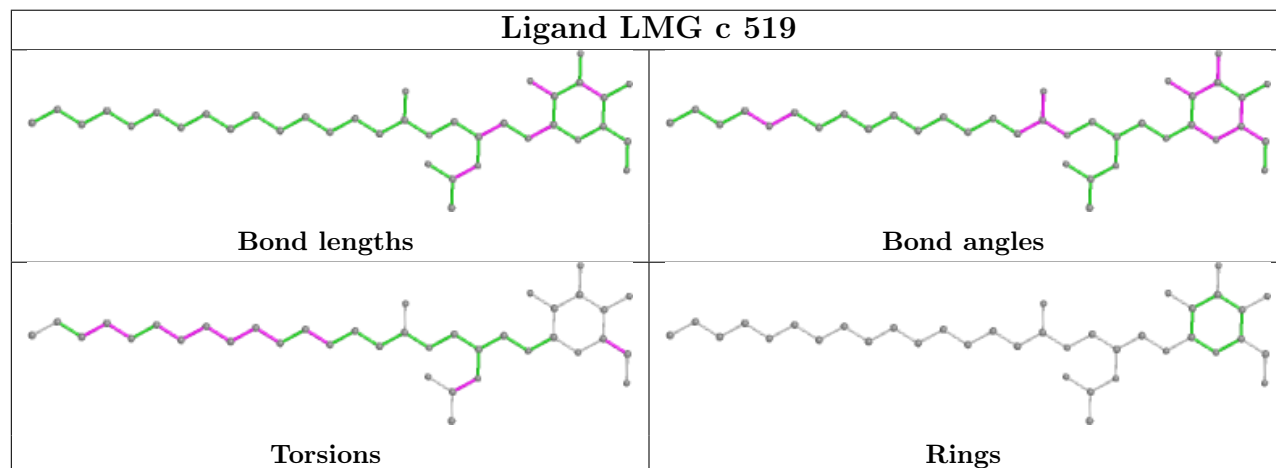
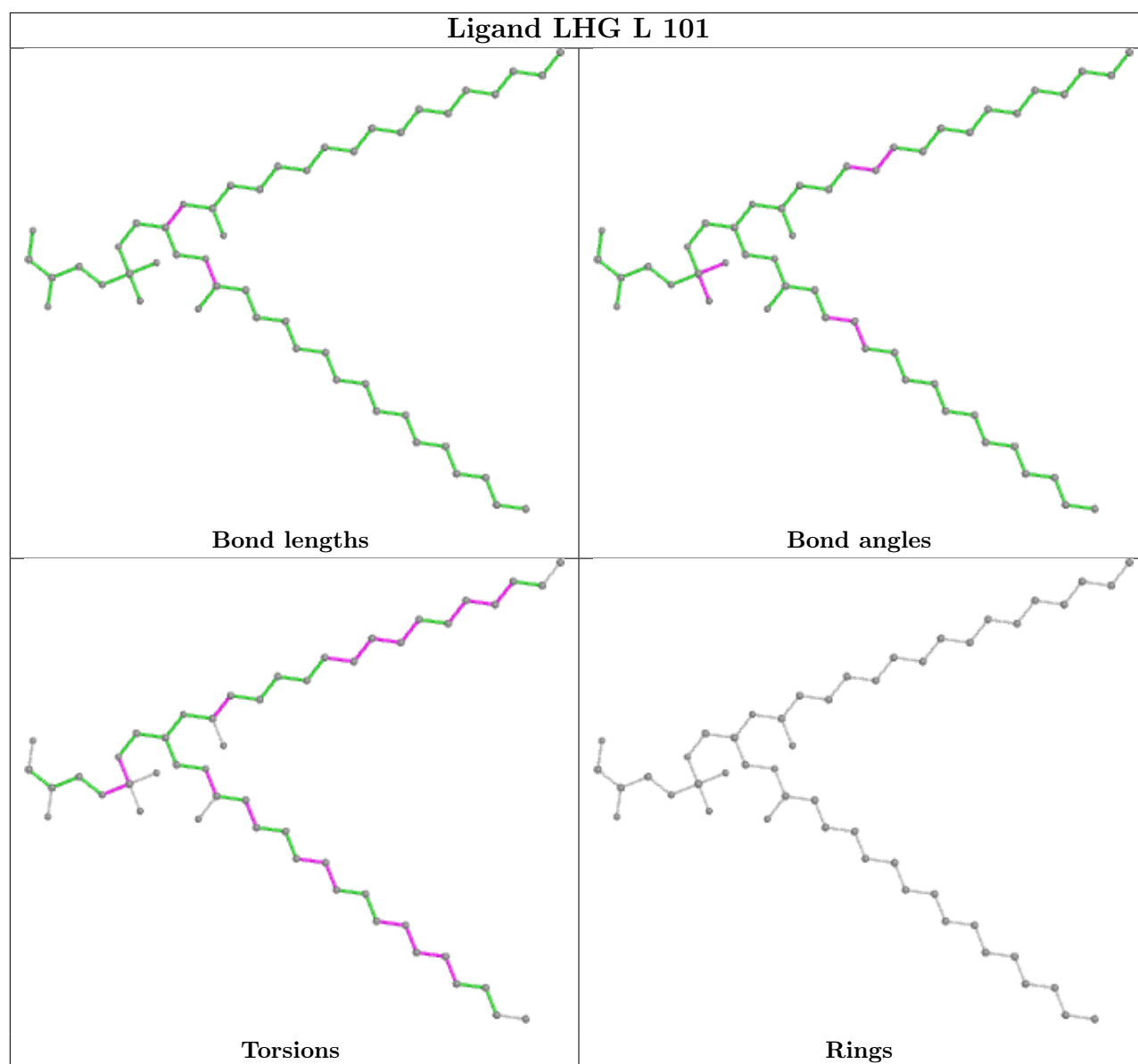
Ligand CLA b 603

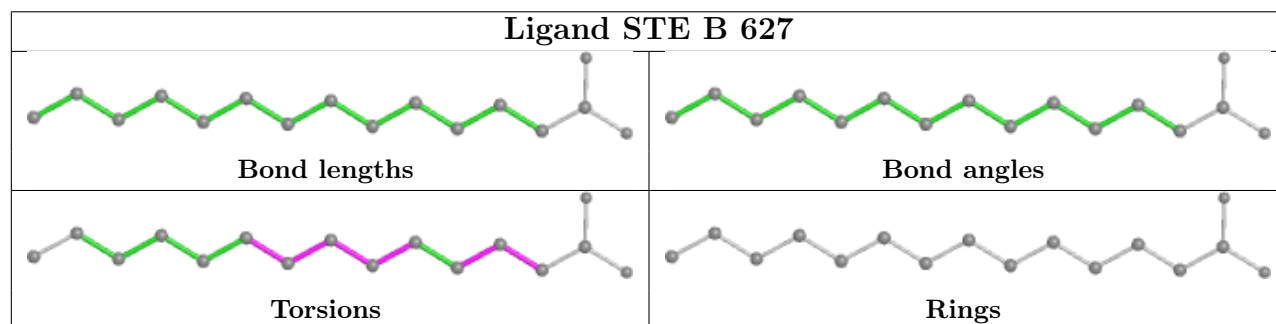
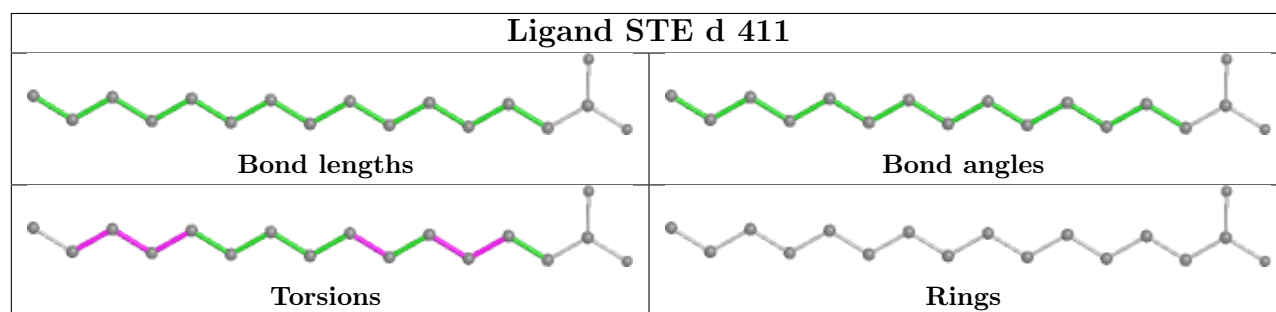
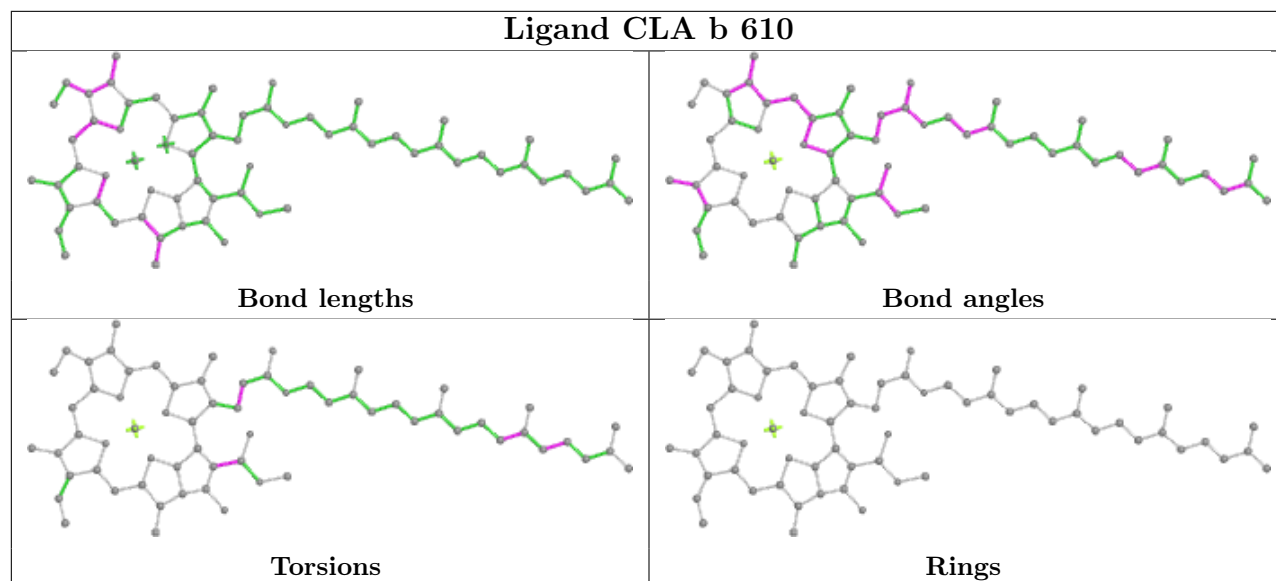
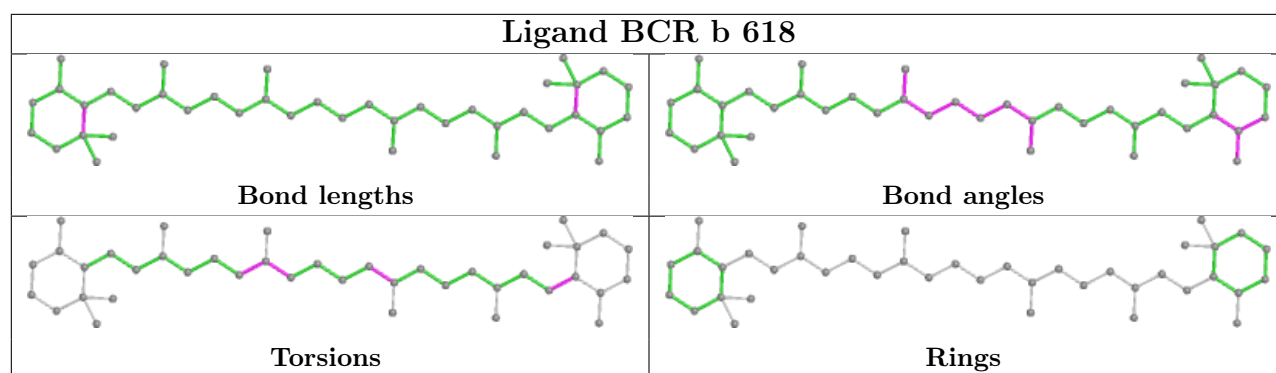


Ligand DGD C 517

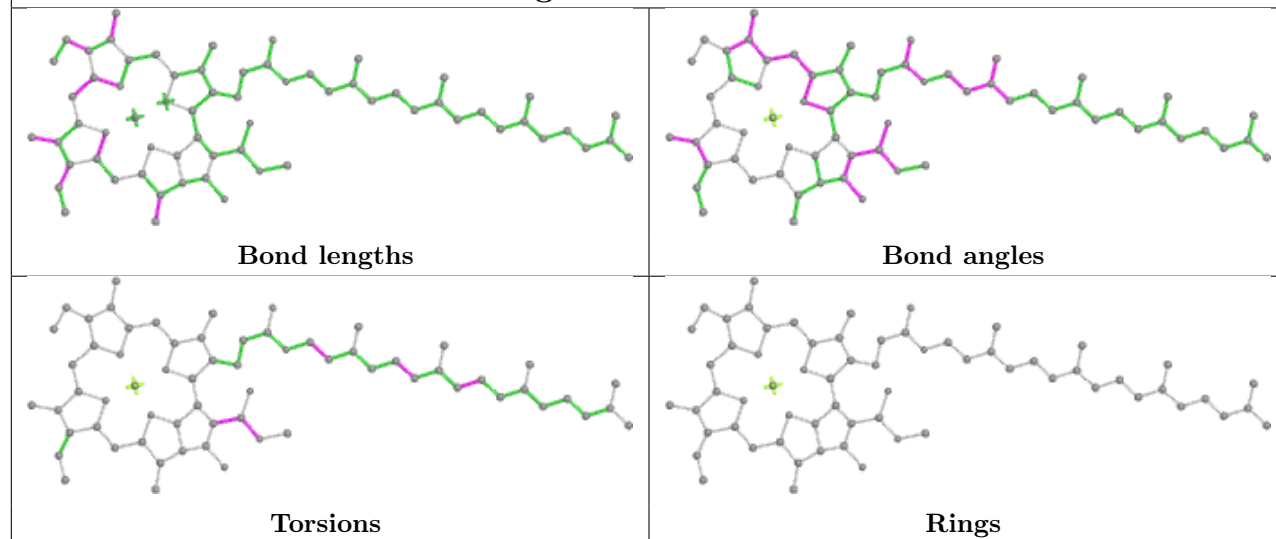




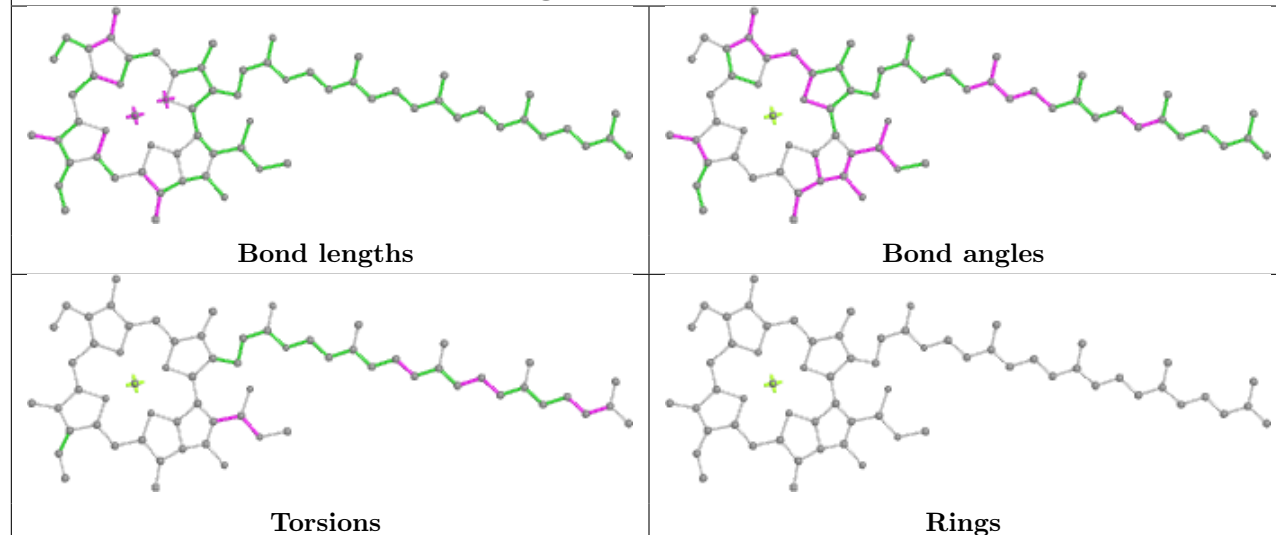




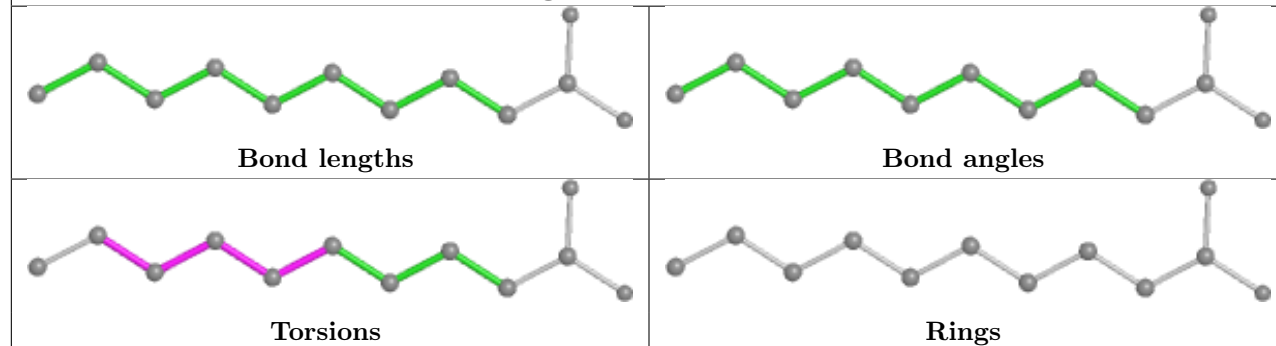
Ligand CLA d 405



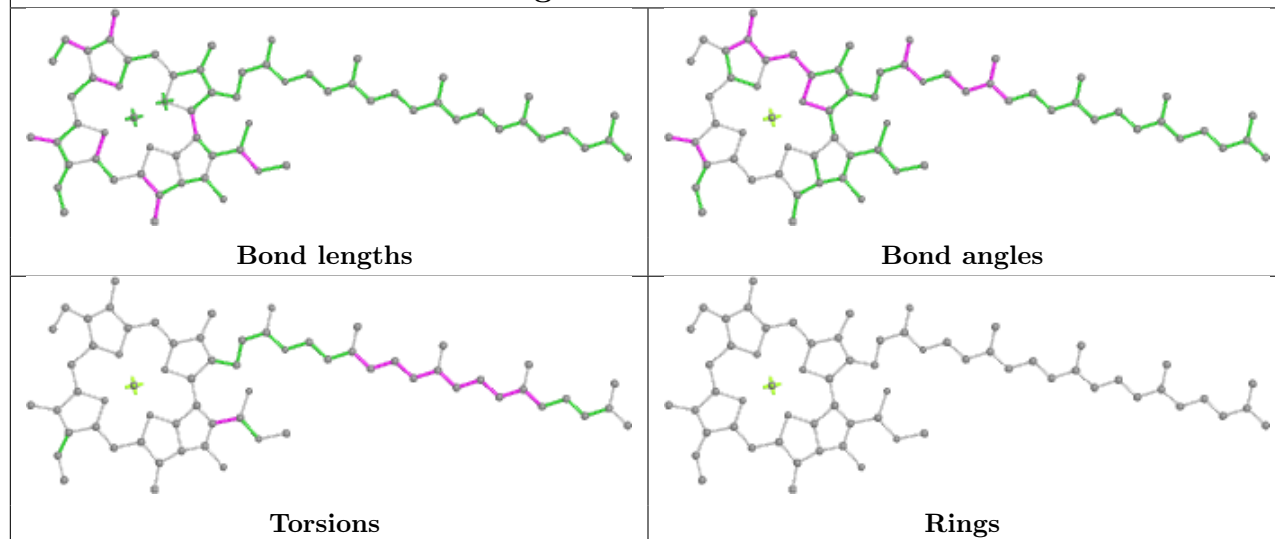
Ligand CLA c 503



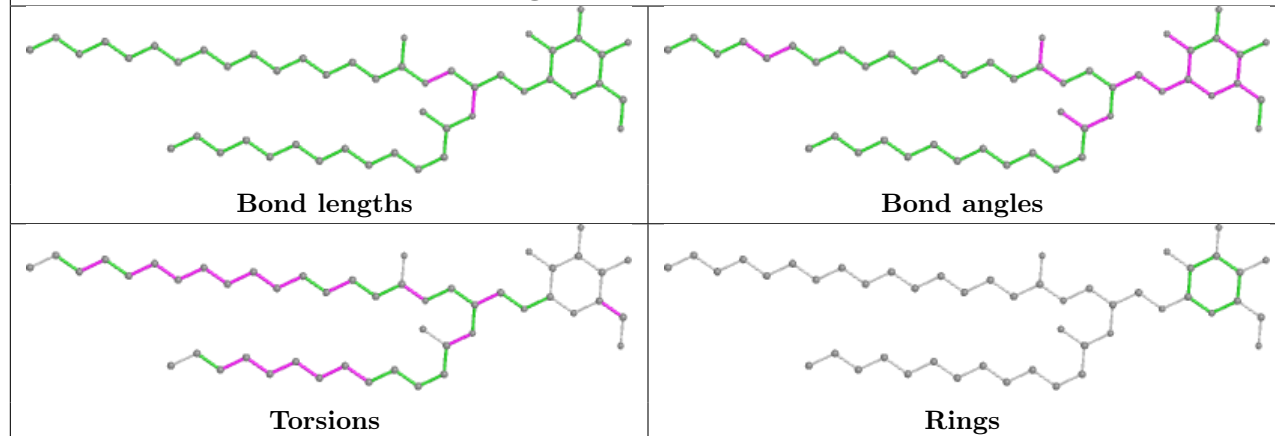
Ligand STE a 415



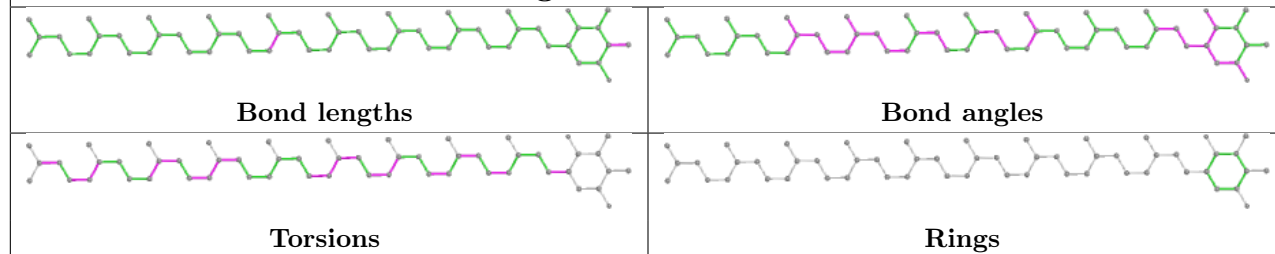
Ligand CLA b 614



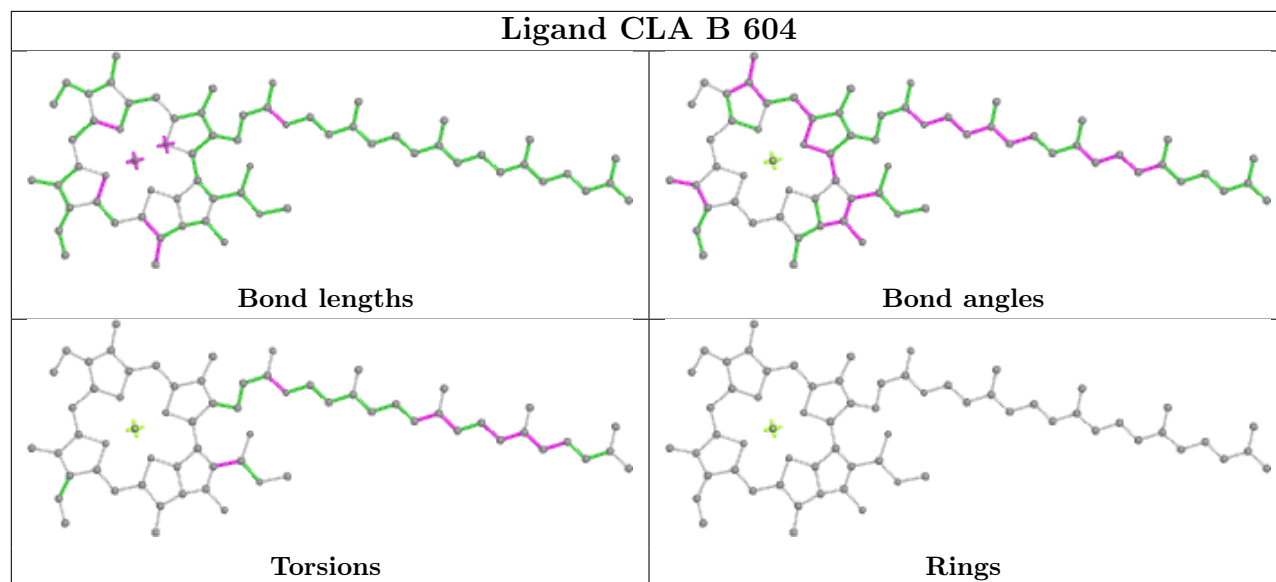
Ligand LMG Y 101



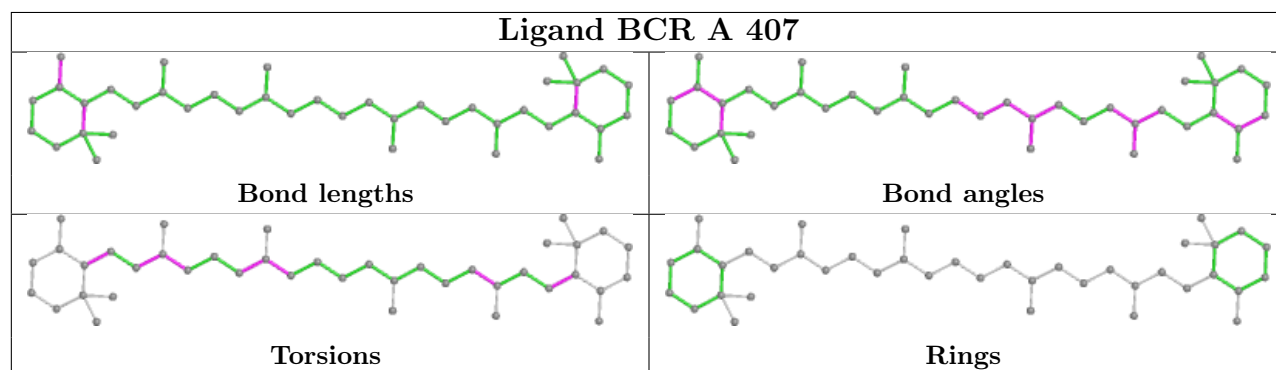
Ligand PL9 A 410



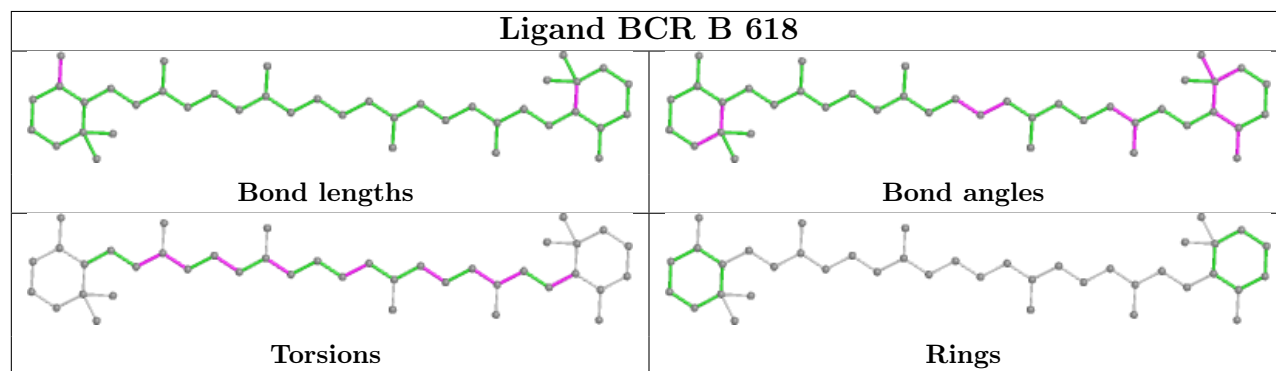
Ligand CLA B 604

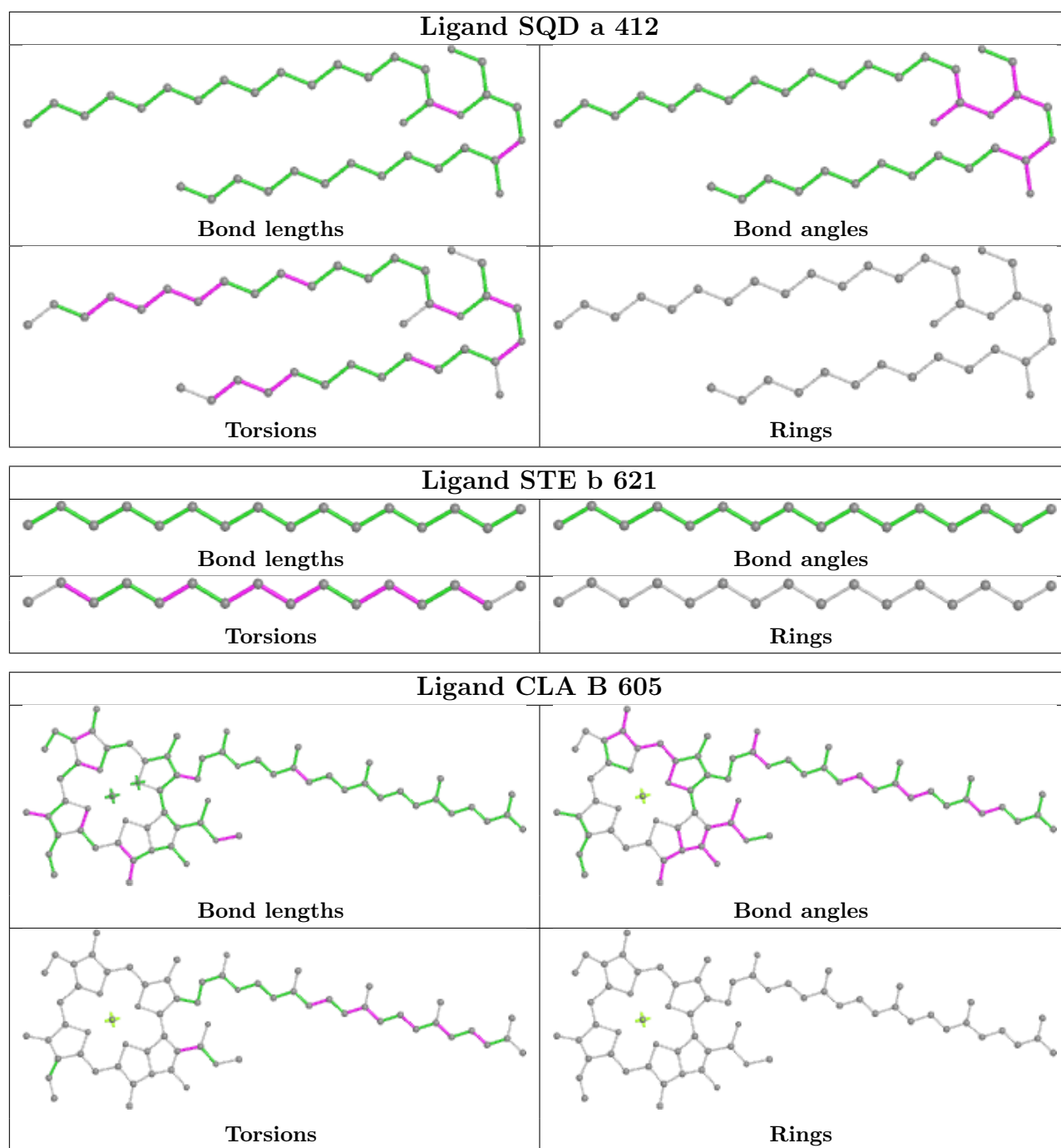


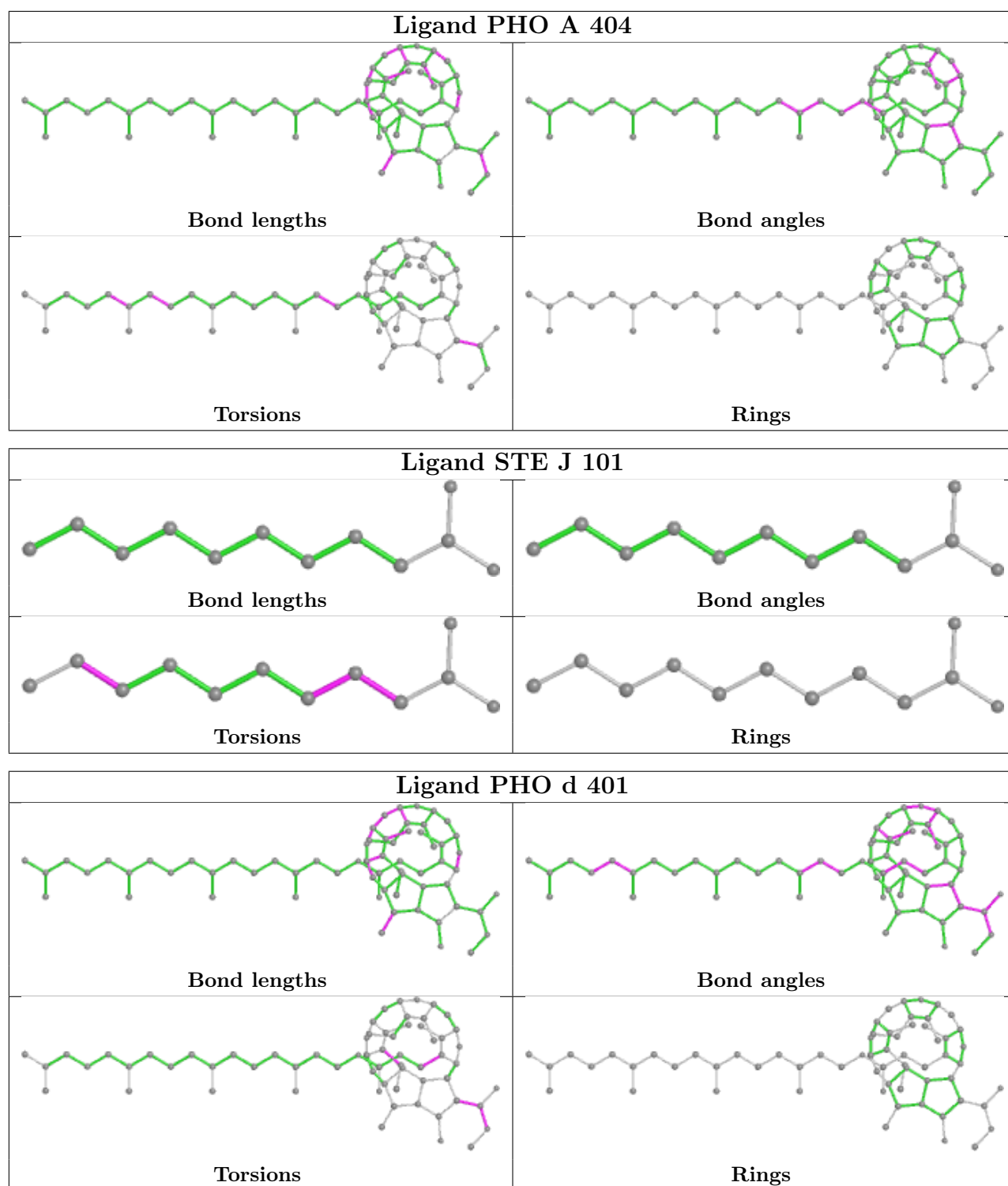
Ligand BCR A 407



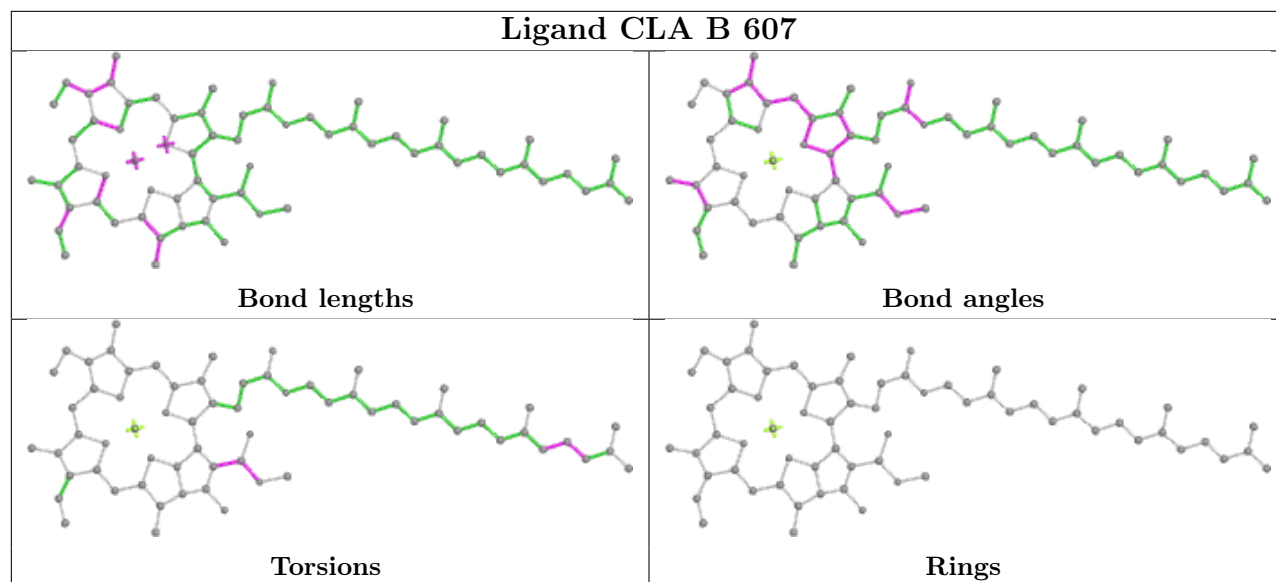
Ligand BCR B 618



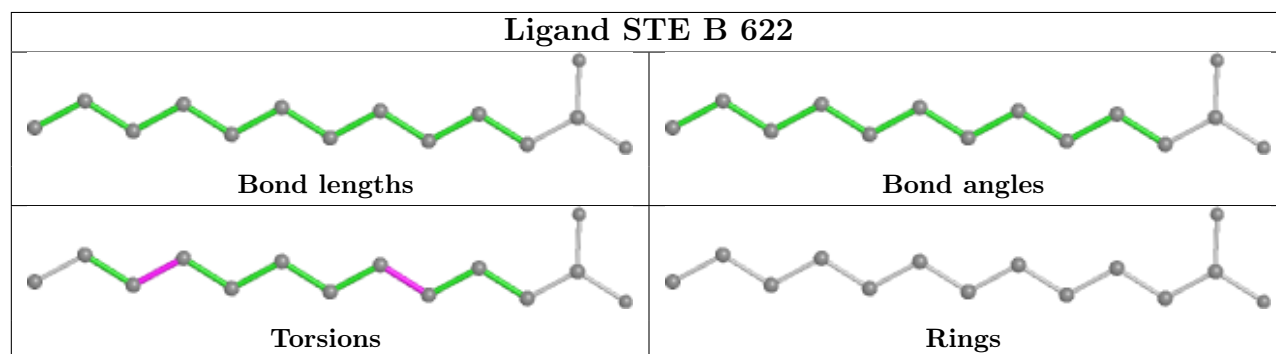




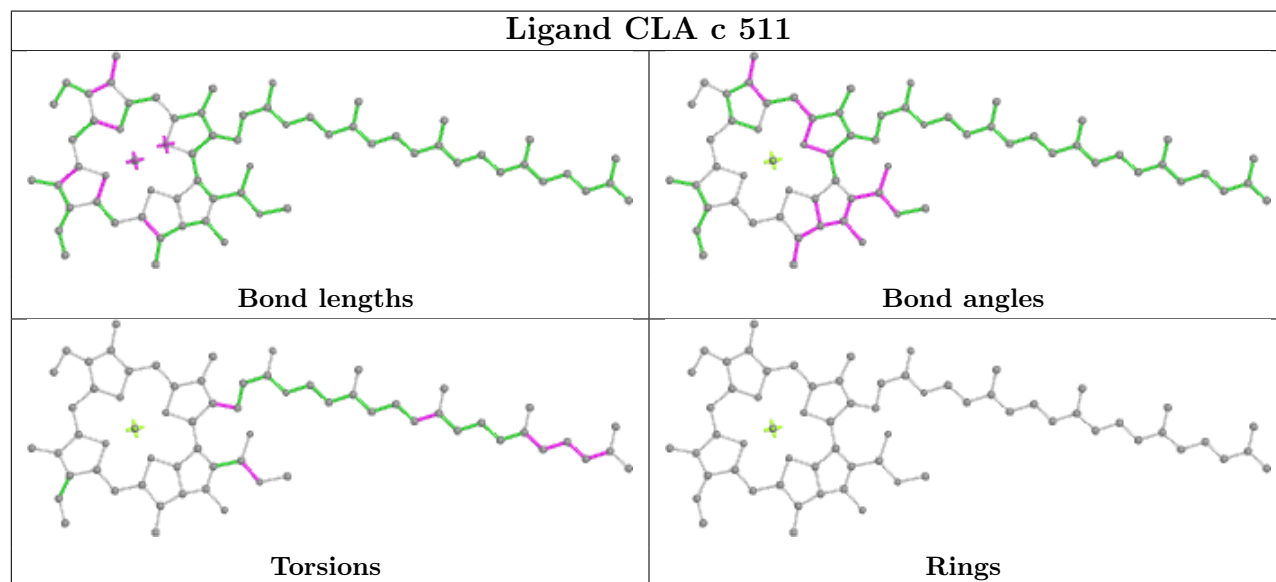
Ligand CLA B 607

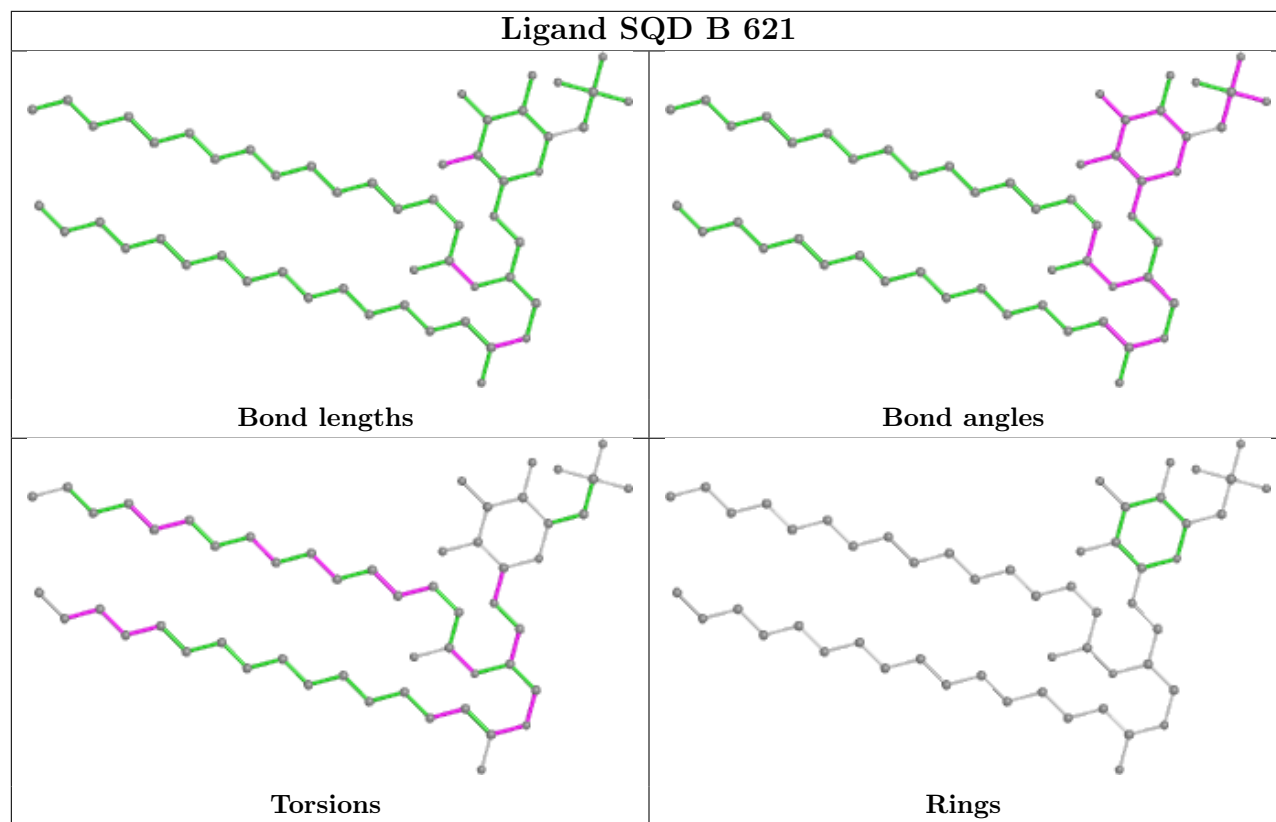
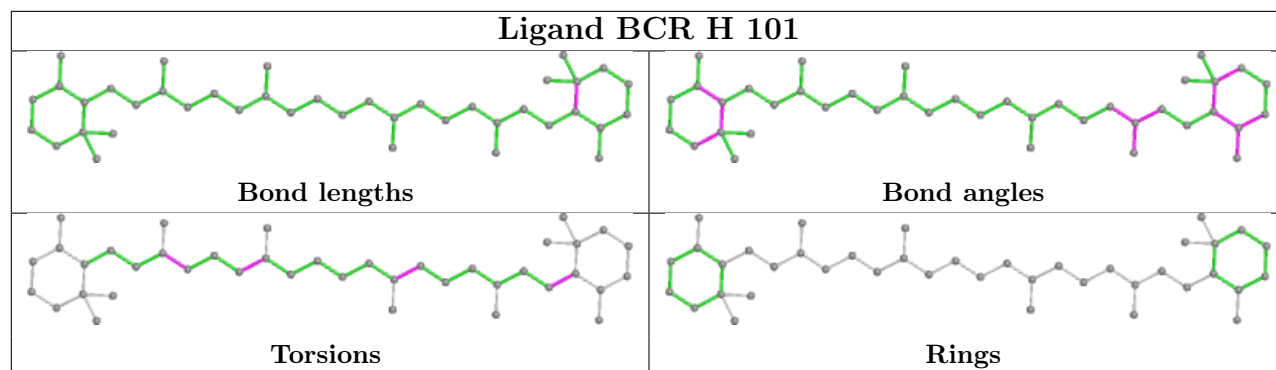


