



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 6, 2020 – 09:10 am BST

PDB ID : 6W1T
Title : RT XFEL structure of Photosystem II 250 microseconds after the second illumination at 2.01 Angstrom resolution
Authors : Ibrahim, M.; Fransson, T.; Chatterjee, R.; Cheah, M.H.; Hussein, R.; Lassalle, L.; Sutherlin, K.D.; Young, I.D.; Fuller, F.D.; Gul, S.; Kim, I.-S.; Simon, P.S.; de Lichtenberg, C.; Chernev, P.; Bogacz, I.; Pham, C.; Orville, A.M.; Saichek, N.; Northen, T.R.; Batyuk, A.; Carbajo, S.; Alonso-Mori, R.; Tono, K.; Owada, S.; Bhowmick, A.; Bolotovskii, R.; Mendez, D.; Moriarty, N.W.; Holton, J.M.; Dobbek, H.; Brewster, A.S.; Adams, P.D.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on : 2020-03-04
Resolution : 2.01 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 ⓘ](#)) 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	:	2.11
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)

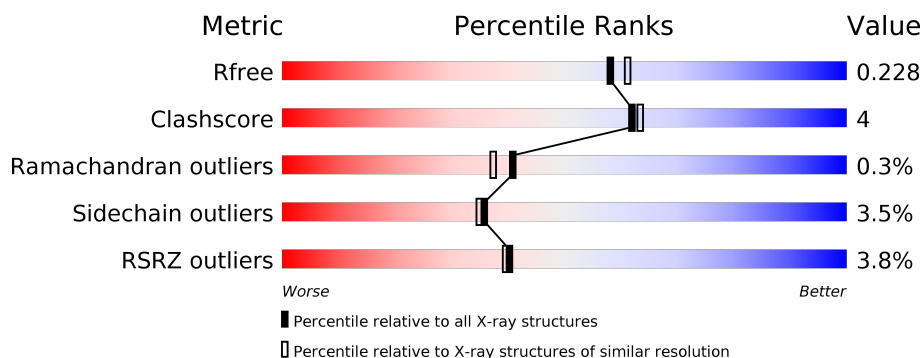
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)


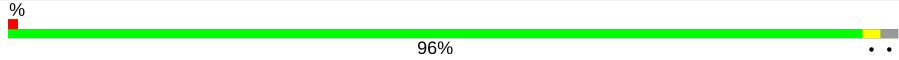

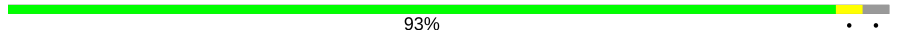

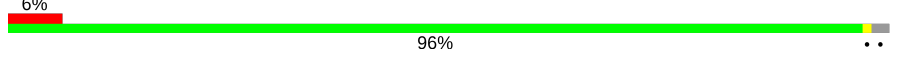



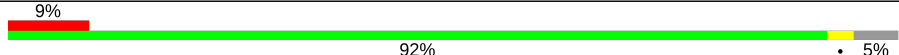
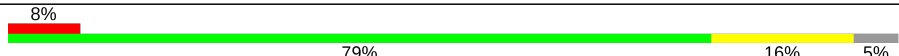
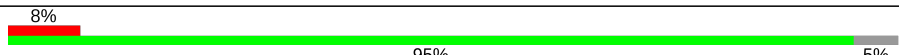
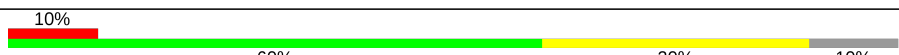



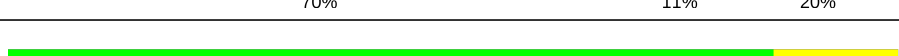

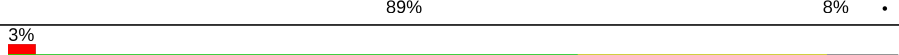


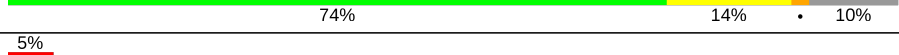



The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Mol	Chain	Length	Quality of chain
1	A	344	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>.</div> </div> </div>
1	a	344	<div> <div>93%</div> <div>.</div> <div>.</div> </div>
2	B	506	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>16%</div> </div> </div>
2	b	506	<div> <div>3%</div> <div>98%</div> <div>.</div> </div>

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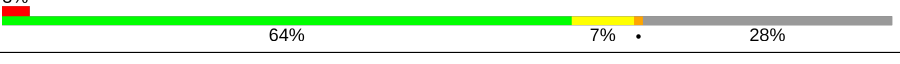

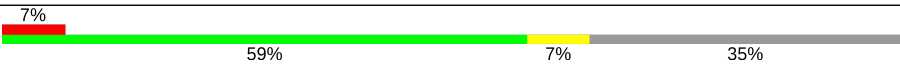



Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

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Mol	Chain	Length	Quality of chain
3	C	461	
3	c	461	
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	40	
14	r	40	
15	T	30	

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Mol	Chain	Length	Quality of chain
15	t	30	
16	U	134	
16	u	134	
17	V	163	
17	v	163	
18	X	41	
18	x	41	
19	Y	46	
19	y	46	
20	Z	62	
20	z	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	402	X	-	-	-
22	CLA	A	403	X	-	-	-
22	CLA	A	406	X	-	-	-
22	CLA	B	601	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	508	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	402	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	D	404	X	-	-	-
22	CLA	a	402	X	-	-	-
22	CLA	a	404	X	-	-	-
22	CLA	b	601	X	-	-	-
22	CLA	b	602	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
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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	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
22	CLA	d	401	X	-	-	-
22	CLA	d	403	X	-	-	-
22	CLA	d	404	X	-	-	-
22	CLA	d	405	X	-	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 105978 atoms, of which 52553 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	60	0
			6031	2014	2942	509	547	19			
1	a	334	Total	C	H	N	O	S	0	60	0
			6019	2011	2933	509	547	19			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	H	N	O	S	0	5	0
			7864	2631	3859	666	695	13			
2	b	505	Total	C	H	N	O	S	0	0	0
			7800	2610	3822	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	10	0
			6876	2283	3397	580	602	14			
3	c	451	Total	C	H	N	O	S	0	10	0
			7021	2324	3468	596	619	14			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	341	Total	C	H	N	O	S	0	1	0
			5350	1806	2624	445	463	12			
4	d	341	Total	C	H	N	O	S	0	2	0
			5362	1810	2630	445	465	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	82	Total	C	H	N	O	0	1	0
			1316	436	650	107	123			
5	e	82	Total	C	H	N	O	0	0	0
			1311	434	647	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
			556	187	281	45	42			
6	f	34	Total	C	H	N	O	0	0	0
			556	187	281	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
			3698	1168	1828	313	385			
13	o	244	Total	C	H	N	O	0	0	0
			3718	1170	1844	317	383			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	R	34	Total	C	H	N	O	0	0	0
			569	184	298	47	40			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	r	31	Total	C	H	N	O	0	0	0
			493	162	253	42	36			

- 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
			1546	491	772	129	154			
16	u	97	Total	C	H	N	O	0	0	0
			1546	491	772	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
			2132	675	1068	177	208	4		
17	v	137	Total	C	H	N	O	S	0	0
			2132	675	1068	177	208	4		

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

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

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

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

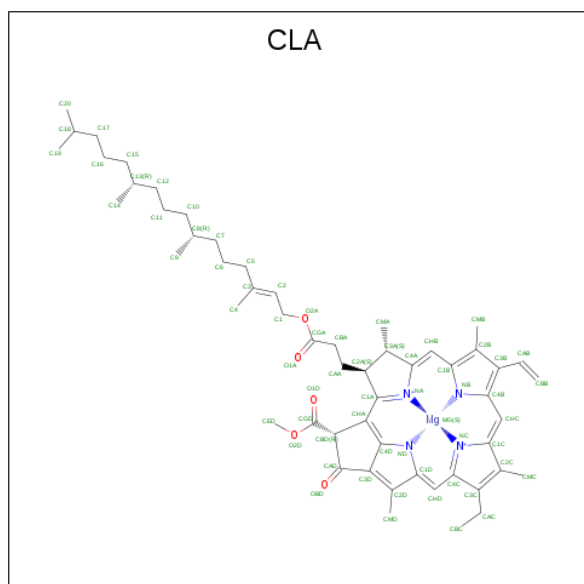
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

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

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

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



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

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

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

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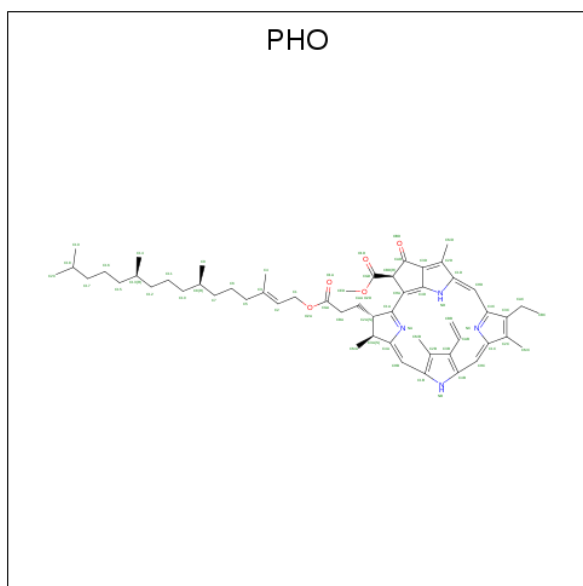
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	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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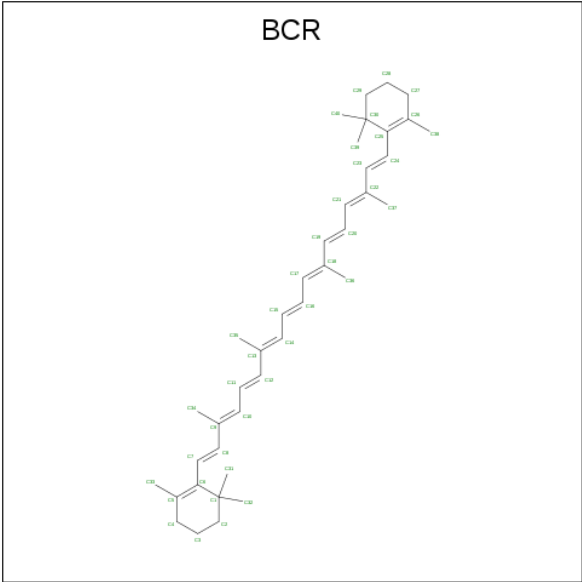
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	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	A	1	Total	C	H	N	O		0	0
			138	55	74	4	5			
23	a	1	Total	C	H	N	O		0	0
			138	55	74	4	5			
23	d	1	Total	C	H	N	O		0	0
			138	55	74	4	5			

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



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

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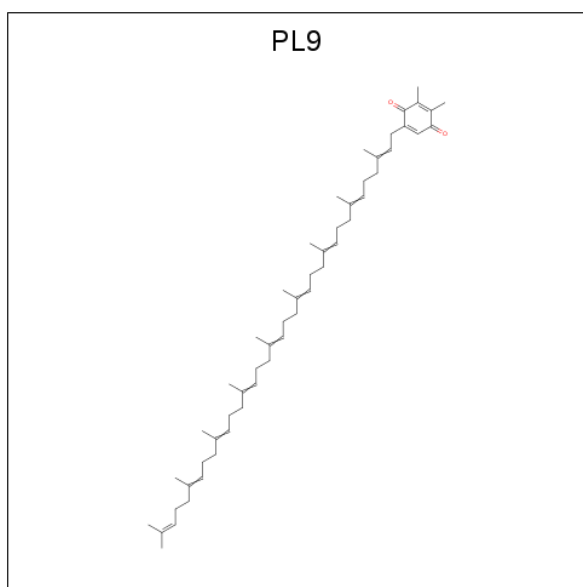
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	b	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	d	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40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

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

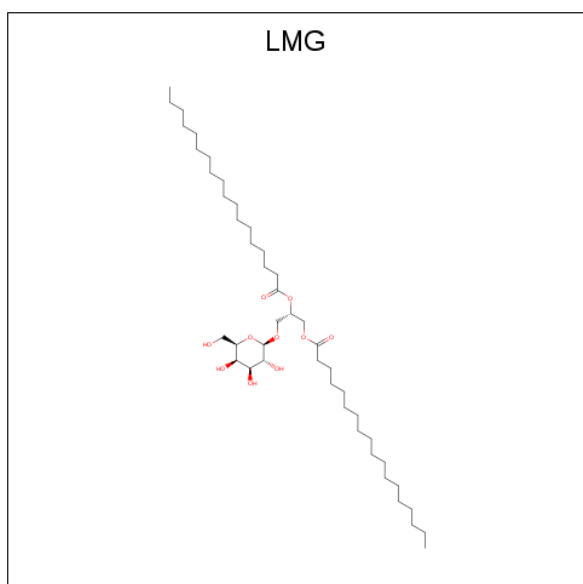
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	2	Total	Cl	0	0
			2	2		
25	a	2	Total	Cl	0	0
			2	2		

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



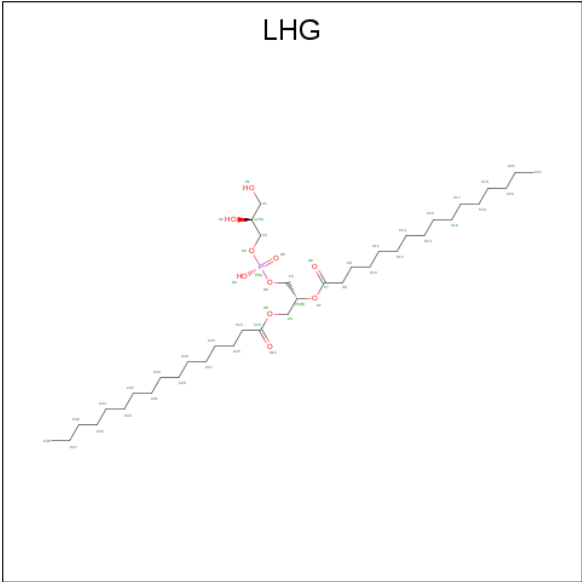
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	H	O	0	0
			135	53	80	2		
26	D	1	Total	C	H	O	0	0
			135	53	80	2		
26	a	1	Total	C	H	O	0	0
			135	53	80	2		
26	d	1	Total	C	H	O	0	0
			135	53	80	2		

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



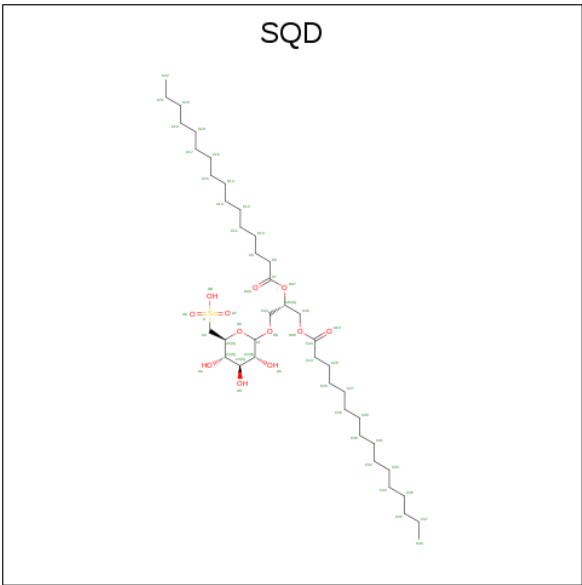
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	H	O	0	0
			113	38	65	10		
27	C	1	Total	C	H	O	0	0
			113	38	65	10		
27	D	1	Total	C	H	O	0	0
			122	41	71	10		
27	D	1	Total	C	H	O	0	0
			78	27	45	6		
27	D	1	Total	C	H	O	0	0
			68	24	40	4		
27	M	1	Total	C	H	O	0	0
			120	41	69	10		
27	a	1	Total	C	H	O	0	0
			138	45	83	10		
27	b	1	Total	C	H	O	0	0
			140	45	85	10		
27	c	1	Total	C	H	O	0	0
			78	27	41	10		
27	c	1	Total	C	H	O	0	0
			116	38	68	10		
27	c	1	Total	C	H	O	0	0
			117	39	68	10		
27	d	1	Total	C	H	O	0	0
			101	34	57	10		
27	m	1	Total	C	H	O	0	0
			120	41	69	10		

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



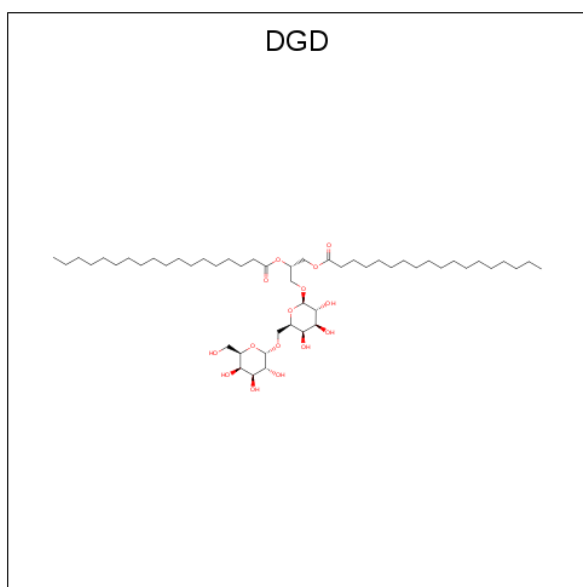
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	A	1	Total	C	H	O	P	0	0
			112	36	65	10	1		
28	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	B	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
28	D	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
28	E	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
28	a	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
28	d	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
28	d	1	Total	C	H	O	P	0	0
			88	28	49	10	1		
28	e	1	Total	C	H	O	P	0	0
			97	31	55	10	1		
28	l	1	Total	C	H	O	P	0	0
			122	38	73	10	1		

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



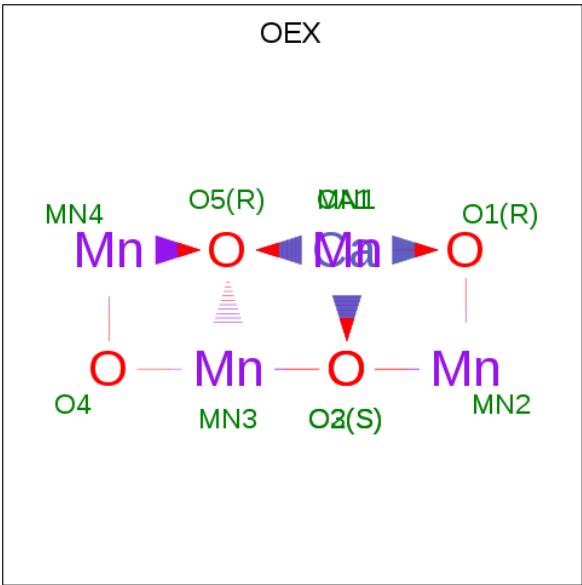
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	S	0	0
			123	39	71	12	1		
29	A	1	Total	C	H	O		0	0
			104	35	65	4			
29	B	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
29	D	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
29	a	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
29	a	1	Total	C	H	O		0	0
			92	31	56	5			
29	b	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
29	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



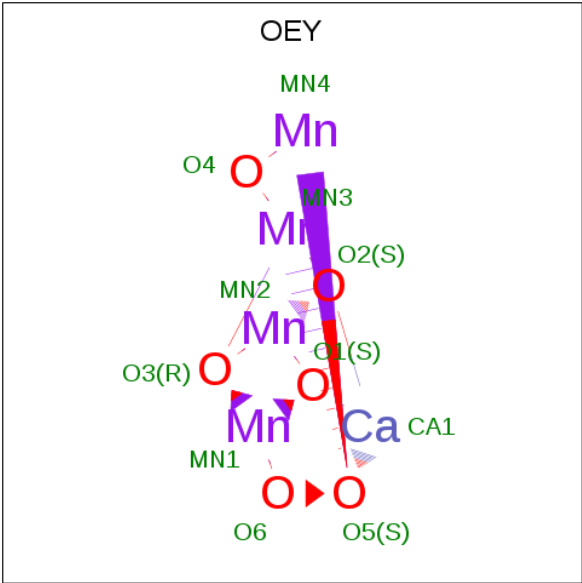
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	H	O	0	0
			160	51	94	15		
30	C	1	Total	C	H	O	0	0
			143	47	81	15		
30	C	1	Total	C	H	O	0	0
			142	47	80	15		
30	C	1	Total	C	H	O	0	0
			142	47	80	15		
30	H	1	Total	C	H	O	0	0
			142	47	80	15		
30	c	1	Total	C	H	O	0	0
			140	47	78	15		
30	c	1	Total	C	H	O	0	0
			138	47	76	15		
30	c	1	Total	C	H	O	0	0
			142	47	80	15		
30	h	1	Total	C	H	O	0	0
			139	47	77	15		

- Molecule 31 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



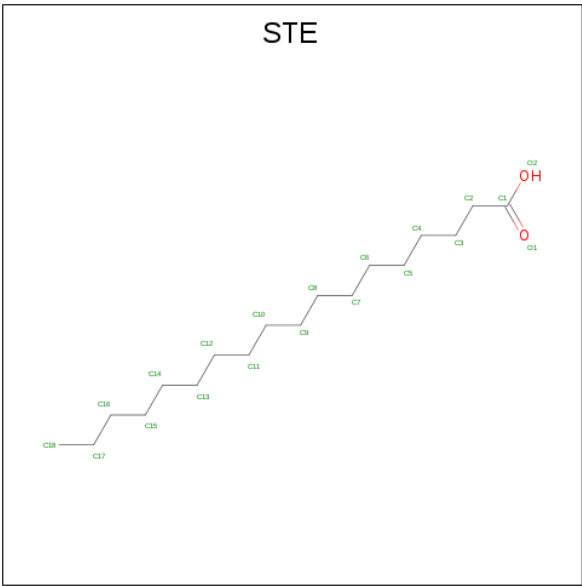
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
31	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 32 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula: CaMn_4O_6).



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

- Molecule 33 is STEARIC ACID (three-letter code: STE) (formula: C₁₈H₃₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total C H O 43 15 26 2	0	0
33	B	1	Total C H O 28 10 16 2	0	0
33	B	1	Total C H 47 16 31	0	0
33	B	1	Total C H O 28 10 16 2	0	0
33	C	1	Total C H O 28 10 16 2	0	0
33	C	1	Total C H 47 16 31	0	0
33	C	1	Total C H O 28 10 16 2	0	0
33	D	1	Total C H O 55 18 35 2	0	0
33	H	1	Total C H 53 18 35	0	0
33	I	1	Total C H 41 15 26	0	0
33	J	1	Total C H O 28 10 16 2	0	0
33	M	1	Total C H O 37 13 22 2	0	0
33	M	1	Total C H 26 10 16	0	0

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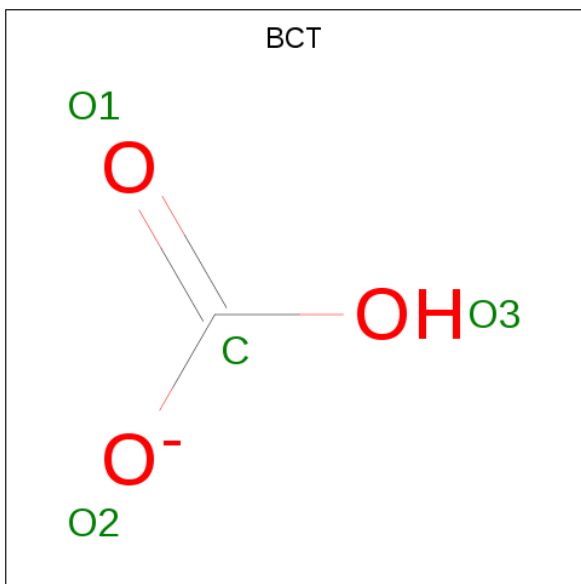
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	R	1	Total C H O 28 10 16 2	0	0
33	T	1	Total C H 44 15 29	0	0
33	Z	1	Total C H 20 8 12	0	0
33	a	1	Total C H 26 10 16	0	0
33	a	1	Total C H O 28 10 16 2	0	0
33	a	1	Total C H 41 15 26	0	0
33	b	1	Total C H 47 16 31	0	0
33	b	1	Total C H O 55 18 35 2	0	0
33	b	1	Total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

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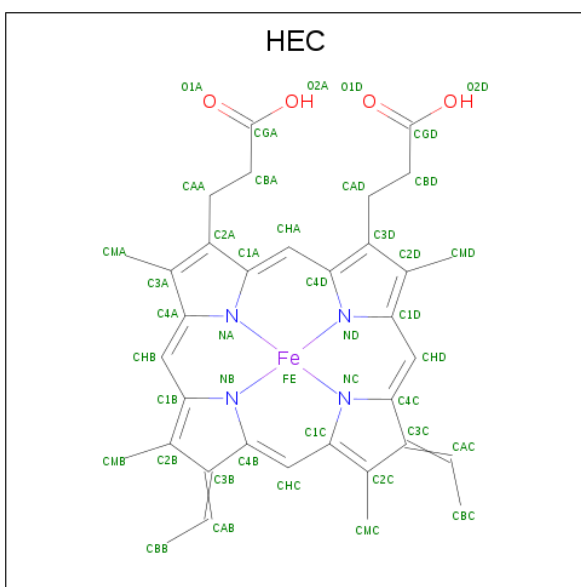
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	t	1	Total	C	H	O	0	0
			46	16	28	2		

- Molecule 34 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



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

- Molecule 35 is HEME C (three-letter code: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
35	F	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
			73	34	1	30	4	4		
35	f	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
			73	34	1	30	4	4		

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	146	Total	O	0	8
			146	146		
36	B	211	Total	O	0	0
			211	211		
36	C	185	Total	O	0	0
			185	185		
36	D	129	Total	O	0	0
			129	129		
36	E	34	Total	O	0	0
			34	34		
36	F	13	Total	O	0	0
			13	13		
36	H	33	Total	O	0	0
			33	33		
36	I	11	Total	O	0	0
			11	11		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	J	15	Total 15	O 15	0	0
36	K	9	Total 9	O 9	0	0
36	L	9	Total 9	O 9	0	0
36	M	5	Total 5	O 5	0	0
36	O	104	Total 104	O 104	0	0
36	R	13	Total 13	O 13	0	0
36	T	15	Total 15	O 15	0	0
36	U	51	Total 51	O 51	0	0
36	V	70	Total 70	O 70	0	0
36	X	11	Total 11	O 11	0	0
36	Y	2	Total 2	O 2	0	0
36	Z	5	Total 5	O 5	0	0
36	a	130	Total 130	O 130	0	8
36	b	215	Total 215	O 215	0	0
36	c	190	Total 190	O 190	0	0
36	d	122	Total 122	O 122	0	0
36	e	30	Total 30	O 30	0	0
36	f	9	Total 9	O 9	0	0
36	h	22	Total 22	O 22	0	0
36	i	9	Total 9	O 9	0	0
36	j	10	Total 10	O 10	0	0

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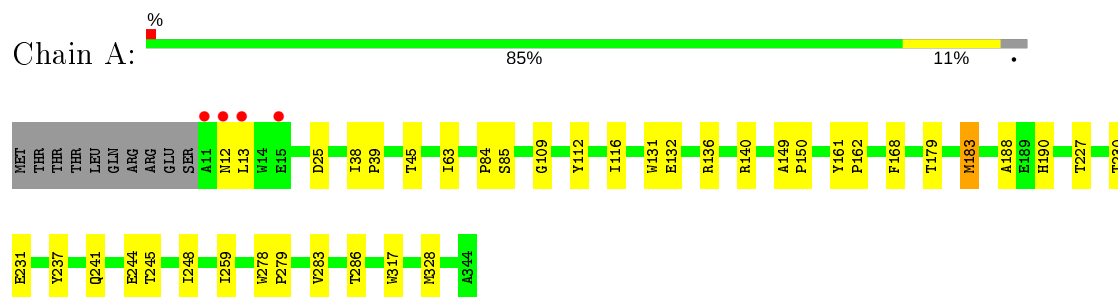
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	k	10	Total 10	O 10	0	0
36	l	9	Total 9	O 9	0	0
36	m	8	Total 8	O 8	0	0
36	o	103	Total 103	O 103	0	0
36	r	2	Total 2	O 2	0	0
36	t	11	Total 11	O 11	0	0
36	u	66	Total 66	O 66	0	0
36	v	58	Total 58	O 58	0	0
36	x	10	Total 10	O 10	0	0
36	y	6	Total 6	O 6	0	0
36	z	6	Total 6	O 6	0	0

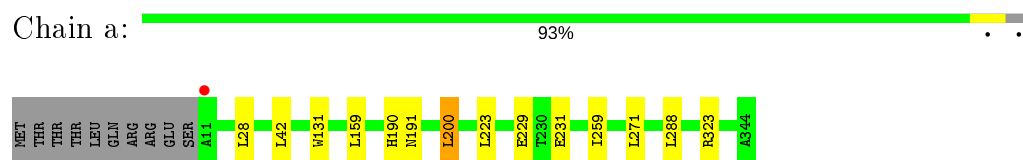
3 Residue-property plots [i](#)

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

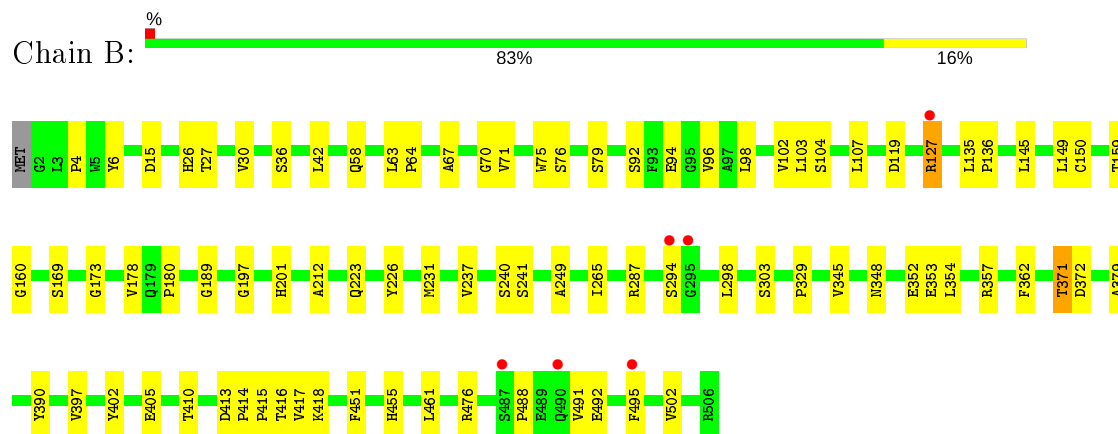
- Molecule 1: Photosystem II protein D1 1



- Molecule 1: Photosystem II protein D1 1

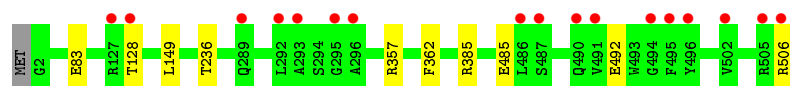


- Molecule 2: Photosystem II CP47 reaction center protein

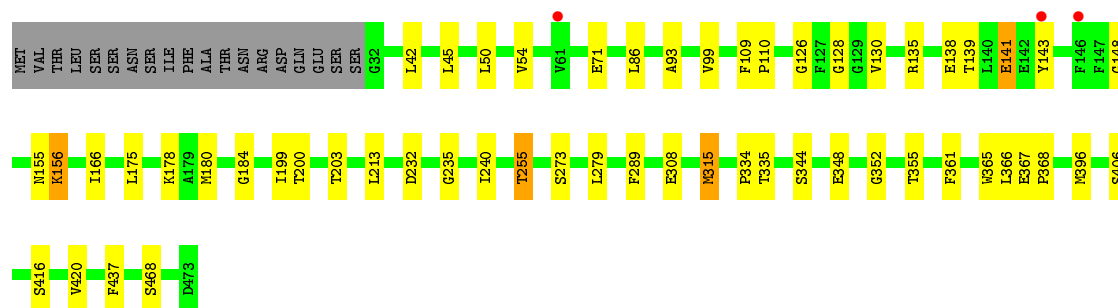
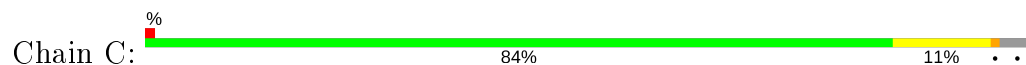


- Molecule 2: Photosystem II CP47 reaction center protein





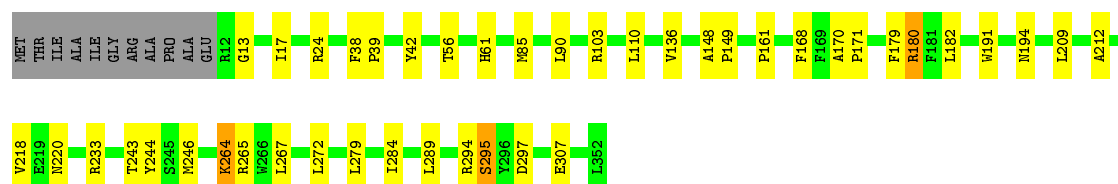
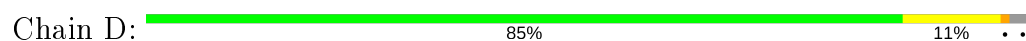
- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 4: Photosystem II D2 protein



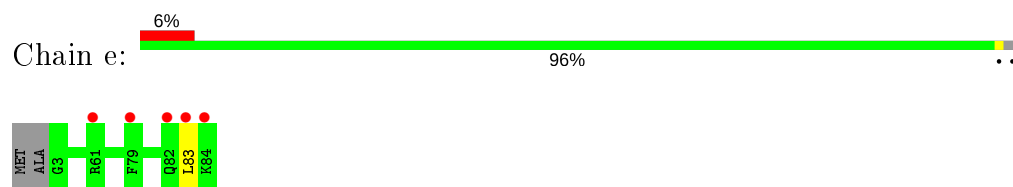
- Molecule 4: Photosystem II D2 protein



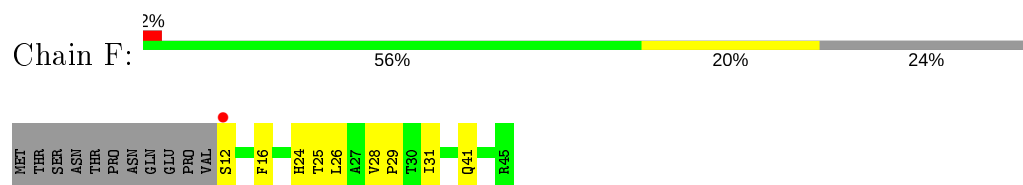
- Molecule 5: Cytochrome b559 subunit alpha



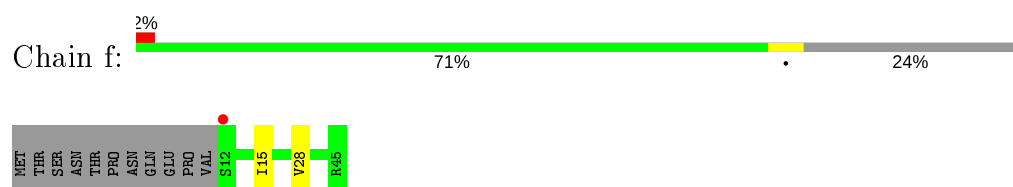
- Molecule 5: Cytochrome b559 subunit alpha



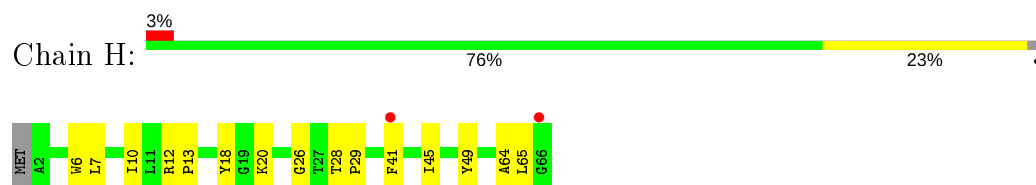
- Molecule 6: Cytochrome b559 subunit beta



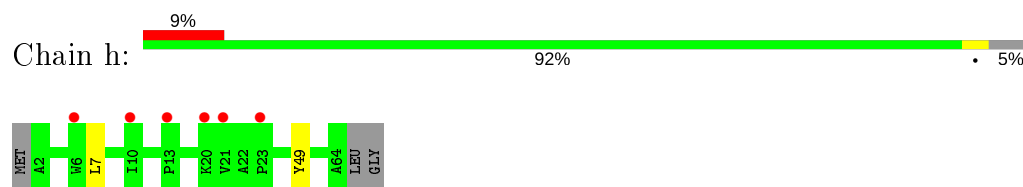
- Molecule 6: Cytochrome b559 subunit beta



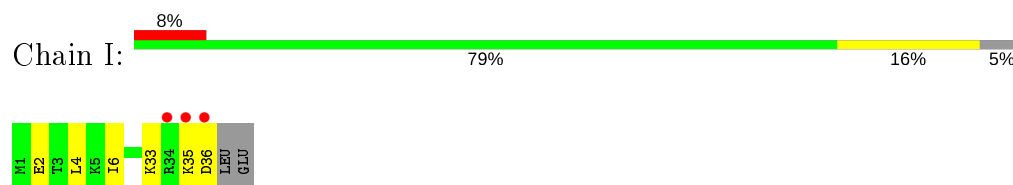
- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H

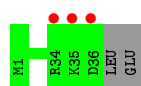


- Molecule 8: Photosystem II reaction center protein I

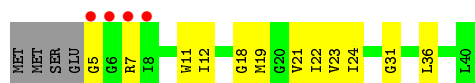


- Molecule 8: Photosystem II reaction center protein I

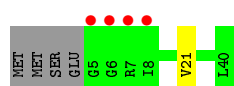
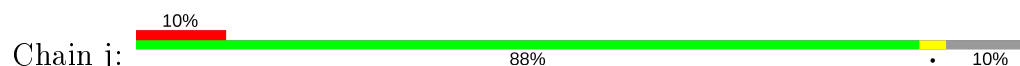




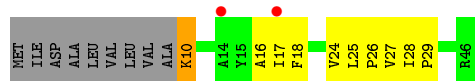
- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



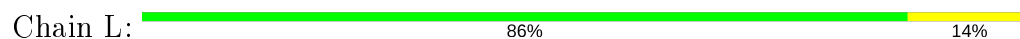
- Molecule 10: Photosystem II reaction center protein K



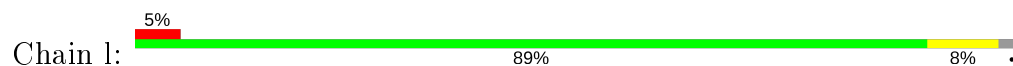
- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



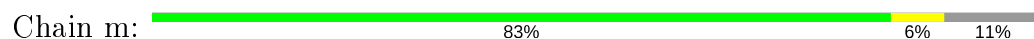
- Molecule 11: Photosystem II reaction center protein L



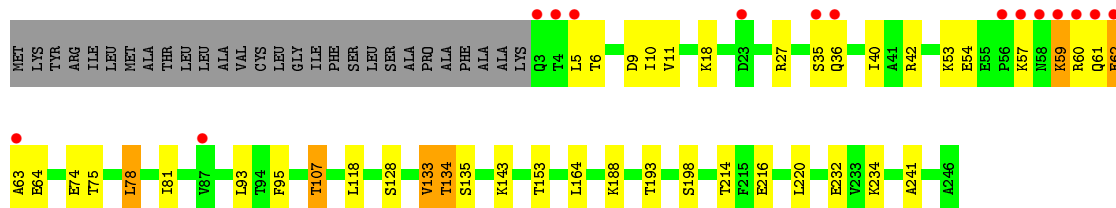
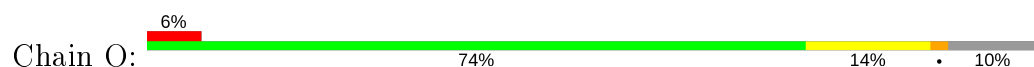
- Molecule 12: Photosystem II reaction center protein M



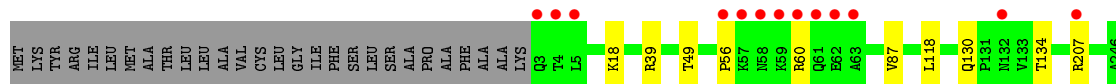
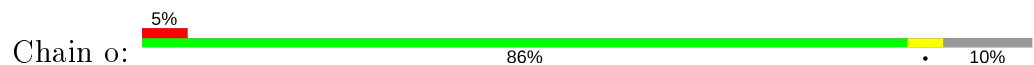
- Molecule 12: Photosystem II reaction center protein M



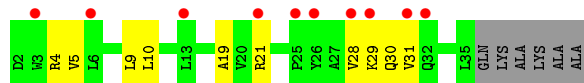
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



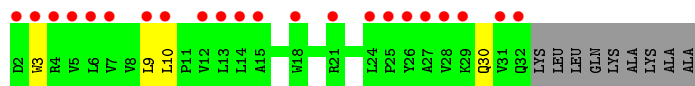
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 14: Photosystem II protein Y



- Molecule 14: Photosystem II protein Y



- Molecule 15: Photosystem II reaction center protein T

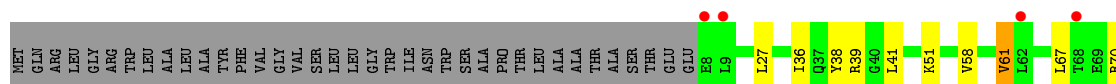




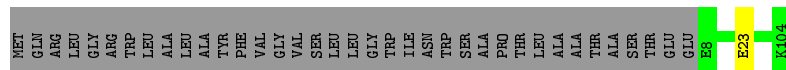
- Molecule 15: Photosystem II reaction center protein T



- Molecule 16: Photosystem II 12 kDa extrinsic protein



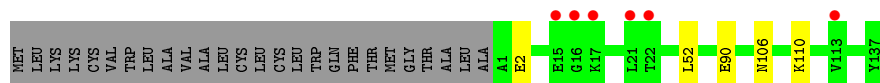
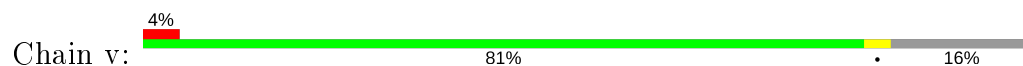
- Molecule 16: Photosystem II 12 kDa extrinsic protein



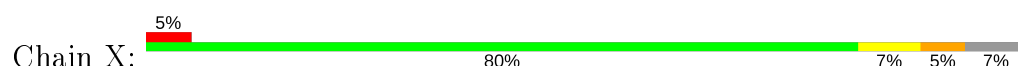
- Molecule 17: Cytochrome c-550

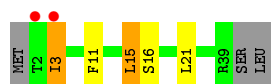


- Molecule 17: Cytochrome c-550

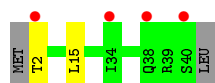
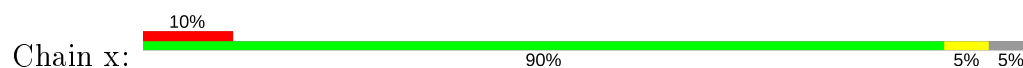


- Molecule 18: Photosystem II reaction center X protein

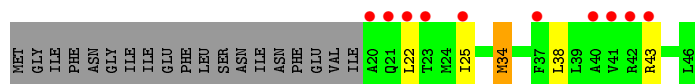




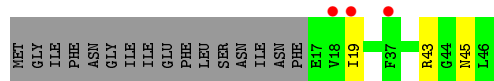
- Molecule 18: Photosystem II reaction center X protein



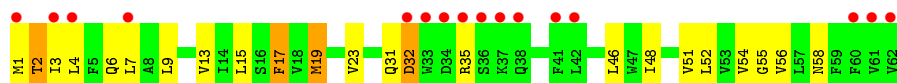
- Molecule 19: Photosystem II reaction center protein Ycf12



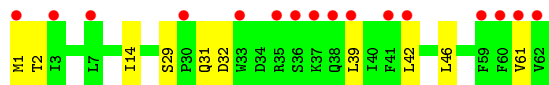
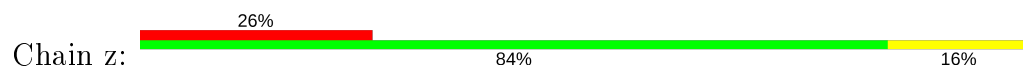
- Molecule 19: Photosystem II reaction center protein Ycf12



- 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	117.04Å 221.92Å 308.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.59 – 2.01 33.59 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (33.59-2.01) 86.7 (33.59-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.57 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.175 , 0.228 0.175 , 0.228	Depositor DCC
R_{free} test set	4767 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 66.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	105978	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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: LHG, STE, OEY, OEX, PHO, DGD, CL, CLA, PL9, LMG, FE2, HEC, BCT, FME, BCR, SQD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.62	0/3187	0.66	2/4342 (0.0%)
1	a	0.60	0/3184	0.82	11/4338 (0.3%)
2	B	0.64	0/4161	0.69	1/5669 (0.0%)
2	b	0.61	0/4118	0.68	1/5611 (0.0%)
3	C	0.62	1/3621 (0.0%)	0.66	1/4930 (0.0%)
3	c	0.59	0/3693	0.66	0/5026
4	D	0.67	0/2820	0.69	2/3840 (0.1%)
4	d	0.64	0/2829	0.70	1/3852 (0.0%)
5	E	0.57	0/688	0.62	0/940
5	e	0.51	0/683	0.62	0/932
6	F	0.54	0/284	0.58	0/387
6	f	0.53	0/284	0.60	0/387
7	H	0.63	0/523	0.68	0/713
7	h	0.58	0/511	0.68	0/697
8	I	0.61	0/293	0.68	0/396
8	i	0.66	0/293	0.63	0/396
9	J	0.49	0/263	0.63	0/356
9	j	0.53	0/263	0.63	0/356
10	K	0.50	0/303	0.65	0/416
10	k	0.54	0/303	0.64	0/416
11	L	0.60	0/311	0.65	0/422
11	l	0.66	0/303	0.69	0/412
12	M	0.63	0/249	0.67	0/341
12	m	0.62	0/244	0.76	0/334
13	O	0.61	0/1904	0.70	0/2585
13	o	0.61	0/1905	0.72	0/2583
14	R	0.47	0/277	0.56	0/380
14	r	0.36	0/246	0.51	0/339
15	T	0.71	0/257	0.63	0/349
15	t	0.75	0/255	0.63	0/346
16	U	0.55	0/785	0.67	0/1064
16	u	0.60	0/785	0.68	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	V	0.58	0/1085	0.70	1/1473 (0.1%)
17	v	0.55	0/1085	0.63	0/1473
18	X	0.51	0/284	0.60	0/384
18	x	0.44	0/289	0.55	0/391
19	Y	0.48	0/197	0.59	0/264
19	y	0.45	0/219	0.61	0/294
20	Z	0.45	0/490	0.58	0/669
20	z	0.41	0/488	0.52	0/666
All	All	0.60	1/43962 (0.0%)	0.68	20/59833 (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
1	A	0	1
17	V	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	468	SER	C-N	-5.64	1.21	1.34

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	190[A]	HIS	O-C-N	-14.28	99.85	122.70
1	a	190[B]	HIS	O-C-N	-14.28	99.85	122.70
1	a	190[A]	HIS	CA-C-N	11.07	141.56	117.20
1	a	190[B]	HIS	CA-C-N	11.07	141.56	117.20
1	a	190[A]	HIS	C-N-CA	9.85	146.32	121.70
1	a	190[B]	HIS	C-N-CA	9.85	146.32	121.70
17	V	63	THR	C-N-CD	-6.23	106.89	120.60
2	B	15	ASP	CB-CG-OD2	-5.74	113.14	118.30
2	b	385	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	183[A]	MET	CA-CB-CG	5.31	122.32	113.30
1	A	183[B]	MET	CA-CB-CG	5.31	122.32	113.30
4	d	297	ASP	CB-CG-OD1	5.26	123.03	118.30
4	D	297	ASP	CB-CG-OD1	5.22	123.00	118.30
3	C	396	MET	CG-SD-CE	-5.20	91.88	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	294	ARG	NE-CZ-NH1	-5.19	117.70	120.30
1	a	323	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	a	200	LEU	CA-CB-CG	5.09	127.01	115.30
1	a	131	TRP	CA-CB-CG	-5.08	104.05	113.70
1	a	191[A]	ASN	O-C-N	5.01	130.71	122.70
1	a	191[B]	ASN	O-C-N	5.01	130.71	122.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	190[A]	HIS	Mainchain
17	V	63	THR	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3089	2942	2956	28	0
1	a	3086	2933	2946	0	0
2	B	4005	3859	3867	62	0
2	b	3978	3822	3836	0	0
3	C	3479	3397	3383	38	0
3	c	3553	3468	3466	0	0
4	D	2726	2624	2632	36	0
4	d	2732	2630	2638	0	0
5	E	666	650	651	22	0
5	e	664	647	648	0	0
6	F	275	281	282	10	0
6	f	275	281	282	0	0
7	H	510	532	532	10	0
7	h	498	518	518	0	0
8	I	296	311	311	2	0
8	i	296	311	311	0	0
9	J	257	268	268	9	0
9	j	257	268	268	0	0
10	K	293	305	305	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	k	293	305	305	0	0
11	L	304	316	316	4	0
11	l	296	304	304	0	0
12	M	256	269	269	9	0
12	m	251	267	267	0	0
13	O	1870	1828	1830	25	0
13	o	1874	1844	1846	0	0
14	R	271	298	298	7	0
14	r	240	253	250	0	0
15	T	258	261	261	3	0
15	t	256	256	256	0	0
16	U	774	772	773	7	0
16	u	774	772	773	0	0
17	V	1064	1068	1073	9	0
17	v	1064	1068	1073	0	0
18	X	281	312	312	5	0
18	x	286	316	314	0	0
19	Y	196	217	217	4	0
19	y	218	241	241	0	0
20	Z	479	516	516	19	0
20	z	477	509	509	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	184	192	192	6	0
22	B	1035	1139	1139	49	0
22	C	839	922	922	32	0
22	D	195	216	216	6	0
22	a	130	144	144	0	0
22	b	1035	1139	1139	0	0
22	c	839	919	919	0	0
22	d	260	288	288	0	0
23	A	128	148	148	2	0
23	a	64	74	74	0	0
23	d	64	74	74	0	0
24	A	40	56	56	1	0
24	B	120	168	168	11	0
24	C	120	168	168	6	0
24	D	40	56	56	2	0
24	H	40	56	56	4	0
24	T	40	56	56	6	0
24	Y	40	56	56	2	0
24	a	40	56	56	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	b	120	168	168	0	0
24	c	120	168	168	0	0
24	d	40	56	56	0	0
24	k	40	56	56	0	0
24	t	40	56	56	0	0
24	x	40	56	56	0	0
25	A	2	0	0	0	0
25	a	2	0	0	0	0
26	A	55	80	80	8	0
26	D	55	80	80	0	0
26	a	55	80	80	0	0
26	d	55	80	80	0	0
27	A	48	65	66	0	0
27	C	48	65	66	0	0
27	D	112	156	157	0	0
27	M	51	69	72	2	0
27	a	55	83	86	0	0
27	b	55	85	86	0	0
27	c	134	177	181	0	0
27	d	44	57	58	0	0
27	m	51	69	72	0	0
28	A	47	65	67	0	0
28	B	98	146	148	1	0
28	D	49	73	74	0	0
28	E	49	73	74	3	0
28	a	49	72	74	0	0
28	d	88	121	125	0	0
28	e	42	55	57	0	0
28	l	49	73	74	0	0
29	A	91	136	136	1	0
29	B	54	77	77	2	0
29	D	36	45	46	0	0
29	a	90	133	132	0	0
29	b	49	65	65	0	0
29	f	41	48	48	0	0
30	A	66	94	95	1	0
30	C	186	241	246	2	0
30	H	62	80	81	0	0
30	c	186	234	246	0	0
30	h	62	77	79	0	0
31	A	10	0	0	0	0
31	a	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	A	11	0	0	1	0
32	a	11	0	0	0	0
33	B	57	89	86	3	0
33	C	40	63	60	1	0
33	D	20	35	35	4	0
33	H	18	35	35	0	0
33	I	15	26	26	0	0
33	J	12	16	16	0	0
33	M	25	38	38	1	0
33	R	12	16	16	0	0
33	T	15	29	26	1	0
33	Z	8	12	12	0	0
33	a	37	58	58	0	0
33	b	96	168	165	0	0
33	c	20	35	35	0	0
33	d	57	96	96	0	0
33	j	12	16	16	0	0
33	k	12	16	16	0	0
33	l	18	35	35	0	0
33	m	12	16	16	0	0
33	t	32	48	48	0	0
34	D	4	1	1	0	0
34	a	4	1	1	0	0
35	F	43	32	32	11	0
35	V	43	30	30	6	0
35	f	43	32	32	0	0
35	v	43	30	30	0	0
36	A	146	0	0	3	0
36	B	211	0	0	8	0
36	C	185	0	0	5	0
36	D	129	0	0	5	0
36	E	34	0	0	3	0
36	F	13	0	0	2	0
36	H	33	0	0	1	0
36	I	11	0	0	0	0
36	J	15	0	0	3	0
36	K	9	0	0	1	0
36	L	9	0	0	0	0
36	M	5	0	0	4	0
36	O	104	0	0	3	0
36	R	13	0	0	0	0
36	T	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	U	51	0	0	1	0
36	V	70	0	0	2	0
36	X	11	0	0	0	0
36	Y	2	0	0	0	0
36	Z	5	0	0	1	0
36	a	130	0	0	0	0
36	b	215	0	0	0	0
36	c	190	0	0	0	0
36	d	122	0	0	0	0
36	e	30	0	0	0	0
36	f	9	0	0	0	0
36	h	22	0	0	0	0
36	i	9	0	0	0	0
36	j	10	0	0	0	0
36	k	10	0	0	0	0
36	l	9	0	0	0	0
36	m	8	0	0	0	0
36	o	103	0	0	0	0
36	r	2	0	0	0	0
36	t	11	0	0	0	0
36	u	66	0	0	0	0
36	v	58	0	0	0	0
36	x	10	0	0	0	0
36	y	6	0	0	0	0
36	z	6	0	0	0	0
All	All	53425	52553	52659	400	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (400) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:315:MET:SD	36:C:768:HOH:O	13.15	0.94
32:A:417[B]:OEY:O6	32:A:417[B]:OEY:O5	1.92	0.88
5:E:71:GLU:OE1	36:E:201:HOH:O	50.17	0.86
30:C:517:DGD:O1A	36:C:601:HOH:O	44.91	0.86
1:A:25:ASP:OD1	36:A:501:HOH:O	1.94	0.84
35:F:101:HEC:HHD	35:F:101:HEC:HBC3	1.59	0.84
16:U:58:VAL:O	16:U:61:VAL:HG22	1.80	0.82
35:V:201:HEC:HMC1	35:V:201:HEC:HBC3	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:40:CYS:SG	35:V:201:HEC:C3C	2.72	0.78
2:B:410:THR:O	36:B:701:HOH:O	2.01	0.78
7:H:64:ALA:O	36:H:201:HOH:O	25.06	0.76
6:F:12:SER:N	36:F:201:HOH:O	9.45	0.75
24:T:101:BCR:HC8	24:T:101:BCR:H321	1.82	0.74
22:D:403:CLA:HBB1	22:D:403:CLA:HMB1	1.69	0.74
26:A:410:PL9:H361	6:F:25:THR:HG21	1.69	0.74
10:K:24:VAL:HG13	19:Y:25:ILE:HD13	1.69	0.73
22:B:613:CLA:HBB1	22:B:613:CLA:HMB1	1.71	0.73
2:B:491:VAL:HG12	4:D:136:VAL:HG13	1.87	0.72
9:J:5:GLY:N	36:J:201:HOH:O	2.23	0.72
3:C:141:GLU:OE1	36:C:601:HOH:O	2.08	0.71
3:C:143:TYR:CE1	22:C:513:CLA:HED3	2.25	0.71
12:M:30:GLU:OE2	36:M:201:HOH:O	35.10	0.70
22:D:404:CLA:HMB1	22:D:404:CLA:HBB1	1.73	0.69
22:C:513:CLA:HMB1	22:C:513:CLA:HBB1	1.73	0.68
24:D:405:BCR:H23C	24:D:405:BCR:H392	1.76	0.68
22:C:511:CLA:HBB1	22:C:511:CLA:HMB1	1.75	0.68
10:K:10:LYS:NZ	36:K:101:HOH:O	2.20	0.67
3:C:148:GLY:O	3:C:156:LYS:NZ	2.27	0.67
22:C:509:CLA:HBB1	22:C:509:CLA:HMB1	1.76	0.67
22:B:609:CLA:HBB1	22:B:609:CLA:HMB1	1.99	0.66
3:C:279:LEU:HD12	22:C:509:CLA:HED2	1.77	0.66
1:A:63[B]:ILE:HB	3:C:335:THR:HG21	1.79	0.65
2:B:371:THR:HG23	2:B:372:ASP:O	1.96	0.65
22:C:510:CLA:HBB1	22:C:510:CLA:HMB1	1.78	0.65
24:C:514:BCR:C8	24:C:514:BCR:H331	2.26	0.64
22:B:602:CLA:HBB1	22:B:602:CLA:HMB1	1.79	0.64
2:B:223:GLN:OE1	36:B:703:HOH:O	2.15	0.64
13:O:35:SER:OG	13:O:36:GLN:N	2.27	0.64
13:O:62:GLU:OE1	13:O:63:ALA:N	6.16	0.64
35:F:101:HEC:HMB1	35:F:101:HEC:HBB2	1.80	0.64
33:B:624:STE:O1	36:B:704:HOH:O	2.15	0.63
6:F:24:HIS:O	6:F:28:VAL:HG13	5.48	0.63
2:B:102:VAL:HG21	22:B:606:CLA:H141	3.83	0.63
3:C:279:LEU:CD1	22:C:509:CLA:HED2	2.29	0.62
1:A:188[A]:ALA:HB2	1:A:328[A]:MET:HB2	1.81	0.62
2:B:492:GLU:OE2	2:B:495:PHE:CE1	6.27	0.62
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.35	0.61
13:O:27:ARG:O	13:O:27:ARG:HG2	2.00	0.61
22:A:402:CLA:HMB1	22:A:402:CLA:HBB1	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:LEU:HD22	22:B:604:CLA:H193	1.82	0.61
22:B:604:CLA:HMD2	22:B:612:CLA:H202	1.83	0.61
6:F:28:VAL:HG22	6:F:29:PRO:HD3	4.67	0.60
16:U:38:TYR:HB2	16:U:41:LEU:HD12	1.82	0.60
5:E:30:LEU:HD11	35:F:101:HEC:CBB	3.84	0.60
36:A:585:HOH:O	13:O:107:THR:HG21	2.01	0.59
5:E:26:THR:HB	35:F:101:HEC:HBB2	3.85	0.59
20:Z:51:VAL:O	20:Z:54:VAL:O	2.20	0.59
26:A:410:PL9:H152	28:E:101:LHG:H381	1.83	0.59
20:Z:32:ASP:OD1	20:Z:32:ASP:N	3.49	0.58
24:B:618:BCR:H331	24:B:618:BCR:C8	2.35	0.58
2:B:169:SER:O	7:H:65:LEU:HD22	2.03	0.58
22:B:607:CLA:H193	11:L:27:LEU:HD11	1.84	0.58
3:C:45:LEU:HD22	3:C:138:GLU:HG2	1.86	0.58
12:M:4:ASN:ND2	27:M:101:LMG:O10	2.89	0.58
4:D:209:LEU:HD23	4:D:209:LEU:C	2.24	0.58
22:B:612:CLA:HMB1	22:B:612:CLA:HBB1	2.04	0.58
22:B:614:CLA:HBB1	22:B:614:CLA:HMB1	1.85	0.58
8:I:33:LYS:O	8:I:35:LYS:NZ	2.92	0.57
2:B:357:ARG:NE	36:B:702:HOH:O	2.10	0.57
22:C:504:CLA:H91	22:C:508:CLA:C17	4.19	0.57
5:E:22[A]:ILE:HG23	5:E:23:HIS:ND1	2.19	0.57
2:B:348:ASN:HB3	2:B:354:LEU:HD11	2.33	0.57
3:C:406:SER:HA	3:C:420:VAL:HG23	1.88	0.57
22:C:504:CLA:H142	22:C:508:CLA:H121	7.11	0.57
23:A:405:PHO:HBC3	4:D:279:LEU:HD22	1.86	0.57
4:D:267:LEU:HD23	4:D:267:LEU:C	2.49	0.56
2:B:30:VAL:HG12	22:B:605:CLA:HHD	2.15	0.56
1:A:241:GLN:NE2	1:A:245:THR:HG23	6.11	0.56
2:B:345:VAL:HG13	2:B:353:GLU:OE2	4.14	0.56
2:B:27:THR:HG22	2:B:107:LEU:HD13	1.88	0.56
2:B:352:GLU:OE1	36:B:705:HOH:O	2.18	0.56
20:Z:31:GLN:NE2	36:Z:201:HOH:O	2.38	0.56
1:A:188[B]:ALA:HB2	1:A:328[B]:MET:HB2	1.99	0.56
13:O:6:THR:HG22	13:O:9:ASP:OD2	2.06	0.56
4:D:272:LEU:HD23	4:D:272:LEU:C	2.42	0.56
22:B:608:CLA:HBB1	22:B:608:CLA:HMB1	2.08	0.55
3:C:178:LYS:NZ	3:C:184:GLY:O	2.50	0.55
23:A:405:PHO:HMB1	23:A:405:PHO:HBB1	1.87	0.55
5:E:68:ASP:O	5:E:72:ALA:HB2	2.12	0.54
17:V:40:CYS:SG	35:V:201:HEC:CBC	2.76	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:602:CLA:H43	7:H:45:ILE:HG22	2.14	0.54
24:B:619:BCR:C8	24:B:619:BCR:H331	2.37	0.54
9:J:18:GLY:O	9:J:22:ILE:HD13	4.75	0.54
9:J:36:LEU:O	36:J:201:HOH:O	45.36	0.54
24:Y:101:BCR:H322	20:Z:17:PHE:CE2	2.43	0.54
13:O:164:LEU:HD13	13:O:188:LYS:O	2.71	0.53
2:B:127:ARG:NH1	7:H:18:TYR:O	10.53	0.53
1:A:183[B]:MET:HA	22:A:402:CLA:HMD2	1.91	0.53
3:C:232:ASP:OD2	36:C:604:HOH:O	31.27	0.53
13:O:59:LYS:O	13:O:61:GLN:N	2.41	0.53
33:B:624:STE:C1	36:B:704:HOH:O	2.57	0.53
2:B:249:ALA:HB2	22:B:604:CLA:HBC3	2.35	0.52
16:U:58:VAL:HG12	16:U:79:LEU:HD22	2.28	0.52
17:V:104:MET:HA	17:V:107:LEU:HD22	5.05	0.52
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.45	0.52
13:O:54:GLU:O	13:O:63:ALA:HB3	2.09	0.52
3:C:437:PHE:CZ	22:C:510:CLA:HMB3	2.54	0.52
1:A:179[A]:THR:O	1:A:183[A]:MET:HG3	4.30	0.52
1:A:283:VAL:HA	1:A:286:THR:HG22	2.20	0.52
18:X:3:ILE:O	18:X:3:ILE:HG13	2.10	0.51
20:Z:1:MET:HB3	20:Z:4:LEU:HD23	7.63	0.51
22:C:511:CLA:HMB1	22:C:511:CLA:CBB	2.38	0.51
6:F:16:PHE:H	14:R:30:GLN:HE22	2.47	0.51
3:C:166:ILE:HG21	22:C:512:CLA:H202	4.88	0.51
22:B:604:CLA:HAB	22:B:611:CLA:H191	3.62	0.51
22:C:505:CLA:HBC2	24:C:515:BCR:H341	1.93	0.51
20:Z:52:LEU:O	20:Z:56:VAL:HG23	2.10	0.51
24:H:101:BCR:H331	24:H:101:BCR:C8	2.39	0.51
10:K:18:PHE:HE2	20:Z:9:LEU:HD21	1.75	0.51
5:E:30:LEU:HD11	35:F:101:HEC:HBB3	4.30	0.51
35:F:101:HEC:CHD	35:F:101:HEC:HBC3	2.34	0.51
13:O:133:VAL:C	13:O:134:THR:HG23	2.31	0.51
33:D:412:STE:H92	18:X:16:SER:HB3	1.93	0.51
4:D:179:PHE:HA	4:D:182:LEU:HD22	5.50	0.51
9:J:19:MET:O	9:J:23:VAL:HG23	2.16	0.51
22:B:610:CLA:HHC	22:B:610:CLA:CBB	2.41	0.50
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.03	0.50
7:H:41:PHE:CE1	7:H:45:ILE:HD11	2.46	0.50
22:B:606:CLA:H102	22:B:606:CLA:H142	4.48	0.50
22:C:503:CLA:HBB1	22:C:503:CLA:HMB1	1.94	0.50
35:F:101:HEC:HHC	35:F:101:HEC:CBB	3.98	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:26:PRO:O	10:K:29:PRO:HD2	2.25	0.50
12:M:5:GLN:O	36:M:201:HOH:O	2.20	0.50
15:T:15:ALA:HB2	24:T:101:BCR:H14C	2.21	0.50
3:C:213:LEU:HG	22:C:506:CLA:H193	1.93	0.50
4:D:148:ALA:HB3	4:D:149:PRO:CD	2.41	0.50
22:B:604:CLA:HBD	22:B:605:CLA:H43	1.94	0.50
13:O:216:GLU:OE2	13:O:234:LYS:HD2	3.21	0.50
14:R:30:GLN:N	14:R:31:VAL:HA	4.83	0.50
22:B:615:CLA:HBB1	22:B:615:CLA:HHC	4.13	0.49
24:D:405:BCR:C8	24:D:405:BCR:H331	2.41	0.49
4:D:85:MET:HE1	5:E:72:ALA:HB2	1.93	0.49
5:E:20:TRP:O	5:E:24:SER:OG	2.99	0.49
2:B:212:ALA:HB2	22:B:609:CLA:HMC3	2.02	0.49
2:B:414:PRO:O	2:B:418:LYS:HG3	2.12	0.49
22:C:501:CLA:H192	22:C:507:CLA:HBB1	4.80	0.49
20:Z:19:MET:O	20:Z:23:VAL:HG23	2.84	0.49
22:C:503:CLA:HMB3	33:C:522:STE:H111	1.95	0.49
10:K:18:PHE:HE2	20:Z:13:VAL:HG21	5.53	0.49
1:A:230:THR:HG21	11:L:8:GLN:NE2	2.27	0.49
22:B:604:CLA:H42	22:B:605:CLA:H42	1.95	0.49
2:B:70:GLY:HA2	2:B:178:VAL:HG21	2.14	0.49
22:A:406:CLA:HBB1	22:A:406:CLA:HMB1	1.94	0.48
26:A:410:PL9:H152	28:E:101:LHG:C38	2.42	0.48
22:B:611:CLA:HBB1	22:B:611:CLA:HMB1	1.94	0.48
3:C:45:LEU:HA	3:C:139:THR:HG22	2.27	0.48
13:O:18:LYS:NZ	13:O:74:GLU:OE1	4.98	0.48
10:K:24:VAL:CG1	19:Y:25:ILE:HD13	2.39	0.48
13:O:78:LEU:HB3	13:O:81:ILE:HD11	1.95	0.48
22:A:403:CLA:HMB1	22:A:403:CLA:HBB1	1.94	0.48
2:B:492:GLU:OE1	5:E:3:GLY:N	5.46	0.48
1:A:112:TYR:O	1:A:116:ILE:HG12	2.37	0.48
2:B:102:VAL:HA	24:B:618:BCR:C40	2.44	0.48
2:B:249:ALA:CB	22:B:604:CLA:HBC3	2.87	0.48
2:B:119:ASP:H	11:L:1:MET:HE1	1.78	0.48
2:B:102:VAL:HG11	22:B:606:CLA:H142	3.86	0.48
4:D:194:ASN:HA	4:D:295:SER:OG	2.34	0.48
6:F:31:ILE:HG13	35:F:101:HEC:HMC1	1.95	0.47
1:A:131:TRP:CE3	1:A:132:GLU:HA	2.49	0.47
1:A:183[A]:MET:HA	22:A:402:CLA:HMD2	1.97	0.47
2:B:26:HIS:HB2	22:B:612:CLA:HMB2	1.96	0.47
5:E:17:VAL:HG23	9:J:7:ARG:HD3	4.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:3:ILE:HG22	20:Z:7:LEU:HD23	8.96	0.47
1:A:227:THR:HB	1:A:231:GLU:HG3	1.97	0.47
2:B:27:THR:HG22	2:B:107:LEU:CD1	2.44	0.47
2:B:461:LEU:HD21	4:D:284:ILE:HD11	2.38	0.47
22:B:604:CLA:H42	22:B:605:CLA:H2	4.19	0.47
3:C:315:MET:CE	3:C:365:TRP:HZ3	4.32	0.47
4:D:61:HIS:CE1	4:D:168:PHE:CE1	3.59	0.47
10:K:17:ILE:HD11	20:Z:6:GLN:HG2	9.29	0.47
7:H:6:TRP:CZ2	7:H:10:ILE:HD11	2.50	0.47
15:T:29:ILE:H	15:T:29:ILE:HD12	4.35	0.47
2:B:502:VAL:O	2:B:502:VAL:HG22	2.15	0.46
3:C:315:MET:CE	36:C:768:HOH:O	14.56	0.46
12:M:31:SER:HB2	12:M:32:GLN:OE1	8.87	0.46
2:B:287:ARG:HD3	36:B:709:HOH:O	2.14	0.46
2:B:397:VAL:HG12	2:B:417:VAL:HG11	1.97	0.46
2:B:103:LEU:HD21	22:B:605:CLA:HMC3	1.97	0.46
9:J:5:GLY:N	36:J:205:HOH:O	2.49	0.46
13:O:27:ARG:HH11	13:O:27:ARG:HG3	1.81	0.46
7:H:28:THR:HB	7:H:29:PRO:HD3	2.31	0.46
12:M:30:GLU:HA	12:M:30:GLU:OE1	2.15	0.46
5:E:22[A]:ILE:HD12	5:E:23:HIS:CE1	2.50	0.46
2:B:67:ALA:HA	2:B:71:VAL:O	2.16	0.46
4:D:218:VAL:HG13	4:D:244:TYR:CD1	2.62	0.46
35:F:101:HEC:HBB3	35:F:101:HEC:HHC	4.20	0.46
17:V:76:MET:CE	17:V:112:LEU:HD22	4.26	0.46
3:C:42:LEU:HD21	22:C:511:CLA:H2A	2.14	0.46
5:E:8:ARG:NH2	5:E:12:ASP:OD2	2.68	0.46
13:O:53:LYS:NZ	13:O:232:GLU:OE1	3.01	0.46
14:R:28:VAL:O	14:R:31:VAL:CB	3.85	0.46
22:C:513:CLA:C4B	24:C:514:BCR:H383	2.86	0.46
4:D:170:ALA:HB1	4:D:171:PRO:HD2	1.97	0.46
1:A:241:GLN:HE22	1:A:245:THR:HG23	5.70	0.45
2:B:413:ASP:OD2	2:B:416:THR:OG1	2.27	0.45
3:C:315:MET:HE3	3:C:365:TRP:CZ3	5.27	0.45
2:B:189:GLY:O	2:B:197:GLY:HA3	2.51	0.45
2:B:150:CYS:HB2	22:B:603:CLA:HMC3	2.05	0.45
4:D:246:MET:HE3	4:D:264:LYS:CG	3.27	0.45
22:B:606:CLA:H112	22:B:606:CLA:H93	1.78	0.45
24:B:619:BCR:H383	24:B:619:BCR:H23C	1.98	0.45
4:D:13:GLY:N	36:D:510:HOH:O	22.81	0.45
3:C:203:THR:O	3:C:235:GLY:HA3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:V:201:HEC:HMB1	35:V:201:HEC:HBB3	1.99	0.45
22:C:504:CLA:H91	22:C:508:CLA:H172	3.66	0.45
24:C:514:BCR:H24C	24:C:514:BCR:H371	1.72	0.45
9:J:18:GLY:O	9:J:21:VAL:HG13	5.60	0.45
16:U:27:LEU:HD13	16:U:61:VAL:HG13	1.99	0.45
3:C:344:SER:O	13:O:75:THR:HG22	2.17	0.45
16:U:36:ILE:HG22	16:U:36:ILE:O	2.16	0.45
17:V:99:ASP:N	17:V:99:ASP:OD1	2.60	0.45
2:B:414:PRO:N	2:B:415:PRO:HD2	2.31	0.45
12:M:20:VAL:HG11	12:M:20:VAL:HG22	2.97	0.45
17:V:41:HIS:HA	17:V:45:ILE:O	2.17	0.45
2:B:451:PHE:CE2	2:B:455:HIS:CE1	3.17	0.45
22:B:614:CLA:H192	27:M:101:LMG:H421	6.02	0.45
20:Z:2:THR:HG22	20:Z:3:ILE:N	2.31	0.45
24:H:101:BCR:HC8	24:H:101:BCR:H331	1.99	0.44
7:H:6:TRP:CE2	7:H:10:ILE:HD11	2.51	0.44
10:K:25:LEU:HD22	24:Y:101:BCR:H332	2.00	0.44
19:Y:22:LEU:HA	19:Y:25:ILE:HG22	2.10	0.44
24:B:618:BCR:H351	24:B:618:BCR:H15C	1.83	0.44
22:B:615:CLA:H161	7:H:7:LEU:HD11	3.99	0.44
1:A:38:ILE:HB	1:A:39:PRO:HD3	1.98	0.44
3:C:308:GLU:HB2	3:C:361:PHE:CE1	2.52	0.44
2:B:298:LEU:HD23	2:B:402:TYR:CZ	2.53	0.44
2:B:241:SER:HB3	22:B:612:CLA:HED3	2.00	0.44
3:C:180:MET:HG2	3:C:199:ILE:O	2.18	0.44
3:C:367:GLU:N	3:C:368:PRO:CD	2.87	0.44
24:T:101:BCR:H23C	24:T:101:BCR:H382	2.01	0.44
20:Z:3:ILE:O	20:Z:7:LEU:HD23	4.62	0.44
26:A:410:PL9:H371	36:F:211:HOH:O	2.17	0.44
4:D:233:ARG:NH1	36:D:506:HOH:O	54.75	0.44
5:E:30:LEU:HD12	35:F:101:HEC:HMC3	2.00	0.44
16:U:70:ARG:HD2	36:U:213:HOH:O	2.18	0.44
1:A:84:PRO:HA	1:A:112:TYR:CG	2.59	0.44
22:B:613:CLA:CBB	22:B:613:CLA:HMB1	2.45	0.44
26:A:410:PL9:C15	28:E:101:LHG:H381	2.46	0.44
5:E:22[A]:ILE:HG23	5:E:23:HIS:HD1	1.83	0.44
13:O:42:ARG:O	13:O:241:ALA:HA	2.18	0.44
1:A:162[A]:PRO:HB3	1:A:168[A]:PHE:HA	2.04	0.43
26:A:410:PL9:H513	36:D:629:HOH:O	2.17	0.43
13:O:5:LEU:HD12	13:O:10:ILE:HD11	2.00	0.43
1:A:279:PRO:HG2	4:D:212:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:27:VAL:O	10:K:27:VAL:HG12	2.18	0.43
17:V:69:ILE:HD12	17:V:120:LEU:HD12	4.44	0.43
2:B:145:LEU:CD2	22:B:604:CLA:H193	2.47	0.43
22:B:609:CLA:H141	22:B:609:CLA:H172	4.25	0.43
5:E:25:ILE:N	5:E:25:ILE:HD12	4.45	0.43
10:K:18:PHE:CE2	20:Z:13:VAL:HG21	4.98	0.43
2:B:160:GLY:HA3	2:B:180:PRO:HB3	2.00	0.43
4:D:56:THR:HG22	36:E:213:HOH:O	42.00	0.43
7:H:12:ARG:HB3	7:H:13:PRO:HD3	2.00	0.43
24:B:618:BCR:HC8	24:B:618:BCR:H331	2.23	0.43
3:C:315:MET:CE	3:C:366:LEU:HD13	4.28	0.43
24:T:101:BCR:HC7	24:T:101:BCR:H331	1.81	0.43
2:B:149[A]:LEU:HD21	22:B:606:CLA:HBB2	2.01	0.43
2:B:379:ALA:HA	2:B:390:TYR:HB3	2.01	0.43
24:B:618:BCR:H371	24:B:618:BCR:H24C	1.77	0.43
2:B:42:LEU:HD13	2:B:94:GLU:HG3	2.00	0.43
12:M:32:GLN:C	36:M:205:HOH:O	7.08	0.43
13:O:93:LEU:O	13:O:128:SER:HA	2.19	0.43
15:T:29:ILE:HD12	15:T:29:ILE:N	4.70	0.43
2:B:226:TYR:HA	2:B:231:MET:HG3	2.30	0.43
13:O:27:ARG:NH1	36:O:304:HOH:O	2.41	0.43
22:C:506:CLA:HBB1	22:C:506:CLA:HMB1	2.01	0.43
22:C:509:CLA:H141	22:C:509:CLA:H171	2.00	0.43
29:A:414:SQD:H383	22:B:606:CLA:H93	73.77	0.42
22:B:610:CLA:HHC	22:B:610:CLA:HBB1	2.01	0.42
3:C:315:MET:CE	3:C:365:TRP:CZ3	5.19	0.42
3:C:71:GLU:HB3	3:C:86:LEU:HD22	2.01	0.42
33:M:102:STE:O1	36:M:202:HOH:O	2.21	0.42
12:M:9:ILE:HG13	12:M:13:LEU:HD22	4.80	0.42
35:V:201:HEC:HMD2	36:V:337:HOH:O	2.19	0.42
20:Z:1:MET:CB	20:Z:4:LEU:HD23	7.45	0.42
2:B:413:ASP:OD1	36:B:706:HOH:O	2.21	0.42
3:C:155:ASN:OD1	3:C:255:THR:HG22	3.02	0.42
3:C:50:LEU:O	3:C:54:VAL:HG23	2.19	0.42
4:D:307:GLU:HG3	36:D:530:HOH:O	2.18	0.42
5:E:65:LEU:O	5:E:67:THR:HG23	2.19	0.42
4:D:103:ARG:HH21	5:E:77:GLU:HG3	1.83	0.42
6:F:26:LEU:O	6:F:29:PRO:HD2	2.40	0.42
2:B:201:HIS:HB2	22:B:602:CLA:CHB	2.50	0.42
33:D:412:STE:H172	18:X:21:LEU:HD21	2.01	0.42
10:K:18:PHE:CE2	20:Z:9:LEU:HD21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:298:LEU:HA	2:B:298:LEU:HD12	1.89	0.42
3:C:128:GLY:HA3	22:C:513:CLA:C3C	2.51	0.42
22:C:504:CLA:H92	22:C:504:CLA:H62	2.44	0.42
22:C:509:CLA:H91	22:C:509:CLA:H112	1.81	0.42
30:C:518:DGD:HA41	30:C:518:DGD:O1A	2.19	0.42
3:C:93:ALA:HB1	3:C:99:VAL:HG21	2.96	0.42
4:D:42:TYR:CZ	6:F:25:THR:HG23	2.77	0.42
13:O:143:LYS:HE3	36:O:359:HOH:O	22.62	0.42
14:R:5:VAL:HG12	14:R:9:LEU:HD12	2.01	0.42
20:Z:55:GLY:HA2	20:Z:58:ASN:CB	2.49	0.42
1:A:140:ARG:HB2	4:D:220:ASN:HA	2.03	0.42
1:A:237:TYR:HB2	1:A:245:THR:HG21	3.49	0.42
5:E:14:ILE:O	5:E:20:TRP:NE1	2.50	0.42
17:V:78:ASN:OD1	17:V:96:ARG:NH1	2.53	0.42
22:B:608:CLA:H141	22:B:608:CLA:H161	2.01	0.42
22:B:616:CLA:HBB1	22:B:616:CLA:HMB1	2.02	0.42
24:H:101:BCR:H341	24:H:101:BCR:H11C	1.86	0.42
22:B:601:CLA:H92	24:H:101:BCR:H21C	2.01	0.42
22:B:610:CLA:H151	22:B:610:CLA:H203	5.10	0.42
2:B:92:SER:O	2:B:96:VAL:HG23	2.34	0.42
8:I:2:GLU:O	8:I:6:ILE:HG12	2.20	0.42
22:B:604:CLA:C3B	22:B:613:CLA:HMC3	2.49	0.42
3:C:352:GLY:O	3:C:355[A]:THR:HG22	2.41	0.42
22:D:404:CLA:H43	22:D:404:CLA:O1A	4.42	0.42
5:E:45:ASP:OD2	14:R:4:ARG:NH2	2.47	0.42
26:A:410:PL9:H451	26:A:410:PL9:H471	1.91	0.42
2:B:298:LEU:HA	2:B:298:LEU:HD23	4.42	0.42
10:K:25:LEU:N	10:K:26:PRO:CD	2.82	0.42
24:A:407:BCR:H24C	24:A:407:BCR:H371	1.78	0.41
2:B:173:GLY:HA3	2:B:265:ILE:HD11	2.35	0.41
2:B:104:SER:OG	29:B:623:SQD:H221	2.20	0.41
5:E:6:GLY:HA2	36:E:218:HOH:O	2.20	0.41
9:J:11:TRP:CZ2	9:J:12:ILE:HD11	3.11	0.41
22:A:403:CLA:HMD3	4:D:182:LEU:HD11	2.02	0.41
22:B:607:CLA:H191	28:B:622:LHG:H142	2.02	0.41
22:B:616:CLA:O1A	22:B:616:CLA:C2	2.67	0.41
2:B:36:SER:OG	24:B:618:BCR:H362	2.36	0.41
24:B:619:BCR:H383	24:B:619:BCR:C23	2.50	0.41
29:B:623:SQD:H352	29:B:623:SQD:H383	1.86	0.41
1:A:245:THR:HB	4:D:265:ARG:HE	3.69	0.41
2:B:488:PRO:O	2:B:492:GLU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:GLN:C	2:B:329:PRO:HB3	2.51	0.41
30:A:415:DGD:HD5	2:B:75:TRP:HB3	65.61	0.41
4:D:90:LEU:HA	4:D:90:LEU:HD23	1.90	0.41
10:K:28:ILE:N	10:K:29:PRO:CD	2.83	0.41
5:E:22[A]:ILE:HG13	14:R:19:ALA:CB	2.51	0.41
20:Z:6:GLN:O	20:Z:7:LEU:HD23	2.20	0.41
3:C:175:LEU:HD22	22:C:501:CLA:C3D	2.82	0.41
22:C:505:CLA:HBC2	24:C:515:BCR:C34	2.50	0.41
4:D:103:ARG:NH2	36:D:518:HOH:O	43.95	0.41
4:D:42:TYR:CE1	6:F:25:THR:HG22	2.77	0.41
2:B:159:THR:O	2:B:180:PRO:HB3	2.63	0.41
35:V:201:HEC:HMC1	35:V:201:HEC:CBC	2.44	0.41
2:B:237:VAL:HG12	22:B:612:CLA:HMD1	2.02	0.41
4:D:161:PRO:HG3	4:D:170:ALA:HB2	2.10	0.41
3:C:348:GLU:OE2	13:O:11:VAL:HA	2.20	0.41
19:Y:34:MET:O	19:Y:38:LEU:HG	2.21	0.41
20:Z:48:ILE:O	20:Z:52:LEU:HG	5.10	0.41
4:D:13:GLY:O	4:D:17:ILE:HG12	2.21	0.41
22:D:403:CLA:C4A	22:D:403:CLA:HBA1	2.50	0.41
35:F:101:HEC:HMB3	14:R:19:ALA:CB	2.75	0.41
1:A:278:TRP:HB3	1:A:279:PRO:HD3	2.05	0.41
3:C:135:ARG:HD3	3:C:135:ARG:O	2.20	0.41
22:C:507:CLA:H61	22:C:507:CLA:H92	2.01	0.41
18:X:11:PHE:O	18:X:15:LEU:HD23	2.21	0.41
1:A:161[B]:TYR:HB3	1:A:162[B]:PRO:HD3	2.03	0.41
1:A:85:SER:HA	1:A:109:GLY:HA3	2.03	0.41
16:U:27:LEU:HD13	16:U:61:VAL:CG1	2.51	0.41
2:B:135:LEU:N	2:B:136:PRO:CD	2.98	0.41
22:B:604:CLA:H142	33:B:620:STE:H142	2.02	0.41
2:B:63:LEU:N	2:B:64:PRO:HD2	2.45	0.41
3:C:109:PHE:N	3:C:110:PRO:CD	2.87	0.41
3:C:126:GLY:O	3:C:130:VAL:HG13	2.21	0.41
22:C:509:CLA:H142	22:C:509:CLA:H111	4.02	0.41
22:B:605:CLA:H143	22:B:610:CLA:HMA2	2.02	0.40
2:B:4:PRO:HB2	2:B:6:TYR:CE1	2.56	0.40
3:C:334:PRO:HA	13:O:153:THR:OG1	2.27	0.40
4:D:246:MET:HE2	4:D:246:MET:HA	2.03	0.40
4:D:38:PHE:N	4:D:39:PRO:CD	2.84	0.40
1:A:132:GLU:O	1:A:136:ARG:HG2	2.28	0.40
1:A:149:ALA:HB3	1:A:150:PRO:CD	2.51	0.40
26:A:410:PL9:H422	26:A:410:PL9:H401	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:619:BCR:C38	24:B:619:BCR:C23	2.98	0.40
4:D:110:LEU:HA	4:D:110:LEU:HD23	1.93	0.40
4:D:244:TYR:CE2	4:D:246:MET:HE2	2.56	0.40
13:O:193:THR:HG21	13:O:220:LEU:HD12	2.02	0.40
1:A:45:THR:HG23	22:D:403:CLA:H191	2.03	0.40
24:C:516:BCR:H15C	24:C:516:BCR:H351	1.95	0.40
36:A:503:HOH:O	4:D:243:THR:HG22	2.21	0.40
22:D:404:CLA:C4B	33:D:412:STE:H151	2.52	0.40
12:M:8:LEU:HD11	33:T:102:STE:H111	2.03	0.40
24:B:618:BCR:H361	24:B:618:BCR:H20C	1.78	0.40
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.57	0.40
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.24	0.40
24:T:101:BCR:H341	24:T:101:BCR:H11C	2.10	0.40
22:B:615:CLA:H2	22:B:616:CLA:HBB2	2.05	0.40
22:C:501:CLA:CAD	22:C:503:CLA:H12	2.52	0.40
22:C:506:CLA:O1A	22:C:506:CLA:C2	3.64	0.40
22:C:513:CLA:C4	22:C:513:CLA:O2A	2.70	0.40
33:D:412:STE:H71	18:X:16:SER:HB3	5.27	0.40
11:L:2:GLU:N	11:L:3:PRO:CD	4.31	0.40
13:O:27:ARG:HG3	36:O:304:HOH:O	2.22	0.40
24:T:101:BCR:H361	24:T:101:BCR:H20C	1.92	0.40
17:V:57:GLU:OE1	36:V:301:HOH:O	4.05	0.40

There are no symmetry-related clashes.

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	391/344 (114%)	387 (99%)	3 (1%)	1 (0%)	41 37
1	a	391/344 (114%)	387 (99%)	3 (1%)	1 (0%)	41 37
2	B	508/506 (100%)	497 (98%)	10 (2%)	1 (0%)	47 44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	503/506 (99%)	491 (98%)	12 (2%)	0	100	100
3	C	450/461 (98%)	440 (98%)	9 (2%)	1 (0%)	47	44
3	c	459/461 (100%)	443 (96%)	15 (3%)	1 (0%)	47	44
4	D	339/352 (96%)	329 (97%)	10 (3%)	0	100	100
4	d	340/352 (97%)	331 (97%)	9 (3%)	0	100	100
5	E	81/84 (96%)	81 (100%)	0	0	100	100
5	e	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	30 (94%)	2 (6%)	0	100	100
7	H	63/66 (96%)	58 (92%)	4 (6%)	1 (2%)	9	4
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	31 (91%)	3 (9%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	34 (97%)	0	1 (3%)	4	1
10	k	35/46 (76%)	35 (100%)	0	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%)	30 (97%)	1 (3%)	0	100	100
12	m	30/36 (83%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	227 (93%)	12 (5%)	4 (2%)	9	4
13	o	242/272 (89%)	233 (96%)	8 (3%)	1 (0%)	34	30
14	R	32/40 (80%)	30 (94%)	2 (6%)	0	100	100
14	r	29/40 (72%)	27 (93%)	2 (7%)	0	100	100
15	T	28/30 (93%)	28 (100%)	0	0	100	100
15	t	28/30 (93%)	28 (100%)	0	0	100	100
16	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
16	u	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
17	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	22	16
17	v	135/163 (83%)	129 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	57 (95%)	3 (5%)	0	100	100
20	z	60/62 (97%)	55 (92%)	3 (5%)	2 (3%)	4	1
All	All	5374/5686 (94%)	5216 (97%)	141 (3%)	17 (0%)	41	37

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
10	K	16	ALA
13	O	60	ARG
17	V	64	PRO
3	c	416	SER
13	O	62	GLU
20	z	2	THR
7	H	26	GLY
13	O	59	LYS
19	Y	43	ARG
19	y	43	ARG
2	B	294	SER
13	O	133	VAL
13	o	56	PRO
1	a	259	ILE
20	z	61	VAL
1	A	259	ILE

5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	320/280 (114%)	316 (99%)	4 (1%)	69	74
1	a	319/280 (114%)	310 (97%)	9 (3%)	43	44
2	B	408/404 (101%)	399 (98%)	9 (2%)	52	55
2	b	402/404 (100%)	393 (98%)	9 (2%)	52	55
3	C	353/362 (98%)	345 (98%)	8 (2%)	50	53
3	c	361/362 (100%)	353 (98%)	8 (2%)	52	55
4	D	277/283 (98%)	273 (99%)	4 (1%)	67	72
4	d	278/283 (98%)	267 (96%)	11 (4%)	31	29
5	E	72/73 (99%)	67 (93%)	5 (7%)	15	11
5	e	71/73 (97%)	70 (99%)	1 (1%)	67	72
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	26 (93%)	2 (7%)	14	10
7	H	54/55 (98%)	52 (96%)	2 (4%)	34	32
7	h	53/55 (96%)	51 (96%)	2 (4%)	33	31
8	I	32/34 (94%)	30 (94%)	2 (6%)	18	13
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	23 (96%)	1 (4%)	30	27
9	j	24/28 (86%)	23 (96%)	1 (4%)	30	27
10	K	30/37 (81%)	29 (97%)	1 (3%)	38	37
10	k	30/37 (81%)	25 (83%)	5 (17%)	2	1
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	31 (91%)	3 (9%)	10	6
12	M	28/32 (88%)	27 (96%)	1 (4%)	35	34
12	m	28/32 (88%)	26 (93%)	2 (7%)	14	10
13	O	206/228 (90%)	197 (96%)	9 (4%)	28	25
13	o	207/228 (91%)	198 (96%)	9 (4%)	29	26
14	R	28/32 (88%)	25 (89%)	3 (11%)	6	3
14	r	23/32 (72%)	19 (83%)	4 (17%)	2	1
15	T	26/26 (100%)	26 (100%)	0	100	100
15	t	25/26 (96%)	25 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	U	84/112 (75%)	80 (95%)	4 (5%)	25	22
16	u	84/112 (75%)	83 (99%)	1 (1%)	71	76
17	V	117/138 (85%)	114 (97%)	3 (3%)	46	48
17	v	117/138 (85%)	112 (96%)	5 (4%)	29	26
18	X	31/34 (91%)	29 (94%)	2 (6%)	17	12
18	x	31/34 (91%)	29 (94%)	2 (6%)	17	12
19	Y	19/37 (51%)	18 (95%)	1 (5%)	22	18
19	y	22/37 (60%)	20 (91%)	2 (9%)	9	5
20	Z	52/52 (100%)	45 (86%)	7 (14%)	4	2
20	z	51/52 (98%)	43 (84%)	8 (16%)	2	1
All	All	4444/4642 (96%)	4294 (97%)	150 (3%)	36	36

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	13	LEU
1	A	244	GLU
1	A	248	ILE
2	B	76	SER
2	B	79	SER
2	B	98	LEU
2	B	127	ARG
2	B	240	SER
2	B	362	PHE
2	B	371	THR
2	B	405	GLU
2	B	476	ARG
3	C	141	GLU
3	C	156	LYS
3	C	200	THR
3	C	240	ILE
3	C	255	THR
3	C	273	SER
3	C	289	PHE
3	C	315	MET
4	D	24	ARG
4	D	180	ARG

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Mol	Chain	Res	Type
4	D	264	LYS
4	D	295	SER
5	E	11	SER
5	E	22[A]	ILE
5	E	22[B]	ILE
5	E	61	ARG
5	E	81	GLU
7	H	20	LYS
7	H	49	TYR
8	I	4	LEU
8	I	36	ASP
9	J	24	ILE
10	K	10	LYS
12	M	25	LEU
13	O	57	LYS
13	O	64	GLU
13	O	78	LEU
13	O	107	THR
13	O	118	LEU
13	O	134	THR
13	O	135	SER
13	O	198	SER
13	O	214	THR
14	R	10	LEU
14	R	21	ARG
14	R	29	LYS
16	U	39	ARG
16	U	51	LYS
16	U	61	VAL
16	U	67	LEU
17	V	3	LEU
17	V	7	VAL
17	V	86	GLN
18	X	3	ILE
18	X	15	LEU
19	Y	34	MET
20	Z	2	THR
20	Z	15	LEU
20	Z	17	PHE
20	Z	19	MET
20	Z	32	ASP
20	Z	35	ARG

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Mol	Chain	Res	Type
20	Z	46	LEU
1	a	28	LEU
1	a	42	LEU
1	a	159	LEU
1	a	200	LEU
1	a	223	LEU
1	a	229	GLU
1	a	231	GLU
1	a	271	LEU
1	a	288	LEU
2	b	83	GLU
2	b	128	THR
2	b	149	LEU
2	b	236	THR
2	b	357	ARG
2	b	362	PHE
2	b	485	GLU
2	b	492	GLU
2	b	506	ARG
3	c	24	THR
3	c	72	LEU
3	c	124	VAL
3	c	125	LEU
3	c	135	ARG
3	c	165	LEU
3	c	240	ILE
3	c	289	PHE
4	d	90	LEU
4	d	180	ARG
4	d	182	LEU
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
4	d	329	MET
5	e	83	LEU
6	f	15	ILE
6	f	28	VAL
7	h	7	LEU

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Mol	Chain	Res	Type
7	h	49	TYR
9	j	21	VAL
10	k	10	LYS
10	k	13	GLU
10	k	24	VAL
10	k	30	VAL
10	k	35	LEU
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
12	m	16	LEU
13	o	18	LYS
13	o	39	ARG
13	o	49	THR
13	o	60	ARG
13	o	87	VAL
13	o	118	LEU
13	o	130	GLN
13	o	134	THR
13	o	207	ARG
14	r	3	TRP
14	r	9	LEU
14	r	10	LEU
14	r	30	GLN
16	u	23	GLU
17	v	2	GLU
17	v	52	LEU
17	v	90	GLU
17	v	106	ASN
17	v	110	LYS
18	x	2	THR
18	x	15	LEU
19	y	19	ILE
19	y	45	ASN
20	z	1	MET
20	z	14	ILE
20	z	29	SER
20	z	31	GLN
20	z	32	ASP
20	z	39	LEU
20	z	42	LEU

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Mol	Chain	Res	Type
20	z	46	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	497	GLN
11	L	8	GLN
13	O	88	ASN
17	V	86	GLN
18	X	38	GLN
20	Z	31	GLN
1	a	234	ASN
2	b	179	GLN
3	c	378	ASN
5	e	82	GLN
13	o	80	GLN
14	r	30	GLN
18	x	33	GLN
20	z	31	GLN
20	z	58	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	i	1	8	8,9,10	1.13	1 (12%)	7,9,11	1.14	1 (14%)
12	FME	M	1	12	8,9,10	1.08	1 (12%)	7,9,11	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	FME	m	1	12	8,9,10	0.98	1 (12%)	7,9,11	0.82	0
15	FME	T	1	15	8,9,10	1.02	1 (12%)	7,9,11	1.53	2 (28%)
15	FME	t	1	15	8,9,10	1.53	1 (12%)	7,9,11	0.45	0
8	FME	I	1	8	8,9,10	0.92	0	7,9,11	1.05	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	-	0/7/9/11	-
12	FME	M	1	12	-	0/7/9/11	-
12	FME	m	1	12	-	1/7/9/11	-
15	FME	T	1	15	-	2/7/9/11	-
15	FME	t	1	15	-	1/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-3.60	1.41	1.46
8	i	1	FME	CA-N	-2.48	1.42	1.46
15	T	1	FME	CA-N	-2.27	1.43	1.46
12	M	1	FME	CA-N	-2.11	1.43	1.46
12	m	1	FME	CA-N	-2.08	1.43	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	1	FME	O1-CN-N	-2.57	118.51	125.27
8	i	1	FME	CA-N-CN	-2.13	119.54	122.82
8	I	1	FME	C-CA-N	2.02	113.37	109.73
15	T	1	FME	C-CA-N	2.01	113.35	109.73

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	m	1	FME	O-C-CA-CB

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
24	BCR	c	514	-	41,41,41	1.15	2 (4%)	56,56,56	1.33	7 (12%)
24	BCR	b	619	-	41,41,41	1.02	2 (4%)	56,56,56	1.27	7 (12%)
22	CLA	c	513	-	59,73,73	1.39	7 (11%)	67,113,113	1.39	8 (11%)
22	CLA	A	402	-	59,73,73	1.58	6 (10%)	67,113,113	1.46	11 (16%)
22	CLA	c	508	-	58,72,73	1.43	7 (12%)	65,111,113	1.62	13 (20%)
24	BCR	x	101	-	41,41,41	1.04	2 (4%)	56,56,56	1.27	8 (14%)
33	STE	t	102	-	10,13,19	0.49	0	9,13,19	0.70	0
22	CLA	B	605	-	59,73,73	1.17	4 (6%)	67,113,113	1.54	10 (14%)
27	LMG	m	101	-	51,51,55	0.95	2 (3%)	59,59,63	1.48	8 (13%)
22	CLA	C	508	-	59,73,73	1.52	7 (11%)	67,113,113	1.83	12 (17%)
22	CLA	b	610	36	59,73,73	1.33	10 (16%)	67,113,113	1.69	16 (23%)
27	LMG	c	522	-	48,48,55	1.05	5 (10%)	56,56,63	1.28	4 (7%)
22	CLA	C	512	-	59,73,73	1.37	9 (15%)	67,113,113	1.60	13 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	STE	b	627	-	13,13,19	0.51	0	12,12,19	0.46	0
22	CLA	D	402	-	59,73,73	1.36	6 (10%)	67,113,113	1.61	12 (17%)
23	PHO	A	404	-	67,69,69	1.14	6 (8%)	85,99,99	1.13	5 (5%)
22	CLA	c	503	-	59,73,73	1.42	8 (13%)	67,113,113	1.59	10 (14%)
33	STE	C	522	-	15,15,19	0.46	0	14,14,19	0.65	0
33	STE	a	413	-	9,9,19	0.52	0	8,8,19	0.52	0
33	STE	j	101	-	8,11,19	0.59	0	7,11,19	0.57	0
22	CLA	b	614	-	59,73,73	1.37	5 (8%)	67,113,113	1.72	13 (19%)
22	CLA	C	506	-	59,73,73	1.52	8 (13%)	67,113,113	1.37	9 (13%)
33	STE	J	101	-	8,11,19	0.37	0	7,11,19	1.01	0
24	BCR	b	618	-	41,41,41	1.17	2 (4%)	56,56,56	1.29	8 (14%)
33	STE	a	415	-	14,14,19	0.39	0	13,13,19	0.73	0
22	CLA	C	507	36	59,73,73	1.36	6 (10%)	67,113,113	1.76	13 (19%)
33	STE	b	624	-	12,15,19	0.47	0	11,15,19	0.62	0
30	DGD	c	517	-	63,63,67	1.20	10 (15%)	77,77,81	1.42	15 (19%)
26	PL9	d	407	-	55,55,55	1.57	10 (18%)	68,69,69	1.89	20 (29%)
22	CLA	c	509	-	59,73,73	1.22	3 (5%)	67,113,113	1.74	11 (16%)
28	LHG	l	101	-	48,48,48	0.84	1 (2%)	51,54,54	1.29	7 (13%)
22	CLA	c	511	3	59,73,73	1.69	6 (10%)	67,113,113	1.56	12 (17%)
33	STE	t	103	-	14,17,19	0.37	0	13,17,19	0.86	0
24	BCR	B	619	-	41,41,41	1.14	2 (4%)	56,56,56	1.34	5 (8%)
28	LHG	A	412	-	46,46,48	1.15	5 (10%)	49,52,54	1.37	7 (14%)
22	CLA	B	609	-	59,73,73	1.60	7 (11%)	67,113,113	1.60	14 (20%)
22	CLA	a	402	-	59,73,73	1.49	6 (10%)	67,113,113	1.56	8 (11%)
22	CLA	B	603	-	59,73,73	1.38	9 (15%)	67,113,113	1.87	15 (22%)
22	CLA	b	612	-	59,73,73	1.65	6 (10%)	67,113,113	1.70	13 (19%)
30	DGD	A	415	-	67,67,67	1.39	11 (16%)	81,81,81	1.34	11 (13%)
22	CLA	d	405	-	59,73,73	1.57	9 (15%)	67,113,113	1.43	11 (16%)
22	CLA	b	608	-	59,73,73	1.38	7 (11%)	67,113,113	1.38	9 (13%)
33	STE	b	626	-	9,9,19	0.48	0	8,8,19	0.55	0
24	BCR	t	101	-	41,41,41	1.07	4 (9%)	56,56,56	1.42	11 (19%)
35	HEC	V	201	17	26,50,50	2.18	3 (11%)	18,82,82	1.96	5 (27%)
22	CLA	a	404	-	59,73,73	1.40	5 (8%)	67,113,113	1.56	15 (22%)
22	CLA	C	511	3	59,73,73	1.53	6 (10%)	67,113,113	1.52	8 (11%)
22	CLA	B	611	-	59,73,73	1.50	5 (8%)	67,113,113	1.93	13 (19%)
22	CLA	b	602	-	59,73,73	1.16	7 (11%)	67,113,113	1.75	15 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	d	403	-	59,73,73	1.63	7 (11%)	67,113,113	1.53	12 (17%)
22	CLA	b	609	-	59,73,73	1.45	7 (11%)	67,113,113	1.86	15 (22%)
24	BCR	D	405	-	41,41,41	1.18	3 (7%)	56,56,56	1.37	9 (16%)
22	CLA	A	406	-	48,62,73	1.43	6 (12%)	53,99,113	1.61	10 (18%)
27	LMG	c	520	-	37,37,55	1.23	5 (13%)	45,45,63	1.34	8 (17%)
22	CLA	C	510	-	59,73,73	1.36	7 (11%)	67,113,113	1.58	10 (14%)
33	STE	b	621	-	15,15,19	0.40	0	14,14,19	0.80	0
24	BCR	C	514	-	41,41,41	1.13	3 (7%)	56,56,56	1.39	12 (21%)
24	BCR	d	406	-	41,41,41	1.08	2 (4%)	56,56,56	1.29	6 (10%)
24	BCR	B	618	-	41,41,41	1.11	2 (4%)	56,56,56	1.31	8 (14%)
28	LHG	e	101	-	41,41,48	0.94	3 (7%)	44,47,54	1.30	5 (11%)
22	CLA	A	403	36	59,73,73	1.48	7 (11%)	67,113,113	1.50	12 (17%)
30	DGD	C	518	-	63,63,67	1.20	8 (12%)	77,77,81	1.35	10 (12%)
33	STE	Z	101	-	7,7,19	0.45	0	6,6,19	0.54	0
33	STE	M	103	-	9,9,19	0.42	0	8,8,19	0.81	0
33	STE	I	101	-	14,14,19	0.54	0	13,13,19	0.53	0
22	CLA	c	501	-	59,73,73	1.25	5 (8%)	67,113,113	1.64	11 (16%)
35	HEC	f	101	5,6	26,50,50	2.53	3 (11%)	18,82,82	2.29	5 (27%)
29	SQD	a	411	-	53,54,54	1.03	5 (9%)	62,65,65	1.85	11 (17%)
22	CLA	c	504	36	54,68,73	1.55	7 (12%)	61,107,113	1.61	12 (19%)
33	STE	M	102	-	11,14,19	0.28	0	10,14,19	1.05	0
33	STE	a	414	-	8,11,19	0.56	0	7,11,19	0.52	0
22	CLA	b	616	-	54,68,73	1.36	9 (16%)	61,107,113	1.68	10 (16%)
33	STE	b	622	-	16,19,19	0.35	0	15,19,19	0.81	0
24	BCR	c	516	-	41,41,41	1.08	3 (7%)	56,56,56	1.15	3 (5%)
23	PHO	d	402	-	67,69,69	1.27	10 (14%)	85,99,99	1.13	6 (7%)
29	SQD	f	102	-	40,41,54	1.09	4 (10%)	49,52,65	2.11	10 (20%)
22	CLA	D	404	-	59,73,73	1.50	9 (15%)	67,113,113	1.34	8 (11%)
24	BCR	a	405	-	41,41,41	0.97	3 (7%)	56,56,56	1.27	8 (14%)
33	STE	b	625	-	16,19,19	0.49	0	15,19,19	0.65	0
33	STE	m	102	-	8,11,19	0.46	0	7,11,19	0.44	0
22	CLA	C	504	36	53,67,73	1.27	6 (11%)	59,105,113	1.49	11 (18%)
24	BCR	A	407	-	41,41,41	1.13	4 (9%)	56,56,56	1.47	11 (19%)
22	CLA	b	601	36	59,73,73	1.52	8 (13%)	67,113,113	1.46	7 (10%)
22	CLA	d	401	36	59,73,73	1.61	10 (16%)	67,113,113	1.60	14 (20%)
33	STE	T	102	-	14,14,19	0.46	0	13,13,19	0.65	0
24	BCR	Y	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.36	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	DGD	c	518	-	63,63,67	1.25	10 (15%)	77,77,81	1.38	10 (12%)
22	CLA	c	502	-	59,73,73	1.37	5 (8%)	67,113,113	1.46	7 (10%)
22	CLA	b	615	-	59,73,73	1.65	6 (10%)	67,113,113	1.76	11 (16%)
24	BCR	C	515	-	41,41,41	1.16	4 (9%)	56,56,56	1.33	9 (16%)
27	LMG	d	410	-	44,44,55	1.11	3 (6%)	52,52,63	1.29	7 (13%)
28	LHG	E	101	-	48,48,48	0.90	2 (4%)	51,54,54	1.24	5 (9%)
22	CLA	b	607	36	59,73,73	1.37	9 (15%)	67,113,113	1.34	8 (11%)
24	BCR	b	617	-	41,41,41	1.08	3 (7%)	56,56,56	1.48	9 (16%)
27	LMG	A	411	-	48,48,55	1.09	4 (8%)	56,56,63	1.33	7 (12%)
34	BCT	D	401	21	0,3,3	0.00	-	0,3,3	0.00	-
27	LMG	c	523	-	49,49,55	0.85	1 (2%)	57,57,63	1.29	6 (10%)
33	STE	B	624	-	8,11,19	0.36	0	7,11,19	0.97	0
35	HEC	v	201	17	26,50,50	2.42	3 (11%)	18,82,82	2.12	9 (50%)
29	SQD	D	408	-	35,36,54	1.00	4 (11%)	42,45,65	2.21	10 (23%)
22	CLA	c	506	-	59,73,73	1.38	8 (13%)	67,113,113	1.66	12 (17%)
22	CLA	b	611	-	59,73,73	1.15	6 (10%)	67,113,113	1.44	10 (14%)
27	LMG	a	416	-	55,55,55	1.05	2 (3%)	63,63,63	1.37	7 (11%)
22	CLA	D	403	36	59,73,73	1.36	7 (11%)	67,113,113	1.47	9 (13%)
22	CLA	B	616	-	54,68,73	1.60	8 (14%)	61,107,113	1.89	10 (16%)
22	CLA	C	513	-	59,73,73	1.30	8 (13%)	67,113,113	1.59	8 (11%)
24	BCR	c	515	-	41,41,41	1.21	3 (7%)	56,56,56	1.45	12 (21%)
28	LHG	d	408	-	48,48,48	0.95	2 (4%)	51,54,54	1.18	4 (7%)
33	STE	c	521	-	16,19,19	0.35	0	15,19,19	0.77	0
30	DGD	C	517	-	63,63,67	1.29	10 (15%)	77,77,81	1.42	11 (14%)
22	CLA	B	614	-	59,73,73	1.43	5 (8%)	67,113,113	1.52	13 (19%)
22	CLA	d	404	36	59,73,73	1.73	6 (10%)	67,113,113	1.77	11 (16%)
34	BCT	a	408	21	0,3,3	0.00	-	0,3,3	0.00	-
33	STE	C	521	-	8,11,19	0.50	0	7,11,19	0.65	0
30	DGD	c	519	-	63,63,67	1.11	4 (6%)	77,77,81	1.38	7 (9%)
30	DGD	H	102	-	63,63,67	1.41	13 (20%)	77,77,81	1.42	10 (12%)
23	PHO	A	405	-	67,69,69	1.21	6 (8%)	85,99,99	1.12	8 (9%)
33	STE	d	412	-	16,19,19	0.47	0	15,19,19	0.71	0
22	CLA	B	612	-	59,73,73	1.53	4 (6%)	67,113,113	1.79	12 (17%)
33	STE	R	101	-	8,11,19	0.51	0	7,11,19	0.57	0
33	STE	B	626	-	8,11,19	0.49	0	7,11,19	0.53	0
28	LHG	d	409	-	38,38,48	1.02	2 (5%)	41,44,54	1.16	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	OEY	a	418[B]	1,3,36	0,16,16	0.00	-	-		
27	LMG	D	407	-	51,51,55	0.98	5 (9%)	59,59,63	1.25	4 (6%)
22	CLA	C	501	-	59,73,73	1.51	5 (8%)	67,113,113	1.56	9 (13%)
28	LHG	B	621	-	48,48,48	0.89	2 (4%)	51,54,54	1.12	2 (3%)
27	LMG	D	410	-	31,31,55	1.11	3 (9%)	33,33,63	1.10	2 (6%)
33	STE	C	523	-	8,11,19	0.37	0	7,11,19	1.14	1 (14%)
33	STE	D	412	-	16,19,19	0.21	0	15,19,19	1.14	1 (6%)
24	BCR	C	516	-	41,41,41	1.15	3 (7%)	56,56,56	1.20	4 (7%)
28	LHG	B	622	-	48,48,48	0.89	3 (6%)	51,54,54	1.27	5 (9%)
31	OEX	a	417[A]	1,3,36	0,15,15	0.00	-	-		
27	LMG	C	520	-	48,48,55	0.86	3 (6%)	56,56,63	1.36	8 (14%)
29	SQD	A	414	-	38,38,54	1.02	4 (10%)	40,40,65	1.60	4 (10%)
22	CLA	b	605	-	59,73,73	1.30	5 (8%)	67,113,113	1.70	13 (19%)
29	SQD	B	623	-	53,54,54	0.97	4 (7%)	62,65,65	1.88	14 (22%)
28	LHG	a	410	-	48,48,48	0.89	2 (4%)	51,54,54	1.47	8 (15%)
22	CLA	C	509	-	59,73,73	1.24	6 (10%)	67,113,113	1.66	11 (16%)
29	SQD	A	413	-	51,52,54	1.08	7 (13%)	60,63,65	2.05	13 (21%)
33	STE	B	620	-	13,16,19	0.39	0	12,16,19	1.03	0
22	CLA	B	610	36	59,73,73	1.57	8 (13%)	67,113,113	1.60	12 (17%)
29	SQD	a	412	-	35,35,54	1.08	2 (5%)	37,37,65	1.62	5 (13%)
22	CLA	b	603	-	59,73,73	1.68	8 (13%)	67,113,113	1.68	14 (20%)
22	CLA	B	607	36	59,73,73	1.21	7 (11%)	67,113,113	1.43	8 (11%)
22	CLA	c	512	-	59,73,73	1.30	7 (11%)	67,113,113	1.50	14 (20%)
22	CLA	b	606	-	59,73,73	1.70	8 (13%)	67,113,113	1.85	11 (16%)
22	CLA	B	606	-	59,73,73	1.71	10 (16%)	67,113,113	1.67	12 (17%)
26	PL9	A	410	-	55,55,55	1.25	6 (10%)	68,69,69	1.46	11 (16%)
22	CLA	B	613	-	59,73,73	1.58	10 (16%)	67,113,113	1.20	9 (13%)
22	CLA	B	604	-	59,73,73	1.49	8 (13%)	67,113,113	1.80	10 (14%)
33	STE	k	102	-	8,11,19	0.49	0	7,11,19	0.79	0
32	OEY	A	417[B]	1,3,36	0,16,16	0.00	-	-		
30	DGD	C	519	-	63,63,67	1.21	7 (11%)	77,77,81	1.33	7 (9%)
24	BCR	k	101	-	41,41,41	1.05	4 (9%)	56,56,56	1.08	3 (5%)
35	HEC	F	101	5,6	26,50,50	2.37	5 (19%)	18,82,82	2.73	7 (38%)
29	SQD	b	620	-	48,49,54	0.98	2 (4%)	57,60,65	1.97	14 (24%)
30	DGD	h	101	-	63,63,67	1.18	7 (11%)	77,77,81	1.36	8 (10%)
26	PL9	D	406	-	55,55,55	1.70	7 (12%)	68,69,69	1.76	18 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	STE	d	413	-	16,19,19	0.32	0	15,19,19	0.85	0
22	CLA	c	507	36	59,73,73	1.10	5 (8%)	67,113,113	1.62	11 (16%)
22	CLA	b	613	-	59,73,73	1.33	6 (10%)	67,113,113	1.44	11 (16%)
27	LMG	M	101	-	51,51,55	1.01	4 (7%)	59,59,63	1.55	9 (15%)
23	PHO	a	403	-	67,69,69	1.18	6 (8%)	85,99,99	1.12	8 (9%)
33	STE	d	411	-	13,16,19	0.30	0	12,16,19	1.17	1 (8%)
33	STE	B	625	-	15,15,19	0.45	0	14,14,19	0.62	0
22	CLA	C	502	-	59,73,73	1.49	8 (13%)	67,113,113	1.36	10 (14%)
22	CLA	c	505	-	59,73,73	1.47	7 (11%)	67,113,113	1.64	11 (16%)
27	LMG	D	411	-	20,26,55	0.45	0	18,26,63	1.16	0
22	CLA	C	503	-	59,73,73	1.59	6 (10%)	67,113,113	2.01	14 (20%)
22	CLA	B	608	-	59,73,73	1.21	6 (10%)	67,113,113	1.46	12 (17%)
33	STE	H	103	-	17,17,19	0.49	0	16,16,19	0.69	0
27	LMG	b	623	-	55,55,55	0.99	3 (5%)	63,63,63	1.49	9 (14%)
24	BCR	T	101	-	41,41,41	1.04	3 (7%)	56,56,56	1.42	6 (10%)
22	CLA	B	615	-	59,73,73	1.49	8 (13%)	67,113,113	1.44	10 (14%)
22	CLA	b	604	-	59,73,73	1.40	5 (8%)	67,113,113	1.83	21 (31%)
24	BCR	H	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.36	9 (16%)
22	CLA	B	602	-	59,73,73	1.57	5 (8%)	67,113,113	1.37	10 (14%)
22	CLA	C	505	-	59,73,73	1.53	6 (10%)	67,113,113	1.64	10 (14%)
24	BCR	B	617	-	41,41,41	1.10	4 (9%)	56,56,56	1.30	12 (21%)
33	STE	l	102	-	17,17,19	0.37	0	16,16,19	0.91	0
26	PL9	a	409	-	55,55,55	1.09	5 (9%)	68,69,69	1.67	13 (19%)
22	CLA	B	601	36	59,73,73	1.56	8 (13%)	67,113,113	1.58	7 (10%)
22	CLA	c	510	-	59,73,73	1.66	8 (13%)	67,113,113	1.63	15 (22%)
28	LHG	D	409	-	48,48,48	1.09	3 (6%)	51,54,54	1.24	6 (11%)
31	OEX	A	416[A]	1,3,36	0,15,15	0.00	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	c	514	-	-	15/29/63/63	0/2/2/2
24	BCR	b	619	-	-	0/29/63/63	0/2/2/2
22	CLA	c	513	-	2/2/25/25	6/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	402	-	3/3/25/25	5/37/135/135	-
22	CLA	b	615	-	3/3/25/25	7/37/135/135	-
24	BCR	x	101	-	-	5/29/63/63	0/2/2/2
33	STE	t	102	-	-	3/9/11/17	-
22	CLA	C	507	36	3/3/25/25	10/37/135/135	-
27	LMG	m	101	-	-	25/46/66/70	0/1/1/1
22	CLA	C	508	-	2/2/25/25	11/37/135/135	-
22	CLA	b	610	36	3/3/25/25	4/37/135/135	-
27	LMG	c	522	-	-	24/43/63/70	0/1/1/1
22	CLA	C	512	-	3/3/25/25	13/37/135/135	-
33	STE	b	627	-	-	5/11/11/17	-
22	CLA	D	402	-	2/2/25/25	6/37/135/135	-
23	PHO	A	404	-	-	3/53/103/103	0/5/6/6
22	CLA	c	503	-	3/3/25/25	7/37/135/135	-
33	STE	C	522	-	-	5/13/13/17	-
33	STE	a	413	-	-	3/7/7/17	-
33	STE	j	101	-	-	3/7/9/17	-
22	CLA	b	614	-	3/3/25/25	14/37/135/135	-
22	CLA	C	506	-	3/3/25/25	8/37/135/135	-
33	STE	J	101	-	-	4/7/9/17	-
24	BCR	b	618	-	-	6/29/63/63	0/2/2/2
33	STE	a	415	-	-	6/12/12/17	-
22	CLA	B	605	-	3/3/25/25	9/37/135/135	-
33	STE	b	624	-	-	6/11/13/17	-
30	DGD	c	517	-	-	27/51/91/95	0/2/2/2
26	PL9	d	407	-	-	12/53/73/73	0/1/1/1
22	CLA	c	509	-	3/3/25/25	9/37/135/135	-
28	LHG	l	101	-	-	15/53/53/53	-
22	CLA	c	511	3	3/3/25/25	11/37/135/135	-
33	STE	t	103	-	-	6/13/15/17	-
24	BCR	B	619	-	-	4/29/63/63	0/2/2/2
28	LHG	A	412	-	-	19/51/51/53	-
22	CLA	B	609	-	-	6/37/135/135	-
22	CLA	a	402	-	3/3/25/25	6/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	501	-	3/3/25/25	3/37/135/135	-
22	CLA	b	612	-	3/3/25/25	4/37/135/135	-
30	DGD	A	415	-	-	20/55/95/95	0/2/2/2
22	CLA	d	405	-	3/3/25/25	12/37/135/135	-
22	CLA	b	608	-	1/1/25/25	1/37/135/135	-
33	STE	b	626	-	-	4/7/7/17	-
24	BCR	t	101	-	-	6/29/63/63	0/2/2/2
35	HEC	V	201	17	-	0/6/54/54	-
22	CLA	a	404	-	3/3/25/25	8/37/135/135	-
22	CLA	C	511	3	3/3/25/25	4/37/135/135	-
22	CLA	B	611	-	3/3/25/25	9/37/135/135	-
22	CLA	b	602	-	1/1/25/25	4/37/135/135	-
22	CLA	d	403	-	2/2/25/25	7/37/135/135	-
22	CLA	b	609	-	2/2/25/25	10/37/135/135	-
24	BCR	D	405	-	-	6/29/63/63	0/2/2/2
22	CLA	A	406	-	3/3/22/25	3/24/122/135	-
27	LMG	c	520	-	-	10/31/51/70	0/1/1/1
22	CLA	C	510	-	3/3/25/25	9/37/135/135	-
33	STE	b	621	-	-	8/13/13/17	-
22	CLA	C	502	-	2/2/25/25	8/37/135/135	-
24	BCR	d	406	-	-	8/29/63/63	0/2/2/2
24	BCR	B	618	-	-	2/29/63/63	0/2/2/2
28	LHG	e	101	-	-	31/46/46/53	-
22	CLA	A	403	36	3/3/25/25	13/37/135/135	-
30	DGD	C	518	-	-	23/51/91/95	0/2/2/2
33	STE	Z	101	-	-	2/5/5/17	-
33	STE	M	103	-	-	2/7/7/17	-
33	STE	I	101	-	-	3/12/12/17	-
22	CLA	c	501	-	3/3/25/25	2/37/135/135	-
35	HEC	f	101	5,6	-	0/6/54/54	-
22	CLA	b	616	-	3/3/24/25	7/31/129/135	-
22	CLA	c	504	36	3/3/24/25	8/31/129/135	-
33	STE	M	102	-	-	3/10/12/17	-
33	STE	a	414	-	-	3/7/9/17	-
29	SQD	a	411	-	-	22/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	STE	b	622	-	-	8/15/17/17	-
24	BCR	c	516	-	-	3/29/63/63	0/2/2/2
23	PHO	d	402	-	-	2/53/103/103	0/5/6/6
29	SQD	f	102	-	-	11/36/56/69	0/1/1/1
22	CLA	D	404	-	2/2/25/25	10/37/135/135	-
24	BCR	a	405	-	-	1/29/63/63	0/2/2/2
33	STE	b	625	-	-	9/15/17/17	-
33	STE	m	102	-	-	4/7/9/17	-
22	CLA	B	606	-	3/3/25/25	9/37/135/135	-
24	BCR	A	407	-	-	10/29/63/63	0/2/2/2
22	CLA	b	601	36	3/3/25/25	13/37/135/135	-
22	CLA	d	401	36	2/2/25/25	13/37/135/135	-
33	STE	T	102	-	-	11/12/12/17	-
24	BCR	Y	101	-	-	6/29/63/63	0/2/2/2
30	DGD	c	518	-	-	19/51/91/95	0/2/2/2
22	CLA	c	502	-	2/2/25/25	5/37/135/135	-
22	CLA	c	508	-	2/2/24/25	11/36/134/135	-
22	CLA	C	503	-	2/2/25/25	5/37/135/135	-
27	LMG	d	410	-	-	10/39/59/70	0/1/1/1
28	LHG	E	101	-	-	23/53/53/53	-
22	CLA	b	607	36	3/3/25/25	13/37/135/135	-
24	BCR	b	617	-	-	7/29/63/63	0/2/2/2
27	LMG	A	411	-	-	21/43/63/70	0/1/1/1
27	LMG	c	523	-	-	20/44/64/70	0/1/1/1
33	STE	B	624	-	-	3/7/9/17	-
35	HEC	v	201	17	-	0/6/54/54	-
29	SQD	D	408	-	-	12/28/48/69	0/1/1/1
22	CLA	c	506	-	3/3/25/25	17/37/135/135	-
22	CLA	b	611	-	3/3/25/25	6/37/135/135	-
27	LMG	a	416	-	-	30/50/70/70	0/1/1/1
22	CLA	D	403	36	1/1/25/25	7/37/135/135	-
22	CLA	B	616	-	3/3/24/25	7/31/129/135	-
22	CLA	C	513	-	2/2/25/25	9/37/135/135	-
24	BCR	c	515	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LHG	d	408	-	-	17/53/53/53	-
33	STE	c	521	-	-	5/15/17/17	-
30	DGD	C	517	-	-	25/51/91/95	0/2/2/2
22	CLA	B	614	-	3/3/25/25	18/37/135/135	-
22	CLA	d	404	36	2/2/25/25	4/37/135/135	-
33	STE	C	521	-	-	5/7/9/17	-
30	DGD	c	519	-	-	13/51/91/95	0/2/2/2
30	DGD	H	102	-	-	16/51/91/95	0/2/2/2
22	CLA	c	505	-	2/2/25/25	10/37/135/135	-
33	STE	d	412	-	-	6/15/17/17	-
22	CLA	B	612	-	3/3/25/25	6/37/135/135	-
33	STE	R	101	-	-	4/7/9/17	-
33	STE	B	626	-	-	4/7/9/17	-
28	LHG	d	409	-	-	14/43/43/53	-
27	LMG	D	407	-	-	15/46/66/70	0/1/1/1
22	CLA	B	603	-	3/3/25/25	5/37/135/135	-
28	LHG	B	621	-	-	25/53/53/53	-
27	LMG	D	410	-	-	15/33/33/70	-
33	STE	C	523	-	-	3/7/9/17	-
33	STE	D	412	-	-	8/15/17/17	-
24	BCR	C	516	-	-	10/29/63/63	0/2/2/2
28	LHG	B	622	-	-	18/53/53/53	-
27	LMG	C	520	-	-	12/43/63/70	0/1/1/1
29	SQD	A	414	-	-	21/39/39/69	-
22	CLA	b	605	-	3/3/25/25	4/37/135/135	-
29	SQD	B	623	-	-	24/49/69/69	0/1/1/1
28	LHG	a	410	-	-	23/53/53/53	-
22	CLA	C	509	-	3/3/25/25	12/37/135/135	-
29	SQD	A	413	-	-	16/47/67/69	0/1/1/1
33	STE	B	620	-	-	5/12/14/17	-
22	CLA	B	610	36	3/3/25/25	6/37/135/135	-
29	SQD	a	412	-	-	18/37/37/69	-
22	CLA	b	603	-	3/3/25/25	6/37/135/135	-
22	CLA	C	505	-	2/2/25/25	11/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	512	-	3/3/25/25	18/37/135/135	-
22	CLA	b	606	-	3/3/25/25	7/37/135/135	-
22	CLA	C	504	36	3/3/23/25	6/30/128/135	-
26	PL9	A	410	-	-	24/53/73/73	0/1/1/1
22	CLA	B	613	-	3/3/25/25	11/37/135/135	-
22	CLA	B	604	-	3/3/25/25	10/37/135/135	-
33	STE	k	102	-	-	5/7/9/17	-
24	BCR	C	515	-	-	6/29/63/63	0/2/2/2
30	DGD	C	519	-	-	11/51/91/95	0/2/2/2
24	BCR	k	101	-	-	10/29/63/63	0/2/2/2
35	HEC	F	101	5,6	-	0/6/54/54	-
29	SQD	b	620	-	-	20/44/64/69	0/1/1/1
30	DGD	h	101	-	-	19/51/91/95	0/2/2/2
26	PL9	D	406	-	-	10/53/73/73	0/1/1/1
33	STE	d	413	-	-	8/15/17/17	-
22	CLA	c	507	36	3/3/25/25	6/37/135/135	-
22	CLA	b	613	-	3/3/25/25	10/37/135/135	-
27	LMG	M	101	-	-	22/46/66/70	0/1/1/1
23	PHO	a	403	-	-	2/53/103/103	0/5/6/6
33	STE	d	411	-	-	6/12/14/17	-
33	STE	B	625	-	-	9/13/13/17	-
24	BCR	C	514	-	-	11/29/63/63	0/2/2/2
23	PHO	A	405	-	-	2/53/103/103	0/5/6/6
27	LMG	D	411	-	-	6/18/22/70	-
22	CLA	B	601	36	2/2/25/25	12/37/135/135	-
22	CLA	B	608	-	2/2/25/25	1/37/135/135	-
33	STE	H	103	-	-	10/15/15/17	-
27	LMG	b	623	-	-	22/50/70/70	0/1/1/1
24	BCR	T	101	-	-	7/29/63/63	0/2/2/2
22	CLA	B	615	-	3/3/25/25	9/37/135/135	-
22	CLA	b	604	-	3/3/25/25	9/37/135/135	-
24	BCR	H	101	-	-	6/29/63/63	0/2/2/2
22	CLA	B	602	-	3/3/25/25	5/37/135/135	-
22	CLA	B	607	36	3/3/25/25	5/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	B	617	-	-	8/29/63/63	0/2/2/2
33	STE	l	102	-	-	9/15/15/17	-
26	PL9	a	409	-	-	27/53/73/73	0/1/1/1
22	CLA	c	510	-	3/3/25/25	11/37/135/135	-
28	LHG	D	409	-	-	20/53/53/53	-

