



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 4, 2021 – 10:51 AM EDT

PDB ID : 7RF7
Title : RT XFEL structure of Photosystem II 400 microseconds after the second illumination at 2.09 Angstrom resolution
Authors : Hussein, R.; Ibrahim, M.; Bhowmick, A.; Simon, P.S.; Chatterjee, R.; Lassalle, L.; Doyle, M.D.; Bogacz, I.; Kim, I.-S.; Cheah, M.H.; Gul, S.; de Lichtenberg, C.; Chernev, P.; Pham, C.C.; Young, I.D.; Carbajo, S.; Fuller, F.D.; Alonso-Mori, R.; Batyuk, A.; Sutherlin, K.D.; Brewster, A.S.; Bolotovskii, R.; Mendez, D.; Holton, J.M.; Moriarty, N.W.; Adams, P.D.; Bergmann, U.; Sauter, N.K.; Dobbek, H.; Messinger, J.; Zouni, A.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on : 2021-07-13
Resolution : 2.09 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:

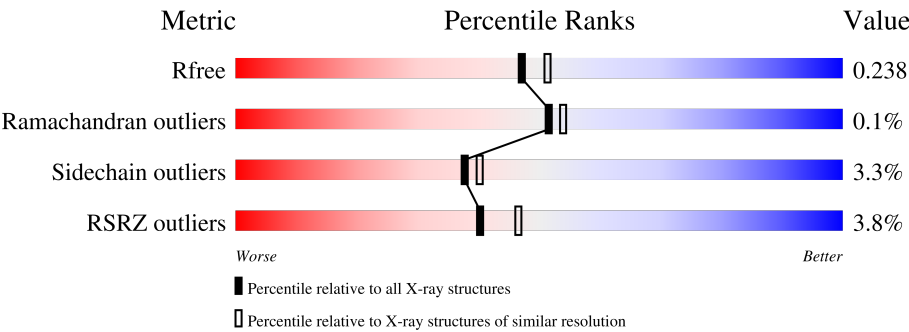
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.09 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.



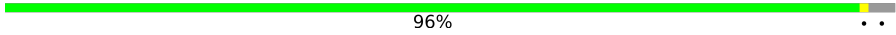
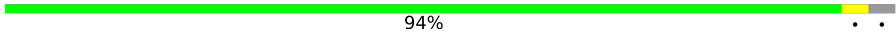
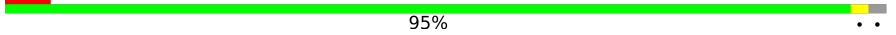
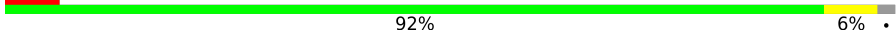


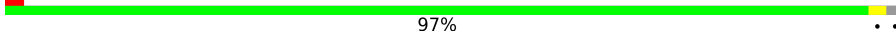







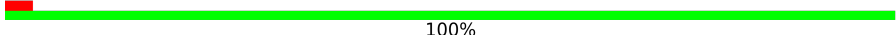







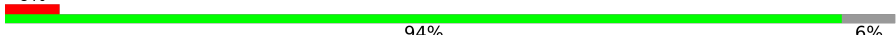


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	5197 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	 96% ..
4	d	352	 94% . .
5	E	84	 95% ..
5	e	84	 92% 6% .
6	F	45	 76% 24%
6	f	45	 69% 7% 24%
7	H	66	 97% ..
7	h	66	 91% 8% 5% 5%
8	I	38	 82% 13% 5%
8	i	38	 92% . 5%
9	J	40	 90% 10%
9	j	40	 88% . 10%
10	K	46	 80% 20%
10	k	46	 72% 9% 20%
11	L	37	 100%
11	l	37	 86% 11% .
12	M	36	 89% . 8%
12	m	36	 83% 6% 11%
13	O	272	 85% 5% 10%
13	o	272	 87% . 10%
14	R	41	 59% 22% 10% 32%
14	r	41	 63% 49% 5% 32%
15	T	32	 94% 6%
15	t	32	 88% 6% 6% 6%
16	U	134	 69% . 28%

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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	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	502	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	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	402	X	-	-	-
22	CLA	a	402	X	-	-	-
22	CLA	a	404	X	-	-	-
22	CLA	b	601	X	-	-	-
22	CLA	b	602	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	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	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	403	X	-	-	-
22	CLA	d	404	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 106082 atoms, of which 52760 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	334	Total	C	H	N	O	S	0	66	0
			6098	2030	2985	513	551	19			
1	a	334	Total	C	H	N	O	S	0	66	0
			6086	2027	2976	513	551	19			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	H	N	O	S	0	5	0
			7878	2631	3873	666	695	13			
2	b	505	Total	C	H	N	O	S	0	0	0
			7814	2610	3836	665	690	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	442	Total	C	H	N	O	S	0	14	0
			6941	2302	3432	586	607	14			
3	c	451	Total	C	H	N	O	S	0	14	0
			7086	2343	3503	602	624	14			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	341	Total	C	H	N	O	S	0	2	0
			5368	1809	2637	446	464	12			
4	d	341	Total	C	H	N	O	S	0	3	0
			5380	1813	2643	446	466	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	82	Total	C	H	N	O	16	1	0
			1317	436	651	107	123			
5	e	82	Total	C	H	N	O	0	0	0
			1312	434	648	108	122			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
15	T	30	Total	C	H	N	O	S	0	0	0
			519	181	261	36	39	2			
15	t	30	Total	C	H	N	O	S	0	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	0
			2135	675	1071	177	208	4			
17	v	137	Total	C	H	N	O	S	0	0	0
			2135	675	1071	177	208	4			

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

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

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

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

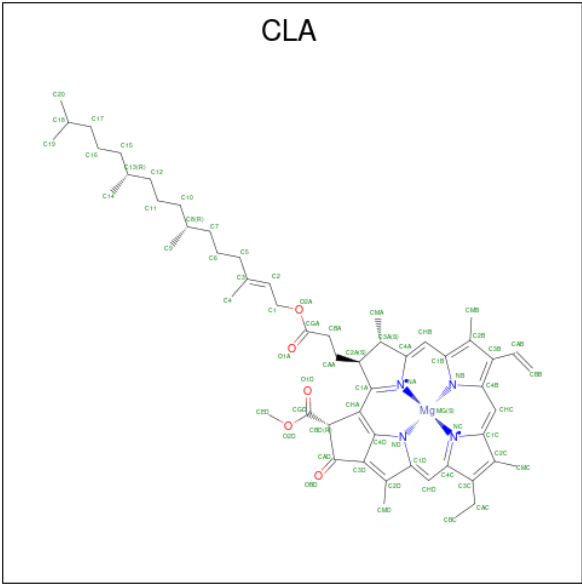
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

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

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

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



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

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

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

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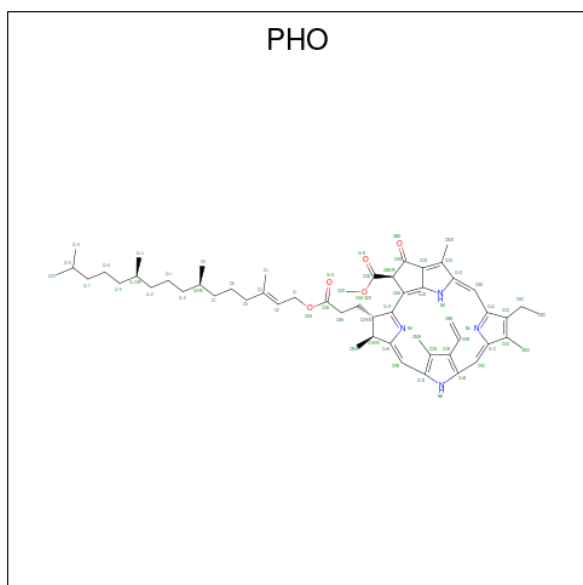
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total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

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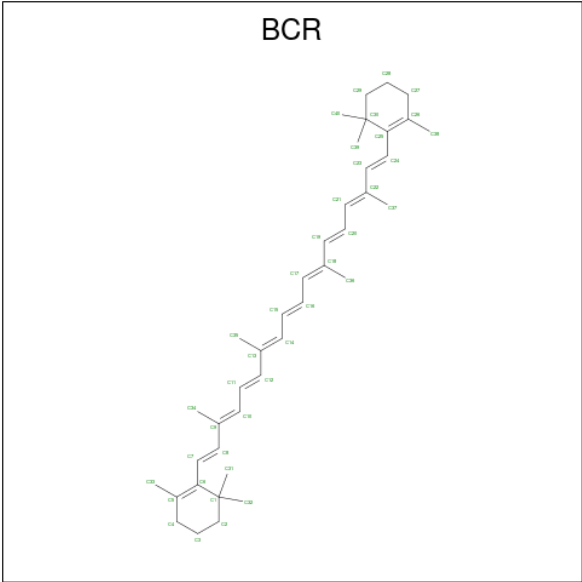
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	D	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	d	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	T	1	Total	C	H	0	0
			96	40	56		
24	Y	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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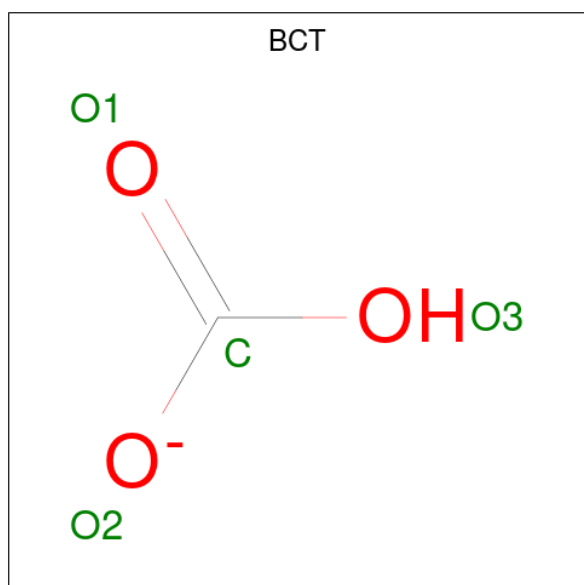
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	b	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	d	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40	56		
24	t	1	Total	C	H	0	0
			96	40	56		
24	x	1	Total	C	H	0	0
			96	40	56		

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

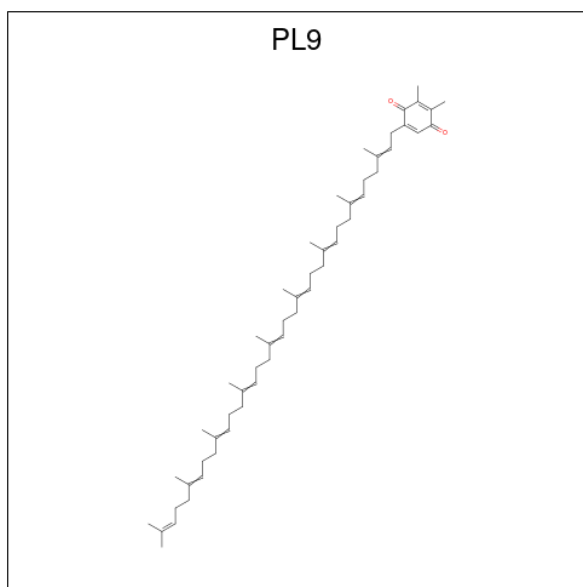
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	2	Total	Cl	0	0
			2	2		
25	a	2	Total	Cl	0	0
			2	2		

- Molecule 26 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



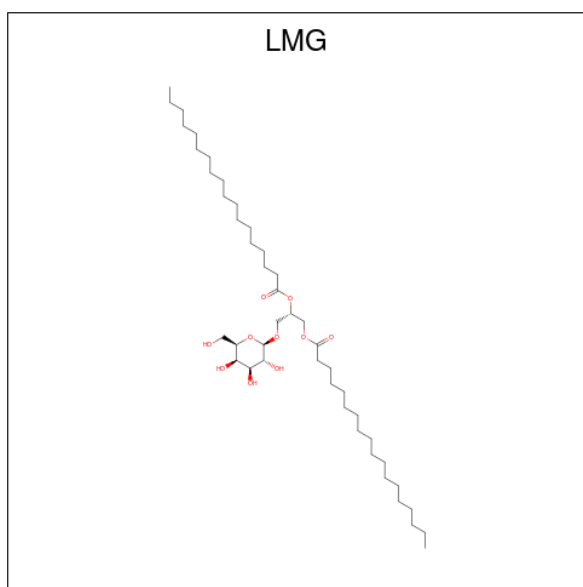
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	H	O	0	0
			5	1	1	3		
26	a	1	Total	C	H	O	0	0
			5	1	1	3		

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



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

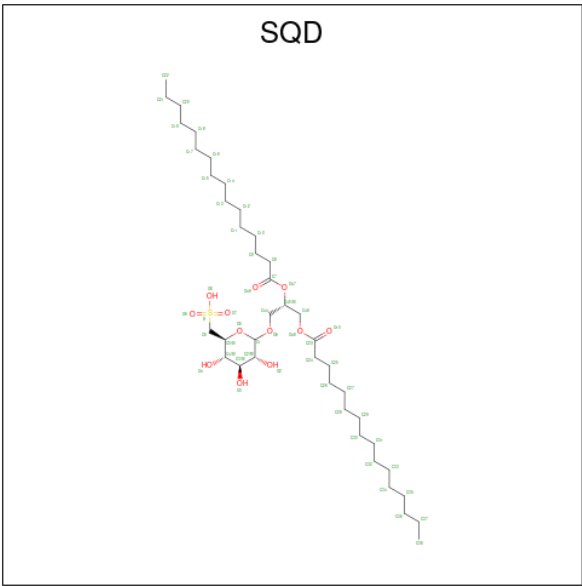
- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



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

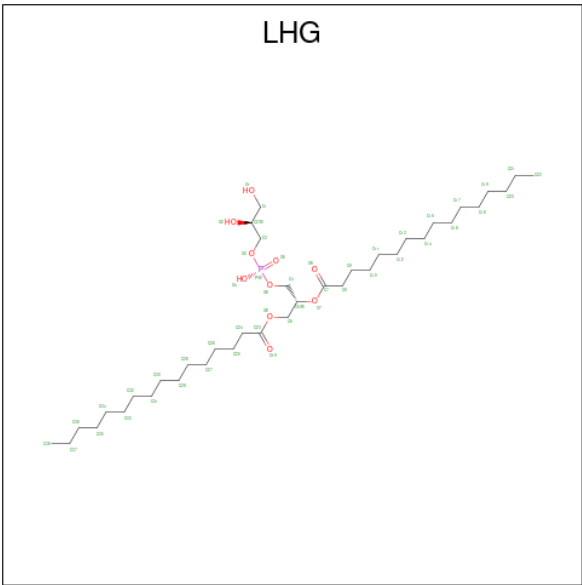
- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



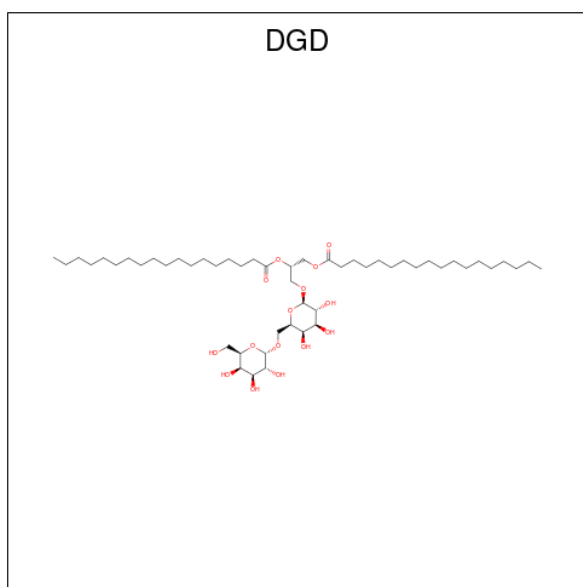
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
29	A	1	Total	C	H	O		0	0
			104	35	65	4			
29	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
29	D	1	Total	C	H	O	S	0	0
			82	25	46	10	1		
29	a	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
29	a	1	Total	C	H	O		0	0
			92	31	56	5			
29	b	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
29	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



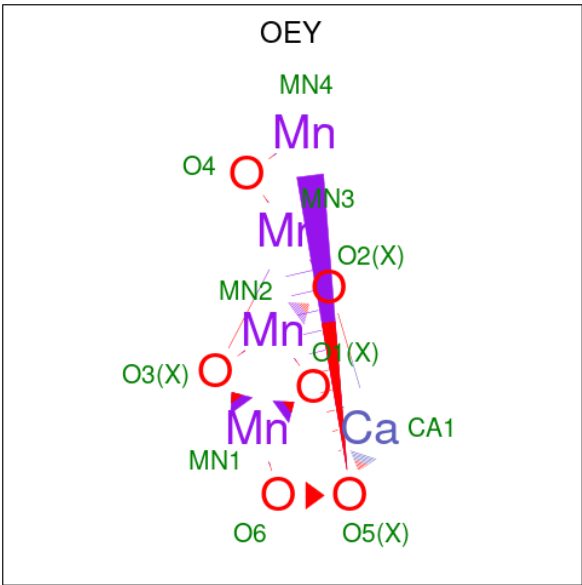
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
30	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
30	d	1	Total	C	H	O	P	0	0
			123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

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



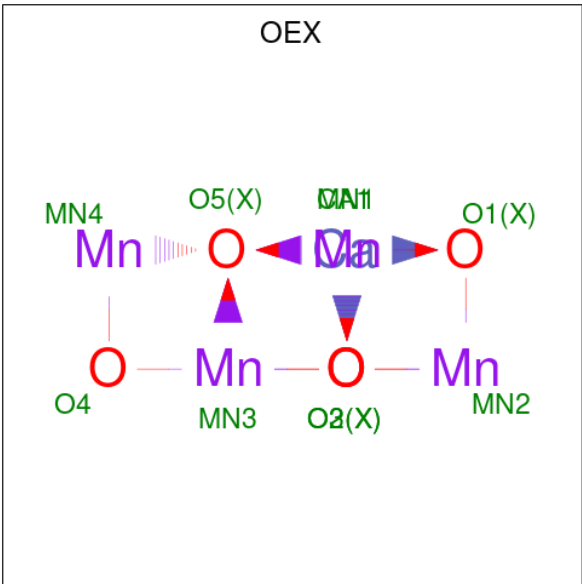
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	H	O	0	0
			162	51	96	15		
31	C	1	Total	C	H	O	0	0
			144	47	82	15		
31	C	1	Total	C	H	O	0	0
			144	47	82	15		
31	C	1	Total	C	H	O	0	0
			144	47	82	15		
31	H	1	Total	C	H	O	0	0
			144	47	82	15		
31	c	1	Total	C	H	O	0	0
			144	47	82	15		
31	c	1	Total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

- Molecule 32 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula: CaMn_4O_6) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 33 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



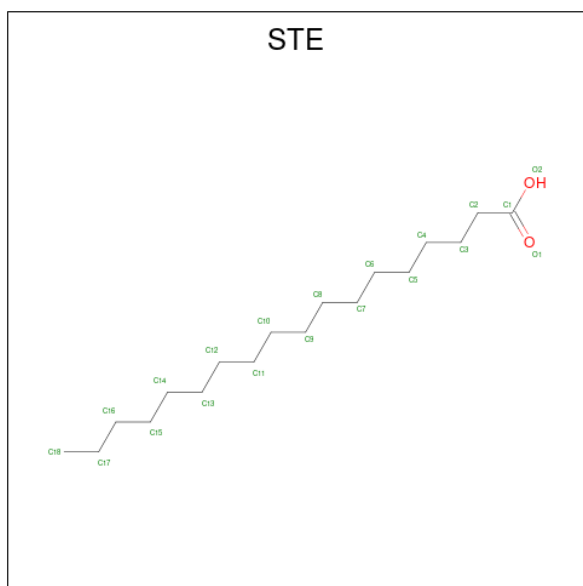
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

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

- Molecule 34 is STEARIC ACID (three-letter code: STE) (formula: $C_{18}H_{36}O_2$).



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

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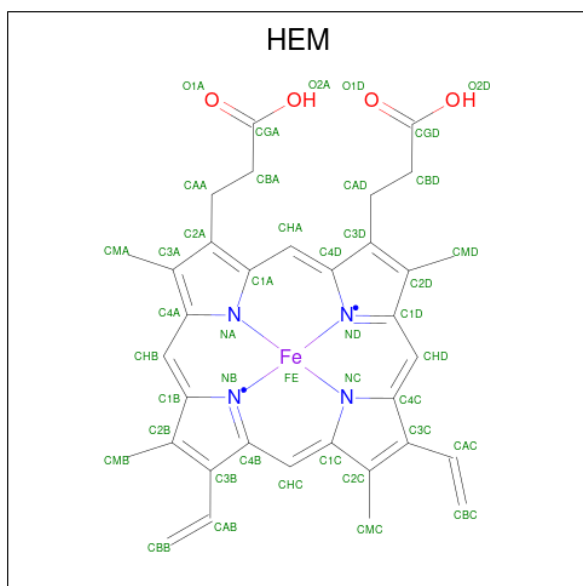
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	J	1	Total C H O 28 10 16 2	0	0
34	L	1	Total C H O 28 10 16 2	0	0
34	M	1	Total C H O 37 13 22 2	0	0
34	M	1	Total C H 26 10 16	0	0
34	R	1	Total C H O 28 10 16 2	0	0
34	T	1	Total C H 44 15 29	0	0
34	X	1	Total C H O 55 18 35 2	0	0
34	Z	1	Total C H 20 8 12	0	0
34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

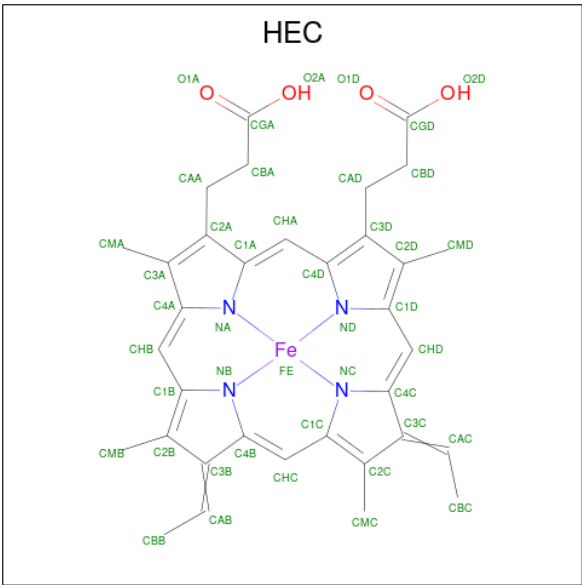
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	h	1	Total	C	H	0	0
			41	14	27		
34	j	1	Total	C	H	O	0
			28	10	16	2	
34	l	1	Total	C	H	0	0
			53	18	35		
34	t	1	Total	C	H	O	0
			34	12	20	2	

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





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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	151	Total	O	0	8
			151	151		
37	B	204	Total	O	0	0
			204	204		
37	C	173	Total	O	0	0
			173	173		
37	D	131	Total	O	0	0
			131	131		
37	E	33	Total	O	0	0
			33	33		
37	F	8	Total	O	0	0
			8	8		
37	H	34	Total	O	0	0
			34	34		
37	I	17	Total	O	0	0
			17	17		
37	J	24	Total	O	0	0
			24	24		
37	K	15	Total	O	0	0
			15	15		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	L	10	Total 10	O 10	0	0
37	M	8	Total 8	O 8	0	0
37	O	86	Total 86	O 86	0	0
37	R	4	Total 4	O 4	0	0
37	T	8	Total 8	O 8	0	0
37	U	34	Total 34	O 34	0	0
37	V	64	Total 64	O 64	0	0
37	X	15	Total 15	O 15	0	0
37	Y	3	Total 3	O 3	0	0
37	Z	10	Total 10	O 10	0	0
37	a	132	Total 132	O 132	0	8
37	b	172	Total 172	O 172	0	0
37	c	157	Total 157	O 157	0	0
37	d	110	Total 110	O 110	0	0
37	e	28	Total 28	O 28	0	0
37	f	6	Total 6	O 6	0	0
37	h	20	Total 20	O 20	0	0
37	i	11	Total 11	O 11	0	0
37	j	8	Total 8	O 8	0	0
37	k	5	Total 5	O 5	0	0
37	l	8	Total 8	O 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	m	7	Total 7	O 7	0	0
37	o	100	Total 100	O 100	0	0
37	r	7	Total 7	O 7	0	0
37	t	8	Total 8	O 8	0	0
37	u	48	Total 48	O 48	0	0
37	v	59	Total 59	O 59	0	0
37	x	11	Total 11	O 11	0	0
37	y	4	Total 4	O 4	0	0
37	z	12	Total 12	O 12	0	0

3 Residue-property plots [i](#)

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

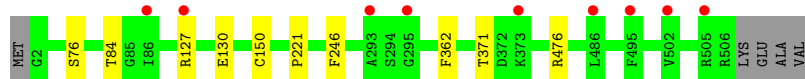
- Molecule 1: Photosystem II protein D1 1



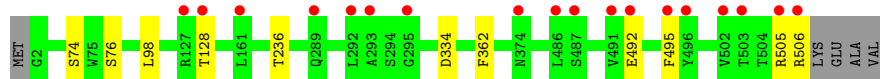
- Molecule 1: Photosystem II protein D1 1



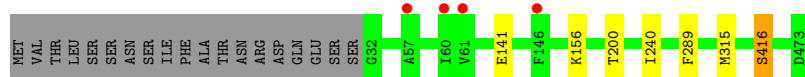
- Molecule 2: Photosystem II CP47 reaction center protein



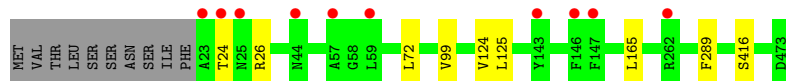
- Molecule 2: Photosystem II CP47 reaction center protein



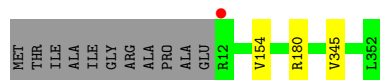
- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein



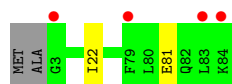
- Molecule 4: Photosystem II D2 protein



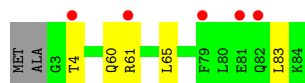
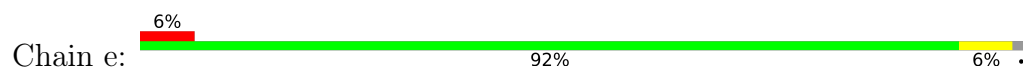
- Molecule 4: Photosystem II D2 protein



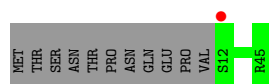
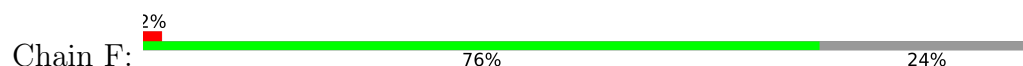
- Molecule 5: Cytochrome b559 subunit alpha



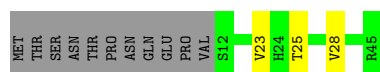
- Molecule 5: Cytochrome b559 subunit alpha



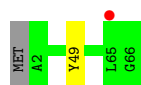
- Molecule 6: Cytochrome b559 subunit beta



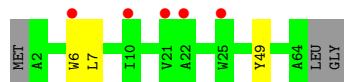
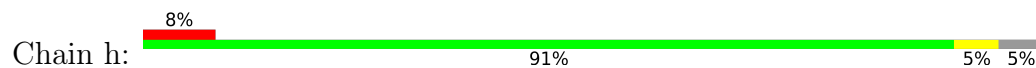
- Molecule 6: Cytochrome b559 subunit beta



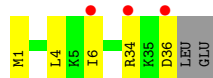
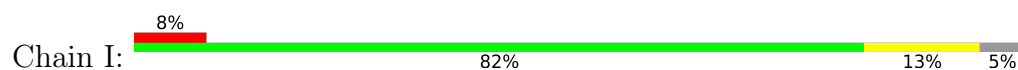
- Molecule 7: Photosystem II reaction center protein H



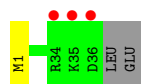
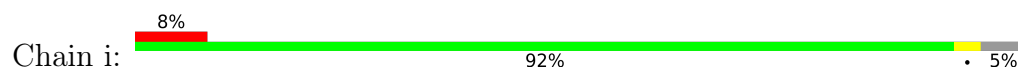
- Molecule 7: Photosystem II reaction center protein H



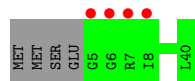
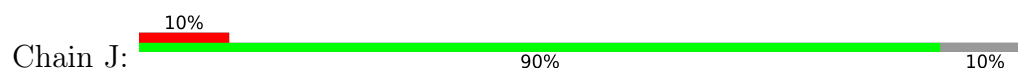
- Molecule 8: Photosystem II reaction center protein I



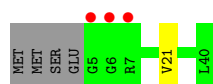
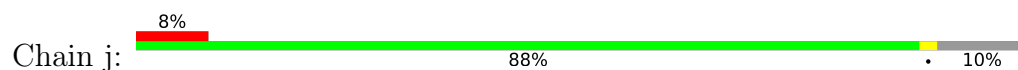
- Molecule 8: Photosystem II reaction center protein I



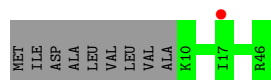
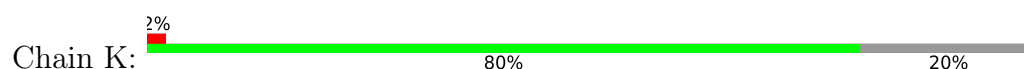
- Molecule 9: Photosystem II reaction center protein J



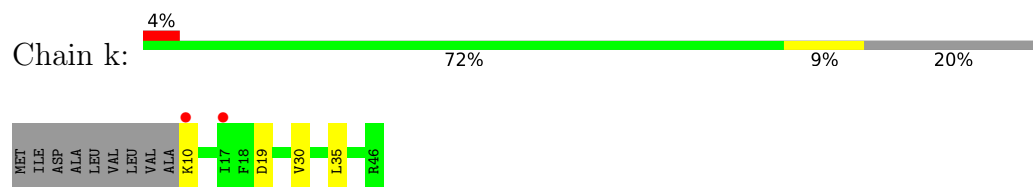
- Molecule 9: Photosystem II reaction center protein J



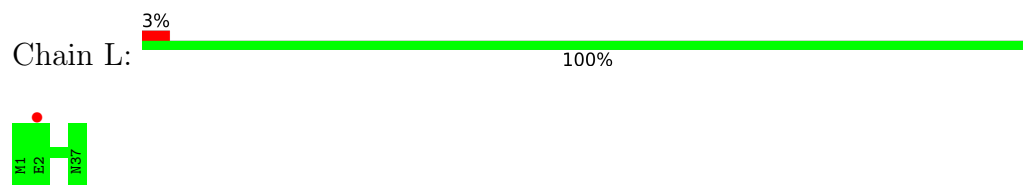
- Molecule 10: Photosystem II reaction center protein K



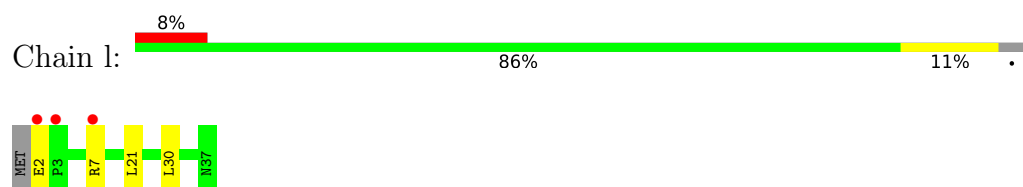
- Molecule 10: Photosystem II reaction center protein K



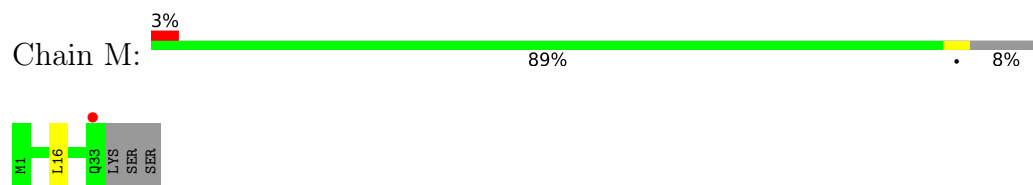
- Molecule 11: Photosystem II reaction center protein L



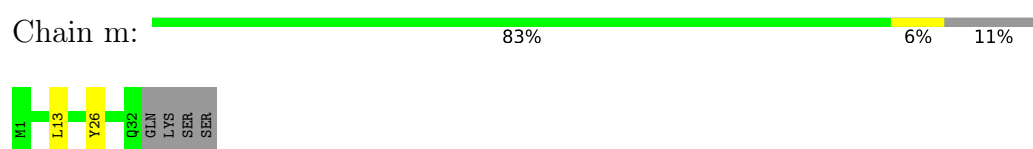
- Molecule 11: Photosystem II reaction center protein L



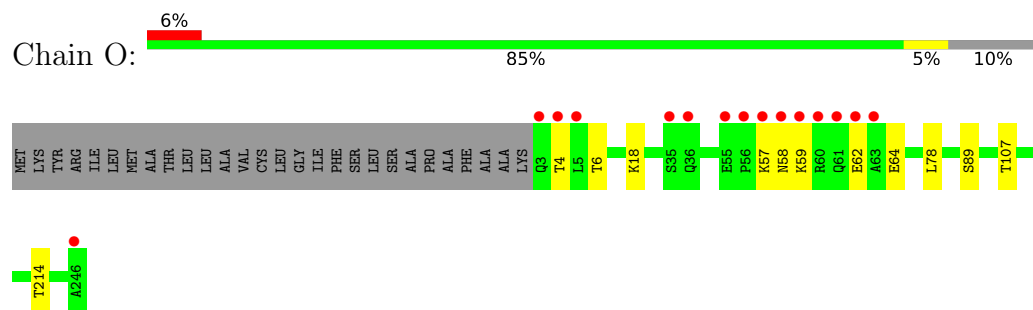
- Molecule 12: Photosystem II reaction center protein M



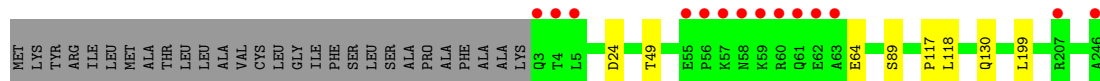
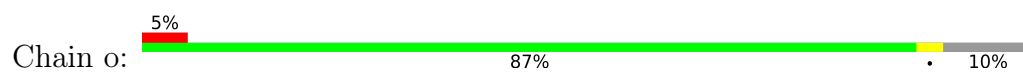
- Molecule 12: Photosystem II reaction center protein M



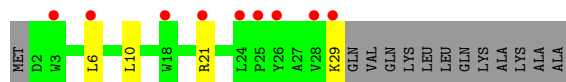
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



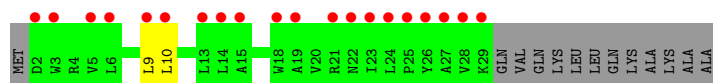
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



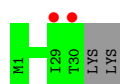
- Molecule 14: Photosystem II protein Y



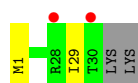
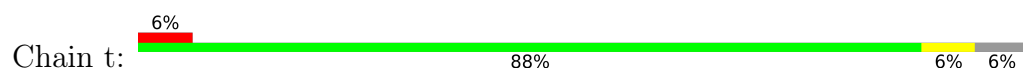
- Molecule 14: Photosystem II protein Y



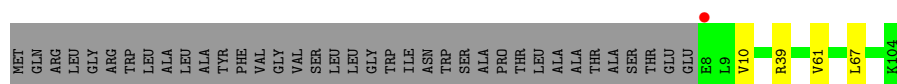
- Molecule 15: Photosystem II reaction center protein T



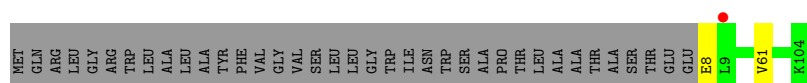
- Molecule 15: Photosystem II reaction center protein T




- Molecule 16: Photosystem II 12 kDa extrinsic protein

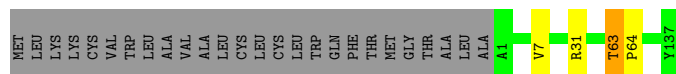


- Molecule 16: Photosystem II 12 kDa extrinsic protein




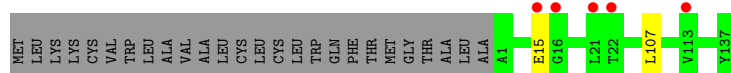
- Molecule 17: Cytochrome c-550

Chain V:  82% .. 16%




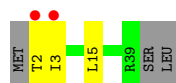
- Molecule 17: Cytochrome c-550

Chain v:  83% . 16%




- Molecule 18: Photosystem II reaction center X protein

Chain X:  85% 7% 7%



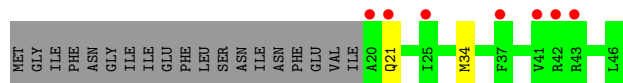
- Molecule 18: Photosystem II reaction center X protein

Chain x:  90% 5% 5%



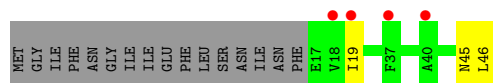
- Molecule 19: Photosystem II reaction center protein Ycf12

Chain Y:  54% . 41%




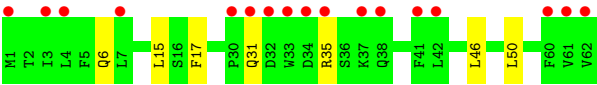
- Molecule 19: Photosystem II reaction center protein Ycf12

Chain y:  59% 7% 35%

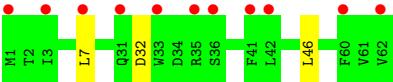
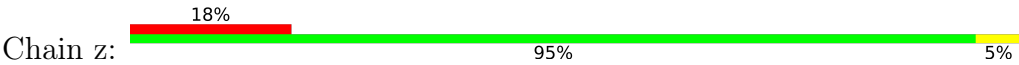


- Molecule 20: Photosystem II reaction center protein Z

Chain Z:  89% 11%



● Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.97Å 221.71Å 308.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.65 – 2.09 33.65 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.7 (33.65-2.09) 86.0 (33.65-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.72 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.186 , 0.239 0.186 , 0.238	Depositor DCC
R_{free} test set	4171 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 63.1	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	106082	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.57	0/3227	0.64	1/4397 (0.0%)
1	a	0.57	0/3224	0.64	0/4393
2	B	0.61	2/4161 (0.0%)	0.66	0/5669
2	b	0.60	0/4118	0.66	1/5611 (0.0%)
3	C	0.57	0/3647	0.65	0/4965
3	c	0.54	0/3719	0.64	0/5061
4	D	0.62	0/2825	0.67	0/3847
4	d	0.59	0/2834	0.68	0/3859
5	E	0.56	0/688	0.61	0/940
5	e	0.50	0/683	0.63	0/932
6	F	0.52	0/284	0.55	0/387
6	f	0.45	0/284	0.56	0/387
7	H	0.60	0/523	0.71	0/713
7	h	0.53	0/511	0.69	0/697
8	I	0.57	0/293	0.64	0/396
8	i	0.60	0/293	0.64	0/396
9	J	0.55	0/263	0.63	0/356
9	j	0.47	0/263	0.66	0/356
10	K	0.51	0/303	0.60	0/416
10	k	0.49	0/303	0.62	0/416
11	L	0.58	0/311	0.68	0/422
11	l	0.64	0/303	0.66	0/412
12	M	0.57	0/249	0.62	0/341
12	m	0.78	1/244 (0.4%)	0.64	0/334
13	O	0.57	0/1904	0.72	0/2585
13	o	0.58	0/1905	0.71	0/2583
14	R	0.39	0/227	0.55	0/313
14	r	0.35	0/227	0.54	0/313
15	T	0.67	0/257	0.70	0/349
15	t	0.66	0/255	0.61	0/346
16	U	0.54	0/785	0.67	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	u	0.61	0/785	0.68	0/1064
17	V	0.59	0/1085	0.66	1/1473 (0.1%)
17	v	0.55	0/1085	0.65	0/1473
18	X	0.52	0/284	0.66	0/384
18	x	0.44	0/289	0.58	0/391
19	Y	0.45	0/197	0.58	0/264
19	y	0.36	0/219	0.57	0/294
20	Z	0.45	0/490	0.54	0/669
20	z	0.40	0/488	0.51	0/666
All	All	0.57	3/44035 (0.0%)	0.65	3/59934 (0.0%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	m	26	TYR	CD1-CE1	-6.25	1.29	1.39
2	B	150	CYS	CB-SG	-5.75	1.72	1.81
2	B	221	PRO	CA-C	-5.37	1.42	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	V	63	THR	C-N-CD	-5.33	108.87	120.60
2	b	334	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	131	TRP	CA-CB-CG	-5.05	104.10	113.70

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

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	397/344 (115%)	390 (98%)	6 (2%)	1 (0%)	41	41
1	a	397/344 (115%)	388 (98%)	9 (2%)	0	100	100
2	B	508/510 (100%)	501 (99%)	7 (1%)	0	100	100
2	b	503/510 (99%)	493 (98%)	10 (2%)	0	100	100
3	C	454/461 (98%)	444 (98%)	9 (2%)	1 (0%)	47	49
3	c	463/461 (100%)	452 (98%)	10 (2%)	1 (0%)	47	49
4	D	340/352 (97%)	330 (97%)	10 (3%)	0	100	100
4	d	341/352 (97%)	332 (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%)	31 (97%)	1 (3%)	0	100	100
7	H	63/66 (96%)	57 (90%)	6 (10%)	0	100	100
7	h	61/66 (92%)	56 (92%)	5 (8%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100

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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%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	231 (95%)	9 (4%)	3 (1%)	13	8
13	o	242/272 (89%)	235 (97%)	7 (3%)	0	100	100
14	R	26/41 (63%)	26 (100%)	0	0	100	100
14	r	26/41 (63%)	26 (100%)	0	0	100	100
15	T	28/32 (88%)	28 (100%)	0	0	100	100
15	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
16	U	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
16	u	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
17	V	135/163 (83%)	130 (96%)	4 (3%)	1 (1%)	22	18
17	v	135/163 (83%)	128 (95%)	7 (5%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	35 (95%)	2 (5%)	0	100	100
19	Y	25/46 (54%)	23 (92%)	2 (8%)	0	100	100
19	y	28/46 (61%)	25 (89%)	3 (11%)	0	100	100
20	Z	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
20	z	60/62 (97%)	55 (92%)	5 (8%)	0	100	100
All	All	5387/5700 (94%)	5241 (97%)	139 (3%)	7 (0%)	51	54

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
17	V	64	PRO
3	c	416	SER
13	O	59	LYS
13	O	62	GLU
13	O	58	ASN
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	324/280 (116%)	322 (99%)	2 (1%)	86	90
1	a	323/280 (115%)	313 (97%)	10 (3%)	40	43
2	B	408/407 (100%)	400 (98%)	8 (2%)	55	60
2	b	402/407 (99%)	392 (98%)	10 (2%)	47	52
3	C	356/362 (98%)	349 (98%)	7 (2%)	55	60
3	c	364/362 (101%)	356 (98%)	8 (2%)	52	57
4	D	277/283 (98%)	274 (99%)	3 (1%)	73	79
4	d	278/283 (98%)	269 (97%)	9 (3%)	39	41
5	E	72/73 (99%)	69 (96%)	3 (4%)	30	30
5	e	71/73 (97%)	66 (93%)	5 (7%)	15	12
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	25 (89%)	3 (11%)	6	3
7	H	54/55 (98%)	53 (98%)	1 (2%)	57	63
7	h	53/55 (96%)	50 (94%)	3 (6%)	20	18
8	I	32/34 (94%)	28 (88%)	4 (12%)	4	2
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	23 (96%)	1 (4%)	30	30
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	26 (87%)	4 (13%)	4	2
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	2
12	M	28/32 (88%)	27 (96%)	1 (4%)	35	36
12	m	28/32 (88%)	27 (96%)	1 (4%)	35	36
13	O	206/228 (90%)	195 (95%)	11 (5%)	22	20
13	o	207/228 (91%)	199 (96%)	8 (4%)	32	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	R	22/33 (67%)	18 (82%)	4 (18%)	1	1
14	r	22/33 (67%)	20 (91%)	2 (9%)	9	6
15	T	26/28 (93%)	26 (100%)	0	100	100
15	t	25/28 (89%)	24 (96%)	1 (4%)	31	32
16	U	84/112 (75%)	80 (95%)	4 (5%)	25	24
16	u	84/112 (75%)	82 (98%)	2 (2%)	49	53
17	V	117/138 (85%)	115 (98%)	2 (2%)	60	67
17	v	117/138 (85%)	115 (98%)	2 (2%)	60	67
18	X	31/34 (91%)	28 (90%)	3 (10%)	8	5
18	x	31/34 (91%)	29 (94%)	2 (6%)	17	14
19	Y	19/37 (51%)	17 (90%)	2 (10%)	7	4
19	y	22/37 (60%)	19 (86%)	3 (14%)	3	2
20	Z	52/52 (100%)	45 (86%)	7 (14%)	4	2
20	z	51/52 (98%)	48 (94%)	3 (6%)	19	17
All	All	4451/4654 (96%)	4308 (97%)	143 (3%)	38	41

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	270	SER
2	B	76	SER
2	B	84	THR
2	B	127	ARG
2	B	130	GLU
2	B	246	PHE
2	B	362	PHE
2	B	371	THR
2	B	476	ARG
3	C	141	GLU
3	C	156	LYS
3	C	200	THR
3	C	240	ILE
3	C	289	PHE
3	C	315	MET
3	C	416	SER
4	D	154	VAL

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Mol	Chain	Res	Type
4	D	180	ARG
4	D	345	VAL
5	E	22[A]	ILE
5	E	22[B]	ILE
5	E	81	GLU
7	H	49	TYR
8	I	4	LEU
8	I	6	ILE
8	I	34	ARG
8	I	36	ASP
12	M	16	LEU
13	O	4	THR
13	O	6	THR
13	O	18	LYS
13	O	57	LYS
13	O	64	GLU
13	O	78	LEU
13	O	89	SER
13	O	107	THR
13	O	118	LEU
13	O	135	SER
13	O	214	THR
14	R	6	LEU
14	R	10	LEU
14	R	21	ARG
14	R	29	LYS
16	U	10	VAL
16	U	39	ARG
16	U	61	VAL
16	U	67	LEU
17	V	7	VAL
17	V	31	ARG
18	X	2	THR
18	X	3	ILE
18	X	15	LEU
19	Y	21	GLN
19	Y	34	MET
20	Z	6	GLN
20	Z	15	LEU
20	Z	17	PHE
20	Z	31	GLN
20	Z	35	ARG

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Mol	Chain	Res	Type
20	Z	46	LEU
20	Z	50	LEU
1	a	16	ARG
1	a	28	LEU
1	a	42	LEU
1	a	121	LEU
1	a	159[A]	LEU
1	a	159[B]	LEU
1	a	200	LEU
1	a	223	LEU
1	a	245	THR
1	a	288	LEU
2	b	74	SER
2	b	76	SER
2	b	98	LEU
2	b	128	THR
2	b	236	THR
2	b	362	PHE
2	b	492	GLU
2	b	495	PHE
2	b	505	ARG
2	b	506	ARG
3	c	24	THR
3	c	26	ARG
3	c	72	LEU
3	c	99	VAL
3	c	124	VAL
3	c	125	LEU
3	c	165	LEU
3	c	289	PHE
4	d	90	LEU
4	d	180	ARG
4	d	182	LEU
4	d	230	SER
4	d	259	ILE
4	d	272	LEU
4	d	291	LEU
4	d	307	GLU
4	d	321	LEU
5	e	4	THR
5	e	60	GLN
5	e	61	ARG

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Mol	Chain	Res	Type
5	e	65	LEU
5	e	83	LEU
6	f	23	VAL
6	f	25	THR
6	f	28	VAL
7	h	6	TRP
7	h	7	LEU
7	h	49	TYR
9	j	21	VAL
10	k	10	LYS
10	k	19	ASP
10	k	30	VAL
10	k	35	LEU
11	l	2	GLU
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
13	o	24	ASP
13	o	49	THR
13	o	64	GLU
13	o	89	SER
13	o	117	PRO
13	o	118	LEU
13	o	130	GLN
13	o	199	LEU
14	r	9	LEU
14	r	10	LEU
15	t	29	ILE
16	u	8	GLU
16	u	61	VAL
17	v	15	GLU
17	v	107	LEU
18	x	2	THR
18	x	15	LEU
19	y	19	ILE
19	y	45	ASN
19	y	46	LEU
20	z	7	LEU
20	z	32	ASP
20	z	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	GLN
2	B	409	GLN
11	L	8	GLN
12	M	32	GLN
13	O	36	GLN
13	O	88	ASN
14	R	22	ASN
17	V	86	GLN
18	X	38	GLN
19	Y	21	GLN
1	a	234	ASN
2	b	179	GLN
2	b	409	GLN
3	c	28	GLN
3	c	378	ASN
5	e	82	GLN
7	h	59	ASN
13	o	36	GLN
13	o	132	ASN
16	u	37	GLN
18	x	33	GLN
20	z	31	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	FME	T	1	15	8,9,10	1.04	0	7,9,11	1.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	FME	i	1	8	8,9,10	0.89	0	7,9,11	1.41	1 (14%)
12	FME	M	1	12	8,9,10	0.83	0	7,9,11	0.82	0
12	FME	m	1	12	8,9,10	0.98	0	7,9,11	1.13	0
15	FME	t	1	15	8,9,10	1.10	1 (12%)	7,9,11	1.13	0
8	FME	I	1	8	8,9,10	1.08	1 (12%)	7,9,11	1.26	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	FME	T	1	15	-	3/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
15	FME	t	1	15	-	2/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	1	FME	CA-N	-2.69	1.42	1.46
15	t	1	FME	CA-N	-2.35	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	CA-N-CN	-3.15	117.98	122.82
8	I	1	FME	CA-N-CN	-2.05	119.67	122.82

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	T	1	FME	N-CA-CB-CG
15	t	1	FME	O-C-CA-CB
15	t	1	FME	CB-CG-SD-CE
15	T	1	FME	CB-CG-SD-CE
15	T	1	FME	C-CA-CB-CG

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
22	CLA	D	402	-	56,73,73	1.37	5 (8%)	55,113,113	1.65	9 (16%)
22	CLA	a	402	-	56,73,73	1.62	7 (12%)	55,113,113	1.70	9 (16%)
26	BCT	A	409	21	0,3,3	-	-	0,3,3	-	-
22	CLA	A	405	-	45,62,73	1.65	5 (11%)	41,99,113	1.74	12 (29%)
24	BCR	t	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.35	8 (14%)
22	CLA	B	611	-	56,73,73	1.60	7 (12%)	55,113,113	1.81	14 (25%)
31	DGD	h	101	-	63,63,67	1.04	5 (7%)	77,77,81	1.48	11 (14%)
22	CLA	c	512	-	56,73,73	1.63	6 (10%)	55,113,113	1.78	10 (18%)
24	BCR	Y	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.16	3 (5%)
22	CLA	C	503	-	56,73,73	1.84	7 (12%)	55,113,113	1.92	9 (16%)
24	BCR	c	515	-	41,41,41	1.13	3 (7%)	56,56,56	1.23	7 (12%)
22	CLA	c	502	-	56,73,73	1.83	9 (16%)	55,113,113	1.69	8 (14%)
29	SQD	A	413	-	51,52,54	0.96	5 (9%)	60,63,65	1.83	12 (20%)
22	CLA	a	410	37	56,73,73	1.90	6 (10%)	55,113,113	1.66	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	a	405	-	41,41,41	1.09	2 (4%)	56,56,56	1.38	8 (14%)
22	CLA	b	606	-	56,73,73	1.85	12 (21%)	55,113,113	2.20	13 (23%)
29	SQD	a	411	-	53,54,54	1.02	5 (9%)	62,65,65	1.79	12 (19%)
22	CLA	c	506	-	56,73,73	1.47	7 (12%)	55,113,113	1.66	11 (20%)
28	LMG	a	416	-	55,55,55	1.21	4 (7%)	63,63,63	1.49	7 (11%)
35	HEM	e	101	5,6	27,50,50	2.04	5 (18%)	17,82,82	2.13	4 (23%)
22	CLA	B	609	-	56,73,73	1.73	8 (14%)	55,113,113	1.62	10 (18%)
22	CLA	C	513	-	56,73,73	1.68	7 (12%)	55,113,113	1.52	10 (18%)
22	CLA	C	508	-	56,73,73	1.65	6 (10%)	55,113,113	1.89	10 (18%)
22	CLA	A	402	-	56,73,73	1.57	9 (16%)	55,113,113	1.60	8 (14%)
22	CLA	d	403	-	56,73,73	1.58	8 (14%)	55,113,113	1.59	10 (18%)
24	BCR	d	405	-	41,41,41	1.19	2 (4%)	56,56,56	1.18	6 (10%)
22	CLA	b	608	-	56,73,73	1.70	8 (14%)	55,113,113	1.49	11 (20%)
24	BCR	A	406	-	41,41,41	1.08	2 (4%)	56,56,56	1.32	7 (12%)
26	BCT	a	408	21	0,3,3	-	-	0,3,3	-	-
22	CLA	C	504	37	50,67,73	1.68	7 (14%)	47,105,113	1.67	13 (27%)
22	CLA	b	615	-	56,73,73	1.68	9 (16%)	55,113,113	1.69	8 (14%)
34	STE	d	411	-	13,16,19	0.32	0	12,16,19	1.16	1 (8%)
22	CLA	B	616	-	51,68,73	1.81	10 (19%)	49,107,113	2.15	16 (32%)
34	STE	B	626	-	15,15,19	0.44	0	14,14,19	0.62	0
22	CLA	c	503	-	56,73,73	1.54	9 (16%)	55,113,113	1.69	9 (16%)
22	CLA	C	505	-	56,73,73	1.68	5 (8%)	55,113,113	1.57	11 (20%)
22	CLA	a	403	37	56,73,73	1.56	6 (10%)	55,113,113	1.56	9 (16%)
27	PL9	a	409	-	55,55,55	1.18	5 (9%)	68,69,69	1.58	14 (20%)
28	LMG	D	411	-	20,26,55	0.42	0	18,26,63	1.19	0
29	SQD	a	412	-	35,35,54	1.10	2 (5%)	37,37,65	1.44	4 (10%)
36	HEC	v	201	17	26,50,50	2.37	4 (15%)	18,82,82	2.14	5 (27%)
23	PHO	d	401	-	67,69,69	1.13	6 (8%)	85,99,99	1.03	5 (5%)
24	BCR	K	102	-	41,41,41	1.09	3 (7%)	56,56,56	1.18	5 (8%)
29	SQD	f	101	-	40,41,54	1.12	5 (12%)	49,52,65	2.05	11 (22%)
28	LMG	D	406	-	51,51,55	0.87	3 (5%)	59,59,63	1.43	9 (15%)
34	STE	B	625	-	14,17,19	0.37	0	13,17,19	1.03	0
22	CLA	b	604	-	56,73,73	1.45	7 (12%)	55,113,113	1.84	12 (21%)
23	PHO	D	401	-	67,69,69	1.15	5 (7%)	85,99,99	1.25	10 (11%)
24	BCR	c	514	-	41,41,41	1.15	2 (4%)	56,56,56	1.21	6 (10%)
34	STE	H	103	-	17,17,19	0.43	0	16,16,19	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	STE	l	102	-	17,17,19	0.31	0	16,16,19	1.00	0
31	DGD	c	516	-	63,63,67	1.26	11 (17%)	77,77,81	1.43	13 (16%)
30	LHG	l	101	-	48,48,48	0.74	1 (2%)	51,54,54	1.17	4 (7%)
29	SQD	b	620	-	48,49,54	0.95	4 (8%)	57,60,65	2.15	17 (29%)
22	CLA	B	612	-	56,73,73	1.63	5 (8%)	55,113,113	1.86	12 (21%)
34	STE	B	620	-	13,16,19	0.32	0	12,16,19	1.10	0
30	LHG	D	409	-	46,46,48	0.98	3 (6%)	49,52,54	1.32	4 (8%)
34	STE	C	519	-	8,11,19	0.39	0	7,11,19	0.81	0
30	LHG	A	414	-	48,48,48	0.85	3 (6%)	51,54,54	1.18	4 (7%)
34	STE	J	101	-	8,11,19	0.33	0	7,11,19	0.99	0
34	STE	L	101	-	8,11,19	0.44	0	7,11,19	0.70	0
28	LMG	C	518	-	48,48,55	1.15	5 (10%)	56,56,63	1.34	6 (10%)
30	LHG	D	408	-	48,48,48	1.05	3 (6%)	51,54,54	1.27	7 (13%)
22	CLA	B	601	37	56,73,73	1.62	9 (16%)	55,113,113	1.99	13 (23%)
34	STE	c	523	-	8,11,19	0.38	0	7,11,19	0.77	0
27	PL9	D	405	-	55,55,55	1.71	9 (16%)	68,69,69	1.72	14 (20%)
32	OEY	a	418[B]	37,1,3	0,16,16	-	-	-	-	-
22	CLA	b	607	37	56,73,73	1.39	6 (10%)	55,113,113	1.89	11 (20%)
24	BCR	C	514	-	41,41,41	1.27	3 (7%)	56,56,56	1.37	5 (8%)
28	LMG	D	410	-	31,31,55	0.89	2 (6%)	33,33,63	1.16	2 (6%)
22	CLA	c	508	-	55,72,73	1.66	8 (14%)	53,111,113	1.67	11 (20%)
30	LHG	d	409	-	38,38,48	0.71	1 (2%)	41,44,54	1.13	3 (7%)
34	STE	d	413	-	16,19,19	0.39	0	15,19,19	0.76	0
28	LMG	c	522	-	49,49,55	0.92	3 (6%)	57,57,63	1.32	4 (7%)
34	STE	C	521	-	8,11,19	0.29	0	7,11,19	1.29	1 (14%)
24	BCR	B	618	-	41,41,41	1.14	3 (7%)	56,56,56	1.26	7 (12%)
22	CLA	c	504	37	51,68,73	1.58	6 (11%)	49,107,113	1.51	8 (16%)
22	CLA	b	605	-	56,73,73	1.50	8 (14%)	55,113,113	1.70	12 (21%)
22	CLA	b	611	-	56,73,73	1.52	5 (8%)	55,113,113	1.62	8 (14%)
31	DGD	c	518	-	63,63,67	1.01	4 (6%)	77,77,81	1.38	12 (15%)
33	OEX	A	418[A]	37,1,3	0,15,15	-	-	-	-	-
36	HEC	V	201	17	26,50,50	2.07	3 (11%)	18,82,82	2.17	6 (33%)
34	STE	b	627	-	9,9,19	0.48	0	8,8,19	0.55	0
34	STE	B	624	-	8,11,19	0.32	0	7,11,19	0.93	0
22	CLA	B	614	-	56,73,73	1.63	8 (14%)	55,113,113	1.77	13 (23%)
34	STE	t	102	-	10,13,19	0.41	0	9,13,19	0.92	0
22	CLA	b	602	-	56,73,73	1.51	7 (12%)	55,113,113	1.88	10 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	STE	T	102	-	14,14,19	0.39	0	13,13,19	0.83	0
35	HEM	F	101	5,6	27,50,50	1.95	5 (18%)	17,82,82	2.37	8 (47%)
22	CLA	c	501	-	56,73,73	1.56	5 (8%)	55,113,113	1.75	11 (20%)
22	CLA	b	613	-	56,73,73	1.57	7 (12%)	55,113,113	1.98	14 (25%)
24	BCR	D	404	-	41,41,41	1.19	2 (4%)	56,56,56	1.11	3 (5%)
24	BCR	T	101	-	41,41,41	1.10	4 (9%)	56,56,56	1.25	5 (8%)
32	OEY	A	417[B]	37,1,3	0,16,16	-	-	-	-	-
28	LMG	A	412	-	48,48,55	1.04	3 (6%)	56,56,63	1.35	7 (12%)
22	CLA	A	403	37	56,73,73	1.56	8 (14%)	55,113,113	1.52	9 (16%)
22	CLA	B	605	-	56,73,73	1.43	6 (10%)	55,113,113	1.42	9 (16%)
22	CLA	C	501	-	56,73,73	1.69	8 (14%)	55,113,113	1.72	6 (10%)
22	CLA	B	608	-	56,73,73	1.40	8 (14%)	55,113,113	1.70	9 (16%)
34	STE	b	623	-	16,19,19	0.36	0	15,19,19	0.82	0
28	LMG	c	521	-	48,48,55	1.08	4 (8%)	56,56,63	1.31	6 (10%)
22	CLA	B	610	37	56,73,73	1.72	7 (12%)	55,113,113	1.85	14 (25%)
23	PHO	A	404	-	67,69,69	1.22	9 (13%)	85,99,99	1.24	8 (9%)
34	STE	a	414	-	8,11,19	0.47	0	7,11,19	0.79	0
24	BCR	k	102	-	41,41,41	1.04	2 (4%)	56,56,56	1.25	5 (8%)
28	LMG	M	101	-	51,51,55	1.05	6 (11%)	59,59,63	1.43	9 (15%)
34	STE	b	621	-	15,15,19	0.40	0	14,14,19	0.78	0
24	BCR	H	101	-	41,41,41	1.08	1 (2%)	56,56,56	1.33	8 (14%)
28	LMG	c	519	-	37,37,55	1.23	5 (13%)	45,45,63	1.33	7 (15%)
22	CLA	C	509	-	56,73,73	1.38	7 (12%)	55,113,113	1.97	9 (16%)
34	STE	b	625	-	12,15,19	0.40	0	11,15,19	0.71	0
22	CLA	b	614	-	56,73,73	1.71	8 (14%)	55,113,113	1.49	9 (16%)
28	LMG	b	622	-	51,51,55	1.01	5 (9%)	59,59,63	1.47	7 (11%)
31	DGD	C	515	-	63,63,67	1.11	3 (4%)	77,77,81	1.39	13 (16%)
30	LHG	e	102	-	41,41,48	1.04	4 (9%)	44,47,54	1.36	5 (11%)
27	PL9	A	410	-	55,55,55	1.25	4 (7%)	68,69,69	1.83	16 (23%)
22	CLA	b	601	37	56,73,73	1.63	4 (7%)	55,113,113	1.92	8 (14%)
34	STE	Z	101	-	7,7,19	0.33	0	6,6,19	0.67	0
34	STE	h	102	-	13,13,19	0.42	0	12,12,19	0.63	0
22	CLA	C	510	-	56,73,73	1.55	6 (10%)	55,113,113	1.58	6 (10%)
24	BCR	b	617	-	41,41,41	1.16	4 (9%)	56,56,56	1.40	8 (14%)
27	PL9	d	406	-	55,55,55	1.64	7 (12%)	68,69,69	1.69	15 (22%)
31	DGD	c	517	-	63,63,67	0.97	4 (6%)	77,77,81	1.42	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	LMG	d	410	-	44,44,55	1.01	2 (4%)	52,52,63	1.36	8 (15%)
30	LHG	B	621	-	48,48,48	0.99	2 (4%)	51,54,54	1.09	3 (5%)
34	STE	a	413	-	9,9,19	0.49	0	8,8,19	0.52	0
22	CLA	b	616	-	51,68,73	1.44	10 (19%)	49,107,113	1.80	9 (18%)
24	BCR	b	618	-	41,41,41	1.24	3 (7%)	56,56,56	1.26	8 (14%)
34	STE	b	626	-	16,19,19	0.45	0	15,19,19	0.72	0
34	STE	c	520	-	16,19,19	0.37	0	15,19,19	0.80	0
22	CLA	c	505	-	56,73,73	1.36	6 (10%)	55,113,113	1.58	9 (16%)
24	BCR	B	619	-	41,41,41	1.15	3 (7%)	56,56,56	1.29	7 (12%)
29	SQD	D	407	-	35,36,54	0.97	2 (5%)	42,45,65	2.28	12 (28%)
22	CLA	A	411	37	56,73,73	1.56	8 (14%)	55,113,113	1.59	9 (16%)
31	DGD	A	416	-	67,67,67	1.27	10 (14%)	81,81,81	1.44	11 (13%)
31	DGD	C	517	-	63,63,67	0.90	5 (7%)	77,77,81	1.32	6 (7%)
22	CLA	c	509	-	56,73,73	1.46	4 (7%)	55,113,113	1.86	12 (21%)
30	LHG	B	622	-	48,48,48	0.87	3 (6%)	51,54,54	1.40	8 (15%)
22	CLA	B	602	-	56,73,73	1.63	6 (10%)	55,113,113	1.75	10 (18%)
24	BCR	K	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.32	8 (14%)
34	STE	C	520	-	15,15,19	0.39	0	14,14,19	0.80	0
22	CLA	C	507	37	56,73,73	1.60	5 (8%)	55,113,113	1.88	12 (21%)
34	STE	X	101	-	16,19,19	0.29	0	15,19,19	1.10	1 (6%)
34	STE	M	103	-	9,9,19	0.37	0	8,8,19	0.68	0
22	CLA	C	506	-	56,73,73	1.66	9 (16%)	55,113,113	1.55	10 (18%)
30	LHG	d	408	-	48,48,48	0.92	3 (6%)	51,54,54	1.19	4 (7%)
28	LMG	b	624	-	55,55,55	0.87	3 (5%)	63,63,63	1.49	10 (15%)
22	CLA	c	513	-	56,73,73	1.54	5 (8%)	55,113,113	1.49	9 (16%)
22	CLA	C	511	3	56,73,73	1.92	6 (10%)	55,113,113	1.56	4 (7%)
22	CLA	D	403	-	56,73,73	1.57	11 (19%)	55,113,113	1.65	12 (21%)
34	STE	M	102	-	11,14,19	0.43	0	10,14,19	0.71	0
22	CLA	c	510	-	56,73,73	1.65	8 (14%)	55,113,113	1.69	9 (16%)
22	CLA	B	607	37	56,73,73	1.61	10 (17%)	55,113,113	1.69	7 (12%)
22	CLA	d	404	-	56,73,73	1.65	8 (14%)	55,113,113	1.56	10 (18%)
22	CLA	c	511	3	56,73,73	1.53	6 (10%)	55,113,113	1.75	8 (14%)
22	CLA	b	610	37	56,73,73	1.48	8 (14%)	55,113,113	1.67	12 (21%)
23	PHO	d	402	-	67,69,69	1.24	7 (10%)	85,99,99	1.16	6 (7%)
22	CLA	b	603	-	56,73,73	1.56	8 (14%)	55,113,113	1.74	12 (21%)
22	CLA	B	615	-	56,73,73	1.64	7 (12%)	55,113,113	1.52	11 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	STE	B	627	-	8,11,19	0.35	0	7,11,19	0.58	0
22	CLA	C	512	-	56,73,73	1.59	10 (17%)	55,113,113	1.57	12 (21%)
31	DGD	C	516	-	63,63,67	1.25	8 (12%)	77,77,81	1.34	9 (11%)
34	STE	j	101	-	8,11,19	0.54	0	7,11,19	0.39	0
34	STE	a	415	-	14,14,19	0.41	0	13,13,19	0.86	0
34	STE	I	101	-	14,14,19	0.45	0	13,13,19	0.59	0
22	CLA	b	612	-	56,73,73	1.38	6 (10%)	55,113,113	1.76	13 (23%)
34	STE	d	412	-	16,19,19	0.41	0	15,19,19	0.63	0
24	BCR	x	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.30	7 (12%)
22	CLA	a	404	-	56,73,73	1.70	10 (17%)	55,113,113	1.76	11 (20%)
31	DGD	H	102	-	63,63,67	1.23	8 (12%)	77,77,81	1.47	12 (15%)
24	BCR	b	619	-	41,41,41	1.16	2 (4%)	56,56,56	1.32	7 (12%)
30	LHG	d	407	-	48,48,48	0.95	2 (4%)	51,54,54	1.35	7 (13%)
33	OEX	a	417[A]	37,1,3	0,15,15	-	-	-	-	-
34	STE	R	101	-	8,11,19	0.42	0	7,11,19	0.64	0
22	CLA	C	502	-	56,73,73	1.54	6 (10%)	55,113,113	1.79	9 (16%)
29	SQD	A	415	-	38,38,54	1.00	3 (7%)	40,40,65	1.29	4 (10%)
24	BCR	k	101	-	41,41,41	1.09	3 (7%)	56,56,56	1.05	3 (5%)
22	CLA	B	613	-	56,73,73	1.64	9 (16%)	55,113,113	1.84	9 (16%)
22	CLA	B	604	-	56,73,73	1.51	6 (10%)	55,113,113	2.02	14 (25%)
24	BCR	B	617	-	41,41,41	1.17	3 (7%)	56,56,56	1.28	6 (10%)
22	CLA	B	606	-	56,73,73	1.75	8 (14%)	55,113,113	1.47	9 (16%)
22	CLA	c	507	37	56,73,73	1.29	7 (12%)	55,113,113	1.73	14 (25%)
29	SQD	B	623	-	53,54,54	0.97	3 (5%)	62,65,65	1.76	11 (17%)
22	CLA	b	609	-	56,73,73	1.67	9 (16%)	55,113,113	1.59	10 (18%)
22	CLA	B	603	-	56,73,73	1.62	8 (14%)	55,113,113	1.52	11 (20%)

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	D	402	-	1/1/20/20	9/37/115/115	-
22	CLA	a	402	-	1/1/20/20	6/37/115/115	-
22	CLA	A	405	-	1/1/17/20	6/24/102/115	-
24	BCR	t	101	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	611	-	1/1/20/20	7/37/115/115	-
31	DGD	h	101	-	-	16/51/91/95	0/2/2/2
22	CLA	c	512	-	1/1/20/20	21/37/115/115	-
24	BCR	Y	101	-	-	9/29/63/63	0/2/2/2
22	CLA	C	503	-	-	4/37/115/115	-
24	BCR	c	515	-	-	8/29/63/63	0/2/2/2
22	CLA	c	502	-	1/1/20/20	8/37/115/115	-
29	SQD	A	413	-	-	17/47/67/69	0/1/1/1
22	CLA	a	410	37	-	6/37/115/115	-
24	BCR	a	405	-	-	2/29/63/63	0/2/2/2
22	CLA	b	606	-	1/1/20/20	14/37/115/115	-
29	SQD	a	411	-	-	25/49/69/69	0/1/1/1
22	CLA	c	506	-	1/1/20/20	16/37/115/115	-
28	LMG	a	416	-	-	25/50/70/70	0/1/1/1
35	HEM	e	101	5,6	-	0/6/54/54	-
22	CLA	B	609	-	-	7/37/115/115	-
22	CLA	C	513	-	1/1/20/20	11/37/115/115	-
22	CLA	C	508	-	-	6/37/115/115	-
22	CLA	A	402	-	1/1/20/20	4/37/115/115	-
22	CLA	d	403	-	1/1/20/20	9/37/115/115	-
24	BCR	d	405	-	-	6/29/63/63	0/2/2/2
22	CLA	b	608	-	1/1/20/20	8/37/115/115	-
24	BCR	A	406	-	-	4/29/63/63	0/2/2/2
22	CLA	C	504	37	1/1/18/20	9/30/108/115	-
22	CLA	b	615	-	1/1/20/20	12/37/115/115	-
34	STE	d	411	-	-	9/12/14/17	-
22	CLA	B	616	-	1/1/19/20	9/31/109/115	-
34	STE	B	626	-	-	10/13/13/17	-
22	CLA	c	503	-	-	4/37/115/115	-
22	CLA	C	505	-	1/1/20/20	14/37/115/115	-
22	CLA	a	403	37	-	13/37/115/115	-
27	PL9	a	409	-	-	23/53/73/73	0/1/1/1
28	LMG	D	411	-	-	9/18/22/70	-
29	SQD	a	412	-	-	14/37/37/69	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	HEC	v	201	17	-	0/6/54/54	-
23	PHO	d	401	-	-	6/53/103/103	0/5/6/6
24	BCR	K	102	-	-	6/29/63/63	0/2/2/2
29	SQD	f	101	-	-	15/36/56/69	0/1/1/1
28	LMG	D	406	-	-	16/46/66/70	0/1/1/1
34	STE	B	625	-	-	7/13/15/17	-
22	CLA	b	604	-	1/1/20/20	5/37/115/115	-
23	PHO	D	401	-	-	1/53/103/103	0/5/6/6
24	BCR	c	514	-	-	7/29/63/63	0/2/2/2
34	STE	H	103	-	-	11/15/15/17	-
34	STE	l	102	-	-	9/15/15/17	-
31	DGD	c	516	-	-	26/51/91/95	0/2/2/2
30	LHG	l	101	-	-	18/53/53/53	-
29	SQD	b	620	-	-	20/44/64/69	0/1/1/1
22	CLA	B	612	-	1/1/20/20	11/37/115/115	-
34	STE	B	620	-	-	6/12/14/17	-
30	LHG	D	409	-	-	26/51/51/53	-
34	STE	C	519	-	-	5/7/9/17	-
30	LHG	A	414	-	-	31/53/53/53	-
34	STE	J	101	-	-	2/7/9/17	-
34	STE	L	101	-	-	4/7/9/17	-
28	LMG	C	518	-	-	20/43/63/70	0/1/1/1
30	LHG	D	408	-	-	24/53/53/53	-
22	CLA	B	601	37	1/1/20/20	20/37/115/115	-
34	STE	c	523	-	-	3/7/9/17	-
27	PL9	D	405	-	-	10/53/73/73	0/1/1/1
22	CLA	b	607	37	1/1/20/20	17/37/115/115	-
24	BCR	C	514	-	-	7/29/63/63	0/2/2/2
28	LMG	D	410	-	-	14/33/33/70	-
22	CLA	c	508	-	-	16/36/114/115	-
30	LHG	d	409	-	-	19/43/43/53	-
34	STE	d	413	-	-	9/15/17/17	-
28	LMG	c	522	-	-	19/44/64/70	0/1/1/1
34	STE	C	521	-	-	4/7/9/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	B	618	-	-	8/29/63/63	0/2/2/2
22	CLA	c	504	37	1/1/19/20	9/31/109/115	-
22	CLA	b	605	-	1/1/20/20	11/37/115/115	-
22	CLA	b	611	-	1/1/20/20	9/37/115/115	-
31	DGD	c	518	-	-	16/51/91/95	0/2/2/2
36	HEC	V	201	17	-	0/6/54/54	-
34	STE	b	627	-	-	5/7/7/17	-
34	STE	B	624	-	-	3/7/9/17	-
22	CLA	B	614	-	1/1/20/20	14/37/115/115	-
34	STE	t	102	-	-	3/9/11/17	-
22	CLA	b	602	-	1/1/20/20	12/37/115/115	-
34	STE	T	102	-	-	7/12/12/17	-
35	HEM	F	101	5,6	-	0/6/54/54	-
22	CLA	c	501	-	1/1/20/20	5/37/115/115	-
22	CLA	b	613	-	1/1/20/20	4/37/115/115	-
24	BCR	D	404	-	-	5/29/63/63	0/2/2/2
24	BCR	T	101	-	-	6/29/63/63	0/2/2/2
28	LMG	A	412	-	-	17/43/63/70	0/1/1/1
22	CLA	A	403	37	1/1/20/20	14/37/115/115	-
22	CLA	B	605	-	1/1/20/20	11/37/115/115	-
22	CLA	C	501	-	1/1/20/20	2/37/115/115	-
22	CLA	B	608	-	-	1/37/115/115	-
34	STE	b	623	-	-	9/15/17/17	-
28	LMG	c	521	-	-	24/43/63/70	0/1/1/1
22	CLA	B	610	37	1/1/20/20	7/37/115/115	-
23	PHO	A	404	-	-	4/53/103/103	0/5/6/6
34	STE	a	414	-	-	4/7/9/17	-
24	BCR	k	102	-	-	7/29/63/63	0/2/2/2
28	LMG	M	101	-	-	17/46/66/70	0/1/1/1
34	STE	b	621	-	-	5/13/13/17	-
24	BCR	H	101	-	-	1/29/63/63	0/2/2/2
28	LMG	c	519	-	-	10/31/51/70	0/1/1/1
22	CLA	C	509	-	1/1/20/20	9/37/115/115	-
34	STE	b	625	-	-	4/11/13/17	-
22	CLA	b	614	-	1/1/20/20	20/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMG	b	622	-	-	24/46/66/70	0/1/1/1
31	DGD	C	515	-	-	22/51/91/95	0/2/2/2
30	LHG	e	102	-	-	25/46/46/53	-
27	PL9	A	410	-	-	22/53/73/73	0/1/1/1
22	CLA	b	601	37	1/1/20/20	17/37/115/115	-
34	STE	Z	101	-	-	3/5/5/17	-
34	STE	h	102	-	-	5/11/11/17	-
22	CLA	C	510	-	1/1/20/20	9/37/115/115	-
24	BCR	b	617	-	-	5/29/63/63	0/2/2/2
27	PL9	d	406	-	-	14/53/73/73	0/1/1/1
31	DGD	c	517	-	-	20/51/91/95	0/2/2/2
28	LMG	d	410	-	-	12/39/59/70	0/1/1/1
30	LHG	B	621	-	-	26/53/53/53	-
34	STE	a	413	-	-	3/7/7/17	-
22	CLA	b	616	-	1/1/19/20	13/31/109/115	-
24	BCR	b	618	-	-	1/29/63/63	0/2/2/2
34	STE	b	626	-	-	4/15/17/17	-
34	STE	c	520	-	-	9/15/17/17	-
22	CLA	c	505	-	1/1/20/20	7/37/115/115	-
24	BCR	B	619	-	-	4/29/63/63	0/2/2/2
29	SQD	D	407	-	-	10/28/48/69	0/1/1/1
22	CLA	A	411	37	-	11/37/115/115	-
31	DGD	A	416	-	-	24/55/95/95	0/2/2/2
31	DGD	C	517	-	-	15/51/91/95	0/2/2/2
22	CLA	c	509	-	1/1/20/20	10/37/115/115	-
30	LHG	B	622	-	-	22/53/53/53	-
22	CLA	B	602	-	-	6/37/115/115	-
24	BCR	K	101	-	-	14/29/63/63	0/2/2/2
34	STE	C	520	-	-	5/13/13/17	-
22	CLA	C	507	37	1/1/20/20	6/37/115/115	-
34	STE	X	101	-	-	9/15/17/17	-
34	STE	M	103	-	-	1/7/7/17	-
22	CLA	C	506	-	1/1/20/20	12/37/115/115	-
30	LHG	d	408	-	-	22/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMG	b	624	-	-	29/50/70/70	0/1/1/1
22	CLA	c	513	-	1/1/20/20	9/37/115/115	-
22	CLA	C	511	3	1/1/20/20	12/37/115/115	-
22	CLA	D	403	-	-	10/37/115/115	-
34	STE	M	102	-	-	4/10/12/17	-
22	CLA	c	510	-	1/1/20/20	12/37/115/115	-
22	CLA	B	607	37	1/1/20/20	10/37/115/115	-
22	CLA	d	404	-	1/1/20/20	9/37/115/115	-
22	CLA	c	511	3	1/1/20/20	13/37/115/115	-
22	CLA	b	610	37	1/1/20/20	7/37/115/115	-
23	PHO	d	402	-	-	9/53/103/103	0/5/6/6
22	CLA	b	603	-	1/1/20/20	7/37/115/115	-
22	CLA	B	615	-	1/1/20/20	8/37/115/115	-
34	STE	B	627	-	-	5/7/9/17	-
22	CLA	C	512	-	1/1/20/20	15/37/115/115	-
31	DGD	C	516	-	-	20/51/91/95	0/2/2/2
34	STE	j	101	-	-	4/7/9/17	-
34	STE	a	415	-	-	7/12/12/17	-
34	STE	I	101	-	-	6/12/12/17	-
22	CLA	b	612	-	1/1/20/20	6/37/115/115	-
34	STE	d	412	-	-	10/15/17/17	-
24	BCR	x	101	-	-	6/29/63/63	0/2/2/2
22	CLA	a	404	-	1/1/20/20	8/37/115/115	-
31	DGD	H	102	-	-	18/51/91/95	0/2/2/2
24	BCR	b	619	-	-	3/29/63/63	0/2/2/2
30	LHG	d	407	-	-	22/53/53/53	-
34	STE	R	101	-	-	4/7/9/17	-
22	CLA	C	502	-	1/1/20/20	6/37/115/115	-
29	SQD	A	415	-	-	11/39/39/69	-
24	BCR	k	101	-	-	9/29/63/63	0/2/2/2
22	CLA	B	613	-	1/1/20/20	12/37/115/115	-
22	CLA	B	604	-	1/1/20/20	10/37/115/115	-
24	BCR	B	617	-	-	7/29/63/63	0/2/2/2
22	CLA	B	606	-	1/1/20/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	507	37	1/1/20/20	8/37/115/115	-
29	SQD	B	623	-	-	24/49/69/69	0/1/1/1
22	CLA	b	609	-	-	4/37/115/115	-
22	CLA	B	603	-	1/1/20/20	12/37/115/115	-

All (792) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	606	CLA	MG-NA	8.45	2.26	2.06
22	C	511	CLA	MG-NA	8.43	2.26	2.06
22	B	613	CLA	C4B-NB	8.39	1.42	1.35
22	B	614	CLA	C4B-NB	8.14	1.42	1.35
22	a	410	CLA	MG-NA	7.99	2.25	2.06
22	b	614	CLA	C4B-NB	7.87	1.42	1.35
22	c	504	CLA	C4B-NB	7.74	1.42	1.35
22	C	513	CLA	C4B-NB	7.74	1.42	1.35
22	C	504	CLA	C4B-NB	7.55	1.41	1.35
22	c	502	CLA	C4B-NB	7.47	1.41	1.35
36	v	201	HEC	C3B-C2B	-7.47	1.33	1.40
22	c	512	CLA	C4B-NB	7.43	1.41	1.35
22	b	609	CLA	C4B-NB	7.33	1.41	1.35
22	B	612	CLA	C4B-NB	7.29	1.41	1.35
22	A	402	CLA	C4B-NB	7.28	1.41	1.35
22	B	601	CLA	C4B-NB	7.28	1.41	1.35
22	B	616	CLA	C4C-NC	7.22	1.41	1.35
22	A	405	CLA	C4B-NB	7.21	1.41	1.35
22	a	410	CLA	C4B-NB	7.20	1.41	1.35
22	c	502	CLA	C4C-NC	7.17	1.41	1.35
22	C	501	CLA	C4B-NB	7.15	1.41	1.35
22	a	403	CLA	C4B-NB	7.14	1.41	1.35
22	c	509	CLA	C4B-NB	7.11	1.41	1.35
22	B	615	CLA	C4B-NB	7.08	1.41	1.35
22	B	610	CLA	C4B-NB	7.07	1.41	1.35
22	C	505	CLA	C4B-NB	7.07	1.41	1.35
22	C	508	CLA	C4B-NB	7.07	1.41	1.35
22	C	507	CLA	C4B-NB	7.01	1.41	1.35
22	C	506	CLA	C4B-NB	7.00	1.41	1.35
22	b	602	CLA	C4B-NB	6.96	1.41	1.35
22	d	404	CLA	C4B-NB	6.89	1.41	1.35
22	b	608	CLA	C4B-NB	6.89	1.41	1.35
22	d	403	CLA	C4B-NB	6.88	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	608	CLA	C4C-NC	6.84	1.41	1.35
22	C	510	CLA	C4B-NB	6.80	1.41	1.35
22	C	511	CLA	C4B-NB	6.80	1.41	1.35
22	B	610	CLA	C4C-NC	6.79	1.41	1.35
22	c	513	CLA	C4B-NB	6.78	1.41	1.35
22	C	502	CLA	C4C-NC	6.75	1.41	1.35
22	B	604	CLA	MG-NA	6.75	2.22	2.06
22	c	501	CLA	C4B-NB	6.74	1.41	1.35
22	c	503	CLA	C4B-NB	6.74	1.41	1.35
22	B	609	CLA	C4C-NC	6.70	1.41	1.35
22	D	402	CLA	C4B-NB	6.69	1.41	1.35
22	B	602	CLA	C4B-NB	6.68	1.41	1.35
22	C	503	CLA	C4B-NB	6.61	1.41	1.35
22	B	612	CLA	C4C-NC	6.59	1.41	1.35
22	b	604	CLA	C4B-NB	6.59	1.41	1.35
22	C	503	CLA	MG-NA	6.54	2.21	2.06
35	e	101	HEM	C3B-C2B	-6.54	1.31	1.40
22	C	507	CLA	MG-NA	6.49	2.21	2.06
22	C	503	CLA	C4C-NC	6.48	1.41	1.35
22	B	607	CLA	C4B-NB	6.41	1.40	1.35
22	a	402	CLA	C4C-NC	6.37	1.40	1.35
22	a	404	CLA	C4C-NC	6.34	1.40	1.35
27	A	410	PL9	C7-C3	-6.33	1.44	1.51
22	B	603	CLA	C4C-NC	6.31	1.40	1.35
22	C	505	CLA	C4C-NC	6.31	1.40	1.35
22	A	403	CLA	C4B-NB	6.29	1.40	1.35
22	B	609	CLA	C4B-NB	6.27	1.40	1.35
22	b	611	CLA	C4C-NC	6.26	1.40	1.35
22	b	601	CLA	C4B-NB	6.26	1.40	1.35
22	d	404	CLA	C4C-NC	6.21	1.40	1.35
22	c	501	CLA	C4C-NC	6.18	1.40	1.35
22	c	511	CLA	C4B-NB	6.16	1.40	1.35
22	B	602	CLA	C4C-NC	6.14	1.40	1.35
22	c	508	CLA	C4C-NC	6.14	1.40	1.35
22	B	606	CLA	C4C-NC	6.08	1.40	1.35
22	b	605	CLA	C4B-NB	6.07	1.40	1.35
22	A	411	CLA	C4B-NB	6.07	1.40	1.35
22	C	512	CLA	C4B-NB	6.04	1.40	1.35
27	d	406	PL9	C6-C1	-6.04	1.37	1.48
22	B	611	CLA	C4C-NC	6.00	1.40	1.35
22	c	508	CLA	C4B-NB	5.99	1.40	1.35
22	b	614	CLA	C4C-NC	5.97	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	511	CLA	C4C-NC	5.95	1.40	1.35
22	b	613	CLA	C4B-NB	5.94	1.40	1.35
22	a	404	CLA	C4B-NB	5.93	1.40	1.35
22	C	510	CLA	C4C-NC	5.89	1.40	1.35
22	b	615	CLA	C4B-NB	5.87	1.40	1.35
22	c	510	CLA	C4C-NC	5.85	1.40	1.35
22	D	403	CLA	C4B-NB	5.84	1.40	1.35
22	c	506	CLA	C4B-NB	5.82	1.40	1.35
22	b	611	CLA	C4B-NB	5.82	1.40	1.35
22	B	606	CLA	C4B-NB	5.78	1.40	1.35
22	B	615	CLA	C4C-NC	5.77	1.40	1.35
22	c	510	CLA	C4B-NB	5.72	1.40	1.35
36	V	201	HEC	C3B-C2B	-5.67	1.34	1.40
36	V	201	HEC	C3C-C2C	-5.66	1.34	1.40
22	B	603	CLA	MG-NA	5.61	2.19	2.06
22	a	402	CLA	C4B-NB	5.60	1.40	1.35
22	B	616	CLA	MG-NA	5.58	2.19	2.06
22	C	509	CLA	C4B-NB	5.57	1.40	1.35
22	b	610	CLA	C4C-NC	5.57	1.40	1.35
22	c	512	CLA	C4C-NC	5.56	1.40	1.35
22	b	613	CLA	C4C-NC	5.53	1.40	1.35
22	b	606	CLA	C4B-NB	5.52	1.40	1.35
22	b	603	CLA	MG-NA	5.50	2.19	2.06
22	B	606	CLA	MG-NA	5.49	2.19	2.06
22	b	615	CLA	C4C-NC	5.48	1.40	1.35
22	A	403	CLA	C4C-NC	5.48	1.40	1.35
22	c	505	CLA	C4B-NB	5.48	1.40	1.35
22	b	615	CLA	MG-NA	5.44	2.19	2.06
22	b	612	CLA	C4B-NB	5.42	1.40	1.35
22	b	601	CLA	C4C-NC	5.40	1.40	1.35
22	c	513	CLA	C4C-NC	5.35	1.40	1.35
22	b	601	CLA	MG-NA	5.31	2.18	2.06
22	b	607	CLA	C4B-NB	5.31	1.39	1.35
22	D	403	CLA	C4C-NC	5.30	1.39	1.35
22	b	603	CLA	C4B-NB	5.30	1.39	1.35
22	B	607	CLA	C4C-NC	5.27	1.39	1.35
27	D	405	PL9	C7-C3	-5.27	1.45	1.51
22	C	506	CLA	C4C-NC	5.22	1.39	1.35
22	C	512	CLA	C4C-NC	5.18	1.39	1.35
22	B	605	CLA	C4B-NB	5.16	1.39	1.35
22	c	507	CLA	C4B-NB	5.15	1.39	1.35
35	F	101	HEM	C3B-C2B	-5.14	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	605	CLA	C4C-NC	5.13	1.39	1.35
22	B	608	CLA	C4B-NB	5.12	1.39	1.35
22	c	510	CLA	MG-NA	5.08	2.18	2.06
36	v	201	HEC	C3C-C2C	-5.07	1.35	1.40
35	F	101	HEM	C3C-C2C	-5.05	1.33	1.40
22	a	410	CLA	C4C-NC	5.03	1.39	1.35
22	B	611	CLA	MG-NA	5.02	2.18	2.06
22	a	403	CLA	C4C-NC	5.00	1.39	1.35
22	C	513	CLA	C4C-NC	4.99	1.39	1.35
22	a	404	CLA	MG-NA	4.95	2.18	2.06
22	b	605	CLA	C4C-NC	4.91	1.39	1.35
22	B	614	CLA	C4C-NC	4.90	1.39	1.35
22	b	610	CLA	C4B-NB	4.90	1.39	1.35
22	C	501	CLA	MG-NA	4.90	2.17	2.06
22	C	501	CLA	C4C-NC	4.88	1.39	1.35
22	C	509	CLA	C4C-NC	4.85	1.39	1.35
36	v	201	HEC	C3D-C2D	4.81	1.51	1.37
22	c	503	CLA	C4C-NC	4.80	1.39	1.35
22	B	611	CLA	C4B-NB	4.79	1.39	1.35
22	C	502	CLA	C4B-NB	4.77	1.39	1.35
27	D	405	PL9	C6-C1	-4.75	1.40	1.48
28	a	416	LMG	C4-C5	4.74	1.63	1.53
22	C	508	CLA	C4C-NC	4.73	1.39	1.35
22	b	616	CLA	C4C-NC	4.72	1.39	1.35
22	c	508	CLA	MG-NA	4.72	2.17	2.06
22	c	511	CLA	MG-NA	4.72	2.17	2.06
22	c	509	CLA	C4C-NC	4.70	1.39	1.35
22	A	402	CLA	C4C-NC	4.70	1.39	1.35
22	b	602	CLA	C4C-NC	4.70	1.39	1.35
22	b	612	CLA	C4C-NC	4.68	1.39	1.35
22	A	411	CLA	C4C-NC	4.68	1.39	1.35
22	B	608	CLA	C4C-NC	4.68	1.39	1.35
22	c	506	CLA	C4C-NC	4.68	1.39	1.35
22	b	613	CLA	MG-NA	4.67	2.17	2.06
36	V	201	HEC	C3D-C2D	4.65	1.51	1.37
22	b	607	CLA	MG-NA	4.62	2.17	2.06
22	C	513	CLA	MG-NA	4.53	2.17	2.06
22	B	616	CLA	C4B-NB	4.51	1.39	1.35
22	C	505	CLA	MG-NA	4.46	2.16	2.06
22	B	604	CLA	C4B-NB	4.43	1.39	1.35
27	d	406	PL9	C3-C4	-4.42	1.42	1.49
22	B	601	CLA	C4C-NC	4.42	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	H	101	BCR	C30-C25	-4.33	1.47	1.53
24	C	514	BCR	C1-C6	-4.28	1.47	1.53
22	b	609	CLA	C4C-NC	4.27	1.39	1.35
22	C	504	CLA	C4C-NC	4.26	1.39	1.35
22	b	606	CLA	C1B-NB	4.24	1.39	1.35
31	A	416	DGD	C4E-C5E	4.23	1.61	1.53
22	d	403	CLA	MG-NA	4.23	2.16	2.06
22	a	402	CLA	MG-NA	4.21	2.16	2.06
24	Y	101	BCR	C30-C25	-4.21	1.48	1.53
30	B	621	LHG	O7-C5	-4.20	1.36	1.46
22	c	511	CLA	C4C-NC	4.19	1.38	1.35
22	c	505	CLA	C4C-NC	4.18	1.38	1.35
22	C	508	CLA	MG-NA	4.17	2.16	2.06
22	B	603	CLA	C4B-NB	4.08	1.38	1.35
22	b	604	CLA	C4C-NC	4.07	1.38	1.35
22	B	606	CLA	C3B-C2B	-4.07	1.34	1.40
31	c	516	DGD	C4D-C3D	4.02	1.62	1.52
22	C	506	CLA	MG-NA	3.98	2.15	2.06
24	b	618	BCR	C30-C25	-3.94	1.48	1.53
22	A	405	CLA	C4C-NC	3.93	1.38	1.35
24	D	404	BCR	C30-C25	-3.92	1.48	1.53
22	b	603	CLA	C4C-NC	3.92	1.38	1.35
22	B	610	CLA	C3B-C2B	-3.88	1.35	1.40
24	b	617	BCR	C1-C6	-3.83	1.48	1.53
29	a	411	SQD	O48-C23	3.79	1.44	1.33
27	D	405	PL9	C52-C5	-3.76	1.42	1.50
22	b	610	CLA	C3B-C2B	-3.76	1.35	1.40
28	C	518	LMG	C4-C5	3.74	1.60	1.53
27	D	405	PL9	C11-C9	-3.73	1.43	1.51
27	D	405	PL9	C41-C39	-3.72	1.43	1.51
35	e	101	HEM	C3C-C2C	-3.72	1.35	1.40
30	D	408	LHG	O8-C6	-3.71	1.36	1.45
22	A	411	CLA	MG-NA	3.69	2.15	2.06
24	d	405	BCR	C1-C6	-3.68	1.48	1.53
22	c	502	CLA	MG-NA	3.66	2.15	2.06
31	C	516	DGD	C4D-C3D	3.66	1.61	1.52
22	c	504	CLA	C4C-NC	3.65	1.38	1.35
31	H	102	DGD	C4E-C5E	3.64	1.60	1.53
24	B	617	BCR	C1-C6	-3.64	1.48	1.53
27	a	409	PL9	C3-C4	-3.63	1.43	1.49
24	B	618	BCR	C30-C25	-3.62	1.48	1.53
29	B	623	SQD	O47-C7	3.58	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	512	CLA	MG-NA	3.57	2.14	2.06
24	B	617	BCR	C30-C25	-3.56	1.48	1.53
24	c	514	BCR	C1-C6	-3.56	1.48	1.53
24	x	101	BCR	C30-C25	-3.54	1.48	1.53
28	A	412	LMG	O1-C7	-3.49	1.37	1.43
27	d	406	PL9	C46-C44	-3.49	1.44	1.51
27	d	406	PL9	C53-C6	-3.49	1.43	1.50
24	b	619	BCR	C30-C25	-3.48	1.49	1.53
29	a	412	SQD	O47-C7	3.46	1.44	1.34
30	d	408	LHG	O7-C5	-3.45	1.37	1.46
28	a	416	LMG	C4-C3	3.45	1.61	1.52
24	c	515	BCR	C1-C6	-3.45	1.49	1.53
22	b	616	CLA	C3B-CAB	-3.43	1.40	1.47
24	d	405	BCR	C30-C25	-3.43	1.49	1.53
35	e	101	HEM	C3C-CAC	3.43	1.54	1.47
29	a	412	SQD	O48-C23	3.43	1.43	1.33
31	C	516	DGD	O3E-C3E	-3.38	1.35	1.43
22	D	403	CLA	MG-NA	3.38	2.14	2.06
29	A	415	SQD	O48-C23	3.37	1.43	1.33
24	K	101	BCR	C30-C25	-3.36	1.49	1.53
24	k	101	BCR	C30-C25	-3.36	1.49	1.53
22	b	609	CLA	MG-NA	3.35	2.14	2.06
22	C	508	CLA	C1D-C2D	3.35	1.50	1.42
24	Y	101	BCR	C1-C6	-3.35	1.49	1.53
27	a	409	PL9	C6-C1	-3.35	1.42	1.48
28	d	410	LMG	O1-C7	-3.34	1.37	1.43
31	C	515	DGD	C4D-C3D	3.34	1.60	1.52
24	A	406	BCR	C1-C6	-3.31	1.49	1.53
24	c	514	BCR	C30-C25	-3.31	1.49	1.53
22	d	403	CLA	C4C-NC	3.31	1.38	1.35
24	T	101	BCR	C30-C25	-3.30	1.49	1.53
22	b	609	CLA	CMB-C2B	-3.30	1.44	1.51
22	c	507	CLA	C4C-NC	3.29	1.38	1.35
22	B	613	CLA	MG-NA	3.29	2.14	2.06
30	d	407	LHG	O7-C5	-3.28	1.38	1.46
24	B	619	BCR	C30-C25	-3.28	1.49	1.53
22	B	601	CLA	C3B-C2B	-3.27	1.35	1.40
28	c	522	LMG	O7-C8	-3.26	1.38	1.46
28	d	410	LMG	O7-C8	-3.24	1.38	1.46
28	c	521	LMG	O1-C1	3.23	1.45	1.40
23	d	402	PHO	C3B-C4B	3.21	1.49	1.43
31	A	416	DGD	C3G-C2G	3.20	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	609	CLA	C3B-C2B	-3.20	1.35	1.40
35	F	101	HEM	C3B-CAB	3.20	1.54	1.47
22	B	601	CLA	MG-NA	3.19	2.13	2.06
22	c	510	CLA	CMB-C2B	-3.19	1.45	1.51
24	B	619	BCR	C1-C6	-3.18	1.49	1.53
22	C	504	CLA	MG-NA	3.18	2.13	2.06
31	C	515	DGD	O2E-C2E	-3.18	1.35	1.43
28	a	416	LMG	O8-C9	-3.17	1.37	1.45
23	D	401	PHO	C3B-C4B	3.17	1.49	1.43
22	c	502	CLA	CMD-C2D	-3.16	1.44	1.51
22	B	602	CLA	C1D-C2D	3.16	1.49	1.42
22	a	410	CLA	CMB-C2B	-3.16	1.45	1.51
35	e	101	HEM	C3B-CAB	3.16	1.54	1.47
31	c	518	DGD	O2G-C2G	-3.15	1.38	1.46
31	A	416	DGD	C4D-C3D	3.15	1.60	1.52
24	b	618	BCR	C1-C6	-3.14	1.49	1.53
29	D	407	SQD	O48-C23	3.14	1.42	1.33
24	K	101	BCR	C1-C6	-3.12	1.49	1.53
23	d	401	PHO	C4C-C3C	3.11	1.50	1.45
22	d	404	CLA	CMD-C2D	-3.11	1.44	1.51
22	C	511	CLA	CMB-C2B	-3.10	1.45	1.51
24	b	619	BCR	C1-C6	-3.10	1.49	1.53
31	H	102	DGD	O5D-C1E	3.09	1.45	1.40
22	B	604	CLA	C4C-NC	3.09	1.38	1.35
22	C	503	CLA	C1D-C2D	3.09	1.49	1.42
22	C	502	CLA	MG-NA	3.07	2.13	2.06
29	b	620	SQD	O47-C7	3.07	1.43	1.34
30	D	409	LHG	P-O6	3.04	1.71	1.59
22	B	610	CLA	CMB-C2B	-3.03	1.45	1.51
22	B	603	CLA	C3B-CAB	-3.03	1.41	1.47
29	b	620	SQD	O48-C23	3.03	1.42	1.33
30	e	102	LHG	P-O6	3.02	1.71	1.59
29	A	415	SQD	O47-C7	3.02	1.42	1.34
22	B	609	CLA	C3B-CAB	-3.01	1.41	1.47
22	b	616	CLA	C4B-NB	3.00	1.37	1.35
27	d	406	PL9	C11-C9	-3.00	1.45	1.51
22	C	501	CLA	C3B-C2B	-3.00	1.36	1.40
22	c	512	CLA	CMB-C2B	-2.99	1.45	1.51
30	D	408	LHG	O7-C5	-2.98	1.39	1.46
28	c	521	LMG	C3-C2	2.97	1.59	1.52
24	C	514	BCR	C30-C25	-2.97	1.49	1.53
29	f	101	SQD	O48-C23	2.96	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	d	406	PL9	C16-C14	-2.96	1.45	1.51
22	c	507	CLA	C3B-C2B	-2.96	1.36	1.40
24	K	102	BCR	C30-C25	-2.95	1.49	1.53
22	c	505	CLA	C1B-NB	2.95	1.37	1.35
30	B	622	LHG	O7-C5	-2.95	1.39	1.46
35	F	101	HEM	C3C-CAC	2.94	1.53	1.47
23	A	404	PHO	C4C-NC	2.93	1.43	1.36
22	b	602	CLA	CAC-C3C	-2.93	1.44	1.52
22	B	616	CLA	C3B-CAB	-2.93	1.42	1.47
22	b	615	CLA	CMD-C2D	-2.93	1.44	1.51
22	c	504	CLA	CAC-C3C	-2.93	1.44	1.52
28	c	519	LMG	O1-C1	2.93	1.45	1.40
22	d	403	CLA	CMB-C2B	-2.93	1.45	1.51
22	B	608	CLA	CMD-C2D	-2.92	1.44	1.51
23	D	401	PHO	CMB-C2B	-2.92	1.44	1.50
22	B	613	CLA	C4C-NC	2.92	1.37	1.35
29	f	101	SQD	O47-C7	2.91	1.42	1.34
28	b	624	LMG	C3-C2	2.91	1.59	1.52
28	D	410	LMG	C7-C8	2.91	1.58	1.51
22	B	603	CLA	C1D-C2D	2.90	1.49	1.42
29	a	411	SQD	O47-C7	2.90	1.42	1.34
22	b	609	CLA	C3B-C2B	-2.90	1.36	1.40
22	a	402	CLA	CMB-C2B	-2.90	1.45	1.51
28	c	519	LMG	C1-C2	2.90	1.60	1.52
22	B	616	CLA	CMC-C2C	-2.90	1.44	1.51
24	k	102	BCR	C30-C25	-2.89	1.49	1.53
22	b	601	CLA	C1D-C2D	2.89	1.49	1.42
28	M	101	LMG	O4-C4	-2.89	1.36	1.43
22	b	609	CLA	CAC-C3C	-2.89	1.45	1.52
24	c	515	BCR	C30-C25	-2.88	1.49	1.53
22	B	611	CLA	CMB-C2B	-2.88	1.45	1.51
22	C	512	CLA	CMB-C2B	-2.88	1.45	1.51
22	c	513	CLA	CMB-C2B	-2.88	1.45	1.51
22	B	605	CLA	C3B-C2B	-2.87	1.36	1.40
22	B	607	CLA	CMB-C2B	-2.86	1.45	1.51
28	A	412	LMG	C4-C3	2.86	1.59	1.52
24	b	617	BCR	C30-C25	-2.85	1.49	1.53
31	C	516	DGD	O5D-C6D	-2.85	1.38	1.43
29	B	623	SQD	O48-C23	2.85	1.41	1.33
22	b	613	CLA	CMD-C2D	-2.85	1.44	1.51
22	c	512	CLA	C3B-C2B	-2.85	1.36	1.40
22	b	609	CLA	C3B-CAB	-2.84	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	512	CLA	C1D-C2D	2.84	1.49	1.42
22	B	609	CLA	CMD-C2D	-2.84	1.44	1.51
24	k	101	BCR	C1-C6	-2.83	1.49	1.53
30	d	408	LHG	O8-C6	-2.83	1.38	1.45
31	c	516	DGD	O3G-C1D	-2.83	1.35	1.40
22	B	601	CLA	C1D-C2D	2.83	1.49	1.42
22	c	506	CLA	CMD-C2D	-2.82	1.44	1.51
31	C	516	DGD	C1E-C2E	2.82	1.60	1.52
22	a	404	CLA	CMC-C2C	-2.82	1.44	1.51
28	c	519	LMG	C3-C2	2.82	1.59	1.52
22	d	404	CLA	CMB-C2B	-2.82	1.45	1.51
22	B	602	CLA	CMB-C2B	-2.82	1.45	1.51
28	C	518	LMG	O8-C9	-2.81	1.38	1.45
22	b	605	CLA	CMD-C2D	-2.81	1.44	1.51
23	A	404	PHO	C1A-NA	2.81	1.43	1.37
22	c	505	CLA	CMB-C2B	-2.80	1.45	1.51
24	t	101	BCR	C30-C25	-2.80	1.49	1.53
22	c	509	CLA	CMB-C2B	-2.80	1.45	1.51
29	A	413	SQD	O2-C2	-2.80	1.36	1.43
28	b	624	LMG	O1-C7	-2.79	1.38	1.43
22	b	614	CLA	CMC-C2C	-2.78	1.44	1.51
23	d	402	PHO	CHC-C1C	2.78	1.44	1.38
22	C	503	CLA	CMD-C2D	-2.77	1.45	1.51
22	C	513	CLA	CMB-C2B	-2.77	1.45	1.51
22	B	606	CLA	CMD-C2D	-2.77	1.45	1.51
30	D	409	LHG	C8-C7	-2.77	1.42	1.50
22	a	404	CLA	CAC-C3C	-2.77	1.45	1.52
31	C	516	DGD	C6E-C5E	2.76	1.61	1.51
22	B	607	CLA	MG-NA	2.76	2.12	2.06
31	c	517	DGD	O2G-C2G	-2.76	1.39	1.46
22	B	608	CLA	C1D-C2D	2.76	1.48	1.42
22	C	501	CLA	C1D-C2D	2.76	1.48	1.42
22	c	511	CLA	C1D-C2D	2.75	1.48	1.42
22	b	603	CLA	C1D-C2D	2.74	1.48	1.42
22	b	606	CLA	C4C-NC	2.74	1.37	1.35
30	B	621	LHG	O8-C6	-2.74	1.38	1.45
27	D	405	PL9	C36-C34	-2.74	1.45	1.51
24	a	405	BCR	C1-C6	-2.73	1.50	1.53
27	A	410	PL9	C31-C29	-2.73	1.45	1.51
22	c	501	CLA	CAC-C3C	-2.73	1.45	1.52
27	a	409	PL9	C53-C6	-2.73	1.45	1.50
23	A	404	PHO	CMC-C2C	-2.72	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	612	CLA	CMB-C2B	-2.70	1.46	1.51
22	C	508	CLA	CMB-C2B	-2.70	1.46	1.51
22	b	612	CLA	CMC-C2C	-2.70	1.45	1.51
27	D	405	PL9	C53-C6	-2.69	1.45	1.50
24	K	102	BCR	C1-C6	-2.69	1.50	1.53
30	e	102	LHG	O8-C23	2.69	1.41	1.33
31	c	518	DGD	O3D-C3D	-2.69	1.36	1.43
22	A	405	CLA	CMB-C2B	-2.69	1.46	1.51
31	h	101	DGD	C4D-C3D	2.68	1.59	1.52
22	c	506	CLA	CAC-C3C	-2.68	1.45	1.52
22	A	411	CLA	C1D-C2D	2.68	1.48	1.42
22	b	615	CLA	C3B-C2B	-2.68	1.36	1.40
22	b	613	CLA	CMB-C2B	-2.68	1.46	1.51
23	D	401	PHO	CHC-C1C	2.68	1.43	1.38
22	C	504	CLA	CMB-C2B	-2.67	1.46	1.51
22	c	506	CLA	C1D-C2D	2.67	1.48	1.42
22	C	510	CLA	CMC-C2C	-2.67	1.45	1.51
22	b	608	CLA	CMB-C2B	-2.67	1.46	1.51
28	c	519	LMG	C7-C8	2.66	1.58	1.50
23	A	404	PHO	C1C-NC	-2.66	1.32	1.38
22	C	512	CLA	C3B-C2B	-2.65	1.36	1.40
30	A	414	LHG	C24-C23	2.65	1.58	1.50
31	A	416	DGD	C4D-C5D	2.65	1.58	1.53
28	C	518	LMG	O7-C8	-2.65	1.40	1.46
31	h	101	DGD	C4E-C5E	2.65	1.58	1.53
28	b	622	LMG	C4-C3	2.64	1.59	1.52
22	A	411	CLA	CAC-C3C	-2.64	1.45	1.52
31	h	101	DGD	O2D-C2D	-2.64	1.36	1.43
22	c	513	CLA	C1D-C2D	2.64	1.48	1.42
22	b	616	CLA	CMB-C2B	-2.63	1.46	1.51
22	b	616	CLA	C1D-C2D	2.62	1.48	1.42
27	A	410	PL9	C3-C4	-2.62	1.45	1.49
22	b	605	CLA	C1D-C2D	2.62	1.48	1.42
22	b	608	CLA	C1D-C2D	2.62	1.48	1.42
22	C	503	CLA	CMB-C2B	-2.62	1.46	1.51
27	D	405	PL9	C46-C44	-2.62	1.45	1.51
22	a	410	CLA	C1D-C2D	2.61	1.48	1.42
24	T	101	BCR	C1-C6	-2.61	1.50	1.53
28	c	522	LMG	O1-C7	-2.61	1.39	1.43
24	D	404	BCR	C1-C6	-2.61	1.50	1.53
22	B	615	CLA	CAC-C3C	-2.61	1.45	1.52
29	A	415	SQD	O47-C45	-2.61	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	607	CLA	C3B-CAB	-2.61	1.42	1.47
28	b	622	LMG	C4-C5	2.60	1.58	1.53
22	B	613	CLA	CMB-C2B	-2.60	1.46	1.51
22	B	613	CLA	CMD-C2D	-2.60	1.45	1.51
22	A	405	CLA	CMD-C2D	-2.59	1.45	1.51
22	B	605	CLA	CMD-C2D	-2.59	1.45	1.51
31	c	516	DGD	O6E-C5E	-2.59	1.38	1.44
22	b	606	CLA	CAC-C3C	-2.59	1.45	1.52
22	B	611	CLA	C3B-C2B	-2.58	1.36	1.40
28	c	519	LMG	C4-C5	2.58	1.58	1.53
22	A	411	CLA	CMD-C2D	-2.58	1.45	1.51
22	C	505	CLA	CMC-C2C	-2.58	1.45	1.51
31	c	517	DGD	O3G-C3G	-2.57	1.39	1.43
22	C	502	CLA	CMB-C2B	-2.57	1.46	1.51
22	B	609	CLA	MG-NA	2.57	2.12	2.06
31	c	518	DGD	C6D-C5D	2.57	1.59	1.51
22	C	507	CLA	C1D-C2D	2.57	1.48	1.42
31	A	416	DGD	C1E-C2E	2.57	1.59	1.52
22	b	612	CLA	CMD-C2D	-2.56	1.45	1.51
22	c	504	CLA	MG-NA	-2.56	2.00	2.06
29	B	623	SQD	O2-C2	-2.56	1.36	1.43
23	d	402	PHO	CHC-C4B	-2.56	1.34	1.40
22	B	610	CLA	CMC-C2C	-2.55	1.45	1.51
22	B	615	CLA	MG-NA	2.55	2.12	2.06
22	C	510	CLA	CMB-C2B	-2.55	1.46	1.51
23	A	404	PHO	CHC-C1C	2.55	1.43	1.38
22	d	403	CLA	C1D-C2D	2.55	1.48	1.42
22	C	506	CLA	C1D-C2D	2.55	1.48	1.42
22	B	615	CLA	CMB-C2B	-2.55	1.46	1.51
23	d	401	PHO	C4C-NC	2.55	1.42	1.36
22	b	610	CLA	CMB-C2B	-2.55	1.46	1.51
22	A	402	CLA	O2D-CED	-2.55	1.39	1.45
24	C	514	BCR	C36-C18	-2.54	1.45	1.50
22	b	609	CLA	C1D-C2D	2.54	1.48	1.42
31	c	516	DGD	O4D-C4D	-2.54	1.37	1.43
22	d	403	CLA	CMD-C2D	-2.54	1.45	1.51
23	A	404	PHO	C3B-C4B	2.54	1.48	1.43
22	b	608	CLA	C3B-C2B	-2.54	1.36	1.40
22	C	509	CLA	CMC-C2C	-2.54	1.45	1.51
27	D	405	PL9	C3-C4	-2.54	1.45	1.49
22	b	602	CLA	CMB-C2B	-2.54	1.46	1.51
29	f	101	SQD	O3-C3	-2.54	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	604	CLA	CMC-C2C	-2.53	1.45	1.51
30	A	414	LHG	P-O6	2.53	1.69	1.59
22	a	402	CLA	C1D-C2D	2.53	1.48	1.42
22	b	604	CLA	C1D-C2D	2.53	1.48	1.42
22	A	411	CLA	CMB-C2B	-2.53	1.46	1.51
22	b	603	CLA	CMD-C2D	-2.52	1.45	1.51
23	d	402	PHO	C4C-C3C	2.52	1.49	1.45
29	A	413	SQD	O48-C23	2.51	1.40	1.33
31	h	101	DGD	O2G-C1B	2.51	1.41	1.34
22	c	506	CLA	CMB-C2B	-2.51	1.46	1.51
31	C	517	DGD	O2G-C2G	-2.51	1.40	1.46
23	d	401	PHO	C3B-C4B	2.51	1.48	1.43
22	A	402	CLA	C1D-C2D	2.51	1.48	1.42
24	T	101	BCR	C27-C26	-2.50	1.46	1.51
22	b	616	CLA	C3B-C2B	-2.50	1.36	1.40
29	A	413	SQD	O47-C7	2.50	1.41	1.34
22	a	403	CLA	C3B-CAB	-2.50	1.42	1.47
29	f	101	SQD	O2-C2	-2.49	1.37	1.43
22	B	606	CLA	C3B-CAB	-2.49	1.42	1.47
24	b	618	BCR	C38-C26	-2.49	1.46	1.50
31	A	416	DGD	O2G-C1B	2.49	1.41	1.34
28	D	410	LMG	C9-C8	2.49	1.58	1.50
23	d	402	PHO	C1C-NC	-2.49	1.33	1.38
22	b	606	CLA	C3B-C2B	-2.49	1.36	1.40
22	B	601	CLA	CMB-C2B	-2.49	1.46	1.51
22	b	606	CLA	CMD-C2D	-2.49	1.45	1.51
22	b	605	CLA	C3B-C2B	-2.49	1.36	1.40
22	c	503	CLA	C1D-C2D	2.48	1.48	1.42
22	c	503	CLA	CMC-C2C	-2.48	1.45	1.51
28	c	521	LMG	C4-C3	2.48	1.58	1.52
22	C	513	CLA	C1D-C2D	2.48	1.48	1.42
22	b	604	CLA	CMB-C2B	-2.47	1.46	1.51
28	M	101	LMG	C4-C5	2.47	1.58	1.53
22	C	512	CLA	CMD-C2D	-2.46	1.45	1.51
22	C	508	CLA	CMD-C2D	-2.46	1.45	1.51
22	c	503	CLA	C3B-C2B	-2.46	1.37	1.40
31	H	102	DGD	C6E-C5E	2.46	1.60	1.51
22	b	604	CLA	CAC-C3C	-2.46	1.46	1.52
22	c	503	CLA	CMB-C2B	-2.45	1.46	1.51
24	k	102	BCR	C1-C6	-2.45	1.50	1.53
22	d	404	CLA	CMC-C2C	-2.45	1.45	1.51
22	B	607	CLA	CMC-C2C	-2.45	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	510	CLA	CMD-C2D	-2.45	1.45	1.51
31	H	102	DGD	C4D-C5D	2.45	1.58	1.53
22	b	614	CLA	C1D-C2D	2.44	1.48	1.42
22	C	507	CLA	C4C-NC	2.44	1.37	1.35
22	C	506	CLA	CMA-C3A	-2.44	1.47	1.53
31	C	517	DGD	C4D-C3D	2.43	1.58	1.52
22	b	612	CLA	C1D-C2D	2.43	1.48	1.42
29	D	407	SQD	O2-C2	-2.43	1.37	1.43
31	H	102	DGD	C4D-C3D	2.43	1.58	1.52
22	b	608	CLA	CMD-C2D	-2.42	1.45	1.51
28	b	622	LMG	O6-C1	2.41	1.48	1.41
22	b	606	CLA	C1D-C2D	2.41	1.48	1.42
22	B	607	CLA	CAC-C3C	-2.41	1.46	1.52
31	H	102	DGD	O6E-C1E	2.41	1.48	1.41
22	c	513	CLA	CMC-C2C	-2.41	1.45	1.51
31	c	516	DGD	O2E-C2E	-2.41	1.37	1.43
22	b	610	CLA	C3B-CAB	-2.41	1.43	1.47
30	d	407	LHG	C24-C23	2.41	1.57	1.50
24	b	617	BCR	C33-C5	-2.41	1.47	1.50
22	c	508	CLA	CMC-C2C	-2.40	1.45	1.51
22	C	509	CLA	CMD-C2D	-2.40	1.45	1.51
22	c	502	CLA	CMC-C2C	-2.39	1.45	1.51
22	D	403	CLA	CAC-C3C	-2.39	1.46	1.52
22	D	403	CLA	CMB-C2B	-2.39	1.46	1.51
22	A	402	CLA	C3B-C2B	-2.39	1.37	1.40
29	a	411	SQD	O2-C2	-2.39	1.37	1.43
22	b	607	CLA	CMC-C2C	-2.39	1.45	1.51
22	B	614	CLA	MG-NA	2.39	2.11	2.06
31	C	517	DGD	O3G-C3G	-2.38	1.39	1.43
22	a	403	CLA	CMD-C2D	-2.38	1.45	1.51
22	b	611	CLA	CMD-C2D	-2.38	1.45	1.51
22	c	507	CLA	CMB-C2B	-2.38	1.46	1.51
31	c	516	DGD	O1G-C1A	2.38	1.40	1.33
22	B	607	CLA	C1D-C2D	2.37	1.47	1.42
22	B	611	CLA	CAC-C3C	-2.37	1.46	1.52
22	A	403	CLA	CMB-C2B	-2.37	1.46	1.51
22	B	609	CLA	C1D-C2D	2.37	1.47	1.42
22	b	615	CLA	CMB-C2B	-2.37	1.46	1.51
22	B	616	CLA	CAC-C3C	-2.37	1.46	1.52
22	B	616	CLA	C3B-C2B	-2.36	1.37	1.40
31	c	516	DGD	C3G-C2G	2.36	1.57	1.50
31	C	515	DGD	C2A-C1A	-2.36	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	403	CLA	CMC-C2C	-2.36	1.46	1.51
31	A	416	DGD	O5D-C6D	-2.35	1.39	1.43
22	b	606	CLA	C4B-CHC	-2.35	1.34	1.41
22	c	501	CLA	CMD-C2D	-2.35	1.46	1.51
22	b	605	CLA	MG-NA	2.35	2.11	2.06
28	M	101	LMG	O7-C8	-2.35	1.40	1.46
22	C	502	CLA	C3B-C2B	-2.35	1.37	1.40
22	B	613	CLA	C3B-C2B	-2.35	1.37	1.40
22	B	612	CLA	C1C-C2C	2.34	1.47	1.42
22	B	608	CLA	CMB-C2B	-2.34	1.46	1.51
27	a	409	PL9	C25-C24	-2.34	1.44	1.50
22	C	504	CLA	CMD-C2D	-2.33	1.46	1.51
23	A	404	PHO	C1C-C2C	2.33	1.50	1.45
22	b	611	CLA	CMB-C2B	-2.33	1.46	1.51
22	B	604	CLA	O2D-CGD	2.33	1.38	1.33
22	C	504	CLA	C1D-C2D	2.33	1.47	1.42
22	B	604	CLA	C1D-C2D	2.33	1.47	1.42
22	B	603	CLA	CMD-C2D	-2.33	1.46	1.51
22	B	611	CLA	CMD-C2D	-2.33	1.46	1.51
24	K	101	BCR	C33-C5	-2.33	1.47	1.50
29	b	620	SQD	O2-C2	-2.32	1.37	1.43
22	c	501	CLA	CMB-C2B	-2.32	1.46	1.51
23	d	401	PHO	O2D-CGD	2.32	1.38	1.33
22	c	502	CLA	C1C-C2C	2.31	1.47	1.42
22	c	512	CLA	CMC-C2C	-2.31	1.46	1.51
22	C	512	CLA	CMC-C2C	-2.31	1.46	1.51
22	B	614	CLA	C3B-CAB	-2.31	1.43	1.47
22	C	501	CLA	CAC-C3C	-2.31	1.46	1.52
22	c	510	CLA	C3B-C2B	-2.31	1.37	1.40
36	v	201	HEC	C1D-ND	2.31	1.40	1.36
22	b	607	CLA	C3B-C2B	-2.30	1.37	1.40
22	D	402	CLA	CAC-C3C	-2.30	1.46	1.52
27	A	410	PL9	C53-C6	-2.30	1.45	1.50
22	b	616	CLA	CMC-C2C	-2.30	1.46	1.51
22	a	403	CLA	CMB-C2B	-2.30	1.46	1.51
22	D	403	CLA	C4B-CHC	-2.30	1.34	1.41
24	B	618	BCR	C1-C6	-2.30	1.50	1.53
22	D	402	CLA	CAA-C2A	-2.29	1.49	1.54
22	D	403	CLA	C1D-C2D	2.29	1.47	1.42
23	d	402	PHO	C1A-NA	2.29	1.42	1.37
22	A	402	CLA	CMC-C2C	-2.29	1.46	1.51
22	C	506	CLA	CAC-C3C	-2.29	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	411	SQD	O3-C3	-2.29	1.37	1.43
22	d	403	CLA	C3B-C2B	-2.29	1.37	1.40
30	D	408	LHG	C8-C7	-2.28	1.44	1.50
22	a	404	CLA	C3B-CAB	-2.28	1.43	1.47
22	b	607	CLA	C4C-NC	2.28	1.37	1.35
22	C	505	CLA	C3B-CAB	-2.28	1.43	1.47
22	C	504	CLA	CAC-C3C	-2.28	1.46	1.52
22	b	616	CLA	CMD-C2D	-2.28	1.46	1.51
22	B	610	CLA	C1D-C2D	2.27	1.47	1.42
22	D	402	CLA	C4C-NC	2.27	1.37	1.35
22	B	614	CLA	CMB-C2B	-2.27	1.46	1.51
22	C	503	CLA	CMC-C2C	-2.27	1.46	1.51
22	a	404	CLA	CMB-C2B	-2.27	1.46	1.51
31	A	416	DGD	C3D-C2D	2.27	1.58	1.52
22	A	405	CLA	MG-NA	-2.27	2.00	2.06
22	b	610	CLA	CAC-C3C	-2.27	1.46	1.52
22	C	507	CLA	C3B-CAB	-2.27	1.43	1.47
22	B	612	CLA	CMC-C2C	-2.27	1.46	1.51
22	B	614	CLA	C3B-C2B	-2.27	1.37	1.40
24	a	405	BCR	C38-C26	-2.26	1.47	1.50
22	A	403	CLA	MG-NA	-2.26	2.00	2.06
22	c	507	CLA	C3B-CAB	-2.26	1.43	1.47
22	c	502	CLA	C1D-C2D	2.26	1.47	1.42
24	B	617	BCR	C33-C5	-2.26	1.47	1.50
22	b	611	CLA	C1D-C2D	2.25	1.47	1.42
22	C	509	CLA	CAC-C3C	-2.25	1.46	1.52
31	c	516	DGD	O6D-C1D	2.25	1.47	1.41
22	C	501	CLA	CMD-C2D	-2.25	1.46	1.51
24	A	406	BCR	C33-C5	-2.25	1.47	1.50
22	B	605	CLA	C1D-C2D	2.25	1.47	1.42
22	c	503	CLA	MG-NA	2.25	2.11	2.06
22	b	616	CLA	CAC-C3C	-2.24	1.46	1.52
22	C	512	CLA	CAA-C2A	-2.24	1.49	1.54
23	A	404	PHO	CHD-C4C	-2.24	1.35	1.40
22	b	602	CLA	CMD-C2D	-2.24	1.46	1.51
22	b	602	CLA	C4B-CHC	-2.23	1.34	1.41
22	a	403	CLA	CAC-C3C	-2.23	1.46	1.52
22	d	404	CLA	C4B-CHC	-2.23	1.34	1.41
22	B	607	CLA	C1B-NB	2.23	1.37	1.35
22	B	616	CLA	C1D-C2D	2.23	1.47	1.42
31	H	102	DGD	O2D-C2D	-2.22	1.37	1.43
22	d	403	CLA	CMC-C2C	-2.22	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	x	101	BCR	C33-C5	-2.22	1.47	1.50
30	B	622	LHG	C24-C23	2.22	1.57	1.50
22	D	403	CLA	C3B-CAB	-2.22	1.43	1.47
22	B	615	CLA	C4B-CHC	-2.22	1.34	1.41
29	f	101	SQD	O4-C4	-2.22	1.37	1.43
22	C	506	CLA	CMC-C2C	-2.22	1.46	1.51
22	c	511	CLA	CMB-C2B	-2.21	1.47	1.51
22	D	403	CLA	CMD-C2D	-2.21	1.46	1.51
28	c	521	LMG	C7-C8	2.21	1.57	1.50
22	B	604	CLA	C1B-NB	2.21	1.37	1.35
28	a	416	LMG	O7-C10	2.21	1.40	1.34
22	c	508	CLA	CMB-C2B	-2.20	1.47	1.51
28	D	406	LMG	C4-C3	2.20	1.57	1.52
27	a	409	PL9	C30-C29	-2.20	1.45	1.50
23	d	401	PHO	CHC-C1C	2.20	1.43	1.38
30	e	102	LHG	O7-C5	-2.20	1.41	1.46
22	c	508	CLA	C3B-C2B	-2.20	1.37	1.40
22	B	612	CLA	C1D-C2D	2.20	1.47	1.42
30	e	102	LHG	C4-C5	2.20	1.57	1.50
22	b	614	CLA	CMB-C2B	-2.19	1.47	1.51
22	c	503	CLA	C3B-CAB	-2.19	1.43	1.47
22	C	511	CLA	CMC-C2C	-2.19	1.46	1.51
22	b	608	CLA	C3B-CAB	-2.19	1.43	1.47
22	B	616	CLA	CMD-C2D	-2.19	1.46	1.51
22	B	608	CLA	C3B-C2B	-2.19	1.37	1.40
31	C	516	DGD	O5D-C1E	2.18	1.43	1.40
22	B	614	CLA	C1C-C2C	2.18	1.47	1.42
22	A	403	CLA	CMD-C2D	-2.18	1.46	1.51
22	A	402	CLA	CMB-C2B	-2.18	1.47	1.51
22	b	602	CLA	CMC-C2C	-2.18	1.46	1.51
22	b	605	CLA	CAC-C3C	-2.18	1.46	1.52
22	b	616	CLA	C4B-CHC	-2.18	1.34	1.41
22	c	508	CLA	C1C-C2C	2.18	1.47	1.42
22	c	505	CLA	C3B-CAB	-2.18	1.43	1.47
28	M	101	LMG	O7-C10	2.18	1.40	1.34
30	D	409	LHG	O3-C3	-2.18	1.36	1.44
22	D	402	CLA	C1D-C2D	2.18	1.47	1.42
22	c	508	CLA	CMD-C2D	-2.17	1.46	1.51
22	a	404	CLA	C4B-CHC	-2.17	1.34	1.41
22	A	403	CLA	C4B-CHC	-2.17	1.35	1.41
22	c	507	CLA	CAC-C3C	-2.17	1.46	1.52
22	D	403	CLA	C3B-C2B	-2.17	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	501	CLA	CMB-C2B	-2.17	1.47	1.51
22	C	509	CLA	CMB-C2B	-2.16	1.47	1.51
28	C	518	LMG	O1-C7	-2.16	1.39	1.43
22	B	606	CLA	C4B-CHC	-2.16	1.35	1.41
22	C	512	CLA	C1D-C2D	2.16	1.47	1.42
28	C	518	LMG	C1-C2	2.16	1.58	1.52
23	A	404	PHO	C4C-C3C	2.16	1.49	1.45
22	B	607	CLA	O2D-CGD	2.16	1.38	1.33
22	B	614	CLA	CMC-C2C	-2.16	1.46	1.51
22	c	505	CLA	CMC-C2C	-2.16	1.46	1.51
22	b	607	CLA	CMB-C2B	-2.16	1.47	1.51
22	a	404	CLA	CMD-C2D	-2.16	1.46	1.51
22	A	411	CLA	C1C-C2C	2.15	1.47	1.42
22	C	512	CLA	C3B-CAB	-2.15	1.43	1.47
31	c	516	DGD	O3E-C3E	-2.15	1.37	1.43
30	d	408	LHG	C1-C2	-2.15	1.42	1.51
22	b	603	CLA	C3B-CAB	-2.15	1.43	1.47
31	A	416	DGD	O1G-C1G	-2.15	1.40	1.45
24	B	619	BCR	C38-C26	-2.15	1.47	1.50
22	b	613	CLA	CMC-C2C	-2.15	1.46	1.51
29	b	620	SQD	O3-C3	-2.15	1.37	1.43
22	B	608	CLA	MG-NA	2.15	2.11	2.06
22	b	615	CLA	CMC-C2C	-2.15	1.46	1.51
31	C	516	DGD	C1G-C2G	2.14	1.57	1.50
22	c	502	CLA	C3B-CAB	-2.14	1.43	1.47
22	B	613	CLA	C3B-CAB	-2.14	1.43	1.47
22	B	608	CLA	CMC-C2C	-2.14	1.46	1.51
22	C	511	CLA	C3B-C2B	-2.14	1.37	1.40
22	b	615	CLA	C3B-CAB	-2.14	1.43	1.47
31	C	516	DGD	C6D-C5D	2.14	1.58	1.51
24	K	102	BCR	C27-C26	-2.14	1.46	1.51
22	b	609	CLA	CMD-C2D	-2.14	1.46	1.51
22	B	601	CLA	CMC-C2C	-2.14	1.46	1.51
22	b	610	CLA	C1D-C2D	2.14	1.47	1.42
28	M	101	LMG	C9-C8	2.13	1.57	1.50
22	b	606	CLA	O1D-CGD	2.13	1.26	1.21
22	B	605	CLA	CMC-C2C	-2.13	1.46	1.51
22	b	605	CLA	C4B-CHC	-2.13	1.35	1.41
22	c	511	CLA	C3B-C2B	-2.13	1.37	1.40
27	d	406	PL9	C25-C24	-2.12	1.45	1.50
22	B	616	CLA	CMB-C2B	-2.12	1.47	1.51
22	A	403	CLA	CMC-C2C	-2.12	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	502	CLA	CAC-C3C	-2.12	1.47	1.52
22	C	510	CLA	CAA-C2A	-2.12	1.50	1.54
22	C	506	CLA	C3B-C2B	-2.11	1.37	1.40
28	b	622	LMG	C6-C5	2.11	1.58	1.51
31	H	102	DGD	O3E-C3E	-2.11	1.38	1.43
30	B	622	LHG	P-O4	-2.11	1.45	1.55
31	c	516	DGD	O5D-C6D	2.11	1.47	1.43
35	F	101	HEM	CAD-C3D	2.11	1.55	1.52
22	b	613	CLA	C4B-CHC	-2.10	1.35	1.41
22	b	614	CLA	C3B-C2B	-2.10	1.37	1.40
22	B	603	CLA	CMB-C2B	-2.10	1.47	1.51
22	A	403	CLA	CAC-C3C	-2.10	1.47	1.52
24	T	101	BCR	C38-C26	-2.10	1.47	1.50
22	c	503	CLA	CMD-C2D	-2.09	1.46	1.51
28	A	412	LMG	O7-C8	-2.09	1.41	1.46
22	b	606	CLA	C3B-CAB	-2.09	1.43	1.47
29	a	411	SQD	O4-C4	-2.09	1.38	1.43
22	b	614	CLA	MG-NA	2.09	2.11	2.06
23	d	401	PHO	CHD-C4C	-2.09	1.35	1.40
22	c	509	CLA	C1D-C2D	2.09	1.47	1.42
22	b	603	CLA	CMB-C2B	-2.09	1.47	1.51
23	D	401	PHO	C1A-NA	2.08	1.41	1.37
23	D	401	PHO	C1C-NC	-2.08	1.34	1.38
22	b	614	CLA	C3B-CAB	-2.08	1.43	1.47
22	c	504	CLA	CMD-C2D	-2.08	1.46	1.51
22	B	602	CLA	CAC-C3C	-2.08	1.47	1.52
28	D	406	LMG	O2-C2	-2.08	1.38	1.43
22	b	608	CLA	CMC-C2C	-2.08	1.46	1.51
22	A	402	CLA	C1C-C2C	2.08	1.47	1.42
22	C	502	CLA	CAC-C3C	-2.07	1.47	1.52
22	a	402	CLA	C3D-C2D	-2.07	1.35	1.39
22	c	510	CLA	CMD-C2D	-2.07	1.46	1.51
22	B	601	CLA	CAC-C3C	-2.07	1.47	1.52
22	a	410	CLA	C3B-C2B	-2.07	1.37	1.40
24	b	617	BCR	C4-C5	-2.07	1.46	1.51
28	M	101	LMG	O1-C7	-2.07	1.40	1.43
22	c	510	CLA	C1D-C2D	2.07	1.47	1.42
22	b	603	CLA	CMC-C2C	-2.07	1.46	1.51
22	c	510	CLA	CAC-C3C	-2.07	1.47	1.52
30	A	414	LHG	O7-C5	-2.07	1.41	1.46
22	B	615	CLA	C3B-CAB	-2.06	1.43	1.47
22	B	613	CLA	C1D-C2D	2.06	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	k	101	BCR	C33-C5	-2.06	1.47	1.50
22	b	615	CLA	CAC-C3C	-2.06	1.47	1.52
22	b	610	CLA	CMD-C2D	-2.06	1.46	1.51
22	a	402	CLA	CMC-C2C	-2.05	1.46	1.51
22	A	402	CLA	C3D-C2D	-2.05	1.35	1.39
31	c	517	DGD	O5D-C6D	-2.05	1.40	1.43
22	b	606	CLA	CMB-C2B	-2.05	1.47	1.51
31	C	517	DGD	O4D-C4D	-2.05	1.38	1.43
22	B	613	CLA	C5-C3	-2.05	1.47	1.51
22	C	513	CLA	CMC-C2C	-2.05	1.46	1.51
30	l	101	LHG	C4-C5	2.04	1.57	1.50
31	c	517	DGD	C6E-C5E	2.04	1.58	1.51
31	h	101	DGD	O2E-C2E	-2.04	1.38	1.43
22	C	509	CLA	O2D-CGD	2.04	1.38	1.33
22	c	504	CLA	CMB-C2B	-2.04	1.47	1.51
28	b	624	LMG	C4-C3	2.04	1.57	1.52
22	B	603	CLA	C3B-C2B	-2.04	1.37	1.40
29	A	413	SQD	O4-C4	-2.04	1.38	1.43
28	D	406	LMG	O7-C8	-2.04	1.41	1.46
35	e	101	HEM	C4A-CHB	-2.04	1.35	1.41
22	B	606	CLA	C1D-C2D	2.03	1.47	1.42
22	B	609	CLA	CMC-C2C	-2.03	1.46	1.51
22	C	506	CLA	CMB-C2B	-2.03	1.47	1.51
22	B	602	CLA	C4B-CHC	-2.03	1.35	1.41
22	b	604	CLA	MG-NA	2.03	2.11	2.06
22	d	404	CLA	C1D-C2D	2.03	1.47	1.42
22	C	513	CLA	C3B-CAB	-2.03	1.43	1.47
22	B	610	CLA	CMD-C2D	-2.03	1.46	1.51
29	A	413	SQD	O3-C3	-2.03	1.38	1.43
31	C	517	DGD	O1G-C1G	-2.03	1.40	1.45
28	b	622	LMG	O8-C28	2.03	1.39	1.33
31	A	416	DGD	O3D-C3D	-2.02	1.38	1.43
24	t	101	BCR	C33-C5	-2.02	1.47	1.50
22	a	404	CLA	C1D-C2D	2.02	1.47	1.42
31	c	516	DGD	O1A-C1A	2.01	1.28	1.22
22	c	506	CLA	CMC-C2C	-2.01	1.46	1.51
22	B	601	CLA	C3B-CAB	-2.01	1.43	1.47
24	c	515	BCR	C35-C13	-2.01	1.46	1.50
23	d	402	PHO	CMD-C2D	-2.01	1.46	1.50
24	B	618	BCR	C27-C26	-2.01	1.47	1.51
28	c	522	LMG	C3-C2	2.01	1.57	1.52
31	c	518	DGD	C4E-C5E	-2.00	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	507	CLA	CMC-C2C	-2.00	1.46	1.51
30	d	409	LHG	P-O6	2.00	1.67	1.59
22	d	404	CLA	MG-NA	2.00	2.11	2.06