Ligand STE B 622

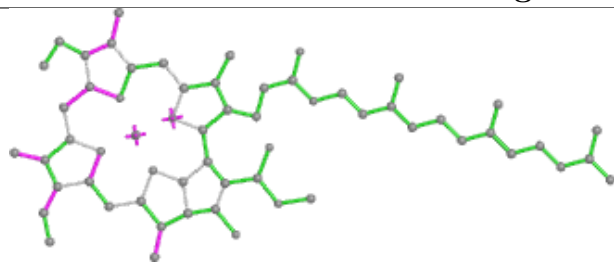


Ligand CLA c 511

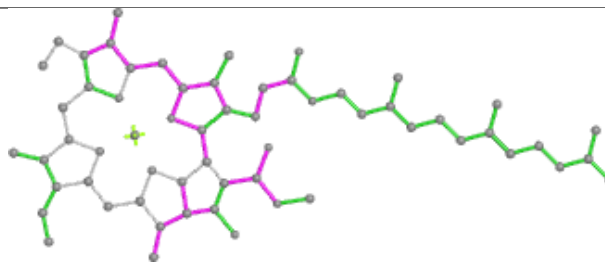




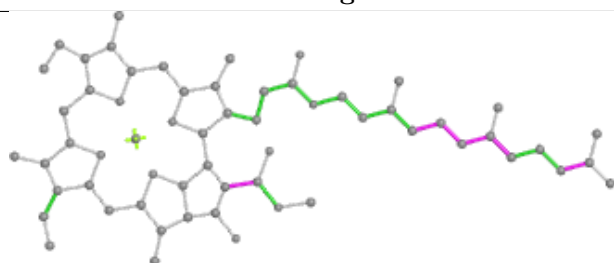
Ligand CLA B 616



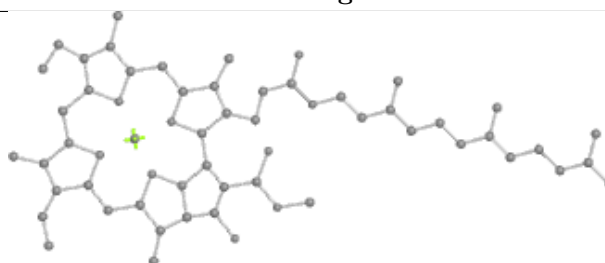
Bond lengths



Bond angles

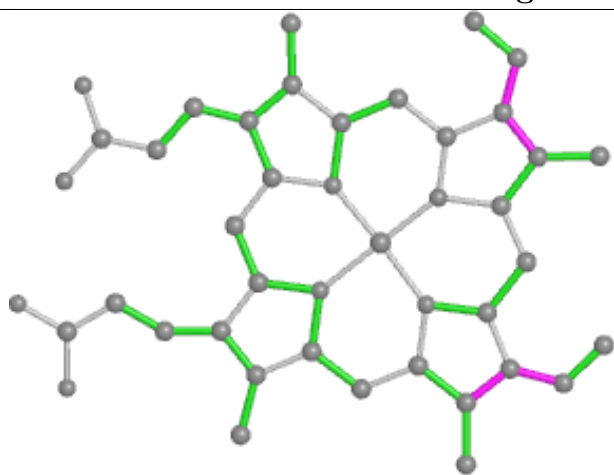


Torsions

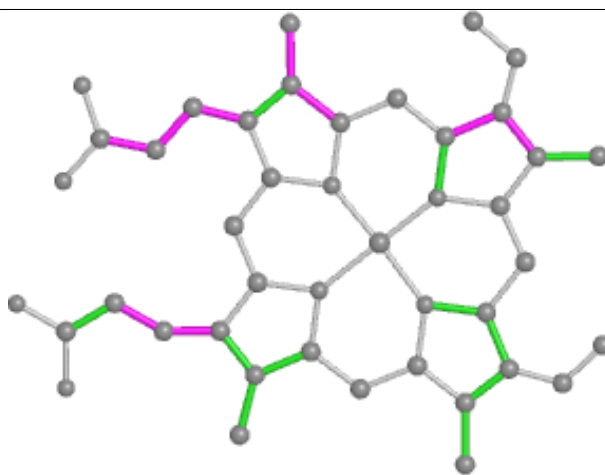


Rings

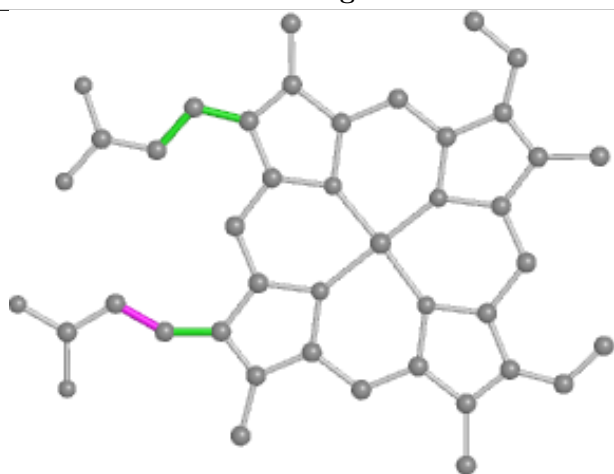
Ligand HEM f 101



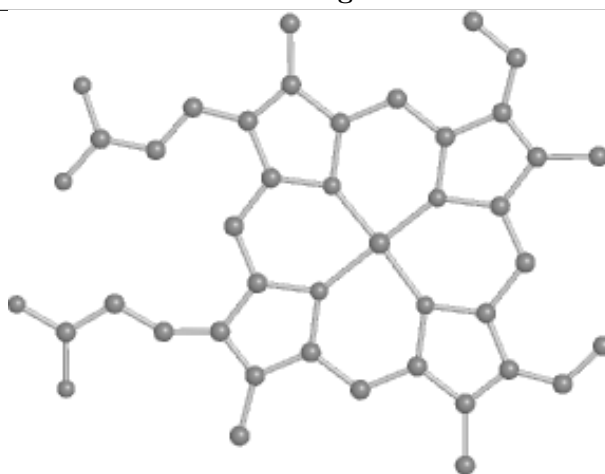
Bond lengths



Bond angles

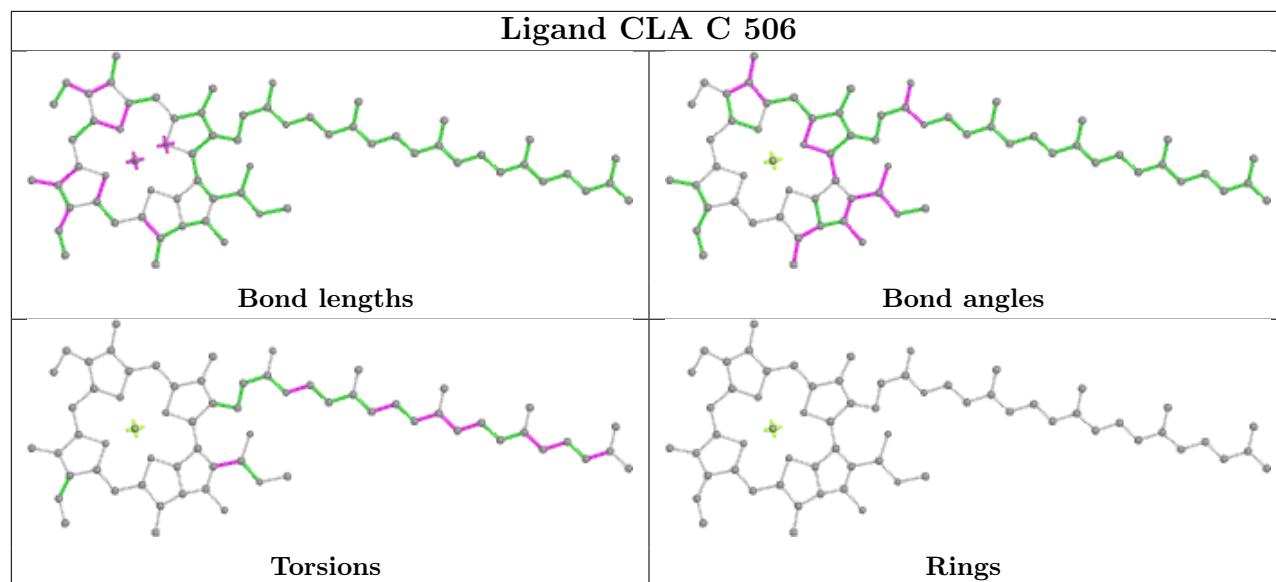


Torsions

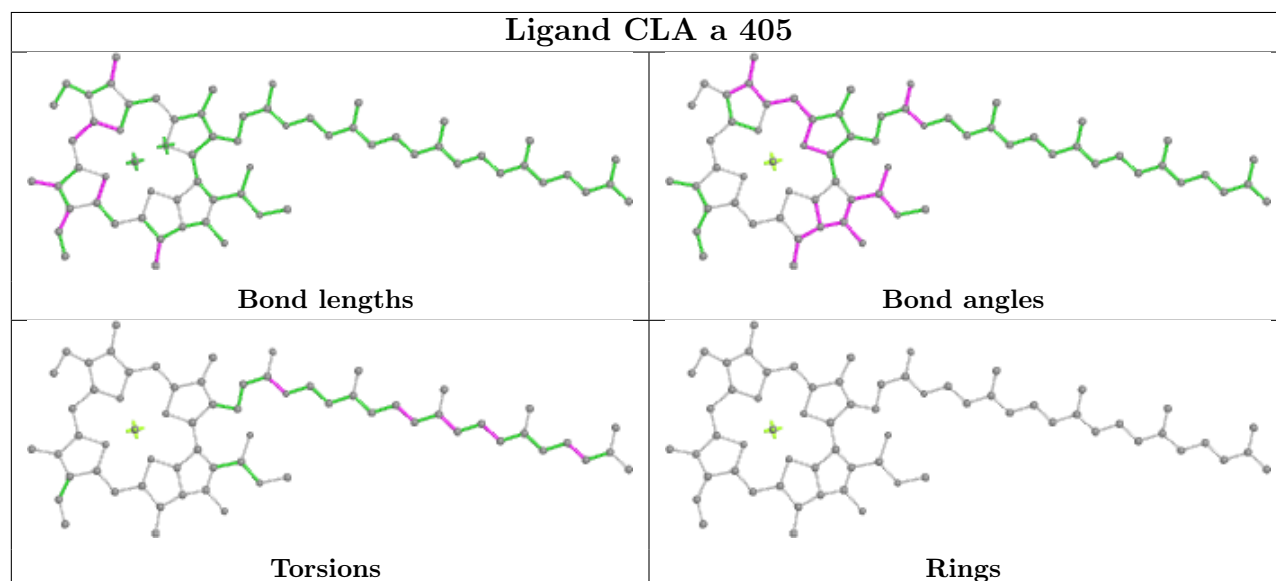


Rings

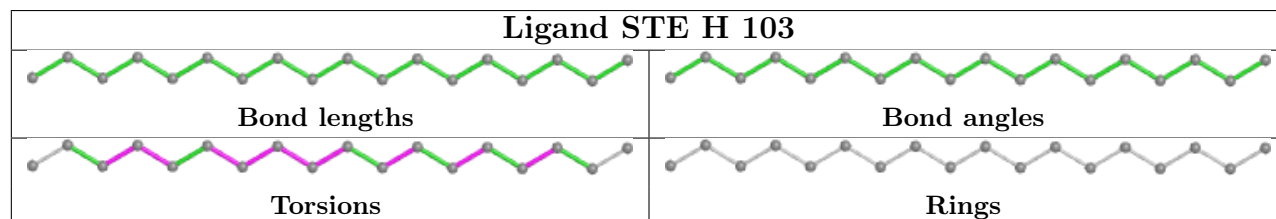
Ligand CLA C 506



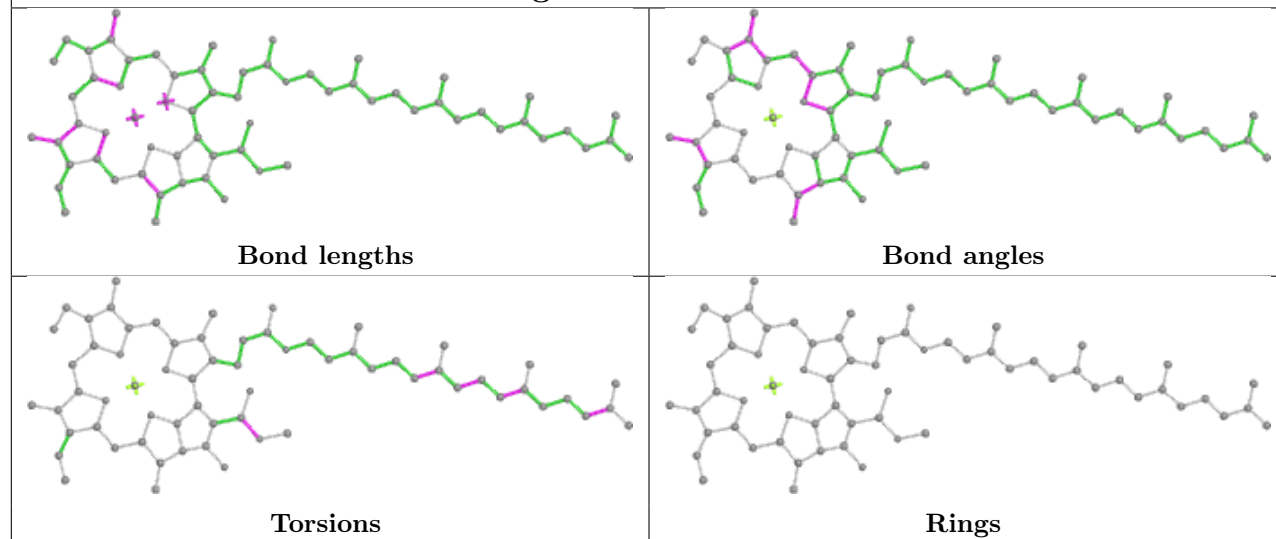
Ligand CLA a 405



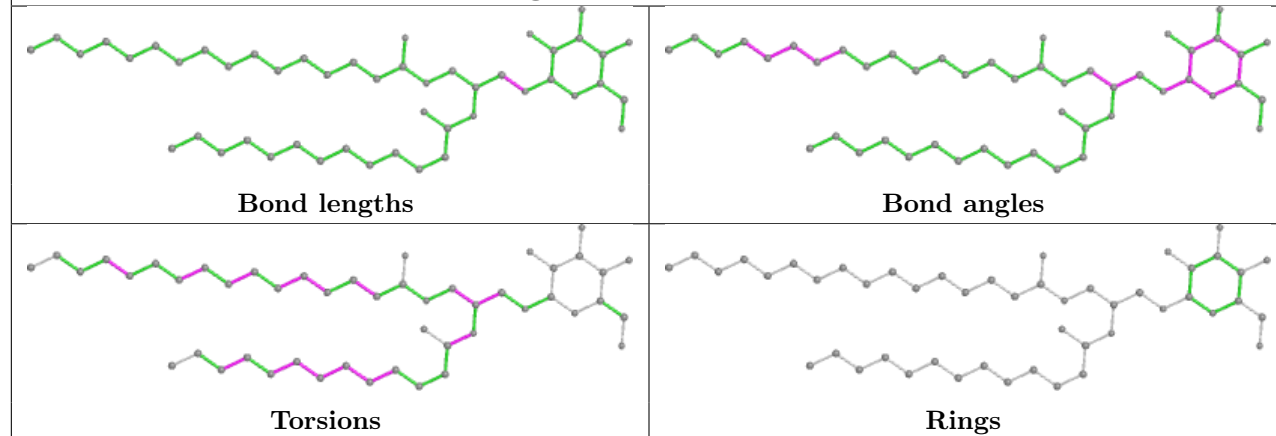
Ligand STE H 103



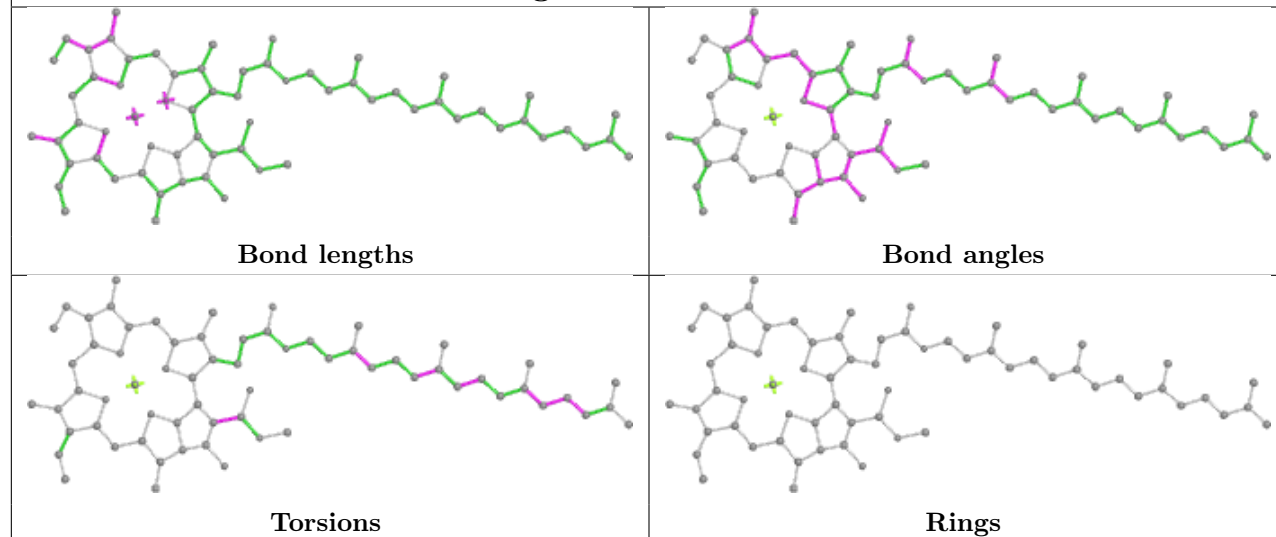
Ligand CLA C 511



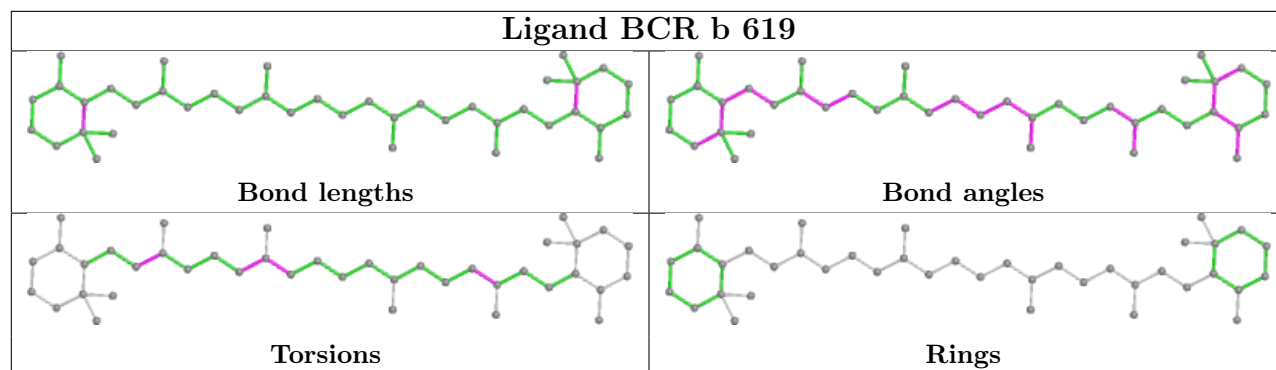
Ligand LMG A 411



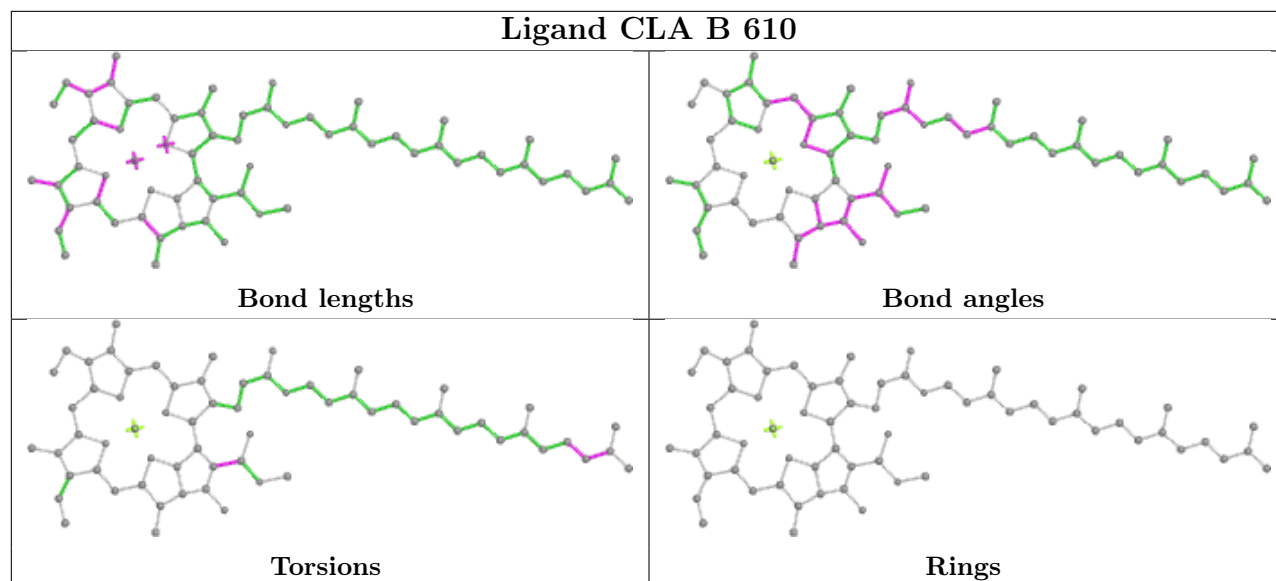
Ligand CLA B 614



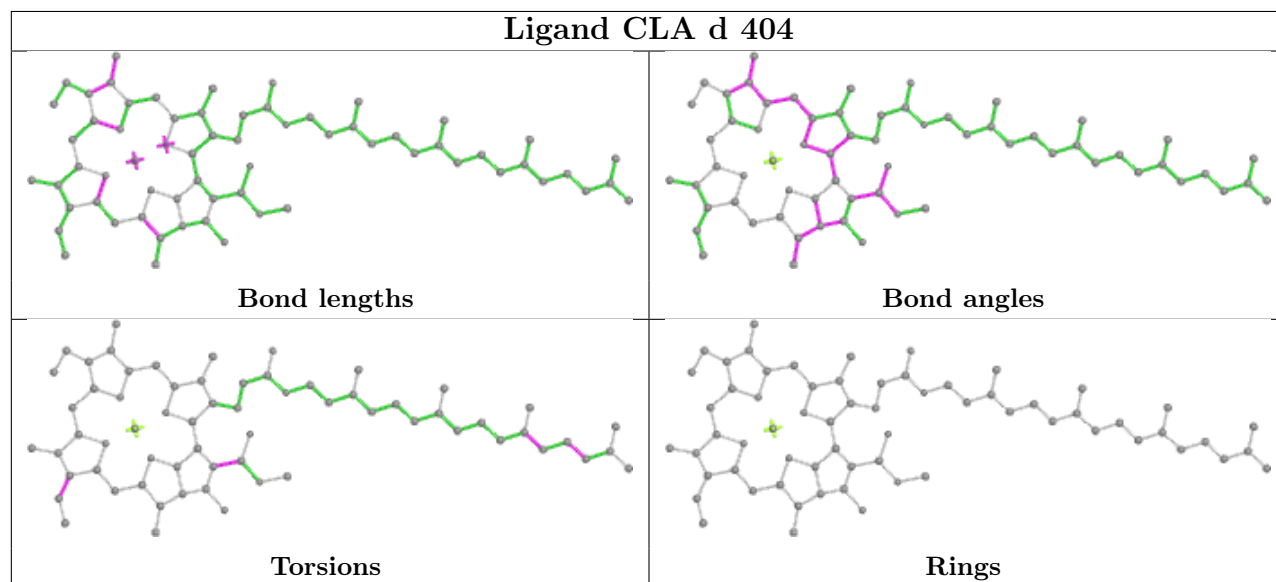
Ligand BCR b 619



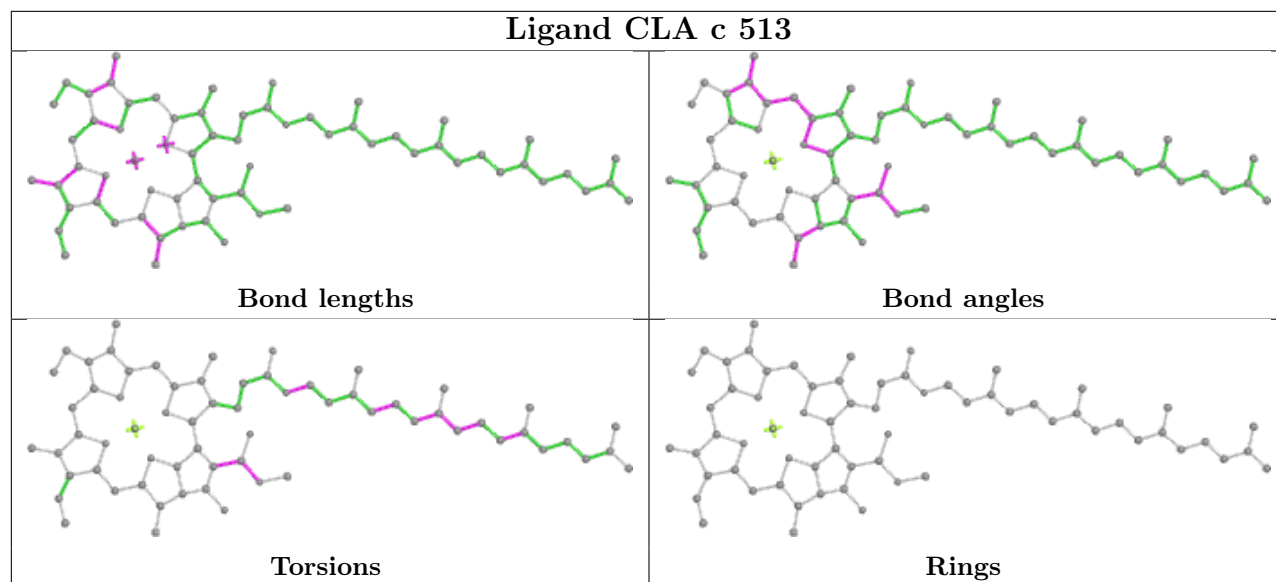
Ligand CLA B 610



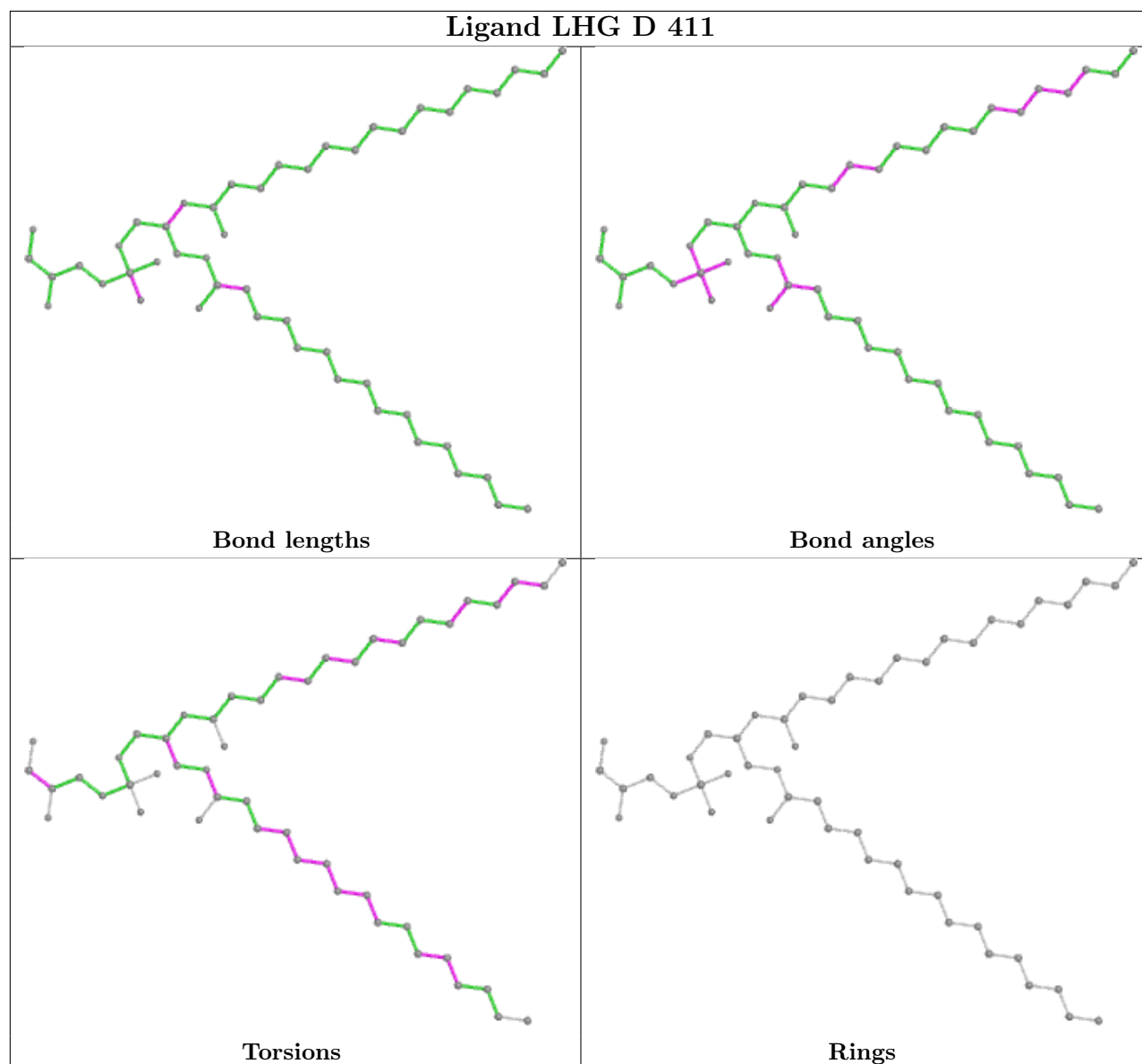
Ligand CLA d 404

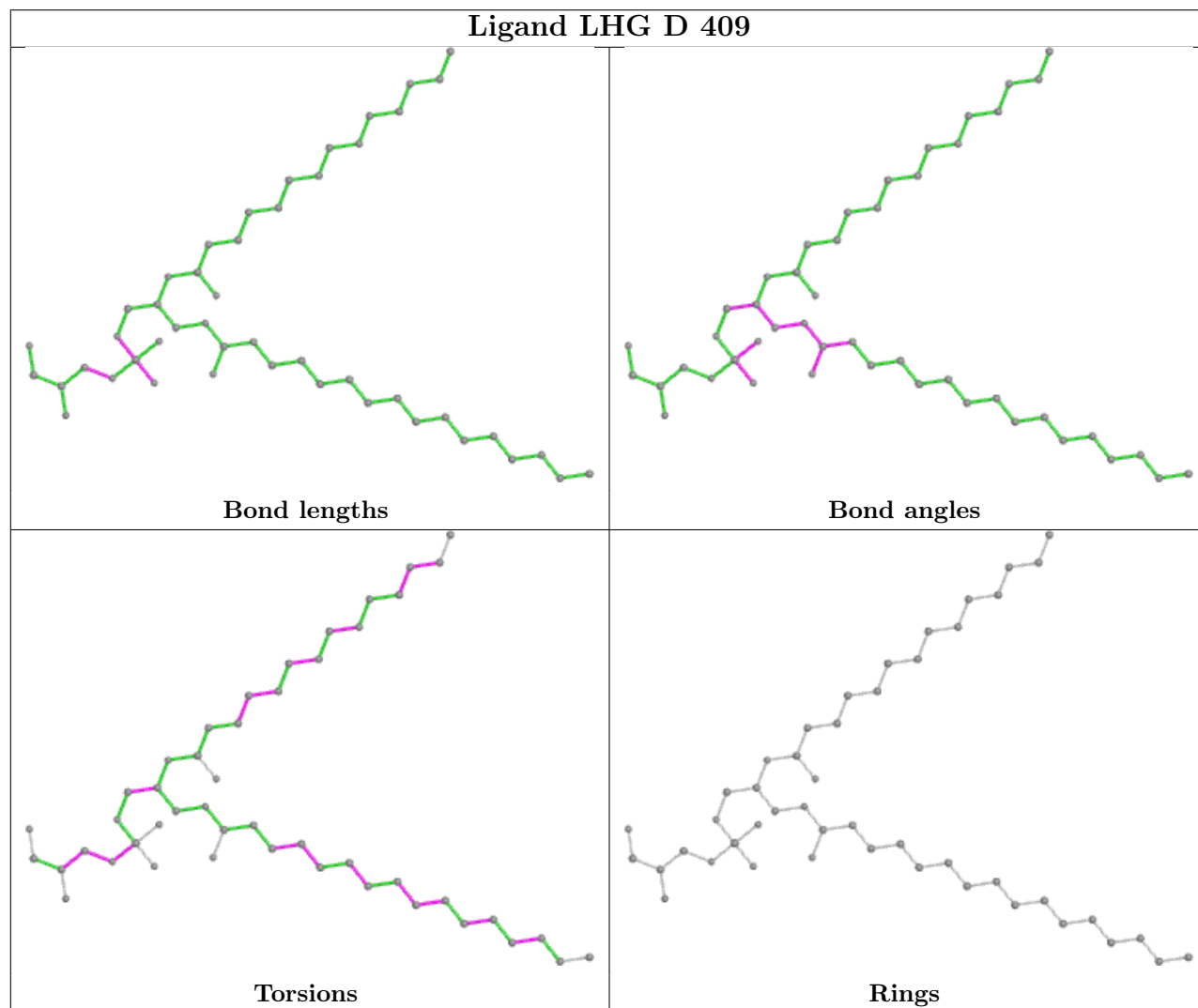
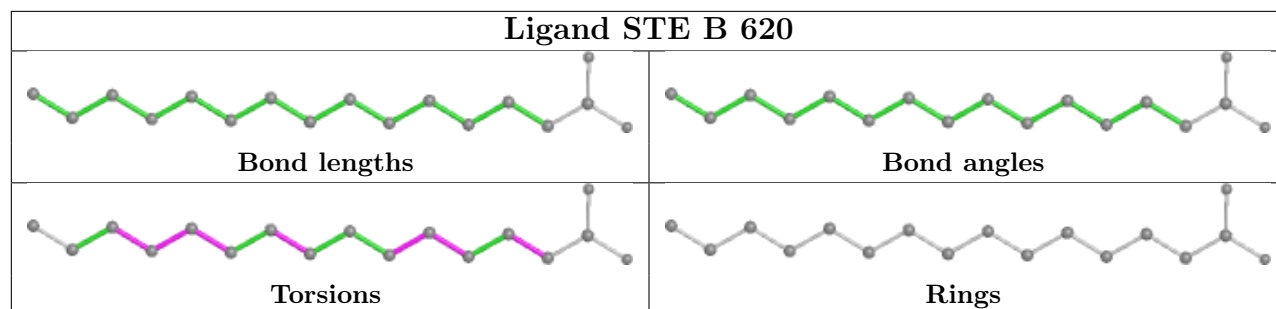


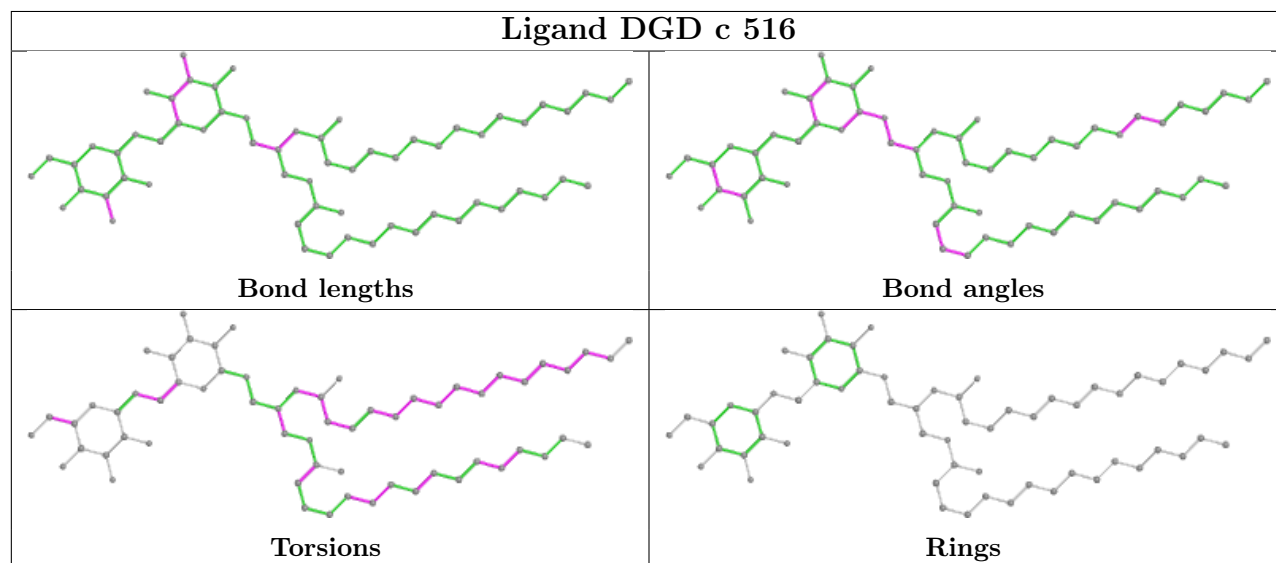
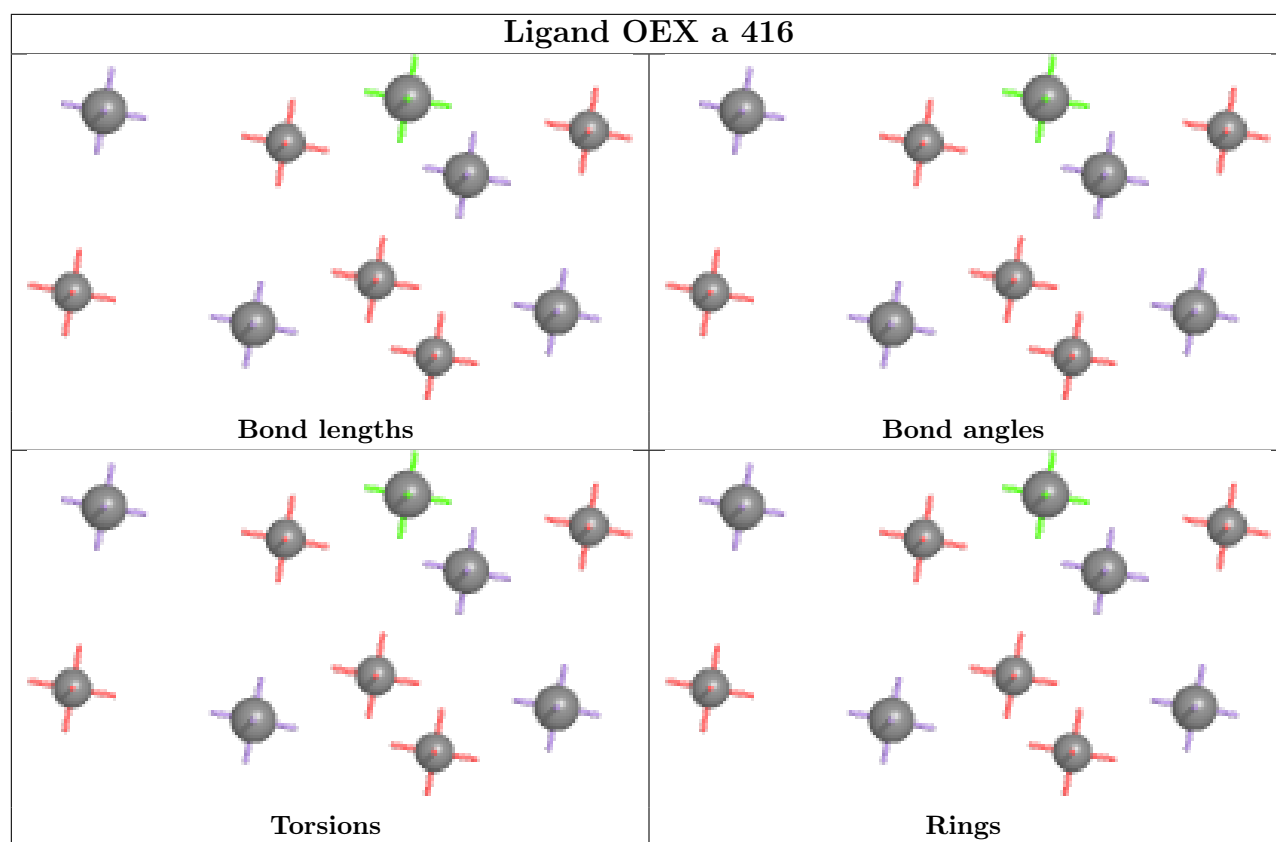
Ligand CLA c 513



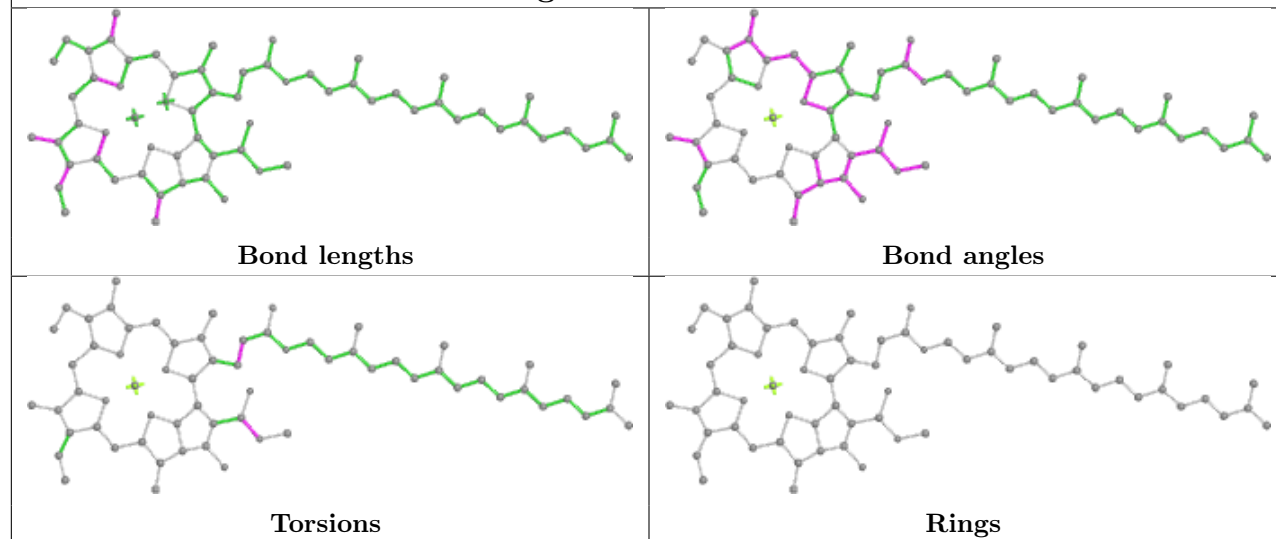
Ligand LHG D 411



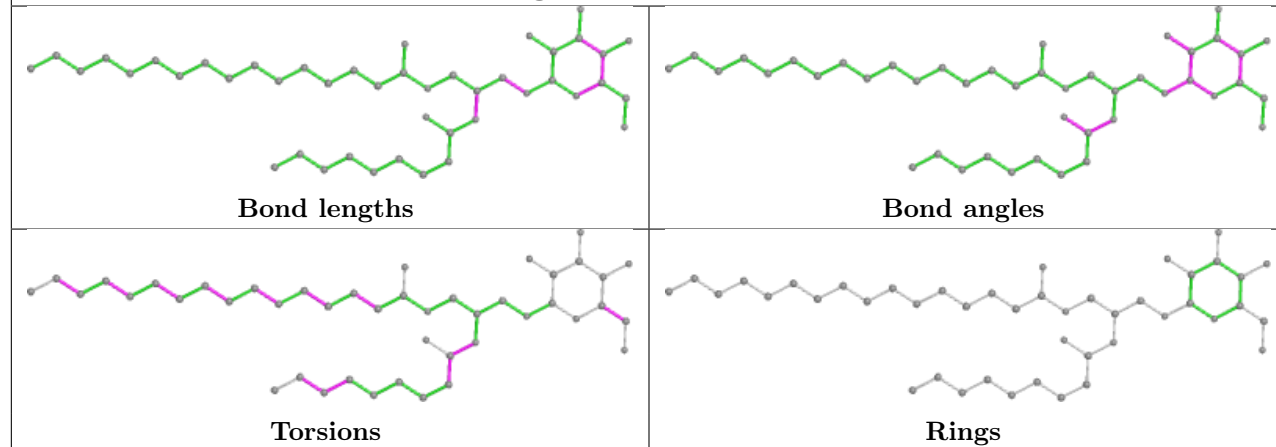




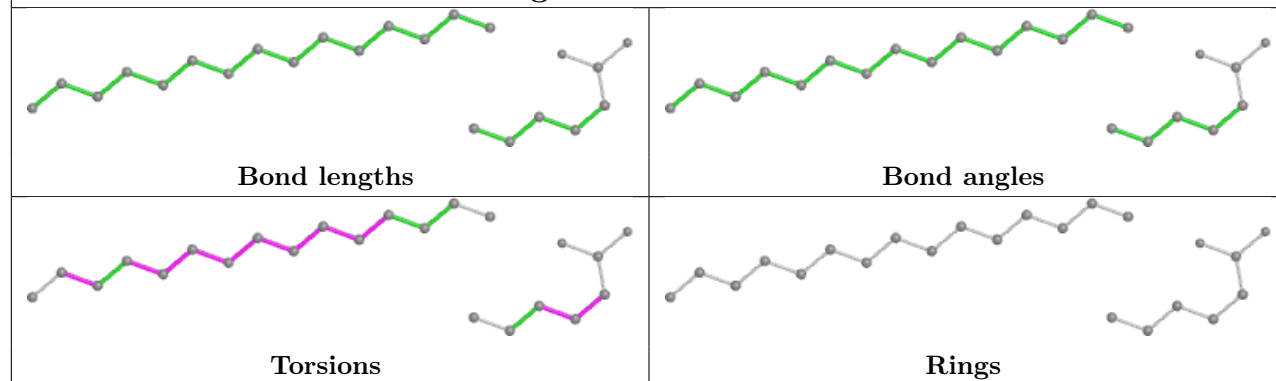
Ligand CLA c 501

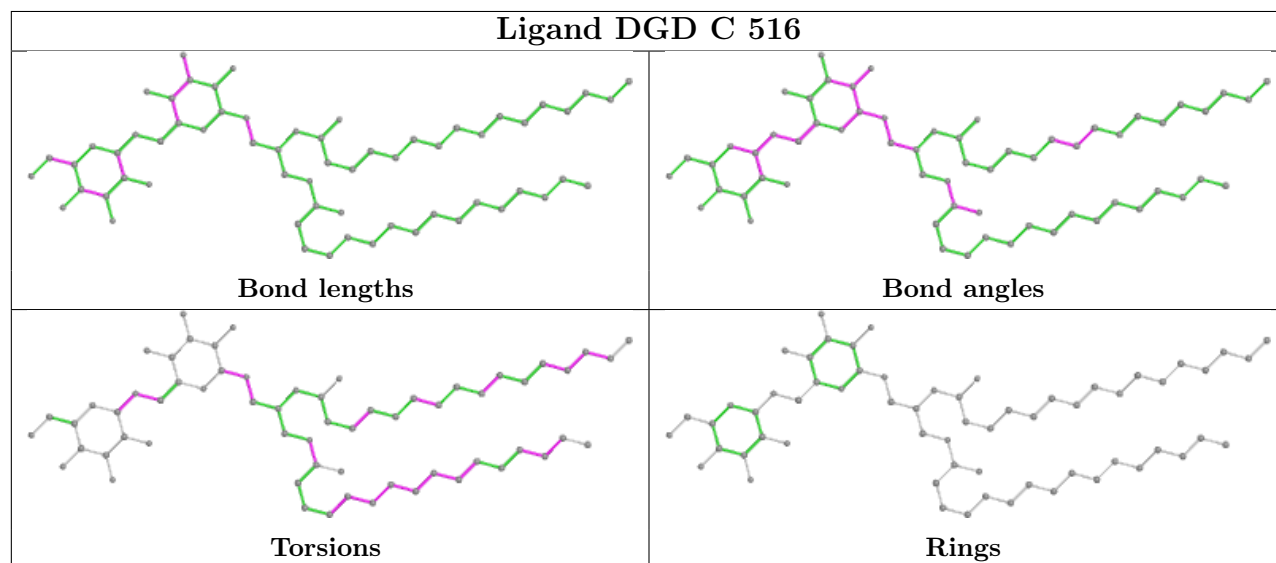
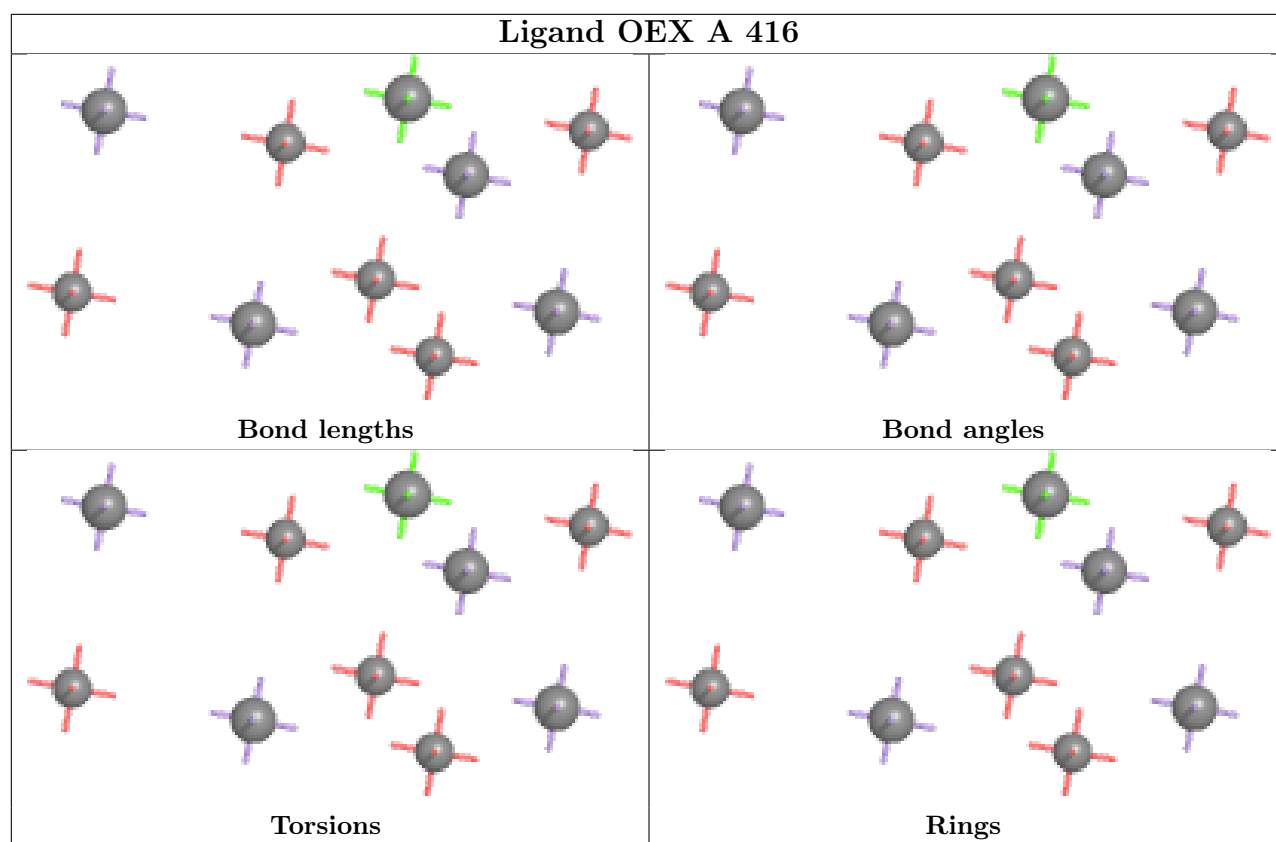


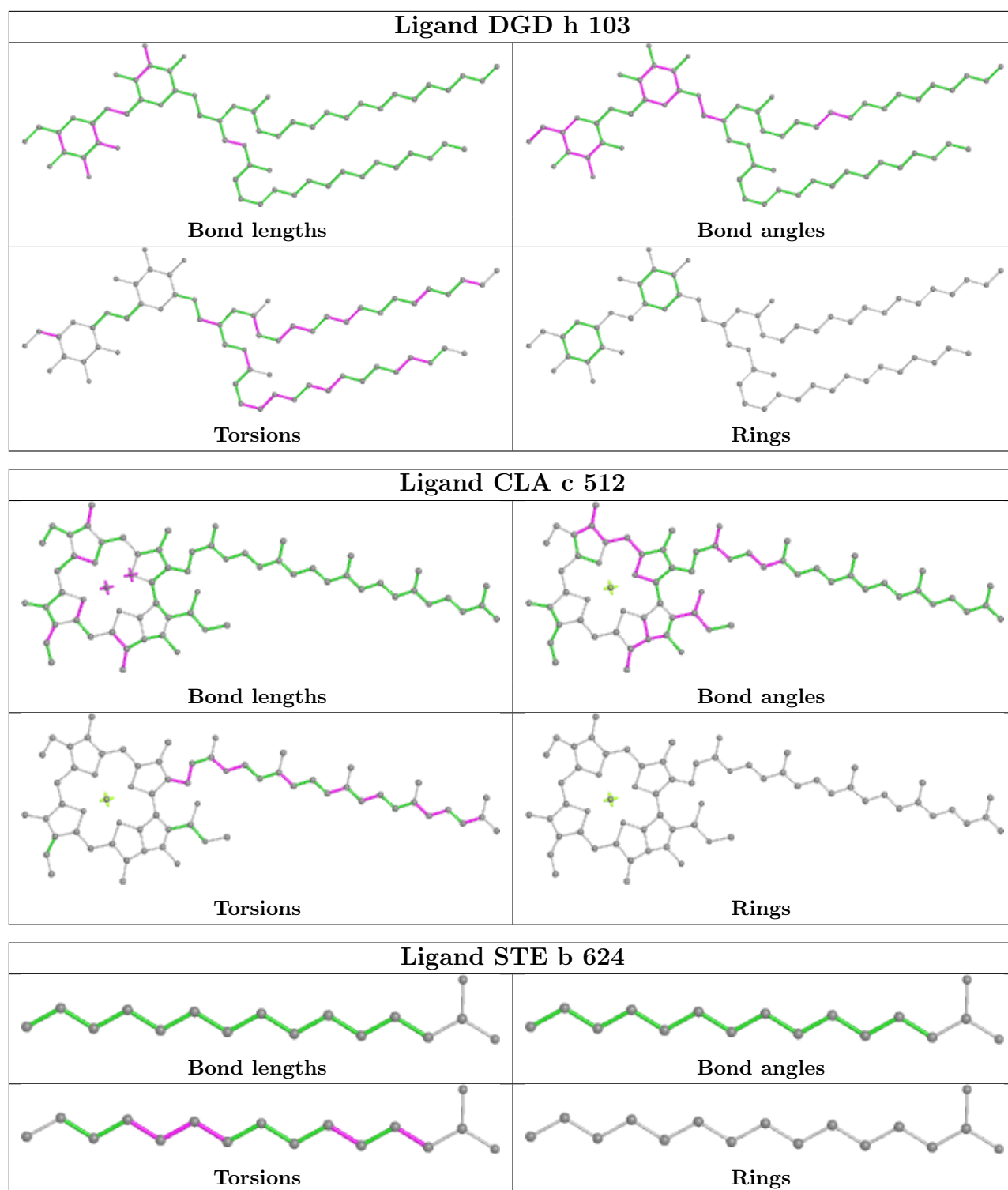
Ligand LMG d 410



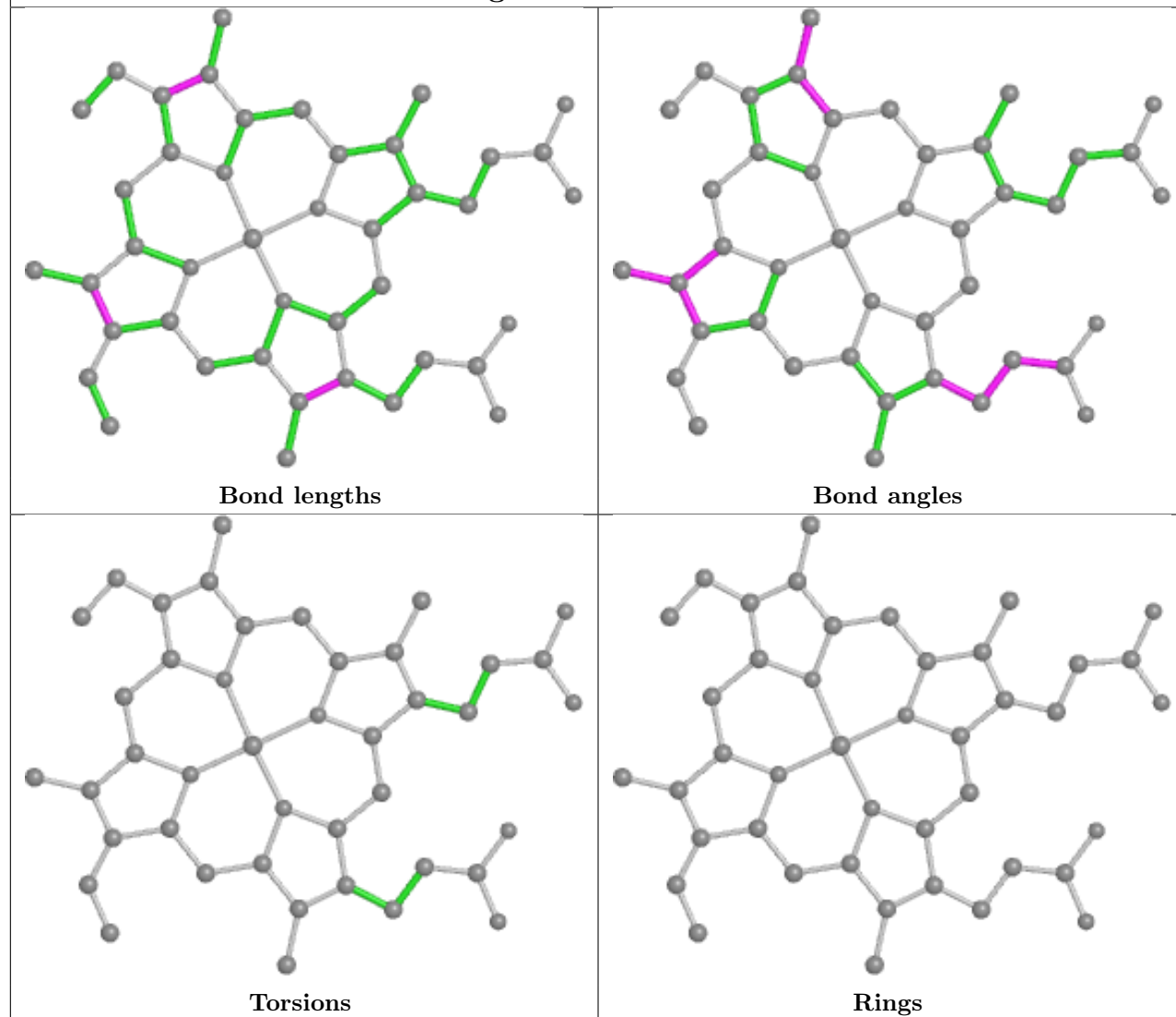
Ligand LMG h 102



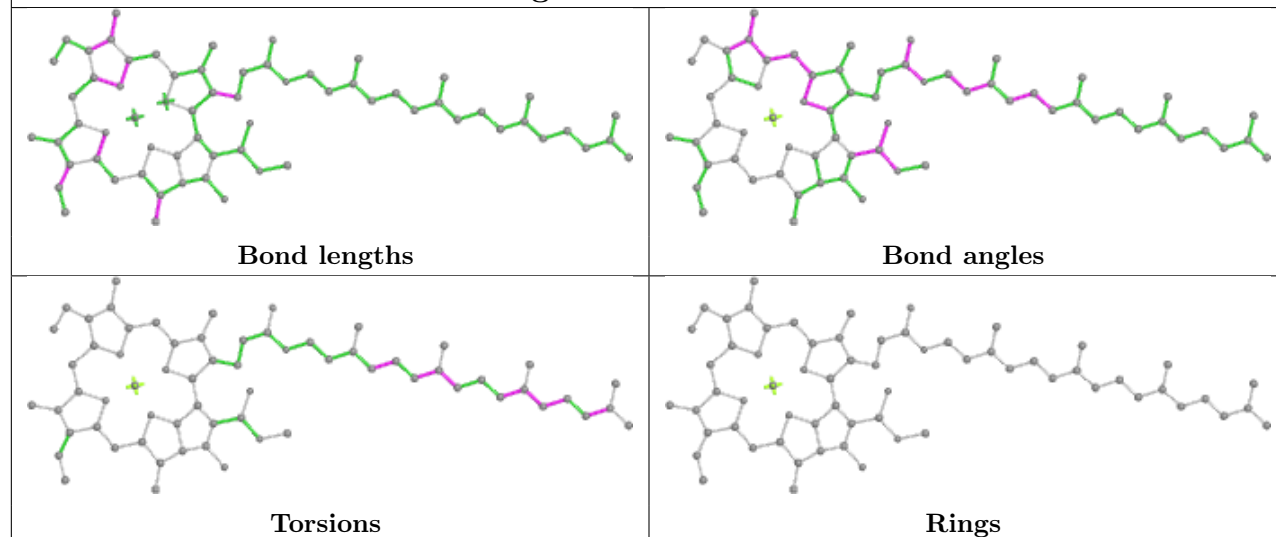




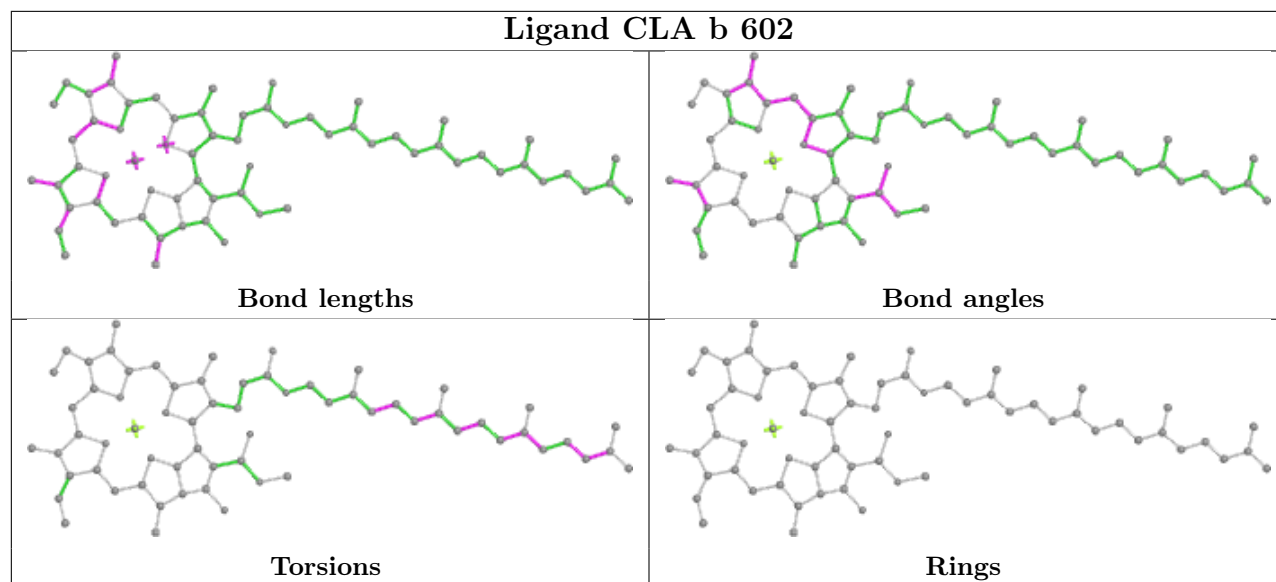
Ligand HEC V 201



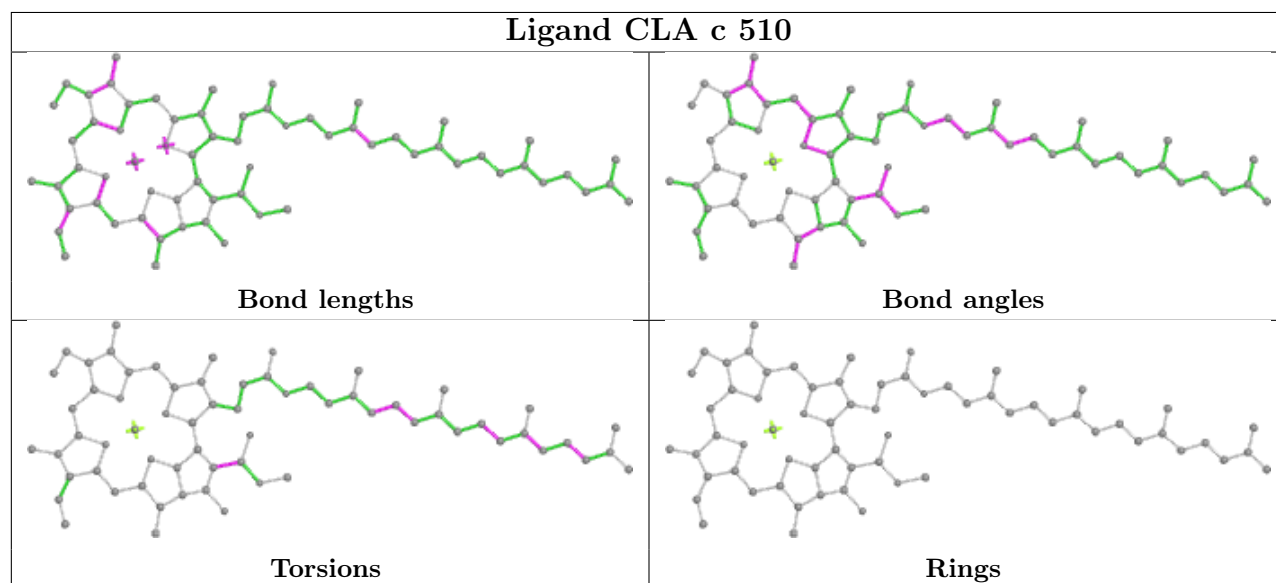
Ligand CLA A 403

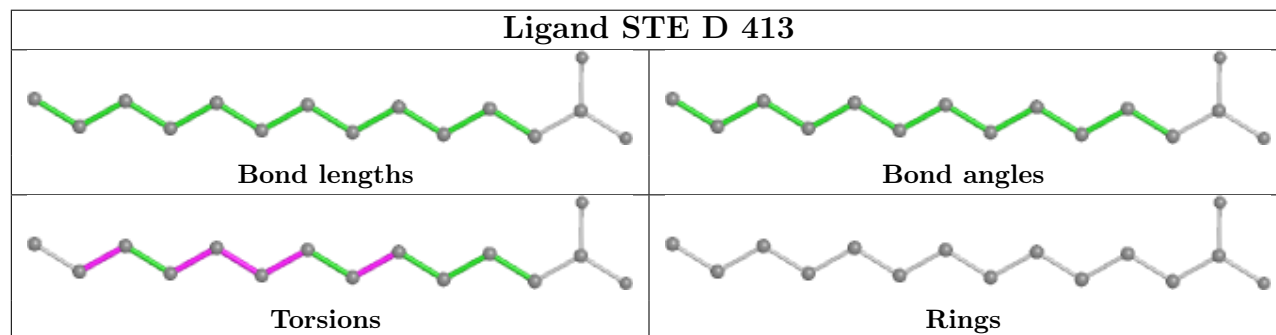
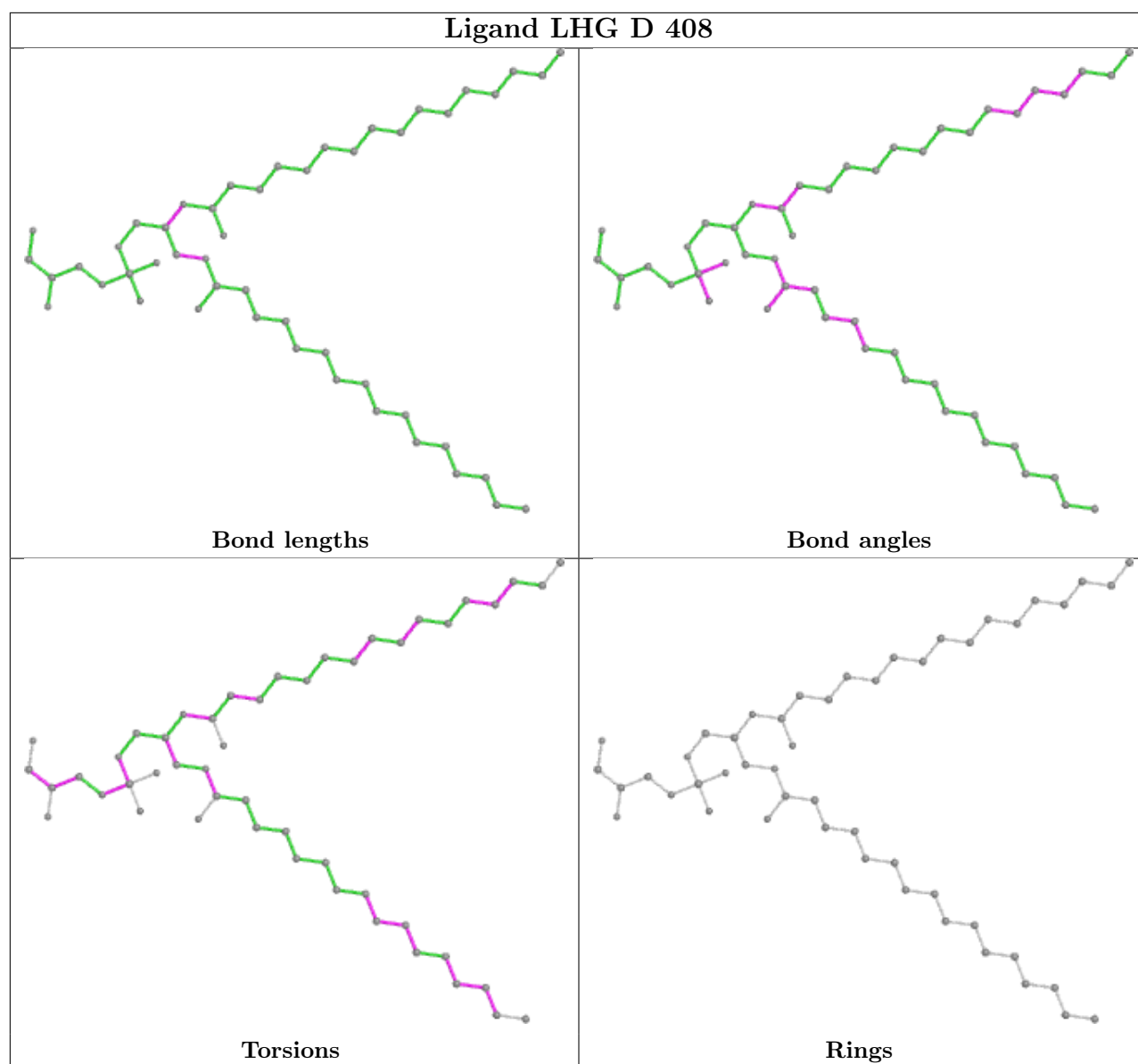