All (787) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	d	403	CLA	C4B-NB	9.29	1.43	1.35
22	b	606	CLA	MG-NA	9.01	2.27	2.06
22	b	603	CLA	C4B-NB	8.74	1.43	1.35
35	f	101	HEC	C3B-C2B	-8.44	1.31	1.40
22	B	602	CLA	C4B-NB	8.29	1.42	1.35
22	B	612	CLA	C4B-NB	8.21	1.42	1.35
22	B	613	CLA	C4B-NB	8.06	1.42	1.35
22	A	402	CLA	C4B-NB	8.01	1.42	1.35
22	B	601	CLA	C4B-NB	7.98	1.42	1.35
22	c	504	CLA	C4B-NB	7.96	1.42	1.35
35	v	201	HEC	C3B-C2B	-7.80	1.32	1.40
22	c	505	CLA	C4B-NB	7.69	1.42	1.35
22	d	404	CLA	MG-NA	7.67	2.24	2.06
22	b	612	CLA	MG-NC	-7.66	1.88	2.06
22	d	401	CLA	C4B-NB	7.59	1.42	1.35
22	A	403	CLA	C4B-NB	7.55	1.41	1.35
26	D	406	PL9	C7-C3	-7.53	1.43	1.51
22	B	614	CLA	C4B-NB	7.50	1.41	1.35
22	b	615	CLA	C4B-NB	7.47	1.41	1.35
22	C	511	CLA	C4B-NB	7.46	1.41	1.35
22	b	601	CLA	C4B-NB	7.42	1.41	1.35
22	d	404	CLA	C4B-NB	7.36	1.41	1.35
22	B	609	CLA	C4B-NB	7.35	1.41	1.35
22	B	610	CLA	C4B-NB	7.32	1.41	1.35
22	C	505	CLA	C4B-NB	7.19	1.41	1.35
22	C	503	CLA	C4B-NB	7.10	1.41	1.35
22	c	511	CLA	MG-NA	7.08	2.23	2.06
22	c	510	CLA	C4B-NB	7.07	1.41	1.35
22	D	404	CLA	C4B-NB	7.05	1.41	1.35
22	C	501	CLA	C4B-NB	6.96	1.41	1.35
22	c	513	CLA	C4B-NB	6.93	1.41	1.35
22	B	606	CLA	C4B-NB	6.91	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	615	CLA	C4B-NB	6.77	1.41	1.35
22	b	613	CLA	C4B-NB	6.76	1.41	1.35
35	F	101	HEC	C3B-C2B	-6.69	1.33	1.40
22	a	404	CLA	C4B-NB	6.63	1.41	1.35
22	B	611	CLA	MG-NA	6.62	2.22	2.06
22	d	405	CLA	C4B-NB	6.61	1.41	1.35
22	c	502	CLA	C4B-NB	6.45	1.41	1.35
22	c	511	CLA	C4B-NB	6.41	1.40	1.35
35	V	201	HEC	C3B-C2B	-6.36	1.34	1.40
22	a	402	CLA	C4B-NB	6.31	1.40	1.35
22	C	510	CLA	C4B-NB	6.31	1.40	1.35
22	c	510	CLA	MG-NA	6.30	2.21	2.06
22	A	406	CLA	C4B-NB	6.30	1.40	1.35
22	C	506	CLA	C4B-NB	6.25	1.40	1.35
22	B	616	CLA	MG-NA	6.24	2.21	2.06
22	b	609	CLA	C4B-NB	6.22	1.40	1.35
22	c	503	CLA	C4B-NB	6.17	1.40	1.35
22	b	604	CLA	C4B-NB	6.13	1.40	1.35
22	b	614	CLA	C4B-NB	6.13	1.40	1.35
22	B	609	CLA	MG-NA	6.11	2.20	2.06
22	C	502	CLA	C4B-NB	6.11	1.40	1.35
22	b	605	CLA	C4B-NB	6.04	1.40	1.35
22	c	509	CLA	C4B-NB	6.04	1.40	1.35
22	c	501	CLA	C4B-NB	5.93	1.40	1.35
22	B	611	CLA	C4B-NB	5.91	1.40	1.35
35	F	101	HEC	C3C-C2C	-5.90	1.34	1.40
26	d	407	PL9	C6-C1	-5.87	1.38	1.48
22	b	612	CLA	C4B-NB	5.82	1.40	1.35
22	D	402	CLA	C4B-NB	5.82	1.40	1.35
22	c	506	CLA	C4B-NB	5.81	1.40	1.35
22	D	403	CLA	C4B-NB	5.81	1.40	1.35
35	V	201	HEC	C3C-C2C	-5.81	1.34	1.40
22	C	507	CLA	C4B-NB	5.77	1.40	1.35
22	B	604	CLA	MG-NC	5.76	2.20	2.06
22	B	616	CLA	C4B-NB	5.75	1.40	1.35
35	v	201	HEC	C3C-C2C	-5.74	1.34	1.40
22	C	505	CLA	MG-NA	5.62	2.19	2.06
22	C	513	CLA	C4B-NB	5.57	1.40	1.35
22	C	508	CLA	MG-NA	5.53	2.19	2.06
22	b	610	CLA	C4B-NB	5.51	1.40	1.35
22	c	512	CLA	C4B-NB	5.49	1.40	1.35
22	c	508	CLA	C4B-NB	5.48	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	f	101	HEC	C3C-C2C	-5.45	1.35	1.40
22	b	608	CLA	C4B-NB	5.43	1.40	1.35
22	B	603	CLA	C4B-NB	5.40	1.40	1.35
22	C	509	CLA	C4B-NB	5.39	1.40	1.35
22	B	606	CLA	MG-NA	5.34	2.19	2.06
22	C	504	CLA	C4B-NB	5.19	1.39	1.35
35	v	201	HEC	C3D-C2D	5.17	1.53	1.37
22	b	616	CLA	C4B-NB	5.16	1.39	1.35
22	B	604	CLA	C4B-NB	5.14	1.39	1.35
22	C	512	CLA	C4B-NB	5.10	1.39	1.35
22	b	607	CLA	C4B-NB	5.04	1.39	1.35
35	f	101	HEC	C3D-C2D	4.94	1.52	1.37
35	F	101	HEC	C3D-C2D	4.91	1.52	1.37
22	C	506	CLA	MG-NA	4.91	2.17	2.06
22	b	615	CLA	MG-NA	4.83	2.17	2.06
22	C	502	CLA	MG-NA	4.82	2.17	2.06
22	C	503	CLA	MG-NA	4.80	2.17	2.06
22	b	609	CLA	MG-NA	4.80	2.17	2.06
22	C	511	CLA	MG-NA	4.65	2.17	2.06
22	B	606	CLA	C3B-C2B	-4.65	1.33	1.40
22	C	507	CLA	MG-NA	4.56	2.17	2.06
22	C	501	CLA	MG-NA	4.55	2.17	2.06
22	c	508	CLA	MG-NA	4.50	2.17	2.06
22	d	405	CLA	MG-NA	4.50	2.16	2.06
28	D	409	LHG	O7-C5	-4.49	1.35	1.46
22	B	612	CLA	MG-NC	4.46	2.16	2.06
22	A	402	CLA	MG-NC	4.42	2.16	2.06
24	c	515	BCR	C1-C6	-4.41	1.47	1.53
24	Y	101	BCR	C30-C25	-4.40	1.47	1.53
22	b	606	CLA	C4B-NB	4.39	1.39	1.35
22	C	508	CLA	C4B-NB	4.39	1.39	1.35
22	B	605	CLA	C4B-NB	4.37	1.39	1.35
30	C	519	DGD	O2G-C2G	-4.36	1.35	1.46
35	V	201	HEC	C3D-C2D	4.33	1.50	1.37
22	b	603	CLA	MG-NA	4.33	2.16	2.06
24	B	618	BCR	C30-C25	-4.33	1.47	1.53
24	C	515	BCR	C1-C6	-4.22	1.48	1.53
30	C	519	DGD	O5D-C1E	4.14	1.47	1.40
24	H	101	BCR	C30-C25	-4.10	1.48	1.53
22	B	607	CLA	C4B-NB	4.06	1.38	1.35
26	d	407	PL9	C53-C6	-4.02	1.42	1.50
28	A	412	LHG	O3-C3	-4.00	1.29	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	602	CLA	C4B-NB	3.97	1.38	1.35
22	C	501	CLA	CHC-C1C	3.95	1.45	1.35
24	D	405	BCR	C30-C25	-3.95	1.48	1.53
26	D	406	PL9	C3-C4	-3.95	1.43	1.49
30	c	517	DGD	O2G-C2G	-3.94	1.36	1.46
22	b	604	CLA	MG-NC	3.89	2.15	2.06
22	a	402	CLA	MG-NA	3.89	2.15	2.06
30	c	519	DGD	O3G-C3G	-3.85	1.36	1.43
24	c	514	BCR	C1-C6	-3.84	1.48	1.53
22	c	505	CLA	CHC-C1C	3.83	1.44	1.35
22	a	402	CLA	MG-NC	3.80	2.15	2.06
30	A	415	DGD	C3E-C2E	3.78	1.62	1.52
30	C	518	DGD	C4D-C3D	3.77	1.61	1.52
30	A	415	DGD	C3G-C2G	3.76	1.62	1.50
27	a	416	LMG	C4-C5	3.75	1.60	1.53
22	b	615	CLA	C3B-C2B	-3.74	1.35	1.40
27	c	520	LMG	C1-C2	3.72	1.63	1.52
26	D	406	PL9	C26-C24	-3.72	1.43	1.51
29	b	620	SQD	O48-C23	3.71	1.44	1.33
24	C	516	BCR	C30-C25	-3.69	1.48	1.53
22	B	601	CLA	C3B-C2B	-3.68	1.35	1.40
24	C	514	BCR	C1-C6	-3.68	1.48	1.53
28	a	410	LHG	C24-C23	3.68	1.61	1.50
22	d	401	CLA	CHC-C1C	3.65	1.44	1.35
28	B	621	LHG	O7-C5	-3.63	1.37	1.46
22	b	607	CLA	MG-NA	3.62	2.14	2.06
22	B	602	CLA	MG-NA	3.62	2.14	2.06
22	C	513	CLA	MG-NA	3.61	2.14	2.06
22	c	511	CLA	MG-NC	-3.59	1.97	2.06
28	A	412	LHG	P-O6	3.59	1.73	1.59
22	D	402	CLA	CHC-C1C	3.59	1.44	1.35
26	A	410	PL9	C7-C3	-3.57	1.47	1.51
22	C	508	CLA	C1D-C2D	3.57	1.50	1.42
22	B	612	CLA	CHC-C1C	3.56	1.44	1.35
22	B	603	CLA	C3B-C2B	-3.55	1.35	1.40
30	A	415	DGD	C4D-C3D	3.54	1.61	1.52
22	c	511	CLA	CHC-C1C	3.54	1.44	1.35
22	C	505	CLA	CHC-C1C	3.53	1.44	1.35
24	B	617	BCR	C1-C6	-3.52	1.48	1.53
22	d	401	CLA	MG-NC	3.52	2.14	2.06
26	d	407	PL9	C31-C29	-3.52	1.44	1.51
22	B	606	CLA	CHC-C1C	3.51	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	610	CLA	C3B-C2B	-3.51	1.35	1.40
30	H	102	DGD	C4E-C5E	3.50	1.60	1.53
22	d	401	CLA	C3B-C2B	-3.50	1.35	1.40
22	C	508	CLA	MG-NC	-3.49	1.98	2.06
22	B	610	CLA	C1B-NB	3.46	1.38	1.35
24	B	619	BCR	C1-C6	-3.44	1.49	1.53
24	C	514	BCR	C30-C25	-3.42	1.49	1.53
22	c	510	CLA	CHC-C1C	3.41	1.43	1.35
24	d	406	BCR	C30-C25	-3.41	1.49	1.53
22	B	608	CLA	MG-NA	3.41	2.14	2.06
29	A	414	SQD	O47-C7	3.41	1.43	1.34
22	B	611	CLA	CHC-C1C	3.41	1.43	1.35
24	b	619	BCR	C1-C6	-3.40	1.49	1.53
30	c	518	DGD	C3E-C2E	3.40	1.61	1.52
22	b	611	CLA	C4B-NB	3.40	1.38	1.35
23	A	405	PHO	C1A-NA	3.39	1.44	1.37
23	A	405	PHO	C1C-NC	-3.39	1.31	1.38
22	b	608	CLA	CMB-C2B	-3.38	1.44	1.51
30	H	102	DGD	O3G-C1D	3.38	1.46	1.40
22	B	605	CLA	CHC-C1C	3.38	1.43	1.35
22	c	507	CLA	C4B-NB	3.37	1.38	1.35
28	E	101	LHG	P-O6	3.37	1.72	1.59
22	c	508	CLA	CHC-C1C	3.36	1.43	1.35
29	B	623	SQD	O48-C23	3.35	1.43	1.33
30	A	415	DGD	C6E-C5E	3.35	1.63	1.51
22	C	508	CLA	CHC-C1C	3.34	1.43	1.35
22	B	615	CLA	CMB-C2B	-3.34	1.44	1.51
22	B	602	CLA	CHC-C1C	3.33	1.43	1.35
30	H	102	DGD	O5D-C1E	3.33	1.45	1.40
29	a	412	SQD	O48-C23	3.32	1.43	1.33
22	b	615	CLA	CMB-C2B	-3.32	1.44	1.51
24	k	101	BCR	C30-C25	-3.31	1.49	1.53
24	x	101	BCR	C30-C25	-3.31	1.49	1.53
22	B	604	CLA	MG-NA	3.31	2.14	2.06
22	B	604	CLA	CHC-C1C	3.30	1.43	1.35
27	d	410	LMG	C4-C5	3.30	1.60	1.53
22	a	404	CLA	CMC-C2C	-3.29	1.43	1.50
22	B	608	CLA	C4B-NB	3.29	1.38	1.35
29	a	412	SQD	O47-C7	3.28	1.43	1.34
22	B	614	CLA	C3B-C2B	-3.28	1.35	1.40
22	B	615	CLA	C1D-C2D	3.28	1.50	1.42
22	B	613	CLA	CMD-C2D	-3.27	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	601	CLA	CHC-C1C	3.27	1.43	1.35
27	c	522	LMG	C3-C2	3.27	1.60	1.52
22	D	403	CLA	CHC-C1C	3.27	1.43	1.35
30	c	518	DGD	C4D-C3D	3.26	1.60	1.52
29	D	408	SQD	O48-C23	3.25	1.42	1.33
29	a	411	SQD	O48-C23	3.25	1.42	1.33
22	c	512	CLA	CHC-C1C	3.25	1.43	1.35
22	c	506	CLA	CHC-C1C	3.24	1.43	1.35
24	c	516	BCR	C1-C6	-3.24	1.49	1.53
22	B	603	CLA	CMB-C2B	-3.24	1.44	1.51
22	c	507	CLA	C3B-C2B	-3.22	1.35	1.40
30	C	518	DGD	C6E-C5E	3.22	1.62	1.51
23	d	402	PHO	C3B-C4B	3.22	1.49	1.43
22	c	504	CLA	CHC-C1C	3.22	1.43	1.35
28	d	409	LHG	P-O6	3.22	1.72	1.59
22	b	605	CLA	CHC-C1C	3.21	1.43	1.35
24	b	617	BCR	C30-C25	-3.21	1.49	1.53
24	c	516	BCR	C30-C25	-3.21	1.49	1.53
22	B	610	CLA	CHC-C1C	3.20	1.43	1.35
22	D	404	CLA	MG-NC	3.20	2.13	2.06
23	A	405	PHO	C3B-C4B	3.20	1.49	1.43
26	d	407	PL9	C7-C3	-3.20	1.48	1.51
22	b	601	CLA	C1D-C2D	3.20	1.49	1.42
22	C	504	CLA	CHC-C1C	3.19	1.43	1.35
22	B	601	CLA	CMB-C2B	-3.19	1.45	1.51
22	b	612	CLA	CHC-C1C	3.18	1.43	1.35
22	b	615	CLA	CHC-C1C	3.17	1.43	1.35
22	C	506	CLA	MG-NC	-3.17	1.98	2.06
30	A	415	DGD	O5D-C6D	-3.17	1.37	1.43
30	c	519	DGD	O1G-C1G	-3.17	1.37	1.45
22	C	503	CLA	C1D-C2D	3.16	1.49	1.42
27	A	411	LMG	C4-C3	3.14	1.60	1.52
24	c	514	BCR	C30-C25	-3.14	1.49	1.53
22	C	503	CLA	MG-NC	3.14	2.13	2.06
29	A	414	SQD	O48-C23	3.13	1.42	1.33
22	b	601	CLA	MG-NA	3.13	2.13	2.06
29	A	413	SQD	O48-C23	3.12	1.42	1.33
22	B	607	CLA	CHC-C1C	3.12	1.43	1.35
22	d	405	CLA	C3B-C2B	-3.12	1.36	1.40
24	b	618	BCR	C1-C6	-3.12	1.49	1.53
22	C	512	CLA	MG-NA	3.11	2.13	2.06
22	B	603	CLA	MG-NA	3.11	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	511	CLA	CHC-C1C	3.11	1.42	1.35
22	b	611	CLA	CHC-C1C	3.11	1.42	1.35
22	b	603	CLA	CMB-C2B	-3.10	1.45	1.51
27	D	410	LMG	C7-C8	3.09	1.58	1.51
22	A	402	CLA	C1D-C2D	3.09	1.49	1.42
26	d	407	PL9	C21-C19	-3.08	1.44	1.51
26	a	409	PL9	C52-C5	-3.08	1.44	1.50
29	B	623	SQD	O47-C7	3.08	1.43	1.34
24	B	617	BCR	C30-C25	-3.08	1.49	1.53
22	B	610	CLA	C1D-C2D	3.07	1.49	1.42
30	h	101	DGD	O2D-C2D	-3.07	1.35	1.43
22	b	608	CLA	CHC-C1C	3.05	1.42	1.35
26	a	409	PL9	C53-C6	-3.05	1.44	1.50
24	b	617	BCR	C1-C6	-3.05	1.49	1.53
22	c	503	CLA	MG-NC	3.05	2.13	2.06
30	C	517	DGD	C6D-C5D	3.05	1.61	1.51
24	Y	101	BCR	C1-C6	-3.04	1.49	1.53
22	C	512	CLA	CMD-C2D	-3.03	1.44	1.51
22	c	510	CLA	CMB-C2B	-3.03	1.45	1.51
22	D	403	CLA	MG-NA	3.03	2.13	2.06
26	D	406	PL9	C30-C29	-3.02	1.42	1.50
28	B	622	LHG	C24-C23	3.02	1.59	1.50
30	c	519	DGD	O2G-C2G	-3.02	1.39	1.46
23	a	403	PHO	C4C-NC	3.02	1.43	1.36
30	c	517	DGD	C4D-C5D	3.02	1.59	1.53
29	f	102	SQD	O48-C23	3.00	1.42	1.33
22	c	511	CLA	C1D-C2D	3.00	1.49	1.42
30	h	101	DGD	C4E-C5E	2.98	1.59	1.53
28	d	409	LHG	C24-C23	2.97	1.59	1.50
24	c	515	BCR	C30-C25	-2.96	1.49	1.53
23	A	404	PHO	C4C-NC	2.96	1.43	1.36
22	C	507	CLA	CMB-C2B	-2.96	1.45	1.51
22	c	512	CLA	C1D-C2D	2.95	1.49	1.42
22	b	607	CLA	CHC-C1C	2.95	1.42	1.35
24	C	516	BCR	C1-C6	-2.95	1.49	1.53
28	D	409	LHG	C8-C7	-2.95	1.42	1.50
22	c	503	CLA	CHC-C1C	2.95	1.42	1.35
22	D	403	CLA	CMB-C2B	-2.95	1.45	1.51
23	d	402	PHO	CMC-C2C	-2.94	1.44	1.50
30	h	101	DGD	O2E-C2E	-2.94	1.36	1.43
22	C	509	CLA	C1B-NB	2.93	1.37	1.35
22	B	602	CLA	CMB-C2B	-2.92	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	613	CLA	CHC-C1C	2.92	1.42	1.35
22	b	614	CLA	CHC-C1C	2.92	1.42	1.35
22	b	608	CLA	C1D-C2D	2.92	1.49	1.42
30	H	102	DGD	O2D-C2D	-2.91	1.36	1.43
24	A	407	BCR	C1-C6	-2.91	1.49	1.53
23	a	403	PHO	CHD-C4C	-2.90	1.33	1.40
22	B	615	CLA	CHC-C1C	2.90	1.42	1.35
29	b	620	SQD	O47-C7	2.90	1.42	1.34
22	b	614	CLA	CMB-C2B	-2.89	1.45	1.51
22	d	404	CLA	CMB-C2B	-2.89	1.45	1.51
22	c	502	CLA	CHC-C1C	2.89	1.42	1.35
22	C	513	CLA	CHC-C1C	2.89	1.42	1.35
27	b	623	LMG	O6-C1	2.88	1.49	1.41
22	C	512	CLA	CHC-C1C	2.88	1.42	1.35
30	C	517	DGD	O5D-C6D	-2.88	1.38	1.43
27	A	411	LMG	O1-C7	-2.88	1.38	1.43
24	T	101	BCR	C30-C25	-2.88	1.49	1.53
26	d	407	PL9	C3-C4	-2.88	1.44	1.49
22	d	403	CLA	MG-NA	2.88	2.13	2.06
22	c	509	CLA	CHC-C1C	2.88	1.42	1.35
22	C	502	CLA	CMB-C2B	-2.87	1.45	1.51
22	B	615	CLA	MG-NA	2.87	2.13	2.06
22	B	610	CLA	C3B-C2B	-2.87	1.36	1.40
22	b	612	CLA	CMB-C2B	-2.87	1.45	1.51
22	b	602	CLA	CHC-C1C	2.86	1.42	1.35
22	D	402	CLA	CMD-C2D	-2.85	1.44	1.51
22	c	502	CLA	CMD-C2D	-2.85	1.44	1.51
24	d	406	BCR	C1-C6	-2.85	1.49	1.53
22	c	513	CLA	C1D-C2D	2.85	1.49	1.42
22	B	608	CLA	C1D-C2D	2.85	1.49	1.42
30	H	102	DGD	C1E-C2E	2.84	1.60	1.52
27	c	523	LMG	C4-C5	2.84	1.59	1.53
27	D	410	LMG	C9-C8	2.83	1.59	1.50
22	D	404	CLA	CMB-C2B	-2.83	1.45	1.51
24	T	101	BCR	C1-C6	-2.83	1.49	1.53
27	b	623	LMG	C3-C2	2.83	1.59	1.52
22	d	403	CLA	CHC-C1C	2.83	1.42	1.35
22	B	609	CLA	C3B-C2B	-2.82	1.36	1.40
22	b	605	CLA	MG-NA	2.82	2.13	2.06
28	B	622	LHG	O7-C5	-2.82	1.39	1.46
22	b	615	CLA	CMD-C2D	-2.82	1.44	1.51
29	a	411	SQD	O47-C7	2.81	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	d	405	CLA	CMC-C2C	-2.81	1.44	1.50
22	d	401	CLA	CMB-C2B	-2.81	1.45	1.51
27	m	101	LMG	C4-C3	2.81	1.59	1.52
22	a	402	CLA	C1D-C2D	2.80	1.48	1.42
24	b	618	BCR	C30-C25	-2.80	1.49	1.53
22	b	616	CLA	CMB-C2B	-2.80	1.45	1.51
26	D	406	PL9	C6-C1	-2.79	1.43	1.48
22	c	513	CLA	CHC-C1C	2.79	1.42	1.35
22	B	608	CLA	CMD-C2D	-2.79	1.44	1.51
22	c	506	CLA	CAC-C3C	-2.79	1.44	1.51
22	B	603	CLA	CHC-C1C	2.78	1.42	1.35
29	f	102	SQD	O47-C7	2.78	1.42	1.34
24	A	407	BCR	C33-C5	-2.78	1.46	1.50
23	d	402	PHO	C1A-NA	2.78	1.43	1.37
28	A	412	LHG	C8-C7	-2.78	1.42	1.50
22	b	612	CLA	MG-NA	2.77	2.12	2.06
30	C	518	DGD	O5D-C6D	-2.77	1.38	1.43
22	b	608	CLA	C3B-CAB	-2.77	1.42	1.47
23	d	402	PHO	CHC-C1C	2.77	1.44	1.38
22	a	402	CLA	CHC-C1C	2.76	1.42	1.35
22	B	605	CLA	C1D-C2D	2.75	1.48	1.42
22	c	513	CLA	MG-NA	2.75	2.12	2.06
22	c	508	CLA	C3B-C2B	-2.75	1.36	1.40
22	B	615	CLA	C3B-C2B	-2.75	1.36	1.40
22	A	403	CLA	CHC-C1C	2.74	1.42	1.35
30	C	517	DGD	C4E-C3E	2.74	1.59	1.52
24	t	101	BCR	C30-C25	-2.74	1.50	1.53
22	B	610	CLA	MG-NA	2.74	2.12	2.06
22	d	405	CLA	CHC-C1C	2.74	1.42	1.35
22	C	510	CLA	CHC-C1C	2.74	1.42	1.35
22	B	607	CLA	CMB-C2B	-2.74	1.45	1.51
24	b	619	BCR	C30-C25	-2.73	1.50	1.53
22	c	505	CLA	CMB-C2B	-2.73	1.46	1.51
30	h	101	DGD	C4D-C3D	2.73	1.59	1.52
22	c	510	CLA	MG-NC	-2.73	1.99	2.06
26	A	410	PL9	C6-C1	-2.73	1.43	1.48
22	b	612	CLA	CMC-C2C	-2.72	1.45	1.50
22	d	405	CLA	MG-NC	-2.71	1.99	2.06
22	b	610	CLA	CMB-C2B	-2.71	1.46	1.51
26	A	410	PL9	C37-C38	2.71	1.59	1.50
30	C	518	DGD	O1G-C1G	-2.71	1.39	1.45
22	C	503	CLA	CHC-C1C	2.70	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	502	CLA	CHC-C1C	2.70	1.41	1.35
30	c	518	DGD	C4D-C5D	2.70	1.58	1.53
30	H	102	DGD	O2G-C2G	-2.69	1.39	1.46
24	a	405	BCR	C1-C6	-2.69	1.50	1.53
30	A	415	DGD	O3G-C1D	2.69	1.44	1.40
24	x	101	BCR	C1-C6	-2.69	1.50	1.53
22	C	506	CLA	CHC-C1C	2.68	1.41	1.35
22	C	510	CLA	O2A-CGA	2.68	1.41	1.33
22	B	610	CLA	CMB-C2B	-2.67	1.46	1.51
23	a	403	PHO	C1C-NC	-2.67	1.32	1.38
22	b	603	CLA	C1D-C2D	2.67	1.48	1.42
29	a	411	SQD	O4-C4	-2.67	1.36	1.43
26	D	406	PL9	C5-C4	-2.67	1.37	1.47
22	d	403	CLA	CMD-C2D	-2.66	1.45	1.51
22	A	403	CLA	CMD-C2D	-2.66	1.45	1.51
22	b	603	CLA	CMC-C2C	-2.66	1.45	1.50
24	D	405	BCR	C1-C6	-2.66	1.50	1.53
22	c	503	CLA	C1D-C2D	2.66	1.48	1.42
22	b	611	CLA	CMC-C2C	-2.65	1.45	1.50
30	A	415	DGD	O3D-C3D	-2.65	1.36	1.43
28	e	101	LHG	P-O6	2.65	1.70	1.59
24	k	101	BCR	C1-C6	-2.65	1.50	1.53
22	b	607	CLA	C3B-C2B	-2.65	1.36	1.40
22	B	606	CLA	MG-NC	2.64	2.12	2.06
22	d	405	CLA	CMD-C2D	-2.64	1.45	1.51
22	d	404	CLA	CHC-C1C	2.64	1.41	1.35
22	B	615	CLA	C4B-CHC	-2.64	1.33	1.41
22	b	606	CLA	C3B-C2B	-2.63	1.36	1.40
30	C	517	DGD	C3G-C2G	2.63	1.58	1.50
30	H	102	DGD	C4E-C3E	2.63	1.59	1.52
29	A	413	SQD	O47-C7	2.63	1.41	1.34
22	B	601	CLA	CHC-C1C	2.62	1.41	1.35
22	b	604	CLA	CHC-C1C	2.62	1.41	1.35
22	c	507	CLA	MG-NC	-2.62	2.00	2.06
22	b	610	CLA	CMD-C2D	-2.61	1.45	1.51
30	c	518	DGD	C6E-C5E	2.61	1.60	1.51
24	C	515	BCR	C30-C25	-2.60	1.50	1.53
22	c	505	CLA	MG-NA	2.60	2.12	2.06
22	D	404	CLA	CMC-C2C	-2.60	1.45	1.50
30	H	102	DGD	C6E-C5E	2.60	1.60	1.51
26	A	410	PL9	C7-C8	-2.60	1.46	1.50
22	C	513	CLA	C1D-C2D	2.59	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	613	CLA	CMB-C2B	-2.59	1.46	1.51
27	A	411	LMG	C4-C5	2.59	1.58	1.53
22	a	404	CLA	CMD-C2D	-2.59	1.45	1.51
22	b	606	CLA	MG-NC	-2.58	2.00	2.06
24	t	101	BCR	C1-C6	-2.58	1.50	1.53
22	B	601	CLA	MG-NA	2.58	2.12	2.06
22	B	616	CLA	CMC-C2C	-2.58	1.45	1.50
30	A	415	DGD	C1E-C2E	2.58	1.59	1.52
22	d	404	CLA	C1D-C2D	2.58	1.48	1.42
22	C	512	CLA	MG-NC	-2.58	2.00	2.06
23	a	403	PHO	CAA-C2A	-2.57	1.49	1.54
22	b	602	CLA	CAC-C3C	-2.57	1.44	1.51
22	C	502	CLA	C1D-C2D	2.57	1.48	1.42
22	b	604	CLA	C1D-C2D	2.57	1.48	1.42
30	C	517	DGD	O1G-C1A	2.57	1.40	1.33
23	d	402	PHO	CAA-C2A	-2.56	1.49	1.54
22	C	506	CLA	C3B-CAB	-2.56	1.42	1.47
22	b	609	CLA	CHC-C1C	2.56	1.41	1.35
22	b	610	CLA	C4B-CHC	-2.56	1.33	1.41
22	A	403	CLA	MG-NA	2.55	2.12	2.06
22	b	614	CLA	CAC-C3C	-2.55	1.44	1.51
22	b	608	CLA	C3B-C2B	-2.55	1.36	1.40
30	C	519	DGD	O3G-C1D	-2.55	1.35	1.40
22	B	607	CLA	MG-NA	2.55	2.12	2.06
22	B	616	CLA	MG-NC	-2.55	2.00	2.06
22	B	604	CLA	CMC-C2C	-2.54	1.45	1.50
22	b	607	CLA	CMD-C2D	-2.54	1.45	1.51
22	c	506	CLA	C3B-CAB	-2.54	1.42	1.47
29	A	414	SQD	O47-C45	-2.54	1.42	1.47
29	f	102	SQD	O3-C3	-2.53	1.37	1.43
22	D	402	CLA	MG-NA	2.53	2.12	2.06
22	B	612	CLA	C1D-C2D	2.52	1.48	1.42
22	b	611	CLA	C1D-C2D	2.52	1.48	1.42
22	B	606	CLA	C4B-CHC	-2.52	1.34	1.41
22	B	613	CLA	C3B-CAB	-2.52	1.42	1.47
22	c	508	CLA	CMD-C2D	-2.52	1.45	1.51
22	C	501	CLA	CMC-C2C	-2.52	1.45	1.50
23	d	402	PHO	CHD-C4C	-2.51	1.34	1.40
26	d	407	PL9	C45-C44	-2.51	1.44	1.50
27	c	522	LMG	O1-C1	2.51	1.44	1.40
22	C	504	CLA	CMD-C2D	-2.51	1.45	1.51
30	H	102	DGD	C3E-C2E	2.51	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	403	PHO	C4C-C3C	2.50	1.49	1.45
23	a	403	PHO	O2D-CGD	2.50	1.39	1.33
30	C	517	DGD	C6E-C5E	2.50	1.60	1.51
27	A	411	LMG	C1-C2	2.49	1.59	1.52
22	c	506	CLA	CMC-C2C	-2.48	1.45	1.50
22	B	606	CLA	CMB-C2B	-2.48	1.46	1.51
22	A	406	CLA	CMD-C2D	-2.48	1.45	1.51
26	A	410	PL9	C25-C24	-2.47	1.44	1.50
23	A	404	PHO	CHB-C1B	-2.47	1.34	1.38
22	B	611	CLA	CMC-C2C	-2.47	1.45	1.50
22	C	510	CLA	C1D-C2D	2.47	1.48	1.42
28	E	101	LHG	O7-C5	-2.47	1.40	1.46
22	c	512	CLA	CMB-C2B	-2.46	1.46	1.51
22	B	607	CLA	C1B-NB	2.46	1.37	1.35
22	B	616	CLA	C3B-CAB	-2.46	1.42	1.47
24	B	619	BCR	C30-C25	-2.46	1.50	1.53
22	b	609	CLA	CMB-C2B	-2.46	1.46	1.51
22	D	404	CLA	C4B-CHC	-2.46	1.34	1.41
22	C	502	CLA	MG-NC	2.46	2.12	2.06
28	B	621	LHG	O1-C1	2.45	1.52	1.42
22	C	511	CLA	CMB-C2B	-2.45	1.46	1.51
22	C	504	CLA	C1D-C2D	2.45	1.48	1.42
30	C	517	DGD	O2G-C1B	2.45	1.41	1.34
22	B	614	CLA	CHC-C1C	2.44	1.41	1.35
27	a	416	LMG	C7-C8	2.44	1.58	1.50
27	c	522	LMG	C4-C3	2.44	1.58	1.52
30	c	517	DGD	O4D-C4D	-2.44	1.37	1.43
27	d	410	LMG	O7-C8	-2.44	1.40	1.46
22	D	402	CLA	CAA-C2A	-2.43	1.49	1.54
22	a	404	CLA	C1D-C2D	2.43	1.48	1.42
23	A	404	PHO	CMC-C2C	-2.43	1.45	1.50
30	c	517	DGD	O3E-C3E	-2.43	1.37	1.43
30	C	517	DGD	C4D-C3D	2.43	1.58	1.52
30	h	101	DGD	C2A-C1A	-2.43	1.43	1.50
22	c	502	CLA	CMB-C2B	-2.42	1.46	1.51
22	b	606	CLA	CMB-C2B	-2.42	1.46	1.51
22	b	602	CLA	CMD-C2D	-2.42	1.45	1.51
22	C	507	CLA	CMD-C2D	-2.42	1.45	1.51
22	C	509	CLA	CHC-C1C	2.42	1.41	1.35
22	d	404	CLA	MG-NC	-2.42	2.00	2.06
22	a	404	CLA	C4B-CHC	-2.42	1.34	1.41
22	c	508	CLA	C1D-C2D	2.42	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	d	403	CLA	C1D-C2D	2.42	1.48	1.42
22	C	510	CLA	CMB-C2B	-2.42	1.46	1.51
27	M	101	LMG	C9-C8	2.41	1.58	1.50
27	C	520	LMG	C4-C3	2.41	1.58	1.52
30	C	518	DGD	O2G-C2G	-2.41	1.40	1.46
22	A	406	CLA	CHC-C1C	2.41	1.41	1.35
29	a	411	SQD	O2-C2	-2.41	1.37	1.43
27	c	520	LMG	C3-C2	2.40	1.58	1.52
22	c	502	CLA	C1D-C2D	2.40	1.48	1.42
22	a	402	CLA	CMB-C2B	-2.40	1.46	1.51
28	A	412	LHG	O7-C7	2.40	1.41	1.34
22	c	513	CLA	CMB-C2B	-2.40	1.46	1.51
22	B	613	CLA	CMC-C2C	-2.40	1.45	1.50
22	c	504	CLA	CMD-C2D	-2.40	1.45	1.51
22	b	609	CLA	C3B-CAB	-2.40	1.43	1.47
22	C	511	CLA	CMC-C2C	-2.39	1.45	1.50
22	c	511	CLA	CMB-C2B	-2.39	1.46	1.51
22	C	506	CLA	CMB-C2B	-2.39	1.46	1.51
22	b	614	CLA	CMC-C2C	-2.39	1.45	1.50
24	b	617	BCR	C33-C5	-2.39	1.47	1.50
22	D	404	CLA	CMD-C2D	-2.39	1.45	1.51
22	A	406	CLA	C1D-C2D	2.39	1.48	1.42
24	A	407	BCR	C38-C26	-2.38	1.47	1.50
27	D	407	LMG	C7-C8	2.38	1.58	1.50
22	D	404	CLA	C1D-C2D	2.38	1.48	1.42
22	B	609	CLA	CMD-C2D	-2.38	1.45	1.51
22	b	616	CLA	CMC-C2C	-2.38	1.45	1.50
22	b	616	CLA	C3B-C2B	-2.38	1.37	1.40
27	m	101	LMG	C1-C2	2.37	1.59	1.52
27	D	407	LMG	C9-C8	2.37	1.58	1.50
22	b	616	CLA	C1D-C2D	2.37	1.47	1.42
22	b	601	CLA	O2A-CGA	2.37	1.40	1.33
26	d	407	PL9	C27-C28	-2.37	1.42	1.50
22	c	504	CLA	C1D-C2D	2.37	1.47	1.42
23	A	405	PHO	CHC-C1C	2.37	1.43	1.38
26	a	409	PL9	C3-C4	-2.37	1.45	1.49
28	D	409	LHG	P-O3	2.36	1.68	1.59
22	c	503	CLA	CMB-C2B	-2.36	1.46	1.51
30	C	517	DGD	O2E-C2E	-2.36	1.37	1.43
22	B	611	CLA	C3B-C2B	-2.36	1.37	1.40
22	b	613	CLA	CHC-C1C	2.36	1.41	1.35
22	c	501	CLA	MG-NA	2.36	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	409	PL9	C6-C1	-2.35	1.44	1.48
22	c	510	CLA	CMC-C2C	-2.35	1.45	1.50
22	B	607	CLA	C1D-C2D	2.35	1.47	1.42
30	A	415	DGD	C4D-C5D	2.35	1.58	1.53
22	B	603	CLA	C3B-CAB	-2.35	1.43	1.47
30	c	517	DGD	C3G-C2G	2.35	1.57	1.50
29	A	413	SQD	O2-C2	-2.35	1.37	1.43
27	c	520	LMG	C4-C3	2.34	1.58	1.52
22	B	609	CLA	C3B-CAB	-2.34	1.43	1.47
22	D	403	CLA	C1D-C2D	2.34	1.47	1.42
22	B	608	CLA	CHC-C1C	2.34	1.41	1.35
29	D	408	SQD	O2-C2	-2.34	1.37	1.43
22	c	503	CLA	C5-C3	-2.34	1.46	1.51
22	B	605	CLA	CMD-C2D	-2.34	1.46	1.51
22	D	403	CLA	C3B-C2B	-2.34	1.37	1.40
23	A	405	PHO	CMB-C2B	-2.34	1.45	1.50
22	C	510	CLA	CMC-C2C	-2.33	1.45	1.50
30	A	415	DGD	O5D-C1E	2.33	1.44	1.40
22	C	510	CLA	CMD-C2D	-2.33	1.46	1.51
27	D	410	LMG	O8-C28	2.32	1.40	1.33
22	b	603	CLA	CHC-C1C	2.32	1.40	1.35
22	B	608	CLA	C3B-C2B	-2.32	1.37	1.40
22	C	501	CLA	C1D-C2D	2.32	1.47	1.42
22	A	403	CLA	C1D-C2D	2.32	1.47	1.42
22	C	507	CLA	CHC-C1C	2.32	1.40	1.35
22	C	506	CLA	C1D-C2D	2.31	1.47	1.42
24	B	617	BCR	C33-C5	-2.31	1.47	1.50
22	c	512	CLA	CMD-C2D	-2.31	1.46	1.51
22	d	405	CLA	C4B-CHC	-2.31	1.34	1.41
22	C	512	CLA	CMC-C2C	-2.30	1.45	1.50
30	c	518	DGD	O3E-C3E	-2.30	1.37	1.43
30	h	101	DGD	C1E-C2E	2.30	1.59	1.52
27	M	101	LMG	C29-C28	-2.30	1.44	1.50
22	C	509	CLA	CMB-C2B	-2.30	1.46	1.51
30	c	517	DGD	O2E-C2E	-2.30	1.37	1.43
29	D	408	SQD	O3-C3	-2.29	1.37	1.43
23	A	404	PHO	CHD-C4C	-2.29	1.35	1.40
23	d	402	PHO	C1C-NC	-2.29	1.33	1.38
24	A	407	BCR	C30-C25	-2.29	1.50	1.53
22	b	616	CLA	CHC-C1C	2.28	1.40	1.35
22	A	402	CLA	CMD-C2D	-2.28	1.46	1.51
29	A	413	SQD	O4-C4	-2.28	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	507	CLA	C1D-C2D	2.28	1.47	1.42
22	B	606	CLA	C3B-CAB	-2.28	1.43	1.47
22	B	610	CLA	CMA-C3A	-2.27	1.48	1.53
24	c	515	BCR	C33-C5	-2.27	1.47	1.50
22	b	606	CLA	CHC-C1C	2.27	1.40	1.35
22	C	512	CLA	CMB-C2B	-2.27	1.46	1.51
30	c	518	DGD	O3G-C3G	-2.27	1.39	1.43
22	d	403	CLA	CMB-C2B	-2.27	1.46	1.51
30	H	102	DGD	O6E-C1E	2.27	1.47	1.41
22	C	513	CLA	C4B-CHC	-2.26	1.34	1.41
24	a	405	BCR	C30-C25	-2.26	1.50	1.53
22	C	512	CLA	C1D-C2D	2.26	1.47	1.42
22	C	508	CLA	C1B-NB	2.26	1.37	1.35
22	c	505	CLA	MG-NC	2.26	2.11	2.06
22	D	403	CLA	CMD-C2D	-2.25	1.46	1.51
22	B	603	CLA	CMC-C2C	-2.25	1.46	1.50
22	d	405	CLA	C3B-CAB	-2.25	1.43	1.47
27	M	101	LMG	O7-C8	-2.25	1.41	1.46
22	C	506	CLA	C3B-C2B	-2.25	1.37	1.40
27	D	407	LMG	C4-C5	2.25	1.57	1.53
22	B	614	CLA	C3B-CAB	-2.25	1.43	1.47
30	c	517	DGD	C6D-C5D	2.25	1.58	1.51
22	d	401	CLA	MG-NA	-2.25	2.00	2.06
22	B	613	CLA	C3D-C2D	-2.25	1.35	1.39
22	C	504	CLA	CMB-C2B	-2.25	1.47	1.51
22	c	506	CLA	CMD-C2D	-2.25	1.46	1.51
22	A	406	CLA	C4B-CHC	-2.24	1.34	1.41
22	b	605	CLA	C4B-CHC	-2.24	1.34	1.41
22	b	613	CLA	CMC-C2C	-2.24	1.46	1.50
22	C	513	CLA	C3B-CAB	-2.23	1.43	1.47
24	T	101	BCR	C38-C26	-2.23	1.47	1.50
22	b	611	CLA	CMD-C2D	-2.23	1.46	1.51
22	C	502	CLA	CMC-C2C	-2.23	1.46	1.50
30	C	519	DGD	C6E-C5E	2.23	1.59	1.51
22	C	503	CLA	CMD-C2D	-2.23	1.46	1.51
22	b	601	CLA	C1B-NB	2.23	1.37	1.35
22	C	502	CLA	C3B-C2B	-2.23	1.37	1.40
22	B	606	CLA	C1B-NB	2.23	1.37	1.35
22	B	616	CLA	CMD-C2D	-2.23	1.46	1.51
28	d	408	LHG	O6-C4	-2.23	1.36	1.44
22	b	616	CLA	CMD-C2D	-2.22	1.46	1.51
22	d	401	CLA	C1D-C2D	2.22	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	d	403	CLA	C4B-CHC	-2.22	1.34	1.41
24	C	516	BCR	C33-C5	-2.22	1.47	1.50
27	c	520	LMG	O1-C1	2.21	1.44	1.40
28	B	622	LHG	P-O4	-2.21	1.44	1.55
22	b	613	CLA	C3B-C2B	-2.21	1.37	1.40
22	B	613	CLA	MG-NC	2.21	2.11	2.06
30	C	518	DGD	C1E-C2E	2.20	1.58	1.52
30	C	519	DGD	C6D-C5D	2.20	1.58	1.51
22	b	616	CLA	C4B-CHC	-2.20	1.34	1.41
22	B	609	CLA	CHC-C1C	2.20	1.40	1.35
22	b	602	CLA	MG-NA	-2.19	2.01	2.06
24	C	514	BCR	C38-C26	-2.19	1.47	1.50
30	H	102	DGD	C6D-C5D	2.19	1.58	1.51
29	A	413	SQD	O3-C3	-2.19	1.37	1.43
22	b	607	CLA	C1D-C2D	2.18	1.47	1.42
22	b	602	CLA	C1D-C2D	2.18	1.47	1.42
30	c	518	DGD	C4E-C5E	2.18	1.57	1.53
22	C	511	CLA	CMD-C2D	-2.18	1.46	1.51
22	c	512	CLA	MG-NA	2.18	2.11	2.06
22	D	402	CLA	C1C-NC	-2.18	1.34	1.37
22	C	508	CLA	CMC-C2C	-2.17	1.46	1.50
22	c	501	CLA	CHC-C1C	2.17	1.40	1.35
30	C	518	DGD	C6D-C5D	2.17	1.58	1.51
22	C	513	CLA	CMB-C2B	-2.17	1.47	1.51
22	B	606	CLA	C1D-C2D	2.17	1.47	1.42
27	D	407	LMG	C6-C5	2.17	1.59	1.51
22	c	504	CLA	CMB-C2B	-2.17	1.47	1.51
27	c	520	LMG	O2-C2	-2.17	1.37	1.43
24	t	101	BCR	C27-C26	-2.17	1.46	1.51
22	B	601	CLA	C3B-CAB	-2.17	1.43	1.47
35	F	101	HEC	CAD-C3D	2.17	1.55	1.52
23	A	404	PHO	CHC-C4B	-2.16	1.35	1.40
22	A	402	CLA	C4B-CHC	-2.16	1.35	1.41
22	b	616	CLA	CAC-C3C	-2.16	1.45	1.51
22	c	504	CLA	CMC-C2C	-2.16	1.46	1.50
22	c	503	CLA	CMC-C2C	-2.16	1.46	1.50
22	B	601	CLA	CMC-C2C	-2.16	1.46	1.50
27	d	410	LMG	O1-C1	2.15	1.43	1.40
22	c	507	CLA	CHC-C1C	2.15	1.40	1.35
22	d	401	CLA	C4B-CHC	-2.15	1.35	1.41
24	D	405	BCR	C36-C18	-2.15	1.46	1.50
23	d	402	PHO	CMD-C2D	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	518	DGD	O4E-C4E	-2.15	1.37	1.43
24	a	405	BCR	C27-C26	-2.15	1.46	1.51
26	D	406	PL9	C46-C44	-2.15	1.46	1.51
22	c	503	CLA	C3B-C2B	-2.15	1.37	1.40
30	c	518	DGD	O3D-C3D	-2.15	1.37	1.43
22	b	611	CLA	O2D-CGD	2.15	1.38	1.33
22	C	509	CLA	C1D-C2D	2.15	1.47	1.42
22	B	601	CLA	C1D-C2D	2.14	1.47	1.42
22	b	607	CLA	CMB-C2B	-2.14	1.47	1.51
22	b	610	CLA	C1C-NC	-2.14	1.34	1.37
22	C	509	CLA	CMD-C2D	-2.14	1.46	1.51
29	A	414	SQD	C46-C45	2.14	1.55	1.50
22	B	604	CLA	C1B-NB	2.14	1.37	1.35
23	d	402	PHO	C4C-C3C	2.14	1.49	1.45
22	C	512	CLA	C4B-CHC	-2.14	1.35	1.41
22	b	603	CLA	C3B-CAB	-2.14	1.43	1.47
26	A	410	PL9	C3-C4	-2.13	1.46	1.49
26	d	407	PL9	C51-C49	-2.13	1.44	1.50
22	c	505	CLA	C3B-C2B	-2.13	1.37	1.40
22	B	613	CLA	C3B-C2B	-2.13	1.37	1.40
29	B	623	SQD	O4-C4	-2.13	1.38	1.43
22	c	510	CLA	C4B-CHC	-2.13	1.35	1.41
22	c	513	CLA	CMD-C2D	-2.13	1.46	1.51
22	b	605	CLA	C1A-CHA	-2.13	1.34	1.43
22	B	616	CLA	C1D-C2D	2.13	1.47	1.42
22	A	403	CLA	C4C-C3C	2.12	1.48	1.45
22	C	505	CLA	MG-NC	-2.12	2.01	2.06
22	b	606	CLA	C1B-NB	2.12	1.37	1.35
28	e	101	LHG	C24-C23	2.12	1.56	1.50
22	B	616	CLA	CMB-C2B	-2.12	1.47	1.51
22	b	613	CLA	C1D-C2D	2.12	1.47	1.42
22	b	607	CLA	MG-NC	2.12	2.11	2.06
30	h	101	DGD	O2G-C2G	-2.12	1.41	1.46
22	D	404	CLA	C3B-C2B	-2.12	1.37	1.40
22	b	601	CLA	CMC-C2C	-2.12	1.46	1.50
29	A	413	SQD	O6-C44	-2.12	1.39	1.43
22	B	609	CLA	C1D-C2D	2.12	1.47	1.42
22	c	505	CLA	CMC-C2C	-2.11	1.46	1.50
30	C	517	DGD	O3G-C3G	-2.11	1.39	1.43
27	C	520	LMG	O7-C8	-2.11	1.41	1.46
22	c	513	CLA	CMC-C2C	-2.11	1.46	1.50
30	C	519	DGD	C4D-C3D	2.11	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	610	CLA	CHC-C1C	2.11	1.40	1.35
22	C	504	CLA	C4B-CHC	-2.10	1.35	1.41
22	c	501	CLA	MG-NC	-2.10	2.01	2.06
28	e	101	LHG	O8-C23	2.10	1.39	1.33
29	A	413	SQD	O47-C45	-2.10	1.41	1.46
27	c	522	LMG	C1-C2	2.10	1.58	1.52
30	c	517	DGD	O1G-C1G	-2.10	1.40	1.45
22	d	401	CLA	CMD-C2D	-2.10	1.46	1.51
27	M	101	LMG	O3-C3	-2.10	1.38	1.43
22	b	610	CLA	MG-NA	2.09	2.11	2.06
27	D	407	LMG	O7-C10	2.09	1.40	1.34
24	C	515	BCR	C38-C26	-2.09	1.47	1.50
30	H	102	DGD	O5D-C6D	2.09	1.47	1.43
22	B	614	CLA	CMC-C2C	-2.09	1.46	1.50
22	C	505	CLA	CMC-C2C	-2.09	1.46	1.50
22	b	604	CLA	CMB-C2B	-2.08	1.47	1.51
22	D	404	CLA	C1C-NC	-2.08	1.34	1.37
22	c	508	CLA	C4B-CHC	-2.08	1.35	1.41
22	B	604	CLA	C3B-C2B	-2.08	1.37	1.40
30	A	415	DGD	C3D-C2D	2.08	1.57	1.52
22	A	406	CLA	C3B-CAB	-2.08	1.43	1.47
24	k	101	BCR	C36-C18	-2.08	1.46	1.50
26	a	409	PL9	C46-C44	-2.08	1.47	1.51
28	a	410	LHG	O7-C5	-2.08	1.41	1.46
22	b	609	CLA	O2D-CGD	2.08	1.38	1.33
22	b	610	CLA	C1D-C2D	2.07	1.47	1.42
28	l	101	LHG	O7-C5	-2.07	1.41	1.46
29	B	623	SQD	O2-C2	-2.07	1.38	1.43
22	B	613	CLA	C5-C3	-2.07	1.47	1.51
27	b	623	LMG	C7-C8	2.07	1.57	1.50
30	H	102	DGD	O3E-C3E	-2.07	1.38	1.43
22	b	607	CLA	C1B-NB	-2.06	1.33	1.35
22	B	603	CLA	CMD-C2D	-2.06	1.46	1.51
29	a	411	SQD	O3-C3	-2.06	1.38	1.43
22	c	504	CLA	C3B-CAB	-2.06	1.43	1.47
27	c	522	LMG	O7-C8	-2.06	1.41	1.46
27	C	520	LMG	C4-C5	2.06	1.57	1.53
26	d	407	PL9	C46-C44	-2.06	1.47	1.51
22	A	402	CLA	CHC-C1C	2.05	1.40	1.35
30	c	518	DGD	O3G-C1D	-2.05	1.36	1.40
22	A	403	CLA	C3B-C2B	-2.05	1.37	1.40
24	B	618	BCR	C27-C26	-2.05	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	f	102	SQD	O2-C2	-2.05	1.38	1.43
22	c	506	CLA	CMB-C2B	-2.04	1.47	1.51
22	b	606	CLA	C4B-CHC	-2.04	1.35	1.41
23	A	405	PHO	CMD-C2D	-2.04	1.46	1.50
22	b	609	CLA	C3B-C2B	-2.04	1.37	1.40
24	k	101	BCR	C33-C5	-2.04	1.47	1.50
35	F	101	HEC	C1C-CHC	-2.04	1.35	1.41
22	d	401	CLA	CMC-C2C	-2.04	1.46	1.50
22	b	601	CLA	CMD-C2D	-2.04	1.46	1.51
30	c	519	DGD	O3E-C3E	-2.04	1.38	1.43
30	c	517	DGD	O3G-C3G	-2.04	1.40	1.43
24	c	516	BCR	C38-C26	-2.04	1.47	1.50
22	B	607	CLA	CMD-C2D	-2.04	1.46	1.51
28	d	408	LHG	C4-C5	2.03	1.56	1.50
23	d	402	PHO	C4C-NC	2.03	1.41	1.36
22	c	506	CLA	C1D-C2D	2.03	1.47	1.42
22	b	608	CLA	CMD-C2D	-2.03	1.46	1.51
24	B	617	BCR	C38-C26	-2.03	1.47	1.50
24	t	101	BCR	C31-C1	-2.03	1.49	1.53
28	A	412	LHG	C3-C2	2.02	1.58	1.51
22	c	510	CLA	C1D-C2D	2.02	1.47	1.42
22	B	604	CLA	C3C-C2C	2.02	1.41	1.36
22	c	507	CLA	CMB-C2B	-2.02	1.47	1.51
30	C	518	DGD	O6E-C5E	-2.02	1.39	1.44
22	B	615	CLA	C3B-CAB	-2.02	1.43	1.47
22	b	610	CLA	C3B-CAB	-2.02	1.43	1.47
22	C	505	CLA	C4B-CHC	-2.02	1.35	1.41
24	C	515	BCR	C33-C5	-2.02	1.47	1.50
22	B	603	CLA	C1D-C2D	2.02	1.47	1.42
29	D	408	SQD	O4-C4	-2.01	1.38	1.43
22	c	501	CLA	CMC-C2C	-2.01	1.46	1.50
22	C	513	CLA	CMD-C2D	-2.01	1.46	1.51
22	b	602	CLA	C4B-CHC	-2.01	1.35	1.41
22	c	509	CLA	C3B-CAB	-2.01	1.43	1.47
22	c	512	CLA	MG-NC	2.00	2.11	2.06
22	B	602	CLA	C1D-C2D	2.00	1.47	1.42
22	b	603	CLA	O2D-CGD	2.00	1.38	1.33
23	A	404	PHO	C1D-ND	2.00	1.42	1.38
22	B	613	CLA	C1D-C2D	2.00	1.47	1.42
30	C	519	DGD	C1G-C2G	2.00	1.56	1.50
30	c	517	DGD	O3D-C3D	-2.00	1.38	1.43

