



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 4, 2021 – 10:46 AM EDT

PDB ID : 7RF4
Title : RT XFEL structure of Photosystem II 50 microseconds after the second illumination at 2.27 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 : 2.27 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.

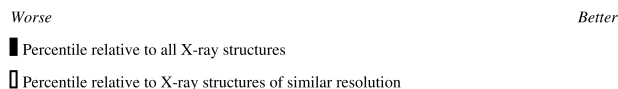
The following versions of software and data (see [references](#) ①) were used in the production of this report:

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

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X-RAY DIFFRACTION

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.



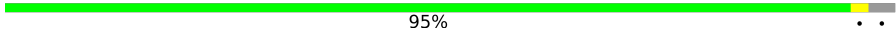
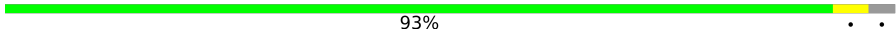
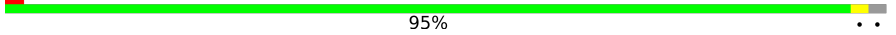
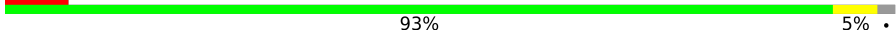


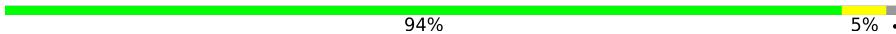







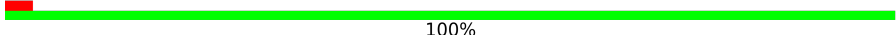










Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6980 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	344	<div> <div></div> <div>96%</div> <div>..</div> </div>
1	a	344	<div> <div></div> <div>94%</div> <div>..</div> </div>
2	B	510	<div> <div></div> <div>96%</div> <div>..</div> </div>
2	b	510	<div> <div>4%</div> <div>96%</div> <div>..</div> </div>
3	C	461	<div> <div>2%</div> <div>94%</div> <div>..</div> </div>
3	c	461	<div> <div>2%</div> <div>95%</div> <div>..</div> </div>

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	402	X	-	-	-
22	CLA	A	405	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	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	C	501	X	-	-	-
22	CLA	C	502	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	c	501	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
22	CLA	d	403	X	-	-	-
22	CLA	d	404	X	-	-	-
22	CLA	d	405	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 103252 atoms, of which 51649 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	334	Total	C	H	N	O	S	0	0	0
			5141	1717	2519	431	459	15			
1	a	334	Total	C	H	N	O	S	0	0	0
			5129	1714	2510	431	459	15			

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

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	442	Total	C	H	N	O	S	0	2	0
			6781	2249	3355	571	593	13			
3	c	451	Total	C	H	N	O	S	0	2	0
			6926	2290	3426	587	610	13			

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	H	N	O	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			

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

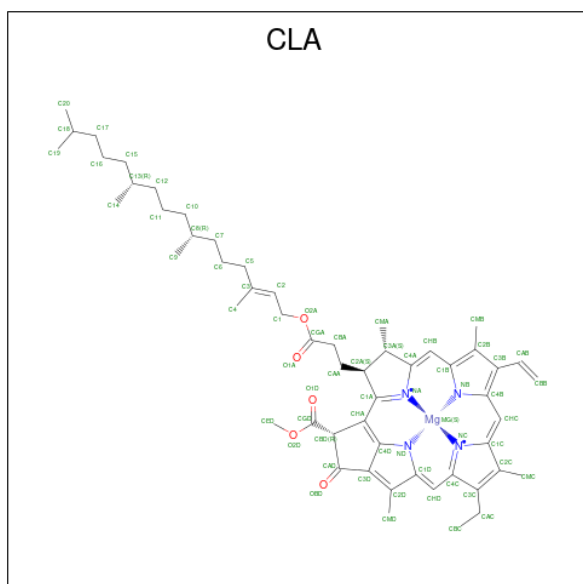
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

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

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

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



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

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	A	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	A	1	Total 102	C 44	H 48	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	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 119	C 50	H 59	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0

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

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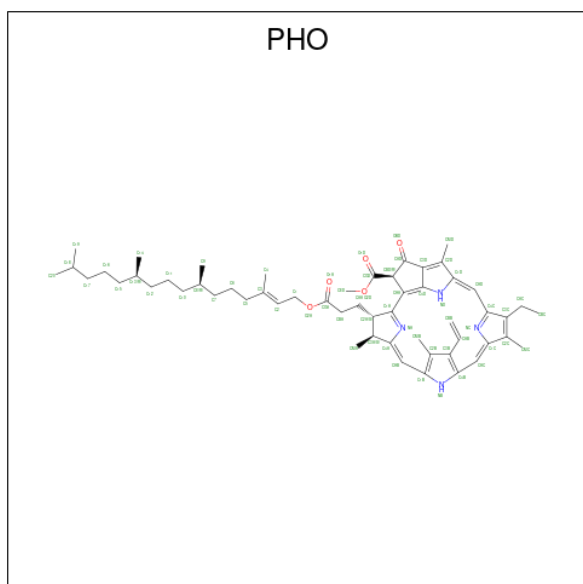
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total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

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

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

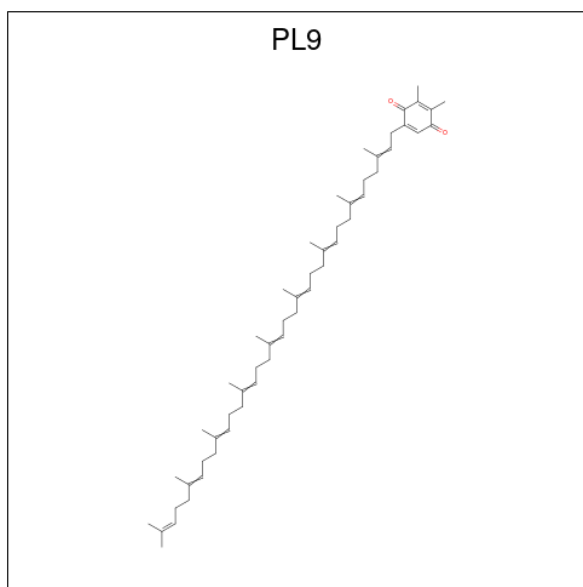


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	A	1	Total	C	H	N	O		0	0
			138	55	74	4	5			
23	D	1	Total	C	H	N	O		0	0
			138	55	74	4	5			
23	a	1	Total	C	H	N	O		0	0
			138	55	74	4	5			
23	d	1	Total	C	H	N	O		0	0
			138	55	74	4	5			

- Molecule 24 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

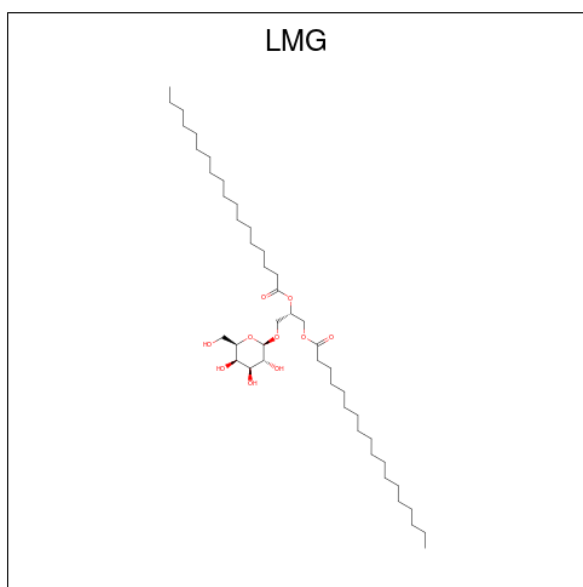
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	2	Total Cl 2 2	0	0
24	a	2	Total Cl 2 2	0	0

- Molecule 25 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
25	A	1	Total C H O 135 53 80 2	0	0
25	D	1	Total C H O 135 53 80 2	0	0
25	a	1	Total C H O 135 53 80 2	0	0
25	d	1	Total C H O 135 53 80 2	0	0

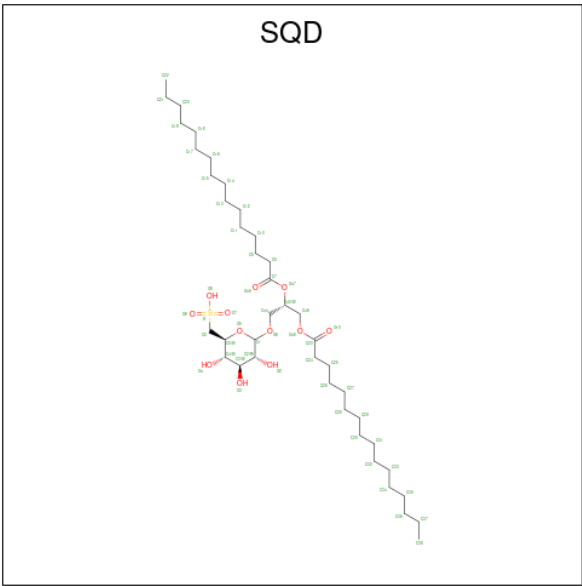
- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



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

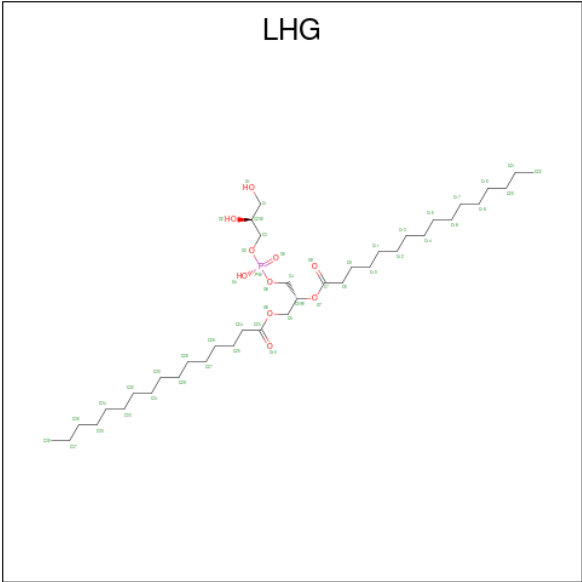
- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

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



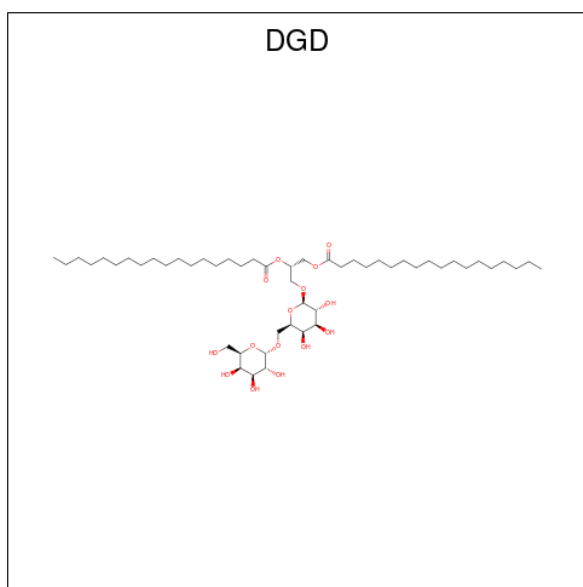
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
27	A	1	Total	C	H	O		0	0
			104	35	65	4			
27	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
27	D	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
27	L	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
27	a	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
27	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		
27	t	1	Total	C	H	O		0	0
			92	31	56	5			

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



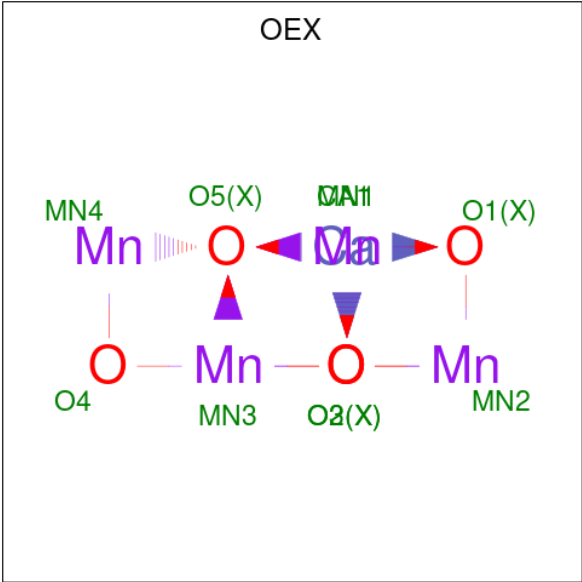
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
28	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	a	1	Total	C	H	O	P	0	0
			123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

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



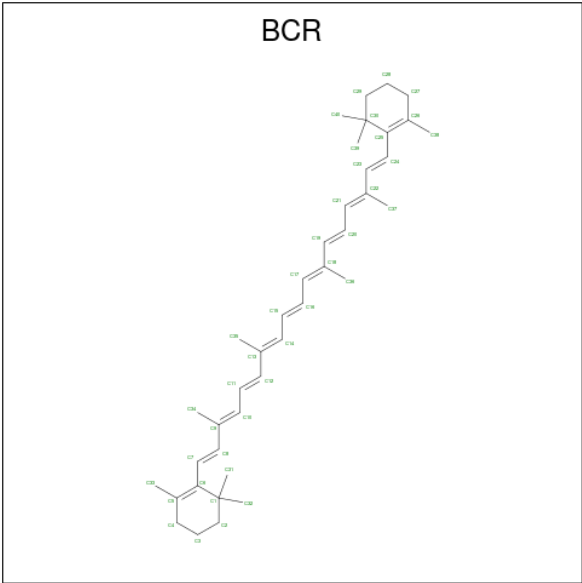
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	H	O	0	0
			162	51	96	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	H	1	Total	C	H	O	0	0
			144	47	82	15		
29	c	1	Total	C	H	O	0	0
			144	47	82	15		
29	c	1	Total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

- Molecule 30 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 31 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



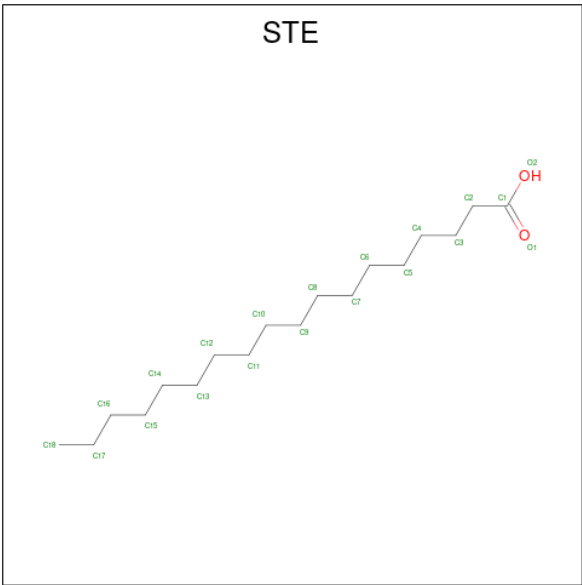
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	H	0	0
			96	40	56		
31	B	1	Total	C	H	0	0
			96	40	56		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	H	0	0
			96	40	56		
31	C	1	Total	C	H	0	0
			96	40	56		
31	D	1	Total	C	H	0	0
			96	40	56		
31	H	1	Total	C	H	0	0
			96	40	56		
31	I	1	Total	C	H	0	0
			96	40	56		
31	K	1	Total	C	H	0	0
			96	40	56		
31	K	1	Total	C	H	0	0
			96	40	56		
31	T	1	Total	C	H	0	0
			96	40	56		
31	Z	1	Total	C	H	0	0
			96	40	56		
31	a	1	Total	C	H	0	0
			96	40	56		
31	b	1	Total	C	H	0	0
			96	40	56		
31	b	1	Total	C	H	0	0
			96	40	56		
31	b	1	Total	C	H	0	0
			96	40	56		
31	c	1	Total	C	H	0	0
			96	40	56		
31	c	1	Total	C	H	0	0
			96	40	56		
31	d	1	Total	C	H	0	0
			96	40	56		
31	k	1	Total	C	H	0	0
			96	40	56		
31	k	1	Total	C	H	0	0
			96	40	56		
31	t	1	Total	C	H	0	0
			96	40	56		
31	x	1	Total	C	H	0	0
			96	40	56		

- Molecule 32 is STEARIC ACID (three-letter code: STE) (formula: $C_{18}H_{36}O_2$).



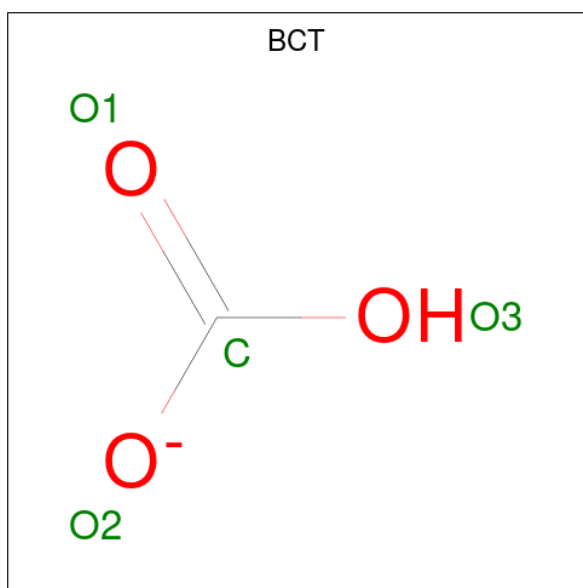
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	H	O	0	0
			43	15	26	2		
32	B	1	Total	C	H	O	0	0
			28	10	16	2		
32	B	1	Total	C	H	O	0	0
			46	16	28	2		
32	B	1	Total	C	H		0	0
			47	16	31			
32	B	1	Total	C	H	O	0	0
			28	10	16	2		
32	C	1	Total	C	H	O	0	0
			28	10	16	2		
32	C	1	Total	C	H		0	0
			47	16	31			
32	C	1	Total	C	H	O	0	0
			28	10	16	2		
32	H	1	Total	C	H		0	0
			53	18	35			
32	I	1	Total	C	H		0	0
			41	15	26			
32	J	1	Total	C	H	O	0	0
			28	10	16	2		
32	L	1	Total	C	H	O	0	0
			28	10	16	2		
32	M	1	Total	C	H	O	0	0
			37	13	22	2		
32	M	1	Total	C	H		0	0
			26	10	16			

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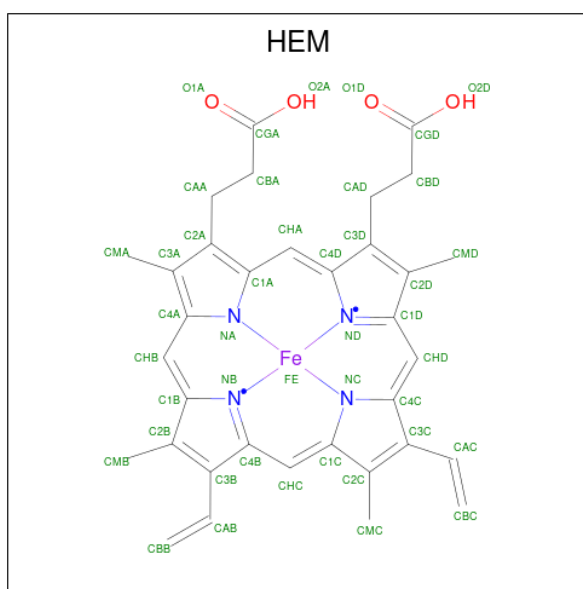
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	R	1	Total C H O 28 10 16 2	0	0
32	X	1	Total C H O 55 18 35 2	0	0
32	Z	1	Total C H 20 8 12	0	0
32	a	1	Total C H O 28 10 16 2	0	0
32	a	1	Total C H 41 15 26	0	0
32	b	1	Total C H 47 16 31	0	0
32	b	1	Total C H O 55 18 35 2	0	0
32	b	1	Total C H O 40 14 24 2	0	0
32	b	1	Total C H 44 15 29	0	0
32	b	1	Total C H O 55 18 35 2	0	0
32	b	1	Total C H 26 10 16	0	0
32	b	1	Total C H 41 14 27	0	0
32	c	1	Total C H O 55 18 35 2	0	0
32	c	1	Total C H O 28 10 16 2	0	0
32	d	1	Total C H O 43 15 26 2	0	0
32	d	1	Total C H O 55 18 35 2	0	0
32	j	1	Total C H O 28 10 16 2	0	0
32	l	1	Total C H 53 18 35	0	0
32	t	1	Total C H O 34 12 20 2	0	0
32	t	1	Total C H 26 10 16	0	0
32	x	1	Total C H O 55 18 35 2	0	0

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



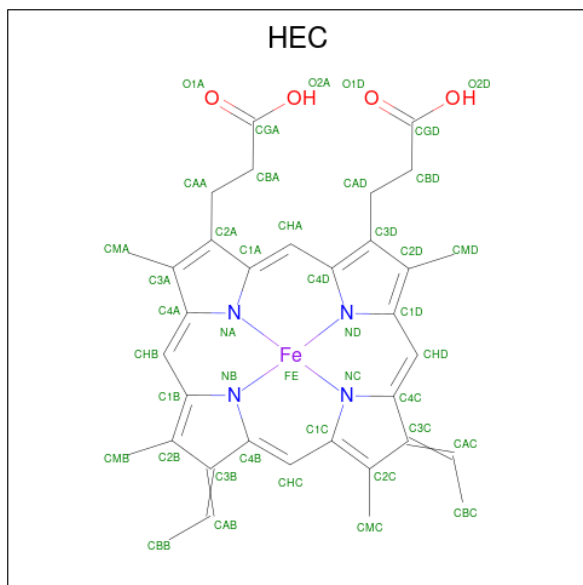
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	D	1	Total	C	H	O	0	0
			5	1	1	3		
33	a	1	Total	C	H	O	0	0
			5	1	1	3		

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



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

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



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

- Molecule 36 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	V	1	Total	Na	0	0
			1	1		

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	125	Total	O	0	0
			125	125		
37	B	135	Total	O	0	0
			135	135		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	C	119	Total 119	O 119	0	0
37	D	103	Total 103	O 103	0	0
37	E	20	Total 20	O 20	0	0
37	F	5	Total 5	O 5	0	0
37	H	22	Total 22	O 22	0	0
37	I	12	Total 12	O 12	0	0
37	J	11	Total 11	O 11	0	0
37	K	6	Total 6	O 6	0	0
37	L	9	Total 9	O 9	0	0
37	M	6	Total 6	O 6	0	0
37	O	68	Total 68	O 68	0	0
37	R	8	Total 8	O 8	0	0
37	T	7	Total 7	O 7	0	0
37	U	30	Total 30	O 30	0	0
37	V	49	Total 49	O 49	0	0
37	X	9	Total 9	O 9	0	0
37	Y	3	Total 3	O 3	0	0
37	Z	6	Total 6	O 6	0	0
37	a	99	Total 99	O 99	0	0
37	b	114	Total 114	O 114	0	0
37	c	120	Total 120	O 120	0	0

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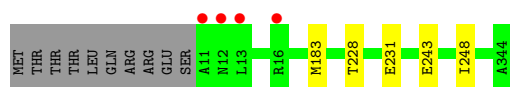
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	d	88	Total 88	O 88	0	0
37	e	18	Total 18	O 18	0	0
37	f	5	Total 5	O 5	0	0
37	h	22	Total 22	O 22	0	0
37	i	8	Total 8	O 8	0	0
37	j	9	Total 9	O 9	0	0
37	k	2	Total 2	O 2	0	0
37	l	11	Total 11	O 11	0	0
37	m	2	Total 2	O 2	0	0
37	o	70	Total 70	O 70	0	0
37	t	11	Total 11	O 11	0	0
37	u	35	Total 35	O 35	0	0
37	v	32	Total 32	O 32	0	0
37	x	7	Total 7	O 7	0	0
37	y	6	Total 6	O 6	0	0
37	z	11	Total 11	O 11	0	0

3 Residue-property plots [i](#)

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

- Molecule 1: Photosystem II protein D1 1



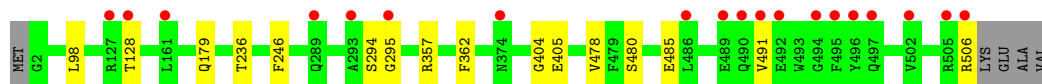
- Molecule 1: Photosystem II protein D1 1



- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein



D473

- Molecule 3: Photosystem II CP43 reaction center protein

Chain c:  2% 95%

MET	VAL	THR	LEU	SER	ASN	SER	ILE	PHE	A23	T24	N25	R26	E29	A57	L72	A123	V124	L125	Y143	S144	S145	F146	F147	L165	T200	T255	R262	L279	F289	K315	T355	S416	D473
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

- Molecule 4: Photosystem II D2 protein

Chain D:  95%

MET	THR	ILE	ALA	ILE	GLY	ARG	ALA	PRO	ALA	ALA	GLU	R12	R180	Q224	E227	T238	Y296	M329	D333	V345	L352
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------

- Molecule 4: Photosystem II D2 protein

Chain d:  93%

MET	THR	ILE	ALA	ILE	GLY	ARG	ALA	PRO	ALA	ALA	GLU	R12	L90	R180	F181	L182	E227	S230	R233	T259	L291	N292	L293	D297	E307	L321	L352
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------

- Molecule 5: Cytochrome b559 subunit alpha

Chain E:  2% 95%


MET	ALA	G3	I22	R61	F79	K84
-----	-----	----	-----	-----	-----	-----

- Molecule 5: Cytochrome b559 subunit alpha

Chain e:  7% 93% 5%


MET	ALA	T4	Q60	R61	L65	E71	Q74	Q75	F79	Q82	L83	K84
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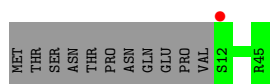
- Molecule 6: Cytochrome b559 subunit beta

Chain F:  2% 73% 24%

MET	THR	SER	ASN	THR	PRO	ASN	GLN	PRO	PRO	VAL	S12	R45
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 6: Cytochrome b559 subunit beta

Chain f:  2% 76% 24%



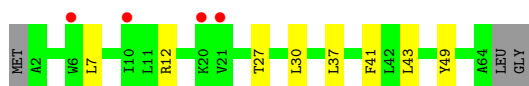
- Molecule 7: Photosystem II reaction center protein H

Chain H: 94% 5%



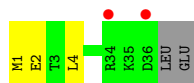
- Molecule 7: Photosystem II reaction center protein H

Chain h: 6% 83% 12% 5%



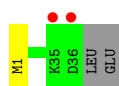
- Molecule 8: Photosystem II reaction center protein I

Chain I: 5% 87% 8% 5%



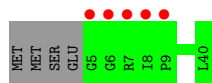
- Molecule 8: Photosystem II reaction center protein I

Chain i: 5% 92% 5%



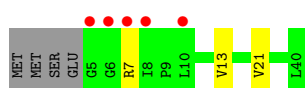
- Molecule 9: Photosystem II reaction center protein J

Chain J: 12% 90% 10%

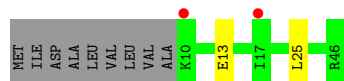
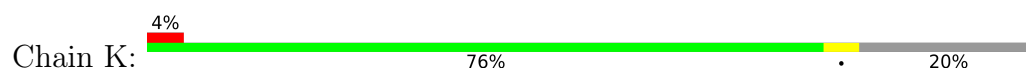


- Molecule 9: Photosystem II reaction center protein J

Chain j: 12% 82% 8% 10%



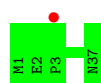
- Molecule 10: Photosystem II reaction center protein K



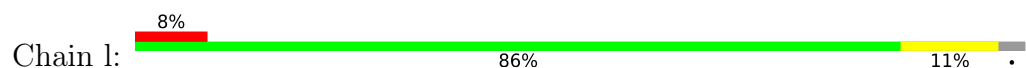
- Molecule 10: Photosystem II reaction center protein K



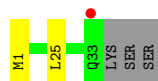
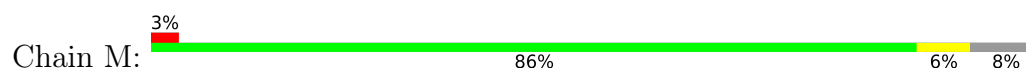
- Molecule 11: Photosystem II reaction center protein L



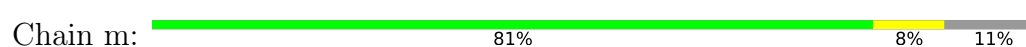
- Molecule 11: Photosystem II reaction center protein L



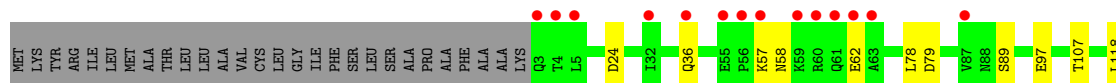
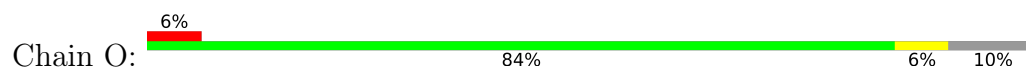
- Molecule 12: Photosystem II reaction center protein M



- Molecule 12: Photosystem II reaction center protein M

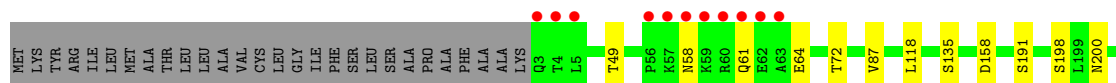
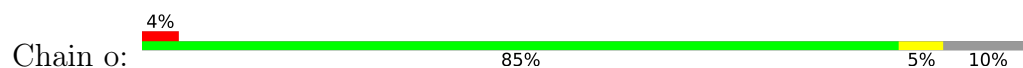


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

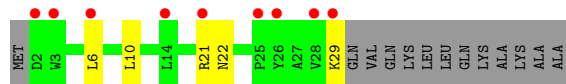




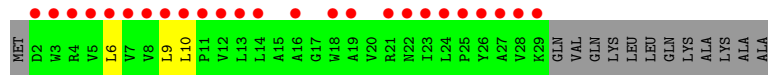
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



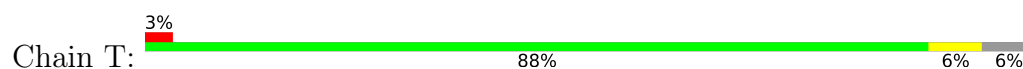
- Molecule 14: Photosystem II protein Y



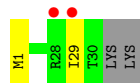
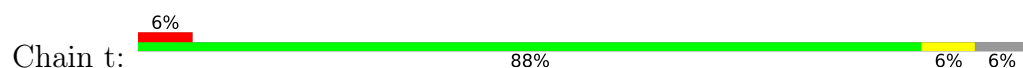
- Molecule 14: Photosystem II protein Y



- Molecule 15: Photosystem II reaction center protein T

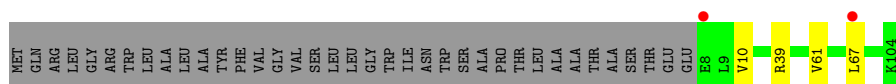


- Molecule 15: Photosystem II reaction center protein T

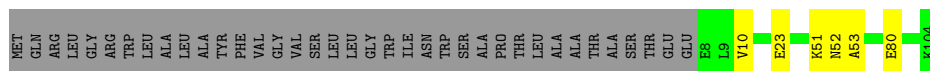


- Molecule 16: Photosystem II 12 kDa extrinsic protein

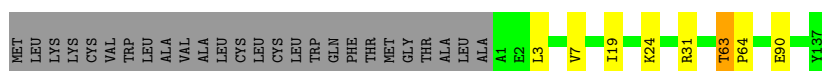
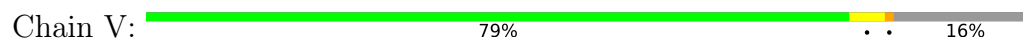




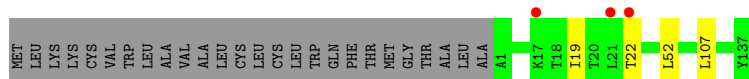
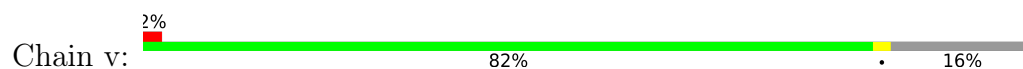
- Molecule 16: Photosystem II 12 kDa extrinsic protein



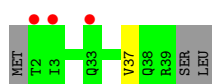
- Molecule 17: Cytochrome c-550



- Molecule 17: Cytochrome c-550



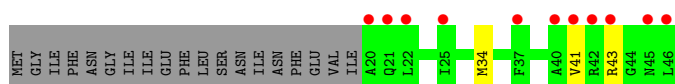
- Molecule 18: Photosystem II reaction center X protein



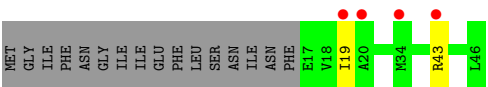
- Molecule 18: Photosystem II reaction center X protein



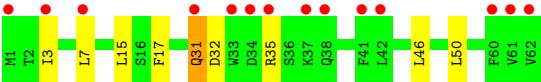
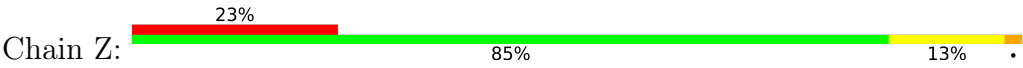
- Molecule 19: Photosystem II reaction center protein Ycf12



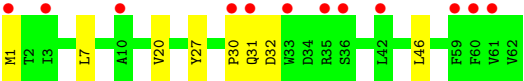
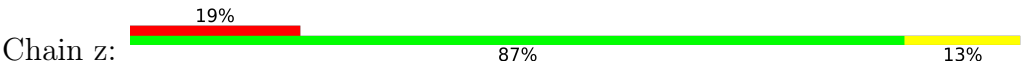
- Molecule 19: Photosystem II reaction center protein Ycf12



• Molecule 20: Photosystem II reaction center protein Z



• Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.07Å 222.05Å 308.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.45 – 2.27 33.45 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.5 (33.45-2.27) 84.3 (33.45-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.58 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.182 , 0.244 0.182 , 0.245	Depositor DCC
R_{free} test set	3275 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	103252	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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: LMG, CL, OEX, DGD, FE2, STE, PL9, LHG, HEM, SQD, FME, BCT, HEC, PHO, CLA, NA, BCR

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	0.66	0/2707	0.70	1/3692 (0.0%)
1	a	0.66	0/2704	0.68	0/3688
2	B	0.66	1/4161 (0.0%)	0.68	1/5669 (0.0%)
2	b	0.64	0/4118	0.68	0/5611
3	C	0.62	1/3547 (0.0%)	0.68	1/4830 (0.0%)
3	c	0.58	0/3619	0.68	0/4926
4	D	0.68	1/2812 (0.0%)	0.70	2/3832 (0.1%)
4	d	0.64	0/2821	0.70	1/3844 (0.0%)
5	E	0.59	0/688	0.59	0/940
5	e	0.54	0/683	0.62	0/932
6	F	0.49	0/284	0.63	0/387
6	f	0.47	0/284	0.64	0/387
7	H	0.65	0/523	0.65	0/713
7	h	0.59	0/511	0.69	0/697
8	I	0.63	0/293	0.72	0/396
8	i	0.64	0/293	0.66	0/396
9	J	0.56	0/263	0.64	0/356
9	j	0.52	0/263	0.63	0/356
10	K	0.56	0/303	0.61	0/416
10	k	0.47	0/303	0.62	0/416
11	L	0.61	0/311	0.68	0/422
11	l	0.68	0/303	0.68	0/412
12	M	0.62	0/249	0.60	0/341
12	m	0.68	0/244	0.70	0/334
13	O	0.60	0/1904	0.75	1/2585 (0.0%)
13	o	0.63	0/1905	0.77	1/2583 (0.0%)
14	R	0.42	0/227	0.61	0/313
14	r	0.38	0/227	0.52	0/313
15	T	0.82	0/257	0.76	0/349
15	t	0.68	0/255	0.64	0/346
16	U	0.57	0/785	0.70	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	u	0.64	0/785	0.74	0/1064
17	V	0.59	0/1085	0.70	1/1473 (0.1%)
17	v	0.54	0/1085	0.67	0/1473
18	X	0.56	0/284	0.67	0/384
18	x	0.49	0/289	0.63	0/391
19	Y	0.44	0/197	0.62	0/264
19	y	0.36	0/219	0.54	0/294
20	Z	0.47	0/490	0.55	0/669
20	z	0.43	0/488	0.53	0/666
All	All	0.62	3/42769 (0.0%)	0.68	9/58224 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
16	u	0	1
17	V	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	468	SER	C-N	-6.11	1.20	1.34
2	B	193	TYR	CD2-CE2	-5.45	1.31	1.39
4	D	296	TYR	CE1-CZ	-5.44	1.31	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	158	ASP	CB-CG-OD1	6.71	124.34	118.30
1	A	183	MET	CA-CB-CG	6.10	123.68	113.30
4	D	333	ASP	CB-CG-OD2	-5.80	113.08	118.30
4	d	297	ASP	CB-CG-OD1	5.76	123.48	118.30
3	C	460	ASP	CB-CG-OD1	5.72	123.45	118.30
17	V	63	THR	C-N-CD	-5.66	108.14	120.60
4	D	333	ASP	CB-CG-OD1	5.57	123.31	118.30
13	O	79	ASP	CB-CG-OD1	5.26	123.03	118.30
2	B	49	ASP	CB-CG-OD1	5.25	123.03	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	V	63	THR	Peptide
16	u	52	ASN	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/344 (96%)	325 (98%)	7 (2%)	0	100	100
1	a	332/344 (96%)	323 (97%)	9 (3%)	0	100	100
2	B	508/510 (100%)	500 (98%)	8 (2%)	0	100	100
2	b	503/510 (99%)	487 (97%)	13 (3%)	3 (1%)	25	29
3	C	442/461 (96%)	424 (96%)	17 (4%)	1 (0%)	47	57
3	c	451/461 (98%)	437 (97%)	13 (3%)	1 (0%)	47	57
4	D	339/352 (96%)	329 (97%)	10 (3%)	0	100	100
4	d	340/352 (97%)	329 (97%)	11 (3%)	0	100	100
5	E	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
5	e	80/84 (95%)	77 (96%)	3 (4%)	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%)	61 (97%)	1 (2%)	1 (2%)	9	8
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	31 (91%)	3 (9%)	0	100	100
10	K	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
10	k	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	228 (94%)	12 (5%)	3 (1%)	13	12
13	o	242/272 (89%)	228 (94%)	13 (5%)	1 (0%)	34	40
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%)	28 (100%)	0	0	100	100
16	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
16	u	95/134 (71%)	91 (96%)	3 (3%)	1 (1%)	14	14
17	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	22	25
17	v	135/163 (83%)	131 (97%)	4 (3%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Y	25/46 (54%)	23 (92%)	1 (4%)	1 (4%)	3	1
19	y	28/46 (61%)	25 (89%)	2 (7%)	1 (4%)	3	1
20	Z	60/62 (97%)	55 (92%)	3 (5%)	2 (3%)	4	2
20	z	60/62 (97%)	56 (93%)	3 (5%)	1 (2%)	9	7
All	All	5231/5700 (92%)	5049 (96%)	165 (3%)	17 (0%)	41	49

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
17	V	64	PRO
20	Z	31	GLN
3	c	416	SER
16	u	53	ALA

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Mol	Chain	Res	Type
13	O	58	ASN
13	O	62	GLU
13	o	61	GLN
19	Y	43	ARG
20	Z	32	ASP
2	b	294	SER
19	y	43	ARG
2	b	295	GLY
13	O	57	LYS
2	b	404	GLY
20	z	30	PRO
7	H	60	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/280 (96%)	266 (98%)	4 (2%)	65	77
1	a	269/280 (96%)	258 (96%)	11 (4%)	30	41
2	B	408/407 (100%)	397 (97%)	11 (3%)	44	59
2	b	402/407 (99%)	389 (97%)	13 (3%)	39	52
3	C	346/362 (96%)	339 (98%)	7 (2%)	55	70
3	c	354/362 (98%)	341 (96%)	13 (4%)	34	45
4	D	276/283 (98%)	271 (98%)	5 (2%)	59	72
4	d	277/283 (98%)	264 (95%)	13 (5%)	26	34
5	E	72/73 (99%)	69 (96%)	3 (4%)	30	39
5	e	71/73 (97%)	67 (94%)	4 (6%)	21	27
6	F	28/39 (72%)	27 (96%)	1 (4%)	35	47
6	f	28/39 (72%)	28 (100%)	0	100	100
7	H	54/55 (98%)	52 (96%)	2 (4%)	34	45
7	h	53/55 (96%)	45 (85%)	8 (15%)	3	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	32/34 (94%)	30 (94%)	2 (6%)	18	22
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%)	21 (88%)	3 (12%)	4	4
10	K	30/37 (81%)	28 (93%)	2 (7%)	16	19
10	k	30/37 (81%)	24 (80%)	6 (20%)	1	1
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	5
12	M	28/32 (88%)	27 (96%)	1 (4%)	35	47
12	m	28/32 (88%)	26 (93%)	2 (7%)	14	17
13	O	206/228 (90%)	195 (95%)	11 (5%)	22	29
13	o	207/228 (91%)	196 (95%)	11 (5%)	22	29
14	R	22/33 (67%)	17 (77%)	5 (23%)	1	0
14	r	22/33 (67%)	19 (86%)	3 (14%)	3	3
15	T	26/28 (93%)	25 (96%)	1 (4%)	33	44
15	t	25/28 (89%)	24 (96%)	1 (4%)	31	42
16	U	84/112 (75%)	80 (95%)	4 (5%)	25	34
16	u	84/112 (75%)	80 (95%)	4 (5%)	25	34
17	V	117/138 (85%)	111 (95%)	6 (5%)	24	31
17	v	117/138 (85%)	113 (97%)	4 (3%)	37	49
18	X	31/34 (91%)	30 (97%)	1 (3%)	39	52
18	x	31/34 (91%)	29 (94%)	2 (6%)	17	21
19	Y	19/37 (51%)	17 (90%)	2 (10%)	7	7
19	y	22/37 (60%)	21 (96%)	1 (4%)	27	36
20	Z	52/52 (100%)	44 (85%)	8 (15%)	2	2
20	z	51/52 (98%)	44 (86%)	7 (14%)	3	3
All	All	4321/4654 (93%)	4135 (96%)	186 (4%)	29	38

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	THR
1	A	231	GLU

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Mol	Chain	Res	Type
1	A	243	GLU
1	A	248	ILE
2	B	98	LEU
2	B	101	ILE
2	B	127	ARG
2	B	138	MET
2	B	289	GLN
2	B	297	THR
2	B	350	GLU
2	B	353	GLU
2	B	362	PHE
2	B	371	THR
2	B	385	ARG
3	C	141	GLU
3	C	201	ASN
3	C	279	LEU
3	C	289	PHE
3	C	315	MET
3	C	386	PRO
3	C	418	ASN
4	D	180	ARG
4	D	224	GLN
4	D	238	THR
4	D	329	MET
4	D	345	VAL
5	E	22[A]	ILE
5	E	22[B]	ILE
5	E	61	ARG
6	F	12	SER
7	H	49	TYR
7	H	56	ASP
8	I	2	GLU
8	I	4	LEU
10	K	13	GLU
10	K	25	LEU
12	M	25	LEU
13	O	24	ASP
13	O	36	GLN
13	O	78	LEU
13	O	89	SER
13	O	97	GLU
13	O	107	THR

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Mol	Chain	Res	Type
13	O	118	LEU
13	O	191	SER
13	O	214	THR
13	O	218	GLU
13	O	225	MET
14	R	6	LEU
14	R	10	LEU
14	R	21	ARG
14	R	22	ASN
14	R	29	LYS
15	T	25	GLU
16	U	10	VAL
16	U	39	ARG
16	U	61	VAL
16	U	67	LEU
17	V	3	LEU
17	V	7	VAL
17	V	19	ILE
17	V	24	LYS
17	V	31	ARG
17	V	90	GLU
18	X	37	VAL
19	Y	34	MET
19	Y	41	VAL
20	Z	3	ILE
20	Z	7	LEU
20	Z	15	LEU
20	Z	17	PHE
20	Z	31	GLN
20	Z	35	ARG
20	Z	46	LEU
20	Z	50	LEU
1	a	28	LEU
1	a	42	LEU
1	a	121	LEU
1	a	159	LEU
1	a	200	LEU
1	a	223	LEU
1	a	226	GLU
1	a	230	THR
1	a	245	THR
1	a	248	ILE

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Mol	Chain	Res	Type
1	a	288	LEU
2	b	98	LEU
2	b	128	THR
2	b	179	GLN
2	b	236	THR
2	b	246	PHE
2	b	357	ARG
2	b	362	PHE
2	b	405	GLU
2	b	478	VAL
2	b	480	SER
2	b	485	GLU
2	b	491	VAL
2	b	506	ARG
3	c	24	THR
3	c	26	ARG
3	c	29	GLU
3	c	72	LEU
3	c	124	VAL
3	c	125	LEU
3	c	165	LEU
3	c	200	THR
3	c	255	THR
3	c	279	LEU
3	c	289	PHE
3	c	315	MET
3	c	355	THR
4	d	12	ARG
4	d	90	LEU
4	d	180	ARG
4	d	182	LEU
4	d	227[A]	GLU
4	d	227[B]	GLU
4	d	230	SER
4	d	233	ARG
4	d	259	ILE
4	d	291	LEU
4	d	293	LEU
4	d	307	GLU
4	d	321	LEU
5	e	4	THR
5	e	65	LEU

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Mol	Chain	Res	Type
5	e	75	GLN
5	e	84	LYS
7	h	7	LEU
7	h	12	ARG
7	h	27	THR
7	h	30	LEU
7	h	37	LEU
7	h	41	PHE
7	h	43	LEU
7	h	49	TYR
9	j	7	ARG
9	j	13	VAL
9	j	21	VAL
10	k	10	LYS
10	k	13	GLU
10	k	17	ILE
10	k	30	VAL
10	k	35	LEU
10	k	46	ARG
11	l	2	GLU
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
12	m	16	LEU
13	o	49	THR
13	o	58	ASN
13	o	64	GLU
13	o	72	THR
13	o	87	VAL
13	o	118	LEU
13	o	135	SER
13	o	191	SER
13	o	198	SER
13	o	200	ASN
13	o	207	ARG
14	r	6	LEU
14	r	9	LEU
14	r	10	LEU
15	t	29	ILE
16	u	10	VAL
16	u	23	GLU

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Mol	Chain	Res	Type
16	u	51	LYS
16	u	80	GLU
17	v	19	ILE
17	v	22	THR
17	v	52	LEU
17	v	107	LEU
18	x	8	LYS
18	x	15	LEU
19	y	19	ILE
20	z	1	MET
20	z	7	LEU
20	z	20	VAL
20	z	27	TYR
20	z	31	GLN
20	z	32	ASP
20	z	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	ASN
1	A	338	ASN
2	B	216	HIS
2	B	289	GLN
3	C	56	HIS
3	C	327	ASN
4	D	236	ASN
13	O	36	GLN
13	O	88	ASN
18	X	38	GLN
19	Y	45	ASN
20	Z	6	GLN
20	Z	31	GLN
1	a	181	ASN
1	a	234	ASN
3	c	28	GLN
13	o	61	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	$\# Z > 2$
8	FME	I	1	8	8,9,10	1.10	1 (12%)	7,9,11	0.80	0
12	FME	m	1	12	8,9,10	1.03	0	7,9,11	1.37	1 (14%)
12	FME	M	1	12	8,9,10	1.03	1 (12%)	7,9,11	0.98	0
8	FME	i	1	8	8,9,10	1.09	1 (12%)	7,9,11	1.13	0
15	FME	T	1	15	8,9,10	0.96	0	7,9,11	1.11	1 (14%)
15	FME	t	1	15	8,9,10	1.46	1 (12%)	7,9,11	1.22	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
8	FME	I	1	8	-	4/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
8	FME	i	1	8	-	2/7/9/11	-
15	FME	T	1	15	-	4/7/9/11	-
15	FME	t	1	15	-	3/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-3.80	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	1	FME	CA-N	-2.13	1.43	1.46
8	I	1	FME	CA-N	-2.01	1.43	1.46
8	i	1	FME	CA-N	-2.01	1.43	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	m	1	FME	CA-N-CN	2.98	127.41	122.82
15	t	1	FME	CA-N-CN	-2.26	119.35	122.82
15	T	1	FME	CG-CB-CA	2.21	119.09	112.95

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	N-CA-CB-CG
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
8	I	1	FME	CB-CG-SD-CE
15	T	1	FME	C-CA-CB-CG
15	t	1	FME	C-CA-CB-CG
15	t	1	FME	N-CA-CB-CG
8	i	1	FME	CB-CG-SD-CE
8	I	1	FME	C-CA-CB-CG
8	I	1	FME	CB-CA-N-CN
8	i	1	FME	CB-CA-N-CN
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 190 ligands modelled in this entry, 7 are monoatomic - leaving 183 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
22	CLA	b	608	-	56,73,73	1.56	9 (16%)	55,113,113	1.49	10 (18%)
31	BCR	c	514	-	41,41,41	1.19	2 (4%)	56,56,56	1.39	9 (16%)
27	SQD	B	622	-	53,54,54	1.01	3 (5%)	62,65,65	1.98	13 (20%)
22	CLA	C	506	-	56,73,73	1.53	10 (17%)	55,113,113	1.61	12 (21%)
32	STE	c	520	-	16,19,19	0.40	0	15,19,19	0.71	0
28	LHG	D	410	-	48,48,48	0.92	3 (6%)	51,54,54	1.22	6 (11%)
31	BCR	c	515	-	41,41,41	1.17	4 (9%)	56,56,56	1.32	8 (14%)
32	STE	l	102	-	17,17,19	0.42	0	16,16,19	0.82	0
32	STE	j	101	-	8,11,19	0.44	0	7,11,19	0.68	0
22	CLA	B	614	-	56,73,73	1.74	7 (12%)	55,113,113	1.55	12 (21%)
32	STE	R	101	-	8,11,19	0.39	0	7,11,19	0.72	0
22	CLA	B	604	-	56,73,73	1.44	6 (10%)	55,113,113	2.17	17 (30%)
33	BCT	a	408	21	0,3,3	-	-	0,3,3	-	-
25	PL9	A	408	-	55,55,55	1.79	4 (7%)	68,69,69	1.57	15 (22%)
27	SQD	t	102	-	35,35,54	1.10	2 (5%)	37,37,65	1.36	4 (10%)
33	BCT	D	402	21	0,3,3	-	-	0,3,3	-	-
22	CLA	B	605	-	56,73,73	1.39	6 (10%)	55,113,113	1.54	10 (18%)
22	CLA	C	501	-	56,73,73	1.61	8 (14%)	55,113,113	1.72	9 (16%)
22	CLA	b	607	37	56,73,73	1.51	12 (21%)	55,113,113	1.51	7 (12%)
22	CLA	b	614	-	56,73,73	1.54	8 (14%)	55,113,113	1.68	11 (20%)
32	STE	b	621	-	16,19,19	0.41	0	15,19,19	0.87	0
22	CLA	B	616	-	51,68,73	1.67	8 (15%)	49,107,113	1.82	10 (20%)
32	STE	b	627	-	13,13,19	0.45	0	12,12,19	0.55	0
31	BCR	H	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.16	6 (10%)
22	CLA	B	607	37	56,73,73	1.63	10 (17%)	55,113,113	1.61	8 (14%)
31	BCR	B	619	-	41,41,41	1.23	3 (7%)	56,56,56	1.50	12 (21%)
32	STE	b	623	-	12,15,19	0.43	0	11,15,19	0.76	0
32	STE	a	413	-	14,14,19	0.46	0	13,13,19	0.70	0
31	BCR	k	102	-	41,41,41	1.14	3 (7%)	56,56,56	1.22	5 (8%)
26	LMG	M	101	-	51,51,55	1.04	4 (7%)	59,59,63	1.39	9 (15%)
28	LHG	l	101	-	48,48,48	0.80	2 (4%)	51,54,54	1.12	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	d	403	-	56,73,73	1.62	11 (19%)	55,113,113	1.44	7 (12%)
31	BCR	C	514	-	41,41,41	1.24	2 (4%)	56,56,56	1.35	8 (14%)
26	LMG	b	622	-	55,55,55	1.14	7 (12%)	63,63,63	1.37	7 (11%)
32	STE	X	101	-	16,19,19	0.28	0	15,19,19	1.14	0
27	SQD	D	409	-	35,36,54	1.03	3 (8%)	42,45,65	2.04	10 (23%)
28	LHG	D	413	-	48,48,48	0.98	3 (6%)	51,54,54	1.35	6 (11%)
30	OEX	A	414	3,37,1	0,15,15	-	-	-	-	-
32	STE	d	412	-	16,19,19	0.37	0	15,19,19	0.81	0
22	CLA	c	510	-	56,73,73	1.55	8 (14%)	55,113,113	1.59	9 (16%)
31	BCR	b	617	-	41,41,41	1.12	3 (7%)	56,56,56	1.28	6 (10%)
22	CLA	b	616	-	51,68,73	1.60	9 (17%)	49,107,113	1.97	12 (24%)
25	PL9	d	407	-	55,55,55	1.53	10 (18%)	68,69,69	1.59	16 (23%)
22	CLA	B	601	37	56,73,73	1.80	8 (14%)	55,113,113	1.57	8 (14%)
26	LMG	d	410	-	44,44,55	1.25	5 (11%)	52,52,63	1.28	5 (9%)
32	STE	t	103	-	10,13,19	0.51	0	9,13,19	0.67	0
22	CLA	B	603	-	56,73,73	1.49	9 (16%)	55,113,113	1.84	16 (29%)
29	DGD	A	413	-	67,67,67	1.24	8 (11%)	81,81,81	1.37	11 (13%)
28	LHG	d	408	-	48,48,48	0.70	1 (2%)	51,54,54	1.18	4 (7%)
22	CLA	d	405	-	56,73,73	1.79	9 (16%)	55,113,113	1.57	7 (12%)
22	CLA	d	401	37	56,73,73	1.68	6 (10%)	55,113,113	1.37	10 (18%)
32	STE	M	103	-	9,9,19	0.61	0	8,8,19	0.46	0
22	CLA	b	610	37	56,73,73	1.51	11 (19%)	55,113,113	1.58	10 (18%)
22	CLA	C	502	-	56,73,73	1.68	7 (12%)	55,113,113	1.70	12 (21%)
22	CLA	D	405	-	56,73,73	1.62	7 (12%)	55,113,113	1.50	10 (18%)
32	STE	b	624	-	14,14,19	0.34	0	13,13,19	1.00	0
30	OEX	a	414	3,37,1	0,15,15	-	-	-	-	-
22	CLA	B	609	-	56,73,73	1.48	7 (12%)	55,113,113	1.70	13 (23%)
22	CLA	b	615	-	56,73,73	1.88	8 (14%)	55,113,113	1.61	10 (18%)
22	CLA	c	509	-	56,73,73	1.39	6 (10%)	55,113,113	1.78	12 (21%)
26	LMG	D	408	-	51,51,55	0.88	1 (1%)	59,59,63	1.27	3 (5%)
27	SQD	A	410	-	51,52,54	1.09	4 (7%)	60,63,65	2.09	14 (23%)
22	CLA	A	405	-	45,62,73	1.79	8 (17%)	41,99,113	1.89	11 (26%)
22	CLA	b	606	-	56,73,73	1.90	11 (19%)	55,113,113	1.84	7 (12%)
27	SQD	f	102	-	40,41,54	1.14	4 (10%)	49,52,65	1.91	11 (22%)
32	STE	d	411	-	13,16,19	0.38	0	12,16,19	0.88	0
28	LHG	e	101	-	41,41,48	1.03	3 (7%)	44,47,54	1.29	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	HEM	f	101	6,5	27,50,50	1.98	5 (18%)	17,82,82	2.12	6 (35%)
27	SQD	A	412	-	38,38,54	1.06	3 (7%)	40,40,65	1.42	4 (10%)
22	CLA	b	612	-	56,73,73	1.59	9 (16%)	55,113,113	1.91	12 (21%)
22	CLA	A	402	-	56,73,73	1.83	6 (10%)	55,113,113	1.70	11 (20%)
22	CLA	c	513	-	56,73,73	1.57	7 (12%)	55,113,113	1.44	9 (16%)
22	CLA	b	611	-	56,73,73	1.70	9 (16%)	55,113,113	1.68	14 (25%)
26	LMG	Y	101	-	48,48,55	1.07	7 (14%)	56,56,63	1.24	6 (10%)
26	LMG	c	522	-	49,49,55	1.20	5 (10%)	57,57,63	1.42	7 (12%)
32	STE	B	623	-	8,11,19	0.42	0	7,11,19	0.80	0
22	CLA	c	504	37	51,68,73	1.62	5 (9%)	49,107,113	1.69	12 (24%)
32	STE	x	102	-	16,19,19	0.47	0	15,19,19	0.63	0
34	HEM	F	101	6,5	27,50,50	1.98	5 (18%)	17,82,82	2.26	6 (35%)
22	CLA	C	510	-	56,73,73	1.62	8 (14%)	55,113,113	1.87	7 (12%)
29	DGD	c	516	-	63,63,67	1.29	8 (12%)	77,77,81	1.45	13 (16%)
22	CLA	c	508	-	55,72,73	1.61	7 (12%)	53,111,113	1.38	8 (15%)
35	HEC	v	201	17	26,50,50	2.40	5 (19%)	18,82,82	2.53	6 (33%)
31	BCR	K	102	-	41,41,41	1.11	3 (7%)	56,56,56	1.22	5 (8%)
22	CLA	c	507	37	56,73,73	1.66	11 (19%)	55,113,113	1.78	17 (30%)
22	CLA	b	601	37	56,73,73	1.70	9 (16%)	55,113,113	1.66	10 (18%)
26	LMG	A	409	-	48,48,55	1.17	3 (6%)	56,56,63	1.43	9 (16%)
32	STE	L	103	-	8,11,19	0.45	0	7,11,19	0.75	0
22	CLA	b	604	-	56,73,73	1.52	6 (10%)	55,113,113	1.92	16 (29%)
25	PL9	a	409	-	55,55,55	1.02	3 (5%)	68,69,69	1.66	16 (23%)
22	CLA	C	504	37	50,67,73	1.78	9 (18%)	47,105,113	1.57	9 (19%)
22	CLA	C	511	3	56,73,73	1.61	9 (16%)	55,113,113	1.75	9 (16%)
32	STE	H	103	-	17,17,19	0.44	0	16,16,19	0.68	0
35	HEC	V	201	17	26,50,50	2.13	3 (11%)	18,82,82	2.41	6 (33%)
26	LMG	D	412	-	31,31,55	1.02	3 (9%)	33,33,63	1.16	4 (12%)
22	CLA	b	602	-	56,73,73	1.68	10 (17%)	55,113,113	1.78	13 (23%)
22	CLA	c	506	-	56,73,73	1.75	8 (14%)	55,113,113	1.52	6 (10%)
26	LMG	B	626	-	55,55,55	1.21	6 (10%)	63,63,63	1.31	5 (7%)
31	BCR	b	618	-	41,41,41	1.52	3 (7%)	56,56,56	1.30	7 (12%)
22	CLA	B	611	-	56,73,73	1.55	9 (16%)	55,113,113	2.02	12 (21%)
25	PL9	D	407	-	55,55,55	1.43	8 (14%)	68,69,69	1.60	15 (22%)
28	LHG	L	102	-	48,48,48	0.81	2 (4%)	51,54,54	1.16	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	DGD	h	101	-	63,63,67	1.09	4 (6%)	77,77,81	1.41	14 (18%)
22	CLA	B	613	-	56,73,73	1.65	7 (12%)	55,113,113	1.64	12 (21%)
32	STE	c	523	-	8,11,19	0.40	0	7,11,19	0.77	0
32	STE	b	620	-	15,15,19	0.44	0	14,14,19	0.80	0
22	CLA	c	505	-	56,73,73	1.55	5 (8%)	55,113,113	1.61	10 (18%)
22	CLA	C	509	-	56,73,73	1.50	7 (12%)	55,113,113	1.79	12 (21%)
22	CLA	B	606	-	56,73,73	2.00	9 (16%)	55,113,113	1.44	9 (16%)
28	LHG	a	410	-	48,48,48	0.89	1 (2%)	51,54,54	1.27	6 (11%)
26	LMG	c	519	-	37,37,55	1.43	7 (18%)	45,45,63	1.36	5 (11%)
26	LMG	B	621	-	20,26,55	0.64	0	18,26,63	1.09	1 (5%)
22	CLA	B	610	37	56,73,73	1.59	9 (16%)	55,113,113	1.77	12 (21%)
28	LHG	A	411	-	48,48,48	0.86	3 (6%)	51,54,54	1.23	6 (11%)
29	DGD	c	517	-	63,63,67	1.07	6 (9%)	77,77,81	1.55	13 (16%)
28	LHG	d	409	-	38,38,48	0.91	2 (5%)	41,44,54	1.21	5 (12%)
22	CLA	D	403	-	56,73,73	1.54	6 (10%)	55,113,113	1.51	10 (18%)
22	CLA	b	613	-	56,73,73	1.62	8 (14%)	55,113,113	1.91	13 (23%)
31	BCR	I	101	-	41,41,41	1.24	4 (9%)	56,56,56	1.40	9 (16%)
22	CLA	B	615	-	56,73,73	1.65	11 (19%)	55,113,113	1.59	9 (16%)
22	CLA	d	404	37	56,73,73	1.79	7 (12%)	55,113,113	1.74	10 (18%)
31	BCR	t	101	-	41,41,41	1.20	4 (9%)	56,56,56	1.36	8 (14%)
32	STE	C	520	-	8,11,19	0.35	0	7,11,19	1.19	0
32	STE	a	412	-	8,11,19	0.47	0	7,11,19	0.68	0
29	DGD	C	515	-	63,63,67	1.34	10 (15%)	77,77,81	1.36	11 (14%)
32	STE	B	620	-	13,16,19	0.36	0	12,16,19	0.95	0
31	BCR	d	406	-	41,41,41	1.17	2 (4%)	56,56,56	1.33	8 (14%)
22	CLA	D	404	37	56,73,73	1.75	9 (16%)	55,113,113	1.66	11 (20%)
26	LMG	c	521	-	48,48,55	1.08	4 (8%)	56,56,63	1.34	7 (12%)
22	CLA	b	609	-	56,73,73	1.68	8 (14%)	55,113,113	1.71	11 (20%)
32	STE	B	627	-	8,11,19	0.42	0	7,11,19	0.72	0
29	DGD	C	516	-	63,63,67	1.23	9 (14%)	77,77,81	1.49	16 (20%)
31	BCR	D	406	-	41,41,41	1.20	2 (4%)	56,56,56	1.18	6 (10%)
22	CLA	b	603	-	56,73,73	1.83	10 (17%)	55,113,113	2.08	14 (25%)
29	DGD	H	102	-	63,63,67	1.33	8 (12%)	77,77,81	1.54	12 (15%)
22	CLA	C	507	37	56,73,73	1.47	9 (16%)	55,113,113	1.87	11 (20%)
32	STE	b	625	-	16,19,19	0.50	0	15,19,19	0.70	0
22	CLA	C	512	-	56,73,73	1.51	7 (12%)	55,113,113	1.69	10 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	BCR	x	101	-	41,41,41	1.07	3 (7%)	56,56,56	1.41	9 (16%)
22	CLA	A	403	37	56,73,73	2.09	8 (14%)	55,113,113	1.55	10 (18%)
22	CLA	B	612	-	56,73,73	1.34	6 (10%)	55,113,113	1.86	10 (18%)
31	BCR	k	101	-	41,41,41	1.13	3 (7%)	56,56,56	1.06	3 (5%)
22	CLA	B	602	-	56,73,73	1.77	9 (16%)	55,113,113	1.68	14 (25%)
23	PHO	d	402	-	67,69,69	1.29	7 (10%)	85,99,99	1.23	11 (12%)
31	BCR	T	101	-	41,41,41	1.12	3 (7%)	56,56,56	1.28	6 (10%)
31	BCR	b	619	-	41,41,41	1.14	2 (4%)	56,56,56	1.30	8 (14%)
32	STE	C	519	-	15,15,19	0.49	0	14,14,19	0.67	0
31	BCR	B	617	-	41,41,41	1.16	3 (7%)	56,56,56	1.40	7 (12%)
31	BCR	B	618	-	41,41,41	1.15	3 (7%)	56,56,56	1.34	5 (8%)
22	CLA	C	503	-	56,73,73	1.63	8 (14%)	55,113,113	1.99	12 (21%)
22	CLA	C	508	-	56,73,73	1.57	8 (14%)	55,113,113	1.58	8 (14%)
31	BCR	K	101	-	41,41,41	1.24	3 (7%)	56,56,56	1.21	5 (8%)
22	CLA	b	605	-	56,73,73	1.60	8 (14%)	55,113,113	1.75	12 (21%)
22	CLA	c	502	-	56,73,73	1.63	9 (16%)	55,113,113	1.73	11 (20%)
27	SQD	a	411	-	53,54,54	1.05	4 (7%)	62,65,65	1.72	11 (17%)
27	SQD	L	101	-	48,49,54	0.97	3 (6%)	57,60,65	2.20	16 (28%)
32	STE	M	102	-	11,14,19	0.46	0	10,14,19	0.79	0
32	STE	B	625	-	15,15,19	0.47	0	14,14,19	0.84	0
22	CLA	a	404	-	56,73,73	1.23	7 (12%)	55,113,113	1.50	11 (20%)
29	DGD	C	517	-	63,63,67	1.18	8 (12%)	77,77,81	1.56	12 (15%)
22	CLA	c	503	-	56,73,73	1.58	8 (14%)	55,113,113	1.50	8 (14%)
32	STE	B	624	-	14,17,19	0.36	0	13,17,19	0.94	0
22	CLA	a	402	-	56,73,73	1.70	7 (12%)	55,113,113	1.83	11 (20%)
31	BCR	a	405	-	41,41,41	1.21	4 (9%)	56,56,56	1.44	8 (14%)
22	CLA	B	608	-	56,73,73	1.73	10 (17%)	55,113,113	1.43	10 (18%)
22	CLA	c	511	3	56,73,73	1.75	5 (8%)	55,113,113	1.83	7 (12%)
22	CLA	C	513	-	56,73,73	1.70	8 (14%)	55,113,113	1.69	11 (20%)
32	STE	t	104	-	9,9,19	0.54	0	8,8,19	0.45	0
32	STE	b	626	-	9,9,19	0.49	0	8,8,19	0.50	0
23	PHO	A	404	-	67,69,69	1.30	10 (14%)	85,99,99	1.24	8 (9%)
23	PHO	a	403	-	67,69,69	1.23	8 (11%)	85,99,99	1.12	5 (5%)
32	STE	I	102	-	14,14,19	0.51	0	13,13,19	0.51	0
32	STE	J	101	-	8,11,19	0.31	0	7,11,19	1.01	0
22	CLA	c	501	-	56,73,73	1.62	8 (14%)	55,113,113	1.95	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	DGD	c	518	-	63,63,67	1.23	9 (14%)	77,77,81	1.40	11 (14%)
31	BCR	Z	101	-	41,41,41	1.19	2 (4%)	56,56,56	1.34	5 (8%)
28	LHG	D	411	-	46,46,48	1.00	3 (6%)	49,52,54	1.20	3 (6%)
23	PHO	D	401	-	67,69,69	1.27	7 (10%)	85,99,99	1.10	4 (4%)
32	STE	Z	102	-	7,7,19	0.49	0	6,6,19	0.29	0
22	CLA	c	512	-	56,73,73	1.76	7 (12%)	55,113,113	1.60	13 (23%)
22	CLA	C	505	-	56,73,73	1.58	6 (10%)	55,113,113	1.68	11 (20%)
32	STE	C	518	-	8,11,19	0.50	0	7,11,19	0.72	0
26	LMG	m	101	-	51,51,55	1.30	6 (11%)	59,59,63	1.39	8 (13%)

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	b	608	-	1/1/20/20	6/37/115/115	-
31	BCR	c	514	-	-	8/29/63/63	0/2/2/2
27	SQD	B	622	-	-	25/49/69/69	0/1/1/1
22	CLA	C	506	-	1/1/20/20	21/37/115/115	-
32	STE	c	520	-	-	7/15/17/17	-
28	LHG	D	410	-	-	25/53/53/53	-
31	BCR	c	515	-	-	6/29/63/63	0/2/2/2
32	STE	l	102	-	-	7/15/15/17	-
32	STE	j	101	-	-	2/7/9/17	-
22	CLA	B	614	-	1/1/20/20	21/37/115/115	-
32	STE	R	101	-	-	4/7/9/17	-
22	CLA	B	604	-	1/1/20/20	16/37/115/115	-
25	PL9	A	408	-	-	19/53/73/73	0/1/1/1
27	SQD	t	102	-	-	14/37/37/69	-
22	CLA	B	605	-	1/1/20/20	14/37/115/115	-
22	CLA	C	501	-	1/1/20/20	2/37/115/115	-
22	CLA	b	607	37	1/1/20/20	16/37/115/115	-
22	CLA	b	614	-	1/1/20/20	19/37/115/115	-
32	STE	b	621	-	-	8/15/17/17	-
22	CLA	B	616	-	1/1/19/20	10/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	STE	b	627	-	-	7/11/11/17	-
31	BCR	H	101	-	-	10/29/63/63	0/2/2/2
22	CLA	B	607	37	1/1/20/20	13/37/115/115	-
31	BCR	B	619	-	-	6/29/63/63	0/2/2/2
32	STE	b	623	-	-	9/11/13/17	-
32	STE	a	413	-	-	8/12/12/17	-
31	BCR	k	102	-	-	4/29/63/63	0/2/2/2
26	LMG	M	101	-	-	20/46/66/70	0/1/1/1
28	LHG	l	101	-	-	17/53/53/53	-
22	CLA	d	403	-	1/1/20/20	10/37/115/115	-
31	BCR	C	514	-	-	7/29/63/63	0/2/2/2
26	LMG	b	622	-	-	30/50/70/70	0/1/1/1
32	STE	X	101	-	-	11/15/17/17	-
27	SQD	D	409	-	-	13/28/48/69	0/1/1/1
28	LHG	D	413	-	-	20/53/53/53	-
32	STE	d	412	-	-	7/15/17/17	-
22	CLA	c	510	-	1/1/20/20	16/37/115/115	-
31	BCR	b	617	-	-	9/29/63/63	0/2/2/2
22	CLA	b	616	-	1/1/19/20	10/31/109/115	-
25	PL9	d	407	-	-	16/53/73/73	0/1/1/1
22	CLA	B	601	37	1/1/20/20	16/37/115/115	-
26	LMG	d	410	-	-	10/39/59/70	0/1/1/1
32	STE	t	103	-	-	4/9/11/17	-
22	CLA	B	603	-	1/1/20/20	14/37/115/115	-
29	DGD	A	413	-	-	32/55/95/95	0/2/2/2
28	LHG	d	408	-	-	26/53/53/53	-
22	CLA	d	405	-	1/1/20/20	12/37/115/115	-
22	CLA	d	401	37	-	14/37/115/115	-
32	STE	M	103	-	-	2/7/7/17	-
22	CLA	b	610	37	1/1/20/20	7/37/115/115	-
22	CLA	C	502	-	1/1/20/20	10/37/115/115	-
22	CLA	D	405	-	-	13/37/115/115	-
32	STE	b	624	-	-	7/12/12/17	-
22	CLA	B	609	-	-	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	615	-	1/1/20/20	11/37/115/115	-
22	CLA	c	509	-	1/1/20/20	9/37/115/115	-
26	LMG	D	408	-	-	15/46/66/70	0/1/1/1
27	SQD	A	410	-	-	20/47/67/69	0/1/1/1
22	CLA	A	405	-	1/1/17/20	5/24/102/115	-
22	CLA	b	606	-	1/1/20/20	5/37/115/115	-
27	SQD	f	102	-	-	14/36/56/69	0/1/1/1
32	STE	d	411	-	-	6/12/14/17	-
28	LHG	e	101	-	-	24/46/46/53	-
34	HEM	f	101	6,5	-	0/6/54/54	-
27	SQD	A	412	-	-	19/39/39/69	-
22	CLA	b	612	-	1/1/20/20	5/37/115/115	-
22	CLA	A	402	-	1/1/20/20	7/37/115/115	-
22	CLA	c	513	-	1/1/20/20	10/37/115/115	-
22	CLA	b	611	-	-	10/37/115/115	-
26	LMG	Y	101	-	-	22/43/63/70	0/1/1/1
26	LMG	c	522	-	-	25/44/64/70	0/1/1/1
32	STE	B	623	-	-	4/7/9/17	-
22	CLA	c	504	37	1/1/19/20	9/31/109/115	-
32	STE	x	102	-	-	11/15/17/17	-
34	HEM	F	101	6,5	-	0/6/54/54	-
22	CLA	C	510	-	1/1/20/20	12/37/115/115	-
29	DGD	c	516	-	-	20/51/91/95	0/2/2/2
22	CLA	c	508	-	-	12/36/114/115	-
35	HEC	v	201	17	-	0/6/54/54	-
31	BCR	K	102	-	-	9/29/63/63	0/2/2/2
22	CLA	c	507	37	1/1/20/20	11/37/115/115	-
22	CLA	b	601	37	1/1/20/20	23/37/115/115	-
26	LMG	A	409	-	-	18/43/63/70	0/1/1/1
32	STE	L	103	-	-	5/7/9/17	-
22	CLA	b	604	-	1/1/20/20	11/37/115/115	-
25	PL9	a	409	-	-	28/53/73/73	0/1/1/1
22	CLA	C	504	37	1/1/18/20	8/30/108/115	-
22	CLA	C	511	3	1/1/20/20	6/37/115/115	-
32	STE	H	103	-	-	8/15/15/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HEC	V	201	17	-	0/6/54/54	-
26	LMG	D	412	-	-	19/33/33/70	-
22	CLA	b	602	-	1/1/20/20	12/37/115/115	-
22	CLA	c	506	-	1/1/20/20	14/37/115/115	-
26	LMG	B	626	-	-	35/50/70/70	0/1/1/1
31	BCR	b	618	-	-	2/29/63/63	0/2/2/2
22	CLA	B	611	-	-	6/37/115/115	-
25	PL9	D	407	-	-	13/53/73/73	0/1/1/1
28	LHG	L	102	-	-	23/53/53/53	-
29	DGD	h	101	-	-	17/51/91/95	0/2/2/2
22	CLA	B	613	-	1/1/20/20	11/37/115/115	-
32	STE	c	523	-	-	5/7/9/17	-
32	STE	b	620	-	-	7/13/13/17	-
22	CLA	c	505	-	1/1/20/20	10/37/115/115	-
22	CLA	C	509	-	1/1/20/20	15/37/115/115	-
22	CLA	B	606	-	1/1/20/20	10/37/115/115	-
28	LHG	a	410	-	-	22/53/53/53	-
26	LMG	c	519	-	-	12/31/51/70	0/1/1/1
26	LMG	B	621	-	-	10/18/22/70	-
22	CLA	B	610	37	1/1/20/20	10/37/115/115	-
28	LHG	A	411	-	-	23/53/53/53	-
29	DGD	c	517	-	-	21/51/91/95	0/2/2/2
28	LHG	d	409	-	-	11/43/43/53	-
22	CLA	D	403	-	1/1/20/20	6/37/115/115	-
22	CLA	b	613	-	1/1/20/20	11/37/115/115	-
31	BCR	I	101	-	-	5/29/63/63	0/2/2/2
22	CLA	B	615	-	1/1/20/20	6/37/115/115	-
22	CLA	d	404	37	1/1/20/20	6/37/115/115	-
31	BCR	t	101	-	-	13/29/63/63	0/2/2/2
32	STE	C	520	-	-	2/7/9/17	-
32	STE	a	412	-	-	4/7/9/17	-
29	DGD	C	515	-	-	24/51/91/95	0/2/2/2
32	STE	B	620	-	-	5/12/14/17	-
31	BCR	d	406	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	D	404	37	1/1/20/20	9/37/115/115	-
26	LMG	c	521	-	-	22/43/63/70	0/1/1/1
22	CLA	b	609	-	1/1/20/20	13/37/115/115	-
32	STE	B	627	-	-	4/7/9/17	-
29	DGD	C	516	-	-	26/51/91/95	0/2/2/2
31	BCR	D	406	-	-	7/29/63/63	0/2/2/2
22	CLA	b	603	-	1/1/20/20	8/37/115/115	-
29	DGD	H	102	-	-	18/51/91/95	0/2/2/2
22	CLA	C	507	37	1/1/20/20	7/37/115/115	-
32	STE	b	625	-	-	7/15/17/17	-
22	CLA	C	512	-	1/1/20/20	14/37/115/115	-
31	BCR	x	101	-	-	7/29/63/63	0/2/2/2
22	CLA	A	403	37	-	12/37/115/115	-
22	CLA	B	612	-	1/1/20/20	10/37/115/115	-
31	BCR	k	101	-	-	12/29/63/63	0/2/2/2
22	CLA	B	602	-	1/1/20/20	10/37/115/115	-
23	PHO	d	402	-	-	9/53/103/103	0/5/6/6
31	BCR	T	101	-	-	12/29/63/63	0/2/2/2
31	BCR	b	619	-	-	7/29/63/63	0/2/2/2
32	STE	C	519	-	-	5/13/13/17	-
31	BCR	B	617	-	-	9/29/63/63	0/2/2/2
31	BCR	B	618	-	-	10/29/63/63	0/2/2/2
22	CLA	C	503	-	1/1/20/20	9/37/115/115	-
22	CLA	C	508	-	-	10/37/115/115	-
31	BCR	K	101	-	-	12/29/63/63	0/2/2/2
22	CLA	b	605	-	1/1/20/20	15/37/115/115	-
22	CLA	c	502	-	-	12/37/115/115	-
27	SQD	a	411	-	-	23/49/69/69	0/1/1/1
27	SQD	L	101	-	-	29/44/64/69	0/1/1/1
32	STE	M	102	-	-	4/10/12/17	-
32	STE	B	625	-	-	7/13/13/17	-
22	CLA	a	404	-	1/1/20/20	8/37/115/115	-
29	DGD	C	517	-	-	13/51/91/95	0/2/2/2
22	CLA	c	503	-	1/1/20/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	STE	B	624	-	-	11/13/15/17	-
22	CLA	a	402	-	-	2/37/115/115	-
31	BCR	a	405	-	-	3/29/63/63	0/2/2/2
22	CLA	B	608	-	1/1/20/20	11/37/115/115	-
22	CLA	c	511	3	1/1/20/20	14/37/115/115	-
22	CLA	C	513	-	1/1/20/20	9/37/115/115	-
32	STE	t	104	-	-	3/7/7/17	-
32	STE	b	626	-	-	4/7/7/17	-
23	PHO	A	404	-	-	7/53/103/103	0/5/6/6
23	PHO	a	403	-	-	6/53/103/103	0/5/6/6
32	STE	I	102	-	-	4/12/12/17	-
32	STE	J	101	-	-	6/7/9/17	-
22	CLA	c	501	-	1/1/20/20	10/37/115/115	-
29	DGD	c	518	-	-	17/51/91/95	0/2/2/2
31	BCR	Z	101	-	-	13/29/63/63	0/2/2/2
28	LHG	D	411	-	-	19/51/51/53	-
23	PHO	D	401	-	-	3/53/103/103	0/5/6/6
32	STE	Z	102	-	-	4/5/5/17	-
22	CLA	c	512	-	1/1/20/20	20/37/115/115	-
22	CLA	C	505	-	1/1/20/20	9/37/115/115	-
32	STE	C	518	-	-	2/7/9/17	-
26	LMG	m	101	-	-	24/46/66/70	0/1/1/1

All (879) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	403	CLA	C4B-NB	10.45	1.44	1.35
22	B	606	CLA	MG-NA	9.77	2.29	2.06
25	A	408	PL9	C7-C3	-9.72	1.41	1.51
22	B	614	CLA	C4B-NB	9.21	1.43	1.35
22	A	402	CLA	C4B-NB	9.03	1.43	1.35
22	c	512	CLA	C4B-NB	8.92	1.43	1.35
22	B	602	CLA	C4B-NB	8.50	1.42	1.35
22	B	613	CLA	C4B-NB	8.42	1.42	1.35
22	b	609	CLA	C4B-NB	8.26	1.42	1.35
22	c	511	CLA	C4B-NB	8.07	1.42	1.35
22	d	404	CLA	C4B-NB	7.92	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	606	CLA	C4B-NB	7.68	1.42	1.35
35	v	201	HEC	C3B-C2B	-7.68	1.32	1.40
22	b	615	CLA	C4B-NB	7.63	1.42	1.35
22	a	402	CLA	C4C-NC	7.62	1.42	1.35
22	c	513	CLA	C4B-NB	7.60	1.42	1.35
22	A	403	CLA	C4C-NC	7.55	1.41	1.35
22	b	606	CLA	MG-NA	7.55	2.24	2.06
22	C	504	CLA	C4B-NB	7.29	1.41	1.35
22	B	601	CLA	MG-NA	7.27	2.23	2.06
22	D	404	CLA	MG-NA	7.24	2.23	2.06
22	A	402	CLA	C4C-NC	7.19	1.41	1.35
22	B	615	CLA	C4B-NB	7.19	1.41	1.35
22	c	505	CLA	C4B-NB	7.17	1.41	1.35
22	B	608	CLA	MG-NA	7.11	2.23	2.06
22	C	513	CLA	C4B-NB	7.09	1.41	1.35
22	d	401	CLA	C4B-NB	7.08	1.41	1.35
22	b	602	CLA	C4B-NB	7.08	1.41	1.35
22	c	501	CLA	C4B-NB	7.04	1.41	1.35
22	A	405	CLA	C4B-NB	7.03	1.41	1.35
22	c	504	CLA	C4B-NB	6.98	1.41	1.35
22	b	612	CLA	C4B-NB	6.98	1.41	1.35
22	b	611	CLA	C4B-NB	6.98	1.41	1.35
22	b	614	CLA	C4B-NB	6.98	1.41	1.35
22	C	505	CLA	C4B-NB	6.91	1.41	1.35
22	b	613	CLA	C4B-NB	6.86	1.41	1.35
22	b	601	CLA	C4B-NB	6.86	1.41	1.35
22	C	506	CLA	C4B-NB	6.85	1.41	1.35
22	C	513	CLA	C4C-NC	6.84	1.41	1.35
22	b	604	CLA	C4B-NB	6.82	1.41	1.35
22	b	605	CLA	C4B-NB	6.81	1.41	1.35
35	V	201	HEC	C3C-C2C	-6.81	1.33	1.40
22	D	405	CLA	C4B-NB	6.78	1.41	1.35
22	C	503	CLA	C4B-NB	6.78	1.41	1.35
22	d	404	CLA	MG-NA	6.77	2.22	2.06
22	b	615	CLA	MG-NA	6.77	2.22	2.06
22	B	601	CLA	C4B-NB	6.73	1.41	1.35
22	c	506	CLA	C4B-NB	6.73	1.41	1.35
22	B	616	CLA	C4B-NB	6.69	1.41	1.35
22	c	510	CLA	C4C-NC	6.66	1.41	1.35
22	d	403	CLA	C4B-NB	6.64	1.41	1.35
22	C	502	CLA	C4C-NC	6.63	1.41	1.35
22	C	510	CLA	C4B-NB	6.58	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	603	CLA	C4C-NC	6.56	1.41	1.35
22	c	502	CLA	C4C-NC	6.55	1.41	1.35
22	b	616	CLA	C4B-NB	6.52	1.41	1.35
22	b	610	CLA	C4C-NC	6.46	1.41	1.35
22	D	404	CLA	C4B-NB	6.45	1.41	1.35
22	C	504	CLA	C4C-NC	6.44	1.41	1.35
22	B	608	CLA	C4C-NC	6.39	1.40	1.35
22	B	612	CLA	C4B-NB	6.39	1.40	1.35
22	b	608	CLA	C4C-NC	6.31	1.40	1.35
22	c	503	CLA	C4B-NB	6.30	1.40	1.35
22	b	607	CLA	C4B-NB	6.29	1.40	1.35
22	c	506	CLA	C4C-NC	6.29	1.40	1.35
34	f	101	HEM	C3B-C2B	-6.28	1.31	1.40
22	D	403	CLA	C4B-NB	6.28	1.40	1.35
22	C	508	CLA	C4B-NB	6.27	1.40	1.35
22	c	508	CLA	C4B-NB	6.23	1.40	1.35
22	b	613	CLA	C4C-NC	6.23	1.40	1.35
22	C	502	CLA	C4B-NB	6.22	1.40	1.35
22	C	501	CLA	MG-NA	6.21	2.21	2.06
22	c	508	CLA	C4C-NC	6.19	1.40	1.35
22	c	507	CLA	MG-NA	6.17	2.20	2.06
22	B	610	CLA	C4C-NC	6.17	1.40	1.35
22	c	502	CLA	C4B-NB	6.13	1.40	1.35
22	C	511	CLA	C4B-NB	6.11	1.40	1.35
22	b	603	CLA	C4B-NB	6.04	1.40	1.35
22	b	605	CLA	C4C-NC	6.03	1.40	1.35
22	B	609	CLA	C4B-NB	5.96	1.40	1.35
35	v	201	HEC	C3C-C2C	-5.96	1.34	1.40
22	c	512	CLA	C4C-NC	5.91	1.40	1.35
22	d	405	CLA	MG-NA	5.88	2.20	2.06
22	C	505	CLA	C4C-NC	5.86	1.40	1.35
22	B	611	CLA	MG-NA	5.84	2.20	2.06
22	d	401	CLA	C4C-NC	5.81	1.40	1.35
22	d	405	CLA	C4B-NB	5.79	1.40	1.35
22	d	405	CLA	C4C-NC	5.77	1.40	1.35
22	B	611	CLA	C4B-NB	5.76	1.40	1.35
22	C	512	CLA	C4B-NB	5.73	1.40	1.35
22	C	510	CLA	C4C-NC	5.72	1.40	1.35
22	B	606	CLA	C4C-NC	5.70	1.40	1.35
22	c	509	CLA	C4C-NC	5.58	1.40	1.35
22	B	603	CLA	C4B-NB	5.58	1.40	1.35
22	b	601	CLA	C4C-NC	5.55	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	603	CLA	MG-NA	5.55	2.19	2.06
35	V	201	HEC	C3B-C2B	-5.52	1.35	1.40
34	F	101	HEM	C3B-C2B	-5.52	1.32	1.40
22	b	608	CLA	C4B-NB	5.52	1.40	1.35
22	C	503	CLA	C4C-NC	5.51	1.40	1.35
31	b	618	BCR	C30-C25	-5.48	1.46	1.53
22	D	405	CLA	C4C-NC	5.47	1.40	1.35
22	D	403	CLA	C4C-NC	5.47	1.40	1.35
22	B	606	CLA	C4B-NB	5.46	1.40	1.35
22	B	607	CLA	C4C-NC	5.42	1.40	1.35
22	C	511	CLA	MG-NA	5.41	2.19	2.06
22	c	505	CLA	C4C-NC	5.39	1.40	1.35
22	B	605	CLA	C4B-NB	5.38	1.40	1.35
22	c	511	CLA	MG-NA	5.36	2.19	2.06
22	c	507	CLA	C4B-NB	5.32	1.40	1.35
22	C	509	CLA	C4B-NB	5.30	1.39	1.35
22	B	607	CLA	C4B-NB	5.28	1.39	1.35
22	c	503	CLA	C4C-NC	5.27	1.39	1.35
22	B	604	CLA	C4B-NB	5.23	1.39	1.35
22	b	604	CLA	C4C-NC	5.17	1.39	1.35
26	m	101	LMG	C4-C3	5.17	1.65	1.52
22	a	402	CLA	MG-NA	5.17	2.18	2.06
29	c	516	DGD	O5D-C6D	-5.17	1.34	1.43
22	B	614	CLA	C4C-NC	5.13	1.39	1.35
22	b	611	CLA	C4C-NC	5.13	1.39	1.35
22	C	507	CLA	C4B-NB	5.12	1.39	1.35
22	c	511	CLA	C4C-NC	5.07	1.39	1.35
22	c	504	CLA	C4C-NC	5.01	1.39	1.35
22	b	616	CLA	C4C-NC	4.99	1.39	1.35
22	c	510	CLA	C4B-NB	4.98	1.39	1.35
22	b	602	CLA	C4C-NC	4.97	1.39	1.35
22	C	501	CLA	C4B-NB	4.96	1.39	1.35
22	B	602	CLA	C4C-NC	4.93	1.39	1.35
29	C	515	DGD	O5D-C6D	-4.91	1.34	1.43
22	B	610	CLA	C4B-NB	4.90	1.39	1.35
22	A	405	CLA	C4C-NC	4.89	1.39	1.35
31	C	514	BCR	C1-C6	-4.89	1.47	1.53
22	b	615	CLA	C4C-NC	4.87	1.39	1.35
22	b	612	CLA	C4C-NC	4.84	1.39	1.35
22	B	607	CLA	MG-NA	4.82	2.17	2.06
22	a	404	CLA	C4B-NB	4.79	1.39	1.35
22	a	402	CLA	C4B-NB	4.78	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	616	CLA	C4C-NC	4.75	1.39	1.35
22	b	609	CLA	C4C-NC	4.74	1.39	1.35
22	c	501	CLA	C4C-NC	4.73	1.39	1.35
35	v	201	HEC	C3D-C2D	4.72	1.51	1.37
22	C	512	CLA	C4C-NC	4.72	1.39	1.35
26	A	409	LMG	O1-C7	-4.71	1.35	1.43
25	d	407	PL9	C3-C4	-4.63	1.41	1.49
22	c	507	CLA	C4C-NC	4.62	1.39	1.35
22	b	601	CLA	MG-NA	4.61	2.17	2.06
22	c	509	CLA	C4B-NB	4.59	1.39	1.35
22	C	509	CLA	C4C-NC	4.54	1.39	1.35
22	C	512	CLA	MG-NA	4.52	2.17	2.06
31	K	101	BCR	C30-C25	-4.50	1.47	1.53
25	A	408	PL9	C7-C8	-4.47	1.44	1.50
22	B	604	CLA	MG-NA	4.46	2.16	2.06
22	d	403	CLA	C4C-NC	4.43	1.39	1.35
25	d	407	PL9	C53-C6	-4.41	1.41	1.50
22	D	404	CLA	C4C-NC	4.39	1.39	1.35
22	C	508	CLA	MG-NA	4.39	2.16	2.06
22	C	507	CLA	C4C-NC	4.39	1.39	1.35
22	C	508	CLA	C4C-NC	4.35	1.39	1.35
22	B	601	CLA	C4C-NC	4.31	1.39	1.35
22	C	509	CLA	MG-NA	4.28	2.16	2.06
22	b	614	CLA	C4C-NC	4.28	1.39	1.35
22	B	605	CLA	C4C-NC	4.27	1.39	1.35
22	B	609	CLA	C4C-NC	4.25	1.39	1.35
26	B	626	LMG	C4-C5	4.22	1.61	1.53
25	A	408	PL9	C3-C4	-4.19	1.42	1.49
22	C	511	CLA	C4C-NC	4.18	1.38	1.35
26	d	410	LMG	C4-C5	4.16	1.61	1.53
22	c	513	CLA	C4C-NC	4.15	1.38	1.35
34	F	101	HEM	C3C-C2C	-4.14	1.34	1.40
22	c	501	CLA	MG-NA	4.12	2.16	2.06
22	b	610	CLA	C4B-NB	4.10	1.38	1.35
22	b	602	CLA	MG-NA	4.10	2.16	2.06
22	B	603	CLA	C4C-NC	4.08	1.38	1.35
22	C	507	CLA	C1B-NB	-4.01	1.31	1.35
31	H	101	BCR	C30-C25	-3.97	1.48	1.53
25	D	407	PL9	C52-C5	-3.97	1.42	1.50
31	D	406	BCR	C30-C25	-3.93	1.48	1.53
23	A	404	PHO	C1C-NC	-3.93	1.30	1.38
34	F	101	HEM	C3B-CAB	3.92	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	V	201	HEC	C3D-C2D	3.91	1.49	1.37
22	B	615	CLA	CMB-C2B	-3.89	1.43	1.51
22	C	501	CLA	C4C-NC	3.89	1.38	1.35
34	f	101	HEM	C3C-C2C	-3.88	1.35	1.40
22	B	606	CLA	C3B-C2B	-3.87	1.35	1.40
31	K	101	BCR	C1-C6	-3.86	1.48	1.53
29	A	413	DGD	C4D-C5D	3.85	1.61	1.53
31	b	619	BCR	C1-C6	-3.84	1.48	1.53
31	b	617	BCR	C1-C6	-3.84	1.48	1.53
23	a	403	PHO	C1C-NC	-3.83	1.30	1.38
22	B	610	CLA	C3B-C2B	-3.82	1.35	1.40
26	c	519	LMG	C4-C5	3.80	1.61	1.53
31	t	101	BCR	C30-C25	-3.79	1.48	1.53
31	k	102	BCR	C30-C25	-3.79	1.48	1.53
31	c	514	BCR	C1-C6	-3.78	1.48	1.53
31	k	101	BCR	C30-C25	-3.76	1.48	1.53
22	B	608	CLA	C4B-NB	3.74	1.38	1.35
23	D	401	PHO	CHC-C1C	3.72	1.45	1.38
31	a	405	BCR	C30-C25	-3.71	1.48	1.53
29	A	413	DGD	C4E-C5E	3.71	1.60	1.53
22	B	612	CLA	MG-NA	3.70	2.15	2.06
22	B	610	CLA	MG-NA	3.69	2.15	2.06
22	c	503	CLA	MG-NA	3.68	2.15	2.06
26	c	522	LMG	C3-C2	3.67	1.61	1.52
26	m	101	LMG	O1-C7	-3.66	1.37	1.43
22	b	603	CLA	C3B-C2B	-3.65	1.35	1.40
27	a	411	SQD	O48-C23	3.65	1.44	1.33
26	Y	101	LMG	C4-C5	3.64	1.60	1.53
22	c	506	CLA	MG-NA	3.64	2.14	2.06
27	t	102	SQD	O47-C7	3.64	1.44	1.34
28	D	413	LHG	O7-C5	-3.63	1.37	1.46
27	L	101	SQD	O48-C23	3.61	1.43	1.33
22	B	604	CLA	C4C-NC	3.61	1.38	1.35
27	A	412	SQD	O47-C7	3.60	1.44	1.34
26	c	522	LMG	C1-C2	3.57	1.62	1.52
22	b	611	CLA	MG-NA	3.57	2.14	2.06
27	B	622	SQD	O47-C7	3.56	1.44	1.34
31	b	618	BCR	C1-C6	-3.56	1.48	1.53
27	A	412	SQD	O48-C23	3.56	1.43	1.33
26	d	410	LMG	O1-C7	-3.55	1.37	1.43
25	a	409	PL9	C53-C6	-3.54	1.43	1.50
31	Z	101	BCR	C30-C25	-3.53	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	501	CLA	C3B-C2B	-3.52	1.35	1.40
31	B	619	BCR	C1-C6	-3.51	1.48	1.53
31	T	101	BCR	C30-C25	-3.51	1.48	1.53
27	A	410	SQD	O47-C7	3.49	1.44	1.34
29	H	102	DGD	O2D-C2D	-3.49	1.34	1.43
22	D	405	CLA	C3B-C2B	-3.48	1.35	1.40
27	A	410	SQD	O48-C23	3.47	1.43	1.33
28	D	411	LHG	P-O6	3.47	1.73	1.59
26	D	412	LMG	C7-C8	3.45	1.59	1.51
22	A	403	CLA	MG-NA	3.44	2.14	2.06
22	B	602	CLA	CMB-C2B	-3.44	1.44	1.51
22	b	610	CLA	C3B-C2B	-3.42	1.35	1.40
29	H	102	DGD	C1E-C2E	3.42	1.62	1.52
23	D	401	PHO	C3B-C4B	3.41	1.50	1.43
29	C	515	DGD	O1G-C1A	3.40	1.43	1.33
25	D	407	PL9	C11-C9	-3.40	1.44	1.51
27	B	622	SQD	O48-C23	3.38	1.43	1.33
22	B	615	CLA	C3B-C2B	-3.37	1.35	1.40
22	B	615	CLA	C4C-NC	3.37	1.38	1.35
26	b	622	LMG	O1-C7	-3.37	1.37	1.43
31	I	101	BCR	C1-C6	-3.36	1.49	1.53
22	b	606	CLA	C4C-NC	3.35	1.38	1.35
22	b	612	CLA	CMB-C2B	-3.35	1.44	1.51
29	C	517	DGD	O1G-C1G	-3.34	1.37	1.45
22	b	606	CLA	C1B-NB	3.34	1.38	1.35
22	B	610	CLA	CMB-C2B	-3.34	1.44	1.51
25	D	407	PL9	C6-C1	-3.31	1.42	1.48
34	F	101	HEM	C3C-CAC	3.31	1.54	1.47
22	B	613	CLA	C4C-NC	3.30	1.38	1.35
22	B	615	CLA	C3B-CAB	-3.29	1.41	1.47
31	c	515	BCR	C1-C6	-3.28	1.49	1.53
26	b	622	LMG	C4-C3	3.28	1.60	1.52
22	b	605	CLA	CMC-C2C	-3.27	1.43	1.51
31	Z	101	BCR	C1-C6	-3.26	1.49	1.53
31	d	406	BCR	C30-C25	-3.25	1.49	1.53
22	d	401	CLA	C3B-CAB	-3.24	1.41	1.47
22	B	601	CLA	C3B-C2B	-3.23	1.35	1.40
26	c	521	LMG	O1-C1	3.23	1.45	1.40
23	d	402	PHO	C3B-C4B	3.23	1.50	1.43
22	C	506	CLA	C4C-NC	3.22	1.38	1.35
31	c	514	BCR	C30-C25	-3.22	1.49	1.53
22	B	604	CLA	C1D-C2D	3.21	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	603	CLA	MG-NA	3.21	2.13	2.06
29	H	102	DGD	C6D-C5D	3.20	1.61	1.51
25	d	407	PL9	C7-C8	-3.19	1.46	1.50
22	d	403	CLA	CMB-C2B	-3.19	1.45	1.51
22	B	609	CLA	CMD-C2D	-3.18	1.44	1.51
29	c	518	DGD	O4E-C4E	-3.18	1.35	1.43
26	M	101	LMG	C1-C2	3.18	1.61	1.52
31	D	406	BCR	C1-C6	-3.17	1.49	1.53
27	D	409	SQD	O48-C23	3.16	1.42	1.33
29	C	516	DGD	C1E-C2E	3.16	1.61	1.52
22	c	510	CLA	CMB-C2B	-3.15	1.45	1.51
27	t	102	SQD	O48-C23	3.15	1.42	1.33
31	x	101	BCR	C30-C25	-3.15	1.49	1.53
29	h	101	DGD	O5D-C6D	-3.14	1.38	1.43
31	B	617	BCR	C30-C25	-3.14	1.49	1.53
29	C	517	DGD	O3G-C3G	-3.13	1.38	1.43
22	C	510	CLA	MG-NA	3.12	2.13	2.06
31	d	406	BCR	C1-C6	-3.12	1.49	1.53
26	c	519	LMG	C1-C2	3.11	1.61	1.52
22	C	502	CLA	MG-NA	3.11	2.13	2.06
26	d	410	LMG	O7-C8	-3.10	1.38	1.46
22	C	505	CLA	CMB-C2B	-3.09	1.45	1.51
27	L	101	SQD	O47-C7	3.07	1.43	1.34
22	d	404	CLA	CMB-C2B	-3.07	1.45	1.51
31	B	617	BCR	C1-C6	-3.07	1.49	1.53
22	d	404	CLA	C4C-NC	3.07	1.37	1.35
22	C	502	CLA	C3B-C2B	-3.07	1.36	1.40
22	D	403	CLA	MG-NA	3.06	2.13	2.06
22	B	607	CLA	C3B-C2B	-3.05	1.36	1.40
26	c	522	LMG	C4-C5	3.05	1.59	1.53
29	H	102	DGD	O5D-C1E	3.05	1.45	1.40
22	C	503	CLA	MG-NA	3.05	2.13	2.06
22	B	613	CLA	CMD-C2D	-3.05	1.44	1.51
22	c	501	CLA	CMC-C2C	-3.04	1.44	1.51
22	c	506	CLA	CMB-C2B	-3.04	1.45	1.51
22	b	611	CLA	C3B-C2B	-3.04	1.36	1.40
23	d	402	PHO	CHC-C1C	3.03	1.44	1.38
22	d	405	CLA	C3B-CAB	-3.03	1.41	1.47
22	b	602	CLA	CMD-C2D	-3.03	1.44	1.51
29	h	101	DGD	O5D-C1E	3.03	1.45	1.40
22	a	402	CLA	CMB-C2B	-3.02	1.45	1.51
26	c	519	LMG	C7-C8	3.02	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	603	CLA	CMB-C2B	-3.02	1.45	1.51
22	D	405	CLA	CMB-C2B	-3.02	1.45	1.51
25	A	408	PL9	C6-C1	-3.01	1.43	1.48
22	c	501	CLA	CMB-C2B	-3.00	1.45	1.51
22	B	603	CLA	C3B-CAB	-3.00	1.41	1.47
29	H	102	DGD	C4E-C5E	2.99	1.59	1.53
22	b	607	CLA	C4C-NC	2.99	1.37	1.35
23	d	402	PHO	C1C-NC	-2.99	1.32	1.38
22	A	403	CLA	CMB-C2B	-2.98	1.45	1.51
22	b	610	CLA	C4B-CHC	-2.98	1.32	1.41
22	C	511	CLA	CMB-C2B	-2.98	1.45	1.51
22	C	513	CLA	CMB-C2B	-2.97	1.45	1.51
27	f	102	SQD	O48-C23	2.97	1.42	1.33
28	a	410	LHG	O7-C5	-2.97	1.39	1.46
26	A	409	LMG	C4-C3	2.97	1.59	1.52
23	D	401	PHO	C1A-NA	2.96	1.43	1.37
22	b	615	CLA	CMB-C2B	-2.96	1.45	1.51
29	c	516	DGD	C4D-C3D	2.96	1.59	1.52
26	c	521	LMG	C3-C2	2.96	1.59	1.52
22	C	503	CLA	CMB-C2B	-2.96	1.45	1.51
22	C	503	CLA	C1D-C2D	2.95	1.49	1.42
22	c	512	CLA	C1D-C2D	2.95	1.49	1.42
22	d	401	CLA	C3B-C2B	-2.95	1.36	1.40
29	C	516	DGD	C4D-C3D	2.95	1.59	1.52
22	b	611	CLA	CMD-C2D	-2.95	1.44	1.51
22	B	601	CLA	CMB-C2B	-2.94	1.45	1.51
29	C	517	DGD	O2G-C2G	-2.93	1.39	1.46
27	f	102	SQD	O47-C7	2.92	1.42	1.34
22	d	405	CLA	CMD-C2D	-2.92	1.44	1.51
22	d	405	CLA	CMB-C2B	-2.92	1.45	1.51
29	c	518	DGD	C2A-C1A	-2.92	1.42	1.50
31	t	101	BCR	C1-C6	-2.92	1.49	1.53
29	C	516	DGD	O3G-C3G	-2.92	1.38	1.43
22	C	501	CLA	CAC-C3C	-2.92	1.44	1.52
22	c	506	CLA	C3B-C2B	-2.91	1.36	1.40
22	A	405	CLA	C3B-CAB	-2.91	1.42	1.47
22	b	608	CLA	C1D-C2D	2.91	1.49	1.42
29	c	516	DGD	O2G-C2G	-2.91	1.39	1.46
26	c	519	LMG	C3-C2	2.90	1.59	1.52
22	B	616	CLA	CMB-C2B	-2.90	1.45	1.51
22	B	611	CLA	CMD-C2D	-2.90	1.44	1.51
28	D	410	LHG	O8-C6	-2.90	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	515	DGD	C3G-C2G	2.89	1.59	1.50
26	m	101	LMG	C1-C2	2.89	1.60	1.52
22	B	603	CLA	C3B-C2B	-2.88	1.36	1.40
25	d	407	PL9	C16-C14	-2.88	1.45	1.51
27	a	411	SQD	O47-C7	2.88	1.42	1.34
22	B	616	CLA	CMD-C2D	-2.88	1.44	1.51
22	c	513	CLA	CMB-C2B	-2.88	1.45	1.51
22	b	605	CLA	C1D-C2D	2.88	1.49	1.42
22	c	507	CLA	C3B-C2B	-2.88	1.36	1.40
29	A	413	DGD	O5D-C6D	-2.88	1.38	1.43
34	f	101	HEM	C3C-CAC	2.88	1.53	1.47
31	K	102	BCR	C30-C25	-2.88	1.49	1.53
22	D	405	CLA	CMD-C2D	-2.87	1.44	1.51
22	C	506	CLA	C3B-C2B	-2.86	1.36	1.40
22	B	602	CLA	CAC-C3C	-2.86	1.45	1.52
23	d	402	PHO	CHC-C4B	-2.86	1.33	1.40
29	c	518	DGD	O2E-C2E	-2.86	1.36	1.43
22	b	602	CLA	CMB-C2B	-2.86	1.45	1.51
22	b	603	CLA	CMC-C2C	-2.85	1.44	1.51
22	C	509	CLA	CMD-C2D	-2.84	1.44	1.51
22	c	513	CLA	CMD-C2D	-2.84	1.44	1.51
22	d	401	CLA	CMD-C2D	-2.83	1.44	1.51
31	b	619	BCR	C30-C25	-2.83	1.49	1.53
22	b	609	CLA	CMB-C2B	-2.83	1.45	1.51
22	B	607	CLA	C3B-CAB	-2.83	1.42	1.47
27	D	409	SQD	O2-C2	-2.83	1.36	1.43
26	B	626	LMG	C3-C2	2.82	1.59	1.52
22	b	615	CLA	CMD-C2D	-2.82	1.44	1.51
26	b	622	LMG	O8-C28	2.82	1.41	1.33
23	a	403	PHO	C3B-C4B	2.81	1.49	1.43
26	m	101	LMG	O4-C4	-2.81	1.36	1.43
29	A	413	DGD	C3G-C2G	2.81	1.59	1.50
26	D	412	LMG	C9-C8	2.81	1.59	1.50
22	C	507	CLA	C3B-C2B	-2.80	1.36	1.40
26	b	622	LMG	C3-C2	2.80	1.59	1.52
31	K	102	BCR	C1-C6	-2.80	1.49	1.53
22	b	608	CLA	C1C-C2C	2.79	1.48	1.42
22	C	509	CLA	CMB-C2B	-2.79	1.45	1.51
23	D	401	PHO	CMD-C2D	-2.78	1.44	1.50
22	C	506	CLA	CAC-C3C	-2.78	1.45	1.52
28	D	411	LHG	O3-C3	-2.78	1.34	1.44
29	C	516	DGD	C6D-C5D	2.78	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	617	BCR	C33-C5	-2.78	1.46	1.50
22	C	513	CLA	C1D-C2D	2.77	1.48	1.42
22	D	404	CLA	CMB-C2B	-2.77	1.45	1.51
25	D	407	PL9	C26-C24	-2.77	1.45	1.51
22	b	601	CLA	CMB-C2B	-2.76	1.45	1.51
22	b	608	CLA	C3B-CAB	-2.76	1.42	1.47
22	A	405	CLA	C1D-C2D	2.76	1.48	1.42
22	c	511	CLA	C1D-C2D	2.76	1.48	1.42
29	h	101	DGD	C4D-C3D	2.75	1.59	1.52
28	L	102	LHG	O7-C5	-2.75	1.39	1.46
22	b	602	CLA	CAC-C3C	-2.75	1.45	1.52
29	C	517	DGD	O2D-C2D	-2.75	1.36	1.43
31	I	101	BCR	C33-C5	-2.75	1.46	1.50
23	A	404	PHO	CHC-C1C	2.74	1.44	1.38
22	b	607	CLA	C3B-C2B	-2.74	1.36	1.40
22	B	611	CLA	C4C-NC	2.74	1.37	1.35
22	B	602	CLA	MG-NA	2.74	2.12	2.06
22	b	613	CLA	CMB-C2B	-2.74	1.46	1.51
22	d	401	CLA	CMB-C2B	-2.73	1.46	1.51
31	a	405	BCR	C1-C6	-2.73	1.50	1.53
22	b	602	CLA	C3B-C2B	-2.72	1.36	1.40
22	C	505	CLA	C3B-CAB	-2.72	1.42	1.47
29	C	515	DGD	C4E-C3E	2.72	1.59	1.52
22	B	616	CLA	C1D-C2D	2.71	1.48	1.42
34	f	101	HEM	C3B-CAB	2.71	1.53	1.47
22	B	602	CLA	C1D-C2D	2.71	1.48	1.42
22	b	616	CLA	CMD-C2D	-2.71	1.45	1.51
22	C	507	CLA	CMB-C2B	-2.70	1.46	1.51
22	b	607	CLA	CMB-C2B	-2.70	1.46	1.51
28	e	101	LHG	O8-C23	2.70	1.41	1.33
28	e	101	LHG	P-O6	2.70	1.70	1.59
22	A	403	CLA	CMD-C2D	-2.69	1.45	1.51
23	A	404	PHO	CMD-C2D	-2.69	1.45	1.50
27	f	102	SQD	O2-C2	-2.68	1.36	1.43
22	B	601	CLA	C1D-C2D	2.68	1.48	1.42
22	b	603	CLA	CMD-C2D	-2.68	1.45	1.51
29	C	517	DGD	O2E-C2E	-2.68	1.36	1.43
28	l	101	LHG	P-O6	2.67	1.70	1.59
31	k	102	BCR	C1-C6	-2.67	1.50	1.53
22	c	512	CLA	CMB-C2B	-2.67	1.46	1.51
22	c	504	CLA	CMD-C2D	-2.66	1.45	1.51
29	c	518	DGD	O3D-C3D	-2.66	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	605	CLA	CAC-C3C	-2.65	1.45	1.52
22	d	403	CLA	C1D-C2D	2.65	1.48	1.42
23	A	404	PHO	C1D-C2D	-2.65	1.40	1.45
26	c	521	LMG	C4-C3	2.64	1.59	1.52
28	l	101	LHG	O7-C5	-2.64	1.40	1.46
22	C	501	CLA	CMD-C2D	-2.64	1.45	1.51
23	a	403	PHO	CHC-C4B	-2.64	1.34	1.40
22	b	603	CLA	C3B-CAB	-2.63	1.42	1.47
22	b	605	CLA	CMD-C2D	-2.63	1.45	1.51
22	c	502	CLA	CMD-C2D	-2.63	1.45	1.51
22	B	615	CLA	C4B-CHC	-2.62	1.33	1.41
31	B	618	BCR	C30-C25	-2.62	1.50	1.53
22	B	607	CLA	CMB-C2B	-2.62	1.46	1.51
22	B	611	CLA	CMB-C2B	-2.62	1.46	1.51
22	C	504	CLA	CMB-C2B	-2.62	1.46	1.51
28	A	411	LHG	P-O6	2.61	1.69	1.59
22	b	614	CLA	C3B-C2B	-2.61	1.36	1.40
29	c	517	DGD	O3D-C3D	-2.61	1.36	1.43
28	d	409	LHG	P-O6	2.60	1.69	1.59
29	H	102	DGD	O6E-C1E	2.60	1.48	1.41
25	a	409	PL9	C3-C4	-2.60	1.45	1.49
22	B	607	CLA	CAC-C3C	-2.59	1.45	1.52
22	B	612	CLA	C4C-NC	2.59	1.37	1.35
29	C	516	DGD	O2G-C2G	-2.59	1.40	1.46
22	B	614	CLA	C3B-CAB	-2.59	1.42	1.47
22	b	610	CLA	C3B-CAB	-2.59	1.42	1.47
22	c	503	CLA	CAC-C3C	-2.59	1.45	1.52
29	c	516	DGD	O3E-C3E	-2.59	1.36	1.43
22	b	601	CLA	C1D-C2D	2.59	1.48	1.42
31	b	618	BCR	C33-C5	-2.59	1.46	1.50
27	A	410	SQD	O2-C2	-2.58	1.36	1.43
22	c	504	CLA	CAC-C3C	-2.58	1.45	1.52
22	b	609	CLA	C1D-C2D	2.58	1.48	1.42
22	c	507	CLA	C4B-CHC	-2.58	1.33	1.41
29	A	413	DGD	C1E-C2E	2.57	1.59	1.52
29	c	517	DGD	O2E-C2E	-2.57	1.36	1.43
28	A	411	LHG	C24-C23	2.57	1.58	1.50
22	B	603	CLA	C4B-CHC	-2.56	1.33	1.41
22	b	613	CLA	CMD-C2D	-2.56	1.45	1.51
22	B	611	CLA	C4B-CHC	-2.55	1.33	1.41
22	C	506	CLA	C1D-C2D	2.55	1.48	1.42
22	C	502	CLA	CMB-C2B	-2.55	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	502	CLA	CMC-C2C	-2.54	1.45	1.51
26	Y	101	LMG	O7-C8	-2.54	1.40	1.46
22	c	506	CLA	C1D-C2D	2.53	1.48	1.42
27	a	411	SQD	O2-C2	-2.53	1.37	1.43
22	a	404	CLA	C4B-CHC	-2.52	1.34	1.41
22	B	613	CLA	CMB-C2B	-2.52	1.46	1.51
29	c	516	DGD	C4E-C3E	2.52	1.58	1.52
28	D	411	LHG	O7-C7	2.52	1.41	1.34
22	B	609	CLA	CMC-C2C	-2.51	1.45	1.51
22	c	507	CLA	CMB-C2B	-2.51	1.46	1.51
22	B	613	CLA	C3B-C2B	-2.50	1.36	1.40
28	L	102	LHG	P-O6	2.50	1.69	1.59
25	d	407	PL9	C40-C39	-2.50	1.44	1.50
22	C	507	CLA	C3B-CAB	-2.50	1.42	1.47
22	b	601	CLA	O2A-CGA	2.50	1.40	1.33
29	A	413	DGD	O1G-C1A	2.50	1.40	1.33
22	c	508	CLA	CMD-C2D	-2.50	1.45	1.51
23	a	403	PHO	C4C-NC	2.50	1.42	1.36
23	D	401	PHO	C1C-NC	-2.50	1.33	1.38
22	b	615	CLA	CAC-C3C	-2.49	1.46	1.52
28	D	410	LHG	O7-C5	-2.49	1.40	1.46
22	B	606	CLA	CMA-C3A	-2.49	1.47	1.53
22	b	607	CLA	C4B-CHC	-2.49	1.34	1.41
31	B	619	BCR	C30-C25	-2.49	1.50	1.53
22	B	608	CLA	CMC-C2C	-2.49	1.45	1.51
22	b	616	CLA	C3B-CAB	-2.48	1.42	1.47
22	b	611	CLA	C4B-CHC	-2.48	1.34	1.41
22	a	402	CLA	C1D-C2D	2.48	1.48	1.42
28	D	413	LHG	O8-C23	2.48	1.40	1.33
22	C	512	CLA	CMD-C2D	-2.47	1.45	1.51
22	c	509	CLA	C1D-C2D	2.47	1.48	1.42
22	b	604	CLA	CMC-C2C	-2.47	1.45	1.51
22	B	613	CLA	CMC-C2C	-2.47	1.45	1.51
22	d	403	CLA	CMD-C2D	-2.47	1.45	1.51
22	b	606	CLA	CMB-C2B	-2.47	1.46	1.51
22	C	508	CLA	CMB-C2B	-2.46	1.46	1.51
22	B	616	CLA	CMC-C2C	-2.46	1.45	1.51
22	B	608	CLA	CMD-C2D	-2.46	1.45	1.51
22	B	603	CLA	CMB-C2B	-2.46	1.46	1.51
25	D	407	PL9	C53-C6	-2.46	1.45	1.50
26	d	410	LMG	O6-C5	-2.45	1.38	1.44
22	b	614	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	509	CLA	CMB-C2B	-2.45	1.46	1.51
29	C	516	DGD	C4E-C5E	2.45	1.58	1.53
22	A	405	CLA	CMD-C2D	-2.45	1.45	1.51
27	a	411	SQD	O3-C3	-2.45	1.37	1.43
29	c	518	DGD	O2G-C2G	-2.45	1.40	1.46
22	C	508	CLA	C1D-C2D	2.45	1.48	1.42
29	c	517	DGD	O6D-C5D	-2.44	1.38	1.44
26	Y	101	LMG	C3-C2	2.44	1.58	1.52
23	A	404	PHO	CHD-C4C	-2.44	1.34	1.40
22	a	402	CLA	CMC-C2C	-2.43	1.45	1.51
22	c	511	CLA	CMB-C2B	-2.43	1.46	1.51
22	b	610	CLA	CMD-C2D	-2.43	1.45	1.51
22	d	403	CLA	CAC-C3C	-2.43	1.46	1.52
26	A	409	LMG	C4-C5	2.42	1.58	1.53
22	b	601	CLA	CAC-C3C	-2.42	1.46	1.52
22	B	616	CLA	CAC-C3C	-2.42	1.46	1.52
22	c	513	CLA	C3B-C2B	-2.42	1.37	1.40
31	b	617	BCR	C30-C25	-2.42	1.50	1.53
22	B	605	CLA	CMD-C2D	-2.42	1.45	1.51
22	B	602	CLA	C4B-CHC	-2.42	1.34	1.41
22	B	604	CLA	C3B-C2B	-2.41	1.37	1.40
22	b	612	CLA	CMC-C2C	-2.41	1.45	1.51
31	C	514	BCR	C33-C5	-2.41	1.47	1.50
27	f	102	SQD	O3-C3	-2.41	1.37	1.43
22	c	503	CLA	CMC-C2C	-2.41	1.45	1.51
22	C	502	CLA	CAC-C3C	-2.41	1.46	1.52
22	b	604	CLA	C1D-C2D	2.40	1.48	1.42
22	b	610	CLA	CAC-C3C	-2.40	1.46	1.52
22	C	512	CLA	C1D-C2D	2.40	1.48	1.42
29	C	515	DGD	O5D-C1E	2.40	1.44	1.40
22	c	507	CLA	C1D-C2D	2.40	1.48	1.42
23	d	402	PHO	CMC-C2C	-2.40	1.45	1.50
22	C	510	CLA	CMB-C2B	-2.40	1.46	1.51
22	C	510	CLA	C1C-C2C	2.40	1.48	1.42
22	c	503	CLA	C1D-C2D	2.40	1.48	1.42
22	b	609	CLA	CMD-C2D	-2.40	1.45	1.51
29	c	518	DGD	C4D-C5D	2.40	1.58	1.53
22	a	404	CLA	CMB-C2B	-2.40	1.46	1.51
31	k	101	BCR	C1-C6	-2.40	1.50	1.53
29	c	517	DGD	C4E-C5E	2.39	1.58	1.53
22	A	405	CLA	C4B-CHC	-2.39	1.34	1.41
22	b	607	CLA	CMD-C2D	-2.39	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	615	CLA	C3B-C2B	-2.39	1.37	1.40
22	C	508	CLA	CMD-C2D	-2.39	1.45	1.51
26	c	521	LMG	C7-C8	2.39	1.58	1.50
22	c	507	CLA	CMC-C2C	-2.38	1.45	1.51
29	c	516	DGD	C3G-C2G	2.38	1.58	1.50
22	c	506	CLA	OBD-CAD	2.38	1.25	1.22
22	c	508	CLA	C3B-C2B	-2.38	1.37	1.40
22	b	612	CLA	C1D-C2D	2.38	1.48	1.42
22	C	502	CLA	C1C-C2C	2.38	1.48	1.42
22	d	404	CLA	C1D-C2D	2.38	1.48	1.42
22	b	606	CLA	C1D-C2D	2.38	1.47	1.42
23	A	404	PHO	C4C-NC	2.37	1.42	1.36
26	c	519	LMG	O7-C10	2.37	1.40	1.35
26	d	410	LMG	O2-C2	-2.37	1.37	1.43
26	m	101	LMG	C4-C5	2.36	1.58	1.53
22	A	403	CLA	CAC-C3C	-2.36	1.46	1.52
28	D	413	LHG	P-O6	2.36	1.68	1.59
22	b	614	CLA	CMB-C2B	-2.36	1.46	1.51
31	b	617	BCR	C33-C5	-2.36	1.47	1.50
22	B	609	CLA	C3B-CAB	-2.35	1.43	1.47
26	b	622	LMG	O6-C1	2.35	1.47	1.41
22	c	505	CLA	CMB-C2B	-2.35	1.46	1.51
22	C	506	CLA	CMB-C2B	-2.35	1.46	1.51
22	b	611	CLA	C1D-C2D	2.34	1.47	1.42
22	c	508	CLA	C3B-CAB	-2.34	1.43	1.47
22	c	508	CLA	CMC-C2C	-2.34	1.46	1.51
22	B	608	CLA	CMB-C2B	-2.34	1.46	1.51
22	D	403	CLA	CAC-C3C	-2.33	1.46	1.52
22	b	616	CLA	C1D-C2D	2.33	1.47	1.42
22	c	501	CLA	C4B-CHC	-2.33	1.34	1.41
22	d	405	CLA	C1D-C2D	2.33	1.47	1.42
26	M	101	LMG	O7-C8	-2.33	1.40	1.46
27	B	622	SQD	O2-C2	-2.33	1.37	1.43
22	b	608	CLA	CMB-C2B	-2.33	1.46	1.51
22	B	614	CLA	MG-NA	2.33	2.11	2.06
22	c	509	CLA	C4B-CHC	-2.33	1.34	1.41
26	c	522	LMG	O6-C5	-2.33	1.38	1.44
22	b	616	CLA	MG-NA	2.33	2.11	2.06
23	a	403	PHO	CHD-C4C	-2.32	1.35	1.40
22	c	503	CLA	C3B-C2B	-2.32	1.37	1.40
23	a	403	PHO	CMB-C2B	-2.32	1.45	1.50
27	A	410	SQD	O3-C3	-2.32	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	510	CLA	CMC-C2C	-2.32	1.46	1.51
22	B	611	CLA	CAC-C3C	-2.32	1.46	1.52
22	A	403	CLA	C3B-CAB	-2.31	1.43	1.47
23	d	402	PHO	CHD-C1D	2.31	1.43	1.38
22	B	605	CLA	C1D-C2D	2.31	1.47	1.42
22	b	606	CLA	CMD-C2D	-2.30	1.46	1.51
22	C	510	CLA	CAC-C3C	-2.30	1.46	1.52
22	b	607	CLA	CMC-C2C	-2.30	1.46	1.51
22	C	510	CLA	CMD-C2D	-2.30	1.46	1.51
22	c	504	CLA	CMB-C2B	-2.30	1.46	1.51
22	D	404	CLA	CAC-C3C	-2.30	1.46	1.52
22	C	513	CLA	MG-NA	2.30	2.11	2.06
22	C	505	CLA	CMC-C2C	-2.30	1.46	1.51
22	B	608	CLA	C1D-C2D	2.29	1.47	1.42
26	Y	101	LMG	O8-C9	-2.29	1.39	1.45
22	b	611	CLA	C3B-CAB	-2.29	1.43	1.47
29	c	518	DGD	C1D-C2D	2.29	1.59	1.52
22	d	405	CLA	C4B-CHC	-2.29	1.34	1.41
22	D	405	CLA	CMC-C2C	-2.29	1.46	1.51
22	B	610	CLA	CAC-C3C	-2.29	1.46	1.52
22	b	604	CLA	CAC-C3C	-2.29	1.46	1.52
22	c	503	CLA	CMB-C2B	-2.29	1.46	1.51
22	C	510	CLA	C1D-C2D	2.29	1.47	1.42
31	a	405	BCR	C38-C26	-2.29	1.47	1.50
22	C	504	CLA	C1D-C2D	2.29	1.47	1.42
22	b	611	CLA	CAC-C3C	-2.28	1.46	1.52
22	B	612	CLA	CMC-C2C	-2.28	1.46	1.51
22	C	512	CLA	CMB-C2B	-2.28	1.46	1.51
23	a	403	PHO	C1A-NA	2.28	1.42	1.37
29	C	515	DGD	O2G-C2G	-2.28	1.40	1.46
26	c	522	LMG	C4-C3	2.27	1.58	1.52
29	c	518	DGD	C3G-C2G	2.27	1.57	1.50
22	c	512	CLA	CMC-C2C	-2.27	1.46	1.51
22	C	501	CLA	CMC-C2C	-2.27	1.46	1.51
22	c	507	CLA	CAC-C3C	-2.27	1.46	1.52
22	B	614	CLA	C1D-C2D	2.27	1.47	1.42
23	A	404	PHO	CHC-C4B	-2.26	1.35	1.40
22	b	607	CLA	CAC-C3C	-2.26	1.46	1.52
22	A	405	CLA	CMC-C2C	-2.26	1.46	1.51
22	A	402	CLA	MG-NA	2.26	2.11	2.06
22	b	603	CLA	CAC-C3C	-2.26	1.46	1.52
31	k	101	BCR	C33-C5	-2.26	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	606	CLA	C3B-C2B	-2.26	1.37	1.40
22	c	508	CLA	CMB-C2B	-2.26	1.46	1.51
22	B	615	CLA	CMD-C2D	-2.26	1.46	1.51
31	I	101	BCR	C34-C9	-2.25	1.46	1.50
22	C	503	CLA	CAC-C3C	-2.25	1.46	1.52
22	B	606	CLA	CMB-C2B	-2.25	1.47	1.51
22	B	607	CLA	CMC-C2C	-2.25	1.46	1.51
25	d	407	PL9	C26-C24	-2.25	1.46	1.51
22	B	612	CLA	C1D-C2D	2.25	1.47	1.42
27	A	412	SQD	O47-C45	-2.25	1.43	1.47
22	A	402	CLA	C1D-C2D	2.25	1.47	1.42
22	d	405	CLA	O1D-CGD	2.24	1.26	1.21
22	C	506	CLA	CMC-C2C	-2.24	1.46	1.51
22	B	607	CLA	C4B-CHC	-2.24	1.34	1.41
28	e	101	LHG	C24-C23	2.24	1.57	1.50
25	D	407	PL9	C51-C49	-2.24	1.44	1.50
22	c	513	CLA	C1D-C2D	2.24	1.47	1.42
29	C	517	DGD	O6D-C5D	-2.23	1.38	1.44
22	B	615	CLA	C3D-C2D	-2.23	1.35	1.39
22	b	602	CLA	C3B-CAB	-2.23	1.43	1.47
25	D	407	PL9	C46-C44	-2.23	1.46	1.51
22	c	509	CLA	MG-NA	2.23	2.11	2.06
22	B	613	CLA	C3B-CAB	-2.23	1.43	1.47
22	C	512	CLA	CMC-C2C	-2.23	1.46	1.51
22	b	606	CLA	O2D-CED	-2.22	1.40	1.45
22	A	403	CLA	CMC-C2C	-2.22	1.46	1.51
22	b	603	CLA	C1D-C2D	2.22	1.47	1.42
29	A	413	DGD	O5D-C1E	2.22	1.44	1.40
29	C	517	DGD	C2B-C1B	-2.22	1.44	1.50
22	C	504	CLA	CAC-C3C	-2.22	1.46	1.52
22	b	616	CLA	CMC-C2C	-2.22	1.46	1.51
22	C	504	CLA	CMD-C2D	-2.22	1.46	1.51
31	B	618	BCR	C1-C6	-2.22	1.50	1.53
22	c	510	CLA	CMD-C2D	-2.22	1.46	1.51
22	c	505	CLA	MG-NA	2.21	2.11	2.06
29	C	515	DGD	C2A-C1A	-2.21	1.44	1.50
22	a	404	CLA	CAC-C3C	-2.21	1.46	1.52
22	C	507	CLA	CMD-C2D	-2.21	1.46	1.51
25	d	407	PL9	C16-C17	2.21	1.61	1.53
22	B	611	CLA	C1D-C2D	2.21	1.47	1.42
22	c	502	CLA	C4B-CHC	-2.21	1.34	1.41
31	c	515	BCR	C30-C25	-2.21	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	404	CLA	C1D-C2D	2.21	1.47	1.42
22	c	502	CLA	CAC-C3C	-2.21	1.46	1.52
22	c	507	CLA	C3B-CAB	-2.21	1.43	1.47
22	b	607	CLA	C1D-C2D	2.21	1.47	1.42
22	B	615	CLA	CAC-C3C	-2.21	1.46	1.52
22	B	615	CLA	O2A-CGA	2.20	1.39	1.33
22	b	609	CLA	CMC-C2C	-2.20	1.46	1.51
22	B	606	CLA	C3B-CAB	-2.20	1.43	1.47
22	C	503	CLA	CMC-C2C	-2.20	1.46	1.51
22	B	610	CLA	C1D-C2D	2.20	1.47	1.42
28	d	409	LHG	C6-C5	2.20	1.57	1.50
26	Y	101	LMG	O1-C1	2.20	1.43	1.40
22	b	609	CLA	C3B-CAB	-2.20	1.43	1.47
29	H	102	DGD	C4D-C3D	2.20	1.57	1.52
22	C	507	CLA	CAC-C3C	-2.20	1.46	1.52
22	b	606	CLA	CAC-C3C	-2.20	1.46	1.52
22	B	614	CLA	CMB-C2B	-2.20	1.47	1.51
31	I	101	BCR	C38-C26	-2.19	1.47	1.50
22	C	504	CLA	O2D-CGD	2.19	1.38	1.33
26	D	408	LMG	C7-C8	2.19	1.57	1.50
22	c	512	CLA	C3B-CAB	-2.19	1.43	1.47
22	c	501	CLA	CAC-C3C	-2.19	1.46	1.52
22	C	501	CLA	C1D-C2D	2.19	1.47	1.42
29	c	516	DGD	O5D-C1E	2.18	1.43	1.40
26	Y	101	LMG	C1-C2	2.18	1.58	1.52
22	b	616	CLA	C3B-C2B	-2.18	1.37	1.40
22	B	608	CLA	O2A-CGA	2.18	1.39	1.33
31	t	101	BCR	C33-C5	-2.18	1.47	1.50
29	c	517	DGD	C3E-C2E	2.18	1.57	1.52
22	b	607	CLA	O2D-CGD	2.18	1.38	1.33
26	b	622	LMG	C4-C5	2.18	1.57	1.53
23	d	402	PHO	CHD-C4C	-2.18	1.35	1.40
23	A	404	PHO	C3B-C4B	2.18	1.47	1.43
22	b	606	CLA	C4B-CHC	-2.17	1.35	1.41
29	C	515	DGD	O1A-C1A	2.17	1.29	1.22
22	C	513	CLA	CMC-C2C	-2.17	1.46	1.51
22	B	605	CLA	C3B-C2B	-2.17	1.37	1.40
25	d	407	PL9	C10-C9	-2.17	1.45	1.50
22	b	613	CLA	C1D-C2D	2.17	1.47	1.42
22	a	404	CLA	CMD-C2D	-2.17	1.46	1.51
22	B	601	CLA	C3B-CAB	-2.17	1.43	1.47
31	x	101	BCR	C33-C5	-2.17	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	M	101	LMG	C7-C8	2.16	1.57	1.50
22	B	616	CLA	CAA-C2A	-2.16	1.50	1.54
22	c	512	CLA	CMD-C2D	-2.16	1.46	1.51
26	D	412	LMG	O8-C28	2.16	1.39	1.33
23	a	403	PHO	O2D-CGD	2.16	1.38	1.33
22	D	404	CLA	C3B-C2B	-2.16	1.37	1.40
29	C	516	DGD	O1G-C1G	-2.16	1.40	1.45
22	B	608	CLA	C3B-CAB	-2.16	1.43	1.47
29	C	516	DGD	C1G-C2G	2.16	1.57	1.50
22	B	602	CLA	CMD-C2D	-2.15	1.46	1.51
31	K	102	BCR	C27-C26	-2.15	1.46	1.51
29	c	516	DGD	O4D-C4D	-2.15	1.37	1.43
29	C	515	DGD	C1D-C2D	2.15	1.58	1.52
22	C	511	CLA	C1D-C2D	2.15	1.47	1.42
22	b	613	CLA	CMC-C2C	-2.15	1.46	1.51
22	A	402	CLA	C3D-C2D	-2.15	1.35	1.39
22	b	610	CLA	C1D-C2D	2.14	1.47	1.42
22	C	511	CLA	C1B-NB	2.14	1.37	1.35
22	C	513	CLA	C3B-CAB	-2.14	1.43	1.47
23	D	401	PHO	C4C-NC	2.14	1.41	1.36
22	c	501	CLA	CMD-C2D	-2.14	1.46	1.51
22	b	608	CLA	O2A-CGA	2.14	1.39	1.33
22	b	612	CLA	CMD-C2D	-2.14	1.46	1.51
34	f	101	HEM	C1A-CHA	-2.13	1.35	1.41
22	B	609	CLA	C1D-C2D	2.13	1.47	1.42
26	M	101	LMG	O6-C1	2.13	1.47	1.41
23	D	401	PHO	CAC-C3C	-2.13	1.45	1.51
26	c	519	LMG	O2-C2	-2.13	1.38	1.43
29	h	101	DGD	C4E-C5E	2.13	1.57	1.53
22	B	611	CLA	C3B-CAB	-2.13	1.43	1.47
22	B	610	CLA	CMC-C2C	-2.13	1.46	1.51
22	b	604	CLA	CMB-C2B	-2.13	1.47	1.51
22	c	502	CLA	C3B-CAB	-2.13	1.43	1.47
26	m	101	LMG	C6-C5	2.12	1.59	1.51
22	d	403	CLA	C1C-C2C	2.12	1.47	1.42
27	D	409	SQD	O3-C3	-2.12	1.38	1.43
22	a	404	CLA	CMC-C2C	-2.12	1.46	1.51
22	C	513	CLA	C4B-CHC	-2.12	1.35	1.41
22	c	505	CLA	C3B-CAB	-2.12	1.43	1.47
31	x	101	BCR	C1-C6	-2.12	1.50	1.53
22	B	608	CLA	C4B-CHC	-2.12	1.35	1.41
31	t	101	BCR	C27-C26	-2.12	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	516	DGD	C2B-C1B	-2.12	1.44	1.50
22	C	509	CLA	CAC-C3C	-2.12	1.47	1.52
22	B	603	CLA	CMC-C2C	-2.11	1.46	1.51
29	c	518	DGD	O4D-C4D	-2.11	1.38	1.43
22	B	603	CLA	CAC-C3C	-2.11	1.47	1.52
29	H	102	DGD	C1G-C2G	2.11	1.57	1.50
26	c	519	LMG	O1-C1	2.11	1.43	1.40
22	d	403	CLA	C4B-CHC	-2.11	1.35	1.41
22	C	504	CLA	MG-NA	-2.11	2.01	2.06
31	a	405	BCR	C33-C5	-2.11	1.47	1.50
22	C	508	CLA	CAC-C3C	-2.11	1.47	1.52
22	b	601	CLA	CMC-C2C	-2.10	1.46	1.51
22	b	610	CLA	CMC-C2C	-2.10	1.46	1.51
31	T	101	BCR	C1-C6	-2.10	1.50	1.53
28	A	411	LHG	O7-C5	-2.10	1.41	1.46
22	C	503	CLA	C3B-C2B	-2.10	1.37	1.40
29	c	517	DGD	O2G-C2G	-2.10	1.41	1.46
22	c	507	CLA	CMD-C2D	-2.10	1.46	1.51
22	b	616	CLA	CAC-C3C	-2.10	1.47	1.52
22	d	404	CLA	CMD-C2D	-2.10	1.46	1.51
31	T	101	BCR	C38-C26	-2.10	1.47	1.50
28	d	408	LHG	P-O3	2.09	1.67	1.59
22	B	609	CLA	CAC-C3C	-2.09	1.47	1.52
23	A	404	PHO	O2D-CGD	2.09	1.38	1.33
22	d	403	CLA	C3B-C2B	-2.09	1.37	1.40
22	b	614	CLA	C1B-NB	-2.09	1.33	1.35
22	B	602	CLA	C1B-NB	2.09	1.37	1.35
34	F	101	HEM	CAD-C3D	2.09	1.55	1.52
22	b	612	CLA	C1C-C2C	2.09	1.47	1.42
22	c	513	CLA	CAC-C3C	-2.09	1.47	1.52
22	C	506	CLA	C3B-CAB	-2.09	1.43	1.47
22	C	511	CLA	C4B-CHC	-2.09	1.35	1.41
22	b	605	CLA	C4B-CHC	-2.08	1.35	1.41
22	b	601	CLA	CMD-C2D	-2.08	1.46	1.51
22	B	615	CLA	C1D-C2D	2.08	1.47	1.42
31	c	515	BCR	C35-C13	-2.08	1.46	1.50
22	a	402	CLA	CAC-C3C	-2.08	1.47	1.52
22	b	612	CLA	C3B-CAB	-2.08	1.43	1.47
22	b	610	CLA	C1A-CHA	-2.08	1.34	1.43
22	D	405	CLA	C1D-C2D	2.08	1.47	1.42
22	B	606	CLA	CMD-C2D	-2.08	1.46	1.51
22	b	608	CLA	CMC-C2C	-2.08	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	404	CLA	C1D-C2D	2.08	1.47	1.42
22	B	605	CLA	C5-C3	-2.07	1.47	1.51
31	K	101	BCR	C33-C5	-2.07	1.47	1.50
22	d	403	CLA	CMC-C2C	-2.07	1.46	1.51
22	B	607	CLA	C1C-C2C	2.07	1.47	1.42
25	D	407	PL9	C2-C1	2.07	1.50	1.44
22	C	511	CLA	CMD-C2D	-2.07	1.46	1.51
22	b	602	CLA	C1D-C2D	2.07	1.47	1.42
25	d	407	PL9	C46-C44	-2.07	1.47	1.51
31	B	619	BCR	C33-C5	-2.07	1.47	1.50
22	b	610	CLA	CMB-C2B	-2.07	1.47	1.51
22	C	508	CLA	CMC-C2C	-2.06	1.46	1.51
26	B	626	LMG	O7-C10	2.06	1.40	1.34
22	C	506	CLA	CAA-C2A	-2.06	1.50	1.54
29	A	413	DGD	C3D-C2D	2.06	1.57	1.52
22	B	604	CLA	CMB-C2B	-2.06	1.47	1.51
22	c	510	CLA	C1D-C2D	2.06	1.47	1.42
22	d	404	CLA	C1B-NB	2.06	1.37	1.35
22	B	601	CLA	CMC-C2C	-2.06	1.46	1.51
25	a	409	PL9	C6-C1	-2.05	1.44	1.48
22	D	404	CLA	O2D-CED	-2.05	1.40	1.45
22	C	507	CLA	C1C-C2C	2.05	1.47	1.42
22	A	405	CLA	CMA-C3A	-2.05	1.48	1.53
22	D	404	CLA	CMD-C2D	-2.05	1.46	1.51
31	k	102	BCR	C33-C5	-2.05	1.47	1.50
22	b	615	CLA	CMC-C2C	-2.05	1.46	1.51
22	C	504	CLA	C4B-CHC	-2.05	1.35	1.41
31	B	618	BCR	C35-C13	-2.05	1.46	1.50
22	b	608	CLA	CMA-C3A	-2.05	1.48	1.53
27	L	101	SQD	O2-C2	-2.05	1.38	1.43
26	B	626	LMG	C7-C8	2.04	1.57	1.50
22	B	612	CLA	CMD-C2D	-2.04	1.46	1.51
22	b	613	CLA	CAA-C2A	-2.04	1.50	1.54
22	b	609	CLA	C3B-C2B	-2.04	1.37	1.40
26	B	626	LMG	O1-C7	2.04	1.47	1.43
31	c	515	BCR	C27-C26	-2.04	1.47	1.51
22	c	502	CLA	C3B-C2B	-2.04	1.37	1.40
22	b	614	CLA	CAC-C3C	-2.04	1.47	1.52
22	c	510	CLA	O2D-CGD	2.03	1.38	1.33
23	A	404	PHO	CMB-C2B	-2.03	1.46	1.50
29	C	515	DGD	C4D-C3D	2.03	1.57	1.52
22	C	509	CLA	O2D-CGD	2.03	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	d	403	CLA	MG-NA	-2.03	2.01	2.06
22	b	607	CLA	MG-NA	2.03	2.11	2.06
22	b	602	CLA	C4B-CHC	-2.03	1.35	1.41
22	b	607	CLA	C3B-CAB	-2.03	1.43	1.47
25	d	407	PL9	C6-C1	-2.03	1.45	1.48
22	b	614	CLA	C1A-CHA	-2.03	1.34	1.43
22	D	403	CLA	C4B-CHC	-2.02	1.35	1.41
22	B	614	CLA	C4B-CHC	-2.02	1.35	1.41
26	B	626	LMG	O8-C9	-2.02	1.40	1.45
22	C	505	CLA	C1D-C2D	2.02	1.47	1.42
22	C	506	CLA	O2D-CGD	2.02	1.38	1.33
22	D	403	CLA	CMB-C2B	-2.02	1.47	1.51
22	B	610	CLA	CMD-C2D	-2.02	1.46	1.51
26	Y	101	LMG	C6-C5	2.02	1.58	1.51
26	b	622	LMG	C1-C2	2.01	1.58	1.52
29	C	517	DGD	C2A-C1A	-2.01	1.44	1.50
35	v	201	HEC	C1D-CHD	-2.01	1.35	1.41
22	C	511	CLA	CMC-C2C	-2.01	1.46	1.51
22	B	606	CLA	C1C-C2C	2.01	1.47	1.42
22	c	506	CLA	CMD-C2D	-2.01	1.46	1.51
22	b	612	CLA	C3B-C2B	-2.01	1.37	1.40
22	b	613	CLA	CAC-C3C	-2.01	1.47	1.52
35	v	201	HEC	C3B-C4B	2.00	1.46	1.43
22	c	510	CLA	CAC-C3C	-2.00	1.47	1.52
28	D	410	LHG	C8-C7	-2.00	1.44	1.50
22	b	605	CLA	C1A-CHA	-2.00	1.34	1.43
22	c	502	CLA	MG-NA	2.00	2.11	2.06
22	A	402	CLA	CMB-C2B	-2.00	1.47	1.51