All (1282) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	606	CLA	C4A-NA-C1A	10.68	111.51	106.71
22	B	601	CLA	C4A-NA-C1A	10.55	111.45	106.71
22	b	601	CLA	C4A-NA-C1A	9.46	110.96	106.71
22	B	604	CLA	C4A-NA-C1A	9.36	110.91	106.71
29	b	620	SQD	O6-C1-C2	9.26	122.76	108.30
29	D	407	SQD	O6-C1-C2	8.93	122.24	108.30
22	b	607	CLA	C4A-NA-C1A	8.71	110.62	106.71
22	C	503	CLA	C4A-NA-C1A	8.68	110.61	106.71
22	B	616	CLA	C4A-NA-C1A	8.65	110.60	106.71
22	c	511	CLA	C4A-NA-C1A	8.44	110.50	106.71
22	C	507	CLA	C4A-NA-C1A	8.34	110.46	106.71
22	C	509	CLA	C4A-NA-C1A	8.19	110.39	106.71
22	C	508	CLA	C4A-NA-C1A	8.04	110.32	106.71
22	a	404	CLA	C4A-NA-C1A	7.80	110.21	106.71
22	b	602	CLA	C4A-NA-C1A	7.52	110.09	106.71
22	B	609	CLA	C4A-NA-C1A	7.48	110.07	106.71
29	a	411	SQD	O6-C1-C2	7.41	119.88	108.30
22	C	501	CLA	C4A-NA-C1A	7.38	110.03	106.71
22	c	502	CLA	C4A-NA-C1A	7.38	110.03	106.71
29	f	101	SQD	O7-S-C6	7.31	115.62	106.94
22	C	511	CLA	C4A-NA-C1A	7.26	109.97	106.71
22	a	410	CLA	C4A-NA-C1A	7.22	109.95	106.71
29	B	623	SQD	O6-C1-C2	7.21	119.56	108.30
22	c	503	CLA	C4A-NA-C1A	7.15	109.92	106.71
29	A	413	SQD	O6-C1-C2	7.07	119.35	108.30
22	C	502	CLA	C4A-NA-C1A	6.69	109.71	106.71
22	b	615	CLA	C4A-NA-C1A	6.40	109.58	106.71
22	B	607	CLA	C4A-NA-C1A	6.39	109.58	106.71
27	D	405	PL9	C7-C3-C4	6.33	122.02	116.88
22	c	510	CLA	C4A-NA-C1A	6.33	109.55	106.71
22	B	612	CLA	C4A-NA-C1A	6.30	109.54	106.71
22	a	402	CLA	C4A-NA-C1A	6.29	109.53	106.71
22	b	604	CLA	C4A-NA-C1A	6.28	109.53	106.71
22	A	411	CLA	C4A-NA-C1A	6.26	109.52	106.71
29	D	407	SQD	O9-S-C6	6.21	114.32	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	510	CLA	C4A-NA-C1A	6.09	109.44	106.71
22	B	611	CLA	C4A-NA-C1A	5.94	109.38	106.71
22	d	404	CLA	CMB-C2B-C1B	-5.94	119.34	128.46
35	e	101	HEM	CBD-CAD-C3D	-5.94	101.54	112.48
22	b	613	CLA	CMB-C2B-C1B	-5.93	119.35	128.46
27	A	410	PL9	C7-C3-C4	5.91	121.68	116.88
22	B	610	CLA	O2D-CGD-O1D	-5.72	112.65	123.84
22	D	403	CLA	C4A-NA-C1A	5.69	109.26	106.71
22	B	610	CLA	C4A-NA-C1A	5.56	109.20	106.71
22	C	502	CLA	C4D-C3D-CAD	-5.56	105.37	108.47
22	C	509	CLA	CMB-C2B-C1B	-5.55	119.94	128.46
29	b	620	SQD	O7-S-C6	5.54	113.52	106.94
22	c	509	CLA	C4A-NA-C1A	5.52	109.19	106.71
22	B	613	CLA	C4A-NA-C1A	5.51	109.19	106.71
29	f	101	SQD	O6-C1-C2	5.51	116.90	108.30
22	c	513	CLA	CMB-C2B-C1B	-5.47	120.06	128.46
22	c	512	CLA	C4A-NA-C1A	5.45	109.16	106.71
22	C	513	CLA	C4A-NA-C1A	5.41	109.14	106.71
22	a	402	CLA	CMB-C2B-C1B	-5.41	120.15	128.46
22	B	607	CLA	CMB-C2B-C1B	-5.38	120.19	128.46
27	d	406	PL9	C7-C3-C4	5.37	121.24	116.88
22	c	501	CLA	C4A-NA-C1A	5.35	109.11	106.71
22	B	613	CLA	CMB-C2B-C1B	-5.35	120.24	128.46
35	F	101	HEM	CBA-CAA-C2A	-5.34	102.63	112.49
22	A	402	CLA	C4A-NA-C1A	5.30	109.09	106.71
22	C	508	CLA	CMB-C2B-C1B	-5.27	120.37	128.46
36	V	201	HEC	CMC-C2C-C1C	-5.24	120.40	128.46
22	c	509	CLA	CMB-C2B-C1B	-5.23	120.43	128.46
22	B	602	CLA	O2D-CGD-CBD	5.22	120.54	111.27
22	b	616	CLA	C4A-NA-C1A	5.22	109.05	106.71
22	B	608	CLA	CMB-C2B-C1B	-5.21	120.45	128.46
22	c	508	CLA	CMB-C2B-C1B	-5.20	120.47	128.46
22	d	404	CLA	CMB-C2B-C3B	5.19	134.39	124.68
22	c	501	CLA	O2D-CGD-O1D	-5.16	113.75	123.84
22	C	509	CLA	CMB-C2B-C3B	5.16	134.33	124.68
28	b	624	LMG	C1-O6-C5	-5.15	103.57	113.69
36	v	201	HEC	CBD-CAD-C3D	-5.10	103.09	112.49
22	A	403	CLA	CMB-C2B-C1B	-5.05	120.70	128.46
22	c	507	CLA	C4A-NA-C1A	5.02	108.97	106.71
22	b	605	CLA	C4A-NA-C1A	4.97	108.94	106.71
22	B	602	CLA	CMB-C2B-C1B	-4.95	120.85	128.46
29	a	411	SQD	O7-S-C6	4.94	112.81	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	606	CLA	CMB-C2B-C1B	-4.92	120.91	128.46
22	C	503	CLA	CMB-C2B-C1B	-4.86	121.00	128.46
22	b	610	CLA	C4A-NA-C1A	4.86	108.89	106.71
22	b	616	CLA	CMB-C2B-C3B	4.86	133.76	124.68
22	A	403	CLA	CMB-C2B-C3B	4.85	133.76	124.68
27	a	409	PL9	C7-C3-C4	4.85	120.82	116.88
22	B	611	CLA	CMB-C2B-C1B	-4.85	121.00	128.46
22	B	606	CLA	C4A-NA-C1A	4.78	108.86	106.71
22	B	602	CLA	O2D-CGD-O1D	-4.77	114.50	123.84
22	B	612	CLA	CMB-C2B-C1B	-4.77	121.14	128.46
22	C	501	CLA	O2D-CGD-O1D	-4.75	114.55	123.84
22	b	614	CLA	C4A-NA-C1A	4.73	108.83	106.71
22	c	510	CLA	CMB-C2B-C1B	-4.73	121.19	128.46
22	c	506	CLA	CMB-C2B-C1B	-4.70	121.25	128.46
22	b	612	CLA	CMB-C2B-C1B	-4.69	121.26	128.46
28	a	416	LMG	C1-C2-C3	-4.65	100.30	110.00
22	C	506	CLA	C4A-NA-C1A	4.65	108.80	106.71
22	b	609	CLA	C4A-NA-C1A	4.64	108.79	106.71
22	B	604	CLA	CMB-C2B-C1B	-4.64	121.34	128.46
29	A	413	SQD	C1-C2-C3	-4.63	100.35	110.00
22	c	506	CLA	C4A-NA-C1A	4.62	108.78	106.71
30	D	409	LHG	O4-P-O5	4.59	134.93	112.24
22	c	513	CLA	CMB-C2B-C3B	4.59	133.27	124.68
22	c	508	CLA	C4A-NA-C1A	4.58	108.76	106.71
22	C	506	CLA	CMB-C2B-C1B	-4.57	121.44	128.46
22	d	403	CLA	C4A-NA-C1A	4.57	108.76	106.71
22	b	613	CLA	C4A-NA-C1A	4.56	108.75	106.71
22	b	601	CLA	O2D-CGD-O1D	-4.55	114.95	123.84
29	A	413	SQD	O47-C7-C8	4.54	121.29	111.50
22	c	509	CLA	CMB-C2B-C3B	4.54	133.17	124.68
22	B	615	CLA	C4A-NA-C1A	4.53	108.74	106.71
22	C	511	CLA	CMB-C2B-C1B	-4.52	121.52	128.46
22	b	613	CLA	C1-C2-C3	-4.51	118.25	126.04
27	a	409	PL9	C35-C34-C36	4.48	122.81	115.27
22	b	616	CLA	CMB-C2B-C1B	-4.46	121.61	128.46
31	C	516	DGD	O3G-C3G-C2G	-4.46	100.15	110.90
22	D	403	CLA	CMB-C2B-C1B	-4.45	121.62	128.46
22	c	509	CLA	C4D-C3D-CAD	-4.45	105.99	108.47
22	b	603	CLA	C4A-NA-C1A	4.45	108.70	106.71
22	b	607	CLA	CMB-C2B-C1B	-4.41	121.69	128.46
22	b	603	CLA	O2D-CGD-O1D	-4.41	115.22	123.84
22	D	402	CLA	CMB-C2B-C1B	-4.38	121.74	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	613	CLA	CMB-C2B-C3B	4.37	132.86	124.68
22	c	505	CLA	CMB-C2B-C1B	-4.36	121.76	128.46
22	b	606	CLA	CMB-C2B-C3B	4.36	132.84	124.68
28	b	622	LMG	O3-C3-C2	-4.35	100.30	110.35
22	b	615	CLA	CMB-C2B-C1B	-4.35	121.78	128.46
22	C	510	CLA	CMB-C2B-C1B	-4.34	121.79	128.46
31	C	517	DGD	O3G-C3G-C2G	-4.34	100.43	110.90
22	b	603	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
22	c	508	CLA	CMB-C2B-C3B	4.33	132.77	124.68
22	c	504	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
22	B	607	CLA	CMB-C2B-C3B	4.32	132.77	124.68
31	H	102	DGD	O3G-C3G-C2G	-4.32	100.47	110.90
22	C	508	CLA	O2D-CGD-O1D	-4.31	115.41	123.84
22	b	602	CLA	CMB-C2B-C1B	-4.31	121.85	128.46
22	B	613	CLA	CMB-C2B-C3B	4.29	132.70	124.68
30	A	414	LHG	O4-P-O5	4.27	133.35	112.24
22	b	611	CLA	O2D-CGD-CBD	4.27	118.86	111.27
31	c	518	DGD	O3G-C3G-C2G	-4.26	100.62	110.90
27	A	410	PL9	C7-C3-C2	-4.26	117.70	123.30
22	b	602	CLA	O2D-CGD-CBD	4.25	118.83	111.27
22	C	512	CLA	CMB-C2B-C1B	-4.24	121.94	128.46
28	a	416	LMG	C1-O6-C5	-4.23	105.38	113.69
22	B	608	CLA	CMB-C2B-C3B	4.22	132.57	124.68
22	a	403	CLA	CMB-C2B-C1B	-4.22	121.98	128.46
22	a	402	CLA	CMB-C2B-C3B	4.21	132.56	124.68
22	b	612	CLA	C4A-NA-C1A	4.21	108.60	106.71
22	b	605	CLA	O2D-CGD-O1D	-4.19	115.64	123.84
35	F	101	HEM	CBD-CAD-C3D	-4.19	104.76	112.48
22	B	614	CLA	C4A-NA-C1A	4.18	108.59	106.71
22	b	611	CLA	O2D-CGD-O1D	-4.16	115.71	123.84
27	d	406	PL9	C36-C34-C33	-4.16	112.70	121.12
22	b	612	CLA	CMB-C2B-C3B	4.15	132.44	124.68
22	c	501	CLA	CMB-C2B-C1B	-4.14	122.09	128.46
36	V	201	HEC	CBD-CAD-C3D	-4.14	104.85	112.49
31	c	517	DGD	O2D-C2D-C1D	-4.14	99.99	110.05
22	B	613	CLA	OBD-CAD-C3D	4.13	134.84	127.98
22	B	614	CLA	C4D-C3D-CAD	-4.12	106.17	108.47
22	c	505	CLA	CMD-C2D-C3D	4.11	132.38	124.68
22	c	505	CLA	C4D-C3D-CAD	-4.11	106.18	108.47
22	b	601	CLA	CHB-C4A-NA	4.11	130.20	124.51
22	B	616	CLA	CMB-C2B-C3B	4.11	132.36	124.68
29	B	623	SQD	O7-S-C6	4.10	111.81	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	603	CLA	C4A-NA-C1A	4.10	108.55	106.71
22	B	614	CLA	CMD-C2D-C3D	4.10	132.34	124.68
30	e	102	LHG	O4-P-O5	4.08	132.43	112.24
22	B	602	CLA	CMB-C2B-C3B	4.08	132.31	124.68
22	c	502	CLA	O2D-CGD-O1D	-4.07	115.87	123.84
22	B	608	CLA	O2D-CGD-O1D	-4.07	115.87	123.84
22	B	608	CLA	C4A-NA-C1A	4.07	108.53	106.71
30	l	101	LHG	O4-P-O5	4.07	132.34	112.24
29	a	412	SQD	O48-C23-O10	-4.06	113.33	123.59
22	C	502	CLA	CMD-C2D-C3D	4.05	132.26	124.68
24	T	101	BCR	C7-C8-C9	-4.05	120.12	126.23
22	C	503	CLA	CMB-C2B-C3B	4.05	132.25	124.68
22	b	603	CLA	CMB-C2B-C3B	4.04	132.24	124.68
29	B	623	SQD	O47-C7-C8	4.04	120.20	111.50
30	B	622	LHG	O4-P-O5	4.03	132.17	112.24
29	D	407	SQD	O8-S-C6	4.03	112.16	105.74
35	e	101	HEM	CBA-CAA-C2A	-4.03	105.06	112.49
29	b	620	SQD	C1-C2-C3	-4.02	101.62	110.00
22	D	402	CLA	C4A-NA-C1A	4.01	108.51	106.71
22	C	505	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
29	a	412	SQD	O48-C23-C24	4.00	124.46	111.91
22	b	611	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
22	b	602	CLA	O2D-CGD-O1D	-3.99	116.04	123.84
29	A	413	SQD	C1-O5-C5	-3.98	105.88	113.69
22	b	616	CLA	CHB-C4A-NA	3.98	130.01	124.51
22	D	402	CLA	CMB-C2B-C3B	3.97	132.11	124.68
22	C	504	CLA	O2D-CGD-O1D	-3.97	116.07	123.84
22	B	615	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
22	B	613	CLA	OBD-CAD-CBD	-3.96	120.23	125.89
22	A	402	CLA	CMB-C2B-C1B	-3.96	122.37	128.46
30	B	621	LHG	O4-P-O5	3.96	131.81	112.24
22	b	610	CLA	O2D-CGD-O1D	-3.95	116.11	123.84
22	B	612	CLA	CMB-C2B-C3B	3.95	132.06	124.68
30	d	409	LHG	O4-P-O5	3.95	131.75	112.24
22	B	616	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
28	b	622	LMG	O1-C1-C2	-3.94	102.15	108.30
24	C	514	BCR	C15-C16-C17	-3.94	115.41	123.47
22	a	410	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
36	v	201	HEC	CMC-C2C-C1C	-3.93	122.42	128.46
22	b	609	CLA	CMB-C2B-C1B	-3.93	122.43	128.46
22	b	616	CLA	O2D-CGD-O1D	-3.91	116.19	123.84
22	A	402	CLA	CMB-C2B-C3B	3.90	131.98	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	504	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
29	f	101	SQD	O9-S-O7	-3.90	100.45	113.95
22	A	411	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
22	c	506	CLA	CMB-C2B-C3B	3.86	131.90	124.68
29	a	411	SQD	O9-S-C6	3.86	111.53	106.94
22	C	507	CLA	C1-C2-C3	-3.85	119.38	126.04
30	D	408	LHG	O4-P-O5	3.85	131.27	112.24
30	d	407	LHG	O4-P-O5	3.84	131.23	112.24
22	C	509	CLA	CHB-C4A-NA	3.84	129.82	124.51
22	c	501	CLA	O2D-CGD-CBD	3.84	118.08	111.27
22	A	405	CLA	CMB-C2B-C1B	-3.83	122.57	128.46
22	A	402	CLA	CHB-C4A-NA	3.82	129.79	124.51
22	c	512	CLA	C1-C2-C3	-3.82	119.44	126.04
22	c	509	CLA	CMD-C2D-C3D	3.79	131.77	124.68
22	C	501	CLA	O2D-CGD-CBD	3.79	118.00	111.27
22	D	403	CLA	CMB-C2B-C3B	3.79	131.77	124.68
22	B	603	CLA	CMB-C2B-C3B	3.77	131.74	124.68
22	a	403	CLA	CMB-C2B-C3B	3.77	131.73	124.68
22	b	604	CLA	OBD-CAD-CBD	-3.77	120.51	125.89
23	D	401	PHO	CAC-C3C-C4C	-3.77	121.11	125.22
22	b	605	CLA	C4-C3-C5	3.76	121.60	115.27
22	C	508	CLA	CMB-C2B-C3B	3.76	131.71	124.68
22	B	613	CLA	C1-C2-C3	-3.75	119.55	126.04
31	h	101	DGD	O3G-C3G-C2G	-3.75	101.85	110.90
22	C	507	CLA	C4-C3-C5	3.75	121.57	115.27
23	A	404	PHO	CMD-C2D-C1D	3.71	130.78	125.06
24	b	617	BCR	C2-C1-C6	3.70	116.18	110.48
22	B	614	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
22	A	411	CLA	CMB-C2B-C3B	3.70	131.60	124.68
22	C	504	CLA	C4D-C3D-CAD	-3.70	106.41	108.47
24	B	619	BCR	C2-C1-C6	3.70	116.17	110.48
22	C	504	CLA	C4A-NA-C1A	3.69	108.37	106.71
22	B	611	CLA	O2D-CGD-O1D	-3.68	116.64	123.84
22	c	505	CLA	CMB-C2B-C3B	3.68	131.57	124.68
27	A	410	PL9	C40-C39-C41	3.68	121.46	115.27
22	b	604	CLA	C1-C2-C3	-3.68	119.68	126.04
22	B	614	CLA	O2D-CGD-O1D	-3.68	116.65	123.84
27	D	405	PL9	C7-C3-C2	-3.68	118.46	123.30
24	C	514	BCR	C36-C18-C17	-3.68	117.78	122.92
30	d	408	LHG	O4-P-O5	3.67	130.41	112.24
22	c	503	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
22	b	608	CLA	C4A-NA-C1A	3.67	108.36	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	408	LHG	O8-C23-O10	-3.66	114.35	123.59
22	c	509	CLA	O2A-CGA-O1A	-3.66	114.36	123.59
22	c	504	CLA	CMB-C2B-C3B	3.65	131.51	124.68
28	b	624	LMG	O2-C2-C1	-3.65	101.18	110.05
22	c	502	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
36	v	201	HEC	C1D-C2D-C3D	-3.63	104.47	107.00
22	b	610	CLA	C1B-CHB-C4A	-3.63	122.92	130.12
22	b	604	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
22	b	614	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
22	c	512	CLA	O2D-CGD-O1D	-3.62	116.76	123.84
22	b	612	CLA	CMD-C2D-C3D	3.62	131.46	124.68
22	c	511	CLA	C4D-C3D-CAD	-3.61	106.46	108.47
22	c	510	CLA	CMB-C2B-C3B	3.61	131.43	124.68
22	b	608	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
22	c	512	CLA	O2A-CGA-O1A	-3.60	114.51	123.59
22	c	512	CLA	C4D-C3D-CAD	-3.60	106.46	108.47
22	c	507	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
22	b	611	CLA	CHB-C4A-NA	3.59	129.48	124.51
22	a	403	CLA	C4A-NA-C1A	3.59	108.32	106.71
30	e	102	LHG	O8-C23-C24	3.58	123.15	111.91
29	f	101	SQD	O47-C7-C8	3.58	120.78	110.80
22	B	612	CLA	CMD-C2D-C3D	3.57	131.36	124.68
22	c	501	CLA	CMB-C2B-C3B	3.57	131.36	124.68
22	c	507	CLA	OBD-CAD-CBD	-3.57	120.80	125.89
23	D	401	PHO	O2D-CGD-O1D	-3.57	116.86	123.84
22	b	608	CLA	C1B-CHB-C4A	-3.56	123.07	130.12
22	B	605	CLA	OBD-CAD-CBD	-3.56	120.81	125.89
30	B	622	LHG	O8-C23-C24	3.55	123.06	111.91
22	D	403	CLA	O2D-CGD-O1D	-3.55	116.90	123.84
31	A	416	DGD	C3G-C2G-C1G	-3.54	103.42	111.79
22	B	611	CLA	CMB-C2B-C3B	3.53	131.29	124.68
22	C	505	CLA	CMB-C2B-C3B	3.53	131.29	124.68
29	b	620	SQD	O47-C7-C8	3.53	119.11	111.50
27	A	410	PL9	C27-C28-C29	-3.52	119.19	127.66
27	D	405	PL9	C42-C43-C44	-3.51	119.20	127.66
22	c	506	CLA	C4-C3-C5	3.51	121.17	115.27
27	a	409	PL9	C22-C23-C24	-3.51	119.21	127.66
22	C	505	CLA	O2D-CGD-O1D	-3.51	116.98	123.84
22	B	606	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
22	c	504	CLA	CMD-C2D-C3D	3.50	131.22	124.68
35	F	101	HEM	C1D-C2D-C3D	3.49	109.43	107.00
22	b	613	CLA	CHB-C4A-NA	3.49	129.34	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	507	CLA	CMD-C2D-C3D	3.49	131.20	124.68
22	C	505	CLA	CMD-C2D-C3D	3.48	131.19	124.68
22	A	405	CLA	O2D-CGD-O1D	-3.48	117.04	123.84
22	B	610	CLA	C1B-CHB-C4A	-3.48	123.23	130.12
22	b	615	CLA	CMB-C2B-C3B	3.48	131.18	124.68
22	C	512	CLA	CMB-C2B-C3B	3.47	131.17	124.68
22	C	510	CLA	CMB-C2B-C3B	3.47	131.16	124.68
22	B	604	CLA	CMB-C2B-C3B	3.46	131.15	124.68
22	c	502	CLA	CMB-C2B-C3B	3.45	131.13	124.68
29	A	415	SQD	C45-O47-C7	3.45	122.31	117.88
22	C	513	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
23	A	404	PHO	CMB-C2B-C1B	-3.44	119.76	125.06
22	b	604	CLA	OBD-CAD-C3D	3.44	133.69	127.98
22	B	602	CLA	CHB-C4A-NA	3.43	129.26	124.51
31	C	515	DGD	O3G-C3G-C2G	-3.43	102.64	110.90
22	A	405	CLA	O2D-CGD-CBD	3.42	117.34	111.27
22	c	507	CLA	CMB-C2B-C3B	3.41	131.06	124.68
24	t	101	BCR	C15-C16-C17	-3.41	116.48	123.47
22	B	615	CLA	CHB-C4A-NA	3.41	129.23	124.51
29	A	413	SQD	O9-S-O7	-3.41	102.16	113.95
36	V	201	HEC	C1D-C2D-C3D	-3.41	104.63	107.00
22	b	607	CLA	CMB-C2B-C3B	3.40	131.04	124.68
22	D	402	CLA	CED-O2D-CGD	3.40	123.63	115.94
22	B	601	CLA	OBD-CAD-CBD	-3.40	121.04	125.89
31	c	517	DGD	O3G-C3G-C2G	-3.39	102.71	110.90
22	c	511	CLA	CMD-C2D-C3D	3.39	131.02	124.68
23	d	402	PHO	CMB-C2B-C1B	-3.39	119.84	125.06
22	c	510	CLA	OBD-CAD-CBD	-3.38	121.06	125.89
22	d	403	CLA	C1B-CHB-C4A	-3.38	123.42	130.12
22	b	613	CLA	O2D-CGD-O1D	-3.37	117.24	123.84
22	a	410	CLA	CMB-C2B-C3B	3.37	130.98	124.68
30	d	407	LHG	O8-C23-C24	3.37	122.48	111.91
22	b	602	CLA	CMB-C2B-C3B	3.37	130.98	124.68
22	B	612	CLA	C4D-C3D-CAD	-3.36	106.60	108.47
27	d	406	PL9	C40-C39-C41	3.36	120.92	115.27
22	b	608	CLA	CMB-C2B-C3B	3.35	130.95	124.68
22	A	405	CLA	C4A-NA-C1A	3.35	108.21	106.71
22	b	612	CLA	CMC-C2C-C3C	3.35	131.25	124.94
22	A	402	CLA	O1D-CGD-CBD	3.34	131.31	124.48
29	D	407	SQD	O5-C1-C2	-3.33	103.30	110.35
24	x	101	BCR	C36-C18-C17	-3.32	118.27	122.92
27	D	405	PL9	C7-C8-C9	-3.31	121.28	126.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	616	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
22	B	603	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
22	D	402	CLA	C1B-CHB-C4A	-3.29	123.61	130.12
22	c	512	CLA	OBD-CAD-CBD	-3.28	121.20	125.89
22	a	404	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
22	d	403	CLA	O2A-CGA-O1A	-3.28	115.31	123.59
22	C	502	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
22	C	506	CLA	CMB-C2B-C3B	3.28	130.81	124.68
27	D	405	PL9	C22-C23-C24	-3.27	119.79	127.66
22	A	405	CLA	CMB-C2B-C3B	3.27	130.79	124.68
29	f	101	SQD	C1-C2-C3	-3.27	103.19	110.00
22	B	601	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
22	b	615	CLA	CMD-C2D-C3D	3.26	130.77	124.68
29	a	411	SQD	O9-S-O7	-3.26	102.68	113.95
22	B	616	CLA	C4D-C3D-CAD	-3.25	106.66	108.47
22	c	504	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
22	a	404	CLA	C4-C3-C5	3.25	120.74	115.27
22	d	404	CLA	C1B-CHB-C4A	-3.25	123.69	130.12
22	B	612	CLA	CHB-C4A-NA	3.25	129.00	124.51
22	C	512	CLA	C4A-NA-C1A	3.24	108.16	106.71
22	a	403	CLA	CED-O2D-CGD	-3.24	108.61	115.94
24	H	101	BCR	C16-C15-C14	-3.23	116.85	123.47
22	b	611	CLA	CMB-C2B-C3B	3.23	130.72	124.68
31	h	101	DGD	C1D-C2D-C3D	-3.23	103.27	110.00
31	A	416	DGD	O2D-C2D-C1D	-3.22	102.22	110.05
22	b	607	CLA	CMD-C2D-C3D	3.22	130.71	124.68
29	b	620	SQD	O8-S-C6	3.22	110.88	105.74
23	D	401	PHO	CMB-C2B-C1B	-3.22	120.10	125.06
22	B	608	CLA	O2D-CGD-CBD	3.22	116.99	111.27
31	C	517	DGD	O6D-C1D-O3G	-3.22	102.35	109.97
22	B	605	CLA	C4D-C3D-CAD	-3.22	106.68	108.47
22	B	610	CLA	O2A-CGA-O1A	-3.21	115.48	123.59
22	B	614	CLA	C4-C3-C5	3.21	120.68	115.27
22	c	508	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
22	c	507	CLA	C1B-CHB-C4A	-3.21	123.77	130.12
22	C	503	CLA	C7-C6-C5	-3.20	104.66	113.36
27	A	410	PL9	C35-C34-C36	3.19	120.63	115.27
22	b	609	CLA	OBD-CAD-CBD	-3.19	121.34	125.89
22	b	601	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
22	c	510	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
22	a	403	CLA	CHB-C4A-NA	3.17	128.90	124.51
22	C	506	CLA	OBD-CAD-CBD	-3.17	121.36	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	604	CLA	OBD-CAD-CBD	-3.17	121.36	125.89
22	b	606	CLA	CMC-C2C-C3C	3.16	130.91	124.94
22	a	404	CLA	CMB-C2B-C3B	3.16	130.60	124.68
22	C	502	CLA	O1D-CGD-CBD	3.16	130.96	124.48
31	H	102	DGD	O2D-C2D-C1D	-3.16	102.37	110.05
22	B	610	CLA	O1D-CGD-CBD	3.16	130.95	124.48
29	a	412	SQD	O47-C7-C8	3.16	118.31	111.50
36	v	201	HEC	CMB-C2B-C1B	-3.15	123.62	128.46
22	C	505	CLA	OBD-CAD-CBD	-3.15	121.39	125.89
22	b	602	CLA	CHB-C4A-NA	3.15	128.87	124.51
29	a	411	SQD	O48-C23-C24	3.15	121.79	111.91
28	M	101	LMG	C1-O6-C5	-3.15	107.51	113.69
24	a	405	BCR	C37-C22-C21	-3.15	118.52	122.92
22	b	609	CLA	CED-O2D-CGD	3.15	123.05	115.94
27	d	406	PL9	C37-C38-C39	-3.15	120.09	127.66
22	C	507	CLA	CMB-C2B-C1B	-3.15	123.63	128.46
22	b	604	CLA	C11-C12-C13	-3.14	105.76	115.92
27	A	410	PL9	C36-C34-C33	-3.14	114.76	121.12
22	a	403	CLA	C1B-CHB-C4A	-3.14	123.90	130.12
24	B	618	BCR	C37-C22-C21	-3.14	118.53	122.92
28	C	518	LMG	O1-C7-C8	-3.13	103.34	110.90
22	C	513	CLA	O2A-CGA-O1A	-3.13	115.70	123.59
24	x	101	BCR	C37-C22-C21	-3.12	118.55	122.92
22	B	611	CLA	O2D-CGD-CBD	3.12	116.82	111.27
31	A	416	DGD	O5D-C1E-C2E	3.12	113.18	108.30
27	a	409	PL9	C7-C3-C2	-3.12	119.19	123.30
29	D	407	SQD	C44-O6-C1	3.12	119.01	113.84
24	b	617	BCR	C3-C4-C5	-3.12	108.51	114.08
23	d	402	PHO	O1D-CGD-CBD	3.11	130.86	124.48
22	b	606	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
22	b	612	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
28	D	406	LMG	O1-C7-C8	-3.10	103.42	110.90
22	C	512	CLA	CMD-C2D-C3D	3.10	130.47	124.68
22	b	613	CLA	CMC-C2C-C3C	3.09	130.78	124.94
31	H	102	DGD	C3D-C4D-C5D	-3.09	104.72	110.24
31	C	516	DGD	O2D-C2D-C1D	-3.09	102.54	110.05
22	c	511	CLA	CHB-C4A-NA	3.09	128.78	124.51
35	F	101	HEM	CMD-C2D-C1D	-3.09	123.72	128.46
22	c	506	CLA	CBC-CAC-C3C	-3.09	104.41	112.27
22	C	507	CLA	CMB-C2B-C3B	3.07	130.43	124.68
24	K	101	BCR	C35-C13-C14	-3.07	118.62	122.92
22	b	606	CLA	CGD-CBD-CAD	-3.07	100.79	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	513	CLA	CHB-C4A-NA	3.07	128.76	124.51
31	h	101	DGD	C4D-C3D-C2D	-3.07	105.47	110.82
22	b	605	CLA	O1D-CGD-CBD	3.06	130.75	124.48
22	c	512	CLA	CHB-C4A-NA	3.06	128.74	124.51
24	t	101	BCR	C3-C4-C5	-3.04	108.65	114.08
30	D	409	LHG	O8-C23-C24	3.04	121.45	111.91
24	a	405	BCR	C27-C26-C25	3.04	127.14	122.73
22	B	605	CLA	CMD-C2D-C3D	3.04	130.36	124.68
24	b	619	BCR	C2-C1-C6	3.03	115.15	110.48
22	B	616	CLA	CHB-C4A-NA	3.03	128.71	124.51
30	d	407	LHG	O8-C23-O10	-3.03	115.94	123.59
29	B	623	SQD	O8-S-C6	3.03	110.57	105.74
31	C	516	DGD	O6D-C1D-O3G	-3.03	102.79	109.97
22	b	616	CLA	C1B-CHB-C4A	-3.03	124.12	130.12
29	A	415	SQD	O48-C23-C24	3.03	121.41	111.91
22	B	605	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
22	b	613	CLA	O2A-CGA-O1A	-3.02	115.97	123.59
28	d	410	LMG	O6-C1-O1	-3.02	102.83	109.97
28	d	410	LMG	O1-C1-C2	-3.02	103.59	108.30
22	d	403	CLA	CMD-C2D-C3D	3.02	130.32	124.68
22	c	503	CLA	CMD-C2D-C3D	3.01	130.32	124.68
24	x	101	BCR	C38-C26-C25	-3.01	121.14	124.53
27	d	406	PL9	C7-C3-C2	-3.01	119.34	123.30
22	a	402	CLA	C1B-CHB-C4A	-3.00	124.17	130.12
22	c	510	CLA	CMD-C2D-C3D	3.00	130.30	124.68
22	b	603	CLA	C1B-CHB-C4A	-3.00	124.18	130.12
31	C	515	DGD	O6D-C1D-O3G	-2.99	102.88	109.97
27	A	410	PL9	C22-C23-C24	-2.99	120.45	127.66
22	b	605	CLA	C1-C2-C3	-2.98	120.88	126.04
28	A	412	LMG	C1-O6-C5	-2.98	107.83	113.69
22	a	403	CLA	O2D-CGD-CBD	2.98	116.57	111.27
23	A	404	PHO	O2D-CGD-O1D	-2.98	118.01	123.84
22	c	507	CLA	C4D-C3D-CAD	-2.98	106.81	108.47
22	b	601	CLA	O2D-CGD-CBD	2.98	116.56	111.27
24	B	617	BCR	C2-C1-C6	2.97	115.05	110.48
29	B	623	SQD	O48-C23-C24	2.97	121.23	111.91
27	d	406	PL9	C22-C23-C24	-2.97	120.52	127.66
22	C	503	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
28	A	412	LMG	C38-C37-C36	-2.97	99.37	114.42
22	d	403	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
22	c	507	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
23	d	402	PHO	O2D-CGD-O1D	-2.96	118.06	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	611	CLA	C4A-NA-C1A	2.95	108.03	106.71
24	A	406	BCR	C38-C26-C25	-2.95	121.22	124.53
22	C	502	CLA	C1-C2-C3	-2.94	120.95	126.04
24	t	101	BCR	C7-C8-C9	-2.93	121.80	126.23
22	b	613	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
22	C	506	CLA	C4D-C3D-CAD	-2.92	106.84	108.47
22	B	612	CLA	O2A-CGA-O1A	-2.92	116.22	123.59
22	b	604	CLA	CMB-C2B-C3B	2.92	130.14	124.68
22	b	605	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
24	H	101	BCR	C2-C1-C6	2.91	114.96	110.48
22	B	615	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
31	h	101	DGD	C3D-C4D-C5D	-2.91	105.06	110.24
22	c	507	CLA	O2A-CGA-O1A	-2.91	116.26	123.59
24	Y	101	BCR	C27-C26-C25	2.90	126.95	122.73
27	A	410	PL9	C25-C24-C26	2.90	120.15	115.27
22	B	609	CLA	CMB-C2B-C1B	-2.90	124.00	128.46
22	C	513	CLA	CMB-C2B-C3B	2.90	130.10	124.68
24	H	101	BCR	C37-C22-C21	-2.90	118.86	122.92
22	D	402	CLA	C4-C3-C5	2.90	120.14	115.27
22	B	610	CLA	O2D-CGD-CBD	2.89	116.40	111.27
22	b	612	CLA	CHB-C4A-NA	2.89	128.51	124.51
22	b	609	CLA	CMB-C2B-C3B	2.89	130.08	124.68
24	K	102	BCR	C37-C22-C21	-2.89	118.88	122.92
28	M	101	LMG	C1-C2-C3	-2.89	103.98	110.00
29	a	411	SQD	C1-O5-C5	-2.89	108.02	113.69
22	c	502	CLA	C1-C2-C3	-2.88	121.06	126.04
27	A	410	PL9	O2-C1-C6	2.88	125.58	120.59
31	C	515	DGD	C3G-C2G-C1G	-2.88	104.97	111.79
22	C	501	CLA	O2A-CGA-O1A	-2.88	116.32	123.59
22	B	609	CLA	OBD-CAD-CBD	-2.88	121.78	125.89
22	a	404	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
22	A	411	CLA	CHB-C4A-NA	2.88	128.49	124.51
22	B	615	CLA	CMB-C2B-C3B	2.87	130.05	124.68
22	c	509	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
22	c	503	CLA	CMB-C2B-C3B	2.87	130.05	124.68
36	V	201	HEC	CMB-C2B-C1B	-2.87	124.06	128.46
22	b	607	CLA	C4D-C3D-CAD	-2.87	106.87	108.47
22	c	512	CLA	CMD-C2D-C3D	2.86	130.03	124.68
29	A	413	SQD	O47-C7-O49	-2.86	116.79	123.70
28	D	406	LMG	O6-C1-O1	-2.86	103.20	109.97
22	C	513	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
34	C	521	STE	C4-C3-C2	-2.85	102.66	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	610	CLA	CMD-C2D-C3D	2.85	130.01	124.68
22	b	605	CLA	CMB-C2B-C3B	2.85	130.01	124.68
24	b	617	BCR	C36-C18-C17	-2.85	118.93	122.92
22	b	612	CLA	C1B-CHB-C4A	-2.85	124.48	130.12
22	a	403	CLA	CMD-C2D-C3D	2.85	130.00	124.68
28	b	622	LMG	C1-O6-C5	-2.84	108.10	113.69
22	c	503	CLA	C7-C6-C5	-2.84	105.64	113.36
22	b	614	CLA	CMB-C2B-C3B	2.84	130.00	124.68
22	c	504	CLA	O2A-CGA-O1A	-2.84	116.42	123.59
22	b	614	CLA	CHB-C4A-NA	2.84	128.44	124.51
24	B	617	BCR	C15-C16-C17	-2.84	117.66	123.47
22	b	613	CLA	CMD-C2D-C3D	2.83	129.97	124.68
27	D	405	PL9	C37-C38-C39	-2.83	120.84	127.66
29	a	412	SQD	O49-C7-C8	-2.83	112.69	123.73
31	C	516	DGD	C4E-C3E-C2E	-2.83	105.89	110.82
22	c	507	CLA	CMC-C2C-C3C	2.83	130.27	124.94
29	B	623	SQD	O9-S-C6	2.82	110.30	106.94
24	T	101	BCR	C27-C26-C25	2.82	126.83	122.73
22	C	513	CLA	CMD-C2D-C3D	2.82	129.96	124.68
24	x	101	BCR	C27-C26-C25	2.82	126.82	122.73
22	c	513	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
24	d	405	BCR	C27-C26-C25	2.82	126.82	122.73
28	b	622	LMG	C38-C37-C36	-2.82	100.12	114.42
24	K	101	BCR	C11-C10-C9	-2.82	123.29	127.31
24	b	619	BCR	C36-C18-C17	-2.81	118.98	122.92
22	b	614	CLA	C4-C3-C5	2.81	120.00	115.27
22	B	611	CLA	CHB-C4A-NA	2.81	128.40	124.51
22	c	506	CLA	OBD-CAD-CBD	-2.81	121.89	125.89
24	b	619	BCR	C29-C30-C25	2.81	114.80	110.48
36	v	201	HEC	CBA-CAA-C2A	-2.80	107.31	112.48
31	c	516	DGD	O2G-C1B-O1B	-2.80	116.93	123.70
22	c	511	CLA	CMB-C2B-C1B	-2.80	124.16	128.46
22	C	506	CLA	CMD-C2D-C3D	2.80	129.91	124.68
31	c	516	DGD	O3E-C3E-C2E	-2.80	103.89	110.35
35	F	101	HEM	CAD-CBD-CGD	2.79	117.36	112.67
22	C	501	CLA	OBD-CAD-CBD	-2.79	121.90	125.89
22	C	507	CLA	C2A-C1A-CHA	2.79	128.74	123.86
30	d	408	LHG	C20-C19-C18	-2.79	100.25	114.42
22	c	502	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
22	b	615	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
22	B	616	CLA	O2A-C1-C2	2.79	115.96	108.64
24	a	405	BCR	C29-C30-C25	2.79	114.77	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	403	CLA	C1B-CHB-C4A	-2.78	124.60	130.12
29	f	101	SQD	O48-C23-O10	-2.78	116.57	123.59
28	D	406	LMG	O3-C3-C2	-2.78	103.92	110.35
29	b	620	SQD	O9-S-O7	-2.78	104.33	113.95
22	d	403	CLA	CHB-C4A-NA	2.78	128.35	124.51
28	b	624	LMG	O5-C6-C5	-2.78	101.77	111.29
24	k	102	BCR	C11-C10-C9	-2.77	123.35	127.31
31	C	515	DGD	O1G-C1A-C2A	-2.77	103.21	111.91
31	c	518	DGD	O3E-C3E-C2E	-2.77	103.95	110.35
22	B	603	CLA	OBD-CAD-CBD	-2.77	121.94	125.89
22	b	614	CLA	C1-C2-C3	-2.76	121.26	126.04
22	b	601	CLA	CMB-C2B-C3B	2.76	129.84	124.68
22	B	605	CLA	C7-C6-C5	-2.76	105.86	113.36
22	b	614	CLA	OBD-CAD-CBD	-2.76	121.95	125.89
24	c	515	BCR	C27-C26-C25	2.76	126.74	122.73
28	c	521	LMG	O3-C3-C2	-2.76	103.97	110.35
22	b	612	CLA	O2A-CGA-O1A	-2.76	116.63	123.59
22	B	603	CLA	O2A-CGA-O1A	-2.75	116.64	123.59
22	B	614	CLA	OBD-CAD-CBD	-2.75	121.96	125.89
22	c	505	CLA	OBD-CAD-CBD	-2.75	121.96	125.89
28	a	416	LMG	O6-C1-C2	-2.75	104.52	110.35
24	k	102	BCR	C27-C26-C25	2.75	126.72	122.73
22	b	608	CLA	CMD-C2D-C3D	2.75	129.82	124.68
31	H	102	DGD	C3E-C4E-C5E	-2.75	105.33	110.24
22	B	609	CLA	OBD-CAD-C3D	2.75	132.54	127.98
22	B	601	CLA	CMD-C2D-C3D	2.75	129.82	124.68
31	c	517	DGD	O3D-C3D-C4D	-2.75	104.00	110.35
22	a	410	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
24	A	406	BCR	C27-C26-C25	2.74	126.71	122.73
28	d	410	LMG	O2-C2-C1	-2.74	103.39	110.05
31	h	101	DGD	C3G-C2G-C1G	-2.74	105.31	111.79
29	f	101	SQD	C3-C4-C5	2.74	115.13	110.24
28	c	521	LMG	O7-C10-O9	-2.74	117.08	123.70
31	h	101	DGD	C4E-C3E-C2E	-2.74	106.04	110.82
22	B	616	CLA	O1D-CGD-CBD	2.74	130.08	124.48
22	B	606	CLA	CMD-C2D-C3D	2.73	129.79	124.68
24	a	405	BCR	C7-C8-C9	-2.73	122.11	126.23
22	C	511	CLA	CMB-C2B-C3B	2.73	129.78	124.68
22	a	410	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
22	C	504	CLA	CMC-C2C-C3C	2.72	130.07	124.94
22	C	510	CLA	CMD-C2D-C3D	2.72	129.76	124.68
22	A	402	CLA	O2D-CGD-O1D	-2.72	118.53	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	405	BCR	C30-C25-C26	-2.72	118.79	122.61
22	C	512	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
29	D	407	SQD	O8-S-O9	-2.71	104.64	111.27
22	C	503	CLA	C1B-CHB-C4A	-2.71	124.74	130.12
27	d	406	PL9	C7-C8-C9	-2.71	122.28	126.79
24	b	618	BCR	C27-C26-C25	2.71	126.66	122.73
23	A	404	PHO	CHD-C1D-ND	-2.71	118.94	124.58
22	C	508	CLA	CMC-C2C-C3C	2.71	130.05	124.94
22	b	610	CLA	CHB-C4A-NA	2.71	128.26	124.51
30	A	414	LHG	O8-C23-C24	2.71	120.40	111.91
22	B	604	CLA	C11-C12-C13	-2.70	107.18	115.92
27	a	409	PL9	C26-C24-C23	-2.70	115.64	121.12
22	C	512	CLA	CHB-C4A-NA	2.70	128.25	124.51
22	b	615	CLA	CHB-C4A-NA	2.70	128.25	124.51
22	B	603	CLA	C3B-C4B-NB	-2.70	105.72	109.21
22	b	609	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
23	d	402	PHO	C1-C2-C3	-2.70	121.37	126.04
22	B	611	CLA	OBD-CAD-CBD	-2.70	122.04	125.89
22	a	404	CLA	OBD-CAD-CBD	-2.70	122.04	125.89
24	a	405	BCR	C37-C22-C23	2.70	122.33	118.08
22	b	614	CLA	C1B-CHB-C4A	-2.70	124.78	130.12
24	d	405	BCR	C38-C26-C25	-2.69	121.50	124.53
30	B	622	LHG	O3-P-O5	-2.69	98.54	109.07
22	C	504	CLA	CMB-C2B-C3B	2.69	129.72	124.68
22	b	610	CLA	C1-C2-C3	-2.69	121.39	126.04
22	c	504	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
28	c	519	LMG	C40-C39-C38	-2.69	100.76	114.42
28	c	521	LMG	O1-C1-C2	-2.69	104.10	108.30
22	B	612	CLA	C11-C12-C13	-2.69	107.23	115.92
24	c	515	BCR	C38-C26-C25	-2.69	121.51	124.53
24	k	101	BCR	C38-C26-C25	-2.68	121.52	124.53
22	B	604	CLA	O2D-CGD-CBD	2.68	116.03	111.27
31	H	102	DGD	C4D-C3D-C2D	-2.68	106.14	110.82
30	D	408	LHG	O8-C23-C24	2.68	120.31	111.91
22	d	403	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
23	D	401	PHO	O1D-CGD-CBD	2.68	129.96	124.48
22	B	614	CLA	CMB-C2B-C3B	2.68	129.68	124.68
24	t	101	BCR	C2-C1-C6	2.67	114.60	110.48
22	d	403	CLA	CMB-C2B-C3B	2.67	129.68	124.68
27	A	410	PL9	C20-C19-C21	2.67	119.77	115.27
22	B	611	CLA	CMD-C2D-C3D	2.67	129.68	124.68
22	c	508	CLA	C1B-CHB-C4A	-2.67	124.83	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	412	LMG	O6-C1-O1	-2.67	103.65	109.97
22	C	502	CLA	OBD-CAD-CBD	-2.67	122.08	125.89
22	B	610	CLA	CMB-C2B-C1B	-2.67	124.36	128.46
22	B	612	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
22	b	608	CLA	CHB-C4A-NA	2.67	128.20	124.51
27	A	410	PL9	O2-C1-C2	-2.66	115.69	121.78
29	b	620	SQD	O48-C23-C24	2.66	120.25	111.91
22	c	503	CLA	C4D-C3D-CAD	-2.66	106.99	108.47
24	B	619	BCR	C29-C30-C25	2.66	114.57	110.48
31	C	515	DGD	CDB-CCB-CBB	-2.66	100.94	114.42
24	D	404	BCR	C27-C26-C25	2.65	126.58	122.73
22	D	402	CLA	CMC-C2C-C3C	2.65	129.94	124.94
31	H	102	DGD	O2G-C1B-O1B	-2.65	117.29	123.70
28	b	624	LMG	C3-C4-C5	-2.65	105.51	110.24
22	B	604	CLA	OBD-CAD-C3D	2.65	132.38	127.98
22	D	402	CLA	OBD-CAD-CBD	-2.65	122.11	125.89
22	c	508	CLA	CHB-C4A-NA	2.65	128.17	124.51
22	B	604	CLA	CHB-C4A-NA	2.64	128.17	124.51
31	c	516	DGD	O6E-C5E-C4E	2.64	114.49	109.69
22	B	616	CLA	C1-O2A-CGA	2.64	123.37	116.44
24	B	618	BCR	C15-C16-C17	-2.64	118.07	123.47
29	a	411	SQD	O47-C7-C8	2.64	117.18	111.50
22	a	402	CLA	C7-C6-C5	-2.64	106.20	113.36
29	B	623	SQD	O9-S-O7	-2.63	104.84	113.95
29	b	620	SQD	C3-C4-C5	2.63	114.94	110.24
28	c	522	LMG	O6-C1-O1	-2.63	103.74	109.97
30	B	622	LHG	O8-C23-O10	-2.63	116.95	123.59
29	A	413	SQD	O8-S-C6	2.63	109.93	105.74
22	C	507	CLA	C4-C3-C2	-2.63	116.93	123.68
22	b	612	CLA	C11-C12-C13	-2.63	107.43	115.92
22	a	403	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
28	c	522	LMG	C40-C39-C38	-2.63	101.10	114.42
31	H	102	DGD	C1D-C2D-C3D	-2.63	104.53	110.00
22	b	608	CLA	O2D-CGD-CBD	2.62	115.93	111.27
22	b	610	CLA	C11-C12-C13	-2.62	107.44	115.92
22	b	607	CLA	C6-C7-C8	-2.62	107.45	115.92
31	c	516	DGD	O2D-C2D-C1D	-2.62	103.68	110.05
22	a	404	CLA	CMD-C2D-C3D	2.62	129.58	124.68
22	b	607	CLA	OBD-CAD-CBD	-2.62	122.15	125.89
22	C	513	CLA	C4D-C3D-CAD	-2.62	107.01	108.47
22	B	616	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
31	c	518	DGD	C1D-C2D-C3D	-2.62	104.55	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	620	SQD	O2-C2-C1	2.62	116.40	110.05
23	D	401	PHO	C1B-NB-C4B	2.62	111.44	106.51
22	b	603	CLA	C7-C6-C5	-2.61	106.26	113.36
24	k	102	BCR	C16-C15-C14	-2.61	118.13	123.47
30	d	407	LHG	C11-C10-C9	-2.61	101.18	114.42
24	D	404	BCR	C38-C26-C25	-2.61	121.60	124.53
27	D	405	PL9	C35-C34-C36	2.61	119.66	115.27
24	D	404	BCR	C24-C23-C22	-2.61	122.30	126.23
22	B	614	CLA	CHB-C4A-NA	2.60	128.11	124.51
30	e	102	LHG	C20-C19-C18	-2.60	101.21	114.42
22	c	506	CLA	C4-C3-C2	-2.60	117.00	123.68
22	c	506	CLA	OBD-CAD-C3D	2.60	132.30	127.98
24	A	406	BCR	C37-C22-C21	-2.60	119.28	122.92
22	B	606	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
22	a	410	CLA	C2A-C1A-CHA	2.59	128.39	123.86
22	c	501	CLA	CHB-C4A-NA	2.59	128.10	124.51
24	b	617	BCR	C15-C16-C17	-2.59	118.17	123.47
27	d	406	PL9	C30-C29-C31	-2.59	110.92	115.27
29	A	413	SQD	O48-C23-C24	2.59	120.02	111.91
22	b	606	CLA	O1D-CGD-CBD	2.58	129.77	124.48
31	c	518	DGD	O6D-C1D-O3G	-2.58	103.86	109.97
28	a	416	LMG	O5-C6-C5	-2.58	102.44	111.29
24	B	618	BCR	C2-C1-C6	2.58	114.45	110.48
22	B	606	CLA	CMB-C2B-C3B	2.58	129.51	124.68
29	f	101	SQD	C1-O5-C5	-2.58	108.63	113.69
30	l	101	LHG	O8-C23-C24	2.58	120.00	111.91
22	B	602	CLA	CMC-C2C-C3C	2.58	129.80	124.94
22	A	403	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
22	b	609	CLA	OBD-CAD-C3D	2.58	132.26	127.98
22	c	512	CLA	O1D-CGD-CBD	2.58	129.75	124.48
31	c	516	DGD	CDB-CCB-CBB	-2.57	101.36	114.42
29	b	620	SQD	O5-C5-C4	2.57	114.37	109.69
22	B	606	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
22	C	506	CLA	CHB-C4A-NA	2.57	128.07	124.51
31	c	516	DGD	O3D-C3D-C4D	-2.57	104.41	110.35
22	B	608	CLA	CHB-C4A-NA	2.57	128.06	124.51
22	c	512	CLA	CMB-C2B-C1B	-2.57	124.52	128.46
22	B	602	CLA	C4A-NA-C1A	2.57	107.86	106.71
22	b	606	CLA	C6-C5-C3	-2.56	106.73	113.45
31	A	416	DGD	C4E-C3E-C2E	-2.56	106.35	110.82
24	b	618	BCR	C38-C26-C25	-2.56	121.65	124.53
31	C	517	DGD	O3E-C3E-C2E	-2.56	104.43	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	V	201	HEC	CMC-C2C-C3C	2.56	128.83	125.82
23	A	404	PHO	C1B-NB-C4B	2.56	111.33	106.51
22	b	603	CLA	O1D-CGD-CBD	2.56	129.72	124.48
22	b	602	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
22	C	512	CLA	CMC-C2C-C3C	2.55	129.76	124.94
22	C	509	CLA	C1-C2-C3	-2.55	121.63	126.04
31	c	516	DGD	O6D-C1D-C2D	2.55	115.75	110.35
24	b	619	BCR	C37-C22-C21	-2.55	119.35	122.92
31	A	416	DGD	O6D-C1D-O3G	-2.55	103.94	109.97
22	C	504	CLA	OBD-CAD-CBD	-2.55	122.25	125.89
23	D	401	PHO	C3C-C4C-NC	-2.55	106.33	110.28
27	D	405	PL9	C12-C13-C14	-2.55	121.53	127.66
22	c	508	CLA	C4D-C3D-CAD	-2.55	107.05	108.47
24	a	405	BCR	C38-C26-C27	-2.55	108.72	113.62
22	d	403	CLA	C4-C3-C5	2.54	119.55	115.27
22	B	614	CLA	CHA-C1A-NA	-2.54	120.57	126.40
27	a	409	PL9	C27-C28-C29	-2.54	121.54	127.66
22	b	603	CLA	O2A-CGA-O1A	-2.54	117.18	123.59
22	b	616	CLA	CMD-C2D-C3D	2.54	129.43	124.68
22	c	501	CLA	O2A-CGA-O1A	-2.54	117.19	123.59
24	c	514	BCR	C15-C16-C17	-2.53	118.28	123.47
24	c	514	BCR	C27-C26-C25	2.53	126.41	122.73
22	A	411	CLA	CMD-C2D-C3D	2.53	129.41	124.68
22	C	510	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
23	A	404	PHO	CBD-CHA-C4D	-2.53	105.69	108.54
22	A	402	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
31	c	517	DGD	O6D-C1D-O3G	-2.53	103.99	109.97
22	C	510	CLA	CHB-C4A-NA	2.52	128.00	124.51
24	H	101	BCR	C37-C22-C23	2.52	122.05	118.08
22	B	601	CLA	OBD-CAD-C3D	2.52	132.16	127.98
31	c	516	DGD	O5E-C6E-C5E	-2.52	102.65	111.29
24	K	101	BCR	C36-C18-C17	-2.52	119.40	122.92
22	c	509	CLA	OBD-CAD-CBD	-2.52	122.30	125.89
31	c	518	DGD	CDB-CCB-CBB	-2.52	101.66	114.42
29	b	620	SQD	O5-C1-C2	-2.52	105.03	110.35
22	c	509	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
24	H	101	BCR	C27-C26-C25	2.51	126.38	122.73
22	b	601	CLA	CMC-C2C-C3C	2.51	129.68	124.94
24	B	617	BCR	C27-C26-C25	2.51	126.38	122.73
29	a	411	SQD	C1-C2-C3	-2.51	104.77	110.00
30	d	409	LHG	C26-C25-C24	2.51	122.21	113.19
22	a	404	CLA	C1B-CHB-C4A	-2.51	125.15	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	616	CLA	C5-C3-C2	2.51	126.19	121.12
22	B	611	CLA	C7-C6-C5	-2.51	106.55	113.36
27	a	409	PL9	C7-C8-C9	-2.51	122.62	126.79
22	B	616	CLA	OBD-CAD-CBD	-2.51	122.31	125.89
22	c	508	CLA	C7-C6-C5	-2.50	106.56	113.36
22	c	505	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
24	A	406	BCR	C36-C18-C19	2.50	122.02	118.08
28	b	622	LMG	C9-C8-C7	-2.50	105.87	111.79
24	B	619	BCR	C1-C6-C5	-2.50	119.09	122.61
24	C	514	BCR	C15-C14-C13	-2.50	123.74	127.31
29	D	407	SQD	C46-C45-C44	-2.50	105.39	113.70
22	c	513	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
24	K	101	BCR	C2-C1-C6	2.50	114.32	110.48
22	d	404	CLA	CHA-C1A-NA	-2.49	120.69	126.40
22	B	602	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
29	D	407	SQD	O48-C23-O10	-2.49	117.30	123.59
22	d	404	CLA	O2A-CGA-O1A	-2.49	117.30	123.59
24	b	617	BCR	C8-C7-C6	-2.49	120.21	127.20
22	a	410	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	B	616	CLA	C2A-C3A-C4A	2.49	105.88	101.87
22	B	611	CLA	C1-C2-C3	-2.48	121.75	126.04
22	D	403	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
22	b	602	CLA	CMC-C2C-C3C	2.48	129.61	124.94
22	b	603	CLA	O2A-C1-C2	-2.48	102.13	108.64
22	C	508	CLA	O2D-CGD-CBD	2.47	115.66	111.27
29	b	620	SQD	O48-C23-O10	-2.47	117.35	123.59
24	A	406	BCR	C2-C1-C6	2.47	114.29	110.48
22	b	603	CLA	C4-C3-C5	2.47	119.43	115.27
22	B	607	CLA	C4-C3-C5	2.47	119.43	115.27
22	b	611	CLA	CED-O2D-CGD	-2.47	110.35	115.94
31	c	516	DGD	O3G-C3G-C2G	-2.47	104.94	110.90
22	c	506	CLA	CHB-C4A-NA	2.47	127.92	124.51
24	k	102	BCR	C37-C22-C21	-2.47	119.47	122.92
22	C	506	CLA	CHA-C1A-NA	-2.46	120.75	126.40
30	B	621	LHG	C27-C26-C25	-2.46	101.93	114.42
24	B	618	BCR	C40-C30-C25	2.46	114.29	110.30
22	c	503	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
22	a	404	CLA	O2D-CGD-CBD	2.46	115.64	111.27
28	D	406	LMG	C1-C2-C3	-2.46	104.88	110.00
31	A	416	DGD	O3G-C3G-C2G	-2.46	104.97	110.90
31	c	516	DGD	O1G-C1A-C2A	-2.46	104.20	111.91
31	h	101	DGD	O3E-C3E-C2E	-2.46	104.67	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	D	403	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
22	A	405	CLA	CMD-C2D-C3D	2.45	129.26	124.68
22	D	402	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
22	c	507	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	c	508	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
31	c	517	DGD	O3G-C1D-C2D	-2.45	104.48	108.30
29	A	413	SQD	O5-C1-O6	2.45	115.77	109.97
30	B	622	LHG	C20-C19-C18	-2.45	102.01	114.42
24	b	618	BCR	C31-C1-C6	2.44	114.26	110.30
29	b	620	SQD	C1-O5-C5	-2.44	108.89	113.69
24	c	515	BCR	C7-C8-C9	-2.44	122.54	126.23
22	B	615	CLA	O2A-CGA-O1A	-2.44	117.42	123.59
22	c	506	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
24	t	101	BCR	C37-C22-C23	2.44	121.92	118.08
31	A	416	DGD	O6E-C5E-C4E	2.44	114.12	109.69
28	C	518	LMG	C38-C37-C36	-2.44	102.05	114.42
22	B	607	CLA	O2A-C1-C2	-2.44	102.23	108.64
22	B	607	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
24	B	617	BCR	C37-C22-C21	-2.44	119.51	122.92
27	d	406	PL9	C31-C32-C33	-2.43	103.88	111.88
22	B	605	CLA	O1D-CGD-CBD	2.43	129.46	124.48
31	H	102	DGD	O3E-C3E-C2E	-2.43	104.73	110.35
31	H	102	DGD	C7B-C6B-C5B	-2.43	102.08	114.42
24	d	405	BCR	C24-C23-C22	-2.43	122.56	126.23
29	B	623	SQD	C3-C4-C5	2.43	114.58	110.24
24	b	619	BCR	C15-C16-C17	-2.43	118.50	123.47
22	A	405	CLA	CMC-C2C-C3C	2.43	129.52	124.94
24	b	617	BCR	C29-C30-C25	2.43	114.22	110.48
31	c	517	DGD	C3E-C4E-C5E	-2.42	105.91	110.24
27	A	410	PL9	C31-C32-C33	-2.42	103.92	111.88
22	C	506	CLA	O1D-CGD-CBD	2.42	129.44	124.48
29	D	407	SQD	C1-C2-C3	-2.42	104.96	110.00
22	B	615	CLA	C2A-C3A-C4A	2.42	105.78	101.87
29	A	413	SQD	O7-S-C6	2.41	109.81	106.94
29	D	407	SQD	O9-S-O7	-2.41	105.59	113.95
27	D	405	PL9	C36-C34-C33	-2.41	116.23	121.12
22	b	605	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
27	d	406	PL9	C20-C19-C21	2.41	119.32	115.27
22	B	612	CLA	O1D-CGD-CBD	2.41	129.41	124.48
24	c	514	BCR	C37-C22-C21	-2.41	119.55	122.92
22	B	604	CLA	CMC-C2C-C3C	2.40	129.47	124.94
22	b	606	CLA	C1B-CHB-C4A	-2.40	125.36	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	506	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
22	b	606	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
24	c	514	BCR	C20-C21-C22	-2.40	123.89	127.31
22	b	610	CLA	CAA-CBA-CGA	-2.40	106.24	113.25
22	b	602	CLA	C4D-C3D-CAD	-2.40	107.13	108.47
22	B	609	CLA	CMB-C2B-C3B	2.40	129.16	124.68
35	F	101	HEM	CMB-C2B-C3B	2.40	129.16	124.68
28	d	410	LMG	O1-C7-C8	-2.40	105.12	110.90
22	c	502	CLA	O1D-CGD-CBD	2.39	129.38	124.48
22	b	608	CLA	OBD-CAD-CBD	-2.39	122.48	125.89
30	l	101	LHG	C11-C10-C9	-2.39	102.30	114.42
28	b	622	LMG	O1-C7-C8	-2.39	105.14	110.90
22	b	606	CLA	C2A-C1A-CHA	2.38	128.03	123.86
22	c	501	CLA	C1B-CHB-C4A	-2.38	125.39	130.12
31	A	416	DGD	O1G-C1A-O1A	-2.38	117.58	123.59
22	b	605	CLA	CMD-C2D-C3D	2.38	129.13	124.68
24	K	101	BCR	C24-C23-C22	-2.38	122.64	126.23
31	c	518	DGD	C6B-C5B-C4B	-2.38	102.36	114.42
29	A	415	SQD	O47-C7-C8	2.38	116.62	111.50
22	c	505	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
31	C	516	DGD	O5D-C6D-C5D	-2.38	104.65	109.05
24	K	101	BCR	C7-C8-C9	-2.38	122.65	126.23
31	C	515	DGD	CCB-CBB-CAB	-2.37	102.37	114.42
31	A	416	DGD	O5D-C6D-C5D	-2.37	104.66	109.05
22	C	509	CLA	CMD-C2D-C3D	2.37	129.11	124.68
22	C	504	CLA	C4-C3-C5	2.37	119.26	115.27
24	C	514	BCR	C7-C8-C9	-2.37	122.66	126.23
27	d	406	PL9	C42-C43-C44	-2.37	121.97	127.66
22	C	513	CLA	CHB-C4A-NA	2.36	127.78	124.51
27	D	405	PL9	C20-C19-C21	2.36	119.25	115.27
30	e	102	LHG	C11-C10-C9	-2.36	102.43	114.42
24	b	618	BCR	C37-C22-C21	-2.36	119.62	122.92
22	B	603	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
22	B	609	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
22	a	402	CLA	CHB-C4A-NA	2.36	127.77	124.51
31	C	516	DGD	CDB-CCB-CBB	-2.36	102.45	114.42
22	c	509	CLA	CHB-C4A-NA	2.36	127.77	124.51
22	B	601	CLA	O2D-CGD-CBD	2.36	115.46	111.27
22	c	509	CLA	O1D-CGD-CBD	2.36	129.31	124.48
22	C	505	CLA	CGD-CBD-CAD	-2.36	103.10	110.73
22	B	610	CLA	CHB-C4A-NA	2.36	127.77	124.51
27	d	406	PL9	C15-C14-C13	-2.35	117.64	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	508	CLA	CHB-C4A-NA	2.35	127.77	124.51
27	D	405	PL9	C41-C39-C38	-2.35	116.36	121.12
22	B	605	CLA	CHB-C4A-NA	2.35	127.76	124.51
28	c	519	LMG	O2-C2-C1	-2.35	104.34	110.05
22	b	616	CLA	C4-C3-C5	2.35	119.22	115.27
24	k	101	BCR	C27-C26-C25	2.35	126.14	122.73
31	c	518	DGD	O5D-C1E-C2E	2.34	111.96	108.30
22	B	603	CLA	CHB-C4A-NA	2.34	127.75	124.51
22	C	505	CLA	C4D-C3D-CAD	-2.34	107.17	108.47
29	f	101	SQD	O5-C1-O6	2.34	115.52	109.97
22	A	403	CLA	C3D-CAD-CBD	-2.34	104.53	107.61
22	B	602	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
22	b	603	CLA	OBD-CAD-CBD	-2.33	122.56	125.89
24	a	405	BCR	C15-C16-C17	-2.33	118.69	123.47
22	B	605	CLA	OBD-CAD-C3D	2.33	131.85	127.98
22	A	403	CLA	CED-O2D-CGD	-2.33	110.66	115.94
28	c	519	LMG	C1-O6-C5	-2.33	109.11	113.69
28	c	521	LMG	O2-C2-C1	-2.33	104.38	110.05
22	c	510	CLA	O1D-CGD-CBD	2.33	129.25	124.48
24	b	619	BCR	C12-C13-C14	-2.33	115.37	118.94
22	A	402	CLA	CAA-CBA-CGA	-2.33	106.45	113.25
24	c	515	BCR	C15-C16-C17	-2.33	118.70	123.47
27	a	409	PL9	C36-C34-C33	-2.33	116.41	121.12
30	D	408	LHG	C29-C28-C27	-2.33	102.61	114.42
22	a	402	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
22	b	604	CLA	C4D-C3D-CAD	-2.32	107.18	108.47
31	c	518	DGD	C3D-C4D-C5D	-2.32	106.11	110.24
29	B	623	SQD	C1-O5-C5	-2.31	109.14	113.69
30	A	414	LHG	C11-C10-C9	-2.31	102.68	114.42
28	C	518	LMG	O6-C1-O1	-2.31	104.50	109.97
24	K	101	BCR	C27-C26-C25	2.31	126.09	122.73
22	c	508	CLA	CMD-C2D-C3D	2.31	129.00	124.68
22	c	510	CLA	OBD-CAD-C3D	2.31	131.82	127.98
29	a	411	SQD	O5-C5-C4	2.31	113.89	109.69
22	B	608	CLA	C6-C7-C8	-2.31	108.46	115.92
24	Y	101	BCR	C16-C15-C14	-2.31	118.75	123.47
31	C	515	DGD	C6D-O5D-C1E	2.31	118.25	113.74
22	c	505	CLA	CMC-C2C-C3C	2.30	129.29	124.94
22	B	606	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
22	b	613	CLA	CHA-C1A-NA	-2.30	121.12	126.40
22	A	411	CLA	CMC-C2C-C3C	2.30	129.28	124.94
22	C	503	CLA	CMD-C2D-C3D	2.30	128.98	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	406	LMG	O2-C2-C1	-2.30	104.46	110.05
28	b	624	LMG	O6-C5-C6	2.30	112.15	106.44
22	d	404	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
29	f	101	SQD	C46-C45-C44	-2.29	106.36	111.79
28	C	518	LMG	O3-C3-C2	-2.29	105.04	110.35
31	c	517	DGD	C3G-O3G-C1D	2.29	118.22	113.74
22	C	507	CLA	CHB-C4A-NA	2.29	127.68	124.51
31	C	516	DGD	C1D-C2D-C3D	-2.29	105.23	110.00
22	B	613	CLA	CHA-C1A-NA	-2.29	121.16	126.40
22	b	616	CLA	O1D-CGD-CBD	2.29	129.17	124.48
29	f	101	SQD	O9-S-C6	2.29	109.66	106.94
22	b	610	CLA	C4D-C3D-CAD	-2.29	107.19	108.47
30	D	408	LHG	C27-C26-C25	-2.29	102.81	114.42
22	C	512	CLA	C1-C2-C3	-2.29	122.09	126.04
22	c	510	CLA	CHB-C4A-NA	2.29	127.67	124.51
24	d	405	BCR	C16-C15-C14	-2.29	118.79	123.47
22	C	503	CLA	O1D-CGD-CBD	2.28	129.16	124.48
28	M	101	LMG	O1-C7-C8	-2.28	105.39	110.90
22	A	403	CLA	CHB-C4A-NA	2.28	127.67	124.51
29	A	415	SQD	O47-C45-C44	2.28	113.15	107.93
22	B	615	CLA	C4-C3-C5	2.28	119.11	115.27
29	b	620	SQD	O8-S-O7	-2.28	105.70	111.27
28	c	519	LMG	O6-C1-O1	-2.28	104.57	109.97
22	B	608	CLA	OBD-CAD-CBD	-2.28	122.64	125.89
22	D	403	CLA	C6-C7-C8	-2.28	108.55	115.92
31	H	102	DGD	C3G-C2G-C1G	-2.28	106.40	111.79
24	b	618	BCR	C36-C18-C17	-2.28	119.73	122.92
22	B	601	CLA	C4-C3-C5	2.27	119.10	115.27
22	C	507	CLA	CMC-C2C-C3C	2.27	129.23	124.94
31	c	517	DGD	O5D-C6D-C5D	-2.27	104.84	109.05
28	D	406	LMG	C3-C4-C5	-2.27	106.19	110.24
30	d	408	LHG	O7-C7-C8	-2.27	106.61	111.50
22	A	405	CLA	CHB-C4A-NA	2.27	127.65	124.51
24	t	101	BCR	C29-C30-C25	2.27	113.97	110.48
24	H	101	BCR	C16-C17-C18	-2.27	124.07	127.31
22	B	610	CLA	OBD-CAD-CBD	-2.27	122.65	125.89
22	A	405	CLA	C4-C3-C5	2.27	119.09	115.27
22	B	614	CLA	C1-C2-C3	-2.27	122.12	126.04
27	D	405	PL9	C32-C33-C34	-2.27	122.20	127.66
22	B	607	CLA	CED-O2D-CGD	2.27	121.06	115.94
22	b	612	CLA	C4D-C3D-CAD	-2.27	107.21	108.47
22	D	403	CLA	C4D-C3D-CAD	-2.26	107.21	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	405	PL9	C11-C12-C13	-2.26	104.44	111.88
24	B	617	BCR	C37-C22-C23	2.26	121.64	118.08
22	b	609	CLA	CMC-C2C-C3C	2.26	129.20	124.94
22	D	403	CLA	CMD-C2D-C3D	2.26	128.90	124.68
22	a	410	CLA	O2D-CGD-CBD	2.26	115.28	111.27
28	M	101	LMG	O3-C3-C2	-2.26	105.13	110.35
30	A	414	LHG	C20-C19-C18	-2.26	102.97	114.42
28	c	519	LMG	C9-C8-C7	-2.25	106.45	111.79
22	B	614	CLA	O1D-CGD-CBD	2.25	129.10	124.48
31	C	515	DGD	O3E-C3E-C2E	-2.25	105.14	110.35
22	a	402	CLA	CGD-CBD-CAD	-2.25	103.44	110.73
22	c	513	CLA	CMD-C2D-C3D	2.25	128.89	124.68
22	C	509	CLA	C4D-C3D-CAD	-2.25	107.22	108.47
22	c	501	CLA	CED-O2D-CGD	-2.25	110.85	115.94
22	C	509	CLA	C2A-C1A-CHA	2.25	127.79	123.86
22	B	616	CLA	CMD-C2D-C3D	2.25	128.88	124.68
31	c	516	DGD	O6D-C1D-O3G	-2.25	104.65	109.97
22	b	602	CLA	C11-C12-C13	-2.25	108.66	115.92
31	A	416	DGD	CBB-CAB-C9B	-2.24	103.03	114.42
22	b	610	CLA	O2D-CGD-CBD	2.24	115.25	111.27
27	A	410	PL9	C7-C8-C9	-2.24	123.06	126.79
22	C	504	CLA	CMD-C2D-C3D	2.24	128.87	124.68
22	B	601	CLA	CHB-C4A-NA	2.24	127.61	124.51
28	D	406	LMG	O8-C28-O10	-2.24	117.94	123.59
22	b	614	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
24	b	617	BCR	C38-C26-C25	-2.24	122.01	124.53
24	A	406	BCR	C15-C16-C17	-2.24	118.89	123.47
28	c	521	LMG	C42-C41-C40	-2.24	103.06	114.42
29	D	407	SQD	O5-C5-C4	2.24	113.76	109.69
22	a	410	CLA	CMD-C2D-C3D	2.24	128.86	124.68
36	V	201	HEC	CBA-CAA-C2A	-2.23	108.36	112.48
23	D	401	PHO	C7-C6-C5	-2.23	107.30	113.36
22	c	513	CLA	C11-C12-C13	-2.23	108.71	115.92
29	a	411	SQD	O10-C23-C24	-2.23	115.03	123.73
22	C	505	CLA	O1D-CGD-CBD	2.23	129.04	124.48
22	d	404	CLA	O1D-CGD-CBD	2.23	129.04	124.48
30	d	409	LHG	O8-C23-O10	-2.23	117.97	123.59
23	d	401	PHO	CMB-C2B-C1B	-2.23	121.63	125.06
28	b	624	LMG	C40-C39-C38	-2.23	103.12	114.42
23	D	401	PHO	CHB-C1B-NB	2.22	129.20	124.58
31	h	101	DGD	O6D-C1D-O3G	-2.22	104.71	109.97
22	B	606	CLA	C4-C3-C5	2.22	119.01	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	622	LHG	C11-C10-C9	-2.22	103.16	114.42
23	A	404	PHO	O2A-CGA-O1A	-2.22	117.99	123.59
22	b	608	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
22	b	606	CLA	C4D-C3D-CAD	-2.22	107.23	108.47
24	k	102	BCR	C8-C7-C6	-2.22	120.97	127.20
27	D	405	PL9	C50-C49-C48	-2.22	116.24	122.65
22	A	411	CLA	CHA-C1A-NA	-2.22	121.32	126.40
30	d	407	LHG	C20-C19-C18	-2.22	103.17	114.42
27	d	406	PL9	C12-C13-C14	-2.22	122.32	127.66
24	c	514	BCR	C7-C8-C9	-2.22	122.89	126.23
22	B	604	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
23	d	402	PHO	C1B-NB-C4B	2.21	110.68	106.51
22	B	615	CLA	CMD-C2D-C3D	2.21	128.82	124.68
22	c	501	CLA	CMC-C2C-C3C	2.21	129.11	124.94
30	d	407	LHG	C27-C26-C25	-2.21	103.19	114.42
22	b	601	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
24	b	618	BCR	C30-C25-C26	-2.21	119.50	122.61
27	A	410	PL9	C41-C39-C38	-2.21	116.65	121.12
24	K	102	BCR	C38-C26-C25	-2.21	122.05	124.53
28	M	101	LMG	O6-C1-O1	-2.21	104.74	109.97
22	B	601	CLA	C1-O2A-CGA	2.21	122.24	116.44
35	e	101	HEM	CAD-CBD-CGD	2.21	116.38	112.67
22	C	512	CLA	CAA-CBA-CGA	-2.21	106.80	113.25
22	B	610	CLA	CMB-C2B-C3B	2.21	128.81	124.68
24	d	405	BCR	C2-C1-C6	2.21	113.88	110.48
22	C	512	CLA	O2D-CGD-CBD	2.21	115.19	111.27
23	D	401	PHO	C2B-C1B-NB	-2.20	106.47	109.79
22	b	608	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
24	K	102	BCR	C7-C8-C9	-2.20	122.91	126.23
27	a	409	PL9	C11-C12-C13	-2.20	104.65	111.88
22	b	604	CLA	CED-O2D-CGD	-2.20	110.96	115.94
24	t	101	BCR	C31-C1-C6	2.20	113.87	110.30
24	t	101	BCR	C1-C6-C5	-2.20	119.52	122.61
22	b	613	CLA	OBD-CAD-CBD	-2.20	122.76	125.89
22	b	607	CLA	CMC-C2C-C3C	2.19	129.08	124.94
22	C	504	CLA	O1D-CGD-CBD	2.19	128.97	124.48
28	d	410	LMG	O3-C3-C2	-2.19	105.28	110.35
22	B	615	CLA	C6-C7-C8	-2.19	108.83	115.92
23	d	401	PHO	C1B-NB-C4B	2.19	110.64	106.51
22	B	601	CLA	C4D-C3D-CAD	-2.19	107.25	108.47
22	B	611	CLA	C2A-C3A-C4A	2.19	105.41	101.87
22	B	604	CLA	CMD-C2D-C3D	2.19	128.77	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	623	SQD	O5-C5-C4	2.19	113.67	109.69
22	b	605	CLA	O2A-C1-C2	-2.19	102.89	108.64
22	C	508	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
22	c	501	CLA	CMD-C2D-C3D	2.19	128.77	124.68
22	B	603	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
22	C	507	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
22	d	404	CLA	CMC-C2C-C3C	2.18	129.06	124.94
27	d	406	PL9	C47-C48-C49	-2.18	120.28	127.75
24	d	405	BCR	C7-C8-C9	-2.18	122.94	126.23
22	B	601	CLA	C1-C2-C3	-2.18	122.27	126.04
30	D	408	LHG	C18-C17-C16	-2.18	103.35	114.42
22	c	503	CLA	C3A-C2A-C1A	2.18	104.61	101.34
31	C	516	DGD	CBB-CAB-C9B	-2.18	103.37	114.42
24	x	101	BCR	C15-C16-C17	-2.18	119.02	123.47
24	b	618	BCR	C8-C7-C6	-2.18	121.09	127.20
28	M	101	LMG	C38-C37-C36	-2.17	103.39	114.42
22	b	609	CLA	C4D-C3D-CAD	-2.17	107.26	108.47
22	A	403	CLA	C4A-NA-C1A	2.17	107.68	106.71
22	C	512	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
23	D	401	PHO	O2A-CGA-O1A	-2.17	118.11	123.59
22	b	611	CLA	C7-C6-C5	-2.17	107.47	113.36
31	H	102	DGD	CAB-C9B-C8B	-2.17	103.41	114.42
35	F	101	HEM	C4C-C3C-C2C	2.17	108.41	106.90
28	D	406	LMG	C38-C37-C36	-2.17	103.42	114.42
29	a	411	SQD	O8-S-C6	2.17	109.19	105.74
28	a	416	LMG	O6-C5-C4	2.17	113.63	109.69
22	C	507	CLA	CMD-C2D-C3D	2.17	128.73	124.68
22	C	505	CLA	OBD-CAD-C3D	2.17	131.58	127.98
22	c	513	CLA	C4A-NA-C1A	2.16	107.68	106.71
28	b	624	LMG	O8-C28-O10	-2.16	118.13	123.59
29	A	413	SQD	O4-C4-C3	-2.16	105.35	110.35
22	C	508	CLA	C4D-C3D-CAD	-2.16	107.26	108.47
22	d	403	CLA	CMC-C2C-C3C	2.16	129.02	124.94
31	c	518	DGD	O3D-C3D-C4D	-2.16	105.35	110.35
24	T	101	BCR	C38-C26-C27	-2.16	109.46	113.62
22	C	504	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
22	B	614	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
22	c	504	CLA	CHB-C4A-NA	2.16	127.50	124.51
35	F	101	HEM	C3C-C4C-NC	-2.16	106.87	110.94
22	b	612	CLA	OBD-CAD-CBD	-2.16	122.81	125.89
22	d	404	CLA	C1-C2-C3	-2.16	122.31	126.04
24	A	406	BCR	C36-C18-C17	-2.16	119.90	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	609	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
28	c	519	LMG	C38-C37-C36	-2.15	103.49	114.42
28	b	624	LMG	O7-C10-O9	-2.15	118.50	123.70
22	B	616	CLA	CAA-CBA-CGA	-2.15	106.96	113.25
29	a	411	SQD	C45-O47-C7	2.15	123.09	117.79
22	A	411	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
22	b	615	CLA	C11-C10-C8	-2.15	108.96	115.92
22	D	403	CLA	O1D-CGD-CBD	2.15	128.89	124.48
27	a	409	PL9	C20-C19-C21	2.15	118.89	115.27
22	b	604	CLA	CMC-C2C-C3C	2.15	129.00	124.94
24	B	618	BCR	C28-C27-C26	-2.15	110.24	114.08
31	h	101	DGD	O6E-C5E-C6E	-2.15	101.09	106.44
22	c	506	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
22	B	601	CLA	CMC-C2C-C3C	2.15	128.99	124.94
22	c	505	CLA	O2D-CGD-CBD	2.15	115.08	111.27
22	C	502	CLA	CHB-C4A-NA	2.14	127.48	124.51
30	B	622	LHG	C27-C26-C25	-2.14	103.55	114.42
28	D	406	LMG	O1-C1-C2	-2.14	104.96	108.30
22	C	507	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
22	c	513	CLA	O2D-CGD-CBD	2.14	115.07	111.27
22	c	511	CLA	CMC-C2C-C3C	2.14	128.97	124.94
31	C	517	DGD	CDB-CCB-CBB	-2.14	103.57	114.42
31	C	515	DGD	C6B-C5B-C4B	-2.14	103.58	114.42
24	B	619	BCR	C2-C3-C4	-2.14	106.60	111.38
31	C	516	DGD	O3D-C3D-C4D	-2.14	105.41	110.35
31	A	416	DGD	O4D-C4D-C3D	2.14	115.29	110.35
22	A	403	CLA	CMC-C2C-C3C	2.13	128.97	124.94
22	C	505	CLA	C1B-CHB-C4A	-2.13	125.89	130.12
28	A	412	LMG	O8-C28-O10	-2.13	118.21	123.59
30	D	408	LHG	C20-C19-C18	-2.13	103.60	114.42
28	A	412	LMG	C12-C11-C10	-2.13	105.87	113.62
28	a	416	LMG	C9-C8-C7	-2.13	106.75	111.79
31	C	515	DGD	C9B-C8B-C7B	-2.13	103.62	114.42
28	D	410	LMG	O8-C28-O10	-2.13	118.23	123.59
28	C	518	LMG	C40-C39-C38	-2.13	103.63	114.42
31	c	516	DGD	O4D-C4D-C5D	-2.12	104.02	109.30
29	B	623	SQD	C25-C24-C23	-2.12	105.90	113.62
29	b	620	SQD	O9-S-C6	2.12	109.46	106.94
22	b	610	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
24	c	515	BCR	C36-C18-C17	-2.12	119.95	122.92
22	B	604	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
24	Y	101	BCR	C30-C25-C26	-2.12	119.63	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	d	404	CLA	CMD-C2D-C3D	2.12	128.64	124.68
24	B	619	BCR	C38-C26-C25	-2.12	122.15	124.53
24	x	101	BCR	C2-C1-C6	2.12	113.74	110.48
22	B	602	CLA	CMD-C2D-C3D	2.11	128.63	124.68
35	e	101	HEM	C1D-C2D-C3D	2.11	108.47	107.00
31	c	518	DGD	O5D-C6D-C5D	-2.11	105.14	109.05
28	d	410	LMG	C3-C4-C5	-2.11	106.47	110.24
22	C	501	CLA	OBD-CAD-C3D	2.11	131.49	127.98
22	b	604	CLA	CMD-C2D-C3D	2.11	128.63	124.68
22	C	513	CLA	O1D-CGD-CBD	2.11	128.81	124.48
22	B	605	CLA	CHA-C1A-NA	-2.11	121.56	126.40
30	B	621	LHG	C20-C19-C18	-2.11	103.70	114.42
22	B	612	CLA	CMA-C3A-C4A	-2.11	106.10	111.77
22	b	609	CLA	O1D-CGD-CBD	2.11	128.80	124.48
31	C	517	DGD	O3D-C3D-C4D	-2.11	105.47	110.35
23	d	401	PHO	O2A-CGA-O1A	-2.11	118.27	123.59
29	A	413	SQD	O48-C23-O10	-2.11	118.27	123.59
22	C	505	CLA	C6-C7-C8	-2.11	109.11	115.92
27	a	409	PL9	C25-C24-C23	-2.11	118.28	123.68
22	b	605	CLA	C4D-C3D-CAD	-2.11	107.30	108.47
29	D	407	SQD	O48-C23-C24	2.11	118.51	111.91
22	b	613	CLA	C16-C15-C13	-2.10	109.12	115.92
24	c	515	BCR	C37-C22-C21	-2.10	119.98	122.92
24	b	617	BCR	C15-C14-C13	-2.10	124.31	127.31
22	C	508	CLA	O1D-CGD-CBD	2.10	128.78	124.48
22	a	404	CLA	OBD-CAD-C3D	2.10	131.47	127.98
22	b	610	CLA	CMD-C2D-C3D	2.10	128.61	124.68
30	e	102	LHG	C18-C17-C16	-2.10	103.77	114.42
22	a	404	CLA	CHB-C4A-NA	2.10	127.41	124.51
23	d	402	PHO	CMC-C2C-C1C	-2.10	121.83	125.06
22	b	603	CLA	O2D-CGD-CBD	2.10	115.00	111.27
22	B	613	CLA	C3D-CAD-CBD	-2.09	104.85	107.61
22	b	615	CLA	C3B-C4B-NB	-2.09	106.50	109.21
28	b	624	LMG	O1-C1-C2	-2.09	105.03	108.30
28	b	624	LMG	C38-C37-C36	-2.09	103.80	114.42
24	B	617	BCR	C8-C7-C6	-2.09	121.33	127.20
28	d	410	LMG	C6-C5-C4	-2.09	108.11	113.00
22	B	603	CLA	OBD-CAD-C3D	2.09	131.45	127.98
22	c	502	CLA	CMD-C2D-C3D	2.09	128.59	124.68
28	M	101	LMG	O8-C28-O10	-2.09	118.32	123.59
31	H	102	DGD	O6D-C1D-O3G	-2.09	105.03	109.97
22	b	607	CLA	O2D-CGD-O1D	-2.09	119.76	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	503	CLA	C1-O2A-CGA	2.08	121.91	116.44
29	b	620	SQD	C45-O47-C7	2.08	122.92	117.79
31	C	515	DGD	O6E-C5E-C4E	2.08	113.48	109.69
28	c	522	LMG	O7-C10-O9	-2.08	118.67	123.70
30	B	622	LHG	C18-C17-C16	-2.08	103.86	114.42
22	c	511	CLA	CMB-C2B-C3B	2.08	128.57	124.68
27	a	409	PL9	C42-C43-C44	-2.08	122.65	127.66
22	a	402	CLA	C2A-C1A-CHA	2.08	127.50	123.86
22	B	613	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
24	K	102	BCR	C15-C16-C17	-2.08	119.22	123.47
34	d	411	STE	C6-C5-C4	-2.08	103.88	114.42
24	T	101	BCR	C1-C6-C5	-2.08	119.69	122.61
22	C	513	CLA	C1B-CHB-C4A	-2.08	126.01	130.12
24	C	514	BCR	C27-C26-C25	2.07	125.74	122.73
22	B	603	CLA	O1A-CGA-CBA	2.07	131.82	123.73
22	B	610	CLA	C1-C2-C3	-2.07	122.46	126.04
31	c	516	DGD	C3G-C2G-C1G	-2.07	106.89	111.79
28	A	412	LMG	O7-C10-C11	2.07	115.97	111.50
22	B	610	CLA	C11-C10-C8	-2.07	109.22	115.92
31	c	518	DGD	CAB-C9B-C8B	-2.07	103.91	114.42
29	b	620	SQD	O47-C45-C46	2.07	115.90	108.40
24	k	101	BCR	C1-C6-C5	-2.07	119.70	122.61
22	C	504	CLA	O2D-CGD-CBD	2.07	114.94	111.27
22	B	606	CLA	CHB-C4A-NA	2.07	127.37	124.51
28	A	412	LMG	C35-C34-C33	-2.07	103.93	114.42
22	B	608	CLA	C2A-C3A-C4A	2.07	105.21	101.87
24	B	618	BCR	C8-C7-C6	-2.07	121.40	127.20
24	H	101	BCR	C34-C9-C8	-2.06	114.82	118.08
28	b	622	LMG	O6-C5-C6	2.06	111.56	106.44
22	b	604	CLA	C2A-C1A-CHA	2.06	127.47	123.86
24	H	101	BCR	C38-C26-C25	-2.06	122.21	124.53
22	D	403	CLA	CMC-C2C-C3C	2.06	128.83	124.94
22	B	612	CLA	C1B-CHB-C4A	-2.06	126.04	130.12
22	c	508	CLA	O2D-CGD-CBD	2.06	114.92	111.27
22	b	610	CLA	CBC-CAC-C3C	2.06	117.51	112.27
24	T	101	BCR	C31-C1-C6	2.06	113.63	110.30
22	C	509	CLA	CMC-C2C-C3C	2.06	128.82	124.94
22	B	610	CLA	CAA-C2A-C3A	-2.06	107.15	112.78
24	B	618	BCR	C29-C30-C25	2.05	113.64	110.48
31	c	518	DGD	CBB-CAB-C9B	-2.05	104.02	114.42
23	d	401	PHO	CBD-CHA-C4D	-2.05	106.23	108.54
28	D	410	LMG	O1-C7-C8	-2.05	106.35	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	x	101	BCR	C36-C18-C19	2.05	121.30	118.08
22	b	606	CLA	CHB-C4A-NA	2.05	127.34	124.51
22	B	609	CLA	CHA-C1A-NA	-2.05	121.71	126.40
22	C	512	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
22	c	509	CLA	O2A-CGA-CBA	2.05	118.33	111.91
22	B	601	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
27	d	406	PL9	C8-C7-C3	2.04	117.76	111.98
28	M	101	LMG	C22-C21-C20	-2.04	104.05	114.42
28	C	518	LMG	O2-C2-C1	-2.04	105.08	110.05
30	D	409	LHG	O7-C7-C8	-2.04	107.10	111.50
31	h	101	DGD	O6E-C1E-O5D	-2.04	105.14	109.97
22	C	504	CLA	CHB-C4A-NA	2.04	127.33	124.51
27	A	410	PL9	C42-C43-C44	-2.04	122.75	127.66
27	a	409	PL9	C32-C33-C34	-2.04	122.75	127.66
24	B	619	BCR	C28-C27-C26	-2.04	110.44	114.08
24	c	515	BCR	C35-C13-C14	-2.04	120.07	122.92
28	M	101	LMG	C37-C36-C35	-2.04	104.08	114.42
24	K	102	BCR	C27-C26-C25	2.04	125.69	122.73
22	B	615	CLA	C14-C13-C15	-2.04	103.92	111.29
22	C	502	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
22	B	609	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
22	B	611	CLA	C14-C13-C15	-2.04	103.92	111.29
24	b	618	BCR	C15-C16-C17	-2.03	119.31	123.47
22	B	604	CLA	C1B-CHB-C4A	-2.03	126.09	130.12
22	C	511	CLA	CMD-C2D-C3D	2.03	128.48	124.68
22	B	611	CLA	CMC-C2C-C3C	2.03	128.78	124.94
30	d	408	LHG	O8-C23-C24	2.03	118.28	111.91
31	c	517	DGD	C5B-C4B-C3B	-2.03	104.11	114.42
31	C	515	DGD	C3D-C4D-C5D	-2.03	106.62	110.24
22	c	511	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
23	A	404	PHO	CAB-C3B-C4B	-2.03	118.71	126.21
22	A	405	CLA	CHA-C1A-NA	-2.03	121.76	126.40
30	l	101	LHG	C20-C19-C18	-2.03	104.14	114.42
22	D	403	CLA	CHA-C1A-NA	-2.03	121.76	126.40
28	a	416	LMG	O8-C28-O10	-2.03	118.48	123.59
24	B	619	BCR	C27-C26-C25	2.02	125.67	122.73
22	B	609	CLA	CMD-C2D-C3D	2.02	128.46	124.68
31	C	517	DGD	C5B-C4B-C3B	-2.02	104.17	114.42
34	X	101	STE	C12-C11-C10	-2.02	104.17	114.42
22	b	607	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
28	c	522	LMG	C38-C37-C36	-2.02	104.17	114.42
22	c	504	CLA	O1A-CGA-CBA	2.02	131.61	123.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	517	DGD	O2E-C2E-C1E	-2.02	105.14	110.05
22	A	411	CLA	C2A-C1A-CHA	2.02	127.39	123.86
27	a	409	PL9	C31-C32-C33	-2.02	105.25	111.88
22	A	405	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
22	c	507	CLA	O1D-CGD-CBD	2.02	128.61	124.48
27	A	410	PL9	C12-C13-C14	-2.02	122.81	127.66
23	d	401	PHO	CBC-CAC-C3C	2.01	117.99	112.43
22	b	612	CLA	O2A-C1-C2	-2.01	103.34	108.64
22	b	608	CLA	C11-C10-C8	-2.01	109.41	115.92
22	c	507	CLA	OBD-CAD-C3D	2.01	131.32	127.98
28	c	521	LMG	C40-C39-C38	-2.01	104.21	114.42
22	b	613	CLA	C4D-C3D-CAD	-2.01	107.35	108.47
22	c	503	CLA	C1B-CHB-C4A	-2.01	126.13	130.12
28	d	410	LMG	C9-C8-C7	-2.01	107.03	111.79
22	B	611	CLA	C1B-CHB-C4A	-2.01	126.13	130.12
22	b	607	CLA	C1B-CHB-C4A	-2.01	126.13	130.12
22	A	405	CLA	C6-C5-C3	2.01	118.73	113.45
24	b	619	BCR	C16-C15-C14	-2.01	119.36	123.47
28	c	519	LMG	O8-C28-O10	-2.01	118.52	123.59
31	C	515	DGD	O2D-C2D-C1D	-2.01	105.17	110.05
31	h	101	DGD	O5D-C6D-C5D	-2.01	105.33	109.05
22	b	605	CLA	C4-C3-C2	-2.01	118.53	123.68
30	d	407	LHG	O2-C2-C3	-2.01	102.52	109.56
22	B	604	CLA	CHA-C1A-NA	-2.01	121.80	126.40
24	c	514	BCR	C2-C1-C6	2.01	113.57	110.48
22	c	507	CLA	C4-C3-C5	2.01	118.64	115.27
22	B	616	CLA	C4-C3-C2	-2.00	118.54	123.68
30	D	409	LHG	C27-C26-C25	-2.00	104.27	114.42
24	K	101	BCR	C38-C26-C25	-2.00	122.28	124.53

All (58) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
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
22	B	605	CLA	ND
22	B	606	CLA	ND
22	B	607	CLA	ND

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Mol	Chain	Res	Type	Atom
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	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	402	CLA	ND
22	a	402	CLA	ND
22	a	404	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	608	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	504	CLA	ND
22	c	505	CLA	ND
22	c	506	CLA	ND
22	c	507	CLA	ND

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Mol	Chain	Res	Type	Atom
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	403	CLA	ND
22	d	404	CLA	ND

All (1883) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	402	CLA	C2C-C3C-CAC-CBC
22	A	405	CLA	C2-C3-C5-C6
22	A	405	CLA	C4-C3-C5-C6
22	A	411	CLA	CHA-CBD-CGD-O1D
22	A	411	CLA	CHA-CBD-CGD-O2D
22	B	601	CLA	CBA-CGA-O2A-C1
22	B	601	CLA	O1A-CGA-O2A-C1
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	C	504	CLA	C2-C3-C5-C6
22	C	504	CLA	C4-C3-C5-C6
22	C	508	CLA	CHA-CBD-CGD-O1D
22	C	512	CLA	C1A-C2A-CAA-CBA
22	D	402	CLA	C11-C10-C8-C9
22	a	410	CLA	CHA-CBD-CGD-O2D
22	b	605	CLA	C4-C3-C5-C6
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	CHA-CBD-CGD-O2D
22	b	614	CLA	CAD-CBD-CGD-O1D
22	b	614	CLA	CBD-CGD-O2D-CED
22	b	614	CLA	C2-C3-C5-C6
22	b	616	CLA	C2-C3-C5-C6
22	b	616	CLA	C4-C3-C5-C6
22	c	508	CLA	CHA-CBD-CGD-O1D
22	c	508	CLA	CHA-CBD-CGD-O2D
22	c	511	CLA	C14-C13-C15-C16
24	A	406	BCR	C37-C22-C23-C24
24	B	618	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
24	C	514	BCR	C11-C12-C13-C14
24	C	514	BCR	C36-C18-C19-C20
24	D	404	BCR	C37-C22-C23-C24
24	K	101	BCR	C7-C8-C9-C34
24	K	101	BCR	C11-C12-C13-C35
24	K	101	BCR	C35-C13-C14-C15
24	K	101	BCR	C16-C17-C18-C36
24	K	102	BCR	C17-C18-C19-C20
24	K	102	BCR	C36-C18-C19-C20
24	T	101	BCR	C7-C8-C9-C10
24	T	101	BCR	C7-C8-C9-C34
24	T	101	BCR	C18-C19-C20-C21
24	Y	101	BCR	C11-C12-C13-C35
24	Y	101	BCR	C21-C22-C23-C24
24	Y	101	BCR	C37-C22-C23-C24
24	b	617	BCR	C1-C6-C7-C8
24	b	619	BCR	C37-C22-C23-C24
24	c	515	BCR	C7-C8-C9-C34
24	c	515	BCR	C35-C13-C14-C15
24	c	515	BCR	C20-C21-C22-C37
24	d	405	BCR	C21-C22-C23-C24
24	d	405	BCR	C37-C22-C23-C24
24	d	405	BCR	C23-C24-C25-C30
24	k	101	BCR	C1-C6-C7-C8
24	k	101	BCR	C5-C6-C7-C8
24	k	101	BCR	C7-C8-C9-C34
24	k	102	BCR	C37-C22-C23-C24
24	t	101	BCR	C17-C18-C19-C20
24	t	101	BCR	C36-C18-C19-C20
24	x	101	BCR	C11-C10-C9-C8
27	A	410	PL9	C12-C13-C14-C15
27	A	410	PL9	C13-C14-C16-C17
27	A	410	PL9	C17-C18-C19-C21
27	A	410	PL9	C20-C19-C21-C22
27	A	410	PL9	C25-C24-C26-C27
27	A	410	PL9	C37-C38-C39-C40
27	A	410	PL9	C37-C38-C39-C41
27	A	410	PL9	C40-C39-C41-C42
27	A	410	PL9	C43-C44-C46-C47
27	D	405	PL9	C32-C33-C34-C35
27	D	405	PL9	C32-C33-C34-C36
27	a	409	PL9	C19-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
27	a	409	PL9	C22-C23-C24-C25
27	a	409	PL9	C22-C23-C24-C26
27	a	409	PL9	C33-C34-C36-C37
27	a	409	PL9	C35-C34-C36-C37
27	a	409	PL9	C39-C41-C42-C43
27	a	409	PL9	C42-C43-C44-C45
27	a	409	PL9	C42-C43-C44-C46
27	d	406	PL9	C27-C28-C29-C30
27	d	406	PL9	C32-C33-C34-C36
27	d	406	PL9	C33-C34-C36-C37
27	d	406	PL9	C42-C43-C44-C45
27	d	406	PL9	C42-C43-C44-C46
28	A	412	LMG	O9-C10-O7-C8
28	D	410	LMG	C11-C10-O7-C8
28	D	411	LMG	C28-C29-C30-C31
28	b	624	LMG	C11-C10-O7-C8
28	c	521	LMG	C11-C10-O7-C8
28	c	522	LMG	O6-C1-O1-C7
29	B	623	SQD	O5-C1-O6-C44
29	B	623	SQD	O49-C7-O47-C45
29	B	623	SQD	C8-C7-O47-C45
29	D	407	SQD	O5-C1-O6-C44
29	a	411	SQD	O6-C44-C45-O47
29	a	411	SQD	C5-C6-S-O7
29	a	411	SQD	C5-C6-S-O8
29	a	411	SQD	C5-C6-S-O9
29	a	412	SQD	C8-C7-O47-C45
29	b	620	SQD	O49-C7-O47-C45
29	b	620	SQD	C8-C7-O47-C45
29	f	101	SQD	C2-C1-O6-C44
29	f	101	SQD	O5-C1-O6-C44
30	A	414	LHG	O1-C1-C2-O2
30	A	414	LHG	O1-C1-C2-C3
30	A	414	LHG	C4-O6-P-O4
30	B	621	LHG	C3-O3-P-O4
30	B	621	LHG	C4-O6-P-O4
30	B	621	LHG	C4-O6-P-O5
30	B	622	LHG	O1-C1-C2-C3
30	B	622	LHG	C3-O3-P-O4
30	D	408	LHG	O1-C1-C2-C3
30	D	408	LHG	O2-C2-C3-O3
30	D	408	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
30	D	408	LHG	C4-O6-P-O4
30	D	409	LHG	C3-O3-P-O6
30	d	408	LHG	O1-C1-C2-C3
30	d	408	LHG	C3-O3-P-O4
30	d	408	LHG	C4-O6-P-O3
30	d	408	LHG	C4-O6-P-O4
30	d	408	LHG	C4-O6-P-O5
30	d	409	LHG	C4-O6-P-O4
30	e	102	LHG	C1-C2-C3-O3
30	e	102	LHG	C3-O3-P-O5
30	e	102	LHG	O10-C23-O8-C6
30	e	102	LHG	C24-C23-O8-C6
30	l	101	LHG	C3-O3-P-O4
30	l	101	LHG	C4-O6-P-O4
30	l	101	LHG	C4-O6-P-O5
31	A	416	DGD	C2B-C1B-O2G-C2G
31	A	416	DGD	O1B-C1B-O2G-C2G
31	A	416	DGD	O2G-C2G-C3G-O3G
34	B	620	STE	C1-C2-C3-C4
34	B	625	STE	C1-C2-C3-C4
34	C	519	STE	C1-C2-C3-C4
34	J	101	STE	C1-C2-C3-C4
34	R	101	STE	C1-C2-C3-C4
34	b	623	STE	C1-C2-C3-C4
34	b	625	STE	C1-C2-C3-C4
34	d	412	STE	C1-C2-C3-C4
34	d	413	STE	C1-C2-C3-C4
34	j	101	STE	C1-C2-C3-C4
28	c	522	LMG	O10-C28-O8-C9
29	a	412	SQD	O10-C23-O48-C46
30	A	414	LHG	O10-C23-O8-C6
28	c	522	LMG	C29-C28-O8-C9
29	D	407	SQD	C24-C23-O48-C46
22	B	601	CLA	CBD-CGD-O2D-CED
22	C	511	CLA	CBD-CGD-O2D-CED
22	b	601	CLA	CBD-CGD-O2D-CED
28	M	101	LMG	O10-C28-O8-C9
28	c	521	LMG	O10-C28-O8-C9
29	b	620	SQD	O10-C23-O48-C46
22	B	603	CLA	CBD-CGD-O2D-CED
22	b	614	CLA	O1D-CGD-O2D-CED
28	D	410	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
28	b	624	LMG	O9-C10-O7-C8
28	c	521	LMG	O9-C10-O7-C8
22	A	405	CLA	C3-C5-C6-C7
28	c	521	LMG	C29-C28-O8-C9
29	a	412	SQD	C24-C23-O48-C46
29	b	620	SQD	C24-C23-O48-C46
29	f	101	SQD	C24-C23-O48-C46
28	A	412	LMG	C11-C10-O7-C8
27	D	405	PL9	C47-C48-C49-C51
22	c	501	CLA	CBD-CGD-O2D-CED
22	c	508	CLA	CBD-CGD-O2D-CED
23	d	402	PHO	CBD-CGD-O2D-CED
31	A	416	DGD	O6E-C5E-C6E-O5E
22	b	614	CLA	C4-C3-C5-C6
22	c	506	CLA	C4-C3-C5-C6
27	A	410	PL9	C23-C24-C26-C27
22	B	604	CLA	C3-C5-C6-C7
22	b	602	CLA	C3-C5-C6-C7
22	b	614	CLA	C3-C5-C6-C7
28	M	101	LMG	C29-C28-O8-C9
29	B	623	SQD	C24-C23-O48-C46
30	A	414	LHG	C24-C23-O8-C6
27	D	405	PL9	C47-C48-C49-C50
27	A	410	PL9	C12-C13-C14-C16
29	B	623	SQD	O10-C23-O48-C46
29	f	101	SQD	O10-C23-O48-C46
31	H	102	DGD	C4E-C5E-C6E-O5E
30	d	407	LHG	O2-C2-C3-O3
30	d	408	LHG	O2-C2-C3-O3
30	e	102	LHG	O2-C2-C3-O3
29	D	407	SQD	O10-C23-O48-C46
28	b	624	LMG	O6-C5-C6-O5
22	B	614	CLA	C15-C16-C17-C18
22	b	607	CLA	CBD-CGD-O2D-CED
22	d	404	CLA	CBD-CGD-O2D-CED
34	C	521	STE	C4-C5-C6-C7
30	B	621	LHG	C7-C8-C9-C10
34	a	415	STE	C4-C5-C6-C7
28	b	624	LMG	O10-C28-O8-C9
22	B	614	CLA	C4-C3-C5-C6
22	C	507	CLA	C4-C3-C5-C6
22	c	507	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	B	614	CLA	C2-C3-C5-C6
22	C	507	CLA	C2-C3-C5-C6
22	b	605	CLA	C2-C3-C5-C6
22	c	507	CLA	C2-C3-C5-C6
27	a	409	PL9	C23-C24-C26-C27
28	d	410	LMG	C10-C11-C12-C13
22	B	606	CLA	C2A-CAA-CBA-CGA
22	b	606	CLA	C2A-CAA-CBA-CGA
31	H	102	DGD	O6E-C5E-C6E-O5E
27	A	410	PL9	C9-C11-C12-C13
27	A	410	PL9	C34-C36-C37-C38
27	A	410	PL9	C39-C41-C42-C43
27	A	410	PL9	C44-C46-C47-C48
27	a	409	PL9	C9-C11-C12-C13
27	d	406	PL9	C34-C36-C37-C38
28	b	622	LMG	C29-C28-O8-C9
31	A	416	DGD	C4E-C5E-C6E-O5E
27	a	409	PL9	C7-C8-C9-C10
22	B	601	CLA	O1D-CGD-O2D-CED
30	D	408	LHG	C1-C2-C3-O3
30	d	407	LHG	C1-C2-C3-O3
30	d	408	LHG	C1-C2-C3-O3
22	b	601	CLA	CBA-CGA-O2A-C1
22	c	506	CLA	CBA-CGA-O2A-C1
22	b	601	CLA	O1D-CGD-O2D-CED
22	B	613	CLA	C8-C10-C11-C12
22	b	611	CLA	C15-C16-C17-C18
22	c	507	CLA	C5-C6-C7-C8
30	e	102	LHG	O6-C4-C5-O7
22	C	506	CLA	C13-C15-C16-C17
22	C	513	CLA	C5-C6-C7-C8
28	D	406	LMG	C10-C11-C12-C13
31	C	515	DGD	C1B-C2B-C3B-C4B
29	B	623	SQD	C2-C1-O6-C44
29	D	407	SQD	C2-C1-O6-C44
29	B	623	SQD	O6-C44-C45-O47
22	b	601	CLA	O1A-CGA-O2A-C1
22	A	403	CLA	C14-C13-C15-C16
22	B	601	CLA	C6-C7-C8-C9
22	B	604	CLA	C11-C10-C8-C9
22	B	606	CLA	C11-C12-C13-C14
22	B	609	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	B	616	CLA	C11-C10-C8-C9
22	C	503	CLA	C11-C10-C8-C9
22	C	507	CLA	C11-C10-C8-C9
22	C	509	CLA	C11-C10-C8-C9
22	C	512	CLA	C11-C10-C8-C9
22	b	601	CLA	C14-C13-C15-C16
22	b	605	CLA	C11-C10-C8-C9
22	b	606	CLA	C14-C13-C15-C16
22	b	607	CLA	C11-C10-C8-C9
22	b	611	CLA	C14-C13-C15-C16
22	b	614	CLA	C6-C7-C8-C9
22	b	616	CLA	C6-C7-C8-C9
22	c	509	CLA	C6-C7-C8-C9
22	c	509	CLA	C11-C12-C13-C14
22	c	510	CLA	C11-C10-C8-C9
22	c	512	CLA	C6-C7-C8-C9
22	b	606	CLA	C15-C16-C17-C18
22	c	512	CLA	C13-C15-C16-C17
24	B	618	BCR	C37-C22-C23-C24
24	T	101	BCR	C36-C18-C19-C20
24	c	514	BCR	C7-C8-C9-C34
24	k	101	BCR	C36-C18-C19-C20
28	C	518	LMG	C11-C10-O7-C8
28	C	518	LMG	C28-C29-C30-C31
28	c	521	LMG	C28-C29-C30-C31
29	B	623	SQD	C23-C24-C25-C26
22	c	506	CLA	O1A-CGA-O2A-C1
28	C	518	LMG	O10-C28-O8-C9
22	C	507	CLA	C10-C11-C12-C13
22	b	604	CLA	C15-C16-C17-C18
22	b	614	CLA	C10-C11-C12-C13
22	c	504	CLA	C5-C6-C7-C8
30	d	409	LHG	C30-C31-C32-C33
22	B	601	CLA	C5-C6-C7-C8
22	B	606	CLA	C15-C16-C17-C18
22	B	609	CLA	C15-C16-C17-C18
22	B	611	CLA	C13-C15-C16-C17
22	C	510	CLA	C15-C16-C17-C18
22	C	513	CLA	C15-C16-C17-C18
22	b	609	CLA	C15-C16-C17-C18
22	c	503	CLA	C8-C10-C11-C12
29	b	620	SQD	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
30	A	414	LHG	C7-C8-C9-C10
31	c	518	DGD	C1A-C2A-C3A-C4A
30	d	409	LHG	C24-C25-C26-C27
22	B	602	CLA	C8-C10-C11-C12
22	B	603	CLA	C8-C10-C11-C12
22	B	604	CLA	C13-C15-C16-C17
22	C	503	CLA	C5-C6-C7-C8
22	C	509	CLA	C10-C11-C12-C13
22	b	602	CLA	C8-C10-C11-C12
22	b	603	CLA	C5-C6-C7-C8
22	b	615	CLA	C10-C11-C12-C13
22	c	509	CLA	C13-C15-C16-C17
22	c	511	CLA	C13-C15-C16-C17
29	A	413	SQD	C11-C12-C13-C14
30	d	408	LHG	C28-C29-C30-C31
27	d	406	PL9	C12-C13-C14-C15
28	D	410	LMG	C10-C11-C12-C13
28	M	101	LMG	C28-C29-C30-C31
28	c	519	LMG	C28-C29-C30-C31
30	d	407	LHG	C23-C24-C25-C26
30	d	409	LHG	C23-C24-C25-C26
22	C	505	CLA	C10-C11-C12-C13
22	C	506	CLA	C8-C10-C11-C12
22	b	607	CLA	C10-C11-C12-C13
22	b	611	CLA	C13-C15-C16-C17
29	A	413	SQD	C30-C31-C32-C33
22	C	511	CLA	O1D-CGD-O2D-CED
29	a	412	SQD	O49-C7-O47-C45
22	D	402	CLA	C15-C16-C17-C18
28	D	410	LMG	C28-C29-C30-C31
29	A	413	SQD	C7-C8-C9-C10
30	D	409	LHG	C7-C8-C9-C10
22	C	508	CLA	C15-C16-C17-C18
22	b	601	CLA	C8-C10-C11-C12
22	c	511	CLA	C15-C16-C17-C18
22	B	604	CLA	C6-C7-C8-C10
22	a	403	CLA	C6-C7-C8-C10
22	b	613	CLA	C12-C13-C15-C16
22	b	614	CLA	C6-C7-C8-C10
22	b	615	CLA	C11-C12-C13-C15
22	c	506	CLA	C12-C13-C15-C16
22	c	510	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
28	a	416	LMG	O10-C28-O8-C9
28	b	624	LMG	C29-C28-O8-C9
22	B	603	CLA	O1D-CGD-O2D-CED
22	B	605	CLA	C13-C15-C16-C17
22	B	614	CLA	C8-C10-C11-C12
22	B	616	CLA	C5-C6-C7-C8
28	b	622	LMG	O6-C1-O1-C7
22	B	602	CLA	C13-C15-C16-C17
22	B	613	CLA	C13-C15-C16-C17
27	A	410	PL9	C29-C31-C32-C33
27	a	409	PL9	C14-C16-C17-C18
27	a	409	PL9	C24-C26-C27-C28
27	a	409	PL9	C34-C36-C37-C38
34	B	626	STE	C11-C12-C13-C14
28	d	410	LMG	C28-C29-C30-C31
24	B	617	BCR	C10-C11-C12-C13
24	B	619	BCR	C10-C11-C12-C13
24	c	515	BCR	C18-C19-C20-C21
28	b	624	LMG	C4-C5-C6-O5
22	B	601	CLA	C8-C10-C11-C12
22	B	607	CLA	C5-C6-C7-C8
22	B	614	CLA	C13-C15-C16-C17
22	b	615	CLA	C15-C16-C17-C18
22	c	505	CLA	C15-C16-C17-C18
22	c	509	CLA	C10-C11-C12-C13
28	C	518	LMG	C29-C28-O8-C9
28	b	622	LMG	C38-C39-C40-C41
22	A	411	CLA	C15-C16-C17-C18
22	B	615	CLA	C5-C6-C7-C8
22	C	511	CLA	C8-C10-C11-C12
22	a	402	CLA	C15-C16-C17-C18
22	b	613	CLA	C15-C16-C17-C18
28	c	519	LMG	O9-C10-O7-C8
22	b	616	CLA	CBD-CGD-O2D-CED
22	B	601	CLA	C13-C15-C16-C17
22	B	607	CLA	C10-C11-C12-C13
22	B	612	CLA	C10-C11-C12-C13
22	B	615	CLA	C13-C15-C16-C17
22	C	509	CLA	C13-C15-C16-C17
30	B	621	LHG	C4-O6-P-O3
30	D	408	LHG	C3-O3-P-O6
30	D	408	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
30	d	408	LHG	C3-O3-P-O6
30	l	101	LHG	C4-O6-P-O3
22	B	616	CLA	C3-C5-C6-C7
22	B	607	CLA	C8-C10-C11-C12
22	b	607	CLA	C8-C10-C11-C12
22	d	404	CLA	C15-C16-C17-C18
22	c	508	CLA	O1D-CGD-O2D-CED
22	B	611	CLA	C8-C10-C11-C12
22	C	510	CLA	C16-C17-C18-C20
22	c	504	CLA	C11-C12-C13-C14
23	d	402	PHO	O1D-CGD-O2D-CED
22	c	512	CLA	CBA-CGA-O2A-C1
28	a	416	LMG	C29-C28-O8-C9
28	b	624	LMG	C10-C11-C12-C13
28	c	522	LMG	C12-C13-C14-C15
29	D	407	SQD	C31-C32-C33-C34
30	d	408	LHG	C11-C10-C9-C8
34	d	412	STE	C3-C4-C5-C6
22	A	402	CLA	C15-C16-C17-C18
24	A	406	BCR	C20-C21-C22-C37
24	B	617	BCR	C11-C10-C9-C34
24	B	617	BCR	C35-C13-C14-C15
24	B	617	BCR	C16-C17-C18-C36
24	B	619	BCR	C20-C21-C22-C37
24	C	514	BCR	C35-C13-C14-C15
24	C	514	BCR	C20-C21-C22-C37
24	D	404	BCR	C20-C21-C22-C37
24	a	405	BCR	C11-C10-C9-C34
24	a	405	BCR	C20-C21-C22-C37
24	b	618	BCR	C11-C10-C9-C34
24	b	619	BCR	C35-C13-C14-C15
24	c	514	BCR	C35-C13-C14-C15
24	t	101	BCR	C20-C21-C22-C37
28	C	518	LMG	C32-C33-C34-C35
28	b	622	LMG	C33-C34-C35-C36
28	c	521	LMG	C16-C17-C18-C19
28	c	521	LMG	C30-C31-C32-C33
28	c	522	LMG	C30-C31-C32-C33
28	c	522	LMG	C39-C40-C41-C42
29	a	412	SQD	C11-C10-C9-C8
30	A	414	LHG	C24-C25-C26-C27
30	A	414	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
30	B	621	LHG	C29-C30-C31-C32
30	B	621	LHG	C34-C35-C36-C37
30	D	408	LHG	C12-C13-C14-C15
30	d	407	LHG	C32-C33-C34-C35
31	C	516	DGD	C7B-C8B-C9B-CAB
31	c	516	DGD	C4A-C5A-C6A-C7A
31	h	101	DGD	CBA-CCA-CDA-CEA
34	b	623	STE	C14-C15-C16-C17
34	c	520	STE	C2-C3-C4-C5
34	d	411	STE	C10-C11-C12-C13
34	d	412	STE	C10-C11-C12-C13
34	l	102	STE	C4-C5-C6-C7
22	B	612	CLA	C16-C17-C18-C20
22	B	613	CLA	C16-C17-C18-C20
22	a	402	CLA	C16-C17-C18-C20
28	a	416	LMG	C36-C37-C38-C39
29	b	620	SQD	C27-C28-C29-C30
29	f	101	SQD	C29-C30-C31-C32
30	D	409	LHG	C11-C10-C9-C8
30	D	409	LHG	C9-C10-C11-C12
30	l	101	LHG	C17-C18-C19-C20
31	A	416	DGD	C4B-C5B-C6B-C7B
31	c	516	DGD	C4B-C5B-C6B-C7B
31	c	517	DGD	C5A-C6A-C7A-C8A
31	c	517	DGD	CAB-CBB-CCB-CDB
34	B	620	STE	C6-C7-C8-C9
34	B	626	STE	C13-C14-C15-C16
34	b	621	STE	C6-C7-C8-C9
29	b	620	SQD	C46-C45-O47-C7
28	D	406	LMG	O6-C5-C6-O5
28	D	410	LMG	C14-C15-C16-C17
29	f	101	SQD	C31-C32-C33-C34
30	B	622	LHG	C29-C30-C31-C32
30	D	408	LHG	C10-C11-C12-C13
34	H	103	STE	C10-C11-C12-C13
34	b	623	STE	C7-C8-C9-C10
34	b	626	STE	C12-C13-C14-C15
34	b	626	STE	C14-C15-C16-C17
34	c	520	STE	C9-C10-C11-C12
28	M	101	LMG	C13-C14-C15-C16
28	c	519	LMG	C33-C34-C35-C36
28	d	410	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
29	b	620	SQD	C25-C26-C27-C28
30	A	414	LHG	C26-C27-C28-C29
30	d	408	LHG	C11-C12-C13-C14
31	C	516	DGD	C5A-C6A-C7A-C8A
31	c	517	DGD	CBB-CCB-CDB-CEB
34	B	626	STE	C4-C5-C6-C7
34	d	413	STE	C14-C15-C16-C17
34	h	102	STE	C11-C12-C13-C14
28	a	416	LMG	C12-C13-C14-C15
30	D	408	LHG	C34-C35-C36-C37
30	e	102	LHG	C14-C15-C16-C17
31	c	517	DGD	C6A-C7A-C8A-C9A
34	B	620	STE	C4-C5-C6-C7
22	B	605	CLA	C3-C5-C6-C7
22	c	509	CLA	C3-C5-C6-C7
30	B	622	LHG	C7-C8-C9-C10
24	B	619	BCR	C11-C10-C9-C8
24	C	514	BCR	C11-C10-C9-C8
24	K	101	BCR	C12-C13-C14-C15
24	K	101	BCR	C16-C17-C18-C19
24	c	515	BCR	C12-C13-C14-C15
24	c	515	BCR	C20-C21-C22-C23
24	t	101	BCR	C20-C21-C22-C23
31	C	516	DGD	C2E-C1E-O5D-C6D
31	c	517	DGD	C2E-C1E-O5D-C6D
22	C	513	CLA	CBA-CGA-O2A-C1
29	a	411	SQD	C17-C18-C19-C20
29	a	411	SQD	C25-C26-C27-C28
29	a	412	SQD	C15-C16-C17-C18
30	B	621	LHG	C31-C32-C33-C34
30	D	408	LHG	C32-C33-C34-C35
30	d	407	LHG	C10-C11-C12-C13
30	d	408	LHG	C29-C30-C31-C32
31	h	101	DGD	C9A-CAA-CBA-CCA
22	c	512	CLA	O1A-CGA-O2A-C1
31	C	517	DGD	O1A-C1A-O1G-C1G
22	B	614	CLA	C16-C17-C18-C19
22	B	616	CLA	C11-C12-C13-C15
22	b	602	CLA	C16-C17-C18-C20
22	c	511	CLA	C16-C17-C18-C19
22	B	609	CLA	C4-C3-C5-C6
22	C	510	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	a	409	PL9	C27-C28-C29-C30
28	b	622	LMG	C32-C33-C34-C35
28	c	521	LMG	C39-C40-C41-C42
29	A	415	SQD	C12-C13-C14-C15
29	B	623	SQD	C33-C34-C35-C36
30	B	621	LHG	C12-C13-C14-C15
30	D	409	LHG	C25-C26-C27-C28
30	e	102	LHG	C11-C10-C9-C8
30	e	102	LHG	C16-C17-C18-C19
31	H	102	DGD	C3B-C4B-C5B-C6B
31	c	516	DGD	C5B-C6B-C7B-C8B
31	c	517	DGD	C5B-C6B-C7B-C8B
34	B	626	STE	C5-C6-C7-C8
34	a	415	STE	C7-C8-C9-C10
34	l	102	STE	C13-C14-C15-C16
22	C	512	CLA	C11-C12-C13-C14
22	a	404	CLA	C11-C10-C8-C9
22	a	404	CLA	C14-C13-C15-C16
22	b	605	CLA	C11-C12-C13-C14
22	b	615	CLA	C11-C12-C13-C14
22	d	404	CLA	C14-C13-C15-C16
23	A	404	PHO	C14-C13-C15-C16
28	A	412	LMG	C16-C17-C18-C19
28	D	406	LMG	C35-C36-C37-C38
28	D	411	LMG	C14-C15-C16-C17
28	D	411	LMG	C30-C31-C32-C33
28	c	521	LMG	C31-C32-C33-C34
29	B	623	SQD	C11-C12-C13-C14
30	D	408	LHG	C11-C12-C13-C14
30	d	409	LHG	C32-C33-C34-C35
31	H	102	DGD	C7A-C8A-C9A-CAA
31	c	516	DGD	C6B-C7B-C8B-C9B
31	c	517	DGD	C7A-C8A-C9A-CAA
31	c	517	DGD	C8A-C9A-CAA-CBA
31	c	517	DGD	CBA-CCA-CDA-CEA
31	h	101	DGD	C5B-C6B-C7B-C8B
34	a	415	STE	C5-C6-C7-C8
34	c	520	STE	C11-C12-C13-C14
34	c	523	STE	C5-C6-C7-C8
22	c	512	CLA	C2A-CAA-CBA-CGA
24	B	619	BCR	C37-C22-C23-C24
24	K	102	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
28	D	411	LMG	C31-C32-C33-C34
28	b	622	LMG	C18-C19-C20-C21
29	a	412	SQD	C10-C11-C12-C13
31	C	516	DGD	C6A-C7A-C8A-C9A
34	Z	101	STE	C11-C12-C13-C14
34	j	101	STE	C4-C5-C6-C7
34	t	102	STE	C4-C5-C6-C7
30	D	409	LHG	O1-C1-C2-C3
30	d	407	LHG	O1-C1-C2-C3
30	d	409	LHG	O1-C1-C2-C3
24	k	101	BCR	C17-C18-C19-C20
22	A	411	CLA	C13-C15-C16-C17
28	M	101	LMG	C16-C17-C18-C19
28	b	624	LMG	C11-C12-C13-C14
29	B	623	SQD	C13-C14-C15-C16
29	b	620	SQD	C28-C29-C30-C31
34	b	627	STE	C6-C7-C8-C9
30	A	414	LHG	C23-C24-C25-C26
28	A	412	LMG	C34-C35-C36-C37
28	C	518	LMG	C31-C32-C33-C34
28	M	101	LMG	C12-C13-C14-C15
28	M	101	LMG	C36-C37-C38-C39
28	b	624	LMG	C17-C18-C19-C20
28	b	624	LMG	C32-C33-C34-C35
29	A	413	SQD	C13-C14-C15-C16
29	D	407	SQD	C30-C31-C32-C33
30	A	414	LHG	C15-C16-C17-C18
30	B	622	LHG	C10-C11-C12-C13
30	D	409	LHG	C10-C11-C12-C13
30	d	408	LHG	C12-C13-C14-C15
30	l	101	LHG	C27-C28-C29-C30
30	l	101	LHG	C32-C33-C34-C35
31	C	517	DGD	C5A-C6A-C7A-C8A
31	c	517	DGD	C6B-C7B-C8B-C9B
31	c	518	DGD	C5B-C6B-C7B-C8B
34	H	103	STE	C7-C8-C9-C10
34	I	101	STE	C11-C10-C9-C8
34	a	415	STE	C9-C10-C11-C12
34	d	413	STE	C9-C10-C11-C12
22	B	601	CLA	C16-C17-C18-C20
22	B	603	CLA	C16-C17-C18-C20
22	B	605	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
22	B	606	CLA	C16-C17-C18-C19
22	B	611	CLA	C16-C17-C18-C19
22	C	510	CLA	C16-C17-C18-C19
22	D	403	CLA	C16-C17-C18-C19
22	b	607	CLA	C16-C17-C18-C19
22	b	607	CLA	C16-C17-C18-C20
22	b	615	CLA	C16-C17-C18-C19
22	d	403	CLA	C16-C17-C18-C19
22	d	403	CLA	C16-C17-C18-C20
28	C	518	LMG	O6-C1-O1-C7
31	C	516	DGD	O6E-C1E-O5D-C6D
31	c	517	DGD	O6E-C1E-O5D-C6D
22	B	601	CLA	C15-C16-C17-C18
28	c	522	LMG	C17-C18-C19-C20
28	d	410	LMG	C33-C34-C35-C36
29	a	411	SQD	C27-C28-C29-C30
30	l	101	LHG	C26-C27-C28-C29
34	H	103	STE	C13-C14-C15-C16
34	T	102	STE	C12-C13-C14-C15
34	l	102	STE	C10-C11-C12-C13
22	c	511	CLA	CBD-CGD-O2D-CED
22	c	512	CLA	CBD-CGD-O2D-CED
28	c	521	LMG	C34-C35-C36-C37
28	c	522	LMG	C33-C34-C35-C36
29	B	623	SQD	C34-C35-C36-C37
29	a	412	SQD	C9-C10-C11-C12
30	D	408	LHG	C9-C10-C11-C12
30	d	407	LHG	C31-C32-C33-C34
30	e	102	LHG	C24-C25-C26-C27
31	A	416	DGD	C2B-C3B-C4B-C5B
31	A	416	DGD	C6B-C7B-C8B-C9B
31	C	515	DGD	C2A-C3A-C4A-C5A
31	c	518	DGD	C7A-C8A-C9A-CAA
34	M	102	STE	C11-C10-C9-C8
34	X	101	STE	C11-C10-C9-C8
34	b	623	STE	C13-C14-C15-C16
34	d	411	STE	C5-C6-C7-C8
34	d	412	STE	C9-C10-C11-C12
34	l	102	STE	C12-C13-C14-C15
28	b	622	LMG	C28-C29-C30-C31
22	A	403	CLA	C15-C16-C17-C18
22	c	513	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
28	D	406	LMG	C39-C40-C41-C42
28	M	101	LMG	C29-C30-C31-C32
31	C	515	DGD	C6B-C7B-C8B-C9B
31	c	518	DGD	C9B-CAB-CBB-CCB
34	B	626	STE	C11-C10-C9-C8
34	a	413	STE	C2-C3-C4-C5
29	a	411	SQD	C24-C25-C26-C27
30	d	407	LHG	C16-C17-C18-C19
30	d	407	LHG	C25-C26-C27-C28
31	A	416	DGD	CBB-CCB-CDB-CEB
34	B	626	STE	C12-C13-C14-C15
34	R	101	STE	C3-C4-C5-C6
22	C	512	CLA	C3A-C2A-CAA-CBA
22	c	512	CLA	C3A-C2A-CAA-CBA
22	c	512	CLA	C5-C6-C7-C8
23	d	402	PHO	C5-C6-C7-C8
28	D	411	LMG	C32-C33-C34-C35
29	a	411	SQD	C32-C33-C34-C35
29	b	620	SQD	C26-C27-C28-C29
30	D	409	LHG	C32-C33-C34-C35
31	A	416	DGD	C4A-C5A-C6A-C7A
34	b	627	STE	C2-C3-C4-C5
34	h	102	STE	C9-C10-C11-C12
22	D	403	CLA	C16-C17-C18-C20
22	a	402	CLA	C16-C17-C18-C19
22	b	615	CLA	C16-C17-C18-C20
22	c	504	CLA	C11-C12-C13-C15
22	c	511	CLA	C16-C17-C18-C20
28	b	622	LMG	C37-C38-C39-C40
29	b	620	SQD	C29-C30-C31-C32
30	A	414	LHG	C11-C12-C13-C14
28	a	416	LMG	O1-C7-C8-C9
29	f	101	SQD	C28-C29-C30-C31
30	D	409	LHG	C31-C32-C33-C34
24	K	101	BCR	C14-C15-C16-C17
24	c	515	BCR	C14-C15-C16-C17
28	a	416	LMG	C30-C31-C32-C33
28	b	624	LMG	C31-C32-C33-C34
34	d	411	STE	C4-C5-C6-C7
28	D	410	LMG	O10-C28-O8-C9
22	c	510	CLA	C4-C3-C5-C6
22	C	510	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	c	510	CLA	C2-C3-C5-C6
23	A	404	PHO	C2-C3-C5-C6
27	A	410	PL9	C28-C29-C31-C32
28	a	416	LMG	C11-C10-O7-C8
34	H	103	STE	C12-C13-C14-C15
34	d	411	STE	C9-C10-C11-C12
30	B	622	LHG	O1-C1-C2-O2
30	D	408	LHG	O1-C1-C2-O2
30	D	409	LHG	O1-C1-C2-O2
28	C	518	LMG	C18-C19-C20-C21
30	D	408	LHG	C30-C31-C32-C33
31	C	517	DGD	C6A-C7A-C8A-C9A
31	c	518	DGD	C6A-C7A-C8A-C9A
31	h	101	DGD	C2B-C3B-C4B-C5B
34	X	101	STE	C4-C5-C6-C7
34	X	101	STE	C7-C8-C9-C10
22	c	501	CLA	O1D-CGD-O2D-CED
31	c	518	DGD	O1A-C1A-O1G-C1G
31	c	516	DGD	O6D-C5D-C6D-O5D
22	c	512	CLA	C16-C17-C18-C19
31	c	516	DGD	C3B-C4B-C5B-C6B
29	b	620	SQD	C24-C25-C26-C27
28	c	522	LMG	C15-C16-C17-C18
28	d	410	LMG	C38-C39-C40-C41
29	A	413	SQD	C16-C17-C18-C19
31	H	102	DGD	CCA-CDA-CEA-CFA
34	C	521	STE	C5-C6-C7-C8
22	c	506	CLA	C2-C1-O2A-CGA
30	d	407	LHG	C34-C35-C36-C37
31	A	416	DGD	C5B-C6B-C7B-C8B
31	C	516	DGD	C9A-CAA-CBA-CCA
34	B	625	STE	C9-C10-C11-C12
34	X	101	STE	C12-C13-C14-C15
34	b	623	STE	C9-C10-C11-C12
22	b	609	CLA	C13-C15-C16-C17
22	C	513	CLA	O1A-CGA-O2A-C1
30	D	409	LHG	C24-C25-C26-C27
31	H	102	DGD	C7B-C8B-C9B-CAB
22	b	601	CLA	C3-C5-C6-C7
24	D	404	BCR	C23-C24-C25-C26
24	D	404	BCR	C23-C24-C25-C30
24	T	101	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	T	101	BCR	C5-C6-C7-C8
24	Y	101	BCR	C1-C6-C7-C8
24	Y	101	BCR	C5-C6-C7-C8
24	d	405	BCR	C23-C24-C25-C26
24	k	102	BCR	C1-C6-C7-C8
24	k	102	BCR	C5-C6-C7-C8
30	D	409	LHG	C30-C31-C32-C33
31	C	516	DGD	C5B-C6B-C7B-C8B
22	B	603	CLA	C5-C6-C7-C8
28	D	406	LMG	C21-C22-C23-C24
28	b	622	LMG	C14-C15-C16-C17
34	H	103	STE	C5-C6-C7-C8
28	b	622	LMG	O10-C28-O8-C9
28	A	412	LMG	C28-C29-C30-C31
22	C	504	CLA	C11-C12-C13-C14
28	b	622	LMG	C11-C12-C13-C14
31	H	102	DGD	CAB-CBB-CCB-CDB
22	B	605	CLA	C8-C10-C11-C12
30	B	621	LHG	C18-C19-C20-C21
30	d	407	LHG	C33-C34-C35-C36
30	d	408	LHG	C14-C15-C16-C17
31	H	102	DGD	CAA-CBA-CCA-CDA
31	c	518	DGD	C5A-C6A-C7A-C8A
23	A	404	PHO	C4-C3-C5-C6
27	D	405	PL9	C30-C29-C31-C32
22	A	403	CLA	C6-C7-C8-C10
22	A	403	CLA	C12-C13-C15-C16
22	B	601	CLA	C6-C7-C8-C10
22	B	606	CLA	C6-C7-C8-C10
22	B	606	CLA	C11-C10-C8-C7
22	B	609	CLA	C2-C3-C5-C6
22	B	611	CLA	C12-C13-C15-C16
22	C	509	CLA	C11-C10-C8-C7
22	C	511	CLA	C6-C7-C8-C10
22	C	511	CLA	C11-C12-C13-C15
22	C	512	CLA	C11-C12-C13-C15
22	a	404	CLA	C11-C10-C8-C7
22	b	601	CLA	C11-C12-C13-C15
22	b	603	CLA	C6-C7-C8-C10
22	b	605	CLA	C11-C12-C13-C15
22	b	606	CLA	C11-C10-C8-C7
22	b	606	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	b	611	CLA	C12-C13-C15-C16
22	b	614	CLA	C12-C13-C15-C16
22	d	404	CLA	C12-C13-C15-C16
27	D	405	PL9	C13-C14-C16-C17
31	c	518	DGD	CBA-CCA-CDA-CEA
22	C	504	CLA	C8-C10-C11-C12
30	d	407	LHG	C7-C8-C9-C10
31	c	518	DGD	C2A-C3A-C4A-C5A
22	C	509	CLA	C8-C10-C11-C12
30	A	414	LHG	C32-C33-C34-C35
30	l	101	LHG	C33-C34-C35-C36
34	X	101	STE	C2-C3-C4-C5
28	a	416	LMG	C11-C12-C13-C14
30	A	414	LHG	C30-C31-C32-C33
31	A	416	DGD	CAB-CBB-CCB-CDB
31	C	515	DGD	C5A-C6A-C7A-C8A
31	H	102	DGD	C9A-CAA-CBA-CCA
34	H	103	STE	C14-C15-C16-C17
34	b	623	STE	C10-C11-C12-C13
34	t	102	STE	C11-C10-C9-C8
22	d	403	CLA	C3-C5-C6-C7
23	d	402	PHO	C2C-C3C-CAC-CBC
28	a	416	LMG	C39-C40-C41-C42
29	a	411	SQD	C29-C30-C31-C32
34	l	102	STE	C9-C10-C11-C12
24	B	618	BCR	C22-C23-C24-C25
22	a	403	CLA	C16-C17-C18-C20
22	c	504	CLA	C8-C10-C11-C12
22	b	607	CLA	O1D-CGD-O2D-CED
28	C	518	LMG	C30-C31-C32-C33
34	C	519	STE	C2-C3-C4-C5
31	c	517	DGD	C1A-C2A-C3A-C4A
24	d	405	BCR	C10-C11-C12-C13
28	a	416	LMG	C32-C33-C34-C35
30	A	414	LHG	C28-C29-C30-C31
31	h	101	DGD	C6B-C7B-C8B-C9B
34	d	412	STE	C6-C7-C8-C9
22	b	614	CLA	C5-C6-C7-C8
27	d	406	PL9	C47-C48-C49-C51
29	A	413	SQD	C34-C35-C36-C37
30	d	407	LHG	C27-C28-C29-C30
34	X	101	STE	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
34	d	411	STE	C6-C7-C8-C9
30	B	621	LHG	O9-C7-O7-C5
30	D	408	LHG	C33-C34-C35-C36
30	d	407	LHG	C29-C30-C31-C32
31	c	518	DGD	C8A-C9A-CAA-CBA
34	H	103	STE	C11-C12-C13-C14
34	b	625	STE	C6-C7-C8-C9
28	c	522	LMG	C2-C1-O1-C7
28	c	521	LMG	O1-C7-C8-O7
28	c	519	LMG	O6-C5-C6-O5
28	a	416	LMG	C33-C34-C35-C36
28	d	410	LMG	C14-C15-C16-C17
31	h	101	DGD	CAB-CBB-CCB-CDB
34	b	623	STE	C2-C3-C4-C5
22	B	616	CLA	C11-C12-C13-C14
28	a	416	LMG	C34-C35-C36-C37
30	D	409	LHG	C27-C28-C29-C30
30	d	407	LHG	C15-C16-C17-C18
31	C	516	DGD	C3A-C4A-C5A-C6A
34	c	523	STE	C6-C7-C8-C9
22	b	606	CLA	C10-C11-C12-C13
27	A	410	PL9	C45-C44-C46-C47
22	c	506	CLA	C2-C3-C5-C6
29	A	415	SQD	C18-C19-C20-C21
34	M	102	STE	C9-C10-C11-C12
22	A	403	CLA	C6-C7-C8-C9
22	A	411	CLA	C11-C12-C13-C14
22	B	604	CLA	C6-C7-C8-C9
22	B	606	CLA	C11-C10-C8-C9
22	B	614	CLA	C11-C12-C13-C14
22	B	615	CLA	C11-C12-C13-C14
22	C	511	CLA	C11-C12-C13-C14
22	a	403	CLA	C6-C7-C8-C9
22	b	601	CLA	C11-C12-C13-C14
22	b	613	CLA	C14-C13-C15-C16
22	b	614	CLA	C14-C13-C15-C16
22	c	510	CLA	C14-C13-C15-C16
31	c	516	DGD	O6E-C5E-C6E-O5E
28	b	624	LMG	C16-C17-C18-C19
34	L	101	STE	C4-C5-C6-C7
22	d	404	CLA	O1D-CGD-O2D-CED
29	a	411	SQD	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
30	d	408	LHG	C16-C17-C18-C19
31	C	516	DGD	C9B-CAB-CBB-CCB
28	c	521	LMG	O6-C5-C6-O5
24	C	514	BCR	C11-C12-C13-C35
24	b	617	BCR	C36-C18-C19-C20
28	b	624	LMG	C30-C31-C32-C33
29	A	413	SQD	C9-C10-C11-C12
30	B	621	LHG	C30-C31-C32-C33
31	H	102	DGD	C5B-C6B-C7B-C8B
34	d	411	STE	C7-C8-C9-C10
30	d	409	LHG	O10-C23-O8-C6
22	B	601	CLA	C1A-C2A-CAA-CBA
22	a	404	CLA	C1A-C2A-CAA-CBA
22	c	511	CLA	C1A-C2A-CAA-CBA
22	c	512	CLA	C1A-C2A-CAA-CBA
22	B	601	CLA	C16-C17-C18-C19
22	B	612	CLA	C16-C17-C18-C19
22	B	614	CLA	C16-C17-C18-C20
22	a	403	CLA	C16-C17-C18-C19
31	c	516	DGD	O1B-C1B-O2G-C2G
28	D	411	LMG	C16-C17-C18-C19
28	a	416	LMG	C18-C19-C20-C21
28	d	410	LMG	C30-C31-C32-C33
30	D	409	LHG	C11-C12-C13-C14
30	l	101	LHG	C15-C16-C17-C18
34	B	625	STE	C11-C12-C13-C14
22	b	613	CLA	C13-C15-C16-C17
31	c	518	DGD	CBB-CCB-CDB-CEB
22	c	509	CLA	C15-C16-C17-C18
28	a	416	LMG	O6-C5-C6-O5
30	B	621	LHG	C32-C33-C34-C35
28	b	624	LMG	C34-C35-C36-C37
30	e	102	LHG	C27-C28-C29-C30
34	C	520	STE	C4-C5-C6-C7
22	B	606	CLA	C16-C17-C18-C20
34	B	626	STE	C6-C7-C8-C9
34	I	101	STE	C5-C6-C7-C8
28	c	521	LMG	C41-C42-C43-C44
34	C	519	STE	C4-C5-C6-C7
34	a	415	STE	C6-C7-C8-C9
34	h	102	STE	C6-C7-C8-C9
28	D	406	LMG	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
28	a	416	LMG	C38-C39-C40-C41
34	d	411	STE	C11-C12-C13-C14
22	C	505	CLA	C4-C3-C5-C6
30	D	408	LHG	C13-C14-C15-C16
34	M	103	STE	C4-C5-C6-C7
29	B	623	SQD	C9-C10-C11-C12
22	c	512	CLA	C16-C17-C18-C20
28	C	518	LMG	O1-C7-C8-C9
28	c	522	LMG	O1-C7-C8-C9
29	B	623	SQD	O6-C44-C45-C46
29	a	411	SQD	O6-C44-C45-C46
30	d	407	LHG	C19-C20-C21-C22
30	d	409	LHG	C4-C5-C6-O8
31	c	516	DGD	O1G-C1G-C2G-C3G
34	a	413	STE	C7-C8-C9-C10
28	c	519	LMG	C34-C35-C36-C37
28	c	522	LMG	C31-C32-C33-C34
30	A	414	LHG	C19-C20-C21-C22
30	D	408	LHG	C25-C26-C27-C28
34	B	626	STE	C14-C15-C16-C17
34	b	623	STE	C5-C6-C7-C8
24	B	618	BCR	C14-C15-C16-C17
28	a	416	LMG	C8-C7-O1-C1
31	C	516	DGD	C2G-C3G-O3G-C1D
31	C	516	DGD	C5D-C6D-O5D-C1E
31	c	517	DGD	C5D-C6D-O5D-C1E
29	B	623	SQD	C35-C36-C37-C38
30	D	409	LHG	C35-C36-C37-C38
30	d	409	LHG	C26-C27-C28-C29
31	c	516	DGD	C1A-C2A-C3A-C4A
29	a	412	SQD	C28-C29-C30-C31
31	C	517	DGD	CDB-CEB-CFB-CGB
22	C	506	CLA	C3-C5-C6-C7
22	C	506	CLA	C5-C6-C7-C8
28	c	521	LMG	C12-C13-C14-C15
30	A	414	LHG	C16-C17-C18-C19
31	h	101	DGD	C7A-C8A-C9A-CAA
34	h	102	STE	C7-C8-C9-C10
28	d	410	LMG	O6-C5-C6-O5
31	C	515	DGD	O6E-C5E-C6E-O5E
30	d	407	LHG	O1-C1-C2-O2
30	d	408	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
28	c	519	LMG	C36-C37-C38-C39
29	A	413	SQD	C17-C18-C19-C20
30	B	621	LHG	C27-C28-C29-C30
30	d	409	LHG	C35-C36-C37-C38
34	c	520	STE	C3-C4-C5-C6
34	l	102	STE	C7-C8-C9-C10
31	C	517	DGD	C3A-C4A-C5A-C6A
34	B	625	STE	C13-C14-C15-C16
34	B	627	STE	C2-C3-C4-C5
30	B	622	LHG	C18-C19-C20-C21
22	d	404	CLA	C8-C10-C11-C12
24	B	617	BCR	C20-C21-C22-C37
28	b	624	LMG	C12-C13-C14-C15
31	C	515	DGD	CBA-CCA-CDA-CEA
34	B	627	STE	C7-C8-C9-C10
27	D	405	PL9	C28-C29-C31-C32
27	d	406	PL9	C13-C14-C16-C17
22	b	616	CLA	O1D-CGD-O2D-CED
22	c	510	CLA	C16-C17-C18-C20
31	h	101	DGD	O6E-C5E-C6E-O5E
29	A	415	SQD	C19-C20-C21-C22
34	C	520	STE	C3-C4-C5-C6
22	C	513	CLA	C8-C10-C11-C12
22	a	404	CLA	C5-C6-C7-C8
29	a	412	SQD	C31-C32-C33-C34
31	C	517	DGD	C8B-C9B-CAB-CBB
34	H	103	STE	C3-C4-C5-C6
34	I	101	STE	C1-C2-C3-C4
22	C	505	CLA	C15-C16-C17-C18
22	c	508	CLA	C16-C17-C18-C19
28	b	624	LMG	C42-C43-C44-C45
30	d	407	LHG	C18-C19-C20-C21
34	B	626	STE	C3-C4-C5-C6
34	b	621	STE	C7-C8-C9-C10
34	B	624	STE	C7-C8-C9-C10
34	b	621	STE	C10-C11-C12-C13
34	c	520	STE	C4-C5-C6-C7
34	d	412	STE	C7-C8-C9-C10
29	A	413	SQD	C28-C29-C30-C31
29	a	411	SQD	C35-C36-C37-C38
30	B	622	LHG	C27-C28-C29-C30
22	c	503	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	c	509	CLA	C8-C10-C11-C12
28	A	412	LMG	C12-C13-C14-C15
28	A	412	LMG	C33-C34-C35-C36
28	b	622	LMG	C31-C32-C33-C34
30	B	622	LHG	C28-C29-C30-C31
30	e	102	LHG	C11-C12-C13-C14
34	X	101	STE	C10-C11-C12-C13
31	c	516	DGD	C4D-C5D-C6D-O5D
30	l	101	LHG	C7-C8-C9-C10
22	C	511	CLA	C15-C16-C17-C18
22	b	605	CLA	C5-C6-C7-C8
30	B	622	LHG	C24-C25-C26-C27
28	c	522	LMG	O1-C7-C8-O7
28	D	406	LMG	C32-C33-C34-C35
30	D	409	LHG	C33-C34-C35-C36
34	d	413	STE	C2-C3-C4-C5
22	C	508	CLA	C10-C11-C12-C13
31	c	516	DGD	CDB-CEB-CFB-CGB
31	h	101	DGD	C3B-C4B-C5B-C6B
34	c	523	STE	C7-C8-C9-C10
29	f	101	SQD	C35-C36-C37-C38
22	A	411	CLA	C11-C12-C13-C15
22	B	603	CLA	C12-C13-C15-C16
22	B	606	CLA	C11-C12-C13-C15
22	B	615	CLA	C11-C10-C8-C7
22	B	615	CLA	C11-C12-C13-C15
22	C	503	CLA	C11-C10-C8-C7
22	C	513	CLA	C11-C10-C8-C7
22	a	403	CLA	C12-C13-C15-C16
22	b	601	CLA	C12-C13-C15-C16
22	b	607	CLA	C11-C10-C8-C7
22	b	607	CLA	C11-C12-C13-C15
22	c	505	CLA	C6-C7-C8-C10
22	c	512	CLA	C6-C7-C8-C10
22	c	512	CLA	C11-C12-C13-C15
22	c	513	CLA	C11-C12-C13-C15
27	A	410	PL9	C33-C34-C36-C37
31	C	515	DGD	C4B-C5B-C6B-C7B
31	C	516	DGD	CDA-CEA-CFA-CGA
22	B	603	CLA	C14-C13-C15-C16
22	B	604	CLA	C14-C13-C15-C16
22	B	607	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	B	614	CLA	C11-C10-C8-C9
22	B	616	CLA	C6-C7-C8-C9
22	C	506	CLA	C6-C7-C8-C9
22	C	511	CLA	C6-C7-C8-C9
22	C	511	CLA	C11-C10-C8-C9
22	C	513	CLA	C11-C10-C8-C9
22	a	403	CLA	C14-C13-C15-C16
22	b	607	CLA	C11-C12-C13-C14
22	b	607	CLA	C14-C13-C15-C16
22	b	608	CLA	C11-C12-C13-C14
22	b	615	CLA	C6-C7-C8-C9
22	c	506	CLA	C6-C7-C8-C9
22	c	512	CLA	C11-C12-C13-C14
28	c	519	LMG	C31-C32-C33-C34
34	C	519	STE	C3-C4-C5-C6
34	b	623	STE	C6-C7-C8-C9
22	C	510	CLA	C10-C11-C12-C13
28	a	416	LMG	C23-C24-C25-C26
31	C	516	DGD	C6B-C7B-C8B-C9B
31	C	517	DGD	CBA-CCA-CDA-CEA
34	d	411	STE	C12-C13-C14-C15
28	C	518	LMG	C39-C40-C41-C42
34	R	101	STE	C6-C7-C8-C9
22	c	513	CLA	C3-C5-C6-C7
30	B	622	LHG	C1-C2-C3-O3
28	a	416	LMG	C37-C38-C39-C40
29	B	623	SQD	C27-C28-C29-C30
31	A	416	DGD	CFA-CGA-CHA-CIA
31	c	518	DGD	C2A-C1A-O1G-C1G
30	B	621	LHG	C23-C24-C25-C26
22	b	607	CLA	C13-C15-C16-C17
31	A	416	DGD	CCA-CDA-CEA-CFA
22	C	501	CLA	CBD-CGD-O2D-CED
22	a	402	CLA	CBD-CGD-O2D-CED
30	d	408	LHG	O6-C4-C5-C6
30	e	102	LHG	O6-C4-C5-C6
34	R	101	STE	C4-C5-C6-C7
28	C	518	LMG	C19-C20-C21-C22
34	C	521	STE	C6-C7-C8-C9
22	B	608	CLA	C13-C15-C16-C17
31	A	416	DGD	CEB-CFB-CGB-CHB
31	c	518	DGD	C6B-C7B-C8B-C9B