All (1387) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	503	CLA	C4A-NA-C1A	10.58	111.46	106.71
22	B	604	CLA	C4A-NA-C1A	9.47	110.96	106.71
22	B	611	CLA	C4A-NA-C1A	8.94	110.72	106.71
22	C	507	CLA	C4A-NA-C1A	8.89	110.70	106.71
22	B	601	CLA	C4A-NA-C1A	8.84	110.68	106.71
29	D	408	SQD	O6-C1-C2	8.61	121.75	108.30
29	a	411	SQD	O6-C1-C2	8.58	121.69	108.30
22	b	615	CLA	C4A-NA-C1A	8.46	110.51	106.71
22	C	511	CLA	C4A-NA-C1A	8.11	110.35	106.71
22	b	606	CLA	C4A-NA-C1A	7.96	110.28	106.71
22	B	612	CLA	C4A-NA-C1A	7.85	110.23	106.71
29	f	102	SQD	O7-S-C6	7.64	116.02	106.94
22	C	513	CLA	C4A-NA-C1A	7.58	110.11	106.71
22	B	603	CLA	C4A-NA-C1A	7.54	110.09	106.71
22	c	509	CLA	C4A-NA-C1A	7.52	110.09	106.71
22	b	609	CLA	C4A-NA-C1A	7.38	110.03	106.71
29	A	413	SQD	O7-S-C6	7.34	115.66	106.94
22	B	616	CLA	C4A-NA-C1A	7.27	109.98	106.71
22	B	609	CLA	C4A-NA-C1A	7.26	109.97	106.71
22	C	509	CLA	C4A-NA-C1A	7.16	109.93	106.71
29	b	620	SQD	O6-C1-C2	7.13	119.43	108.30
22	b	601	CLA	C4A-NA-C1A	7.10	109.90	106.71
35	f	101	HEC	CBD-CAD-C3D	-6.77	100.00	112.49
29	B	623	SQD	O6-C1-C2	6.77	118.86	108.30
22	d	403	CLA	C4A-NA-C1A	6.66	109.70	106.71
22	b	614	CLA	C4A-NA-C1A	6.64	109.69	106.71
22	B	606	CLA	C4A-NA-C1A	6.56	109.65	106.71
35	F	101	HEC	CBD-CAD-C3D	-6.52	100.46	112.49
22	b	604	CLA	C4A-NA-C1A	6.50	109.63	106.71
22	C	508	CLA	C4A-NA-C1A	6.47	109.61	106.71
26	d	407	PL9	C7-C3-C4	6.46	122.12	116.88
29	A	413	SQD	O6-C1-C2	6.39	118.28	108.30
22	d	404	CLA	C4A-NA-C1A	6.38	109.58	106.71
22	c	510	CLA	C4A-NA-C1A	6.36	109.57	106.71
22	a	402	CLA	C4A-NA-C1A	6.34	109.56	106.71
29	f	102	SQD	O6-C1-C2	6.33	118.19	108.30
22	b	616	CLA	C4A-NA-C1A	6.32	109.55	106.71
22	d	404	CLA	CMB-C2B-C1B	-6.25	118.86	128.46
22	c	511	CLA	C4A-NA-C1A	6.23	109.51	106.71
29	A	414	SQD	C45-O47-C7	6.00	125.60	117.88
26	a	409	PL9	C7-C3-C4	5.98	121.74	116.88
22	D	403	CLA	C4A-NA-C1A	5.87	109.34	106.71
22	C	505	CLA	C4A-NA-C1A	5.86	109.34	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	502	CLA	C4A-NA-C1A	5.84	109.33	106.71
22	C	508	CLA	C4D-C3D-CAD	-5.83	105.22	108.47
35	F	101	HEC	CMC-C2C-C1C	-5.83	119.51	128.46
29	a	412	SQD	O47-C7-C8	5.68	123.75	111.50
22	d	401	CLA	C4A-NA-C1A	5.64	109.24	106.71
22	C	502	CLA	C4A-NA-C1A	5.61	109.23	106.71
22	c	501	CLA	O2D-CGD-O1D	-5.58	112.93	123.84
22	c	506	CLA	C4A-NA-C1A	5.55	109.20	106.71
22	c	508	CLA	C4A-NA-C1A	5.54	109.19	106.71
22	B	615	CLA	C4A-NA-C1A	5.52	109.19	106.71
22	c	501	CLA	C4A-NA-C1A	5.46	109.16	106.71
22	B	616	CLA	CMB-C2B-C1B	-5.40	120.16	128.46
22	b	603	CLA	CMB-C2B-C1B	-5.40	120.17	128.46
22	b	612	CLA	C4D-C3D-CAD	-5.29	105.52	108.47
22	C	501	CLA	O2D-CGD-O1D	-5.28	113.52	123.84
22	b	606	CLA	O2D-CGD-O1D	-5.17	113.72	123.84
26	d	407	PL9	C40-C39-C41	5.17	123.97	115.27
22	c	505	CLA	C4A-NA-C1A	5.17	109.03	106.71
29	a	412	SQD	O48-C23-O10	-5.12	110.67	123.59
22	B	605	CLA	C4A-NA-C1A	5.09	108.99	106.71
22	A	403	CLA	C4A-NA-C1A	5.08	108.99	106.71
22	D	404	CLA	C4A-NA-C1A	5.06	108.98	106.71
22	a	402	CLA	CMB-C2B-C1B	-5.05	120.71	128.46
22	D	402	CLA	CMD-C2D-C3D	5.04	134.11	124.68
22	B	610	CLA	O2D-CGD-O1D	-4.96	114.14	123.84
22	c	505	CLA	C4D-C3D-CAD	-4.96	105.71	108.47
29	D	408	SQD	O8-S-C6	4.93	113.59	105.74
22	B	616	CLA	CMB-C2B-C3B	4.91	133.86	124.68
22	C	510	CLA	O2D-CGD-O1D	-4.91	114.25	123.84
22	C	501	CLA	C4A-NA-C1A	4.90	108.91	106.71
22	c	503	CLA	C4D-C3D-CAD	-4.89	105.74	108.47
22	B	611	CLA	O2D-CGD-O1D	-4.88	114.30	123.84
22	B	612	CLA	CMB-C2B-C1B	-4.84	121.02	128.46
29	A	413	SQD	C1-C2-C3	-4.84	99.91	110.00
22	b	610	CLA	C4A-NA-C1A	4.83	108.88	106.71
22	b	602	CLA	C4A-NA-C1A	4.81	108.87	106.71
22	b	612	CLA	CMD-C2D-C3D	4.81	133.68	124.68
29	A	413	SQD	O9-S-O7	-4.79	97.37	113.95
22	B	607	CLA	C4A-NA-C1A	4.79	108.86	106.71
22	C	505	CLA	CMB-C2B-C1B	-4.77	121.12	128.46
22	c	504	CLA	C4A-NA-C1A	4.70	108.82	106.71
22	c	507	CLA	CMB-C2B-C1B	-4.67	121.28	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	608	CLA	CMB-C2B-C1B	-4.67	121.29	128.46
22	b	605	CLA	CMB-C2B-C1B	-4.66	121.30	128.46
22	C	501	CLA	O2D-CGD-CBD	4.65	119.53	111.27
27	b	623	LMG	O1-C1-C2	-4.63	101.07	108.30
22	C	508	CLA	OBD-CAD-CBD	-4.63	119.28	125.89
35	V	201	HEC	CBD-CAD-C3D	-4.56	104.08	112.49
22	B	606	CLA	OBD-CAD-CBD	-4.56	119.39	125.89
29	A	413	SQD	C1-O5-C5	-4.55	104.75	113.69
28	A	412	LHG	O4-P-O5	4.53	134.64	112.24
22	B	616	CLA	C4D-C3D-CAD	-4.50	105.96	108.47
22	c	512	CLA	C4A-NA-C1A	4.50	108.73	106.71
22	b	609	CLA	OBD-CAD-CBD	-4.48	119.49	125.89
22	b	605	CLA	O2D-CGD-O1D	-4.48	115.09	123.84
22	b	607	CLA	CMB-C2B-C1B	-4.48	121.58	128.46
22	a	404	CLA	C4A-NA-C1A	4.47	108.72	106.71
22	b	609	CLA	CMB-C2B-C1B	-4.47	121.59	128.46
22	C	512	CLA	C4A-NA-C1A	4.47	108.72	106.71
22	c	504	CLA	CMB-C2B-C1B	-4.44	121.64	128.46
29	b	620	SQD	O7-S-C6	4.43	112.21	106.94
22	c	513	CLA	C4A-NA-C1A	4.43	108.70	106.71
29	f	102	SQD	O9-S-O7	-4.43	98.62	113.95
22	b	614	CLA	CMB-C2B-C1B	-4.43	121.66	128.46
27	b	623	LMG	C1-O6-C5	-4.41	105.04	113.69
22	b	611	CLA	O2D-CGD-CBD	4.40	119.08	111.27
22	A	402	CLA	CMB-C2B-C3B	4.39	132.89	124.68
24	T	101	BCR	C35-C13-C14	-4.38	116.79	122.92
22	C	510	CLA	O2D-CGD-CBD	4.38	119.05	111.27
22	b	615	CLA	CMB-C2B-C1B	-4.38	121.74	128.46
22	b	603	CLA	OBD-CAD-CBD	-4.37	119.65	125.89
22	c	507	CLA	C4A-NA-C1A	4.37	108.67	106.71
22	B	610	CLA	C1B-CHB-C4A	-4.35	121.49	130.12
22	c	507	CLA	CMB-C2B-C3B	4.35	132.81	124.68
22	b	610	CLA	O2D-CGD-O1D	-4.35	115.34	123.84
22	B	608	CLA	O2D-CGD-O1D	-4.33	115.37	123.84
24	Y	101	BCR	C39-C30-C25	-4.33	103.28	110.30
22	b	612	CLA	CHB-C4A-NA	4.32	130.49	124.51
23	d	402	PHO	O1D-CGD-CBD	4.30	133.28	124.48
29	D	408	SQD	C1-O5-C5	-4.30	105.25	113.69
22	C	512	CLA	CMB-C2B-C1B	-4.30	121.86	128.46
22	d	404	CLA	CMB-C2B-C3B	4.29	132.70	124.68
29	A	413	SQD	O47-C7-C8	4.28	120.72	111.50
22	b	608	CLA	CMB-C2B-C3B	4.27	132.66	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	602	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
22	b	602	CLA	CMB-C2B-C3B	4.25	132.64	124.68
29	B	623	SQD	O7-S-C6	4.24	111.98	106.94
22	b	616	CLA	CMB-C2B-C1B	-4.22	121.98	128.46
22	b	607	CLA	C4A-NA-C1A	4.21	108.60	106.71
29	B	623	SQD	C1-O5-C5	-4.20	105.44	113.69
22	C	510	CLA	C4A-NA-C1A	4.19	108.59	106.71
28	a	410	LHG	O8-C23-O10	-4.16	113.09	123.59
29	B	623	SQD	O48-C23-C24	4.16	124.96	111.91
22	c	505	CLA	CMB-C2B-C1B	-4.16	122.08	128.46
28	E	101	LHG	O4-P-O5	4.15	132.78	112.24
22	c	502	CLA	CMB-C2B-C1B	-4.15	122.09	128.46
22	B	612	CLA	CMB-C2B-C3B	4.14	132.43	124.68
22	d	401	CLA	CHB-C4A-NA	4.14	130.24	124.51
22	D	402	CLA	C4A-NA-C1A	4.14	108.57	106.71
30	C	519	DGD	O3G-C3G-C2G	-4.13	100.94	110.90
22	B	614	CLA	C4D-C3D-CAD	-4.12	106.17	108.47
22	b	602	CLA	O2D-CGD-O1D	-4.08	115.85	123.84
22	a	402	CLA	CMB-C2B-C3B	4.08	132.32	124.68
22	d	404	CLA	CMD-C2D-C3D	4.08	132.31	124.68
22	c	509	CLA	CHB-C4A-NA	4.08	130.15	124.51
29	D	408	SQD	O9-S-C6	4.07	111.78	106.94
28	e	101	LHG	O4-P-O5	4.06	132.32	112.24
22	A	403	CLA	CMB-C2B-C1B	-4.05	122.23	128.46
22	b	603	CLA	O2D-CGD-O1D	-4.04	115.94	123.84
22	c	503	CLA	C4A-NA-C1A	4.04	108.52	106.71
22	b	603	CLA	CMB-C2B-C3B	4.03	132.22	124.68
22	D	402	CLA	C4D-C3D-CAD	-4.02	106.23	108.47
22	b	602	CLA	O2D-CGD-CBD	4.02	118.42	111.27
26	a	409	PL9	C35-C34-C36	4.02	122.03	115.27
22	b	609	CLA	C4D-C3D-CAD	-4.02	106.23	108.47
24	b	617	BCR	C2-C1-C6	4.02	116.67	110.48
22	B	602	CLA	O2D-CGD-CBD	4.01	118.40	111.27
30	H	102	DGD	O3G-C3G-C2G	-4.01	101.22	110.90
35	F	101	HEC	CBA-CAA-C2A	-4.01	105.08	112.48
22	c	509	CLA	C4D-C3D-CAD	-4.01	106.23	108.47
22	C	512	CLA	CMB-C2B-C3B	4.01	132.18	124.68
22	c	505	CLA	CMD-C2D-C3D	4.01	132.18	124.68
28	a	410	LHG	O4-P-O5	3.99	131.96	112.24
28	d	409	LHG	O4-P-O5	3.99	131.94	112.24
22	d	405	CLA	CMD-C2D-C3D	3.97	132.10	124.68
28	B	622	LHG	O4-P-O5	3.97	131.85	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	402	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
27	M	101	LMG	O1-C1-C2	-3.95	102.13	108.30
28	d	408	LHG	O4-P-O5	3.95	131.76	112.24
30	C	519	DGD	O6D-C1D-O3G	-3.94	100.64	109.97
26	D	406	PL9	C30-C29-C31	-3.93	108.66	115.27
22	C	509	CLA	CMB-C2B-C3B	3.93	132.03	124.68
22	C	509	CLA	CMB-C2B-C1B	-3.93	122.43	128.46
28	D	409	LHG	O4-P-O5	3.92	131.60	112.24
22	c	510	CLA	CMD-C2D-C3D	3.91	131.99	124.68
22	A	406	CLA	O2D-CGD-O1D	-3.90	116.21	123.84
30	c	519	DGD	C3D-C4D-C5D	-3.89	103.30	110.24
26	a	409	PL9	C7-C3-C2	-3.89	118.19	123.30
22	B	603	CLA	C5-C3-C2	-3.87	113.28	121.12
22	B	614	CLA	O2D-CGD-O1D	-3.87	116.27	123.84
22	c	504	CLA	CMB-C2B-C3B	3.86	131.90	124.68
27	m	101	LMG	O7-C10-O9	-3.86	114.38	123.70
22	b	605	CLA	O1D-CGD-CBD	3.85	132.36	124.48
26	D	406	PL9	C7-C3-C4	3.85	120.00	116.88
22	b	613	CLA	CHB-C4A-NA	3.84	129.82	124.51
22	C	510	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
22	b	606	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
22	b	607	CLA	CMB-C2B-C3B	3.83	131.84	124.68
26	d	407	PL9	C7-C3-C2	-3.83	118.27	123.30
29	f	102	SQD	C1-C2-C3	-3.82	102.03	110.00
26	D	406	PL9	C36-C34-C33	-3.82	113.38	121.12
22	C	504	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
22	C	506	CLA	C4A-NA-C1A	3.81	108.42	106.71
29	B	623	SQD	O8-S-C6	3.81	111.80	105.74
22	B	616	CLA	CMD-C2D-C3D	3.80	131.79	124.68
22	C	508	CLA	CMB-C2B-C1B	-3.79	122.63	128.46
22	c	513	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
22	b	605	CLA	C4-C3-C5	3.79	121.64	115.27
22	b	612	CLA	C1B-CHB-C4A	-3.79	122.62	130.12
22	B	611	CLA	O2D-CGD-CBD	3.79	118.00	111.27
22	c	503	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
22	c	509	CLA	O2A-CGA-O1A	-3.78	114.04	123.59
22	C	503	CLA	C7-C6-C5	-3.78	103.08	113.36
29	b	620	SQD	O9-S-C6	3.78	111.43	106.94
22	C	508	CLA	O2D-CGD-O1D	-3.78	116.46	123.84
22	b	616	CLA	CMB-C2B-C3B	3.77	131.73	124.68
22	C	505	CLA	CMB-C2B-C3B	3.76	131.71	124.68
22	C	513	CLA	O2D-CGD-O1D	-3.75	116.51	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	C	517	DGD	C3D-C4D-C5D	-3.75	103.56	110.24
22	c	504	CLA	CHB-C4A-NA	3.74	129.68	124.51
22	c	509	CLA	CMD-C2D-C3D	3.74	131.67	124.68
22	D	403	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
22	C	508	CLA	CMB-C2B-C3B	3.73	131.66	124.68
22	B	603	CLA	O2D-CGD-O1D	-3.72	116.57	123.84
22	B	603	CLA	C4-C3-C5	3.72	121.52	115.27
28	B	621	LHG	O4-P-O5	3.70	130.56	112.24
22	D	402	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
22	B	606	CLA	OBD-CAD-C3D	3.70	134.12	127.98
28	l	101	LHG	O4-P-O5	3.70	130.51	112.24
22	c	510	CLA	O2D-CGD-O1D	-3.70	116.61	123.84
22	B	610	CLA	C4A-NA-C1A	3.69	108.37	106.71
22	C	507	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
27	a	416	LMG	C1-C2-C3	-3.69	102.31	110.00
29	b	620	SQD	O5-C5-C4	3.69	116.39	109.69
22	c	508	CLA	C4D-C3D-CAD	-3.68	106.42	108.47
22	c	511	CLA	C1D-CHD-C4C	3.68	127.42	122.56
22	C	503	CLA	C1D-CHD-C4C	3.68	127.41	122.56
22	D	402	CLA	CED-O2D-CGD	3.68	124.25	115.94
26	A	410	PL9	C7-C3-C4	3.67	119.86	116.88
29	a	411	SQD	O47-C7-C8	3.67	119.40	111.50
22	b	615	CLA	C11-C10-C8	-3.65	104.11	115.92
22	c	501	CLA	CMB-C2B-C3B	3.65	131.51	124.68
29	D	408	SQD	C1-C2-C3	-3.65	102.40	110.00
22	B	604	CLA	CHB-C4A-NA	3.64	129.54	124.51
22	b	602	CLA	CHB-C4A-NA	3.63	129.53	124.51
28	a	410	LHG	O8-C23-C24	3.63	123.29	111.91
24	B	619	BCR	C2-C1-C6	3.62	116.06	110.48
22	a	404	CLA	OBD-CAD-CBD	-3.61	120.73	125.89
22	b	606	CLA	C4D-C3D-CAD	-3.61	106.46	108.47
22	b	605	CLA	CMB-C2B-C3B	3.60	131.42	124.68
29	A	414	SQD	O48-C23-C24	3.60	123.19	111.91
22	c	507	CLA	C4D-C3D-CAD	-3.59	106.47	108.47
22	b	611	CLA	CMB-C2B-C3B	3.59	131.39	124.68
22	c	506	CLA	CMB-C2B-C1B	-3.58	122.95	128.46
22	C	506	CLA	O2D-CGD-O1D	-3.58	116.83	123.84
35	V	201	HEC	CMC-C2C-C1C	-3.58	122.96	128.46
22	b	613	CLA	C1-C2-C3	-3.58	119.86	126.04
26	D	406	PL9	C35-C34-C36	3.57	121.27	115.27
26	D	406	PL9	C20-C19-C21	3.56	121.25	115.27
22	B	608	CLA	CMB-C2B-C3B	3.56	131.33	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	507	CLA	O2D-CGD-O1D	-3.56	116.89	123.84
22	c	506	CLA	CMD-C2D-C3D	3.55	131.33	124.68
30	c	519	DGD	O3G-C3G-C2G	-3.54	102.35	110.90
22	B	611	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
24	c	515	BCR	C35-C13-C14	-3.54	117.97	122.92
22	C	503	CLA	O1D-CGD-CBD	3.54	131.72	124.48
35	v	201	HEC	CBD-CAD-C3D	-3.53	105.97	112.49
22	a	404	CLA	CMB-C2B-C1B	-3.53	123.03	128.46
30	C	518	DGD	O3G-C3G-C2G	-3.53	102.38	110.90
22	c	506	CLA	CHB-C4A-NA	3.53	129.39	124.51
22	b	606	CLA	CMD-C2D-C3D	3.53	131.28	124.68
23	d	402	PHO	C1-C2-C3	-3.52	119.95	126.04
23	A	405	PHO	O2D-CGD-O1D	-3.52	116.96	123.84
22	a	404	CLA	CMB-C2B-C3B	3.51	131.25	124.68
22	b	604	CLA	OBD-CAD-CBD	-3.51	120.88	125.89
26	D	406	PL9	C27-C28-C29	-3.51	119.21	127.66
29	a	411	SQD	O9-S-C6	3.51	111.11	106.94
22	D	402	CLA	CMB-C2B-C3B	3.51	131.24	124.68
22	c	508	CLA	CMD-C2D-C3D	3.50	131.23	124.68
22	c	513	CLA	O2D-CGD-O1D	-3.50	117.00	123.84
22	d	403	CLA	O2D-CGD-O1D	-3.49	117.01	123.84
22	c	506	CLA	CMB-C2B-C3B	3.49	131.21	124.68
22	C	503	CLA	O2A-C1-C2	-3.49	99.46	108.64
22	c	502	CLA	CMB-C2B-C3B	3.48	131.20	124.68
24	A	407	BCR	C27-C26-C25	3.48	127.79	122.73
22	c	511	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
27	d	410	LMG	O1-C1-C2	-3.48	102.87	108.30
29	b	620	SQD	C3-C4-C5	3.48	116.44	110.24
22	C	512	CLA	OBD-CAD-CBD	-3.48	120.93	125.89
22	c	508	CLA	O2D-CGD-O1D	-3.48	117.04	123.84
22	B	607	CLA	CMB-C2B-C1B	-3.47	123.12	128.46
30	C	517	DGD	O3G-C3G-C2G	-3.47	102.52	110.90
22	d	401	CLA	C4D-C3D-CAD	-3.47	106.53	108.47
22	C	505	CLA	C4D-C3D-CAD	-3.47	106.54	108.47
22	B	601	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
22	b	609	CLA	CMB-C2B-C3B	3.46	131.16	124.68
22	c	512	CLA	C1-C2-C3	-3.46	120.06	126.04
22	B	602	CLA	CMD-C2D-C3D	3.46	131.15	124.68
22	c	501	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
35	v	201	HEC	CMC-C2C-C1C	-3.45	123.17	128.46
24	b	619	BCR	C29-C30-C25	3.45	115.79	110.48
22	A	403	CLA	CED-O2D-CGD	-3.44	108.14	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	614	CLA	O2A-CGA-O1A	-3.44	114.92	123.59
22	c	501	CLA	O2D-CGD-CBD	3.43	117.37	111.27
22	d	403	CLA	O2D-CGD-CBD	3.43	117.36	111.27
22	b	603	CLA	C1B-CHB-C4A	-3.43	123.33	130.12
22	b	610	CLA	O1D-CGD-CBD	3.43	131.50	124.48
29	a	411	SQD	C1-C2-C3	-3.43	102.86	110.00
22	B	608	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
22	C	505	CLA	C1D-CHD-C4C	3.42	127.06	122.56
22	D	403	CLA	CMD-C2D-C3D	3.41	131.06	124.68
29	a	411	SQD	C1-O5-C5	-3.41	107.00	113.69
26	d	407	PL9	C37-C38-C39	-3.41	119.46	127.66
22	C	510	CLA	CMB-C2B-C3B	3.41	131.05	124.68
22	B	606	CLA	C1D-CHD-C4C	3.40	127.05	122.56
22	c	508	CLA	CHB-C4A-NA	3.40	129.22	124.51
22	C	512	CLA	C1-C2-C3	-3.40	120.16	126.04
29	b	620	SQD	C1-C2-C3	-3.40	102.92	110.00
30	A	415	DGD	C4E-C3E-C2E	-3.40	104.89	110.82
24	c	514	BCR	C33-C5-C6	-3.39	120.72	124.53
22	b	604	CLA	C1D-CHD-C4C	3.39	127.04	122.56
22	B	612	CLA	C4D-C3D-CAD	-3.39	106.58	108.47
22	c	503	CLA	C7-C6-C5	-3.39	104.16	113.36
26	D	406	PL9	C42-C43-C44	-3.37	119.54	127.66
26	A	410	PL9	C20-C19-C21	3.37	120.93	115.27
22	A	406	CLA	C4-C3-C5	3.36	120.92	115.27
22	b	615	CLA	O2D-CGD-CBD	3.35	117.23	111.27
22	c	512	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
22	B	610	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
22	b	611	CLA	O2D-CGD-O1D	-3.34	117.30	123.84
29	b	620	SQD	O8-S-C6	3.34	111.06	105.74
22	b	616	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
22	C	506	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
35	v	201	HEC	CMB-C2B-C1B	-3.34	123.33	128.46
22	b	603	CLA	O2D-CGD-CBD	3.33	117.19	111.27
22	A	406	CLA	C1B-CHB-C4A	-3.33	123.52	130.12
22	b	605	CLA	C4D-C3D-CAD	-3.33	106.61	108.47
22	C	505	CLA	CMD-C2D-C3D	3.33	130.90	124.68
22	b	611	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
22	b	610	CLA	O2A-CGA-O1A	-3.32	115.21	123.59
22	B	615	CLA	C1B-CHB-C4A	-3.31	123.55	130.12
22	c	503	CLA	CMD-C2D-C3D	3.31	130.88	124.68
22	c	506	CLA	OBD-CAD-C3D	3.31	133.47	127.98
22	A	403	CLA	CMB-C2B-C3B	3.31	130.86	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	514	BCR	C33-C5-C6	-3.29	120.83	124.53
22	b	614	CLA	CMB-C2B-C3B	3.28	130.82	124.68
22	d	405	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
22	b	612	CLA	CAC-C3C-C4C	3.28	129.07	124.81
24	B	618	BCR	C35-C13-C14	-3.28	118.33	122.92
22	b	610	CLA	CAC-C3C-C4C	3.28	129.06	124.81
22	A	406	CLA	O2D-CGD-CBD	3.27	117.08	111.27
24	C	514	BCR	C2-C1-C6	3.27	115.52	110.48
22	d	403	CLA	CMD-C2D-C3D	3.27	130.79	124.68
30	h	101	DGD	O3G-C3G-C2G	-3.26	103.03	110.90
22	B	604	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
22	b	602	CLA	C1B-CHB-C4A	-3.26	123.66	130.12
29	f	102	SQD	O9-S-C6	3.26	110.81	106.94
26	a	409	PL9	C36-C34-C33	-3.25	114.54	121.12
23	A	405	PHO	CAC-C3C-C4C	-3.24	121.69	125.22
22	c	502	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
29	a	411	SQD	O8-S-C6	3.24	110.90	105.74
27	M	101	LMG	C1-O6-C5	-3.24	107.33	113.69
22	c	510	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
22	b	602	CLA	CMD-C2D-C3D	3.23	130.73	124.68
22	b	616	CLA	CMD-C2D-C3D	3.23	130.73	124.68
26	A	410	PL9	O1-C4-C3	-3.23	117.16	120.72
26	A	410	PL9	C36-C34-C33	-3.23	114.58	121.12
22	C	504	CLA	C4-C3-C5	3.23	120.70	115.27
24	c	515	BCR	C27-C26-C25	3.23	127.42	122.73
22	C	510	CLA	CMD-C2D-C3D	3.23	130.72	124.68
27	A	411	LMG	O6-C1-O1	-3.22	102.34	109.97
22	c	503	CLA	OBD-CAD-CBD	-3.22	121.29	125.89
22	c	501	CLA	CMD-C2D-C3D	3.22	130.70	124.68
22	A	402	CLA	C1B-CHB-C4A	-3.22	123.75	130.12
29	D	408	SQD	O48-C23-C24	3.21	121.99	111.91
27	b	623	LMG	O2-C2-C1	-3.21	102.25	110.05
22	b	604	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
22	B	603	CLA	CMD-C2D-C3D	3.21	130.68	124.68
22	C	504	CLA	O2A-CGA-O1A	-3.20	115.51	123.59
22	B	611	CLA	CMB-C2B-C3B	3.20	130.66	124.68
22	d	405	CLA	CMB-C2B-C3B	3.19	130.66	124.68
22	b	613	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
22	b	606	CLA	OBD-CAD-CBD	-3.19	121.34	125.89
22	B	602	CLA	C4A-NA-C1A	3.18	108.14	106.71
22	c	506	CLA	OBD-CAD-CBD	-3.18	121.36	125.89
26	d	407	PL9	C42-C43-C44	-3.18	120.02	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	620	SQD	O48-C23-C24	3.17	121.87	111.91
29	a	411	SQD	O9-S-O7	-3.17	102.97	113.95
24	H	101	BCR	C16-C15-C14	-3.17	116.98	123.47
30	C	518	DGD	O6D-C1D-O3G	-3.17	102.47	109.97
24	b	617	BCR	C27-C26-C25	3.16	127.33	122.73
22	a	404	CLA	C1B-CHB-C4A	-3.16	123.86	130.12
24	C	515	BCR	C15-C16-C17	-3.16	117.00	123.47
28	e	101	LHG	O8-C23-C24	3.16	121.82	111.91
24	T	101	BCR	C38-C26-C27	-3.16	107.55	113.62
30	C	517	DGD	O5D-C6D-C5D	-3.16	103.21	109.05
30	H	102	DGD	C1E-O6E-C5E	3.15	119.88	113.69
22	b	606	CLA	O2D-CGD-CBD	3.15	116.87	111.27
24	C	514	BCR	C11-C10-C9	-3.15	122.82	127.31
35	F	101	HEC	CMB-C2B-C1B	-3.14	123.64	128.46
22	b	614	CLA	OBD-CAD-CBD	-3.14	121.41	125.89
22	C	502	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
29	f	102	SQD	O47-C7-C8	3.13	119.54	110.80
22	B	613	CLA	C1-C2-C3	-3.13	120.63	126.04
22	c	513	CLA	CMB-C2B-C3B	3.13	130.53	124.68
30	c	517	DGD	O3G-C3G-C2G	-3.12	103.36	110.90
24	t	101	BCR	C7-C8-C9	-3.12	121.52	126.23
24	A	407	BCR	C35-C13-C14	-3.11	118.56	122.92
24	c	515	BCR	C33-C5-C6	-3.11	121.03	124.53
23	d	402	PHO	O2D-CGD-O1D	-3.11	117.76	123.84
30	C	517	DGD	O6D-C1D-O3G	-3.11	102.61	109.97
22	B	611	CLA	CMD-C2D-C3D	3.11	130.49	124.68
22	B	611	CLA	OBD-CAD-CBD	-3.11	121.46	125.89
22	B	611	CLA	C11-C12-C13	-3.11	105.88	115.92
30	C	518	DGD	O5D-C6D-C5D	-3.11	103.30	109.05
22	c	511	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
28	d	409	LHG	C26-C25-C24	3.10	124.33	113.19
22	C	504	CLA	C4A-NA-C1A	3.10	108.10	106.71
22	d	401	CLA	CAC-C3C-C4C	3.09	128.82	124.81
22	C	512	CLA	CMD-C2D-C3D	3.09	130.46	124.68
22	D	404	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
27	m	101	LMG	O1-C7-C8	-3.09	103.45	110.90
22	B	604	CLA	CMB-C2B-C3B	3.09	130.46	124.68
24	d	406	BCR	C38-C26-C25	-3.09	121.06	124.53
22	b	601	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
22	b	602	CLA	C4D-C3D-CAD	-3.08	106.75	108.47
22	A	402	CLA	CHB-C4A-NA	3.07	128.76	124.51
22	b	606	CLA	CMB-C2B-C3B	3.07	130.42	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	f	101	HEC	C1D-C2D-C3D	-3.07	104.86	107.00
22	C	511	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
22	D	403	CLA	CMB-C2B-C3B	3.06	130.40	124.68
22	A	403	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
27	m	101	LMG	O3-C3-C2	-3.05	103.30	110.35
22	B	602	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
22	b	605	CLA	OBD-CAD-CBD	-3.05	121.54	125.89
22	b	604	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
29	b	620	SQD	O9-S-O7	-3.04	103.42	113.95
22	c	508	CLA	O2D-CGD-CBD	3.04	116.67	111.27
22	B	609	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
22	D	404	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
29	B	623	SQD	C3-C4-C5	3.04	115.66	110.24
24	T	101	BCR	C7-C8-C9	-3.04	121.64	126.23
22	B	610	CLA	O2A-CGA-O1A	-3.03	115.93	123.59
22	c	506	CLA	CBC-CAC-C3C	-3.03	104.06	112.43
23	A	404	PHO	CBD-CHA-C4D	-3.03	105.12	108.54
22	C	501	CLA	OBD-CAD-CBD	-3.03	121.56	125.89
35	f	101	HEC	CMC-C2C-C1C	-3.03	123.80	128.46
22	c	505	CLA	CMB-C2B-C3B	3.03	130.35	124.68
26	A	410	PL9	C22-C23-C24	-3.03	120.36	127.66
22	C	512	CLA	C1B-CHB-C4A	-3.03	124.11	130.12
22	C	503	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
24	c	516	BCR	C29-C30-C25	3.03	115.14	110.48
30	H	102	DGD	C3E-C4E-C5E	-3.02	104.85	110.24
22	b	605	CLA	CMD-C2D-C3D	3.02	130.33	124.68
22	d	401	CLA	OBD-CAD-CBD	-3.02	121.58	125.89
24	b	618	BCR	C15-C14-C13	-3.02	123.00	127.31
22	B	614	CLA	C4A-NA-C1A	3.02	108.06	106.71
30	c	518	DGD	O3G-C1D-C2D	-3.02	103.59	108.30
22	B	603	CLA	O2A-CGA-O1A	-3.01	115.99	123.59
35	v	201	HEC	C1D-C2D-C3D	-3.01	104.90	107.00
24	A	407	BCR	C2-C1-C6	3.01	115.11	110.48
22	c	501	CLA	CED-O2D-CGD	-3.00	109.14	115.94
27	d	410	LMG	O2-C2-C1	-3.00	102.75	110.05
24	Y	101	BCR	C30-C25-C26	-3.00	118.39	122.61
22	d	404	CLA	CHB-C4A-NA	3.00	128.65	124.51
22	C	507	CLA	CMB-C2B-C3B	2.99	130.28	124.68
22	c	511	CLA	OBD-CAD-CBD	-2.99	121.62	125.89
22	B	605	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
24	B	617	BCR	C2-C1-C6	2.99	115.08	110.48
27	C	520	LMG	O6-C1-O1	-2.98	102.91	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	407	BCR	C37-C22-C21	-2.97	118.76	122.92
22	C	504	CLA	CMB-C2B-C3B	2.97	130.24	124.68
22	B	614	CLA	CMD-C2D-C3D	2.97	130.24	124.68
27	m	101	LMG	C1-O6-C5	-2.97	107.85	113.69
22	B	611	CLA	CHB-C4A-NA	2.97	128.62	124.51
22	c	503	CLA	CMB-C2B-C3B	2.96	130.22	124.68
22	B	615	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
22	b	615	CLA	CHB-C4A-NA	2.96	128.61	124.51
22	b	612	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
22	B	603	CLA	C4D-C3D-CAD	-2.96	106.82	108.47
29	A	414	SQD	O47-C45-C46	2.96	112.99	106.13
22	d	401	CLA	CMD-C2D-C3D	2.96	130.21	124.68
22	B	605	CLA	CMB-C2B-C3B	2.96	130.21	124.68
22	b	614	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
22	B	603	CLA	CMB-C2B-C1B	-2.95	123.92	128.46
22	d	404	CLA	O2D-CGD-CBD	2.95	116.51	111.27
27	b	623	LMG	O6-C5-C6	2.95	113.77	106.44
22	B	614	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
30	c	518	DGD	O3G-C3G-C2G	-2.95	103.78	110.90
22	b	609	CLA	OBD-CAD-C3D	2.94	132.86	127.98
27	a	416	LMG	C9-C8-C7	-2.93	104.85	111.79
35	V	201	HEC	CMB-C2B-C1B	-2.93	123.96	128.46
22	A	406	CLA	CMB-C2B-C3B	2.93	130.15	124.68
29	A	413	SQD	O47-C7-O49	-2.92	116.64	123.70
28	a	410	LHG	C11-C10-C9	-2.92	99.59	114.42
22	C	509	CLA	CED-O2D-CGD	2.91	122.53	115.94
22	b	616	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
22	B	614	CLA	C1D-CHD-C4C	2.90	126.39	122.56
22	b	614	CLA	OBD-CAD-C3D	2.90	132.80	127.98
24	T	101	BCR	C27-C26-C25	2.90	126.95	122.73
22	b	616	CLA	CHB-C4A-NA	2.90	128.52	124.51
22	B	605	CLA	CMB-C2B-C1B	-2.90	124.01	128.46
22	B	614	CLA	O1D-CGD-CBD	2.90	130.41	124.48
22	C	503	CLA	CMB-C2B-C1B	-2.90	124.01	128.46
27	a	416	LMG	O7-C10-O9	-2.90	116.70	123.70
28	B	622	LHG	O8-C23-O10	-2.90	116.28	123.59
27	D	407	LMG	O6-C1-O1	-2.90	103.11	109.97
24	Y	101	BCR	C27-C26-C25	2.90	126.94	122.73
22	C	506	CLA	O1D-CGD-CBD	2.90	130.41	124.48
30	H	102	DGD	CDB-CCB-CBB	-2.89	99.73	114.42
22	B	612	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
27	m	101	LMG	C38-C37-C36	-2.89	99.74	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	509	CLA	CHB-C4A-NA	2.89	128.51	124.51
22	C	513	CLA	O2A-CGA-O1A	-2.89	116.30	123.59
22	B	606	CLA	CHA-C1A-NA	-2.88	119.79	126.40
24	d	406	BCR	C3-C4-C5	-2.88	108.93	114.08
28	B	622	LHG	O8-C23-C24	2.88	120.95	111.91
27	M	101	LMG	O3-C3-C2	-2.88	103.69	110.35
22	c	512	CLA	CMD-C2D-C3D	2.87	130.05	124.68
22	c	507	CLA	C4-C3-C5	2.87	120.10	115.27
29	B	623	SQD	O5-C5-C4	2.87	114.91	109.69
22	b	611	CLA	C4A-NA-C1A	2.87	108.00	106.71
22	c	512	CLA	CMB-C2B-C1B	-2.87	124.06	128.46
24	B	619	BCR	C3-C4-C5	-2.87	108.96	114.08
23	A	405	PHO	O1D-CGD-CBD	2.86	130.35	124.48
22	b	610	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
24	d	406	BCR	C2-C1-C6	2.86	114.88	110.48
22	B	616	CLA	O2A-CGA-O1A	-2.86	116.38	123.59
24	k	101	BCR	C33-C5-C6	-2.86	121.32	124.53
22	B	615	CLA	CAC-C3C-C4C	2.85	128.51	124.81
22	b	615	CLA	CMB-C2B-C3B	2.85	130.02	124.68
22	b	614	CLA	C1D-CHD-C4C	2.85	126.32	122.56
22	c	505	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
22	b	602	CLA	CHC-C1C-NC	2.85	128.53	124.20
22	D	403	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
22	B	605	CLA	CHB-C4A-NA	2.85	128.46	124.51
22	B	603	CLA	CHD-C4C-NC	2.85	128.70	124.20
22	B	610	CLA	CMB-C2B-C3B	2.85	130.00	124.68
24	b	617	BCR	C29-C30-C25	2.84	114.86	110.48
22	C	512	CLA	CHB-C4A-NA	2.84	128.44	124.51
22	B	606	CLA	C4-C3-C5	2.84	120.05	115.27
22	B	607	CLA	CMB-C2B-C3B	2.84	129.99	124.68
28	l	101	LHG	C20-C19-C18	-2.84	100.00	114.42
24	H	101	BCR	C29-C30-C25	2.84	114.85	110.48
22	a	404	CLA	O2D-CGD-CBD	2.84	116.31	111.27
35	F	101	HEC	CAD-CBD-CGD	2.84	117.43	112.67
22	c	512	CLA	CMB-C2B-C3B	2.84	129.98	124.68
22	c	504	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
22	A	402	CLA	CMD-C2D-C3D	2.83	129.98	124.68
22	b	604	CLA	CMD-C2D-C3D	2.83	129.98	124.68
35	v	201	HEC	CBA-CAA-C2A	-2.83	107.26	112.48
22	d	401	CLA	CHC-C1C-NC	2.83	128.50	124.20
22	b	604	CLA	O2A-CGA-O1A	-2.83	116.45	123.59
22	d	405	CLA	OBD-CAD-CBD	-2.83	121.85	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	623	LMG	C3-C4-C5	-2.83	105.19	110.24
27	M	101	LMG	C31-C30-C29	-2.83	103.03	113.19
22	c	507	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
22	A	406	CLA	CMB-C2B-C1B	-2.83	124.12	128.46
22	a	404	CLA	CHB-C4A-NA	2.83	128.42	124.51
22	C	513	CLA	CMB-C2B-C3B	2.82	129.96	124.68
22	c	509	CLA	CMB-C2B-C1B	-2.81	124.14	128.46
22	b	613	CLA	C7-C6-C5	-2.81	105.73	113.36
22	C	513	CLA	CHB-C4A-NA	2.81	128.40	124.51
27	c	522	LMG	O3-C3-C2	-2.81	103.86	110.35
22	b	609	CLA	O2A-CGA-O1A	-2.80	116.53	123.59
27	A	411	LMG	O3-C3-C2	-2.80	103.88	110.35
22	a	402	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
27	c	523	LMG	O6-C1-O1	-2.80	103.35	109.97
22	b	612	CLA	CMB-C2B-C3B	2.80	129.91	124.68
23	d	402	PHO	C1B-NB-C4B	2.80	111.78	106.51
22	d	401	CLA	CMA-C3A-C4A	-2.79	104.27	111.77
22	b	614	CLA	CAC-C3C-C4C	2.79	128.43	124.81
22	c	509	CLA	CMB-C2B-C3B	2.79	129.90	124.68
22	B	602	CLA	CMB-C2B-C1B	-2.79	124.18	128.46
30	h	101	DGD	O6E-C5E-C4E	2.79	114.76	109.69
24	D	405	BCR	C24-C23-C22	-2.78	122.03	126.23
24	b	618	BCR	C35-C13-C14	-2.78	119.03	122.92
30	c	517	DGD	C8B-C7B-C6B	-2.78	100.33	114.42
22	c	510	CLA	OBD-CAD-CBD	-2.78	121.93	125.89
22	C	508	CLA	C1D-CHD-C4C	2.77	126.22	122.56
22	b	604	CLA	CMB-C2B-C3B	2.77	129.86	124.68
22	B	605	CLA	C1D-CHD-C4C	2.77	126.22	122.56
22	B	609	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
22	B	612	CLA	C11-C12-C13	-2.77	106.98	115.92
22	c	510	CLA	C4D-C3D-CAD	-2.77	106.93	108.47
22	b	610	CLA	C2A-C1A-CHA	2.76	128.69	123.86
22	b	607	CLA	C1-O2A-CGA	2.76	123.68	116.44
28	l	101	LHG	C11-C10-C9	-2.76	100.43	114.42
22	c	511	CLA	O2D-CGD-CBD	2.76	116.17	111.27
22	a	404	CLA	CMD-C2D-C3D	2.76	129.84	124.68
22	b	603	CLA	OBD-CAD-C3D	2.76	132.56	127.98
22	C	507	CLA	O2D-CGD-CBD	2.75	116.16	111.27
29	B	623	SQD	O48-C23-O10	-2.75	116.64	123.59
30	C	518	DGD	C6D-O5D-C1E	2.75	119.11	113.74
22	c	505	CLA	C1D-CHD-C4C	2.75	126.19	122.56
24	a	405	BCR	C29-C30-C25	2.75	114.71	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	504	CLA	C1D-CHD-C4C	2.74	126.18	122.56
22	C	513	CLA	CMB-C2B-C1B	-2.74	124.25	128.46
22	b	601	CLA	CMB-C2B-C1B	-2.74	124.25	128.46
22	b	610	CLA	C2C-C1C-NC	2.74	112.54	109.97
22	B	612	CLA	C1D-CHD-C4C	2.74	126.17	122.56
24	C	514	BCR	C15-C16-C17	-2.74	117.86	123.47
22	C	506	CLA	CMB-C2B-C3B	2.74	129.80	124.68
22	A	402	CLA	C4D-C3D-CAD	-2.73	106.94	108.47
22	B	602	CLA	C1B-CHB-C4A	-2.73	124.70	130.12
27	a	416	LMG	C1-O6-C5	-2.73	108.32	113.69
22	b	604	CLA	OBD-CAD-C3D	2.73	132.52	127.98
22	c	507	CLA	CHB-C4A-NA	2.73	128.29	124.51
22	b	610	CLA	C4D-C3D-CAD	-2.73	106.95	108.47
22	C	505	CLA	OBD-CAD-CBD	-2.73	121.99	125.89
22	b	612	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
24	D	405	BCR	C3-C4-C5	-2.73	109.20	114.08
22	c	501	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
26	D	406	PL9	C40-C39-C38	-2.73	116.68	123.68
22	b	610	CLA	CHB-C4A-NA	2.73	128.28	124.51
28	E	101	LHG	O8-C23-C24	2.73	120.46	111.91
22	C	505	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
22	A	403	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
22	B	610	CLA	O2D-CGD-CBD	2.73	116.11	111.27
30	A	415	DGD	CDB-CCB-CBB	-2.72	100.59	114.42
22	b	609	CLA	CMD-C2D-C3D	2.72	129.77	124.68
22	B	601	CLA	CMD-C2D-C3D	2.72	129.77	124.68
26	a	409	PL9	C20-C19-C21	2.72	119.85	115.27
23	A	405	PHO	C1B-NB-C4B	2.72	111.63	106.51
22	B	605	CLA	OBD-CAD-CBD	-2.72	122.01	125.89
26	d	407	PL9	C20-C19-C21	2.72	119.84	115.27
22	d	403	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
22	d	405	CLA	C4D-C3D-CAD	-2.71	106.96	108.47
22	d	403	CLA	C4-C3-C5	2.71	119.83	115.27
29	a	412	SQD	O49-C7-C8	-2.71	113.16	123.73
22	c	512	CLA	C4D-C3D-CAD	-2.71	106.96	108.47
26	d	407	PL9	C22-C23-C24	-2.70	121.15	127.66
22	B	603	CLA	OBD-CAD-CBD	-2.70	122.03	125.89
24	H	101	BCR	C2-C1-C6	2.70	114.64	110.48
29	b	620	SQD	O2-C2-C1	2.70	116.60	110.05
22	C	501	CLA	CMB-C2B-C1B	-2.69	124.32	128.46
27	a	416	LMG	C7-O1-C1	2.69	119.00	113.74
24	b	618	BCR	C37-C22-C21	-2.69	119.15	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	618	BCR	C29-C30-C25	2.69	114.62	110.48
24	C	515	BCR	C36-C18-C17	-2.69	119.16	122.92
22	c	507	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
22	C	508	CLA	CHB-C4A-NA	2.69	128.23	124.51
22	c	511	CLA	C4D-C3D-CAD	-2.69	106.97	108.47
22	a	404	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
30	C	519	DGD	CDB-CCB-CBB	-2.68	100.84	114.42
22	c	510	CLA	O2A-CGA-O1A	-2.68	116.84	123.59
27	c	520	LMG	C1-O6-C5	-2.68	108.44	113.69
22	B	606	CLA	CGD-CBD-CAD	-2.67	102.07	110.73
22	B	604	CLA	OBD-CAD-CBD	-2.67	122.07	125.89
24	H	101	BCR	C37-C22-C21	-2.67	119.19	122.92
22	c	501	CLA	CHB-C4A-NA	2.67	128.20	124.51
30	c	518	DGD	CBB-CAB-C9B	-2.67	100.89	114.42
30	C	517	DGD	C6B-C5B-C4B	-2.66	100.90	114.42
22	C	513	CLA	CMD-C2D-C3D	2.66	129.66	124.68
26	A	410	PL9	C40-C39-C41	2.66	119.75	115.27
26	d	407	PL9	C36-C34-C33	-2.66	115.73	121.12
22	B	601	CLA	O2A-CGA-O1A	-2.66	116.88	123.59
22	c	513	CLA	CHB-C4A-NA	2.66	128.19	124.51
22	d	403	CLA	CHB-C4A-NA	2.65	128.18	124.51
22	c	512	CLA	CHB-C4A-NA	2.65	128.18	124.51
22	B	614	CLA	CMB-C2B-C3B	2.65	129.64	124.68
22	B	614	CLA	C4-C3-C5	2.65	119.73	115.27
29	a	411	SQD	O48-C23-C24	2.65	120.22	111.91
22	B	605	CLA	C7-C6-C5	-2.65	106.16	113.36
22	b	604	CLA	C11-C12-C13	-2.65	107.36	115.92
22	d	404	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
22	B	613	CLA	CHA-C1A-NA	-2.65	120.33	126.40
24	b	619	BCR	C7-C8-C9	-2.65	122.23	126.23
22	B	609	CLA	CMB-C2B-C3B	2.65	129.63	124.68
22	d	404	CLA	C1B-CHB-C4A	-2.64	124.88	130.12
22	b	610	CLA	CHA-C1A-NA	-2.64	120.35	126.40
22	b	603	CLA	O2A-C1-C2	-2.64	101.69	108.64
22	C	506	CLA	CMD-C2D-C3D	2.64	129.62	124.68
24	C	514	BCR	C27-C26-C25	2.64	126.56	122.73
24	H	101	BCR	C27-C26-C25	2.64	126.56	122.73
22	c	502	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
30	C	518	DGD	C3E-C4E-C5E	-2.64	105.53	110.24
22	D	403	CLA	C17-C16-C15	-2.64	101.12	113.24
26	a	409	PL9	C25-C24-C26	2.64	119.71	115.27
22	B	606	CLA	C1-C2-C3	-2.64	121.48	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	409	PL9	C37-C38-C39	-2.63	121.32	127.66
24	B	619	BCR	C29-C30-C25	2.63	114.53	110.48
27	m	101	LMG	O6-C1-O1	-2.63	103.74	109.97
22	c	509	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
29	a	412	SQD	C46-O48-C23	2.63	126.86	117.12
23	a	403	PHO	O2A-CGA-O1A	-2.63	116.96	123.59
22	b	601	CLA	CHB-C4A-NA	2.63	128.15	124.51
24	x	101	BCR	C35-C13-C14	-2.63	119.24	122.92
22	b	608	CLA	C1B-CHB-C4A	-2.63	124.92	130.12
22	c	508	CLA	CMB-C2B-C3B	2.63	129.59	124.68
30	c	518	DGD	O2D-C2D-C1D	-2.62	103.67	110.05
29	B	623	SQD	O9-S-C6	-2.62	103.82	106.94
22	B	608	CLA	C4A-NA-C1A	2.62	107.89	106.71
22	d	401	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
35	v	201	HEC	CMD-C2D-C3D	2.62	129.88	124.94
27	c	520	LMG	C3-C4-C5	-2.62	105.57	110.24
22	d	404	CLA	C1D-CHD-C4C	2.61	126.01	122.56
22	C	503	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
22	B	604	CLA	O2A-C1-C2	2.61	115.50	108.64
22	B	613	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
30	c	519	DGD	O6D-C1D-O3G	-2.61	103.80	109.97
27	c	522	LMG	O6-C1-O1	-2.61	103.80	109.97
29	a	411	SQD	O7-S-C6	2.61	110.04	106.94
26	D	406	PL9	C22-C23-C24	-2.60	121.39	127.66
28	l	101	LHG	C18-C17-C16	-2.60	101.20	114.42
24	x	101	BCR	C38-C26-C25	-2.60	121.61	124.53
22	B	603	CLA	CHC-C1C-NC	2.60	128.15	124.20
22	C	507	CLA	CHB-C4A-NA	2.60	128.11	124.51
30	C	517	DGD	CDB-CCB-CBB	-2.60	101.22	114.42
22	b	611	CLA	C1D-CHD-C4C	2.60	125.99	122.56
22	B	603	CLA	CMB-C2B-C3B	2.60	129.54	124.68
22	B	604	CLA	C1D-CHD-C4C	2.60	125.99	122.56
29	B	623	SQD	O9-S-O7	-2.60	104.96	113.95
22	d	403	CLA	CMB-C2B-C1B	-2.60	124.47	128.46
35	V	201	HEC	C1D-C2D-C3D	-2.60	105.19	107.00
24	b	619	BCR	C27-C26-C25	2.60	126.50	122.73
22	B	602	CLA	O2A-CGA-O1A	-2.60	117.04	123.59
22	A	406	CLA	CAA-CBA-CGA	-2.60	105.67	113.25
22	A	406	CLA	CHB-C4A-NA	2.59	128.10	124.51
22	B	604	CLA	O2A-CGA-O1A	-2.59	117.05	123.59
22	B	614	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
22	B	615	CLA	CMB-C2B-C3B	2.58	129.51	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	615	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
22	b	604	CLA	CAC-C3C-C4C	2.58	128.16	124.81
30	A	415	DGD	C3G-C2G-C1G	-2.58	105.68	111.79
26	D	406	PL9	C37-C38-C39	-2.58	121.44	127.66
30	c	517	DGD	O6E-C5E-C4E	2.58	114.38	109.69
22	b	609	CLA	C1D-CHD-C4C	2.57	125.96	122.56
24	t	101	BCR	C15-C16-C17	-2.57	118.20	123.47
22	b	612	CLA	O2A-C1-C2	-2.57	101.87	108.64
22	B	610	CLA	O1D-CGD-CBD	2.57	129.75	124.48
22	A	402	CLA	C4A-NA-C1A	2.57	107.86	106.71
22	b	614	CLA	C4-C3-C5	2.57	119.60	115.27
24	d	406	BCR	C24-C23-C22	-2.57	122.35	126.23
22	d	405	CLA	C1-C2-C3	-2.57	121.59	126.04
30	h	101	DGD	O2D-C2D-C1D	-2.57	103.80	110.05
24	c	514	BCR	C7-C8-C9	-2.57	122.35	126.23
27	c	523	LMG	C38-C37-C36	-2.57	101.40	114.42
22	C	512	CLA	OBD-CAD-C3D	2.56	132.24	127.98
24	b	617	BCR	C15-C16-C17	-2.56	118.22	123.47
22	C	506	CLA	CHB-C4A-NA	2.56	128.06	124.51
27	C	520	LMG	O1-C7-C8	-2.56	104.71	110.90
22	b	604	CLA	CMA-C3A-C4A	2.56	118.66	111.77
22	c	507	CLA	O2A-CGA-O1A	-2.56	117.12	123.59
22	b	615	CLA	C1-O2A-CGA	2.56	123.16	116.44
22	C	503	CLA	CMB-C2B-C3B	2.56	129.47	124.68
22	C	510	CLA	C11-C10-C8	-2.56	107.65	115.92
27	D	407	LMG	O2-C2-C1	-2.56	103.84	110.05
22	c	511	CLA	CMB-C2B-C3B	2.56	129.46	124.68
26	d	407	PL9	C7-C8-C9	-2.55	122.54	126.79
22	c	511	CLA	CMD-C2D-C3D	2.55	129.45	124.68
22	C	508	CLA	OBD-CAD-C3D	2.55	132.22	127.98
24	c	514	BCR	C24-C23-C22	-2.55	122.38	126.23
22	C	509	CLA	C1-C2-C3	-2.55	121.64	126.04
27	A	411	LMG	C1-O6-C5	-2.54	108.70	113.69
24	c	515	BCR	C34-C9-C10	-2.54	119.36	122.92
22	b	610	CLA	OBD-CAD-CBD	-2.54	122.27	125.89
22	B	611	CLA	C9-C8-C10	-2.54	102.10	111.29
29	B	623	SQD	O47-C7-C8	2.54	116.97	111.50
24	c	514	BCR	C15-C16-C17	-2.54	118.28	123.47
35	F	101	HEC	CMB-C2B-C3B	2.54	128.80	125.82
26	a	409	PL9	C11-C12-C13	-2.53	103.55	111.88
26	D	406	PL9	C50-C49-C48	-2.53	115.32	122.65
29	D	408	SQD	O5-C1-C2	-2.53	104.99	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	606	CLA	C2A-C1A-CHA	2.53	128.29	123.86
28	D	409	LHG	O8-C23-C24	2.53	119.86	111.91
22	a	402	CLA	CAC-C3C-C4C	2.53	128.10	124.81
24	x	101	BCR	C27-C26-C25	2.53	126.41	122.73
22	B	611	CLA	C1D-CHD-C4C	2.53	125.90	122.56
27	C	520	LMG	O7-C10-O9	-2.53	117.59	123.70
24	c	514	BCR	C11-C10-C9	-2.53	123.70	127.31
24	C	515	BCR	C34-C9-C10	-2.53	119.38	122.92
24	c	515	BCR	C2-C1-C6	2.53	114.37	110.48
22	b	609	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
30	c	517	DGD	O3E-C3E-C2E	-2.52	104.51	110.35
22	C	501	CLA	OBD-CAD-C3D	2.52	132.17	127.98
22	C	502	CLA	C4D-C3D-CAD	-2.52	107.06	108.47
22	C	513	CLA	O2D-CGD-CBD	2.52	115.75	111.27
24	A	407	BCR	C16-C15-C14	-2.52	118.31	123.47
22	c	501	CLA	O1D-CGD-CBD	2.52	129.64	124.48
24	B	617	BCR	C36-C18-C17	-2.52	119.39	122.92
26	a	409	PL9	C40-C39-C41	2.52	119.51	115.27
22	d	401	CLA	O2A-CGA-O1A	-2.51	117.25	123.59
22	B	612	CLA	CMD-C2D-C3D	2.51	129.38	124.68
30	C	518	DGD	C1D-C2D-C3D	-2.51	104.77	110.00
26	D	406	PL9	C8-C7-C3	2.51	119.08	111.98
30	c	517	DGD	O6D-C1D-O3G	-2.51	104.03	109.97
24	C	514	BCR	C24-C23-C22	-2.51	122.45	126.23
22	b	605	CLA	O1A-CGA-CBA	2.51	133.51	123.73
30	c	517	DGD	CDB-CCB-CBB	-2.50	101.71	114.42
22	b	613	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
29	D	408	SQD	O9-S-O7	-2.50	105.29	113.95
22	b	610	CLA	C1-C2-C3	-2.50	121.72	126.04
24	B	619	BCR	C16-C15-C14	-2.50	118.36	123.47
22	c	510	CLA	CMB-C2B-C3B	2.50	129.35	124.68
24	D	405	BCR	C35-C13-C14	-2.50	119.43	122.92
22	B	610	CLA	C2C-C1C-NC	2.49	112.31	109.97
24	c	516	BCR	C27-C26-C25	2.49	126.35	122.73
29	A	414	SQD	O47-C7-C8	2.49	116.86	111.50
22	b	602	CLA	C1-C2-C3	-2.49	121.74	126.04
22	b	612	CLA	C11-C12-C13	-2.49	107.88	115.92
24	x	101	BCR	C2-C1-C6	2.49	114.31	110.48
22	b	613	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
29	f	102	SQD	C1-O5-C5	-2.49	108.81	113.69
24	H	101	BCR	C11-C10-C9	-2.48	123.77	127.31
24	c	515	BCR	C7-C8-C9	-2.48	122.48	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	617	BCR	C15-C14-C13	-2.48	123.77	127.31
22	B	615	CLA	CED-O2D-CGD	2.48	121.54	115.94
22	c	503	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
22	b	615	CLA	C6-C5-C3	-2.47	106.97	113.45
30	h	101	DGD	O5E-C6E-C5E	-2.47	102.82	111.29
22	B	616	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
22	D	402	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
24	B	618	BCR	C24-C23-C22	-2.47	122.51	126.23
22	C	506	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
22	C	509	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
28	D	409	LHG	C11-C10-C9	-2.47	101.91	114.42
29	A	413	SQD	O8-S-C6	2.46	109.67	105.74
22	c	504	CLA	CMD-C2D-C3D	2.46	129.29	124.68
28	A	412	LHG	C27-C26-C25	-2.46	101.92	114.42
22	c	504	CLA	O1A-CGA-CBA	2.46	133.33	123.73
30	C	519	DGD	C1D-C2D-C3D	-2.46	104.87	110.00
24	B	618	BCR	C7-C8-C9	-2.46	122.52	126.23
24	B	617	BCR	C3-C4-C5	-2.46	109.69	114.08
22	C	511	CLA	CMD-C2D-C3D	2.46	129.28	124.68
22	D	403	CLA	C7-C6-C5	-2.46	106.69	113.36
30	H	102	DGD	O5D-C1E-C2E	2.46	112.14	108.30
22	c	512	CLA	OBD-CAD-CBD	-2.46	122.39	125.89
27	c	520	LMG	O6-C1-O1	-2.45	104.16	109.97
22	C	501	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
22	C	507	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
30	h	101	DGD	C3D-C4D-C5D	-2.45	105.86	110.24
28	e	101	LHG	O8-C23-O10	-2.45	117.41	123.59
24	D	405	BCR	C36-C18-C19	-2.45	114.22	118.08
28	d	409	LHG	O8-C23-O10	-2.45	117.42	123.59
24	A	407	BCR	C38-C26-C25	-2.45	121.78	124.53
30	H	102	DGD	C3D-C4D-C5D	-2.45	105.88	110.24
22	b	604	CLA	C6-C5-C3	-2.44	107.05	113.45
27	d	410	LMG	O6-C1-O1	-2.44	104.19	109.97
22	C	511	CLA	O2A-CGA-O1A	-2.44	117.43	123.59
22	b	601	CLA	C1D-CHD-C4C	2.44	125.78	122.56
28	D	409	LHG	C20-C19-C18	-2.44	102.03	114.42
22	C	504	CLA	C4D-C3D-CAD	-2.44	107.11	108.47
22	b	602	CLA	OBD-CAD-CBD	-2.44	122.41	125.89
22	b	608	CLA	CHA-C1A-NA	-2.44	120.81	126.40
22	b	609	CLA	O1D-CGD-CBD	2.44	129.47	124.48
22	b	605	CLA	C4A-NA-C1A	2.44	107.80	106.71
22	b	604	CLA	C2C-C1C-NC	2.43	112.25	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	613	CLA	CHA-C1A-NA	-2.43	120.83	126.40
29	b	620	SQD	C45-O47-C7	2.43	123.78	117.79
22	c	508	CLA	CMB-C2B-C1B	-2.43	124.73	128.46
35	f	101	HEC	CBA-CAA-C2A	-2.43	108.00	112.48
22	d	404	CLA	C4D-C3D-CAD	-2.43	107.11	108.47
22	c	510	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
22	c	509	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
30	A	415	DGD	C1D-C2D-C3D	-2.43	104.94	110.00
24	k	101	BCR	C38-C26-C25	-2.43	121.80	124.53
22	a	402	CLA	O2A-CGA-O1A	-2.43	117.47	123.59
22	d	405	CLA	O2A-CGA-O1A	-2.42	117.47	123.59
24	x	101	BCR	C29-C30-C25	2.42	114.21	110.48
29	f	102	SQD	O5-C1-O6	2.42	115.71	109.97
22	B	606	CLA	C4D-C3D-CAD	-2.42	107.12	108.47
35	f	101	HEC	C4C-C3C-C2C	2.41	108.96	106.35
22	c	510	CLA	CHB-C4A-NA	2.41	127.85	124.51
22	B	609	CLA	CMD-C2D-C3D	2.41	129.19	124.68
24	x	101	BCR	C16-C15-C14	-2.41	118.54	123.47
22	B	612	CLA	C16-C15-C13	-2.41	108.14	115.92
22	d	401	CLA	CMB-C2B-C1B	-2.41	124.77	128.46
24	T	101	BCR	C33-C5-C6	-2.41	121.83	124.53
22	b	616	CLA	C4D-C3D-CAD	-2.40	107.13	108.47
26	d	407	PL9	C31-C32-C33	-2.40	103.98	111.88
22	b	604	CLA	C6-C7-C8	-2.40	108.15	115.92
30	C	517	DGD	O2D-C2D-C1D	-2.40	104.21	110.05
29	A	413	SQD	O48-C23-C24	2.40	119.45	111.91
22	B	607	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
24	b	617	BCR	C11-C10-C9	-2.40	123.88	127.31
22	c	513	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
30	h	101	DGD	O3E-C3E-C2E	-2.40	104.80	110.35
22	D	402	CLA	OBD-CAD-CBD	-2.40	122.47	125.89
24	Y	101	BCR	C12-C13-C14	-2.40	115.26	118.94
24	t	101	BCR	C33-C5-C6	-2.40	121.84	124.53
23	A	404	PHO	O2A-CGA-O1A	-2.40	117.54	123.59
26	A	410	PL9	C12-C13-C14	-2.40	121.89	127.66
24	b	619	BCR	C2-C1-C6	2.40	114.17	110.48
24	a	405	BCR	C27-C26-C25	2.39	126.21	122.73
28	A	412	LHG	O8-C6-C5	-2.39	101.46	108.43
24	c	514	BCR	C27-C26-C25	2.39	126.20	122.73
22	b	603	CLA	C4A-NA-C1A	2.39	107.78	106.71
24	B	617	BCR	C29-C30-C25	2.39	114.16	110.48
22	A	403	CLA	O2D-CGD-CBD	2.39	115.51	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	609	CLA	C6-C5-C3	2.39	119.72	113.45
22	b	615	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
30	h	101	DGD	CDB-CCB-CBB	-2.39	102.31	114.42
30	A	415	DGD	O2D-C2D-C1D	-2.39	104.25	110.05
22	B	607	CLA	CED-O2D-CGD	2.39	121.33	115.94
22	b	602	CLA	C4-C3-C5	2.38	119.28	115.27
22	B	608	CLA	O1D-CGD-CBD	2.38	129.36	124.48
30	C	517	DGD	O1G-C1A-C2A	-2.38	104.43	111.91
22	c	513	CLA	O2D-CGD-CBD	2.38	115.50	111.27
22	C	508	CLA	CMD-C2D-C3D	2.38	129.13	124.68
27	m	101	LMG	O1-C1-C2	-2.38	104.59	108.30
22	b	613	CLA	C4D-C3D-CAD	-2.38	107.14	108.47
28	E	101	LHG	C11-C10-C9	-2.38	102.36	114.42
26	D	406	PL9	C31-C29-C28	2.37	125.92	121.12
22	b	609	CLA	CHB-C4A-NA	2.37	127.80	124.51
22	b	607	CLA	CHA-C1A-NA	-2.37	120.96	126.40
22	C	502	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
22	C	502	CLA	CMB-C2B-C3B	2.37	129.12	124.68
30	c	518	DGD	O4E-C4E-C3E	-2.37	104.86	110.35
22	B	613	CLA	C1D-CHD-C4C	2.37	125.69	122.56
22	c	509	CLA	CHC-C1C-NC	2.37	127.80	124.20
22	b	614	CLA	C7-C6-C5	-2.37	106.92	113.36
22	B	601	CLA	C4-C3-C5	2.37	119.26	115.27
24	t	101	BCR	C2-C1-C6	2.37	114.13	110.48
35	V	201	HEC	CAD-CBD-CGD	-2.37	108.70	112.67
22	d	405	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
22	c	508	CLA	CHD-C4C-NC	2.37	127.93	124.20
28	l	101	LHG	O8-C23-C24	2.36	119.33	111.91
22	B	602	CLA	C1-C2-C3	-2.36	121.96	126.04
26	d	407	PL9	C30-C29-C31	-2.36	111.30	115.27
26	D	406	PL9	C32-C33-C34	-2.36	121.97	127.66
27	c	520	LMG	O8-C28-O10	-2.36	117.64	123.59
30	c	517	DGD	O2D-C2D-C3D	-2.36	104.89	110.35
30	c	517	DGD	O3D-C3D-C4D	-2.36	104.90	110.35
22	B	616	CLA	OBD-CAD-CBD	-2.36	122.53	125.89
22	b	614	CLA	C1-C2-C3	-2.36	121.97	126.04
22	C	512	CLA	CAA-CBA-CGA	-2.36	106.37	113.25
30	c	517	DGD	C6D-O5D-C1E	2.35	118.33	113.74
22	B	609	CLA	O2D-CGD-CBD	2.35	115.44	111.27
22	b	609	CLA	C7-C6-C5	-2.35	106.98	113.36
28	d	408	LHG	O8-C23-C24	2.35	119.27	111.91
29	D	408	SQD	O48-C23-O10	-2.34	117.67	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	605	CLA	C1-C2-C3	2.34	130.09	126.04
26	A	410	PL9	C31-C32-C33	-2.34	104.18	111.88
22	c	512	CLA	O1D-CGD-CBD	2.34	129.27	124.48
24	B	618	BCR	C27-C26-C25	2.34	126.13	122.73
22	B	615	CLA	CHB-C4A-NA	2.34	127.75	124.51
22	A	402	CLA	CED-O2D-CGD	2.34	121.23	115.94
27	c	523	LMG	C1-O6-C5	-2.34	109.10	113.69
22	b	603	CLA	C4D-C3D-CAD	-2.34	107.17	108.47
22	c	505	CLA	OBD-CAD-CBD	-2.34	122.56	125.89
29	D	408	SQD	O5-C5-C4	2.33	113.93	109.69
28	a	410	LHG	O3-P-O5	-2.33	99.95	109.07
24	d	406	BCR	C27-C26-C25	2.33	126.12	122.73
26	d	407	PL9	C8-C7-C3	2.33	118.57	111.98
22	d	405	CLA	CHA-C1A-NA	-2.33	121.06	126.40
24	D	405	BCR	C27-C26-C25	2.33	126.11	122.73
29	b	620	SQD	O47-C45-C46	2.33	116.83	108.40
27	D	407	LMG	O3-C3-C2	-2.33	104.96	110.35
22	C	505	CLA	CHA-C1A-NA	-2.33	121.06	126.40
22	c	508	CLA	C7-C6-C5	-2.33	107.03	113.36
22	C	503	CLA	CMD-C2D-C3D	2.33	129.03	124.68
29	a	411	SQD	C3-C4-C5	2.33	114.39	110.24
22	C	508	CLA	O2D-CGD-CBD	2.33	115.40	111.27
22	c	502	CLA	CHB-C4A-NA	2.32	127.72	124.51
22	D	403	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
23	d	402	PHO	C2B-C1B-NB	-2.32	106.30	109.79
22	b	608	CLA	O2A-CGA-O1A	-2.32	117.75	123.59
35	F	101	HEC	C4C-C3C-C2C	2.31	108.85	106.35
24	C	515	BCR	C33-C5-C6	-2.31	121.93	124.53
22	d	405	CLA	O2A-C1-C2	-2.31	102.56	108.64
24	B	617	BCR	C33-C5-C6	-2.31	121.93	124.53
22	B	601	CLA	O2D-CGD-CBD	2.31	115.38	111.27
24	A	407	BCR	C36-C18-C17	-2.31	119.69	122.92
26	A	410	PL9	C35-C34-C36	2.31	119.16	115.27
22	B	615	CLA	C2C-C1C-NC	2.30	112.13	109.97
28	d	408	LHG	C20-C19-C18	-2.30	102.74	114.42
22	a	402	CLA	CMD-C2D-C3D	2.30	128.98	124.68
24	C	515	BCR	C38-C26-C27	-2.30	109.20	113.62
22	c	503	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
27	c	520	LMG	C9-C8-C7	-2.30	106.36	111.79
22	c	506	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
23	a	403	PHO	CBD-CHA-C4D	-2.29	105.95	108.54
22	c	513	CLA	OBD-CAD-CBD	-2.29	122.62	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	619	BCR	C33-C5-C6	-2.29	121.95	124.53
27	m	101	LMG	C9-C8-C7	-2.29	106.37	111.79
22	c	508	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
30	c	517	DGD	O1G-C1A-O1A	-2.29	117.81	123.59
28	d	408	LHG	C18-C17-C16	-2.29	102.79	114.42
22	c	512	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
23	a	403	PHO	O2D-CGD-O1D	-2.29	119.36	123.84
22	b	612	CLA	C1-C2-C3	-2.29	122.08	126.04
22	B	610	CLA	C1-C2-C3	-2.29	122.08	126.04
28	B	622	LHG	C11-C10-C9	-2.29	102.81	114.42
26	D	406	PL9	C11-C12-C13	-2.29	104.36	111.88
24	k	101	BCR	C27-C26-C25	2.29	126.05	122.73
22	c	508	CLA	C11-C10-C8	-2.29	108.52	115.92
27	A	411	LMG	O1-C7-C8	-2.28	105.39	110.90
30	A	415	DGD	C3E-C4E-C5E	-2.28	106.16	110.24
24	x	101	BCR	C35-C13-C12	2.28	121.68	118.08
27	D	407	LMG	C3-C4-C5	-2.28	106.17	110.24
29	b	620	SQD	O10-C23-C24	-2.28	114.83	123.73
22	B	616	CLA	C5-C3-C2	2.28	125.74	121.12
28	E	101	LHG	C18-C17-C16	-2.28	102.84	114.42
22	a	404	CLA	CBC-CAC-C3C	-2.28	106.14	112.43
22	c	507	CLA	C2C-C1C-NC	2.28	112.11	109.97
24	C	514	BCR	C8-C7-C6	-2.28	120.80	127.20
22	B	609	CLA	O2A-CGA-O1A	-2.28	117.85	123.59
33	C	523	STE	C4-C3-C2	-2.28	104.91	113.76
27	c	520	LMG	C40-C39-C38	-2.28	102.87	114.42
24	C	515	BCR	C27-C26-C25	2.27	126.03	122.73
26	d	407	PL9	C12-C13-C14	-2.27	122.18	127.66
22	c	506	CLA	CHC-C1C-NC	2.27	127.65	124.20
22	B	603	CLA	CHB-C4A-NA	2.27	127.65	124.51
22	b	612	CLA	OBD-CAD-CBD	-2.27	122.66	125.89
22	c	506	CLA	C4-C3-C2	-2.27	117.86	123.68
27	c	522	LMG	O2-C2-C1	-2.27	104.54	110.05
22	b	604	CLA	O1D-CGD-CBD	2.27	129.12	124.48
27	M	101	LMG	C6-C5-C4	-2.27	107.70	113.00
22	B	603	CLA	C3C-C4C-NC	-2.26	108.03	110.57
35	v	201	HEC	CMC-C2C-C3C	2.26	128.48	125.82
26	d	407	PL9	C46-C47-C48	-2.26	104.44	111.88
26	D	406	PL9	C12-C13-C14	-2.26	122.21	127.66
22	B	605	CLA	C16-C15-C13	-2.26	108.61	115.92
29	B	623	SQD	C1-C2-C3	-2.26	105.29	110.00
30	C	517	DGD	C8B-C7B-C6B	-2.26	102.95	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	614	CLA	CHB-C4A-NA	2.26	127.64	124.51
24	b	617	BCR	C35-C13-C14	-2.26	119.76	122.92
22	b	613	CLA	CMB-C2B-C3B	2.26	128.91	124.68
22	c	510	CLA	O1D-CGD-CBD	2.26	129.11	124.48
22	b	606	CLA	C2C-C1C-NC	2.26	112.09	109.97
22	C	507	CLA	CMD-C2D-C3D	2.26	128.90	124.68
22	A	403	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
22	D	404	CLA	C2C-C1C-NC	2.26	112.09	109.97
24	C	514	BCR	C32-C1-C6	-2.26	106.64	110.30
30	c	517	DGD	O2G-C2G-C1G	-2.26	100.24	108.40
23	A	405	PHO	C1-C2-C3	-2.25	122.14	126.04
24	A	407	BCR	C15-C16-C17	-2.25	118.86	123.47
22	D	403	CLA	CHB-C4A-NA	2.25	127.63	124.51
22	B	608	CLA	O2D-CGD-CBD	2.25	115.27	111.27
22	C	501	CLA	CMD-C2D-C3D	2.25	128.89	124.68
22	b	607	CLA	OBD-CAD-CBD	-2.25	122.68	125.89
30	C	517	DGD	O3E-C3E-C2E	-2.25	105.15	110.35
35	v	201	HEC	CAD-CBD-CGD	-2.25	108.90	112.67
23	a	403	PHO	C1B-NB-C4B	2.25	110.74	106.51
24	C	514	BCR	C15-C14-C13	-2.25	124.10	127.31
22	C	510	CLA	CHB-C4A-NA	2.25	127.62	124.51
30	h	101	DGD	O6D-C1D-O3G	-2.24	104.66	109.97
24	H	101	BCR	C38-C26-C25	-2.24	122.01	124.53
22	b	601	CLA	CMB-C2B-C3B	2.24	128.86	124.68
22	D	404	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
22	C	501	CLA	CMB-C2B-C3B	2.24	128.86	124.68
22	C	502	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
22	b	611	CLA	CHB-C4A-NA	2.24	127.60	124.51
22	c	505	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
24	D	405	BCR	C2-C3-C4	-2.23	106.38	111.38
26	d	407	PL9	C15-C14-C13	-2.23	117.95	123.68
24	b	619	BCR	C16-C15-C14	-2.23	118.90	123.47
22	C	511	CLA	CHB-C4A-NA	2.23	127.60	124.51
22	B	607	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
22	A	403	CLA	C1-O2A-CGA	2.23	122.30	116.44
26	D	406	PL9	C31-C32-C33	-2.23	104.54	111.88
22	c	510	CLA	O1A-CGA-CBA	2.23	132.44	123.73
22	b	608	CLA	C4A-NA-C1A	2.23	107.71	106.71
22	B	612	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
22	c	504	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
30	C	519	DGD	O3D-C3D-C4D	-2.23	105.19	110.35
22	C	504	CLA	CHC-C1C-NC	2.23	127.58	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	601	CLA	CHB-C4A-NA	2.23	127.59	124.51
22	A	402	CLA	O2D-CGD-CBD	-2.23	107.31	111.27
22	C	503	CLA	C2C-C1C-NC	2.23	112.06	109.97
22	B	613	CLA	CHB-C4A-NA	2.23	127.59	124.51
22	c	512	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
33	D	412	STE	C12-C11-C10	-2.23	103.13	114.42
29	f	102	SQD	O5-C1-C2	-2.22	105.64	110.35
27	b	623	LMG	O8-C28-O10	-2.22	117.98	123.59
22	B	611	CLA	C7-C6-C5	-2.22	107.32	113.36
27	D	410	LMG	O1-C7-C8	-2.22	105.89	111.78
26	a	409	PL9	O2-C1-C2	-2.22	116.69	121.78
22	b	604	CLA	CHC-C1C-C2C	-2.22	120.58	126.72
22	C	507	CLA	C4D-C3D-CAD	-2.22	107.23	108.47
22	C	510	CLA	C4D-C3D-CAD	-2.22	107.23	108.47
22	b	606	CLA	O1D-CGD-CBD	2.22	129.02	124.48
23	a	403	PHO	C2B-C1B-NB	-2.22	106.44	109.79
27	d	410	LMG	O7-C10-O9	-2.22	118.34	123.70
22	b	614	CLA	CHB-C4A-NA	2.22	127.58	124.51
22	b	609	CLA	C2C-C1C-NC	2.22	112.05	109.97
30	c	518	DGD	O2E-C2E-C1E	-2.22	104.66	110.05
24	t	101	BCR	C1-C6-C5	-2.22	119.49	122.61
24	a	405	BCR	C37-C22-C21	-2.22	119.82	122.92
28	e	101	LHG	C11-C10-C9	-2.22	103.18	114.42
22	A	402	CLA	O1D-CGD-CBD	2.21	129.01	124.48
22	B	609	CLA	C2C-C1C-NC	2.21	112.05	109.97
24	B	618	BCR	C3-C4-C5	-2.21	110.12	114.08
24	H	101	BCR	C35-C13-C14	-2.21	119.82	122.92
24	B	618	BCR	C15-C16-C17	-2.21	118.94	123.47
27	A	411	LMG	C12-C11-C10	-2.21	105.57	113.62
28	a	410	LHG	C25-C24-C23	2.21	121.67	113.62
22	B	611	CLA	C1-C2-C3	-2.21	122.22	126.04
30	c	517	DGD	CBB-CAB-C9B	-2.21	103.19	114.42
22	c	504	CLA	O2D-CGD-CBD	2.21	115.20	111.27
24	H	101	BCR	C1-C6-C5	-2.21	119.50	122.61
23	a	403	PHO	CHC-C4B-NB	2.21	129.56	124.93
22	B	610	CLA	CHB-C4A-NA	2.21	127.57	124.51
28	B	622	LHG	O3-P-O5	-2.21	100.43	109.07
22	B	608	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
27	M	101	LMG	O1-C7-C8	-2.21	105.57	110.90
22	B	604	CLA	C6-C7-C8	-2.21	108.79	115.92
29	f	102	SQD	O48-C23-C24	2.21	118.83	111.91
24	b	618	BCR	C36-C18-C17	-2.21	119.83	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	404	CLA	OBD-CAD-C3D	2.21	131.64	127.98
22	B	609	CLA	CHA-C1A-NA	-2.21	121.35	126.40
22	B	615	CLA	C6-C7-C8	-2.20	108.79	115.92
22	C	502	CLA	CHA-C1A-NA	-2.20	121.35	126.40
22	b	603	CLA	O1A-CGA-CBA	2.20	132.33	123.73
22	D	402	CLA	C6-C5-C3	2.20	119.23	113.45
30	A	415	DGD	CAB-C9B-C8B	-2.20	103.24	114.42
24	B	617	BCR	C15-C16-C17	-2.20	118.96	123.47
28	l	101	LHG	C27-C26-C25	-2.20	103.25	114.42
24	B	617	BCR	C11-C10-C9	-2.20	124.17	127.31
28	a	410	LHG	C18-C17-C16	-2.20	103.25	114.42
23	a	403	PHO	C3A-C4A-CHB	-2.20	118.03	121.83
30	c	517	DGD	CAB-C9B-C8B	-2.20	103.26	114.42
22	D	402	CLA	CBA-CAA-C2A	-2.20	107.37	113.86
24	Y	101	BCR	C1-C6-C5	-2.20	119.52	122.61
24	D	405	BCR	C2-C1-C6	2.20	113.86	110.48
22	C	506	CLA	CAA-CBA-CGA	-2.20	106.83	113.25
24	B	617	BCR	C27-C26-C25	2.20	125.92	122.73
22	c	508	CLA	C3C-C4C-NC	-2.20	108.11	110.57
29	A	413	SQD	O5-C1-O6	2.19	115.17	109.97
24	t	101	BCR	C36-C18-C19	2.19	121.53	118.08
22	C	509	CLA	C1D-CHD-C4C	2.19	125.45	122.56
22	c	511	CLA	CHB-C4A-NA	2.19	127.54	124.51
22	b	616	CLA	O1D-CGD-CBD	2.19	128.97	124.48
22	b	609	CLA	CHA-C1A-NA	-2.19	121.38	126.40
22	C	507	CLA	C2A-C1A-CHA	2.19	127.69	123.86
22	c	505	CLA	C11-C10-C8	-2.19	108.84	115.92
28	D	409	LHG	C27-C26-C25	-2.19	103.32	114.42
22	b	605	CLA	CHA-C1A-NA	-2.19	121.39	126.40
24	C	516	BCR	C35-C13-C14	-2.19	119.86	122.92
22	d	403	CLA	O2A-CGA-O1A	-2.19	118.08	123.59
22	C	512	CLA	CMA-C3A-C2A	-2.19	105.01	113.83
24	B	617	BCR	C8-C7-C6	-2.18	121.07	127.20
30	c	517	DGD	C5B-C4B-C3B	-2.18	103.34	114.42
22	B	602	CLA	C4-C3-C5	2.18	118.94	115.27
22	C	512	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
24	c	515	BCR	C36-C18-C17	-2.18	119.86	122.92
22	A	403	CLA	C1D-CHD-C4C	2.18	125.44	122.56
24	D	405	BCR	C16-C15-C14	-2.18	119.00	123.47
22	d	401	CLA	O2D-CGD-CBD	2.18	115.14	111.27
24	A	407	BCR	C19-C18-C17	-2.18	115.59	118.94
30	A	415	DGD	O3G-C3G-C2G	-2.18	105.65	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	512	CLA	C1D-CHD-C4C	2.17	125.43	122.56
22	a	404	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
27	c	520	LMG	O2-C2-C1	-2.17	104.77	110.05
22	B	613	CLA	OBD-CAD-CBD	-2.17	122.79	125.89
22	b	612	CLA	CHC-C1C-NC	2.17	127.50	124.20
23	A	405	PHO	CAC-C3C-C2C	2.17	131.25	127.53
30	c	518	DGD	O3E-C3E-C4E	-2.17	105.33	110.35
24	a	405	BCR	C16-C15-C14	-2.17	119.02	123.47
24	T	101	BCR	C30-C25-C26	-2.17	119.55	122.61
30	c	518	DGD	C8B-C7B-C6B	-2.17	103.40	114.42
22	C	511	CLA	C4-C3-C5	2.17	118.92	115.27
22	C	504	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
22	D	402	CLA	CHB-C4A-NA	2.17	127.51	124.51
26	D	406	PL9	C7-C3-C2	-2.17	120.45	123.30
22	B	606	CLA	CMD-C2D-C3D	2.17	128.73	124.68
22	C	510	CLA	C1D-CHD-C4C	2.17	125.42	122.56
27	M	101	LMG	C18-C17-C16	-2.16	103.44	114.42
22	B	609	CLA	C1C-C2C-C3C	-2.16	104.68	106.96
30	C	518	DGD	C1D-O6D-C5D	-2.16	109.44	113.69
22	B	613	CLA	O1D-CGD-CBD	2.16	128.91	124.48
30	c	517	DGD	C4A-C3A-C2A	-2.16	105.42	113.19
28	a	410	LHG	C20-C19-C18	-2.16	103.45	114.42
22	B	606	CLA	O1A-CGA-CBA	2.16	132.16	123.73
24	C	515	BCR	C2-C1-C6	2.16	113.81	110.48
22	b	608	CLA	C6-C7-C8	-2.16	108.95	115.92
22	B	607	CLA	C1B-CHB-C4A	-2.15	125.85	130.12
22	A	403	CLA	C3D-CAD-CBD	-2.15	104.77	107.61
24	b	617	BCR	C3-C4-C5	-2.15	110.23	114.08
22	C	502	CLA	CAC-C3C-C4C	2.15	127.60	124.81
24	b	617	BCR	C33-C5-C6	-2.15	122.11	124.53
22	a	402	CLA	C16-C17-C18	-2.15	105.85	115.98
24	b	618	BCR	C33-C5-C6	-2.15	122.11	124.53
22	D	402	CLA	C3B-C4B-NB	-2.15	106.43	109.21
22	b	613	CLA	OBD-CAD-CBD	-2.15	122.82	125.89
22	B	602	CLA	CHB-C4A-NA	2.15	127.48	124.51
22	A	406	CLA	C1-C2-C3	-2.15	122.33	126.04
22	B	608	CLA	CHB-C4A-NA	2.15	127.48	124.51
30	c	519	DGD	O1G-C1G-C2G	-2.15	102.18	108.43
22	c	504	CLA	CHD-C4C-NC	2.15	127.59	124.20
22	B	616	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
27	M	101	LMG	C40-C39-C38	-2.15	103.52	114.42
22	b	605	CLA	O2A-CGA-O1A	-2.15	118.17	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	407	PL9	C11-C9-C8	-2.15	116.77	121.12
27	d	410	LMG	O3-C3-C2	-2.15	105.39	110.35
28	E	101	LHG	O8-C23-O10	-2.15	118.18	123.59
22	c	511	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
24	Y	101	BCR	C33-C5-C6	-2.14	122.12	124.53
30	C	519	DGD	O4D-C4D-C5D	-2.14	103.98	109.30
22	C	507	CLA	C2C-C1C-NC	2.14	111.98	109.97
27	C	520	LMG	O2-C2-C1	-2.14	104.85	110.05
26	a	409	PL9	O2-C1-C6	2.14	124.30	120.59
22	B	614	CLA	CAC-C3C-C4C	2.14	127.58	124.81
22	d	403	CLA	C6-C5-C3	2.14	119.06	113.45
27	c	523	LMG	C3-C4-C5	-2.14	106.43	110.24
22	c	510	CLA	C7-C6-C5	-2.13	107.56	113.36
30	C	517	DGD	O3G-C1D-C2D	-2.13	104.97	108.30
27	c	523	LMG	C40-C39-C38	-2.13	103.59	114.42
22	d	405	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
24	d	406	BCR	C11-C10-C9	-2.13	124.27	127.31
24	t	101	BCR	C28-C27-C26	-2.13	110.27	114.08
27	d	410	LMG	C40-C39-C38	-2.13	103.60	114.42
27	c	522	LMG	C1-O6-C5	-2.13	109.51	113.69
22	b	604	CLA	C3A-C2A-C1A	2.13	104.53	101.34
22	b	611	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
22	c	501	CLA	C4D-C3D-CAD	-2.13	107.28	108.47
22	D	404	CLA	OBD-CAD-CBD	-2.13	122.86	125.89
22	B	612	CLA	CHB-C4A-NA	2.13	127.45	124.51
30	H	102	DGD	O3E-C3E-C2E	-2.13	105.43	110.35
24	b	617	BCR	C15-C14-C13	-2.13	124.28	127.31
28	D	409	LHG	O4-P-O3	-2.13	97.87	107.75
26	A	410	PL9	C7-C8-C9	-2.12	123.26	126.79
22	B	607	CLA	CHD-C4C-NC	2.12	127.55	124.20
24	B	617	BCR	C24-C23-C22	-2.12	123.03	126.23
28	A	412	LHG	O8-C23-C24	2.12	118.56	111.91
22	B	613	CLA	CMB-C2B-C1B	-2.12	125.21	128.46
30	H	102	DGD	O1G-C1A-O1A	-2.12	118.24	123.59
22	D	404	CLA	CMB-C2B-C3B	2.12	128.64	124.68
22	b	602	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
22	d	403	CLA	CMB-C2B-C3B	2.12	128.64	124.68
22	b	603	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
26	d	407	PL9	C40-C39-C38	-2.11	118.25	123.68
22	b	605	CLA	C1-C2-C3	-2.11	122.39	126.04
27	c	523	LMG	C9-C8-C7	-2.11	106.79	111.79
22	b	607	CLA	C2A-C1A-CHA	2.11	127.56	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	c	518	DGD	O6D-C1D-O3G	-2.11	104.97	109.97
26	d	407	PL9	C41-C39-C38	-2.11	116.84	121.12
29	a	411	SQD	O4-C4-C3	-2.11	105.47	110.35
24	C	516	BCR	C20-C21-C22	-2.11	124.30	127.31
23	A	404	PHO	CMD-C2D-C1D	2.11	128.32	125.06
22	B	604	CLA	CGD-CBD-CAD	-2.11	103.90	110.73
35	v	201	HEC	CMD-C2D-C1D	-2.11	125.22	128.46
30	H	102	DGD	O2D-C2D-C1D	-2.11	104.92	110.05
22	C	504	CLA	CED-O2D-CGD	2.11	120.71	115.94
22	B	608	CLA	C2C-C1C-NC	2.11	111.95	109.97
22	c	510	CLA	C1-C2-C3	-2.11	122.40	126.04
30	C	518	DGD	O2D-C2D-C1D	-2.11	104.93	110.05
22	a	404	CLA	CAA-C2A-C3A	-2.11	107.01	112.78
22	B	614	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
22	B	609	CLA	OBD-CAD-C3D	2.10	131.47	127.98
22	B	603	CLA	O2D-CGD-CBD	2.10	115.00	111.27
24	Y	101	BCR	C15-C16-C17	-2.10	119.18	123.47
24	c	516	BCR	C2-C1-C6	2.10	113.71	110.48
24	t	101	BCR	C39-C30-C25	2.10	113.70	110.30
28	A	412	LHG	O3-P-O5	-2.10	100.88	109.07
26	a	409	PL9	C7-C8-C9	-2.09	123.31	126.79
22	b	616	CLA	C2A-C3A-C4A	2.09	105.25	101.87
24	a	405	BCR	C35-C13-C14	-2.09	119.99	122.92
27	M	101	LMG	C38-C37-C36	-2.09	103.80	114.42
24	C	516	BCR	C27-C26-C25	2.09	125.77	122.73
24	a	405	BCR	C7-C8-C9	-2.09	123.08	126.23
22	A	403	CLA	CMD-C2D-C3D	2.09	128.59	124.68
22	C	509	CLA	C3C-C4C-NC	-2.09	108.23	110.57
22	a	404	CLA	CHA-C1A-NA	-2.09	121.62	126.40
22	C	503	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
22	c	512	CLA	C3B-C4B-NB	-2.09	106.51	109.21
24	A	407	BCR	C24-C23-C22	-2.09	123.08	126.23
24	A	407	BCR	C8-C7-C6	-2.08	121.35	127.20
22	c	503	CLA	C11-C12-C13	-2.08	109.18	115.92
22	c	506	CLA	C4-C3-C5	2.08	118.78	115.27
24	Y	101	BCR	C38-C26-C25	-2.08	122.19	124.53
28	d	409	LHG	O8-C23-C24	2.08	118.44	111.91
33	d	411	STE	C6-C5-C4	-2.08	103.86	114.42
22	c	509	CLA	C3A-C2A-C1A	2.08	104.45	101.34
22	b	604	CLA	C2A-C1A-CHA	2.08	127.50	123.86
22	a	404	CLA	C2C-C1C-NC	2.08	111.92	109.97
24	B	617	BCR	C34-C9-C10	-2.08	120.01	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	512	CLA	O2D-CGD-O1D	-2.08	119.78	123.84
22	c	504	CLA	O2D-CGD-O1D	-2.08	119.78	123.84
22	B	609	CLA	OBD-CAD-CBD	-2.08	122.93	125.89
24	C	514	BCR	C38-C26-C25	-2.08	122.20	124.53
24	C	515	BCR	C1-C6-C5	-2.08	119.69	122.61
22	C	511	CLA	C1B-CHB-C4A	-2.08	126.01	130.12
26	A	410	PL9	C27-C28-C29	-2.08	122.66	127.66
28	e	101	LHG	C20-C19-C18	-2.08	103.89	114.42
22	b	601	CLA	C3C-C4C-NC	-2.07	108.24	110.57
22	b	610	CLA	CMD-C2D-C3D	2.07	128.56	124.68
22	c	505	CLA	C1-C2-C3	-2.07	122.46	126.04
22	b	611	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
24	c	514	BCR	C2-C1-C6	2.07	113.67	110.48
23	d	402	PHO	CBD-CHA-C4D	-2.07	106.21	108.54
27	A	411	LMG	O8-C28-O10	-2.07	118.37	123.59
26	a	409	PL9	C22-C23-C24	-2.07	122.68	127.66
27	d	410	LMG	C3-C4-C5	-2.07	106.55	110.24
22	b	603	CLA	CHD-C4C-NC	2.07	127.46	124.20
22	C	507	CLA	CBC-CAC-C3C	-2.07	106.73	112.43
22	b	610	CLA	CAA-CBA-CGA	-2.07	107.22	113.25
26	d	407	PL9	C17-C16-C14	2.07	119.77	112.98
22	B	608	CLA	CMD-C2D-C3D	2.06	128.54	124.68
29	a	412	SQD	O48-C23-C24	2.06	118.38	111.91
27	C	520	LMG	C38-C37-C36	-2.06	103.95	114.42
27	b	623	LMG	C38-C37-C36	-2.06	103.96	114.42
24	c	515	BCR	C1-C6-C5	-2.06	119.71	122.61
24	C	515	BCR	C34-C9-C8	2.06	121.32	118.08
24	t	101	BCR	C27-C26-C25	2.06	125.72	122.73
24	D	405	BCR	C33-C5-C6	-2.06	122.22	124.53
22	b	603	CLA	C4-C3-C5	2.06	118.73	115.27
22	C	509	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
22	B	609	CLA	C7-C6-C5	-2.06	107.78	113.36
23	A	404	PHO	O2A-C1-C2	2.06	114.04	108.64
26	d	407	PL9	C45-C44-C46	-2.06	111.81	115.27
22	b	610	CLA	C1D-CHD-C4C	2.05	125.27	122.56
22	b	613	CLA	CMD-C2D-C3D	2.05	128.52	124.68
22	C	504	CLA	CHD-C4C-NC	2.05	127.44	124.20
22	B	610	CLA	OBD-CAD-CBD	-2.05	122.97	125.89
29	B	623	SQD	C27-C26-C25	-2.05	104.02	114.42
24	c	515	BCR	C8-C9-C10	2.05	122.09	118.94
22	B	615	CLA	C1-C2-C3	2.05	129.59	126.04
22	b	608	CLA	CHB-C4A-NA	2.05	127.34	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	615	CLA	CHC-C1C-NC	2.05	127.31	124.20
30	A	415	DGD	C5B-C4B-C3B	-2.05	104.03	114.42
30	c	518	DGD	O5D-C6D-C5D	-2.05	105.26	109.05
24	b	618	BCR	C30-C25-C26	-2.05	119.73	122.61
24	b	619	BCR	C15-C16-C17	-2.05	119.28	123.47
24	b	618	BCR	C15-C16-C17	-2.05	119.28	123.47
22	C	511	CLA	C1-C2-C3	-2.04	122.51	126.04
22	b	604	CLA	CGD-CBD-CAD	-2.04	104.12	110.73
22	b	606	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
22	C	507	CLA	C4-C3-C5	2.04	118.71	115.27
27	C	520	LMG	C20-C19-C18	-2.04	104.06	114.42
23	A	405	PHO	C2B-C1B-NB	-2.04	106.71	109.79
30	A	415	DGD	O5D-C6D-C5D	-2.04	105.28	109.05
22	C	508	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
22	b	607	CLA	OBD-CAD-C3D	2.04	131.36	127.98
27	a	416	LMG	C32-C31-C30	-2.04	104.09	114.42
24	C	514	BCR	C35-C13-C14	-2.04	120.07	122.92
30	c	519	DGD	CDB-CCB-CBB	-2.03	104.10	114.42
22	B	613	CLA	C6-C7-C8	-2.03	109.35	115.92
24	t	101	BCR	C4-C5-C6	2.03	125.68	122.73
24	b	618	BCR	C7-C8-C9	-2.03	123.16	126.23
22	B	612	CLA	C1-C2-C3	-2.03	122.53	126.04
27	C	520	LMG	O3-C3-C2	-2.03	105.65	110.35
22	d	404	CLA	C17-C16-C15	-2.03	103.91	113.24
27	b	623	LMG	C40-C39-C38	-2.03	104.11	114.42
28	B	621	LHG	C20-C19-C18	-2.03	104.11	114.42
24	B	618	BCR	C2-C1-C6	2.03	113.61	110.48
24	c	515	BCR	C35-C13-C12	2.03	121.28	118.08
27	c	520	LMG	O7-C10-O9	-2.03	118.93	122.96
30	C	519	DGD	O3E-C3E-C2E	-2.03	105.66	110.35
24	b	619	BCR	C36-C18-C17	-2.03	120.08	122.92
28	l	101	LHG	C13-C12-C11	-2.03	104.13	114.42
29	B	623	SQD	C25-C24-C23	-2.03	106.25	113.62
27	D	410	LMG	O8-C28-O10	-2.03	118.48	123.59
29	b	620	SQD	O48-C23-O10	-2.03	118.48	123.59
30	c	519	DGD	O2D-C2D-C1D	-2.02	105.13	110.05
22	c	510	CLA	O2A-C1-C2	-2.02	103.31	108.64
28	A	412	LHG	O4-P-O3	2.02	117.15	107.75
24	a	405	BCR	C30-C25-C26	-2.02	119.76	122.61
24	C	516	BCR	C24-C23-C22	-2.02	123.18	126.23
24	C	514	BCR	C34-C9-C10	-2.02	120.09	122.92
24	a	405	BCR	C38-C26-C27	-2.02	109.73	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	507	CLA	CHC-C1C-C2C	-2.02	121.14	126.72
27	a	416	LMG	C4-C3-C2	-2.02	107.30	110.82
27	A	411	LMG	C9-C8-C7	-2.02	107.01	111.79
28	A	412	LHG	O8-C23-O10	-2.02	118.50	123.59
22	A	406	CLA	C4A-NA-C1A	2.02	107.61	106.71
22	b	608	CLA	C2A-C1A-CHA	2.02	127.39	123.86
22	d	403	CLA	CHA-C1A-NA	-2.02	121.78	126.40
22	C	503	CLA	CHB-C4A-NA	2.02	127.30	124.51
27	C	520	LMG	C40-C39-C38	-2.02	104.19	114.42
27	b	623	LMG	O1-C7-C8	-2.02	106.03	110.90
24	c	515	BCR	C28-C27-C26	-2.02	110.48	114.08
23	A	405	PHO	CMB-C2B-C1B	-2.01	121.96	125.06
22	c	511	CLA	O1A-CGA-CBA	2.01	131.59	123.73
22	C	509	CLA	C2A-C3A-C4A	2.01	105.12	101.87
23	A	404	PHO	CED-O2D-CGD	2.01	120.49	115.94
22	d	401	CLA	C3C-C4C-NC	-2.01	108.31	110.57
22	C	504	CLA	CHB-C4A-NA	2.01	127.30	124.51
22	b	611	CLA	CAC-C3C-C4C	2.01	127.42	124.81
30	C	518	DGD	CDB-CCB-CBB	-2.01	104.21	114.42
22	C	502	CLA	O1D-CGD-CBD	2.01	128.60	124.48
22	d	401	CLA	CAC-C3C-C2C	-2.01	124.09	127.53
22	B	608	CLA	CED-O2D-CGD	-2.01	111.39	115.94
29	A	413	SQD	O8-S-O9	2.01	116.19	111.27
30	H	102	DGD	C6D-O5D-C1E	2.01	117.67	113.74
24	x	101	BCR	C33-C5-C6	-2.01	122.27	124.53
22	b	602	CLA	CHC-C1C-C2C	-2.01	121.17	126.72
22	C	503	CLA	OBD-CAD-CBD	-2.01	123.03	125.89
30	c	519	DGD	O5D-C1E-C2E	2.01	111.44	108.30
29	A	413	SQD	O9-S-C6	2.01	109.33	106.94
24	c	515	BCR	C38-C26-C27	-2.01	109.76	113.62
22	B	608	CLA	CMA-C3A-C4A	-2.01	106.38	111.77
23	a	403	PHO	CHB-C4A-NA	2.01	128.39	124.94
24	t	101	BCR	C15-C14-C13	-2.01	124.45	127.31
22	C	505	CLA	OBD-CAD-C3D	2.01	131.31	127.98
22	D	404	CLA	OBD-CAD-C3D	2.00	131.31	127.98
22	c	502	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
30	A	415	DGD	O3D-C3D-C4D	-2.00	105.72	110.35
22	b	604	CLA	CHB-C4A-NA	2.00	127.28	124.51
22	C	502	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
29	A	413	SQD	C3-C4-C5	2.00	113.81	110.24
22	A	402	CLA	C1C-C2C-C3C	-2.00	104.85	106.96
30	C	518	DGD	CBB-CAB-C9B	-2.00	104.27	114.42

All (184) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	c	513	CLA	NC
22	c	513	CLA	NA
22	A	402	CLA	NC
22	A	402	CLA	ND
22	A	402	CLA	NA
22	c	508	CLA	NC
22	c	508	CLA	NA
22	B	605	CLA	NC
22	B	605	CLA	ND
22	B	605	CLA	NA
22	C	508	CLA	NC
22	C	508	CLA	NA
22	b	610	CLA	NA
22	b	610	CLA	NC
22	b	610	CLA	ND
22	C	512	CLA	NC
22	C	512	CLA	ND
22	C	512	CLA	NA
22	D	402	CLA	ND
22	D	402	CLA	NA
22	c	503	CLA	NC
22	c	503	CLA	ND
22	c	503	CLA	NA
22	b	614	CLA	NC
22	b	614	CLA	ND
22	b	614	CLA	NA
22	C	506	CLA	NC
22	C	506	CLA	ND
22	C	506	CLA	NA
22	C	507	CLA	NC
22	C	507	CLA	ND
22	C	507	CLA	NA
22	c	509	CLA	NC
22	c	509	CLA	ND
22	c	509	CLA	NA
22	c	511	CLA	NC
22	c	511	CLA	ND
22	c	511	CLA	NA
22	a	402	CLA	NC
22	a	402	CLA	ND
22	a	402	CLA	NA
22	B	603	CLA	NC

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Mol	Chain	Res	Type	Atom
22	B	603	CLA	ND
22	B	603	CLA	NA
22	b	612	CLA	NC
22	b	612	CLA	ND
22	b	612	CLA	NA
22	d	405	CLA	NC
22	d	405	CLA	ND
22	d	405	CLA	NA
22	b	608	CLA	NA
22	a	404	CLA	NC
22	a	404	CLA	ND
22	a	404	CLA	NA
22	C	511	CLA	NC
22	C	511	CLA	ND
22	C	511	CLA	NA
22	B	611	CLA	NC
22	B	611	CLA	ND
22	B	611	CLA	NA
22	b	602	CLA	NA
22	d	403	CLA	ND
22	d	403	CLA	NA
22	b	609	CLA	NC
22	b	609	CLA	ND
22	A	406	CLA	NC
22	A	406	CLA	ND
22	A	406	CLA	NA
22	C	510	CLA	NA
22	C	510	CLA	NC
22	C	510	CLA	ND
22	C	502	CLA	NC
22	C	502	CLA	NA
22	A	403	CLA	NC
22	A	403	CLA	ND
22	A	403	CLA	NA
22	c	501	CLA	NC
22	c	501	CLA	ND
22	c	501	CLA	NA
22	b	616	CLA	NA
22	b	616	CLA	NC
22	b	616	CLA	ND
22	c	504	CLA	NC
22	c	504	CLA	ND

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Mol	Chain	Res	Type	Atom
22	c	504	CLA	NA
22	D	404	CLA	NC
22	D	404	CLA	NA
22	C	504	CLA	NC
22	C	504	CLA	ND
22	C	504	CLA	NA
22	b	601	CLA	NC
22	b	601	CLA	ND
22	b	601	CLA	NA
22	d	401	CLA	NC
22	d	401	CLA	NA
22	c	502	CLA	NC
22	c	502	CLA	NA
22	b	615	CLA	NC
22	b	615	CLA	ND
22	b	615	CLA	NA
22	B	601	CLA	ND
22	B	601	CLA	NA
22	b	607	CLA	NC
22	b	607	CLA	ND
22	b	607	CLA	NA
22	c	506	CLA	NC
22	c	506	CLA	ND
22	c	506	CLA	NA
22	b	611	CLA	NC
22	b	611	CLA	ND
22	b	611	CLA	NA
22	D	403	CLA	NA
22	B	616	CLA	NA
22	B	616	CLA	NC
22	B	616	CLA	ND
22	C	513	CLA	NC
22	C	513	CLA	NA
22	B	614	CLA	NC
22	B	614	CLA	ND
22	B	614	CLA	NA
22	d	404	CLA	ND
22	d	404	CLA	NA
22	B	612	CLA	NC
22	B	612	CLA	ND
22	B	612	CLA	NA
22	C	501	CLA	NC

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Mol	Chain	Res	Type	Atom
22	C	501	CLA	ND
22	C	501	CLA	NA
22	b	605	CLA	NC
22	b	605	CLA	ND
22	b	605	CLA	NA
22	C	509	CLA	NC
22	C	509	CLA	ND
22	C	509	CLA	NA
22	B	610	CLA	NC
22	B	610	CLA	ND
22	B	610	CLA	NA
22	b	603	CLA	NC
22	b	603	CLA	ND
22	b	603	CLA	NA
22	B	607	CLA	NC
22	B	607	CLA	ND
22	B	607	CLA	NA
22	c	512	CLA	NC
22	c	512	CLA	ND
22	c	512	CLA	NA
22	b	606	CLA	NC
22	b	606	CLA	ND
22	b	606	CLA	NA
22	B	606	CLA	NC
22	B	606	CLA	ND
22	B	606	CLA	NA
22	B	613	CLA	NA
22	B	613	CLA	NC
22	B	613	CLA	ND
22	B	604	CLA	NC
22	B	604	CLA	ND
22	B	604	CLA	NA
22	c	507	CLA	NC
22	c	507	CLA	NA
22	c	507	CLA	ND
22	b	613	CLA	NC
22	b	613	CLA	ND
22	b	613	CLA	NA
22	c	505	CLA	ND
22	c	505	CLA	NA
22	C	503	CLA	NC
22	C	503	CLA	ND

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Mol	Chain	Res	Type	Atom
22	B	608	CLA	NC
22	B	608	CLA	NA
22	B	615	CLA	NC
22	B	615	CLA	ND
22	B	615	CLA	NA
22	b	604	CLA	NC
22	b	604	CLA	ND
22	b	604	CLA	NA
22	B	602	CLA	NC
22	B	602	CLA	ND
22	B	602	CLA	NA
22	C	505	CLA	ND
22	C	505	CLA	NA
22	c	510	CLA	NC
22	c	510	CLA	ND
22	c	510	CLA	NA

All (1738) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	c	514	BCR	C7-C8-C9-C34
24	c	514	BCR	C11-C12-C13-C35
24	c	514	BCR	C35-C13-C14-C15
24	c	514	BCR	C16-C17-C18-C19
24	c	514	BCR	C16-C17-C18-C36
24	c	514	BCR	C20-C21-C22-C23
24	c	514	BCR	C20-C21-C22-C37
22	c	513	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	CHA-CBD-CGD-O1D
22	C	512	CLA	C11-C10-C8-C9
33	j	101	STE	C1-C2-C3-C4
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	CAD-CBD-CGD-O2D
22	b	614	CLA	C4-C3-C5-C6
24	b	618	BCR	C16-C17-C18-C36
33	b	624	STE	C1-C2-C3-C4
26	d	407	PL9	C32-C33-C34-C36
26	d	407	PL9	C38-C39-C41-C42

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Mol	Chain	Res	Type	Atoms
26	d	407	PL9	C42-C43-C44-C45
28	A	412	LHG	C3-O3-P-O5
30	A	415	DGD	C2B-C1B-O2G-C2G
30	A	415	DGD	O1B-C1B-O2G-C2G
24	t	101	BCR	C7-C8-C9-C34
22	A	406	CLA	C2-C3-C5-C6
22	A	406	CLA	C4-C3-C5-C6
24	d	406	BCR	C37-C22-C23-C24
28	e	101	LHG	C1-C2-C3-O3
28	e	101	LHG	O2-C2-C3-O3
28	e	101	LHG	C3-O3-P-O5
28	e	101	LHG	C4-O6-P-O5
28	e	101	LHG	O6-C4-C5-O7
28	e	101	LHG	O10-C23-O8-C6
22	b	616	CLA	CBD-CGD-O2D-CED
29	f	102	SQD	C2-C1-O6-C44
29	f	102	SQD	O5-C1-O6-C44
33	b	625	STE	C1-C2-C3-C4
24	A	407	BCR	C36-C18-C19-C20
24	Y	101	BCR	C1-C6-C7-C8
24	Y	101	BCR	C5-C6-C7-C8
24	Y	101	BCR	C37-C22-C23-C24
28	D	409	LHG	O1-C1-C2-C3
28	D	409	LHG	C3-O3-P-O5
28	D	409	LHG	C4-O6-P-O4
22	B	601	CLA	C1A-C2A-CAA-CBA
28	E	101	LHG	O1-C1-C2-C3
28	E	101	LHG	O10-C23-O8-C6
24	b	617	BCR	C1-C6-C7-C8
24	b	617	BCR	C20-C21-C22-C37
27	A	411	LMG	O9-C10-O7-C8
27	c	523	LMG	O6-C1-O1-C7
29	D	408	SQD	O5-C1-O6-C44
22	C	513	CLA	O2A-C1-C2-C3
28	d	408	LHG	O1-C1-C2-C3
28	d	408	LHG	C3-O3-P-O4
28	d	408	LHG	C4-O6-P-O4
28	d	408	LHG	C4-O6-P-O5
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	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	B	614	CLA	C2-C3-C5-C6
22	B	614	CLA	C4-C3-C5-C6
22	d	404	CLA	CHA-CBD-CGD-O1D
22	d	404	CLA	CHA-CBD-CGD-O2D
33	C	521	STE	C1-C2-C3-C4
33	R	101	STE	C1-C2-C3-C4
33	B	626	STE	C1-C2-C3-C4
27	D	410	LMG	O1-C7-C8-C9
27	D	410	LMG	O1-C7-C8-O7
24	C	516	BCR	C7-C8-C9-C34
24	C	516	BCR	C17-C18-C19-C20
24	C	516	BCR	C36-C18-C19-C20
24	C	516	BCR	C37-C22-C23-C24
28	B	622	LHG	O1-C1-C2-C3
29	A	414	SQD	C46-C45-O47-C7
29	B	623	SQD	O5-C1-O6-C44
29	B	623	SQD	O6-C44-C45-O47
29	B	623	SQD	O49-C7-O47-C45
28	a	410	LHG	C3-O3-P-O4
29	a	412	SQD	O6-C44-C45-O47
22	b	603	CLA	C4-C3-C5-C6
22	b	606	CLA	CHA-CBD-CGD-O1D
22	B	606	CLA	CHA-CBD-CGD-O1D
22	B	606	CLA	CHA-CBD-CGD-O2D
26	A	410	PL9	C9-C11-C12-C13
26	A	410	PL9	C12-C13-C14-C15
26	A	410	PL9	C12-C13-C14-C16
26	A	410	PL9	C22-C23-C24-C26
26	A	410	PL9	C23-C24-C26-C27
26	A	410	PL9	C37-C38-C39-C40
26	A	410	PL9	C37-C38-C39-C41
26	A	410	PL9	C43-C44-C46-C47
24	D	405	BCR	C36-C18-C19-C20
24	D	405	BCR	C23-C24-C25-C26
24	D	405	BCR	C23-C24-C25-C30
24	C	515	BCR	C11-C12-C13-C14
24	C	515	BCR	C37-C22-C23-C24
24	k	101	BCR	C5-C6-C7-C8
24	k	101	BCR	C7-C8-C9-C34
29	b	620	SQD	O10-C23-O48-C46
26	D	406	PL9	C32-C33-C34-C36
26	D	406	PL9	C33-C34-C36-C37

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Mol	Chain	Res	Type	Atoms
22	c	507	CLA	C4-C3-C5-C6
24	C	514	BCR	C11-C12-C13-C14
24	C	514	BCR	C11-C12-C13-C35
27	D	411	LMG	C28-C29-C30-C31
27	b	623	LMG	C11-C10-O7-C8
24	T	101	BCR	C7-C8-C9-C34
24	T	101	BCR	C11-C12-C13-C35
24	H	101	BCR	C11-C12-C13-C35
24	H	101	BCR	C23-C24-C25-C30
24	B	617	BCR	C35-C13-C14-C15
26	a	409	PL9	C12-C13-C14-C15
26	a	409	PL9	C17-C18-C19-C21
26	a	409	PL9	C19-C21-C22-C23
26	a	409	PL9	C22-C23-C24-C25
26	a	409	PL9	C22-C23-C24-C26
26	a	409	PL9	C24-C26-C27-C28
26	a	409	PL9	C32-C33-C34-C36
26	a	409	PL9	C37-C38-C39-C41
26	a	409	PL9	C42-C43-C44-C46
22	c	510	CLA	C11-C12-C13-C14
27	c	523	LMG	O10-C28-O8-C9
29	D	408	SQD	O10-C23-O48-C46
22	b	616	CLA	O1D-CGD-O2D-CED
28	e	101	LHG	C24-C23-O8-C6
28	E	101	LHG	C24-C23-O8-C6
29	D	408	SQD	C24-C23-O48-C46
29	b	620	SQD	C24-C23-O48-C46
27	c	522	LMG	O10-C28-O8-C9
29	f	102	SQD	O10-C23-O48-C46
29	a	412	SQD	O10-C23-O48-C46
27	M	101	LMG	O10-C28-O8-C9
22	c	513	CLA	O1D-CGD-O2D-CED
27	D	410	LMG	O9-C10-O7-C8
29	a	412	SQD	O49-C7-O47-C45
27	b	623	LMG	O9-C10-O7-C8
29	B	623	SQD	C45-C46-O48-C23
22	d	405	CLA	C3-C5-C6-C7
22	b	601	CLA	C3-C5-C6-C7
27	c	522	LMG	C29-C28-O8-C9
29	f	102	SQD	C24-C23-O48-C46
27	c	523	LMG	C29-C28-O8-C9
27	M	101	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
27	A	411	LMG	C11-C10-O7-C8
29	B	623	SQD	C8-C7-O47-C45
29	a	412	SQD	C8-C7-O47-C45
26	A	410	PL9	C47-C48-C49-C50
26	A	410	PL9	C47-C48-C49-C51
27	c	520	LMG	C11-C10-O7-C8
26	a	409	PL9	C35-C34-C36-C37
22	b	603	CLA	C2-C3-C5-C6
26	a	409	PL9	C33-C34-C36-C37
22	C	501	CLA	CBD-CGD-O2D-CED
22	b	606	CLA	C2A-CAA-CBA-CGA
22	b	602	CLA	C3-C5-C6-C7
26	d	407	PL9	C47-C48-C49-C51
26	A	410	PL9	C22-C23-C24-C25
29	A	414	SQD	O49-C7-O47-C45
22	B	601	CLA	O1A-CGA-O2A-C1
27	a	416	LMG	O6-C5-C6-O5
22	C	511	CLA	CBD-CGD-O2D-CED
22	C	510	CLA	CBD-CGD-O2D-CED
22	B	601	CLA	CBA-CGA-O2A-C1
29	a	412	SQD	C24-C23-O48-C46
27	C	520	LMG	C11-C10-O7-C8
29	b	620	SQD	C8-C7-O47-C45
30	C	517	DGD	C1B-C2B-C3B-C4B
22	c	508	CLA	CBD-CGD-O2D-CED
22	c	511	CLA	CBD-CGD-O2D-CED
22	b	609	CLA	CBD-CGD-O2D-CED
22	C	509	CLA	CBD-CGD-O2D-CED
27	a	416	LMG	C4-C5-C6-O5
33	D	412	STE	C13-C14-C15-C16
33	C	523	STE	C4-C5-C6-C7
26	a	409	PL9	C47-C48-C49-C50
26	d	407	PL9	C40-C39-C41-C42
22	B	603	CLA	C4-C3-C5-C6
22	C	504	CLA	C4-C3-C5-C6
22	b	605	CLA	C4-C3-C5-C6
22	b	614	CLA	C2-C3-C5-C6
22	B	603	CLA	C2-C3-C5-C6
22	C	504	CLA	C2-C3-C5-C6
22	b	605	CLA	C2-C3-C5-C6
22	c	507	CLA	C2-C3-C5-C6
29	b	620	SQD	O5-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
26	d	407	PL9	C34-C36-C37-C38
26	A	410	PL9	C34-C36-C37-C38
26	A	410	PL9	C44-C46-C47-C48
26	a	409	PL9	C34-C36-C37-C38
22	C	513	CLA	CBA-CGA-O2A-C1
27	d	410	LMG	C10-C11-C12-C13
27	D	410	LMG	C11-C10-O7-C8
26	d	407	PL9	C32-C33-C34-C35
26	D	406	PL9	C37-C38-C39-C40
28	E	101	LHG	C1-C2-C3-O3
27	a	416	LMG	C29-C28-O8-C9
22	B	616	CLA	CBA-CGA-O2A-C1
29	B	623	SQD	C24-C23-O48-C46
22	B	612	CLA	CBD-CGD-O2D-CED
33	d	412	STE	C2-C3-C4-C5
22	a	404	CLA	C10-C11-C12-C13
27	A	411	LMG	O6-C5-C6-O5
22	b	611	CLA	C15-C16-C17-C18
28	E	101	LHG	O2-C2-C3-O3
27	b	623	LMG	C28-C29-C30-C31
27	c	523	LMG	C2-C1-O1-C7
29	B	623	SQD	C2-C1-O6-C44
26	a	409	PL9	C20-C19-C21-C22
26	a	409	PL9	C23-C24-C26-C27
22	C	507	CLA	C11-C10-C8-C9
22	c	509	CLA	C6-C7-C8-C9
22	c	511	CLA	C14-C13-C15-C16
22	b	602	CLA	C11-C10-C8-C9
22	A	403	CLA	C14-C13-C15-C16
22	D	404	CLA	C11-C12-C13-C14
22	b	601	CLA	C14-C13-C15-C16
22	D	403	CLA	C14-C13-C15-C16
23	A	405	PHO	C6-C7-C8-C9
22	B	613	CLA	C11-C12-C13-C14
22	b	613	CLA	C11-C12-C13-C14
22	D	404	CLA	C10-C11-C12-C13
22	c	506	CLA	C15-C16-C17-C18
24	A	407	BCR	C11-C12-C13-C35
24	Y	101	BCR	C11-C12-C13-C35
24	C	515	BCR	C11-C12-C13-C35
24	C	515	BCR	C36-C18-C19-C20
24	k	101	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
24	H	101	BCR	C37-C22-C23-C24
27	a	416	LMG	C11-C10-O7-C8
28	a	410	LHG	C7-C8-C9-C10
22	B	616	CLA	O1A-CGA-O2A-C1
22	C	513	CLA	C15-C16-C17-C18
22	B	612	CLA	C13-C15-C16-C17
22	c	505	CLA	C5-C6-C7-C8
22	C	505	CLA	C5-C6-C7-C8
22	c	506	CLA	CBA-CGA-O2A-C1
22	a	404	CLA	C15-C16-C17-C18
22	d	401	CLA	C8-C10-C11-C12
22	b	611	CLA	C13-C15-C16-C17
22	C	509	CLA	C8-C10-C11-C12
22	c	512	CLA	C13-C15-C16-C17
22	C	503	CLA	C5-C6-C7-C8
22	B	602	CLA	C13-C15-C16-C17
22	C	505	CLA	C10-C11-C12-C13
22	c	510	CLA	C10-C11-C12-C13
22	c	510	CLA	C15-C16-C17-C18
27	d	410	LMG	C28-C29-C30-C31
28	E	101	LHG	C23-C24-C25-C26
27	D	410	LMG	C28-C29-C30-C31
30	C	519	DGD	C8A-C9A-CAA-CBA
24	C	514	BCR	C14-C15-C16-C17
22	b	607	CLA	C10-C11-C12-C13
22	b	611	CLA	C8-C10-C11-C12
22	B	614	CLA	C13-C15-C16-C17
22	B	613	CLA	C8-C10-C11-C12
28	d	409	LHG	C24-C25-C26-C27
26	A	410	PL9	C7-C8-C9-C10
30	c	517	DGD	C1B-C2B-C3B-C4B
30	c	519	DGD	C1A-C2A-C3A-C4A
27	D	407	LMG	C10-C11-C12-C13
28	B	622	LHG	C7-C8-C9-C10
28	B	622	LHG	C23-C24-C25-C26
28	a	410	LHG	C23-C24-C25-C26
30	h	101	DGD	O6E-C5E-C6E-O5E
22	B	605	CLA	C15-C16-C17-C18
22	C	508	CLA	C15-C16-C17-C18
22	C	512	CLA	C10-C11-C12-C13
22	b	615	CLA	C10-C11-C12-C13
22	B	606	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	B	616	CLA	C2-C1-O2A-CGA
22	C	506	CLA	C8-C10-C11-C12
22	B	609	CLA	C13-C15-C16-C17
22	B	601	CLA	C5-C6-C7-C8
27	c	520	LMG	C28-C29-C30-C31
22	B	611	CLA	C12-C13-C15-C16
22	b	613	CLA	C11-C10-C8-C7
22	c	505	CLA	C11-C10-C8-C7
22	c	510	CLA	C11-C12-C13-C15
22	c	506	CLA	O1A-CGA-O2A-C1
22	C	506	CLA	C15-C16-C17-C18
22	c	509	CLA	C13-C15-C16-C17
22	B	608	CLA	C15-C16-C17-C18
22	c	509	CLA	C10-C11-C12-C13
22	c	506	CLA	C13-C15-C16-C17
22	b	603	CLA	C13-C15-C16-C17
22	c	512	CLA	C8-C10-C11-C12
26	A	410	PL9	C39-C41-C42-C43
24	c	514	BCR	C18-C19-C20-C21
24	B	619	BCR	C10-C11-C12-C13
24	d	406	BCR	C18-C19-C20-C21
24	C	514	BCR	C18-C19-C20-C21
28	a	410	LHG	O2-C2-C3-O3
28	e	101	LHG	O9-C7-O7-C5
22	B	614	CLA	C3-C5-C6-C7
22	c	511	CLA	C13-C15-C16-C17
22	D	404	CLA	C13-C15-C16-C17
22	c	507	CLA	C5-C6-C7-C8
22	C	513	CLA	O1A-CGA-O2A-C1
27	m	101	LMG	C10-C11-C12-C13
22	c	511	CLA	C15-C16-C17-C18
22	b	601	CLA	C8-C10-C11-C12
22	B	601	CLA	C13-C15-C16-C17
27	A	411	LMG	C4-C5-C6-O5
22	c	503	CLA	C8-C10-C11-C12
22	B	611	CLA	C13-C15-C16-C17
22	C	505	CLA	C15-C16-C17-C18
22	c	510	CLA	C8-C10-C11-C12
28	l	101	LHG	C4-O6-P-O3
28	A	412	LHG	C3-O3-P-O6
28	e	101	LHG	C3-O3-P-O6
28	D	409	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
28	d	408	LHG	C3-O3-P-O6
28	d	408	LHG	C4-O6-P-O3
28	B	621	LHG	C4-O6-P-O3
28	a	410	LHG	C1-C2-C3-O3
27	c	522	LMG	O9-C10-O7-C8
26	A	410	PL9	C40-C39-C41-C42
26	A	410	PL9	C32-C33-C34-C36
22	b	614	CLA	C5-C6-C7-C8
22	B	606	CLA	C2A-CAA-CBA-CGA
24	c	514	BCR	C13-C14-C15-C16
33	t	103	STE	C5-C6-C7-C8
28	B	621	LHG	C17-C18-C19-C20
29	A	414	SQD	C12-C13-C14-C15
28	a	410	LHG	C10-C11-C12-C13
27	c	522	LMG	C11-C10-O7-C8
22	B	605	CLA	C8-C10-C11-C12
24	x	101	BCR	C16-C17-C18-C36
24	t	101	BCR	C35-C13-C14-C15
24	t	101	BCR	C16-C17-C18-C36
24	A	407	BCR	C35-C13-C14-C15
24	A	407	BCR	C20-C21-C22-C37
24	c	515	BCR	C16-C17-C18-C36
24	C	516	BCR	C11-C10-C9-C34
24	D	405	BCR	C20-C21-C22-C37
24	k	101	BCR	C35-C13-C14-C15
24	C	514	BCR	C16-C17-C18-C36
24	B	617	BCR	C16-C17-C18-C36
24	B	617	BCR	C20-C21-C22-C37
27	c	522	LMG	C16-C17-C18-C19
28	l	101	LHG	C29-C30-C31-C32
28	A	412	LHG	C29-C30-C31-C32
30	C	518	DGD	C5A-C6A-C7A-C8A
33	b	625	STE	C4-C5-C6-C7
33	m	102	STE	C3-C4-C5-C6
30	C	517	DGD	C5B-C6B-C7B-C8B
30	H	102	DGD	C7A-C8A-C9A-CAA
33	D	412	STE	C9-C10-C11-C12
29	B	623	SQD	C11-C12-C13-C14
29	a	412	SQD	C10-C11-C12-C13
30	C	519	DGD	CBA-CCA-CDA-CEA
27	b	623	LMG	C23-C24-C25-C26
22	d	403	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
22	b	607	CLA	C16-C17-C18-C20
22	c	512	CLA	CBA-CGA-O2A-C1
33	J	101	STE	C5-C6-C7-C8
33	t	103	STE	C11-C12-C13-C14
30	C	518	DGD	C9A-CAA-CBA-CCA
30	c	518	DGD	CCA-CDA-CEA-CFA
30	c	518	DGD	CAB-CBB-CCB-CDB
30	c	518	DGD	CBB-CCB-CDB-CEB
29	a	411	SQD	C17-C18-C19-C20
29	a	411	SQD	C25-C26-C27-C28
27	A	411	LMG	C35-C36-C37-C38
27	c	523	LMG	C15-C16-C17-C18
27	a	416	LMG	C15-C16-C17-C18
33	d	412	STE	C11-C12-C13-C14
28	B	621	LHG	C31-C32-C33-C34
27	C	520	LMG	C18-C19-C20-C21
27	b	623	LMG	C11-C12-C13-C14
22	b	610	CLA	C15-C16-C17-C18
33	b	621	STE	C4-C5-C6-C7
27	d	410	LMG	C33-C34-C35-C36
27	d	410	LMG	C36-C37-C38-C39
27	A	411	LMG	C11-C12-C13-C14
28	d	409	LHG	C32-C33-C34-C35
33	D	412	STE	C2-C3-C4-C5
33	B	620	STE	C4-C5-C6-C7
30	h	101	DGD	C5B-C6B-C7B-C8B
33	d	413	STE	C6-C7-C8-C9
27	D	411	LMG	C16-C17-C18-C19
27	c	522	LMG	C34-C35-C36-C37
30	A	415	DGD	C2A-C3A-C4A-C5A
27	c	520	LMG	C36-C37-C38-C39
30	C	518	DGD	C7B-C8B-C9B-CAB
33	k	102	STE	C6-C7-C8-C9
27	D	407	LMG	C32-C33-C34-C35
27	D	407	LMG	C34-C35-C36-C37
27	D	410	LMG	C14-C15-C16-C17
33	B	620	STE	C9-C10-C11-C12
29	b	620	SQD	C25-C26-C27-C28
30	h	101	DGD	C7A-C8A-C9A-CAA
27	M	101	LMG	C17-C18-C19-C20
27	D	411	LMG	C14-C15-C16-C17
28	A	412	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
28	D	409	LHG	O2-C2-C3-O3
27	A	411	LMG	C38-C39-C40-C41
27	a	416	LMG	C41-C42-C43-C44
28	d	408	LHG	C32-C33-C34-C35
28	B	622	LHG	C14-C15-C16-C17
29	A	414	SQD	C10-C11-C12-C13
22	d	403	CLA	C3-C5-C6-C7
22	c	512	CLA	C3-C5-C6-C7
22	C	501	CLA	O1D-CGD-O2D-CED
24	x	101	BCR	C11-C10-C9-C8
24	x	101	BCR	C16-C17-C18-C19
24	b	618	BCR	C20-C21-C22-C23
30	C	518	DGD	C2E-C1E-O5D-C6D
30	c	518	DGD	C2E-C1E-O5D-C6D
24	b	617	BCR	C20-C21-C22-C23
24	C	516	BCR	C20-C21-C22-C23
24	k	101	BCR	C11-C10-C9-C8
24	C	514	BCR	C11-C10-C9-C8
24	T	101	BCR	C12-C13-C14-C15
29	a	411	SQD	O6-C44-C45-O47
30	c	517	DGD	C7A-C8A-C9A-CAA
28	E	101	LHG	C9-C10-C11-C12
27	A	411	LMG	C14-C15-C16-C17
30	C	517	DGD	C8A-C9A-CAA-CBA
28	B	622	LHG	C27-C28-C29-C30
33	l	102	STE	C14-C15-C16-C17
22	c	511	CLA	C16-C17-C18-C19
22	a	402	CLA	C16-C17-C18-C19
22	B	616	CLA	C11-C12-C13-C15
26	D	406	PL9	C27-C28-C29-C30
26	D	406	PL9	C45-C44-C46-C47
33	b	627	STE	C11-C12-C13-C14
33	a	415	STE	C5-C6-C7-C8
33	a	415	STE	C9-C10-C11-C12
33	t	103	STE	C2-C3-C4-C5
28	A	412	LHG	C11-C12-C13-C14
30	C	518	DGD	CAB-CBB-CCB-CDB
28	D	409	LHG	C33-C34-C35-C36
27	c	523	LMG	C12-C13-C14-C15
28	d	408	LHG	C29-C30-C31-C32
27	D	407	LMG	C17-C18-C19-C20
26	d	407	PL9	C13-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
22	A	402	CLA	C14-C13-C15-C16
22	d	405	CLA	C6-C7-C8-C9
22	C	511	CLA	C6-C7-C8-C9
27	m	101	LMG	C33-C34-C35-C36
33	C	522	STE	C5-C6-C7-C8
28	l	101	LHG	C14-C15-C16-C17
28	A	412	LHG	C14-C15-C16-C17
30	A	415	DGD	CAA-CBA-CCA-CDA
30	C	518	DGD	CBA-CCA-CDA-CEA
28	D	409	LHG	C11-C12-C13-C14
27	A	411	LMG	C31-C32-C33-C34
28	d	409	LHG	C26-C27-C28-C29
33	D	412	STE	C7-C8-C9-C10
27	C	520	LMG	C32-C33-C34-C35
22	b	615	CLA	C5-C6-C7-C8
30	c	519	DGD	O1A-C1A-O1G-C1G
27	m	101	LMG	C14-C15-C16-C17
28	D	409	LHG	C25-C26-C27-C28
29	A	413	SQD	C9-C10-C11-C12
30	h	101	DGD	C9A-CAA-CBA-CCA
33	B	625	STE	C2-C3-C4-C5
33	B	625	STE	C12-C13-C14-C15
28	d	409	LHG	O1-C1-C2-C3
28	a	410	LHG	O1-C1-C2-C3
24	d	406	BCR	C21-C22-C23-C24
24	D	405	BCR	C21-C22-C23-C24
22	C	512	CLA	C3-C5-C6-C7
22	d	405	CLA	C10-C11-C12-C13
22	b	615	CLA	C15-C16-C17-C18
27	m	101	LMG	C32-C33-C34-C35
28	A	412	LHG	C32-C33-C34-C35
29	a	411	SQD	C29-C30-C31-C32
27	d	410	LMG	C30-C31-C32-C33
33	D	412	STE	C11-C12-C13-C14
28	a	410	LHG	C30-C31-C32-C33
27	M	101	LMG	C36-C37-C38-C39
22	b	609	CLA	O1D-CGD-O2D-CED
30	A	415	DGD	C4B-C5B-C6B-C7B
33	b	626	STE	C2-C3-C4-C5
33	c	521	STE	C9-C10-C11-C12
33	b	625	STE	C5-C6-C7-C8
33	T	102	STE	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
29	D	408	SQD	C32-C33-C34-C35
33	M	102	STE	C11-C10-C9-C8
30	H	102	DGD	C5B-C6B-C7B-C8B
33	B	626	STE	C2-C3-C4-C5
28	d	409	LHG	C34-C35-C36-C37
28	B	621	LHG	C14-C15-C16-C17
28	B	622	LHG	C29-C30-C31-C32
29	A	413	SQD	C11-C12-C13-C14
33	d	411	STE	C7-C8-C9-C10
33	B	625	STE	C3-C4-C5-C6
33	B	625	STE	C5-C6-C7-C8
22	a	402	CLA	C16-C17-C18-C20
22	d	405	CLA	C16-C17-C18-C20
22	d	403	CLA	C16-C17-C18-C20
22	b	607	CLA	C16-C17-C18-C19
22	B	606	CLA	C16-C17-C18-C19
22	B	615	CLA	C16-C17-C18-C20
30	C	518	DGD	O6E-C1E-O5D-C6D
22	C	506	CLA	C13-C15-C16-C17
22	C	510	CLA	O1D-CGD-O2D-CED
33	b	627	STE	C7-C8-C9-C10
33	b	621	STE	C7-C8-C9-C10
28	e	101	LHG	C26-C27-C28-C29
29	a	411	SQD	C34-C35-C36-C37
33	b	622	STE	C13-C14-C15-C16
33	T	102	STE	C3-C4-C5-C6
27	a	416	LMG	C12-C13-C14-C15
29	a	412	SQD	C11-C12-C13-C14
29	a	412	SQD	C15-C16-C17-C18
33	d	413	STE	C13-C14-C15-C16
27	b	623	LMG	C16-C17-C18-C19
22	C	513	CLA	CBD-CGD-O2D-CED
22	C	505	CLA	CBD-CGD-O2D-CED
22	c	508	CLA	O1D-CGD-O2D-CED
28	A	412	LHG	C30-C31-C32-C33
27	d	410	LMG	C32-C33-C34-C35
27	A	411	LMG	C36-C37-C38-C39
28	d	409	LHG	C29-C30-C31-C32
29	B	623	SQD	C28-C29-C30-C31
29	B	623	SQD	C34-C35-C36-C37
33	d	411	STE	C11-C12-C13-C14
27	D	411	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
33	H	103	STE	C11-C12-C13-C14
28	d	409	LHG	C23-C24-C25-C26
22	c	505	CLA	C15-C16-C17-C18
27	a	416	LMG	O10-C28-O8-C9
27	m	101	LMG	C16-C17-C18-C19
33	b	627	STE	C9-C10-C11-C12
33	a	415	STE	C2-C3-C4-C5
28	e	101	LHG	C13-C14-C15-C16
33	T	102	STE	C2-C3-C4-C5
27	A	411	LMG	C16-C17-C18-C19
27	a	416	LMG	C33-C34-C35-C36
30	C	517	DGD	C2A-C3A-C4A-C5A
28	B	621	LHG	C27-C28-C29-C30
29	a	412	SQD	C12-C13-C14-C15
22	B	605	CLA	C3-C5-C6-C7
33	t	102	STE	C6-C7-C8-C9
28	A	412	LHG	C34-C35-C36-C37
33	I	101	STE	C4-C5-C6-C7
29	a	411	SQD	C24-C25-C26-C27
27	A	411	LMG	C17-C18-C19-C20
28	d	408	LHG	C33-C34-C35-C36
28	B	622	LHG	C18-C19-C20-C21
30	h	101	DGD	C2B-C3B-C4B-C5B
27	D	411	LMG	C29-C30-C31-C32
22	B	601	CLA	C3A-C2A-CAA-CBA
22	C	512	CLA	C13-C15-C16-C17
22	b	601	CLA	C10-C11-C12-C13
27	m	101	LMG	C39-C40-C41-C42
27	c	522	LMG	C40-C41-C42-C43
30	A	415	DGD	C5B-C6B-C7B-C8B
28	e	101	LHG	C11-C10-C9-C8
29	f	102	SQD	C29-C30-C31-C32
33	T	102	STE	C11-C12-C13-C14
28	E	101	LHG	C27-C28-C29-C30
27	A	411	LMG	C33-C34-C35-C36
27	c	523	LMG	C33-C34-C35-C36
33	R	101	STE	C6-C7-C8-C9
29	B	623	SQD	C33-C34-C35-C36
29	A	413	SQD	C30-C31-C32-C33
22	c	511	CLA	C16-C17-C18-C20
22	B	606	CLA	C16-C17-C18-C20
27	c	522	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
28	A	412	LHG	C27-C28-C29-C30
30	A	415	DGD	CBB-CCB-CDB-CEB
29	a	411	SQD	O6-C44-C45-C46
27	a	416	LMG	O1-C7-C8-C9
33	a	415	STE	C3-C4-C5-C6
27	c	520	LMG	C33-C34-C35-C36
28	a	410	LHG	C14-C15-C16-C17
22	C	512	CLA	O2A-C1-C2-C3
28	E	101	LHG	C33-C34-C35-C36
22	c	512	CLA	O1A-CGA-O2A-C1
22	B	606	CLA	C8-C10-C11-C12
22	c	505	CLA	C2-C3-C5-C6
27	c	523	LMG	C11-C10-O7-C8
33	b	624	STE	C10-C11-C12-C13
29	B	623	SQD	C13-C14-C15-C16
33	H	103	STE	C13-C14-C15-C16
28	D	409	LHG	O1-C1-C2-O2
28	E	101	LHG	O1-C1-C2-O2
33	B	624	STE	C3-C4-C5-C6
33	D	412	STE	C6-C7-C8-C9
30	C	519	DGD	CAB-CBB-CCB-CDB
27	M	101	LMG	C14-C15-C16-C17
33	R	101	STE	C4-C5-C6-C7
22	A	402	CLA	C15-C16-C17-C18
27	c	522	LMG	C11-C12-C13-C14
30	c	517	DGD	C2A-C3A-C4A-C5A
29	A	413	SQD	C24-C25-C26-C27
27	b	623	LMG	C18-C19-C20-C21
33	d	413	STE	C9-C10-C11-C12
29	B	623	SQD	O10-C23-O48-C46
22	B	614	CLA	C8-C10-C11-C12
33	c	521	STE	C2-C3-C4-C5
29	f	102	SQD	C32-C33-C34-C35
27	D	410	LMG	C34-C35-C36-C37
27	M	101	LMG	O9-C10-O7-C8
26	d	407	PL9	C42-C43-C44-C46
33	b	627	STE	C10-C11-C12-C13
33	t	103	STE	C4-C5-C6-C7
27	A	411	LMG	C13-C14-C15-C16
27	a	416	LMG	C13-C14-C15-C16
30	C	517	DGD	CBA-CCA-CDA-CEA
33	d	412	STE	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
29	b	620	SQD	C27-C28-C29-C30
33	H	103	STE	C10-C11-C12-C13
27	b	623	LMG	C41-C42-C43-C44
29	D	408	SQD	C44-C45-C46-O48
30	A	415	DGD	CCB-CDB-CEB-CFB
33	b	621	STE	C5-C6-C7-C8
28	D	409	LHG	C28-C29-C30-C31
28	E	101	LHG	C11-C12-C13-C14
28	E	101	LHG	C32-C33-C34-C35
30	c	519	DGD	C3A-C4A-C5A-C6A
27	M	101	LMG	C38-C39-C40-C41
24	c	514	BCR	C1-C6-C7-C8
24	c	514	BCR	C5-C6-C7-C8
24	d	406	BCR	C23-C24-C25-C26
24	d	406	BCR	C23-C24-C25-C30
24	b	617	BCR	C5-C6-C7-C8
24	k	101	BCR	C1-C6-C7-C8
24	H	101	BCR	C23-C24-C25-C26
24	B	617	BCR	C1-C6-C7-C8
24	B	617	BCR	C5-C6-C7-C8
27	c	520	LMG	C39-C40-C41-C42
33	M	102	STE	C9-C10-C11-C12
33	C	521	STE	C6-C7-C8-C9
30	c	519	DGD	C8B-C9B-CAB-CBB
30	H	102	DGD	C6B-C7B-C8B-C9B
22	C	511	CLA	O1D-CGD-O2D-CED
22	C	510	CLA	C15-C16-C17-C18
28	e	101	LHG	C8-C7-O7-C5
33	b	625	STE	C3-C4-C5-C6
27	c	523	LMG	C37-C38-C39-C40
33	B	620	STE	C2-C3-C4-C5
33	B	625	STE	C9-C10-C11-C12
22	C	509	CLA	C5-C6-C7-C8
33	a	415	STE	C4-C5-C6-C7
30	C	518	DGD	CBB-CCB-CDB-CEB
33	b	625	STE	C7-C8-C9-C10
27	a	416	LMG	C36-C37-C38-C39
30	C	517	DGD	CCB-CDB-CEB-CFB
26	d	407	PL9	C45-C44-C46-C47
22	A	402	CLA	C12-C13-C15-C16
22	C	506	CLA	C12-C13-C15-C16
22	c	511	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	a	404	CLA	C11-C10-C8-C7
22	C	511	CLA	C6-C7-C8-C10
22	b	609	CLA	C2-C3-C5-C6
22	A	403	CLA	C12-C13-C15-C16
22	c	504	CLA	C11-C10-C8-C7
22	b	601	CLA	C11-C12-C13-C15
22	d	401	CLA	C11-C10-C8-C7
22	b	603	CLA	C11-C12-C13-C15
22	C	505	CLA	C12-C13-C15-C16
27	A	411	LMG	C34-C35-C36-C37
27	D	410	LMG	C33-C34-C35-C36
22	D	404	CLA	C5-C6-C7-C8
22	C	507	CLA	C16-C17-C18-C19
22	c	504	CLA	C11-C12-C13-C14
22	B	616	CLA	C11-C12-C13-C14
22	c	505	CLA	C16-C17-C18-C19
27	m	101	LMG	O9-C10-O7-C8
27	c	522	LMG	C10-C11-C12-C13
27	m	101	LMG	C29-C28-O8-C9
29	a	411	SQD	C24-C23-O48-C46
28	E	101	LHG	C29-C30-C31-C32
27	c	523	LMG	C30-C31-C32-C33
27	D	407	LMG	C21-C22-C23-C24
33	H	103	STE	C2-C3-C4-C5
22	B	612	CLA	C10-C11-C12-C13
27	m	101	LMG	C12-C13-C14-C15
28	E	101	LHG	C28-C29-C30-C31
28	B	621	LHG	C12-C13-C14-C15
28	a	410	LHG	C25-C26-C27-C28
33	T	102	STE	C11-C10-C9-C8
29	D	408	SQD	C31-C32-C33-C34
27	D	407	LMG	C38-C39-C40-C41
29	B	623	SQD	C9-C10-C11-C12
27	b	623	LMG	C10-C11-C12-C13
22	C	509	CLA	O1D-CGD-O2D-CED
28	e	101	LHG	C10-C11-C12-C13
22	B	616	CLA	C3-C5-C6-C7
22	c	511	CLA	O1D-CGD-O2D-CED
27	c	522	LMG	C41-C42-C43-C44
30	C	517	DGD	C3A-C4A-C5A-C6A
28	B	621	LHG	C29-C30-C31-C32
33	B	625	STE	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
27	D	410	LMG	C29-C28-O8-C9
22	c	512	CLA	C16-C17-C18-C19
30	c	518	DGD	O6E-C1E-O5D-C6D
26	A	410	PL9	C19-C21-C22-C23
27	m	101	LMG	C18-C19-C20-C21
27	m	101	LMG	C37-C38-C39-C40
28	l	101	LHG	C27-C28-C29-C30
30	C	518	DGD	C6B-C7B-C8B-C9B
29	A	414	SQD	C31-C32-C33-C34
30	h	101	DGD	CCA-CDA-CEA-CFA
27	b	623	LMG	C32-C33-C34-C35
27	M	101	LMG	C11-C10-O7-C8
24	t	101	BCR	C10-C11-C12-C13
33	b	625	STE	C2-C3-C4-C5
33	T	102	STE	C9-C10-C11-C12
27	D	407	LMG	C30-C31-C32-C33
28	a	410	LHG	C15-C16-C17-C18
22	C	509	CLA	C13-C15-C16-C17
33	b	625	STE	C11-C10-C9-C8
29	A	413	SQD	C16-C17-C18-C19
29	D	408	SQD	C2-C1-O6-C44
30	A	415	DGD	O2G-C2G-C3G-O3G
29	a	411	SQD	O47-C45-C46-O48
27	b	623	LMG	O6-C5-C6-O5
33	R	101	STE	C3-C4-C5-C6
22	b	601	CLA	C16-C17-C18-C20
22	D	403	CLA	C16-C17-C18-C20
22	C	509	CLA	C16-C17-C18-C19
33	C	522	STE	C2-C3-C4-C5
33	t	103	STE	C10-C11-C12-C13
33	m	102	STE	C4-C5-C6-C7
27	a	416	LMG	C30-C31-C32-C33
28	B	622	LHG	C28-C29-C30-C31
27	D	407	LMG	O6-C5-C6-O5
22	b	609	CLA	C4-C3-C5-C6
26	D	406	PL9	C35-C34-C36-C37
22	c	505	CLA	C4-C3-C5-C6
22	c	510	CLA	C2-C3-C5-C6
29	D	408	SQD	C30-C31-C32-C33
22	a	402	CLA	C14-C13-C15-C16
22	B	603	CLA	C11-C12-C13-C14
22	d	405	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	a	404	CLA	C11-C10-C8-C9
22	c	504	CLA	C11-C10-C8-C9
22	b	601	CLA	C11-C12-C13-C14
22	B	610	CLA	C14-C13-C15-C16
22	b	603	CLA	C11-C12-C13-C14
22	b	613	CLA	C11-C10-C8-C9
22	c	505	CLA	C11-C10-C8-C9
22	C	505	CLA	C14-C13-C15-C16
28	e	101	LHG	C25-C26-C27-C28
28	E	101	LHG	C15-C16-C17-C18
28	d	409	LHG	C25-C26-C27-C28
30	C	518	DGD	C6A-C7A-C8A-C9A
30	c	518	DGD	C1B-C2B-C3B-C4B
22	C	509	CLA	C10-C11-C12-C13
22	c	512	CLA	C5-C6-C7-C8
22	b	613	CLA	C13-C15-C16-C17
27	c	522	LMG	C14-C15-C16-C17
28	D	409	LHG	C29-C30-C31-C32
27	d	410	LMG	C12-C13-C14-C15
27	c	523	LMG	C31-C32-C33-C34
29	A	413	SQD	C14-C15-C16-C17
30	C	519	DGD	C5A-C6A-C7A-C8A
22	c	513	CLA	C1A-C2A-CAA-CBA
22	c	511	CLA	C1A-C2A-CAA-CBA
22	C	507	CLA	C16-C17-C18-C20
22	C	509	CLA	C16-C17-C18-C20
22	c	512	CLA	C16-C17-C18-C20
27	C	520	LMG	O9-C10-O7-C8
33	b	624	STE	C3-C4-C5-C6
28	l	101	LHG	C17-C18-C19-C20
33	b	621	STE	C10-C11-C12-C13
27	M	101	LMG	C11-C12-C13-C14
22	c	503	CLA	C5-C6-C7-C8
22	B	602	CLA	C8-C10-C11-C12
28	e	101	LHG	C4-O6-P-O3
28	a	410	LHG	C3-O3-P-O6
22	b	613	CLA	CBD-CGD-O2D-CED
22	C	513	CLA	O1D-CGD-O2D-CED
27	a	416	LMG	C23-C24-C25-C26
22	C	512	CLA	C15-C16-C17-C18
28	l	101	LHG	O6-C4-C5-C6
26	a	409	PL9	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
28	e	101	LHG	C7-C8-C9-C10
28	B	621	LHG	C7-C8-C9-C10
29	f	102	SQD	C24-C25-C26-C27
30	C	517	DGD	C8B-C9B-CAB-CBB
22	B	613	CLA	C16-C17-C18-C20
30	A	415	DGD	C5A-C6A-C7A-C8A
29	A	414	SQD	C14-C15-C16-C17
22	C	510	CLA	C10-C11-C12-C13
27	c	523	LMG	C17-C18-C19-C20
27	C	520	LMG	C15-C16-C17-C18
22	c	510	CLA	C4-C3-C5-C6
28	D	409	LHG	C34-C35-C36-C37
33	k	102	STE	C2-C3-C4-C5
27	D	407	LMG	C20-C21-C22-C23
33	B	620	STE	C11-C12-C13-C14
30	h	101	DGD	CBA-CCA-CDA-CEA
27	M	101	LMG	C20-C21-C22-C23
27	M	101	LMG	C29-C30-C31-C32
33	J	101	STE	C6-C7-C8-C9
33	b	622	STE	C10-C11-C12-C13
33	b	622	STE	C14-C15-C16-C17
30	c	519	DGD	C4B-C5B-C6B-C7B
27	D	407	LMG	C15-C16-C17-C18
27	D	407	LMG	C39-C40-C41-C42
27	m	101	LMG	C20-C21-C22-C23
27	c	520	LMG	C38-C39-C40-C41
30	c	518	DGD	C6A-C7A-C8A-C9A
27	c	523	LMG	C13-C14-C15-C16
30	h	101	DGD	C3B-C4B-C5B-C6B
33	d	413	STE	C2-C3-C4-C5
22	B	611	CLA	C8-C10-C11-C12
27	c	522	LMG	C7-C8-C9-O8
30	A	415	DGD	C1G-C2G-C3G-O3G
29	a	411	SQD	C44-C45-C46-O48
28	E	101	LHG	C4-C5-C6-O8
27	c	523	LMG	O1-C7-C8-C9
30	c	519	DGD	CCB-CDB-CEB-CFB
29	B	623	SQD	O6-C44-C45-C46
27	M	101	LMG	C7-C8-C9-O8
30	c	518	DGD	C7B-C8B-C9B-CAB
29	a	412	SQD	C31-C32-C33-C34
30	h	101	DGD	CAB-CBB-CCB-CDB

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Mol	Chain	Res	Type	Atoms
30	c	518	DGD	C1A-C2A-C3A-C4A
28	D	409	LHG	C23-C24-C25-C26
30	C	518	DGD	C2G-C3G-O3G-C1D
30	c	518	DGD	C2G-C3G-O3G-C1D
30	c	518	DGD	C5D-C6D-O5D-C1E
27	a	416	LMG	C8-C7-O1-C1
22	B	612	CLA	O1D-CGD-O2D-CED
33	t	103	STE	C7-C8-C9-C10
27	a	416	LMG	C17-C18-C19-C20
29	B	623	SQD	C29-C30-C31-C32
30	H	102	DGD	O2G-C1B-C2B-C3B
27	D	410	LMG	C10-C11-C12-C13
30	C	517	DGD	CDA-CEA-CFA-CGA
30	C	519	DGD	CDA-CEA-CFA-CGA
29	b	620	SQD	C10-C11-C12-C13
33	B	625	STE	C4-C5-C6-C7
28	B	622	LHG	O1-C1-C2-O2
30	A	415	DGD	CEA-CFA-CGA-CHA
28	E	101	LHG	C19-C20-C21-C22
33	B	624	STE	C7-C8-C9-C10
22	a	404	CLA	C5-C6-C7-C8
30	c	517	DGD	C8B-C9B-CAB-CBB
27	D	410	LMG	C15-C16-C17-C18
33	j	101	STE	C2-C3-C4-C5
33	j	101	STE	C4-C5-C6-C7
27	A	411	LMG	C40-C41-C42-C43
27	b	623	LMG	C24-C25-C26-C27
24	d	406	BCR	C16-C17-C18-C36
24	A	407	BCR	C11-C10-C9-C34
22	C	505	CLA	C4-C3-C5-C6
27	b	623	LMG	C42-C43-C44-C45
30	C	517	DGD	O6E-C5E-C6E-O5E
28	A	412	LHG	C9-C10-C11-C12
30	C	518	DGD	CDA-CEA-CFA-CGA
33	H	103	STE	C1-C2-C3-C4
22	b	607	CLA	CBD-CGD-O2D-CED
22	D	402	CLA	C15-C16-C17-C18
30	c	518	DGD	C5B-C6B-C7B-C8B
33	d	413	STE	C15-C16-C17-C18
29	b	620	SQD	C46-C45-O47-C7
27	d	410	LMG	O6-C5-C6-O5
30	C	518	DGD	O1A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
22	b	614	CLA	C8-C10-C11-C12
22	c	506	CLA	C8-C10-C11-C12
28	A	412	LHG	C17-C18-C19-C20
30	C	518	DGD	CDB-CEB-CFB-CGB
30	c	517	DGD	O6E-C5E-C6E-O5E
27	c	522	LMG	C38-C39-C40-C41
30	H	102	DGD	CBA-CCA-CDA-CEA
28	E	101	LHG	C25-C26-C27-C28
29	b	620	SQD	C19-C20-C21-C22
27	M	101	LMG	C31-C32-C33-C34
22	b	611	CLA	C16-C17-C18-C19
27	c	522	LMG	C29-C30-C31-C32
27	m	101	LMG	C31-C32-C33-C34
22	B	616	CLA	C5-C6-C7-C8
24	B	619	BCR	C12-C13-C14-C15
24	C	514	BCR	C12-C13-C14-C15
29	a	411	SQD	C18-C19-C20-C21
33	m	102	STE	C7-C8-C9-C10
27	D	407	LMG	C35-C36-C37-C38
29	A	413	SQD	C34-C35-C36-C37
33	d	411	STE	C10-C11-C12-C13
28	l	101	LHG	C13-C14-C15-C16
28	e	101	LHG	C14-C15-C16-C17
29	A	413	SQD	C26-C27-C28-C29
26	a	409	PL9	C40-C39-C41-C42
33	c	521	STE	C10-C11-C12-C13
22	c	513	CLA	C11-C12-C13-C15
22	c	508	CLA	C12-C13-C15-C16
22	C	512	CLA	C11-C12-C13-C15
22	C	507	CLA	C11-C10-C8-C7
26	d	407	PL9	C43-C44-C46-C47
22	c	509	CLA	C6-C7-C8-C10
22	a	402	CLA	C12-C13-C15-C16
22	B	603	CLA	C11-C12-C13-C15
22	d	405	CLA	C11-C12-C13-C15
22	b	609	CLA	C12-C13-C15-C16
22	C	502	CLA	C12-C13-C15-C16
22	A	403	CLA	C11-C12-C13-C15
22	d	401	CLA	C6-C7-C8-C10
22	b	607	CLA	C6-C7-C8-C10
22	c	506	CLA	C6-C7-C8-C10
22	c	506	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	B	615	CLA	C6-C7-C8-C10
22	B	615	CLA	C11-C12-C13-C15
30	C	517	DGD	C4B-C5B-C6B-C7B
33	H	103	STE	C3-C4-C5-C6
22	c	513	CLA	C11-C12-C13-C14
22	c	508	CLA	C14-C13-C15-C16
22	C	512	CLA	C11-C12-C13-C14
22	C	506	CLA	C14-C13-C15-C16
22	d	405	CLA	C14-C13-C15-C16
22	B	611	CLA	C14-C13-C15-C16
22	A	403	CLA	C11-C12-C13-C14
22	d	401	CLA	C6-C7-C8-C9
22	d	401	CLA	C11-C10-C8-C9
22	b	607	CLA	C6-C7-C8-C9
22	c	506	CLA	C6-C7-C8-C9
22	c	506	CLA	C11-C12-C13-C14
22	B	604	CLA	C14-C13-C15-C16
22	B	615	CLA	C11-C12-C13-C14
22	b	604	CLA	C14-C13-C15-C16
24	b	617	BCR	C14-C15-C16-C17
33	b	627	STE	C6-C7-C8-C9
33	b	624	STE	C5-C6-C7-C8
30	A	415	DGD	C6B-C7B-C8B-C9B
28	D	409	LHG	C10-C11-C12-C13
28	B	622	LHG	C19-C20-C21-C22
22	D	403	CLA	C13-C15-C16-C17
27	M	101	LMG	C40-C41-C42-C43
24	a	405	BCR	C37-C22-C23-C24
30	c	517	DGD	CBB-CCB-CDB-CEB
29	B	623	SQD	C17-C18-C19-C20
29	A	413	SQD	C17-C18-C19-C20
24	c	514	BCR	C21-C22-C23-C24
27	C	520	LMG	C14-C15-C16-C17
30	c	517	DGD	O6D-C5D-C6D-O5D
33	b	625	STE	C6-C7-C8-C9
28	D	409	LHG	C17-C18-C19-C20
27	a	416	LMG	C32-C33-C34-C35
27	C	520	LMG	C29-C28-O8-C9
27	m	101	LMG	C11-C12-C13-C14
27	m	101	LMG	C22-C23-C24-C25
33	b	624	STE	C11-C12-C13-C14
30	A	415	DGD	CDB-CEB-CFB-CGB