All (1336) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	503	CLA	C4A-NA-C1A	9.61	111.03	106.71
22	c	511	CLA	C4A-NA-C1A	9.46	110.96	106.71
27	L	101	SQD	O6-C1-C2	9.05	122.43	108.30
22	C	511	CLA	C4A-NA-C1A	8.63	110.59	106.71
22	C	510	CLA	C4A-NA-C1A	8.48	110.52	106.71
22	a	402	CLA	C4A-NA-C1A	8.22	110.40	106.71
22	B	604	CLA	C4A-NA-C1A	8.05	110.32	106.71
22	c	501	CLA	C4A-NA-C1A	7.73	110.18	106.71
22	C	507	CLA	C4A-NA-C1A	7.24	109.96	106.71
22	d	404	CLA	C4A-NA-C1A	7.13	109.91	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	609	CLA	C4A-NA-C1A	7.02	109.86	106.71
22	C	501	CLA	C4A-NA-C1A	7.00	109.85	106.71
27	A	410	SQD	O6-C1-C2	6.99	119.21	108.30
22	B	601	CLA	C4A-NA-C1A	6.98	109.84	106.71
22	B	611	CLA	CMB-C2B-C1B	-6.87	117.90	128.46
22	B	616	CLA	C4A-NA-C1A	6.87	109.80	106.71
27	B	622	SQD	O6-C1-C2	6.84	118.98	108.30
22	b	606	CLA	C4A-NA-C1A	6.75	109.74	106.71
27	A	410	SQD	O7-S-C6	6.59	114.77	106.94
27	B	622	SQD	O7-S-C6	6.56	114.73	106.94
22	B	612	CLA	C4A-NA-C1A	6.49	109.62	106.71
22	b	601	CLA	C4A-NA-C1A	6.45	109.61	106.71
22	C	502	CLA	C4A-NA-C1A	6.43	109.60	106.71
27	D	409	SQD	O8-S-C6	6.43	115.99	105.74
22	A	402	CLA	C4A-NA-C1A	6.41	109.59	106.71
22	B	615	CLA	C4A-NA-C1A	6.39	109.58	106.71
22	b	612	CLA	C4A-NA-C1A	6.27	109.53	106.71
22	b	603	CLA	O2D-CGD-O1D	-6.23	111.66	123.84
22	c	507	CLA	C4A-NA-C1A	6.17	109.48	106.71
22	B	610	CLA	C4A-NA-C1A	6.14	109.47	106.71
22	C	513	CLA	C4A-NA-C1A	6.06	109.43	106.71
22	B	606	CLA	C4A-NA-C1A	6.02	109.41	106.71
27	f	102	SQD	O7-S-C6	6.00	114.06	106.94
22	c	502	CLA	C4D-C3D-CAD	-5.95	105.15	108.47
25	a	409	PL9	C7-C3-C4	5.93	121.69	116.88
22	B	607	CLA	C4A-NA-C1A	5.90	109.36	106.71
22	b	613	CLA	CMB-C2B-C1B	-5.78	119.59	128.46
22	C	512	CLA	C4A-NA-C1A	5.77	109.30	106.71
22	C	508	CLA	C4A-NA-C1A	5.74	109.28	106.71
27	D	409	SQD	O9-S-C6	5.72	113.74	106.94
27	a	411	SQD	O6-C1-C2	5.72	117.23	108.30
22	b	613	CLA	C4A-NA-C1A	5.70	109.27	106.71
35	v	201	HEC	CMC-C2C-C1C	-5.61	119.84	128.46
22	c	506	CLA	C4A-NA-C1A	5.60	109.22	106.71
22	B	611	CLA	CMB-C2B-C3B	5.59	135.14	124.68
22	b	603	CLA	C4A-NA-C1A	5.56	109.20	106.71
22	b	606	CLA	O2D-CGD-O1D	-5.54	113.01	123.84
22	d	405	CLA	CMB-C2B-C1B	-5.53	119.96	128.46
22	b	615	CLA	C4A-NA-C1A	5.53	109.19	106.71
22	C	505	CLA	CMB-C2B-C1B	-5.51	120.00	128.46
27	f	102	SQD	O9-S-C6	5.51	113.48	106.94
27	D	409	SQD	O6-C1-C2	5.50	116.89	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	614	CLA	C4A-NA-C1A	5.40	109.13	106.71
22	b	616	CLA	O2D-CGD-O1D	-5.38	113.32	123.84
29	H	102	DGD	O3G-C3G-C2G	-5.28	98.17	110.90
27	f	102	SQD	O6-C1-C2	5.26	116.51	108.30
34	f	101	HEM	CBD-CAD-C3D	-5.23	102.85	112.48
22	B	602	CLA	O2D-CGD-CBD	5.18	120.48	111.27
22	b	603	CLA	OBD-CAD-CBD	-5.15	118.54	125.89
22	D	404	CLA	C4A-NA-C1A	5.10	109.00	106.71
22	b	605	CLA	C4A-NA-C1A	5.09	109.00	106.71
22	B	610	CLA	O2D-CGD-O1D	-5.09	113.89	123.84
22	c	509	CLA	C4A-NA-C1A	5.08	108.99	106.71
22	B	611	CLA	C4A-NA-C1A	5.07	108.98	106.71
35	v	201	HEC	CBD-CAD-C3D	-5.03	103.20	112.49
22	b	611	CLA	C4A-NA-C1A	5.03	108.97	106.71
22	b	616	CLA	C4A-NA-C1A	5.01	108.96	106.71
22	b	612	CLA	CMB-C2B-C1B	-4.98	120.81	128.46
29	C	517	DGD	O3G-C3G-C2G	-4.95	98.95	110.90
25	A	408	PL9	C7-C3-C4	4.90	120.86	116.88
22	B	605	CLA	O2D-CGD-O1D	-4.84	114.37	123.84
27	a	411	SQD	O8-S-C6	4.82	113.42	105.74
22	b	609	CLA	C4A-NA-C1A	4.81	108.87	106.71
22	d	403	CLA	C4A-NA-C1A	4.81	108.87	106.71
22	c	510	CLA	CMB-C2B-C1B	-4.81	121.08	128.46
22	d	405	CLA	CMB-C2B-C3B	4.79	133.63	124.68
22	C	508	CLA	CMB-C2B-C1B	-4.78	121.11	128.46
27	L	101	SQD	O7-S-C6	4.78	112.62	106.94
22	C	510	CLA	CMB-C2B-C1B	-4.78	121.12	128.46
22	C	509	CLA	CMB-C2B-C1B	-4.77	121.14	128.46
22	B	613	CLA	CMB-C2B-C1B	-4.76	121.15	128.46
35	V	201	HEC	CAD-CBD-CGD	-4.75	104.70	112.67
27	B	622	SQD	O47-C7-C8	4.72	121.68	111.50
22	c	505	CLA	O2D-CGD-O1D	-4.71	114.63	123.84
22	c	501	CLA	O2D-CGD-O1D	-4.69	114.67	123.84
22	b	602	CLA	C4A-NA-C1A	4.69	108.81	106.71
22	b	604	CLA	C4A-NA-C1A	4.68	108.81	106.71
22	B	612	CLA	CMB-C2B-C1B	-4.67	121.28	128.46
22	C	513	CLA	O2D-CGD-O1D	-4.63	114.79	123.84
22	c	501	CLA	CMB-C2B-C1B	-4.63	121.36	128.46
34	F	101	HEM	CBD-CAD-C3D	-4.62	103.96	112.48
22	A	402	CLA	CMB-C2B-C1B	-4.62	121.36	128.46
27	A	412	SQD	C45-O47-C7	4.62	123.82	117.88
22	b	603	CLA	O2D-CGD-CBD	4.60	119.44	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	603	CLA	O2D-CGD-O1D	-4.59	114.86	123.84
22	C	509	CLA	C4A-NA-C1A	4.59	108.77	106.71
25	D	407	PL9	C7-C3-C4	4.58	120.60	116.88
22	B	604	CLA	CMB-C2B-C1B	-4.58	121.43	128.46
35	V	201	HEC	CMC-C2C-C1C	-4.56	121.45	128.46
22	C	504	CLA	CMB-C2B-C1B	-4.55	121.48	128.46
22	B	607	CLA	CMB-C2B-C1B	-4.55	121.48	128.46
22	c	509	CLA	O2A-CGA-O1A	-4.54	112.13	123.59
22	A	403	CLA	CMB-C2B-C1B	-4.46	121.61	128.46
22	b	615	CLA	CMB-C2B-C1B	-4.45	121.63	128.46
22	d	404	CLA	CMB-C2B-C1B	-4.44	121.65	128.46
22	b	607	CLA	CMB-C2B-C1B	-4.43	121.66	128.46
22	b	604	CLA	OBD-CAD-CBD	-4.42	119.58	125.89
22	b	604	CLA	CMB-C2B-C1B	-4.41	121.68	128.46
22	B	611	CLA	O2D-CGD-O1D	-4.40	115.23	123.84
27	B	622	SQD	C3-C4-C5	4.40	118.09	110.24
22	B	608	CLA	CMB-C2B-C1B	-4.38	121.73	128.46
22	B	603	CLA	C4D-C3D-CAD	-4.36	106.04	108.47
27	t	102	SQD	O47-C7-C8	4.36	120.89	111.50
22	C	506	CLA	OBD-CAD-CBD	-4.35	119.68	125.89
22	b	602	CLA	O2D-CGD-O1D	-4.33	115.37	123.84
28	D	413	LHG	O4-P-O5	4.32	133.60	112.24
35	v	201	HEC	CBA-CAA-C2A	-4.31	104.53	112.48
22	b	609	CLA	CMB-C2B-C1B	-4.30	121.86	128.46
27	A	410	SQD	O47-C7-C8	4.29	120.74	111.50
22	b	614	CLA	CMB-C2B-C1B	-4.28	121.88	128.46
22	b	606	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
28	A	411	LHG	O4-P-O5	4.26	133.29	112.24
22	b	601	CLA	CMB-C2B-C1B	-4.24	121.95	128.46
22	B	604	CLA	O2A-CGA-O1A	-4.23	112.92	123.59
22	C	505	CLA	CMB-C2B-C3B	4.22	132.58	124.68
22	B	612	CLA	CMB-C2B-C3B	4.21	132.55	124.68
29	C	516	DGD	O3G-C3G-C2G	-4.21	100.74	110.90
29	h	101	DGD	C3D-C4D-C5D	-4.20	102.75	110.24
22	A	405	CLA	C4A-NA-C1A	4.20	108.59	106.71
22	C	507	CLA	CMB-C2B-C1B	-4.18	122.03	128.46
22	b	606	CLA	O2D-CGD-CBD	4.18	118.69	111.27
22	b	607	CLA	C4A-NA-C1A	4.18	108.58	106.71
28	d	408	LHG	O4-P-O5	4.18	132.89	112.24
28	D	411	LHG	O4-P-O5	4.17	132.88	112.24
22	b	613	CLA	CMB-C2B-C3B	4.15	132.45	124.68
27	L	101	SQD	C1-C2-C3	-4.15	101.35	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	e	101	LHG	O4-P-O5	4.15	132.75	112.24
28	d	409	LHG	O4-P-O5	4.14	132.69	112.24
22	c	509	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
22	c	513	CLA	C4A-NA-C1A	4.12	108.56	106.71
27	A	410	SQD	O9-S-O7	-4.10	99.75	113.95
22	b	616	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
22	c	502	CLA	CMB-C2B-C3B	4.10	132.35	124.68
35	v	201	HEC	C1D-C2D-C3D	-4.10	104.14	107.00
22	C	506	CLA	C4A-NA-C1A	4.07	108.54	106.71
22	D	405	CLA	O2D-CGD-O1D	-4.07	115.87	123.84
22	D	404	CLA	CMB-C2B-C1B	-4.07	122.20	128.46
22	b	612	CLA	CMB-C2B-C3B	4.05	132.26	124.68
29	C	517	DGD	C4D-C3D-C2D	-4.04	103.78	110.82
31	B	618	BCR	C37-C22-C21	-4.03	117.27	122.92
35	V	201	HEC	CMB-C2B-C1B	-4.03	122.27	128.46
25	d	407	PL9	C40-C39-C41	4.03	122.05	115.27
22	c	504	CLA	CMB-C2B-C1B	-4.02	122.29	128.46
25	A	408	PL9	O1-C4-C3	-4.02	116.30	120.72
22	B	615	CLA	C1B-CHB-C4A	-4.01	122.18	130.12
28	D	410	LHG	O4-P-O5	4.00	132.03	112.24
22	b	605	CLA	O2D-CGD-O1D	-4.00	116.02	123.84
22	B	603	CLA	OBD-CAD-CBD	-4.00	120.18	125.89
22	C	512	CLA	CHB-C4A-NA	4.00	130.04	124.51
22	c	512	CLA	C4A-NA-C1A	3.99	108.50	106.71
22	d	403	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
34	f	101	HEM	CBA-CAA-C2A	-3.98	105.14	112.49
22	b	604	CLA	C1-C2-C3	-3.98	119.17	126.04
22	c	509	CLA	CMB-C2B-C3B	3.97	132.11	124.68
22	c	510	CLA	C4A-NA-C1A	3.97	108.49	106.71
22	c	502	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
29	c	517	DGD	O3G-C3G-C2G	-3.95	101.36	110.90
25	a	409	PL9	C7-C3-C2	-3.95	118.10	123.30
28	a	410	LHG	O4-P-O5	3.94	131.74	112.24
22	B	608	CLA	CMB-C2B-C3B	3.94	132.05	124.68
35	V	201	HEC	C1D-C2D-C3D	-3.94	104.25	107.00
22	a	404	CLA	CHB-C4A-NA	3.94	129.96	124.51
22	C	506	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
22	c	505	CLA	O2D-CGD-CBD	3.92	118.23	111.27
22	C	510	CLA	CMB-C2B-C3B	3.91	132.00	124.68
25	D	407	PL9	C36-C34-C33	-3.91	113.20	121.12
22	C	510	CLA	O2D-CGD-O1D	-3.90	116.21	123.84
22	C	502	CLA	C4D-C3D-CAD	-3.90	106.29	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	617	BCR	C2-C1-C6	3.90	116.48	110.48
25	A	408	PL9	C36-C34-C33	-3.90	113.23	121.12
22	C	509	CLA	CMB-C2B-C3B	3.89	131.96	124.68
22	C	511	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
35	V	201	HEC	CBD-CAD-C3D	-3.89	105.31	112.49
22	c	510	CLA	CMB-C2B-C3B	3.88	131.93	124.68
22	c	507	CLA	O2A-CGA-O1A	-3.85	113.87	123.59
27	f	102	SQD	O9-S-O7	-3.85	100.64	113.95
22	B	604	CLA	CMB-C2B-C3B	3.84	131.85	124.68
22	c	506	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
22	D	403	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
27	A	412	SQD	O47-C7-C8	3.81	119.72	111.50
22	B	602	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
22	C	507	CLA	O2D-CGD-O1D	-3.81	116.39	123.84
26	c	522	LMG	C1-C2-C3	3.79	117.90	110.00
22	b	605	CLA	C4D-C3D-CAD	-3.79	106.36	108.47
22	b	616	CLA	CMB-C2B-C3B	3.79	131.76	124.68
22	c	505	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
22	A	402	CLA	CHB-C4A-NA	3.77	129.73	124.51
31	Z	101	BCR	C15-C16-C17	-3.76	115.77	123.47
22	B	604	CLA	O2D-CGD-O1D	-3.76	116.48	123.84
31	b	618	BCR	C36-C18-C17	-3.76	117.66	122.92
22	C	507	CLA	C4-C3-C5	3.76	121.59	115.27
28	l	101	LHG	O4-P-O5	3.76	130.81	112.24
22	C	507	CLA	CMB-C2B-C3B	3.75	131.69	124.68
22	C	509	CLA	C4D-C3D-CAD	-3.74	106.38	108.47
22	c	509	CLA	O2D-CGD-O1D	-3.74	116.52	123.84
22	b	616	CLA	OBD-CAD-CBD	-3.74	120.55	125.89
22	c	508	CLA	C4A-NA-C1A	3.73	108.39	106.71
22	b	601	CLA	CHB-C4A-NA	3.73	129.67	124.51
28	L	102	LHG	O4-P-O5	3.73	130.69	112.24
22	c	507	CLA	O2D-CGD-O1D	-3.73	116.54	123.84
22	b	602	CLA	O2D-CGD-CBD	3.73	117.89	111.27
34	F	101	HEM	CBA-CAA-C2A	-3.73	105.61	112.49
22	c	504	CLA	OBD-CAD-CBD	-3.72	120.57	125.89
29	c	517	DGD	C3E-C4E-C5E	-3.72	103.59	110.24
27	L	101	SQD	O5-C5-C4	3.72	116.46	109.69
22	A	403	CLA	O2D-CGD-O1D	-3.72	116.56	123.84
22	a	402	CLA	O1D-CGD-CBD	3.72	132.09	124.48
22	D	405	CLA	C1B-CHB-C4A	-3.72	122.75	130.12
26	c	519	LMG	O6-C1-O1	-3.72	101.17	109.97
22	A	403	CLA	C4A-NA-C1A	3.71	108.38	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	503	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
31	d	406	BCR	C38-C26-C25	-3.71	120.36	124.53
26	b	622	LMG	C1-O6-C5	-3.71	106.41	113.69
22	B	609	CLA	OBD-CAD-CBD	-3.71	120.60	125.89
22	C	512	CLA	O2D-CGD-O1D	-3.70	116.60	123.84
27	L	101	SQD	O48-C23-C24	3.69	123.49	111.91
31	B	618	BCR	C29-C30-C25	3.69	116.16	110.48
22	C	502	CLA	CMD-C2D-C3D	3.69	131.58	124.68
22	b	610	CLA	C1B-CHB-C4A	-3.69	122.81	130.12
22	c	513	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
22	b	616	CLA	O1D-CGD-CBD	3.68	132.01	124.48
29	h	101	DGD	C4D-C3D-C2D	-3.68	104.40	110.82
31	b	617	BCR	C2-C1-C6	3.67	116.13	110.48
22	B	613	CLA	CMB-C2B-C3B	3.67	131.54	124.68
22	b	608	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
22	A	405	CLA	O2D-CGD-CBD	3.66	117.77	111.27
26	m	101	LMG	O3-C3-C2	-3.66	101.89	110.35
22	C	508	CLA	CMB-C2B-C3B	3.65	131.52	124.68
22	C	502	CLA	O1D-CGD-CBD	3.65	131.95	124.48
22	b	612	CLA	O2A-CGA-O1A	-3.65	114.39	123.59
22	c	512	CLA	C1-C2-C3	-3.65	119.74	126.04
27	a	411	SQD	O9-S-C6	3.63	111.26	106.94
22	c	503	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
34	F	101	HEM	C1D-C2D-C3D	3.62	109.51	107.00
22	d	401	CLA	CHB-C4A-NA	3.61	129.51	124.51
22	b	613	CLA	CHB-C4A-NA	3.61	129.50	124.51
25	d	407	PL9	C22-C23-C24	-3.60	118.98	127.66
22	B	607	CLA	CMB-C2B-C3B	3.60	131.42	124.68
22	b	603	CLA	C4D-C3D-CAD	-3.60	106.46	108.47
22	B	613	CLA	C1B-CHB-C4A	-3.60	122.99	130.12
22	A	405	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
22	b	607	CLA	CMB-C2B-C3B	3.59	131.39	124.68
22	b	604	CLA	CMB-C2B-C3B	3.59	131.39	124.68
22	B	604	CLA	CHB-C4A-NA	3.59	129.47	124.51
22	b	613	CLA	O2D-CGD-O1D	-3.58	116.83	123.84
22	C	509	CLA	CMD-C2D-C3D	3.58	131.38	124.68
22	B	602	CLA	O2D-CGD-O1D	-3.58	116.84	123.84
22	C	509	CLA	OBD-CAD-CBD	-3.58	120.78	125.89
22	b	611	CLA	O2D-CGD-O1D	-3.57	116.86	123.84
26	B	626	LMG	C1-C2-C3	-3.57	102.56	110.00
22	B	615	CLA	CHB-C4A-NA	3.57	129.45	124.51
22	B	611	CLA	O2D-CGD-CBD	3.57	117.61	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	512	CLA	O2D-CGD-O1D	-3.56	116.87	123.84
22	D	403	CLA	O2A-CGA-O1A	-3.56	114.62	123.59
27	A	410	SQD	O5-C1-C2	-3.55	102.83	110.35
22	B	616	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
29	c	517	DGD	O6D-C1D-O3G	-3.54	101.59	109.97
22	B	614	CLA	C4A-NA-C1A	3.54	108.30	106.71
26	m	101	LMG	O1-C7-C8	-3.54	102.36	110.90
22	C	513	CLA	O1D-CGD-CBD	3.54	131.72	124.48
22	C	513	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
22	C	505	CLA	CMD-C2D-C3D	3.53	131.29	124.68
27	B	622	SQD	O48-C23-C24	3.53	122.99	111.91
22	c	502	CLA	O2D-CGD-O1D	-3.53	116.94	123.84
22	C	505	CLA	C4D-C3D-CAD	-3.52	106.51	108.47
22	c	502	CLA	C4A-NA-C1A	3.51	108.29	106.71
22	A	403	CLA	CMB-C2B-C3B	3.51	131.24	124.68
22	B	604	CLA	C6-C7-C8	-3.51	104.58	115.92
22	B	602	CLA	C1B-CHB-C4A	-3.51	123.17	130.12
22	b	603	CLA	CMB-C2B-C1B	-3.51	123.08	128.46
31	x	101	BCR	C27-C26-C25	3.50	127.82	122.73
22	b	602	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
22	b	615	CLA	CMD-C2D-C3D	3.50	131.22	124.68
27	L	101	SQD	O8-S-C6	3.50	111.31	105.74
22	C	501	CLA	O2D-CGD-CBD	3.50	117.48	111.27
22	c	501	CLA	CMD-C2D-C3D	3.49	131.22	124.68
27	t	102	SQD	O48-C23-O10	-3.49	114.78	123.59
29	c	518	DGD	O3G-C3G-C2G	-3.49	102.49	110.90
22	c	503	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
22	B	610	CLA	O2A-CGA-O1A	-3.48	114.82	123.59
22	c	501	CLA	C4D-C3D-CAD	-3.48	106.53	108.47
22	b	608	CLA	CMB-C2B-C3B	3.48	131.18	124.68
22	c	501	CLA	CMB-C2B-C3B	3.47	131.17	124.68
22	A	405	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
35	v	201	HEC	CMB-C2B-C1B	-3.46	123.14	128.46
22	b	603	CLA	OBD-CAD-C3D	3.46	133.73	127.98
23	d	402	PHO	CMB-C2B-C1B	-3.45	119.75	125.06
22	D	403	CLA	C4-C3-C5	3.45	121.07	115.27
29	C	516	DGD	C1D-C2D-C3D	-3.44	102.82	110.00
22	b	605	CLA	C4-C3-C5	3.44	121.06	115.27
22	c	509	CLA	CHB-C4A-NA	3.44	129.26	124.51
22	C	503	CLA	C4D-C3D-CAD	-3.44	106.55	108.47
22	c	512	CLA	C4D-C3D-CAD	-3.43	106.56	108.47
26	d	410	LMG	O6-C1-O1	-3.43	101.86	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	605	CLA	O1D-CGD-CBD	3.43	131.49	124.48
22	B	603	CLA	C4A-NA-C1A	3.43	108.25	106.71
29	c	517	DGD	O6E-C1E-O5D	-3.42	101.87	109.97
29	c	518	DGD	O6D-C1D-O3G	-3.42	101.87	109.97
22	c	504	CLA	CMB-C2B-C3B	3.42	131.08	124.68
22	D	404	CLA	C1B-CHB-C4A	-3.42	123.34	130.12
27	D	409	SQD	O8-S-O9	-3.42	102.92	111.27
31	a	405	BCR	C37-C22-C21	-3.41	118.14	122.92
23	a	403	PHO	CMB-C2B-C1B	-3.41	119.81	125.06
31	B	619	BCR	C2-C1-C6	3.41	115.73	110.48
22	B	612	CLA	O2D-CGD-O1D	-3.40	117.19	123.84
22	b	610	CLA	C4D-C3D-CAD	-3.40	106.58	108.47
22	B	616	CLA	C1B-CHB-C4A	-3.39	123.39	130.12
22	b	602	CLA	CHB-C4A-NA	3.39	129.20	124.51
29	A	413	DGD	O5D-C1E-C2E	3.39	113.59	108.30
22	D	404	CLA	CMB-C2B-C3B	3.39	131.02	124.68
31	C	514	BCR	C15-C16-C17	-3.39	116.54	123.47
34	F	101	HEM	CMD-C2D-C1D	-3.38	123.27	128.46
22	c	504	CLA	OBD-CAD-C3D	3.38	133.59	127.98
22	c	508	CLA	O2A-CGA-O1A	-3.38	115.06	123.59
22	c	501	CLA	CED-O2D-CGD	-3.37	108.31	115.94
22	B	614	CLA	CMD-C2D-C3D	3.36	130.96	124.68
22	a	402	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
22	b	610	CLA	CMD-C2D-C3D	3.35	130.95	124.68
22	b	616	CLA	C1B-CHB-C4A	-3.35	123.49	130.12
26	c	522	LMG	C1-O6-C5	-3.34	107.12	113.69
27	a	411	SQD	C1-C2-C3	-3.34	103.03	110.00
22	d	405	CLA	O2A-CGA-O1A	-3.34	115.17	123.59
22	C	505	CLA	OBD-CAD-CBD	-3.34	121.13	125.89
22	C	502	CLA	O2D-CGD-O1D	-3.33	117.32	123.84
27	L	101	SQD	O9-S-C6	3.33	110.89	106.94
22	C	506	CLA	OBD-CAD-C3D	3.33	133.50	127.98
31	c	514	BCR	C37-C22-C21	-3.32	118.27	122.92
29	H	102	DGD	O2D-C2D-C1D	-3.32	101.98	110.05
22	A	405	CLA	CMB-C2B-C3B	3.32	130.89	124.68
22	C	506	CLA	CMB-C2B-C3B	3.31	130.87	124.68
22	C	508	CLA	CMC-C2C-C3C	3.31	131.18	124.94
26	A	409	LMG	O6-C1-O1	-3.31	102.15	109.97
22	B	602	CLA	CHB-C4A-NA	3.30	129.08	124.51
25	D	407	PL9	C40-C39-C41	3.30	120.83	115.27
22	B	614	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
22	A	402	CLA	CMB-C2B-C3B	3.30	130.85	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	404	CLA	O2A-CGA-O1A	-3.30	115.27	123.59
31	C	514	BCR	C36-C18-C17	-3.29	118.31	122.92
22	c	505	CLA	CMB-C2B-C3B	3.29	130.84	124.68
31	b	619	BCR	C37-C22-C21	-3.29	118.31	122.92
22	b	605	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
29	C	515	DGD	O6D-C1D-O3G	-3.29	102.19	109.97
31	B	619	BCR	C38-C26-C25	-3.28	120.84	124.53
22	b	605	CLA	OBD-CAD-CBD	-3.28	121.21	125.89
31	B	619	BCR	C29-C30-C25	3.27	115.52	110.48
22	b	613	CLA	C1B-CHB-C4A	-3.27	123.65	130.12
22	C	507	CLA	CHB-C4A-NA	3.27	129.03	124.51
23	A	404	PHO	C1-C2-C3	-3.26	120.40	126.04
22	C	504	CLA	CMB-C2B-C3B	3.26	130.78	124.68
22	b	602	CLA	CMB-C2B-C3B	3.26	130.77	124.68
31	B	619	BCR	C36-C18-C17	-3.25	118.37	122.92
22	b	609	CLA	O1D-CGD-CBD	3.25	131.13	124.48
22	B	601	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
23	A	404	PHO	C1B-NB-C4B	3.25	112.62	106.51
22	b	609	CLA	CMB-C2B-C3B	3.24	130.75	124.68
22	D	405	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
22	C	509	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
31	T	101	BCR	C7-C8-C9	-3.24	121.34	126.23
31	B	617	BCR	C37-C22-C23	3.24	123.18	118.08
22	B	616	CLA	CMB-C2B-C3B	3.24	130.73	124.68
25	A	408	PL9	C7-C3-C2	-3.23	119.05	123.30
22	B	613	CLA	CHB-C4A-NA	3.23	128.98	124.51
22	b	611	CLA	O2D-CGD-CBD	3.22	117.00	111.27
22	B	604	CLA	C4-C3-C5	3.22	120.69	115.27
22	b	615	CLA	C1B-CHB-C4A	-3.22	123.75	130.12
27	L	101	SQD	C3-C4-C5	3.21	115.96	110.24
22	B	603	CLA	C4-C3-C5	3.20	120.66	115.27
26	c	522	LMG	O6-C1-O1	-3.20	102.40	109.97
22	b	614	CLA	O2A-CGA-O1A	-3.19	115.53	123.59
22	B	605	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
27	a	411	SQD	C1-O5-C5	-3.19	107.43	113.69
27	t	102	SQD	O48-C23-C24	3.19	121.92	111.91
22	D	404	CLA	CMD-C2D-C3D	3.19	130.64	124.68
31	T	101	BCR	C27-C26-C25	3.18	127.35	122.73
22	b	610	CLA	CHB-C4A-NA	3.18	128.91	124.51
22	C	503	CLA	C4-C3-C5	3.18	120.62	115.27
29	C	517	DGD	O6D-C1D-O3G	-3.18	102.45	109.97
23	D	401	PHO	CMB-C2B-C1B	-3.18	120.17	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	411	SQD	O48-C23-C24	3.18	121.87	111.91
22	C	512	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
22	b	616	CLA	CHB-C4A-NA	3.17	128.89	124.51
22	B	615	CLA	CMC-C2C-C3C	3.17	130.92	124.94
22	b	612	CLA	C1B-CHB-C4A	-3.17	123.84	130.12
29	A	413	DGD	O6D-C1D-O3G	-3.16	102.49	109.97
27	a	411	SQD	O9-S-O7	-3.15	103.03	113.95
29	A	413	DGD	O6E-C5E-C4E	3.15	115.42	109.69
22	b	604	CLA	C4D-C3D-CAD	-3.15	106.71	108.47
31	K	102	BCR	C37-C22-C21	-3.15	118.51	122.92
22	B	609	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
22	C	502	CLA	CMB-C2B-C1B	-3.15	123.63	128.46
31	c	514	BCR	C36-C18-C17	-3.14	118.52	122.92
22	B	604	CLA	C1-C2-C3	-3.13	120.62	126.04
22	d	403	CLA	CMB-C2B-C3B	3.13	130.54	124.68
22	b	604	CLA	C4-C3-C5	3.13	120.54	115.27
22	B	610	CLA	CHB-C4A-NA	3.13	128.84	124.51
22	b	606	CLA	CMB-C2B-C3B	3.12	130.52	124.68
22	b	613	CLA	CMD-C2D-C3D	3.12	130.52	124.68
22	c	512	CLA	CMD-C2D-C3D	3.11	130.50	124.68
31	c	514	BCR	C15-C16-C17	-3.11	117.10	123.47
22	b	608	CLA	C1B-CHB-C4A	-3.11	123.96	130.12
29	C	515	DGD	O3G-C3G-C2G	-3.11	103.40	110.90
25	D	407	PL9	C22-C23-C24	-3.11	120.18	127.66
22	b	610	CLA	OBD-CAD-CBD	-3.10	121.46	125.89
22	C	501	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
22	a	402	CLA	CHB-C4A-NA	3.09	128.79	124.51
22	c	513	CLA	C1-C2-C3	-3.09	120.69	126.04
22	b	611	CLA	C1B-CHB-C4A	-3.09	124.00	130.12
22	d	404	CLA	CMB-C2B-C3B	3.09	130.46	124.68
22	c	513	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
22	b	614	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
22	b	614	CLA	C4-C3-C5	3.09	120.46	115.27
22	c	503	CLA	CMB-C2B-C3B	3.08	130.45	124.68
31	H	101	BCR	C24-C23-C22	-3.08	121.58	126.23
22	b	612	CLA	CHB-C4A-NA	3.08	128.77	124.51
22	b	609	CLA	C1B-CHB-C4A	-3.08	124.02	130.12
22	b	602	CLA	C1B-CHB-C4A	-3.08	124.02	130.12
29	C	515	DGD	O1G-C1A-C2A	-3.08	102.25	111.91
27	A	410	SQD	O5-C1-O6	3.08	117.26	109.97
22	d	401	CLA	O2A-CGA-O1A	-3.08	115.83	123.59
22	B	603	CLA	C6-C7-C8	-3.07	105.99	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	L	101	SQD	C45-O47-C7	3.07	125.35	117.79
22	c	502	CLA	OBD-CAD-CBD	-3.07	121.51	125.89
22	c	510	CLA	CHB-C4A-NA	3.07	128.75	124.51
22	A	403	CLA	CMD-C2D-C3D	3.07	130.41	124.68
26	b	622	LMG	O1-C1-C2	-3.06	103.53	108.30
27	A	410	SQD	C1-O5-C5	-3.06	107.68	113.69
25	d	407	PL9	C37-C38-C39	-3.05	120.31	127.66
22	A	405	CLA	CMC-C2C-C3C	3.05	130.69	124.94
22	D	403	CLA	CMB-C2B-C3B	3.05	130.38	124.68
22	B	603	CLA	CMD-C2D-C3D	3.04	130.37	124.68
22	C	509	CLA	CHB-C4A-NA	3.04	128.72	124.51
27	B	622	SQD	O9-S-C6	3.04	110.55	106.94
22	B	604	CLA	OBD-CAD-CBD	-3.04	121.55	125.89
31	d	406	BCR	C3-C4-C5	-3.04	108.65	114.08
22	d	401	CLA	C4A-NA-C1A	3.04	108.07	106.71
31	B	617	BCR	C15-C16-C17	-3.04	117.25	123.47
22	c	503	CLA	CMD-C2D-C3D	3.04	130.36	124.68
22	b	604	CLA	CMC-C2C-C3C	3.04	130.67	124.94
27	L	101	SQD	O47-C7-C8	3.04	118.05	111.50
22	c	504	CLA	C4A-NA-C1A	3.03	108.07	106.71
25	D	407	PL9	C30-C29-C31	-3.02	110.18	115.27
22	D	405	CLA	C4A-NA-C1A	3.02	108.06	106.71
22	d	404	CLA	O2D-CGD-CBD	3.02	116.64	111.27
22	A	403	CLA	CED-O2D-CGD	-3.02	109.10	115.94
26	m	101	LMG	O6-C1-O1	-3.02	102.83	109.97
31	K	102	BCR	C15-C16-C17	-3.02	117.29	123.47
22	b	604	CLA	CHB-C4A-NA	3.01	128.68	124.51
22	c	511	CLA	CMC-C2C-C3C	3.01	130.62	124.94
22	c	507	CLA	OBD-CAD-CBD	-3.01	121.59	125.89
22	b	602	CLA	OBD-CAD-CBD	-3.01	121.59	125.89
23	A	404	PHO	C5-C3-C2	3.01	127.20	121.12
22	c	505	CLA	CMD-C2D-C3D	3.01	130.30	124.68
22	c	504	CLA	CMC-C2C-C3C	3.01	130.61	124.94
28	D	413	LHG	O8-C23-O10	-3.01	116.01	123.59
22	b	609	CLA	CHB-C4A-NA	3.00	128.66	124.51
22	c	511	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
31	I	101	BCR	C37-C22-C21	-3.00	118.72	122.92
22	d	405	CLA	C1B-CHB-C4A	-3.00	124.18	130.12
27	f	102	SQD	O48-C23-O10	-3.00	116.03	123.59
22	D	405	CLA	CMD-C2D-C3D	2.99	130.28	124.68
28	e	101	LHG	O8-C23-C24	2.99	121.30	111.91
22	b	605	CLA	CMD-C2D-C3D	2.99	130.28	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	521	LMG	O2-C2-C1	-2.99	102.78	110.05
27	a	411	SQD	O5-C1-O6	2.99	117.06	109.97
22	C	504	CLA	C4A-NA-C1A	2.99	108.05	106.71
22	B	610	CLA	C4D-C3D-CAD	-2.99	106.80	108.47
26	c	519	LMG	O2-C2-C3	-2.99	103.44	110.35
22	c	506	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
22	d	404	CLA	CHB-C4A-NA	2.98	128.64	124.51
22	B	603	CLA	CMC-C2C-C3C	2.98	130.56	124.94
31	x	101	BCR	C36-C18-C17	-2.98	118.75	122.92
31	D	406	BCR	C7-C8-C9	-2.98	121.73	126.23
22	B	605	CLA	C4D-C3D-CAD	-2.98	106.81	108.47
23	a	403	PHO	C1B-NB-C4B	2.98	112.12	106.51
22	b	601	CLA	CMB-C2B-C3B	2.98	130.25	124.68
25	d	407	PL9	C32-C33-C34	-2.97	120.50	127.66
22	C	507	CLA	CMD-C2D-C3D	2.97	130.24	124.68
27	A	410	SQD	C1-C2-C3	-2.97	103.82	110.00
22	B	612	CLA	C11-C12-C13	-2.96	106.34	115.92
27	A	410	SQD	O8-S-C6	2.96	110.46	105.74
22	c	504	CLA	C4-C3-C5	2.96	120.25	115.27
29	c	517	DGD	C3D-C4D-C5D	-2.96	104.96	110.24
22	B	610	CLA	CMD-C2D-C3D	2.96	130.22	124.68
28	D	413	LHG	O3-P-O5	-2.96	97.51	109.07
22	b	601	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
26	M	101	LMG	O6-C1-O1	-2.96	102.97	109.97
31	D	406	BCR	C27-C26-C25	2.95	127.02	122.73
31	D	406	BCR	C2-C1-C6	2.95	115.03	110.48
22	C	501	CLA	OBD-CAD-CBD	-2.95	121.67	125.89
22	b	603	CLA	CMB-C2B-C3B	2.95	130.19	124.68
22	b	615	CLA	C4D-C3D-CAD	-2.95	106.83	108.47
22	C	504	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
22	B	609	CLA	OBD-CAD-C3D	2.94	132.87	127.98
22	D	404	CLA	C16-C15-C13	-2.94	106.41	115.92
26	c	521	LMG	O1-C1-C2	-2.94	103.71	108.30
22	b	614	CLA	C1-C2-C3	-2.94	120.96	126.04
22	B	610	CLA	O2D-CGD-CBD	2.93	116.47	111.27
29	C	515	DGD	CDB-CCB-CBB	-2.93	99.56	114.42
22	D	405	CLA	O1D-CGD-CBD	2.92	130.46	124.48
29	H	102	DGD	C1D-C2D-C3D	-2.92	103.92	110.00
22	b	612	CLA	CMD-C2D-C3D	2.91	130.12	124.68
23	D	401	PHO	C1B-NB-C4B	2.91	111.99	106.51
22	d	401	CLA	CED-O2D-CGD	-2.91	109.36	115.94
29	H	102	DGD	C4E-C3E-C2E	-2.91	105.75	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	510	CLA	C16-C15-C13	-2.91	106.53	115.92
23	d	402	PHO	C1B-NB-C4B	2.90	111.98	106.51
22	c	508	CLA	CMB-C2B-C1B	-2.90	124.00	128.46
22	b	608	CLA	C3B-C4B-NB	-2.90	105.46	109.21
31	I	101	BCR	C27-C26-C25	2.90	126.94	122.73
29	c	516	DGD	C3G-C2G-C1G	-2.90	104.94	111.79
22	d	404	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
22	b	608	CLA	CHB-C4A-NA	2.89	128.51	124.51
22	c	505	CLA	C4D-C3D-CAD	-2.89	106.86	108.47
31	K	101	BCR	C27-C26-C25	2.89	126.92	122.73
23	d	402	PHO	O2D-CGD-O1D	-2.89	118.19	123.84
22	b	601	CLA	CMD-C2D-C3D	2.88	130.07	124.68
22	c	508	CLA	CMB-C2B-C3B	2.88	130.07	124.68
22	c	506	CLA	CHB-C4A-NA	2.88	128.50	124.51
22	C	505	CLA	O2A-CGA-O1A	-2.88	116.33	123.59
22	D	403	CLA	OBD-CAD-CBD	-2.88	121.78	125.89
27	B	622	SQD	C4-C3-C2	2.88	115.85	110.82
27	D	409	SQD	O48-C23-C24	2.88	120.94	111.91
22	B	614	CLA	CMB-C2B-C1B	-2.88	124.05	128.46
27	f	102	SQD	C1-C2-C3	-2.87	104.01	110.00
22	c	507	CLA	CMB-C2B-C1B	-2.87	124.05	128.46
22	B	605	CLA	C16-C15-C13	-2.87	106.64	115.92
31	x	101	BCR	C37-C22-C21	-2.87	118.91	122.92
22	B	602	CLA	C4A-NA-C1A	2.87	108.00	106.71
22	A	405	CLA	O2A-CGA-O1A	-2.87	116.36	123.59
22	c	513	CLA	CMB-C2B-C3B	2.87	130.04	124.68
23	d	402	PHO	O1D-CGD-CBD	2.86	130.35	124.48
22	B	616	CLA	C2A-C3A-C4A	2.86	106.50	101.87
25	A	408	PL9	C22-C23-C24	-2.86	120.77	127.66
22	b	605	CLA	O1D-CGD-CBD	2.86	130.34	124.48
22	b	615	CLA	CMB-C2B-C3B	2.86	130.03	124.68
29	C	516	DGD	C7B-C6B-C5B	-2.86	99.91	114.42
26	c	522	LMG	O2-C2-C1	-2.86	103.10	110.05
22	B	613	CLA	CHA-C1A-NA	-2.85	119.86	126.40
29	C	517	DGD	O5D-C6D-C5D	-2.85	103.77	109.05
31	Z	101	BCR	C27-C26-C25	2.85	126.87	122.73
22	a	404	CLA	CMB-C2B-C3B	2.85	130.00	124.68
26	b	622	LMG	O2-C2-C1	-2.85	103.13	110.05
22	b	615	CLA	OBD-CAD-CBD	-2.85	121.83	125.89
22	c	507	CLA	C4D-C3D-CAD	-2.85	106.88	108.47
27	L	101	SQD	O47-C45-C46	2.84	118.70	108.40
22	B	613	CLA	O1D-CGD-CBD	2.84	130.30	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	515	DGD	O2D-C2D-C1D	-2.84	103.14	110.05
22	b	614	CLA	CMB-C2B-C3B	2.84	130.00	124.68
22	b	611	CLA	CMB-C2B-C1B	-2.84	124.10	128.46
31	B	618	BCR	C35-C13-C14	-2.84	118.94	122.92
29	c	517	DGD	O5D-C6D-C5D	-2.84	103.79	109.05
31	C	514	BCR	C7-C8-C9	-2.84	121.95	126.23
31	a	405	BCR	C27-C26-C25	2.84	126.85	122.73
22	b	606	CLA	CMC-C2C-C3C	2.83	130.28	124.94
22	C	505	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
31	a	405	BCR	C7-C8-C9	-2.83	121.96	126.23
31	B	617	BCR	C27-C26-C25	2.83	126.84	122.73
31	x	101	BCR	C38-C26-C25	-2.83	121.35	124.53
25	a	409	PL9	C32-C33-C34	-2.83	120.85	127.66
22	d	405	CLA	CMC-C2C-C3C	2.83	130.27	124.94
22	B	603	CLA	O2A-CGA-O1A	-2.83	116.46	123.59
22	b	610	CLA	CAA-CBA-CGA	-2.83	104.99	113.25
22	B	616	CLA	O2D-CGD-O1D	-2.82	118.31	123.84
31	Z	101	BCR	C7-C8-C9	-2.82	121.97	126.23
22	d	404	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
27	A	410	SQD	O5-C5-C4	2.82	114.82	109.69
22	B	612	CLA	O2A-CGA-O1A	-2.82	116.47	123.59
27	B	622	SQD	O9-S-O7	-2.82	104.19	113.95
22	c	503	CLA	C4A-NA-C1A	2.82	107.97	106.71
22	b	611	CLA	CMB-C2B-C3B	2.82	129.95	124.68
29	c	516	DGD	O2D-C2D-C1D	-2.82	103.20	110.05
22	B	612	CLA	CHB-C4A-NA	2.82	128.41	124.51
22	B	611	CLA	C1-C2-C3	-2.81	121.18	126.04
22	B	611	CLA	CHB-C4A-NA	2.81	128.40	124.51
22	B	609	CLA	CMB-C2B-C3B	2.81	129.94	124.68
25	a	409	PL9	C40-C39-C41	2.81	120.00	115.27
31	Z	101	BCR	C36-C18-C17	-2.81	118.99	122.92
22	c	512	CLA	CMB-C2B-C3B	2.81	129.93	124.68
28	D	413	LHG	O8-C23-C24	2.80	120.71	111.91
25	A	408	PL9	C27-C28-C29	-2.80	120.91	127.66
31	b	618	BCR	C37-C22-C21	-2.80	119.00	122.92
22	b	610	CLA	C4A-NA-C1A	2.80	107.97	106.71
28	d	408	LHG	O8-C23-C24	2.80	120.70	111.91
22	C	513	CLA	CMB-C2B-C3B	2.80	129.92	124.68
22	B	614	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
22	B	605	CLA	CMB-C2B-C3B	2.80	129.91	124.68
22	b	611	CLA	CHB-C4A-NA	2.80	128.38	124.51
27	B	622	SQD	O5-C5-C4	2.79	114.76	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	622	SQD	O48-C23-O10	-2.79	116.56	123.59
22	b	612	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
22	c	506	CLA	C1B-CHB-C4A	-2.78	124.60	130.12
22	B	601	CLA	CMD-C2D-C3D	2.78	129.88	124.68
22	D	404	CLA	CHB-C4A-NA	2.78	128.36	124.51
22	D	404	CLA	C3D-CAD-CBD	-2.78	103.94	107.61
31	b	618	BCR	C15-C16-C17	-2.78	117.78	123.47
22	b	604	CLA	C11-C12-C13	-2.78	106.94	115.92
22	C	504	CLA	O2A-CGA-O1A	-2.78	116.58	123.59
22	c	511	CLA	CMB-C2B-C1B	-2.78	124.20	128.46
22	C	508	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
22	c	512	CLA	CHB-C4A-NA	2.77	128.35	124.51
31	b	617	BCR	C15-C16-C17	-2.77	117.79	123.47
31	b	617	BCR	C27-C26-C25	2.77	126.76	122.73
22	C	503	CLA	CMD-C2D-C3D	2.77	129.86	124.68
27	L	101	SQD	O2-C2-C1	2.77	116.78	110.05
22	c	501	CLA	O2D-CGD-CBD	2.77	116.19	111.27
22	c	505	CLA	C4A-NA-C1A	2.77	107.95	106.71
22	b	602	CLA	O2A-CGA-O1A	-2.77	116.61	123.59
22	B	616	CLA	CHB-C4A-NA	2.77	128.34	124.51
22	b	603	CLA	O2A-CGA-O1A	-2.76	116.62	123.59
28	d	409	LHG	C26-C25-C24	2.76	123.11	113.19
29	h	101	DGD	C1D-C2D-C3D	-2.76	104.25	110.00
22	A	403	CLA	CHB-C4A-NA	2.76	128.32	124.51
22	A	405	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
22	c	503	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
22	B	602	CLA	CMB-C2B-C3B	2.75	129.83	124.68
22	B	613	CLA	CMD-C2D-C3D	2.75	129.83	124.68
22	B	603	CLA	CMB-C2B-C3B	2.75	129.82	124.68
22	B	601	CLA	CMB-C2B-C1B	-2.75	124.24	128.46
22	c	510	CLA	CMD-C2D-C3D	2.74	129.81	124.68
23	D	401	PHO	C1-C2-C3	-2.74	121.30	126.04
22	b	605	CLA	CHB-C4A-NA	2.74	128.30	124.51
22	C	513	CLA	C4D-C3D-CAD	-2.74	106.94	108.47
22	c	505	CLA	O2A-CGA-O1A	-2.74	116.69	123.59
22	b	606	CLA	C1B-CHB-C4A	-2.74	124.70	130.12
22	b	611	CLA	O2A-CGA-O1A	-2.73	116.69	123.59
22	b	612	CLA	C11-C10-C8	-2.73	107.08	115.92
31	c	515	BCR	C2-C1-C6	2.73	114.69	110.48
31	d	406	BCR	C27-C26-C25	2.73	126.70	122.73
22	D	403	CLA	C1-C2-C3	-2.73	121.32	126.04
28	l	101	LHG	O8-C23-C24	2.73	120.47	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	403	CLA	O2D-CGD-CBD	2.73	116.11	111.27
22	A	402	CLA	O1D-CGD-CBD	2.73	130.06	124.48
26	A	409	LMG	C9-C8-C7	-2.72	105.35	111.79
22	B	603	CLA	CMB-C2B-C1B	-2.72	124.28	128.46
22	c	512	CLA	CMB-C2B-C1B	-2.72	124.28	128.46
22	C	501	CLA	C4-C3-C5	2.72	119.85	115.27
22	B	608	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
22	C	503	CLA	CMB-C2B-C3B	2.72	129.76	124.68
22	c	501	CLA	CMC-C2C-C3C	2.71	130.06	124.94
29	c	516	DGD	O3G-C3G-C2G	-2.71	104.35	110.90
22	D	405	CLA	CMB-C2B-C3B	2.71	129.75	124.68
31	H	101	BCR	C2-C1-C6	2.71	114.65	110.48
26	M	101	LMG	C38-C37-C36	-2.71	100.69	114.42
22	C	506	CLA	CHB-C4A-NA	2.70	128.25	124.51
23	d	402	PHO	O2A-CGA-O1A	-2.70	116.78	123.59
22	c	512	CLA	O2A-CGA-O1A	-2.70	116.79	123.59
22	C	503	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
31	c	515	BCR	C27-C26-C25	2.69	126.64	122.73
22	B	607	CLA	CMD-C2D-C3D	2.69	129.71	124.68
22	c	503	CLA	C4D-C3D-CAD	-2.68	106.97	108.47
31	k	101	BCR	C38-C26-C25	-2.68	121.51	124.53
22	B	610	CLA	C1B-CHB-C4A	-2.68	124.80	130.12
22	d	404	CLA	C1-C2-C3	-2.68	121.40	126.04
29	c	516	DGD	O6D-C1D-O3G	-2.68	103.62	109.97
22	c	506	CLA	CMB-C2B-C3B	2.68	129.69	124.68
25	a	409	PL9	C20-C19-C21	2.68	119.77	115.27
22	a	402	CLA	CMD-C2D-C3D	2.67	129.68	124.68
29	h	101	DGD	O6E-C5E-C4E	2.67	114.55	109.69
22	C	501	CLA	OBD-CAD-C3D	2.67	132.41	127.98
22	B	607	CLA	OBD-CAD-CBD	-2.67	122.08	125.89
26	d	410	LMG	O1-C1-C2	-2.67	104.14	108.30
25	a	409	PL9	C7-C8-C9	-2.67	122.35	126.79
22	C	511	CLA	OBD-CAD-C3D	2.67	132.41	127.98
22	B	604	CLA	CMC-C2C-C3C	2.67	129.97	124.94
26	c	522	LMG	O3-C3-C2	-2.66	104.19	110.35
28	a	410	LHG	C11-C10-C9	-2.66	100.91	114.42
31	b	618	BCR	C8-C7-C6	-2.66	119.73	127.20
22	B	608	CLA	CMD-C2D-C3D	2.66	129.65	124.68
29	c	516	DGD	O4D-C4D-C5D	-2.66	102.69	109.30
29	c	517	DGD	O5D-C1E-C2E	2.66	112.45	108.30
22	c	510	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
31	D	406	BCR	C24-C23-C22	-2.66	122.22	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	410	LHG	C11-C10-C9	-2.66	100.94	114.42
22	C	510	CLA	O2D-CGD-CBD	2.65	115.98	111.27
22	c	507	CLA	CMC-C2C-C3C	2.65	129.94	124.94
29	H	102	DGD	O6D-C1D-O3G	-2.65	103.71	109.97
22	d	403	CLA	O2A-CGA-O1A	-2.64	116.92	123.59
31	d	406	BCR	C16-C15-C14	-2.64	118.06	123.47
31	d	406	BCR	C11-C10-C9	-2.64	123.54	127.31
22	A	405	CLA	C4-C3-C5	2.64	119.72	115.27
25	a	409	PL9	C12-C13-C14	-2.64	121.30	127.66
22	a	402	CLA	C2A-C1A-CHA	2.64	128.47	123.86
23	A	404	PHO	C2B-C1B-NB	-2.64	105.81	109.79
29	c	518	DGD	CDB-CCB-CBB	-2.64	101.04	114.42
22	C	512	CLA	C1B-CHB-C4A	-2.64	124.90	130.12
31	a	405	BCR	C38-C26-C27	-2.64	108.55	113.62
31	T	101	BCR	C37-C22-C21	-2.63	119.23	122.92
31	t	101	BCR	C7-C8-C9	-2.63	122.26	126.23
31	k	102	BCR	C39-C30-C25	-2.63	106.04	110.30
22	b	616	CLA	CMD-C2D-C3D	2.63	129.59	124.68
22	C	505	CLA	CHB-C4A-NA	2.62	128.14	124.51
22	c	502	CLA	CMD-C2D-C3D	2.62	129.58	124.68
22	B	614	CLA	C4D-C3D-CAD	-2.62	107.01	108.47
22	B	605	CLA	OBD-CAD-CBD	-2.62	122.15	125.89
22	a	404	CLA	CMD-C2D-C3D	2.62	129.58	124.68
31	K	101	BCR	C8-C7-C6	-2.62	119.85	127.20
31	t	101	BCR	C1-C6-C5	-2.62	118.93	122.61
26	D	408	LMG	O8-C28-O10	-2.62	116.99	123.59
29	C	516	DGD	CDB-CCB-CBB	-2.61	101.16	114.42
22	C	512	CLA	CMB-C2B-C3B	2.61	129.57	124.68
22	b	608	CLA	OBD-CAD-CBD	-2.61	122.16	125.89
31	x	101	BCR	C15-C16-C17	-2.61	118.13	123.47
26	A	409	LMG	O3-C3-C2	-2.61	104.32	110.35
22	b	604	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
22	c	504	CLA	CMD-C2D-C3D	2.61	129.56	124.68
22	C	512	CLA	O2A-CGA-O1A	-2.61	117.01	123.59
22	B	605	CLA	CHB-C4A-NA	2.60	128.11	124.51
27	a	411	SQD	O47-C7-C8	2.60	117.11	111.50
31	I	101	BCR	C36-C18-C17	-2.60	119.28	122.92
22	B	616	CLA	O1D-CGD-CBD	2.60	129.81	124.48
29	A	413	DGD	C3G-C2G-C1G	-2.60	105.64	111.79
22	c	502	CLA	C1-C2-C3	-2.60	121.55	126.04
29	c	517	DGD	C8B-C7B-C6B	-2.60	101.24	114.42
26	m	101	LMG	O7-C10-O9	-2.60	117.42	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	t	101	BCR	C15-C16-C17	-2.59	118.16	123.47
22	c	507	CLA	CMD-C2D-C3D	2.59	129.53	124.68
31	b	619	BCR	C29-C30-C25	2.59	114.47	110.48
31	a	405	BCR	C39-C30-C25	-2.59	106.10	110.30
22	B	606	CLA	CMB-C2B-C1B	-2.59	124.48	128.46
26	c	522	LMG	O2-C2-C3	-2.59	104.37	110.35
22	b	608	CLA	O2D-CGD-CBD	2.59	115.87	111.27
27	L	101	SQD	O47-C7-O49	-2.59	117.45	123.70
22	B	612	CLA	CMD-C2D-C3D	2.58	129.51	124.68
29	C	515	DGD	O3E-C3E-C2E	-2.58	104.39	110.35
22	C	502	CLA	OBD-CAD-CBD	-2.58	122.21	125.89
25	a	409	PL9	C30-C29-C28	-2.58	117.06	123.68
22	c	507	CLA	CMB-C2B-C3B	2.58	129.50	124.68
22	a	404	CLA	CMC-C2C-C3C	2.58	129.80	124.94
26	c	521	LMG	O8-C28-O10	-2.57	117.10	123.59
31	c	514	BCR	C15-C14-C13	-2.57	123.64	127.31
29	c	516	DGD	C4E-C3E-C2E	-2.57	106.33	110.82
22	c	509	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
22	b	604	CLA	OBD-CAD-C3D	2.57	132.25	127.98
29	A	413	DGD	O3E-C3E-C2E	-2.57	104.41	110.35
31	c	515	BCR	C35-C13-C14	-2.56	119.33	122.92
28	D	410	LHG	O8-C23-C24	2.56	119.94	111.91
22	c	504	CLA	C6-C7-C8	-2.56	107.65	115.92
22	c	509	CLA	O1D-CGD-CBD	2.56	129.72	124.48
22	b	601	CLA	C4D-C3D-CAD	-2.55	107.05	108.47
22	C	501	CLA	CMD-C2D-C3D	2.55	129.45	124.68
29	c	518	DGD	C3G-C2G-C1G	-2.55	105.76	111.79
22	b	608	CLA	C4D-C3D-CAD	-2.55	107.05	108.47
22	c	502	CLA	C6-C5-C3	-2.55	106.78	113.45
31	a	405	BCR	C16-C17-C18	-2.55	123.67	127.31
22	c	508	CLA	CHB-C4A-NA	2.55	128.03	124.51
25	D	407	PL9	C12-C13-C14	-2.55	121.53	127.66
25	d	407	PL9	C7-C8-C9	-2.55	122.56	126.79
22	c	512	CLA	O1D-CGD-CBD	2.54	129.69	124.48
26	b	622	LMG	C3-C4-C5	-2.54	105.70	110.24
22	b	615	CLA	CAA-CBA-CGA	-2.54	105.83	113.25
22	C	513	CLA	CMD-C2D-C3D	2.54	129.43	124.68
22	B	604	CLA	O2A-CGA-CBA	2.54	119.87	111.91
23	a	403	PHO	C2B-C1B-NB	-2.54	105.97	109.79
22	D	405	CLA	CMC-C2C-C3C	2.53	129.72	124.94
22	C	502	CLA	CHA-C1A-NA	-2.53	120.59	126.40
28	e	101	LHG	C11-C10-C9	-2.53	101.58	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	604	CLA	C6-C7-C8	-2.53	107.74	115.92
22	C	510	CLA	CHB-C4A-NA	2.53	128.01	124.51
27	B	622	SQD	C46-C45-C44	-2.53	105.81	111.79
22	b	614	CLA	CHB-C4A-NA	2.53	128.01	124.51
25	D	407	PL9	C7-C8-C9	-2.52	122.59	126.79
22	b	612	CLA	C11-C12-C13	-2.52	107.76	115.92
22	A	402	CLA	C7-C6-C5	-2.52	106.51	113.36
25	a	409	PL9	C42-C43-C44	-2.52	121.59	127.66
25	D	407	PL9	C11-C12-C13	-2.51	103.62	111.88
22	B	601	CLA	C4-C3-C5	2.51	119.50	115.27
22	B	610	CLA	O1D-CGD-CBD	2.51	129.62	124.48
22	A	402	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
31	C	514	BCR	C37-C22-C21	-2.51	119.41	122.92
22	d	404	CLA	CMD-C2D-C3D	2.51	129.37	124.68
22	B	608	CLA	OBD-CAD-CBD	-2.51	122.31	125.89
25	d	407	PL9	C20-C19-C21	2.51	119.49	115.27
25	d	407	PL9	C42-C43-C44	-2.51	121.62	127.66
22	B	603	CLA	O2A-C1-C2	-2.50	102.05	108.64
22	c	509	CLA	CMC-C2C-C3C	2.50	129.66	124.94
23	A	404	PHO	O2D-CGD-O1D	-2.50	118.94	123.84
27	A	410	SQD	O6-C44-C45	2.50	116.93	110.90
34	f	101	HEM	CMC-C2C-C3C	2.50	129.35	124.68
26	d	410	LMG	O3-C3-C2	-2.50	104.57	110.35
29	c	517	DGD	C4E-C3E-C2E	-2.50	106.46	110.82
22	b	611	CLA	CED-O2D-CGD	-2.50	110.29	115.94
27	L	101	SQD	O9-S-O7	-2.50	105.31	113.95
26	c	521	LMG	O6-C1-O1	-2.50	104.06	109.97
22	a	404	CLA	CMB-C2B-C1B	-2.49	124.63	128.46
29	h	101	DGD	O3G-C3G-C2G	-2.49	104.88	110.90
25	a	409	PL9	C22-C23-C24	-2.49	121.66	127.66
35	V	201	HEC	CMC-C2C-C3C	2.49	128.75	125.82
29	h	101	DGD	C4E-C3E-C2E	-2.49	106.48	110.82
28	A	411	LHG	O8-C23-C24	2.49	119.72	111.91
22	b	601	CLA	O2D-CGD-CBD	2.49	115.69	111.27
22	C	504	CLA	C4D-C3D-CAD	-2.49	107.08	108.47
25	D	407	PL9	C42-C43-C44	-2.49	121.67	127.66
31	K	102	BCR	C28-C27-C26	-2.49	109.64	114.08
31	k	102	BCR	C27-C26-C25	2.48	126.34	122.73
31	H	101	BCR	C27-C26-C25	2.48	126.34	122.73
31	c	514	BCR	C7-C8-C9	-2.48	122.48	126.23
22	B	606	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
22	C	502	CLA	CMB-C2B-C3B	2.48	129.32	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	511	CLA	CMB-C2B-C3B	2.48	129.32	124.68
25	d	407	PL9	C50-C49-C48	-2.48	115.47	122.65
22	B	603	CLA	O1D-CGD-CBD	2.48	129.56	124.48
25	d	407	PL9	C45-C44-C46	-2.48	111.10	115.27
22	B	602	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
28	a	410	LHG	O8-C23-C24	2.48	119.68	111.91
22	c	502	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
22	b	608	CLA	C4A-NA-C1A	2.47	107.82	106.71
22	b	611	CLA	C3A-C2A-C1A	2.47	105.04	101.34
31	c	515	BCR	C37-C22-C21	-2.47	119.46	122.92
22	B	602	CLA	C1-C2-C3	-2.47	121.78	126.04
31	B	618	BCR	C7-C8-C9	-2.46	122.51	126.23
22	a	404	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
27	f	102	SQD	O47-C7-C8	2.46	117.66	110.80
22	B	605	CLA	CMD-C2D-C3D	2.46	129.28	124.68
22	A	402	CLA	C16-C15-C13	-2.46	107.97	115.92
22	B	608	CLA	CHB-C4A-NA	2.46	127.91	124.51
27	B	622	SQD	O47-C45-C46	2.46	117.30	108.40
29	H	102	DGD	C3E-C4E-C5E	-2.46	105.86	110.24
22	b	602	CLA	CMC-C2C-C3C	2.46	129.57	124.94
26	Y	101	LMG	O6-C5-C6	2.45	112.54	106.44
22	b	609	CLA	OBD-CAD-CBD	-2.45	122.39	125.89
31	C	514	BCR	C2-C1-C6	2.45	114.25	110.48
22	a	402	CLA	CMB-C2B-C3B	2.45	129.26	124.68
29	C	516	DGD	CAB-C9B-C8B	-2.45	101.99	114.42
22	b	607	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
31	k	102	BCR	C1-C6-C5	-2.45	119.16	122.61
22	a	404	CLA	CHA-C1A-NA	-2.44	120.80	126.40
26	c	522	LMG	O8-C28-O10	-2.44	117.43	123.59
22	b	614	CLA	O2D-CGD-CBD	2.44	115.61	111.27
26	D	412	LMG	O7-C10-O9	-2.44	117.80	123.70
23	d	402	PHO	C1-C2-C3	-2.44	121.83	126.04
27	A	410	SQD	O48-C23-C24	2.44	119.56	111.91
22	b	612	CLA	OBD-CAD-CBD	-2.44	122.41	125.89
22	a	402	CLA	O2D-CGD-O1D	-2.44	119.08	123.84
22	B	613	CLA	C1-C2-C3	-2.44	121.83	126.04
31	B	617	BCR	C37-C22-C21	-2.44	119.51	122.92
23	a	403	PHO	O2D-CGD-O1D	-2.43	119.08	123.84
22	B	614	CLA	CMC-C2C-C3C	2.43	129.53	124.94
22	A	402	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
22	b	610	CLA	CMB-C2B-C3B	2.43	129.22	124.68
27	D	409	SQD	C1-C2-C3	-2.43	104.94	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	411	LHG	O8-C23-C24	2.43	119.53	111.91
22	a	404	CLA	OBD-CAD-CBD	-2.43	122.43	125.89
22	B	603	CLA	O2D-CGD-CBD	2.42	115.58	111.27
31	T	101	BCR	C37-C22-C23	2.42	121.90	118.08
22	b	604	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
29	C	517	DGD	C3G-C2G-C1G	-2.42	106.07	111.79
22	c	503	CLA	O1D-CGD-CBD	2.42	129.43	124.48
27	A	412	SQD	O47-C45-C44	2.42	113.45	107.93
22	B	602	CLA	C16-C15-C13	-2.42	108.11	115.92
22	c	507	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
29	C	517	DGD	O3E-C3E-C2E	-2.42	104.76	110.35
22	B	613	CLA	OBD-CAD-CBD	-2.41	122.44	125.89
27	D	409	SQD	O48-C23-O10	-2.41	117.50	123.59
22	C	512	CLA	C1-C2-C3	-2.41	121.87	126.04
22	C	503	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
22	b	601	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
31	I	101	BCR	C15-C16-C17	-2.41	118.54	123.47
31	C	514	BCR	C36-C18-C19	2.41	121.87	118.08
22	C	512	CLA	CMD-C2D-C3D	2.41	129.19	124.68
22	c	508	CLA	C7-C6-C5	-2.41	106.83	113.36
22	C	501	CLA	O2A-CGA-O1A	-2.40	117.52	123.59
26	d	410	LMG	O6-C5-C4	2.40	114.06	109.69
22	d	403	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
29	A	413	DGD	O3D-C3D-C4D	-2.40	104.80	110.35
29	H	102	DGD	O2G-C1B-O1B	-2.40	117.90	123.70
31	b	618	BCR	C38-C26-C25	-2.40	121.83	124.53
27	D	409	SQD	O9-S-O7	-2.40	105.64	113.95
25	A	408	PL9	C40-C39-C41	2.40	119.31	115.27
26	Y	101	LMG	O2-C2-C1	-2.40	104.22	110.05
22	B	614	CLA	C4-C3-C5	2.40	119.30	115.27
31	I	101	BCR	C34-C9-C8	-2.40	114.30	118.08
22	c	507	CLA	O2D-CGD-CBD	2.39	115.52	111.27
31	I	101	BCR	C11-C10-C9	-2.39	123.90	127.31
29	H	102	DGD	CDB-CCB-CBB	-2.39	102.28	114.42
22	a	402	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
22	c	510	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
31	c	514	BCR	C27-C26-C25	2.39	126.20	122.73
22	b	611	CLA	CGD-CBD-CAD	-2.39	102.99	110.73
26	b	622	LMG	O6-C5-C6	2.39	112.37	106.44
22	b	604	CLA	CMD-C2D-C3D	2.38	129.14	124.68
22	A	405	CLA	CHB-C4A-NA	2.38	127.81	124.51
31	c	514	BCR	C11-C10-C9	-2.38	123.91	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b	619	BCR	C20-C21-C22	-2.38	123.91	127.31
23	d	402	PHO	C2B-C1B-NB	-2.38	106.20	109.79
22	b	605	CLA	C4-C3-C2	-2.38	117.58	123.68
22	B	612	CLA	O1D-CGD-CBD	2.37	129.34	124.48
31	k	101	BCR	C27-C26-C25	2.37	126.18	122.73
25	a	409	PL9	C37-C38-C39	-2.37	121.95	127.66
22	d	401	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
34	f	101	HEM	C4C-C3C-C2C	2.37	108.55	106.90
22	b	603	CLA	C7-C6-C5	-2.36	106.94	113.36
31	x	101	BCR	C34-C9-C8	-2.36	114.35	118.08
22	C	503	CLA	C3A-C2A-C1A	2.36	104.88	101.34
29	c	517	DGD	CDB-CCB-CBB	-2.36	102.43	114.42
22	b	613	CLA	C7-C6-C5	-2.36	106.94	113.36
22	b	611	CLA	CAA-CBA-CGA	-2.36	106.35	113.25
27	A	410	SQD	O3-C3-C2	2.36	115.81	110.35
29	c	517	DGD	CBB-CAB-C9B	-2.36	102.44	114.42
31	B	619	BCR	C30-C25-C26	-2.36	119.29	122.61
34	F	101	HEM	CAD-CBD-CGD	2.36	116.63	112.67
22	B	613	CLA	C4-C3-C5	2.36	119.24	115.27
22	C	504	CLA	C4-C3-C5	2.36	119.24	115.27
22	c	513	CLA	O1D-CGD-CBD	2.36	129.31	124.48
22	D	405	CLA	C4D-C3D-CAD	-2.36	107.16	108.47
29	h	101	DGD	O6D-C1D-O3G	-2.36	104.39	109.97
22	B	606	CLA	CHB-C4A-NA	2.36	127.77	124.51
22	c	513	CLA	C11-C12-C13	-2.36	108.31	115.92
29	c	516	DGD	O3D-C3D-C4D	-2.35	104.91	110.35
22	B	607	CLA	OBD-CAD-C3D	2.35	131.89	127.98
26	M	101	LMG	O3-C3-C2	-2.35	104.91	110.35
22	d	401	CLA	CMB-C2B-C1B	-2.35	124.85	128.46
22	b	602	CLA	C1-C2-C3	-2.35	121.98	126.04
31	b	617	BCR	C36-C18-C17	-2.35	119.63	122.92
31	d	406	BCR	C7-C8-C9	-2.35	122.68	126.23
26	c	521	LMG	O7-C10-O9	-2.35	118.02	123.70
27	A	412	SQD	O49-C7-C8	-2.35	114.57	123.73
26	c	521	LMG	O3-C3-C2	-2.35	104.92	110.35
25	a	409	PL9	C27-C28-C29	-2.34	122.02	127.66
22	C	513	CLA	CBC-CAC-C3C	2.34	118.23	112.27
22	B	608	CLA	OBD-CAD-C3D	2.34	131.87	127.98
22	C	501	CLA	C4D-C3D-CAD	-2.34	107.17	108.47
22	c	505	CLA	CHB-C4A-NA	2.34	127.75	124.51
22	C	511	CLA	C3D-CAD-CBD	-2.34	104.52	107.61
29	C	516	DGD	O6D-C1D-O3G	-2.34	104.43	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	602	CLA	C4-C3-C5	2.34	119.20	115.27
27	L	101	SQD	O5-C1-C2	-2.34	105.40	110.35
22	D	403	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
25	a	409	PL9	O2-C1-C2	-2.34	116.43	121.78
22	c	511	CLA	CMD-C2D-C3D	2.34	129.05	124.68
31	t	101	BCR	C36-C18-C19	2.33	121.75	118.08
31	x	101	BCR	C7-C8-C9	-2.33	122.71	126.23
25	d	407	PL9	C40-C39-C38	-2.33	117.69	123.68
26	D	408	LMG	C3-C4-C5	-2.33	106.08	110.24
22	C	503	CLA	C1-O2A-CGA	2.33	122.56	116.44
22	C	511	CLA	CMD-C2D-C3D	2.33	129.03	124.68
22	c	513	CLA	CHB-C4A-NA	2.33	127.73	124.51
25	d	407	PL9	C27-C28-C29	-2.33	122.06	127.66
29	A	413	DGD	O5D-C6D-C5D	-2.32	104.75	109.05
22	C	502	CLA	C2A-C1A-CHA	2.32	127.92	123.86
22	c	507	CLA	CHA-C1A-NA	-2.32	121.08	126.40
29	C	516	DGD	O6E-C5E-C4E	2.32	113.91	109.69
22	C	507	CLA	O1D-CGD-CBD	2.32	129.23	124.48
25	d	407	PL9	C7-C3-C4	2.32	118.76	116.88
26	D	412	LMG	C38-C37-C36	-2.32	102.65	114.42
22	B	603	CLA	C5-C3-C2	-2.32	116.42	121.12
26	M	101	LMG	C4-C3-C2	-2.32	106.78	110.82
31	H	101	BCR	C16-C15-C14	-2.32	118.73	123.47
29	H	102	DGD	C8B-C7B-C6B	-2.32	102.67	114.42
23	D	401	PHO	C3A-C4A-CHB	-2.32	117.83	121.83
22	B	609	CLA	CMD-C2D-C3D	2.32	129.01	124.68
29	c	518	DGD	O5E-C6E-C5E	-2.32	103.35	111.29
28	D	410	LHG	C20-C19-C18	-2.31	102.68	114.42
31	B	619	BCR	C37-C22-C21	-2.31	119.68	122.92
22	c	505	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
22	B	604	CLA	C2A-C1A-CHA	2.31	127.90	123.86
22	b	610	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
26	c	519	LMG	C9-C8-C7	-2.31	106.32	111.79
22	C	504	CLA	O2D-CGD-CBD	2.31	115.37	111.27
29	C	516	DGD	O4D-C4D-C3D	2.31	115.69	110.35
26	m	101	LMG	C1-O6-C5	-2.31	109.16	113.69
22	B	615	CLA	CMB-C2B-C1B	-2.31	124.92	128.46
22	B	609	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
22	B	611	CLA	CMC-C2C-C3C	2.30	129.28	124.94
27	A	410	SQD	O48-C46-C45	2.30	115.13	108.43
25	D	407	PL9	C8-C7-C3	2.30	118.48	111.98
26	B	626	LMG	O6-C5-C4	2.30	113.87	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	409	LMG	O5-C6-C5	-2.30	103.41	111.29
22	c	509	CLA	CMD-C2D-C3D	2.30	128.97	124.68
22	C	511	CLA	C1-C2-C3	-2.30	122.07	126.04
22	C	504	CLA	CMC-C2C-C3C	2.29	129.27	124.94
22	C	503	CLA	O1D-CGD-CBD	2.29	129.18	124.48
22	b	603	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
22	c	507	CLA	OBD-CAD-C3D	2.29	131.79	127.98
22	C	512	CLA	O1D-CGD-CBD	2.29	129.17	124.48
26	Y	101	LMG	C3-C4-C5	-2.29	106.15	110.24
22	c	513	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
22	c	504	CLA	O2D-CGD-CBD	2.29	115.33	111.27
22	b	607	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
31	K	101	BCR	C38-C26-C25	-2.29	121.96	124.53
22	A	402	CLA	CMC-C2C-C3C	2.29	129.25	124.94
22	b	609	CLA	CHA-C1A-NA	-2.29	121.17	126.40
22	B	603	CLA	CHB-C4A-NA	2.28	127.67	124.51
22	D	404	CLA	C1-C2-C3	-2.28	122.10	126.04
22	B	609	CLA	C2A-C3A-C4A	2.28	105.56	101.87
22	C	508	CLA	CHB-C4A-NA	2.28	127.67	124.51
31	K	101	BCR	C12-C13-C14	-2.28	115.44	118.94
27	D	409	SQD	C46-C45-C44	-2.28	106.12	113.70
31	B	619	BCR	C1-C6-C5	-2.28	119.41	122.61
26	A	409	LMG	C40-C39-C38	-2.27	102.88	114.42
29	h	101	DGD	C1E-O6E-C5E	2.27	118.15	113.69
29	C	515	DGD	C5B-C4B-C3B	-2.27	102.89	114.42
23	A	404	PHO	CAC-C3C-C2C	2.27	131.42	127.53
22	B	611	CLA	O1A-CGA-CBA	2.27	132.60	123.73
26	b	622	LMG	O7-C10-O9	-2.27	118.21	123.70
22	B	604	CLA	CHA-C1A-NA	-2.27	121.20	126.40
22	B	611	CLA	CMD-C2D-C3D	2.27	128.92	124.68
22	C	506	CLA	CMD-C2D-C3D	2.27	128.92	124.68
31	B	618	BCR	C15-C16-C17	-2.27	118.83	123.47
22	C	503	CLA	CED-O2D-CGD	-2.27	110.81	115.94
29	C	516	DGD	O2G-C1B-C2B	-2.27	106.61	111.50
29	C	516	DGD	C6D-O5D-C1E	2.27	118.17	113.74
22	c	501	CLA	O1D-CGD-CBD	2.26	129.12	124.48
22	c	509	CLA	C1-O2A-CGA	-2.26	110.51	116.44
28	a	410	LHG	C20-C19-C18	-2.26	102.94	114.42
29	C	517	DGD	O3D-C3D-C4D	-2.26	105.12	110.35
31	t	101	BCR	C4-C5-C6	2.26	126.02	122.73
22	B	604	CLA	C11-C10-C8	-2.26	108.61	115.92
22	b	609	CLA	C6-C5-C3	2.26	119.39	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	603	CLA	CMD-C2D-C3D	2.26	128.91	124.68
22	C	513	CLA	CHB-C4A-NA	2.26	127.64	124.51
29	c	516	DGD	O5D-C6D-C5D	-2.26	104.86	109.05
22	b	609	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
22	B	609	CLA	CHB-C4A-NA	2.26	127.64	124.51
22	B	616	CLA	OBD-CAD-CBD	-2.26	122.67	125.89
22	C	510	CLA	C11-C10-C8	-2.26	108.62	115.92
29	c	517	DGD	O3D-C3D-C4D	-2.26	105.13	110.35
26	Y	101	LMG	O6-C1-O1	-2.26	104.63	109.97
22	a	402	CLA	OBD-CAD-CBD	-2.26	122.67	125.89
28	L	102	LHG	C5-O7-C7	-2.26	112.23	117.79
22	B	606	CLA	CMD-C2D-C3D	2.26	128.90	124.68
31	c	514	BCR	C38-C26-C25	-2.25	122.00	124.53
22	C	506	CLA	CGD-CBD-CAD	-2.25	103.44	110.73
31	I	101	BCR	C37-C22-C23	2.25	121.62	118.08
22	b	615	CLA	CHB-C4A-NA	2.25	127.62	124.51
22	B	612	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
29	c	518	DGD	C5B-C4B-C3B	-2.25	103.02	114.42
31	I	101	BCR	C8-C7-C6	-2.25	120.89	127.20
31	b	617	BCR	C3-C4-C5	-2.25	110.07	114.08
22	C	513	CLA	CMC-C2C-C3C	2.24	129.17	124.94
25	A	408	PL9	O2-C1-C2	-2.24	116.64	121.78
31	c	515	BCR	C37-C22-C23	2.24	121.61	118.08
25	d	407	PL9	C12-C13-C14	-2.24	122.26	127.66
26	d	410	LMG	C40-C39-C38	-2.24	103.04	114.42
29	C	516	DGD	C1D-O6D-C5D	-2.24	109.29	113.69
22	B	602	CLA	CGD-CBD-CAD	-2.24	103.48	110.73
22	a	404	CLA	C4A-NA-C1A	2.24	107.71	106.71
31	d	406	BCR	C2-C1-C6	2.24	113.93	110.48
31	D	406	BCR	C3-C4-C5	-2.24	110.08	114.08
22	b	611	CLA	CAA-C2A-C1A	-2.24	104.64	111.97
22	B	614	CLA	OBD-CAD-CBD	-2.24	122.70	125.89
22	B	616	CLA	CMD-C2D-C3D	2.24	128.86	124.68
22	c	504	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
29	C	515	DGD	O5D-C6D-C5D	-2.24	104.91	109.05
22	d	401	CLA	O2D-CGD-CBD	2.24	115.24	111.27
23	d	402	PHO	CHD-C4C-C3C	2.24	129.03	124.49
22	B	615	CLA	C6-C7-C8	-2.24	108.69	115.92
22	C	513	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
22	C	509	CLA	CMC-C2C-C3C	2.23	129.15	124.94
31	T	101	BCR	C30-C25-C26	-2.23	119.47	122.61
22	A	403	CLA	O2A-CGA-O1A	-2.23	117.96	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	516	DGD	O5E-C6E-C5E	-2.23	103.64	111.29
22	C	509	CLA	C2A-C3A-C4A	2.23	105.47	101.87
22	b	605	CLA	OBD-CAD-C3D	2.23	131.68	127.98
31	b	619	BCR	C7-C8-C9	-2.23	122.87	126.23
26	c	519	LMG	C38-C37-C36	-2.23	103.11	114.42
31	t	101	BCR	C35-C13-C14	-2.23	119.81	122.92
22	c	512	CLA	OBD-CAD-CBD	-2.23	122.72	125.89
22	c	502	CLA	O1D-CGD-CBD	2.22	129.03	124.48
22	b	613	CLA	C2A-C3A-C4A	2.22	105.46	101.87
31	B	617	BCR	C3-C4-C5	-2.22	110.11	114.08
22	B	604	CLA	O1D-CGD-CBD	2.22	129.02	124.48
25	A	408	PL9	C36-C37-C38	-2.22	104.60	111.88
31	x	101	BCR	C2-C1-C6	2.22	113.89	110.48
28	D	410	LHG	C27-C26-C25	-2.22	103.18	114.42
22	c	504	CLA	C1-C2-C3	-2.21	122.21	126.04
26	B	626	LMG	C6-C5-C4	-2.21	107.82	113.00
22	b	605	CLA	CMB-C2B-C3B	2.21	128.82	124.68
22	B	611	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
22	A	403	CLA	CHA-C1A-NA	-2.21	121.34	126.40
25	A	408	PL9	C25-C24-C26	2.21	118.98	115.27
31	t	101	BCR	C2-C1-C6	2.20	113.87	110.48
26	A	409	LMG	C3-C4-C5	-2.20	106.31	110.24
29	C	517	DGD	O2D-C2D-C1D	-2.20	104.70	110.05
22	C	507	CLA	CMC-C2C-C3C	2.20	129.09	124.94
26	D	408	LMG	O1-C7-C8	-2.20	105.59	110.90
31	a	405	BCR	C37-C22-C23	2.20	121.54	118.08
22	C	502	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
31	B	619	BCR	C33-C5-C6	-2.20	122.06	124.53
22	B	606	CLA	C4-C3-C5	2.20	118.96	115.27
22	b	616	CLA	C2A-C3A-C4A	2.20	105.42	101.87
29	A	413	DGD	O5E-C6E-C5E	-2.19	103.77	111.29
29	C	516	DGD	C5B-C4B-C3B	-2.19	103.29	114.42
22	b	610	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
22	D	403	CLA	CMD-C2D-C3D	2.19	128.78	124.68
31	a	405	BCR	C29-C30-C25	2.19	113.85	110.48
31	K	101	BCR	C24-C23-C22	-2.19	122.93	126.23
22	B	608	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
28	A	411	LHG	C20-C19-C18	-2.19	103.32	114.42
22	C	505	CLA	OBD-CAD-C3D	2.19	131.61	127.98
28	d	409	LHG	O8-C23-C24	2.19	118.77	111.91
22	a	402	CLA	OBD-CAD-C3D	2.18	131.61	127.98
29	c	517	DGD	O2D-C2D-C1D	-2.18	104.75	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	L	101	SQD	O8-S-O7	-2.18	105.94	111.27
22	b	614	CLA	C4-C3-C2	-2.18	118.08	123.68
29	C	516	DGD	O2D-C2D-C1D	-2.18	104.75	110.05
28	A	411	LHG	C11-C10-C9	-2.18	103.36	114.42
28	e	101	LHG	C20-C19-C18	-2.18	103.36	114.42
25	D	407	PL9	C27-C28-C29	-2.18	122.42	127.66
29	c	516	DGD	O3E-C3E-C2E	-2.18	105.32	110.35
22	d	403	CLA	C1-C2-C3	-2.18	122.28	126.04
31	b	619	BCR	C31-C1-C6	2.18	113.83	110.30
22	b	602	CLA	C16-C15-C13	-2.17	108.89	115.92
22	B	613	CLA	CMC-C2C-C3C	2.17	129.04	124.94
26	D	412	LMG	O1-C7-C8	-2.17	106.02	111.78
31	C	514	BCR	C33-C5-C6	-2.17	122.09	124.53
22	B	606	CLA	C2A-C3A-C4A	2.17	105.38	101.87
26	B	626	LMG	O6-C1-O1	-2.17	104.83	109.97
28	d	408	LHG	C27-C26-C25	-2.17	103.42	114.42
22	C	502	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
31	B	617	BCR	C15-C14-C13	-2.17	124.22	127.31
22	C	511	CLA	C1B-CHB-C4A	-2.17	125.83	130.12
28	D	413	LHG	C11-C10-C9	-2.17	103.43	114.42
22	C	509	CLA	CAA-C2A-C3A	-2.17	106.85	112.78
23	A	404	PHO	CMB-C2B-C1B	-2.16	121.73	125.06
29	h	101	DGD	CBB-CAB-C9B	-2.16	103.44	114.42
29	C	517	DGD	CDB-CCB-CBB	-2.16	103.44	114.42
22	c	511	CLA	O1A-CGA-CBA	2.16	132.17	123.73
31	T	101	BCR	C38-C26-C25	-2.16	122.10	124.53
31	b	618	BCR	C15-C14-C13	-2.16	124.22	127.31
31	k	101	BCR	C2-C1-C6	2.16	113.81	110.48
22	d	401	CLA	O2A-C1-C2	-2.16	102.96	108.64
22	b	602	CLA	CMD-C2D-C3D	2.16	128.72	124.68
22	B	614	CLA	CBC-CAC-C3C	-2.16	106.77	112.27
28	a	410	LHG	O8-C23-O10	-2.16	118.14	123.59
25	a	409	PL9	C41-C39-C38	-2.16	116.75	121.12
31	c	515	BCR	C30-C25-C26	-2.16	119.57	122.61
28	d	408	LHG	C20-C19-C18	-2.16	103.47	114.42
22	B	602	CLA	CMC-C2C-C3C	2.16	129.01	124.94
28	D	411	LHG	C18-C17-C16	-2.15	103.49	114.42
22	D	404	CLA	O2A-C1-C2	-2.15	102.97	108.64
31	c	515	BCR	C38-C26-C27	-2.15	109.48	113.62
26	m	101	LMG	C9-C8-C7	-2.15	106.69	111.79
28	L	102	LHG	C20-C19-C18	-2.15	103.49	114.42
25	A	408	PL9	C41-C39-C38	-2.15	116.76	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Y	101	LMG	C38-C37-C36	-2.15	103.50	114.42
22	b	613	CLA	C4D-C3D-CAD	-2.15	107.27	108.47
29	H	102	DGD	C4D-C3D-C2D	-2.15	107.07	110.82
22	C	507	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
28	D	410	LHG	O8-C23-O10	-2.15	118.16	123.59
22	c	508	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
22	b	603	CLA	CED-O2D-CGD	-2.15	111.08	115.94
31	b	617	BCR	C38-C26-C25	-2.14	122.12	124.53
27	t	102	SQD	O49-C7-C8	-2.14	115.37	123.73
22	B	606	CLA	CHA-C1A-NA	-2.14	121.49	126.40
22	B	609	CLA	C4D-C3D-CAD	-2.14	107.28	108.47
22	c	511	CLA	CHB-C4A-NA	2.14	127.47	124.51
22	B	610	CLA	CMC-C2C-C3C	2.14	128.98	124.94
22	D	403	CLA	CHB-C4A-NA	2.14	127.47	124.51
29	C	517	DGD	C8B-C7B-C6B	-2.14	103.56	114.42
22	a	404	CLA	OBD-CAD-C3D	2.14	131.53	127.98
22	c	509	CLA	C16-C15-C13	-2.14	109.00	115.92
22	B	608	CLA	C1-O2A-CGA	2.14	122.06	116.44
22	B	606	CLA	O2D-CGD-CBD	2.14	115.07	111.27
29	C	517	DGD	C7A-C6A-C5A	-2.14	103.57	114.42
22	b	608	CLA	CBC-CAC-C3C	2.14	117.71	112.27
22	b	613	CLA	CMC-C2C-C3C	2.14	128.97	124.94
22	B	605	CLA	CAA-CBA-CGA	-2.13	107.02	113.25
22	C	505	CLA	C4A-NA-C1A	2.13	107.67	106.71
22	B	607	CLA	C1B-CHB-C4A	-2.13	125.89	130.12
31	b	618	BCR	C27-C26-C25	2.13	125.83	122.73
31	k	102	BCR	C37-C22-C21	-2.13	119.94	122.92
22	b	603	CLA	O1D-CGD-CBD	2.13	128.84	124.48
22	D	405	CLA	CHA-C1A-NA	-2.13	121.52	126.40
29	c	518	DGD	C7B-C6B-C5B	-2.13	103.62	114.42
29	A	413	DGD	O1G-C1A-O1A	-2.13	118.22	123.59
25	A	408	PL9	C40-C39-C38	-2.13	118.22	123.68
22	B	604	CLA	CMD-C2D-C3D	2.13	128.66	124.68
27	f	102	SQD	C46-C45-C44	-2.12	106.76	111.79
27	f	102	SQD	O5-C1-O6	2.12	115.00	109.97
26	M	101	LMG	O5-C6-C5	-2.12	104.01	111.29
29	C	515	DGD	CAB-C9B-C8B	-2.12	103.65	114.42
22	B	610	CLA	C1-C2-C3	-2.12	122.37	126.04
29	c	518	DGD	C3D-C4D-C5D	-2.12	106.45	110.24
31	c	515	BCR	C36-C18-C17	-2.12	119.95	122.92
31	B	619	BCR	C27-C26-C25	2.12	125.81	122.73
31	d	406	BCR	C30-C25-C26	-2.12	119.63	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	F	101	HEM	C3C-C4C-NC	-2.12	106.94	110.94
22	B	607	CLA	CBC-CAC-C3C	-2.12	106.87	112.27
22	B	609	CLA	CBC-CAC-C3C	-2.12	106.87	112.27
29	c	518	DGD	O6E-C1E-O5D	-2.12	104.96	109.97
29	h	101	DGD	C2G-O2G-C1B	2.12	123.00	117.79
26	M	101	LMG	C1-O6-C5	-2.12	109.54	113.69
26	A	409	LMG	C36-C35-C34	-2.11	103.69	114.42
22	d	401	CLA	CMB-C2B-C3B	2.11	128.63	124.68
22	b	612	CLA	C1-C2-C3	-2.11	122.39	126.04
31	b	619	BCR	C1-C6-C5	-2.11	119.64	122.61
22	D	404	CLA	O2D-CGD-CBD	2.11	115.02	111.27
27	a	411	SQD	O5-C5-C4	2.11	113.53	109.69
35	v	201	HEC	CAD-CBD-CGD	-2.11	109.13	112.67
22	B	614	CLA	C6-C7-C8	-2.11	109.09	115.92
29	H	102	DGD	C6D-C5D-C4D	2.11	116.50	112.09
25	D	407	PL9	C50-C49-C48	-2.11	116.55	122.65
28	D	413	LHG	C18-C17-C16	-2.11	103.72	114.42
29	c	516	DGD	O6E-C1E-O5D	-2.11	104.98	109.97
31	t	101	BCR	C12-C13-C14	-2.11	115.70	118.94
22	C	506	CLA	CHA-C1A-NA	-2.11	121.57	126.40
22	C	508	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
22	C	507	CLA	C4D-C3D-CAD	-2.11	107.30	108.47
29	A	413	DGD	CDB-CCB-CBB	-2.11	103.73	114.42
25	d	407	PL9	C11-C9-C8	-2.11	116.86	121.12
28	A	411	LHG	C18-C17-C16	-2.11	103.73	114.42
26	B	626	LMG	C1-O6-C5	-2.11	109.56	113.69
25	D	407	PL9	C37-C38-C39	-2.10	122.59	127.66
34	f	101	HEM	C4A-C3A-C2A	2.10	108.46	107.00
22	b	613	CLA	O2D-CGD-CBD	2.10	115.00	111.27
22	b	601	CLA	CMC-C2C-C3C	2.10	128.90	124.94
29	C	516	DGD	O6E-C1E-O5D	-2.10	105.00	109.97
31	I	101	BCR	C40-C30-C25	2.10	113.70	110.30
22	b	607	CLA	C3A-C2A-C1A	2.10	104.48	101.34
31	K	102	BCR	C2-C1-C6	2.10	113.71	110.48
28	d	409	LHG	C29-C28-C27	-2.10	103.78	114.42
23	d	402	PHO	CMC-C2C-C1C	-2.10	121.84	125.06
22	d	405	CLA	CHA-C1A-NA	-2.09	121.60	126.40
29	c	518	DGD	O6E-C5E-C4E	2.09	113.49	109.69
27	D	409	SQD	C3-C4-C5	2.09	113.97	110.24
22	A	405	CLA	CED-O2D-CGD	-2.09	111.21	115.94
25	a	409	PL9	C45-C44-C43	-2.09	118.32	123.68
22	d	403	CLA	CHB-C4A-NA	2.09	127.40	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	517	DGD	O6E-C1E-O5D	-2.09	105.03	109.97
26	m	101	LMG	C38-C37-C36	-2.09	103.83	114.42
29	c	516	DGD	O6E-C5E-C4E	2.09	113.48	109.69
28	a	410	LHG	O7-C7-C8	-2.08	107.01	111.50
22	C	506	CLA	CMC-C2C-C3C	2.08	128.87	124.94
31	k	102	BCR	C36-C18-C19	2.08	121.36	118.08
22	c	507	CLA	C1-C2-C3	-2.08	122.44	126.04
22	B	615	CLA	C4D-C3D-CAD	2.08	109.63	108.47
22	D	403	CLA	O2D-CGD-O1D	-2.08	119.78	123.84
29	h	101	DGD	CDB-CCB-CBB	-2.08	103.88	114.42
22	B	615	CLA	C3D-CAD-CBD	-2.08	104.87	107.61
29	A	413	DGD	C1D-C2D-C3D	-2.08	105.67	110.00
22	B	609	CLA	CHA-C1A-NA	-2.07	121.65	126.40
26	D	412	LMG	C35-C34-C33	-2.07	103.90	114.42
22	B	601	CLA	O2D-CGD-CBD	2.07	114.95	111.27
31	K	102	BCR	C8-C7-C6	-2.07	121.38	127.20
28	l	101	LHG	O8-C23-O10	-2.07	118.36	123.59
22	c	507	CLA	CHB-C4A-NA	2.07	127.38	124.51
22	c	507	CLA	C7-C6-C5	-2.07	107.73	113.36
31	H	101	BCR	C29-C30-C25	2.07	113.67	110.48
28	A	411	LHG	O8-C23-O10	-2.07	118.37	123.59
26	A	409	LMG	C38-C37-C36	-2.07	103.91	114.42
22	c	508	CLA	C1-C2-C3	-2.07	122.46	126.04
31	b	619	BCR	C15-C16-C17	-2.07	119.23	123.47
31	B	619	BCR	C34-C9-C10	-2.07	120.02	122.92
29	C	516	DGD	O3G-C1D-C2D	-2.07	105.07	108.30
22	b	614	CLA	CMC-C2C-C3C	2.07	128.84	124.94
22	b	609	CLA	C7-C6-C5	-2.07	107.74	113.36
29	C	515	DGD	O6D-C5D-C4D	2.07	113.45	109.69
22	B	601	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
22	B	602	CLA	C6-C5-C3	-2.07	108.04	113.45
29	h	101	DGD	O1G-C1A-O1A	-2.07	118.38	123.59
31	D	406	BCR	C30-C25-C26	-2.06	119.71	122.61
34	f	101	HEM	CAD-CBD-CGD	2.06	116.13	112.67
29	H	102	DGD	O2E-C2E-C3E	-2.06	105.58	110.35
23	d	402	PHO	CBD-CHA-C4D	-2.06	106.22	108.54
22	C	505	CLA	C1-O2A-CGA	-2.06	111.04	116.44
22	b	616	CLA	OBD-CAD-C3D	2.06	131.40	127.98
22	b	604	CLA	CBA-CAA-C2A	-2.06	107.79	113.86
22	B	615	CLA	C4-C3-C5	2.06	118.73	115.27
26	c	521	LMG	C3-C4-C5	-2.06	106.57	110.24
22	b	616	CLA	CMC-C2C-C3C	2.06	128.82	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	509	CLA	C1-O2A-CGA	2.05	121.83	116.44
22	c	507	CLA	C2A-C1A-CHA	2.05	127.45	123.86
22	B	610	CLA	O2A-CGA-CBA	2.05	118.35	111.91
22	C	506	CLA	C1B-CHB-C4A	-2.05	126.05	130.12
31	c	514	BCR	C33-C5-C6	-2.05	122.22	124.53
25	A	408	PL9	C26-C24-C23	-2.05	116.97	121.12
26	m	101	LMG	O8-C28-O10	-2.05	118.42	123.59
22	A	402	CLA	CBC-CAC-C3C	2.05	117.49	112.27
22	c	510	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
31	H	101	BCR	C37-C22-C21	-2.05	120.05	122.92
23	a	403	PHO	O2A-CGA-O1A	-2.05	118.42	123.59
26	A	409	LMG	O8-C28-O10	-2.05	118.42	123.59
22	c	501	CLA	CHB-C4A-NA	2.05	127.34	124.51
22	d	401	CLA	CMD-C2D-C3D	2.05	128.51	124.68
23	A	404	PHO	CMD-C2D-C1D	2.05	128.22	125.06
28	L	102	LHG	C27-C26-C25	-2.05	104.04	114.42
31	b	619	BCR	C16-C15-C14	-2.05	119.28	123.47
31	x	101	BCR	C20-C21-C22	-2.04	124.39	127.31
22	b	611	CLA	C1-O2A-CGA	-2.04	111.08	116.44
29	h	101	DGD	C3E-C4E-C5E	-2.04	106.59	110.24
26	B	621	LMG	C38-C37-C36	-2.04	104.06	114.42
22	c	512	CLA	C3B-C4B-NB	-2.04	106.57	109.21
27	f	102	SQD	C1-O5-C5	-2.04	109.68	113.69
22	B	614	CLA	O2D-CGD-CBD	2.04	114.89	111.27
22	C	506	CLA	O2A-C1-C2	-2.04	103.28	108.64
31	B	619	BCR	C40-C30-C29	-2.04	100.76	108.91
26	b	622	LMG	C40-C39-C38	-2.04	104.09	114.42
27	a	411	SQD	C45-O47-C7	2.04	122.80	117.79
27	f	102	SQD	O47-C7-O49	-2.03	118.79	123.70
25	d	407	PL9	C11-C12-C13	-2.03	105.20	111.88
22	c	512	CLA	C1B-CHB-C4A	-2.03	126.09	130.12
22	c	501	CLA	CHA-C1A-NA	-2.03	121.75	126.40
25	D	407	PL9	C25-C24-C26	2.03	118.68	115.27
25	A	408	PL9	C12-C13-C14	-2.03	122.78	127.66
25	A	408	PL9	C31-C32-C33	-2.03	105.22	111.88
22	C	508	CLA	O1D-CGD-CBD	2.03	128.63	124.48
22	b	613	CLA	OBD-CAD-CBD	-2.03	123.00	125.89
26	Y	101	LMG	C40-C39-C38	-2.02	104.14	114.42
22	d	405	CLA	C4A-NA-C1A	2.02	107.62	106.71
31	Z	101	BCR	C15-C14-C13	-2.02	124.42	127.31
22	d	404	CLA	C2A-C1A-CHA	2.02	127.39	123.86
29	C	516	DGD	O4D-C4D-C5D	-2.02	104.28	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	613	CLA	O2A-C1-C2	-2.02	103.32	108.64
29	c	516	DGD	C5B-C4B-C3B	-2.02	104.17	114.42
31	C	514	BCR	C15-C14-C13	-2.02	124.43	127.31
29	C	515	DGD	C8B-C7B-C6B	-2.02	104.17	114.42
22	B	608	CLA	C4A-NA-C1A	2.02	107.61	106.71
22	b	615	CLA	C3A-C2A-C1A	2.02	104.36	101.34
22	B	609	CLA	C1B-CHB-C4A	-2.02	126.12	130.12
25	d	407	PL9	O1-C4-C3	-2.02	118.50	120.72
25	D	407	PL9	C20-C19-C21	2.02	118.67	115.27
22	B	611	CLA	CBC-CAC-C3C	-2.02	107.13	112.27
22	b	607	CLA	CMD-C2D-C3D	2.01	128.45	124.68
25	a	409	PL9	C21-C19-C18	-2.01	117.04	121.12
29	h	101	DGD	CAB-C9B-C8B	-2.01	104.21	114.42
22	C	511	CLA	CMC-C2C-C3C	2.01	128.73	124.94
28	d	409	LHG	O8-C23-O10	-2.01	118.52	123.59
26	M	101	LMG	C9-C8-C7	-2.01	107.04	111.79
26	M	101	LMG	C37-C36-C35	-2.01	104.23	114.42
31	B	619	BCR	C15-C16-C17	-2.01	119.36	123.47
23	d	402	PHO	CBA-CAA-C2A	-2.01	107.94	113.86
29	c	518	DGD	O3D-C3D-C4D	-2.01	105.71	110.35
22	B	601	CLA	CHB-C4A-NA	2.01	127.28	124.51
26	M	101	LMG	O1-C7-C8	-2.00	106.06	110.90
26	c	519	LMG	C40-C39-C38	-2.00	104.26	114.42
27	B	622	SQD	O8-S-C6	2.00	108.93	105.74

All (60) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	402	CLA	ND
22	A	405	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	612	CLA	ND
22	B	613	CLA	ND
22	B	614	CLA	ND

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Mol	Chain	Res	Type	Atom
22	B	615	CLA	ND
22	B	616	CLA	ND
22	C	501	CLA	ND
22	C	502	CLA	ND
22	C	503	CLA	ND
22	C	504	CLA	ND
22	C	505	CLA	ND
22	C	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	403	CLA	ND
22	D	404	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	609	CLA	ND
22	b	610	CLA	ND
22	b	612	CLA	ND
22	b	613	CLA	ND
22	b	614	CLA	ND
22	b	615	CLA	ND
22	b	616	CLA	ND
22	c	501	CLA	ND
22	c	503	CLA	ND
22	c	504	CLA	ND
22	c	505	CLA	ND
22	c	506	CLA	ND
22	c	507	CLA	ND
22	c	509	CLA	ND
22	c	510	CLA	ND
22	c	511	CLA	ND
22	c	512	CLA	ND

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Mol	Chain	Res	Type	Atom
22	c	513	CLA	ND
22	d	403	CLA	ND
22	d	404	CLA	ND
22	d	405	CLA	ND

All (2059) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	402	CLA	C2C-C3C-CAC-CBC
22	A	403	CLA	CHA-CBD-CGD-O1D
22	A	403	CLA	CHA-CBD-CGD-O2D
22	B	603	CLA	C4-C3-C5-C6
22	B	612	CLA	CHA-CBD-CGD-O1D
22	B	612	CLA	CHA-CBD-CGD-O2D
22	B	614	CLA	CHA-CBD-CGD-O1D
22	B	614	CLA	CHA-CBD-CGD-O2D
22	C	502	CLA	CHA-CBD-CGD-O1D
22	C	502	CLA	CHA-CBD-CGD-O2D
22	C	502	CLA	CAD-CBD-CGD-O1D
22	C	502	CLA	C14-C13-C15-C16
22	C	507	CLA	C2-C3-C5-C6
22	C	507	CLA	C4-C3-C5-C6
22	C	508	CLA	CHA-CBD-CGD-O1D
22	C	508	CLA	CHA-CBD-CGD-O2D
22	C	512	CLA	C1A-C2A-CAA-CBA
22	D	405	CLA	C11-C12-C13-C14
22	b	601	CLA	C1A-C2A-CAA-CBA
22	b	605	CLA	C2-C3-C5-C6
22	b	605	CLA	C4-C3-C5-C6
22	b	608	CLA	C2C-C3C-CAC-CBC
22	b	611	CLA	CHA-CBD-CGD-O1D
22	b	613	CLA	C11-C10-C8-C7
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	C4-C3-C5-C6
22	c	506	CLA	C1A-C2A-CAA-CBA
22	c	506	CLA	C3A-C2A-CAA-CBA
22	c	506	CLA	CBD-CGD-O2D-CED
22	c	508	CLA	CHA-CBD-CGD-O1D
22	c	508	CLA	CHA-CBD-CGD-O2D
22	c	508	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	c	509	CLA	C6-C7-C8-C9
22	c	512	CLA	C1A-C2A-CAA-CBA
22	c	512	CLA	C2A-CAA-CBA-CGA
22	c	513	CLA	C1A-C2A-CAA-CBA
22	c	513	CLA	C3A-C2A-CAA-CBA
22	c	513	CLA	C2A-CAA-CBA-CGA
22	d	401	CLA	CHA-CBD-CGD-O1D
22	d	401	CLA	CHA-CBD-CGD-O2D
22	d	404	CLA	CHA-CBD-CGD-O1D
22	d	404	CLA	CHA-CBD-CGD-O2D
23	d	402	PHO	C6-C7-C8-C9
25	A	408	PL9	C22-C23-C24-C26
25	A	408	PL9	C23-C24-C26-C27
25	A	408	PL9	C24-C26-C27-C28
25	A	408	PL9	C32-C33-C34-C36
25	A	408	PL9	C34-C36-C37-C38
25	A	408	PL9	C37-C38-C39-C40
25	A	408	PL9	C40-C39-C41-C42
25	D	407	PL9	C32-C33-C34-C36
25	D	407	PL9	C42-C43-C44-C45
25	D	407	PL9	C47-C48-C49-C50
25	a	409	PL9	C9-C11-C12-C13
25	a	409	PL9	C12-C13-C14-C15
25	a	409	PL9	C12-C13-C14-C16
25	a	409	PL9	C17-C18-C19-C21
25	a	409	PL9	C19-C21-C22-C23
25	a	409	PL9	C22-C23-C24-C25
25	a	409	PL9	C22-C23-C24-C26
25	a	409	PL9	C24-C26-C27-C28
25	a	409	PL9	C28-C29-C31-C32
25	a	409	PL9	C32-C33-C34-C35
25	a	409	PL9	C37-C38-C39-C40
25	a	409	PL9	C42-C43-C44-C45
25	d	407	PL9	C27-C28-C29-C31
25	d	407	PL9	C40-C39-C41-C42
25	d	407	PL9	C47-C48-C49-C50
26	A	409	LMG	O9-C10-O7-C8
26	B	621	LMG	C28-C29-C30-C31
26	D	412	LMG	C11-C10-O7-C8
26	Y	101	LMG	C11-C10-O7-C8
26	b	622	LMG	C11-C10-O7-C8
26	c	521	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
26	c	522	LMG	O6-C1-O1-C7
27	A	410	SQD	C2-C1-O6-C44
27	A	410	SQD	O5-C1-O6-C44
27	B	622	SQD	C2-C1-O6-C44
27	B	622	SQD	O5-C1-O6-C44
27	B	622	SQD	O6-C44-C45-O47
27	B	622	SQD	O49-C7-O47-C45
27	B	622	SQD	C8-C7-O47-C45
27	L	101	SQD	O49-C7-O47-C45
27	L	101	SQD	C8-C7-O47-C45
27	a	411	SQD	O6-C44-C45-O47
27	f	102	SQD	C2-C1-O6-C44
27	f	102	SQD	O5-C1-O6-C44
27	t	102	SQD	O47-C45-C46-O48
27	t	102	SQD	C8-C7-O47-C45
28	D	410	LHG	O1-C1-C2-C3
28	D	410	LHG	C3-O3-P-O5
28	D	410	LHG	C4-O6-P-O4
28	D	413	LHG	O1-C1-C2-C3
28	D	413	LHG	C1-C2-C3-O3
28	L	102	LHG	C3-O3-P-O4
28	L	102	LHG	C4-O6-P-O4
28	a	410	LHG	C4-O6-P-O3
28	a	410	LHG	C4-O6-P-O4
28	a	410	LHG	C4-O6-P-O5
28	d	408	LHG	C4-O6-P-O4
28	d	409	LHG	C4-O6-P-O4
28	e	101	LHG	O1-C1-C2-O2
28	e	101	LHG	O1-C1-C2-C3
28	e	101	LHG	C3-O3-P-O4
28	e	101	LHG	O6-C4-C5-O7
28	e	101	LHG	O10-C23-O8-C6
28	e	101	LHG	C24-C23-O8-C6
29	A	413	DGD	O2G-C2G-C3G-O3G
31	B	617	BCR	C35-C13-C14-C15
31	B	618	BCR	C11-C10-C9-C34
31	B	618	BCR	C10-C11-C12-C13
31	B	618	BCR	C37-C22-C23-C24
31	B	618	BCR	C23-C24-C25-C30
31	B	619	BCR	C7-C8-C9-C34
31	B	619	BCR	C37-C22-C23-C24
31	C	514	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
31	D	406	BCR	C7-C8-C9-C10
31	D	406	BCR	C37-C22-C23-C24
31	D	406	BCR	C22-C23-C24-C25
31	D	406	BCR	C23-C24-C25-C26
31	H	101	BCR	C11-C12-C13-C14
31	H	101	BCR	C36-C18-C19-C20
31	I	101	BCR	C16-C17-C18-C19
31	K	101	BCR	C16-C17-C18-C36
31	K	101	BCR	C21-C22-C23-C24
31	K	101	BCR	C37-C22-C23-C24
31	K	102	BCR	C11-C10-C9-C34
31	K	102	BCR	C11-C12-C13-C14
31	K	102	BCR	C11-C12-C13-C35
31	T	101	BCR	C1-C6-C7-C8
31	T	101	BCR	C7-C8-C9-C34
31	T	101	BCR	C9-C10-C11-C12
31	T	101	BCR	C11-C12-C13-C14
31	T	101	BCR	C16-C17-C18-C19
31	T	101	BCR	C16-C17-C18-C36
31	Z	101	BCR	C6-C7-C8-C9
31	Z	101	BCR	C7-C8-C9-C34
31	Z	101	BCR	C14-C15-C16-C17
31	Z	101	BCR	C16-C17-C18-C36
31	Z	101	BCR	C36-C18-C19-C20
31	a	405	BCR	C37-C22-C23-C24
31	b	617	BCR	C21-C22-C23-C24
31	b	618	BCR	C37-C22-C23-C24
31	b	619	BCR	C11-C12-C13-C14
31	b	619	BCR	C12-C13-C14-C15
31	b	619	BCR	C35-C13-C14-C15
31	c	514	BCR	C6-C7-C8-C9
31	c	514	BCR	C7-C8-C9-C10
31	c	514	BCR	C18-C19-C20-C21
31	c	514	BCR	C20-C21-C22-C37
31	d	406	BCR	C37-C22-C23-C24
31	d	406	BCR	C22-C23-C24-C25
31	d	406	BCR	C23-C24-C25-C30
31	k	101	BCR	C7-C8-C9-C10
31	k	101	BCR	C7-C8-C9-C34
31	k	101	BCR	C23-C24-C25-C30
31	k	102	BCR	C37-C22-C23-C24
31	t	101	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
31	t	101	BCR	C11-C12-C13-C35
31	t	101	BCR	C35-C13-C14-C15
31	t	101	BCR	C16-C17-C18-C19
31	t	101	BCR	C16-C17-C18-C36
31	t	101	BCR	C36-C18-C19-C20
31	x	101	BCR	C7-C8-C9-C34
32	B	624	STE	C1-C2-C3-C4
32	B	627	STE	C1-C2-C3-C4
32	J	101	STE	C1-C2-C3-C4
32	L	103	STE	C1-C2-C3-C4
32	M	102	STE	C1-C2-C3-C4
32	R	101	STE	C1-C2-C3-C4
32	b	623	STE	C1-C2-C3-C4
32	x	102	STE	C1-C2-C3-C4
26	c	519	LMG	C11-C10-O7-C8
22	C	509	CLA	O1D-CGD-O2D-CED
22	B	614	CLA	C15-C16-C17-C18
22	b	614	CLA	O1D-CGD-O2D-CED
22	B	601	CLA	CBD-CGD-O2D-CED
22	B	612	CLA	CBD-CGD-O2D-CED
22	C	501	CLA	CBD-CGD-O2D-CED
22	C	509	CLA	CBD-CGD-O2D-CED
22	b	601	CLA	CBD-CGD-O2D-CED
22	b	614	CLA	CBD-CGD-O2D-CED
22	c	510	CLA	CBD-CGD-O2D-CED
22	c	513	CLA	CBD-CGD-O2D-CED
22	B	601	CLA	O1A-CGA-O2A-C1
26	c	521	LMG	O10-C28-O8-C9
26	c	522	LMG	O10-C28-O8-C9
22	c	506	CLA	O1D-CGD-O2D-CED
22	c	508	CLA	O1D-CGD-O2D-CED
22	B	601	CLA	CBA-CGA-O2A-C1
25	D	407	PL9	C47-C48-C49-C51
25	a	409	PL9	C47-C48-C49-C50
25	a	409	PL9	C47-C48-C49-C51
25	d	407	PL9	C47-C48-C49-C51
22	B	616	CLA	CBD-CGD-O2D-CED
22	b	607	CLA	CBD-CGD-O2D-CED
22	b	613	CLA	CBD-CGD-O2D-CED
22	B	604	CLA	O1A-CGA-O2A-C1
26	M	101	LMG	O10-C28-O8-C9
27	L	101	SQD	O10-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
26	c	519	LMG	O9-C10-O7-C8
22	d	405	CLA	CBD-CGD-O2D-CED
22	b	601	CLA	O1D-CGD-O2D-CED
26	Y	101	LMG	O9-C10-O7-C8
26	b	622	LMG	O9-C10-O7-C8
27	f	102	SQD	O49-C7-O47-C45
27	t	102	SQD	O49-C7-O47-C45
29	A	413	DGD	O1B-C1B-O2G-C2G
22	B	604	CLA	C3-C5-C6-C7
22	C	506	CLA	C3-C5-C6-C7
22	b	614	CLA	C3-C5-C6-C7
22	B	604	CLA	CBA-CGA-O2A-C1
27	L	101	SQD	C24-C23-O48-C46
26	A	409	LMG	C11-C10-O7-C8
29	A	413	DGD	C2B-C1B-O2G-C2G
26	A	409	LMG	O6-C5-C6-O5
22	A	405	CLA	C4-C3-C5-C6
22	B	614	CLA	C4-C3-C5-C6
25	a	409	PL9	C25-C24-C26-C27
22	B	614	CLA	C2-C3-C5-C6
22	b	614	CLA	C2-C3-C5-C6
25	a	409	PL9	C38-C39-C41-C42
22	D	405	CLA	CBD-CGD-O2D-CED
22	B	606	CLA	C2A-CAA-CBA-CGA
22	b	606	CLA	C2A-CAA-CBA-CGA
22	B	605	CLA	C3-C5-C6-C7
22	b	609	CLA	C3-C5-C6-C7
26	c	522	LMG	C29-C28-O8-C9
25	a	409	PL9	C27-C28-C29-C30
28	d	409	LHG	C24-C25-C26-C27
22	B	601	CLA	O1D-CGD-O2D-CED
26	D	412	LMG	O9-C10-O7-C8
26	c	521	LMG	O9-C10-O7-C8
25	A	408	PL9	C37-C38-C39-C41
25	a	409	PL9	C37-C38-C39-C41
25	a	409	PL9	C42-C43-C44-C46
26	c	521	LMG	O6-C5-C6-O5
22	B	604	CLA	CBD-CGD-O2D-CED
22	b	603	CLA	CBD-CGD-O2D-CED
22	c	511	CLA	CBD-CGD-O2D-CED
28	D	413	LHG	O2-C2-C3-O3
22	C	512	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	b	601	CLA	C3-C5-C6-C7
22	c	510	CLA	C3-C5-C6-C7
26	M	101	LMG	C29-C28-O8-C9
27	t	102	SQD	C24-C23-O48-C46
22	c	510	CLA	O1D-CGD-O2D-CED
22	c	513	CLA	O1D-CGD-O2D-CED
29	A	413	DGD	O6E-C5E-C6E-O5E
31	b	619	BCR	C14-C15-C16-C17
22	B	612	CLA	O1D-CGD-O2D-CED
22	c	501	CLA	CBD-CGD-O2D-CED
22	A	405	CLA	C3-C5-C6-C7
26	c	521	LMG	C29-C28-O8-C9
27	f	102	SQD	C24-C23-O48-C46
29	c	518	DGD	O1A-C1A-O1G-C1G
22	B	604	CLA	C4-C3-C5-C6
22	C	504	CLA	C4-C3-C5-C6
26	A	409	LMG	C4-C5-C6-O5
22	B	603	CLA	C2-C3-C5-C6
22	B	604	CLA	C2-C3-C5-C6
22	C	504	CLA	C2-C3-C5-C6
25	d	407	PL9	C38-C39-C41-C42
26	Y	101	LMG	O6-C5-C6-O5
27	D	409	SQD	O10-C23-O48-C46
25	A	408	PL9	C44-C46-C47-C48
25	D	407	PL9	C44-C46-C47-C48
25	d	407	PL9	C44-C46-C47-C48
22	d	405	CLA	C3-C5-C6-C7
29	C	515	DGD	O6E-C5E-C6E-O5E
29	h	101	DGD	C4E-C5E-C6E-O5E
22	C	501	CLA	O1D-CGD-O2D-CED
27	f	102	SQD	C8-C7-O47-C45
32	B	623	STE	C4-C5-C6-C7
25	A	408	PL9	C17-C18-C19-C20
25	a	409	PL9	C17-C18-C19-C20
22	B	616	CLA	O1D-CGD-O2D-CED
22	b	613	CLA	O1D-CGD-O2D-CED
22	d	405	CLA	O1D-CGD-O2D-CED
26	B	626	LMG	O6-C5-C6-O5
28	e	101	LHG	C1-C2-C3-O3
22	b	602	CLA	C3-C5-C6-C7
26	B	626	LMG	C29-C28-O8-C9
27	B	622	SQD	C24-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
27	D	409	SQD	C24-C23-O48-C46
29	c	518	DGD	C2A-C1A-O1G-C1G
32	c	520	STE	C2-C3-C4-C5
32	b	621	STE	C14-C15-C16-C17
22	C	507	CLA	C5-C6-C7-C8
22	c	507	CLA	C5-C6-C7-C8
22	c	511	CLA	C13-C15-C16-C17
22	c	511	CLA	C15-C16-C17-C18
22	c	512	CLA	C13-C15-C16-C17
28	A	411	LHG	O2-C2-C3-O3
28	d	408	LHG	O2-C2-C3-O3
28	d	409	LHG	C23-C24-C25-C26
29	C	516	DGD	C1B-C2B-C3B-C4B
32	a	413	STE	C4-C5-C6-C7
27	f	102	SQD	O10-C23-O48-C46
22	A	405	CLA	C2-C3-C5-C6
25	D	407	PL9	C33-C34-C36-C37
22	A	403	CLA	C14-C13-C15-C16
22	B	601	CLA	C11-C12-C13-C14
22	B	606	CLA	C11-C10-C8-C9
22	B	607	CLA	C14-C13-C15-C16
22	B	609	CLA	C14-C13-C15-C16
22	B	610	CLA	C14-C13-C15-C16
22	B	614	CLA	C11-C12-C13-C14
22	B	614	CLA	C14-C13-C15-C16
22	C	503	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	C11-C10-C8-C9
22	b	605	CLA	C11-C10-C8-C9
22	b	607	CLA	C11-C10-C8-C9
22	b	613	CLA	C11-C12-C13-C14
22	b	616	CLA	C11-C10-C8-C9
22	c	503	CLA	C11-C12-C13-C14
22	c	512	CLA	C6-C7-C8-C9
22	d	405	CLA	C11-C12-C13-C14
23	A	404	PHO	C14-C13-C15-C16
22	b	607	CLA	O1D-CGD-O2D-CED
22	c	512	CLA	CBD-CGD-O2D-CED
28	A	411	LHG	C32-C33-C34-C35
22	C	506	CLA	C15-C16-C17-C18
31	I	101	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
31	K	102	BCR	C7-C8-C9-C34
31	T	101	BCR	C11-C12-C13-C35
31	b	617	BCR	C7-C8-C9-C34
31	b	619	BCR	C37-C22-C23-C24
31	c	514	BCR	C7-C8-C9-C34
31	t	101	BCR	C7-C8-C9-C34
31	T	101	BCR	C7-C8-C9-C10
26	c	522	LMG	O6-C5-C6-O5
27	B	622	SQD	C11-C10-C9-C8
28	A	411	LHG	C27-C28-C29-C30
26	D	408	LMG	C10-C11-C12-C13
28	a	410	LHG	C7-C8-C9-C10
22	B	609	CLA	C15-C16-C17-C18
22	C	503	CLA	C5-C6-C7-C8
22	c	507	CLA	C8-C10-C11-C12
22	c	512	CLA	CBA-CGA-O2A-C1
22	B	603	CLA	C8-C10-C11-C12
22	B	604	CLA	C5-C6-C7-C8
22	B	606	CLA	C8-C10-C11-C12
22	B	607	CLA	C5-C6-C7-C8
22	B	610	CLA	C8-C10-C11-C12
22	C	509	CLA	C10-C11-C12-C13
22	C	510	CLA	C13-C15-C16-C17
22	a	404	CLA	C5-C6-C7-C8
22	b	605	CLA	C5-C6-C7-C8
22	b	608	CLA	C8-C10-C11-C12
27	A	410	SQD	C7-C8-C9-C10
27	L	101	SQD	C7-C8-C9-C10
32	B	625	STE	C9-C10-C11-C12
22	B	614	CLA	C13-C15-C16-C17
22	C	502	CLA	C15-C16-C17-C18
22	C	508	CLA	C10-C11-C12-C13
22	D	404	CLA	C13-C15-C16-C17
22	b	603	CLA	C10-C11-C12-C13
22	b	611	CLA	C10-C11-C12-C13
22	c	505	CLA	C15-C16-C17-C18
22	c	510	CLA	C5-C6-C7-C8
25	A	408	PL9	C47-C48-C49-C51
28	D	410	LHG	O1-C1-C2-O2
26	B	626	LMG	C10-C11-C12-C13
26	D	412	LMG	C28-C29-C30-C31
26	M	101	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	d	410	LMG	C28-C29-C30-C31
26	m	101	LMG	C10-C11-C12-C13
27	B	622	SQD	C7-C8-C9-C10
28	l	101	LHG	C23-C24-C25-C26
26	c	521	LMG	C4-C5-C6-O5
22	B	613	CLA	C8-C10-C11-C12
22	C	505	CLA	C10-C11-C12-C13
25	a	409	PL9	C27-C28-C29-C31
32	B	627	STE	C5-C6-C7-C8
22	B	607	CLA	C8-C10-C11-C12
22	D	403	CLA	C15-C16-C17-C18
22	D	405	CLA	C10-C11-C12-C13
22	c	510	CLA	C10-C11-C12-C13
27	B	622	SQD	C23-C24-C25-C26
28	d	408	LHG	C7-C8-C9-C10
22	b	605	CLA	CBD-CGD-O2D-CED
22	c	502	CLA	CBD-CGD-O2D-CED
32	b	625	STE	C2-C3-C4-C5
22	B	610	CLA	C15-C16-C17-C18
22	B	611	CLA	C13-C15-C16-C17
26	Y	101	LMG	C4-C5-C6-O5
22	C	510	CLA	C12-C13-C15-C16
22	b	609	CLA	C11-C12-C13-C15
22	b	613	CLA	C11-C12-C13-C15
22	b	615	CLA	C11-C12-C13-C15
22	d	405	CLA	C6-C7-C8-C10
22	b	601	CLA	C2A-CAA-CBA-CGA
22	B	614	CLA	C8-C10-C11-C12
22	C	506	CLA	C8-C10-C11-C12
22	b	606	CLA	C10-C11-C12-C13
22	b	610	CLA	C13-C15-C16-C17
22	b	615	CLA	C8-C10-C11-C12
22	C	502	CLA	CBD-CGD-O2D-CED
26	Y	101	LMG	O6-C1-O1-C7
26	m	101	LMG	O6-C1-O1-C7
29	c	517	DGD	O6E-C1E-O5D-C6D
22	B	608	CLA	C15-C16-C17-C18
25	D	407	PL9	C34-C36-C37-C38
25	a	409	PL9	C14-C16-C17-C18
31	B	618	BCR	C18-C19-C20-C21
31	H	101	BCR	C10-C11-C12-C13
31	K	101	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	K	102	BCR	C18-C19-C20-C21
31	T	101	BCR	C18-C19-C20-C21
31	Z	101	BCR	C18-C19-C20-C21
31	c	515	BCR	C18-C19-C20-C21
31	k	101	BCR	C10-C11-C12-C13
28	e	101	LHG	O2-C2-C3-O3
22	c	509	CLA	C10-C11-C12-C13
26	B	626	LMG	O10-C28-O8-C9
27	A	410	SQD	C23-C24-C25-C26
22	B	601	CLA	C13-C15-C16-C17
22	C	509	CLA	C13-C15-C16-C17
22	C	510	CLA	C15-C16-C17-C18
22	d	401	CLA	C8-C10-C11-C12
22	d	401	CLA	C13-C15-C16-C17
22	C	513	CLA	C13-C15-C16-C17
22	D	404	CLA	C15-C16-C17-C18
22	b	607	CLA	C8-C10-C11-C12
22	b	614	CLA	C8-C10-C11-C12
22	b	615	CLA	C15-C16-C17-C18
28	D	411	LHG	C3-O3-P-O6
28	d	408	LHG	C4-O6-P-O3
28	e	101	LHG	C3-O3-P-O6
22	C	511	CLA	C8-C10-C11-C12
22	C	513	CLA	C15-C16-C17-C18
22	b	614	CLA	C13-C15-C16-C17
26	b	622	LMG	C28-C29-C30-C31
26	d	410	LMG	C10-C11-C12-C13
28	A	411	LHG	C1-C2-C3-O3
22	b	604	CLA	C4-C3-C5-C6
28	D	413	LHG	C31-C32-C33-C34
22	B	606	CLA	C16-C17-C18-C20
29	h	101	DGD	O6E-C5E-C6E-O5E
22	b	604	CLA	C3-C5-C6-C7
22	b	607	CLA	CBA-CGA-O2A-C1
26	c	521	LMG	C41-C42-C43-C44
32	b	625	STE	C4-C5-C6-C7
27	A	412	SQD	C12-C13-C14-C15
27	B	622	SQD	C28-C29-C30-C31
27	L	101	SQD	C24-C25-C26-C27
28	l	101	LHG	C15-C16-C17-C18
29	A	413	DGD	C2B-C3B-C4B-C5B
32	C	518	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
32	d	412	STE	C4-C5-C6-C7
31	B	617	BCR	C16-C17-C18-C36
31	B	617	BCR	C20-C21-C22-C37
31	B	618	BCR	C20-C21-C22-C37
31	B	619	BCR	C35-C13-C14-C15
31	C	514	BCR	C16-C17-C18-C36
31	D	406	BCR	C11-C10-C9-C34
31	D	406	BCR	C20-C21-C22-C37
31	I	101	BCR	C16-C17-C18-C36
31	I	101	BCR	C20-C21-C22-C37
31	K	101	BCR	C11-C10-C9-C34
31	Z	101	BCR	C20-C21-C22-C37
31	b	617	BCR	C35-C13-C14-C15
31	b	617	BCR	C20-C21-C22-C37
31	c	515	BCR	C16-C17-C18-C36
31	c	515	BCR	C20-C21-C22-C37
31	d	406	BCR	C20-C21-C22-C37
31	t	101	BCR	C20-C21-C22-C37
26	b	622	LMG	C19-C20-C21-C22
26	c	519	LMG	C31-C32-C33-C34
27	t	102	SQD	C30-C31-C32-C33
28	A	411	LHG	C26-C27-C28-C29
28	a	410	LHG	C32-C33-C34-C35
29	A	413	DGD	C4B-C5B-C6B-C7B
29	C	517	DGD	C4B-C5B-C6B-C7B
32	B	624	STE	C10-C11-C12-C13
32	Z	102	STE	C13-C14-C15-C16
32	a	413	STE	C7-C8-C9-C10
32	b	627	STE	C13-C14-C15-C16
32	d	412	STE	C12-C13-C14-C15
22	B	601	CLA	C16-C17-C18-C19
22	b	602	CLA	C16-C17-C18-C20
22	c	503	CLA	C16-C17-C18-C20
26	M	101	LMG	C12-C13-C14-C15
26	M	101	LMG	C37-C38-C39-C40
26	b	622	LMG	C11-C12-C13-C14
26	c	522	LMG	C17-C18-C19-C20
26	c	522	LMG	C30-C31-C32-C33
27	t	102	SQD	C15-C16-C17-C18
28	d	408	LHG	C11-C12-C13-C14
28	d	409	LHG	C29-C30-C31-C32
29	A	413	DGD	C2A-C3A-C4A-C5A