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Mol	Chain	Res	Type	Atoms
34	d	413	STE	C3-C4-C5-C6
22	B	610	CLA	C16-C17-C18-C20
22	b	601	CLA	C16-C17-C18-C20
28	D	406	LMG	C11-C12-C13-C14
29	a	412	SQD	C14-C15-C16-C17
30	A	414	LHG	C9-C10-C11-C12
30	B	622	LHG	C31-C32-C33-C34
28	D	410	LMG	C29-C28-O8-C9
28	D	410	LMG	C35-C36-C37-C38
28	b	622	LMG	C34-C35-C36-C37
22	B	601	CLA	C3A-C2A-CAA-CBA
30	B	622	LHG	C25-C26-C27-C28
31	C	516	DGD	C2A-C3A-C4A-C5A
27	a	409	PL9	C47-C48-C49-C50
24	k	101	BCR	C19-C20-C21-C22
22	A	405	CLA	C6-C7-C8-C9
30	l	101	LHG	C34-C35-C36-C37
34	C	520	STE	C12-C13-C14-C15
34	b	621	STE	C15-C16-C17-C18
28	D	406	LMG	C30-C31-C32-C33
22	b	606	CLA	C5-C6-C7-C8
28	M	101	LMG	C7-C8-C9-O8
28	c	521	LMG	O1-C7-C8-C9
28	c	521	LMG	C7-C8-C9-O8
29	a	412	SQD	C44-C45-C46-O48
30	D	408	LHG	C14-C15-C16-C17
30	l	101	LHG	C13-C14-C15-C16
31	c	516	DGD	C8A-C9A-CAA-CBA
34	L	101	STE	C7-C8-C9-C10
22	b	615	CLA	C8-C10-C11-C12
28	D	406	LMG	C12-C13-C14-C15
28	M	101	LMG	C15-C16-C17-C18
30	d	408	LHG	C17-C18-C19-C20
31	c	517	DGD	CAA-CBA-CCA-CDA
34	B	626	STE	C15-C16-C17-C18
22	c	512	CLA	O1D-CGD-O2D-CED
34	c	520	STE	C7-C8-C9-C10
22	B	610	CLA	C16-C17-C18-C19
22	B	611	CLA	C16-C17-C18-C20
22	C	505	CLA	C16-C17-C18-C19
22	b	601	CLA	C16-C17-C18-C19
22	C	505	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
34	b	621	STE	C5-C6-C7-C8
22	c	511	CLA	O1D-CGD-O2D-CED
22	B	609	CLA	C13-C15-C16-C17
22	c	507	CLA	C8-C10-C11-C12
28	b	624	LMG	C28-C29-C30-C31
30	d	409	LHG	C7-C8-C9-C10
31	A	416	DGD	C1B-C2B-C3B-C4B
30	e	102	LHG	C28-C29-C30-C31
31	C	517	DGD	CAB-CBB-CCB-CDB
34	b	627	STE	C1-C2-C3-C4
28	c	521	LMG	C29-C30-C31-C32
30	l	101	LHG	C9-C10-C11-C12
30	l	101	LHG	C31-C32-C33-C34
31	A	416	DGD	CBA-CCA-CDA-CEA
34	b	627	STE	C4-C5-C6-C7
28	a	416	LMG	C35-C36-C37-C38
28	c	521	LMG	C35-C36-C37-C38
34	l	102	STE	C1-C2-C3-C4
27	D	405	PL9	C7-C8-C9-C10
27	D	405	PL9	C37-C38-C39-C40
27	a	409	PL9	C37-C38-C39-C40
22	B	605	CLA	C16-C17-C18-C20
22	B	610	CLA	C15-C16-C17-C18
30	B	621	LHG	C19-C20-C21-C22
28	C	518	LMG	C38-C39-C40-C41
31	h	101	DGD	CDA-CEA-CFA-CGA
28	c	519	LMG	C30-C31-C32-C33
30	d	407	LHG	C13-C14-C15-C16
34	d	413	STE	C12-C13-C14-C15
28	b	622	LMG	O7-C8-C9-O8
29	A	413	SQD	O6-C44-C45-O47
29	a	411	SQD	O47-C45-C46-O48
29	a	412	SQD	O47-C45-C46-O48
30	A	414	LHG	O7-C5-C6-O8
22	a	402	CLA	O1D-CGD-O2D-CED
30	B	622	LHG	C19-C20-C21-C22
34	l	102	STE	C14-C15-C16-C17
22	B	603	CLA	C16-C17-C18-C19
22	C	505	CLA	C16-C17-C18-C20
22	b	608	CLA	C16-C17-C18-C19
29	a	411	SQD	C16-C17-C18-C19
28	D	410	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
28	c	519	LMG	C11-C10-O7-C8
31	c	518	DGD	C8B-C9B-CAB-CBB
28	C	518	LMG	C37-C38-C39-C40
30	B	622	LHG	C12-C13-C14-C15
31	c	518	DGD	CCA-CDA-CEA-CFA
22	D	403	CLA	C8-C10-C11-C12
22	A	403	CLA	C11-C12-C13-C14
22	B	605	CLA	C14-C13-C15-C16
22	B	610	CLA	C14-C13-C15-C16
22	C	508	CLA	C11-C10-C8-C9
22	C	510	CLA	C11-C10-C8-C9
22	b	602	CLA	C14-C13-C15-C16
22	c	505	CLA	C6-C7-C8-C9
22	c	505	CLA	C11-C10-C8-C9
31	c	516	DGD	C3A-C4A-C5A-C6A
34	B	620	STE	C7-C8-C9-C10
22	C	512	CLA	C13-C15-C16-C17
30	D	409	LHG	C2-C3-O3-P
28	C	518	LMG	C15-C16-C17-C18
31	A	416	DGD	C7B-C8B-C9B-CAB
22	c	501	CLA	C2A-CAA-CBA-CGA
22	B	613	CLA	C16-C17-C18-C19
22	b	602	CLA	C16-C17-C18-C19
24	B	617	BCR	C1-C6-C7-C8
24	B	617	BCR	C5-C6-C7-C8
24	K	101	BCR	C23-C24-C25-C26
24	K	102	BCR	C23-C24-C25-C26
24	K	102	BCR	C23-C24-C25-C30
24	Y	101	BCR	C23-C24-C25-C30
24	b	617	BCR	C5-C6-C7-C8
24	c	514	BCR	C1-C6-C7-C8
24	c	514	BCR	C5-C6-C7-C8
24	k	102	BCR	C23-C24-C25-C26
24	k	102	BCR	C23-C24-C25-C30
24	x	101	BCR	C23-C24-C25-C26
24	x	101	BCR	C23-C24-C25-C30
22	c	510	CLA	C13-C15-C16-C17
22	c	512	CLA	C8-C10-C11-C12
34	M	102	STE	C3-C4-C5-C6
34	H	103	STE	C1-C2-C3-C4
24	K	101	BCR	C11-C12-C13-C14
24	K	101	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
22	c	508	CLA	C8-C10-C11-C12
31	C	515	DGD	C9A-CAA-CBA-CCA
24	A	406	BCR	C14-C15-C16-C17
30	d	407	LHG	C17-C18-C19-C20
28	A	412	LMG	C40-C41-C42-C43
29	a	411	SQD	C10-C11-C12-C13
34	d	412	STE	C15-C16-C17-C18
34	h	102	STE	C10-C11-C12-C13
29	A	415	SQD	C30-C31-C32-C33
30	A	414	LHG	C27-C28-C29-C30
30	D	409	LHG	C14-C15-C16-C17
22	c	505	CLA	C13-C15-C16-C17
28	M	101	LMG	C18-C19-C20-C21
28	b	624	LMG	C37-C38-C39-C40
34	a	413	STE	C4-C5-C6-C7
22	A	403	CLA	C11-C10-C8-C7
22	B	604	CLA	C12-C13-C15-C16
22	B	605	CLA	C12-C13-C15-C16
22	B	607	CLA	C11-C10-C8-C7
22	B	614	CLA	C11-C12-C13-C15
22	B	616	CLA	C6-C7-C8-C10
22	C	508	CLA	C11-C10-C8-C7
22	C	510	CLA	C11-C10-C8-C7
22	C	512	CLA	C11-C10-C8-C7
22	C	512	CLA	C12-C13-C15-C16
22	a	403	CLA	C11-C10-C8-C7
22	b	602	CLA	C12-C13-C15-C16
22	b	603	CLA	C11-C10-C8-C7
22	b	604	CLA	C11-C12-C13-C15
22	b	606	CLA	C11-C12-C13-C15
22	b	608	CLA	C11-C12-C13-C15
22	b	609	CLA	C12-C13-C15-C16
22	b	614	CLA	C11-C10-C8-C7
22	c	506	CLA	C6-C7-C8-C10
22	c	506	CLA	C11-C10-C8-C7
22	c	510	CLA	C11-C10-C8-C7
28	D	410	LMG	C13-C14-C15-C16
34	T	102	STE	C10-C11-C12-C13
34	a	414	STE	C3-C4-C5-C6
34	d	412	STE	C5-C6-C7-C8
34	d	412	STE	C11-C12-C13-C14
28	D	410	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
22	b	612	CLA	C16-C17-C18-C20
30	D	409	LHG	O9-C7-O7-C5
29	a	411	SQD	C11-C10-C9-C8
31	C	516	DGD	CBA-CCA-CDA-CEA
24	B	618	BCR	C16-C17-C18-C36
24	K	102	BCR	C16-C17-C18-C36
24	b	617	BCR	C16-C17-C18-C36
24	b	619	BCR	C20-C21-C22-C37
24	d	405	BCR	C20-C21-C22-C37
24	k	102	BCR	C20-C21-C22-C37
22	b	614	CLA	C8-C10-C11-C12
22	A	405	CLA	CBA-CGA-O2A-C1
31	A	416	DGD	C2A-C1A-O1G-C1G
28	b	624	LMG	C40-C41-C42-C43
30	D	409	LHG	C26-C27-C28-C29
22	c	502	CLA	C13-C15-C16-C17
31	A	416	DGD	C8A-C9A-CAA-CBA
31	c	516	DGD	C5A-C6A-C7A-C8A
34	B	627	STE	C6-C7-C8-C9
22	B	603	CLA	CAD-CBD-CGD-O2D
22	B	610	CLA	CAD-CBD-CGD-O2D
22	b	610	CLA	CAD-CBD-CGD-O2D
22	c	503	CLA	CAD-CBD-CGD-O2D
22	c	513	CLA	CAD-CBD-CGD-O2D
28	D	410	LMG	C9-C8-O7-C10
28	a	416	LMG	C9-C8-O7-C10
28	M	101	LMG	C14-C15-C16-C17
28	b	622	LMG	C13-C14-C15-C16
28	b	622	LMG	C39-C40-C41-C42
28	c	521	LMG	C15-C16-C17-C18
29	f	101	SQD	C24-C25-C26-C27
31	H	102	DGD	C5A-C6A-C7A-C8A
22	b	611	CLA	C10-C11-C12-C13
22	b	616	CLA	C10-C11-C12-C13
28	c	521	LMG	C13-C14-C15-C16
30	d	407	LHG	C28-C29-C30-C31
22	A	411	CLA	C16-C17-C18-C19
30	B	622	LHG	C26-C27-C28-C29
34	H	103	STE	C2-C3-C4-C5
34	c	520	STE	C12-C13-C14-C15
22	c	513	CLA	C13-C15-C16-C17
28	D	406	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
34	d	413	STE	C11-C12-C13-C14
22	D	402	CLA	C2C-C3C-CAC-CBC
22	a	410	CLA	C2C-C3C-CAC-CBC
28	b	622	LMG	C7-C8-C9-O8
28	b	624	LMG	O1-C7-C8-C9
28	b	624	LMG	C7-C8-C9-O8
29	f	101	SQD	C44-C45-C46-O48
30	A	414	LHG	C4-C5-C6-O8
31	A	416	DGD	C1G-C2G-C3G-O3G
28	D	411	LMG	C12-C13-C14-C15
22	b	610	CLA	C2A-CAA-CBA-CGA
22	c	505	CLA	C5-C6-C7-C8
30	B	621	LHG	C16-C17-C18-C19
28	C	518	LMG	O9-C10-O7-C8
30	e	102	LHG	O9-C7-O7-C5
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	C	502	CLA	CHA-CBD-CGD-O1D
22	C	502	CLA	CHA-CBD-CGD-O2D
22	C	504	CLA	CHA-CBD-CGD-O1D
22	C	508	CLA	CHA-CBD-CGD-O2D
22	a	410	CLA	CHA-CBD-CGD-O1D
22	c	502	CLA	CHA-CBD-CGD-O1D
22	c	504	CLA	CHA-CBD-CGD-O1D
22	c	504	CLA	CHA-CBD-CGD-O2D
22	c	506	CLA	CHA-CBD-CGD-O1D
34	b	627	STE	C5-C6-C7-C8
27	a	409	PL9	C12-C13-C14-C16
30	B	622	LHG	C9-C10-C11-C12
24	k	101	BCR	C11-C10-C9-C8
28	C	518	LMG	C2-C1-O1-C7
29	D	407	SQD	C25-C26-C27-C28
34	X	101	STE	C5-C6-C7-C8
28	C	518	LMG	O1-C7-C8-O7
28	M	101	LMG	O7-C8-C9-O8
28	c	521	LMG	O7-C8-C9-O8
22	a	404	CLA	C10-C11-C12-C13
29	b	620	SQD	C12-C13-C14-C15
34	a	415	STE	C1-C2-C3-C4
28	b	622	LMG	C19-C20-C21-C22
31	c	516	DGD	CBB-CCB-CDB-CEB

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Mol	Chain	Res	Type	Atoms
34	B	620	STE	C11-C10-C9-C8
34	C	520	STE	C7-C8-C9-C10
28	b	622	LMG	C12-C13-C14-C15
29	A	413	SQD	C10-C11-C12-C13
27	a	409	PL9	C4-C3-C7-C8
28	b	622	LMG	C16-C17-C18-C19
29	B	623	SQD	C19-C20-C21-C22
30	B	622	LHG	O9-C7-O7-C5
22	C	512	CLA	C14-C13-C15-C16
22	b	609	CLA	C14-C13-C15-C16
22	c	506	CLA	C11-C10-C8-C9
22	c	512	CLA	C14-C13-C15-C16
34	d	413	STE	C4-C5-C6-C7
34	c	520	STE	C10-C11-C12-C13
22	c	510	CLA	C8-C10-C11-C12
31	H	102	DGD	CBB-CCB-CDB-CEB
31	H	102	DGD	CDB-CEB-CFB-CGB
24	c	514	BCR	C17-C18-C19-C20
22	c	508	CLA	C1A-C2A-CAA-CBA
28	D	411	LMG	C10-C11-C12-C13
34	B	624	STE	C1-C2-C3-C4
34	d	411	STE	C1-C2-C3-C4
22	b	616	CLA	C2-C1-O2A-CGA
22	b	604	CLA	C5-C6-C7-C8
30	A	414	LHG	C4-O6-P-O3
34	T	102	STE	C5-C6-C7-C8
29	b	620	SQD	C15-C16-C17-C18
22	C	506	CLA	C4-C3-C5-C6
28	D	406	LMG	C34-C35-C36-C37
30	B	621	LHG	C26-C27-C28-C29
30	d	408	LHG	C15-C16-C17-C18
31	C	515	DGD	CCB-CDB-CEB-CFB
30	A	414	LHG	C3-O3-P-O4
30	D	408	LHG	C4-O6-P-O5
30	D	409	LHG	C3-O3-P-O5
22	b	608	CLA	C16-C17-C18-C20
22	c	502	CLA	C16-C17-C18-C19
34	a	414	STE	C2-C3-C4-C5
27	A	410	PL9	C17-C18-C19-C20
28	a	416	LMG	C29-C30-C31-C32
28	d	410	LMG	C15-C16-C17-C18
22	b	616	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
30	e	102	LHG	C17-C18-C19-C20
30	l	101	LHG	C14-C15-C16-C17
31	C	515	DGD	C4A-C5A-C6A-C7A
22	B	607	CLA	CAD-CBD-CGD-O1D
22	C	502	CLA	CAD-CBD-CGD-O1D
22	C	504	CLA	CAD-CBD-CGD-O1D
22	c	502	CLA	CAD-CBD-CGD-O1D
22	c	504	CLA	CAD-CBD-CGD-O1D
22	c	506	CLA	CAD-CBD-CGD-O1D
29	A	413	SQD	C26-C27-C28-C29
29	a	411	SQD	C23-C24-C25-C26
28	M	101	LMG	C39-C40-C41-C42
31	c	517	DGD	C4E-C5E-C6E-O5E
31	C	517	DGD	C4B-C5B-C6B-C7B
22	A	403	CLA	C11-C12-C13-C15
22	A	411	CLA	C12-C13-C15-C16
22	B	604	CLA	C11-C10-C8-C7
22	B	605	CLA	C11-C10-C8-C7
22	B	609	CLA	C12-C13-C15-C16
22	C	504	CLA	C11-C10-C8-C7
22	C	505	CLA	C6-C7-C8-C10
22	C	505	CLA	C12-C13-C15-C16
22	C	506	CLA	C12-C13-C15-C16
22	C	507	CLA	C11-C10-C8-C7
22	C	509	CLA	C11-C12-C13-C15
22	b	602	CLA	C11-C12-C13-C15
22	b	605	CLA	C12-C13-C15-C16
22	b	607	CLA	C6-C7-C8-C10
22	c	508	CLA	C12-C13-C15-C16
22	c	509	CLA	C11-C12-C13-C15
22	c	511	CLA	C12-C13-C15-C16
22	c	512	CLA	C12-C13-C15-C16
30	d	408	LHG	O6-C4-C5-O7
28	A	412	LMG	C17-C18-C19-C20
30	d	409	LHG	C29-C30-C31-C32
22	C	512	CLA	C3-C5-C6-C7
29	D	407	SQD	C44-C45-C46-O48
31	C	515	DGD	O1G-C1A-C2A-C3A
28	D	406	LMG	C38-C39-C40-C41
28	M	101	LMG	C22-C23-C24-C25
28	c	521	LMG	C38-C39-C40-C41
34	Z	101	STE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	a	403	CLA	C13-C15-C16-C17
31	C	516	DGD	CAB-CBB-CCB-CDB
22	A	405	CLA	O1A-CGA-O2A-C1
30	B	622	LHG	O2-C2-C3-O3
28	A	412	LMG	C14-C15-C16-C17
31	c	516	DGD	C7A-C8A-C9A-CAA
28	a	416	LMG	O1-C7-C8-O7
28	b	624	LMG	O1-C7-C8-O7
28	b	624	LMG	O7-C8-C9-O8
29	b	620	SQD	O47-C45-C46-O48
29	f	101	SQD	O47-C45-C46-O48
30	d	409	LHG	O7-C5-C6-O8
31	c	516	DGD	O1G-C1G-C2G-O2G
31	c	517	DGD	C2G-C3G-O3G-C1D
22	B	603	CLA	C10-C11-C12-C13
22	d	403	CLA	C8-C10-C11-C12
22	b	616	CLA	C3-C5-C6-C7
22	c	512	CLA	C4-C3-C5-C6
28	D	406	LMG	C14-C15-C16-C17
22	B	602	CLA	C14-C13-C15-C16
22	B	605	CLA	C11-C10-C8-C9
22	B	613	CLA	C11-C12-C13-C14
22	C	505	CLA	C6-C7-C8-C9
22	C	505	CLA	C14-C13-C15-C16
22	a	403	CLA	C11-C10-C8-C9
22	b	603	CLA	C6-C7-C8-C9
22	b	603	CLA	C11-C10-C8-C9
22	b	604	CLA	C11-C12-C13-C14
22	c	506	CLA	C14-C13-C15-C16
22	c	513	CLA	C6-C7-C8-C9
28	C	518	LMG	C16-C17-C18-C19
34	j	101	STE	C5-C6-C7-C8
22	c	510	CLA	C16-C17-C18-C19
28	C	518	LMG	C11-C12-C13-C14
34	T	102	STE	C13-C14-C15-C16
23	d	402	PHO	C4C-C3C-CAC-CBC
34	T	102	STE	C15-C16-C17-C18
29	a	411	SQD	C7-C8-C9-C10
30	e	102	LHG	C7-C8-C9-C10
28	c	519	LMG	C39-C40-C41-C42
34	t	102	STE	C7-C8-C9-C10
22	C	512	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	h	101	DGD	C7B-C8B-C9B-CAB
31	c	516	DGD	C2A-C3A-C4A-C5A
34	B	627	STE	C3-C4-C5-C6
28	c	522	LMG	C13-C14-C15-C16
22	c	509	CLA	CAA-CBA-CGA-O2A
29	A	415	SQD	C11-C10-C9-C8
34	I	101	STE	C9-C10-C11-C12
29	f	101	SQD	C44-C45-O47-C7
29	f	101	SQD	C46-C45-O47-C7
22	C	512	CLA	C2A-CAA-CBA-CGA
22	B	613	CLA	C2-C1-O2A-CGA
22	C	507	CLA	C5-C6-C7-C8
34	b	626	STE	C3-C4-C5-C6
22	c	502	CLA	C16-C17-C18-C20
31	H	102	DGD	CBA-CCA-CDA-CEA
24	K	101	BCR	C23-C24-C25-C30
24	Y	101	BCR	C23-C24-C25-C26
31	C	517	DGD	C2A-C1A-O1G-C1G
31	H	102	DGD	O2G-C1B-C2B-C3B
31	c	516	DGD	O1G-C1A-C2A-C3A
31	H	102	DGD	CCB-CDB-CEB-CFB
22	b	612	CLA	C16-C17-C18-C19
31	C	516	DGD	O6D-C1D-O3G-C3G
29	b	620	SQD	C19-C20-C21-C22
24	x	101	BCR	C12-C13-C14-C15
30	d	408	LHG	C9-C10-C11-C12
31	A	416	DGD	O1G-C1G-C2G-O2G
31	C	515	DGD	O1G-C1G-C2G-O2G
29	B	623	SQD	C18-C19-C20-C21
30	A	414	LHG	C3-O3-P-O6
34	d	412	STE	C4-C5-C6-C7
31	C	517	DGD	O6D-C5D-C6D-O5D
30	B	621	LHG	C24-C25-C26-C27
31	H	102	DGD	C6B-C7B-C8B-C9B
22	B	611	CLA	C11-C10-C8-C7
22	B	612	CLA	C6-C7-C8-C10
22	a	404	CLA	C12-C13-C15-C16
22	b	614	CLA	C11-C12-C13-C15
22	c	501	CLA	C11-C12-C13-C15
29	A	415	SQD	C31-C32-C33-C34
30	B	622	LHG	C30-C31-C32-C33
34	b	626	STE	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
22	C	504	CLA	C11-C10-C8-C9
22	C	509	CLA	C11-C12-C13-C14
22	b	602	CLA	C11-C10-C8-C9
22	b	602	CLA	C11-C12-C13-C14
22	b	605	CLA	C14-C13-C15-C16
22	b	614	CLA	C11-C10-C8-C9
22	c	513	CLA	C11-C12-C13-C14
22	b	610	CLA	C16-C17-C18-C20
29	A	413	SQD	C31-C32-C33-C34
22	b	601	CLA	C2A-CAA-CBA-CGA
30	D	409	LHG	C15-C16-C17-C18
31	C	517	DGD	CBB-CCB-CDB-CEB
34	Z	101	STE	C13-C14-C15-C16
22	b	616	CLA	C11-C12-C13-C15
29	B	623	SQD	C30-C31-C32-C33
31	C	515	DGD	C2B-C3B-C4B-C5B
31	c	517	DGD	C4B-C5B-C6B-C7B
30	d	409	LHG	C2-C3-O3-P
22	b	616	CLA	C8-C10-C11-C12
28	c	521	LMG	C36-C37-C38-C39
22	C	511	CLA	CBA-CGA-O2A-C1
30	e	102	LHG	C12-C13-C14-C15
34	b	625	STE	C9-C10-C11-C12
28	b	624	LMG	O6-C1-O1-C7
31	c	516	DGD	O6E-C1E-O5D-C6D
24	c	514	BCR	C13-C14-C15-C16
30	B	621	LHG	O6-C4-C5-C6
29	b	620	SQD	C11-C12-C13-C14
22	D	402	CLA	C10-C11-C12-C13
23	d	401	PHO	C2C-C3C-CAC-CBC
29	D	407	SQD	C34-C35-C36-C37
34	T	102	STE	C9-C10-C11-C12
34	X	101	STE	C9-C10-C11-C12
22	B	601	CLA	C3-C5-C6-C7
22	B	601	CLA	C4-C3-C5-C6
27	d	406	PL9	C28-C29-C31-C32
28	b	622	LMG	C40-C41-C42-C43
31	h	101	DGD	CCB-CDB-CEB-CFB
22	D	402	CLA	C2-C1-O2A-CGA
27	d	406	PL9	C7-C8-C9-C10
30	A	414	LHG	C18-C19-C20-C21
34	B	625	STE	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	D	403	CLA	C3A-C2A-CAA-CBA
30	e	102	LHG	C23-C24-C25-C26
31	h	101	DGD	O2G-C1B-C2B-C3B
29	A	415	SQD	C10-C11-C12-C13
34	B	625	STE	C11-C10-C9-C8
22	C	506	CLA	C2-C3-C5-C6
22	c	512	CLA	C2-C3-C5-C6
27	a	409	PL9	C38-C39-C41-C42
27	A	410	PL9	C4-C3-C7-C8
28	A	412	LMG	C31-C32-C33-C34
34	L	101	STE	C3-C4-C5-C6
22	B	601	CLA	C11-C12-C13-C14
22	B	605	CLA	C6-C7-C8-C9
22	C	513	CLA	C11-C12-C13-C14
22	D	403	CLA	C11-C12-C13-C14
22	b	601	CLA	C11-C10-C8-C9
22	b	610	CLA	C14-C13-C15-C16
22	b	615	CLA	C11-C10-C8-C9
22	c	511	CLA	C11-C10-C8-C9
28	c	522	LMG	C19-C20-C21-C22
30	A	414	LHG	C11-C10-C9-C8
31	h	101	DGD	CCA-CDA-CEA-CFA
29	A	413	SQD	O6-C44-C45-C46
31	C	515	DGD	O1G-C1G-C2G-C3G
27	D	405	PL9	C27-C28-C29-C30
22	C	512	CLA	O2A-C1-C2-C3
22	b	601	CLA	O2A-C1-C2-C3
23	d	401	PHO	O2A-C1-C2-C3
31	C	515	DGD	O6E-C1E-O5D-C6D
28	D	411	LMG	C33-C34-C35-C36
30	d	409	LHG	C25-C26-C27-C28
31	C	515	DGD	C5B-C6B-C7B-C8B
34	B	625	STE	C12-C13-C14-C15
28	D	406	LMG	C33-C34-C35-C36
29	B	623	SQD	C46-C45-O47-C7
22	c	503	CLA	C10-C11-C12-C13
30	d	409	LHG	C27-C28-C29-C30
22	B	612	CLA	C11-C10-C8-C7
22	B	613	CLA	C6-C7-C8-C10
22	B	616	CLA	C11-C10-C8-C7
22	D	402	CLA	C6-C7-C8-C10
22	D	402	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	b	605	CLA	C11-C10-C8-C7
22	b	608	CLA	C11-C10-C8-C7
22	c	502	CLA	C11-C12-C13-C15
22	c	505	CLA	C11-C10-C8-C7
22	c	508	CLA	C6-C7-C8-C10
23	d	401	PHO	C6-C7-C8-C10
24	k	102	BCR	C19-C20-C21-C22
30	e	102	LHG	C19-C20-C21-C22
30	e	102	LHG	C3-O3-P-O6
31	C	517	DGD	C9B-CAB-CBB-CCB
28	d	410	LMG	C34-C35-C36-C37
29	D	407	SQD	C26-C27-C28-C29
31	C	516	DGD	C2B-C3B-C4B-C5B
30	A	414	LHG	C2-C3-O3-P
22	b	614	CLA	C2A-CAA-CBA-CGA
31	C	515	DGD	O6D-C5D-C6D-O5D
29	A	415	SQD	C24-C25-C26-C27
30	D	408	LHG	C28-C29-C30-C31
22	b	612	CLA	C13-C15-C16-C17
34	H	103	STE	C4-C5-C6-C7
22	b	606	CLA	C16-C17-C18-C20
28	D	410	LMG	C33-C34-C35-C36
22	C	502	CLA	C16-C17-C18-C19
24	B	618	BCR	C11-C10-C9-C8
31	c	516	DGD	C8B-C9B-CAB-CBB
29	B	623	SQD	C45-C46-O48-C23
34	d	413	STE	C15-C16-C17-C18
24	Y	101	BCR	C13-C14-C15-C16
22	b	605	CLA	C10-C11-C12-C13
34	a	414	STE	C6-C7-C8-C9
31	C	517	DGD	CCA-CDA-CEA-CFA
28	A	412	LMG	O6-C1-O1-C7
22	C	511	CLA	O1A-CGA-O2A-C1
22	b	603	CLA	C4-C3-C5-C6
27	a	409	PL9	C40-C39-C41-C42
22	a	402	CLA	C2-C1-O2A-CGA
22	b	611	CLA	C8-C10-C11-C12
34	b	625	STE	C10-C11-C12-C13
22	c	502	CLA	C11-C12-C13-C14
29	a	412	SQD	C11-C12-C13-C14
27	A	410	PL9	C11-C12-C13-C14
28	D	406	LMG	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
30	A	414	LHG	C14-C15-C16-C17
30	B	621	LHG	C9-C10-C11-C12
30	B	621	LHG	C11-C12-C13-C14
22	B	601	CLA	C2A-CAA-CBA-CGA
22	A	411	CLA	C16-C17-C18-C20
28	c	521	LMG	C33-C34-C35-C36
22	C	505	CLA	O1A-CGA-O2A-C1
24	B	618	BCR	C23-C24-C25-C30
24	C	514	BCR	C23-C24-C25-C30
24	c	514	BCR	C23-C24-C25-C30
24	c	515	BCR	C23-C24-C25-C30
24	k	101	BCR	C23-C24-C25-C30
22	b	608	CLA	C13-C15-C16-C17
30	B	622	LHG	C15-C16-C17-C18
28	a	416	LMG	O8-C28-C29-C30
28	A	412	LMG	C7-C8-C9-O8
28	M	101	LMG	O1-C7-C8-C9
29	a	411	SQD	C44-C45-C46-O48
28	c	522	LMG	C37-C38-C39-C40
29	A	415	SQD	C15-C16-C17-C18
29	a	411	SQD	C18-C19-C20-C21
22	D	403	CLA	C4-C3-C5-C6
24	A	406	BCR	C17-C18-C19-C20
24	Y	101	BCR	C11-C12-C13-C14
34	M	102	STE	C7-C8-C9-C10
29	a	411	SQD	C11-C12-C13-C14
28	c	522	LMG	C32-C33-C34-C35
34	j	101	STE	C3-C4-C5-C6
30	B	621	LHG	O6-C4-C5-O7
31	C	516	DGD	C8A-C9A-CAA-CBA
31	c	516	DGD	CCB-CDB-CEB-CFB
34	J	101	STE	C5-C6-C7-C8
28	A	412	LMG	O6-C5-C6-O5
30	d	409	LHG	C11-C10-C9-C8
31	C	517	DGD	C3B-C4B-C5B-C6B
27	a	409	PL9	C44-C46-C47-C48
22	C	506	CLA	C6-C7-C8-C10
22	b	603	CLA	C2-C3-C5-C6
22	d	404	CLA	C6-C7-C8-C10
31	c	517	DGD	C4A-C5A-C6A-C7A
30	d	409	LHG	O1-C1-C2-O2
31	h	101	DGD	O1B-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
28	b	624	LMG	C2-C1-O1-C7
31	C	516	DGD	C2D-C1D-O3G-C3G
28	A	412	LMG	C18-C19-C20-C21
22	b	612	CLA	C8-C10-C11-C12
22	c	508	CLA	C10-C11-C12-C13
23	d	402	PHO	C8-C10-C11-C12
22	B	612	CLA	CAA-CBA-CGA-O2A
28	A	412	LMG	C38-C39-C40-C41
30	d	407	LHG	C35-C36-C37-C38
22	a	403	CLA	C8-C10-C11-C12
22	A	402	CLA	C4C-C3C-CAC-CBC
24	H	101	BCR	C35-C13-C14-C15
24	K	101	BCR	C20-C21-C22-C37
24	b	617	BCR	C20-C21-C22-C37
24	x	101	BCR	C20-C21-C22-C37
22	b	608	CLA	C4-C3-C5-C6
23	d	402	PHO	C4-C3-C5-C6
27	a	409	PL9	C25-C24-C26-C27
31	C	515	DGD	CDB-CEB-CFB-CGB
28	b	624	LMG	C15-C16-C17-C18
29	f	101	SQD	C32-C33-C34-C35
22	b	606	CLA	C16-C17-C18-C19
30	B	621	LHG	O7-C7-C8-C9
22	A	403	CLA	C11-C10-C8-C9
22	A	411	CLA	C14-C13-C15-C16
22	B	612	CLA	C11-C10-C8-C9
22	B	615	CLA	C11-C10-C8-C9
22	C	506	CLA	C14-C13-C15-C16
22	C	511	CLA	C14-C13-C15-C16
22	D	403	CLA	C6-C7-C8-C9
22	a	403	CLA	C11-C12-C13-C14
22	b	606	CLA	C11-C10-C8-C9
22	b	606	CLA	C11-C12-C13-C14
22	b	607	CLA	C6-C7-C8-C9
22	c	508	CLA	C6-C7-C8-C9
22	c	508	CLA	C14-C13-C15-C16
23	d	401	PHO	C6-C7-C8-C9
34	a	415	STE	C11-C10-C9-C8
22	B	607	CLA	C3A-C2A-CAA-CBA
22	d	404	CLA	C3A-C2A-CAA-CBA
22	B	604	CLA	CAD-CBD-CGD-O2D
22	B	605	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	B	616	CLA	CAD-CBD-CGD-O2D
22	C	501	CLA	CAD-CBD-CGD-O2D
22	C	503	CLA	CAD-CBD-CGD-O2D
22	C	505	CLA	CAD-CBD-CGD-O2D
22	C	510	CLA	CAD-CBD-CGD-O2D
22	C	512	CLA	CAD-CBD-CGD-O2D
22	b	604	CLA	CAD-CBD-CGD-O2D
22	b	605	CLA	CAD-CBD-CGD-O2D
22	c	512	CLA	CAD-CBD-CGD-O2D
23	d	401	PHO	CAD-CBD-CGD-O2D
28	b	624	LMG	C9-C8-O7-C10
22	B	602	CLA	C16-C17-C18-C19
30	B	621	LHG	C17-C18-C19-C20
34	C	519	STE	C6-C7-C8-C9
22	B	603	CLA	C2A-CAA-CBA-CGA
34	B	620	STE	C2-C3-C4-C5
29	A	413	SQD	C29-C30-C31-C32
30	A	414	LHG	C10-C11-C12-C13
30	d	408	LHG	C25-C26-C27-C28
31	c	517	DGD	C1B-C2B-C3B-C4B
30	D	409	LHG	O8-C23-C24-C25
22	c	508	CLA	C4-C3-C5-C6
22	A	403	CLA	C16-C17-C18-C19
22	B	601	CLA	C2-C3-C5-C6
22	c	511	CLA	O1A-CGA-O2A-C1
24	K	101	BCR	C21-C22-C23-C24
24	k	101	BCR	C7-C8-C9-C10
31	c	517	DGD	C3A-C4A-C5A-C6A
22	A	411	CLA	C2C-C3C-CAC-CBC
22	B	604	CLA	C2C-C3C-CAC-CBC
22	d	403	CLA	C2C-C3C-CAC-CBC
30	e	102	LHG	C4-C5-C6-O8
31	A	416	DGD	O1G-C1G-C2G-C3G
34	I	101	STE	C2-C3-C4-C5
22	b	601	CLA	CAA-CBA-CGA-O2A
29	a	411	SQD	O47-C7-C8-C9
29	B	623	SQD	C29-C30-C31-C32
22	B	601	CLA	O2A-C1-C2-C3
22	C	509	CLA	O2A-C1-C2-C3
22	C	513	CLA	O2A-C1-C2-C3
22	d	403	CLA	O2A-C1-C2-C3
23	A	404	PHO	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
22	C	513	CLA	C16-C17-C18-C19
34	I	102	STE	C2-C3-C4-C5
22	A	403	CLA	CHA-CBD-CGD-O1D
22	A	403	CLA	CHA-CBD-CGD-O2D
22	B	602	CLA	CHA-CBD-CGD-O2D
22	B	603	CLA	CHA-CBD-CGD-O2D
22	B	612	CLA	CHA-CBD-CGD-O1D
22	B	614	CLA	CHA-CBD-CGD-O1D
22	B	614	CLA	CHA-CBD-CGD-O2D
22	C	504	CLA	CHA-CBD-CGD-O2D
22	C	505	CLA	CHA-CBD-CGD-O2D
22	C	506	CLA	CHA-CBD-CGD-O1D
22	a	403	CLA	CHA-CBD-CGD-O1D
22	a	403	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	b	607	CLA	CHA-CBD-CGD-O2D
22	b	611	CLA	CHA-CBD-CGD-O1D
22	b	611	CLA	CHA-CBD-CGD-O2D
22	c	502	CLA	CHA-CBD-CGD-O2D
22	c	506	CLA	CHA-CBD-CGD-O2D
22	c	507	CLA	CHA-CBD-CGD-O1D
22	c	507	CLA	CHA-CBD-CGD-O2D
22	c	509	CLA	CHA-CBD-CGD-O2D
23	d	402	PHO	CHA-CBD-CGD-O1D
23	d	402	PHO	CHA-CBD-CGD-O2D
31	h	101	DGD	CBB-CCB-CDB-CEB
34	C	520	STE	C11-C12-C13-C14
29	b	620	SQD	C17-C18-C19-C20
28	c	522	LMG	C35-C36-C37-C38
28	A	412	LMG	O1-C7-C8-O7
29	b	620	SQD	O6-C44-C45-O47
28	d	410	LMG	C37-C38-C39-C40
22	b	612	CLA	CAA-CBA-CGA-O2A
22	c	510	CLA	CAA-CBA-CGA-O2A
30	e	102	LHG	O8-C23-C24-C25
22	b	616	CLA	CBA-CGA-O2A-C1
22	B	613	CLA	CAA-CBA-CGA-O2A
30	D	408	LHG	C29-C30-C31-C32
34	a	414	STE	C4-C5-C6-C7
22	D	403	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	a	410	CLA	C11-C12-C13-C15
22	b	615	CLA	C11-C10-C8-C7
22	b	615	CLA	C12-C13-C15-C16
22	b	616	CLA	C6-C7-C8-C10
22	c	508	CLA	C11-C10-C8-C7
22	B	606	CLA	C8-C10-C11-C12
22	B	613	CLA	C6-C7-C8-C9
22	C	502	CLA	C11-C12-C13-C14
22	D	402	CLA	C6-C7-C8-C9
22	a	410	CLA	C11-C12-C13-C14
22	b	615	CLA	C14-C13-C15-C16
22	c	501	CLA	C11-C12-C13-C14
22	c	508	CLA	C11-C10-C8-C9
30	B	621	LHG	C11-C10-C9-C8
31	c	516	DGD	C9A-CAA-CBA-CCA
22	B	612	CLA	CBA-CGA-O2A-C1
30	D	409	LHG	O10-C23-C24-C25
29	a	411	SQD	C8-C7-O47-C45
30	e	102	LHG	C8-C7-O7-C5
31	A	416	DGD	CDA-CEA-CFA-CGA
28	d	410	LMG	O7-C10-C11-C12
29	f	101	SQD	O48-C23-C24-C25
22	B	612	CLA	CAA-CBA-CGA-O1A
22	A	403	CLA	C16-C17-C18-C20
27	d	406	PL9	C30-C29-C31-C32
31	c	518	DGD	CAB-CBB-CCB-CDB
22	c	508	CLA	C2-C3-C5-C6
28	b	624	LMG	C23-C24-C25-C26
22	B	602	CLA	C1A-C2A-CAA-CBA
22	B	607	CLA	C1A-C2A-CAA-CBA
22	D	403	CLA	C1A-C2A-CAA-CBA
22	b	601	CLA	C1A-C2A-CAA-CBA
22	c	513	CLA	C1A-C2A-CAA-CBA
22	d	404	CLA	C1A-C2A-CAA-CBA
34	B	627	STE	C1-C2-C3-C4
34	c	520	STE	C1-C2-C3-C4
31	C	515	DGD	O1B-C1B-C2B-C3B
28	b	622	LMG	C11-C10-O7-C8
22	A	402	CLA	C2-C1-O2A-CGA
22	d	403	CLA	C2-C1-O2A-CGA
22	c	511	CLA	CBA-CGA-O2A-C1
29	A	415	SQD	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
30	e	102	LHG	O10-C23-C24-C25
28	a	416	LMG	C22-C23-C24-C25
34	C	521	STE	C3-C4-C5-C6
34	L	101	STE	C5-C6-C7-C8
29	b	620	SQD	C44-C45-C46-O48
22	B	610	CLA	C2A-CAA-CBA-CGA
30	d	409	LHG	C4-O6-P-O3
30	D	409	LHG	C13-C14-C15-C16
34	I	101	STE	C7-C8-C9-C10
23	D	401	PHO	C8-C10-C11-C12
31	c	516	DGD	O1B-C1B-C2B-C3B
24	D	404	BCR	C22-C23-C24-C25
30	A	414	LHG	C3-O3-P-O5
30	A	414	LHG	C4-O6-P-O5
22	c	510	CLA	CAA-CBA-CGA-O1A
30	D	408	LHG	O10-C23-O8-C6
24	x	101	BCR	C11-C10-C9-C34
30	l	101	LHG	C28-C29-C30-C31
24	B	618	BCR	C23-C24-C25-C26
22	B	610	CLA	C10-C11-C12-C13
22	C	513	CLA	C10-C11-C12-C13
28	b	622	LMG	O8-C28-C29-C30
31	C	515	DGD	C3A-C4A-C5A-C6A
28	b	622	LMG	C35-C36-C37-C38
28	b	624	LMG	C18-C19-C20-C21
22	A	403	CLA	CAD-CBD-CGD-O1D
22	B	609	CLA	CAD-CBD-CGD-O1D
22	B	611	CLA	CAD-CBD-CGD-O1D
22	B	612	CLA	CAD-CBD-CGD-O1D
22	C	506	CLA	CAD-CBD-CGD-O1D
22	b	607	CLA	CAD-CBD-CGD-O1D
22	b	611	CLA	CAD-CBD-CGD-O1D
22	c	511	CLA	C3-C5-C6-C7
30	D	408	LHG	C7-C8-C9-C10
31	C	515	DGD	C4D-C5D-C6D-O5D
22	B	613	CLA	C14-C13-C15-C16
22	B	615	CLA	C14-C13-C15-C16
22	C	509	CLA	C14-C13-C15-C16
22	C	512	CLA	C6-C7-C8-C9
22	a	404	CLA	C6-C7-C8-C9
22	b	602	CLA	C6-C7-C8-C9
22	b	608	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	b	614	CLA	C11-C12-C13-C14
22	c	504	CLA	C6-C7-C8-C9
22	c	504	CLA	C11-C10-C8-C9
22	c	506	CLA	C11-C12-C13-C14
22	c	507	CLA	C11-C10-C8-C9
22	d	403	CLA	C6-C7-C8-C9
28	D	410	LMG	C11-C12-C13-C14
29	a	411	SQD	C12-C13-C14-C15
22	b	610	CLA	C5-C6-C7-C8
22	C	505	CLA	CBA-CGA-O2A-C1
28	a	416	LMG	O7-C10-C11-C12
29	A	415	SQD	O48-C23-C24-C25
31	c	516	DGD	O2G-C1B-C2B-C3B
30	B	622	LHG	C32-C33-C34-C35
34	B	624	STE	C3-C4-C5-C6
30	D	409	LHG	C17-C18-C19-C20
29	A	413	SQD	O47-C7-C8-C9
31	C	515	DGD	O2G-C1B-C2B-C3B
22	c	506	CLA	C8-C10-C11-C12
28	M	101	LMG	C17-C18-C19-C20
34	T	102	STE	C4-C5-C6-C7
27	d	406	PL9	C20-C19-C21-C22
24	t	101	BCR	C11-C12-C13-C35
22	B	613	CLA	C12-C13-C15-C16
22	B	615	CLA	C12-C13-C15-C16
22	C	502	CLA	C11-C12-C13-C15
22	D	402	CLA	C11-C10-C8-C7
22	b	610	CLA	C11-C12-C13-C15
22	b	610	CLA	C12-C13-C15-C16
22	c	507	CLA	C11-C10-C8-C7
22	c	513	CLA	C6-C7-C8-C10
22	d	403	CLA	C6-C7-C8-C10
28	c	522	LMG	C11-C12-C13-C14
30	l	101	LHG	O7-C7-C8-C9
24	t	101	BCR	C7-C8-C9-C10
29	B	623	SQD	O10-C23-C24-C25
24	K	101	BCR	C9-C10-C11-C12
22	D	403	CLA	C10-C11-C12-C13
22	a	410	CLA	C8-C10-C11-C12
22	B	613	CLA	CAA-CBA-CGA-O1A
27	d	406	PL9	C39-C41-C42-C43
29	B	623	SQD	C26-C27-C28-C29

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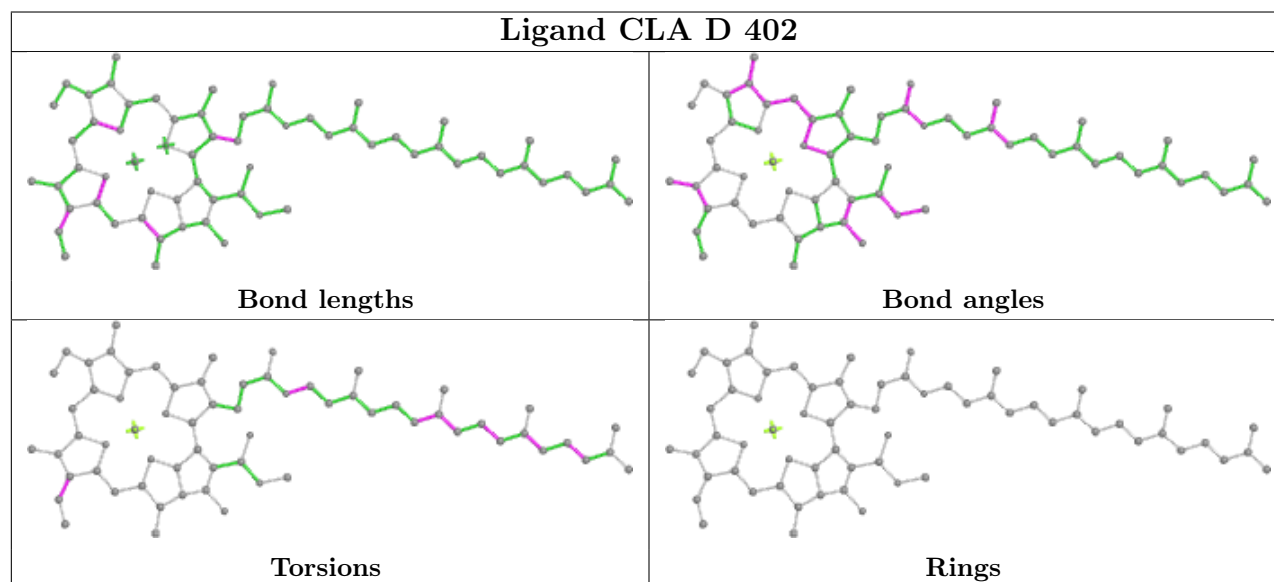
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Mol	Chain	Res	Type	Atoms
31	H	102	DGD	C2B-C3B-C4B-C5B
22	b	612	CLA	CAA-CBA-CGA-O1A
29	A	413	SQD	O49-C7-C8-C9
23	d	401	PHO	C4-C3-C5-C6

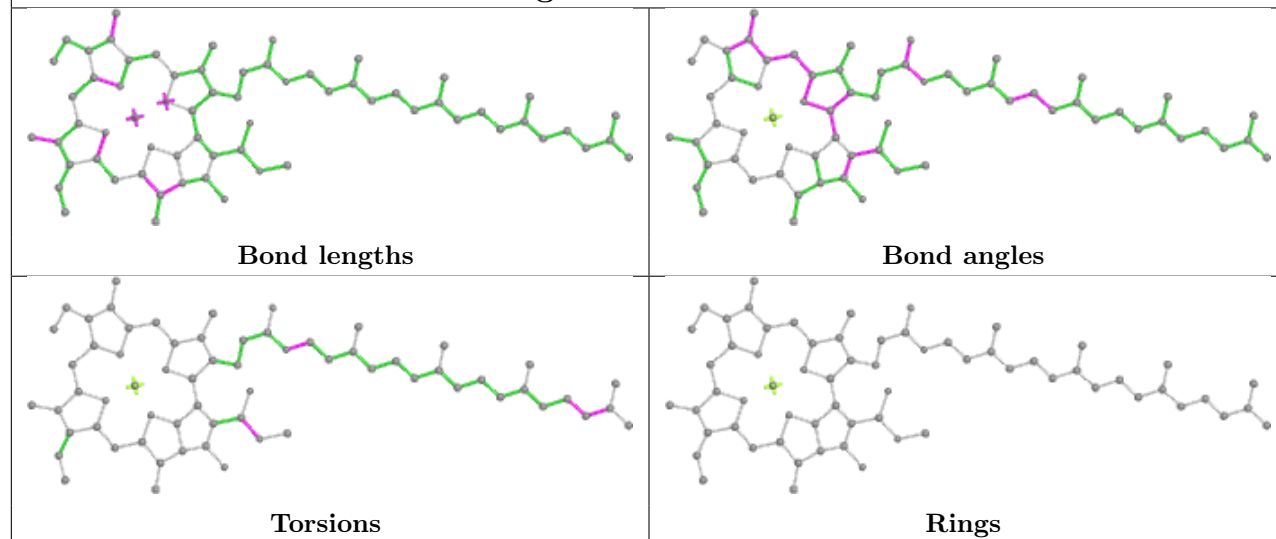
There are no ring outliers.

No monomer is involved in short contacts.

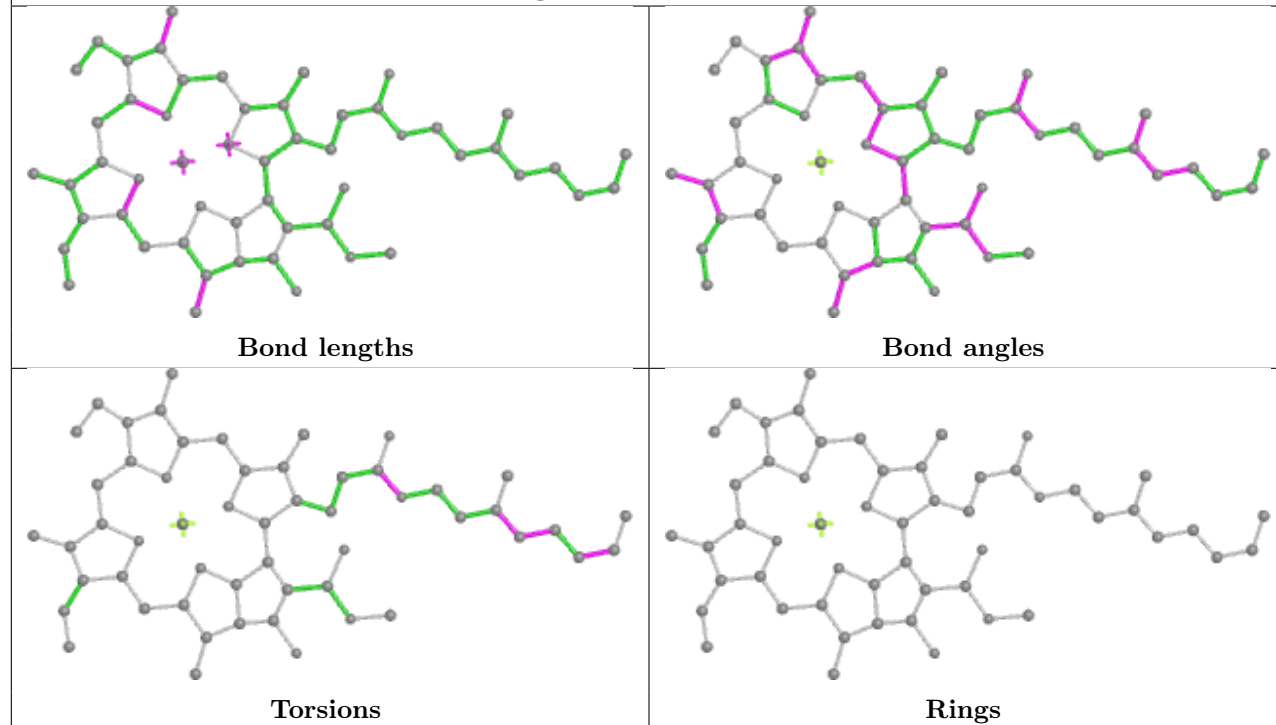
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



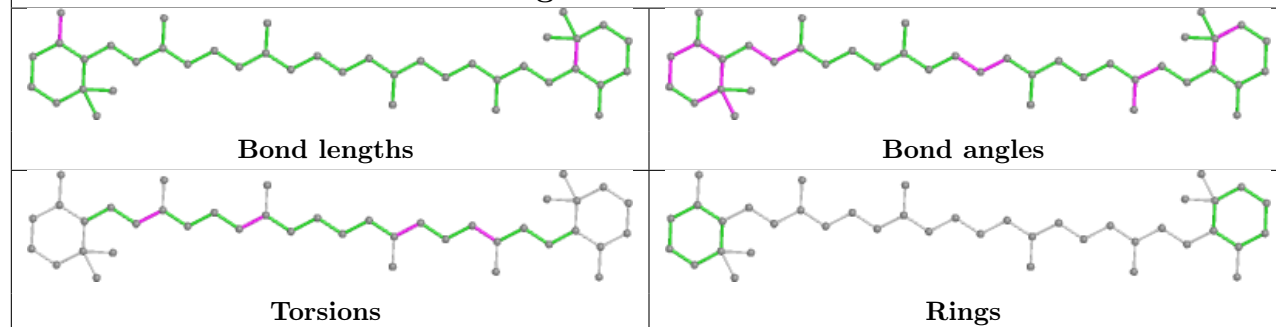
Ligand CLA a 402



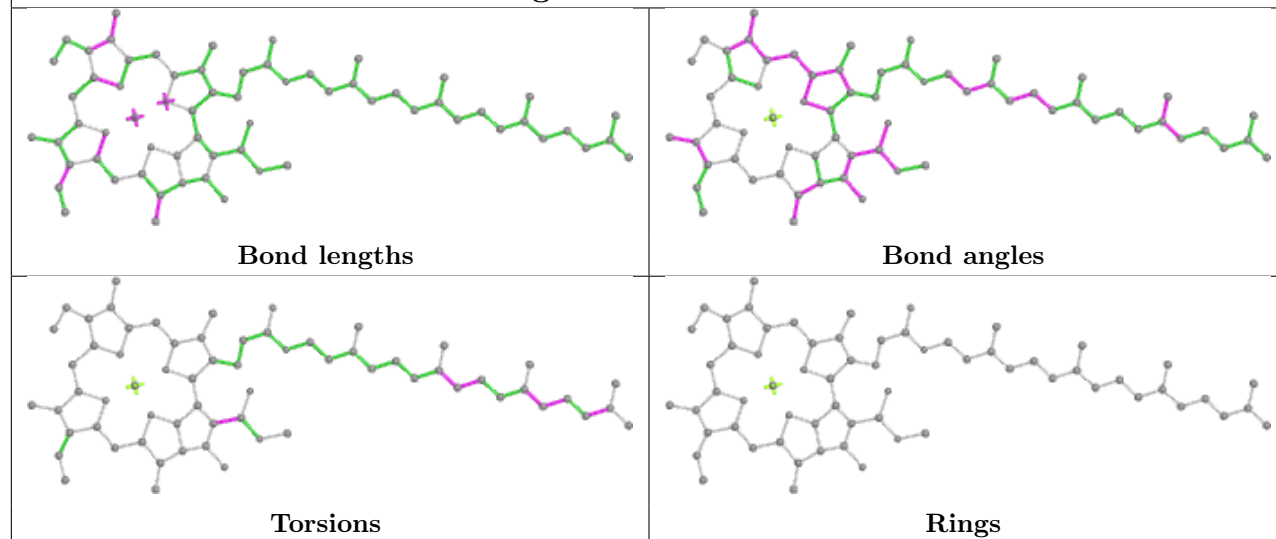
Ligand CLA A 405



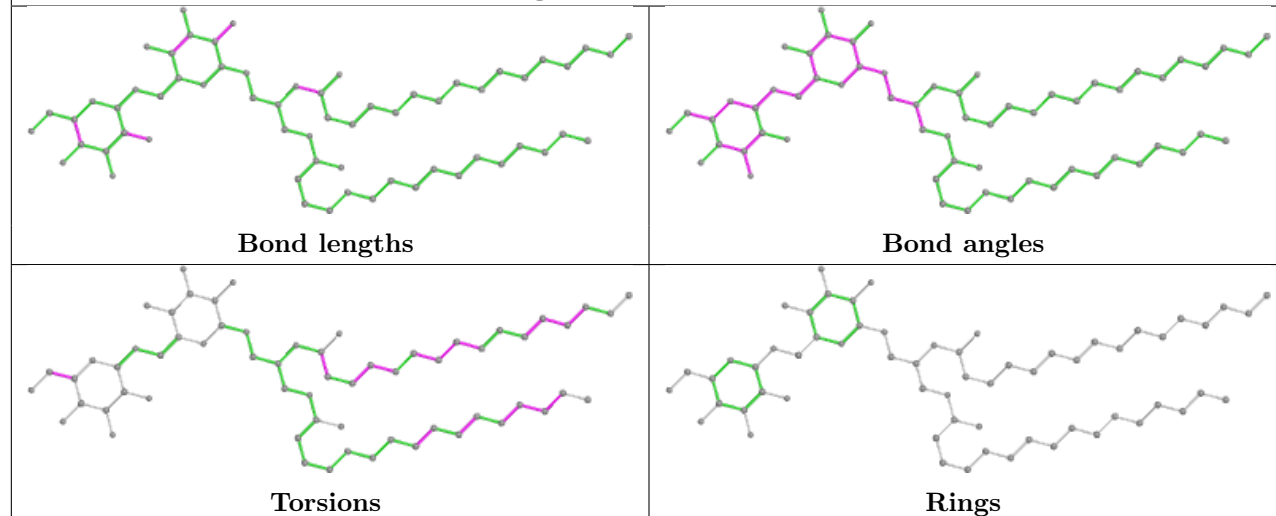
Ligand BCR t 101



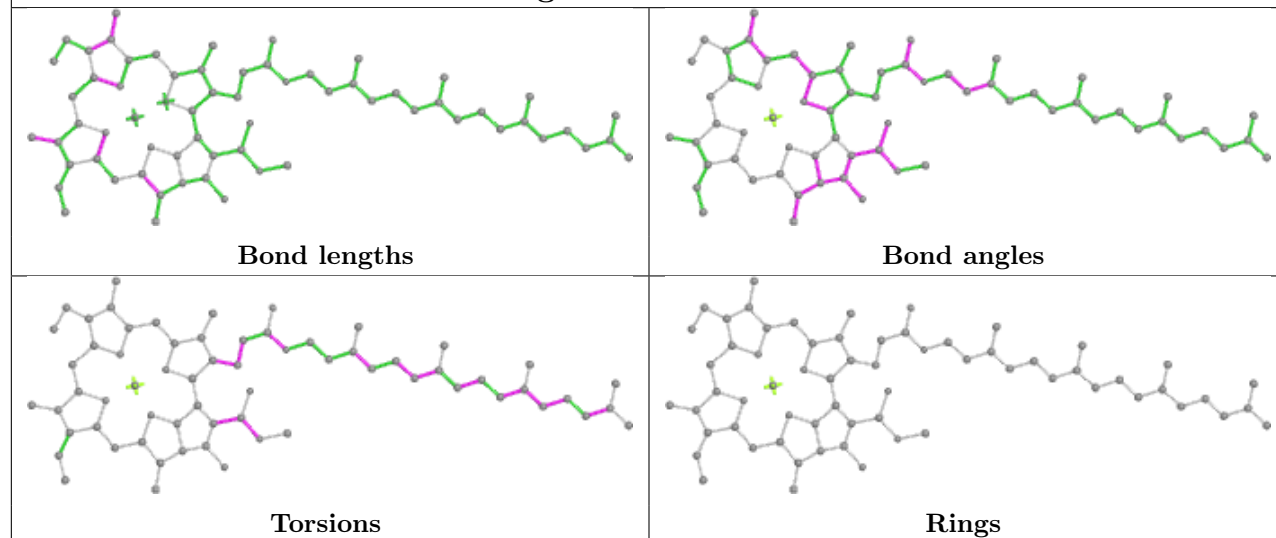
Ligand CLA B 611

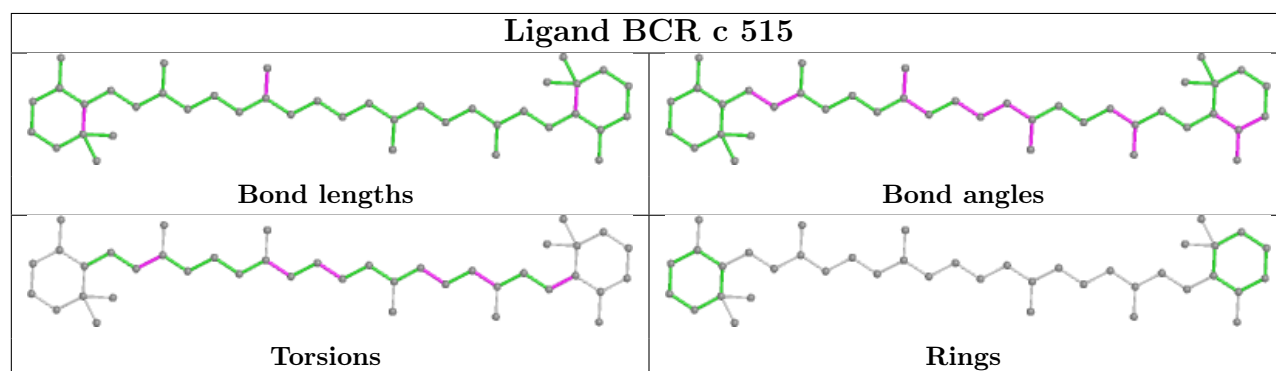
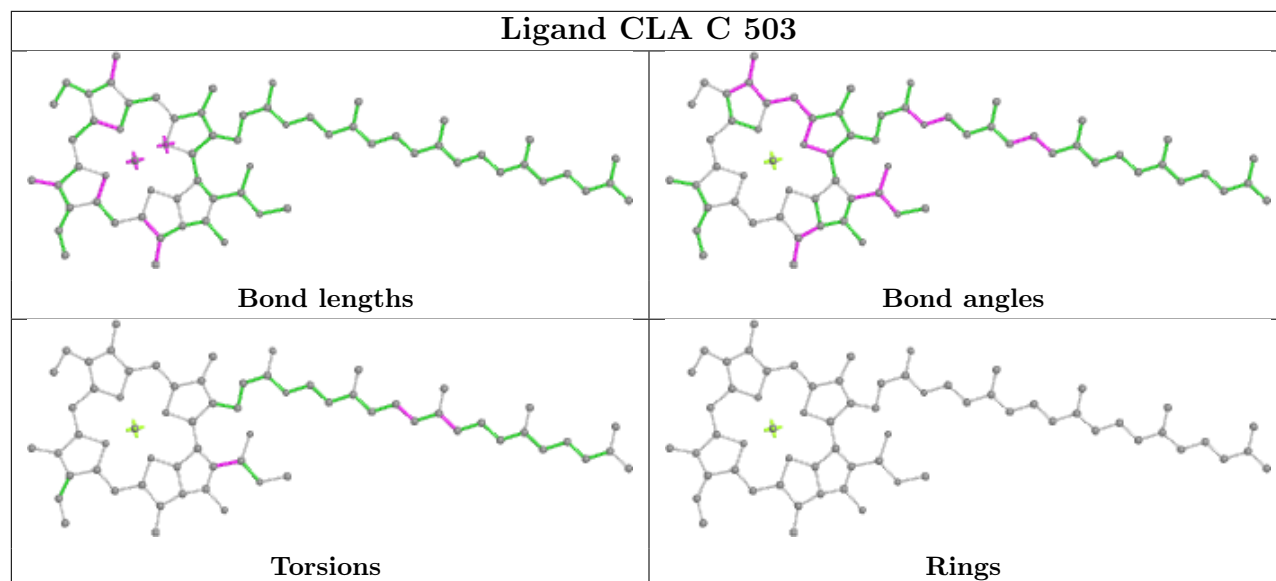
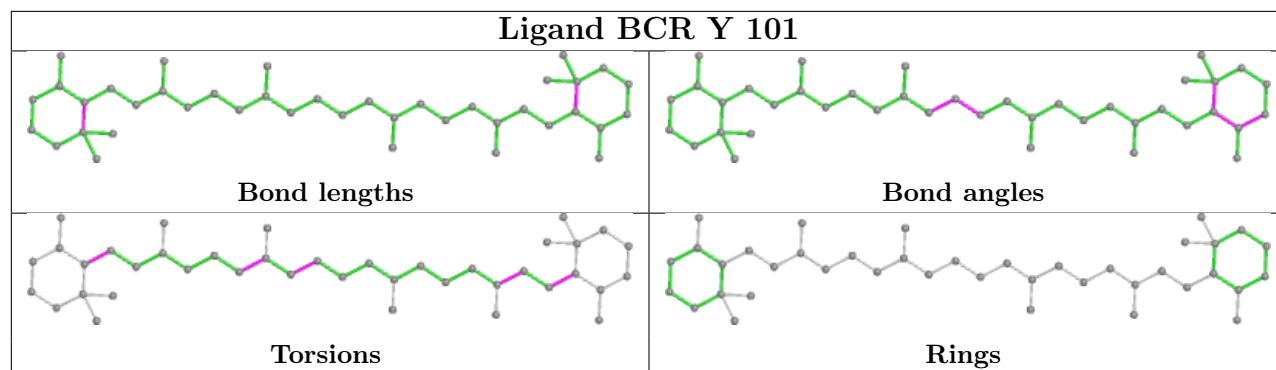


Ligand DGD h 101

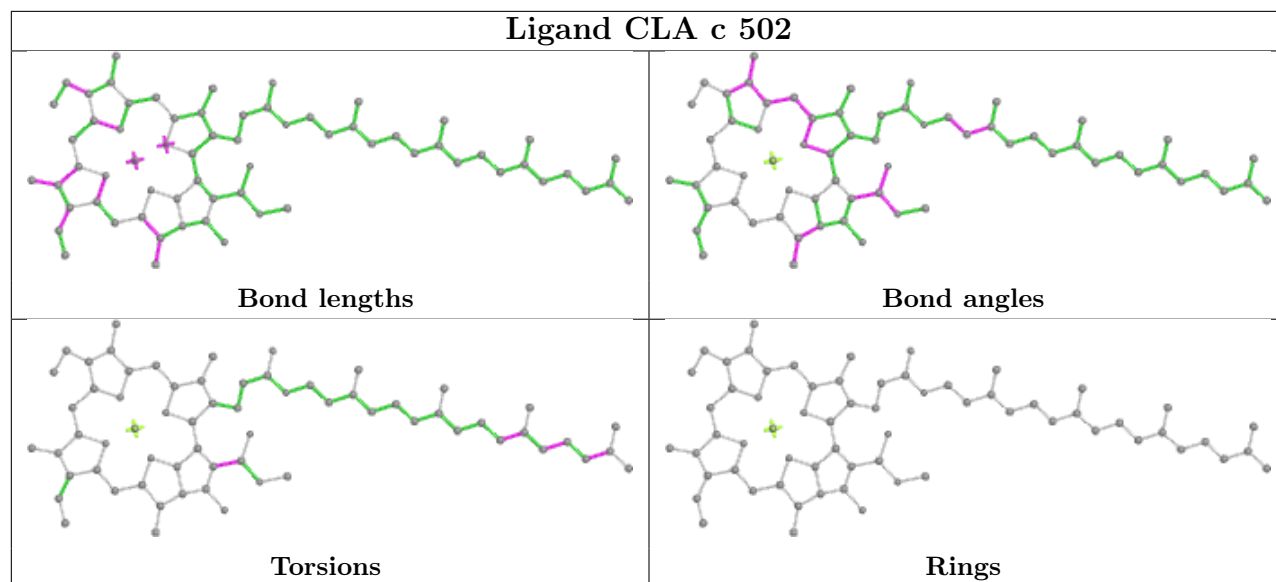


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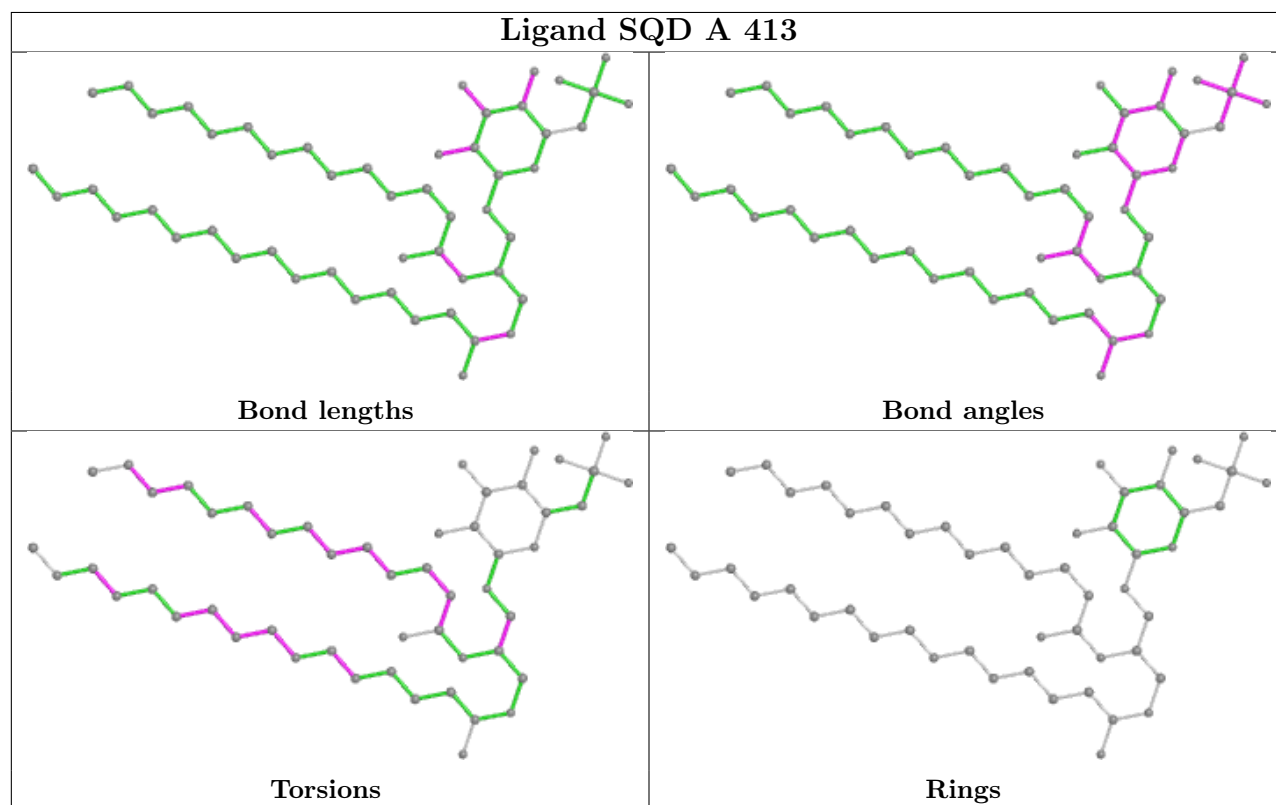




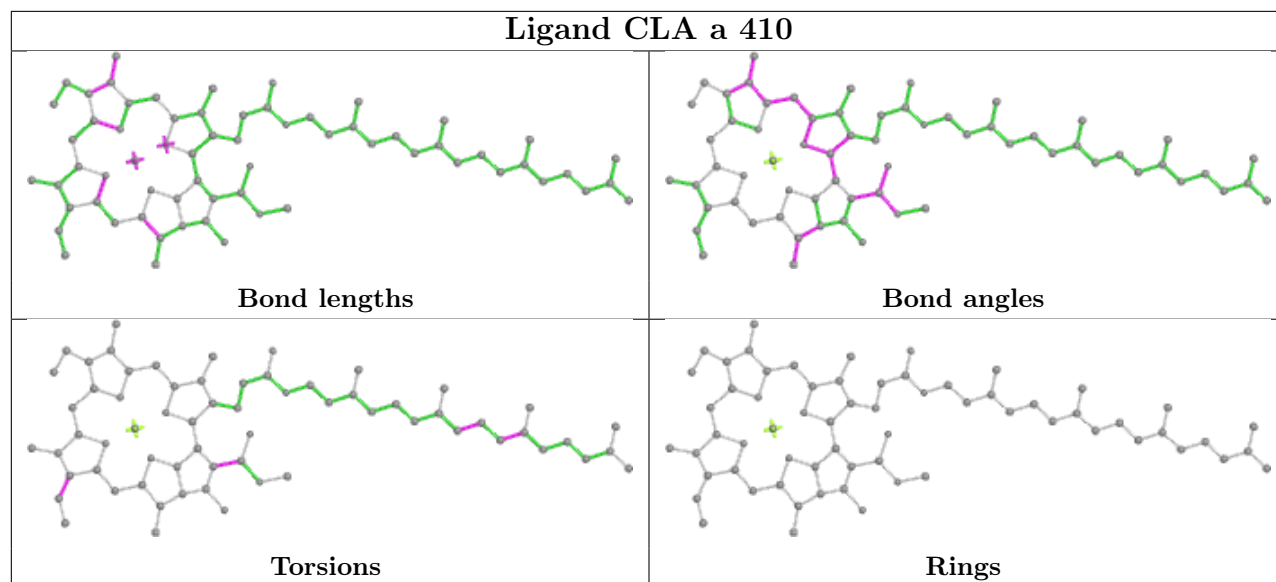
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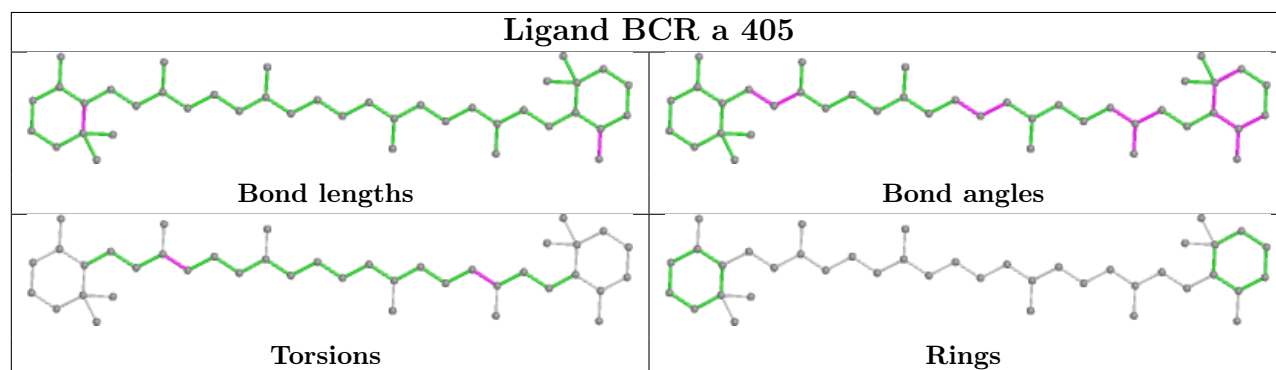
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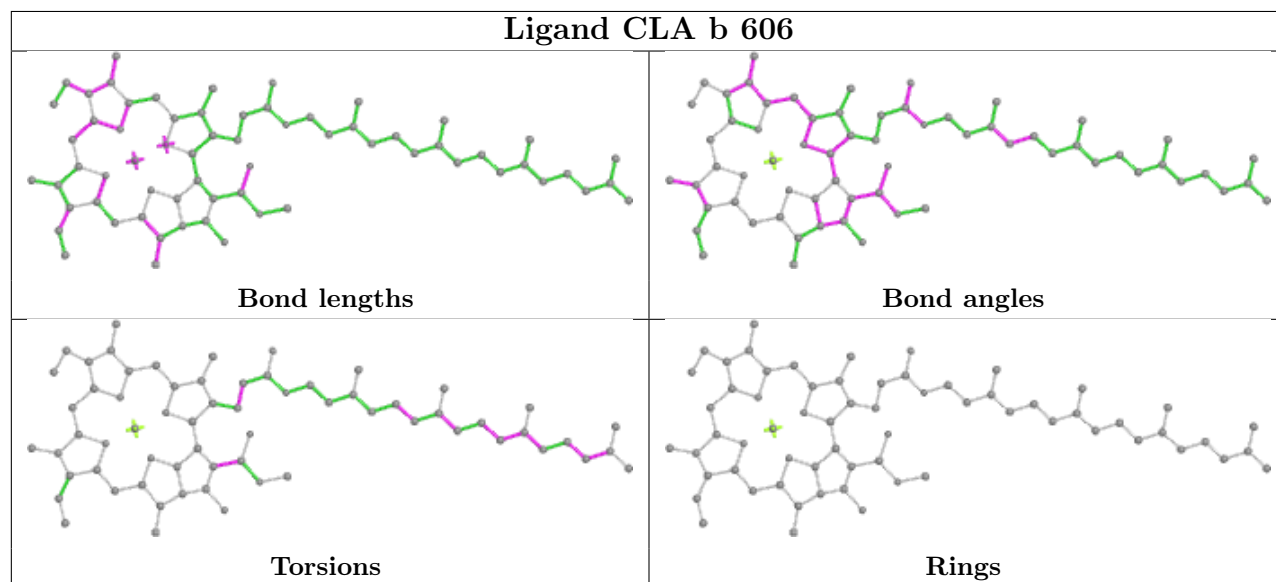
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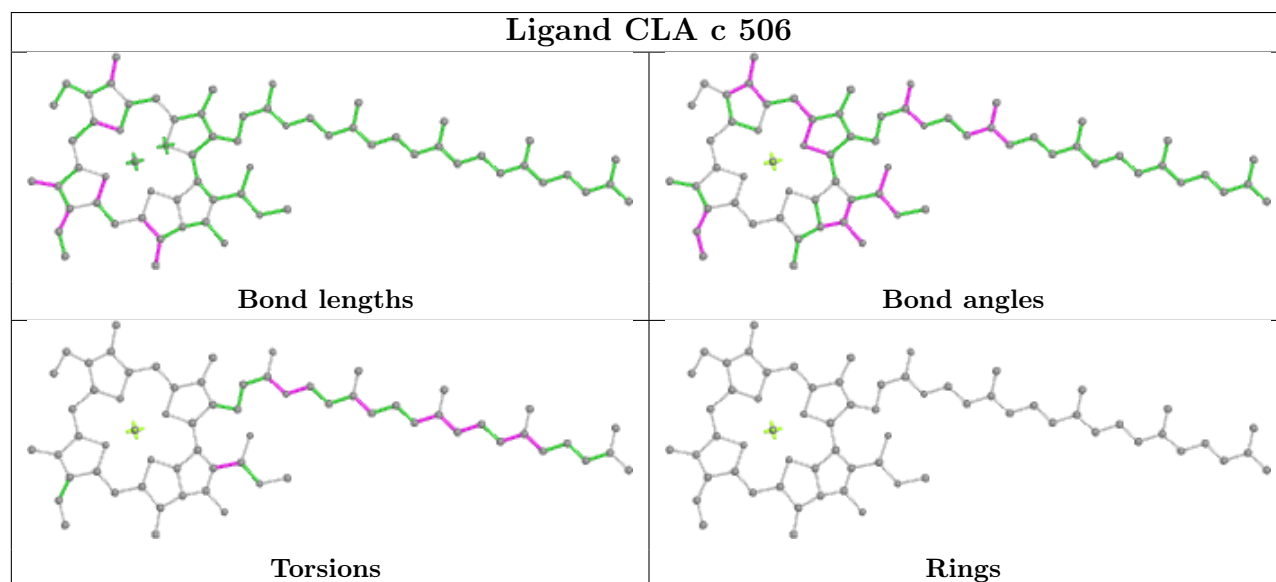
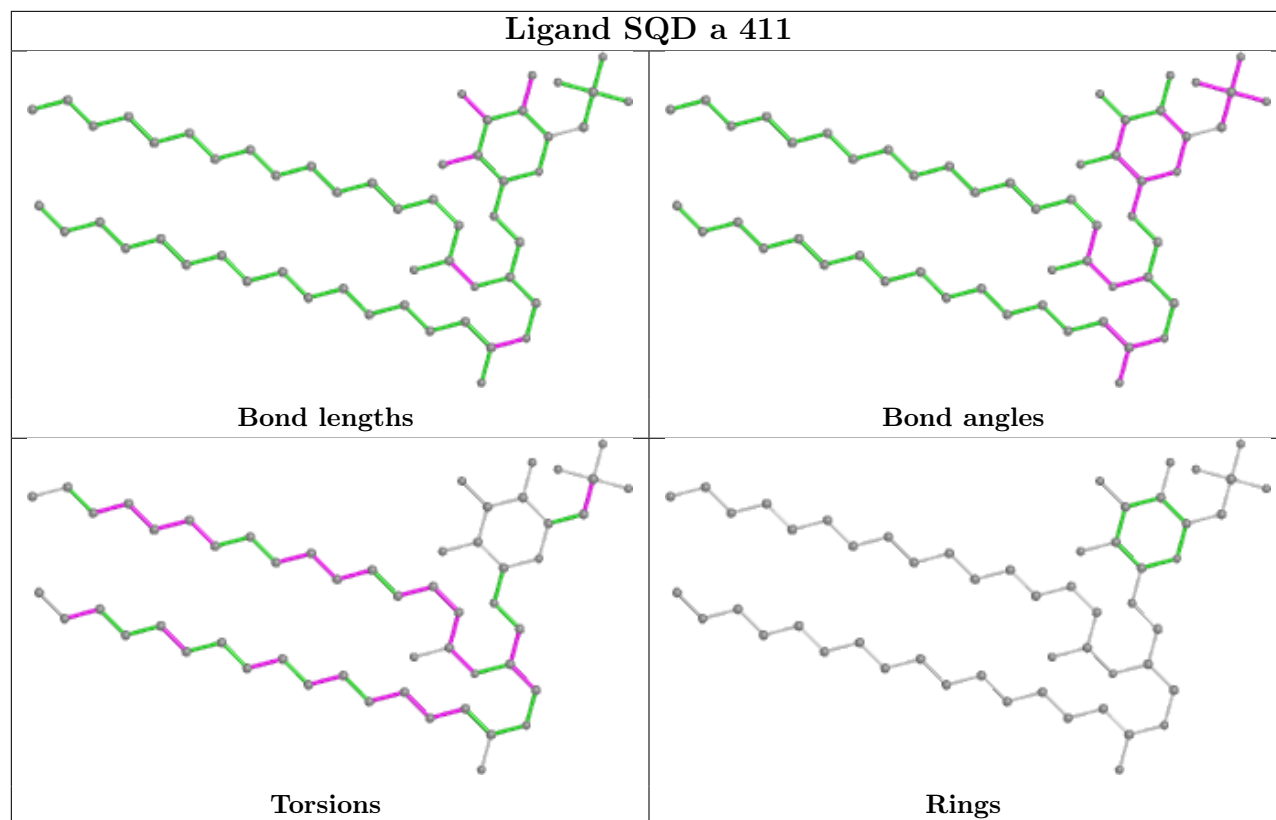


Ligand BCR a 405

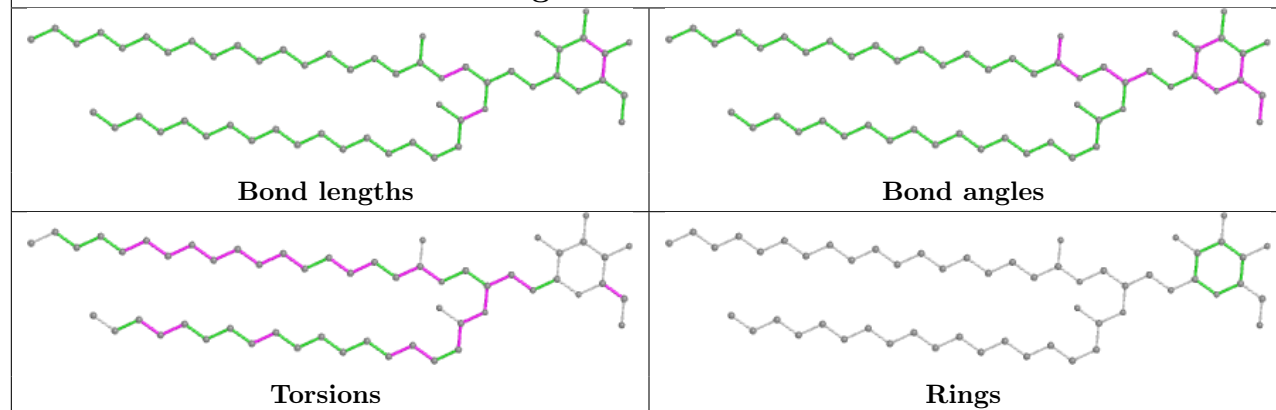


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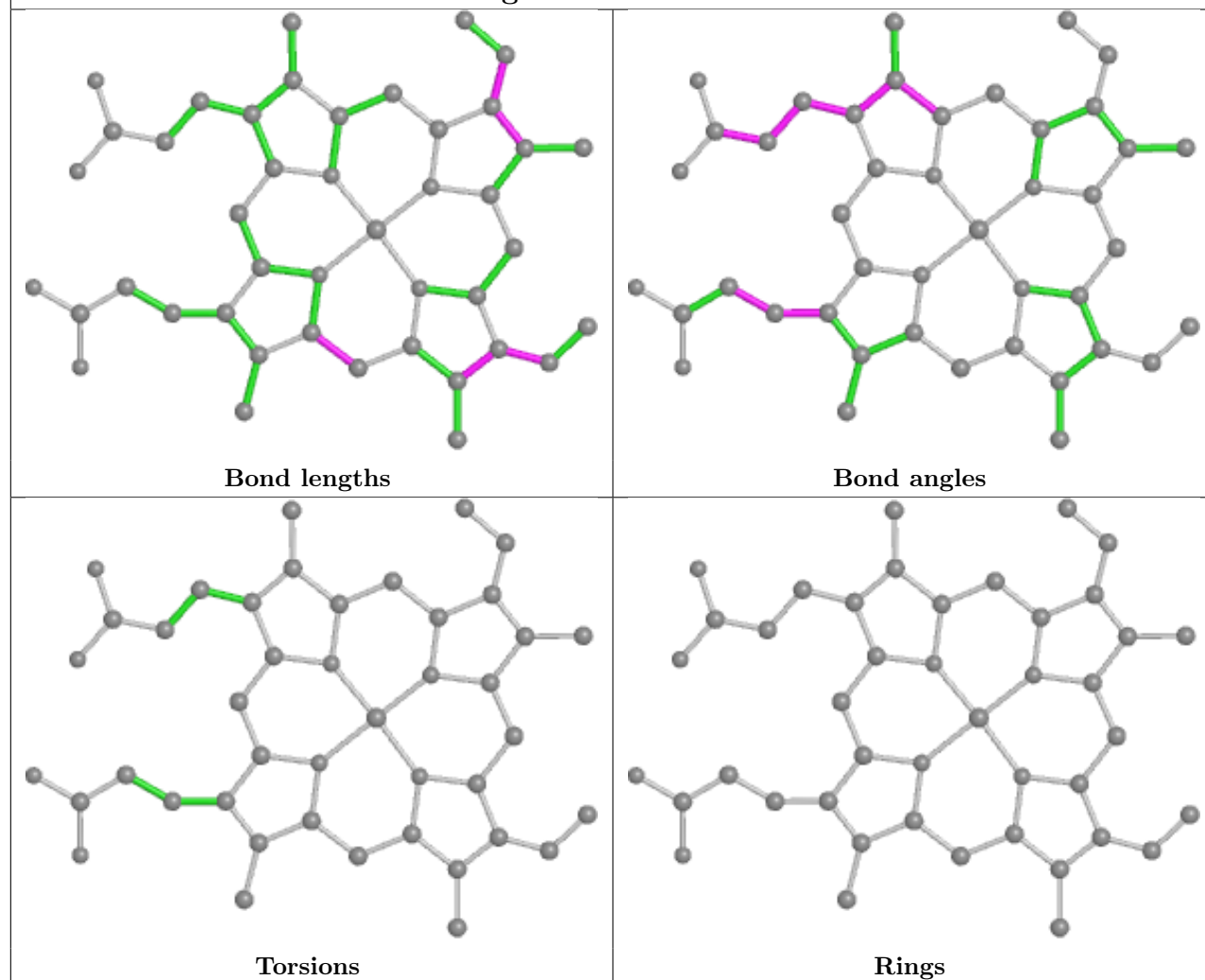




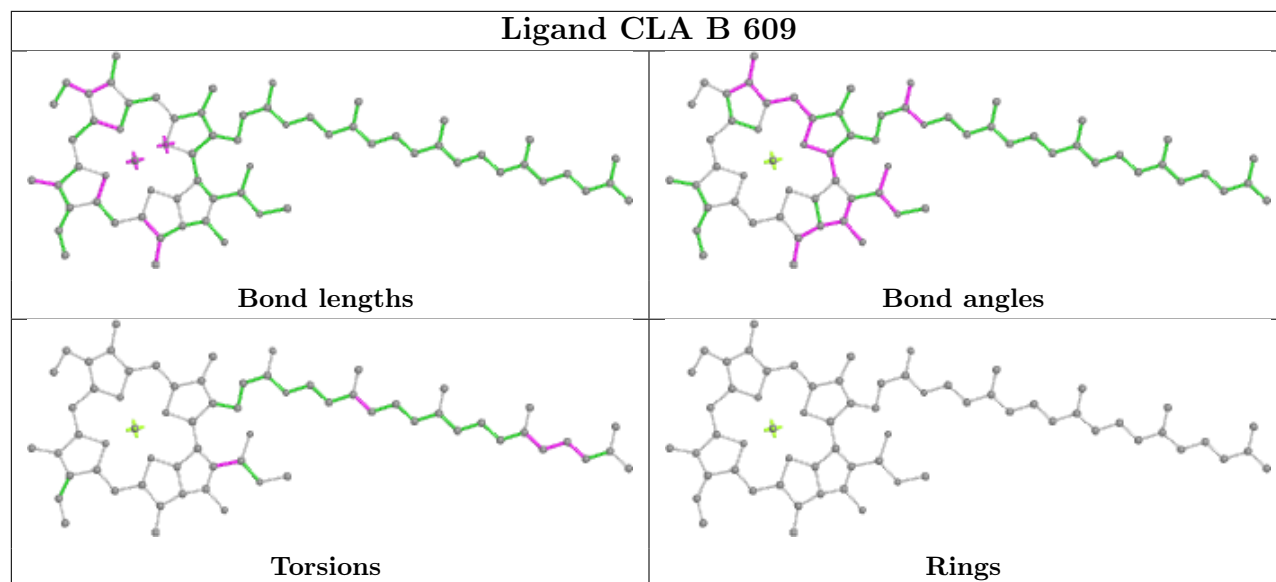
Ligand LMG a 416



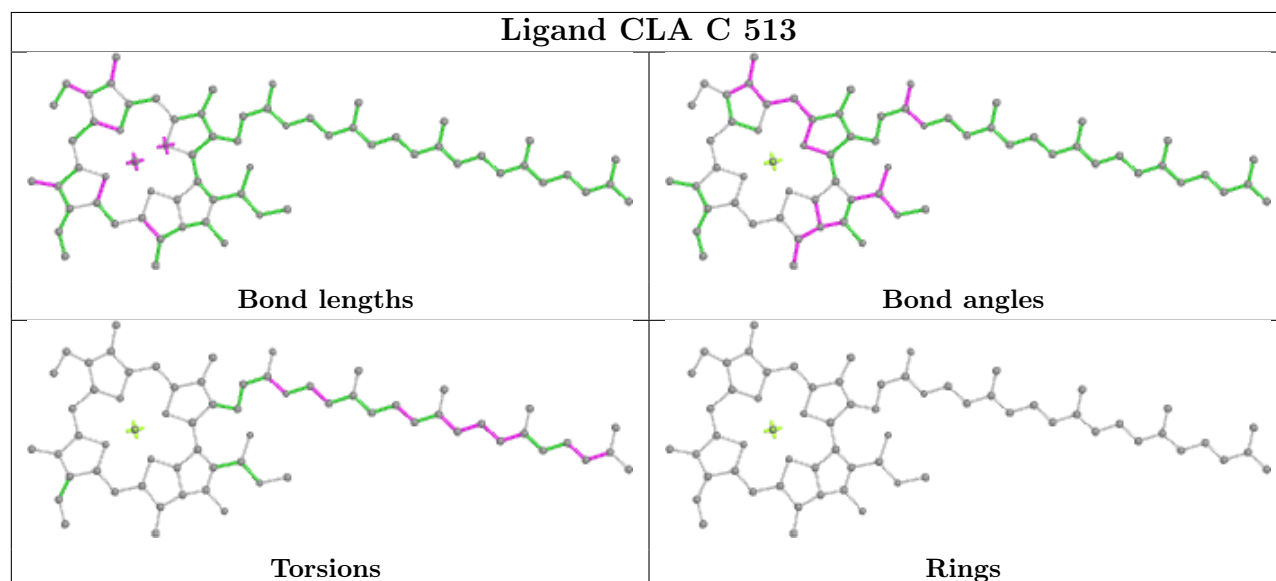
Ligand HEM e 101



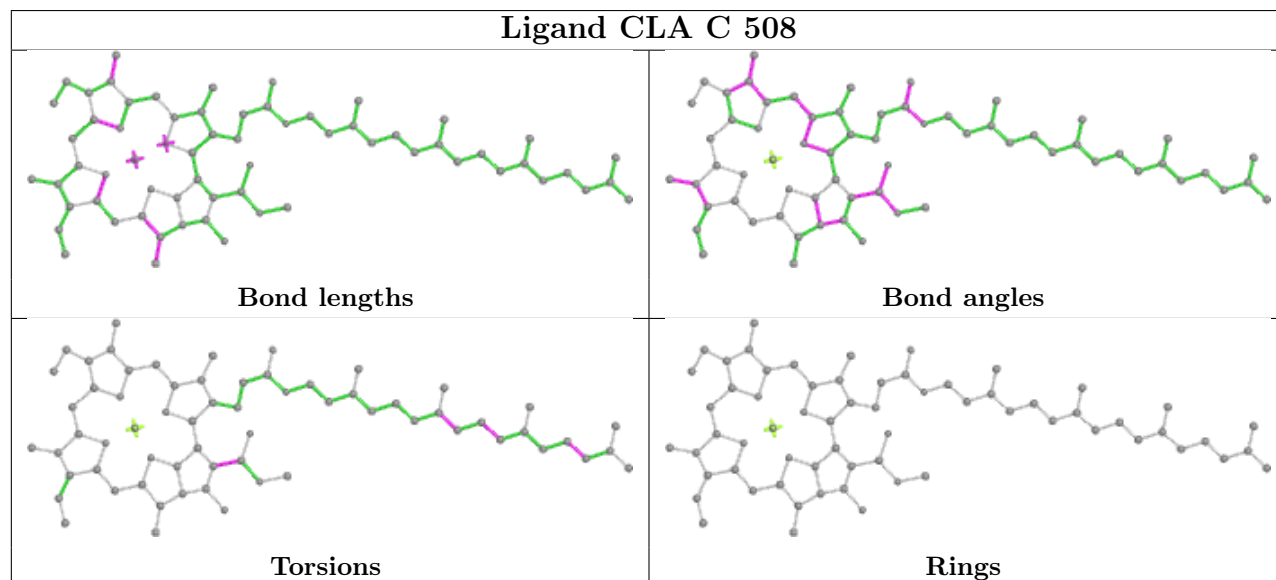
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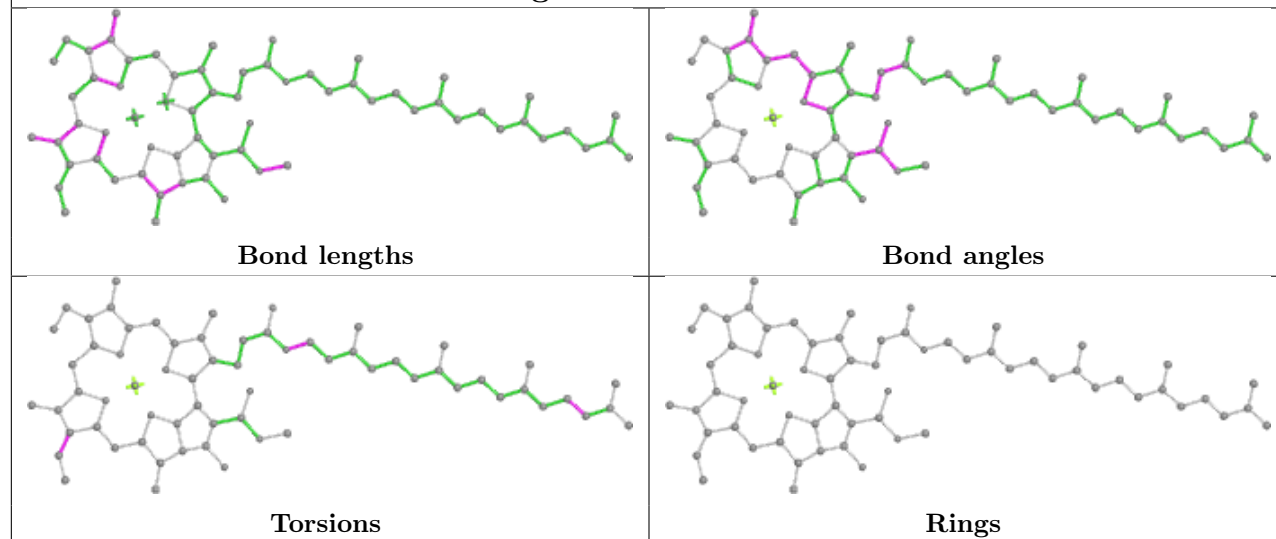
Ligand CLA C 513



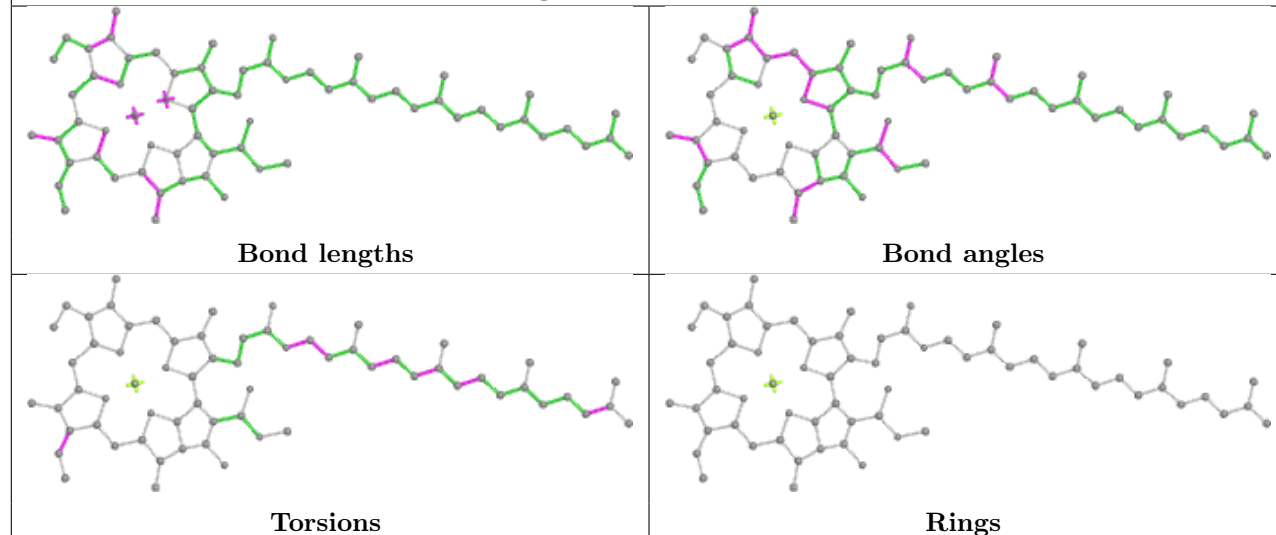
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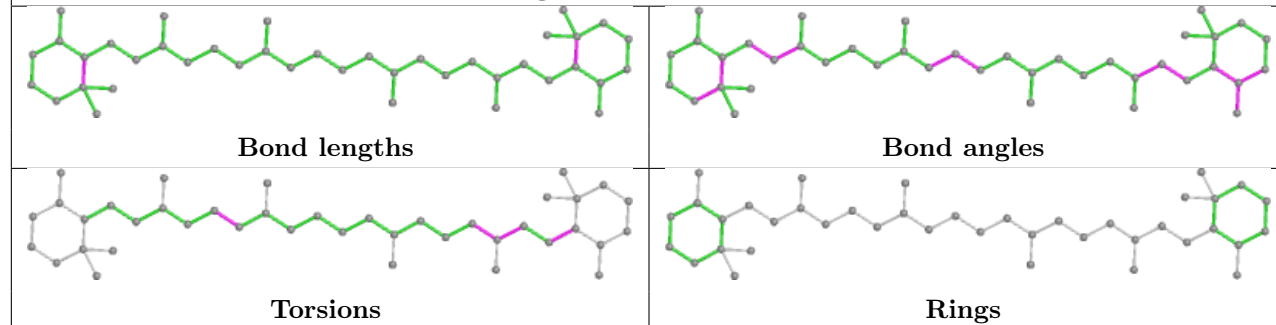
Ligand CLA A 402