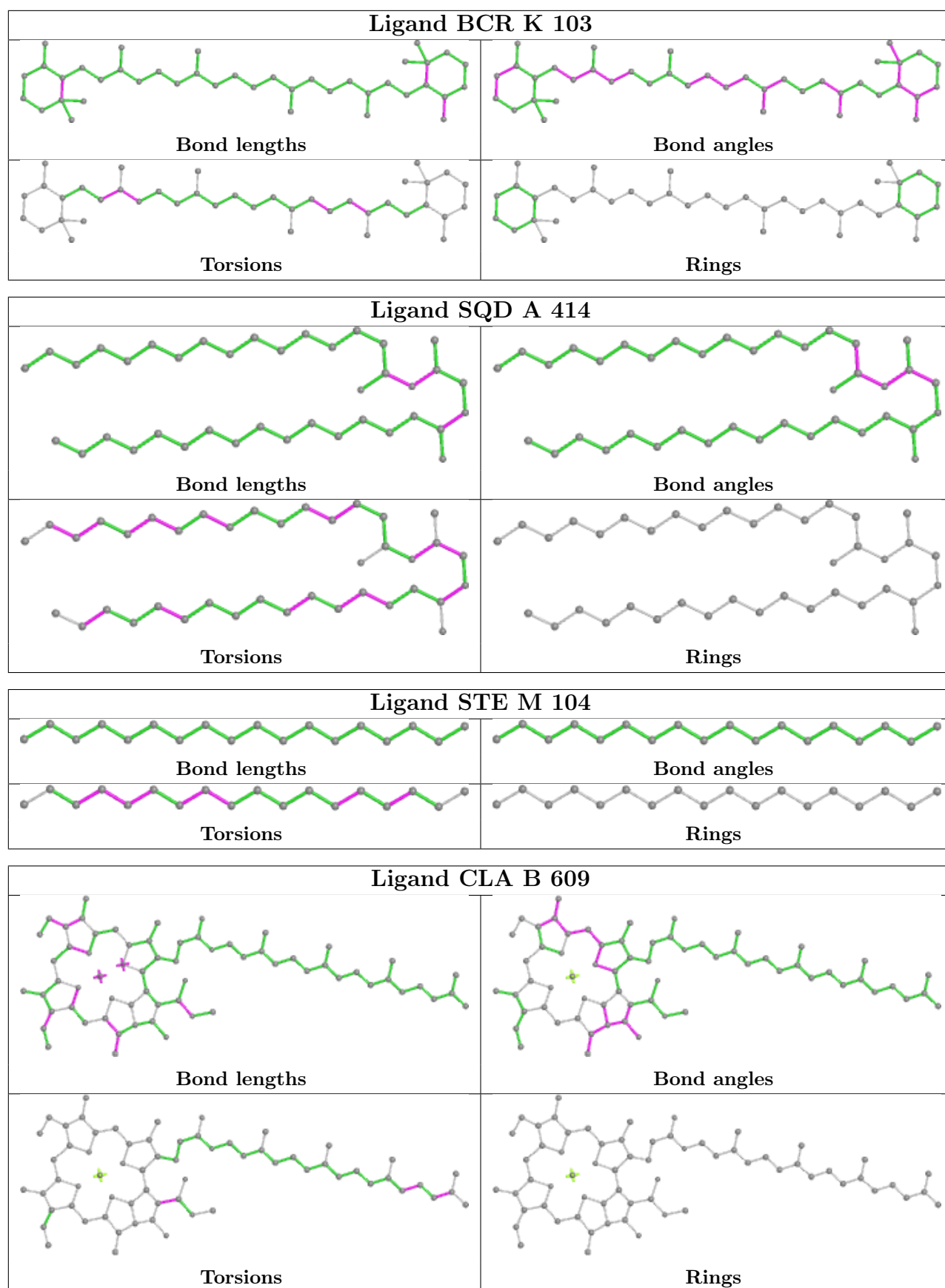
Ligand CLA b 602

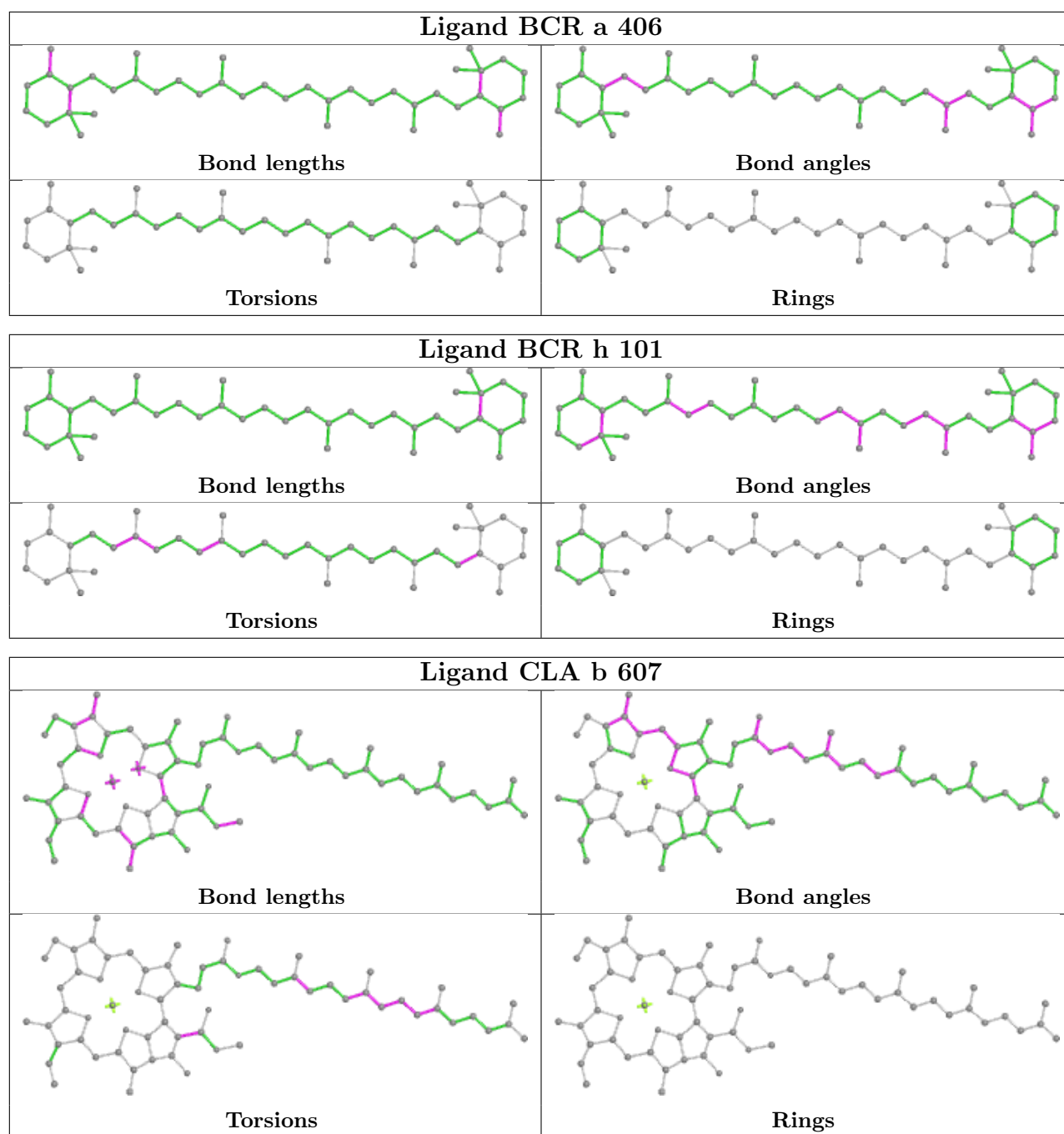


Ligand CLA c 510

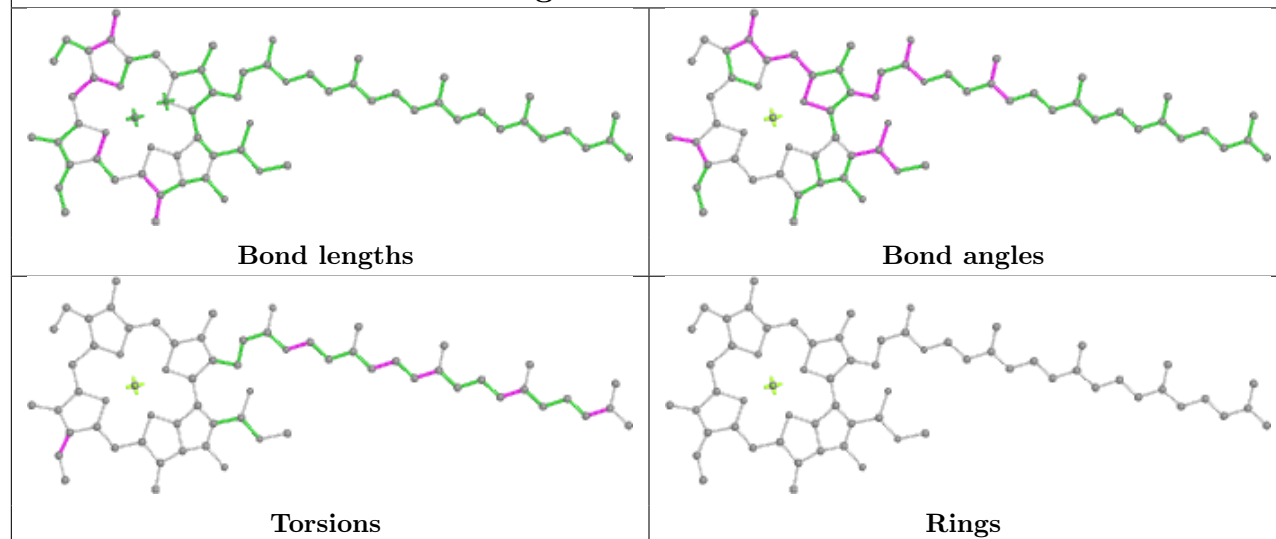




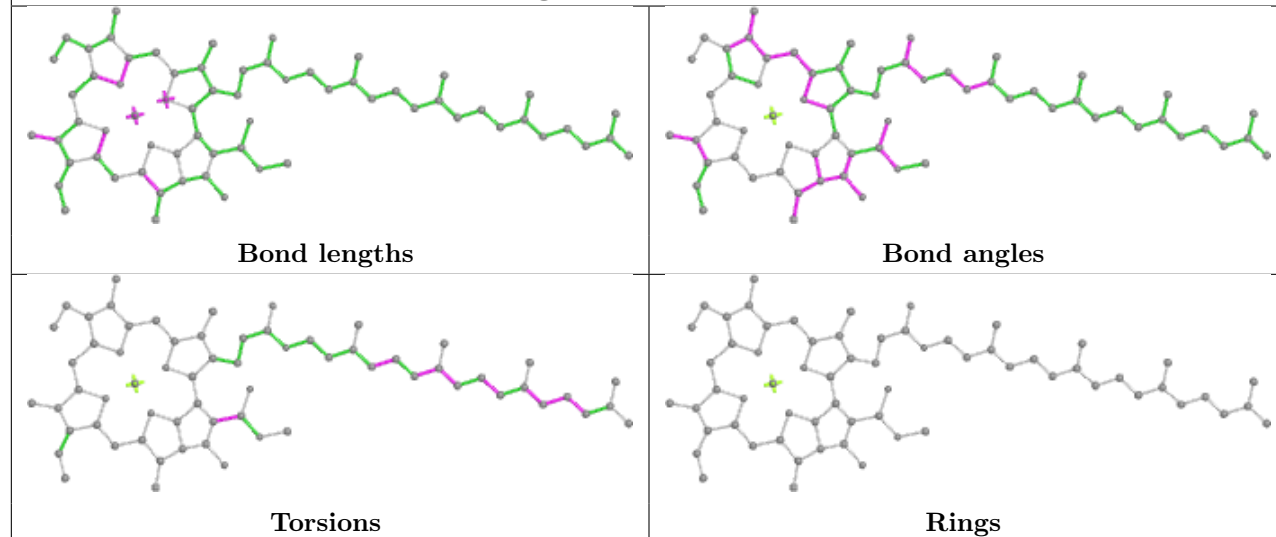




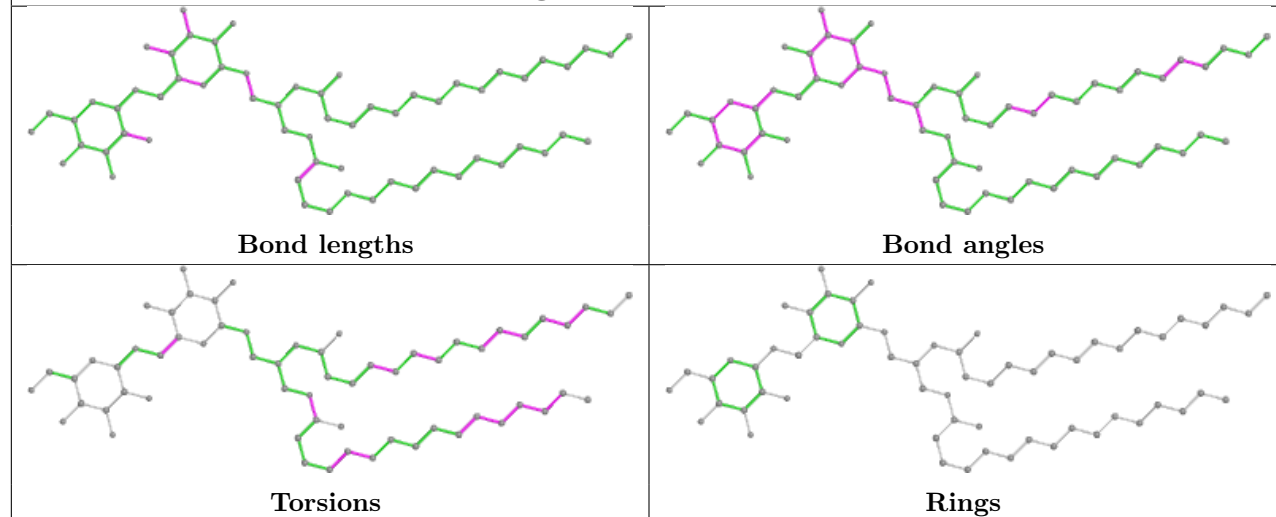
Ligand CLA d 403

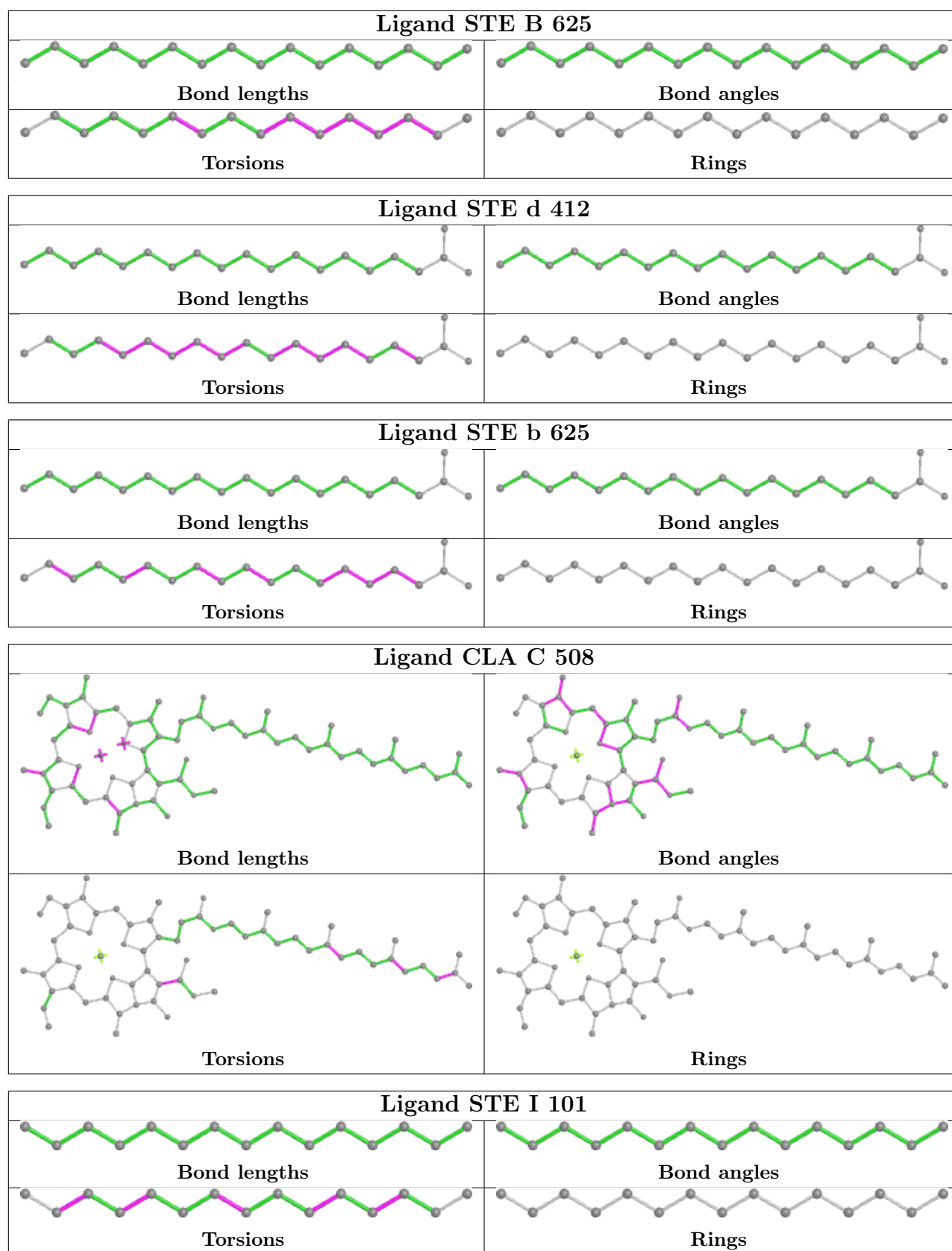


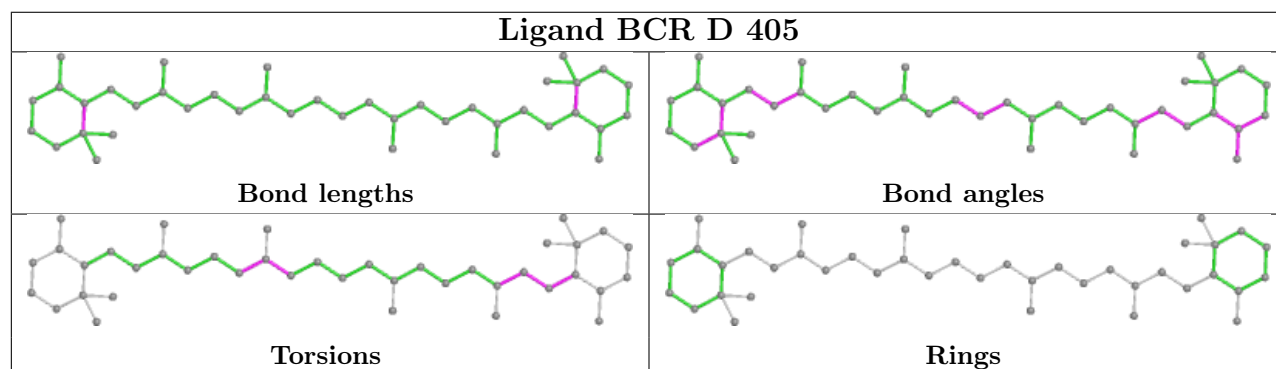
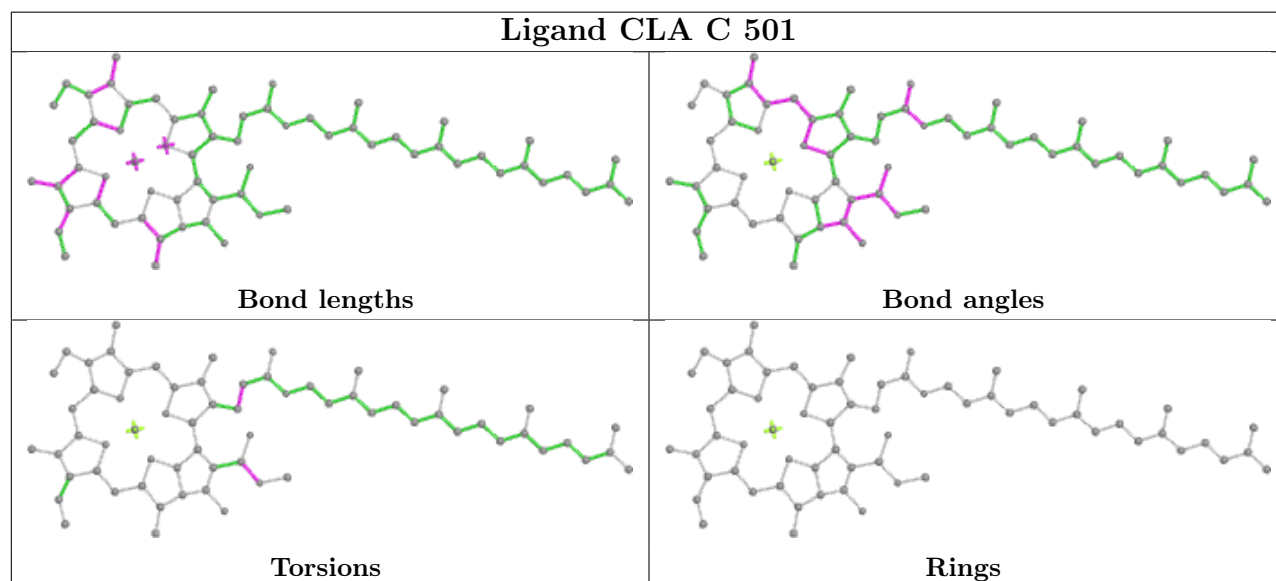
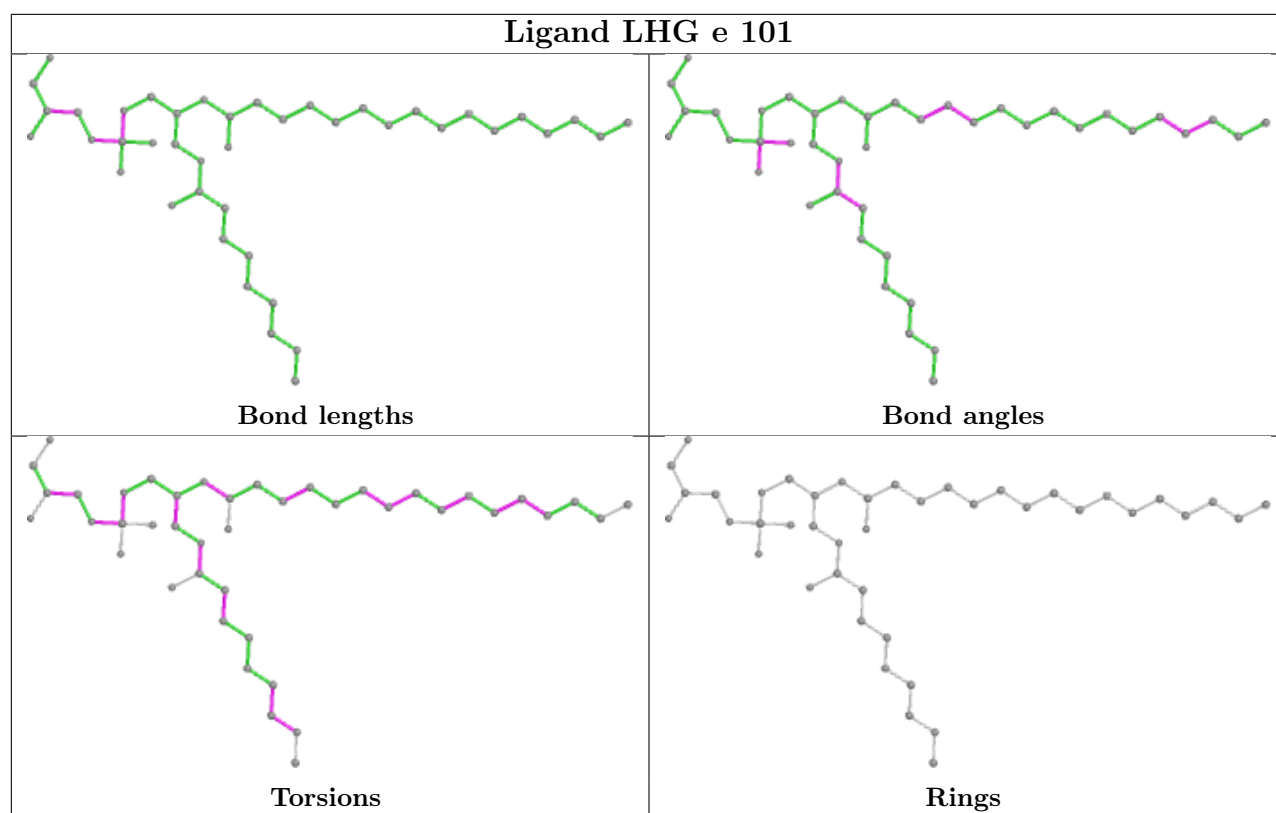
Ligand CLA b 604

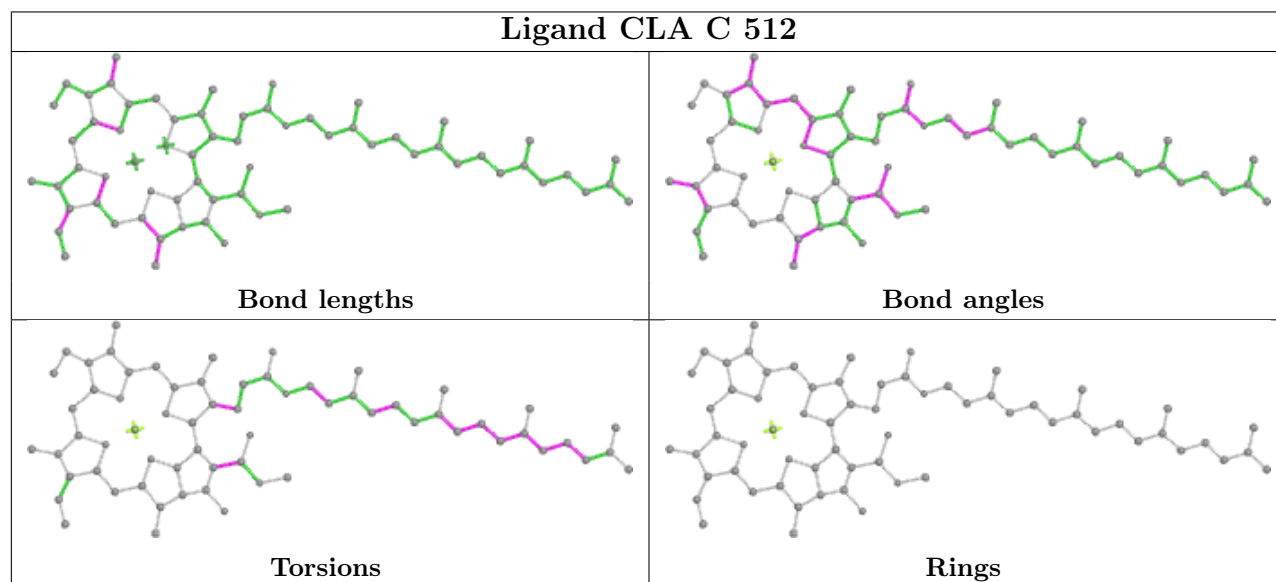
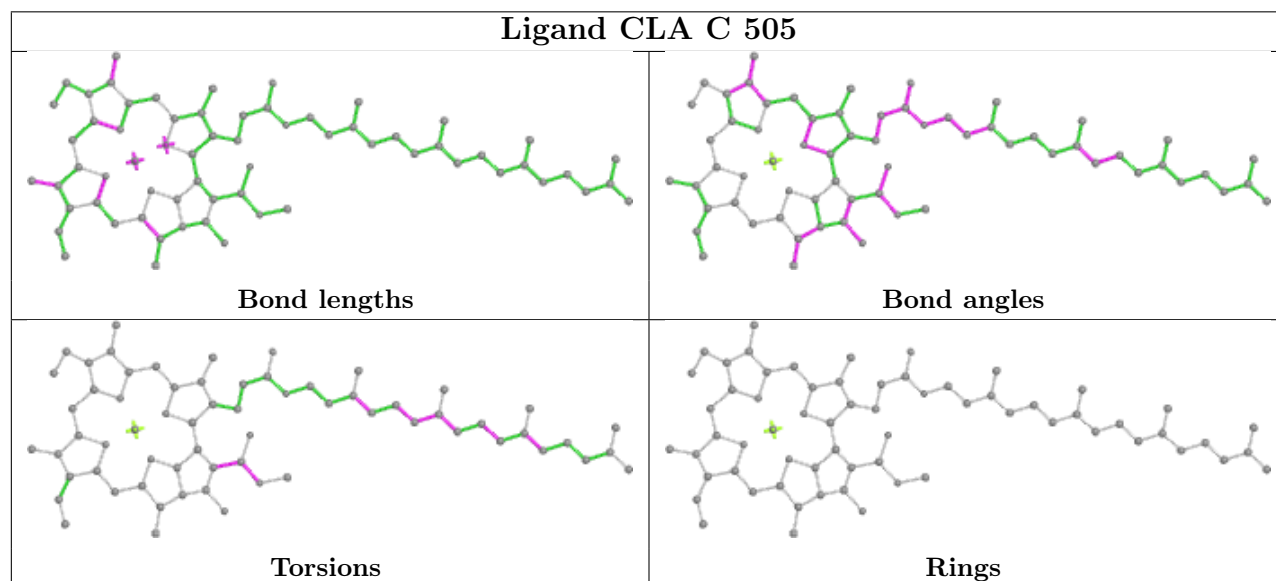
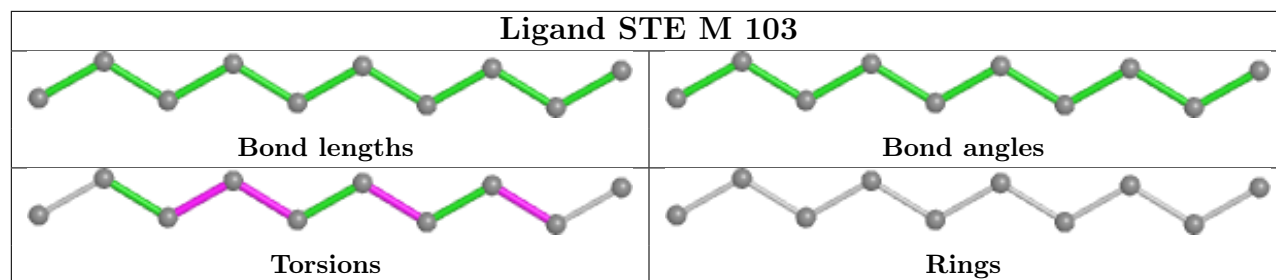


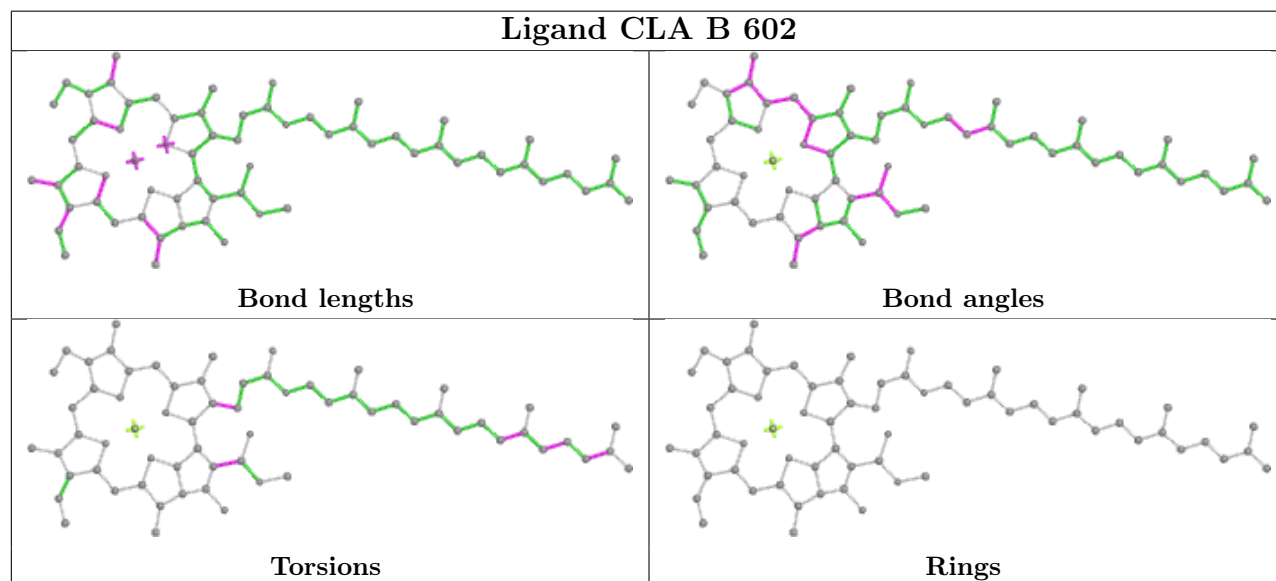
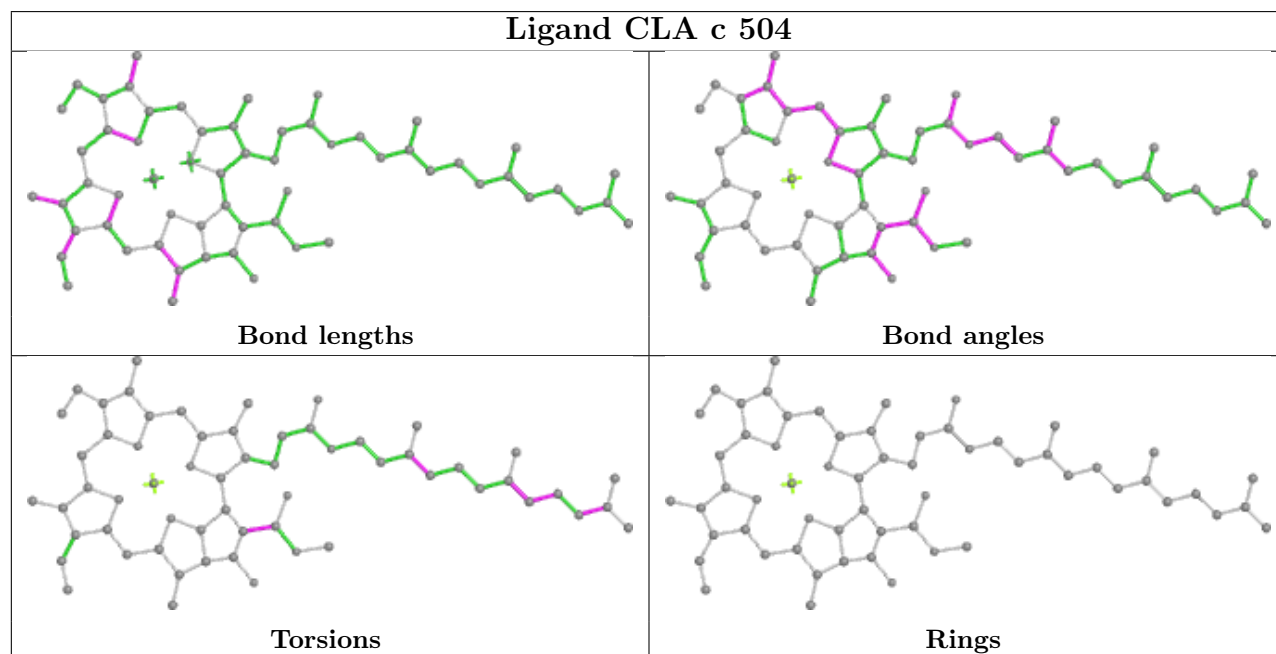
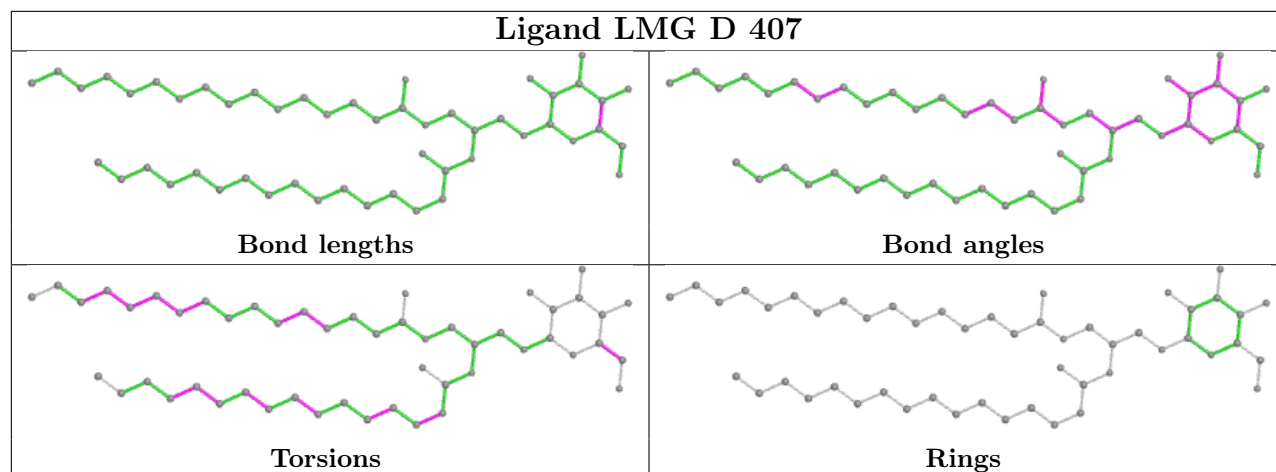
Ligand DGD c 518











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%)	-0.29	4 (1%) 79 81	21, 28, 47, 72	0
1	a	334/344 (97%)	-0.34	0 100 100	21, 30, 54, 71	0
2	B	505/510 (99%)	-0.26	8 (1%) 72 75	23, 32, 59, 82	0
2	b	505/510 (99%)	-0.09	20 (3%) 38 43	21, 35, 66, 97	0
3	C	442/461 (95%)	-0.20	6 (1%) 75 78	24, 35, 49, 72	0
3	c	451/461 (97%)	-0.10	8 (1%) 68 71	26, 38, 56, 85	0
4	D	341/352 (96%)	-0.24	1 (0%) 94 94	20, 29, 46, 74	0
4	d	341/352 (96%)	-0.19	0 100 100	21, 33, 55, 78	0
5	E	82/84 (97%)	0.08	2 (2%) 59 63	32, 49, 66, 74	0
5	e	82/84 (97%)	0.27	3 (3%) 41 46	38, 55, 73, 82	0
6	F	34/45 (75%)	-0.14	1 (2%) 51 56	34, 41, 62, 85	0
6	f	34/45 (75%)	-0.17	2 (5%) 22 26	41, 48, 75, 88	0
7	H	65/66 (98%)	-0.08	1 (1%) 73 76	29, 39, 55, 66	0
7	h	63/66 (95%)	0.26	3 (4%) 30 35	39, 48, 57, 66	0
8	I	35/38 (92%)	-0.06	3 (8%) 10 12	29, 36, 64, 77	0
8	i	35/38 (92%)	-0.17	2 (5%) 23 28	30, 38, 71, 78	0
9	J	36/40 (90%)	0.21	4 (11%) 5 6	32, 47, 75, 86	0
9	j	36/40 (90%)	0.21	4 (11%) 5 6	38, 49, 83, 90	0
10	K	37/46 (80%)	0.26	4 (10%) 5 7	40, 50, 65, 73	0
10	k	37/46 (80%)	0.14	1 (2%) 54 59	45, 53, 64, 70	0
11	L	37/37 (100%)	-0.45	0 100 100	22, 29, 58, 66	0
11	l	36/37 (97%)	-0.26	3 (8%) 11 14	24, 29, 64, 79	0
12	M	32/36 (88%)	-0.06	1 (3%) 49 54	25, 31, 53, 63	0
12	m	31/36 (86%)	-0.20	0 100 100	25, 32, 47, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	0.01	15 (6%) 21 25	24, 38, 75, 127	0
13	o	244/272 (89%)	-0.12	12 (4%) 29 34	22, 37, 74, 103	0
14	R	28/41 (68%)	2.52	16 (57%) 0 0	58, 67, 78, 90	0
14	r	28/41 (68%)	4.52	25 (89%) 0 0	65, 90, 109, 119	0
15	T	29/32 (90%)	-0.39	2 (6%) 16 20	24, 29, 53, 70	0
15	t	29/32 (90%)	-0.17	2 (6%) 16 20	25, 30, 68, 88	0
16	U	97/134 (72%)	-0.22	2 (2%) 63 67	30, 41, 64, 83	0
16	u	97/134 (72%)	-0.36	0 100 100	28, 38, 53, 77	0
17	V	137/163 (84%)	-0.44	0 100 100	29, 38, 54, 70	0
17	v	137/163 (84%)	-0.12	4 (2%) 51 56	30, 44, 62, 83	0
18	X	38/41 (92%)	0.05	2 (5%) 26 31	38, 48, 65, 75	0
18	x	39/41 (95%)	0.54	5 (12%) 3 4	44, 56, 84, 98	0
19	Y	27/46 (58%)	1.48	10 (37%) 0 0	50, 67, 83, 89	0
19	y	30/46 (65%)	0.59	4 (13%) 3 4	57, 70, 79, 89	0
20	Z	62/62 (100%)	1.04	16 (25%) 0 0	51, 66, 106, 117	0
20	z	62/62 (100%)	0.97	12 (19%) 1 1	57, 67, 99, 111	0
All	All	5293/5700 (92%)	-0.08	208 (3%) 39 44	20, 36, 69, 127	0

All (208) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	O	60	ARG	8.5
14	r	14	LEU	8.3
13	o	58	ASN	8.3
15	t	30	THR	8.0
2	b	495	PHE	7.1
14	r	29	LYS	6.9
14	r	28	VAL	6.8
14	r	9	LEU	6.7
20	z	33	TRP	6.4
14	r	18	TRP	6.2
14	r	3	TRP	6.2
20	Z	33	TRP	6.0
14	R	3	TRP	5.7
14	r	26	TYR	5.7
14	r	10	LEU	5.7

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Mol	Chain	Res	Type	RSRZ
14	r	6	LEU	5.6
13	O	62	GLU	5.6
13	o	4	THR	5.4
13	O	59	LYS	5.3
13	O	3	GLN	5.3
20	z	35	ARG	5.3
14	r	25	PRO	5.2
14	r	13	LEU	5.2
13	o	3	GLN	5.1
1	A	13	LEU	5.1
19	Y	41	VAL	5.0
13	O	61	GLN	5.0
14	R	6	LEU	5.0
14	r	24	LEU	5.0
20	Z	37	LYS	5.0
20	Z	62	VAL	4.9
13	O	56	PRO	4.7
3	c	23	ALA	4.7
20	Z	7	LEU	4.7
9	j	6	GLY	4.6
20	Z	32	ASP	4.6
2	B	495	PHE	4.5
14	r	19	ALA	4.5
14	r	2	ASP	4.5
9	j	5	GLY	4.5
14	r	27	ALA	4.4
13	O	4	THR	4.4
14	r	7	VAL	4.4
20	Z	35	ARG	4.3
14	R	26	TYR	4.2
9	J	5	GLY	4.2
19	Y	43	ARG	4.1
13	o	59	LYS	4.1
15	T	30	THR	4.1
3	c	146	PHE	4.1
9	j	7	ARG	4.1
14	R	21	ARG	4.1
20	Z	42	LEU	4.1
14	R	25	PRO	4.0
14	r	5	VAL	4.0
6	F	12	SER	4.0
14	r	4	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
2	b	127	ARG	4.0
14	r	23	ILE	4.0
18	X	2	THR	3.9
5	E	79	PHE	3.9
9	J	8	ILE	3.9
14	r	15	ALA	3.9
9	J	7	ARG	3.8
2	b	488	PRO	3.7
20	Z	34	ASP	3.7
2	b	505	ARG	3.7
14	R	20	VAL	3.7
4	D	12	ARG	3.6
20	Z	3	ILE	3.6
19	y	18	VAL	3.6
2	B	505	ARG	3.6
19	Y	20	ALA	3.6
20	Z	61	VAL	3.5
3	c	147	PHE	3.5
3	c	143	TYR	3.5
14	r	11	PRO	3.5
20	z	62	VAL	3.5
2	b	502	VAL	3.5
5	e	79	PHE	3.5
19	Y	37	PHE	3.5
2	b	85	GLY	3.5
14	r	22	ASN	3.4
20	Z	38	GLN	3.4
18	x	34	ILE	3.4
19	Y	21	GLN	3.4
19	Y	40	ALA	3.4
7	H	66	GLY	3.4
14	R	18	TRP	3.4
18	x	2	THR	3.4
13	o	61	GLN	3.4
1	A	11	ALA	3.3
14	R	10	LEU	3.3
8	I	36	ASP	3.3
3	c	24	THR	3.3
13	o	60	ARG	3.3
13	o	56	PRO	3.3
2	b	486	LEU	3.2
14	r	12	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
13	O	63	ALA	3.2
2	b	487	SER	3.2
19	Y	42	ARG	3.2
13	o	57	LYS	3.2
5	E	83	LEU	3.2
10	K	17	ILE	3.2
20	z	3	ILE	3.2
9	j	8	ILE	3.1
14	R	2	ASP	3.1
14	R	24	LEU	3.1
2	B	127	ARG	3.1
9	J	6	GLY	3.0
18	x	38	GLN	3.0
7	h	6	TRP	3.0
14	R	14	LEU	3.0
14	R	5	VAL	3.0
8	I	34	ARG	3.0
2	b	491	VAL	2.9
20	Z	1	MET	2.9
5	e	61	ARG	2.9
3	C	146	PHE	2.9
14	r	16	ALA	2.9
13	o	5	LEU	2.9
19	y	37	PHE	2.9
20	Z	4	LEU	2.9
2	B	293	ALA	2.8
11	l	3	PRO	2.8
2	b	490	GLN	2.8
2	b	128	THR	2.8
14	R	28	VAL	2.8
20	Z	41	PHE	2.8
15	t	29	ILE	2.8
20	z	1	MET	2.8
14	R	29	LYS	2.8
13	O	5	LEU	2.8
19	Y	25	ILE	2.7
20	Z	60	PHE	2.7
20	z	37	LYS	2.7
19	y	19	ILE	2.7
17	v	15	GLU	2.7
12	M	33	GLN	2.7
2	B	294	SER	2.7

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Mol	Chain	Res	Type	RSRZ
2	b	295	GLY	2.7
14	R	13	LEU	2.7
20	z	36	SER	2.6
13	o	207	ARG	2.6
18	X	3	ILE	2.6
16	U	8	GLU	2.6
2	B	506	ARG	2.5
2	b	289	GLN	2.6
3	c	191	PRO	2.5
7	h	21	VAL	2.5
13	o	132	ASN	2.5
8	i	34	ARG	2.5
20	Z	59	PHE	2.5
20	z	7	LEU	2.5
2	b	293	ALA	2.5
20	z	41	PHE	2.5
2	b	161	LEU	2.5
10	k	17	ILE	2.5
2	B	485	GLU	2.5
6	f	12	SER	2.4
13	O	35	SER	2.4
18	x	37	VAL	2.4
18	x	40	SER	2.4
3	c	262	ARG	2.4
13	O	57	LYS	2.4
13	O	246	ALA	2.4
19	y	40	ALA	2.4
20	z	30	PRO	2.4
2	B	295	GLY	2.4
2	b	496	TYR	2.4
7	h	10	ILE	2.3
6	f	13	TYR	2.3
2	b	503	THR	2.3
2	b	506	ARG	2.3
15	T	29	ILE	2.3
14	R	9	LEU	2.3
2	b	294	SER	2.3
11	l	2	GLU	2.3
11	l	7	ARG	2.3
8	i	36	ASP	2.2
17	v	17	LYS	2.2
20	z	60	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	145	SER	2.2
19	Y	44	GLY	2.2
10	K	18	PHE	2.2
1	A	12	ASN	2.2
3	c	25	ASN	2.2
8	I	35	LYS	2.2
1	A	16	ARG	2.1
14	r	21	ARG	2.1
3	C	57	ALA	2.1
17	v	22	THR	2.1
2	b	292	LEU	2.1
5	e	83	LEU	2.1
13	O	37	THR	2.1
3	C	143	TYR	2.1
19	Y	22	LEU	2.1
17	v	21	LEU	2.0
3	C	61	VAL	2.0
13	o	62	GLU	2.0
3	C	122	SER	2.0
10	K	10	LYS	2.0
13	O	89	SER	2.0
10	K	14	ALA	2.0
16	U	9	LEU	2.0
20	z	2	THR	2.0
13	O	86	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	FME	T	1	10/11	0.94	0.09	27,46,62,62	0
15	FME	t	1	10/11	0.94	0.09	29,43,65,65	0
12	FME	m	1	10/11	0.95	0.11	35,43,58,66	0
8	FME	I	1	10/11	0.96	0.13	40,48,60,60	0
8	FME	i	1	10/11	0.96	0.18	39,48,60,60	0
12	FME	M	1	10/11	0.96	0.11	39,53,66,71	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
32	STE	E	101	12/20	0.68	0.35	52,76,90,92	0
32	STE	B	627	16/20	0.72	0.21	39,47,69,72	0
32	STE	b	625	20/20	0.72	0.22	45,67,80,91	0
32	STE	j	101	12/20	0.74	0.16	42,57,69,72	0
32	STE	H	103	18/20	0.75	0.29	54,82,92,98	0
32	STE	C	519	16/20	0.75	0.17	45,58,76,76	0
32	STE	B	625	16/20	0.75	0.29	37,64,85,88	0
26	PL9	a	409	55/55	0.76	0.29	44,72,88,94	0
27	LMG	h	102	23/55	0.77	0.25	47,65,83,88	0
32	STE	a	415	12/20	0.77	0.23	45,68,76,82	0
32	STE	m	102	12/20	0.77	0.23	49,64,81,90	0
32	STE	b	626	10/20	0.78	0.24	45,57,66,79	0
29	LHG	A	413	49/49	0.78	0.24	48,83,110,124	0
28	SQD	a	412	36/54	0.78	0.18	32,66,92,99	0
32	STE	I	101	15/20	0.79	0.18	43,60,76,80	0
26	PL9	A	410	55/55	0.79	0.30	46,66,88,93	0
32	STE	c	522	12/20	0.80	0.21	58,71,85,89	0
30	DGD	o	301	44/66	0.81	0.16	38,58,81,95	0
32	STE	B	620	17/20	0.81	0.15	35,52,71,82	0
27	LMG	D	410	32/55	0.81	0.18	36,58,75,85	0
27	LMG	c	521	48/55	0.81	0.23	50,77,103,106	0
24	BCR	h	101	40/40	0.81	0.15	34,52,73,80	0
32	STE	d	412	20/20	0.81	0.20	47,65,79,80	0
22	CLA	b	601	65/65	0.81	0.18	46,66,84,89	0
24	BCR	H	101	40/40	0.81	0.15	33,48,66,72	0
30	DGD	A	415	66/66	0.82	0.17	47,63,79,89	0
29	LHG	e	101	42/49	0.82	0.23	64,84,110,118	0
32	STE	a	413	10/20	0.83	0.24	40,65,68,69	0
28	SQD	A	414	39/54	0.83	0.18	44,62,91,95	0
22	CLA	C	512	65/65	0.83	0.17	35,53,82,90	0
32	STE	D	413	15/20	0.83	0.22	33,40,65,65	0
32	STE	c	520	20/20	0.84	0.17	43,58,91,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	c	513	65/65	0.84	0.20	39,65,104,105	0
32	STE	B	623	12/20	0.84	0.12	37,49,69,82	0
22	CLA	c	512	65/65	0.84	0.17	38,54,82,93	0
32	STE	T	102	15/20	0.84	0.18	52,65,79,81	0
32	STE	M	104	18/20	0.85	0.14	35,52,79,82	0
32	STE	b	624	16/20	0.86	0.16	44,61,82,89	0
24	BCR	K	102	40/40	0.86	0.12	36,54,68,73	0
32	STE	M	103	10/20	0.86	0.16	36,47,60,69	0
27	LMG	b	623	55/55	0.86	0.24	46,71,92,102	0
22	CLA	B	601	65/65	0.87	0.15	32,62,87,99	0
28	SQD	b	620	49/54	0.87	0.14	43,59,84,98	0
22	CLA	C	513	65/65	0.87	0.18	39,61,91,95	0
32	STE	d	411	17/20	0.87	0.14	44,57,65,77	0
32	STE	B	624	18/20	0.87	0.12	38,60,76,78	0
24	BCR	K	101	40/40	0.87	0.16	44,58,74,78	0
28	SQD	B	621	54/54	0.87	0.15	42,65,90,100	0
32	STE	J	101	12/20	0.88	0.11	46,58,69,77	0
32	STE	B	622	14/20	0.88	0.12	39,49,62,66	0
27	LMG	Y	101	48/55	0.88	0.15	32,67,84,92	0
24	BCR	k	101	40/40	0.89	0.13	43,60,72,77	0
22	CLA	c	502	65/65	0.89	0.16	30,42,59,62	0
24	BCR	d	406	40/40	0.89	0.13	30,52,86,93	0
32	STE	C	520	12/20	0.89	0.09	35,49,59,59	0
28	SQD	f	102	41/54	0.89	0.20	57,92,112,114	0
27	LMG	A	411	48/55	0.89	0.14	43,58,72,79	0
22	CLA	d	405	65/65	0.89	0.17	29,48,81,89	0
32	STE	b	621	16/20	0.89	0.14	41,52,70,71	0
32	STE	b	622	20/20	0.89	0.22	37,59,81,84	0
32	STE	C	518	12/20	0.90	0.12	45,56,65,67	0
22	CLA	c	508	64/65	0.90	0.15	29,44,87,101	0
22	CLA	D	404	65/65	0.90	0.14	24,41,96,106	0
32	STE	D	412	20/20	0.90	0.14	36,52,75,78	0
27	LMG	m	101	51/55	0.90	0.13	35,54,76,95	0
22	CLA	b	615	65/65	0.90	0.14	25,39,59,59	0
22	CLA	b	616	60/65	0.90	0.13	26,43,84,91	0
27	LMG	M	101	51/55	0.90	0.12	32,49,73,81	0
22	CLA	a	405	65/65	0.90	0.14	18,37,74,82	0
32	STE	M	102	15/20	0.90	0.15	33,50,71,73	0
24	BCR	k	102	40/40	0.90	0.17	42,53,69,69	0
32	STE	B	626	12/20	0.90	0.44	57,69,80,85	0
27	LMG	c	519	37/55	0.90	0.16	40,63,78,78	0
24	BCR	c	514	40/40	0.91	0.15	41,60,71,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	BCR	C	514	40/40	0.91	0.11	25,39,50,58	0
24	BCR	D	405	40/40	0.91	0.12	23,46,83,85	0
22	CLA	B	616	60/65	0.91	0.15	25,38,88,95	0
22	CLA	C	502	65/65	0.91	0.13	27,40,52,54	0
30	DGD	C	516	62/66	0.91	0.13	31,52,95,110	0
27	LMG	a	414	49/55	0.91	0.13	30,59,83,100	0
22	CLA	C	507	65/65	0.91	0.15	21,39,57,60	0
22	CLA	B	604	65/65	0.92	0.13	19,32,70,84	0
27	LMG	D	407	51/55	0.92	0.16	23,55,83,89	0
22	CLA	c	510	65/65	0.92	0.15	30,47,62,65	0
22	CLA	c	511	65/65	0.92	0.12	37,52,68,71	0
24	BCR	K	103	40/40	0.92	0.16	37,51,65,66	0
24	BCR	b	619	40/40	0.92	0.11	31,46,61,65	0
22	CLA	C	506	65/65	0.92	0.12	28,45,78,89	0
30	DGD	H	102	62/66	0.92	0.11	30,47,59,66	0
22	CLA	b	609	65/65	0.92	0.13	29,44,61,69	0
22	CLA	c	503	65/65	0.92	0.14	32,42,53,59	0
24	BCR	B	618	40/40	0.92	0.10	23,39,49,53	0
24	BCR	B	619	40/40	0.92	0.10	27,43,59,67	0
22	CLA	c	505	65/65	0.92	0.17	24,40,64,67	0
22	CLA	c	507	65/65	0.92	0.15	29,44,58,67	0
22	CLA	c	506	65/65	0.93	0.14	31,49,95,99	0
22	CLA	C	510	65/65	0.93	0.13	25,43,59,61	0
30	DGD	c	517	62/66	0.93	0.12	30,50,87,88	0
30	DGD	h	103	62/66	0.93	0.11	27,47,63,72	0
22	CLA	b	602	65/65	0.93	0.15	26,43,62,65	0
24	BCR	T	101	40/40	0.93	0.10	25,37,49,51	0
22	CLA	c	509	65/65	0.93	0.18	31,47,67,72	0
22	CLA	b	606	65/65	0.93	0.12	23,39,67,75	0
24	BCR	c	515	40/40	0.93	0.11	25,44,55,64	0
22	CLA	C	511	65/65	0.93	0.10	28,48,63,72	0
22	CLA	b	610	65/65	0.93	0.18	24,37,50,55	0
22	CLA	b	614	65/65	0.93	0.13	23,39,71,79	0
28	SQD	a	411	54/54	0.93	0.15	40,62,96,97	0
22	CLA	B	614	65/65	0.93	0.16	20,37,67,77	0
22	CLA	C	505	65/65	0.93	0.16	20,40,69,72	0
22	CLA	B	615	65/65	0.93	0.12	20,37,57,63	0
22	CLA	a	403	65/65	0.93	0.14	24,41,88,95	0
22	CLA	c	504	60/65	0.93	0.12	29,44,74,85	0
22	CLA	B	606	65/65	0.93	0.10	23,36,64,71	0
22	CLA	d	404	65/65	0.94	0.13	18,30,45,53	0
22	CLA	C	503	65/65	0.94	0.13	31,41,50,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	BCR	A	407	40/40	0.94	0.09	25,35,44,44	0
22	CLA	C	504	59/65	0.94	0.12	30,42,77,79	0
26	PL9	D	406	55/55	0.94	0.10	21,33,47,53	0
29	LHG	D	409	47/49	0.94	0.12	24,51,77,89	0
22	CLA	B	610	65/65	0.94	0.14	19,33,44,50	0
22	CLA	B	613	65/65	0.94	0.14	18,31,66,75	0
30	DGD	C	515	62/66	0.94	0.13	18,39,69,77	0
22	CLA	B	602	65/65	0.94	0.15	23,35,53,66	0
22	CLA	C	508	65/65	0.94	0.10	26,42,91,97	0
22	CLA	b	604	65/65	0.94	0.14	21,34,68,80	0
30	DGD	c	518	62/66	0.94	0.14	26,52,78,83	0
22	CLA	C	509	65/65	0.94	0.17	25,46,61,69	0
22	CLA	b	608	65/65	0.94	0.15	23,42,61,66	0
22	CLA	A	406	54/65	0.94	0.12	19,31,64,72	0
24	BCR	b	617	40/40	0.94	0.12	24,41,52,54	0
24	BCR	b	618	40/40	0.94	0.11	23,39,52,56	0
27	LMG	d	410	44/55	0.94	0.12	32,54,88,100	0
22	CLA	A	403	65/65	0.94	0.14	22,34,95,103	0
22	CLA	b	612	65/65	0.94	0.17	17,34,48,58	0
22	CLA	b	613	65/65	0.94	0.13	19,35,66,78	0
22	CLA	B	609	65/65	0.94	0.12	26,38,59,66	0
28	SQD	F	102	36/54	0.94	0.19	45,74,95,99	0
22	CLA	B	603	65/65	0.95	0.15	17,32,65,67	0
22	CLA	B	608	65/65	0.95	0.12	20,34,55,59	0
29	LHG	a	410	49/49	0.95	0.13	32,52,70,77	0
29	LHG	d	409	39/49	0.95	0.10	28,41,68,74	0
22	CLA	b	605	65/65	0.95	0.11	21,34,48,52	0
22	CLA	c	501	65/65	0.95	0.13	28,40,52,55	0
24	BCR	a	406	40/40	0.95	0.08	19,33,49,50	0
22	CLA	d	403	65/65	0.95	0.12	18,35,54,59	0
30	DGD	C	517	62/66	0.95	0.10	26,47,73,79	0
22	CLA	A	402	65/65	0.95	0.10	17,27,45,49	0
30	DGD	c	516	62/66	0.95	0.12	22,43,76,81	0
22	CLA	b	607	65/65	0.95	0.12	17,36,64,75	0
23	PHO	A	404	64/64	0.95	0.10	17,28,42,48	0
23	PHO	a	404	64/64	0.95	0.13	20,31,38,44	0
22	CLA	D	402	65/65	0.95	0.12	17,27,53,64	0
24	BCR	B	617	40/40	0.95	0.11	26,38,56,56	0
28	SQD	A	412	52/54	0.95	0.13	35,58,85,88	0
22	CLA	B	605	65/65	0.95	0.14	18,31,47,49	0
22	CLA	C	501	65/65	0.95	0.13	19,35,46,56	0
24	BCR	t	101	40/40	0.95	0.08	26,37,50,54	0

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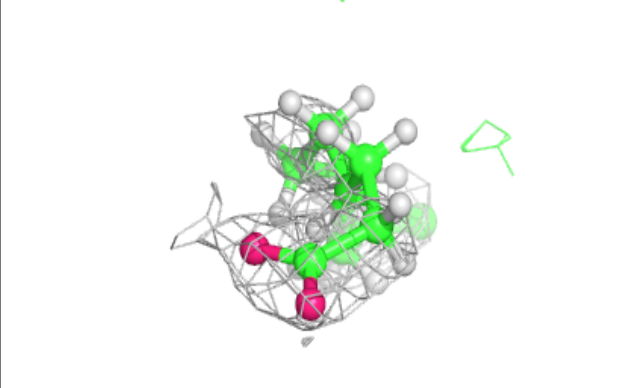
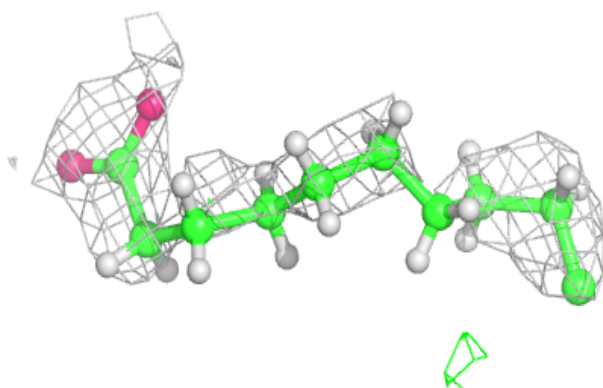
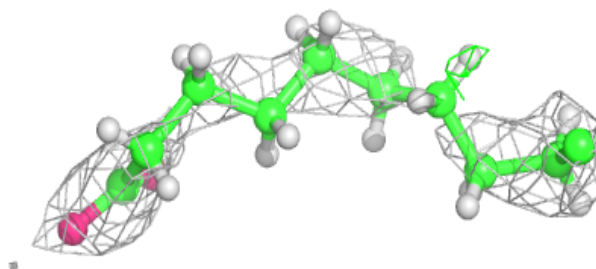
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	b	611	65/65	0.95	0.14	19,35,52,60	0
22	CLA	B	611	65/65	0.95	0.14	20,31,51,54	0
22	CLA	B	612	65/65	0.95	0.14	21,32,45,58	0
26	PL9	d	407	55/55	0.95	0.10	22,34,41,47	0
34	HEM	F	101	43/43	0.95	0.12	37,48,61,62	0
29	LHG	l	101	49/49	0.96	0.10	25,46,58,60	0
23	PHO	A	405	64/64	0.96	0.13	22,32,42,46	0
22	CLA	D	403	65/65	0.96	0.10	19,28,49,59	0
23	PHO	d	401	64/64	0.96	0.10	23,38,47,59	0
29	LHG	D	411	49/49	0.96	0.11	30,45,61,73	0
29	LHG	L	101	49/49	0.96	0.11	26,43,57,64	0
22	CLA	b	603	65/65	0.96	0.12	19,36,61,68	0
22	CLA	B	607	65/65	0.96	0.10	15,35,60,62	0
22	CLA	a	402	65/65	0.96	0.10	20,30,42,55	0
34	HEM	f	101	43/43	0.96	0.13	45,58,77,83	0
29	LHG	D	408	49/49	0.97	0.09	23,42,56,61	0
29	LHG	d	408	49/49	0.97	0.09	22,42,57,67	0
35	HEC	V	201	43/43	0.97	0.13	20,34,42,43	0
35	HEC	v	201	43/43	0.97	0.12	28,36,49,53	0
33	BCT	d	402	4/4	0.98	0.17	32,38,45,52	0
25	CL	a	408	1/1	0.98	0.06	28,28,28,28	0
21	FE2	a	401	1/1	0.98	0.11	35,35,35,35	0
25	CL	A	408	1/1	0.98	0.07	28,28,28,28	0
33	BCT	D	401	4/4	0.98	0.17	22,26,32,35	0
31	OEX	a	416	10/10	0.99	0.13	25,26,31,31	0
25	CL	a	407	1/1	0.99	0.03	28,28,28,28	0
21	FE2	A	401	1/1	0.99	0.10	26,26,26,26	0
31	OEX	A	416	10/10	0.99	0.12	22,26,29,31	0
25	CL	A	409	1/1	1.00	0.04	31,31,31,31	0

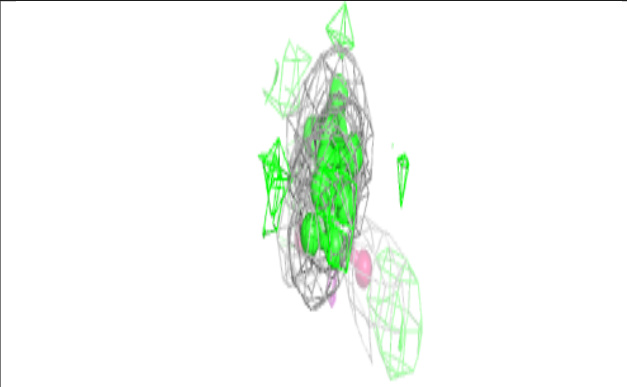
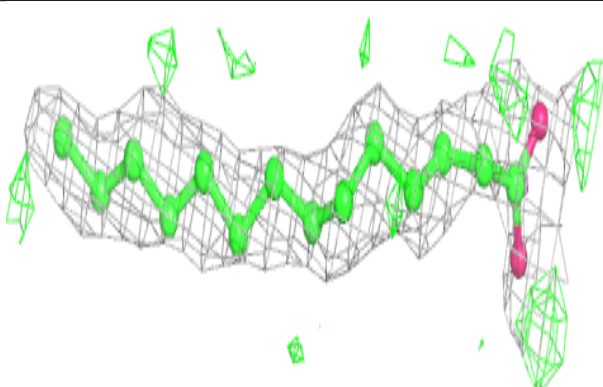
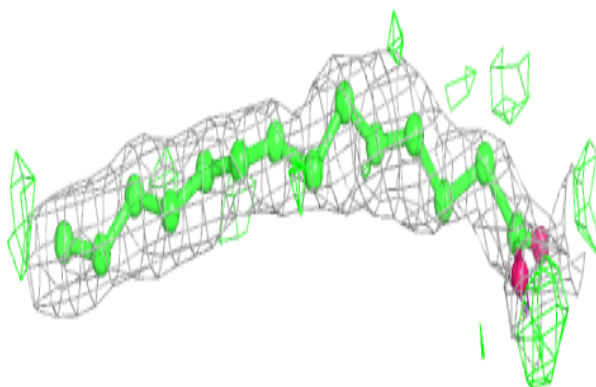
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around STE 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)

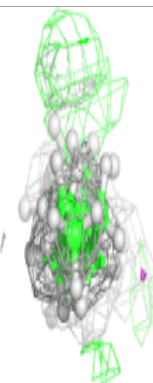
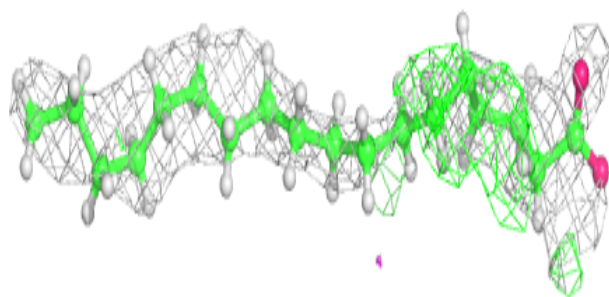
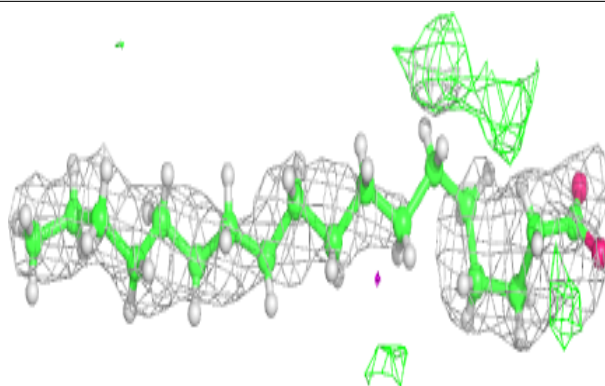
**Electron density around STE B 627:**

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

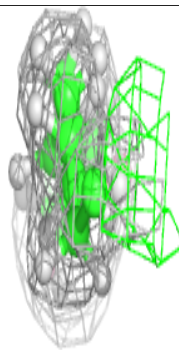
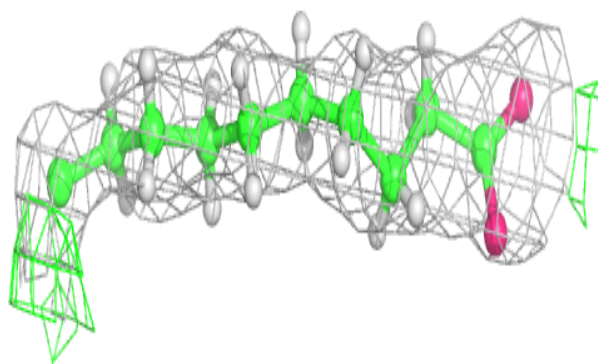
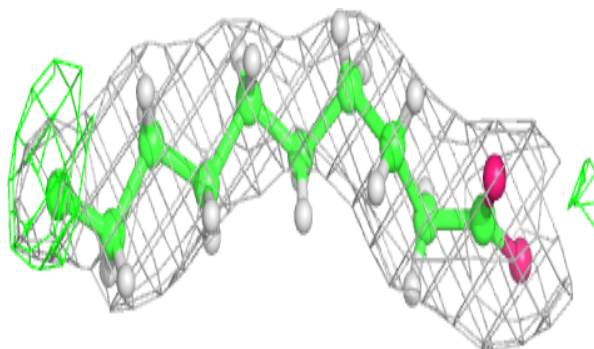


Electron density around STE b 625:

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

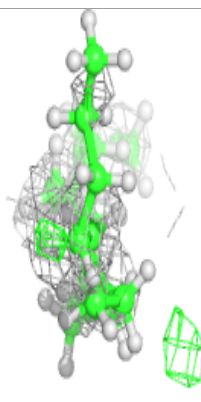
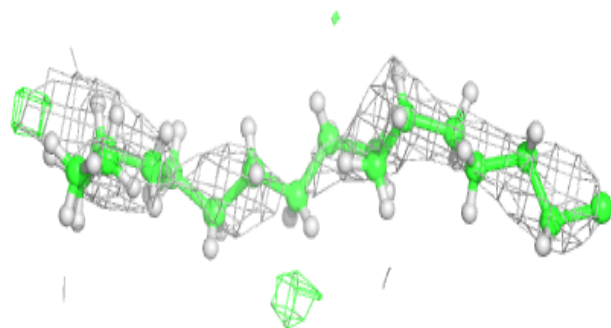
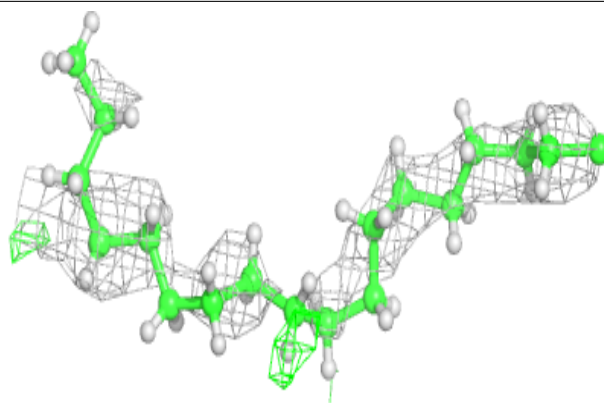
**Electron density around STE j 101:**

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

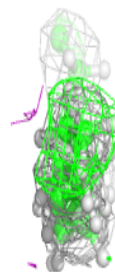
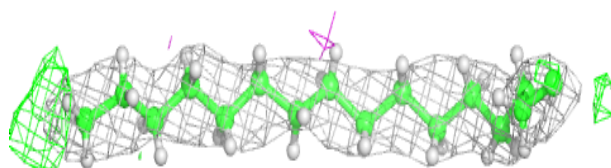
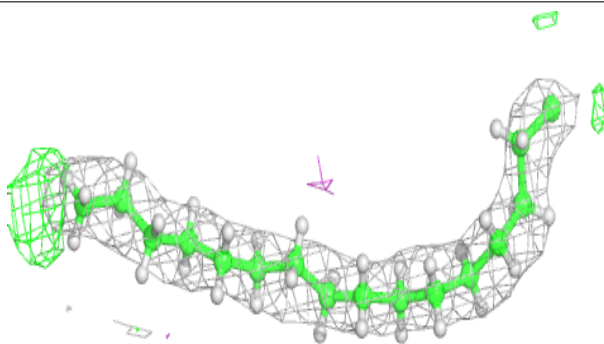


Electron density around STE H 103:

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

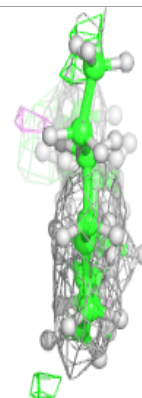
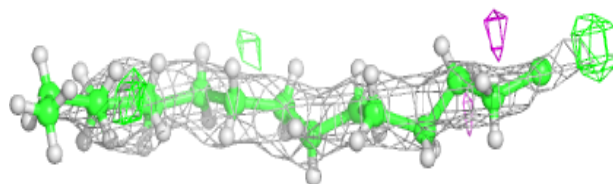
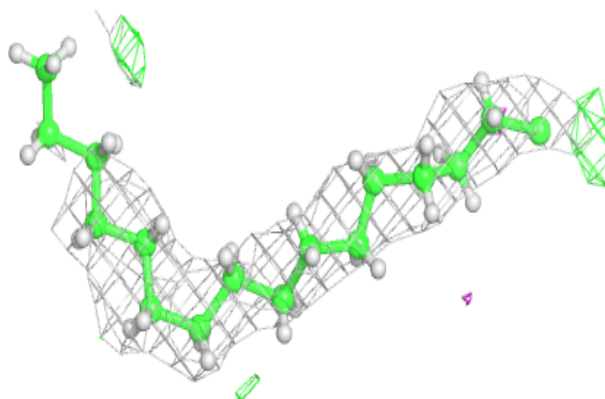
**Electron density around STE C 519:**

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

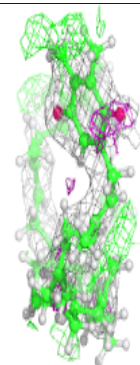
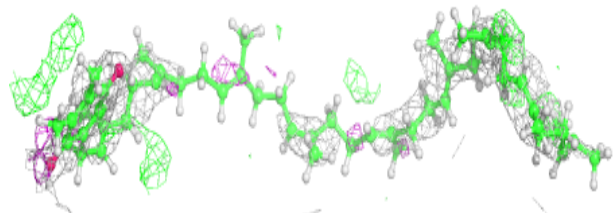
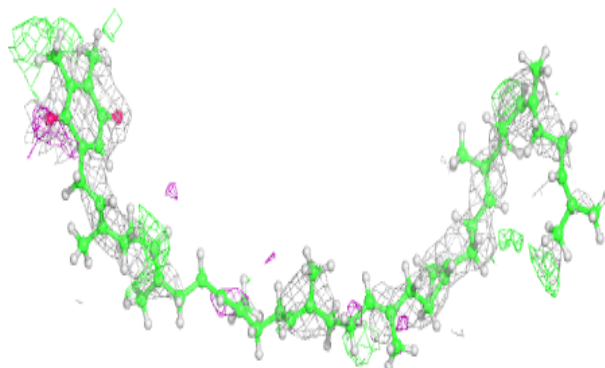