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Mol	Chain	Res	Type	Atoms
29	A	413	DGD	CBB-CCB-CDB-CEB
29	C	516	DGD	C6A-C7A-C8A-C9A
29	C	516	DGD	C9B-CAB-CBB-CCB
29	C	517	DGD	C6A-C7A-C8A-C9A
29	c	516	DGD	C4B-C5B-C6B-C7B
32	b	623	STE	C3-C4-C5-C6
32	b	627	STE	C11-C12-C13-C14
32	d	411	STE	C5-C6-C7-C8
27	L	101	SQD	C46-C45-O47-C7
26	A	409	LMG	C13-C14-C15-C16
26	c	521	LMG	C15-C16-C17-C18
26	c	522	LMG	C32-C33-C34-C35
27	a	411	SQD	C11-C10-C9-C8
27	f	102	SQD	C30-C31-C32-C33
28	a	410	LHG	C15-C16-C17-C18
28	e	101	LHG	C11-C10-C9-C8
28	e	101	LHG	C27-C28-C29-C30
29	C	516	DGD	C3B-C4B-C5B-C6B
32	x	102	STE	C14-C15-C16-C17
26	B	626	LMG	C22-C23-C24-C25
26	c	522	LMG	C11-C12-C13-C14
29	C	516	DGD	C2B-C3B-C4B-C5B
29	c	516	DGD	C3B-C4B-C5B-C6B
29	c	517	DGD	C8A-C9A-CAA-CBA
29	h	101	DGD	C5B-C6B-C7B-C8B
32	b	620	STE	C4-C5-C6-C7
32	b	627	STE	C7-C8-C9-C10
32	x	102	STE	C9-C10-C11-C12
28	D	410	LHG	O2-C2-C3-O3
26	A	409	LMG	C36-C37-C38-C39
26	B	626	LMG	C12-C13-C14-C15
26	M	101	LMG	C30-C31-C32-C33
27	D	409	SQD	C26-C27-C28-C29
27	D	409	SQD	C28-C29-C30-C31
27	a	411	SQD	C16-C17-C18-C19
27	t	102	SQD	C11-C12-C13-C14
28	L	102	LHG	C12-C13-C14-C15
29	c	517	DGD	C7B-C8B-C9B-CAB
32	B	623	STE	C6-C7-C8-C9
32	B	624	STE	C5-C6-C7-C8
32	b	624	STE	C6-C7-C8-C9
32	c	520	STE	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
26	Y	101	LMG	C2-C1-O1-C7
26	c	522	LMG	C2-C1-O1-C7
26	m	101	LMG	C2-C1-O1-C7
29	c	517	DGD	C2E-C1E-O5D-C6D
31	B	617	BCR	C12-C13-C14-C15
31	B	618	BCR	C11-C10-C9-C8
31	B	618	BCR	C12-C13-C14-C15
31	B	619	BCR	C11-C10-C9-C8
31	K	101	BCR	C16-C17-C18-C19
31	K	102	BCR	C11-C10-C9-C8
31	Z	101	BCR	C11-C10-C9-C8
31	Z	101	BCR	C16-C17-C18-C19
31	a	405	BCR	C20-C21-C22-C23
31	b	617	BCR	C11-C10-C9-C8
31	b	617	BCR	C12-C13-C14-C15
31	c	514	BCR	C20-C21-C22-C23
31	c	515	BCR	C12-C13-C14-C15
31	d	406	BCR	C12-C13-C14-C15
31	t	101	BCR	C11-C10-C9-C8
31	x	101	BCR	C11-C10-C9-C8
31	x	101	BCR	C16-C17-C18-C19
26	D	412	LMG	C31-C32-C33-C34
26	c	521	LMG	C34-C35-C36-C37
28	D	411	LHG	C14-C15-C16-C17
28	D	411	LHG	C25-C26-C27-C28
29	A	413	DGD	CCA-CDA-CEA-CFA
29	c	517	DGD	CCB-CDB-CEB-CFB
27	t	102	SQD	O10-C23-O48-C46
22	B	603	CLA	C16-C17-C18-C19
22	B	611	CLA	C16-C17-C18-C19
22	B	614	CLA	C16-C17-C18-C19
22	c	510	CLA	C16-C17-C18-C19
22	d	403	CLA	C16-C17-C18-C19
22	B	604	CLA	O1D-CGD-O2D-CED
22	C	505	CLA	C4-C3-C5-C6
22	C	506	CLA	C4-C3-C5-C6
25	d	407	PL9	C15-C14-C16-C17
25	d	407	PL9	C30-C29-C31-C32
25	d	407	PL9	C45-C44-C46-C47
26	B	626	LMG	C13-C14-C15-C16
26	c	522	LMG	C13-C14-C15-C16
26	c	522	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
27	f	102	SQD	C27-C28-C29-C30
28	D	410	LHG	C17-C18-C19-C20
28	D	413	LHG	C15-C16-C17-C18
28	L	102	LHG	C24-C25-C26-C27
29	A	413	DGD	CEA-CFA-CGA-CHA
29	c	516	DGD	CAB-CBB-CCB-CDB
32	B	623	STE	C2-C3-C4-C5
32	J	101	STE	C6-C7-C8-C9
32	a	413	STE	C6-C7-C8-C9
32	a	413	STE	C10-C11-C12-C13
32	b	620	STE	C2-C3-C4-C5
32	c	523	STE	C5-C6-C7-C8
22	C	510	CLA	C11-C10-C8-C9
22	C	510	CLA	C14-C13-C15-C16
22	a	404	CLA	C6-C7-C8-C9
22	b	602	CLA	C14-C13-C15-C16
22	b	605	CLA	C14-C13-C15-C16
22	b	613	CLA	C14-C13-C15-C16
22	c	502	CLA	C11-C12-C13-C14
22	d	404	CLA	C14-C13-C15-C16
26	B	626	LMG	C30-C31-C32-C33
26	D	412	LMG	C14-C15-C16-C17
26	c	519	LMG	C33-C34-C35-C36
26	m	101	LMG	C12-C13-C14-C15
27	A	410	SQD	C12-C13-C14-C15
27	A	412	SQD	C10-C11-C12-C13
27	a	411	SQD	C10-C11-C12-C13
29	C	516	DGD	C6B-C7B-C8B-C9B
29	H	102	DGD	C4B-C5B-C6B-C7B
32	B	624	STE	C11-C10-C9-C8
32	J	101	STE	C2-C3-C4-C5
32	X	101	STE	C14-C15-C16-C17
32	Z	102	STE	C11-C12-C13-C14
32	b	625	STE	C10-C11-C12-C13
32	l	102	STE	C13-C14-C15-C16
32	x	102	STE	C13-C14-C15-C16
22	c	512	CLA	O1A-CGA-O2A-C1
31	H	101	BCR	C37-C22-C23-C24
31	c	514	BCR	C36-C18-C19-C20
26	B	626	LMG	C17-C18-C19-C20
26	B	626	LMG	C35-C36-C37-C38
26	c	521	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
26	c	522	LMG	C37-C38-C39-C40
26	m	101	LMG	C33-C34-C35-C36
27	A	410	SQD	C25-C26-C27-C28
27	a	411	SQD	C12-C13-C14-C15
27	f	102	SQD	C25-C26-C27-C28
29	C	517	DGD	C6B-C7B-C8B-C9B
29	c	517	DGD	C2A-C3A-C4A-C5A
32	x	102	STE	C3-C4-C5-C6
28	d	409	LHG	O1-C1-C2-C3
22	b	615	CLA	C5-C6-C7-C8
28	A	411	LHG	C13-C14-C15-C16
28	A	411	LHG	C28-C29-C30-C31
28	D	410	LHG	C15-C16-C17-C18
28	D	411	LHG	C12-C13-C14-C15
28	D	411	LHG	C27-C28-C29-C30
28	D	413	LHG	C24-C25-C26-C27
28	d	408	LHG	C11-C10-C9-C8
28	d	408	LHG	C14-C15-C16-C17
29	C	516	DGD	C2A-C3A-C4A-C5A
29	h	101	DGD	C2B-C3B-C4B-C5B
32	I	102	STE	C10-C11-C12-C13
26	c	519	LMG	C28-C29-C30-C31
27	A	412	SQD	C7-C8-C9-C10
26	B	626	LMG	C36-C37-C38-C39
26	B	626	LMG	C38-C39-C40-C41
26	c	519	LMG	C38-C39-C40-C41
26	m	101	LMG	C18-C19-C20-C21
27	L	101	SQD	C14-C15-C16-C17
27	t	102	SQD	C11-C10-C9-C8
27	t	102	SQD	C12-C13-C14-C15
29	A	413	DGD	C5B-C6B-C7B-C8B
29	C	517	DGD	C5A-C6A-C7A-C8A
29	H	102	DGD	C7A-C8A-C9A-CAA
29	c	517	DGD	C4A-C5A-C6A-C7A
32	B	625	STE	C7-C8-C9-C10
22	B	602	CLA	C16-C17-C18-C19
22	B	614	CLA	C16-C17-C18-C20
22	b	601	CLA	C16-C17-C18-C20
22	b	604	CLA	C16-C17-C18-C19
22	b	604	CLA	C16-C17-C18-C20
22	b	605	CLA	C16-C17-C18-C19
22	b	614	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
22	b	614	CLA	C16-C17-C18-C20
22	b	601	CLA	C8-C10-C11-C12
26	B	626	LMG	C33-C34-C35-C36
26	B	626	LMG	C37-C38-C39-C40
26	D	412	LMG	C13-C14-C15-C16
26	Y	101	LMG	C12-C13-C14-C15
26	Y	101	LMG	C33-C34-C35-C36
26	b	622	LMG	C30-C31-C32-C33
26	c	522	LMG	C12-C13-C14-C15
26	d	410	LMG	C34-C35-C36-C37
27	A	412	SQD	C15-C16-C17-C18
28	D	410	LHG	C32-C33-C34-C35
28	D	411	LHG	C33-C34-C35-C36
28	L	102	LHG	C32-C33-C34-C35
29	A	413	DGD	C5A-C6A-C7A-C8A
29	A	413	DGD	CBA-CCA-CDA-CEA
32	B	624	STE	C4-C5-C6-C7
32	X	101	STE	C10-C11-C12-C13
22	b	616	CLA	CBD-CGD-O2D-CED
22	D	405	CLA	O1D-CGD-O2D-CED
26	B	621	LMG	C16-C17-C18-C19
26	B	626	LMG	C23-C24-C25-C26
26	D	408	LMG	C17-C18-C19-C20
26	D	412	LMG	C34-C35-C36-C37
26	m	101	LMG	C20-C21-C22-C23
27	A	410	SQD	C14-C15-C16-C17
27	D	409	SQD	C25-C26-C27-C28
28	D	411	LHG	C11-C12-C13-C14
28	D	413	LHG	C32-C33-C34-C35
28	a	410	LHG	C11-C10-C9-C8
28	d	408	LHG	C33-C34-C35-C36
29	C	517	DGD	C3A-C4A-C5A-C6A
29	c	516	DGD	C4A-C5A-C6A-C7A
29	c	517	DGD	C6A-C7A-C8A-C9A
32	X	101	STE	C3-C4-C5-C6
32	d	411	STE	C11-C12-C13-C14
32	l	102	STE	C4-C5-C6-C7
27	L	101	SQD	C23-C24-C25-C26
22	b	616	CLA	C10-C11-C12-C13
26	m	101	LMG	O10-C28-O8-C9
26	D	408	LMG	C36-C37-C38-C39
26	c	519	LMG	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
26	c	521	LMG	C35-C36-C37-C38
26	m	101	LMG	C17-C18-C19-C20
27	A	412	SQD	C9-C10-C11-C12
27	D	409	SQD	C27-C28-C29-C30
27	a	411	SQD	C9-C10-C11-C12
28	D	413	LHG	C13-C14-C15-C16
28	L	102	LHG	C10-C11-C12-C13
29	C	517	DGD	CCB-CDB-CEB-CFB
32	B	625	STE	C5-C6-C7-C8
32	H	103	STE	C4-C5-C6-C7
32	a	413	STE	C11-C12-C13-C14
26	d	410	LMG	C14-C15-C16-C17
32	j	101	STE	C4-C5-C6-C7
22	c	511	CLA	O1D-CGD-O2D-CED
22	C	512	CLA	C3A-C2A-CAA-CBA
22	c	512	CLA	C3A-C2A-CAA-CBA
22	c	503	CLA	C5-C6-C7-C8
26	m	101	LMG	C16-C17-C18-C19
27	B	622	SQD	C11-C12-C13-C14
28	d	408	LHG	C29-C30-C31-C32
29	C	515	DGD	C4B-C5B-C6B-C7B
29	c	516	DGD	CBA-CCA-CDA-CEA
22	B	602	CLA	C16-C17-C18-C20
22	B	606	CLA	C16-C17-C18-C19
22	B	613	CLA	C16-C17-C18-C20
22	D	404	CLA	C16-C17-C18-C20
22	c	503	CLA	C16-C17-C18-C19
26	A	409	LMG	C11-C12-C13-C14
26	m	101	LMG	C38-C39-C40-C41
27	D	409	SQD	C29-C30-C31-C32
28	D	413	LHG	C9-C10-C11-C12
28	L	102	LHG	C28-C29-C30-C31
28	L	102	LHG	C30-C31-C32-C33
29	c	518	DGD	CCA-CDA-CEA-CFA
29	c	518	DGD	C6B-C7B-C8B-C9B
32	X	101	STE	C9-C10-C11-C12
32	b	627	STE	C10-C11-C12-C13
22	d	401	CLA	CBD-CGD-O2D-CED
26	b	622	LMG	C16-C17-C18-C19
28	D	410	LHG	C11-C12-C13-C14
28	D	411	LHG	C24-C25-C26-C27
31	I	101	BCR	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
26	b	622	LMG	C10-C11-C12-C13
28	L	102	LHG	C31-C32-C33-C34
22	B	611	CLA	C4-C3-C5-C6
22	c	505	CLA	C4-C3-C5-C6
22	b	611	CLA	C2-C3-C5-C6
22	c	505	CLA	C2-C3-C5-C6
23	A	404	PHO	C2-C3-C5-C6
26	B	626	LMG	C11-C10-O7-C8
26	Y	101	LMG	C37-C38-C39-C40
28	e	101	LHG	C17-C18-C19-C20
29	C	517	DGD	CBA-CCA-CDA-CEA
29	c	518	DGD	C3A-C4A-C5A-C6A
22	c	501	CLA	C2A-CAA-CBA-CGA
28	D	413	LHG	O1-C1-C2-O2
26	B	626	LMG	C34-C35-C36-C37
27	L	101	SQD	C11-C12-C13-C14
28	l	101	LHG	C24-C25-C26-C27
29	c	518	DGD	C4B-C5B-C6B-C7B
32	B	620	STE	C11-C12-C13-C14
32	H	103	STE	C5-C6-C7-C8
32	b	624	STE	C4-C5-C6-C7
22	b	607	CLA	O1A-CGA-O2A-C1
22	B	601	CLA	C16-C17-C18-C20
22	B	603	CLA	C16-C17-C18-C20
29	h	101	DGD	C6B-C7B-C8B-C9B
29	A	413	DGD	C4E-C5E-C6E-O5E
26	D	408	LMG	C30-C31-C32-C33
26	D	412	LMG	C12-C13-C14-C15
26	b	622	LMG	C31-C32-C33-C34
27	B	622	SQD	C17-C18-C19-C20
28	D	410	LHG	C29-C30-C31-C32
32	J	101	STE	C5-C6-C7-C8
32	b	627	STE	C6-C7-C8-C9
22	B	605	CLA	C15-C16-C17-C18
22	b	611	CLA	C15-C16-C17-C18
26	A	409	LMG	C18-C19-C20-C21
26	A	409	LMG	C35-C36-C37-C38
26	c	522	LMG	C33-C34-C35-C36
27	a	411	SQD	C34-C35-C36-C37
29	H	102	DGD	C6B-C7B-C8B-C9B
29	H	102	DGD	C8B-C9B-CAB-CBB
32	R	101	STE	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
32	b	624	STE	C7-C8-C9-C10
32	c	523	STE	C4-C5-C6-C7
32	d	411	STE	C2-C3-C4-C5
28	e	101	LHG	O9-C7-O7-C5
22	C	509	CLA	C2-C1-O2A-CGA
26	c	522	LMG	C31-C32-C33-C34
28	d	408	LHG	C32-C33-C34-C35
32	B	624	STE	C3-C4-C5-C6
32	x	102	STE	C4-C5-C6-C7
27	A	412	SQD	C29-C30-C31-C32
27	L	101	SQD	C26-C27-C28-C29
28	l	101	LHG	C34-C35-C36-C37
29	c	518	DGD	C8B-C9B-CAB-CBB
22	d	403	CLA	C16-C17-C18-C20
31	C	514	BCR	C1-C6-C7-C8
31	C	514	BCR	C5-C6-C7-C8
31	D	406	BCR	C23-C24-C25-C30
31	H	101	BCR	C23-C24-C25-C26
31	H	101	BCR	C23-C24-C25-C30
31	K	101	BCR	C1-C6-C7-C8
31	K	101	BCR	C5-C6-C7-C8
31	K	101	BCR	C23-C24-C25-C30
31	T	101	BCR	C5-C6-C7-C8
31	k	101	BCR	C1-C6-C7-C8
31	k	101	BCR	C5-C6-C7-C8
31	k	101	BCR	C23-C24-C25-C26
31	t	101	BCR	C1-C6-C7-C8
26	Y	101	LMG	C30-C31-C32-C33
26	Y	101	LMG	C31-C32-C33-C34
26	b	622	LMG	C15-C16-C17-C18
29	C	516	DGD	C4B-C5B-C6B-C7B
29	c	517	DGD	CAB-CBB-CCB-CDB
22	B	613	CLA	C5-C6-C7-C8
22	C	512	CLA	C8-C10-C11-C12
22	a	404	CLA	C10-C11-C12-C13
22	b	601	CLA	C13-C15-C16-C17
26	c	521	LMG	C33-C34-C35-C36
28	D	413	LHG	C16-C17-C18-C19
32	B	620	STE	C9-C10-C11-C12
28	a	410	LHG	C23-C24-C25-C26
29	h	101	DGD	C9A-CAA-CBA-CCA
22	c	509	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
28	A	411	LHG	C15-C16-C17-C18
23	A	404	PHO	C4-C3-C5-C6
22	A	403	CLA	C12-C13-C15-C16
22	B	604	CLA	C11-C10-C8-C7
22	B	611	CLA	C2-C3-C5-C6
22	B	614	CLA	C12-C13-C15-C16
22	C	505	CLA	C2-C3-C5-C6
22	C	505	CLA	C12-C13-C15-C16
22	C	506	CLA	C11-C12-C13-C15
22	C	506	CLA	C12-C13-C15-C16
22	C	508	CLA	C11-C10-C8-C7
22	C	510	CLA	C11-C10-C8-C7
22	a	404	CLA	C6-C7-C8-C10
22	b	602	CLA	C12-C13-C15-C16
22	b	604	CLA	C2-C3-C5-C6
22	b	605	CLA	C12-C13-C15-C16
22	b	607	CLA	C11-C10-C8-C7
22	c	508	CLA	C11-C10-C8-C7
22	c	508	CLA	C12-C13-C15-C16
25	D	407	PL9	C13-C14-C16-C17
25	d	407	PL9	C13-C14-C16-C17
27	D	409	SQD	C30-C31-C32-C33
22	B	606	CLA	C5-C6-C7-C8
22	C	508	CLA	C15-C16-C17-C18
22	b	601	CLA	C5-C6-C7-C8
22	b	603	CLA	C8-C10-C11-C12
23	A	404	PHO	C15-C16-C17-C18
31	Z	101	BCR	C15-C16-C17-C18
22	B	614	CLA	CBD-CGD-O2D-CED
22	C	506	CLA	CBD-CGD-O2D-CED
22	b	605	CLA	C16-C17-C18-C20
22	c	510	CLA	C16-C17-C18-C20
22	b	603	CLA	O1D-CGD-O2D-CED
26	B	626	LMG	O9-C10-O7-C8
29	c	516	DGD	C1B-C2B-C3B-C4B
22	B	605	CLA	CBA-CGA-O2A-C1
28	D	410	LHG	C13-C14-C15-C16
28	D	410	LHG	C28-C29-C30-C31
22	B	608	CLA	C5-C6-C7-C8
28	D	413	LHG	C25-C26-C27-C28
29	C	517	DGD	C3B-C4B-C5B-C6B
32	d	411	STE	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
32	d	412	STE	C2-C3-C4-C5
32	d	412	STE	C11-C12-C13-C14
26	M	101	LMG	C38-C39-C40-C41
26	M	101	LMG	C39-C40-C41-C42
29	C	516	DGD	C4A-C5A-C6A-C7A
22	B	605	CLA	C8-C10-C11-C12
22	c	507	CLA	C13-C15-C16-C17
27	L	101	SQD	C16-C17-C18-C19
27	a	411	SQD	C14-C15-C16-C17
29	A	413	DGD	C7A-C8A-C9A-CAA
29	c	516	DGD	C5B-C6B-C7B-C8B
29	h	101	DGD	C3B-C4B-C5B-C6B
32	B	620	STE	C4-C5-C6-C7
32	b	624	STE	C2-C3-C4-C5
32	c	523	STE	C2-C3-C4-C5
27	a	411	SQD	C26-C27-C28-C29
23	d	402	PHO	CBD-CGD-O2D-CED
22	C	502	CLA	C16-C17-C18-C19
22	D	405	CLA	C16-C17-C18-C20
22	b	609	CLA	C16-C17-C18-C19
22	b	615	CLA	C16-C17-C18-C19
22	b	616	CLA	C11-C12-C13-C15
26	c	522	LMG	C4-C5-C6-O5
26	b	622	LMG	O6-C1-O1-C7
29	C	516	DGD	O6E-C1E-O5D-C6D
22	c	512	CLA	C8-C10-C11-C12
26	A	409	LMG	C37-C38-C39-C40
27	B	622	SQD	C9-C10-C11-C12
28	D	413	LHG	C17-C18-C19-C20
29	C	515	DGD	C8A-C9A-CAA-CBA
32	b	621	STE	C11-C12-C13-C14
26	c	522	LMG	C11-C10-O7-C8
27	a	411	SQD	C8-C7-O47-C45
27	A	412	SQD	C24-C25-C26-C27
28	l	101	LHG	C30-C31-C32-C33
22	b	602	CLA	C15-C16-C17-C18
22	c	512	CLA	C10-C11-C12-C13
22	b	602	CLA	CBD-CGD-O2D-CED
25	A	408	PL9	C47-C48-C49-C50
27	A	412	SQD	C11-C10-C9-C8
28	D	410	LHG	O9-C7-O7-C5
29	C	516	DGD	C2E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
26	c	521	LMG	O1-C7-C8-O7
26	b	622	LMG	C34-C35-C36-C37
29	C	516	DGD	CBA-CCA-CDA-CEA
29	H	102	DGD	C9B-CAB-CBB-CCB
32	b	627	STE	C12-C13-C14-C15
27	t	102	SQD	C10-C11-C12-C13
28	D	411	LHG	C13-C14-C15-C16
28	l	101	LHG	C11-C12-C13-C14
28	l	101	LHG	C25-C26-C27-C28
28	l	101	LHG	C28-C29-C30-C31
29	c	517	DGD	CBA-CCA-CDA-CEA
32	R	101	STE	C2-C3-C4-C5
32	b	621	STE	C3-C4-C5-C6
22	C	510	CLA	C8-C10-C11-C12
22	b	611	CLA	C4-C3-C5-C6
22	c	504	CLA	C4-C3-C5-C6
22	c	504	CLA	C2-C3-C5-C6
25	D	407	PL9	C4-C3-C7-C8
25	d	407	PL9	C4-C3-C7-C8
27	A	410	SQD	C16-C17-C18-C19
28	a	410	LHG	C25-C26-C27-C28
22	B	603	CLA	C6-C7-C8-C9
22	B	605	CLA	C6-C7-C8-C9
22	B	605	CLA	C11-C10-C8-C9
22	C	505	CLA	C14-C13-C15-C16
22	C	506	CLA	C11-C12-C13-C14
22	C	508	CLA	C11-C10-C8-C9
22	b	605	CLA	C11-C12-C13-C14
22	b	609	CLA	C11-C12-C13-C14
22	c	506	CLA	C11-C12-C13-C14
22	c	508	CLA	C11-C10-C8-C9
22	d	405	CLA	C6-C7-C8-C9
22	c	512	CLA	O1D-CGD-O2D-CED
26	c	522	LMG	C34-C35-C36-C37
27	A	410	SQD	C11-C10-C9-C8
28	D	410	LHG	C30-C31-C32-C33
28	D	411	LHG	C32-C33-C34-C35
32	b	621	STE	C6-C7-C8-C9
32	b	626	STE	C4-C5-C6-C7
22	b	610	CLA	C2A-CAA-CBA-CGA
26	c	521	LMG	C29-C30-C31-C32
26	b	622	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
31	B	617	BCR	C36-C18-C19-C20
26	c	522	LMG	C36-C37-C38-C39
32	H	103	STE	C13-C14-C15-C16
22	B	601	CLA	C1A-C2A-CAA-CBA
22	c	503	CLA	C1A-C2A-CAA-CBA
22	c	508	CLA	C1A-C2A-CAA-CBA
22	b	609	CLA	C16-C17-C18-C20
22	b	615	CLA	C16-C17-C18-C20
23	D	401	PHO	C16-C17-C18-C20
26	D	408	LMG	C35-C36-C37-C38
28	A	411	LHG	C11-C10-C9-C8
28	a	410	LHG	C14-C15-C16-C17
28	l	101	LHG	C32-C33-C34-C35
29	c	516	DGD	CBB-CCB-CDB-CEB
32	b	623	STE	C6-C7-C8-C9
22	c	506	CLA	C10-C11-C12-C13
28	A	411	LHG	C4-O6-P-O3
28	D	410	LHG	C3-O3-P-O6
32	d	412	STE	C9-C10-C11-C12
23	a	403	PHO	CBD-CGD-O2D-CED
28	L	102	LHG	C13-C14-C15-C16
22	C	508	CLA	C13-C15-C16-C17
26	c	521	LMG	C16-C17-C18-C19
27	a	411	SQD	C13-C14-C15-C16
29	C	516	DGD	C8B-C9B-CAB-CBB
29	C	516	DGD	CCB-CDB-CEB-CFB
29	c	516	DGD	C9B-CAB-CBB-CCB
22	C	510	CLA	C10-C11-C12-C13
22	b	601	CLA	C16-C17-C18-C19
29	C	516	DGD	CBB-CCB-CDB-CEB
32	L	103	STE	C3-C4-C5-C6
26	D	412	LMG	C16-C17-C18-C19
27	B	622	SQD	C13-C14-C15-C16
28	A	411	LHG	C25-C26-C27-C28
28	D	413	LHG	C18-C19-C20-C21
28	e	101	LHG	C14-C15-C16-C17
27	A	412	SQD	C24-C23-O48-C46
25	D	407	PL9	C30-C29-C31-C32
22	C	506	CLA	C2-C3-C5-C6
22	b	607	CLA	C10-C11-C12-C13
22	b	613	CLA	C13-C15-C16-C17
27	A	410	SQD	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
32	B	625	STE	C6-C7-C8-C9
32	c	520	STE	C4-C5-C6-C7
27	A	410	SQD	C8-C7-O47-C45
28	a	410	LHG	C28-C29-C30-C31
22	B	615	CLA	C16-C17-C18-C20
26	c	519	LMG	O6-C5-C6-O5
26	B	626	LMG	O1-C7-C8-C9
26	M	101	LMG	C7-C8-C9-O8
26	Y	101	LMG	O1-C7-C8-C9
26	c	521	LMG	C7-C8-C9-O8
26	c	522	LMG	O1-C7-C8-C9
27	B	622	SQD	O6-C44-C45-C46
27	a	411	SQD	O6-C44-C45-C46
27	t	102	SQD	C44-C45-C46-O48
29	A	413	DGD	O1G-C1G-C2G-C3G
29	A	413	DGD	C1G-C2G-C3G-O3G
29	C	515	DGD	O1G-C1G-C2G-C3G
22	C	504	CLA	C8-C10-C11-C12
26	D	412	LMG	C37-C38-C39-C40
26	c	522	LMG	C20-C21-C22-C23
27	L	101	SQD	C27-C28-C29-C30
32	H	103	STE	C12-C13-C14-C15
27	B	622	SQD	O10-C23-O48-C46
26	B	626	LMG	C8-C7-O1-C1
29	C	516	DGD	C2G-C3G-O3G-C1D
28	l	101	LHG	C17-C18-C19-C20
29	h	101	DGD	C7B-C8B-C9B-CAB
32	t	104	STE	C7-C8-C9-C10
22	B	609	CLA	C13-C15-C16-C17
26	B	626	LMG	C4-C5-C6-O5
26	B	621	LMG	C37-C38-C39-C40
26	Y	101	LMG	C13-C14-C15-C16
29	C	515	DGD	C3B-C4B-C5B-C6B
26	D	408	LMG	O6-C5-C6-O5
26	Y	101	LMG	C28-C29-C30-C31
28	l	101	LHG	C9-C10-C11-C12
26	b	622	LMG	C12-C13-C14-C15
26	b	622	LMG	C18-C19-C20-C21
26	c	522	LMG	C19-C20-C21-C22
29	C	516	DGD	C5A-C6A-C7A-C8A
29	C	516	DGD	CDA-CEA-CFA-CGA
32	R	101	STE	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
22	b	614	CLA	CBA-CGA-O2A-C1
27	A	410	SQD	C17-C18-C19-C20
29	C	515	DGD	CDA-CEA-CFA-CGA
32	a	413	STE	C12-C13-C14-C15
32	b	623	STE	C4-C5-C6-C7
27	A	412	SQD	C34-C35-C36-C37
28	d	408	LHG	C15-C16-C17-C18
29	H	102	DGD	C4E-C5E-C6E-O5E
28	d	409	LHG	C31-C32-C33-C34
32	a	412	STE	C3-C4-C5-C6
22	b	608	CLA	C13-C15-C16-C17
22	c	503	CLA	C15-C16-C17-C18
26	d	410	LMG	O6-C5-C6-O5
29	c	516	DGD	O6E-C5E-C6E-O5E
25	d	407	PL9	C28-C29-C31-C32
28	e	101	LHG	C7-C8-C9-C10
22	B	610	CLA	C16-C17-C18-C20
26	m	101	LMG	C37-C38-C39-C40
32	b	623	STE	C11-C12-C13-C14
22	c	504	CLA	C10-C11-C12-C13
26	B	626	LMG	C40-C41-C42-C43
32	Z	102	STE	C12-C13-C14-C15
22	B	616	CLA	C2-C1-O2A-CGA
27	A	412	SQD	C46-C45-O47-C7
28	D	410	LHG	C11-C10-C9-C8
32	d	412	STE	C15-C16-C17-C18
29	c	518	DGD	C7B-C8B-C9B-CAB
32	t	103	STE	C3-C4-C5-C6
22	c	501	CLA	O1D-CGD-O2D-CED
22	d	401	CLA	O1D-CGD-O2D-CED
22	b	616	CLA	C8-C10-C11-C12
26	m	101	LMG	C39-C40-C41-C42
28	a	410	LHG	C19-C20-C21-C22
29	c	518	DGD	CCB-CDB-CEB-CFB
32	a	412	STE	C7-C8-C9-C10
22	C	506	CLA	CBA-CGA-O2A-C1
22	B	605	CLA	O1A-CGA-O2A-C1
28	l	101	LHG	O6-C4-C5-O7
22	c	509	CLA	CAA-CBA-CGA-O2A
22	C	506	CLA	O1D-CGD-O2D-CED
22	C	502	CLA	C16-C17-C18-C20
22	D	405	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
22	b	616	CLA	C11-C12-C13-C14
29	C	516	DGD	C8A-C9A-CAA-CBA
32	b	620	STE	C1-C2-C3-C4
22	B	614	CLA	O1D-CGD-O2D-CED
26	D	412	LMG	C36-C37-C38-C39
22	B	608	CLA	C10-C11-C12-C13
22	b	601	CLA	C15-C16-C17-C18
22	b	609	CLA	C15-C16-C17-C18
26	b	622	LMG	C2-C1-O1-C7
31	c	515	BCR	C20-C21-C22-C23
31	k	102	BCR	C20-C21-C22-C23
29	C	515	DGD	C6B-C7B-C8B-C9B
27	a	411	SQD	O47-C45-C46-O48
26	Y	101	LMG	C11-C12-C13-C14
32	H	103	STE	C6-C7-C8-C9
32	l	102	STE	C3-C4-C5-C6
29	A	413	DGD	O6D-C5D-C6D-O5D
22	b	601	CLA	C10-C11-C12-C13
26	B	626	LMG	C15-C16-C17-C18
26	B	626	LMG	C39-C40-C41-C42
26	b	622	LMG	C38-C39-C40-C41
28	e	101	LHG	C23-C24-C25-C26
27	L	101	SQD	C19-C20-C21-C22
29	H	102	DGD	C5B-C6B-C7B-C8B
22	c	502	CLA	C15-C16-C17-C18
22	A	403	CLA	C6-C7-C8-C10
22	A	403	CLA	C11-C12-C13-C15
22	B	603	CLA	C6-C7-C8-C10
22	B	605	CLA	C11-C10-C8-C7
22	B	610	CLA	C11-C12-C13-C15
22	B	614	CLA	C11-C12-C13-C15
22	C	507	CLA	C11-C10-C8-C7
22	C	509	CLA	C11-C10-C8-C7
22	C	511	CLA	C6-C7-C8-C10
22	C	512	CLA	C11-C10-C8-C7
22	C	513	CLA	C11-C10-C8-C7
22	D	405	CLA	C6-C7-C8-C10
22	b	601	CLA	C11-C12-C13-C15
22	b	604	CLA	C12-C13-C15-C16
22	b	605	CLA	C11-C12-C13-C15
22	b	606	CLA	C11-C10-C8-C7
22	b	607	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	b	607	CLA	C11-C12-C13-C15
22	b	609	CLA	C6-C7-C8-C10
22	b	615	CLA	C12-C13-C15-C16
22	c	501	CLA	C11-C12-C13-C15
22	c	505	CLA	C12-C13-C15-C16
22	c	506	CLA	C11-C10-C8-C7
22	c	506	CLA	C11-C12-C13-C15
22	c	509	CLA	C6-C7-C8-C10
22	c	512	CLA	C12-C13-C15-C16
22	d	401	CLA	C12-C13-C15-C16
22	d	403	CLA	C6-C7-C8-C10
27	A	410	SQD	C30-C31-C32-C33
28	D	411	LHG	C29-C30-C31-C32
28	a	410	LHG	C30-C31-C32-C33
32	t	103	STE	C6-C7-C8-C9
22	A	403	CLA	C6-C7-C8-C9
22	B	602	CLA	C11-C12-C13-C14
22	B	607	CLA	C11-C10-C8-C9
22	B	615	CLA	C11-C12-C13-C14
22	B	616	CLA	C6-C7-C8-C9
22	C	506	CLA	C14-C13-C15-C16
22	C	507	CLA	C11-C10-C8-C9
22	C	511	CLA	C6-C7-C8-C9
22	C	512	CLA	C11-C12-C13-C14
22	C	513	CLA	C11-C10-C8-C9
22	D	404	CLA	C11-C12-C13-C14
22	D	405	CLA	C6-C7-C8-C9
22	D	405	CLA	C11-C10-C8-C9
22	b	601	CLA	C11-C12-C13-C14
22	b	604	CLA	C14-C13-C15-C16
22	b	606	CLA	C11-C10-C8-C9
22	b	607	CLA	C6-C7-C8-C9
22	b	615	CLA	C14-C13-C15-C16
22	c	506	CLA	C11-C10-C8-C9
22	c	509	CLA	C11-C12-C13-C14
22	c	510	CLA	C14-C13-C15-C16
22	c	512	CLA	C14-C13-C15-C16
22	d	403	CLA	C6-C7-C8-C9
22	c	502	CLA	O1D-CGD-O2D-CED
31	B	618	BCR	C14-C15-C16-C17
31	T	101	BCR	C14-C15-C16-C17
29	C	515	DGD	C5A-C6A-C7A-C8A

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Mol	Chain	Res	Type	Atoms
23	D	401	PHO	C16-C17-C18-C19
26	B	621	LMG	C14-C15-C16-C17
27	f	102	SQD	C28-C29-C30-C31
32	B	620	STE	C12-C13-C14-C15
22	A	403	CLA	C3-C5-C6-C7
22	B	607	CLA	C10-C11-C12-C13
22	B	612	CLA	C10-C11-C12-C13
22	B	616	CLA	C5-C6-C7-C8
22	C	509	CLA	C8-C10-C11-C12
29	A	413	DGD	CCB-CDB-CEB-CFB
32	b	626	STE	C7-C8-C9-C10
26	Y	101	LMG	C29-C28-O8-C9
26	D	408	LMG	C15-C16-C17-C18
22	a	404	CLA	C15-C16-C17-C18
28	D	410	LHG	C25-C26-C27-C28
22	c	509	CLA	C15-C16-C17-C18
28	l	101	LHG	O6-C4-C5-C6
26	A	409	LMG	C14-C15-C16-C17
26	m	101	LMG	C40-C41-C42-C43
28	D	411	LHG	C30-C31-C32-C33
22	B	614	CLA	C5-C6-C7-C8
27	a	411	SQD	C25-C26-C27-C28
32	b	624	STE	C9-C10-C11-C12
32	c	520	STE	C11-C12-C13-C14
25	a	409	PL9	C30-C29-C31-C32
22	B	607	CLA	C13-C15-C16-C17
26	Y	101	LMG	C32-C33-C34-C35
28	a	410	LHG	C16-C17-C18-C19
28	A	411	LHG	C10-C11-C12-C13
29	H	102	DGD	CBB-CCB-CDB-CEB
27	a	411	SQD	C24-C23-O48-C46
26	c	521	LMG	C39-C40-C41-C42
27	A	412	SQD	C27-C28-C29-C30
28	A	411	LHG	C18-C19-C20-C21
32	H	103	STE	C11-C10-C9-C8
32	J	101	STE	C7-C8-C9-C10
32	b	620	STE	C9-C10-C11-C12
22	C	506	CLA	C3A-C2A-CAA-CBA
27	D	409	SQD	C45-C44-O6-C1
26	D	408	LMG	C31-C32-C33-C34
28	L	102	LHG	C17-C18-C19-C20
32	M	102	STE	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
27	A	412	SQD	C16-C17-C18-C19
28	d	409	LHG	C26-C27-C28-C29
32	c	523	STE	C7-C8-C9-C10
27	a	411	SQD	C24-C25-C26-C27
28	L	102	LHG	C15-C16-C17-C18
29	c	517	DGD	C9B-CAB-CBB-CCB
29	h	101	DGD	CDB-CEB-CFB-CGB
32	C	520	STE	C5-C6-C7-C8
26	D	412	LMG	C7-C8-C9-O8
26	c	521	LMG	O1-C7-C8-C9
27	L	101	SQD	C44-C45-C46-O48
28	L	102	LHG	O9-C7-O7-C5
32	b	627	STE	C9-C10-C11-C12
32	c	520	STE	C10-C11-C12-C13
22	C	506	CLA	C10-C11-C12-C13
22	b	605	CLA	O1D-CGD-O2D-CED
28	D	413	LHG	C34-C35-C36-C37
28	e	101	LHG	C25-C26-C27-C28
32	C	519	STE	C1-C2-C3-C4
32	b	626	STE	C5-C6-C7-C8
32	l	102	STE	C5-C6-C7-C8
28	L	102	LHG	C33-C34-C35-C36
32	C	519	STE	C13-C14-C15-C16
22	A	403	CLA	C15-C16-C17-C18
25	a	409	PL9	C23-C24-C26-C27
32	B	624	STE	C11-C12-C13-C14
32	a	412	STE	C6-C7-C8-C9
32	x	102	STE	C11-C10-C9-C8
29	H	102	DGD	CCA-CDA-CEA-CFA
32	I	102	STE	C11-C10-C9-C8
28	L	102	LHG	O10-C23-O8-C6
26	d	410	LMG	C15-C16-C17-C18
27	L	101	SQD	C17-C18-C19-C20
32	L	103	STE	C7-C8-C9-C10
32	b	620	STE	C13-C14-C15-C16
22	b	616	CLA	O1D-CGD-O2D-CED
28	a	410	LHG	O1-C1-C2-O2
28	d	408	LHG	O1-C1-C2-O2
28	d	409	LHG	O1-C1-C2-O2
22	C	513	CLA	C8-C10-C11-C12
22	b	609	CLA	C8-C10-C11-C12
29	h	101	DGD	CAB-CBB-CCB-CDB

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Mol	Chain	Res	Type	Atoms
26	d	410	LMG	C30-C31-C32-C33
26	m	101	LMG	C32-C33-C34-C35
22	b	614	CLA	O1A-CGA-O2A-C1
22	B	615	CLA	C16-C17-C18-C19
22	C	512	CLA	C15-C16-C17-C18
32	I	102	STE	C2-C3-C4-C5
29	A	413	DGD	C8A-C9A-CAA-CBA
22	b	612	CLA	C15-C16-C17-C18
22	C	506	CLA	O1A-CGA-O2A-C1
27	B	622	SQD	C24-C25-C26-C27
28	A	411	LHG	C17-C18-C19-C20
29	A	413	DGD	C7B-C8B-C9B-CAB
32	a	413	STE	C1-C2-C3-C4
32	l	102	STE	C12-C13-C14-C15
26	M	101	LMG	O7-C8-C9-O8
26	Y	101	LMG	O1-C7-C8-O7
26	c	522	LMG	O1-C7-C8-O7
29	A	413	DGD	O1G-C1G-C2G-O2G
22	B	611	CLA	C16-C17-C18-C20
26	A	409	LMG	C39-C40-C41-C42
26	B	626	LMG	C32-C33-C34-C35
32	B	624	STE	C12-C13-C14-C15
29	C	515	DGD	O1B-C1B-O2G-C2G
22	c	512	CLA	C4-C3-C5-C6
23	a	403	PHO	O1D-CGD-O2D-CED
22	c	512	CLA	C2-C3-C5-C6
27	B	622	SQD	C32-C33-C34-C35
32	b	626	STE	C1-C2-C3-C4
22	A	402	CLA	C14-C13-C15-C16
22	A	403	CLA	C11-C12-C13-C14
22	B	603	CLA	C11-C12-C13-C14
22	B	610	CLA	C11-C12-C13-C14
22	B	614	CLA	C6-C7-C8-C9
22	C	504	CLA	C11-C10-C8-C9
22	b	607	CLA	C11-C12-C13-C14
22	b	607	CLA	C14-C13-C15-C16
22	b	613	CLA	C6-C7-C8-C9
22	b	613	CLA	C11-C10-C8-C9
22	d	401	CLA	C11-C10-C8-C9
26	B	621	LMG	C29-C30-C31-C32
32	X	101	STE	C13-C14-C15-C16
22	A	402	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
26	B	626	LMG	C24-C25-C26-C27
27	f	102	SQD	C31-C32-C33-C34
29	A	413	DGD	C6B-C7B-C8B-C9B
29	c	518	DGD	C2A-C3A-C4A-C5A
32	B	627	STE	C6-C7-C8-C9
32	c	520	STE	C7-C8-C9-C10
22	B	610	CLA	C16-C17-C18-C19
22	B	613	CLA	C16-C17-C18-C19
22	D	404	CLA	C16-C17-C18-C19
31	B	618	BCR	C23-C24-C25-C26
31	B	619	BCR	C5-C6-C7-C8
31	K	101	BCR	C23-C24-C25-C26
31	K	102	BCR	C5-C6-C7-C8
31	b	617	BCR	C1-C6-C7-C8
31	b	617	BCR	C5-C6-C7-C8
31	d	406	BCR	C23-C24-C25-C26
31	k	102	BCR	C23-C24-C25-C26
31	t	101	BCR	C5-C6-C7-C8
31	x	101	BCR	C23-C24-C25-C30
22	b	604	CLA	C15-C16-C17-C18
22	b	605	CLA	C13-C15-C16-C17
26	D	412	LMG	C30-C31-C32-C33
26	b	622	LMG	C29-C30-C31-C32
29	C	515	DGD	C4E-C5E-C6E-O5E
23	d	402	PHO	O1D-CGD-O2D-CED
31	C	514	BCR	C7-C8-C9-C10
31	C	514	BCR	C11-C12-C13-C14
31	k	101	BCR	C17-C18-C19-C20
22	c	513	CLA	C5-C6-C7-C8
26	b	622	LMG	C35-C36-C37-C38
28	D	411	LHG	C35-C36-C37-C38
29	A	413	DGD	C4A-C5A-C6A-C7A
22	C	502	CLA	O1D-CGD-O2D-CED
28	A	411	LHG	C31-C32-C33-C34
22	C	508	CLA	C16-C17-C18-C19
22	b	602	CLA	C16-C17-C18-C19
28	D	413	LHG	C27-C28-C29-C30
32	x	102	STE	C15-C16-C17-C18
26	d	410	LMG	C12-C13-C14-C15
27	L	101	SQD	C30-C31-C32-C33
32	b	623	STE	C5-C6-C7-C8
22	B	602	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	B	604	CLA	C11-C12-C13-C15
22	B	607	CLA	C11-C10-C8-C7
22	B	610	CLA	C12-C13-C15-C16
22	B	611	CLA	C11-C10-C8-C7
22	B	614	CLA	C11-C10-C8-C7
22	B	615	CLA	C11-C12-C13-C15
22	B	616	CLA	C6-C7-C8-C10
22	C	502	CLA	C12-C13-C15-C16
22	C	504	CLA	C11-C10-C8-C7
22	C	510	CLA	C6-C7-C8-C10
22	C	512	CLA	C11-C12-C13-C15
22	D	404	CLA	C11-C12-C13-C15
22	D	405	CLA	C11-C10-C8-C7
22	b	603	CLA	C6-C7-C8-C10
22	b	605	CLA	C11-C10-C8-C7
22	b	616	CLA	C11-C10-C8-C7
22	c	510	CLA	C12-C13-C15-C16
22	c	511	CLA	C11-C12-C13-C15
22	c	512	CLA	C6-C7-C8-C10
22	d	401	CLA	C11-C10-C8-C7
23	A	404	PHO	C12-C13-C15-C16
22	c	505	CLA	C10-C11-C12-C13
31	t	101	BCR	C15-C16-C17-C18
22	C	503	CLA	CBD-CGD-O2D-CED
26	B	626	LMG	C19-C20-C21-C22
29	H	102	DGD	CBA-CCA-CDA-CEA
26	m	101	LMG	C19-C20-C21-C22
29	C	515	DGD	CAB-CBB-CCB-CDB
29	c	516	DGD	C4D-C5D-C6D-O5D
22	C	505	CLA	C5-C6-C7-C8
31	H	101	BCR	C35-C13-C14-C15
31	K	102	BCR	C20-C21-C22-C37
31	c	514	BCR	C35-C13-C14-C15
32	b	621	STE	C2-C3-C4-C5
28	A	411	LHG	C16-C17-C18-C19
29	C	517	DGD	CAB-CBB-CCB-CDB
22	b	611	CLA	C8-C10-C11-C12
22	a	404	CLA	CBA-CGA-O2A-C1
22	b	609	CLA	CBA-CGA-O2A-C1
28	d	409	LHG	C24-C23-O8-C6
32	Z	102	STE	C14-C15-C16-C17
26	c	519	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
32	M	103	STE	C2-C3-C4-C5
22	b	610	CLA	CBD-CGD-O2D-CED
22	c	507	CLA	CBD-CGD-O2D-CED
26	b	622	LMG	C13-C14-C15-C16
27	A	412	SQD	C13-C14-C15-C16
28	L	102	LHG	C18-C19-C20-C21
32	b	625	STE	C12-C13-C14-C15
22	C	503	CLA	CAD-CBD-CGD-O2D
22	C	512	CLA	CAD-CBD-CGD-O2D
22	a	402	CLA	CAD-CBD-CGD-O2D
22	b	604	CLA	CAD-CBD-CGD-O2D
22	b	610	CLA	CAD-CBD-CGD-O2D
22	b	616	CLA	CAD-CBD-CGD-O2D
22	c	512	CLA	CAD-CBD-CGD-O2D
23	D	401	PHO	CAD-CBD-CGD-O2D
26	D	412	LMG	C9-C8-O7-C10
27	f	102	SQD	C46-C45-O47-C7
22	b	616	CLA	C3-C5-C6-C7
32	H	103	STE	C15-C16-C17-C18
22	c	513	CLA	C8-C10-C11-C12
26	c	519	LMG	C34-C35-C36-C37
28	D	411	LHG	C16-C17-C18-C19
32	C	519	STE	C4-C5-C6-C7
31	B	617	BCR	C6-C7-C8-C9
31	b	617	BCR	C6-C7-C8-C9
32	c	523	STE	C6-C7-C8-C9
26	M	101	LMG	O6-C1-O1-C7
27	L	101	SQD	O5-C1-O6-C44
25	a	409	PL9	C12-C11-C9-C8
26	m	101	LMG	C7-C8-C9-O8
22	b	609	CLA	O1A-CGA-O2A-C1
32	B	627	STE	C2-C3-C4-C5
22	b	611	CLA	C13-C15-C16-C17
22	c	501	CLA	C15-C16-C17-C18
28	l	101	LHG	C33-C34-C35-C36
28	A	411	LHG	C34-C35-C36-C37
22	B	601	CLA	CHA-CBD-CGD-O1D
22	B	601	CLA	CHA-CBD-CGD-O2D
22	B	607	CLA	CHA-CBD-CGD-O1D
22	B	607	CLA	CHA-CBD-CGD-O2D
22	C	509	CLA	CHA-CBD-CGD-O1D
22	C	509	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	D	404	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	506	CLA	CHA-CBD-CGD-O1D
22	c	506	CLA	CHA-CBD-CGD-O2D
23	d	402	PHO	CHA-CBD-CGD-O1D
23	d	402	PHO	CHA-CBD-CGD-O2D
22	B	602	CLA	C10-C11-C12-C13
32	t	103	STE	C11-C10-C9-C8
29	H	102	DGD	C3B-C4B-C5B-C6B
31	B	617	BCR	C20-C21-C22-C23
28	D	411	LHG	C31-C32-C33-C34
26	c	521	LMG	O7-C8-C9-O8
26	m	101	LMG	O7-C8-C9-O8
27	L	101	SQD	O47-C45-C46-O48
22	c	506	CLA	CBA-CGA-O2A-C1
22	B	602	CLA	C15-C16-C17-C18
22	c	506	CLA	O1A-CGA-O2A-C1
26	Y	101	LMG	O10-C28-O8-C9
32	a	412	STE	C2-C3-C4-C5
22	b	607	CLA	C5-C6-C7-C8
27	D	409	SQD	O6-C44-C45-C46
25	a	409	PL9	C4-C3-C7-C8
22	B	604	CLA	C11-C10-C8-C9
22	b	603	CLA	C6-C7-C8-C9
27	B	622	SQD	C25-C26-C27-C28
29	c	517	DGD	C2B-C3B-C4B-C5B
29	h	101	DGD	C6A-C7A-C8A-C9A
32	b	624	STE	C5-C6-C7-C8
22	a	404	CLA	O1A-CGA-O2A-C1
28	a	410	LHG	O10-C23-O8-C6
29	C	516	DGD	O1A-C1A-O1G-C1G
26	c	521	LMG	C32-C33-C34-C35
26	m	101	LMG	C15-C16-C17-C18
29	C	515	DGD	O1G-C1A-C2A-C3A
26	B	621	LMG	C36-C37-C38-C39
31	k	101	BCR	C37-C22-C23-C24
26	Y	101	LMG	C34-C35-C36-C37
28	a	410	LHG	O1-C1-C2-C3
26	M	101	LMG	C19-C20-C21-C22
29	c	518	DGD	CAA-CBA-CCA-CDA

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Mol	Chain	Res	Type	Atoms
29	C	516	DGD	C3A-C4A-C5A-C6A
22	c	511	CLA	C1A-C2A-CAA-CBA
32	X	101	STE	C1-C2-C3-C4
22	D	403	CLA	C16-C17-C18-C19
22	b	608	CLA	C16-C17-C18-C19
29	A	413	DGD	C4D-C5D-C6D-O5D
22	c	513	CLA	C2-C1-O2A-CGA
26	B	621	LMG	C32-C33-C34-C35
32	B	625	STE	C11-C10-C9-C8
28	d	408	LHG	C3-O3-P-O6
27	A	410	SQD	C9-C10-C11-C12
32	j	101	STE	C2-C3-C4-C5
26	D	408	LMG	C37-C38-C39-C40
28	L	102	LHG	C9-C10-C11-C12
28	A	411	LHG	C3-O3-P-O4
28	A	411	LHG	C4-O6-P-O5
28	D	411	LHG	C3-O3-P-O5
28	d	408	LHG	C3-O3-P-O4
22	C	508	CLA	C16-C17-C18-C20
22	C	509	CLA	C16-C17-C18-C19
26	B	626	LMG	O6-C1-O1-C7
22	b	612	CLA	C10-C11-C12-C13
28	e	101	LHG	O6-C4-C5-C6
29	H	102	DGD	CCB-CDB-CEB-CFB
29	h	101	DGD	O2G-C1B-C2B-C3B
26	m	101	LMG	C34-C35-C36-C37
22	C	513	CLA	C16-C17-C18-C19
27	A	410	SQD	C11-C12-C13-C14
32	b	621	STE	C7-C8-C9-C10
22	B	601	CLA	CAD-CBD-CGD-O1D
22	B	607	CLA	CAD-CBD-CGD-O1D
22	B	612	CLA	CAD-CBD-CGD-O1D
22	B	614	CLA	CAD-CBD-CGD-O1D
22	C	504	CLA	CAD-CBD-CGD-O1D
22	C	506	CLA	CAD-CBD-CGD-O1D
22	c	502	CLA	CAD-CBD-CGD-O1D
22	c	506	CLA	CAD-CBD-CGD-O1D
22	A	402	CLA	C15-C16-C17-C18
22	B	603	CLA	C10-C11-C12-C13
29	c	516	DGD	O6D-C5D-C6D-O5D
26	b	622	LMG	C32-C33-C34-C35
28	D	411	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
32	l	102	STE	C9-C10-C11-C12
27	A	412	SQD	C44-C45-O47-C7
28	D	410	LHG	C9-C10-C11-C12
27	A	412	SQD	C23-C24-C25-C26
29	C	515	DGD	O6D-C5D-C6D-O5D
22	b	610	CLA	C16-C17-C18-C19
22	C	503	CLA	C4-C3-C5-C6
22	B	601	CLA	C11-C10-C8-C7
22	B	603	CLA	C11-C12-C13-C15
22	B	604	CLA	C12-C13-C15-C16
22	B	606	CLA	C11-C10-C8-C7
22	B	607	CLA	C11-C12-C13-C15
22	B	607	CLA	C12-C13-C15-C16
22	B	609	CLA	C12-C13-C15-C16
22	B	613	CLA	C12-C13-C15-C16
22	C	503	CLA	C11-C10-C8-C7
22	C	506	CLA	C6-C7-C8-C10
22	D	403	CLA	C11-C12-C13-C15
22	D	405	CLA	C11-C12-C13-C15
22	b	601	CLA	C11-C10-C8-C7
22	b	608	CLA	C11-C10-C8-C7
22	b	611	CLA	C11-C12-C13-C15
22	b	612	CLA	C12-C13-C15-C16
22	c	503	CLA	C11-C12-C13-C15
22	c	505	CLA	C6-C7-C8-C10
22	d	401	CLA	C11-C12-C13-C15
23	a	403	PHO	C6-C7-C8-C10
26	D	408	LMG	C39-C40-C41-C42
27	L	101	SQD	C12-C13-C14-C15
32	d	411	STE	C12-C13-C14-C15
28	A	411	LHG	C23-C24-C25-C26
28	e	101	LHG	C8-C7-O7-C5
32	B	625	STE	C11-C12-C13-C14
26	M	101	LMG	C33-C34-C35-C36
28	d	408	LHG	C9-C10-C11-C12
32	H	103	STE	C2-C3-C4-C5
32	b	625	STE	C14-C15-C16-C17
22	B	612	CLA	C16-C17-C18-C19
22	b	603	CLA	C16-C17-C18-C20
26	B	626	LMG	O1-C7-C8-O7
26	D	412	LMG	O7-C8-C9-O8
27	L	101	SQD	O6-C44-C45-O47

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Mol	Chain	Res	Type	Atoms
29	C	515	DGD	O1G-C1G-C2G-O2G
27	L	101	SQD	C9-C10-C11-C12
32	L	103	STE	C6-C7-C8-C9
22	D	405	CLA	O2A-C1-C2-C3
29	C	516	DGD	C5D-C6D-O5D-C1E
29	c	517	DGD	C2G-C3G-O3G-C1D
29	c	517	DGD	C5D-C6D-O5D-C1E
22	d	404	CLA	C16-C17-C18-C20
23	d	402	PHO	C2C-C3C-CAC-CBC
29	C	515	DGD	CBB-CCB-CDB-CEB
22	b	602	CLA	O1D-CGD-O2D-CED
28	d	409	LHG	C2-C3-O3-P
22	C	513	CLA	C10-C11-C12-C13
22	A	405	CLA	CBA-CGA-O2A-C1
27	L	101	SQD	C29-C30-C31-C32
27	t	102	SQD	C19-C20-C21-C22
29	A	413	DGD	CAA-CBA-CCA-CDA
26	B	626	LMG	O8-C28-C29-C30
22	B	604	CLA	C11-C12-C13-C14
22	B	604	CLA	C14-C13-C15-C16
22	B	607	CLA	C11-C12-C13-C14
22	C	510	CLA	C6-C7-C8-C9
22	b	611	CLA	C11-C12-C13-C14
22	b	615	CLA	C11-C12-C13-C14
22	c	504	CLA	C11-C10-C8-C9
22	c	510	CLA	C11-C10-C8-C9
22	c	511	CLA	C11-C12-C13-C14
27	B	622	SQD	C31-C32-C33-C34
29	A	413	DGD	CFB-CGB-CHB-CIB
22	C	509	CLA	C16-C17-C18-C20
22	b	610	CLA	C16-C17-C18-C20
29	c	517	DGD	C3B-C4B-C5B-C6B
32	x	102	STE	C11-C12-C13-C14
29	h	101	DGD	C1A-C2A-C3A-C4A
22	B	608	CLA	O1A-CGA-O2A-C1
29	H	102	DGD	CAB-CBB-CCB-CDB
29	H	102	DGD	O6E-C5E-C6E-O5E
31	d	406	BCR	C11-C12-C13-C35
32	C	519	STE	C2-C3-C4-C5
32	B	624	STE	C2-C3-C4-C5
25	A	408	PL9	C15-C14-C16-C17
29	H	102	DGD	O2G-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
28	e	101	LHG	C16-C17-C18-C19
25	A	408	PL9	C43-C44-C46-C47
22	C	503	CLA	C10-C11-C12-C13
22	c	501	CLA	C16-C17-C18-C19
22	d	404	CLA	C16-C17-C18-C19
32	C	519	STE	C6-C7-C8-C9
32	x	102	STE	C10-C11-C12-C13
26	c	519	LMG	C32-C33-C34-C35
26	B	626	LMG	C9-C8-O7-C10
28	d	408	LHG	C1-C2-C3-O3
27	A	412	SQD	C28-C29-C30-C31
27	A	410	SQD	C24-C23-O48-C46
22	C	506	CLA	C2-C1-O2A-CGA
22	C	511	CLA	C2-C1-O2A-CGA
22	D	403	CLA	C2-C1-O2A-CGA
22	d	403	CLA	C2-C1-O2A-CGA
29	c	516	DGD	CDB-CEB-CFB-CGB
32	L	103	STE	C4-C5-C6-C7
32	b	623	STE	C10-C11-C12-C13
22	B	608	CLA	C16-C17-C18-C20
22	C	513	CLA	C16-C17-C18-C20
26	B	626	LMG	C16-C17-C18-C19
25	D	407	PL9	C2-C3-C7-C8
27	B	622	SQD	C26-C27-C28-C29
27	a	411	SQD	O10-C23-O48-C46
28	a	410	LHG	C33-C34-C35-C36
22	c	507	CLA	C4-C3-C5-C6
31	B	619	BCR	C1-C6-C7-C8
31	K	102	BCR	C1-C6-C7-C8
31	x	101	BCR	C23-C24-C25-C26
25	a	409	PL9	C43-C44-C46-C47
22	B	613	CLA	C13-C15-C16-C17
22	c	510	CLA	C8-C10-C11-C12
27	L	101	SQD	C10-C11-C12-C13
26	D	408	LMG	C28-C29-C30-C31
29	c	516	DGD	O1G-C1A-C2A-C3A
27	L	101	SQD	C15-C16-C17-C18
32	b	621	STE	C4-C5-C6-C7
27	B	622	SQD	C30-C31-C32-C33
31	T	101	BCR	C12-C13-C14-C15
22	A	403	CLA	C10-C11-C12-C13
29	C	516	DGD	CDB-CEB-CFB-CGB

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Mol	Chain	Res	Type	Atoms
22	d	405	CLA	CBA-CGA-O2A-C1
28	A	411	LHG	C3-O3-P-O6
28	L	102	LHG	C3-O3-P-O6
28	a	410	LHG	C3-O3-P-O6
28	l	101	LHG	C4-O6-P-O3
26	m	101	LMG	C22-C23-C24-C25
22	B	608	CLA	C4-C3-C5-C6
28	a	410	LHG	C29-C30-C31-C32
32	b	625	STE	C11-C12-C13-C14
22	b	610	CLA	O1D-CGD-O2D-CED
22	A	402	CLA	C12-C13-C15-C16
22	B	603	CLA	C11-C10-C8-C7
22	b	613	CLA	C12-C13-C15-C16
22	c	502	CLA	C11-C12-C13-C15
25	D	407	PL9	C28-C29-C31-C32
27	B	622	SQD	C29-C30-C31-C32
22	B	603	CLA	C11-C10-C8-C9
22	D	403	CLA	C11-C12-C13-C14
22	b	608	CLA	C11-C10-C8-C9
22	b	609	CLA	C6-C7-C8-C9
22	c	501	CLA	C11-C12-C13-C14
22	c	505	CLA	C14-C13-C15-C16
22	d	401	CLA	C14-C13-C15-C16
22	B	615	CLA	C5-C6-C7-C8
31	k	101	BCR	C19-C20-C21-C22
26	D	412	LMG	C15-C16-C17-C18
28	d	408	LHG	C16-C17-C18-C19
27	D	409	SQD	O10-C23-C24-C25
28	d	408	LHG	C12-C13-C14-C15
29	c	518	DGD	CDA-CEA-CFA-CGA
29	c	518	DGD	C9B-CAB-CBB-CCB
22	c	507	CLA	O1A-CGA-O2A-C1
29	C	515	DGD	C2B-C3B-C4B-C5B
22	b	614	CLA	C5-C6-C7-C8
31	Z	101	BCR	C7-C8-C9-C10
27	A	410	SQD	C28-C29-C30-C31
26	M	101	LMG	C16-C17-C18-C19
32	M	102	STE	C2-C3-C4-C5
22	C	503	CLA	C2-C3-C5-C6
25	d	407	PL9	C43-C44-C46-C47
32	b	621	STE	C5-C6-C7-C8
27	D	409	SQD	O48-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
22	C	505	CLA	CBD-CGD-O2D-CED
22	c	507	CLA	CBA-CGA-O2A-C1
28	D	410	LHG	C23-C24-C25-C26
29	A	413	DGD	CAB-CBB-CCB-CDB
29	C	515	DGD	O6E-C1E-O5D-C6D
29	c	518	DGD	O6D-C1D-O3G-C3G
31	H	101	BCR	C13-C14-C15-C16
32	c	520	STE	C11-C10-C9-C8
32	d	412	STE	C11-C10-C9-C8
22	b	602	CLA	O1A-CGA-O2A-C1
26	M	101	LMG	C35-C36-C37-C38
28	d	408	LHG	C31-C32-C33-C34
32	t	104	STE	C4-C5-C6-C7
22	A	405	CLA	O1A-CGA-O2A-C1
22	D	403	CLA	C16-C17-C18-C20
22	c	501	CLA	C16-C17-C18-C20
22	c	504	CLA	C11-C12-C13-C14
22	C	509	CLA	C3-C5-C6-C7
32	b	624	STE	C11-C10-C9-C8
22	B	604	CLA	C2-C1-O2A-CGA
29	H	102	DGD	C5A-C6A-C7A-C8A
22	c	507	CLA	O1D-CGD-O2D-CED
26	M	101	LMG	C2-C1-O1-C7
22	B	610	CLA	C2A-CAA-CBA-CGA
22	B	602	CLA	C8-C10-C11-C12
32	B	624	STE	C6-C7-C8-C9
23	A	404	PHO	C10-C11-C12-C13
28	e	101	LHG	C11-C12-C13-C14
31	x	101	BCR	C15-C16-C17-C18
25	A	408	PL9	C4-C3-C7-C8
22	B	601	CLA	C6-C7-C8-C9
22	b	601	CLA	C14-C13-C15-C16
22	b	602	CLA	C11-C10-C8-C9
22	b	606	CLA	C14-C13-C15-C16
22	c	502	CLA	C6-C7-C8-C9
22	c	502	CLA	C14-C13-C15-C16
22	c	508	CLA	C6-C7-C8-C9
22	c	511	CLA	C11-C10-C8-C9
29	c	516	DGD	C6B-C7B-C8B-C9B
32	b	625	STE	C9-C10-C11-C12
29	h	101	DGD	C8A-C9A-CAA-CBA
28	d	408	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
22	D	404	CLA	C8-C10-C11-C12
27	a	411	SQD	C44-C45-C46-O48
29	C	517	DGD	O1G-C1G-C2G-C3G
29	c	518	DGD	O1G-C1G-C2G-C3G
31	a	405	BCR	C35-C13-C14-C15
32	C	518	STE	C7-C8-C9-C10
28	D	410	LHG	C12-C13-C14-C15
22	d	405	CLA	O1A-CGA-O2A-C1
26	D	408	LMG	C32-C33-C34-C35
26	b	622	LMG	C40-C41-C42-C43
26	c	521	LMG	C36-C37-C38-C39
22	B	608	CLA	C16-C17-C18-C19
22	B	601	CLA	O2A-C1-C2-C3
22	B	608	CLA	CBA-CGA-O2A-C1
29	c	517	DGD	O6D-C1D-O3G-C3G
31	K	101	BCR	C7-C8-C9-C34
31	d	406	BCR	C7-C8-C9-C34
28	d	408	LHG	C26-C27-C28-C29
31	H	101	BCR	C17-C18-C19-C20
26	A	409	LMG	C32-C33-C34-C35
26	B	626	LMG	C11-C12-C13-C14
26	M	101	LMG	C7-C8-O7-C10
22	c	501	CLA	C1A-C2A-CAA-CBA
32	M	103	STE	C1-C2-C3-C4
22	B	613	CLA	C6-C7-C8-C10
22	C	503	CLA	C6-C7-C8-C10
22	C	508	CLA	C12-C13-C15-C16
22	D	405	CLA	C12-C13-C15-C16
22	d	405	CLA	C11-C12-C13-C15
26	B	621	LMG	C31-C32-C33-C34
32	b	623	STE	C2-C3-C4-C5
22	B	612	CLA	C13-C15-C16-C17
31	K	101	BCR	C13-C14-C15-C16
28	D	410	LHG	C7-C8-C9-C10
26	m	101	LMG	C29-C28-O8-C9
26	M	101	LMG	C17-C18-C19-C20
28	L	102	LHG	C35-C36-C37-C38
29	C	516	DGD	CAA-CBA-CCA-CDA
29	C	517	DGD	C7A-C8A-C9A-CAA
29	c	516	DGD	C7A-C8A-C9A-CAA
22	B	606	CLA	C15-C16-C17-C18
22	b	603	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	b	605	CLA	C10-C11-C12-C13
32	X	101	STE	C15-C16-C17-C18
22	B	603	CLA	C13-C15-C16-C17
26	b	622	LMG	C42-C43-C44-C45
25	D	407	PL9	C32-C33-C34-C35
28	l	101	LHG	C14-C15-C16-C17
26	D	408	LMG	C12-C13-C14-C15
32	l	102	STE	C11-C12-C13-C14
22	B	609	CLA	C2-C3-C5-C6
32	C	520	STE	C6-C7-C8-C9
22	b	609	CLA	O1D-CGD-O2D-CED
29	c	517	DGD	C7A-C8A-C9A-CAA
26	B	621	LMG	C17-C18-C19-C20
26	D	412	LMG	C33-C34-C35-C36
32	B	620	STE	C11-C10-C9-C8
28	d	408	LHG	C34-C35-C36-C37
22	d	404	CLA	C15-C16-C17-C18
25	A	408	PL9	C35-C34-C36-C37
28	e	101	LHG	C28-C29-C30-C31
22	c	509	CLA	CAA-CBA-CGA-O1A
22	c	502	CLA	C2-C1-O2A-CGA
22	c	512	CLA	C2-C1-O2A-CGA
22	B	608	CLA	C2-C3-C5-C6
22	c	507	CLA	C2-C3-C5-C6
25	A	408	PL9	C13-C14-C16-C17
28	L	102	LHG	C29-C30-C31-C32
22	B	608	CLA	C14-C13-C15-C16
28	D	413	LHG	O10-C23-O8-C6
26	B	626	LMG	C29-C30-C31-C32
29	C	515	DGD	C4D-C5D-C6D-O5D
32	X	101	STE	C11-C12-C13-C14
22	B	614	CLA	C2A-CAA-CBA-CGA
22	A	403	CLA	C16-C17-C18-C20
26	b	622	LMG	C23-C24-C25-C26
26	c	521	LMG	C38-C39-C40-C41
31	B	617	BCR	C1-C6-C7-C8
31	B	617	BCR	C5-C6-C7-C8
31	C	514	BCR	C23-C24-C25-C30
31	Z	101	BCR	C23-C24-C25-C30
31	b	618	BCR	C23-C24-C25-C30
31	k	102	BCR	C23-C24-C25-C30
26	M	101	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
28	A	411	LHG	C29-C30-C31-C32
32	J	101	STE	C3-C4-C5-C6
32	M	102	STE	C11-C10-C9-C8
31	t	101	BCR	C19-C20-C21-C22
22	B	605	CLA	C16-C17-C18-C20
22	c	508	CLA	C8-C10-C11-C12
27	L	101	SQD	C45-C44-O6-C1
27	D	409	SQD	C44-C45-C46-O48
27	a	411	SQD	C11-C12-C13-C14
22	C	512	CLA	C16-C17-C18-C19
32	X	101	STE	C5-C6-C7-C8
22	d	405	CLA	C15-C16-C17-C18
22	b	602	CLA	CBA-CGA-O2A-C1
29	C	515	DGD	CDB-CEB-CFB-CGB
32	I	102	STE	C12-C13-C14-C15
22	c	505	CLA	C5-C6-C7-C8
28	d	408	LHG	C30-C31-C32-C33
27	a	411	SQD	C23-C24-C25-C26
22	c	508	CLA	C4-C3-C5-C6
22	B	606	CLA	C12-C13-C15-C16
22	c	511	CLA	C6-C7-C8-C10
29	A	413	DGD	C1A-C2A-C3A-C4A
29	c	517	DGD	CBB-CCB-CDB-CEB
32	B	624	STE	C9-C10-C11-C12
26	B	626	LMG	O7-C8-C9-O8
26	b	622	LMG	O1-C7-C8-O7
27	f	102	SQD	O6-C44-C45-O47
27	L	101	SQD	C11-C10-C9-C8
32	t	103	STE	C7-C8-C9-C10
26	b	622	LMG	O8-C28-C29-C30
22	A	402	CLA	C4C-C3C-CAC-CBC
31	k	101	BCR	C16-C17-C18-C36
29	H	102	DGD	C1B-C2B-C3B-C4B
28	e	101	LHG	O8-C23-C24-C25
32	B	625	STE	C12-C13-C14-C15
22	B	609	CLA	C4-C3-C5-C6
22	B	616	CLA	C4-C3-C5-C6
23	d	402	PHO	C5-C6-C7-C8
26	c	519	LMG	C36-C37-C38-C39
28	a	410	LHG	C24-C25-C26-C27
22	B	605	CLA	C2-C3-C5-C6
22	C	510	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
28	D	413	LHG	C19-C20-C21-C22
22	B	601	CLA	C11-C10-C8-C9
22	B	613	CLA	C6-C7-C8-C9
22	B	613	CLA	C14-C13-C15-C16
22	C	509	CLA	C14-C13-C15-C16
22	b	604	CLA	C11-C10-C8-C9
22	b	612	CLA	C14-C13-C15-C16
22	b	614	CLA	C6-C7-C8-C9
22	d	401	CLA	C11-C12-C13-C14
22	d	403	CLA	C11-C10-C8-C9
26	D	408	LMG	C38-C39-C40-C41
22	c	512	CLA	C15-C16-C17-C18
22	b	601	CLA	C3A-C2A-CAA-CBA
22	d	401	CLA	C3A-C2A-CAA-CBA
22	d	405	CLA	C3A-C2A-CAA-CBA
22	c	501	CLA	O1A-CGA-O2A-C1
22	B	604	CLA	CAD-CBD-CGD-O2D
22	B	616	CLA	CAD-CBD-CGD-O2D
22	C	505	CLA	CAD-CBD-CGD-O2D
22	b	601	CLA	CAD-CBD-CGD-O2D
22	b	609	CLA	CAD-CBD-CGD-O2D
22	b	614	CLA	CAD-CBD-CGD-O2D
22	c	503	CLA	CAD-CBD-CGD-O2D
22	c	509	CLA	CAD-CBD-CGD-O2D
22	c	510	CLA	CAD-CBD-CGD-O2D
22	c	513	CLA	CAD-CBD-CGD-O2D
23	A	404	PHO	CAD-CBD-CGD-O2D
23	a	403	PHO	CAD-CBD-CGD-O2D
26	A	409	LMG	C7-C8-O7-C10
26	D	408	LMG	C40-C41-C42-C43
26	c	522	LMG	O9-C10-O7-C8
32	b	620	STE	C11-C10-C9-C8
26	D	412	LMG	C11-C12-C13-C14
32	X	101	STE	C6-C7-C8-C9
32	b	620	STE	C7-C8-C9-C10
22	d	403	CLA	C4-C3-C5-C6
25	A	408	PL9	C25-C24-C26-C27
26	m	101	LMG	O8-C28-C29-C30
29	C	517	DGD	CAA-CBA-CCA-CDA
22	C	512	CLA	C2C-C3C-CAC-CBC
22	c	511	CLA	C2C-C3C-CAC-CBC
26	b	622	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
26	m	101	LMG	O1-C7-C8-C9
29	h	101	DGD	C1G-C2G-C3G-O3G
27	t	102	SQD	O48-C23-C24-C25
26	A	409	LMG	C16-C17-C18-C19
27	L	101	SQD	C13-C14-C15-C16
22	b	612	CLA	C8-C10-C11-C12
23	a	403	PHO	O2A-C1-C2-C3
26	b	622	LMG	C14-C15-C16-C17
26	c	522	LMG	C16-C17-C18-C19
27	A	412	SQD	C31-C32-C33-C34
23	d	402	PHO	C8-C10-C11-C12
29	C	515	DGD	C9A-CAA-CBA-CCA
29	C	515	DGD	CCB-CDB-CEB-CFB
32	x	102	STE	C6-C7-C8-C9
22	B	602	CLA	CHA-CBD-CGD-O1D
22	B	602	CLA	CHA-CBD-CGD-O2D
22	B	605	CLA	CHA-CBD-CGD-O2D
22	B	616	CLA	CHA-CBD-CGD-O2D
22	C	504	CLA	CHA-CBD-CGD-O1D
22	C	506	CLA	CHA-CBD-CGD-O1D
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	512	CLA	CHA-CBD-CGD-O2D
22	D	404	CLA	CHA-CBD-CGD-O1D
22	b	601	CLA	CHA-CBD-CGD-O2D
22	b	611	CLA	CHA-CBD-CGD-O2D
22	c	504	CLA	CHA-CBD-CGD-O2D
22	c	507	CLA	CHA-CBD-CGD-O2D
22	c	512	CLA	CHA-CBD-CGD-O2D
31	x	101	BCR	C9-C10-C11-C12
27	B	622	SQD	C10-C11-C12-C13
22	C	512	CLA	C5-C6-C7-C8
29	C	517	DGD	CCA-CDA-CEA-CFA
28	a	410	LHG	O6-C4-C5-C6
31	b	619	BCR	C16-C17-C18-C19
22	B	612	CLA	C16-C17-C18-C20
26	Y	101	LMG	O7-C10-C11-C12
28	L	102	LHG	C25-C26-C27-C28
29	A	413	DGD	CDB-CEB-CFB-CGB
29	c	518	DGD	O1G-C1G-C2G-O2G
26	M	101	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
28	d	408	LHG	C13-C14-C15-C16
28	L	102	LHG	O7-C7-C8-C9
22	c	507	CLA	C2A-CAA-CBA-CGA
22	B	616	CLA	C3-C5-C6-C7
29	c	517	DGD	O2G-C1B-C2B-C3B
22	c	513	CLA	C12-C13-C15-C16
22	d	403	CLA	C11-C12-C13-C15
28	D	411	LHG	C2-C3-O3-P
22	b	601	CLA	CAA-CBA-CGA-O2A
29	C	515	DGD	C8B-C9B-CAB-CBB
22	b	615	CLA	C11-C10-C8-C9
22	c	505	CLA	C6-C7-C8-C9
22	c	505	CLA	C11-C10-C8-C9
23	a	403	PHO	C6-C7-C8-C9
31	H	101	BCR	C15-C16-C17-C18
28	D	411	LHG	C17-C18-C19-C20
32	B	623	STE	C7-C8-C9-C10
27	L	101	SQD	C5-C6-S-O8
22	c	511	CLA	O1A-CGA-O2A-C1
26	b	622	LMG	O10-C28-C29-C30
28	l	101	LHG	C10-C11-C12-C13
28	A	411	LHG	C35-C36-C37-C38
26	d	410	LMG	C31-C32-C33-C34
29	h	101	DGD	C5A-C6A-C7A-C8A
29	c	517	DGD	O1B-C1B-C2B-C3B
25	a	409	PL9	C45-C44-C46-C47
26	D	412	LMG	O10-C28-O8-C9
22	B	613	CLA	CAA-CBA-CGA-O2A
23	d	402	PHO	C4C-C3C-CAC-CBC
31	k	101	BCR	C21-C22-C23-C24
22	c	511	CLA	CBA-CGA-O2A-C1
22	B	602	CLA	C1A-C2A-CAA-CBA
22	C	504	CLA	C1A-C2A-CAA-CBA
22	C	506	CLA	C1A-C2A-CAA-CBA
22	a	404	CLA	C1A-C2A-CAA-CBA
22	b	602	CLA	C1A-C2A-CAA-CBA
22	d	401	CLA	C1A-C2A-CAA-CBA
22	d	405	CLA	C1A-C2A-CAA-CBA
26	d	410	LMG	O9-C10-C11-C12
28	e	101	LHG	O10-C23-C24-C25
25	d	407	PL9	C11-C12-C13-C14
25	d	407	PL9	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
22	a	402	CLA	C15-C16-C17-C18
22	C	511	CLA	CBA-CGA-O2A-C1
28	L	102	LHG	C14-C15-C16-C17
26	A	409	LMG	C7-C8-C9-O8
27	A	410	SQD	C44-C45-C46-O48
27	f	102	SQD	O6-C44-C45-C46
29	c	516	DGD	C1G-C2G-C3G-O3G
28	D	413	LHG	C29-C30-C31-C32
22	A	402	CLA	C16-C17-C18-C20
22	C	511	CLA	O1A-CGA-O2A-C1
22	b	601	CLA	O1A-CGA-O2A-C1
22	C	510	CLA	C4-C3-C5-C6
22	c	502	CLA	C13-C15-C16-C17
26	Y	101	LMG	O9-C10-C11-C12
29	C	515	DGD	C2E-C1E-O5D-C6D
32	a	413	STE	C9-C10-C11-C12
28	D	410	LHG	C3-O3-P-O4
28	d	408	LHG	C4-O6-P-O5
27	A	410	SQD	O49-C7-C8-C9
29	c	516	DGD	O1B-C1B-C2B-C3B
22	b	613	CLA	CAA-CBA-CGA-O2A
22	d	403	CLA	C3-C5-C6-C7
27	B	622	SQD	C14-C15-C16-C17
29	h	101	DGD	CBB-CCB-CDB-CEB
22	c	510	CLA	CAA-CBA-CGA-O2A
29	H	102	DGD	CDB-CEB-CFB-CGB
31	d	406	BCR	C10-C11-C12-C13
27	a	411	SQD	O49-C7-C8-C9
22	B	608	CLA	C13-C15-C16-C17
22	B	605	CLA	C4-C3-C5-C6
27	A	410	SQD	C31-C32-C33-C34
32	X	101	STE	C7-C8-C9-C10
32	d	411	STE	C11-C10-C9-C8
22	B	609	CLA	CAD-CBD-CGD-O1D
22	C	513	CLA	CAD-CBD-CGD-O1D
22	b	607	CLA	CAD-CBD-CGD-O1D
22	c	504	CLA	CAD-CBD-CGD-O1D
22	c	511	CLA	C3-C5-C6-C7
26	A	409	LMG	C9-C8-O7-C10
29	A	413	DGD	O1B-C1B-C2B-C3B
29	c	516	DGD	O2G-C1B-C2B-C3B
22	B	614	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	c	503	CLA	C11-C10-C8-C9
22	c	508	CLA	C14-C13-C15-C16
22	d	403	CLA	C11-C12-C13-C14
22	b	607	CLA	C16-C17-C18-C20
22	B	612	CLA	CAA-CBA-CGA-O2A
26	b	622	LMG	O7-C10-C11-C12
29	C	516	DGD	O2G-C1B-C2B-C3B
22	B	603	CLA	C15-C16-C17-C18
22	c	510	CLA	C15-C16-C17-C18
32	t	104	STE	C3-C4-C5-C6
26	B	621	LMG	C34-C35-C36-C37
32	b	623	STE	C7-C8-C9-C10
22	b	614	CLA	C2A-CAA-CBA-CGA
28	D	410	LHG	C33-C34-C35-C36
28	D	410	LHG	C1-C2-C3-O3
22	B	605	CLA	C10-C11-C12-C13
29	c	517	DGD	CDA-CEA-CFA-CGA
22	B	605	CLA	C6-C7-C8-C10
22	B	606	CLA	C6-C7-C8-C10
22	B	609	CLA	C11-C12-C13-C15
22	B	610	CLA	C11-C10-C8-C7
22	B	615	CLA	C6-C7-C8-C10
22	C	505	CLA	C6-C7-C8-C10
22	C	509	CLA	C12-C13-C15-C16
22	b	615	CLA	C11-C10-C8-C7
22	c	504	CLA	C11-C10-C8-C7
22	c	510	CLA	C11-C10-C8-C7
28	D	413	LHG	O6-C4-C5-O7
27	A	412	SQD	C18-C19-C20-C21
29	c	516	DGD	C6A-C7A-C8A-C9A
22	b	604	CLA	C13-C15-C16-C17
29	A	413	DGD	C3B-C4B-C5B-C6B
31	Z	101	BCR	C11-C12-C13-C14
22	B	613	CLA	CAA-CBA-CGA-O1A
28	d	409	LHG	O10-C23-C24-C25
29	C	515	DGD	O1B-C1B-C2B-C3B
31	b	619	BCR	C13-C14-C15-C16
31	c	515	BCR	C13-C14-C15-C16
28	D	410	LHG	C34-C35-C36-C37
27	a	411	SQD	O47-C7-C8-C9
28	d	408	LHG	C25-C26-C27-C28
22	b	601	CLA	CAA-CBA-CGA-O1A

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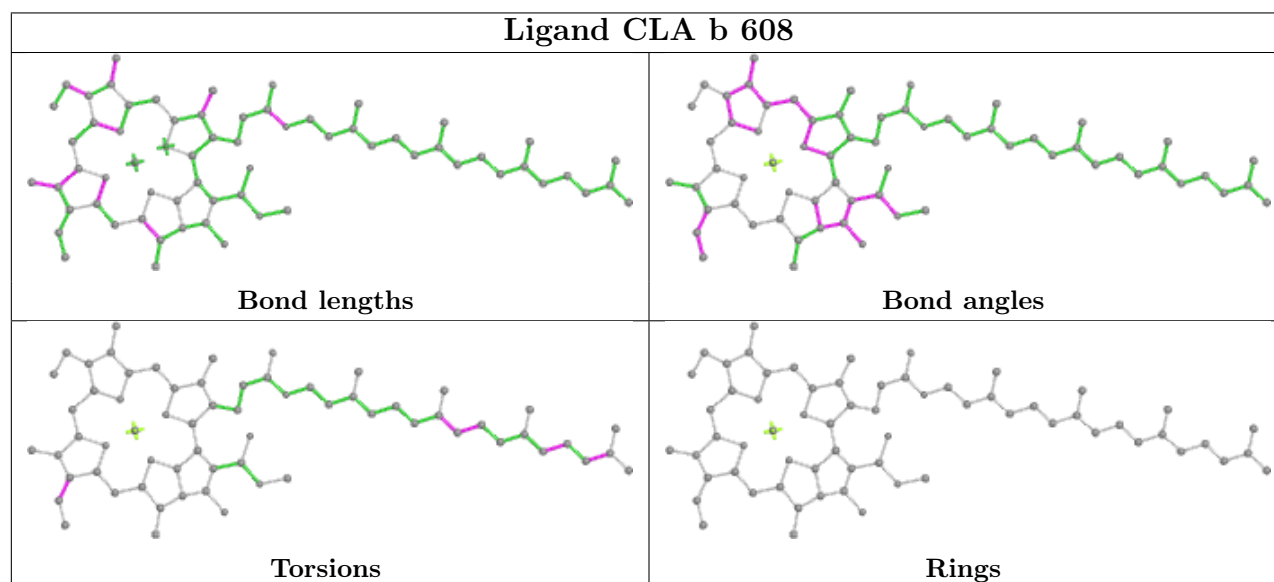
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Mol	Chain	Res	Type	Atoms
22	c	510	CLA	CAA-CBA-CGA-O1A
25	A	408	PL9	C29-C31-C32-C33
22	c	511	CLA	C8-C10-C11-C12
26	A	409	LMG	C19-C20-C21-C22
29	C	516	DGD	O1G-C1A-C2A-C3A
29	c	518	DGD	O1G-C1A-C2A-C3A
25	d	407	PL9	C27-C28-C29-C30
27	a	411	SQD	C35-C36-C37-C38
22	b	614	CLA	CAA-CBA-CGA-O2A

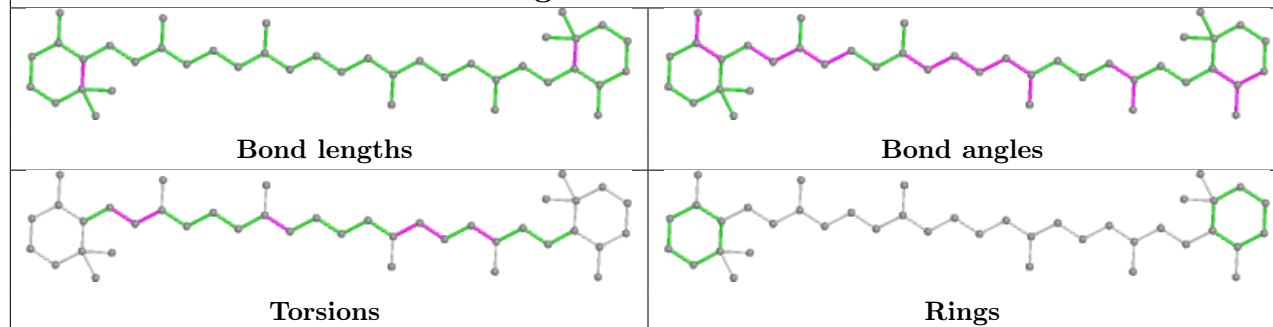
There are no ring outliers.

No monomer is involved in short contacts.

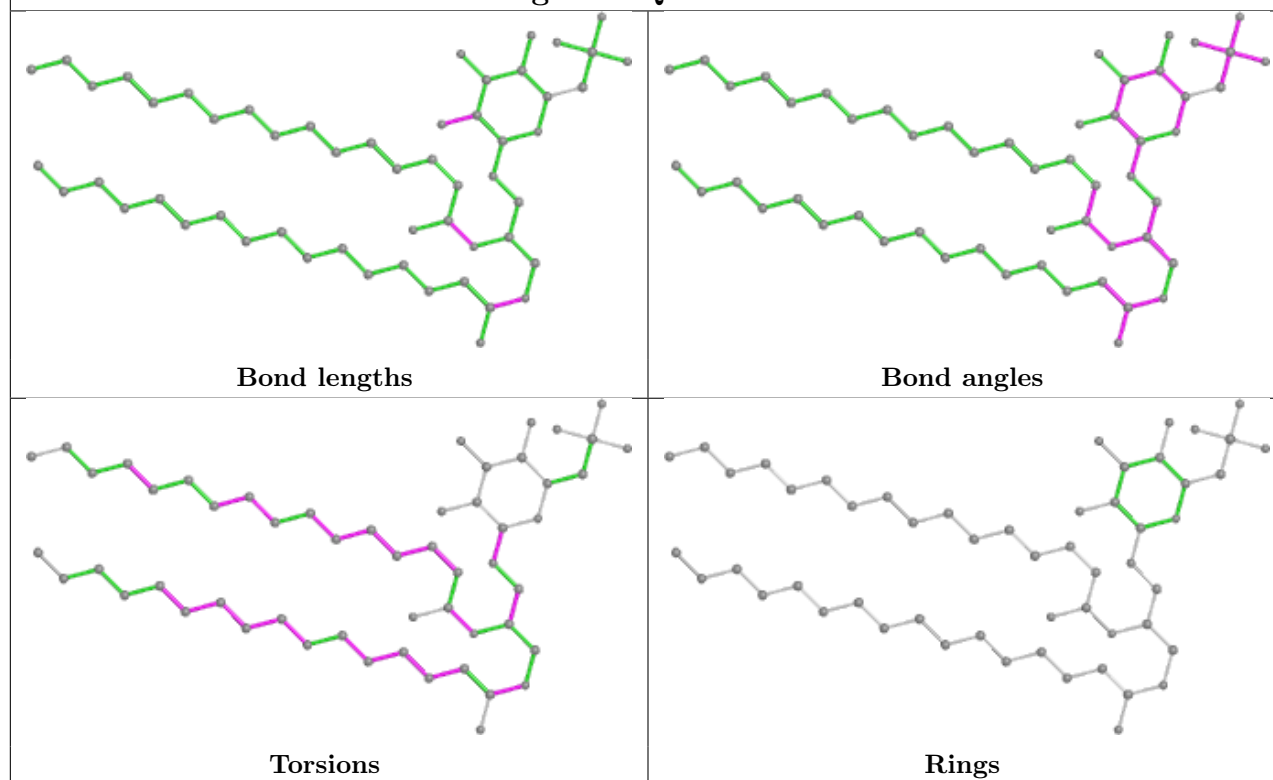
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



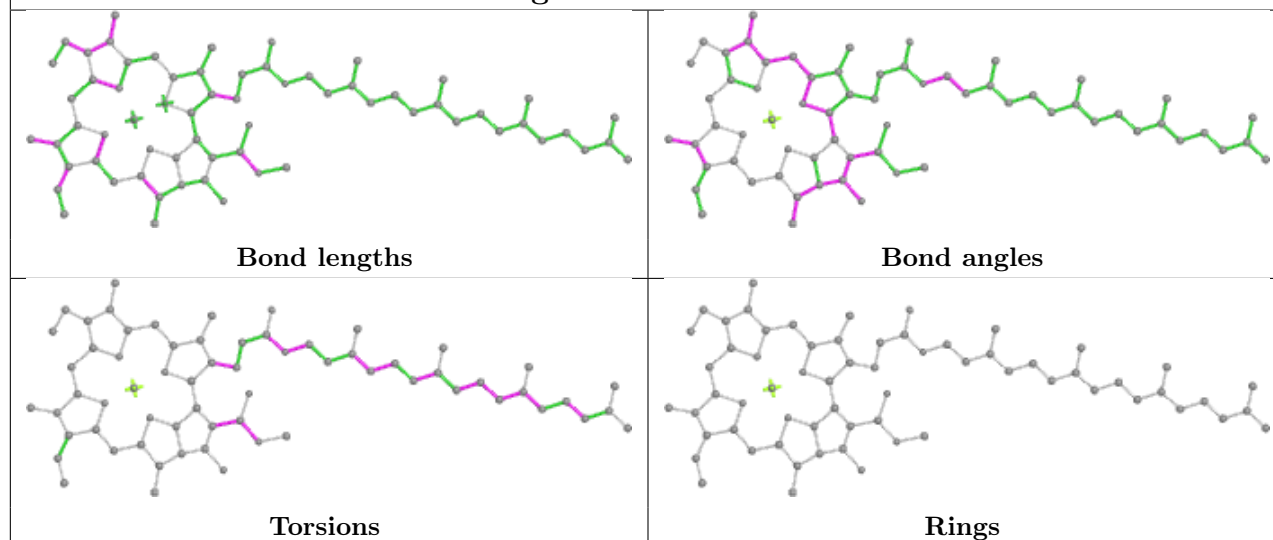
Ligand BCR c 514

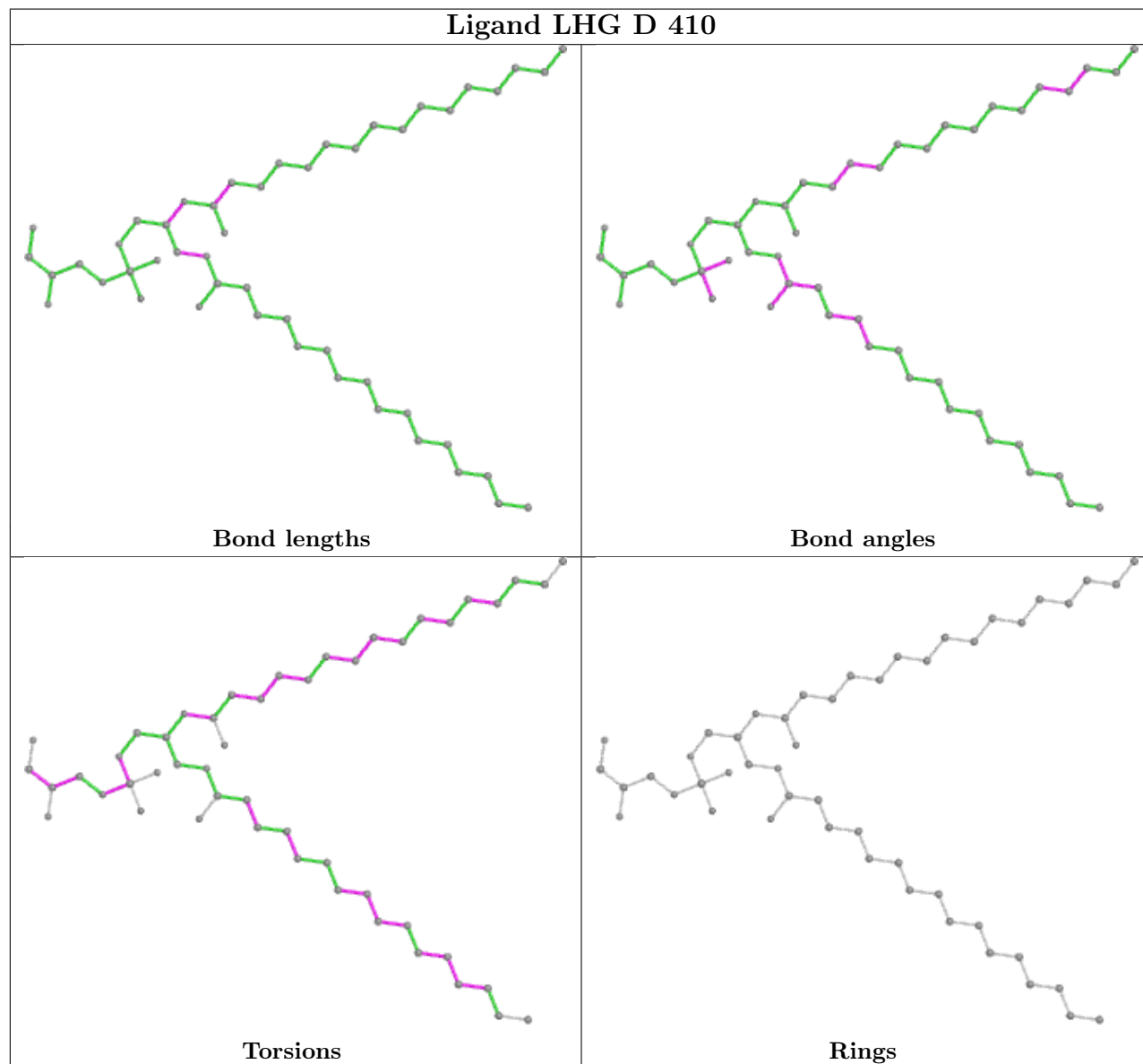
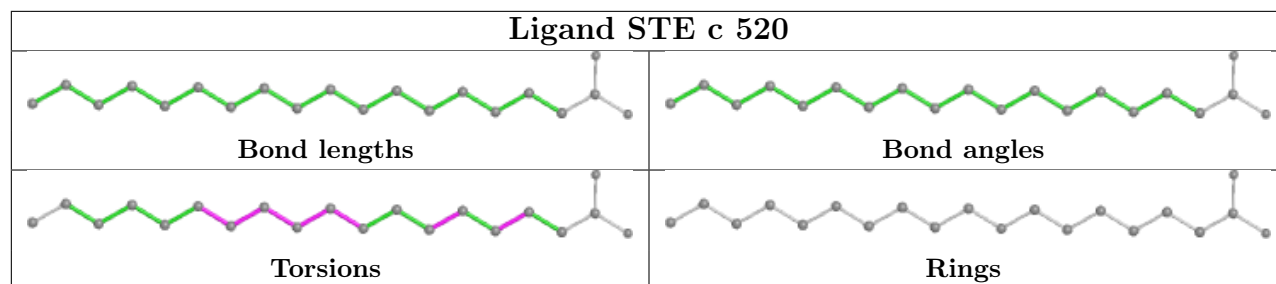


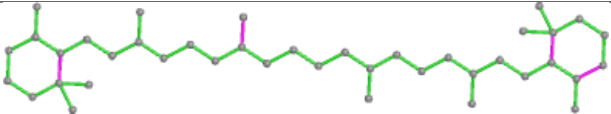
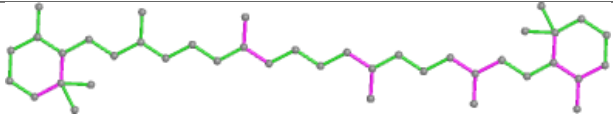
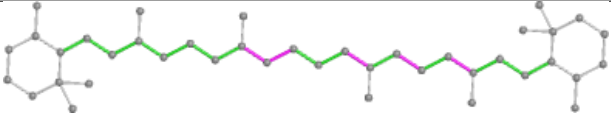
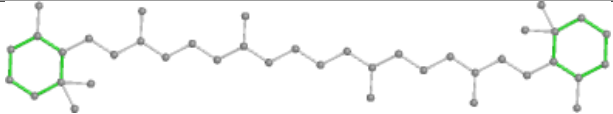
Ligand SQD B 622







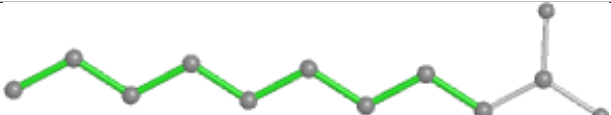
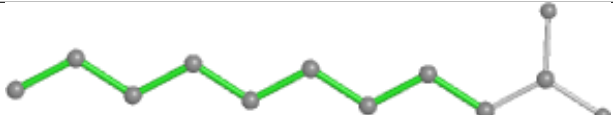
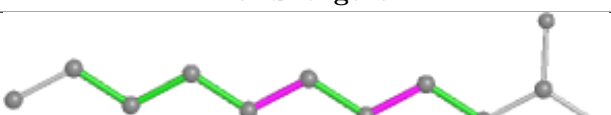
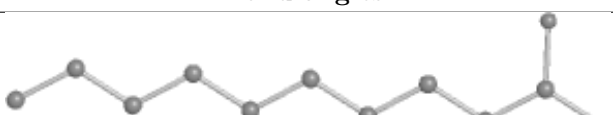
Ligand CLA C 506

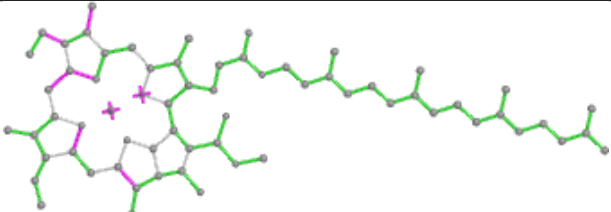
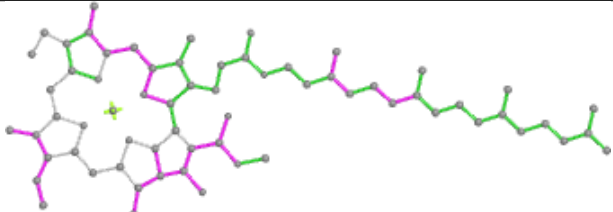
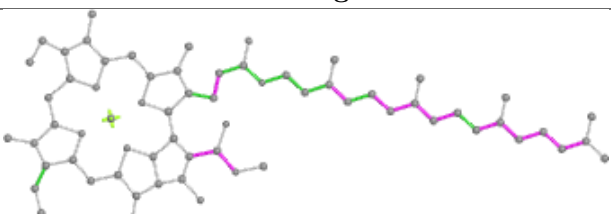
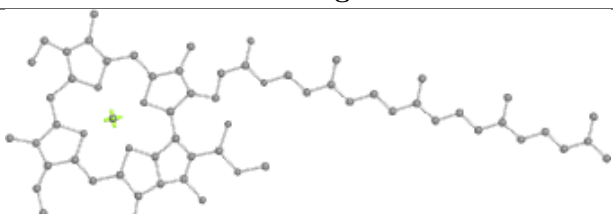


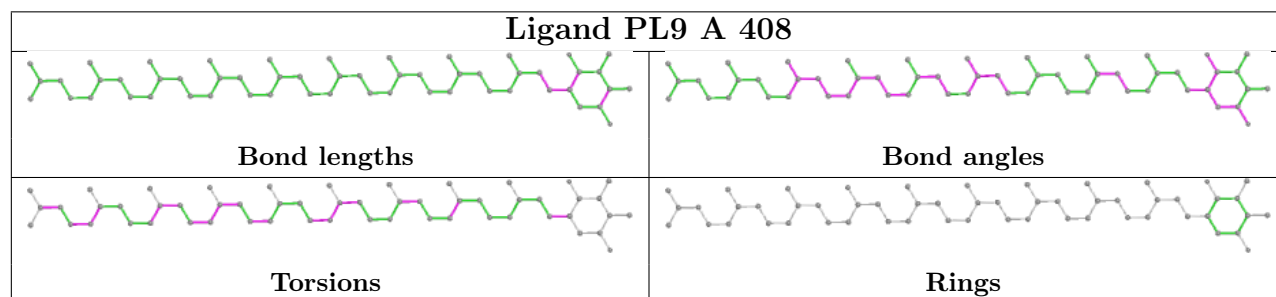
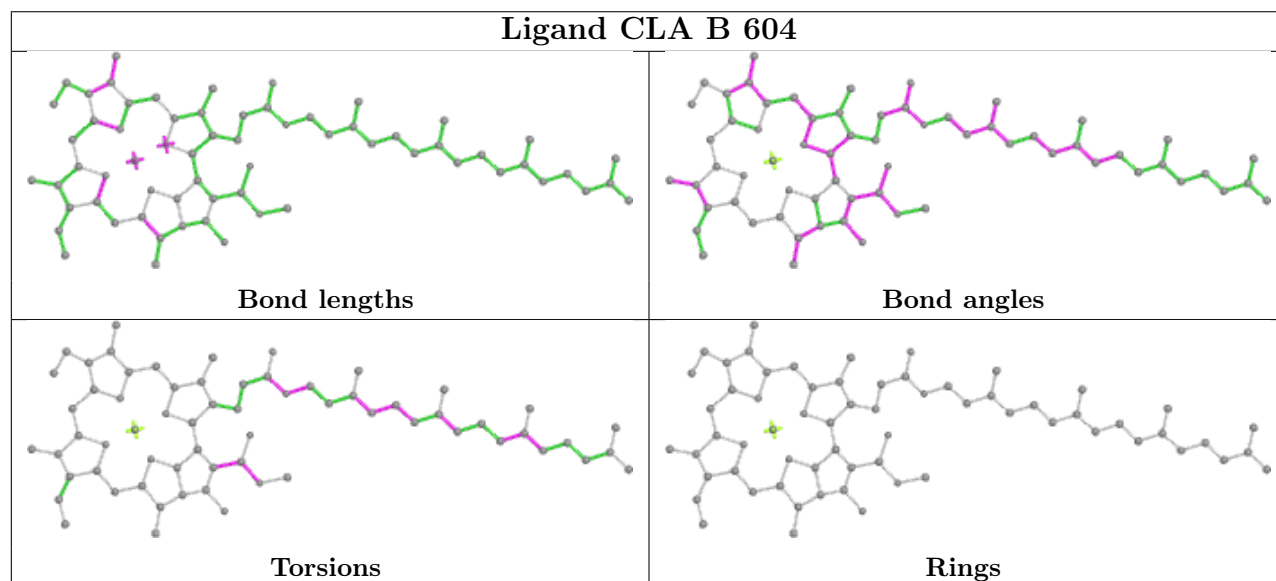
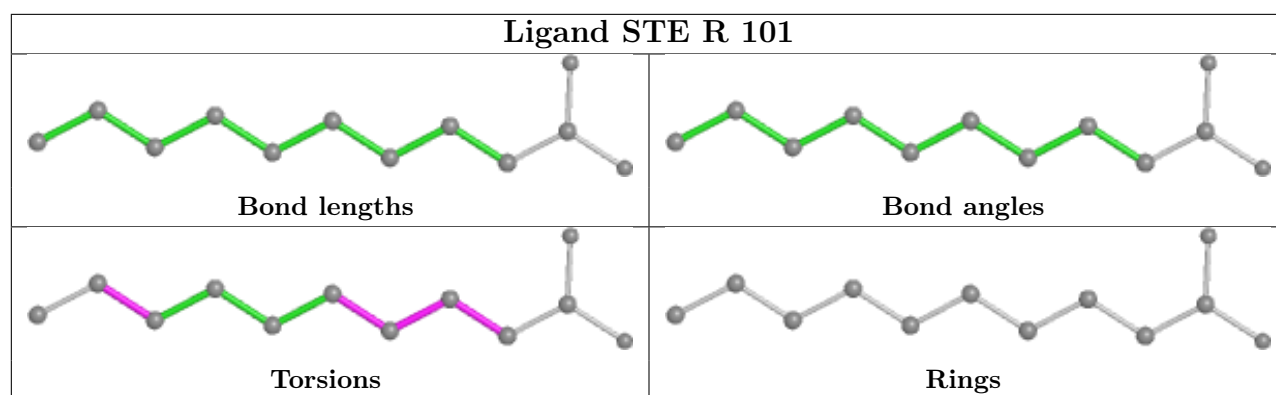


Ligand BCR c 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

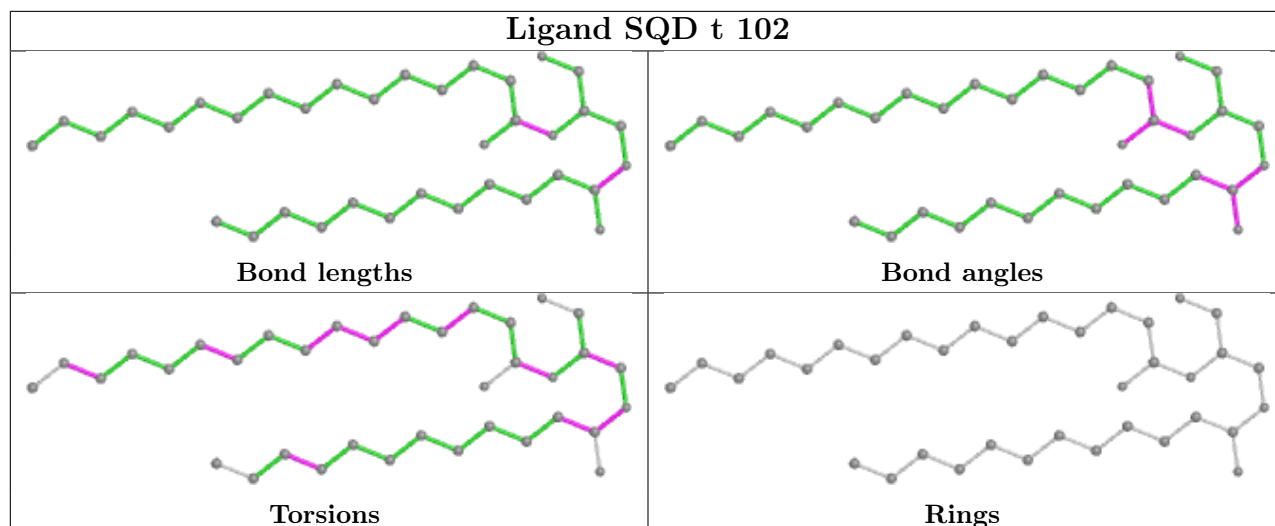
Ligand STE l 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE j 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

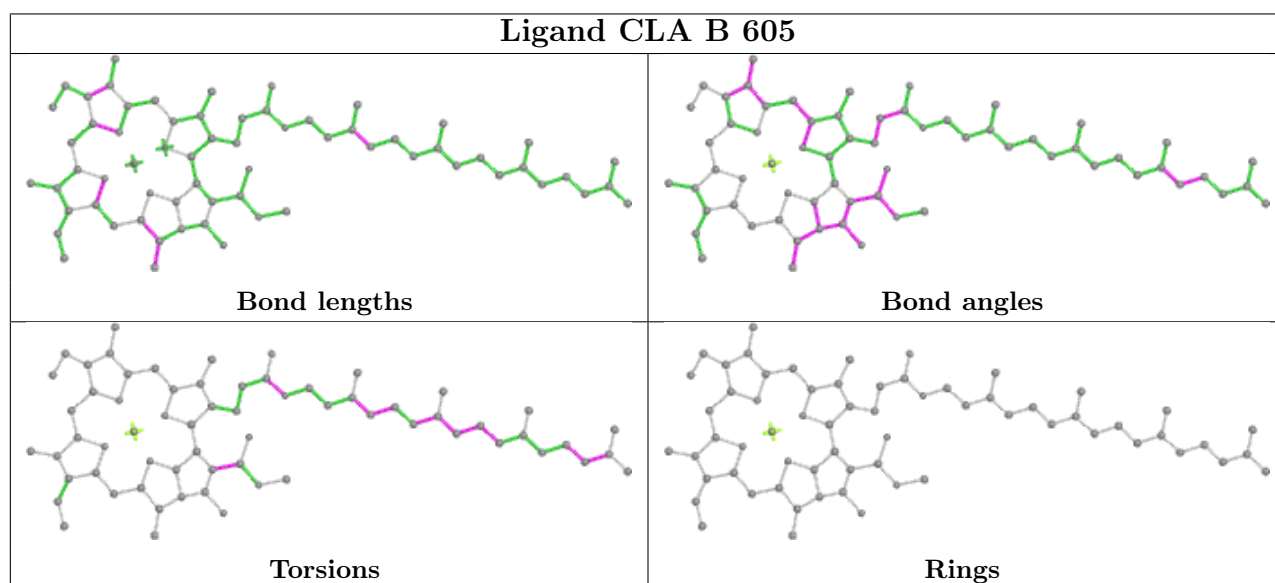
Ligand CLA B 614	
	
Bond lengths	Bond angles
	
Torsions	Rings



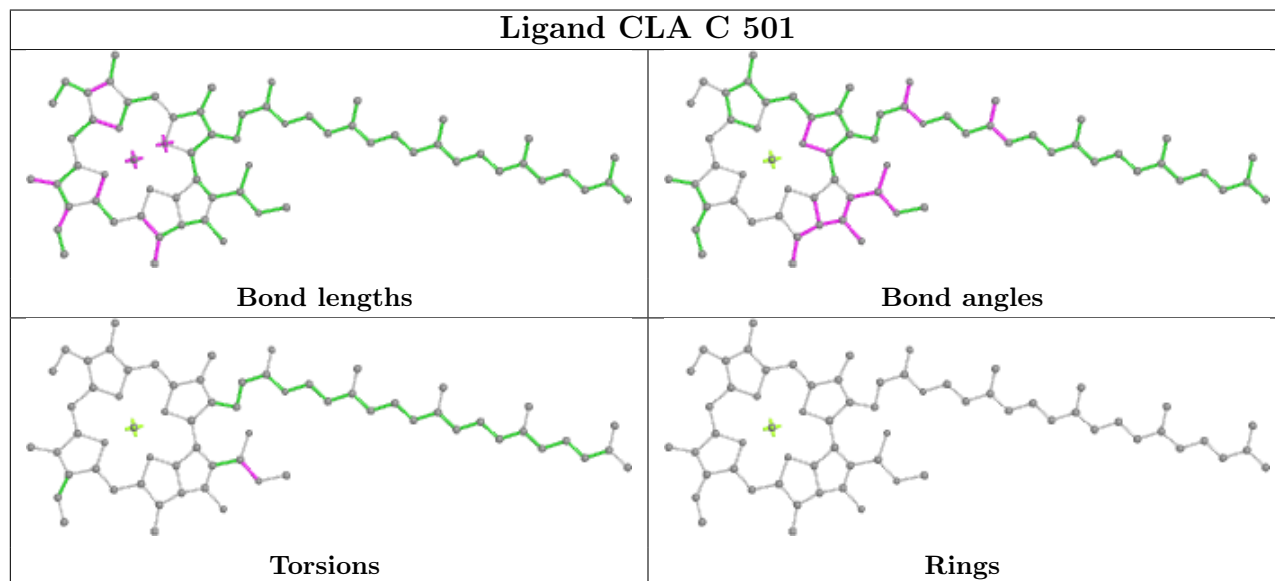
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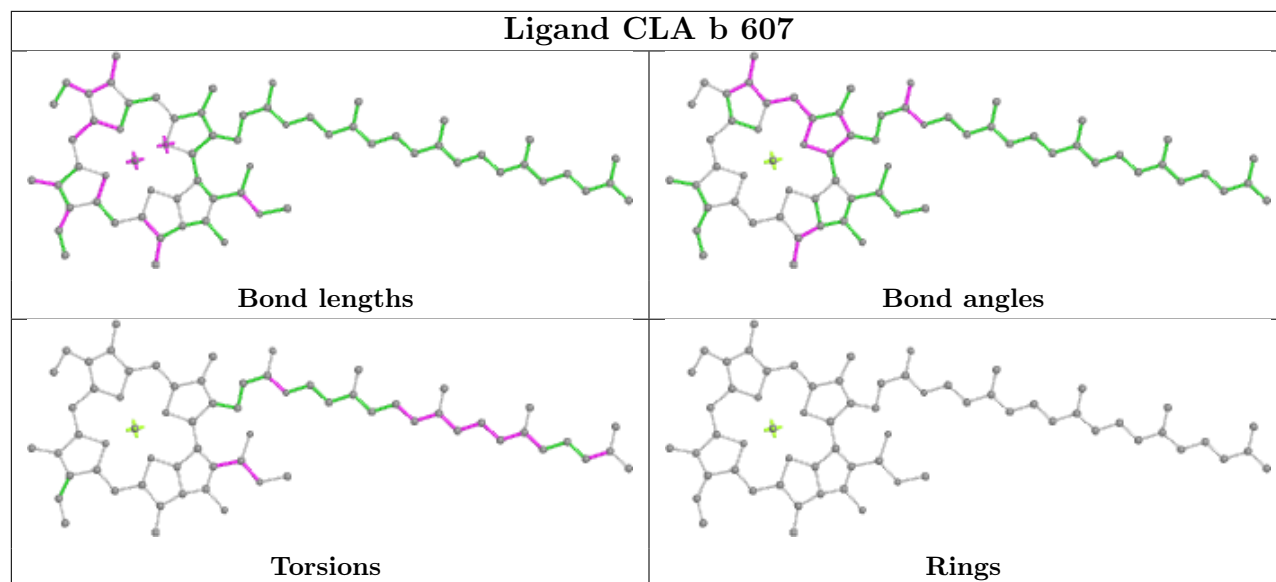
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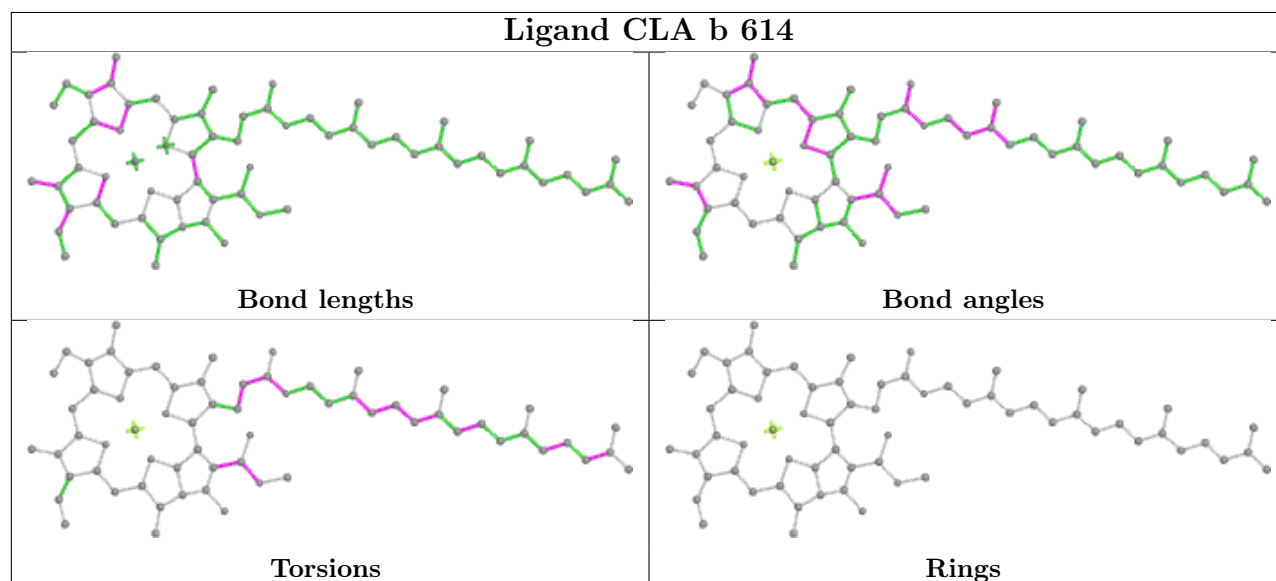
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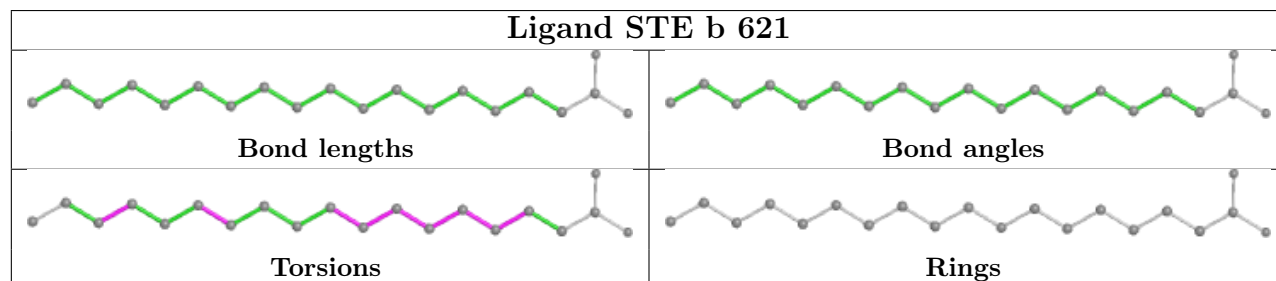
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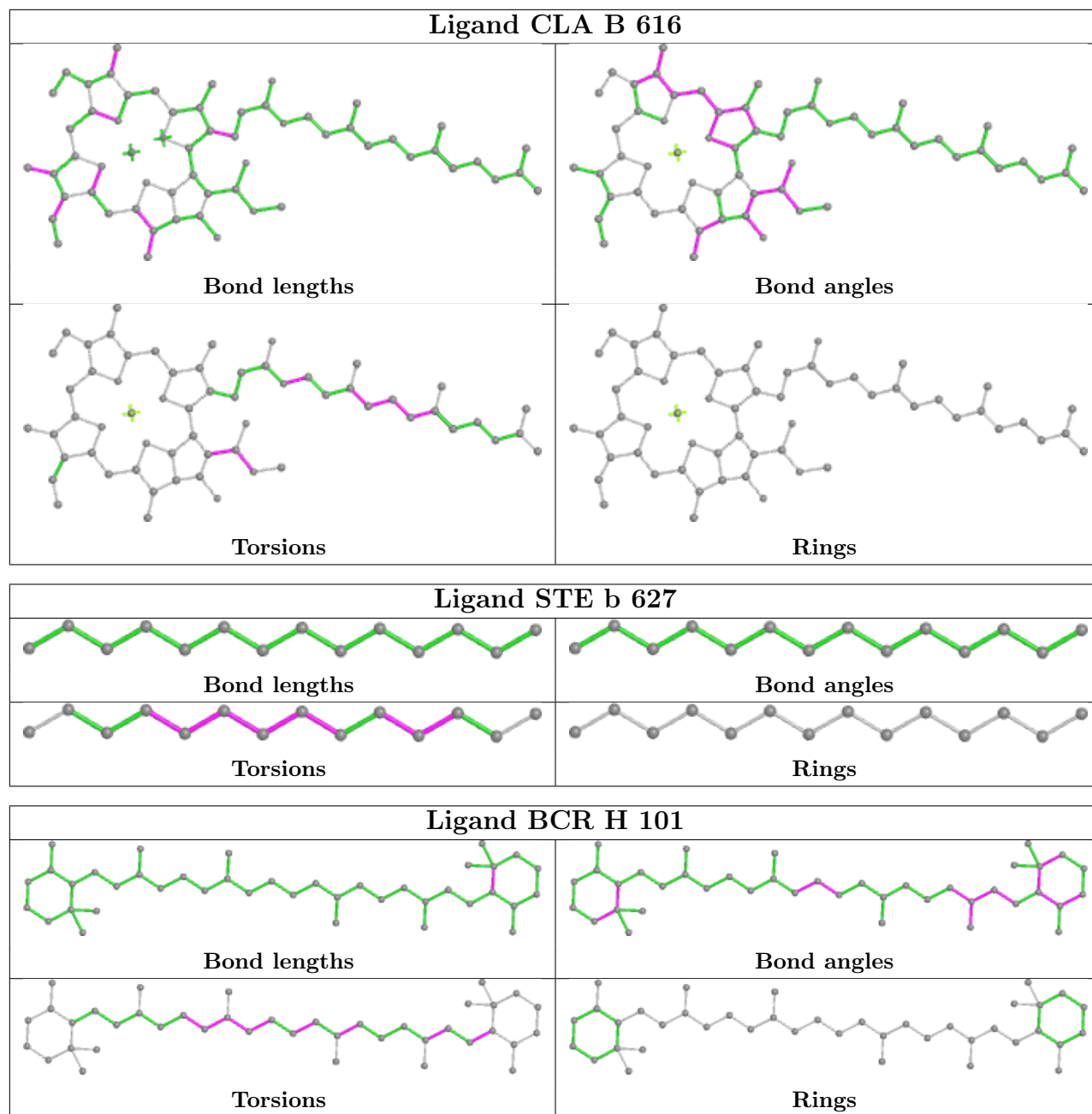


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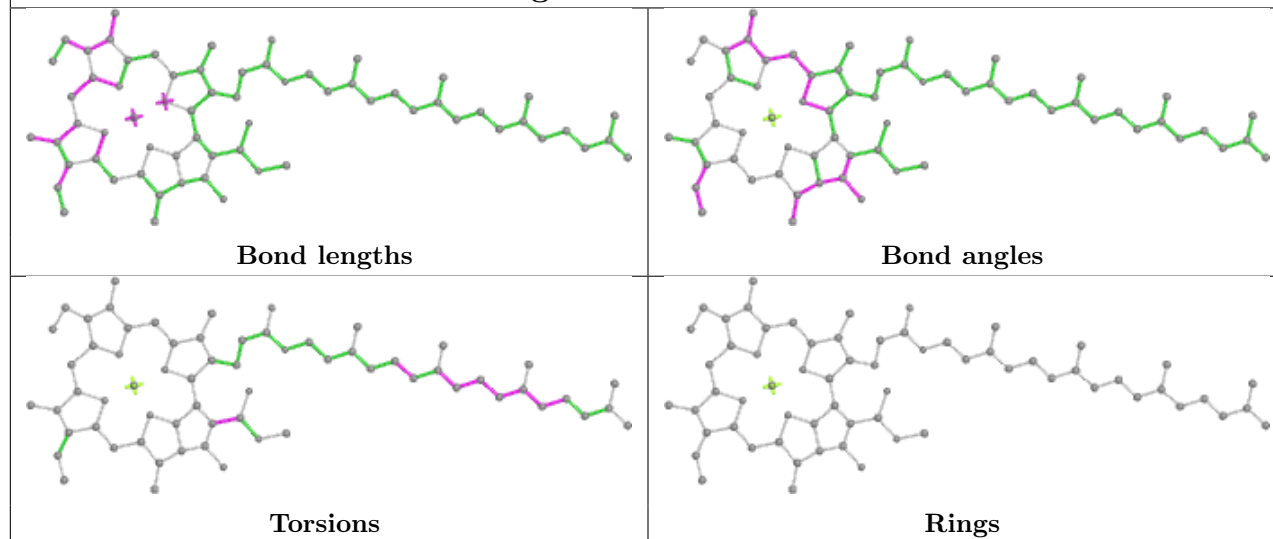


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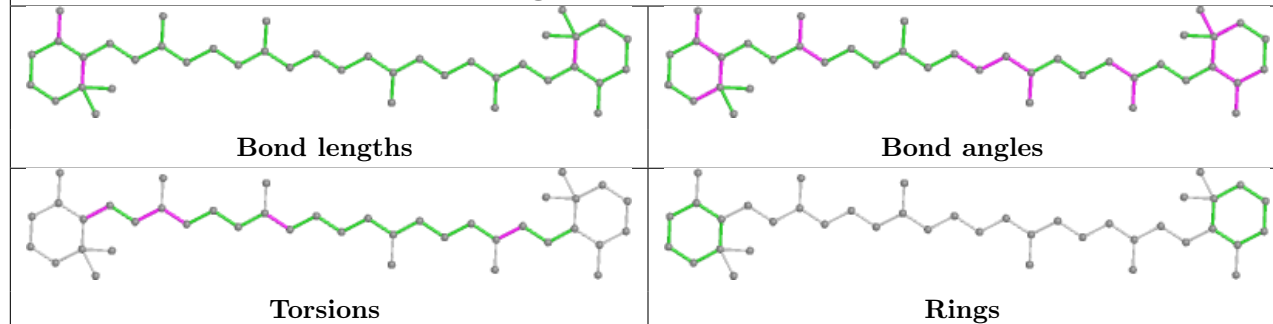




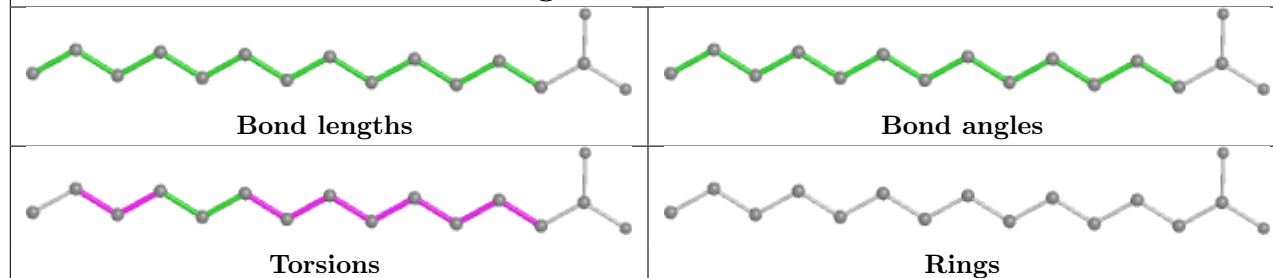
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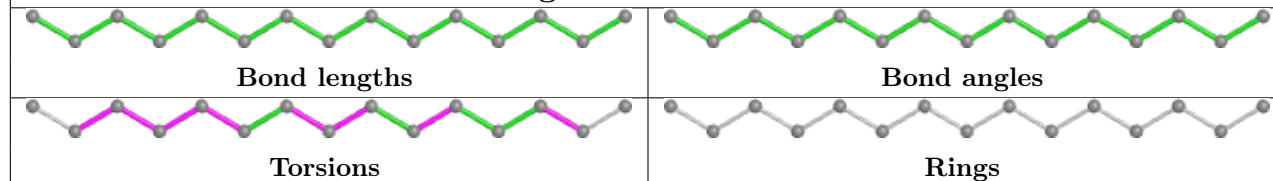
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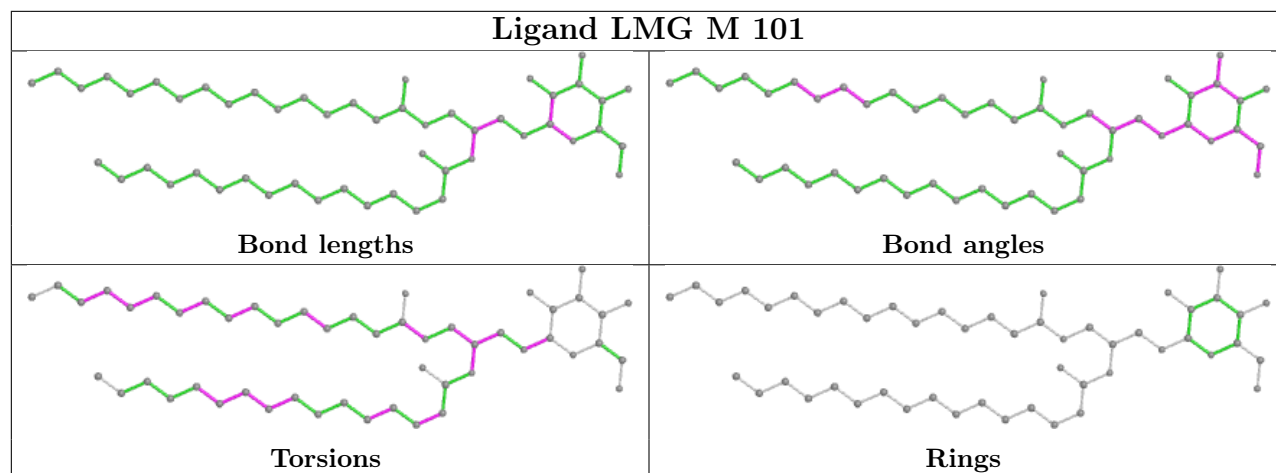
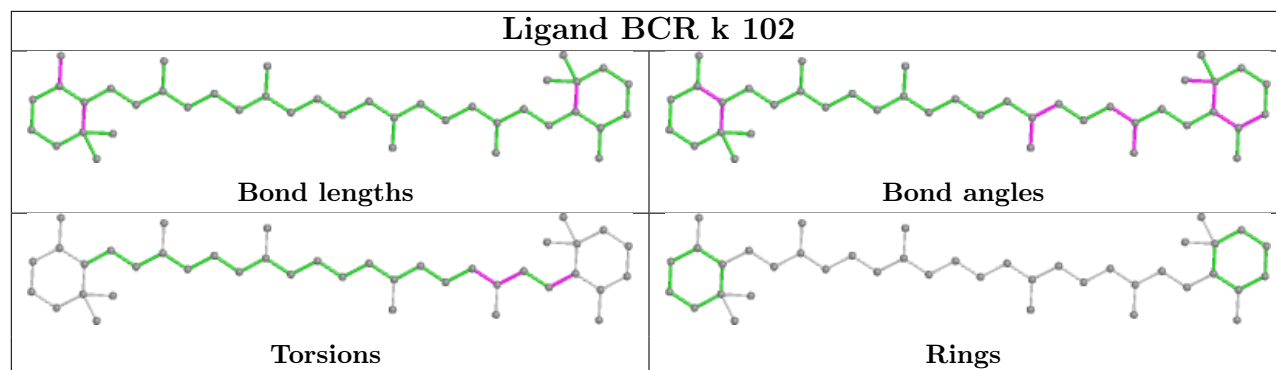


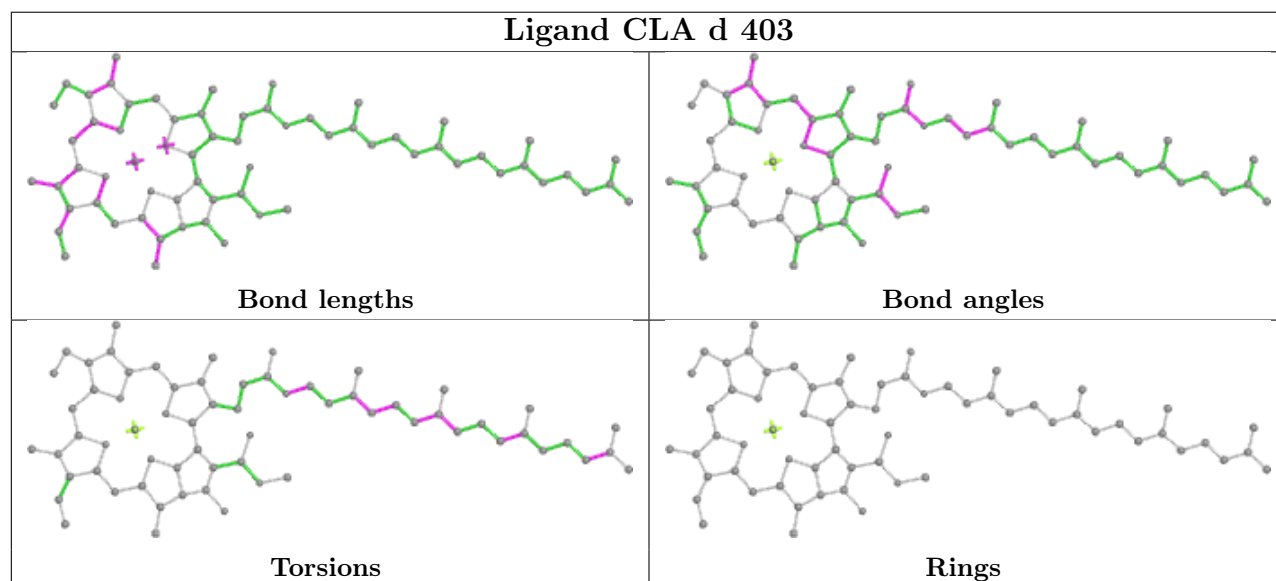
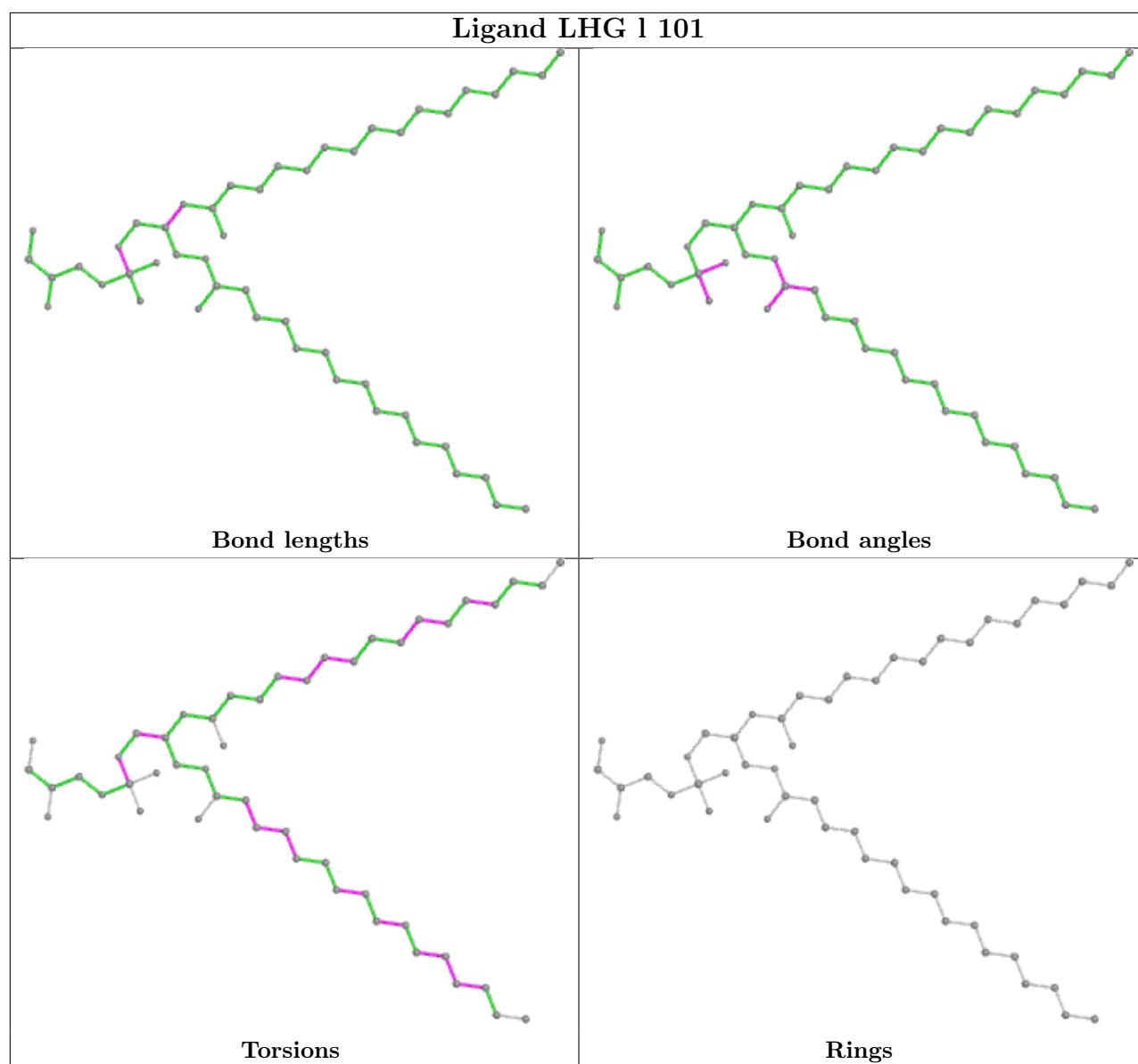
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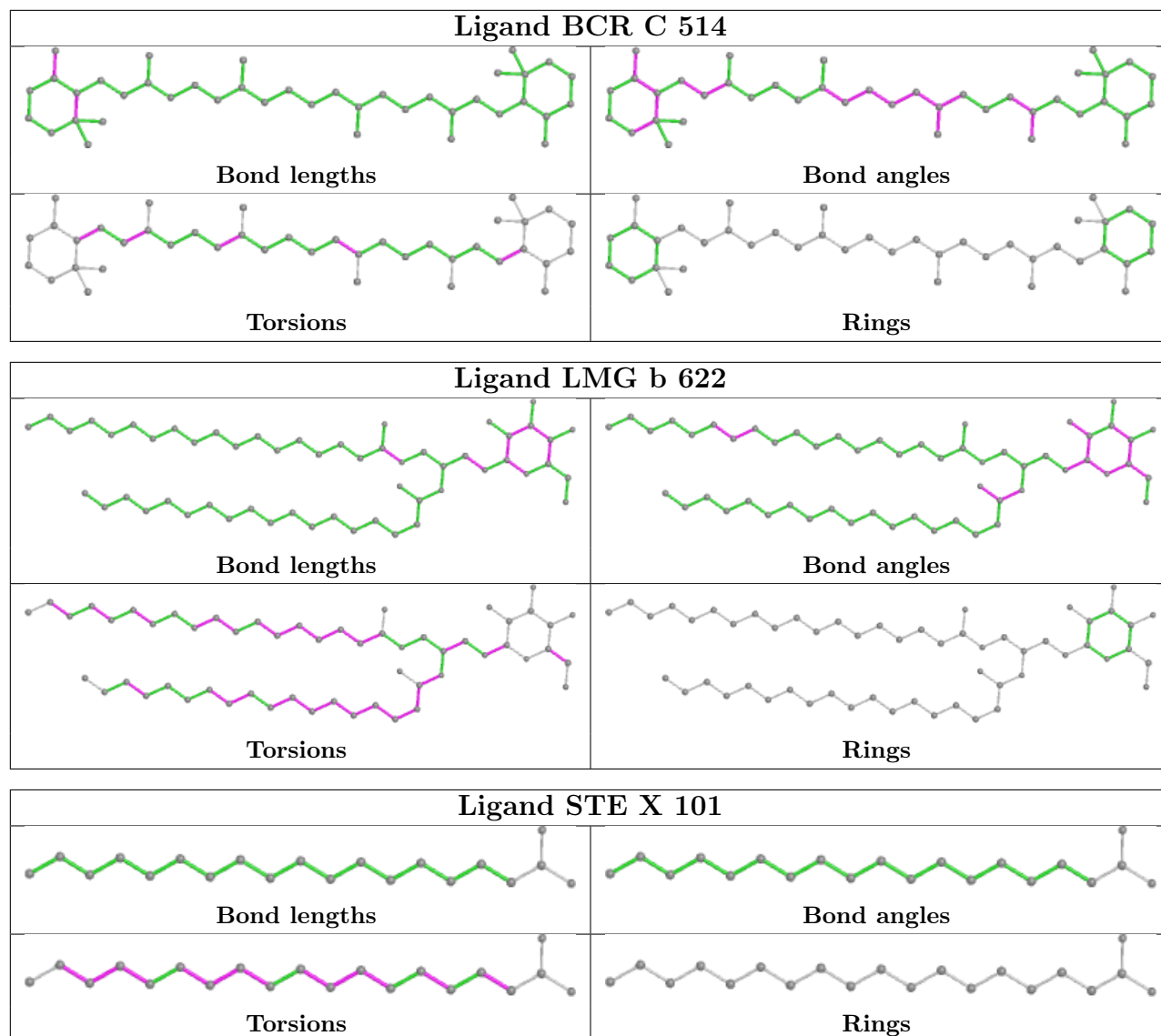