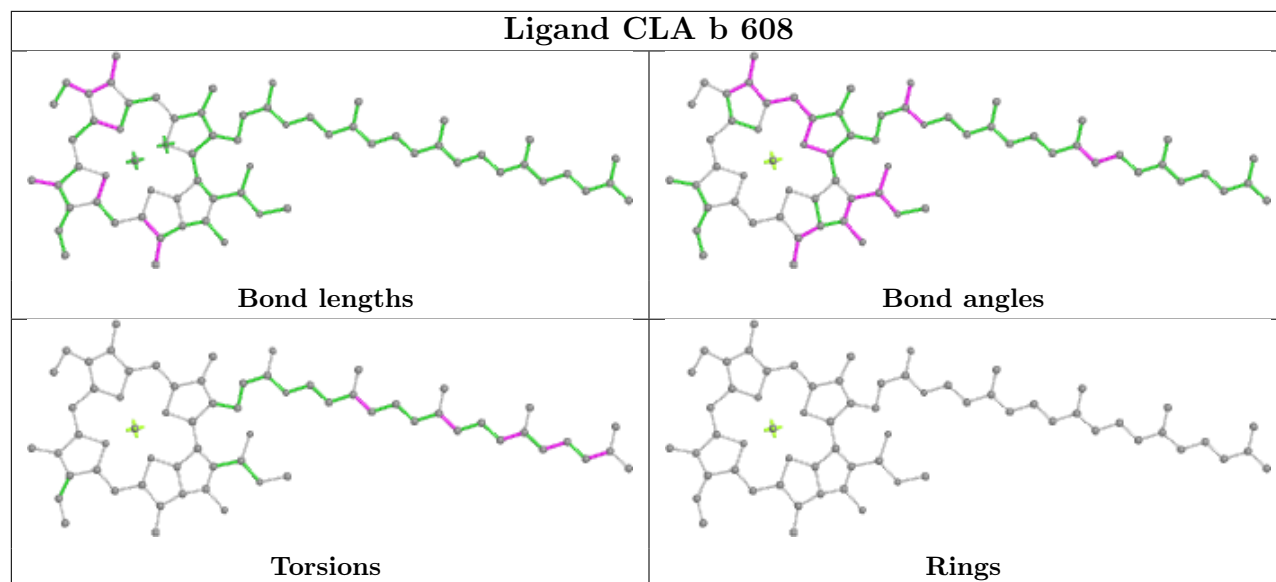
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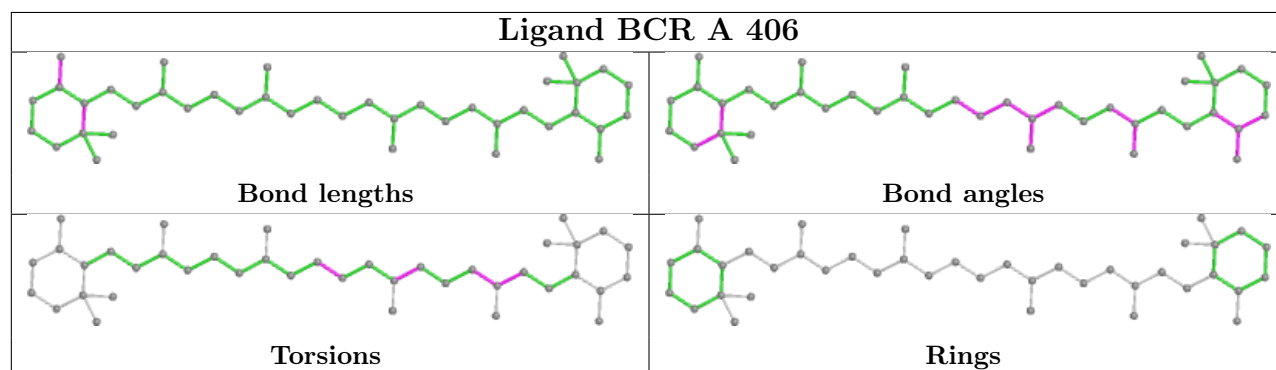
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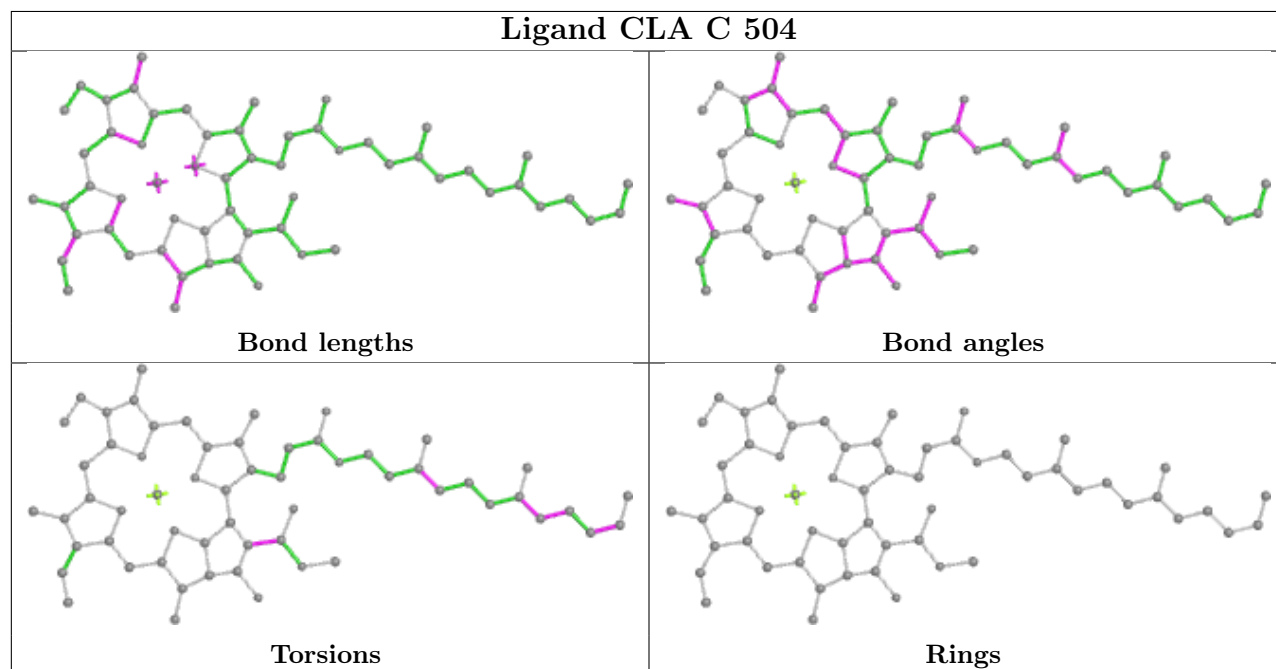
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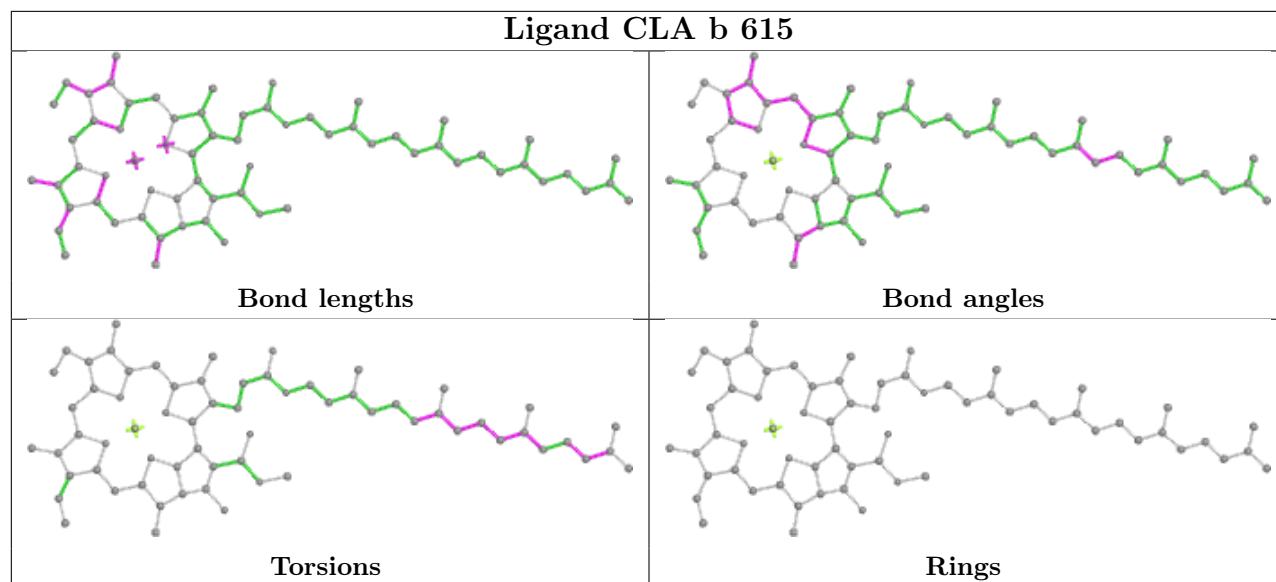
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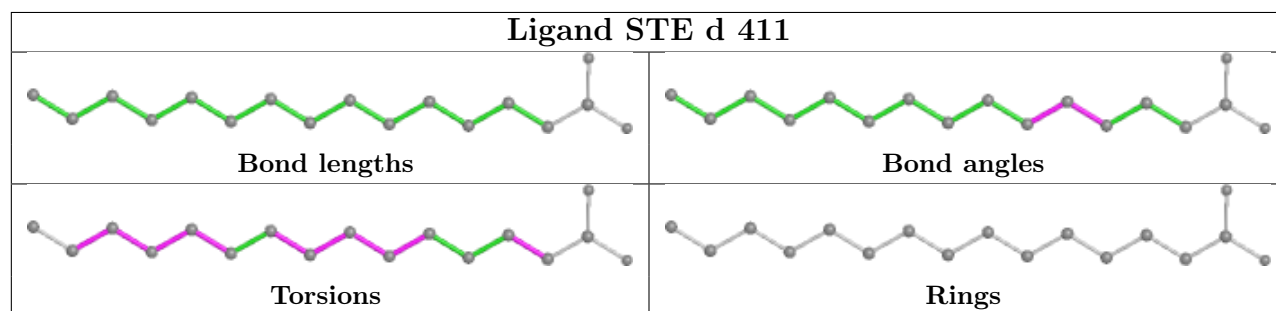
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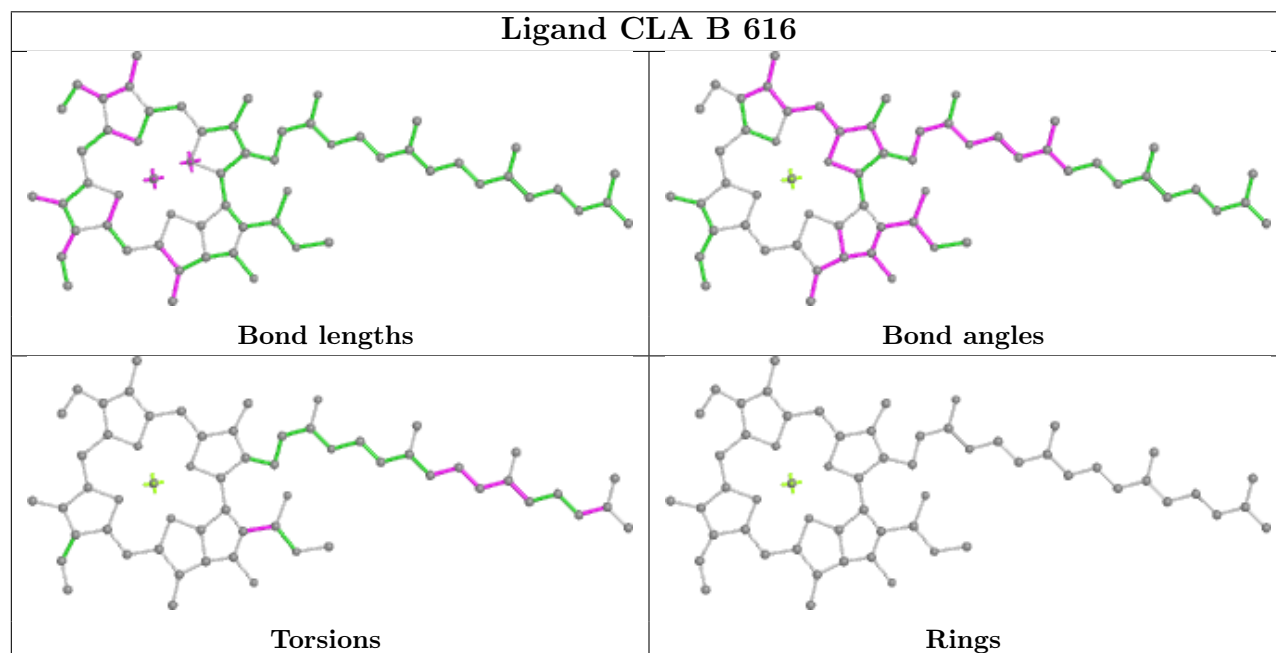
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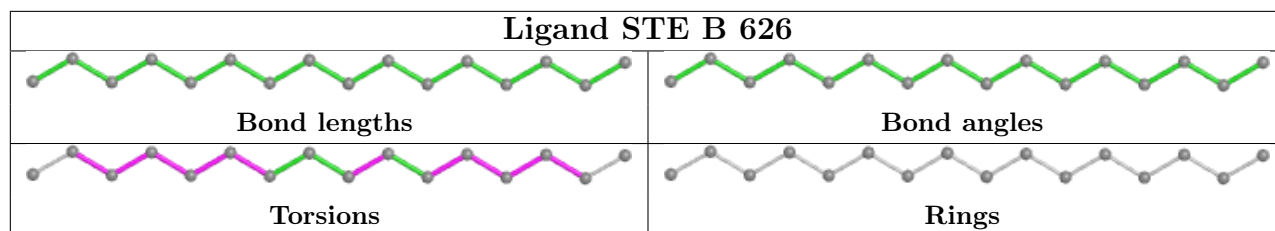
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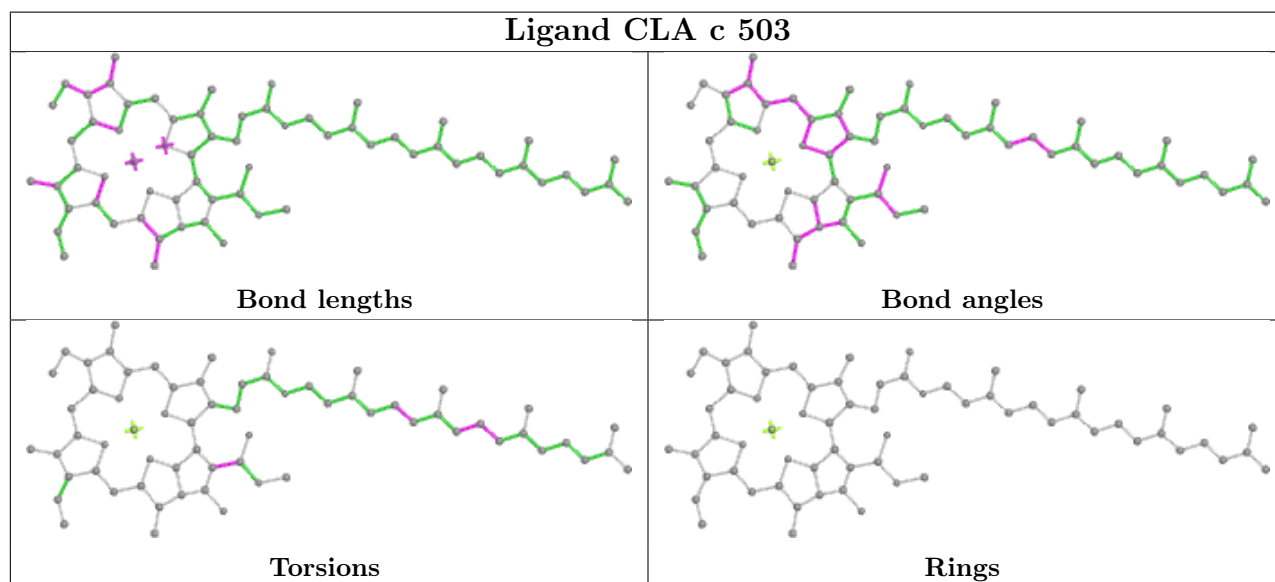
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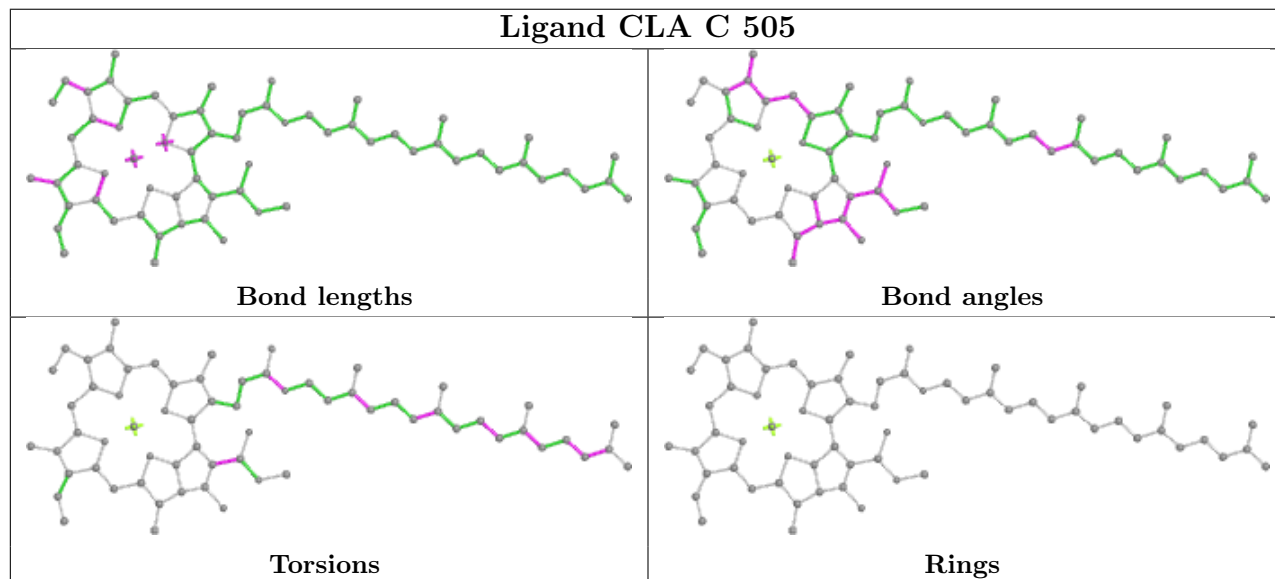
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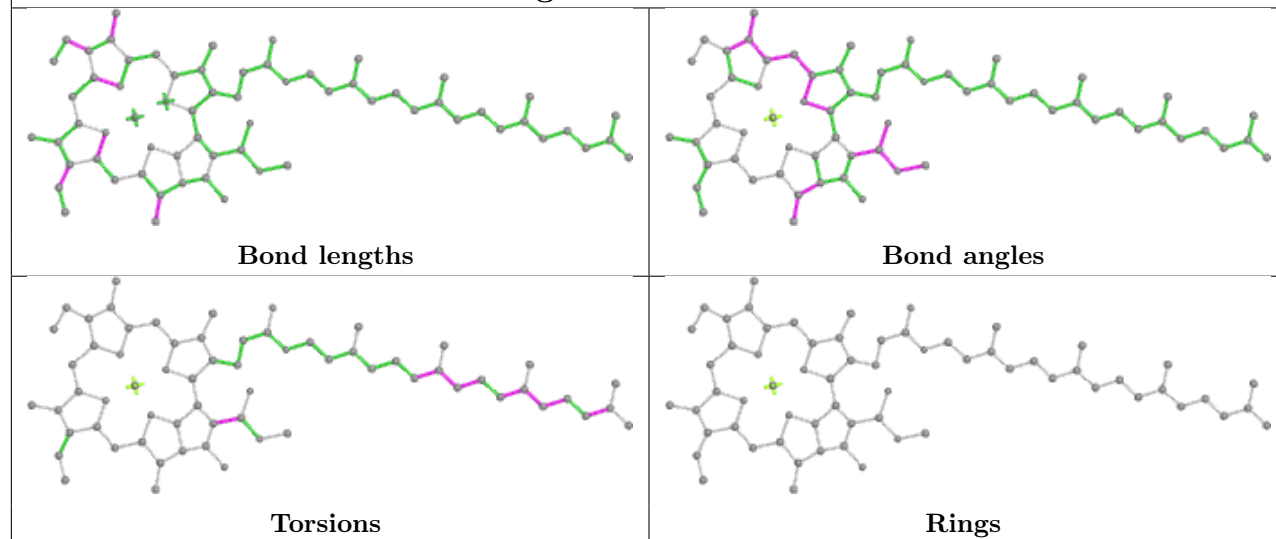
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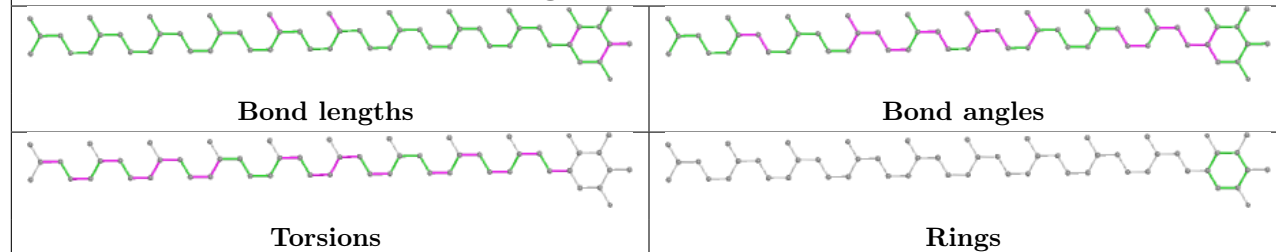
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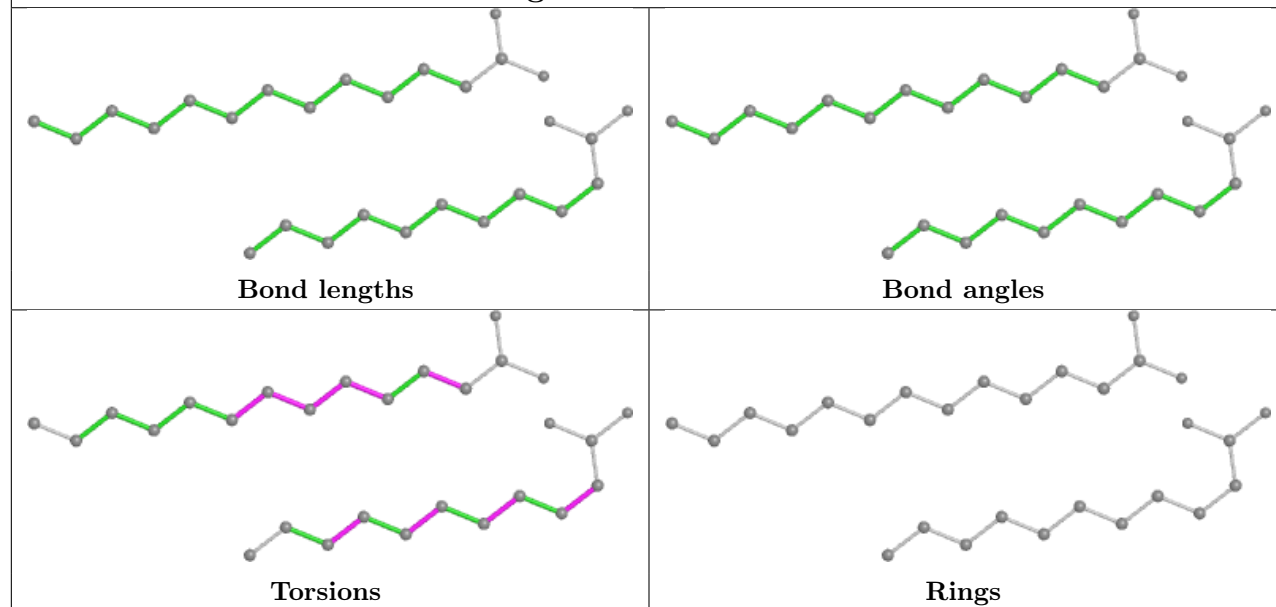
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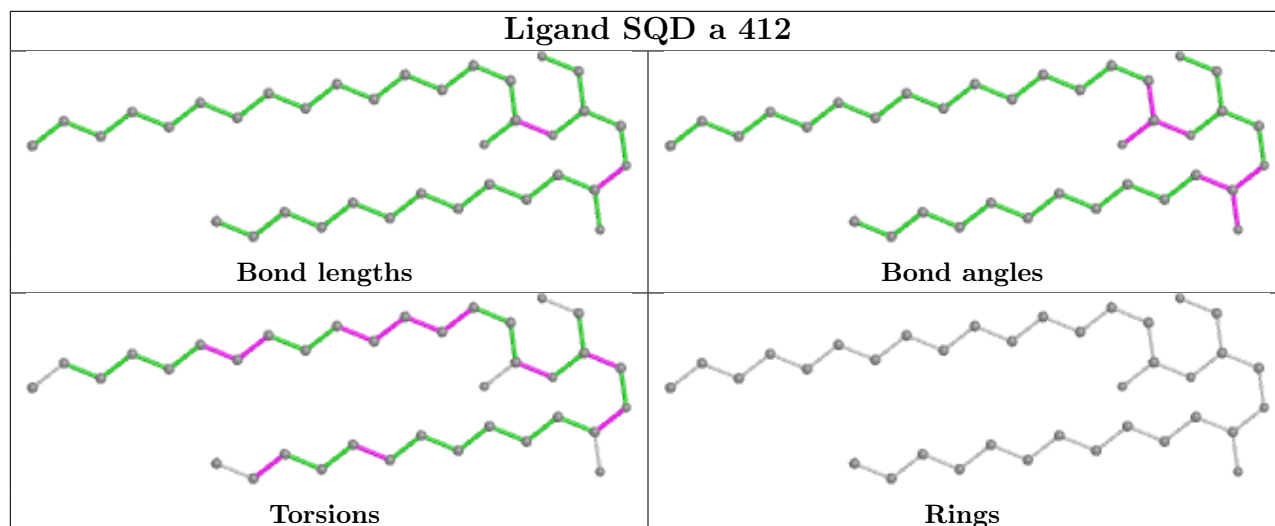
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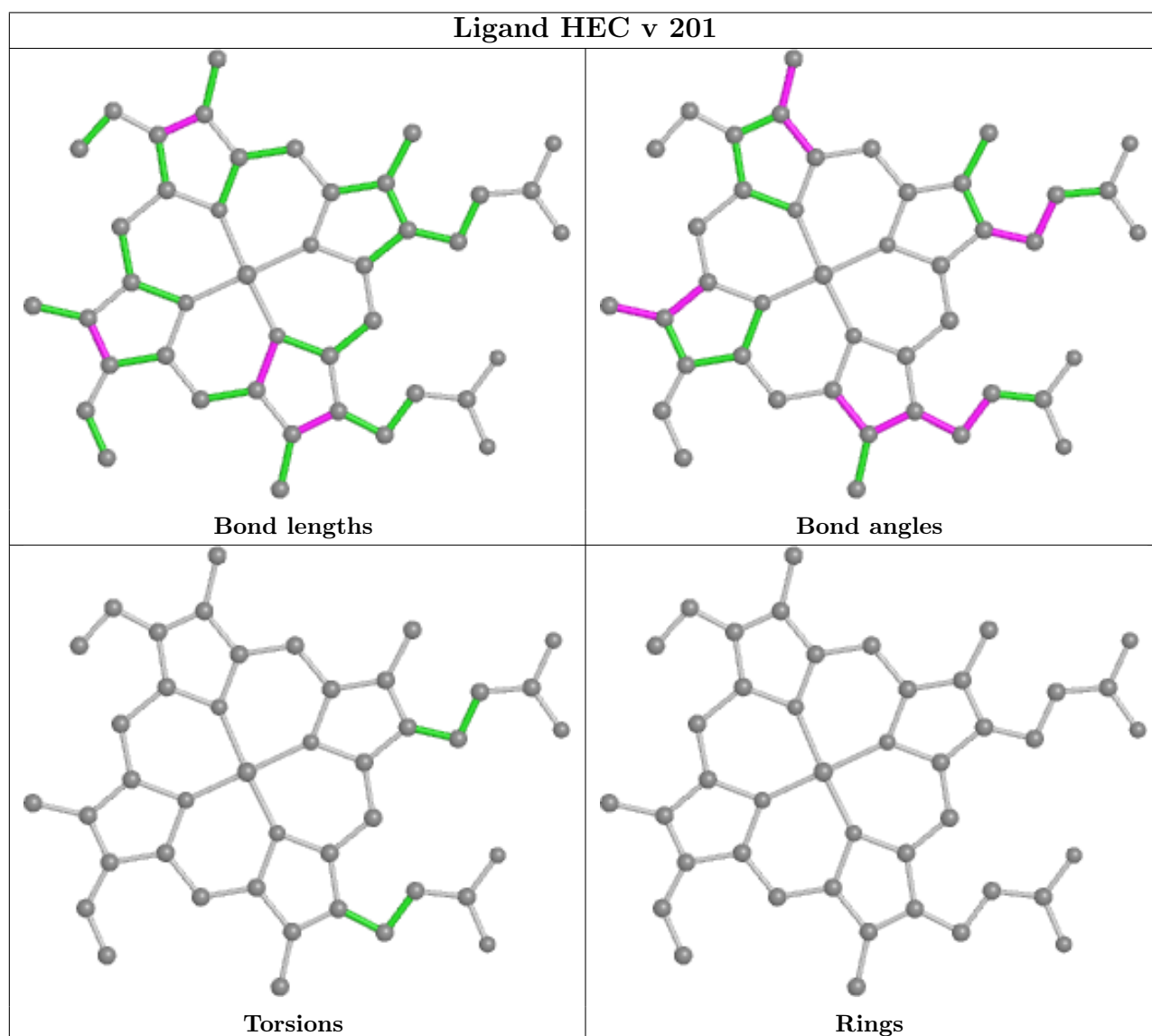
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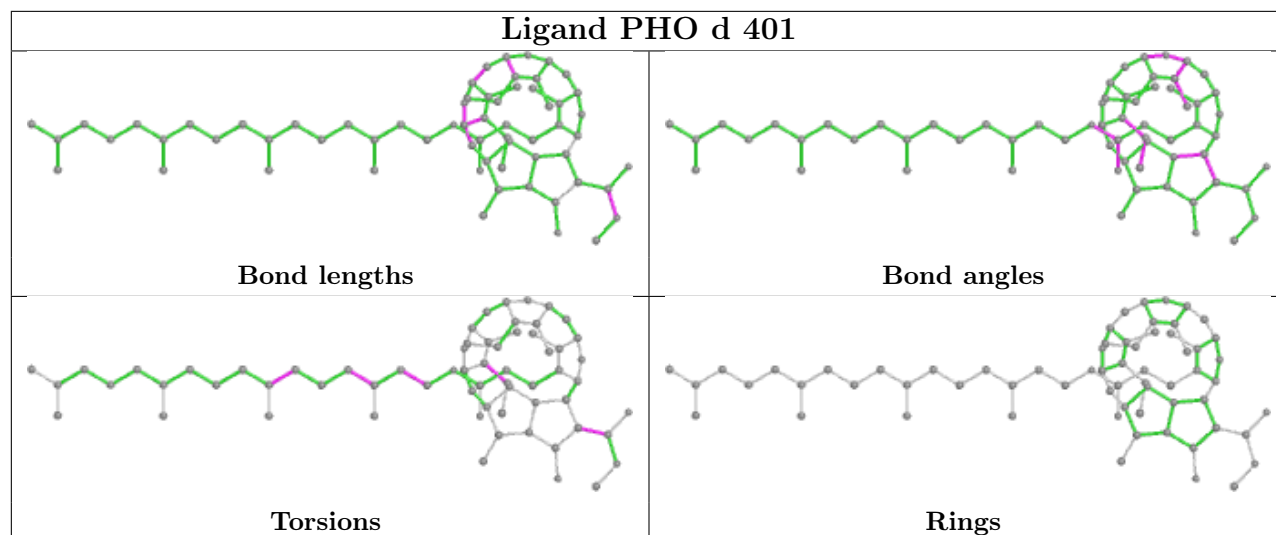
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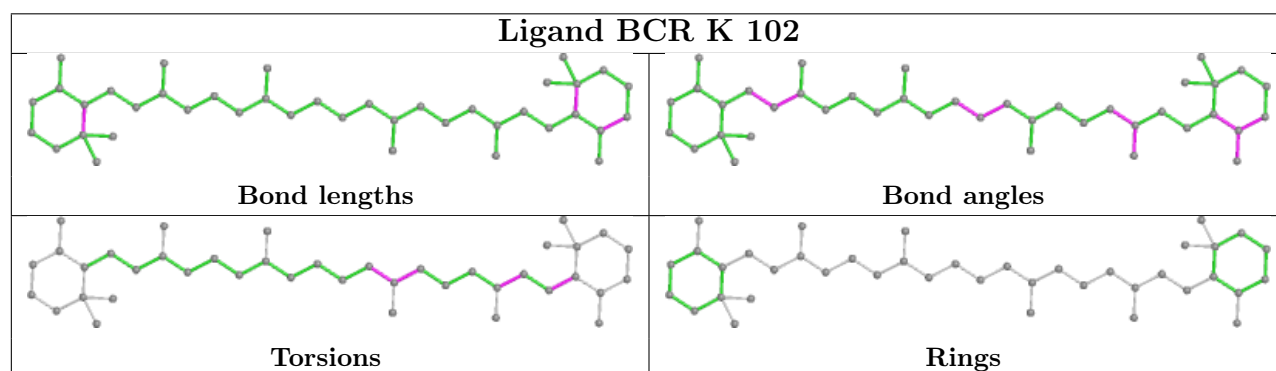
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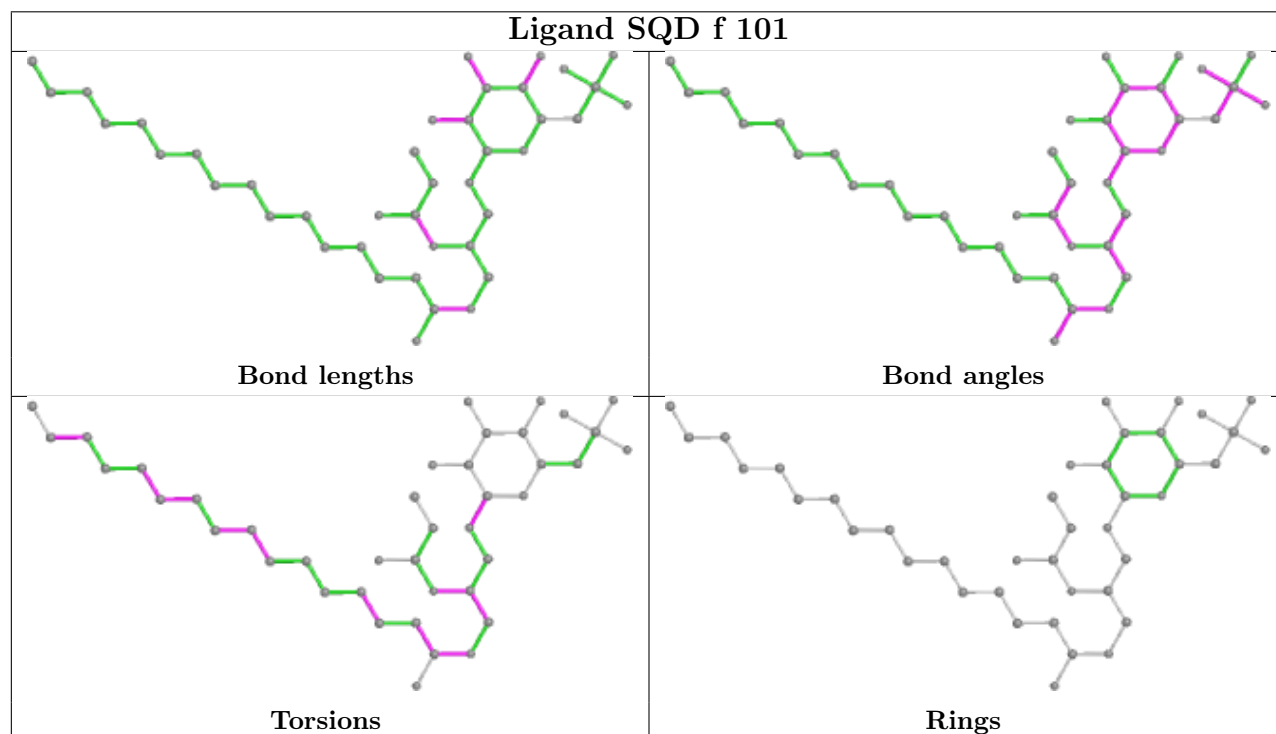
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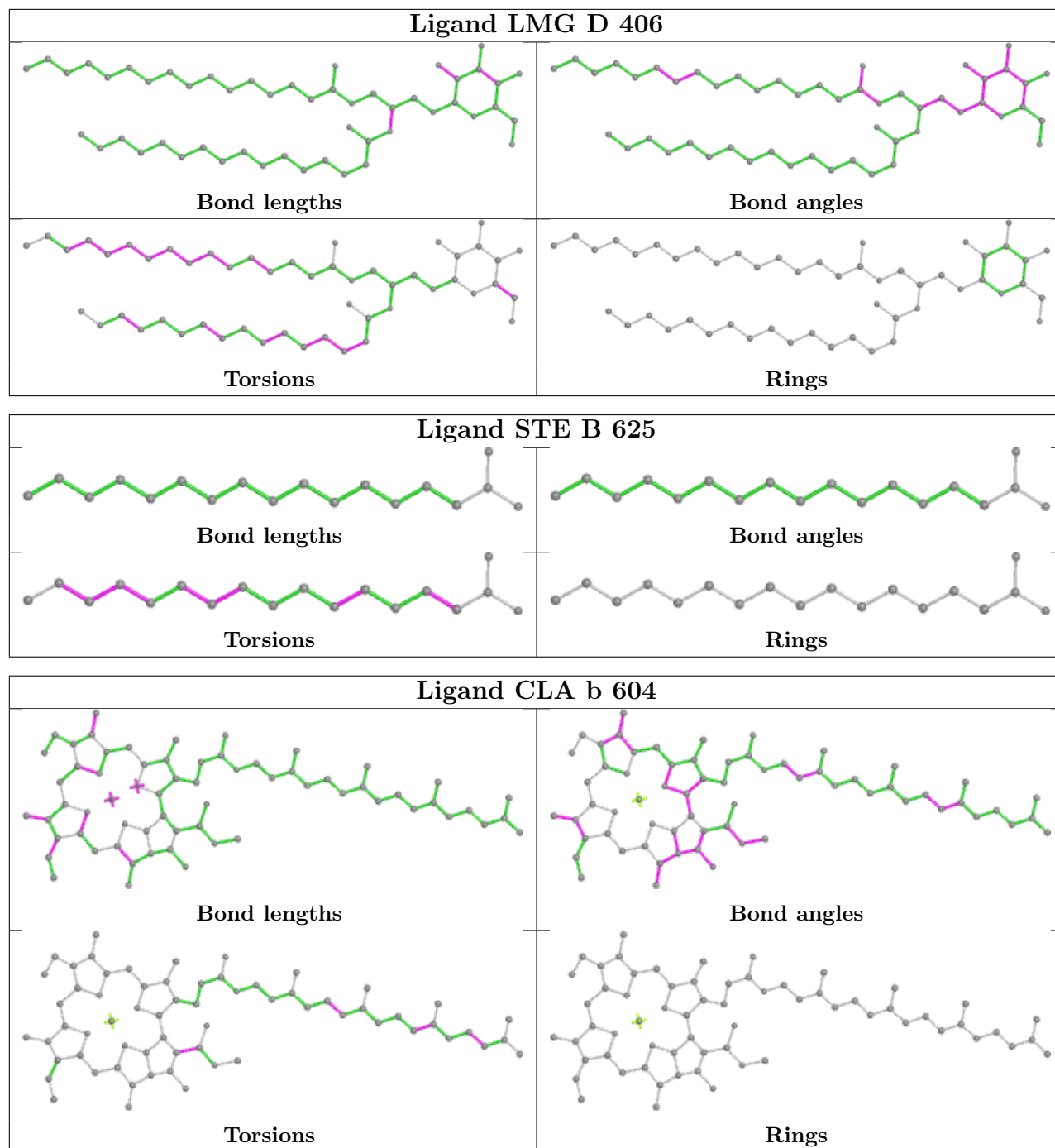


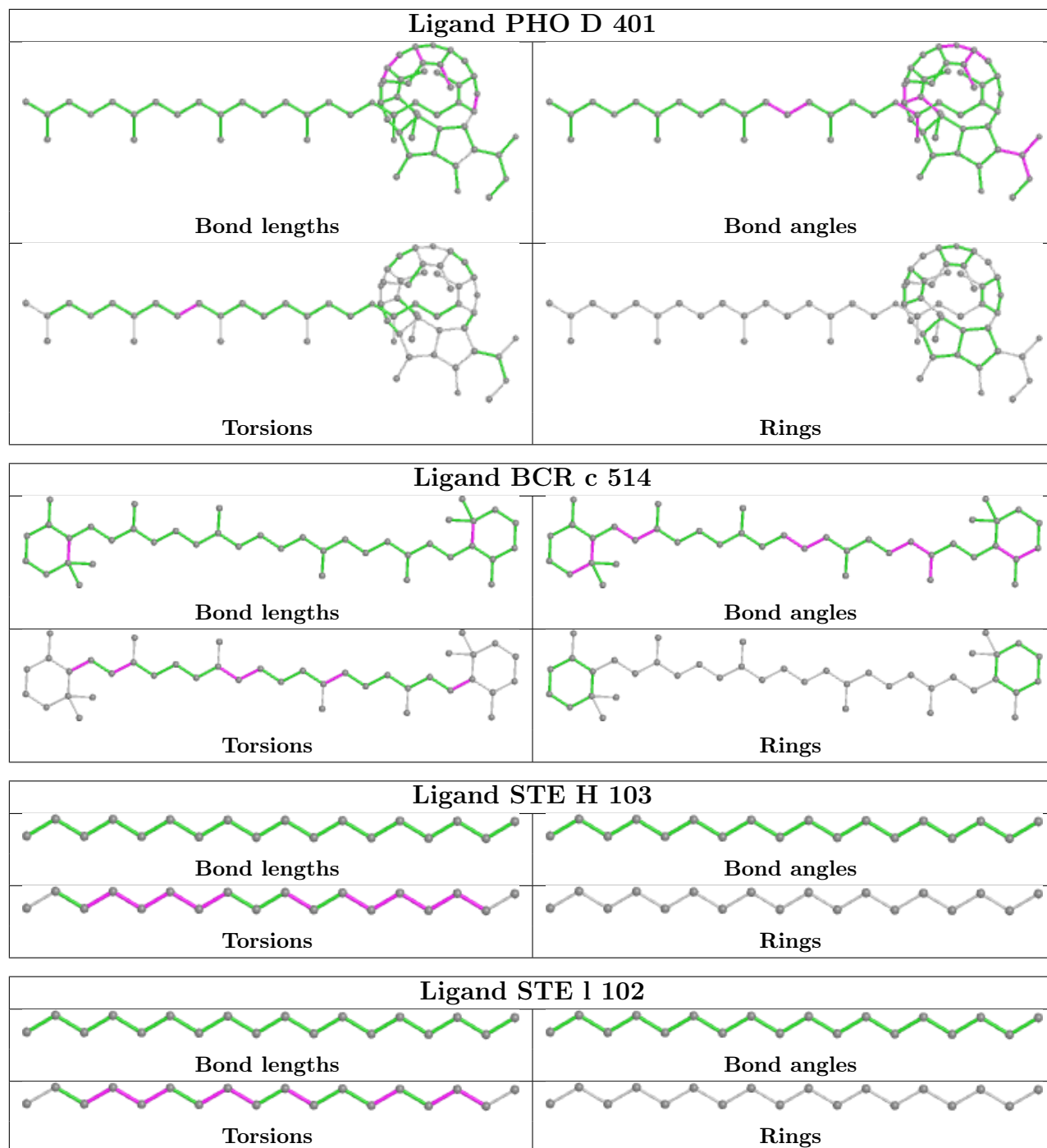
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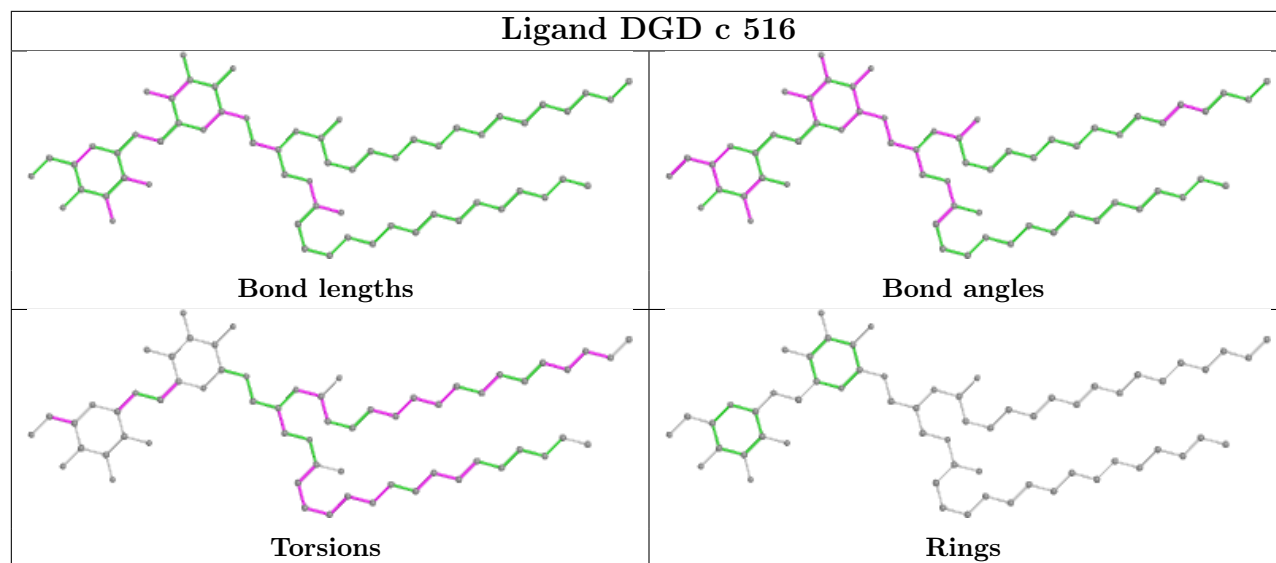
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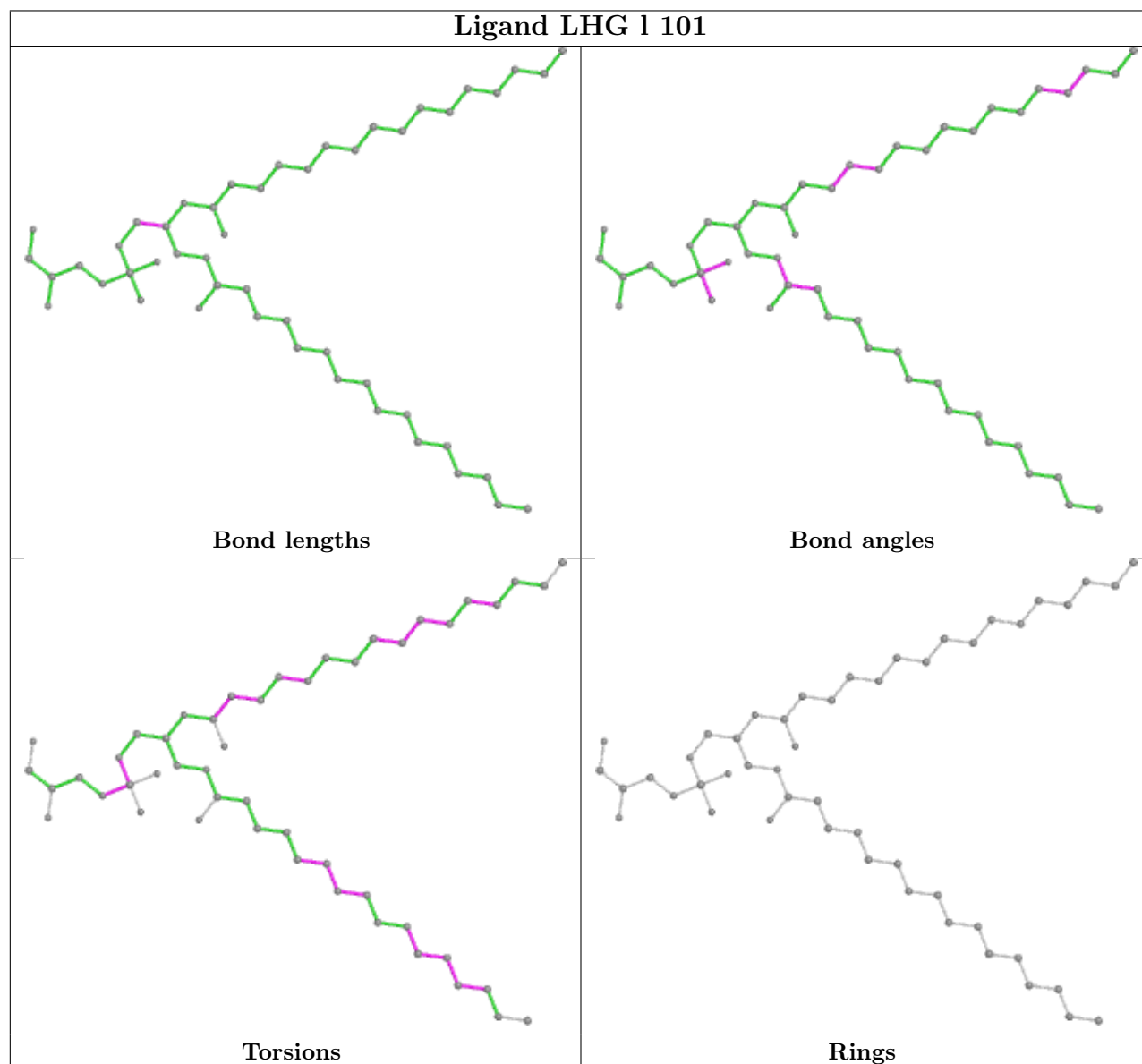


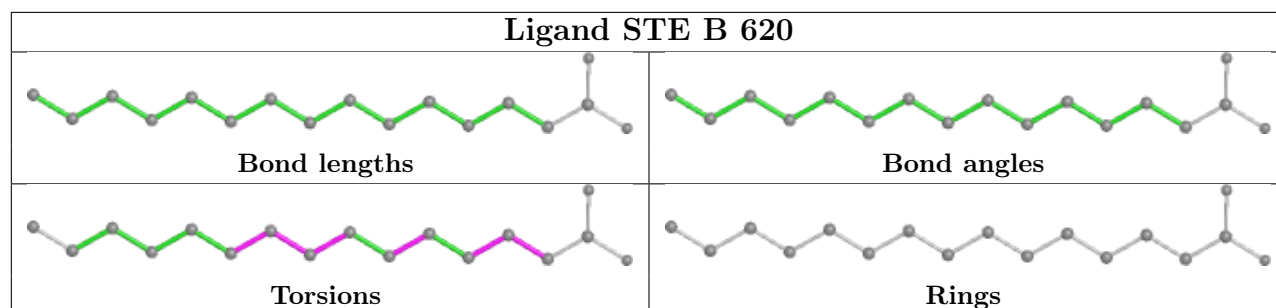
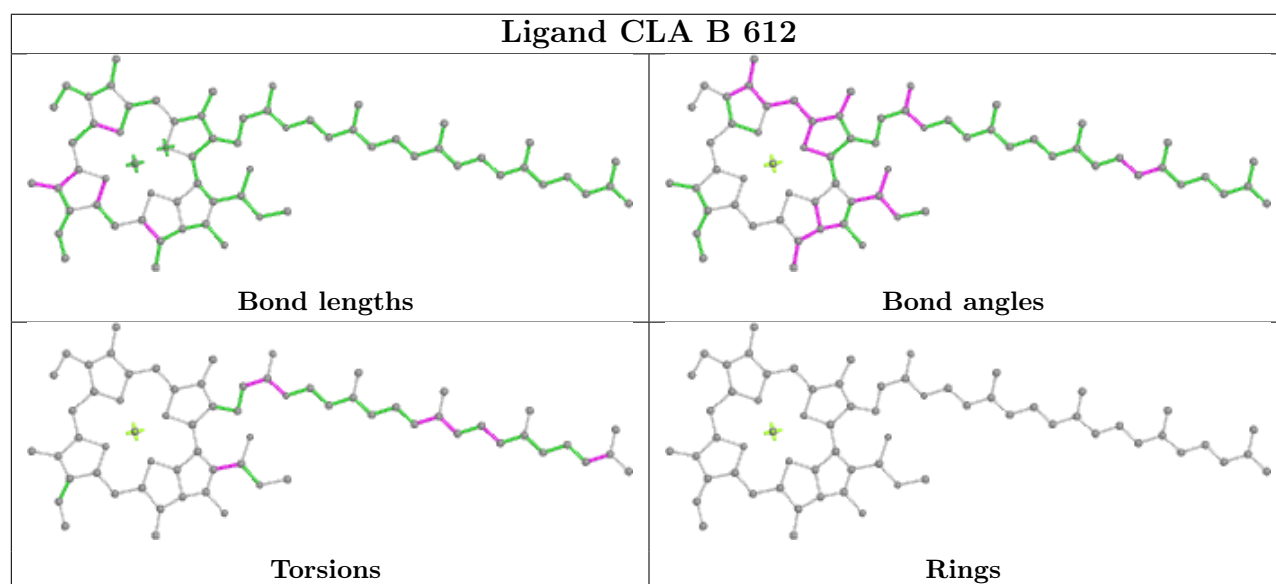
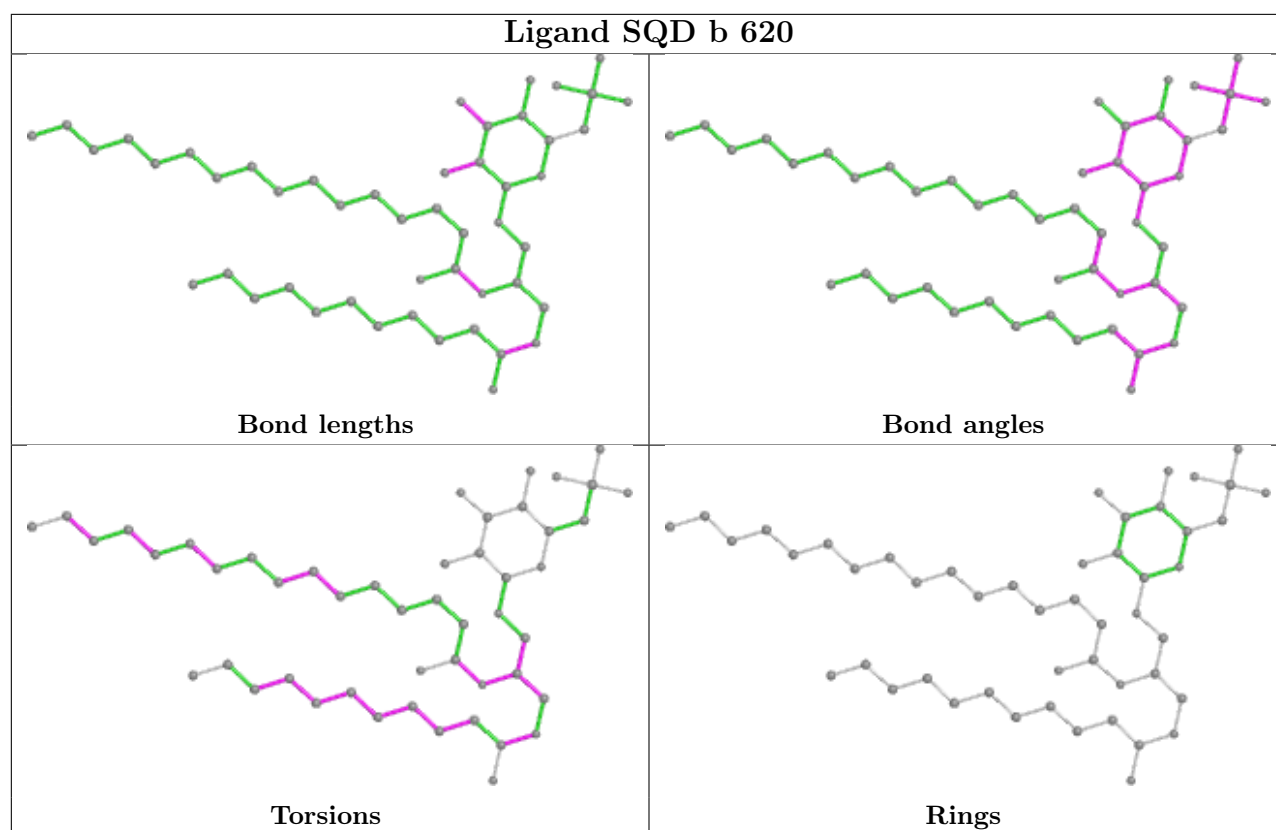


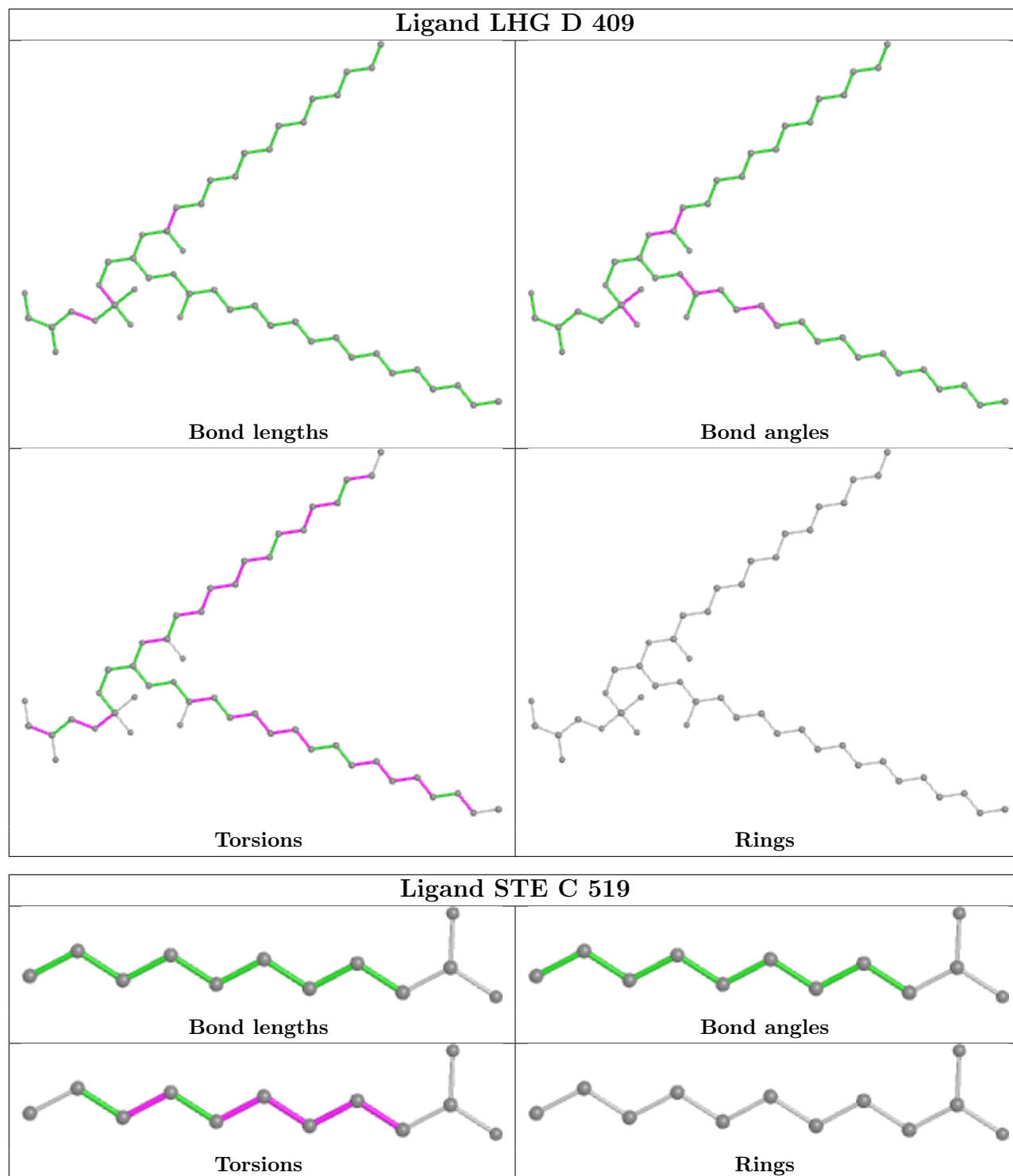
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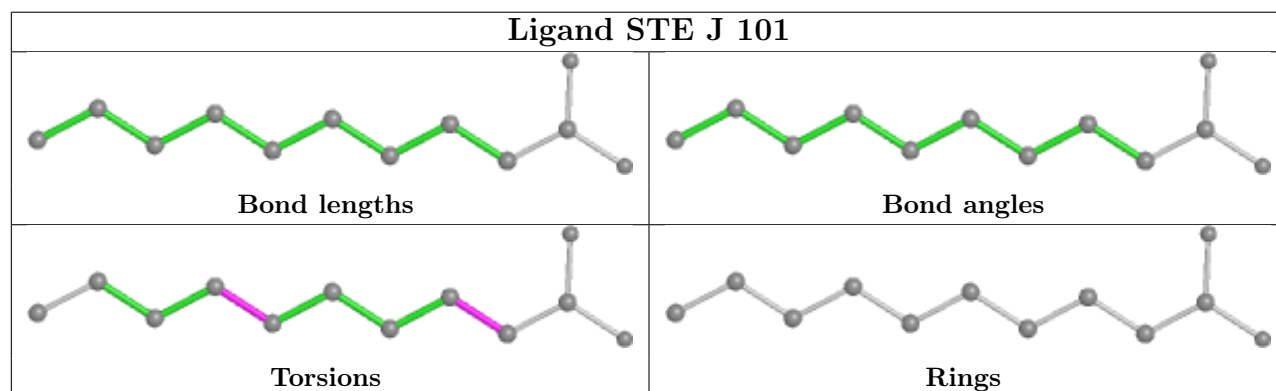
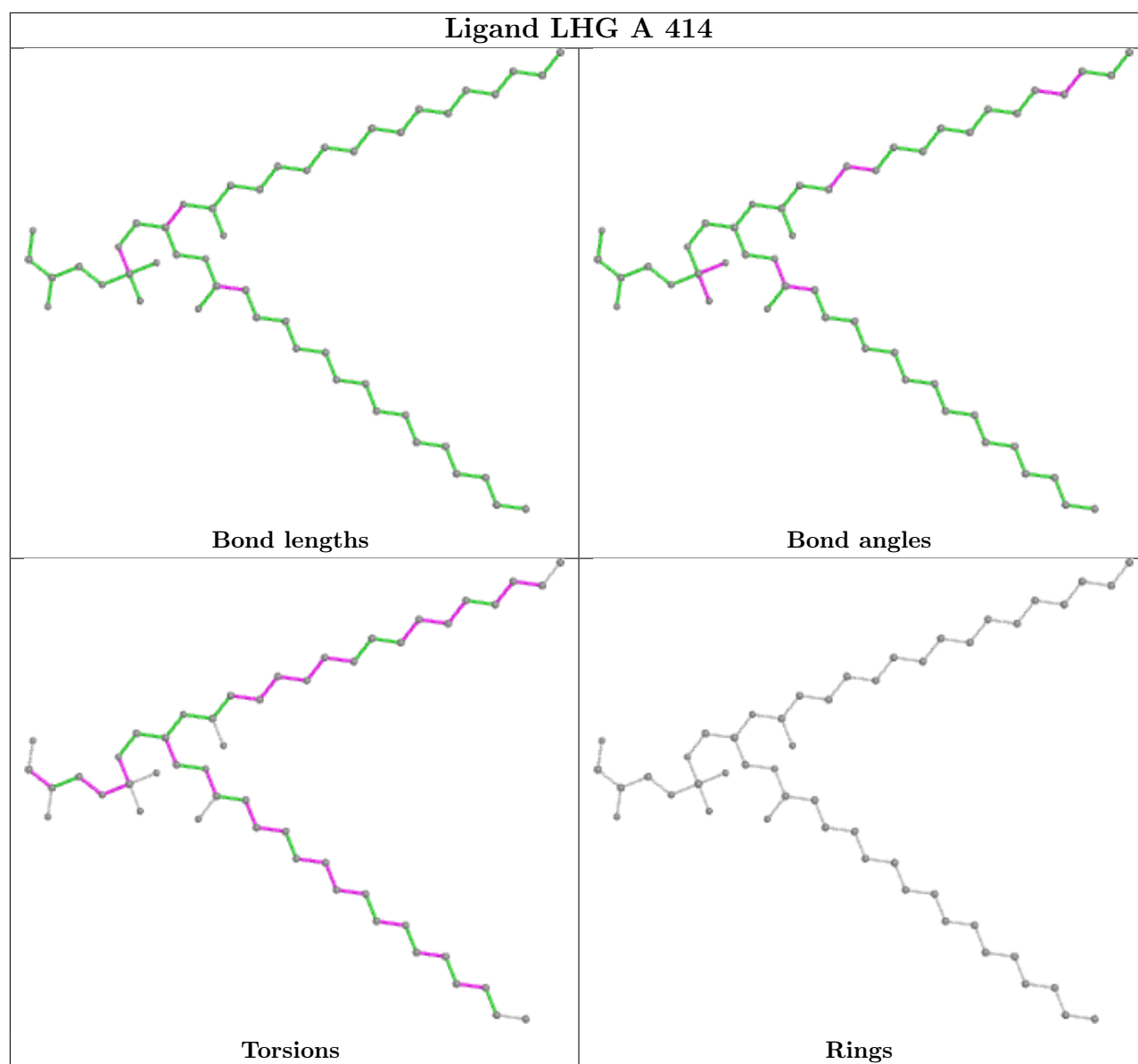


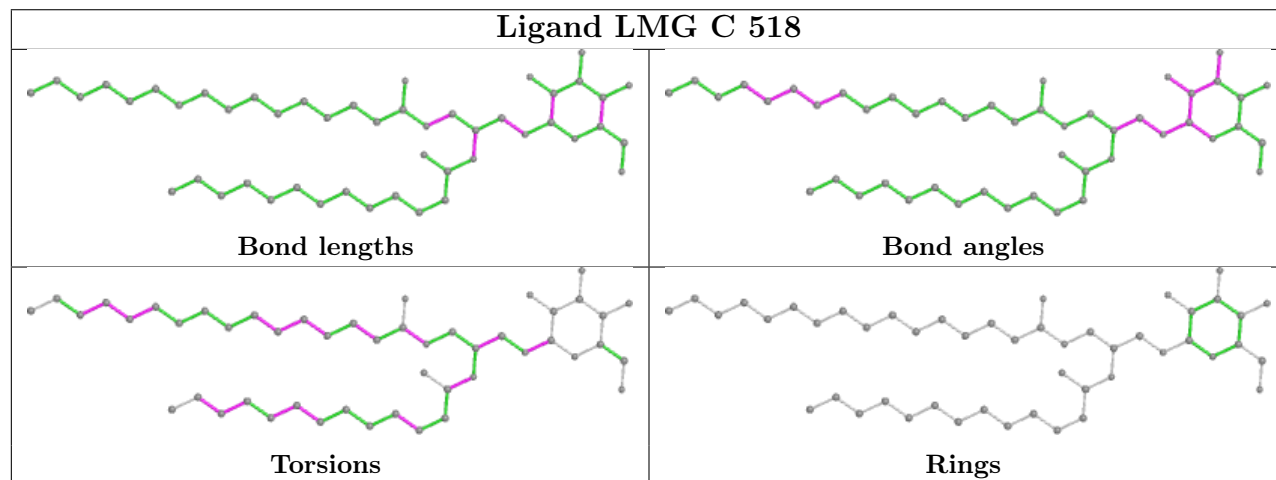
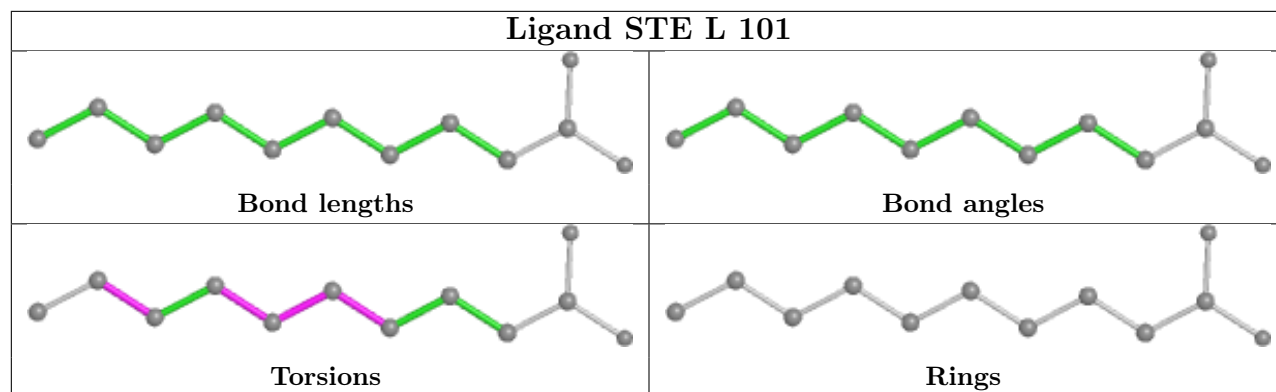
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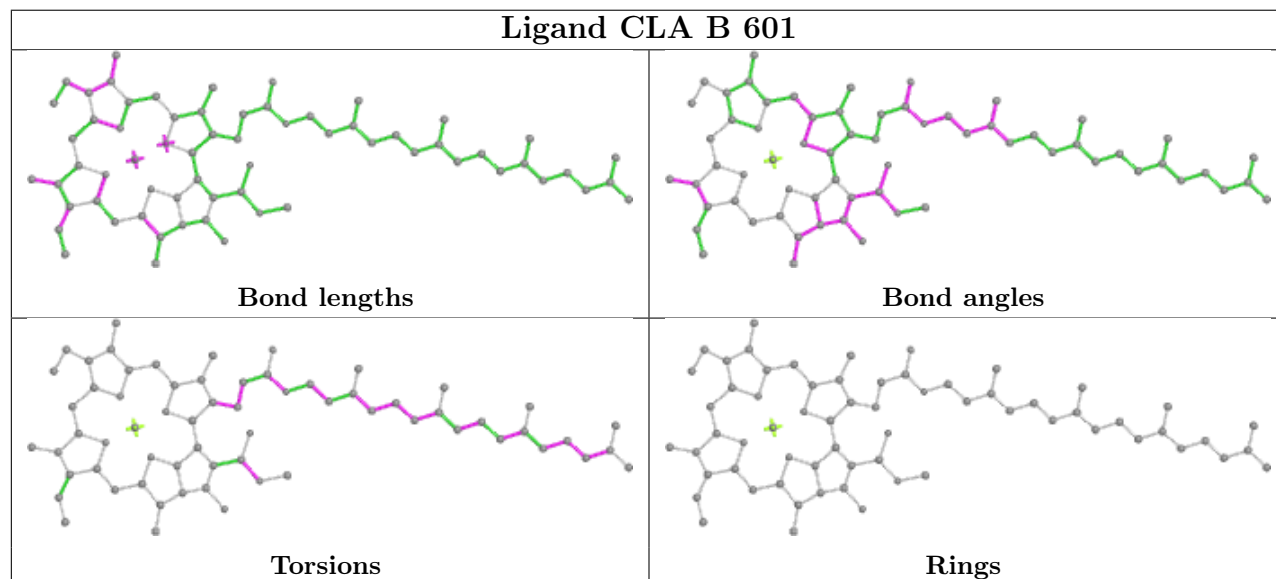
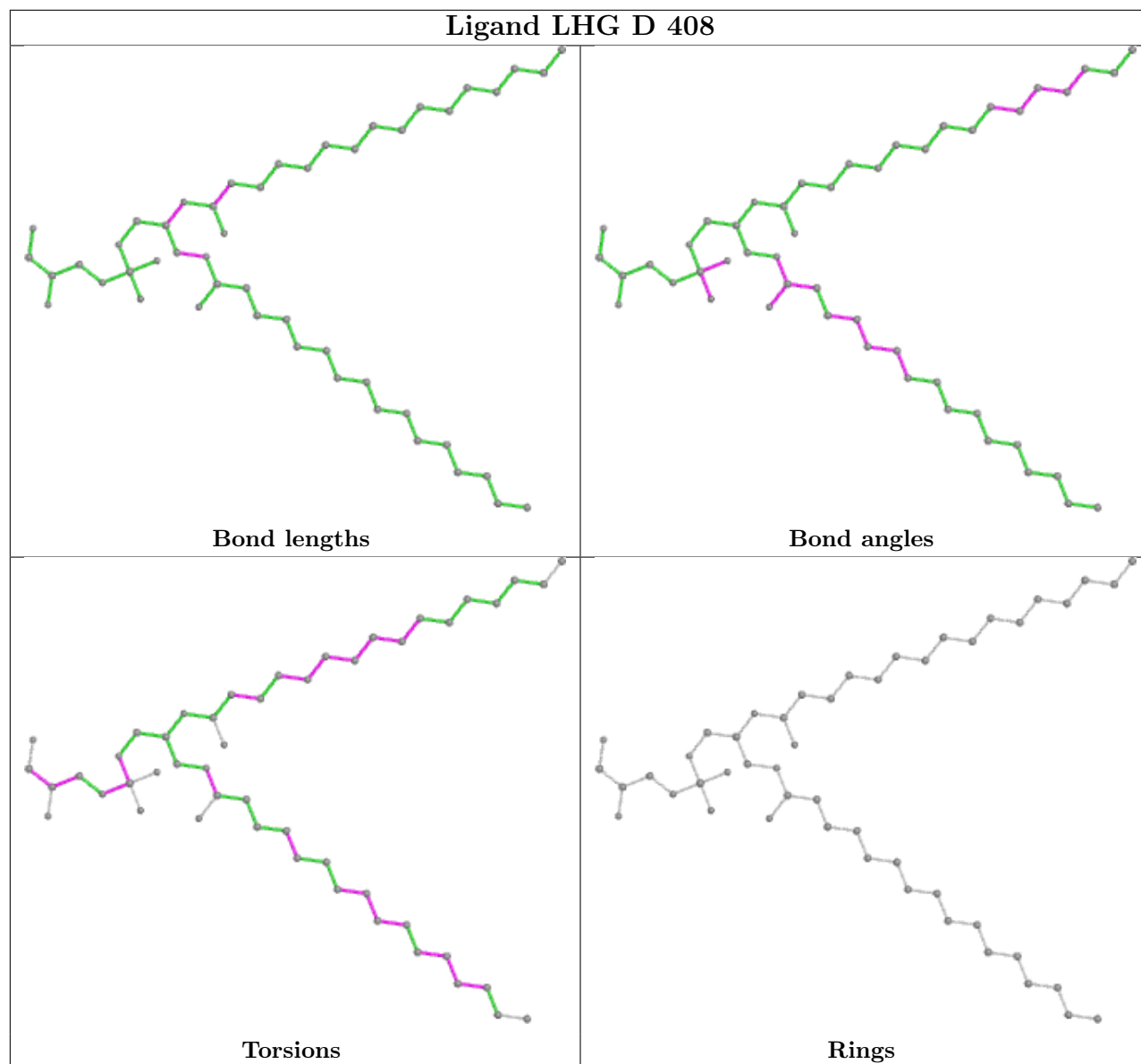


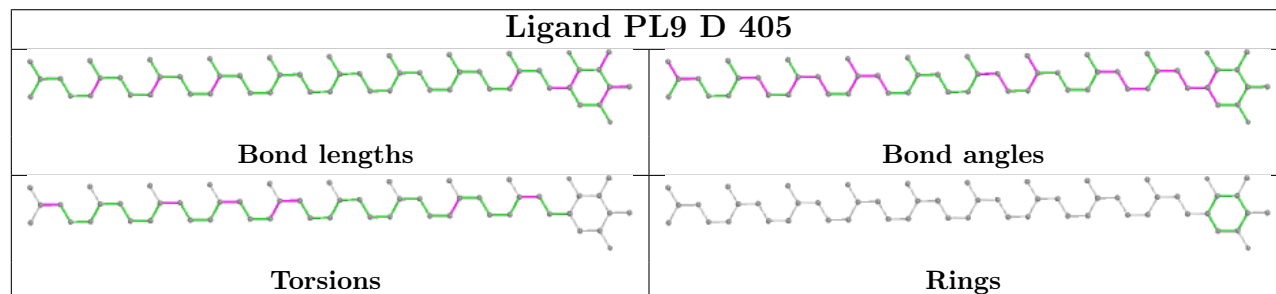
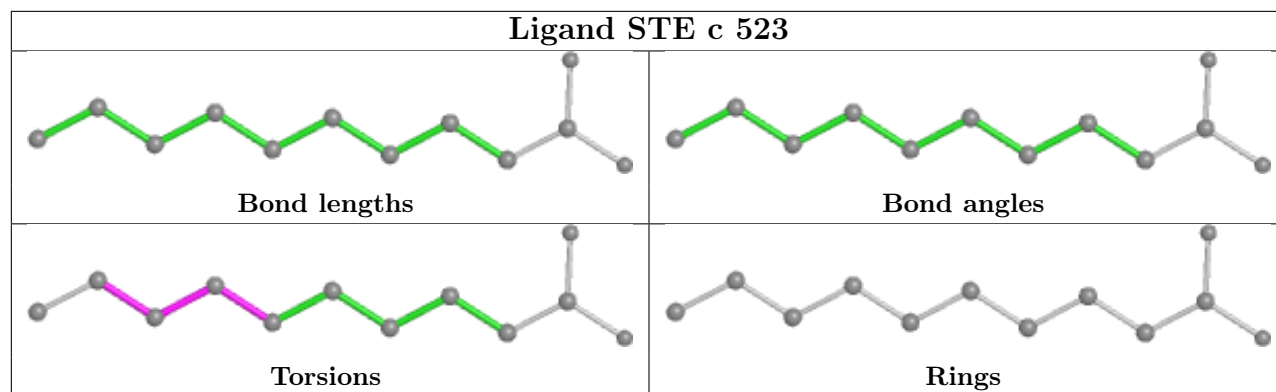




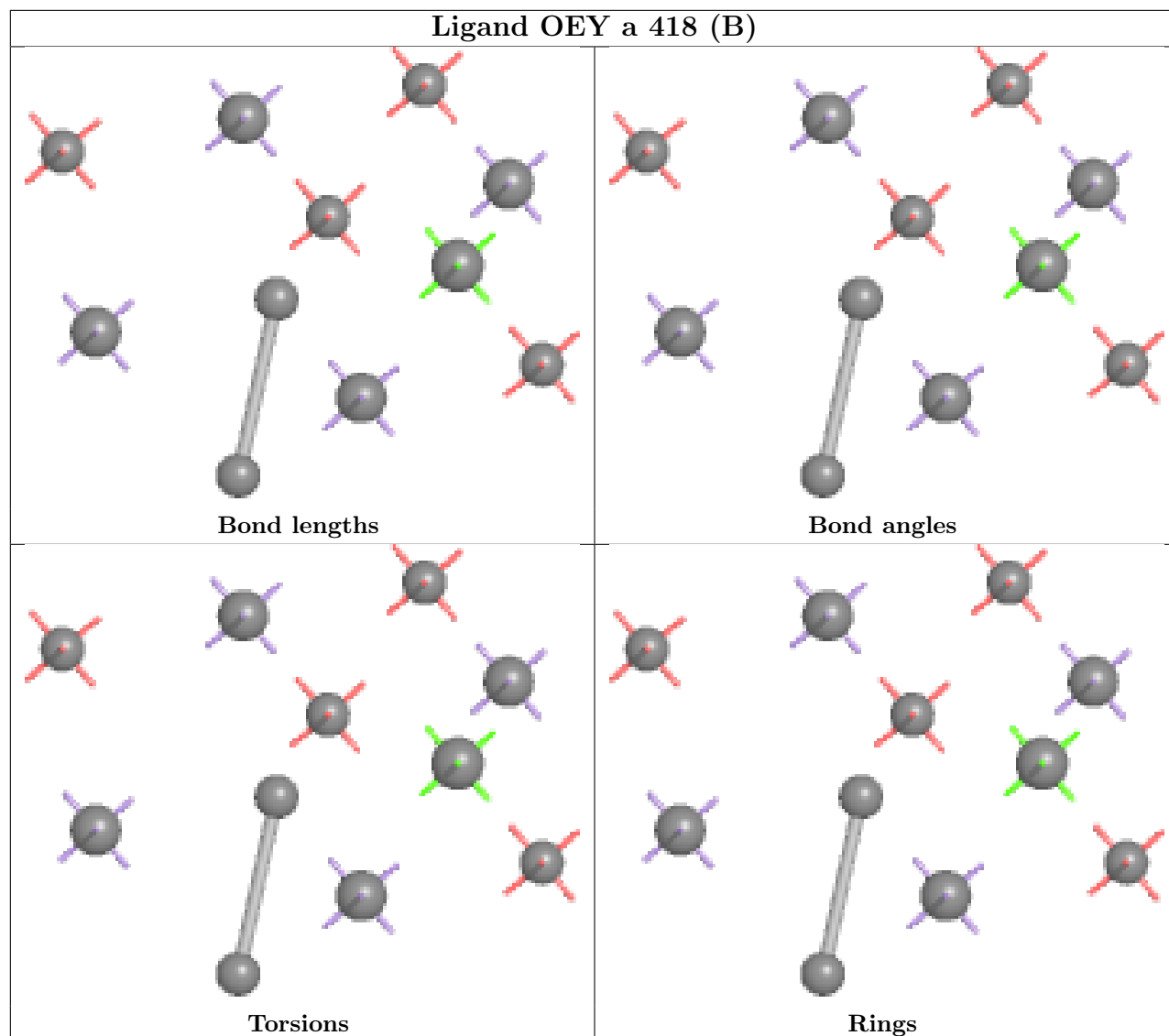




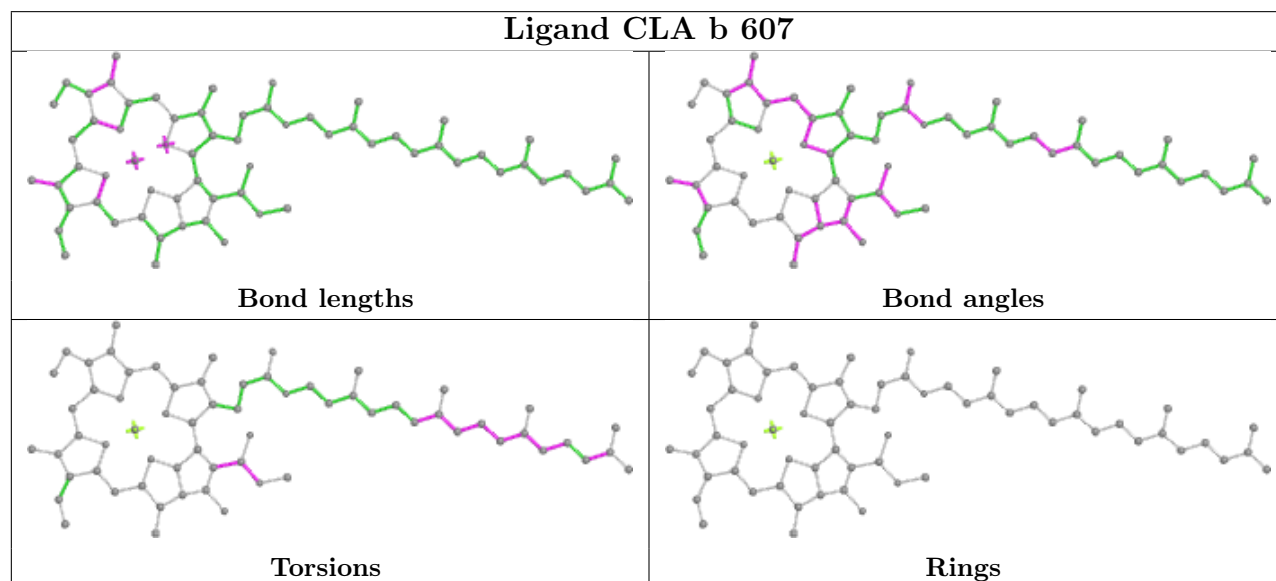


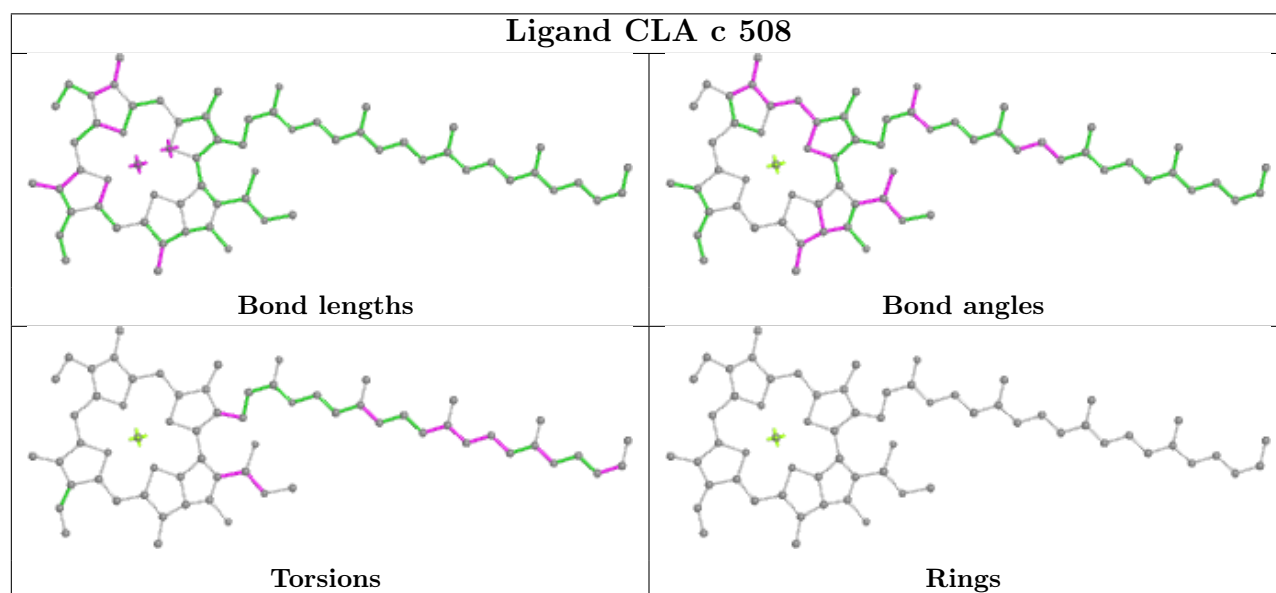
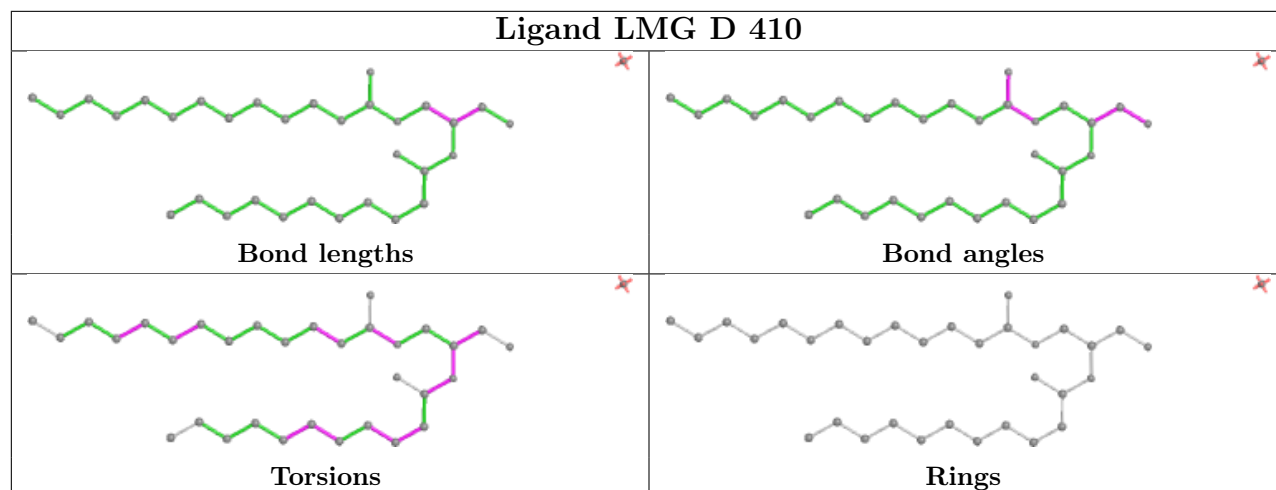
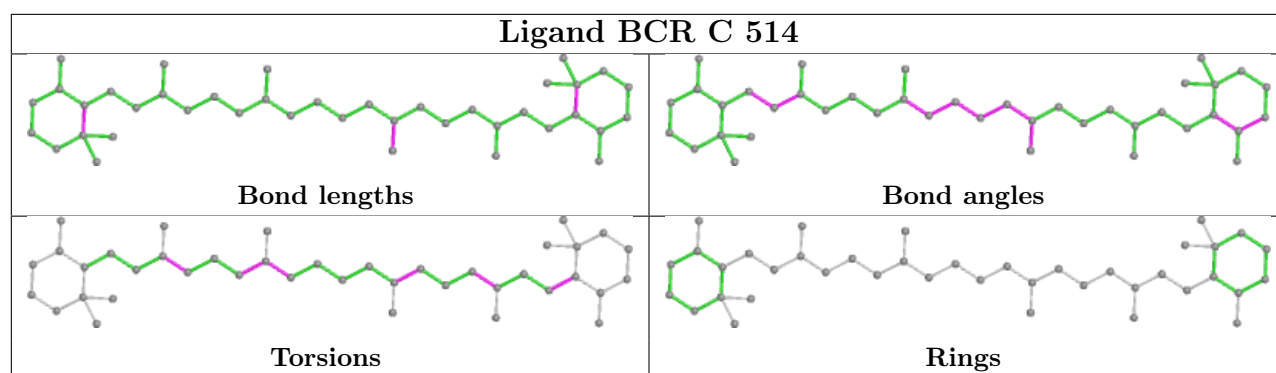


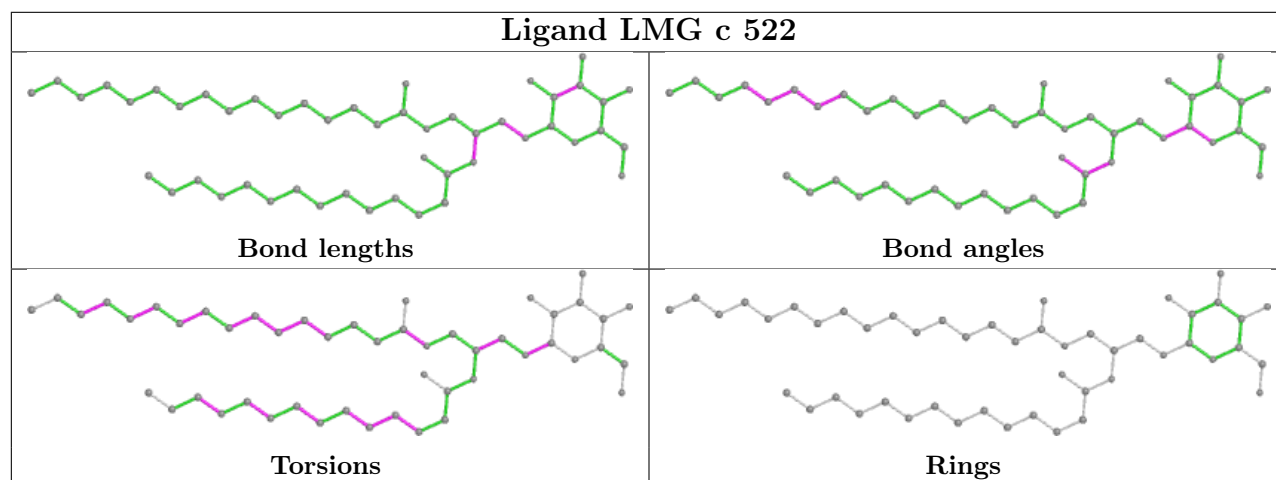
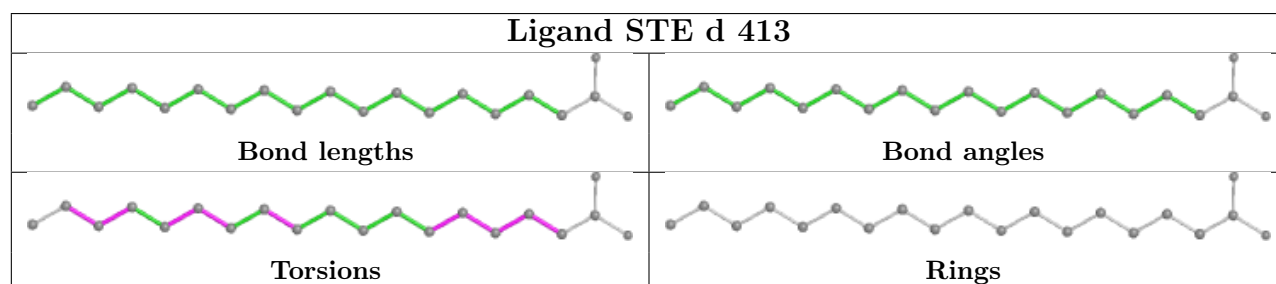
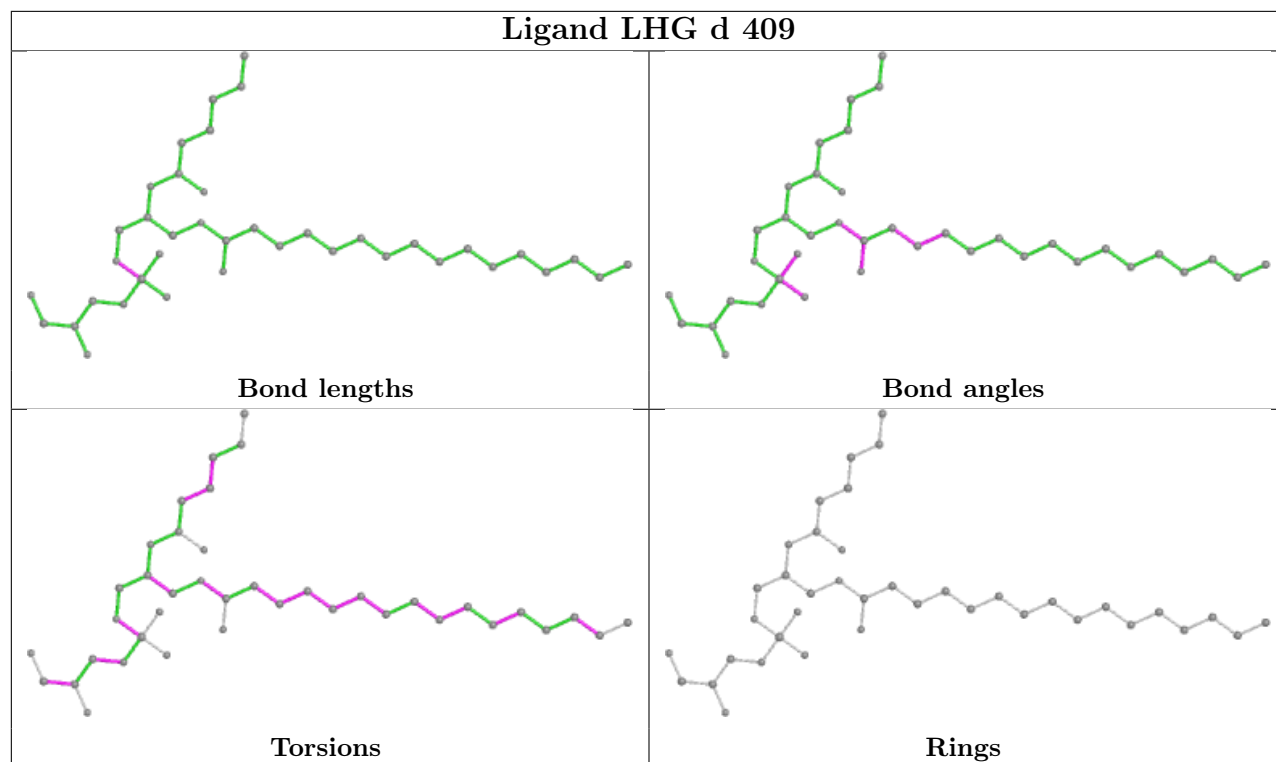
Ligand OEY a 418 (B)

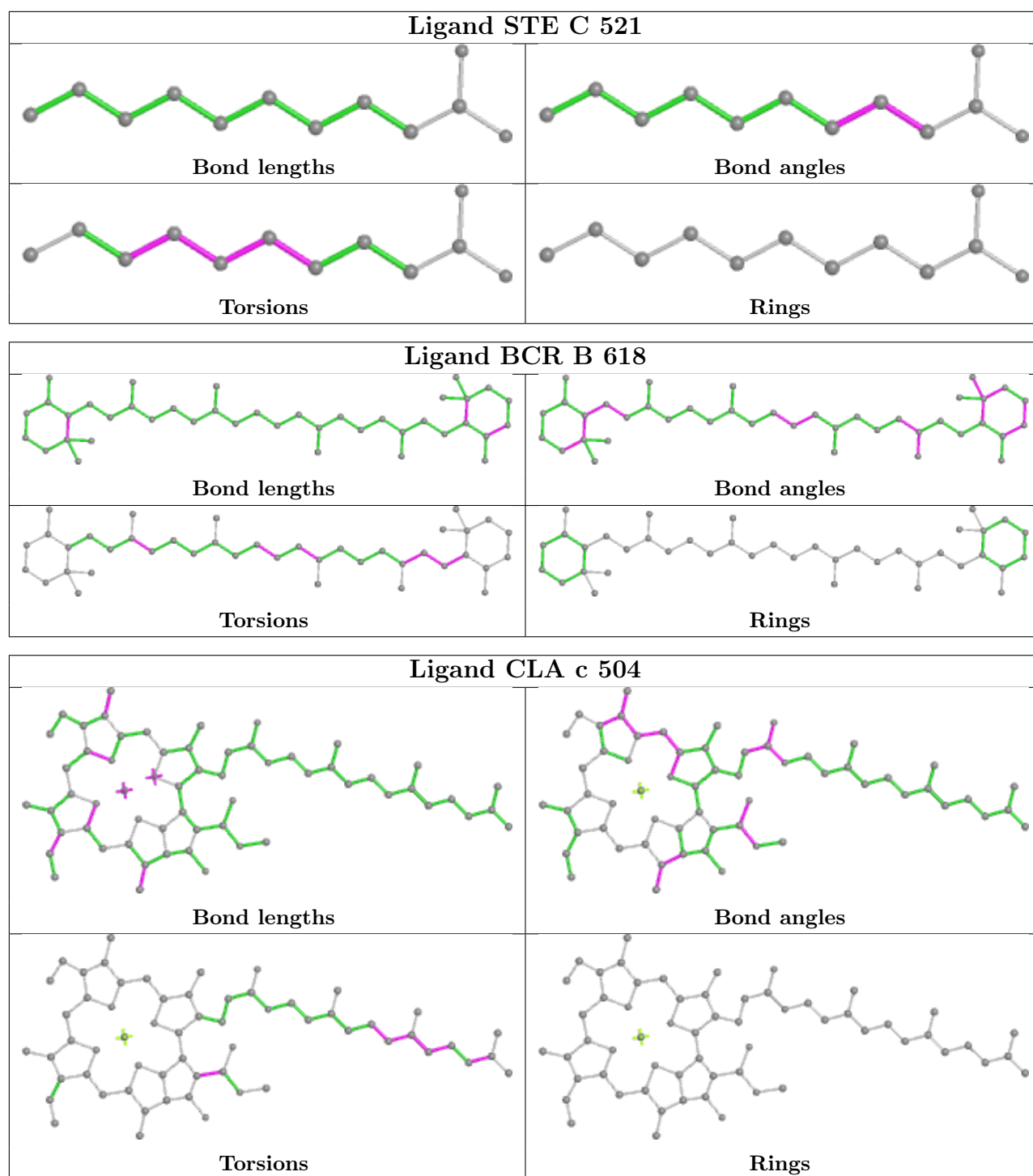


Ligand CLA b 607

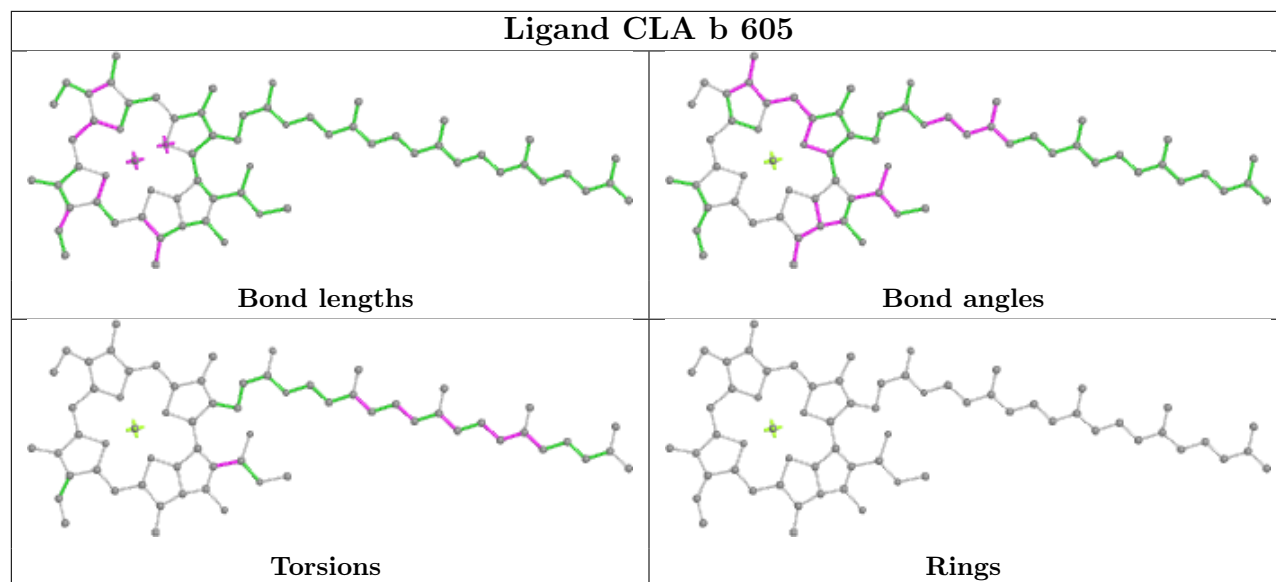




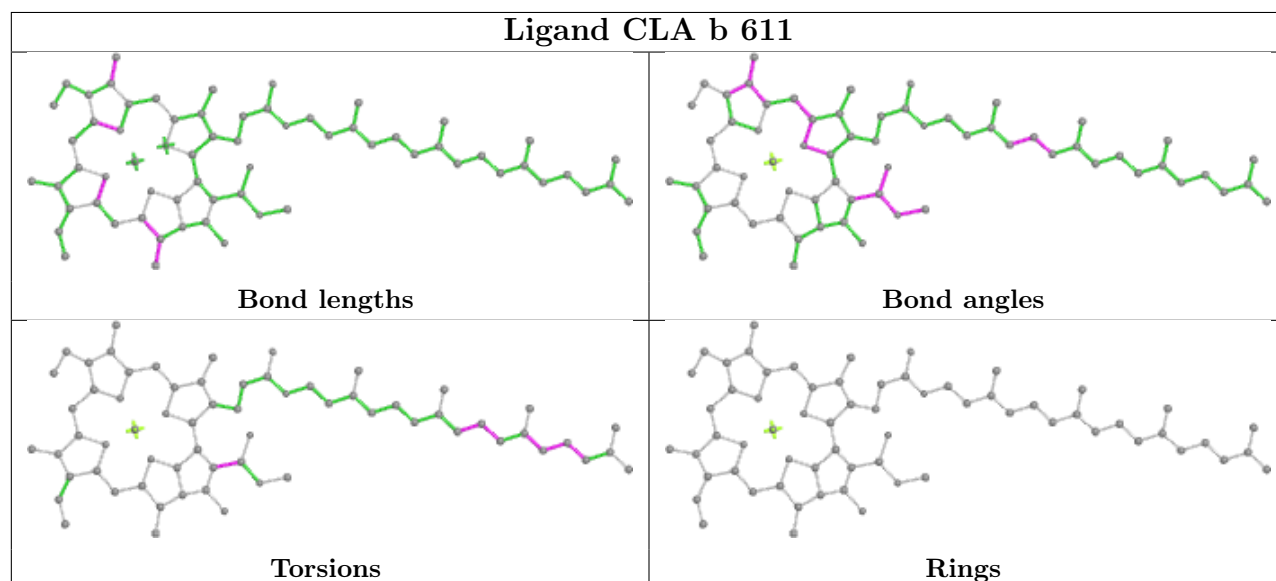




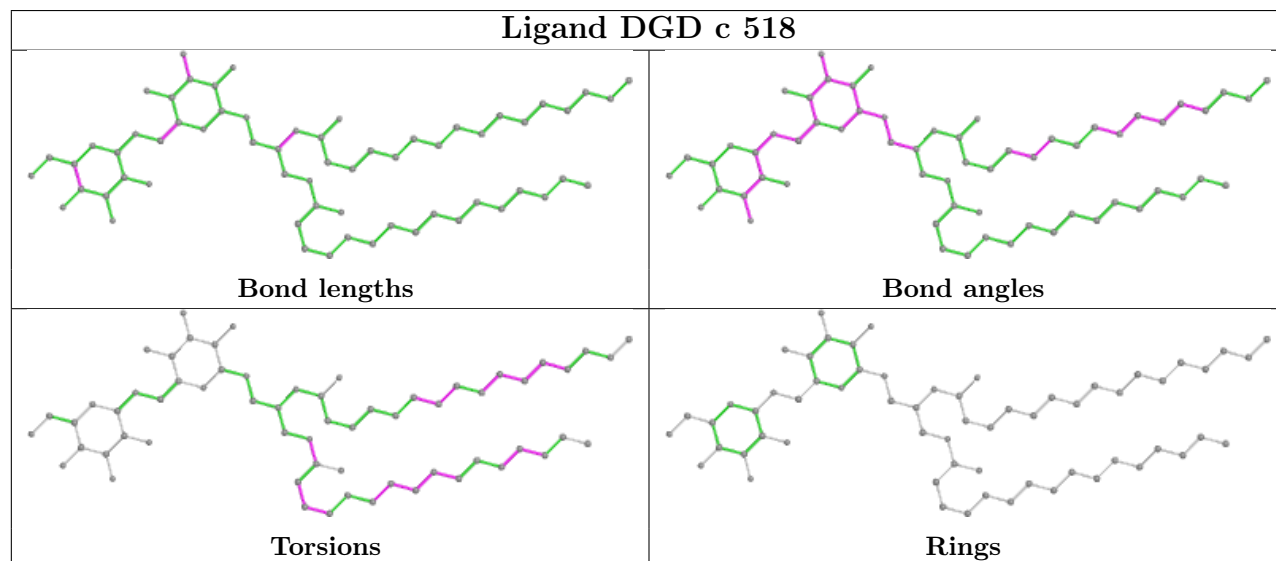
Ligand CLA b 605

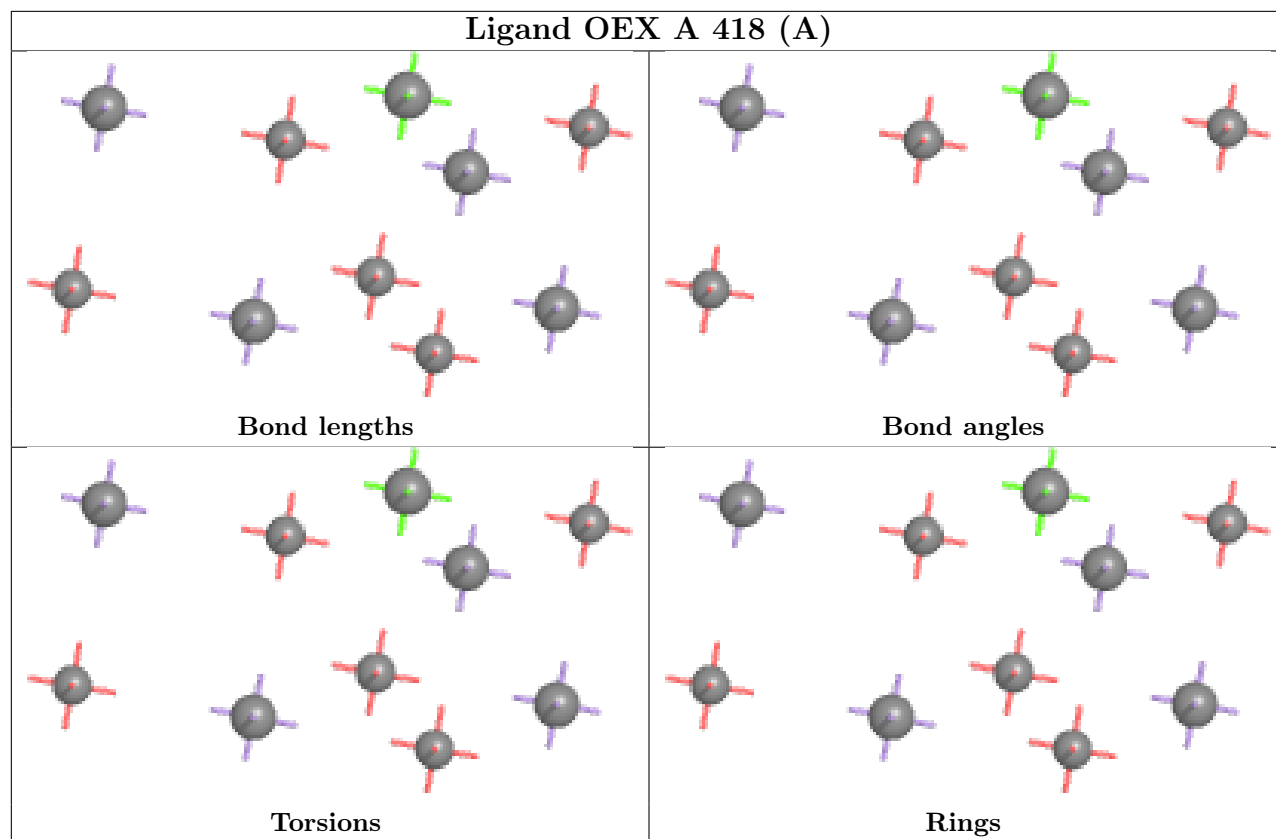


Ligand CLA b 611

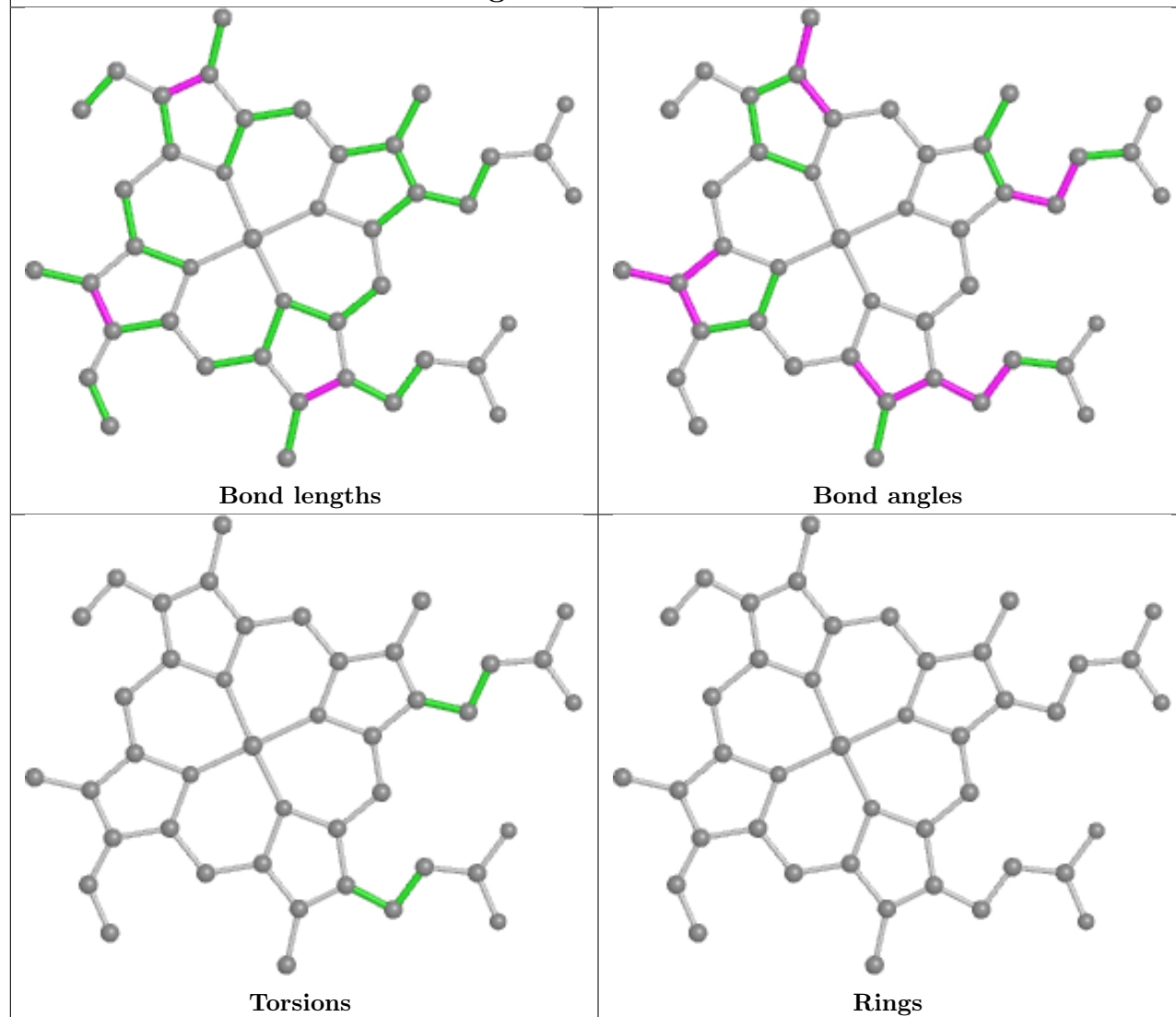


Ligand DGD c 518

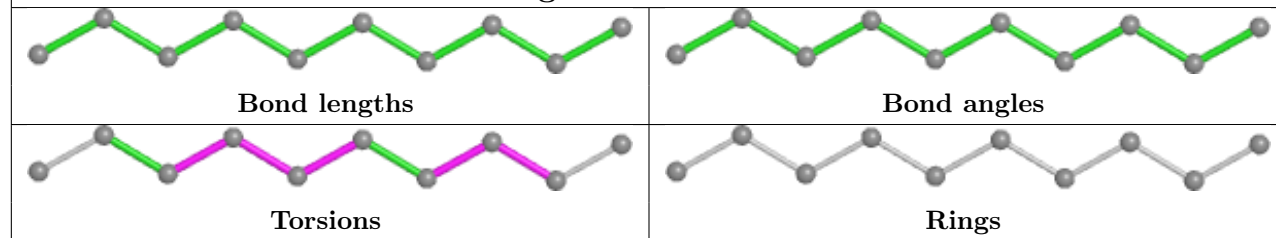




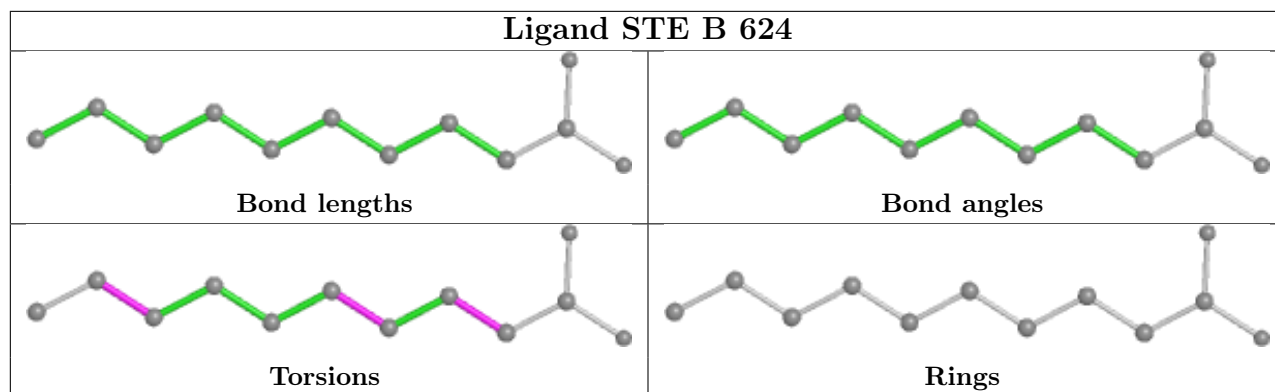
Ligand HEC V 201



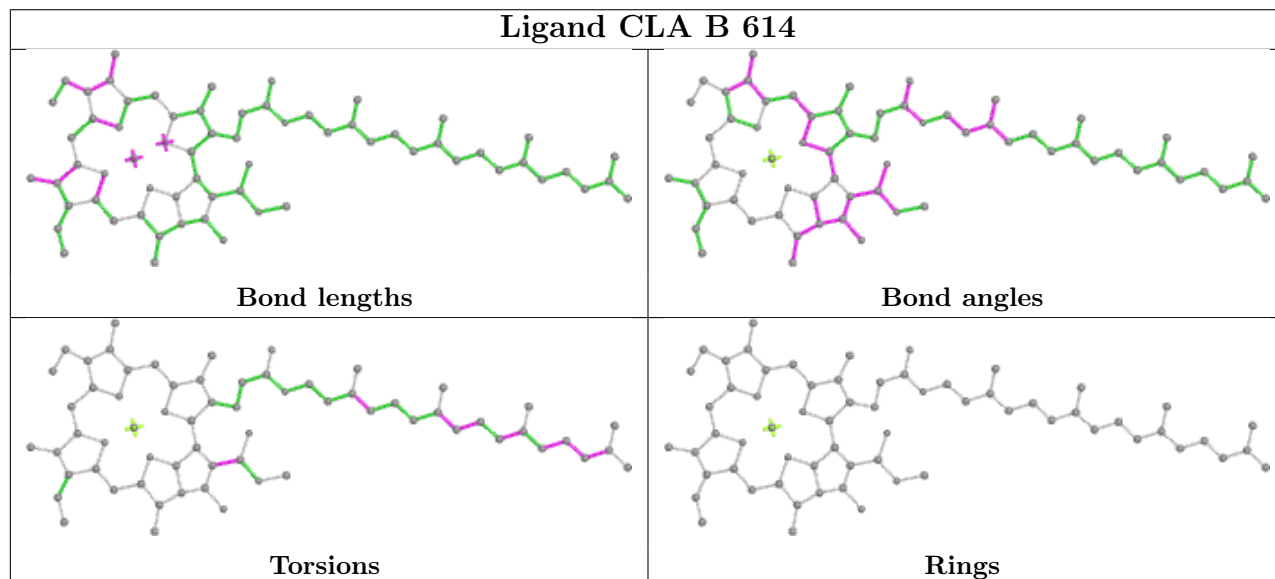
Ligand STE b 627



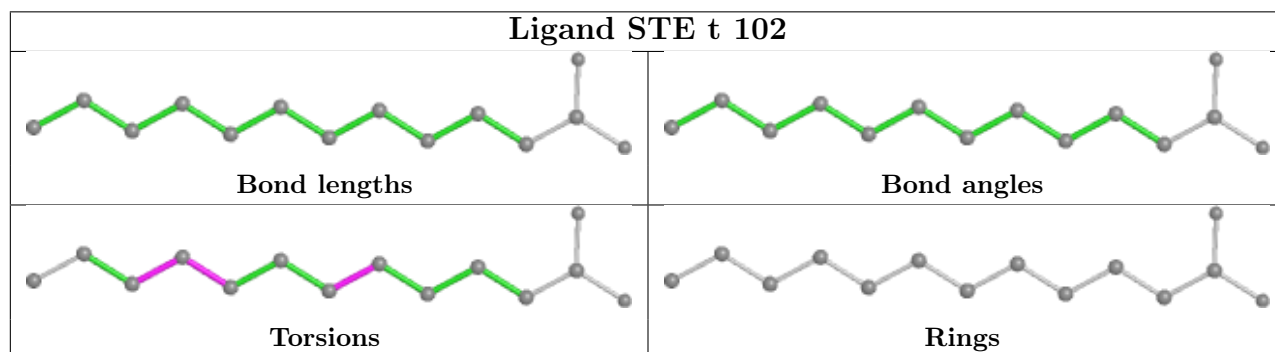
Ligand STE B 624

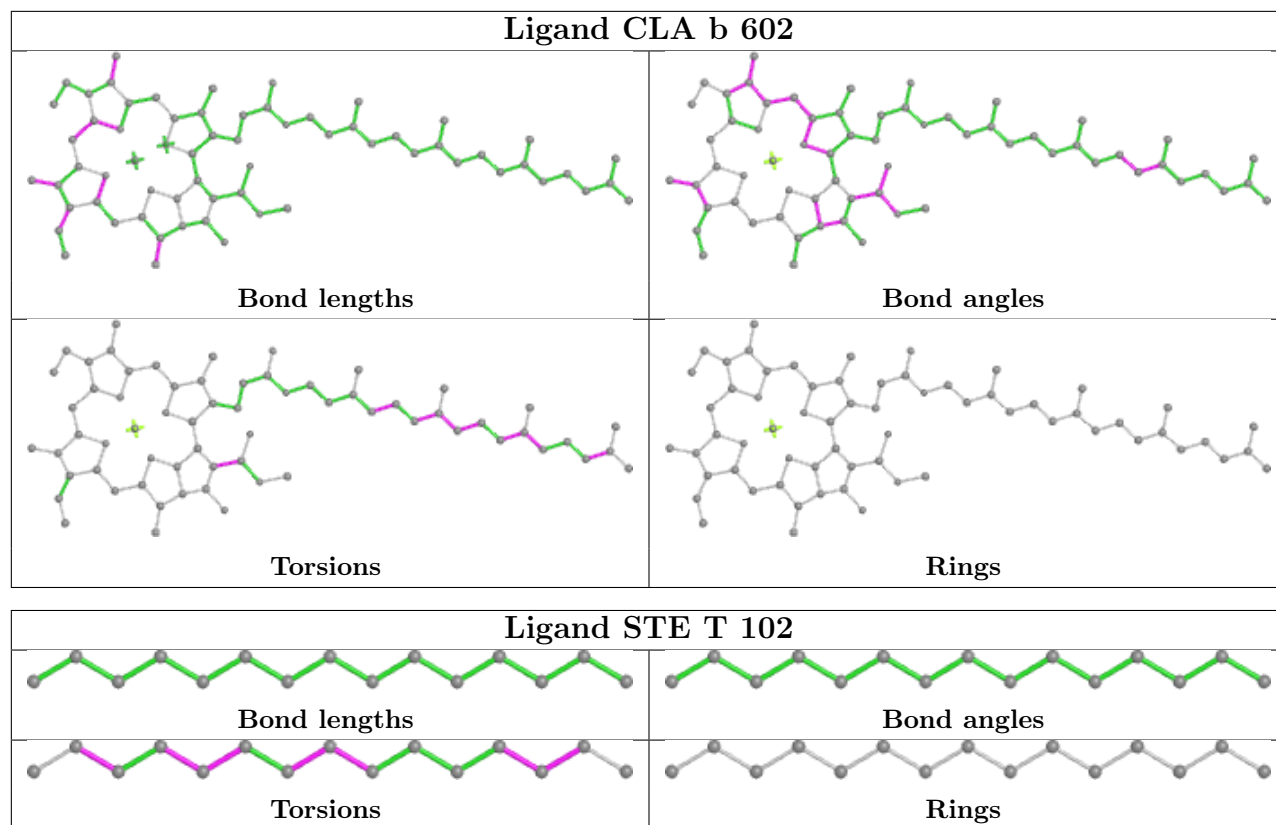


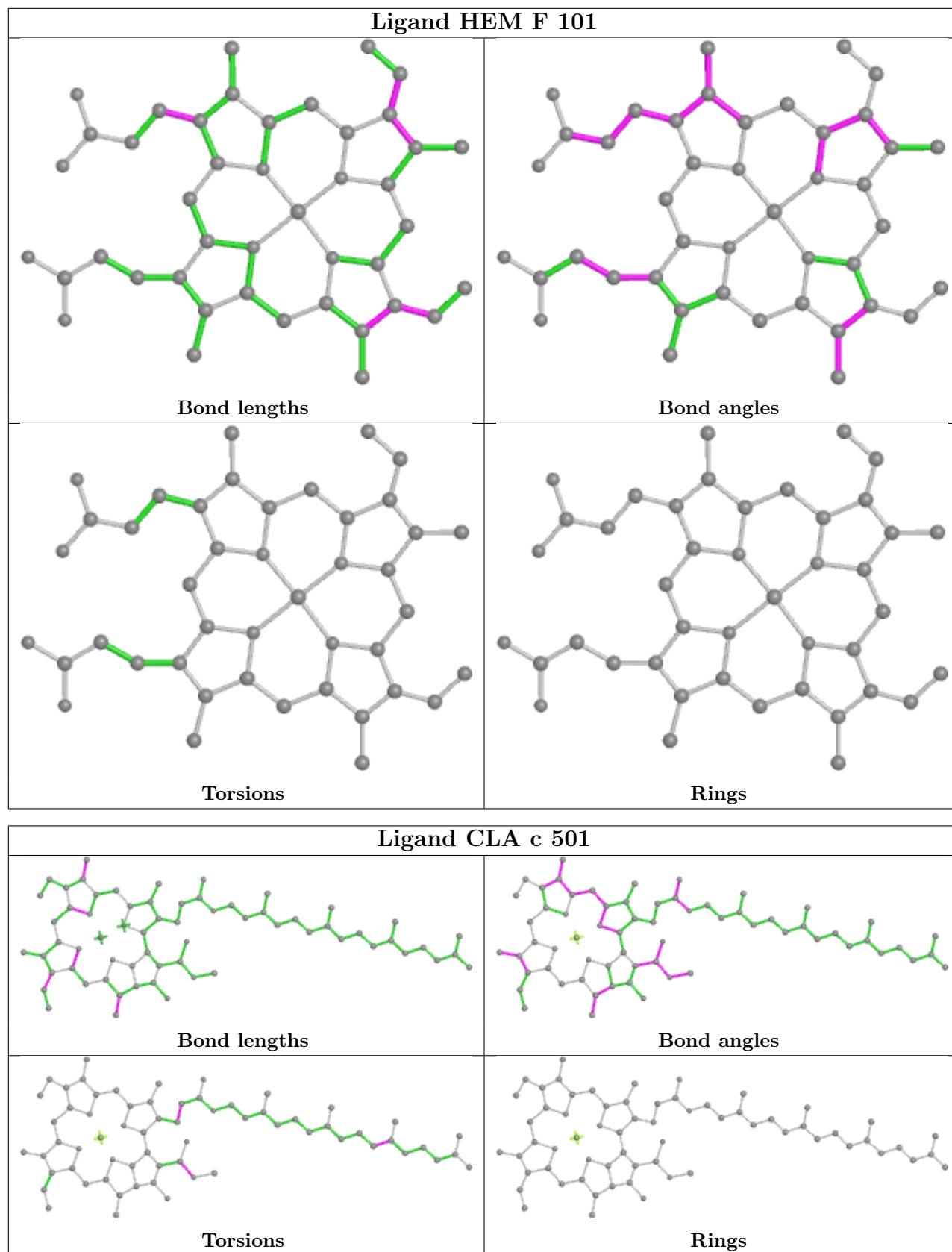
Ligand CLA B 614



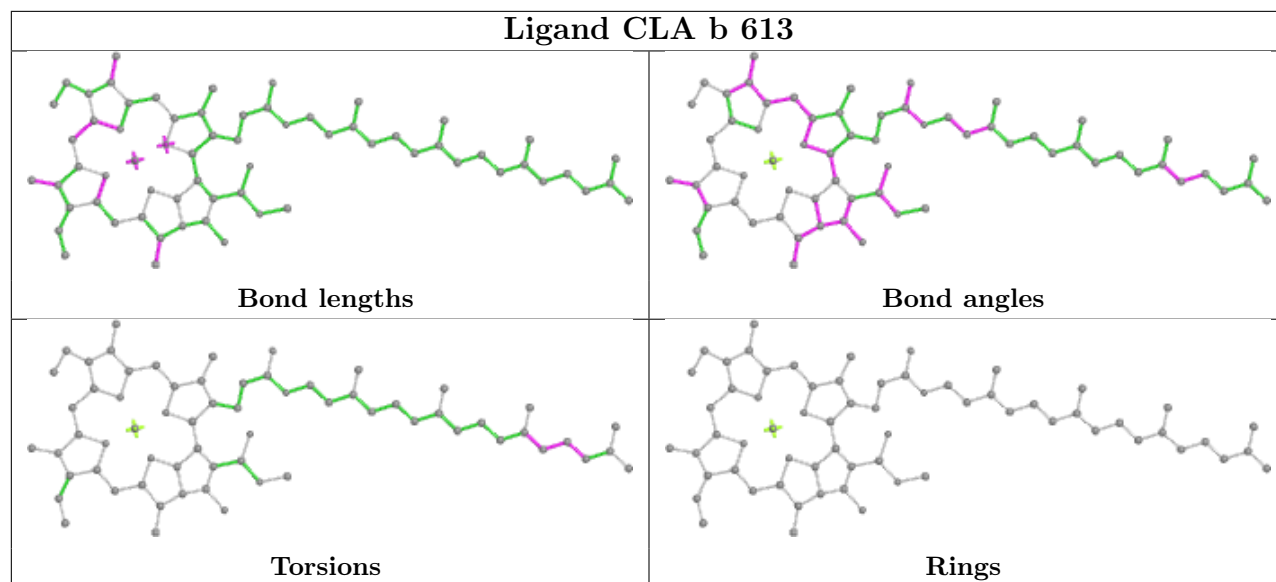
Ligand STE t 102



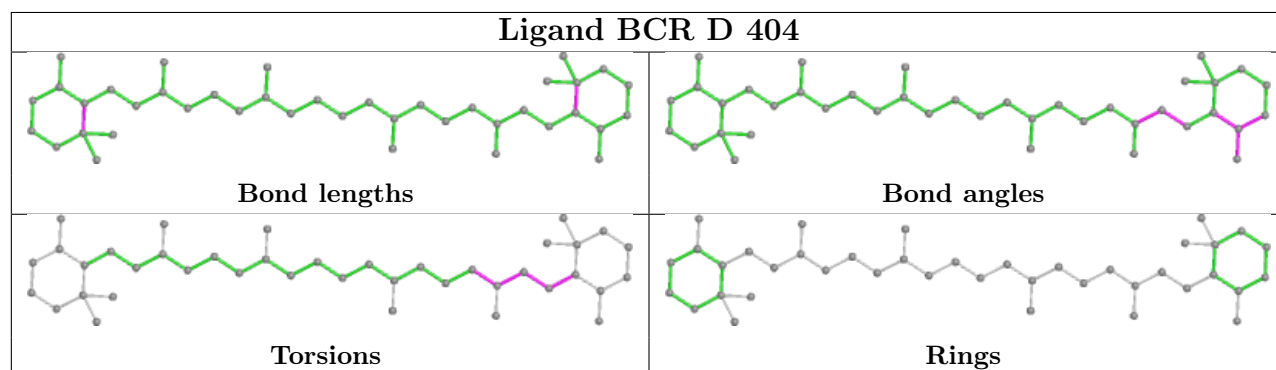




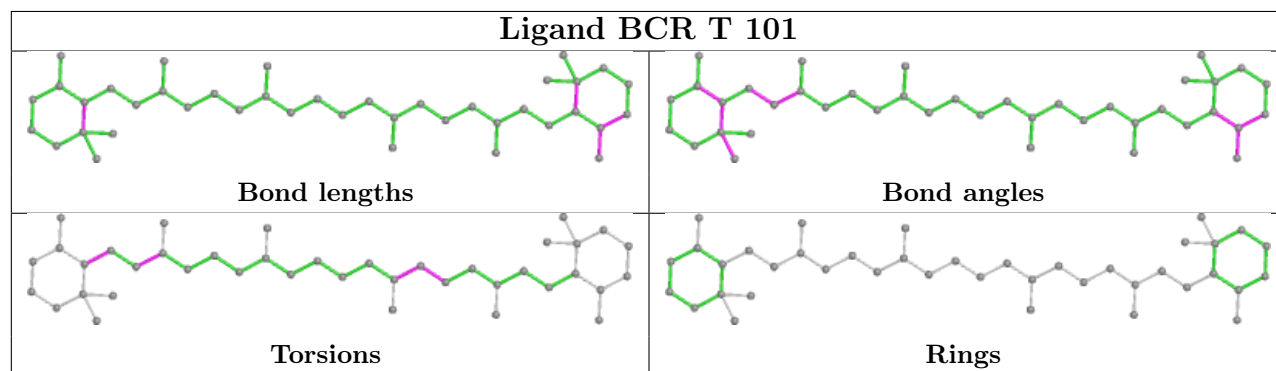
Ligand CLA b 613

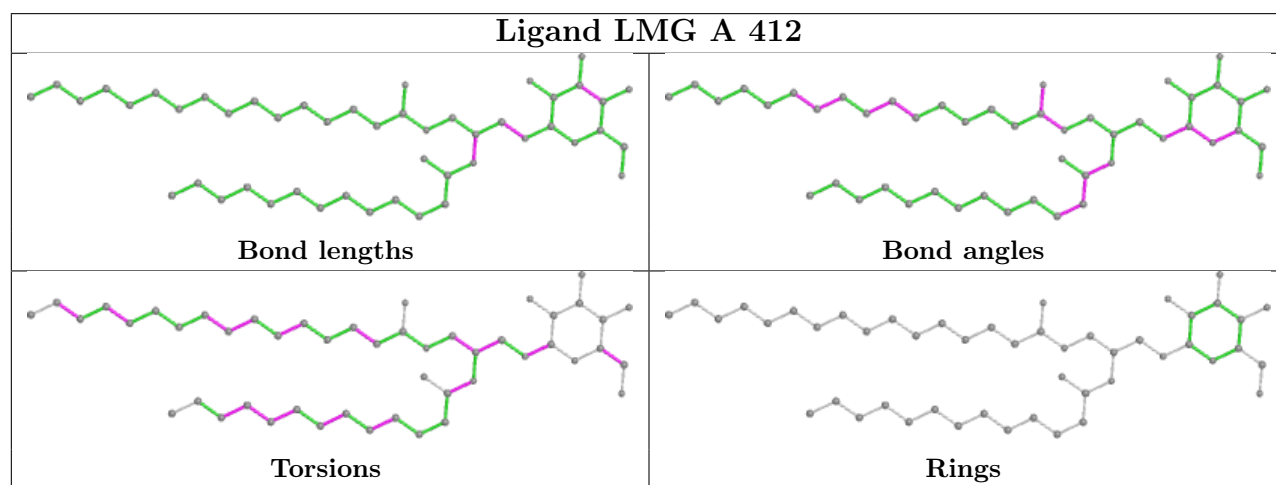
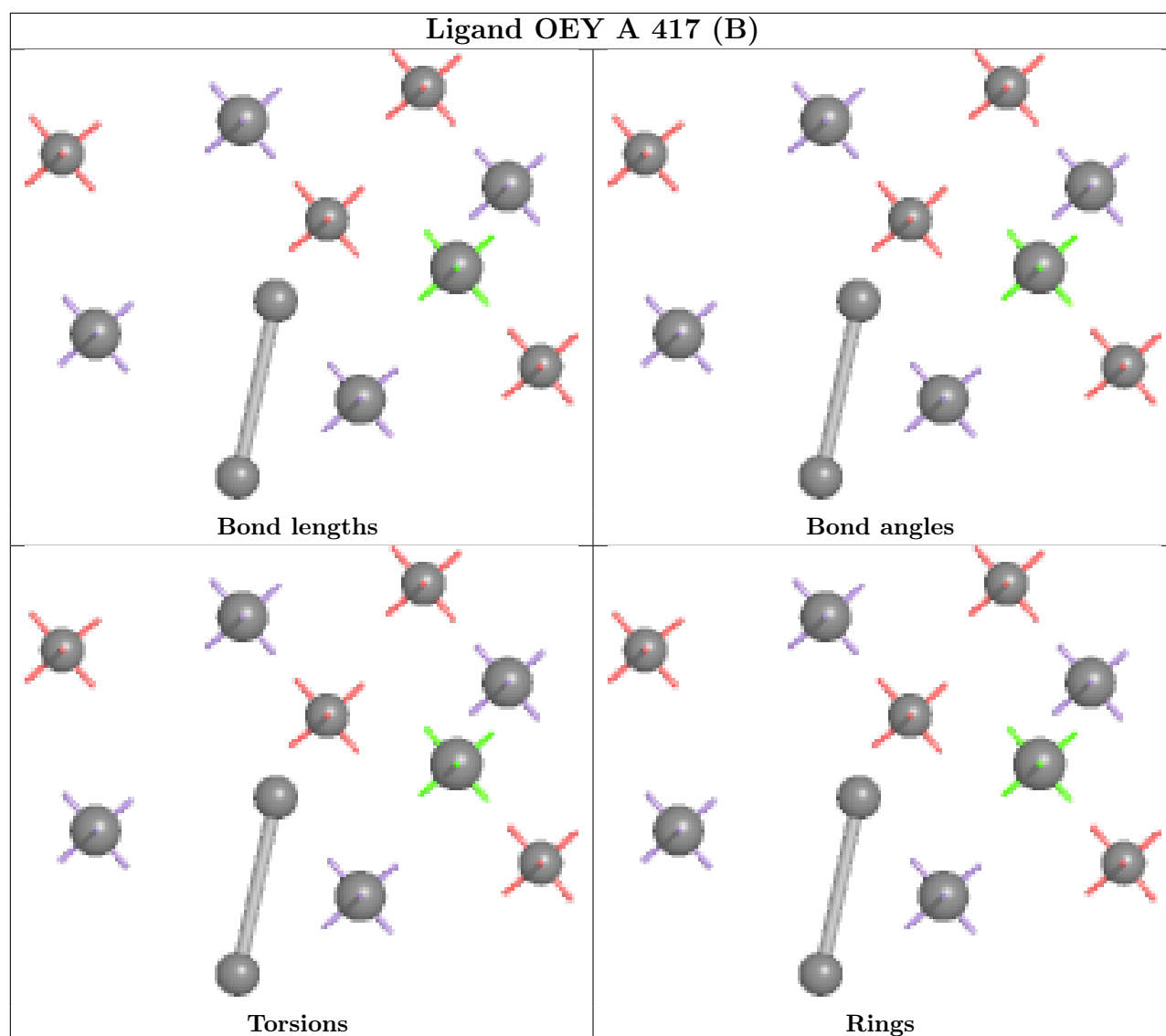