Electron density around STE B 625:

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

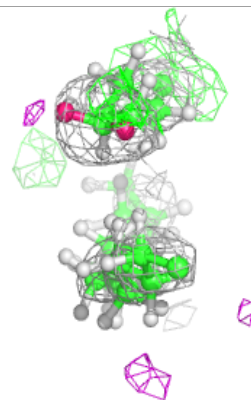
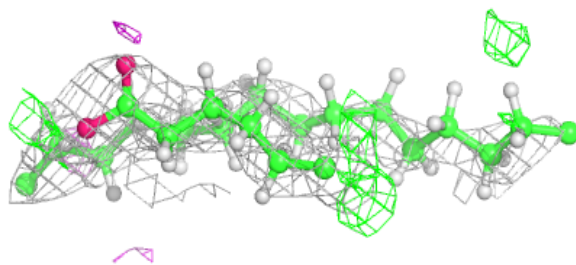
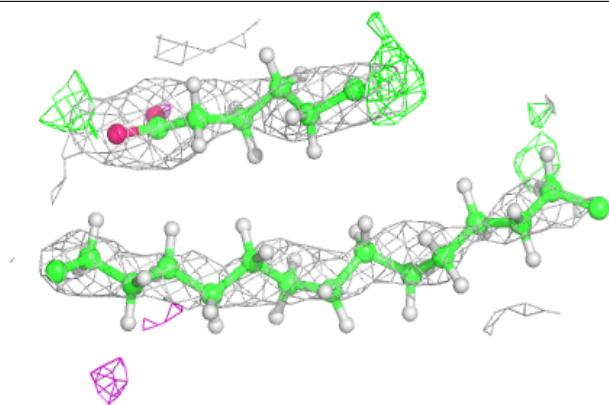
**Electron density around PL9 a 409:**

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

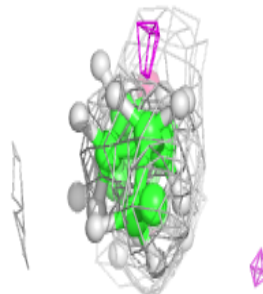
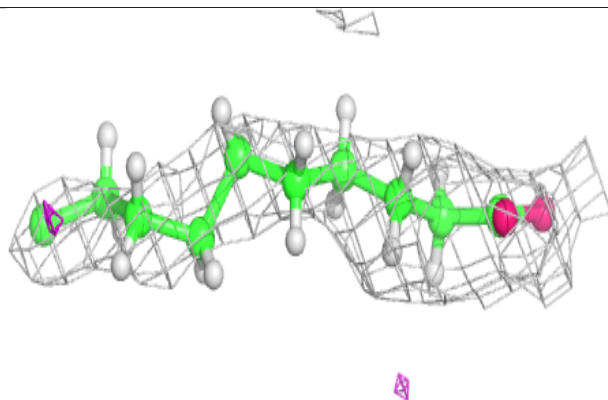
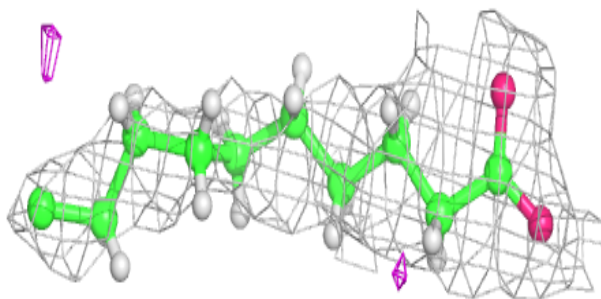


Electron density around LMG h 102:

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

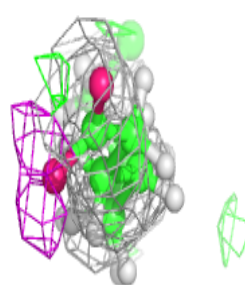
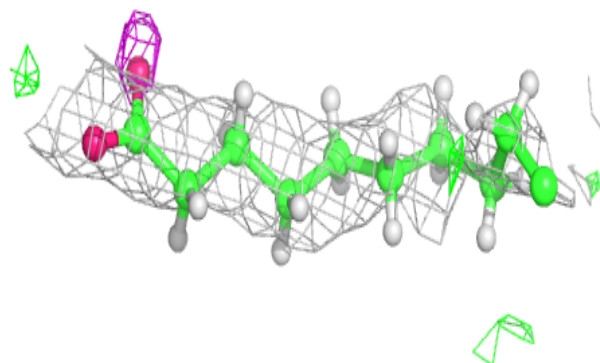
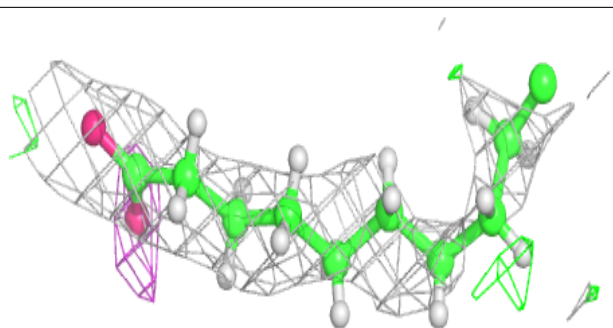
**Electron density around STE a 415:**

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

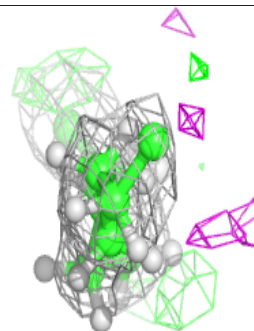
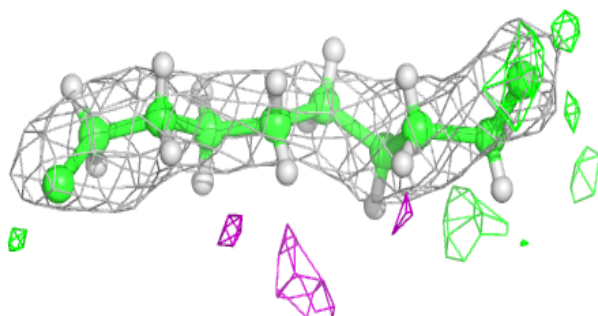
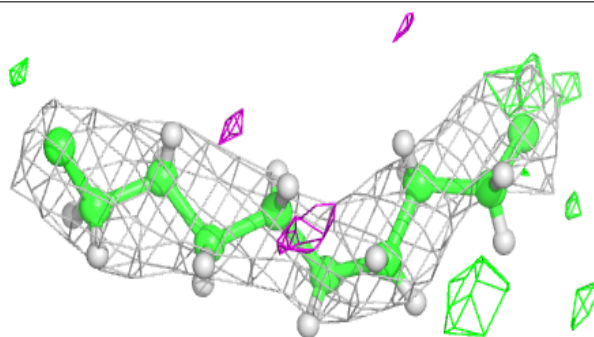


Electron density around STE m 102:

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

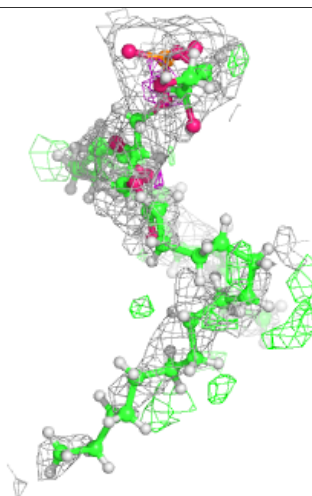
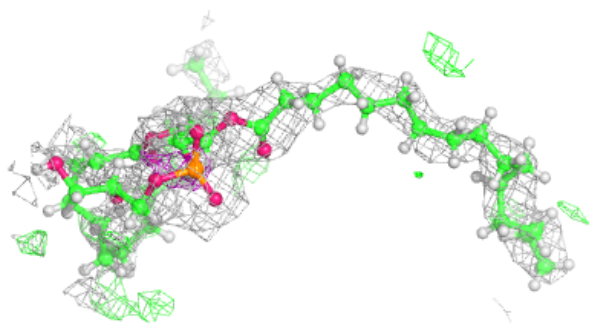
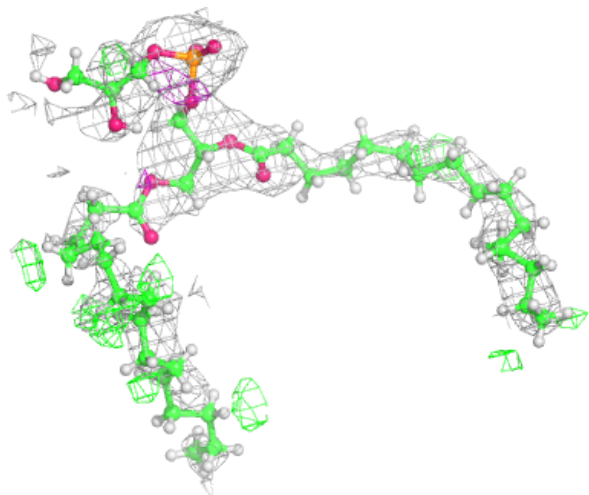
**Electron density around STE b 626:**

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



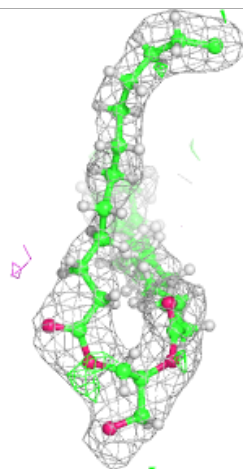
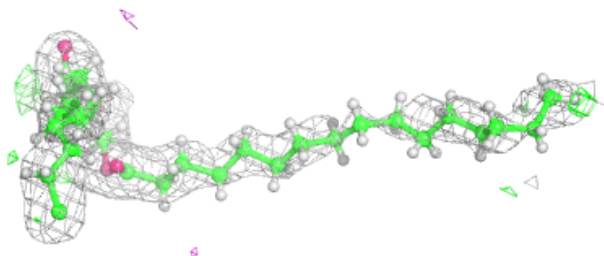
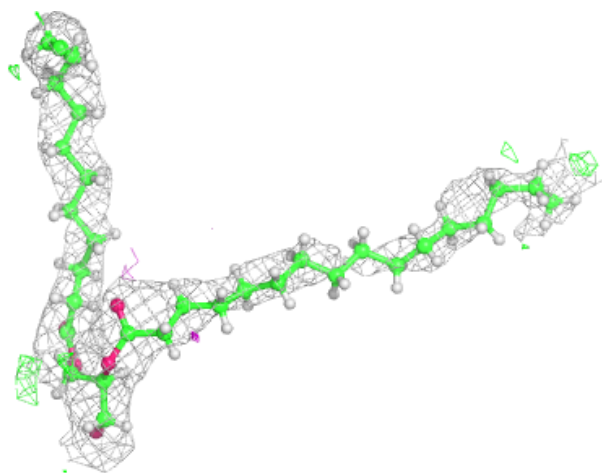
Electron density around LHG A 413:

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



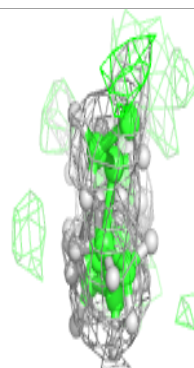
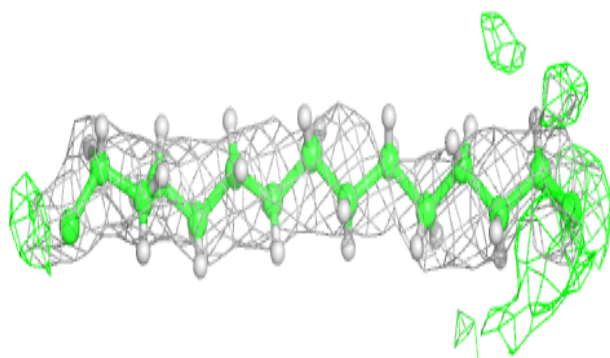
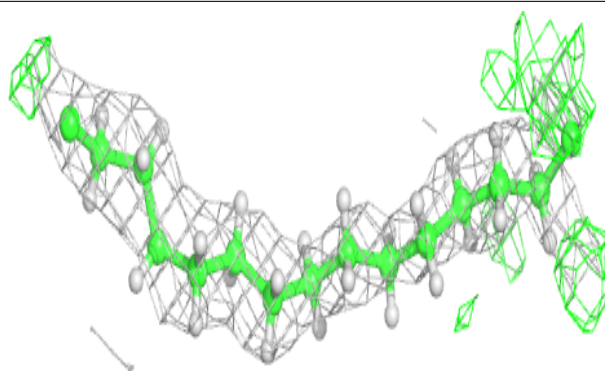
Electron density around SQD a 412:

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

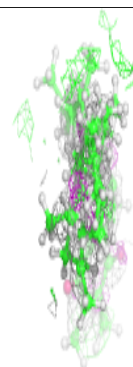
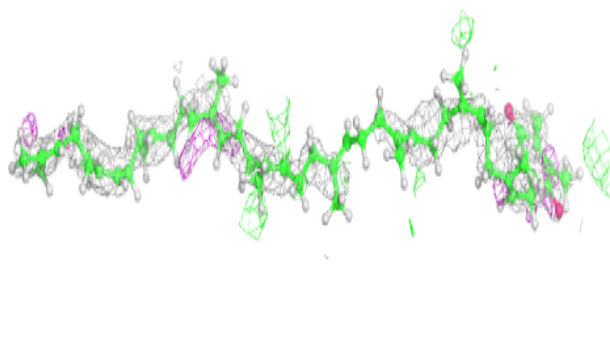
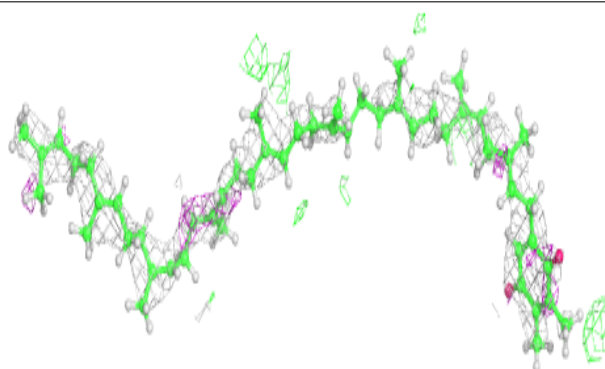


Electron density around STE I 101:

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

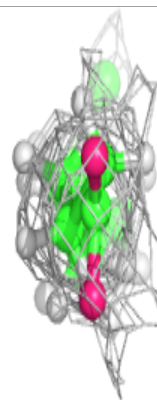
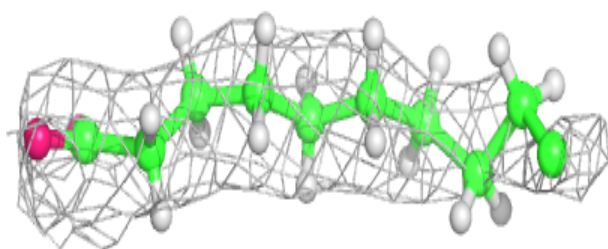
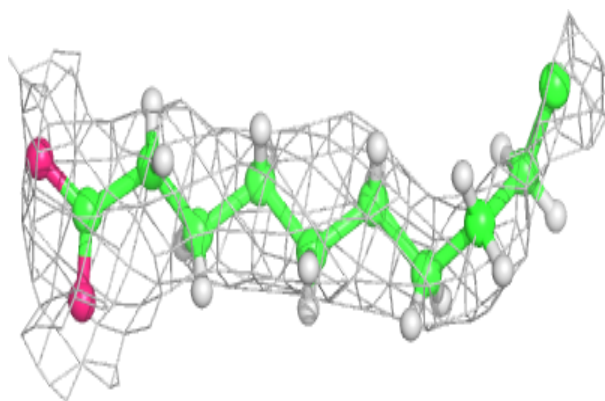
**Electron density around PL9 A 410:**

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

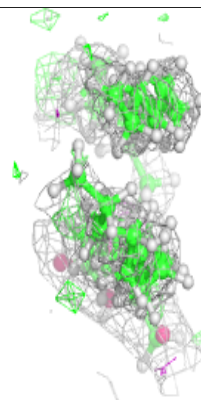
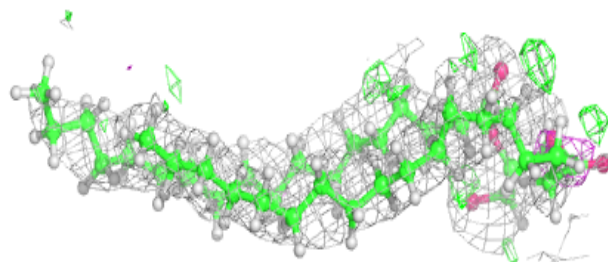
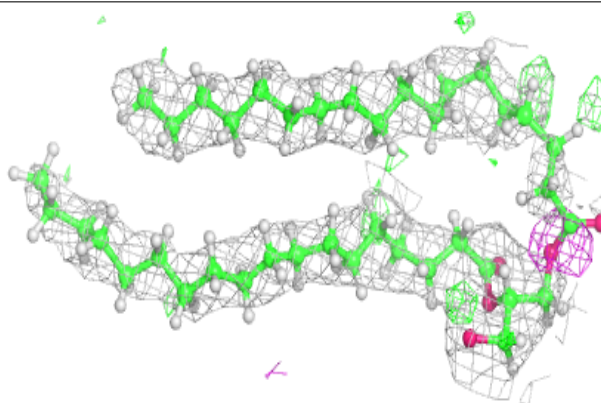


Electron density around STE c 522:

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

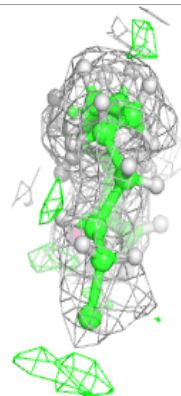
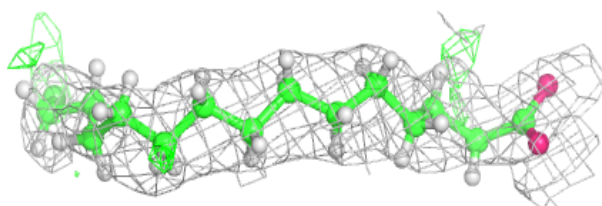
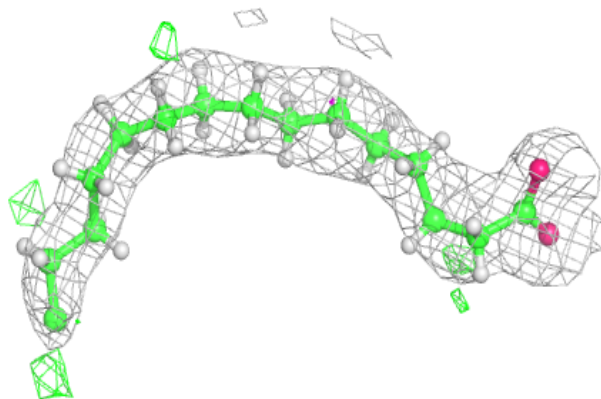
**Electron density around DGD o 301:**

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

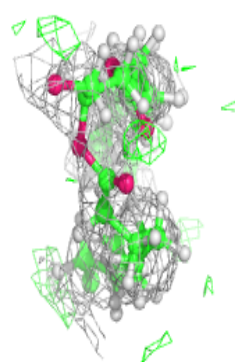
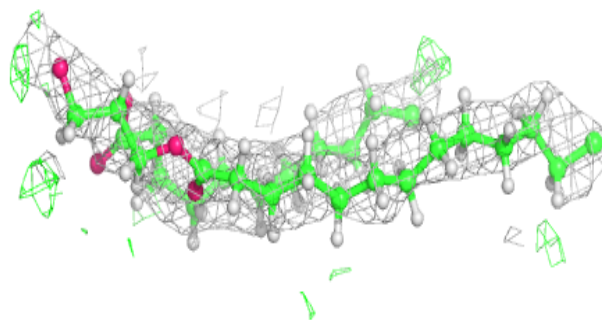
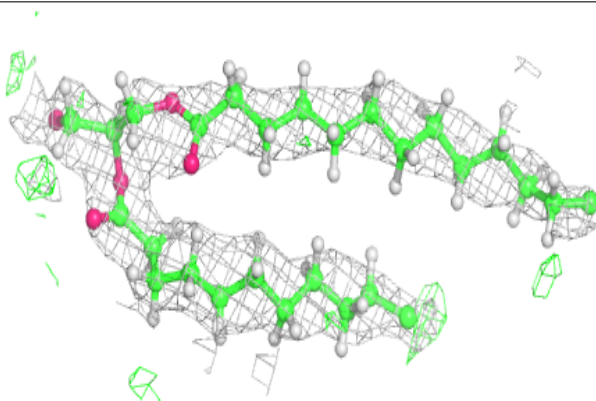


Electron density around STE B 620:

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

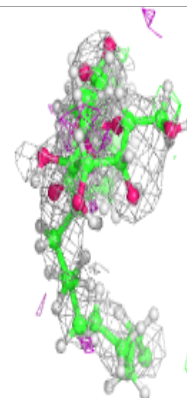
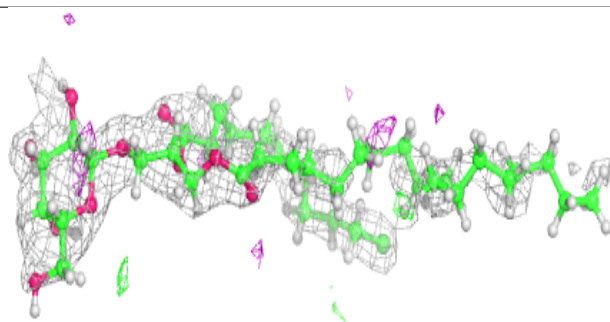
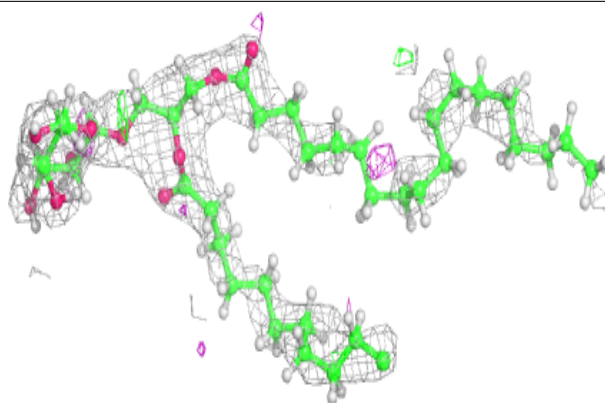
**Electron density around LMG D 410:**

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

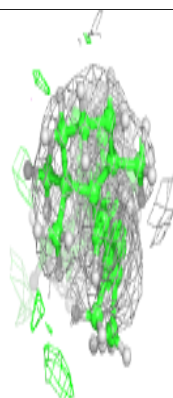
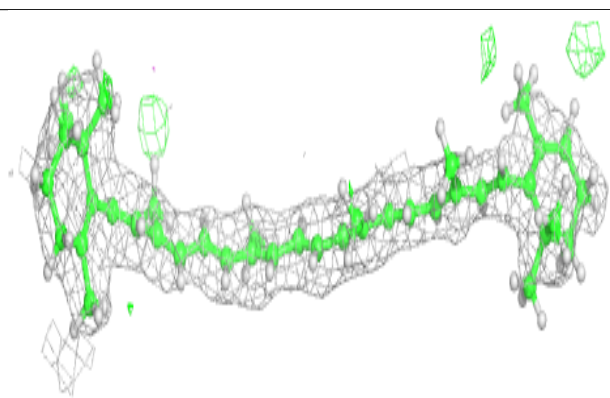
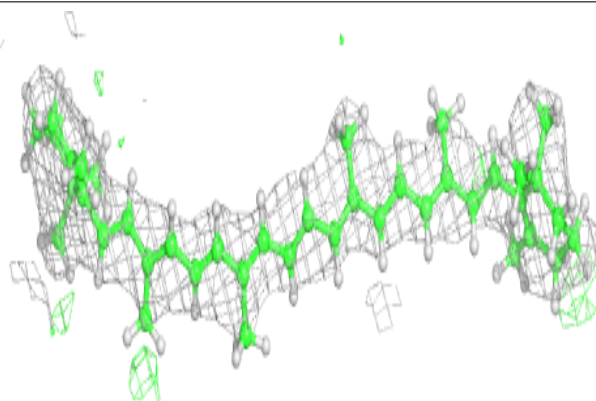


Electron density around LMG c 521:

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

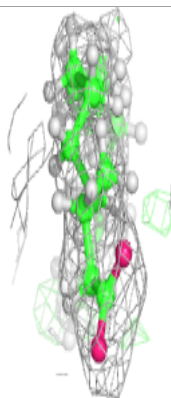
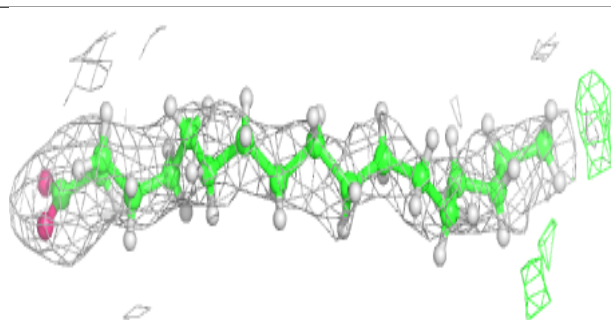
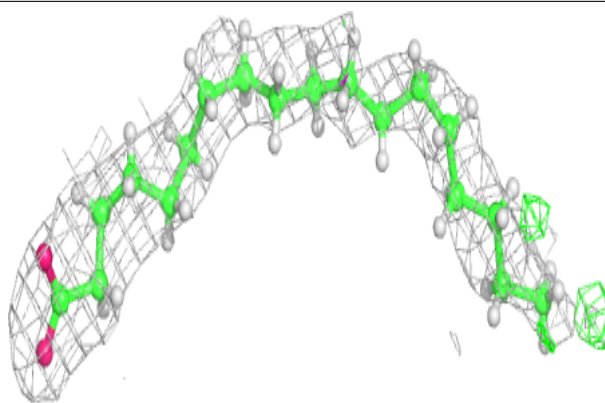
**Electron density around BCR h 101:**

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

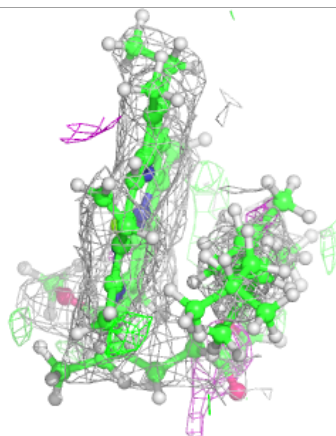
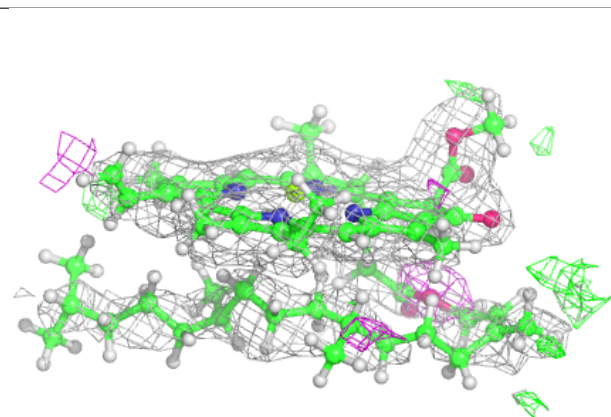
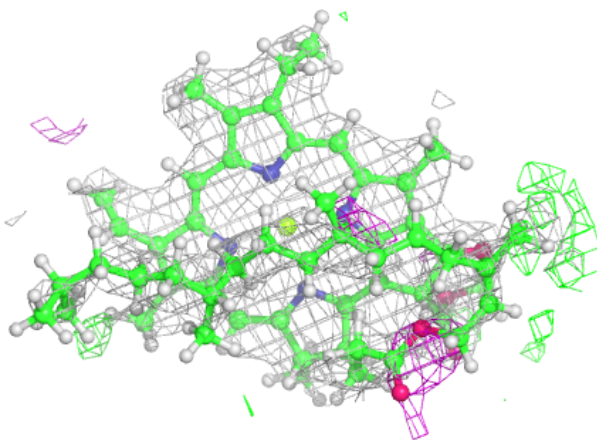


Electron density around STE d 412:

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

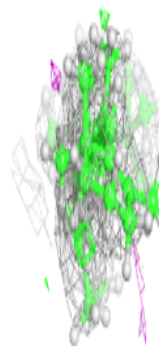
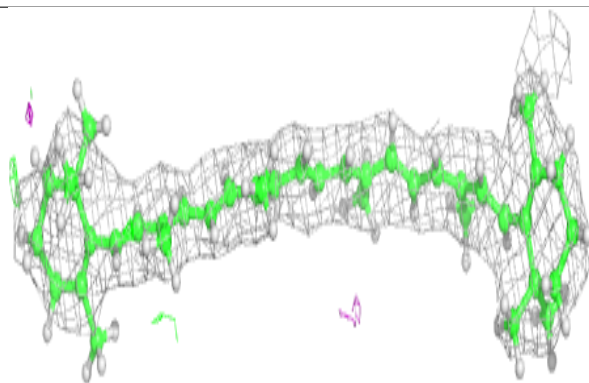
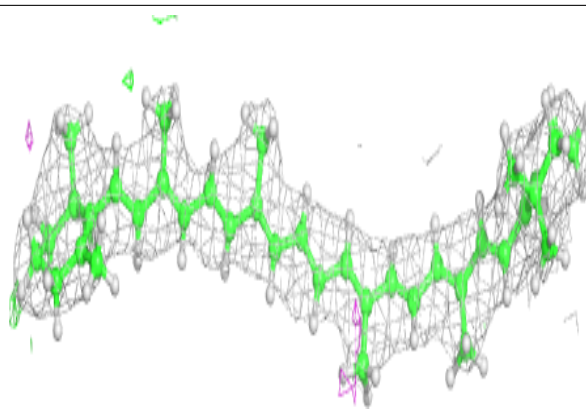
**Electron density around CLA b 601:**

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

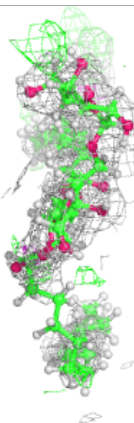
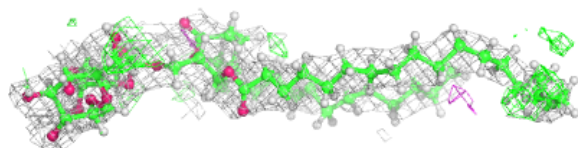
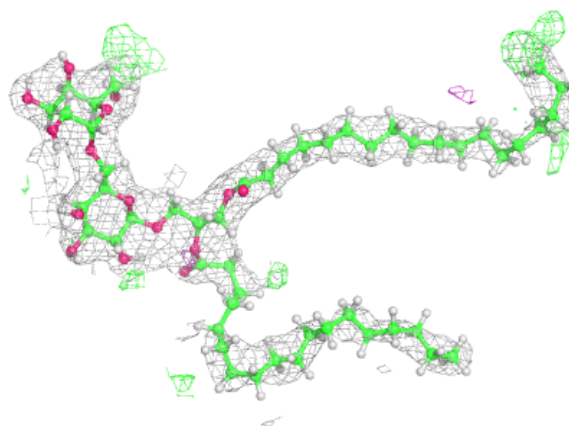


Electron density around BCR H 101:

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

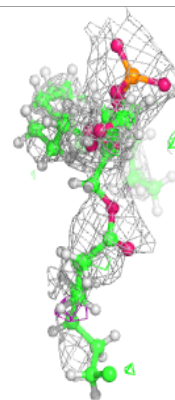
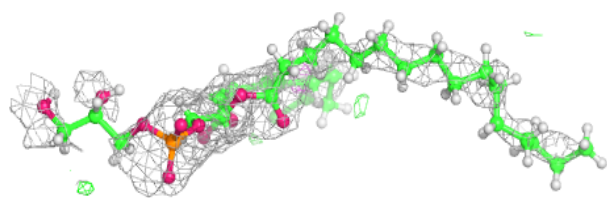
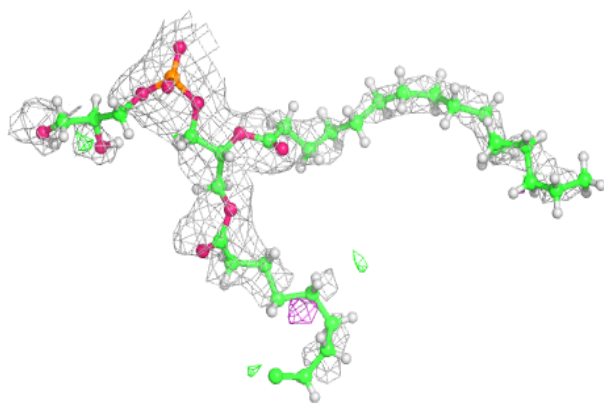
**Electron density around DGD A 415:**

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

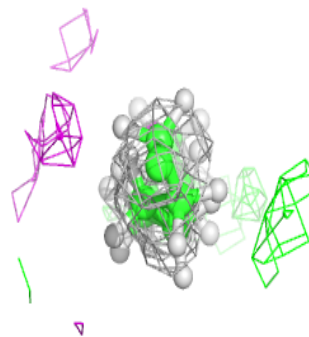
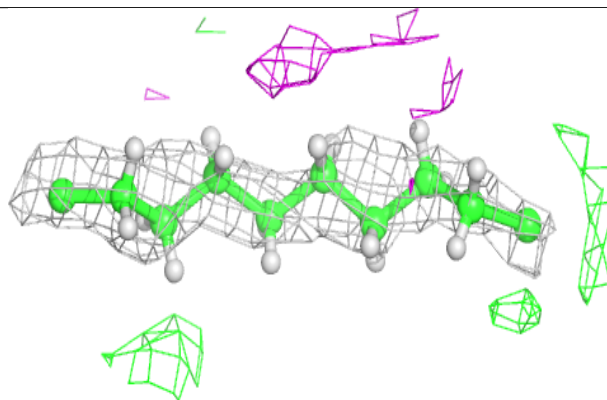
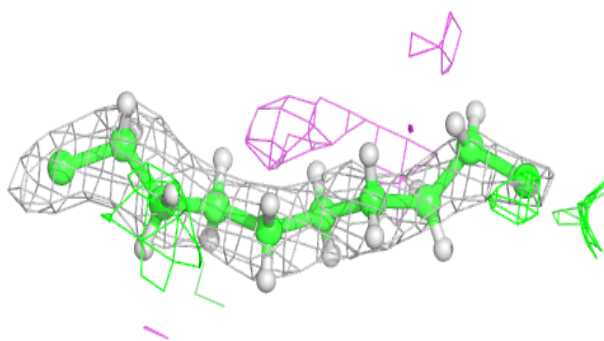


Electron density around LHG e 101:

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

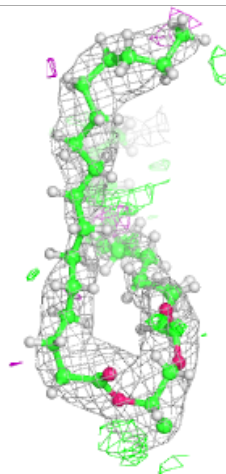
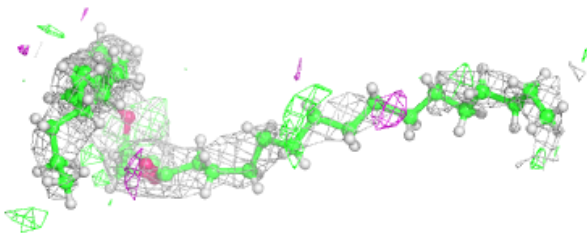
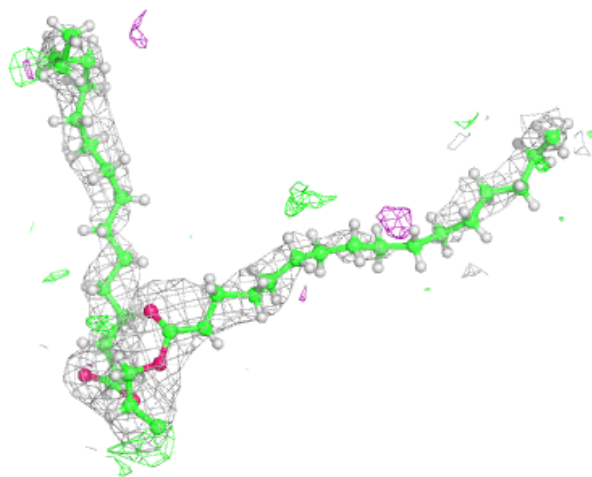
**Electron density around STE a 413:**

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



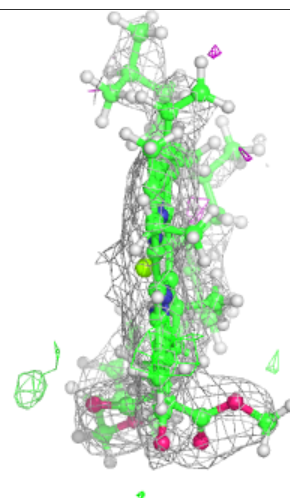
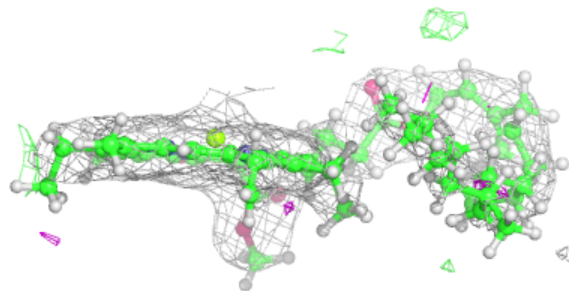
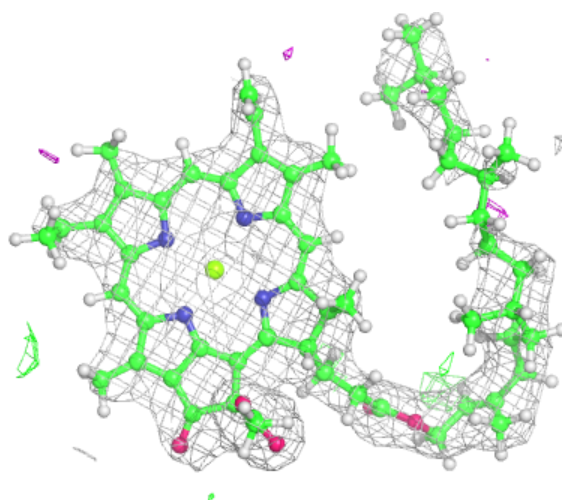
Electron density around SQD A 414:

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



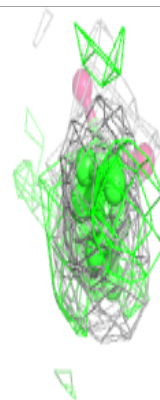
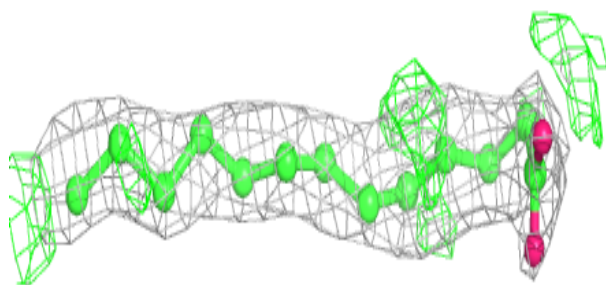
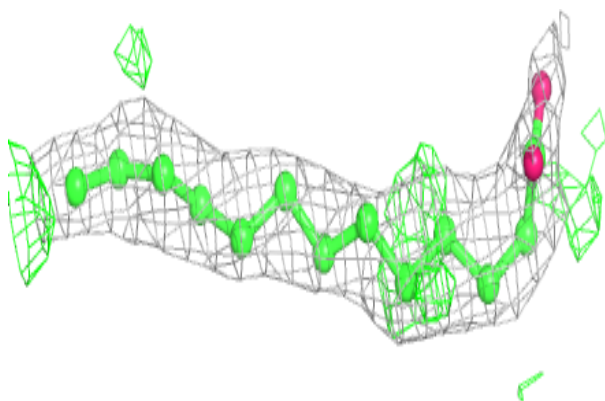
Electron density around CLA C 512:

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

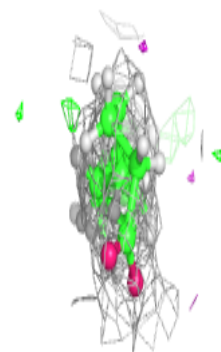
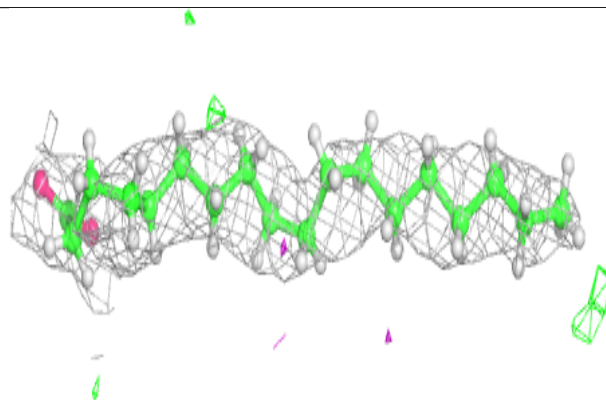
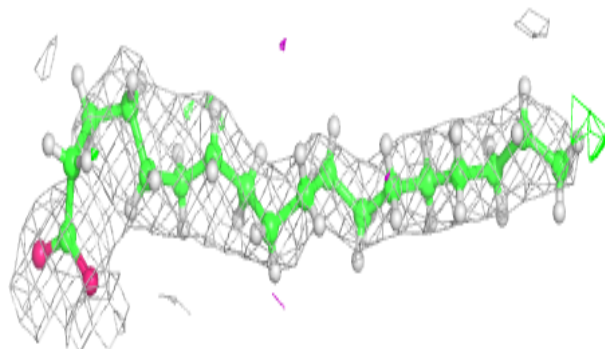


Electron density around STE D 413:

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

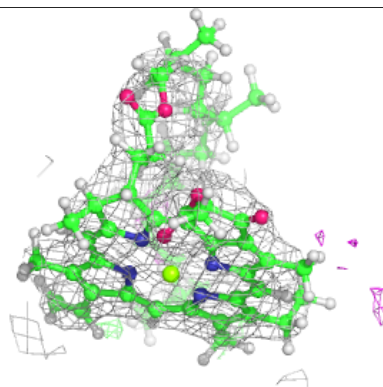
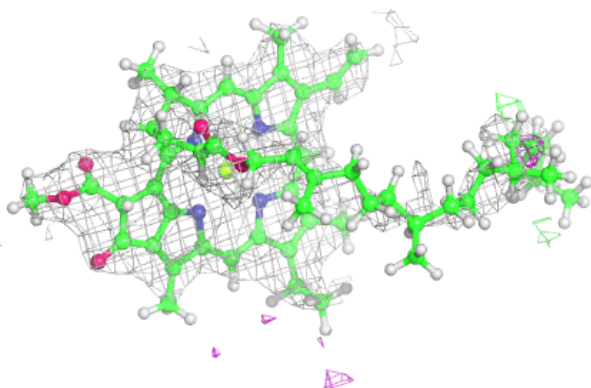
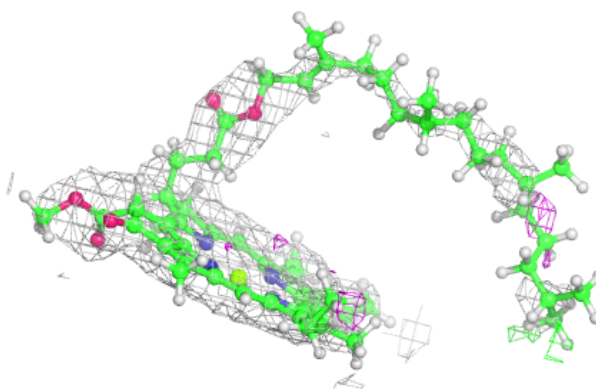
**Electron density around STE c 520:**

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

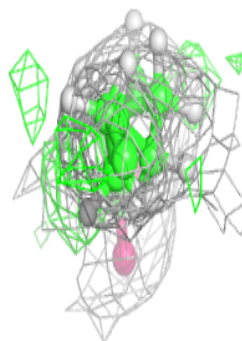
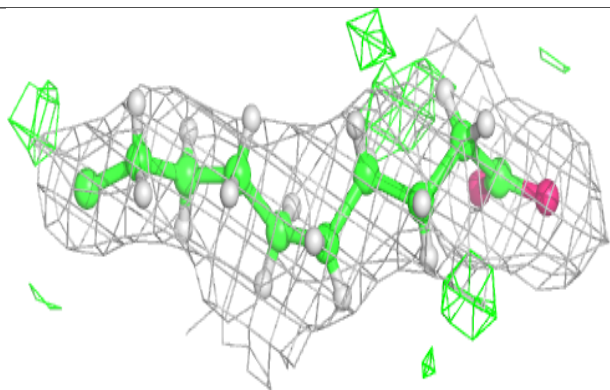
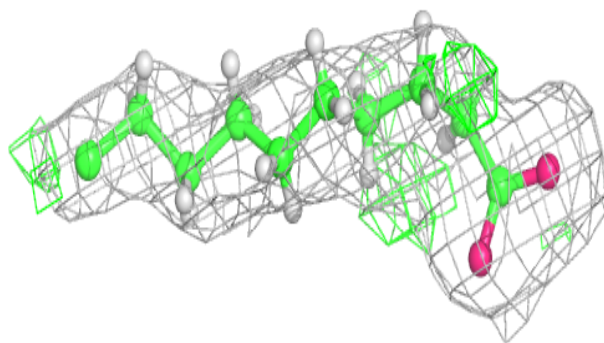


Electron density around CLA c 513:

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

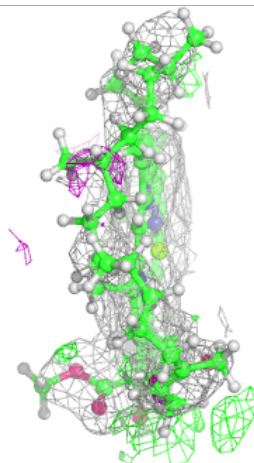
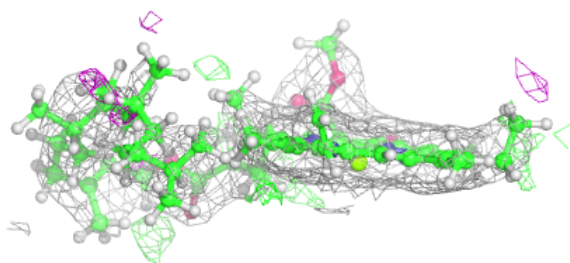
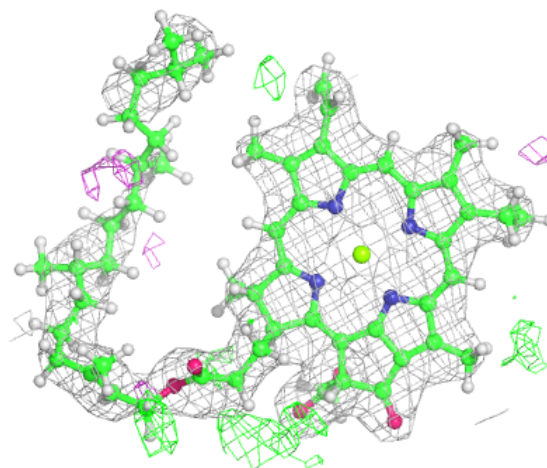
**Electron density around STE B 623:**

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



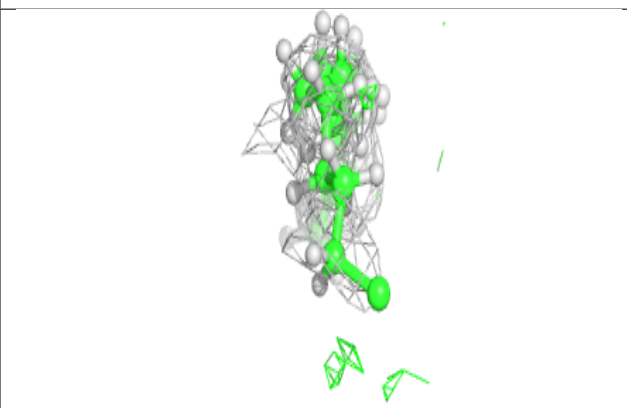
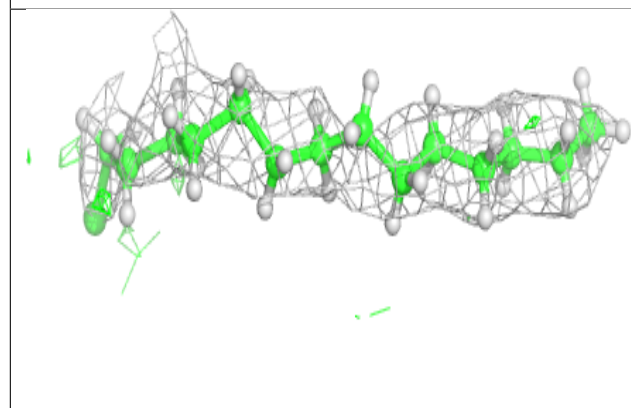
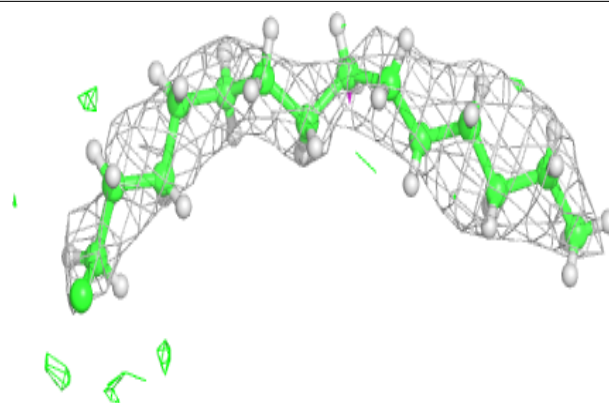
Electron density around CLA c 512:

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

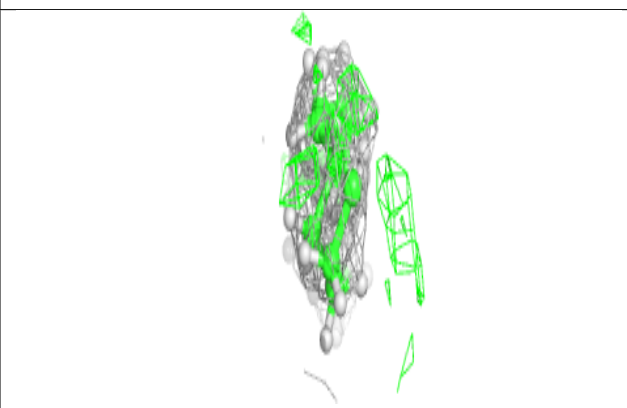
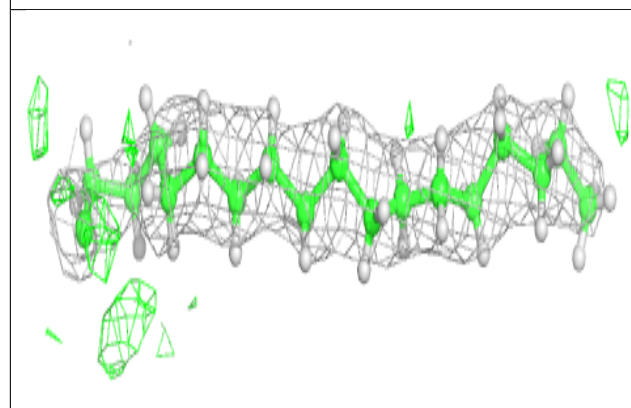
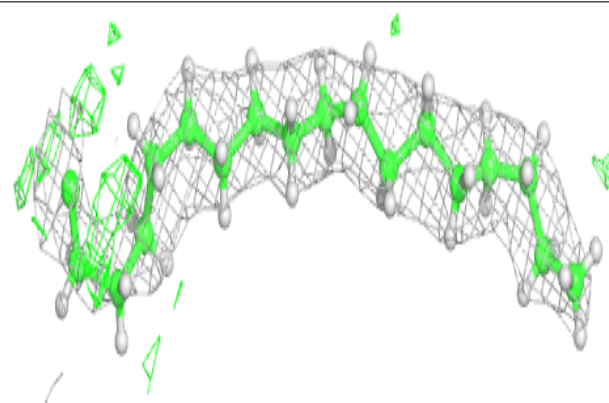


Electron density around STE T 102:

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

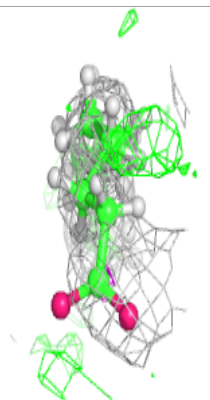
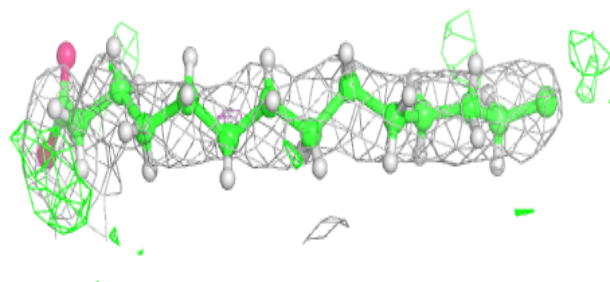
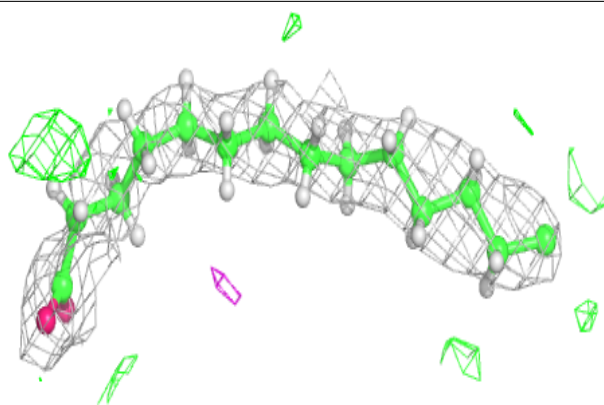
**Electron density around STE M 104:**

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

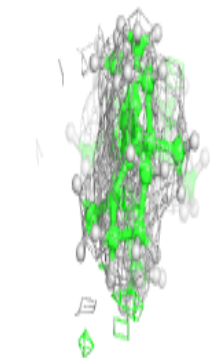
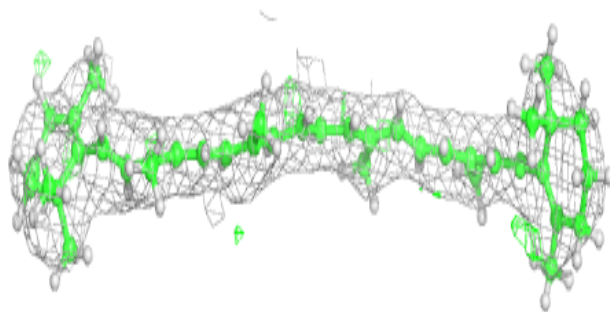
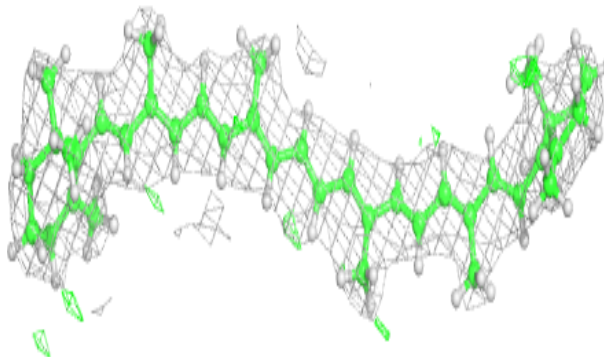


Electron density around STE b 624:

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

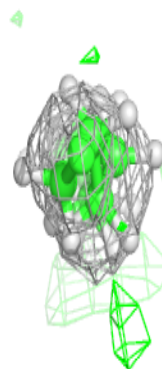
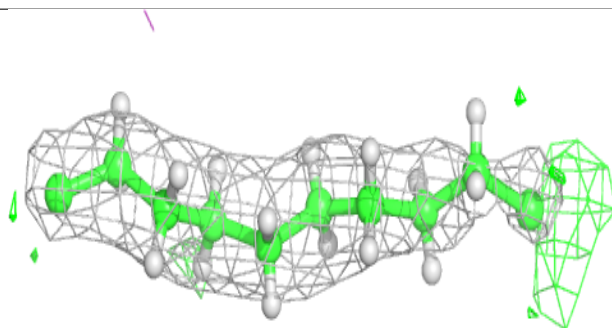
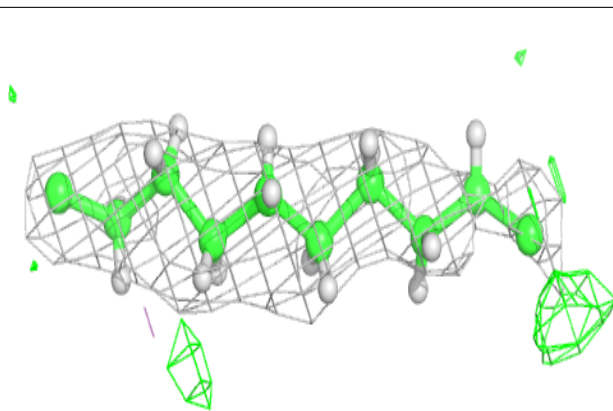
**Electron density around BCR K 102:**

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

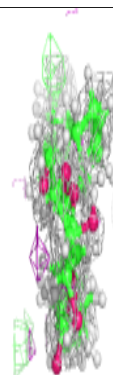
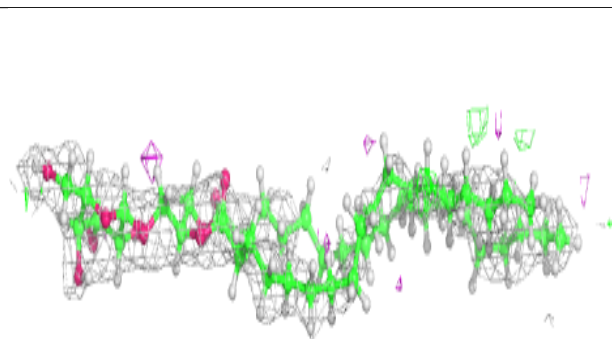
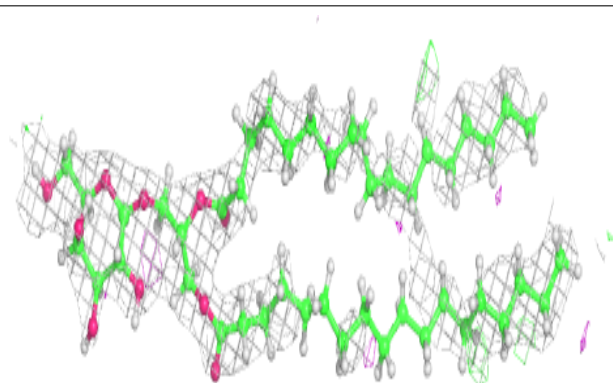


Electron density around STE M 103:

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

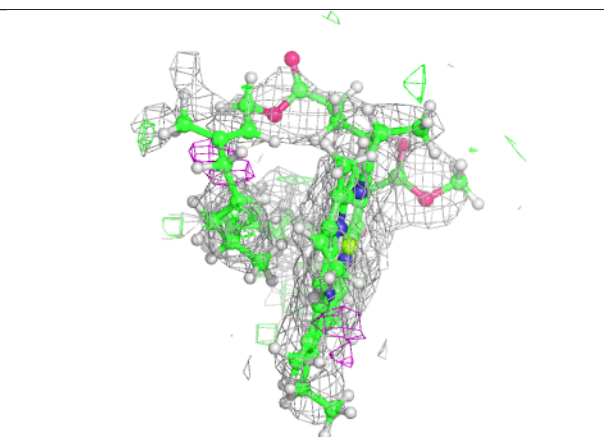
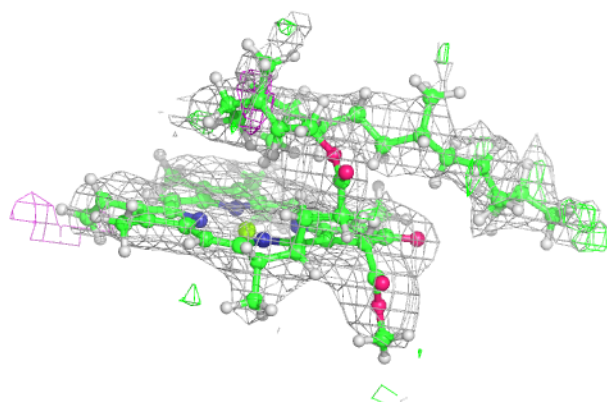
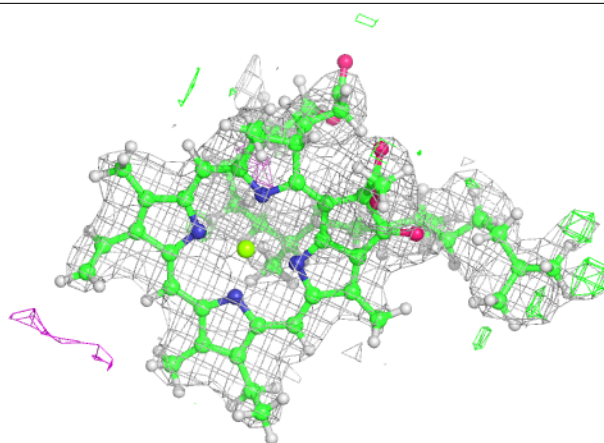
**Electron density around LMG b 623:**

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

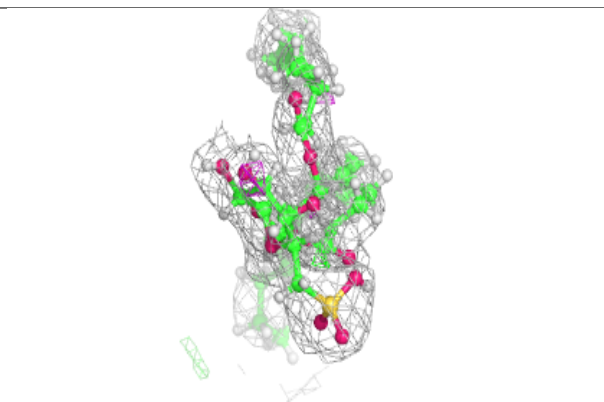
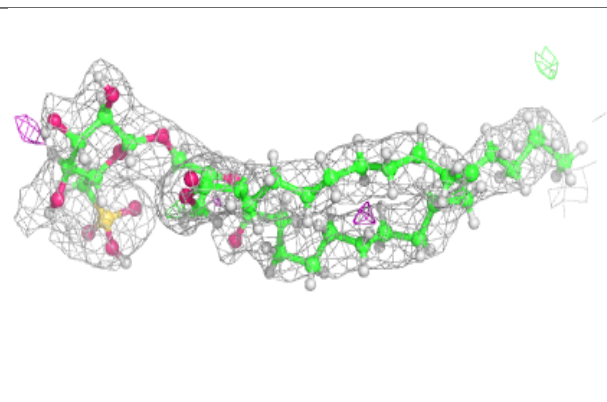
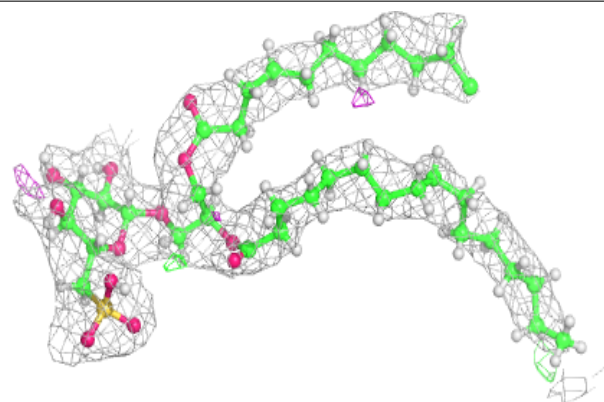


Electron density around CLA B 601:

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

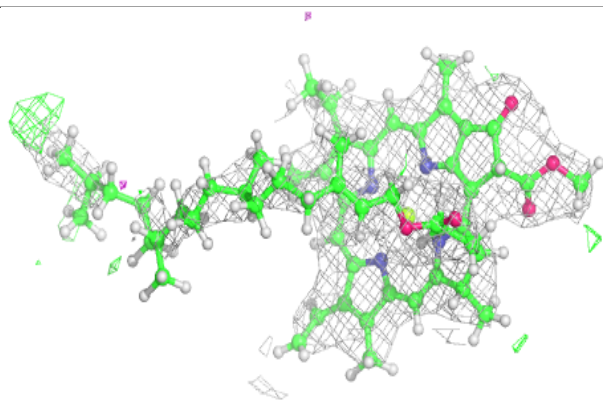
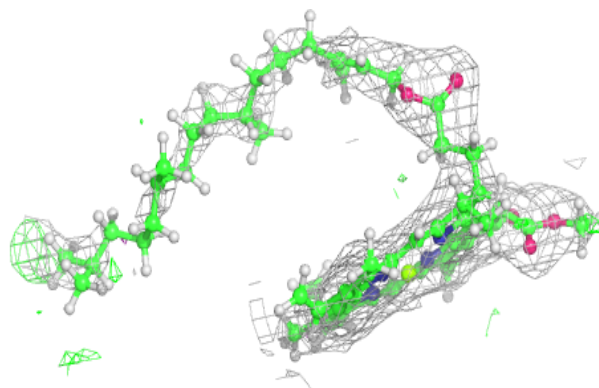
**Electron density around SQD b 620:**