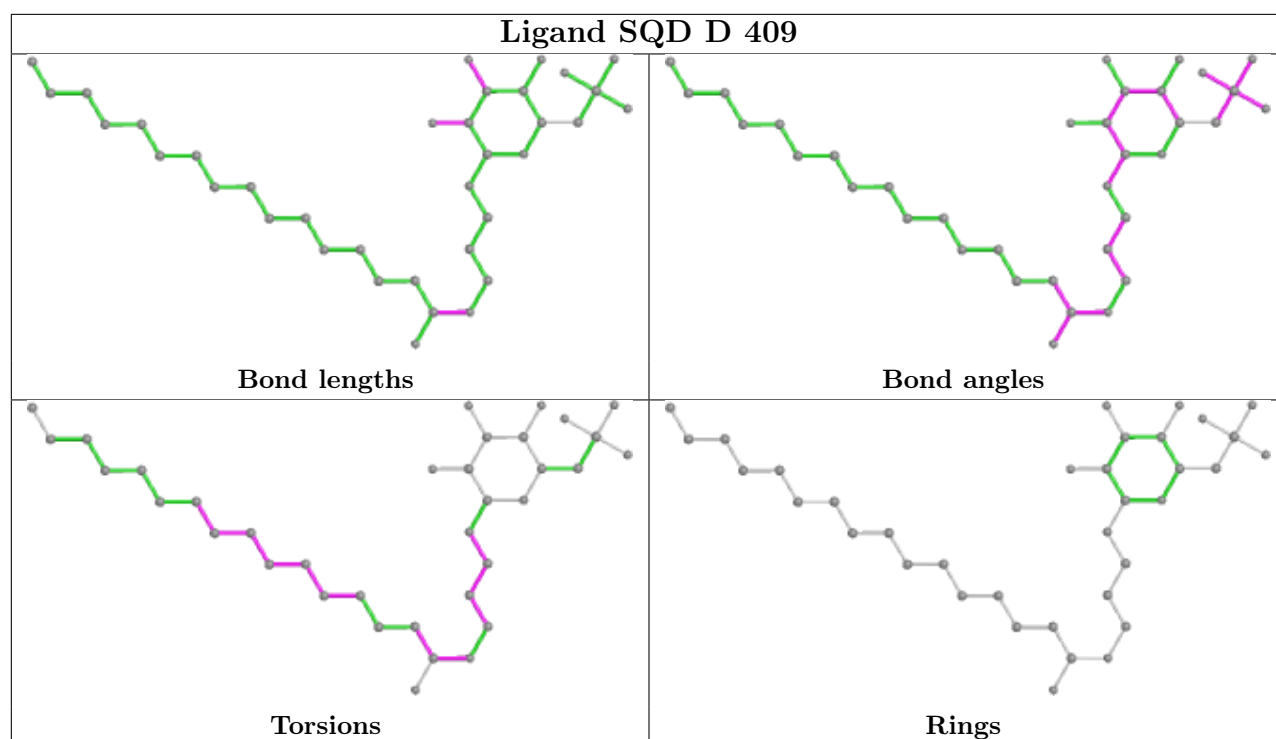
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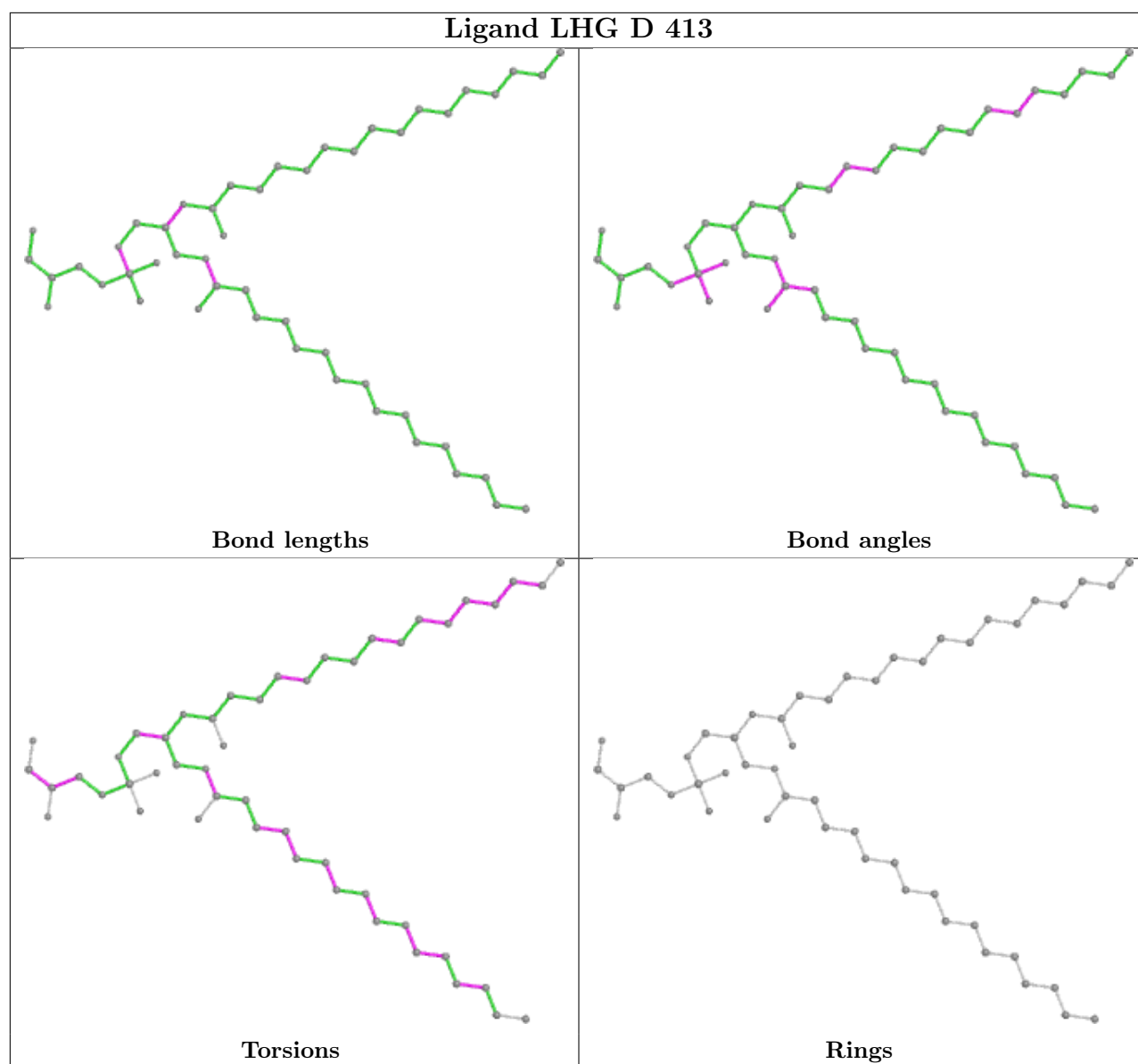


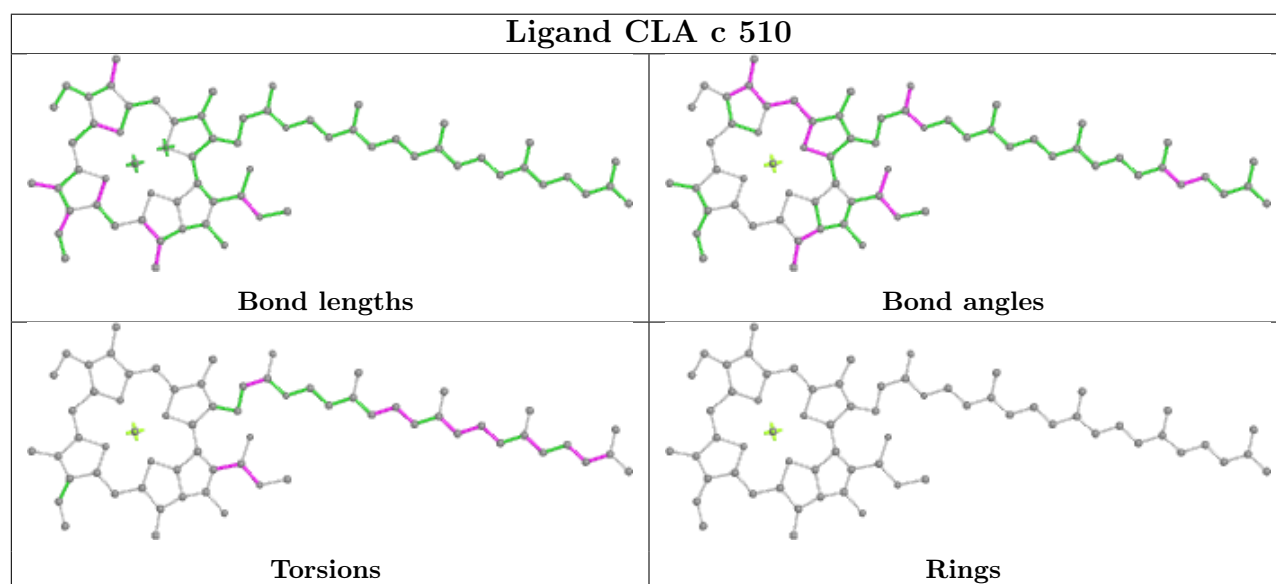
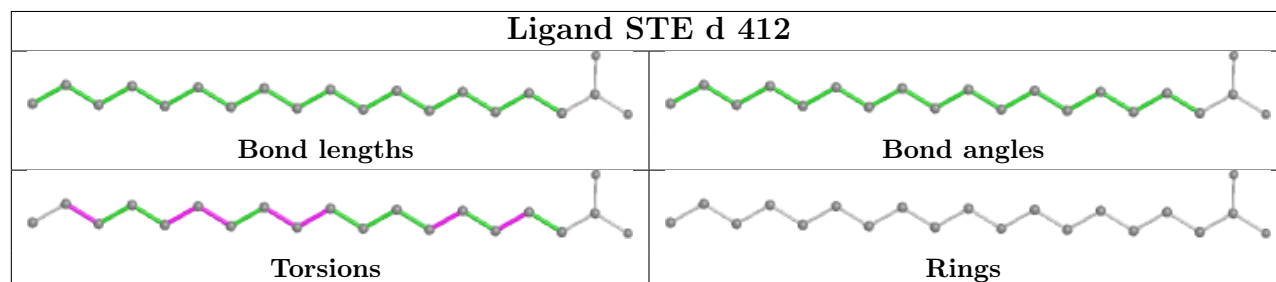
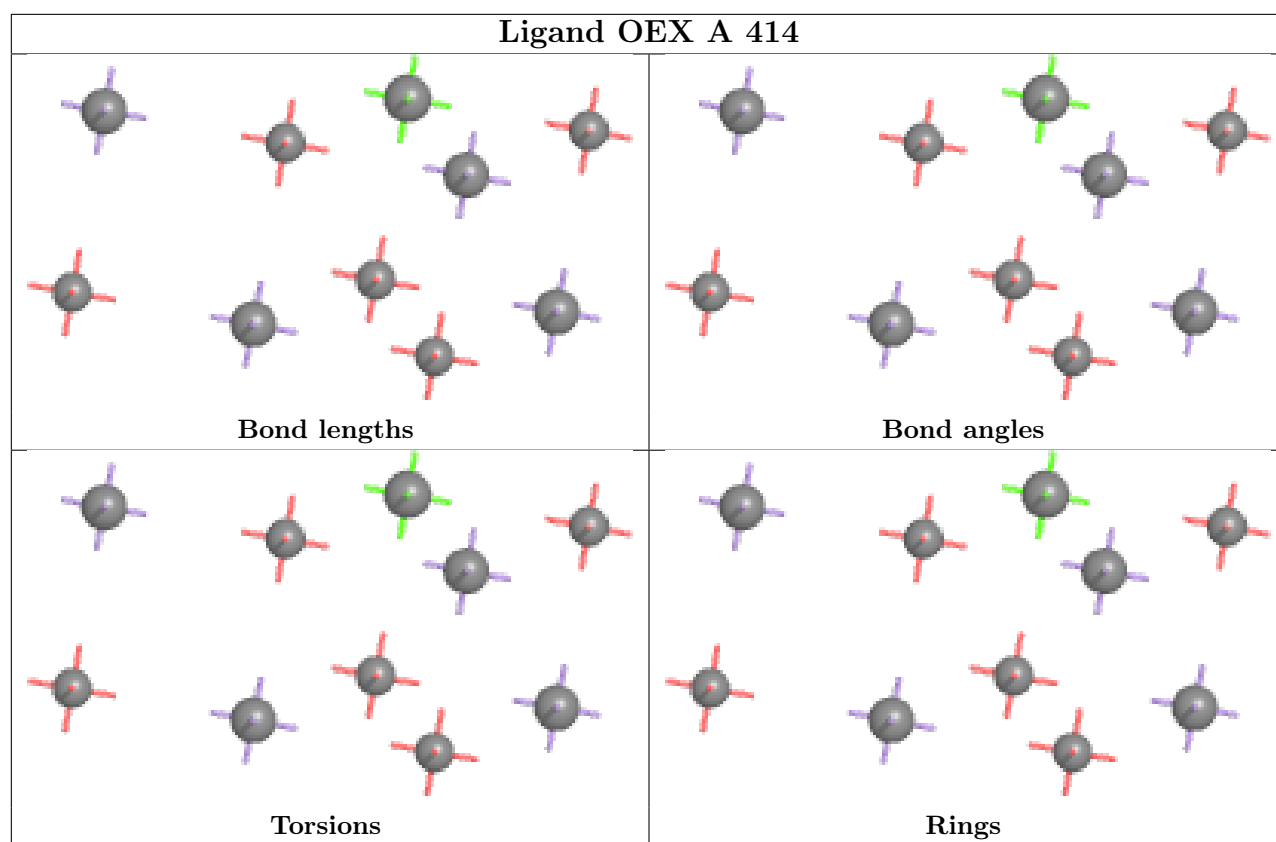




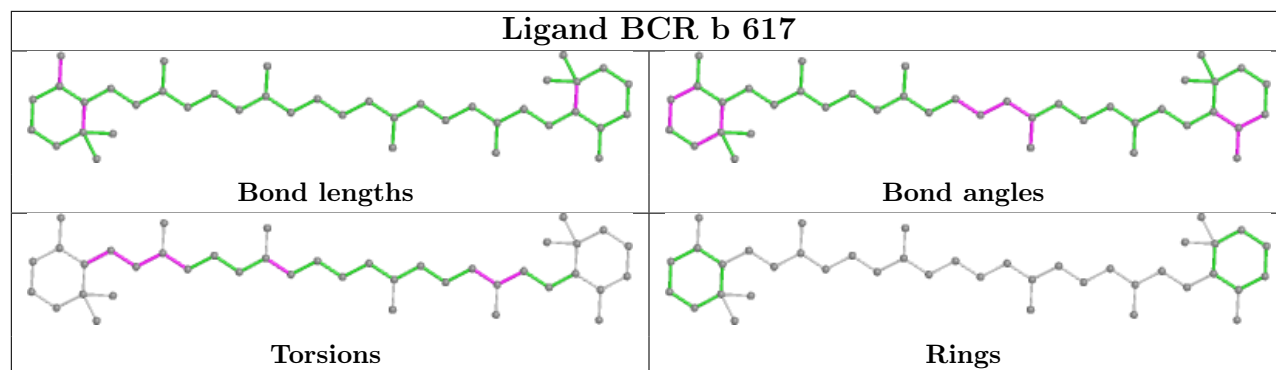




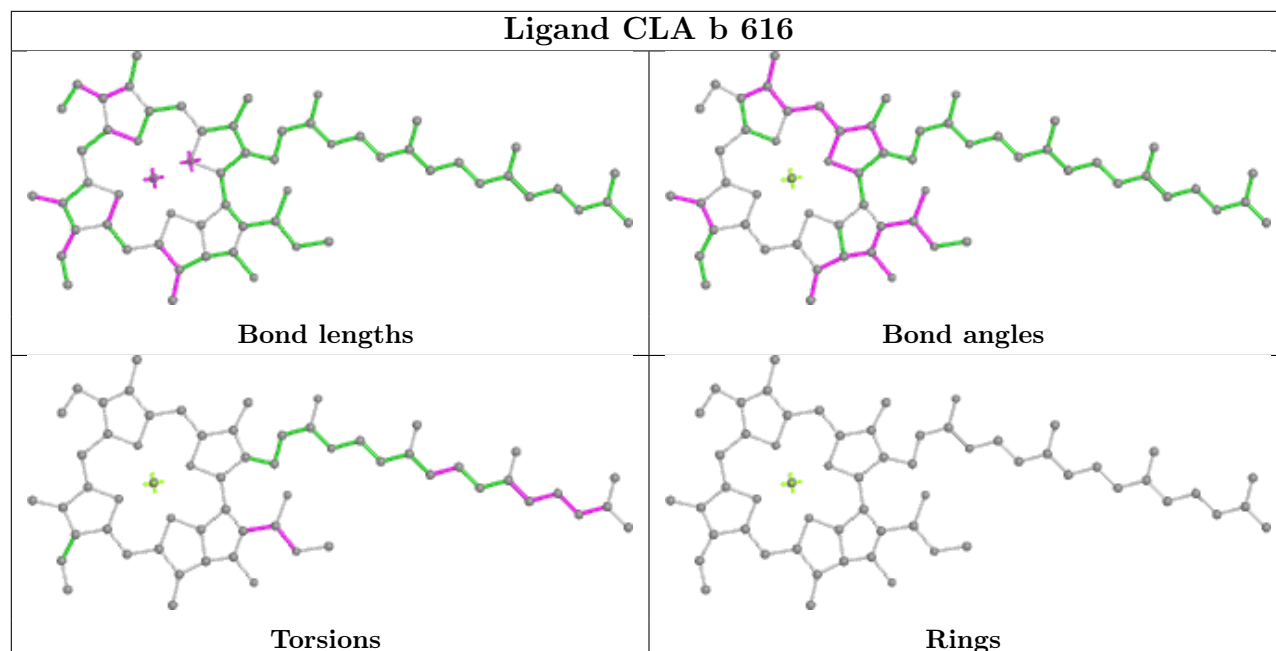




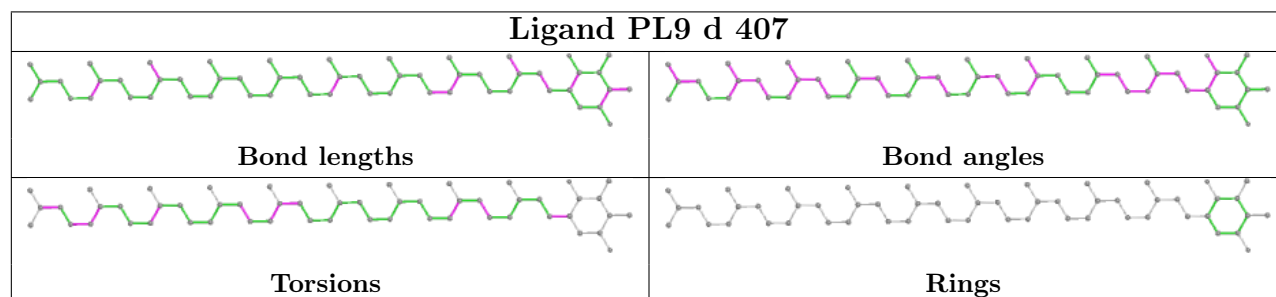
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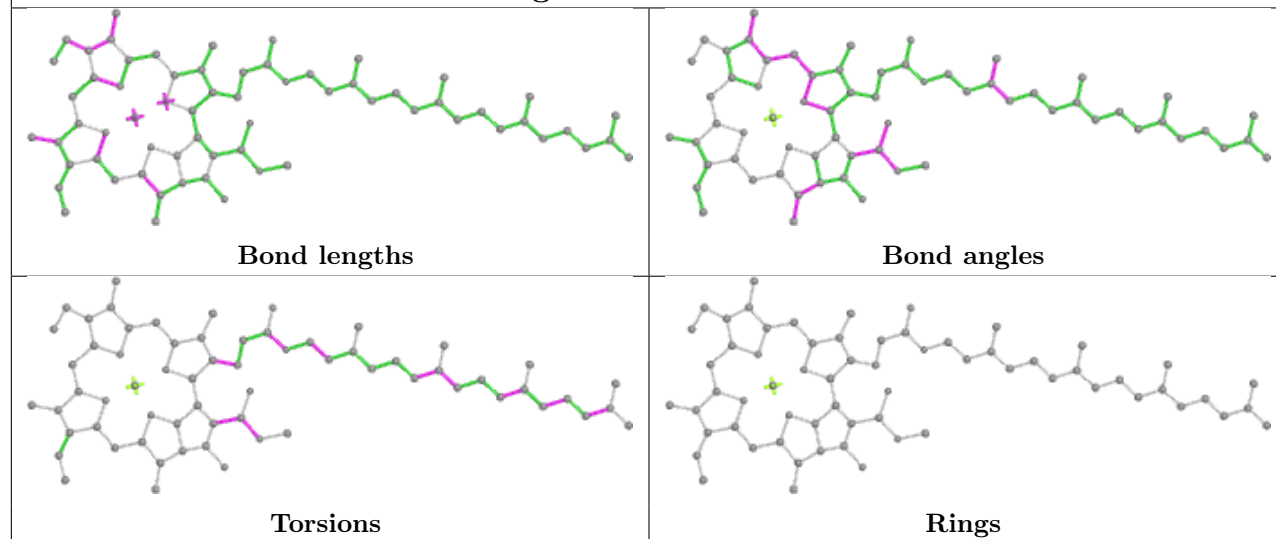
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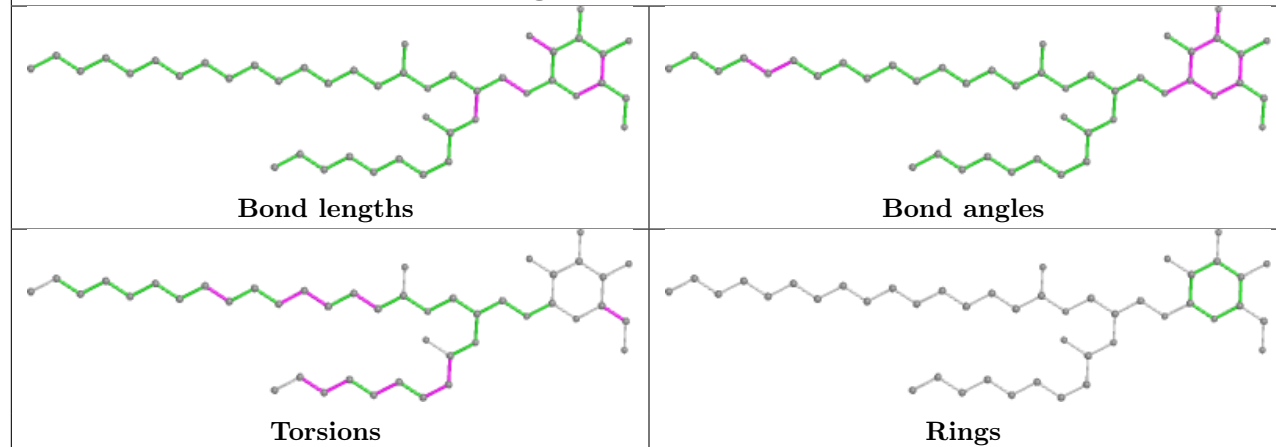
Ligand PL9 d 407



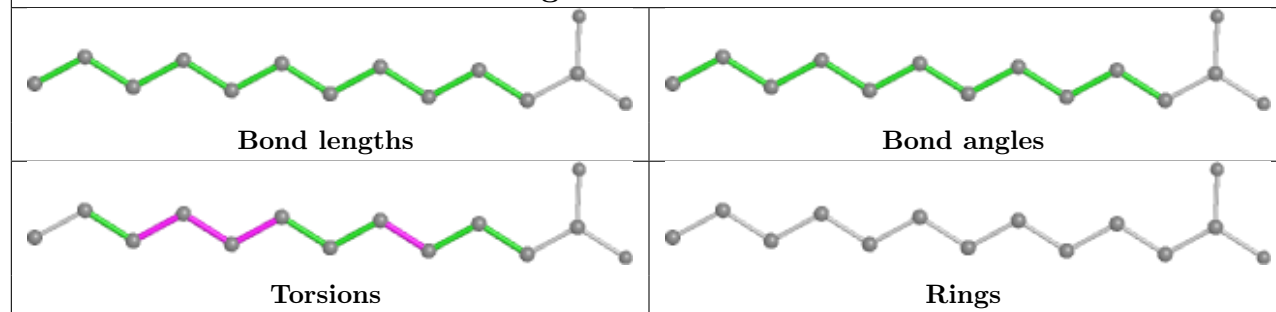
Ligand CLA B 601

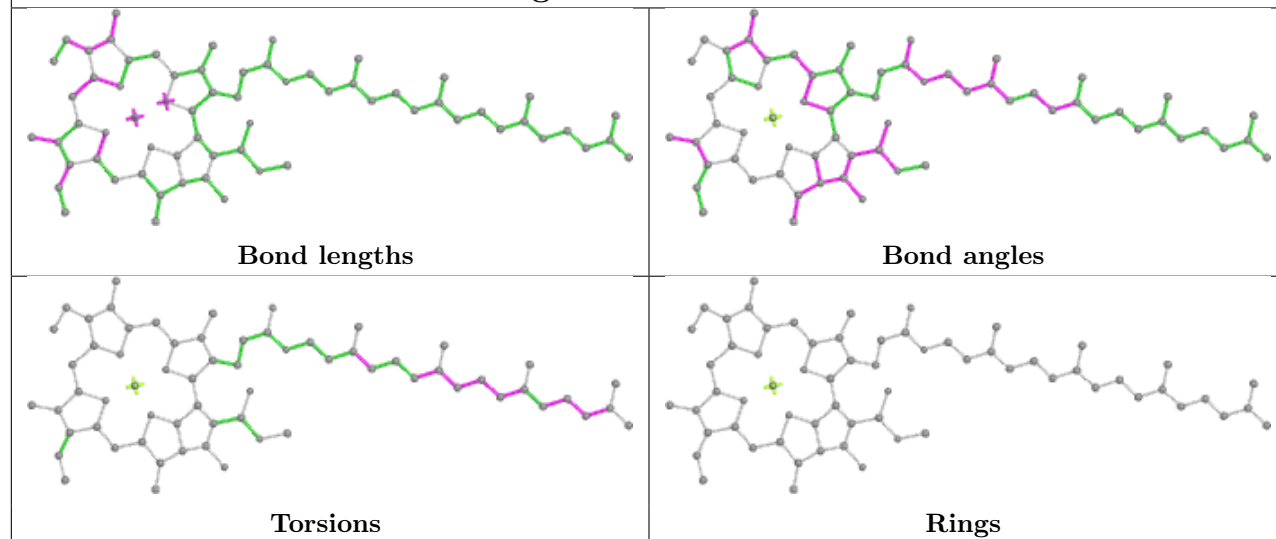
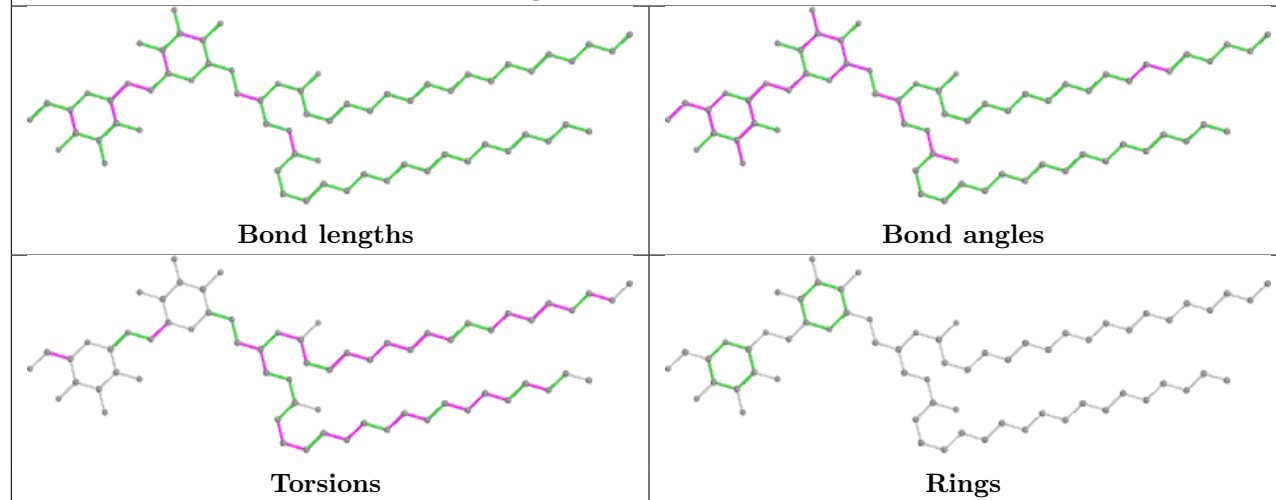


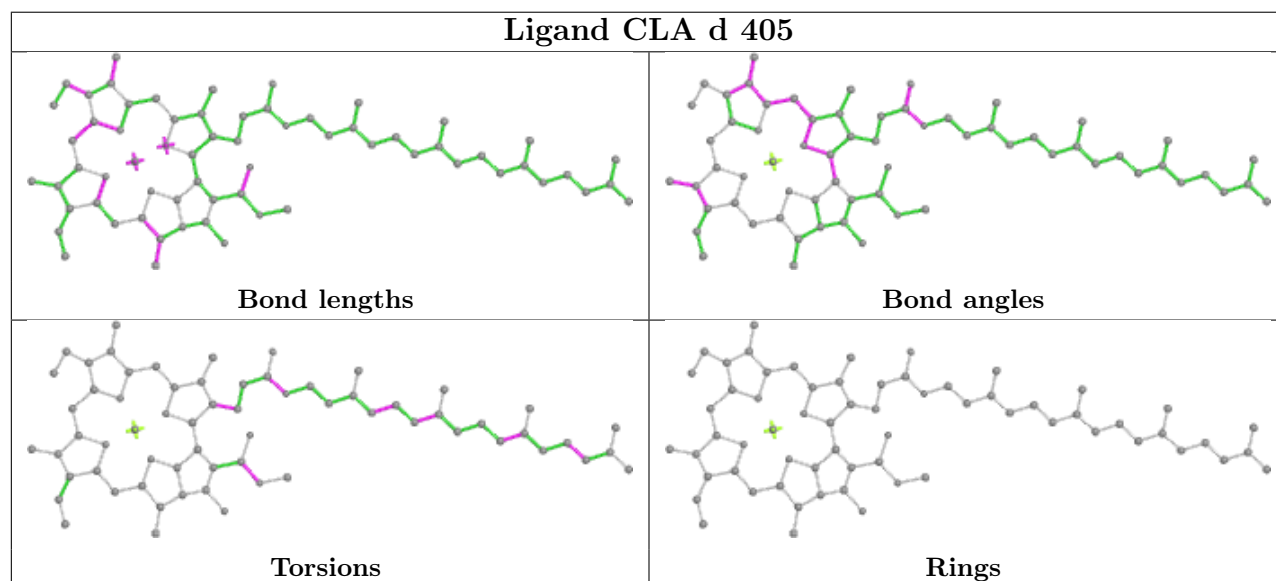
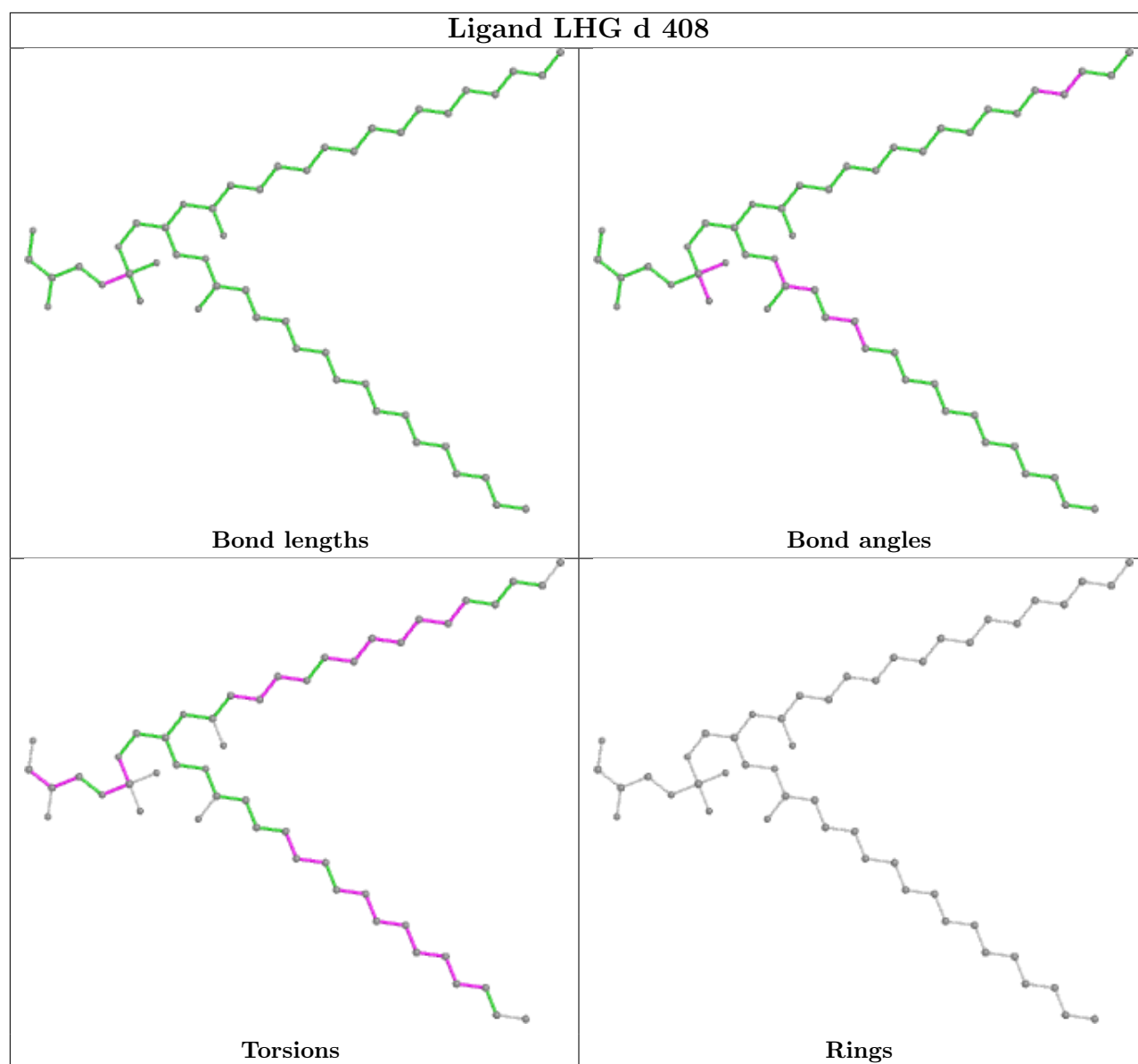
Ligand LMG d 410



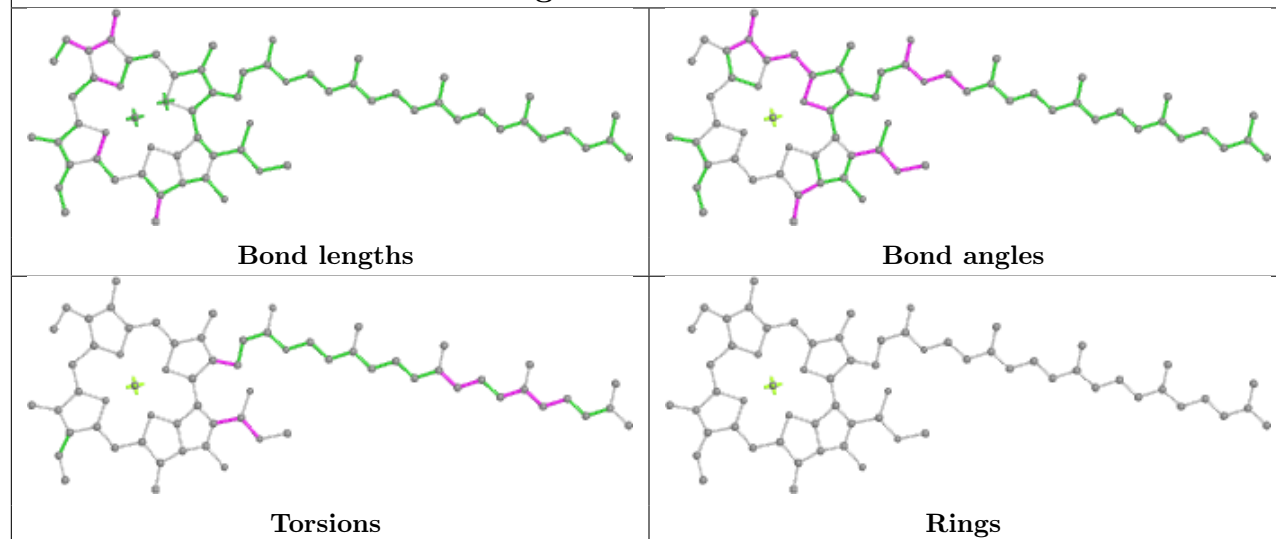
Ligand STE t 103



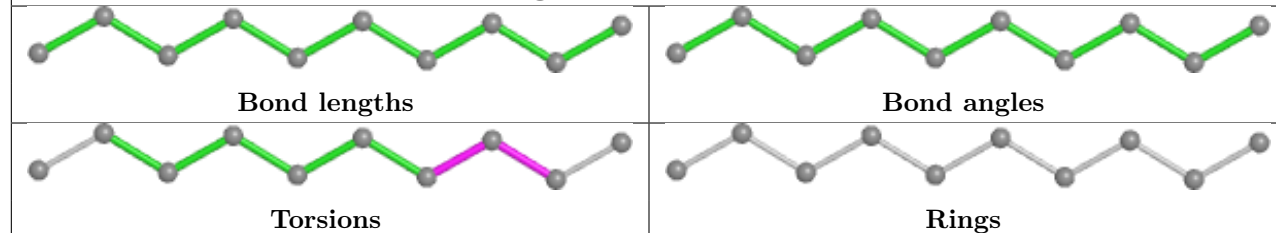
Ligand CLA B 603**Ligand DGD A 413**



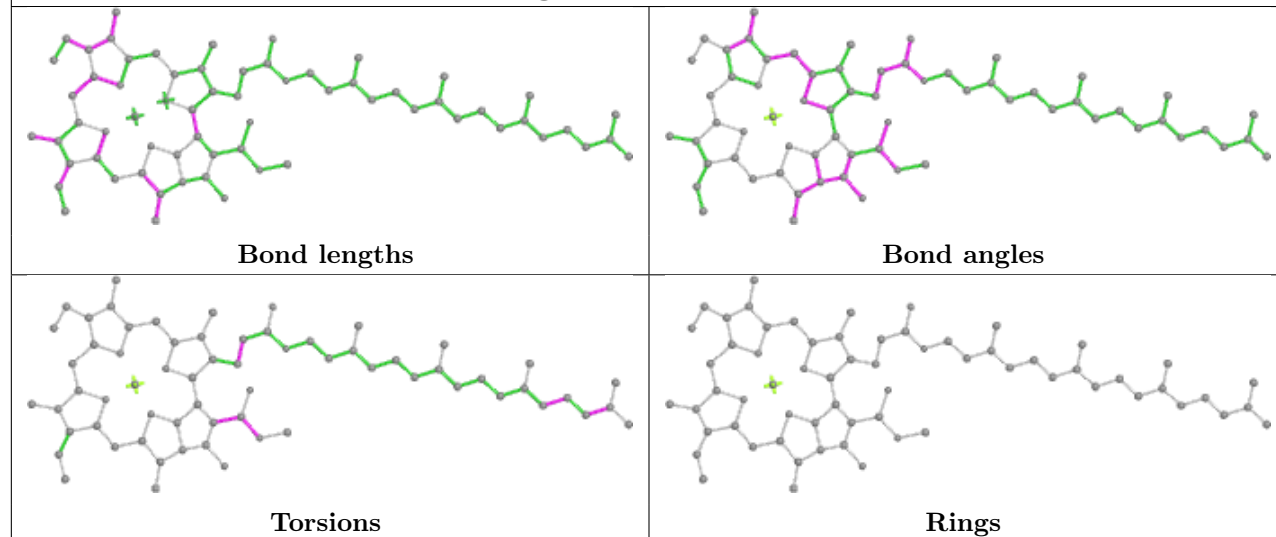
Ligand CLA d 401

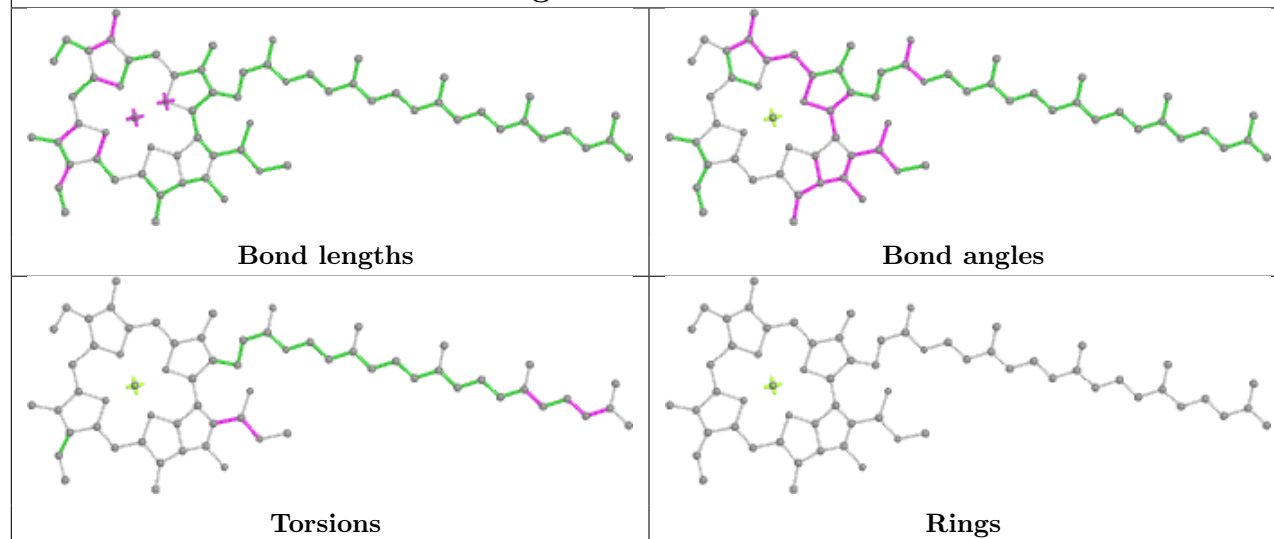
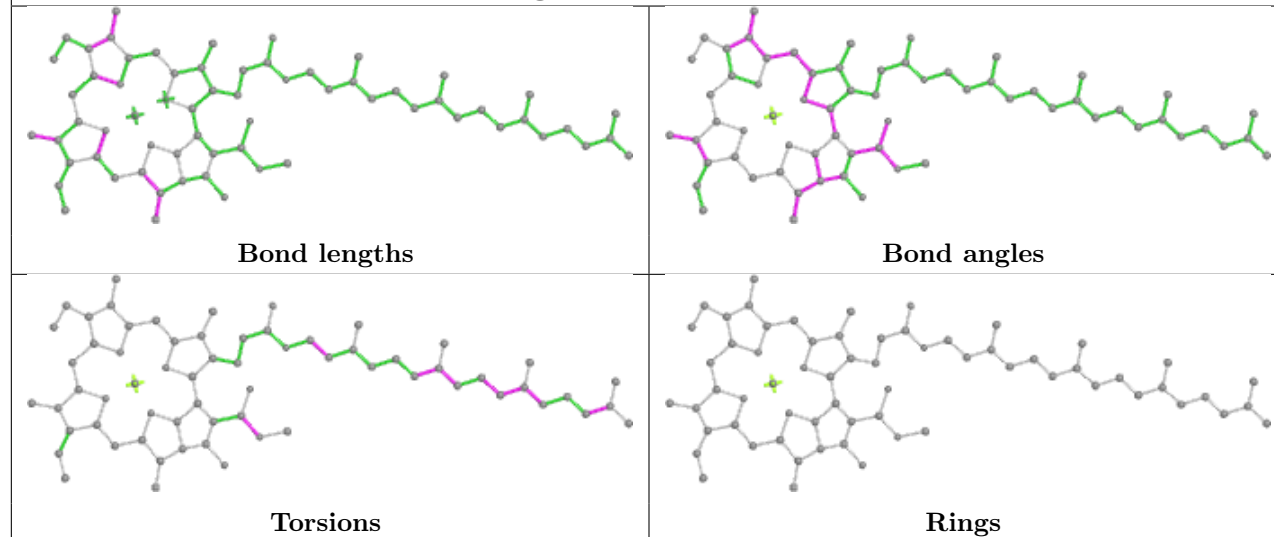
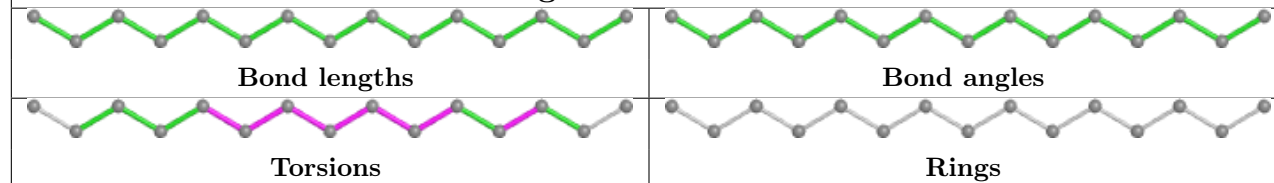


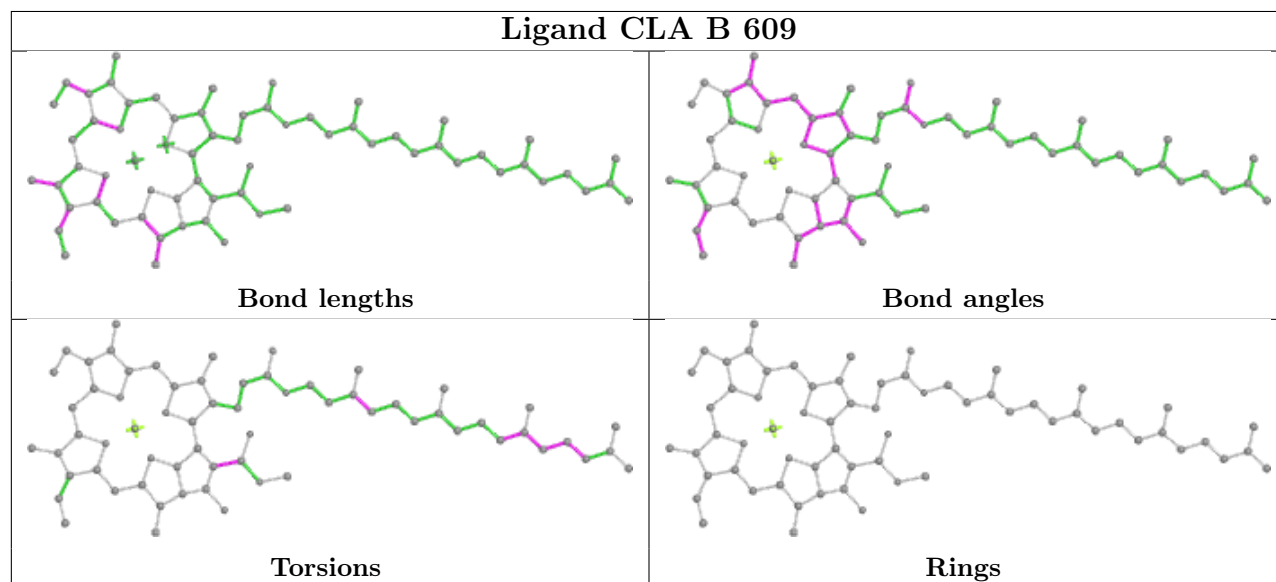
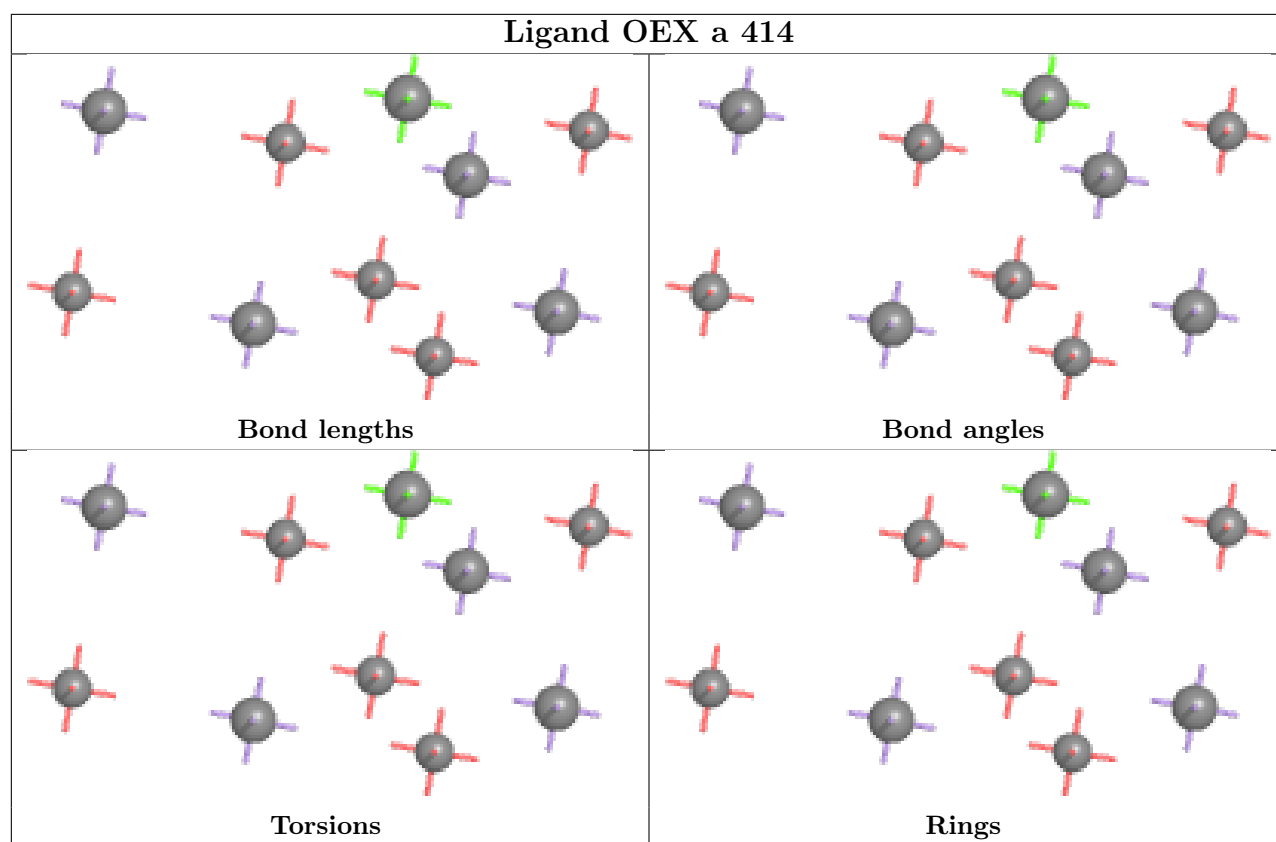
Ligand STE M 103



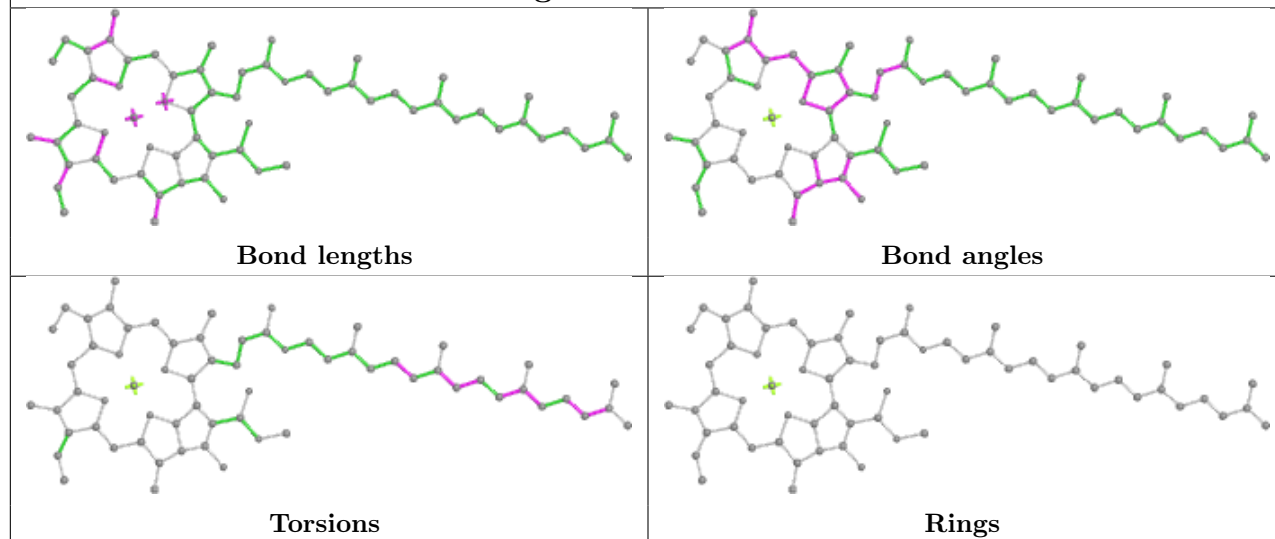
Ligand CLA b 610



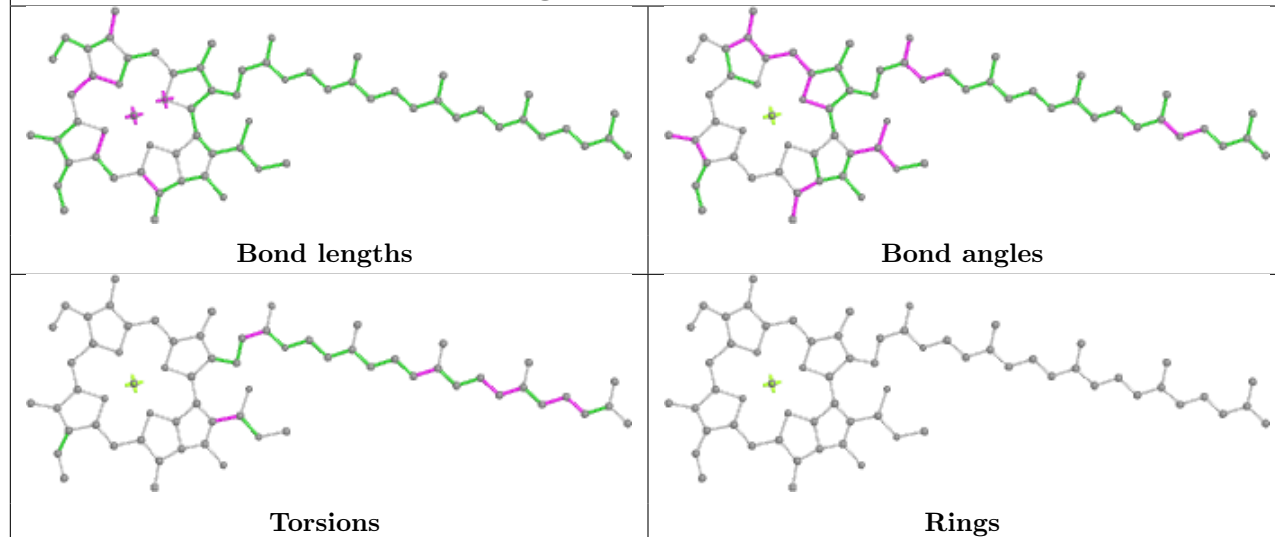
Ligand CLA C 502**Ligand CLA D 405****Ligand STE b 624**



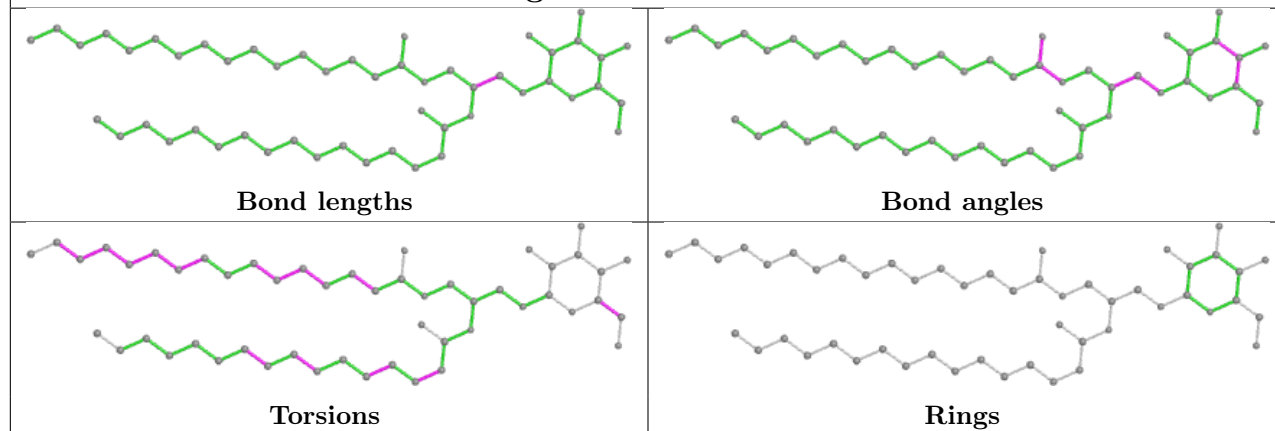
Ligand CLA b 615



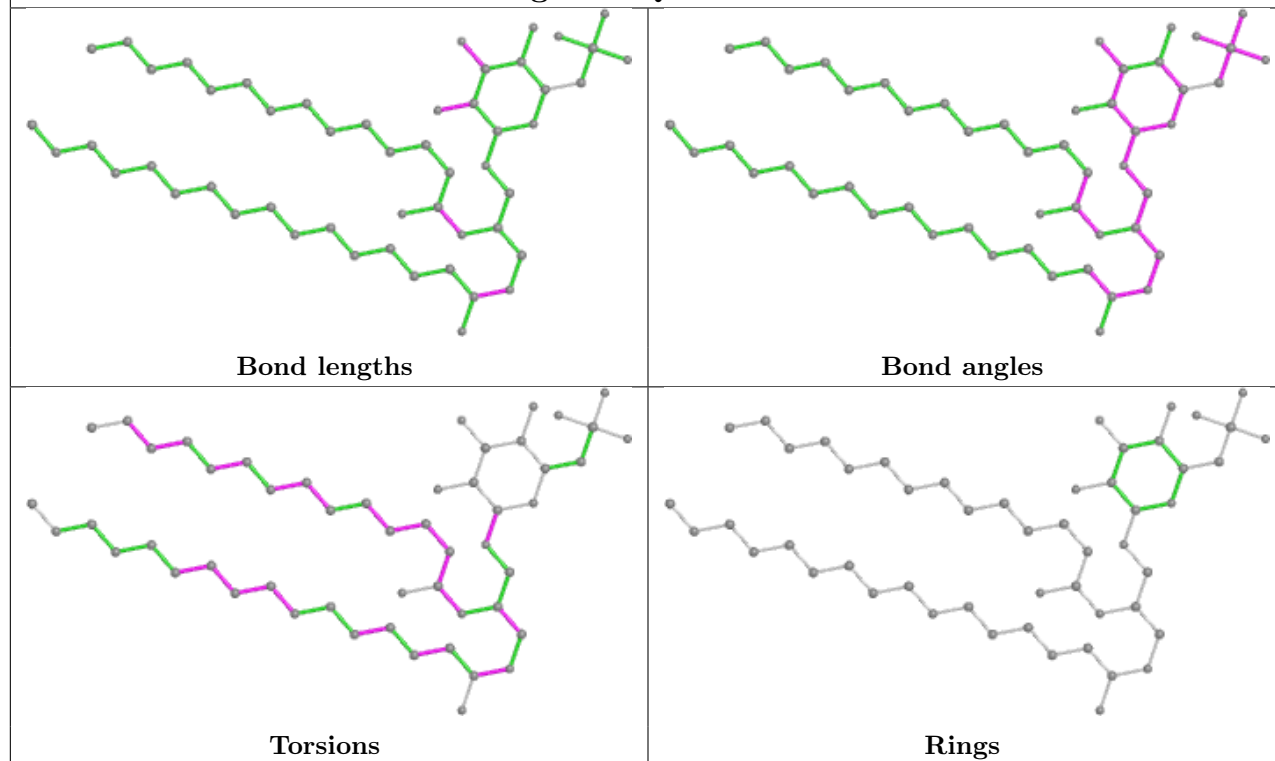
Ligand CLA c 509



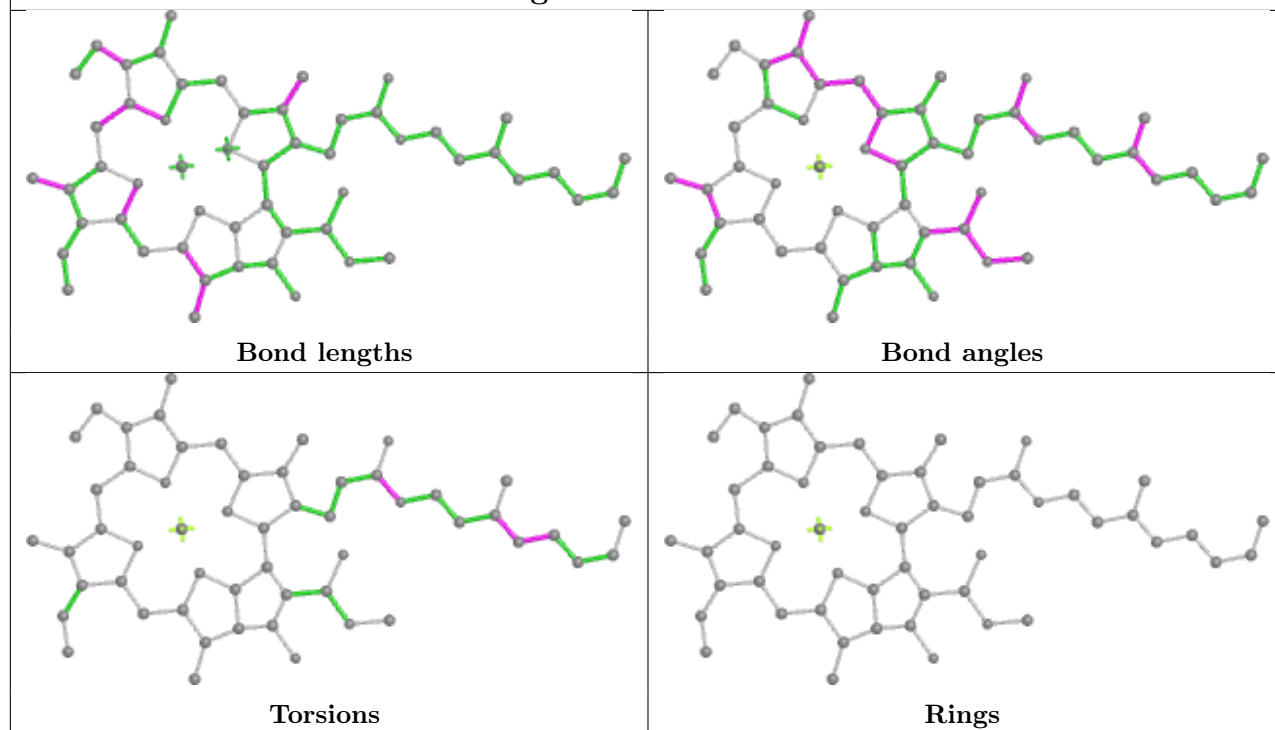
Ligand LMG D 408



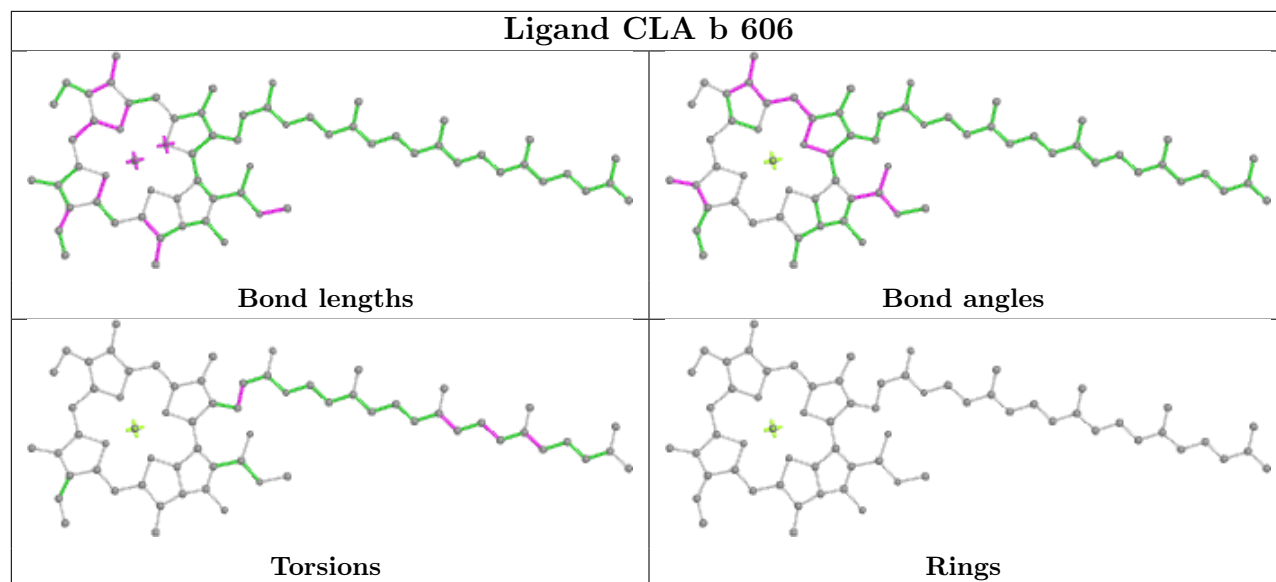
Ligand SQD A 410



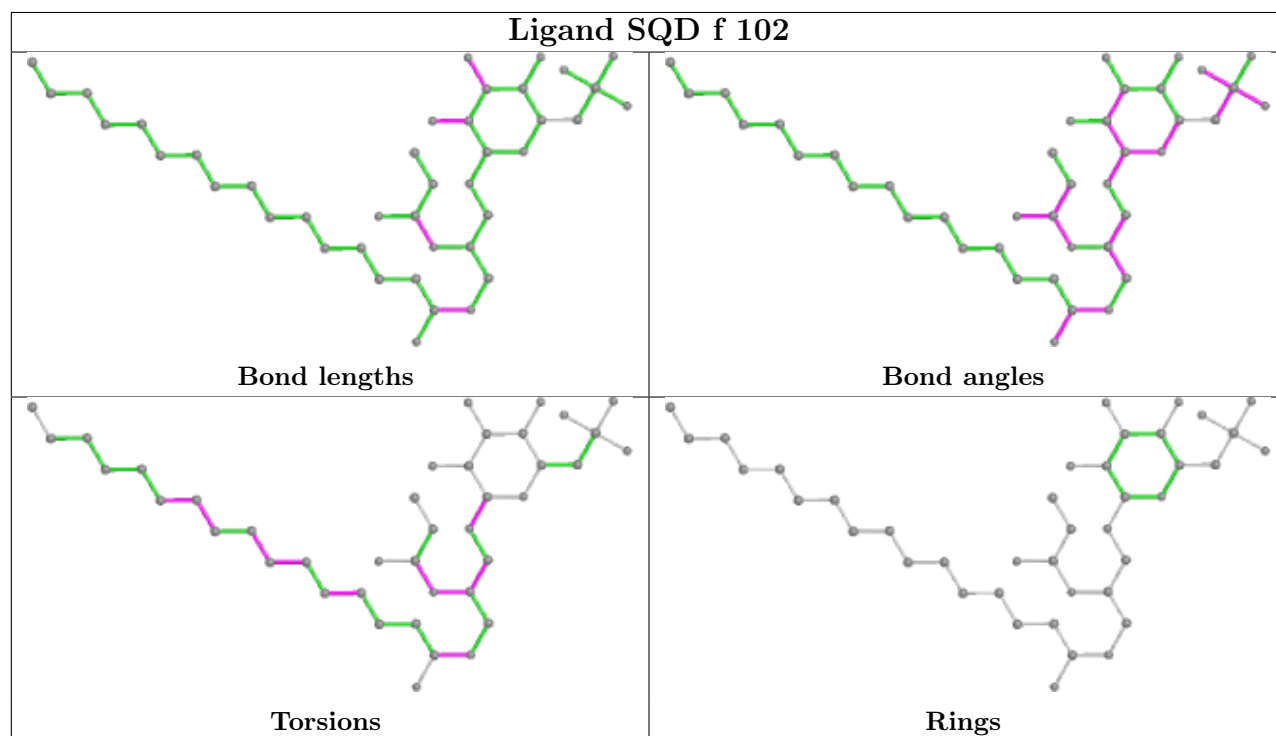
Ligand CLA A 405



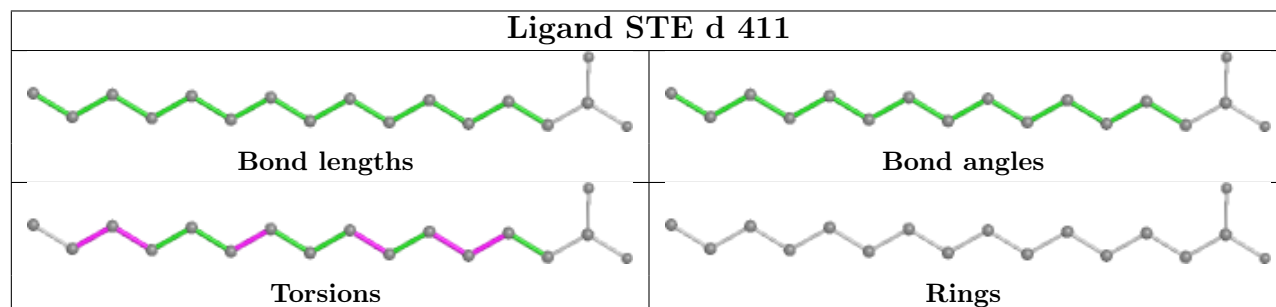
Ligand CLA b 606

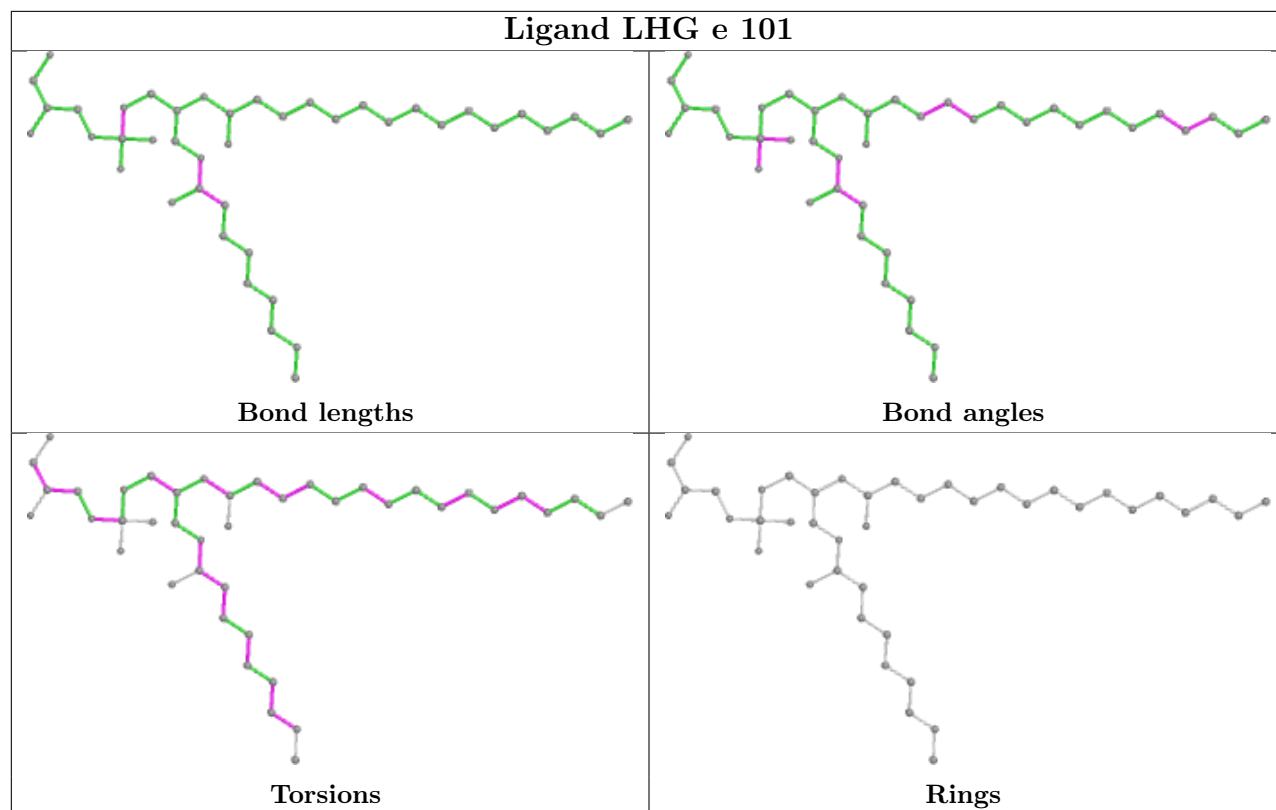


Ligand SQD f 102

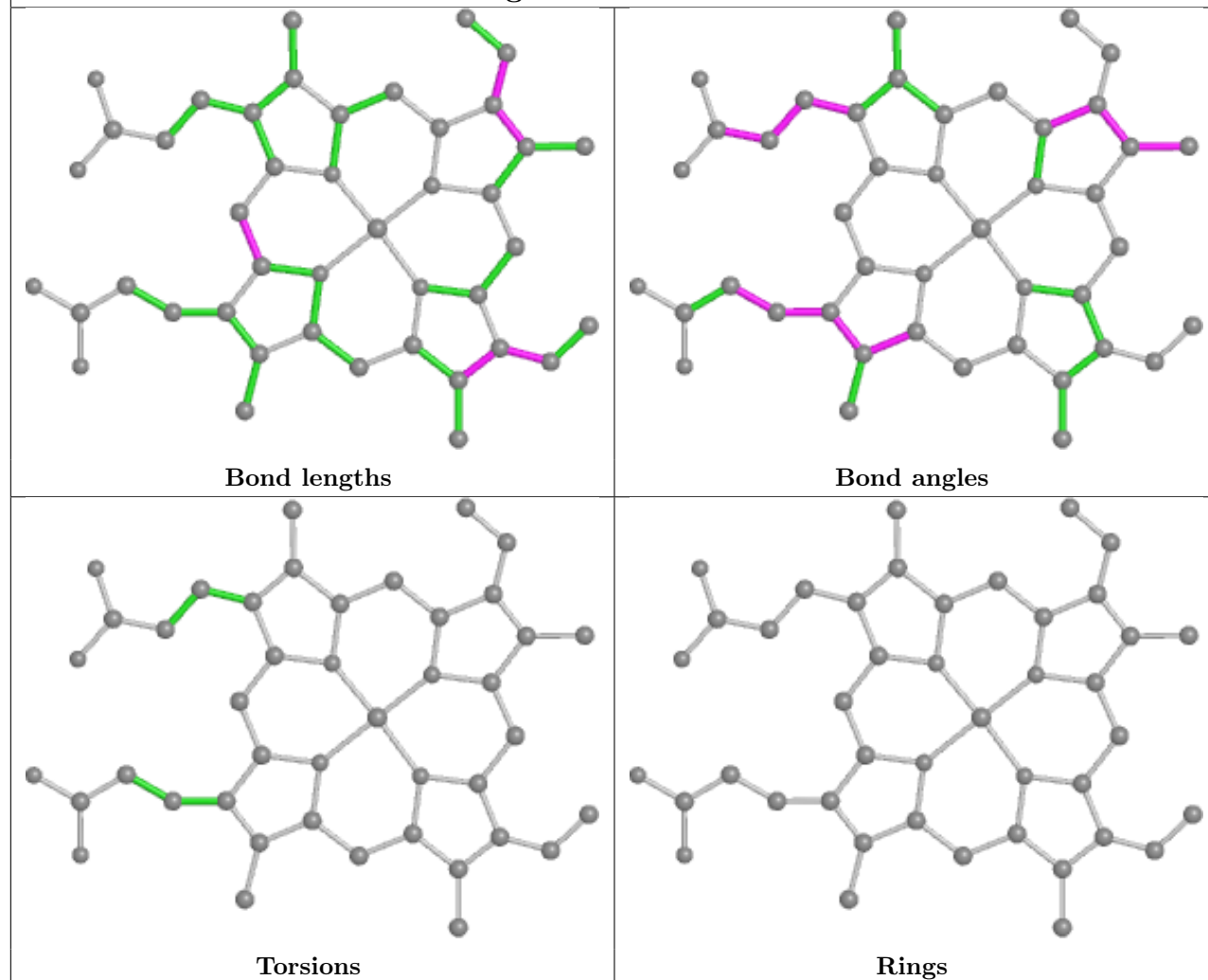


Ligand STE d 411

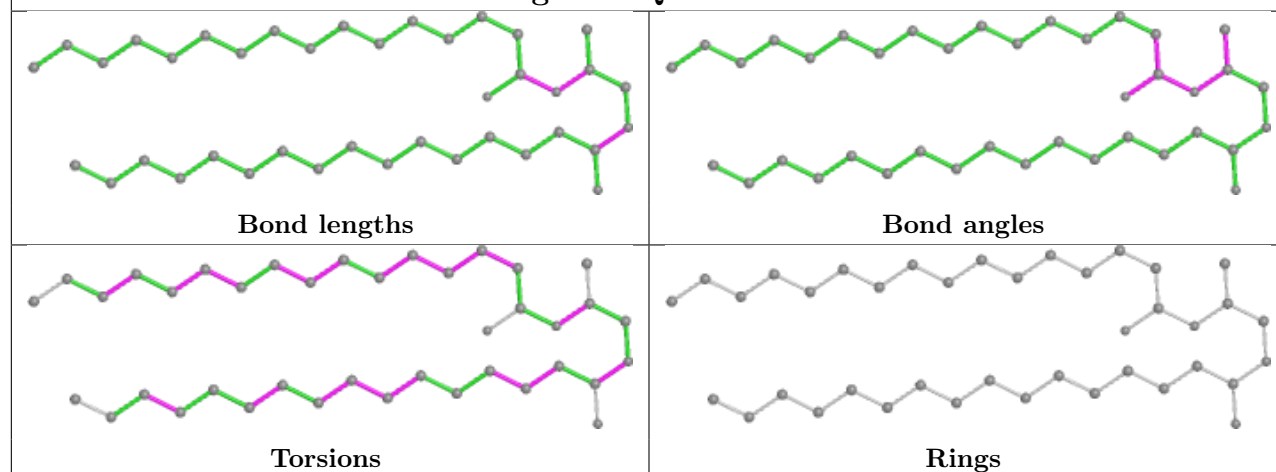




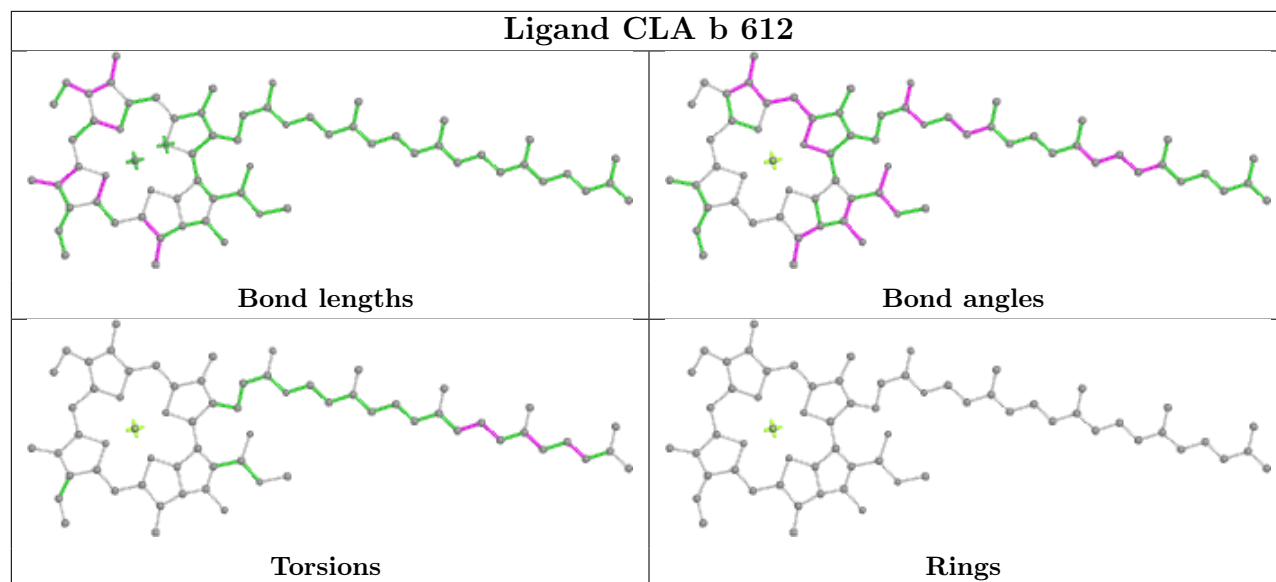
Ligand HEM f 101



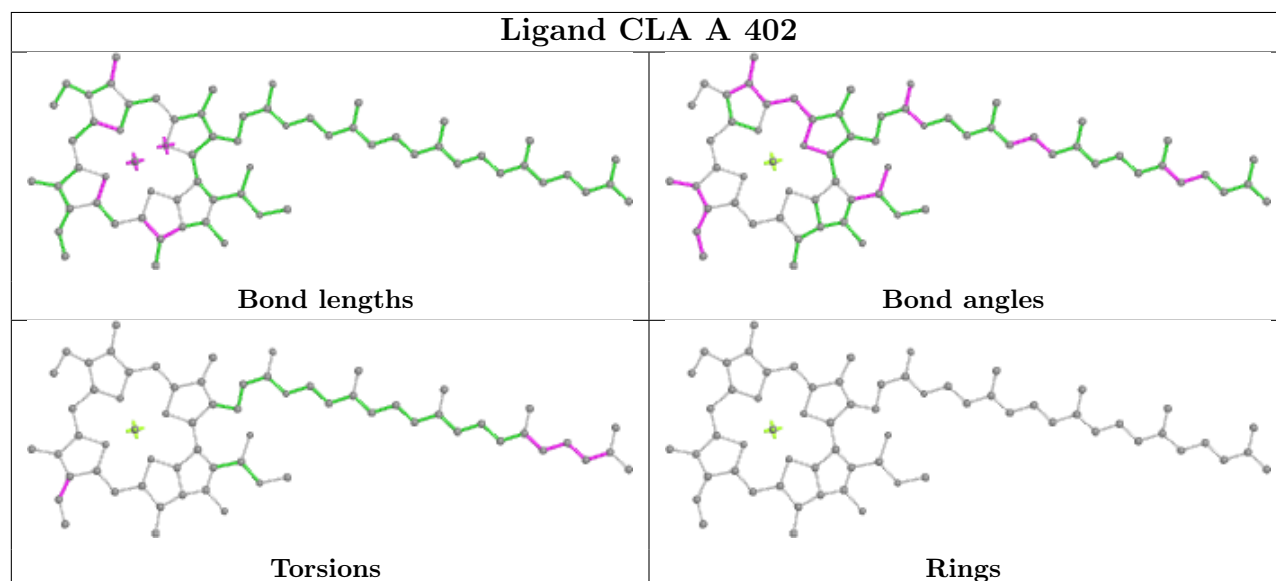
Ligand SQD A 412



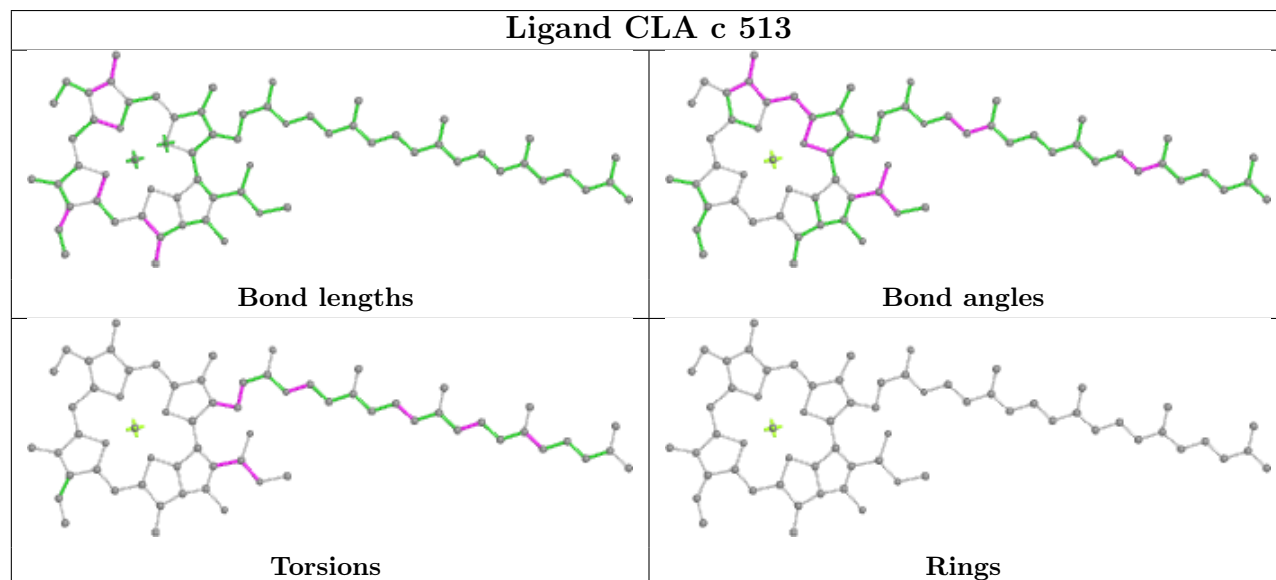
Ligand CLA b 612



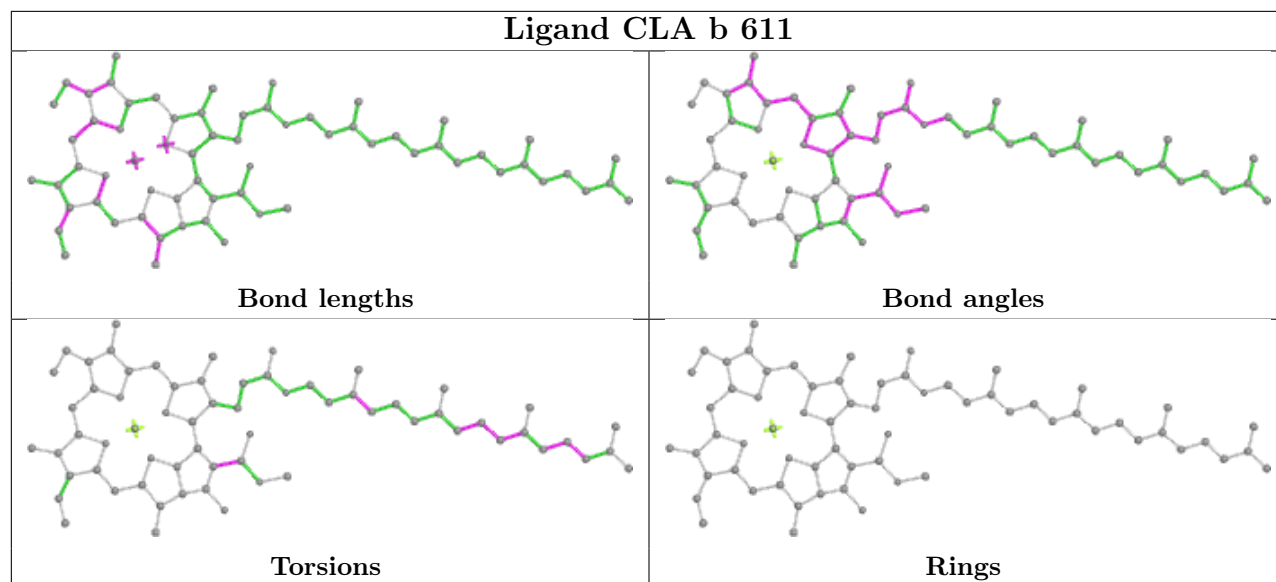
Ligand CLA A 402



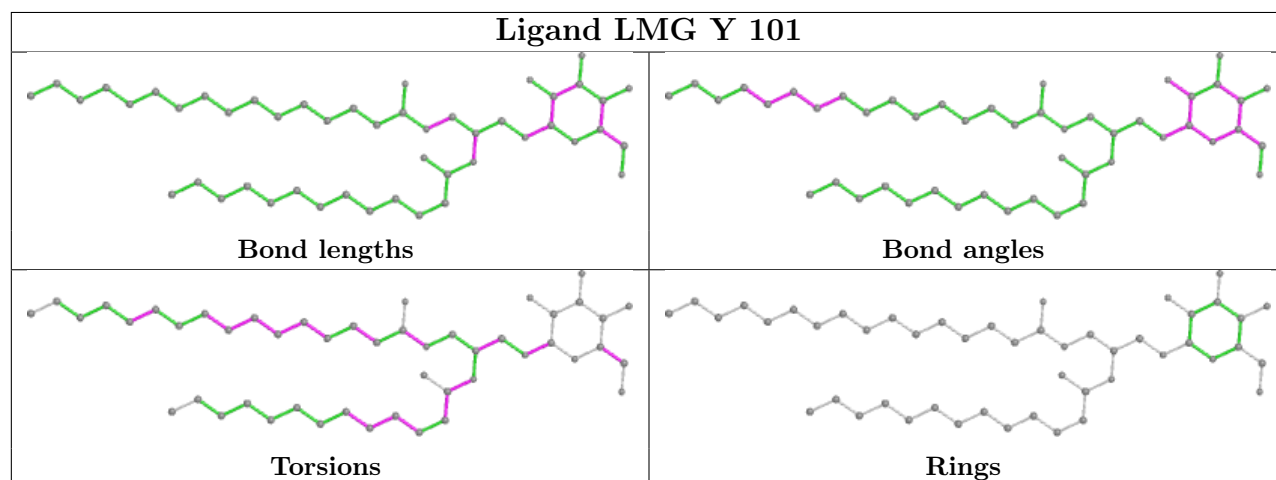
Ligand CLA c 513



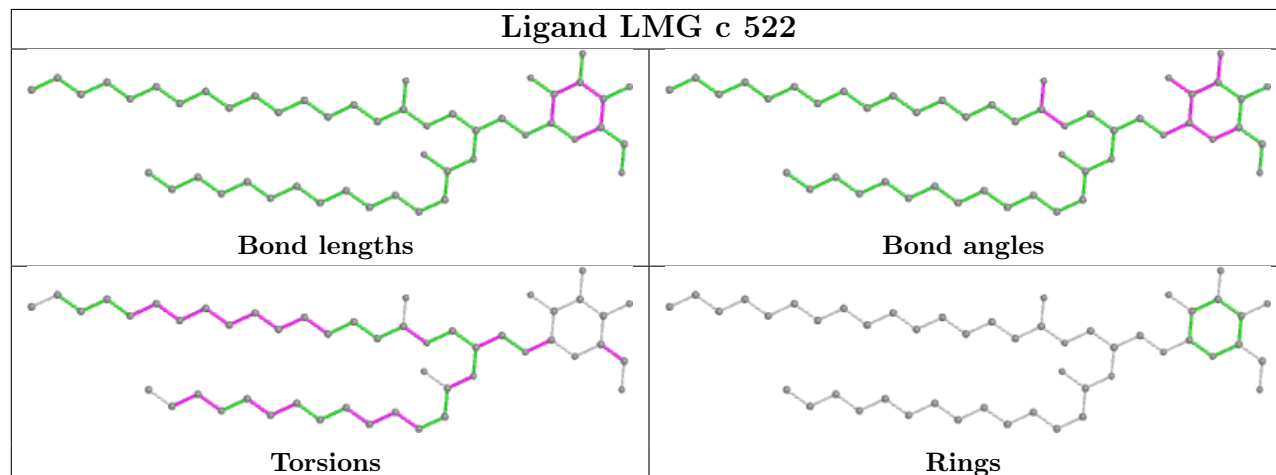
Ligand CLA b 611

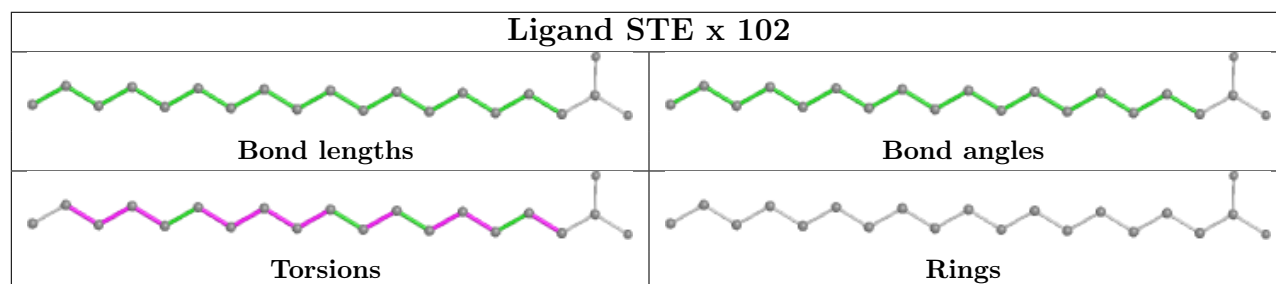
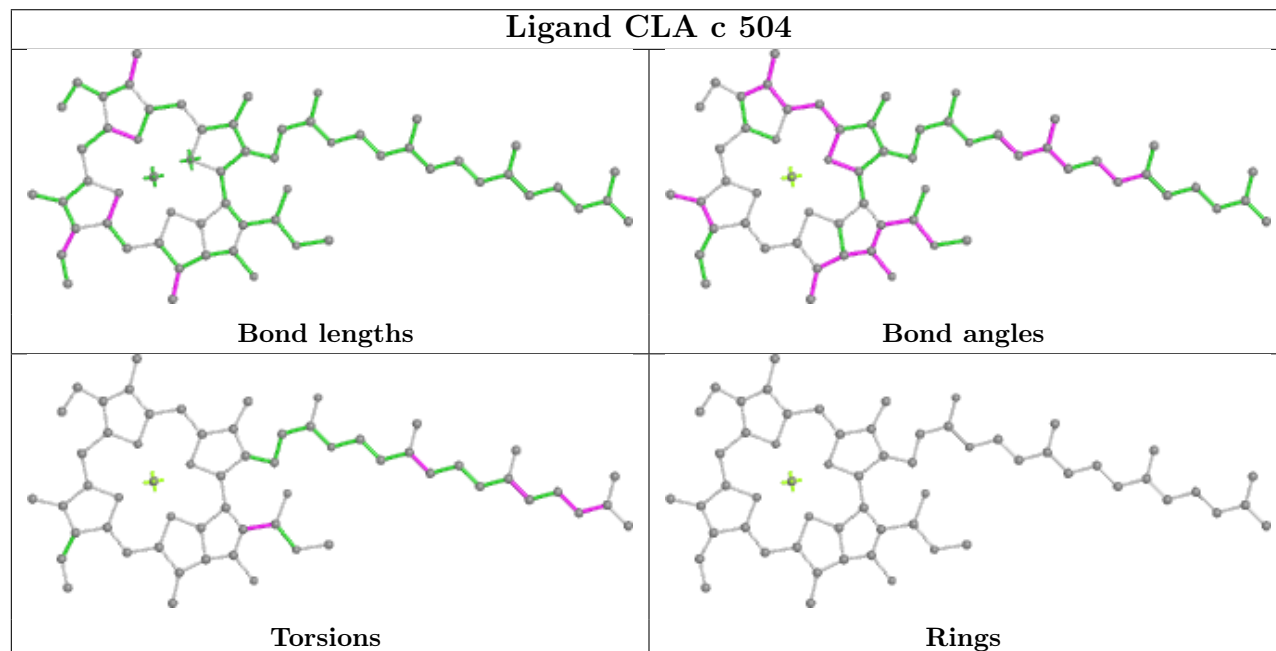
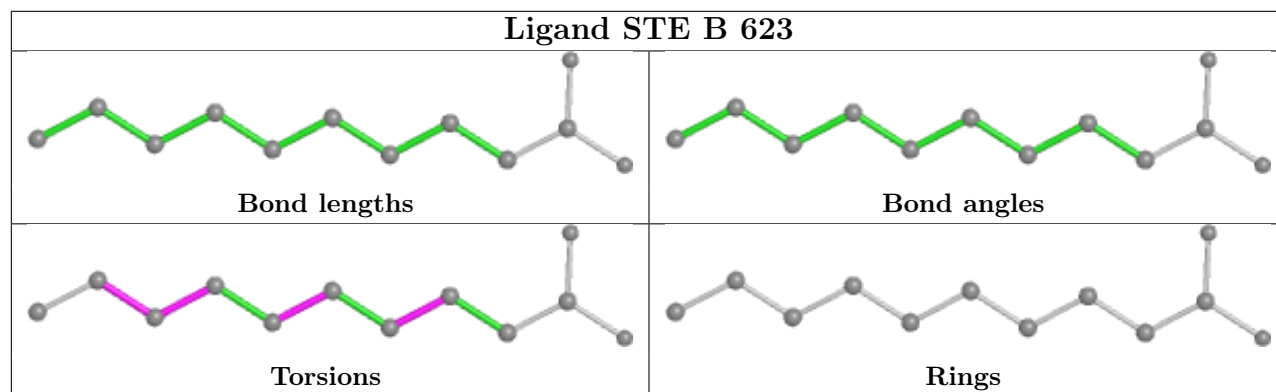


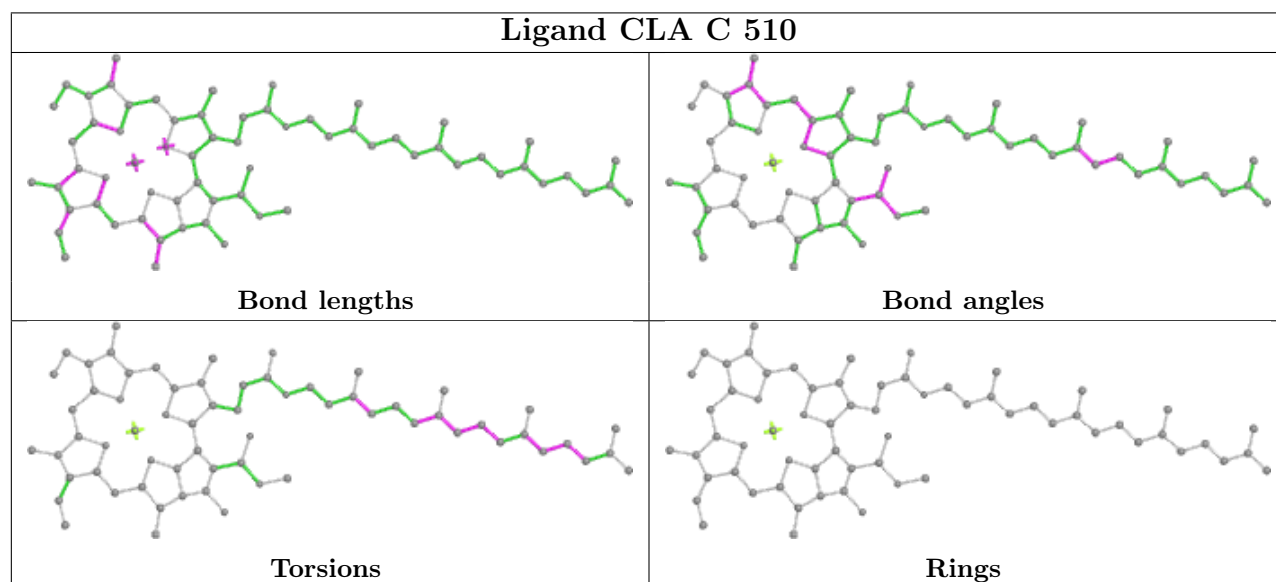
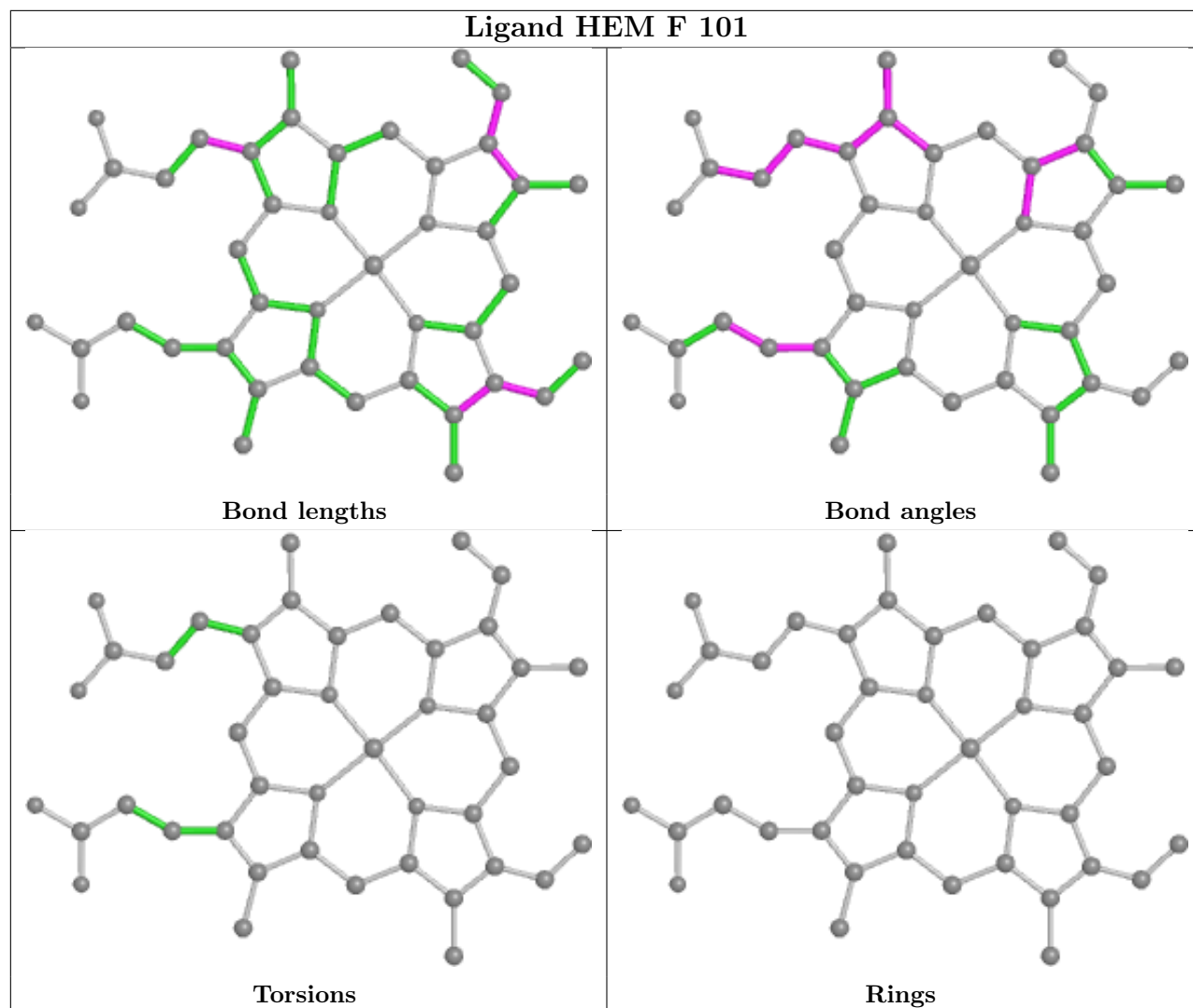
Ligand LMG Y 101



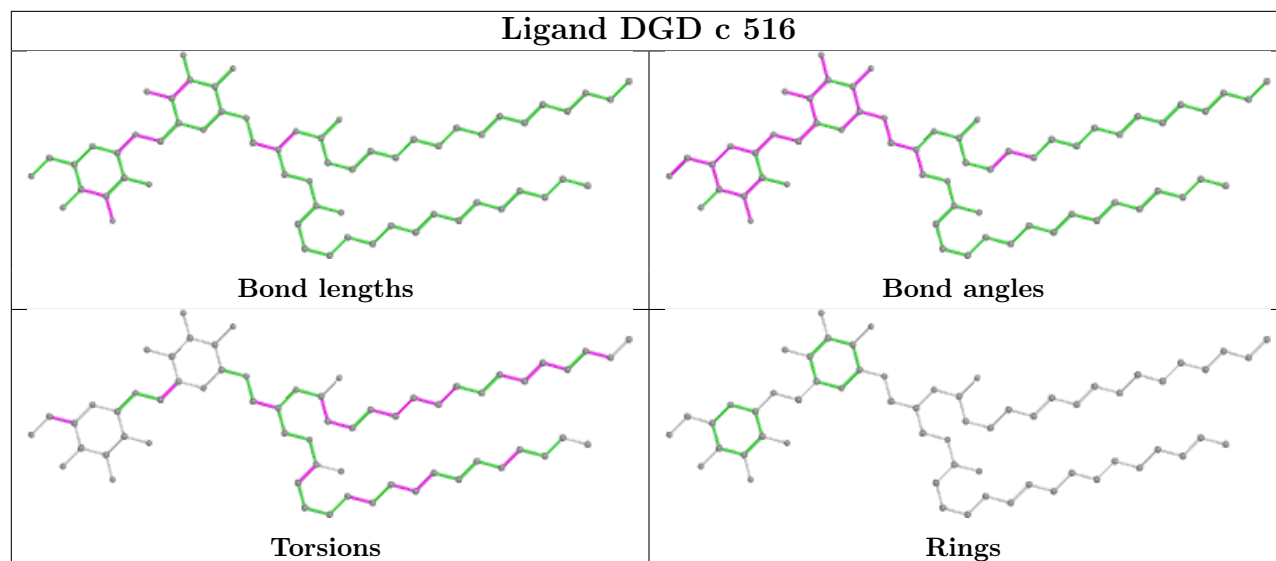
Ligand LMG c 522



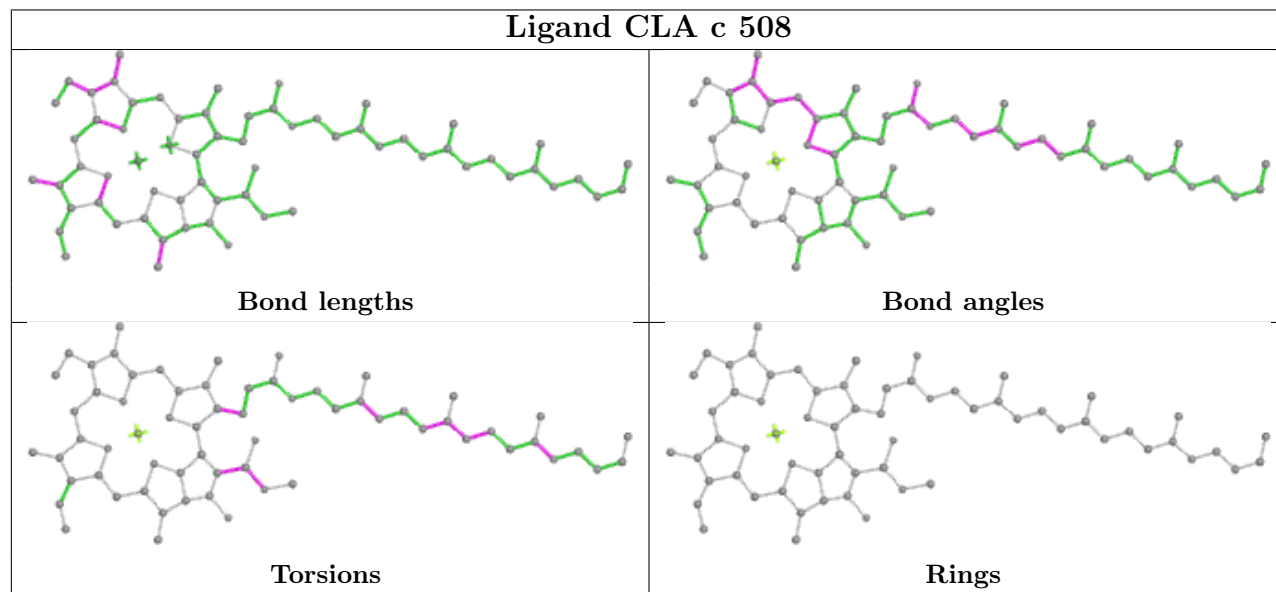




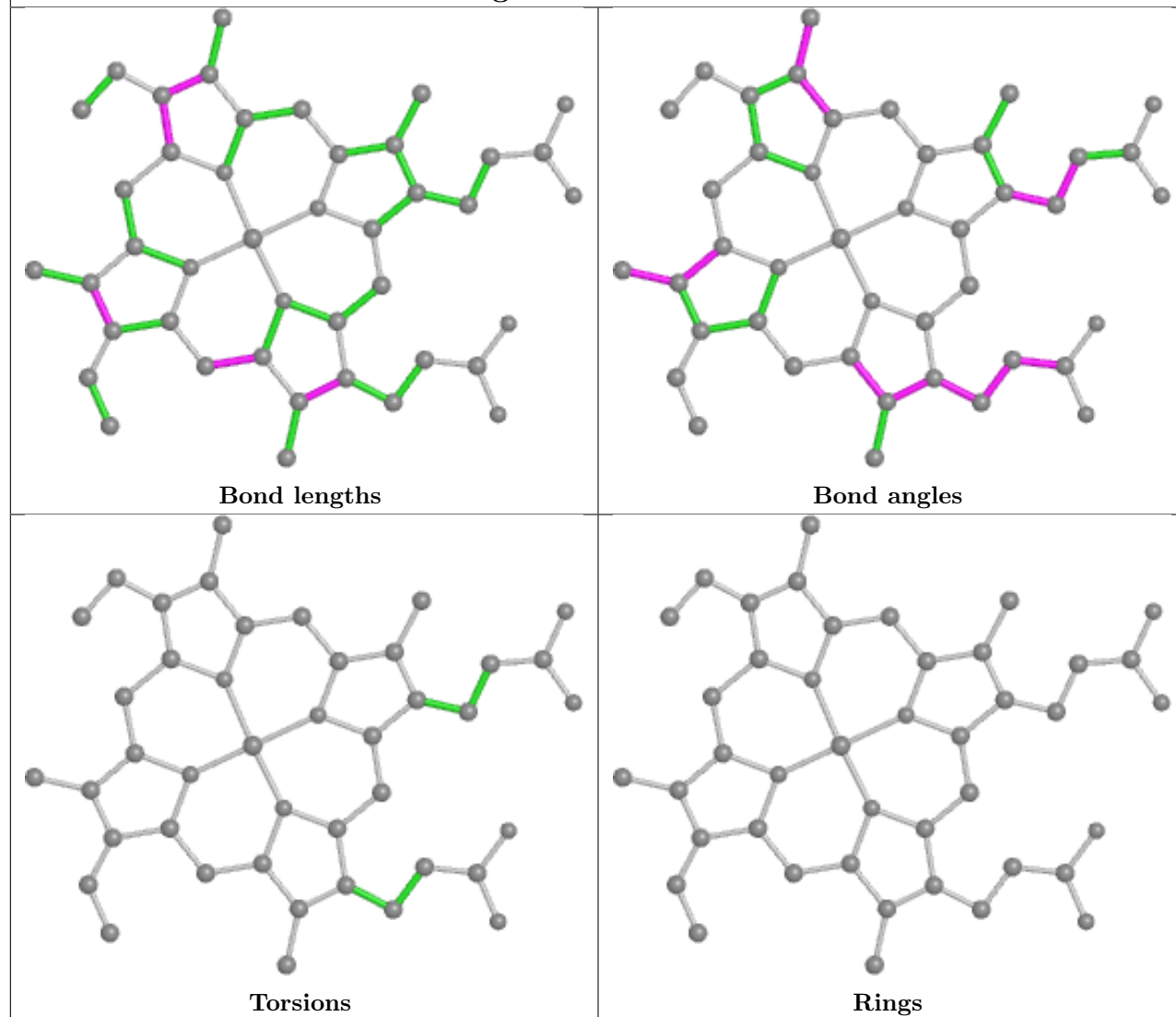
Ligand DGD c 516



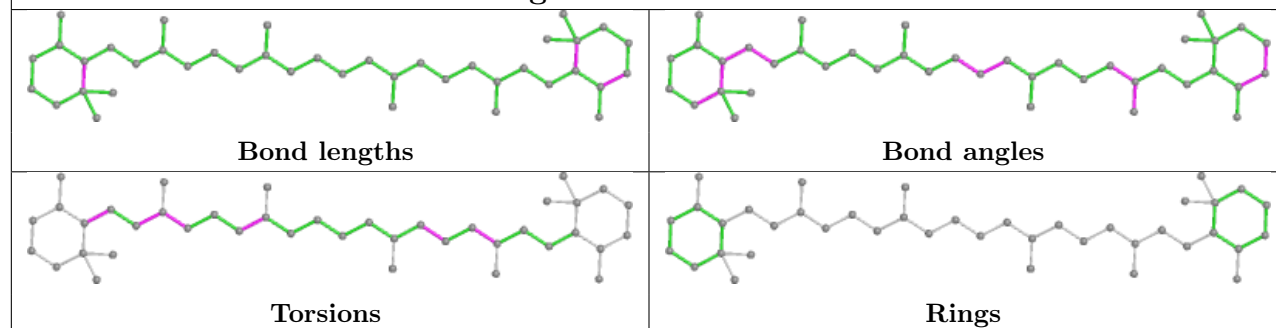
Ligand CLA c 508



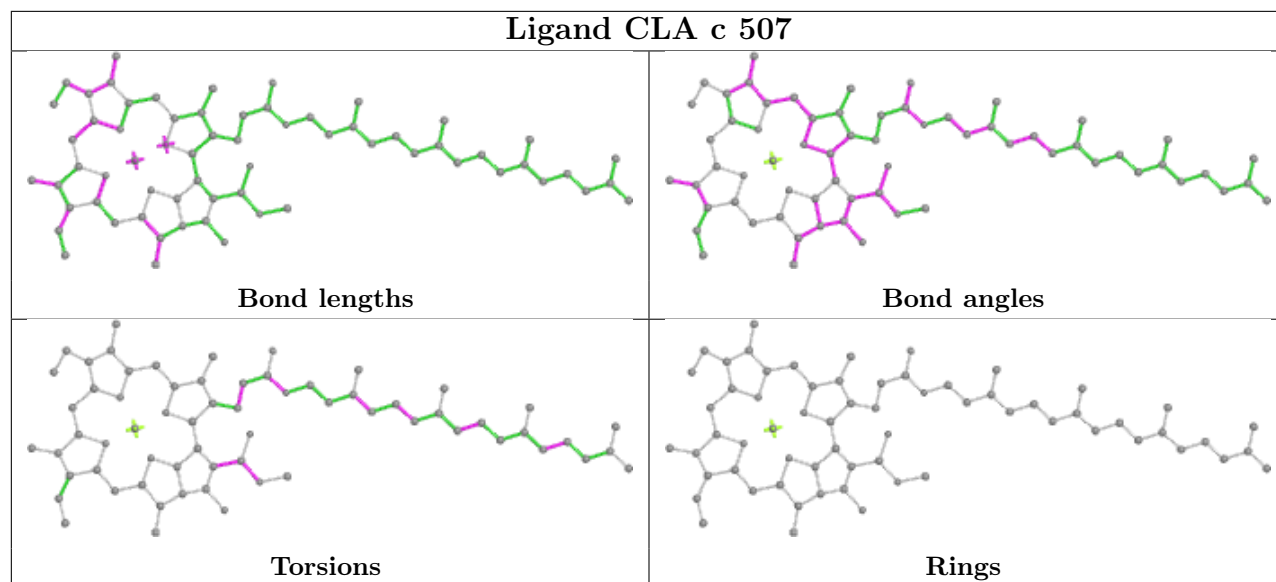
Ligand HEC v 201



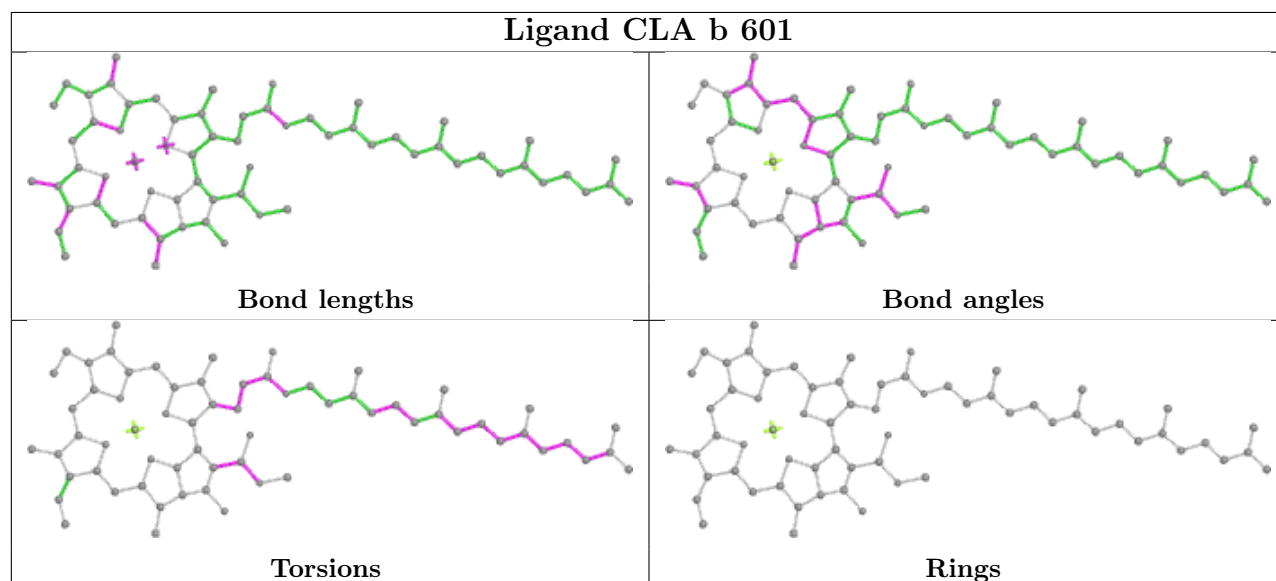
Ligand BCR K 102



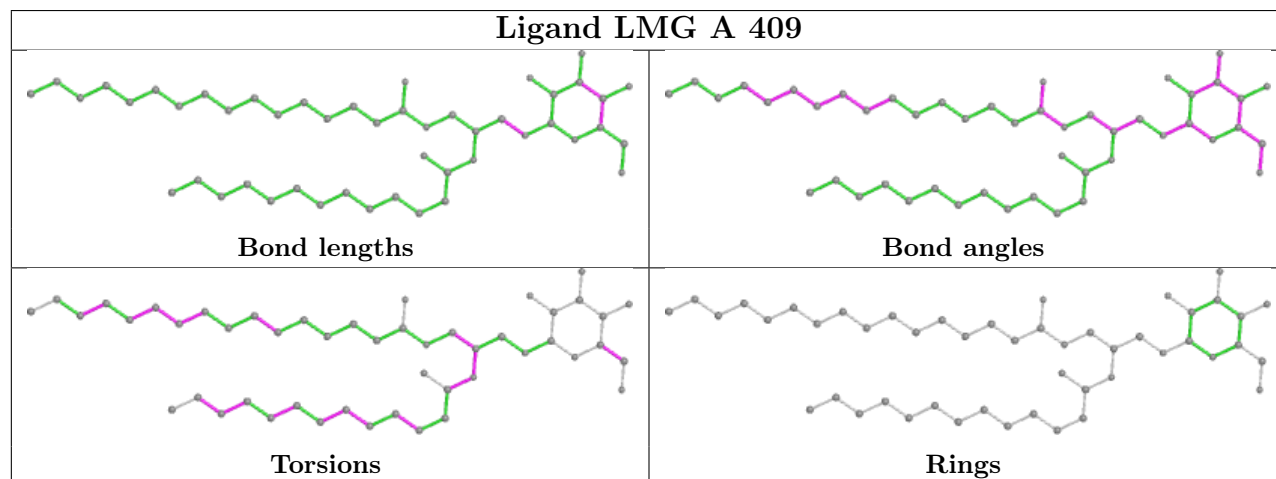
Ligand CLA c 507



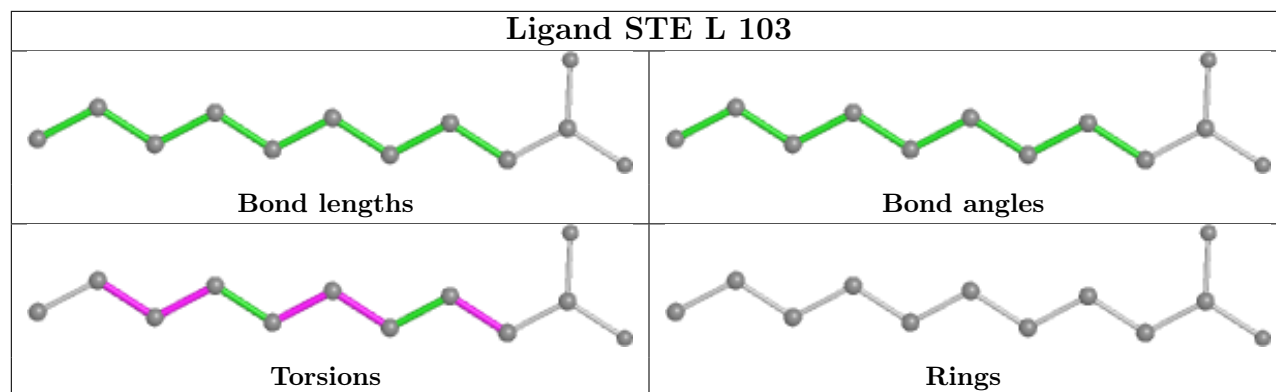
Ligand CLA b 601



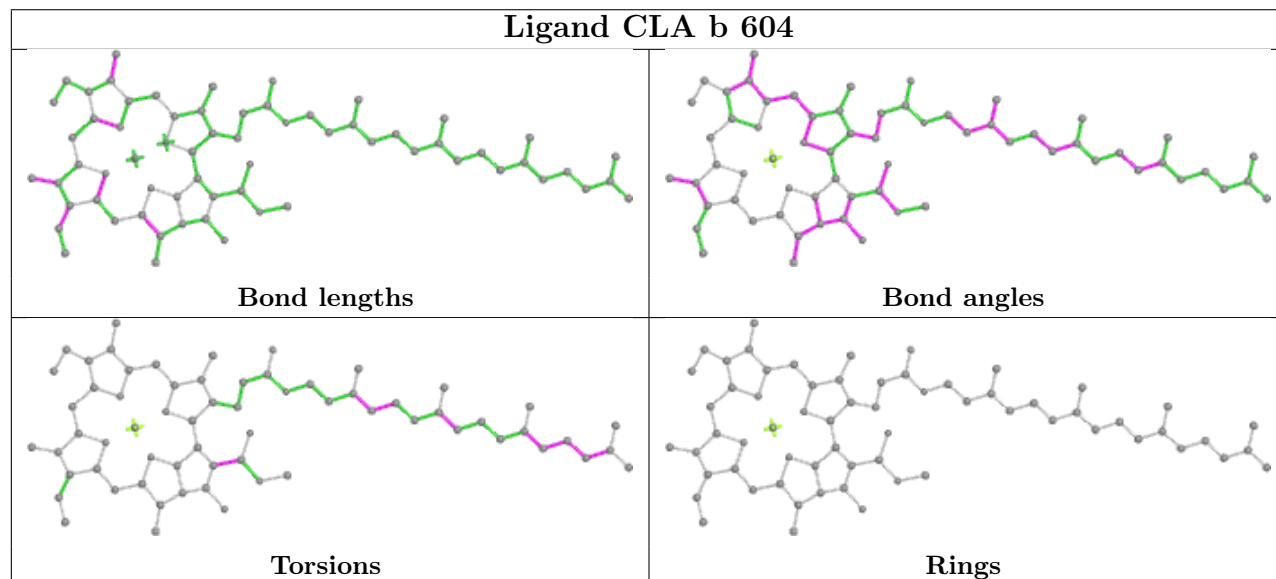
Ligand LMG A 409



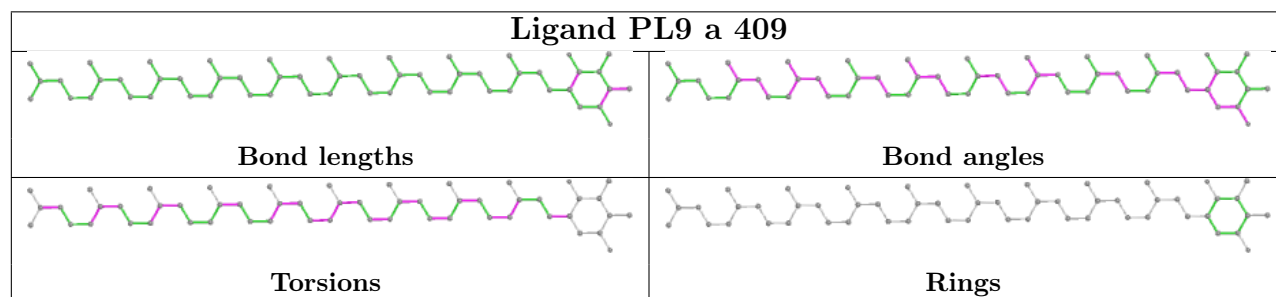
Ligand STE L 103



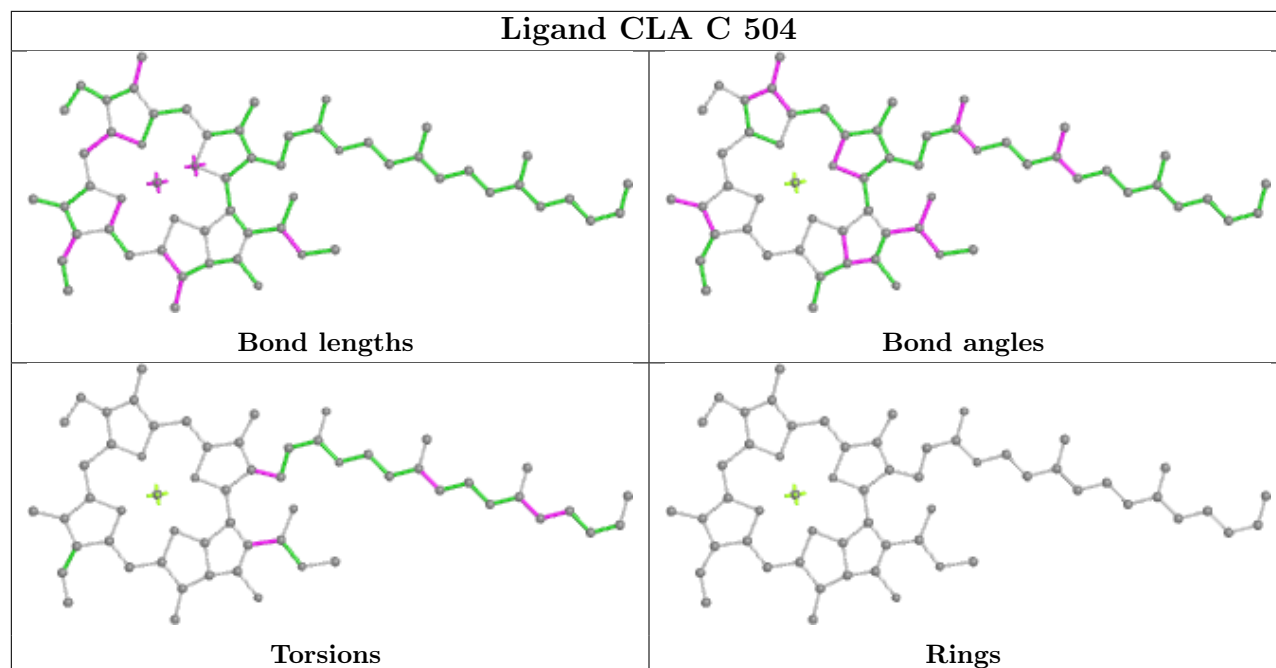
Ligand CLA b 604



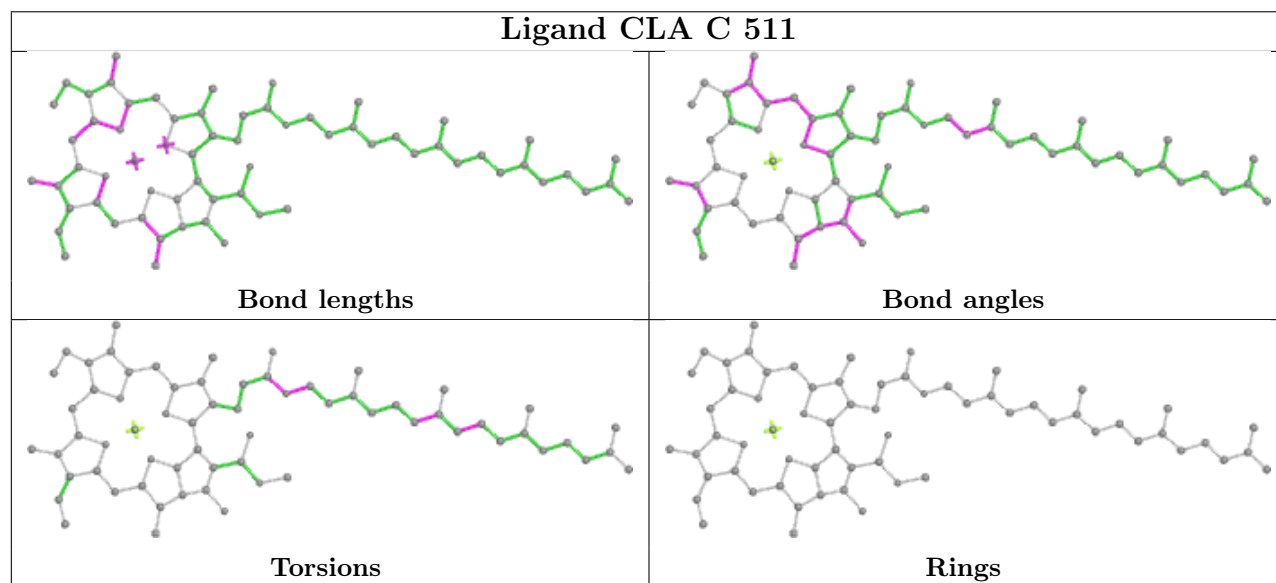
Ligand PL9 a 409



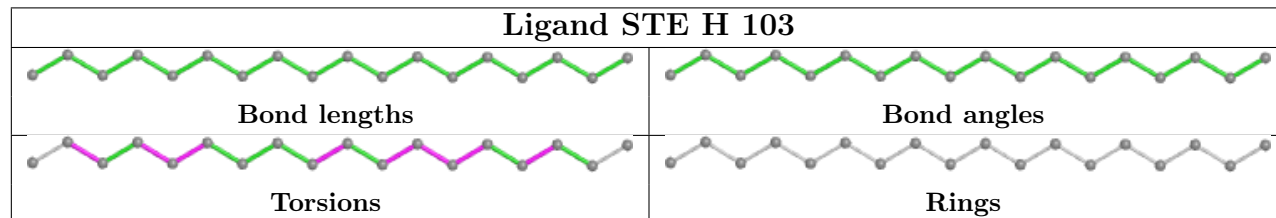
Ligand CLA C 504

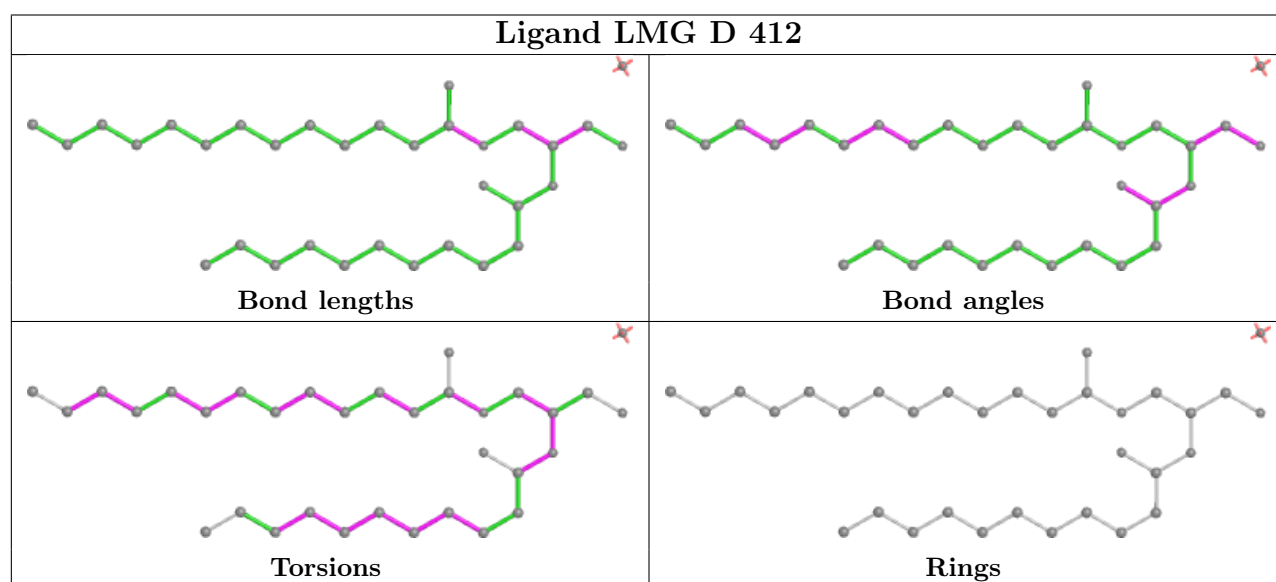
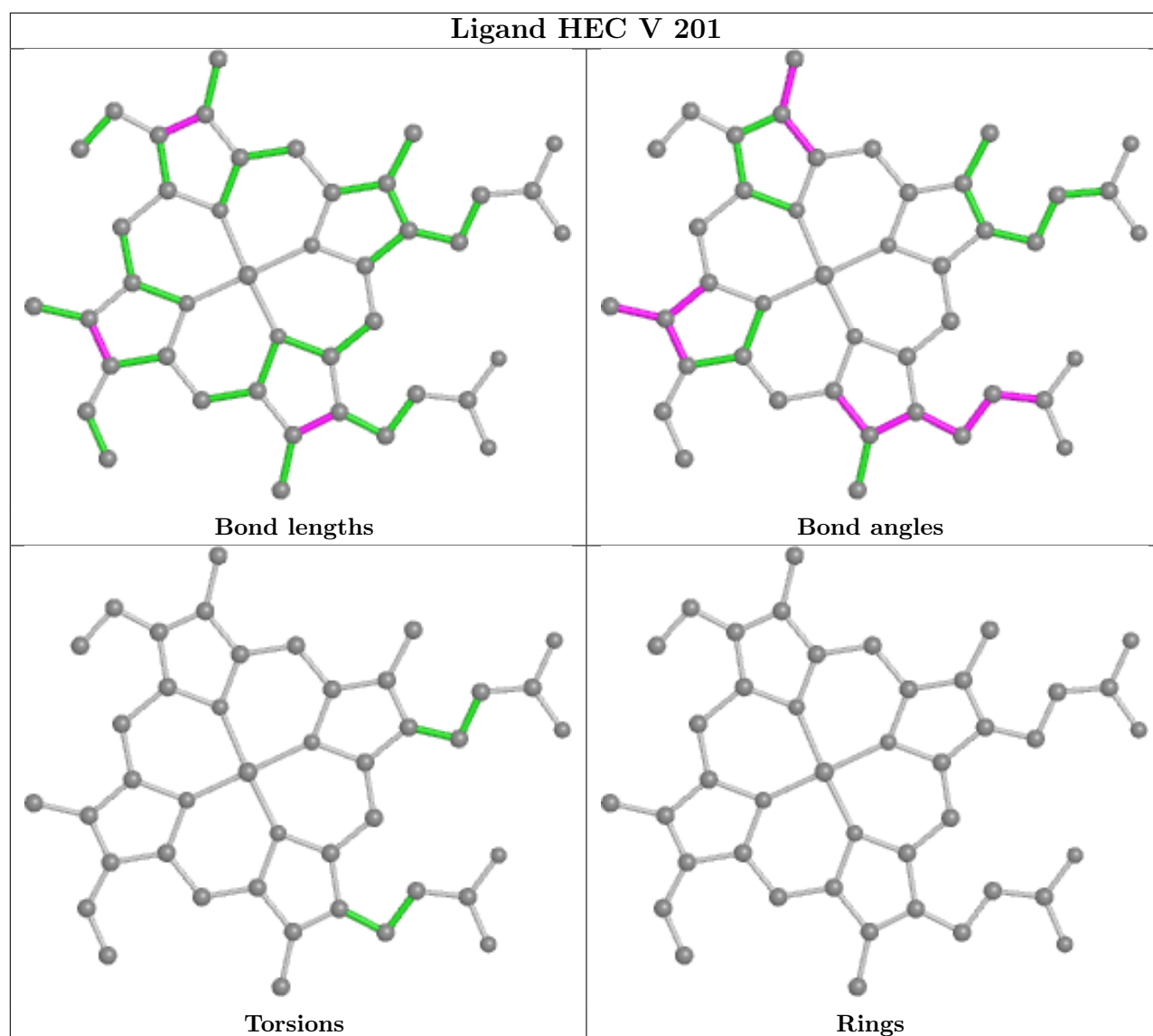