Ligand BCR D 404

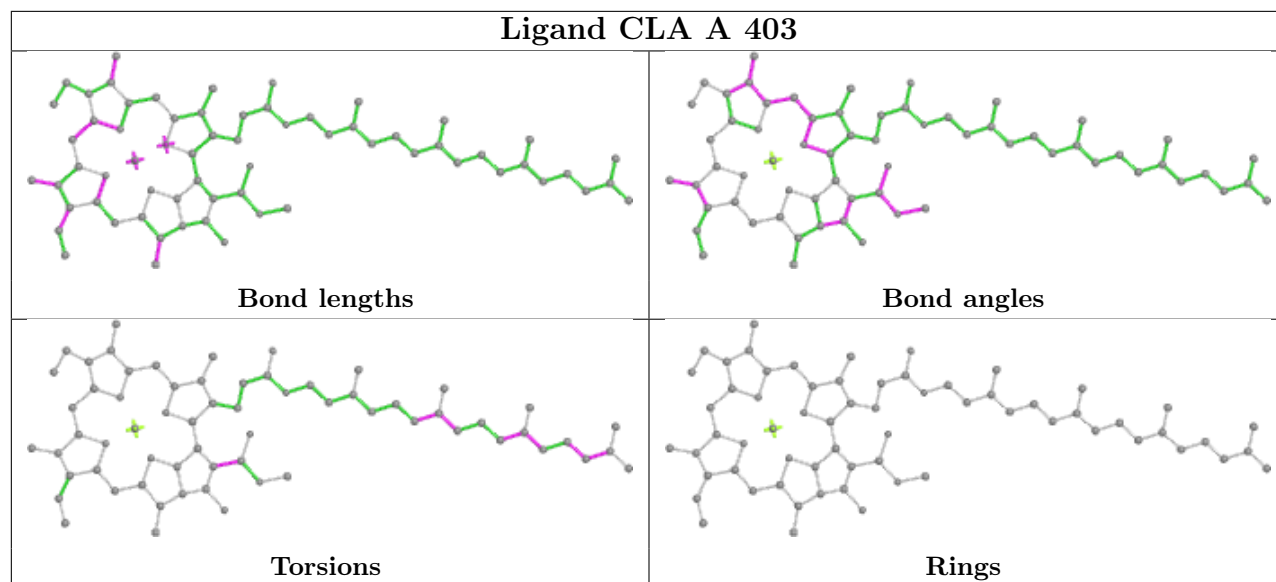


Ligand BCR T 101

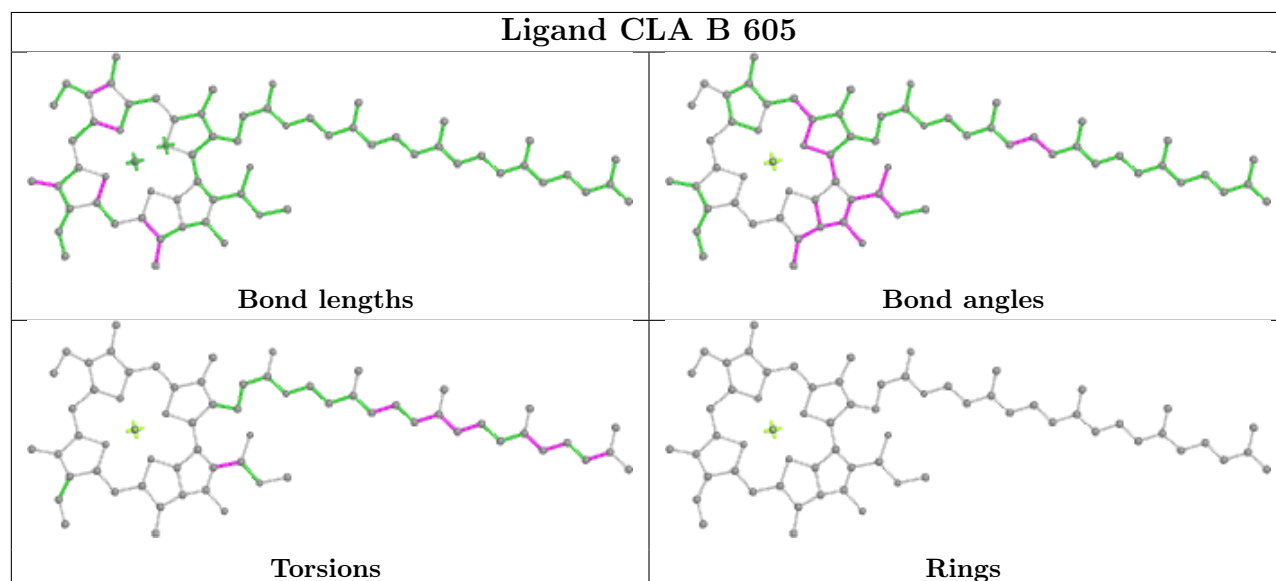




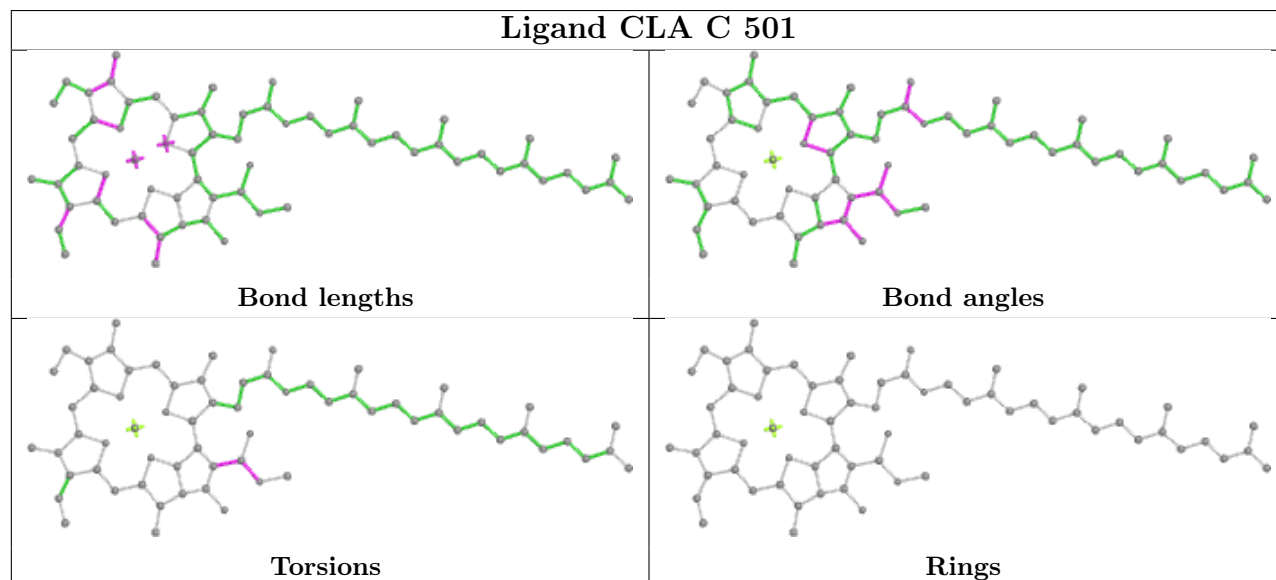
Ligand CLA A 403



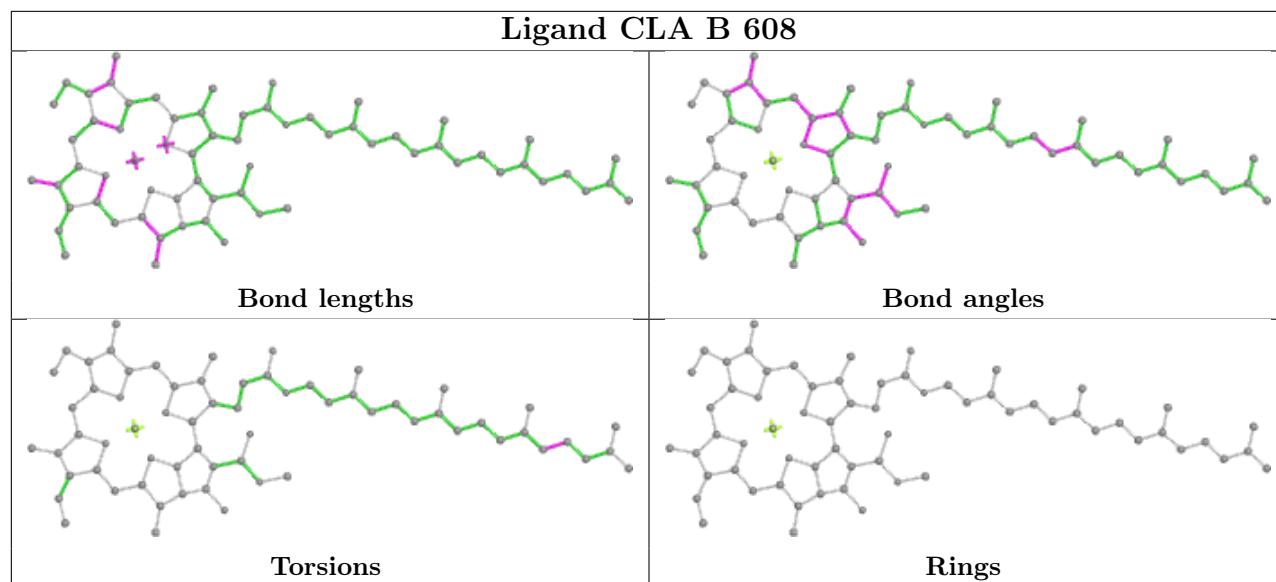
Ligand CLA B 605



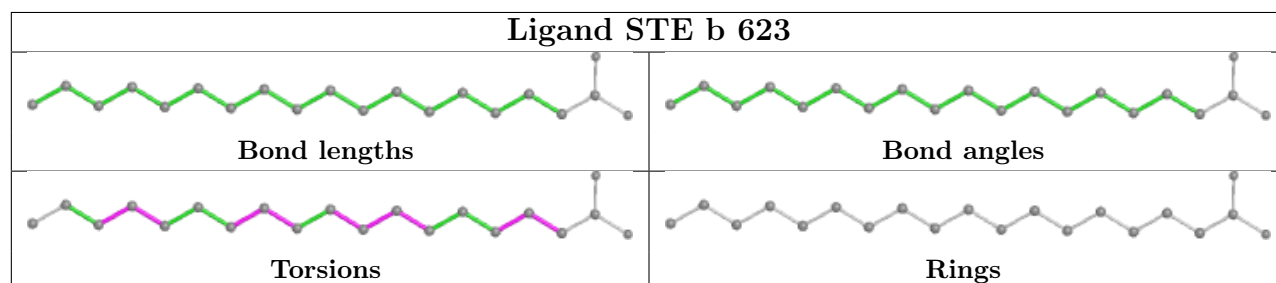
Ligand CLA C 501



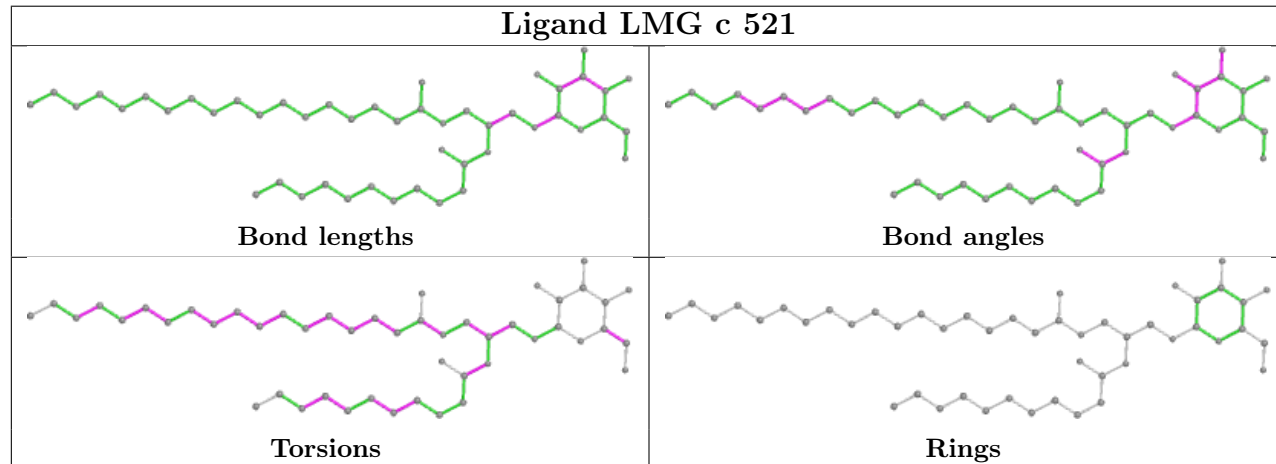
Ligand CLA B 608



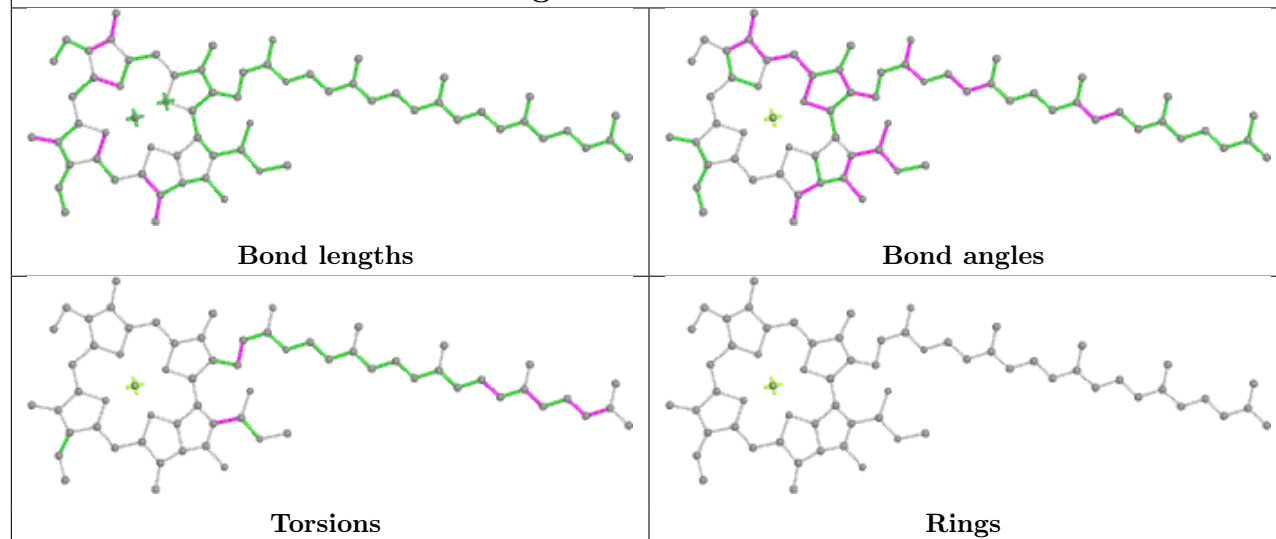
Ligand STE b 623



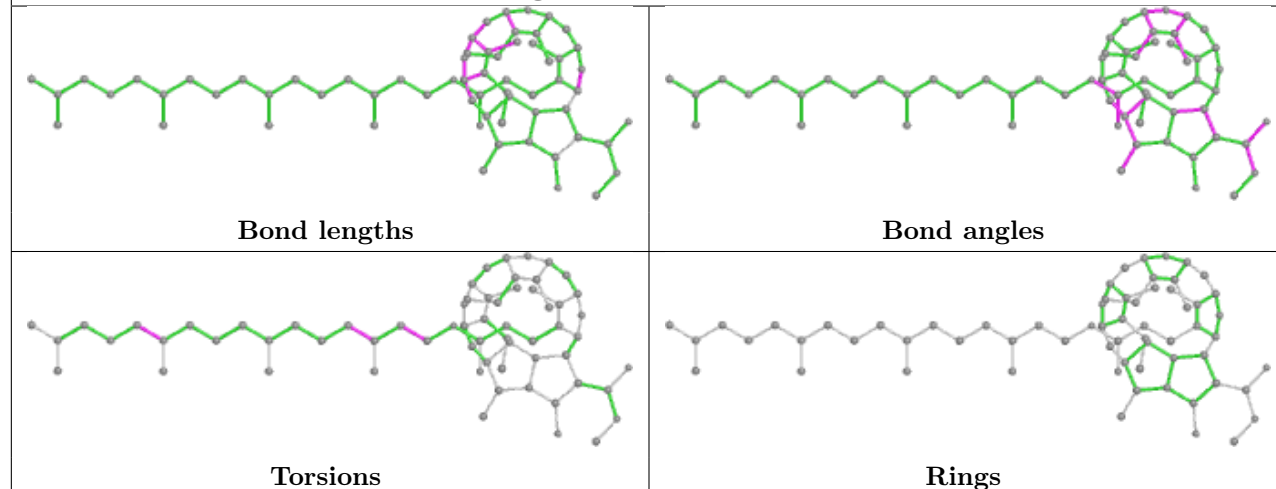
Ligand LMG c 521



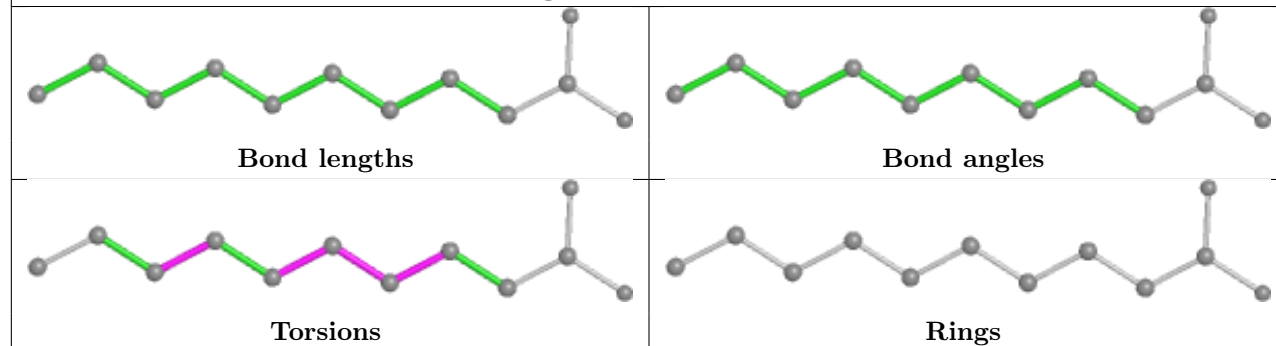
Ligand CLA B 610



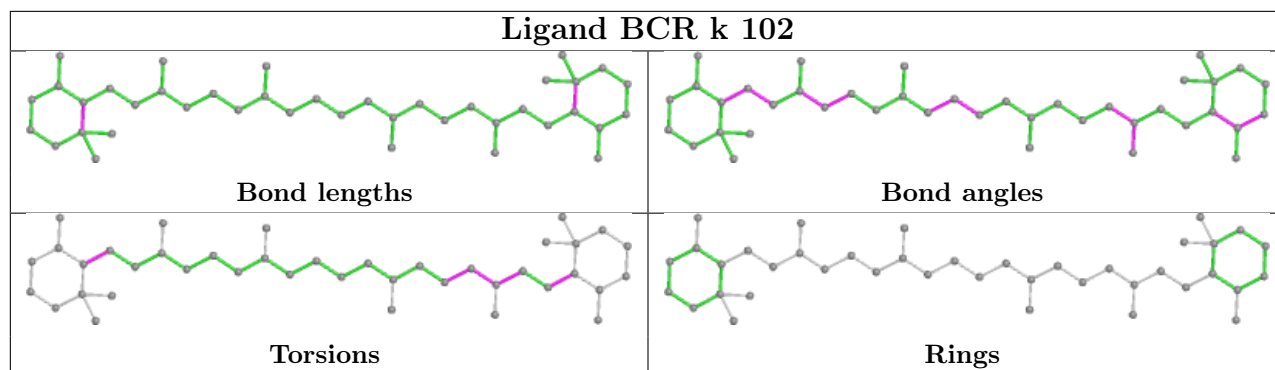
Ligand PHO A 404



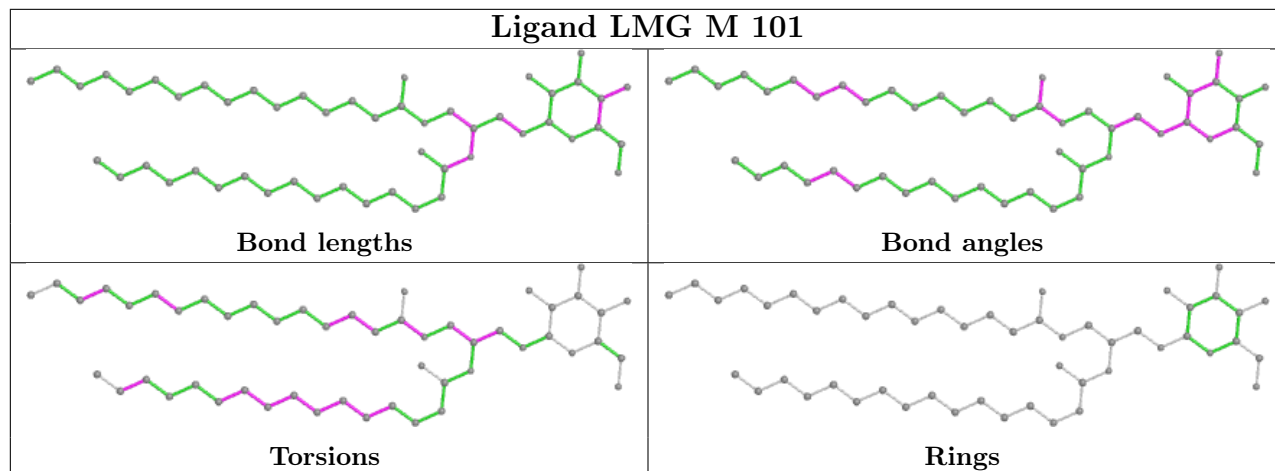
Ligand STE a 414



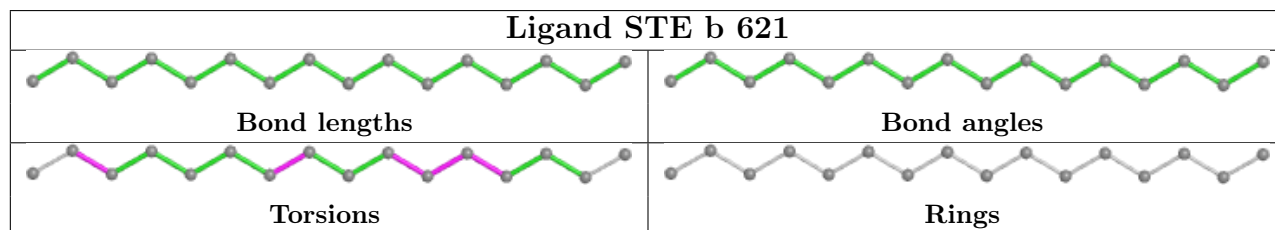
Ligand BCR k 102



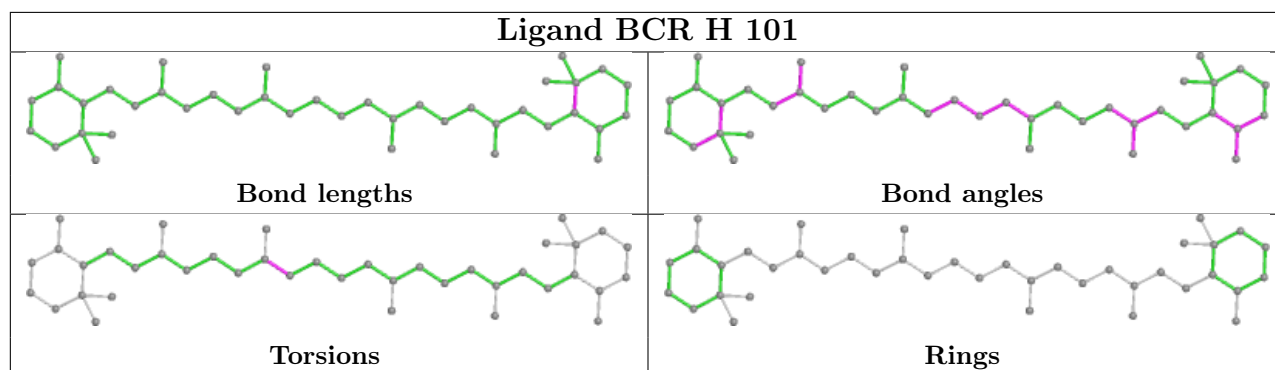
Ligand LMG M 101



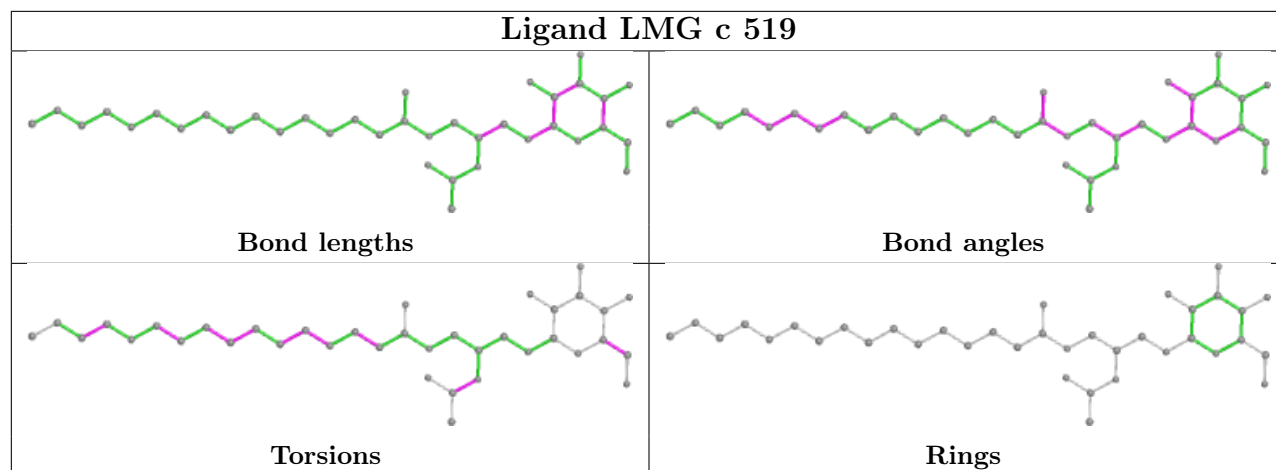
Ligand STE b 621



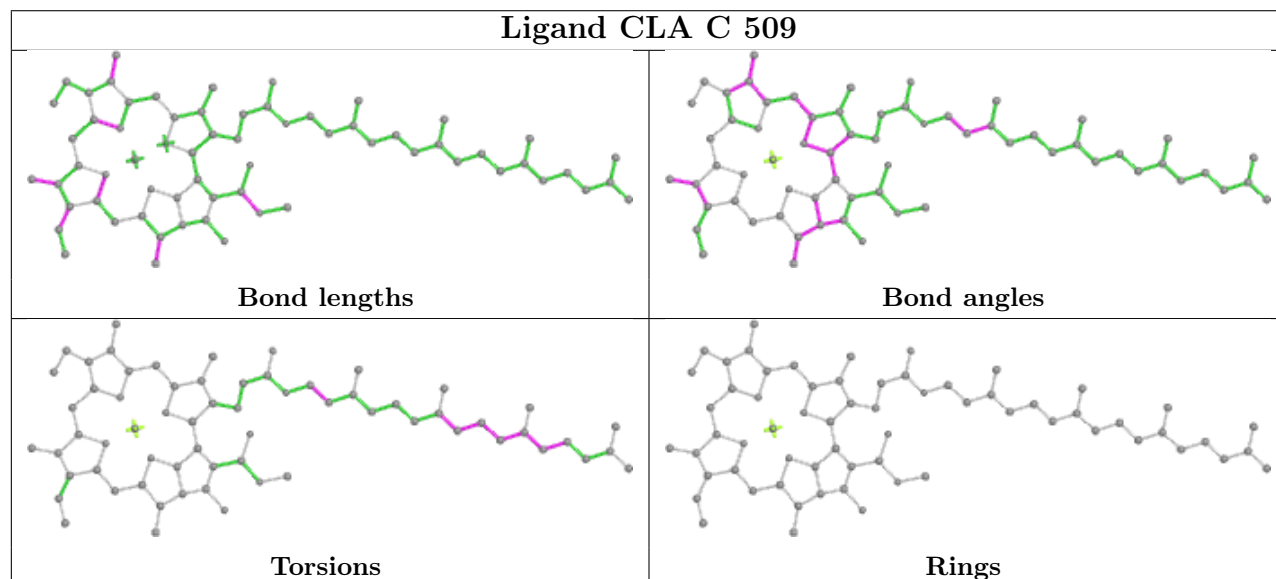
Ligand BCR H 101



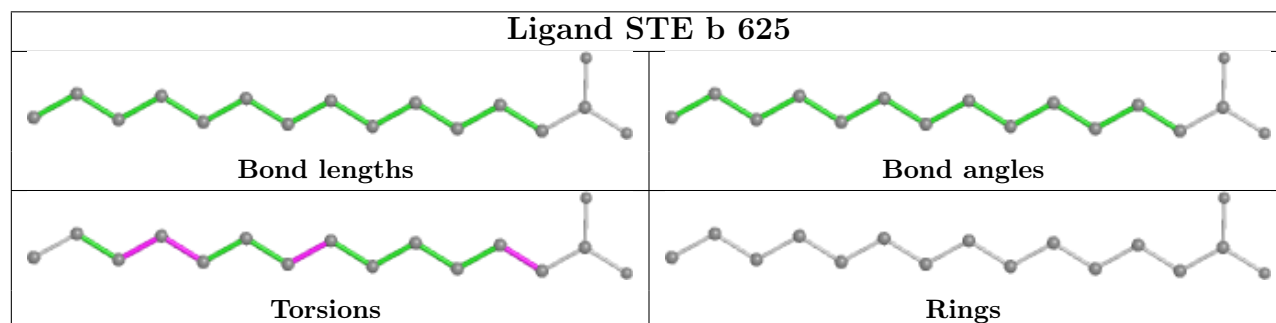
Ligand LMG c 519



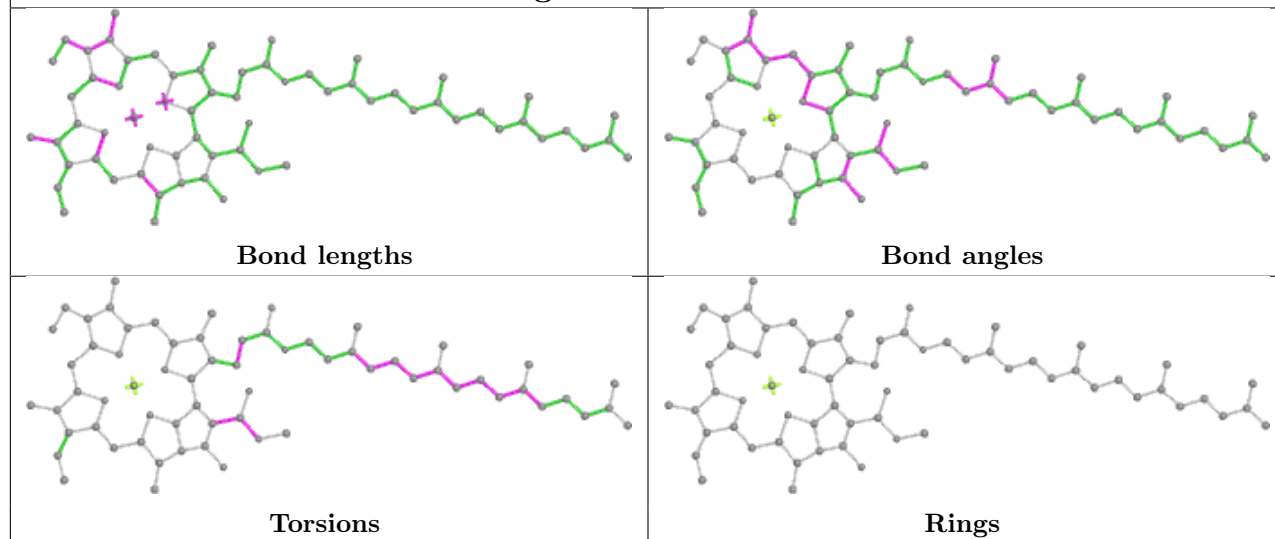
Ligand CLA C 509



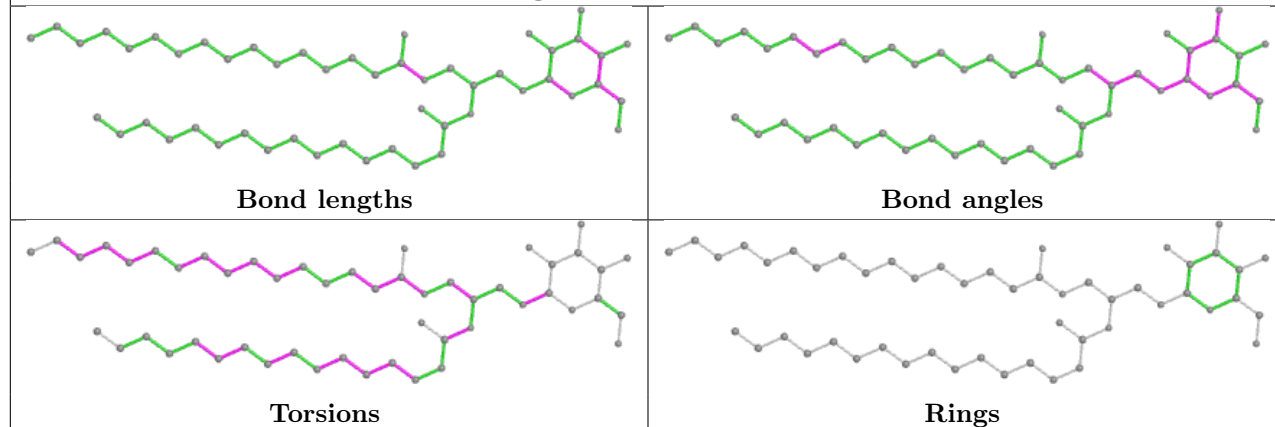
Ligand STE b 625



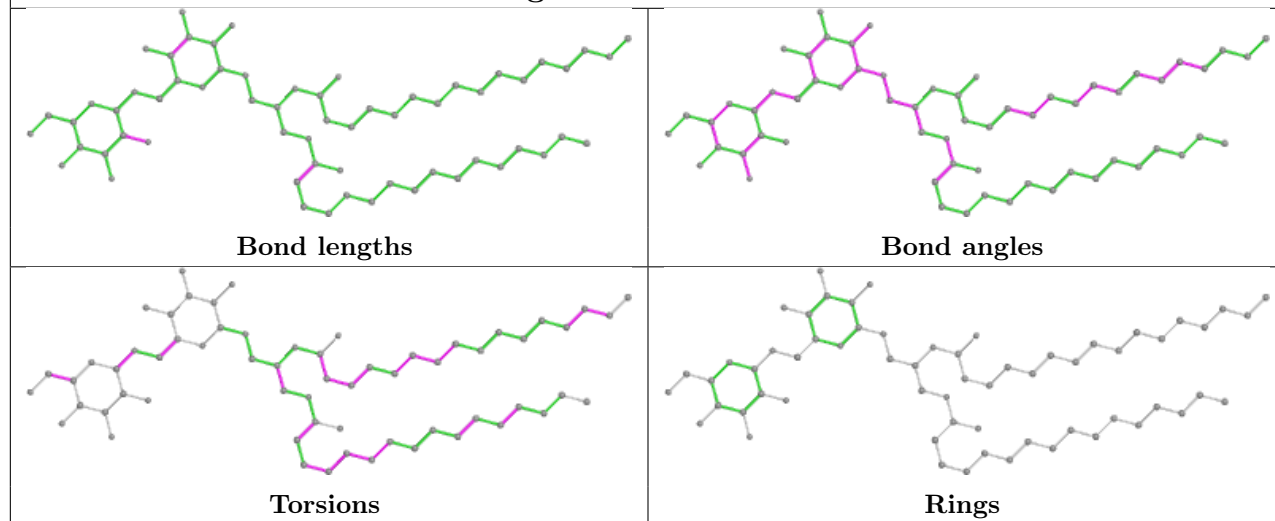
Ligand CLA b 614

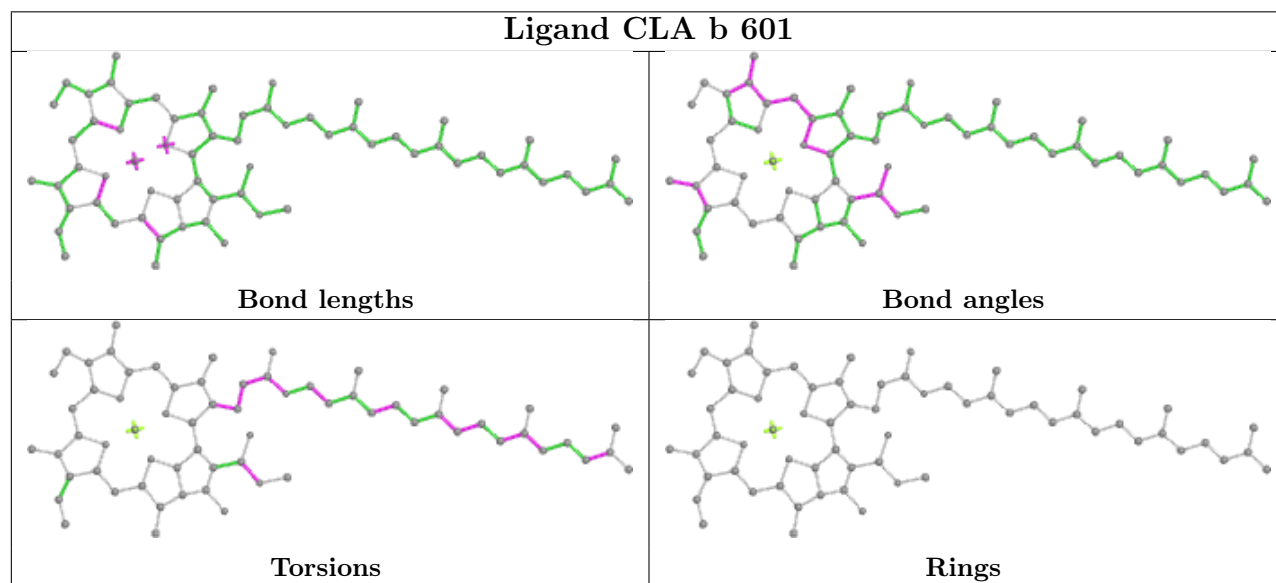
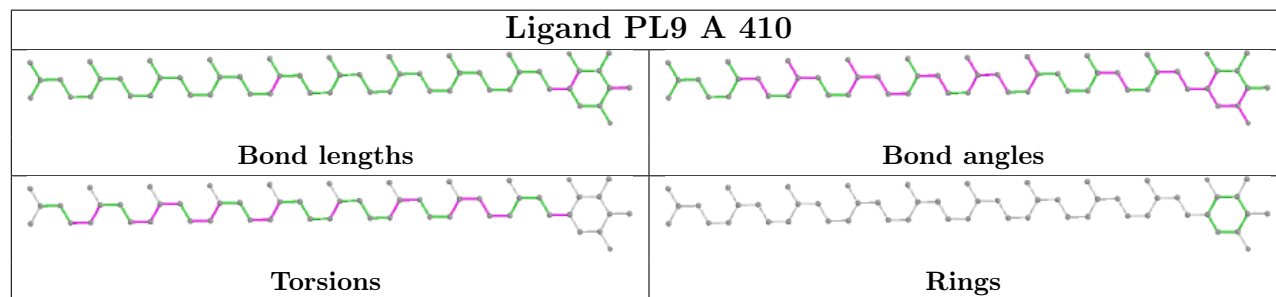
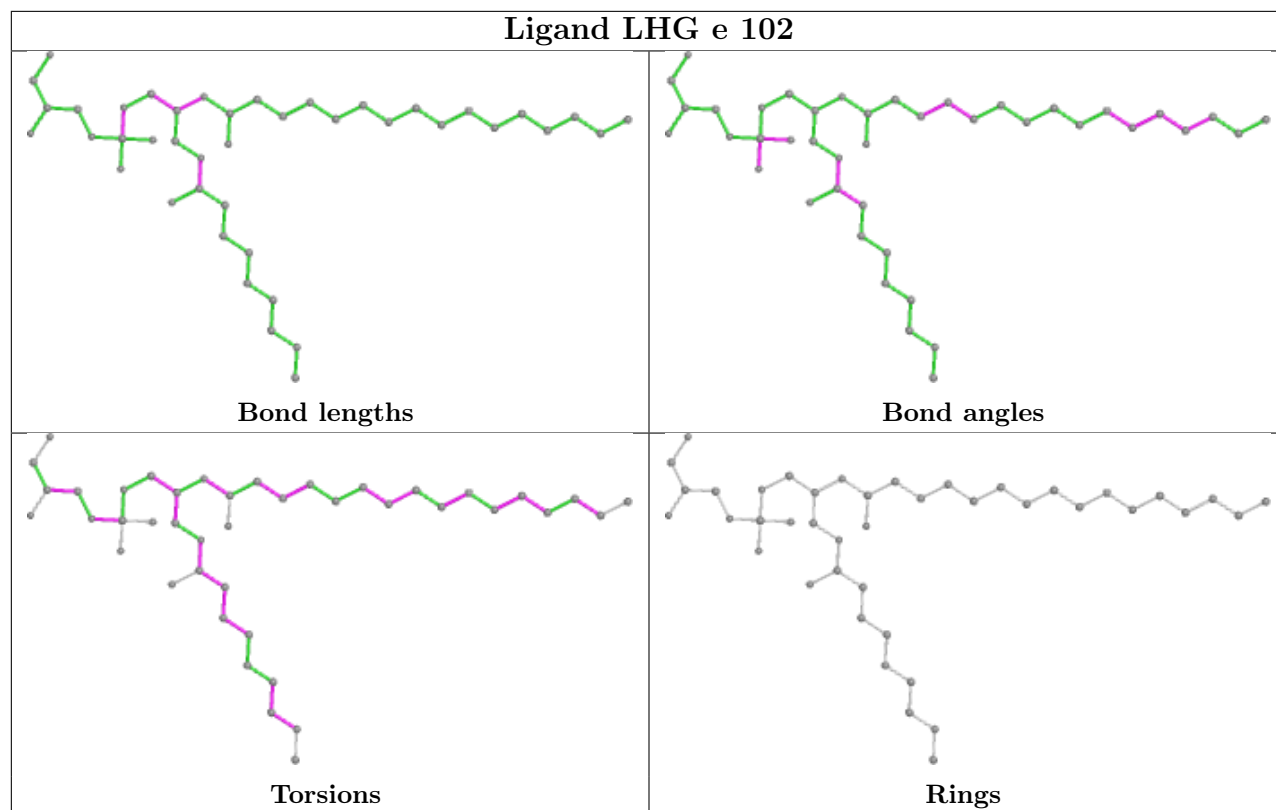


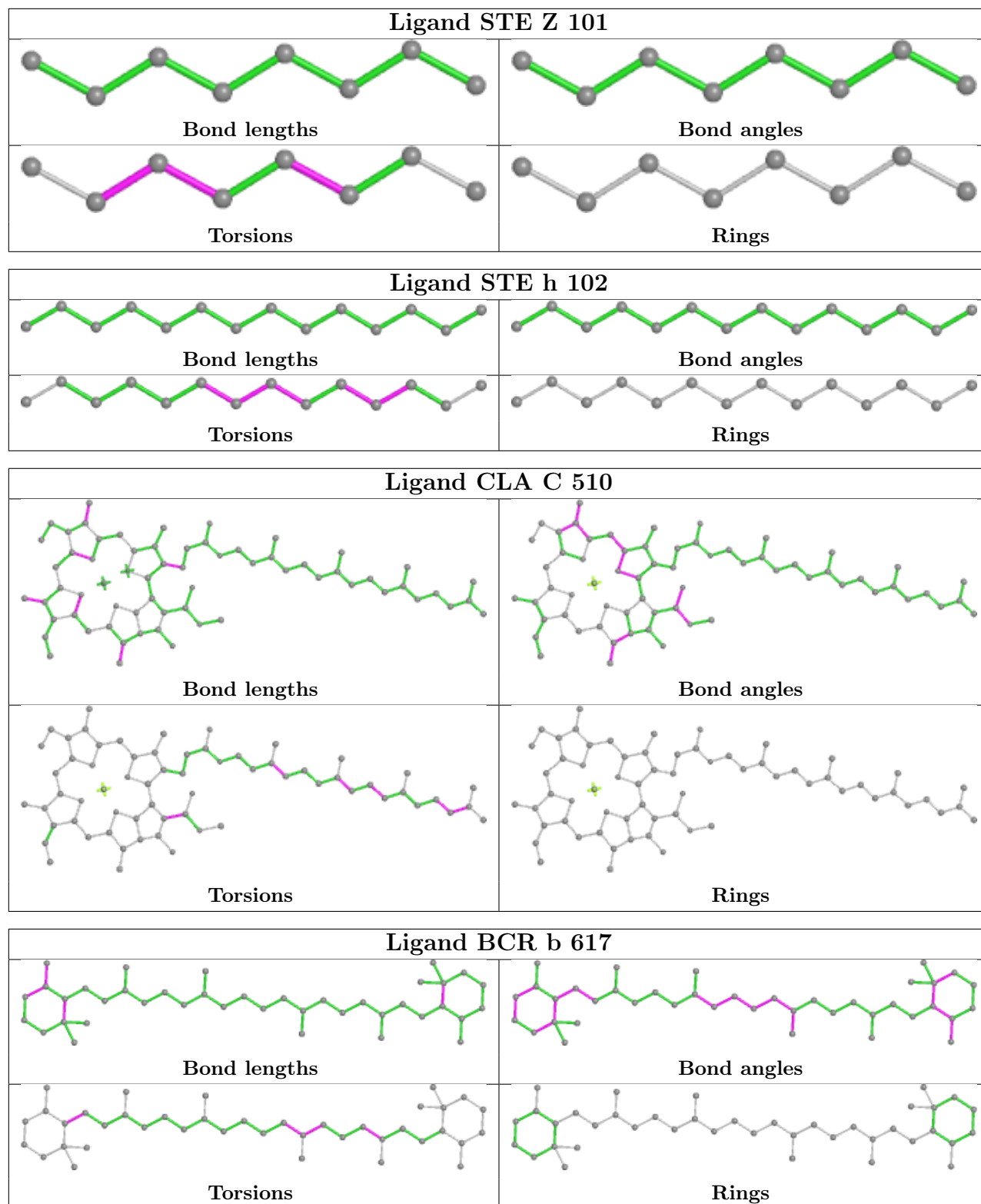
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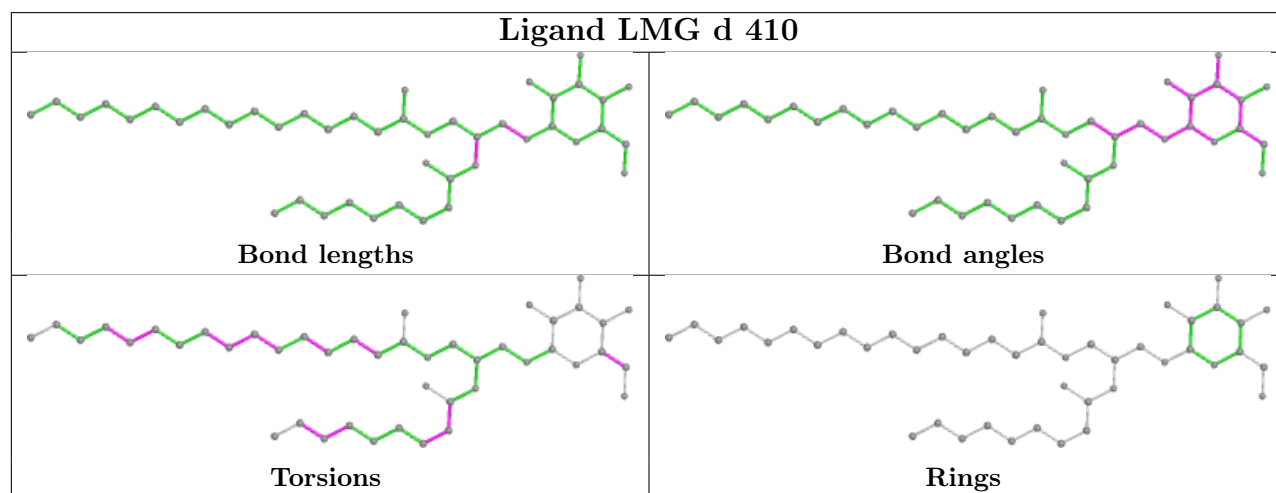
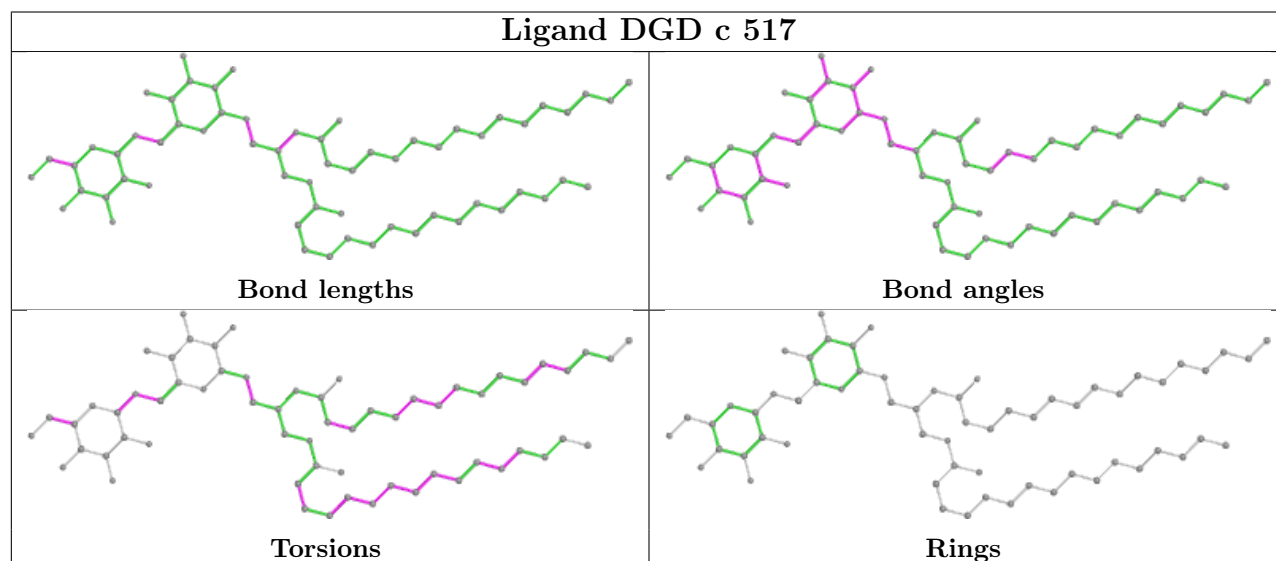
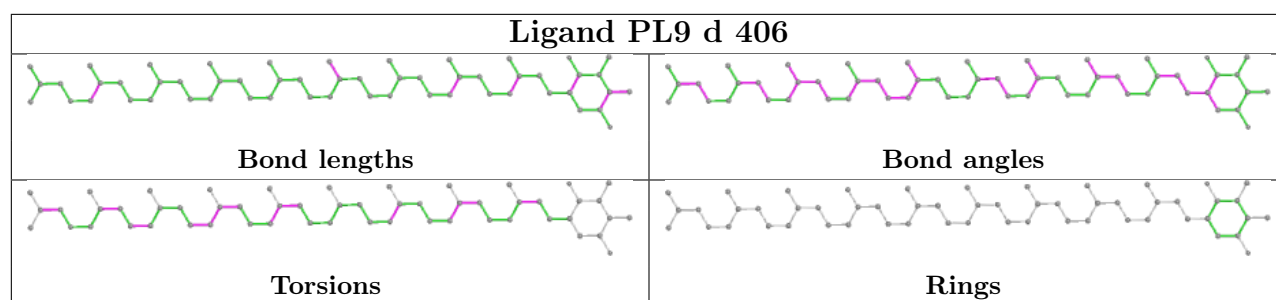


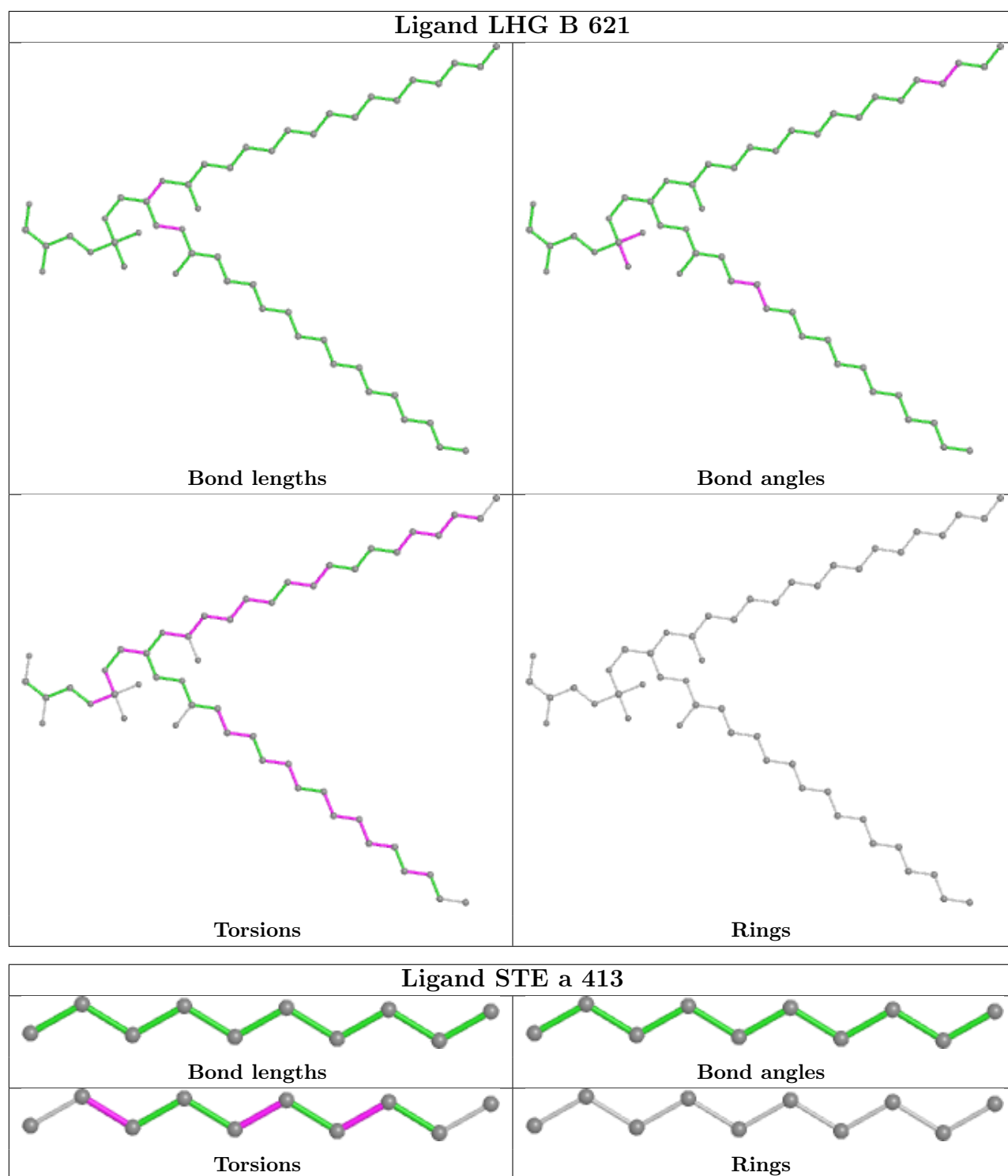
Ligand DGD C 515

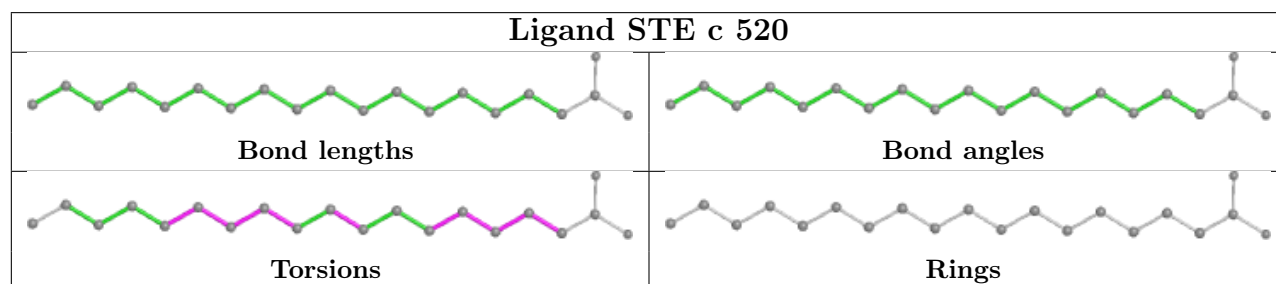
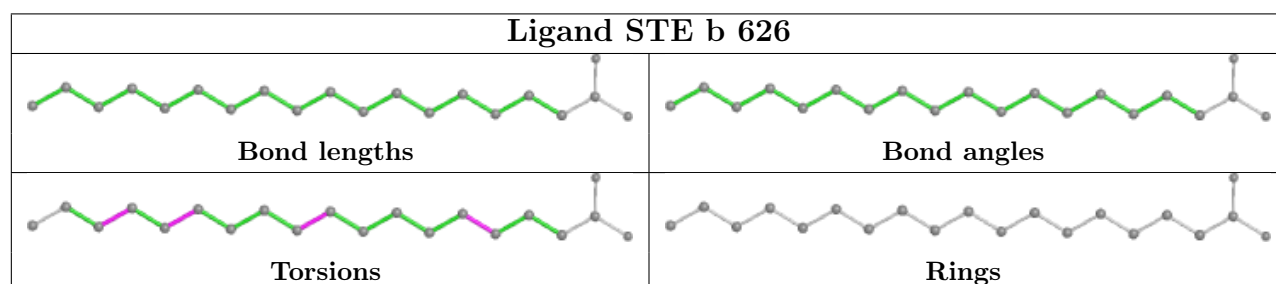
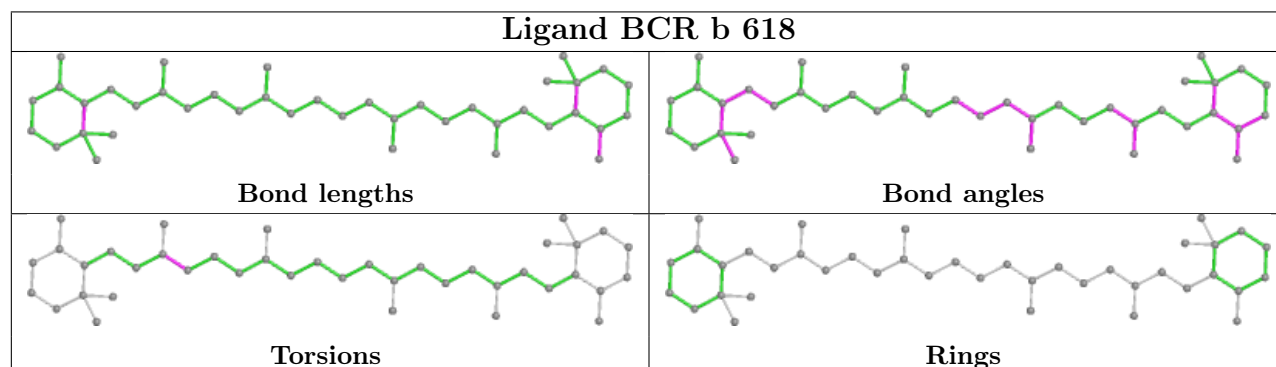
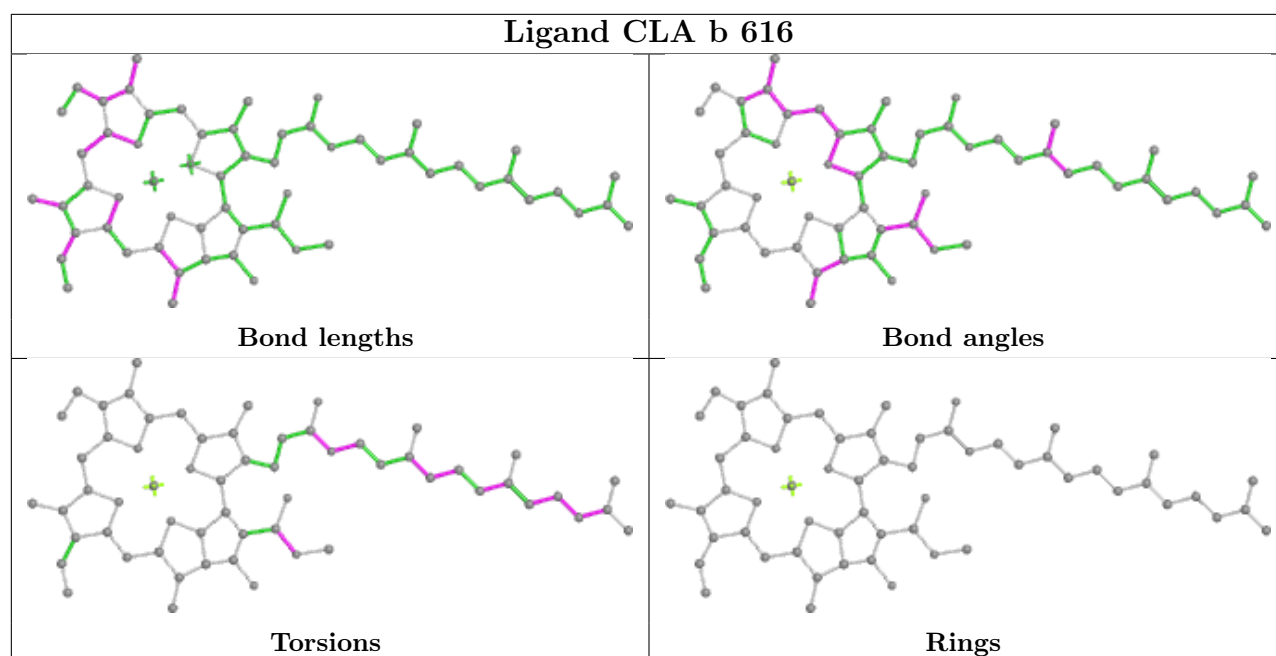




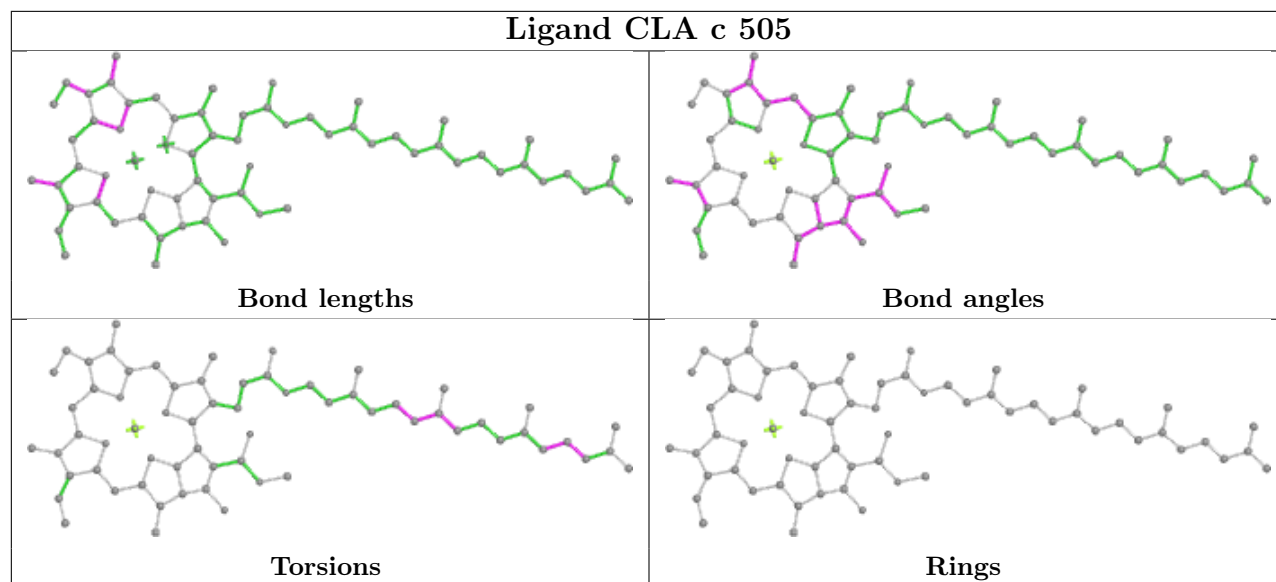




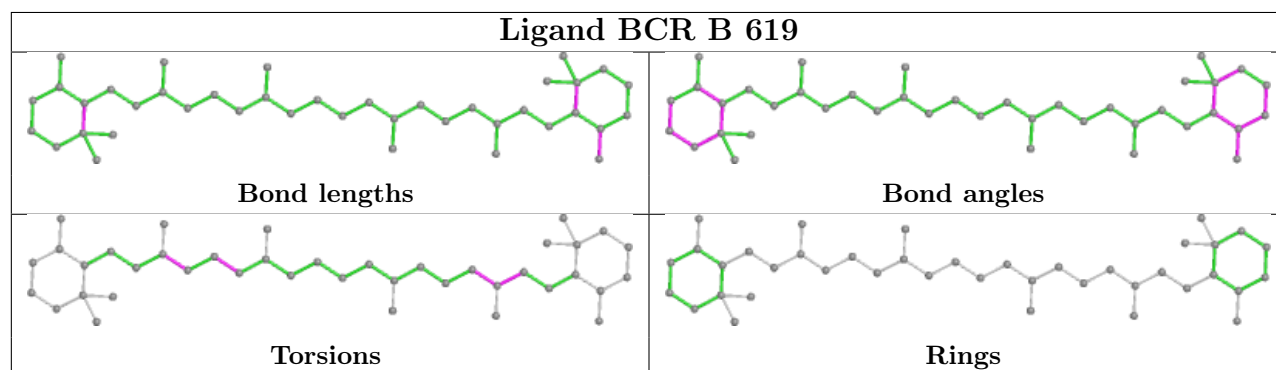




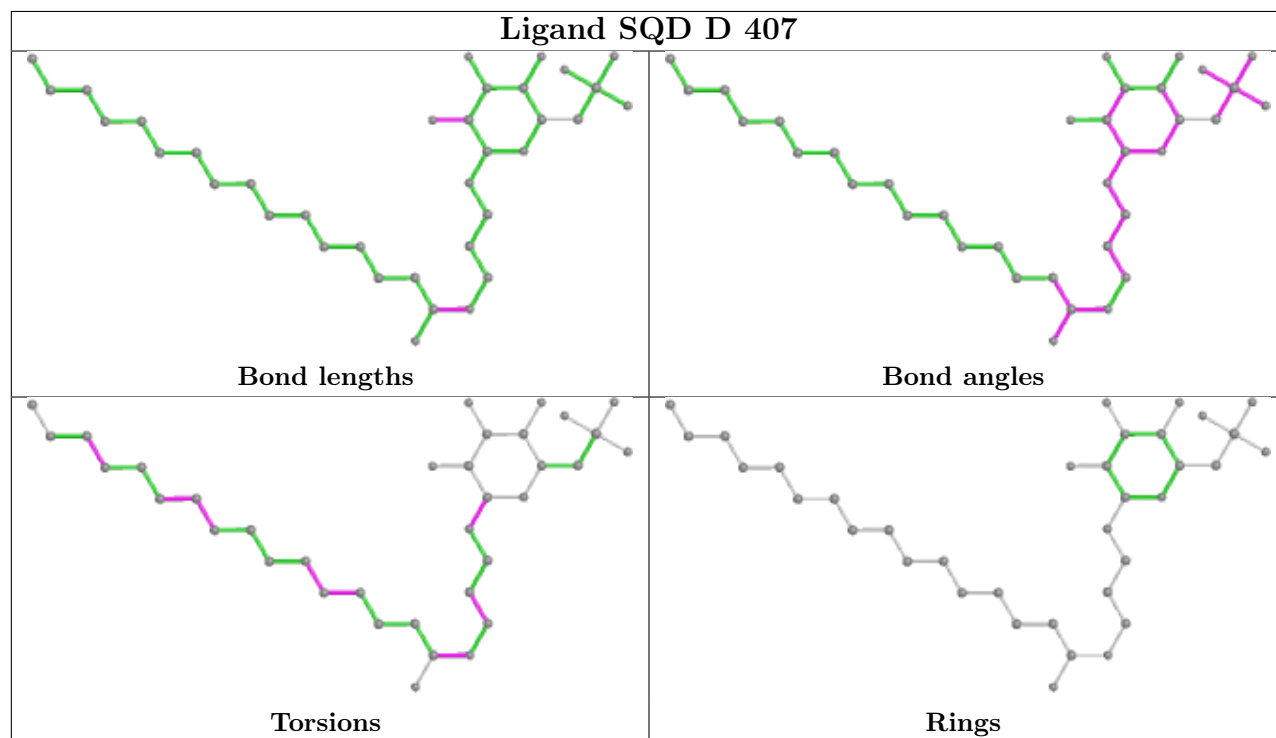
Ligand CLA c 505



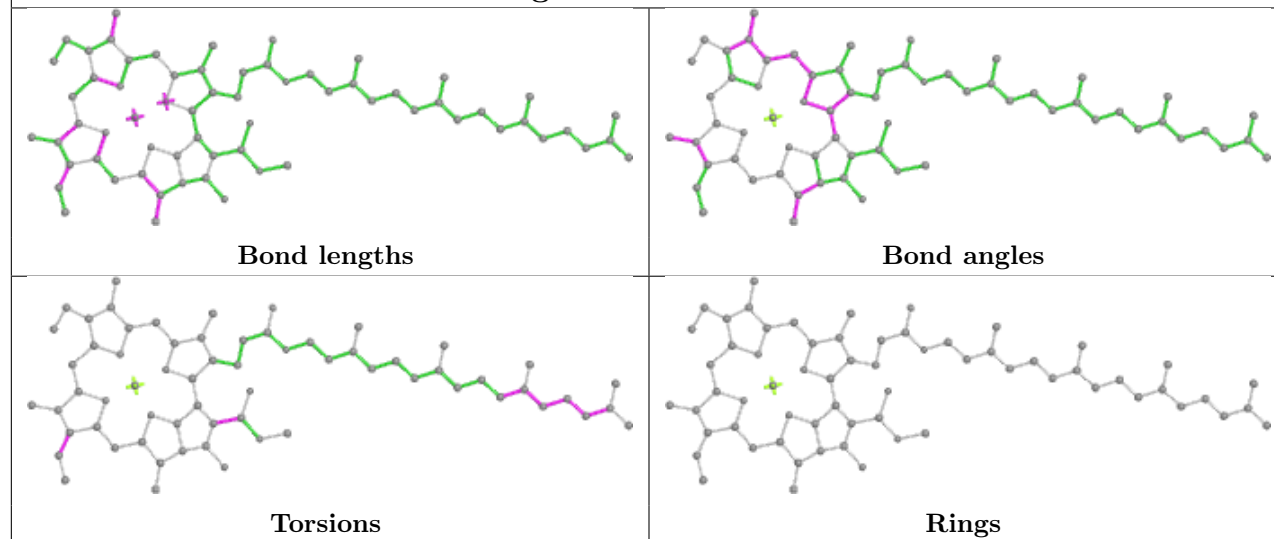
Ligand BCR B 619



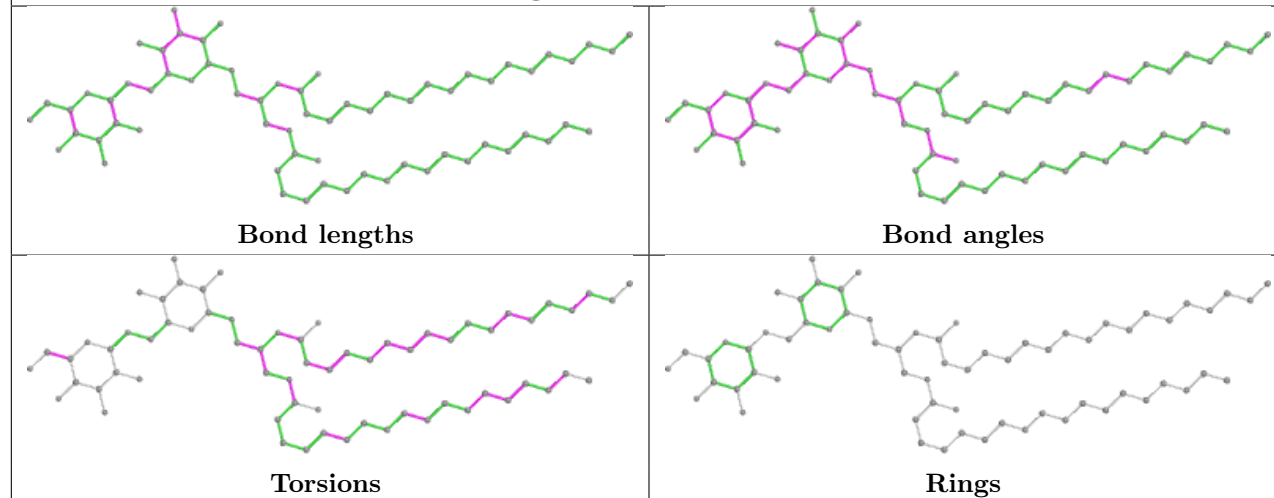
Ligand SQD D 407



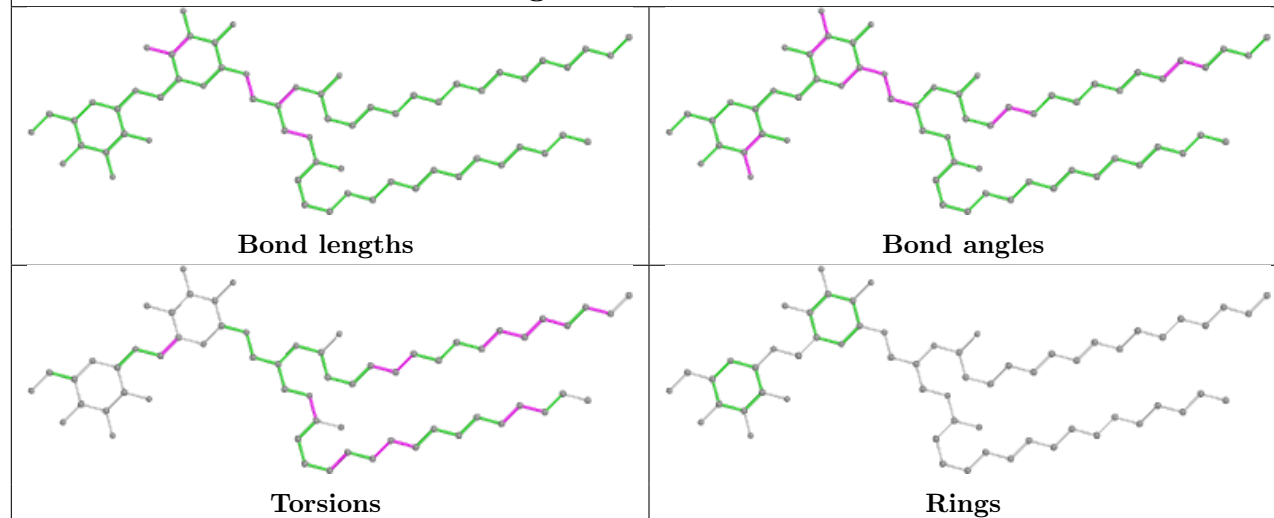
Ligand CLA A 411



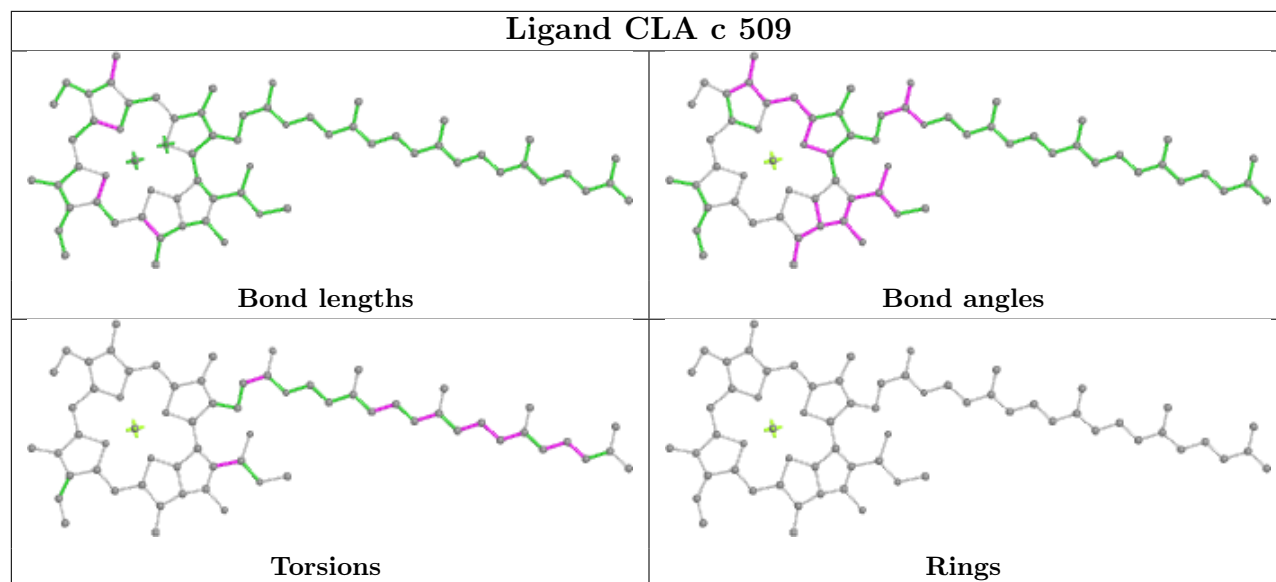
Ligand DGD A 416



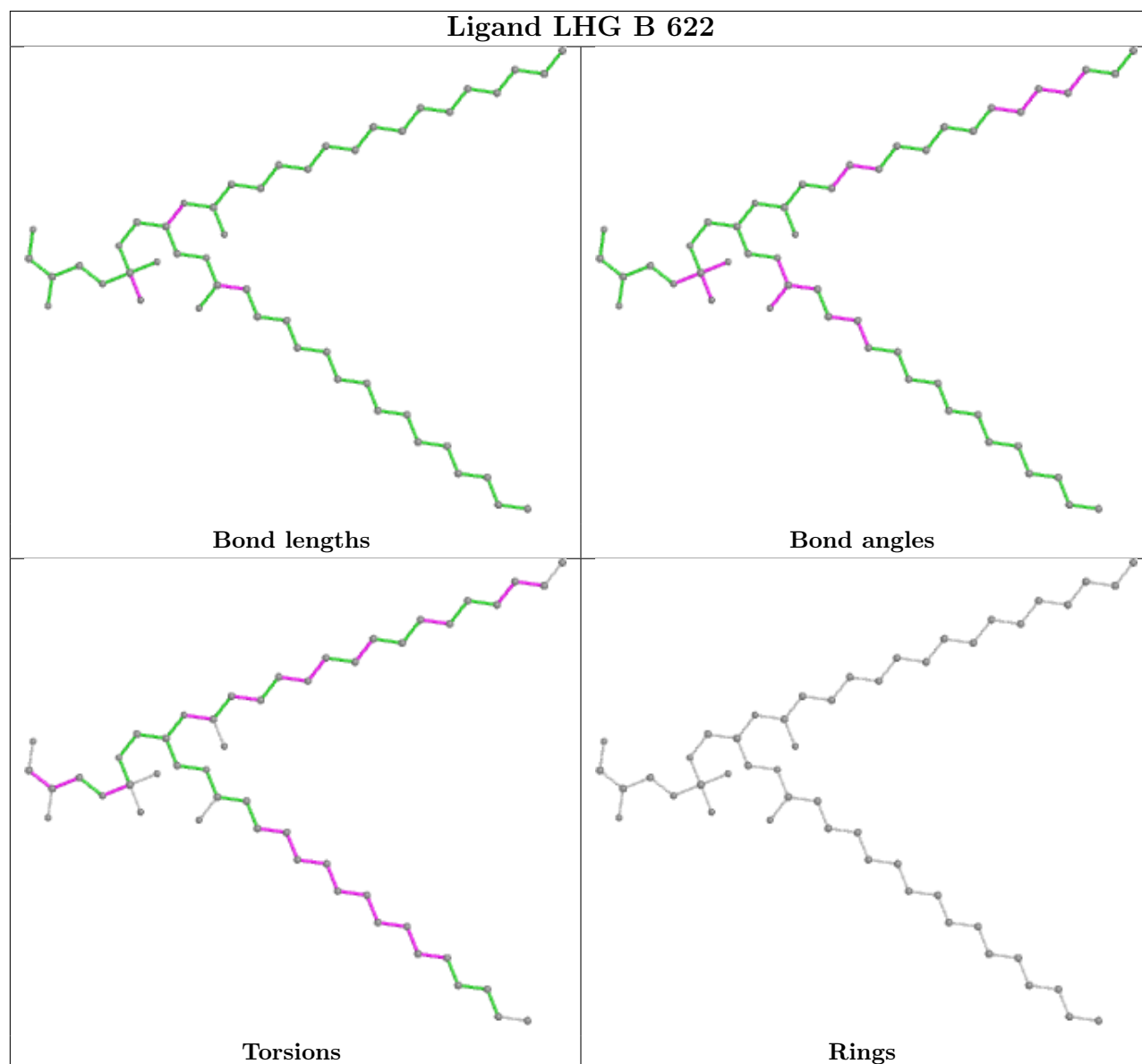
Ligand DGD C 517



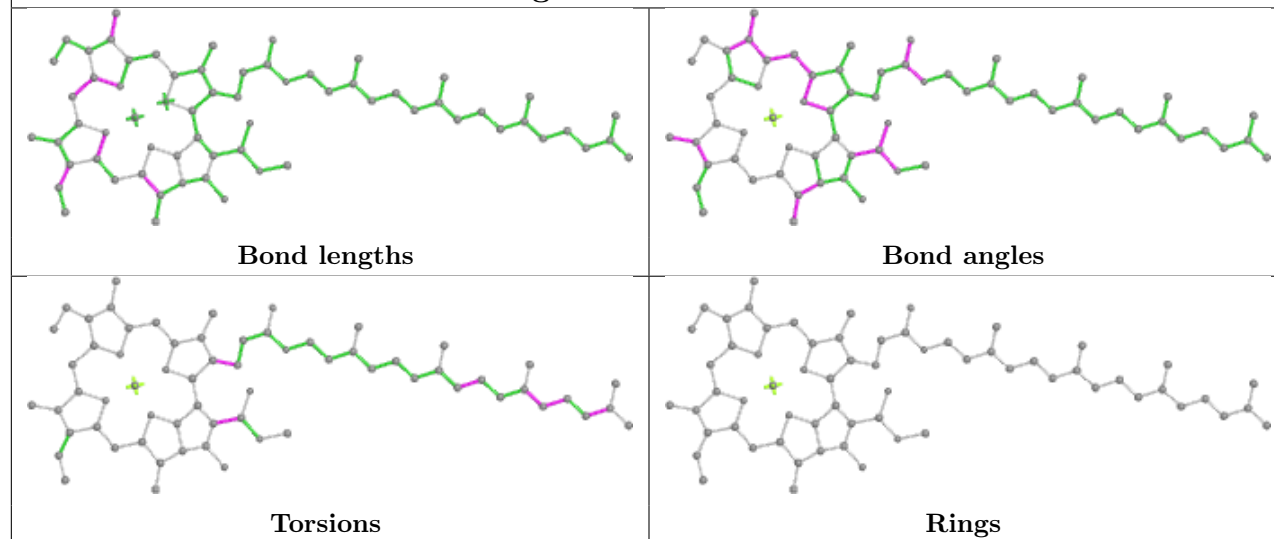
Ligand CLA c 509



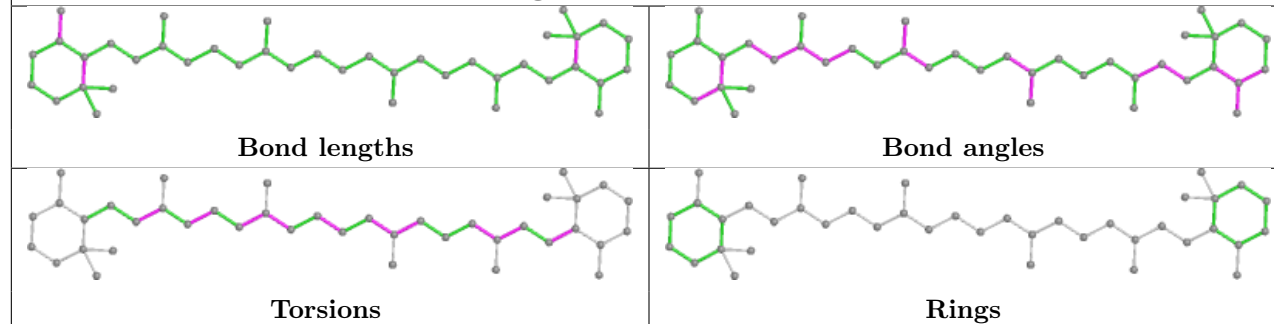
Ligand LHG B 622



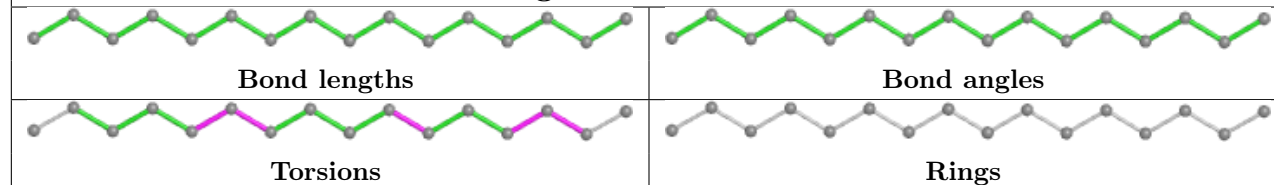
Ligand CLA B 602



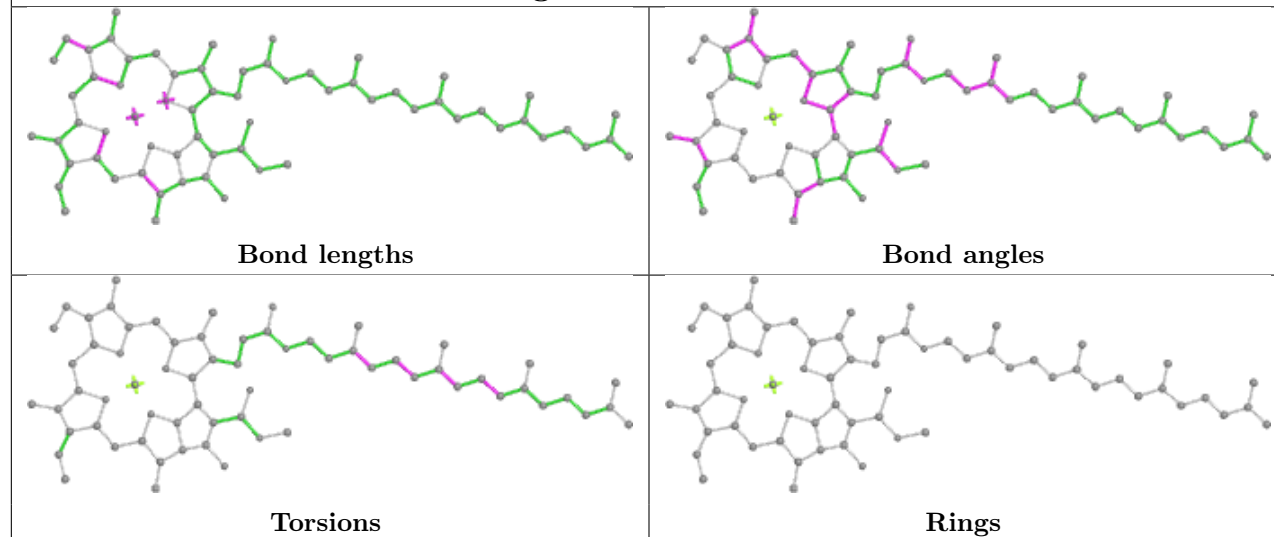
Ligand BCR K 101

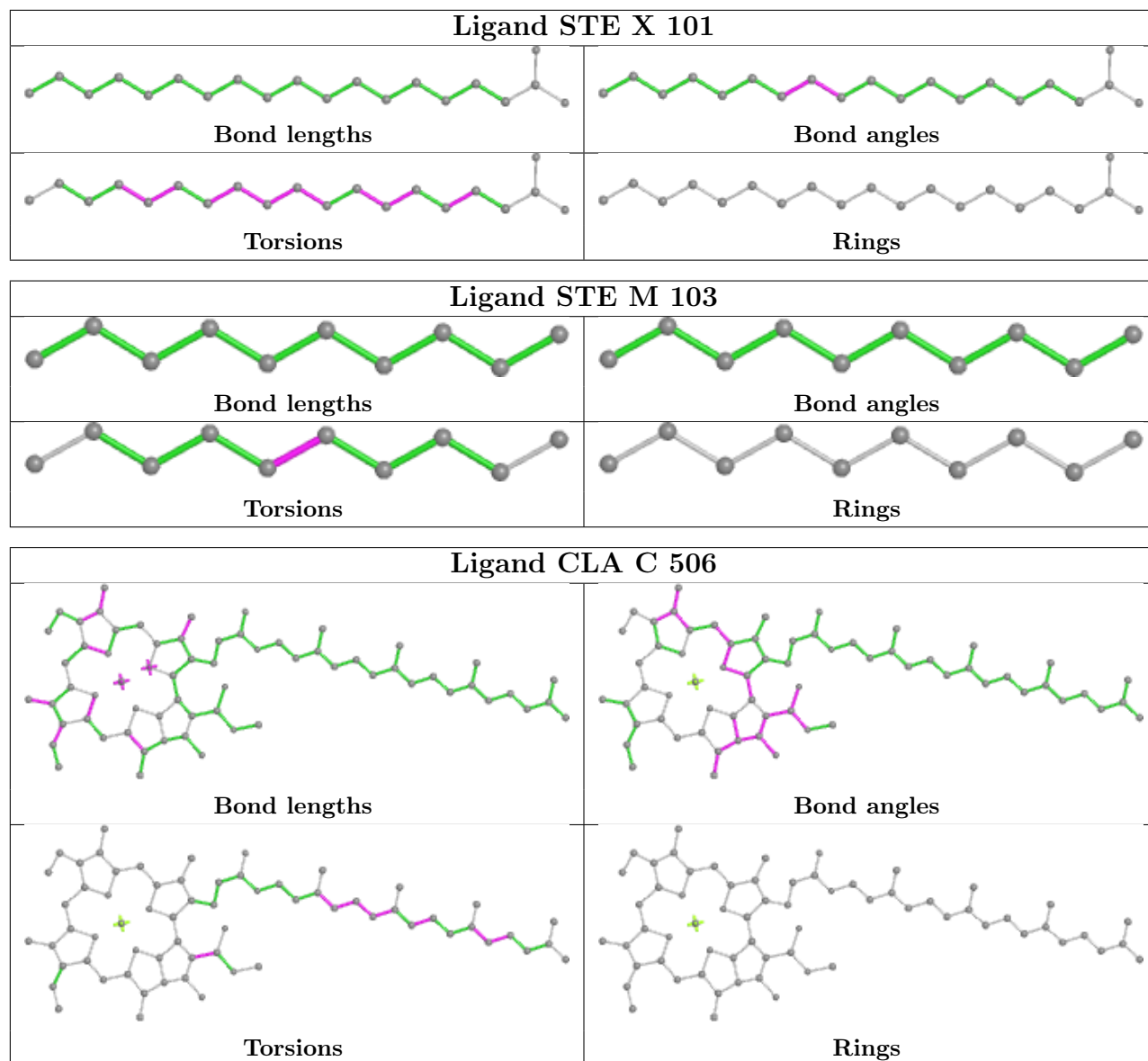


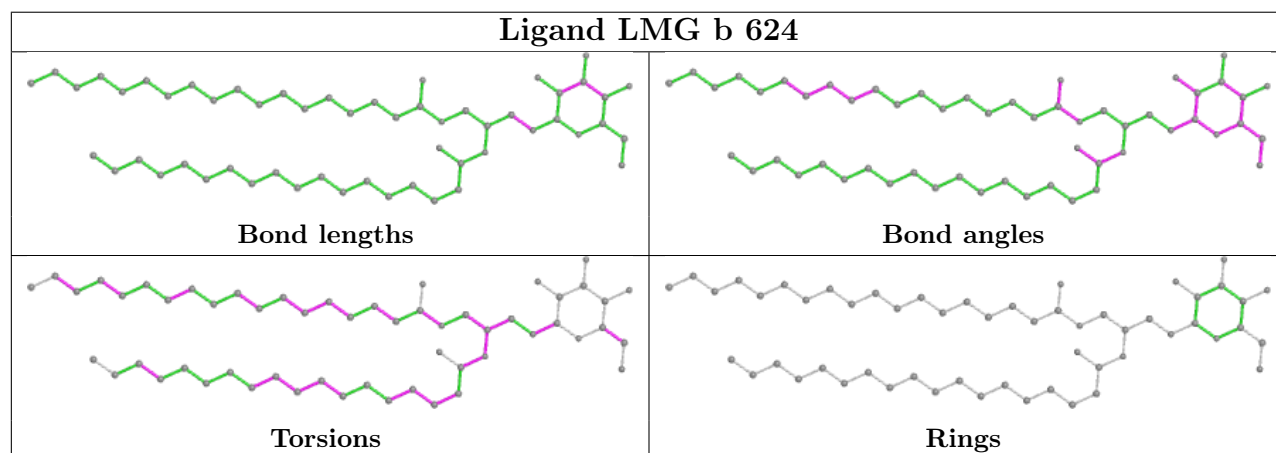
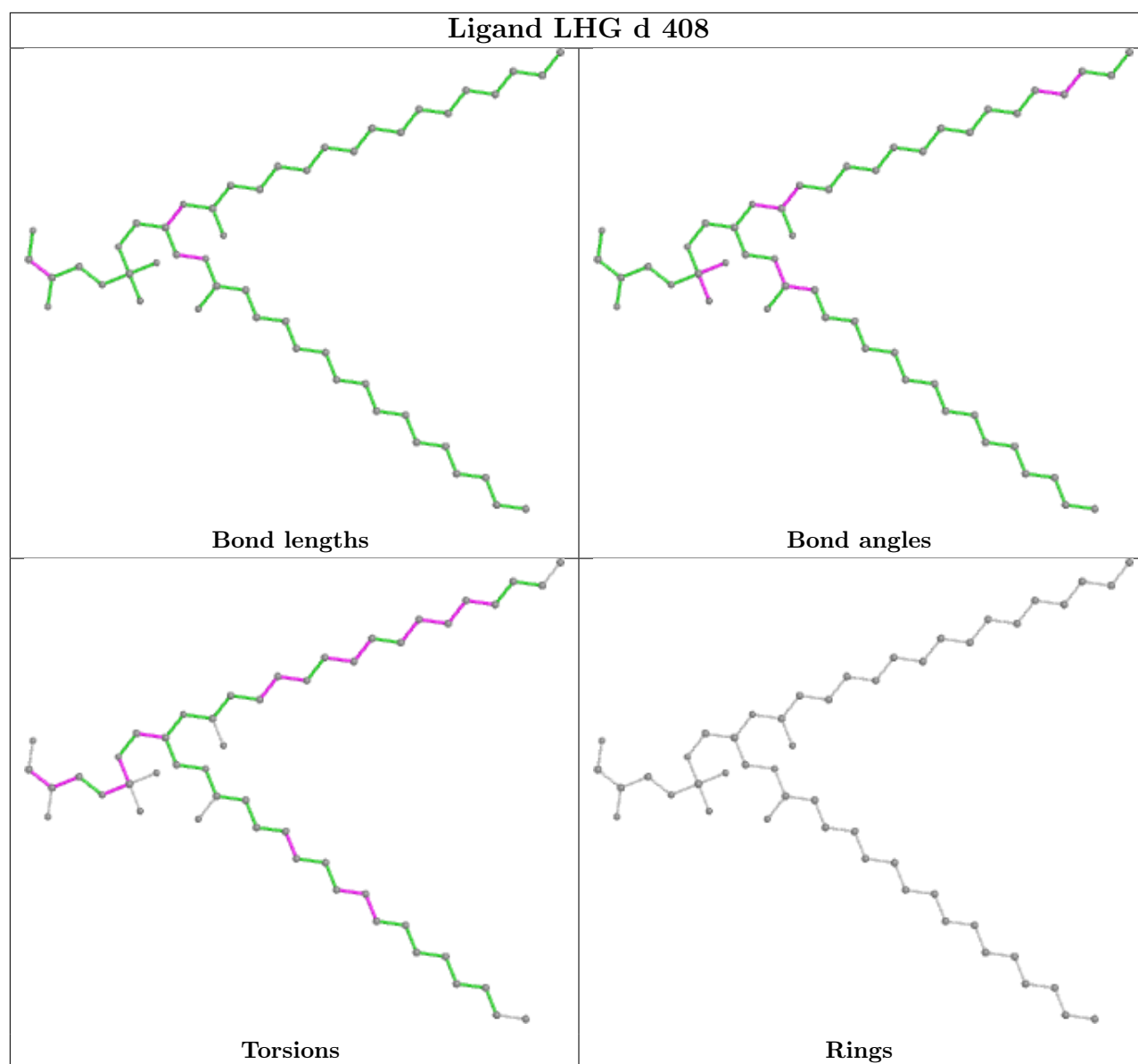
Ligand STE C 520



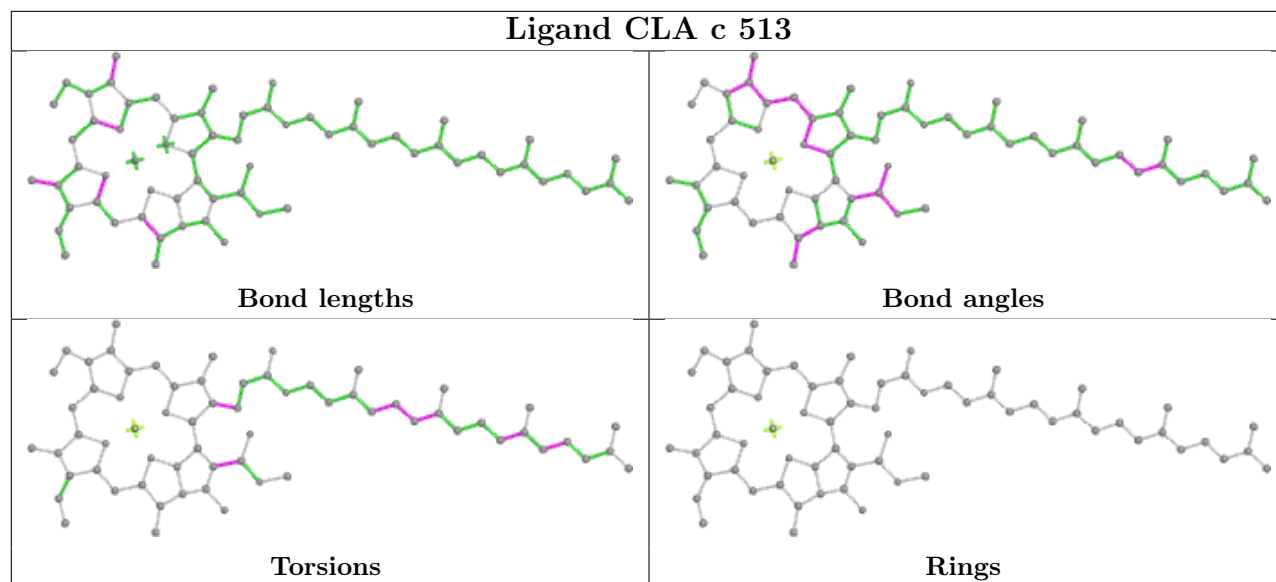
Ligand CLA C 507



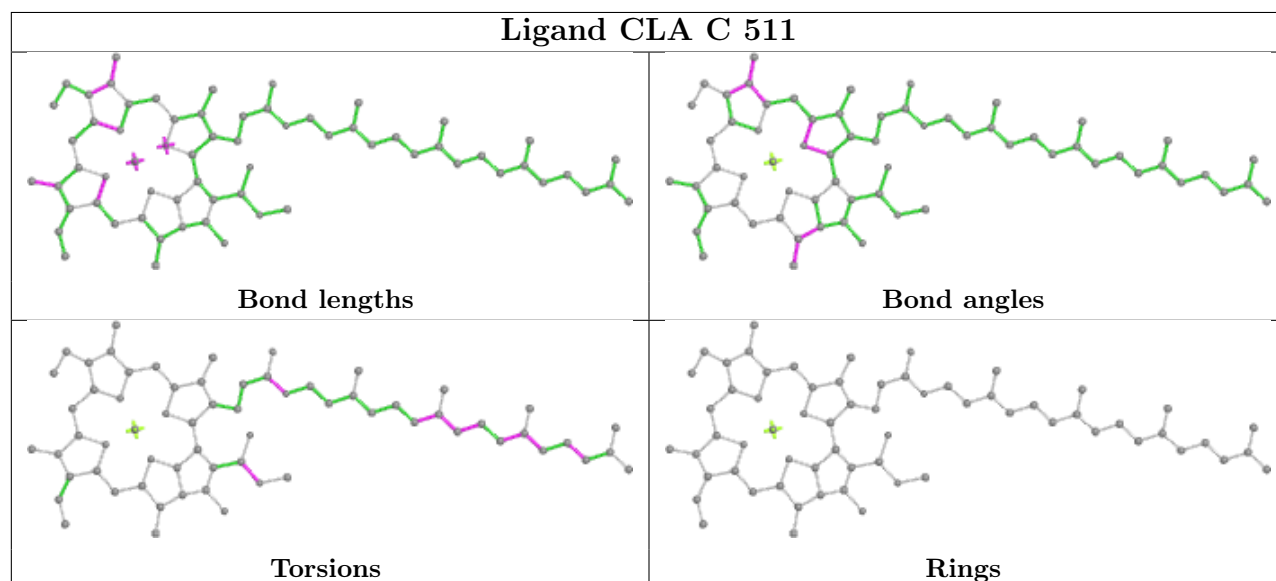




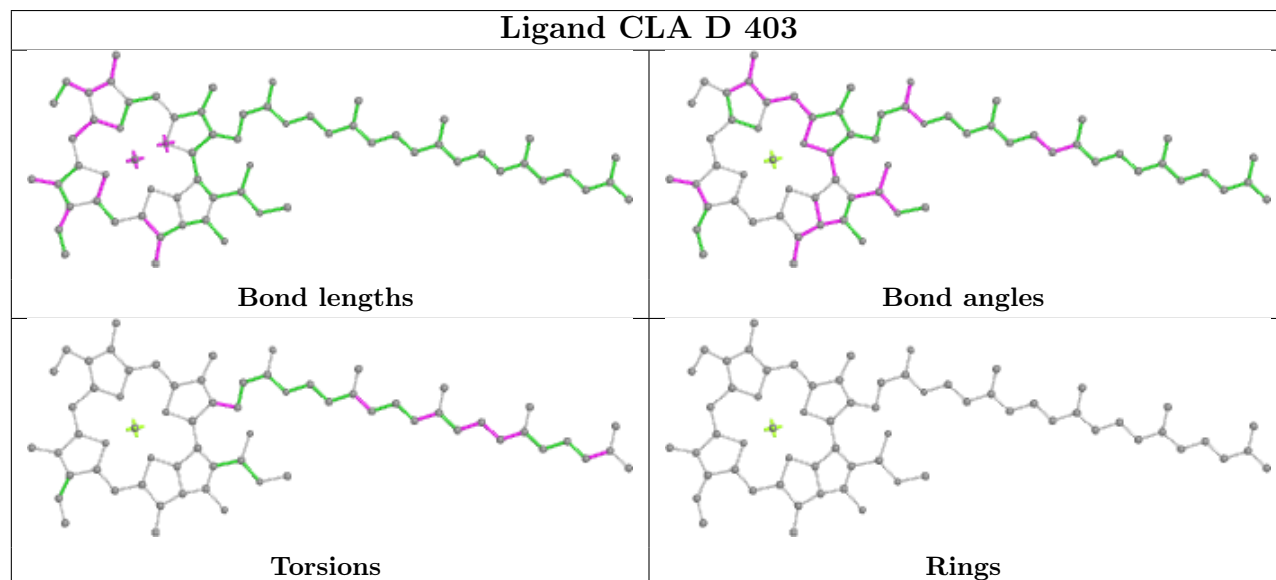
Ligand CLA c 513

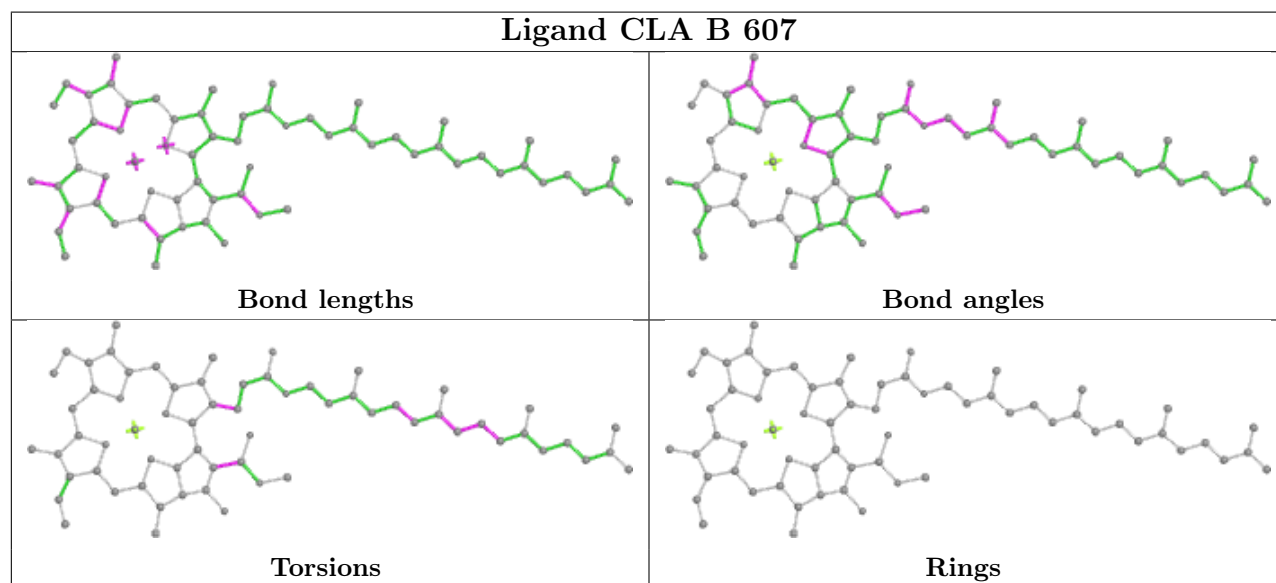
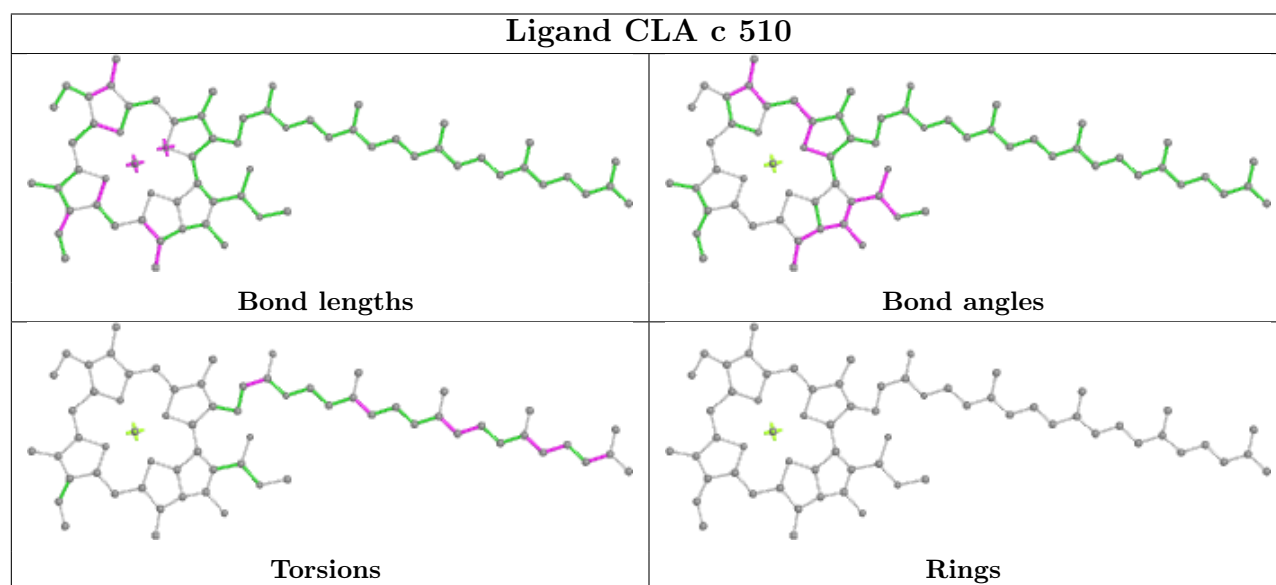
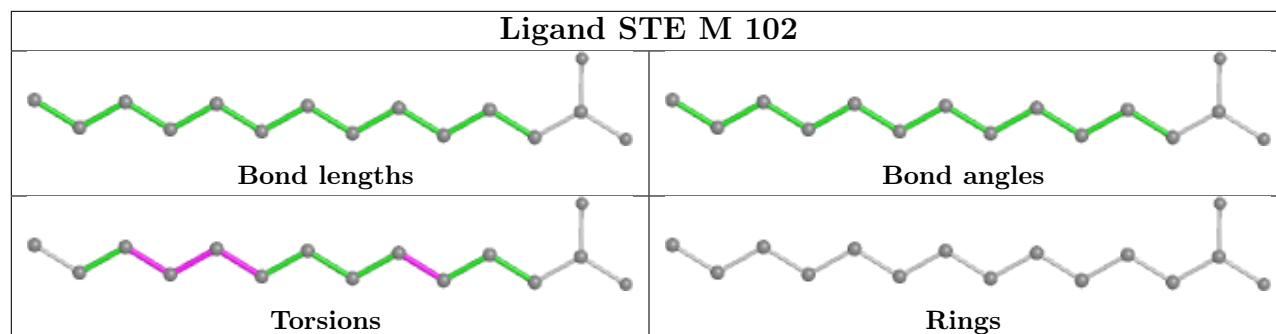


Ligand CLA C 511

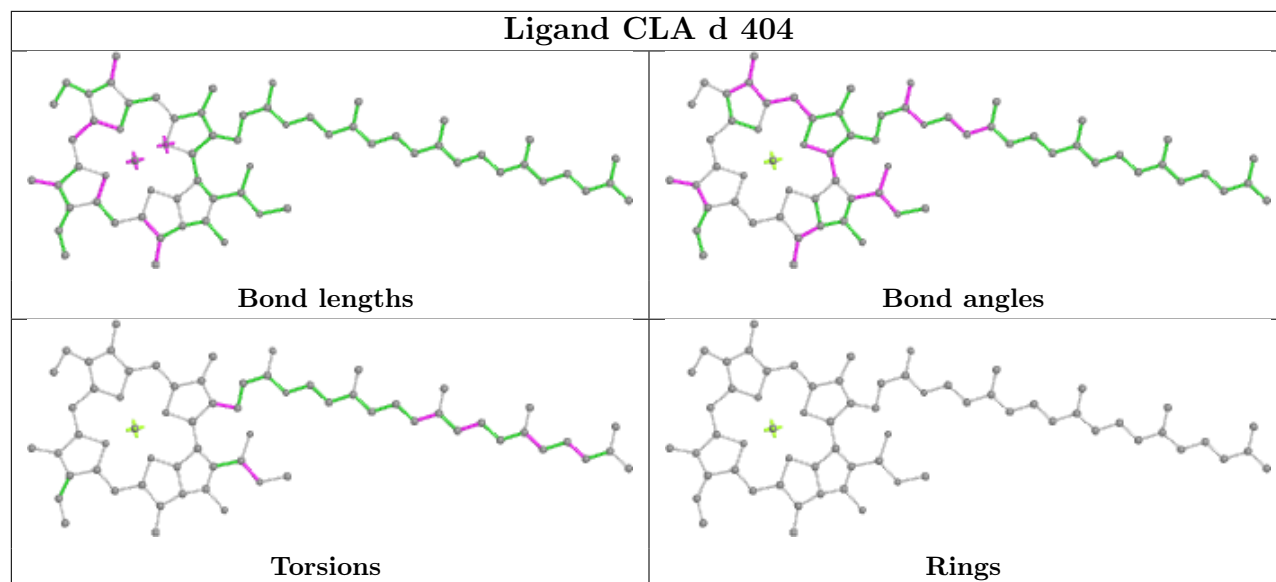


Ligand CLA D 403

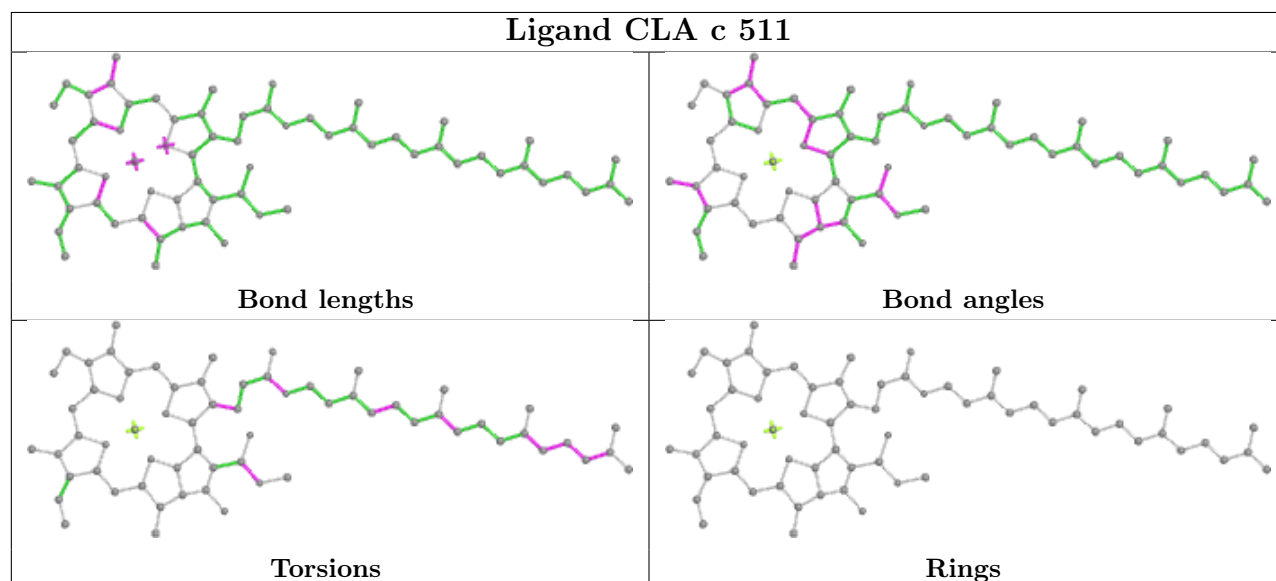




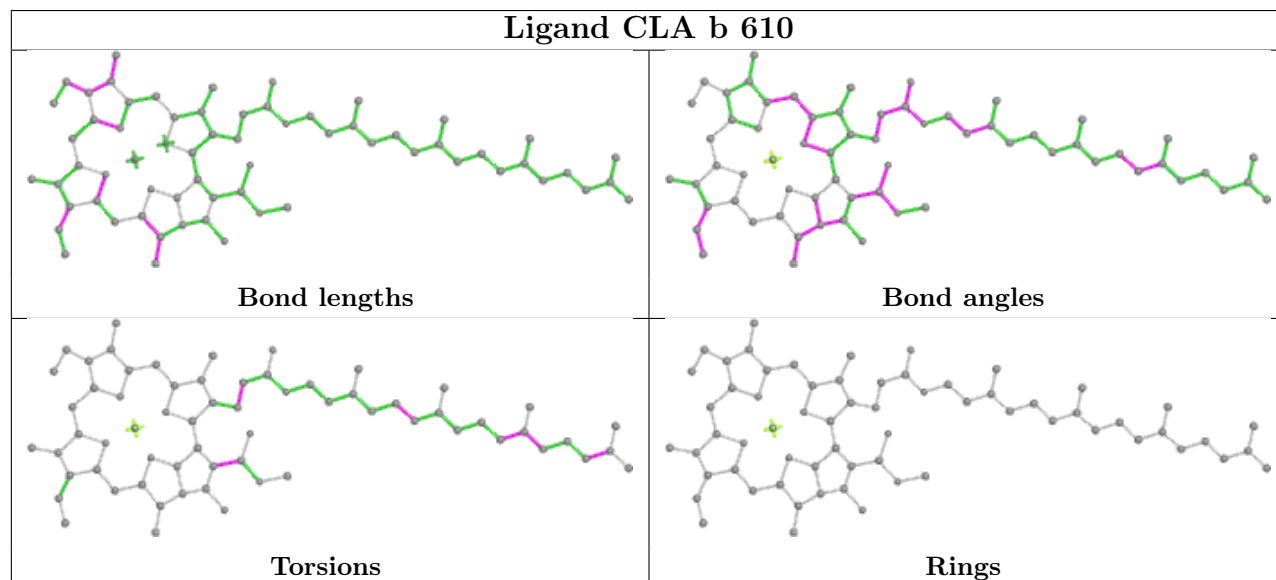
Ligand CLA d 404

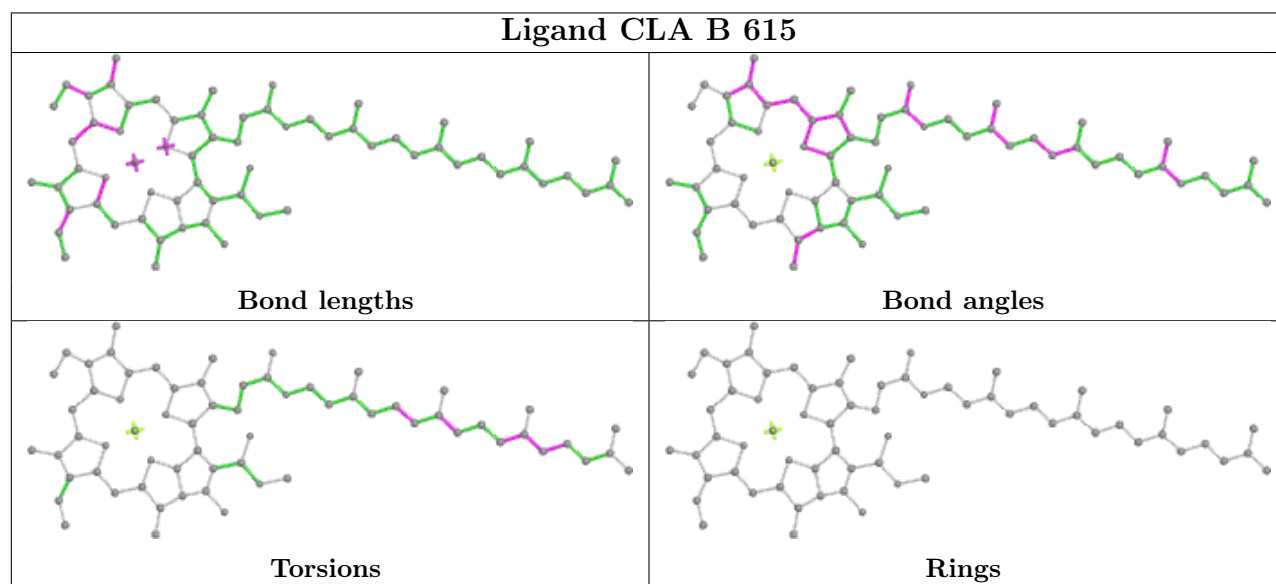
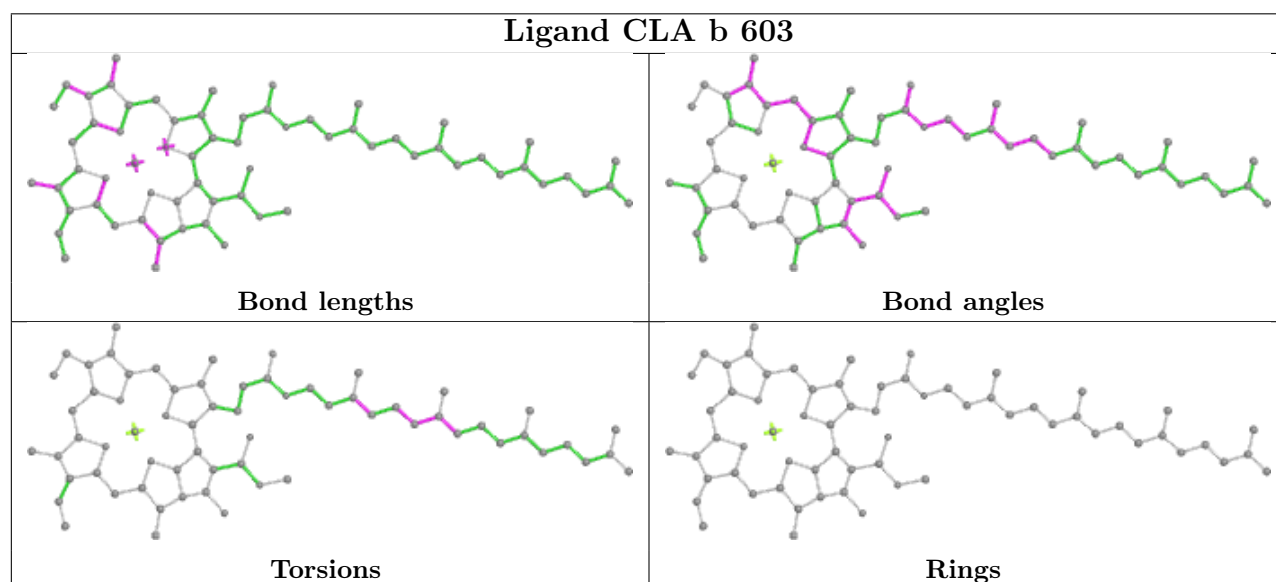
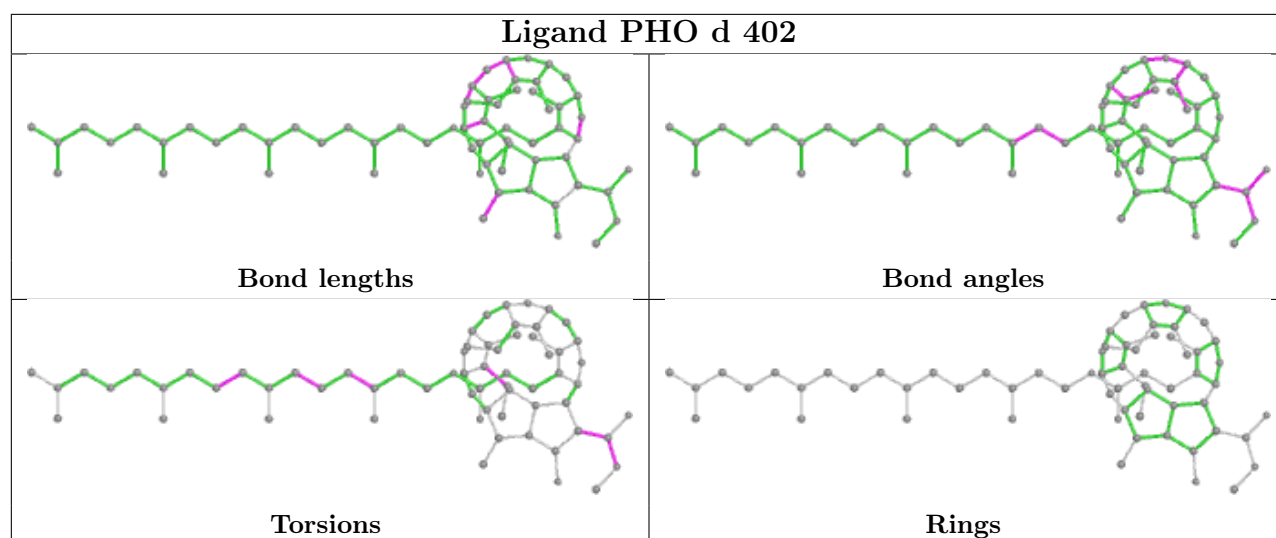


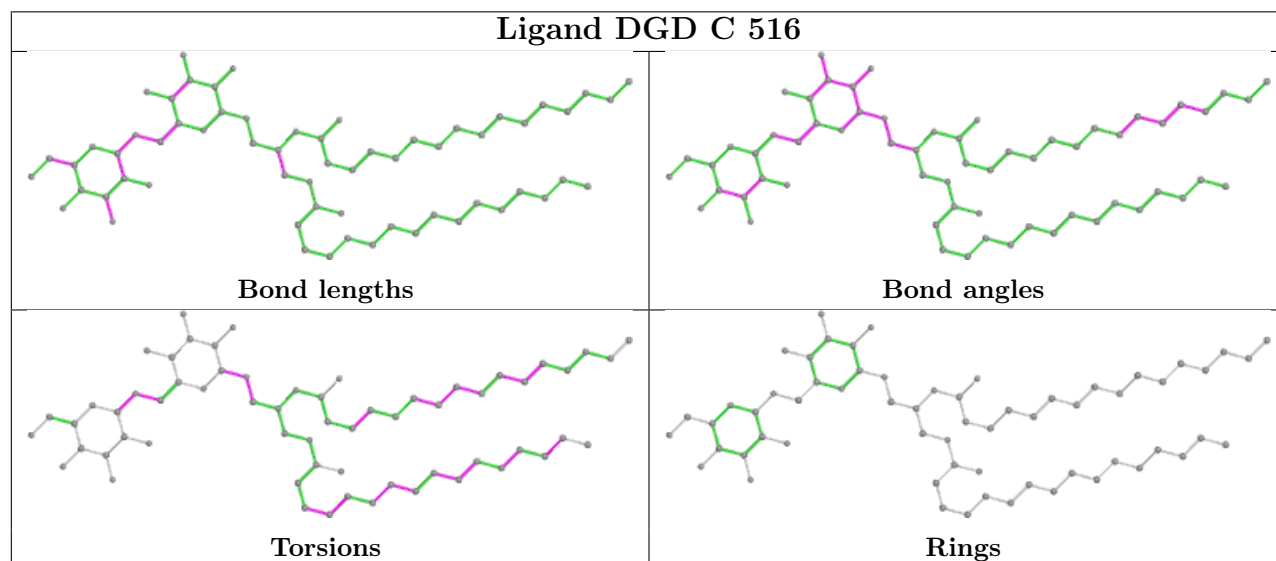
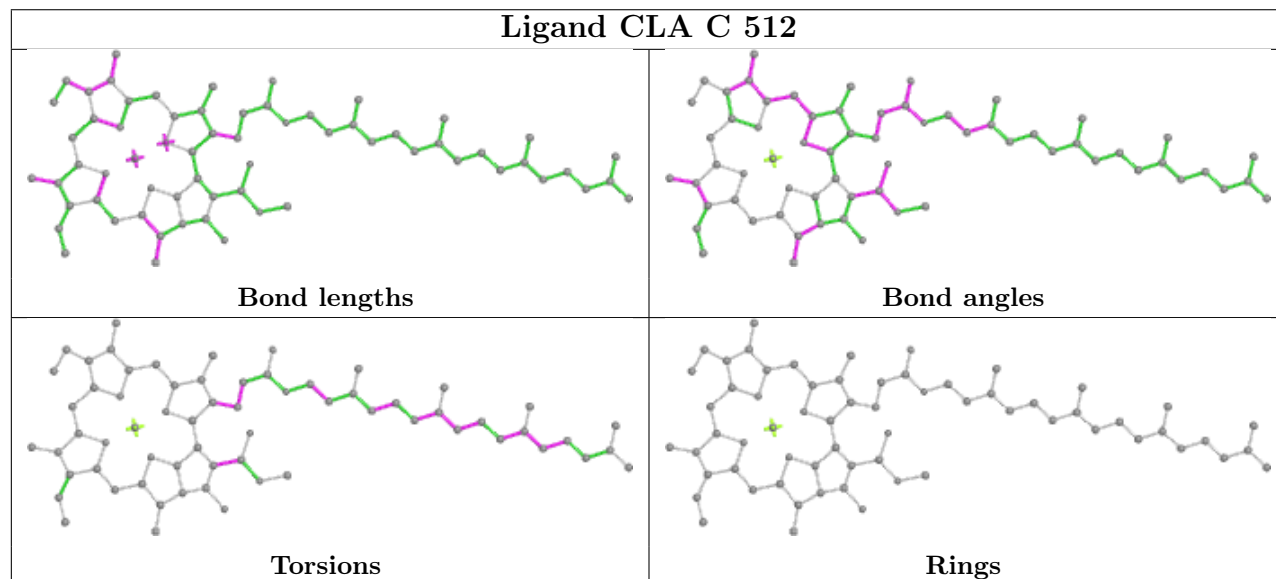
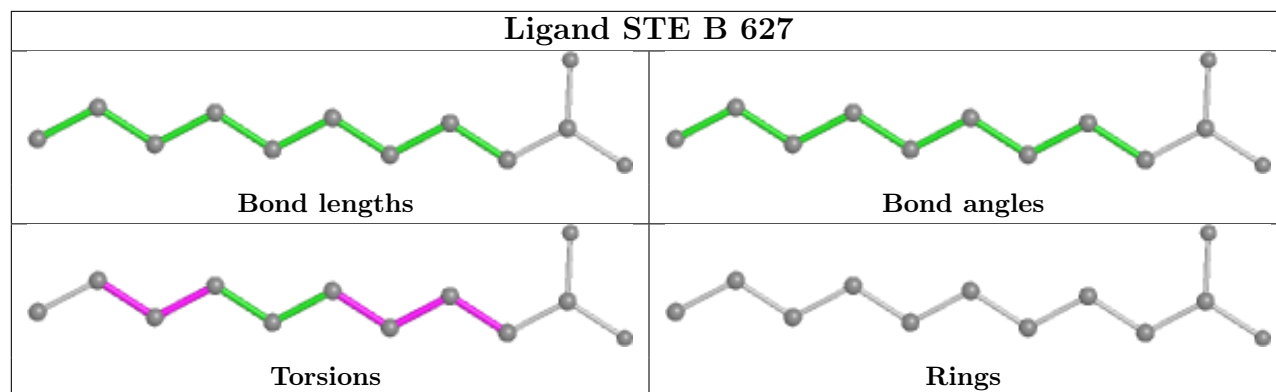
Ligand CLA c 511

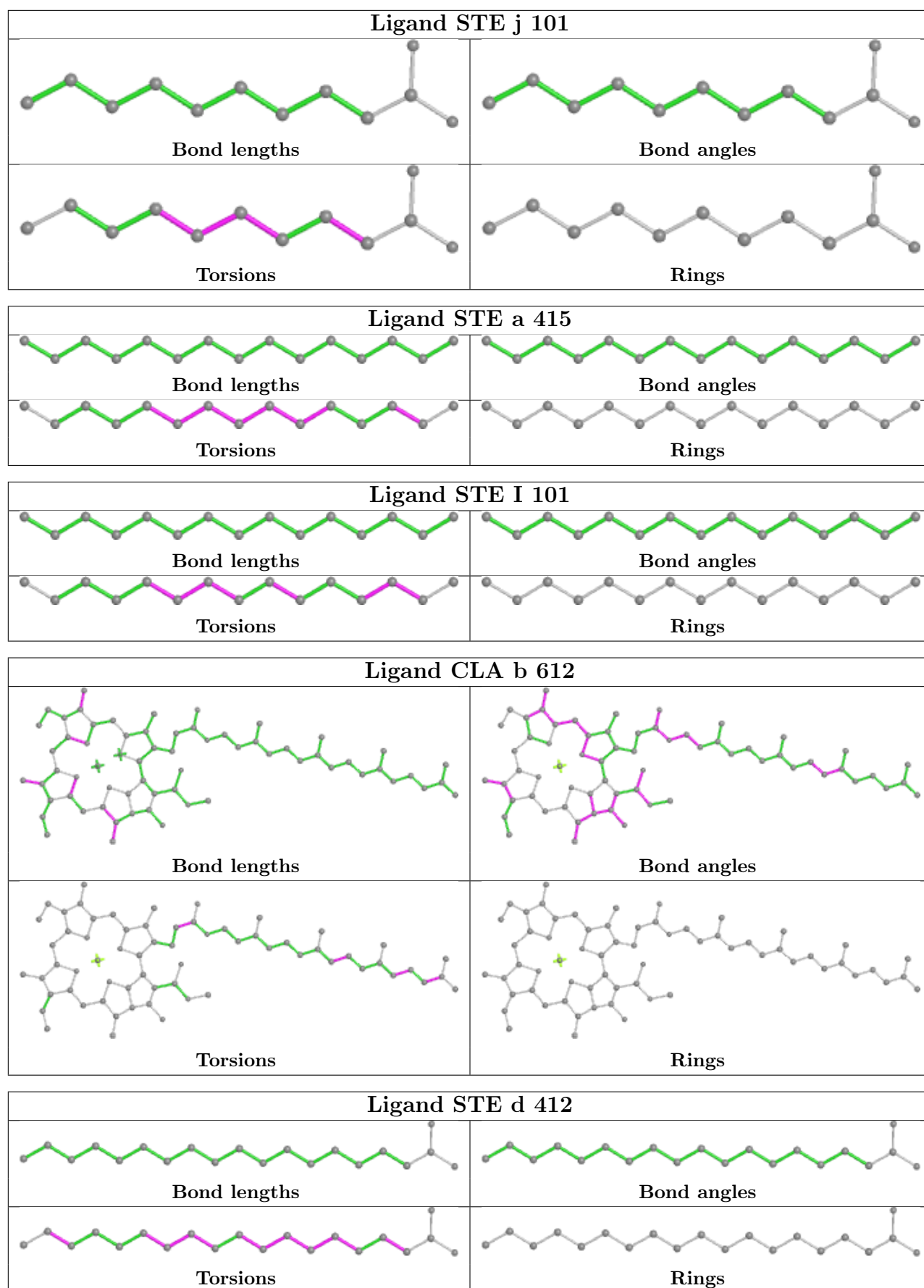


Ligand CLA b 610

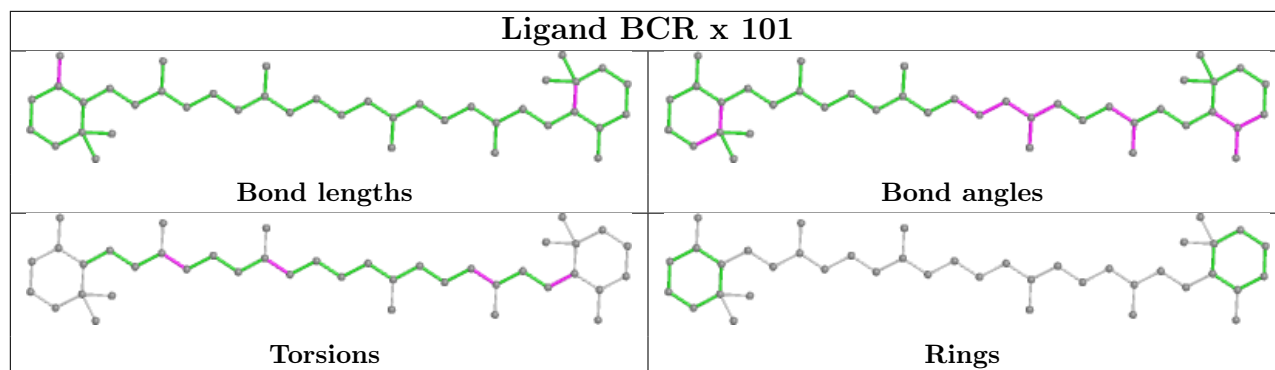




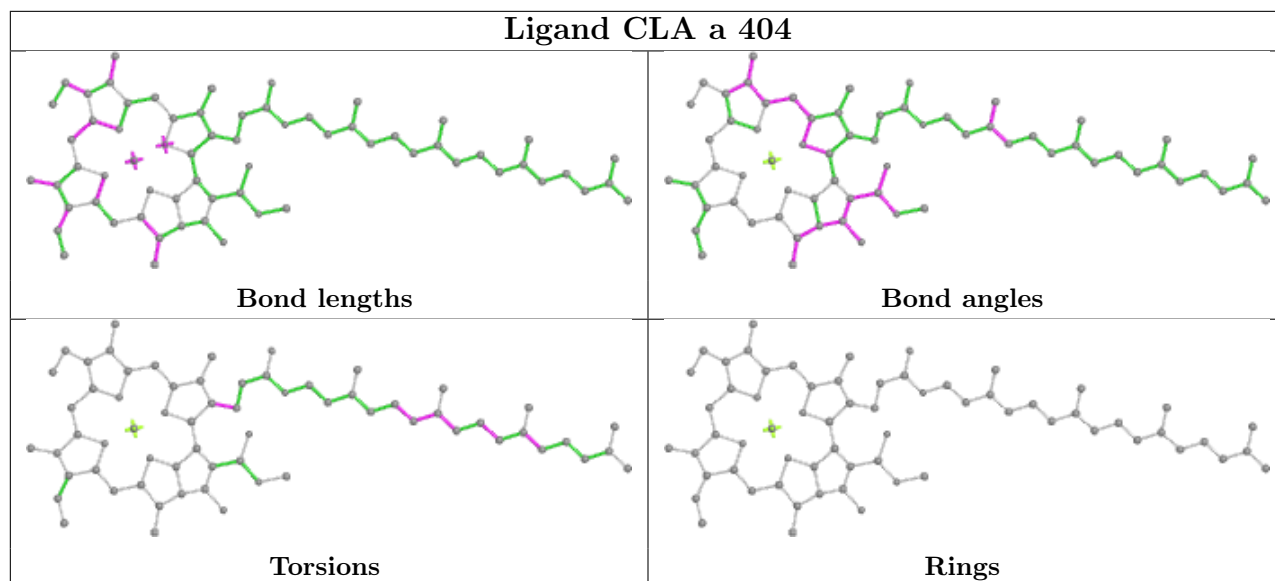




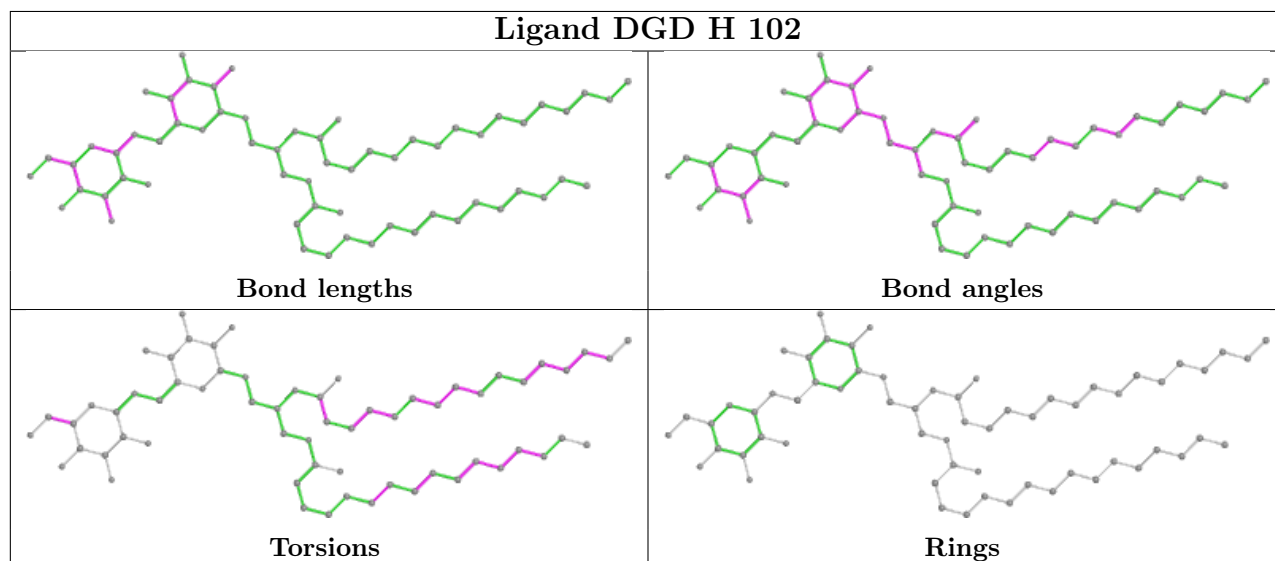
Ligand BCR x 101

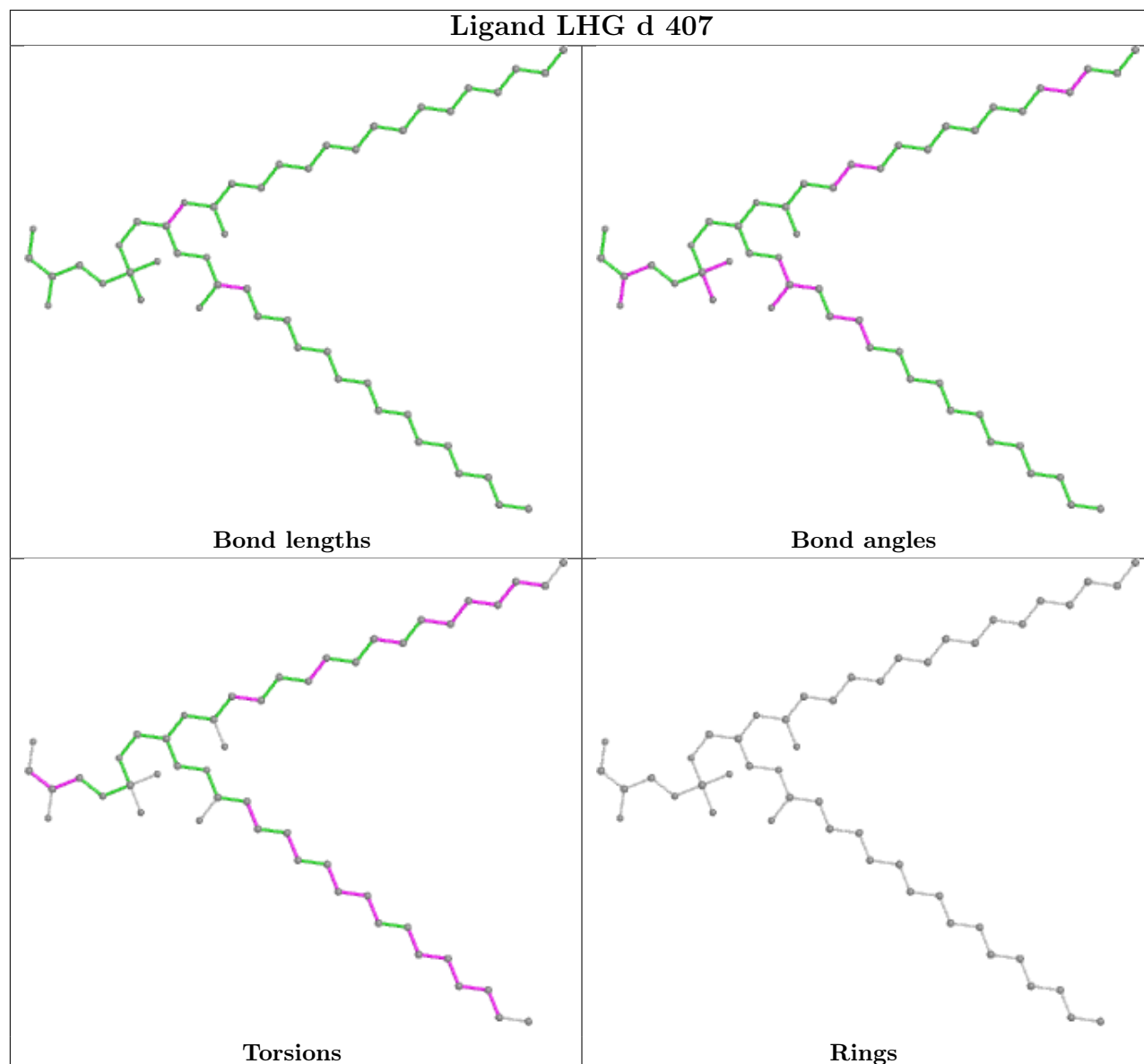
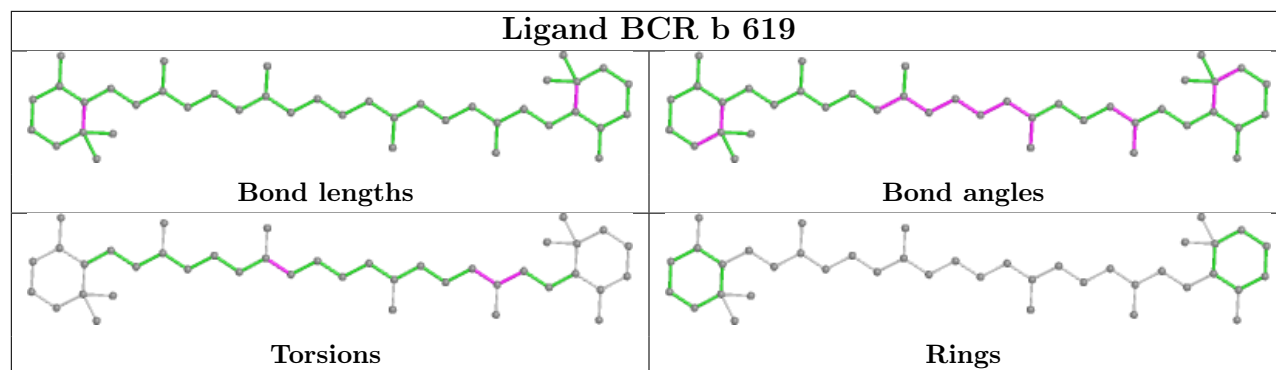