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Mol	Chain	Res	Type	Atoms
30	h	101	DGD	C5A-C6A-C7A-C8A
30	h	101	DGD	C6B-C7B-C8B-C9B
22	C	504	CLA	C5-C6-C7-C8
33	a	413	STE	C2-C3-C4-C5
22	d	405	CLA	C16-C17-C18-C19
22	b	615	CLA	C16-C17-C18-C19
22	A	403	CLA	C15-C16-C17-C18
33	a	413	STE	C4-C5-C6-C7
33	J	101	STE	C3-C4-C5-C6
33	T	102	STE	C6-C7-C8-C9
33	M	102	STE	C4-C5-C6-C7
33	d	412	STE	C3-C4-C5-C6
33	D	412	STE	C11-C10-C9-C8
28	A	412	LHG	C11-C10-C9-C8
30	A	415	DGD	C2B-C3B-C4B-C5B
33	b	621	STE	C13-C14-C15-C16
29	A	414	SQD	C16-C17-C18-C19
27	M	101	LMG	C39-C40-C41-C42
26	a	409	PL9	C25-C24-C26-C27
26	D	406	PL9	C43-C44-C46-C47
22	C	505	CLA	C2-C3-C5-C6
30	c	517	DGD	C1A-C2A-C3A-C4A
33	m	102	STE	C5-C6-C7-C8
30	c	519	DGD	C5B-C6B-C7B-C8B
28	d	408	LHG	O9-C7-O7-C5
22	D	402	CLA	C16-C17-C18-C20
28	A	412	LHG	C25-C26-C27-C28
28	B	621	LHG	C10-C11-C12-C13
30	C	517	DGD	O6D-C5D-C6D-O5D
27	c	522	LMG	C32-C33-C34-C35
30	c	518	DGD	CDA-CEA-CFA-CGA
30	h	101	DGD	CDB-CEB-CFB-CGB
22	C	502	CLA	C15-C16-C17-C18
33	b	626	STE	C5-C6-C7-C8
28	a	410	LHG	C16-C17-C18-C19
30	C	519	DGD	O6D-C5D-C6D-O5D
30	H	102	DGD	CCB-CDB-CEB-CFB
22	b	607	CLA	C8-C10-C11-C12
30	A	415	DGD	O1G-C1G-C2G-C3G
29	A	414	SQD	C44-C45-C46-O48
29	a	412	SQD	C44-C45-C46-O48
29	b	620	SQD	O49-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
28	e	101	LHG	C16-C17-C18-C19
23	a	403	PHO	O2A-C1-C2-C3
22	b	614	CLA	C15-C16-C17-C18
33	b	622	STE	C5-C6-C7-C8
27	C	520	LMG	C30-C31-C32-C33
30	h	101	DGD	C1A-C2A-C3A-C4A
30	c	518	DGD	C7A-C8A-C9A-CAA
30	H	102	DGD	CAB-CBB-CCB-CDB
22	D	403	CLA	C16-C17-C18-C19
30	c	517	DGD	CDB-CEB-CFB-CGB
33	k	102	STE	C5-C6-C7-C8
27	b	623	LMG	C37-C38-C39-C40
28	d	408	LHG	O1-C1-C2-O2
28	d	409	LHG	O1-C1-C2-O2
22	b	616	CLA	C10-C11-C12-C13
27	a	416	LMG	C35-C36-C37-C38
28	a	410	LHG	C29-C30-C31-C32
28	l	101	LHG	O6-C4-C5-O7
28	B	621	LHG	O6-C4-C5-O7
26	a	409	PL9	C17-C18-C19-C20
22	D	402	CLA	C16-C17-C18-C19
22	B	611	CLA	C16-C17-C18-C20
22	c	504	CLA	C11-C12-C13-C15
22	b	601	CLA	C16-C17-C18-C19
22	B	607	CLA	C16-C17-C18-C20
22	c	505	CLA	C16-C17-C18-C20
29	b	620	SQD	C13-C14-C15-C16
30	h	101	DGD	O2G-C1B-C2B-C3B
30	C	518	DGD	C3A-C4A-C5A-C6A
29	a	411	SQD	C11-C12-C13-C14
27	D	410	LMG	C16-C17-C18-C19
30	C	519	DGD	C3A-C4A-C5A-C6A
29	A	414	SQD	O47-C45-C46-O48
30	H	102	DGD	C3B-C4B-C5B-C6B
29	A	413	SQD	O6-C44-C45-O47
28	A	412	LHG	C12-C13-C14-C15
28	e	101	LHG	C28-C29-C30-C31
33	B	626	STE	C5-C6-C7-C8
33	l	102	STE	C9-C10-C11-C12
22	d	403	CLA	C2-C1-O2A-CGA
26	d	407	PL9	C28-C29-C31-C32
33	H	103	STE	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	c	507	CLA	C15-C16-C17-C18
22	c	509	CLA	C11-C12-C13-C14
22	b	616	CLA	C11-C10-C8-C9
22	b	607	CLA	C11-C10-C8-C9
22	b	607	CLA	C11-C12-C13-C14
22	c	512	CLA	C14-C13-C15-C16
30	c	517	DGD	C2B-C3B-C4B-C5B
30	A	415	DGD	CBA-CCA-CDA-CEA
29	A	414	SQD	C9-C10-C11-C12
27	M	101	LMG	C12-C13-C14-C15
22	c	510	CLA	C5-C6-C7-C8
33	b	621	STE	C6-C7-C8-C9
28	e	101	LHG	C27-C28-C29-C30
28	E	101	LHG	C24-C25-C26-C27
28	B	622	LHG	C12-C13-C14-C15
27	C	520	LMG	C12-C13-C14-C15
22	B	604	CLA	C2C-C3C-CAC-CBC
22	B	613	CLA	C16-C17-C18-C19
22	B	615	CLA	C16-C17-C18-C19
24	x	101	BCR	C23-C24-C25-C26
24	x	101	BCR	C23-C24-C25-C30
24	C	516	BCR	C23-C24-C25-C26
24	C	516	BCR	C23-C24-C25-C30
27	d	410	LMG	C14-C15-C16-C17
30	h	101	DGD	C9B-CAB-CBB-CCB
22	a	404	CLA	CBA-CGA-O2A-C1
24	c	515	BCR	C21-C22-C23-C24
24	C	516	BCR	C7-C8-C9-C10
24	k	101	BCR	C17-C18-C19-C20
24	k	101	BCR	C21-C22-C23-C24
30	c	519	DGD	O6D-C5D-C6D-O5D
29	f	102	SQD	O49-C7-O47-C45
24	A	407	BCR	C14-C15-C16-C17
29	A	414	SQD	C8-C7-O47-C45
33	C	522	STE	C1-C2-C3-C4
28	B	622	LHG	C25-C26-C27-C28
33	l	102	STE	C1-C2-C3-C4
28	d	408	LHG	C11-C12-C13-C14
27	M	101	LMG	C19-C20-C21-C22
22	b	611	CLA	C16-C17-C18-C20
30	c	518	DGD	C8B-C9B-CAB-CBB
30	H	102	DGD	CCA-CDA-CEA-CFA

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Mol	Chain	Res	Type	Atoms
28	B	621	LHG	C16-C17-C18-C19
33	d	411	STE	C4-C5-C6-C7
29	D	408	SQD	O6-C44-C45-C46
28	e	101	LHG	O6-C4-C5-C6
28	B	621	LHG	O6-C4-C5-C6
22	B	605	CLA	C11-C10-C8-C7
22	C	512	CLA	C11-C10-C8-C7
22	C	512	CLA	C12-C13-C15-C16
22	d	405	CLA	C12-C13-C15-C16
22	C	510	CLA	C11-C10-C8-C7
22	D	404	CLA	C11-C10-C8-C7
22	d	401	CLA	C11-C12-C13-C15
22	d	401	CLA	C12-C13-C15-C16
22	b	615	CLA	C11-C10-C8-C7
22	b	607	CLA	C11-C12-C13-C15
22	c	512	CLA	C11-C12-C13-C15
22	c	512	CLA	C12-C13-C15-C16
22	B	604	CLA	C11-C12-C13-C15
22	B	604	CLA	C12-C13-C15-C16
22	b	613	CLA	C11-C12-C13-C15
22	b	604	CLA	C12-C13-C15-C16
29	A	414	SQD	C32-C33-C34-C35
24	c	514	BCR	C15-C16-C17-C18
24	C	514	BCR	C9-C10-C11-C12
22	B	607	CLA	C16-C17-C18-C19
30	c	517	DGD	C4B-C5B-C6B-C7B
33	Z	101	STE	C11-C12-C13-C14
30	C	517	DGD	C5A-C6A-C7A-C8A
22	c	512	CLA	C2A-CAA-CBA-CGA
24	c	514	BCR	C11-C10-C9-C34
24	Y	101	BCR	C35-C13-C14-C15
24	c	515	BCR	C20-C21-C22-C37
24	C	515	BCR	C11-C10-C9-C34
24	k	101	BCR	C11-C10-C9-C34
24	C	514	BCR	C20-C21-C22-C37
24	B	617	BCR	C11-C10-C9-C34
29	a	411	SQD	C27-C28-C29-C30
28	d	408	LHG	C31-C32-C33-C34
28	a	410	LHG	C28-C29-C30-C31
22	B	606	CLA	C13-C15-C16-C17
30	c	517	DGD	O1G-C1A-C2A-C3A
27	a	416	LMG	O8-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
30	H	102	DGD	C8B-C9B-CAB-CBB
33	B	626	STE	C4-C5-C6-C7
22	C	513	CLA	C5-C6-C7-C8
27	b	623	LMG	C31-C32-C33-C34
22	c	503	CLA	CAD-CBD-CGD-O2D
22	c	509	CLA	CAD-CBD-CGD-O2D
22	b	616	CLA	CAD-CBD-CGD-O2D
23	a	403	PHO	CAD-CBD-CGD-O2D
22	c	510	CLA	CAD-CBD-CGD-O2D
26	a	409	PL9	C42-C43-C44-C45
33	b	626	STE	C4-C5-C6-C7
30	H	102	DGD	C9A-CAA-CBA-CCA
27	D	407	LMG	C16-C17-C18-C19
28	a	410	LHG	C32-C33-C34-C35
27	b	623	LMG	C12-C13-C14-C15
33	l	102	STE	C7-C8-C9-C10
22	b	609	CLA	C15-C16-C17-C18
29	D	408	SQD	C29-C30-C31-C32
33	C	523	STE	C5-C6-C7-C8
22	C	506	CLA	C4-C3-C5-C6
22	B	609	CLA	C16-C17-C18-C19
27	c	520	LMG	C35-C36-C37-C38
26	A	410	PL9	C24-C26-C27-C28
27	c	522	LMG	O1-C7-C8-C9
30	c	517	DGD	O1G-C1G-C2G-C3G
27	m	101	LMG	C19-C20-C21-C22
33	C	521	STE	C3-C4-C5-C6
33	a	413	STE	C5-C6-C7-C8
33	H	103	STE	C12-C13-C14-C15
22	B	610	CLA	C16-C17-C18-C19
27	m	101	LMG	C38-C39-C40-C41
33	T	102	STE	C5-C6-C7-C8
22	C	508	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	504	CLA	CHA-CBD-CGD-O2D
22	C	504	CLA	CHA-CBD-CGD-O1D
22	C	504	CLA	CHA-CBD-CGD-O2D
22	d	401	CLA	CHA-CBD-CGD-O2D
22	c	502	CLA	CHA-CBD-CGD-O1D
22	c	502	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	B	601	CLA	CHA-CBD-CGD-O1D
22	B	601	CLA	CHA-CBD-CGD-O2D
22	D	403	CLA	CHA-CBD-CGD-O1D
22	D	403	CLA	CHA-CBD-CGD-O2D
22	B	607	CLA	CHA-CBD-CGD-O1D
22	B	607	CLA	CHA-CBD-CGD-O2D
22	b	606	CLA	CHA-CBD-CGD-O2D
22	c	507	CLA	CHA-CBD-CGD-O1D
33	I	101	STE	C7-C8-C9-C10
28	B	621	LHG	C32-C33-C34-C35
27	m	101	LMG	O10-C28-O8-C9
30	c	517	DGD	O1A-C1A-O1G-C1G
33	D	412	STE	C4-C5-C6-C7
24	B	619	BCR	C11-C10-C9-C8
24	B	617	BCR	C12-C13-C14-C15
27	c	522	LMG	O7-C8-C9-O8
30	c	517	DGD	O1G-C1G-C2G-O2G
30	A	415	DGD	O1G-C1G-C2G-O2G
27	c	523	LMG	O1-C7-C8-O7
29	a	412	SQD	O47-C45-C46-O48
29	b	620	SQD	O47-C45-C46-O48
27	a	416	LMG	C20-C21-C22-C23
28	d	408	LHG	C12-C13-C14-C15
30	c	519	DGD	C8A-C9A-CAA-CBA
22	c	509	CLA	CAA-CBA-CGA-O2A
27	c	520	LMG	C31-C32-C33-C34
29	f	102	SQD	C33-C34-C35-C36
22	D	404	CLA	C16-C17-C18-C19
28	a	410	LHG	O1-C1-C2-O2
28	E	101	LHG	C34-C35-C36-C37
29	a	412	SQD	C29-C30-C31-C32
30	c	517	DGD	C4A-C5A-C6A-C7A
28	l	101	LHG	C19-C20-C21-C22
27	b	623	LMG	O10-C28-O8-C9
26	a	409	PL9	C4-C3-C7-C8
30	H	102	DGD	CDA-CEA-CFA-CGA
30	C	517	DGD	O1G-C1A-C2A-C3A
22	B	614	CLA	C6-C7-C8-C9
22	B	604	CLA	C11-C12-C13-C14
22	B	614	CLA	O1D-CGD-O2D-CED
27	m	101	LMG	C30-C31-C32-C33
22	b	604	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	d	401	CLA	C16-C17-C18-C20
27	C	520	LMG	C37-C38-C39-C40
27	c	522	LMG	C36-C37-C38-C39
28	d	408	LHG	C19-C20-C21-C22
33	l	102	STE	C2-C3-C4-C5
30	C	517	DGD	C4D-C5D-C6D-O5D
24	b	618	BCR	C37-C22-C23-C24
24	B	617	BCR	C11-C12-C13-C35
30	C	518	DGD	C9B-CAB-CBB-CCB
30	C	517	DGD	C9B-CAB-CBB-CCB
28	B	621	LHG	C34-C35-C36-C37
22	C	508	CLA	C1A-C2A-CAA-CBA
33	c	521	STE	C1-C2-C3-C4
33	b	622	STE	C1-C2-C3-C4
22	b	601	CLA	C1A-C2A-CAA-CBA
33	k	102	STE	C1-C2-C3-C4
22	C	513	CLA	C1A-C2A-CAA-CBA
22	c	512	CLA	C1A-C2A-CAA-CBA
22	c	506	CLA	C2-C1-O2A-CGA
29	D	408	SQD	C27-C28-C29-C30
29	a	412	SQD	C14-C15-C16-C17
24	T	101	BCR	C13-C14-C15-C16
33	a	415	STE	C10-C11-C12-C13
29	B	623	SQD	C35-C36-C37-C38
33	d	411	STE	C12-C13-C14-C15
28	B	621	LHG	C23-C24-C25-C26
27	m	101	LMG	C17-C18-C19-C20
33	b	622	STE	C11-C12-C13-C14
30	c	517	DGD	C4D-C5D-C6D-O5D
26	A	410	PL9	C18-C19-C21-C22
28	l	101	LHG	C34-C35-C36-C37
27	A	411	LMG	C30-C31-C32-C33
22	d	404	CLA	C2C-C3C-CAC-CBC
33	B	620	STE	C7-C8-C9-C10
28	l	101	LHG	C4-O6-P-O5
28	e	101	LHG	C4-O6-P-O4
28	D	409	LHG	C4-O6-P-O5
28	B	621	LHG	C4-O6-P-O5
28	a	410	LHG	C3-O3-P-O5
22	b	615	CLA	C16-C17-C18-C20
30	A	415	DGD	O6D-C1D-O3G-C3G
22	b	607	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	c	501	CLA	CBD-CGD-O2D-CED
30	c	517	DGD	C3B-C4B-C5B-C6B
28	e	101	LHG	C12-C13-C14-C15
29	a	411	SQD	C10-C11-C12-C13
22	B	610	CLA	C15-C16-C17-C18
28	d	408	LHG	C26-C27-C28-C29
22	c	510	CLA	C16-C17-C18-C19
27	c	522	LMG	C31-C32-C33-C34
29	a	411	SQD	C11-C10-C9-C8
28	D	409	LHG	C11-C10-C9-C8
22	C	506	CLA	CAD-CBD-CGD-O1D
22	C	502	CLA	CAD-CBD-CGD-O1D
22	c	504	CLA	CAD-CBD-CGD-O1D
22	C	504	CLA	CAD-CBD-CGD-O1D
22	c	502	CLA	CAD-CBD-CGD-O1D
22	B	601	CLA	CAD-CBD-CGD-O1D
22	B	607	CLA	CAD-CBD-CGD-O1D
27	m	101	LMG	C28-C29-C30-C31
29	B	623	SQD	C27-C28-C29-C30
33	l	102	STE	C10-C11-C12-C13
30	C	518	DGD	C8B-C9B-CAB-CBB
28	B	622	LHG	C24-C25-C26-C27
33	M	103	STE	C1-C2-C3-C4
33	b	622	STE	C4-C5-C6-C7
22	B	614	CLA	CBD-CGD-O2D-CED
22	B	605	CLA	C12-C13-C15-C16
22	C	508	CLA	C11-C10-C8-C7
22	b	614	CLA	C12-C13-C15-C16
22	d	403	CLA	C6-C7-C8-C10
22	A	403	CLA	C11-C10-C8-C7
22	c	506	CLA	C11-C10-C8-C7
22	C	509	CLA	C11-C12-C13-C15
22	B	613	CLA	C12-C13-C15-C16
22	c	505	CLA	C6-C7-C8-C10
22	B	615	CLA	C12-C13-C15-C16
22	C	505	CLA	C6-C7-C8-C10
27	c	523	LMG	C34-C35-C36-C37
28	B	622	LHG	C32-C33-C34-C35
28	B	621	LHG	C13-C14-C15-C16
30	C	519	DGD	C3B-C4B-C5B-C6B
22	C	507	CLA	C5-C6-C7-C8
29	A	414	SQD	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
33	t	102	STE	C3-C4-C5-C6
30	H	102	DGD	C7B-C8B-C9B-CAB
22	d	401	CLA	C16-C17-C18-C19
33	t	102	STE	C11-C10-C9-C8
27	c	522	LMG	C39-C40-C41-C42
28	E	101	LHG	O7-C5-C6-O8
27	a	416	LMG	O1-C7-C8-O7
29	b	620	SQD	O6-C44-C45-O47
27	M	101	LMG	O7-C8-C9-O8
22	B	604	CLA	O2A-C1-C2-C3
24	b	618	BCR	C14-C15-C16-C17
30	C	518	DGD	C5D-C6D-O5D-C1E
33	l	102	STE	C15-C16-C17-C18
28	d	409	LHG	C2-C3-O3-P
28	E	101	LHG	C16-C17-C18-C19
22	d	404	CLA	C4C-C3C-CAC-CBC
22	C	508	CLA	C5-C6-C7-C8
30	c	517	DGD	CAA-CBA-CCA-CDA
30	c	517	DGD	C5B-C6B-C7B-C8B
22	C	507	CLA	C2-C3-C5-C6
22	B	615	CLA	C5-C6-C7-C8
22	b	609	CLA	C14-C13-C15-C16
22	C	510	CLA	C11-C10-C8-C9
22	d	401	CLA	C14-C13-C15-C16
22	b	615	CLA	C11-C10-C8-C9
22	C	509	CLA	C11-C12-C13-C14
22	c	512	CLA	C11-C12-C13-C14
22	C	505	CLA	C6-C7-C8-C9
33	b	621	STE	C11-C10-C9-C8
30	c	517	DGD	CBA-CCA-CDA-CEA
30	C	519	DGD	C9B-CAB-CBB-CCB
33	d	413	STE	C4-C5-C6-C7
27	D	407	LMG	C37-C38-C39-C40
22	b	613	CLA	C16-C17-C18-C20
27	b	623	LMG	C30-C31-C32-C33
22	b	606	CLA	C10-C11-C12-C13
30	A	415	DGD	CFA-CGA-CHA-CIA
33	B	624	STE	C6-C7-C8-C9
28	B	622	LHG	C9-C10-C11-C12
30	C	517	DGD	C7A-C8A-C9A-CAA
29	b	620	SQD	C9-C10-C11-C12
22	c	504	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	B	619	BCR	C11-C10-C9-C34
24	d	406	BCR	C11-C10-C9-C34
28	d	409	LHG	C27-C28-C29-C30
22	B	601	CLA	CAA-CBA-CGA-O2A
33	c	521	STE	C4-C5-C6-C7
33	b	622	STE	C7-C8-C9-C10
22	a	404	CLA	O1A-CGA-O2A-C1
26	a	409	PL9	C43-C44-C46-C47
22	C	512	CLA	C8-C10-C11-C12
22	b	616	CLA	C11-C12-C13-C14
22	D	404	CLA	C16-C17-C18-C20
22	A	403	CLA	C4C-C3C-CAC-CBC
22	A	406	CLA	C5-C6-C7-C8
29	B	623	SQD	C31-C32-C33-C34
22	b	604	CLA	C3-C5-C6-C7
27	a	416	LMG	C22-C23-C24-C25
29	f	102	SQD	C46-C45-O47-C7
27	a	416	LMG	C9-C8-O7-C10
27	D	410	LMG	C9-C8-O7-C10
29	B	623	SQD	C46-C45-O47-C7
22	B	614	CLA	C2A-CAA-CBA-CGA
28	B	621	LHG	C30-C31-C32-C33
22	D	402	CLA	C2-C1-O2A-CGA
22	B	601	CLA	C2-C1-O2A-CGA
28	A	412	LHG	C33-C34-C35-C36
28	e	101	LHG	C18-C19-C20-C21
27	c	523	LMG	C36-C37-C38-C39
28	B	621	LHG	C24-C25-C26-C27
27	A	411	LMG	C28-C29-C30-C31
24	c	516	BCR	C14-C15-C16-C17
30	h	101	DGD	C7B-C8B-C9B-CAB
22	C	509	CLA	C3-C5-C6-C7
30	C	517	DGD	C2B-C3B-C4B-C5B
30	c	517	DGD	C3A-C4A-C5A-C6A
28	a	410	LHG	C27-C28-C29-C30
33	H	103	STE	C5-C6-C7-C8
22	b	608	CLA	C13-C15-C16-C17
28	d	408	LHG	C17-C18-C19-C20
24	B	618	BCR	C23-C24-C25-C30
24	A	407	BCR	C23-C24-C25-C26
22	C	506	CLA	C2-C3-C5-C6
33	C	523	STE	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
30	C	518	DGD	O6D-C1D-O3G-C3G
29	b	620	SQD	C30-C31-C32-C33
24	A	407	BCR	C16-C17-C18-C19
24	c	515	BCR	C12-C13-C14-C15
27	A	411	LMG	O1-C7-C8-O7
30	C	517	DGD	O1G-C1G-C2G-O2G
33	T	102	STE	C4-C5-C6-C7
27	D	410	LMG	C11-C12-C13-C14
27	D	411	LMG	C13-C14-C15-C16
33	I	101	STE	C11-C10-C9-C8
30	c	519	DGD	C2A-C1A-O1G-C1G
29	A	413	SQD	O6-C44-C45-C46
29	b	620	SQD	C44-C45-C46-O48
22	c	512	CLA	C4-C3-C5-C6
27	a	416	LMG	C16-C17-C18-C19
22	D	402	CLA	C12-C13-C15-C16
22	D	404	CLA	C11-C12-C13-C15
22	B	613	CLA	C11-C12-C13-C15
22	B	606	CLA	C3-C5-C6-C7
22	a	402	CLA	C2C-C3C-CAC-CBC
22	A	403	CLA	C2C-C3C-CAC-CBC
22	B	605	CLA	C11-C10-C8-C9
22	C	508	CLA	C11-C10-C8-C9
22	C	512	CLA	C14-C13-C15-C16
22	B	611	CLA	C6-C7-C8-C9
22	d	403	CLA	C6-C7-C8-C9
22	C	502	CLA	C14-C13-C15-C16
22	B	615	CLA	C6-C7-C8-C9
22	c	510	CLA	C16-C17-C18-C20
28	B	621	LHG	O9-C7-O7-C5
29	A	414	SQD	C11-C12-C13-C14
22	b	605	CLA	C15-C16-C17-C18
30	C	518	DGD	C1B-C2B-C3B-C4B
28	B	621	LHG	C11-C12-C13-C14
28	B	621	LHG	C35-C36-C37-C38
28	A	412	LHG	C2-C3-O3-P
33	C	522	STE	C10-C11-C12-C13
22	b	613	CLA	O1D-CGD-O2D-CED
22	B	609	CLA	C4-C3-C5-C6
22	c	506	CLA	C4-C3-C5-C6
26	a	409	PL9	C12-C13-C14-C16
28	e	101	LHG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
22	B	609	CLA	C16-C17-C18-C20
27	D	410	LMG	C31-C32-C33-C34
29	f	102	SQD	C25-C26-C27-C28
28	B	622	LHG	C16-C17-C18-C19
22	c	506	CLA	C16-C17-C18-C20
22	B	614	CLA	C16-C17-C18-C20
24	T	101	BCR	C9-C10-C11-C12
28	D	409	LHG	O6-C4-C5-C6
22	C	505	CLA	O1D-CGD-O2D-CED
22	b	612	CLA	C10-C11-C12-C13
29	B	623	SQD	C32-C33-C34-C35
33	Z	101	STE	C12-C13-C14-C15
22	B	610	CLA	C16-C17-C18-C20
28	B	621	LHG	C18-C19-C20-C21
22	B	609	CLA	C2-C3-C5-C6
22	c	509	CLA	C15-C16-C17-C18
27	c	523	LMG	O9-C10-O7-C8
27	m	101	LMG	C35-C36-C37-C38
33	b	621	STE	C2-C3-C4-C5
33	T	102	STE	C7-C8-C9-C10
22	b	610	CLA	C2A-CAA-CBA-CGA
26	a	409	PL9	C21-C22-C23-C24
28	e	101	LHG	C2-C3-O3-P
29	a	411	SQD	O49-C7-O47-C45
27	a	416	LMG	C37-C38-C39-C40
30	C	518	DGD	C4A-C5A-C6A-C7A
26	A	410	PL9	C4-C3-C7-C8
28	l	101	LHG	C16-C17-C18-C19
22	B	605	CLA	C6-C7-C8-C9
22	D	404	CLA	C11-C10-C8-C9
22	B	614	CLA	C14-C13-C15-C16
22	c	512	CLA	C6-C7-C8-C9
22	C	503	CLA	C11-C10-C8-C9
22	B	602	CLA	C6-C7-C8-C9
28	E	101	LHG	C10-C11-C12-C13
33	d	413	STE	C7-C8-C9-C10
24	b	617	BCR	C35-C13-C14-C15
30	C	517	DGD	O1G-C1G-C2G-C3G
24	D	405	BCR	C11-C10-C9-C34
27	C	520	LMG	C39-C40-C41-C42
28	A	412	LHG	C23-C24-C25-C26
30	C	517	DGD	C7B-C8B-C9B-CAB

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Mol	Chain	Res	Type	Atoms
33	a	414	STE	C5-C6-C7-C8
30	c	519	DGD	CAA-CBA-CCA-CDA
29	a	412	SQD	C13-C14-C15-C16
22	B	611	CLA	C16-C17-C18-C19
30	c	517	DGD	O6E-C1E-O5D-C6D
27	A	411	LMG	O6-C1-O1-C7
28	d	409	LHG	C9-C10-C11-C12
27	M	101	LMG	C10-C11-C12-C13
28	D	409	LHG	C30-C31-C32-C33
33	a	414	STE	C4-C5-C6-C7
27	c	523	LMG	C9-C8-O7-C10
22	c	508	CLA	C1A-C2A-CAA-CBA
22	b	616	CLA	C11-C12-C13-C15
27	a	416	LMG	O9-C10-O7-C8
22	C	508	CLA	C12-C13-C15-C16
22	b	612	CLA	C6-C7-C8-C10
22	C	502	CLA	C11-C12-C13-C15
22	b	601	CLA	C12-C13-C15-C16
22	D	403	CLA	C12-C13-C15-C16
22	b	604	CLA	C11-C12-C13-C15
24	C	514	BCR	C13-C14-C15-C16
29	a	412	SQD	C19-C20-C21-C22
22	B	614	CLA	C16-C17-C18-C19
28	l	101	LHG	C31-C32-C33-C34
22	B	610	CLA	C2A-CAA-CBA-CGA
22	b	614	CLA	C13-C15-C16-C17
22	b	606	CLA	C5-C6-C7-C8
22	b	606	CLA	C15-C16-C17-C18
29	D	408	SQD	C34-C35-C36-C37
27	M	101	LMG	C13-C14-C15-C16
28	e	101	LHG	C15-C16-C17-C18
28	B	621	LHG	C9-C10-C11-C12
28	a	410	LHG	C18-C19-C20-C21
30	h	101	DGD	C3A-C4A-C5A-C6A
22	b	607	CLA	O1D-CGD-O2D-CED
22	C	507	CLA	C4-C3-C5-C6
22	C	503	CLA	C8-C10-C11-C12
29	a	411	SQD	O10-C23-O48-C46
33	a	414	STE	C6-C7-C8-C9
28	e	101	LHG	C11-C12-C13-C14
24	H	101	BCR	C12-C13-C14-C15
27	c	522	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
28	l	101	LHG	C23-C24-C25-C26
29	A	414	SQD	C30-C31-C32-C33
28	D	409	LHG	C1-C2-C3-O3
29	a	412	SQD	O6-C44-C45-C46
30	c	519	DGD	C7B-C8B-C9B-CAB
26	A	410	PL9	C20-C19-C21-C22
22	B	613	CLA	C2-C1-O2A-CGA
22	c	512	CLA	C2-C3-C5-C6
26	a	409	PL9	C38-C39-C41-C42
22	b	604	CLA	C5-C6-C7-C8
24	c	514	BCR	C10-C11-C12-C13
30	H	102	DGD	O6E-C5E-C6E-O5E
22	c	501	CLA	C2A-CAA-CBA-CGA
24	t	101	BCR	C5-C6-C7-C8
24	B	618	BCR	C23-C24-C25-C26
24	A	407	BCR	C23-C24-C25-C30
30	c	517	DGD	C1G-C2G-C3G-O3G
29	B	623	SQD	C11-C10-C9-C8
22	a	404	CLA	C4-C3-C5-C6
22	C	510	CLA	C4-C3-C5-C6
22	c	506	CLA	C16-C17-C18-C19
33	b	624	STE	C6-C7-C8-C9
27	m	101	LMG	C8-C7-O1-C1
22	c	502	CLA	O1A-CGA-O2A-C1
30	c	518	DGD	C8A-C9A-CAA-CBA
33	b	625	STE	C12-C13-C14-C15
22	C	512	CLA	C2A-CAA-CBA-CGA
30	c	519	DGD	C2A-C3A-C4A-C5A
22	C	508	CLA	C16-C17-C18-C19
27	b	623	LMG	C13-C14-C15-C16
22	c	508	CLA	C4-C3-C5-C6
26	a	409	PL9	C47-C48-C49-C51
22	B	614	CLA	C6-C7-C8-C10
22	b	603	CLA	C6-C7-C8-C10
26	A	410	PL9	C12-C11-C9-C8
27	c	522	LMG	C15-C16-C17-C18
33	C	522	STE	C7-C8-C9-C10
22	c	508	CLA	C16-C17-C18-C19
22	D	402	CLA	C10-C11-C12-C13
30	h	101	DGD	O1B-C1B-C2B-C3B
24	A	407	BCR	C9-C10-C11-C12
30	C	517	DGD	O1A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
30	H	102	DGD	CDB-CEB-CFB-CGB
27	d	410	LMG	O7-C10-C11-C12
22	c	502	CLA	CBA-CGA-O2A-C1
24	d	406	BCR	C20-C21-C22-C37
29	A	414	SQD	O48-C23-C24-C25
22	d	405	CLA	C4-C3-C5-C6
22	B	604	CLA	C4-C3-C5-C6
22	b	604	CLA	C4-C3-C5-C6
29	b	620	SQD	C18-C19-C20-C21
29	a	411	SQD	O47-C7-C8-C9
33	b	626	STE	C3-C4-C5-C6
22	c	508	CLA	C11-C12-C13-C14
22	B	605	CLA	C14-C13-C15-C16
22	c	503	CLA	C11-C10-C8-C9
22	b	614	CLA	C14-C13-C15-C16
22	c	511	CLA	C11-C10-C8-C9
22	d	405	CLA	C11-C10-C8-C9
22	A	403	CLA	C6-C7-C8-C9
22	A	403	CLA	C11-C10-C8-C9
22	d	401	CLA	C11-C12-C13-C14
22	c	506	CLA	C11-C10-C8-C9
22	B	613	CLA	C14-C13-C15-C16
22	B	615	CLA	C14-C13-C15-C16
29	A	414	SQD	C24-C25-C26-C27
29	A	414	SQD	C29-C30-C31-C32
28	a	410	LHG	C17-C18-C19-C20
30	C	519	DGD	C2A-C3A-C4A-C5A
22	c	512	CLA	C3A-C2A-CAA-CBA
22	B	602	CLA	C3A-C2A-CAA-CBA
22	b	610	CLA	CAD-CBD-CGD-O2D
22	B	609	CLA	CAD-CBD-CGD-O2D
22	C	510	CLA	CAD-CBD-CGD-O2D
22	b	601	CLA	CAD-CBD-CGD-O2D
22	c	506	CLA	CAD-CBD-CGD-O2D
22	C	513	CLA	CAD-CBD-CGD-O2D
22	b	605	CLA	CAD-CBD-CGD-O2D
22	B	610	CLA	CAD-CBD-CGD-O2D
22	B	604	CLA	CAD-CBD-CGD-O2D
22	C	503	CLA	CAD-CBD-CGD-O2D
22	b	604	CLA	CAD-CBD-CGD-O2D
30	C	518	DGD	O1B-C1B-O2G-C2G
27	c	522	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
30	c	518	DGD	C3B-C4B-C5B-C6B
33	d	412	STE	C4-C5-C6-C7
30	c	517	DGD	O2G-C1B-C2B-C3B
29	A	414	SQD	C17-C18-C19-C20
29	b	620	SQD	C11-C12-C13-C14
24	b	618	BCR	C6-C7-C8-C9
24	b	618	BCR	C22-C23-C24-C25
22	A	402	CLA	C4C-C3C-CAC-CBC
22	b	601	CLA	C4-C3-C5-C6
26	D	406	PL9	C40-C39-C41-C42
28	a	410	LHG	C33-C34-C35-C36
27	b	623	LMG	C36-C37-C38-C39
23	A	404	PHO	C2-C3-C5-C6
22	C	510	CLA	C2-C3-C5-C6
28	B	621	LHG	O7-C7-C8-C9
29	A	413	SQD	C29-C30-C31-C32
24	b	617	BCR	C21-C22-C23-C24
24	k	101	BCR	C7-C8-C9-C10
24	H	101	BCR	C11-C12-C13-C14
27	C	520	LMG	O1-C7-C8-C9
22	c	503	CLA	O1A-CGA-O2A-C1
27	a	416	LMG	O7-C10-C11-C12
27	D	407	LMG	C12-C13-C14-C15
23	A	404	PHO	O2A-C1-C2-C3
22	d	405	CLA	O2A-C1-C2-C3
22	d	403	CLA	O2A-C1-C2-C3
22	D	404	CLA	O2A-C1-C2-C3
22	C	509	CLA	O2A-C1-C2-C3
33	d	413	STE	C12-C13-C14-C15
33	k	102	STE	C3-C4-C5-C6
33	l	102	STE	C12-C13-C14-C15
22	C	507	CLA	CHA-CBD-CGD-O1D
22	C	507	CLA	CHA-CBD-CGD-O2D
22	b	609	CLA	CHA-CBD-CGD-O1D
22	b	609	CLA	CHA-CBD-CGD-O2D
22	A	403	CLA	CHA-CBD-CGD-O1D
22	A	403	CLA	CHA-CBD-CGD-O2D
23	d	402	PHO	CHA-CBD-CGD-O1D
23	d	402	PHO	CHA-CBD-CGD-O2D
22	d	401	CLA	CHA-CBD-CGD-O1D
22	c	507	CLA	CHA-CBD-CGD-O2D
22	C	503	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
33	M	103	STE	C4-C5-C6-C7
27	c	523	LMG	C32-C33-C34-C35
27	M	101	LMG	C30-C31-C32-C33
29	b	620	SQD	C11-C10-C9-C8
22	b	613	CLA	C16-C17-C18-C19
29	b	620	SQD	O47-C7-C8-C9
22	A	402	CLA	C2C-C3C-CAC-CBC
27	a	416	LMG	O7-C8-C9-O8
22	b	602	CLA	C8-C10-C11-C12
22	b	611	CLA	C10-C11-C12-C13
22	B	611	CLA	C10-C11-C12-C13
29	A	413	SQD	O47-C7-C8-C9
22	B	613	CLA	CAA-CBA-CGA-O2A
27	c	520	LMG	C30-C31-C32-C33
29	a	411	SQD	C28-C29-C30-C31
22	C	501	CLA	C2A-CAA-CBA-CGA
22	c	503	CLA	CBA-CGA-O2A-C1
27	M	101	LMG	C22-C23-C24-C25
28	a	410	LHG	O10-C23-O8-C6
22	B	611	CLA	C6-C7-C8-C10
22	b	607	CLA	C11-C10-C8-C7
22	B	613	CLA	C6-C7-C8-C10
22	B	604	CLA	C11-C10-C8-C7
30	C	517	DGD	O1B-C1B-O2G-C2G
22	a	402	CLA	C4C-C3C-CAC-CBC
22	b	602	CLA	C6-C7-C8-C9
22	C	502	CLA	C11-C12-C13-C14
22	B	604	CLA	C11-C10-C8-C9
22	c	505	CLA	C6-C7-C8-C9
29	a	411	SQD	C5-C6-S-O8
30	h	101	DGD	C4E-C5E-C6E-O5E
28	B	622	LHG	C30-C31-C32-C33
24	c	516	BCR	C37-C22-C23-C24
27	m	101	LMG	O8-C28-C29-C30
26	D	406	PL9	C47-C48-C49-C51
29	a	411	SQD	C19-C20-C21-C22
33	B	625	STE	C13-C14-C15-C16
24	Y	101	BCR	C21-C22-C23-C24
24	T	101	BCR	C7-C8-C9-C10
22	B	614	CLA	C15-C16-C17-C18
22	b	606	CLA	C8-C10-C11-C12
30	H	102	DGD	C4E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
28	A	412	LHG	C1-C2-C3-O3
33	d	412	STE	C1-C2-C3-C4
33	d	411	STE	C1-C2-C3-C4
22	B	602	CLA	C1A-C2A-CAA-CBA
33	T	102	STE	C12-C13-C14-C15
29	B	623	SQD	C10-C11-C12-C13
30	c	517	DGD	C6A-C7A-C8A-C9A
27	c	520	LMG	C34-C35-C36-C37
27	a	416	LMG	C11-C12-C13-C14
33	C	521	STE	C5-C6-C7-C8
27	A	411	LMG	C7-C8-C9-O8
27	a	416	LMG	C34-C35-C36-C37
22	C	507	CLA	C10-C11-C12-C13
22	B	601	CLA	O1D-CGD-O2D-CED
33	l	102	STE	C4-C5-C6-C7
30	C	519	DGD	O1A-C1A-O1G-C1G
28	e	101	LHG	C3-O3-P-O4
28	d	409	LHG	C4-O6-P-O4
28	d	409	LHG	O10-C23-C24-C25
24	t	101	BCR	C1-C6-C7-C8
24	c	516	BCR	C1-C6-C7-C8
24	T	101	BCR	C5-C6-C7-C8
28	B	622	LHG	C31-C32-C33-C34
29	a	411	SQD	O49-C7-C8-C9
30	C	517	DGD	O1B-C1B-C2B-C3B
33	J	101	STE	C7-C8-C9-C10
22	b	612	CLA	CAA-CBA-CGA-O2A
24	C	514	BCR	C10-C11-C12-C13
22	B	603	CLA	C2A-CAA-CBA-CGA
22	c	509	CLA	CAA-CBA-CGA-O1A
24	c	515	BCR	C13-C14-C15-C16
26	A	410	PL9	C33-C34-C36-C37
22	B	605	CLA	CAD-CBD-CGD-O1D
22	b	609	CLA	CAD-CBD-CGD-O1D
22	A	403	CLA	CAD-CBD-CGD-O1D
29	A	413	SQD	C5-C6-S-O7
22	C	508	CLA	O1A-CGA-O2A-C1
22	b	613	CLA	CAA-CBA-CGA-O2A
22	b	610	CLA	C8-C10-C11-C12
22	C	508	CLA	C14-C13-C15-C16
22	b	614	CLA	C11-C10-C8-C9
22	b	604	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
33	C	521	STE	C2-C3-C4-C5
23	A	405	PHO	C8-C10-C11-C12
29	A	414	SQD	C44-C45-O47-C7
29	A	414	SQD	O10-C23-C24-C25
27	b	623	LMG	O10-C28-C29-C30
30	c	518	DGD	C4A-C5A-C6A-C7A
22	c	511	CLA	C8-C10-C11-C12
29	A	413	SQD	C31-C32-C33-C34
33	H	103	STE	C14-C15-C16-C17
30	C	518	DGD	O1G-C1A-C2A-C3A
23	A	404	PHO	C4-C3-C5-C6
26	D	406	PL9	C30-C29-C31-C32
26	a	409	PL9	C45-C44-C46-C47
33	B	625	STE	C10-C11-C12-C13
22	c	508	CLA	C11-C10-C8-C7
22	c	503	CLA	C11-C10-C8-C7
22	b	614	CLA	C11-C10-C8-C7
22	c	506	CLA	C2-C3-C5-C6
27	m	101	LMG	O9-C10-C11-C12
30	c	517	DGD	O1B-C1B-C2B-C3B
27	b	623	LMG	O7-C10-C11-C12
24	c	515	BCR	C7-C8-C9-C10
24	C	516	BCR	C21-C22-C23-C24
24	C	515	BCR	C21-C22-C23-C24
28	e	101	LHG	O10-C23-C24-C25
29	a	412	SQD	O10-C23-C24-C25
30	c	518	DGD	O1B-C1B-C2B-C3B
28	l	101	LHG	O10-C23-O8-C6
30	C	517	DGD	O2G-C1B-C2B-C3B
22	B	612	CLA	CAA-CBA-CGA-O2A
29	A	413	SQD	C25-C26-C27-C28
22	b	612	CLA	CAA-CBA-CGA-O1A
22	B	613	CLA	CAA-CBA-CGA-O1A
22	b	601	CLA	C2A-CAA-CBA-CGA
22	c	513	CLA	C13-C15-C16-C17
22	B	612	CLA	C8-C10-C11-C12

There are no ring outliers.

62 monomers are involved in 162 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	402	CLA	3	0

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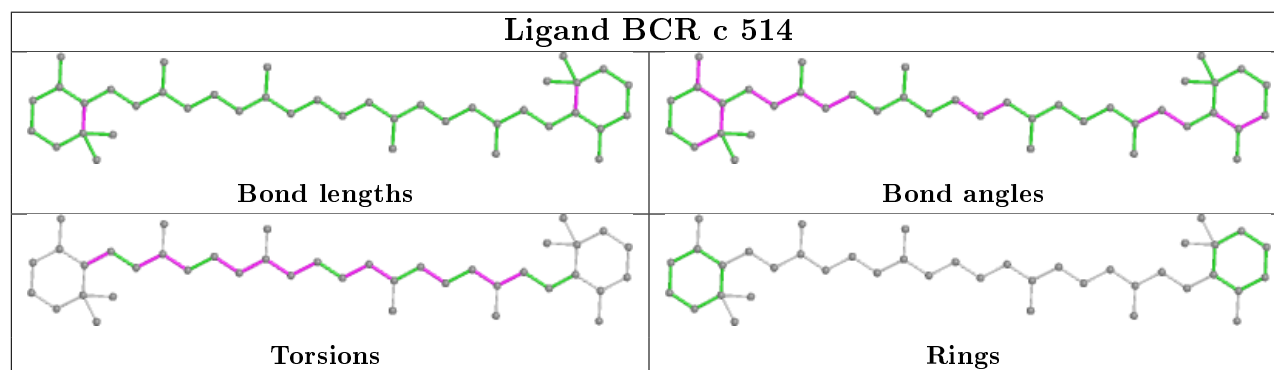
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	605	CLA	6	0
22	C	508	CLA	3	0
22	C	512	CLA	1	0
33	C	522	STE	1	0
22	C	506	CLA	3	0
22	C	507	CLA	2	0
24	B	619	BCR	4	0
22	B	609	CLA	3	0
22	B	603	CLA	1	0
30	A	415	DGD	1	0
35	V	201	HEC	6	0
22	C	511	CLA	3	0
22	B	611	CLA	2	0
24	D	405	BCR	2	0
22	A	406	CLA	1	0
22	C	510	CLA	2	0
24	C	514	BCR	3	0
24	B	618	BCR	7	0
22	A	403	CLA	2	0
30	C	518	DGD	1	0
33	M	102	STE	1	0
22	D	404	CLA	3	0
22	C	504	CLA	4	0
24	A	407	BCR	1	0
33	T	102	STE	1	0
24	Y	101	BCR	2	0
24	C	515	BCR	2	0
28	E	101	LHG	3	0
33	B	624	STE	2	0
22	D	403	CLA	3	0
22	B	616	CLA	3	0
22	C	513	CLA	5	0
30	C	517	DGD	1	0
22	B	614	CLA	2	0
23	A	405	PHO	2	0
22	B	612	CLA	5	0
22	C	501	CLA	3	0
33	D	412	STE	4	0
24	C	516	BCR	1	0
28	B	622	LHG	1	0
29	A	414	SQD	1	0
29	B	623	SQD	2	0

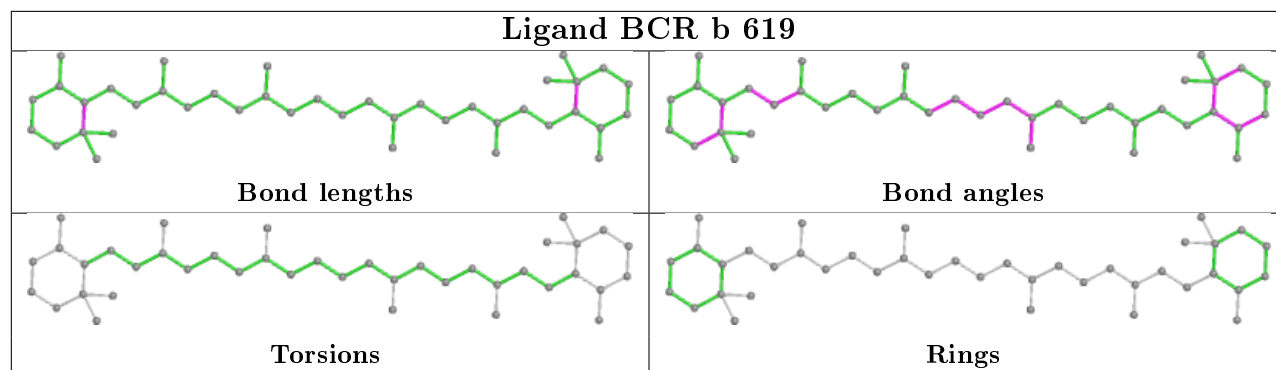
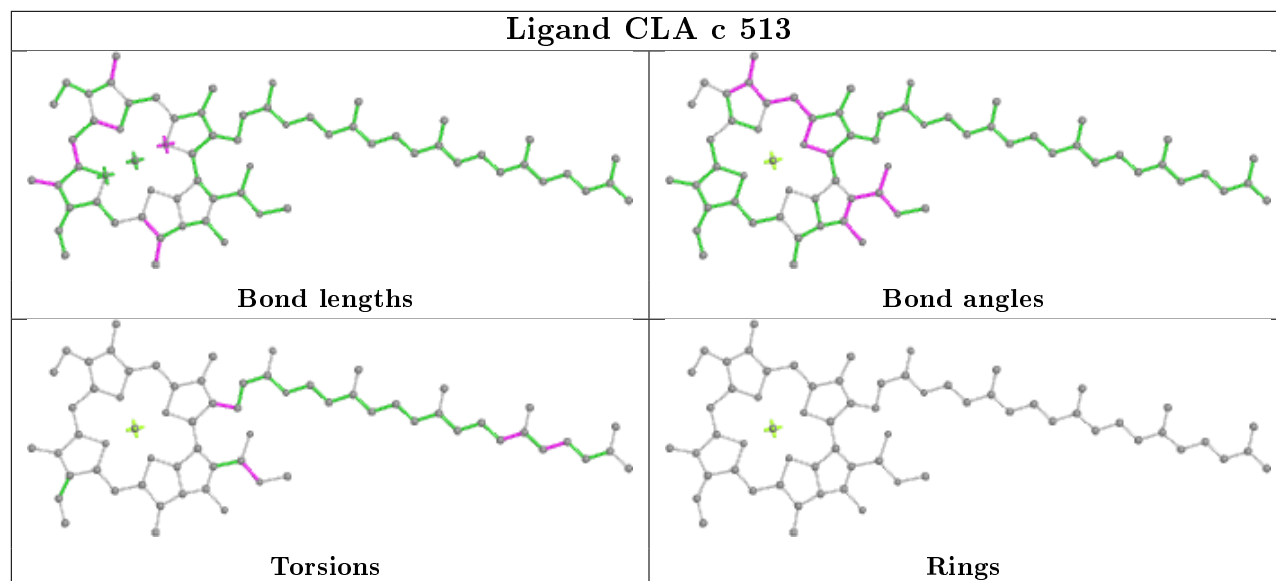
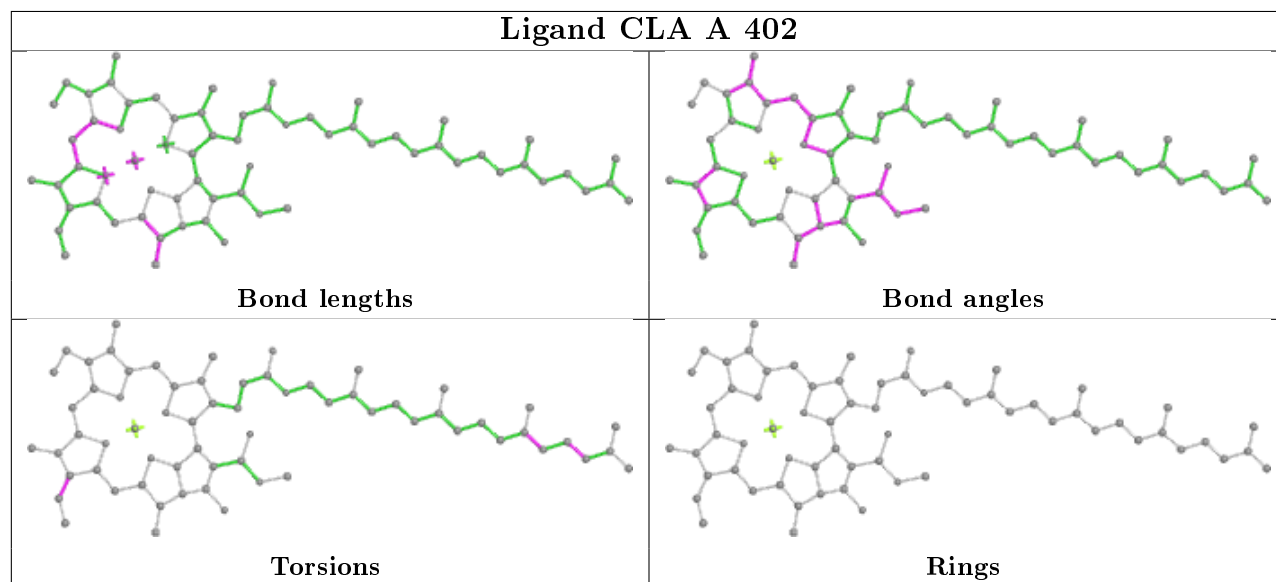
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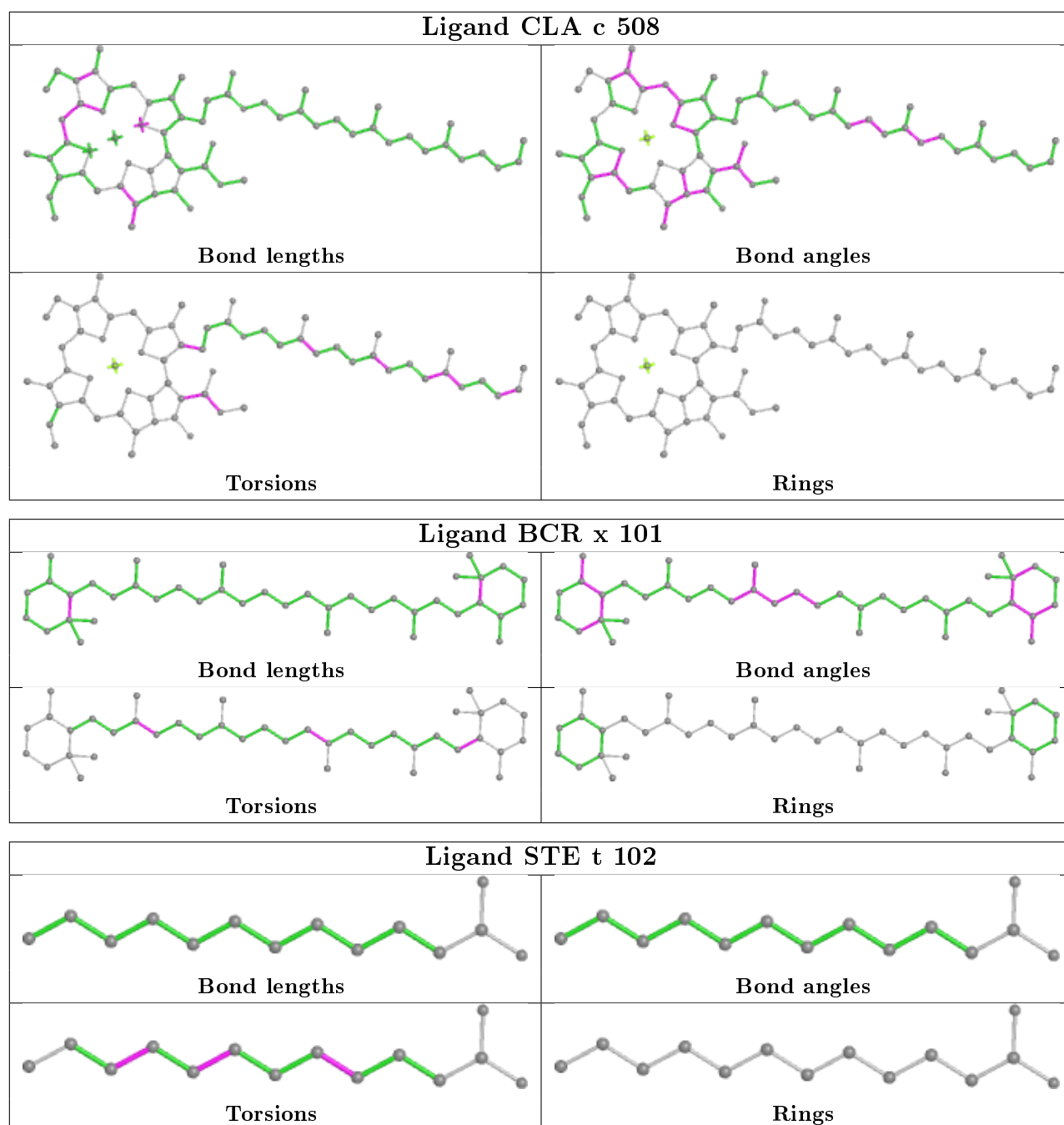
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	509	CLA	6	0
33	B	620	STE	1	0
22	B	610	CLA	4	0
22	B	607	CLA	2	0
22	B	606	CLA	6	0
26	A	410	PL9	8	0
22	B	613	CLA	3	0
22	B	604	CLA	11	0
32	A	417[B]	OEY	1	0
35	F	101	HEC	11	0
27	M	101	LMG	2	0
22	C	503	CLA	3	0
22	B	608	CLA	2	0
24	T	101	BCR	6	0
22	B	615	CLA	3	0
24	H	101	BCR	4	0
22	B	602	CLA	3	0
22	C	505	CLA	2	0
22	B	601	CLA	1	0

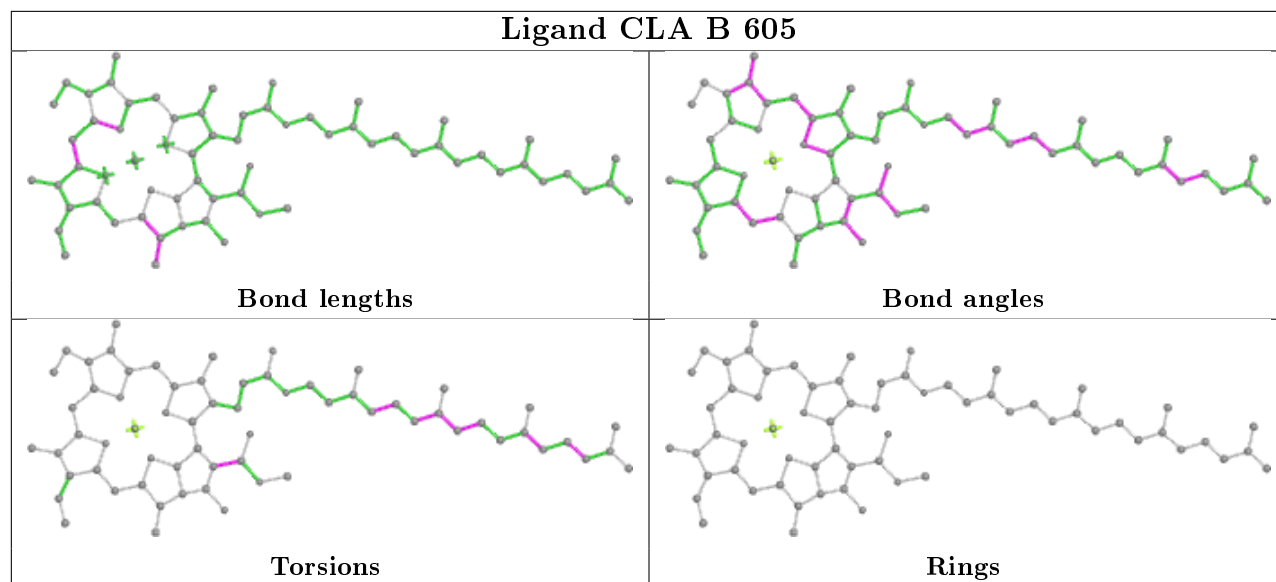
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



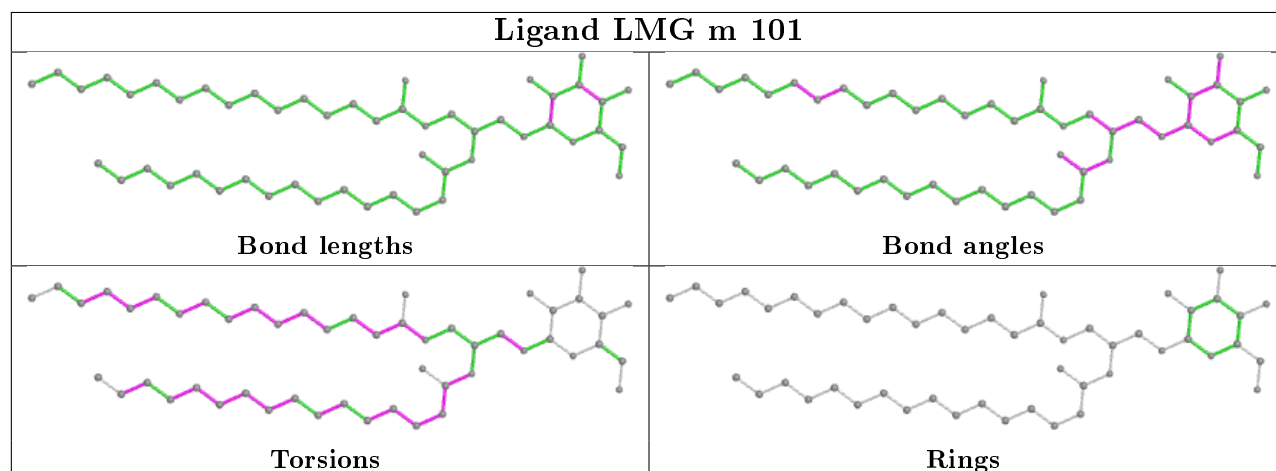
Ligand BCR b 619**Ligand CLA c 513****Ligand CLA A 402**



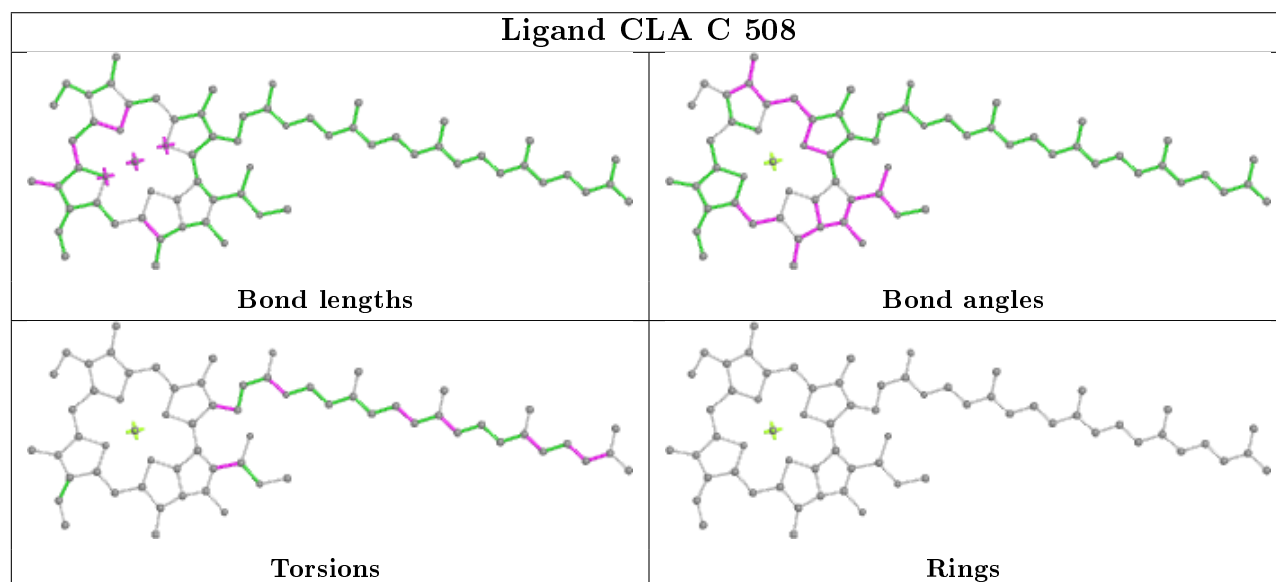
Ligand CLA B 605



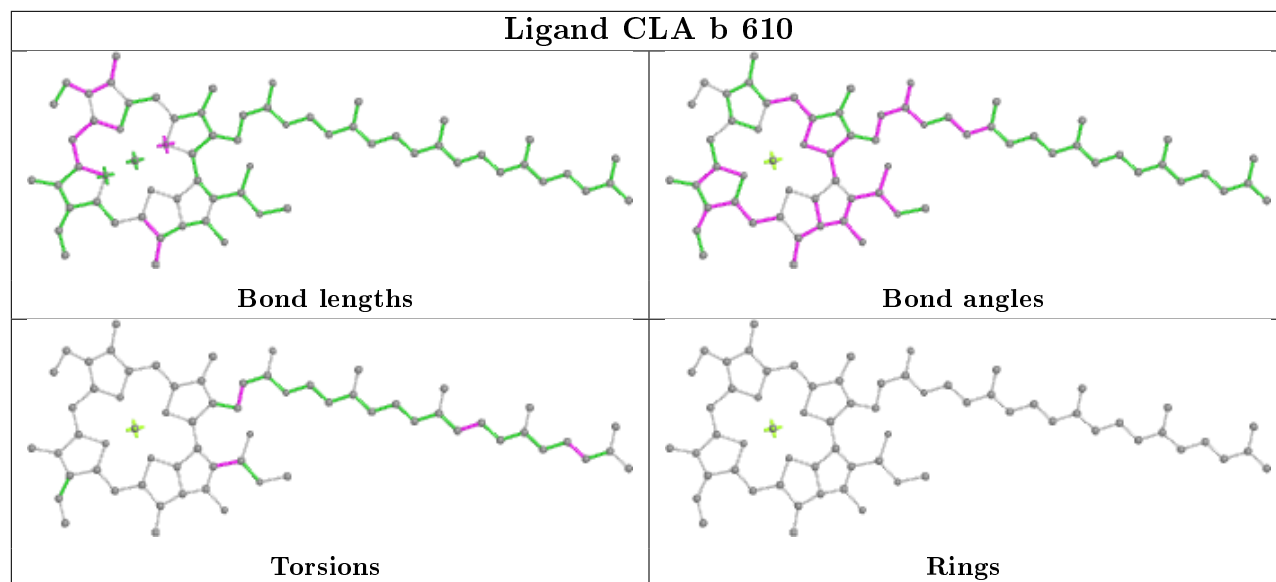
Ligand LMG m 101



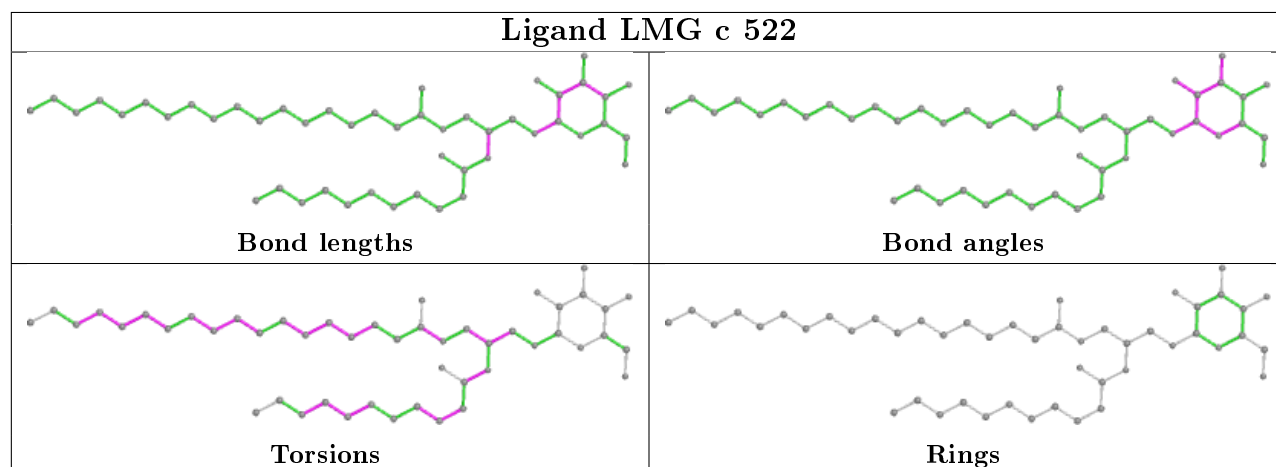
Ligand CLA C 508



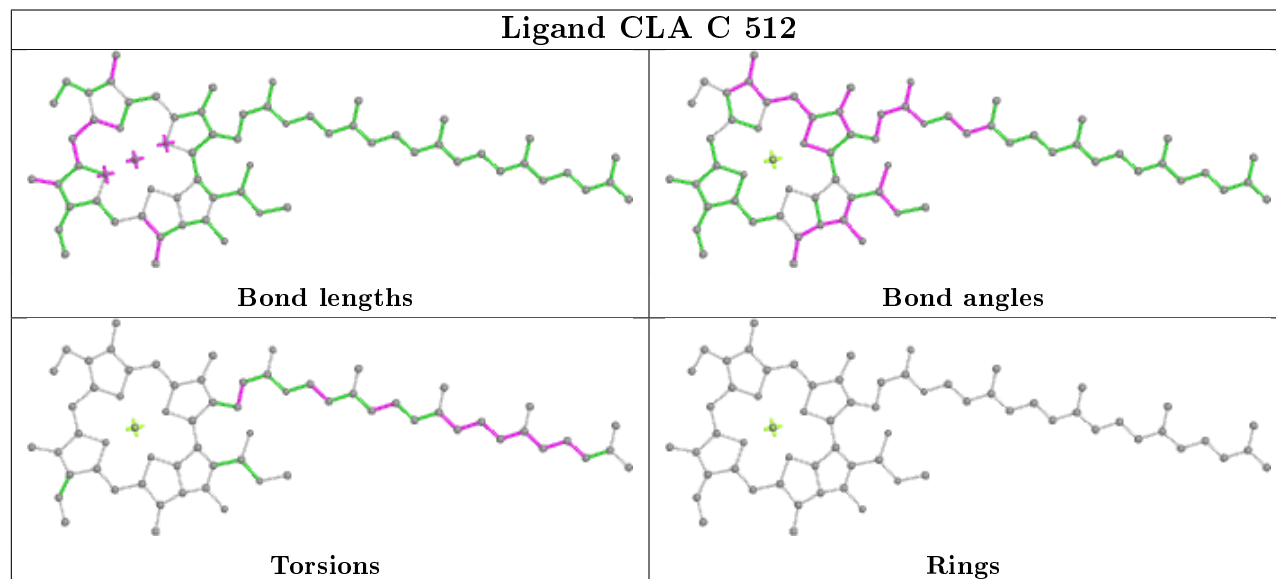
Ligand CLA b 610



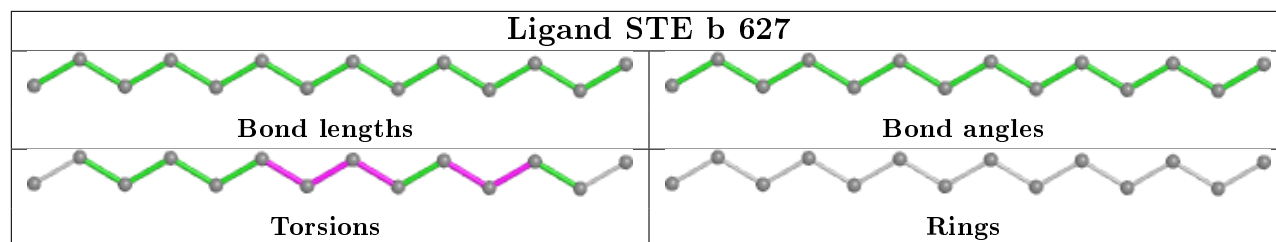
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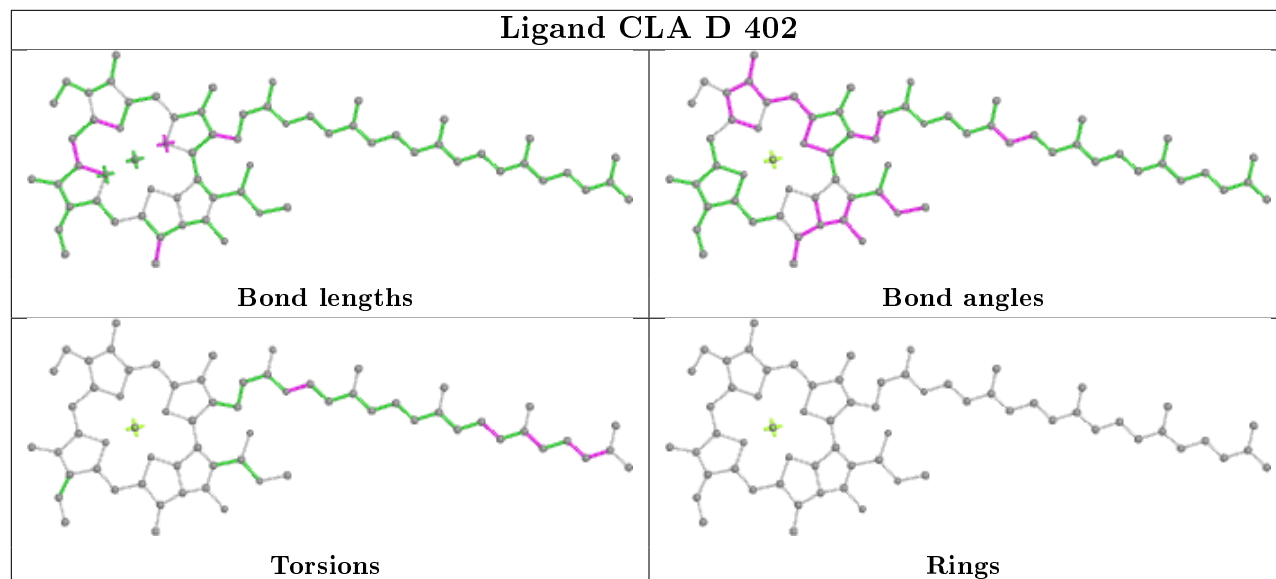
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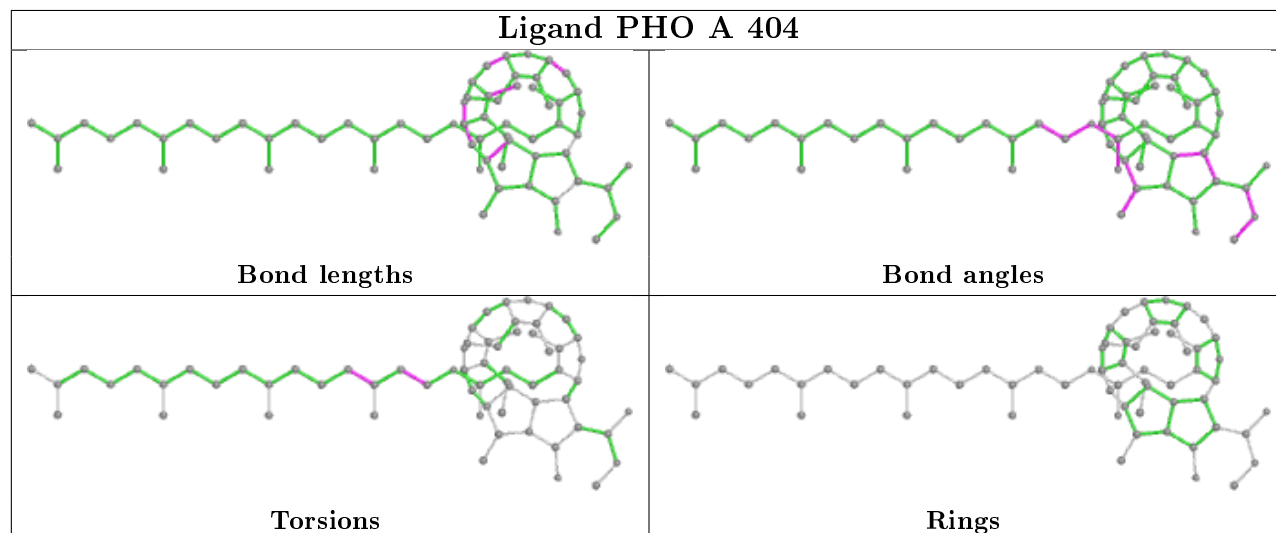
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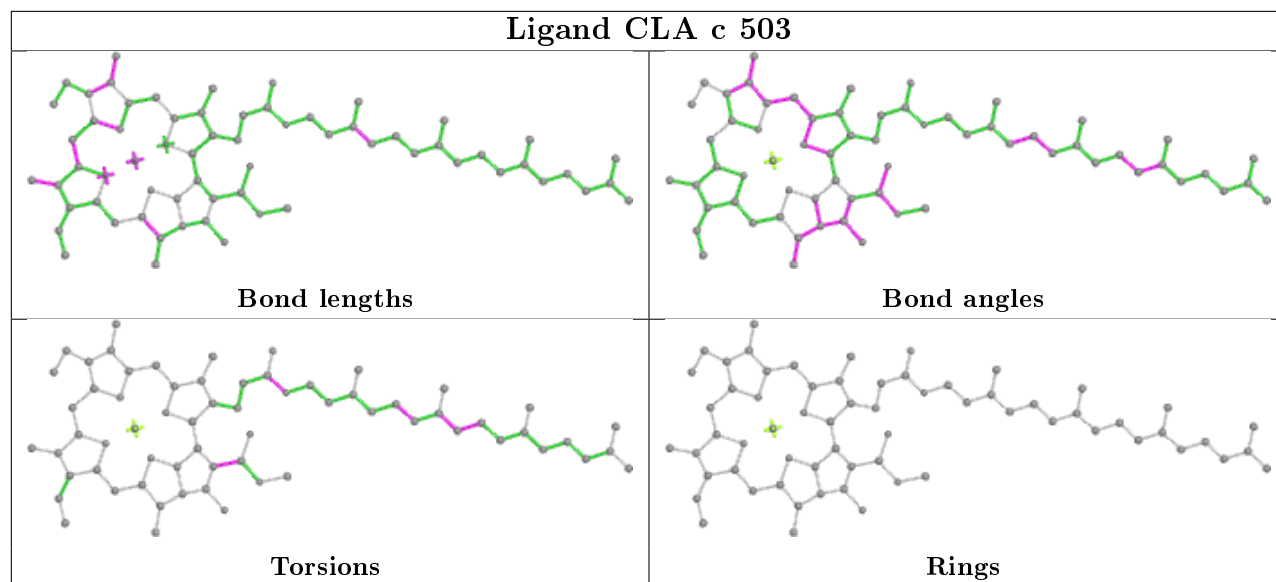
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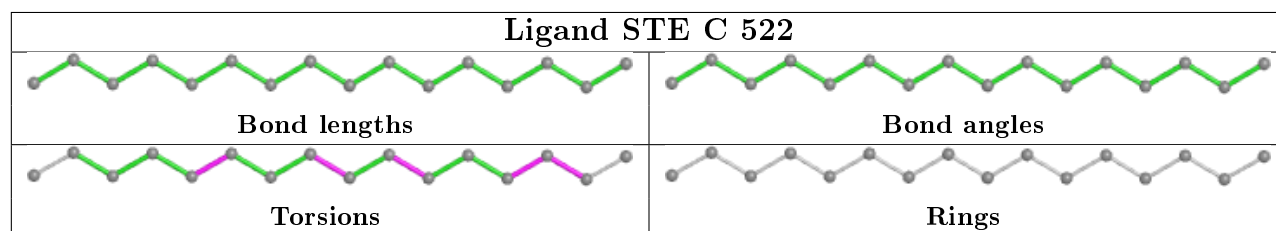
Ligand PHO A 404



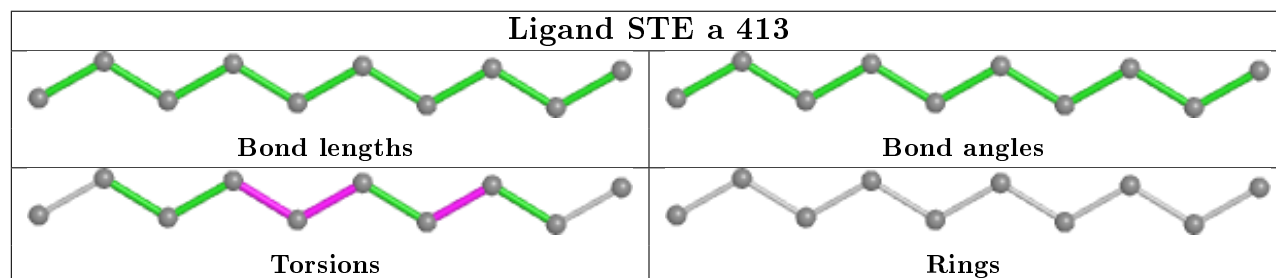
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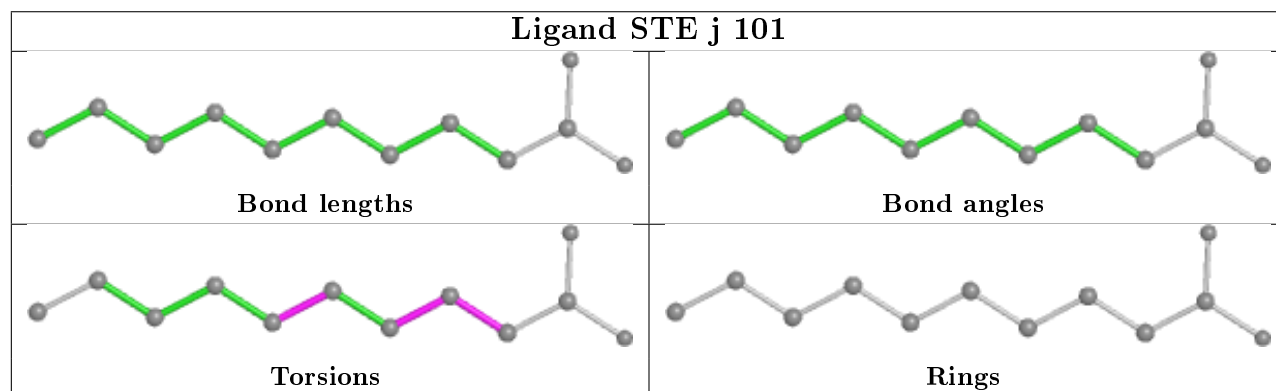
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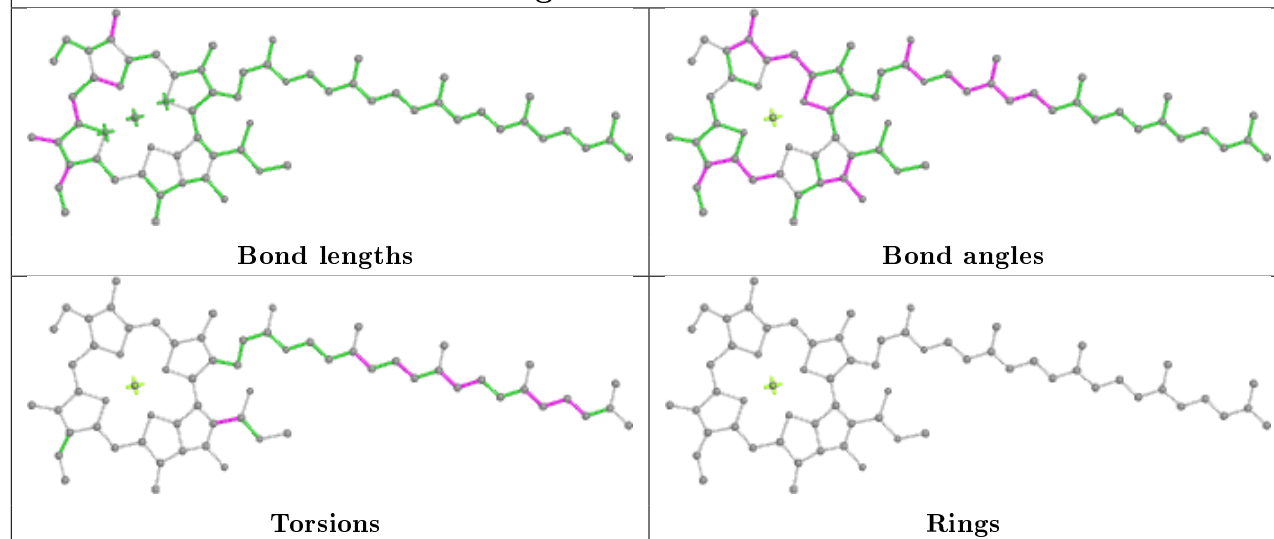
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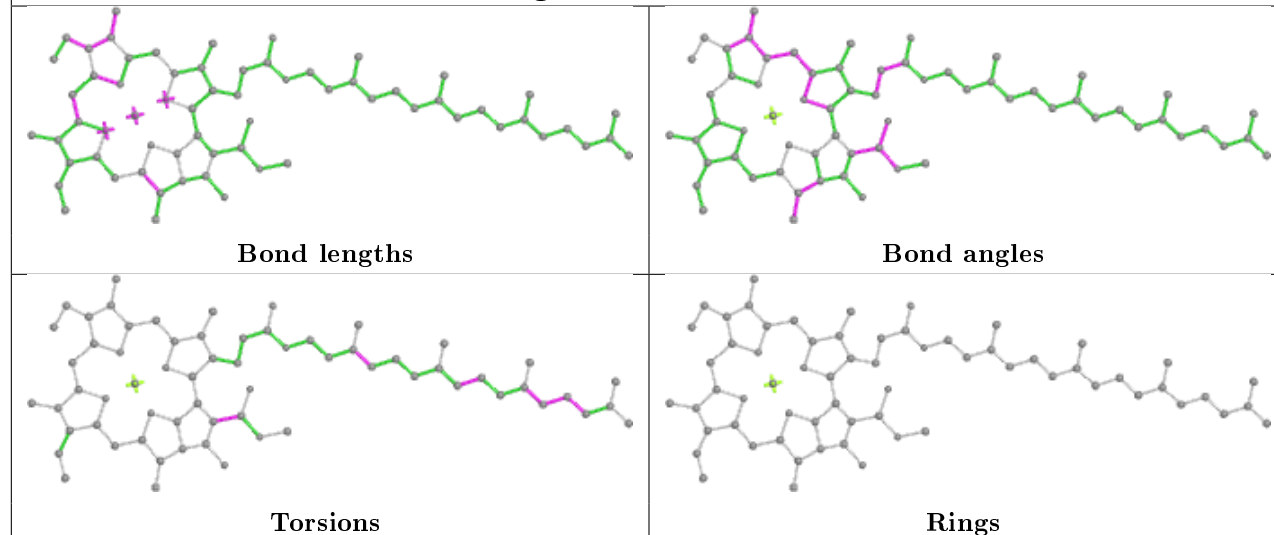
Ligand STE j 101



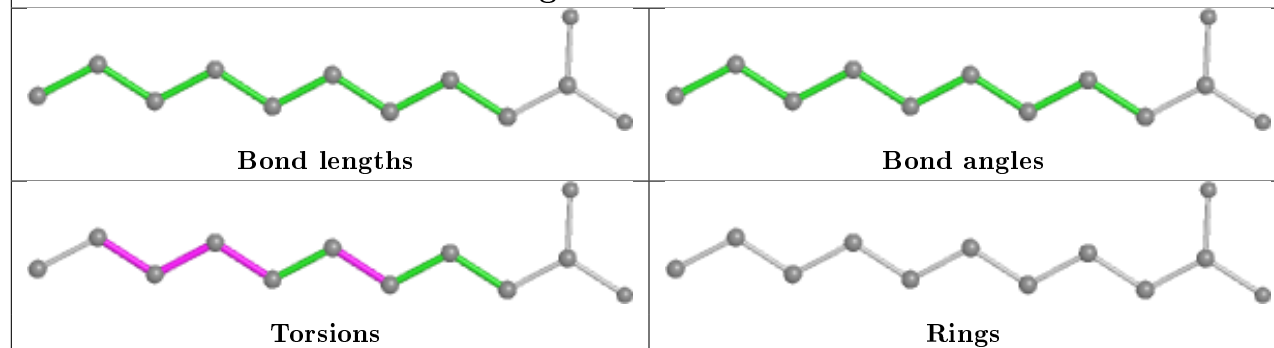
Ligand CLA b 614

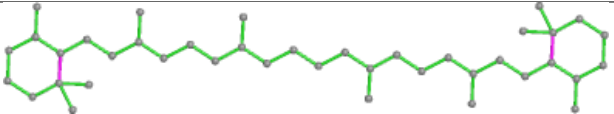
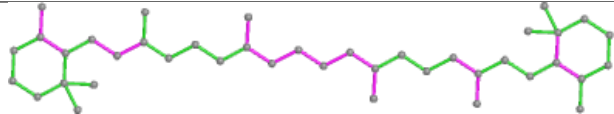
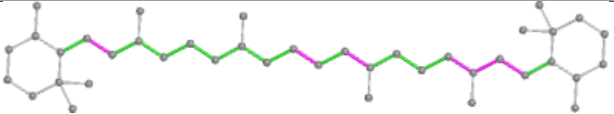
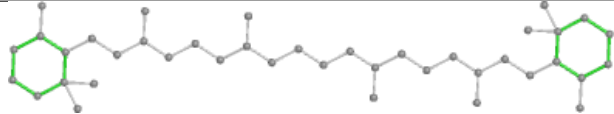






Ligand CLA C 506

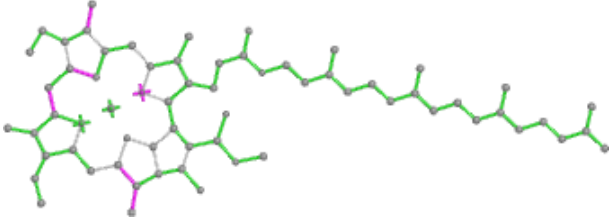
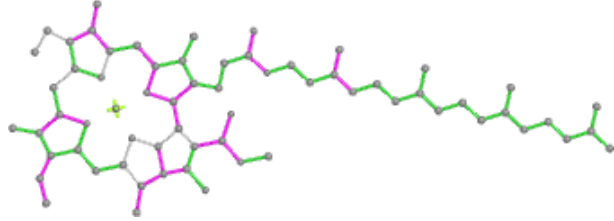
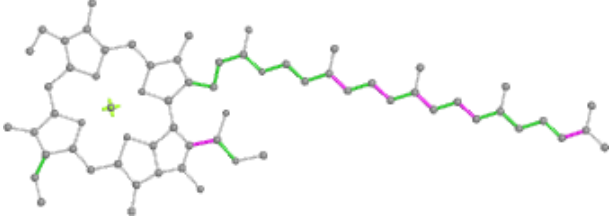
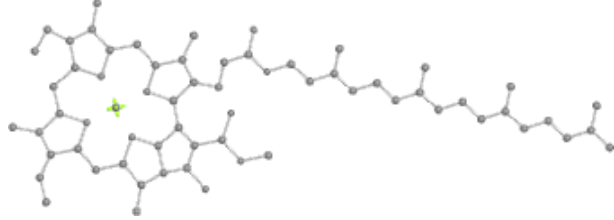


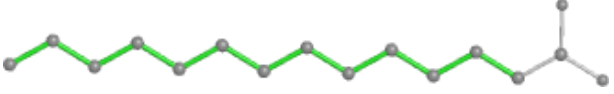
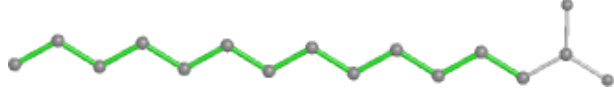
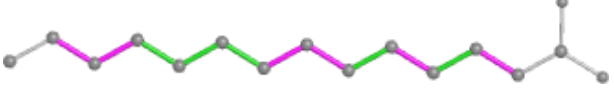
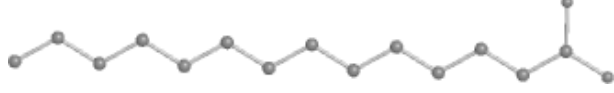
Ligand STE J 101

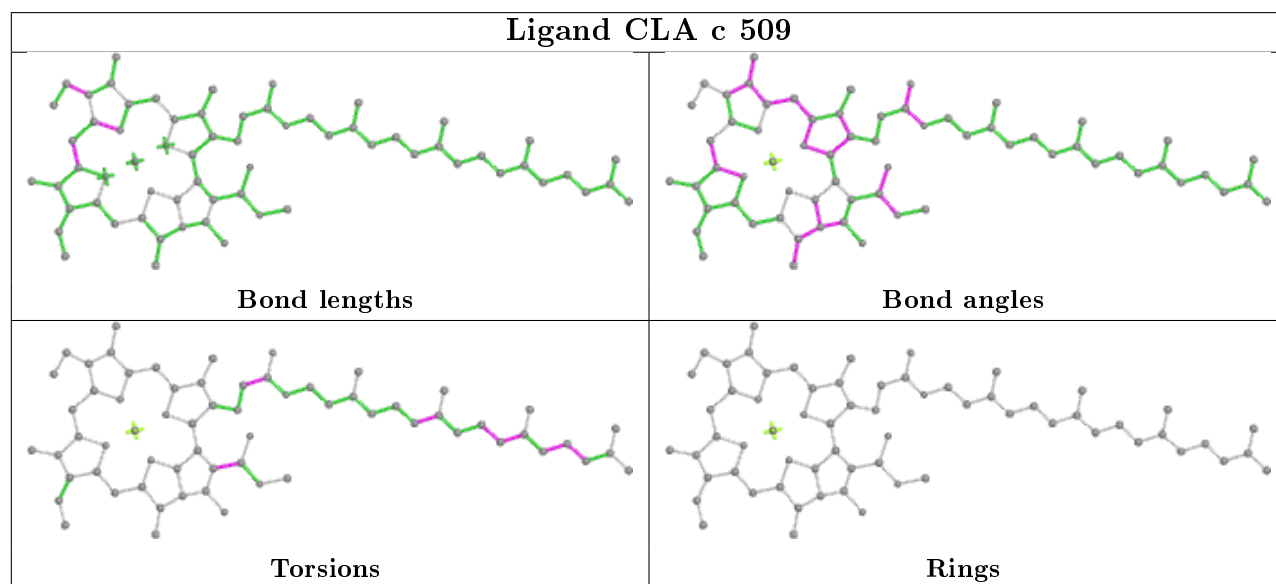
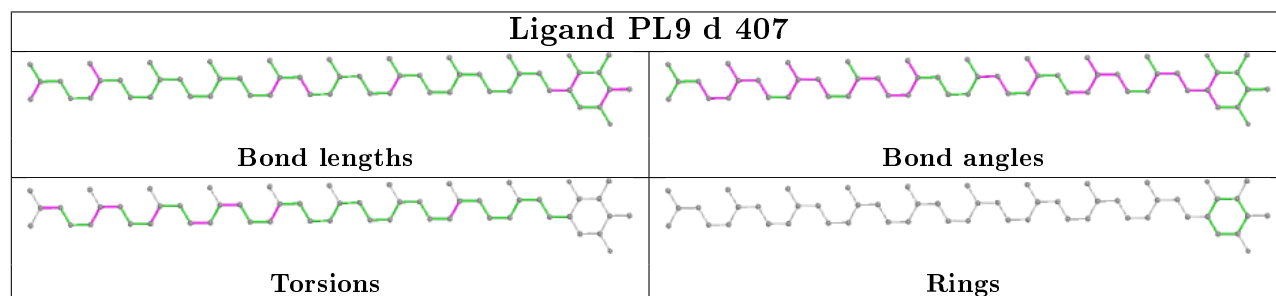
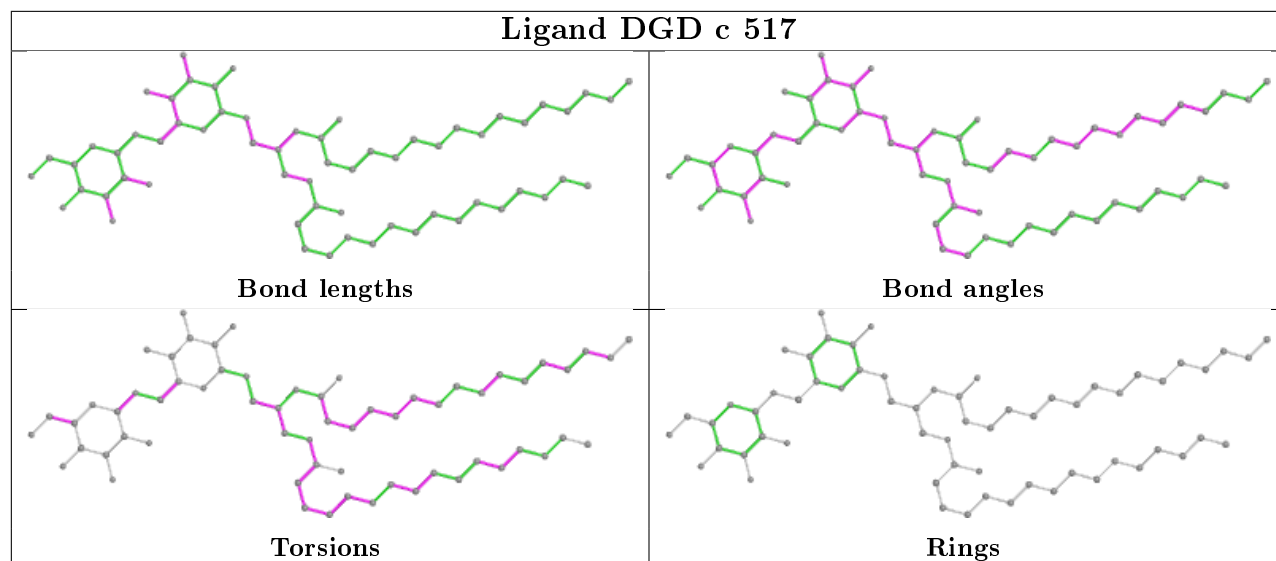


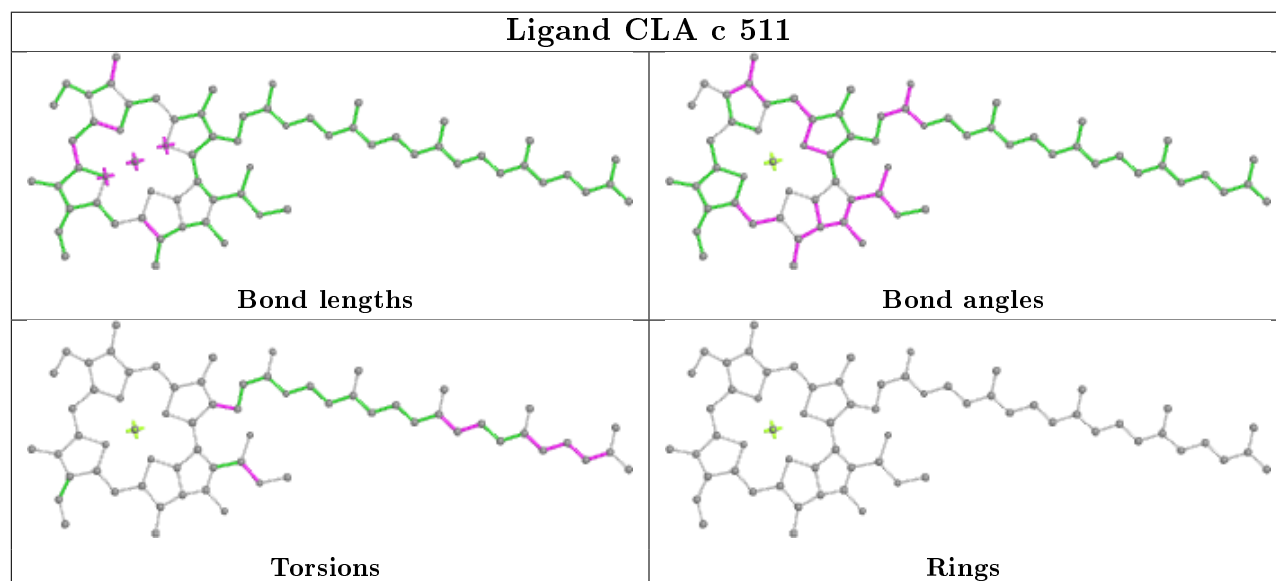
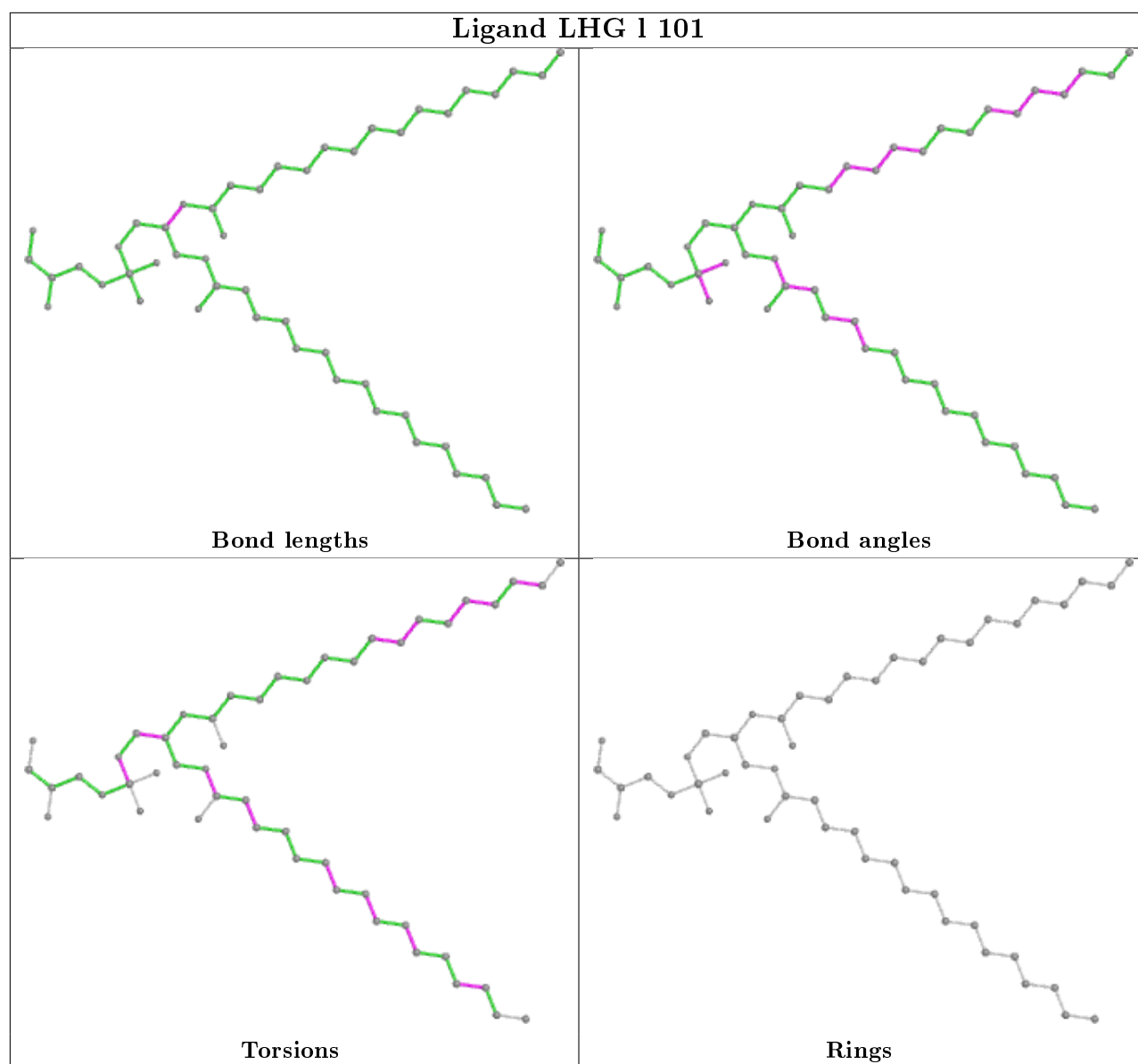
Ligand BCR b 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

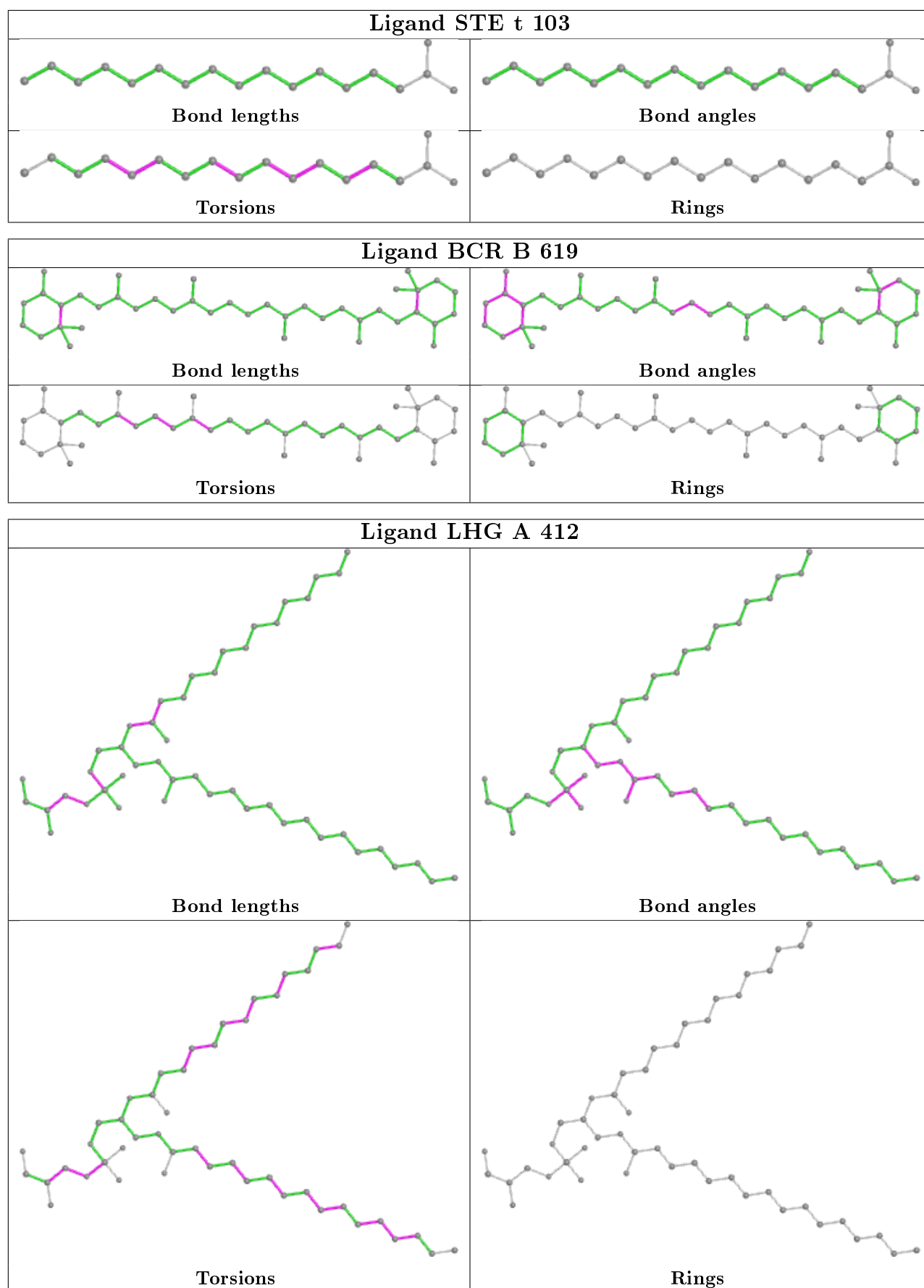
Ligand STE a 415	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