Ligand CLA C 511

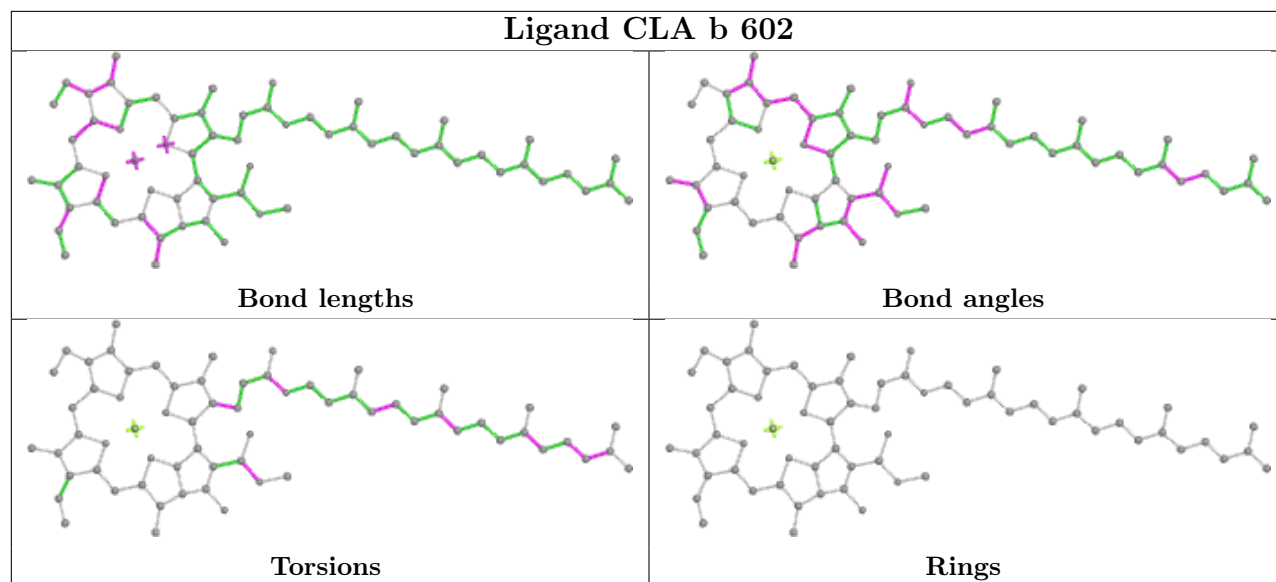


Ligand STE H 103

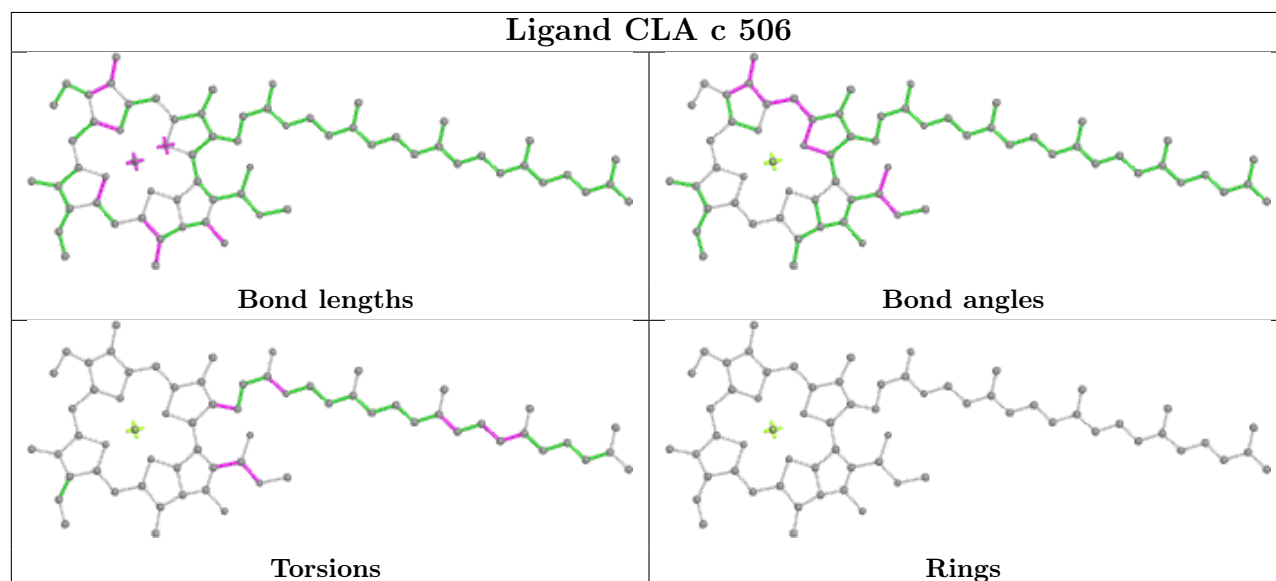




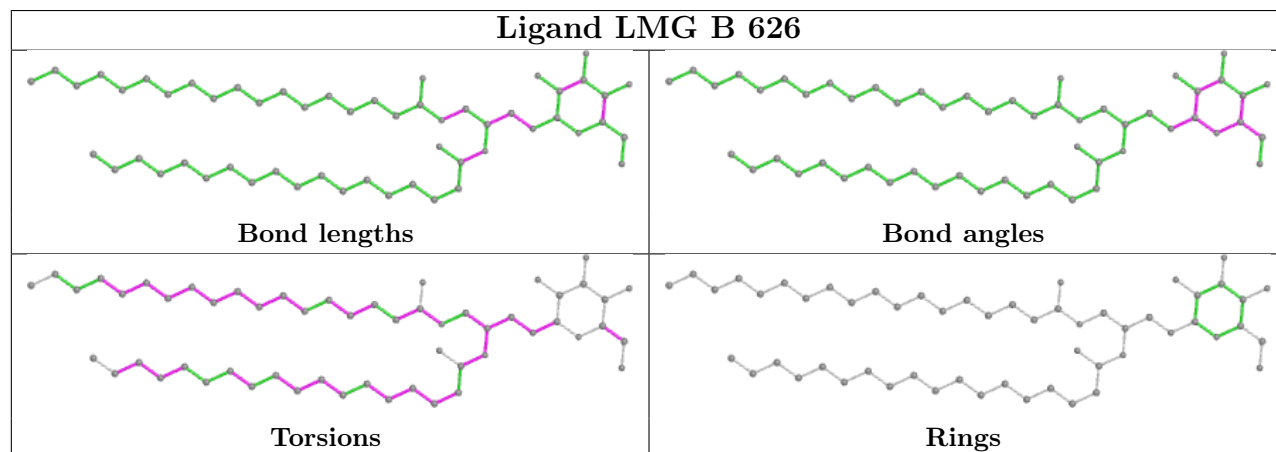
Ligand CLA b 602

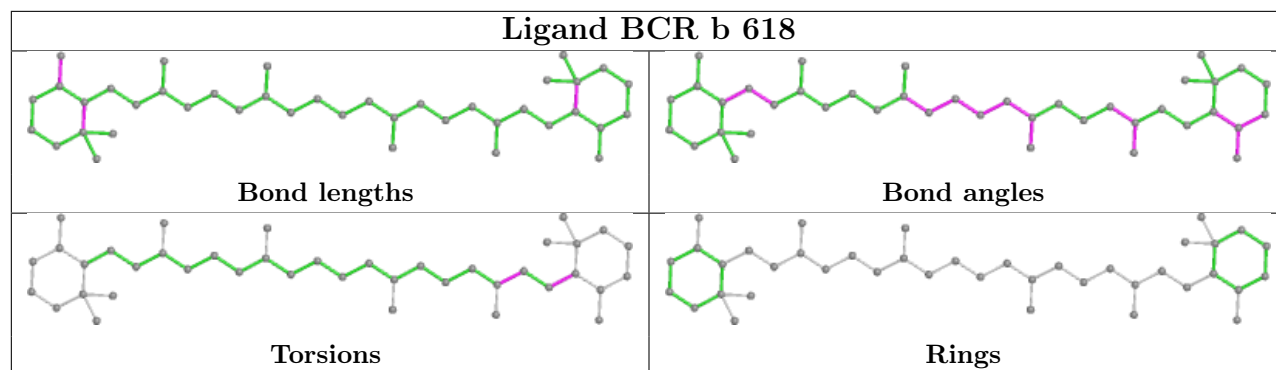
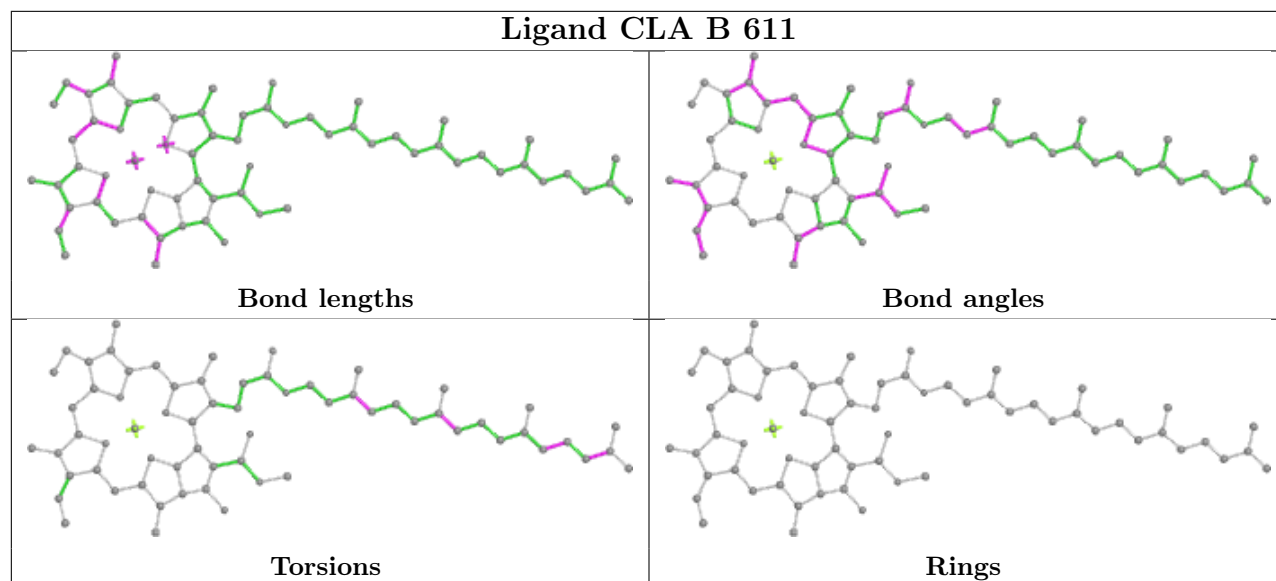
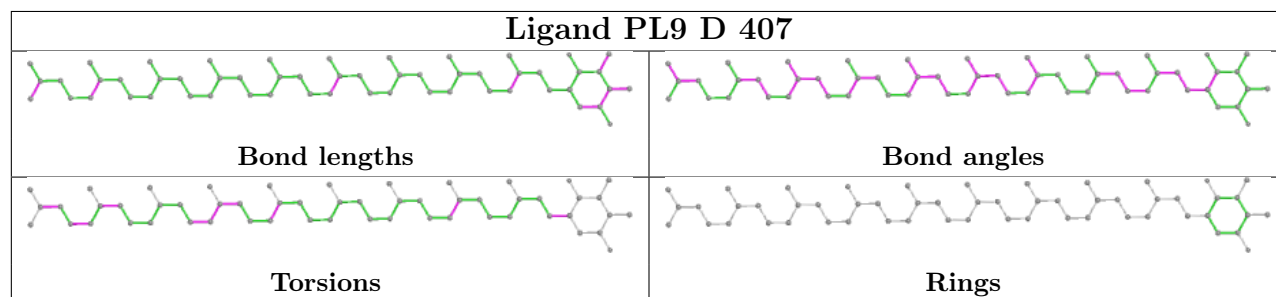


Ligand CLA c 506

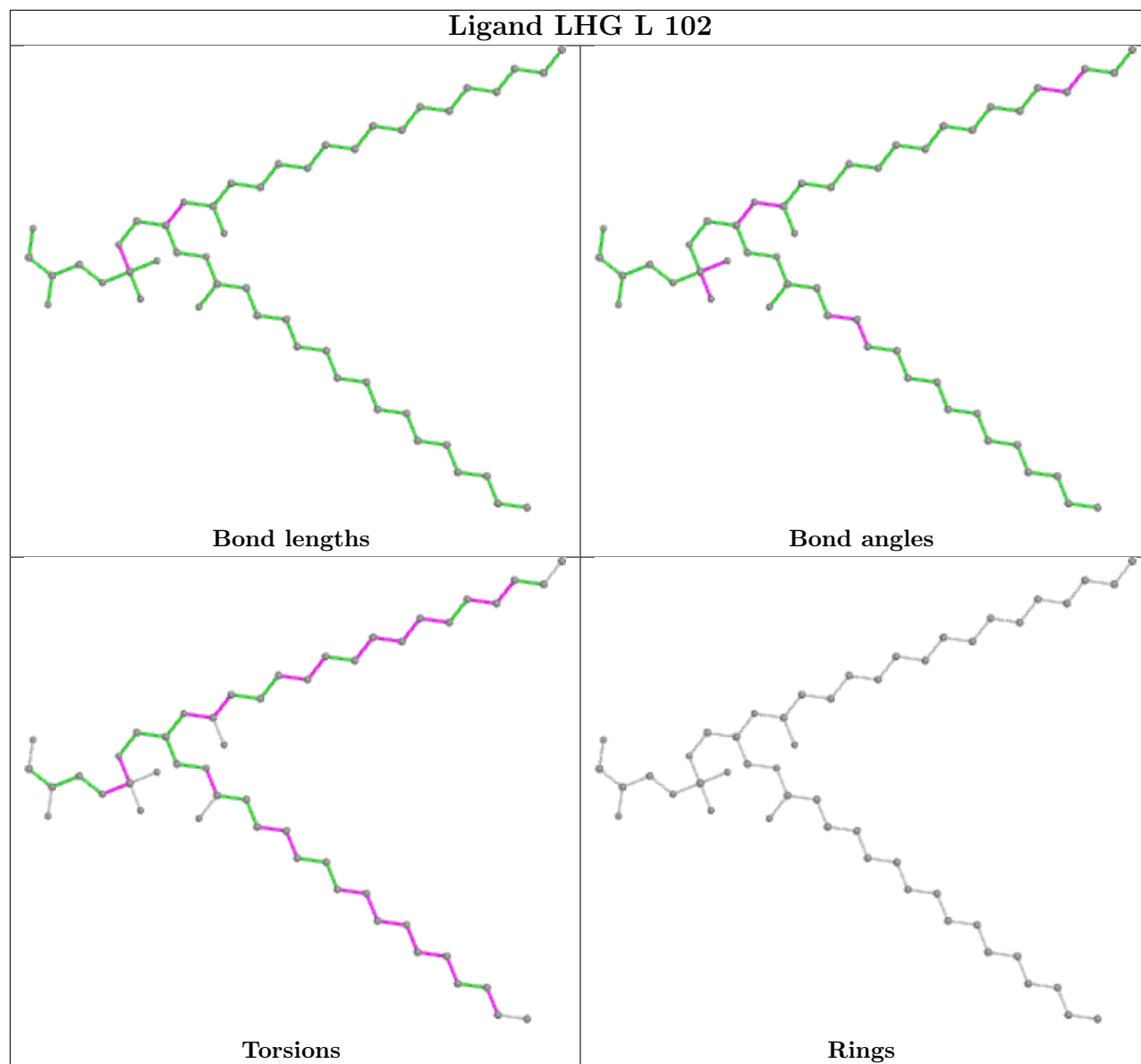


Ligand LMG B 626

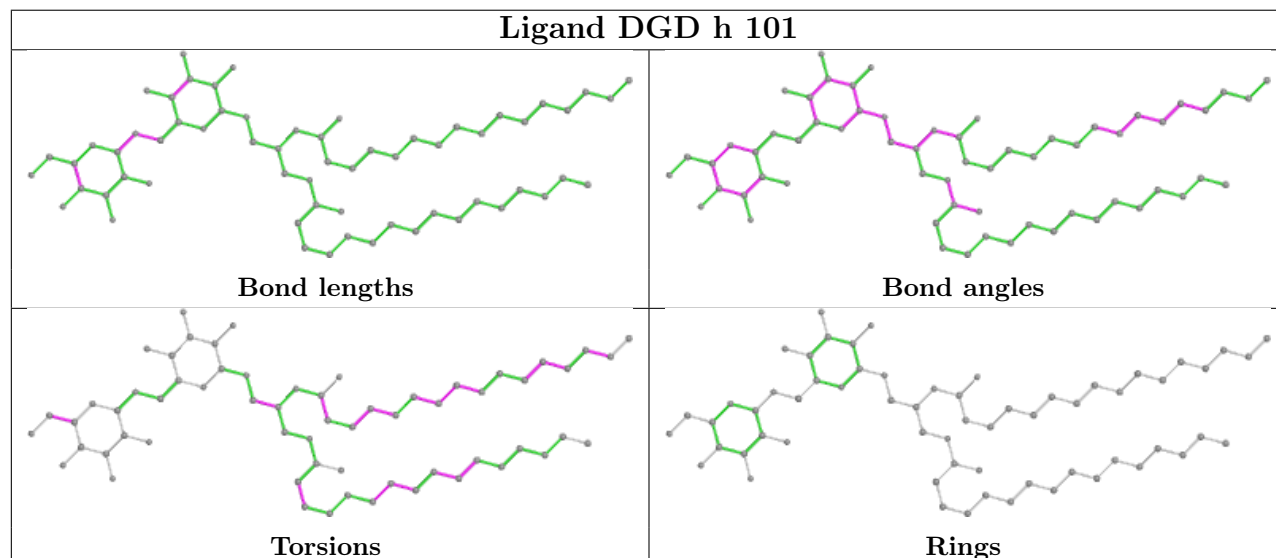


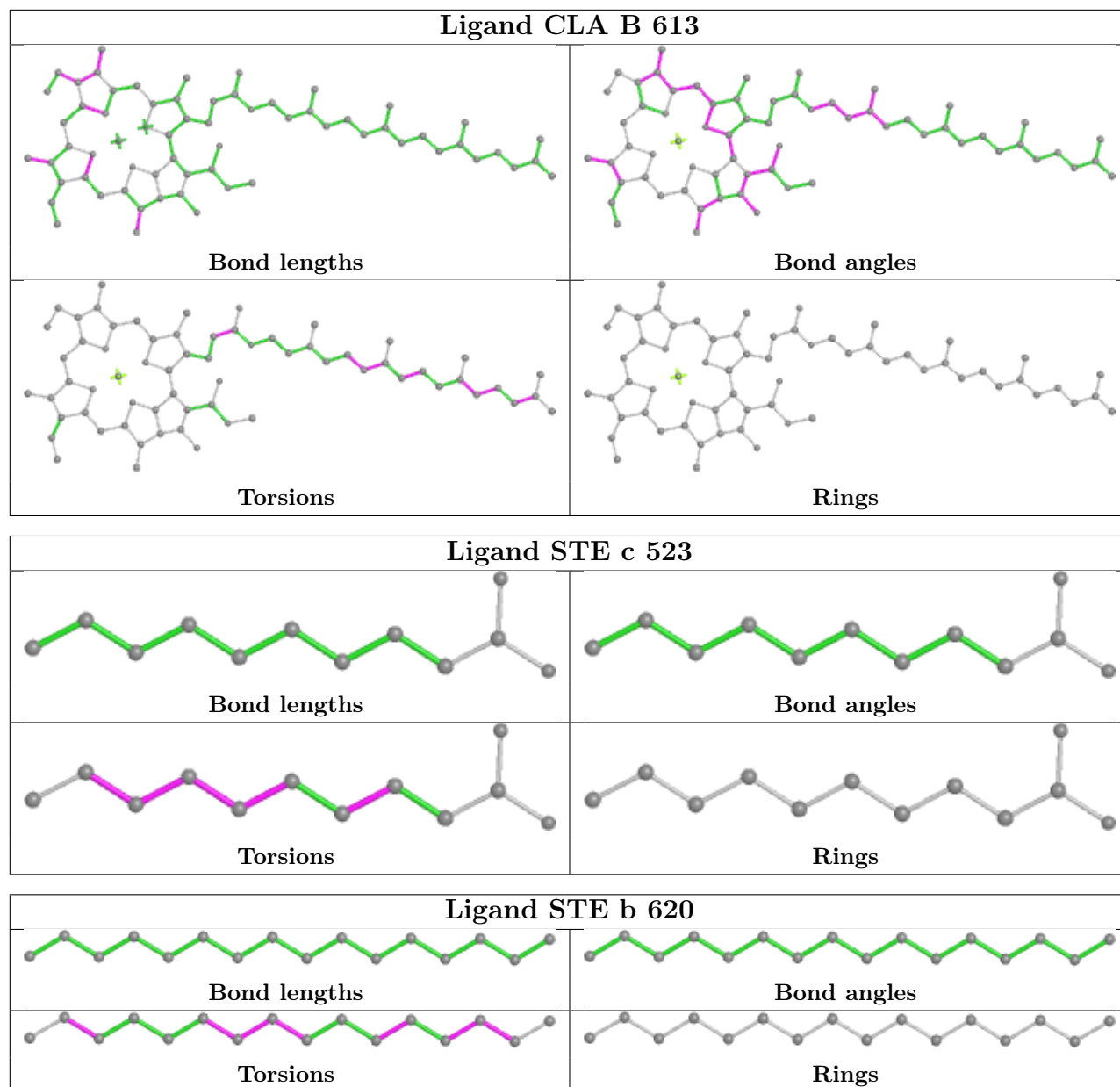
Ligand BCR b 618**Ligand CLA B 611****Ligand PL9 D 407**

Ligand LHG L 102

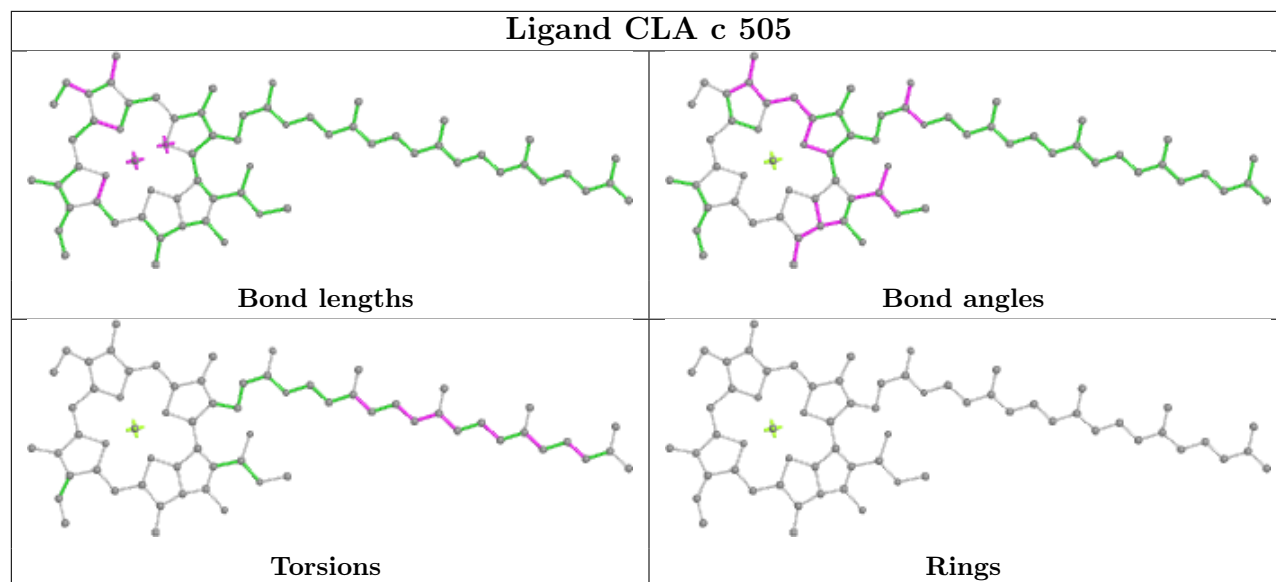


Ligand DGD h 101

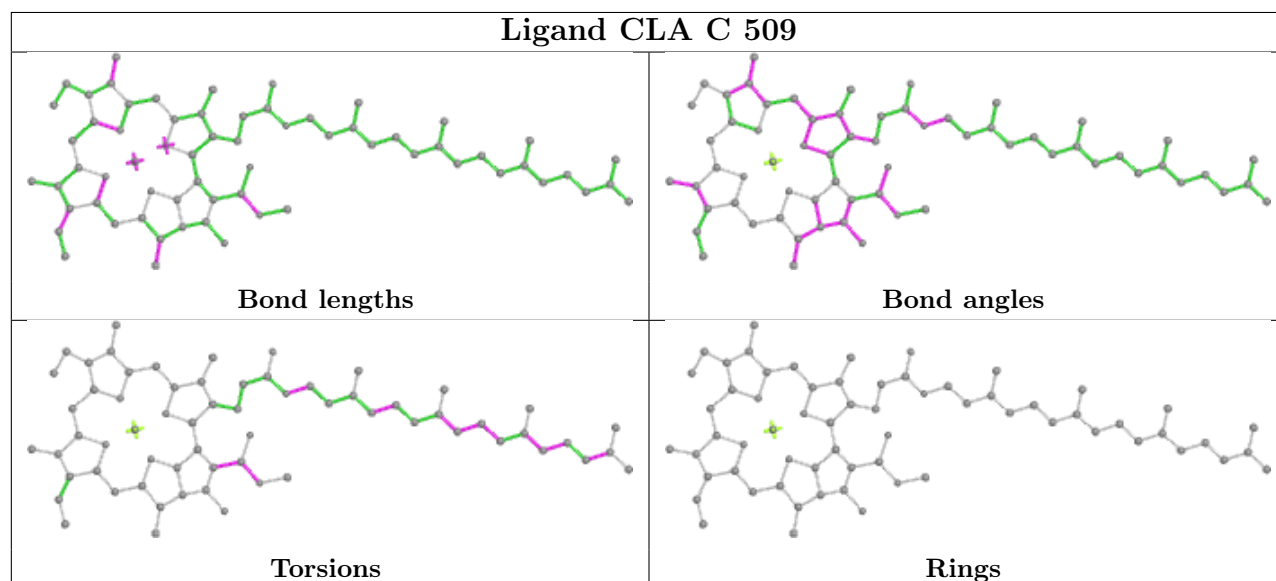




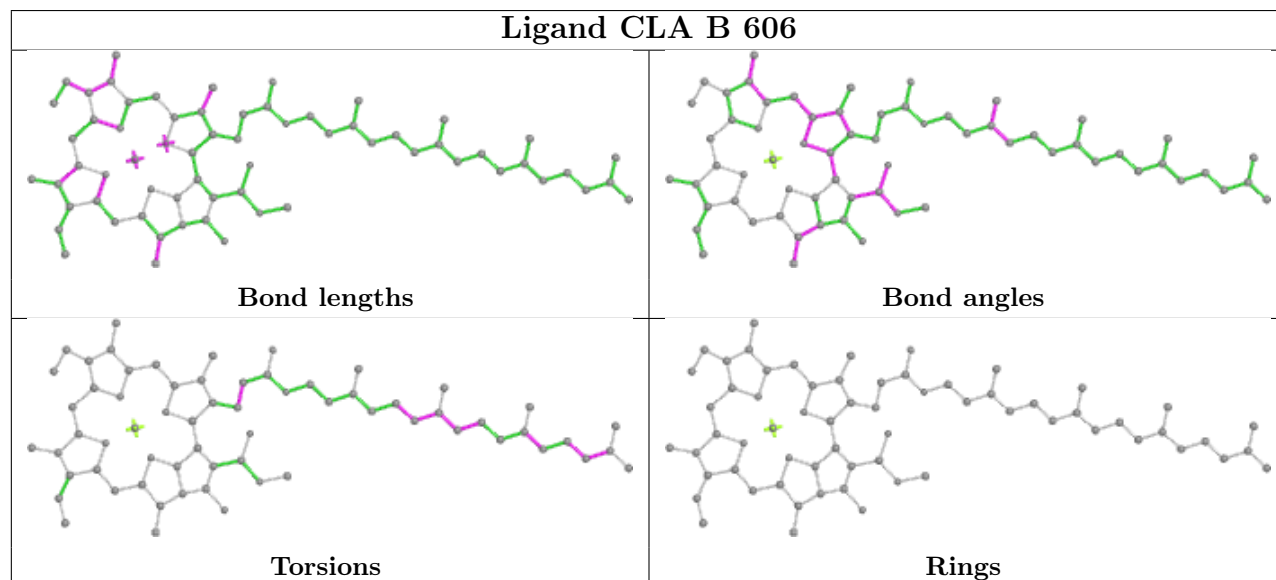
Ligand CLA c 505

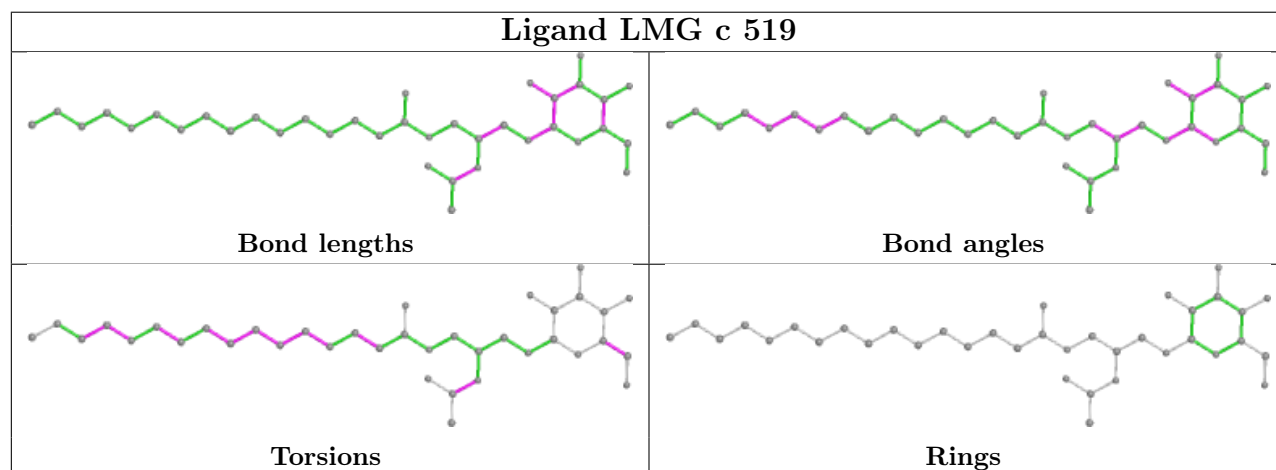
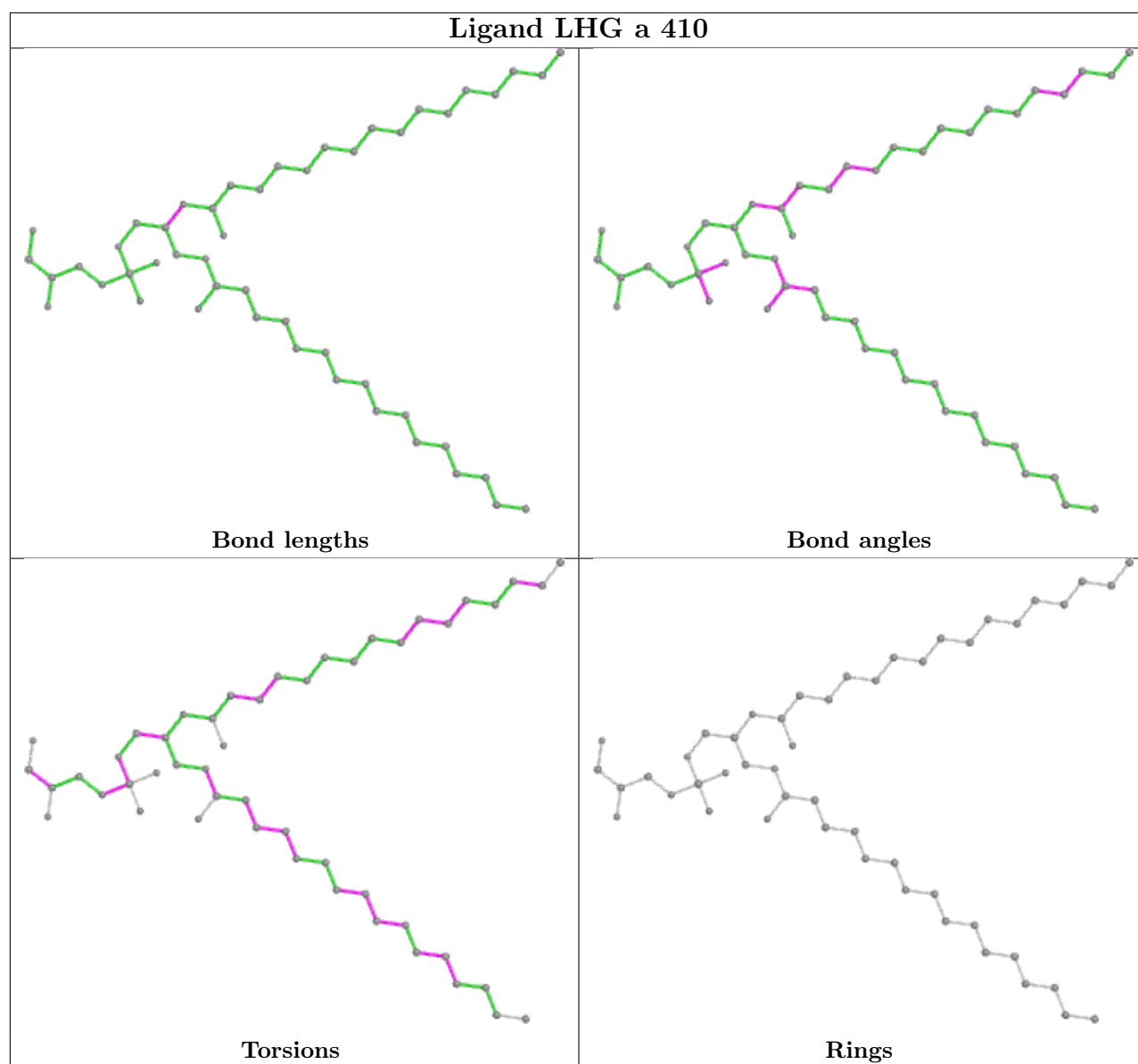


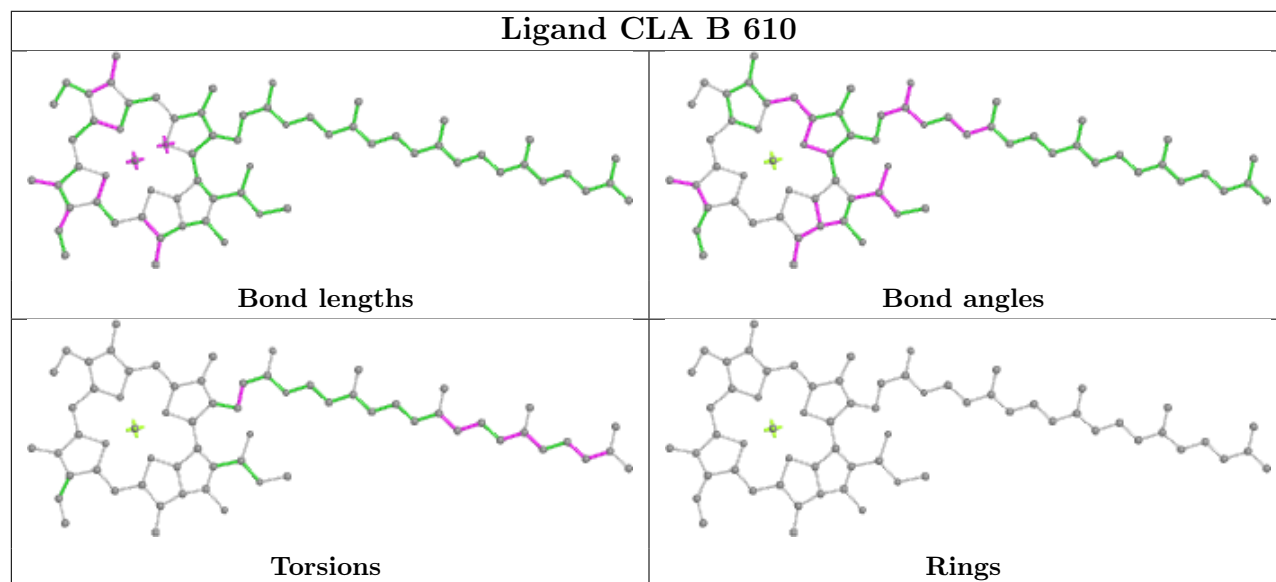
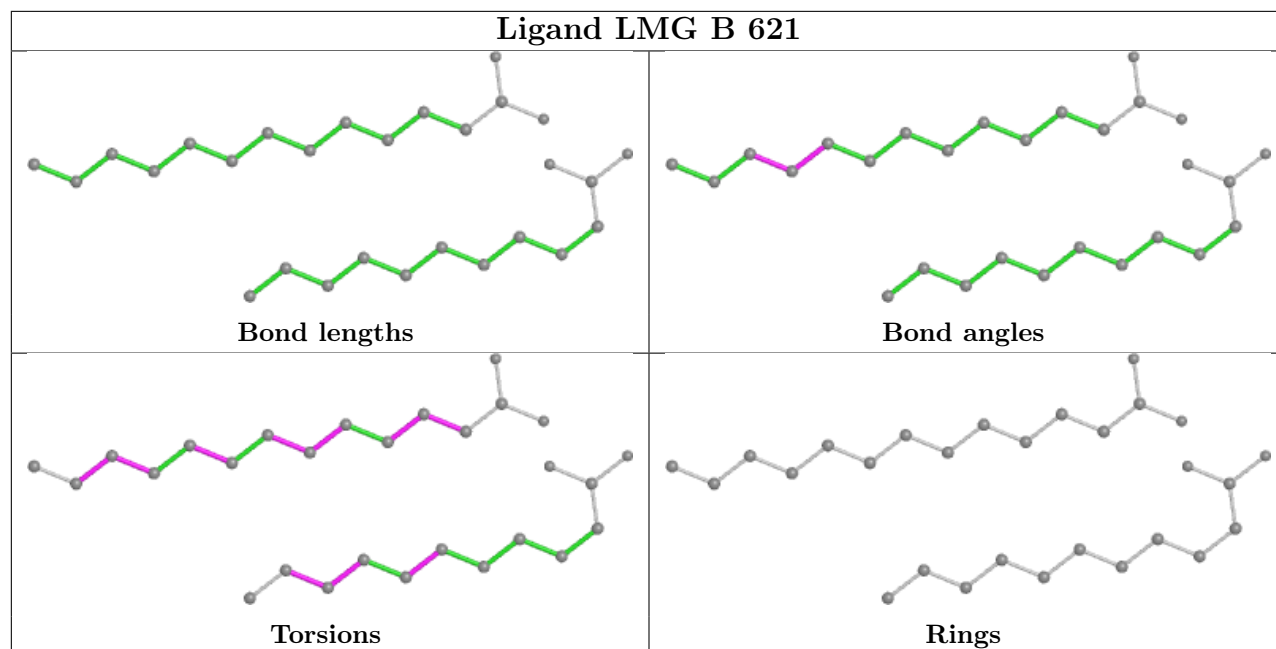
Ligand CLA C 509

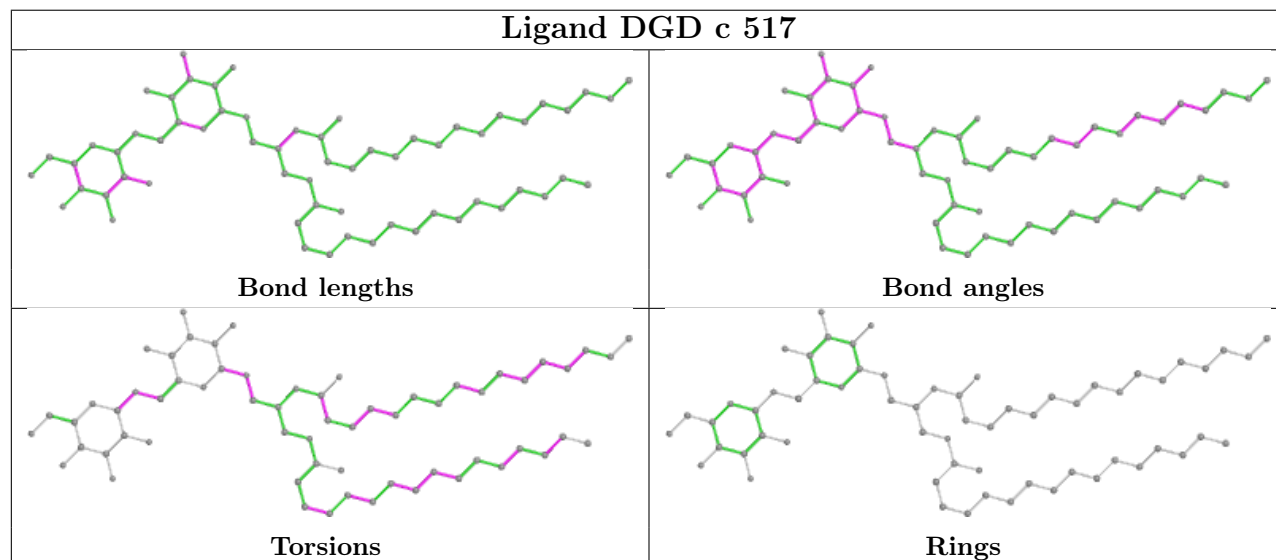
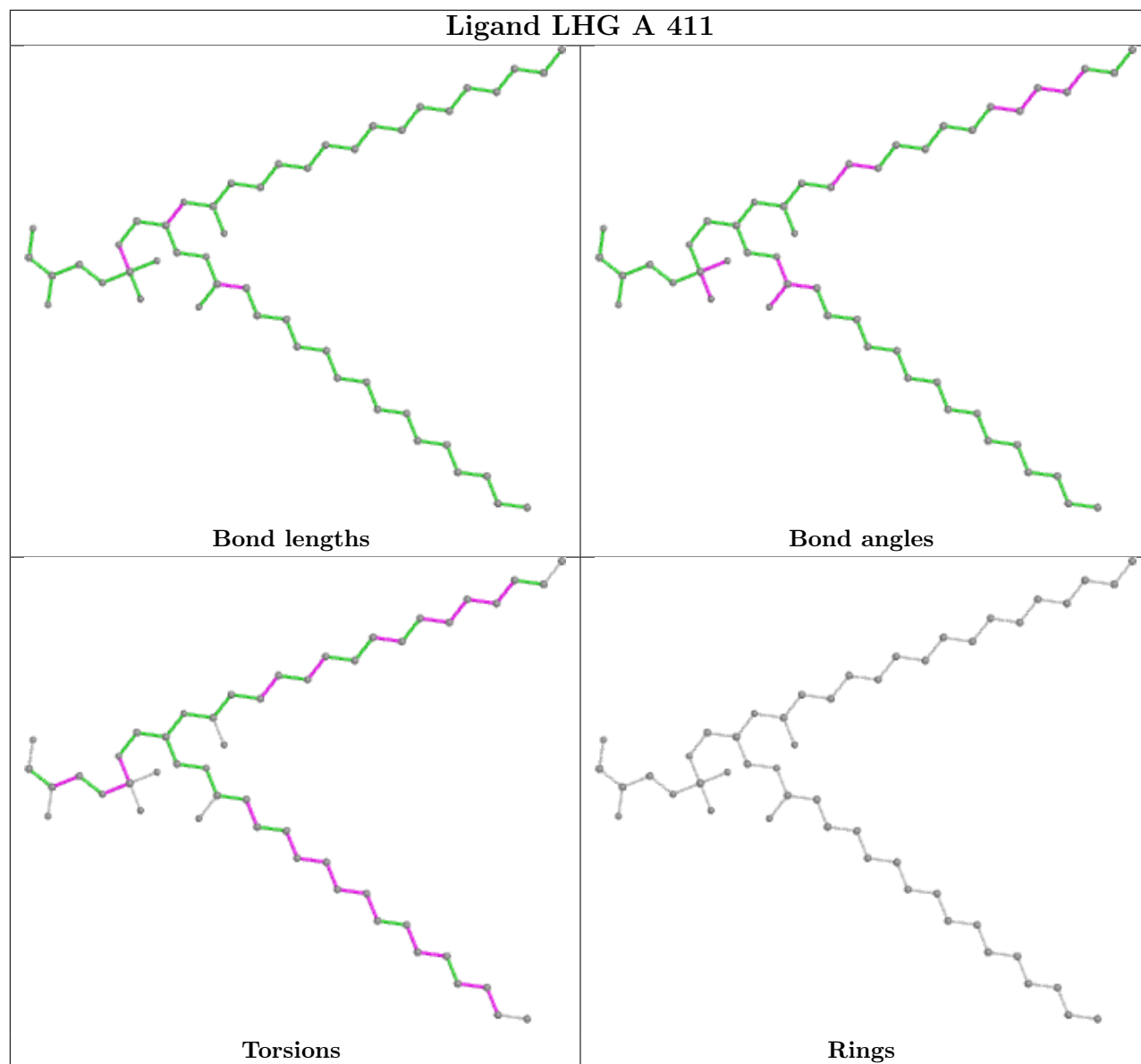


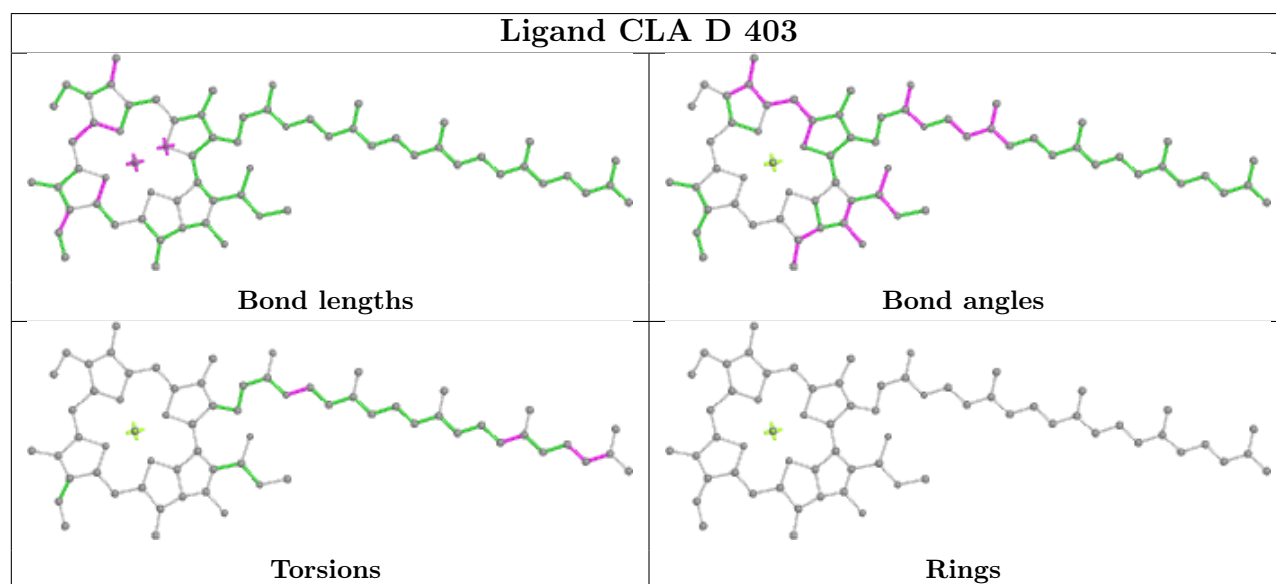
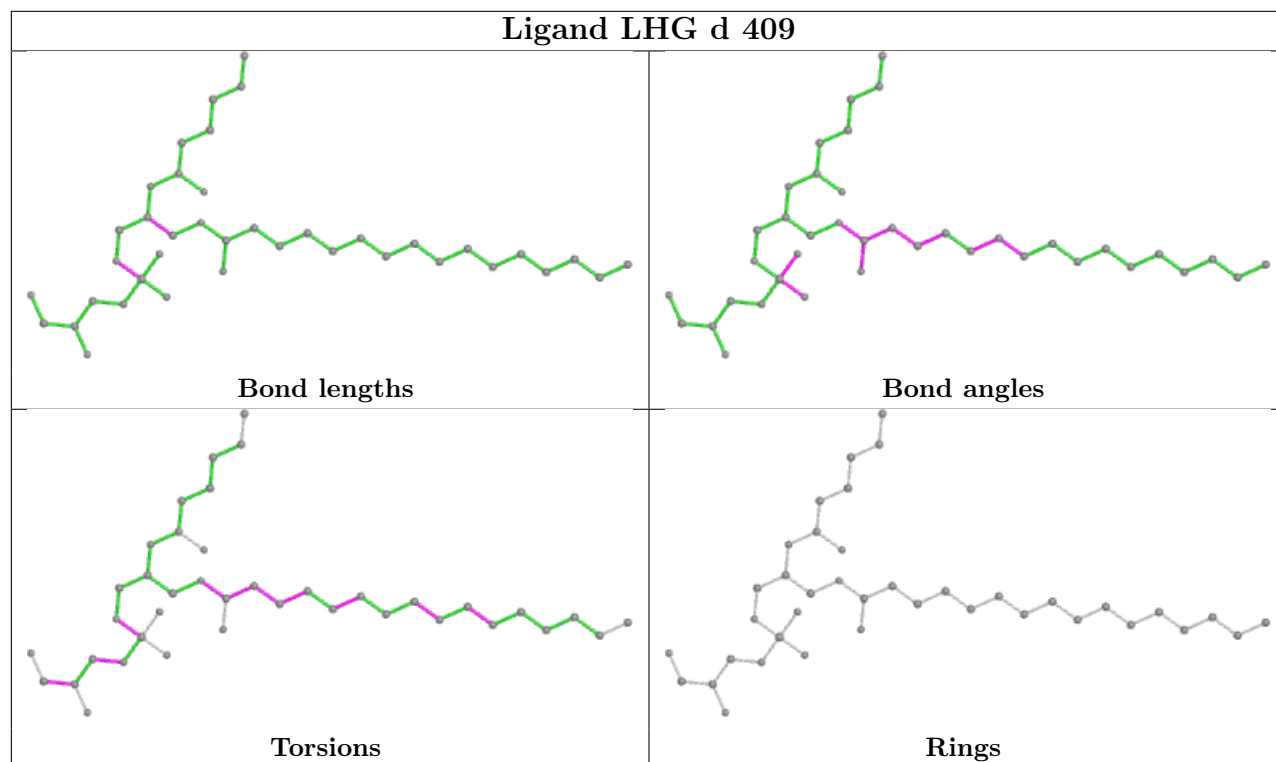
Ligand CLA B 606



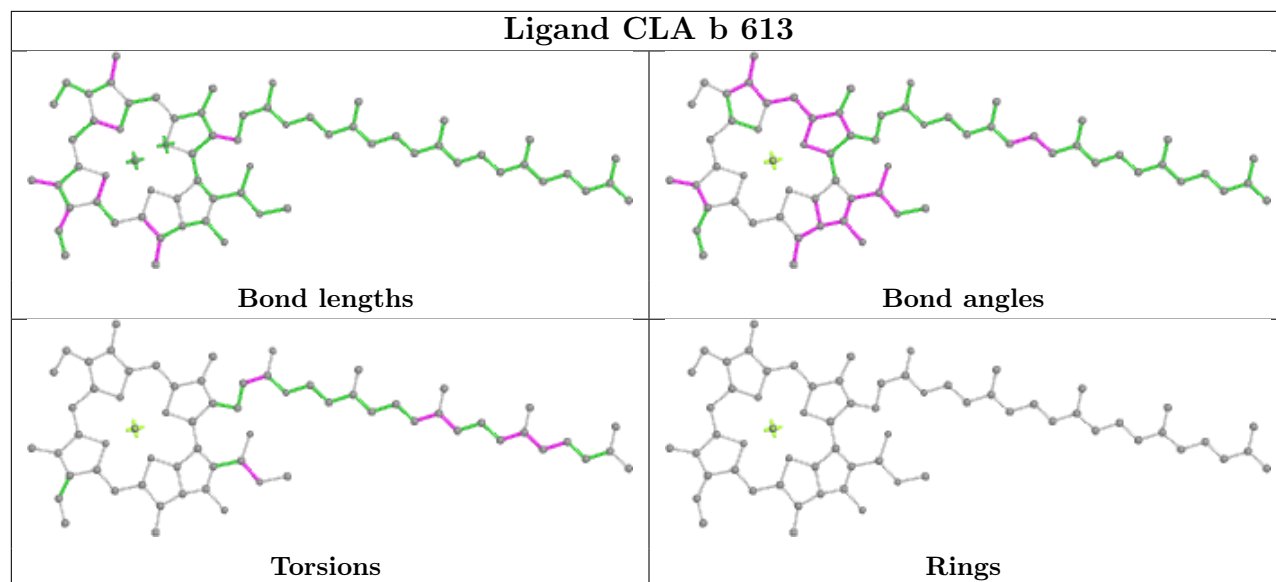




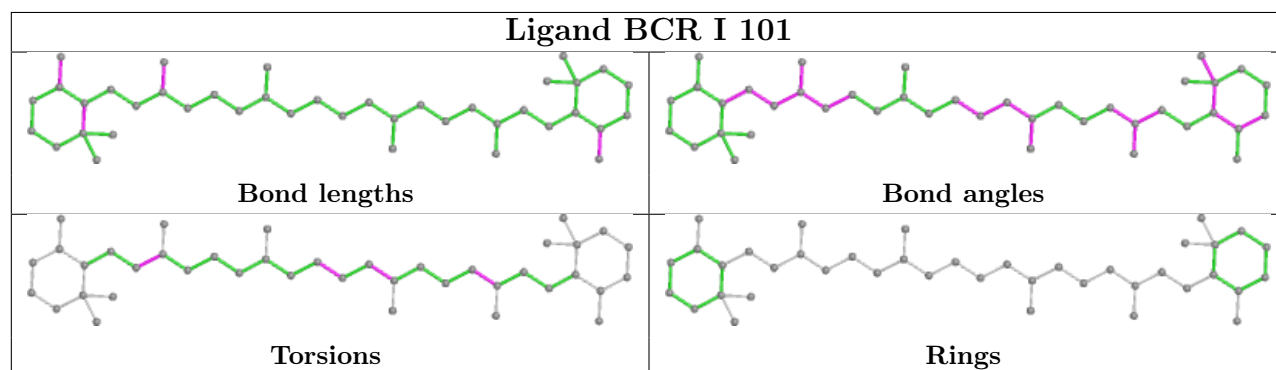




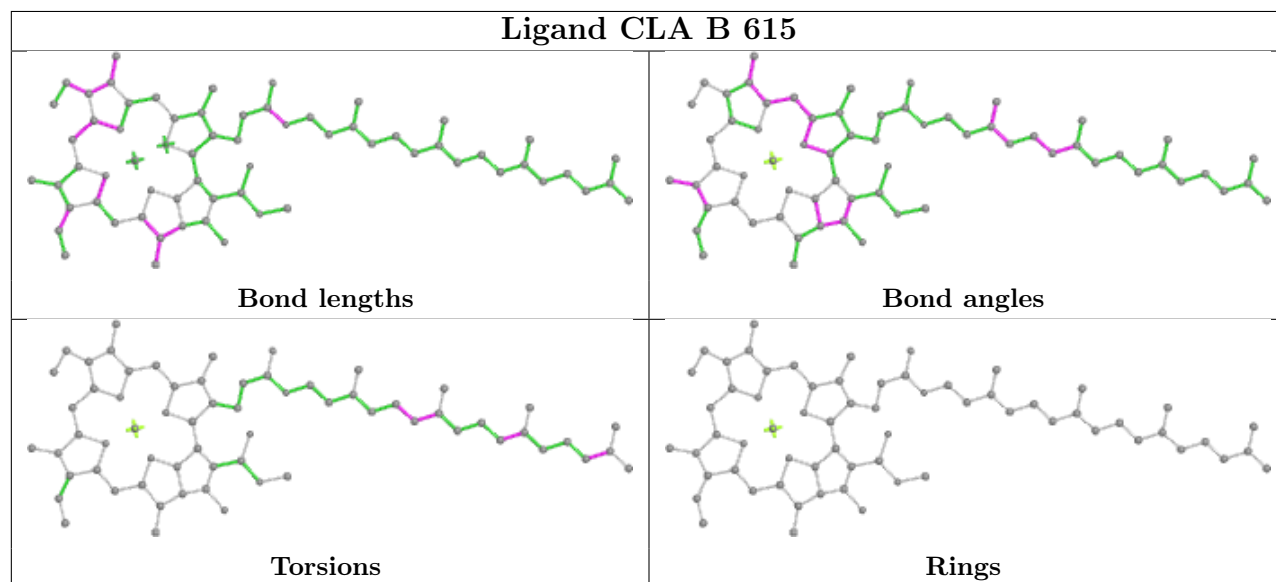
Ligand CLA b 613



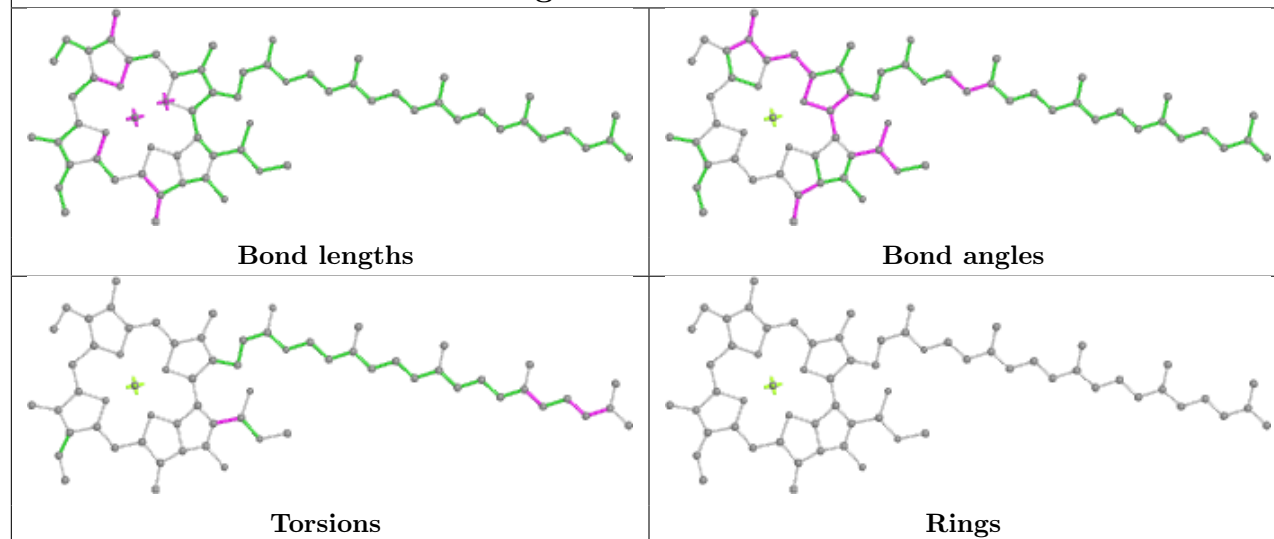
Ligand BCR I 101



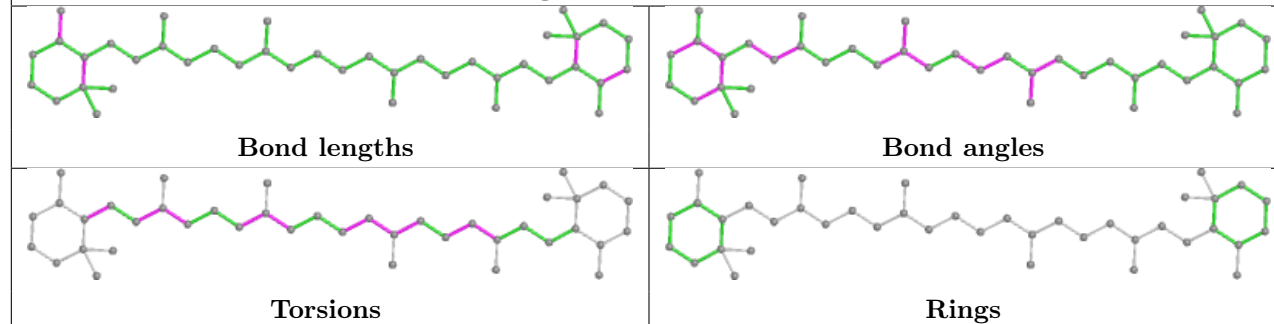
Ligand CLA B 615



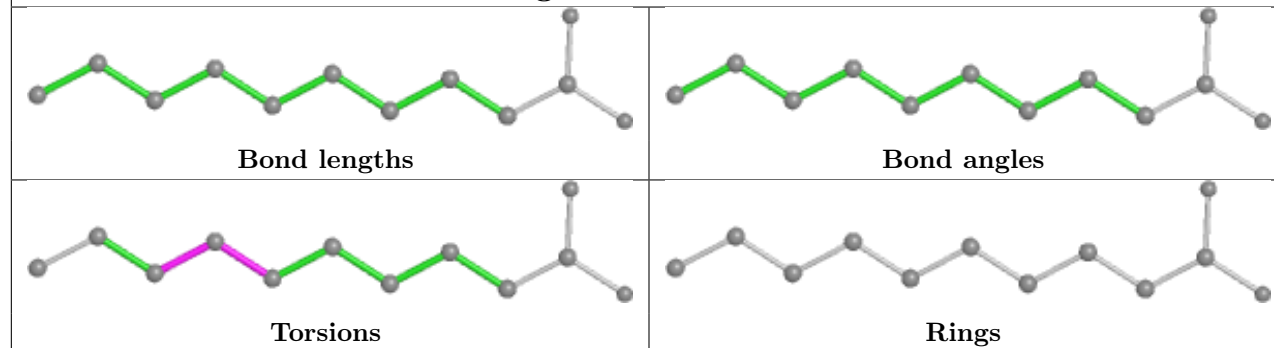
Ligand CLA d 404



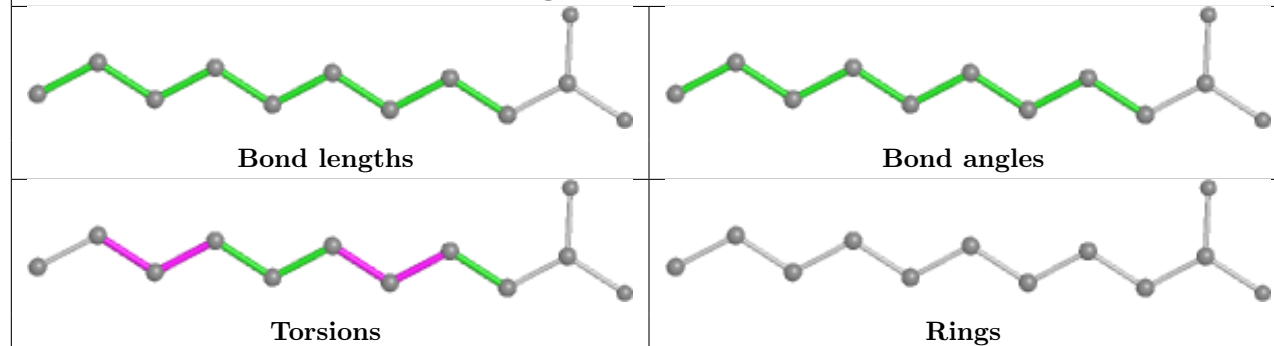
Ligand BCR t 101

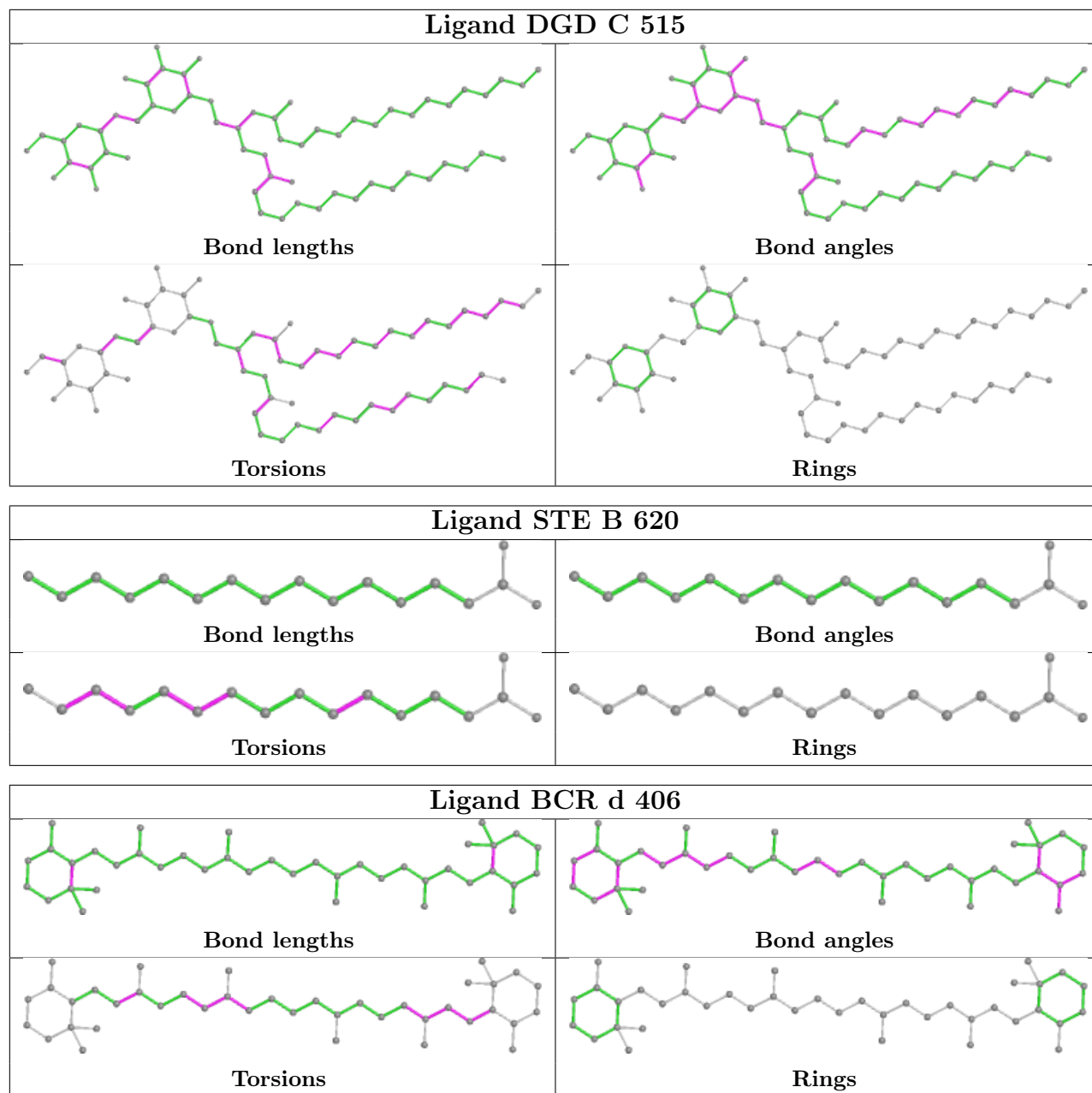


Ligand STE C 520

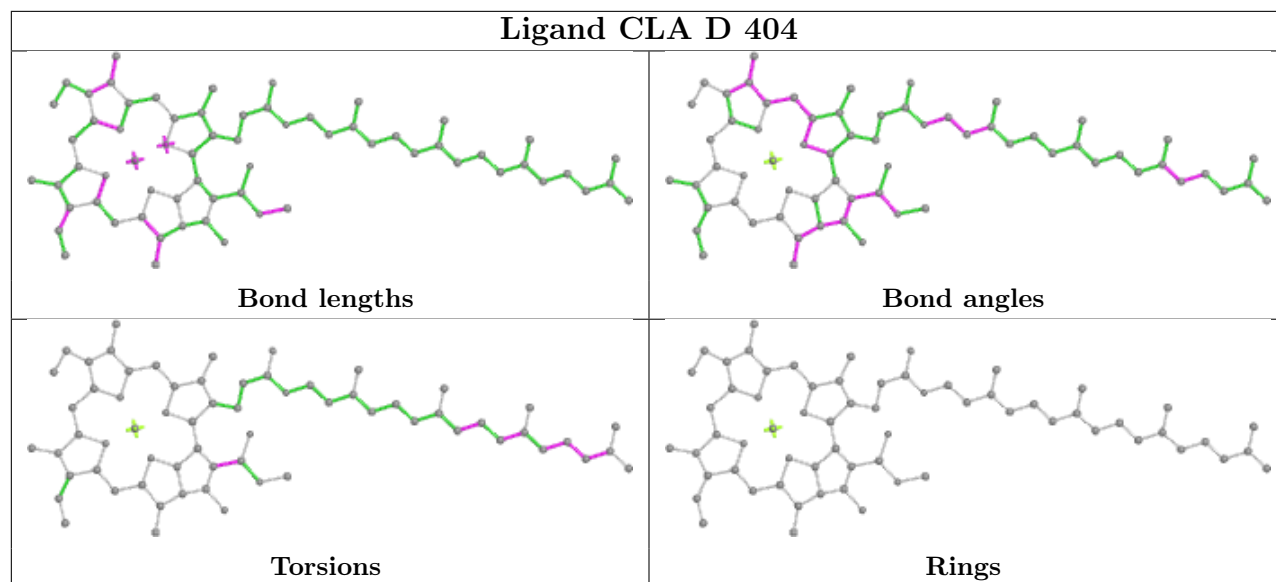


Ligand STE a 412

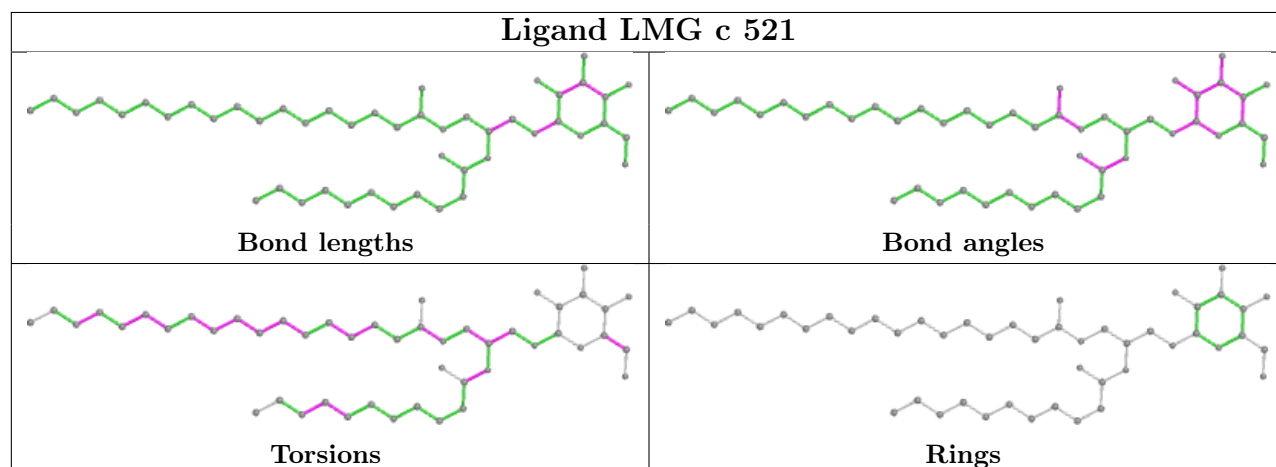




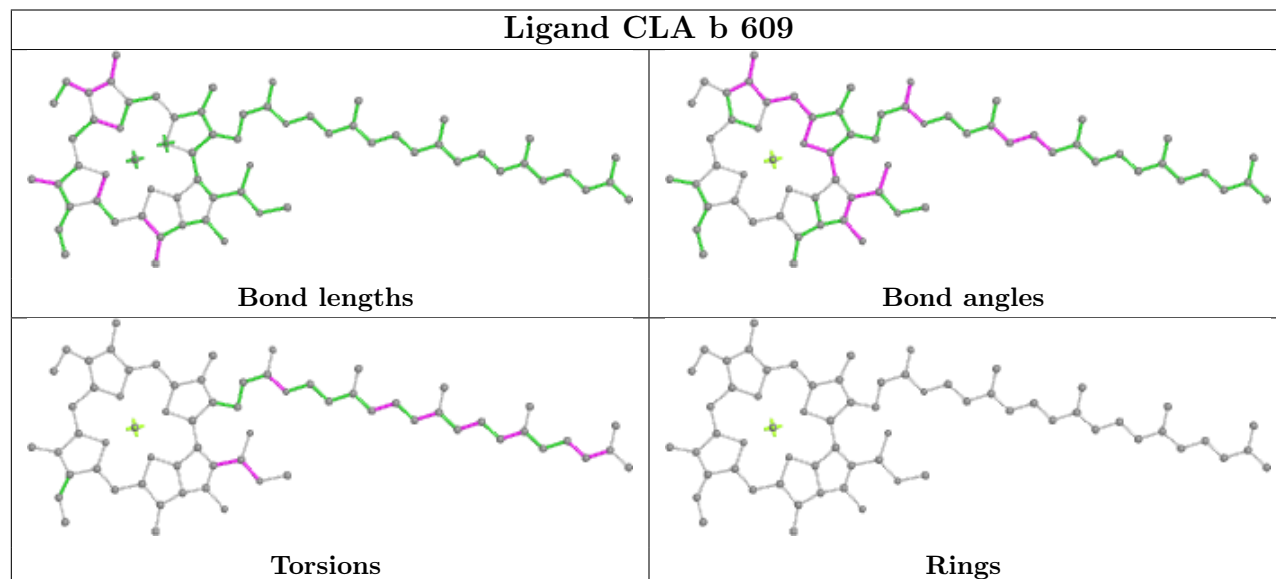
Ligand CLA D 404

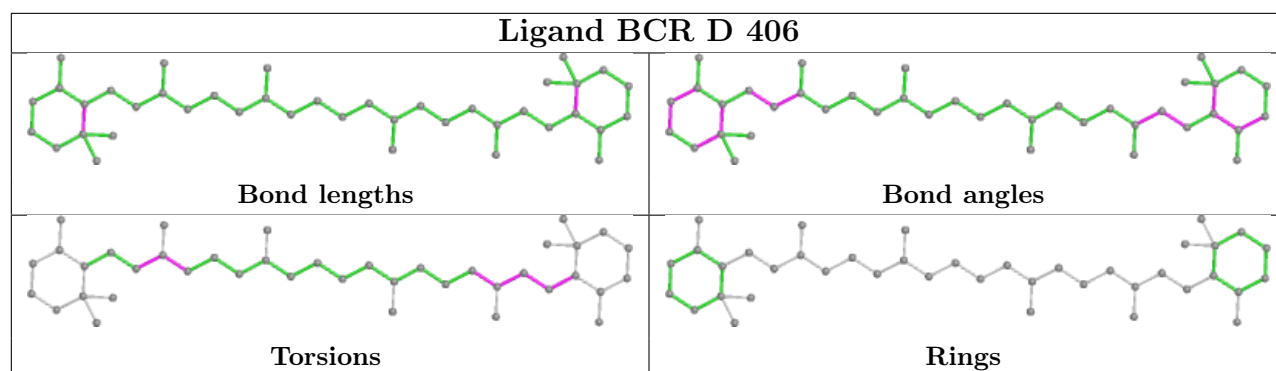
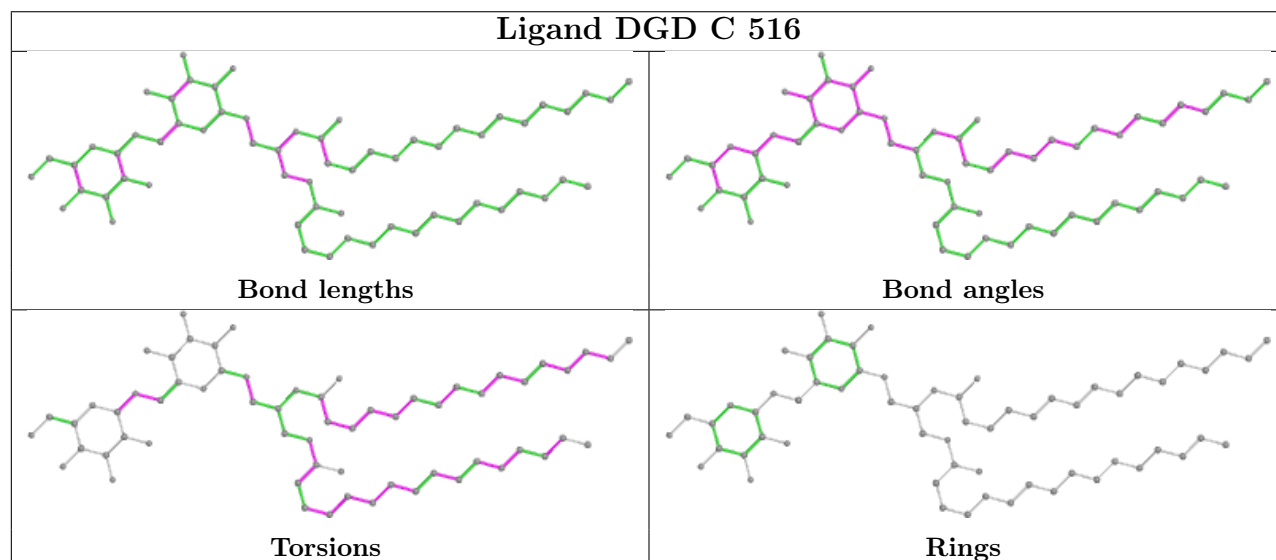
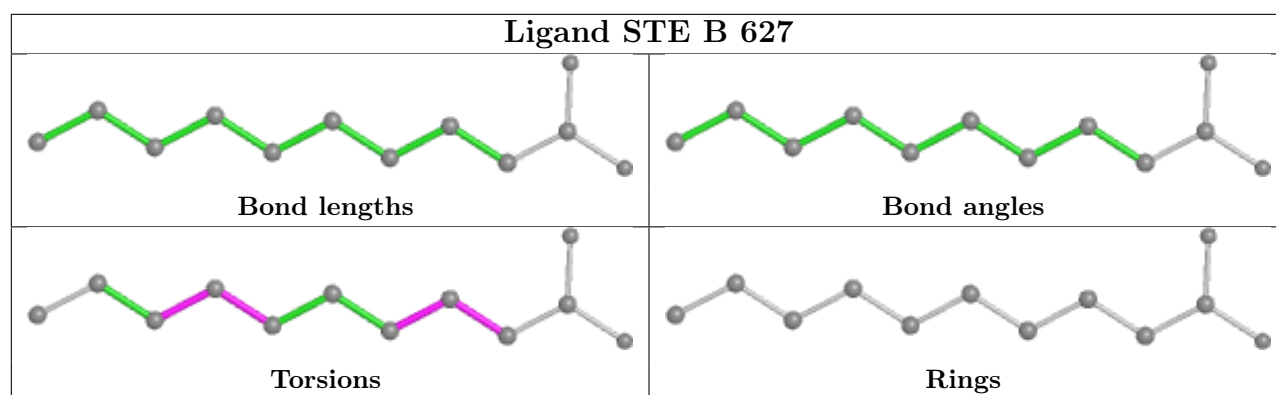


Ligand LMG c 521

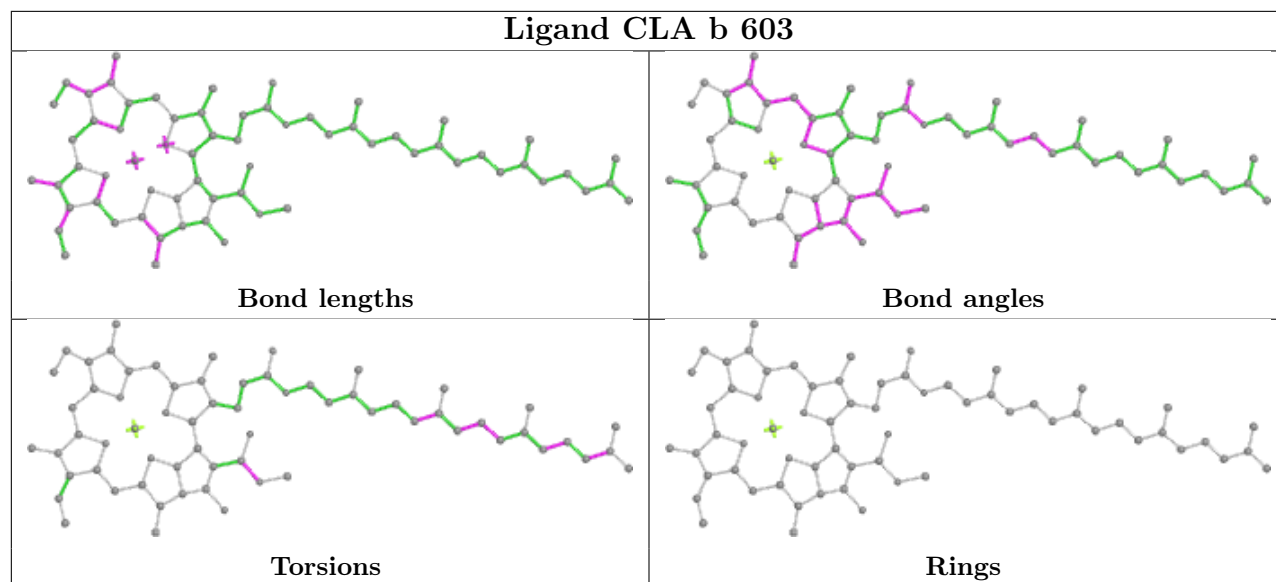


Ligand CLA b 609

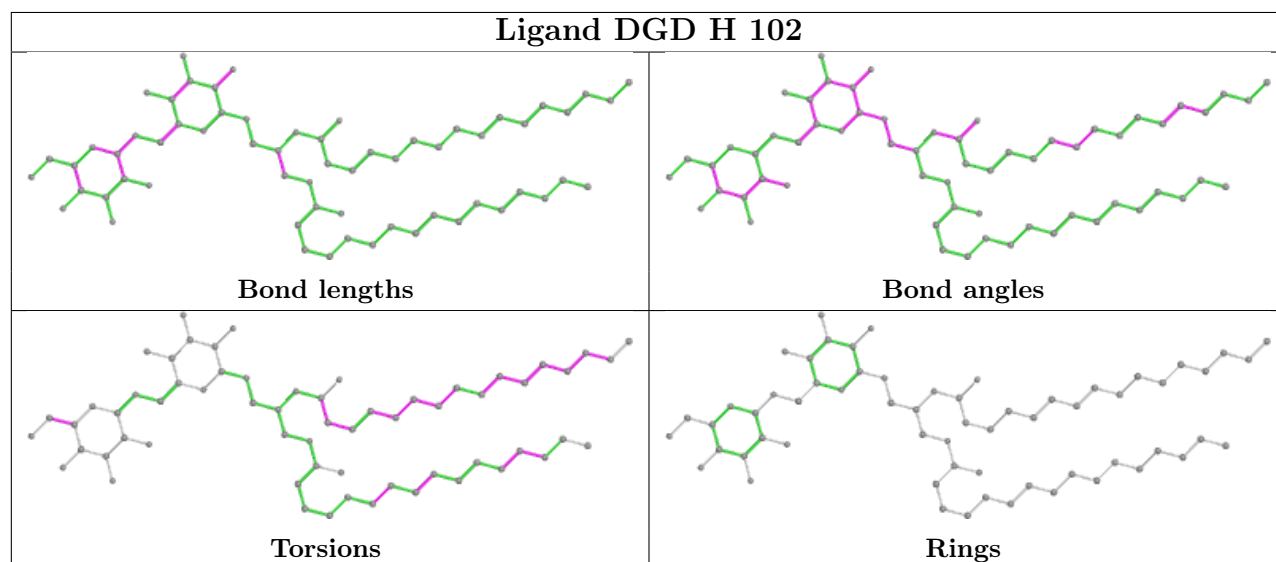




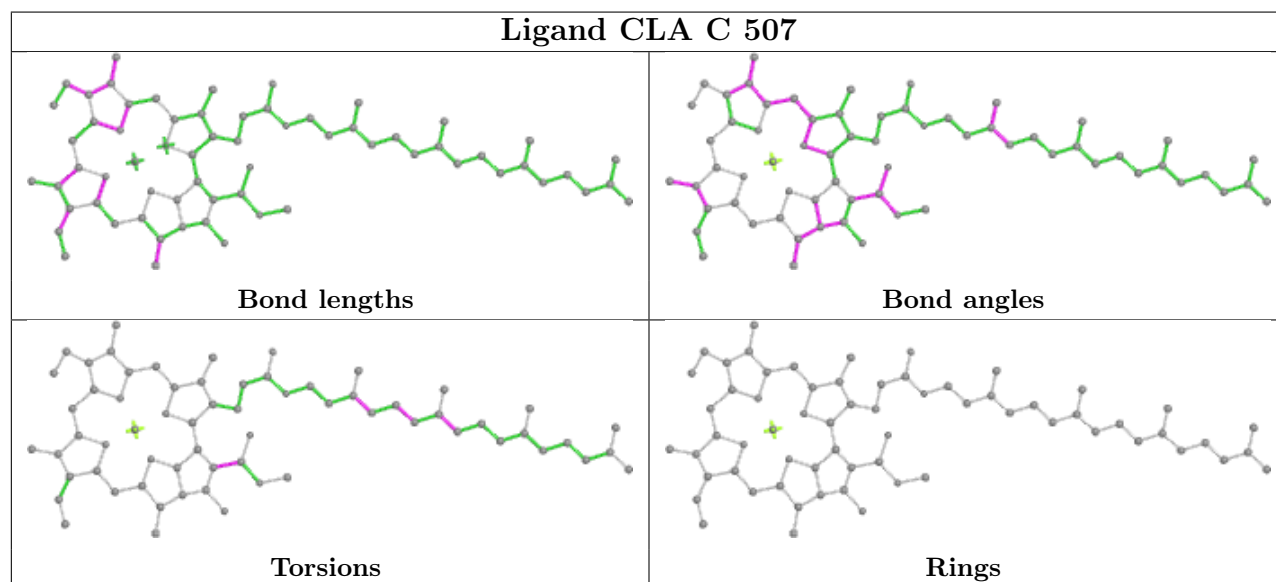
Ligand CLA b 603

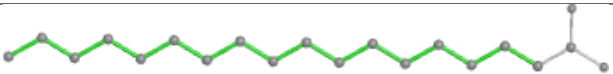
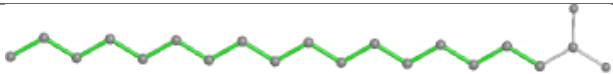
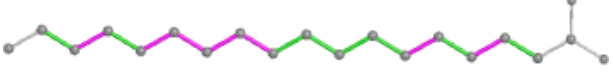
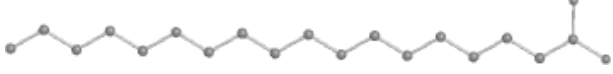


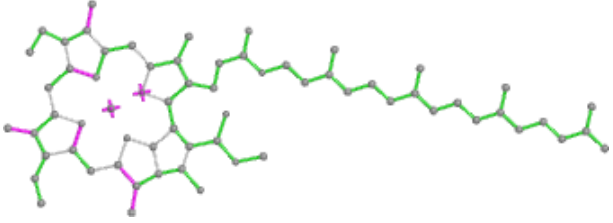
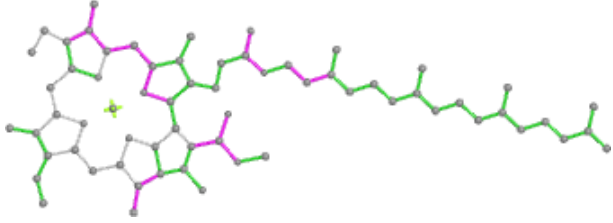
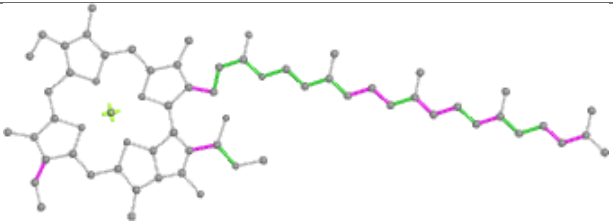
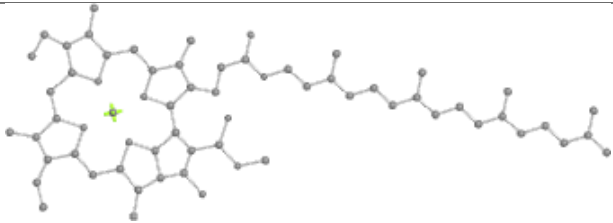
Ligand DGD H 102

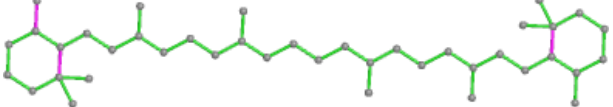
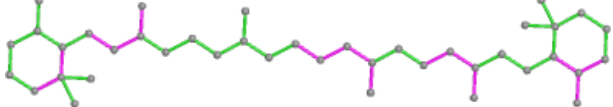
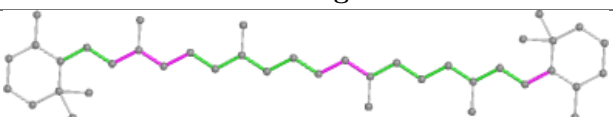
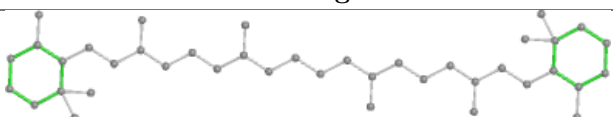


Ligand CLA C 507

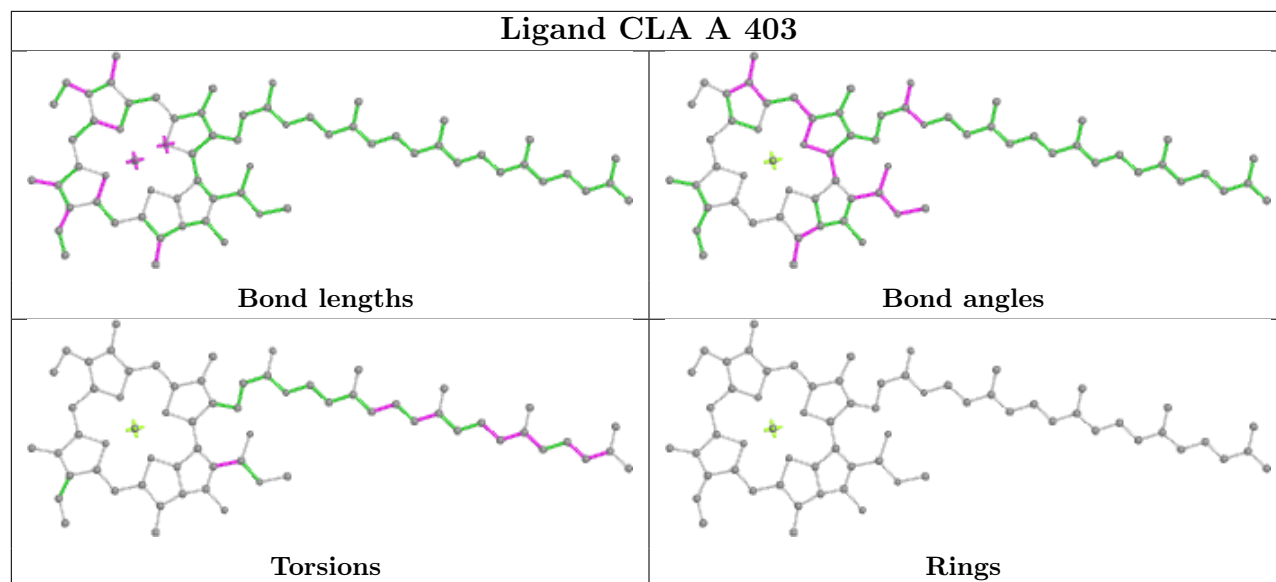


Ligand STE b 625	
 Bond lengths	 Bond angles
 Torsions	 Rings

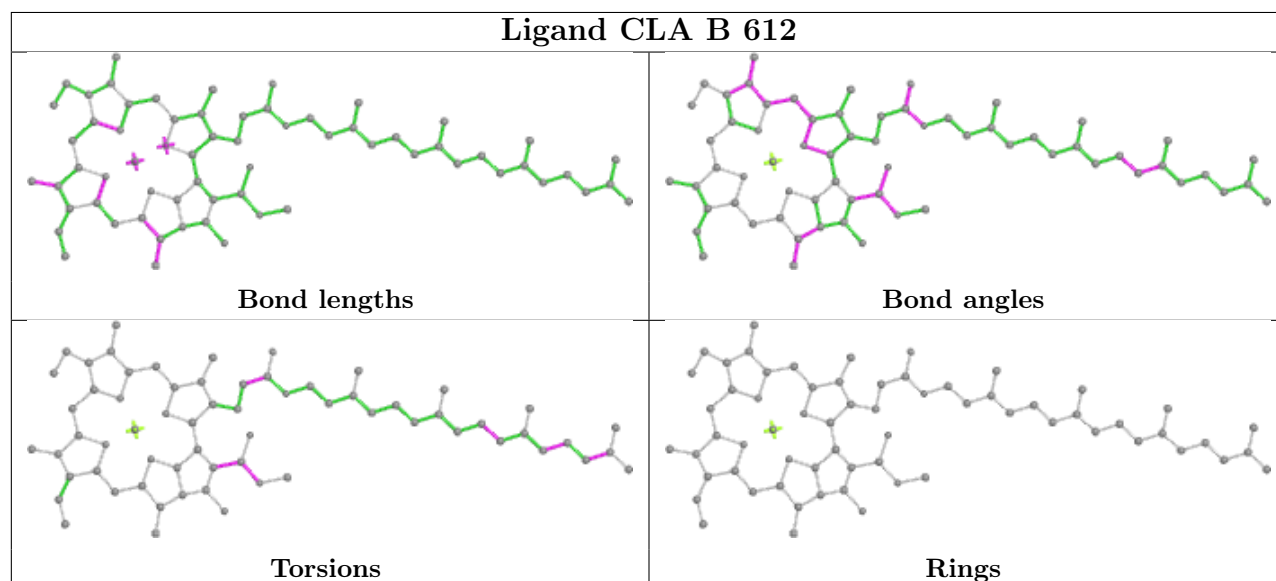
Ligand CLA C 512	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR x 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

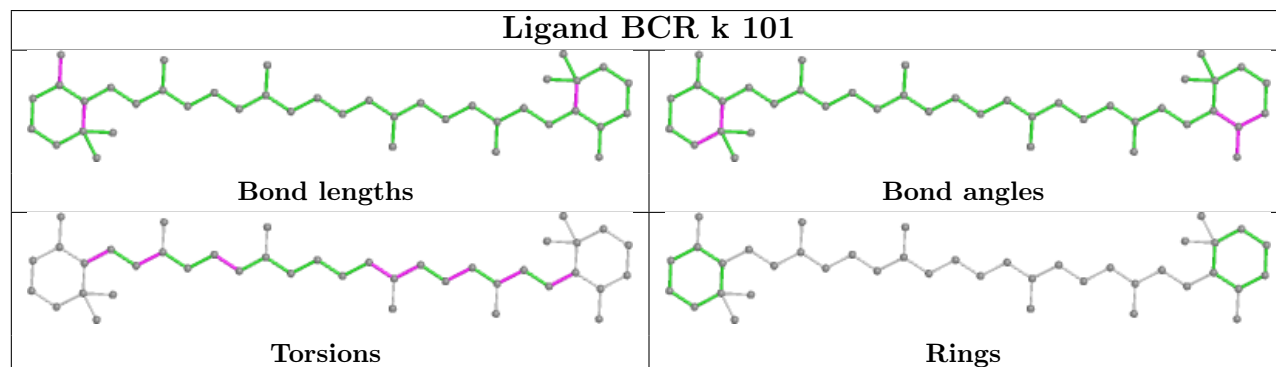
Ligand CLA A 403



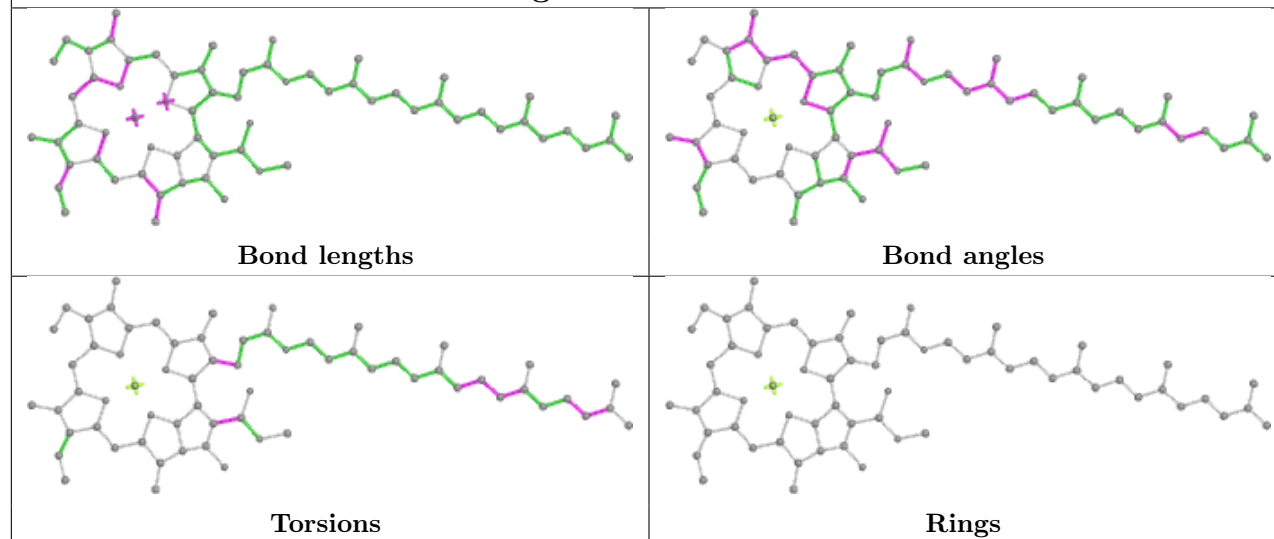
Ligand CLA B 612



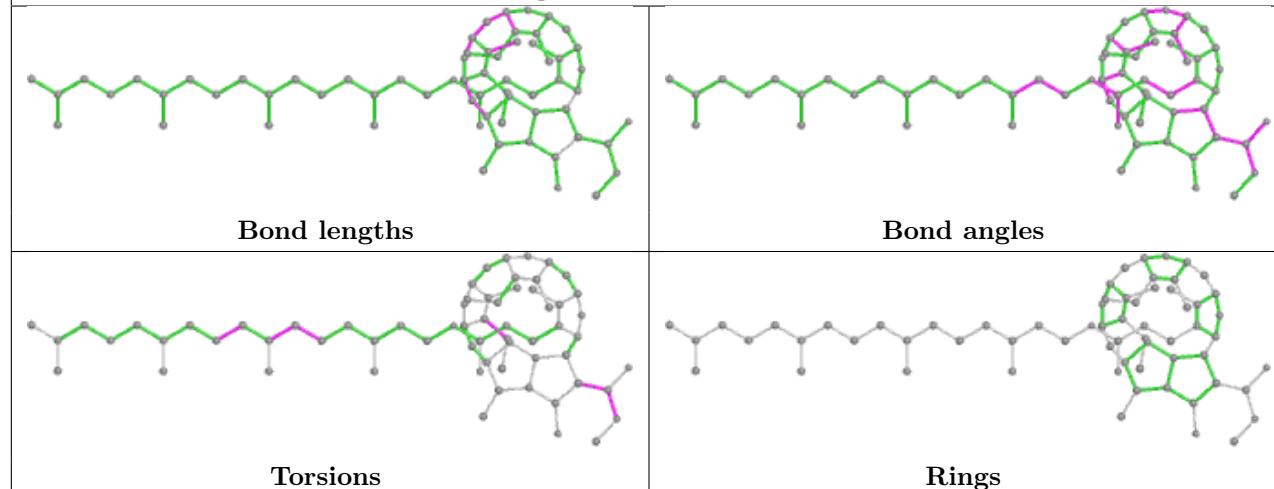
Ligand BCR k 101



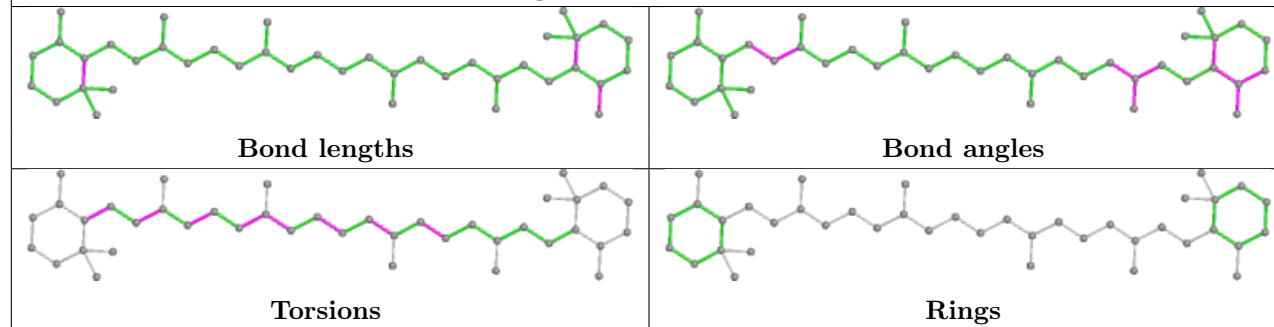
Ligand CLA B 602

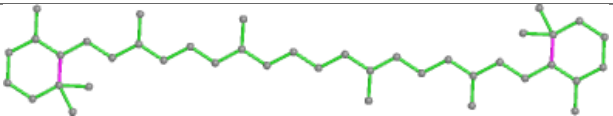
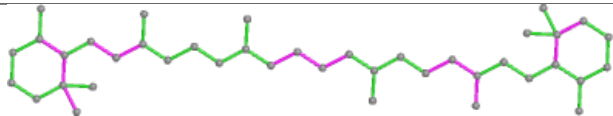
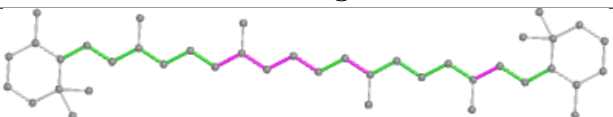
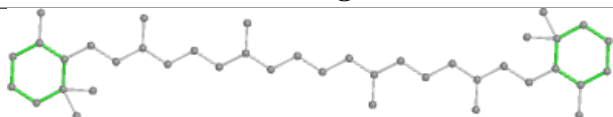





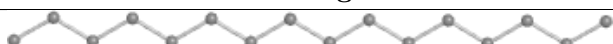
Ligand PHO d 402

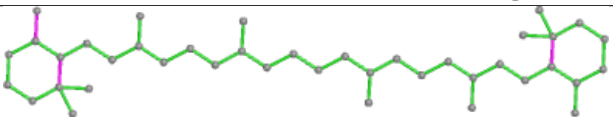
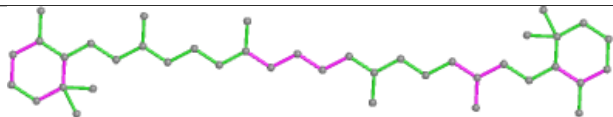
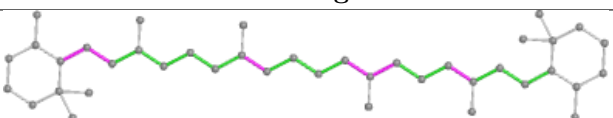
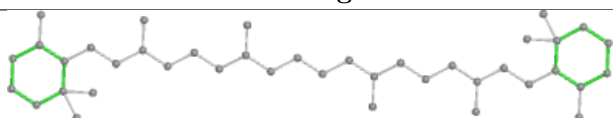


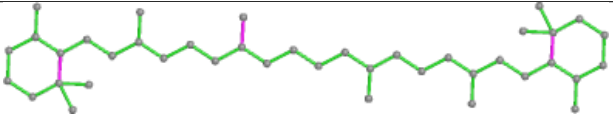
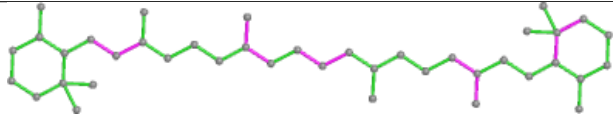
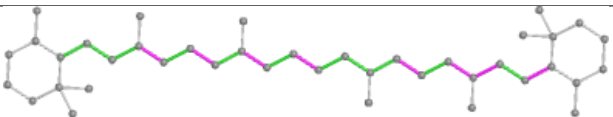
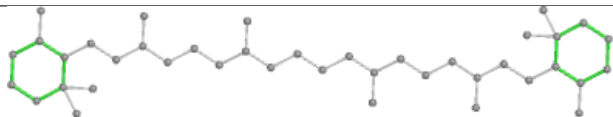
Ligand BCR T 101

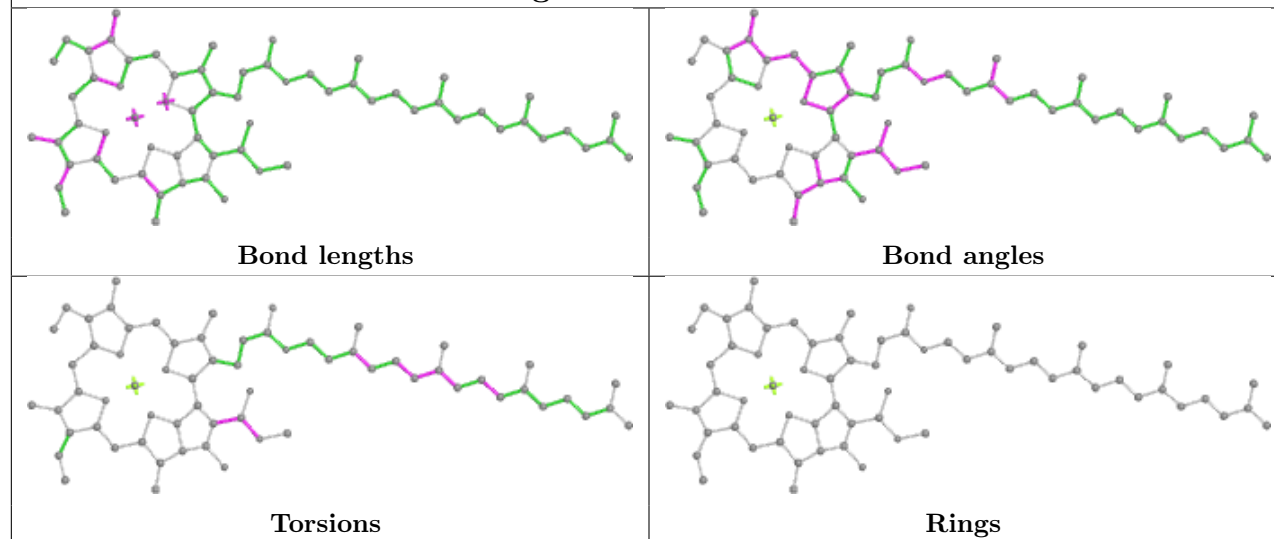
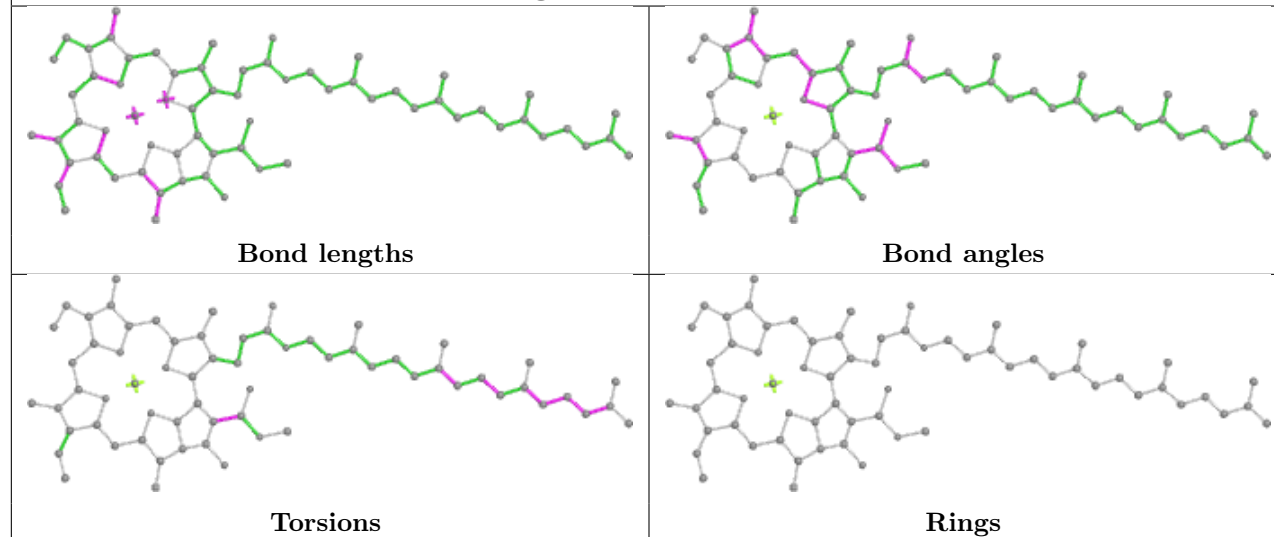
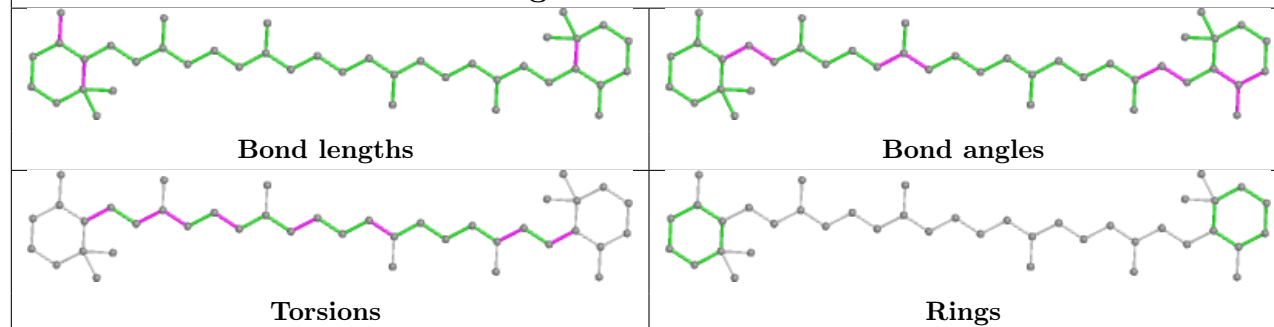


Ligand BCR b 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

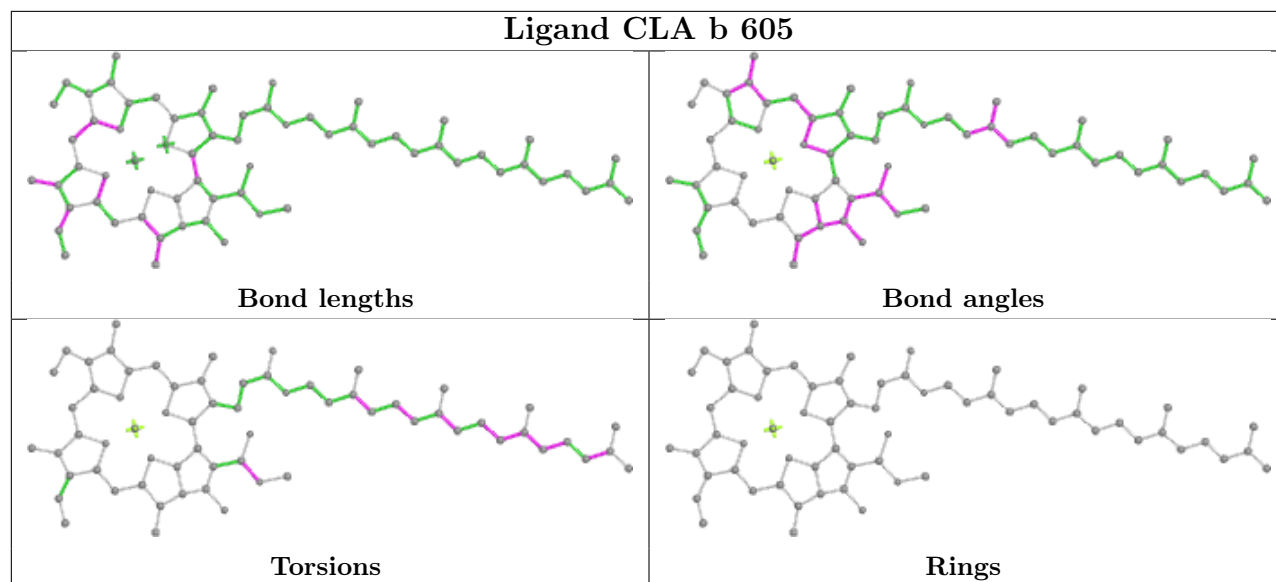
Ligand STE C 519	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR B 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

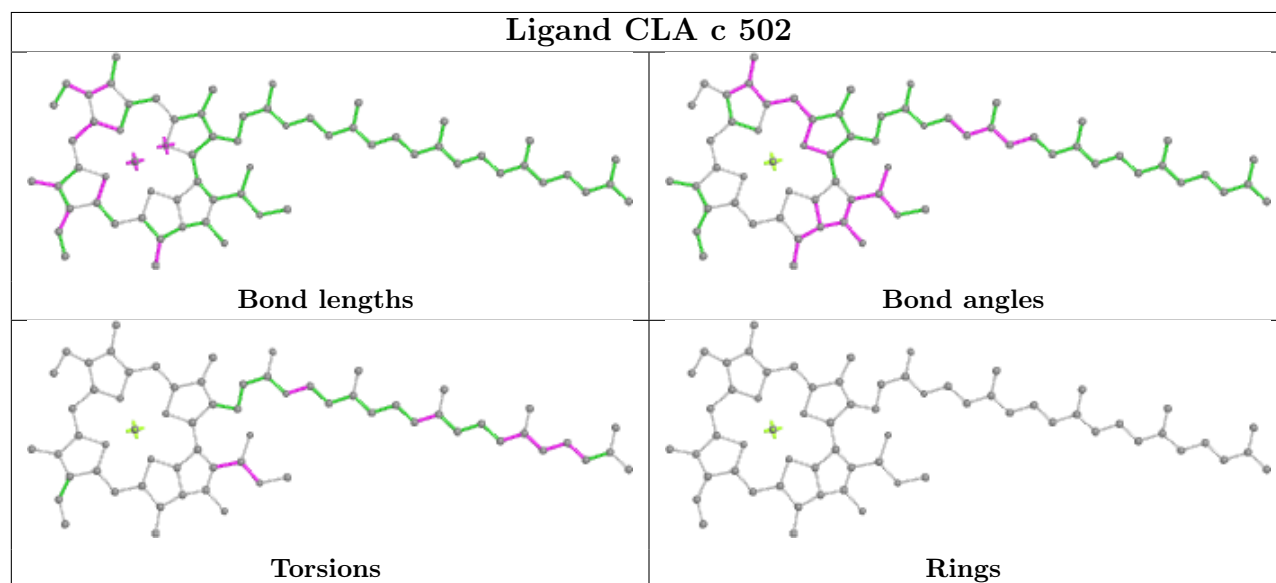
Ligand BCR B 618	
 Bond lengths	 Bond angles
 Torsions	 Rings

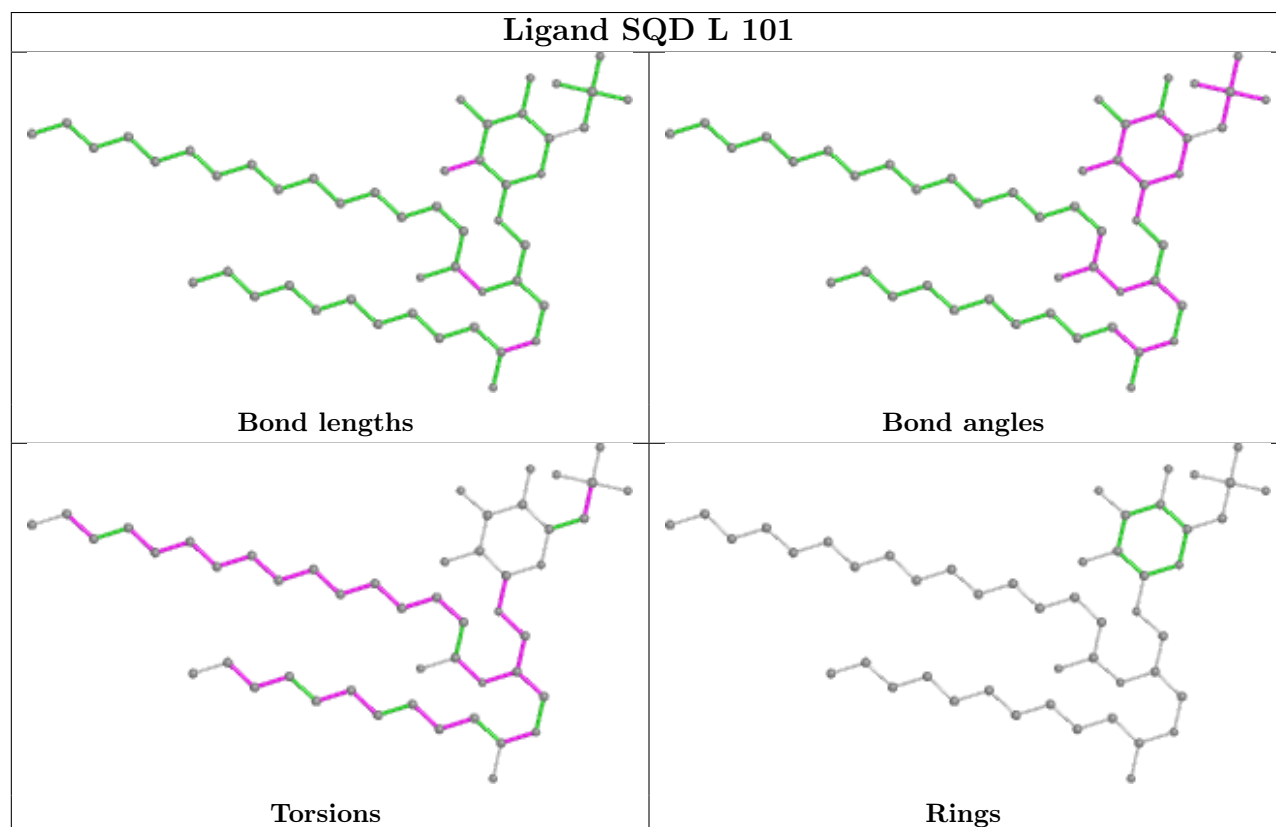
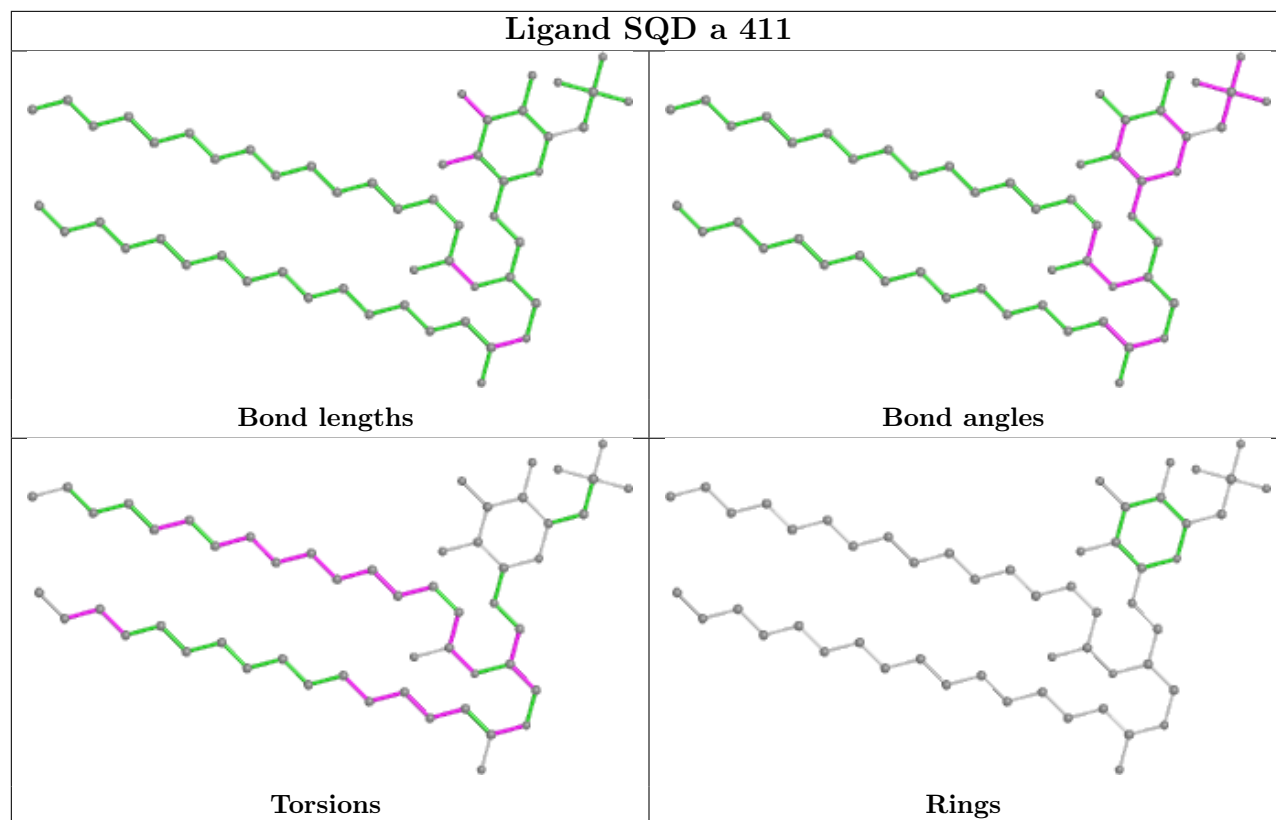
Ligand CLA C 503**Ligand CLA C 508****Ligand BCR K 101**