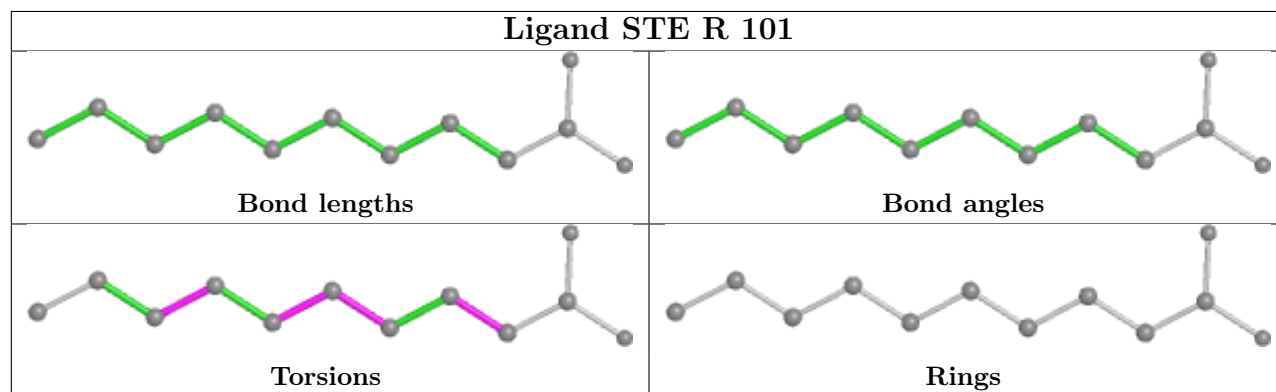
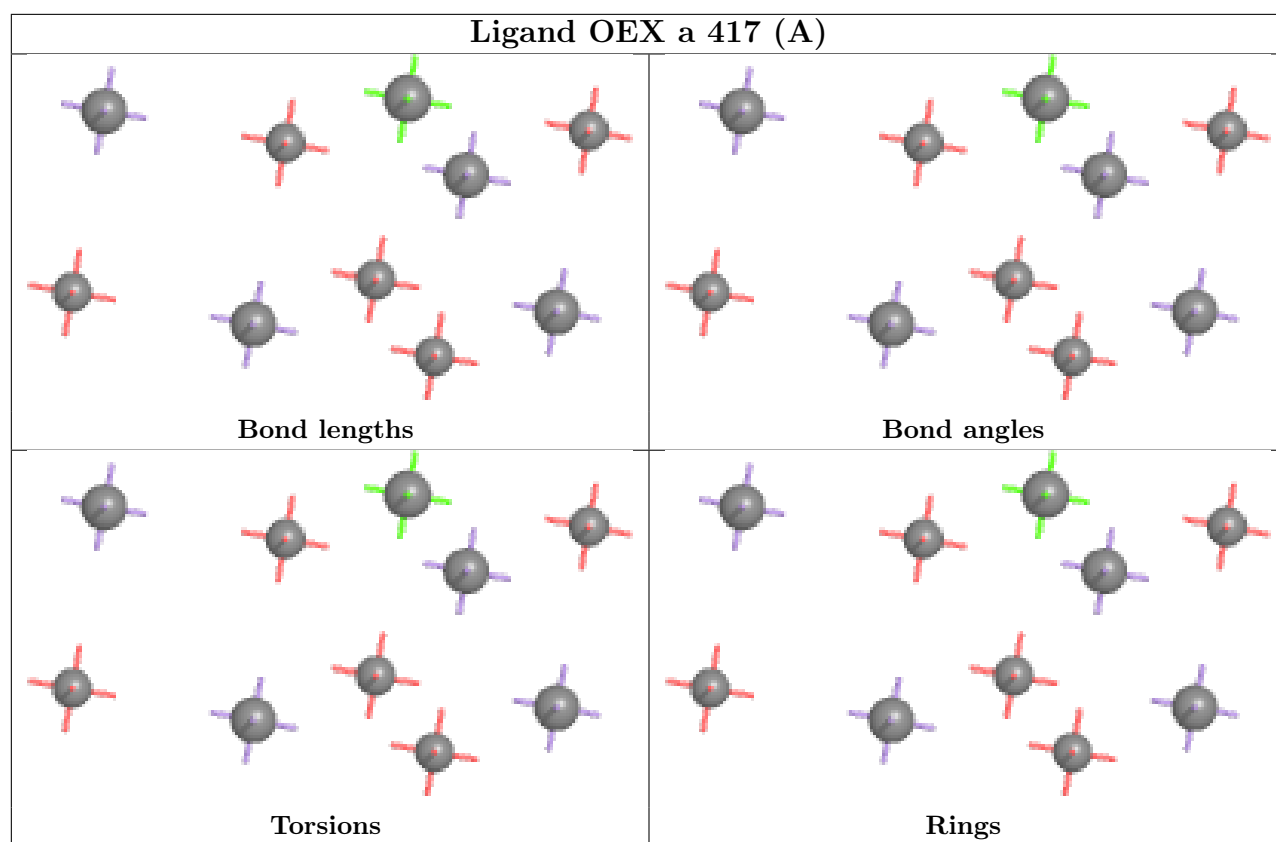
Ligand CLA a 404



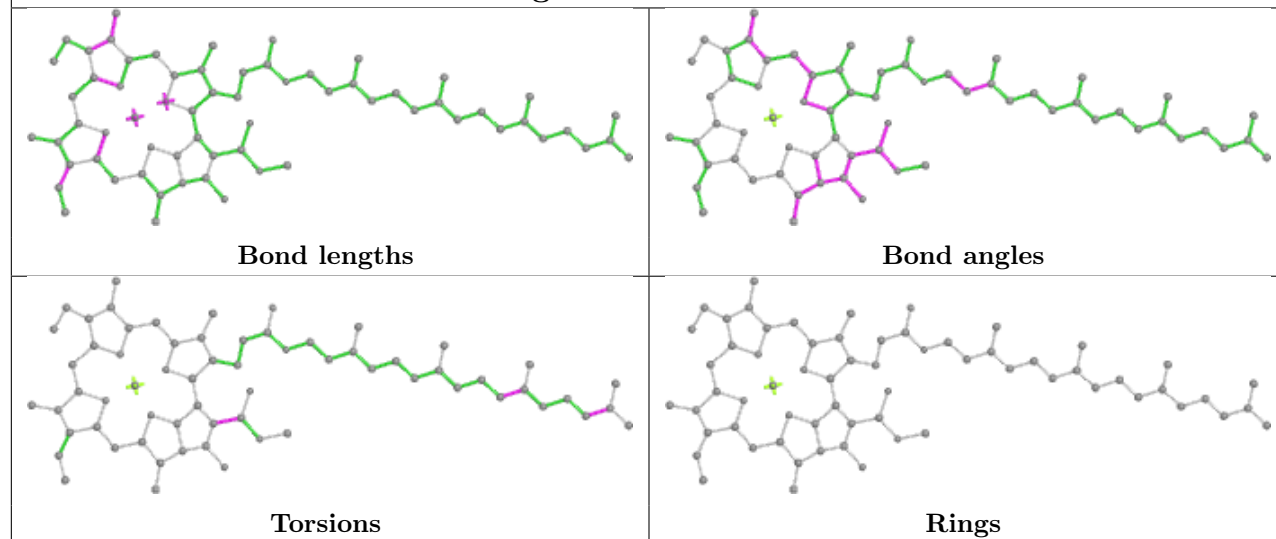
Ligand DGD H 102



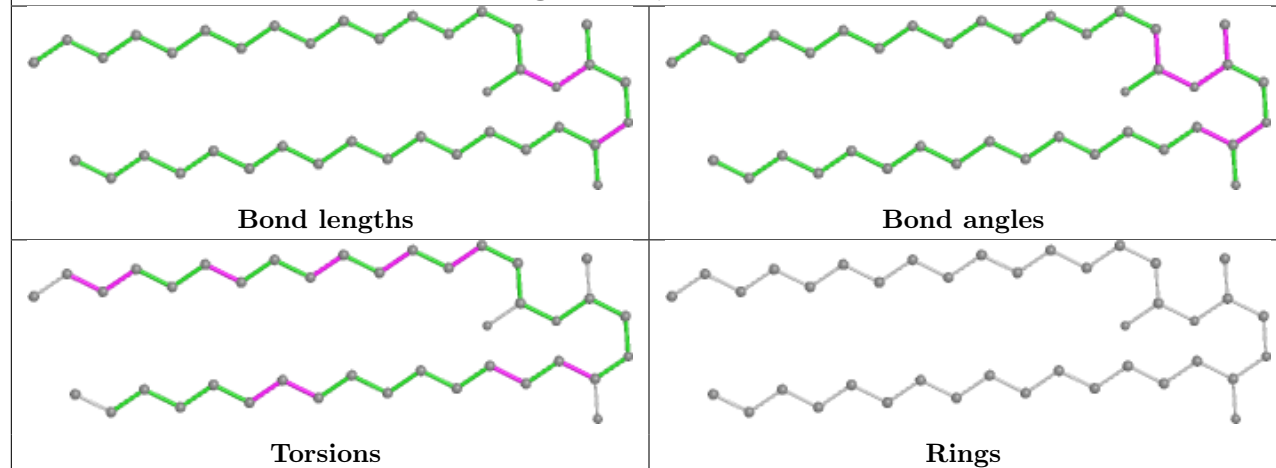




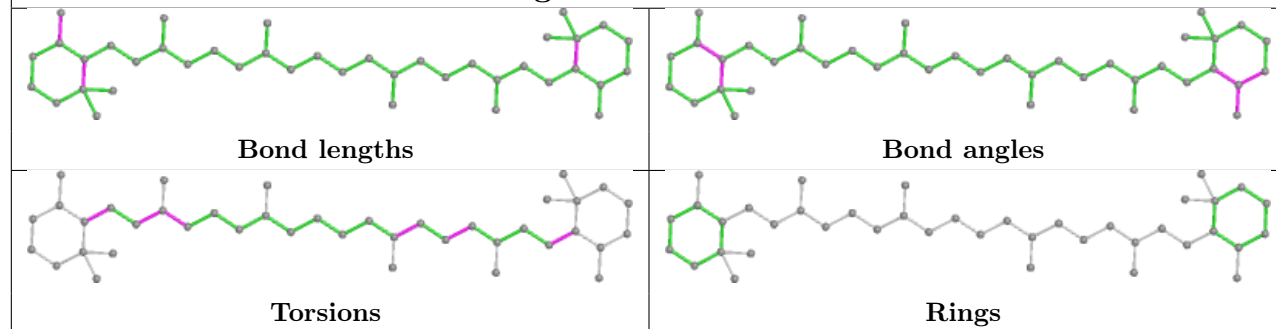
Ligand CLA C 502

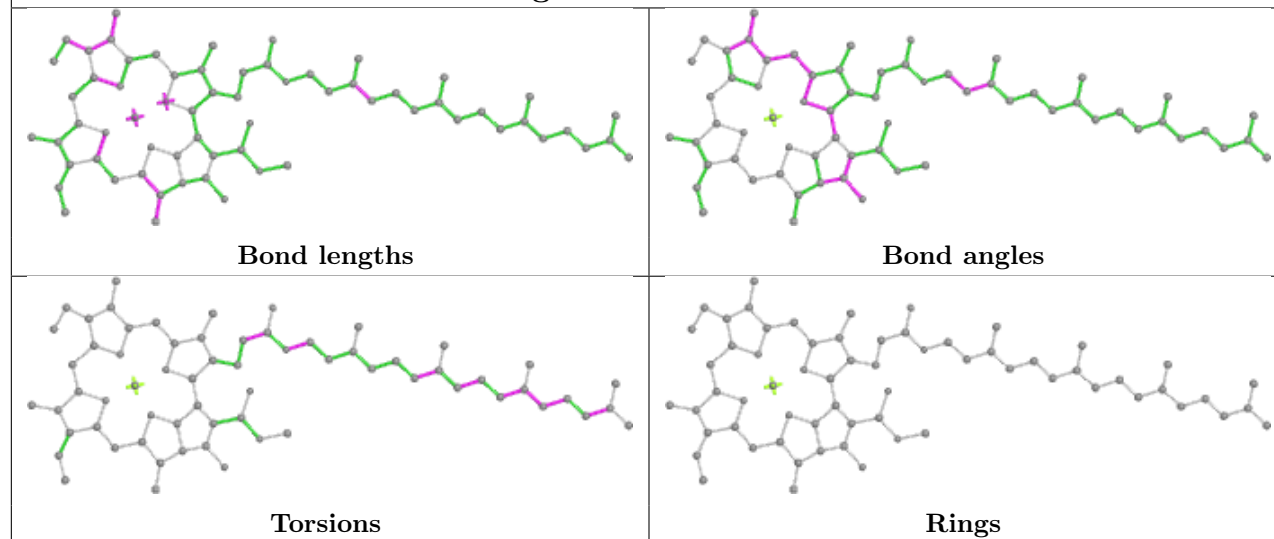
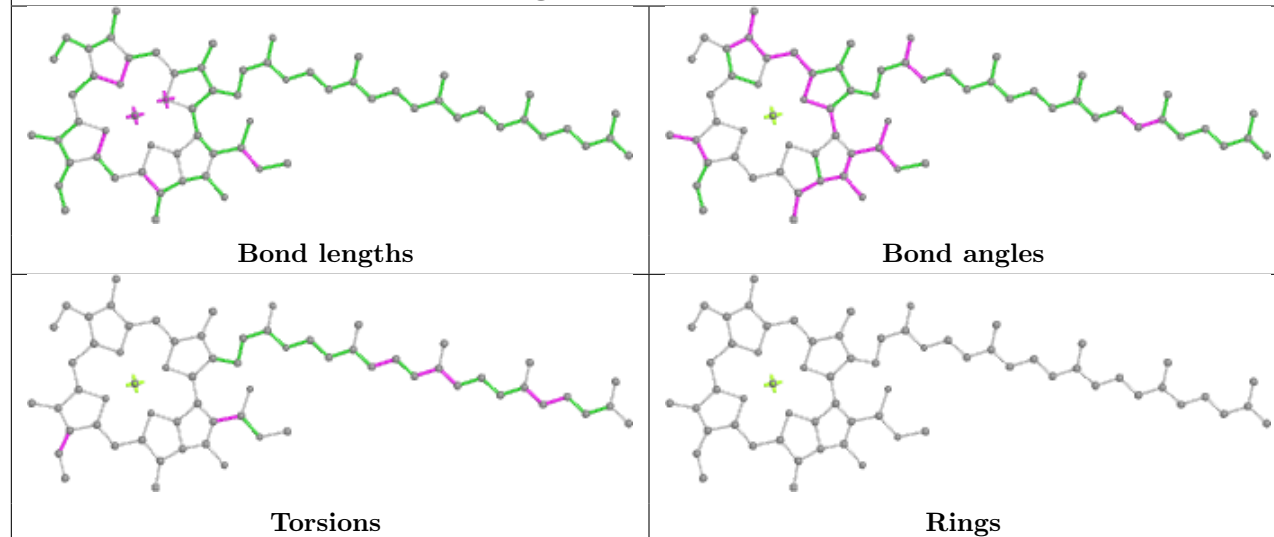
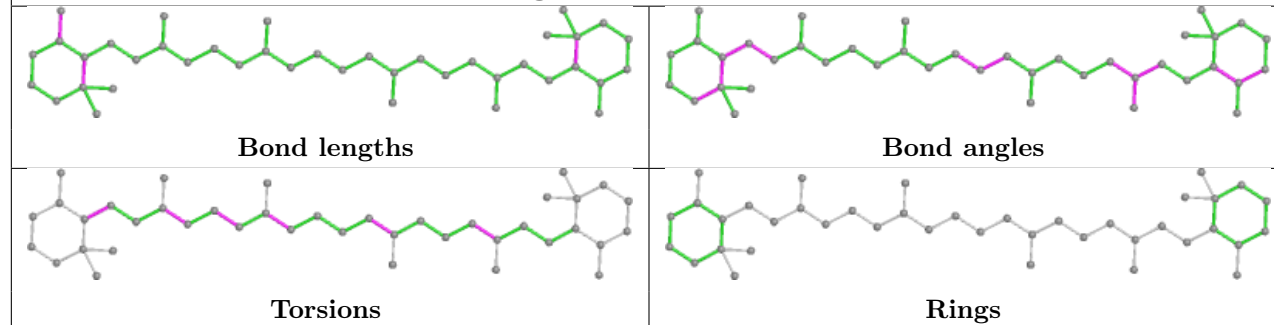


Ligand SQD A 415

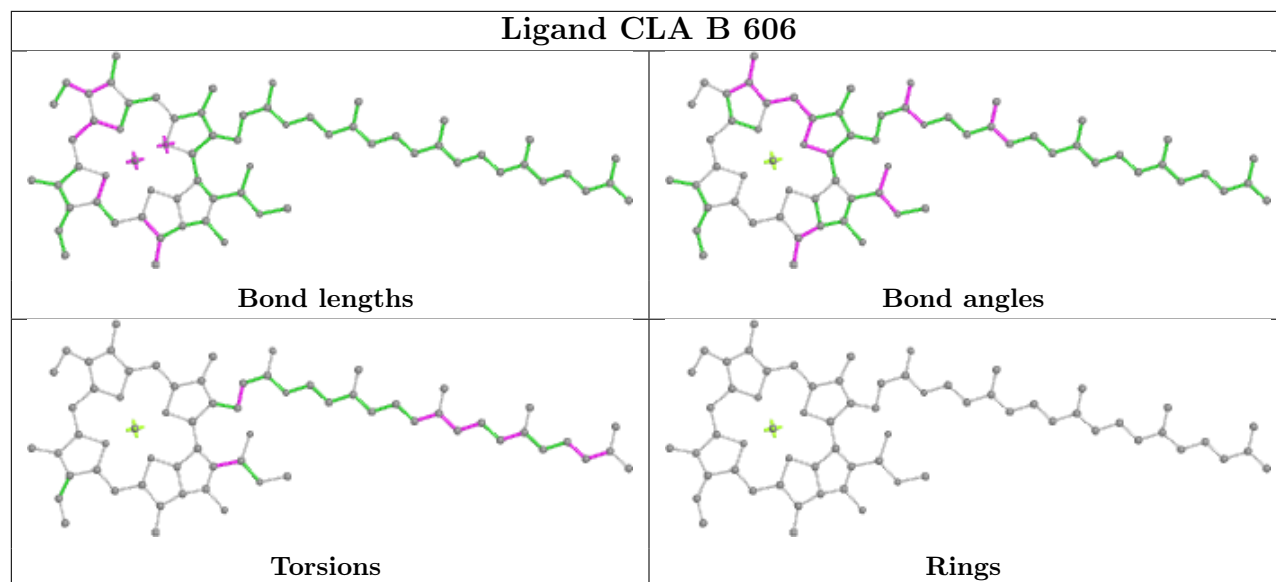


Ligand BCR k 101

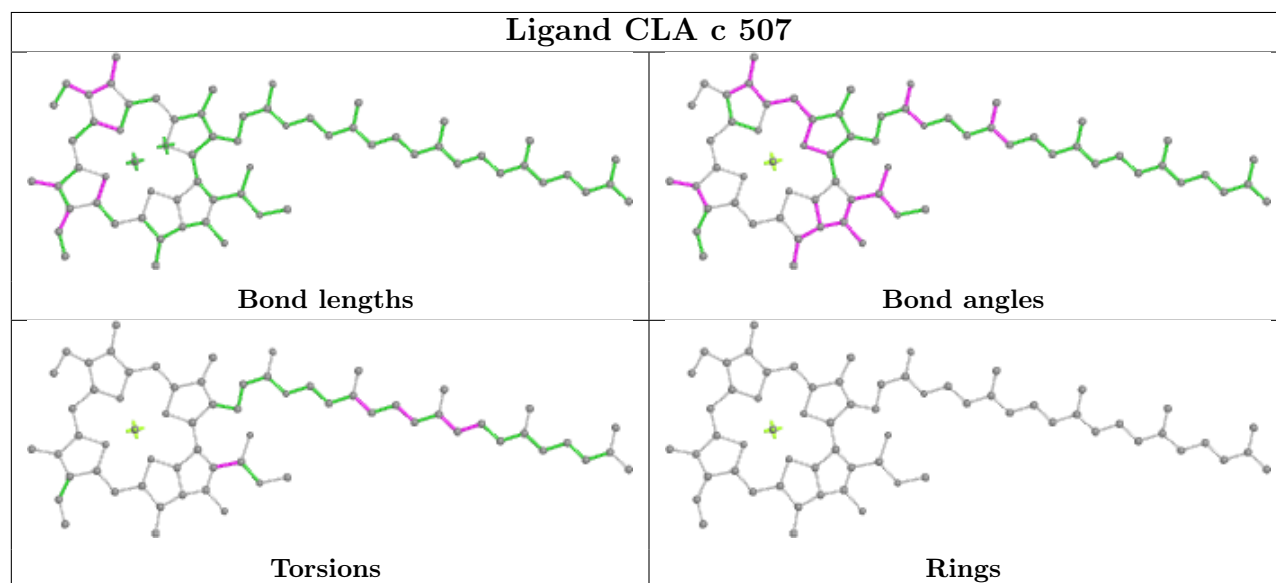


Ligand CLA B 613**Ligand CLA B 604****Ligand BCR B 617**

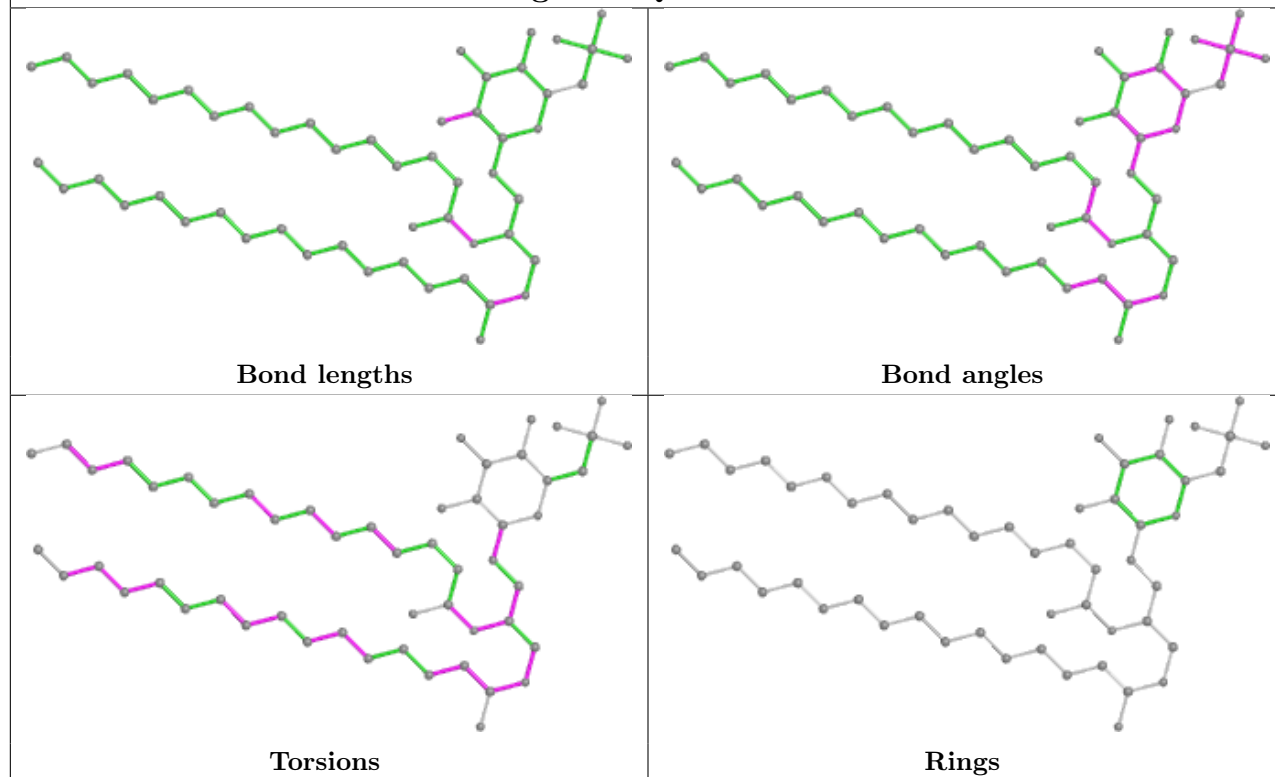
Ligand CLA B 606



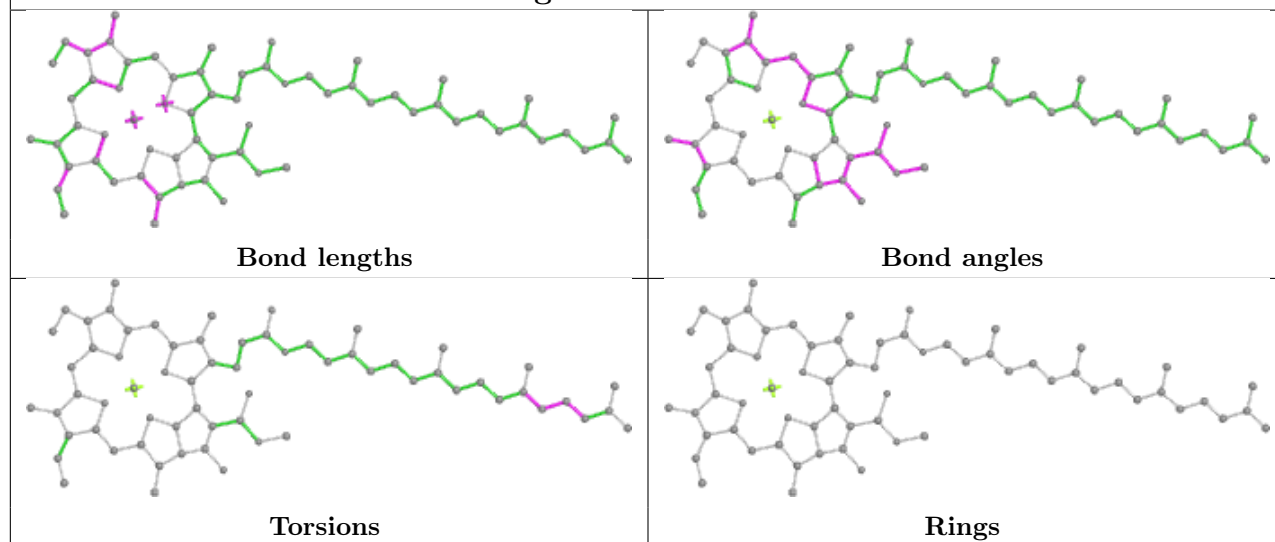
Ligand CLA c 507

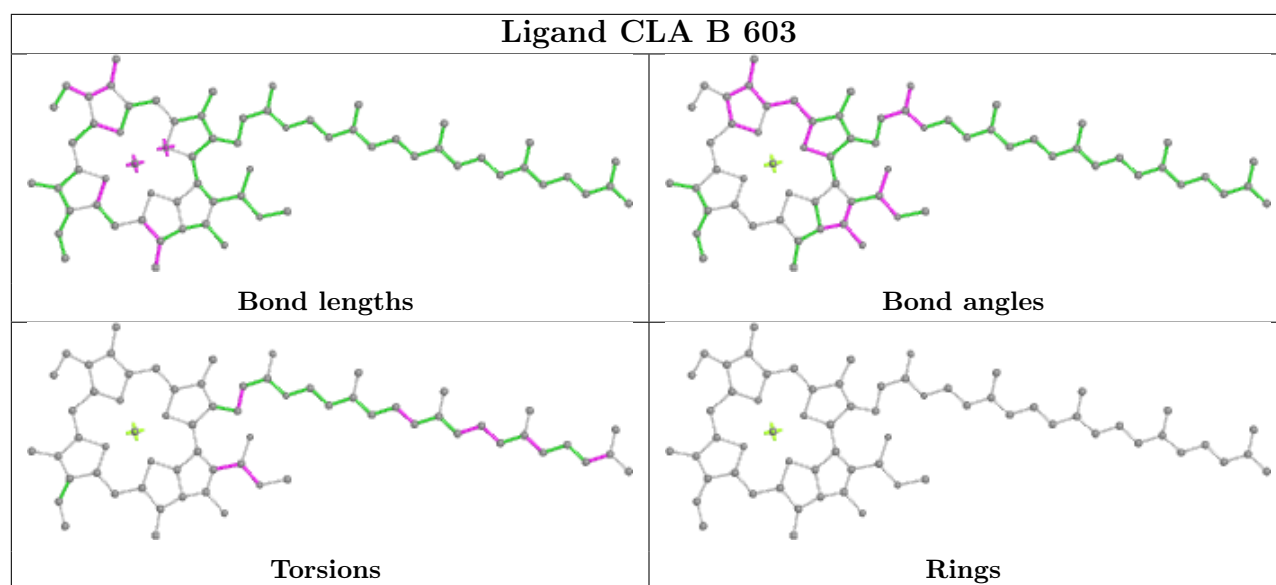


Ligand SQD B 623



Ligand CLA b 609





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%)	-0.36	4 (1%) 79 82	21, 28, 43, 73	0
1	a	334/344 (97%)	-0.39	1 (0%) 94 94	22, 30, 52, 73	0
2	B	505/510 (99%)	-0.36	9 (1%) 68 72	24, 32, 57, 80	0
2	b	505/510 (99%)	-0.15	18 (3%) 42 49	23, 35, 65, 90	0
3	C	442/461 (95%)	-0.26	4 (0%) 84 86	25, 34, 49, 67	0
3	c	451/461 (97%)	-0.18	10 (2%) 62 66	26, 38, 57, 86	0
4	D	341/352 (96%)	-0.32	1 (0%) 94 94	23, 29, 43, 69	0
4	d	341/352 (96%)	-0.29	0 100 100	24, 33, 52, 74	0
5	E	82/84 (97%)	-0.00	4 (4%) 29 35	33, 48, 62, 78	0
5	e	82/84 (97%)	0.27	5 (6%) 21 26	37, 54, 70, 79	0
6	F	34/45 (75%)	-0.36	1 (2%) 51 57	34, 40, 54, 74	0
6	f	34/45 (75%)	-0.22	0 100 100	38, 47, 65, 82	0
7	H	65/66 (98%)	-0.05	1 (1%) 73 77	30, 38, 53, 65	0
7	h	63/66 (95%)	0.27	5 (7%) 12 16	36, 45, 57, 60	0
8	I	35/38 (92%)	-0.23	3 (8%) 10 13	33, 37, 62, 76	0
8	i	35/38 (92%)	-0.12	3 (8%) 10 13	30, 39, 70, 82	0
9	J	36/40 (90%)	-0.04	4 (11%) 5 7	33, 46, 67, 85	0
9	j	36/40 (90%)	0.00	3 (8%) 11 14	34, 48, 78, 86	0
10	K	37/46 (80%)	0.14	1 (2%) 54 60	37, 48, 62, 70	0
10	k	37/46 (80%)	0.03	2 (5%) 25 31	43, 51, 65, 73	0
11	L	37/37 (100%)	-0.44	1 (2%) 54 60	24, 29, 58, 66	0
11	l	36/37 (97%)	-0.19	3 (8%) 11 14	25, 30, 65, 81	0
12	M	32/36 (88%)	-0.04	1 (3%) 49 55	28, 33, 56, 67	0
12	m	31/36 (86%)	-0.11	0 100 100	27, 33, 51, 58	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	0.03	16 (6%) 18 23	24, 41, 77, 133	0
13	o	244/272 (89%)	-0.03	14 (5%) 23 29	25, 40, 77, 114	0
14	R	28/41 (68%)	1.65	9 (32%) 0 0	54, 62, 75, 82	0
14	r	28/41 (68%)	3.12	20 (71%) 0 0	62, 76, 92, 100	0
15	T	29/32 (90%)	-0.32	2 (6%) 16 21	26, 30, 54, 74	0
15	t	29/32 (90%)	-0.20	2 (6%) 16 21	28, 32, 74, 91	0
16	U	97/134 (72%)	-0.23	1 (1%) 82 85	31, 41, 64, 79	0
16	u	97/134 (72%)	-0.39	1 (1%) 82 85	30, 38, 56, 74	0
17	V	137/163 (84%)	-0.45	0 100 100	30, 39, 52, 73	0
17	v	137/163 (84%)	-0.18	5 (3%) 42 49	31, 44, 62, 75	0
18	X	38/41 (92%)	-0.06	2 (5%) 26 32	36, 47, 64, 69	0
18	x	39/41 (95%)	0.37	4 (10%) 6 8	44, 51, 77, 88	0
19	Y	27/46 (58%)	1.15	7 (25%) 0 0	48, 66, 85, 89	0
19	y	30/46 (65%)	0.45	4 (13%) 3 4	56, 67, 78, 86	0
20	Z	62/62 (100%)	0.87	17 (27%) 0 0	49, 62, 97, 104	0
20	z	62/62 (100%)	0.76	11 (17%) 1 1	53, 66, 99, 111	0
All	All	5293/5700 (92%)	-0.15	199 (3%) 40 46	21, 36, 66, 133	0

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	10.5
13	O	56	PRO	6.7
2	b	495	PHE	6.5
14	r	3	TRP	6.0
1	A	13	LEU	6.0
13	O	59	LYS	5.9
13	o	3	GLN	5.9
13	o	57	LYS	5.5
14	r	29	LYS	5.5
13	O	60	ARG	5.4
9	j	5	GLY	5.2
14	r	6	LEU	5.2
14	r	28	VAL	5.1
13	O	3	GLN	5.1
13	o	4	THR	5.0

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Mol	Chain	Res	Type	RSRZ
14	r	24	LEU	5.0
14	r	25	PRO	5.0
20	Z	33	TRP	4.9
13	O	4	THR	4.9
5	e	79	PHE	4.8
14	R	6	LEU	4.8
14	R	3	TRP	4.8
14	r	10	LEU	4.8
20	z	33	TRP	4.8
20	Z	1	MET	4.7
14	r	9	LEU	4.6
20	Z	7	LEU	4.6
20	Z	35	ARG	4.6
20	Z	61	VAL	4.5
2	b	127	ARG	4.5
7	h	21	VAL	4.5
15	t	30	THR	4.5
13	o	60	ARG	4.4
3	c	23	ALA	4.4
18	X	2	THR	4.4
14	R	21	ARG	4.3
13	O	5	LEU	4.3
13	O	61	GLN	4.3
2	b	486	LEU	4.3
20	Z	42	LEU	4.3
14	r	23	ILE	4.2
20	Z	62	VAL	4.2
3	c	143	TYR	4.1
20	Z	3	ILE	4.1
1	A	11	ALA	4.0
3	c	24	THR	4.0
20	z	35	ARG	3.9
13	o	62	GLU	3.9
13	O	62	GLU	3.9
1	a	11	ALA	3.8
13	O	57	LYS	3.8
14	r	27	ALA	3.8
13	o	207	ARG	3.7
15	T	30	THR	3.7
9	j	7	ARG	3.7
14	R	25	PRO	3.7
18	x	34	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
19	Y	43	ARG	3.6
14	r	13	LEU	3.6
14	r	14	LEU	3.6
20	Z	34	ASP	3.5
13	o	56	PRO	3.5
20	z	3	ILE	3.5
14	r	5	VAL	3.4
13	o	59	LYS	3.4
5	e	61	ARG	3.4
13	O	63	ALA	3.4
14	r	18	TRP	3.4
7	h	10	ILE	3.4
19	Y	20	ALA	3.3
9	J	5	GLY	3.3
19	y	40	ALA	3.3
8	i	36	ASP	3.2
8	I	36	ASP	3.2
13	o	61	GLN	3.2
2	b	487	SER	3.2
7	h	6	TRP	3.2
8	I	34	ARG	3.1
5	E	79	PHE	3.1
9	J	7	ARG	3.1
13	O	58	ASN	3.1
18	x	38	GLN	3.1
20	z	7	LEU	3.1
3	C	146	PHE	3.1
6	F	12	SER	3.0
9	J	8	ILE	3.0
17	v	21	LEU	3.0
13	O	246	ALA	3.0
3	c	25	ASN	3.0
19	Y	37	PHE	2.9
2	B	502	VAL	2.9
11	l	3	PRO	2.9
13	O	55	GLU	2.9
18	x	2	THR	2.8
2	b	506	ARG	2.8
14	r	26	TYR	2.8
13	o	5	LEU	2.8
19	y	18	VAL	2.8
17	v	22	THR	2.8

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Mol	Chain	Res	Type	RSRZ
14	r	2	ASP	2.8
1	A	12	ASN	2.8
2	b	491	VAL	2.8
13	O	35	SER	2.8
20	z	41	PHE	2.8
2	b	505	ARG	2.8
16	u	9	LEU	2.8
5	e	81	GLU	2.7
20	z	36	SER	2.7
8	i	34	ARG	2.7
19	Y	25	ILE	2.7
20	Z	32	ASP	2.7
3	c	146	PHE	2.7
3	c	147	PHE	2.7
8	i	35	LYS	2.7
2	b	295	GLY	2.7
20	z	1	MET	2.7
15	t	28	ARG	2.7
2	B	373	LYS	2.7
2	B	486	LEU	2.6
2	b	496	TYR	2.6
2	b	289	GLN	2.6
11	l	7	ARG	2.6
19	Y	42	ARG	2.6
2	b	502	VAL	2.6
14	R	26	TYR	2.6
14	R	24	LEU	2.6
19	y	19	ILE	2.5
20	Z	38	GLN	2.5
14	r	21	ARG	2.5
19	Y	41	VAL	2.5
16	U	8	GLU	2.5
18	X	3	ILE	2.5
3	C	57	ALA	2.5
14	r	15	ALA	2.5
10	k	10	LYS	2.5
20	Z	4	LEU	2.5
20	z	62	VAL	2.5
4	D	12	ARG	2.5
14	r	22	ASN	2.5
20	Z	41	PHE	2.5
13	o	55	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	127	ARG	2.4
5	e	82	GLN	2.4
2	b	128	THR	2.4
2	b	374	ASN	2.4
2	b	503	THR	2.4
20	z	42	LEU	2.4
9	j	6	GLY	2.4
14	R	28	VAL	2.4
13	o	63	ALA	2.4
18	x	40	SER	2.4
2	B	295	GLY	2.4
3	c	262	ARG	2.4
19	Y	21	GLN	2.4
20	Z	30	PRO	2.4
5	E	83	LEU	2.3
5	E	3	GLY	2.3
15	T	29	ILE	2.3
2	b	292	LEU	2.3
20	Z	37	LYS	2.3
10	K	17	ILE	2.3
2	B	293	ALA	2.3
3	C	61	VAL	2.3
2	b	492	GLU	2.2
10	k	17	ILE	2.2
17	v	15	GLU	2.2
20	Z	31	GLN	2.2
2	b	161	LEU	2.2
13	O	36	GLN	2.2
19	y	37	PHE	2.2
11	L	2	GLU	2.2
13	o	246	ALA	2.2
3	c	44	ASN	2.1
3	c	59	LEU	2.1
17	v	113	VAL	2.1
2	B	495	PHE	2.1
1	A	15	GLU	2.1
5	e	4	THR	2.1
14	r	19	ALA	2.1
2	B	86	ILE	2.1
3	C	60	ILE	2.1
2	B	505	ARG	2.1
7	H	65	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
13	O	207	ARG	2.1
20	z	31	GLN	2.1
20	z	60	PHE	2.1
2	b	293	ALA	2.1
5	E	84	LYS	2.1
9	J	6	GLY	2.1
11	l	2	GLU	2.1
7	h	22	ALA	2.1
14	R	29	LYS	2.1
3	c	57	ALA	2.0
20	Z	60	PHE	2.0
17	v	16	GLY	2.0
7	h	25	TRP	2.0
14	R	18	TRP	2.0
8	I	6	ILE	2.0
12	M	33	GLN	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	FME	T	1	10/11	0.93	0.10	29,41,62,62	0
15	FME	t	1	10/11	0.94	0.09	29,43,62,63	0
8	FME	i	1	10/11	0.96	0.16	35,44,57,58	0
12	FME	m	1	10/11	0.97	0.13	33,47,63,74	0
8	FME	I	1	10/11	0.97	0.17	34,41,49,59	0
12	FME	M	1	10/11	0.97	0.13	40,49,68,70	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
34	STE	a	414	12/20	0.68	0.25	50,64,74,78	0
34	STE	b	627	10/20	0.69	0.22	44,59,69,70	0
34	STE	L	101	12/20	0.75	0.16	46,59,75,80	0
34	STE	R	101	12/20	0.76	0.28	51,75,78,85	0
34	STE	H	103	18/20	0.77	0.25	48,66,76,79	0
29	SQD	a	412	36/54	0.79	0.18	33,59,78,86	0
29	SQD	A	415	39/54	0.79	0.18	37,59,88,94	0
30	LHG	A	414	49/49	0.80	0.20	47,70,98,111	0
34	STE	b	625	16/20	0.80	0.17	45,62,72,74	0
28	LMG	c	521	48/55	0.80	0.22	47,69,94,103	0
34	STE	d	412	20/20	0.80	0.23	36,55,71,73	0
34	STE	c	523	12/20	0.81	0.26	49,64,81,82	0
34	STE	b	626	20/20	0.81	0.18	44,62,74,79	0
34	STE	h	102	14/20	0.81	0.26	47,62,75,78	0
34	STE	j	101	12/20	0.81	0.13	42,56,70,73	0
31	DGD	A	416	66/66	0.82	0.17	41,61,75,79	0
22	CLA	C	512	65/65	0.82	0.17	33,53,82,92	0
34	STE	B	626	16/20	0.83	0.24	45,63,72,75	0
28	LMG	D	410	33/55	0.83	0.17	36,55,74,80	0
34	STE	d	413	20/20	0.83	0.16	42,62,76,76	0
30	LHG	e	102	42/49	0.83	0.24	57,79,100,109	0
24	BCR	H	101	40/40	0.83	0.15	26,44,57,61	0
22	CLA	b	601	65/65	0.84	0.17	42,65,85,91	0
34	STE	B	625	18/20	0.84	0.13	38,57,69,74	0
24	BCR	x	101	40/40	0.84	0.14	31,51,66,74	0
22	CLA	c	512	65/65	0.85	0.16	39,57,86,92	0
28	LMG	a	416	55/55	0.85	0.15	38,56,75,80	0
28	LMG	b	624	55/55	0.85	0.28	50,72,91,96	0
34	STE	c	520	20/20	0.85	0.20	43,57,79,88	0
28	LMG	A	412	48/55	0.85	0.16	36,55,74,89	0
28	LMG	c	522	49/55	0.85	0.15	37,55,79,96	0
34	STE	a	413	10/20	0.85	0.17	37,60,68,72	0
34	STE	B	624	12/20	0.85	0.11	44,55,64,66	0
34	STE	a	415	15/20	0.85	0.13	42,58,69,74	0
34	STE	b	621	16/20	0.86	0.18	35,49,65,75	0
24	BCR	Y	101	40/40	0.86	0.13	35,50,68,71	0
34	STE	I	101	15/20	0.86	0.15	39,56,70,70	0
34	STE	B	627	12/20	0.86	0.38	44,59,76,79	0
34	STE	M	102	15/20	0.86	0.14	34,48,63,63	0
34	STE	b	623	20/20	0.87	0.21	39,55,69,79	0
22	CLA	B	601	65/65	0.87	0.16	30,59,82,94	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	0.87	0.17	40,60,87,89	0
34	STE	C	520	16/20	0.87	0.12	36,52,62,69	0
29	SQD	B	623	54/54	0.87	0.15	40,57,86,96	0
34	STE	B	620	17/20	0.88	0.18	36,50,62,62	0
29	SQD	b	620	49/54	0.88	0.14	38,57,85,89	0
22	CLA	c	513	65/65	0.88	0.19	39,68,104,108	0
27	PL9	A	410	55/55	0.88	0.23	34,63,84,90	0
27	PL9	a	409	55/55	0.88	0.19	37,66,80,89	0
34	STE	C	519	12/20	0.88	0.11	46,56,66,67	0
34	STE	X	101	20/20	0.88	0.15	31,48,62,64	0
34	STE	C	521	12/20	0.89	0.09	34,47,54,58	0
24	BCR	k	101	40/40	0.89	0.11	42,61,73,75	0
22	CLA	a	404	65/65	0.89	0.13	20,37,74,79	0
24	BCR	K	101	40/40	0.89	0.15	41,55,70,71	0
22	CLA	d	404	65/65	0.89	0.16	27,46,81,87	0
24	BCR	c	514	40/40	0.89	0.15	43,59,70,72	0
24	BCR	d	405	40/40	0.89	0.13	32,51,85,98	0
34	STE	l	102	18/20	0.89	0.14	34,47,72,80	0
22	CLA	C	502	65/65	0.90	0.14	28,39,61,73	0
28	LMG	c	519	37/55	0.90	0.17	39,61,75,81	0
28	LMG	C	518	48/55	0.90	0.14	36,65,86,89	0
22	CLA	c	502	65/65	0.90	0.15	29,41,61,65	0
22	CLA	c	508	64/65	0.90	0.15	30,45,85,96	0
22	CLA	b	615	65/65	0.91	0.14	26,40,56,60	0
22	CLA	b	616	60/65	0.91	0.13	26,42,85,88	0
34	STE	J	101	12/20	0.91	0.10	45,59,70,72	0
22	CLA	D	403	65/65	0.91	0.13	24,43,100,108	0
24	BCR	B	619	40/40	0.91	0.10	29,41,54,60	0
24	BCR	D	404	40/40	0.91	0.13	25,43,76,85	0
34	STE	T	102	15/20	0.91	0.17	41,56,70,76	0
28	LMG	M	101	51/55	0.91	0.11	29,47,70,84	0
34	STE	Z	101	8/20	0.91	0.15	46,57,66,66	0
24	BCR	k	102	40/40	0.91	0.16	39,54,66,67	0
28	LMG	b	622	51/55	0.91	0.11	29,50,68,80	0
22	CLA	b	602	65/65	0.91	0.15	28,42,60,61	0
34	STE	t	102	14/20	0.91	0.10	33,52,62,65	0
28	LMG	D	411	28/55	0.92	0.13	28,48,59,61	0
29	SQD	f	101	41/54	0.92	0.17	49,76,94,100	0
22	CLA	B	606	65/65	0.92	0.11	24,36,74,79	0
22	CLA	c	503	65/65	0.92	0.16	30,43,53,62	0
24	BCR	C	514	40/40	0.92	0.11	25,41,53,63	0
31	DGD	C	516	62/66	0.92	0.12	30,48,91,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	c	506	65/65	0.92	0.12	30,48,87,97	0
34	STE	d	411	17/20	0.92	0.10	40,54,61,61	0
22	CLA	C	505	65/65	0.92	0.17	24,39,69,74	0
22	CLA	c	511	65/65	0.92	0.13	39,52,71,74	0
22	CLA	C	506	65/65	0.92	0.12	23,42,82,89	0
24	BCR	b	619	40/40	0.92	0.11	28,45,65,68	0
28	LMG	D	406	51/55	0.92	0.16	28,50,76,88	0
22	CLA	C	507	65/65	0.92	0.14	22,40,52,57	0
22	CLA	B	615	65/65	0.93	0.13	23,36,61,64	0
22	CLA	c	510	65/65	0.93	0.15	32,47,64,67	0
22	CLA	B	616	60/65	0.93	0.14	22,38,79,86	0
22	CLA	B	614	65/65	0.93	0.17	21,37,73,79	0
22	CLA	b	606	65/65	0.93	0.11	27,39,69,74	0
31	DGD	H	102	62/66	0.93	0.10	26,41,58,63	0
31	DGD	c	517	62/66	0.93	0.12	33,51,82,89	0
31	DGD	c	518	62/66	0.93	0.14	30,49,77,88	0
34	STE	M	103	10/20	0.93	0.12	35,48,55,58	0
31	DGD	h	101	62/66	0.93	0.12	24,47,62,66	0
22	CLA	c	504	60/65	0.93	0.12	29,42,80,83	0
22	CLA	c	505	65/65	0.93	0.16	26,39,64,73	0
29	SQD	a	411	54/54	0.93	0.15	41,61,84,85	0
22	CLA	b	609	65/65	0.93	0.14	29,45,60,68	0
22	CLA	c	507	65/65	0.93	0.14	27,44,59,61	0
27	PL9	D	405	55/55	0.94	0.10	21,33,46,47	0
24	BCR	B	618	40/40	0.94	0.09	24,37,49,55	0
30	LHG	d	407	49/49	0.94	0.14	32,50,70,76	0
22	CLA	C	508	65/65	0.94	0.12	27,43,95,106	0
22	CLA	C	509	65/65	0.94	0.17	26,43,64,72	0
22	CLA	C	510	65/65	0.94	0.13	25,42,58,62	0
31	DGD	C	517	62/66	0.94	0.12	25,45,68,74	0
22	CLA	b	604	65/65	0.94	0.14	18,35,71,83	0
22	CLA	C	511	65/65	0.94	0.12	28,49,64,66	0
24	BCR	K	102	40/40	0.94	0.14	32,48,61,64	0
22	CLA	B	604	65/65	0.94	0.12	20,34,66,70	0
24	BCR	b	618	40/40	0.94	0.11	25,39,57,61	0
22	CLA	c	509	65/65	0.94	0.17	32,46,62,68	0
22	CLA	b	611	65/65	0.94	0.14	22,34,54,60	0
24	BCR	c	515	40/40	0.94	0.12	27,43,56,61	0
22	CLA	b	614	65/65	0.94	0.13	24,41,73,77	0
28	LMG	d	410	44/55	0.94	0.12	31,50,73,88	0
22	CLA	C	503	65/65	0.94	0.14	26,41,51,57	0
22	CLA	C	504	59/65	0.94	0.13	28,40,76,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
29	SQD	D	407	36/54	0.94	0.14	44,68,83,94	0
24	BCR	t	101	40/40	0.94	0.10	24,39,52,55	0
22	CLA	a	403	65/65	0.94	0.14	23,41,91,95	0
24	BCR	B	617	40/40	0.94	0.11	28,39,55,60	0
22	CLA	b	607	65/65	0.95	0.13	20,36,67,71	0
29	SQD	A	413	52/54	0.95	0.14	29,55,82,90	0
22	CLA	b	608	65/65	0.95	0.14	25,41,58,61	0
22	CLA	C	501	65/65	0.95	0.13	22,36,50,53	0
22	CLA	b	610	65/65	0.95	0.17	24,39,48,56	0
22	CLA	B	603	65/65	0.95	0.14	16,34,59,61	0
22	CLA	b	612	65/65	0.95	0.16	20,34,51,54	0
22	CLA	d	403	65/65	0.95	0.11	20,35,57,67	0
22	CLA	b	613	65/65	0.95	0.14	18,34,72,79	0
23	PHO	A	404	64/64	0.95	0.10	18,28,36,40	0
30	LHG	B	622	49/49	0.95	0.12	27,45,65,70	0
30	LHG	D	409	47/49	0.95	0.12	27,48,73,88	0
23	PHO	d	402	64/64	0.95	0.10	27,38,48,50	0
30	LHG	d	409	39/49	0.95	0.10	28,46,69,71	0
22	CLA	A	403	65/65	0.95	0.13	21,35,85,91	0
30	LHG	l	101	49/49	0.95	0.11	31,43,57,64	0
22	CLA	A	405	54/65	0.95	0.10	18,33,58,67	0
31	DGD	C	515	62/66	0.95	0.12	22,40,74,80	0
22	CLA	B	609	65/65	0.95	0.12	23,37,61,73	0
22	CLA	c	501	65/65	0.95	0.12	23,41,52,56	0
22	CLA	B	610	65/65	0.95	0.14	20,34,46,47	0
31	DGD	c	516	62/66	0.95	0.10	22,41,70,78	0
22	CLA	a	410	65/65	0.95	0.11	20,29,47,54	0
22	CLA	B	613	65/65	0.95	0.14	19,32,63,67	0
22	CLA	A	411	65/65	0.95	0.10	18,27,56,59	0
24	BCR	T	101	40/40	0.95	0.09	22,39,54,62	0
22	CLA	A	402	65/65	0.95	0.10	16,27,41,55	0
24	BCR	a	405	40/40	0.95	0.09	22,33,46,49	0
24	BCR	b	617	40/40	0.95	0.10	23,41,53,57	0
22	CLA	B	602	65/65	0.95	0.14	23,36,55,60	0
35	HEM	F	101	43/43	0.95	0.11	32,45,60,66	0
22	CLA	a	402	65/65	0.96	0.09	18,30,47,60	0
24	BCR	A	406	40/40	0.96	0.08	23,35,45,47	0
27	PL9	d	406	55/55	0.96	0.10	22,34,42,44	0
22	CLA	B	611	65/65	0.96	0.15	22,32,51,54	0
22	CLA	B	612	65/65	0.96	0.15	19,34,46,50	0
22	CLA	B	608	65/65	0.96	0.12	22,35,54,62	0
22	CLA	B	605	65/65	0.96	0.13	21,32,46,53	0

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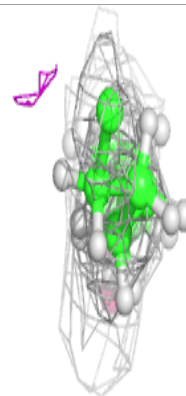
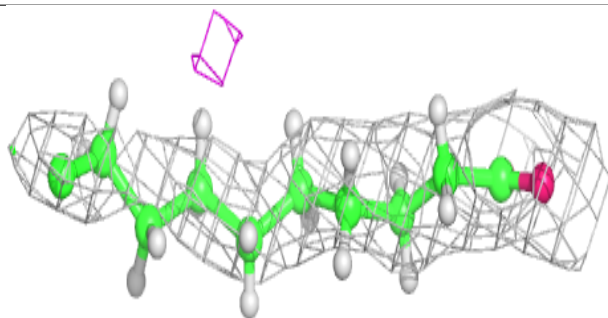
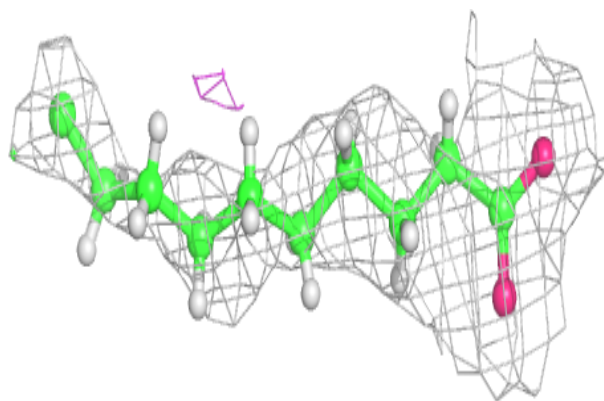
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	D	402	65/65	0.96	0.10	13,30,54,60	0
22	CLA	b	603	65/65	0.96	0.13	23,36,68,70	0
22	CLA	B	607	65/65	0.96	0.10	18,34,60,69	0
22	CLA	b	605	65/65	0.96	0.12	21,35,49,52	0
30	LHG	B	621	49/49	0.96	0.11	27,42,59,64	0
23	PHO	D	401	64/64	0.96	0.13	22,34,43,48	0
26	BCT	a	408	4/4	0.96	0.18	26,32,39,46	0
23	PHO	d	401	64/64	0.96	0.12	18,32,39,48	0
30	LHG	d	408	49/49	0.96	0.10	26,42,52,57	0
35	HEM	e	101	43/43	0.96	0.12	40,51,71,74	0
36	HEC	v	201	43/43	0.96	0.14	25,37,47,49	0
30	LHG	D	408	49/49	0.97	0.10	21,40,51,57	0
36	HEC	V	201	43/43	0.98	0.11	23,33,44,47	0
33	OEX	a	417[A]	10/10	0.99	0.11	26,32,35,35	10
25	CL	a	406	1/1	0.99	0.07	28,28,28,28	0
25	CL	a	407	1/1	0.99	0.02	28,28,28,28	0
26	BCT	A	409	4/4	0.99	0.16	31,32,33,40	0
21	FE2	a	401	1/1	0.99	0.06	32,32,32,32	0
25	CL	A	407	1/1	0.99	0.06	28,28,28,28	0
25	CL	A	408	1/1	0.99	0.03	28,28,28,28	0
32	OXY	A	417[B]	11/11	0.99	0.13	20,26,30,32	11
32	OXY	a	418[B]	11/11	0.99	0.11	22,25,29,31	11
33	OEX	A	418[A]	10/10	0.99	0.13	29,31,35,35	10
21	FE2	A	401	1/1	1.00	0.08	27,27,27,27	0

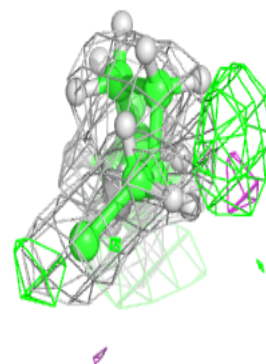
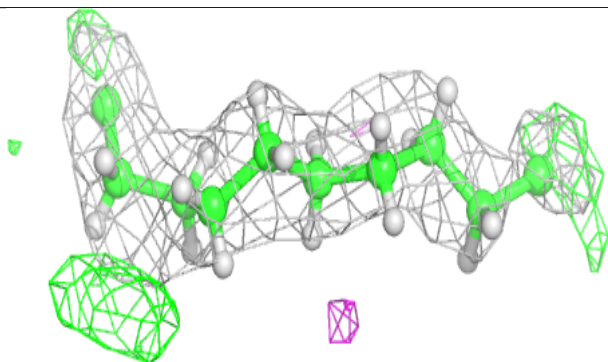
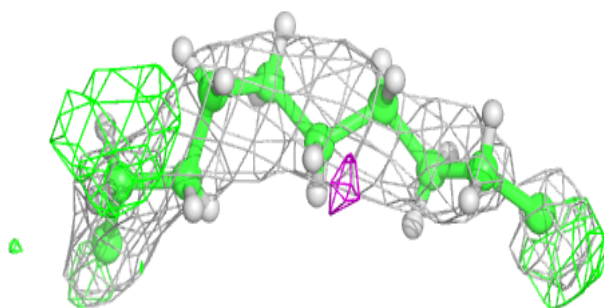
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around STE a 414:

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

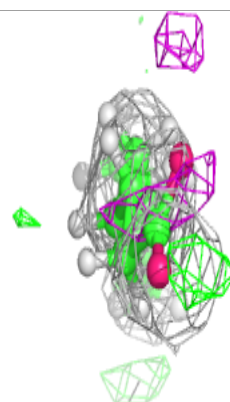
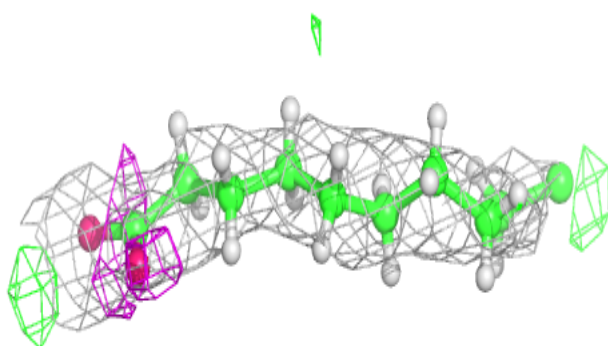
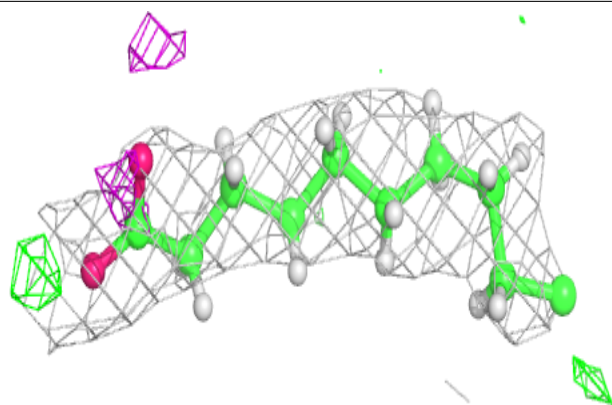
**Electron density around STE b 627:**

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

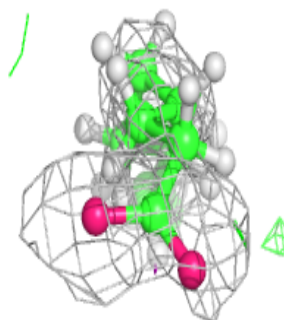
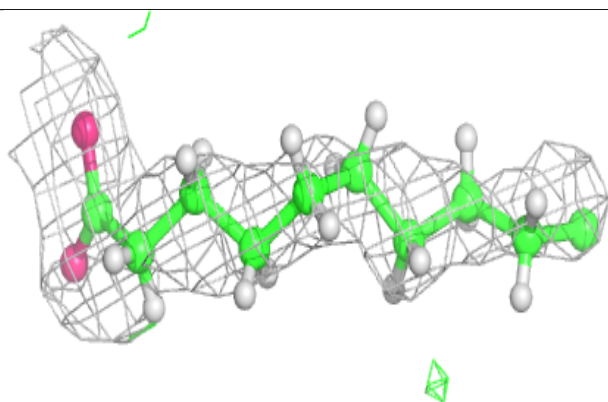
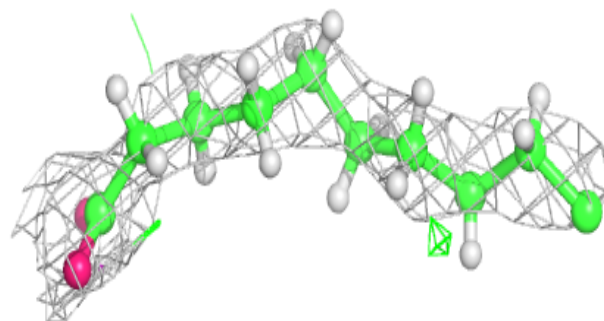


Electron density around STE L 101:

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

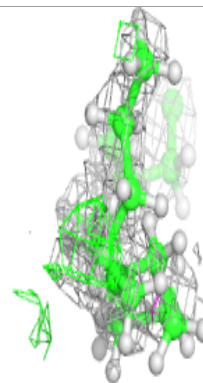
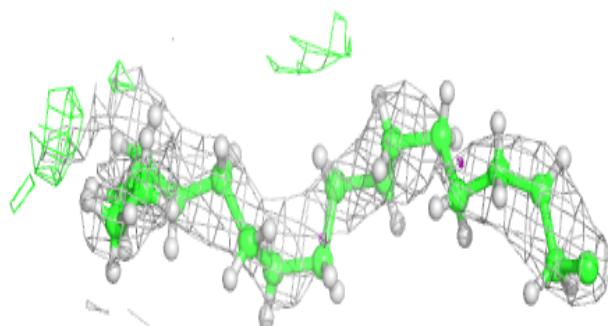
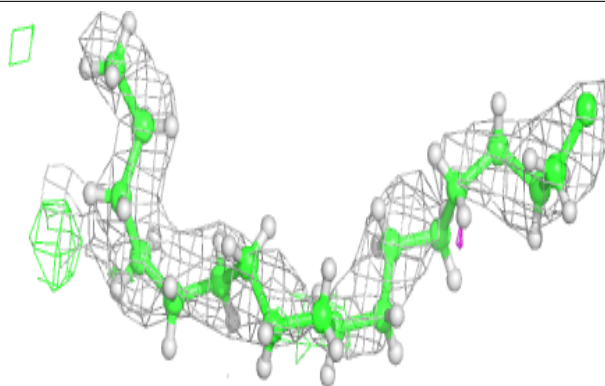
**Electron density around STE R 101:**

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



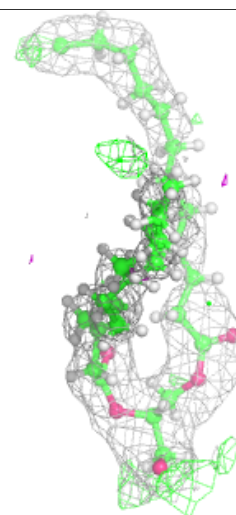
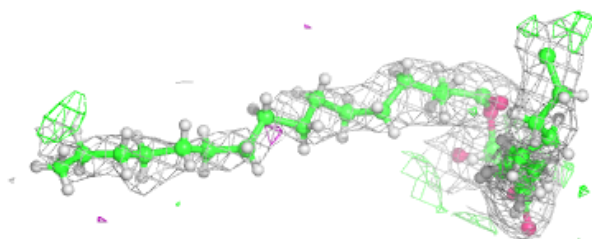
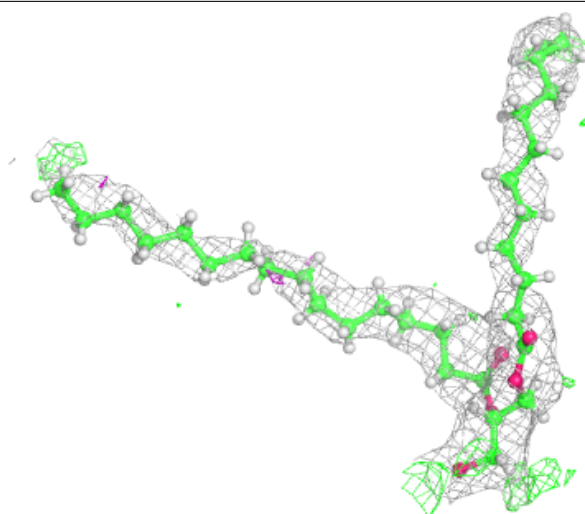
Electron density around STE H 103:

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



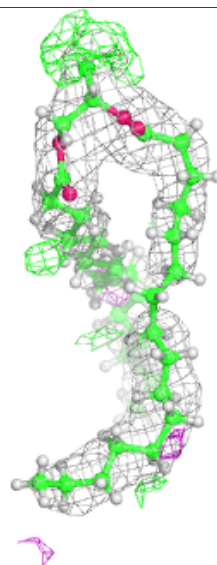
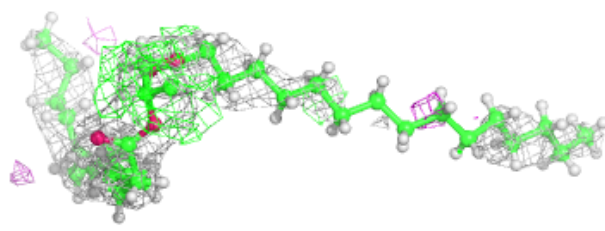
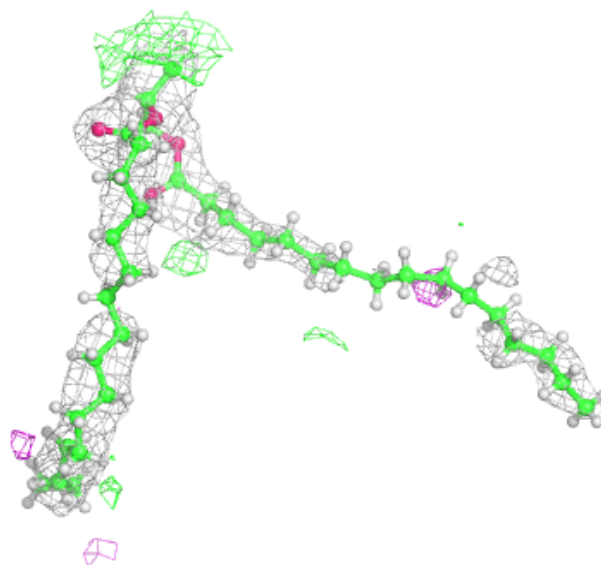
Electron density around SQD a 412:

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



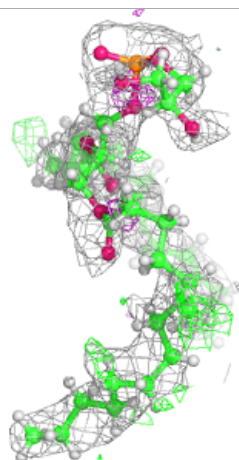
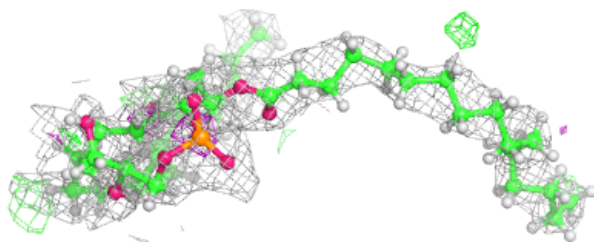
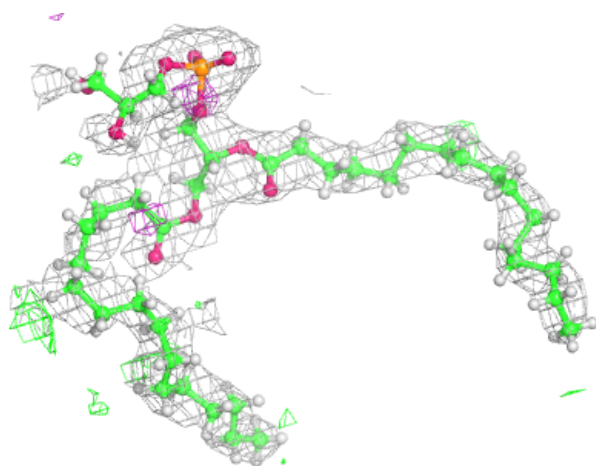
Electron density around SQD A 415:

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



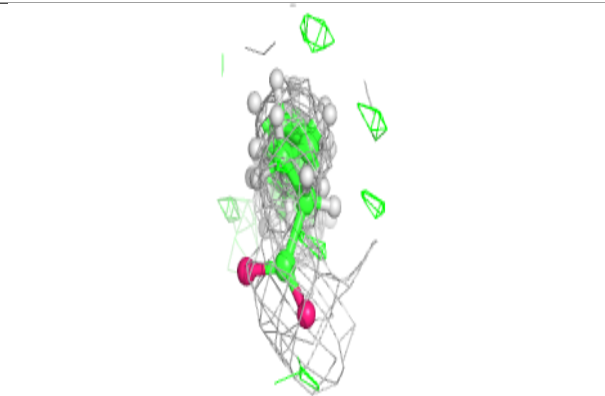
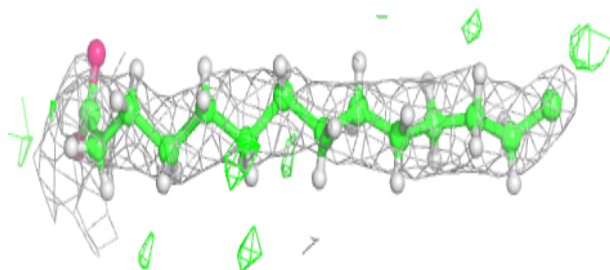
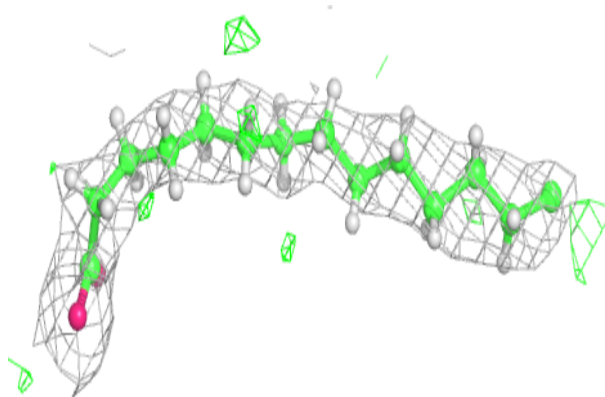
Electron density around LHG A 414:

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

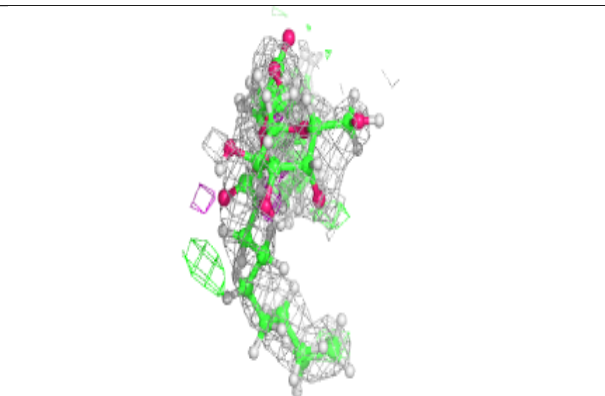
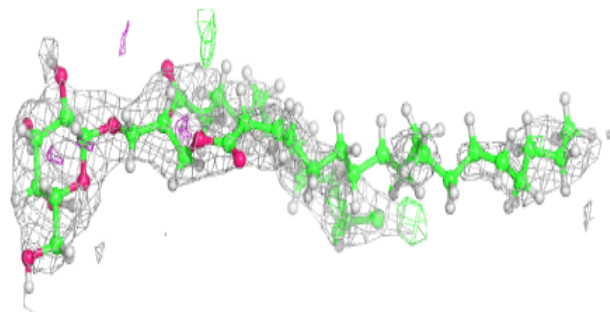
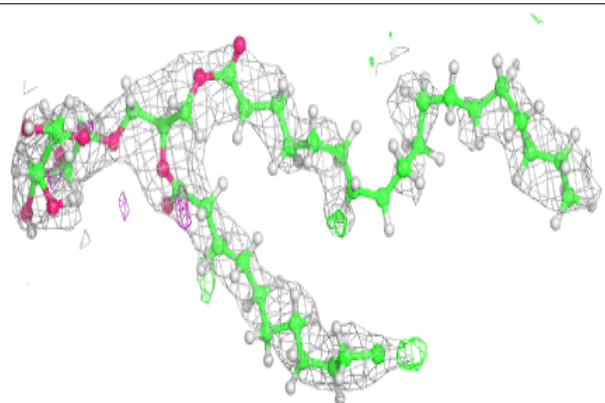


Electron density around STE b 625:

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

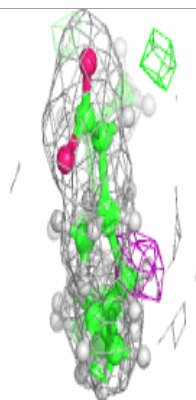
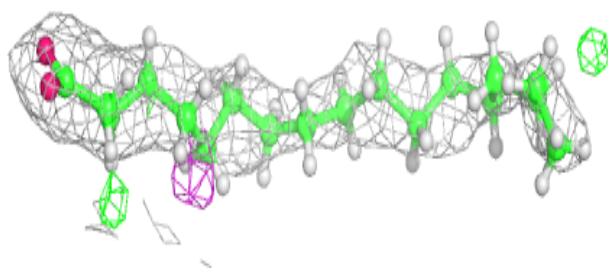
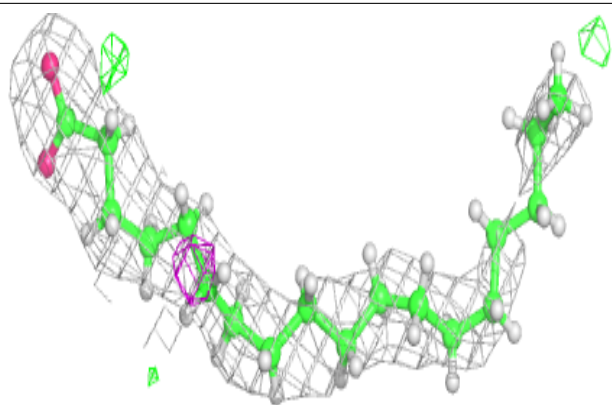
**Electron density around LMG c 521:**

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

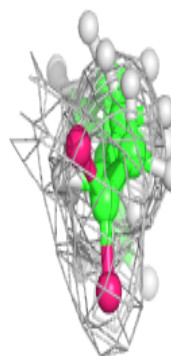
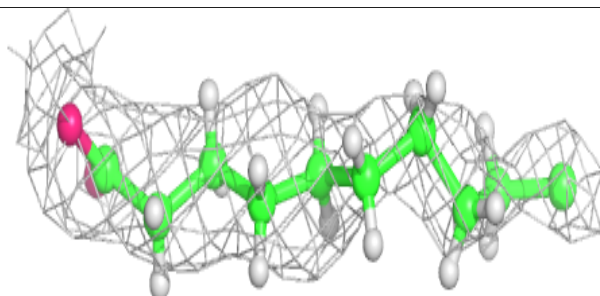
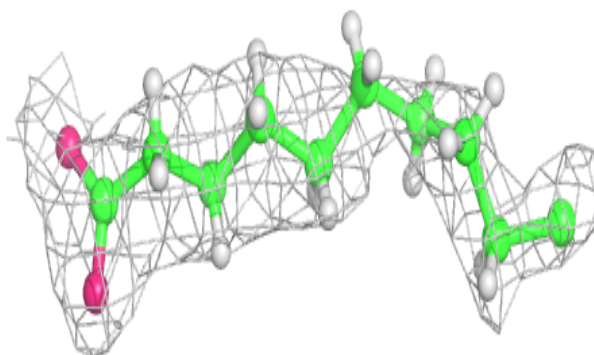


Electron density around STE d 412:

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

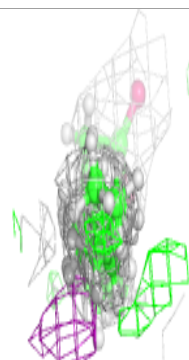
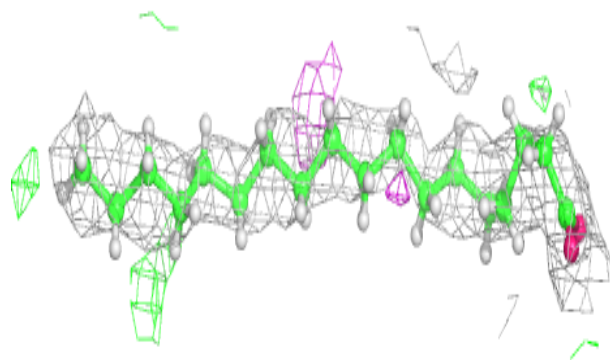
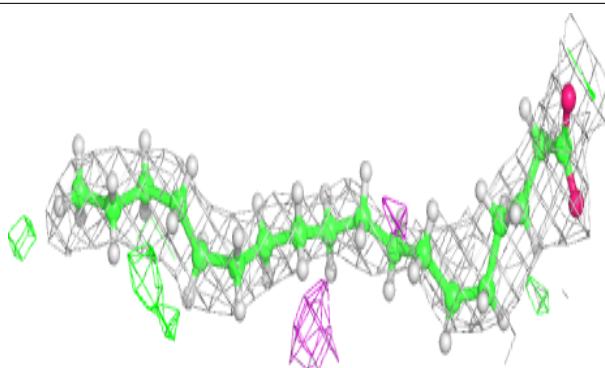
**Electron density around STE c 523:**

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

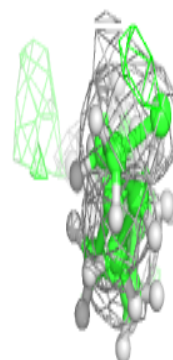
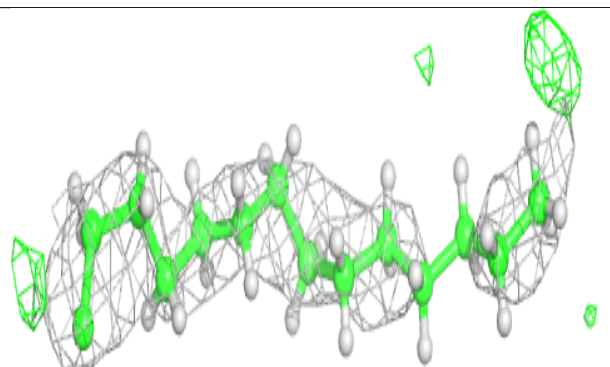
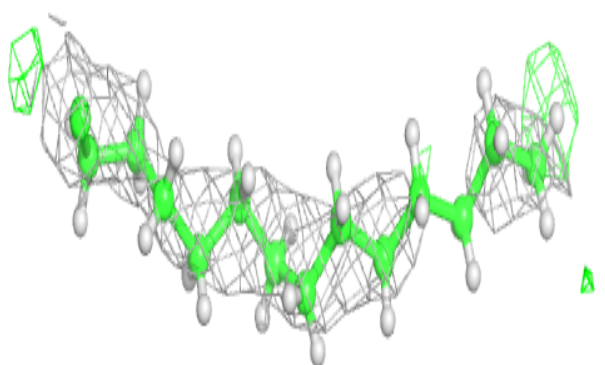


Electron density around STE b 626:

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

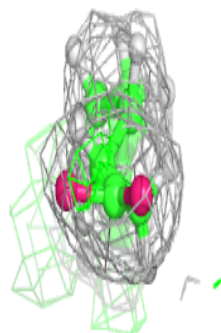
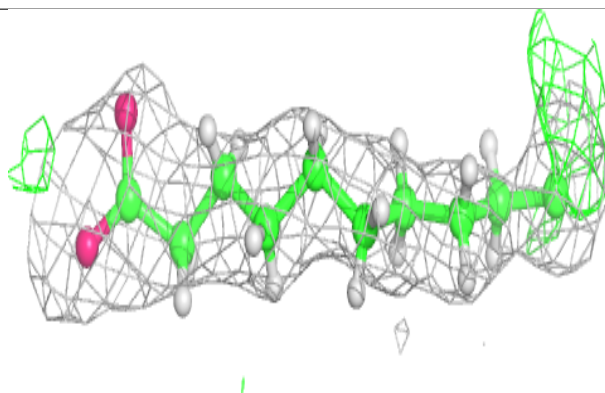
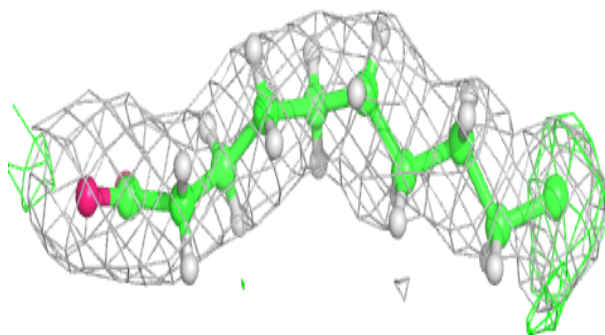
**Electron density around STE h 102:**

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

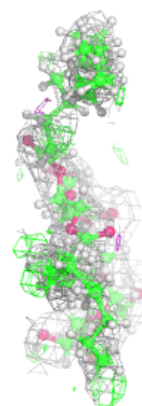
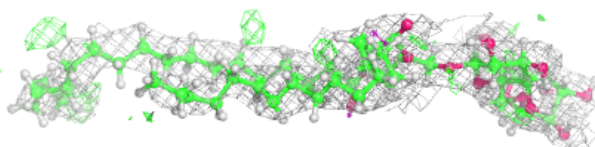
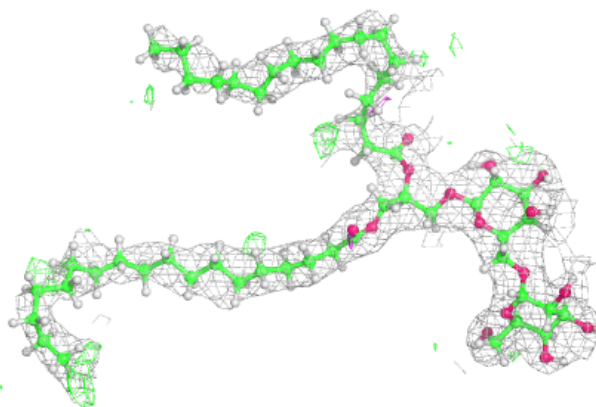


Electron density around STE j 101:

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

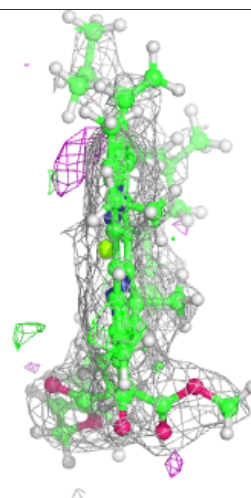
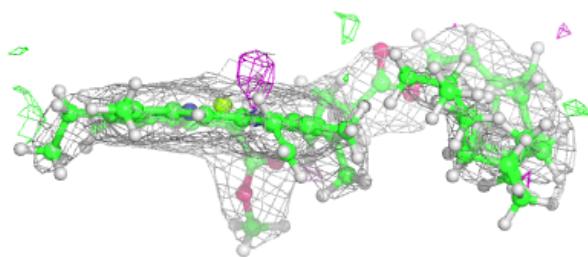
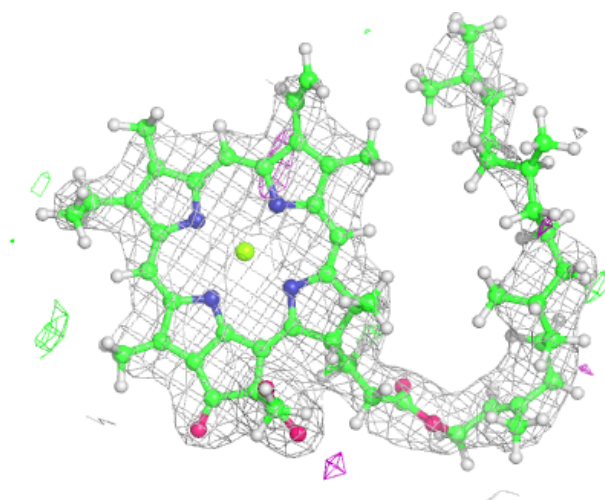
**Electron density around DGD A 416:**

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



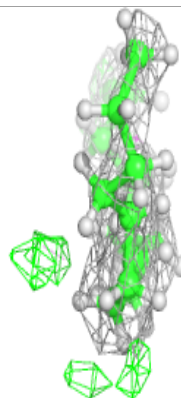
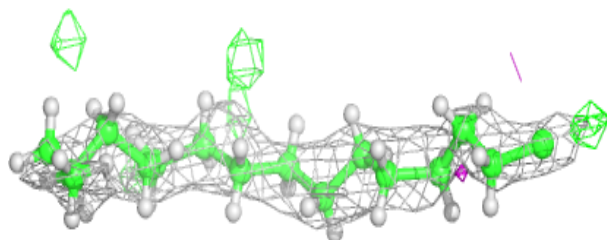
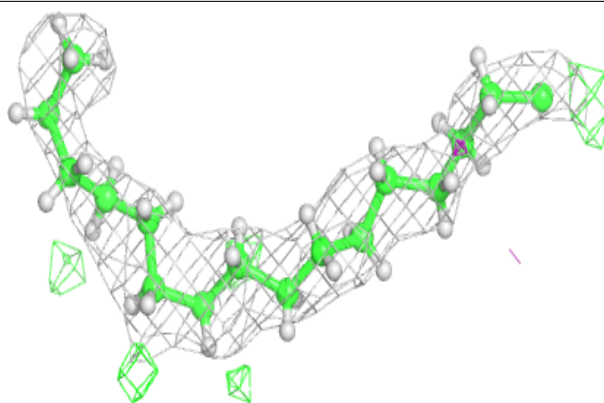
Electron density around CLA C 512:

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

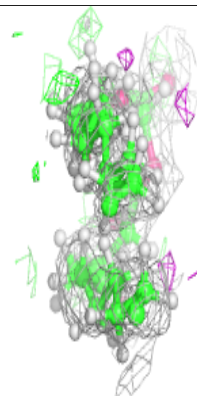
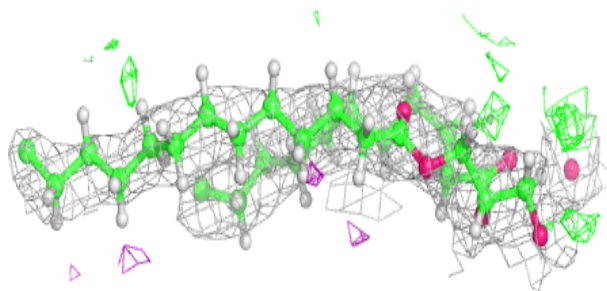
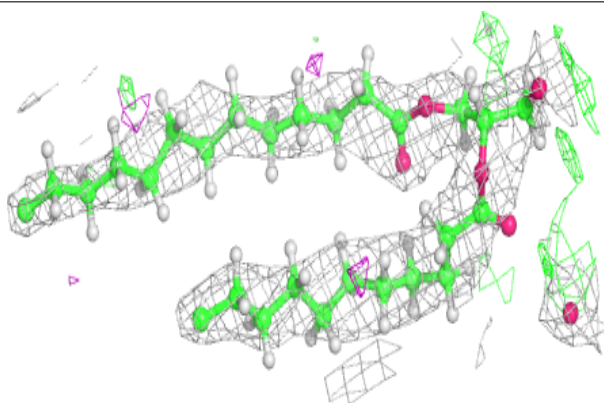


Electron density around STE B 626:

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

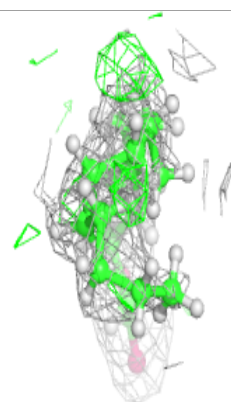
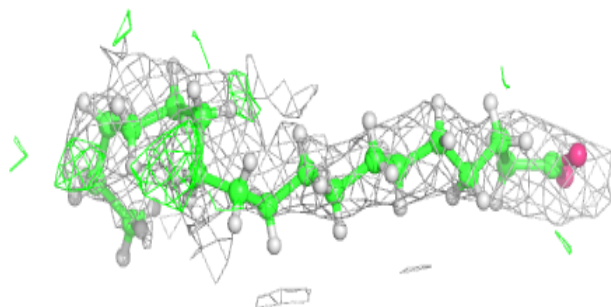
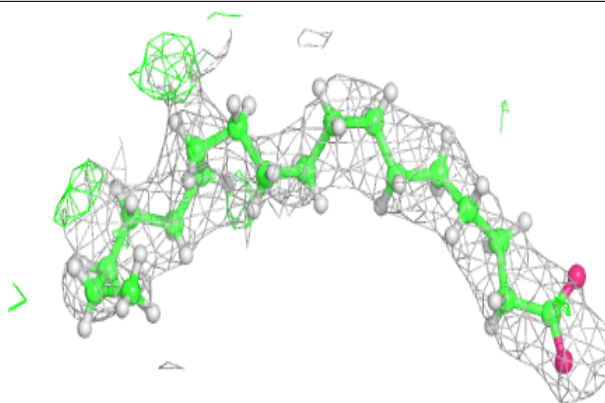
**Electron density around LMG D 410:**

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

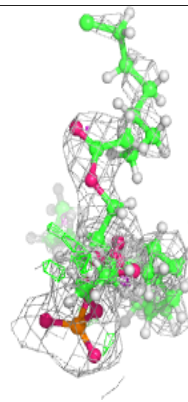
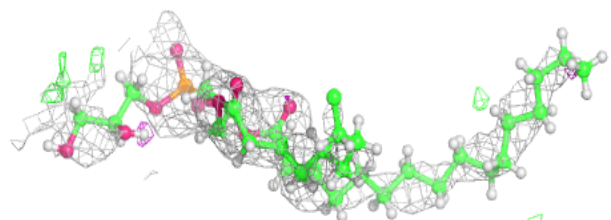
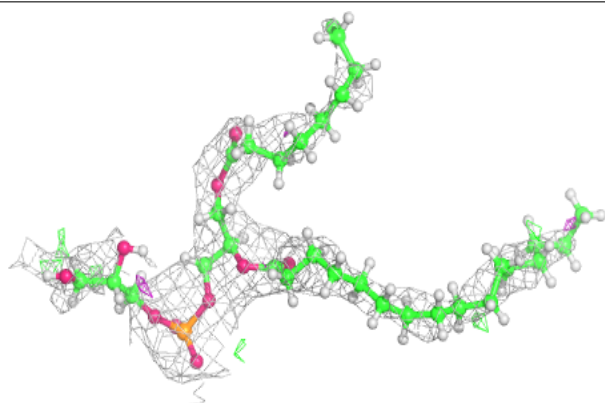


Electron density around STE d 413:

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

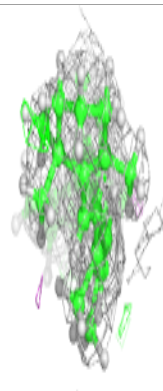
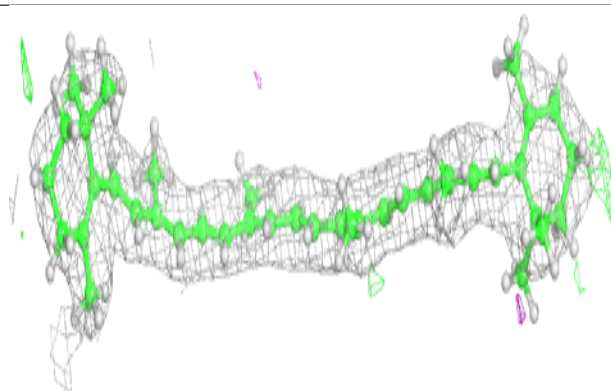
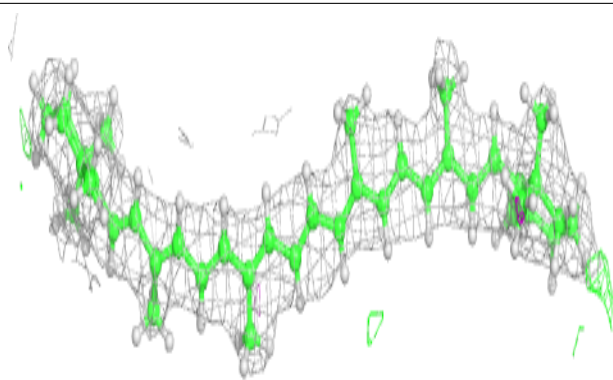
**Electron density around LHG e 102:**

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



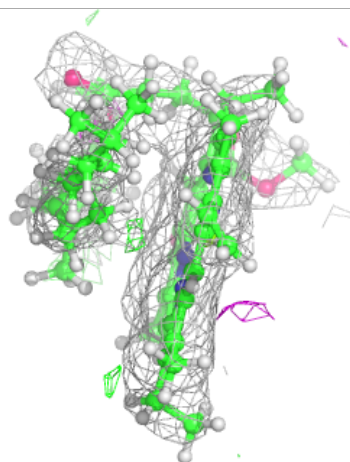
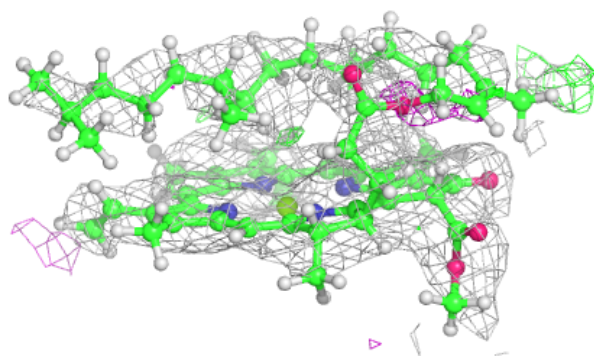
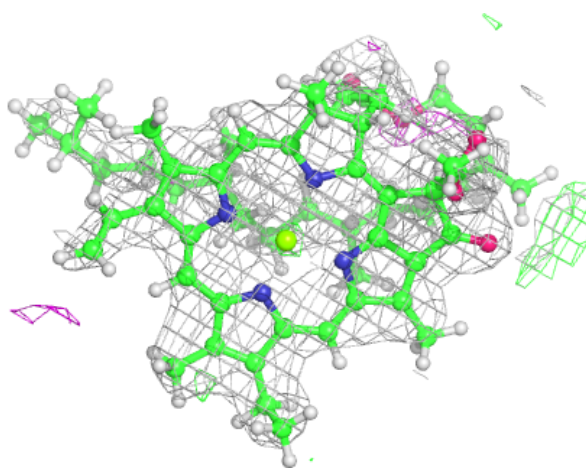
Electron density around BCR H 101:

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



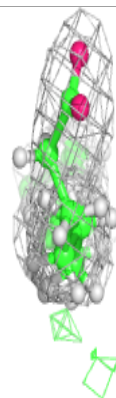
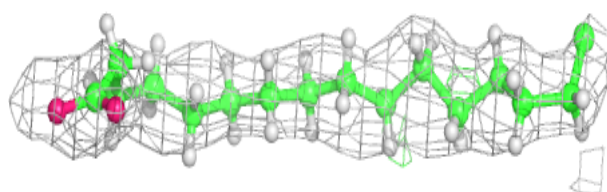
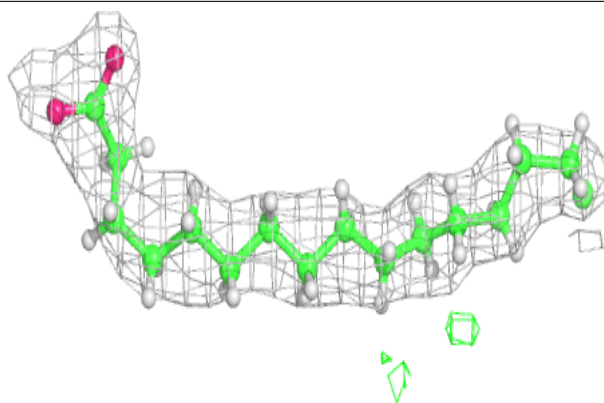
Electron density around CLA b 601:

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

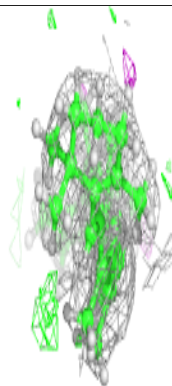
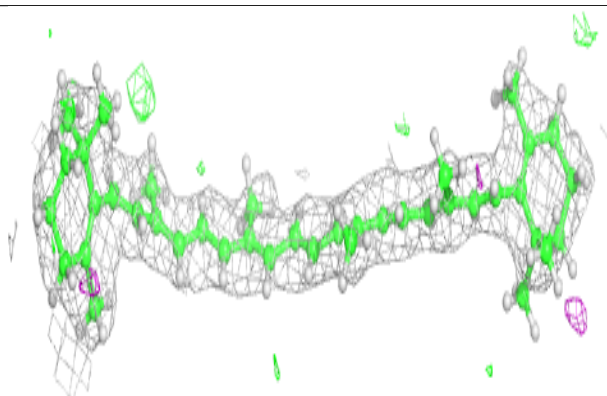
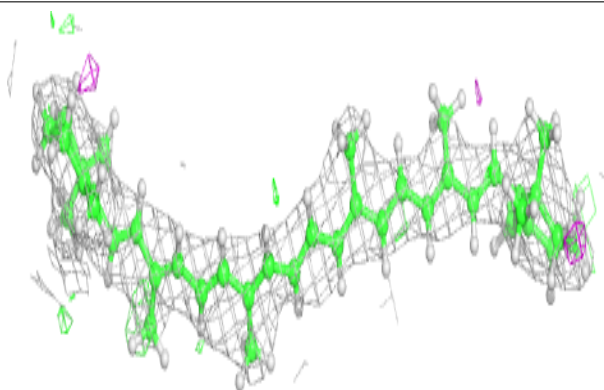


Electron density around STE B 625:

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

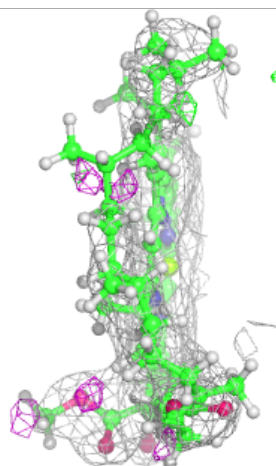
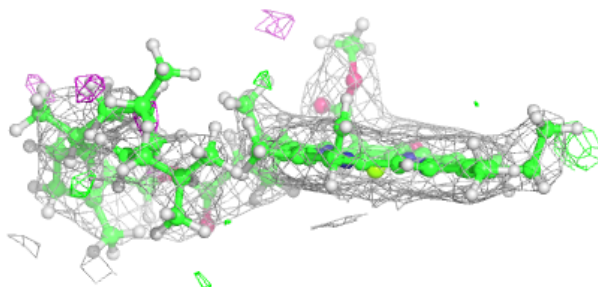
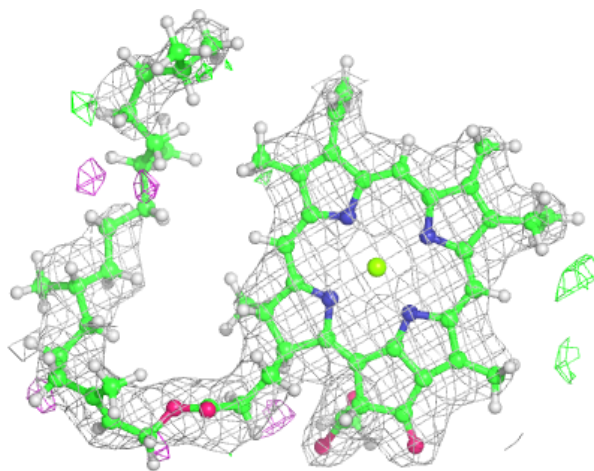
**Electron density around BCR x 101:**

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



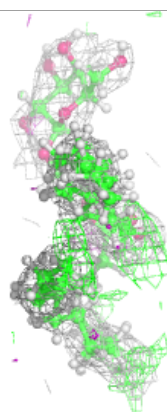
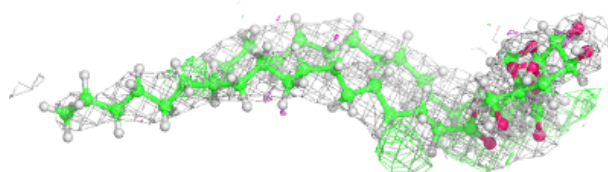
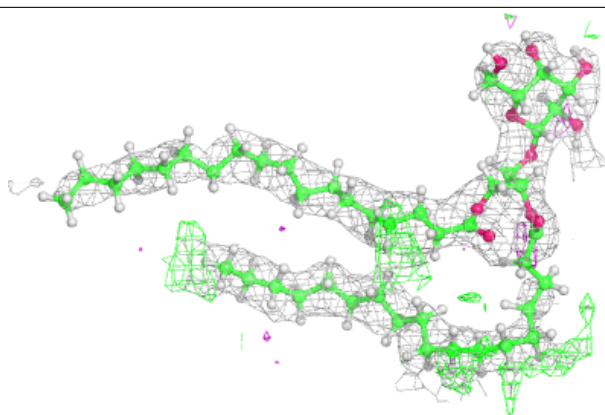
Electron density around CLA c 512:

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

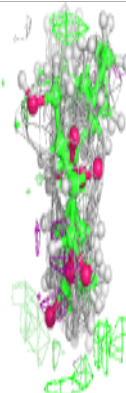
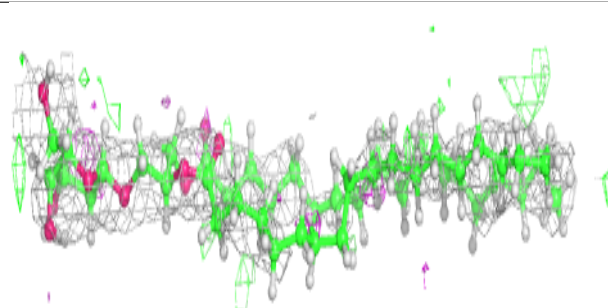
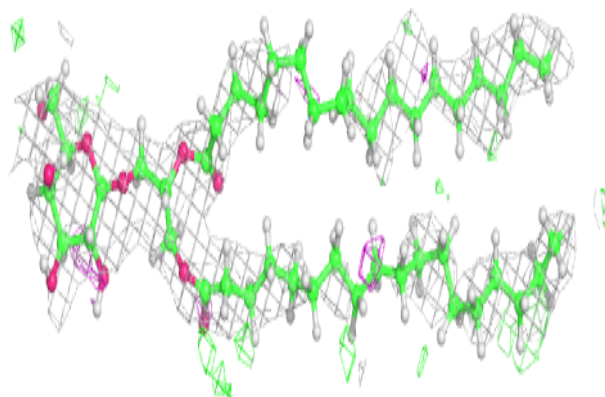


Electron density around LMG a 416:

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

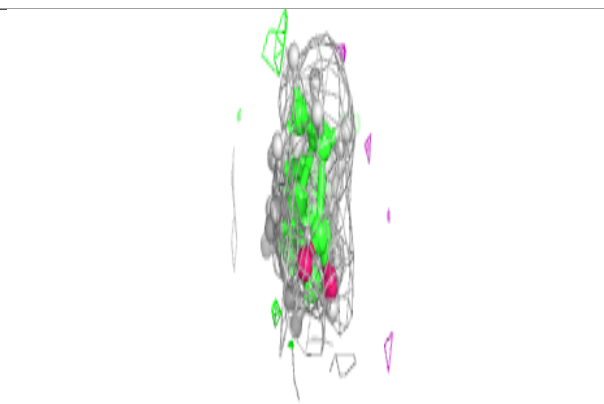
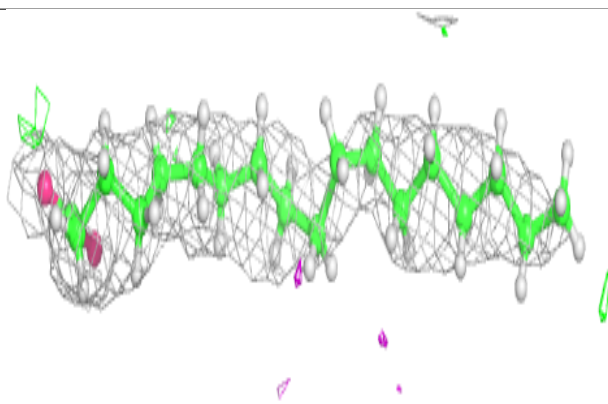
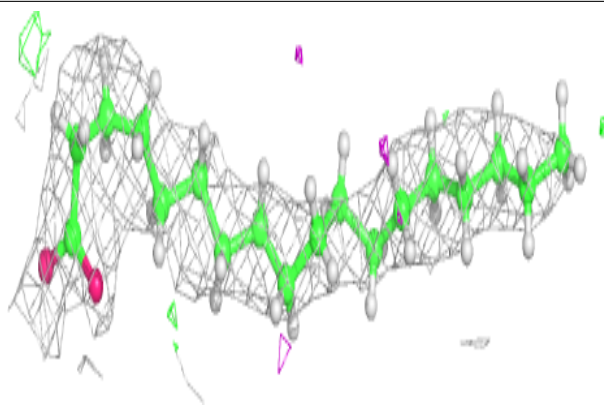
**Electron density around LMG b 624:**

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

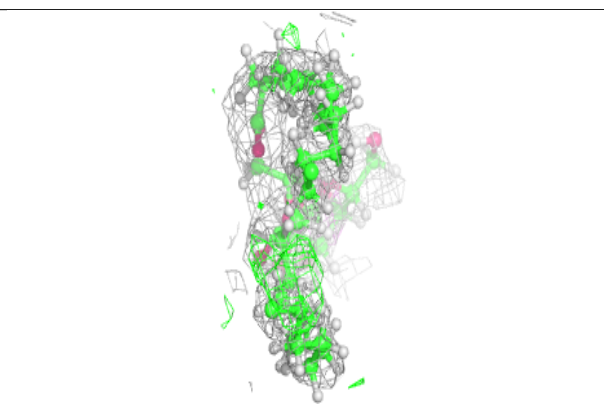
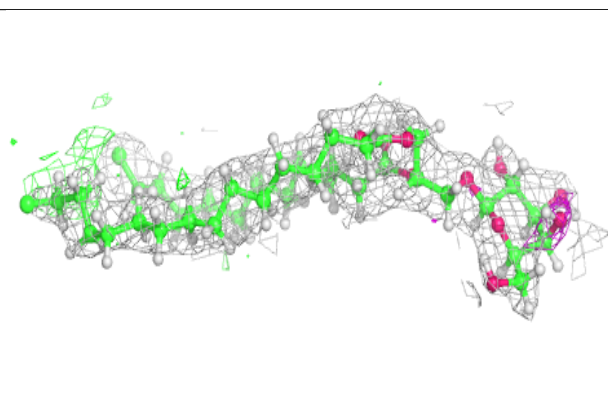
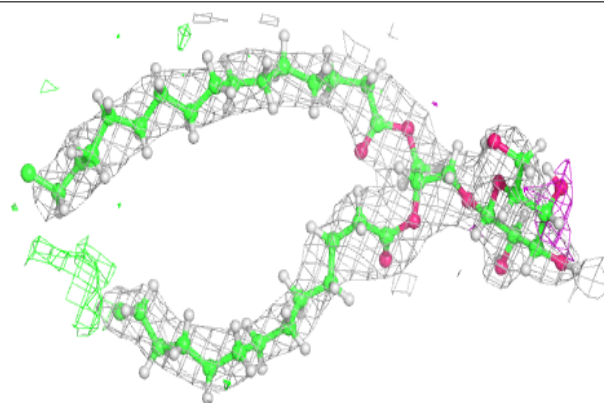


Electron density around STE c 520:

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

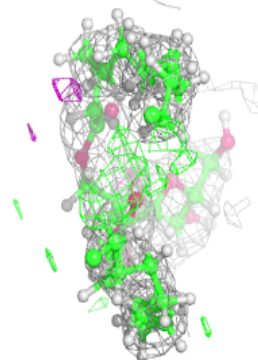
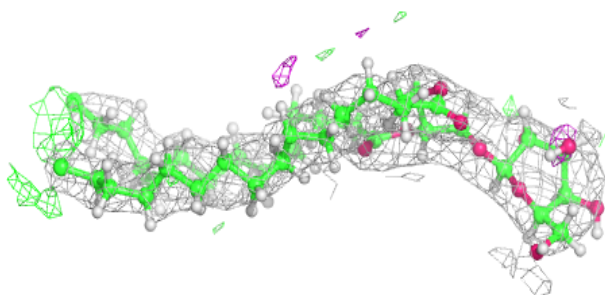
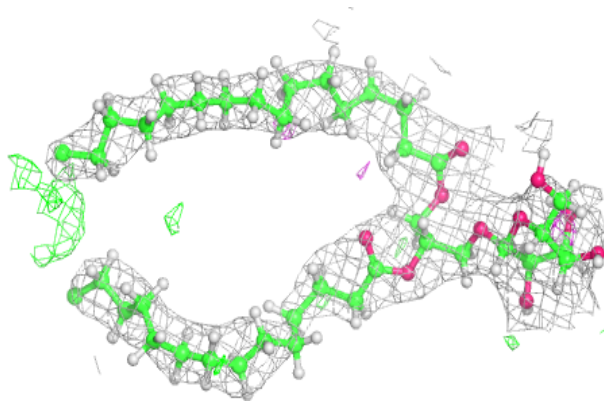
**Electron density around LMG A 412:**

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

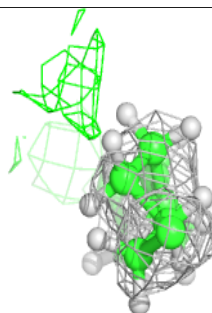
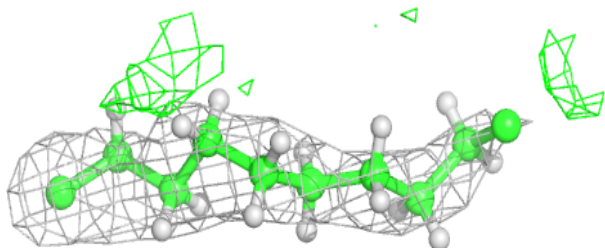
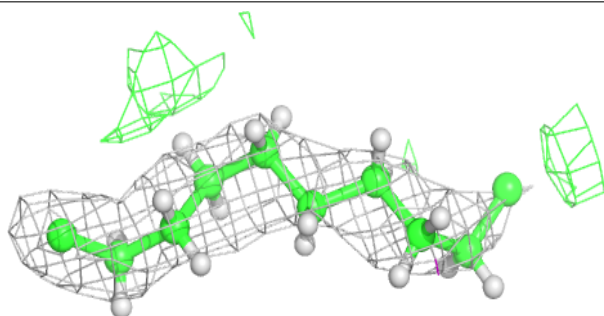


Electron density around LMG c 522:

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

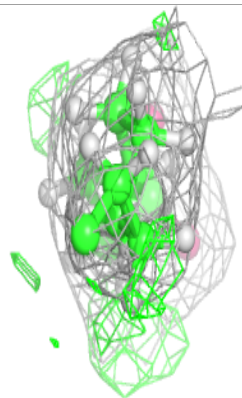
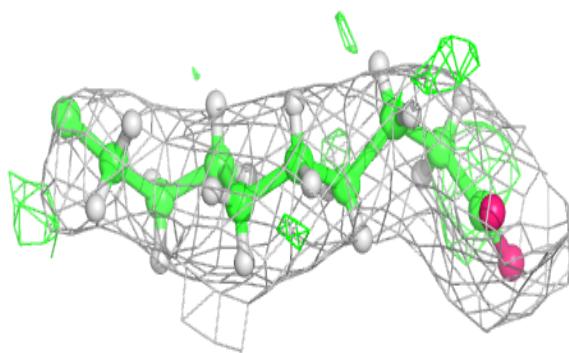
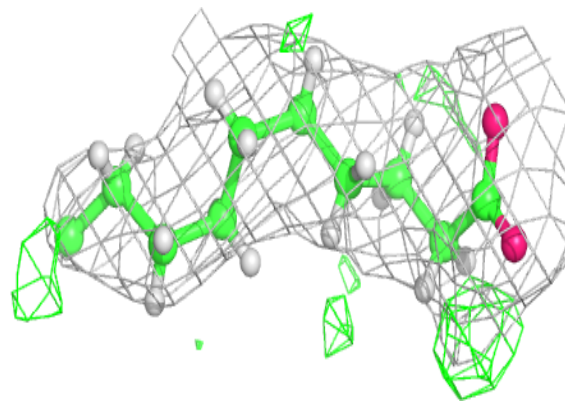
**Electron density around STE a 413:**

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

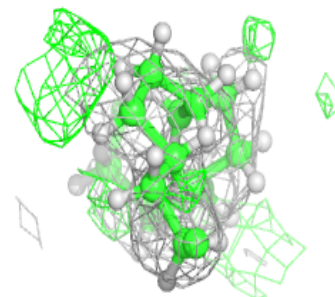
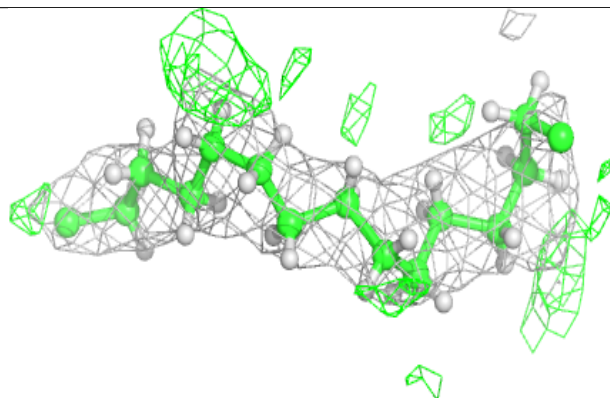
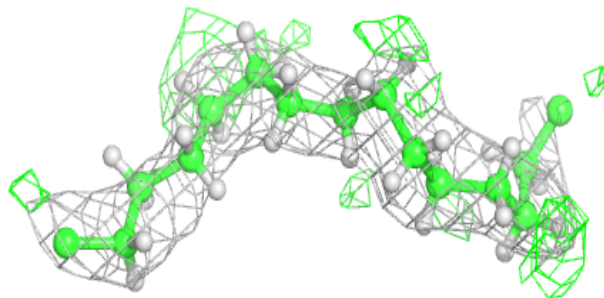


Electron density around STE B 624:

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

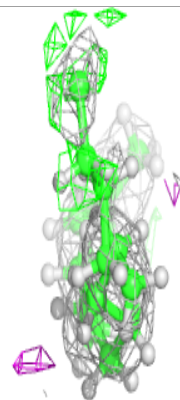
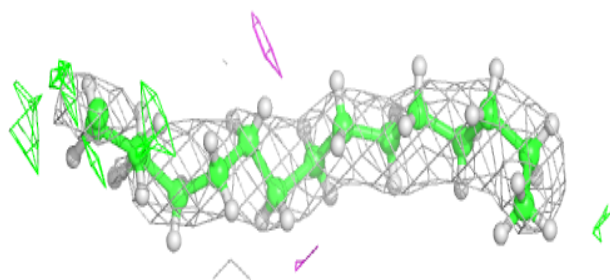
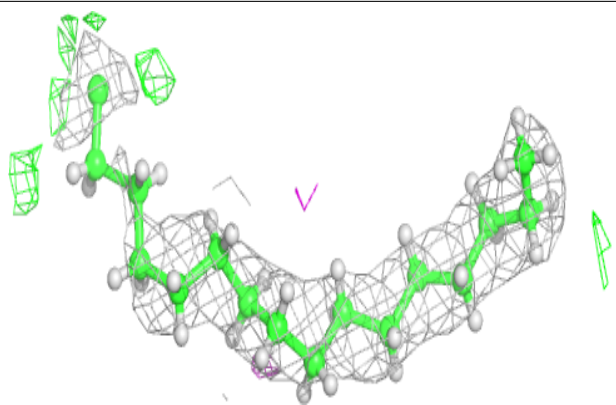
**Electron density around STE a 415:**

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

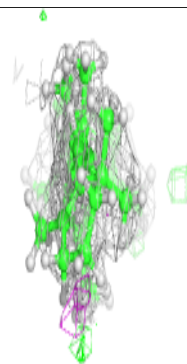
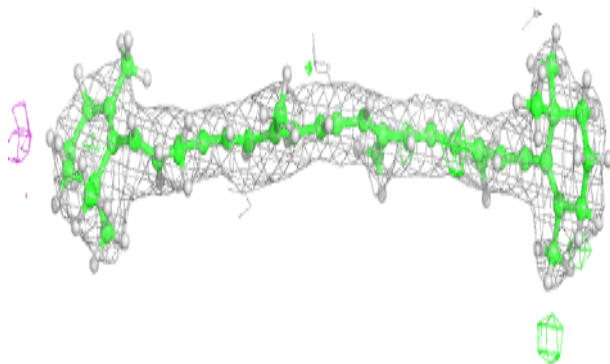
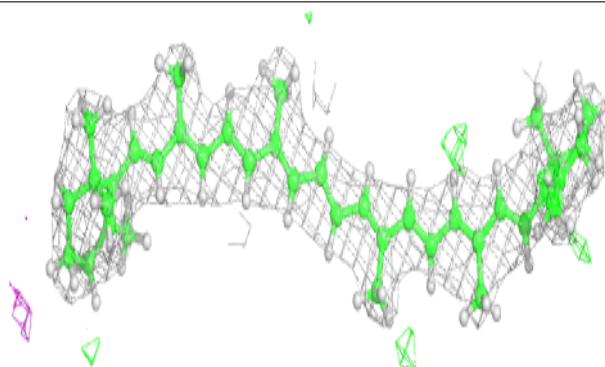


Electron density around STE b 621:

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

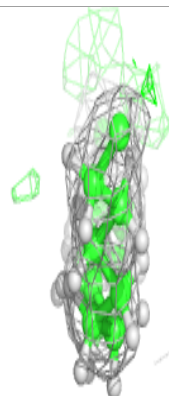
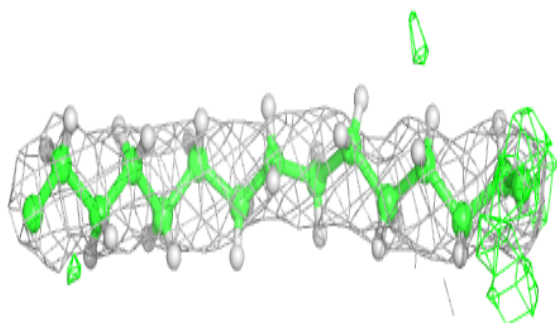
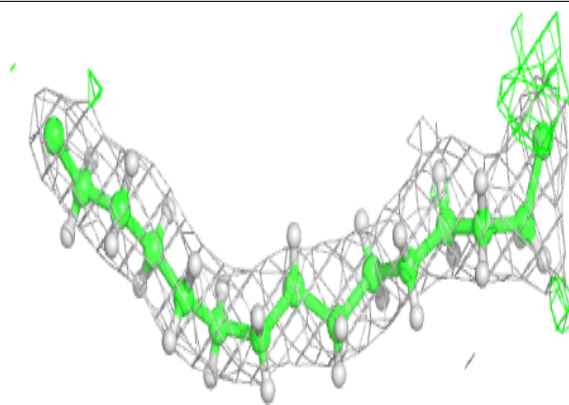
**Electron density around BCR Y 101:**

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

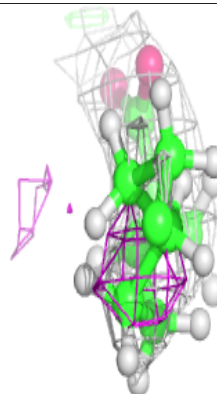
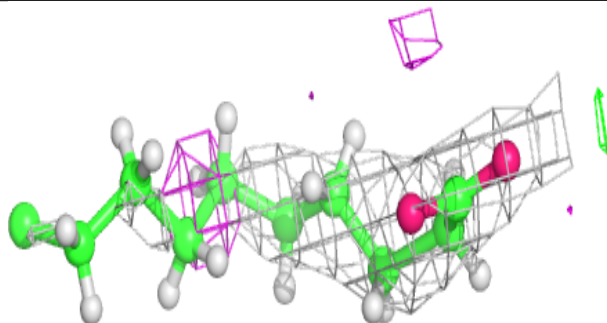
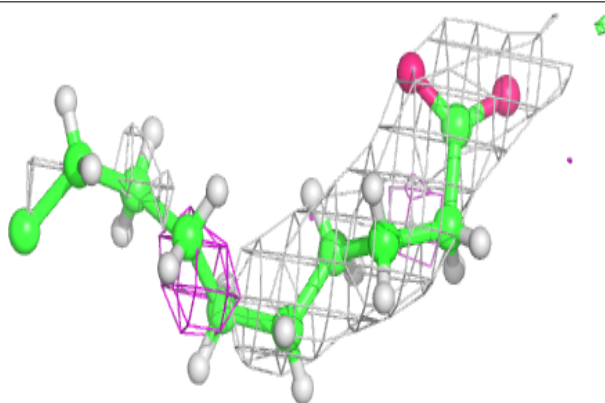


Electron density around STE I 101:

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

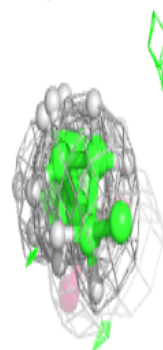
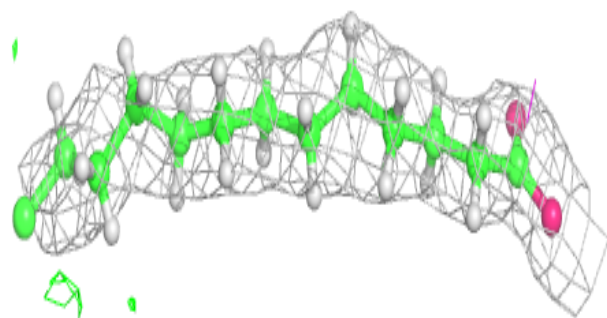
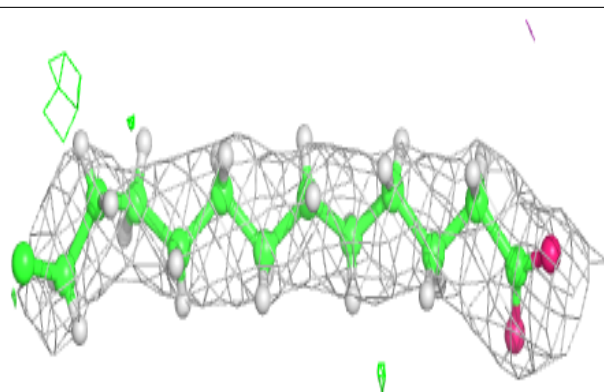
**Electron density around STE B 627:**

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

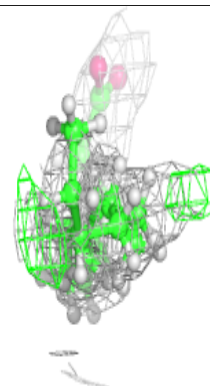
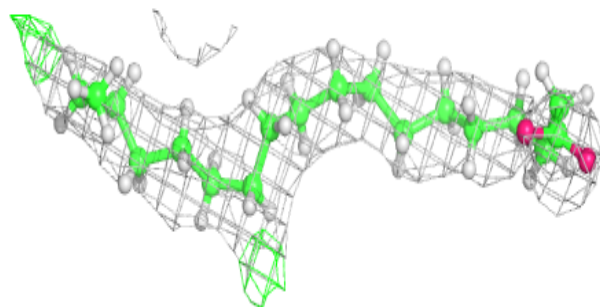
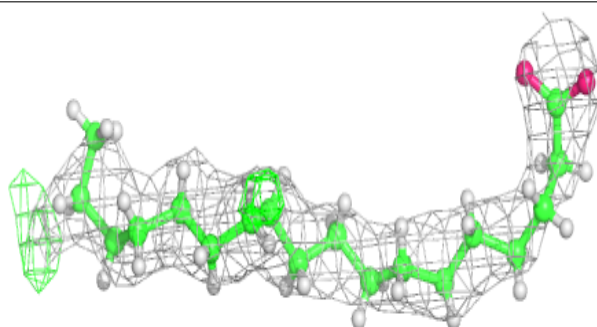


Electron density around STE M 102:

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

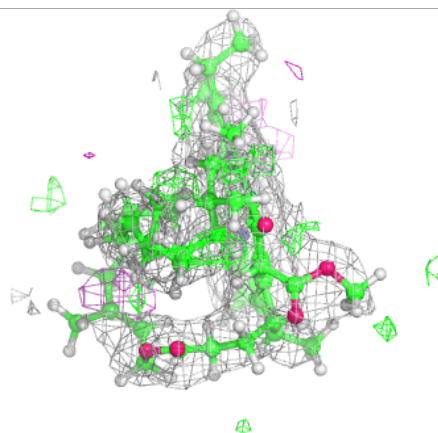
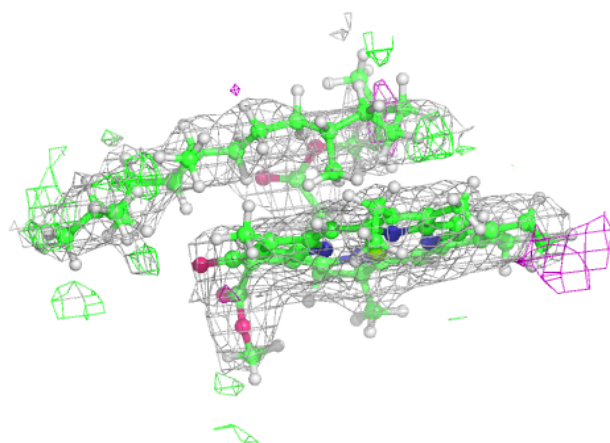
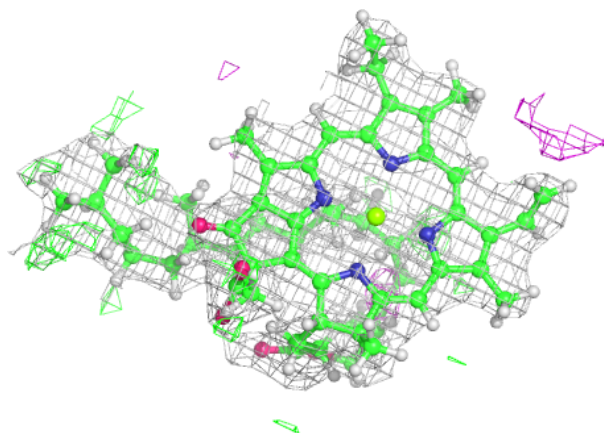
**Electron density around STE b 623:**

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



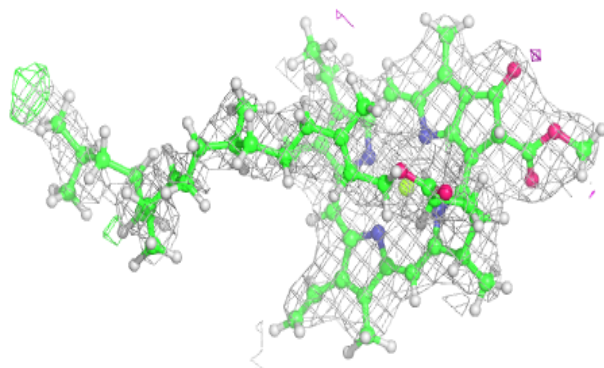
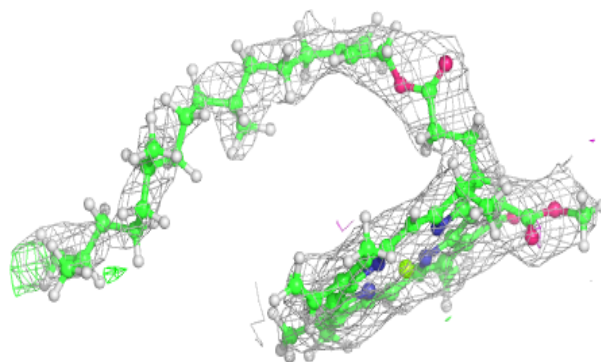
Electron density around CLA B 601:

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

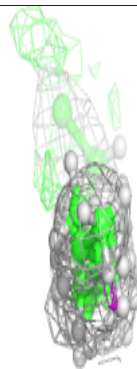
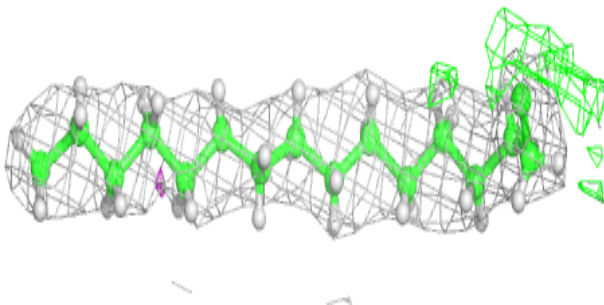
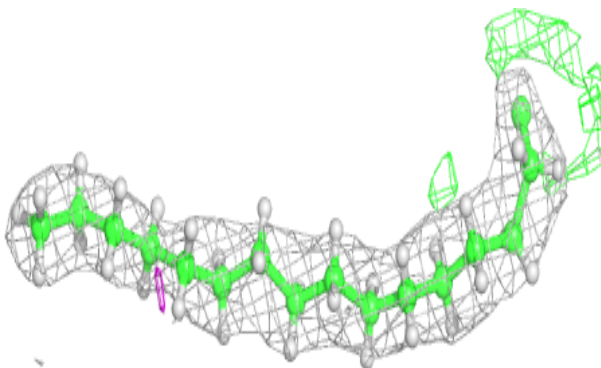


Electron density around CLA C 513:

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

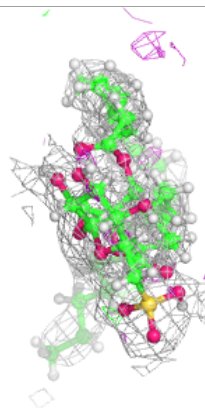
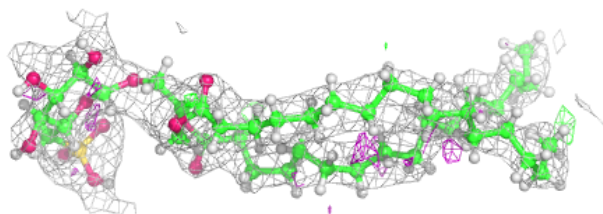
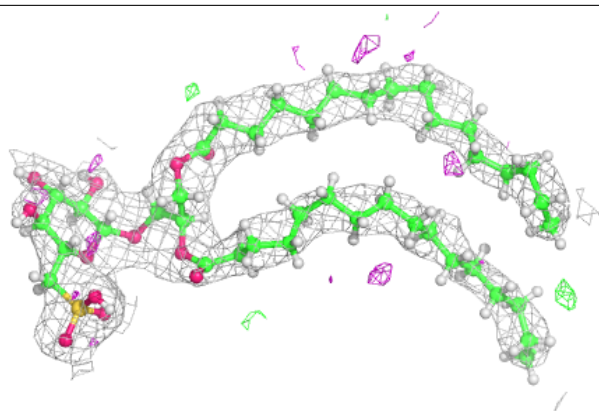
**Electron density around STE C 520:**

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

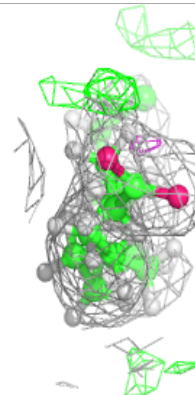
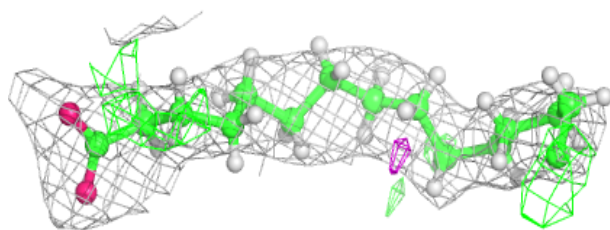
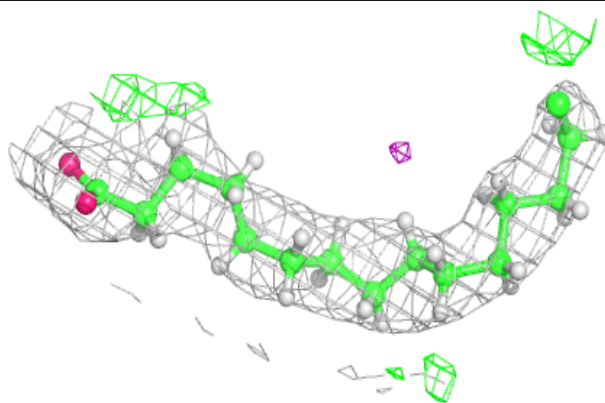


Electron density around SQD B 623:

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

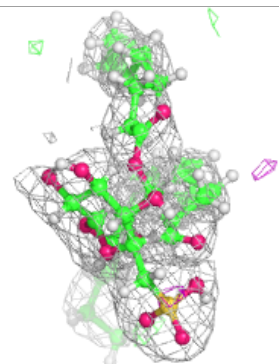
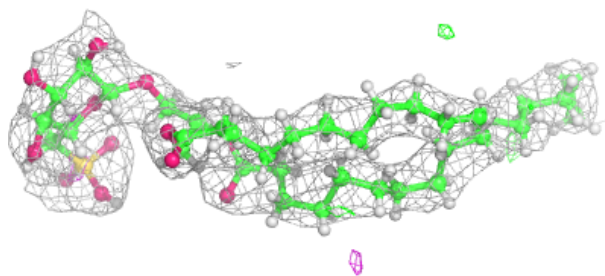
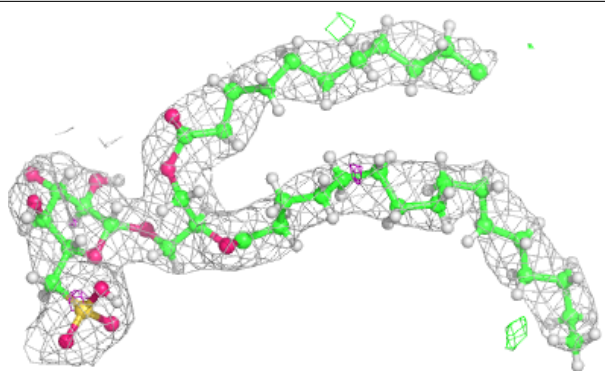
**Electron density around STE B 620:**