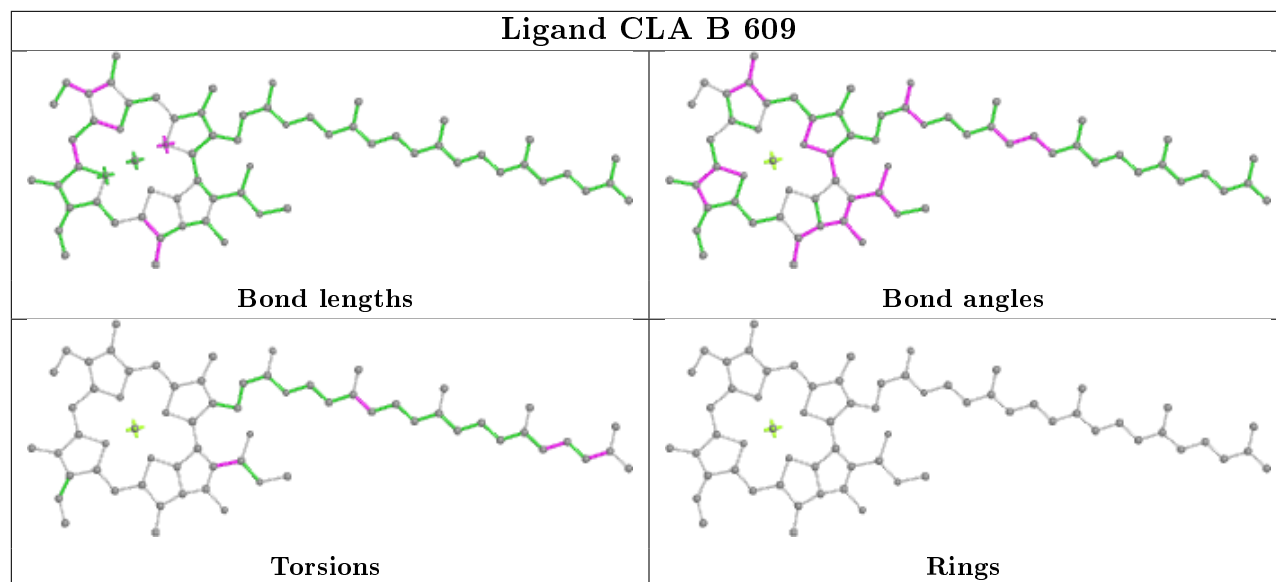
Ligand STE b 624	
	
Bond lengths	Bond angles
	
Torsions	Rings



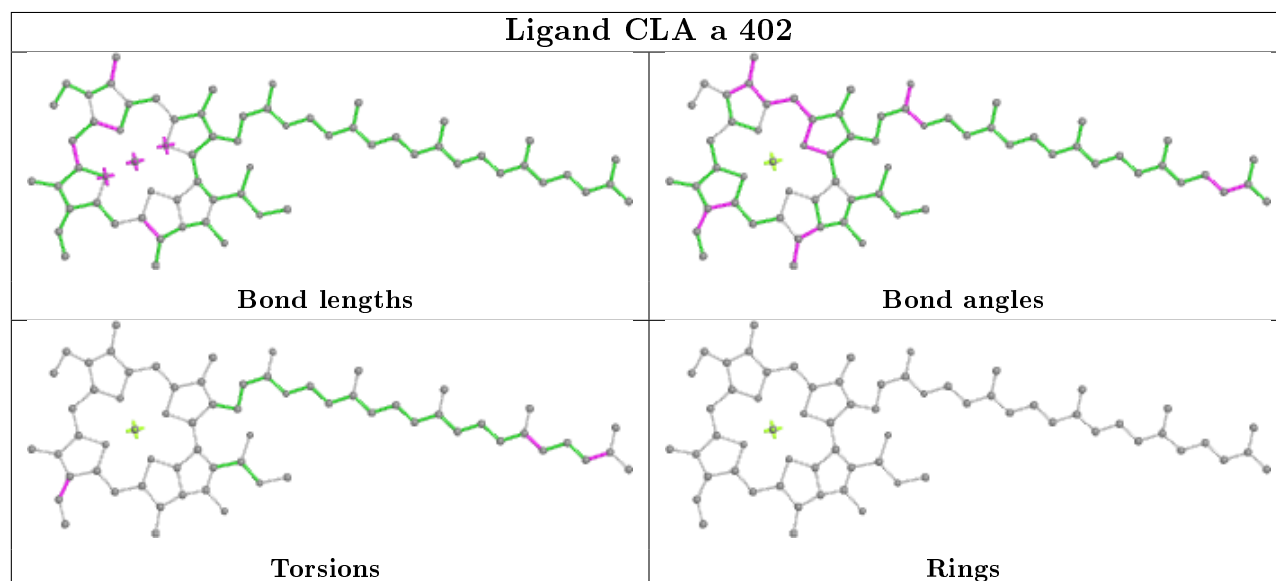




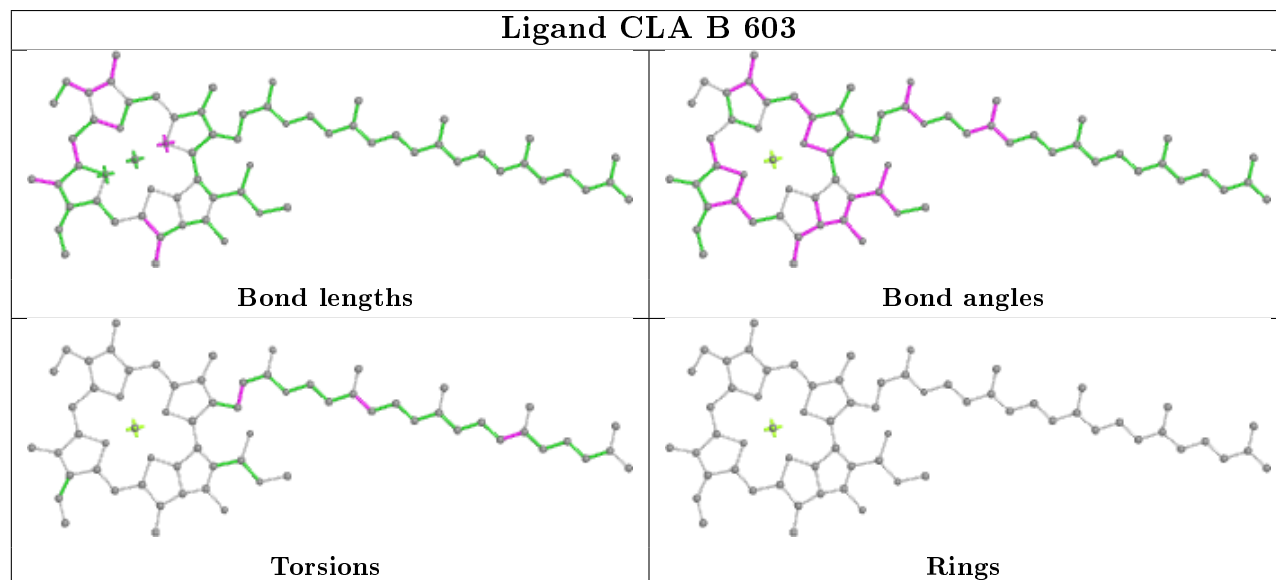
Ligand CLA B 609



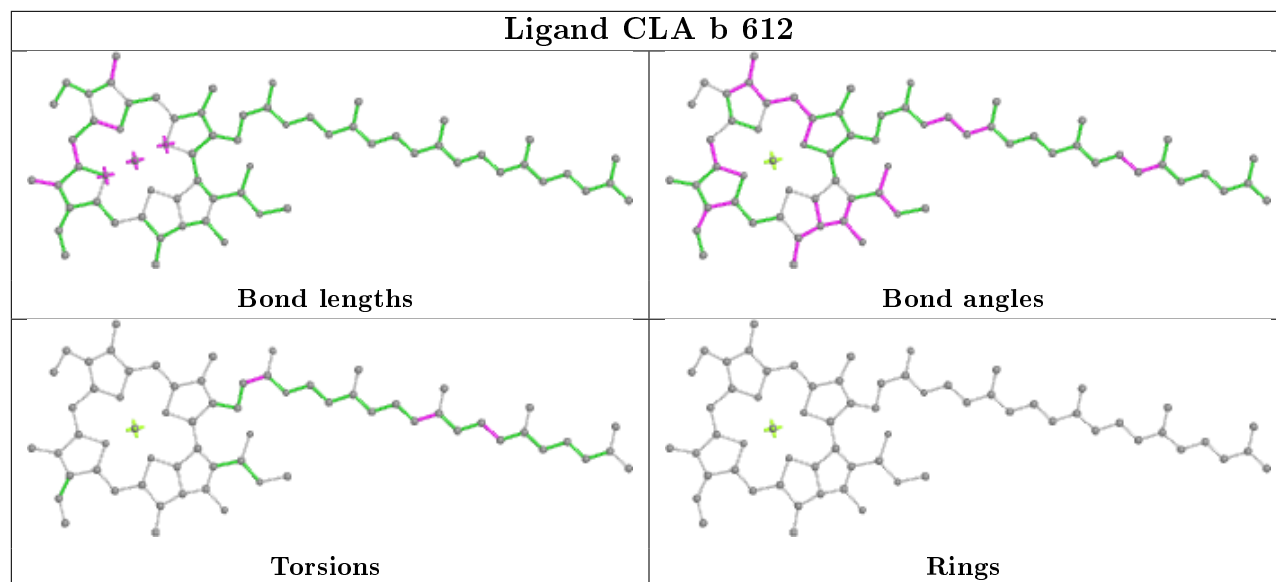
Ligand CLA a 402



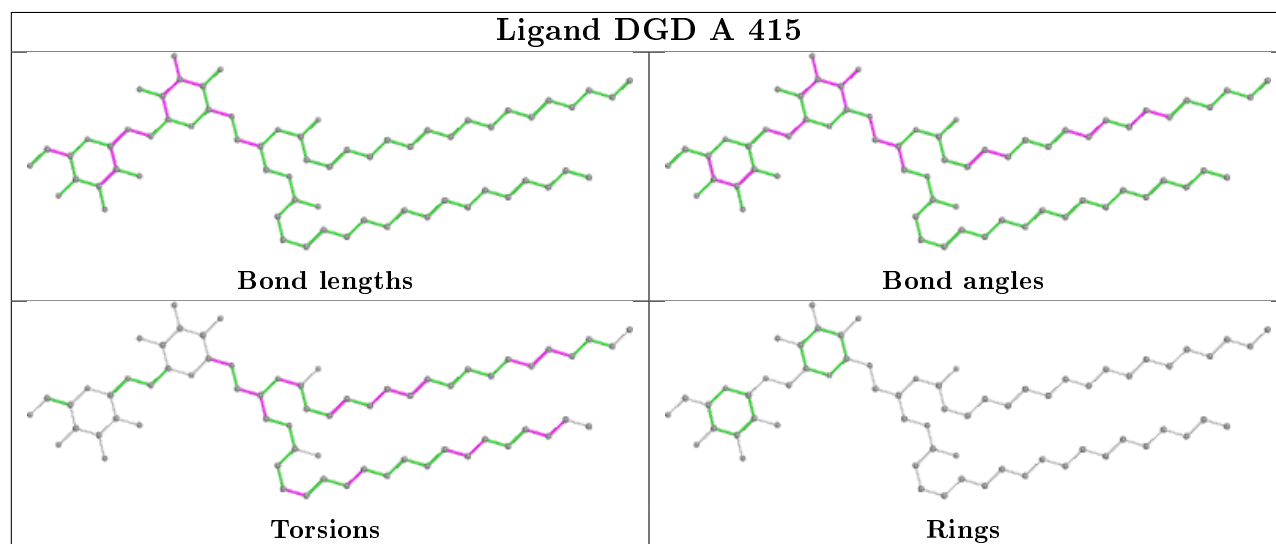
Ligand CLA B 603



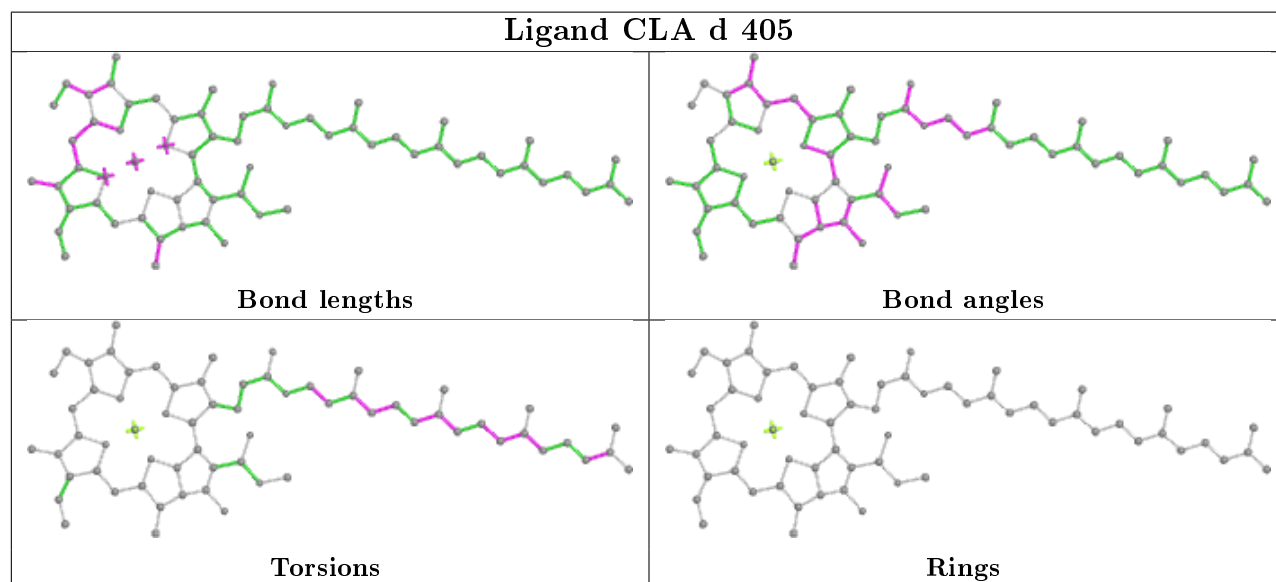
Ligand CLA b 612



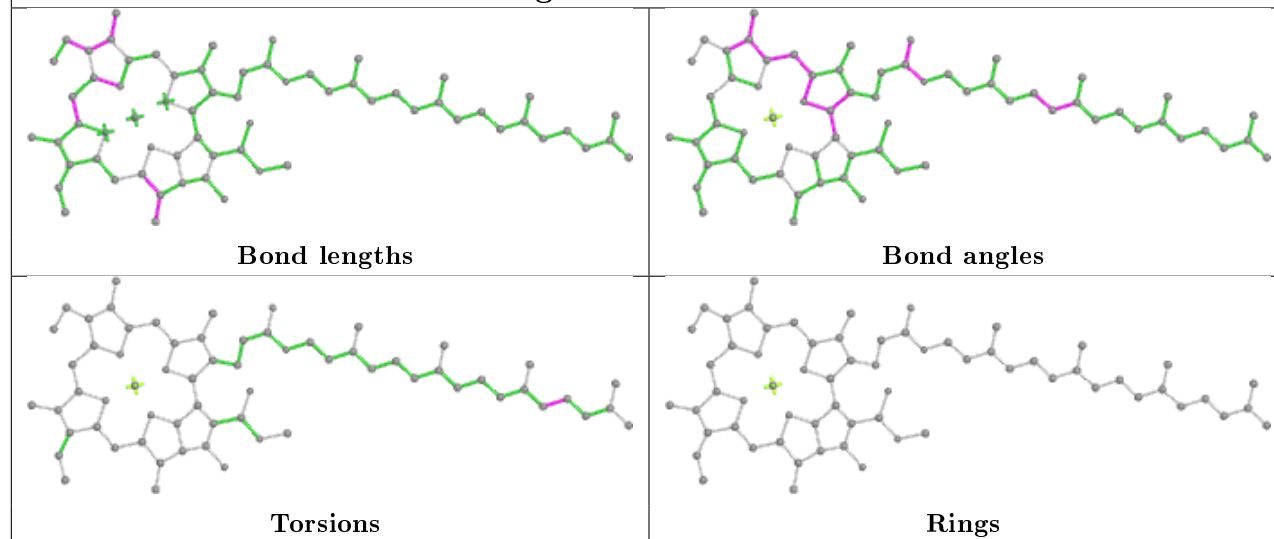
Ligand DGD A 415



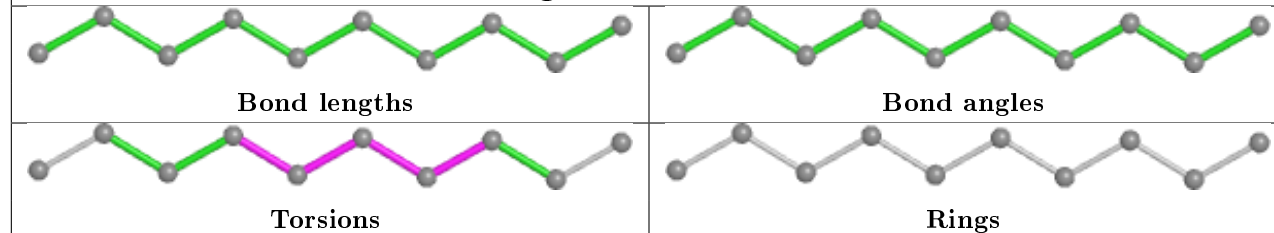
Ligand CLA d 405



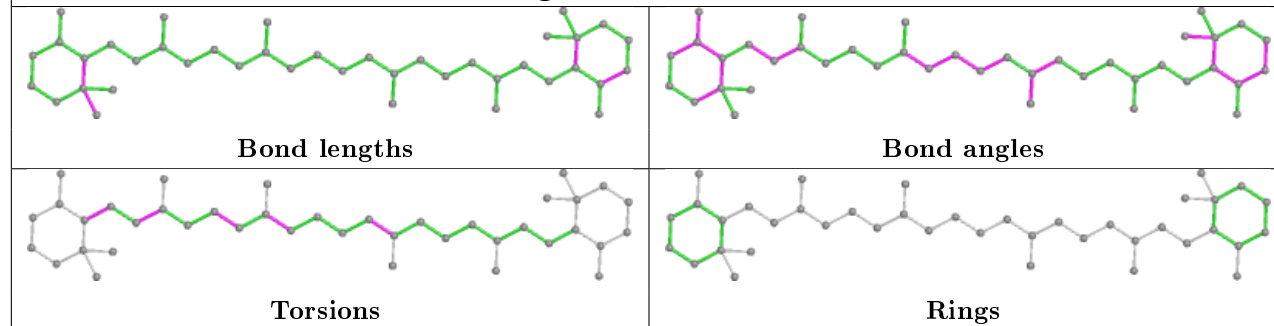
Ligand CLA b 608



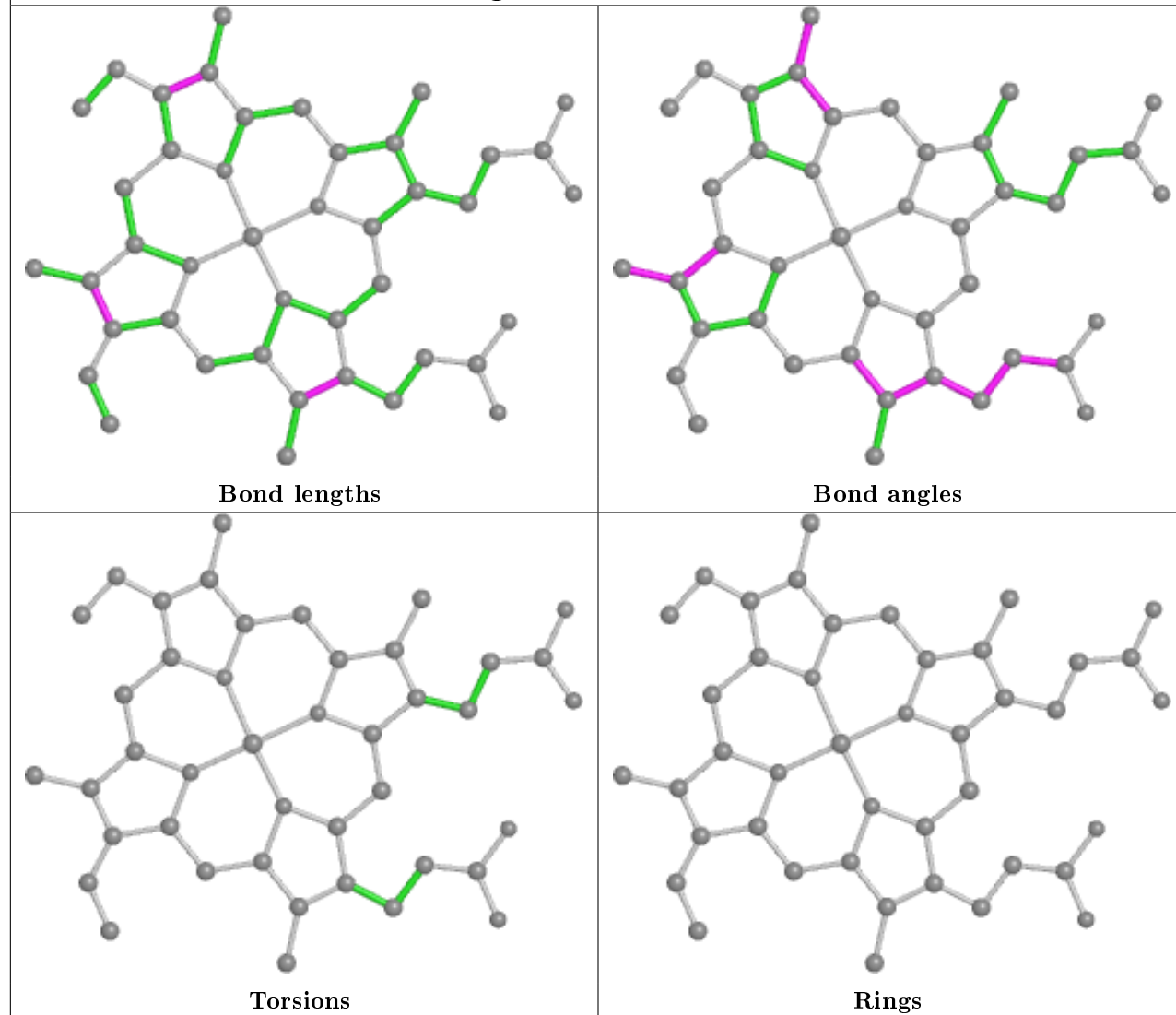
Ligand STE b 626



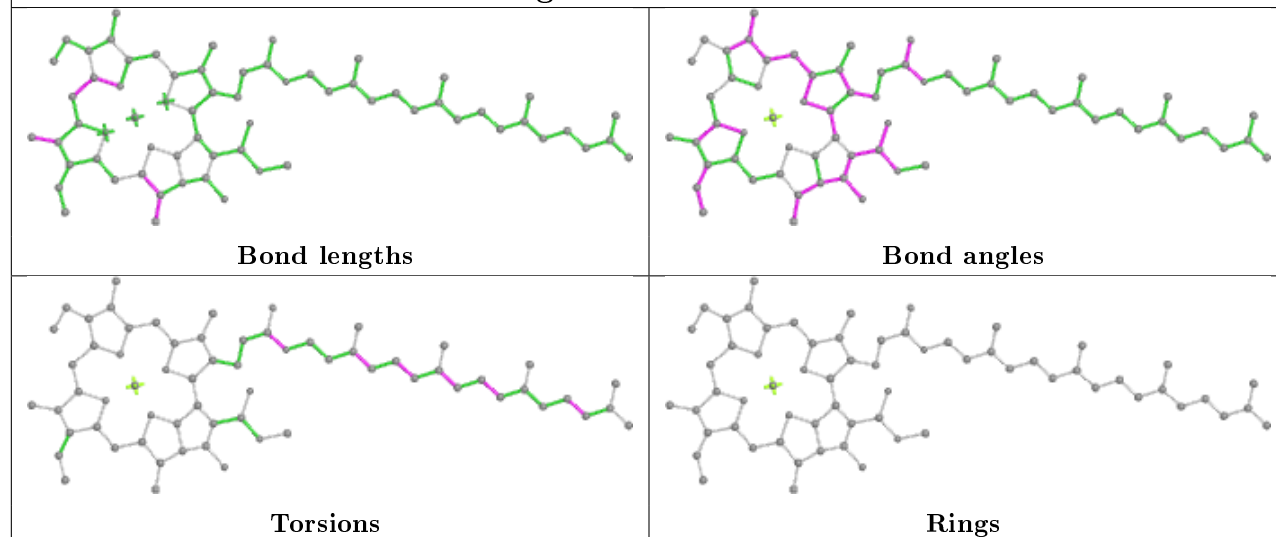
Ligand BCR t 101



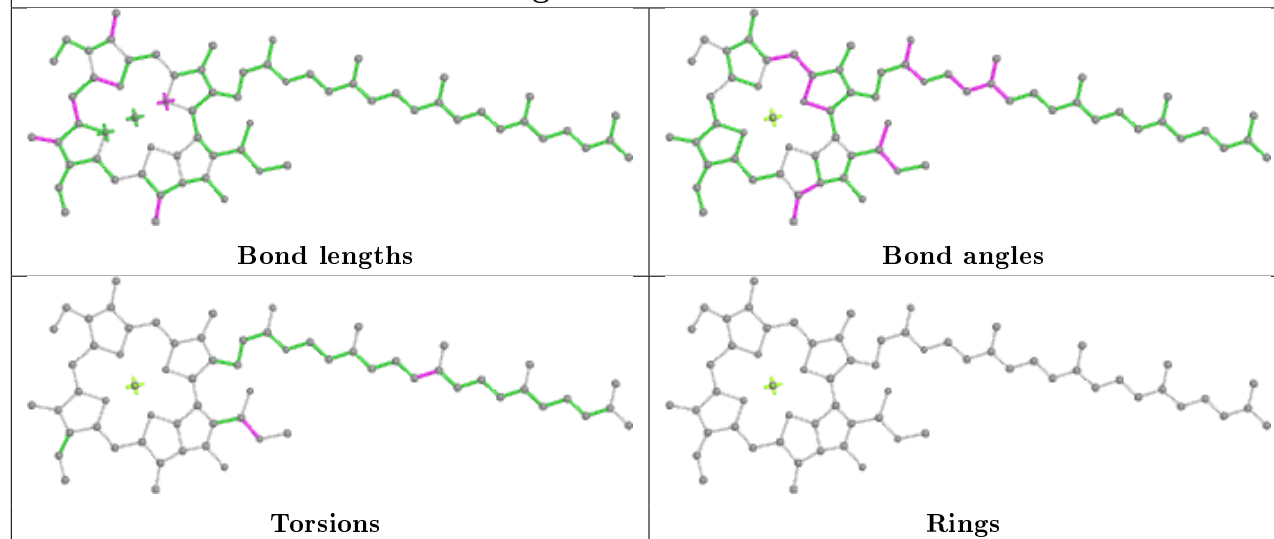
Ligand HEC V 201



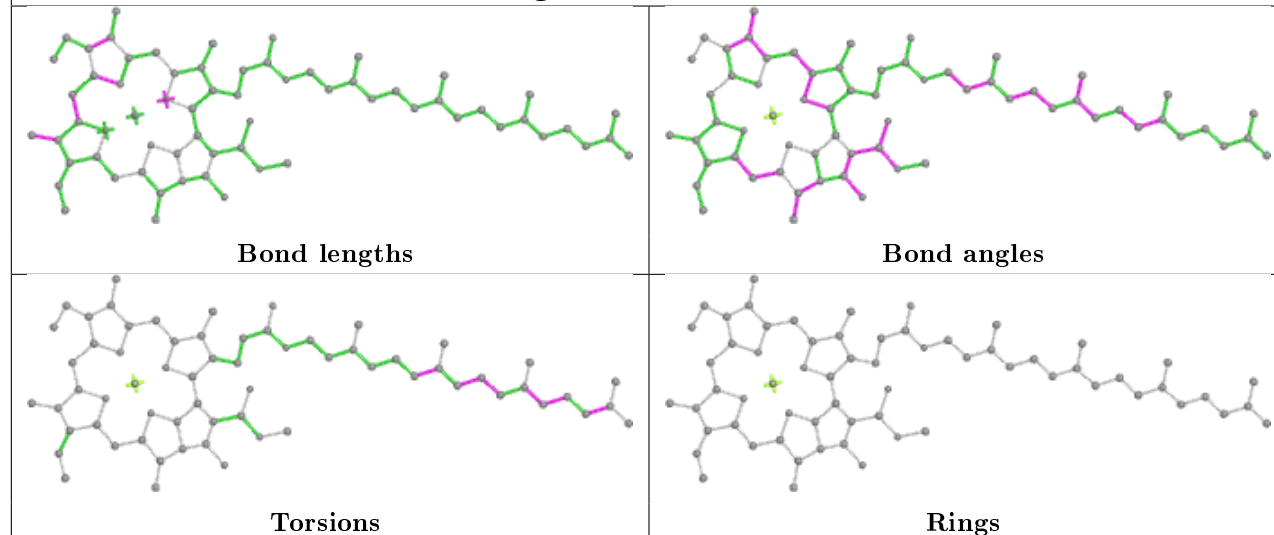
Ligand CLA a 404



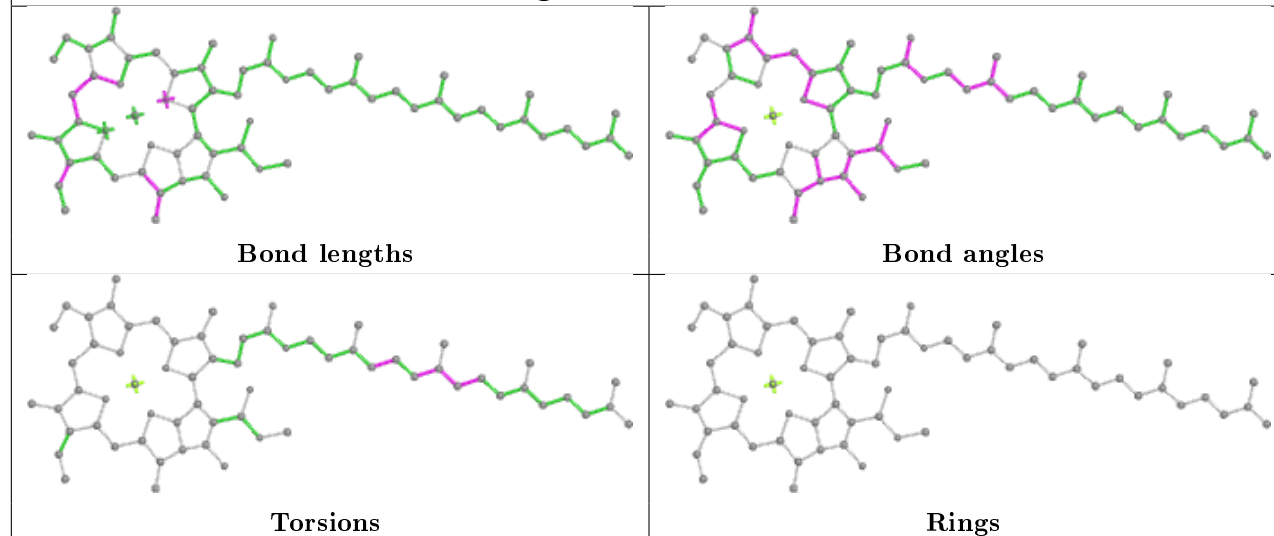
Ligand CLA C 511



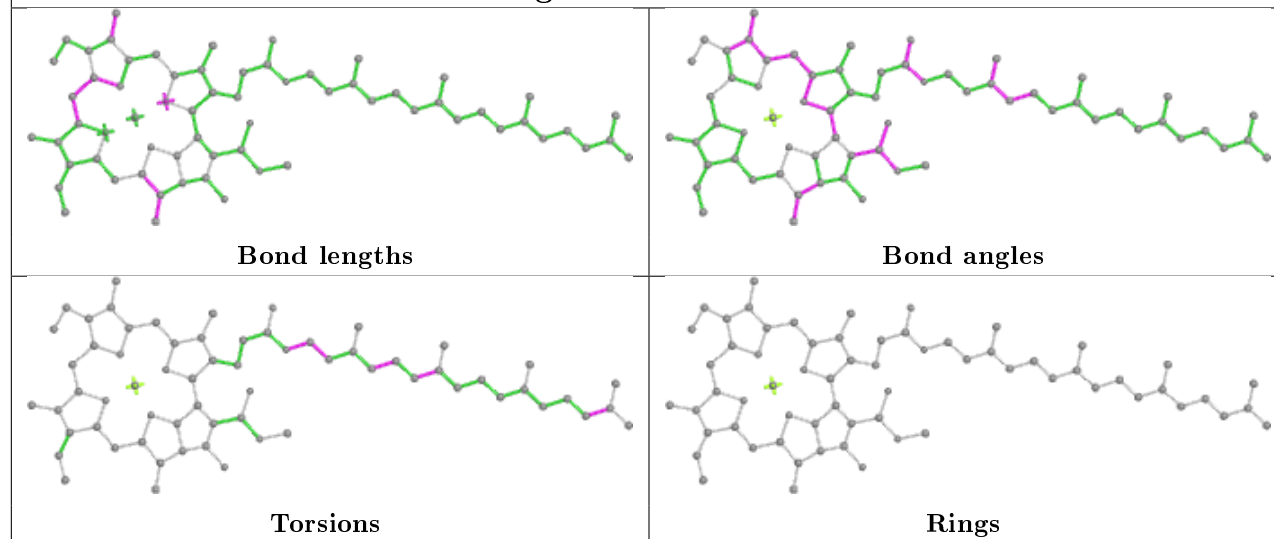
Ligand CLA B 611



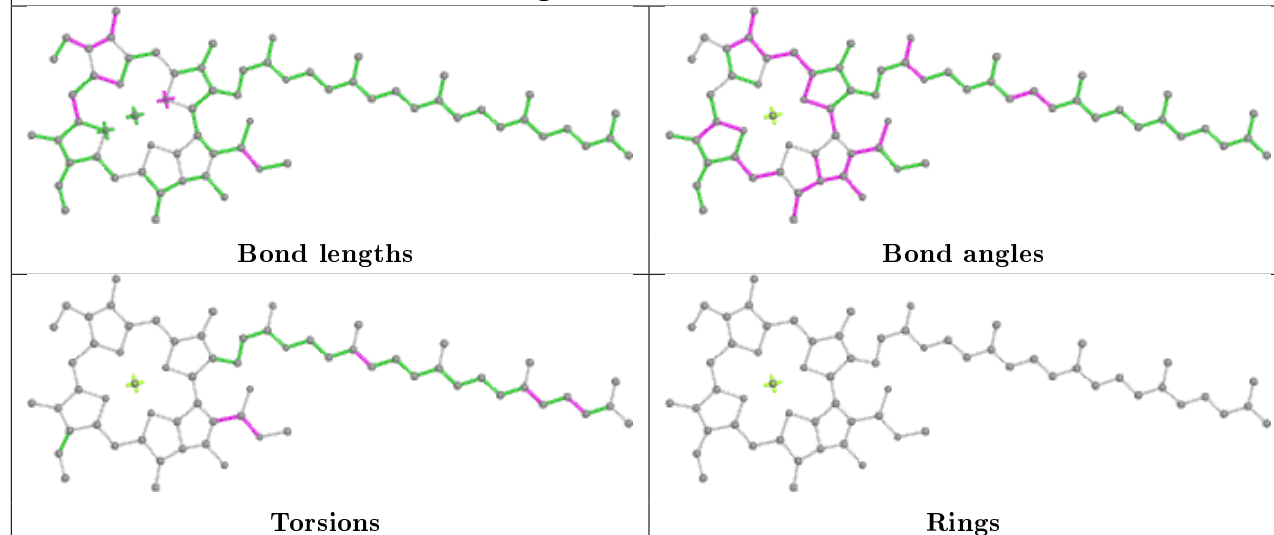
Ligand CLA b 602



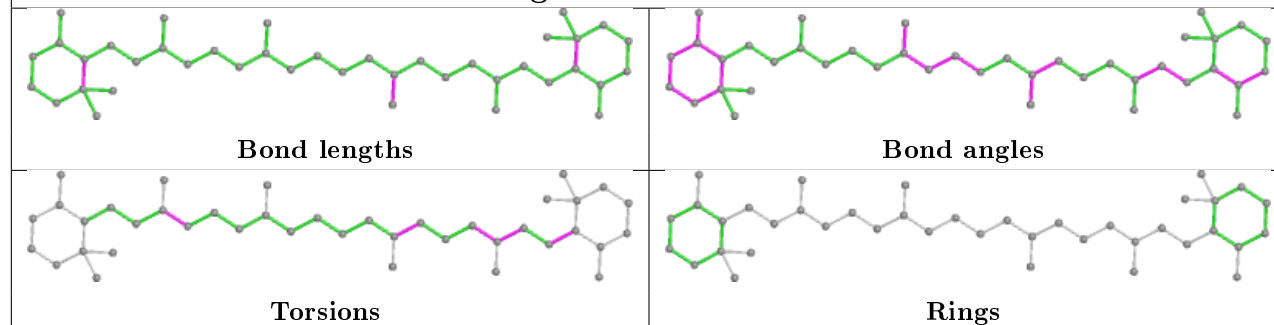
Ligand CLA d 403

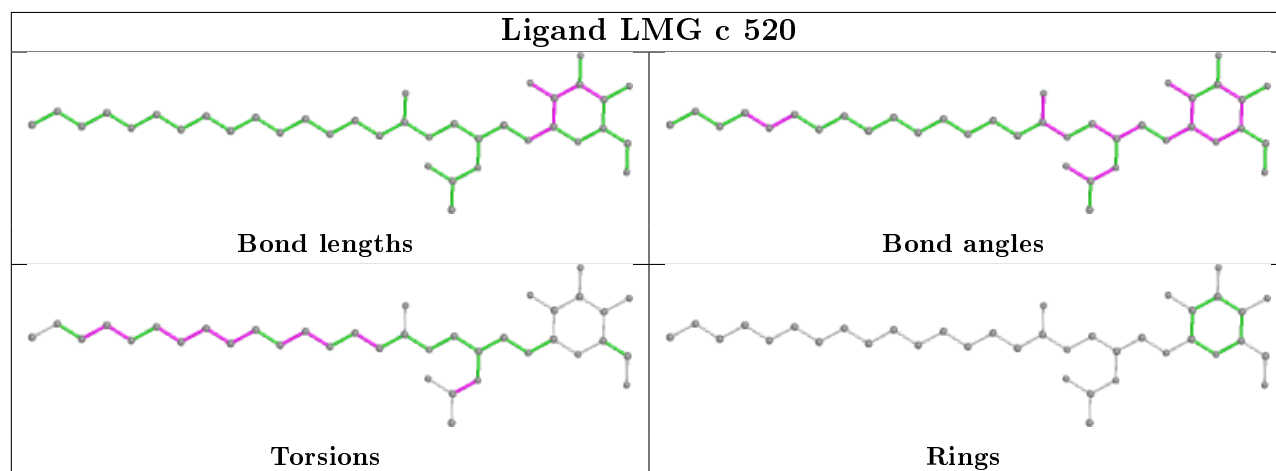
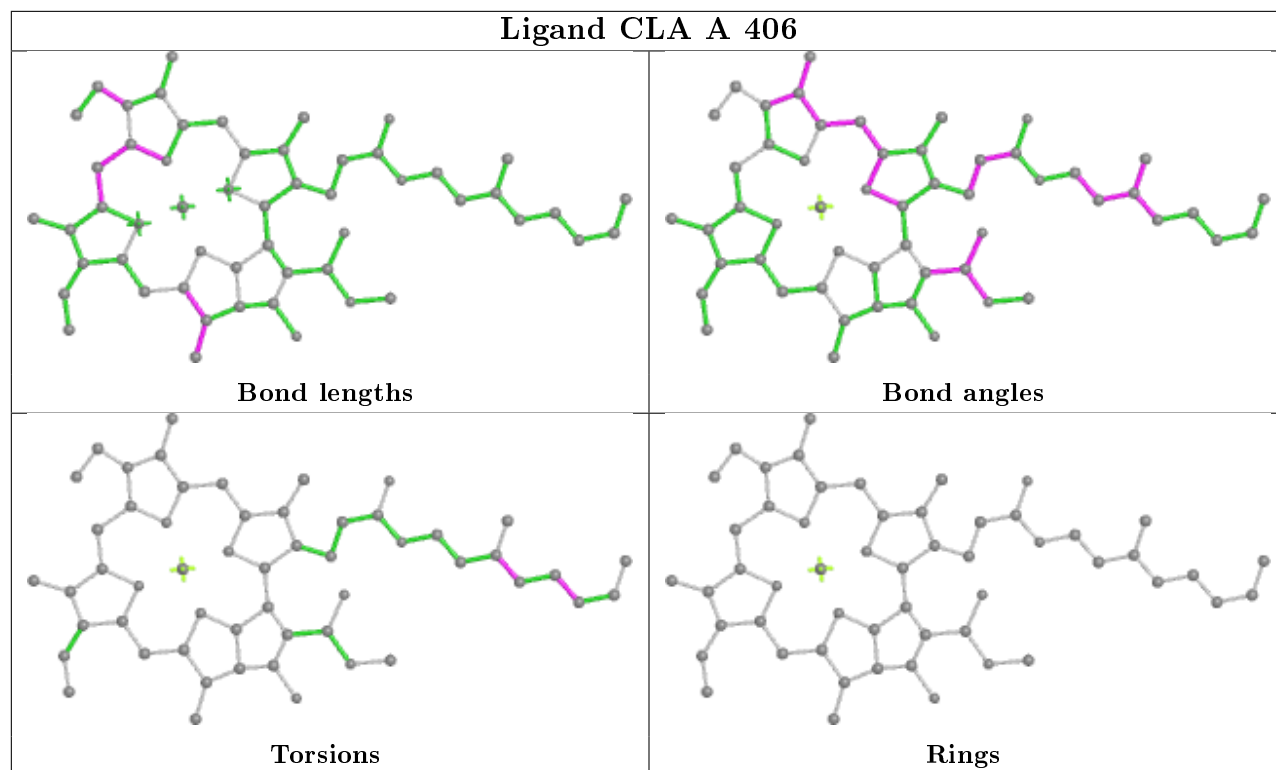


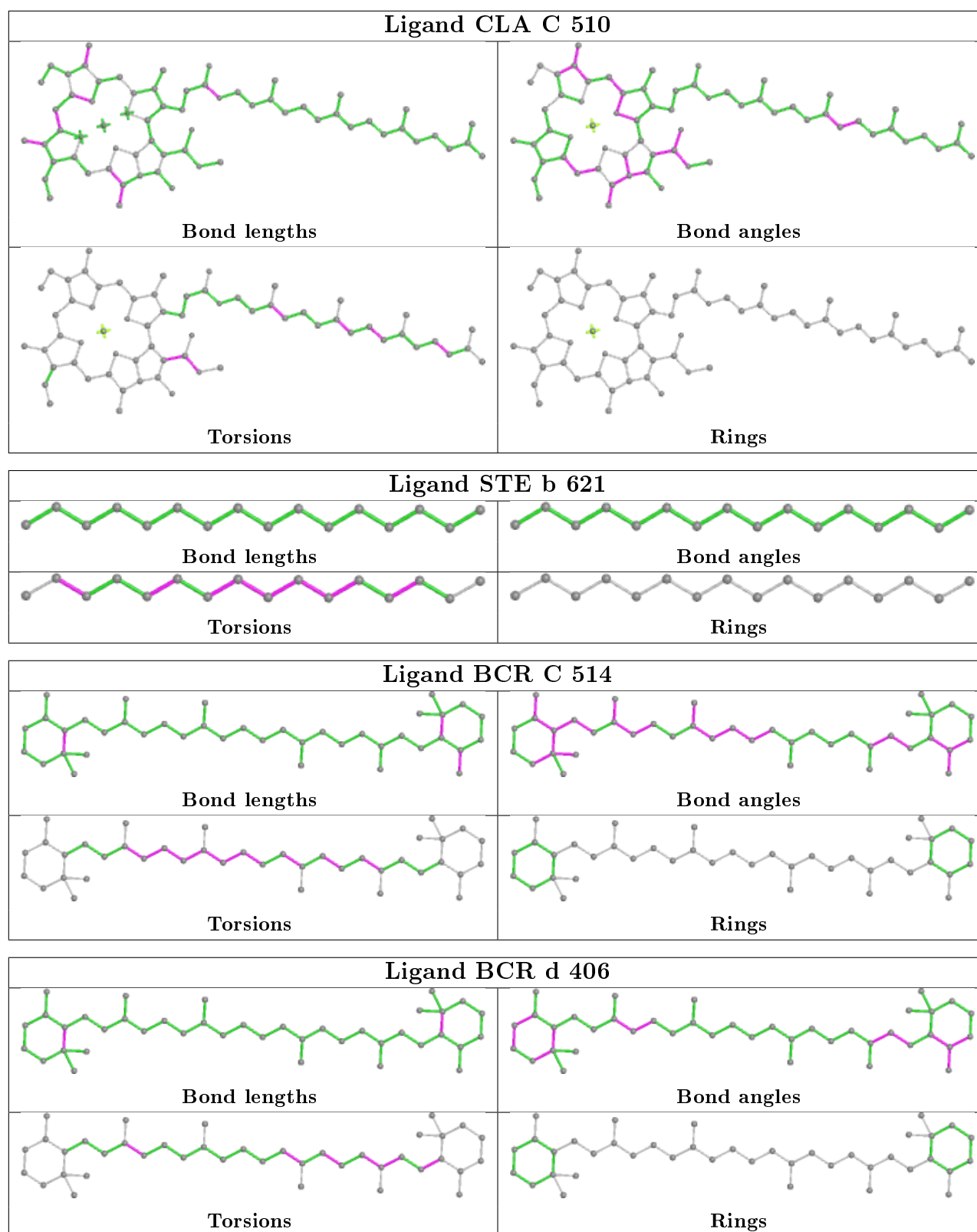
Ligand CLA b 609

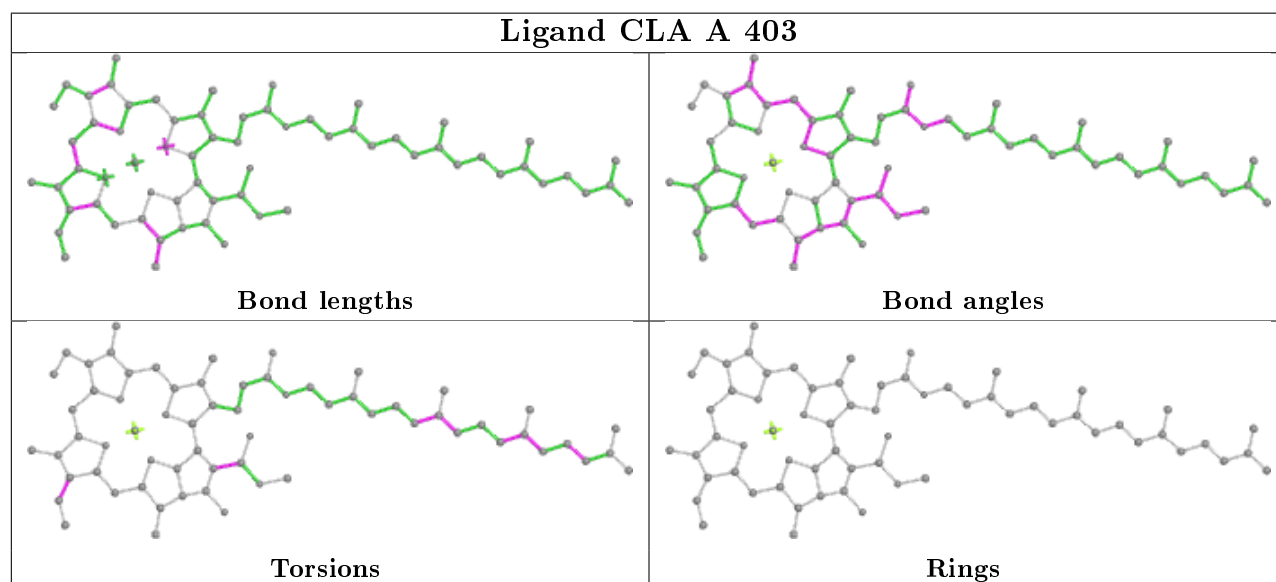
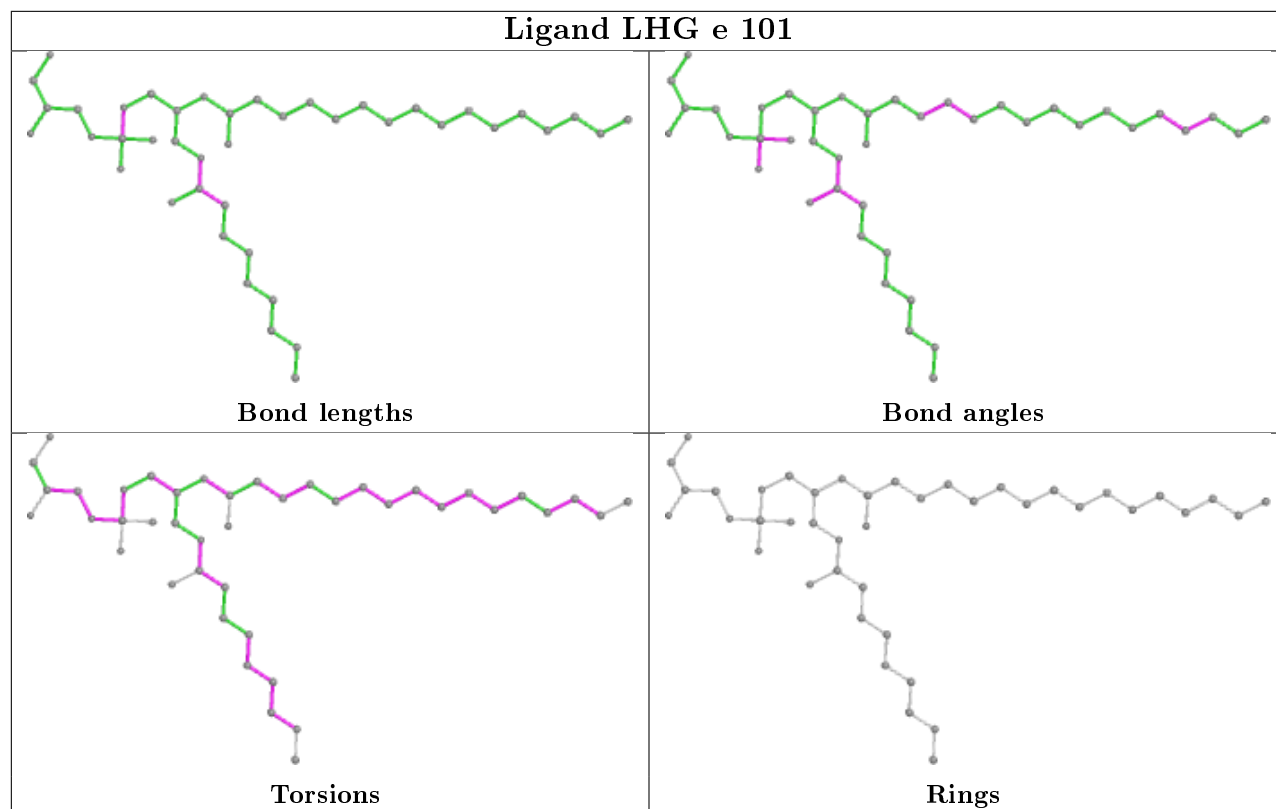
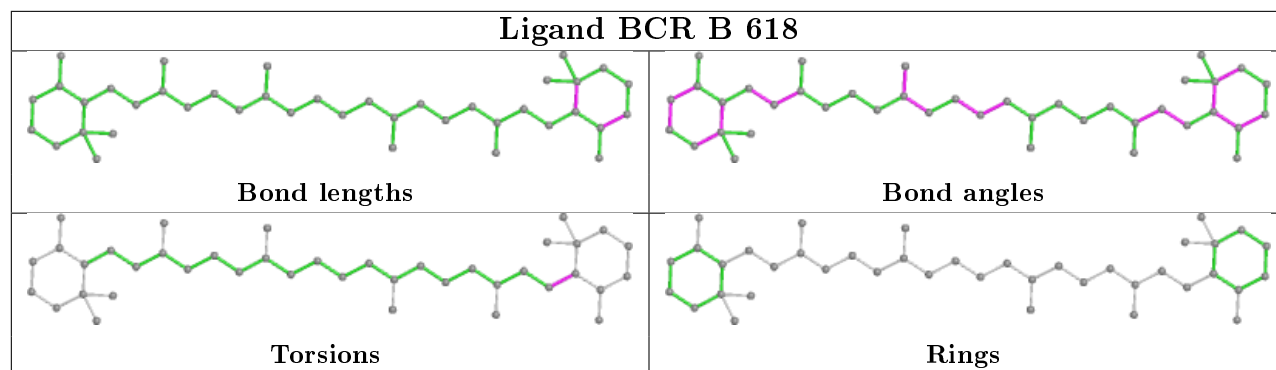


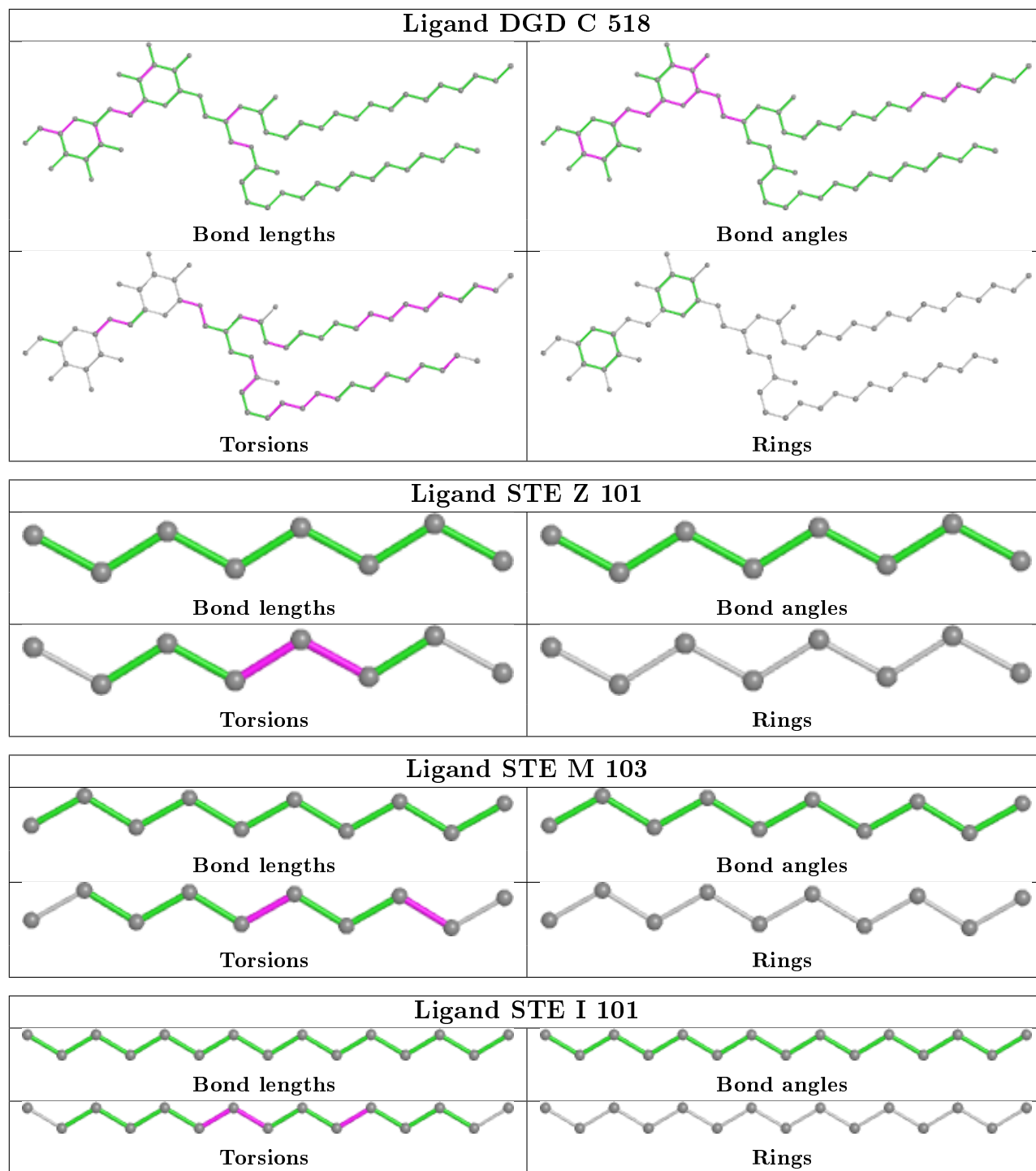
Ligand BCR D 405



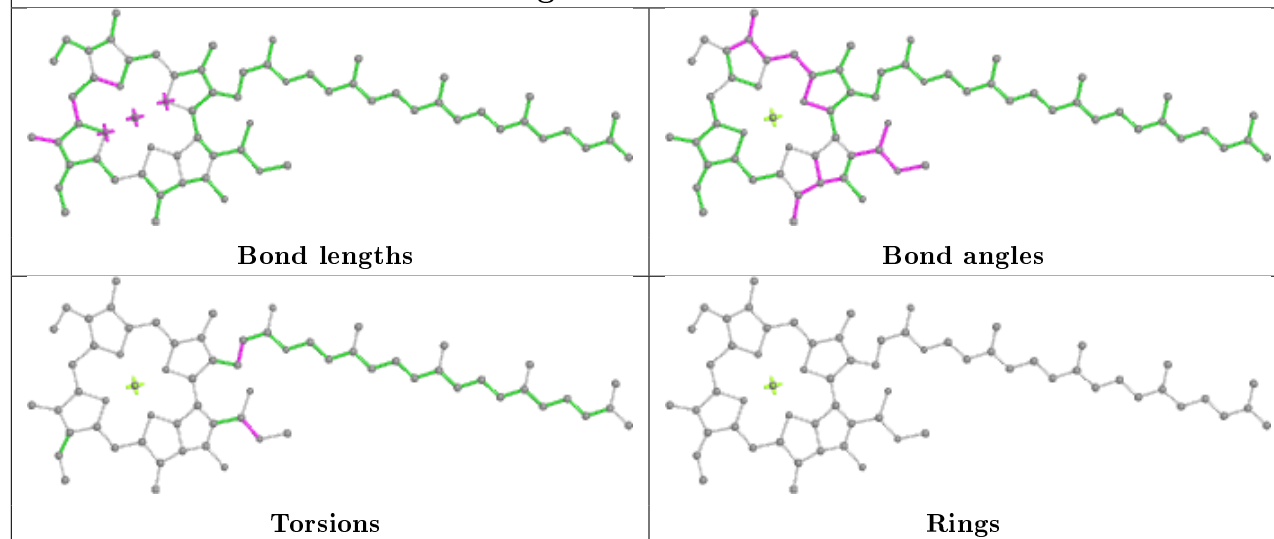




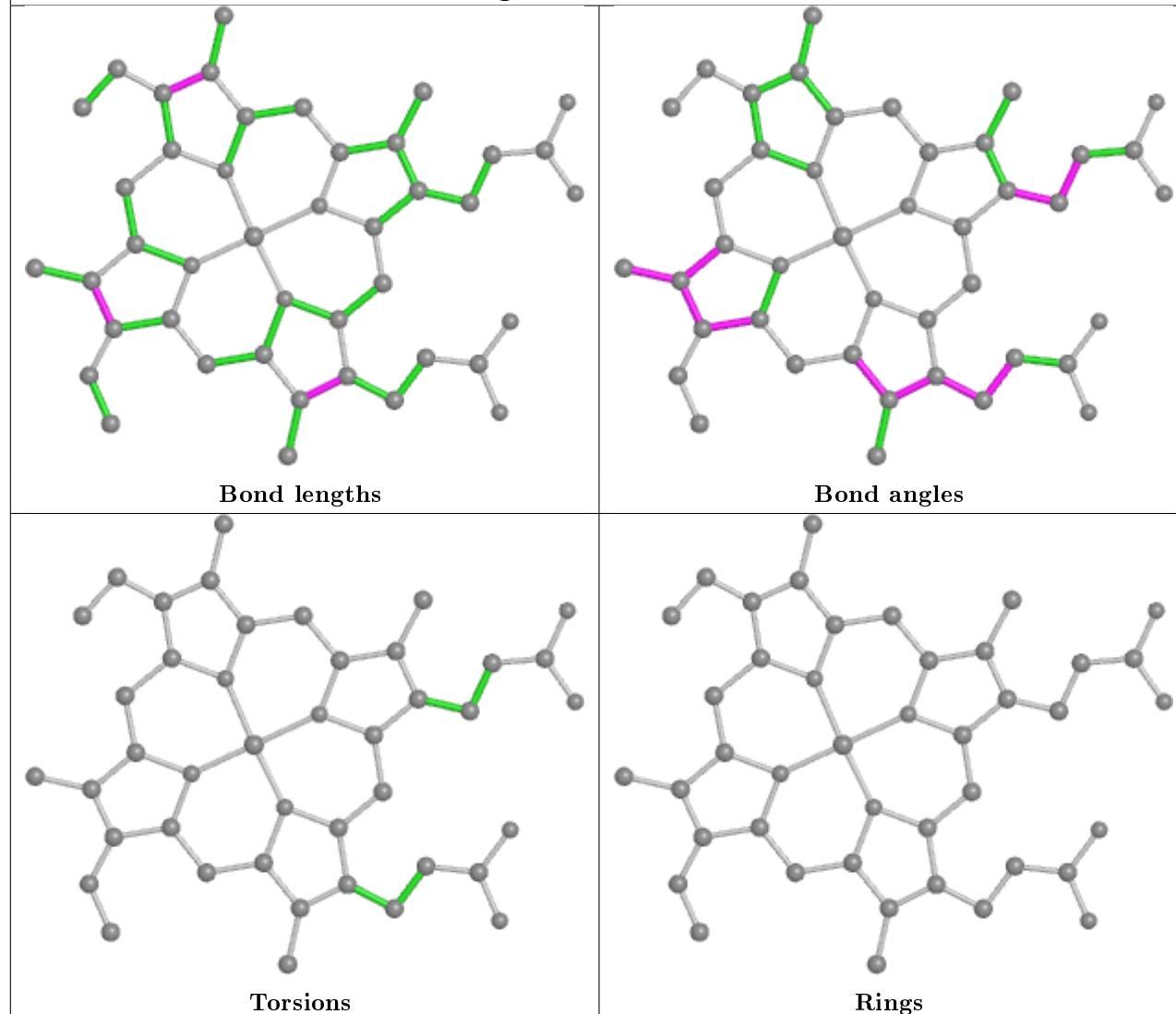




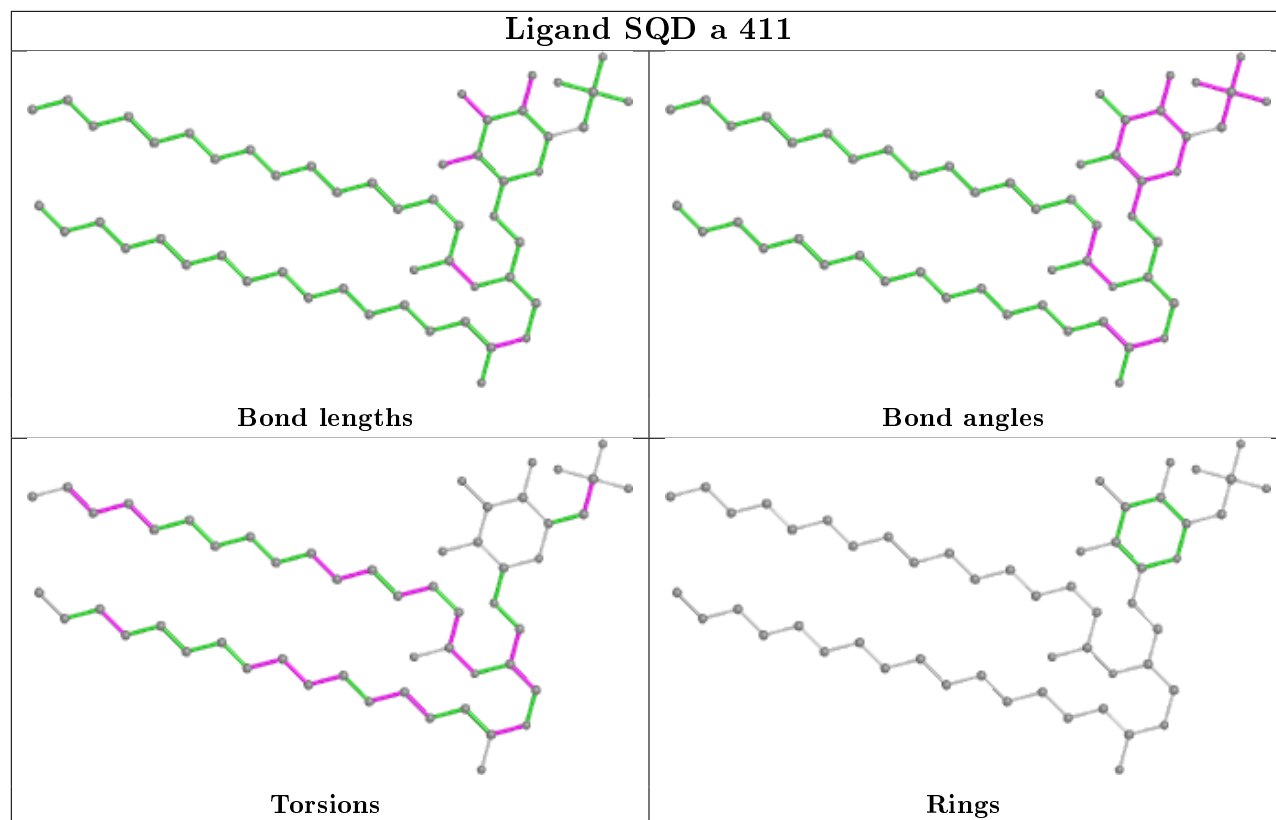
Ligand CLA c 501



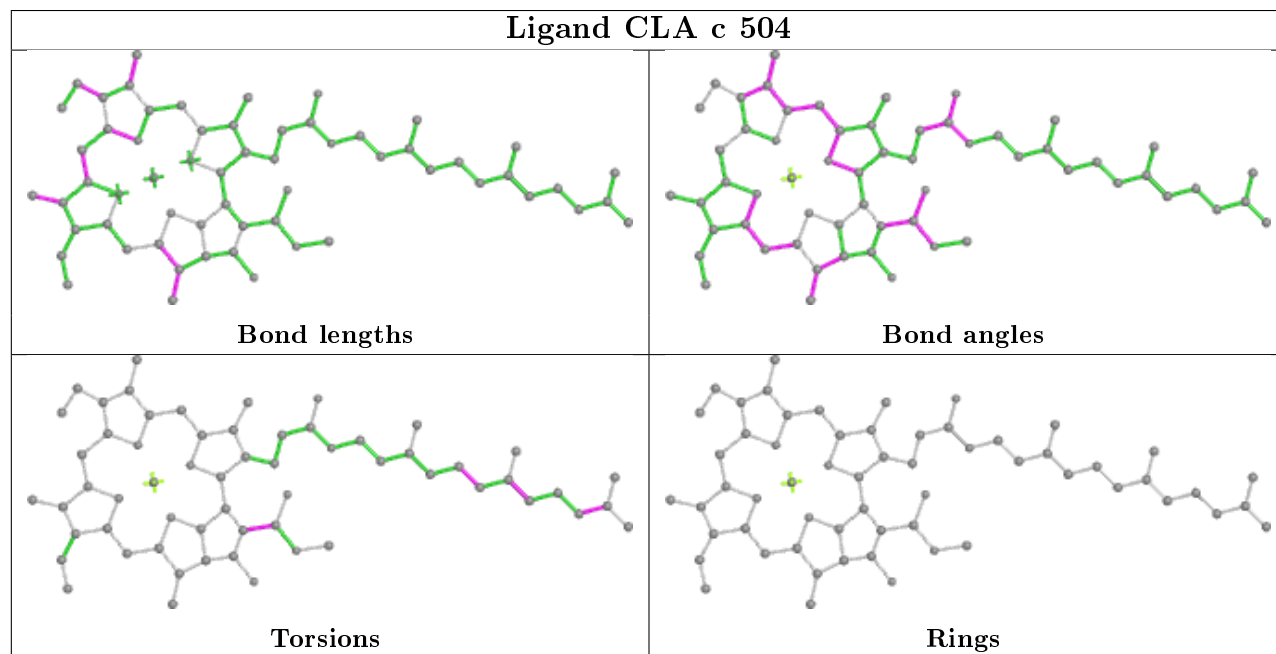
Ligand HEC f 101

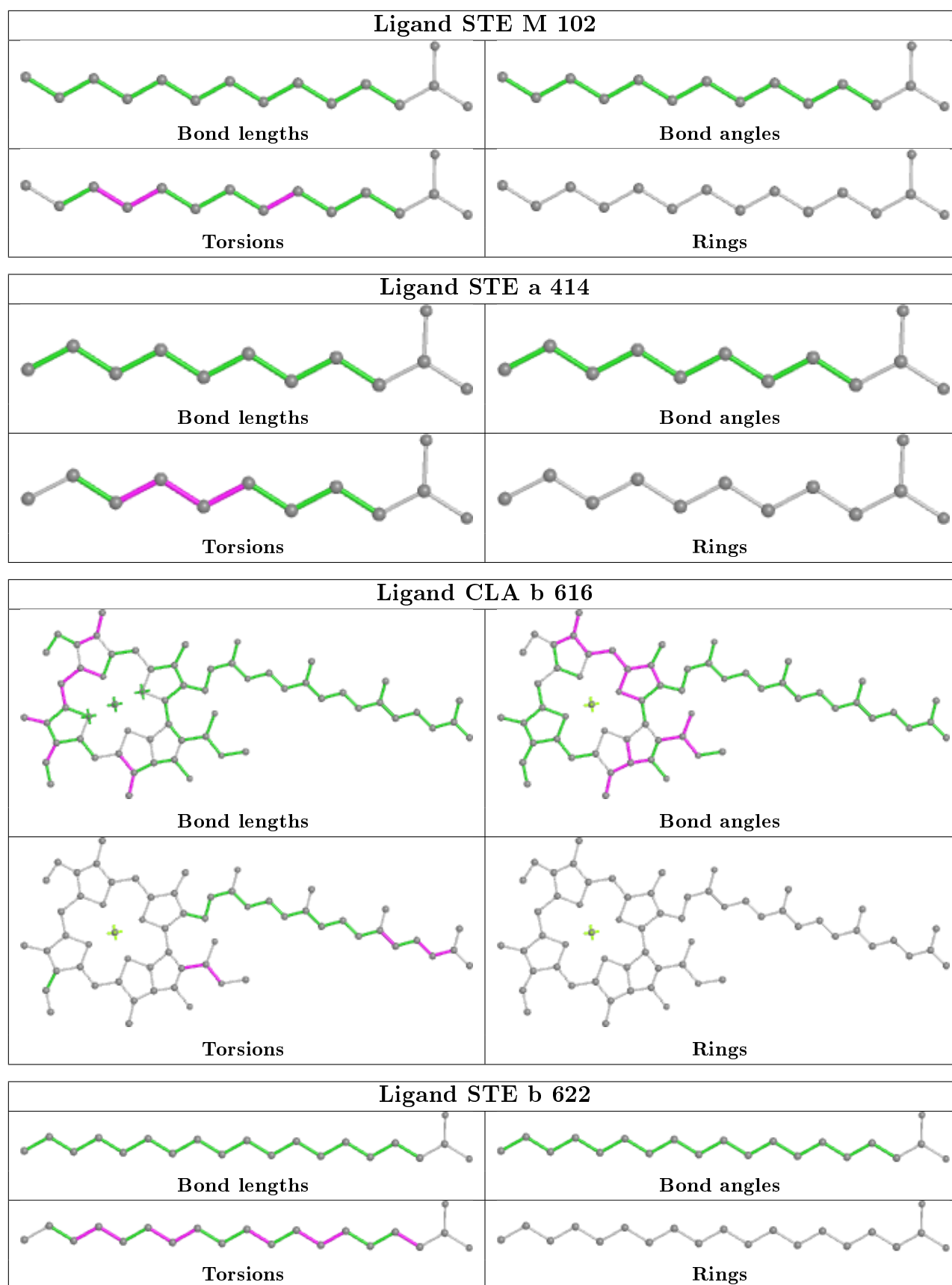


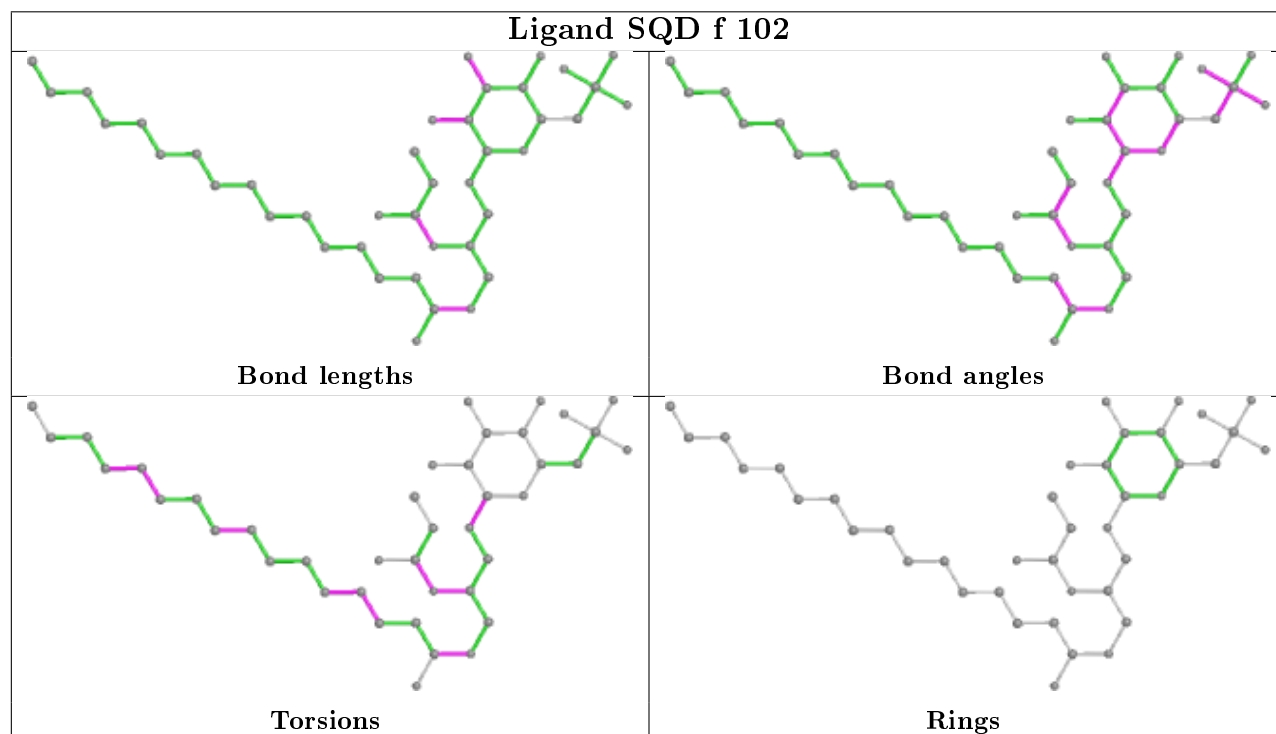
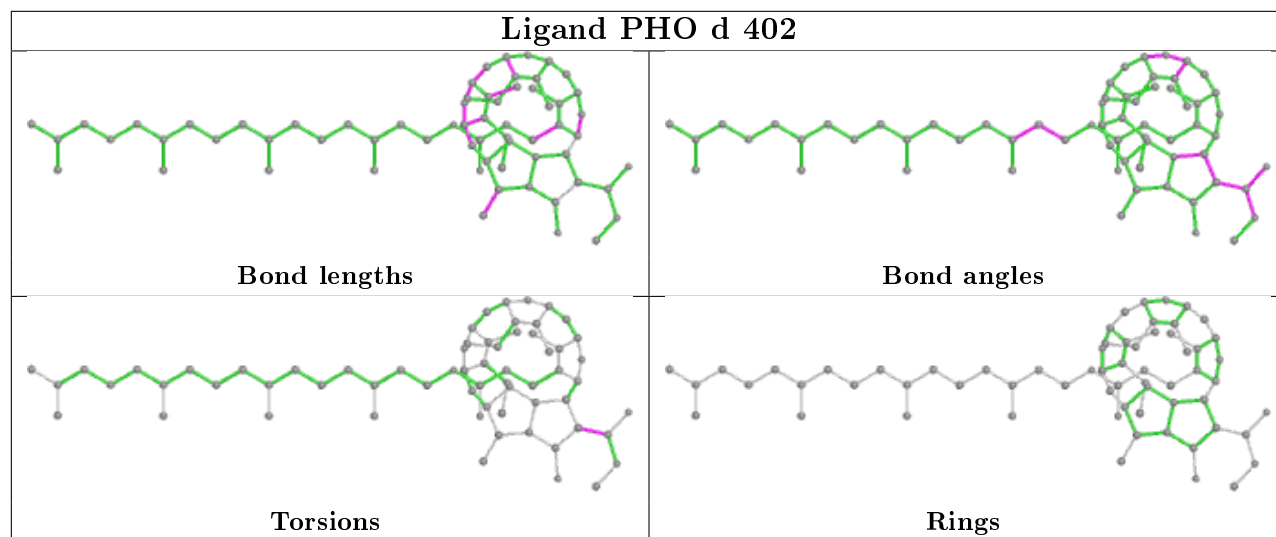
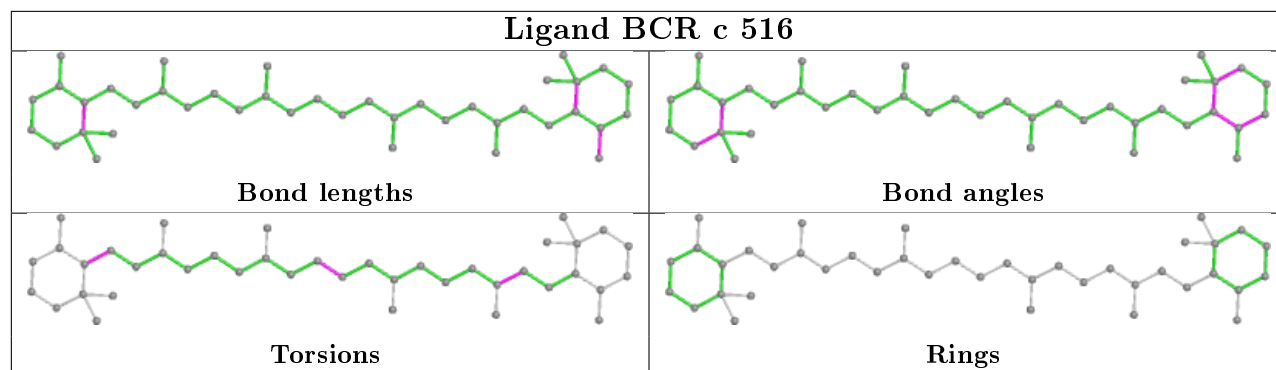
Ligand SQD a 411



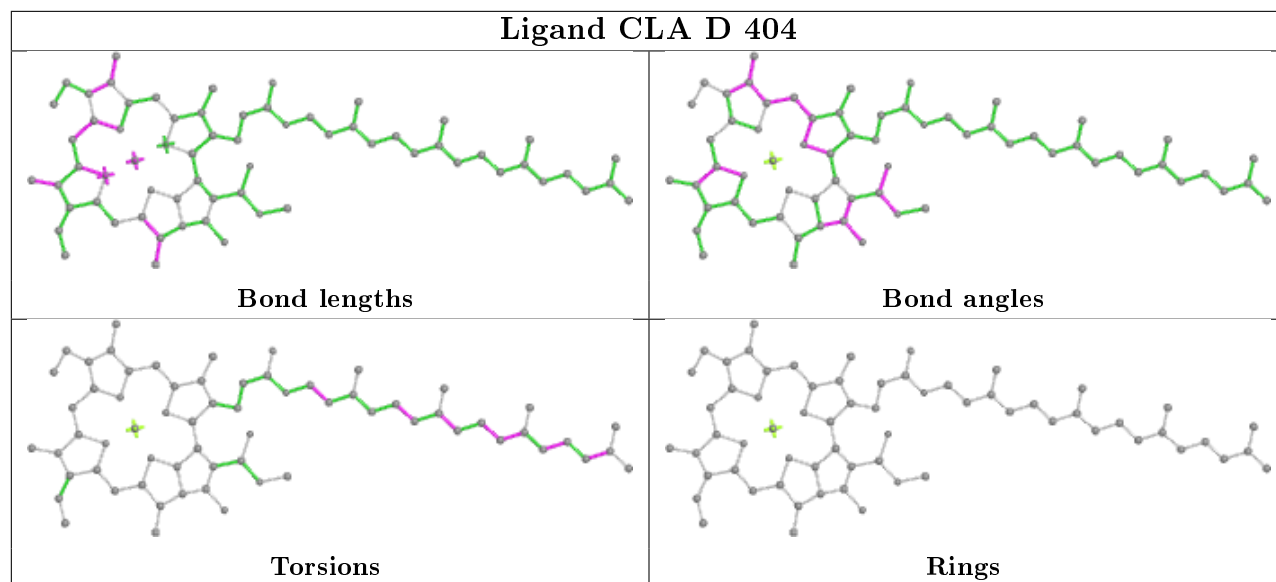
Ligand CLA c 504



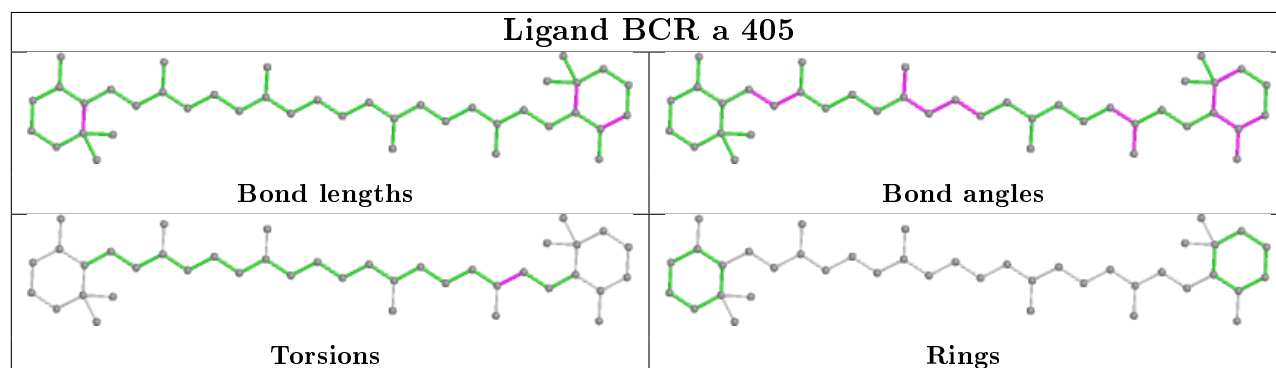




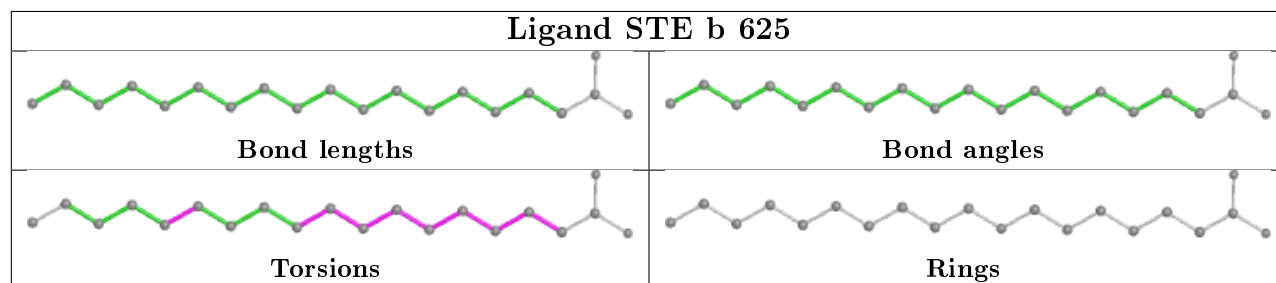
Ligand CLA D 404



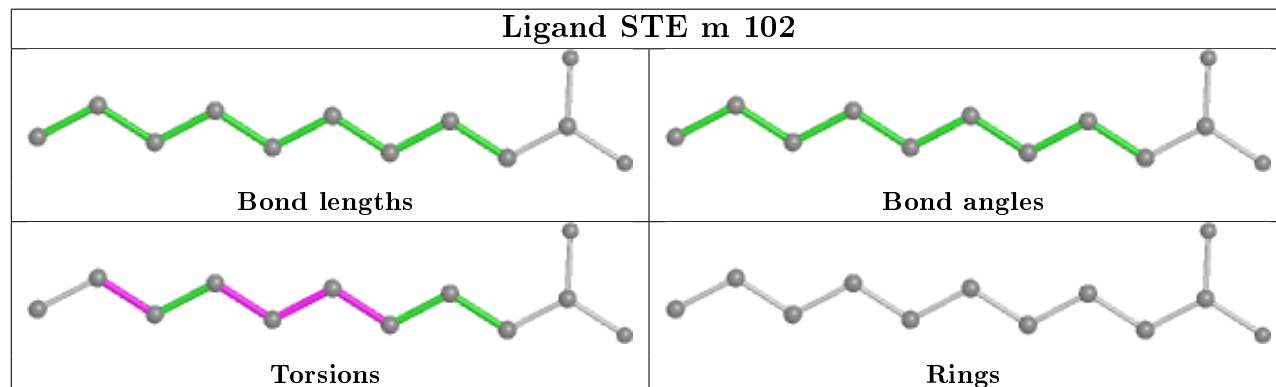
Ligand BCR a 405



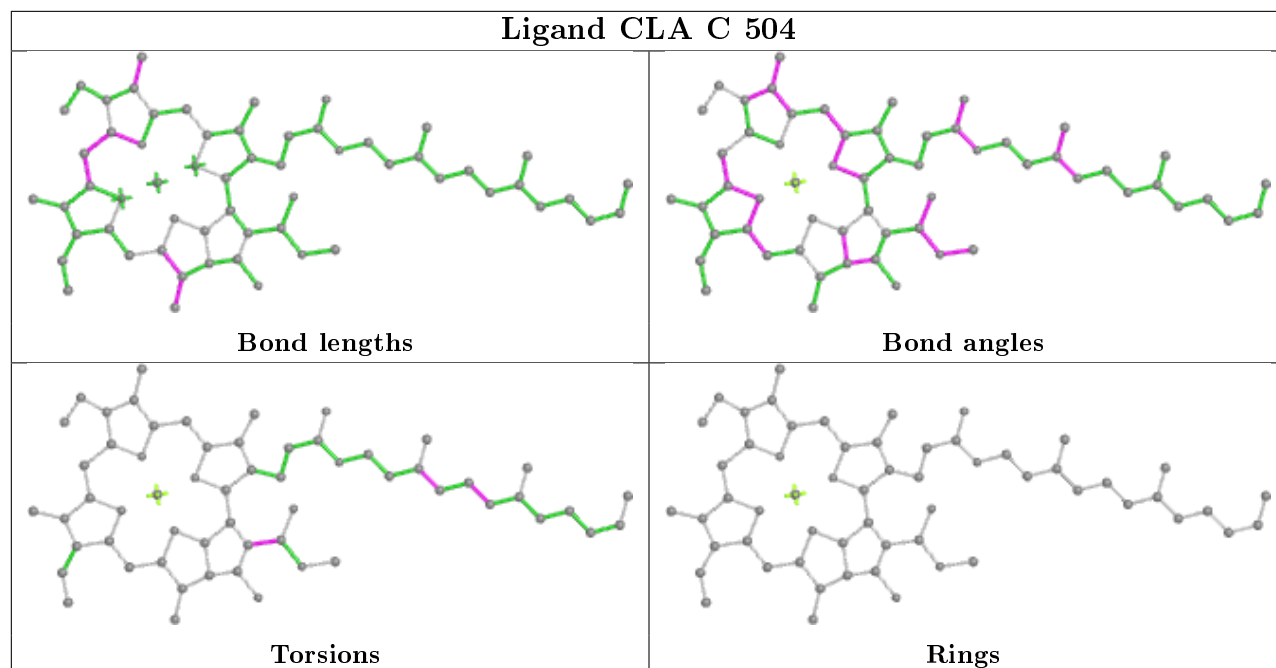
Ligand STE b 625



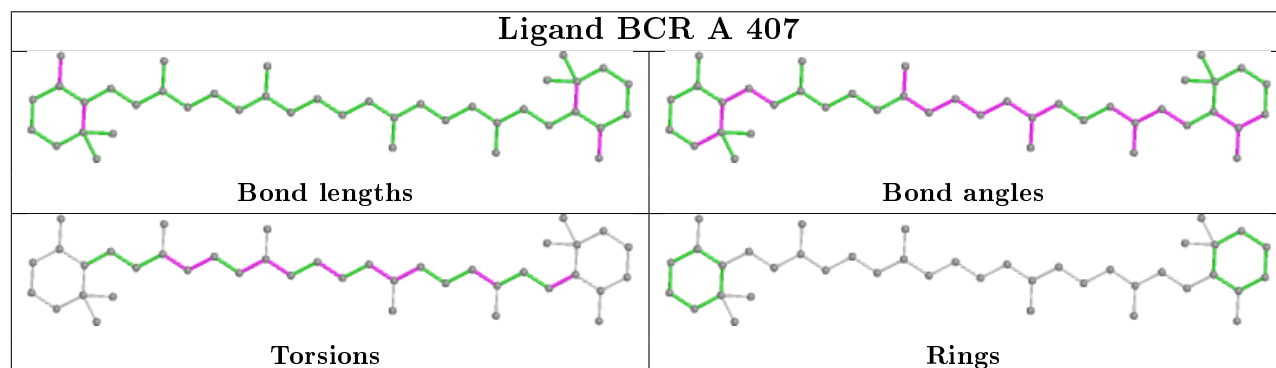
Ligand STE m 102



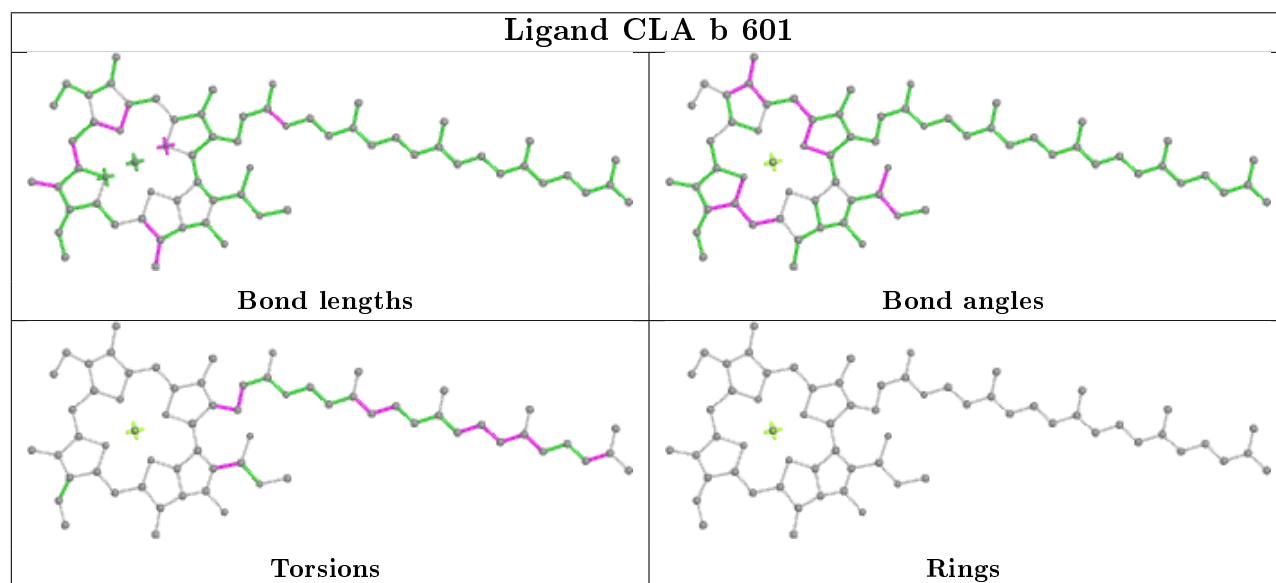
Ligand CLA C 504



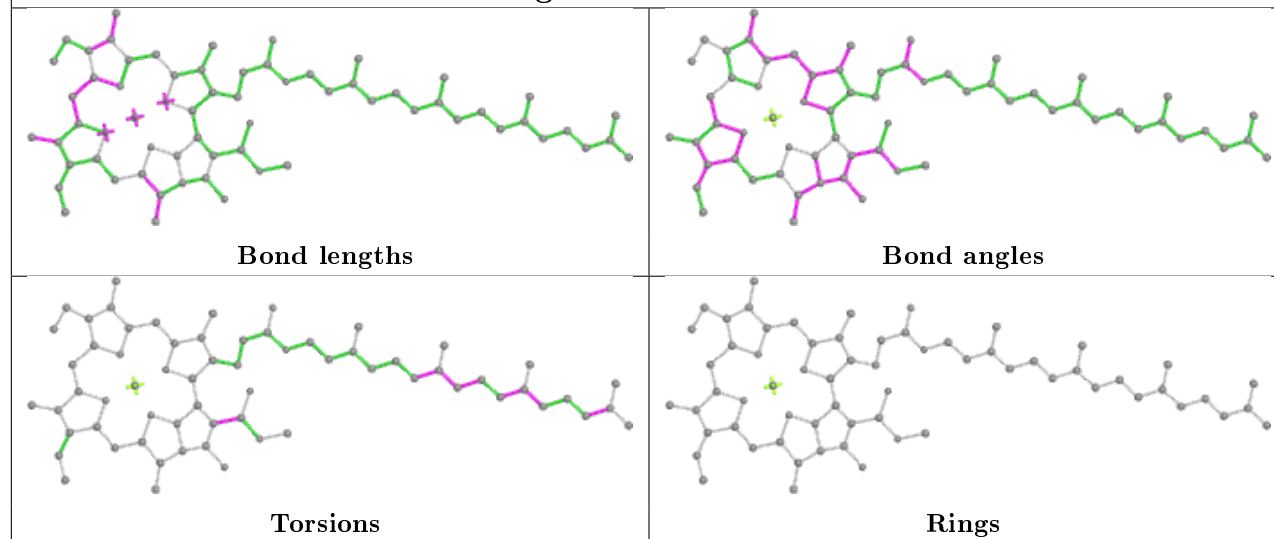
Ligand BCR A 407



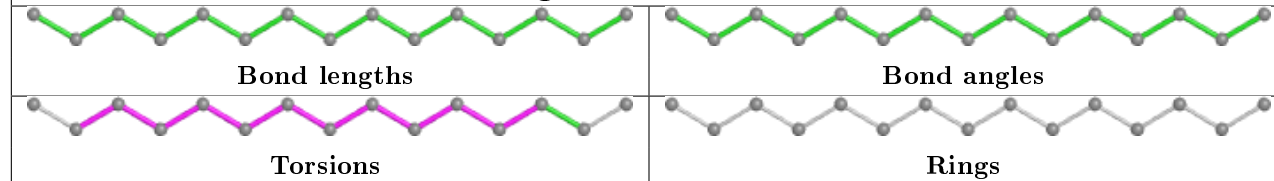
Ligand CLA b 601



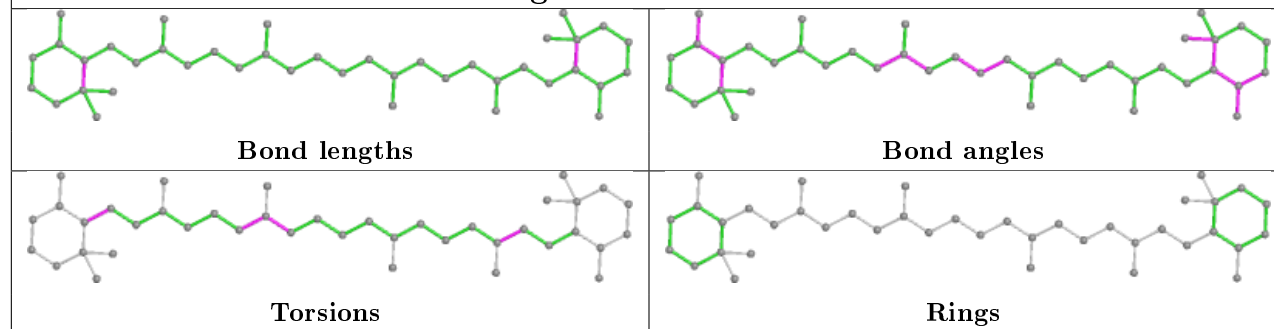
Ligand CLA d 401



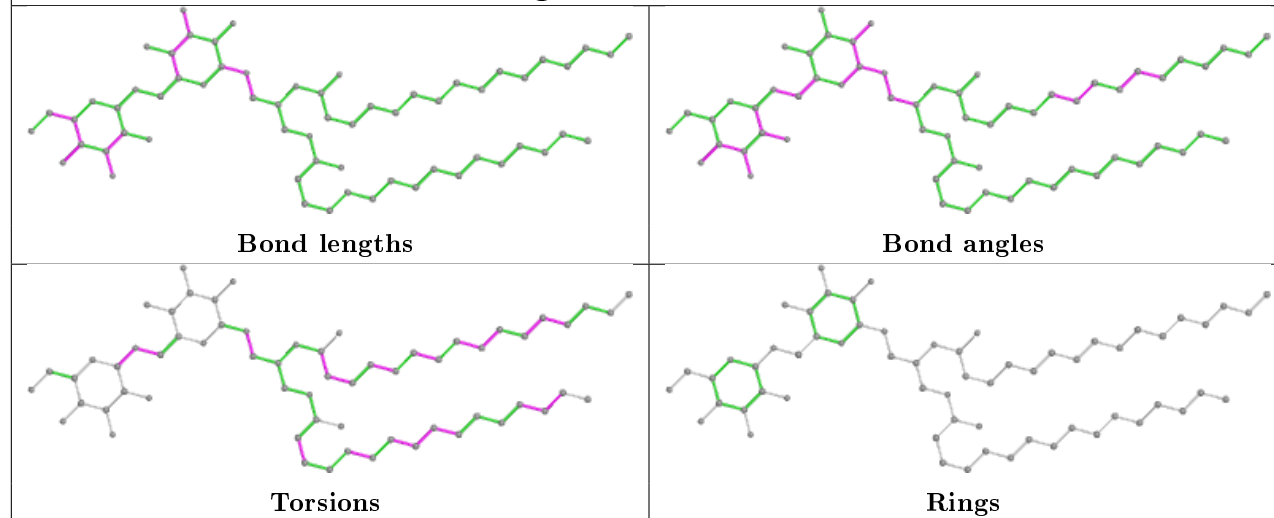
Ligand STE T 102



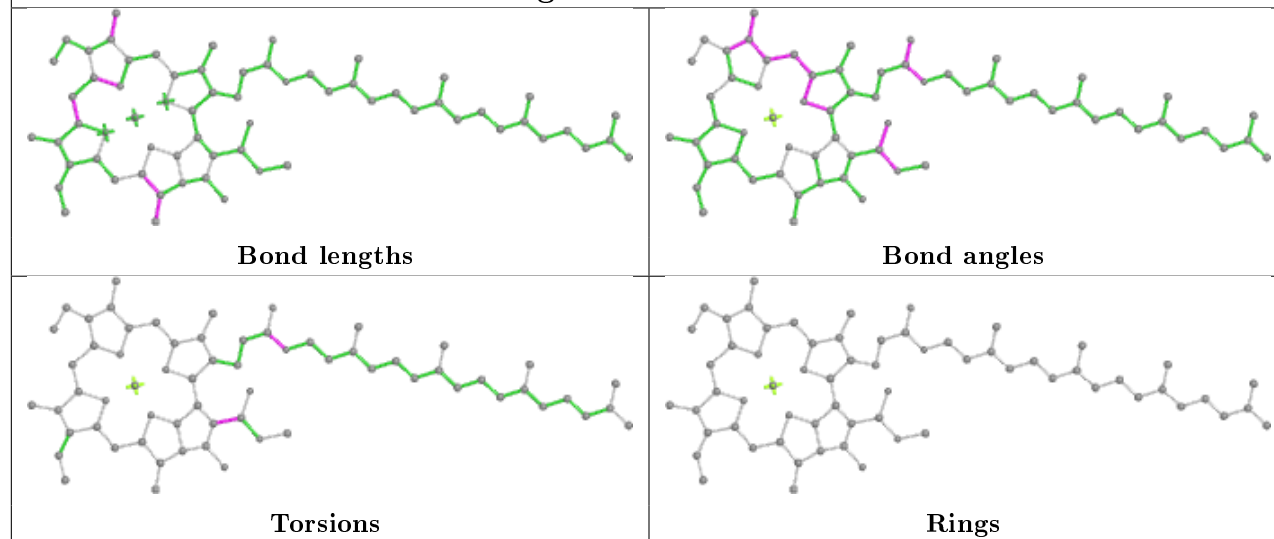
Ligand BCR Y 101



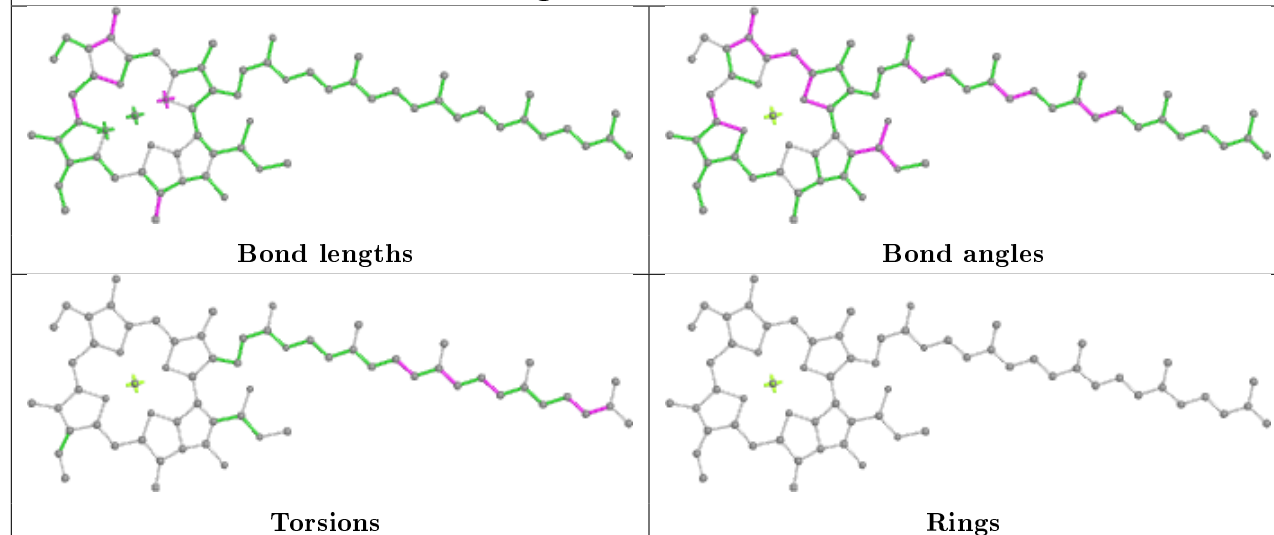
Ligand DGD c 518



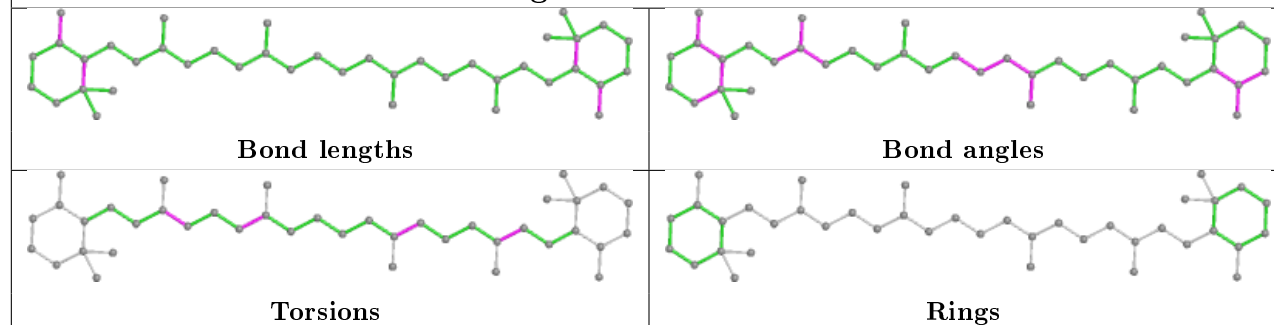
Ligand CLA c 502

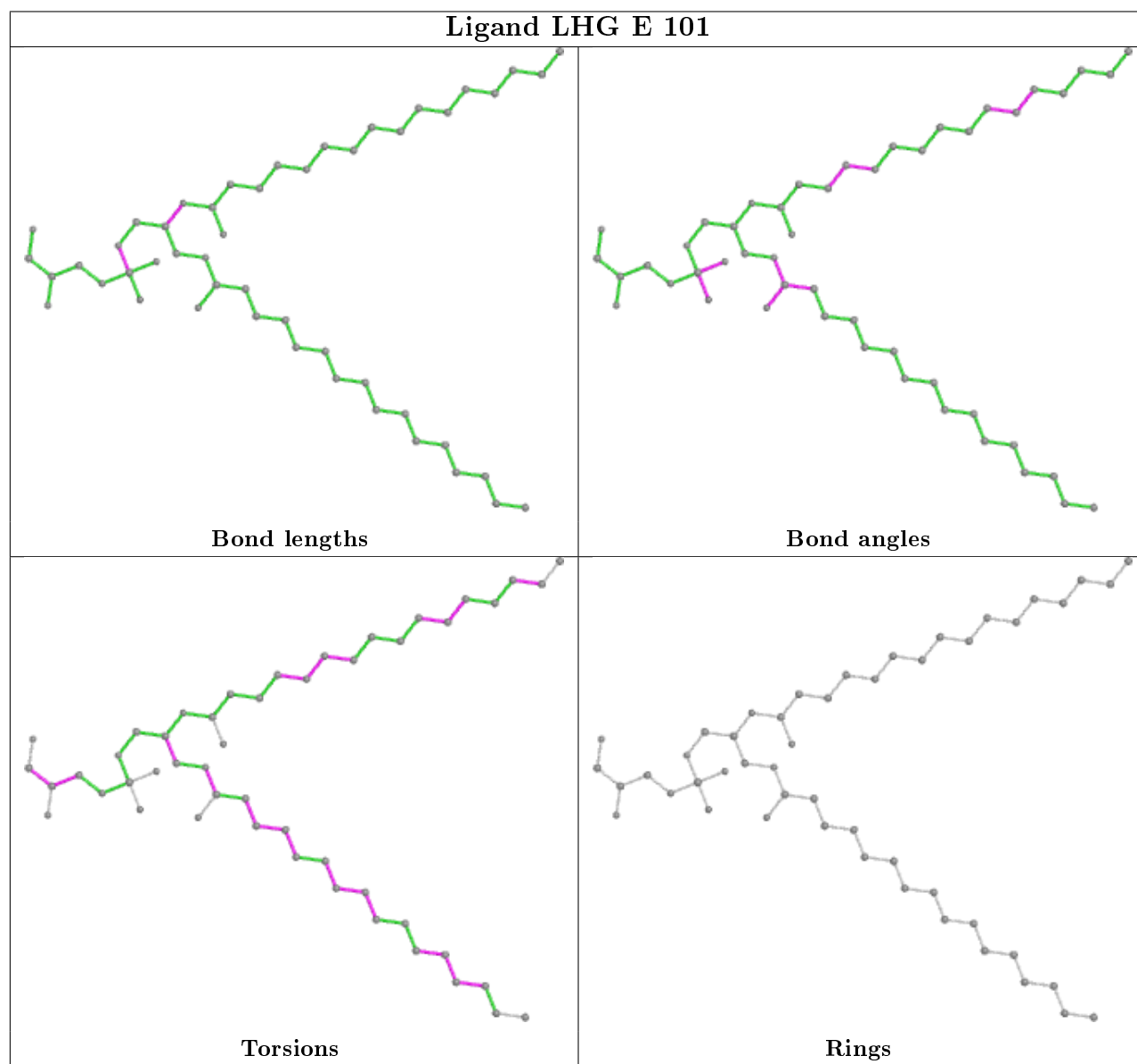
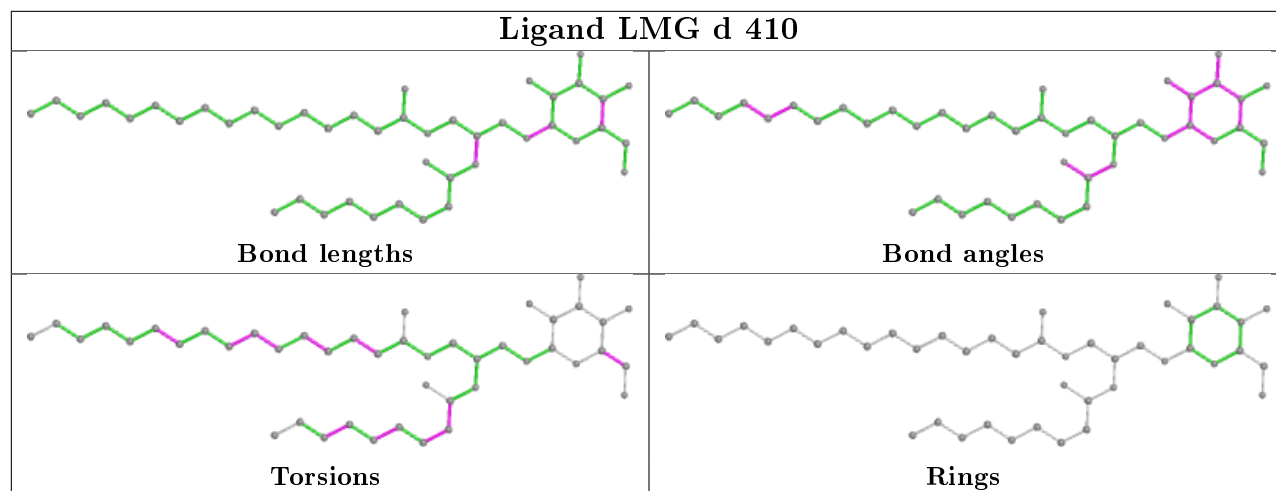


Ligand CLA b 615

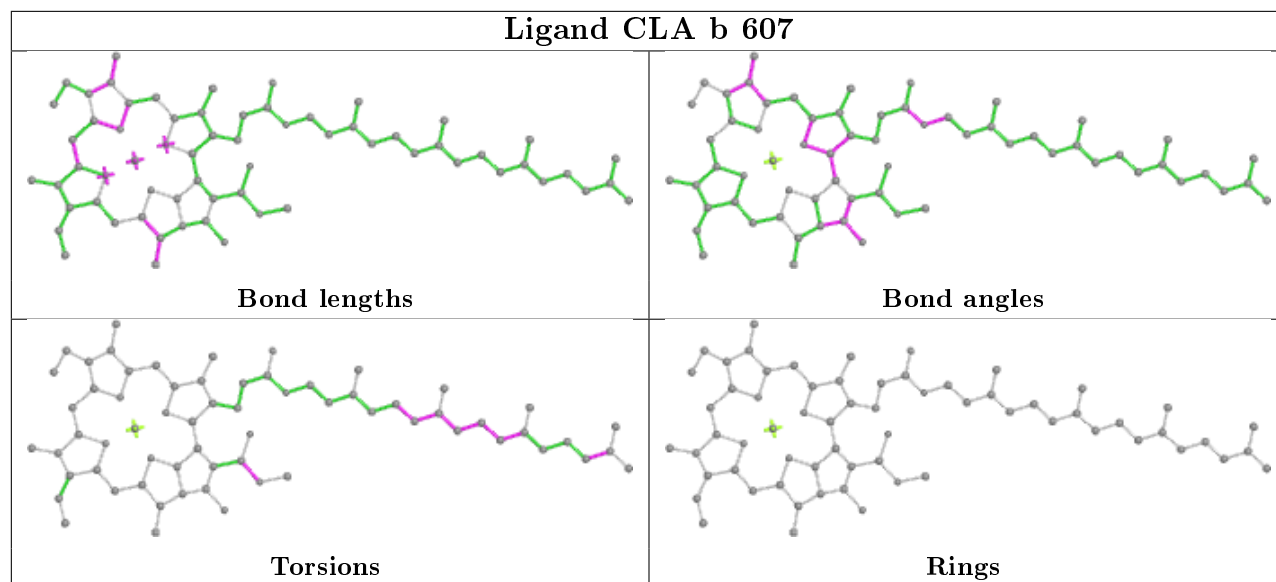


Ligand BCR c 515

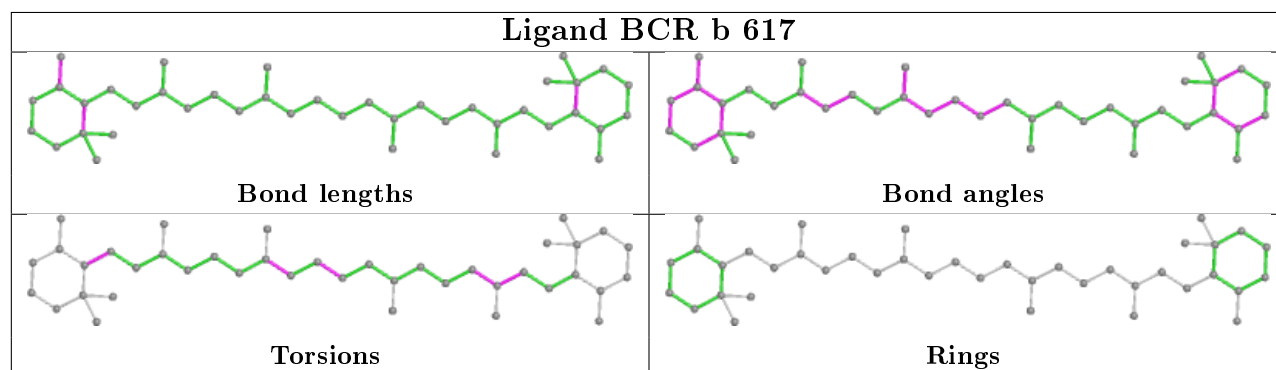




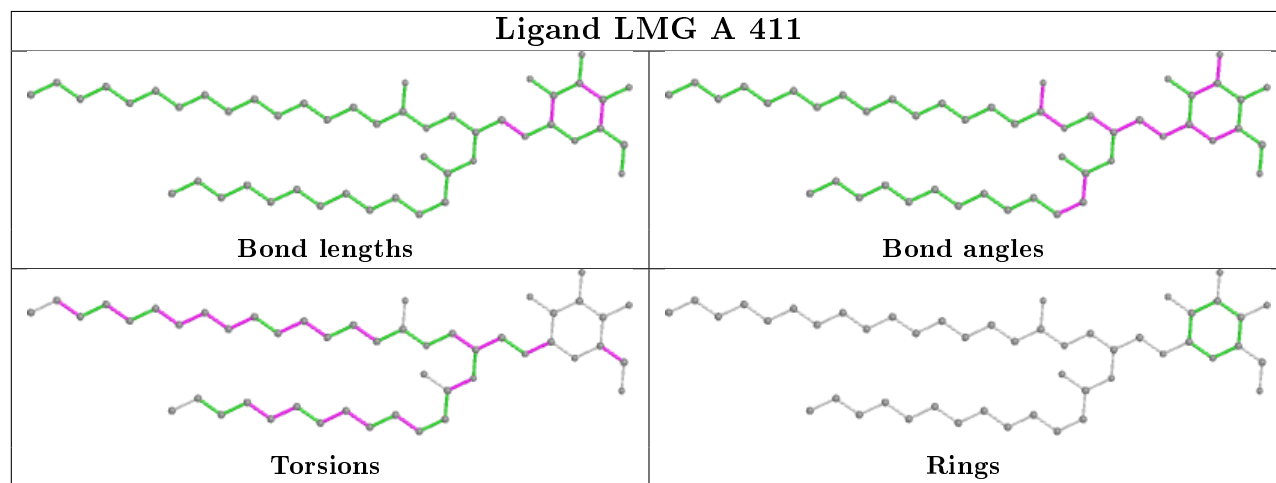
Ligand CLA b 607

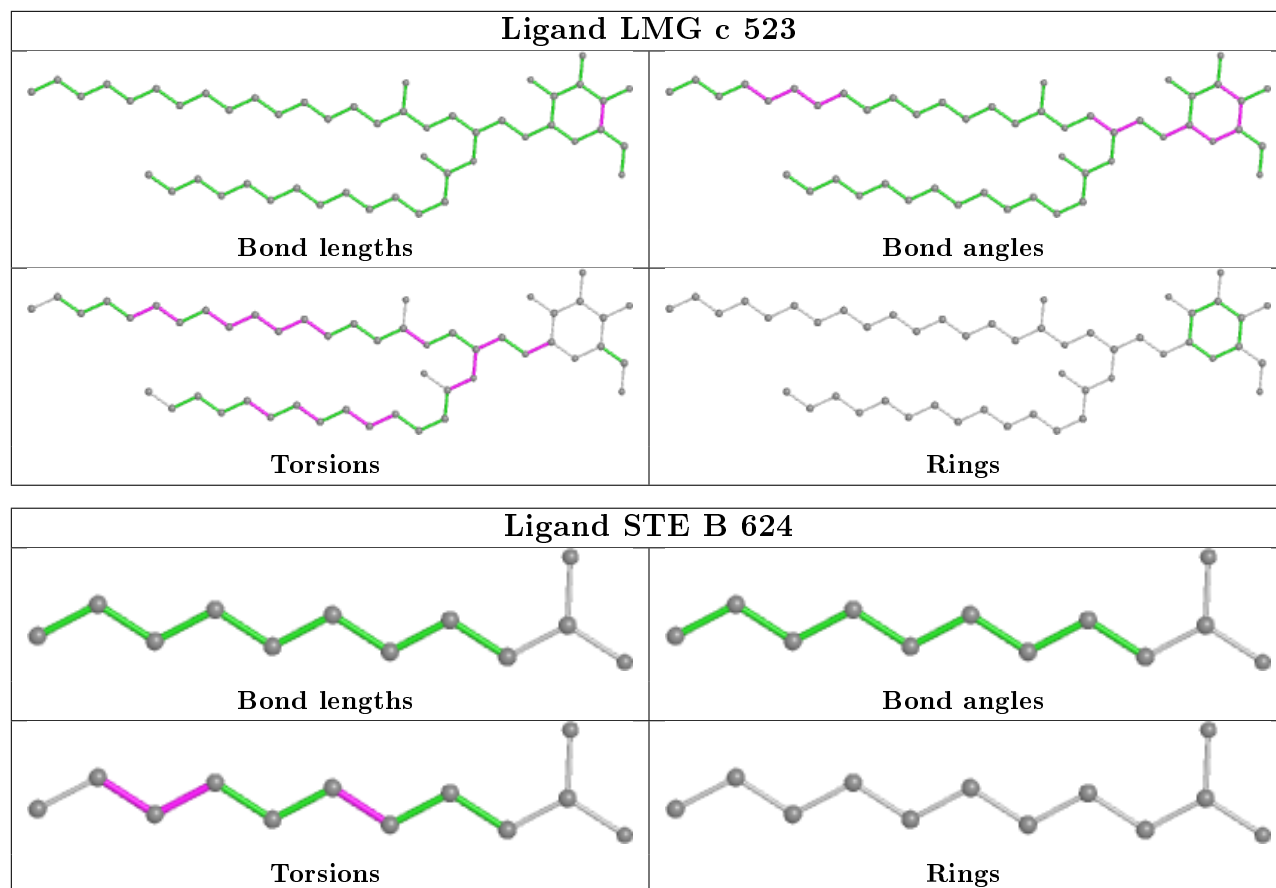


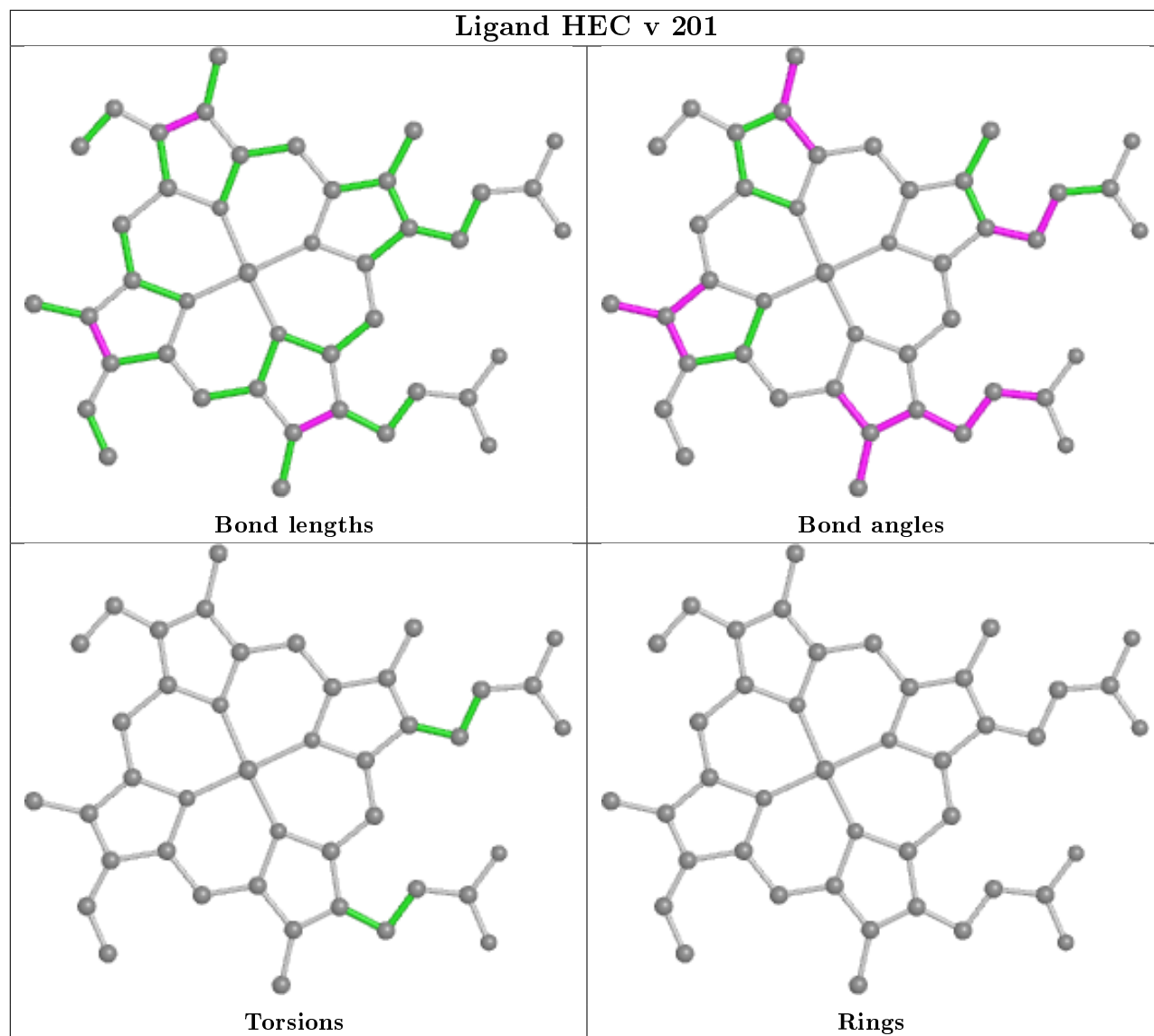
Ligand BCR b 617

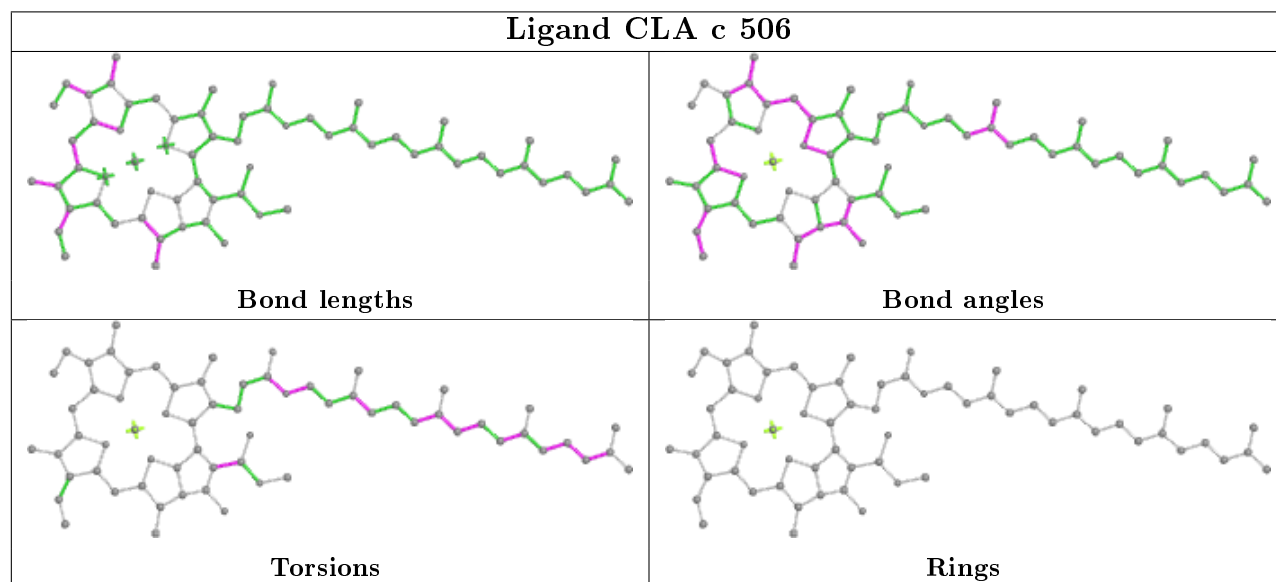
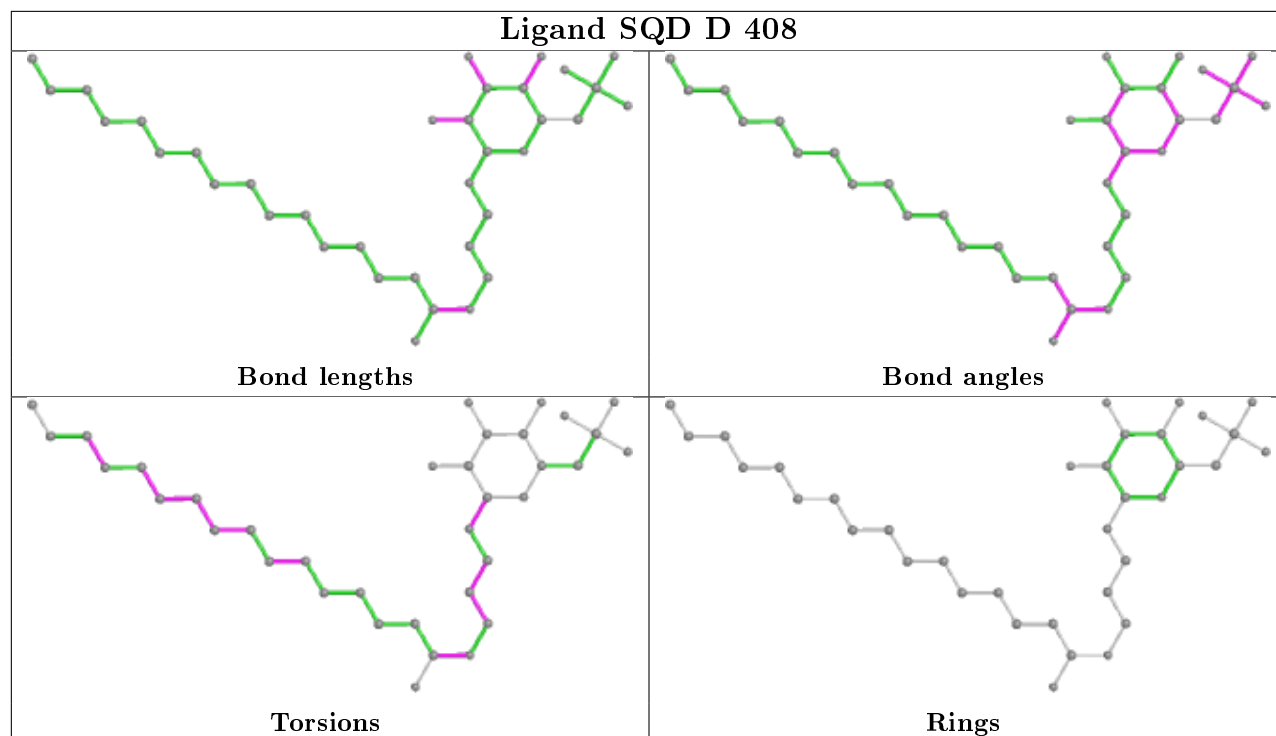