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

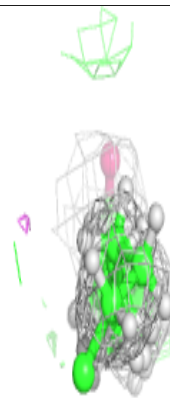
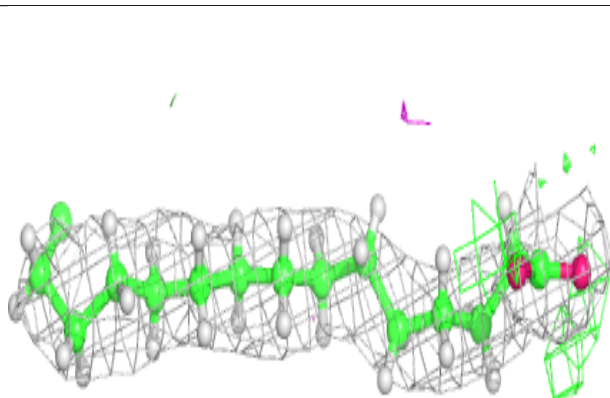
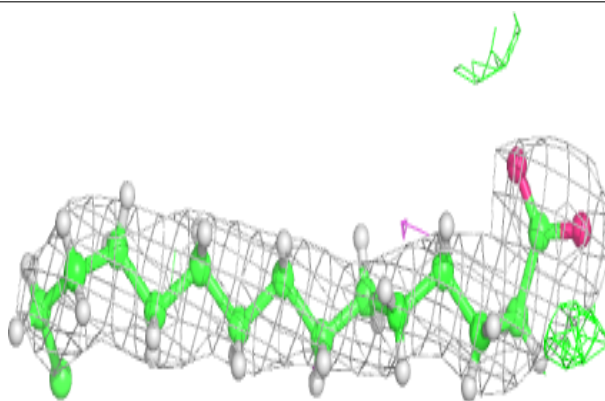


Electron density around CLA C 513:

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

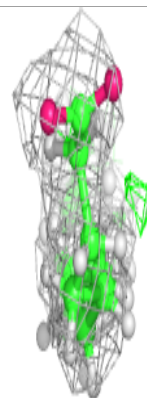
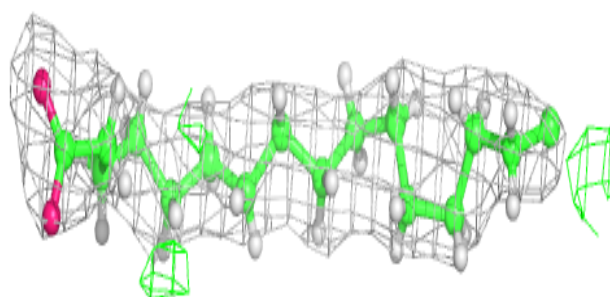
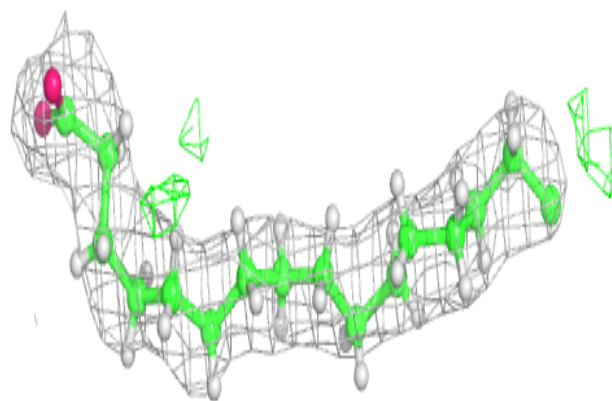
**Electron density around STE d 411:**

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

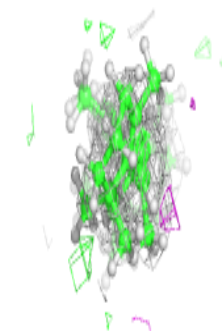
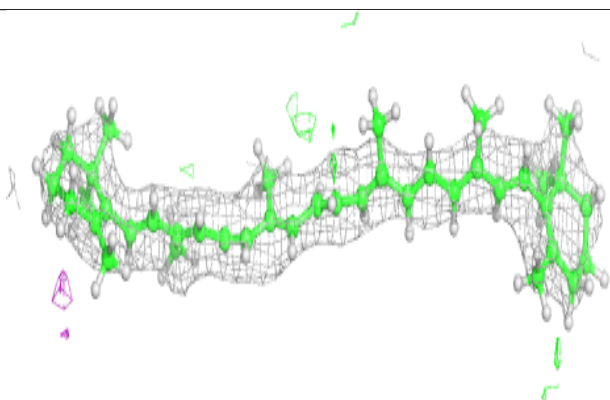
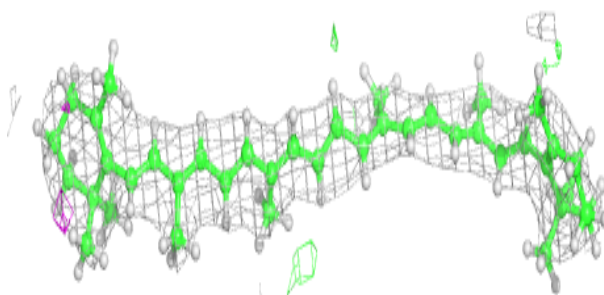


Electron density around STE B 624:

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

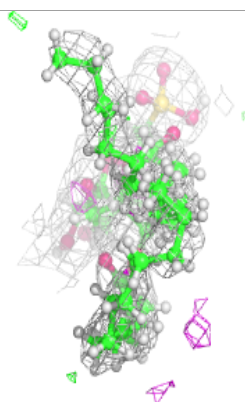
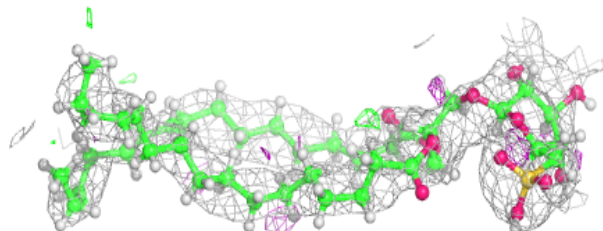
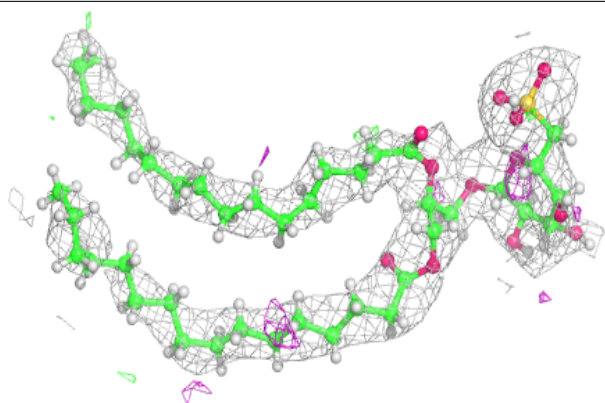
**Electron density around BCR K 101:**

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

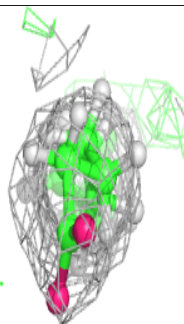
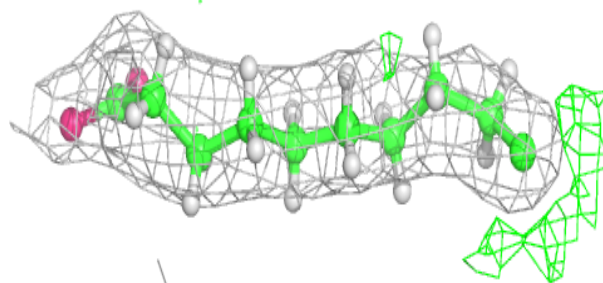
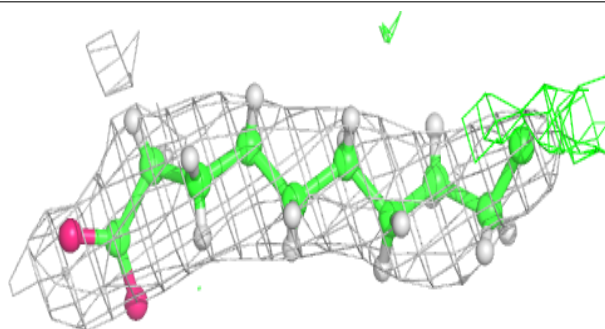


Electron density around SQD B 621:

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

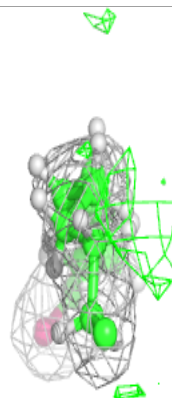
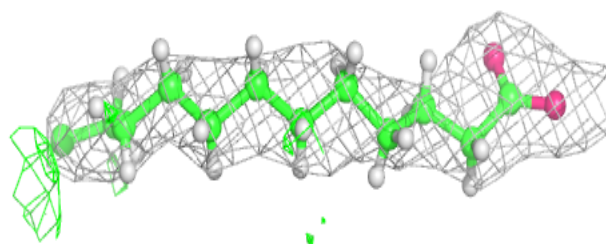
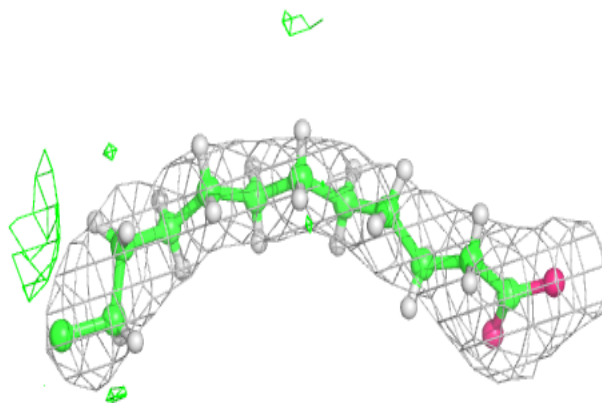
**Electron density around STE J 101:**

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



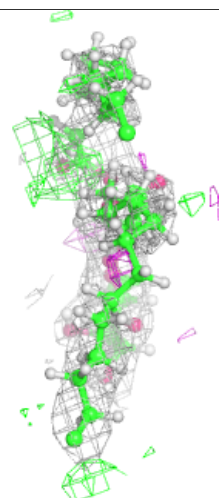
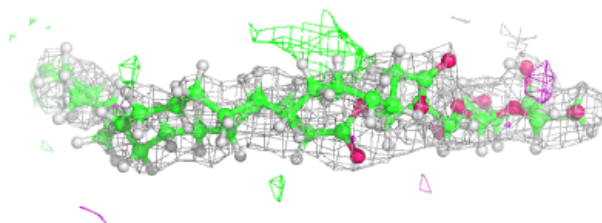
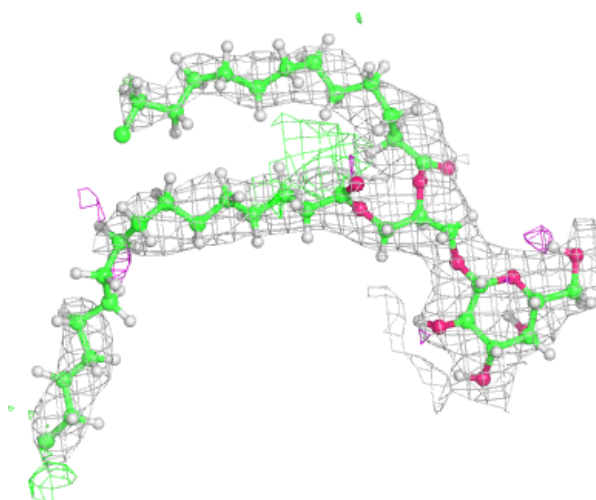
Electron density around STE B 622:

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



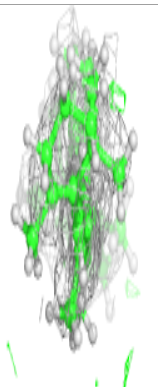
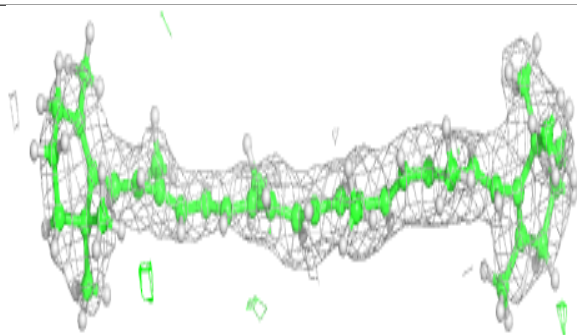
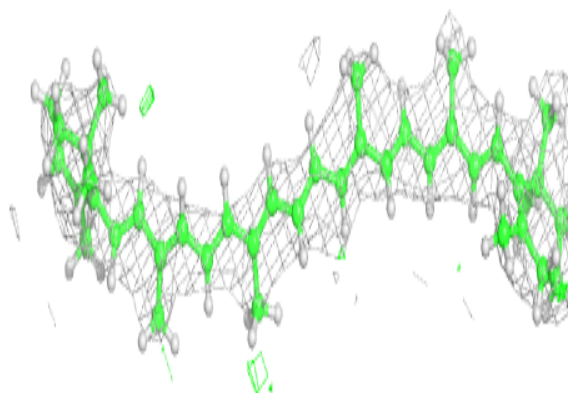
Electron density around LMG Y 101:

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

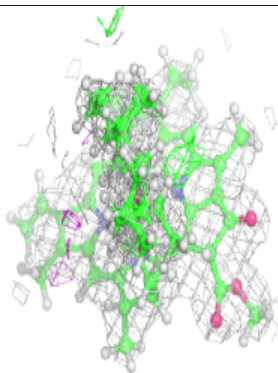
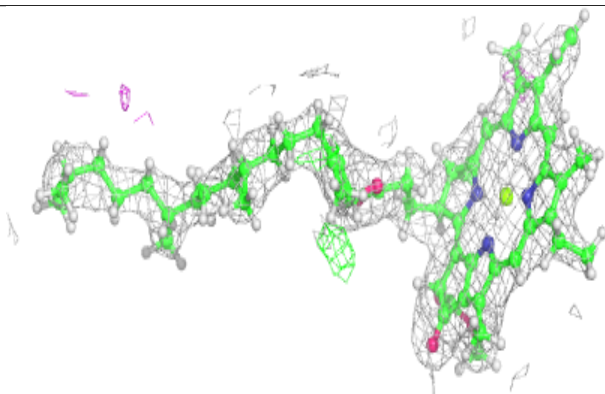
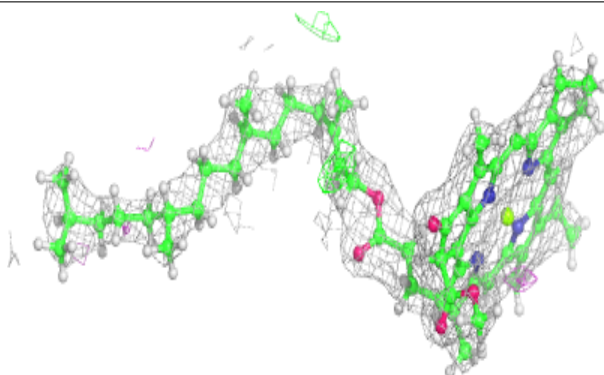


Electron density around BCR k 101:

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

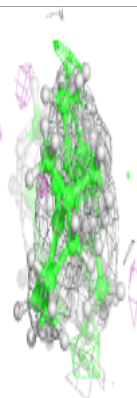
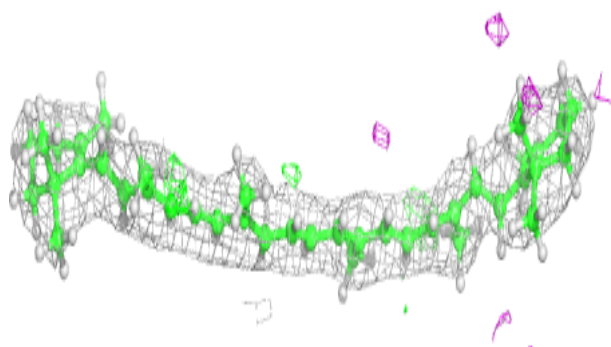
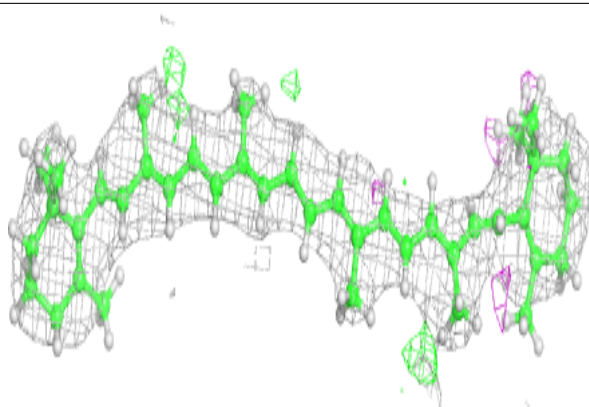
**Electron density around CLA c 502:**

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

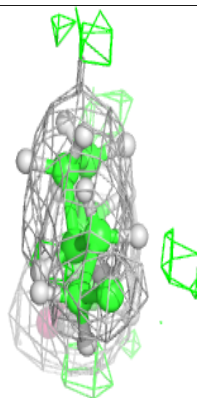
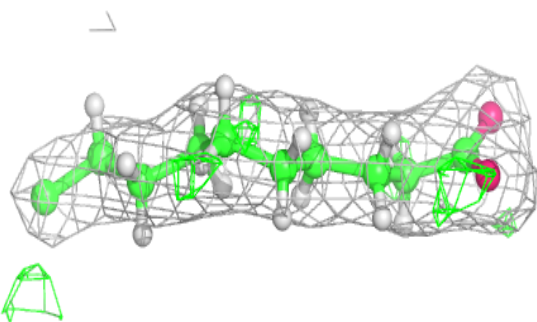
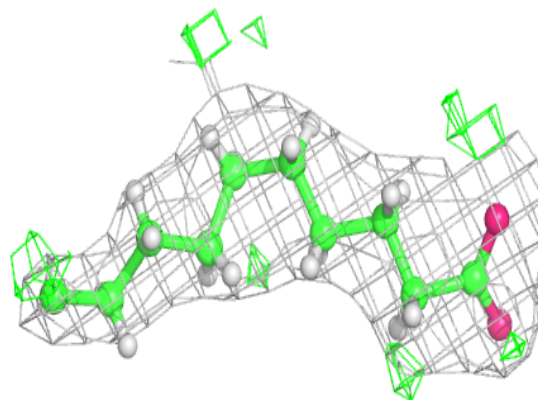


Electron density around BCR d 406:

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

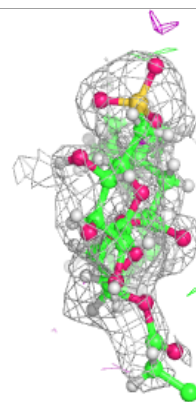
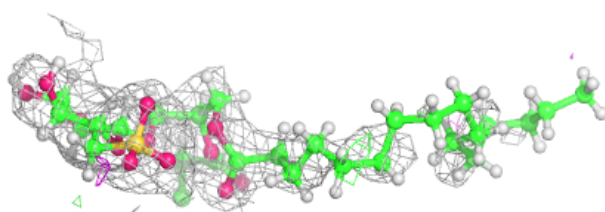
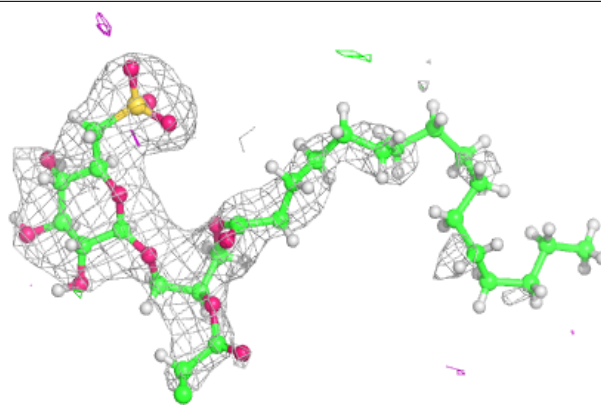
**Electron density around STE C 520:**

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

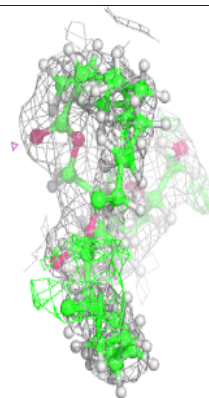
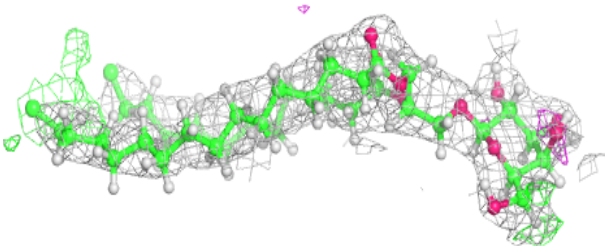
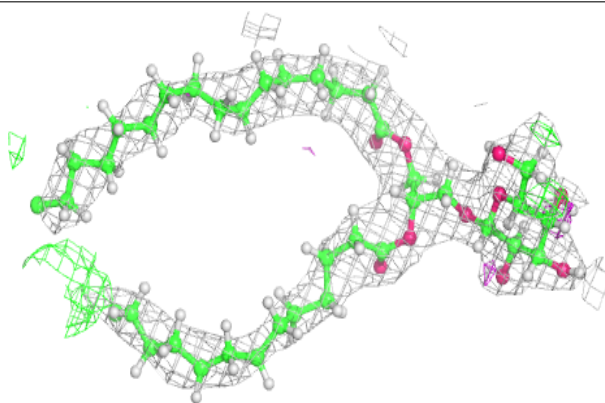


Electron density around SQD f 102:

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

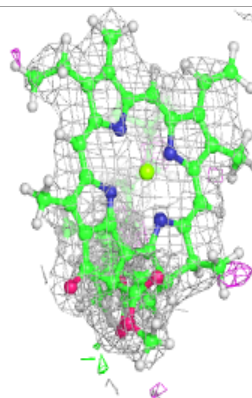
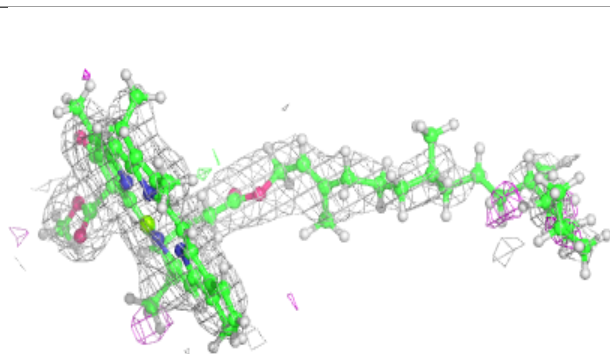
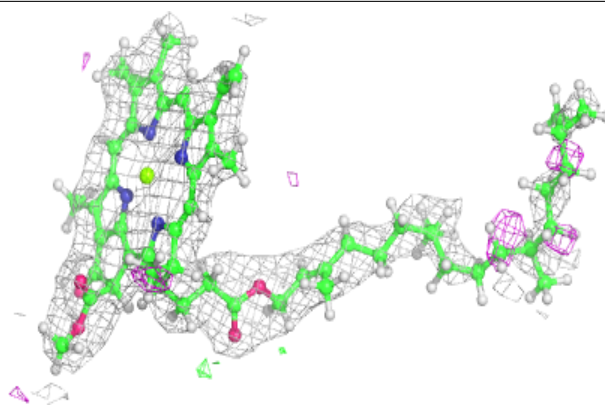
**Electron density around LMG A 411:**

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

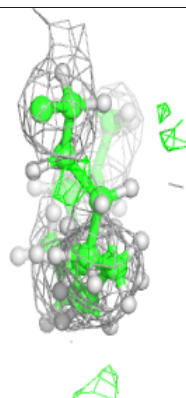
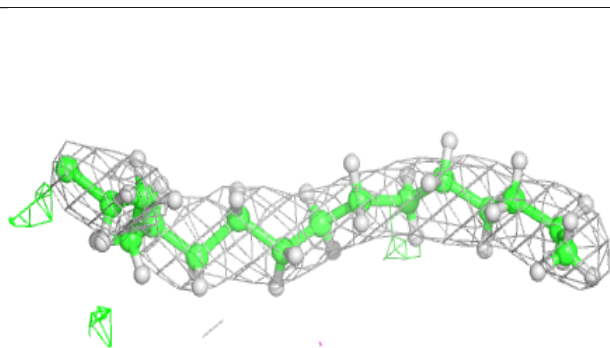
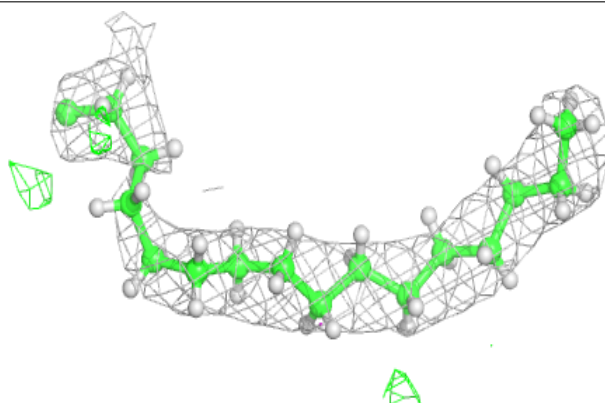


Electron density around CLA d 405:

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

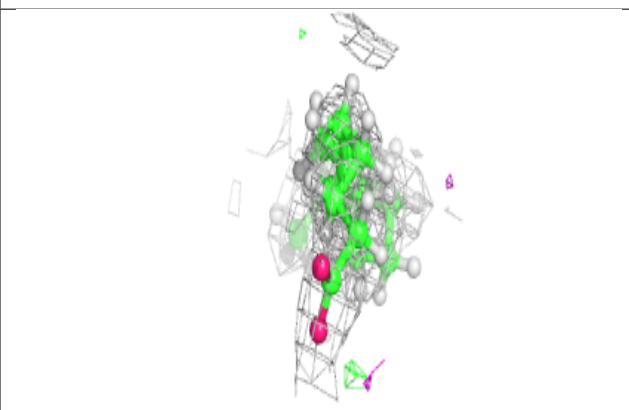
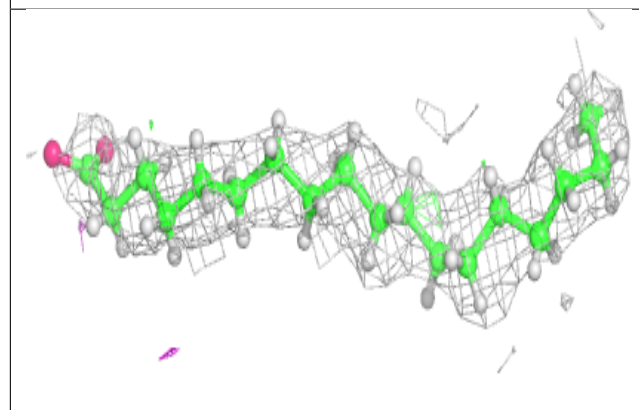
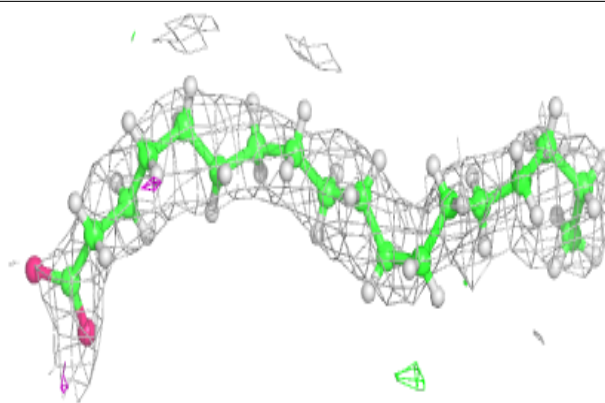
**Electron density around STE b 621:**

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

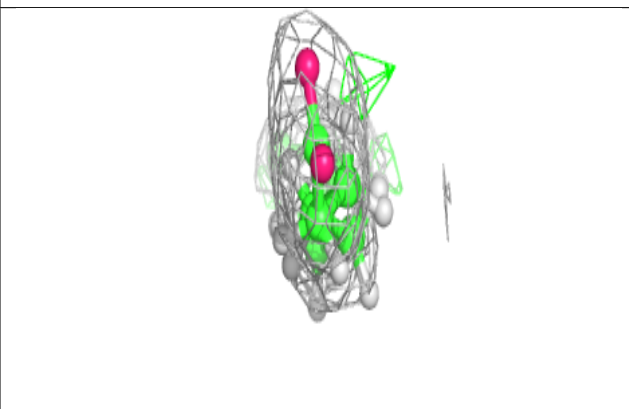
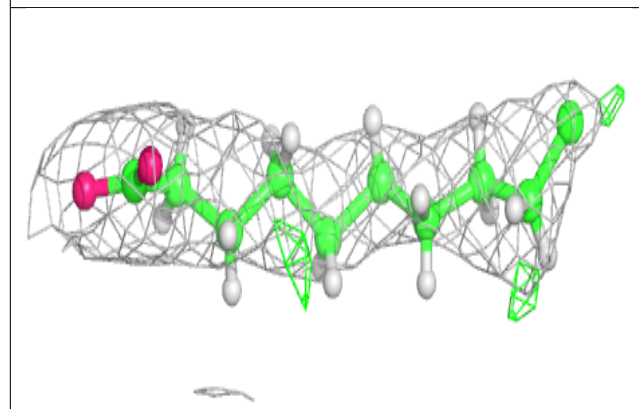
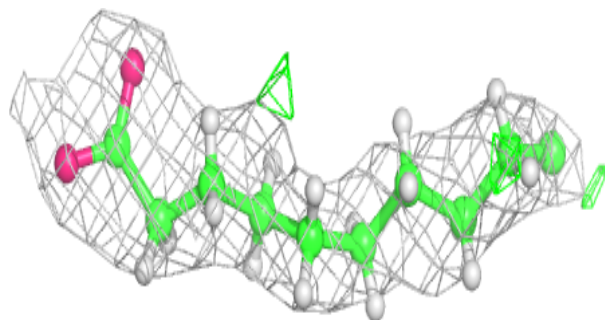


Electron density around STE b 622:

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

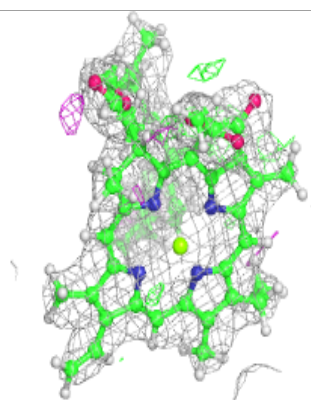
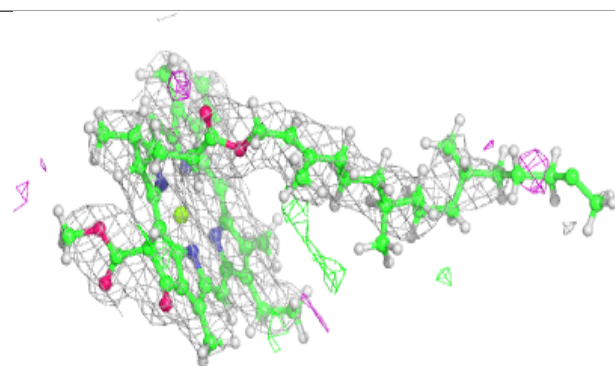
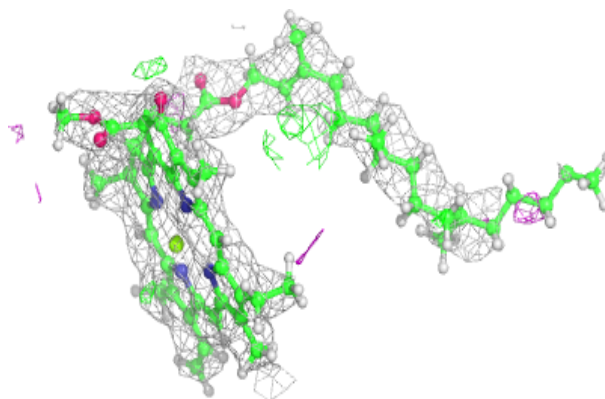
**Electron density around STE C 518:**

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

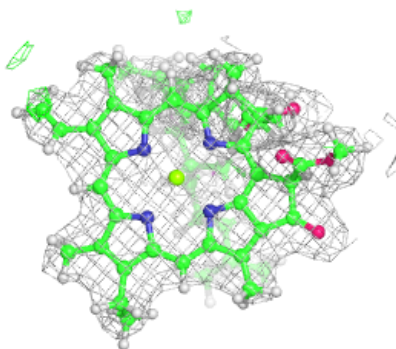
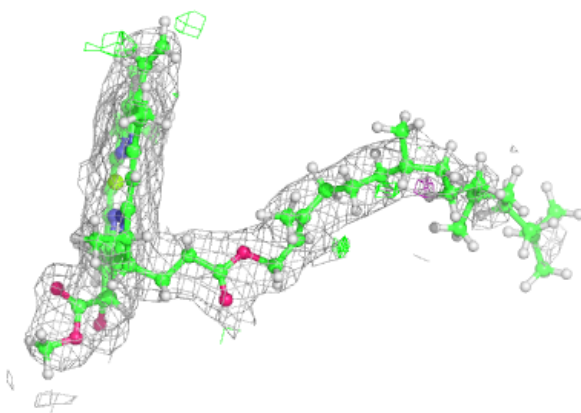
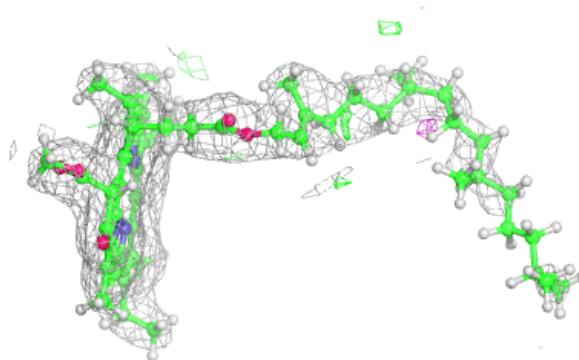


Electron density around CLA c 508:

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

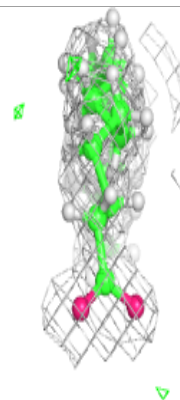
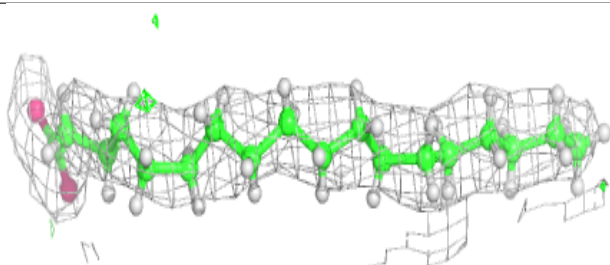
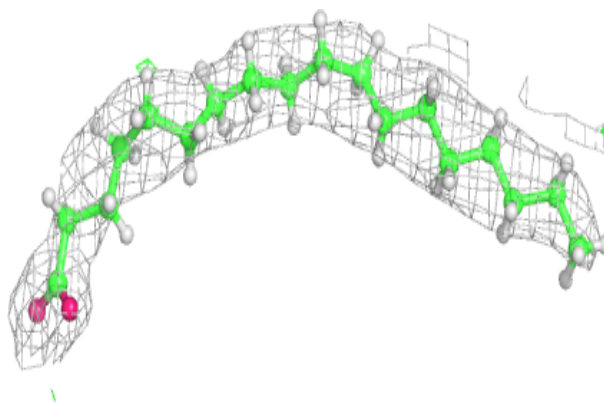
**Electron density around CLA D 404:**

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

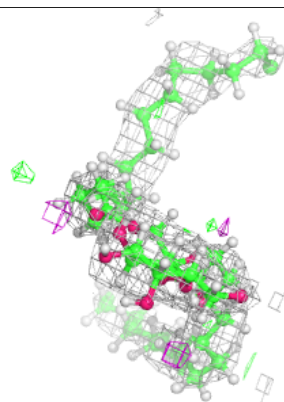
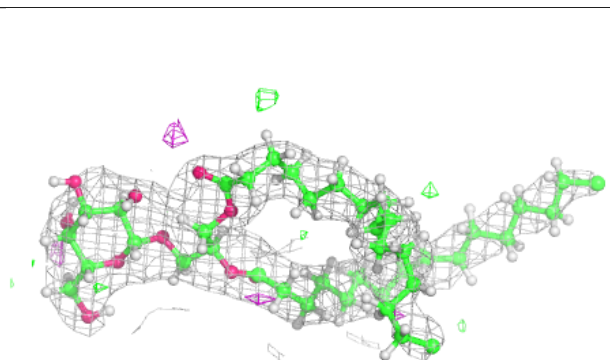
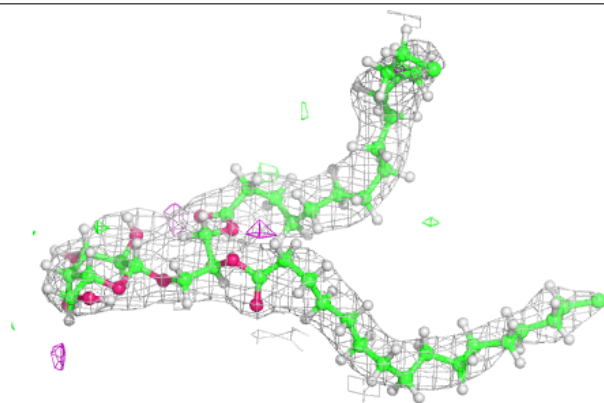


Electron density around STE D 412:

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

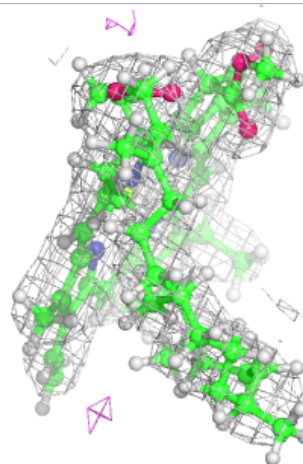
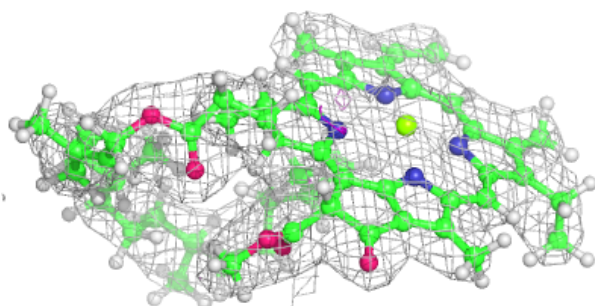
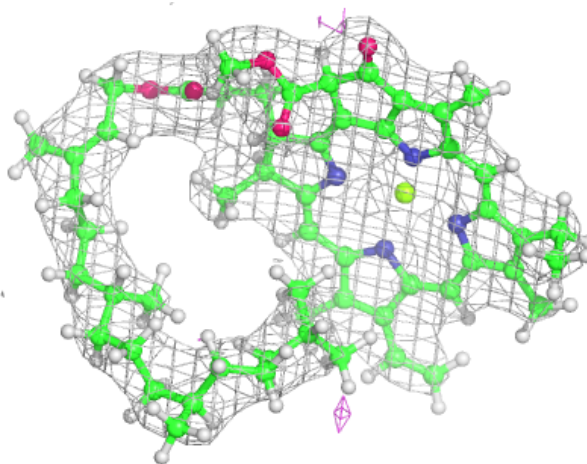
**Electron density around LMG m 101:**

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



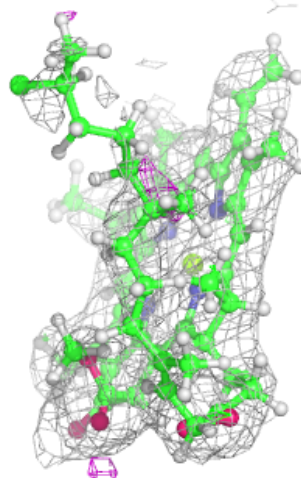
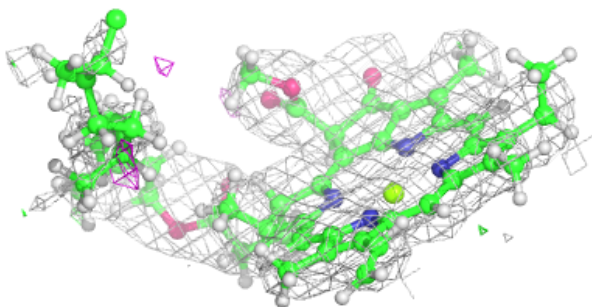
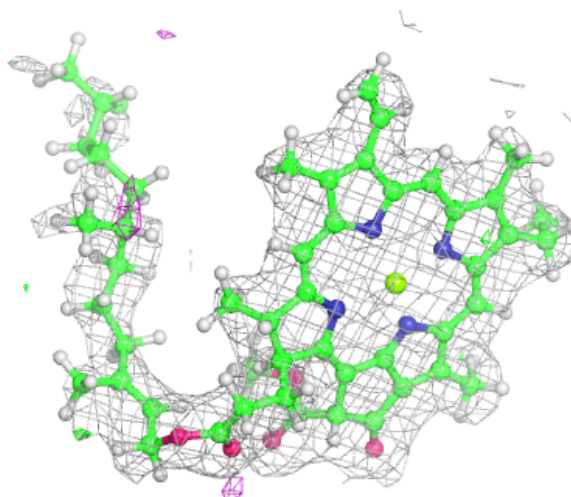
Electron density around CLA b 615:

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



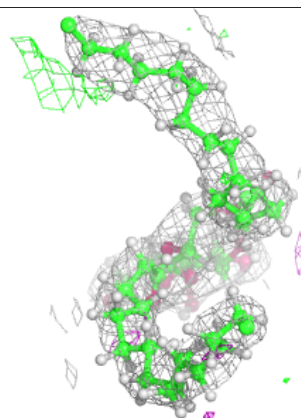
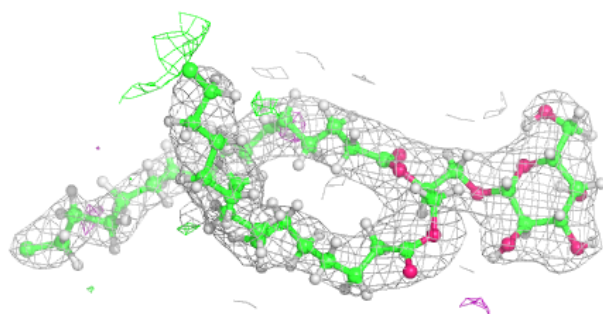
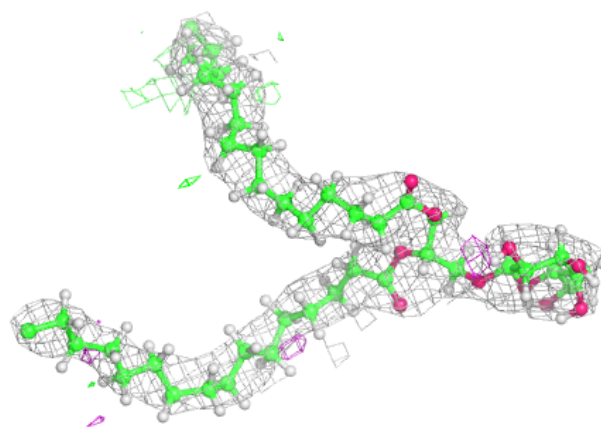
Electron density around CLA b 616:

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



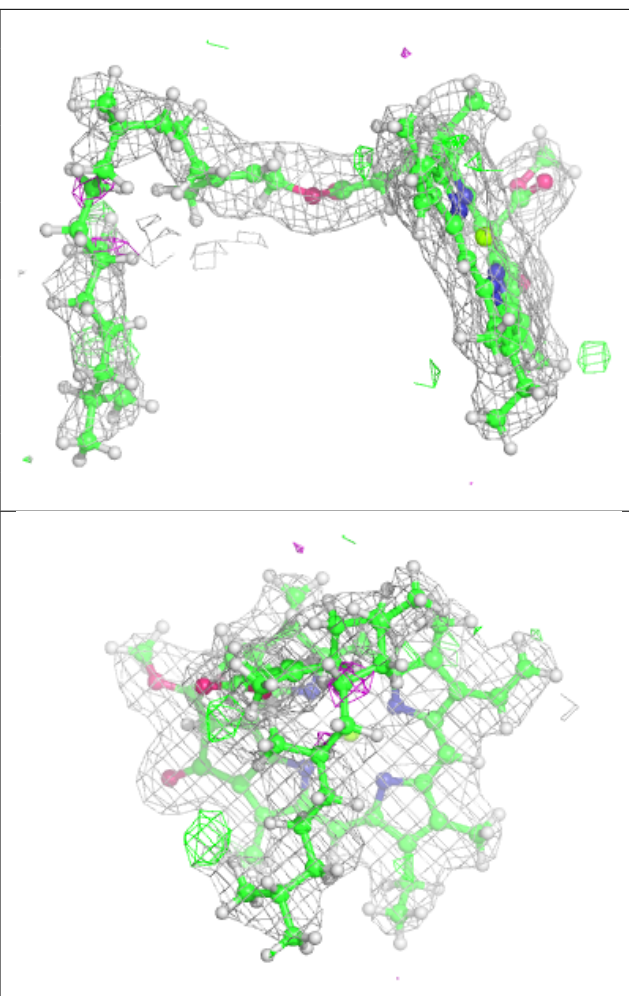
Electron density around LMG M 101:

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



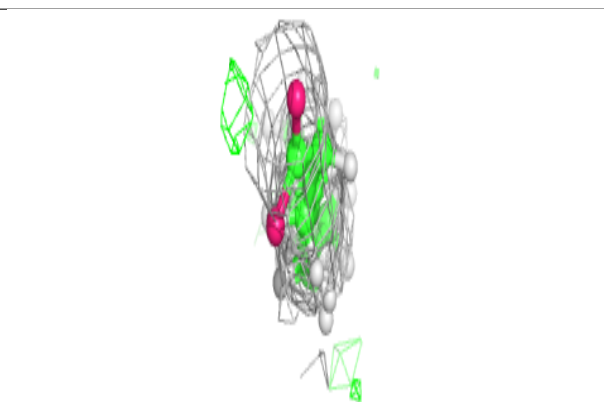
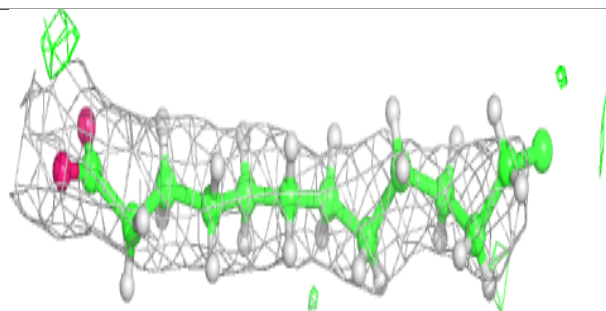
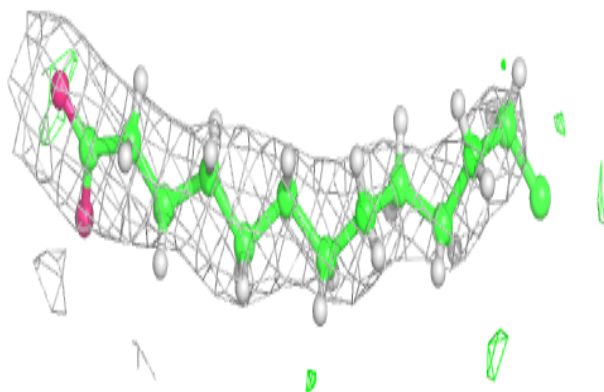
Electron density around CLA a 405:

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

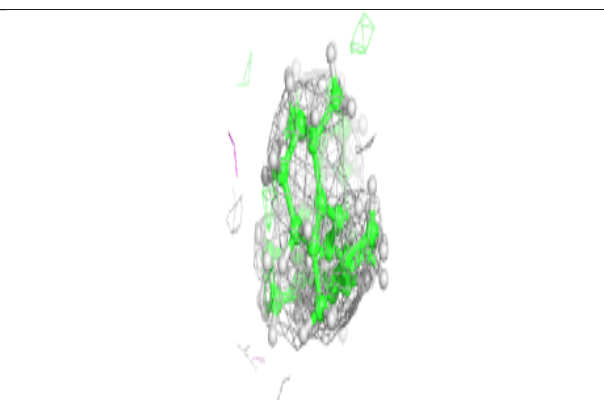
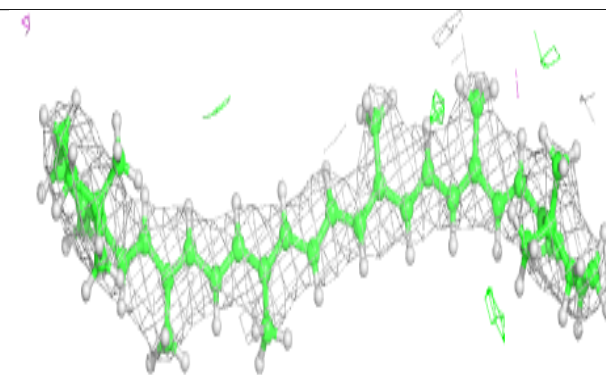
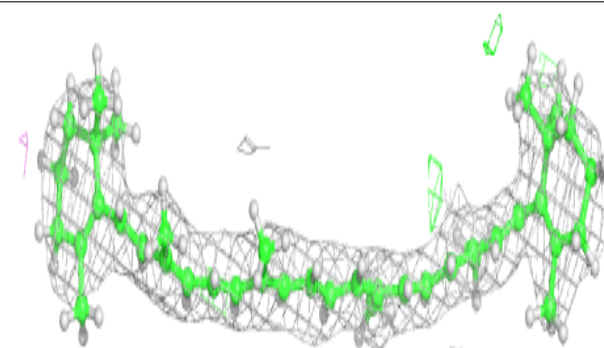


Electron density around STE M 102:

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

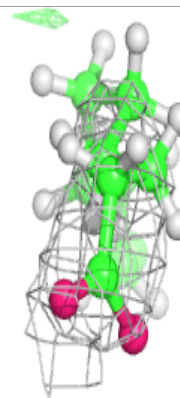
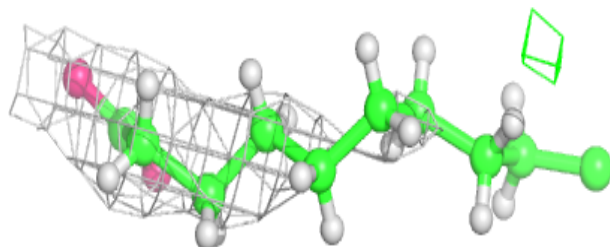
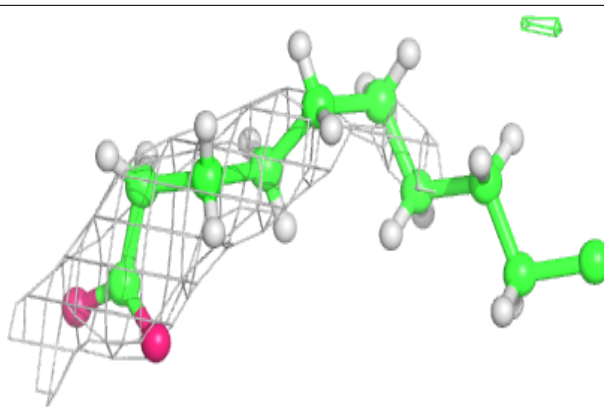
**Electron density around BCR k 102:**

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

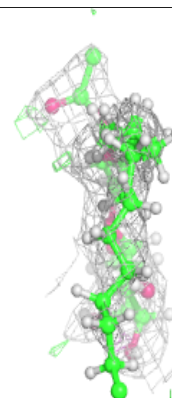
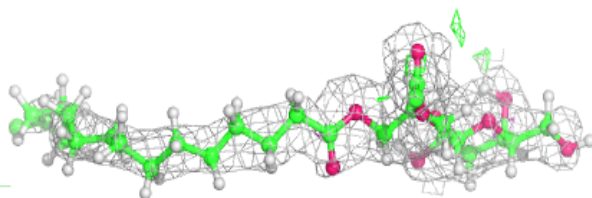
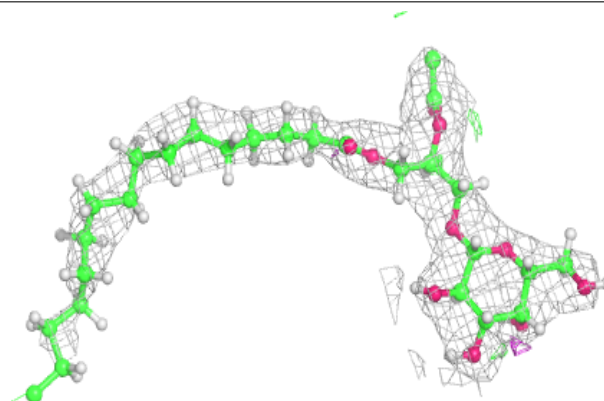


Electron density around STE B 626:

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

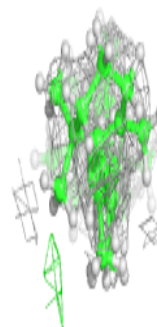
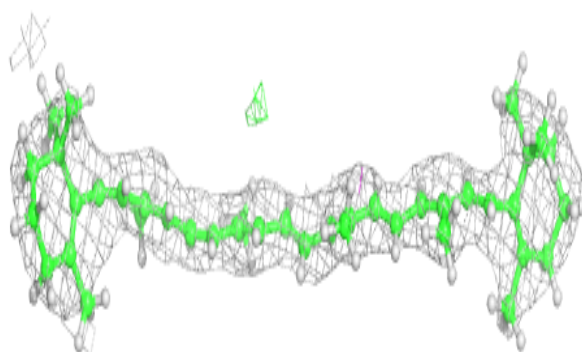
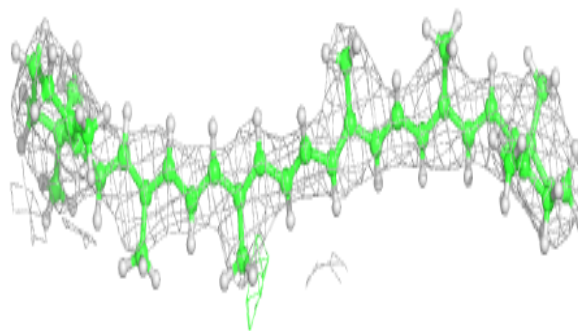
**Electron density around LMG c 519:**

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

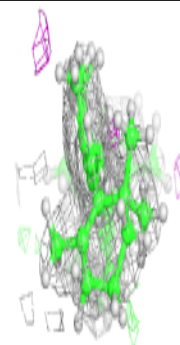
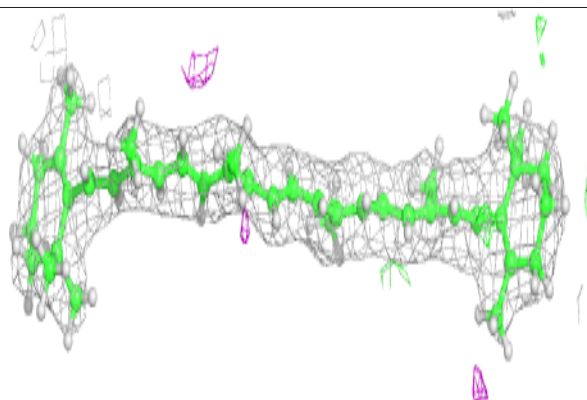
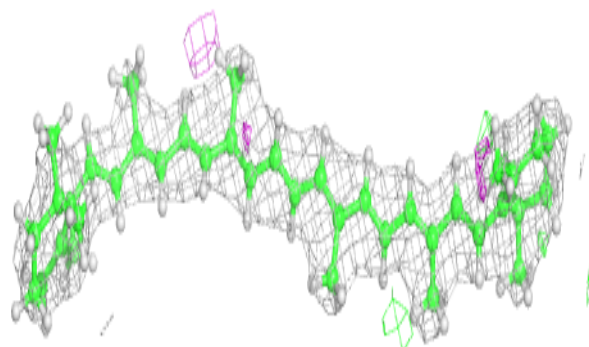


Electron density around BCR c 514:

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

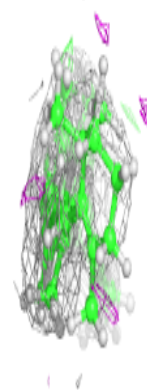
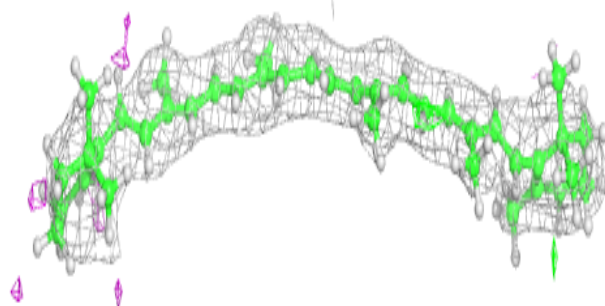
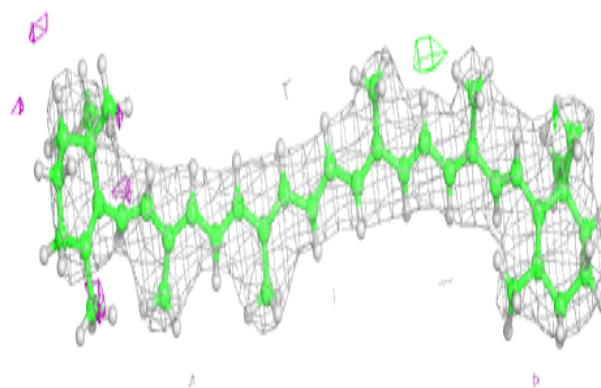
**Electron density around BCR C 514:**

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



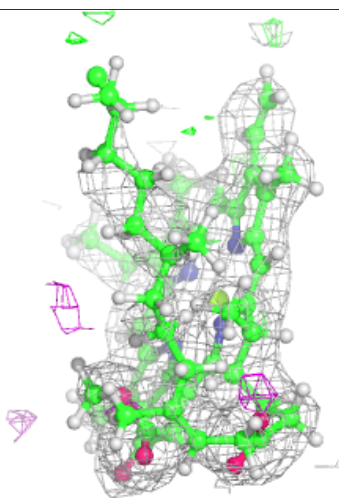
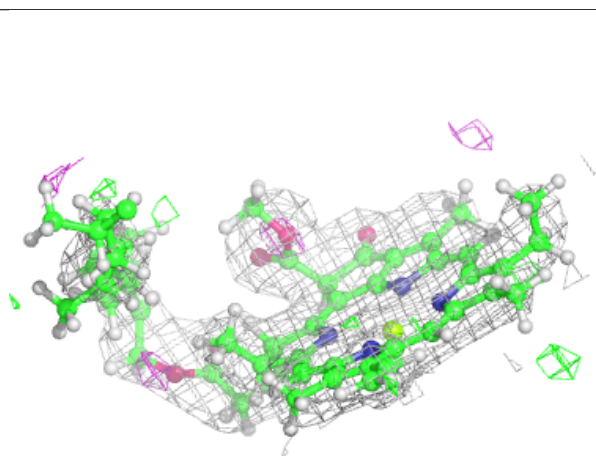
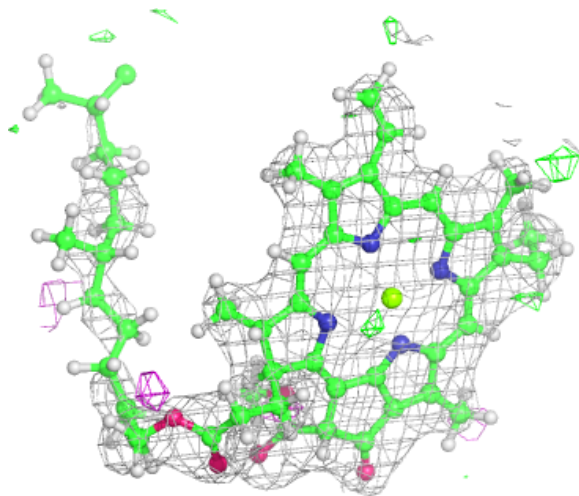
Electron density around BCR D 405:

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



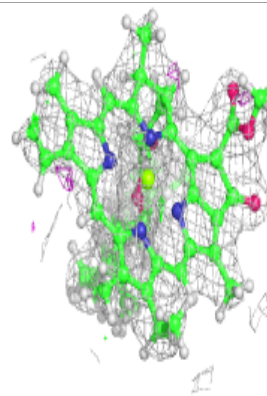
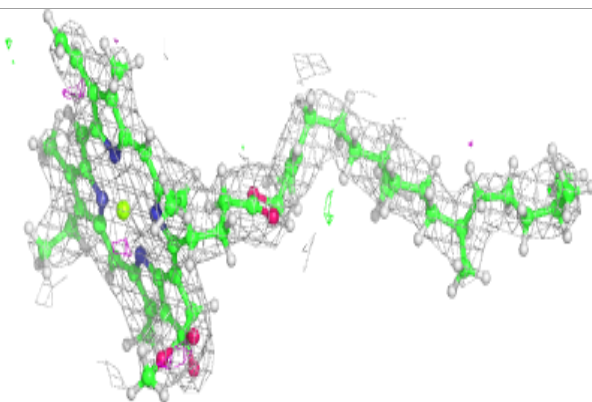
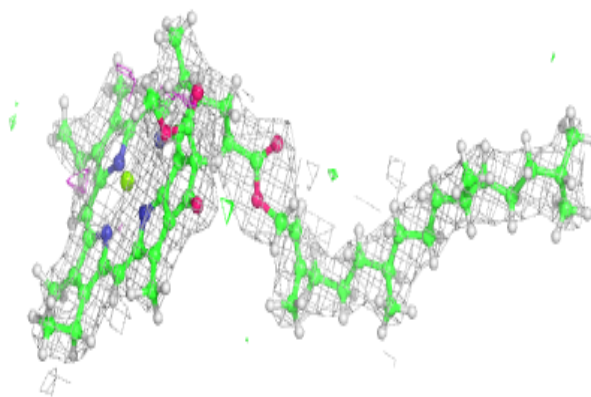
Electron density around CLA B 616:

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



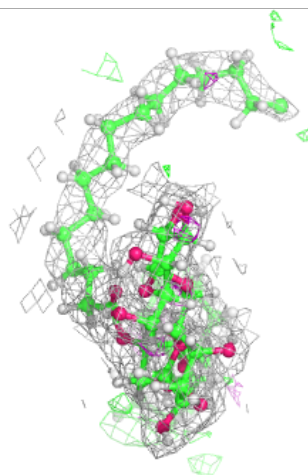
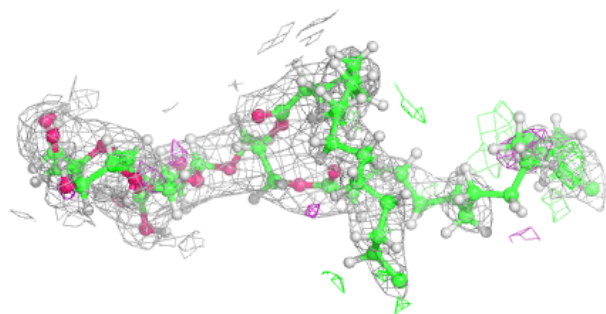
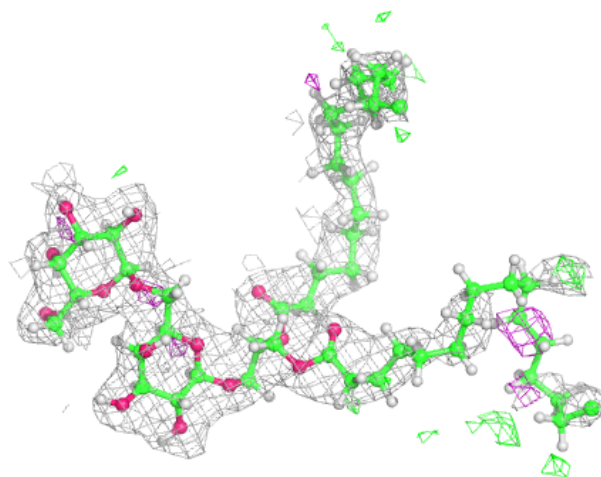
Electron density around CLA C 502:

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



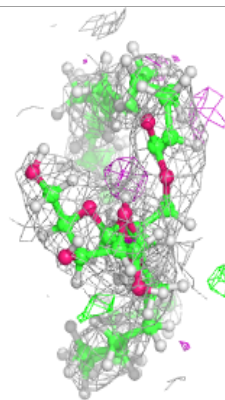
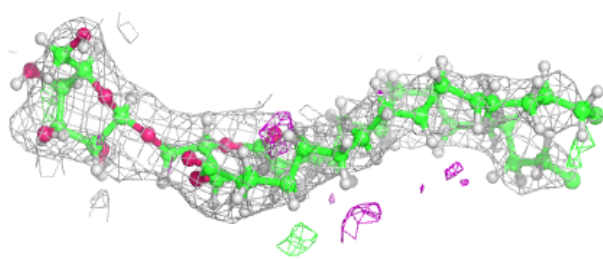
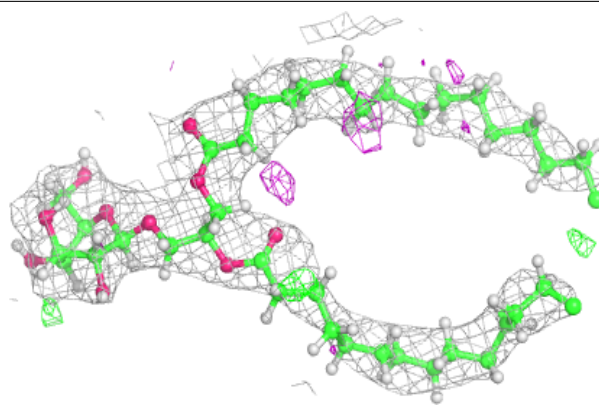
Electron density around DGD C 516:

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



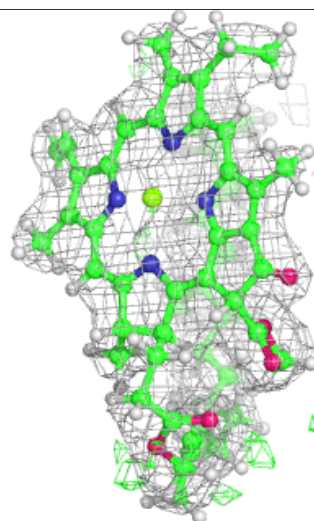
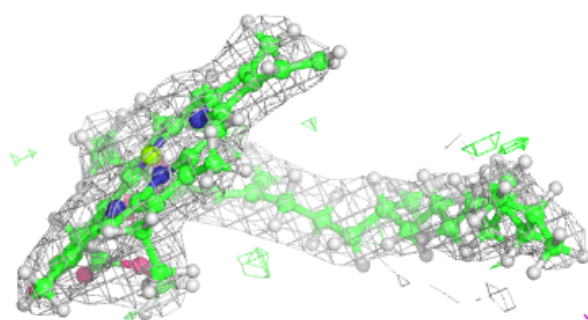
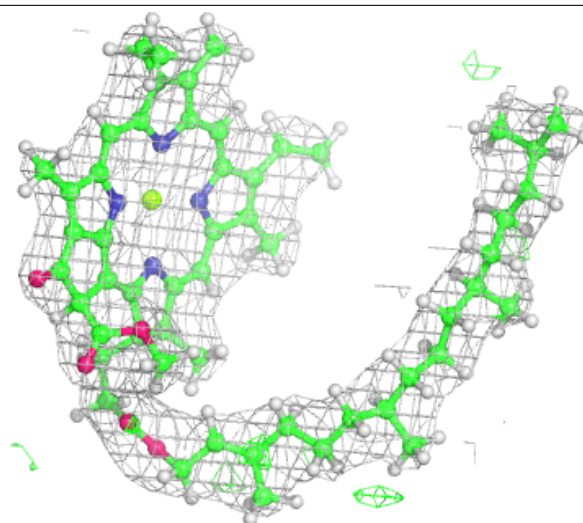
Electron density around LMG a 414:

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



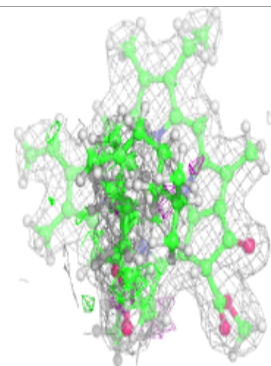
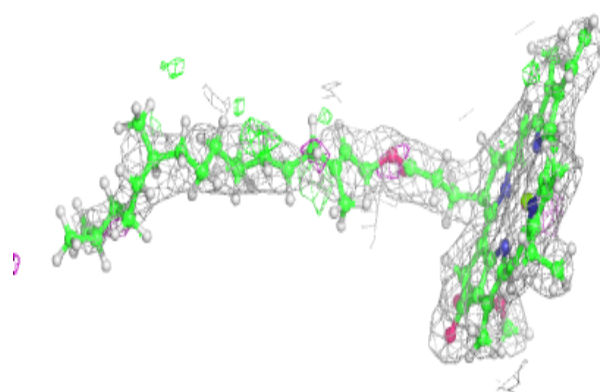
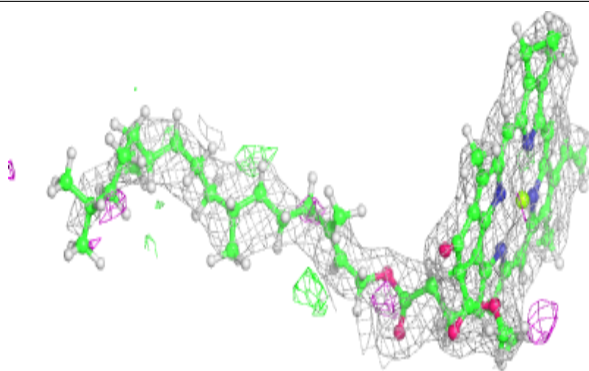
Electron density around CLA C 507:

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

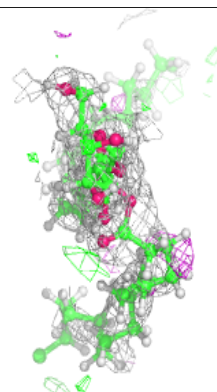
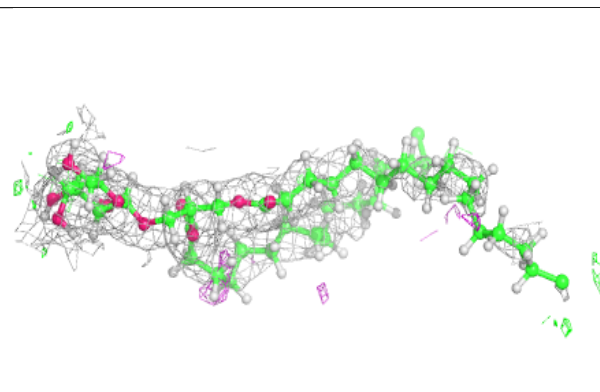
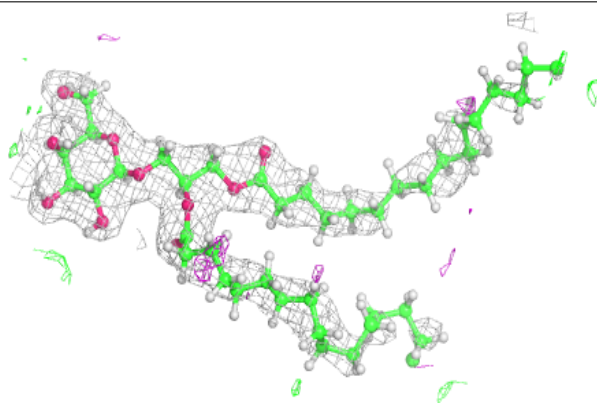


Electron density around CLA B 604:

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

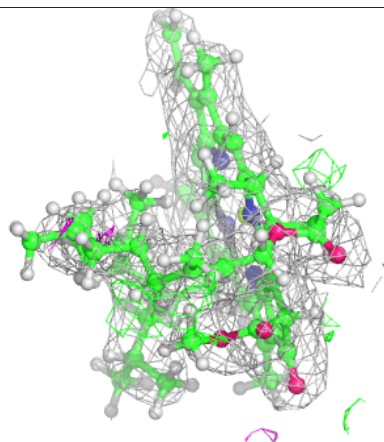
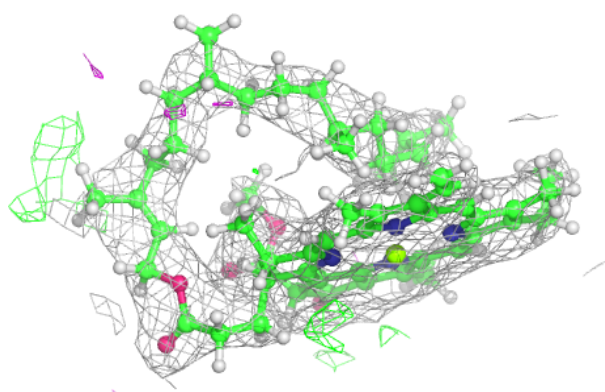
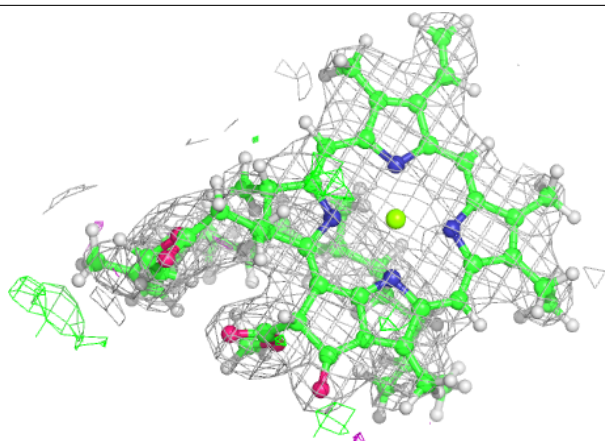
**Electron density around LMG D 407:**

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



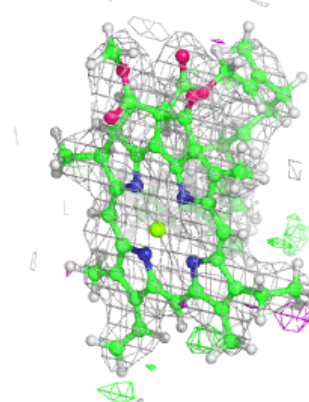
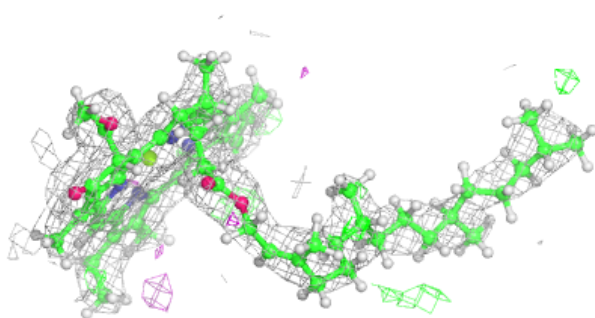
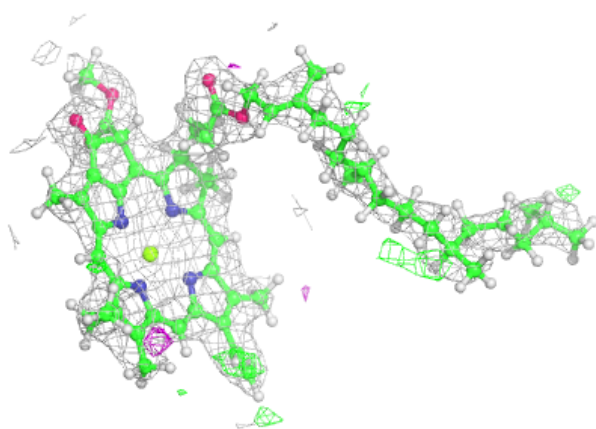
Electron density around CLA c 510:

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

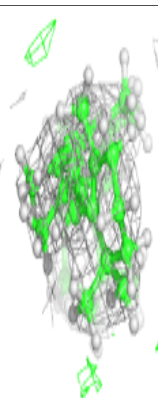
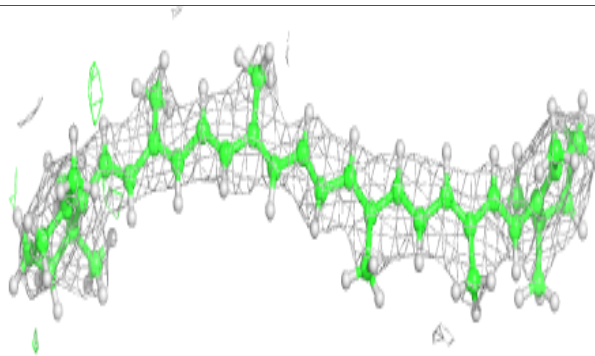
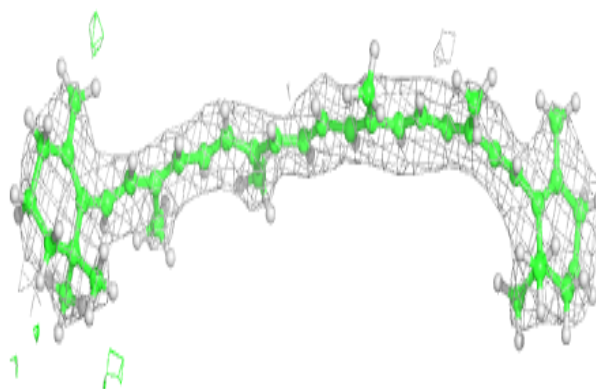


Electron density around CLA c 511:

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

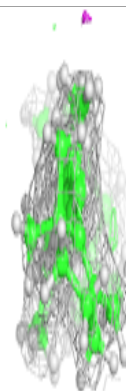
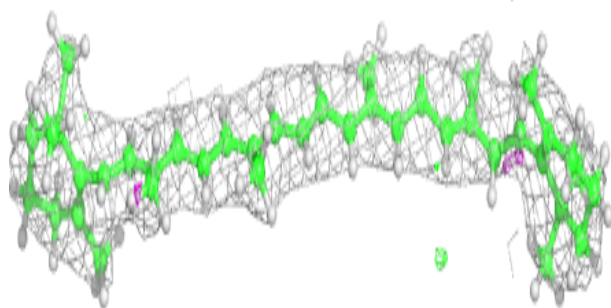
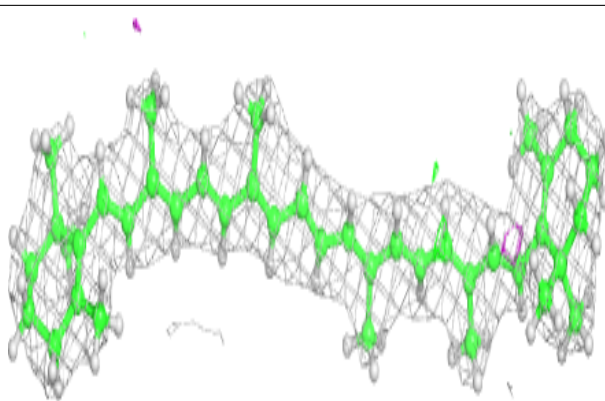
**Electron density around BCR K 103:**

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

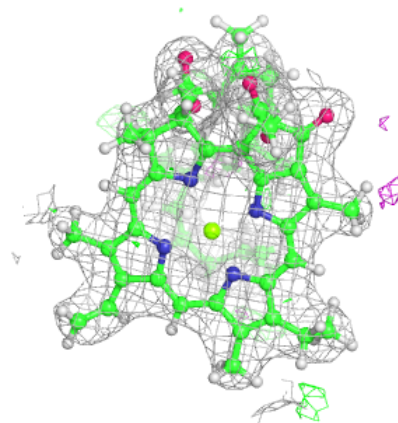
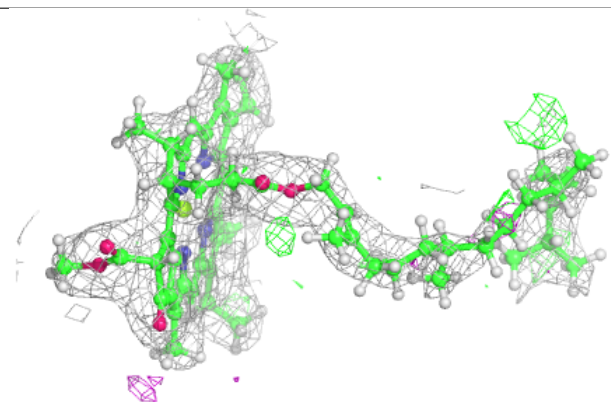
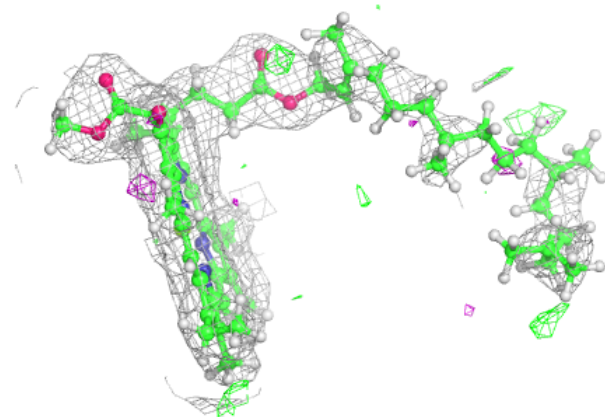


Electron density around BCR b 619:

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

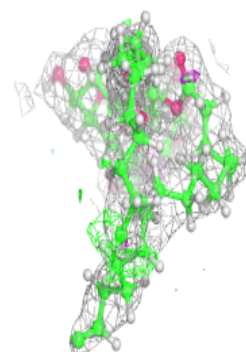
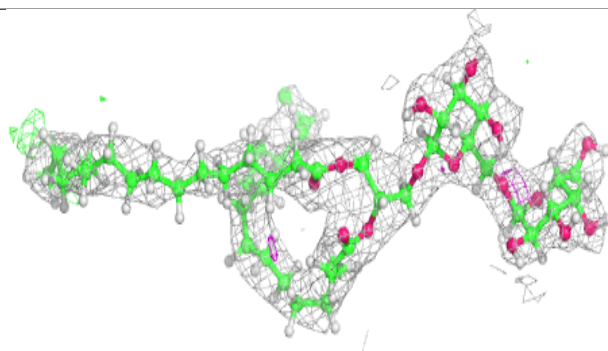
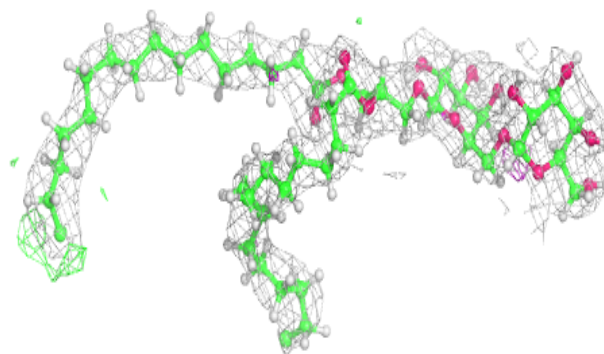
**Electron density around CLA C 506:**

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

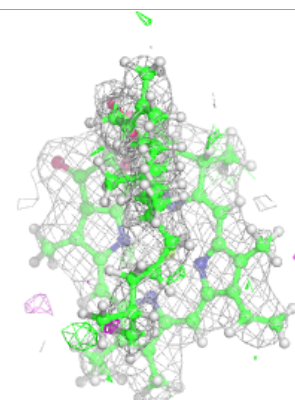
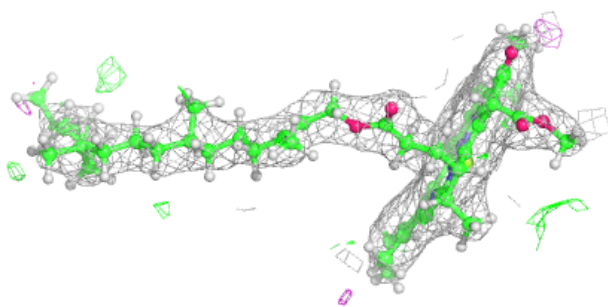
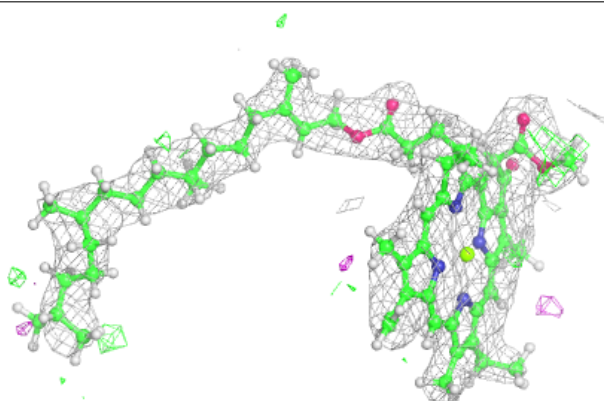


Electron density around DGD H 102:

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

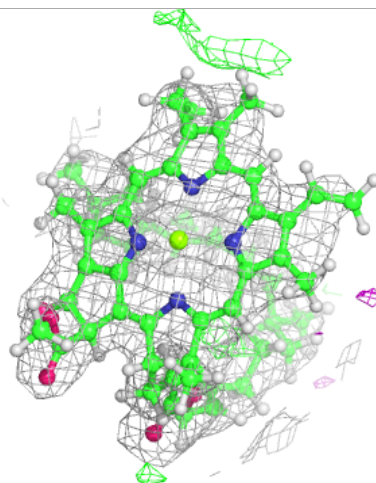
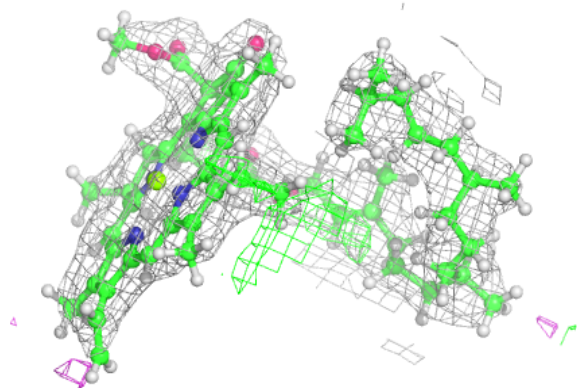
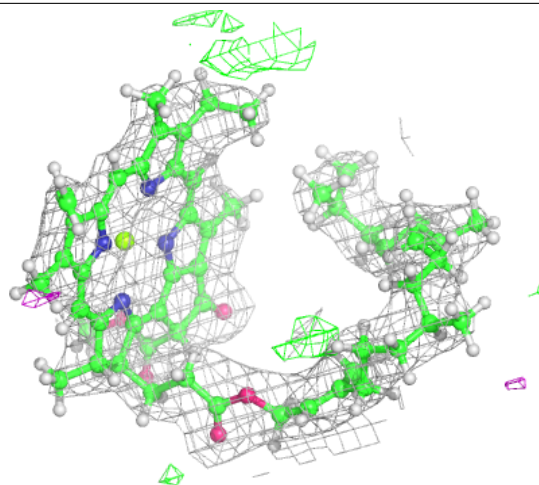
**Electron density around CLA b 609:**

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



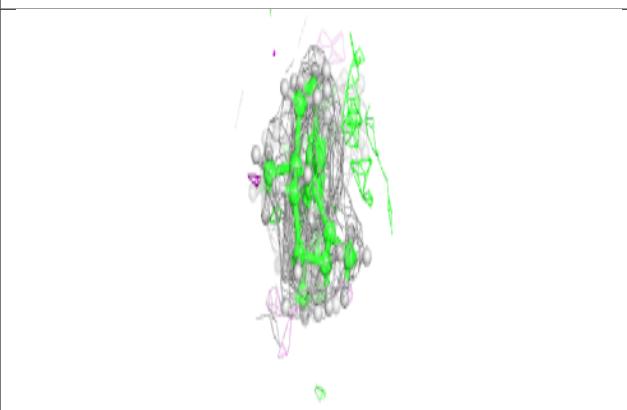
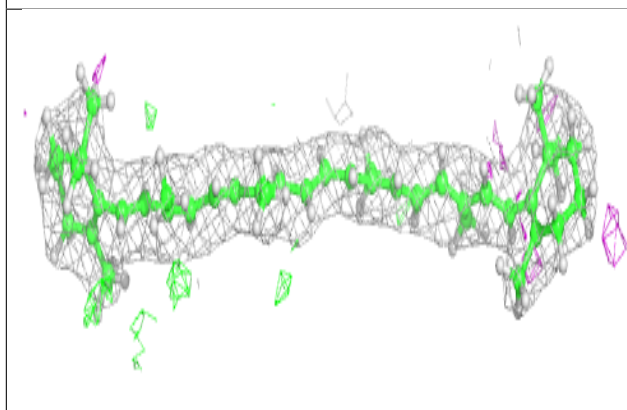
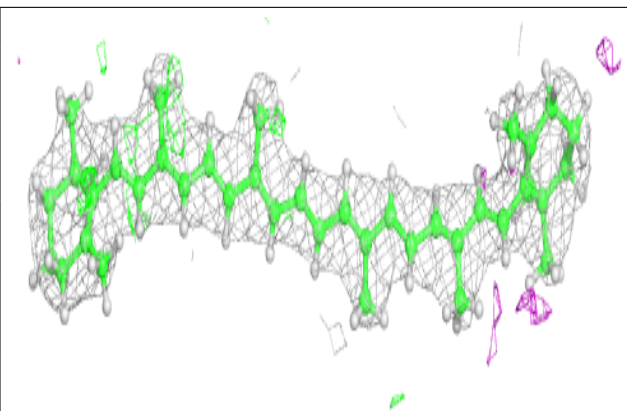
Electron density around CLA c 503:

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

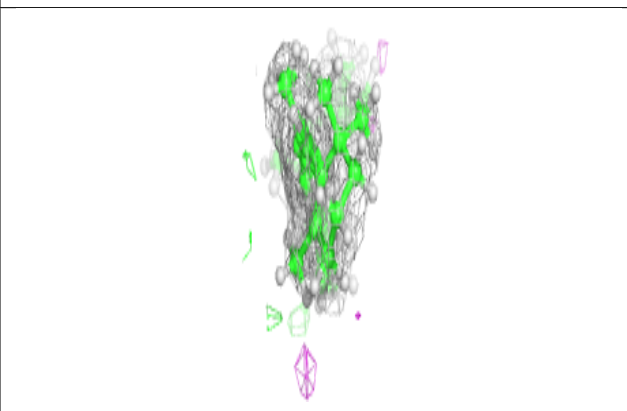
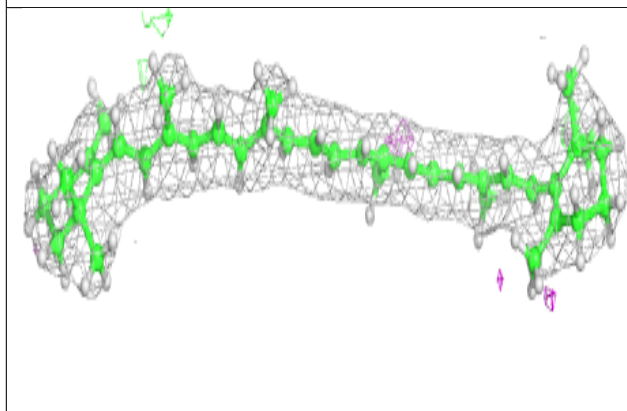
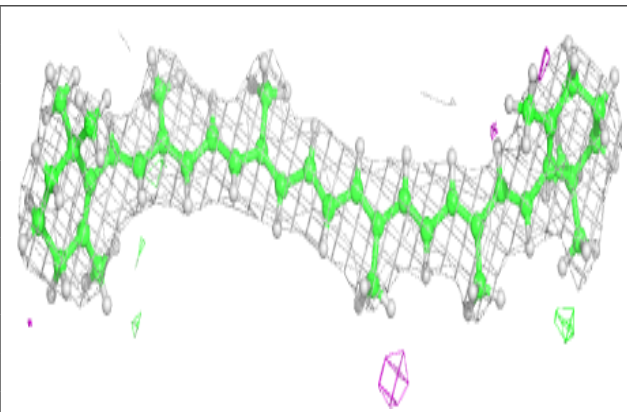


Electron density around BCR B 618:

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

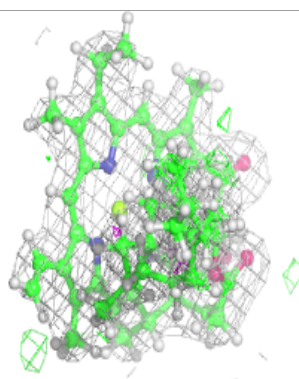
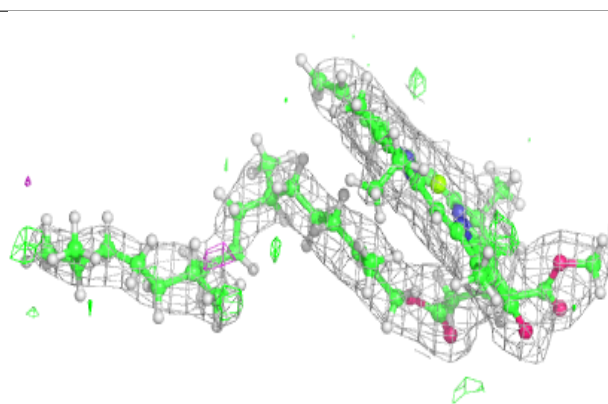
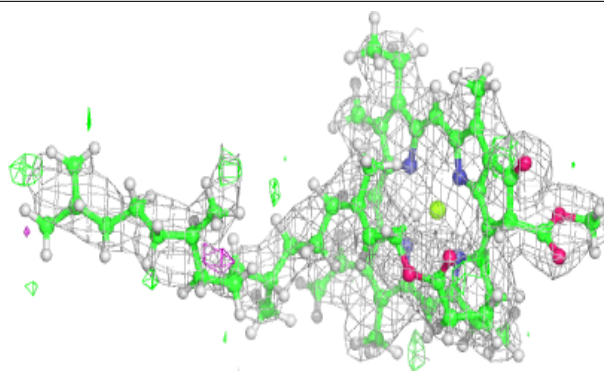
**Electron density around BCR B 619:**

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



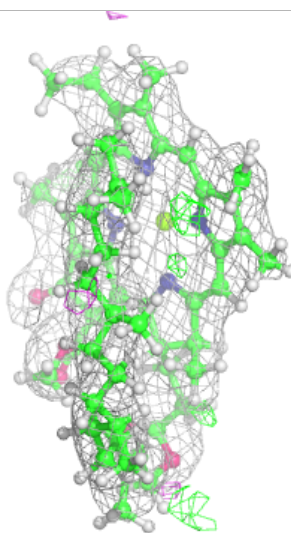
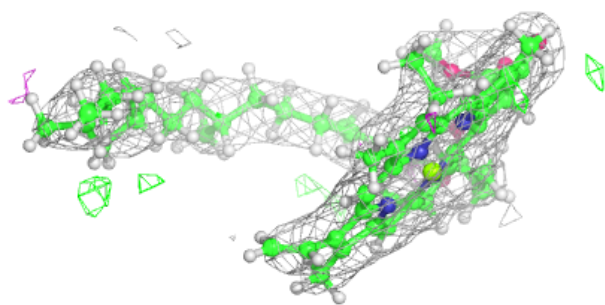
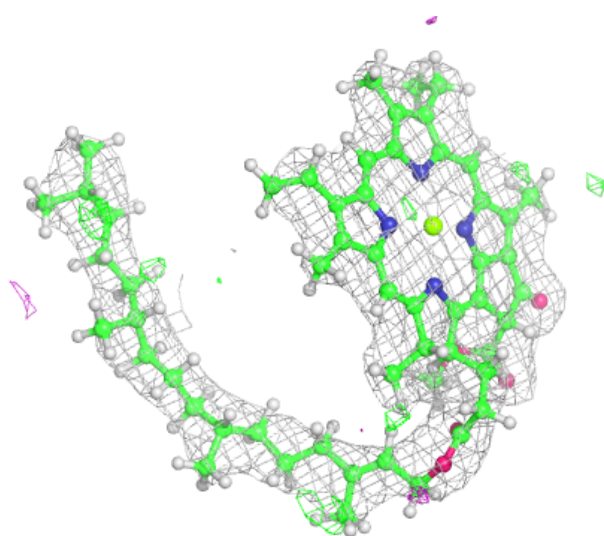
Electron density around CLA c 505:

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



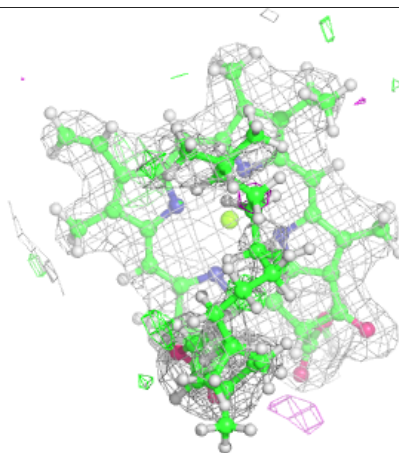
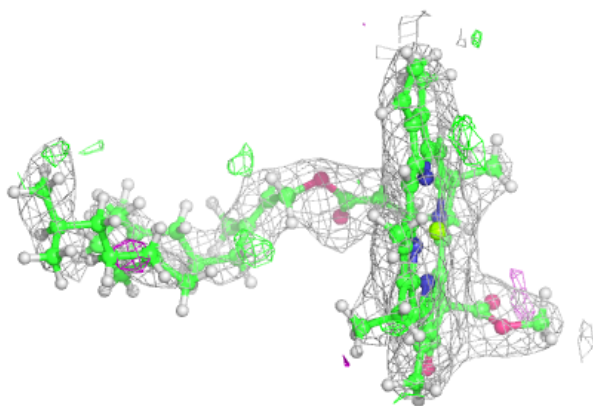
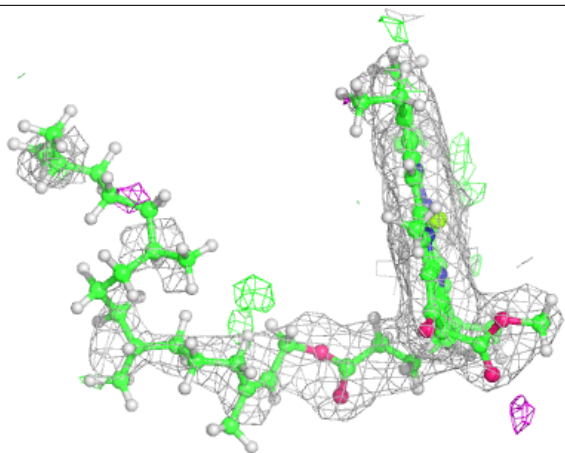
Electron density around CLA c 507:

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



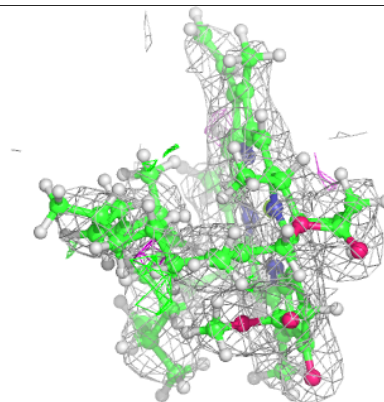
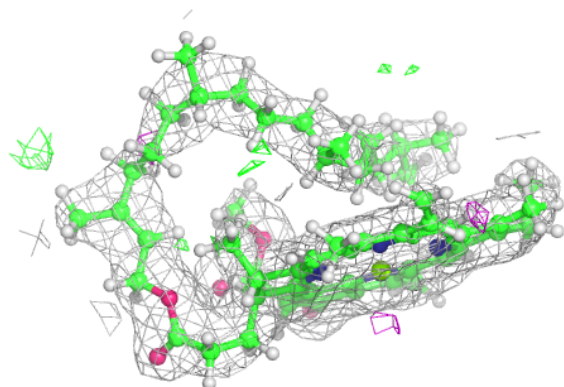
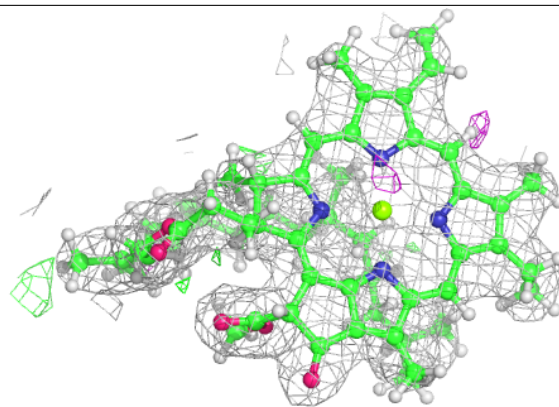
Electron density around CLA c 506:

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

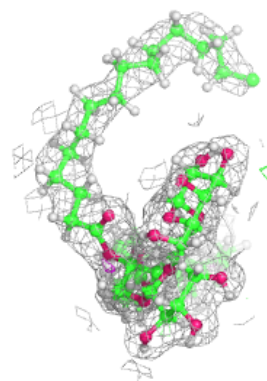
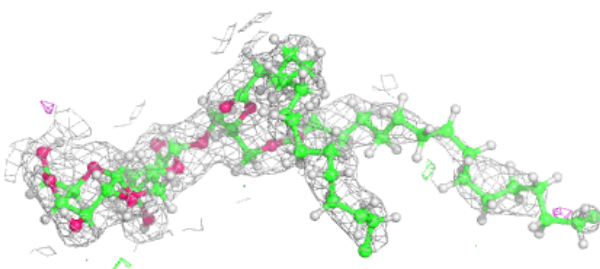
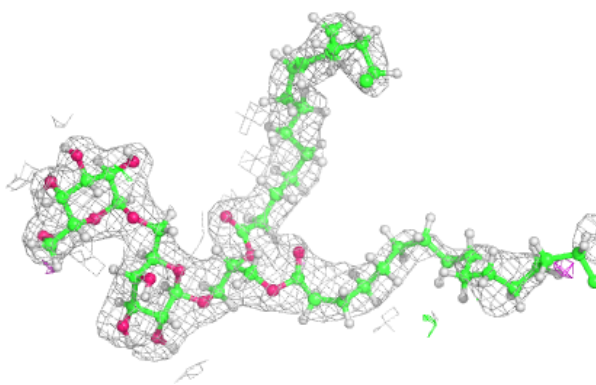


Electron density around CLA C 510:

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

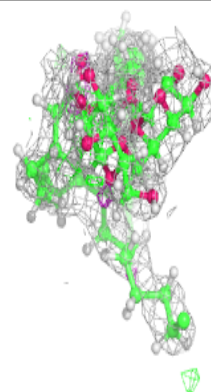
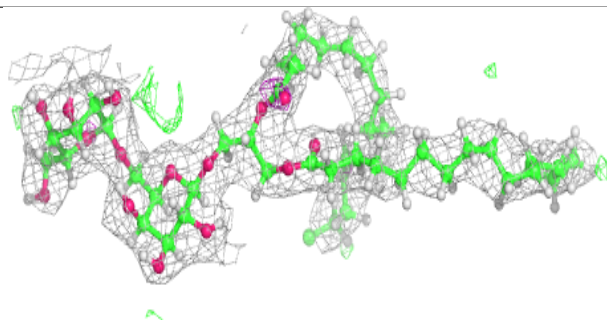
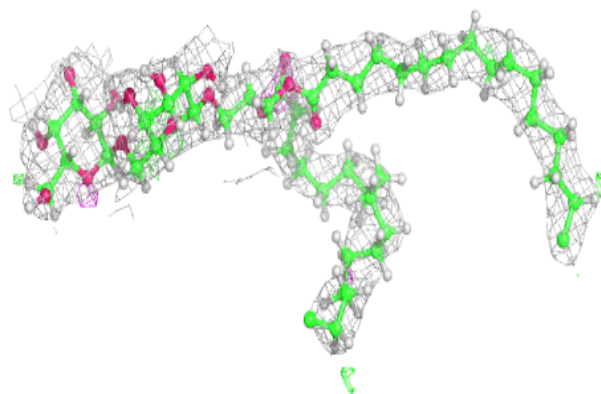
**Electron density around DGD c 517:**

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

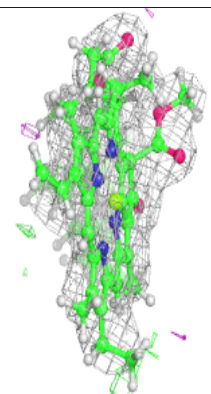
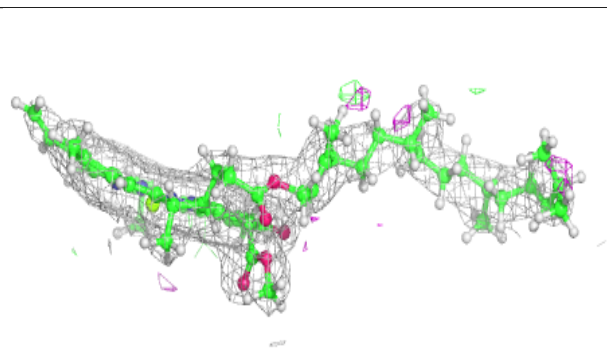
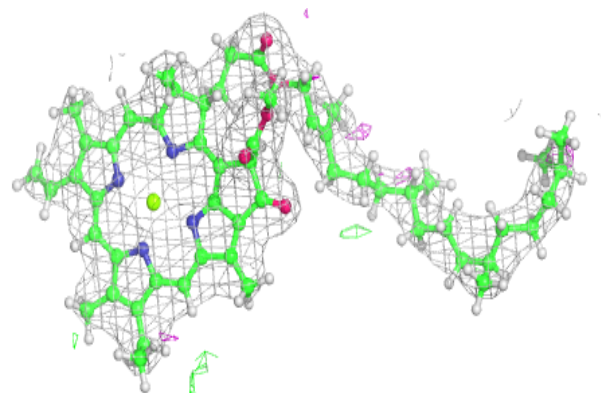


Electron density around DGD h 103:

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

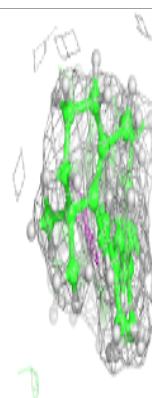
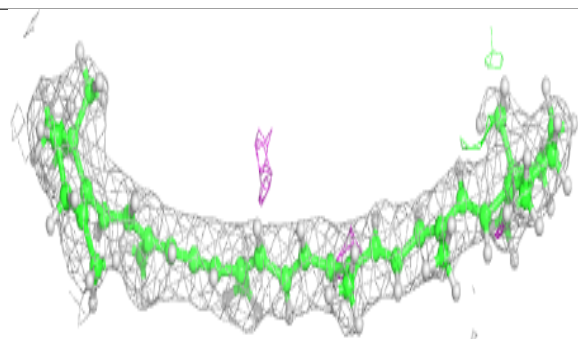
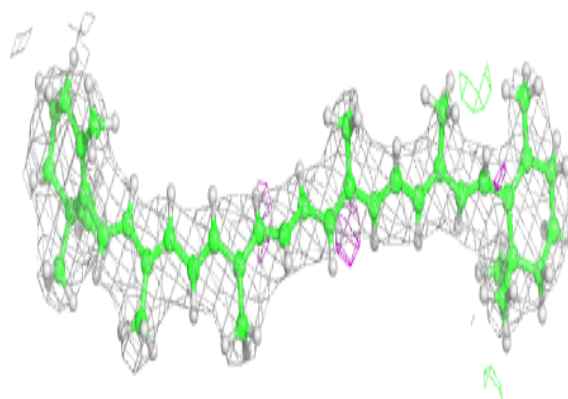
**Electron density around CLA b 602:**

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



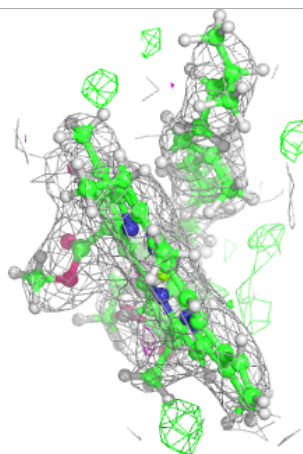
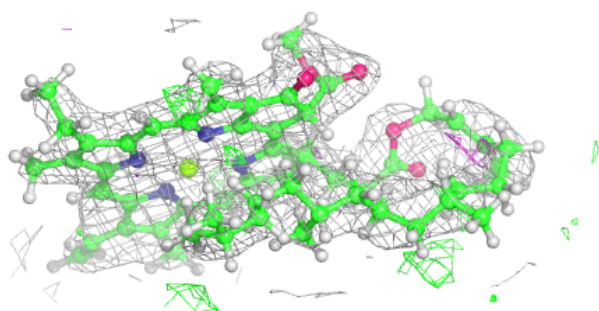
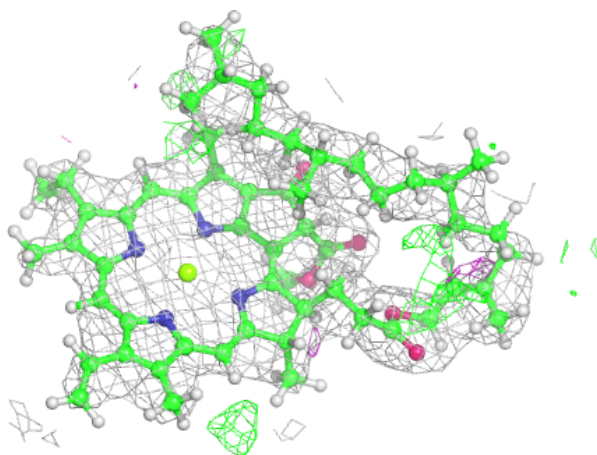
Electron density around BCR T 101:

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



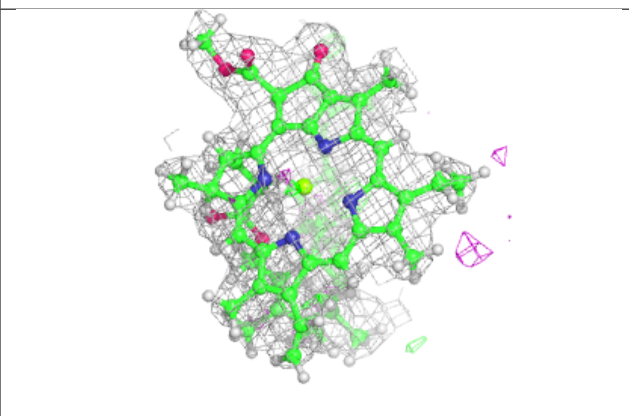
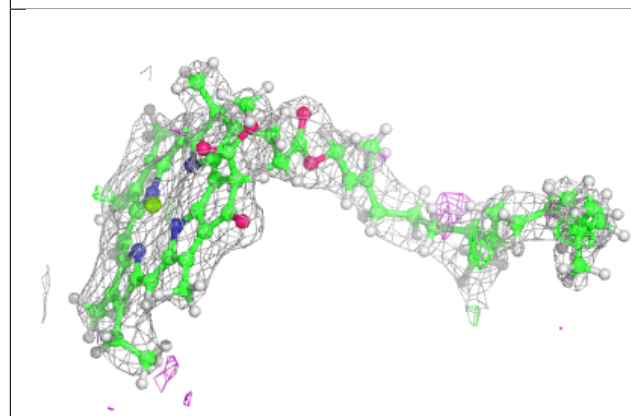
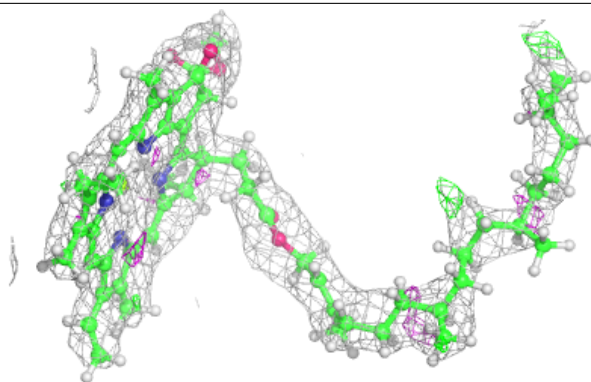
Electron density around CLA c 509:

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

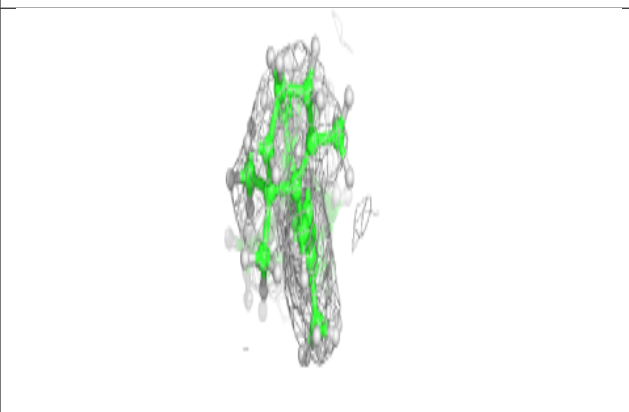
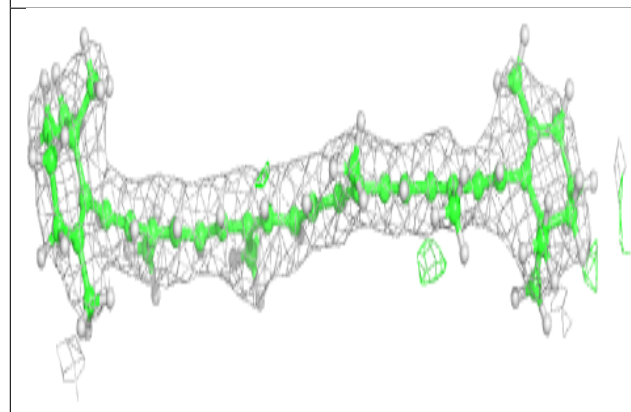
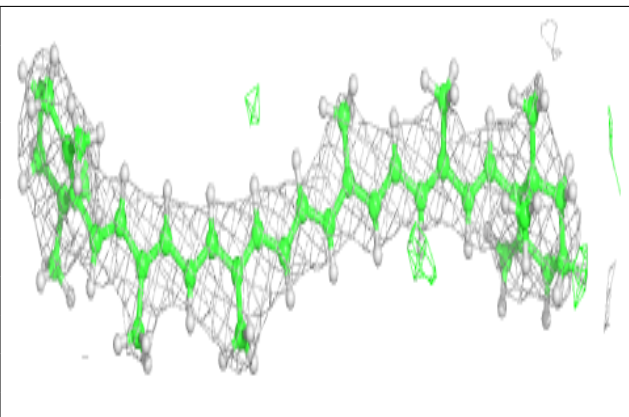


Electron density around CLA b 606:

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

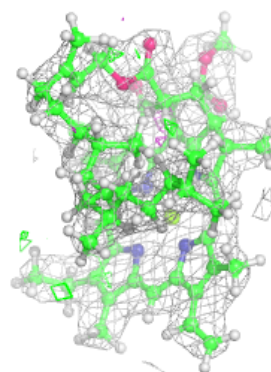
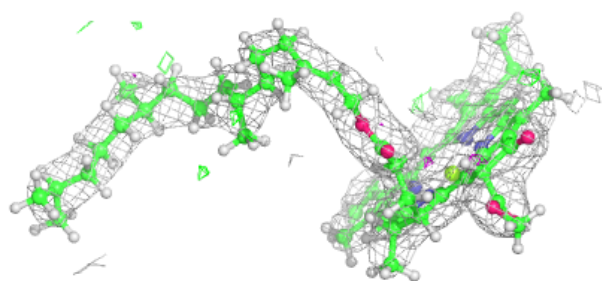
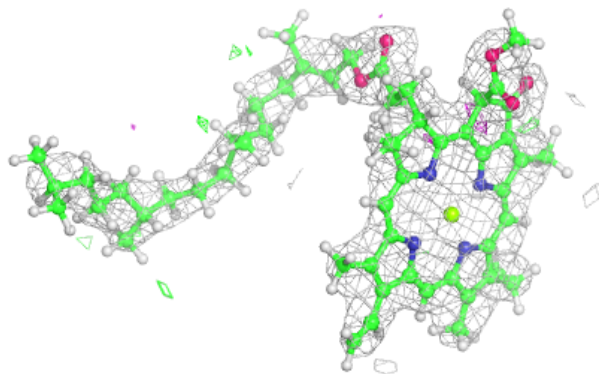
**Electron density around BCR c 515:**

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



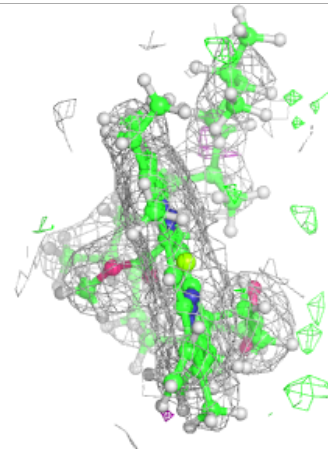
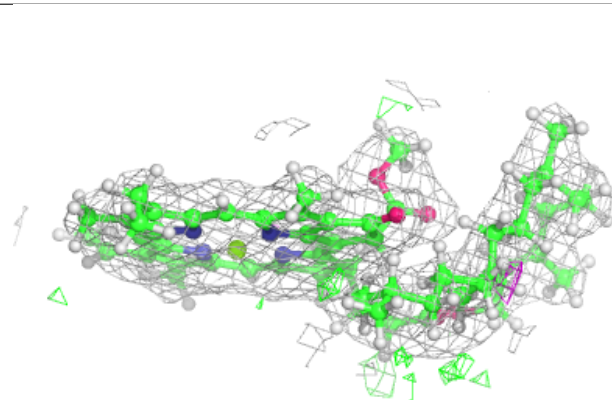
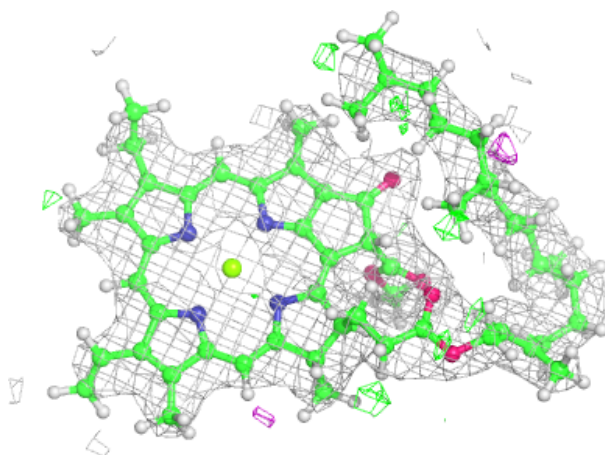
Electron density around CLA C 511:

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



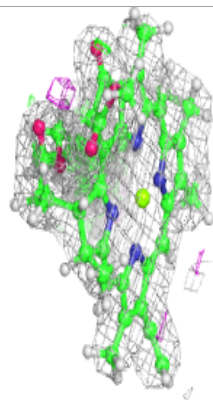
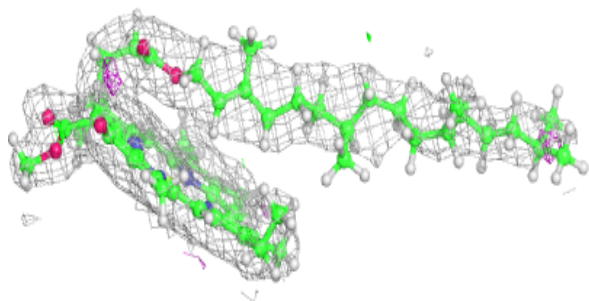
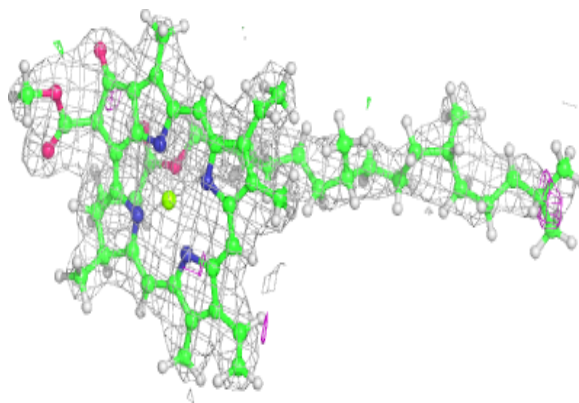
Electron density around CLA b 610:

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



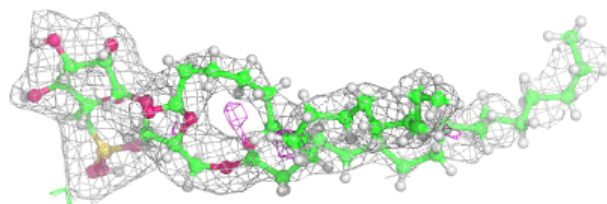
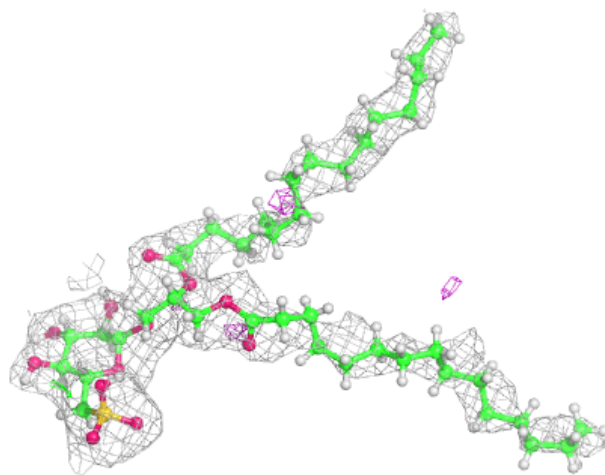
Electron density around CLA b 614:

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



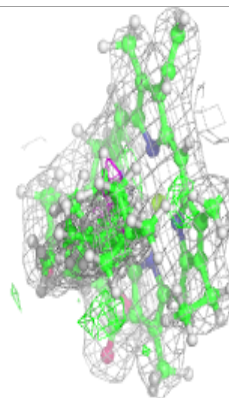
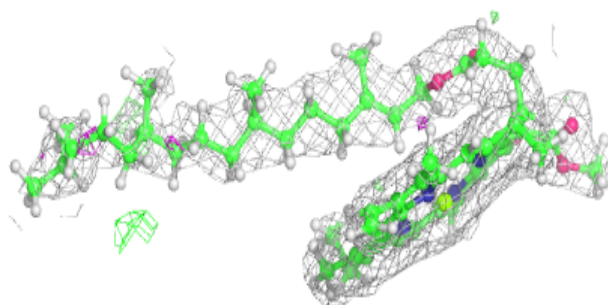
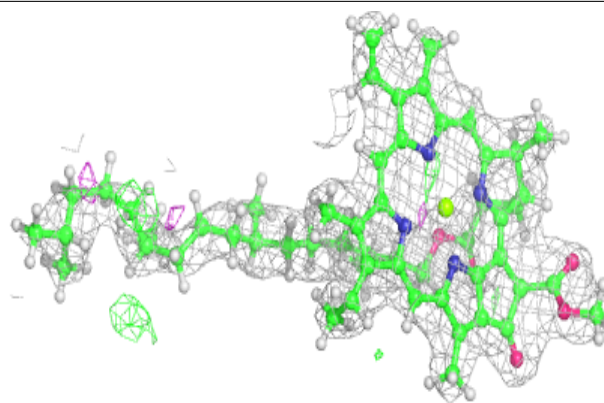
Electron density around SQD a 411:

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

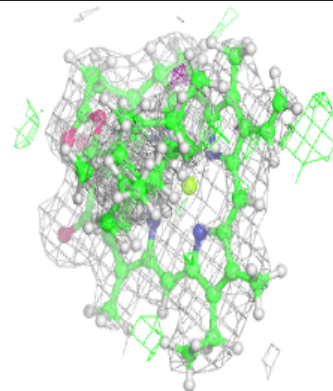
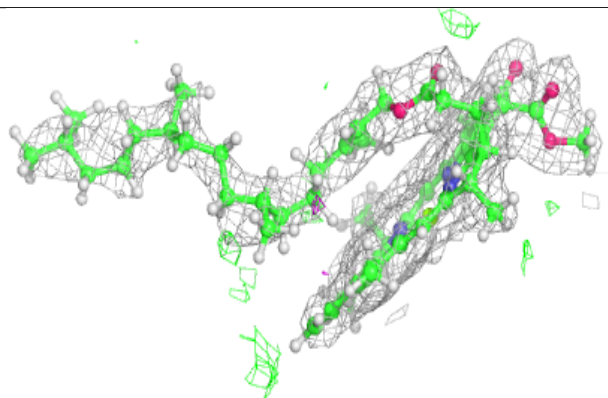
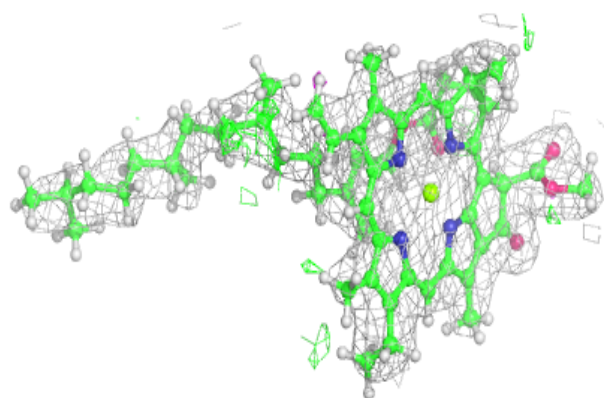


Electron density around CLA B 614:

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

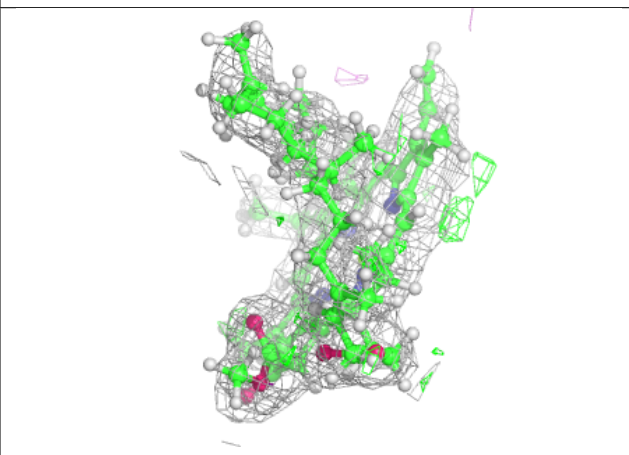
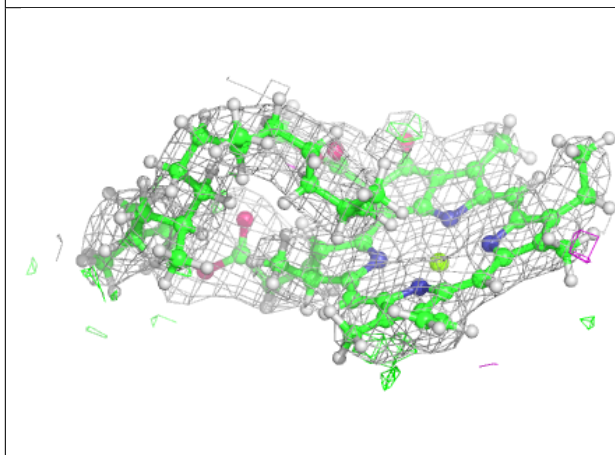
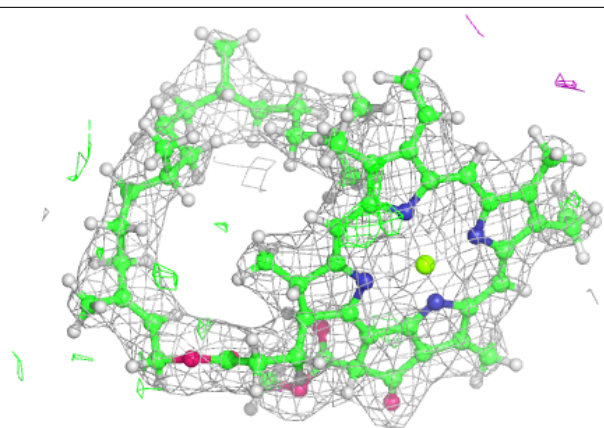
**Electron density around CLA C 505:**

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

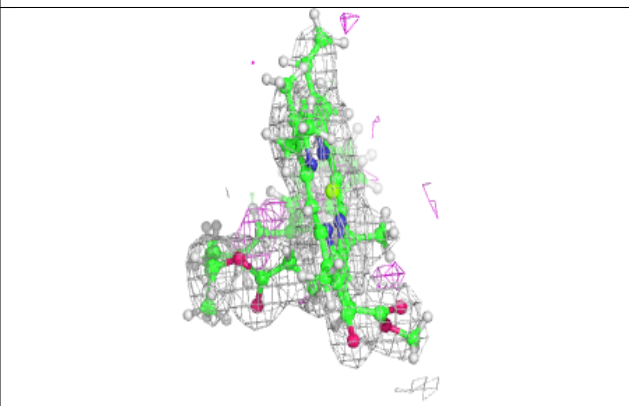
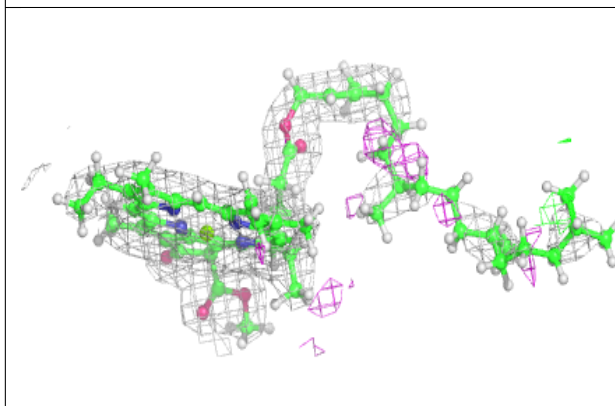
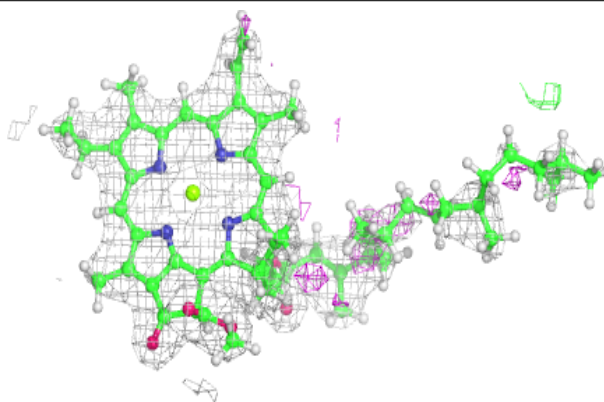