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

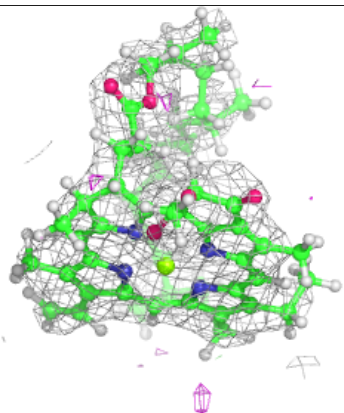
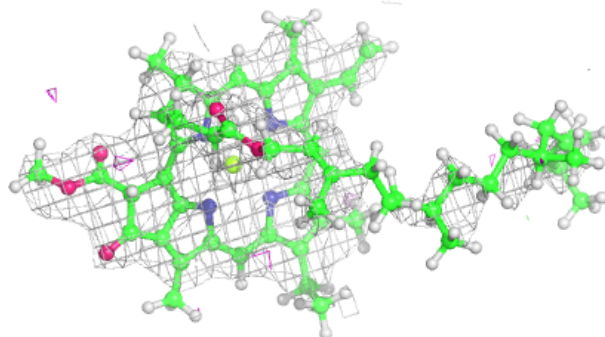
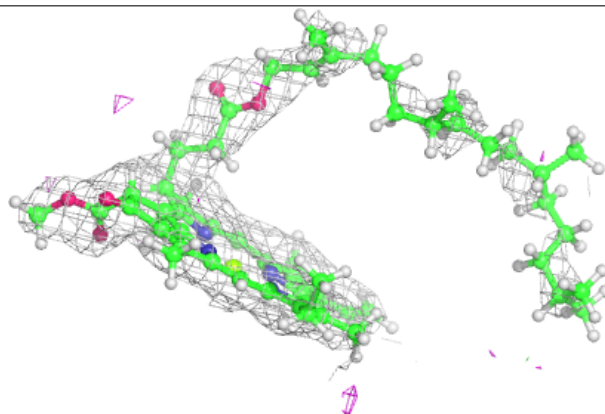


Electron density around SQD b 620:

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

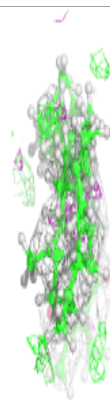
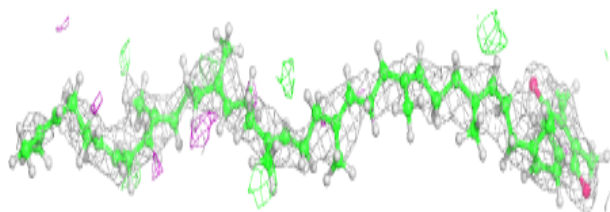
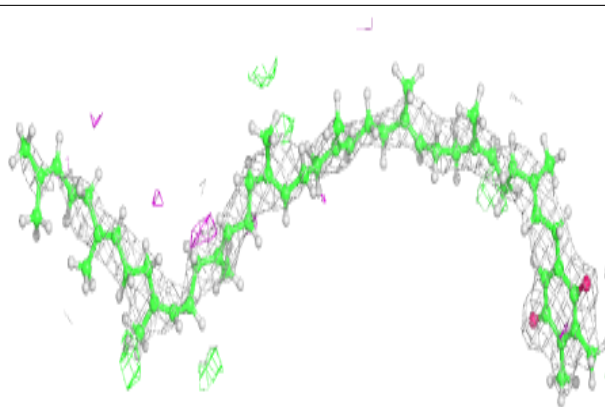
**Electron density around CLA c 513:**

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

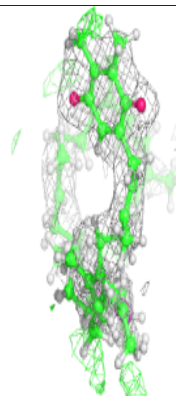
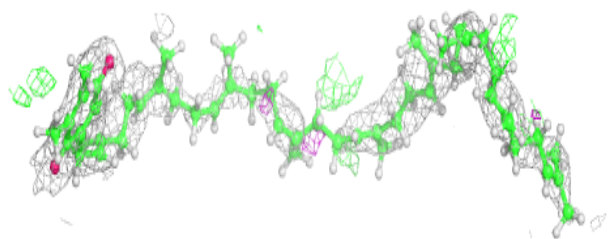
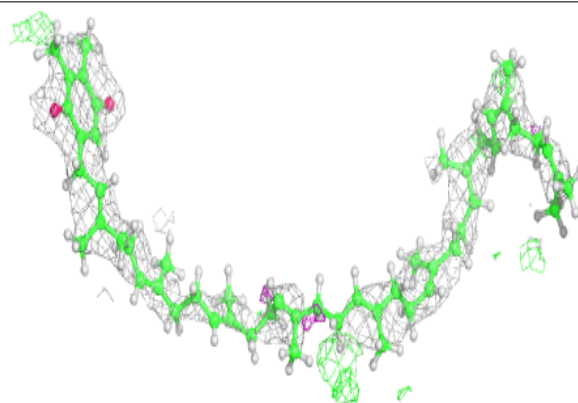


Electron density around PL9 A 410:

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

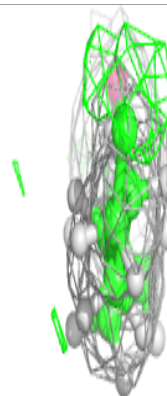
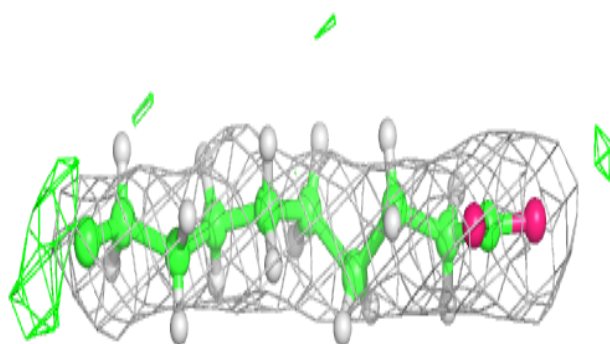
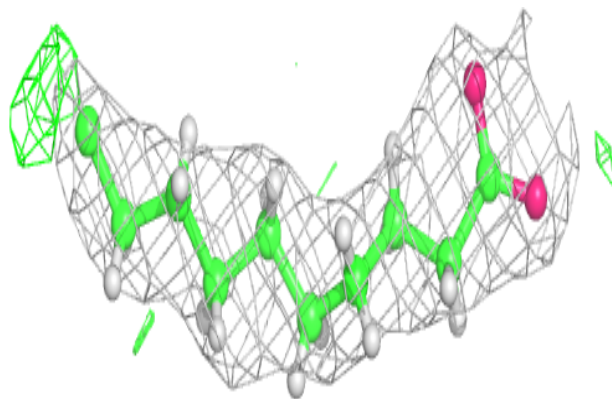
**Electron density around PL9 a 409:**

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

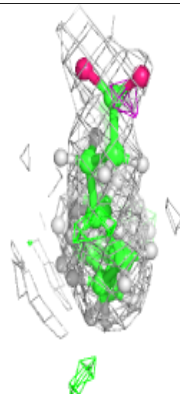
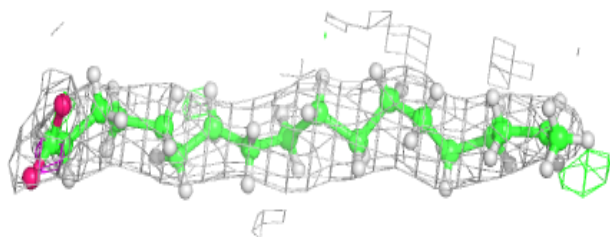
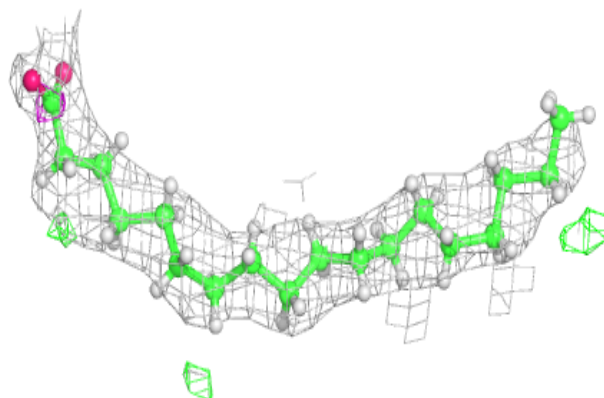


Electron density around STE C 519:

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

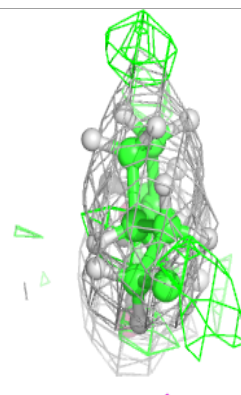
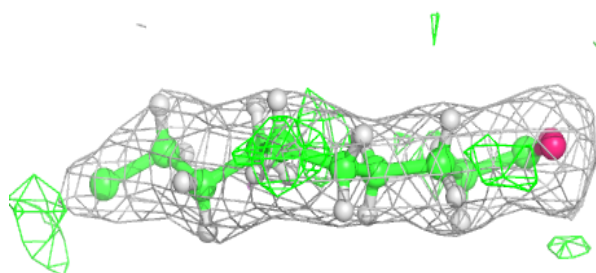
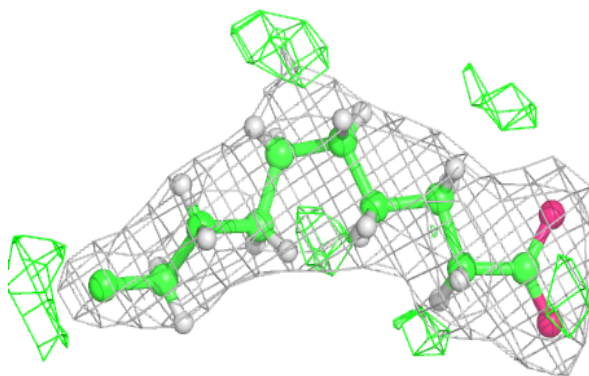
**Electron density around STE X 101:**

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

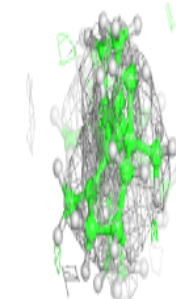
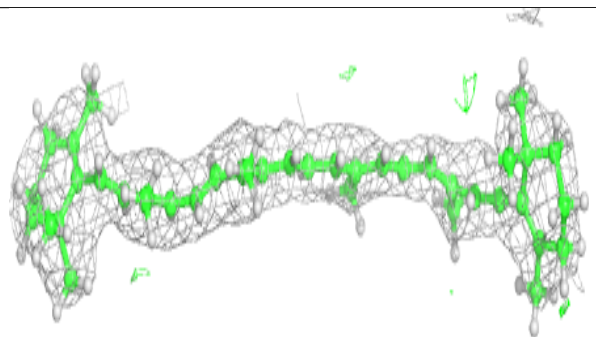
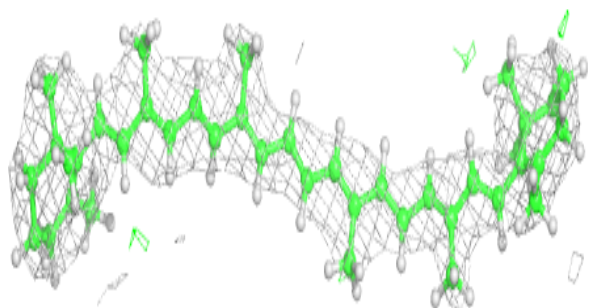


Electron density around STE C 521:

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

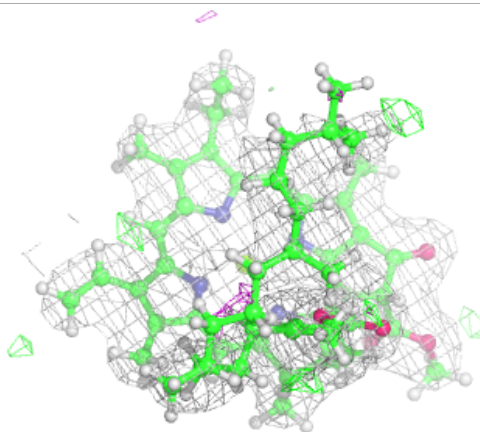
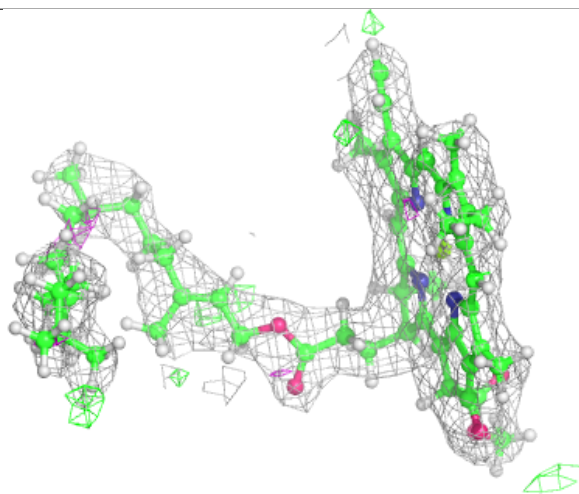
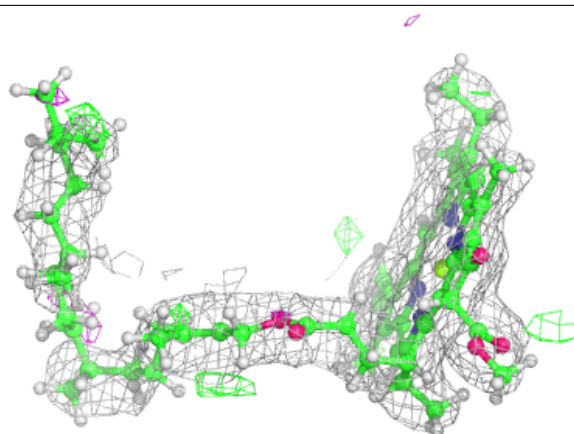
**Electron density around BCR k 101:**

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



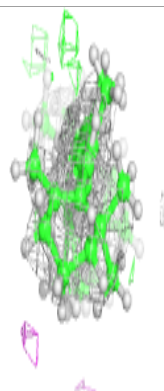
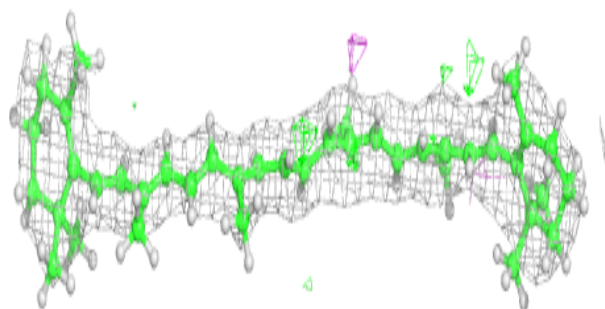
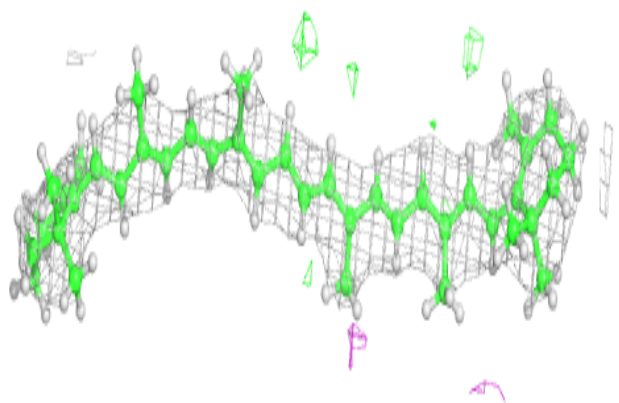
Electron density around CLA a 404:

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

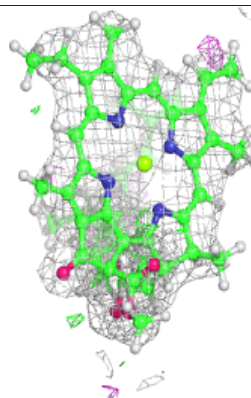
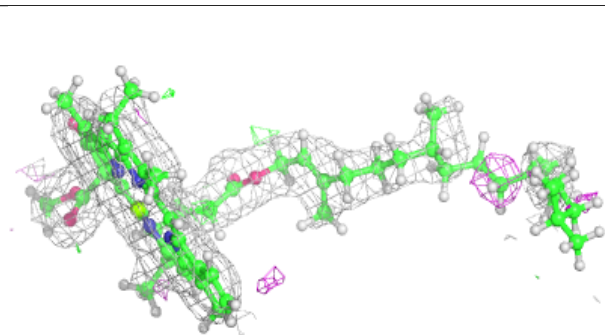
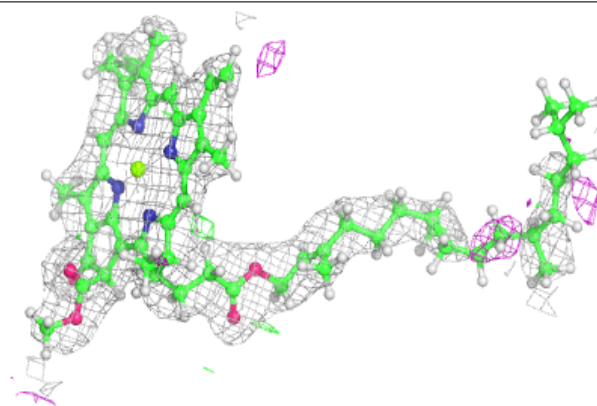


Electron density around BCR K 101:

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

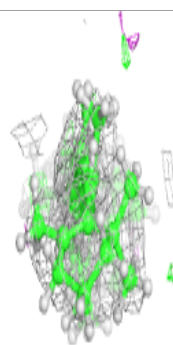
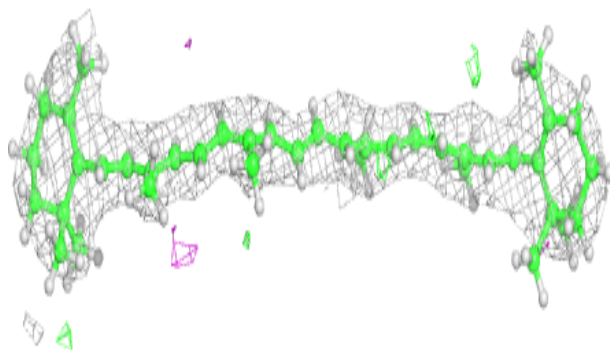
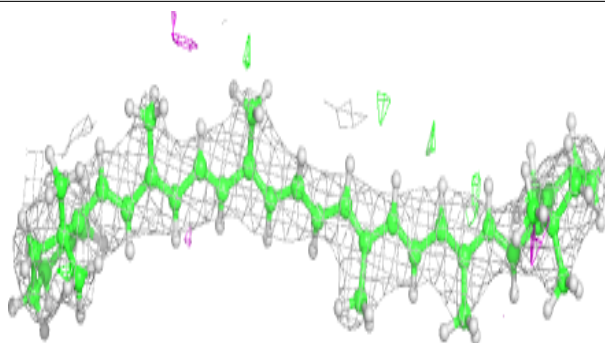
**Electron density around CLA d 404:**

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

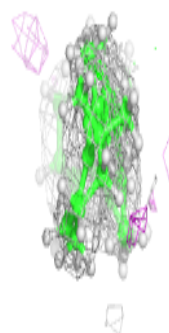
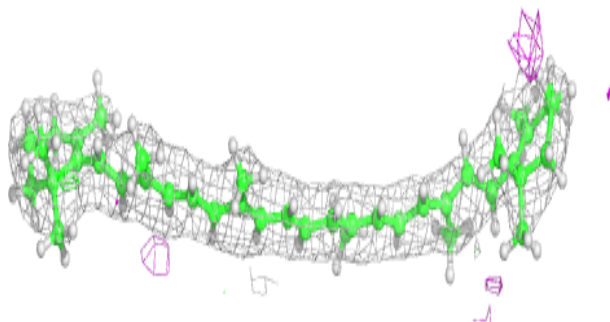
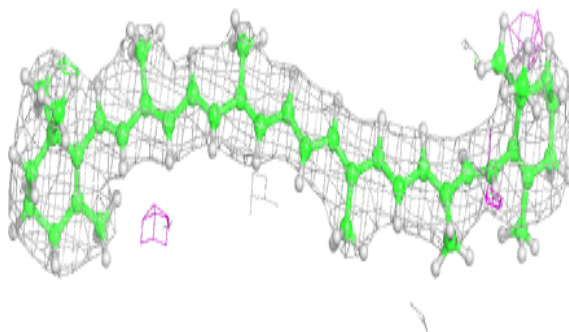


Electron density around BCR c 514:

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

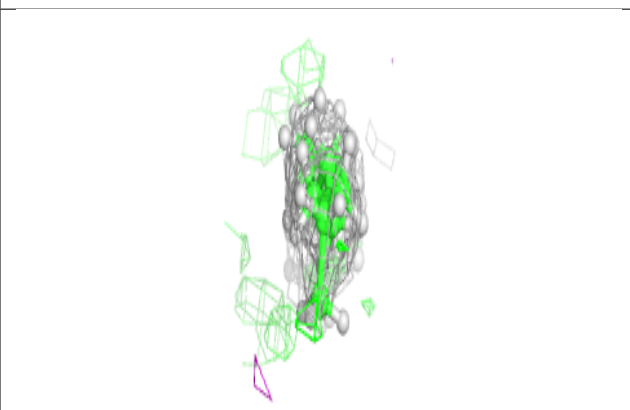
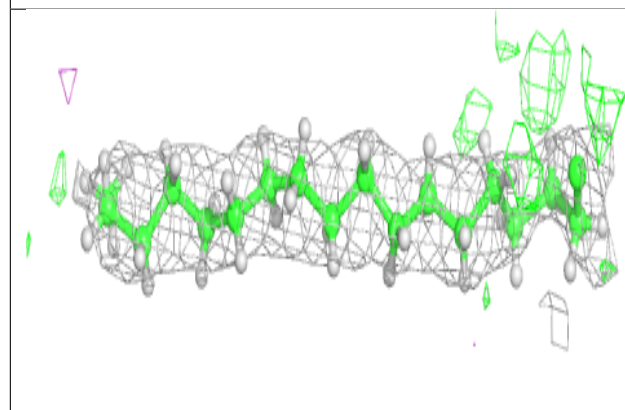
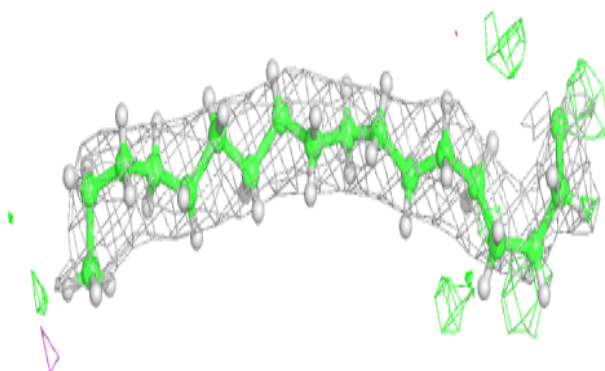
**Electron density around BCR d 405:**

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

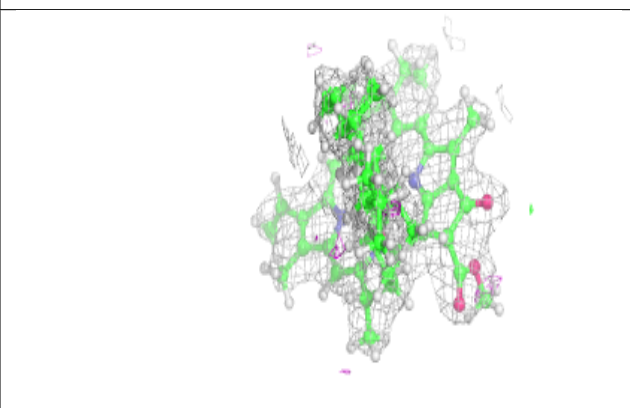
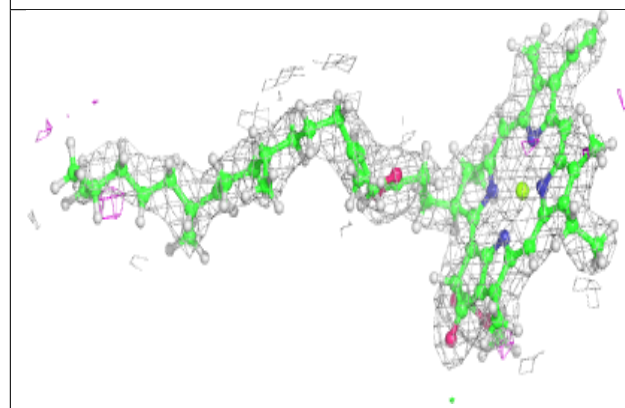
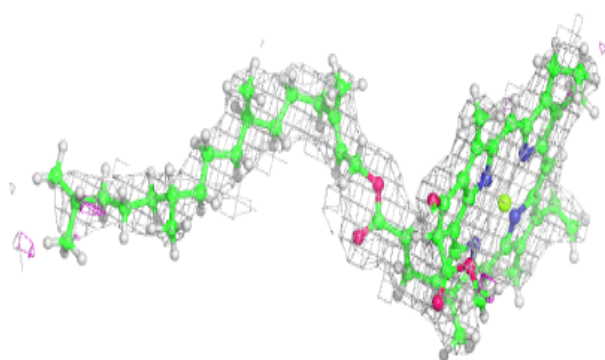


Electron density around STE 1 102:

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

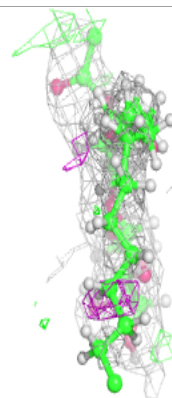
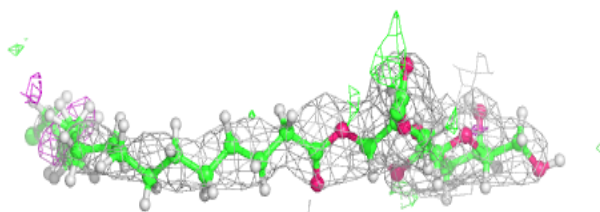
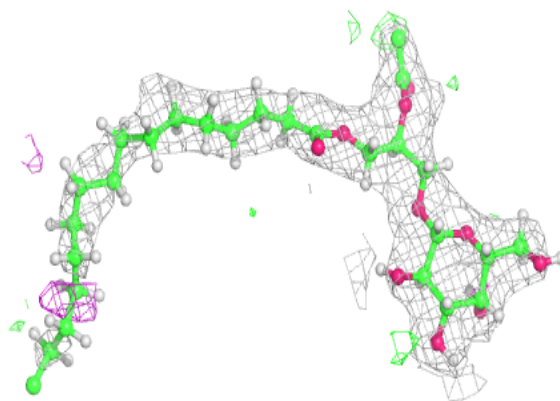
**Electron density around CLA C 502:**

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



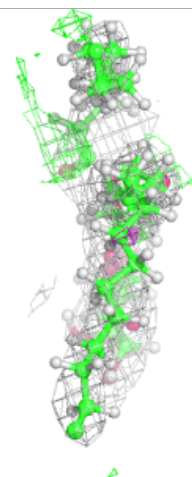
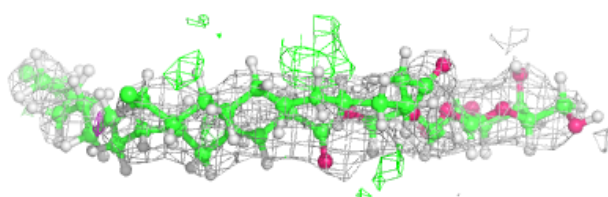
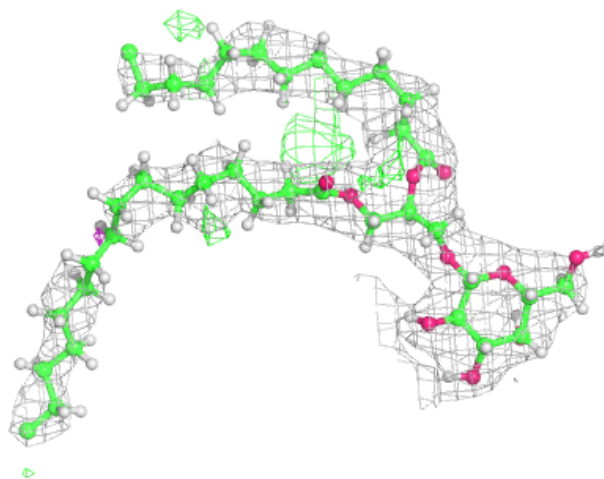
Electron density around LMG c 519:

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



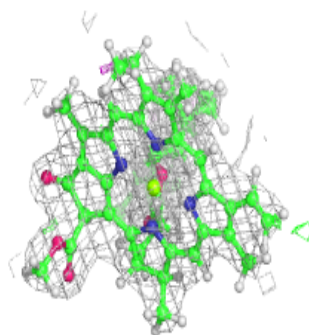
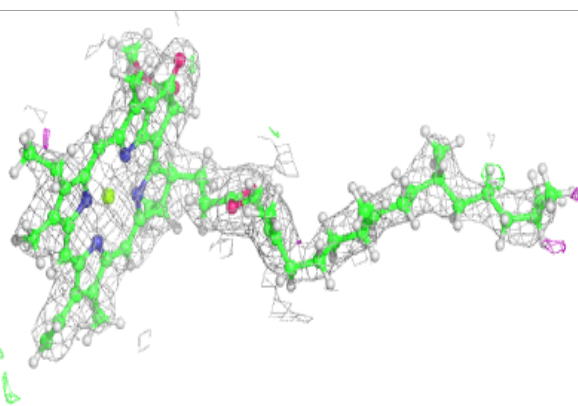
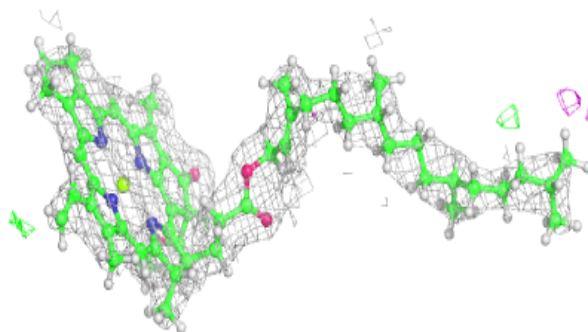
Electron density around LMG C 518:

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

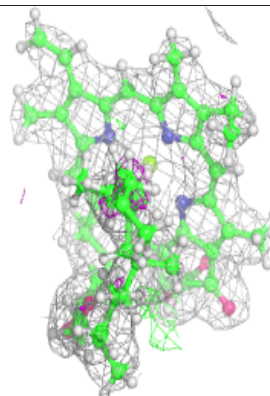
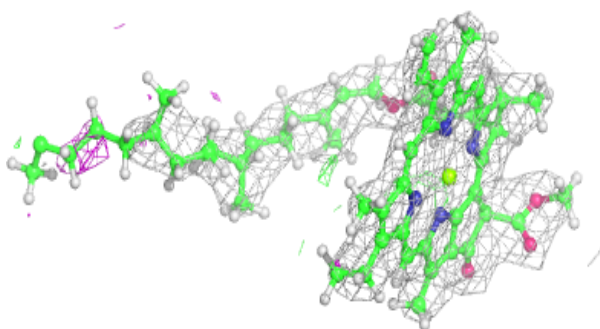
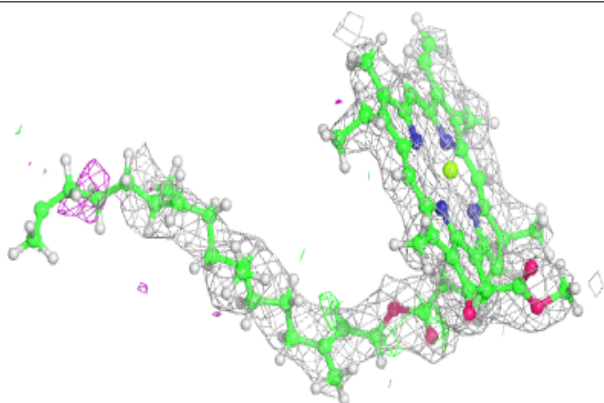


Electron density around CLA c 502:

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

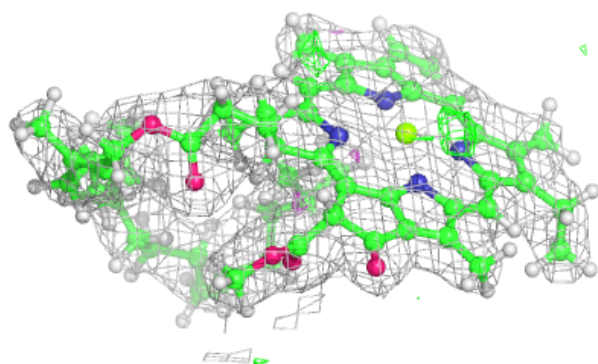
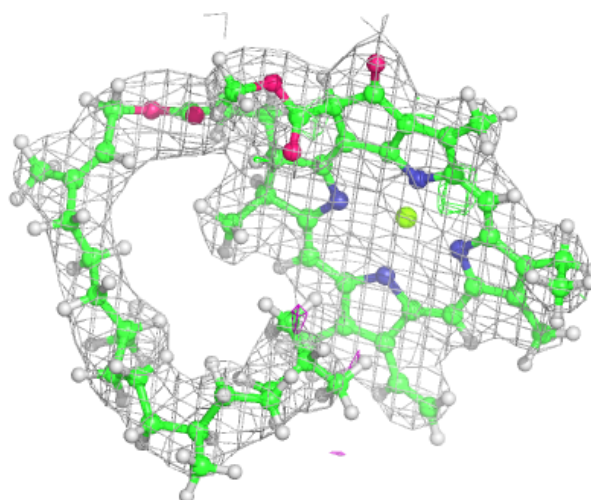
**Electron density around CLA c 508:**

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



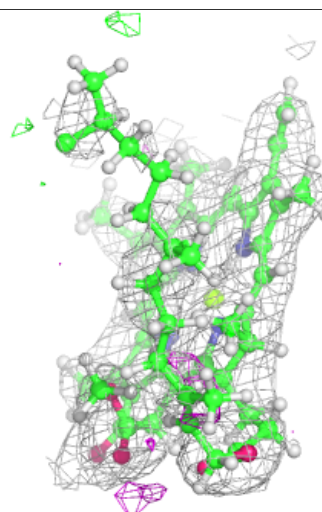
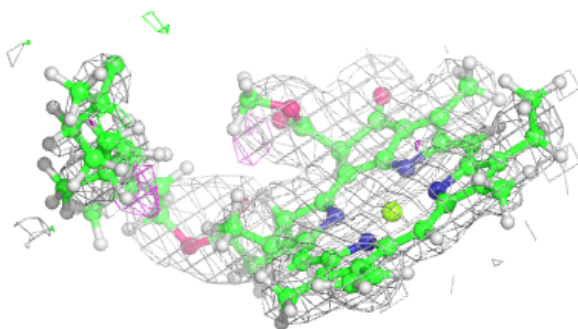
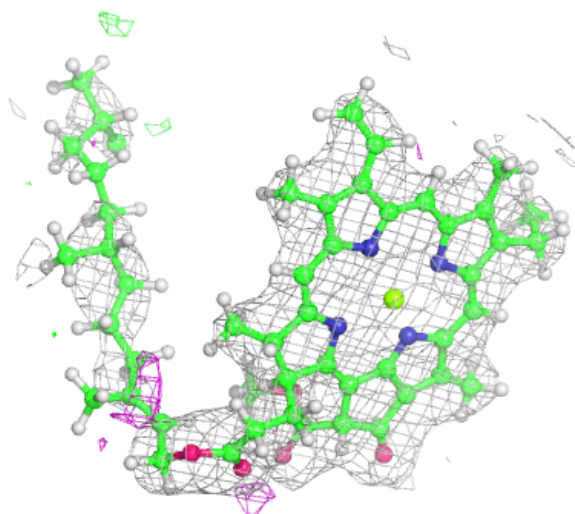
Electron density around CLA b 615:

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



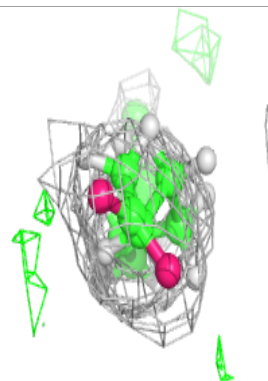
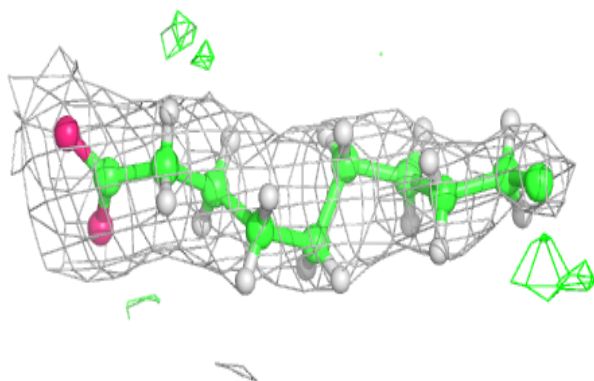
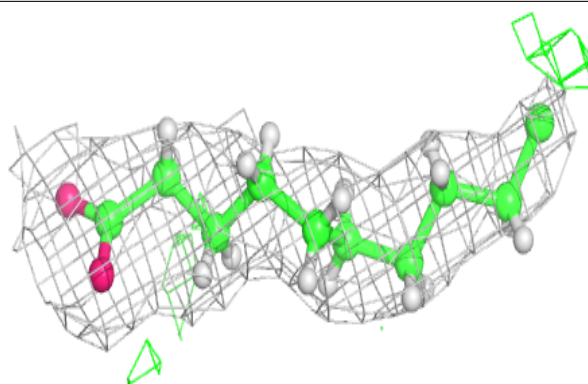
Electron density around CLA b 616:

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

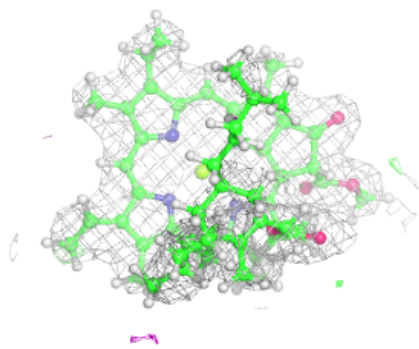
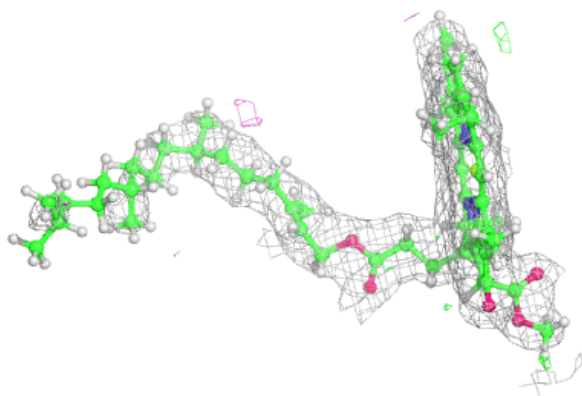
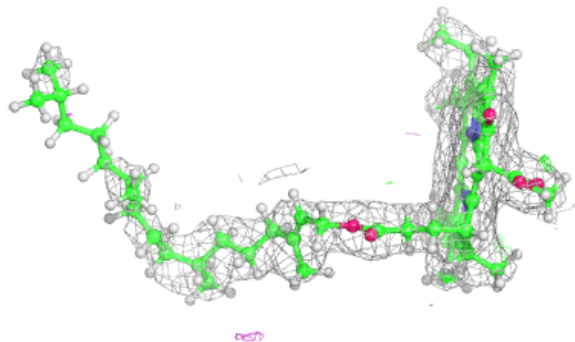


Electron density around STE J 101:

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

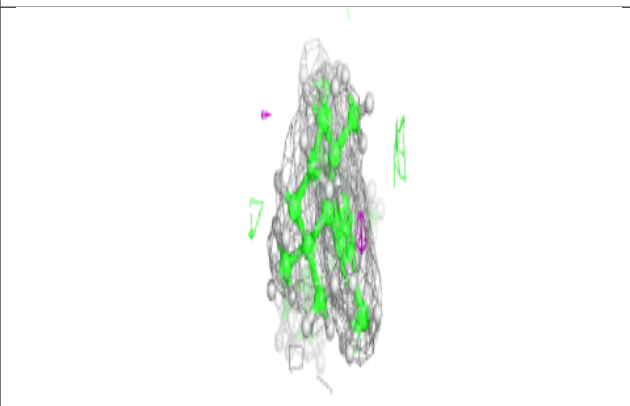
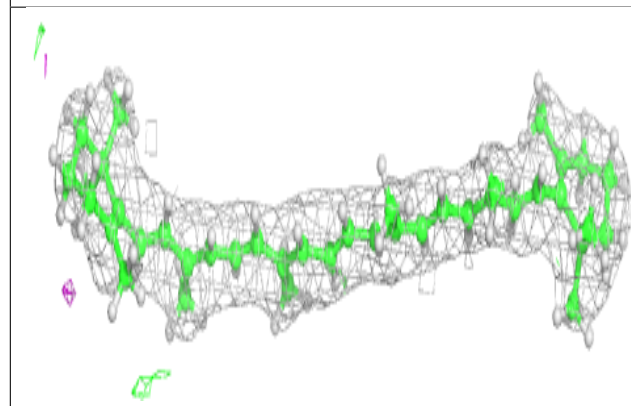
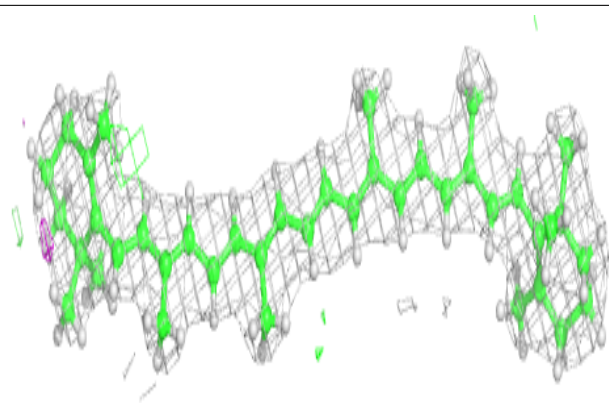
**Electron density around CLA D 403:**

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

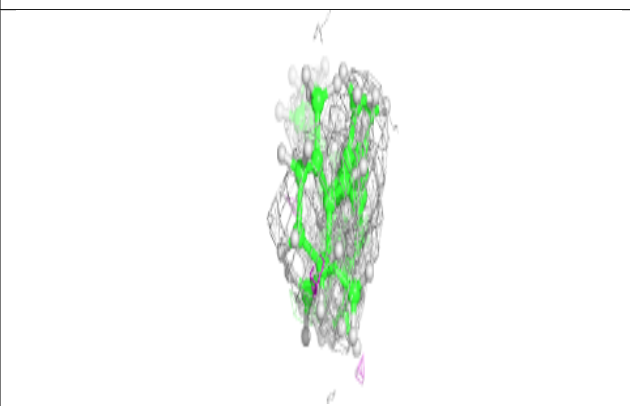
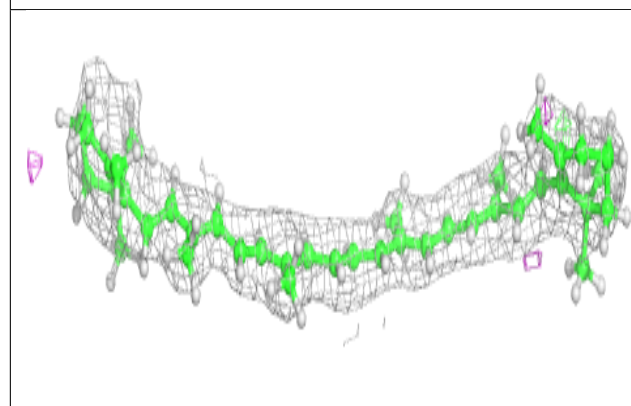
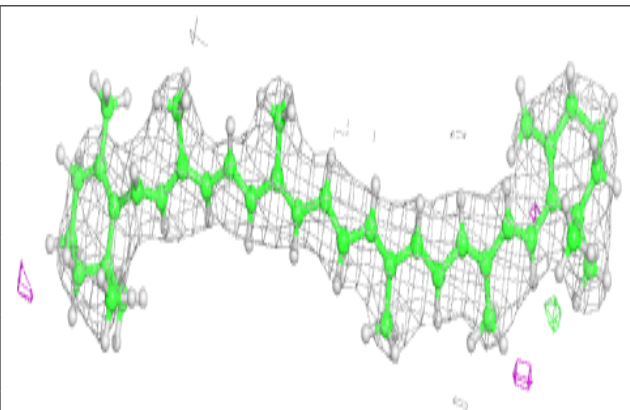


Electron density around BCR B 619:

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

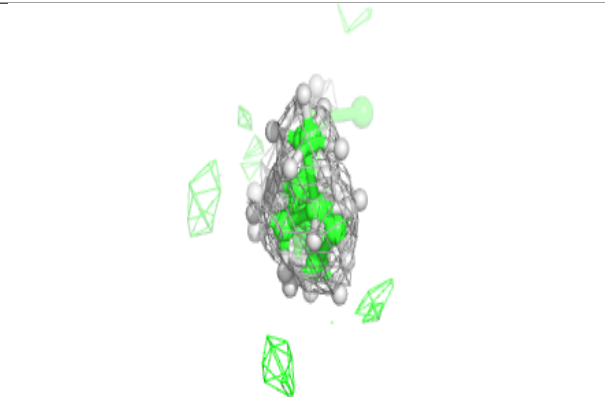
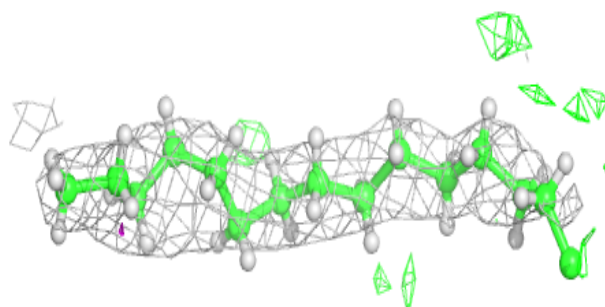
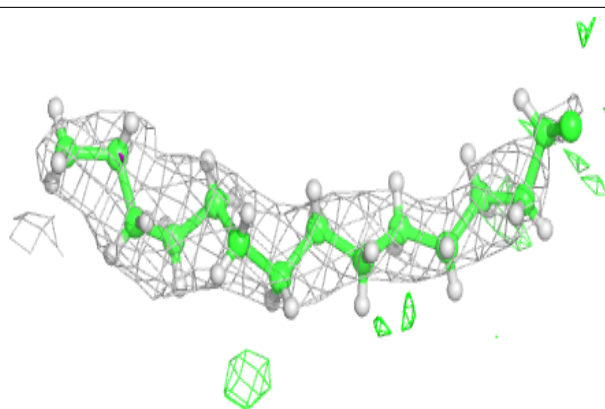
**Electron density around BCR D 404:**

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

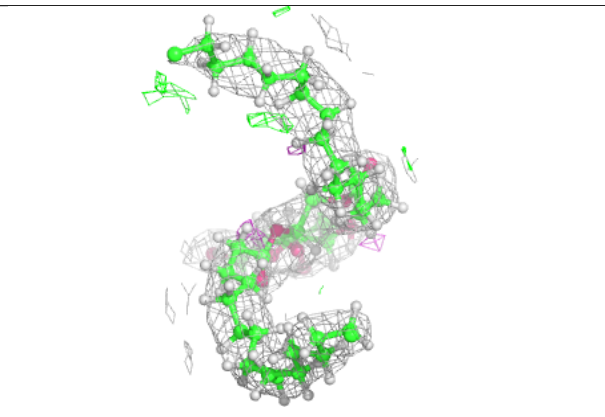
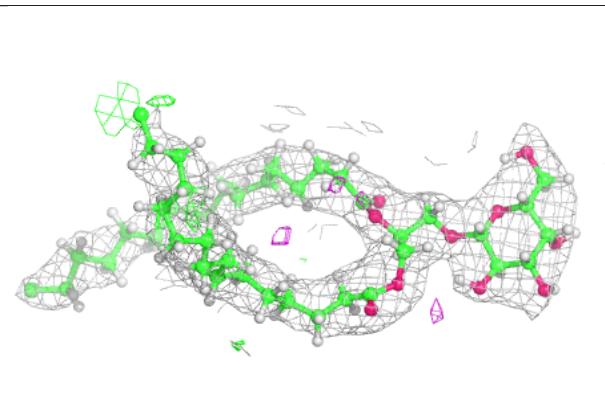
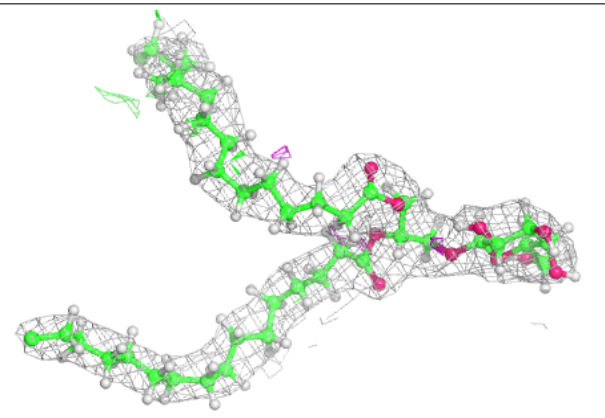


Electron density around STE T 102:

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

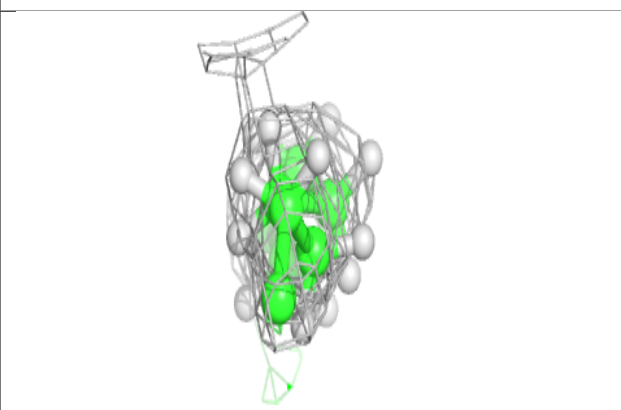
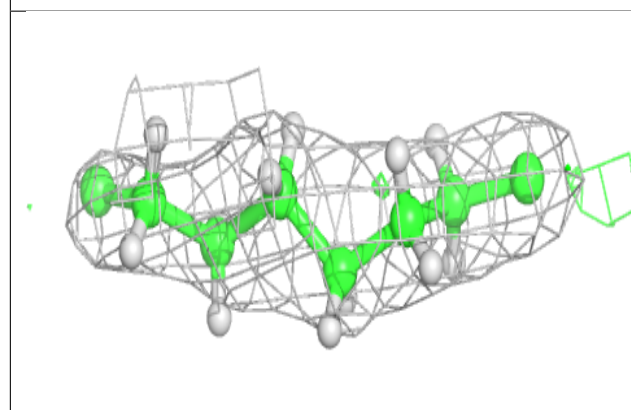
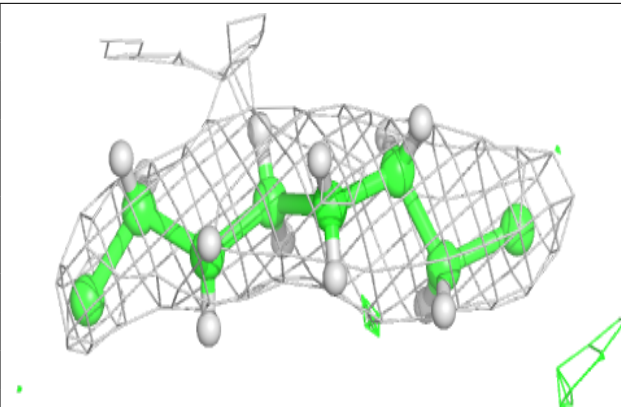
**Electron density around LMG M 101:**

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

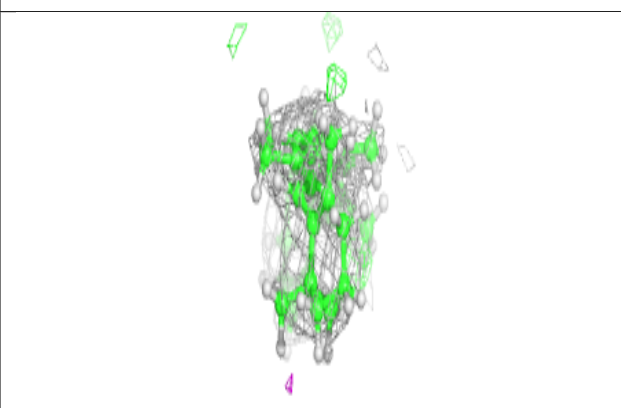
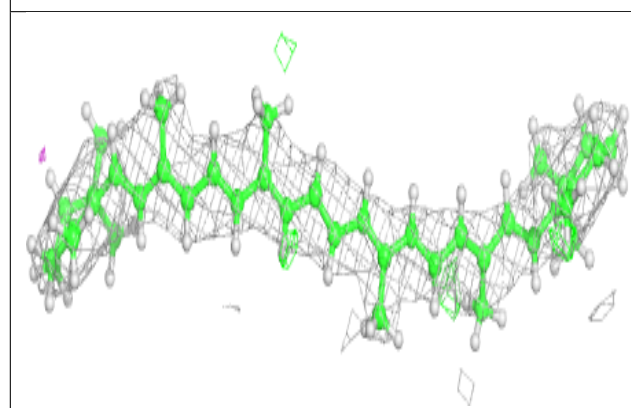
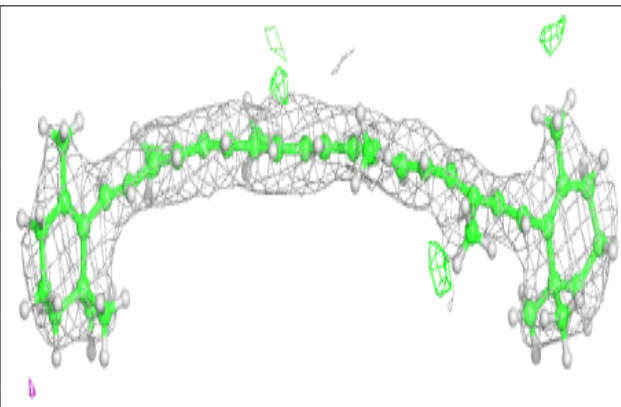


Electron density around STE Z 101:

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

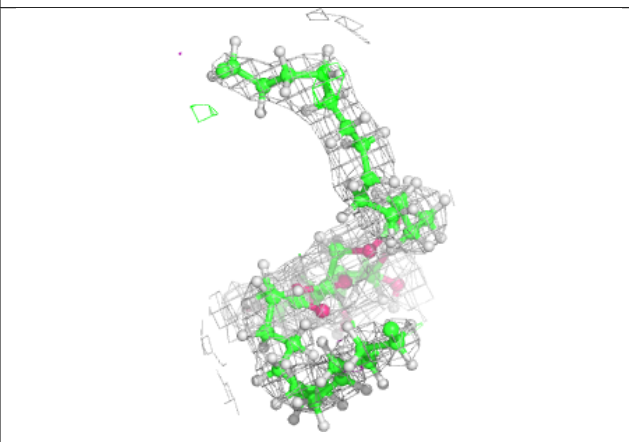
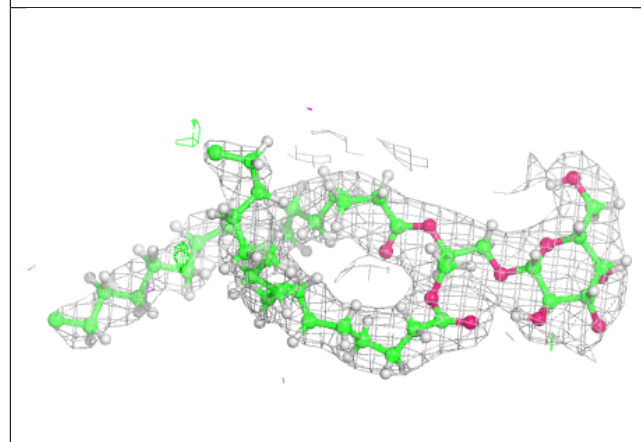
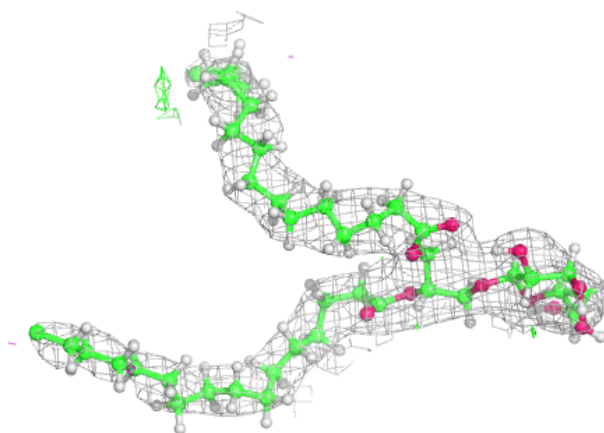
**Electron density around BCR k 102:**

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

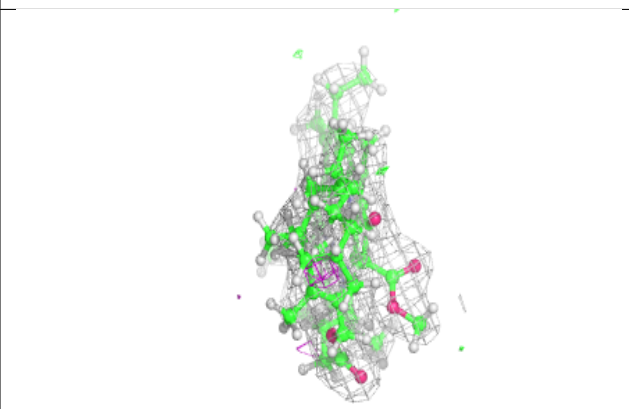
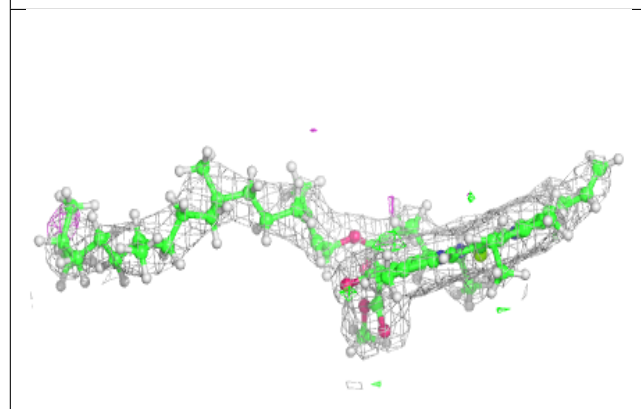
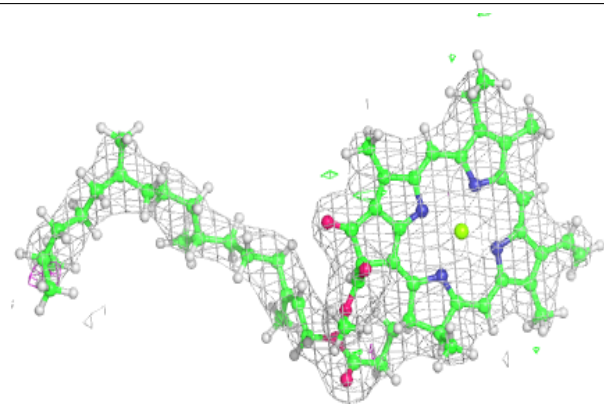


Electron density around LMG b 622:

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

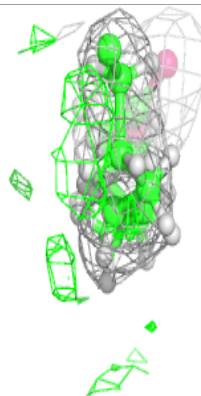
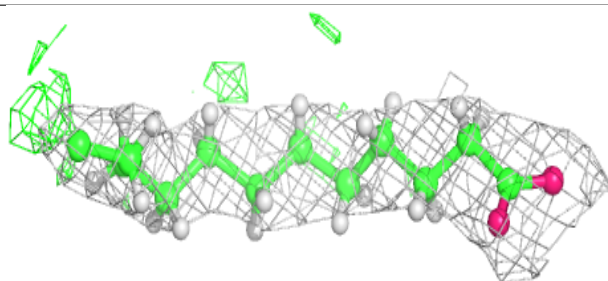
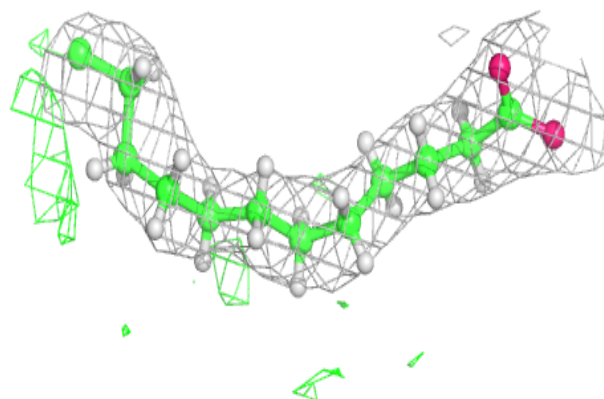
**Electron density around CLA b 602:**

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

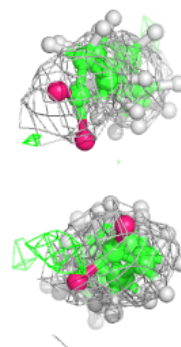
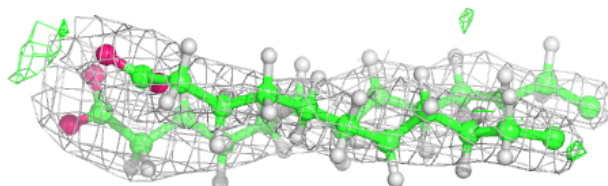
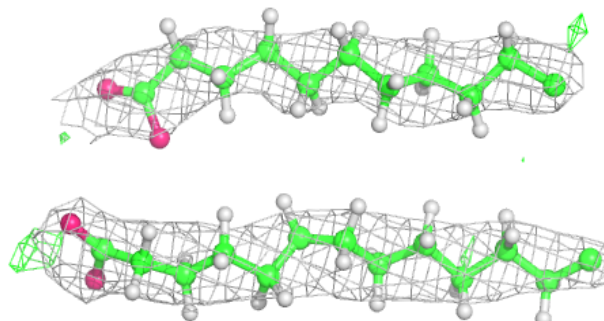


Electron density around STE t 102:

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

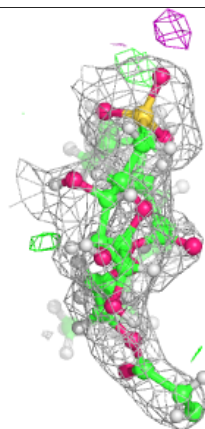
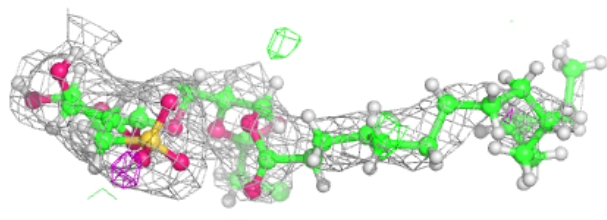
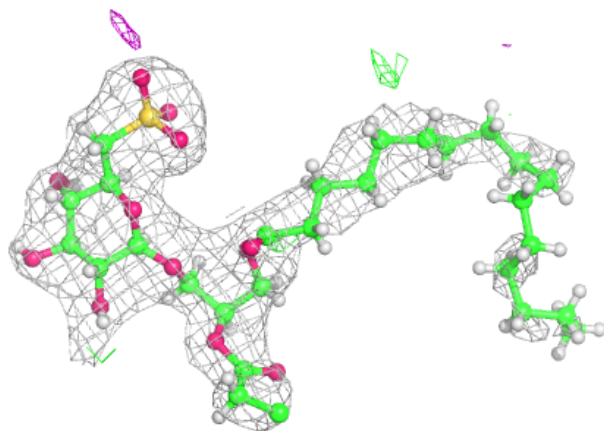
**Electron density around LMG D 411:**

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



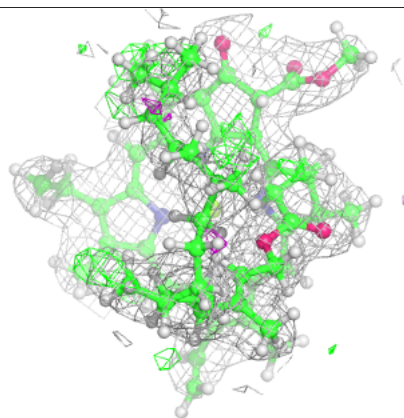
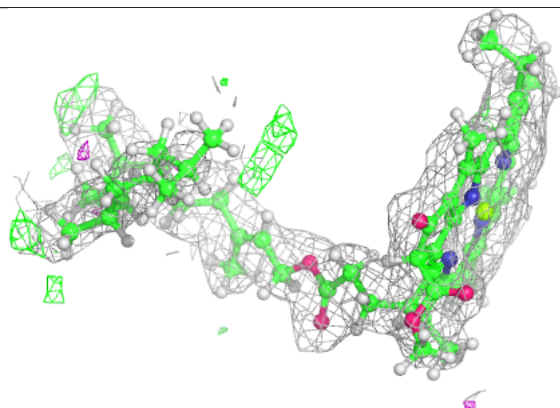
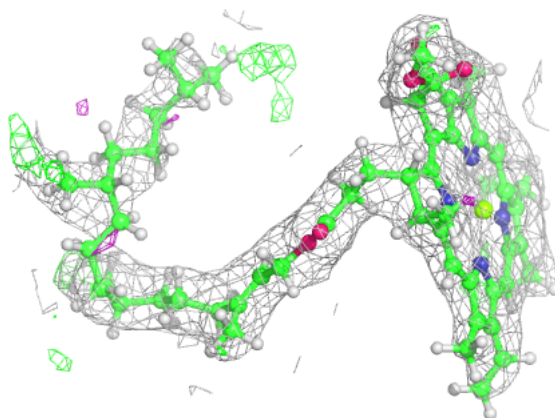
Electron density around SQD f 101:

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



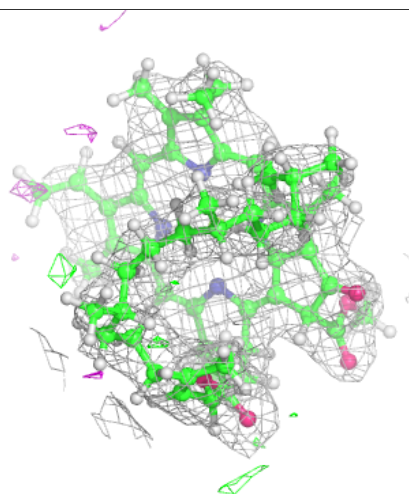
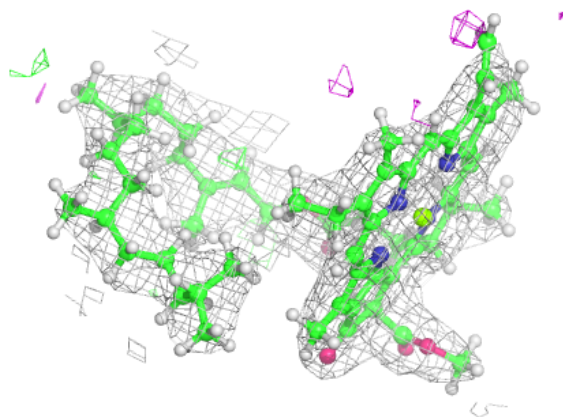
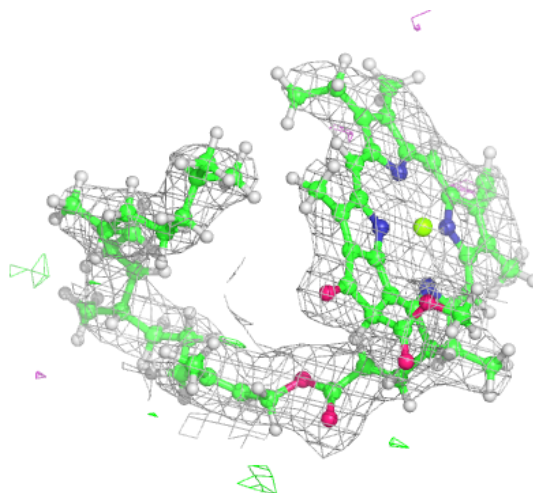
Electron density around CLA B 606:

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



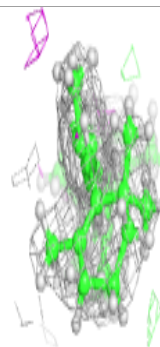
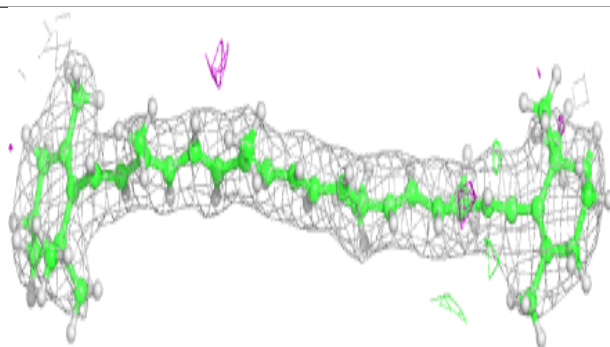
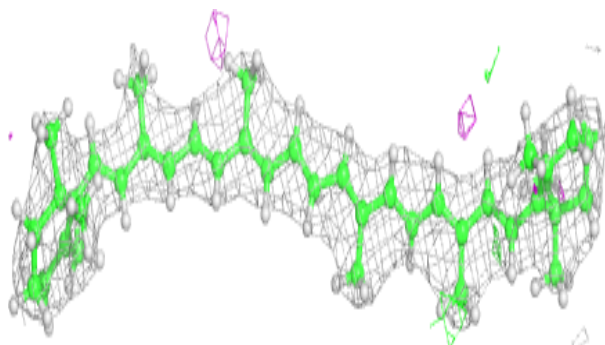
Electron density around CLA c 503:

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

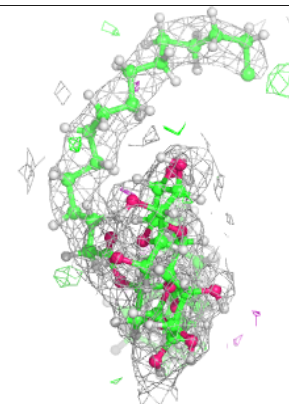
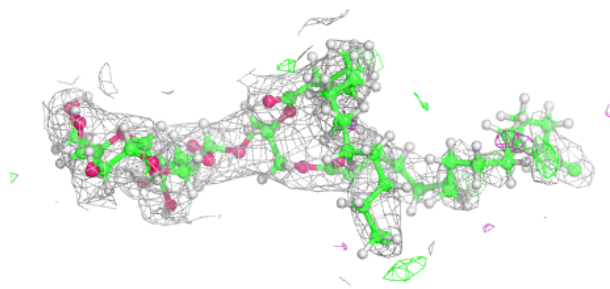
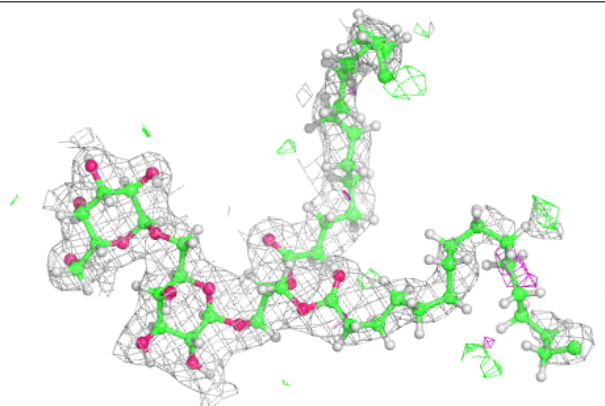


Electron density around BCR C 514:

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

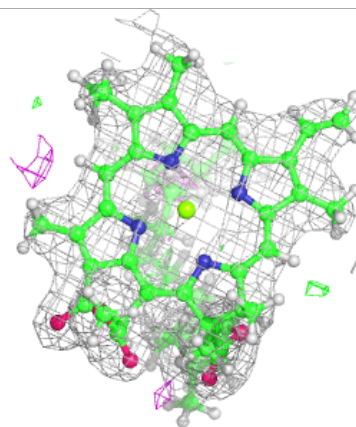
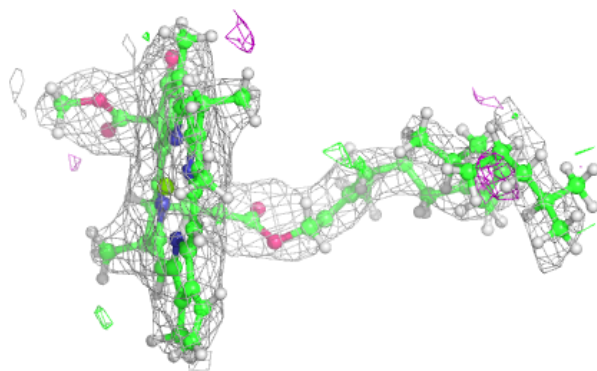
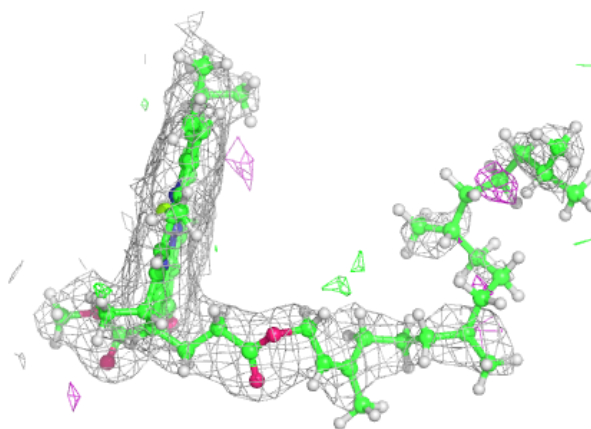
**Electron density around DGD C 516:**

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



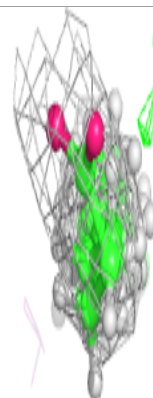
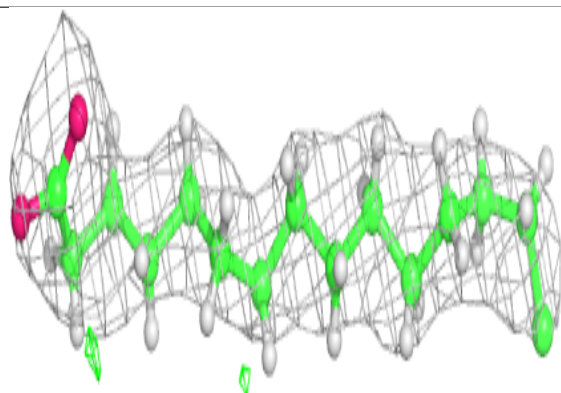
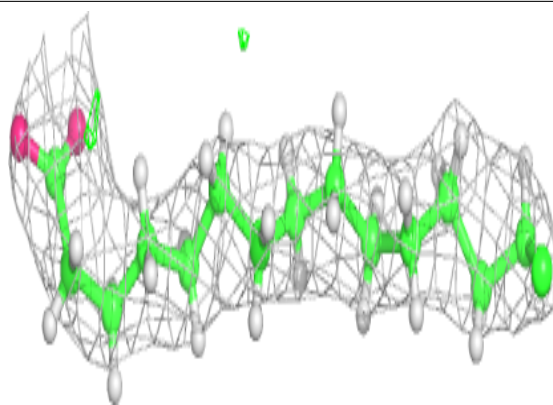
Electron density around CLA c 506:

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

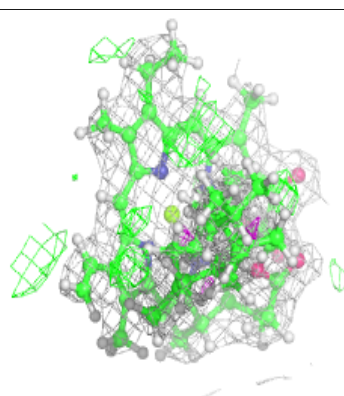
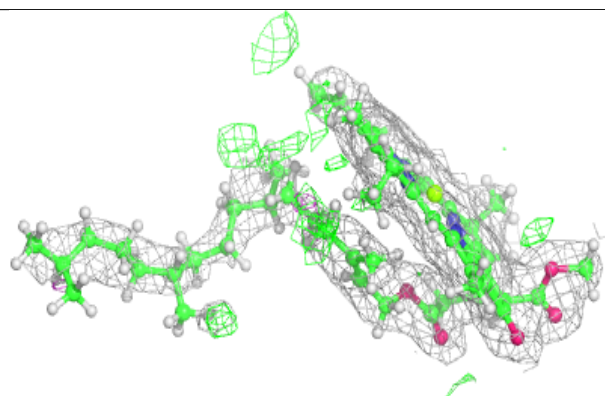
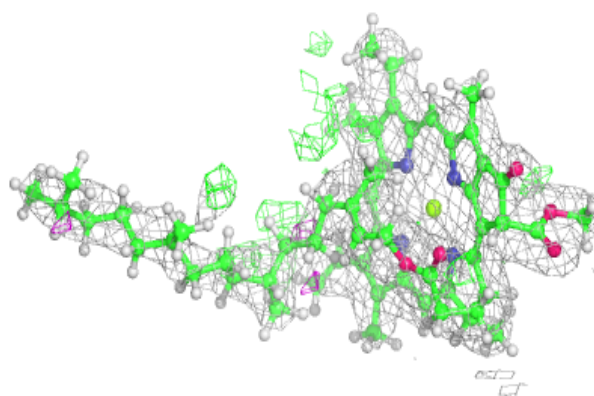


Electron density around STE d 411:

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

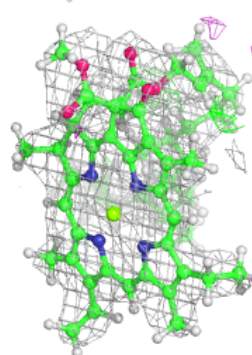
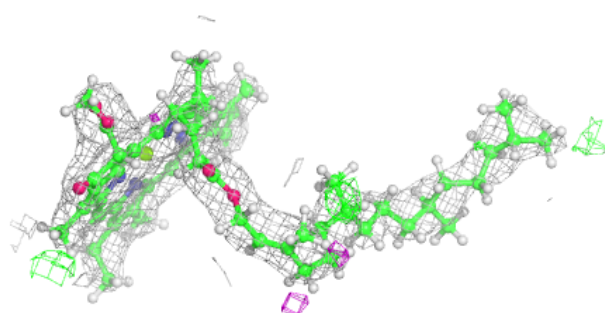
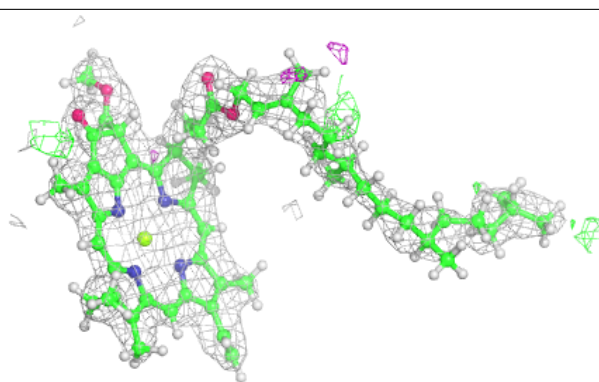
**Electron density around CLA C 505:**

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

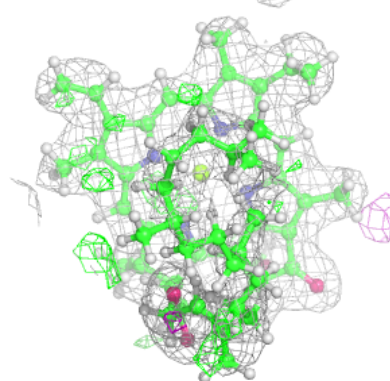
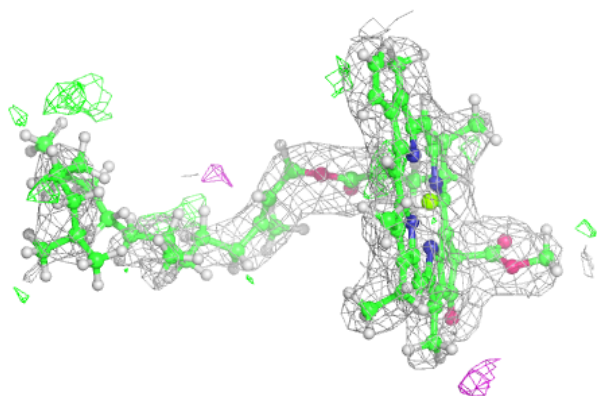
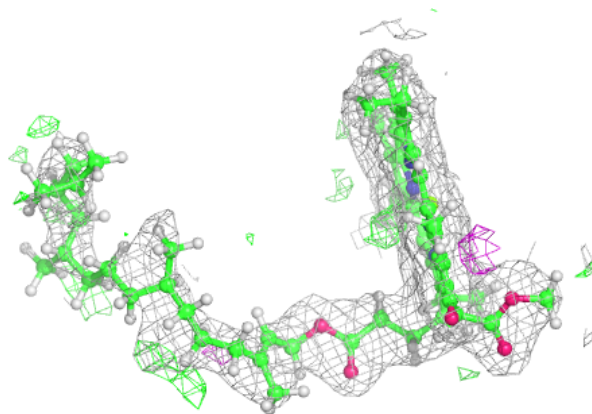


Electron density around CLA c 511:

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

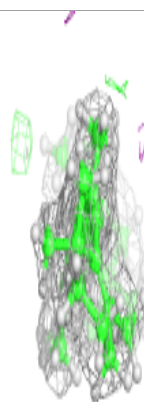
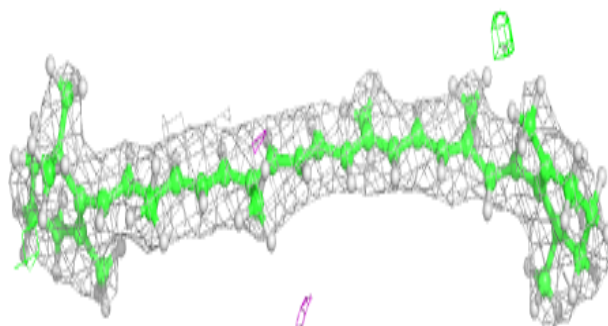
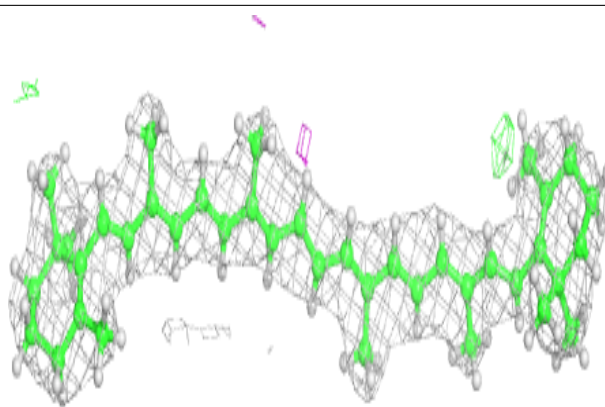
**Electron density around CLA C 506:**

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

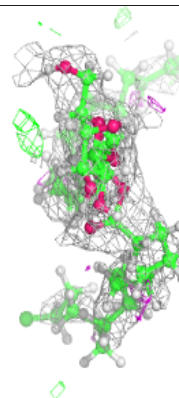
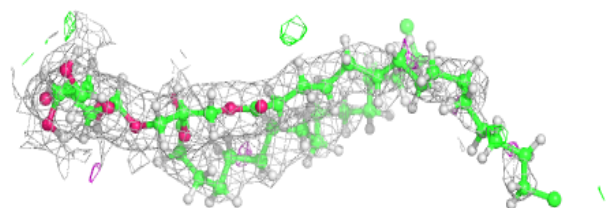
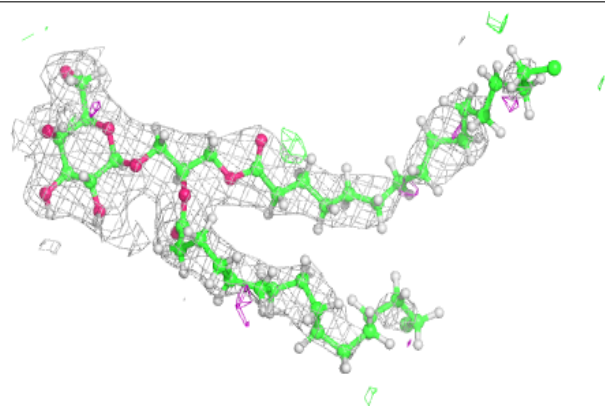


Electron density around BCR b 619:

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

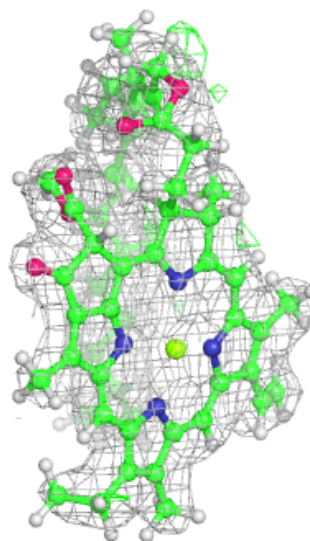
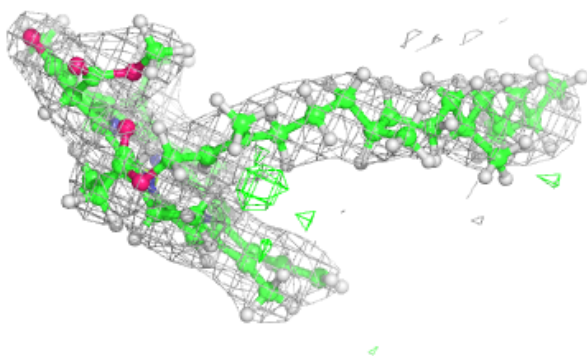
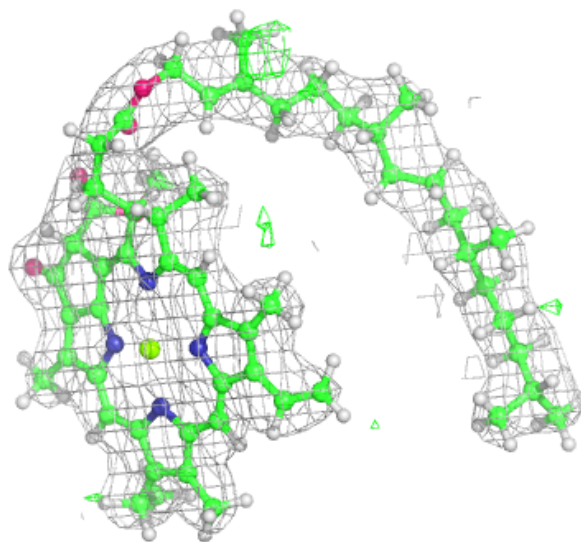
**Electron density around LMG D 406:**

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



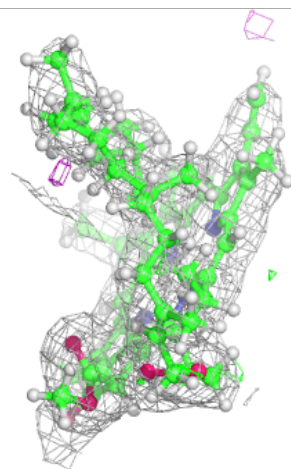
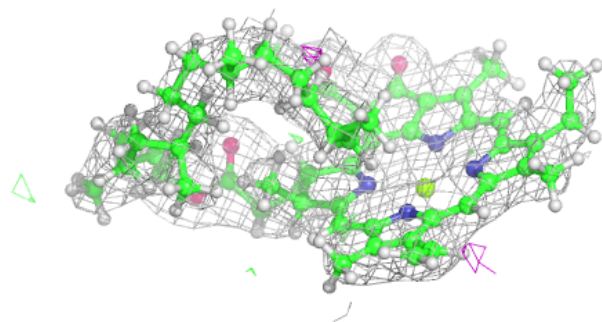
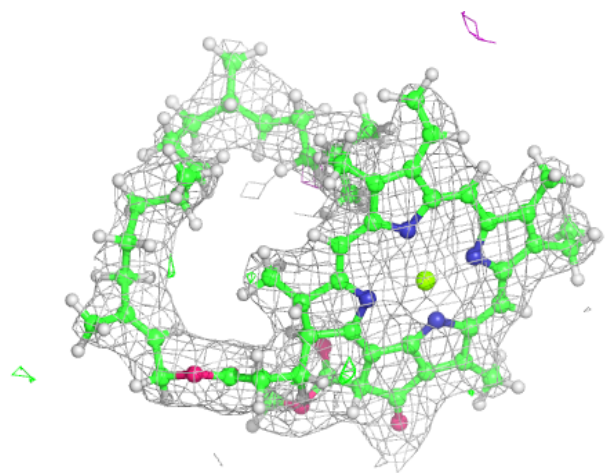
Electron density around CLA C 507:

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



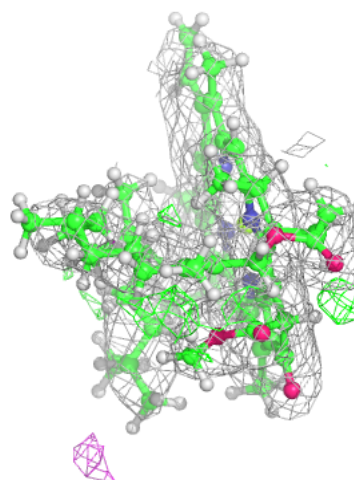
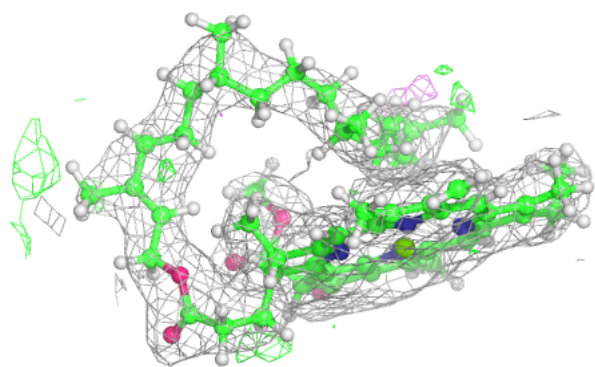
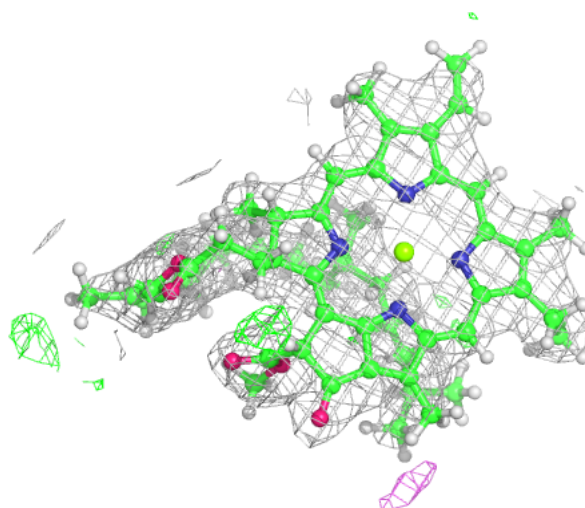
Electron density around CLA B 615:

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



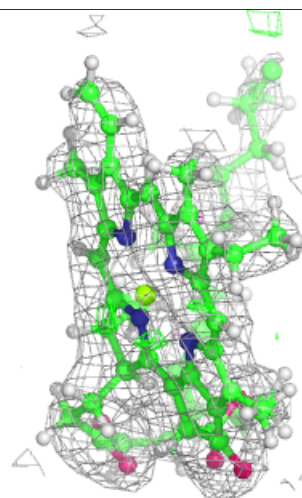
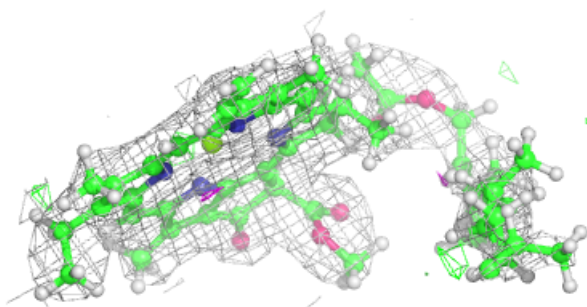
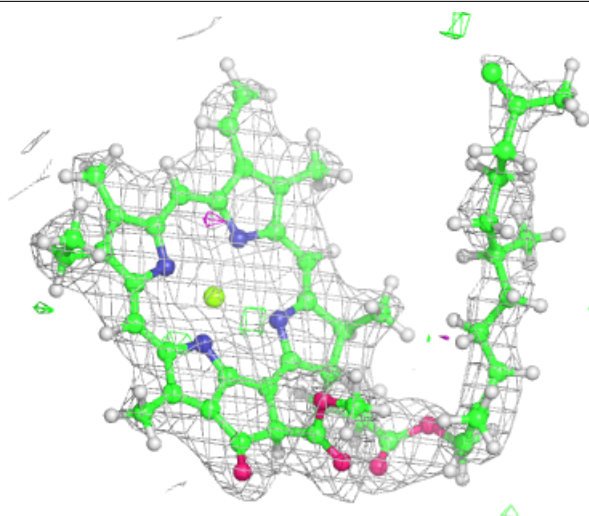
Electron density around CLA c 510:

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



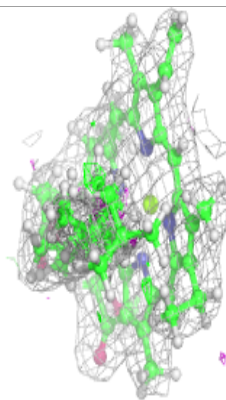
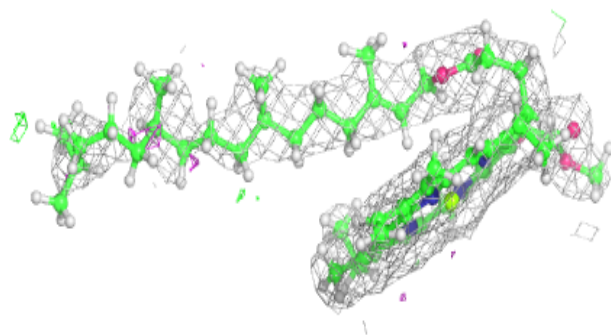
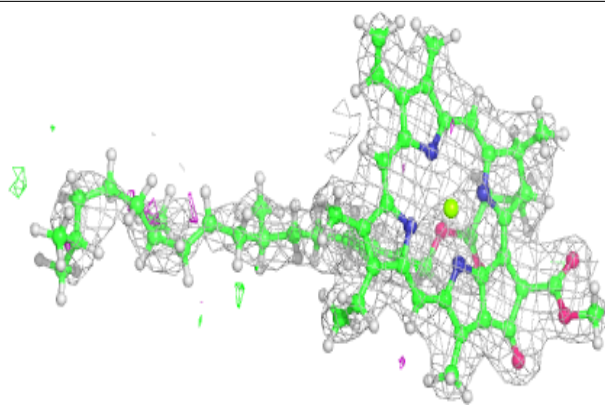
Electron density around CLA B 616:

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

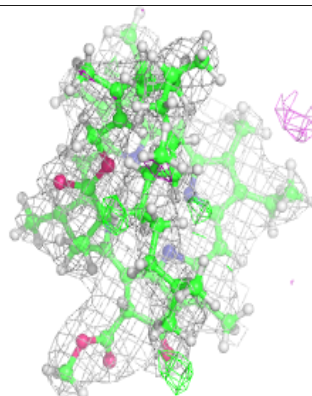
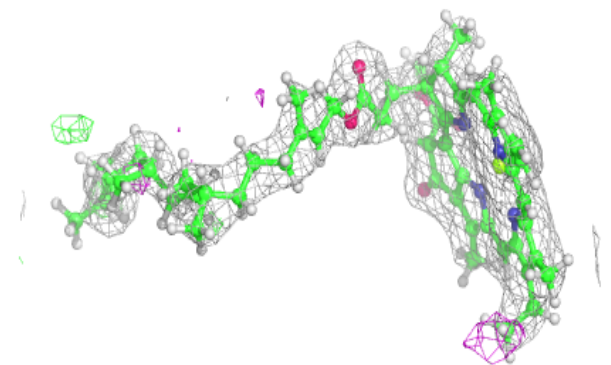
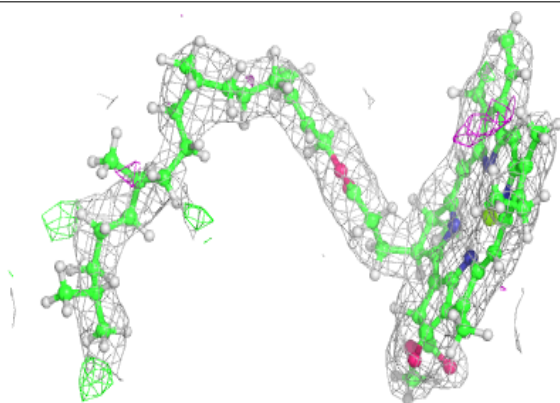


Electron density around CLA B 614:

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

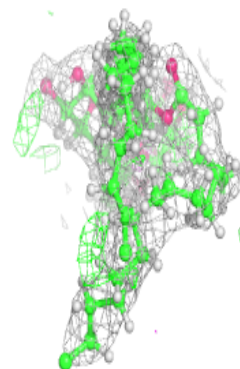
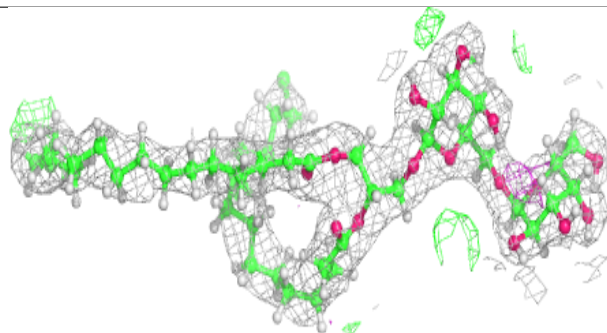
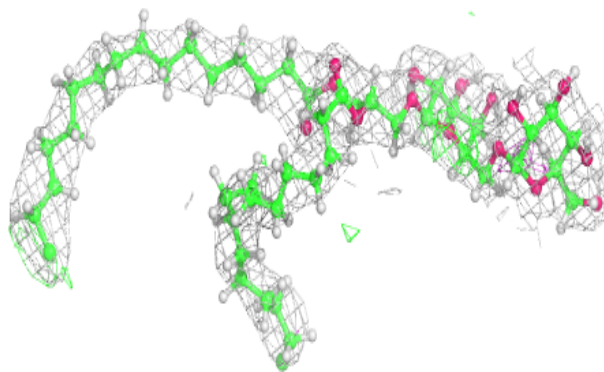
**Electron density around CLA b 606:**

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

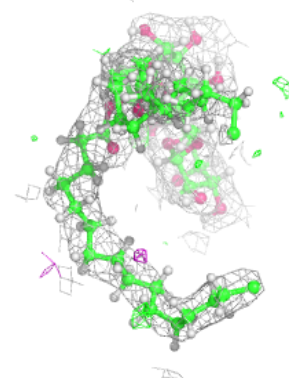
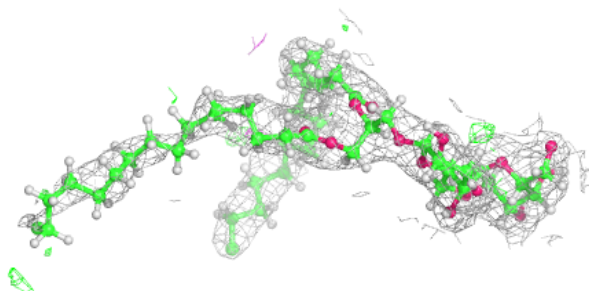
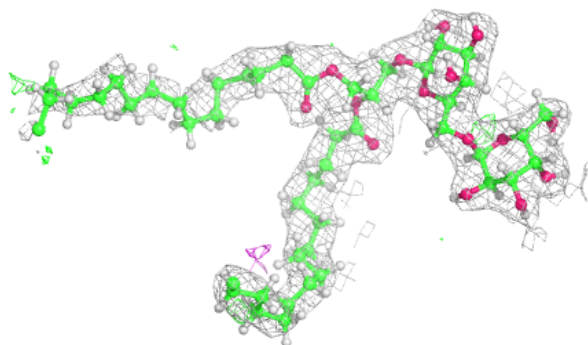


Electron density around DGD H 102:

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

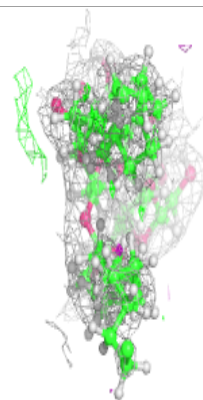
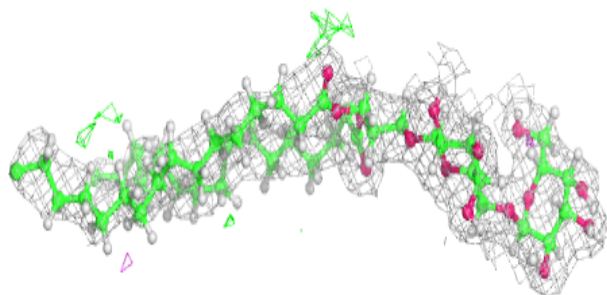
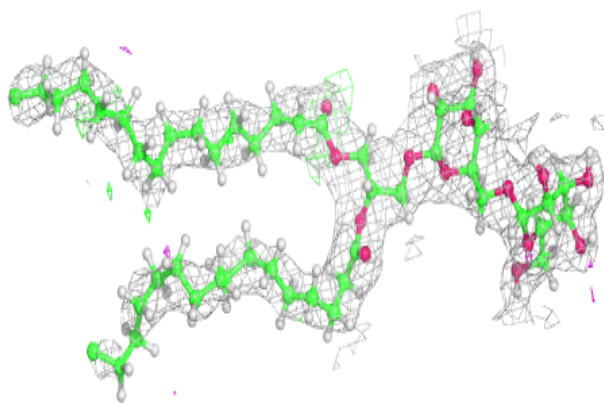
**Electron density around DGD c 517:**

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

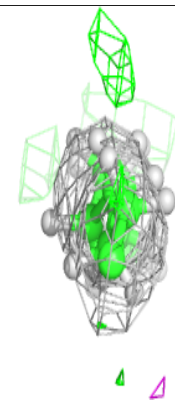
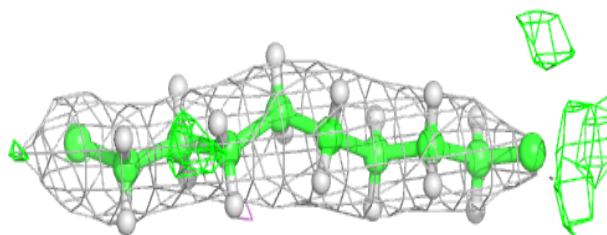
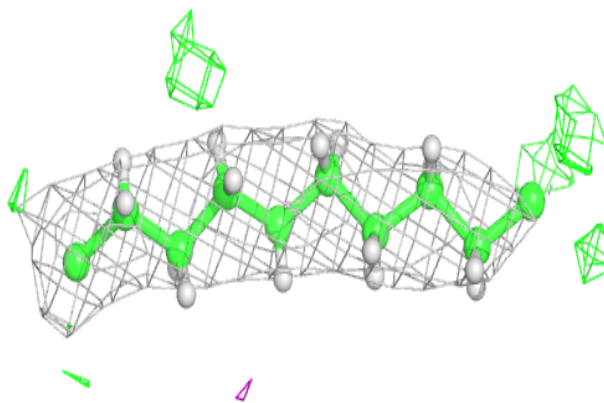


Electron density around DGD c 518:

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

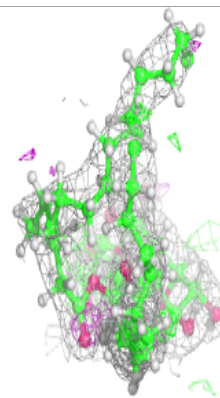
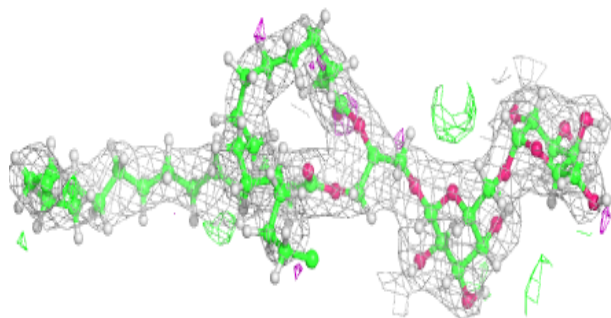
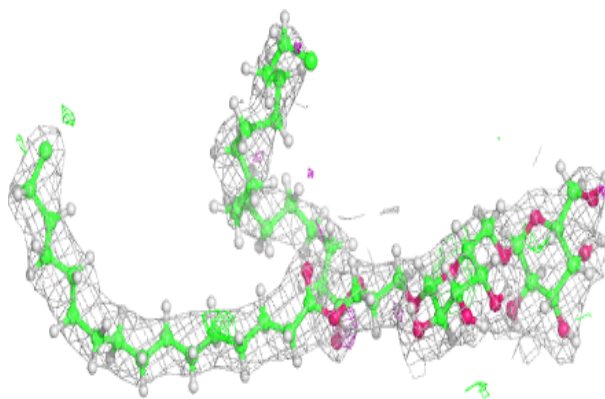
**Electron density around STE M 103:**

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

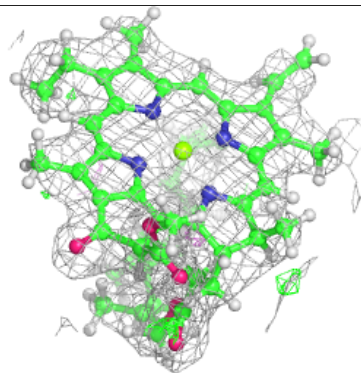
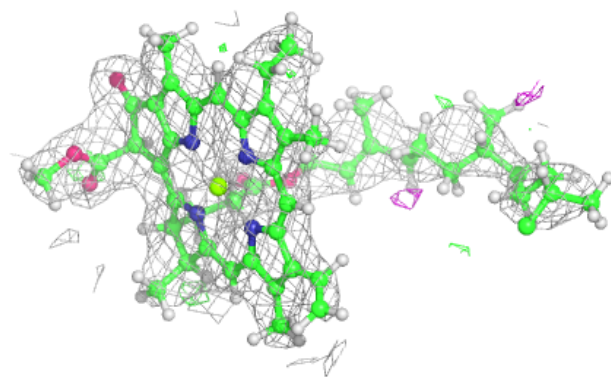
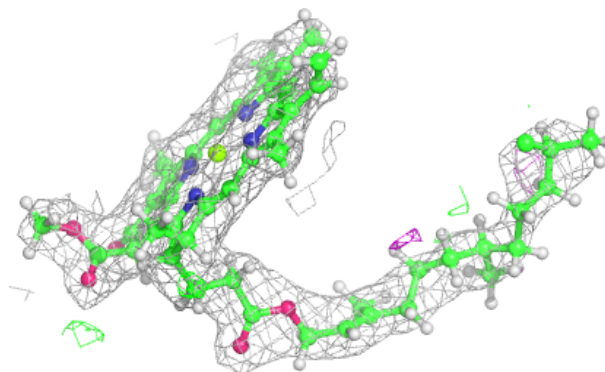


Electron density around DGD h 101:

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

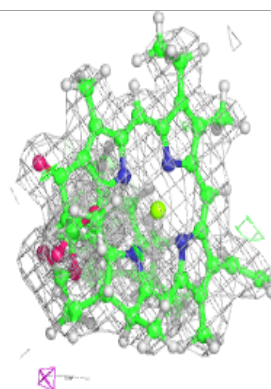
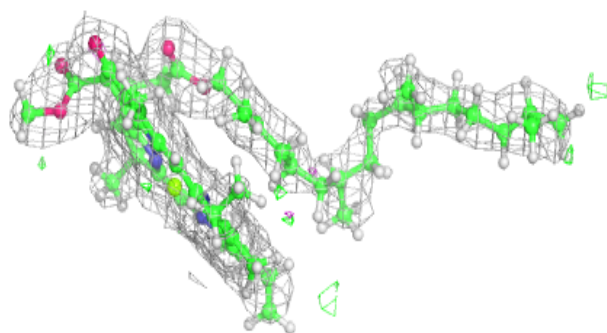
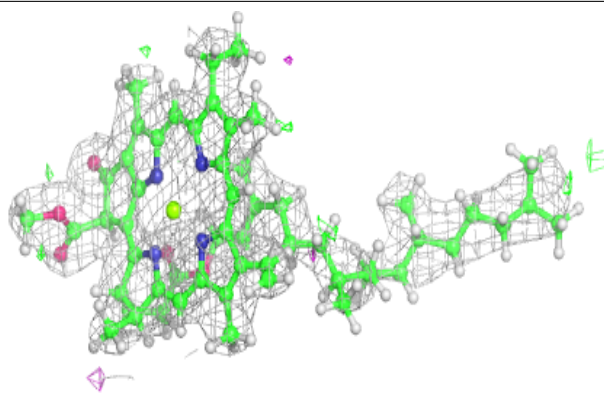
**Electron density around CLA c 504:**

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



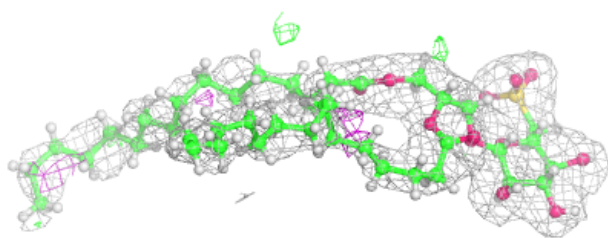
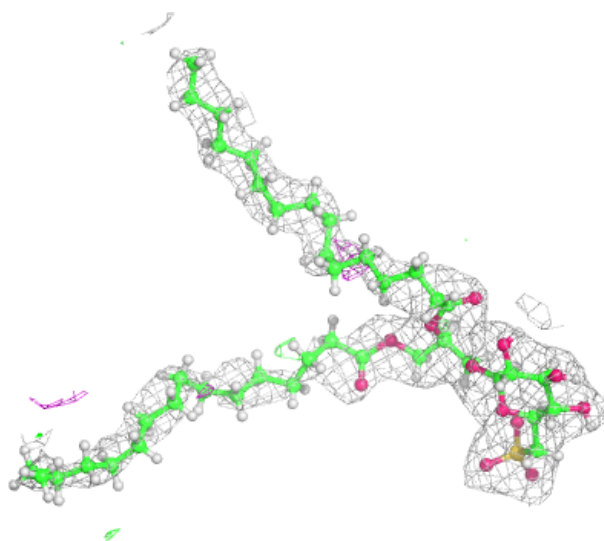
Electron density around CLA c 505:

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



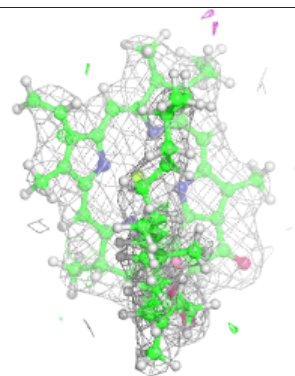
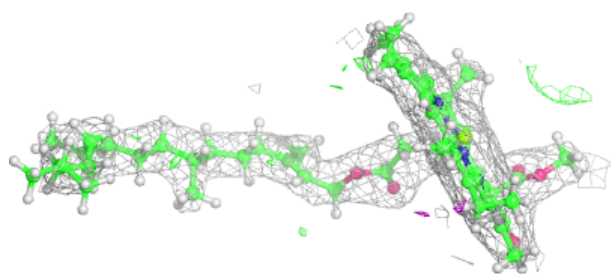
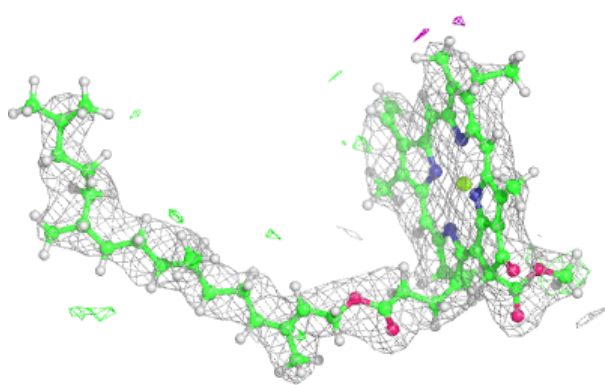
Electron density around SQD a 411:

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



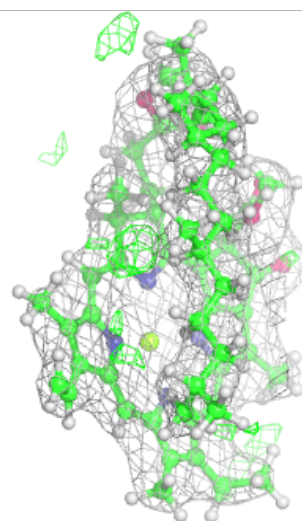
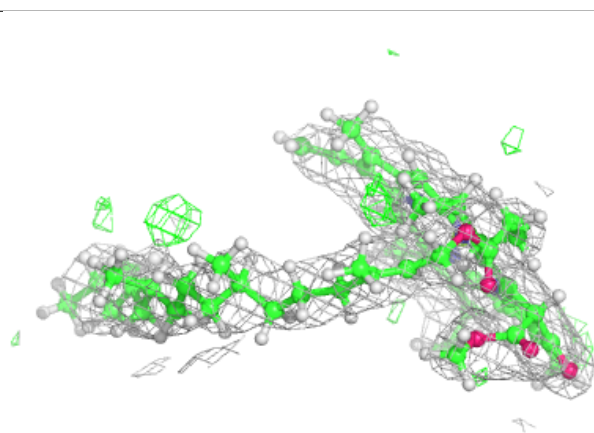
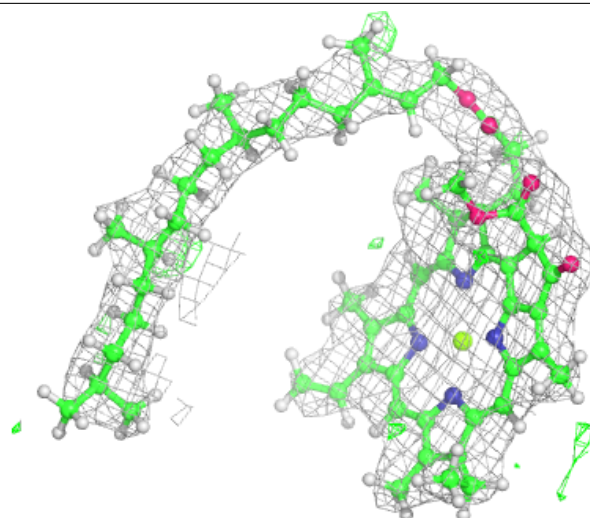
Electron density around CLA b 609:

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



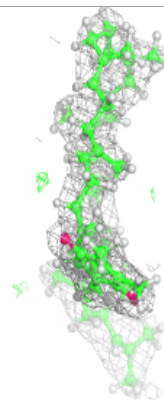
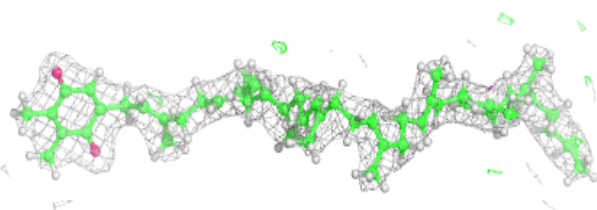
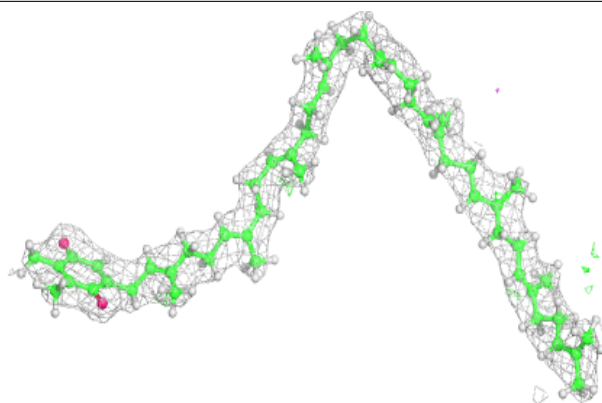
Electron density around CLA c 507:

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

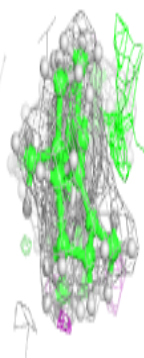
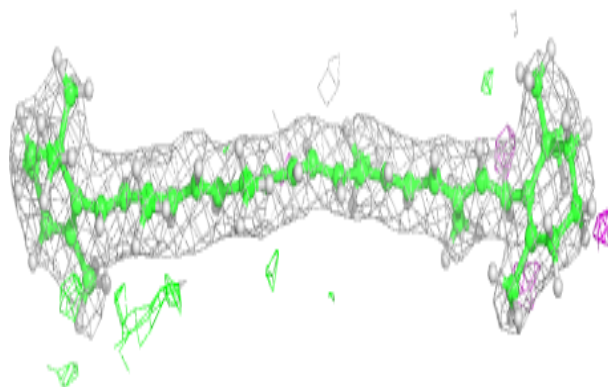
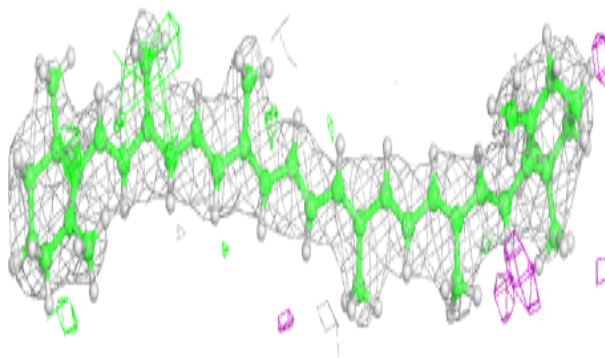


Electron density around PL9 D 405:

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

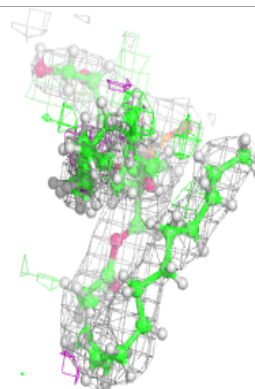
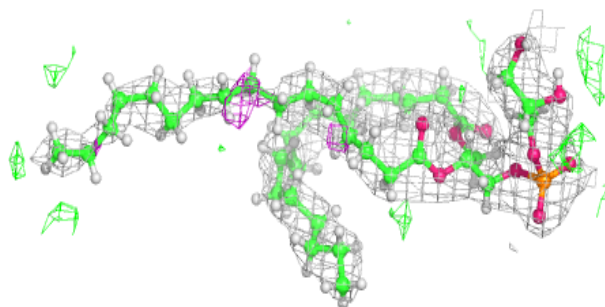
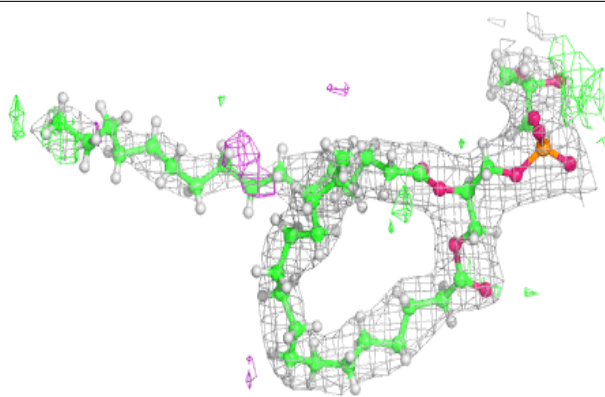
**Electron density around BCR B 618:**

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

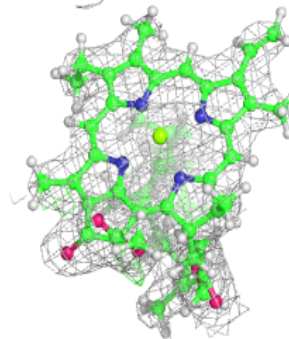
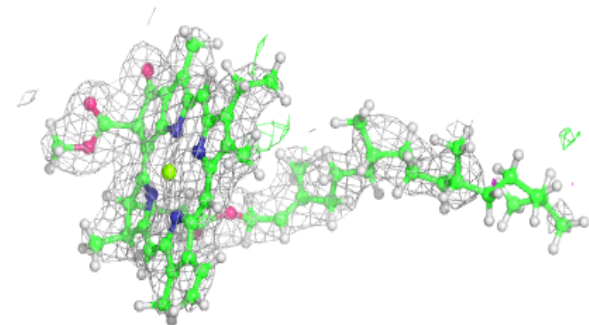
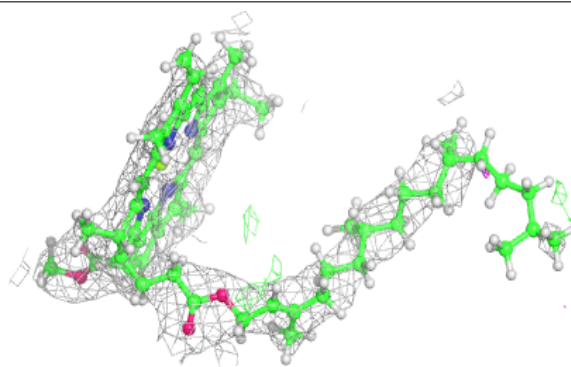


Electron density around LHG d 407:

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

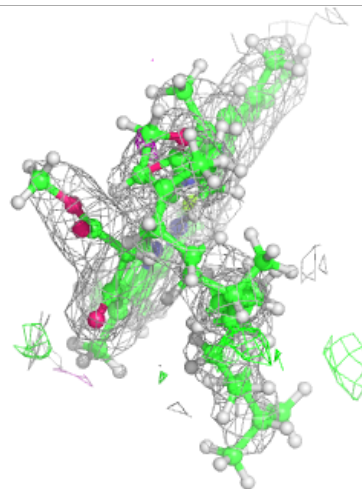
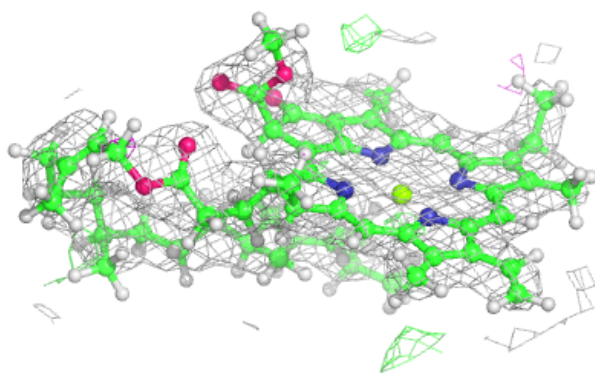
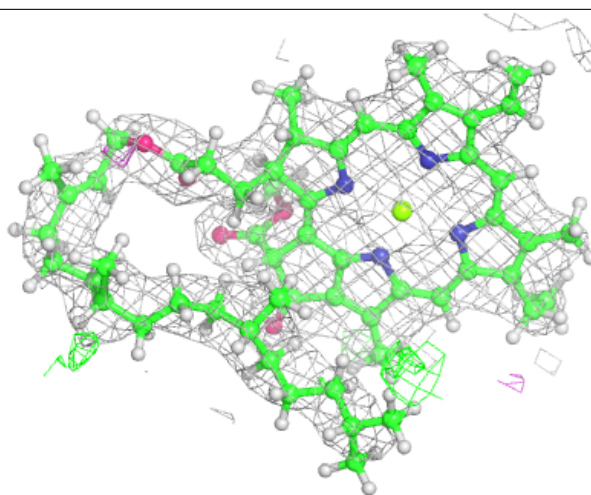
**Electron density around CLA C 508:**

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



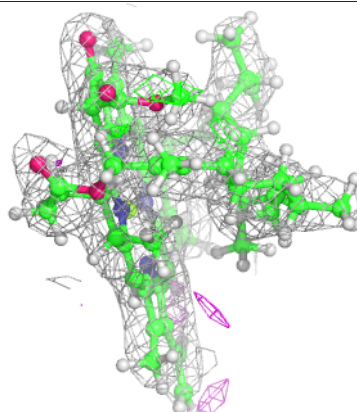
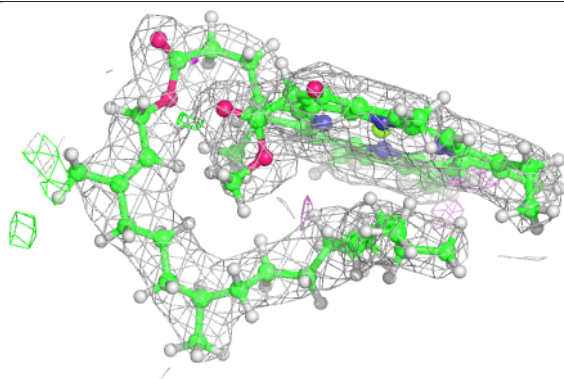
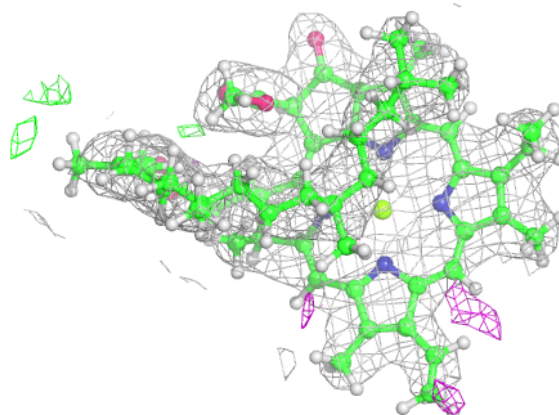
Electron density around CLA C 509:

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

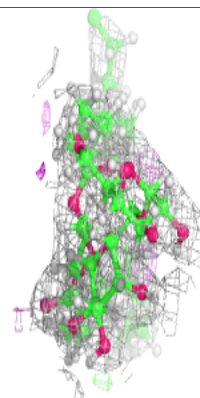
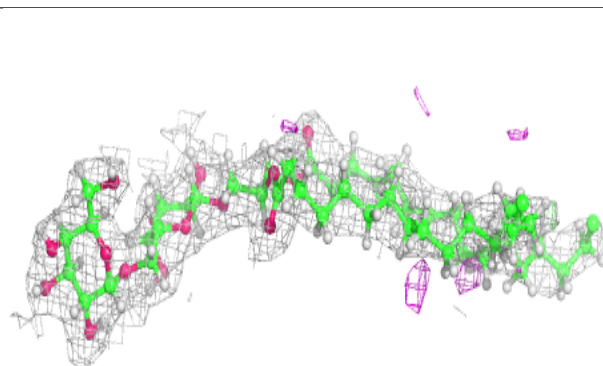
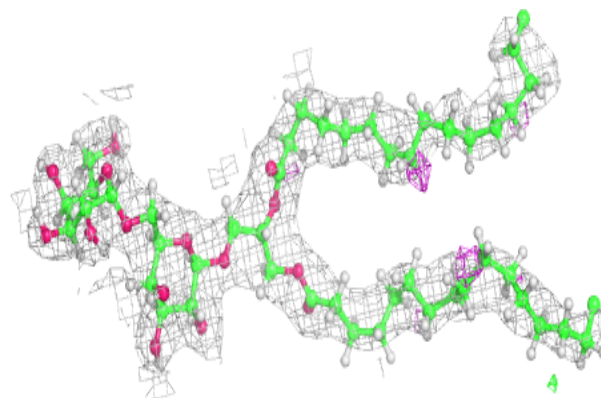


Electron density around CLA C 510:

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

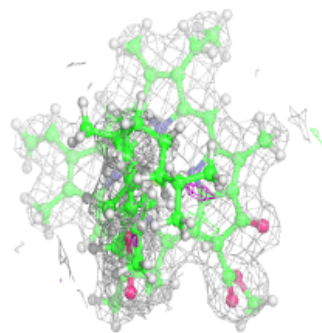
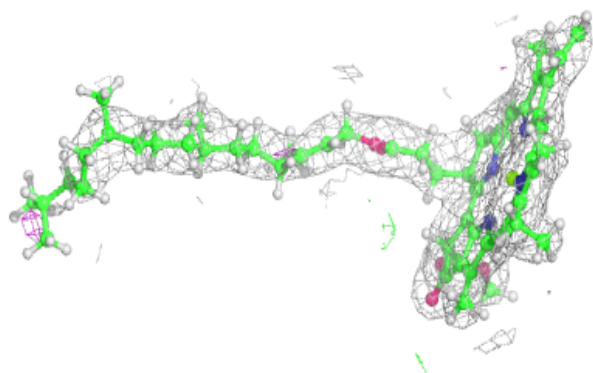
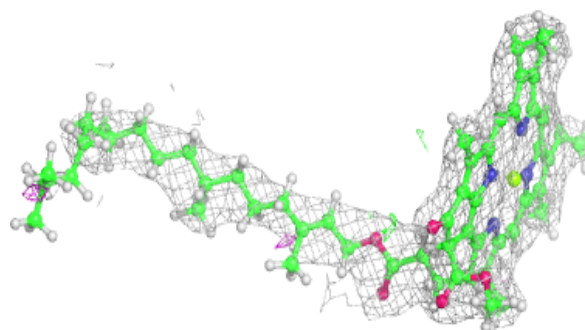
**Electron density around DGD C 517:**

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

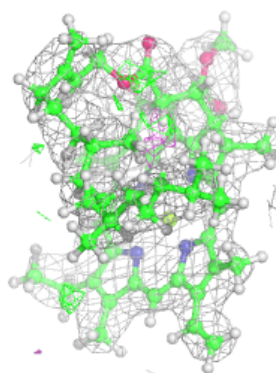
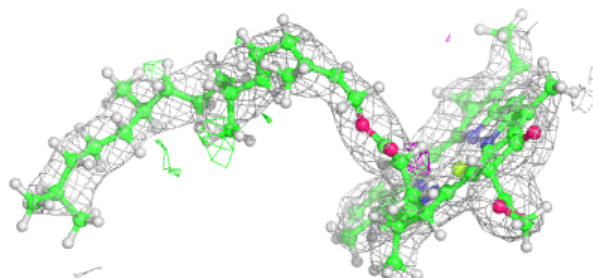
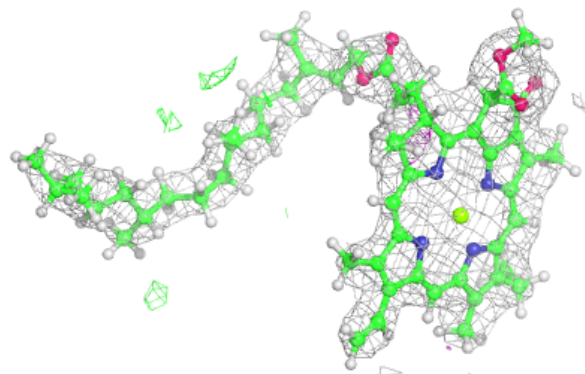


Electron density around CLA b 604:

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

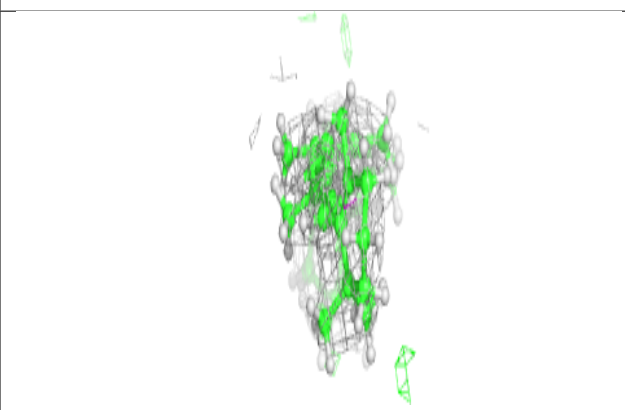
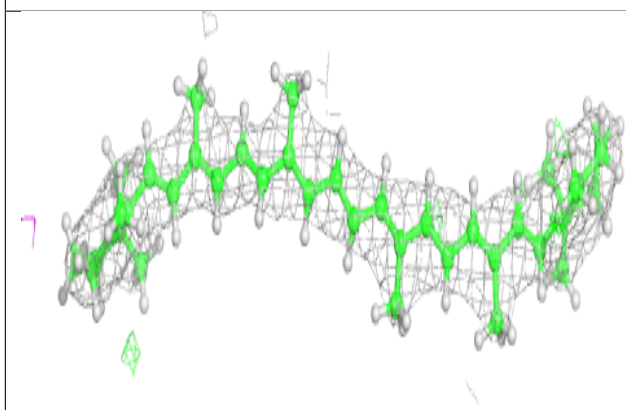
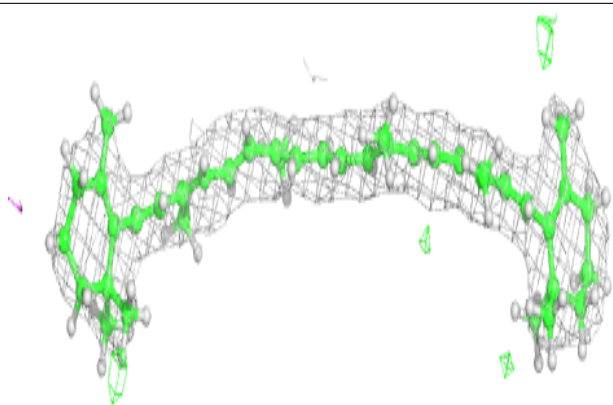
**Electron density around CLA C 511:**