Ligand LMG A 411

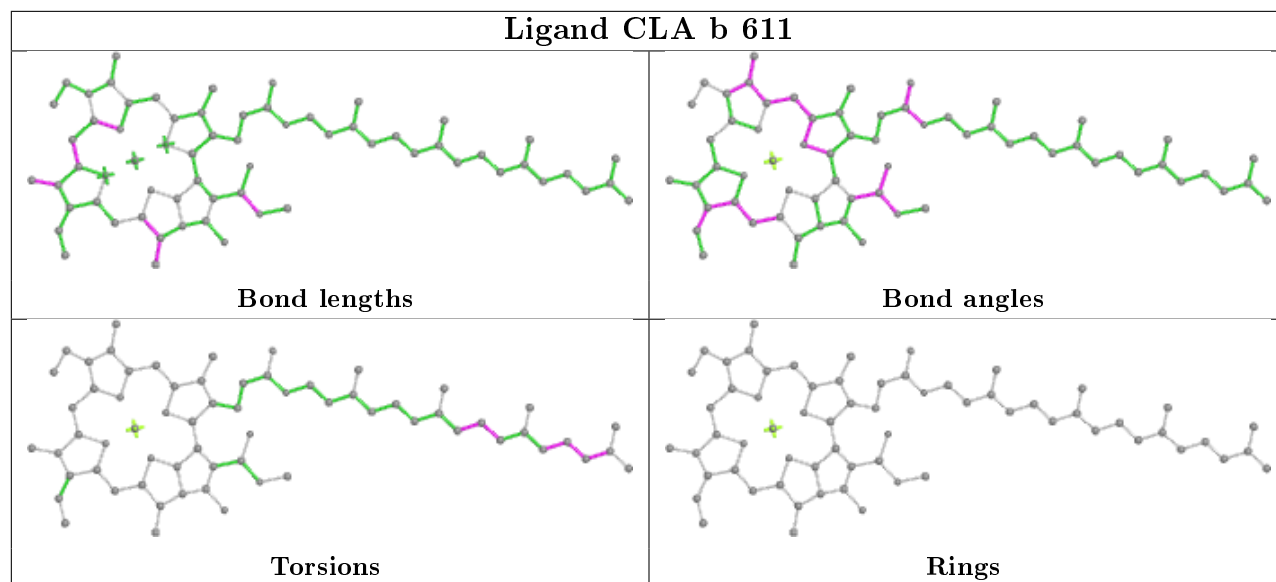




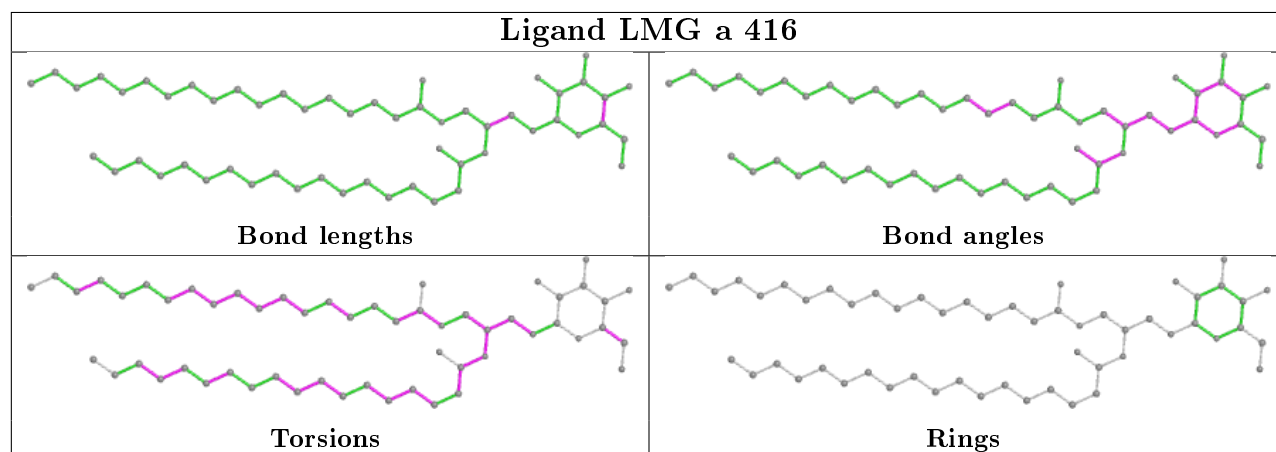




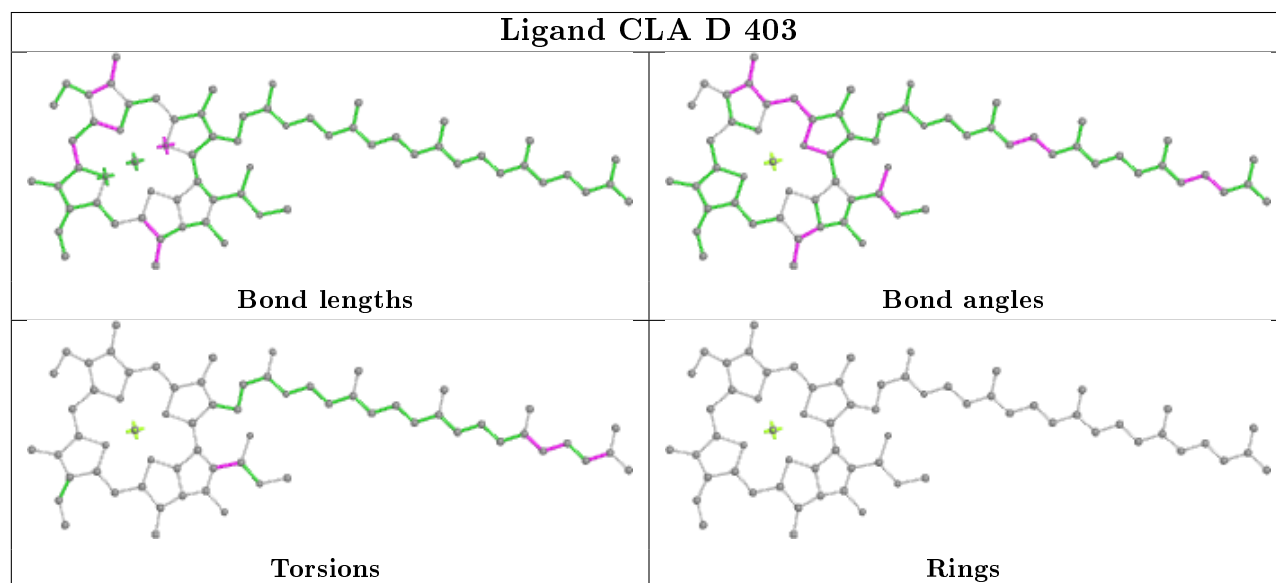
Ligand CLA b 611



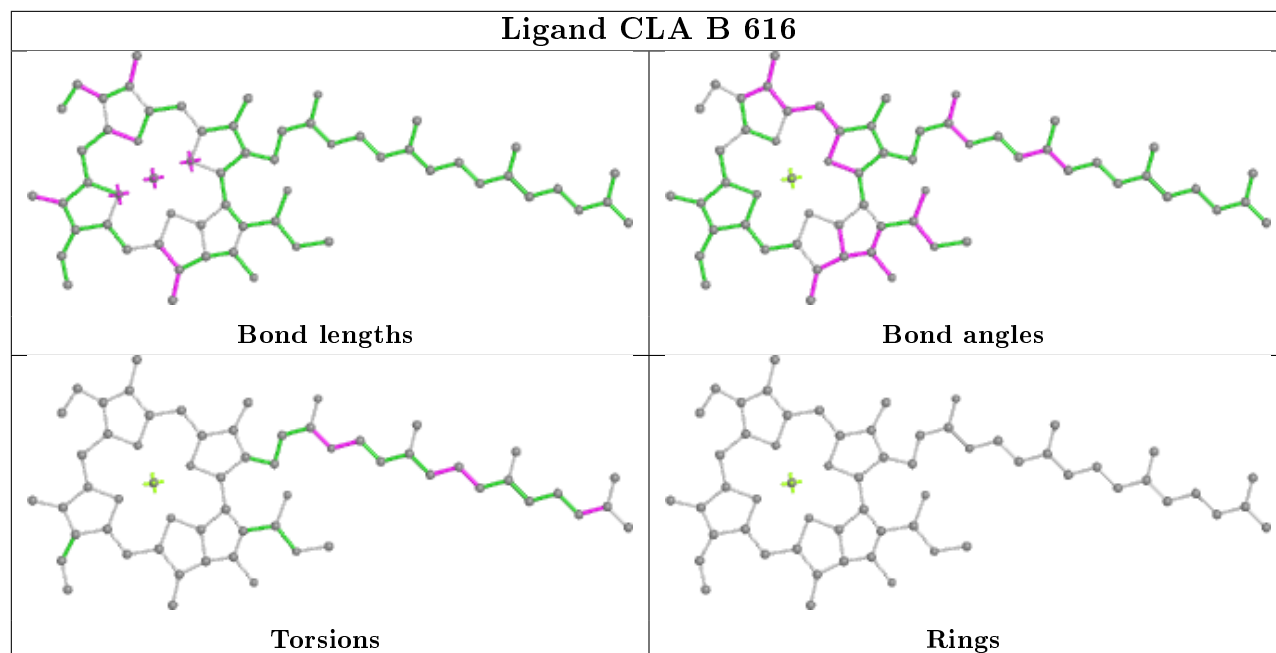
Ligand LMG a 416



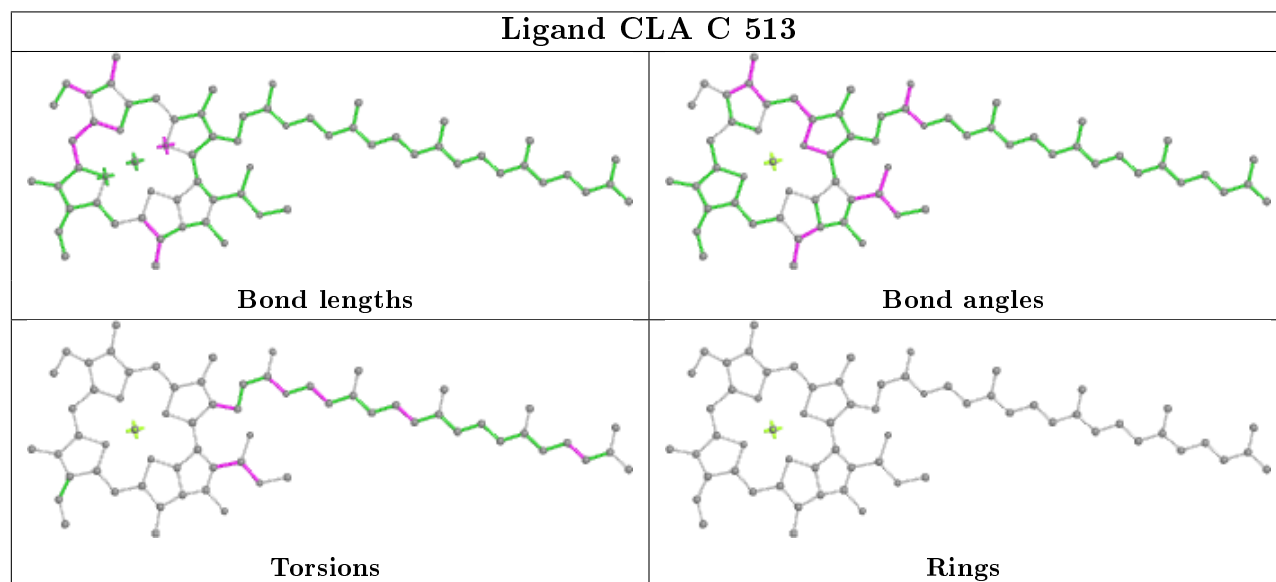
Ligand CLA D 403



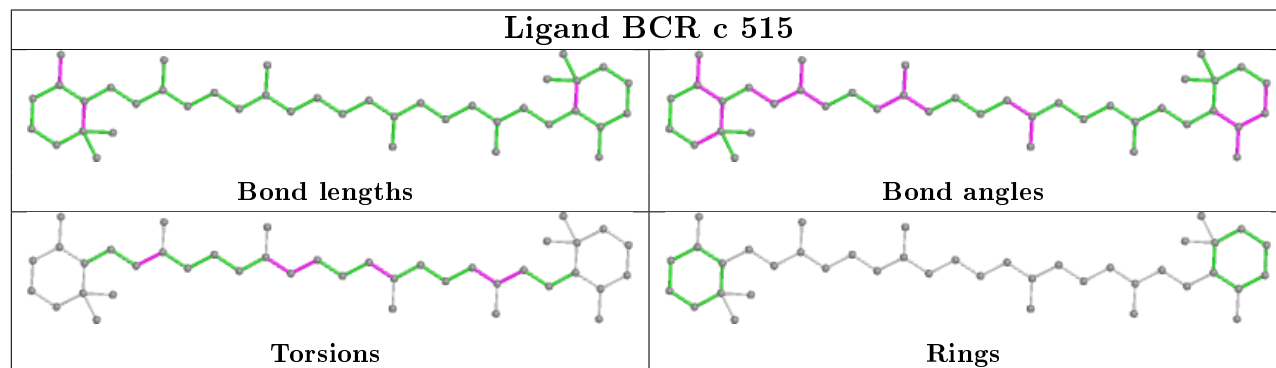
Ligand CLA B 616

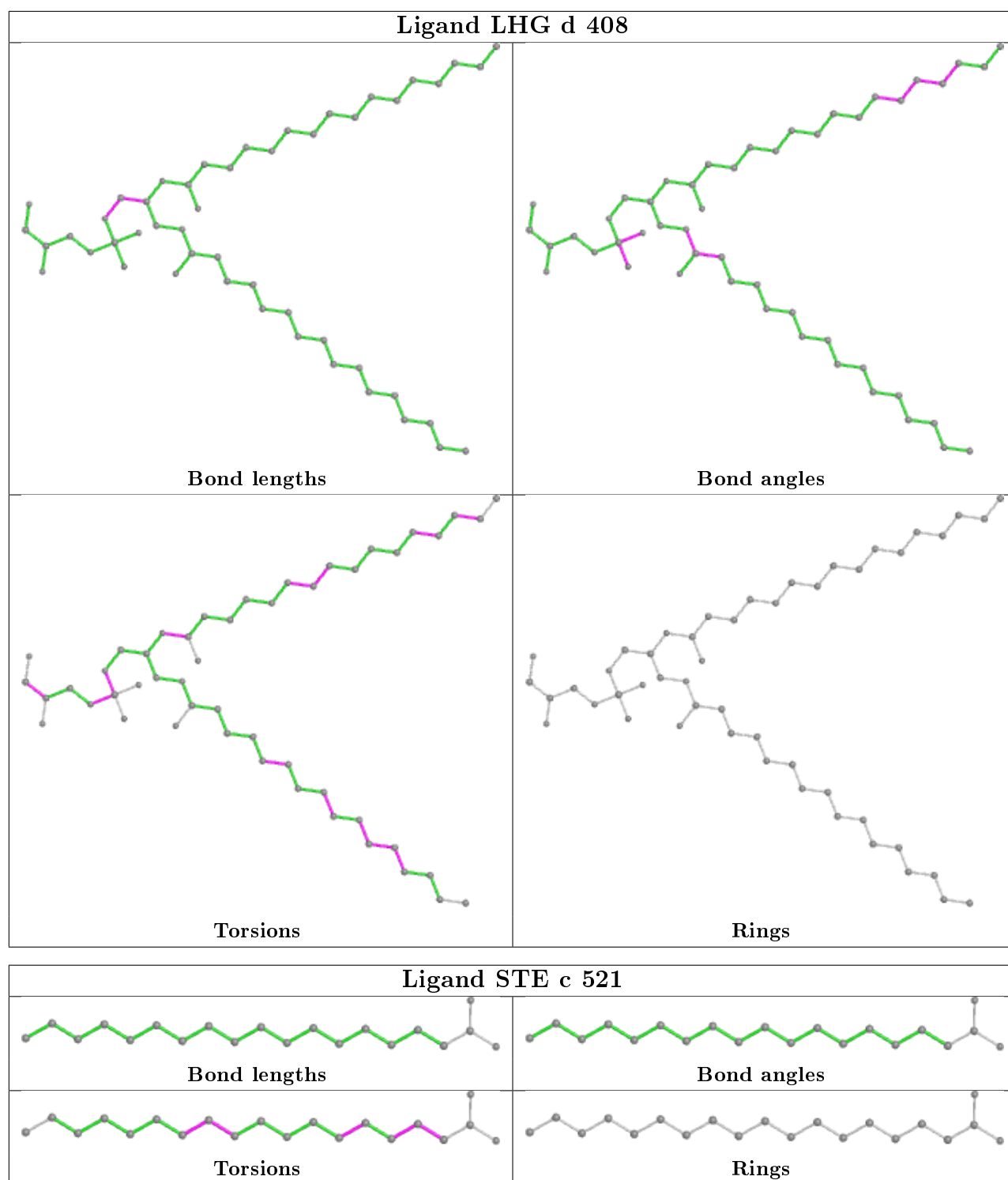


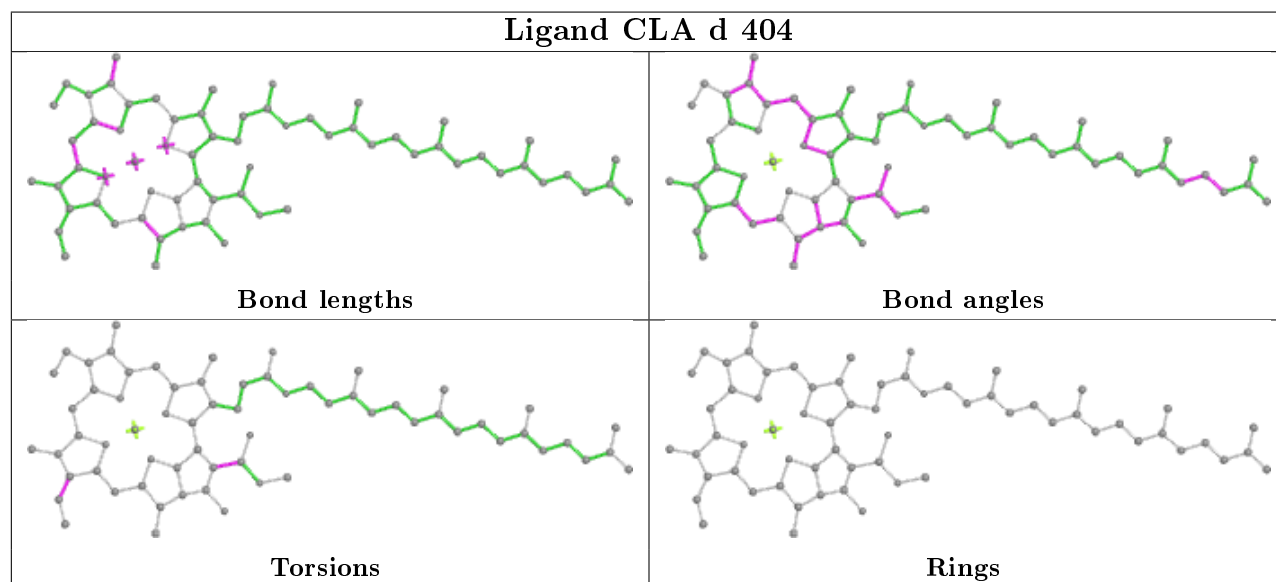
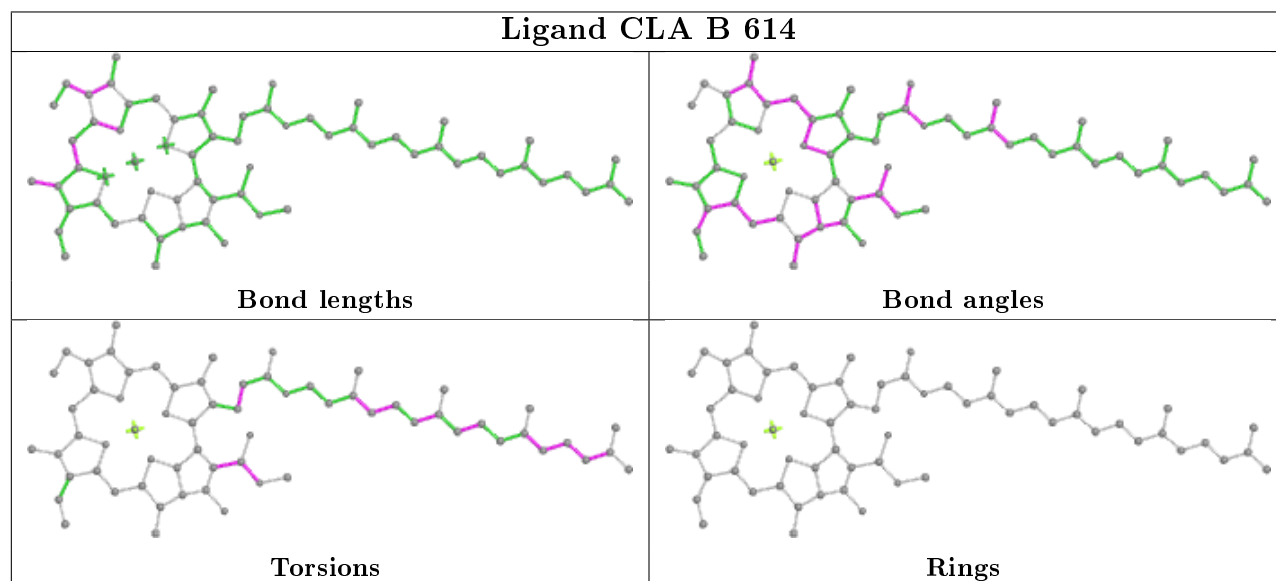
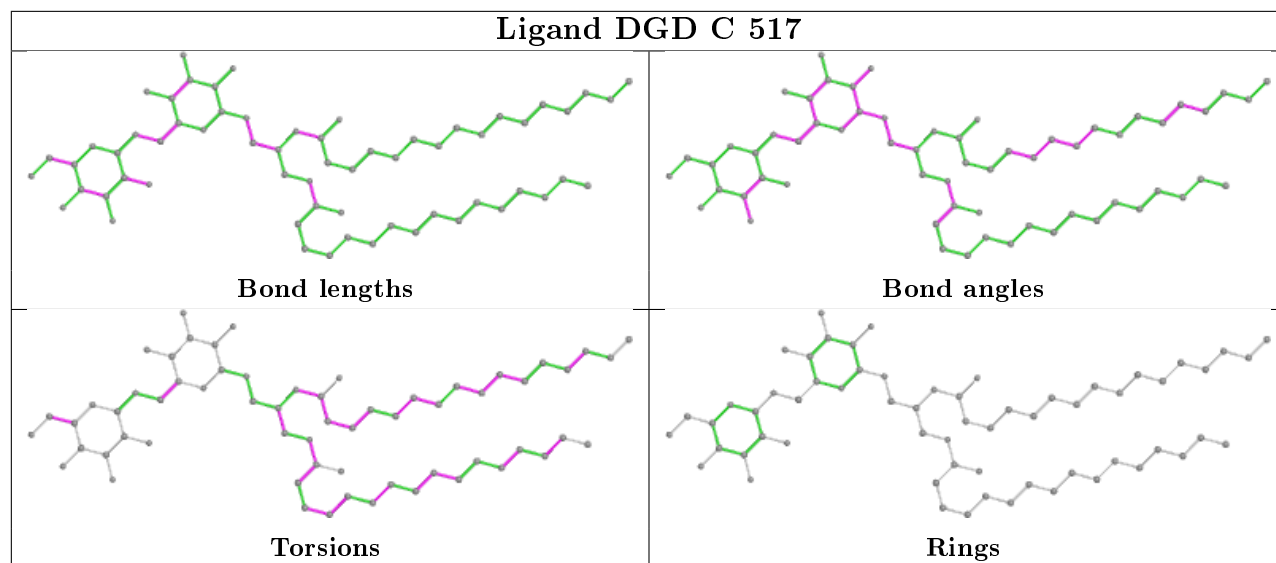
Ligand CLA C 513

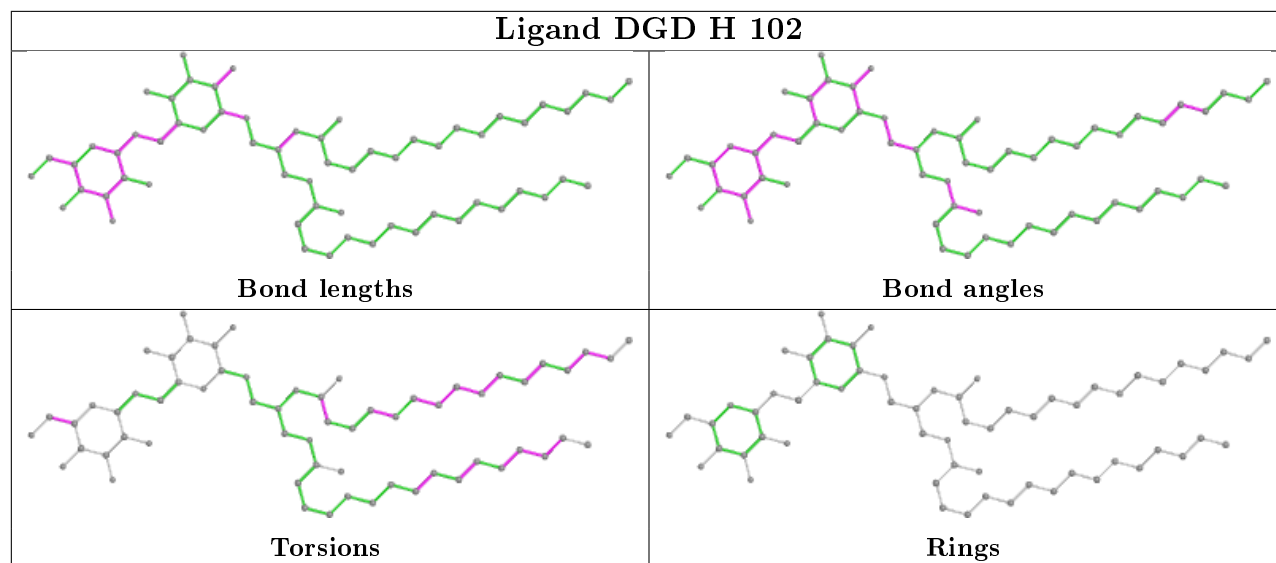
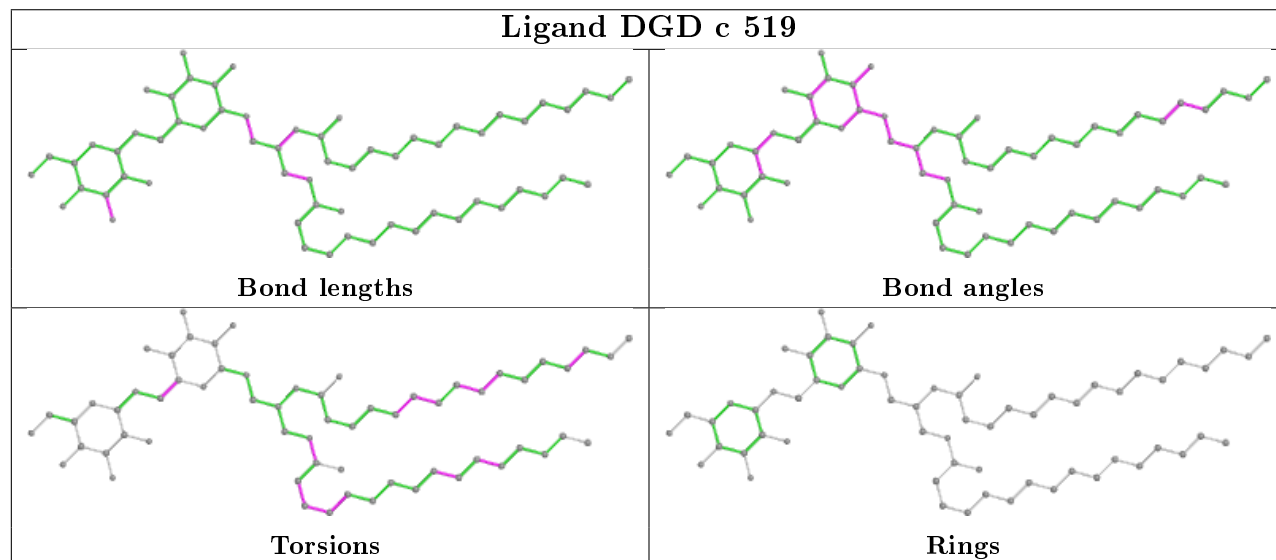
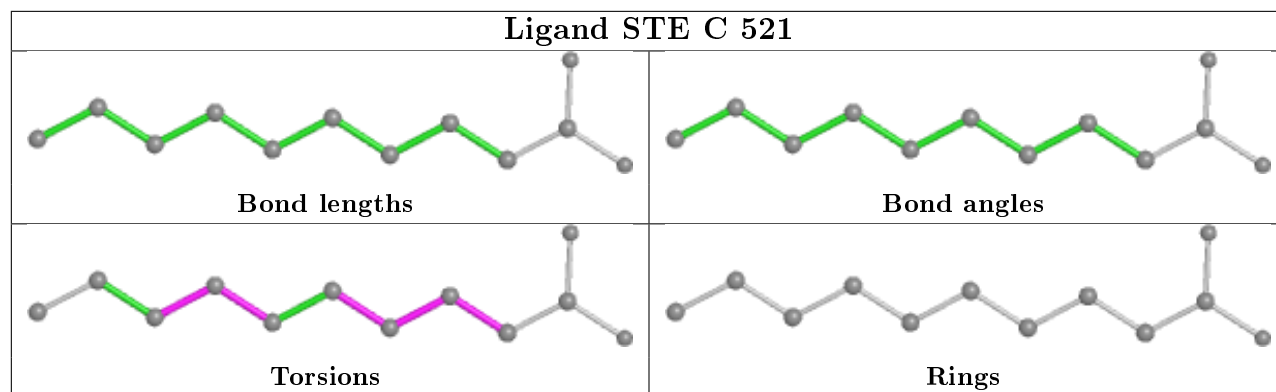


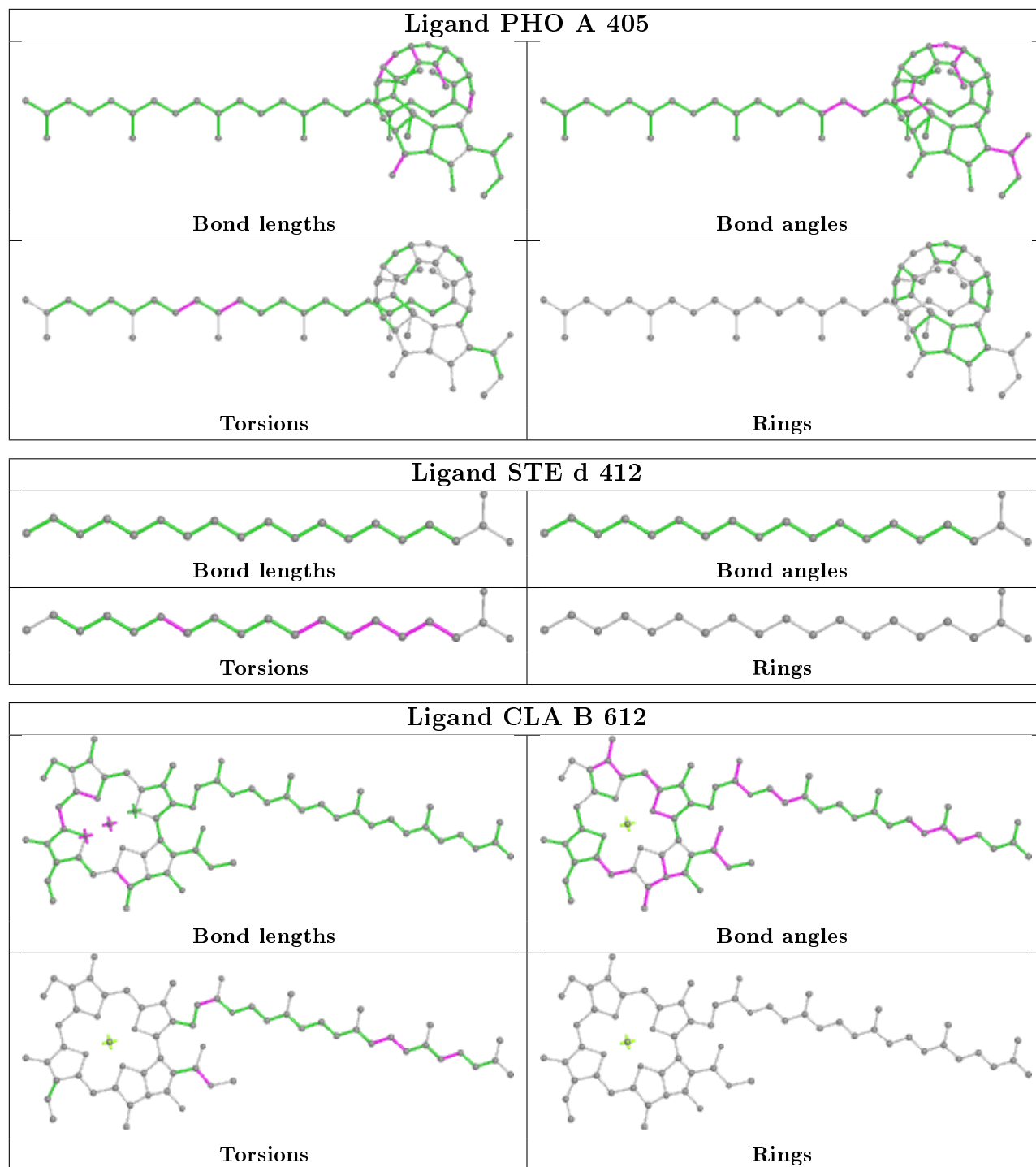
Ligand BCR c 515

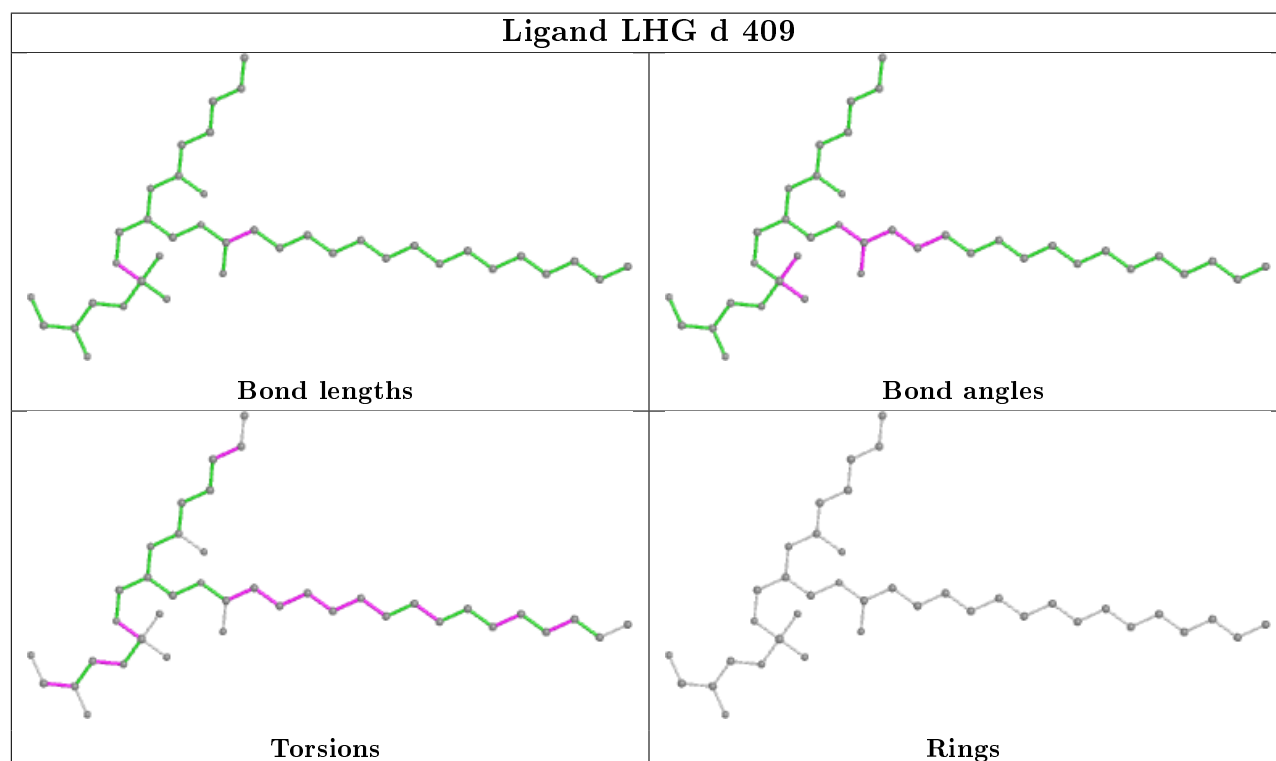
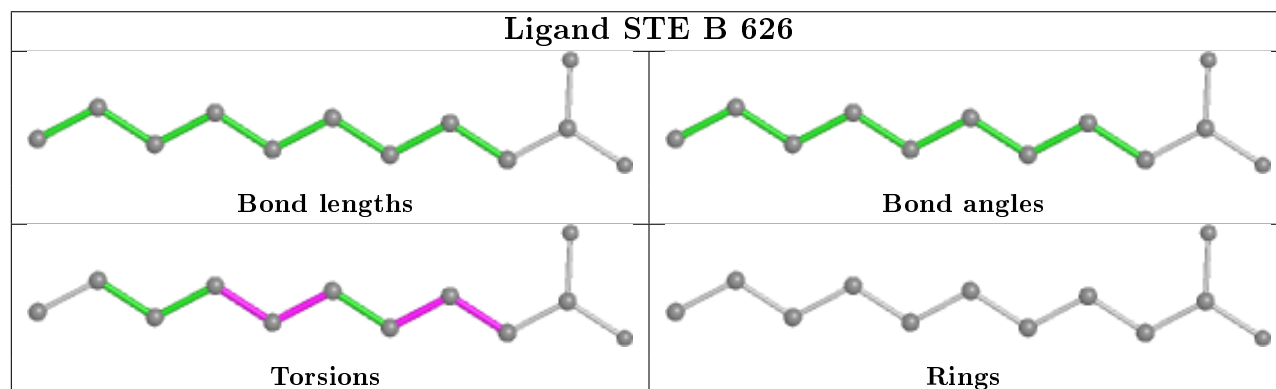
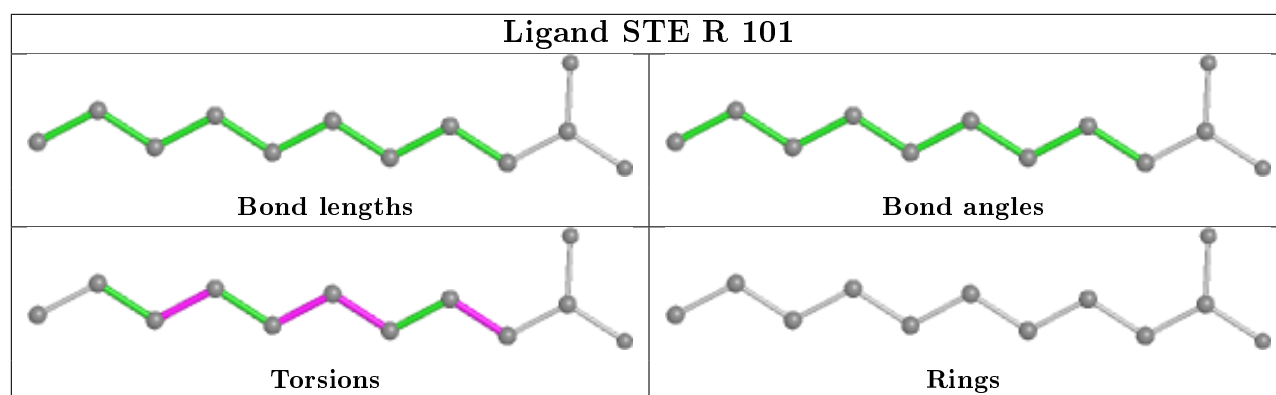


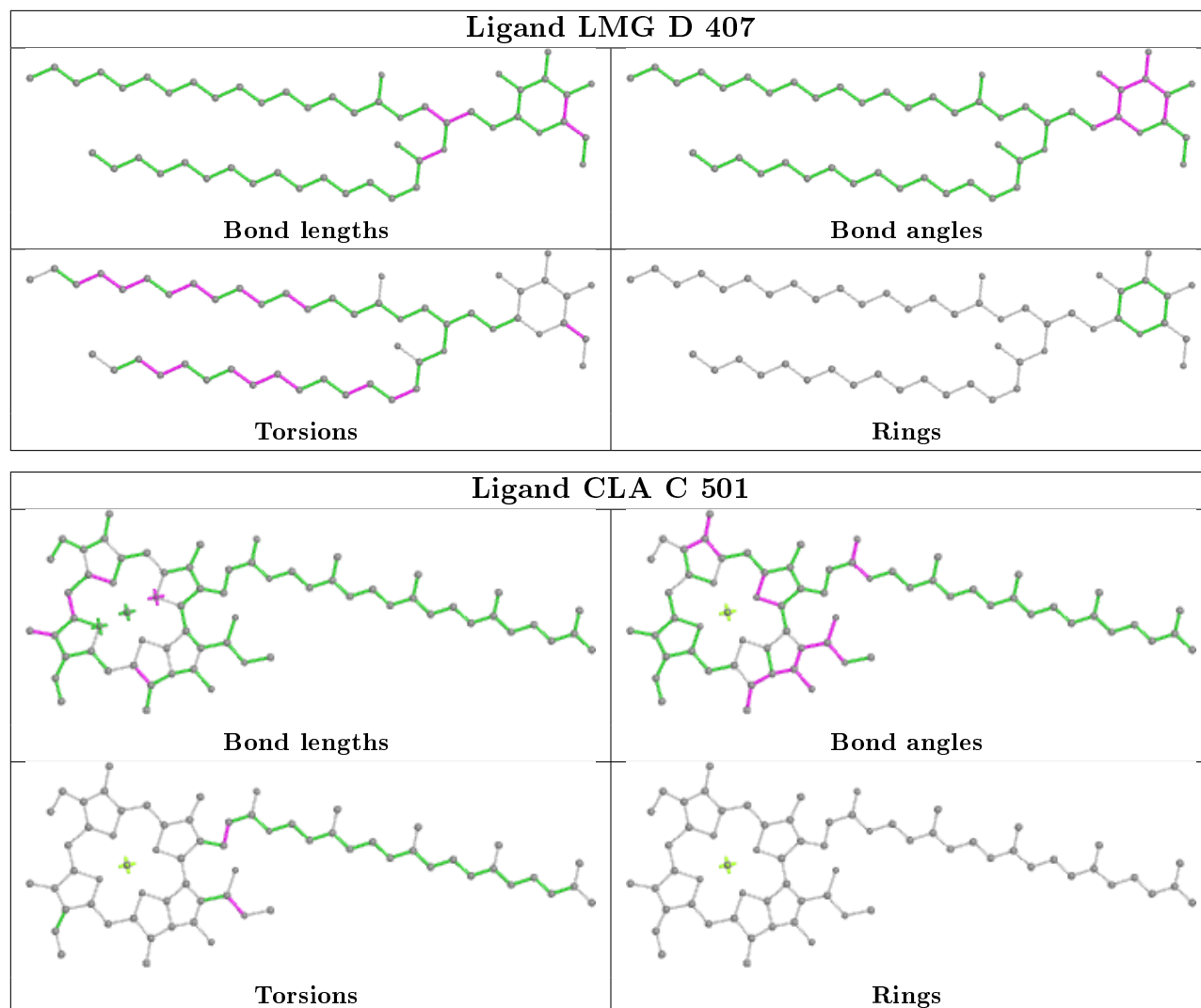


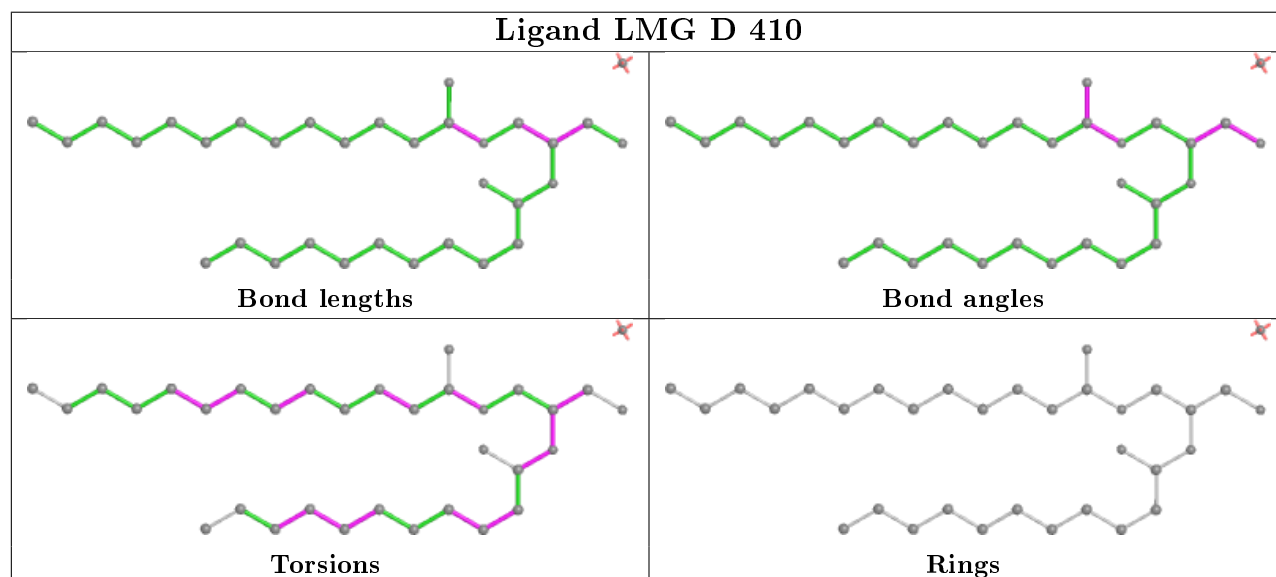
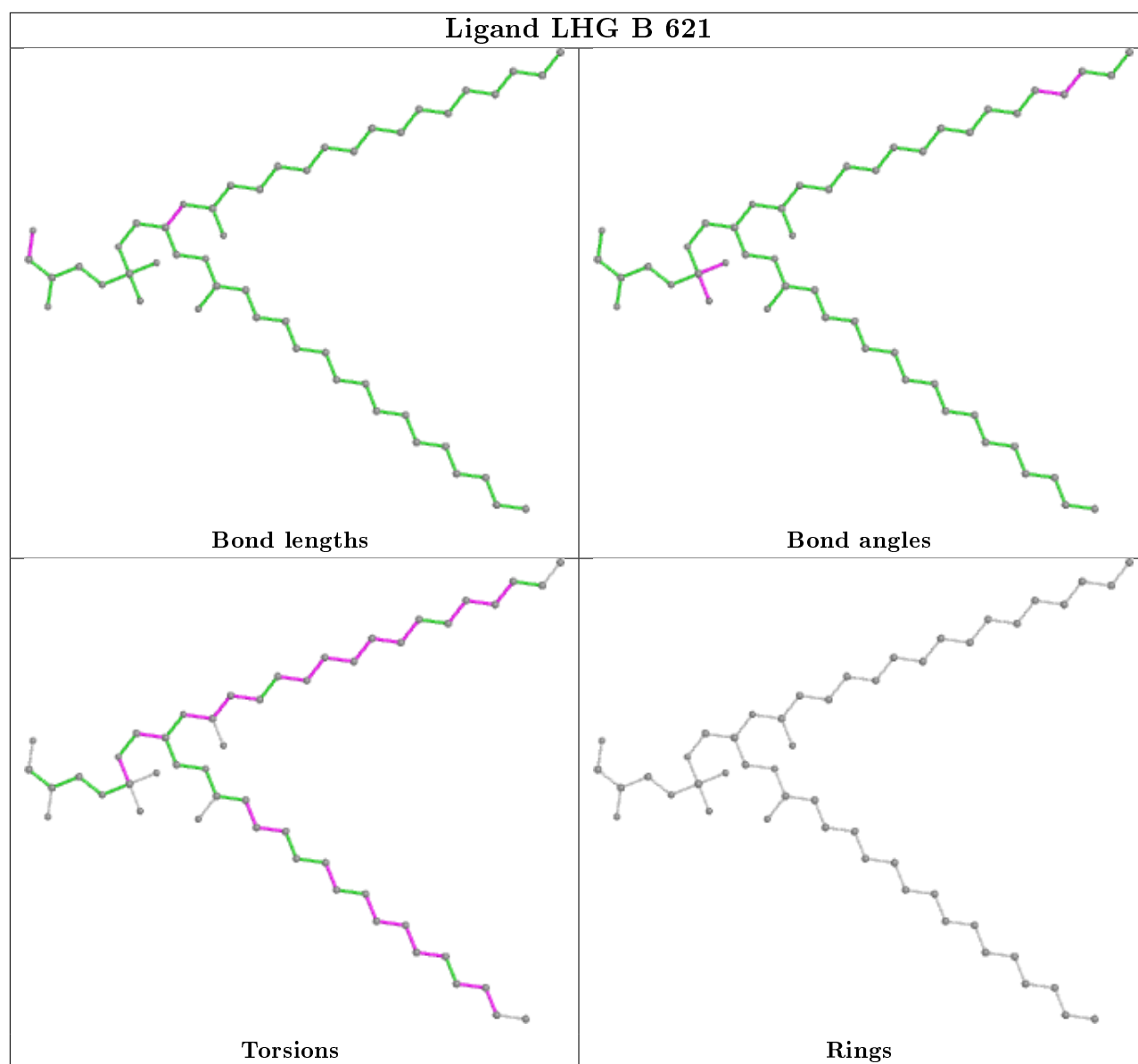


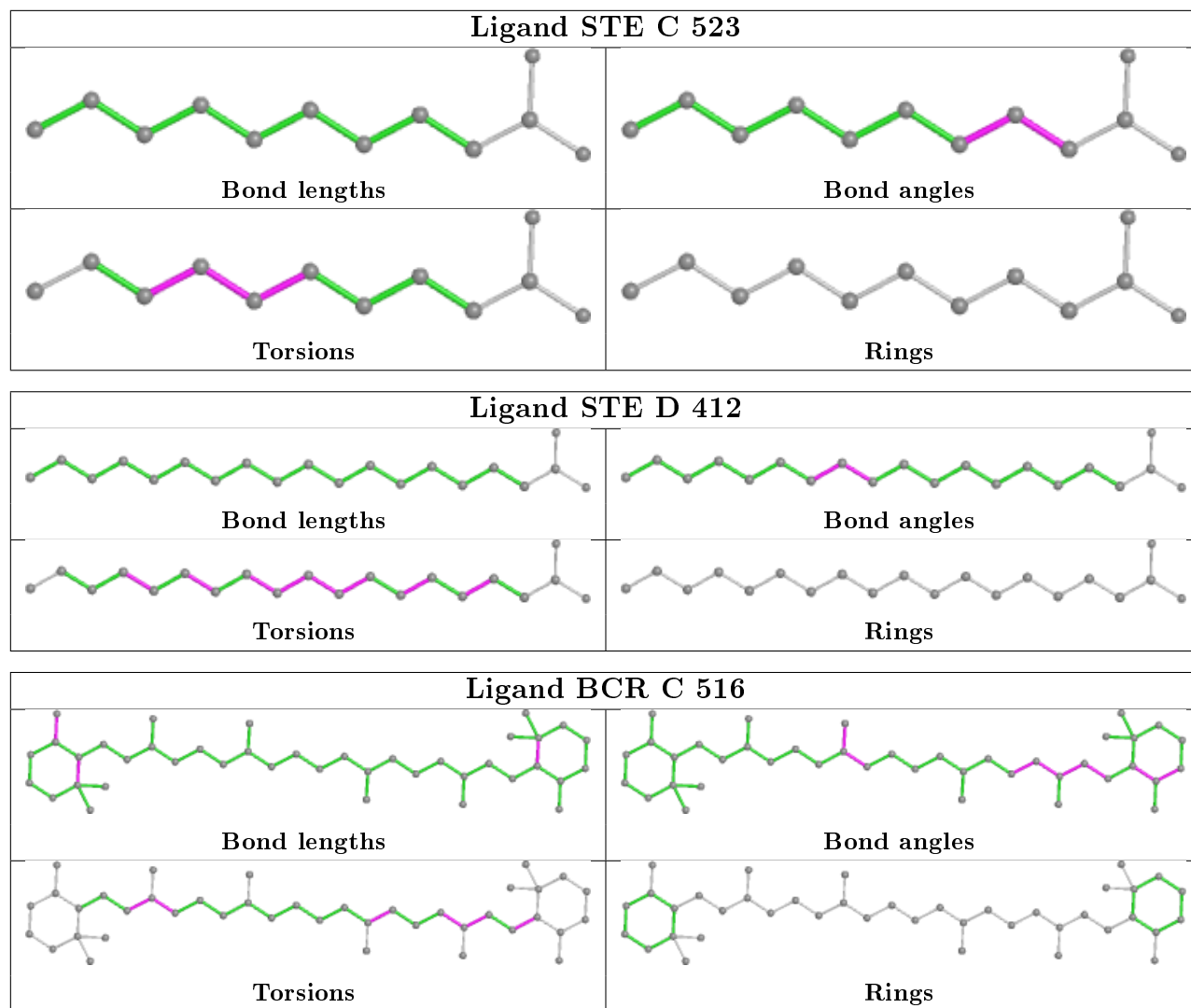


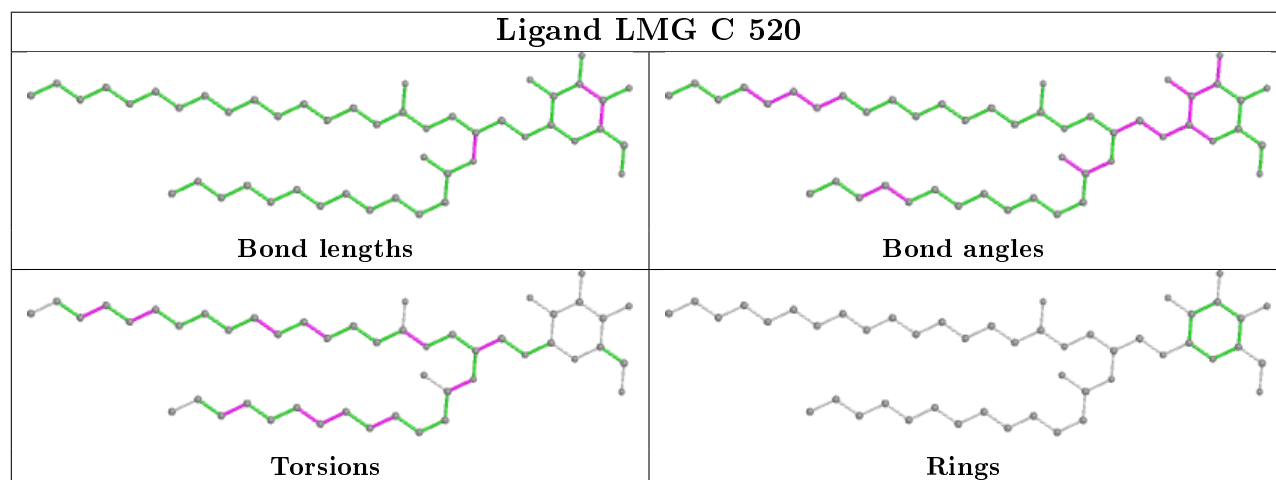
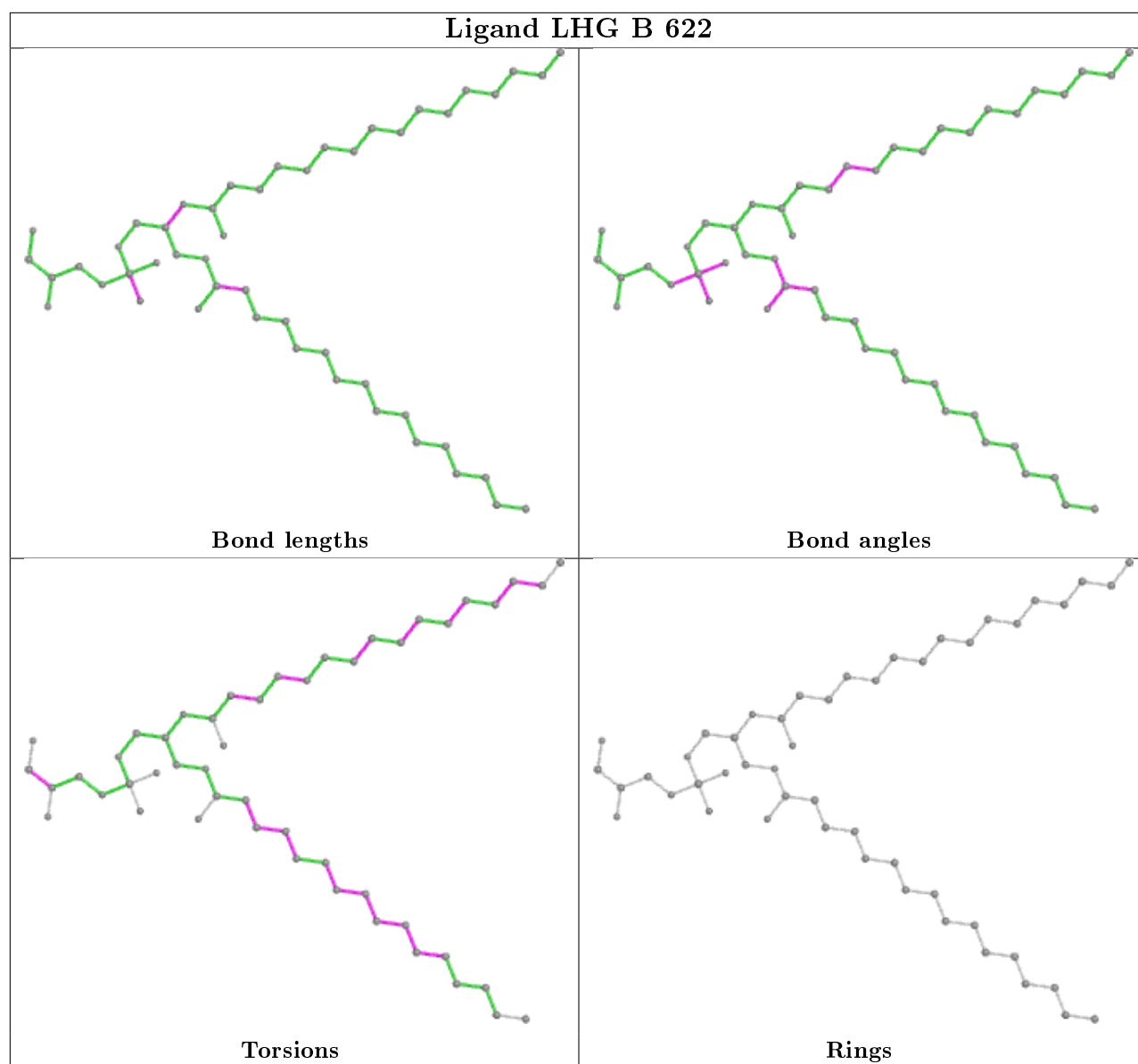


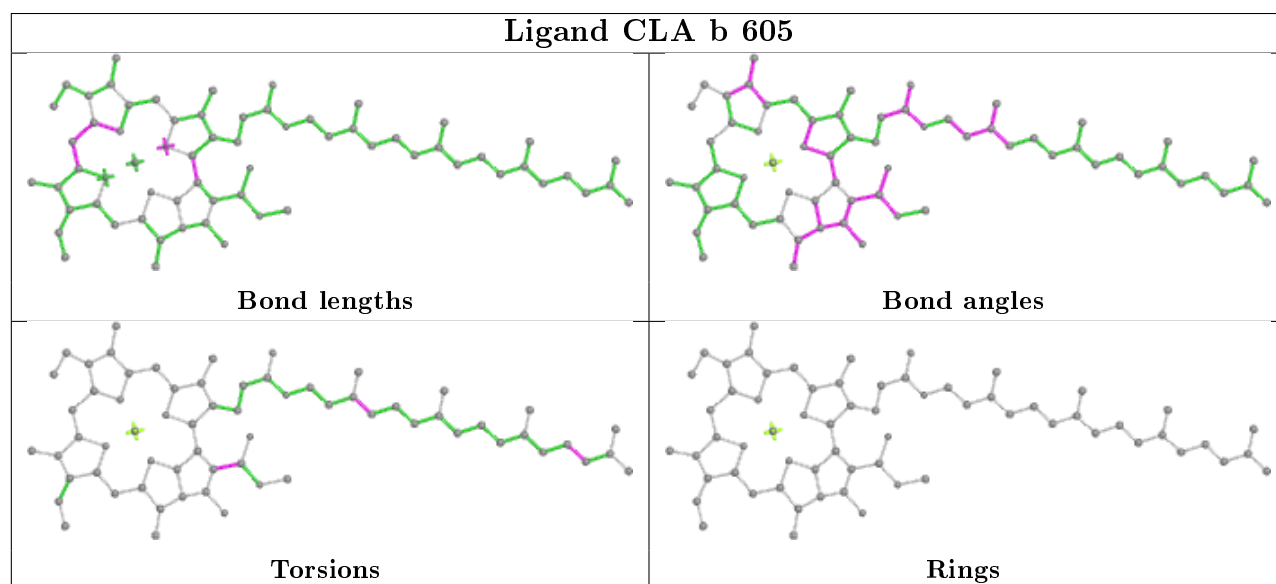
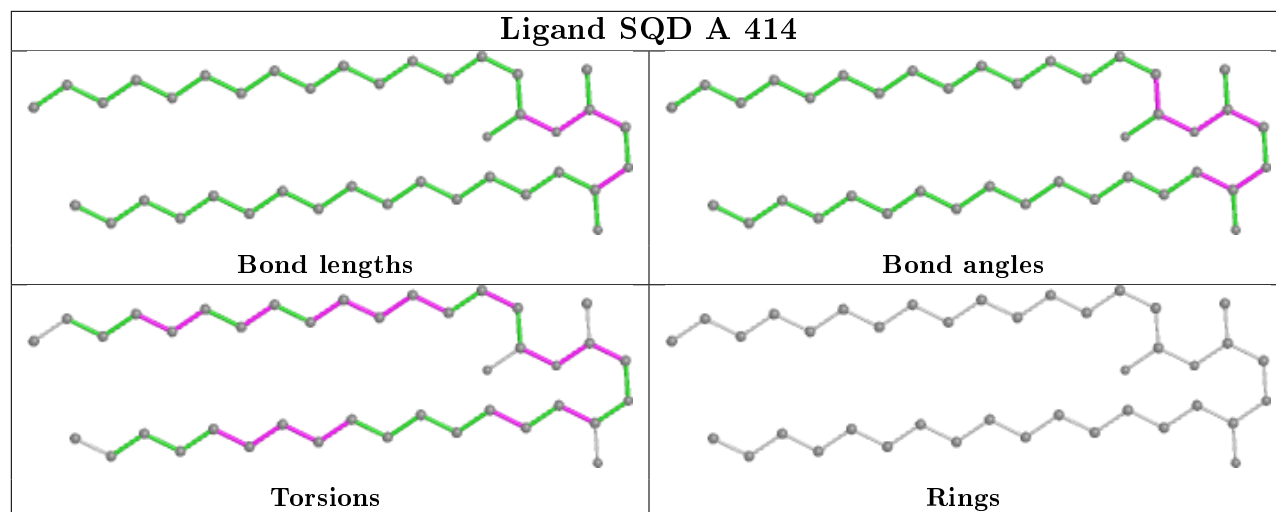


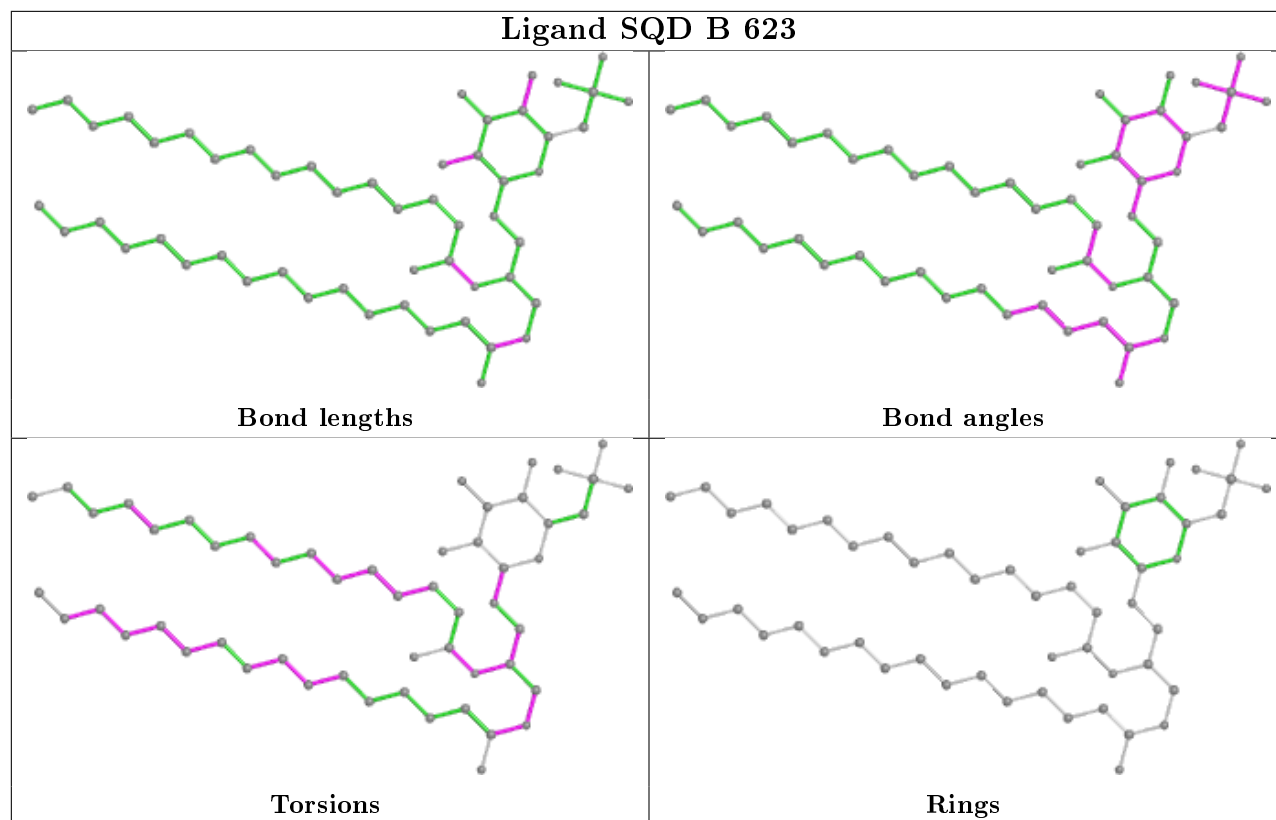




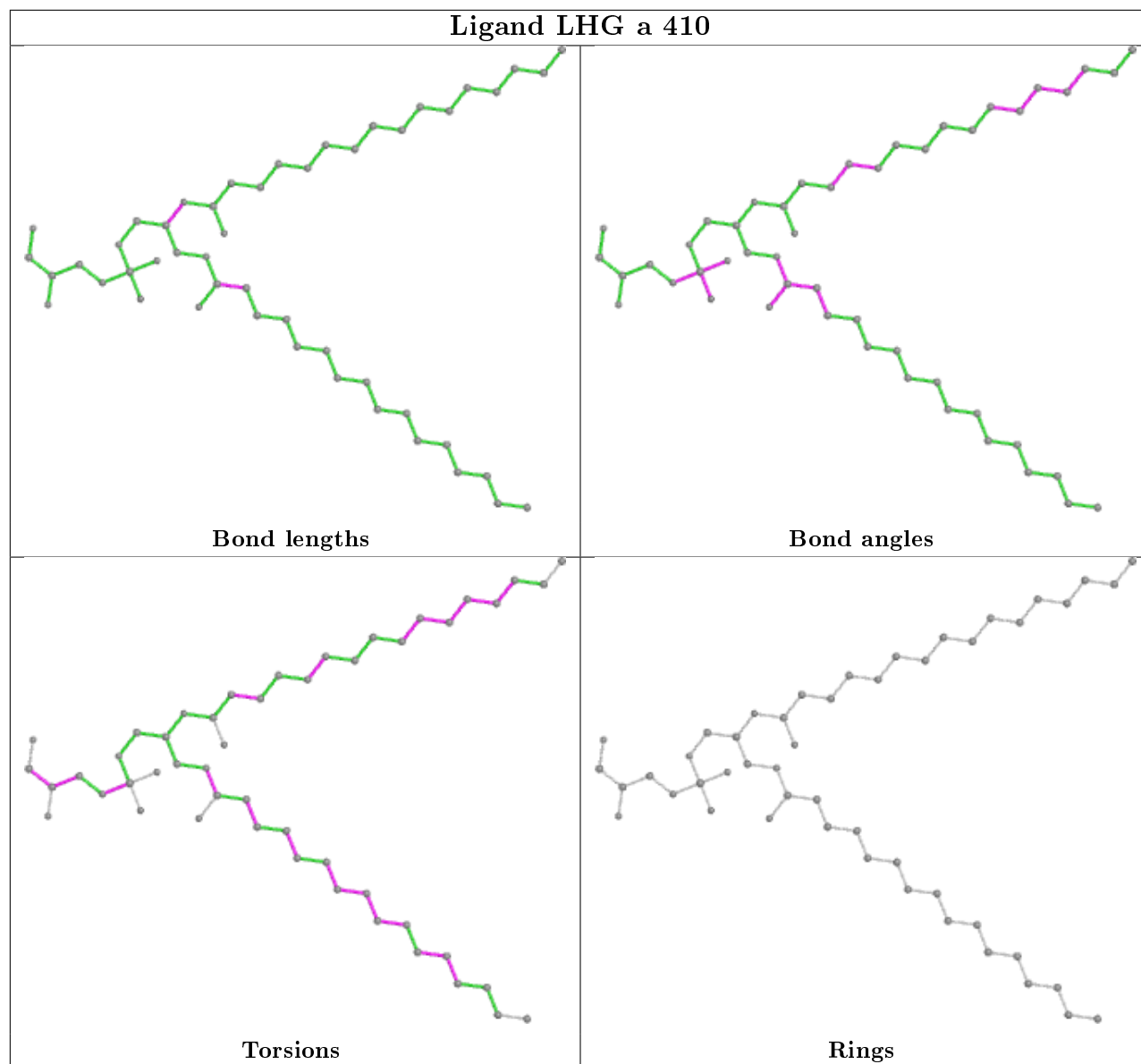




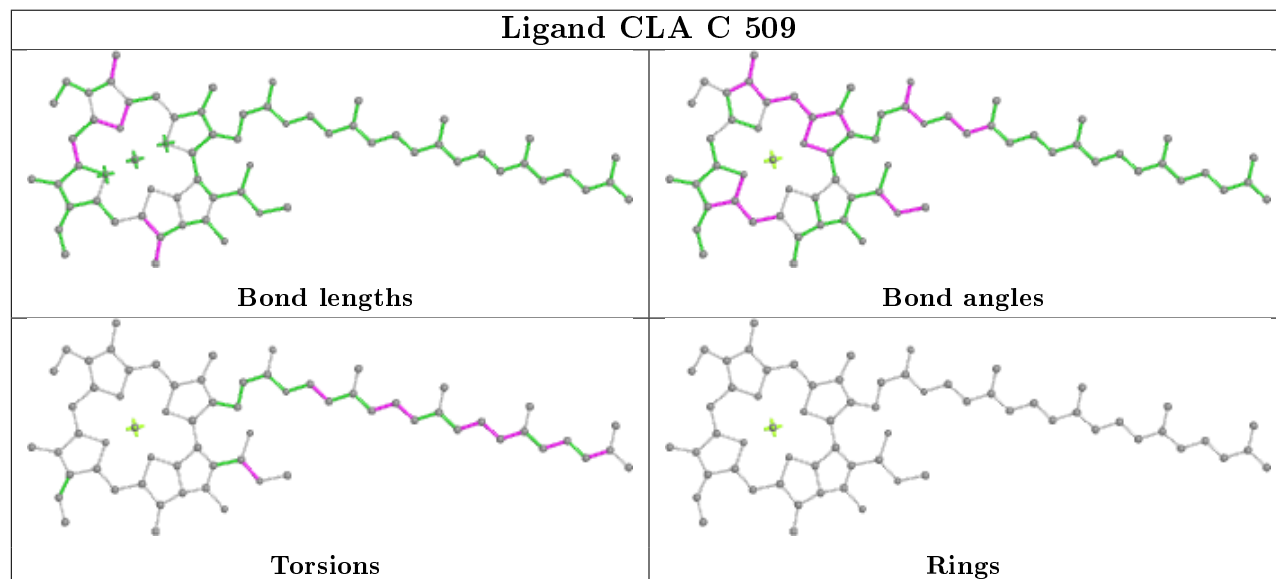


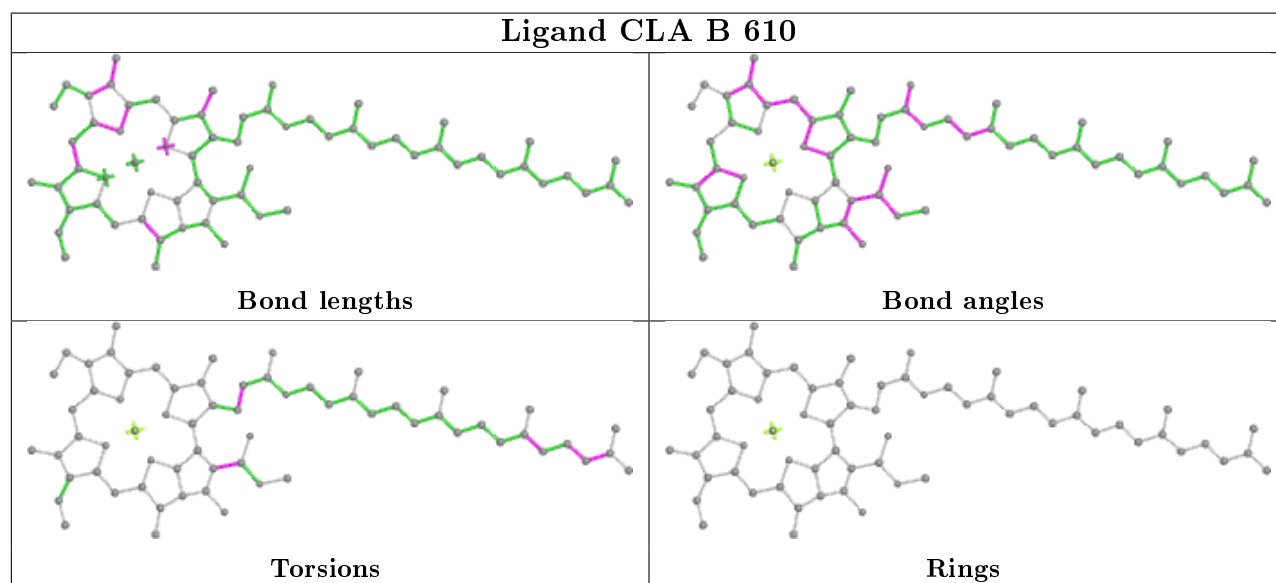
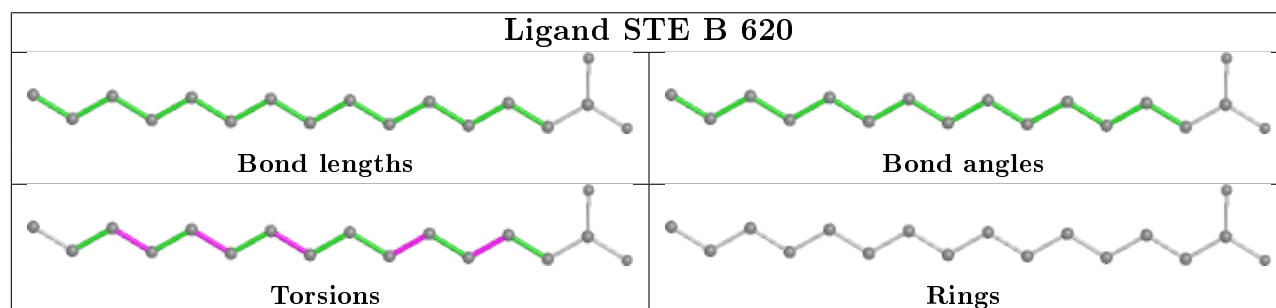
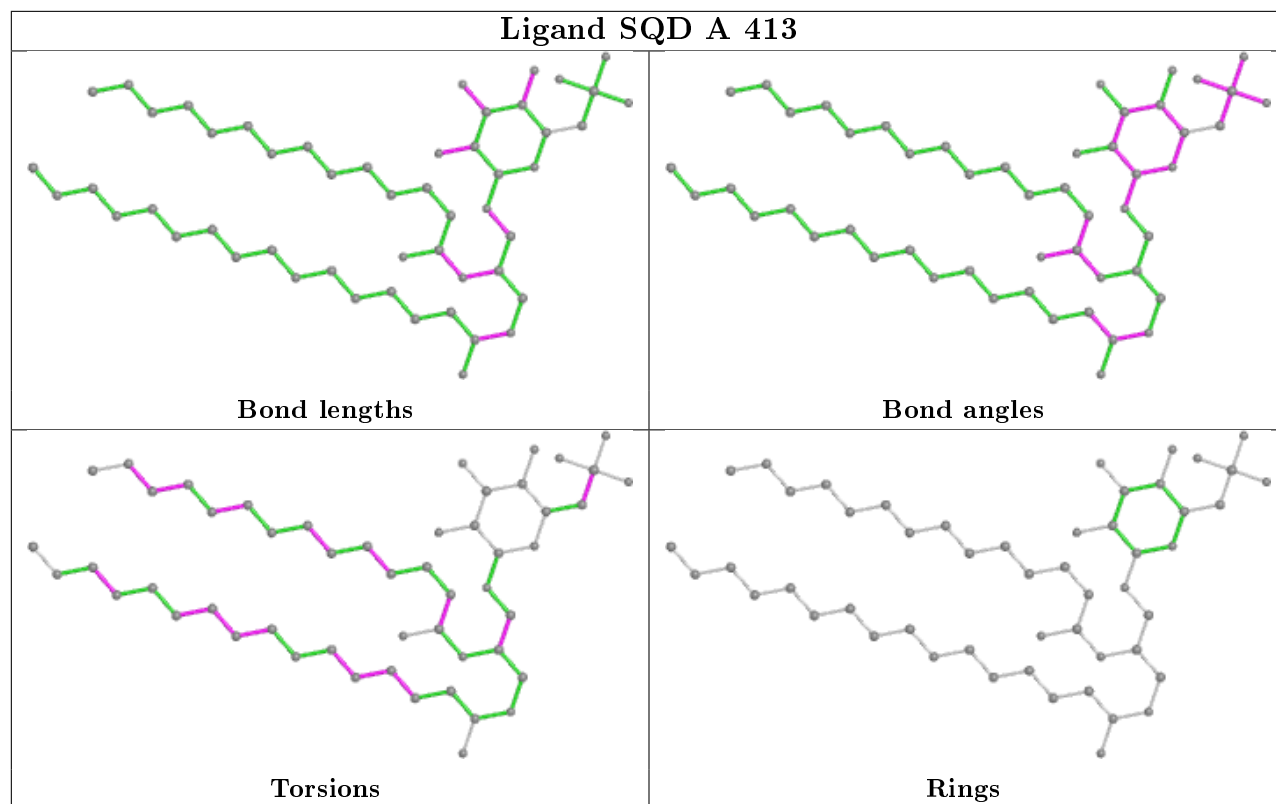


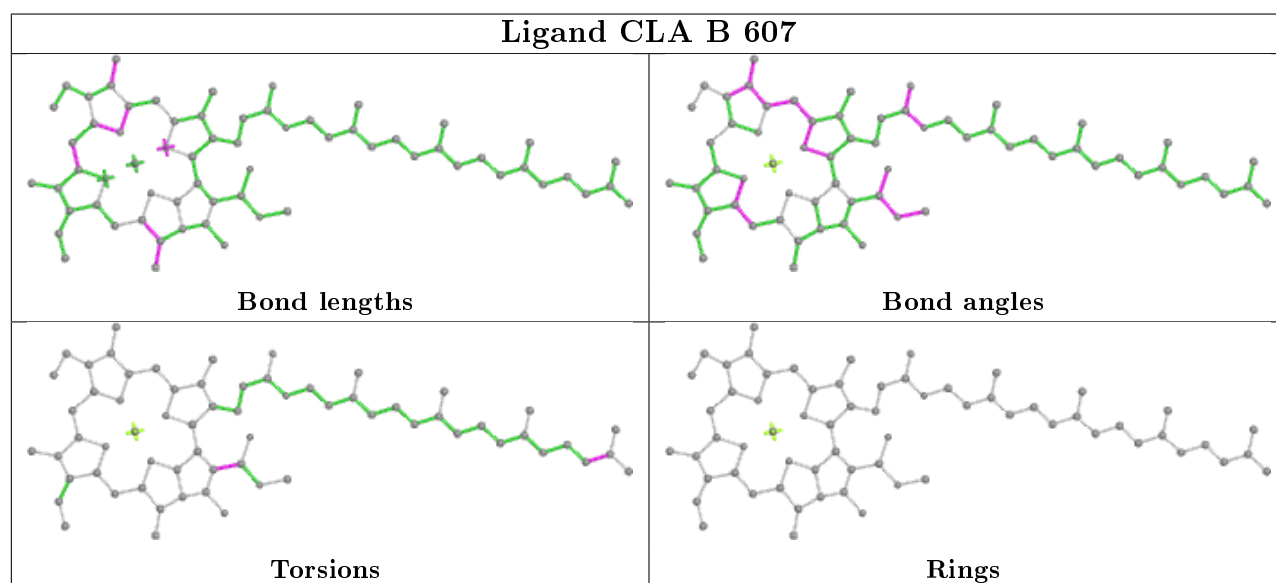
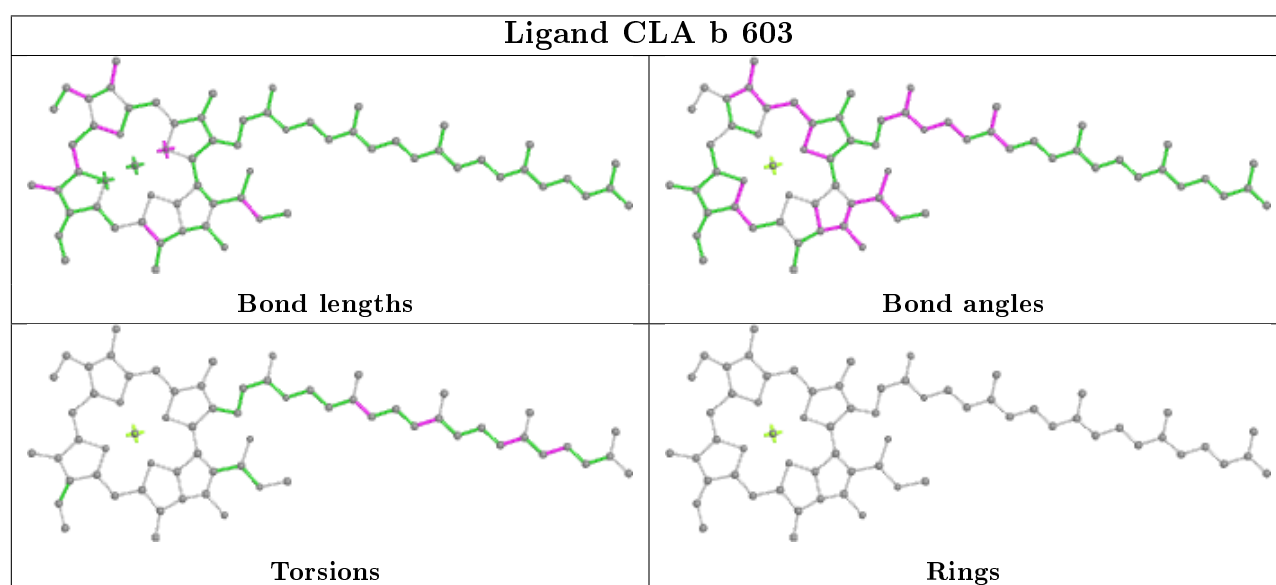
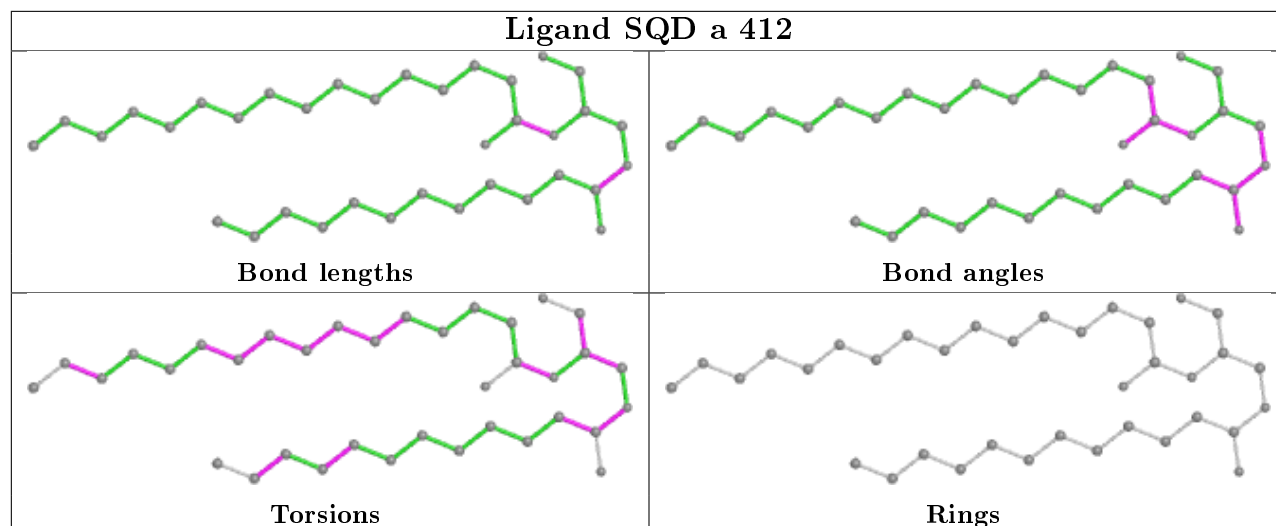
Ligand LHG a 410



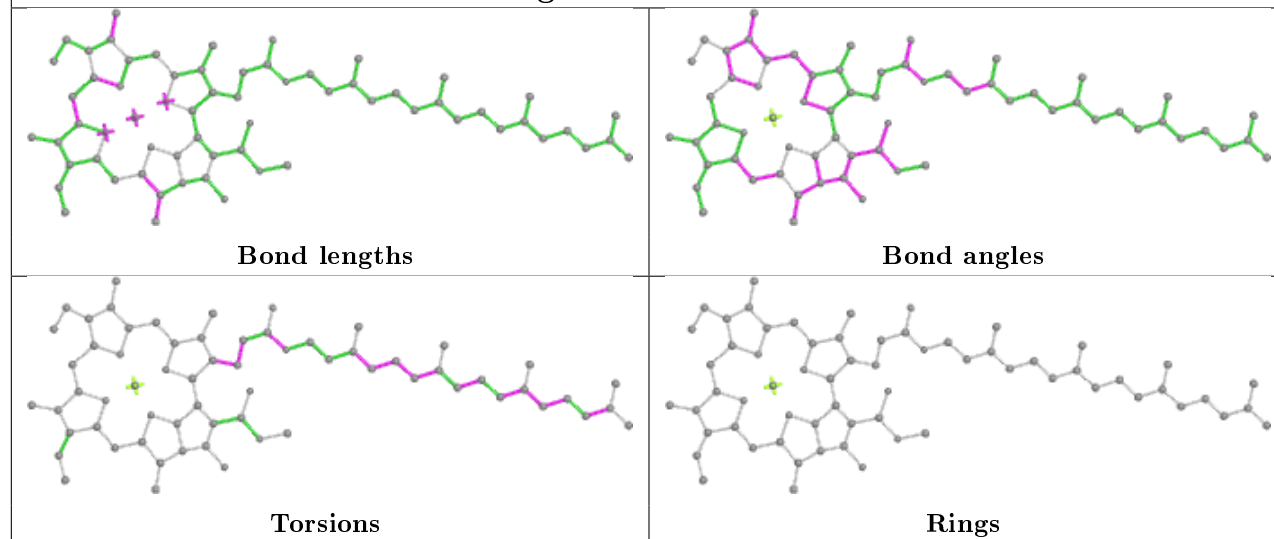
Ligand CLA C 509



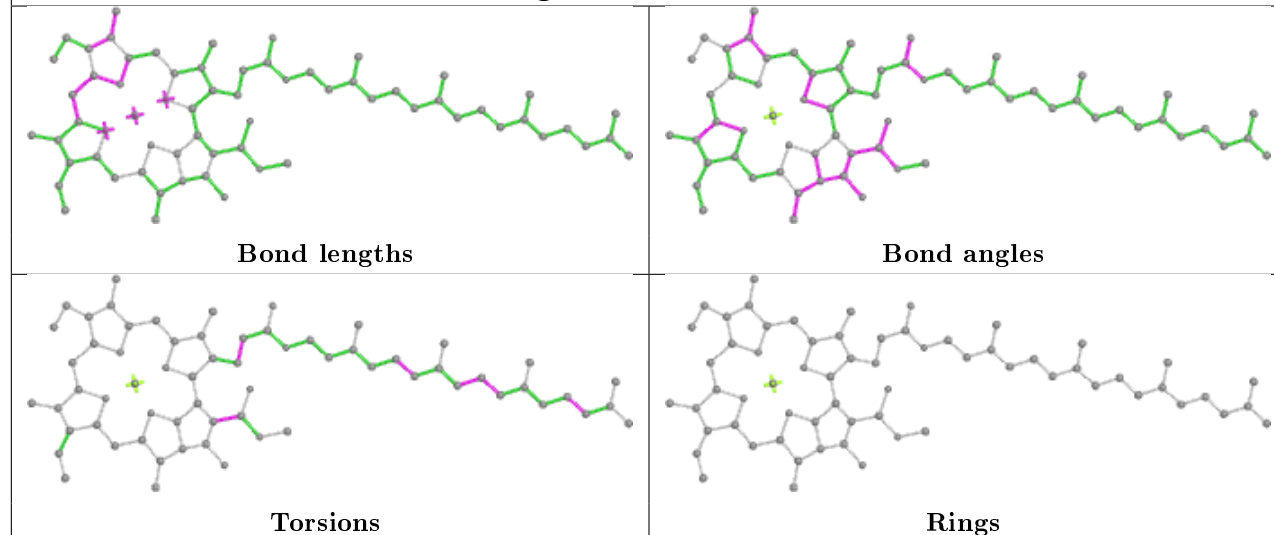




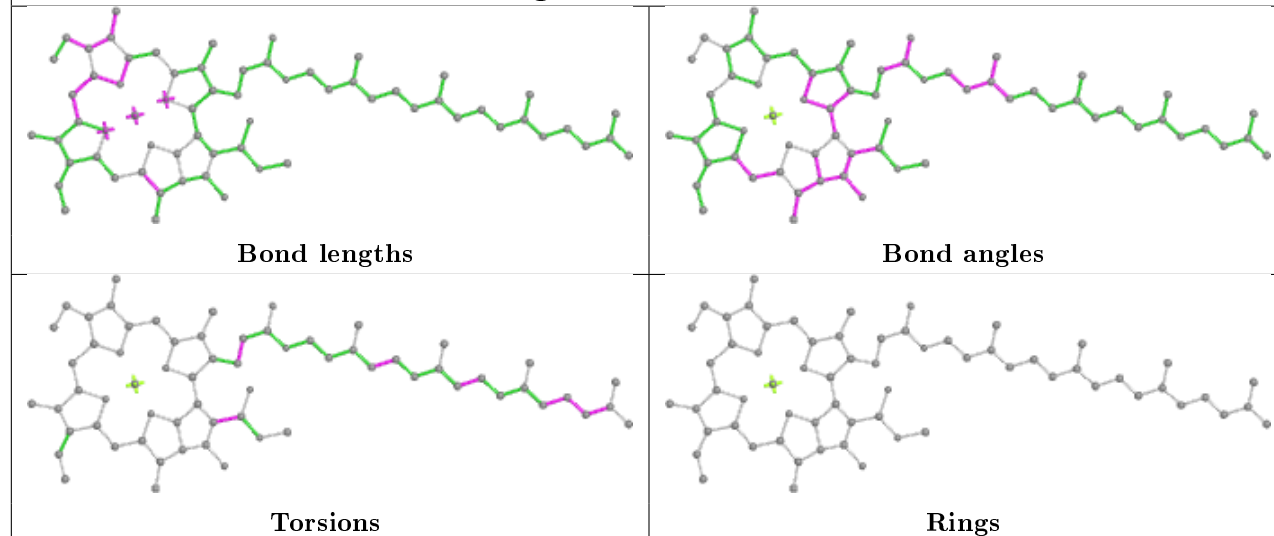
Ligand CLA c 512

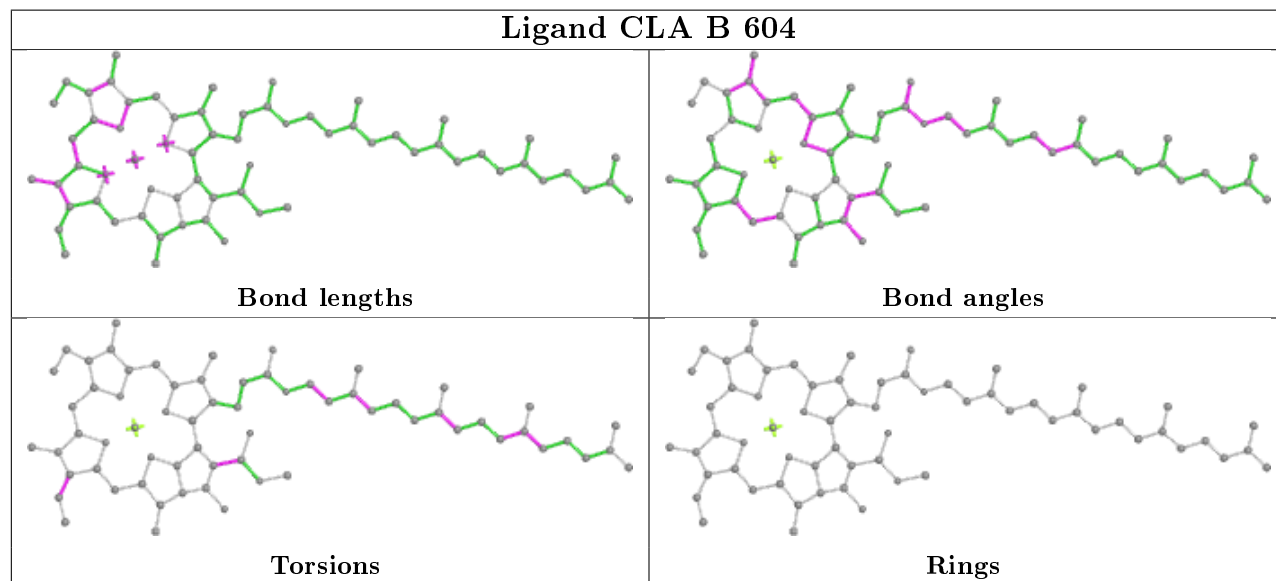
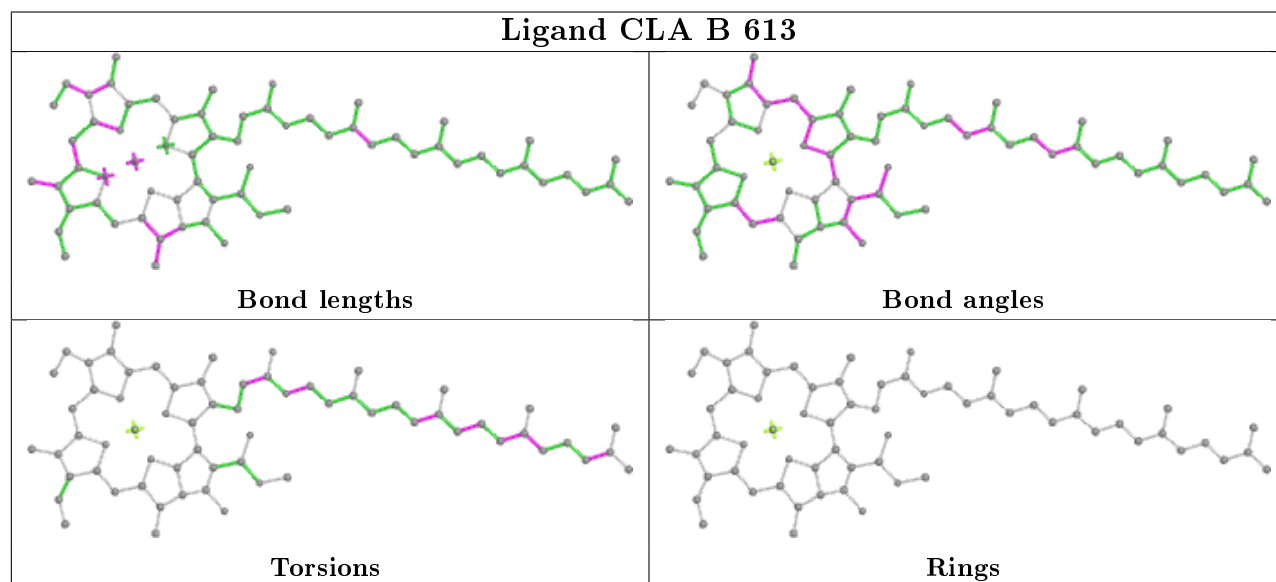
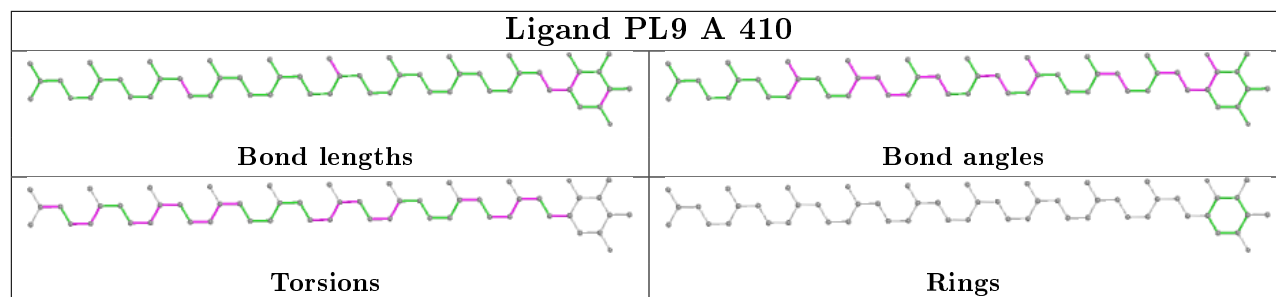


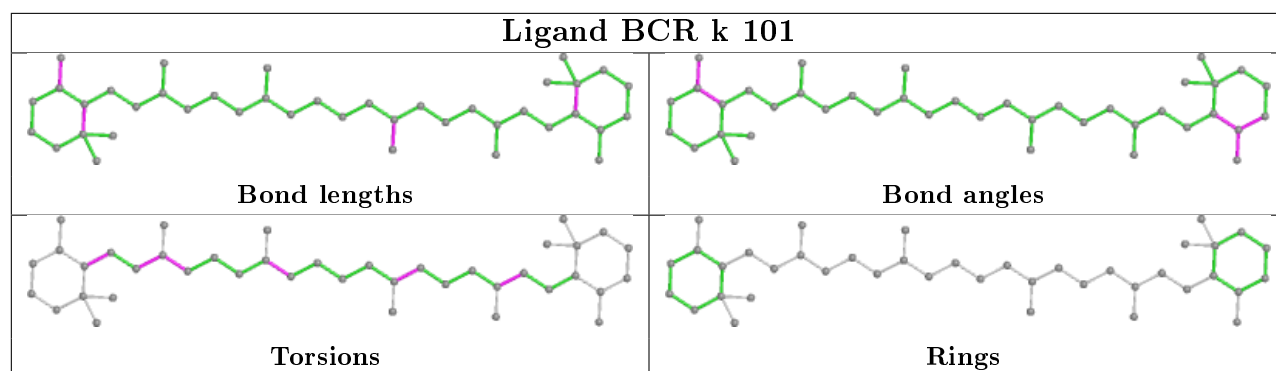
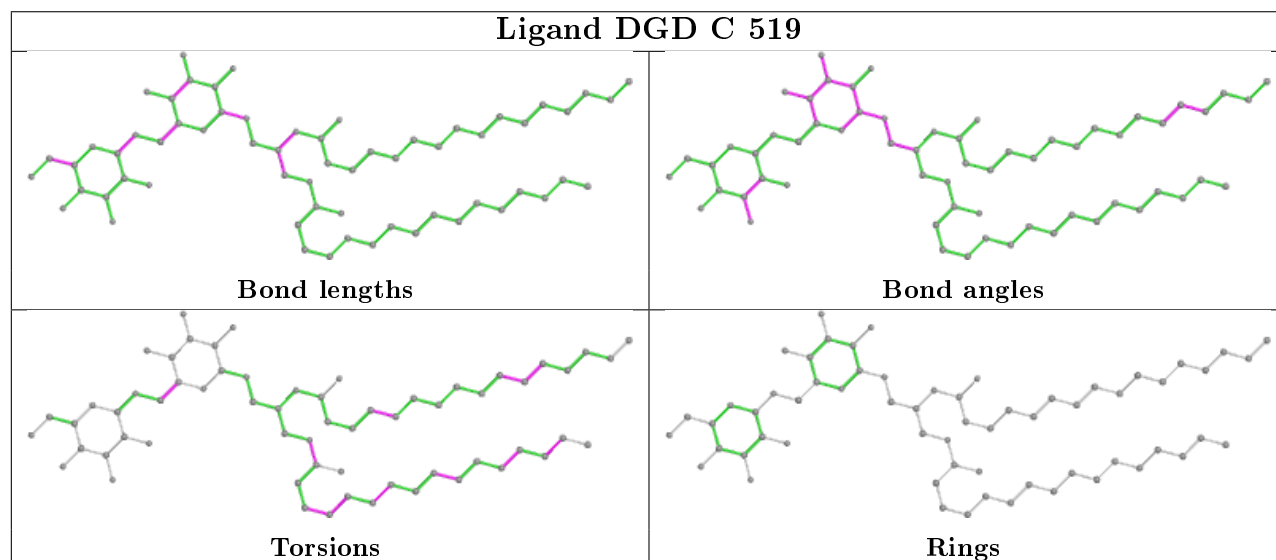
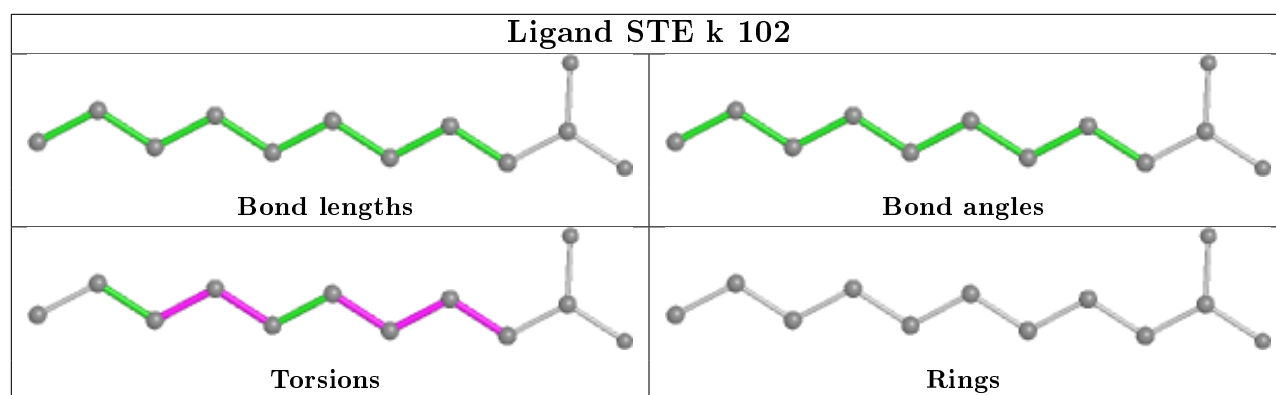
Ligand CLA b 606