Electron density around CLA B 615:

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

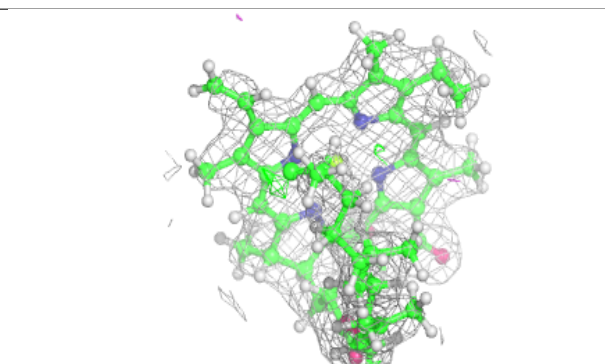
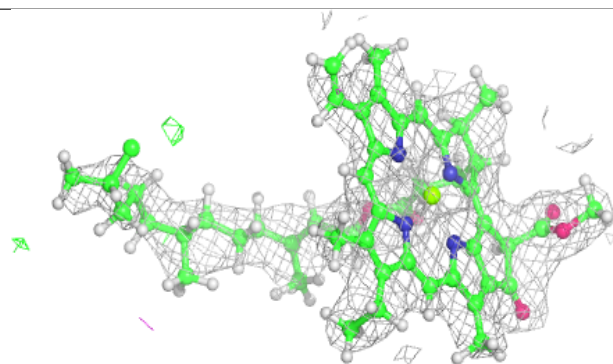
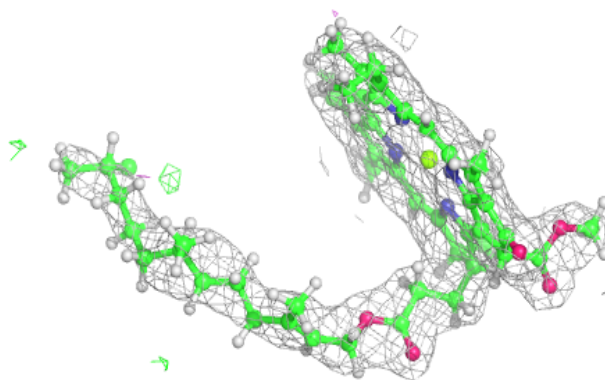
**Electron density around CLA a 403:**

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

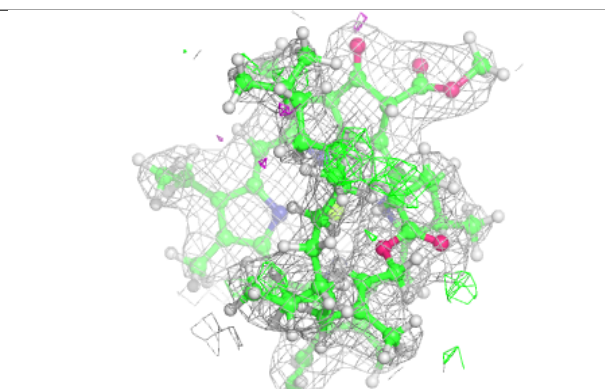
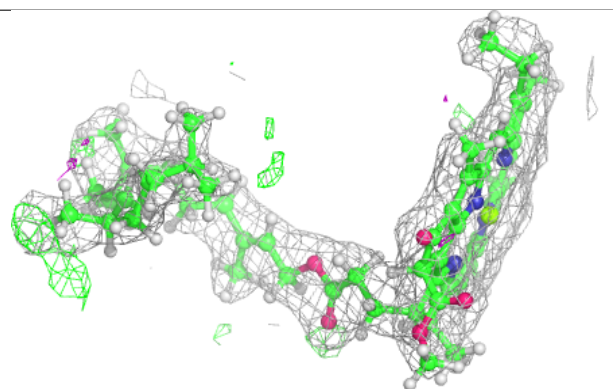
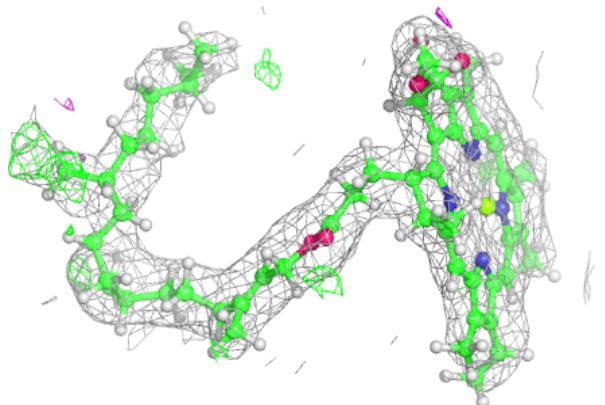


Electron density around CLA c 504:

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

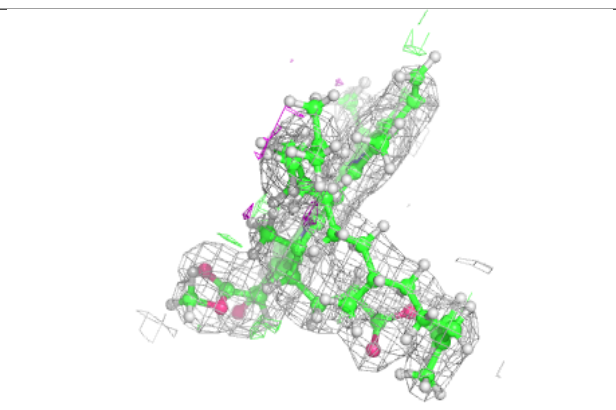
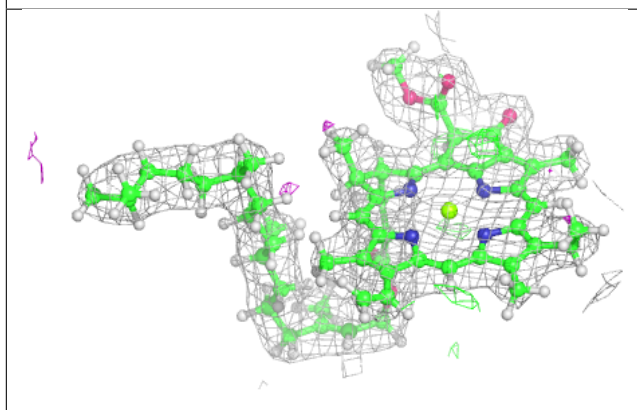
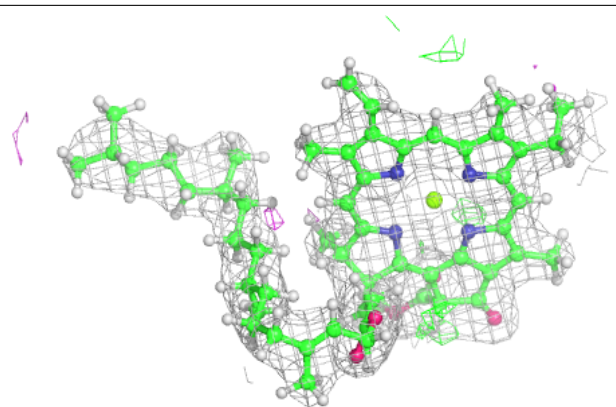
**Electron density around CLA B 606:**

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



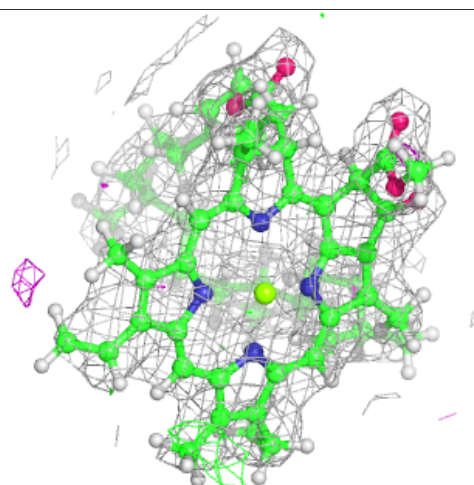
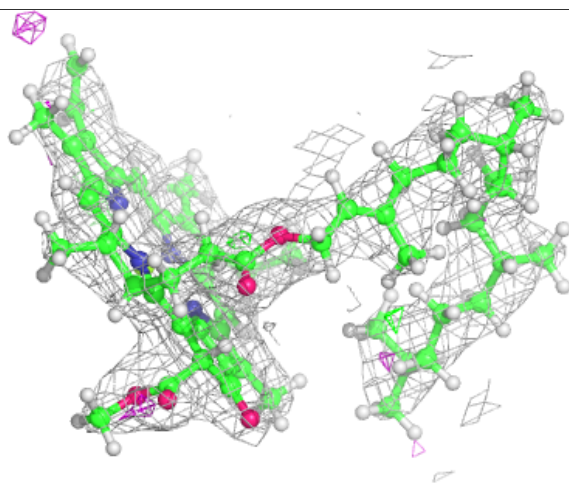
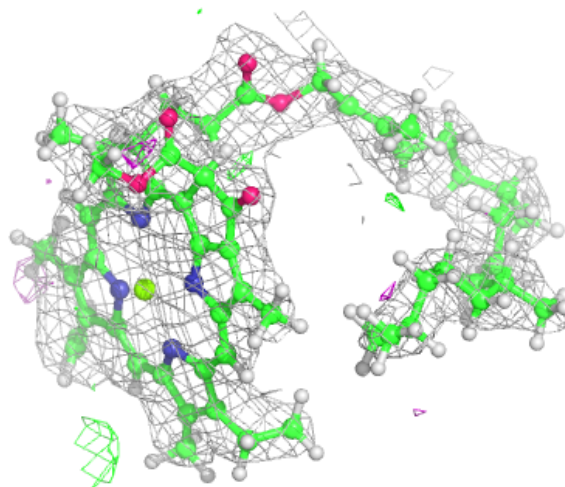
Electron density around CLA d 404:

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



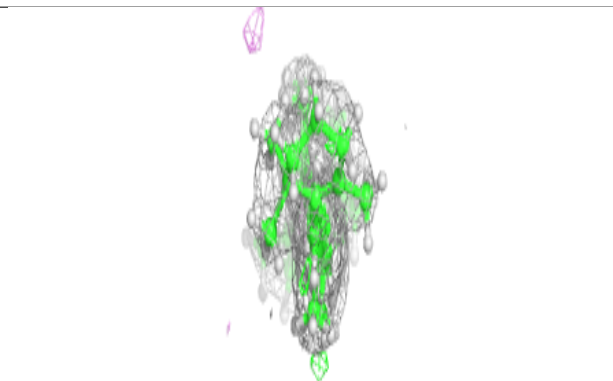
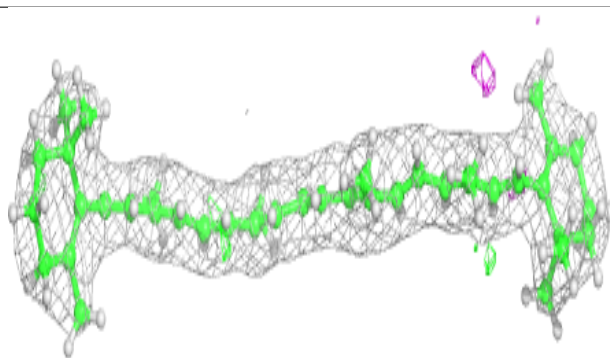
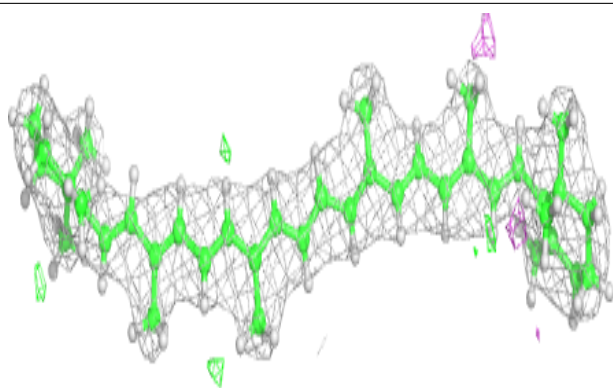
Electron density around CLA C 503:

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

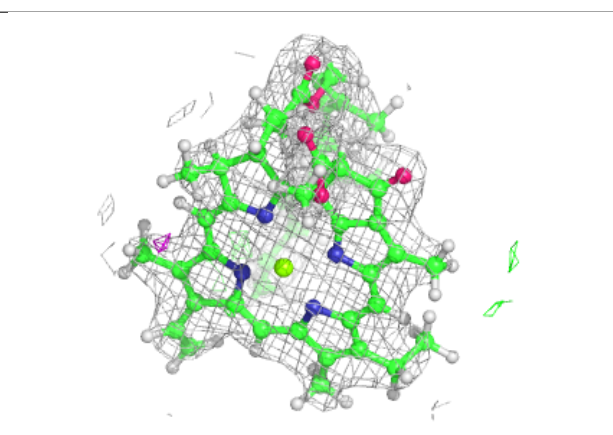
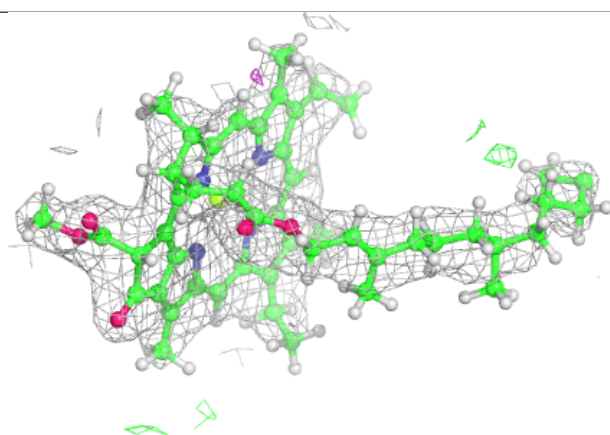
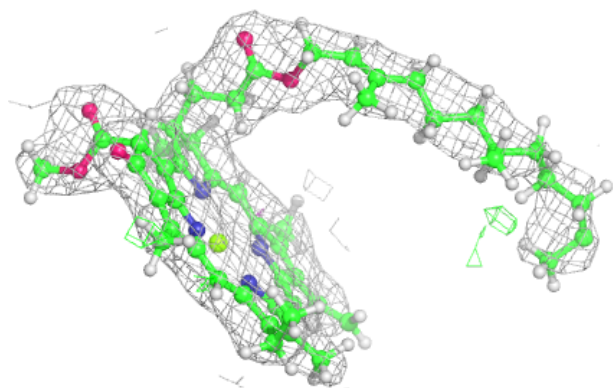


Electron density around BCR A 407:

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

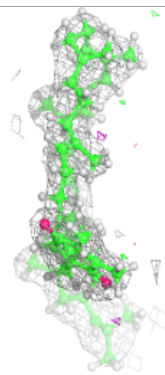
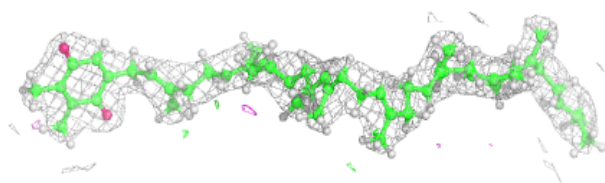
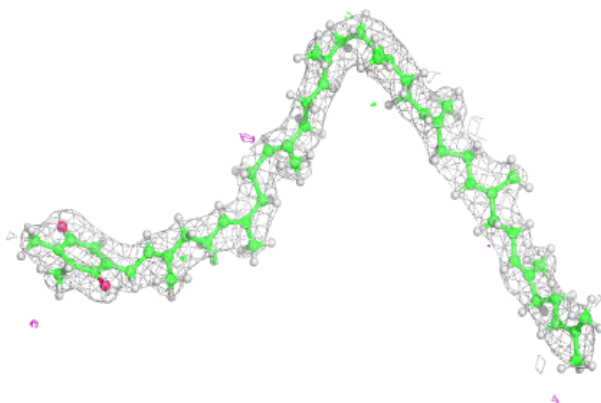
**Electron density around CLA C 504:**

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

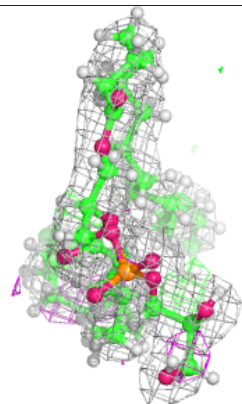
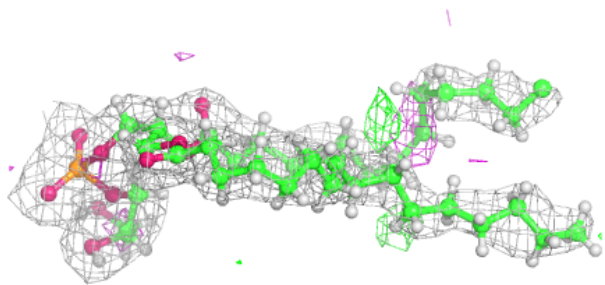
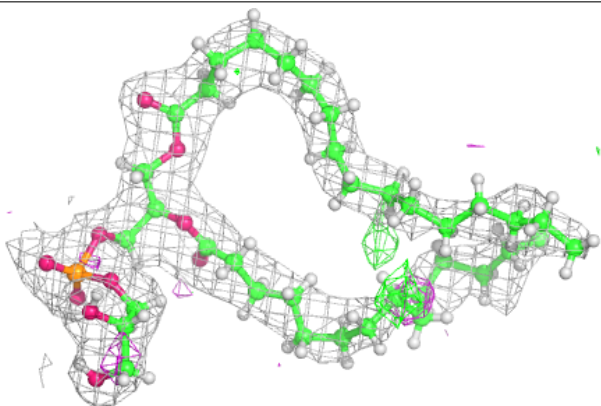


Electron density around PL9 D 406:

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

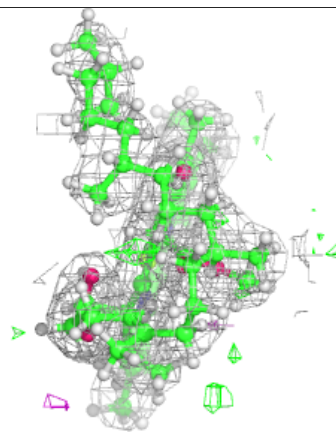
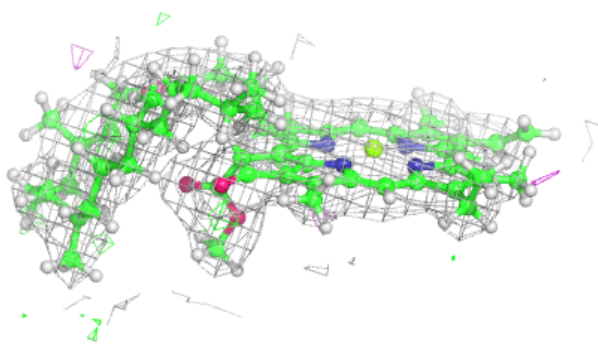
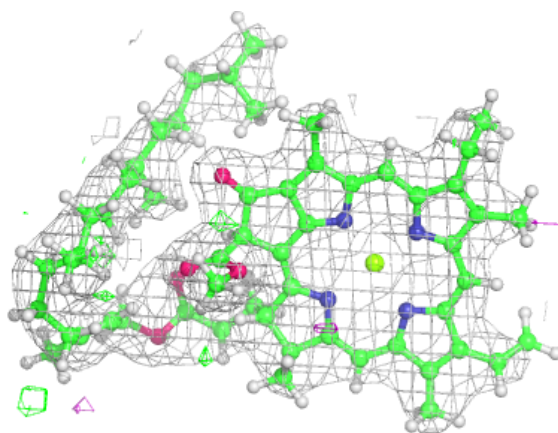
**Electron density around LHG D 409:**

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



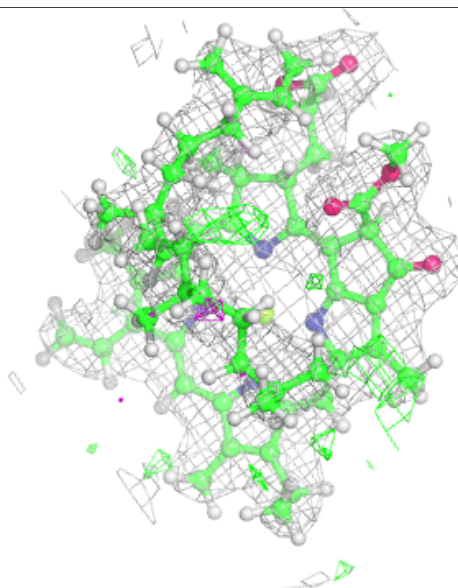
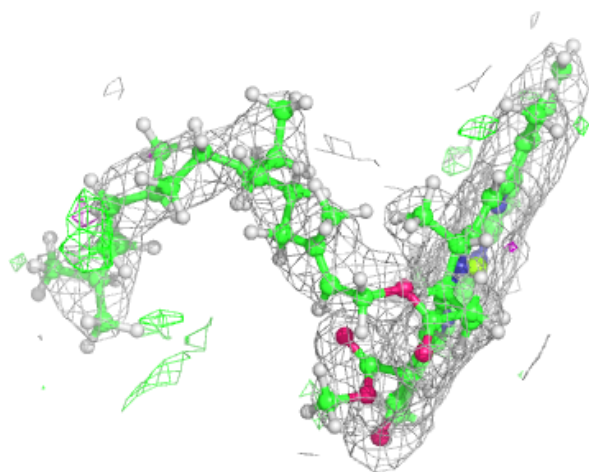
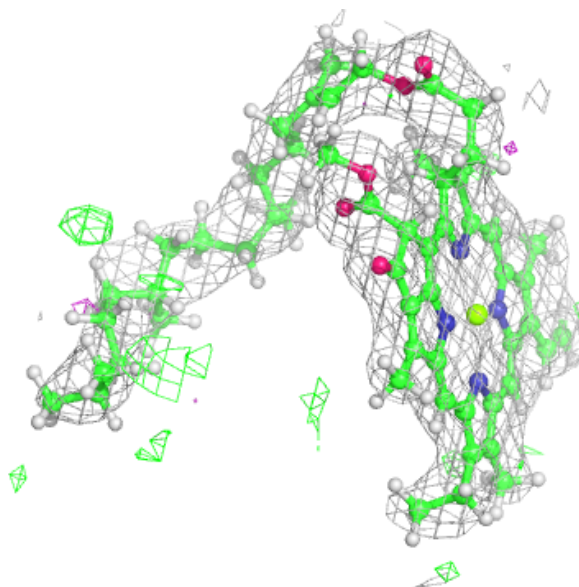
Electron density around CLA B 610:

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



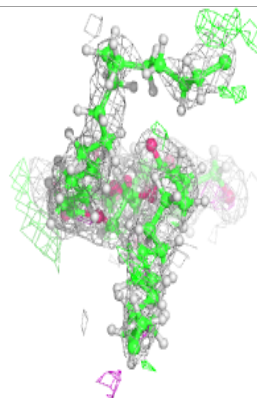
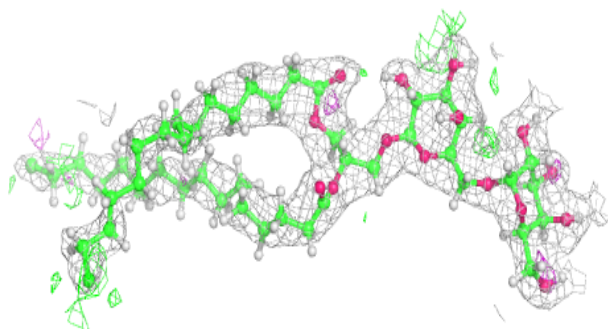
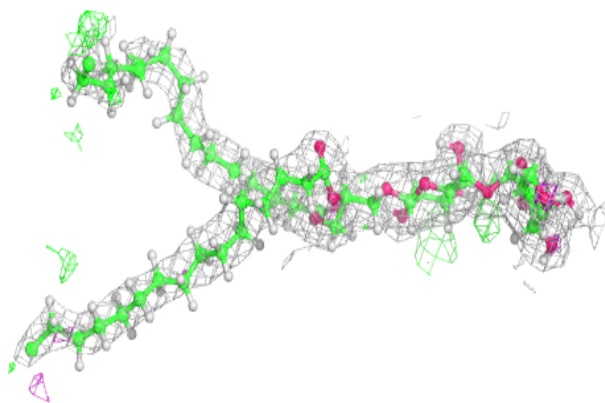
Electron density around CLA B 613:

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

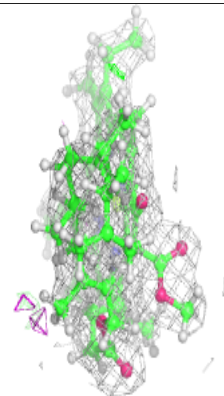
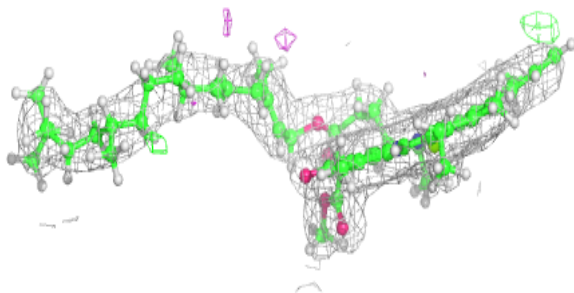
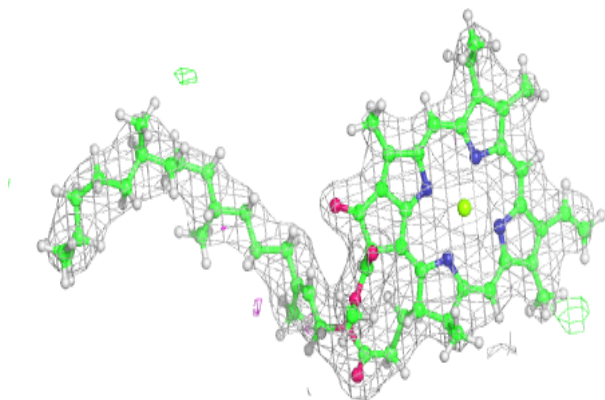


Electron density around DGD C 515:

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

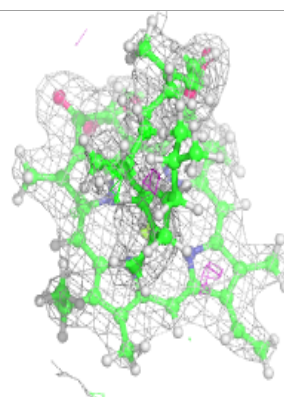
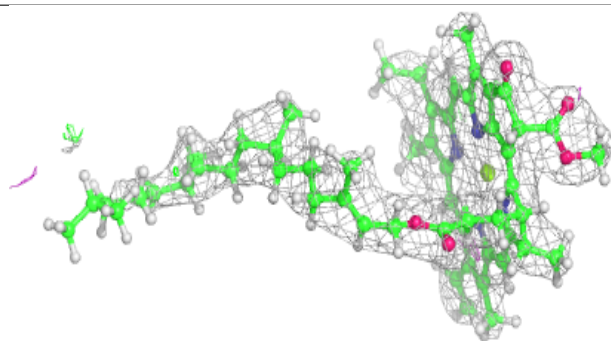
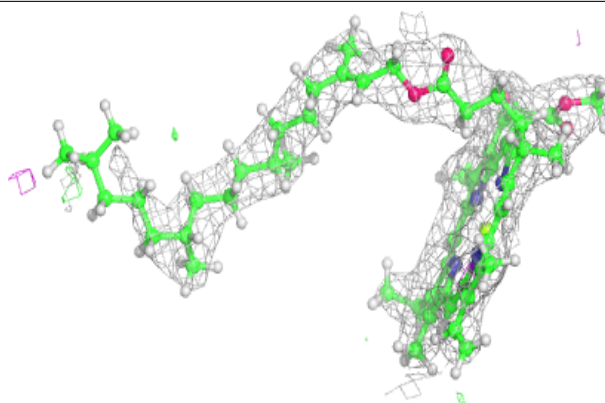
**Electron density around CLA B 602:**

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

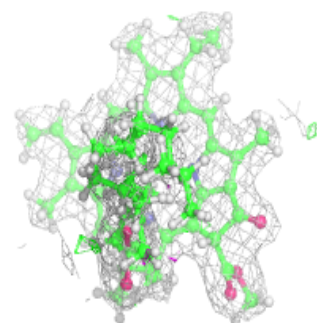
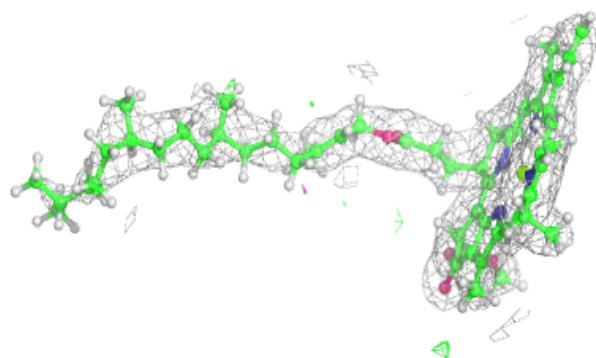
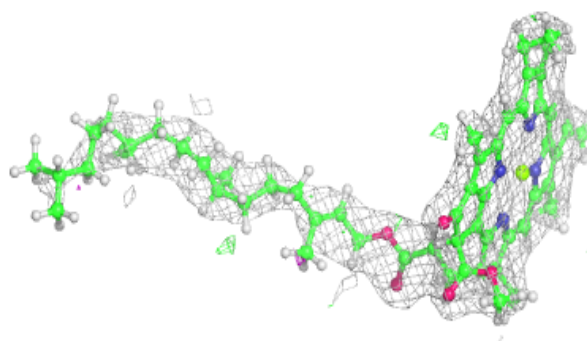


Electron density around CLA C 508:

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

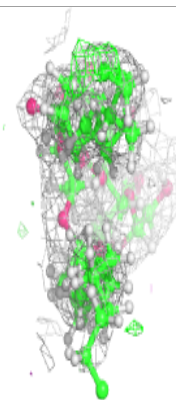
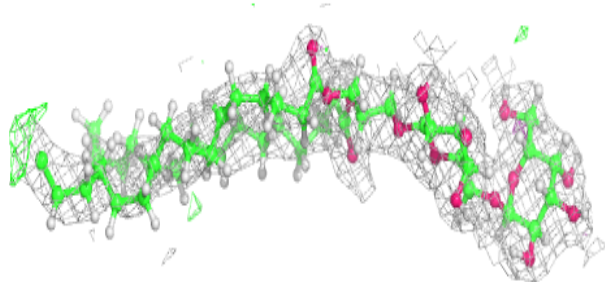
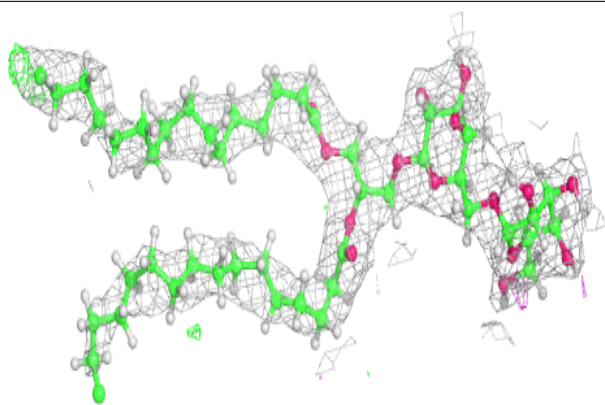
**Electron density around CLA b 604:**

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



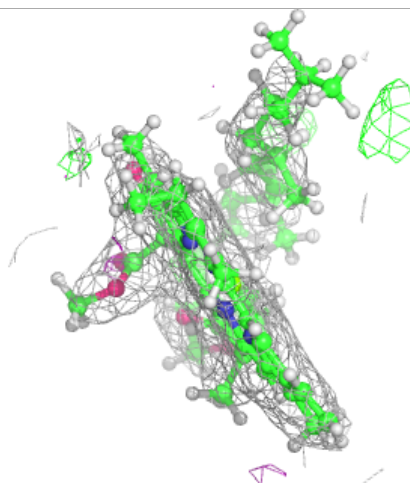
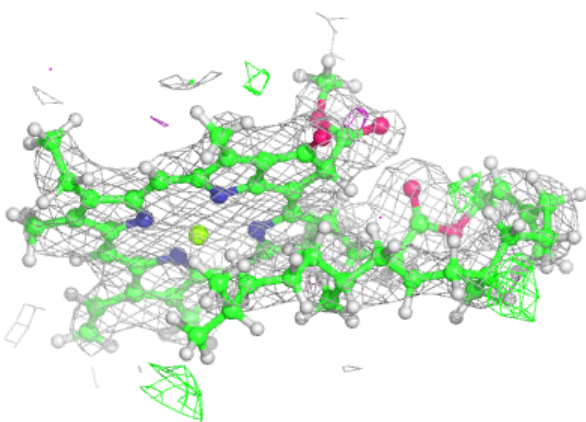
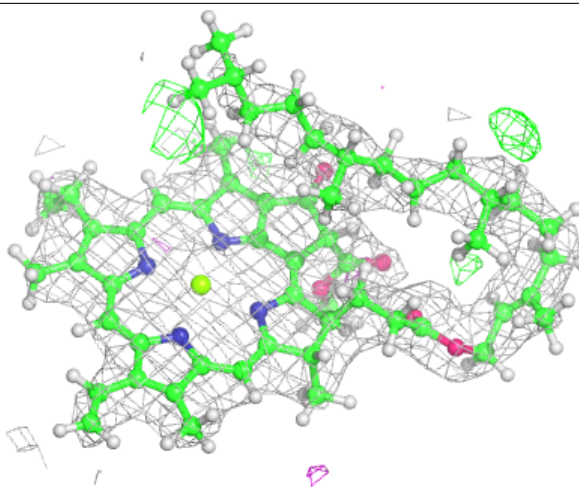
Electron density around DGD c 518:

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



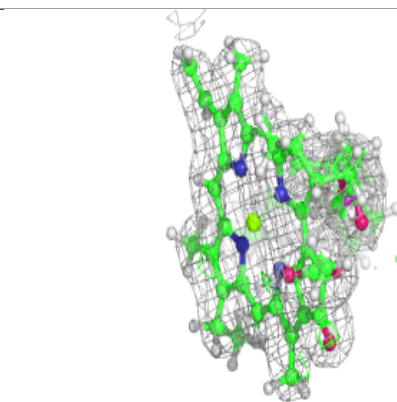
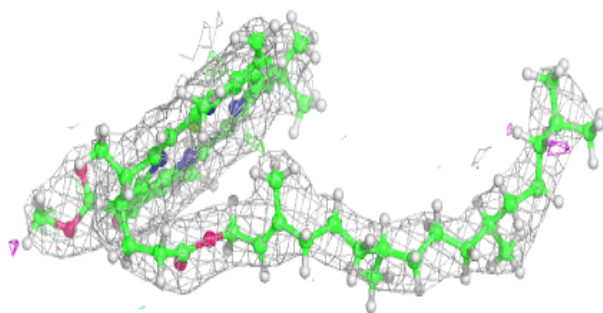
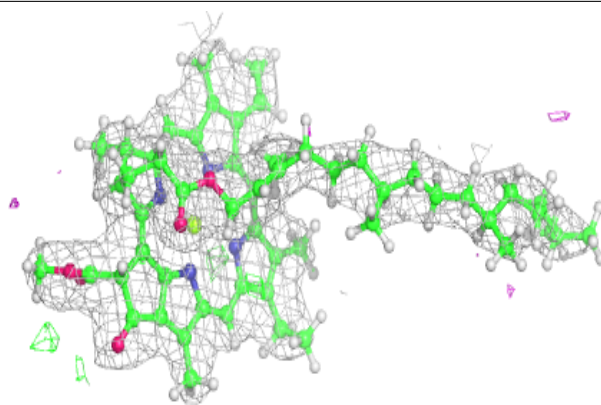
Electron density around CLA C 509:

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

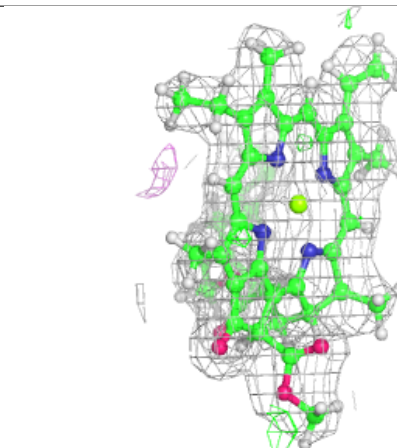
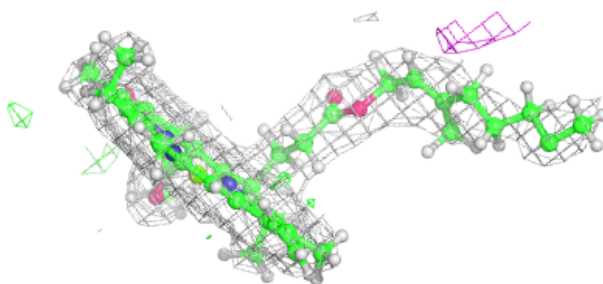
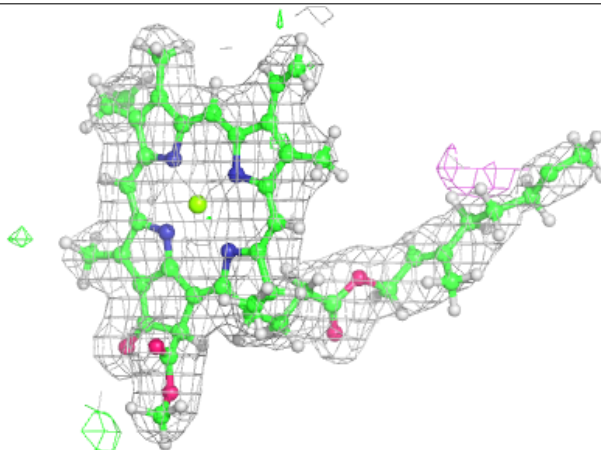


Electron density around CLA b 608:

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

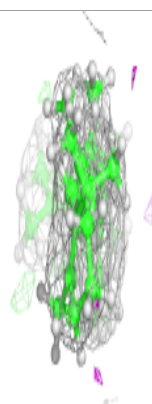
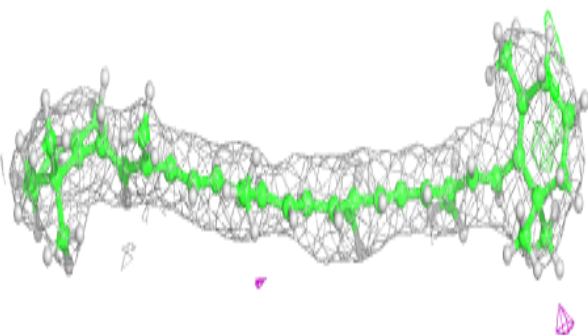
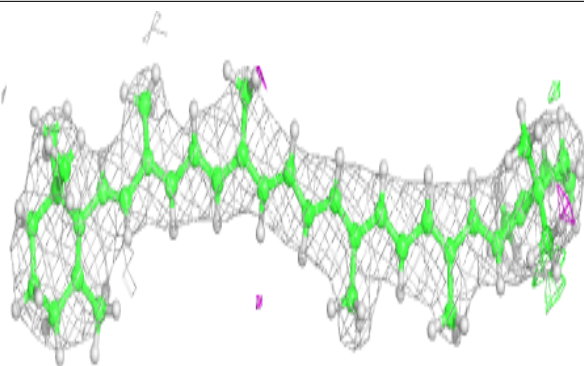
**Electron density around CLA A 406:**

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

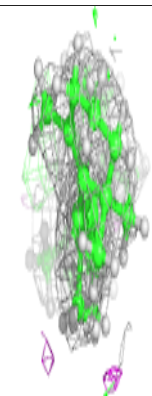
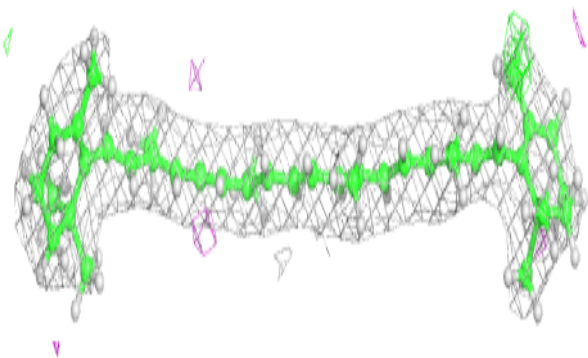
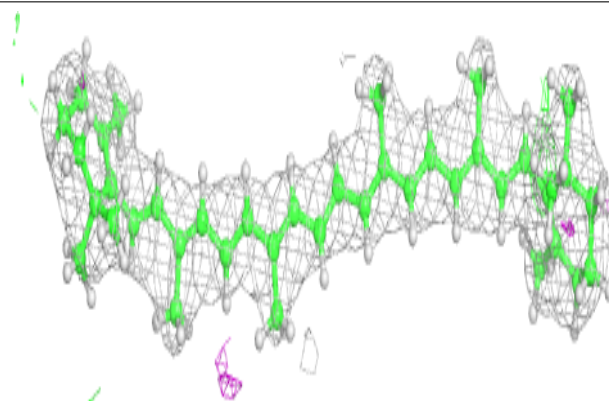


Electron density around BCR b 617:

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

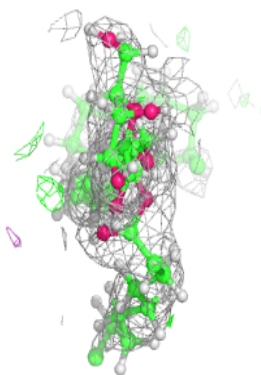
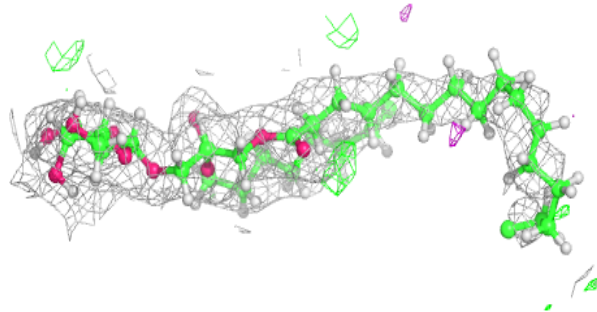
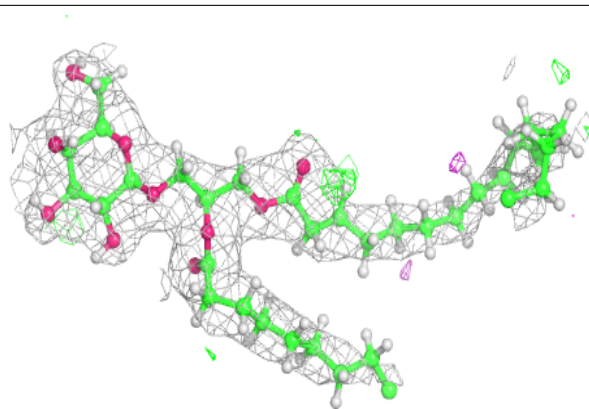
**Electron density around BCR b 618:**

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

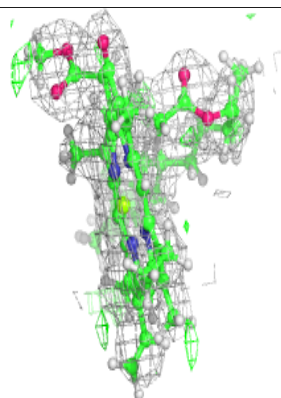
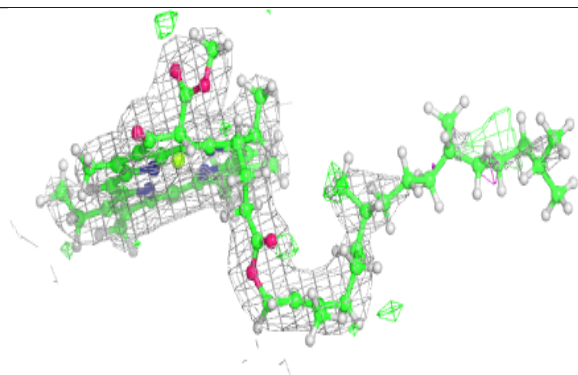
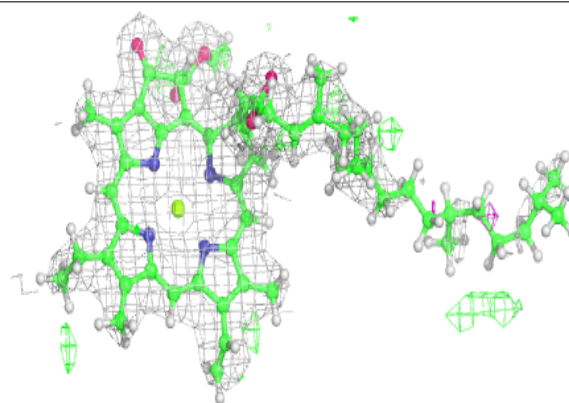


Electron density around LMG d 410:

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

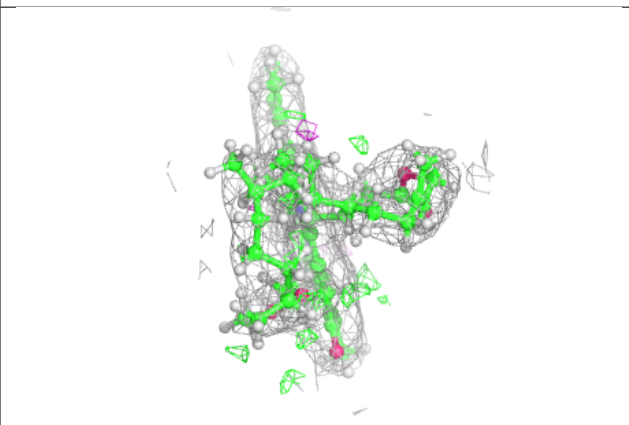
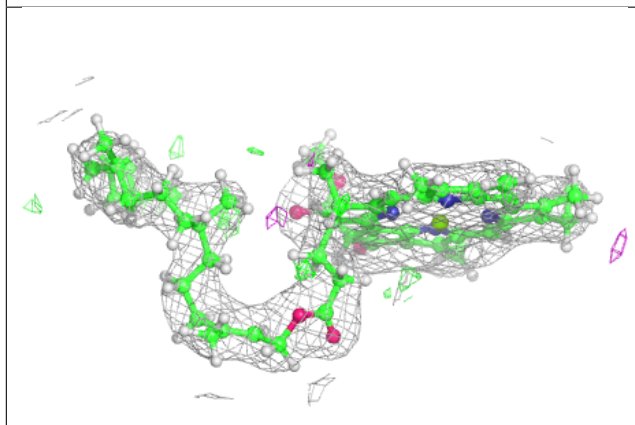
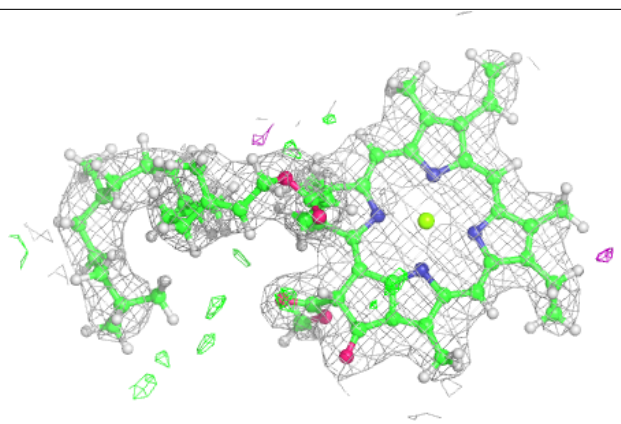
**Electron density around CLA A 403:**

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



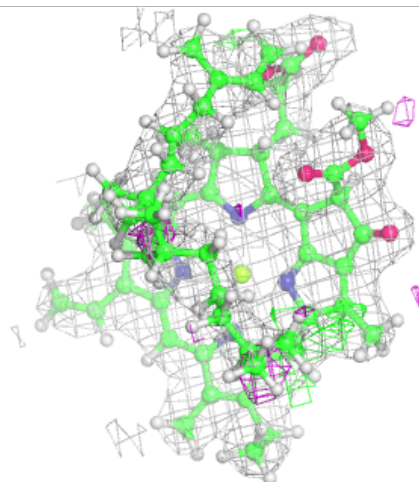
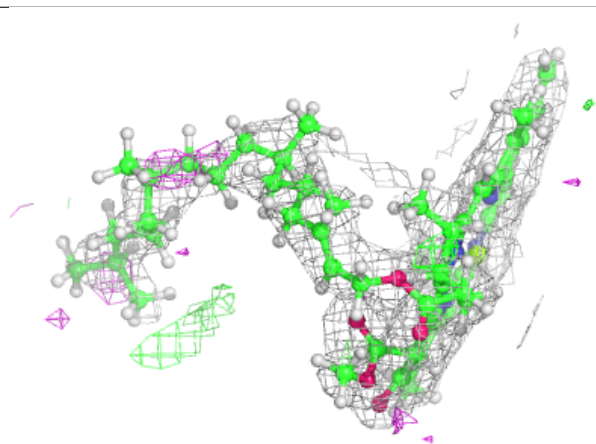
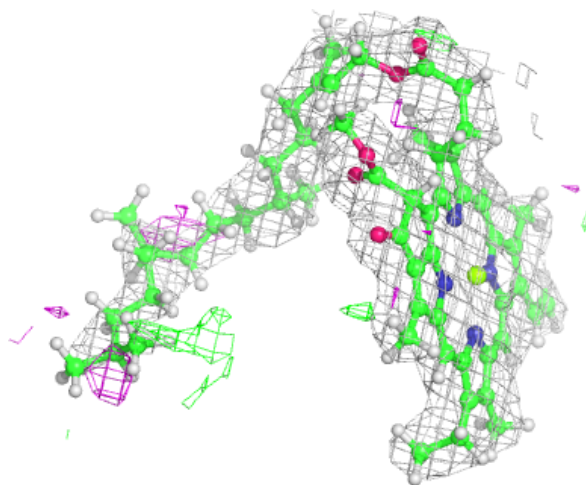
Electron density around CLA b 612:

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



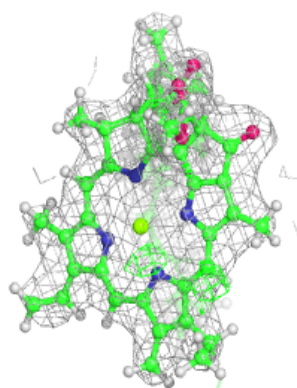
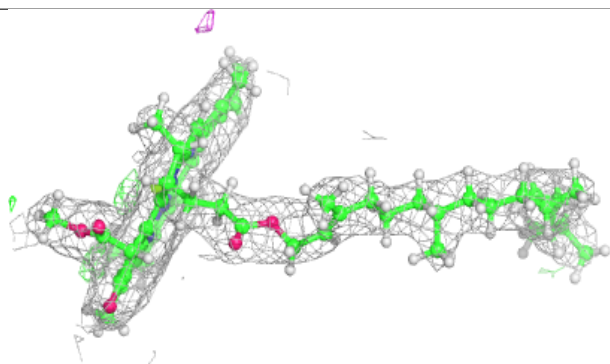
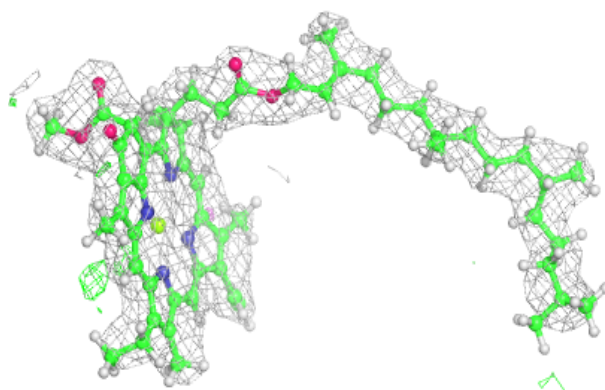
Electron density around CLA b 613:

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

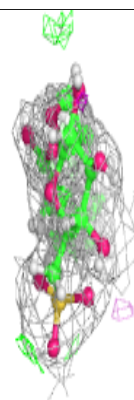
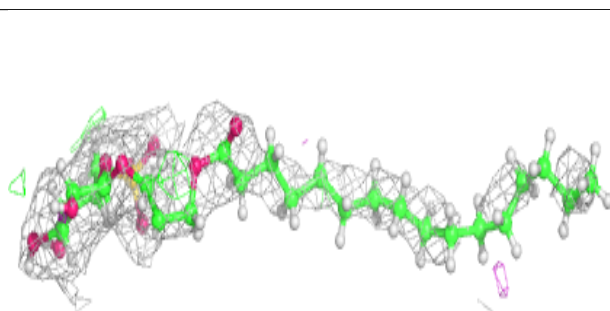
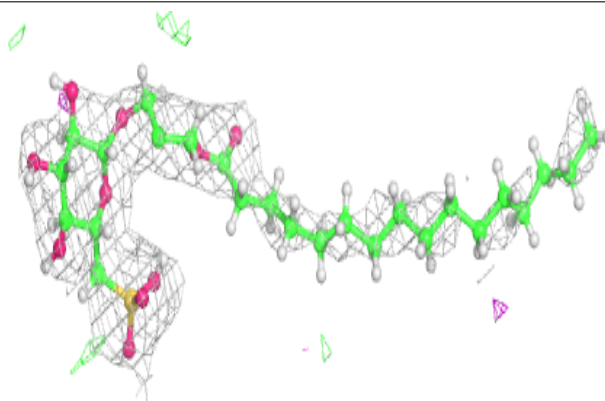


Electron density around CLA B 609:

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

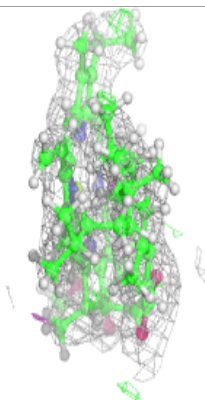
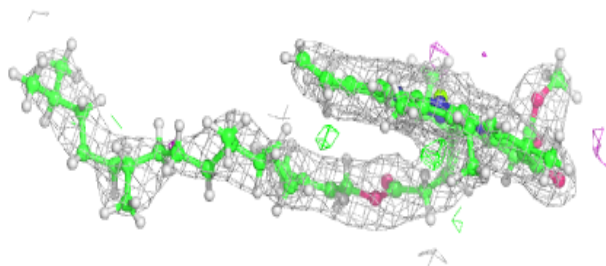
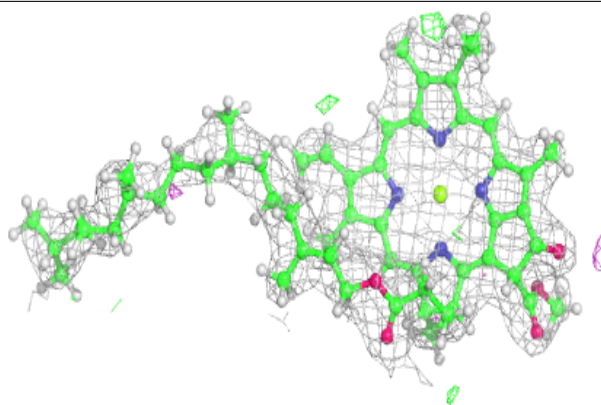
**Electron density around SQD F 102:**

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

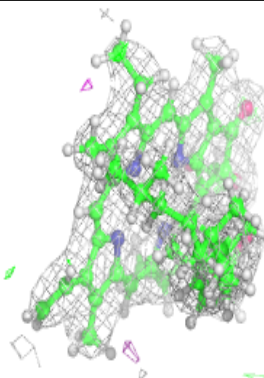
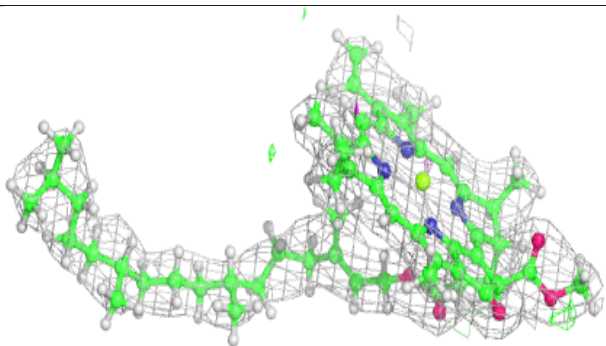
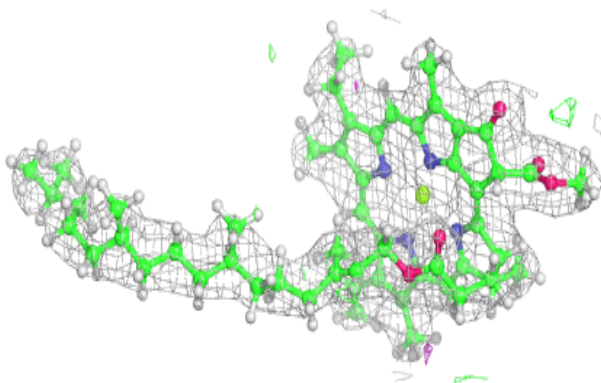


Electron density around CLA B 603:

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

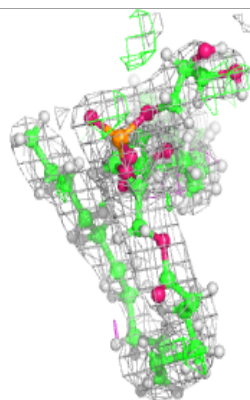
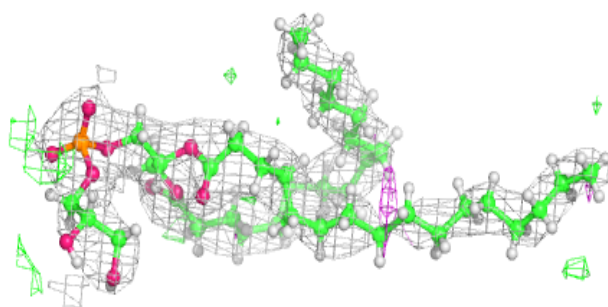
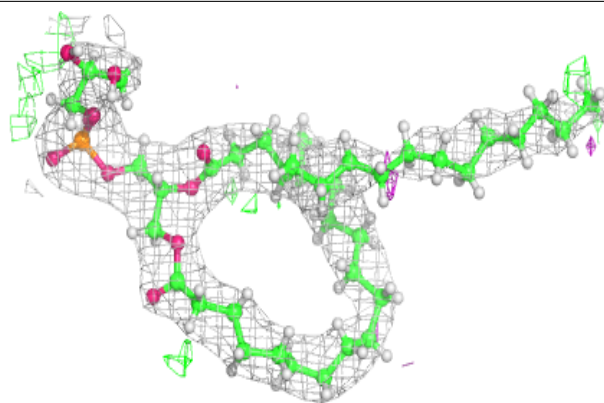
**Electron density around CLA B 608:**

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

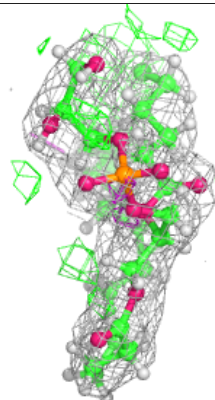
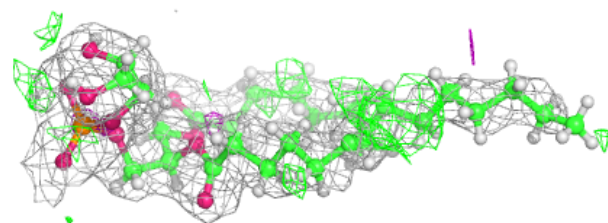
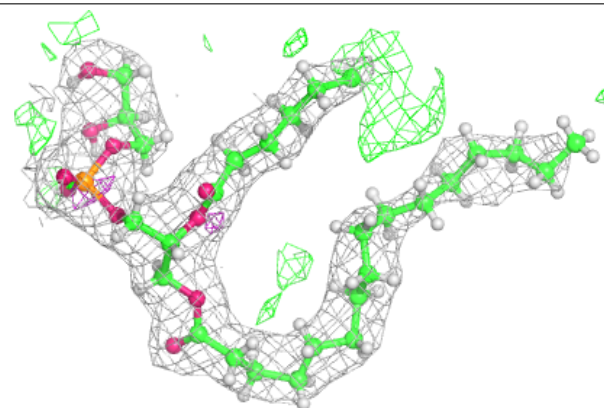


Electron density around LHG a 410:

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

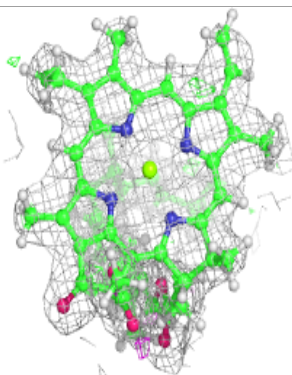
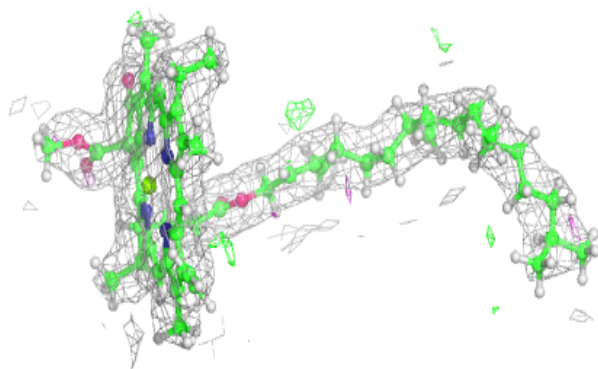
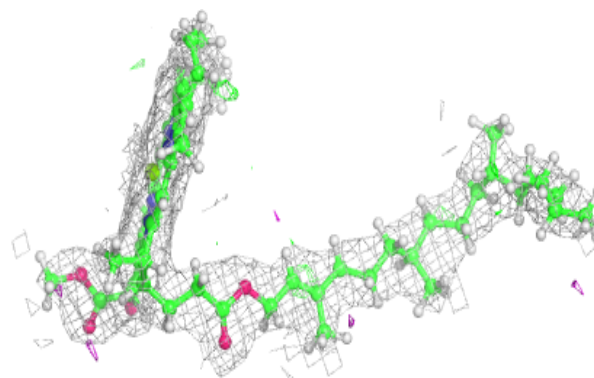
**Electron density around LHG d 409:**

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

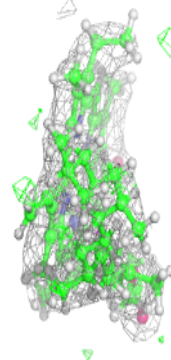
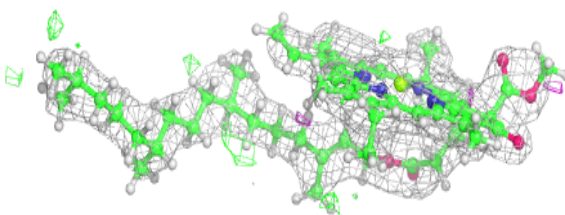
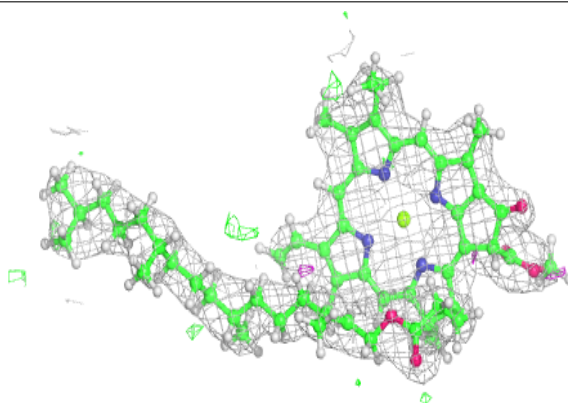


Electron density around CLA b 605:

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

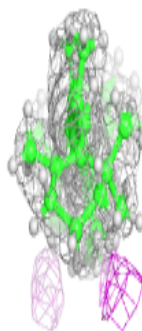
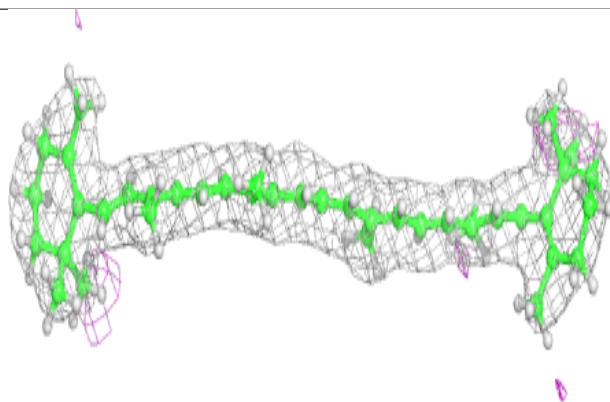
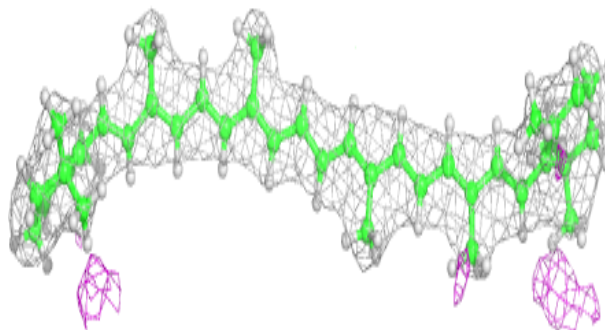
**Electron density around CLA c 501:**