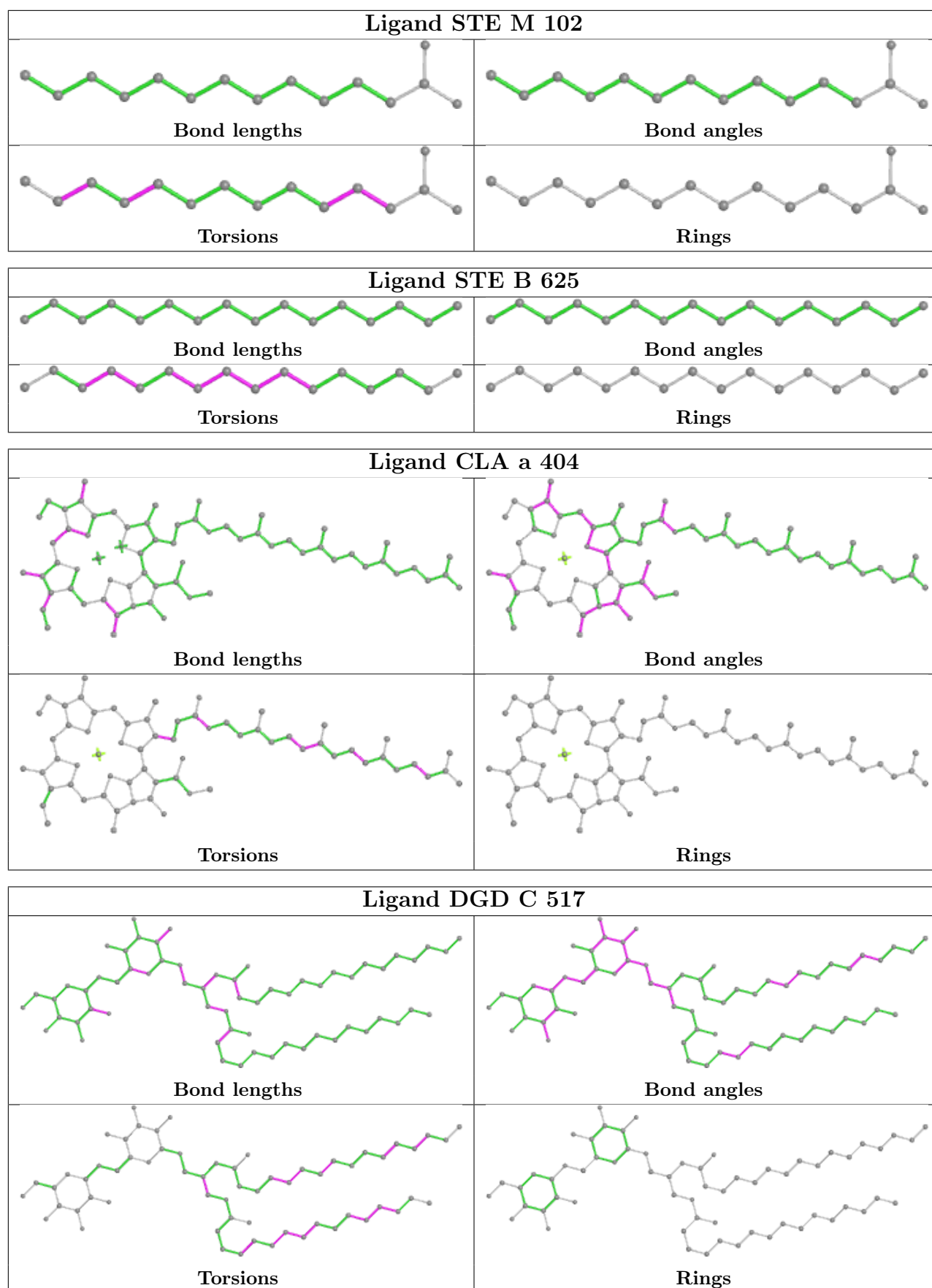
Ligand CLA b 605



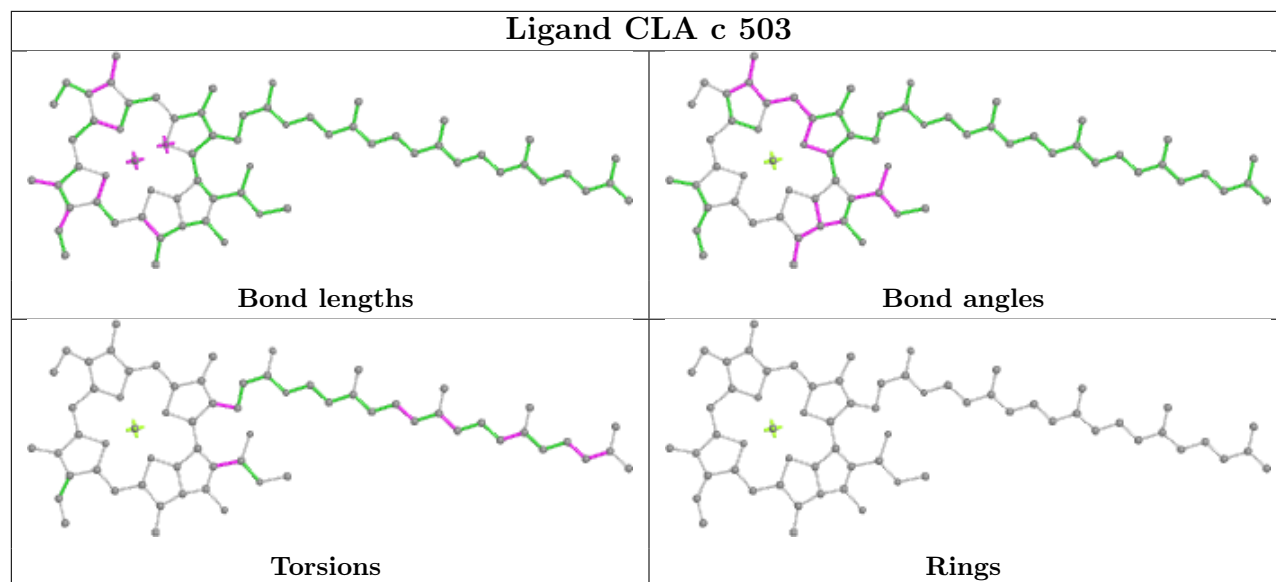
Ligand CLA c 502



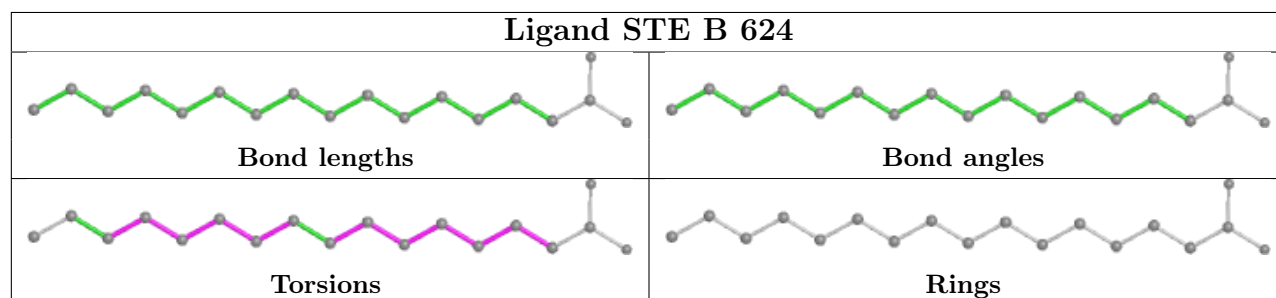




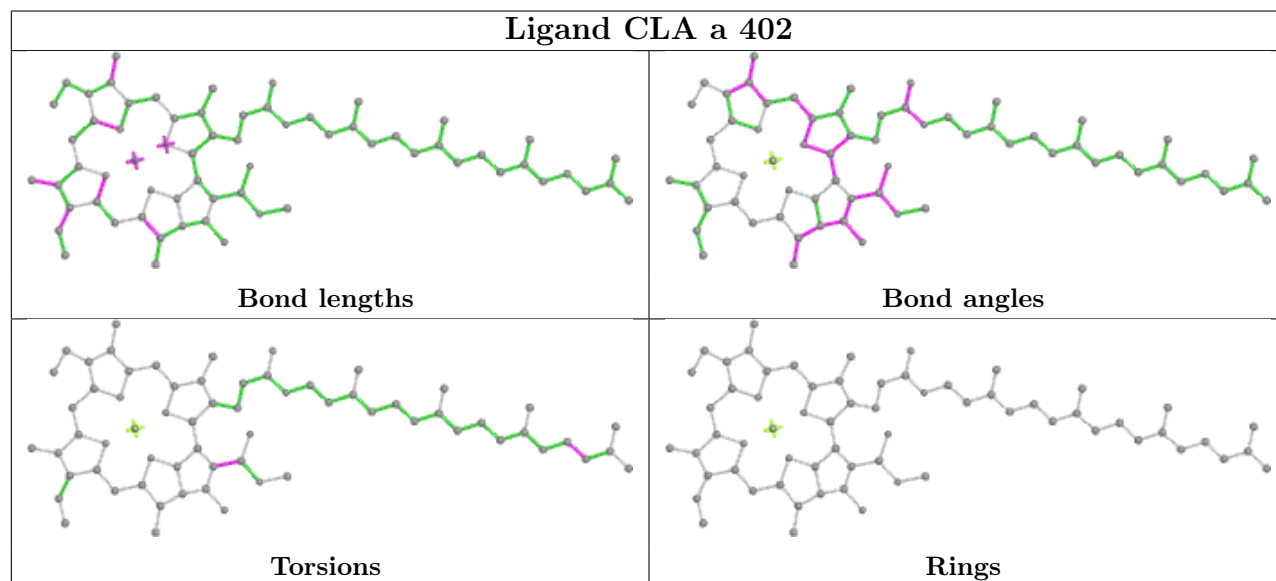
Ligand CLA c 503



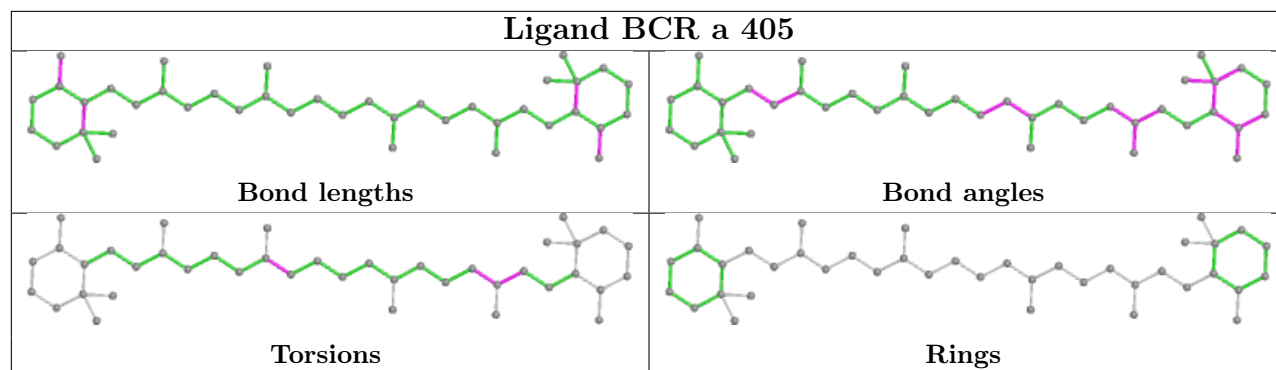
Ligand STE B 624



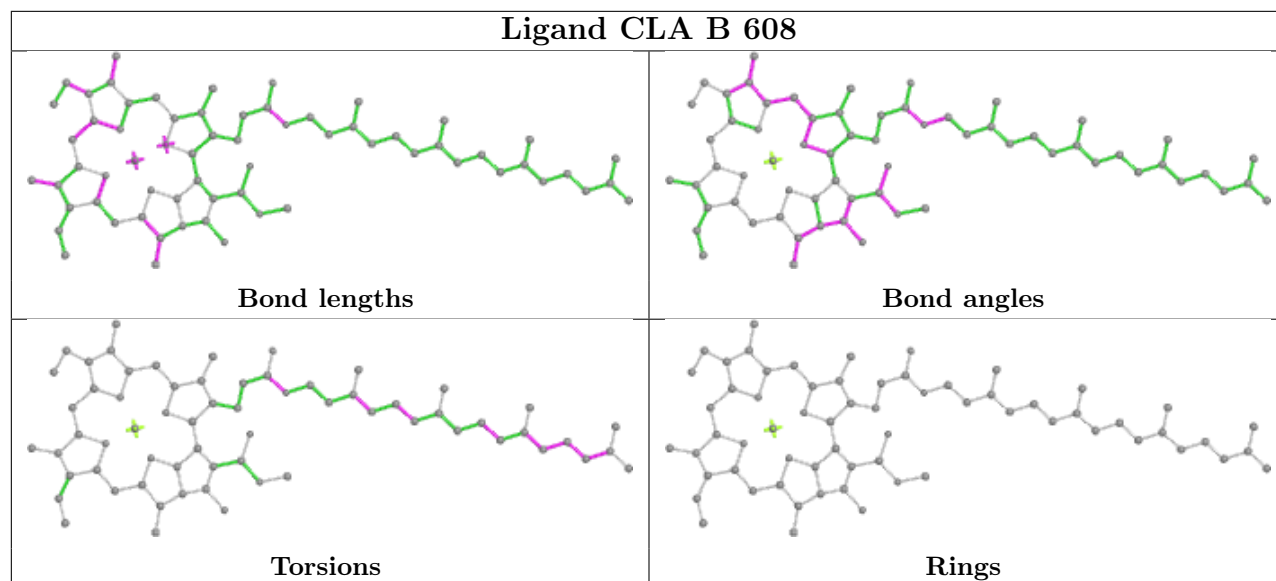
Ligand CLA a 402



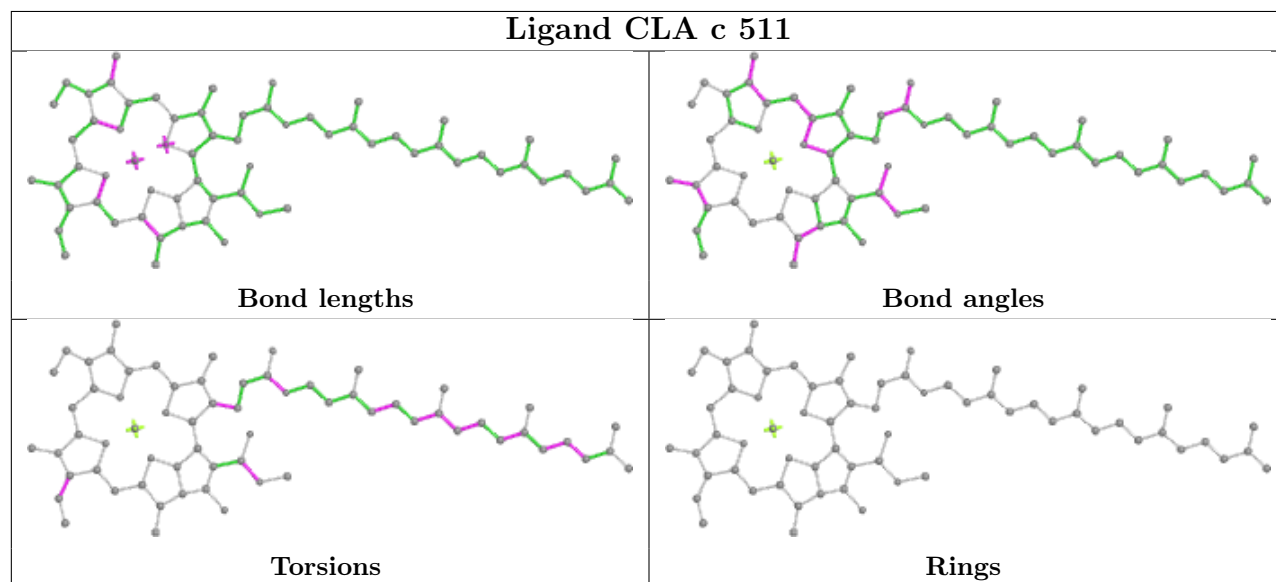
Ligand BCR a 405



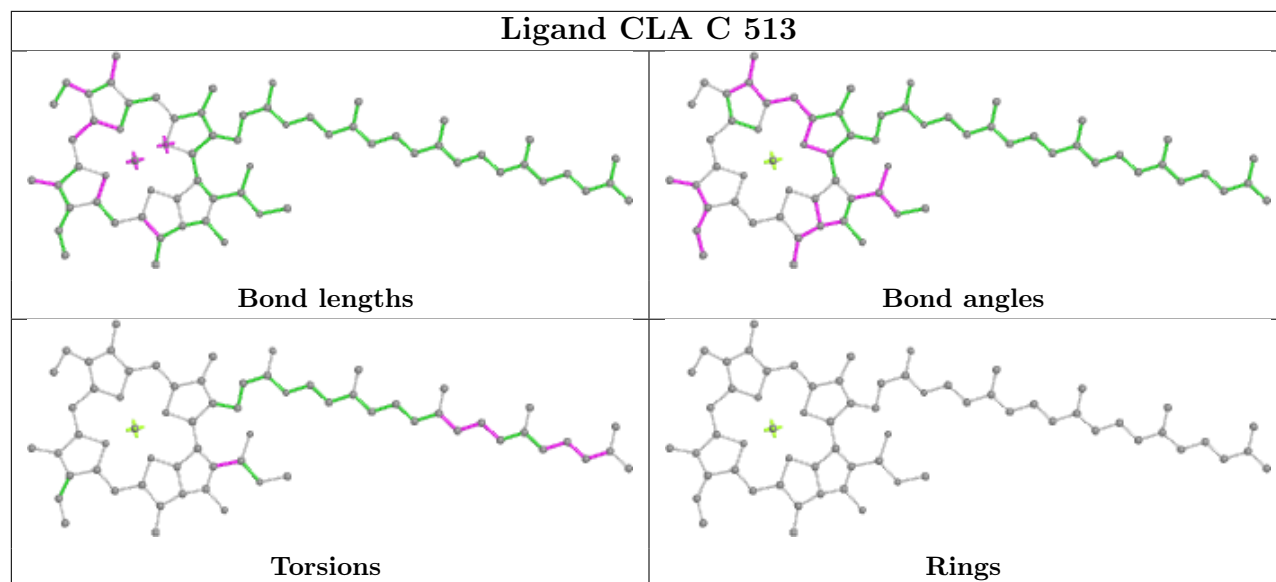
Ligand CLA B 608



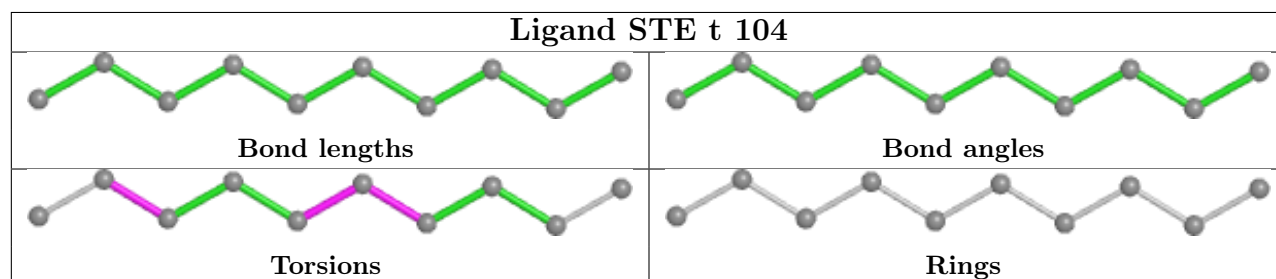
Ligand CLA c 511



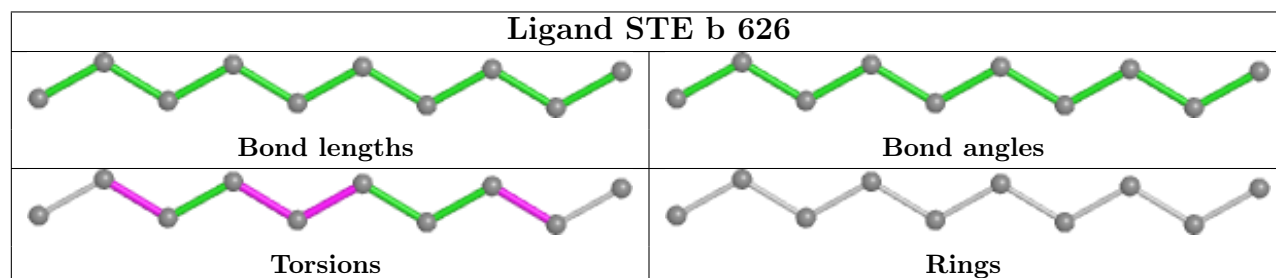
Ligand CLA C 513



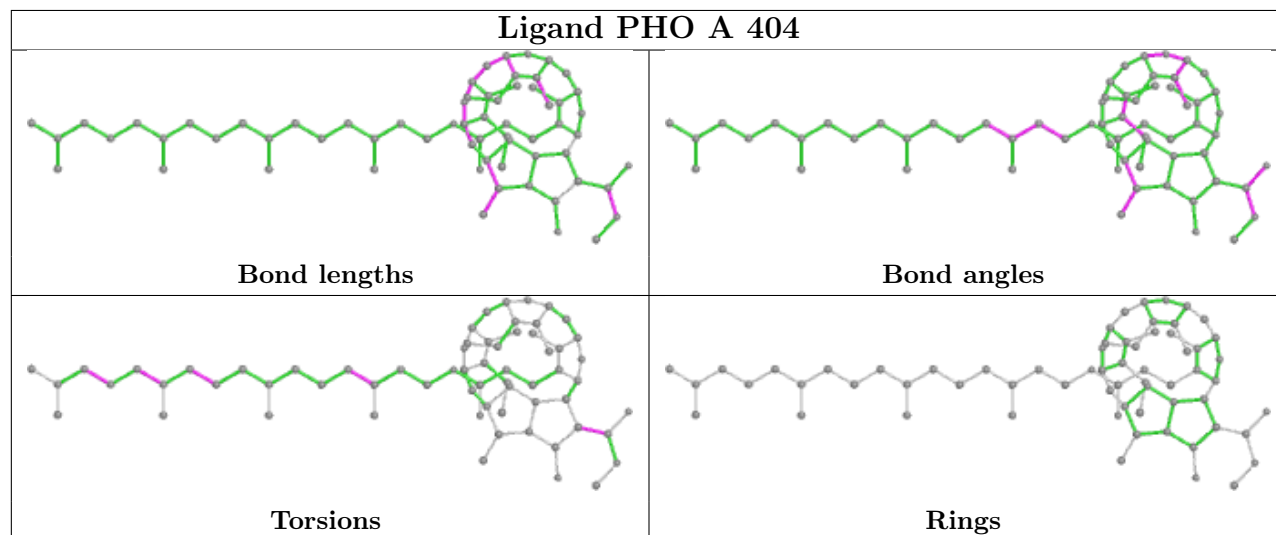
Ligand STE t 104



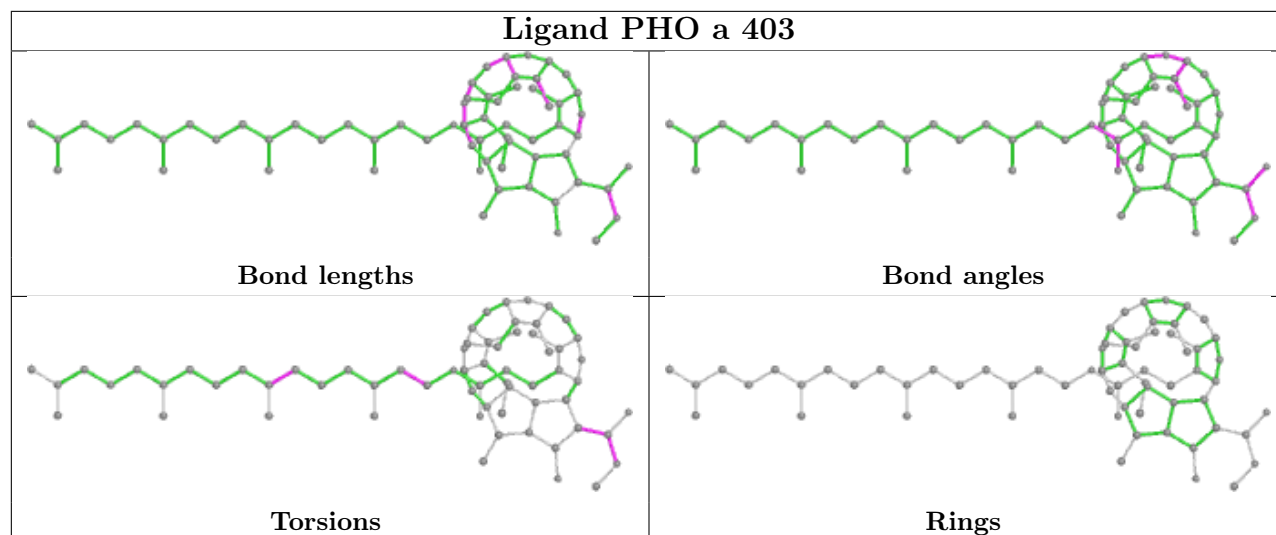
Ligand STE b 626



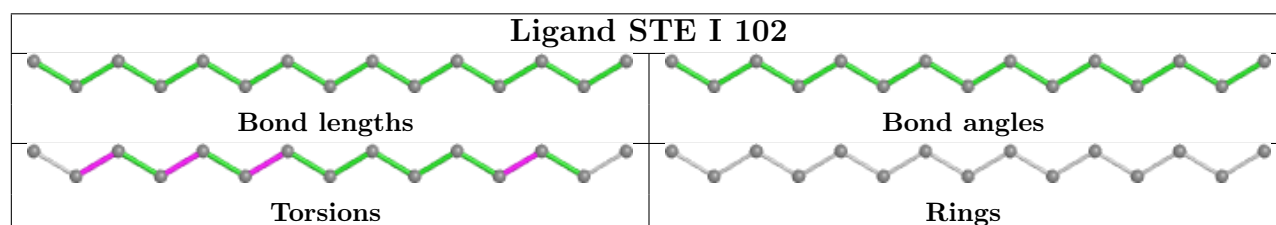
Ligand PHO A 404



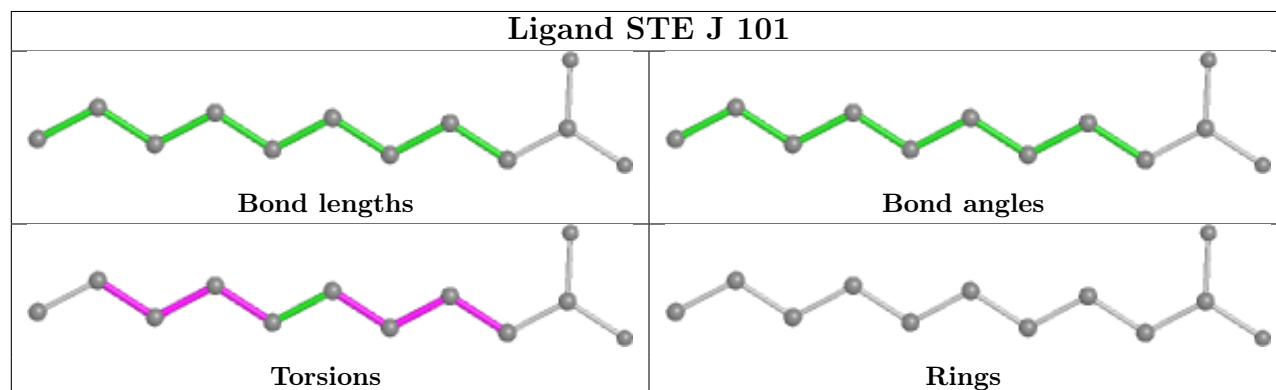
Ligand PHO a 403



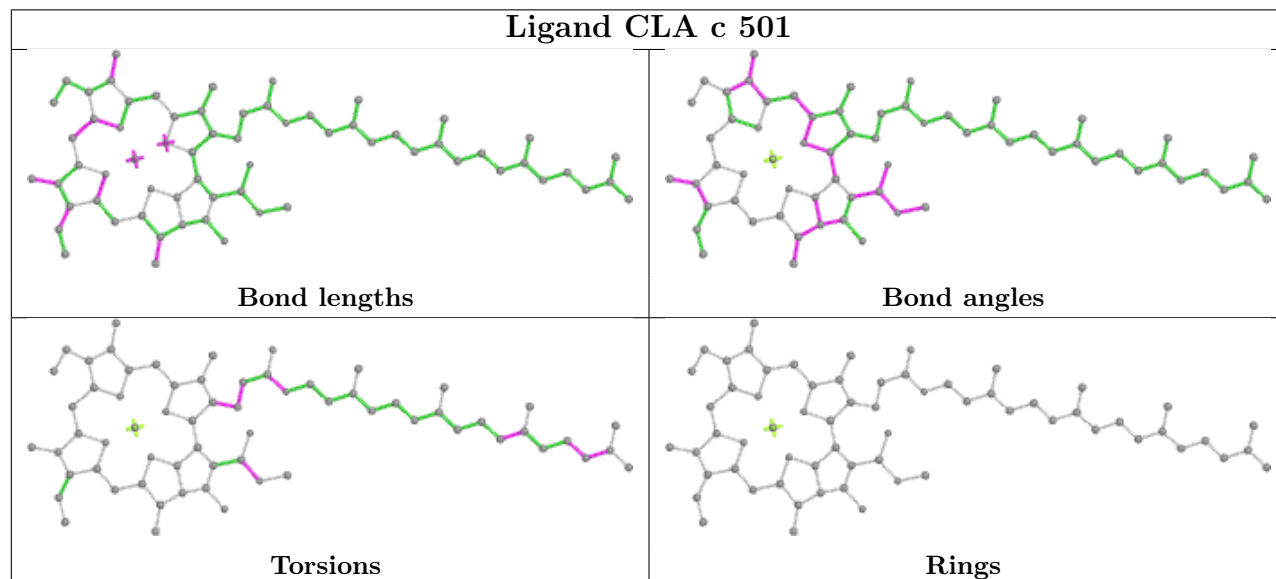
Ligand STE I 102

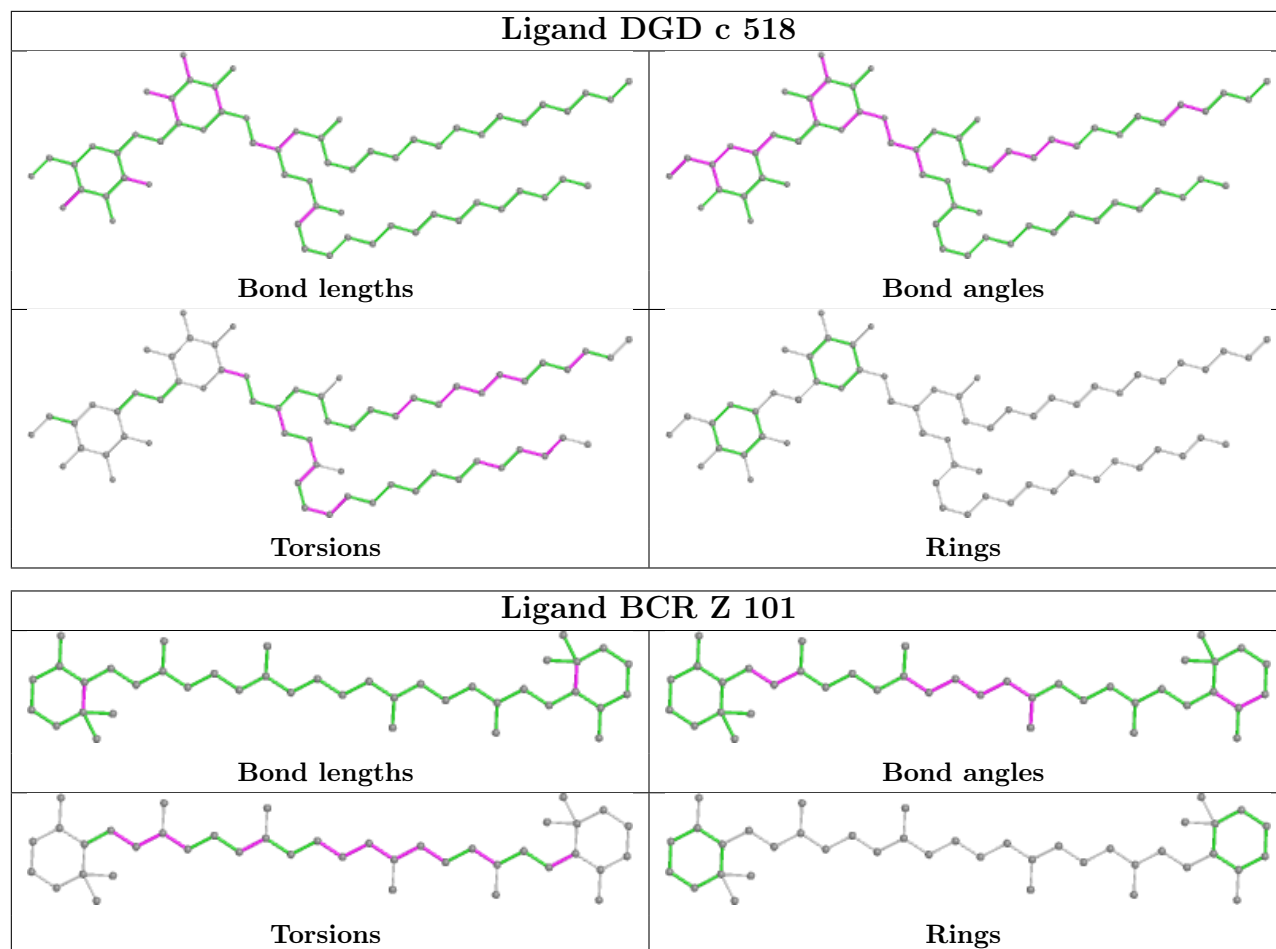


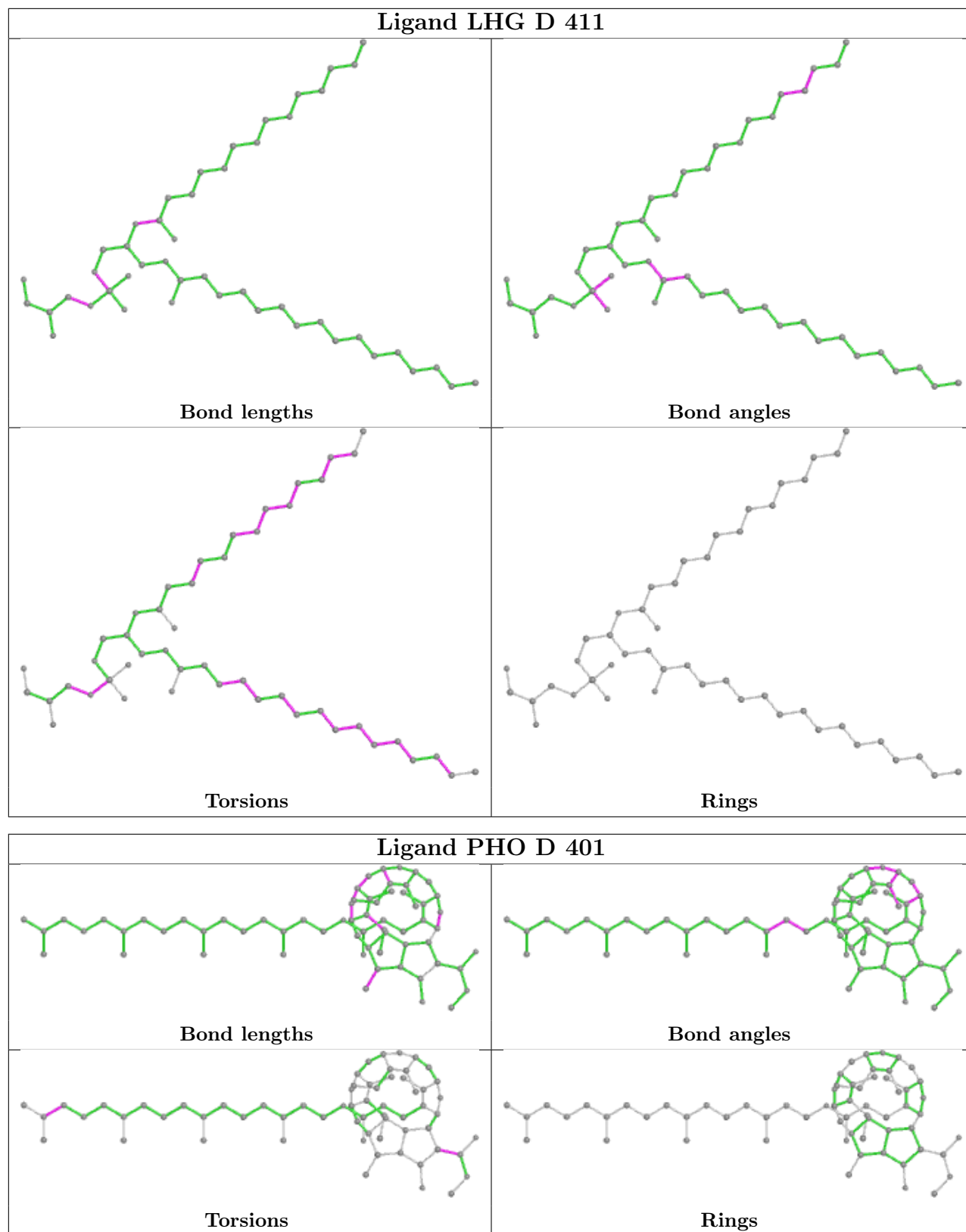
Ligand STE J 101



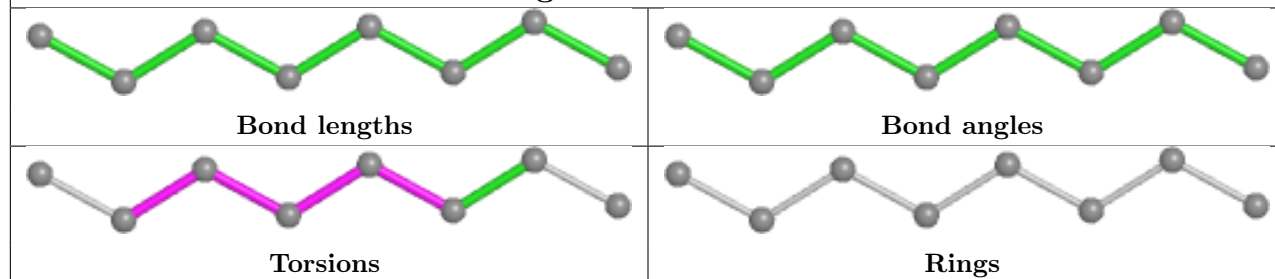
Ligand CLA c 501



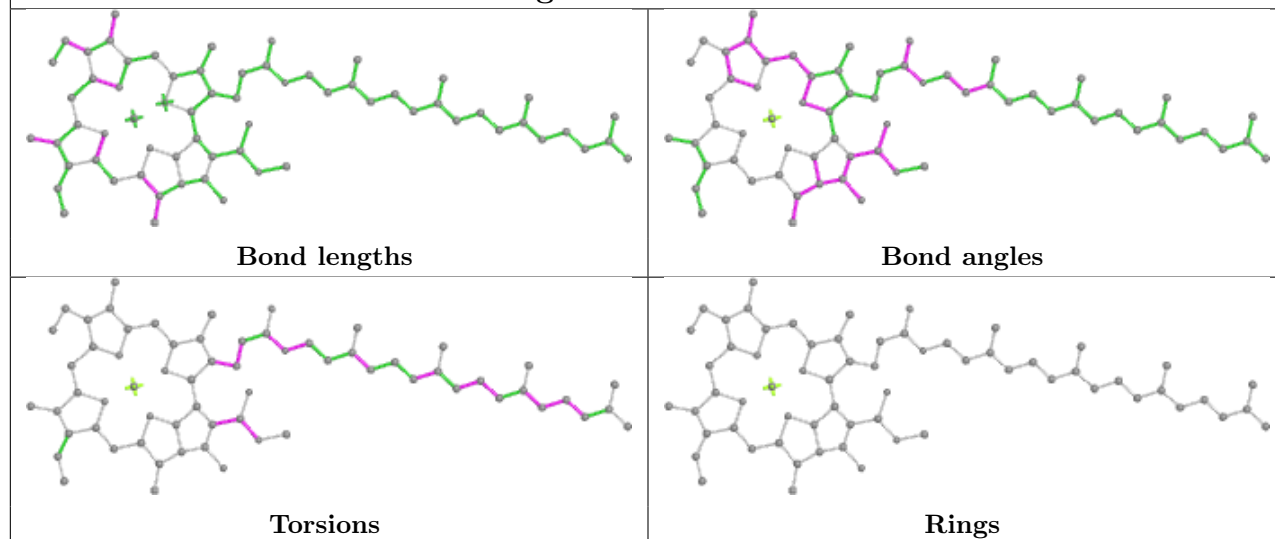




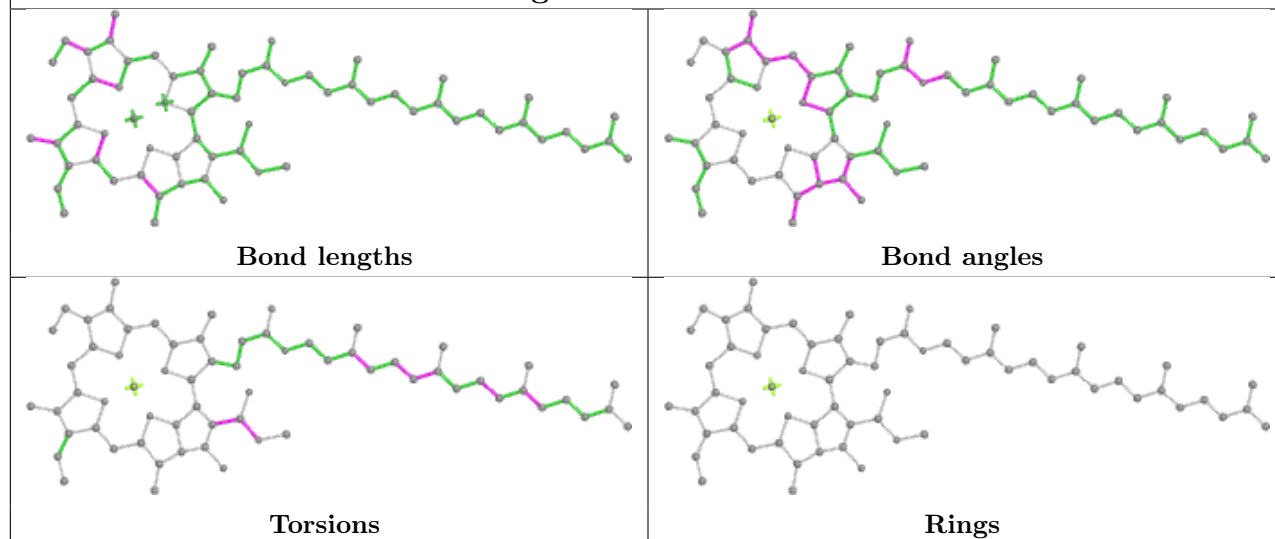
Ligand STE Z 102

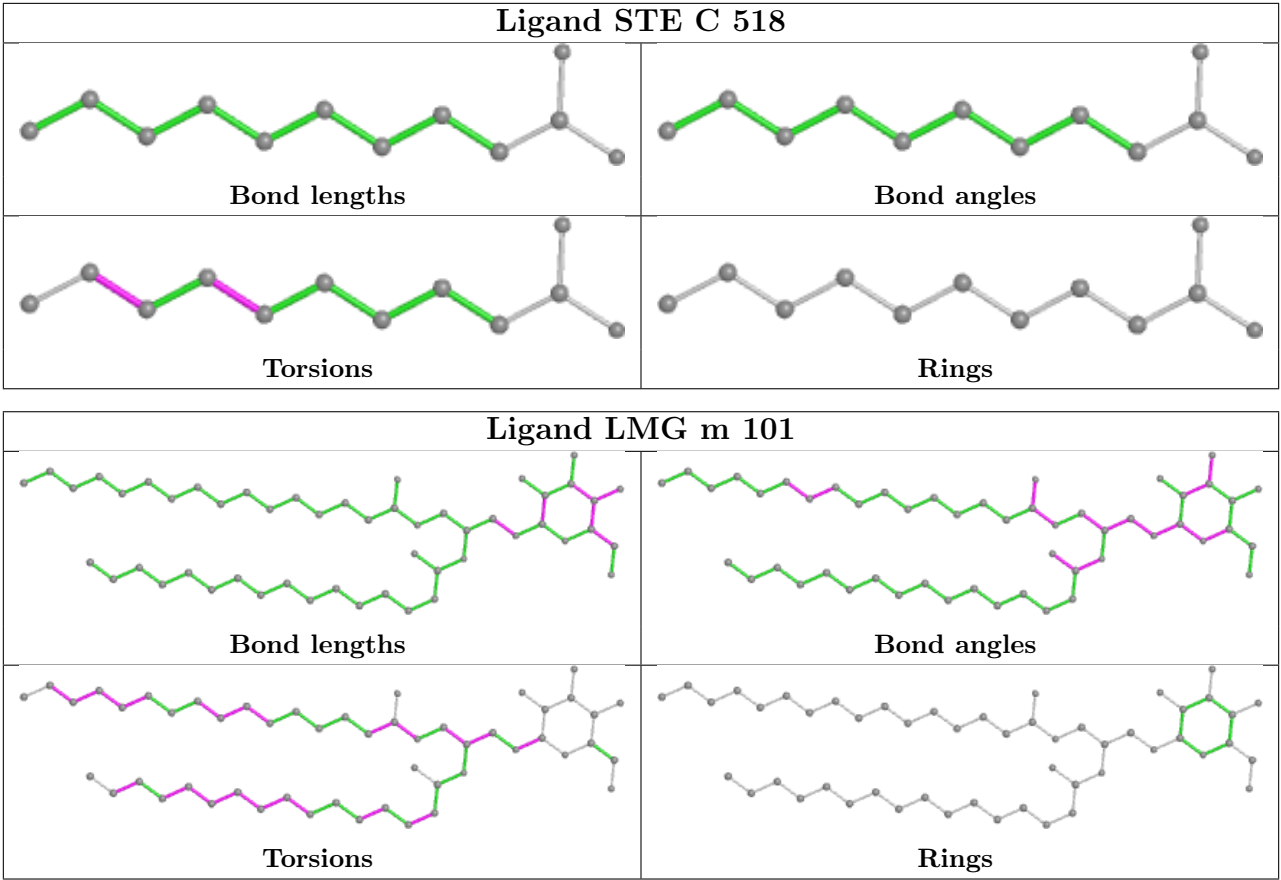


Ligand CLA c 512



Ligand CLA C 505





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	468:SER	C	469:MET	N	1.20

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%)	-0.37	4 (1%) 79 82	26, 34, 52, 83	0
1	a	334/344 (97%)	-0.40	1 (0%) 94 95	28, 36, 61, 81	0
2	B	505/510 (99%)	-0.34	6 (1%) 79 82	27, 38, 66, 87	0
2	b	505/510 (99%)	-0.18	19 (3%) 40 45	30, 41, 72, 102	0
3	C	442/461 (95%)	-0.25	11 (2%) 57 63	28, 41, 58, 80	0
3	c	451/461 (97%)	-0.16	10 (2%) 62 68	29, 45, 65, 98	0
4	D	341/352 (96%)	-0.35	1 (0%) 94 95	27, 35, 53, 78	0
4	d	341/352 (96%)	-0.24	1 (0%) 94 95	26, 39, 62, 85	0
5	E	82/84 (97%)	-0.09	2 (2%) 59 65	37, 56, 73, 84	0
5	e	82/84 (97%)	0.27	6 (7%) 15 18	43, 66, 80, 90	0
6	F	34/45 (75%)	-0.44	1 (2%) 51 57	39, 48, 65, 82	0
6	f	34/45 (75%)	-0.26	1 (2%) 51 57	46, 54, 81, 96	0
7	H	65/66 (98%)	-0.09	0 100 100	36, 45, 61, 69	0
7	h	63/66 (95%)	0.18	4 (6%) 20 24	45, 55, 67, 72	0
8	I	35/38 (92%)	-0.23	2 (5%) 23 28	37, 44, 67, 81	0
8	i	35/38 (92%)	-0.15	2 (5%) 23 28	34, 45, 72, 87	0
9	J	36/40 (90%)	-0.04	5 (13%) 2 3	39, 56, 82, 89	0
9	j	36/40 (90%)	0.21	5 (13%) 2 3	44, 59, 93, 103	0
10	K	37/46 (80%)	0.12	2 (5%) 25 31	45, 55, 70, 75	0
10	k	37/46 (80%)	-0.06	2 (5%) 25 31	53, 60, 77, 83	0
11	L	37/37 (100%)	-0.40	1 (2%) 54 60	29, 35, 64, 73	0
11	l	36/37 (97%)	-0.25	3 (8%) 11 14	31, 36, 73, 85	0
12	M	32/36 (88%)	0.03	1 (3%) 49 54	34, 39, 65, 74	0
12	m	31/36 (86%)	-0.04	0 100 100	32, 38, 57, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.02	15 (6%) 21 26	32, 47, 85, 122	0
13	o	244/272 (89%)	-0.18	12 (4%) 29 35	28, 45, 81, 127	0
14	R	28/41 (68%)	1.58	9 (32%) 0 0	65, 72, 90, 91	0
14	r	28/41 (68%)	3.58	25 (89%) 0 0	83, 99, 117, 127	0
15	T	29/32 (90%)	-0.43	1 (3%) 45 50	30, 36, 61, 81	0
15	t	29/32 (90%)	-0.36	2 (6%) 16 21	33, 37, 78, 89	0
16	U	97/134 (72%)	-0.20	2 (2%) 63 69	33, 49, 76, 95	0
16	u	97/134 (72%)	-0.39	0 100 100	37, 45, 60, 80	0
17	V	137/163 (84%)	-0.52	0 100 100	31, 46, 58, 78	0
17	v	137/163 (84%)	-0.19	3 (2%) 62 68	37, 52, 74, 86	0
18	X	38/41 (92%)	0.18	3 (7%) 12 16	44, 53, 73, 78	0
18	x	39/41 (95%)	0.28	5 (12%) 3 4	53, 62, 90, 101	0
19	Y	27/46 (58%)	1.27	11 (40%) 0 0	58, 77, 95, 102	0
19	y	30/46 (65%)	0.49	4 (13%) 3 4	67, 80, 90, 100	0
20	Z	62/62 (100%)	0.69	14 (22%) 0 1	59, 73, 113, 122	0
20	z	62/62 (100%)	0.84	12 (19%) 1 1	63, 78, 114, 121	0
All	All	5293/5700 (92%)	-0.16	208 (3%) 39 44	26, 43, 77, 127	0

All (208) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	9.3
20	Z	62	VAL	7.7
14	r	9	LEU	6.9
14	r	28	VAL	6.6
1	A	13	LEU	6.3
14	r	3	TRP	6.0
20	Z	1	MET	5.9
14	r	10	LEU	5.9
18	X	2	THR	5.9
13	O	4	THR	5.7
20	z	33	TRP	5.5
14	r	14	LEU	5.4
9	j	5	GLY	5.4
3	c	23	ALA	5.3
14	r	13	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
13	o	3	GLN	5.2
14	R	3	TRP	5.1
13	O	60	ARG	5.1
14	r	6	LEU	4.9
2	b	486	LEU	4.9
14	r	5	VAL	4.8
2	b	127	ARG	4.8
13	O	3	GLN	4.8
13	O	56	PRO	4.6
3	c	143	TYR	4.6
13	o	4	THR	4.6
2	b	495	PHE	4.6
14	r	29	LYS	4.6
5	e	79	PHE	4.5
13	o	62	GLU	4.5
20	Z	61	VAL	4.4
7	h	21	VAL	4.4
13	o	60	ARG	4.4
20	z	3	ILE	4.3
1	A	11	ALA	4.3
9	j	7	ARG	4.2
14	r	25	PRO	4.2
19	Y	40	ALA	4.1
6	f	12	SER	4.0
18	x	38	GLN	4.0
20	z	36	SER	3.9
18	x	40	SER	3.9
14	r	24	LEU	3.9
2	b	505	ARG	3.8
3	c	146	PHE	3.8
13	o	57	LYS	3.8
18	x	2	THR	3.7
14	r	8	VAL	3.7
5	E	79	PHE	3.6
14	R	21	ARG	3.6
20	Z	35	ARG	3.6
13	o	59	LYS	3.6
13	o	56	PRO	3.6
14	R	6	LEU	3.6
20	z	35	ARG	3.5
14	r	4	ARG	3.5
11	l	7	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
19	y	19	ILE	3.4
5	e	61	ARG	3.4
13	o	61	GLN	3.4
14	r	12	VAL	3.4
13	O	62	GLU	3.4
14	r	18	TRP	3.3
14	r	26	TYR	3.3
2	B	295	GLY	3.3
14	R	25	PRO	3.3
19	Y	37	PHE	3.3
2	b	502	VAL	3.3
13	O	59	LYS	3.3
19	Y	20	ALA	3.3
3	C	143	TYR	3.2
14	R	28	VAL	3.2
20	z	31	GLN	3.2
19	y	43	ARG	3.2
9	J	6	GLY	3.2
14	R	29	LYS	3.2
13	O	61	GLN	3.1
11	l	3	PRO	3.1
9	j	6	GLY	3.1
3	c	24	THR	3.1
14	r	21	ARG	3.1
5	e	82	GLN	3.0
20	Z	7	LEU	3.0
9	j	8	ILE	3.0
20	Z	42	LEU	3.0
13	o	63	ALA	2.9
15	t	29	ILE	2.9
2	b	496	TYR	2.9
13	O	32	ILE	2.8
19	Y	41	VAL	2.8
18	X	3	ILE	2.8
13	o	246	ALA	2.8
7	h	6	TRP	2.8
12	M	33	GLN	2.8
13	O	5	LEU	2.8
1	a	11	ALA	2.8
17	v	17	LYS	2.7
3	C	146	PHE	2.7
9	J	7	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
19	Y	43	ARG	2.7
8	i	36	ASP	2.7
19	Y	21	GLN	2.7
19	Y	46	LEU	2.7
9	J	5	GLY	2.7
13	O	63	ALA	2.7
14	r	11	PRO	2.7
11	L	3	PRO	2.6
13	O	55	GLU	2.6
11	l	2	GLU	2.6
14	R	2	ASP	2.6
2	b	497	GLN	2.6
3	C	57	ALA	2.6
2	b	128	THR	2.6
17	v	22	THR	2.6
13	o	5	LEU	2.6
10	K	17	ILE	2.6
13	O	246	ALA	2.6
19	Y	45	ASN	2.6
20	z	59	PHE	2.6
5	e	60	GLN	2.6
14	r	19	ALA	2.6
20	Z	41	PHE	2.6
19	Y	25	ILE	2.6
20	Z	33	TRP	2.5
2	B	127	ARG	2.5
7	h	10	ILE	2.5
20	z	60	PHE	2.5
15	T	30	THR	2.5
20	z	1	MET	2.5
19	Y	42	ARG	2.5
4	D	227	GLU	2.5
14	r	7	VAL	2.5
3	C	62	PHE	2.5
14	r	16	ALA	2.5
14	R	14	LEU	2.5
2	b	489	GLU	2.4
14	r	2	ASP	2.4
3	C	60	ILE	2.4
2	b	293	ALA	2.4
20	Z	38	GLN	2.4
7	h	20	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
14	R	26	TYR	2.4
14	r	23	ILE	2.4
2	b	490	GLN	2.4
13	O	36	GLN	2.4
19	y	34	MET	2.4
2	b	491	VAL	2.4
8	I	34	ARG	2.4
9	j	10	LEU	2.4
2	B	293	ALA	2.4
18	x	34	ILE	2.3
16	U	8	GLU	2.3
2	b	295	GLY	2.3
2	b	161	LEU	2.3
3	C	119	LEU	2.3
9	J	8	ILE	2.3
9	J	9	PRO	2.3
2	b	289	GLN	2.3
1	A	16	ARG	2.3
8	i	35	LYS	2.3
16	U	67	LEU	2.3
20	Z	31	GLN	2.3
3	C	122	SER	2.3
18	X	33	GLN	2.3
20	Z	3	ILE	2.3
2	b	494	GLY	2.2
3	c	25	ASN	2.2
3	c	57	ALA	2.2
18	x	39	ARG	2.2
17	v	21	LEU	2.2
2	b	374	ASN	2.2
3	c	145	SER	2.2
6	F	12	SER	2.2
2	b	506	ARG	2.2
3	c	147	PHE	2.2
8	I	36	ASP	2.2
20	Z	34	ASP	2.2
3	c	262	ARG	2.2
15	t	28	ARG	2.2
2	b	492	GLU	2.2
3	C	61	VAL	2.2
5	e	74	GLN	2.2
2	B	505	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
20	z	30	PRO	2.2
14	r	27	ALA	2.1
5	e	71	GLU	2.1
1	A	12	ASN	2.1
14	r	22	ASN	2.1
13	O	87	VAL	2.1
5	E	84	LYS	2.1
19	Y	22	LEU	2.1
3	c	123	ALA	2.1
10	k	10	LYS	2.1
19	y	20	ALA	2.1
20	z	10	ALA	2.1
2	B	502	VAL	2.1
20	Z	60	PHE	2.1
3	C	66	ALA	2.1
10	k	17	ILE	2.0
20	z	42	LEU	2.0
13	O	57	LYS	2.0
3	C	65	GLY	2.0
3	C	275	SER	2.0
4	d	227[A]	GLU	2.0
20	z	61	VAL	2.0
10	K	10	LYS	2.0
2	B	486	LEU	2.0
20	Z	37	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	FME	t	1	10/11	0.92	0.11	34,54,68,69	0
15	FME	T	1	10/11	0.93	0.13	31,58,77,77	0
8	FME	I	1	10/11	0.95	0.19	46,58,68,81	0
12	FME	m	1	10/11	0.96	0.12	44,53,72,80	0
12	FME	M	1	10/11	0.97	0.12	45,56,70,76	0
8	FME	i	1	10/11	0.97	0.16	42,55,68,74	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
32	STE	a	412	12/20	0.72	0.36	47,74,84,88	0
32	STE	b	625	20/20	0.76	0.28	42,67,89,95	0
32	STE	x	102	20/20	0.76	0.25	50,66,80,86	0
32	STE	B	624	18/20	0.78	0.22	52,72,90,94	0
32	STE	c	520	20/20	0.79	0.26	42,64,85,89	0
32	STE	B	625	16/20	0.79	0.29	40,64,82,85	0
31	BCR	H	101	40/40	0.81	0.17	35,52,66,74	0
26	LMG	c	521	48/55	0.81	0.23	34,77,102,106	0
28	LHG	e	101	42/49	0.81	0.27	62,89,116,133	0
32	STE	R	101	12/20	0.81	0.31	60,82,101,105	0
32	STE	M	103	10/20	0.82	0.19	40,56,67,71	0
32	STE	B	620	17/20	0.83	0.21	37,60,76,76	0
28	LHG	A	411	49/49	0.83	0.23	45,84,111,116	0
26	LMG	D	412	33/55	0.83	0.20	32,62,92,94	0
32	STE	I	102	15/20	0.83	0.16	42,58,80,82	0
22	CLA	b	601	65/65	0.83	0.19	48,73,101,104	0
22	CLA	c	512	65/65	0.84	0.17	42,63,90,104	0
32	STE	a	413	15/20	0.84	0.20	36,63,77,86	0
32	STE	b	621	20/20	0.84	0.25	42,60,79,84	0
32	STE	J	101	12/20	0.84	0.16	49,65,72,74	0
26	LMG	B	626	55/55	0.84	0.18	40,64,84,98	0
32	STE	B	627	12/20	0.84	0.45	42,68,79,82	0
26	LMG	b	622	55/55	0.85	0.27	49,78,102,109	0
22	CLA	C	512	65/65	0.85	0.19	39,61,93,102	0
32	STE	b	623	16/20	0.85	0.17	53,73,83,90	0
32	STE	b	624	15/20	0.85	0.20	50,66,87,92	0
27	SQD	A	412	39/54	0.85	0.20	45,66,96,103	0
32	STE	b	627	14/20	0.85	0.36	54,77,98,104	0
31	BCR	x	101	40/40	0.85	0.16	37,58,76,80	0
32	STE	H	103	18/20	0.85	0.34	52,77,88,89	0
32	STE	L	103	12/20	0.86	0.20	48,66,88,88	0
25	PL9	a	409	55/55	0.86	0.23	41,72,95,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	STE	C	518	12/20	0.86	0.17	39,57,68,69	0
22	CLA	c	513	65/65	0.86	0.21	47,77,104,108	0
29	DGD	A	413	66/66	0.86	0.15	47,64,83,89	0
32	STE	l	102	18/20	0.86	0.17	38,52,75,78	0
27	SQD	t	102	36/54	0.86	0.18	31,66,91,95	0
22	CLA	B	601	65/65	0.87	0.17	40,70,93,104	0
32	STE	C	519	16/20	0.87	0.15	47,62,75,75	0
25	PL9	A	408	55/55	0.87	0.23	32,67,92,100	0
27	SQD	L	101	49/54	0.87	0.16	40,66,100,105	0
32	STE	c	523	12/20	0.87	0.24	55,74,88,90	0
32	STE	d	412	20/20	0.87	0.18	40,68,83,90	0
22	CLA	C	513	65/65	0.87	0.21	41,63,99,108	0
31	BCR	K	101	40/40	0.87	0.15	40,57,75,78	0
32	STE	b	620	16/20	0.88	0.22	40,55,81,91	0
26	LMG	c	519	37/55	0.89	0.18	45,69,89,99	0
22	CLA	c	502	65/65	0.89	0.18	32,48,68,72	0
26	LMG	c	522	49/55	0.89	0.16	28,62,92,100	0
26	LMG	m	101	51/55	0.89	0.15	39,58,78,87	0
22	CLA	c	508	64/65	0.89	0.17	37,55,93,115	0
32	STE	b	626	10/20	0.89	0.33	49,60,69,71	0
31	BCR	k	101	40/40	0.89	0.14	46,68,84,90	0
31	BCR	k	102	40/40	0.89	0.21	46,63,76,78	0
27	SQD	B	622	54/54	0.89	0.18	38,65,89,98	0
26	LMG	Y	101	48/55	0.89	0.19	52,75,93,102	0
27	SQD	f	102	41/54	0.89	0.20	62,87,107,118	0
22	CLA	a	404	65/65	0.89	0.15	24,44,87,96	0
31	BCR	d	406	40/40	0.90	0.14	35,61,97,109	0
32	STE	B	623	12/20	0.90	0.11	38,60,72,73	0
22	CLA	D	405	65/65	0.90	0.15	26,50,128,138	0
32	STE	X	101	20/20	0.90	0.18	39,56,75,81	0
26	LMG	A	409	48/55	0.90	0.16	34,63,79,96	0
32	STE	t	104	10/20	0.90	0.26	43,60,72,77	0
26	LMG	B	621	28/55	0.90	0.16	36,52,67,73	0
26	LMG	d	410	44/55	0.91	0.16	41,61,89,106	0
32	STE	C	520	12/20	0.91	0.12	36,47,59,66	0
26	LMG	M	101	51/55	0.91	0.13	36,54,76,86	0
32	STE	j	101	12/20	0.91	0.13	50,64,71,72	0
26	LMG	D	408	51/55	0.91	0.20	32,65,89,99	0
22	CLA	d	405	65/65	0.91	0.16	32,54,94,107	0
31	BCR	c	514	40/40	0.91	0.16	45,67,82,87	0
22	CLA	C	507	65/65	0.92	0.15	26,46,66,68	0
32	STE	Z	102	8/20	0.92	0.13	43,65,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
29	DGD	c	518	62/66	0.92	0.17	35,62,87,98	0
31	BCR	C	514	40/40	0.92	0.14	29,46,59,77	0
27	SQD	a	411	54/54	0.92	0.16	47,69,98,106	0
22	CLA	b	616	60/65	0.92	0.16	31,49,92,99	0
22	CLA	C	508	65/65	0.92	0.13	30,49,107,117	0
22	CLA	c	506	65/65	0.92	0.14	35,57,100,103	0
22	CLA	B	616	60/65	0.92	0.16	23,43,89,97	0
22	CLA	b	609	65/65	0.93	0.14	31,52,71,79	0
31	BCR	B	619	40/40	0.93	0.12	29,49,73,84	0
22	CLA	b	615	65/65	0.93	0.14	27,46,66,74	0
27	SQD	D	409	36/54	0.93	0.17	51,77,96,105	0
22	CLA	B	606	65/65	0.93	0.13	30,45,78,92	0
31	BCR	Z	101	40/40	0.93	0.13	42,64,78,82	0
22	CLA	C	502	65/65	0.93	0.14	28,47,68,78	0
22	CLA	B	615	65/65	0.93	0.14	27,42,67,84	0
22	CLA	b	602	65/65	0.93	0.17	33,47,65,71	0
32	STE	M	102	15/20	0.93	0.12	38,53,63,66	0
32	STE	d	411	17/20	0.93	0.13	48,63,70,78	0
22	CLA	c	509	65/65	0.93	0.20	30,53,72,80	0
22	CLA	c	510	65/65	0.93	0.15	35,50,66,84	0
22	CLA	c	511	65/65	0.93	0.16	43,63,80,86	0
32	STE	t	103	14/20	0.93	0.15	43,57,69,70	0
29	DGD	C	516	62/66	0.93	0.14	31,54,103,124	0
29	DGD	c	517	62/66	0.93	0.14	38,60,95,104	0
36	NA	V	202	1/1	0.93	0.18	60,60,60,60	0
22	CLA	B	602	65/65	0.94	0.17	26,43,63,67	0
29	DGD	C	517	62/66	0.94	0.13	31,53,79,87	0
29	DGD	H	102	62/66	0.94	0.12	33,51,66,72	0
22	CLA	C	509	65/65	0.94	0.18	30,50,68,77	0
22	CLA	b	604	65/65	0.94	0.14	26,44,80,95	0
29	DGD	h	101	62/66	0.94	0.14	34,52,67,70	0
31	BCR	B	617	40/40	0.94	0.12	30,45,64,65	0
31	BCR	B	618	40/40	0.94	0.10	29,45,60,67	0
22	CLA	b	606	65/65	0.94	0.12	28,46,80,92	0
22	CLA	C	511	65/65	0.94	0.14	32,59,76,80	0
31	BCR	D	406	40/40	0.94	0.11	34,51,88,99	0
22	CLA	b	613	65/65	0.94	0.17	23,41,82,97	0
22	CLA	d	401	65/65	0.94	0.15	28,47,105,111	0
31	BCR	K	102	40/40	0.94	0.16	39,58,71,71	0
27	SQD	A	410	52/54	0.94	0.16	37,66,96,101	0
31	BCR	a	405	40/40	0.94	0.11	24,39,58,59	0
31	BCR	b	617	40/40	0.94	0.13	32,48,65,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	BCR	b	619	40/40	0.94	0.13	30,55,81,85	0
22	CLA	b	614	65/65	0.94	0.15	25,43,80,87	0
31	BCR	c	515	40/40	0.94	0.14	33,53,70,76	0
22	CLA	B	614	65/65	0.94	0.17	26,46,80,96	0
25	PL9	D	407	55/55	0.94	0.12	26,39,54,62	0
22	CLA	C	505	65/65	0.94	0.16	26,47,73,76	0
22	CLA	C	506	65/65	0.94	0.13	30,50,89,98	0
22	CLA	c	503	65/65	0.94	0.16	34,49,61,67	0
22	CLA	c	504	60/65	0.94	0.12	35,51,84,100	0
22	CLA	c	505	65/65	0.94	0.17	31,46,72,76	0
22	CLA	B	604	65/65	0.94	0.14	25,40,87,96	0
22	CLA	c	507	65/65	0.94	0.14	31,50,65,78	0
29	DGD	C	515	62/66	0.94	0.13	27,47,83,98	0
22	CLA	b	610	65/65	0.95	0.18	28,43,58,68	0
22	CLA	b	611	65/65	0.95	0.14	24,41,57,66	0
22	CLA	b	612	65/65	0.95	0.17	27,41,52,54	0
22	CLA	d	403	65/65	0.95	0.14	23,41,64,74	0
22	CLA	d	404	65/65	0.95	0.13	22,37,52,55	0
22	CLA	C	503	65/65	0.95	0.14	31,47,57,61	0
31	BCR	T	101	40/40	0.95	0.10	32,46,58,65	0
23	PHO	a	403	64/64	0.95	0.14	23,36,44,47	0
22	CLA	C	504	59/65	0.95	0.13	32,48,87,92	0
22	CLA	D	403	65/65	0.95	0.12	22,36,54,66	0
31	BCR	b	618	40/40	0.95	0.10	29,44,60,62	0
22	CLA	D	404	65/65	0.95	0.12	23,35,56,65	0
25	PL9	d	407	55/55	0.95	0.11	24,40,53,63	0
28	LHG	a	410	49/49	0.95	0.14	39,57,79,91	0
28	LHG	d	409	39/49	0.95	0.12	32,52,69,75	0
22	CLA	c	501	65/65	0.95	0.14	32,49,65,71	0
22	CLA	B	613	65/65	0.95	0.16	22,40,73,81	0
22	CLA	B	603	65/65	0.95	0.16	23,39,62,68	0
22	CLA	A	403	65/65	0.95	0.15	25,41,95,103	0
22	CLA	A	405	54/65	0.95	0.12	22,39,70,82	0
22	CLA	C	501	65/65	0.95	0.12	26,42,59,65	0
29	DGD	c	516	62/66	0.95	0.11	30,47,80,87	0
22	CLA	b	605	65/65	0.95	0.14	25,38,56,62	0
22	CLA	C	510	65/65	0.95	0.14	29,48,65,73	0
22	CLA	b	607	65/65	0.95	0.13	24,41,81,86	0
22	CLA	b	608	65/65	0.95	0.15	31,48,71,77	0
22	CLA	B	609	65/65	0.95	0.12	28,43,61,65	0
23	PHO	A	404	64/64	0.96	0.12	17,35,45,49	0
23	PHO	D	401	64/64	0.96	0.13	26,40,50,54	0

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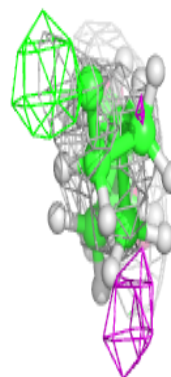
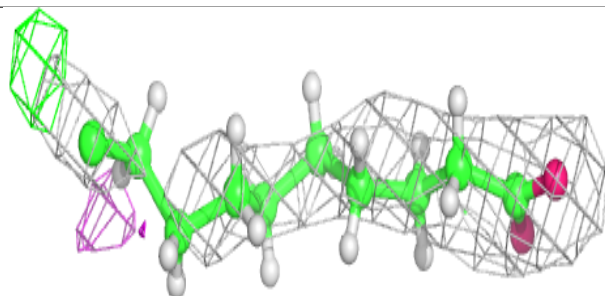
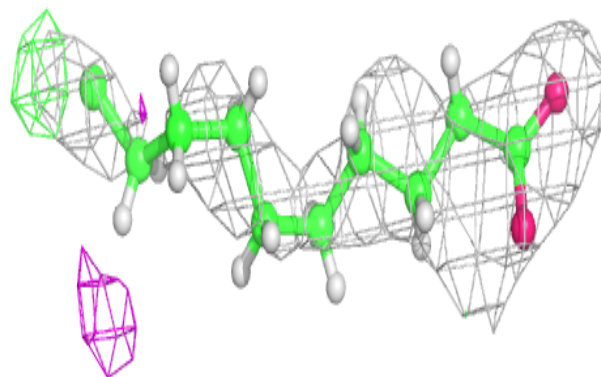
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	B	611	65/65	0.96	0.15	20,36,53,58	0
23	PHO	d	402	64/64	0.96	0.12	28,43,55,68	0
22	CLA	b	603	65/65	0.96	0.15	24,42,74,90	0
22	CLA	B	612	65/65	0.96	0.15	23,36,50,60	0
22	CLA	A	402	65/65	0.96	0.12	20,33,48,57	0
22	CLA	B	608	65/65	0.96	0.13	27,43,64,69	0
28	LHG	D	410	49/49	0.96	0.11	31,46,59,66	0
28	LHG	D	411	47/49	0.96	0.12	28,53,83,89	0
28	LHG	D	413	49/49	0.96	0.13	32,47,74,88	0
22	CLA	a	402	65/65	0.96	0.12	23,36,50,58	0
22	CLA	B	605	65/65	0.96	0.15	21,38,53,60	0
31	BCR	t	101	40/40	0.96	0.10	27,44,59,62	0
22	CLA	B	610	65/65	0.96	0.14	24,38,49,60	0
28	LHG	l	101	49/49	0.96	0.12	34,49,63,70	0
33	BCT	a	408	4/4	0.96	0.16	34,44,53,64	0
34	HEM	F	101	43/43	0.96	0.12	36,54,73,75	0
34	HEM	f	101	43/43	0.96	0.14	43,64,91,99	0
31	BCR	I	101	40/40	0.96	0.09	27,40,50,54	0
28	LHG	L	102	49/49	0.97	0.10	30,45,63,73	0
24	CL	A	407	1/1	0.97	0.08	37,37,37,37	0
28	LHG	d	408	49/49	0.97	0.11	29,47,61,72	0
35	HEC	V	201	43/43	0.97	0.13	24,39,48,49	0
35	HEC	v	201	43/43	0.97	0.13	29,44,55,61	0
22	CLA	B	607	65/65	0.97	0.12	19,40,81,87	0
30	OEX	A	414	10/10	0.98	0.15	27,36,39,39	0
33	BCT	D	402	4/4	0.98	0.17	28,35,45,54	0
24	CL	a	407	1/1	0.99	0.05	34,34,34,34	0
30	OEX	a	414	10/10	0.99	0.14	29,35,39,44	0
21	FE2	a	401	1/1	0.99	0.07	36,36,36,36	0
24	CL	A	406	1/1	0.99	0.08	36,36,36,36	0
21	FE2	A	401	1/1	0.99	0.11	31,31,31,31	0
24	CL	a	406	1/1	0.99	0.06	33,33,33,33	0

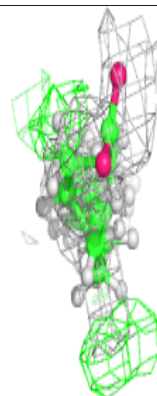
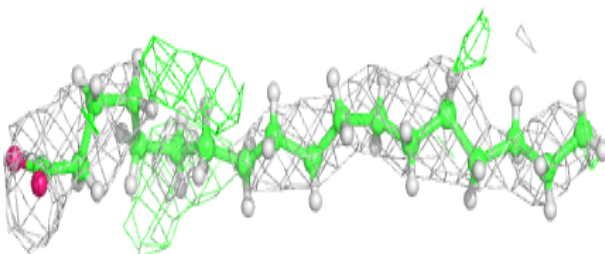
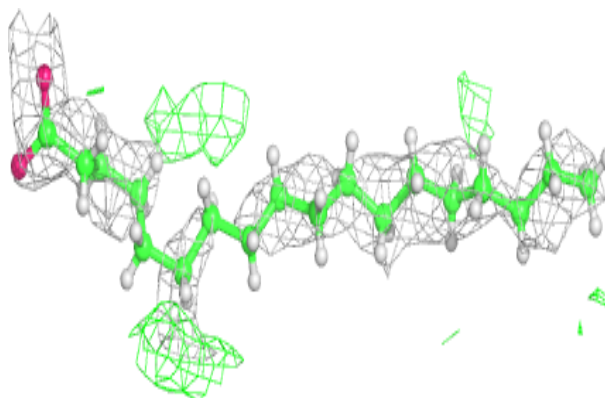
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around STE a 412:

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

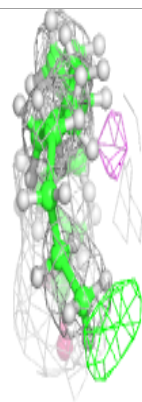
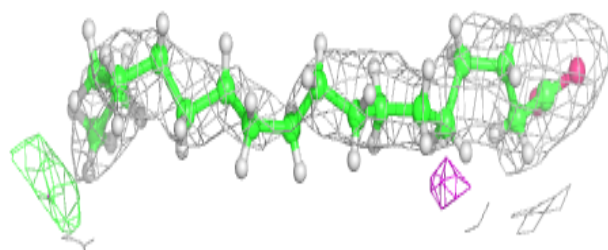
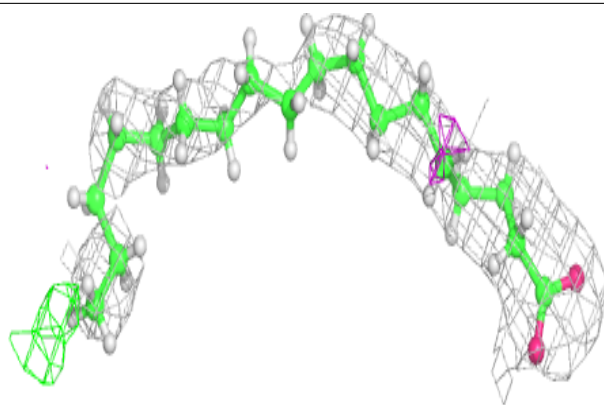
**Electron density around STE b 625:**

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

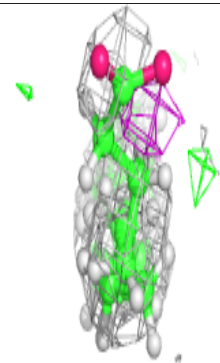
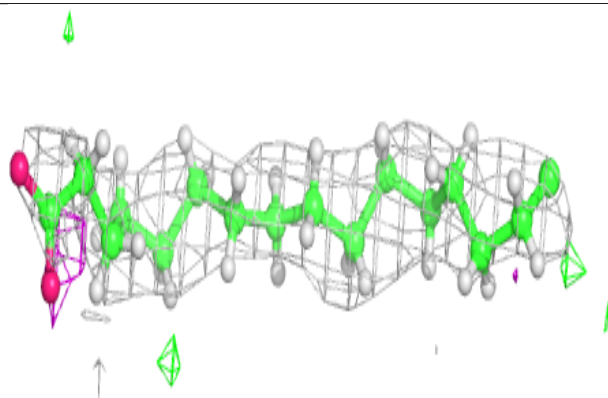
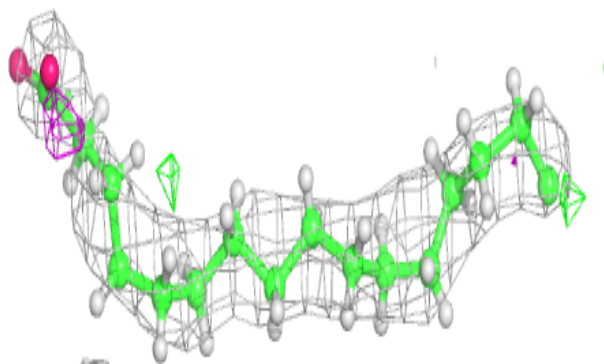


Electron density around STE x 102:

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

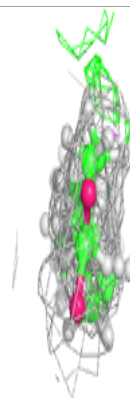
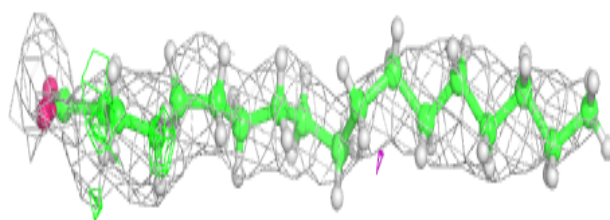
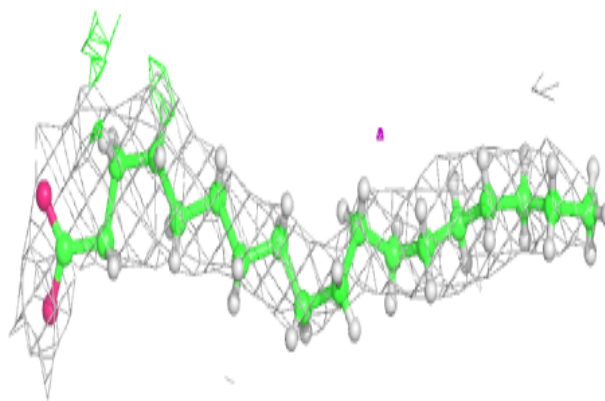
**Electron density around STE B 624:**

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

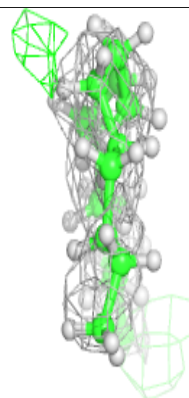
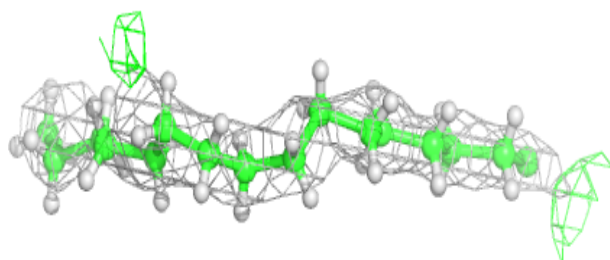
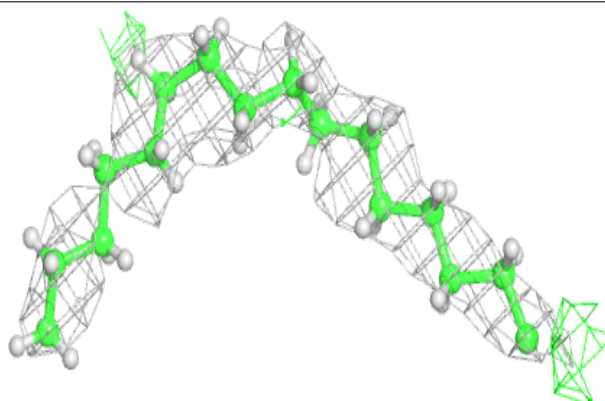


Electron density around STE c 520:

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

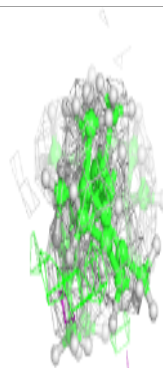
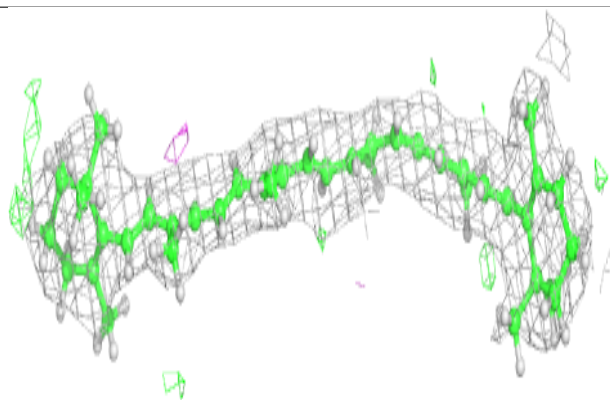
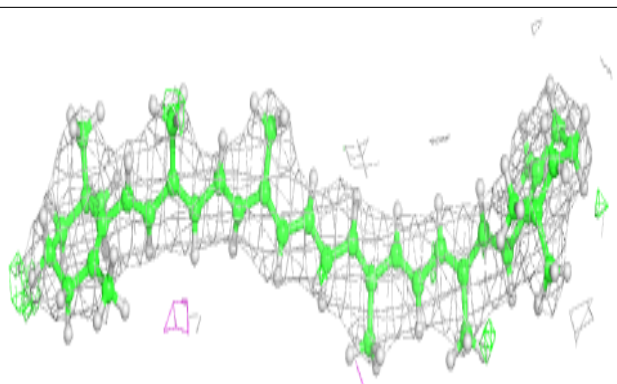
**Electron density around STE B 625:**

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

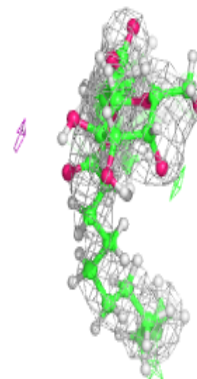
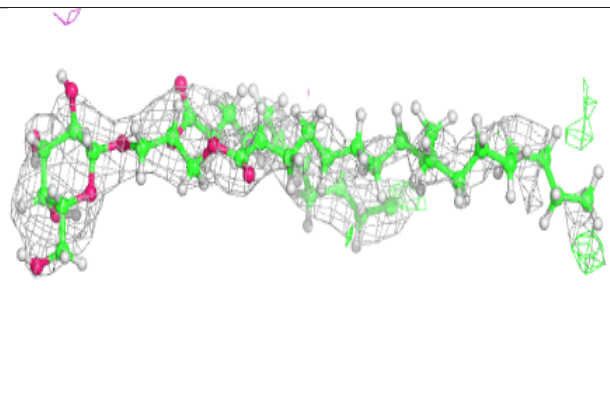
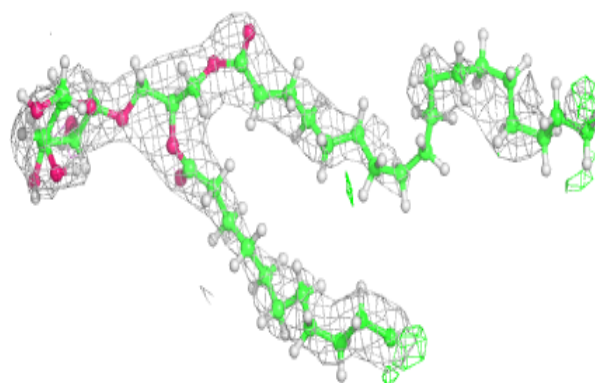


Electron density around BCR H 101:

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

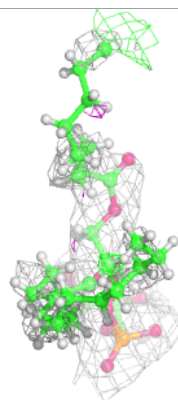
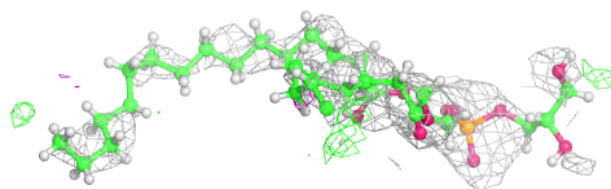
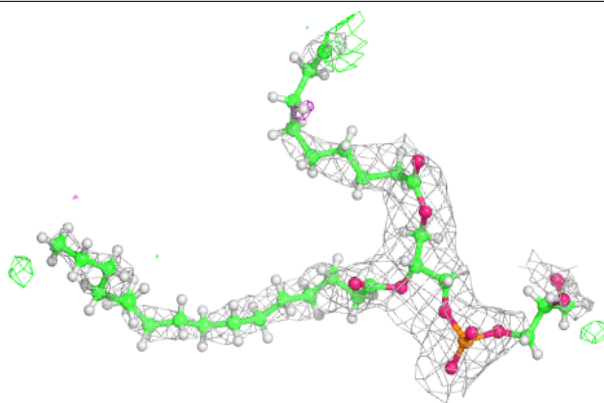
**Electron density around LMG c 521:**

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

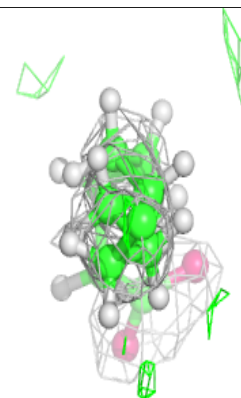
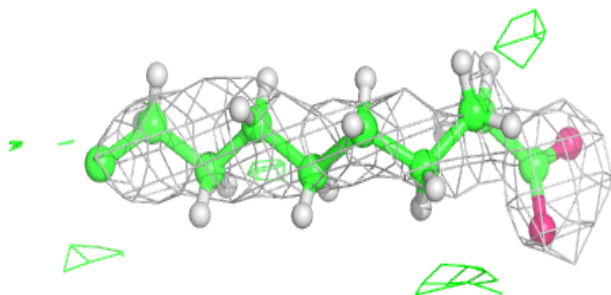
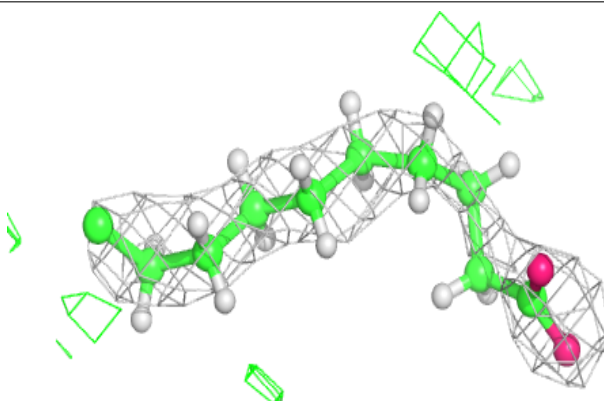


Electron density around LHG e 101:

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

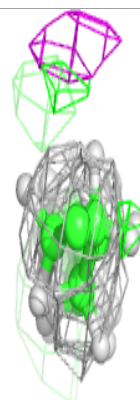
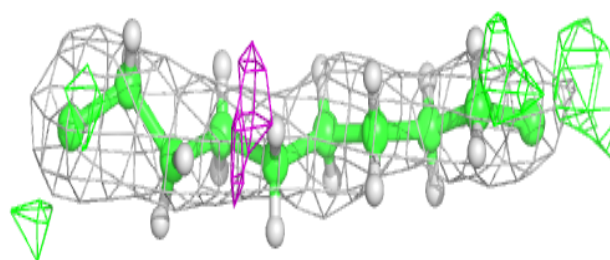
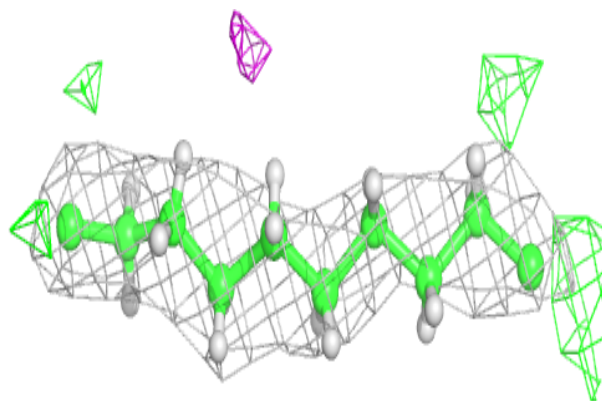
**Electron density around STE R 101:**

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

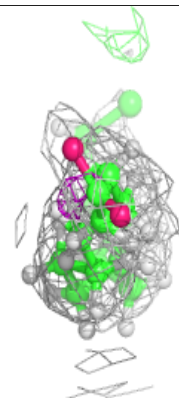
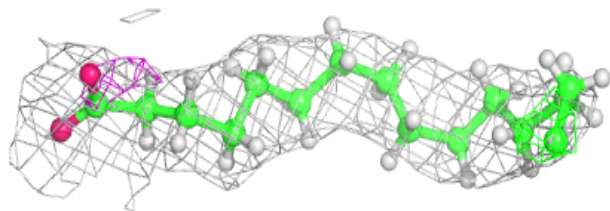
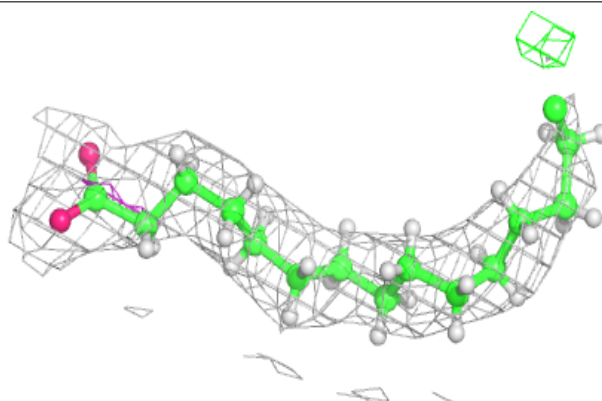


Electron density around STE M 103:

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

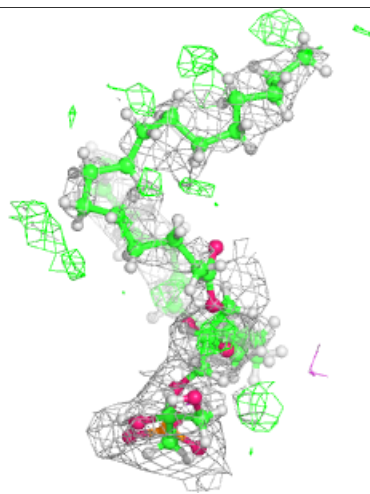
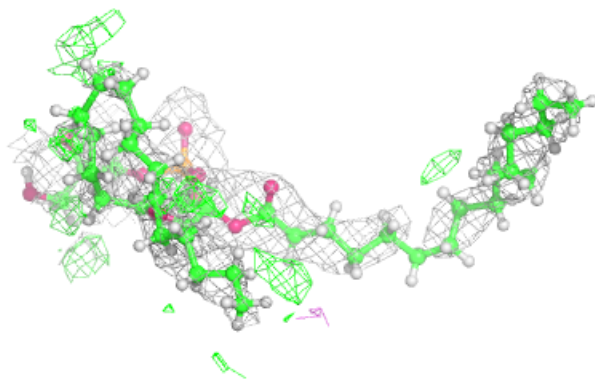
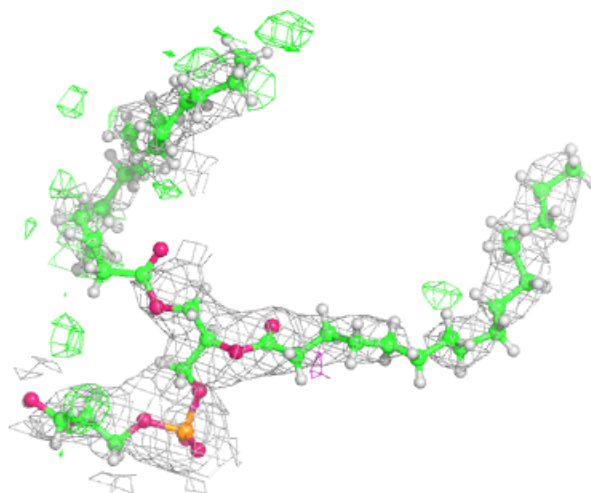
**Electron density around STE B 620:**

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



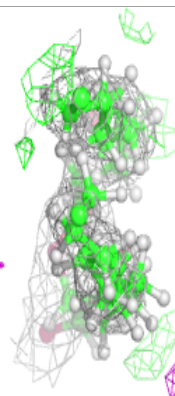
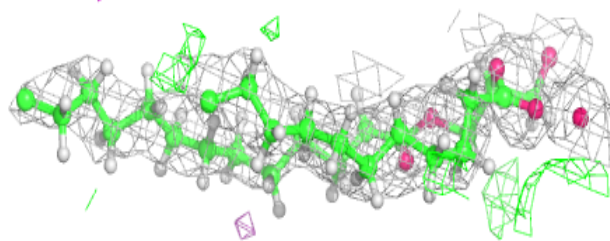
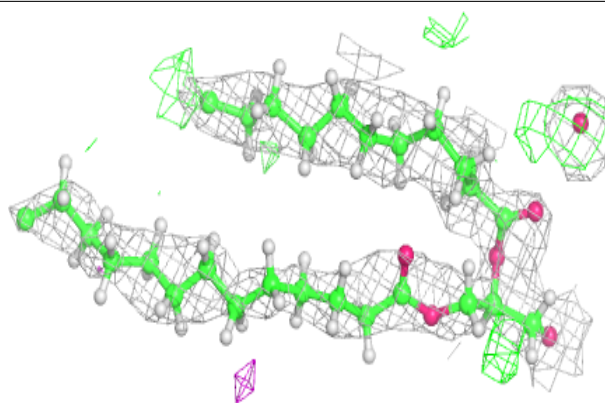
Electron density around LHG A 411:

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

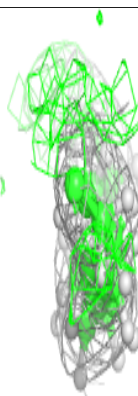
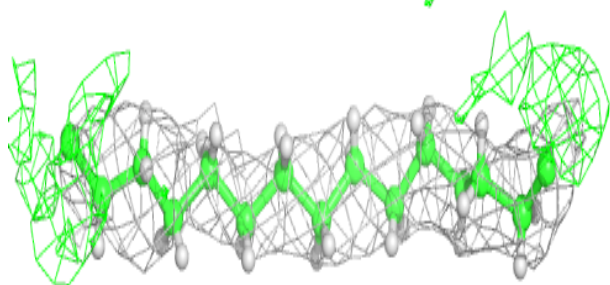
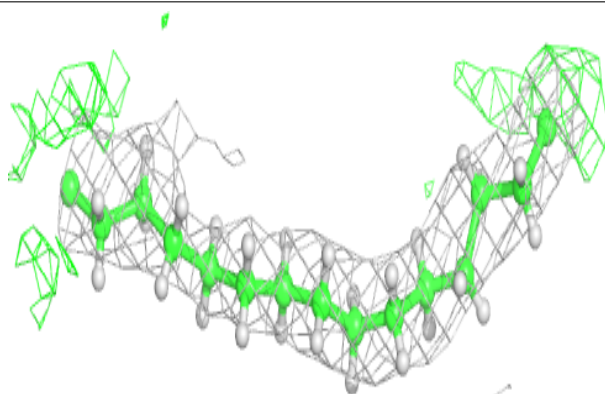


Electron density around LMG D 412:

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

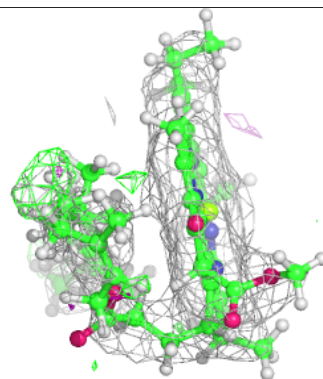
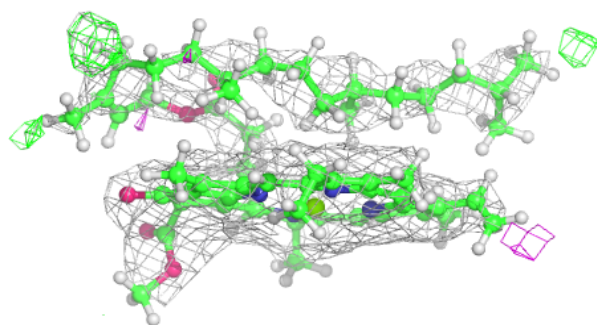
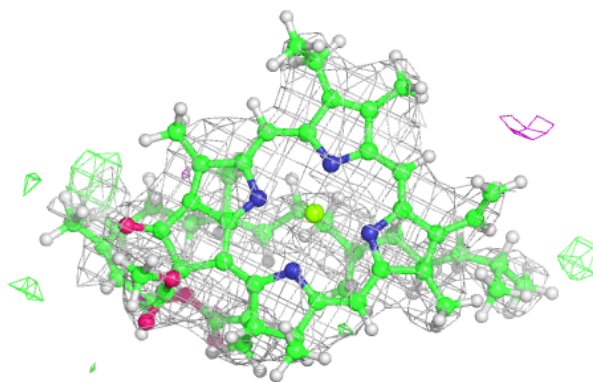
**Electron density around STE I 102:**

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



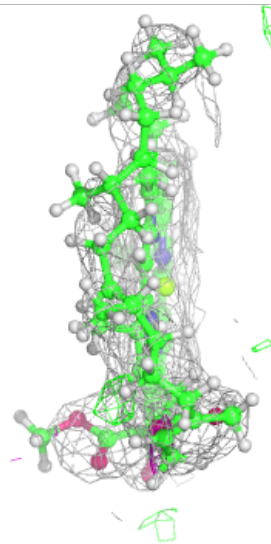
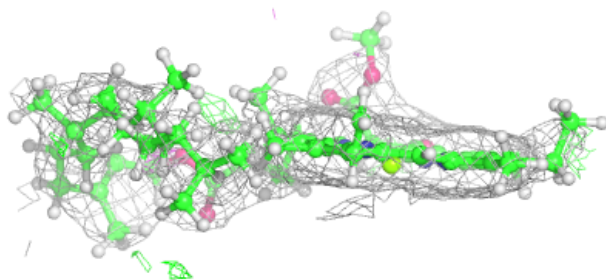
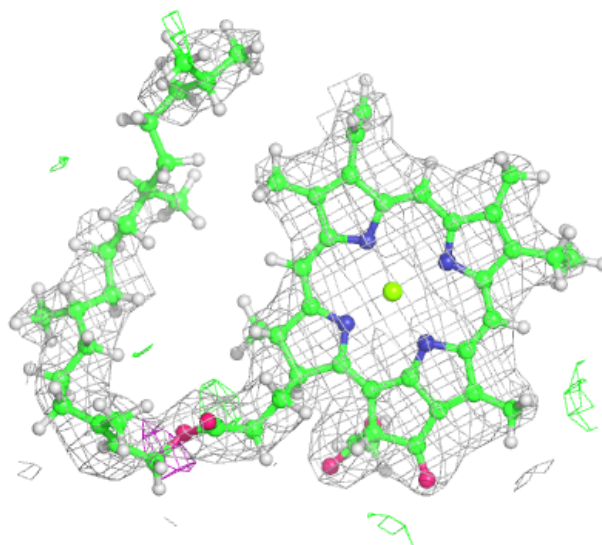
Electron density around CLA b 601:

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



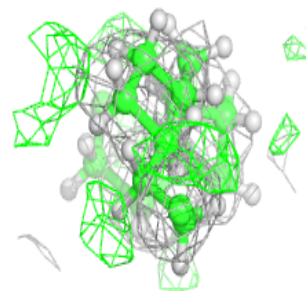
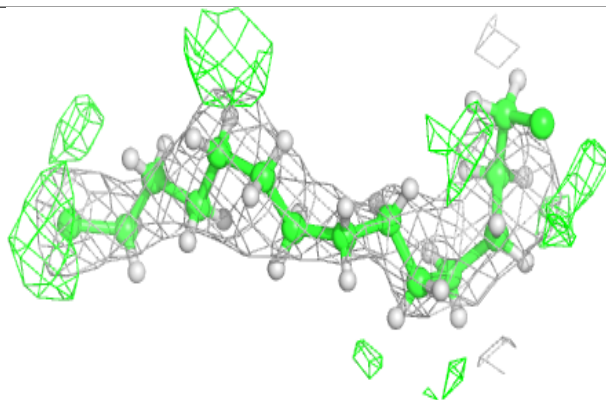
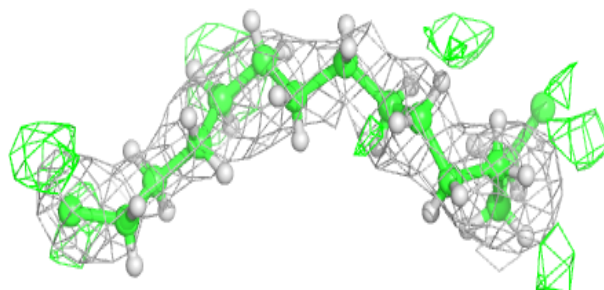
Electron density around CLA c 512:

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

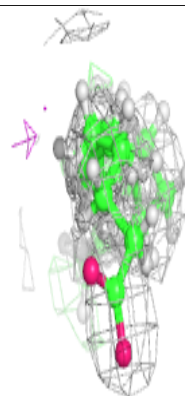
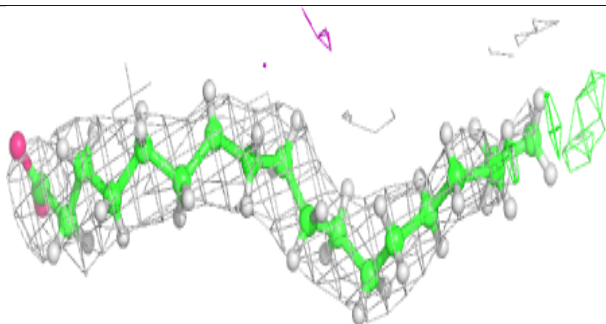
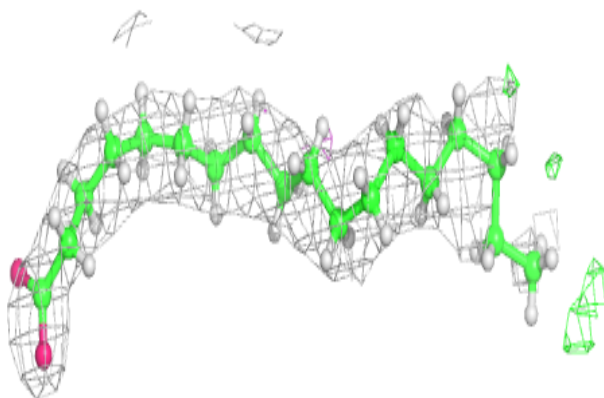


Electron density around STE a 413:

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

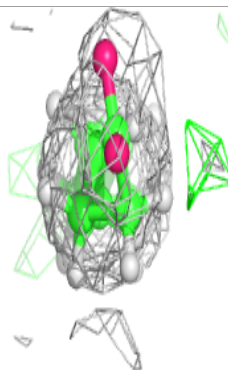
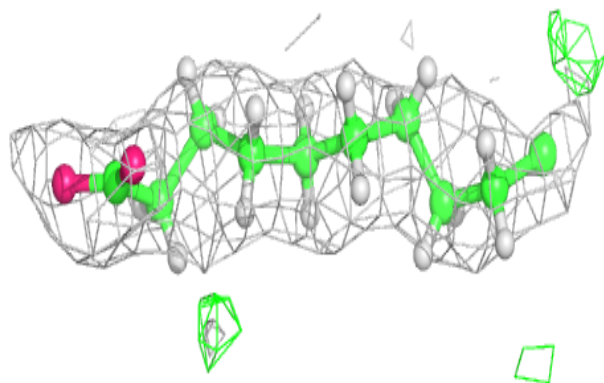
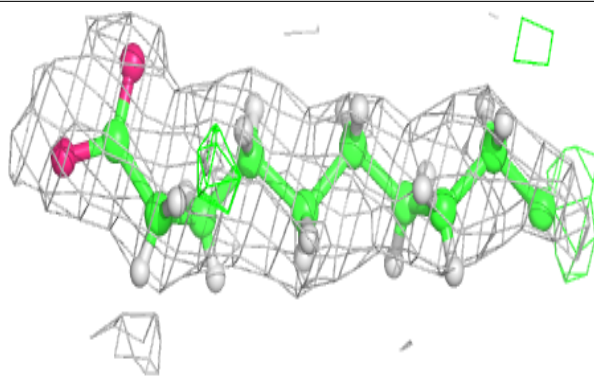
**Electron density around STE b 621:**

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

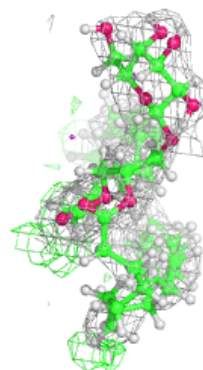
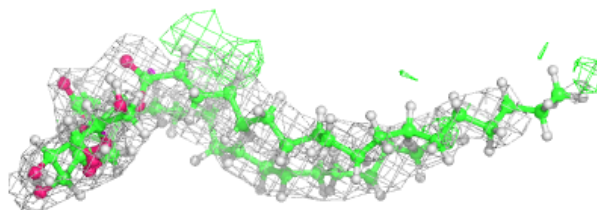
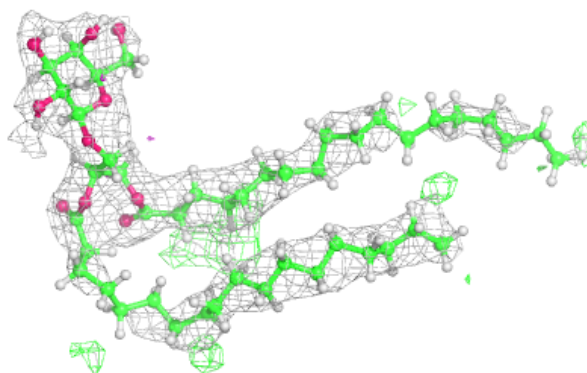


Electron density around STE J 101:

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

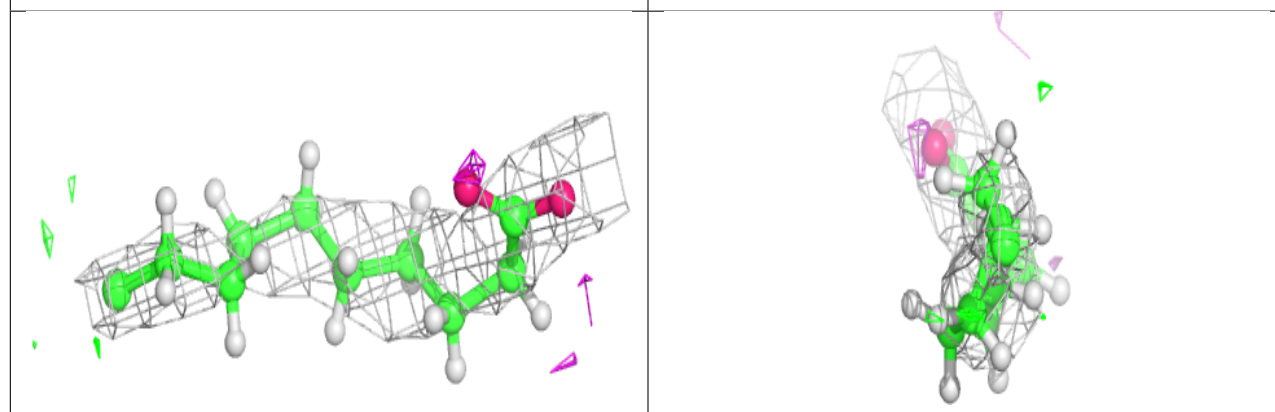
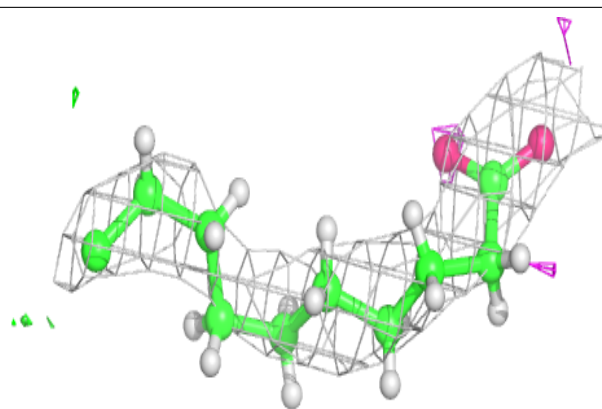
**Electron density around LMG B 626:**

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

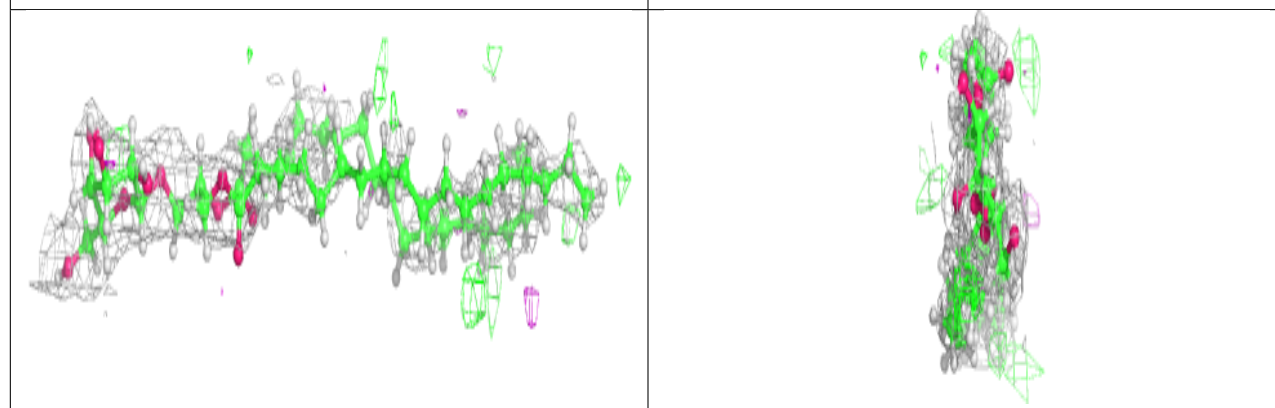
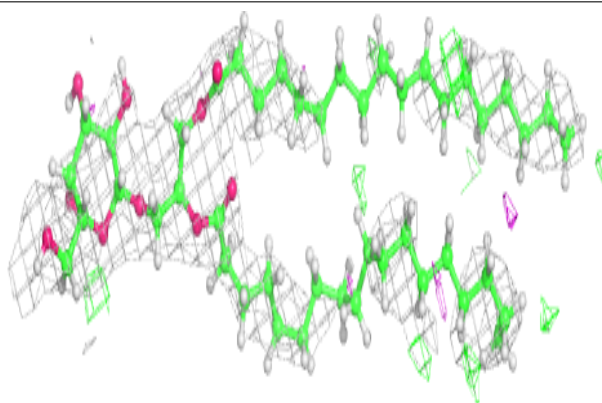


Electron density around STE B 627:

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

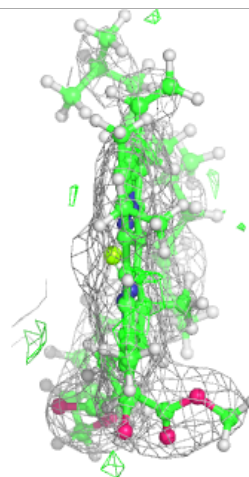
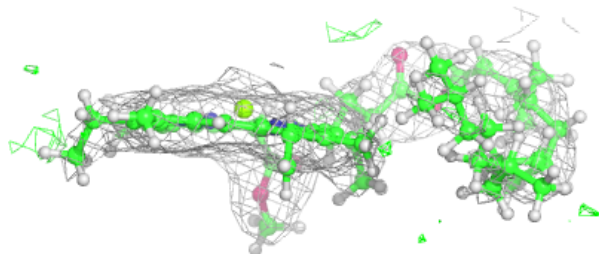
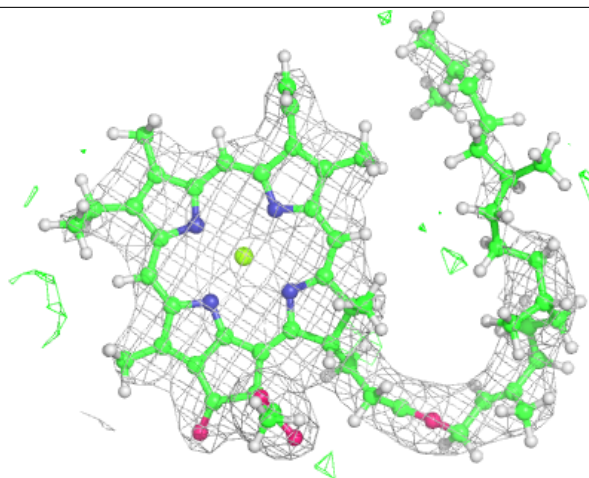
**Electron density around LMG b 622:**

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



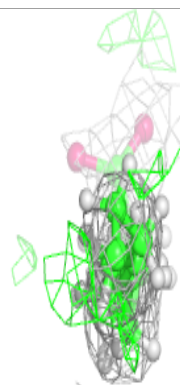
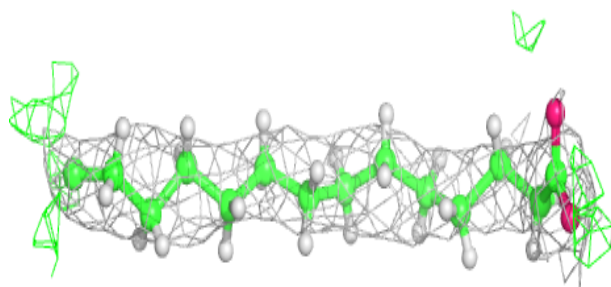
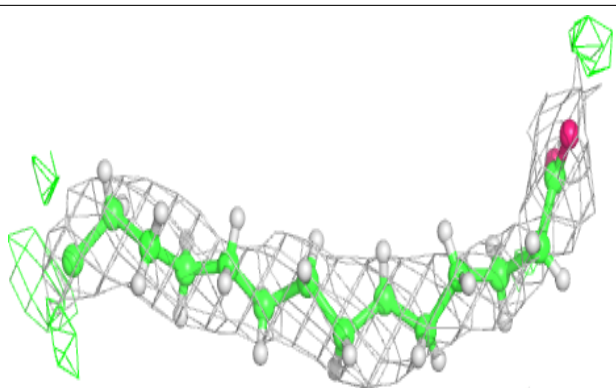
Electron density around CLA C 512:

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

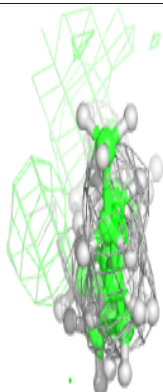
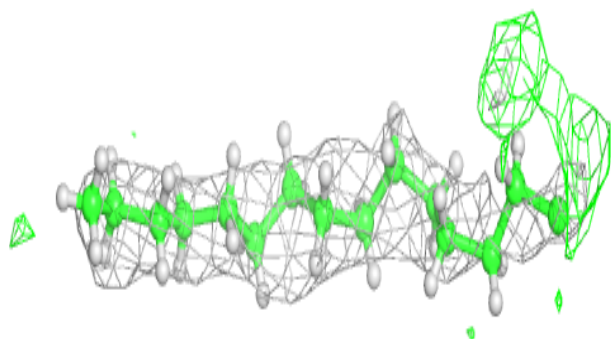
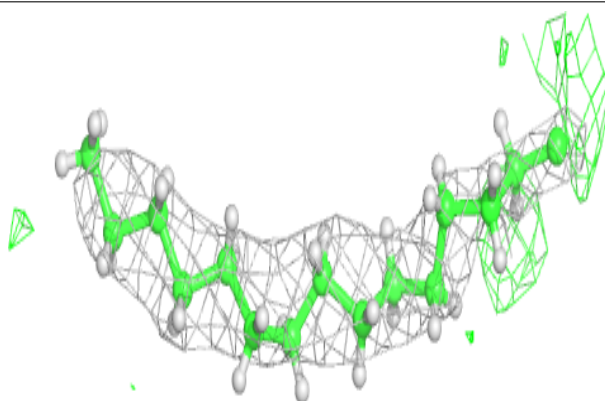


Electron density around STE b 623:

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

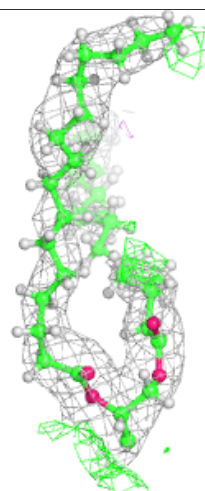
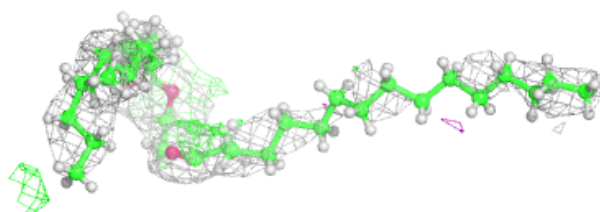
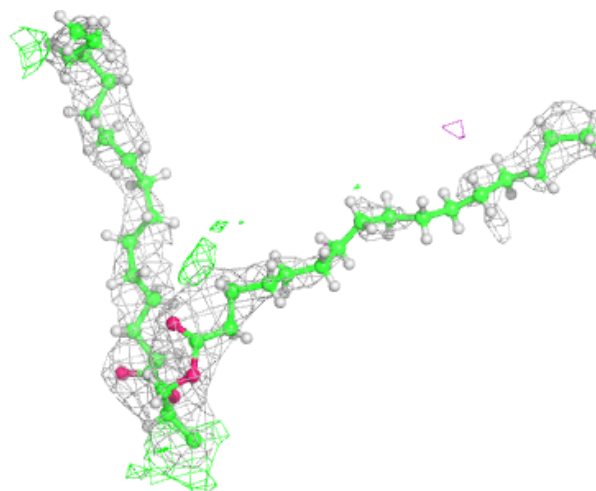
**Electron density around STE b 624:**

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



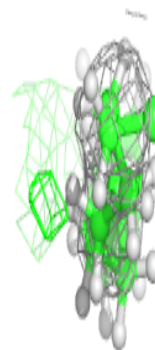
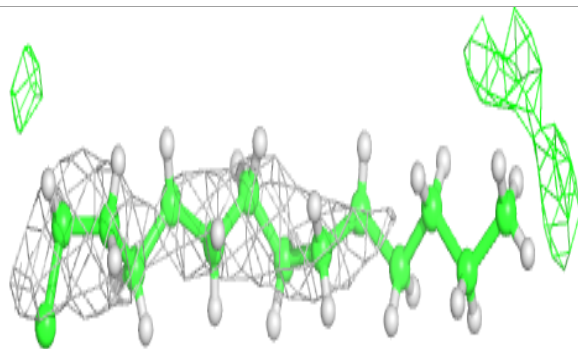
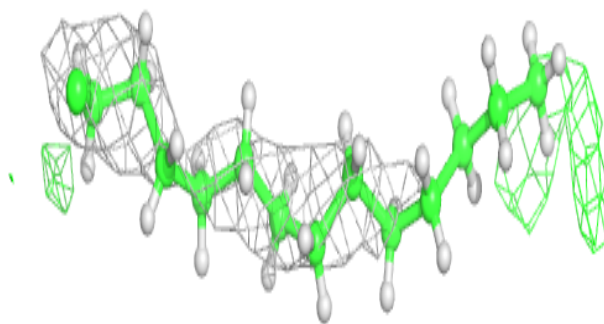
Electron density around SQD A 412:

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

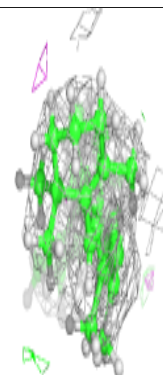
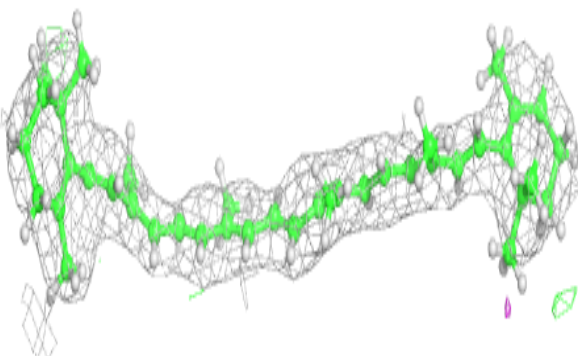
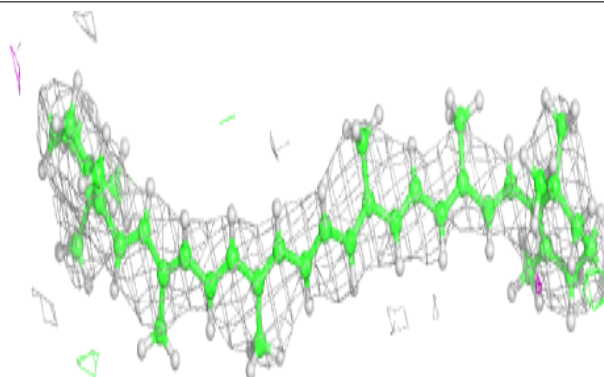


Electron density around STE b 627:

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

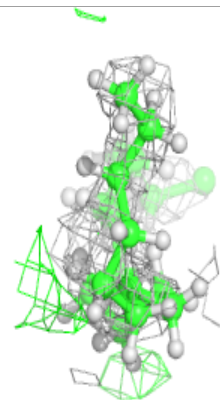
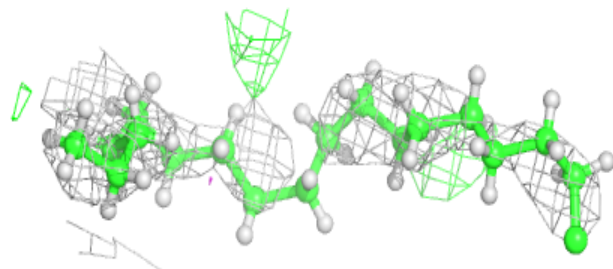
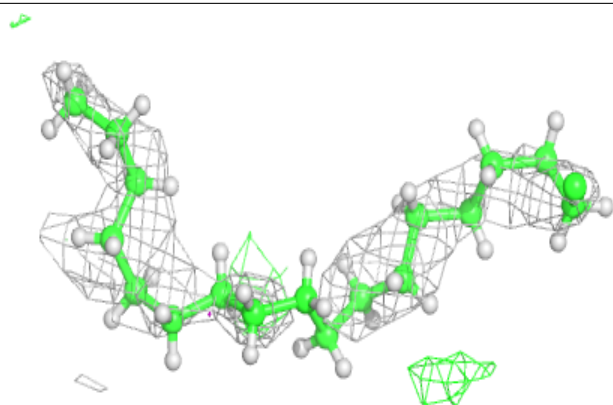
**Electron density around BCR x 101:**

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

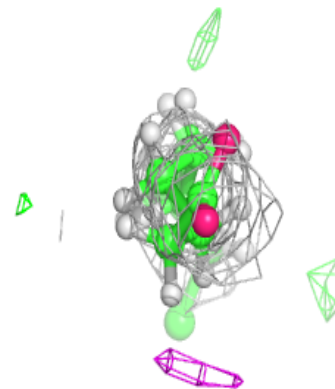
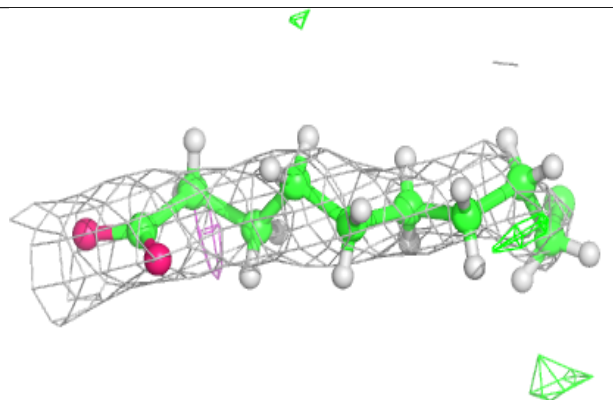
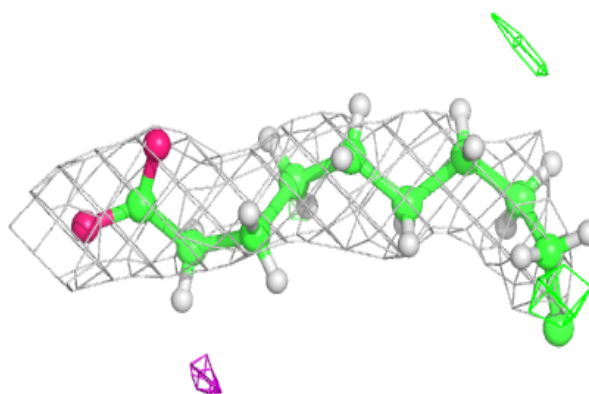


Electron density around STE H 103:

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

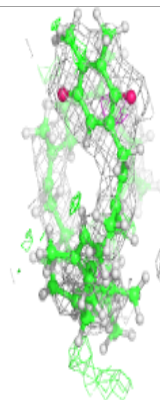
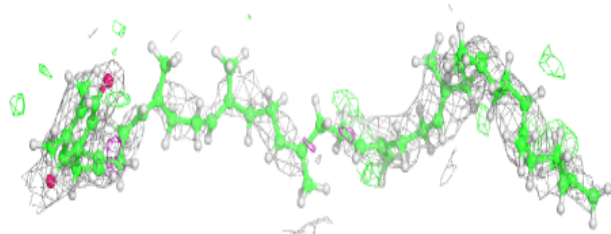
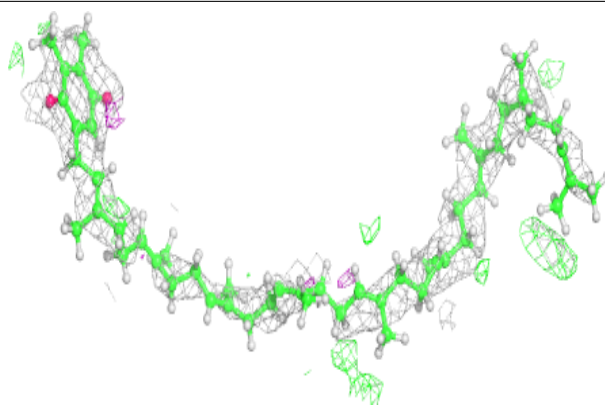
**Electron density around STE L 103:**

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

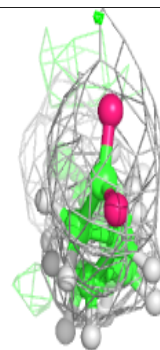
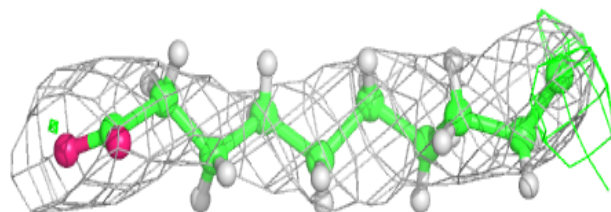
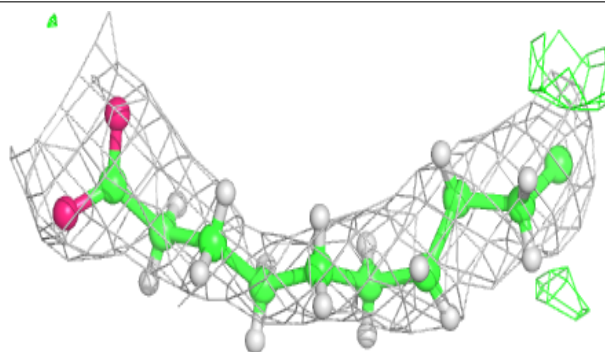


Electron density around PL9 a 409:

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

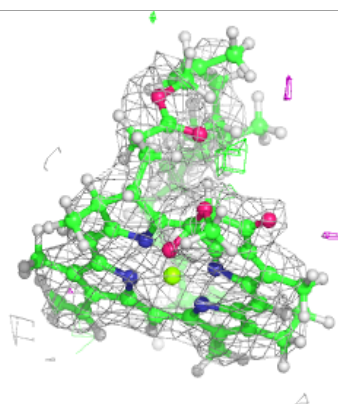
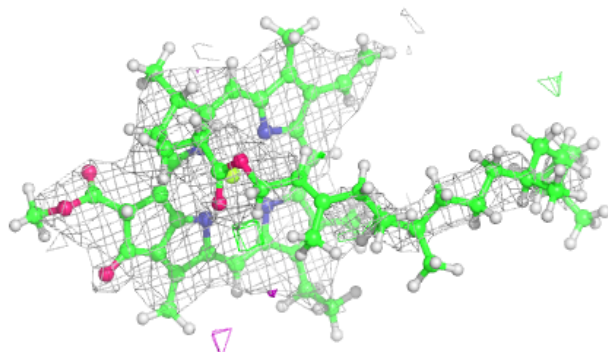
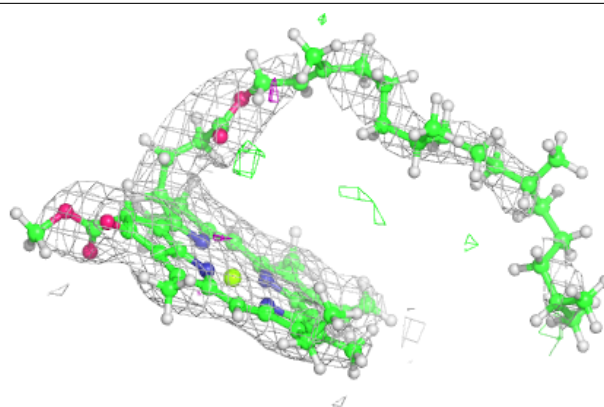
**Electron density around STE C 518:**

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

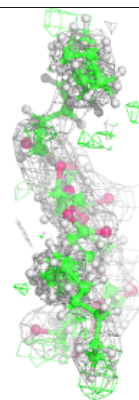
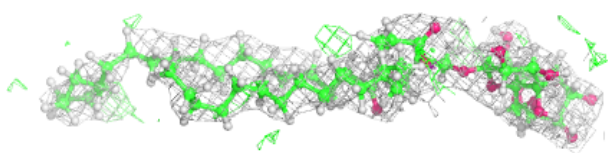
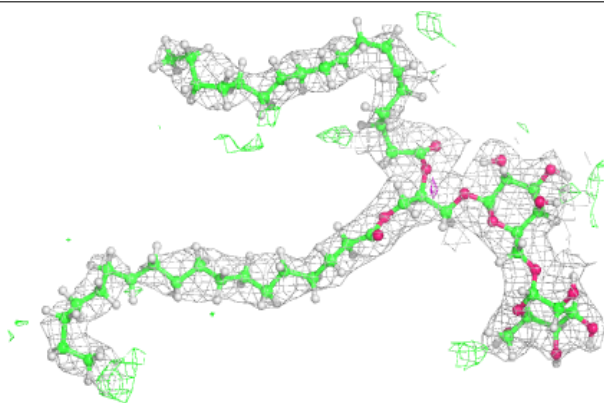


Electron density around CLA c 513:

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

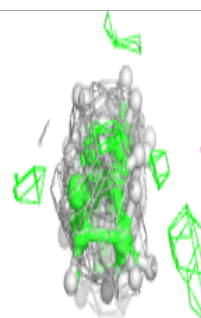
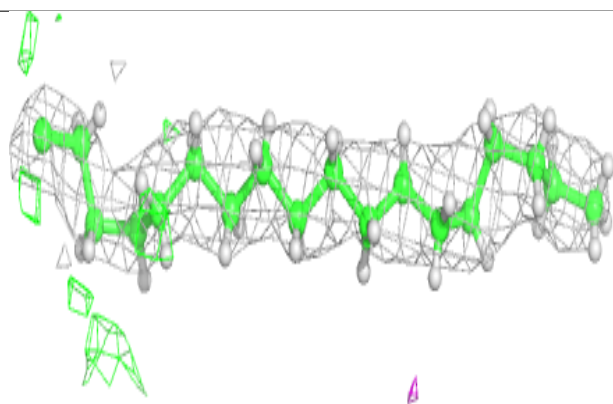
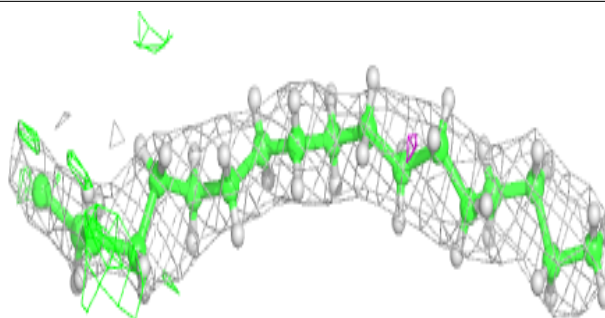
**Electron density around DGD A 413:**

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



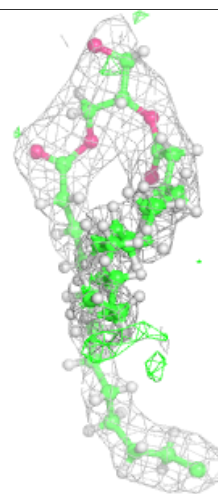
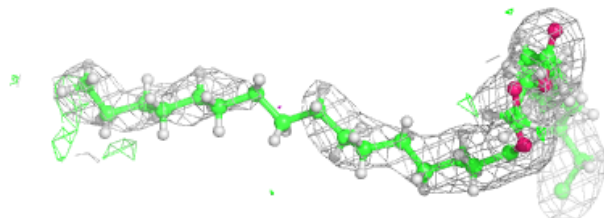
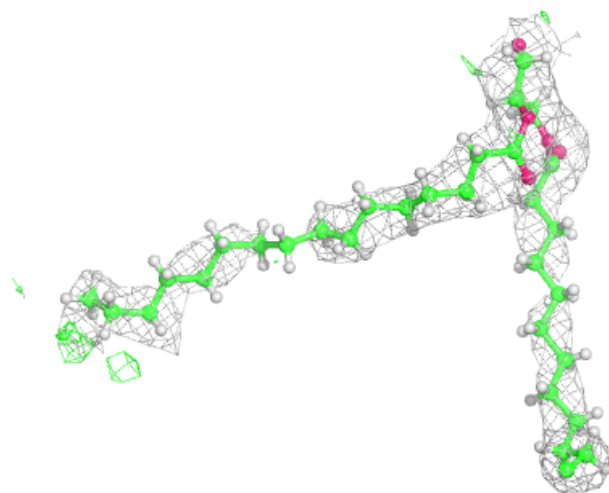
Electron density around STE 1 102:

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



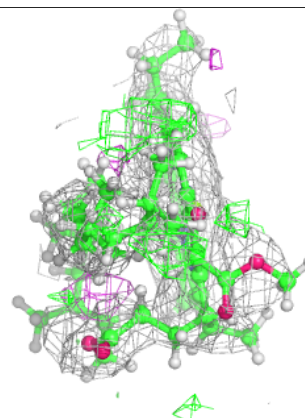
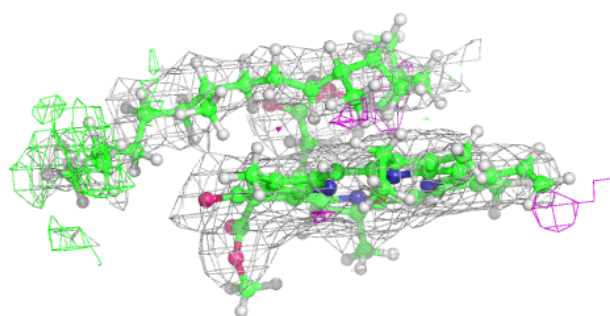
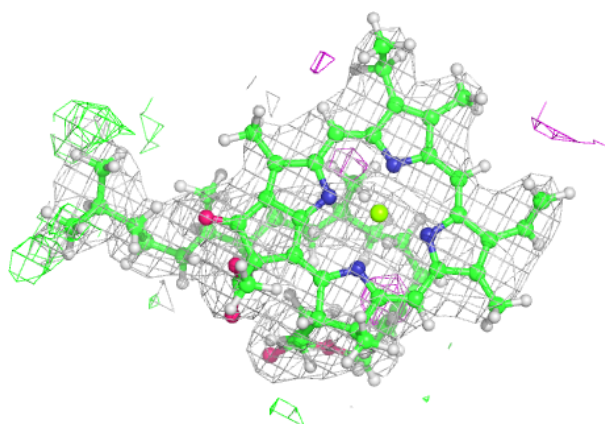
Electron density around SQD t 102:

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

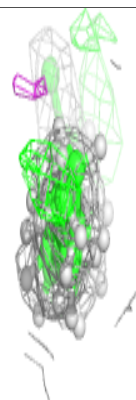
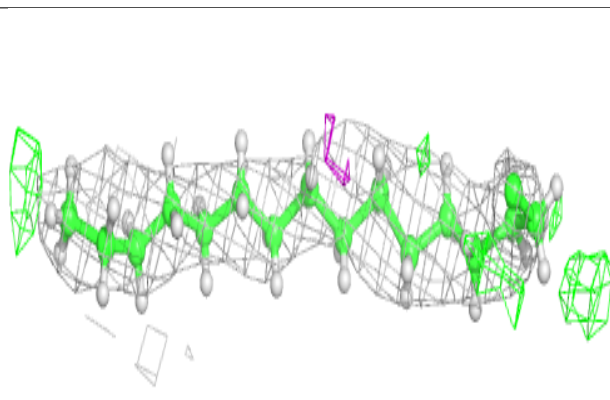
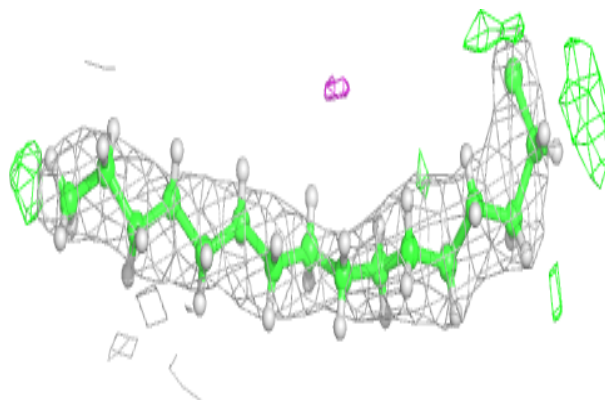


Electron density around CLA B 601:

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

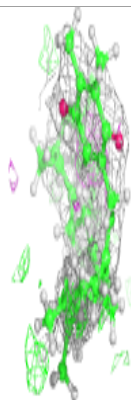
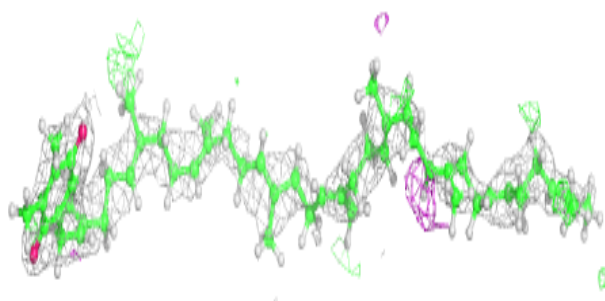
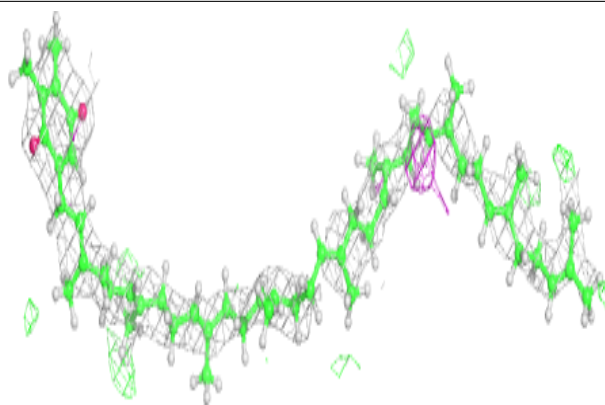
**Electron density around STE C 519:**