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

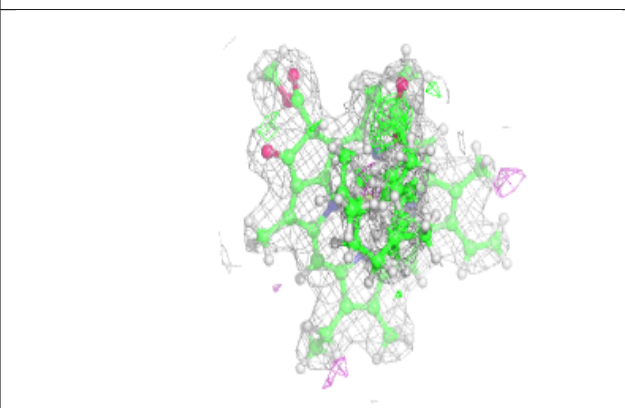
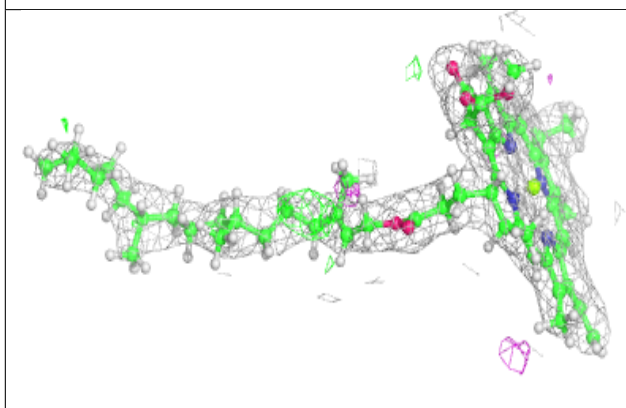
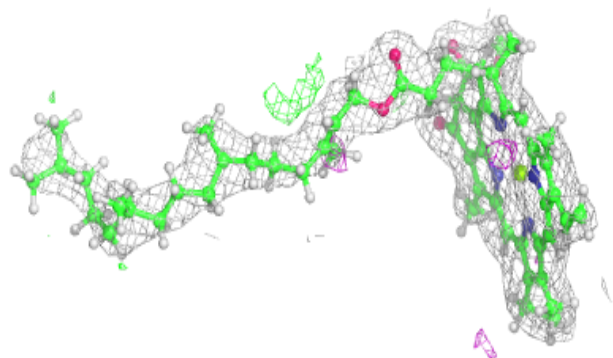


Electron density around BCR K 102:

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

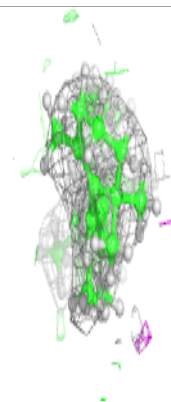
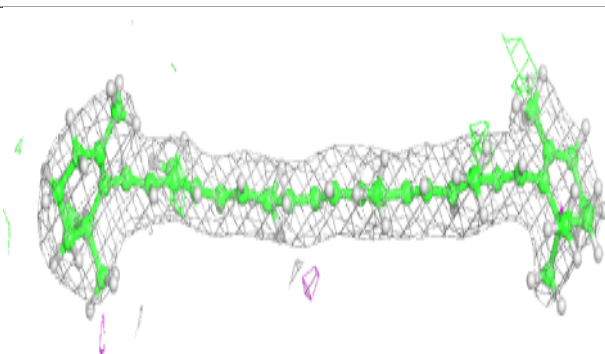
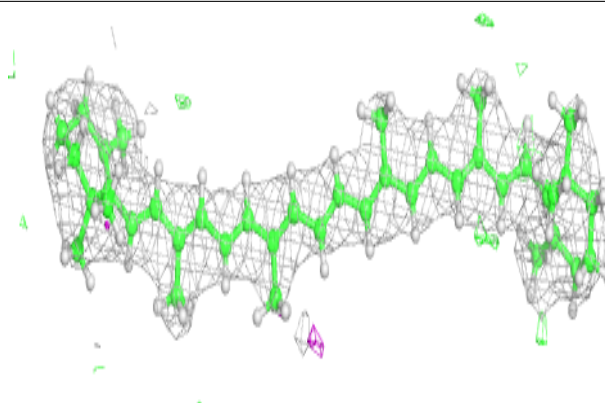
**Electron density around CLA B 604:**

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



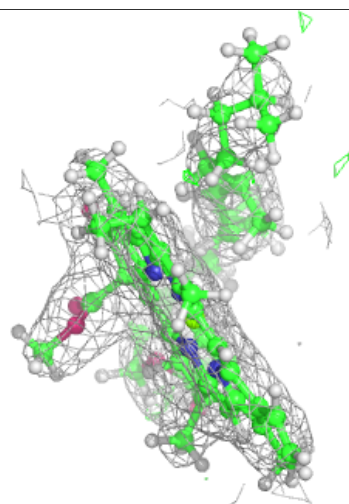
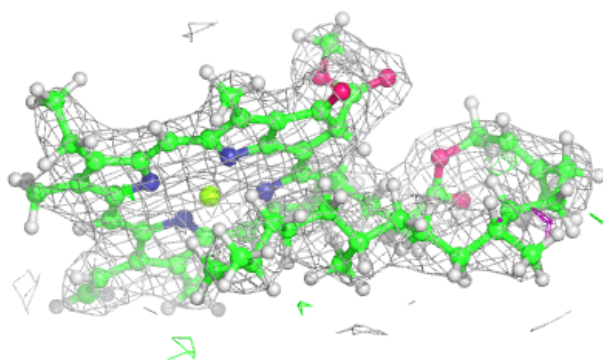
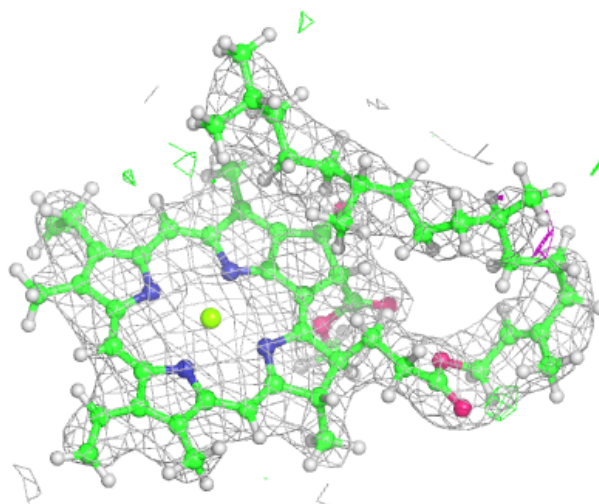
Electron density around BCR b 618:

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



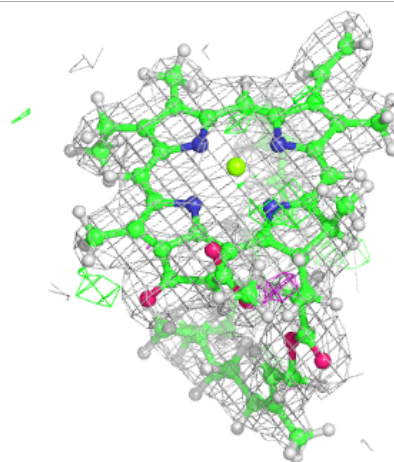
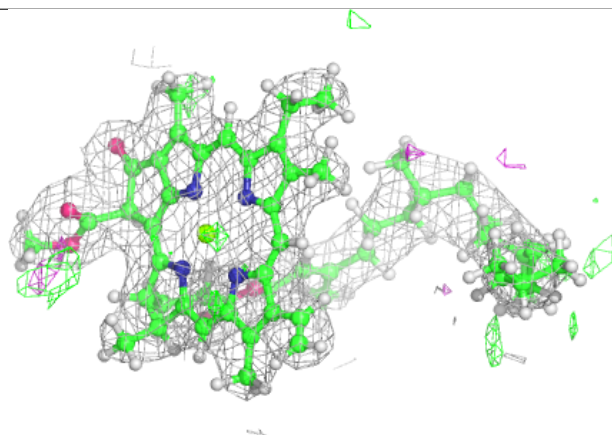
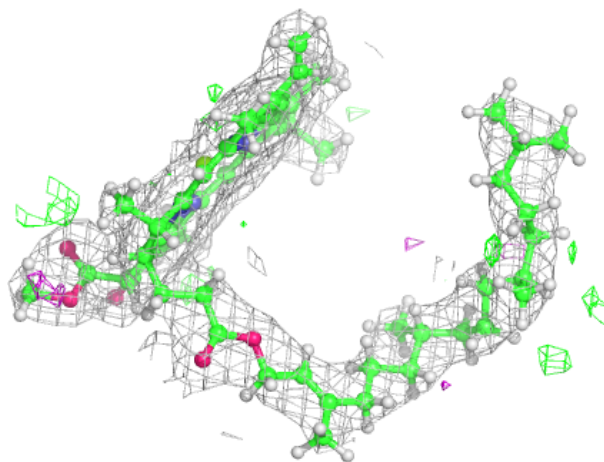
Electron density around CLA c 509:

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



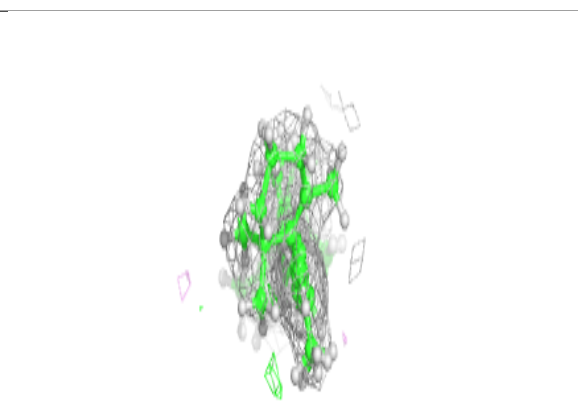
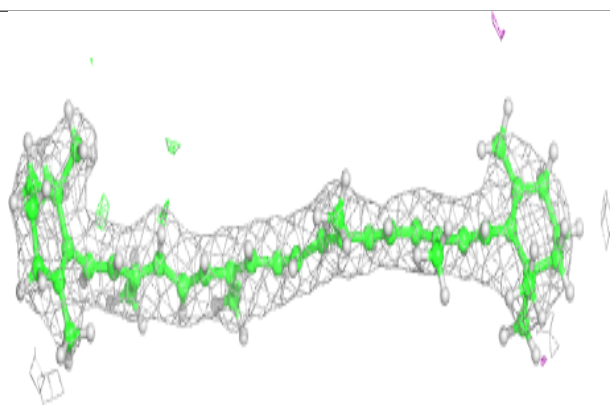
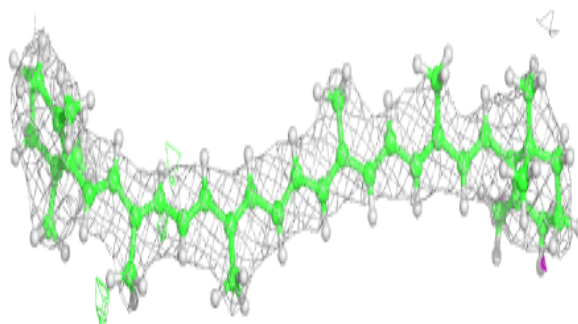
Electron density around CLA b 611:

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

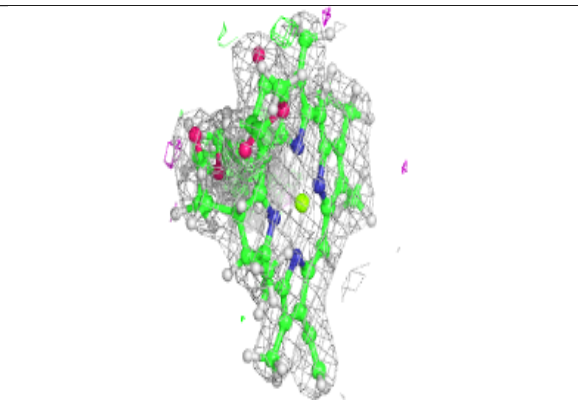
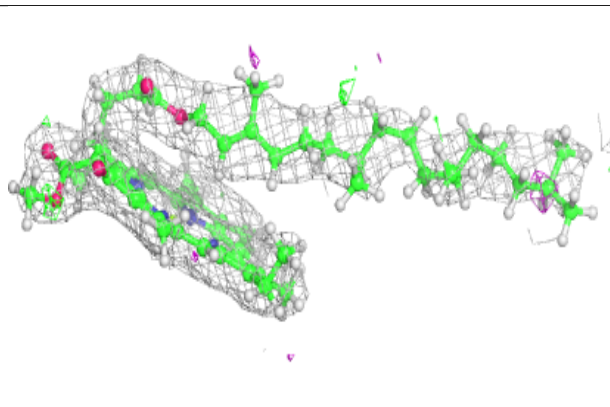
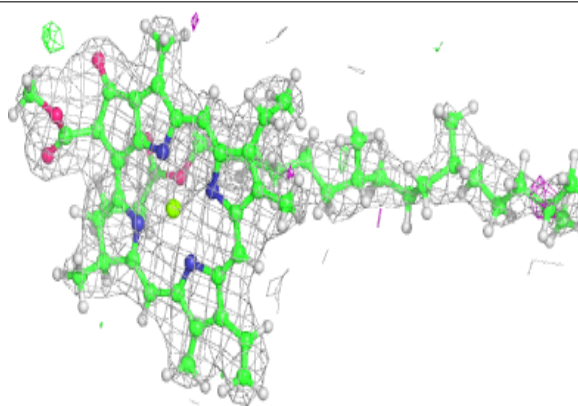


Electron density around BCR c 515:

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

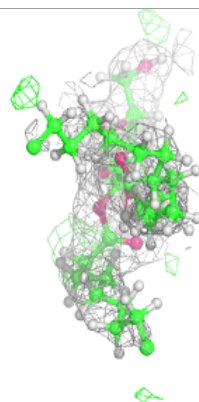
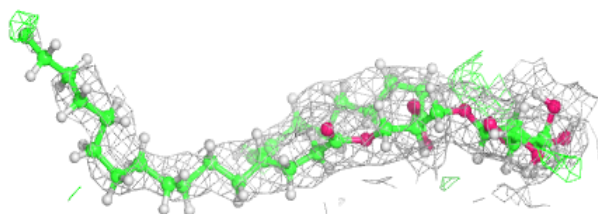
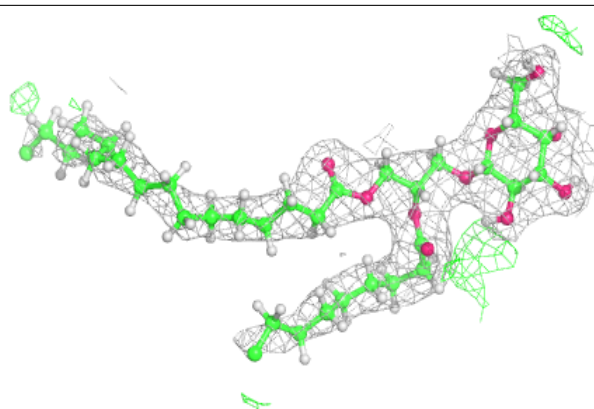
**Electron density around CLA b 614:**

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



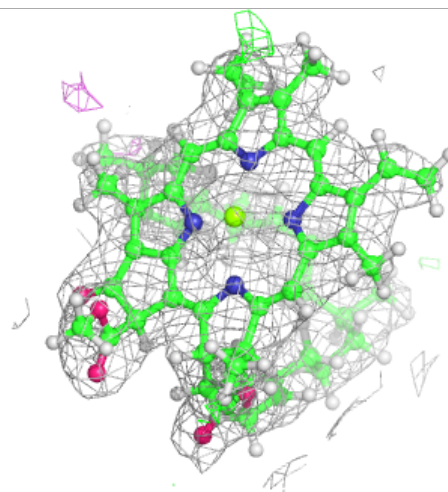
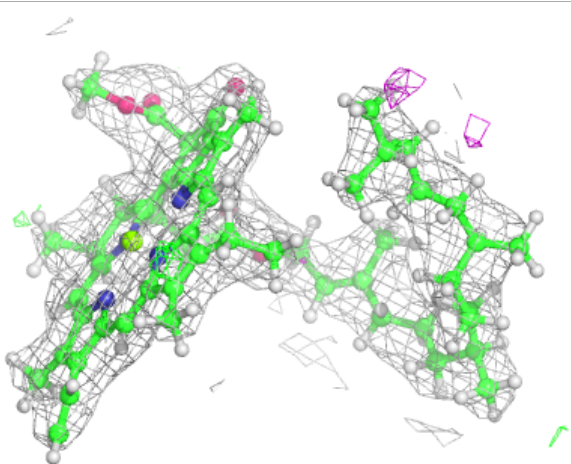
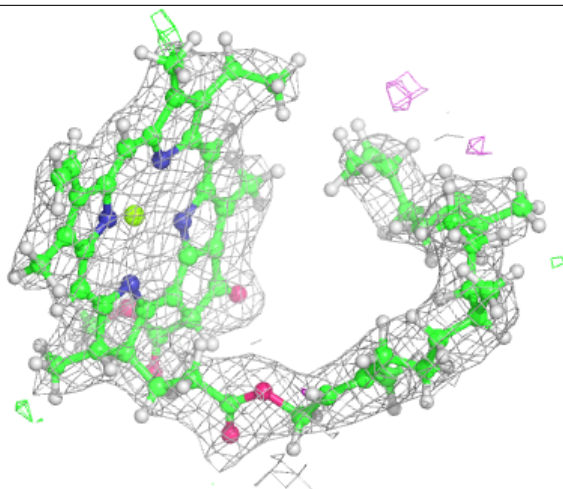
Electron density around LMG d 410:

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



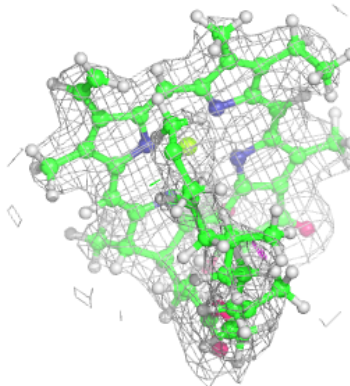
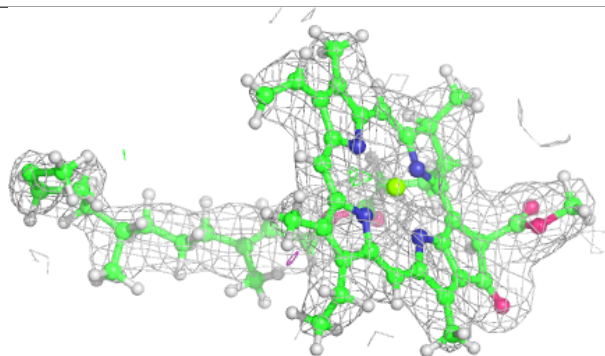
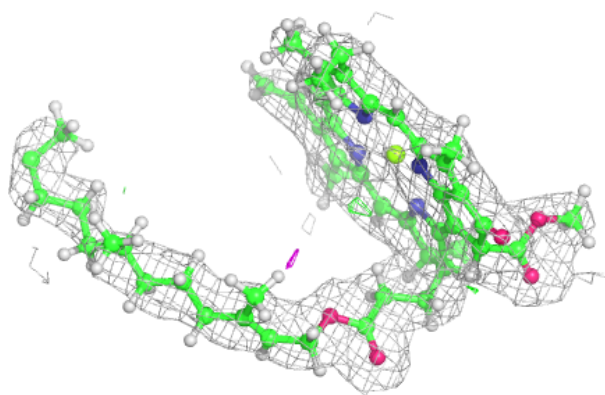
Electron density around CLA C 503:

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

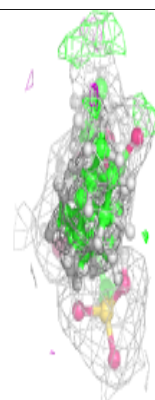
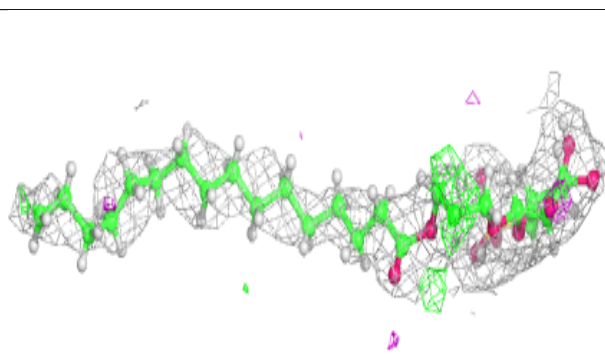
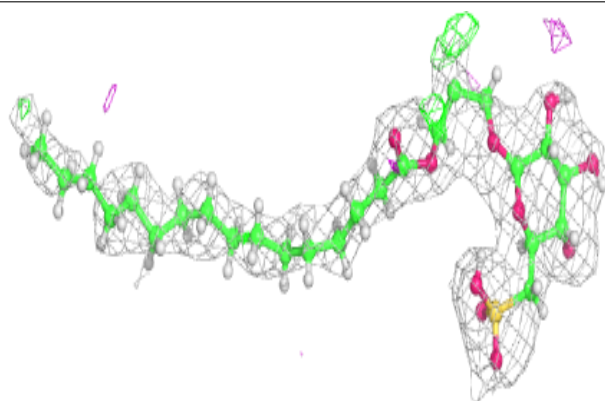


Electron density around CLA C 504:

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

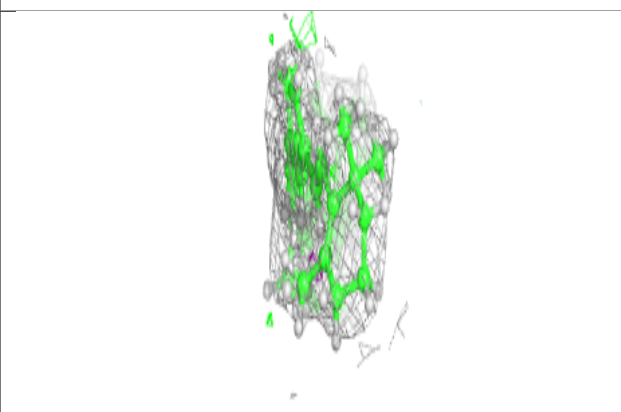
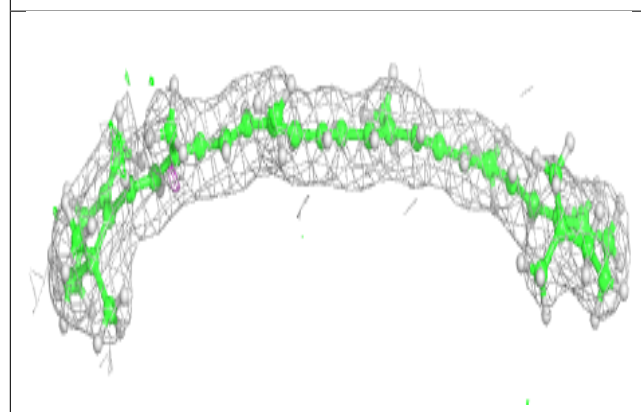
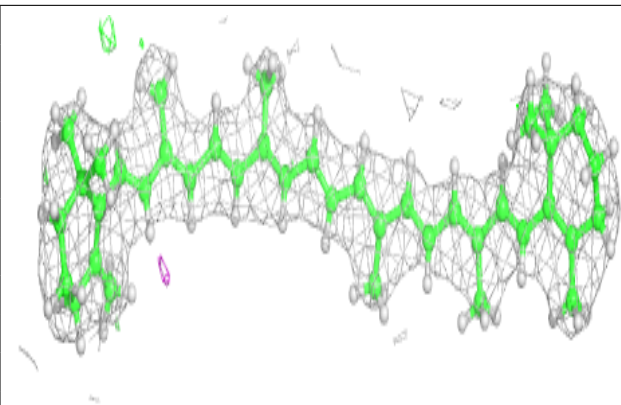
**Electron density around SQD D 407:**

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

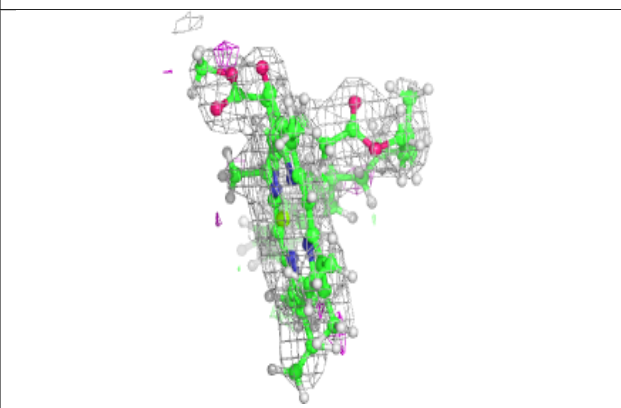
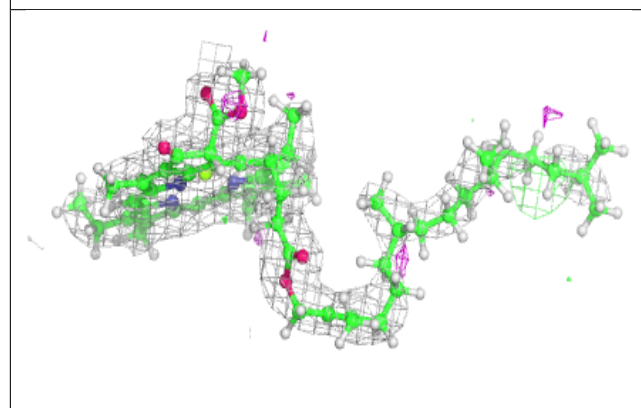
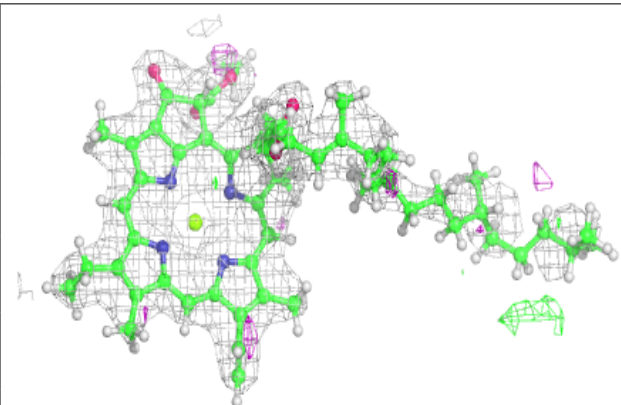


Electron density around BCR t 101:

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

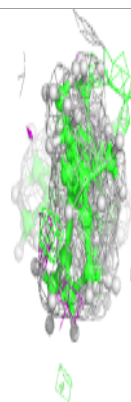
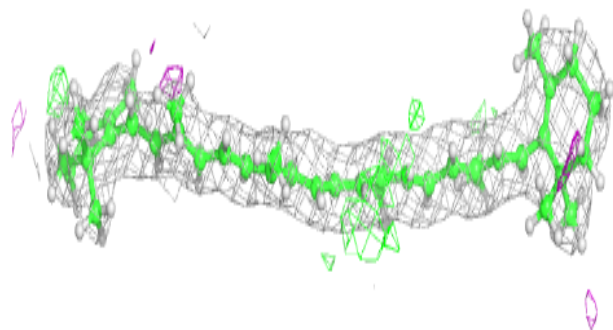
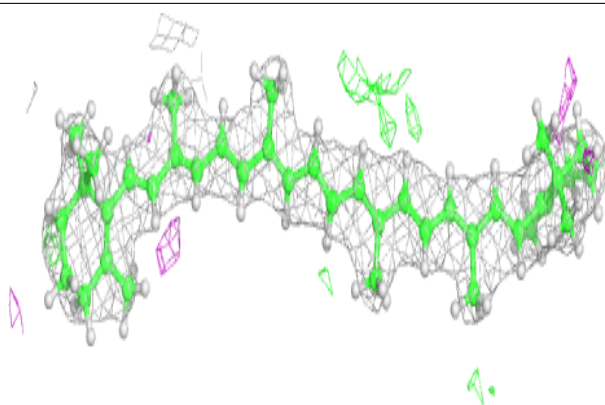
**Electron density around CLA a 403:**

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

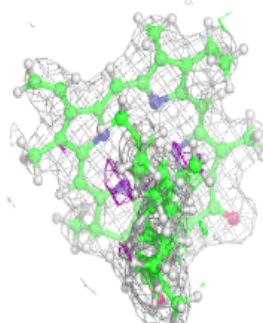
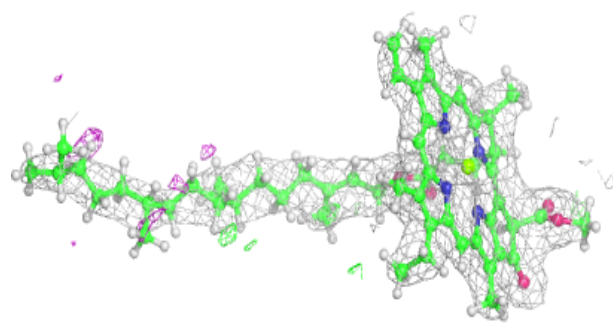
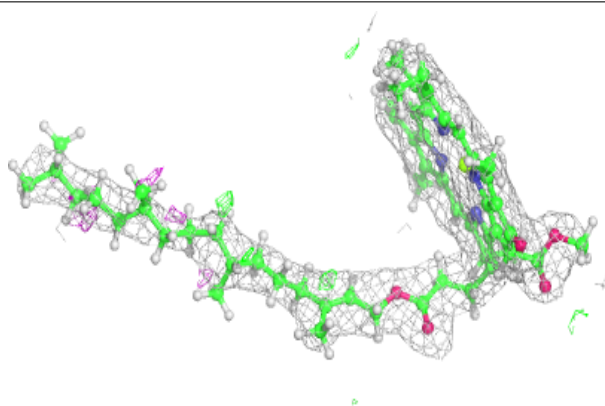


Electron density around BCR B 617:

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

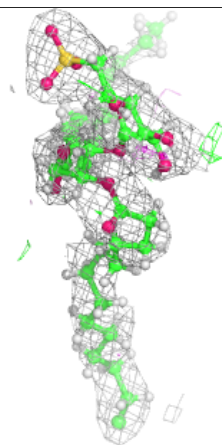
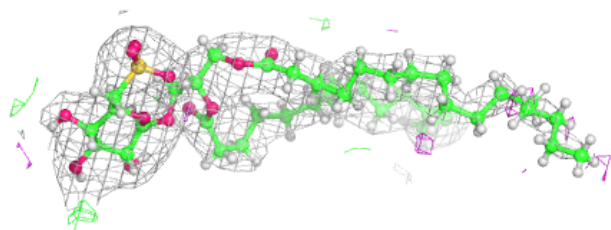
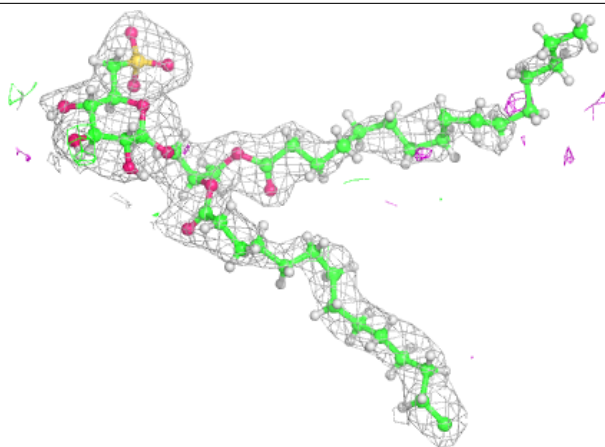
**Electron density around CLA b 607:**

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

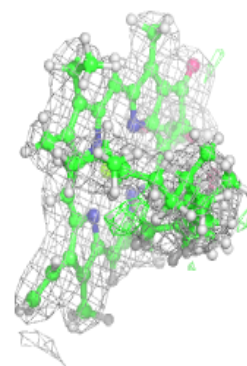
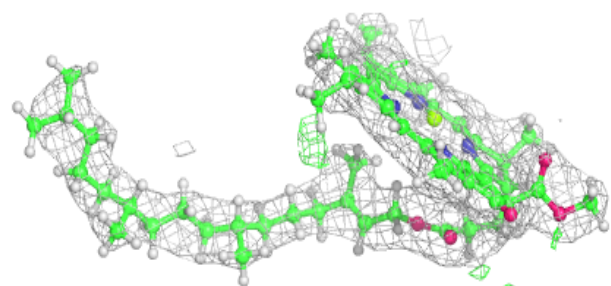
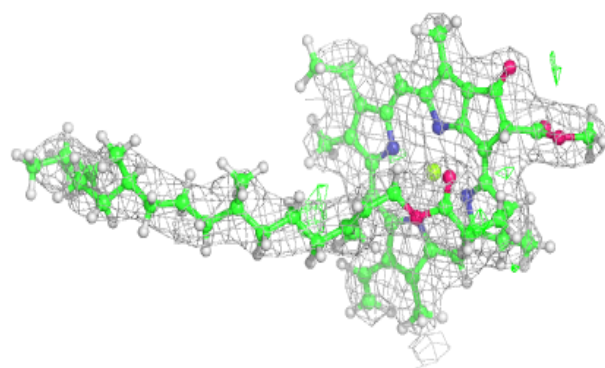


Electron density around SQD A 413:

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

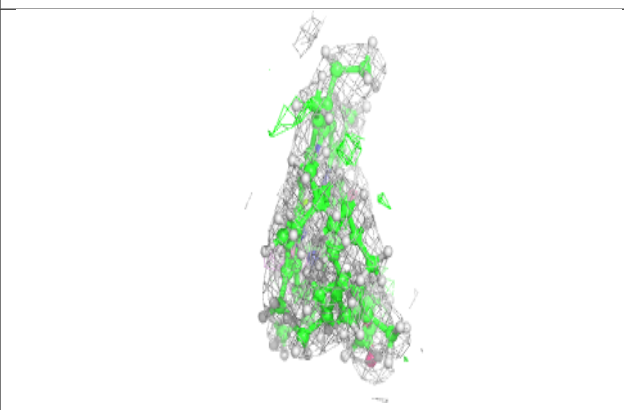
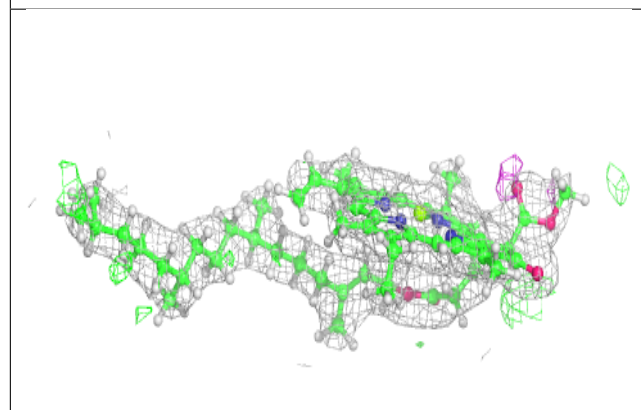
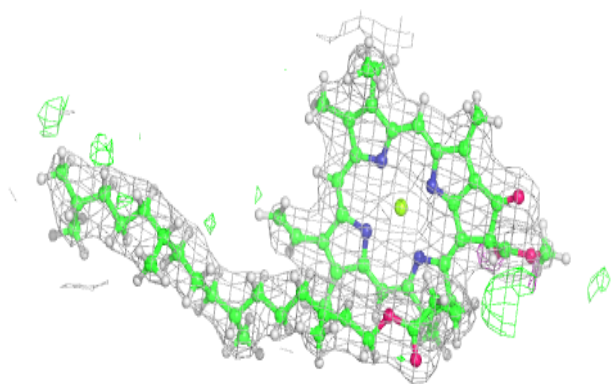
**Electron density around CLA b 608:**

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



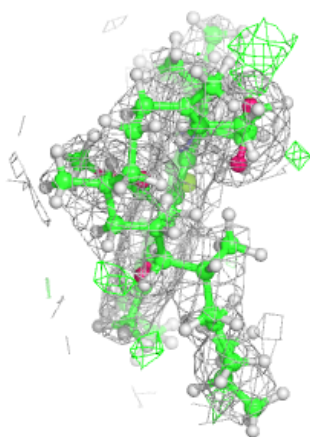
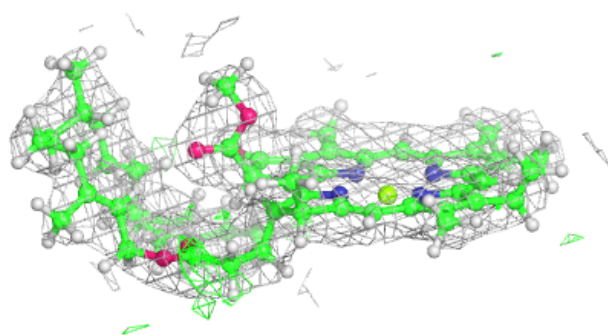
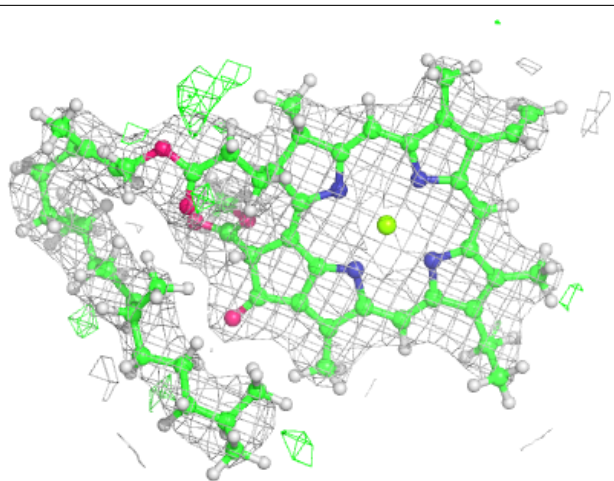
Electron density around CLA C 501:

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



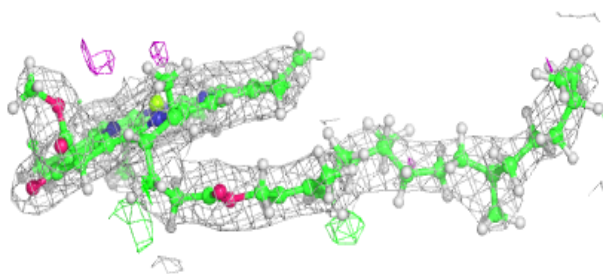
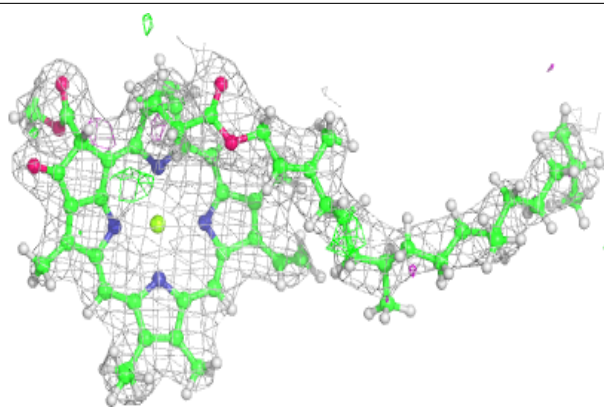
Electron density around CLA b 610:

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

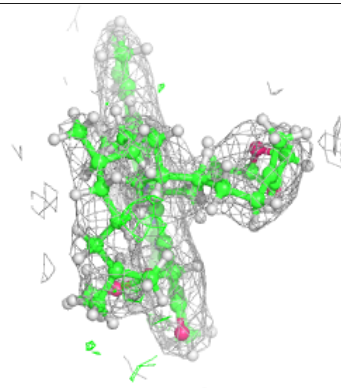
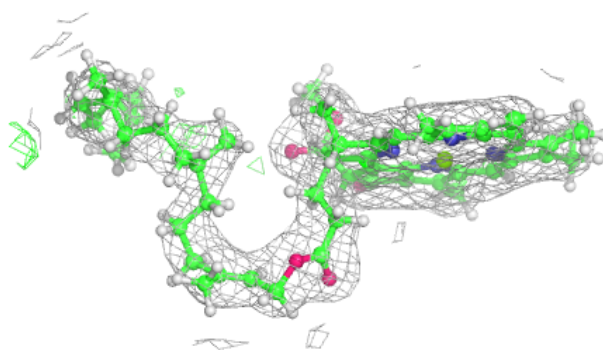
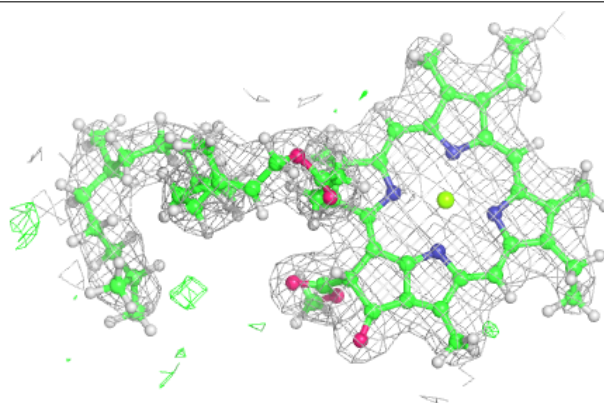


Electron density around CLA B 603:

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

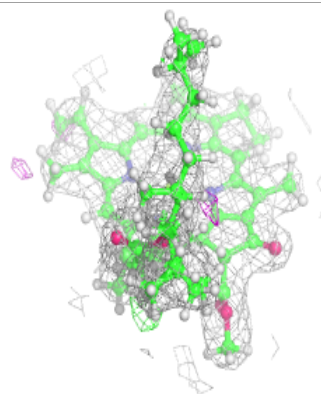
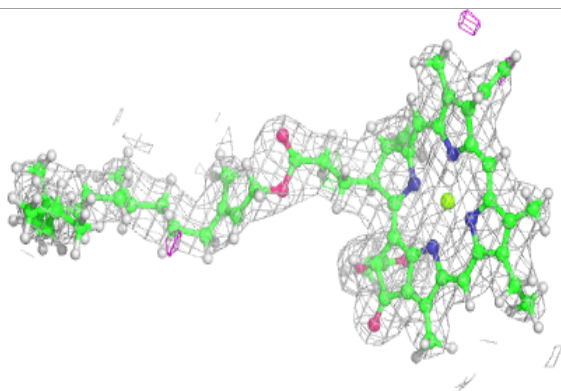
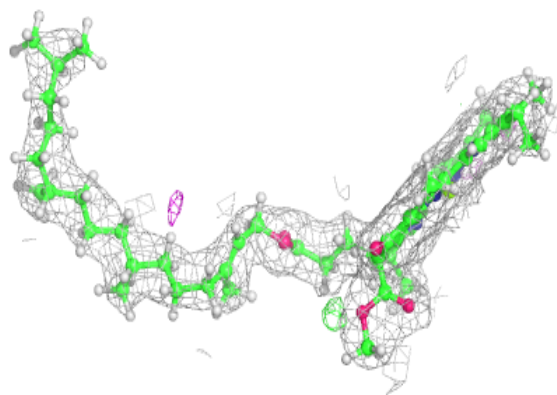
**Electron density around CLA b 612:**

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



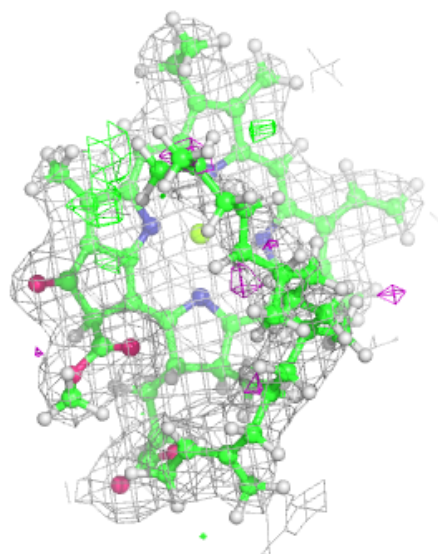
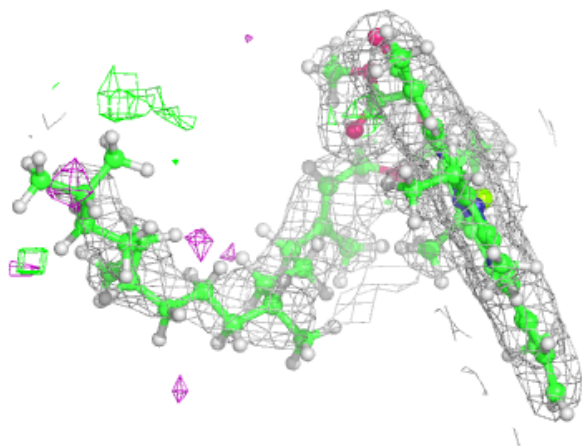
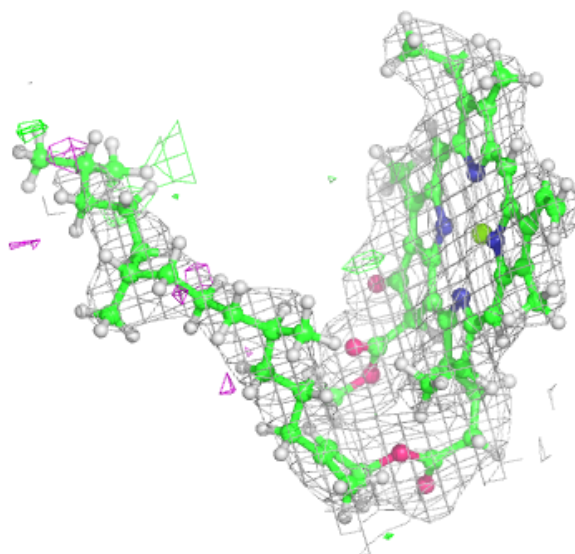
Electron density around CLA d 403:

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



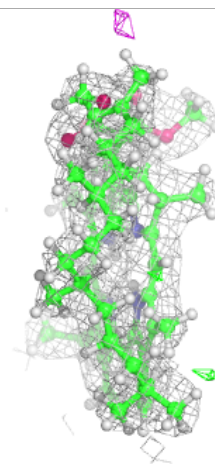
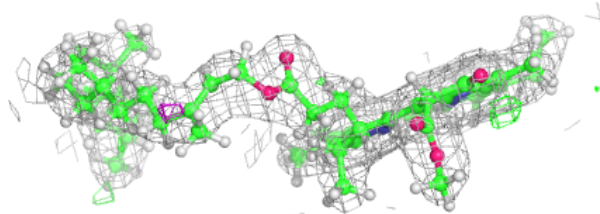
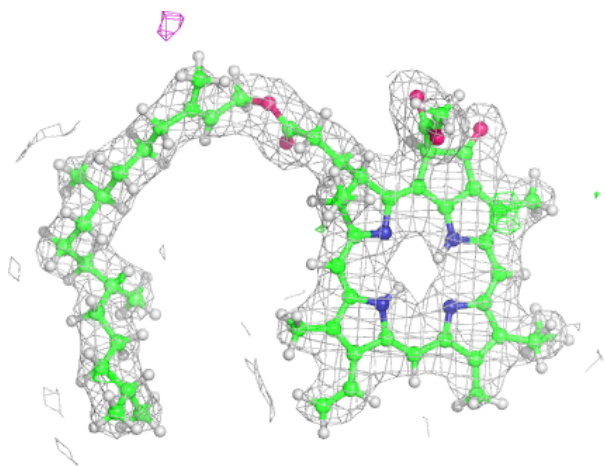
Electron density around CLA b 613:

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



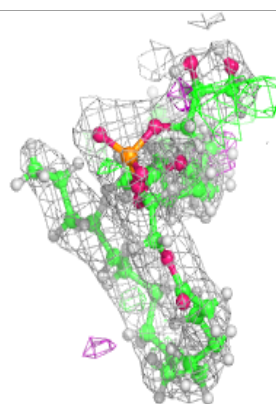
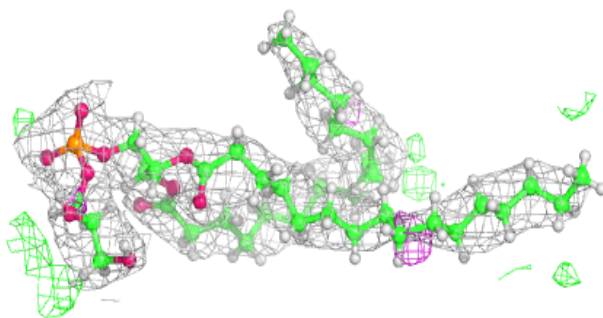
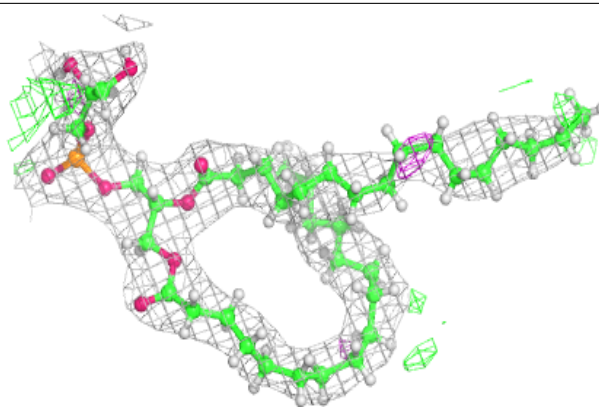
Electron density around PHO A 404:

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

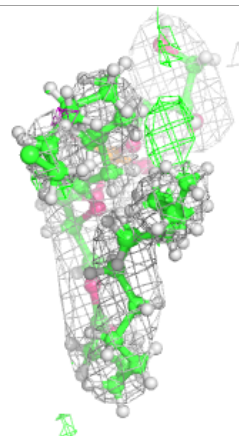
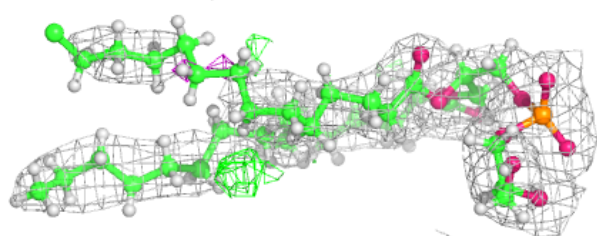
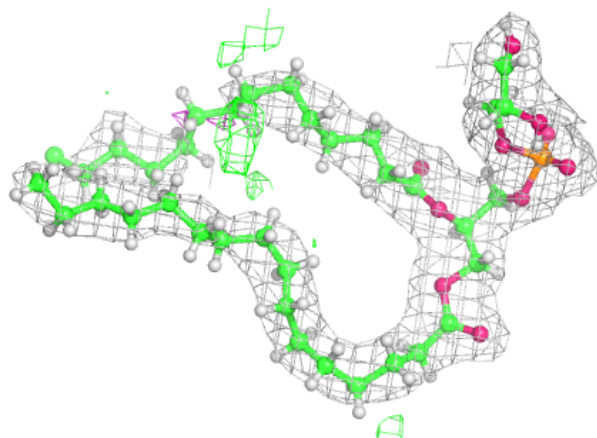


Electron density around LHG B 622:

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

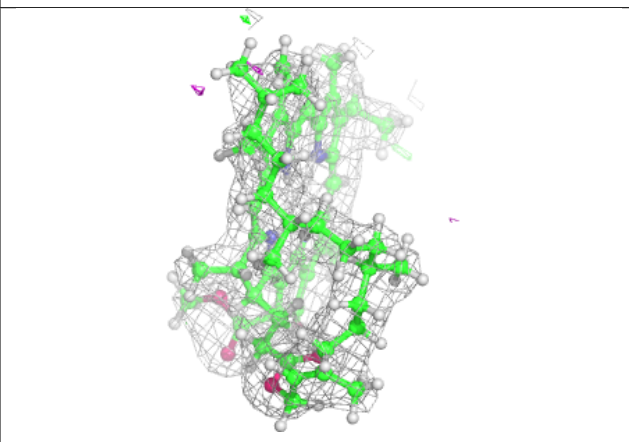
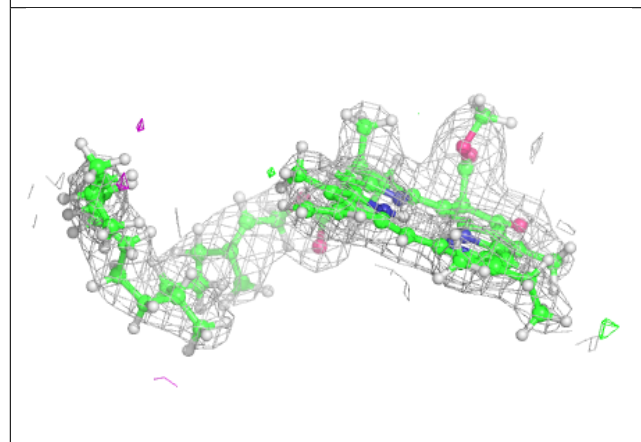
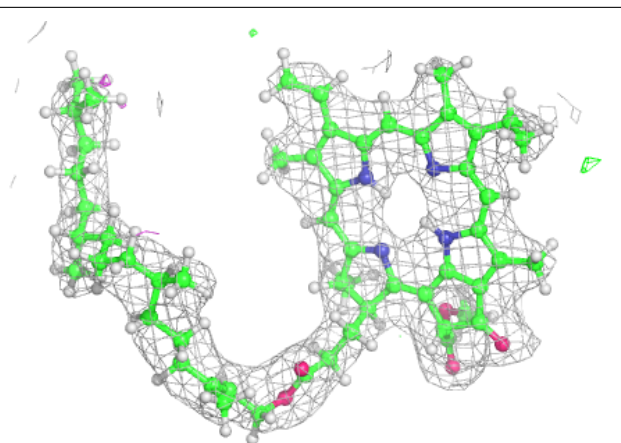
**Electron density around LHG D 409:**

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



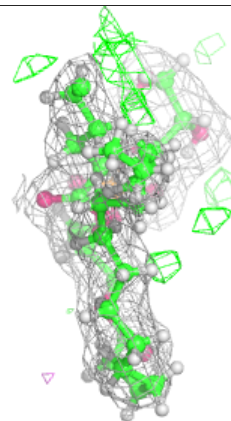
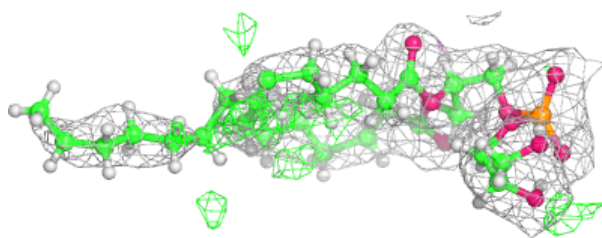
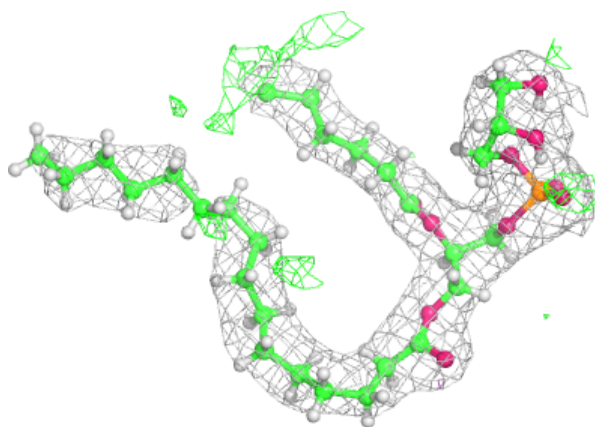
Electron density around PHO d 402:

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

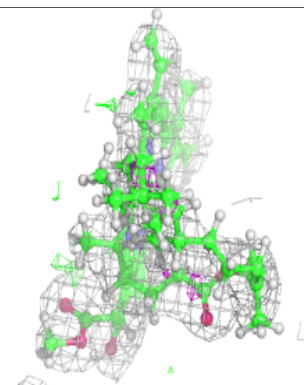
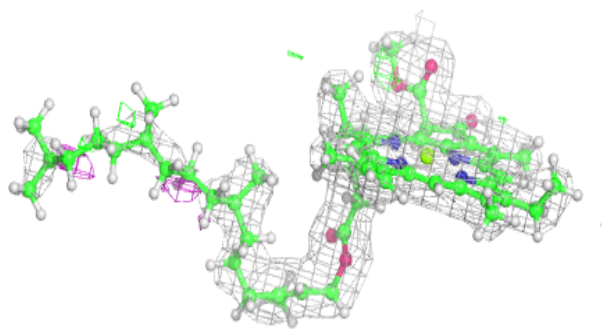
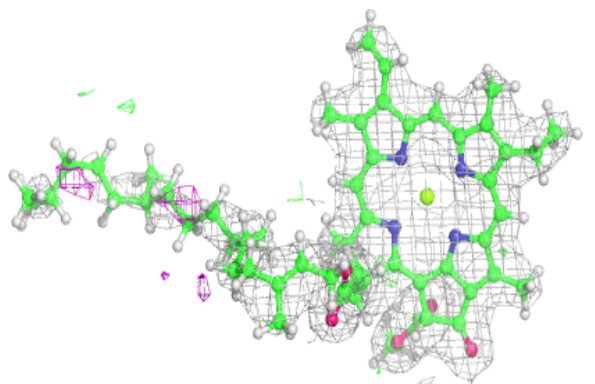


Electron density around LHG d 409:

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

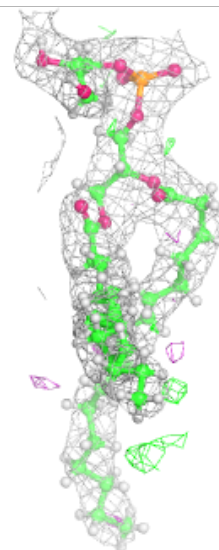
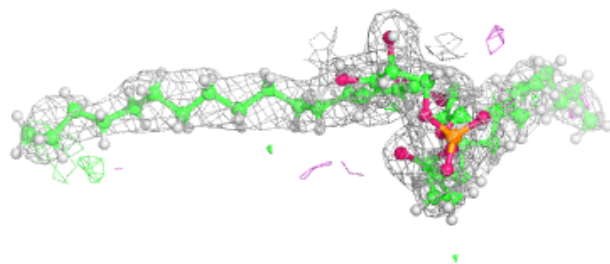
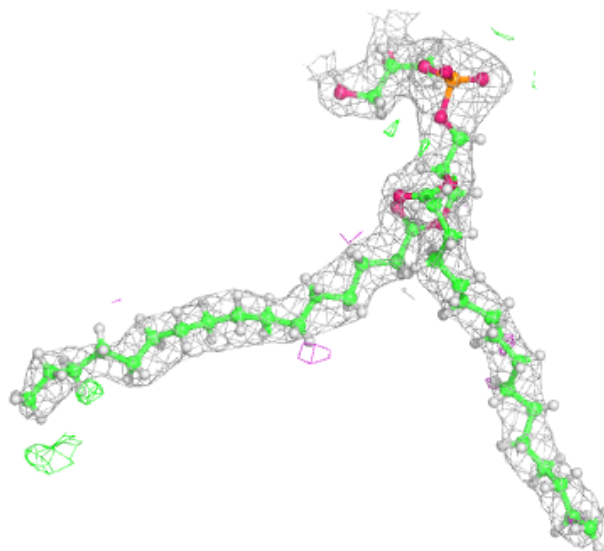
**Electron density around CLA A 403:**

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



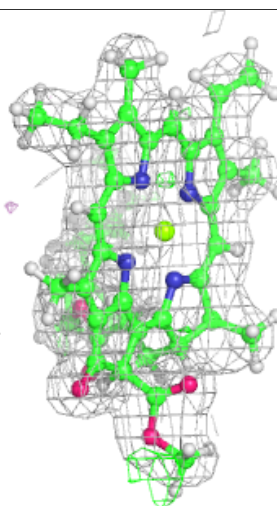
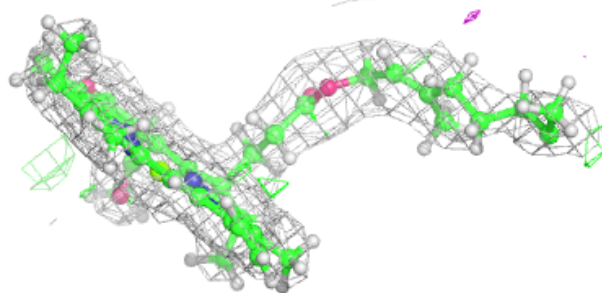
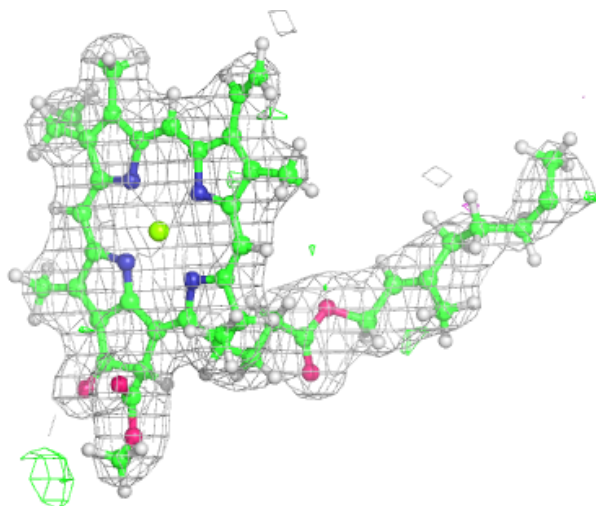
Electron density around LHG 1 101:

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



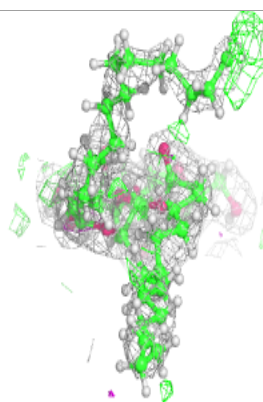
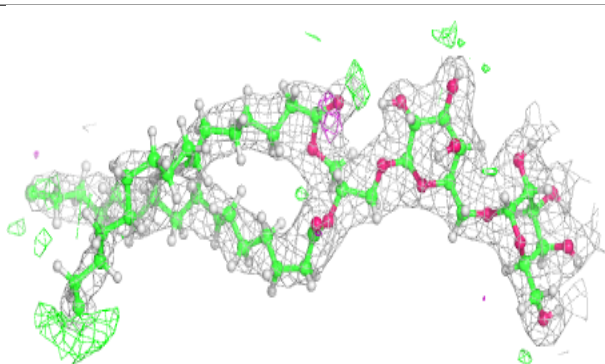
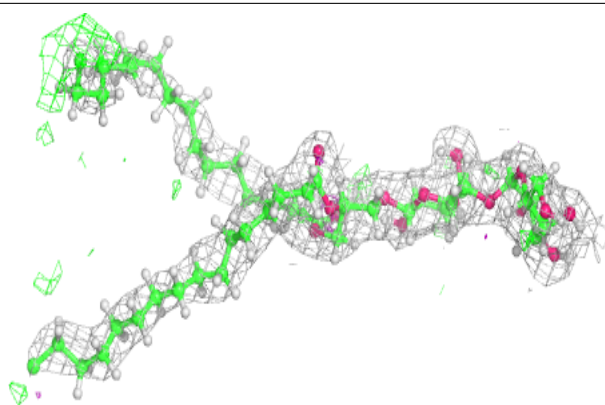
Electron density around CLA A 405:

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

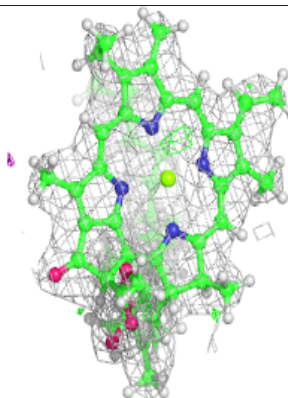
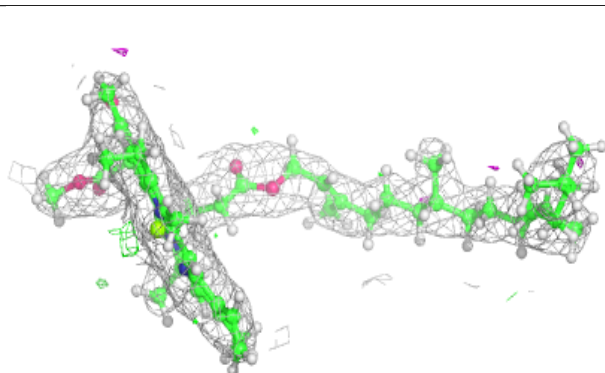
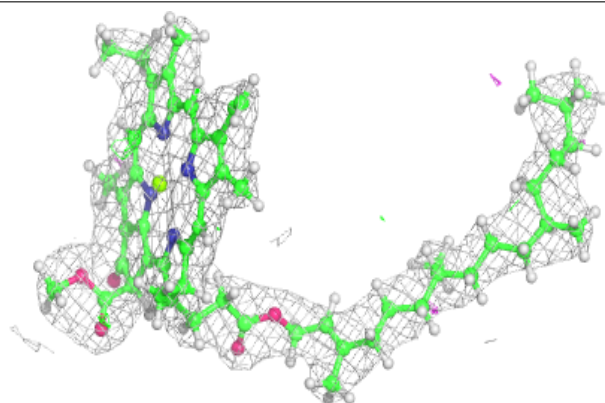


Electron density around DGD C 515:

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

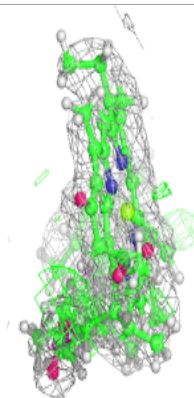
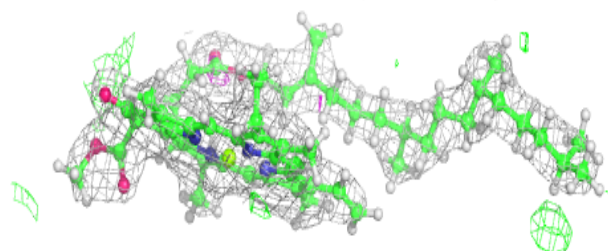
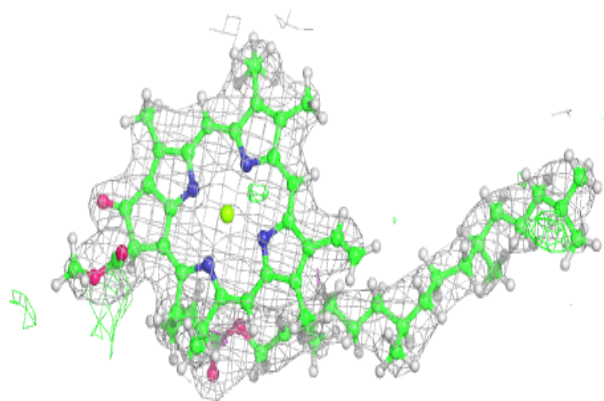
**Electron density around CLA B 609:**

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



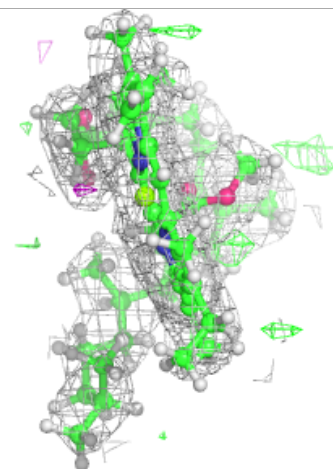
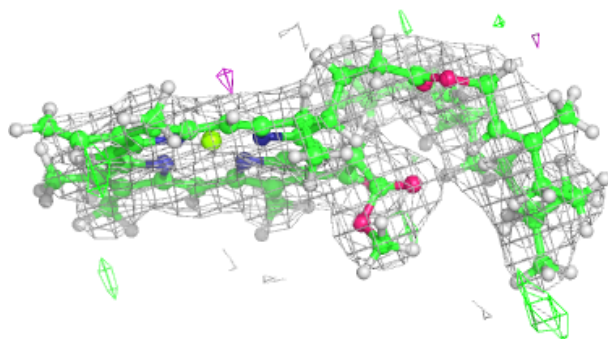
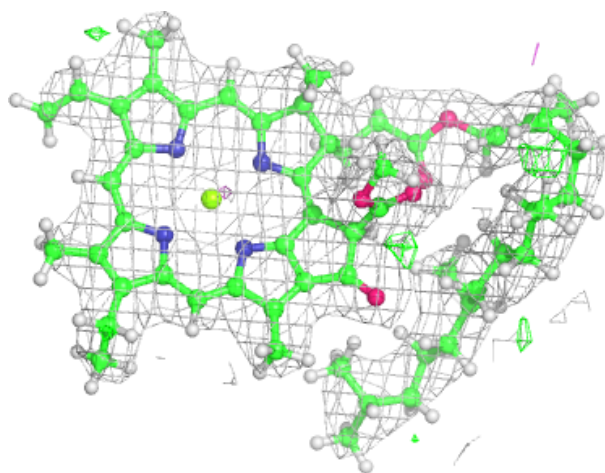
Electron density around CLA c 501:

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



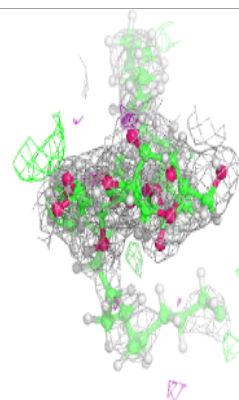
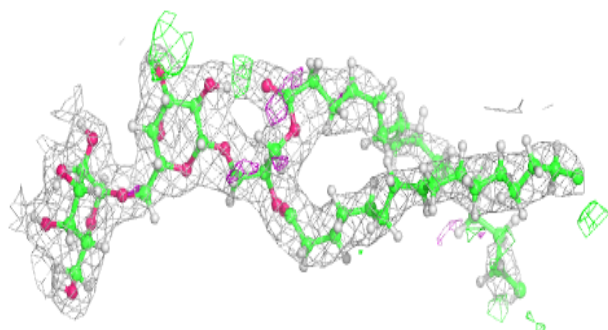
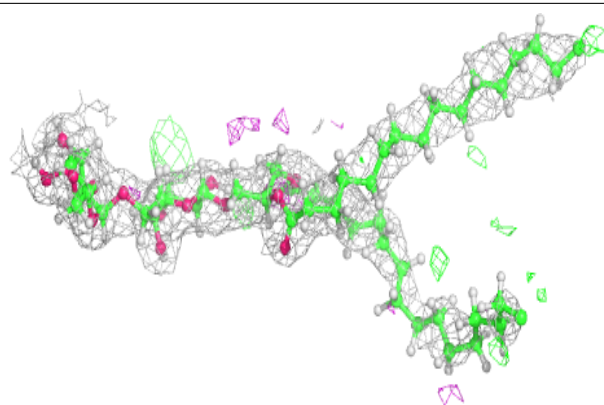
Electron density around CLA B 610:

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

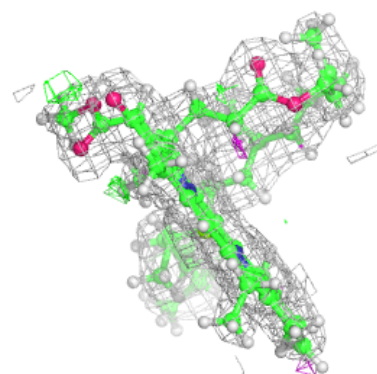
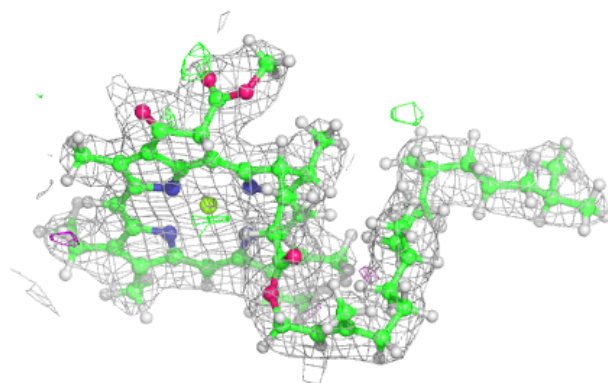
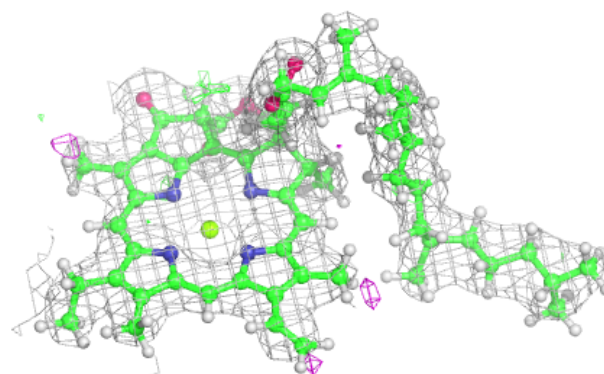


Electron density around DGD c 516:

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

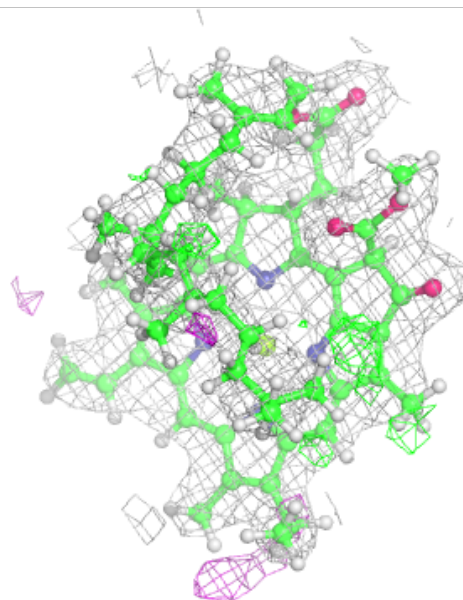
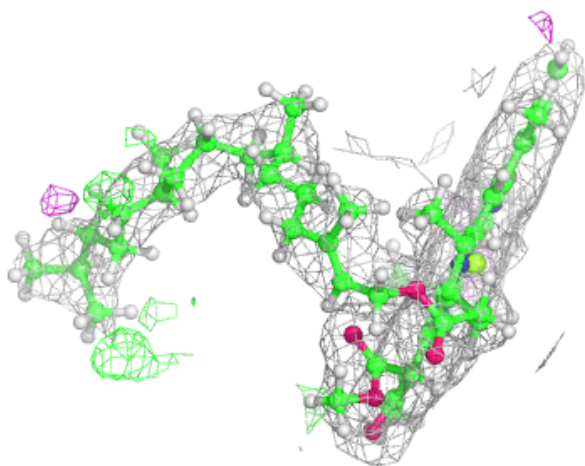
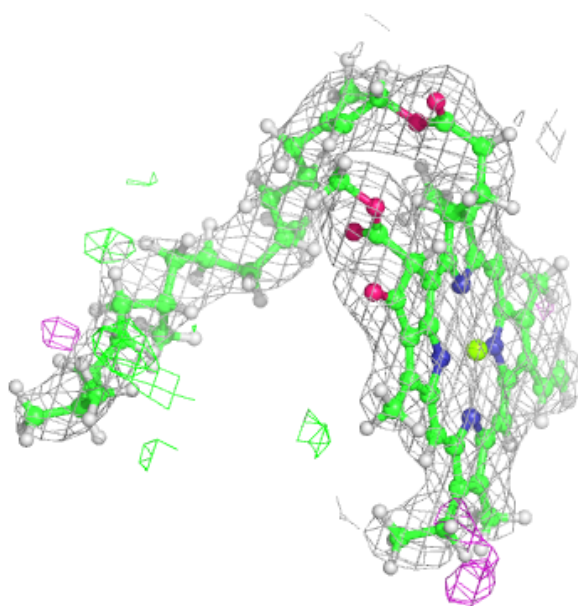
**Electron density around CLA a 410:**

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



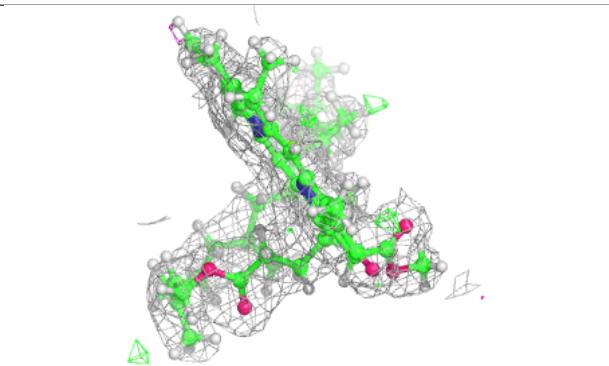
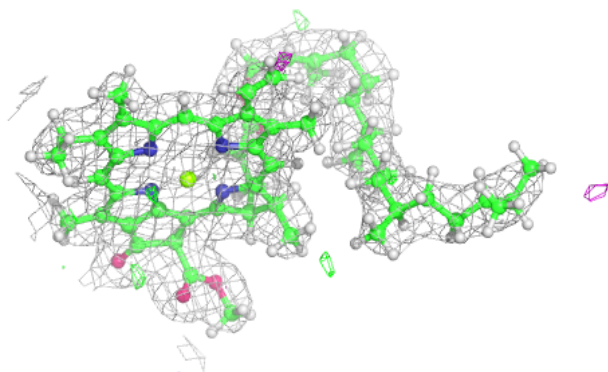
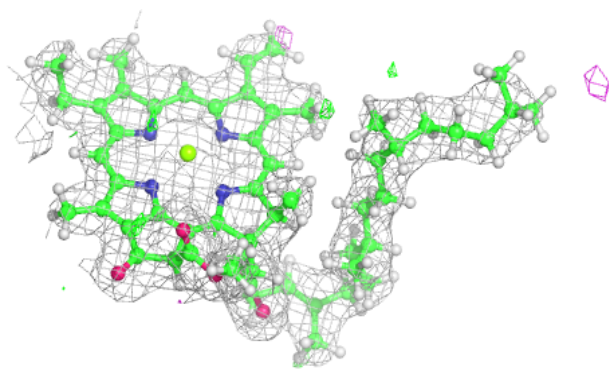
Electron density around CLA B 613:

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

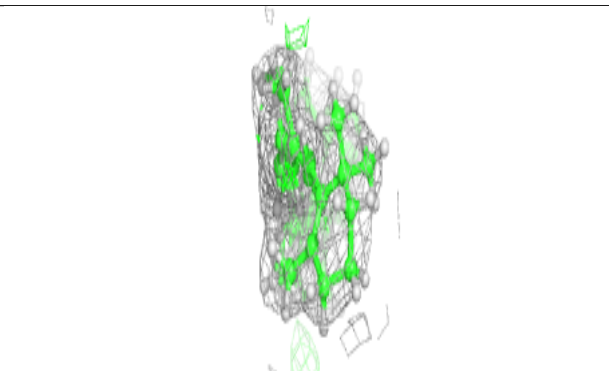
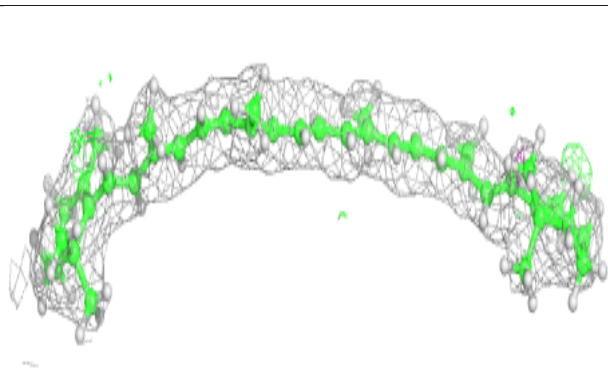
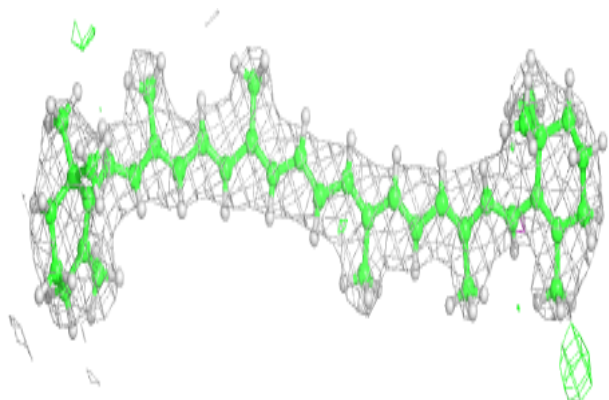


Electron density around CLA A 411:

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

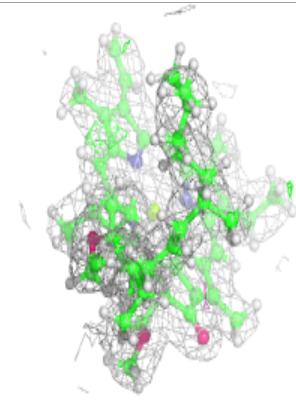
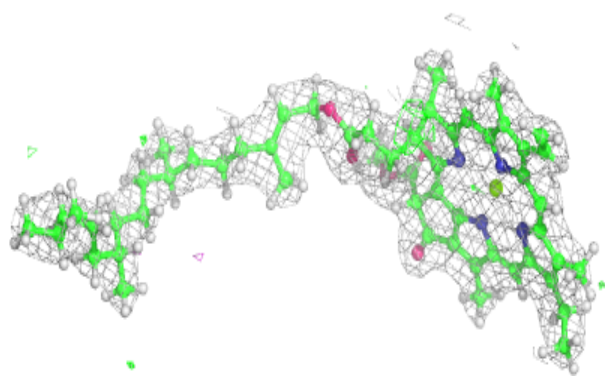
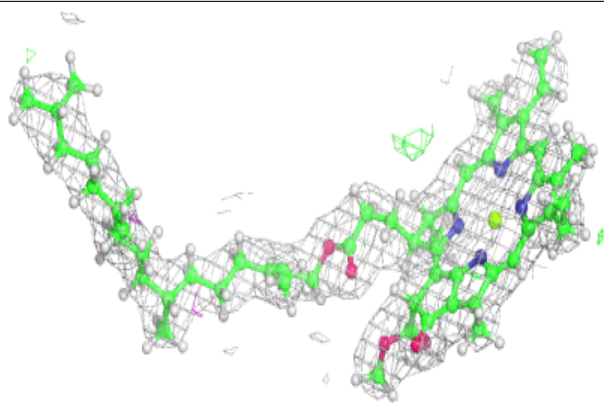
**Electron density around BCR T 101:**

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

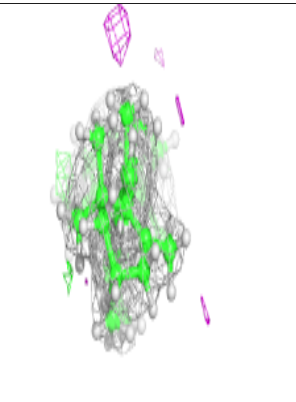
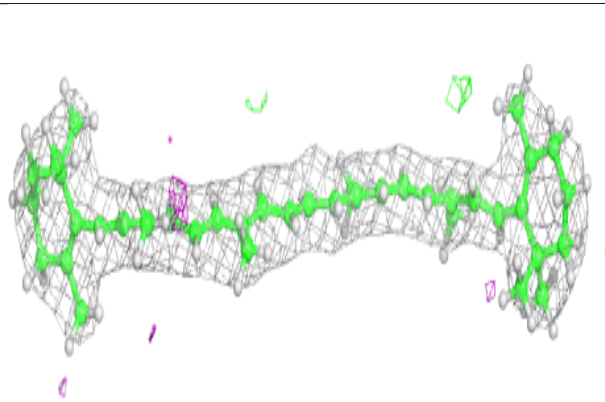
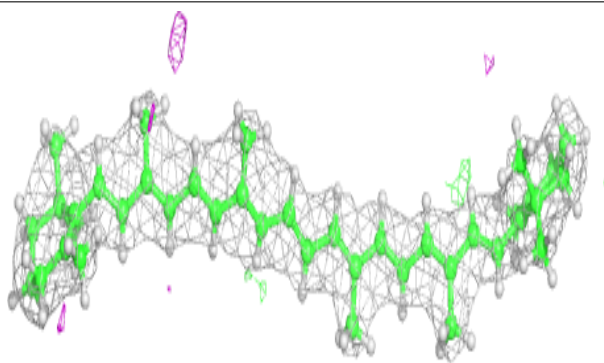


Electron density around CLA A 402:

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

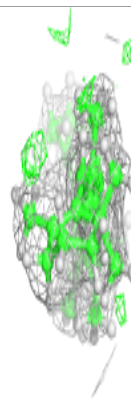
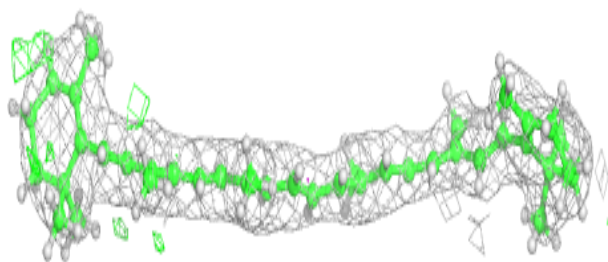
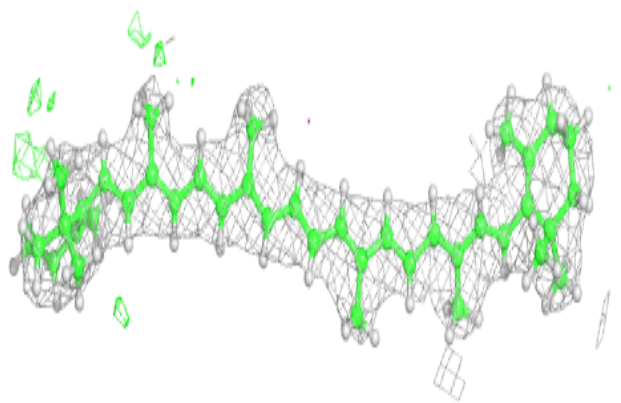
**Electron density around BCR a 405:**

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

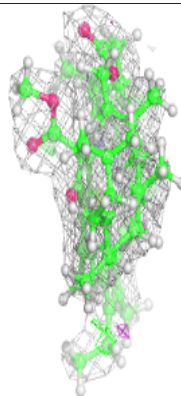
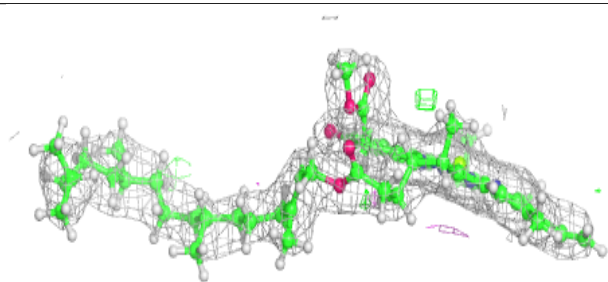
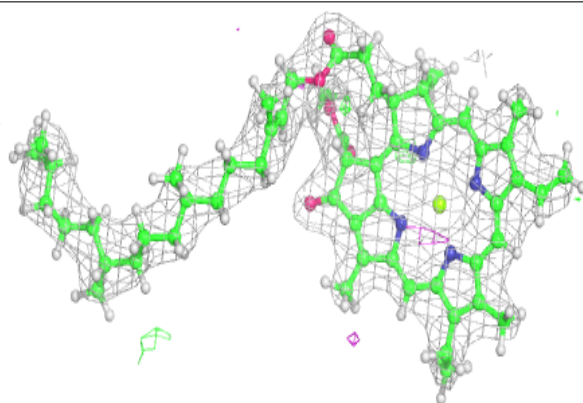


Electron density around BCR b 617:

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

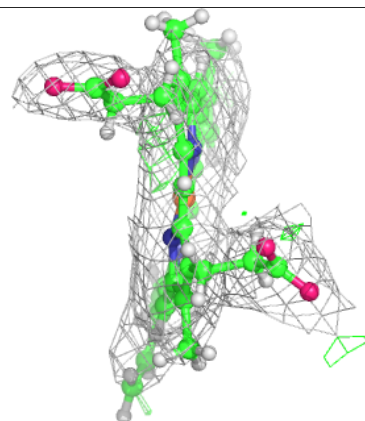
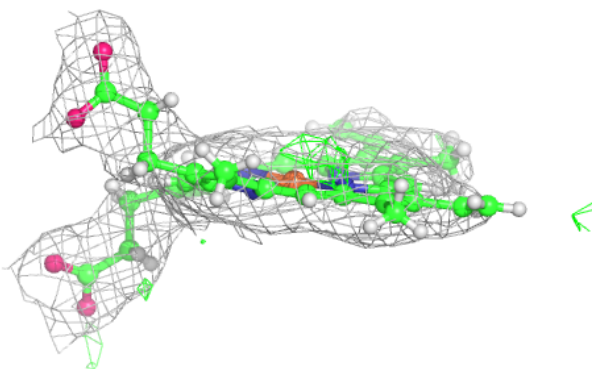
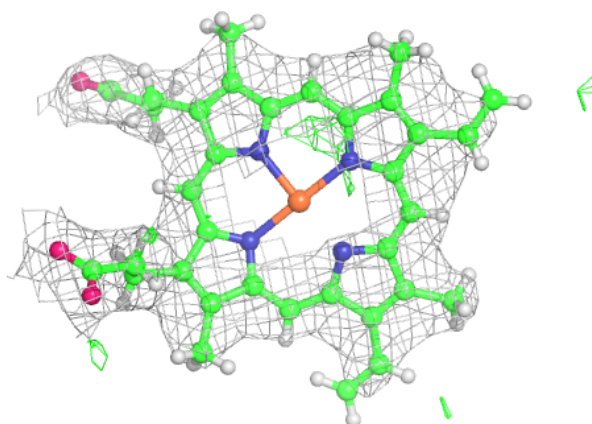
**Electron density around CLA B 602:**

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

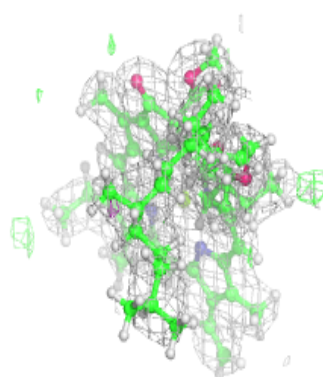
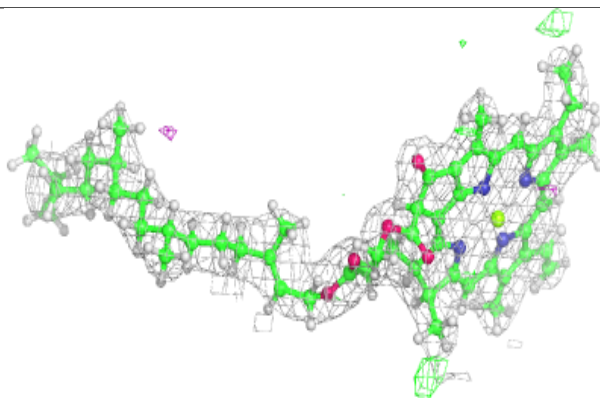
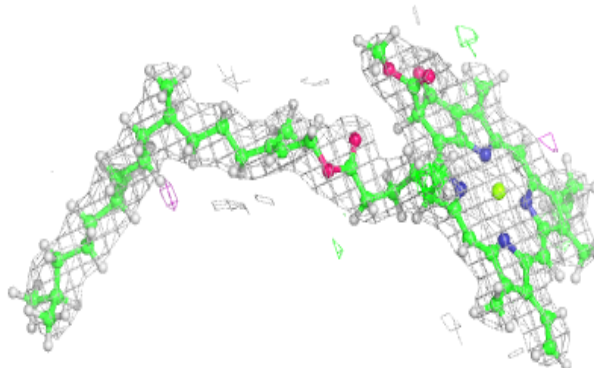


Electron density around HEM F 101:

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

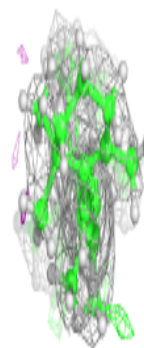
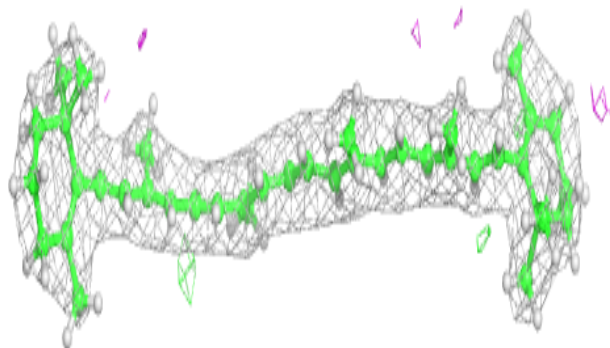
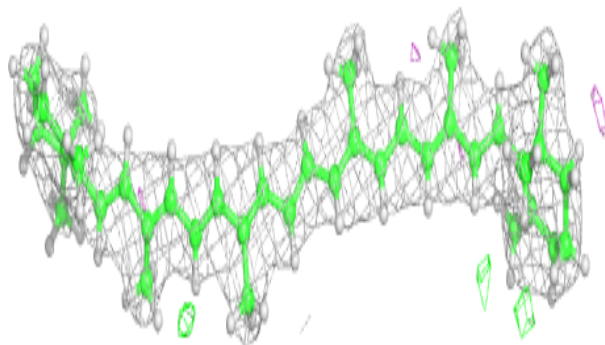
**Electron density around CLA a 402:**

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

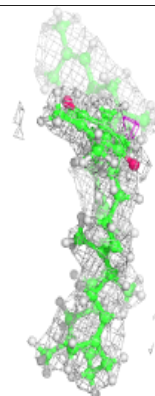
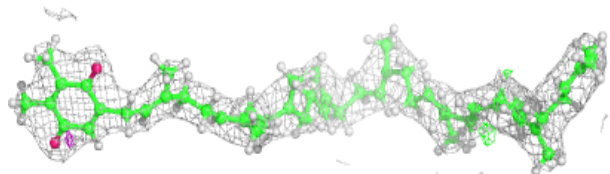
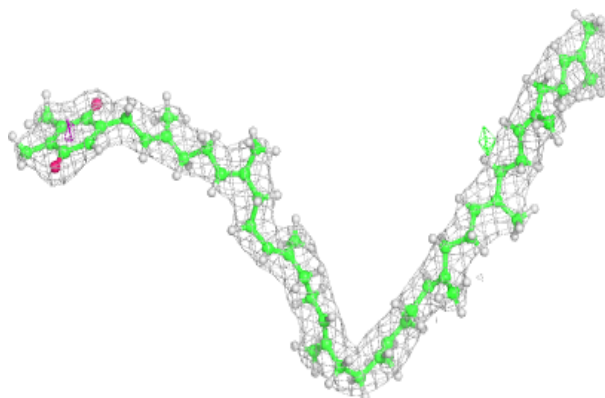


Electron density around BCR A 406:

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

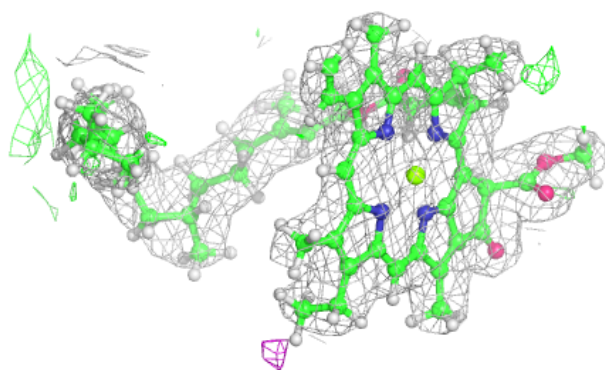
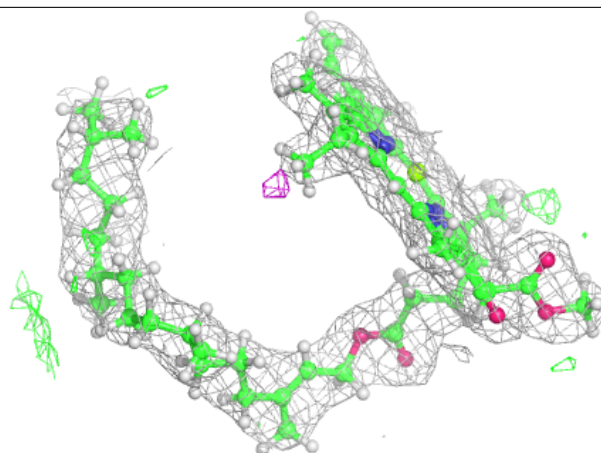
**Electron density around PL9 d 406:**

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



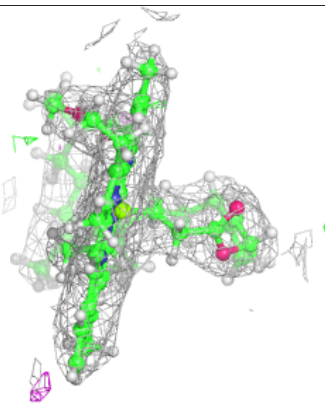
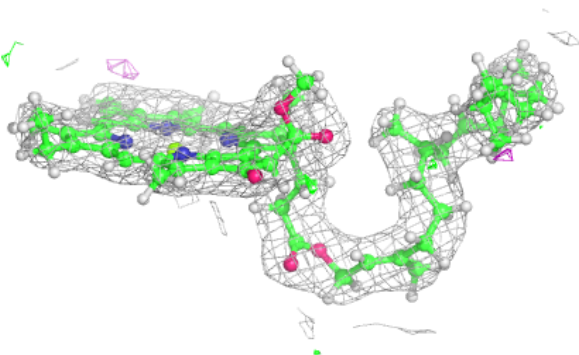
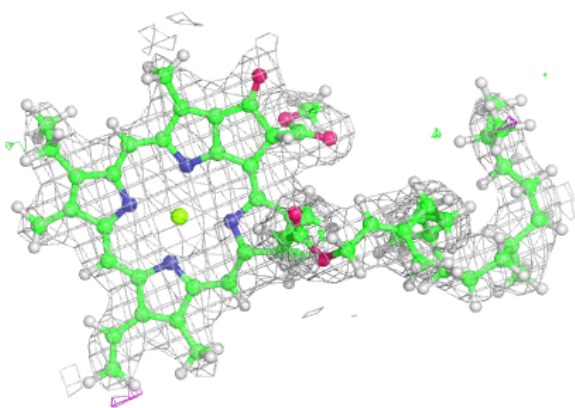
Electron density around CLA B 611:

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

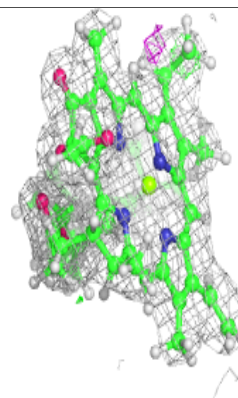
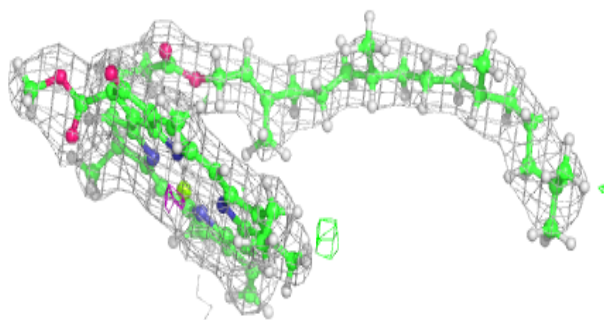
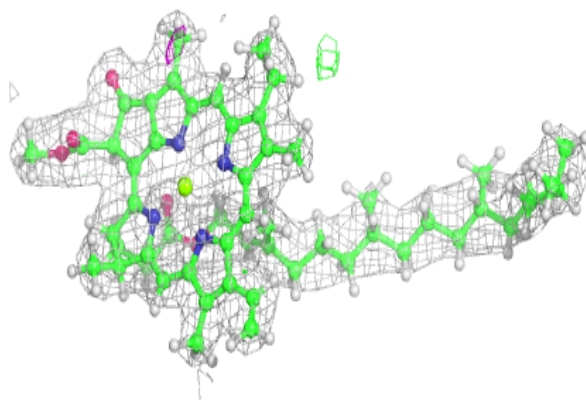


Electron density around CLA B 612:

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

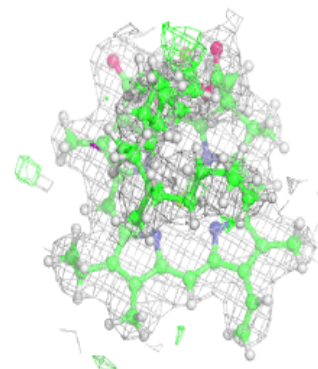
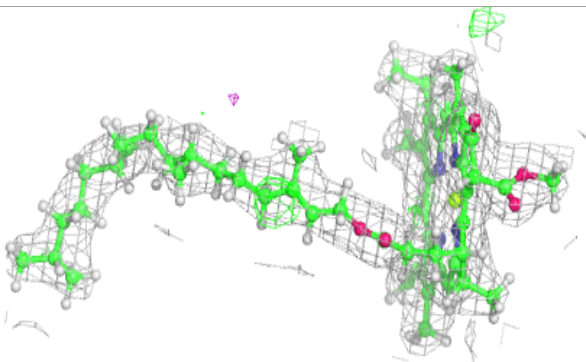
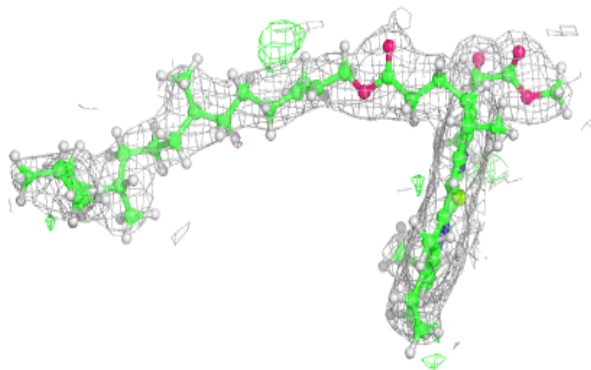
**Electron density around CLA B 608:**

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

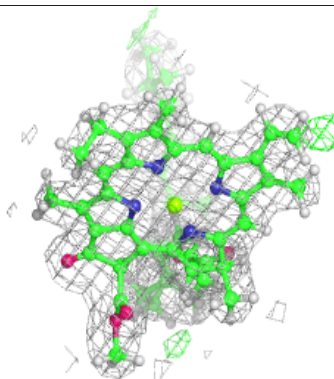
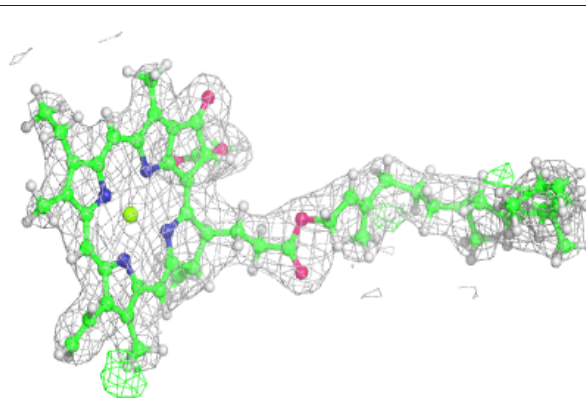
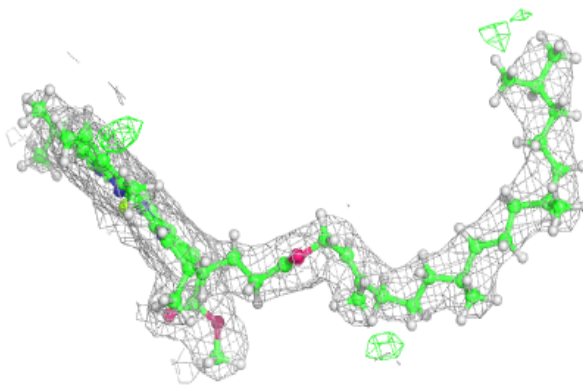


Electron density around CLA B 605:

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

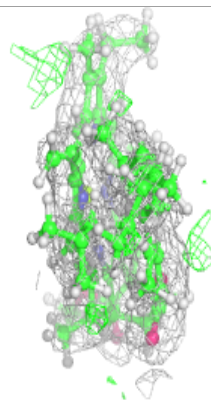
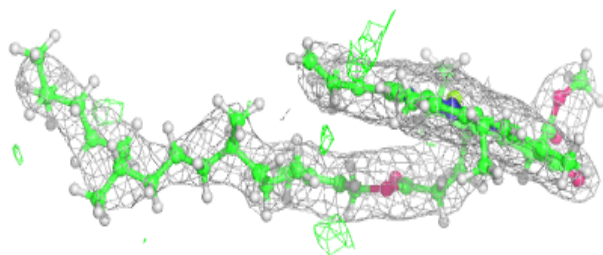
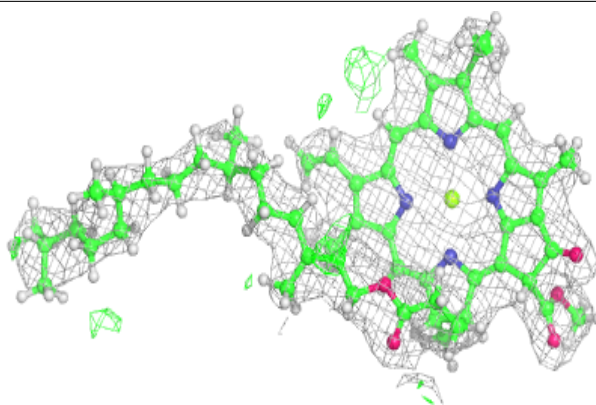
**Electron density around CLA D 402:**

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

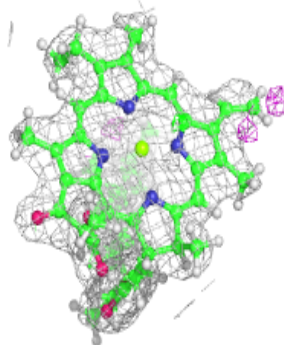
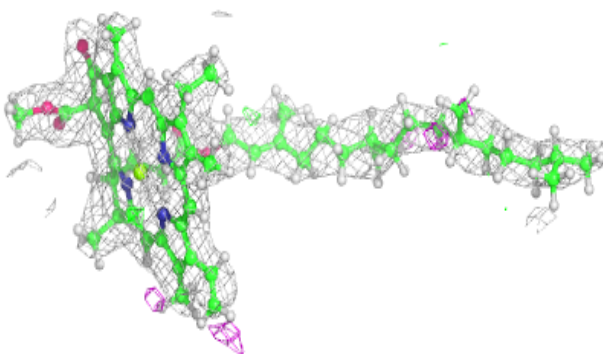
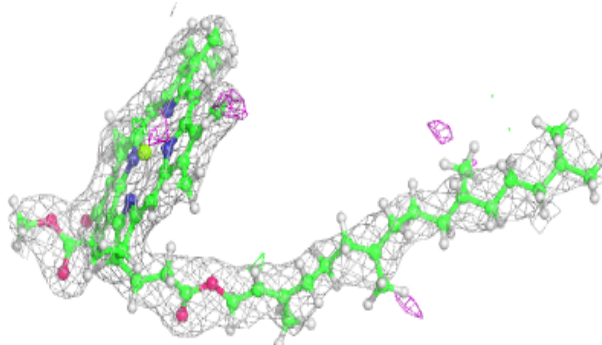


Electron density around CLA b 603:

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

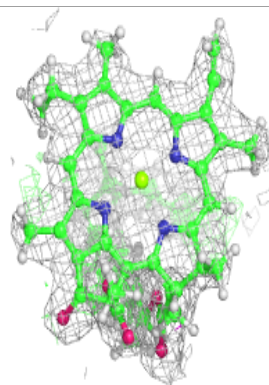
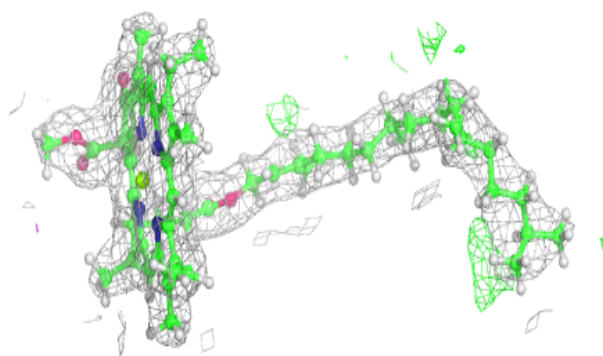
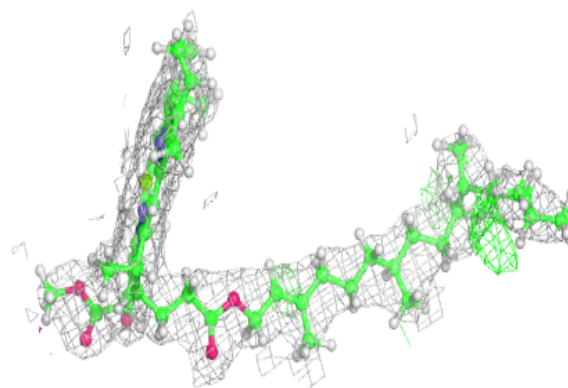
**Electron density around CLA B 607:**

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



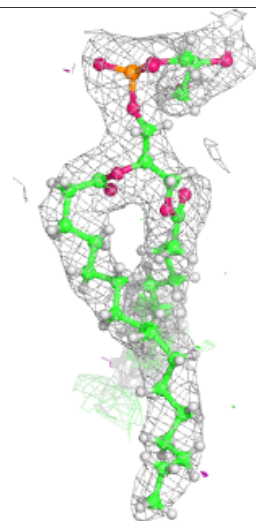
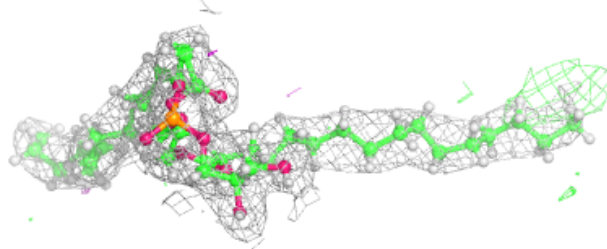
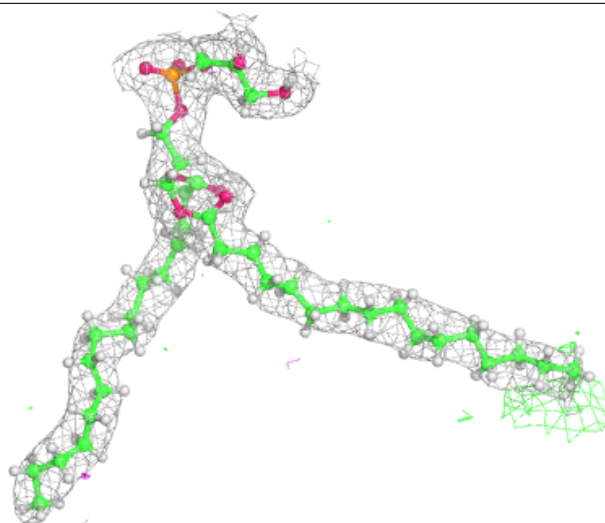
Electron density around CLA b 605:

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



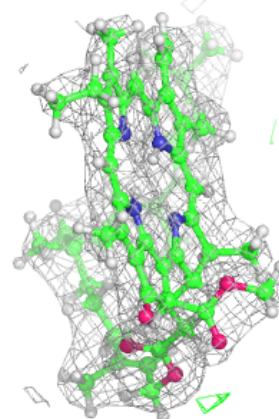
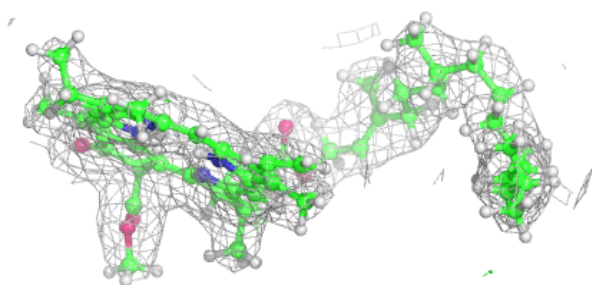
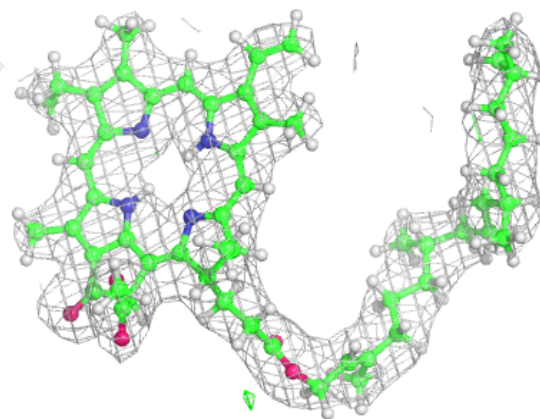
Electron density around LHG B 621:

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



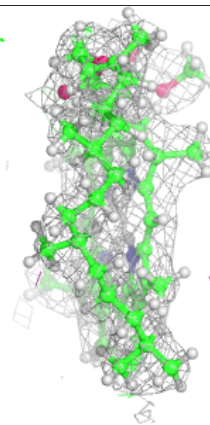
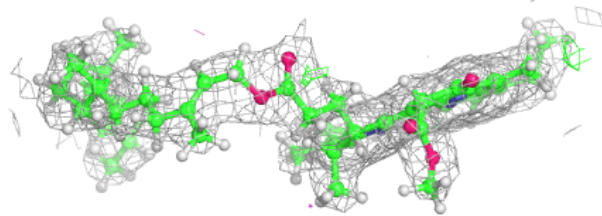
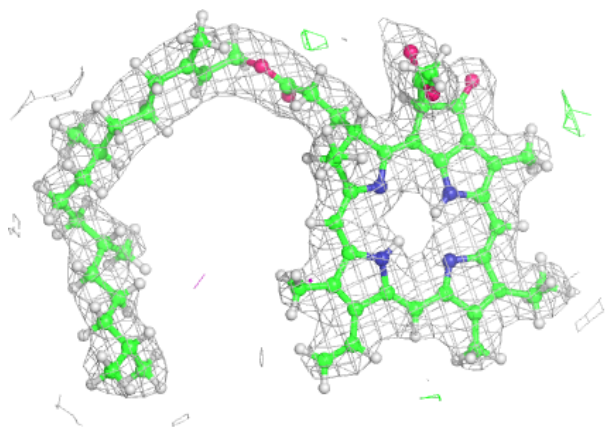
Electron density around PHO D 401:

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

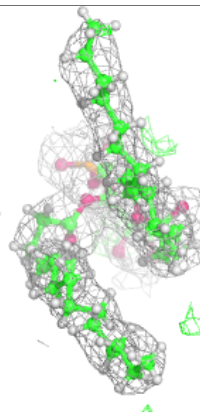
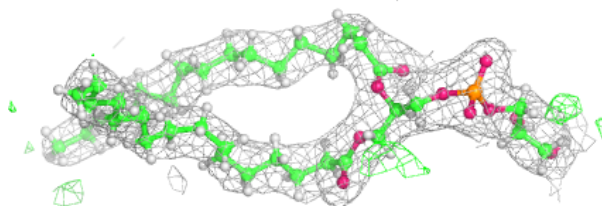
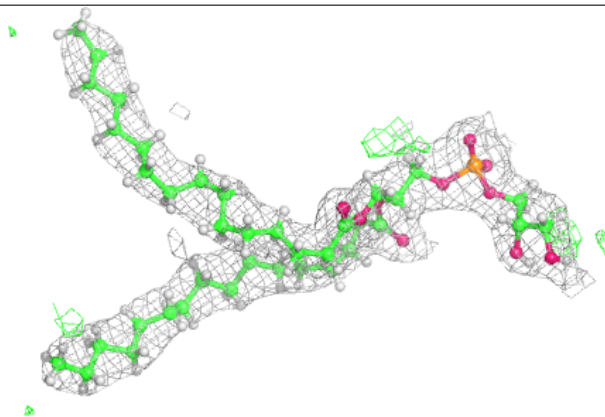


Electron density around PHO d 401:

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

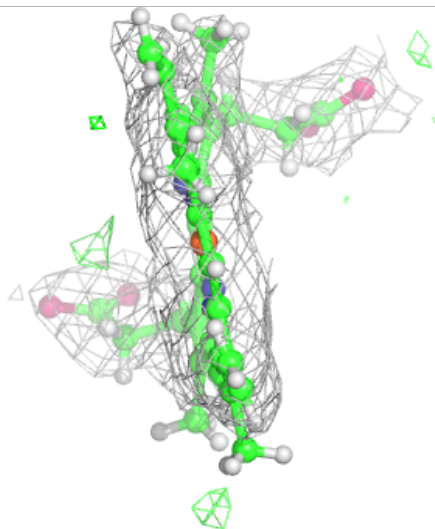
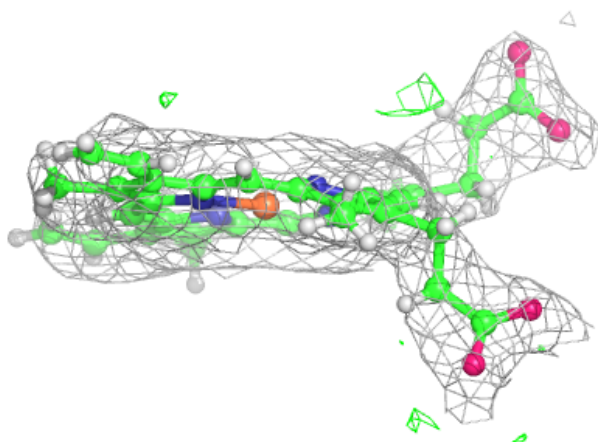
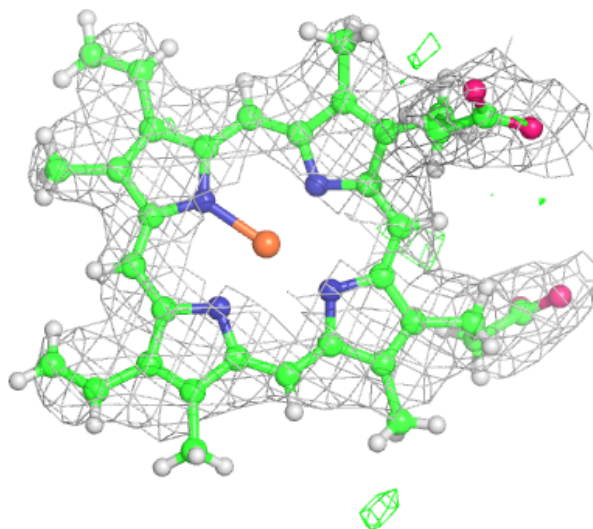
**Electron density around LHG d 408:**

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



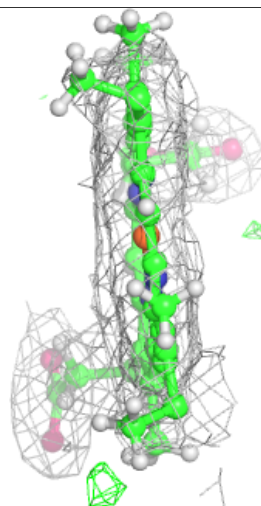
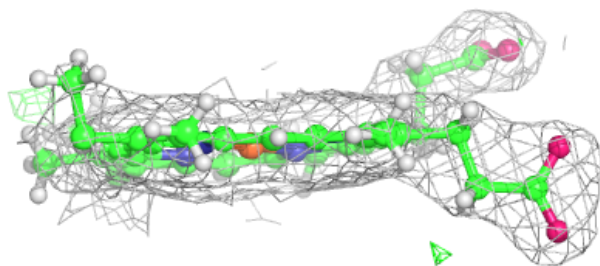
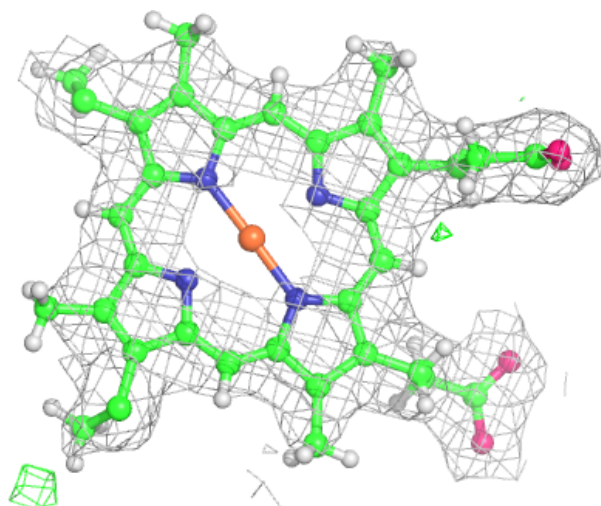
Electron density around HEM e 101:

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



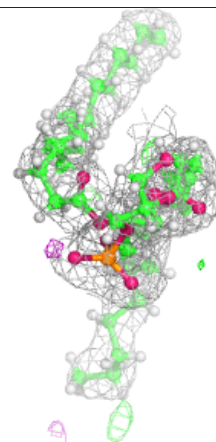
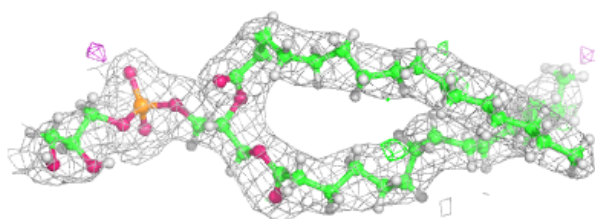
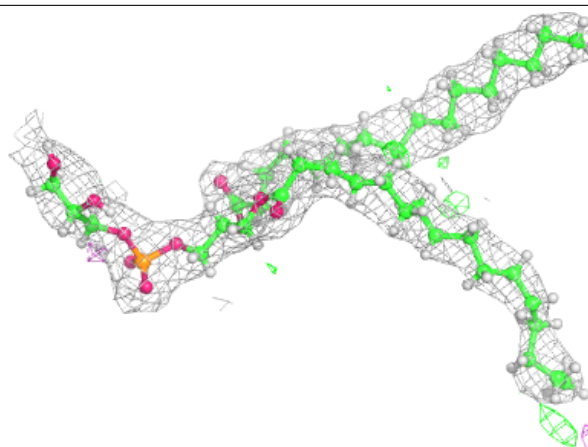
Electron density around HEC v 201:

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



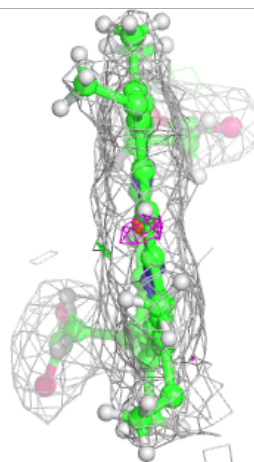
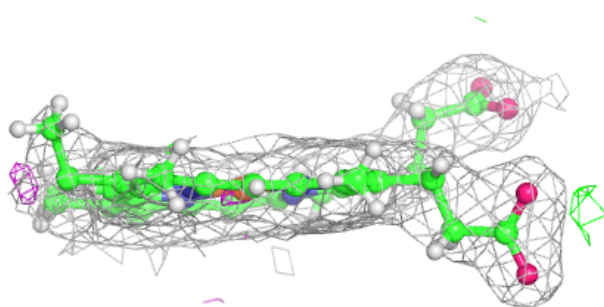
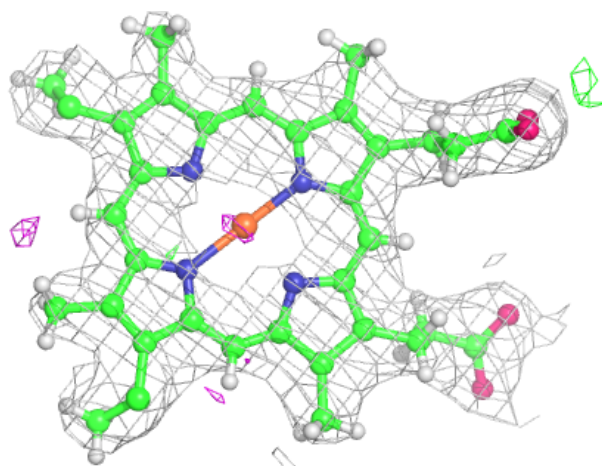
Electron density around LHG D 408:

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



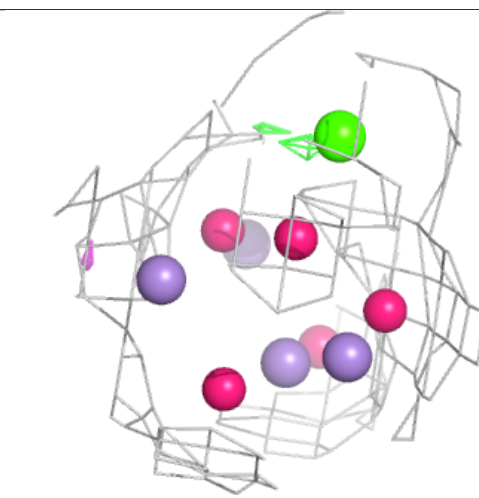
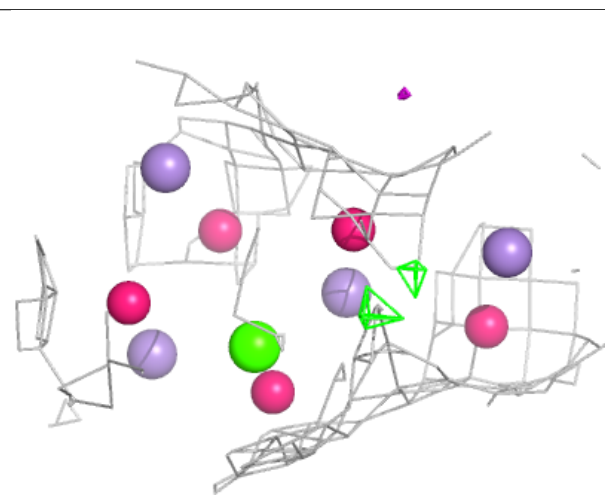
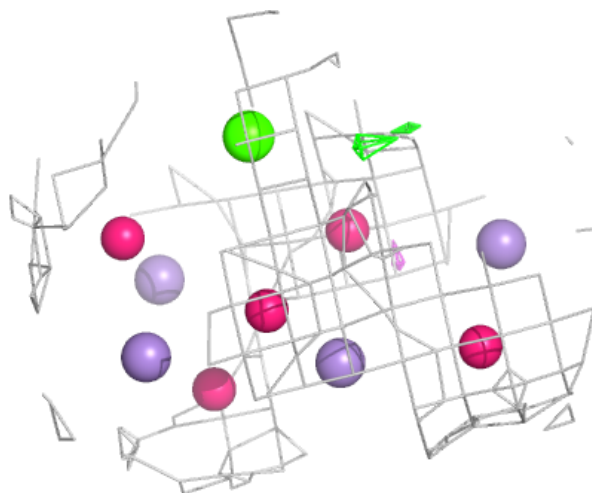
Electron density around HEC V 201:

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



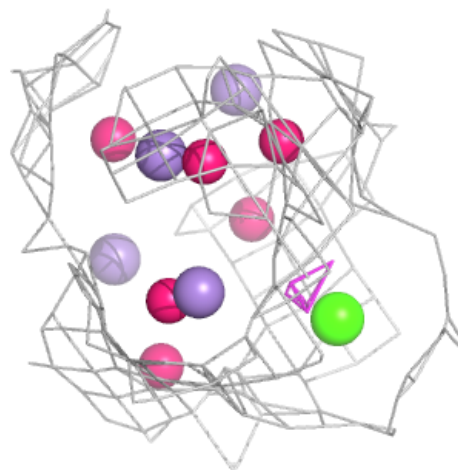
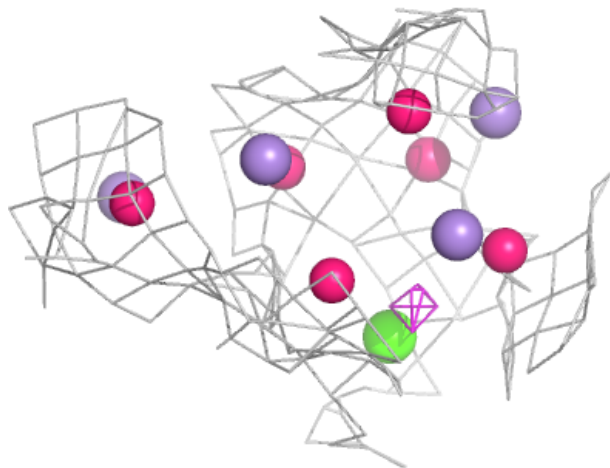
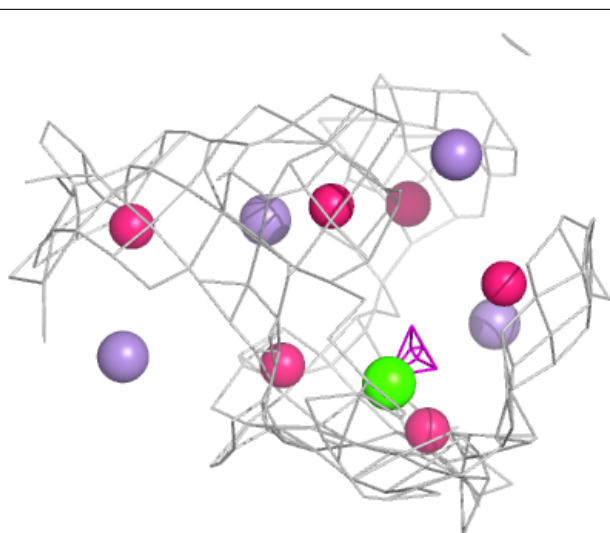
Electron density around OEX a 417 (A):

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



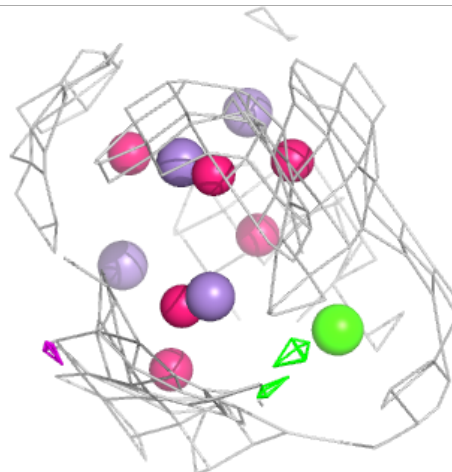
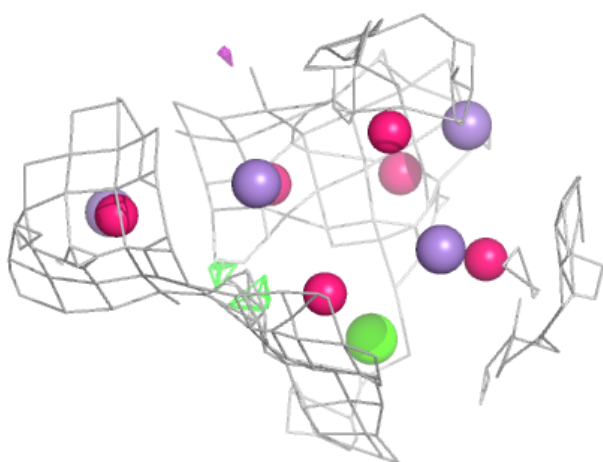
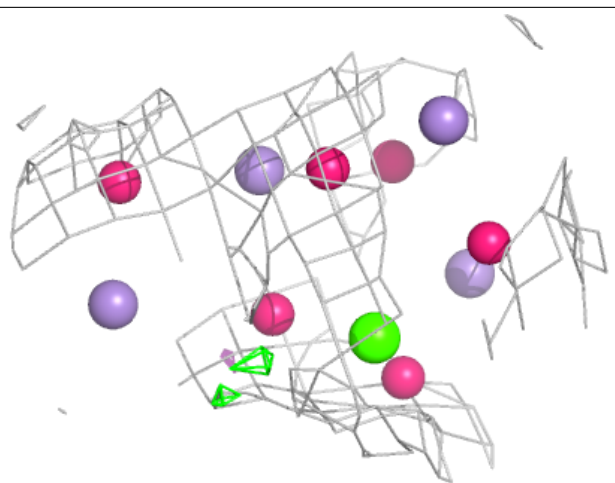
Electron density around OEY A 417 (B):

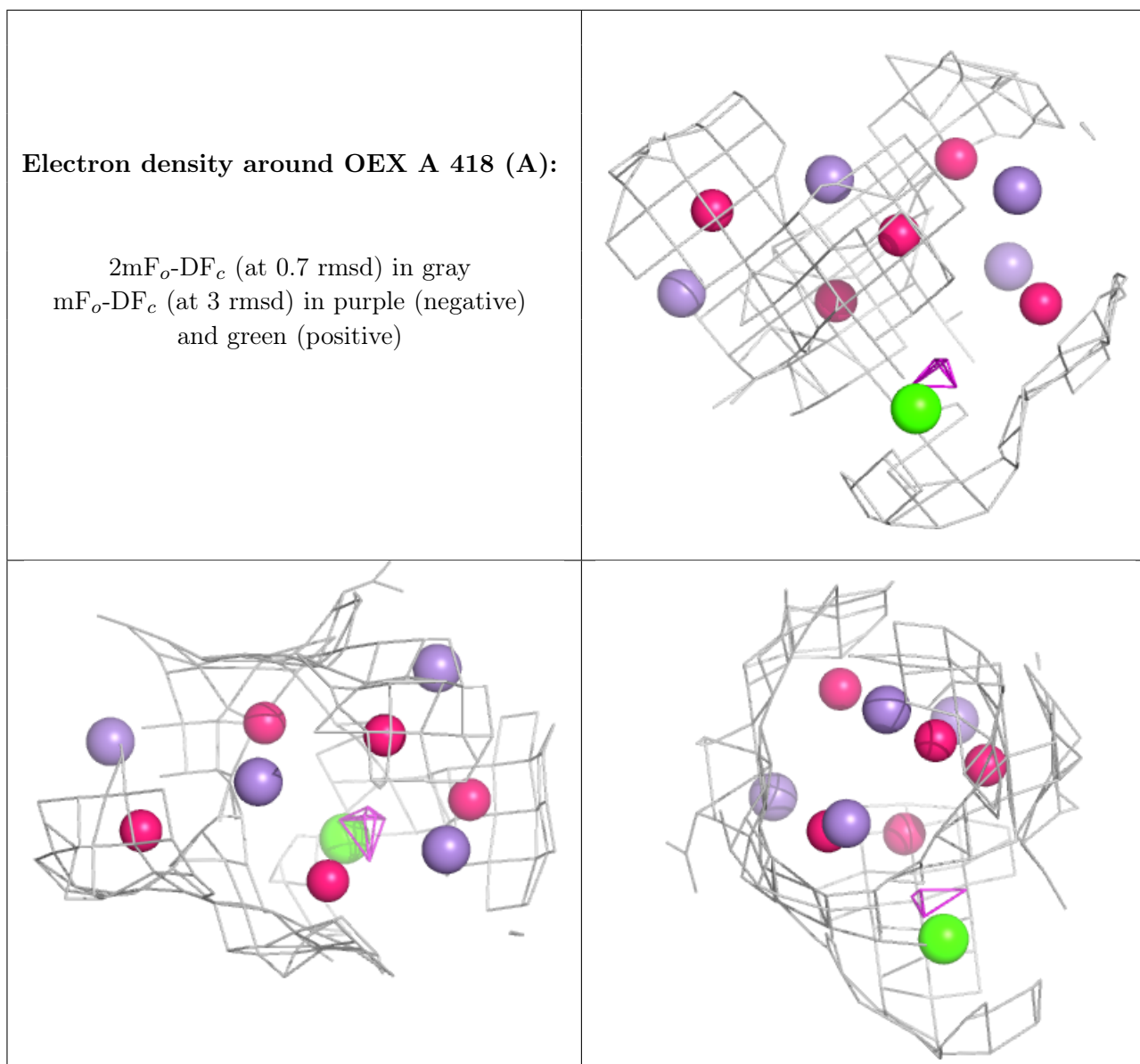
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OEY a 418 (B):

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





6.5 Other polymers ⓘ

There are no such residues in this entry.