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

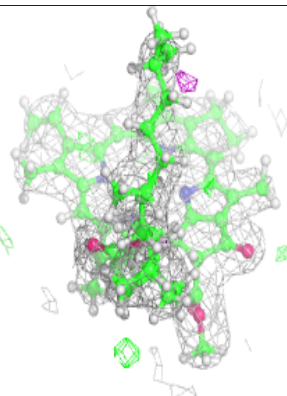
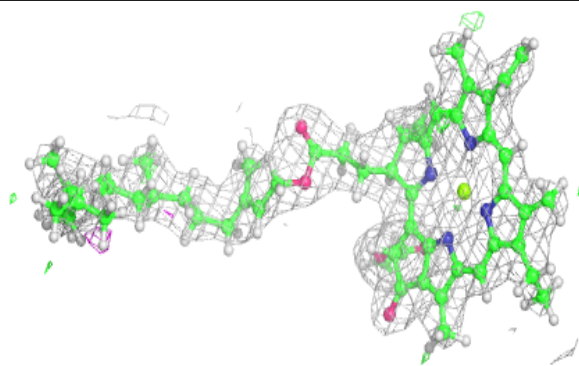
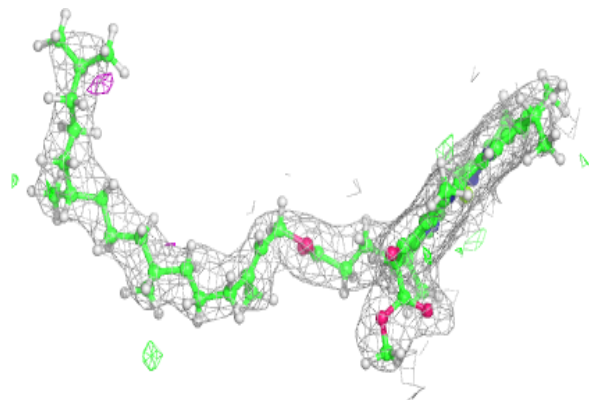


Electron density around BCR a 406:

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

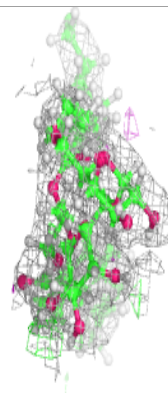
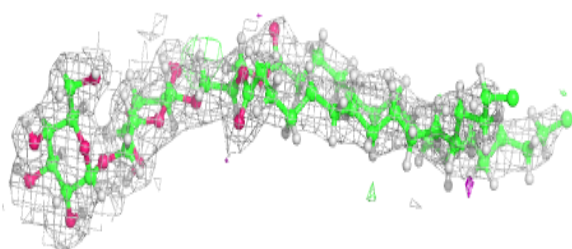
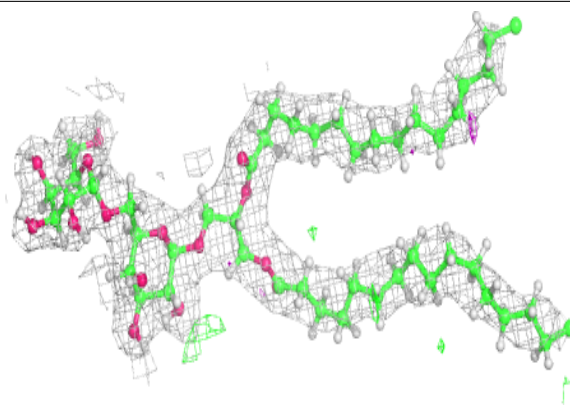
**Electron density around CLA d 403:**

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

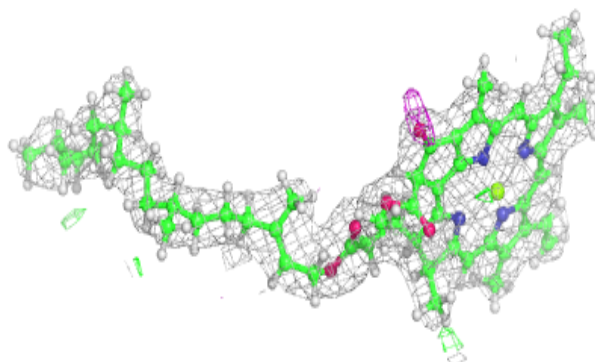
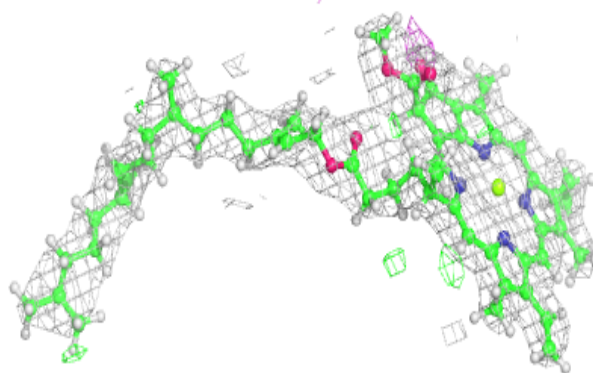


Electron density around DGD C 517:

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

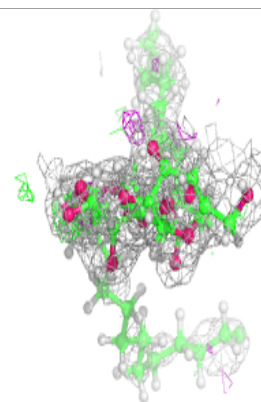
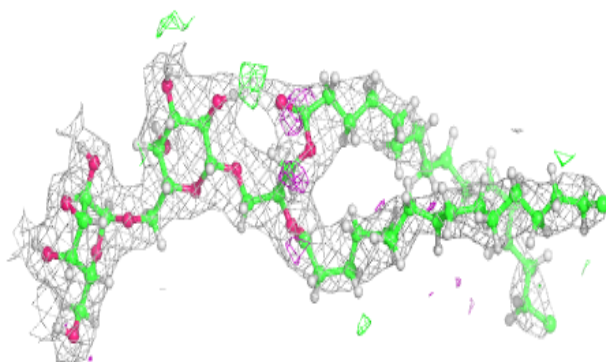
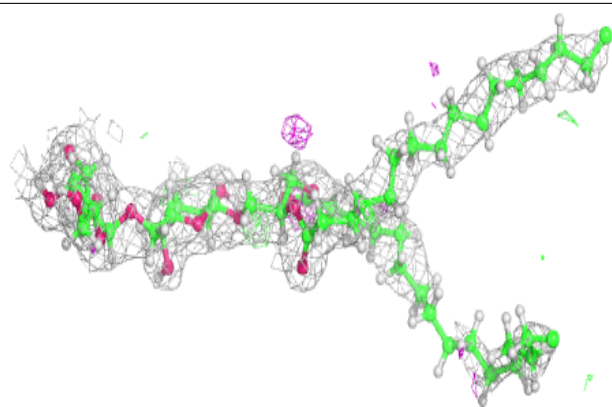
**Electron density around CLA A 402:**

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

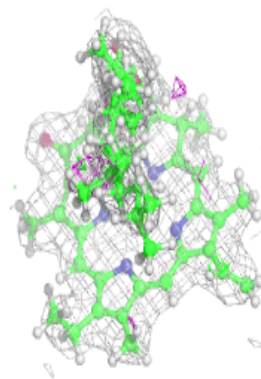
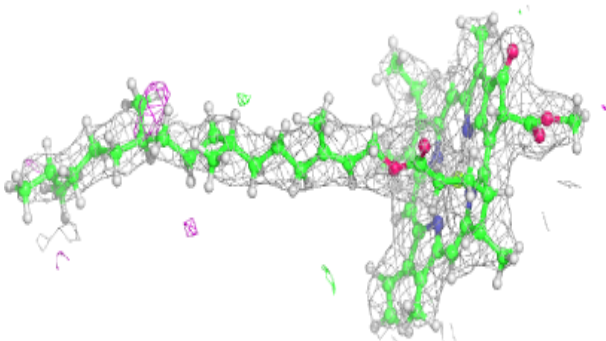
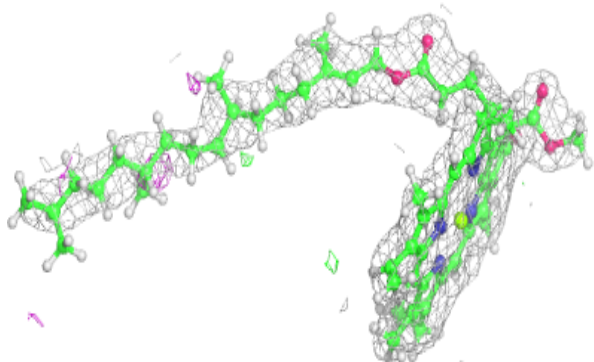


Electron density around DGD c 516:

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

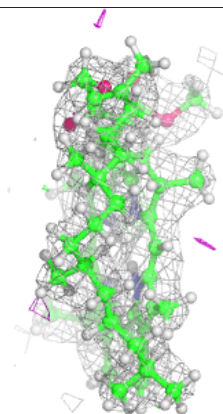
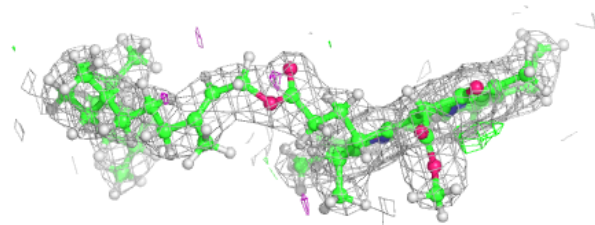
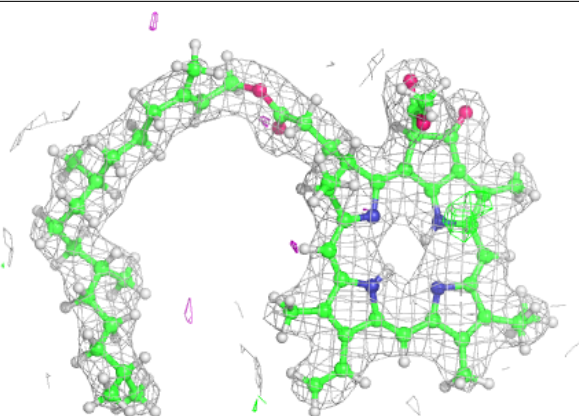
**Electron density around CLA b 607:**

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



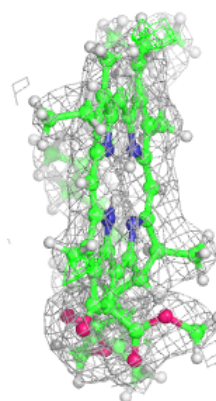
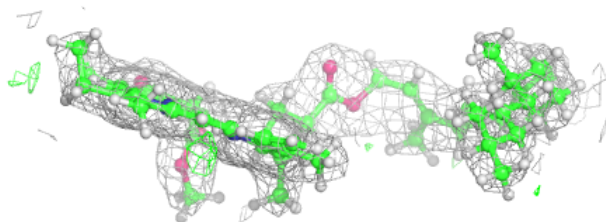
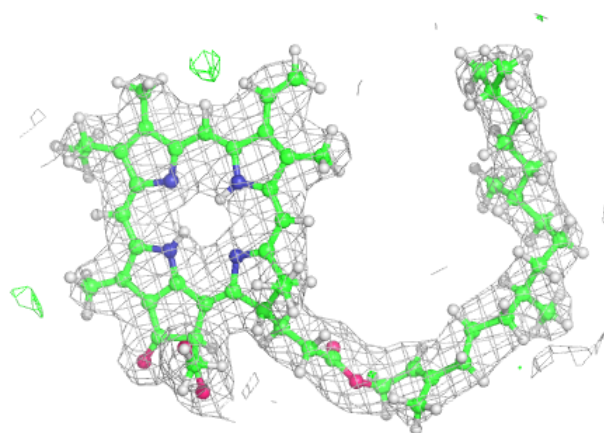
Electron density around PHO A 404:

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



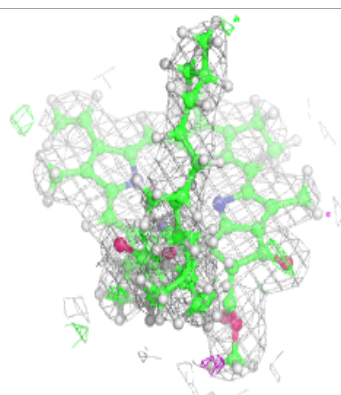
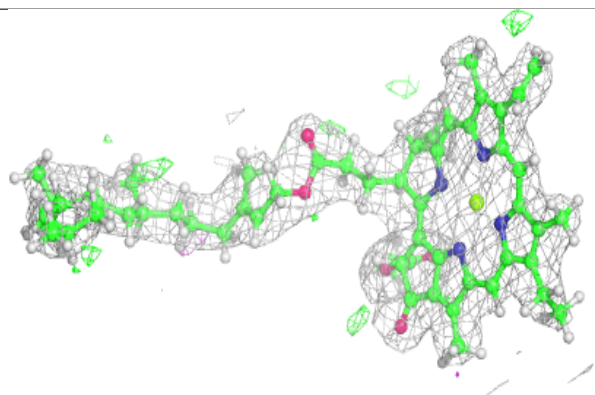
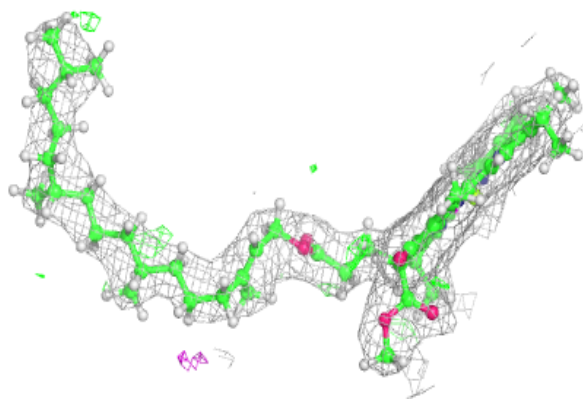
Electron density around PHO a 404:

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

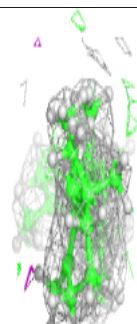
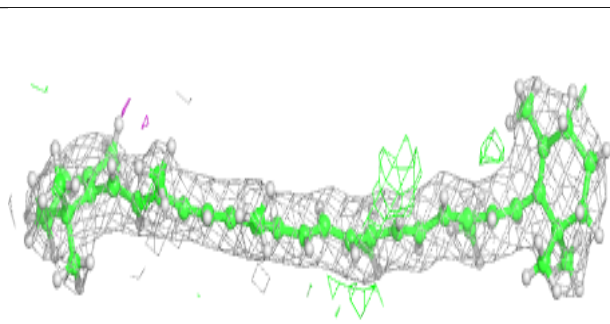
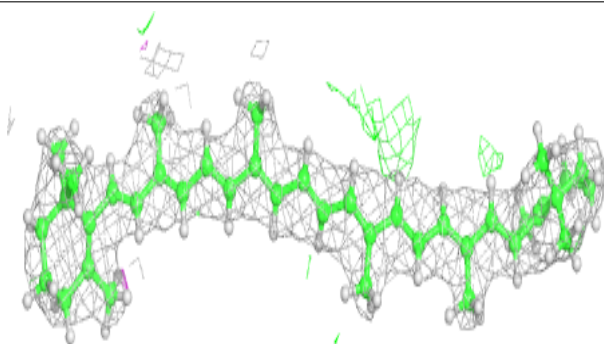


Electron density around CLA D 402:

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

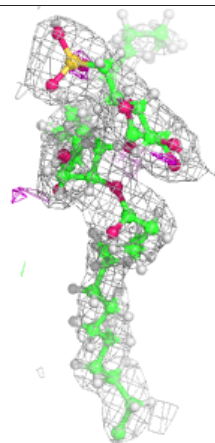
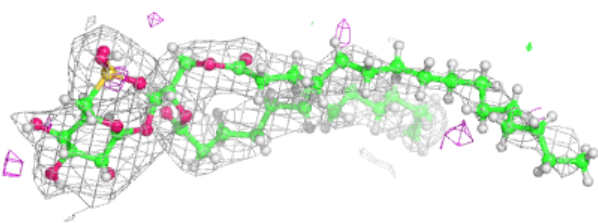
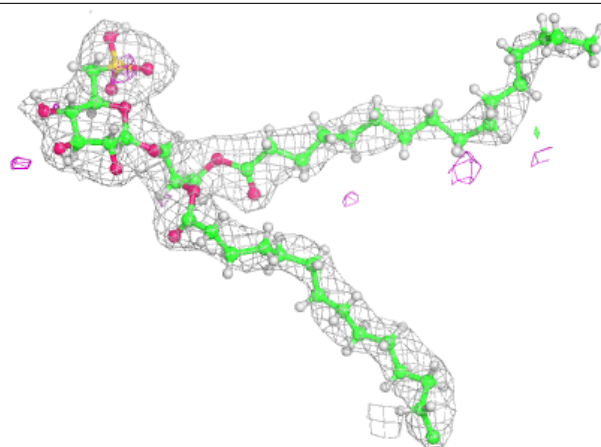
**Electron density around BCR B 617:**

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

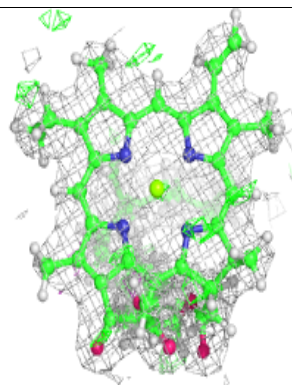
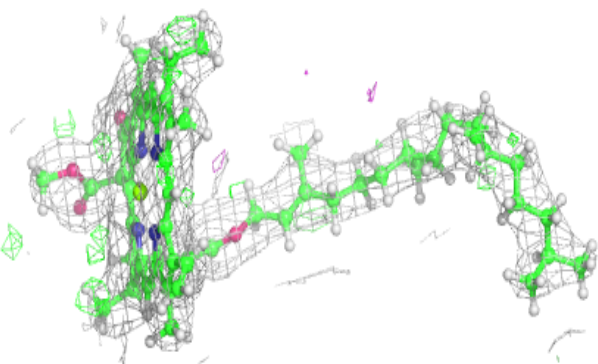
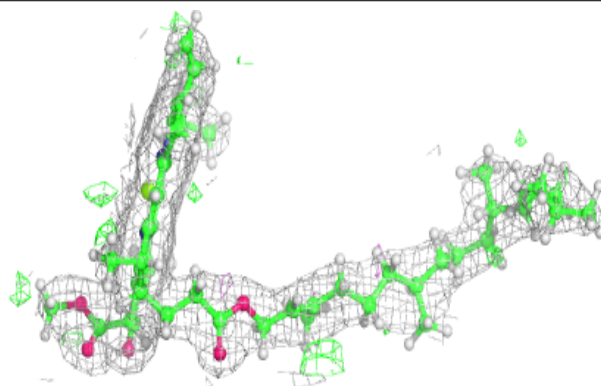


Electron density around SQD A 412:

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

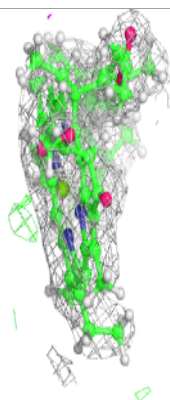
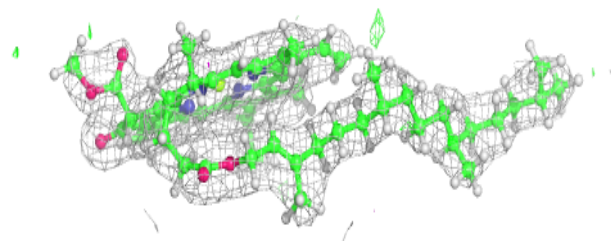
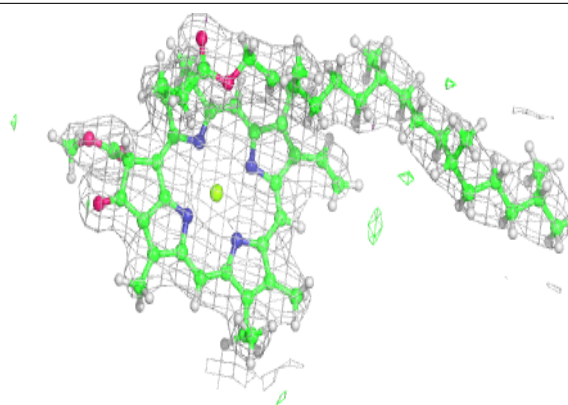
**Electron density around CLA B 605:**

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

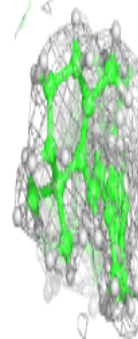
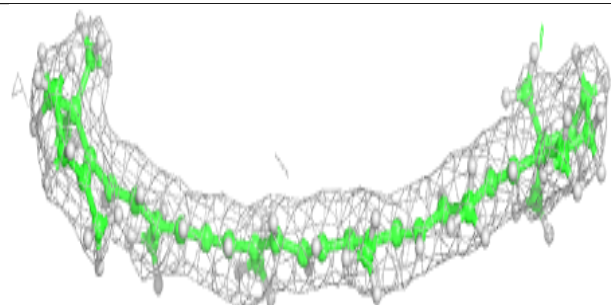
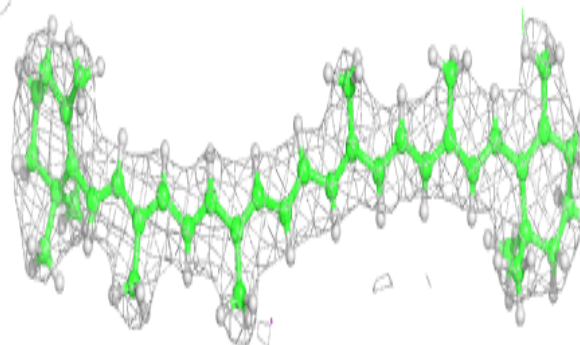


Electron density around CLA C 501:

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

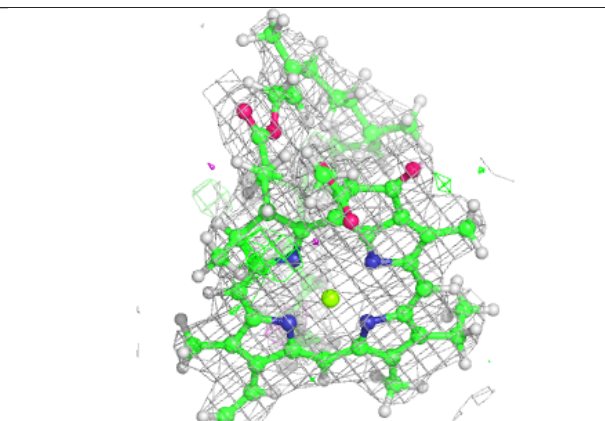
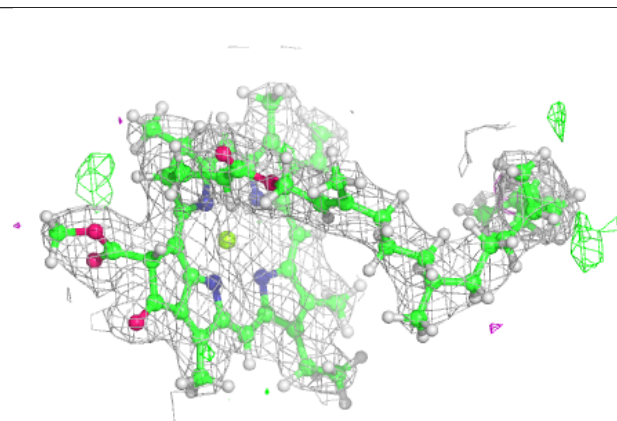
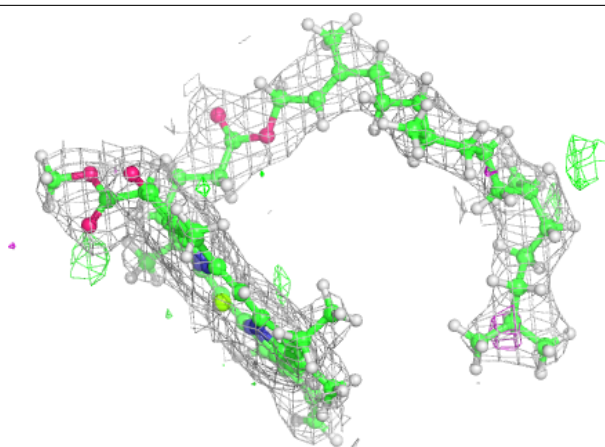
**Electron density around BCR t 101:**

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



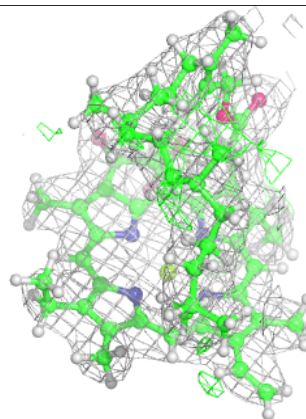
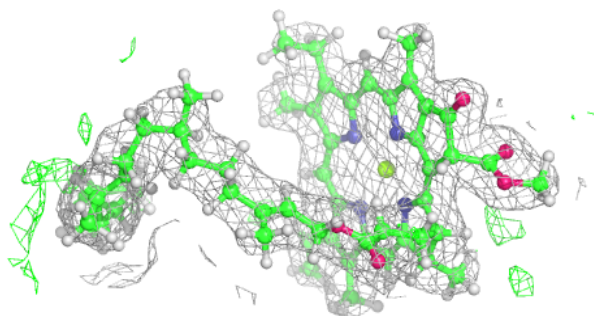
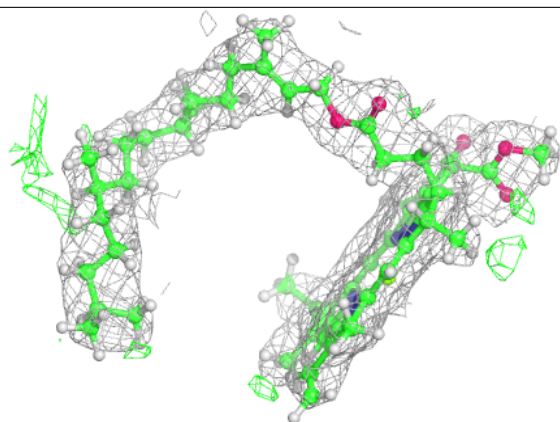
Electron density around CLA b 611:

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



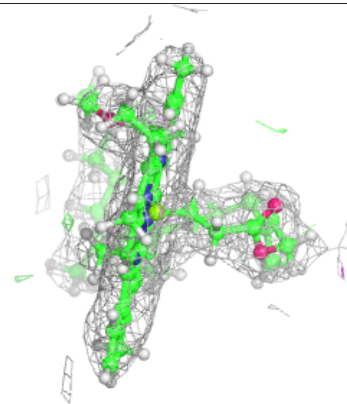
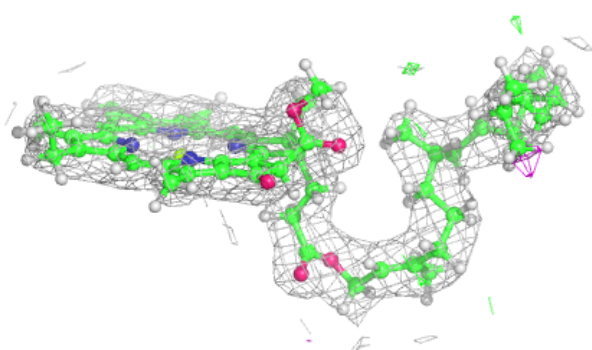
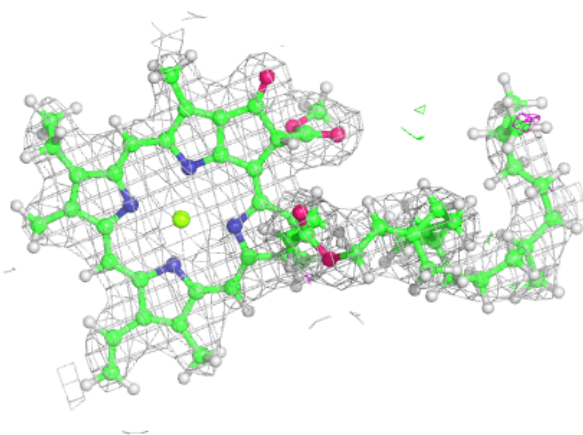
Electron density around CLA B 611:

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

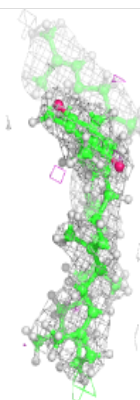
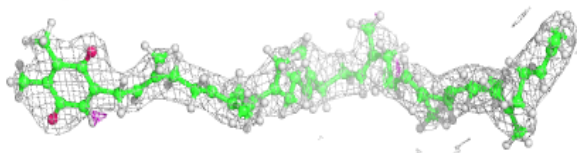
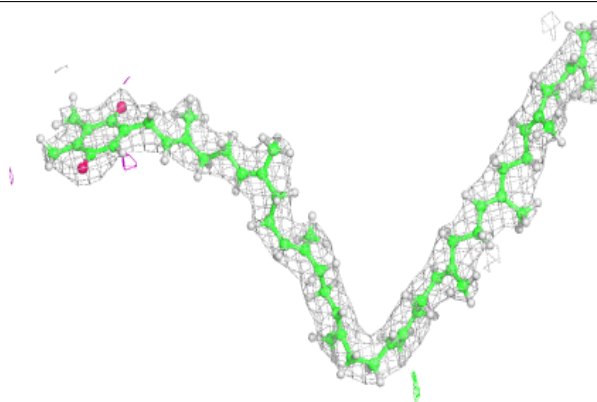


Electron density around CLA B 612:

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

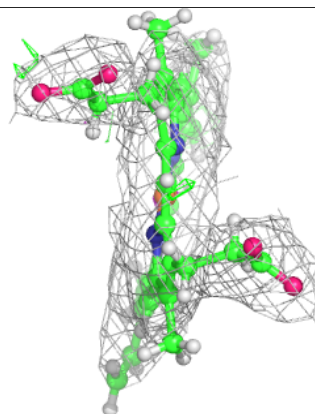
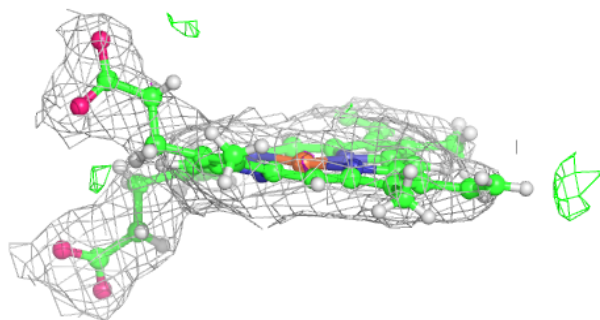
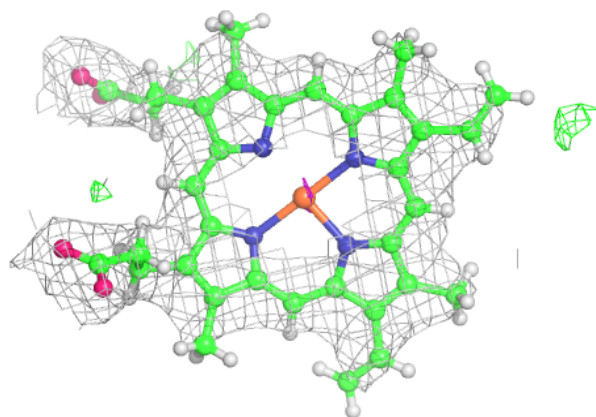
**Electron density around PL9 d 407:**

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



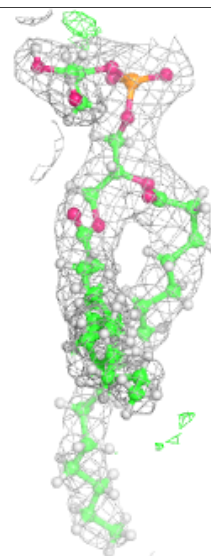
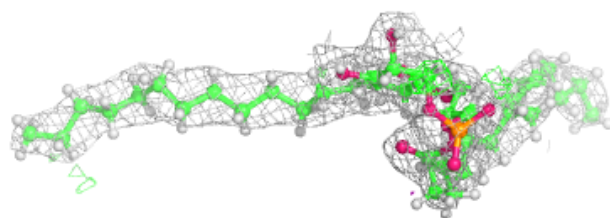
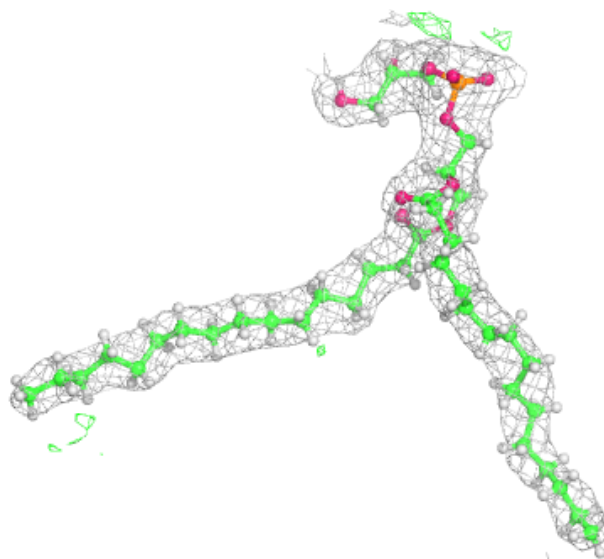
Electron density around HEM F 101:

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



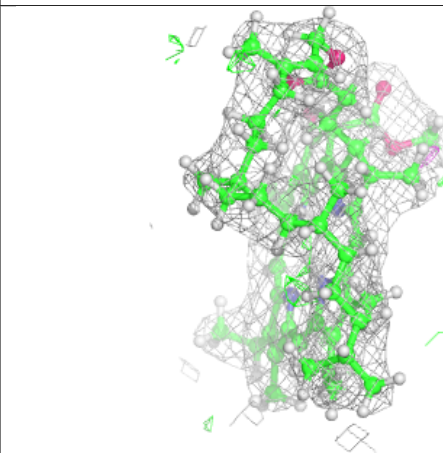
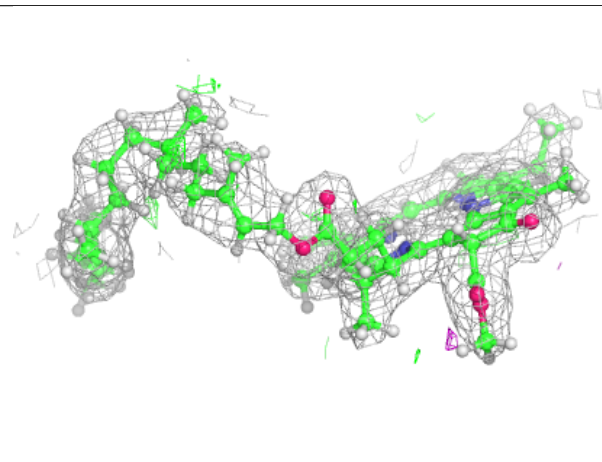
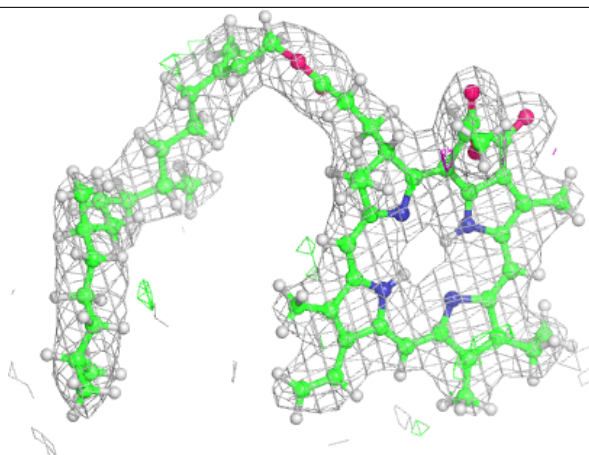
Electron density around LHG 1 101:

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



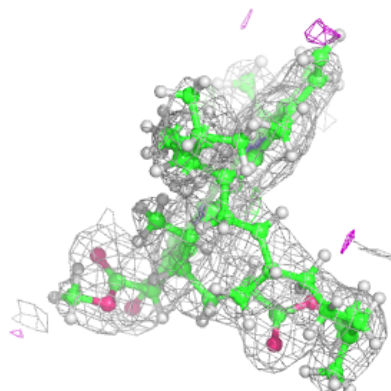
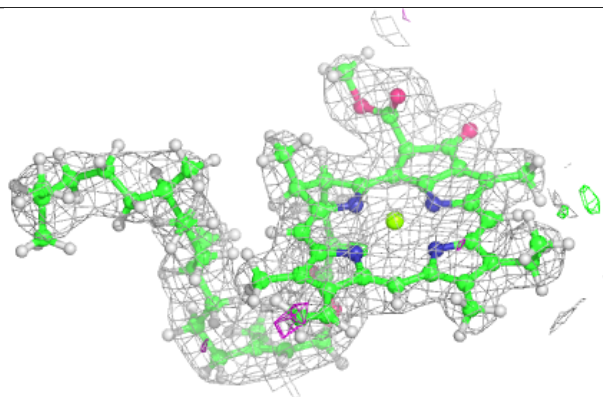
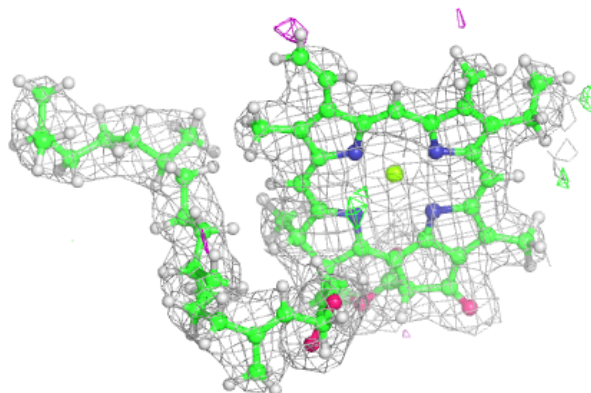
Electron density around PHO A 405:

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

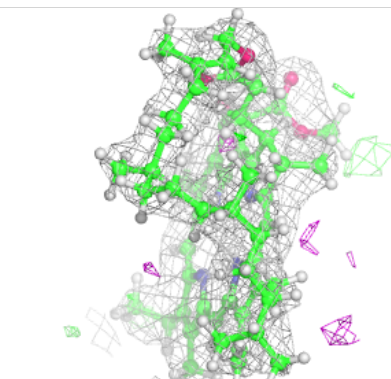
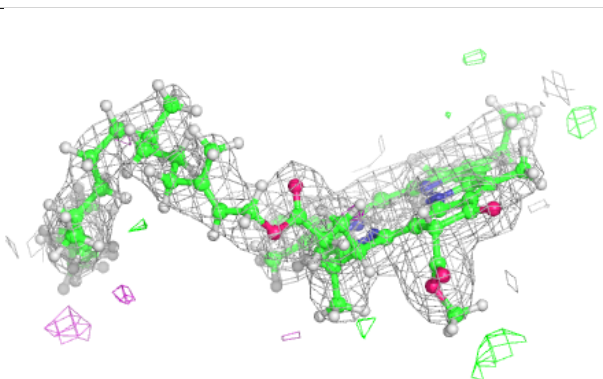
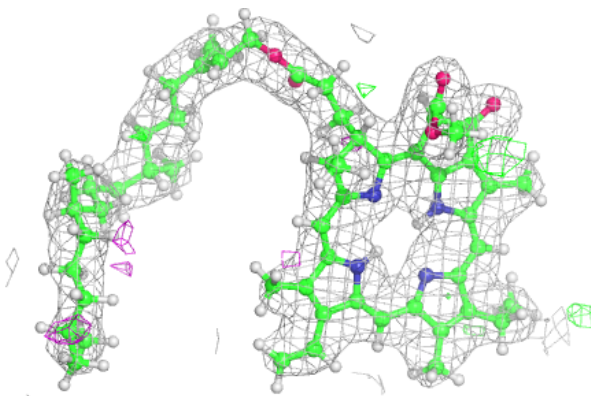


Electron density around CLA D 403:

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

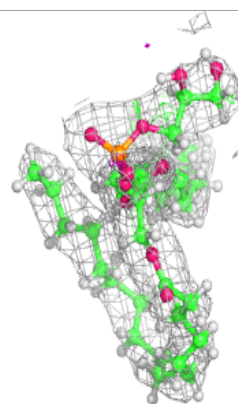
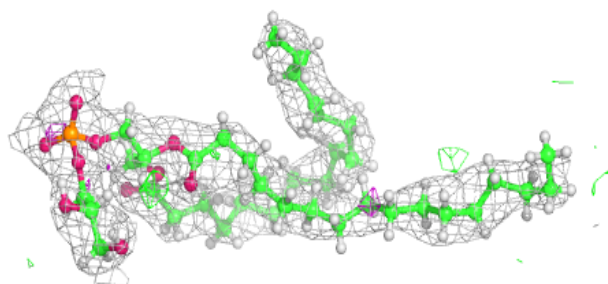
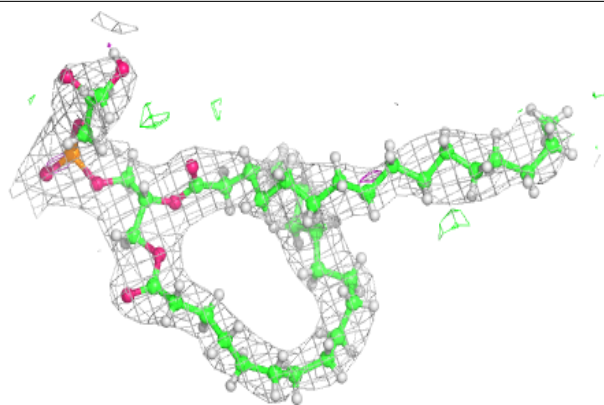
**Electron density around PHO d 401:**

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



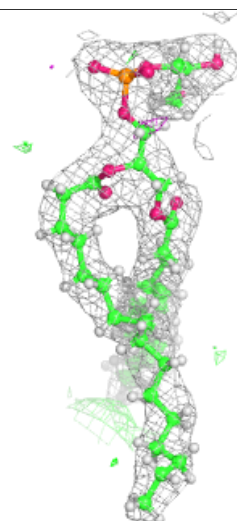
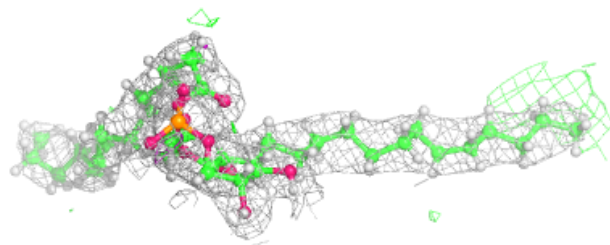
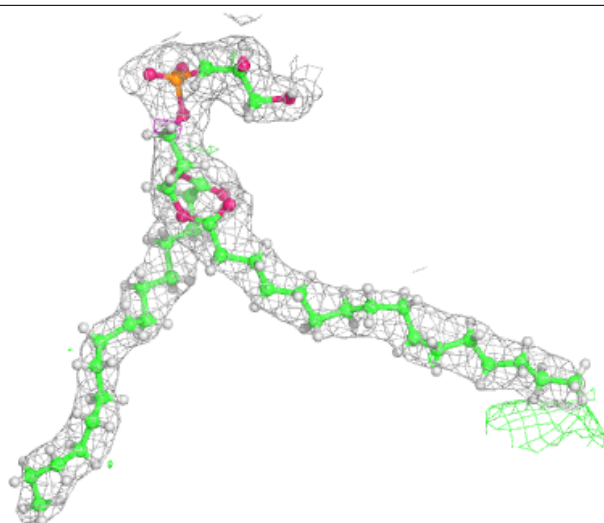
Electron density around LHG D 411:

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



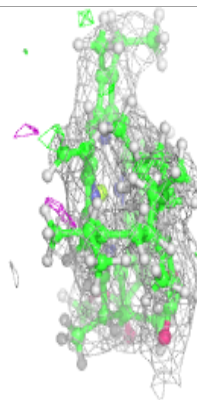
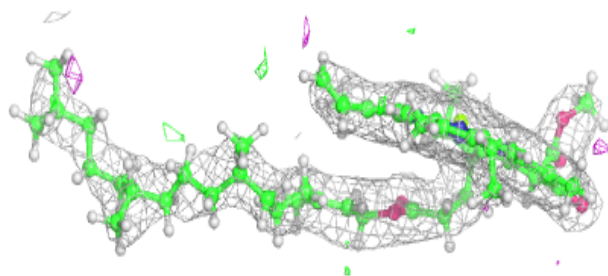
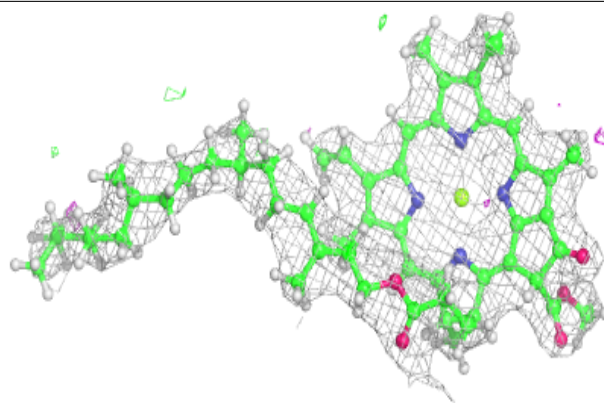
Electron density around LHG L 101:

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

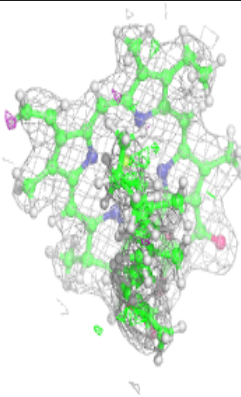
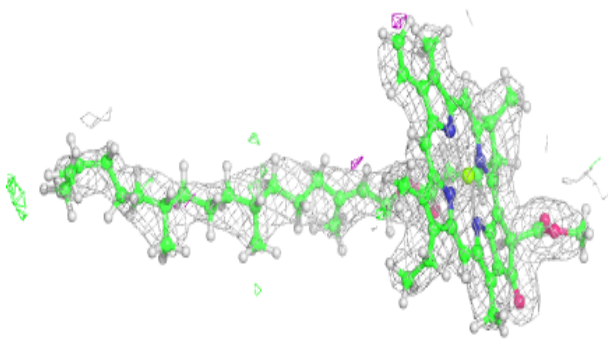
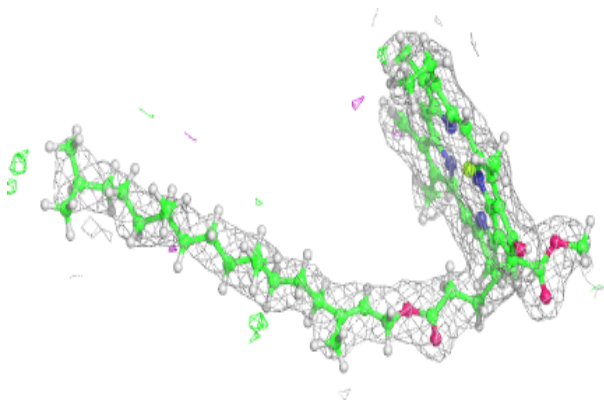


Electron density around CLA b 603:

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

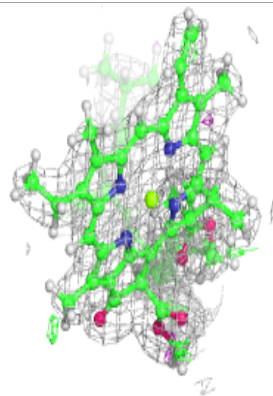
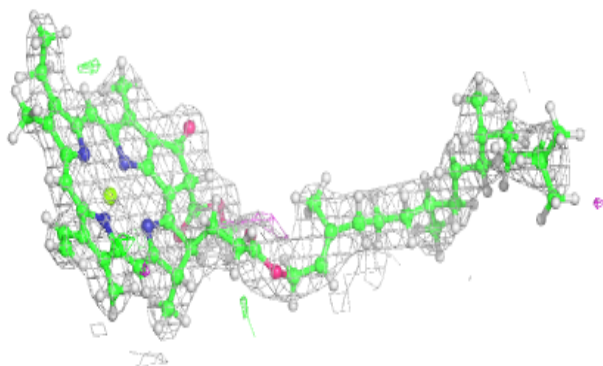
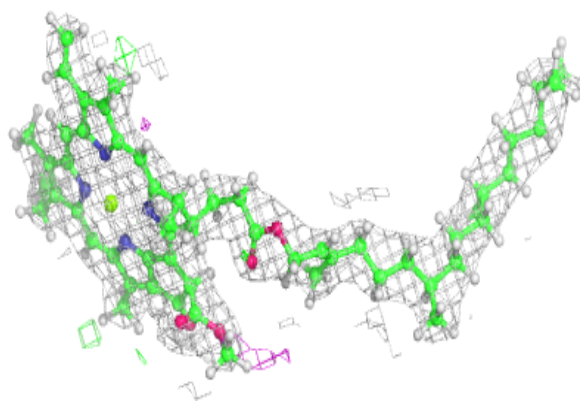
**Electron density around CLA B 607:**

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



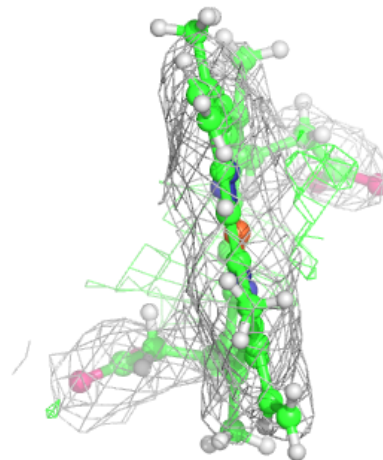
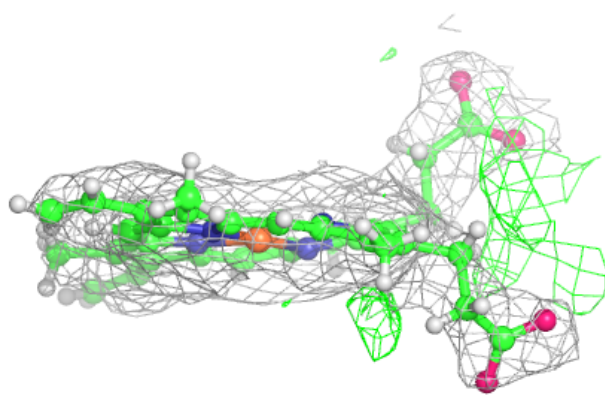
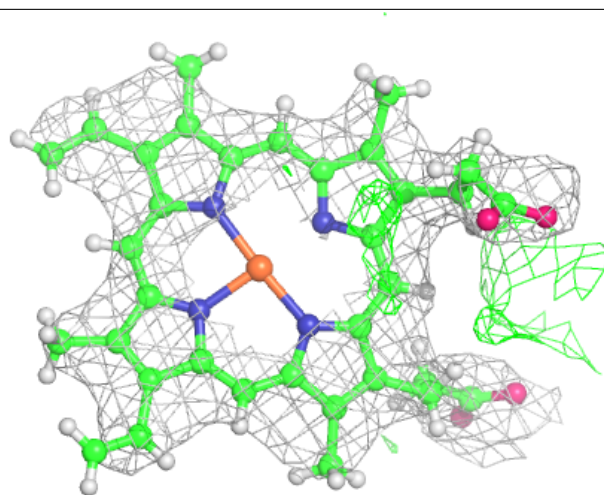
Electron density around CLA a 402:

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



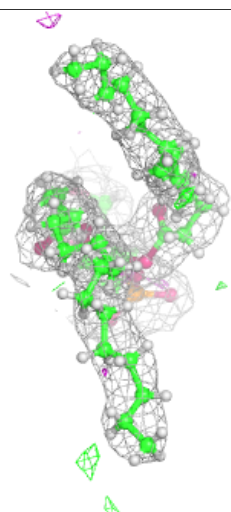
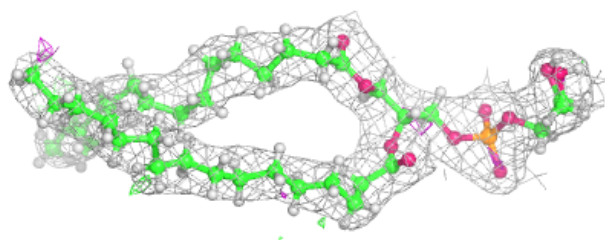
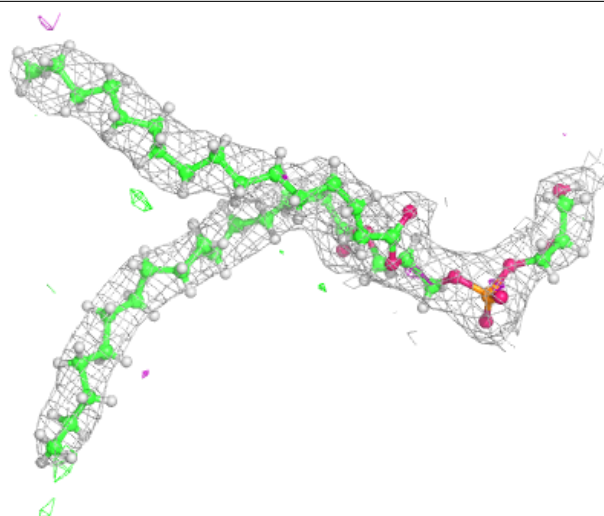
Electron density around HEM f 101:

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



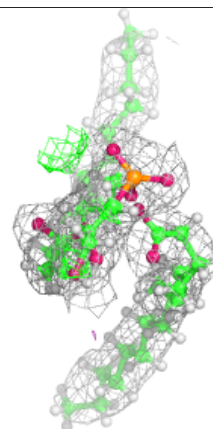
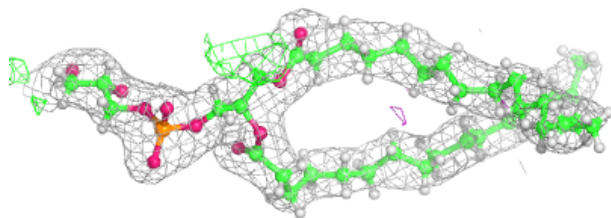
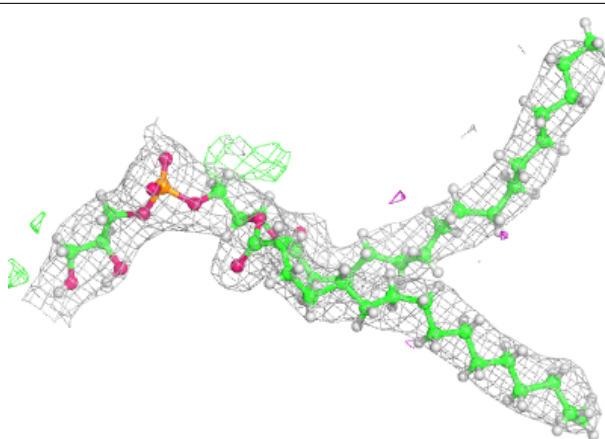
Electron density around LHG D 408:

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



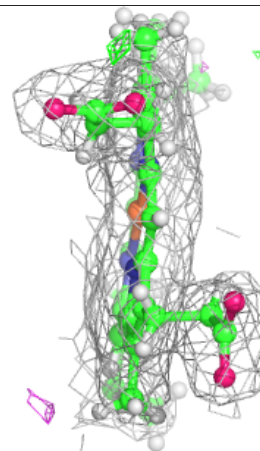
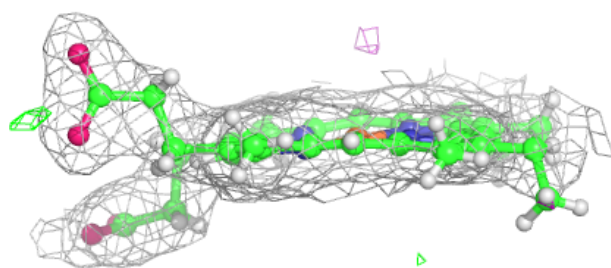
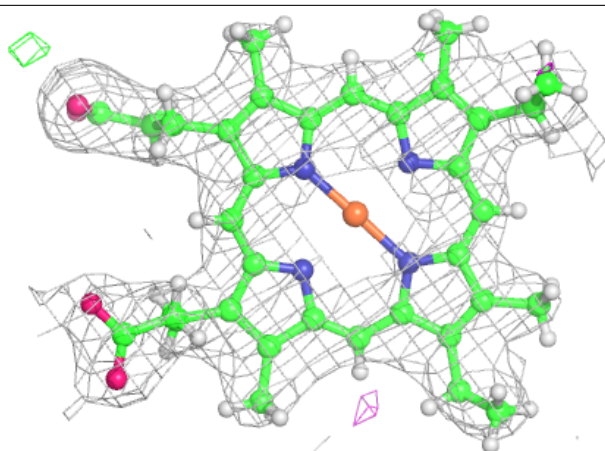
Electron density around LHG d 408:

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



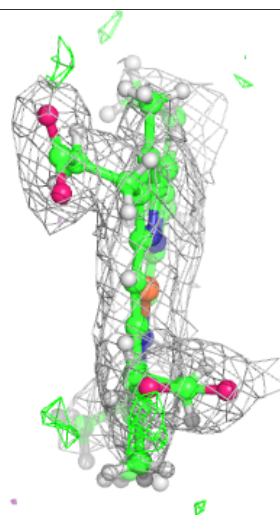
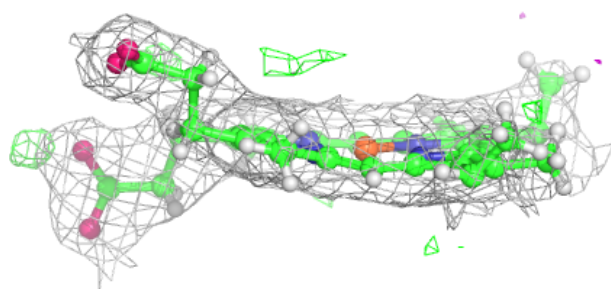
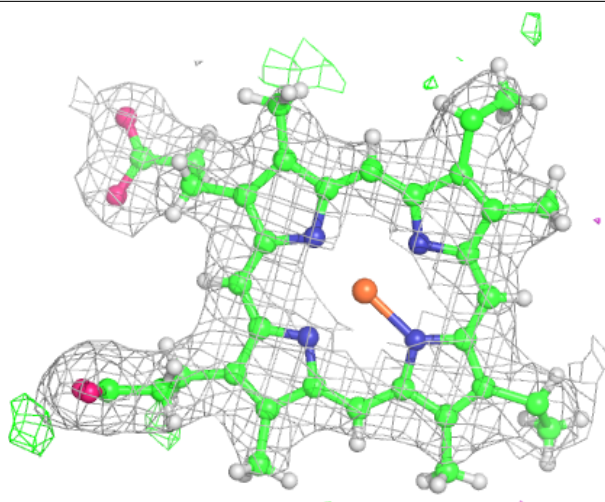
Electron density around HEC V 201:

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



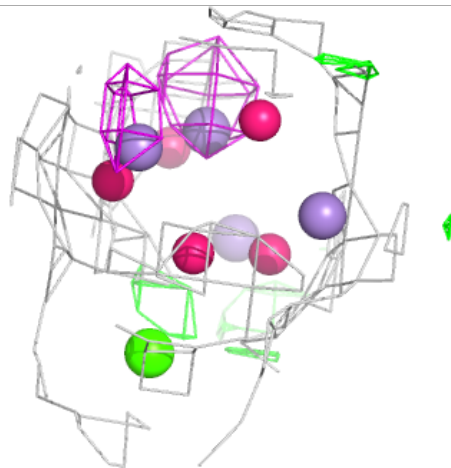
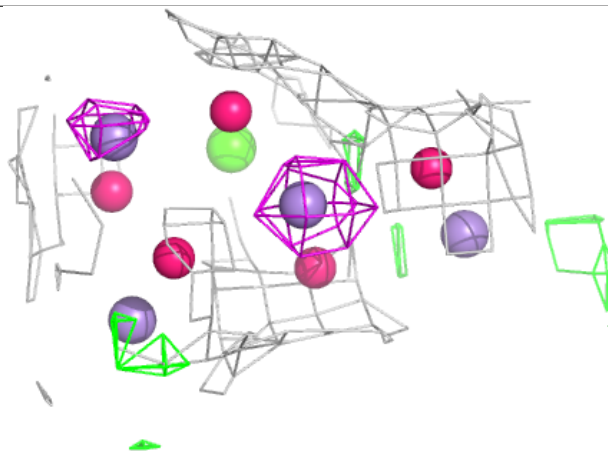
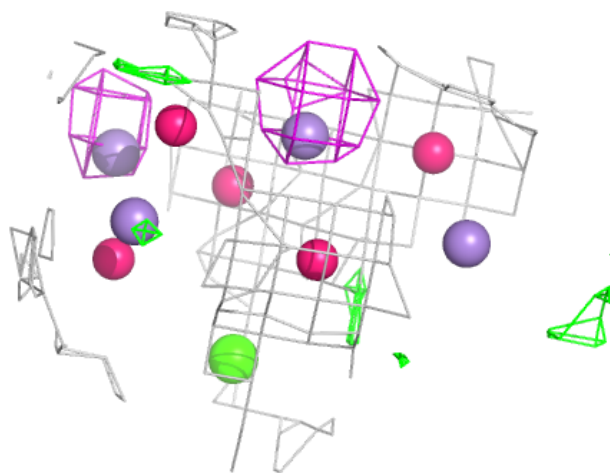
Electron density around HEC v 201:

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



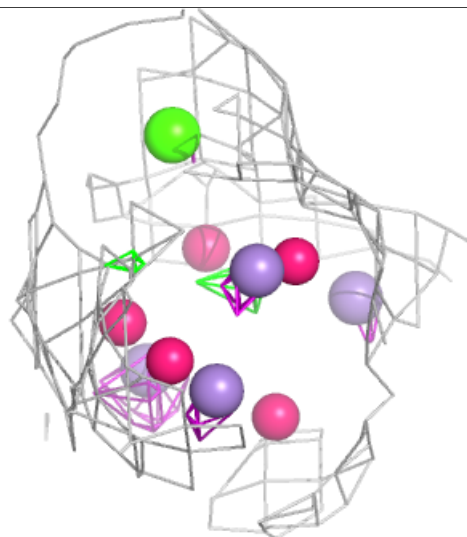
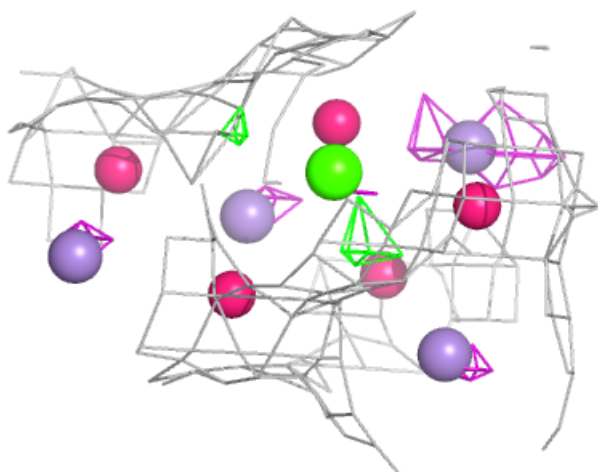
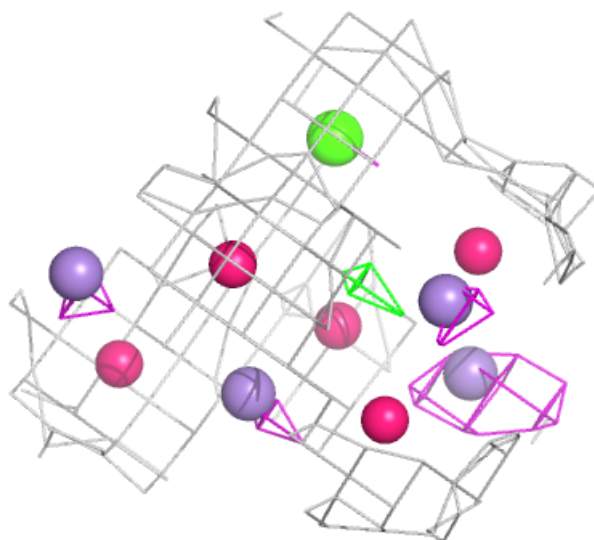
Electron density around OEX a 416:

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



Electron density around OEX 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.