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

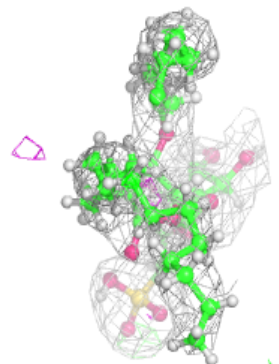
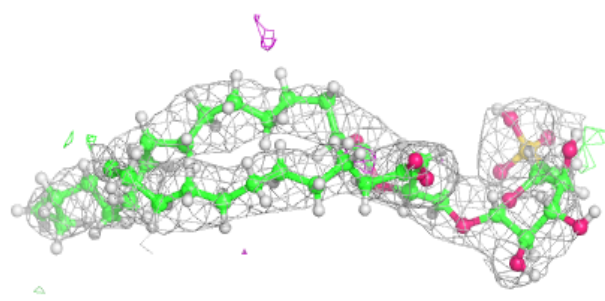
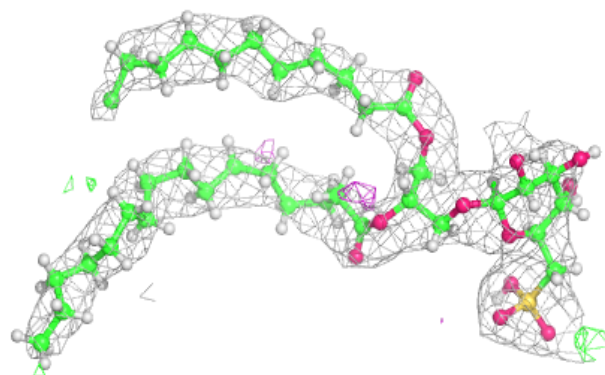


Electron density around PL9 A 408:

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

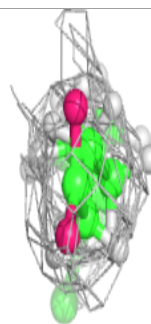
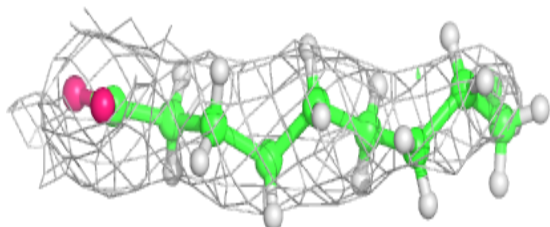
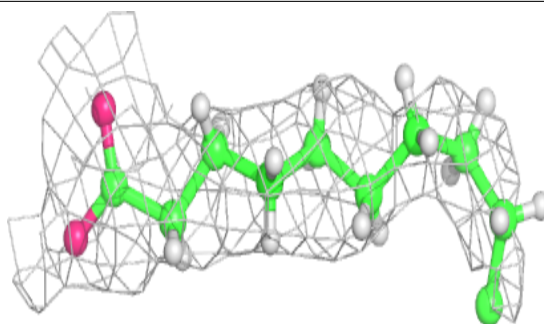
**Electron density around SQD L 101:**

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

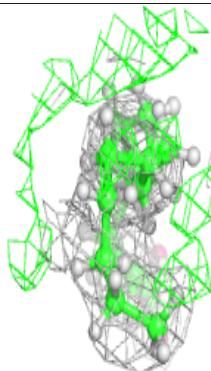
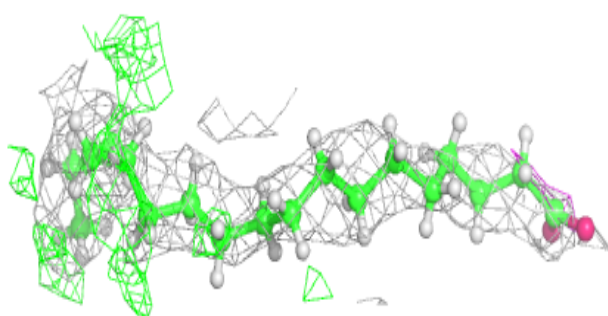
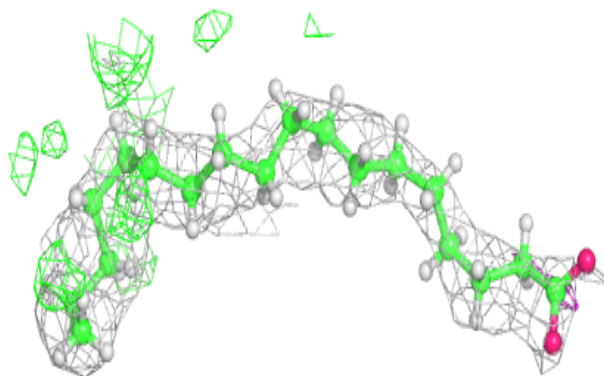


Electron density around STE c 523:

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

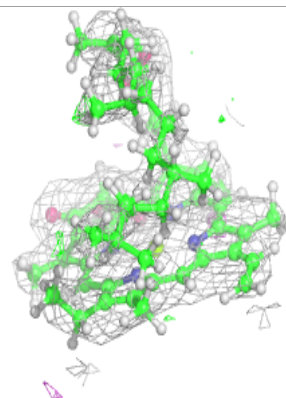
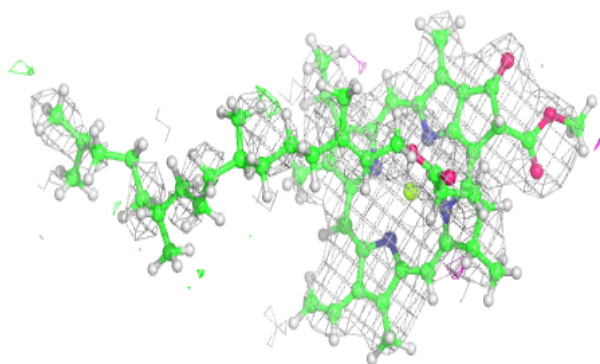
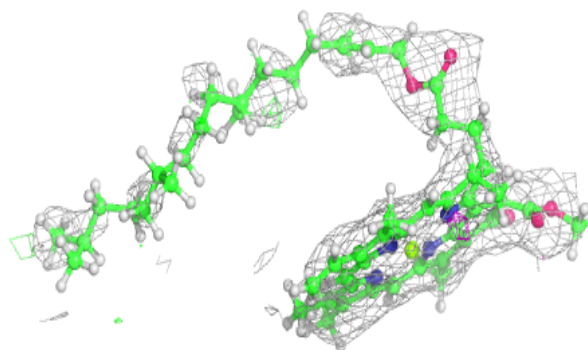
**Electron density around STE d 412:**

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

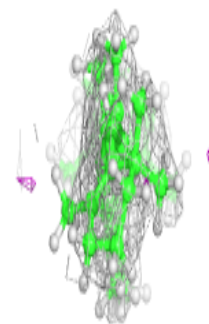
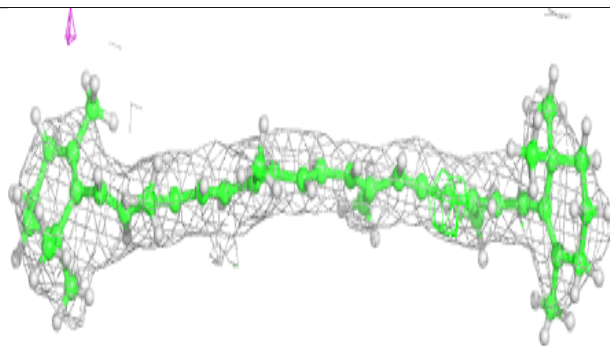
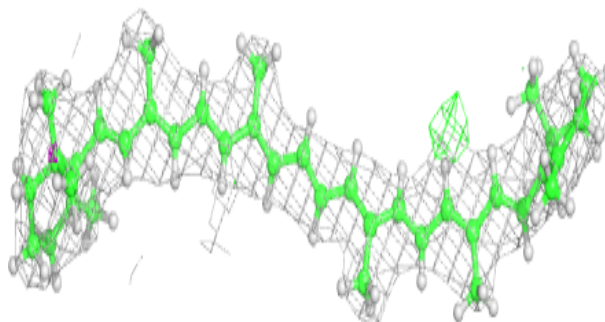


Electron density around CLA C 513:

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

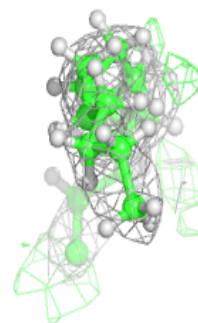
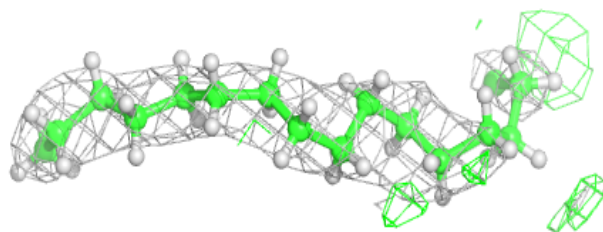
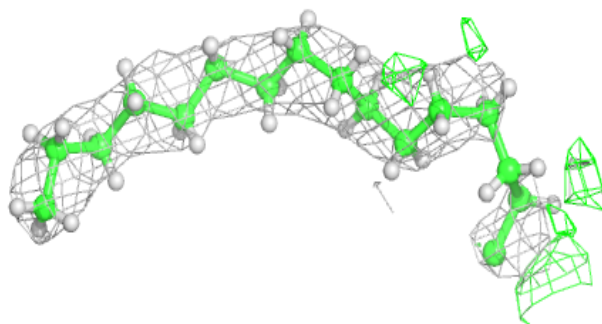
**Electron density around BCR K 101:**

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

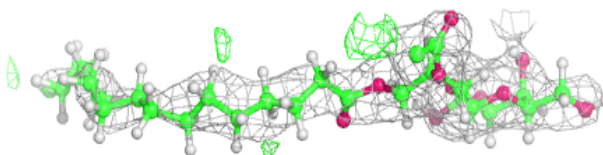
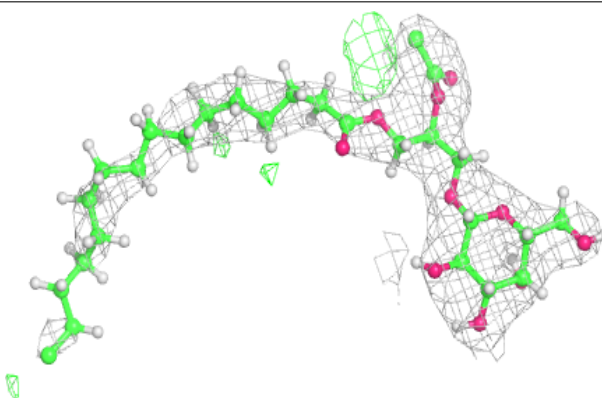


Electron density around STE b 620:

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

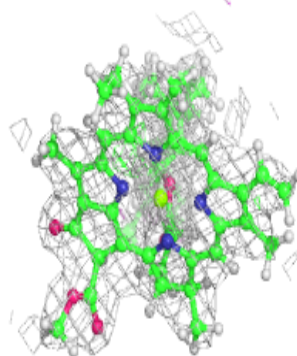
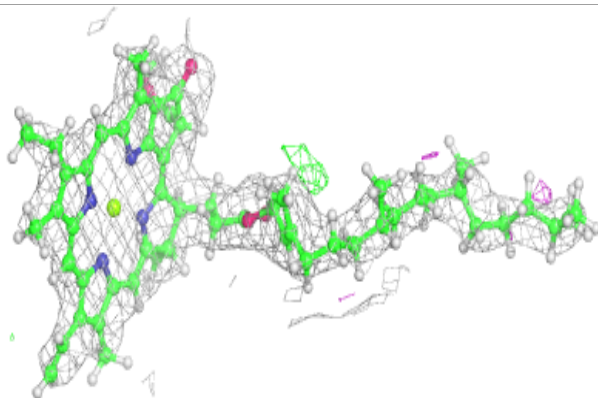
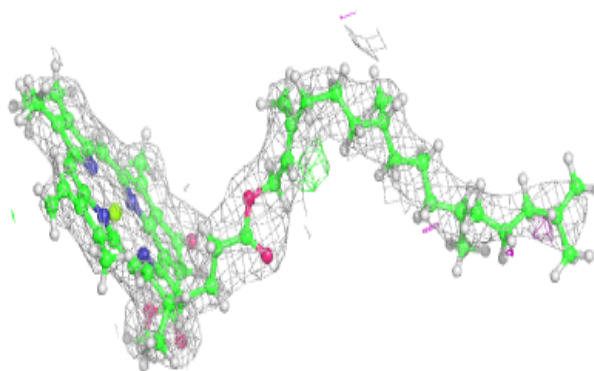
**Electron density around LMG c 519:**

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

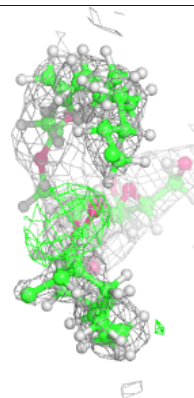
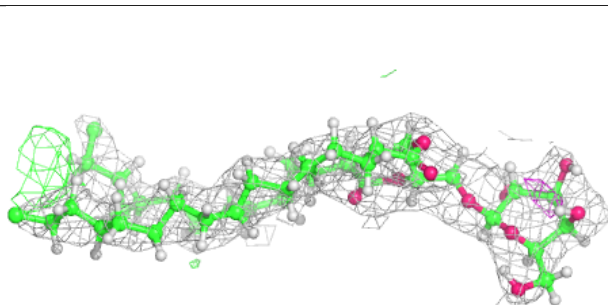
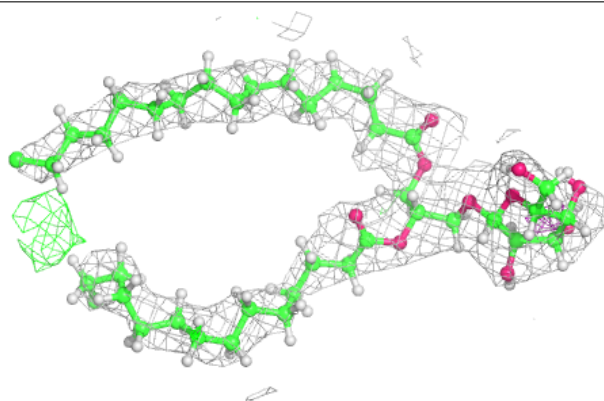


Electron density around CLA c 502:

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

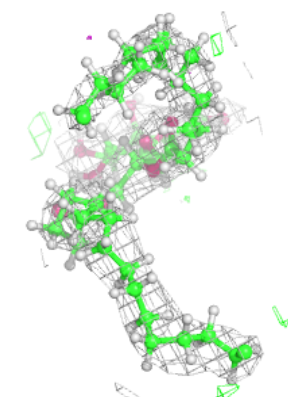
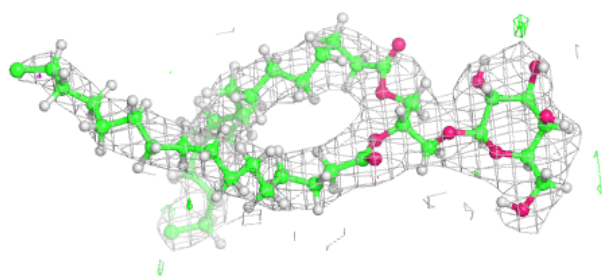
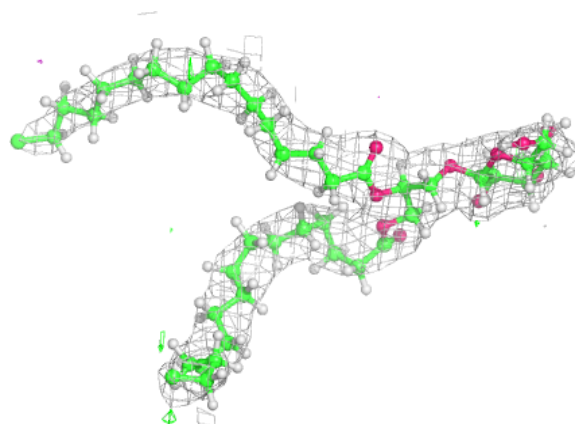
**Electron density around LMG c 522:**

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

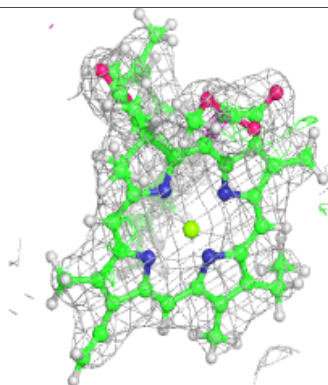
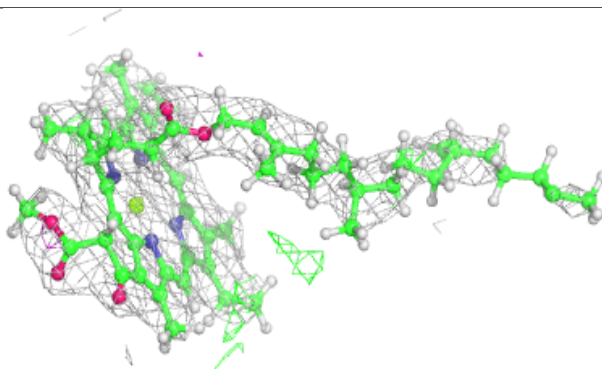
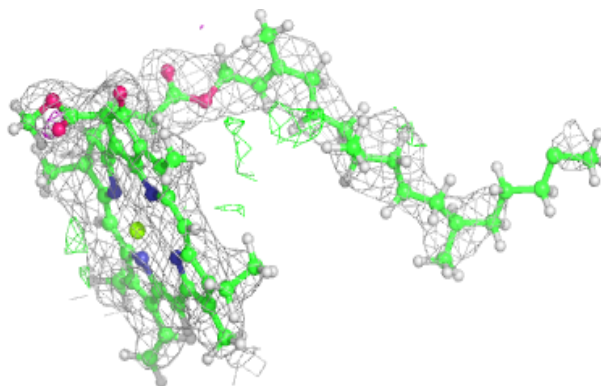


Electron density around LMG m 101:

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

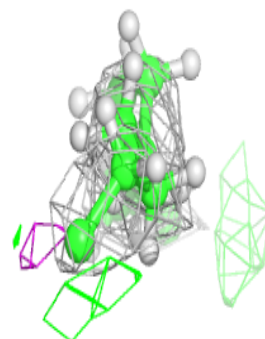
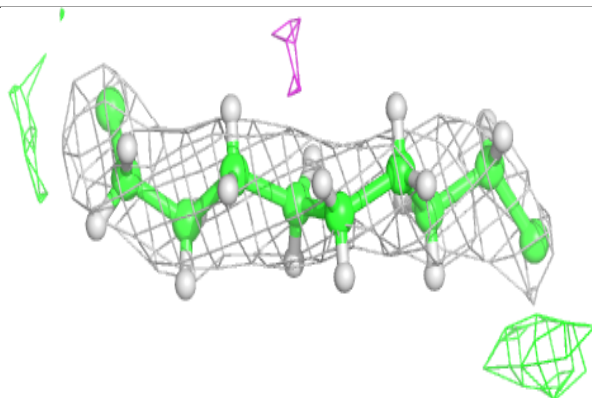
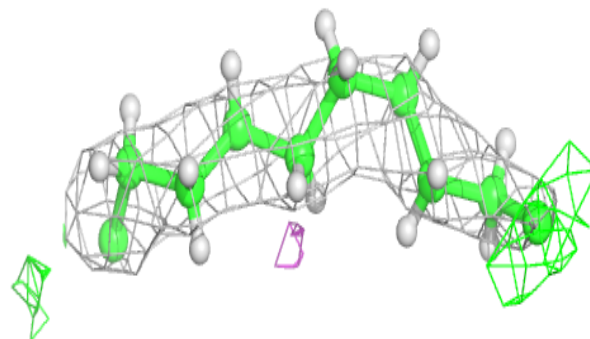
**Electron density around CLA c 508:**

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

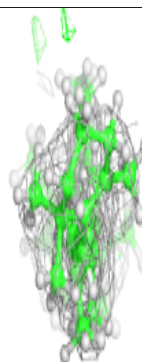
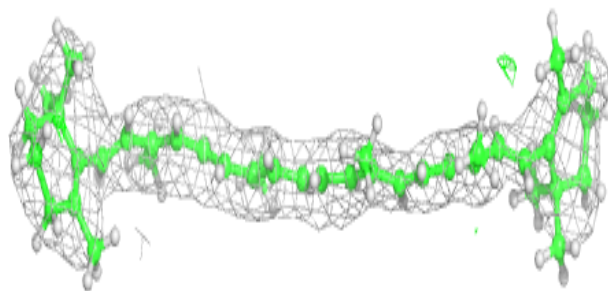
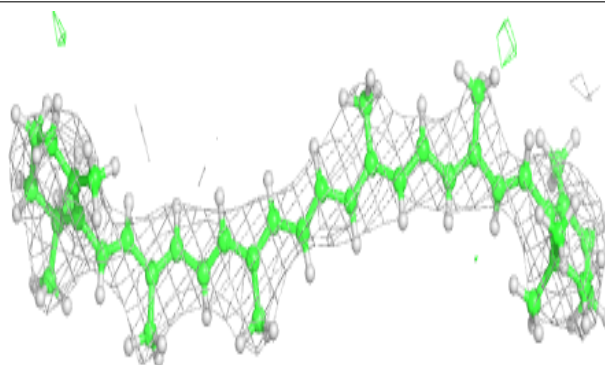


Electron density around STE b 626:

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

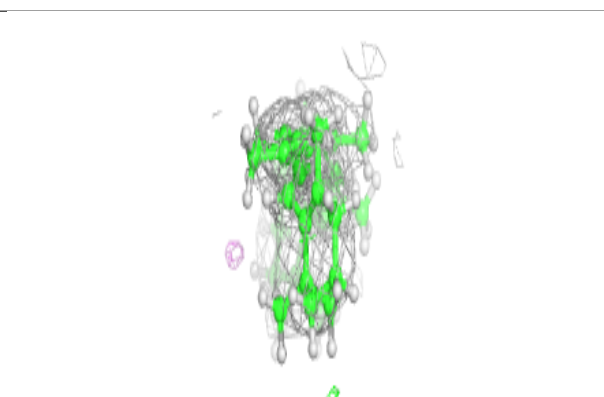
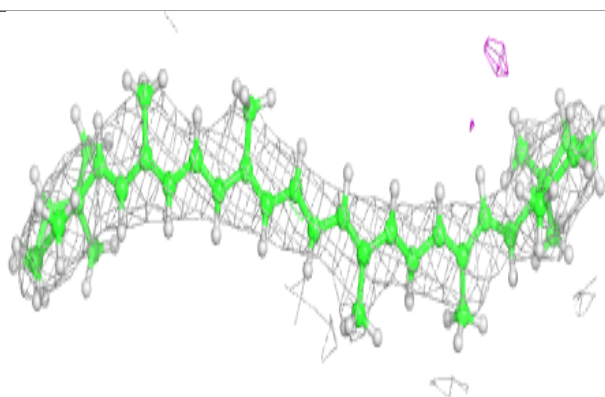
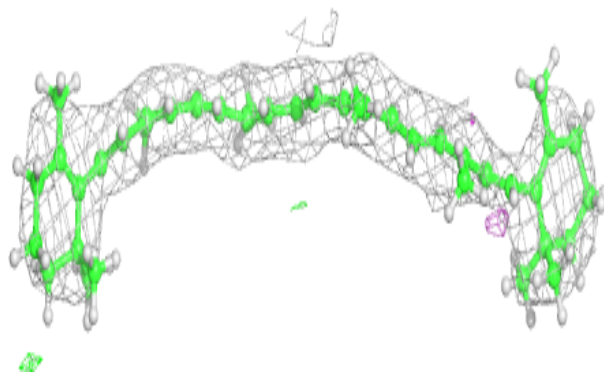
**Electron density around BCR k 101:**

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

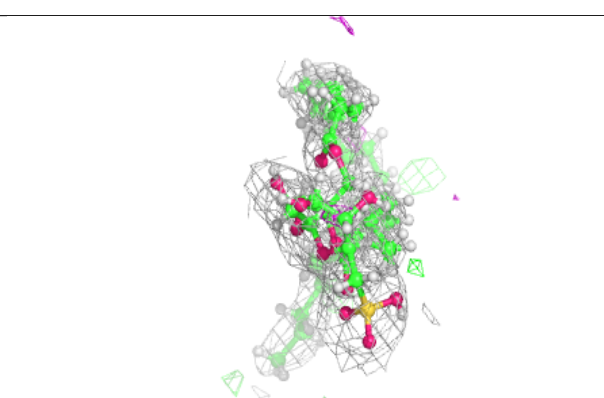
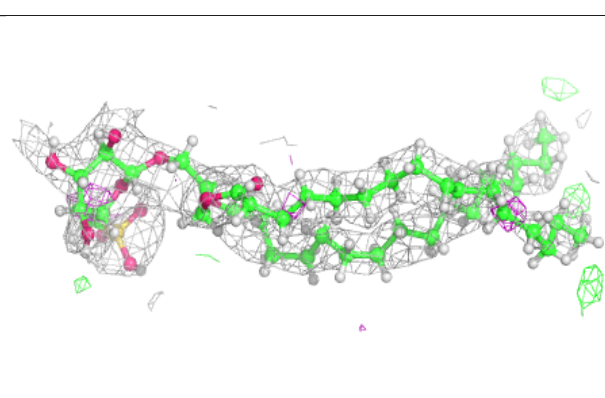
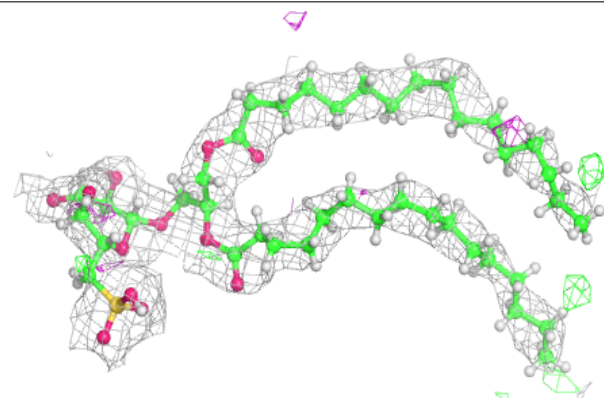


Electron density around BCR k 102:

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

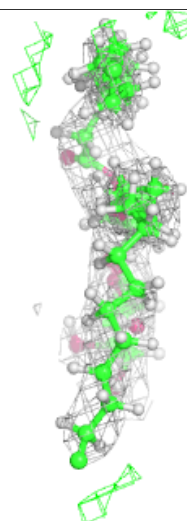
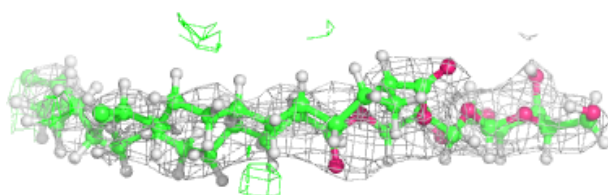
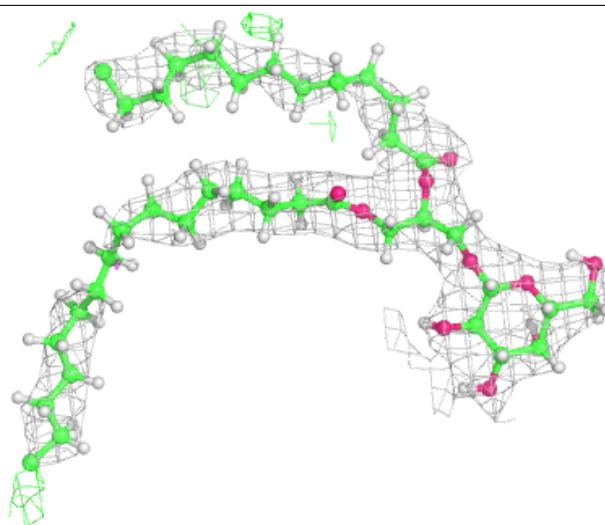
**Electron density around SQD B 622:**

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



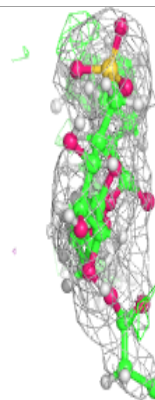
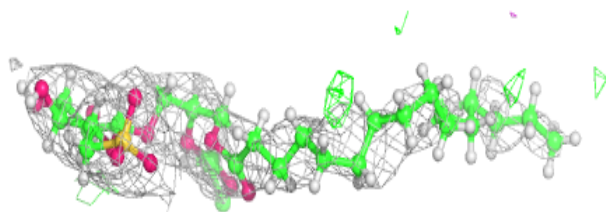
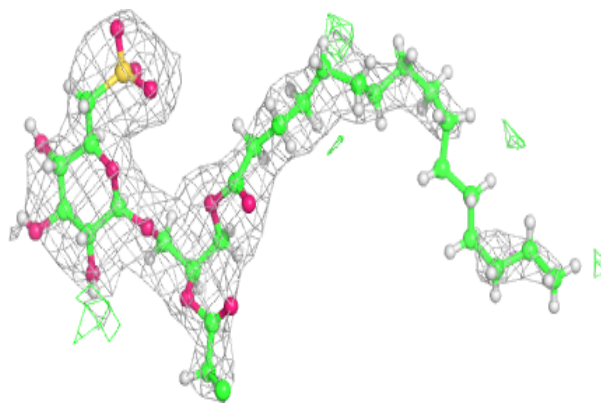
Electron density around LMG Y 101:

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



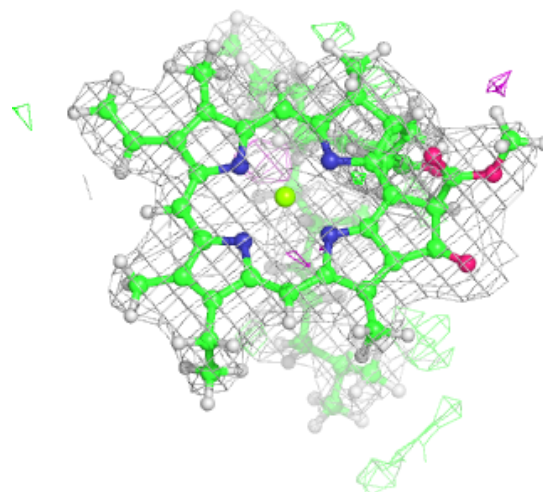
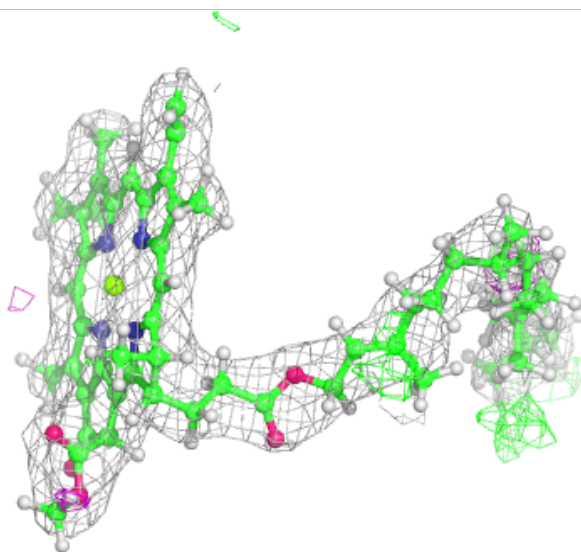
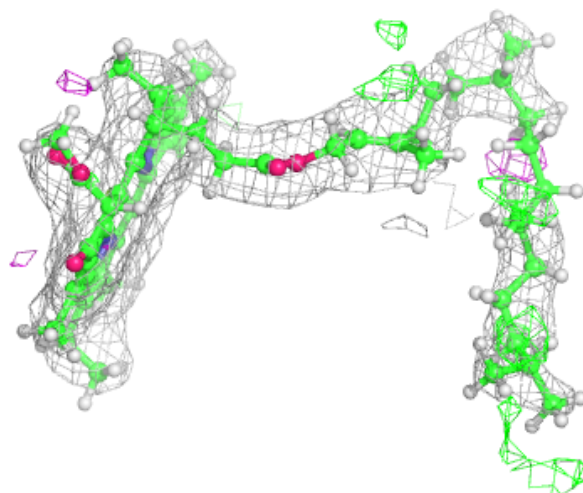
Electron density around SQD f 102:

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



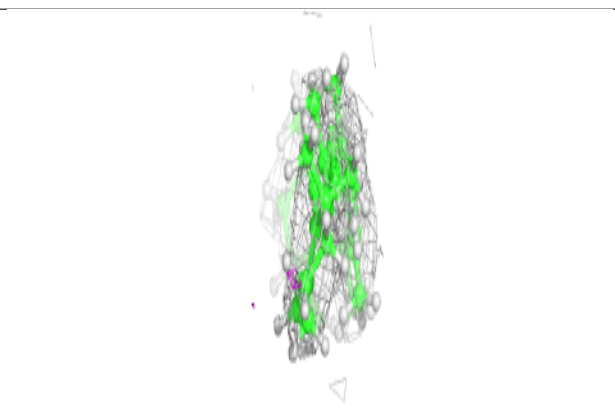
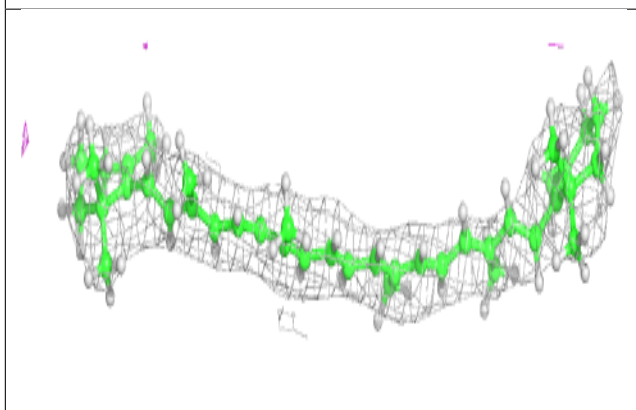
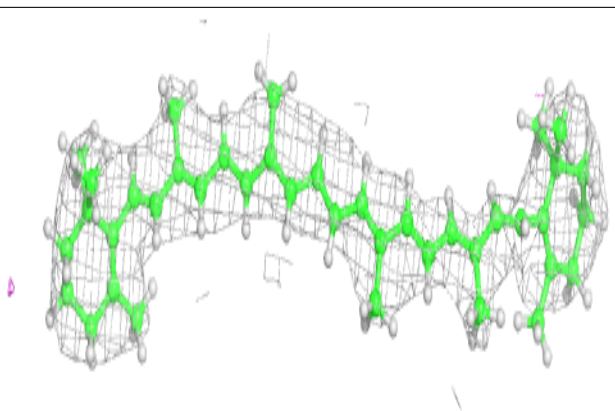
Electron density around CLA a 404:

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

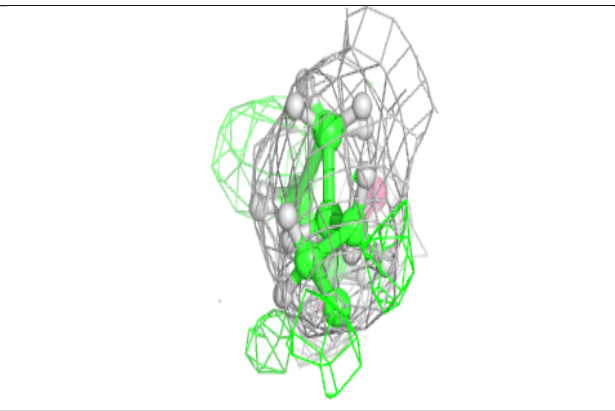
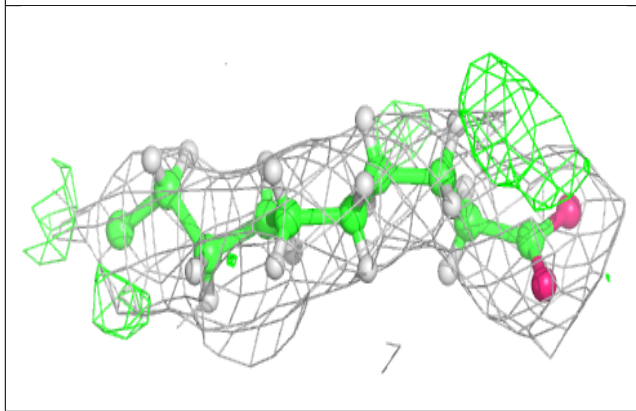
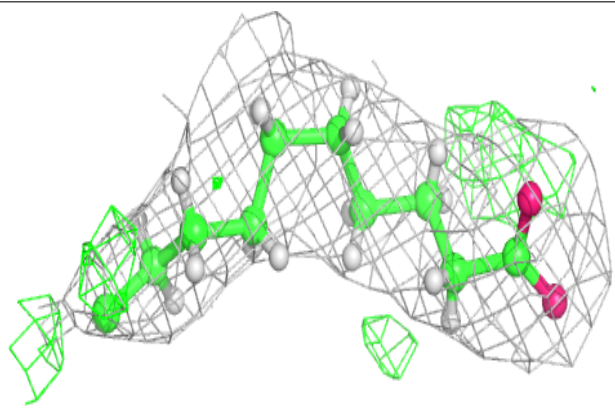


Electron density around BCR d 406:

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

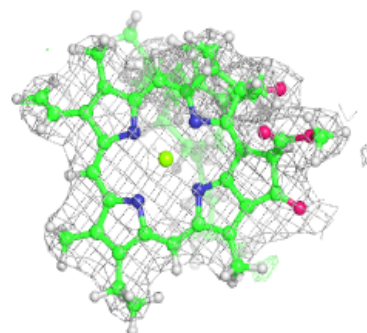
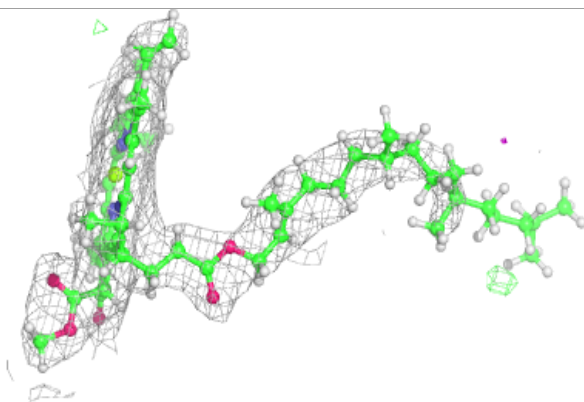
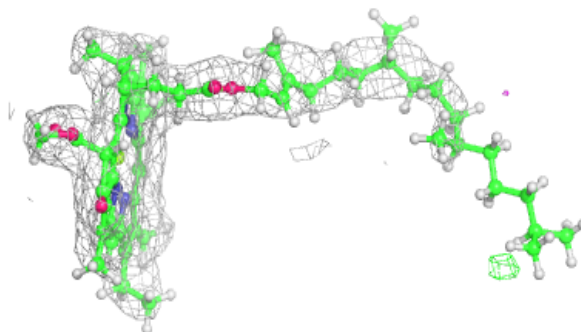
**Electron density around STE B 623:**

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

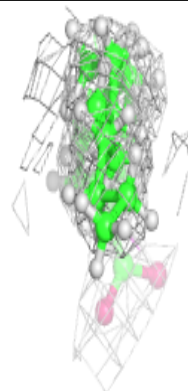
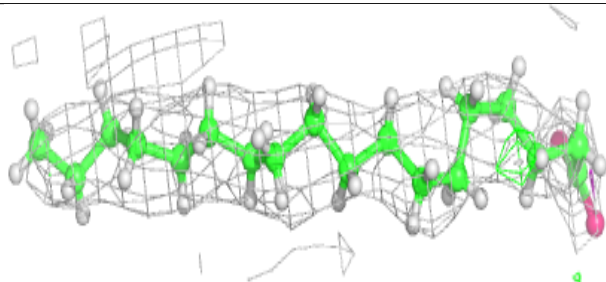
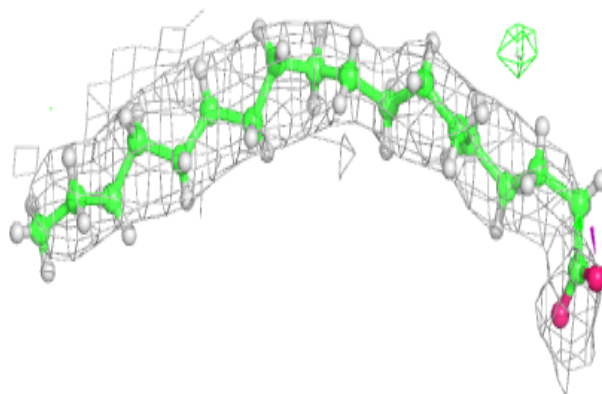


Electron density around CLA D 405:

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

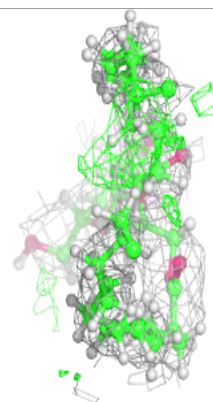
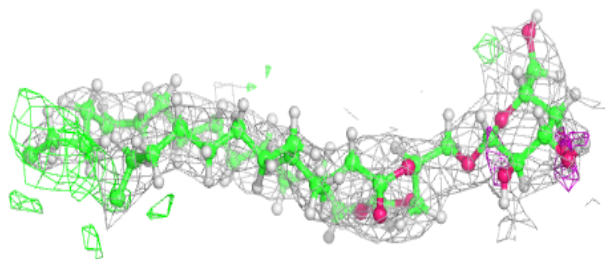
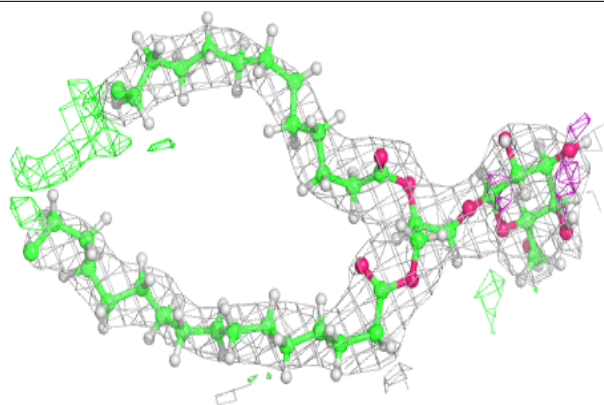
**Electron density around STE X 101:**

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

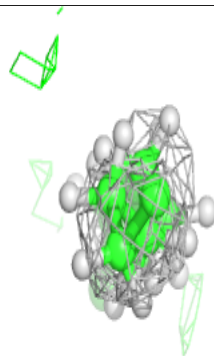
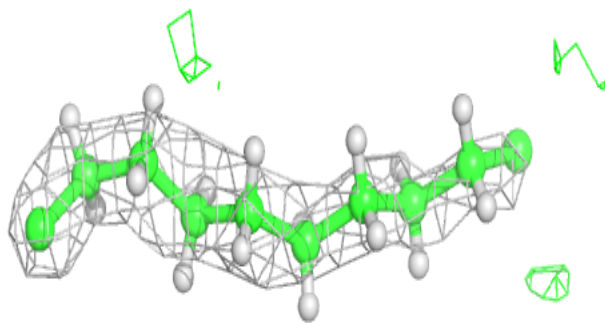
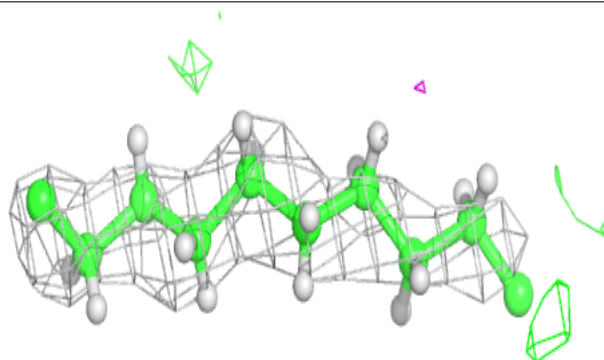


Electron density around LMG A 409:

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

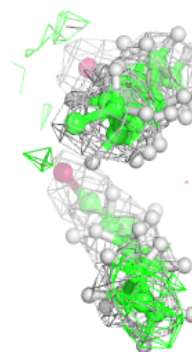
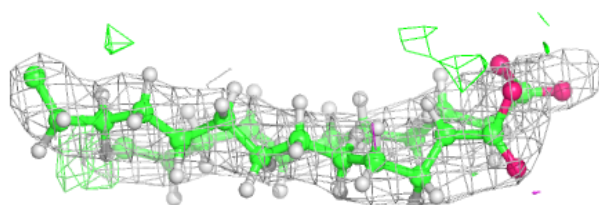
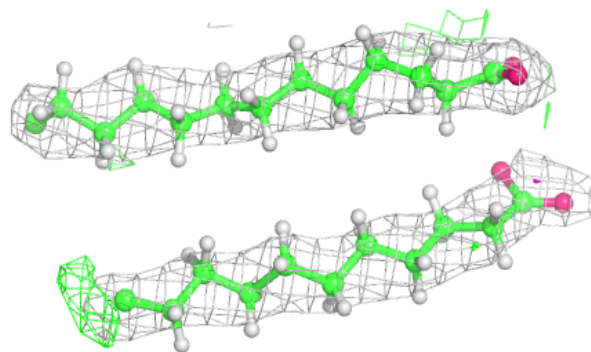
**Electron density around STE t 104:**

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

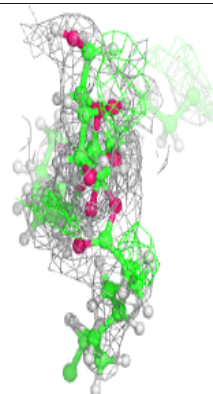
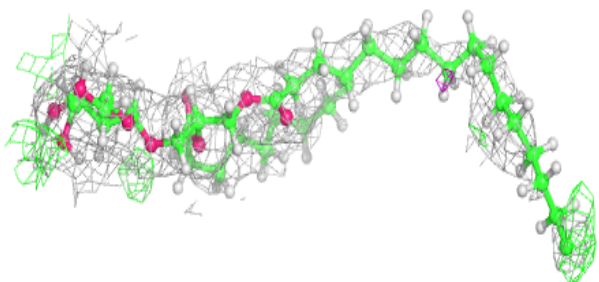
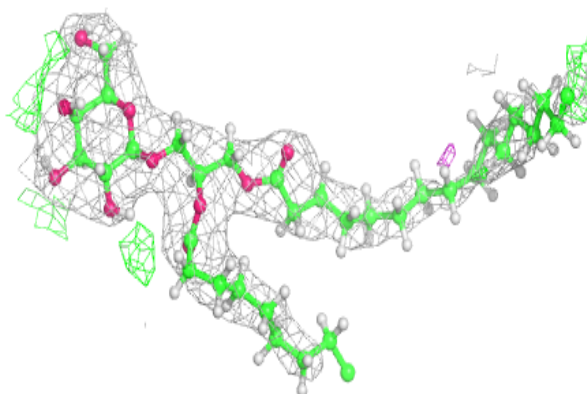


Electron density around LMG B 621:

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

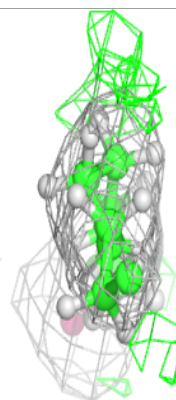
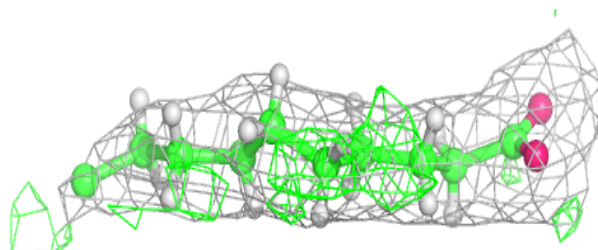
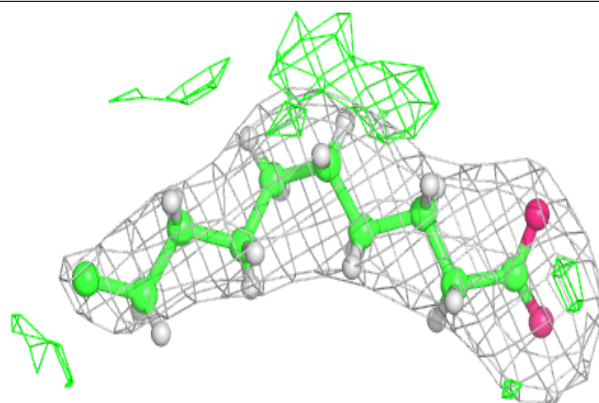
**Electron density around LMG d 410:**

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

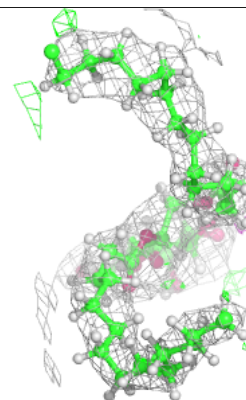
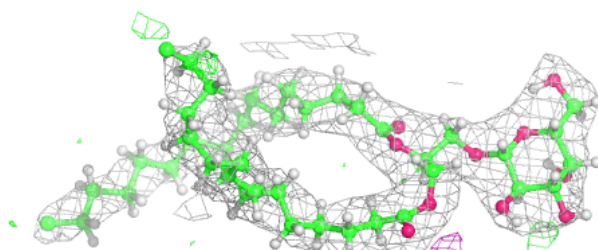
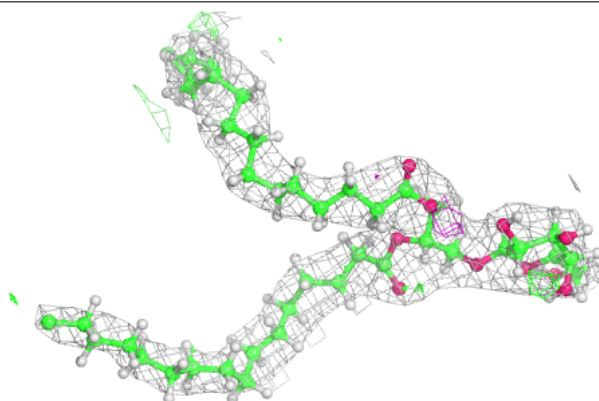


Electron density around STE C 520:

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

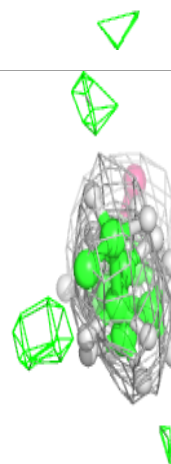
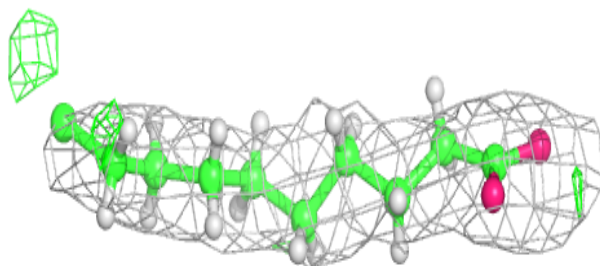
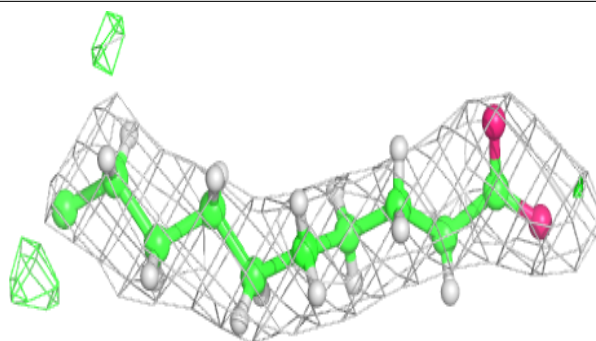
**Electron density around LMG M 101:**

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

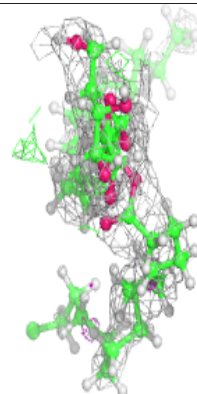
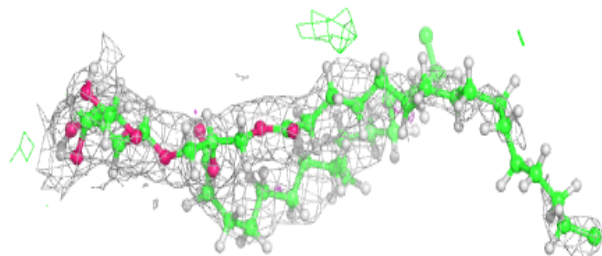
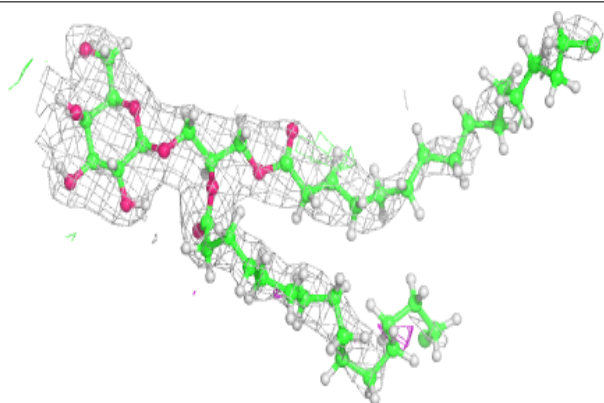


Electron density around STE j 101:

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

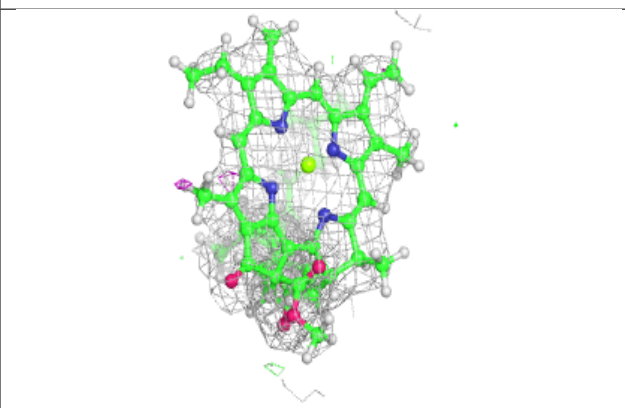
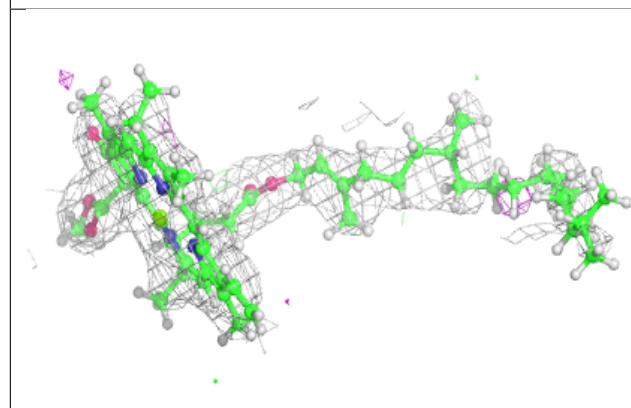
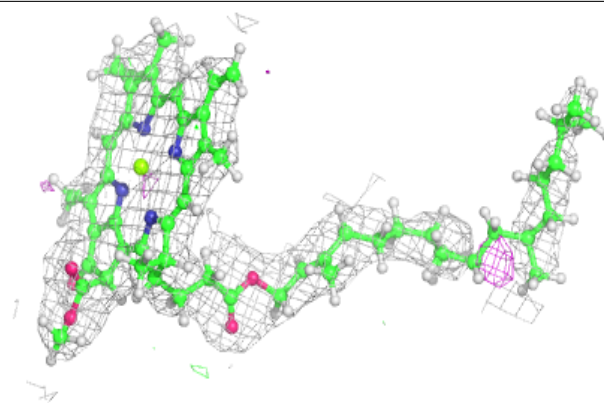
**Electron density around LMG D 408:**

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

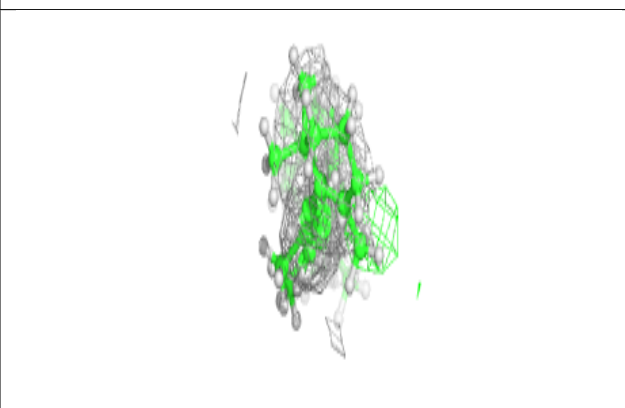
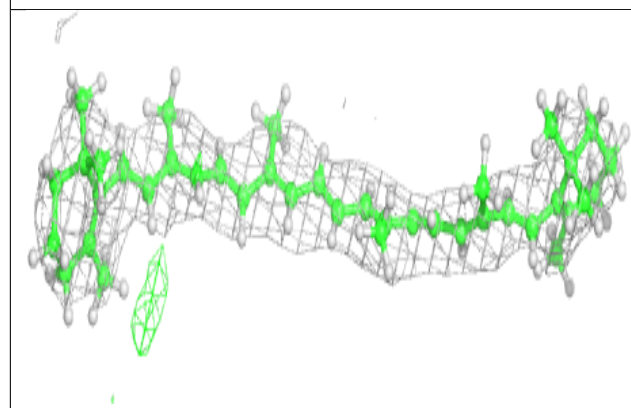
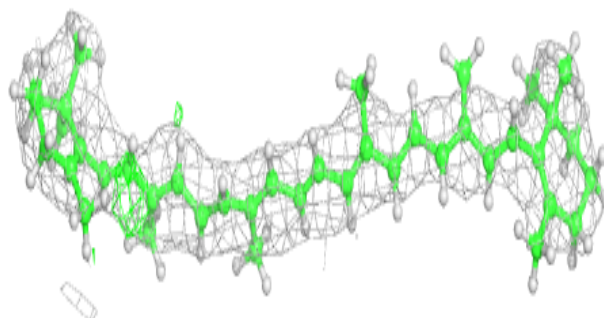


Electron density around CLA d 405:

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

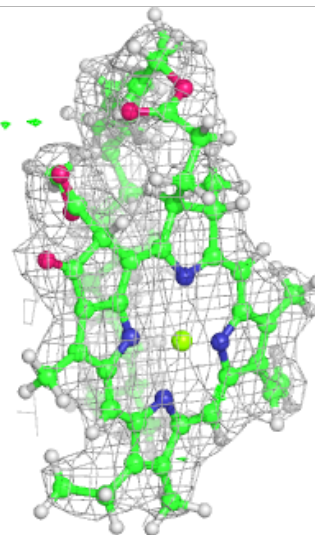
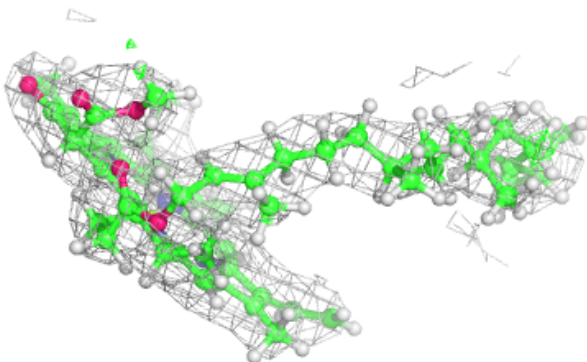
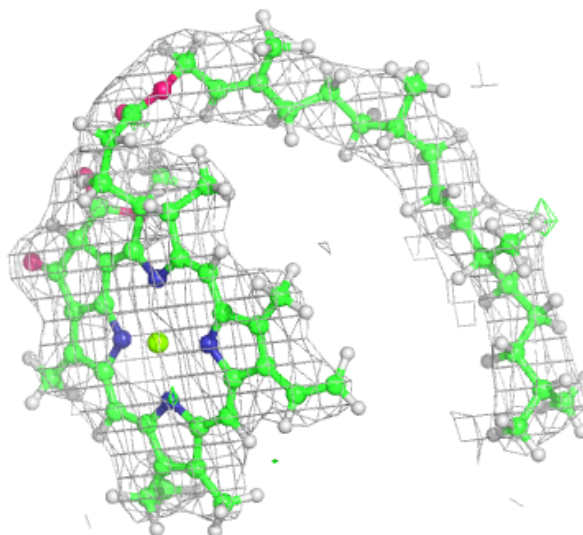
**Electron density around BCR c 514:**

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



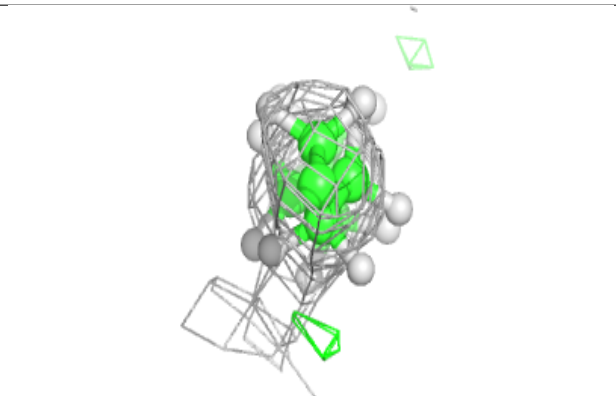
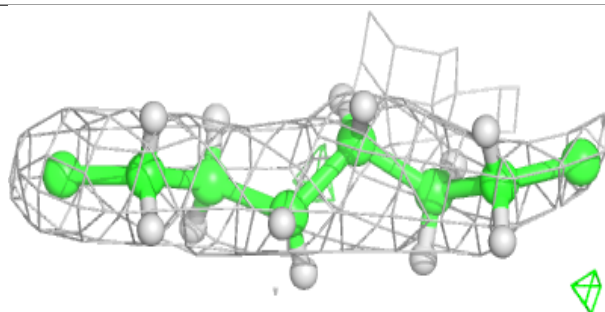
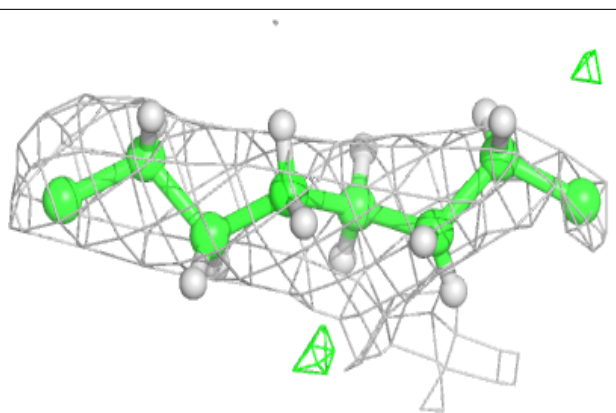
Electron density around CLA C 507:

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

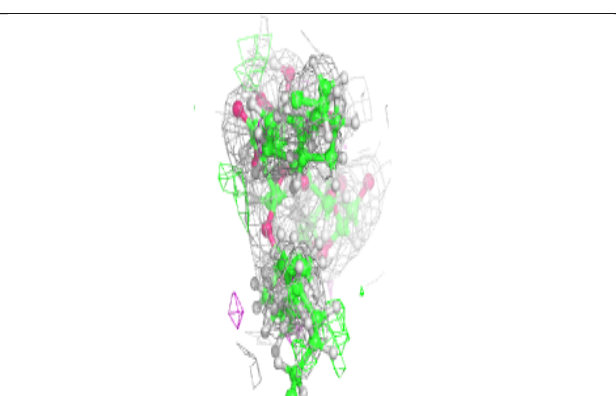
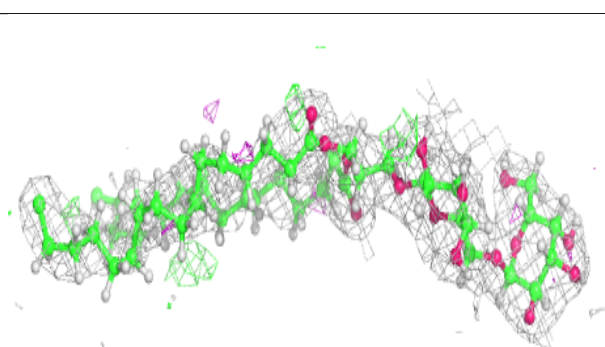
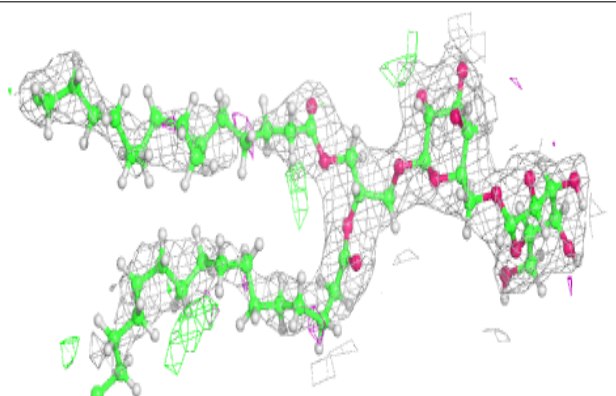


Electron density around STE Z 102:

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

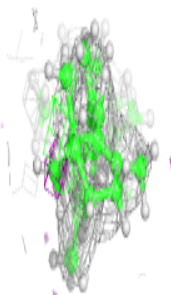
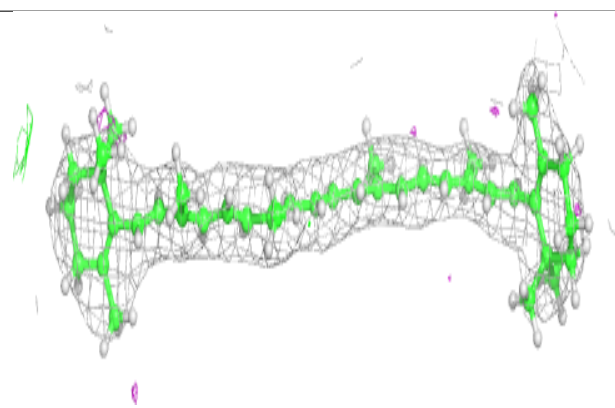
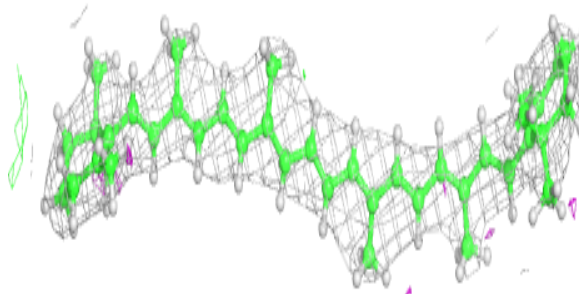
**Electron density around DGD c 518:**

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



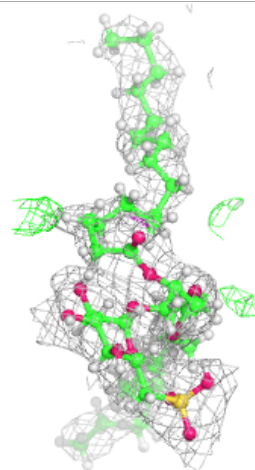
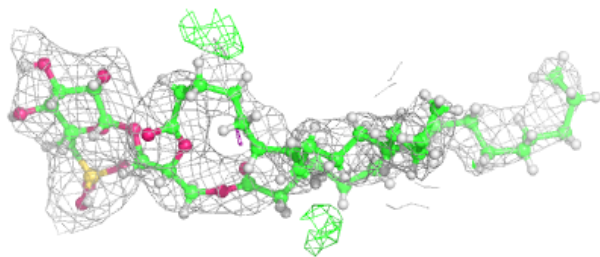
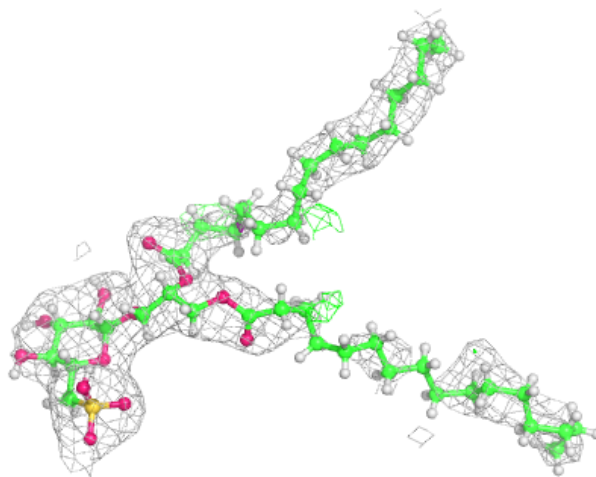
Electron density around BCR C 514:

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



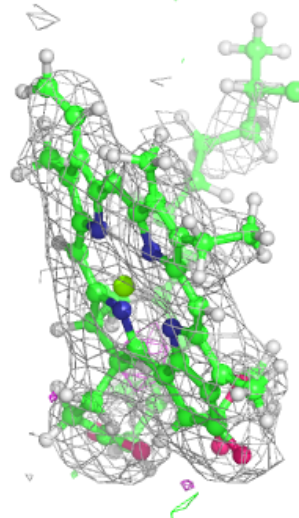
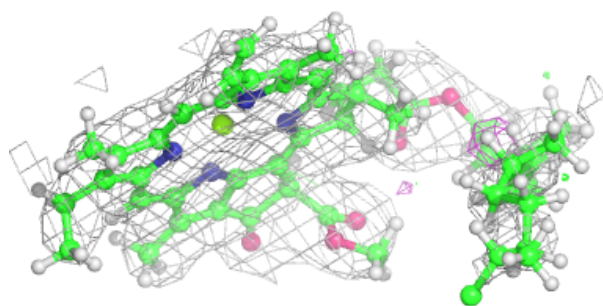
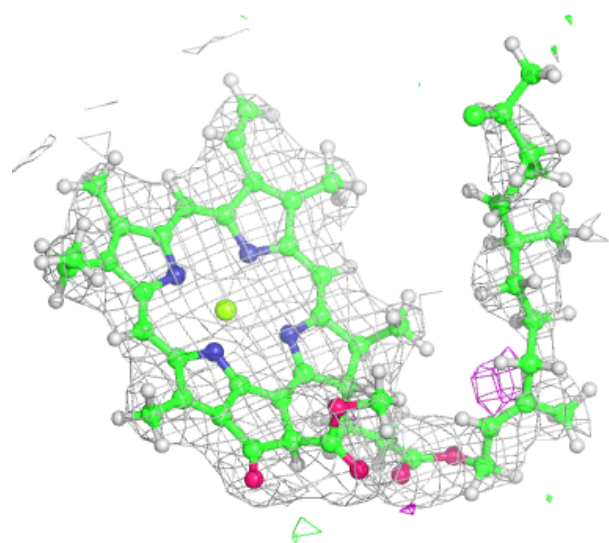
Electron density around SQD a 411:

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



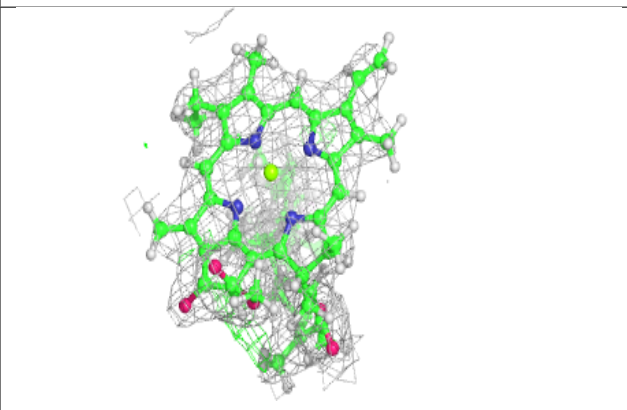
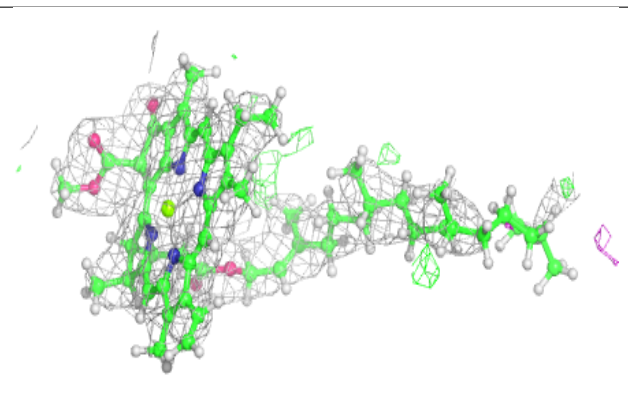
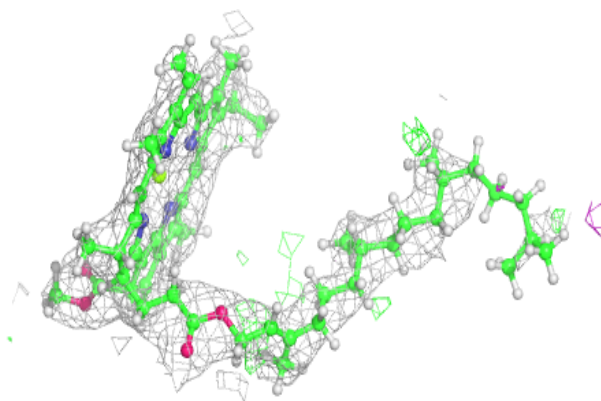
Electron density around CLA b 616:

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



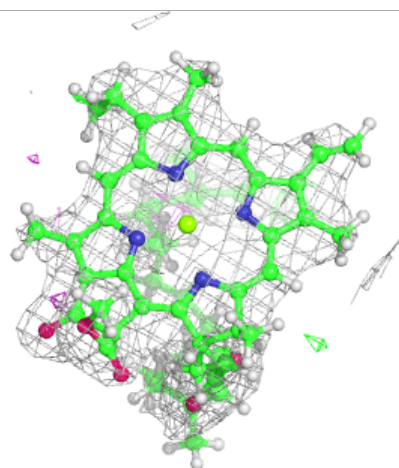
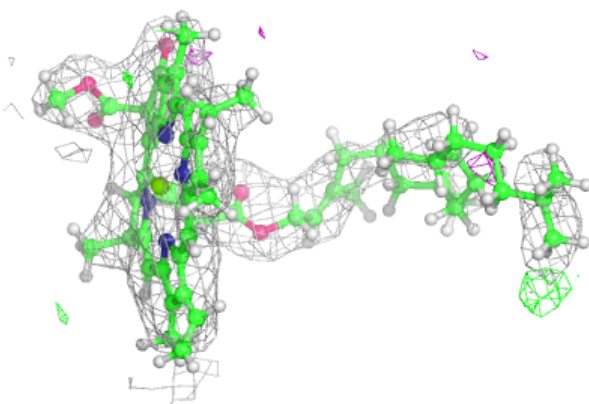
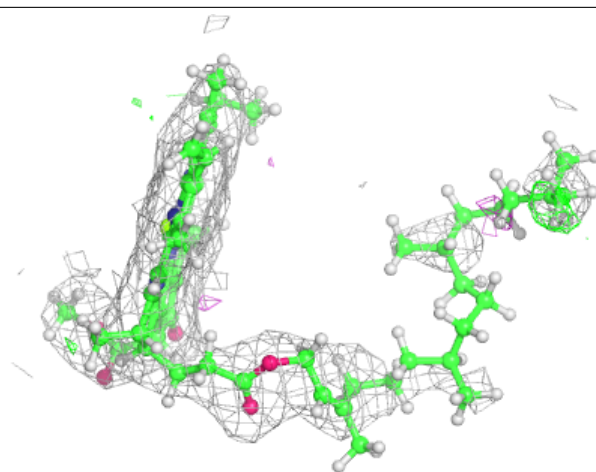
Electron density around CLA C 508:

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



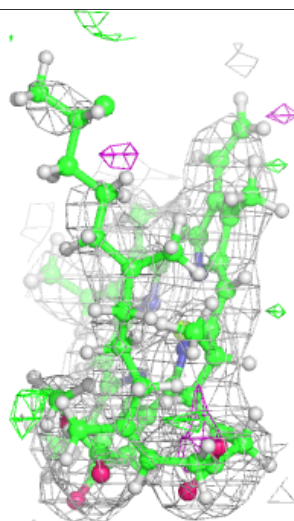
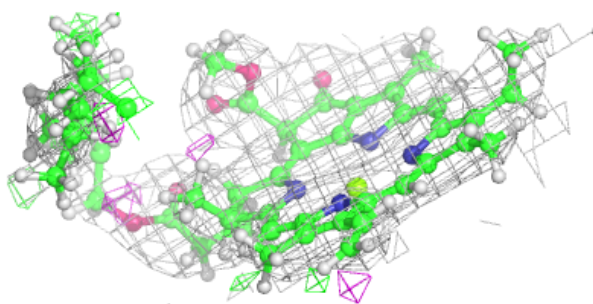
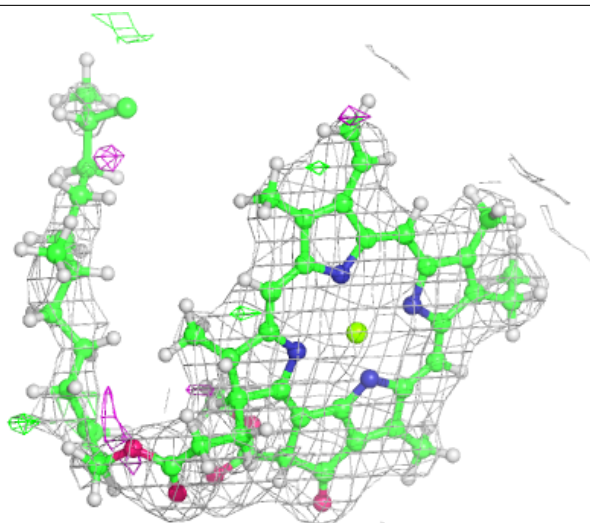
Electron density around CLA c 506:

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



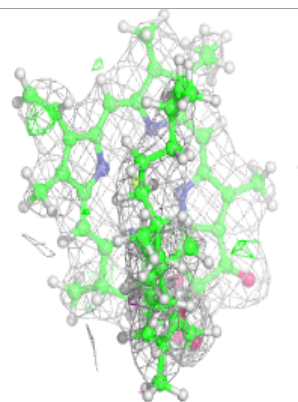
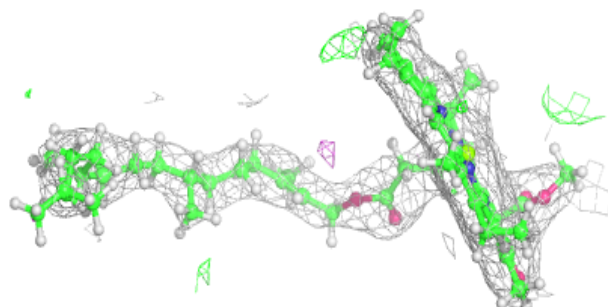
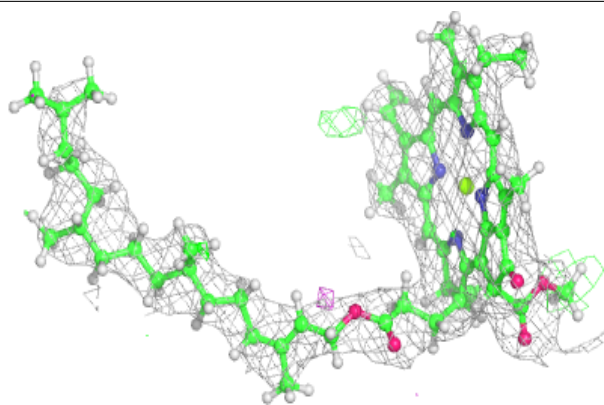
Electron density around CLA B 616:

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

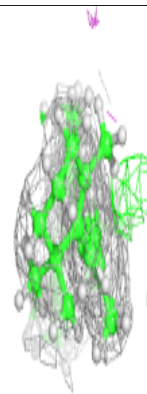
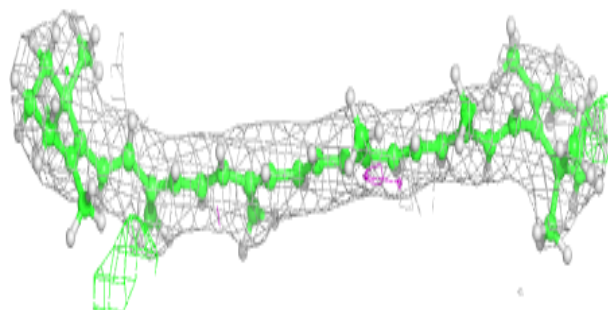
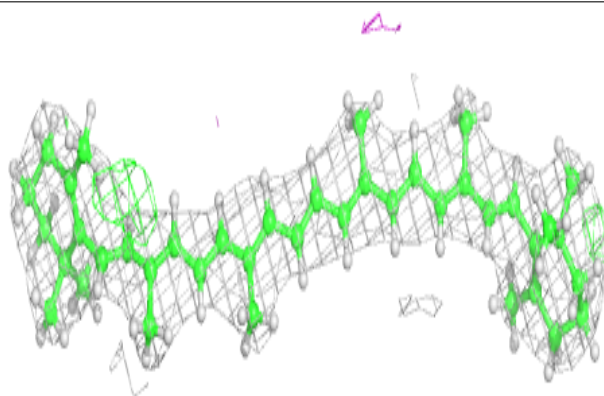


Electron density around CLA b 609:

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

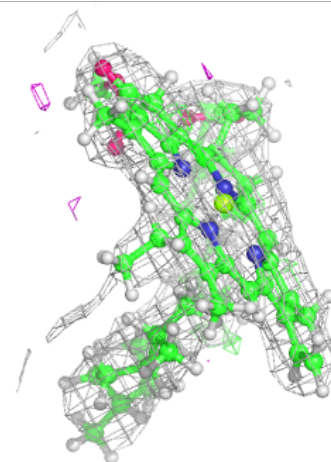
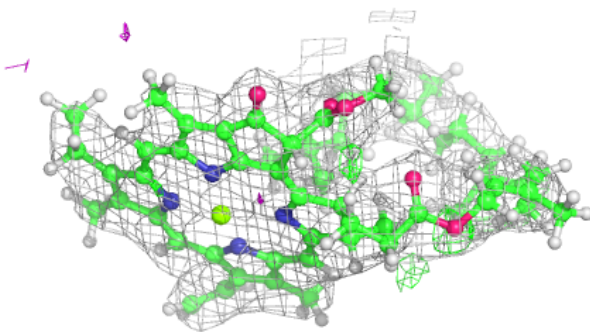
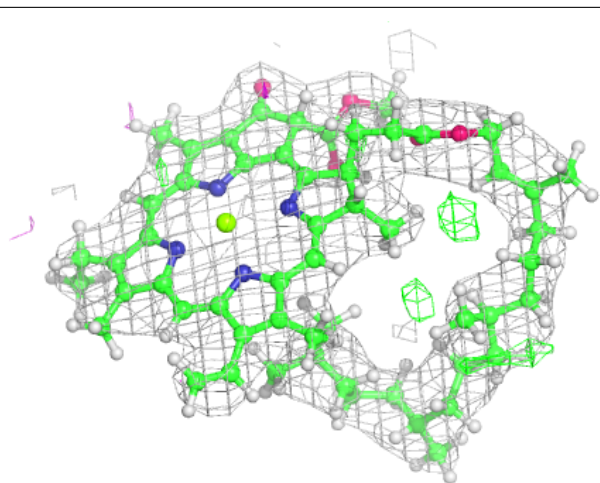
**Electron density around BCR B 619:**

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



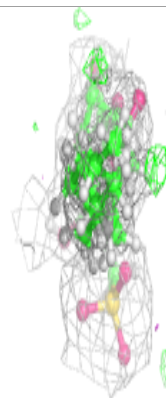
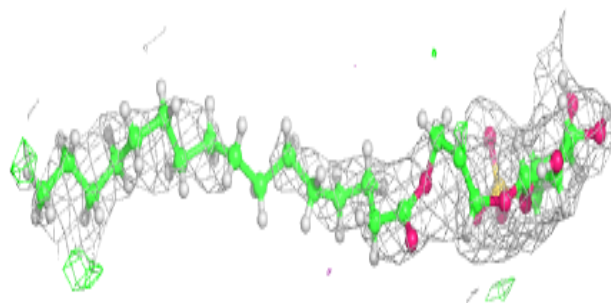
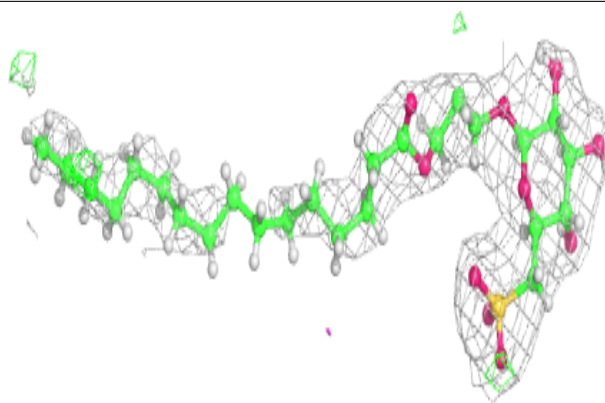
Electron density around CLA b 615:

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



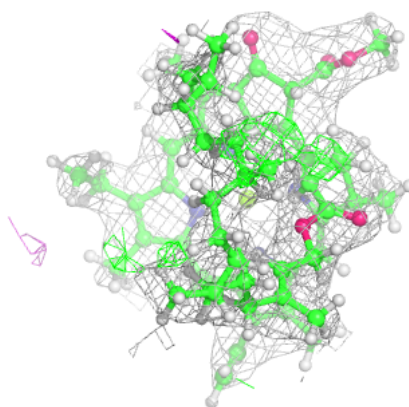
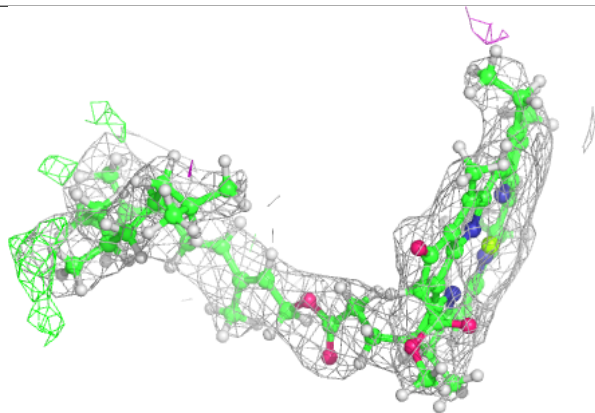
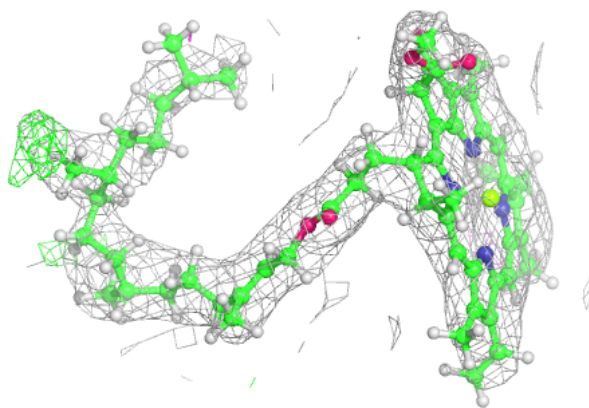
Electron density around SQD D 409:

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



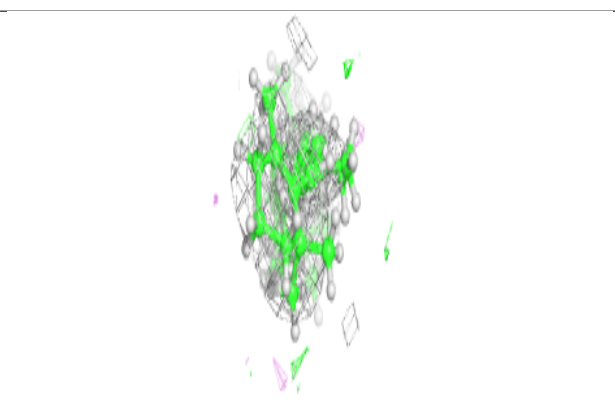
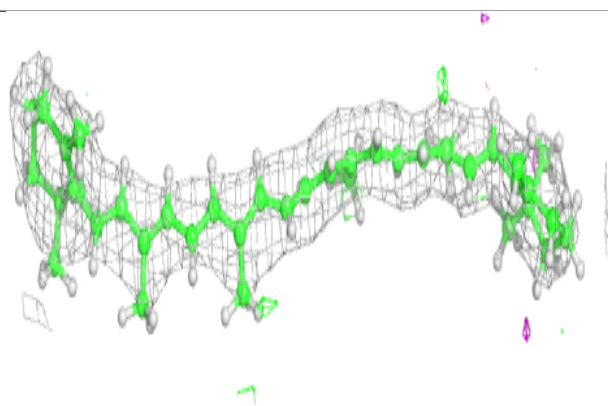
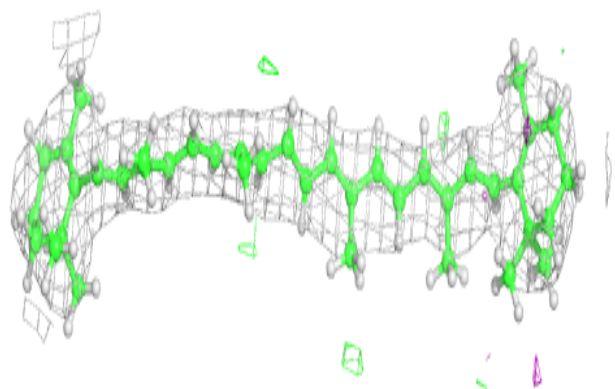
Electron density around CLA B 606:

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

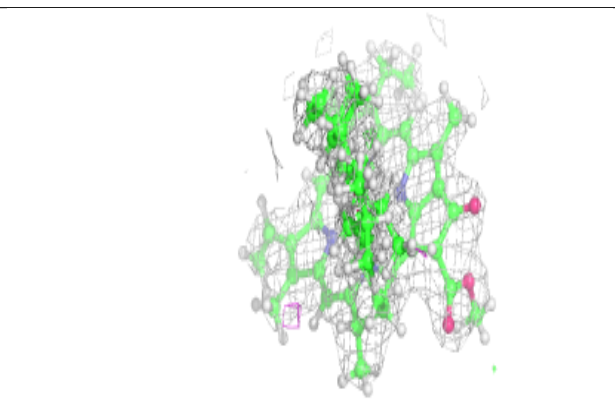
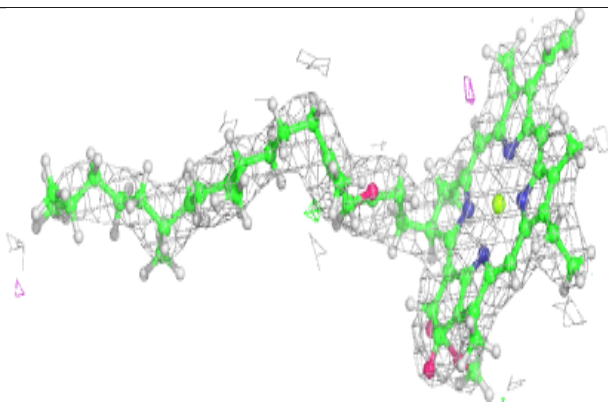
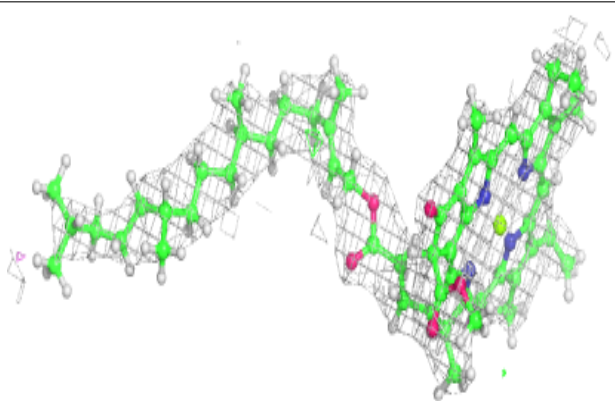


Electron density around BCR Z 101:

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

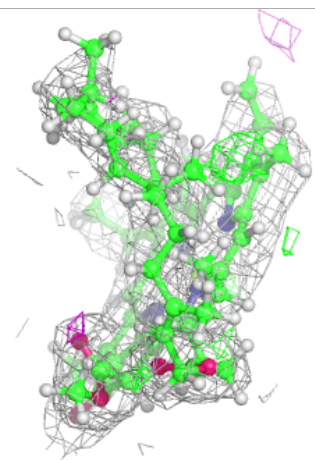
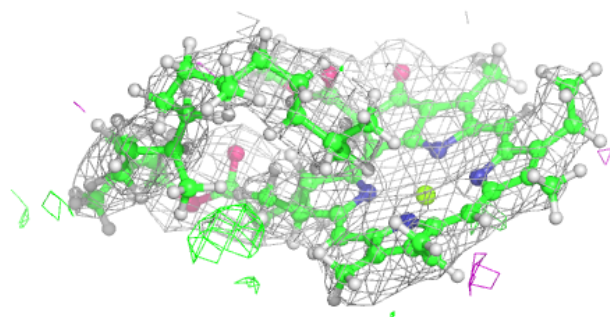
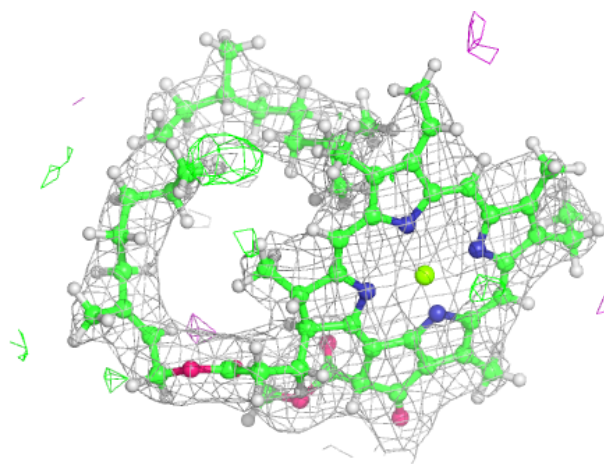
**Electron density around CLA C 502:**

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



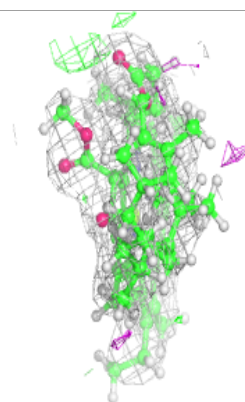
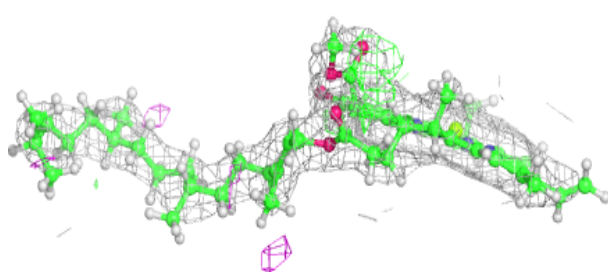
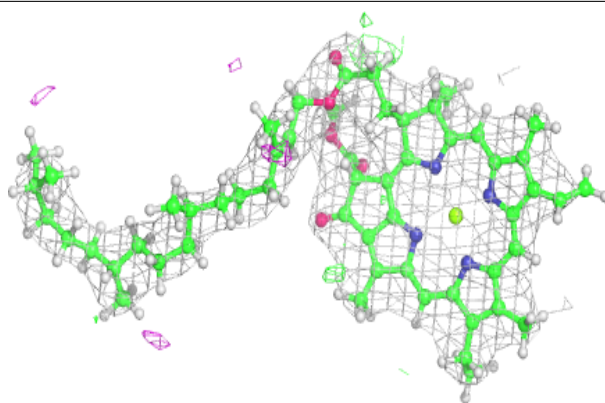
Electron density around CLA B 615:

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

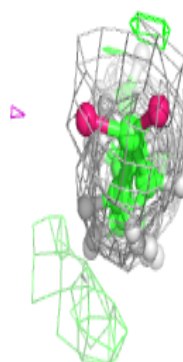
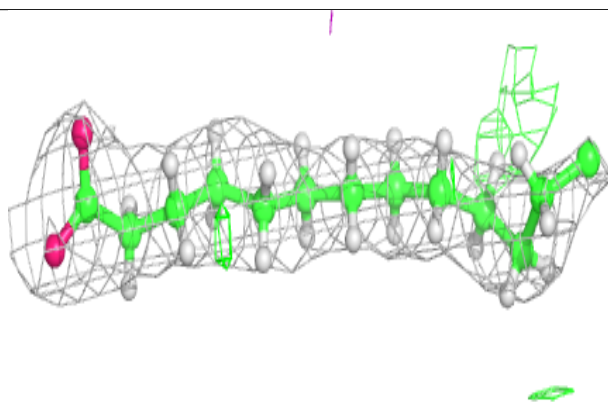
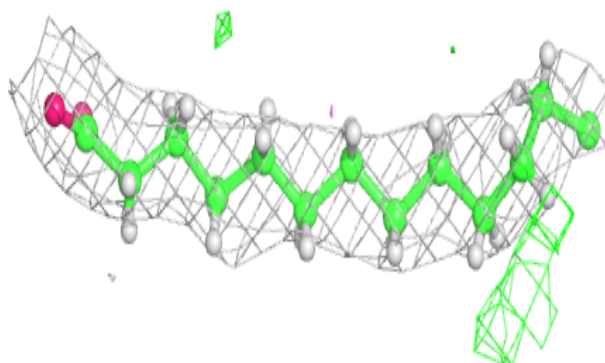


Electron density around CLA b 602:

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

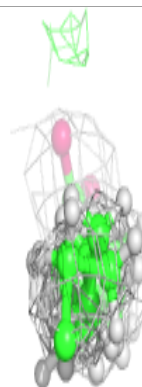
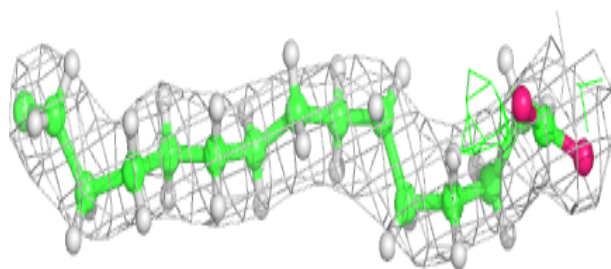
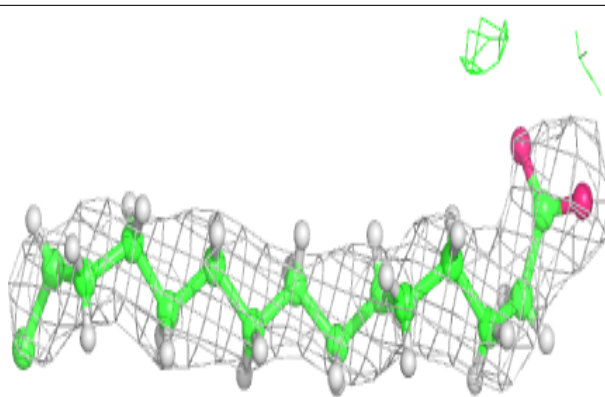
**Electron density around STE M 102:**

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



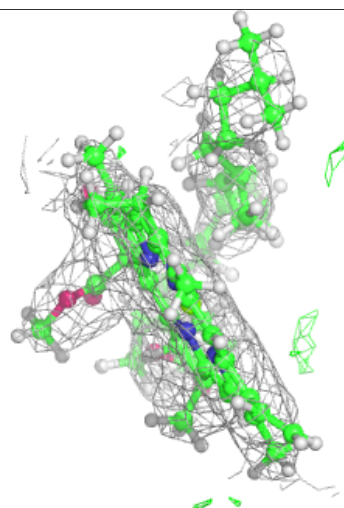
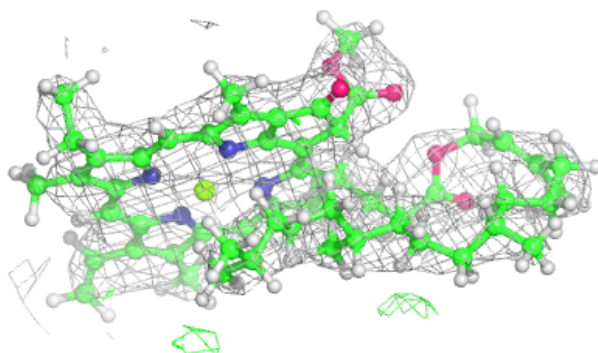
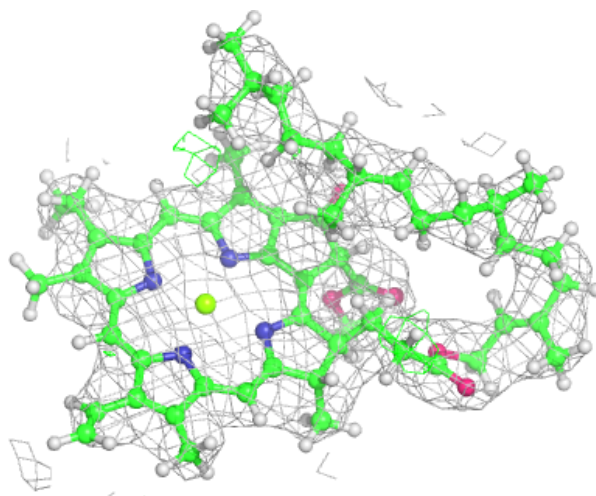
Electron density around STE d 411:

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



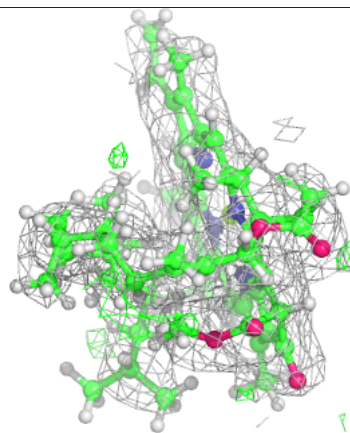
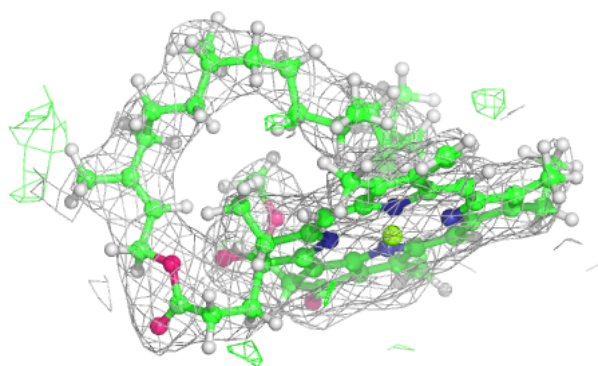
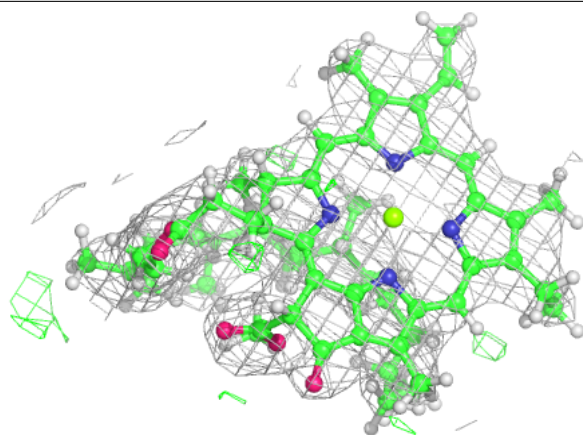
Electron density around CLA c 509:

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

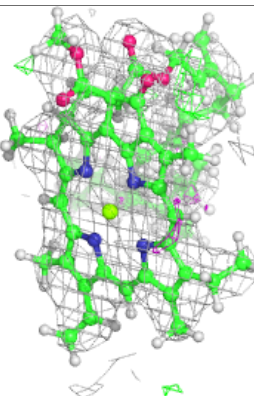
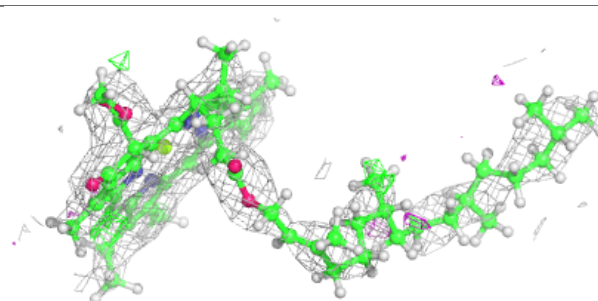
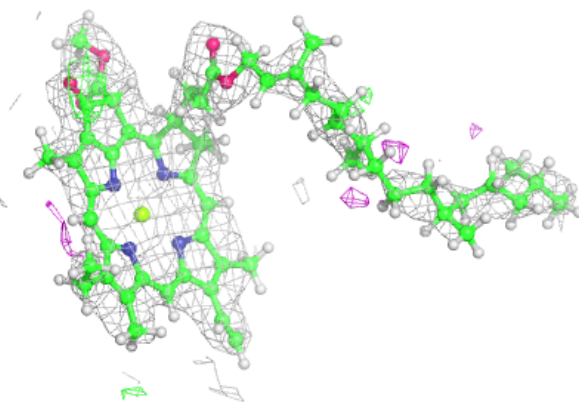


Electron density around CLA c 510:

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

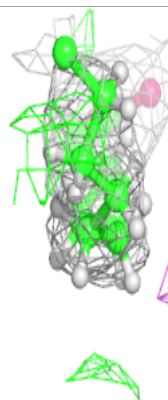
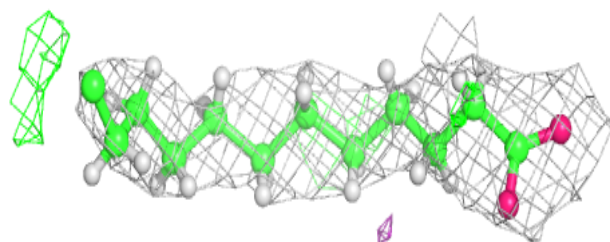
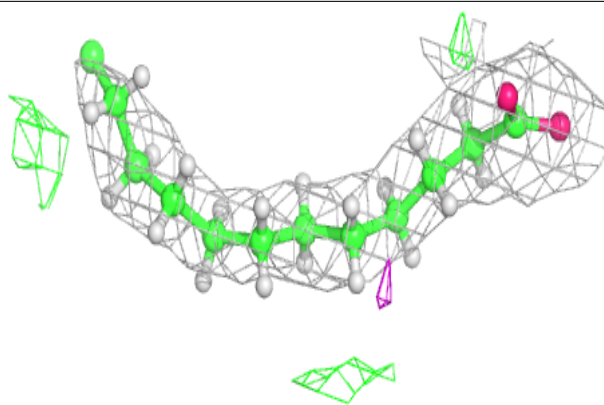
**Electron density around CLA c 511:**

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



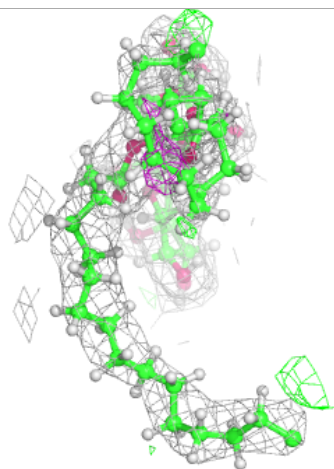
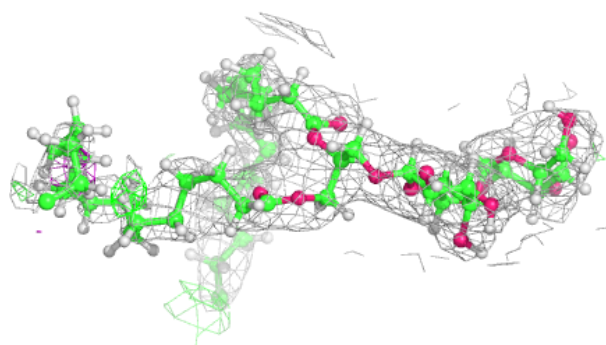
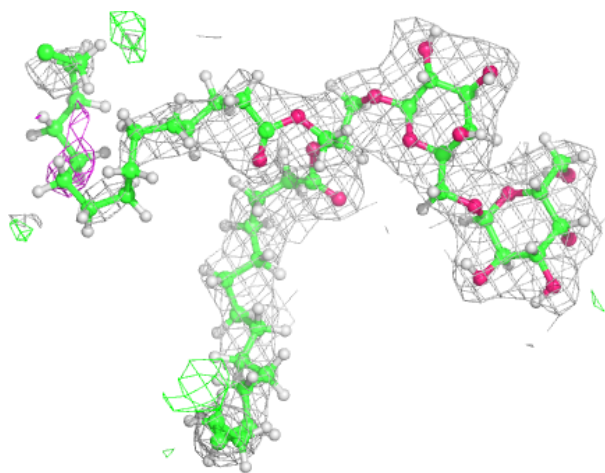
Electron density around STE t 103:

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



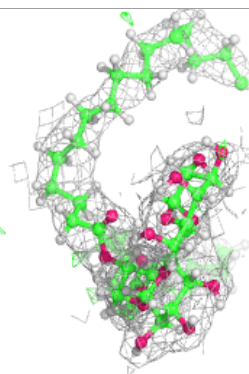
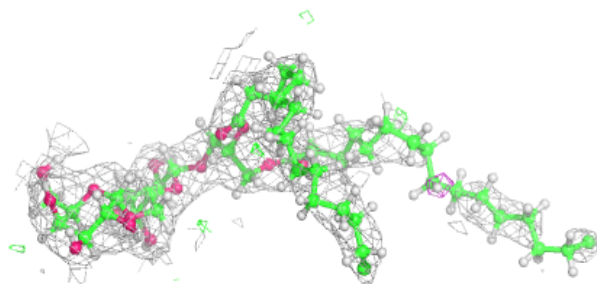
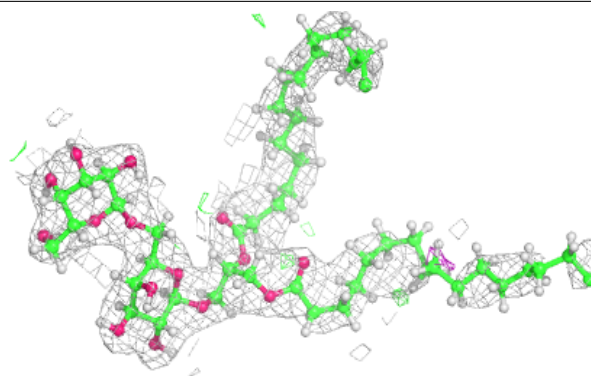
Electron density around DGD C 516:

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

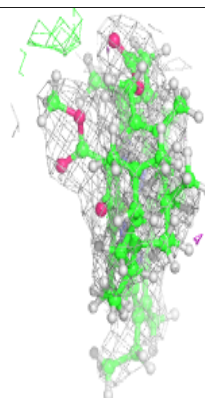
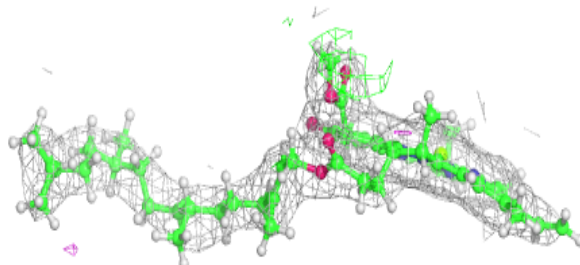
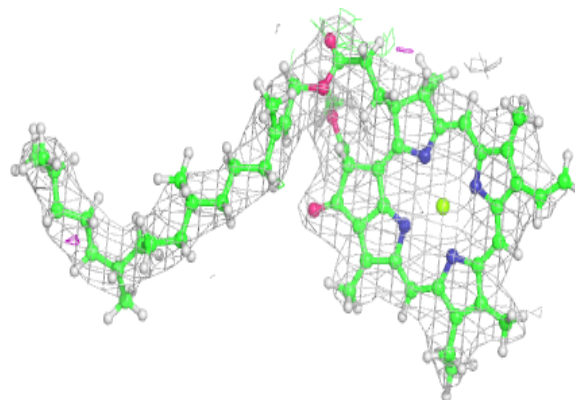


Electron density around DGD c 517:

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

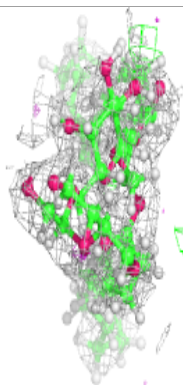
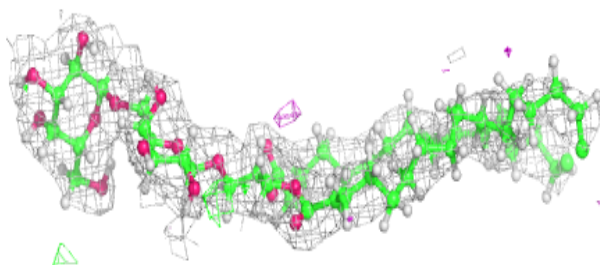
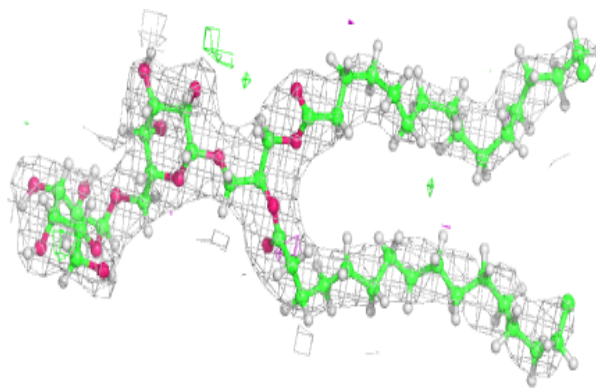
**Electron density around CLA B 602:**

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

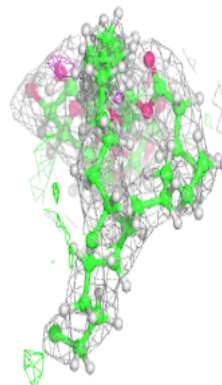
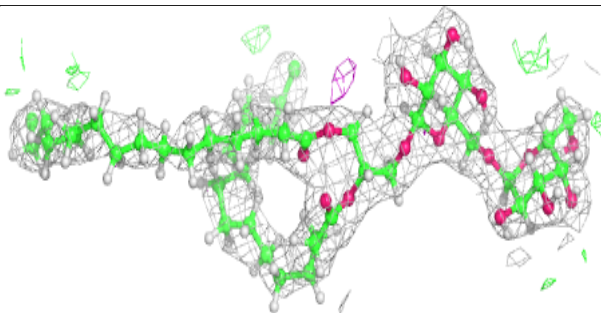
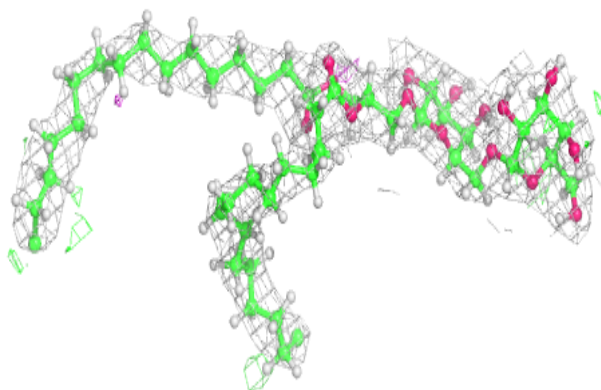


Electron density around DGD C 517:

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

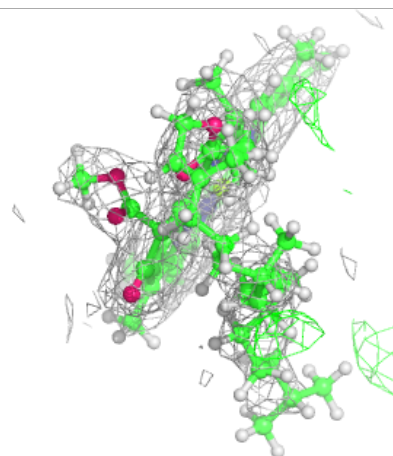
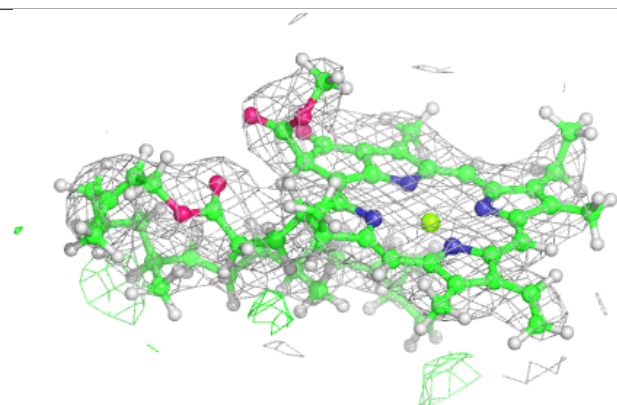
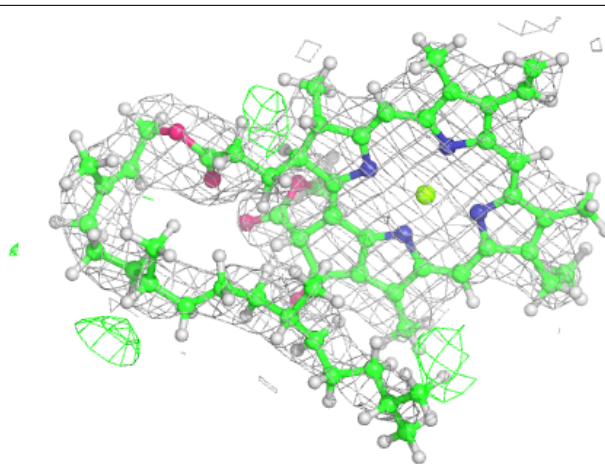
**Electron density around DGD H 102:**

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



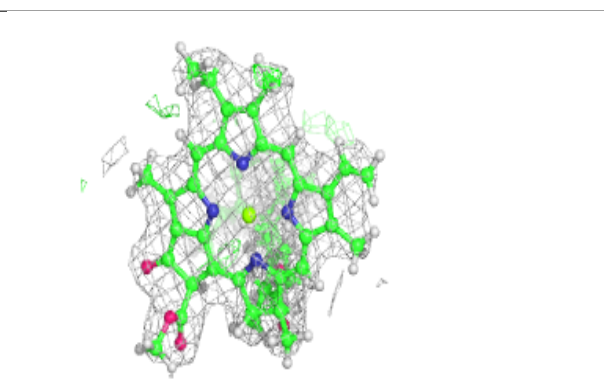
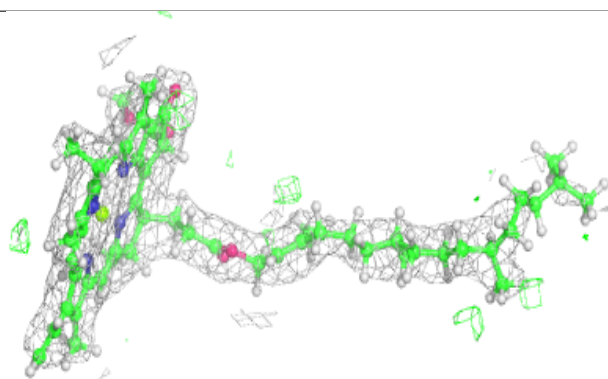
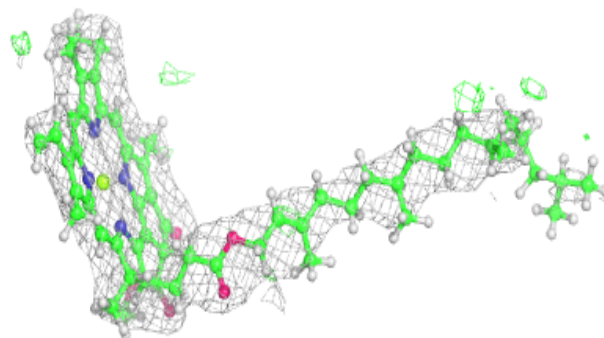
Electron density around CLA C 509:

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

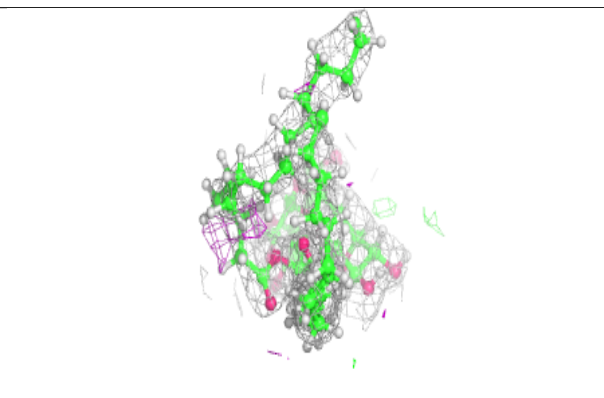
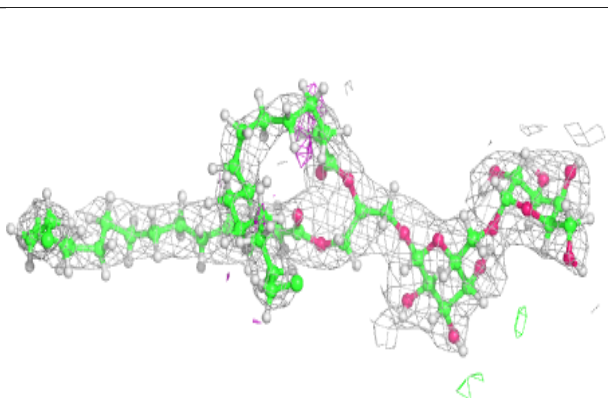
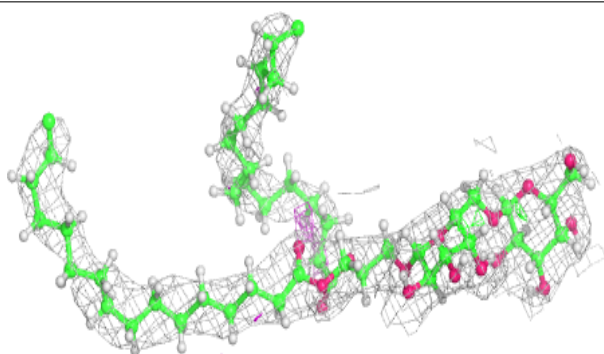


Electron density around CLA b 604:

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

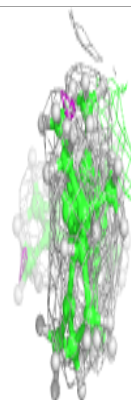
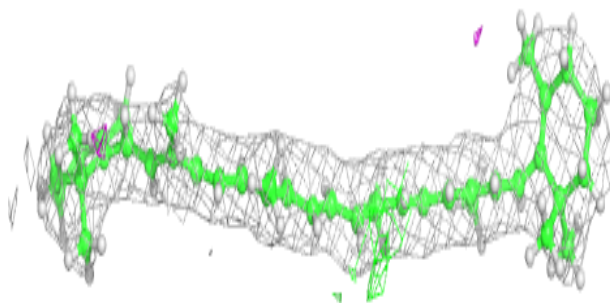
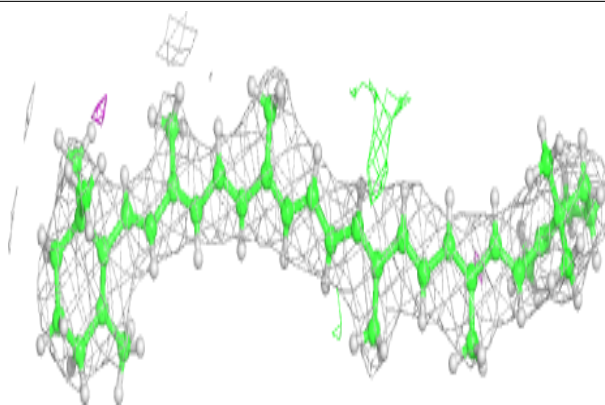
**Electron density around DGD h 101:**

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

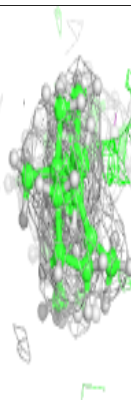
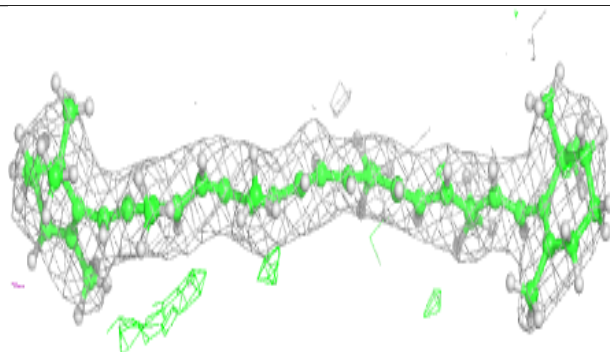
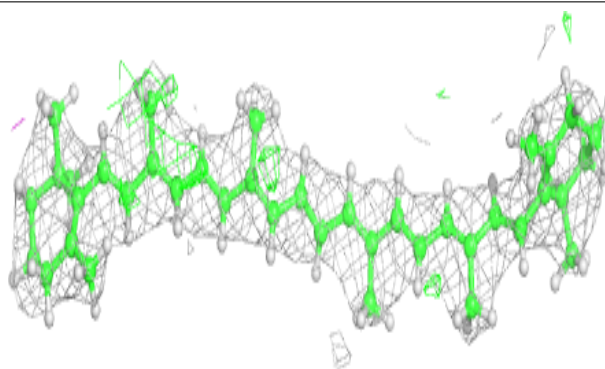


Electron density around BCR B 617:

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

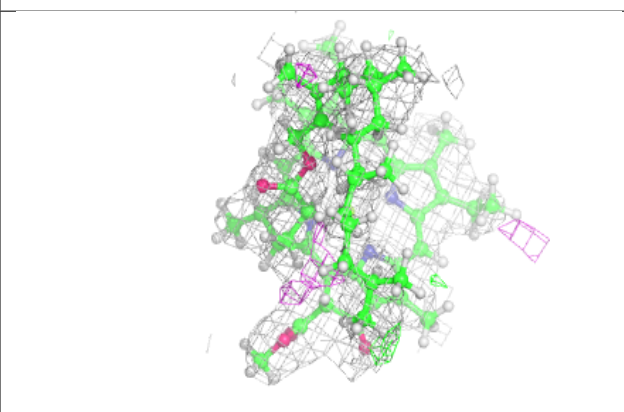
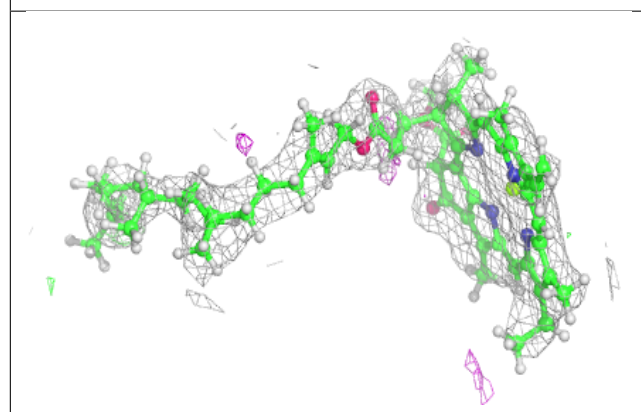
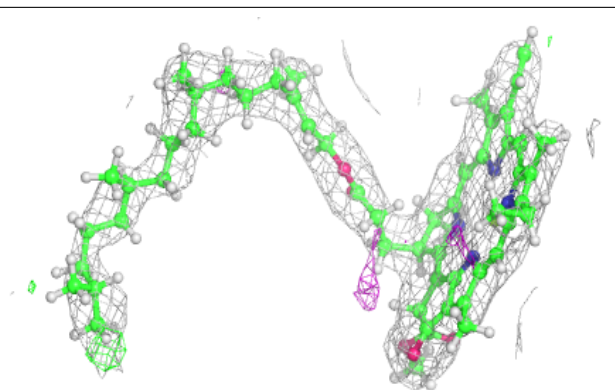
**Electron density around BCR B 618:**

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

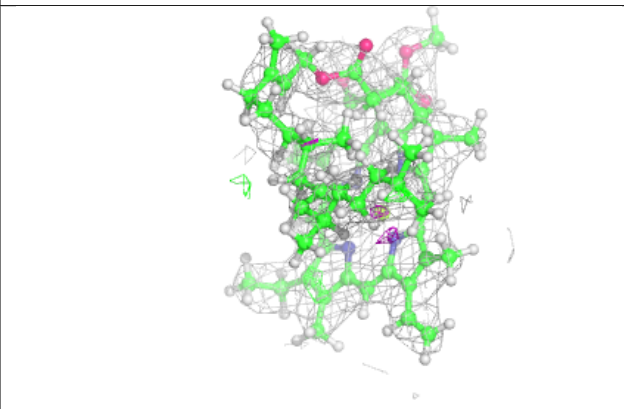
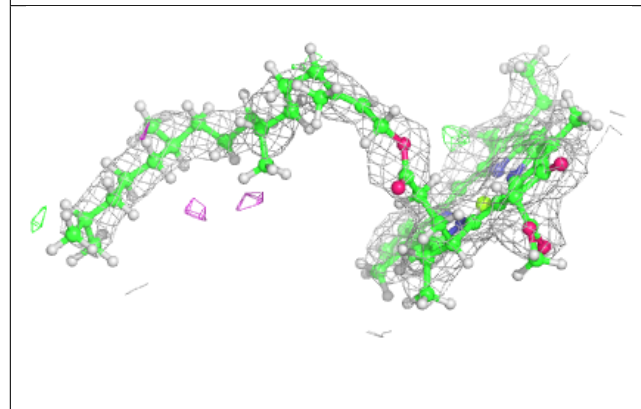
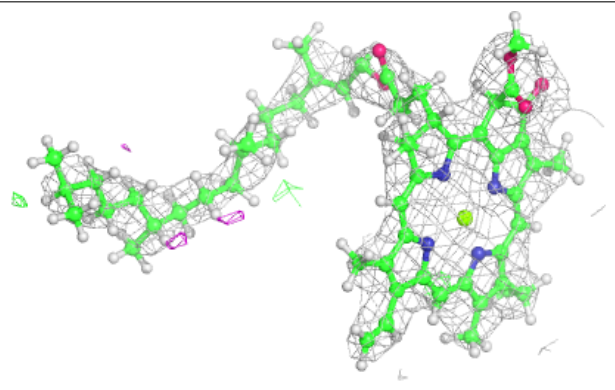


Electron density around CLA b 606:

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

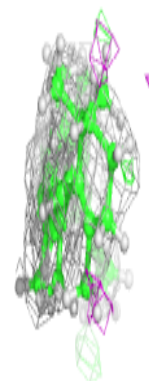
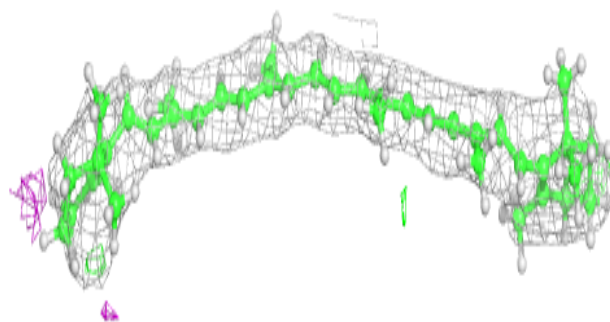
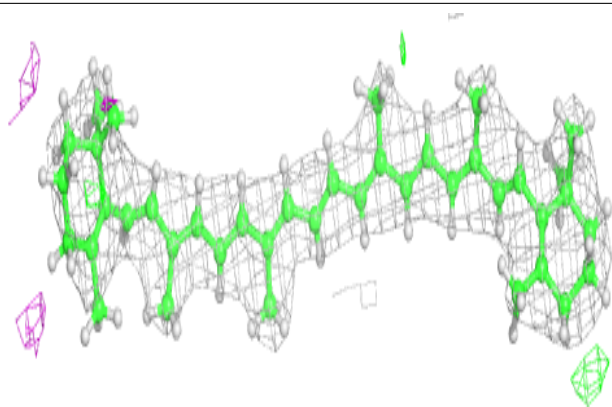
**Electron density around CLA C 511:**

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



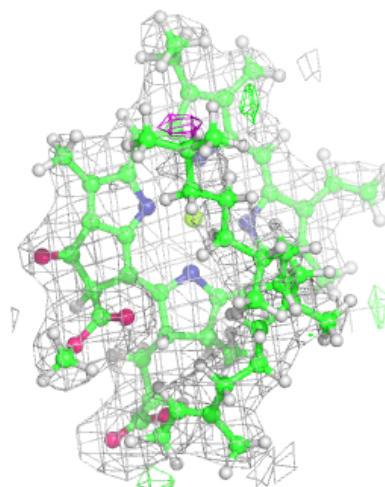
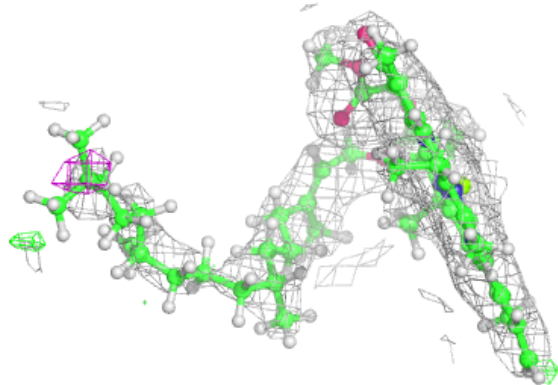
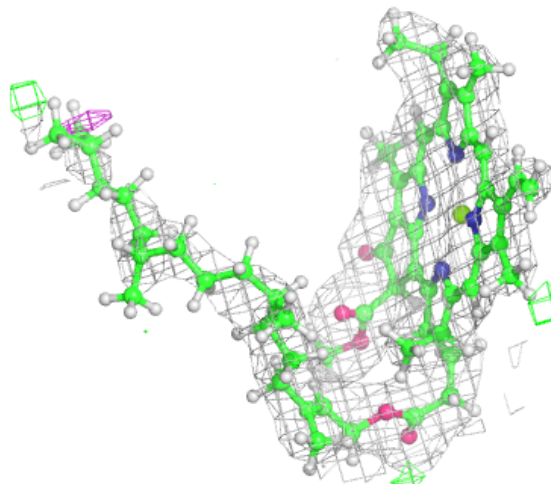
Electron density around BCR D 406:

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



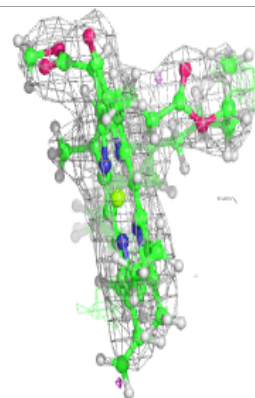
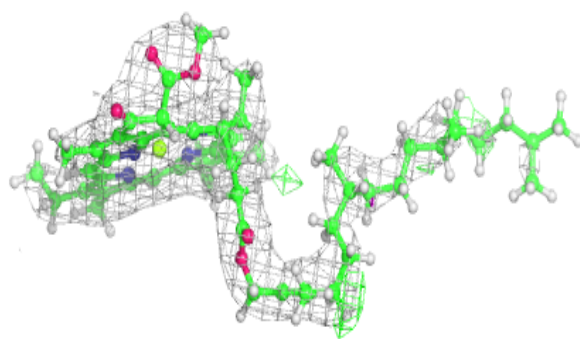
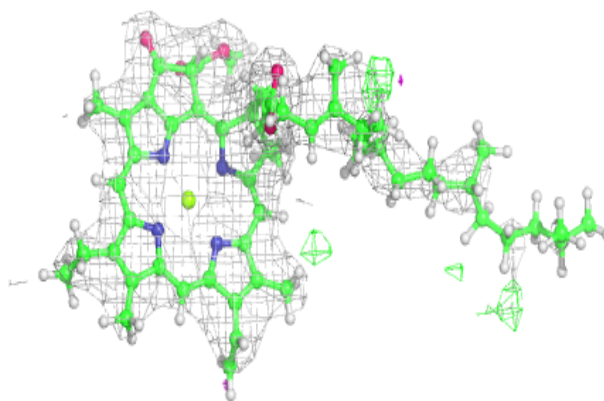
Electron density around CLA b 613:

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

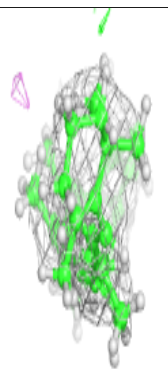
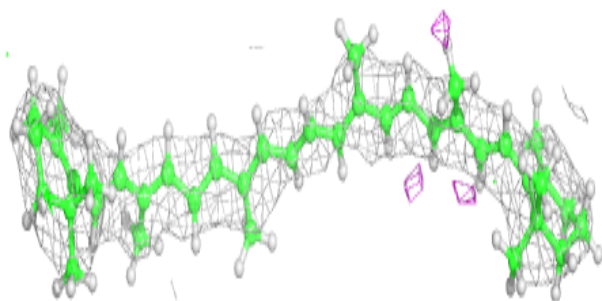
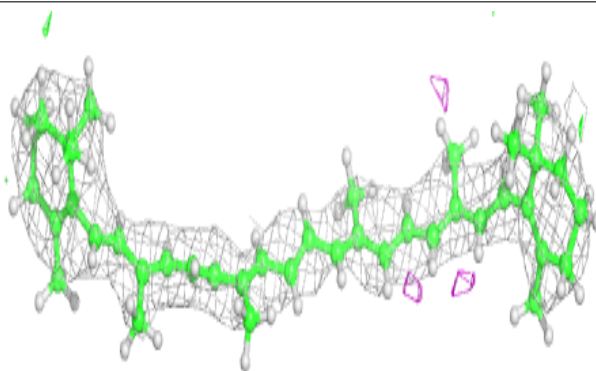


Electron density around CLA d 401:

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

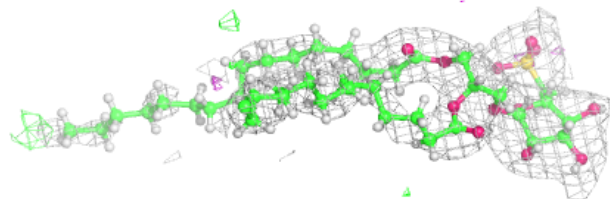
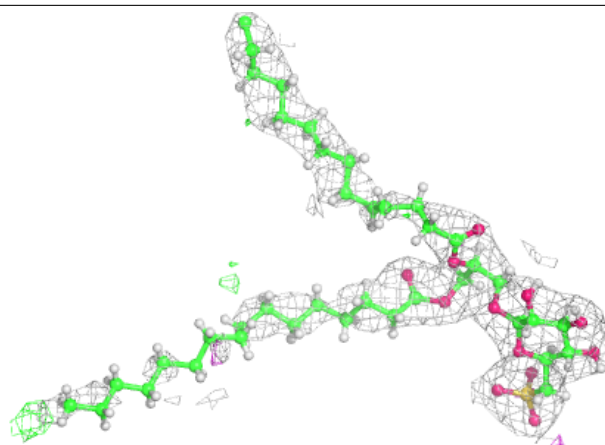
**Electron density around BCR K 102:**

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

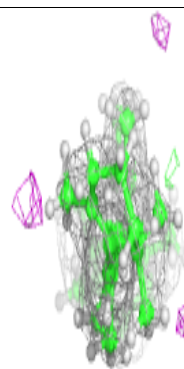
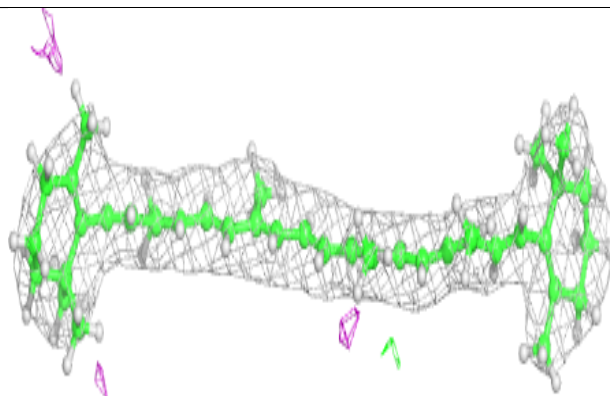
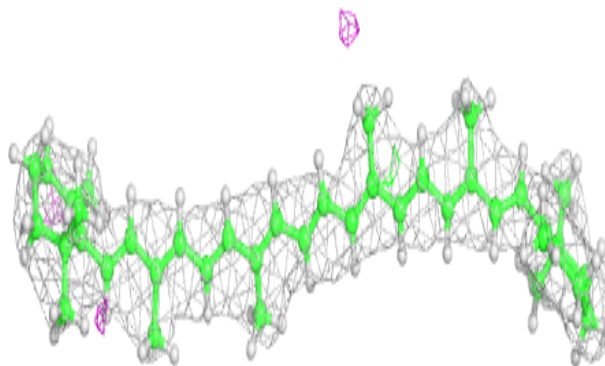


Electron density around SQD A 410:

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

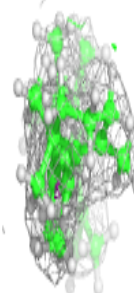
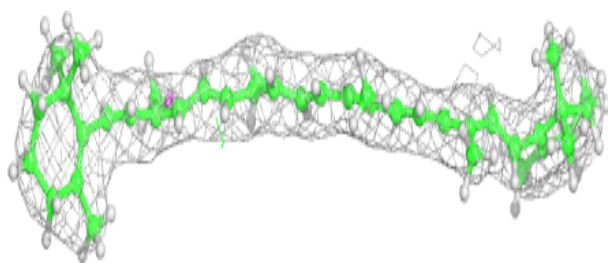
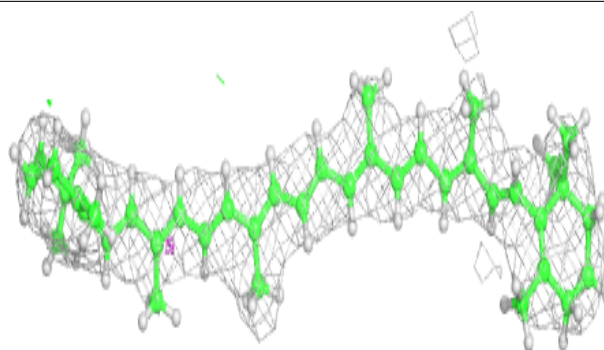
**Electron density around BCR a 405:**

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

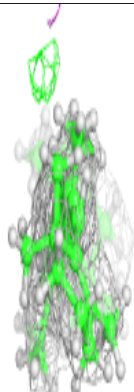
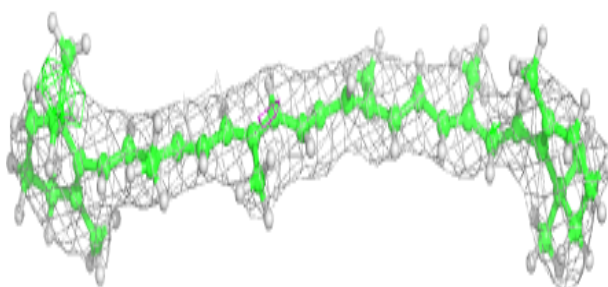
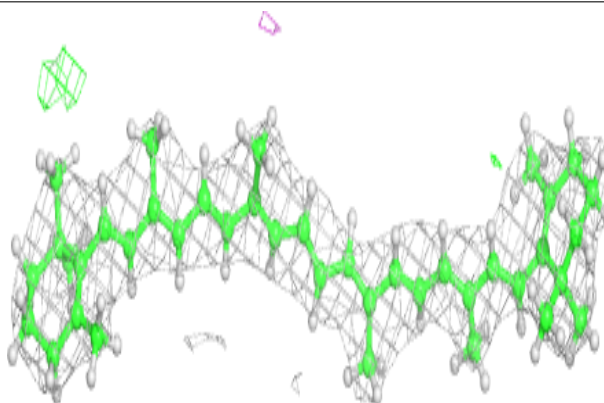


Electron density around BCR b 617:

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

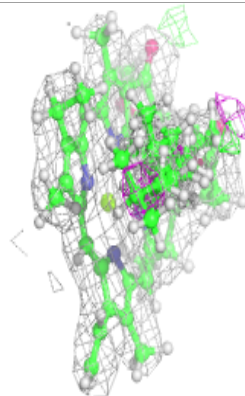
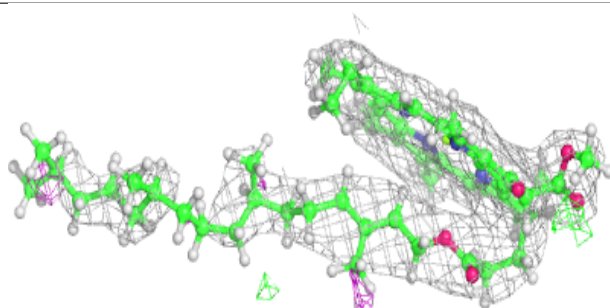
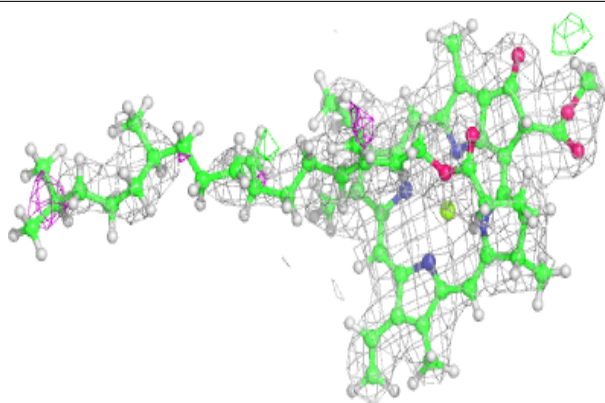
**Electron density around BCR b 619:**

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

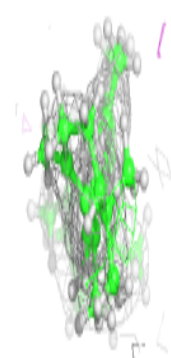
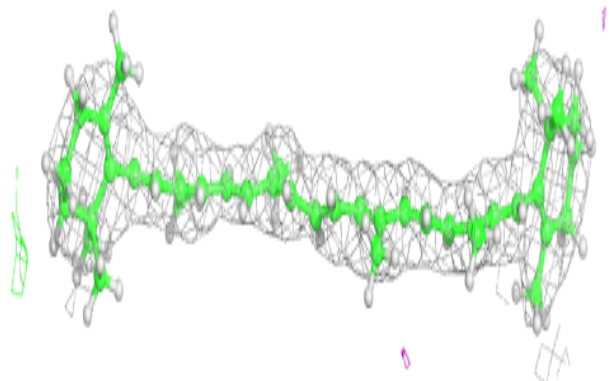
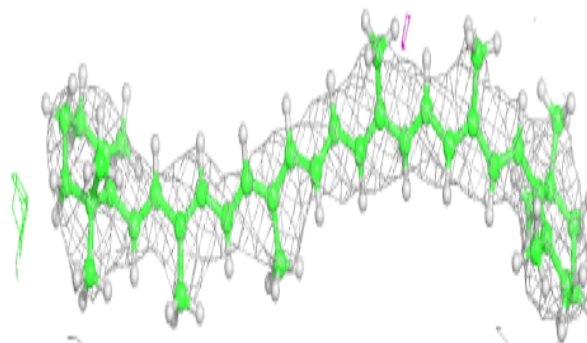


Electron density around CLA b 614:

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

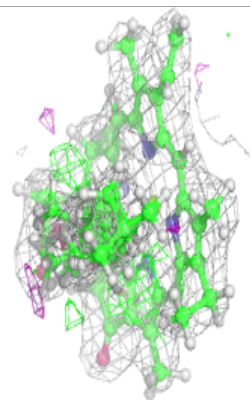
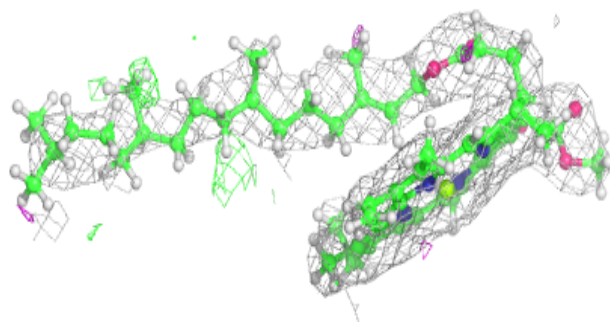
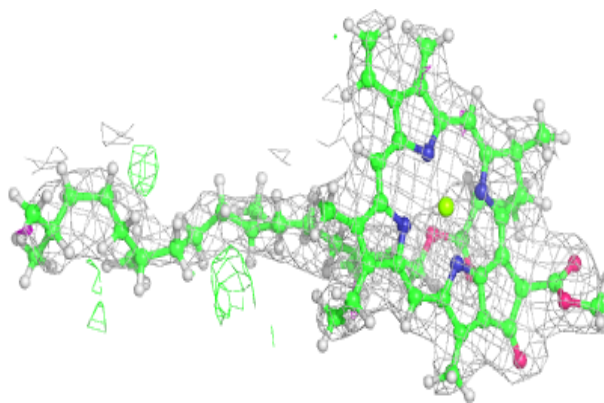
**Electron density around BCR c 515:**

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

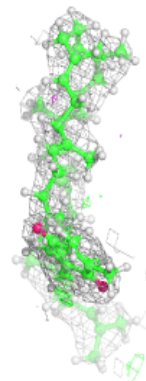
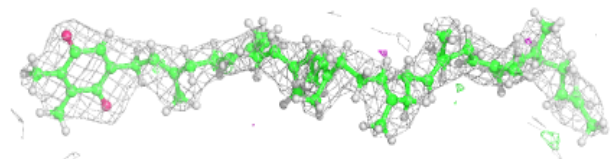
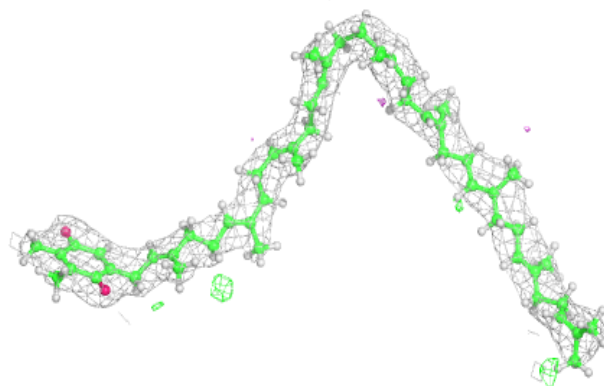


Electron density around CLA B 614:

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

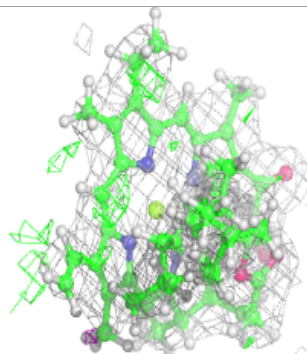
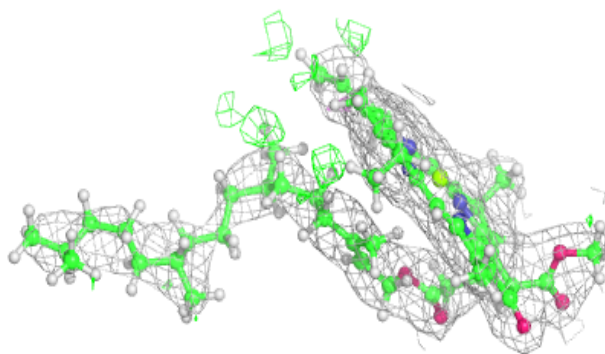
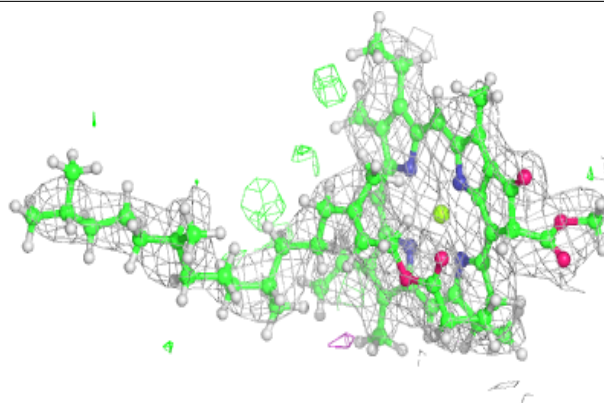
**Electron density around PL9 D 407:**

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

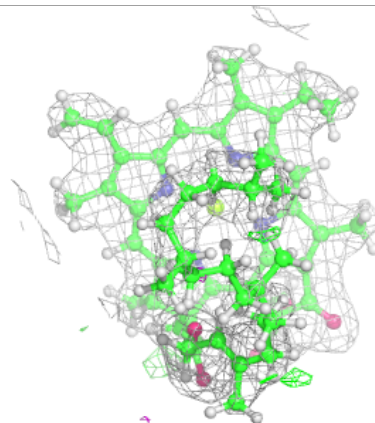
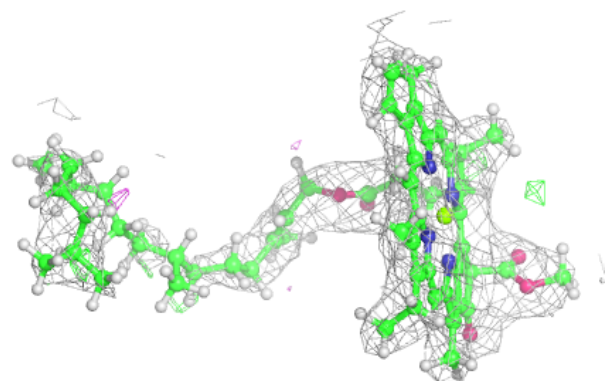
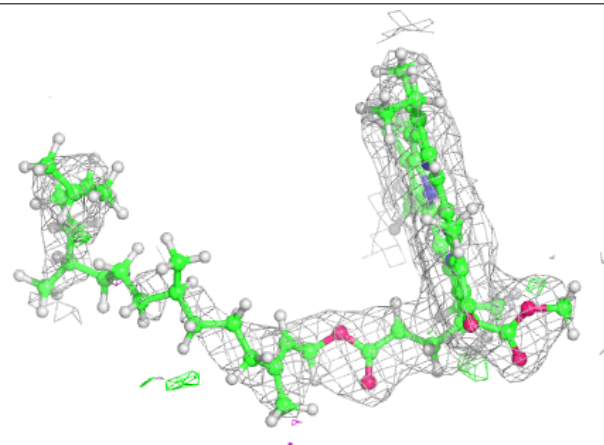


Electron density around CLA C 505:

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

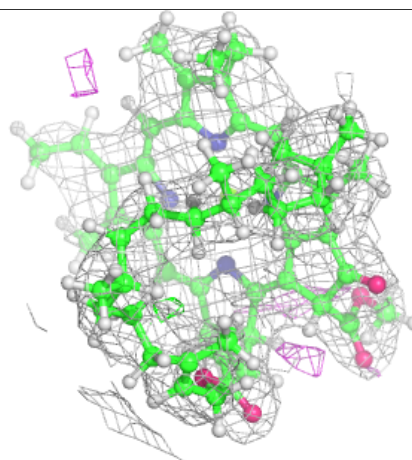
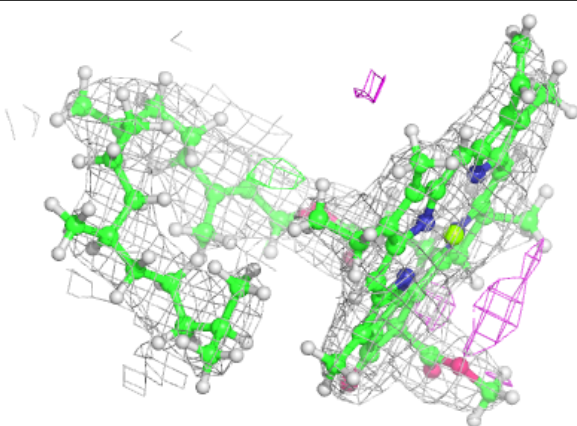
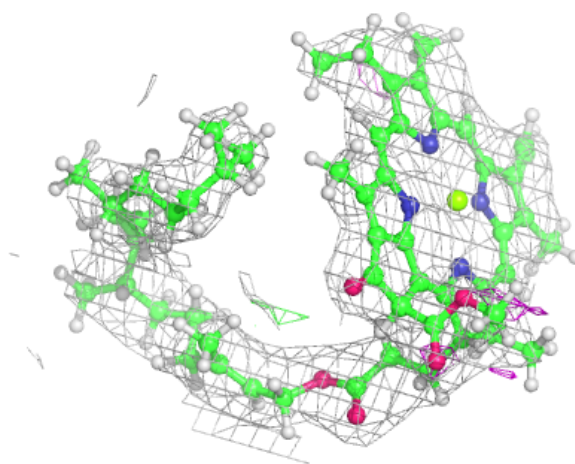
**Electron density around CLA C 506:**

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



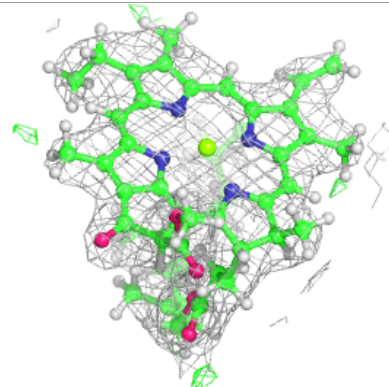
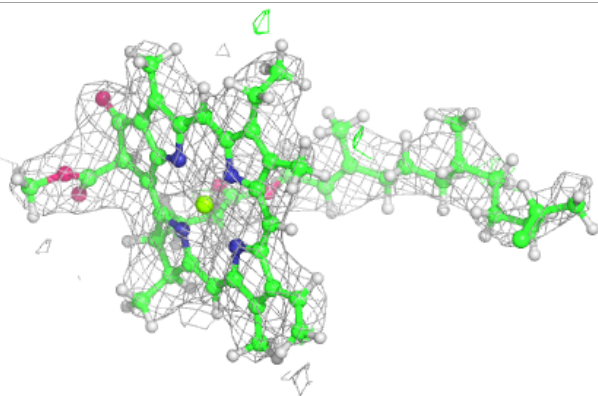
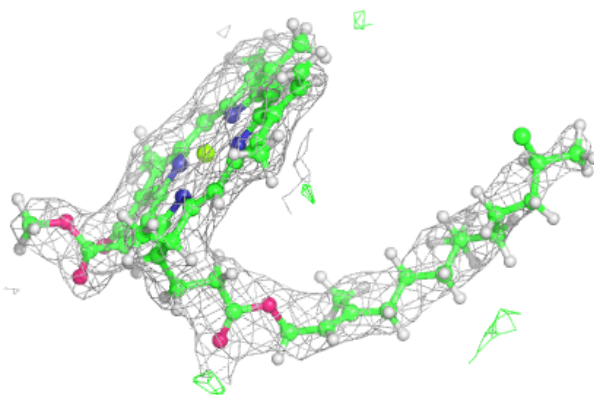
Electron density around CLA c 503:

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

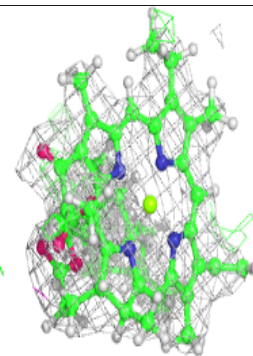
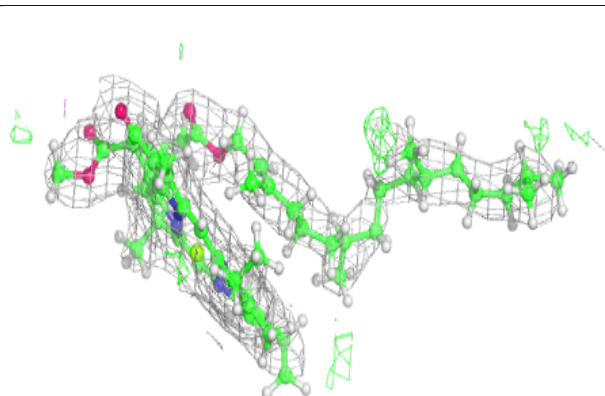
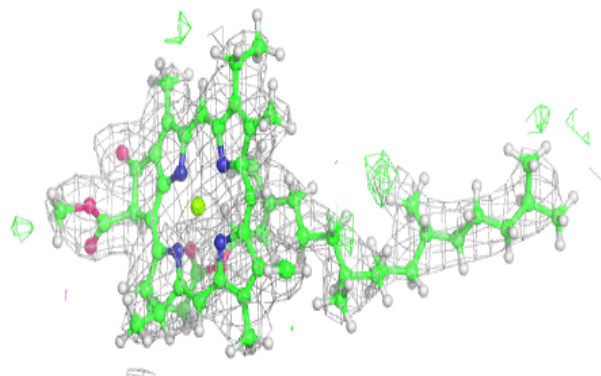


Electron density around CLA c 504:

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

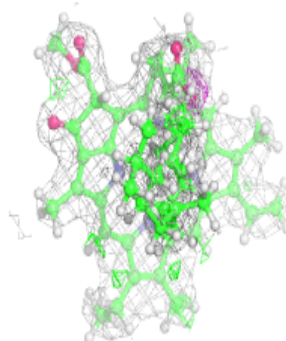
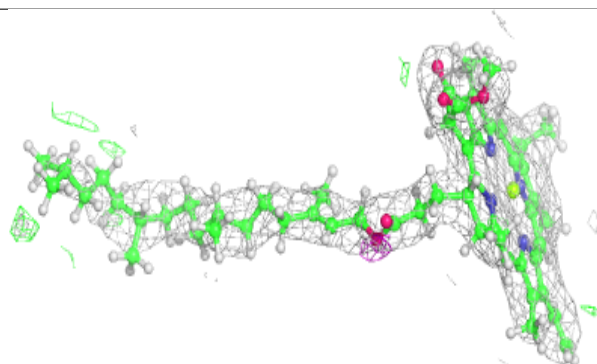
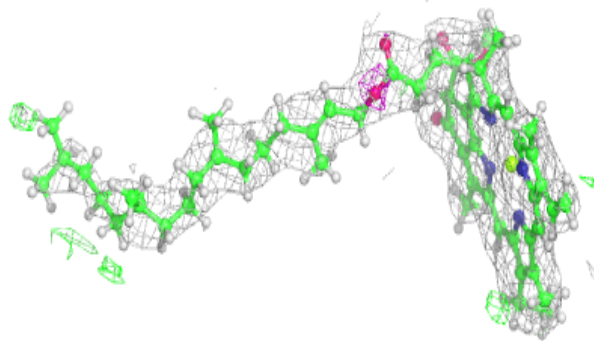
**Electron density around CLA c 505:**

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



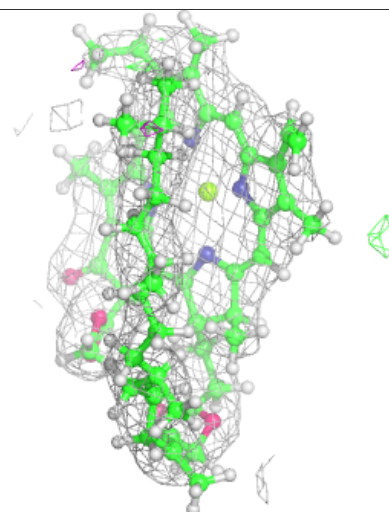
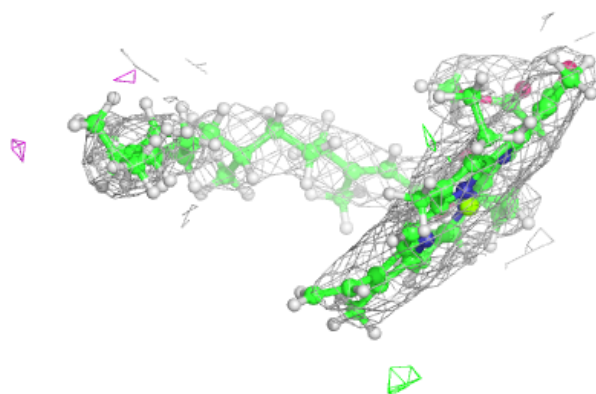
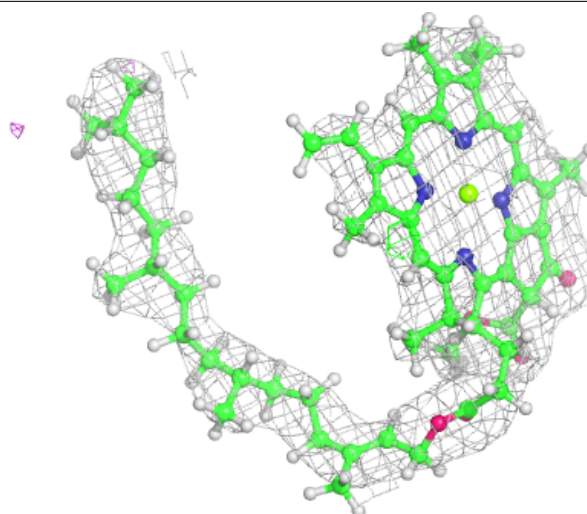
Electron density around CLA B 604:

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



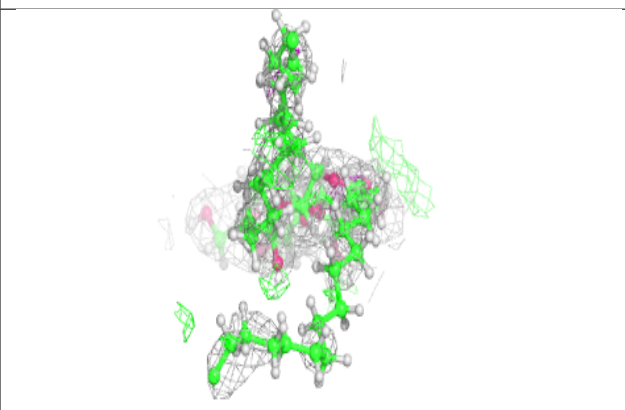
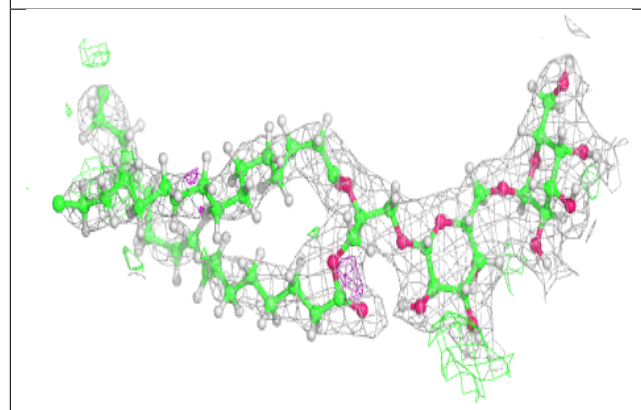
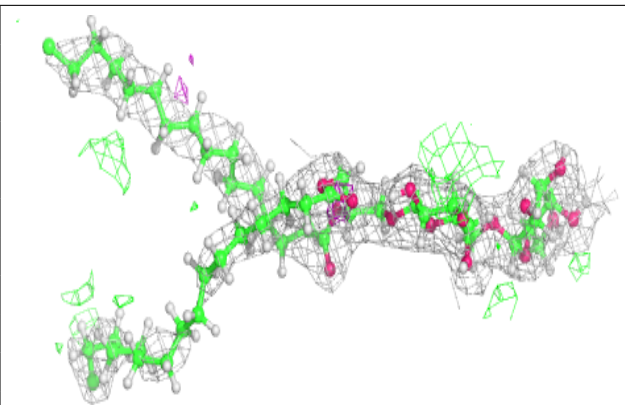
Electron density around CLA c 507:

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

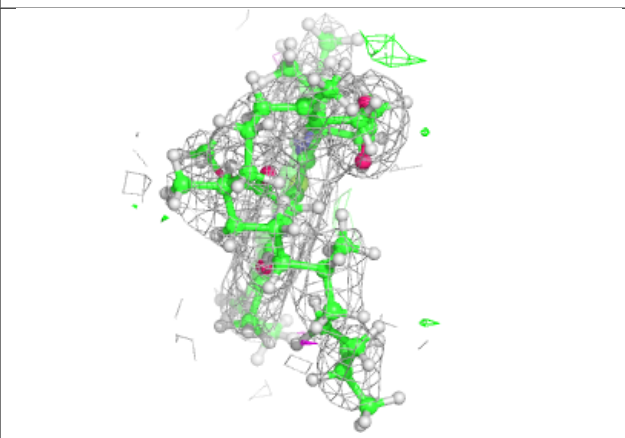
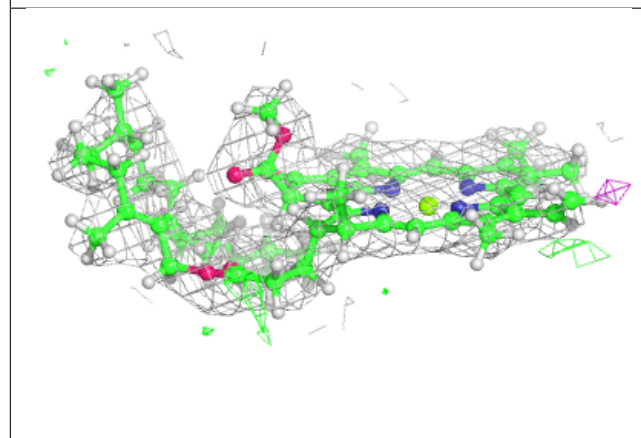
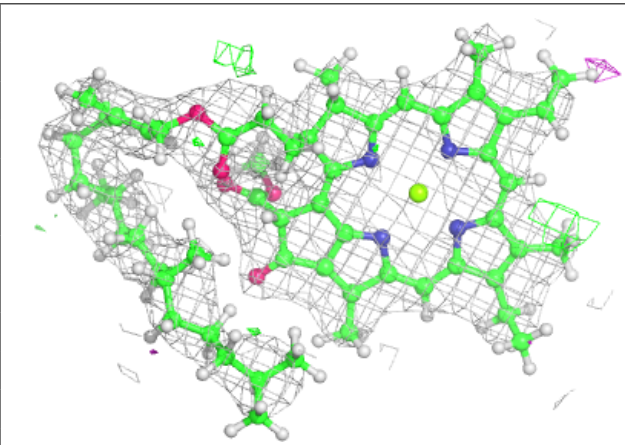


Electron density around DGD C 515:

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

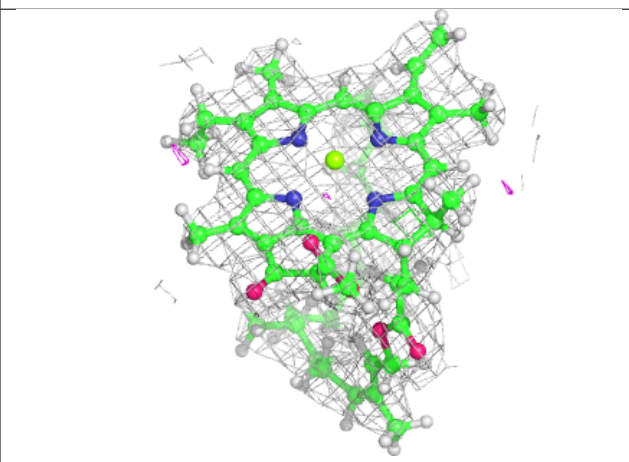
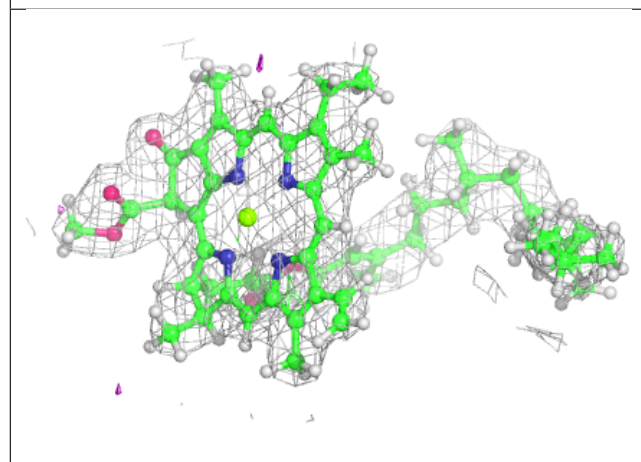
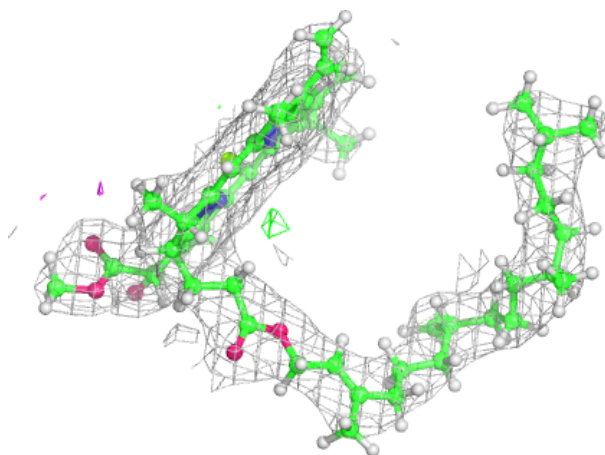
**Electron density around CLA b 610:**

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



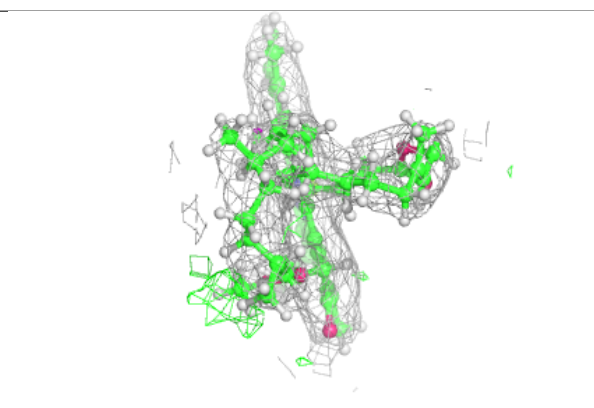
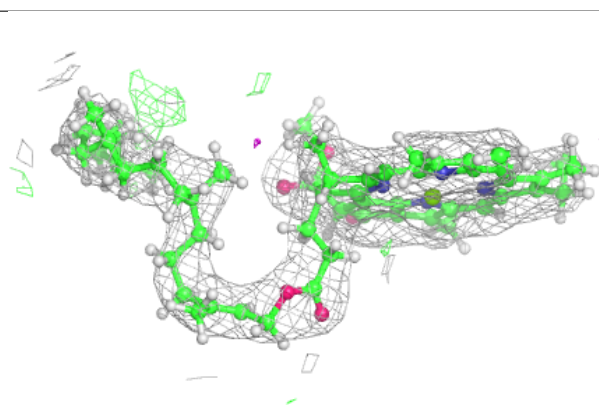
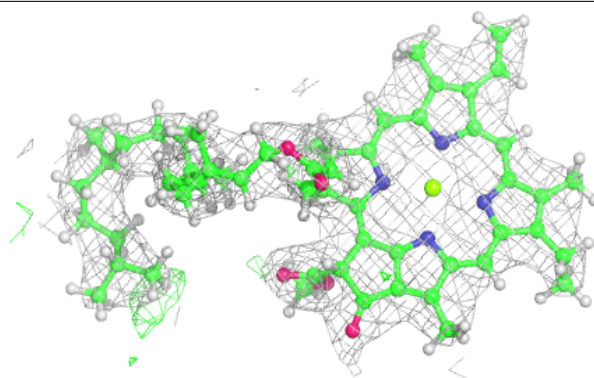
Electron density around CLA b 611:

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

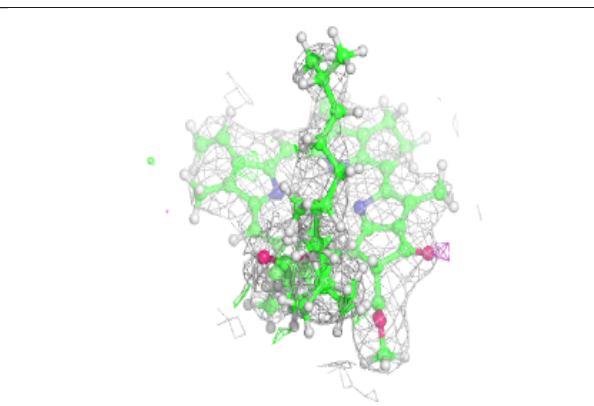
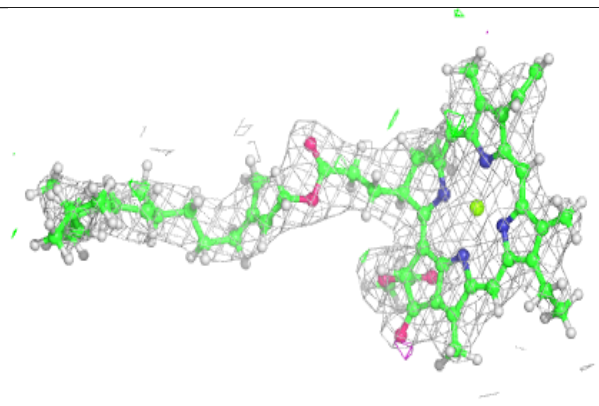
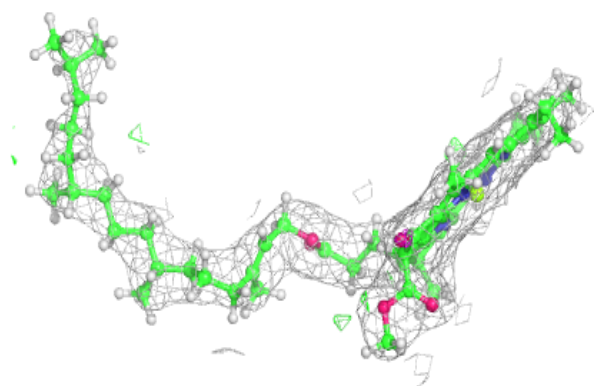


Electron density around CLA b 612:

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

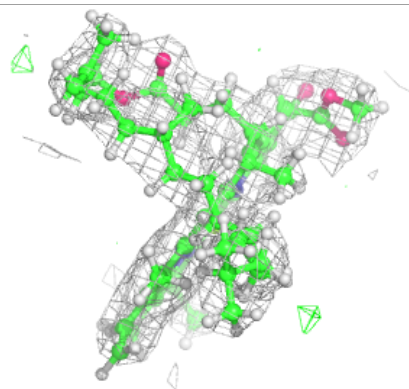
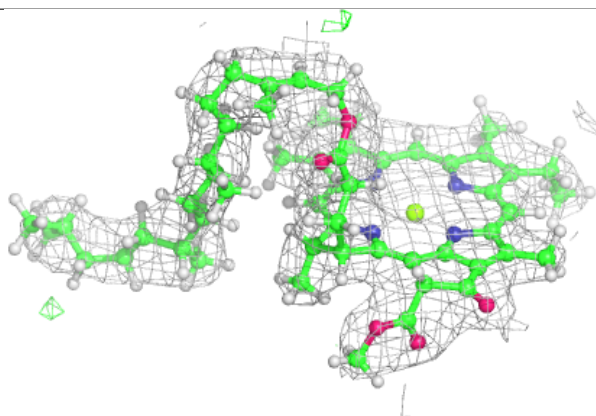
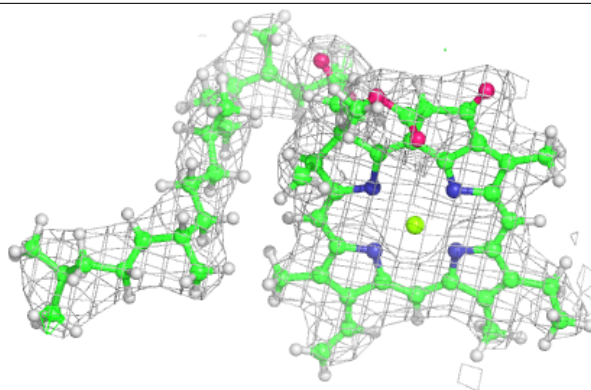
**Electron density around CLA d 403:**

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



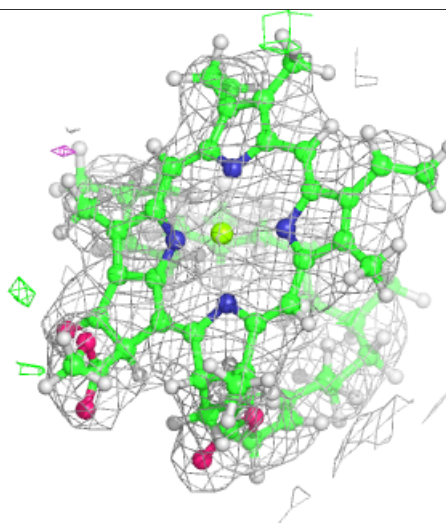
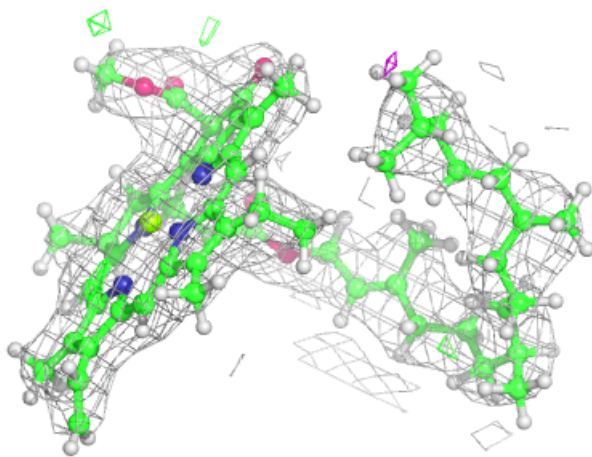
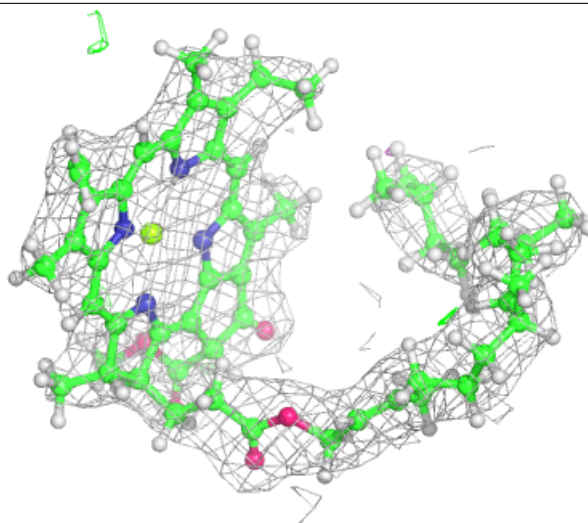
Electron density around CLA d 404:

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



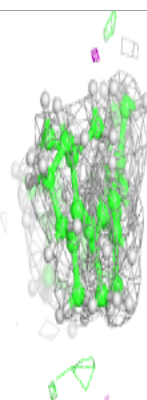
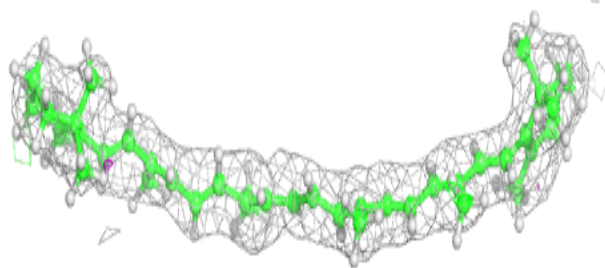
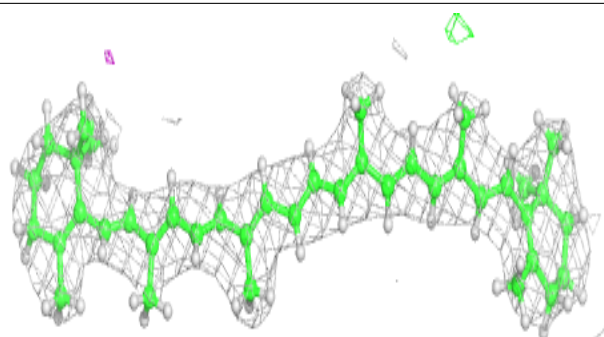
Electron density around CLA C 503:

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

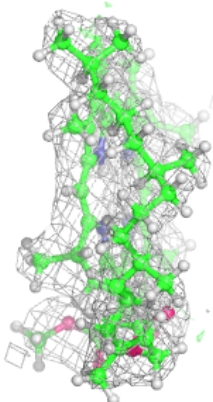
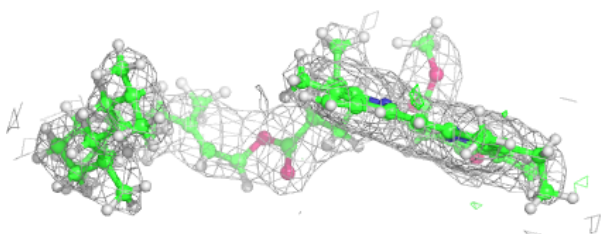
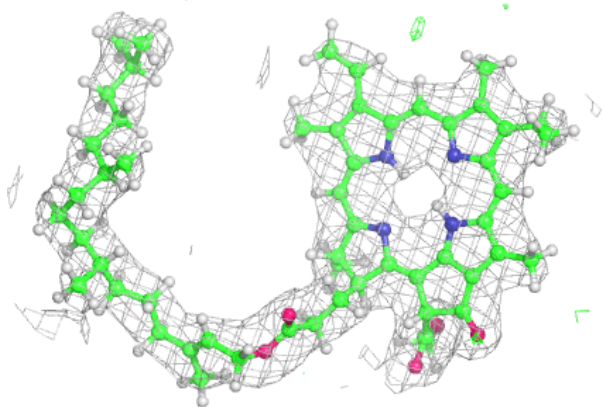


Electron density around BCR T 101:

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

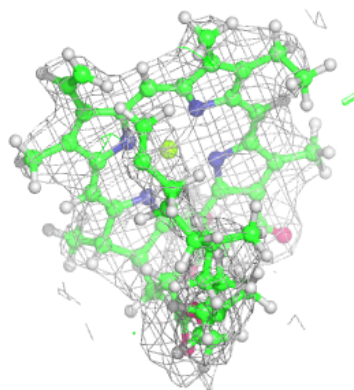
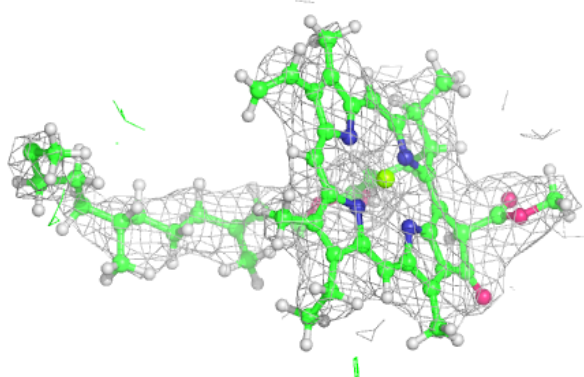
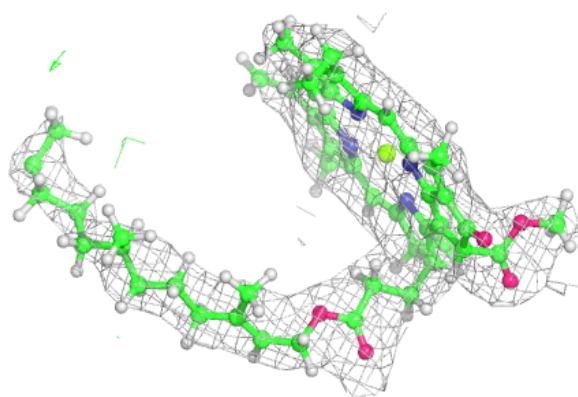
**Electron density around PHO a 403:**

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

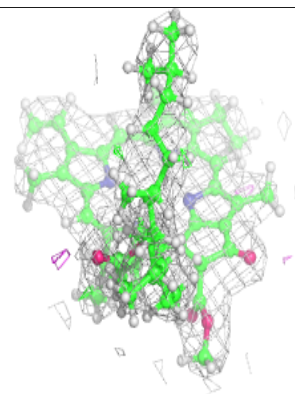
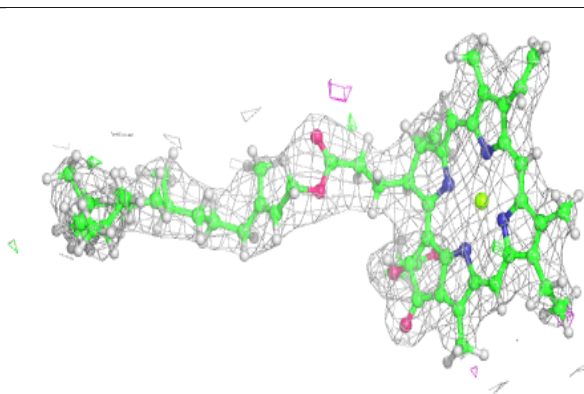
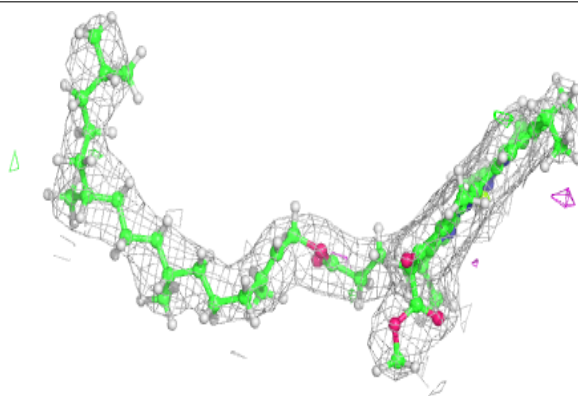


Electron density around CLA C 504:

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

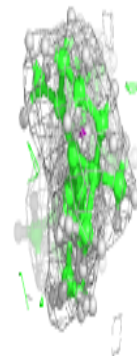
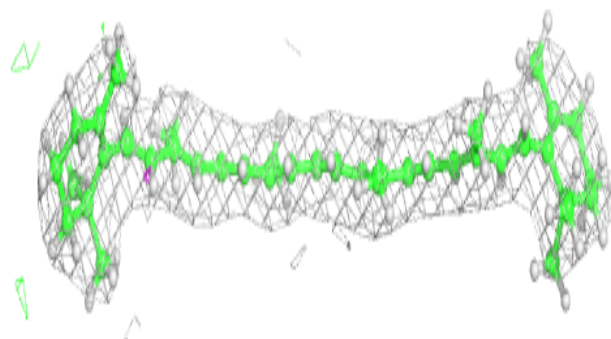
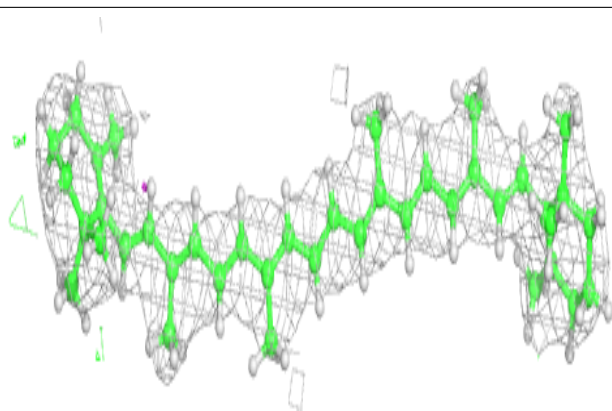
**Electron density around CLA D 403:**

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

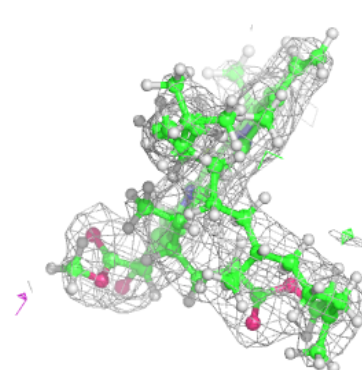
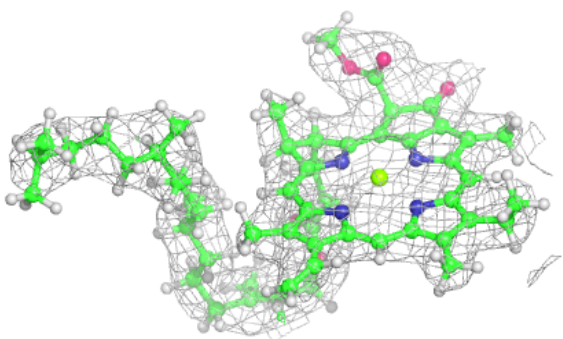
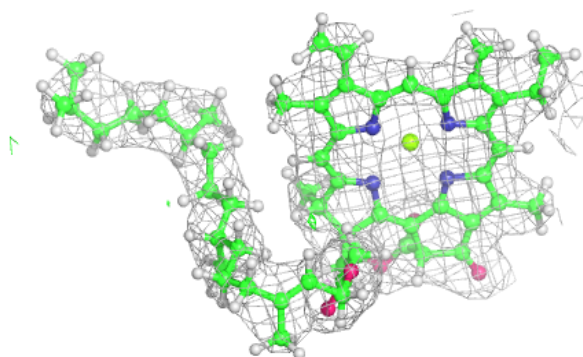


Electron density around BCR b 618:

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

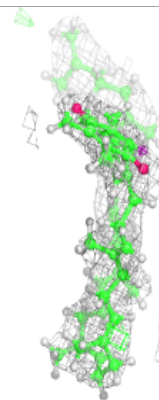
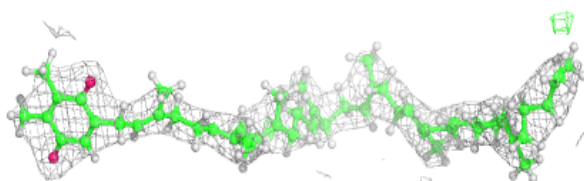
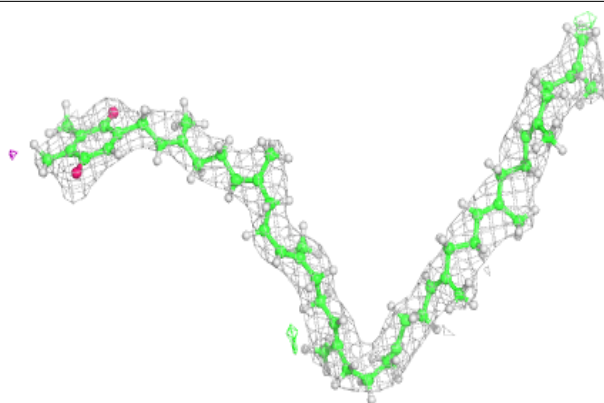
**Electron density around CLA D 404:**

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

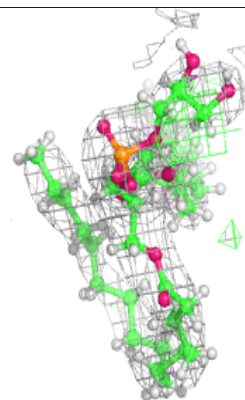
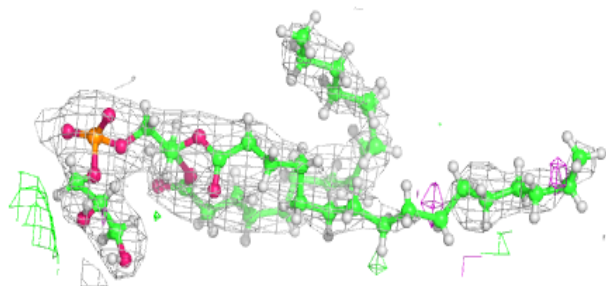
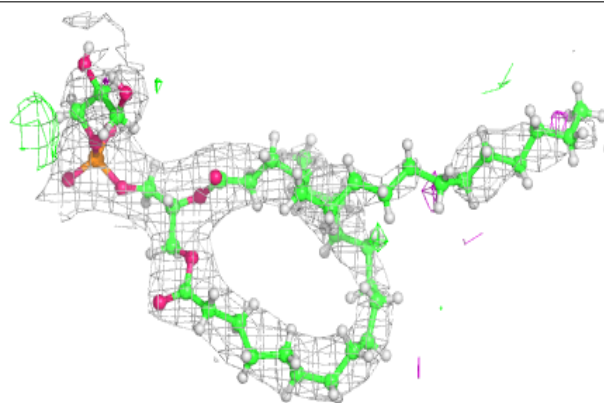


Electron density around PL9 d 407:

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

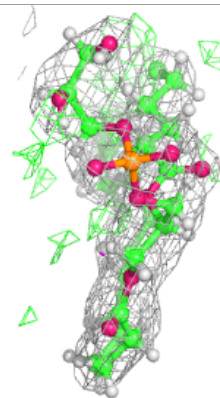
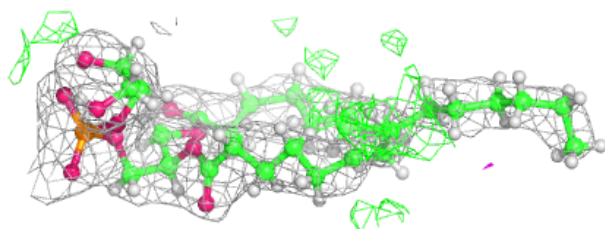
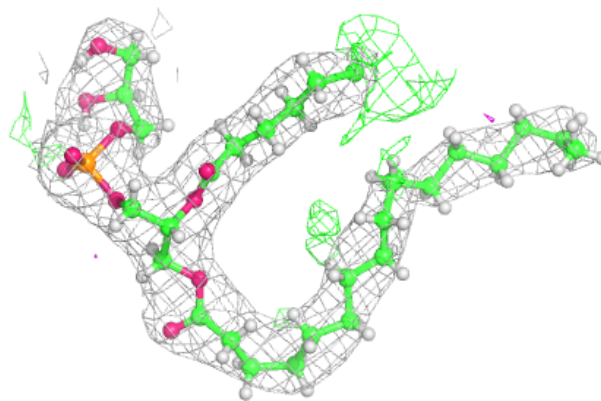
**Electron density around LHG a 410:**

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

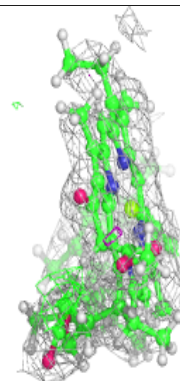
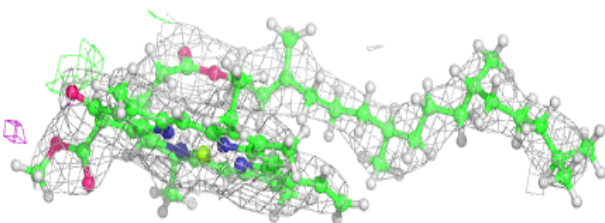
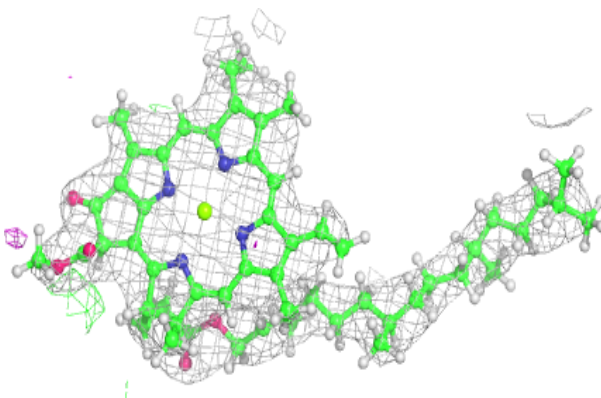


Electron density around LHG d 409:

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

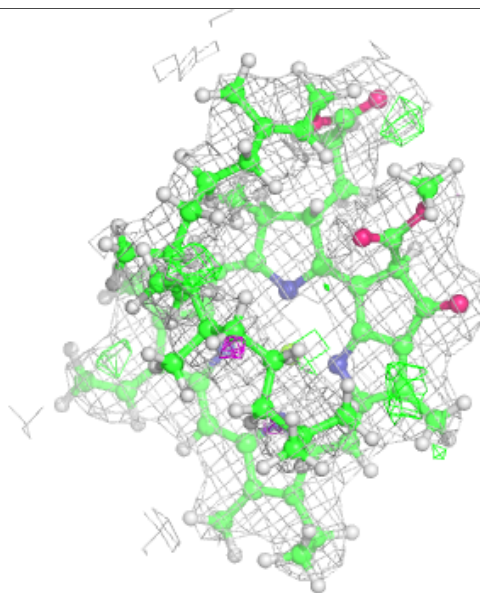
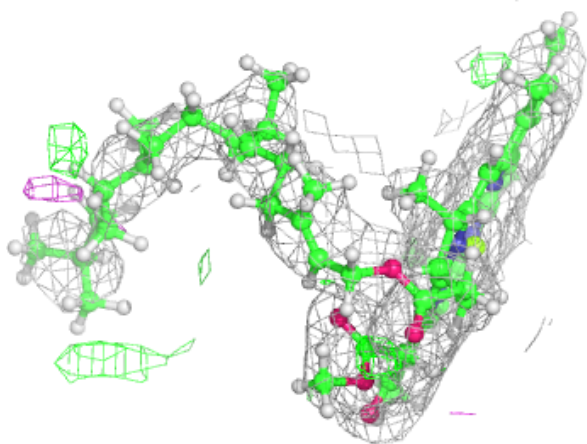
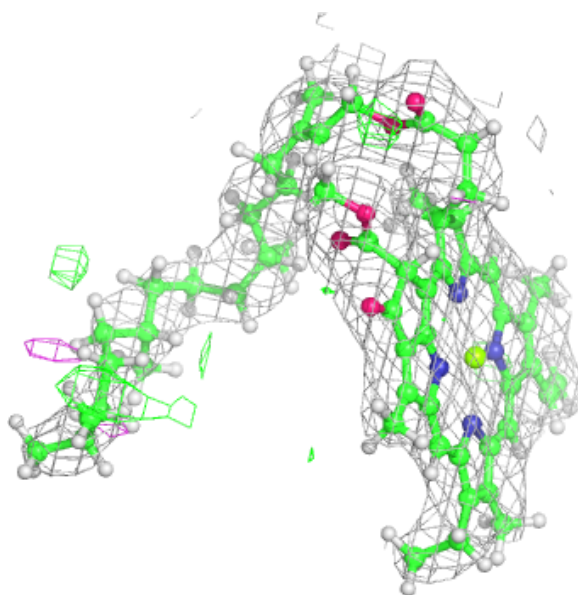
**Electron density around CLA c 501:**

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



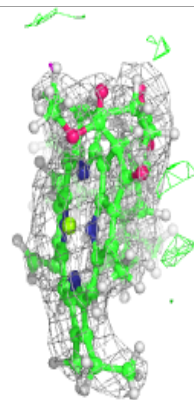
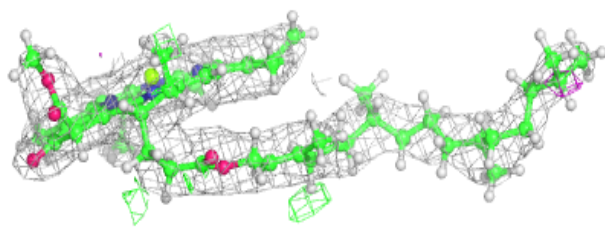
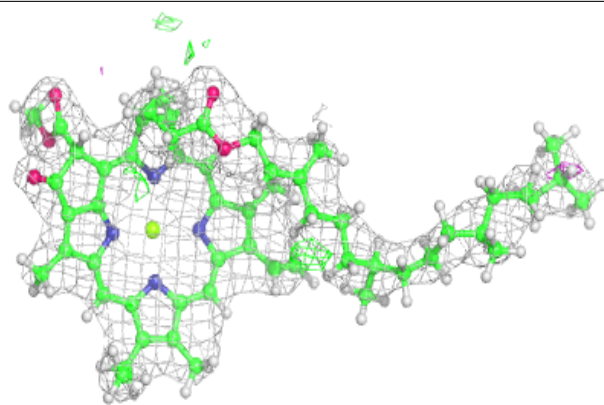
Electron density around CLA B 613:

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

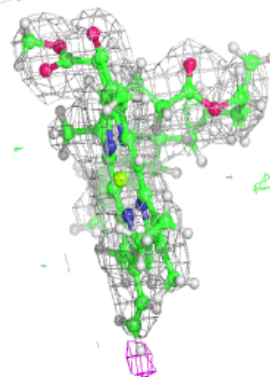
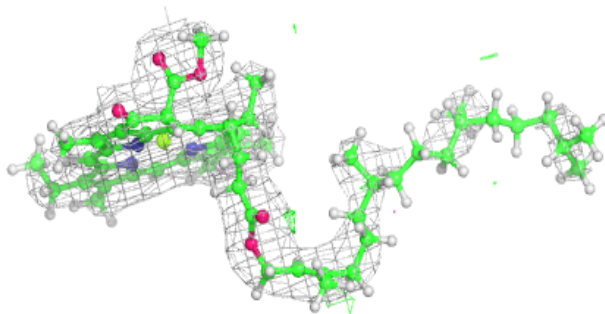
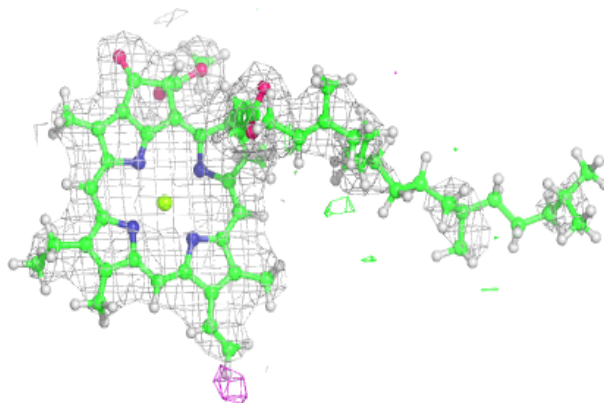


Electron density around CLA B 603:

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

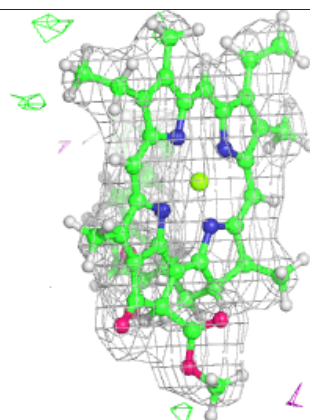
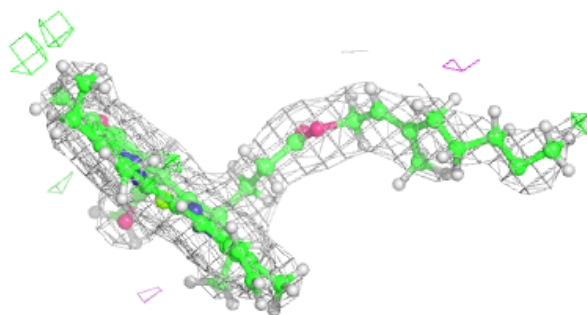
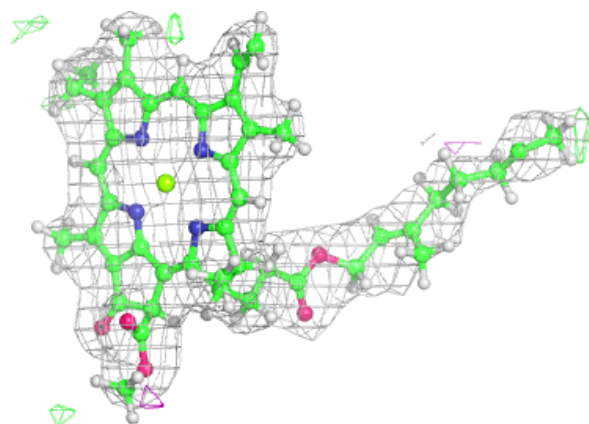
**Electron density around CLA A 403:**

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

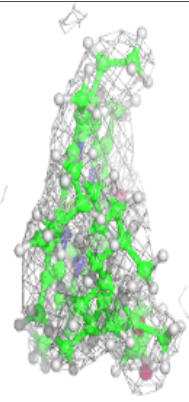
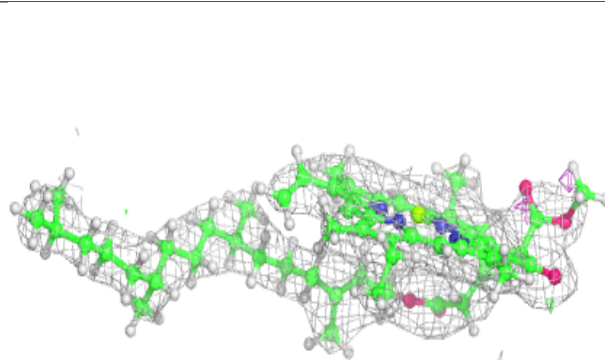
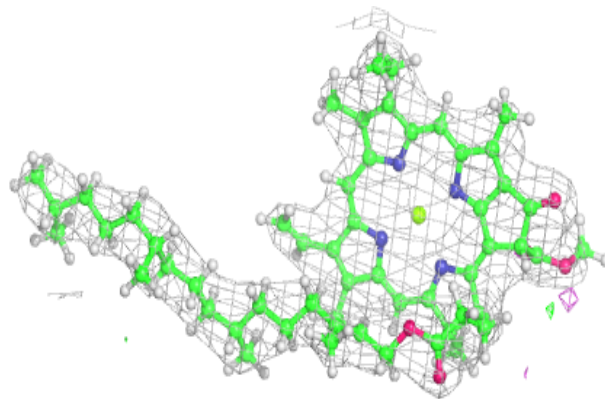


Electron density around CLA A 405:

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

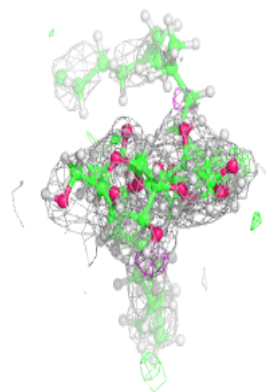
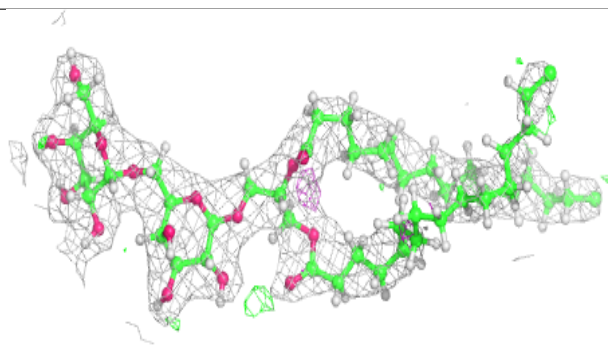
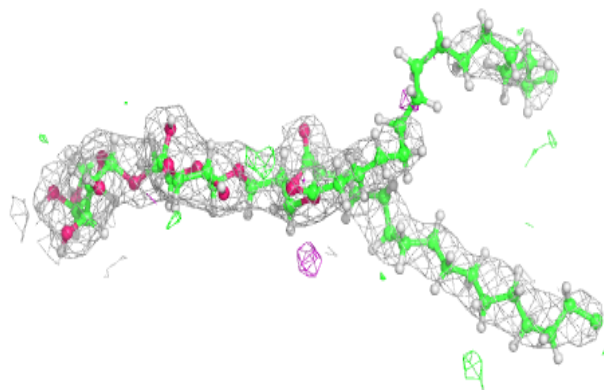
**Electron density around CLA C 501:**

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

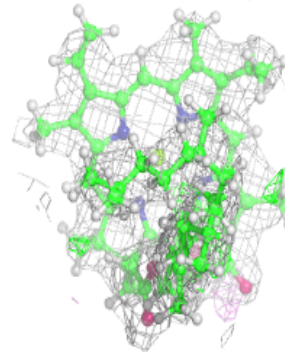
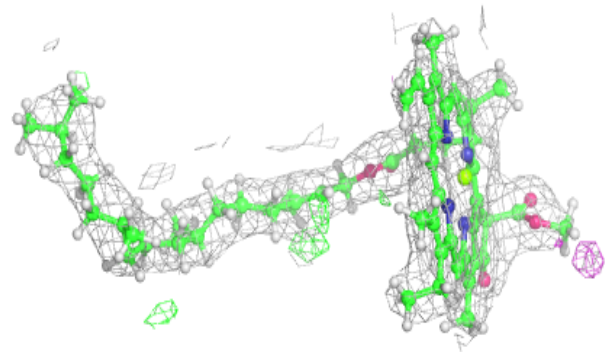
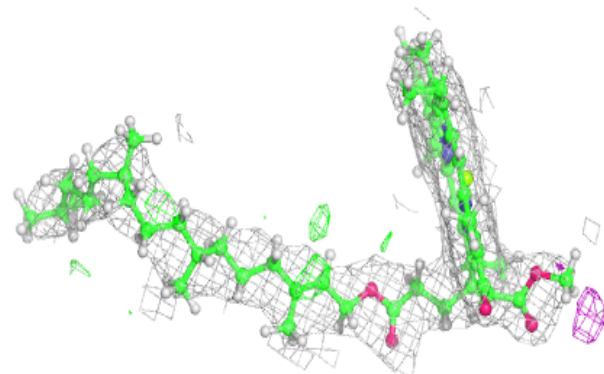


Electron density around DGD c 516:

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

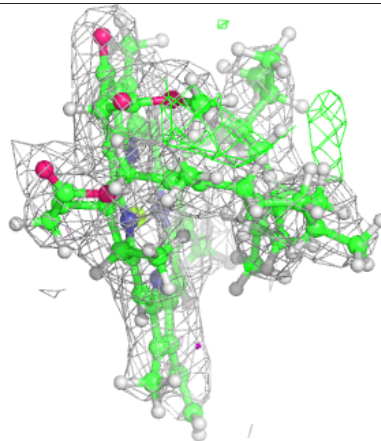
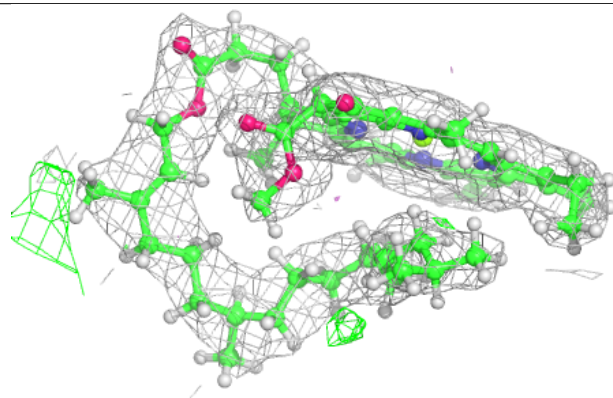
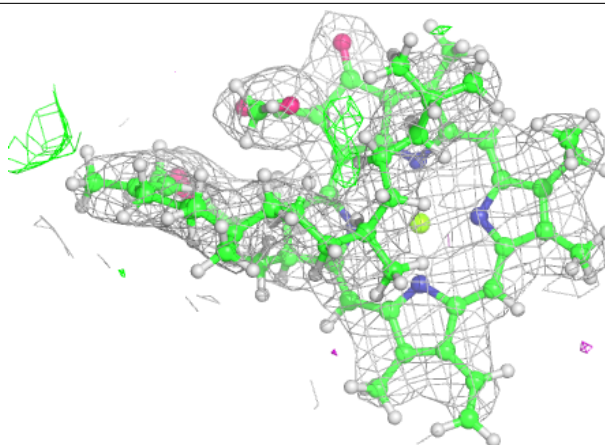
**Electron density around CLA b 605:**

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

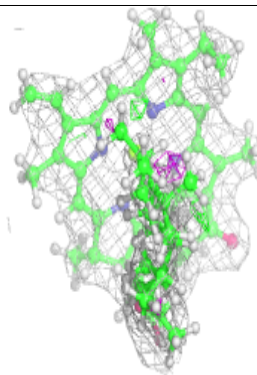
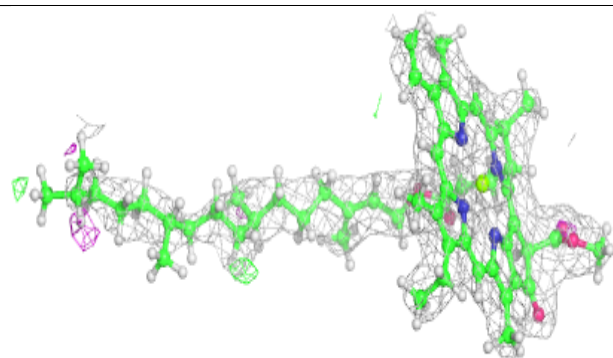
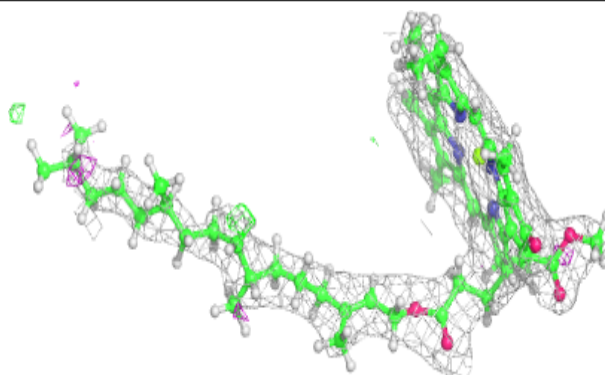


Electron density around CLA C 510:

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

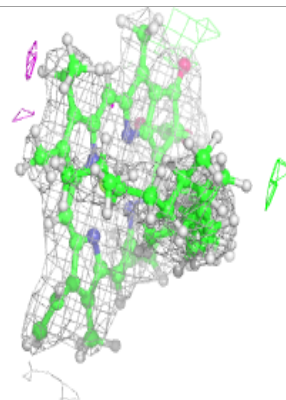
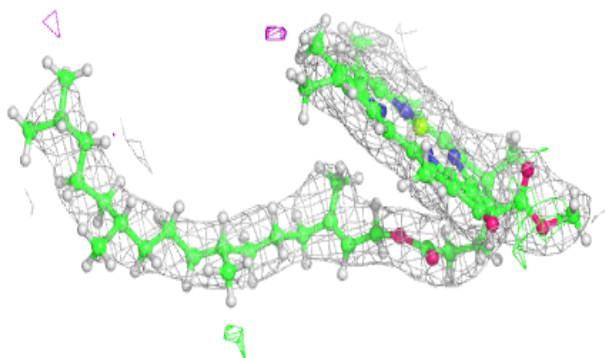
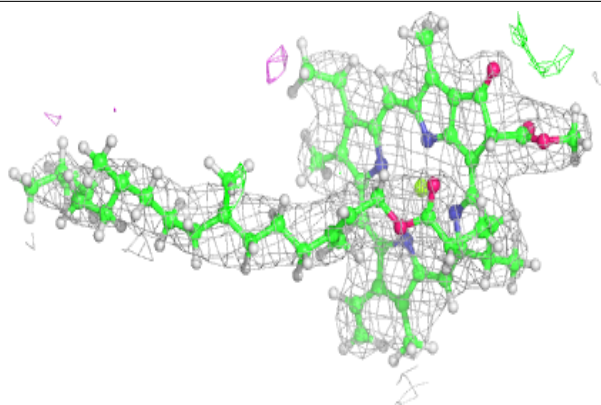
**Electron density around CLA b 607:**

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

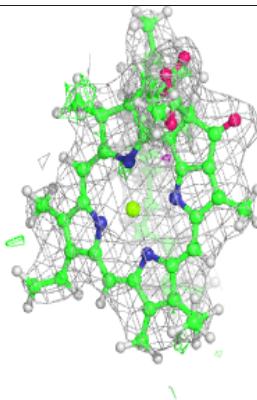
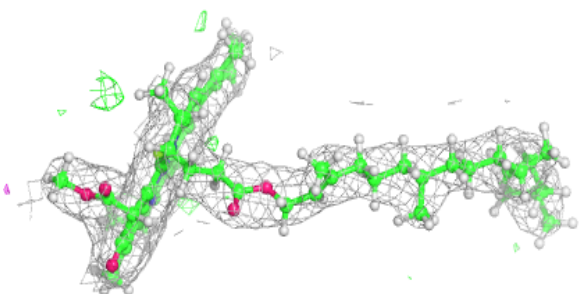
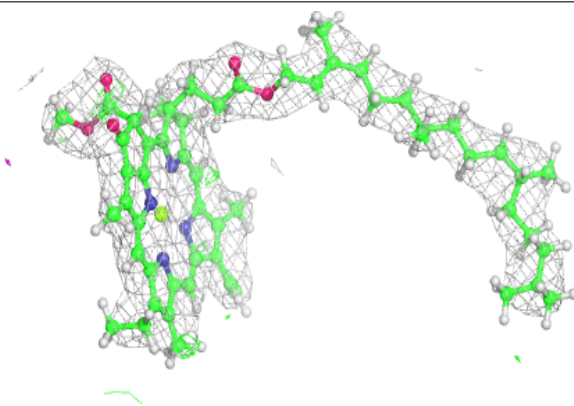


Electron density around CLA b 608:

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

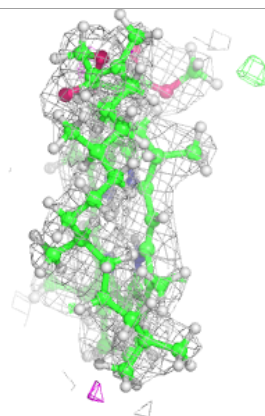
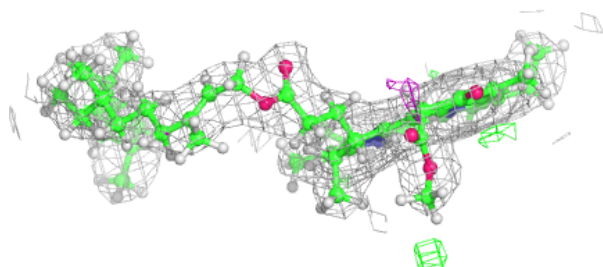
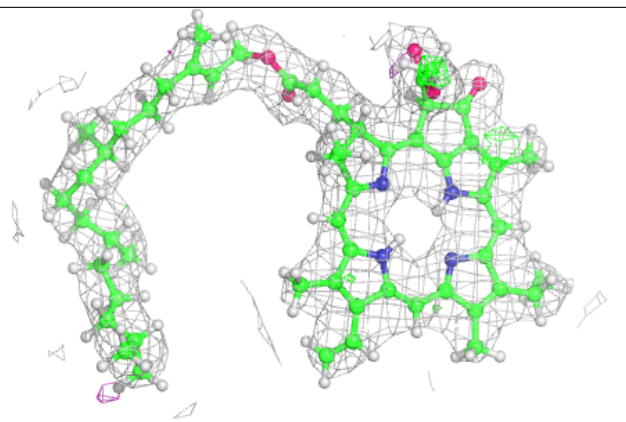
**Electron density around CLA B 609:**

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

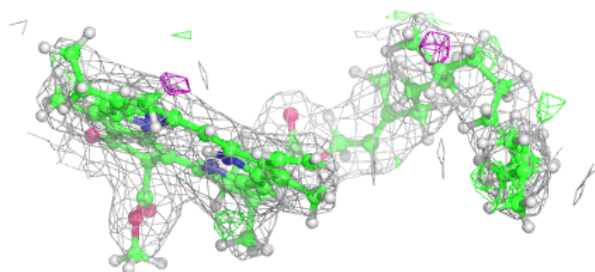
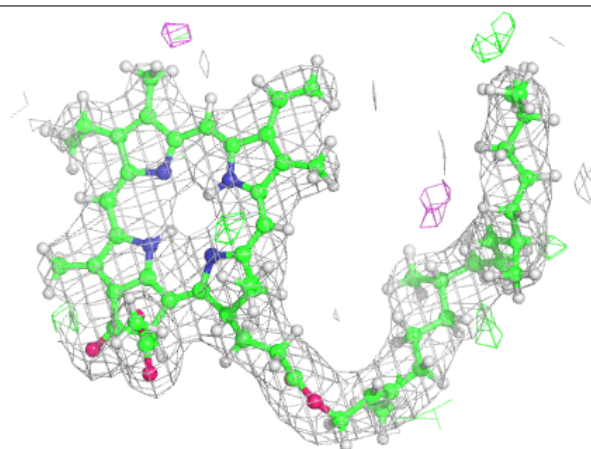


Electron density around PHO A 404:

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

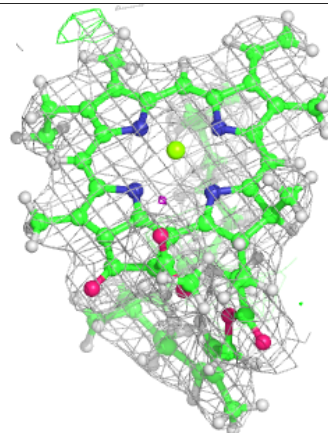
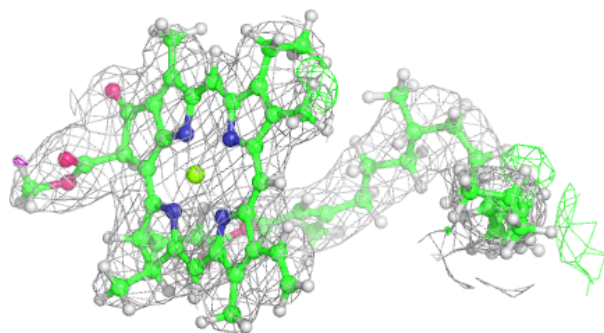
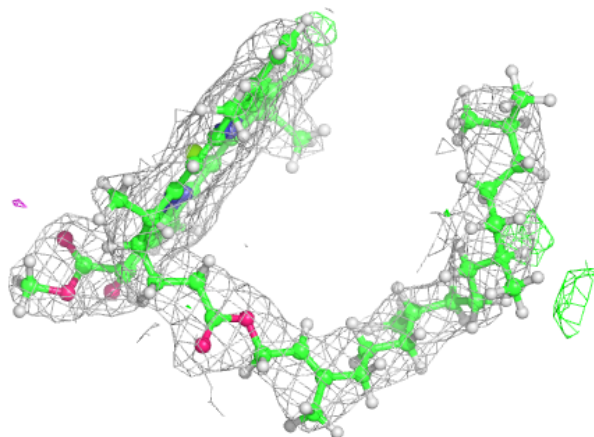
**Electron density around PHO D 401:**

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



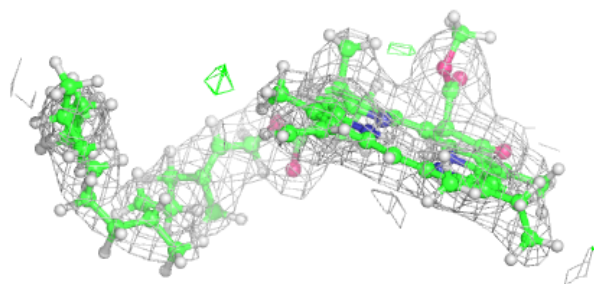
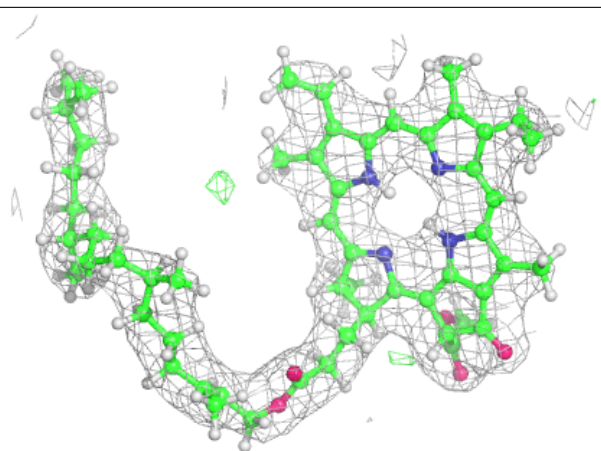
Electron density around CLA B 611:

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

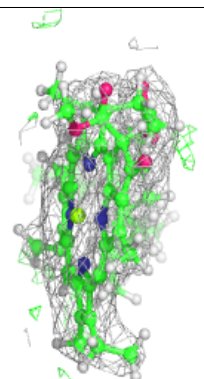
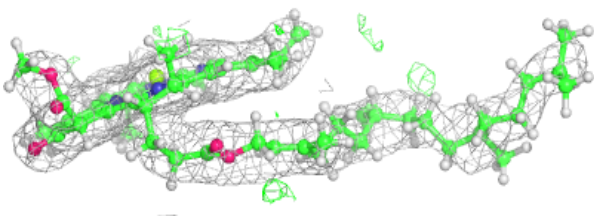
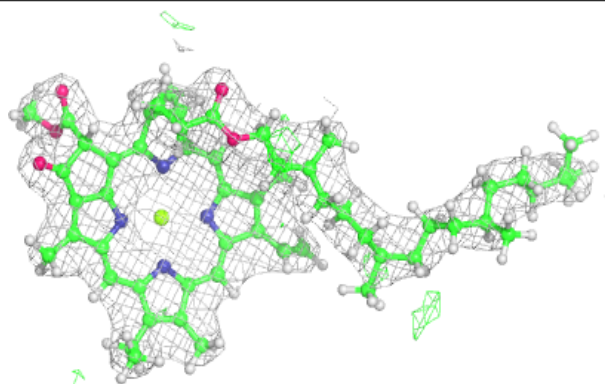


Electron density around PHO d 402:

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

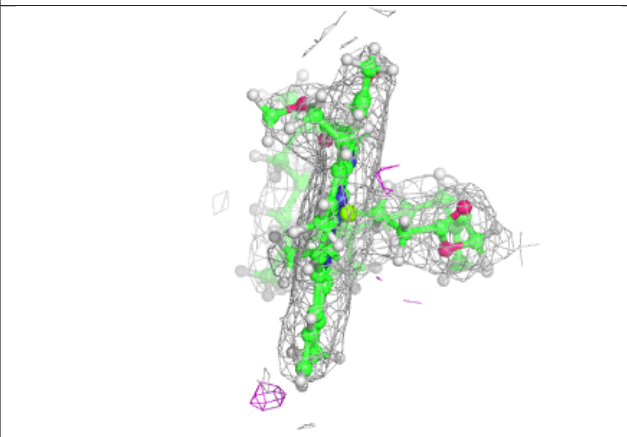
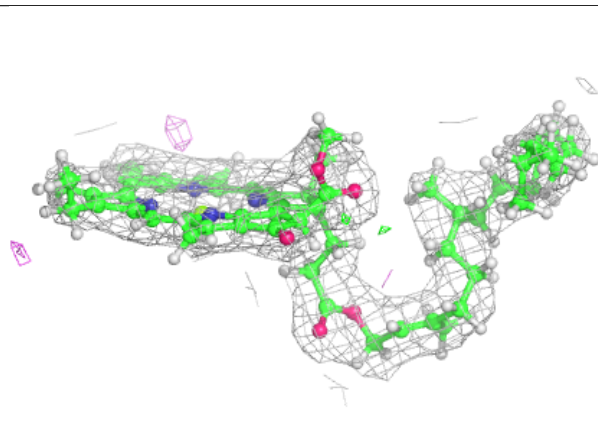
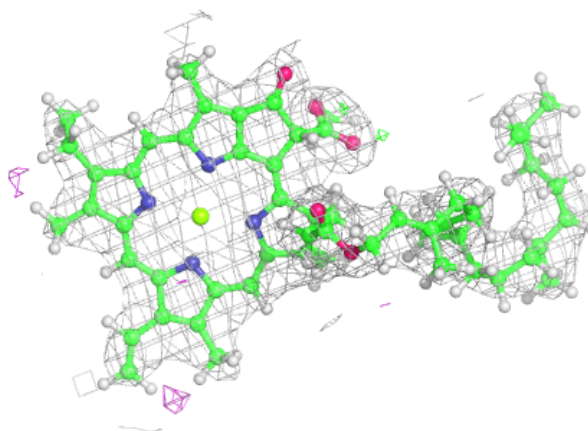
**Electron density around CLA b 603:**

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

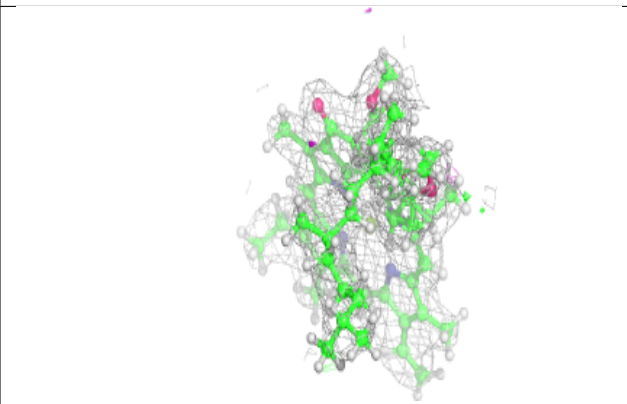
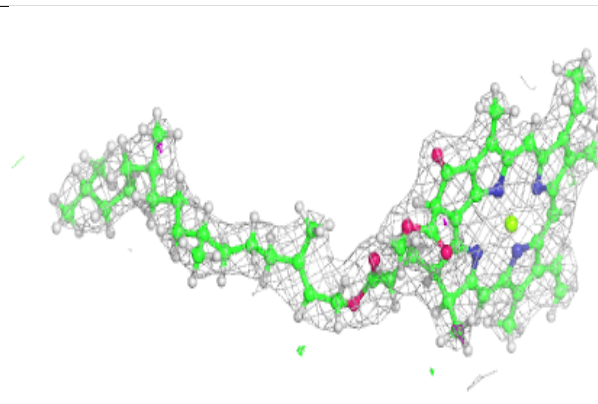
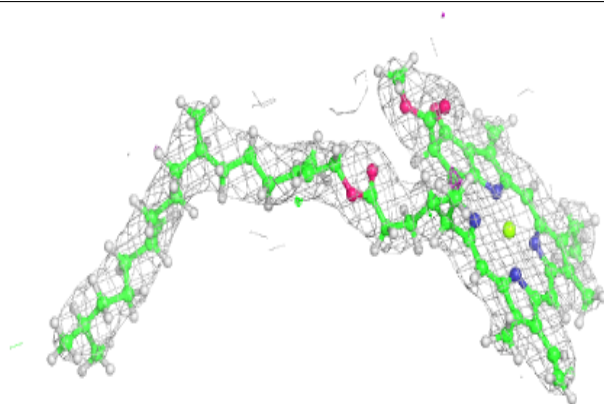


Electron density around CLA B 612:

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

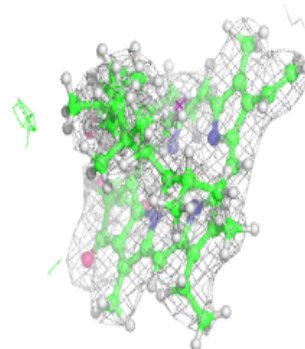
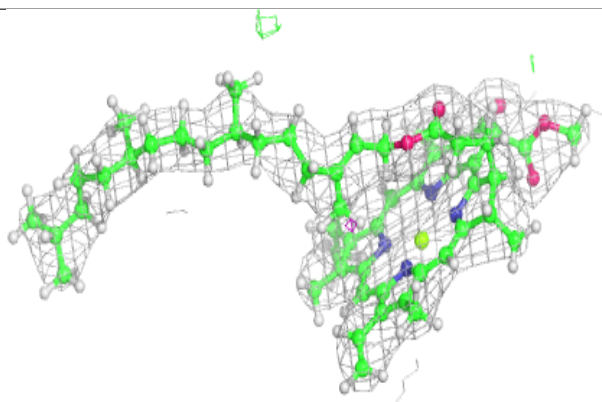
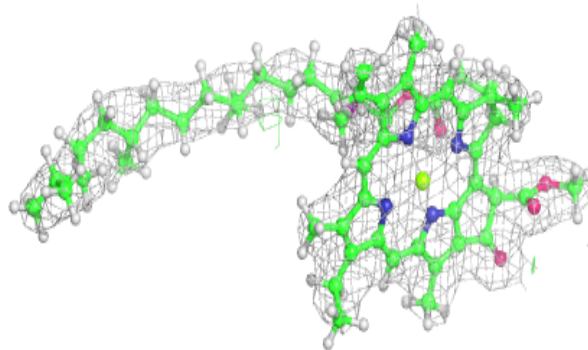
**Electron density around CLA A 402:**

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



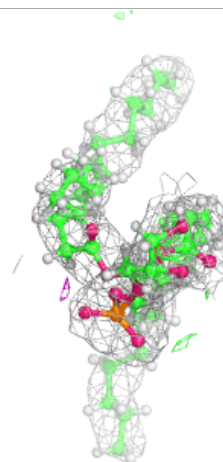
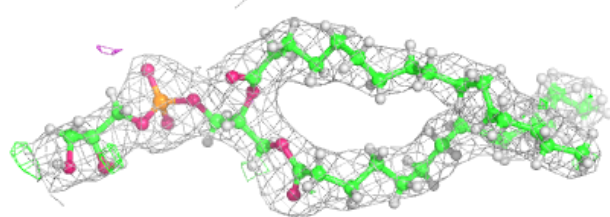
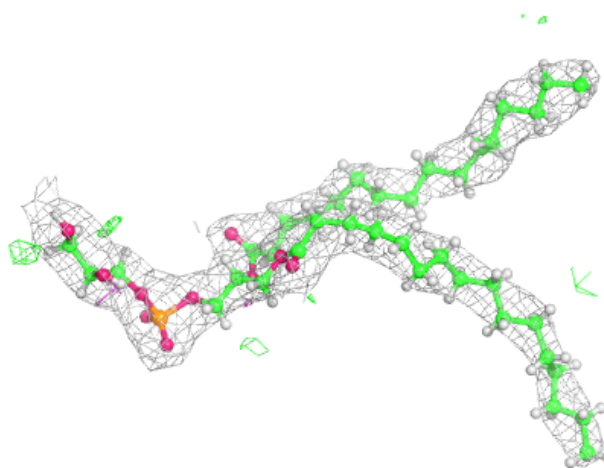
Electron density around CLA B 608:

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



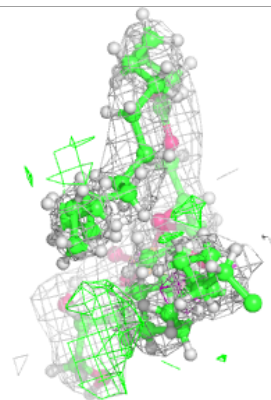
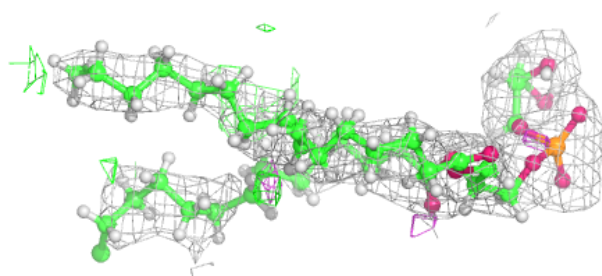
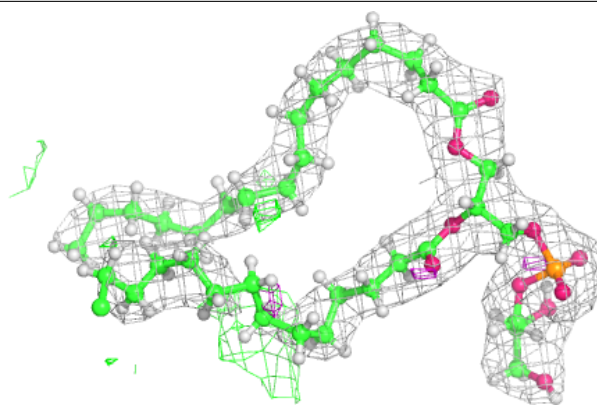
Electron density around LHG D 410:

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

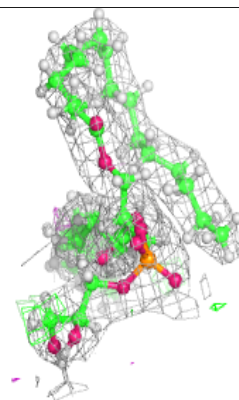
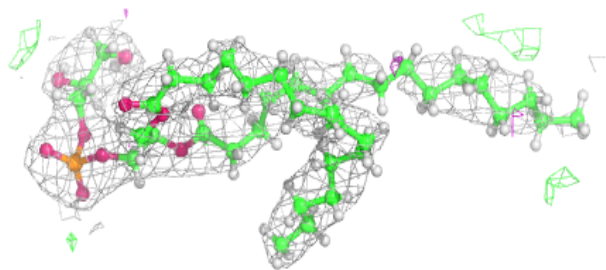
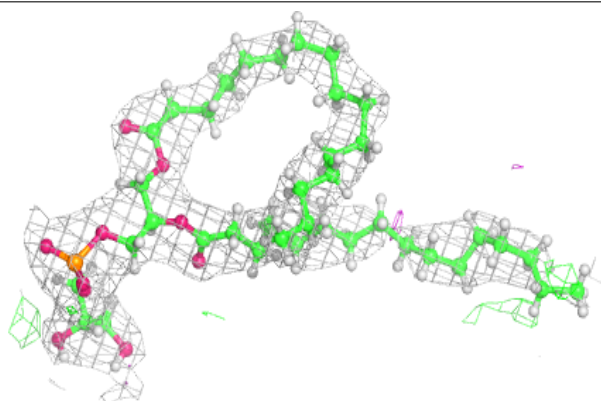


Electron density around LHG D 411:

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

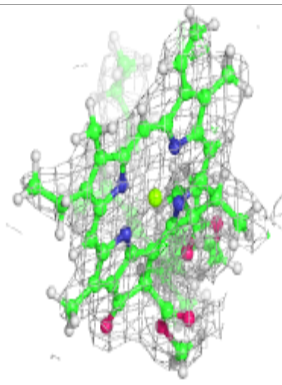
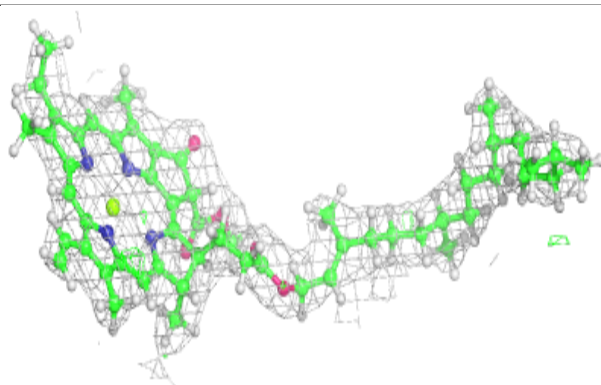
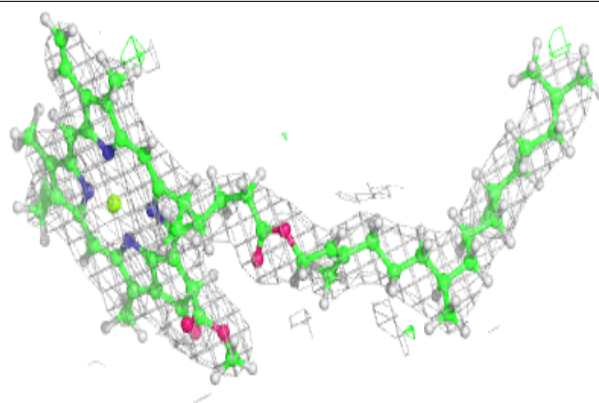
**Electron density around LHG D 413:**

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

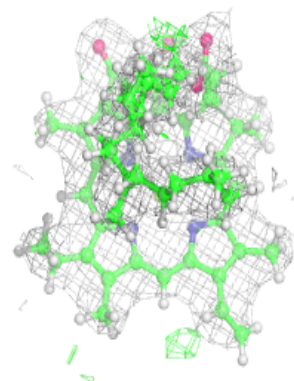
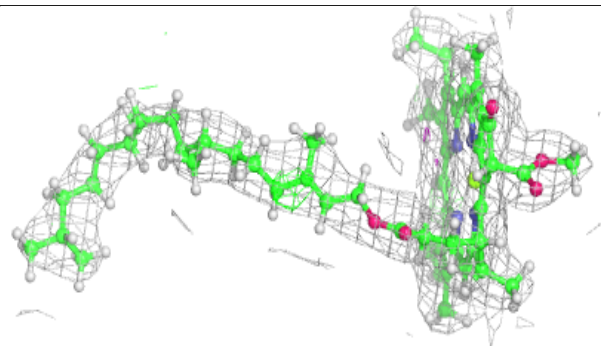
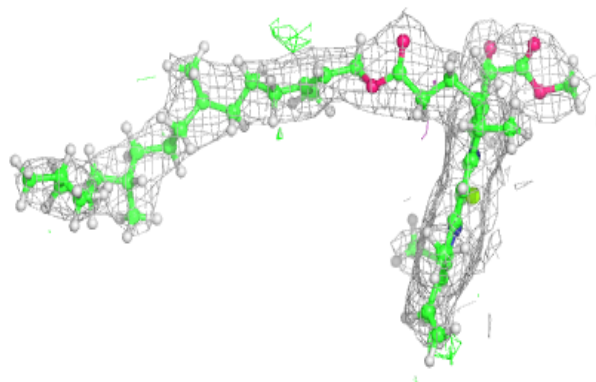


Electron density around CLA a 402:

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

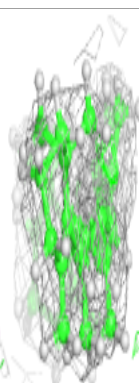
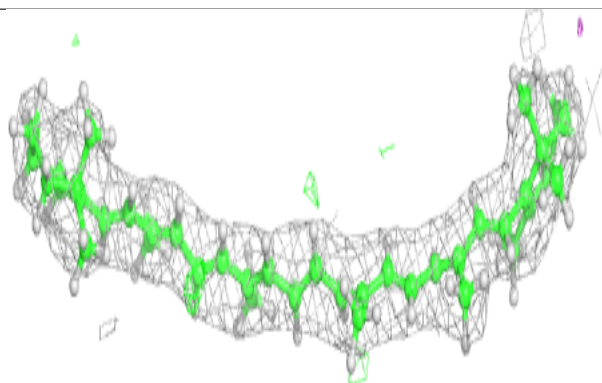
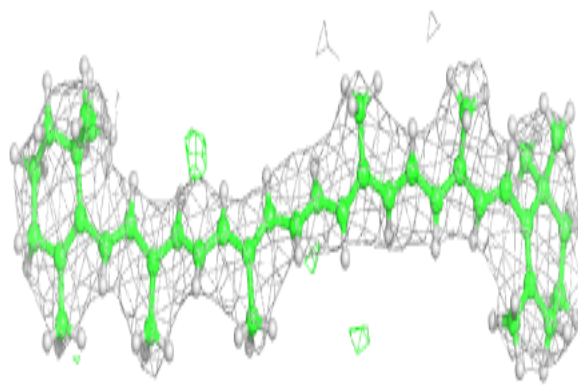
**Electron density around CLA B 605:**

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

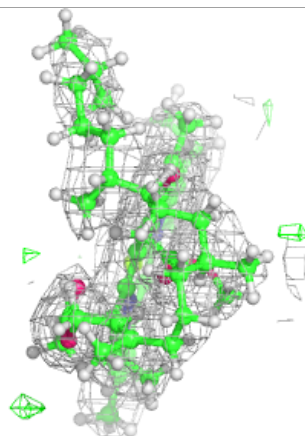
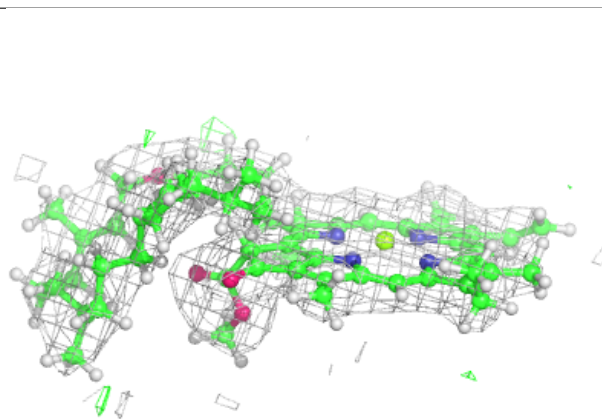
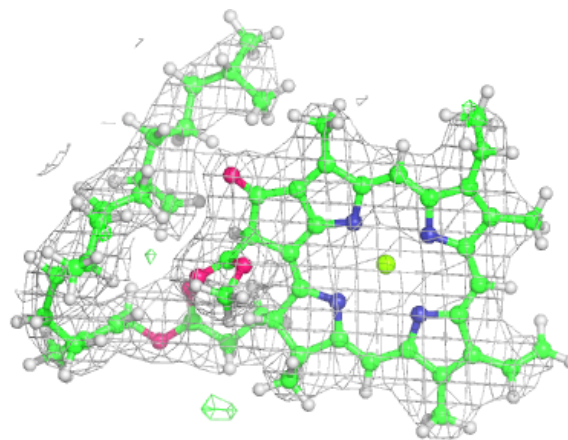


Electron density around BCR t 101:

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

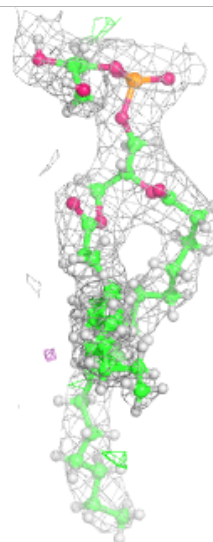
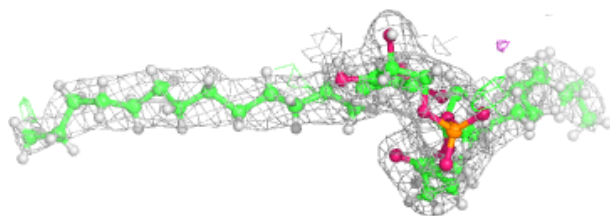
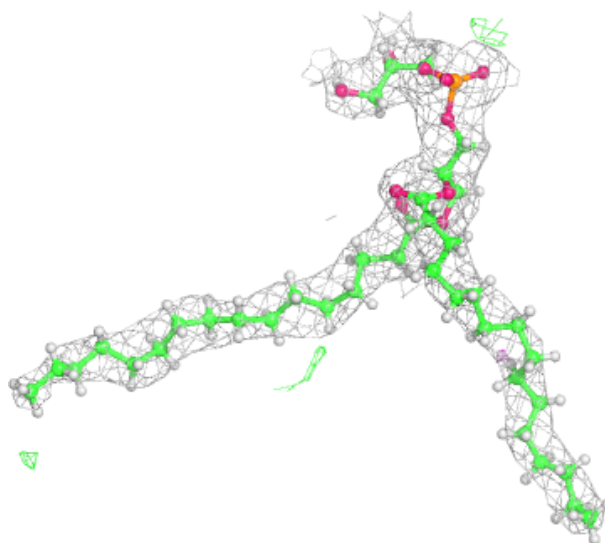
**Electron density around CLA B 610:**

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



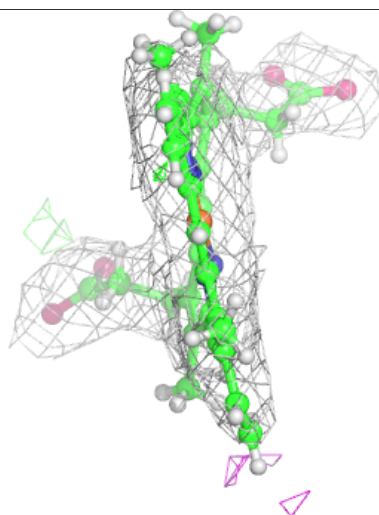
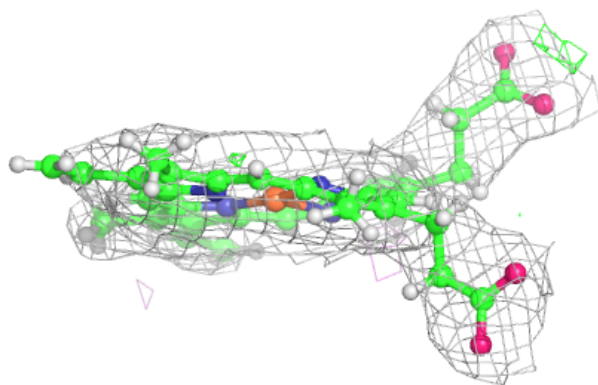
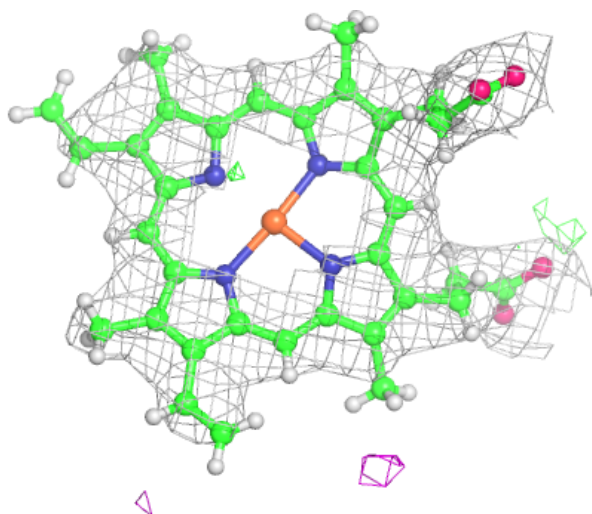
Electron density around LHG 1 101:

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



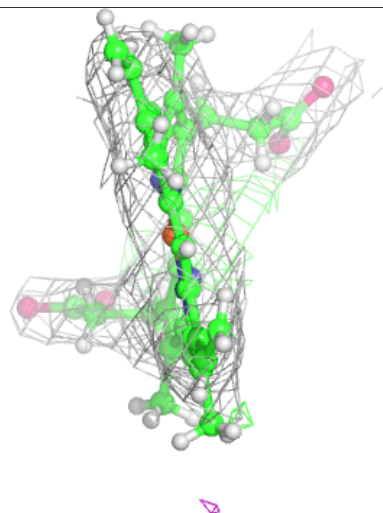
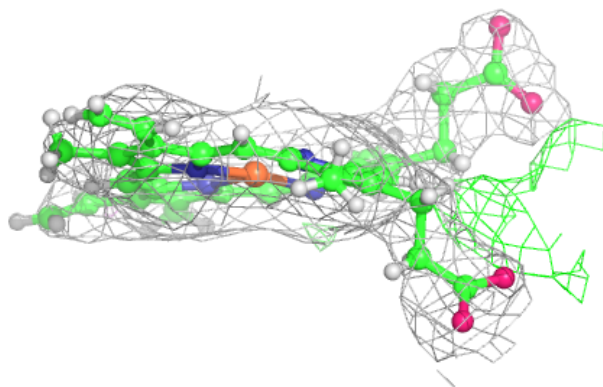
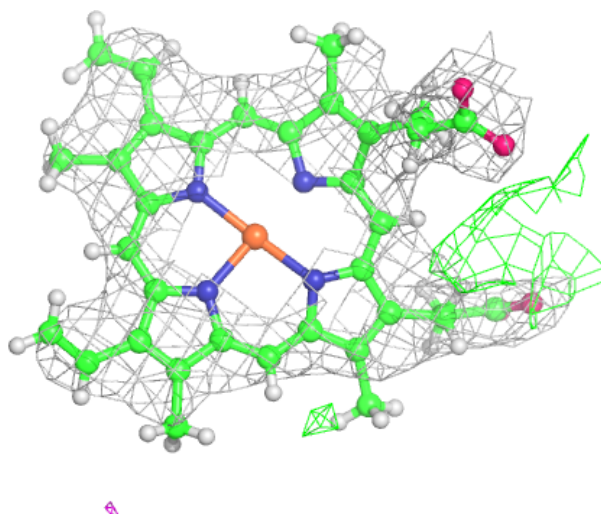
Electron density around HEM F 101:

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



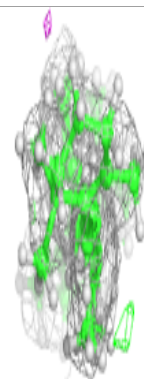
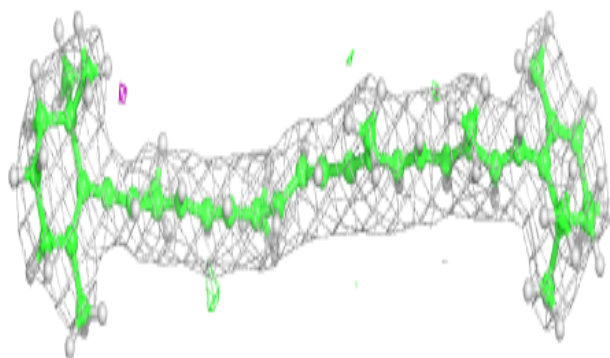
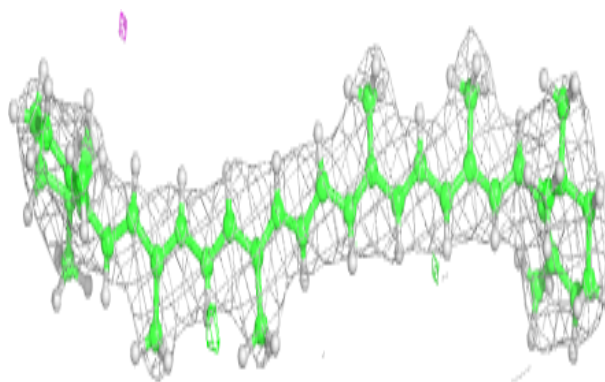
Electron density around HEM f 101:

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



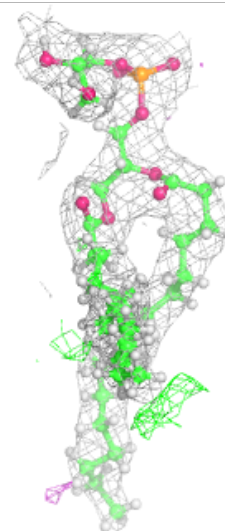
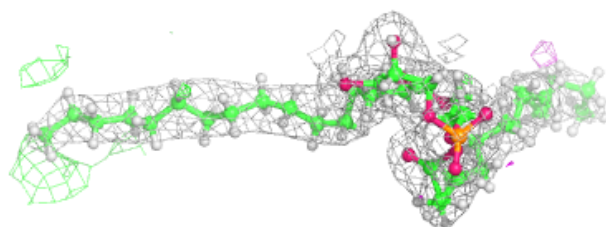
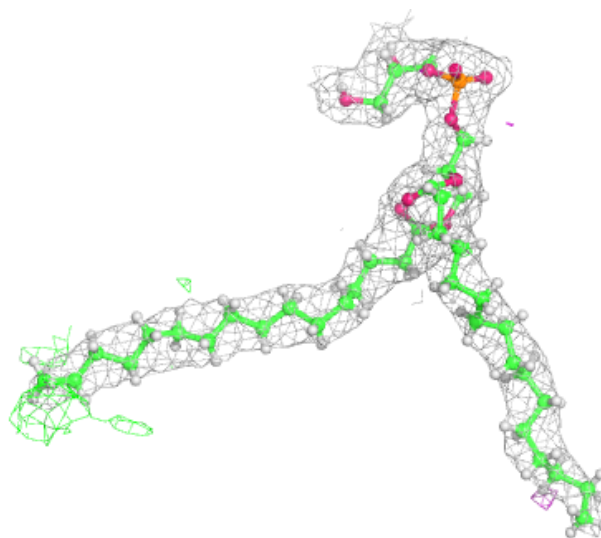
Electron density around BCR I 101:

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



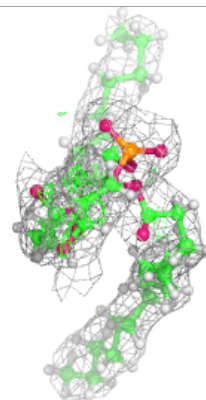
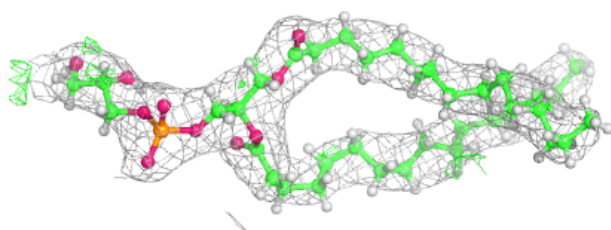
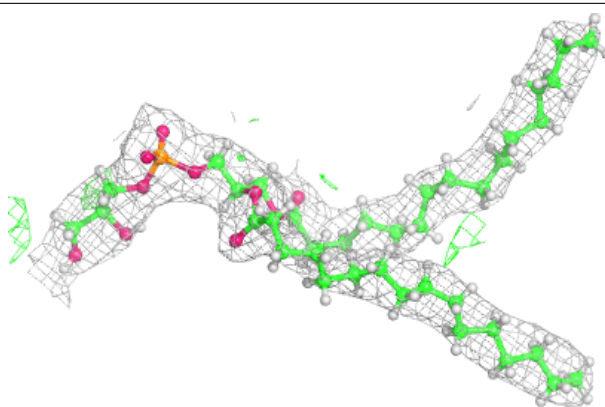
Electron density around LHG L 102:

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



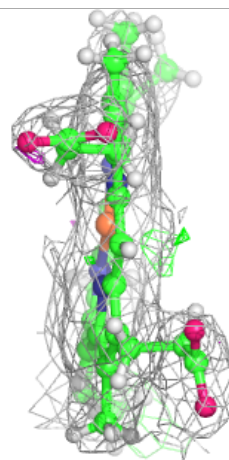
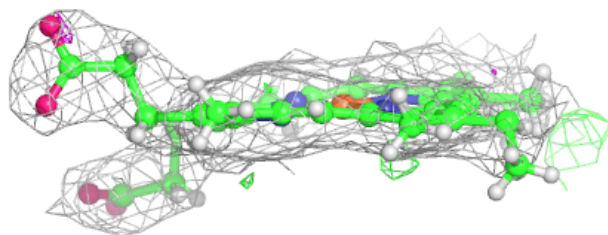
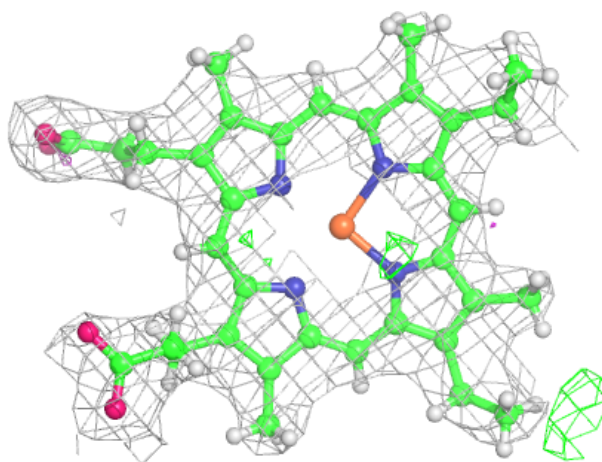
Electron density around LHG d 408:

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



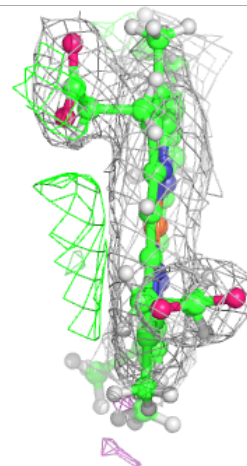
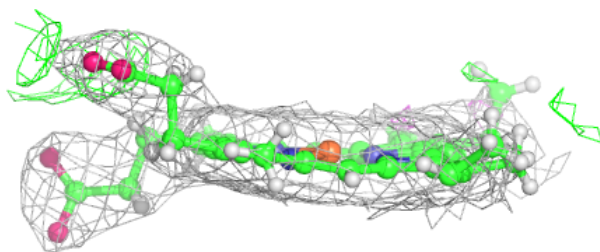
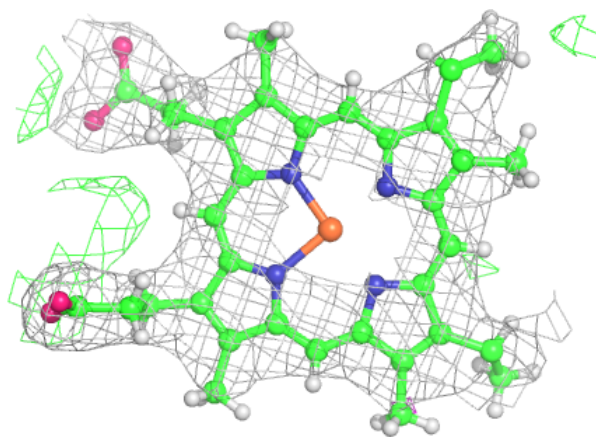
Electron density around HEC V 201:

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



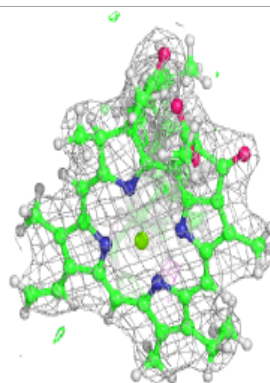
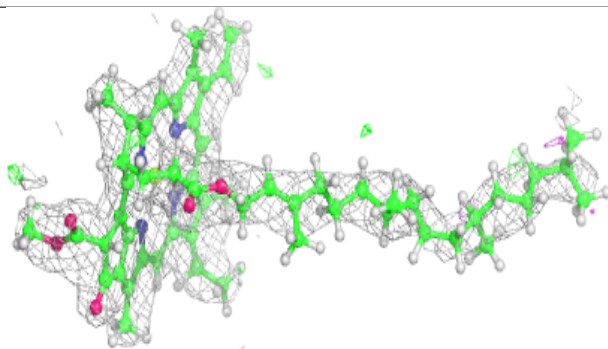
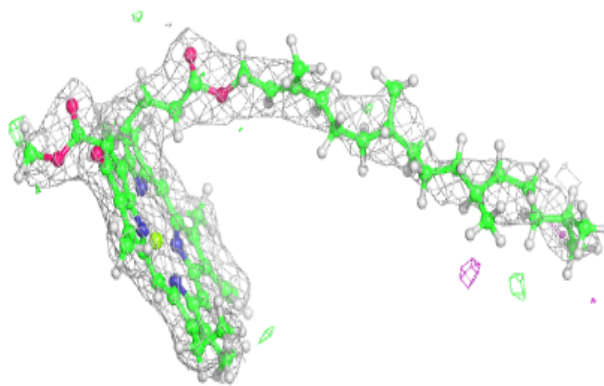
Electron density around HEC v 201:

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



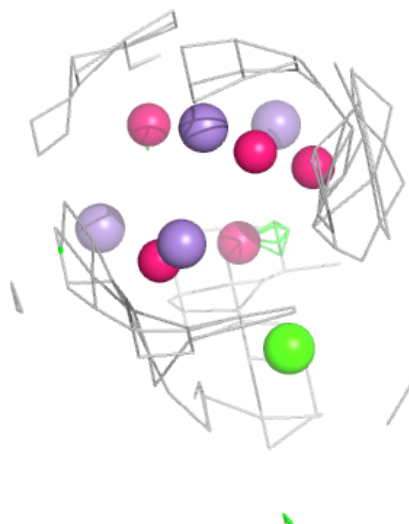
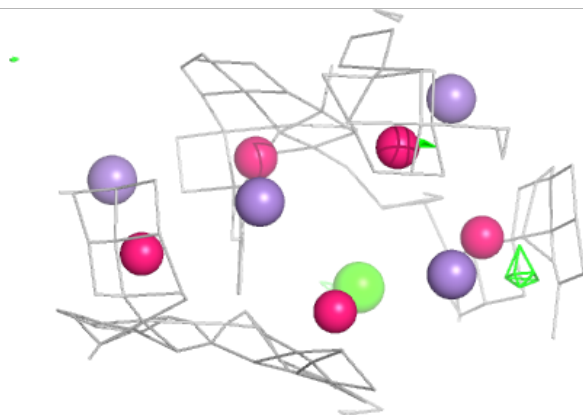
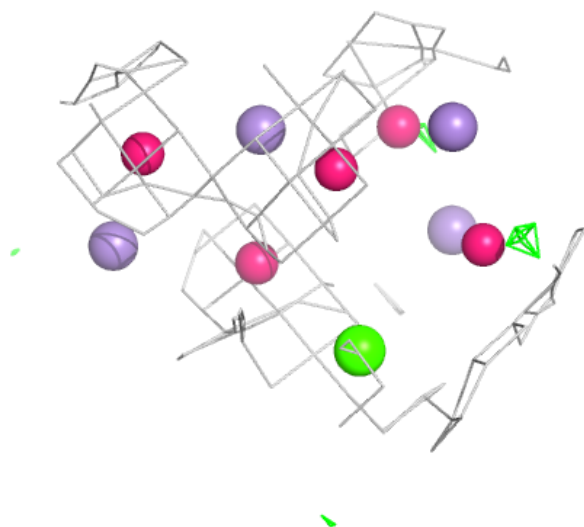
Electron density around CLA B 607:

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



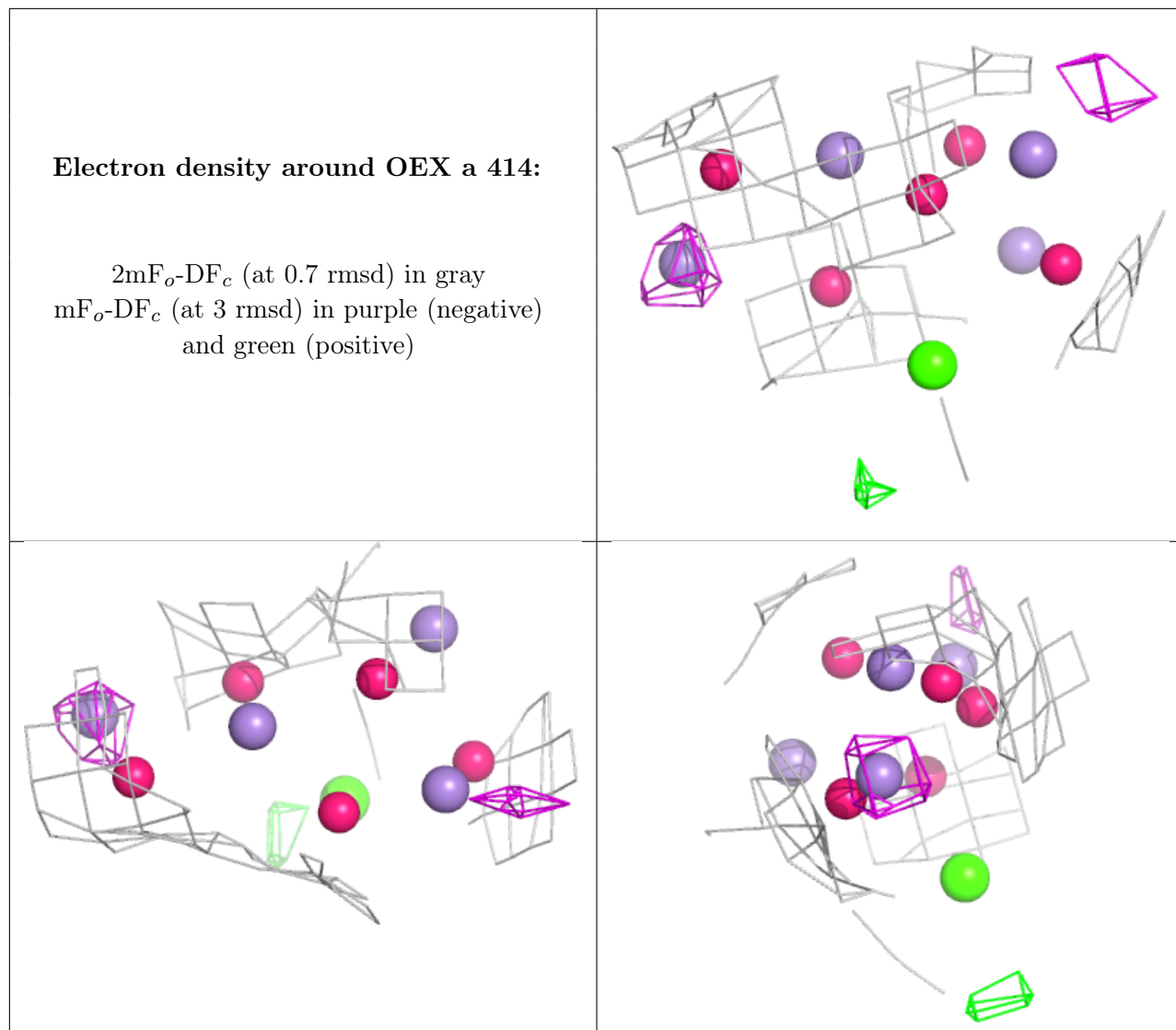
Electron density around OEX A 414:

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



Electron density around OEX 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.