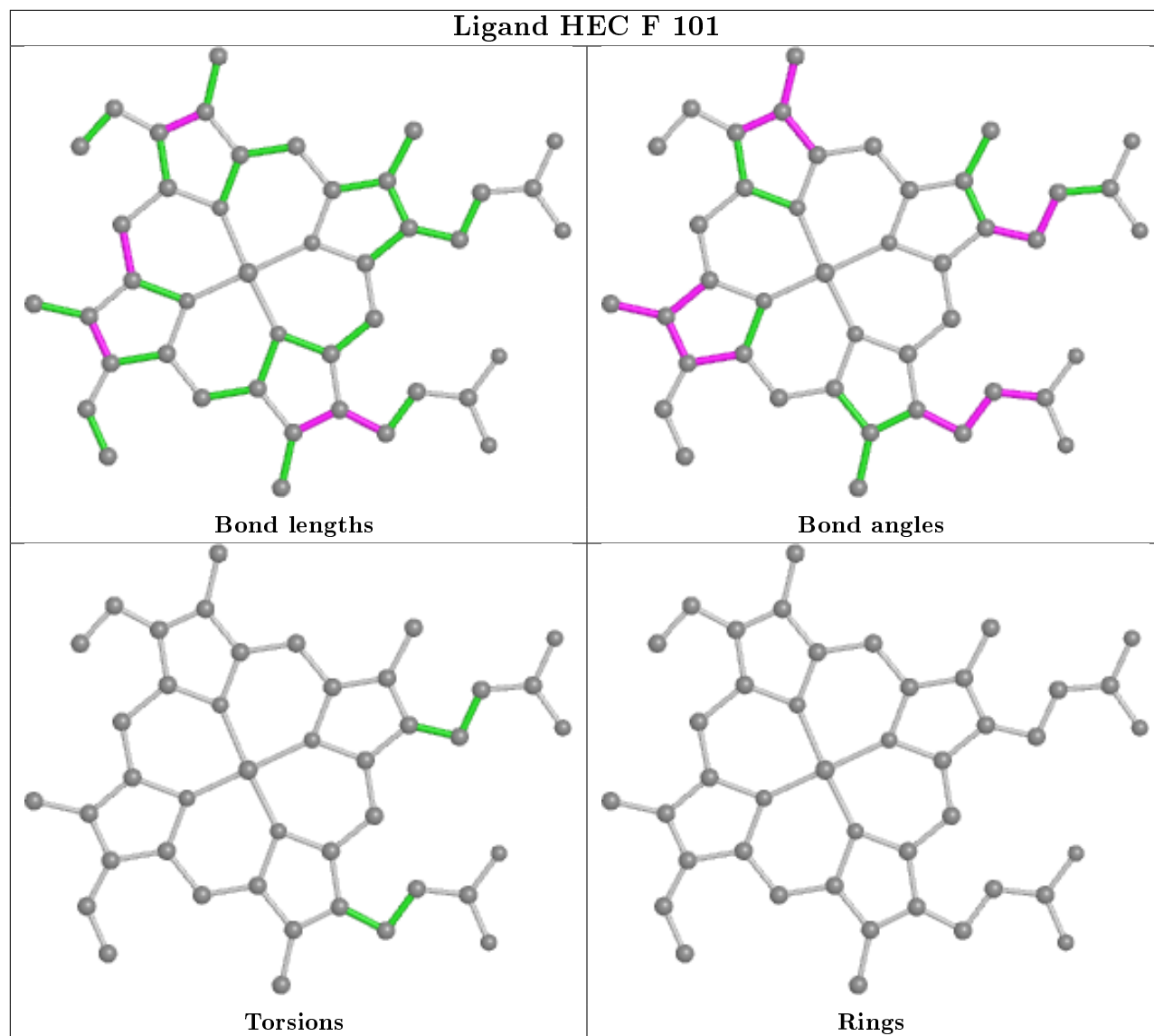
Ligand CLA B 606

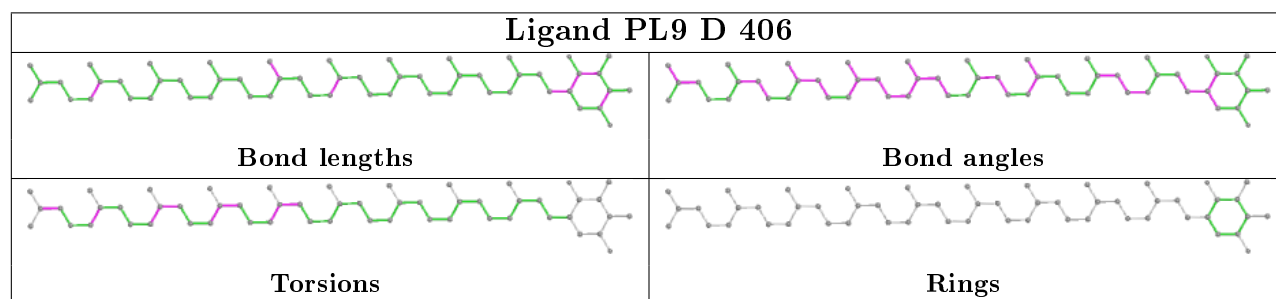
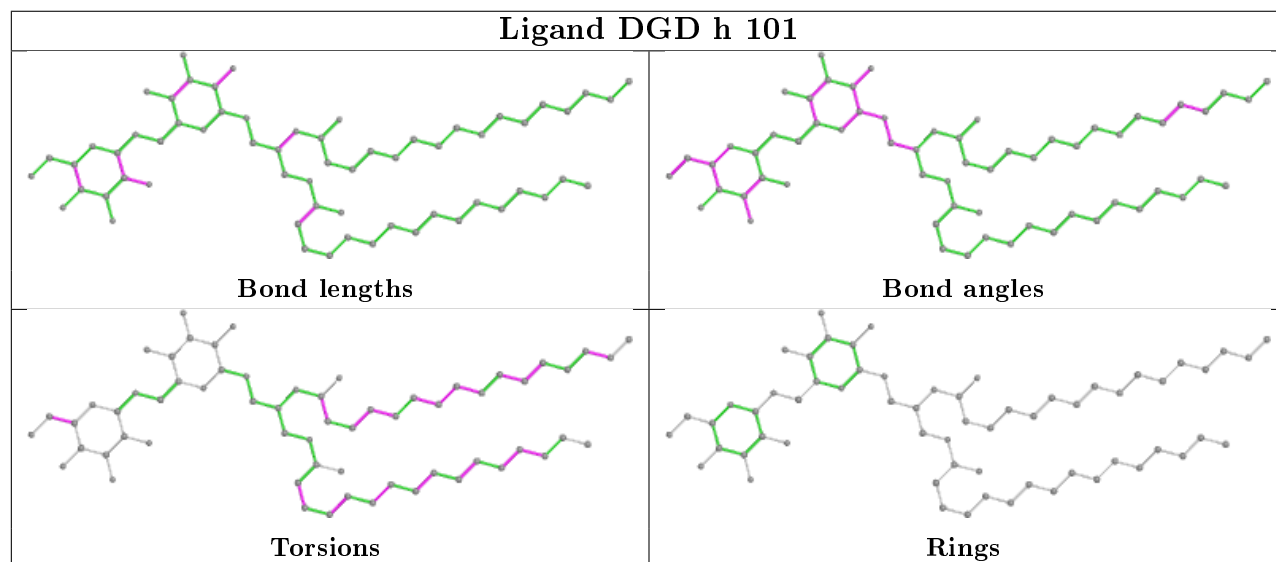
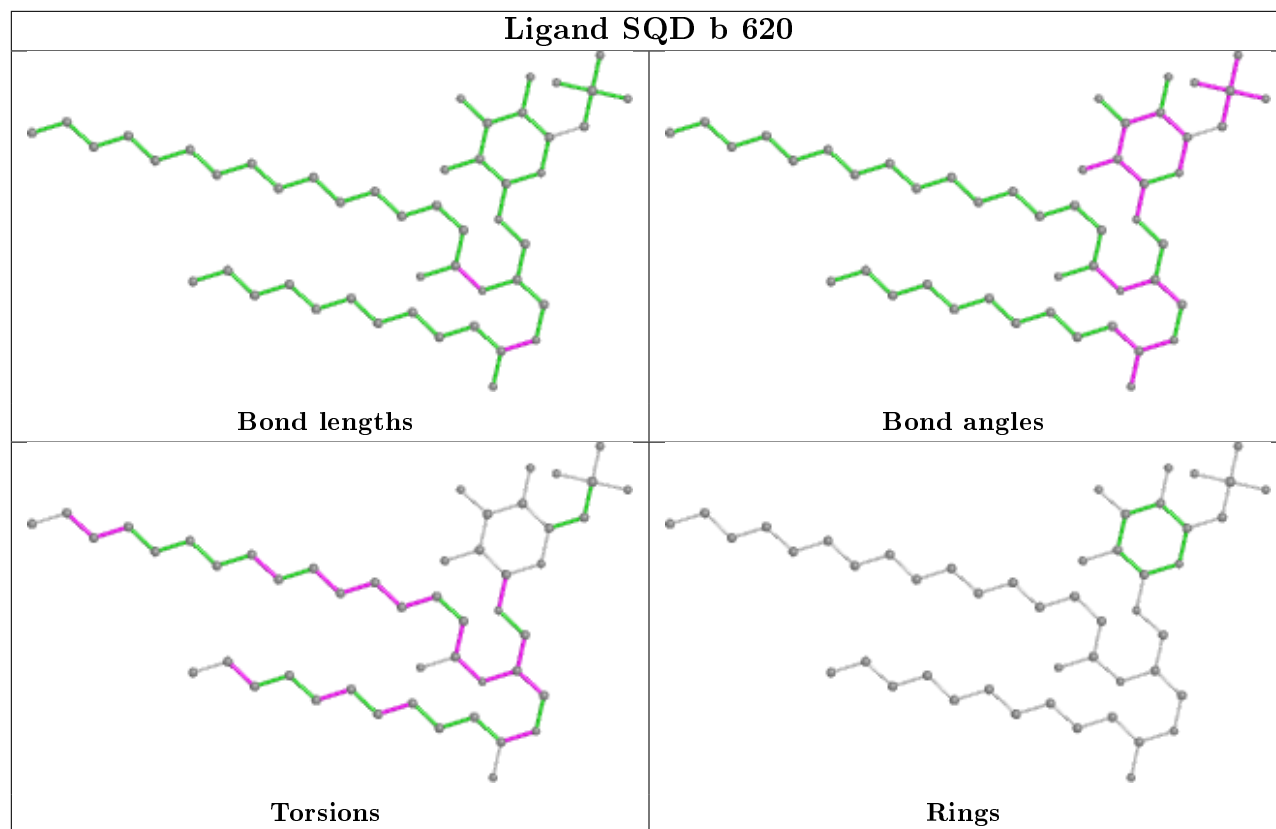




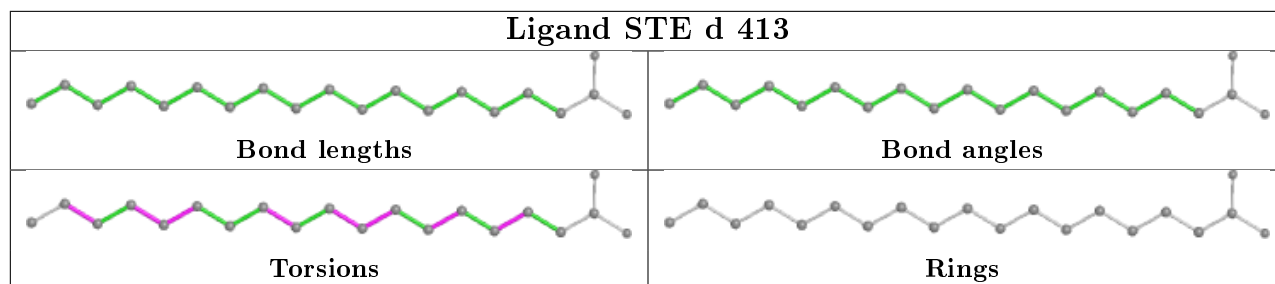


Ligand HEC F 101

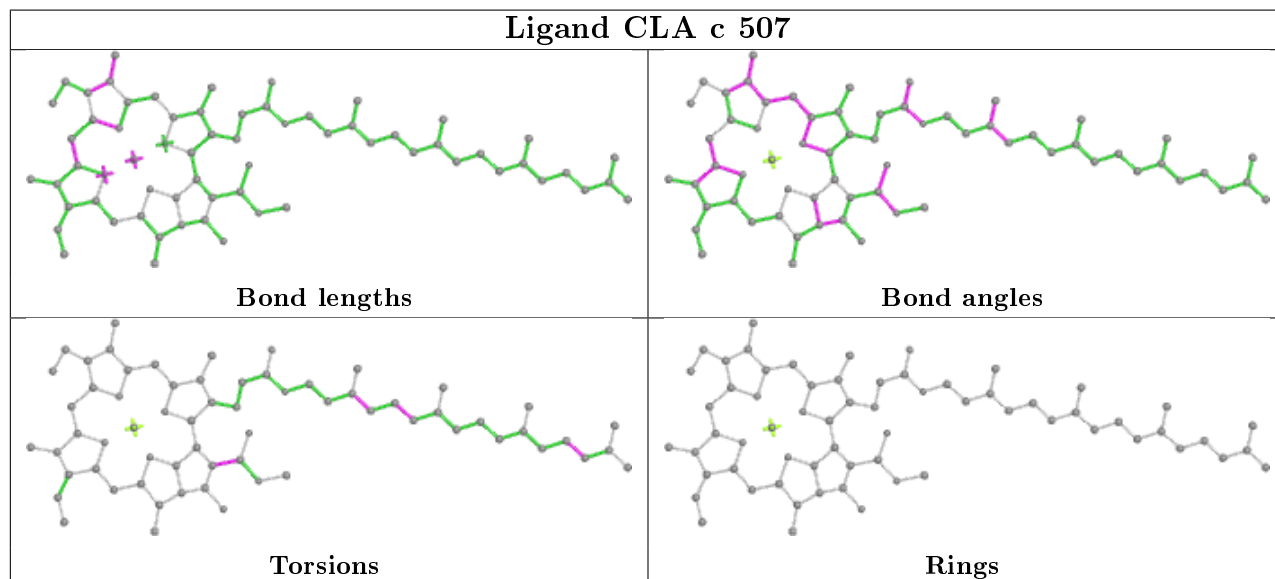




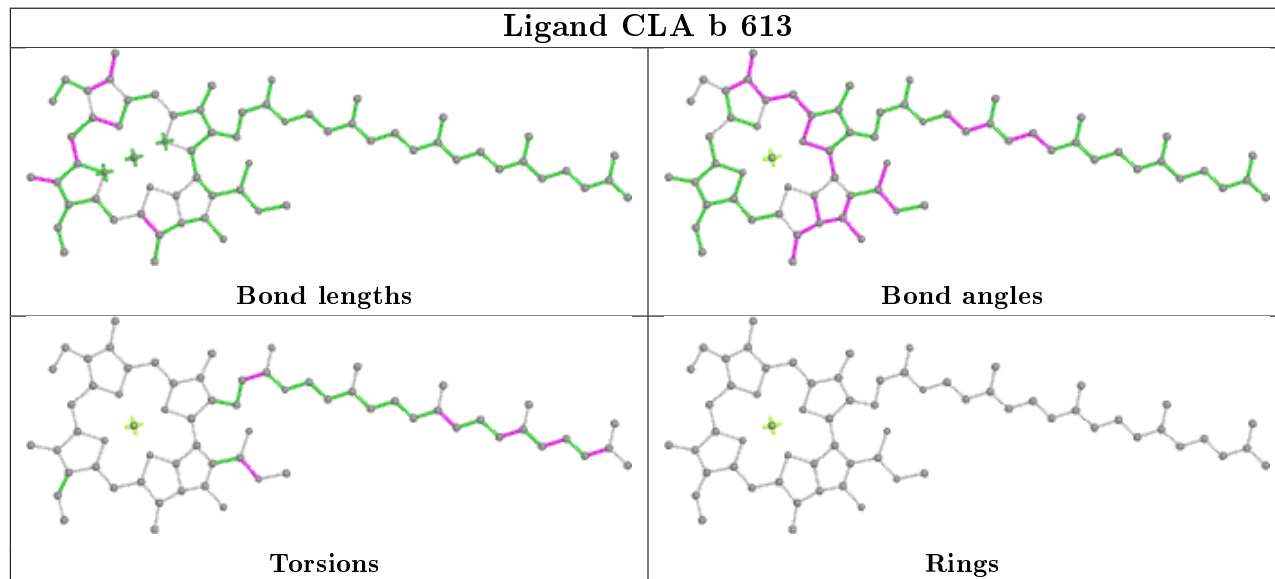
Ligand STE d 413

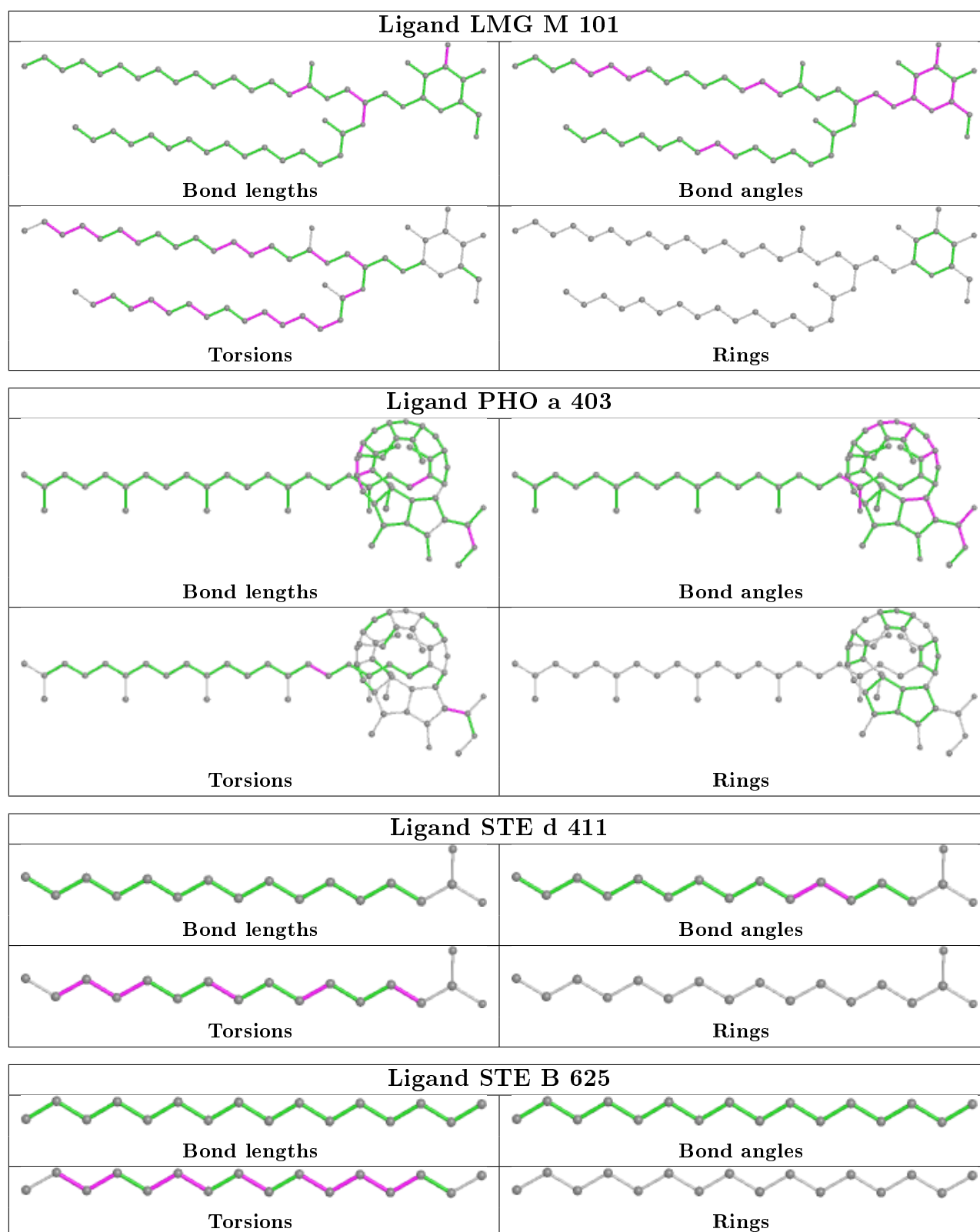


Ligand CLA c 507

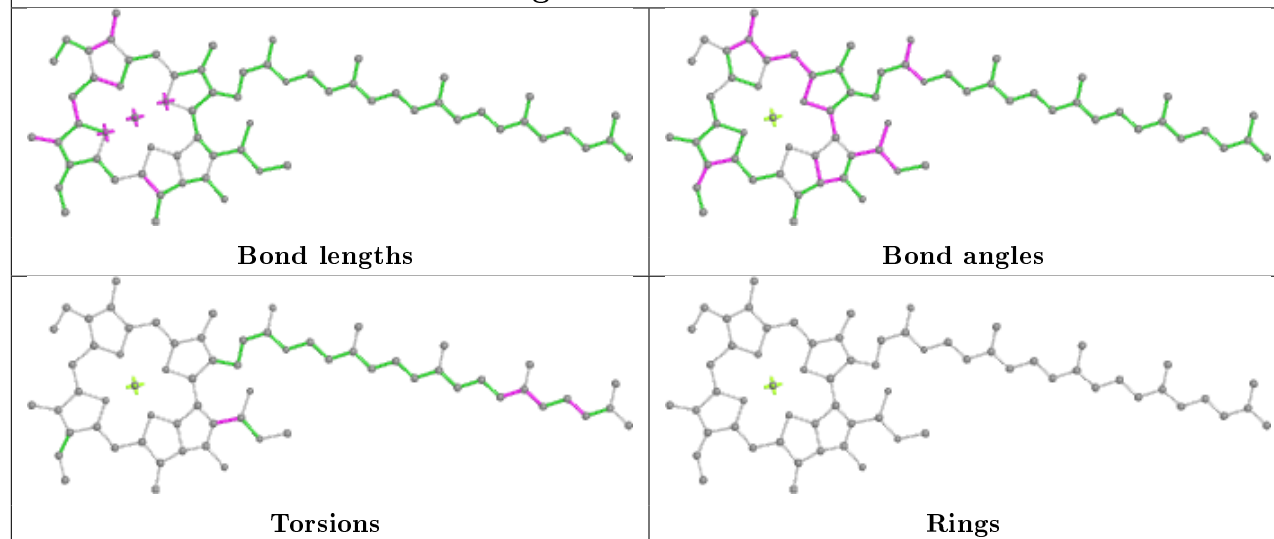


Ligand CLA b 613

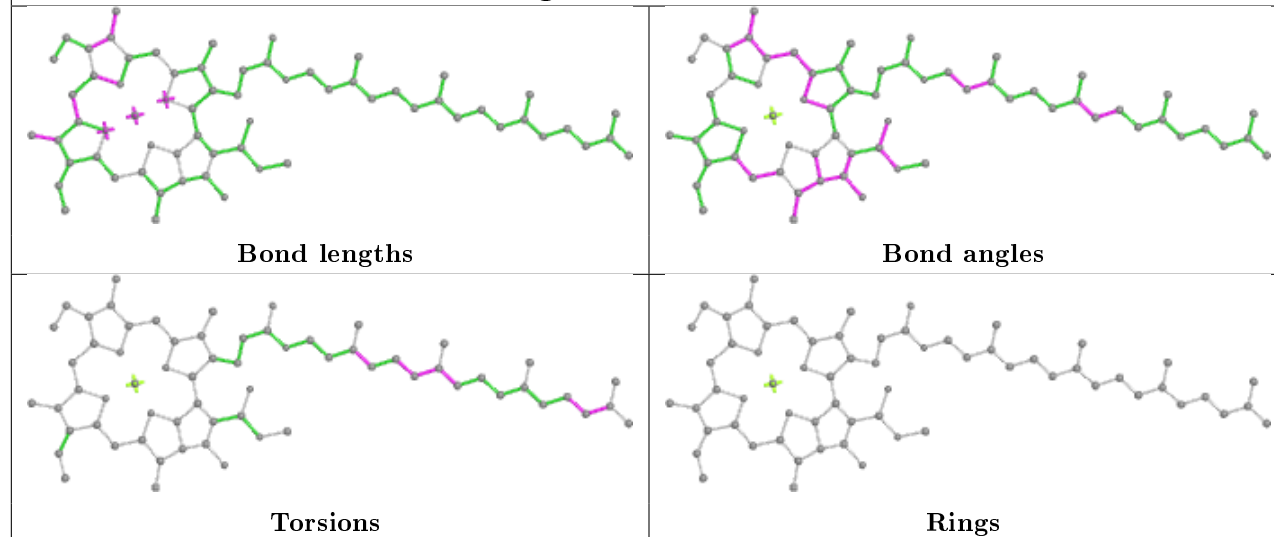


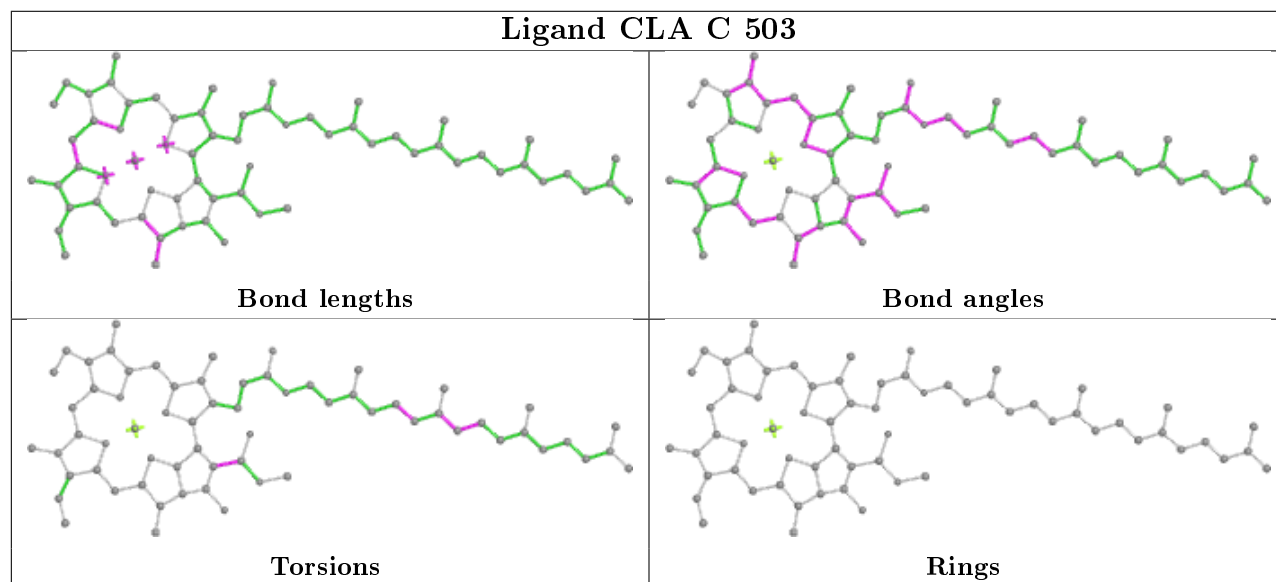
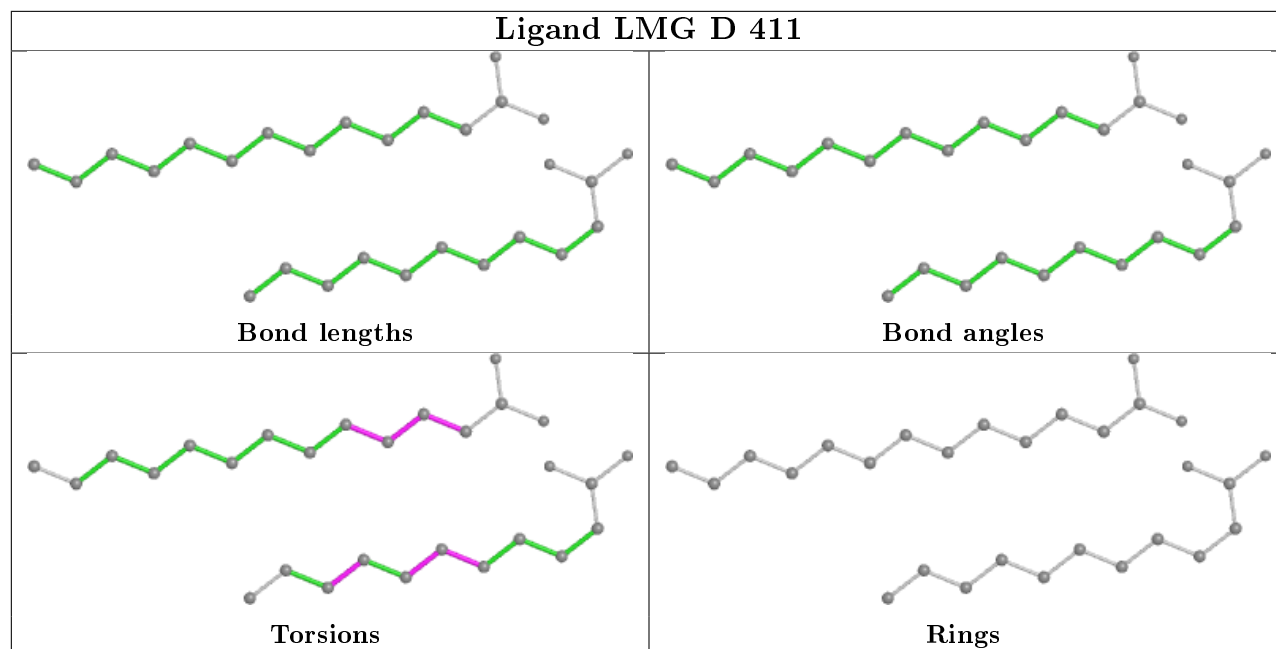


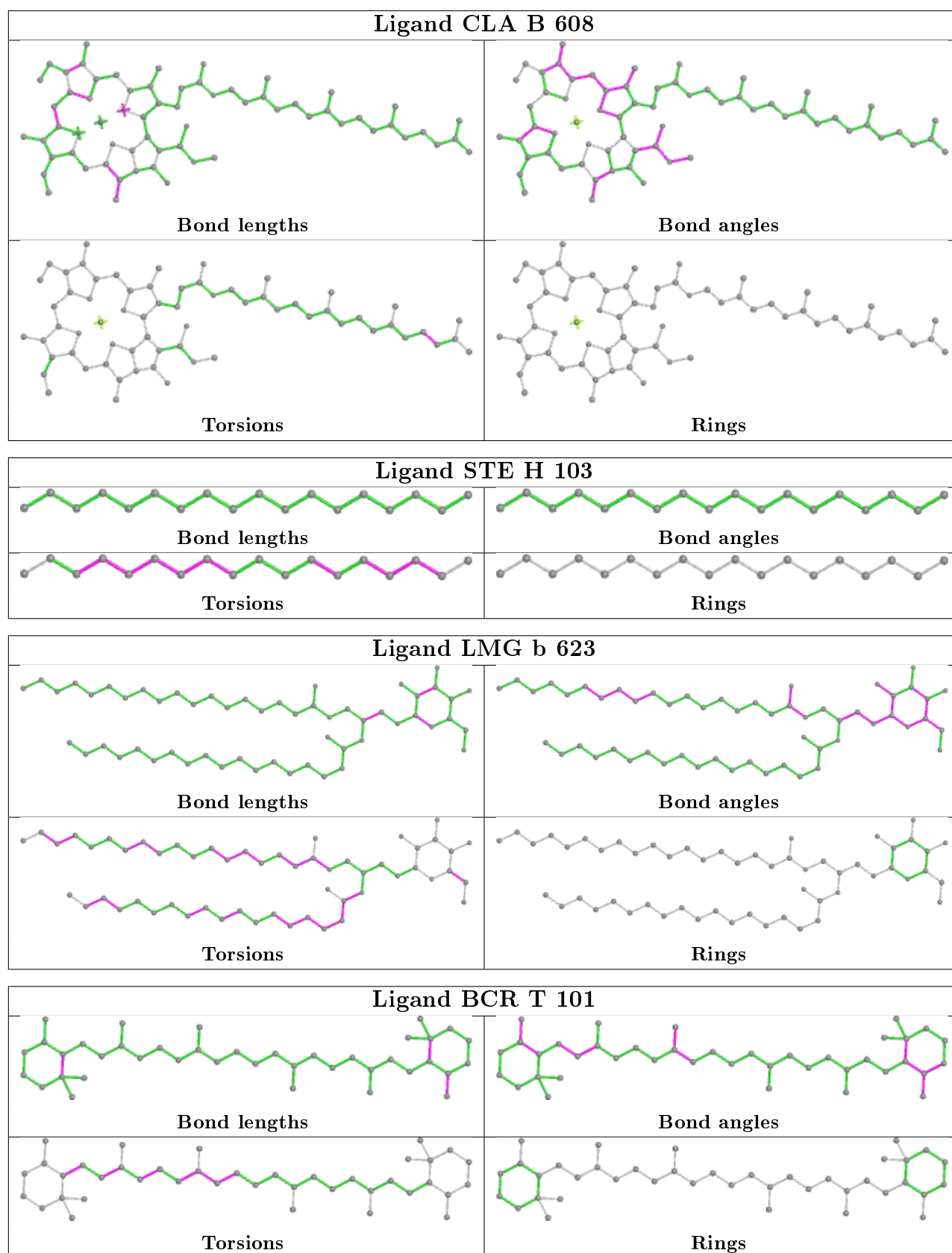
Ligand CLA C 502

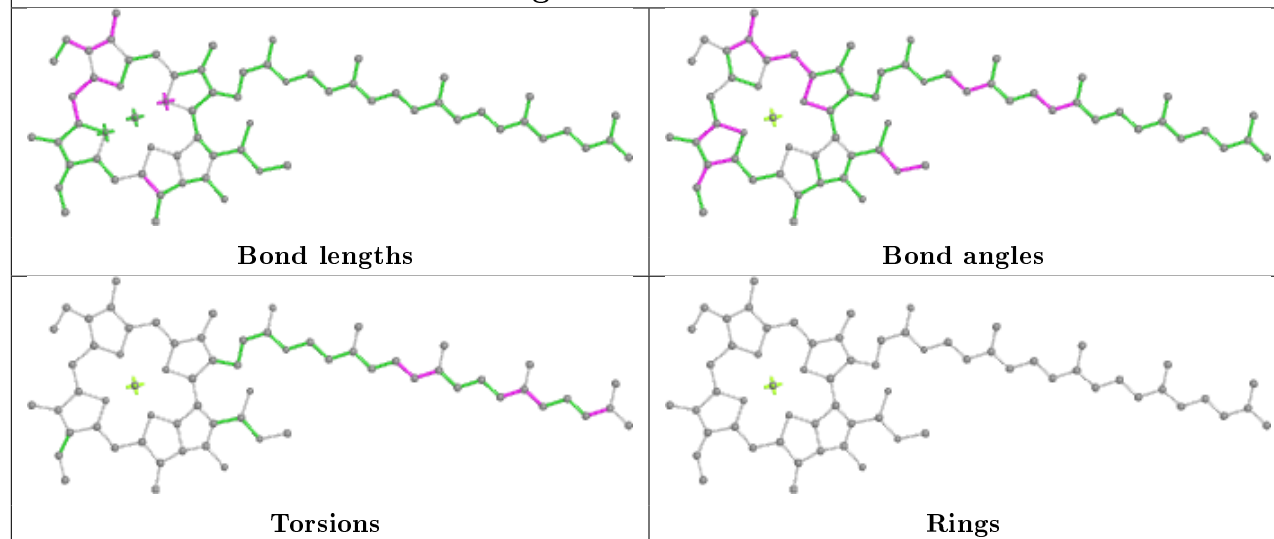
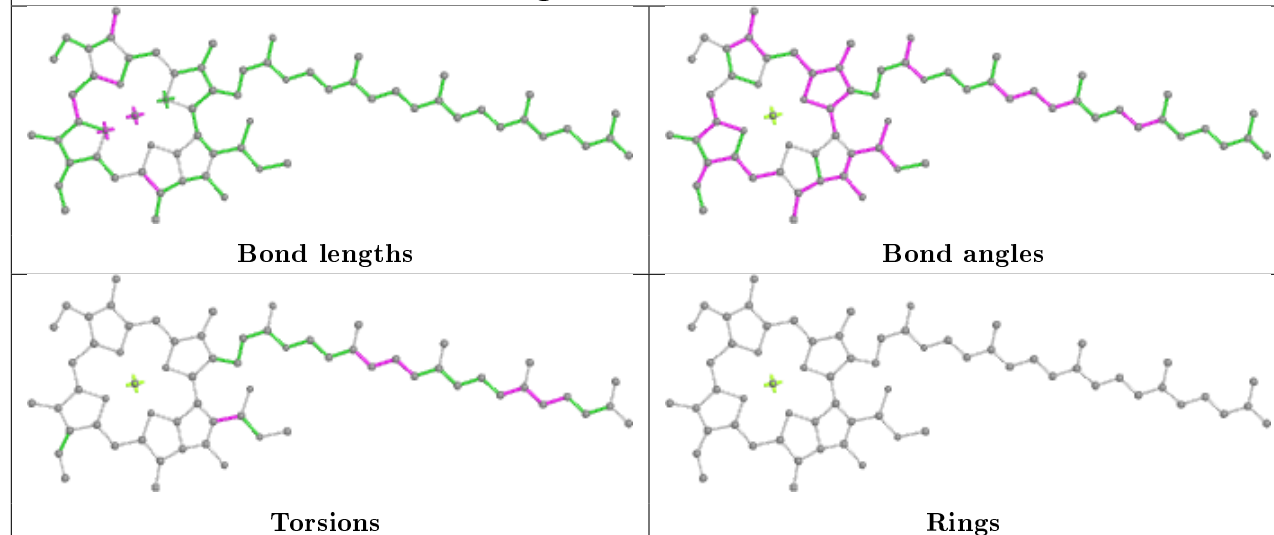
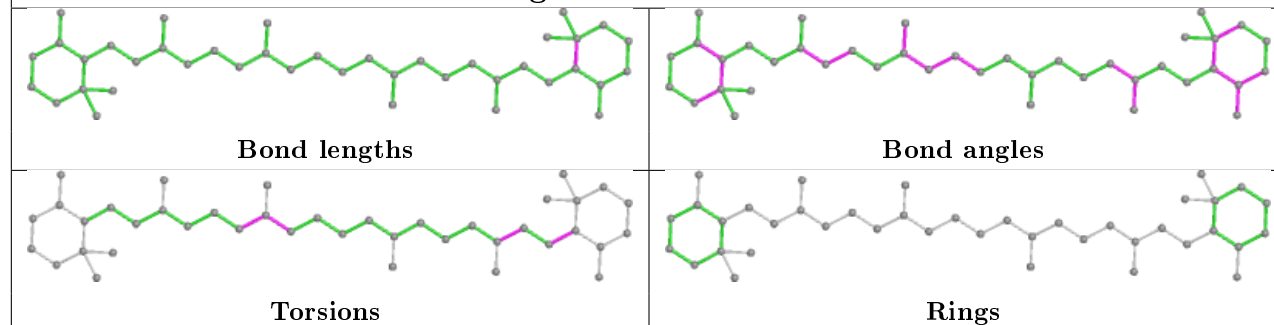


Ligand CLA c 505

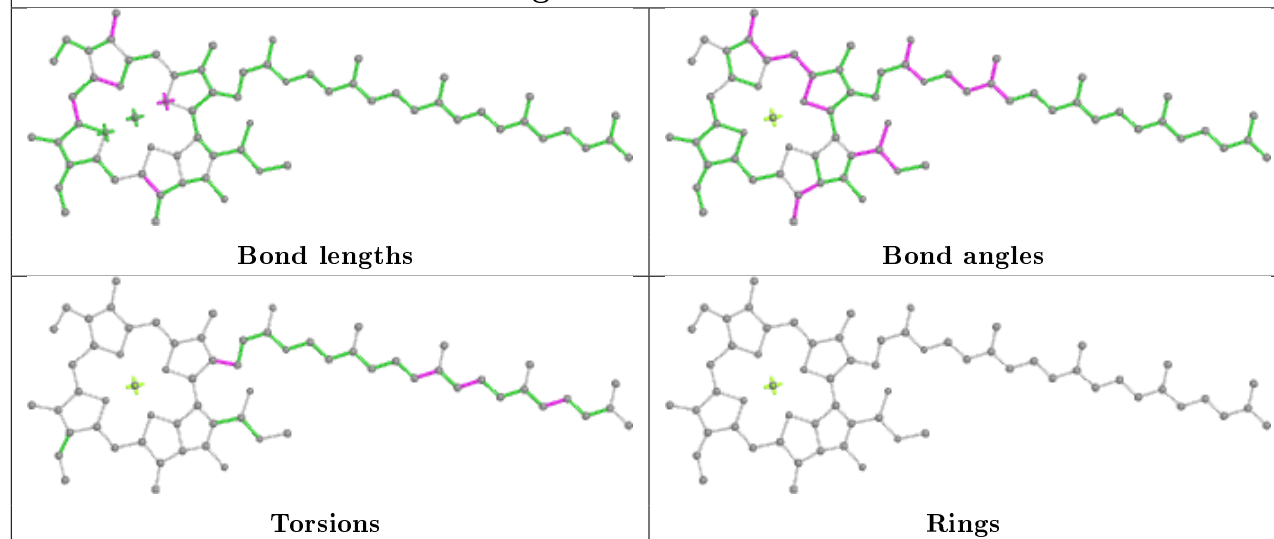




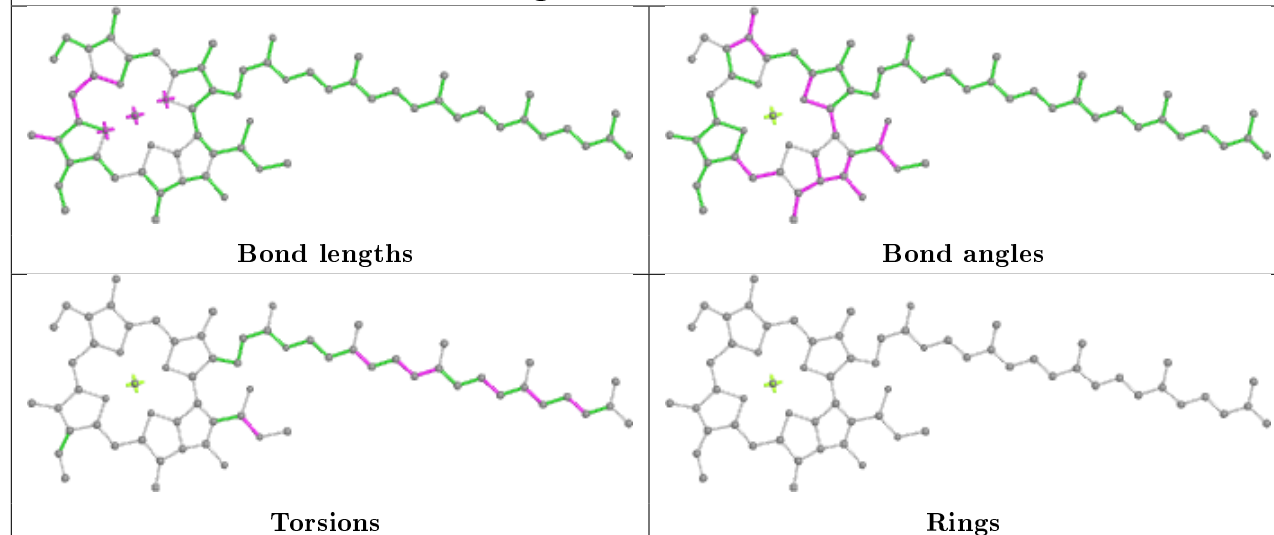


Ligand CLA B 615**Ligand CLA b 604****Ligand BCR H 101**

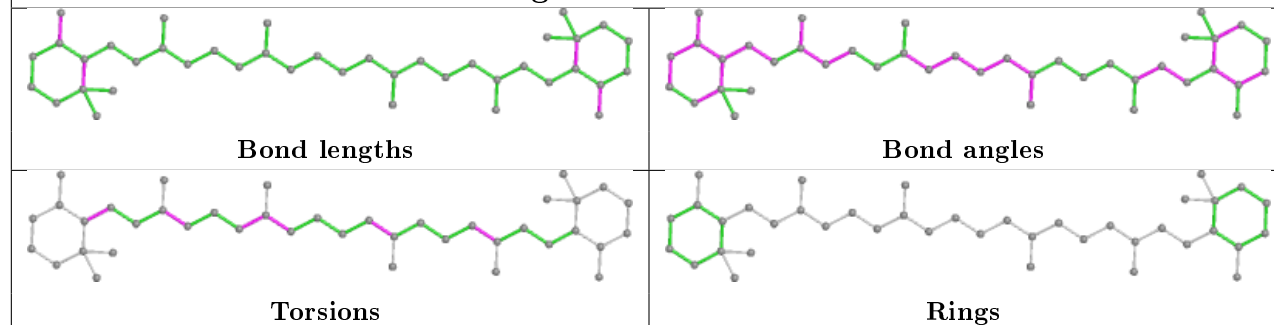
Ligand CLA B 602



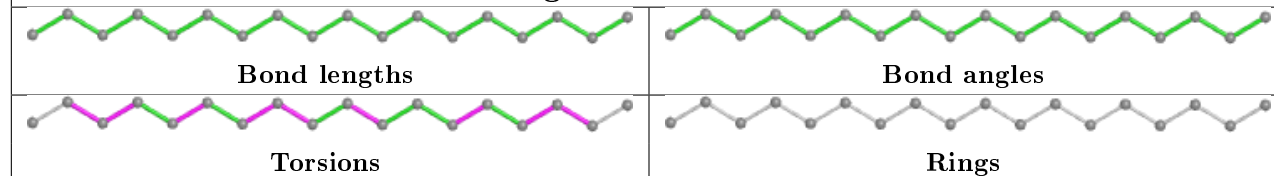
Ligand CLA C 505

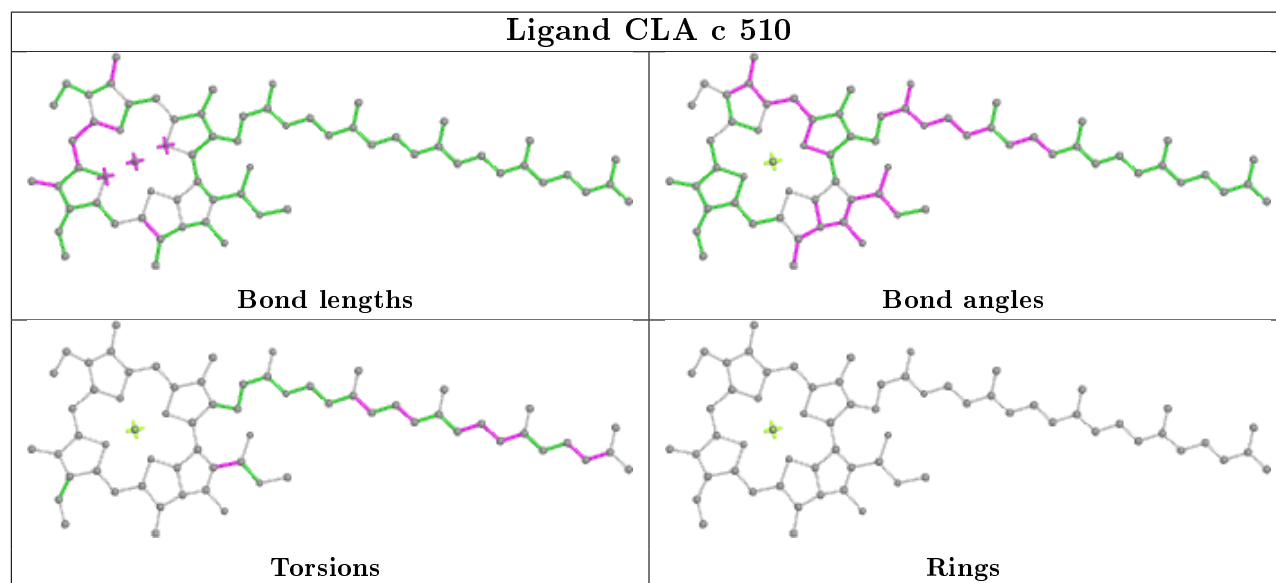
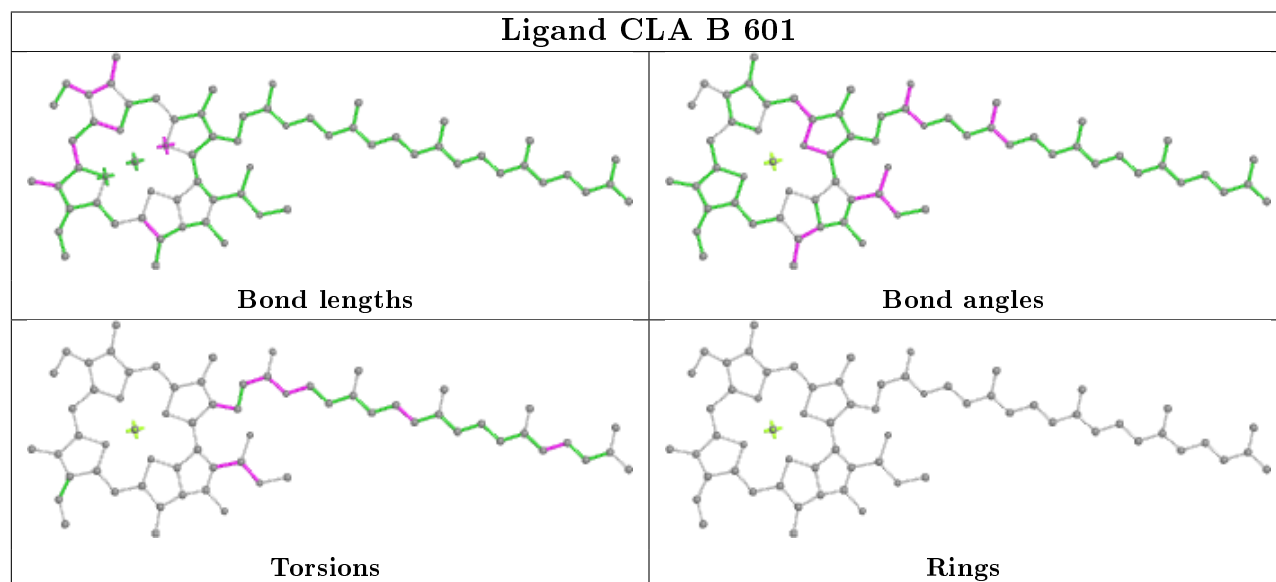
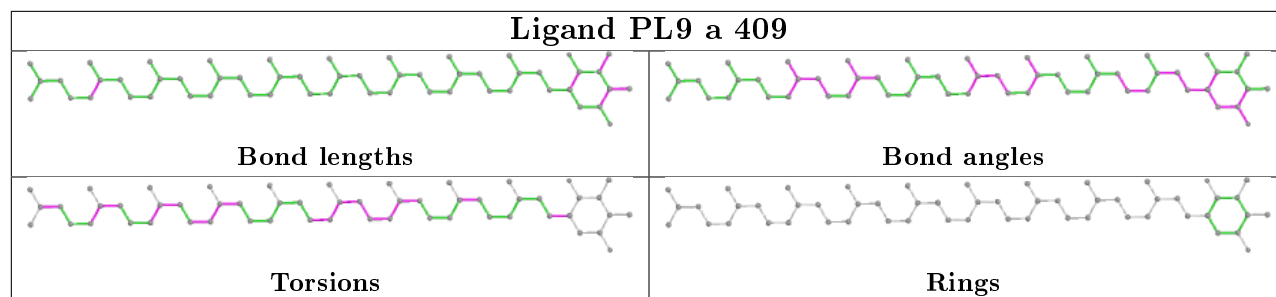


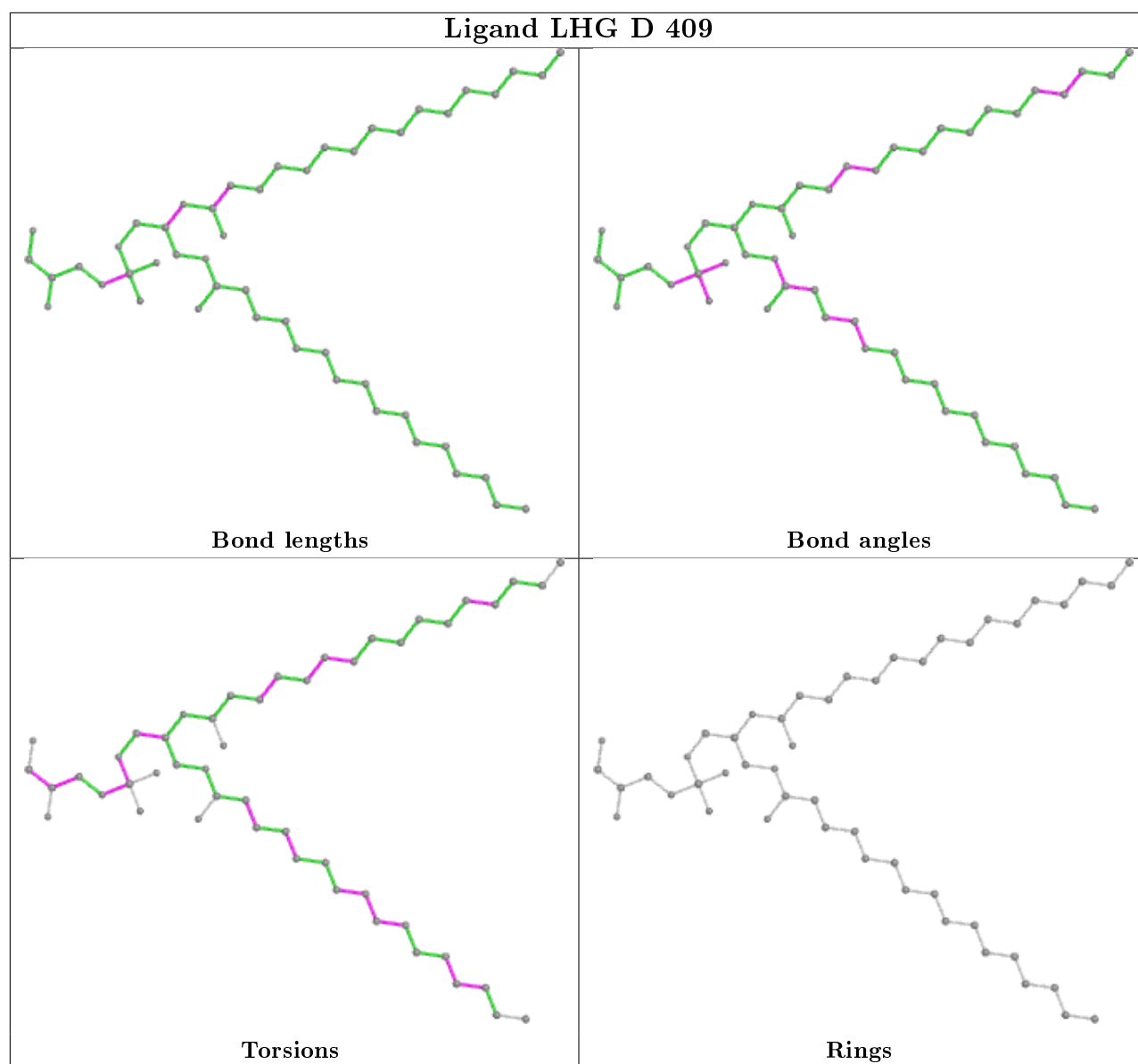
Ligand BCR B 617



Ligand STE 1 102







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.34	4 (1%) 79 78	19, 27, 44, 79	0
1	a	334/344 (97%)	-0.33	1 (0%) 94 93	22, 28, 51, 82	0
2	B	505/506 (99%)	-0.32	6 (1%) 79 78	22, 31, 57, 82	0
2	b	505/506 (99%)	-0.12	17 (3%) 45 44	22, 34, 66, 98	0
3	C	442/461 (95%)	-0.23	3 (0%) 87 87	23, 34, 49, 71	0
3	c	451/461 (97%)	-0.15	6 (1%) 77 76	23, 37, 59, 97	0
4	D	341/352 (96%)	-0.33	0 100 100	21, 28, 44, 76	0
4	d	341/352 (96%)	-0.23	1 (0%) 94 93	23, 31, 53, 75	0
5	E	82/84 (97%)	0.08	4 (4%) 29 28	32, 46, 68, 80	0
5	e	82/84 (97%)	0.31	5 (6%) 21 20	35, 53, 75, 81	0
6	F	34/45 (75%)	-0.38	1 (2%) 51 50	33, 39, 58, 80	0
6	f	34/45 (75%)	-0.13	1 (2%) 51 50	37, 44, 69, 85	0
7	H	65/66 (98%)	0.01	2 (3%) 49 48	30, 37, 56, 68	0
7	h	63/66 (95%)	0.36	6 (9%) 8 7	37, 46, 59, 66	0
8	I	35/38 (92%)	-0.11	3 (8%) 10 9	30, 36, 68, 82	0
8	i	35/38 (92%)	0.04	3 (8%) 10 9	28, 38, 70, 86	0
9	J	36/40 (90%)	0.13	4 (11%) 5 4	31, 46, 66, 87	0
9	j	36/40 (90%)	0.22	4 (11%) 5 4	35, 49, 88, 99	0
10	K	37/46 (80%)	0.14	2 (5%) 25 24	37, 47, 65, 71	0
10	k	37/46 (80%)	0.15	4 (10%) 5 5	44, 50, 63, 76	0
11	L	37/37 (100%)	-0.40	0 100 100	23, 27, 59, 65	0
11	l	36/37 (97%)	-0.14	2 (5%) 24 23	24, 28, 72, 83	0
12	M	32/36 (88%)	0.02	1 (3%) 49 48	24, 32, 60, 69	0
12	m	31/36 (86%)	-0.11	0 100 100	24, 32, 48, 65	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	0.08	15 (6%) 21 20	24, 39, 78, 126	0
13	o	244/272 (89%)	-0.06	13 (5%) 26 25	25, 38, 76, 124	0
14	R	34/40 (85%)	1.52	10 (29%) 0 0	53, 64, 85, 97	0
14	r	31/40 (77%)	3.85	22 (70%) 0 0	66, 82, 100, 106	0
15	T	29/30 (96%)	-0.38	1 (3%) 45 44	25, 29, 60, 72	0
15	t	29/30 (96%)	-0.26	2 (6%) 16 16	25, 29, 76, 80	0
16	U	97/134 (72%)	-0.16	4 (4%) 37 36	30, 40, 66, 85	0
16	u	97/134 (72%)	-0.32	0 100 100	29, 37, 55, 82	0
17	V	137/163 (84%)	-0.38	0 100 100	28, 37, 54, 78	0
17	v	137/163 (84%)	-0.12	6 (4%) 34 33	30, 43, 65, 83	0
18	X	38/41 (92%)	0.12	2 (5%) 26 25	35, 45, 64, 73	0
18	x	39/41 (95%)	0.47	4 (10%) 6 6	44, 52, 78, 94	0
19	Y	27/46 (58%)	1.21	10 (37%) 0 0	48, 63, 88, 92	0
19	y	30/46 (65%)	0.58	3 (10%) 7 6	53, 64, 85, 91	0
20	Z	62/62 (100%)	1.01	16 (25%) 0 0	48, 61, 103, 118	0
20	z	62/62 (100%)	0.96	16 (25%) 0 0	53, 66, 102, 109	0
All	All	5302/5686 (93%)	-0.10	204 (3%) 40 39	19, 35, 69, 126	0

All (204) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	r	32	GLN	16.8
13	o	58	ASN	9.3
13	O	56	PRO	7.8
14	r	6	LEU	6.5
13	o	60	ARG	6.2
2	b	495	PHE	6.1
1	A	13	LEU	6.0
14	r	28	VAL	6.0
14	r	31	VAL	5.9
14	r	13	LEU	5.9
14	r	10	LEU	5.9
14	r	3	TRP	5.9
14	R	3	TRP	5.8
3	c	23	ALA	5.7
13	O	3	GLN	5.5

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Mol	Chain	Res	Type	RSRZ
13	O	4	THR	5.5
14	r	14	LEU	5.4
14	r	25	PRO	5.3
2	b	127	ARG	5.1
3	c	24	THR	5.1
13	o	3	GLN	5.0
14	r	29	LYS	5.0
20	Z	33	TRP	4.9
14	R	6	LEU	4.8
13	O	59	LYS	4.8
20	z	33	TRP	4.8
20	Z	62	VAL	4.8
18	X	2	THR	4.5
14	r	9	LEU	4.5
5	e	79	PHE	4.5
20	z	35	ARG	4.4
15	t	30	THR	4.4
2	b	487	SER	4.3
14	r	24	LEU	4.3
20	Z	35	ARG	4.3
9	j	7	ARG	4.2
20	Z	34	ASP	4.2
15	T	30	THR	4.2
9	j	6	GLY	4.2
9	j	5	GLY	4.1
8	i	36	ASP	4.1
20	Z	1	MET	4.0
14	r	7	VAL	4.0
20	z	30	PRO	4.0
13	O	60	ARG	3.9
1	A	11	ALA	3.9
14	r	15	ALA	3.9
20	z	36	SER	3.9
13	o	61	GLN	3.9
14	r	26	TYR	3.9
9	J	5	GLY	3.8
1	a	11	ALA	3.8
18	x	40	SER	3.8
20	Z	32	ASP	3.8
20	Z	38	GLN	3.8
19	Y	20	ALA	3.8
14	R	32	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
3	c	143	TYR	3.7
13	o	57	LYS	3.7
8	i	34	ARG	3.7
5	e	61	ARG	3.7
19	Y	21	GLN	3.6
13	o	62	GLU	3.6
13	o	4	THR	3.6
5	E	79	PHE	3.6
20	z	3	ILE	3.6
9	J	7	ARG	3.6
20	Z	37	LYS	3.6
20	Z	3	ILE	3.6
20	z	60	PHE	3.6
13	O	5	LEU	3.6
2	b	505	ARG	3.5
9	j	8	ILE	3.5
6	F	12	SER	3.5
2	b	128	THR	3.5
19	Y	41	VAL	3.4
18	x	2	THR	3.4
13	O	61	GLN	3.4
8	I	36	ASP	3.4
3	c	146	PHE	3.4
2	B	127	ARG	3.3
13	o	207	ARG	3.2
18	x	34	ILE	3.2
20	Z	41	PHE	3.2
2	b	506	ARG	3.2
5	e	83	LEU	3.2
14	r	5	VAL	3.2
5	e	82	GLN	3.2
13	O	63	ALA	3.1
5	E	82	GLN	3.1
3	c	25	ASN	3.1
2	b	486	LEU	3.1
13	o	59	LYS	3.1
19	Y	43	ARG	3.1
19	y	37	PHE	3.0
20	Z	61	VAL	3.0
16	U	8	GLU	3.0
20	Z	42	LEU	3.0
13	o	63	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
19	Y	40	ALA	3.0
2	b	292	LEU	3.0
17	v	15	GLU	3.0
20	Z	4	LEU	3.0
2	b	502	VAL	3.0
18	X	3	ILE	3.0
9	J	6	GLY	3.0
7	h	10	ILE	2.9
20	z	61	VAL	2.9
20	z	62	VAL	2.9
2	b	490	GLN	2.9
14	R	21	ARG	2.9
2	b	289	GLN	2.9
10	k	13	GLU	2.9
14	r	4	ARG	2.9
7	H	66	GLY	2.9
3	C	143	TYR	2.9
14	r	21	ARG	2.9
13	O	35	SER	2.9
7	h	6	TRP	2.8
18	x	38	GLN	2.8
2	b	295	GLY	2.8
13	O	58	ASN	2.8
13	o	5	LEU	2.8
13	o	56	PRO	2.8
19	y	18	VAL	2.8
13	O	62	GLU	2.8
7	h	21	VAL	2.8
13	O	57	LYS	2.8
8	I	34	ARG	2.7
8	i	35	LYS	2.7
14	r	18	TRP	2.7
10	k	17	ILE	2.7
15	t	29	ILE	2.7
8	I	35	LYS	2.7
12	M	33	GLN	2.7
5	E	83	LEU	2.7
19	Y	42	ARG	2.7
3	c	147	PHE	2.7
11	l	3	PRO	2.6
20	z	41	PHE	2.6
10	K	17	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
19	Y	22	LEU	2.6
2	B	490	GLN	2.6
2	B	495	PHE	2.6
20	Z	7	LEU	2.6
14	r	12	VAL	2.5
19	Y	23	THR	2.5
20	Z	60	PHE	2.5
2	B	295	GLY	2.5
2	b	494	GLY	2.5
2	b	293	ALA	2.5
1	A	15	GLU	2.5
5	e	84	LYS	2.5
14	R	28	VAL	2.5
17	v	21	LEU	2.4
20	z	7	LEU	2.4
14	R	29	LYS	2.4
19	Y	37	PHE	2.4
16	U	9	LEU	2.4
7	h	20	LYS	2.4
5	E	84	LYS	2.4
2	B	294	SER	2.4
14	R	13	LEU	2.4
20	z	42	LEU	2.3
7	H	41	PHE	2.3
13	O	36	GLN	2.3
14	R	25	PRO	2.3
2	B	487	SER	2.3
7	h	13	PRO	2.3
2	b	296	ALA	2.3
11	l	7	ARG	2.3
20	z	39	LEU	2.3
20	z	1	MET	2.2
16	U	68	THR	2.2
6	f	12	SER	2.2
7	h	23	PRO	2.2
10	K	14	ALA	2.2
3	C	146	PHE	2.2
14	R	26	TYR	2.2
14	r	27	ALA	2.2
17	v	16	GLY	2.2
20	z	38	GLN	2.2
10	k	12	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
13	O	87	VAL	2.1
1	A	12	ASN	2.1
14	r	2	ASP	2.1
14	R	31	VAL	2.1
17	v	22	THR	2.1
4	d	227[A]	GLU	2.1
19	Y	25	ILE	2.1
20	Z	36	SER	2.1
20	z	37	LYS	2.1
20	z	59	PHE	2.1
10	k	10	LYS	2.1
9	J	8	ILE	2.1
3	C	61	VAL	2.1
13	o	132	ASN	2.1
13	O	23	ASP	2.1
17	v	113	VAL	2.1
17	v	17	LYS	2.1
19	y	19	ILE	2.0
2	b	491	VAL	2.0
2	b	496	TYR	2.0
16	U	62	LEU	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	0.93	0.10	32,45,72,72	0
12	FME	M	1	10/11	0.95	0.15	40,51,73,84	0
8	FME	I	1	10/11	0.95	0.18	33,44,65,71	0
15	FME	T	1	10/11	0.96	0.08	27,46,65,65	0
12	FME	m	1	10/11	0.97	0.15	34,45,71,80	0
8	FME	i	1	10/11	0.97	0.16	36,50,62,65	0

6.3 Carbohydrates ⓘ

There are no carbohydrates 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
33	STE	R	101	12/20	0.60	0.31	55,77,85,87	0
33	STE	H	103	18/20	0.69	0.32	51,74,87,90	0
33	STE	b	625	20/20	0.73	0.24	49,66,82,85	0
33	STE	a	414	12/20	0.75	0.24	35,62,69,75	0
33	STE	a	413	10/20	0.80	0.21	40,62,75,75	0
27	LMG	a	416	55/55	0.80	0.18	37,63,101,136	0
33	STE	a	415	15/20	0.81	0.19	39,68,86,93	0
33	STE	b	627	14/20	0.81	0.22	52,65,84,93	0
28	LHG	E	101	49/49	0.82	0.22	43,76,103,113	0
27	LMG	c	522	48/55	0.82	0.26	43,75,106,112	0
33	STE	k	102	12/20	0.83	0.18	43,65,78,83	0
24	BCR	H	101	40/40	0.83	0.16	28,44,58,65	0
33	STE	b	626	10/20	0.84	0.23	39,53,59,69	0
27	LMG	c	523	49/55	0.84	0.18	36,57,92,106	0
28	LHG	e	101	42/49	0.84	0.23	51,78,103,123	0
33	STE	b	624	16/20	0.84	0.15	42,62,79,80	0
30	DGD	A	415	66/66	0.84	0.17	42,64,85,88	0
33	STE	B	626	12/20	0.84	0.32	49,62,79,84	0
27	LMG	D	410	33/55	0.84	0.18	35,55,80,90	0
29	SQD	a	412	36/54	0.84	0.17	31,63,87,91	0
26	PL9	A	410	55/55	0.84	0.25	32,65,86,92	0
33	STE	B	625	16/20	0.84	0.26	43,62,82,84	0
33	STE	m	102	12/20	0.84	0.20	49,62,82,84	0
22	CLA	b	601	65/65	0.84	0.18	46,65,86,102	0
33	STE	d	413	20/20	0.85	0.18	38,68,92,97	0
22	CLA	C	512	65/65	0.86	0.17	32,52,84,94	0
33	STE	c	521	20/20	0.86	0.20	37,59,72,75	0
33	STE	C	523	12/20	0.86	0.12	36,48,55,59	0
29	SQD	A	414	39/54	0.86	0.19	40,64,96,106	0
27	LMG	b	623	55/55	0.86	0.29	49,71,96,103	0
33	STE	t	102	14/20	0.86	0.14	34,50,66,67	0
33	STE	l	102	18/20	0.86	0.15	36,48,82,86	0
24	BCR	Y	101	40/40	0.87	0.13	32,48,64,68	0
22	CLA	C	513	65/65	0.87	0.19	38,62,94,108	0
33	STE	t	103	18/20	0.87	0.14	44,57,78,85	0
24	BCR	x	101	40/40	0.87	0.14	34,49,67,71	0
33	STE	j	101	12/20	0.87	0.14	45,57,71,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
26	PL9	a	409	55/55	0.87	0.18	34,68,87,99	0
33	STE	C	522	16/20	0.88	0.12	34,51,75,83	0
33	STE	d	411	17/20	0.88	0.16	39,56,68,71	0
33	STE	b	621	16/20	0.88	0.18	29,47,69,70	0
29	SQD	B	623	54/54	0.88	0.15	37,61,86,98	0
33	STE	B	620	17/20	0.88	0.19	33,52,69,70	0
33	STE	T	102	15/20	0.88	0.18	42,58,79,80	0
24	BCR	d	406	40/40	0.88	0.14	35,52,96,100	0
24	BCR	k	101	40/40	0.88	0.14	34,57,72,73	0
33	STE	J	101	12/20	0.89	0.15	46,57,67,69	0
27	LMG	A	411	48/55	0.89	0.14	35,56,78,89	0
27	LMG	c	520	37/55	0.89	0.15	43,67,84,90	0
33	STE	Z	101	8/20	0.89	0.16	37,55,66,66	0
33	STE	M	103	10/20	0.89	0.16	32,43,56,63	0
22	CLA	c	513	65/65	0.89	0.20	41,66,110,114	0
33	STE	C	521	12/20	0.89	0.13	41,58,69,70	0
22	CLA	c	512	65/65	0.89	0.15	37,54,91,108	0
22	CLA	B	601	65/65	0.89	0.15	27,57,88,102	0
33	STE	D	412	20/20	0.90	0.19	34,52,73,77	0
24	BCR	C	514	40/40	0.90	0.15	39,54,67,68	0
27	LMG	D	411	28/55	0.90	0.14	34,48,64,74	0
33	STE	b	622	20/20	0.90	0.22	34,60,72,74	0
33	STE	B	624	12/20	0.90	0.10	31,47,59,67	0
29	SQD	b	620	49/54	0.90	0.15	40,58,92,111	0
29	SQD	f	102	41/54	0.90	0.19	52,83,112,115	0
33	STE	d	412	20/20	0.90	0.22	36,54,71,77	0
24	BCR	c	516	40/40	0.91	0.17	35,48,63,67	0
33	STE	I	101	15/20	0.91	0.14	38,55,77,81	0
22	CLA	D	404	65/65	0.91	0.14	22,43,109,119	0
27	LMG	C	520	48/55	0.91	0.15	41,67,88,95	0
22	CLA	a	404	65/65	0.91	0.14	19,35,84,101	0
27	LMG	m	101	51/55	0.91	0.13	34,50,80,88	0
27	LMG	M	101	51/55	0.91	0.12	30,46,67,80	0
27	LMG	D	407	51/55	0.91	0.18	26,54,85,89	0
22	CLA	b	615	65/65	0.92	0.14	26,38,61,66	0
22	CLA	d	405	65/65	0.92	0.14	26,48,89,100	0
24	BCR	c	514	40/40	0.92	0.14	44,57,70,72	0
22	CLA	c	508	64/65	0.92	0.15	28,42,82,101	0
24	BCR	D	405	40/40	0.92	0.12	26,42,77,91	0
22	CLA	c	502	65/65	0.92	0.14	28,39,58,65	0
24	BCR	b	619	40/40	0.93	0.12	27,47,63,72	0
22	CLA	c	507	65/65	0.93	0.14	26,42,60,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	BCR	B	618	40/40	0.93	0.10	24,36,49,50	0
30	DGD	c	519	62/66	0.93	0.14	26,52,87,92	0
29	SQD	a	411	54/54	0.93	0.16	39,62,89,99	0
24	BCR	B	619	40/40	0.93	0.11	24,41,59,71	0
30	DGD	C	518	62/66	0.93	0.13	27,49,99,122	0
22	CLA	b	606	65/65	0.93	0.13	26,39,76,82	0
22	CLA	C	511	65/65	0.93	0.12	27,48,66,69	0
29	SQD	D	408	36/54	0.93	0.16	42,67,91,95	0
22	CLA	C	502	65/65	0.93	0.14	25,39,52,58	0
22	CLA	B	616	60/65	0.93	0.14	23,36,91,109	0
22	CLA	c	510	65/65	0.93	0.15	26,45,59,77	0
24	BCR	C	515	40/40	0.94	0.11	26,39,52,64	0
30	DGD	C	519	62/66	0.94	0.13	24,47,77,91	0
22	CLA	b	616	60/65	0.94	0.13	26,40,82,91	0
22	CLA	d	401	65/65	0.94	0.13	24,37,86,97	0
30	DGD	h	101	62/66	0.94	0.12	32,46,57,68	0
26	PL9	D	406	55/55	0.94	0.12	18,33,46,50	0
22	CLA	C	507	65/65	0.94	0.14	24,39,57,59	0
22	CLA	c	506	65/65	0.94	0.12	29,45,94,103	0
22	CLA	b	602	65/65	0.94	0.15	25,40,64,71	0
22	CLA	b	609	65/65	0.94	0.14	28,42,65,68	0
24	BCR	b	618	40/40	0.94	0.10	27,38,52,52	0
22	CLA	c	509	65/65	0.94	0.18	32,45,61,69	0
27	LMG	d	410	44/55	0.94	0.14	30,49,84,89	0
30	DGD	H	102	62/66	0.94	0.10	26,43,57,60	0
22	CLA	c	511	65/65	0.94	0.13	30,50,70,75	0
22	CLA	B	615	65/65	0.94	0.11	24,35,63,75	0
22	CLA	B	606	65/65	0.94	0.11	20,34,67,72	0
22	CLA	B	602	65/65	0.94	0.15	22,35,55,61	0
22	CLA	C	505	65/65	0.94	0.15	23,38,71,87	0
22	CLA	C	506	65/65	0.94	0.12	26,41,85,102	0
22	CLA	B	604	65/65	0.94	0.12	20,32,74,85	0
30	DGD	c	518	62/66	0.94	0.12	29,51,95,99	0
33	STE	M	102	15/20	0.95	0.11	35,45,62,62	0
22	CLA	B	613	65/65	0.95	0.13	17,31,70,80	0
30	DGD	C	517	62/66	0.95	0.12	22,42,80,92	0
22	CLA	B	614	65/65	0.95	0.15	19,37,81,90	0
22	CLA	C	510	65/65	0.95	0.12	26,42,63,69	0
22	CLA	c	504	60/65	0.95	0.12	29,44,81,89	0
22	CLA	b	608	65/65	0.95	0.14	23,41,63,71	0
22	CLA	b	610	65/65	0.95	0.19	22,35,51,53	0
24	BCR	t	101	40/40	0.95	0.10	24,36,51,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	C	508	65/65	0.95	0.12	24,38,99,119	0
28	LHG	d	409	39/49	0.95	0.12	30,45,75,83	0
24	BCR	b	617	40/40	0.95	0.12	28,40,50,53	0
22	CLA	b	613	65/65	0.95	0.14	16,33,71,82	0
28	LHG	A	412	47/49	0.95	0.13	26,49,84,100	0
22	CLA	A	403	65/65	0.95	0.13	22,33,88,98	0
24	BCR	a	405	40/40	0.95	0.09	23,33,43,46	0
24	BCR	C	516	40/40	0.95	0.15	33,48,64,65	0
22	CLA	c	505	65/65	0.95	0.17	23,40,71,74	0
22	CLA	B	609	65/65	0.95	0.13	24,36,56,65	0
22	CLA	b	612	65/65	0.95	0.16	20,33,47,54	0
22	CLA	C	504	59/65	0.95	0.11	27,40,82,87	0
24	BCR	T	101	40/40	0.95	0.09	23,36,52,54	0
22	CLA	C	509	65/65	0.95	0.17	25,42,62,65	0
22	CLA	b	604	65/65	0.95	0.12	17,37,86,98	0
22	CLA	b	611	65/65	0.95	0.13	21,32,55,60	0
22	CLA	B	610	65/65	0.95	0.14	20,32,40,47	0
22	CLA	c	503	65/65	0.95	0.14	27,42,53,57	0
24	BCR	B	617	40/40	0.95	0.11	25,38,57,65	0
22	CLA	A	406	54/65	0.95	0.11	17,32,63,66	0
22	CLA	b	614	65/65	0.95	0.12	23,37,75,82	0
24	BCR	c	515	40/40	0.95	0.10	28,41,58,63	0
35	HEC	F	101	43/43	0.96	0.11	31,45,59,61	0
22	CLA	D	402	65/65	0.96	0.11	15,28,52,62	0
30	DGD	c	517	62/66	0.96	0.10	20,42,74,76	0
26	PL9	d	407	55/55	0.96	0.11	18,34,43,47	0
22	CLA	b	607	65/65	0.96	0.12	19,35,69,74	0
22	CLA	b	605	65/65	0.96	0.12	20,34,50,55	0
22	CLA	c	501	65/65	0.96	0.13	28,38,50,55	0
28	LHG	a	410	49/49	0.96	0.13	28,48,77,84	0
23	PHO	a	403	64/64	0.96	0.12	19,29,37,48	0
22	CLA	d	404	65/65	0.96	0.11	19,28,45,54	0
29	SQD	A	413	52/54	0.96	0.15	34,58,103,107	0
22	CLA	a	402	65/65	0.96	0.10	17,28,49,59	0
22	CLA	B	603	65/65	0.96	0.15	18,31,65,69	0
24	BCR	A	407	40/40	0.96	0.09	19,33,41,42	0
22	CLA	C	503	65/65	0.96	0.13	26,39,47,50	0
22	CLA	b	603	65/65	0.96	0.14	21,35,71,79	0
22	CLA	B	607	65/65	0.96	0.11	16,31,62,74	0
23	PHO	A	405	64/64	0.96	0.11	21,30,38,40	0
22	CLA	B	611	65/65	0.96	0.14	19,30,46,51	0
22	CLA	B	612	65/65	0.96	0.15	17,31,49,54	0

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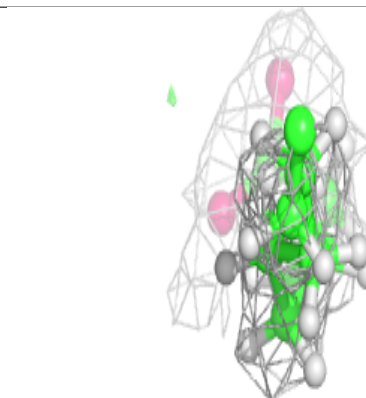
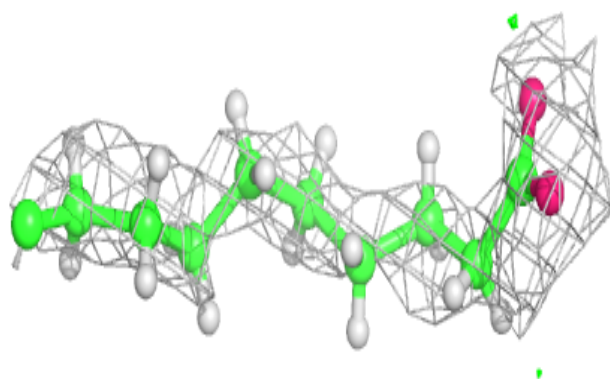
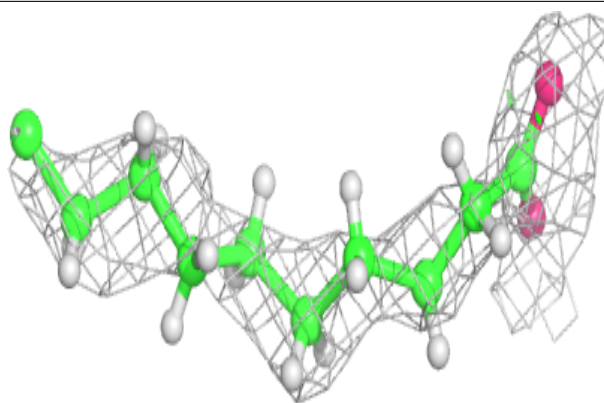
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	PHO	A	404	64/64	0.96	0.10	17,27,36,43	0
22	CLA	d	403	65/65	0.96	0.10	18,31,53,65	0
22	CLA	A	402	65/65	0.96	0.10	16,26,45,55	0
22	CLA	B	605	65/65	0.96	0.13	20,31,46,48	0
22	CLA	C	501	65/65	0.96	0.14	21,35,47,53	0
22	CLA	D	403	65/65	0.96	0.10	18,27,44,55	0
23	PHO	d	402	64/64	0.96	0.10	25,35,45,52	0
28	LHG	B	621	49/49	0.97	0.11	25,39,58,66	0
22	CLA	B	608	65/65	0.97	0.12	17,32,54,58	0
28	LHG	d	408	49/49	0.97	0.09	25,40,51,57	0
35	HEC	f	101	43/43	0.97	0.12	36,52,70,71	0
28	LHG	D	409	49/49	0.97	0.10	22,39,51,55	0
28	LHG	l	101	49/49	0.97	0.09	27,42,52,59	0
28	LHG	B	622	49/49	0.97	0.10	29,43,69,78	0
35	HEC	V	201	43/43	0.98	0.12	22,31,40,41	0
34	BCT	D	401	4/4	0.98	0.19	29,31,31,37	0
34	BCT	a	408	4/4	0.98	0.23	27,33,39,46	0
32	OEY	A	417[B]	11/11	0.98	0.13	18,21,25,25	11
35	HEC	v	201	43/43	0.98	0.13	25,36,44,46	0
31	OEX	A	416[A]	10/10	0.98	0.13	28,31,34,36	10
31	OEX	a	417[A]	10/10	0.99	0.10	25,31,35,35	10
32	OEY	a	418[B]	11/11	0.99	0.10	16,21,24,25	11
25	CL	a	406	1/1	0.99	0.05	26,26,26,26	0
25	CL	A	409	1/1	0.99	0.04	27,27,27,27	0
21	FE2	a	401	1/1	0.99	0.06	29,29,29,29	0
25	CL	A	408	1/1	0.99	0.06	28,28,28,28	0
25	CL	a	407	1/1	1.00	0.02	26,26,26,26	0
21	FE2	A	401	1/1	1.00	0.12	29,29,29,29	0

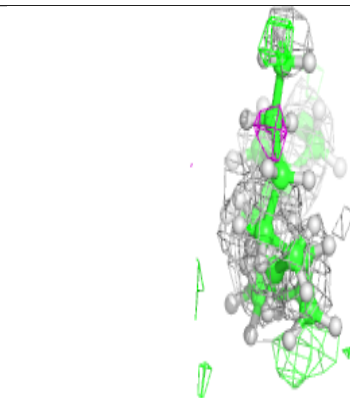
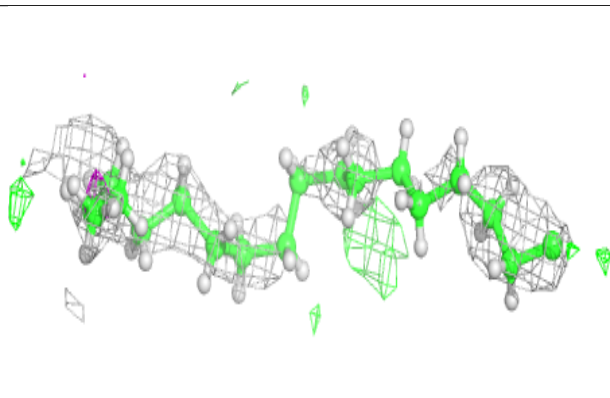
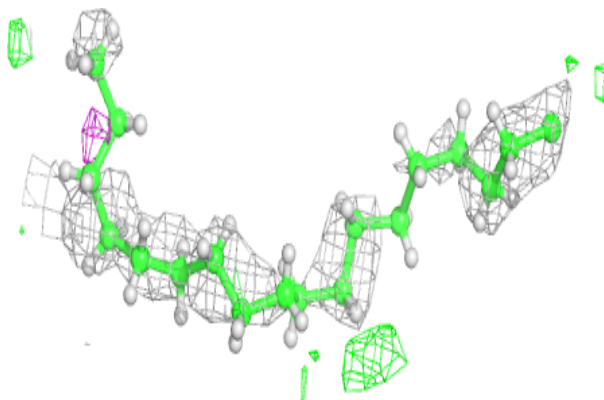
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around STE R 101:

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

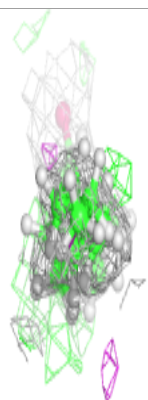
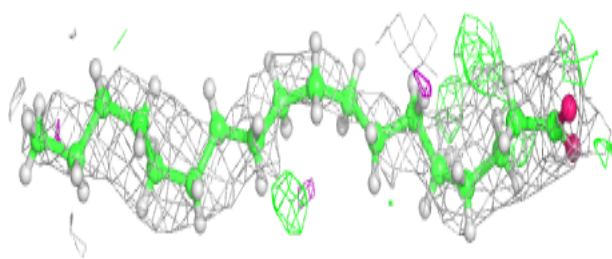
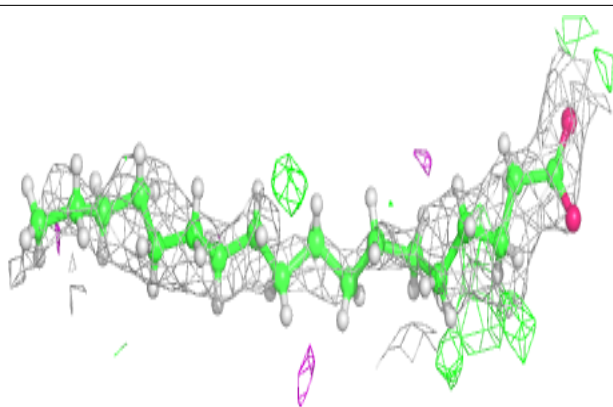
**Electron density around STE H 103:**

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

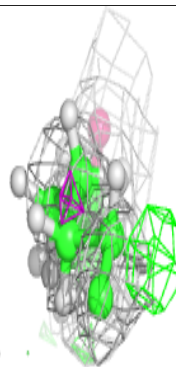
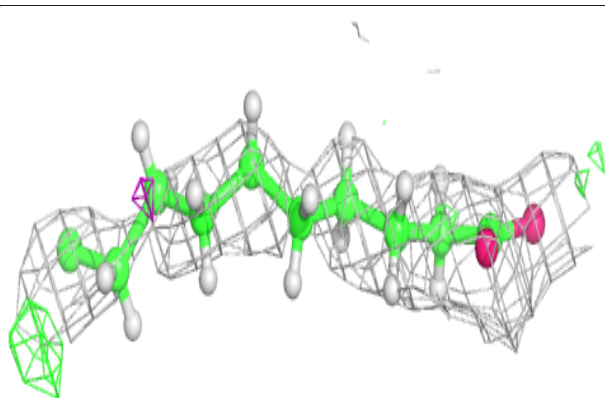
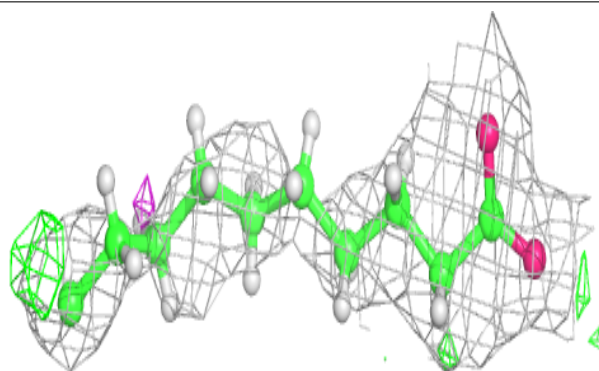


Electron density around STE b 625:

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

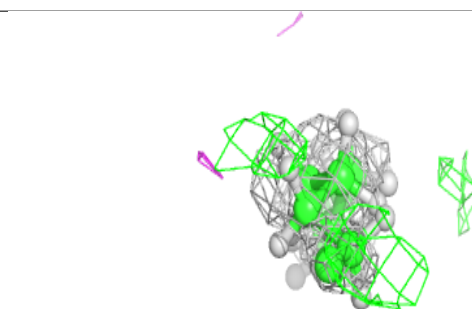
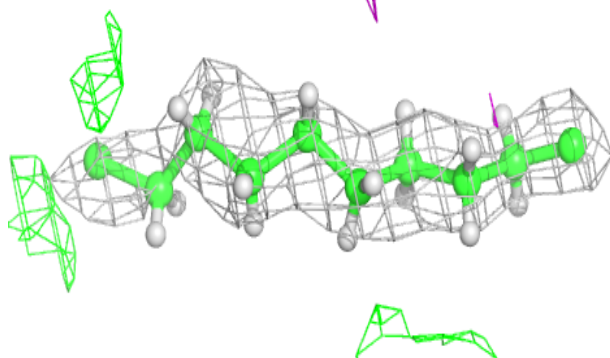
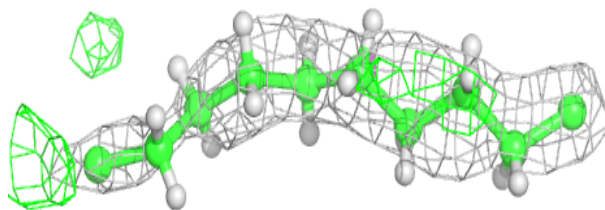
**Electron density around STE a 414:**

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

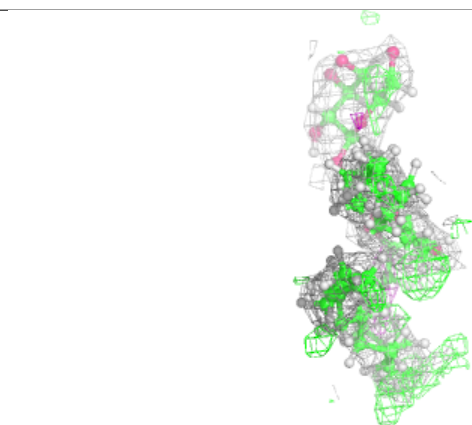
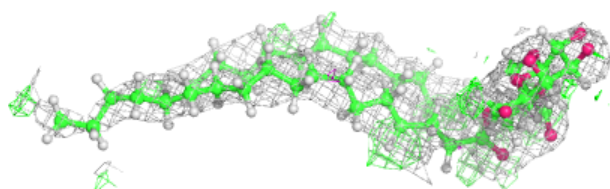
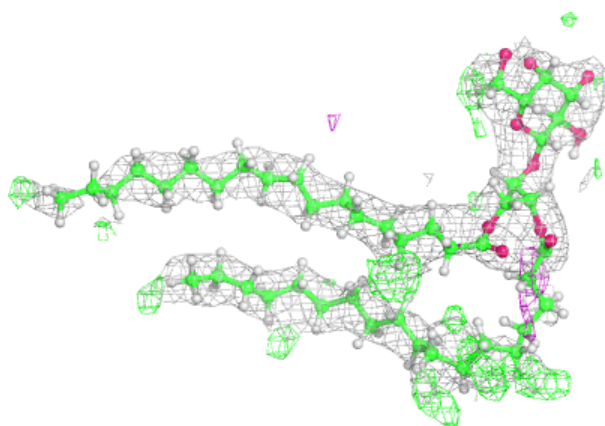


Electron density around STE a 413:

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

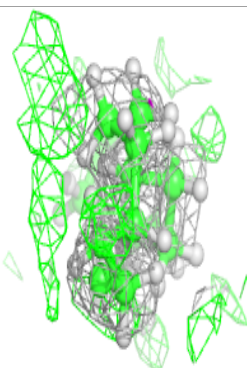
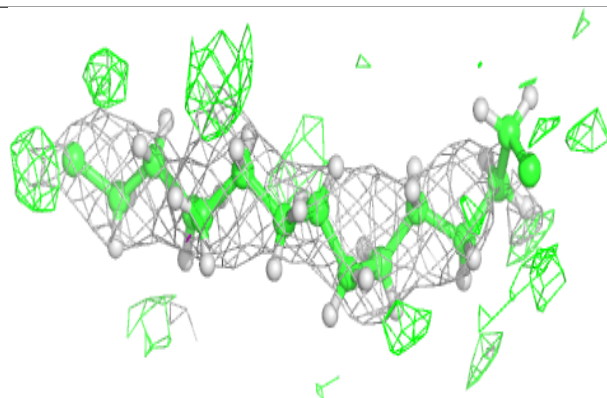
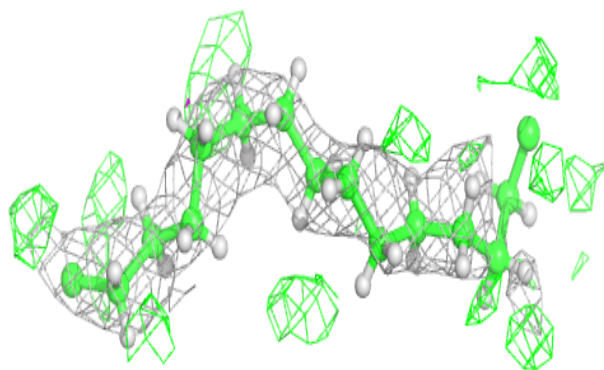
**Electron density around LMG a 416:**

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

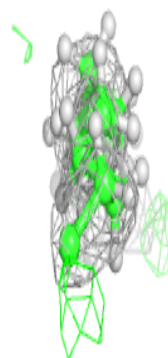
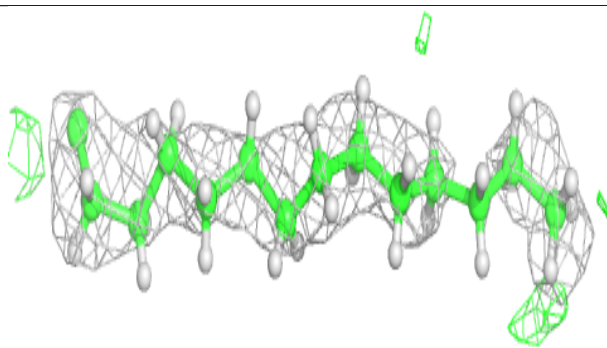
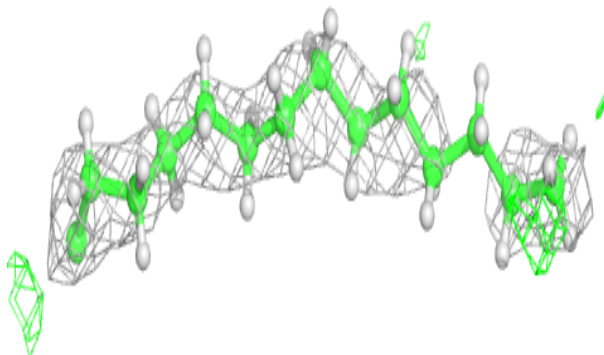


Electron density around STE a 415:

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

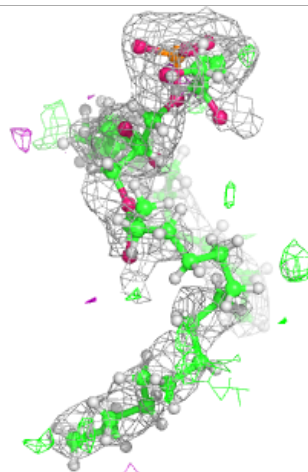
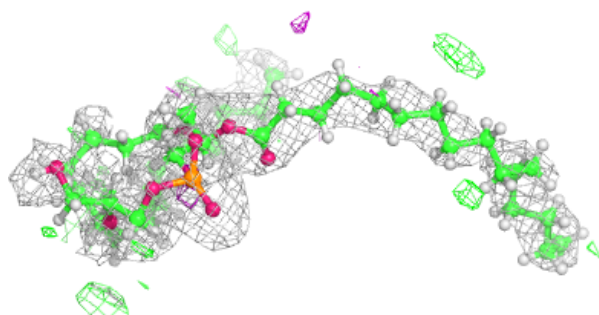
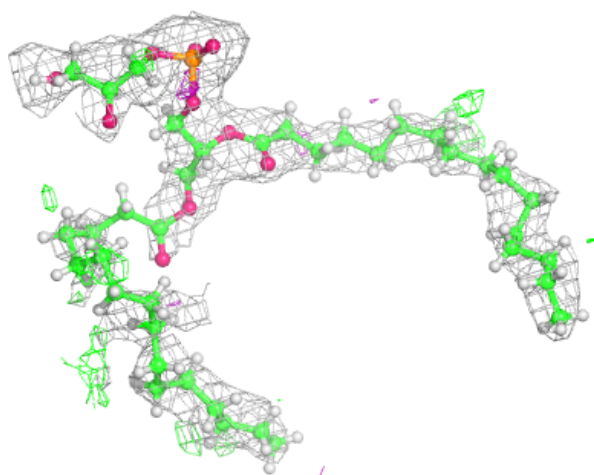
**Electron density around STE b 627:**

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



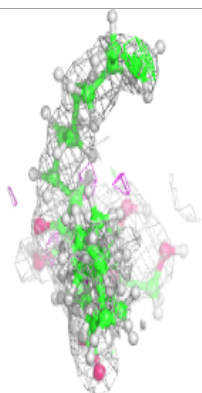
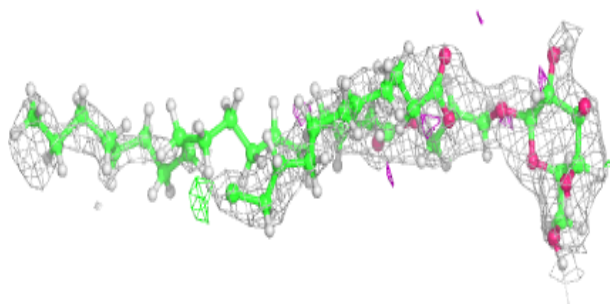
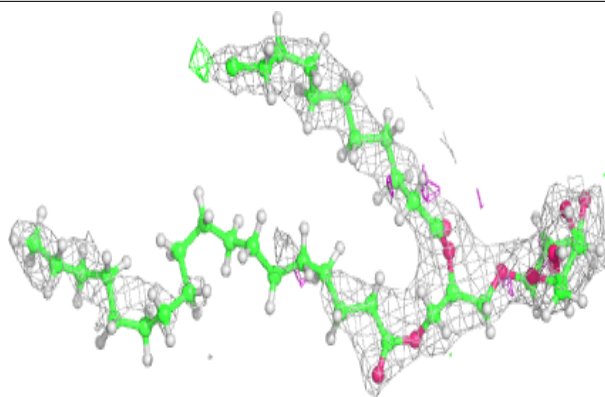
Electron density around LHG E 101:

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

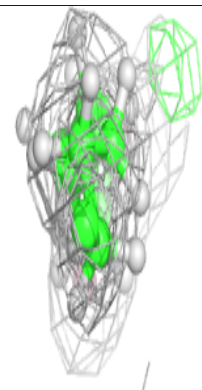
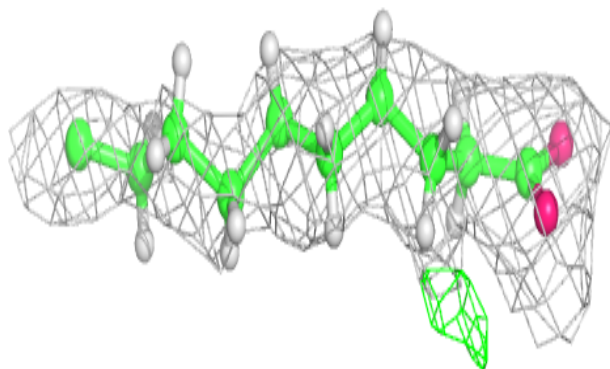
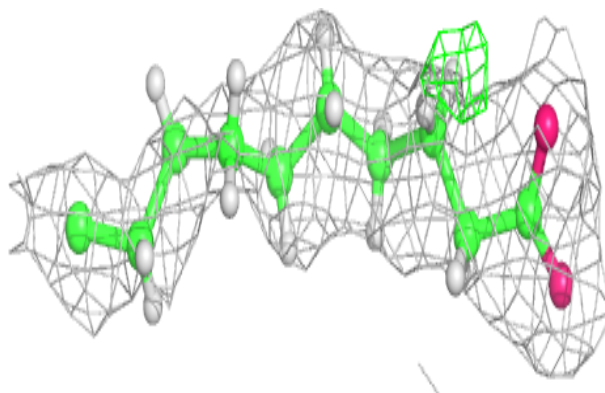


Electron density around LMG c 522:

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

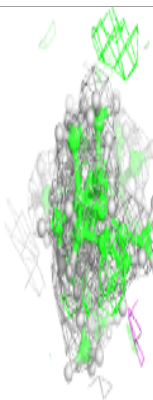
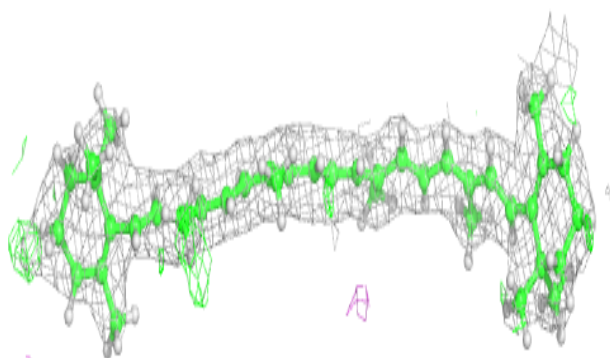
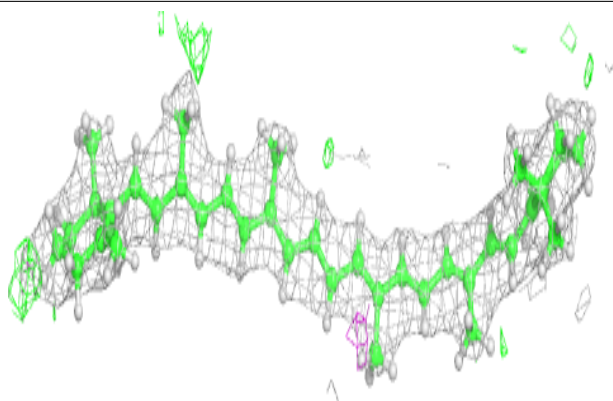
**Electron density around STE k 102:**

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

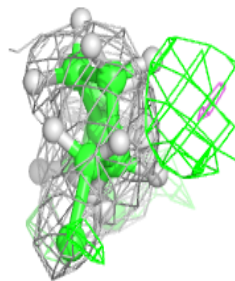
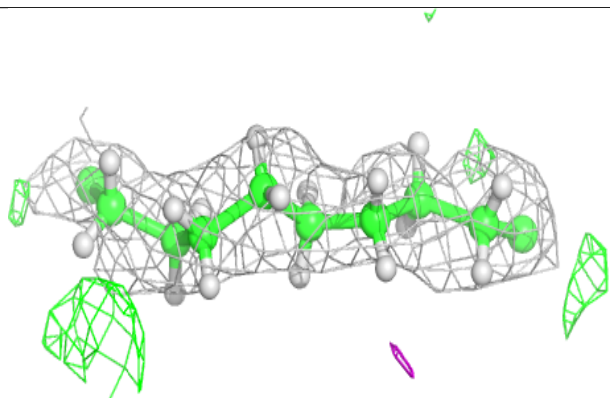
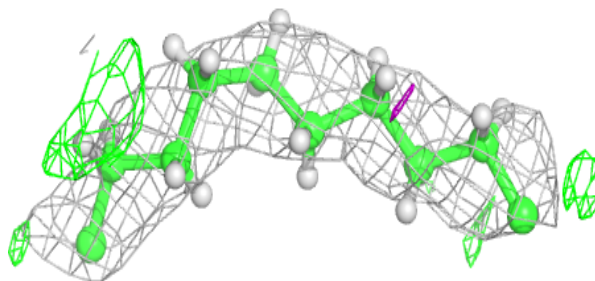


Electron density around BCR H 101:

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

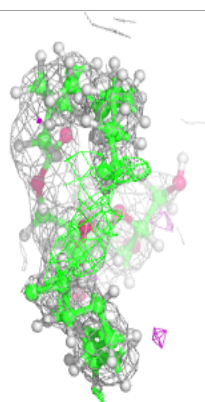
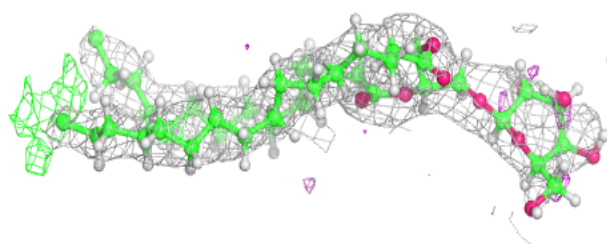
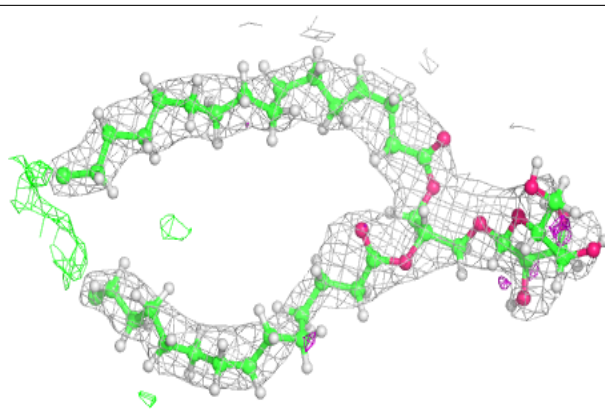
**Electron density around STE b 626:**

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

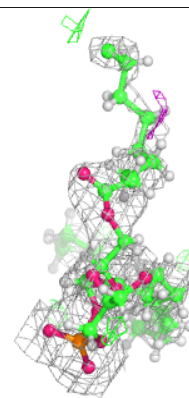
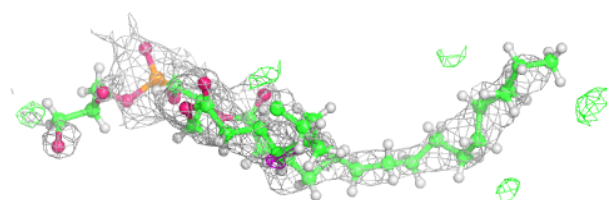
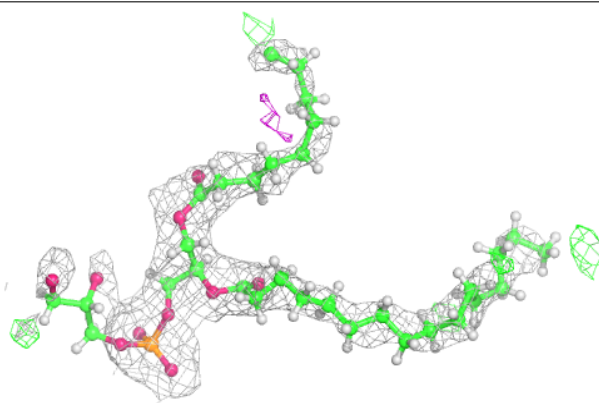


Electron density around LMG c 523:

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

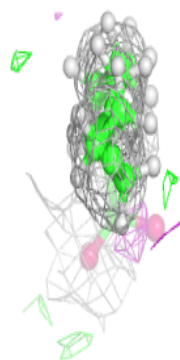
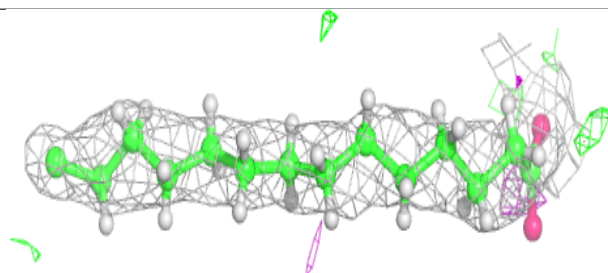
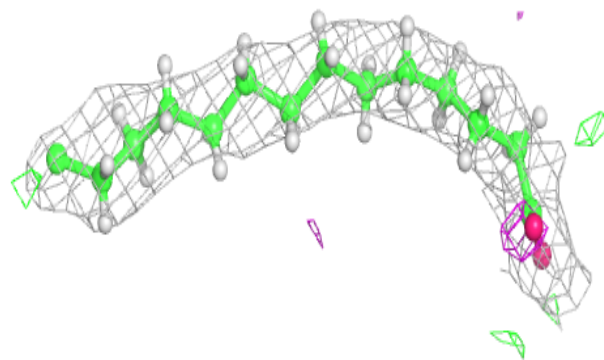
**Electron density around LHG e 101:**

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

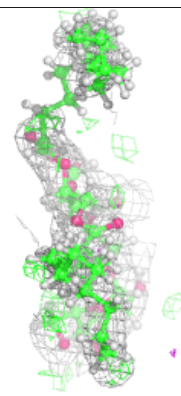
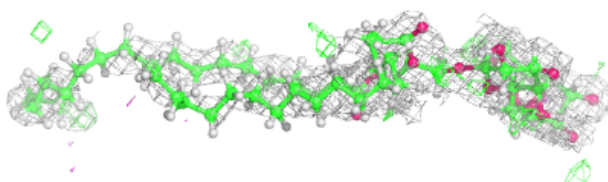
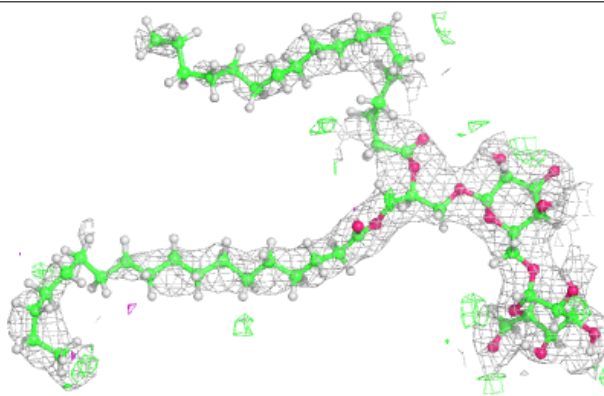


Electron density around STE b 624:

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

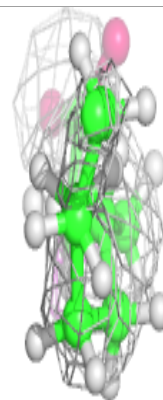
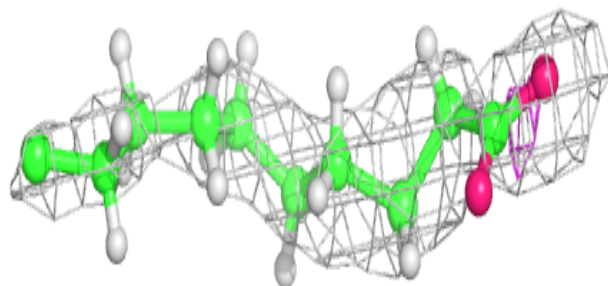
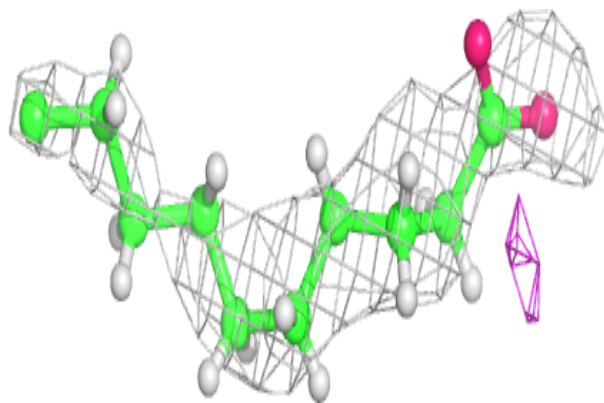
**Electron density around DGD A 415:**

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

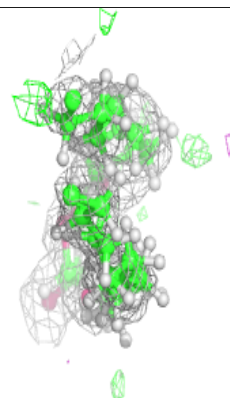
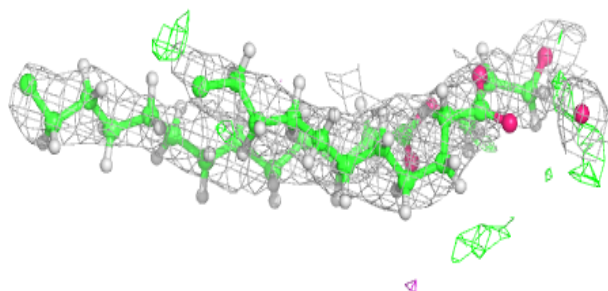
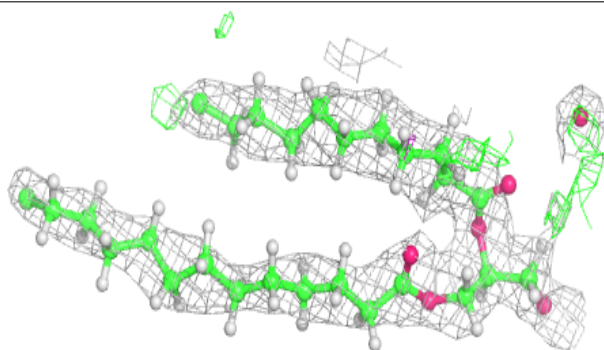


Electron density around STE B 626:

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

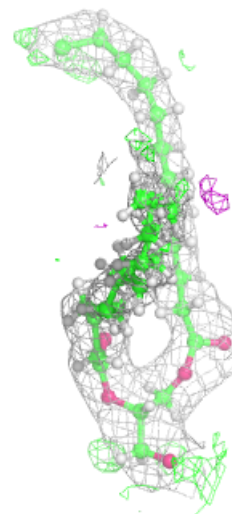
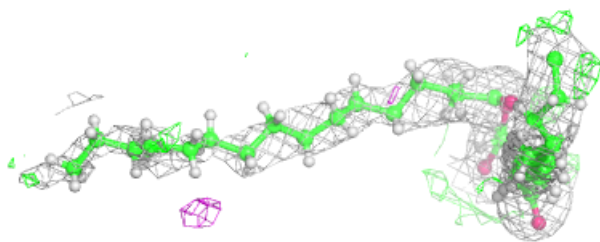
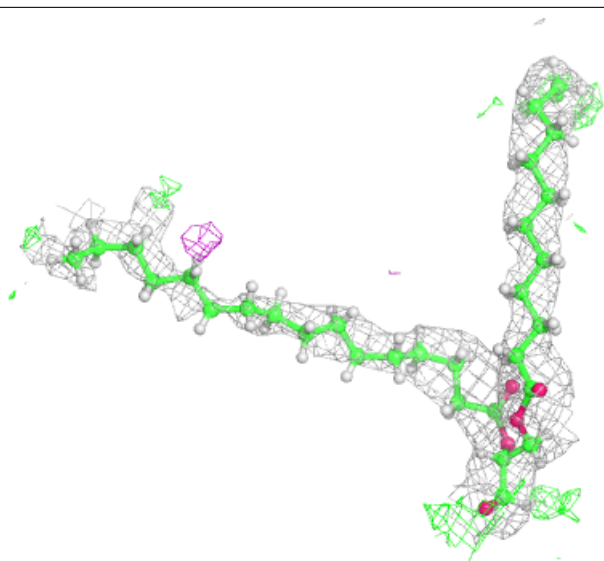
**Electron density around LMG D 410:**

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



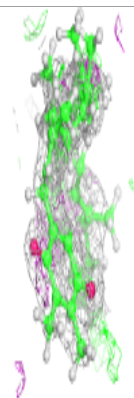
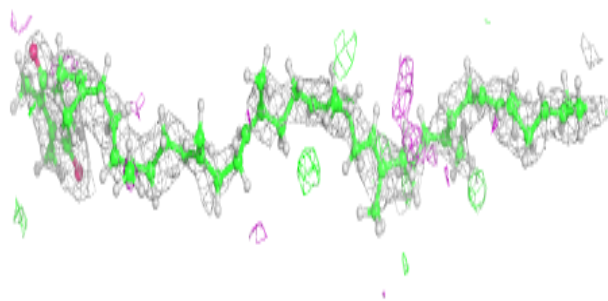
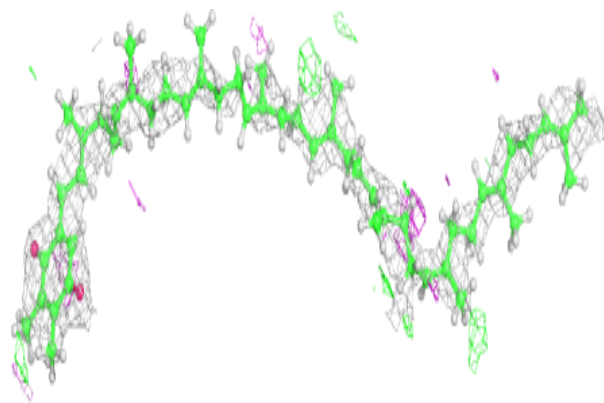
Electron density around SQD a 412:

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

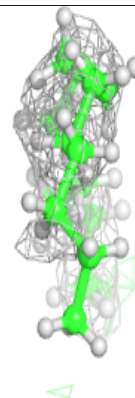
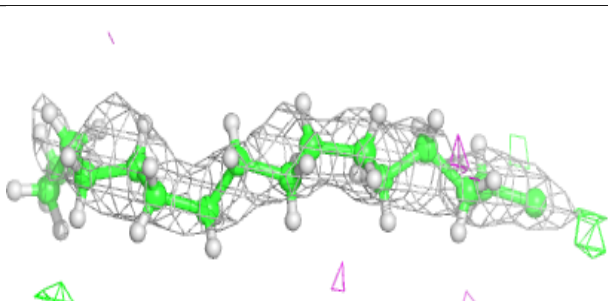
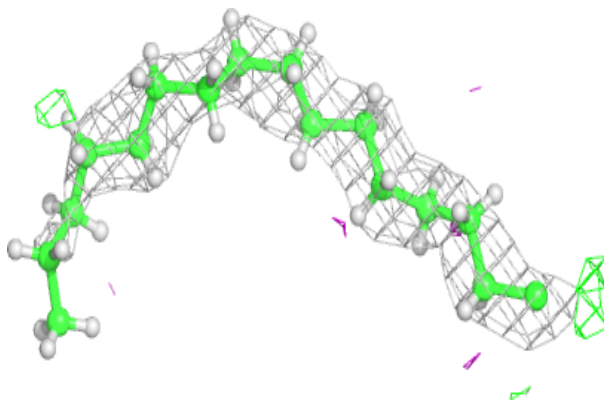


Electron density around PL9 A 410:

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

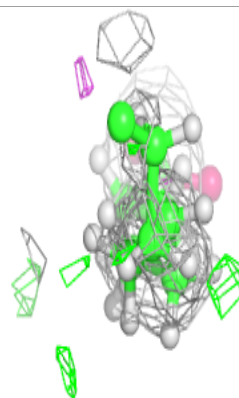
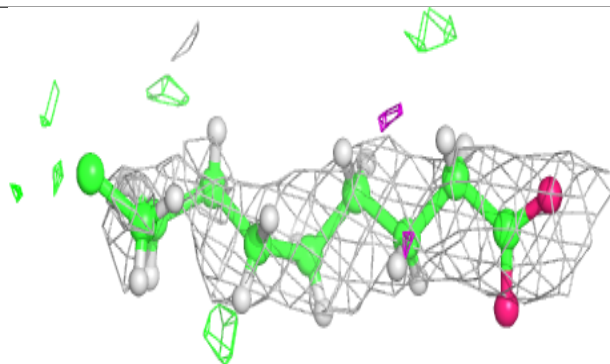
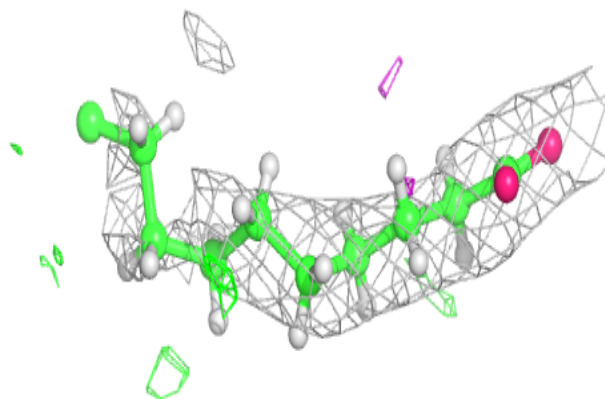
**Electron density around STE B 625:**

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



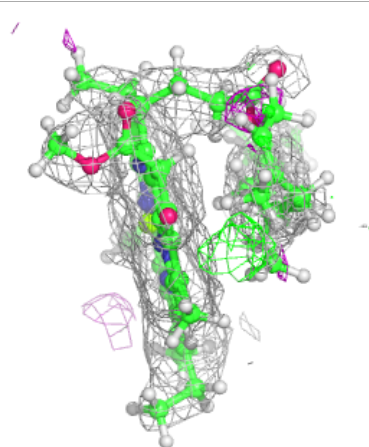
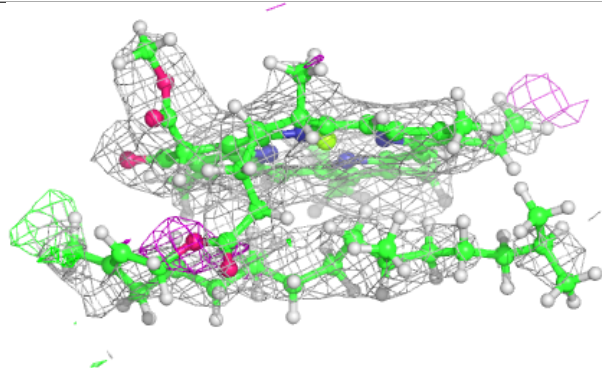
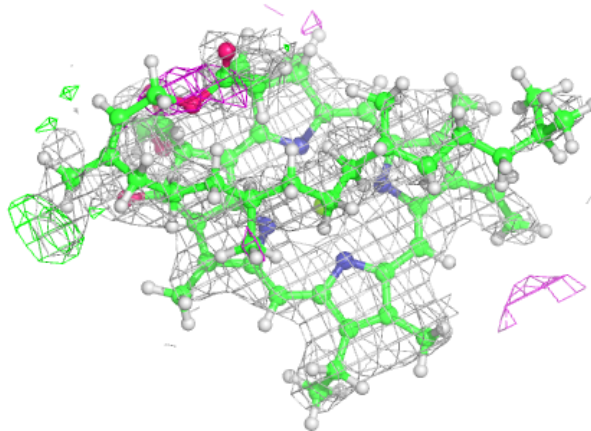
Electron density around STE m 102:

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



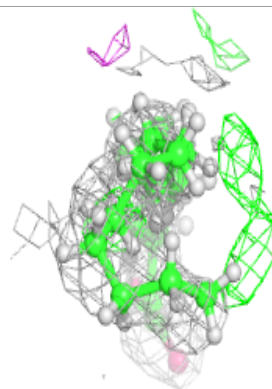
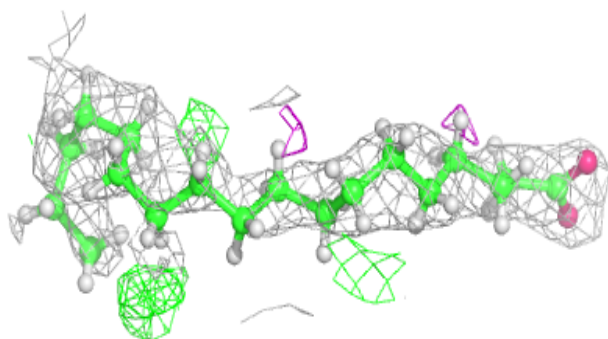
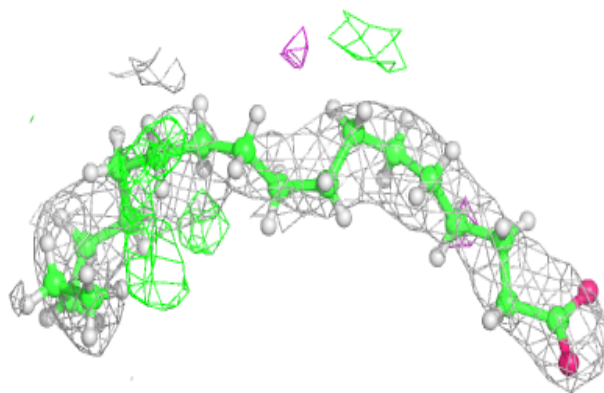
Electron density around CLA b 601:

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



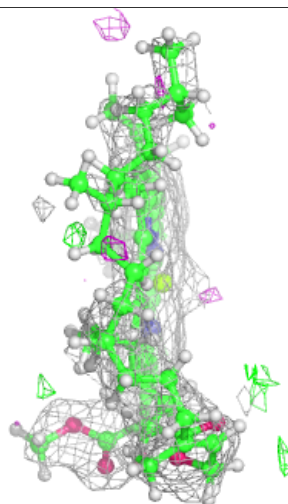
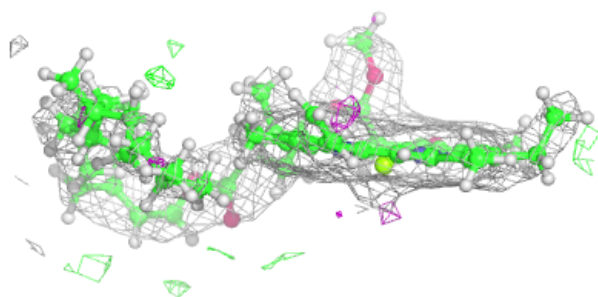
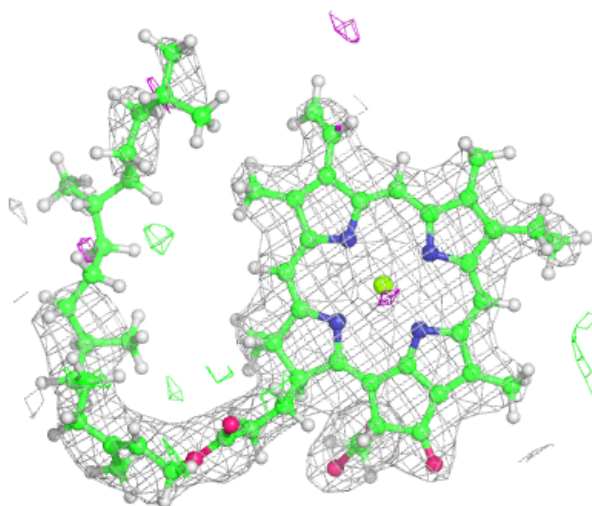
Electron density around STE d 413:

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



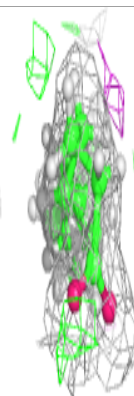
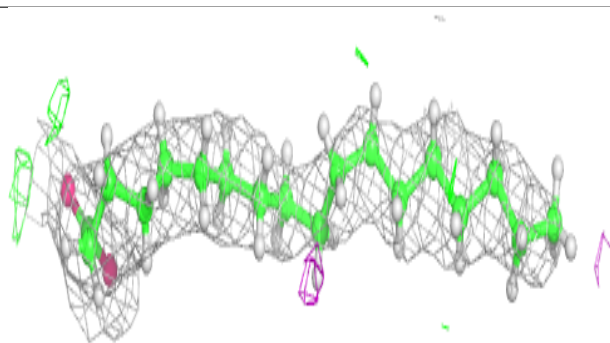
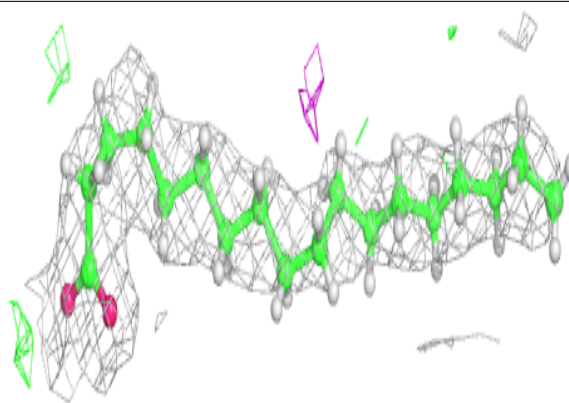
Electron density around CLA C 512:

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

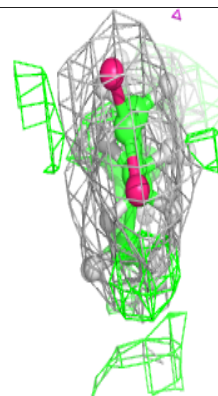
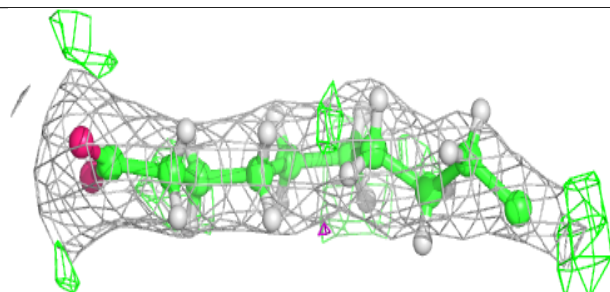
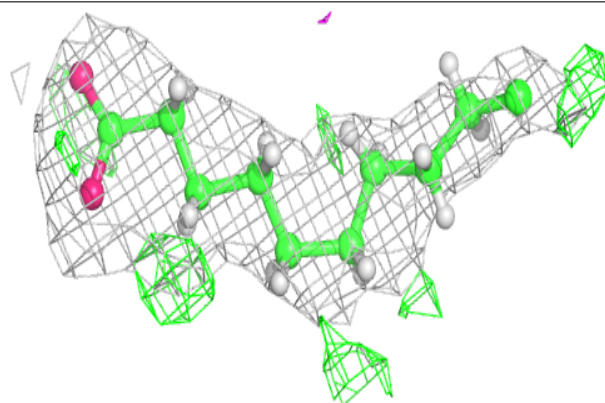


Electron density around STE c 521:

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

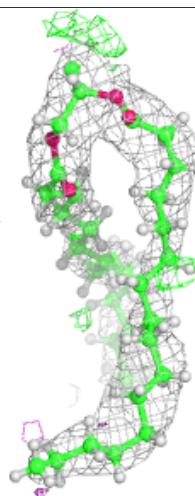
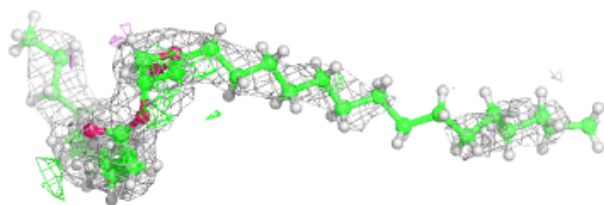
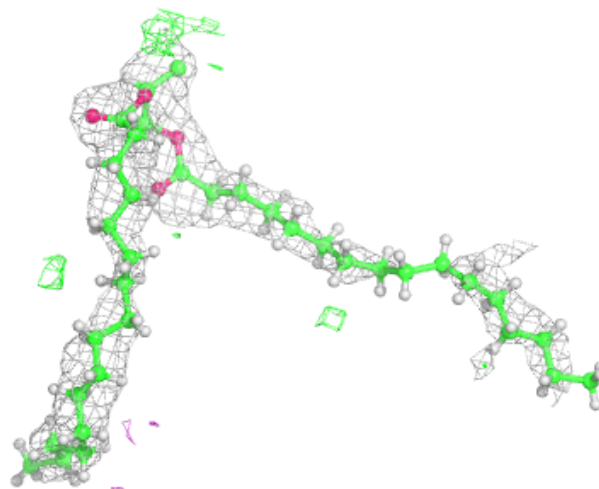
**Electron density around STE C 523:**

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



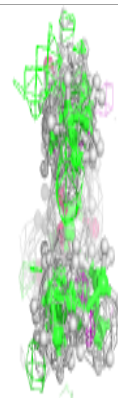
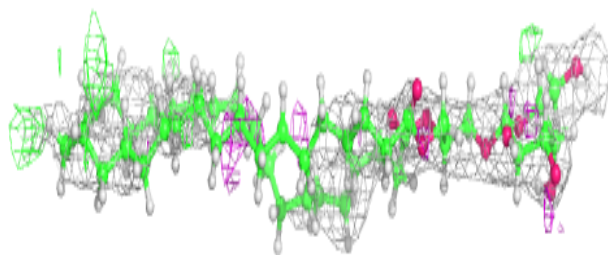
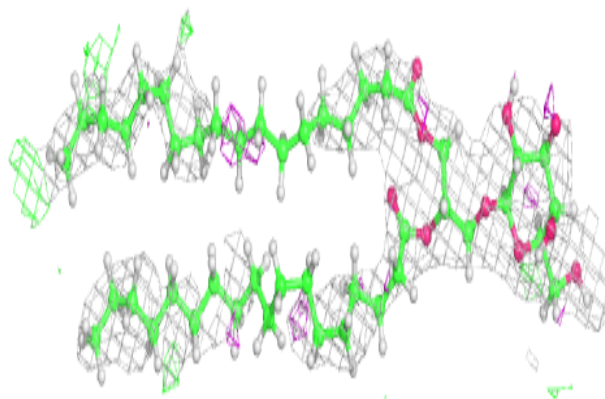
Electron density around SQD A 414:

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

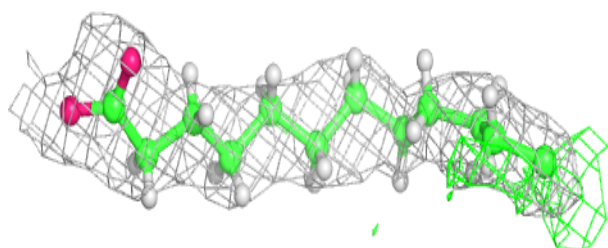
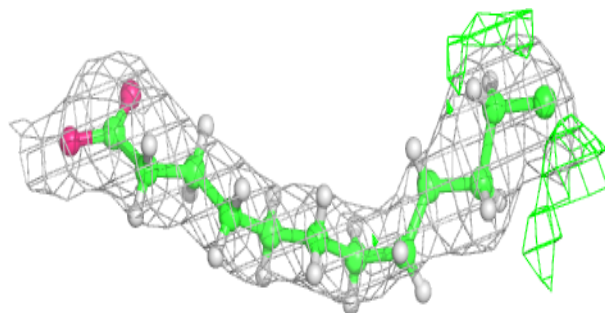


Electron density around LMG b 623:

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

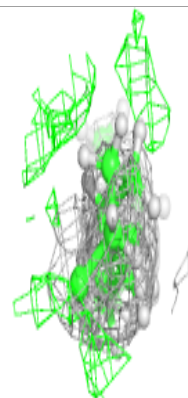
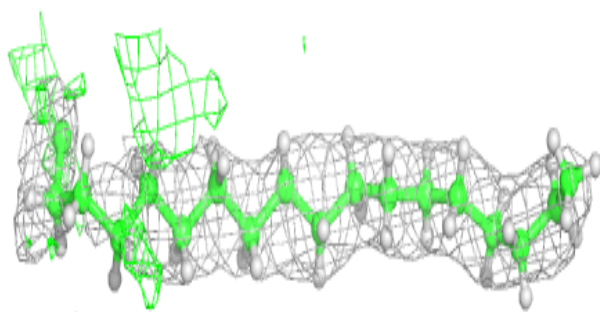
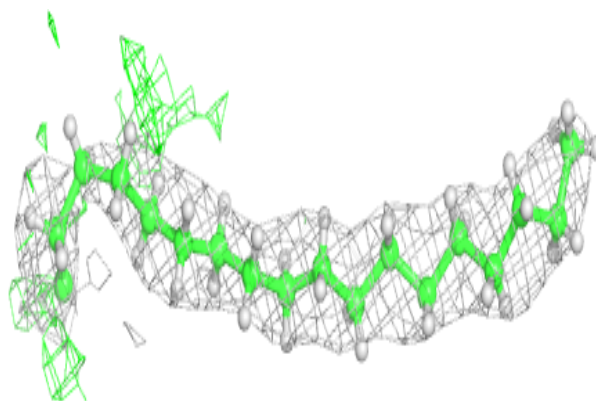
**Electron density around STE t 102:**

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

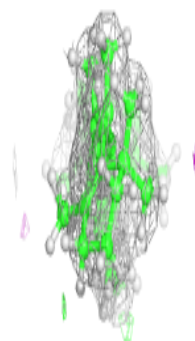
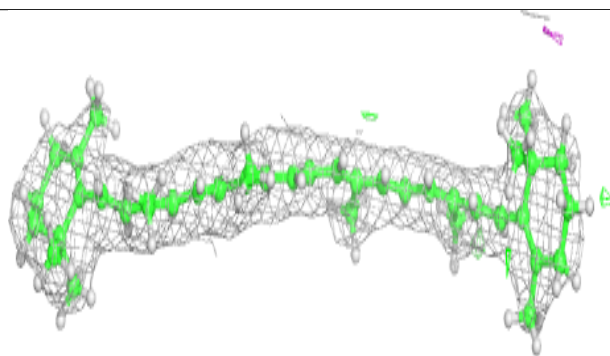
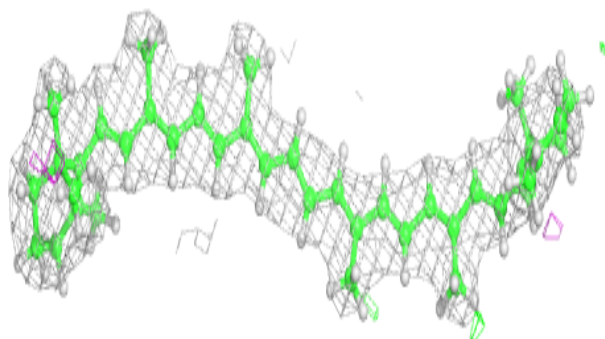


Electron density around STE I 102:

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

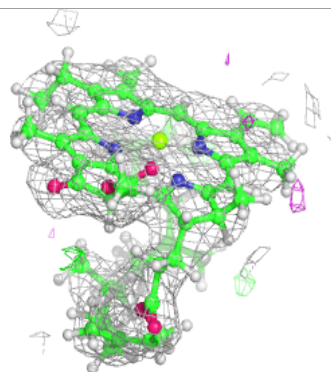
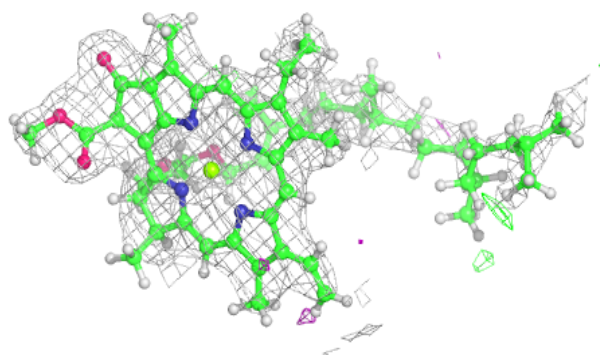
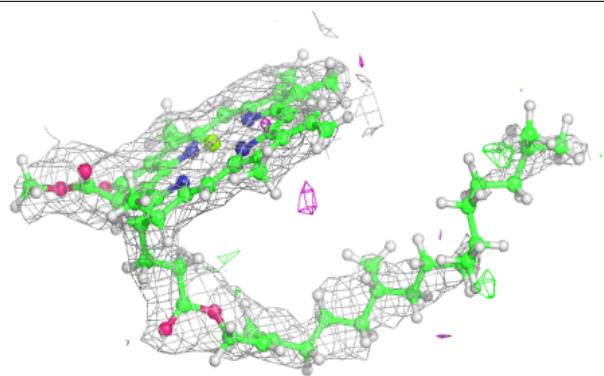
**Electron density around BCR Y 101:**

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

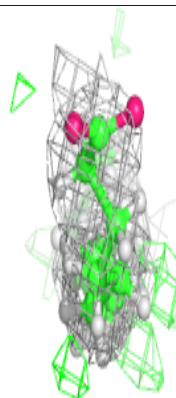
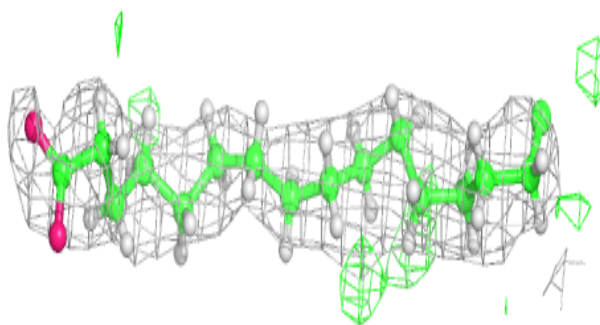
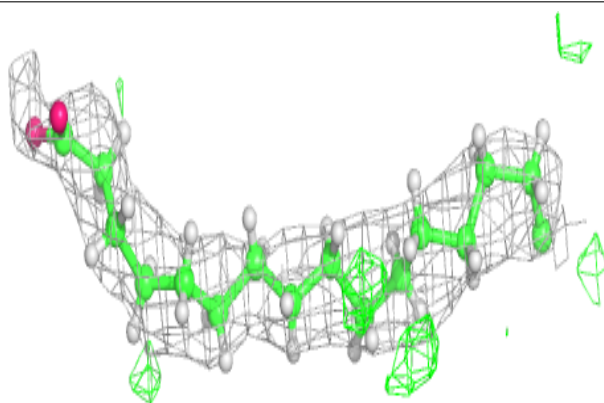


Electron density around CLA C 513:

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

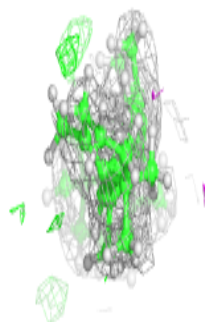
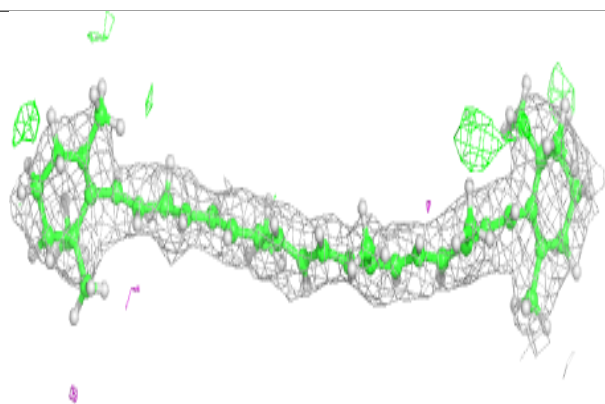
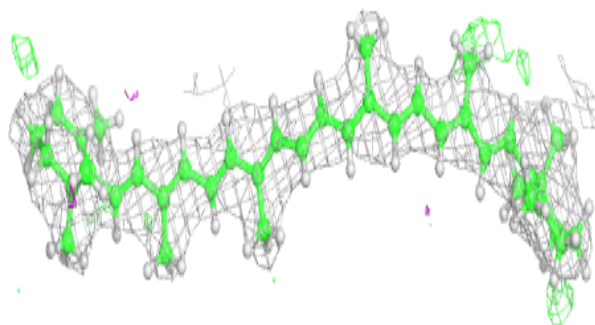
**Electron density around STE t 103:**

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

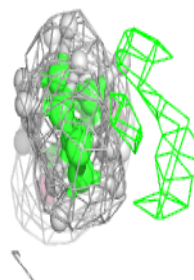
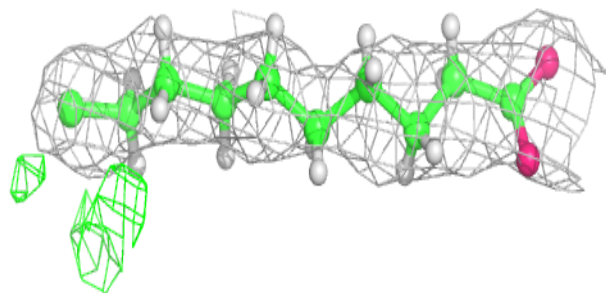
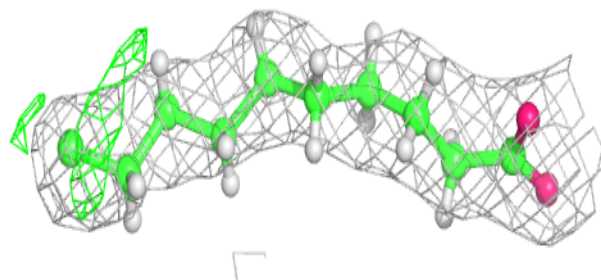


Electron density around BCR x 101:

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

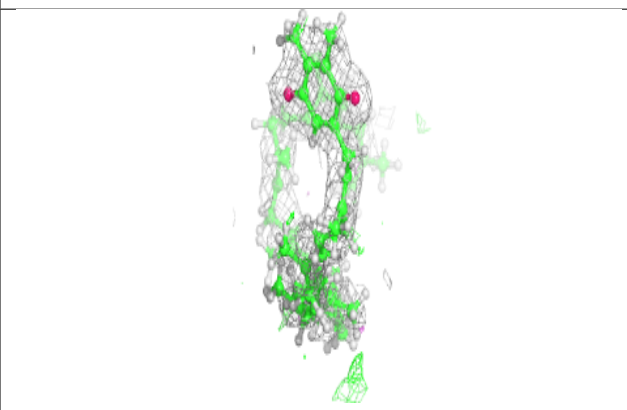
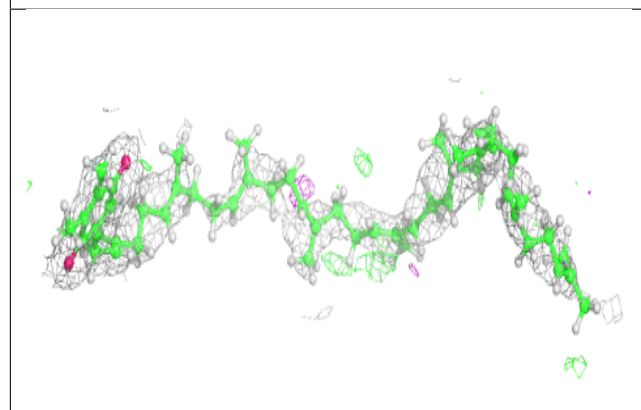
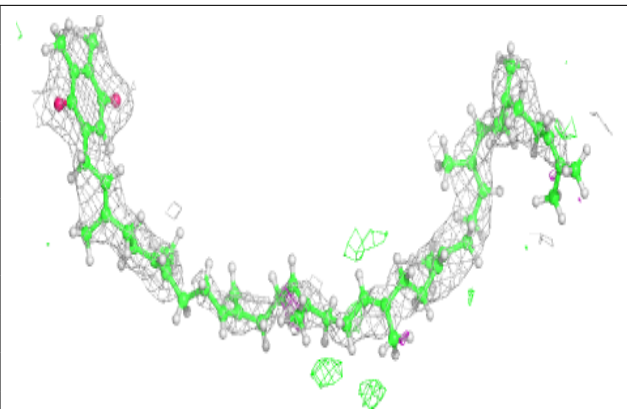
**Electron density around STE j 101:**

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

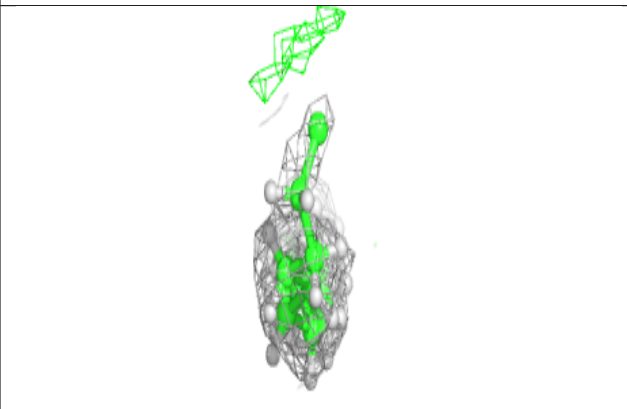
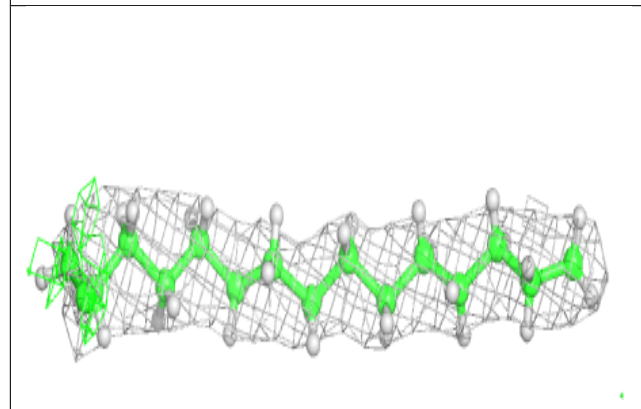
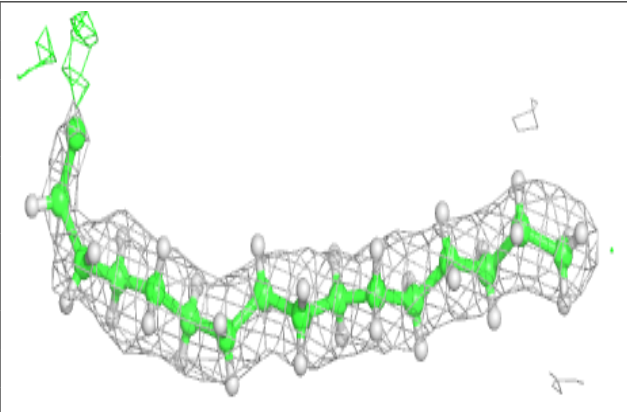


Electron density around PL9 a 409:

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

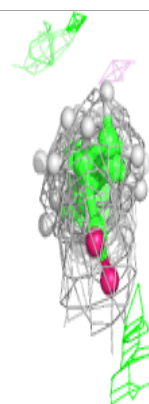
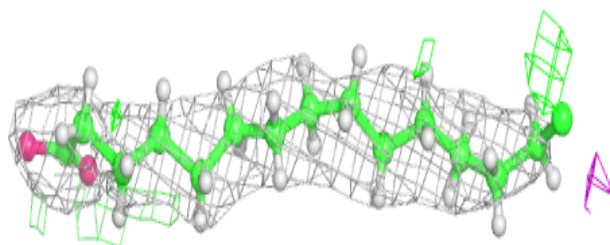
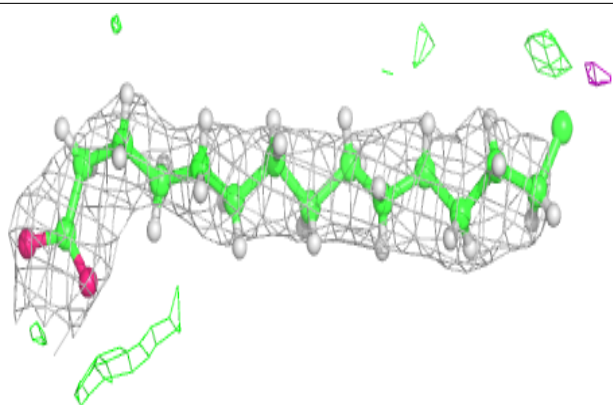
**Electron density around STE C 522:**

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

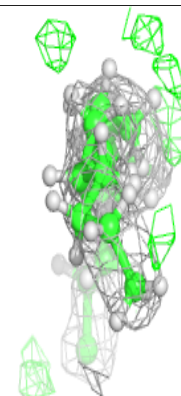
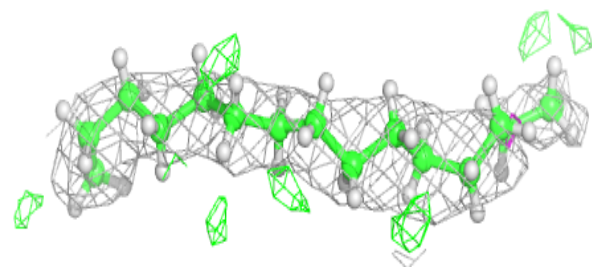
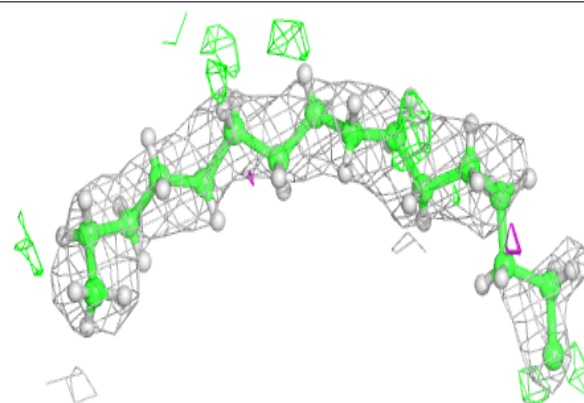


Electron density around STE d 411:

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

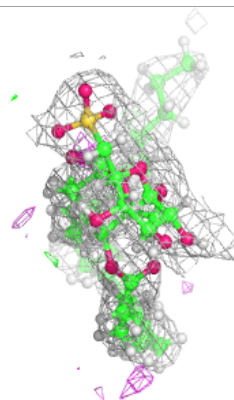
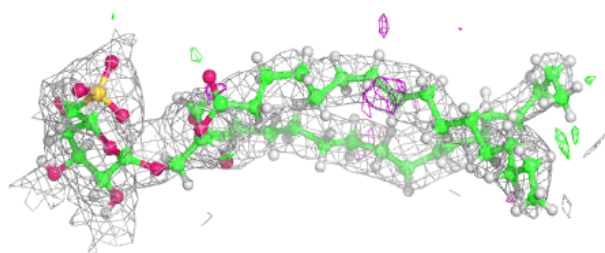
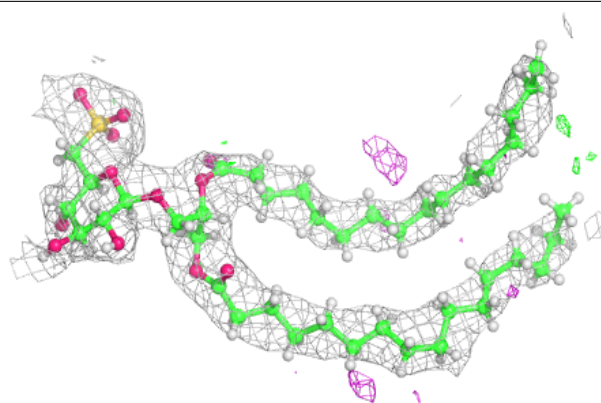
**Electron density around STE b 621:**

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

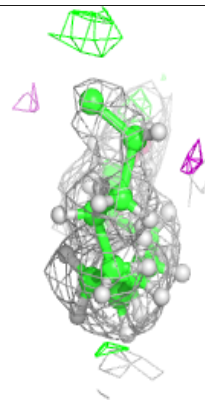
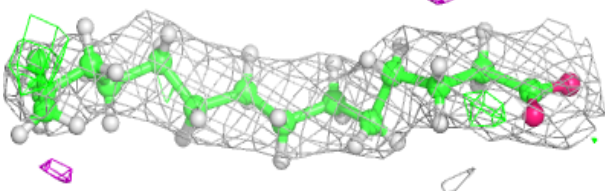
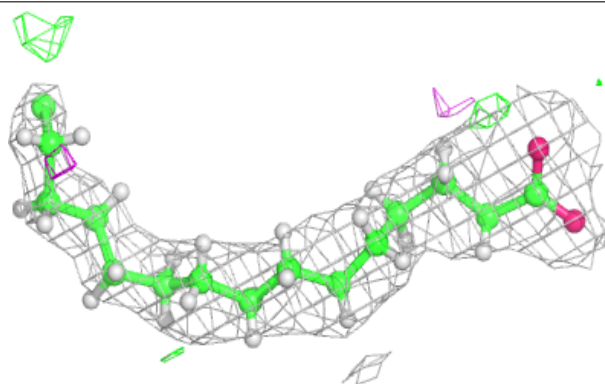


Electron density around SQD B 623:

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

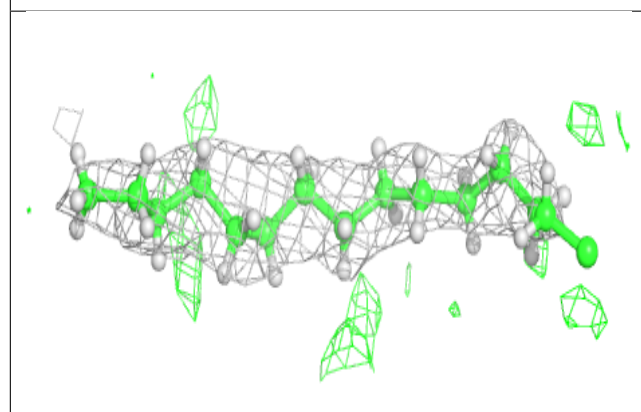
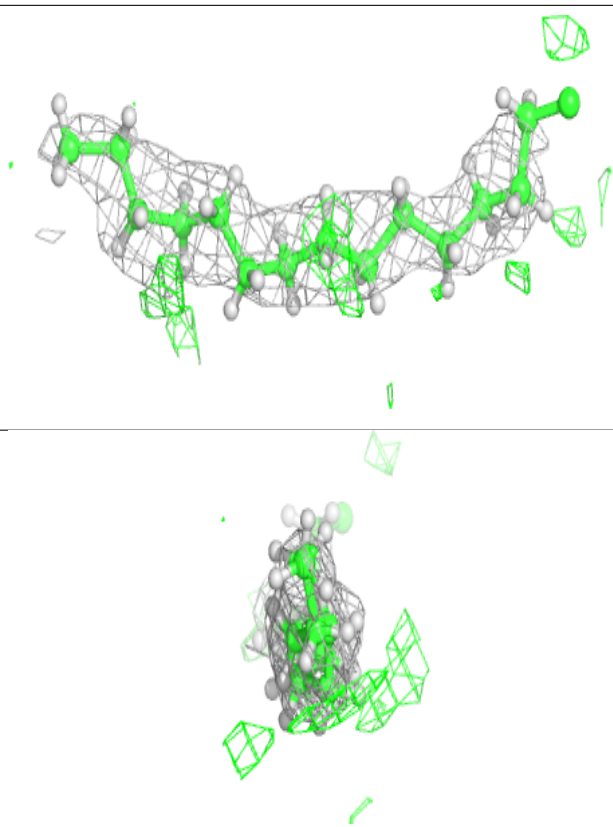
**Electron density around STE B 620:**

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

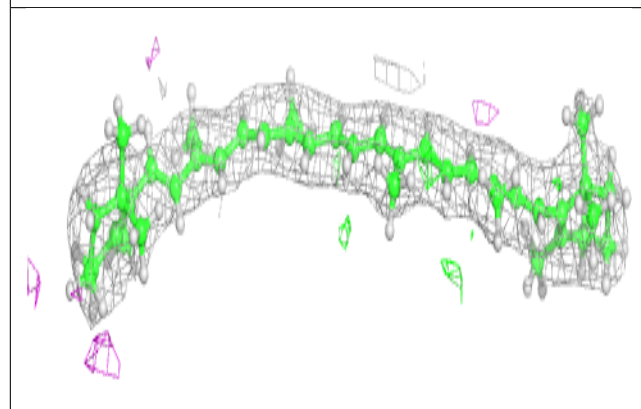
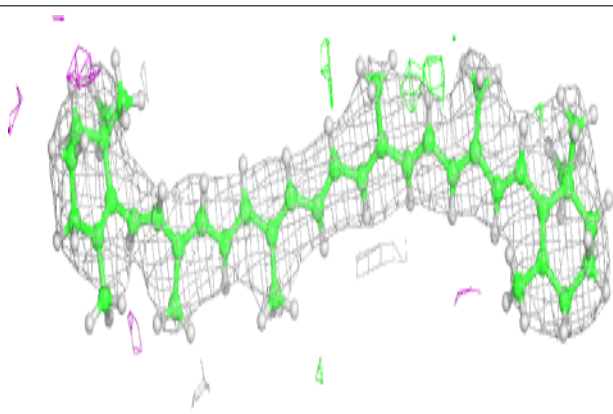


Electron density around STE T 102:

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

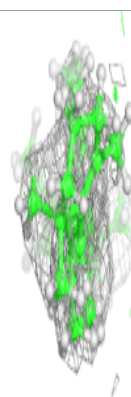
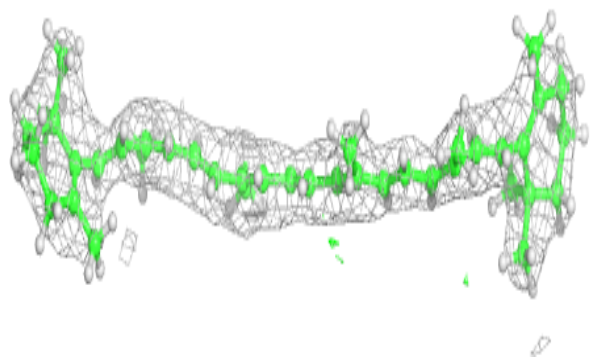
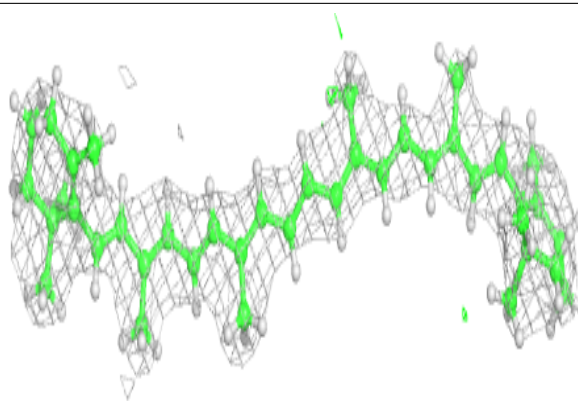
**Electron density around BCR d 406:**

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

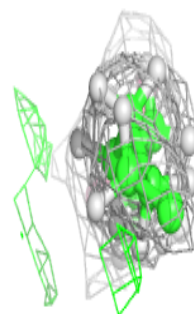
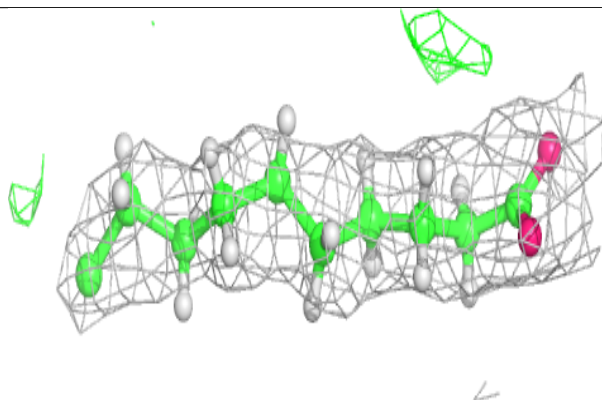
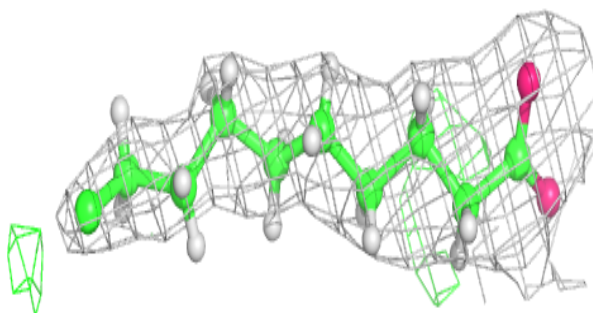


Electron density around BCR k 101:

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

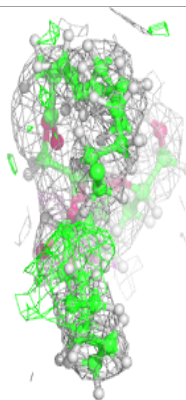
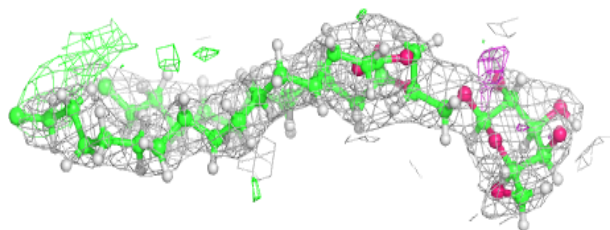
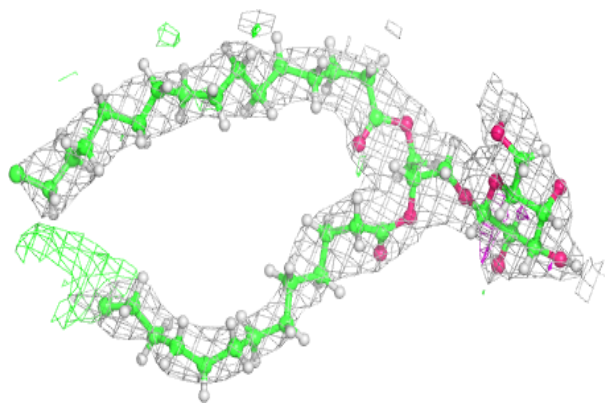
**Electron density around STE J 101:**

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

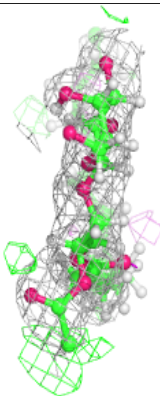
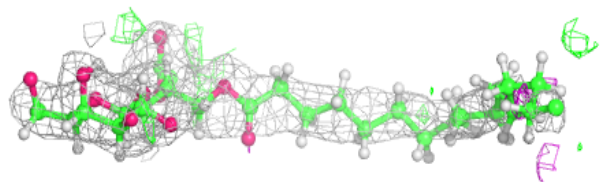
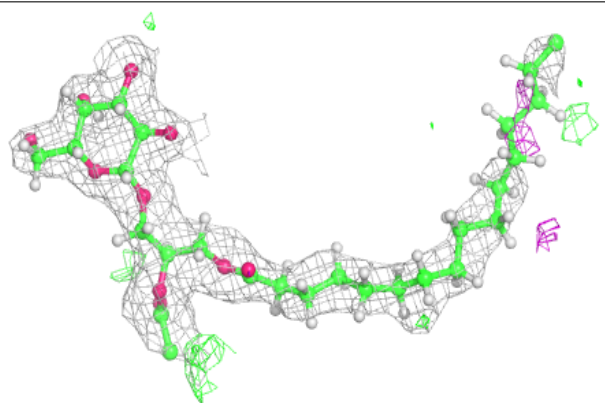


Electron density around LMG A 411:

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

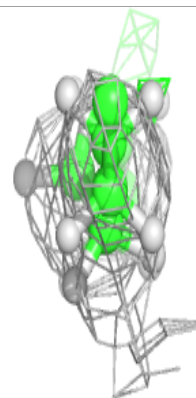
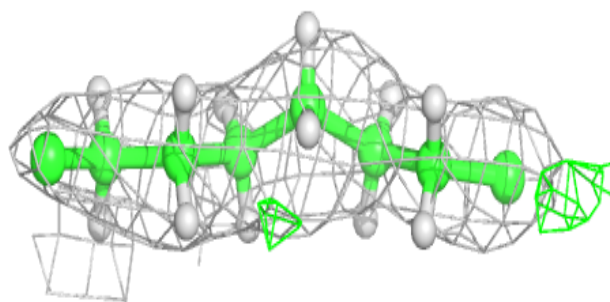
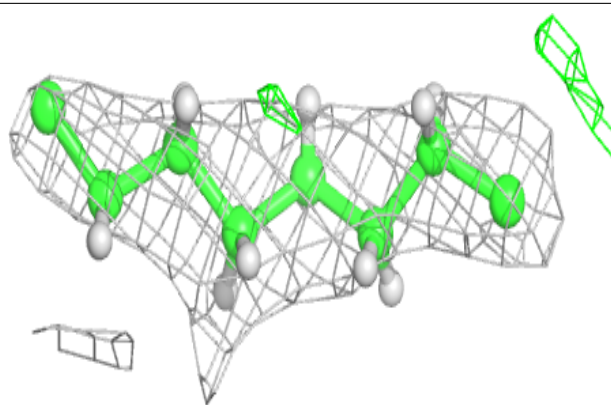
**Electron density around LMG c 520:**

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

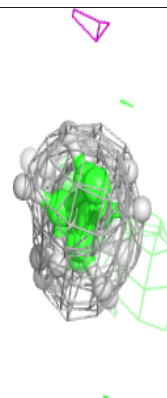
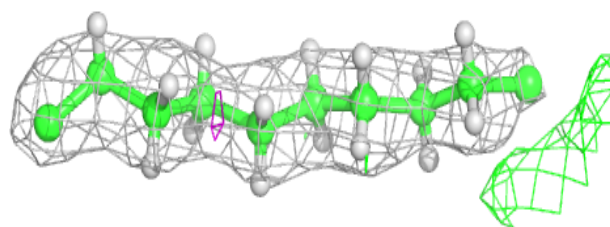
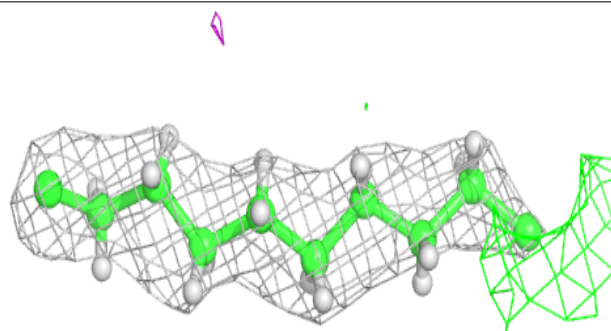


Electron density around STE Z 101:

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

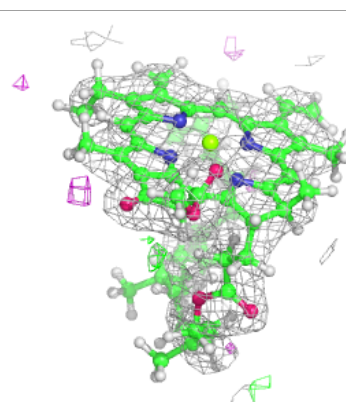
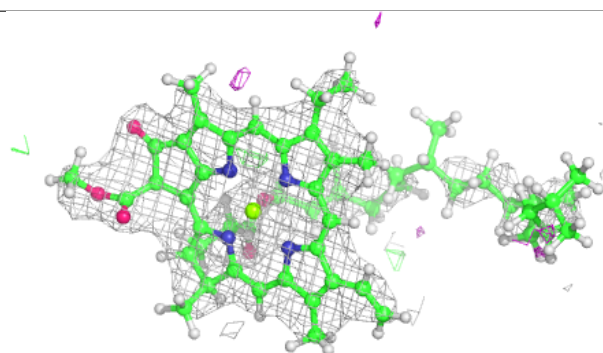
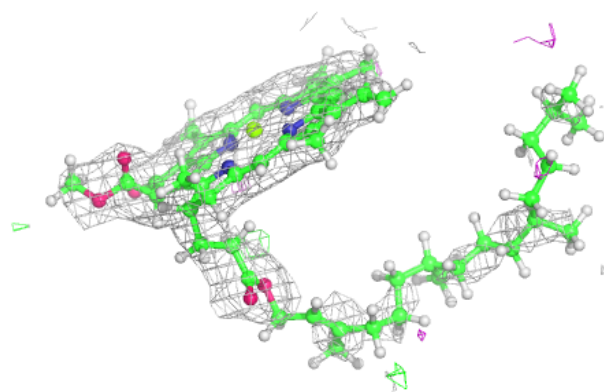
**Electron density around STE M 103:**

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

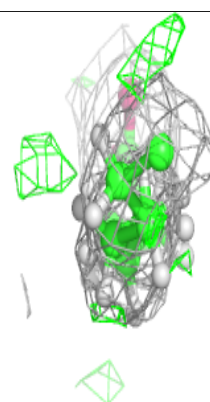
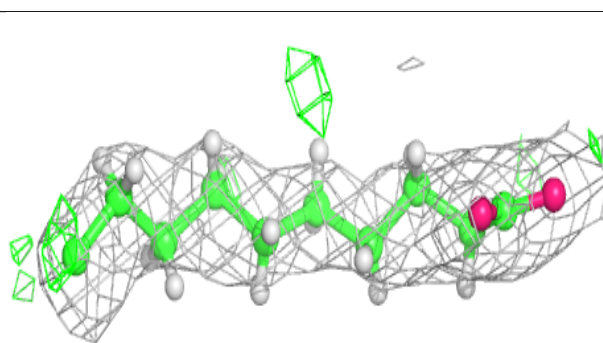
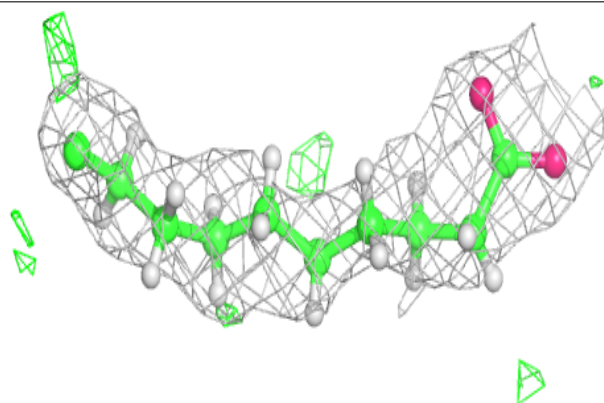


Electron density around CLA c 513:

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

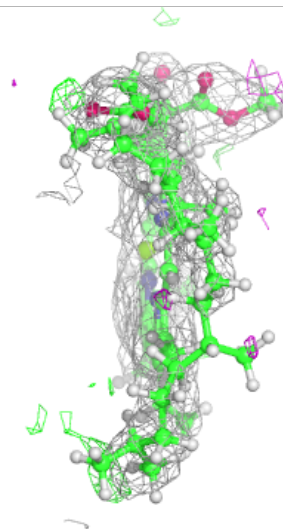
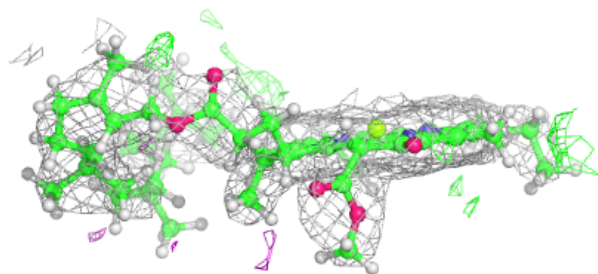
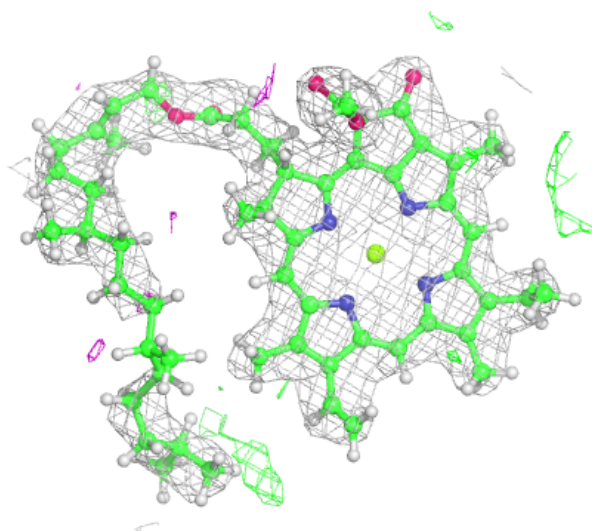
**Electron density around STE C 521:**

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



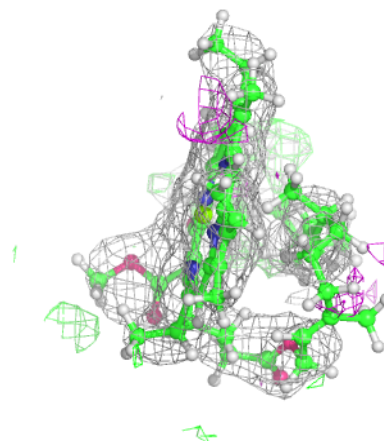
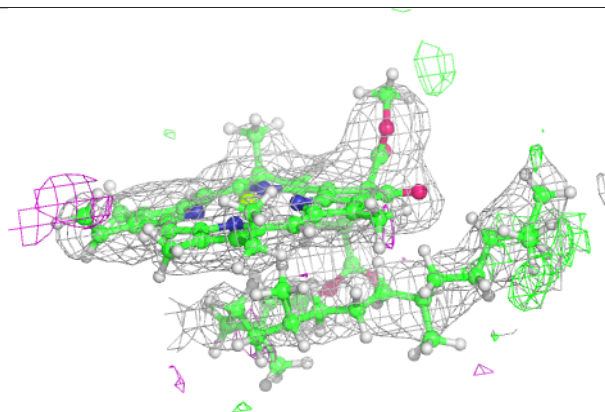
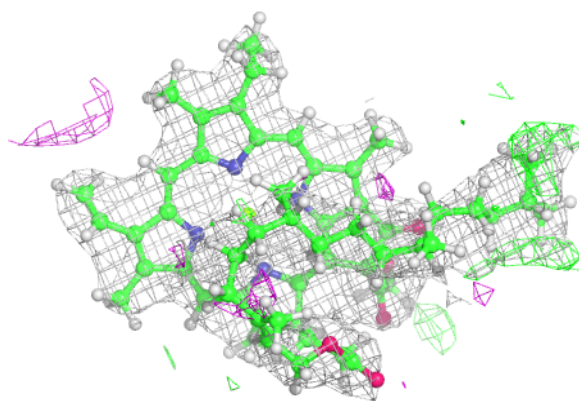
Electron density around CLA c 512:

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

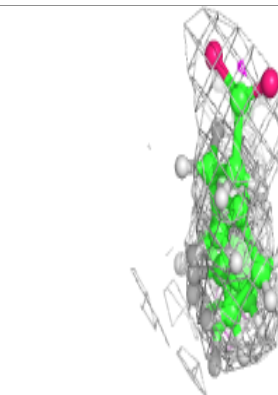
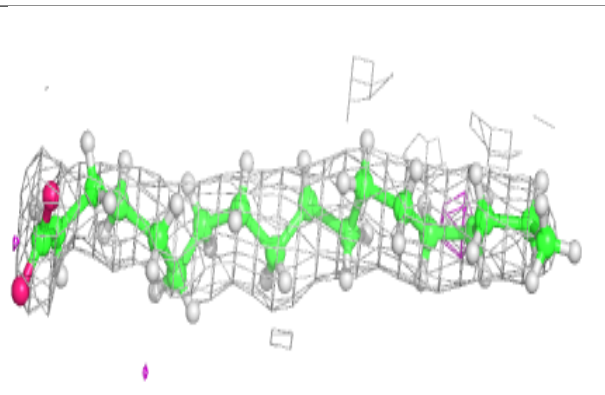
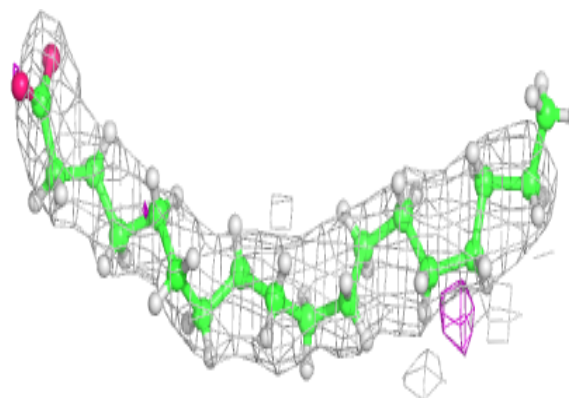


Electron density around CLA B 601:

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

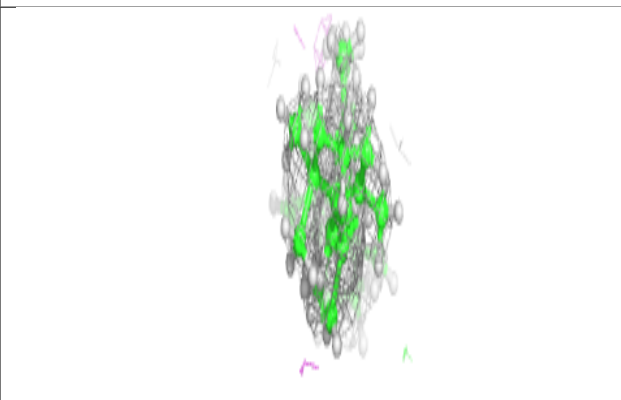
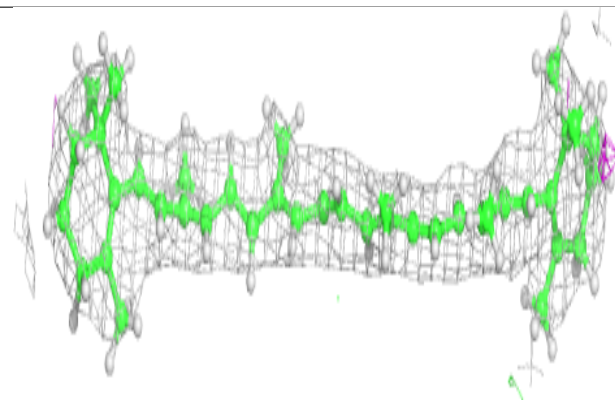
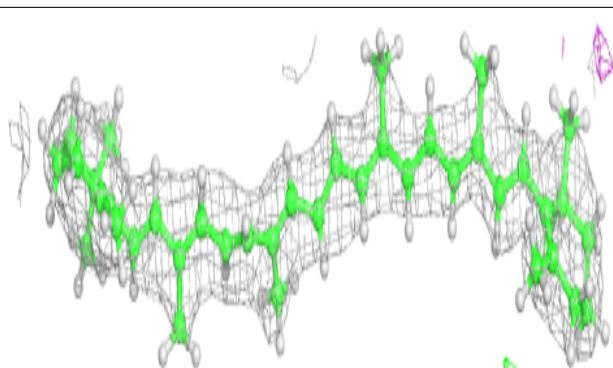
**Electron density around STE D 412:**

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

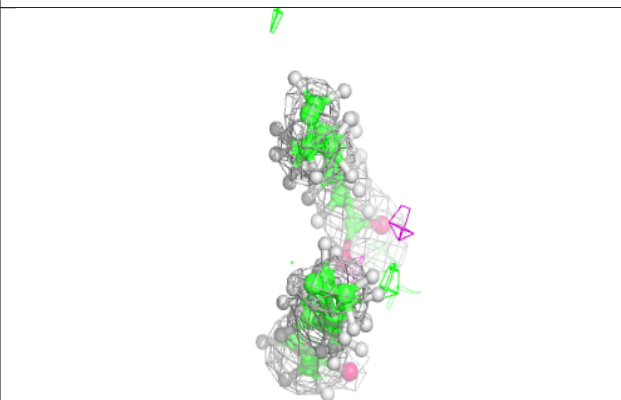
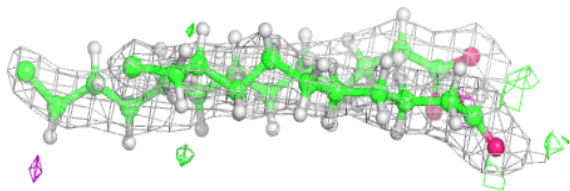
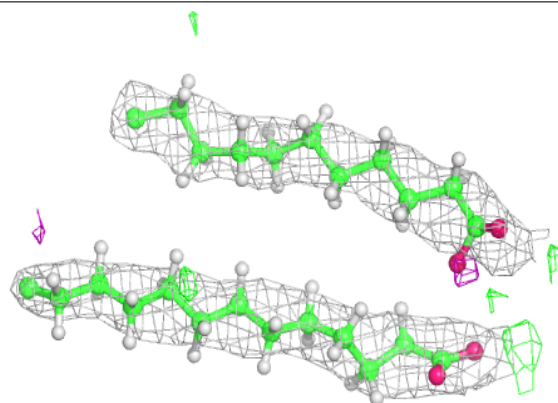


Electron density around BCR C 514:

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

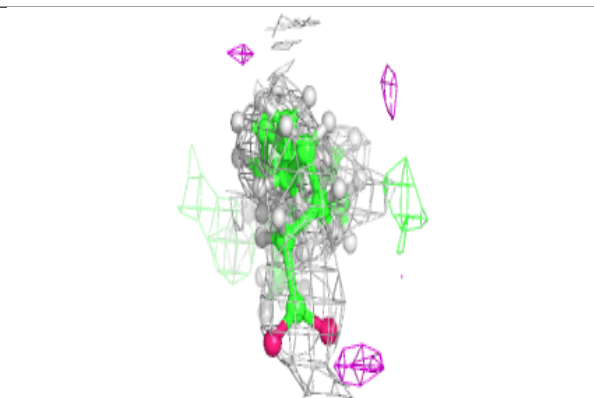
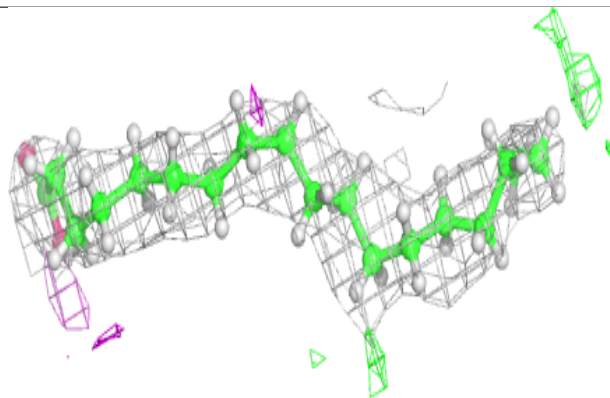
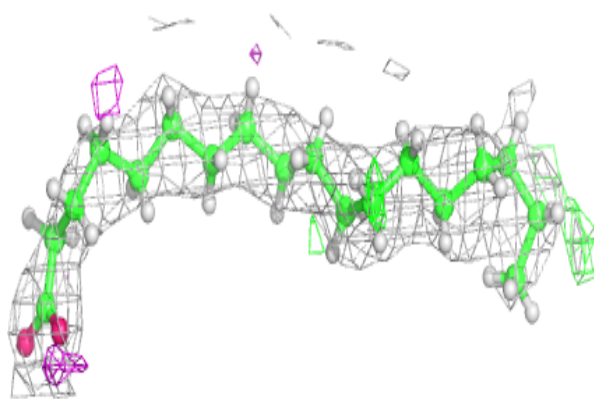
**Electron density around LMG D 411:**

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

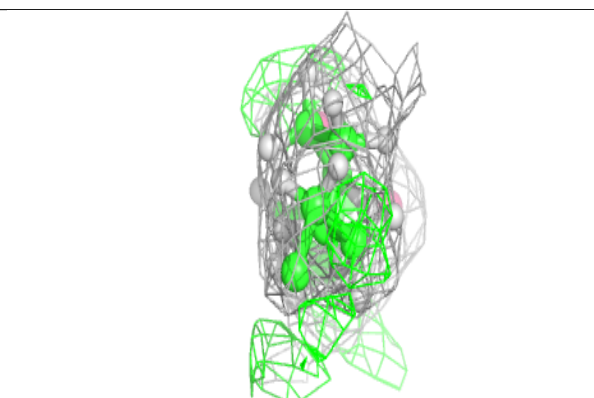
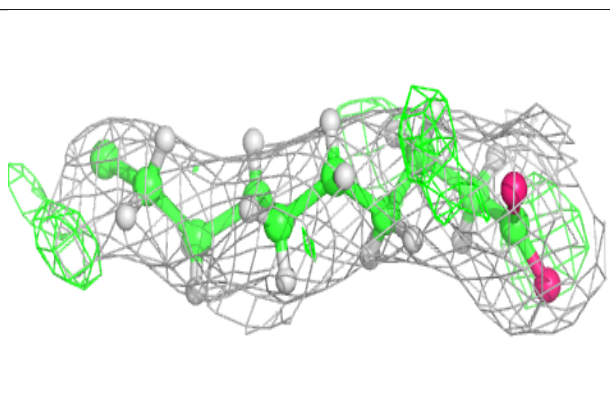
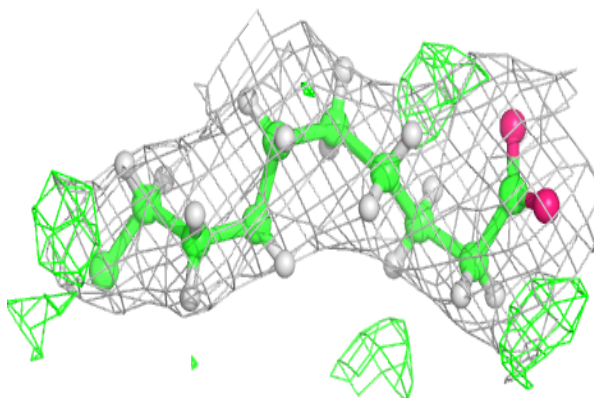


Electron density around STE b 622:

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

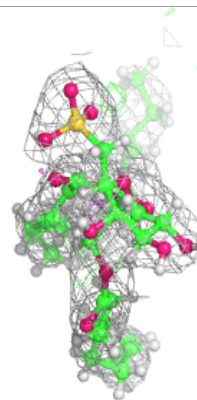
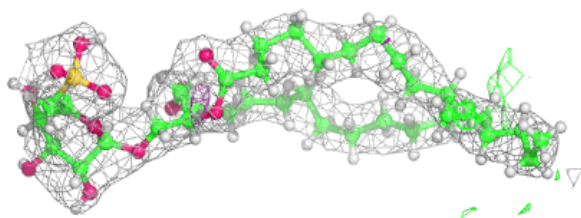
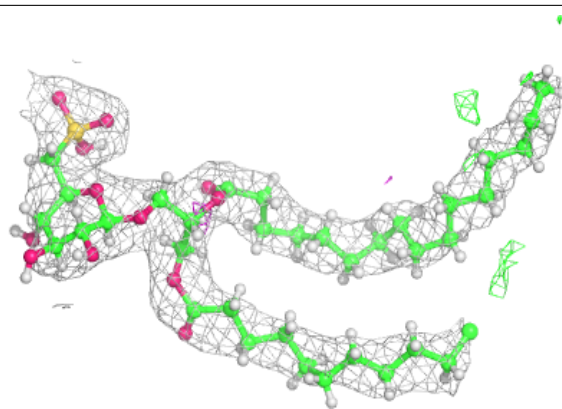
**Electron density around STE B 624:**

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

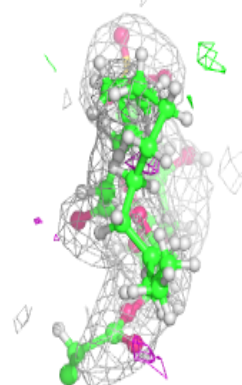
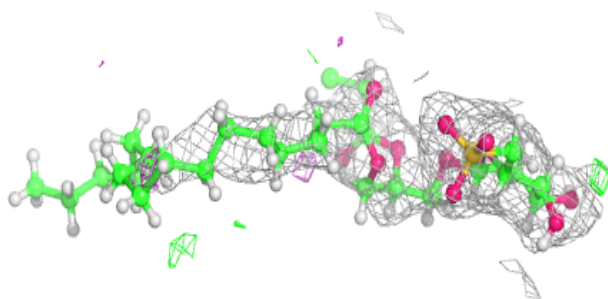
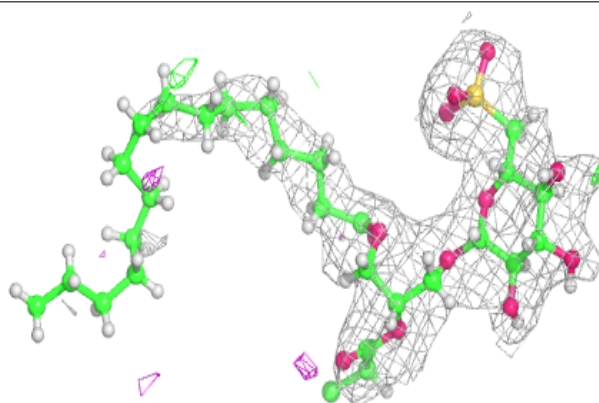


Electron density around SQD b 620:

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

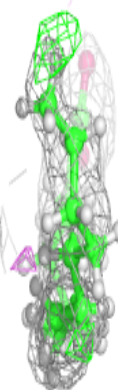
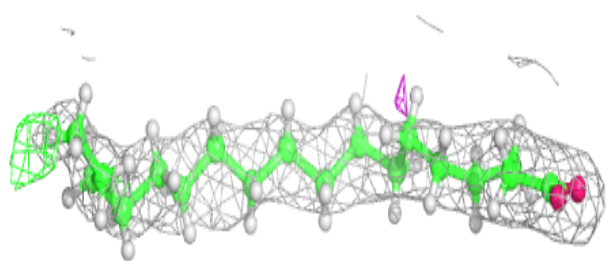
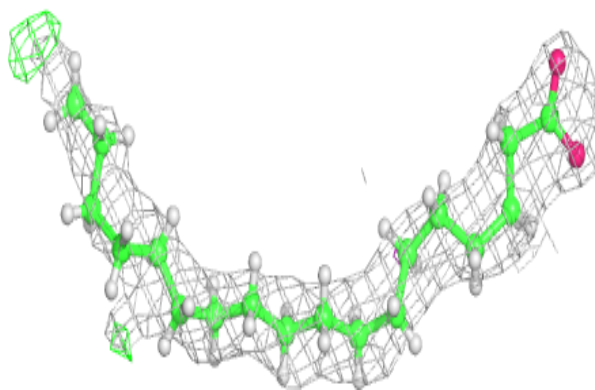
**Electron density around SQD f 102:**

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

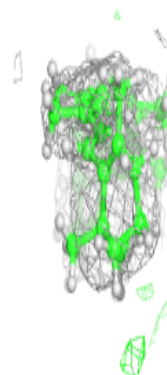
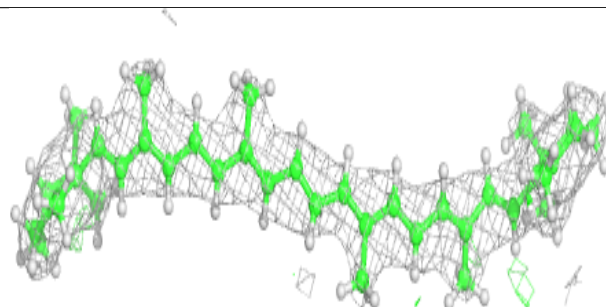
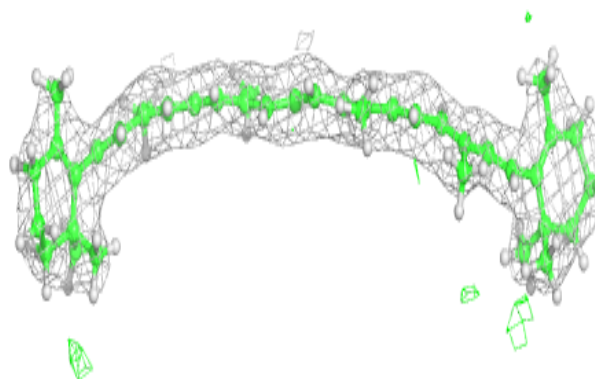


Electron density around STE d 412:

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

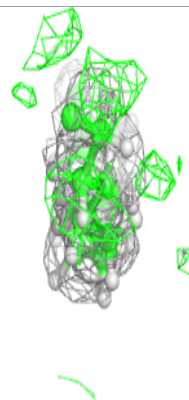
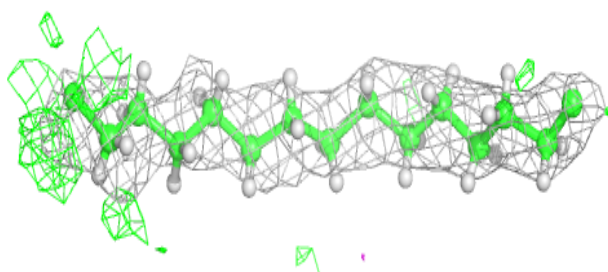
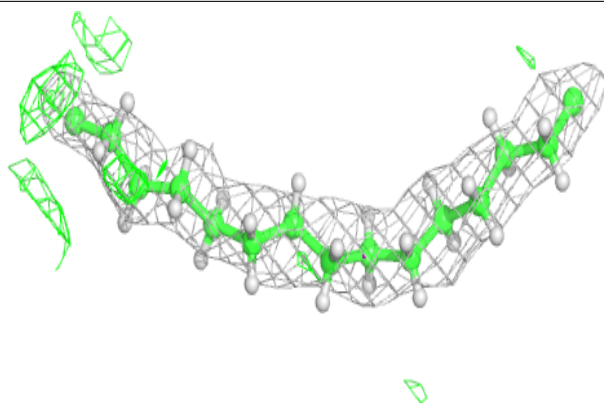
**Electron density around BCR c 516:**

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

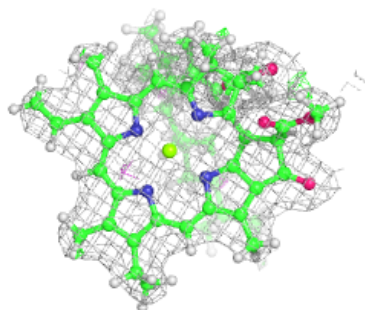
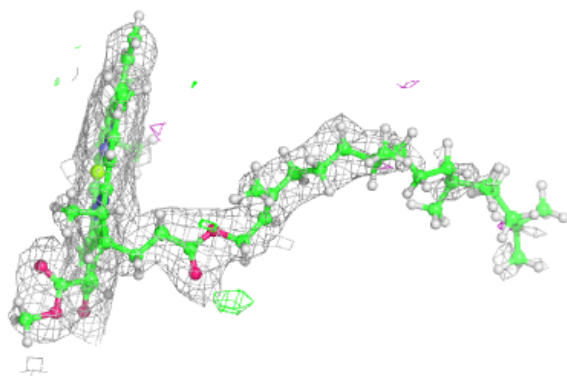
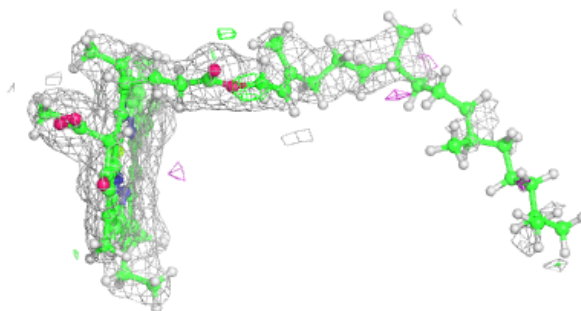


Electron density around STE I 101:

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

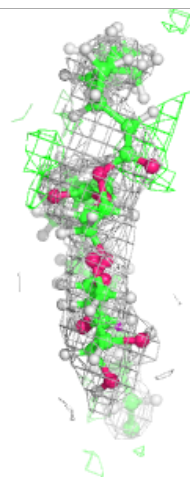
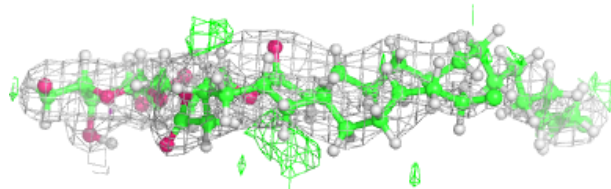
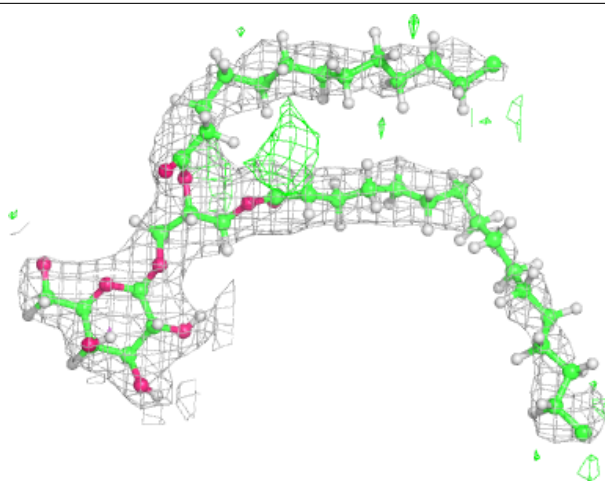
**Electron density around CLA D 404:**

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



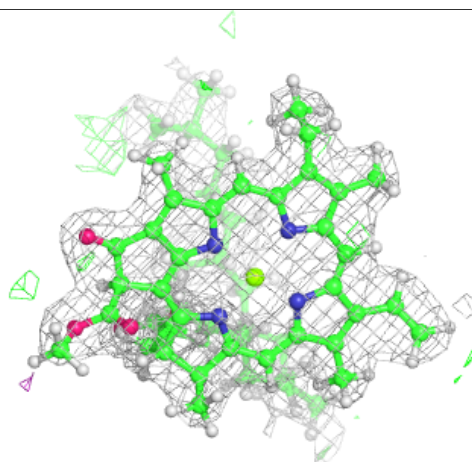
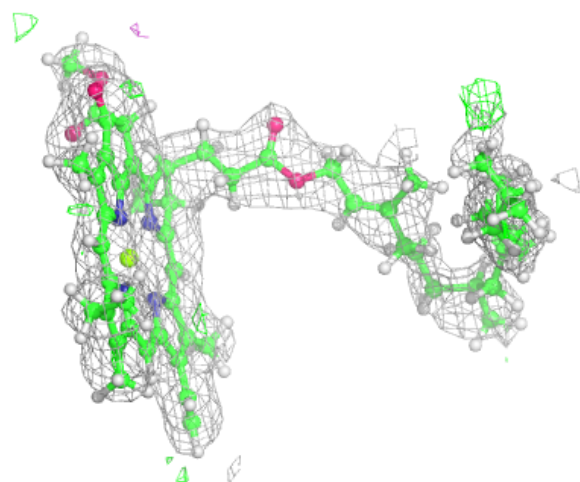
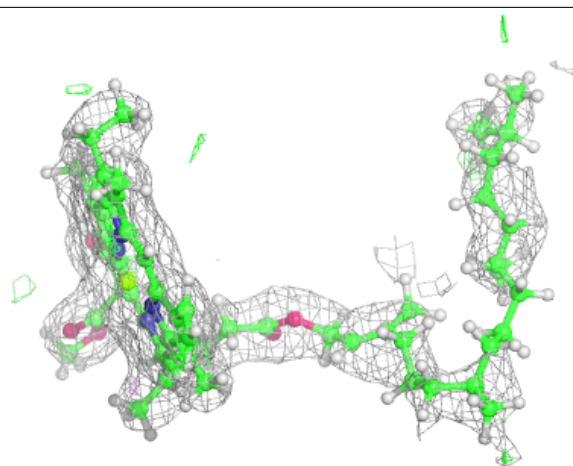
Electron density around LMG C 520:

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



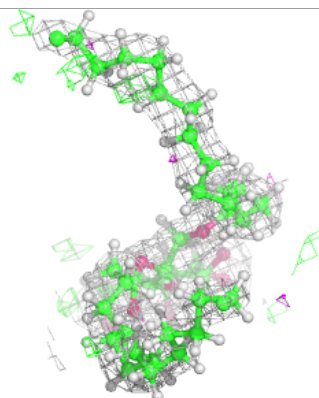
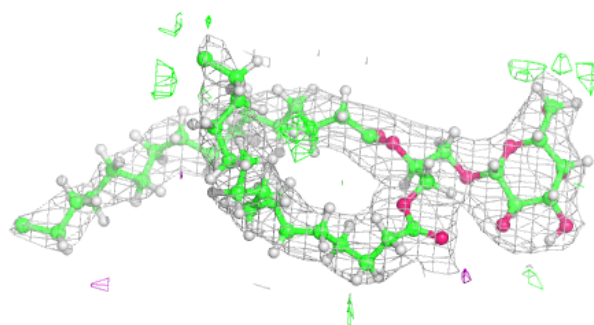
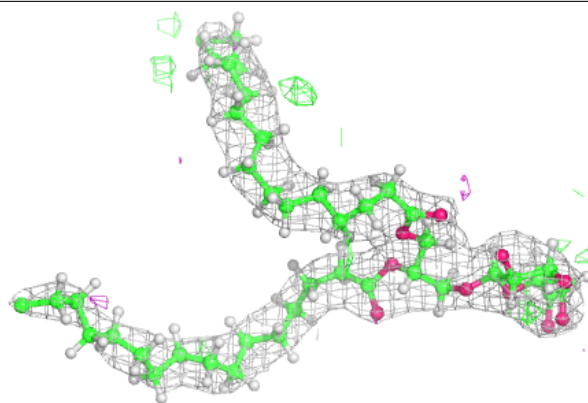
Electron density around CLA a 404:

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

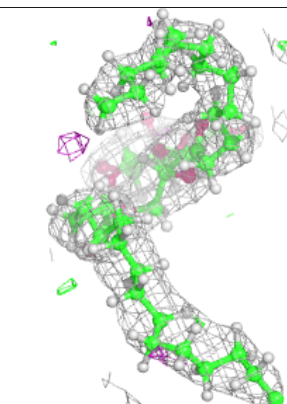
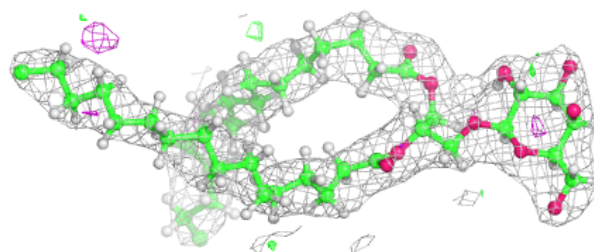
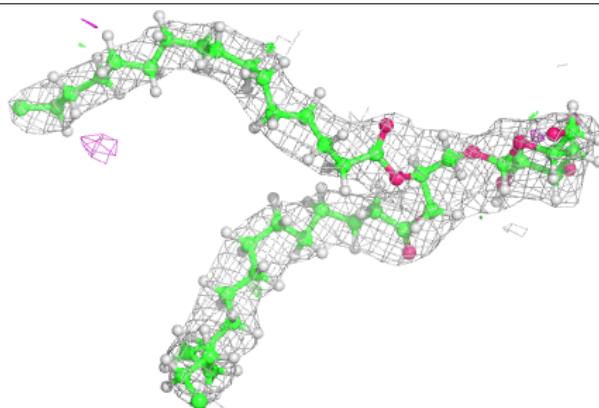


Electron density around LMG m 101:

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

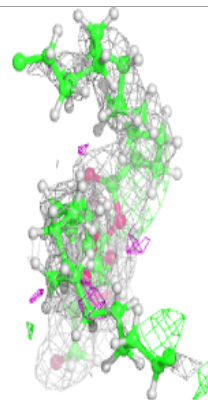
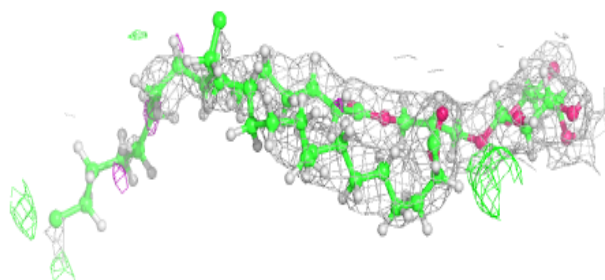
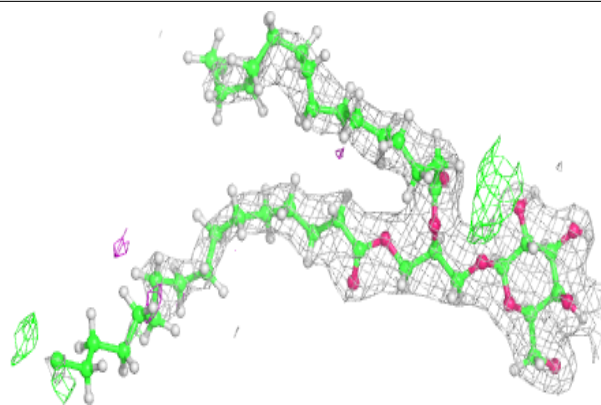
**Electron density around LMG M 101:**

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



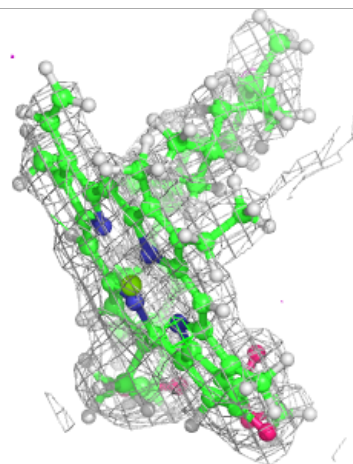
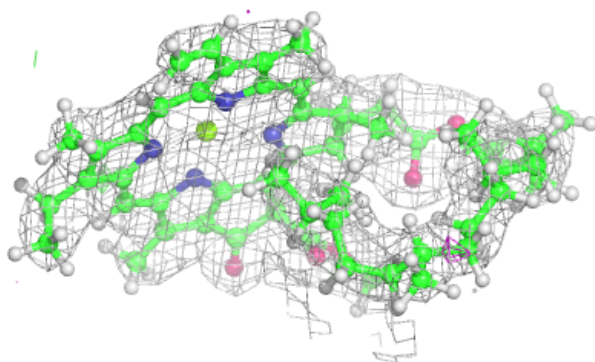
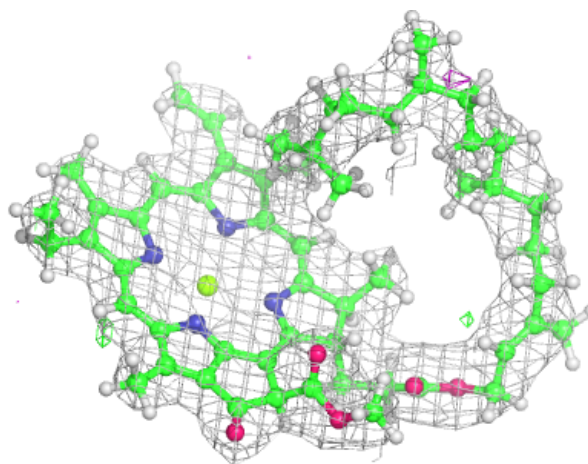
Electron density around LMG D 407:

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



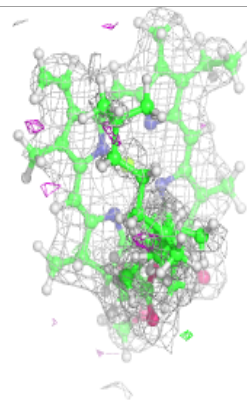
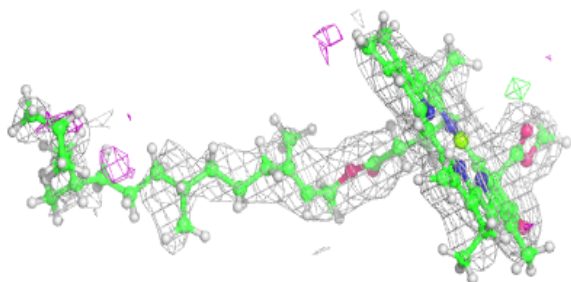
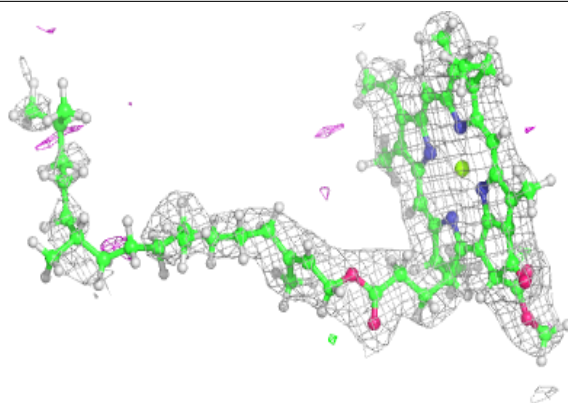
Electron density around CLA b 615:

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

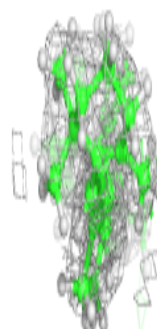
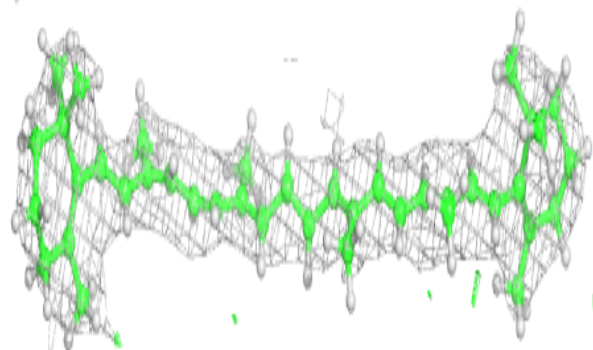
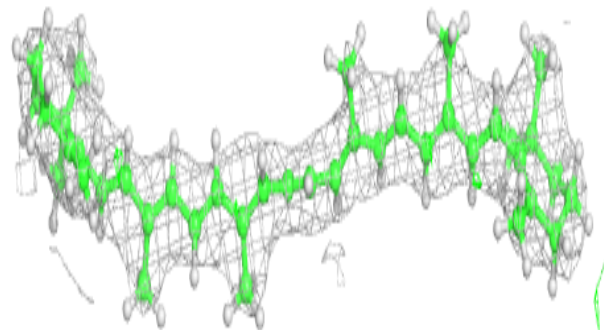


Electron density around CLA d 405:

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

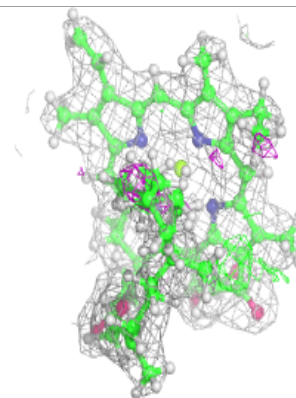
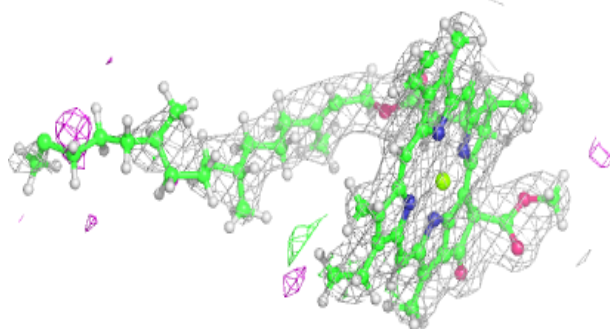
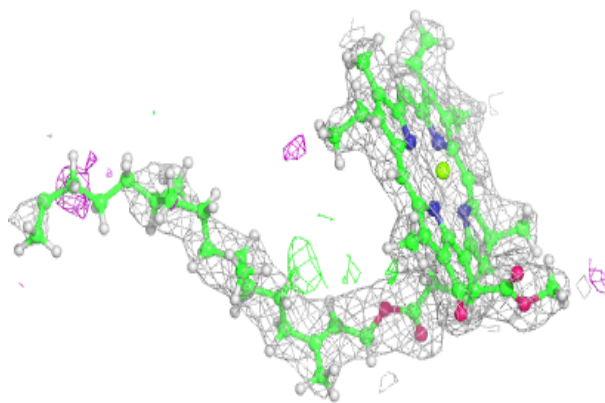
**Electron density around BCR c 514:**

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

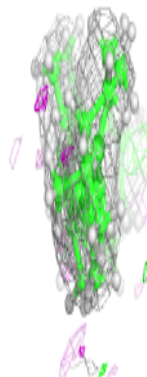
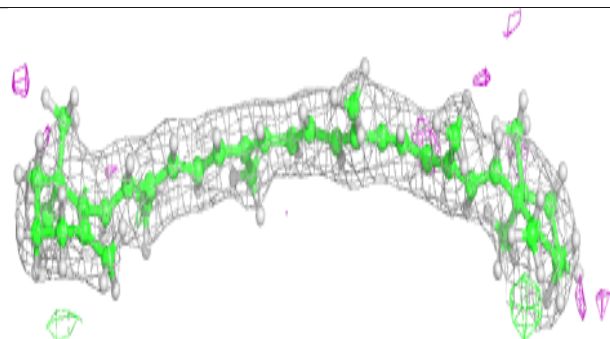
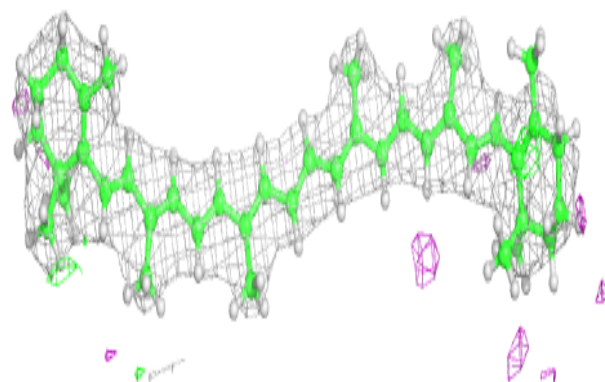


Electron density around CLA c 508:

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

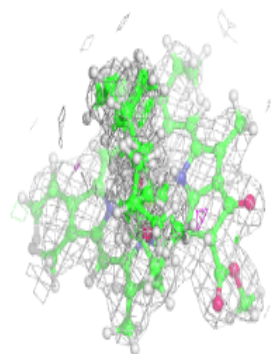
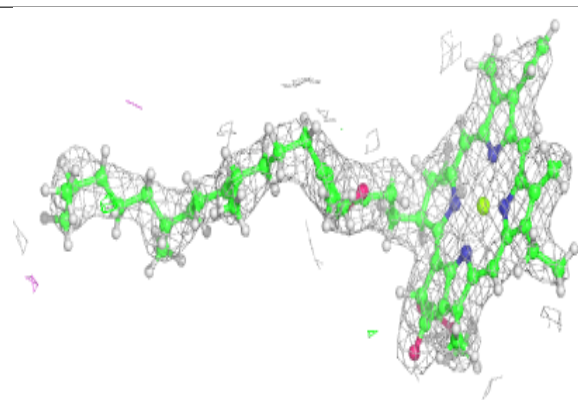
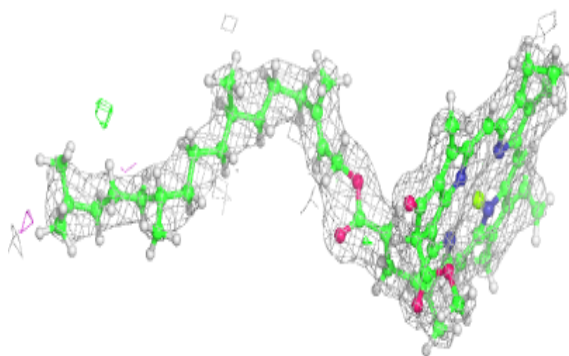
**Electron density around BCR D 405:**

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

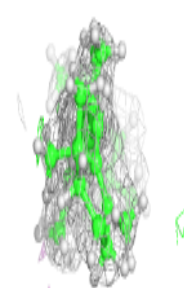
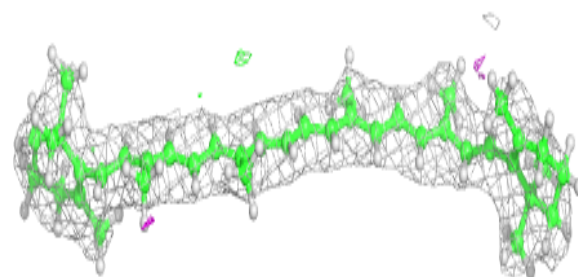
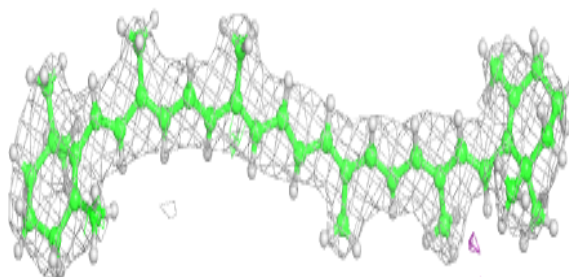


Electron density around CLA c 502:

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

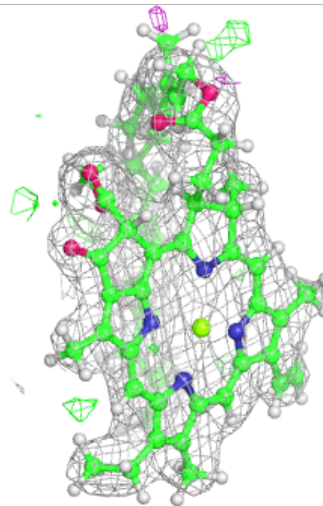
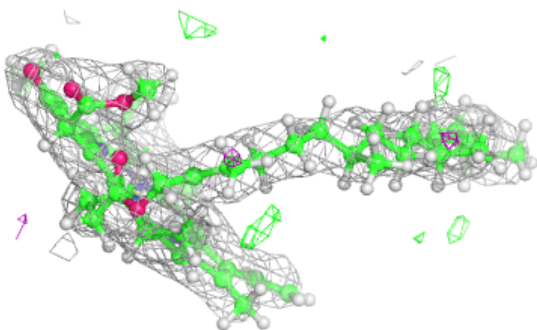
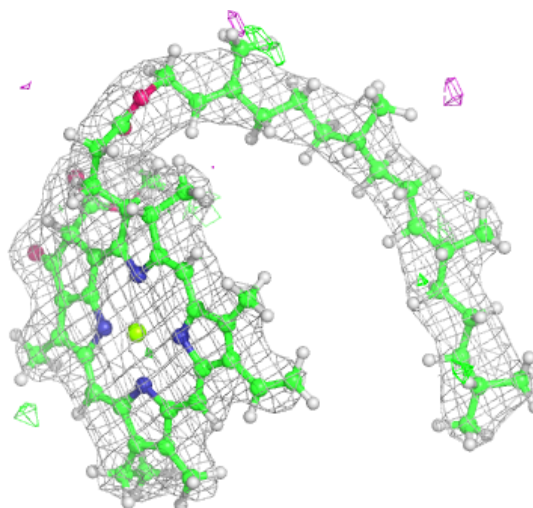
**Electron density around BCR b 619:**

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



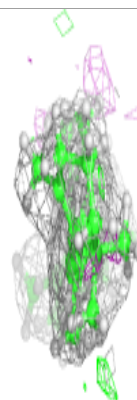
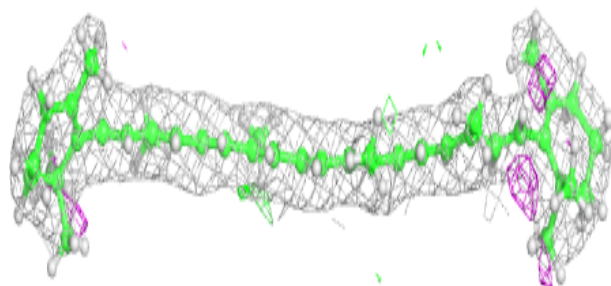
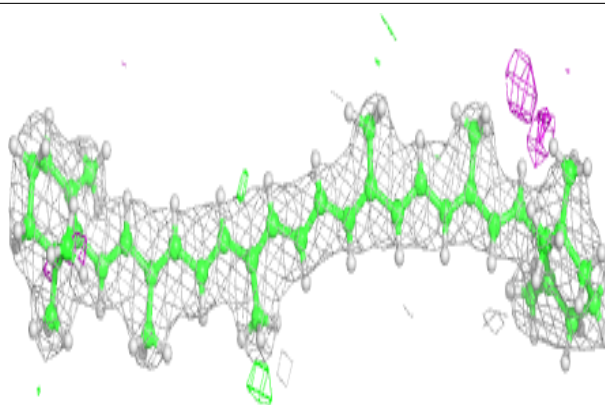
Electron density around CLA c 507:

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

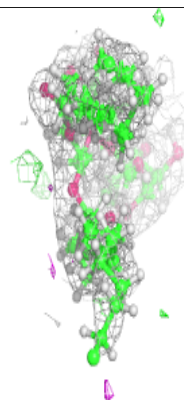
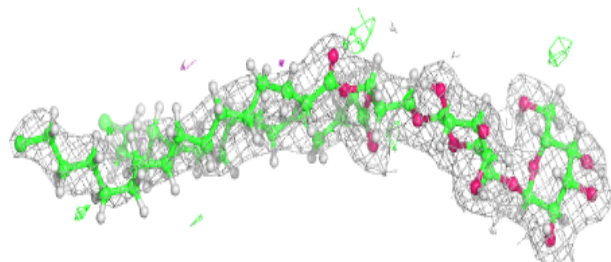
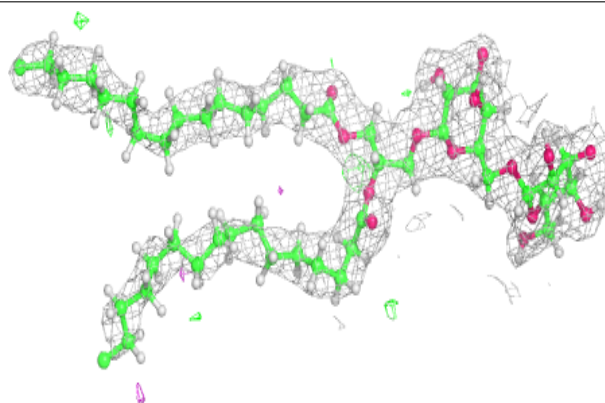


Electron density around BCR B 618:

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

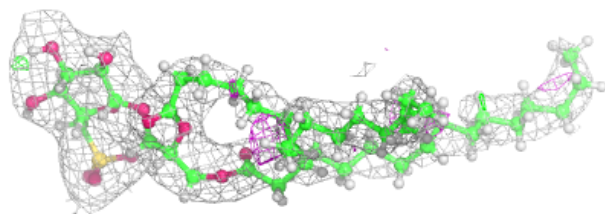
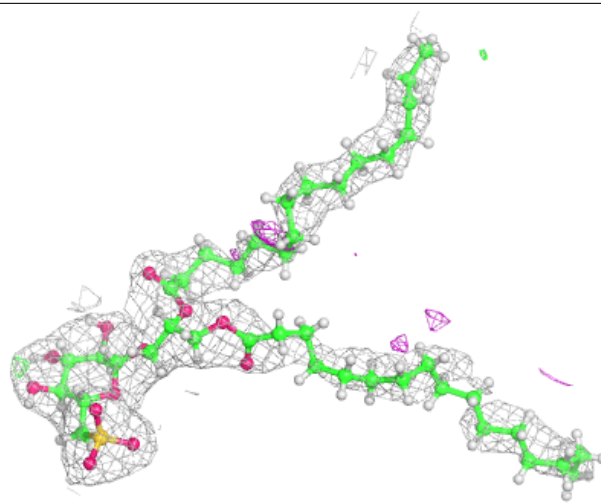
**Electron density around DGD c 519:**

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



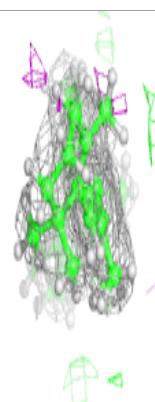
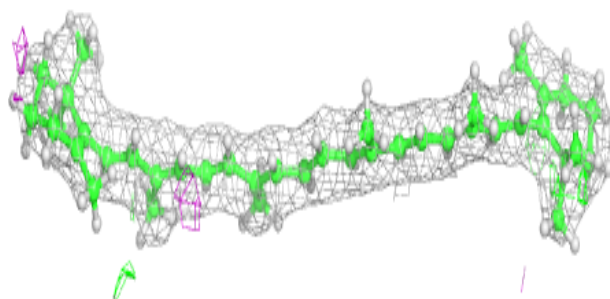
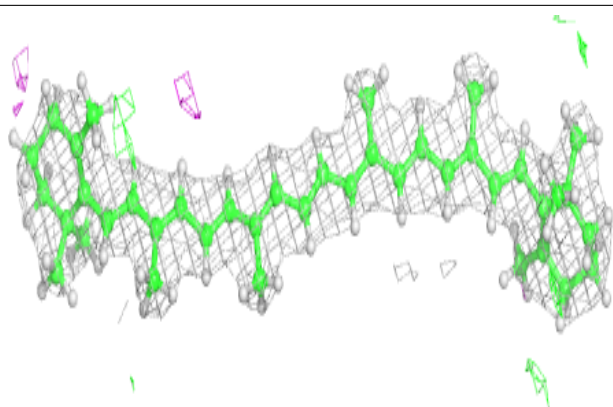
Electron density around SQD a 411:

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

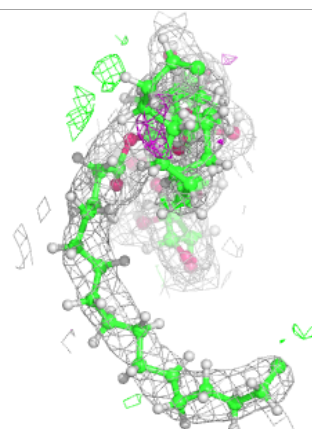
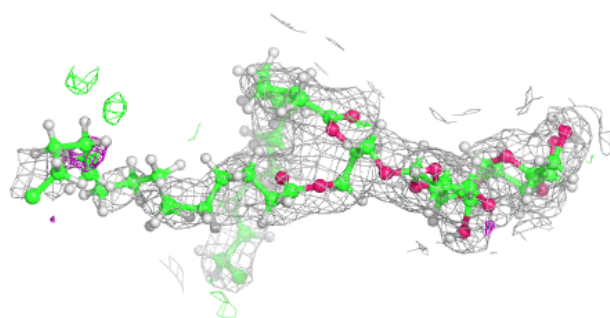
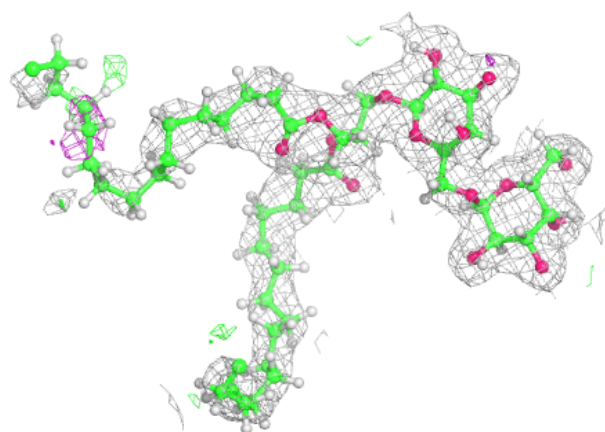


Electron density around BCR B 619:

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

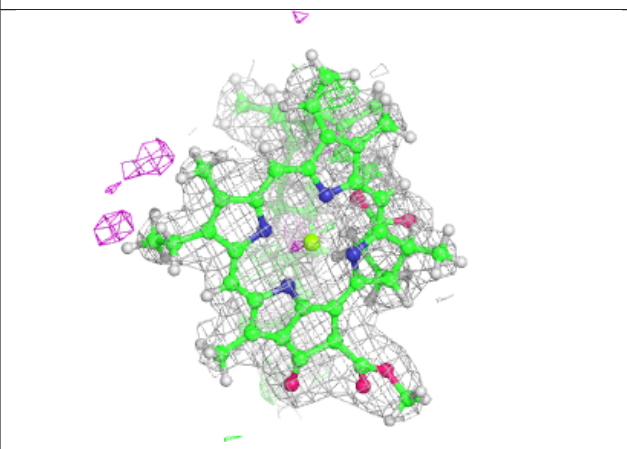
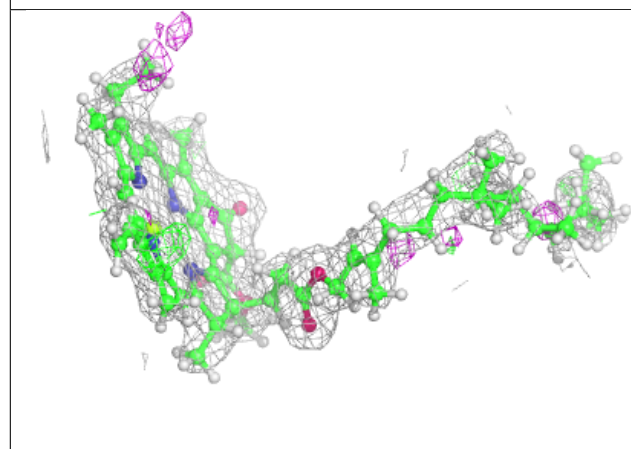
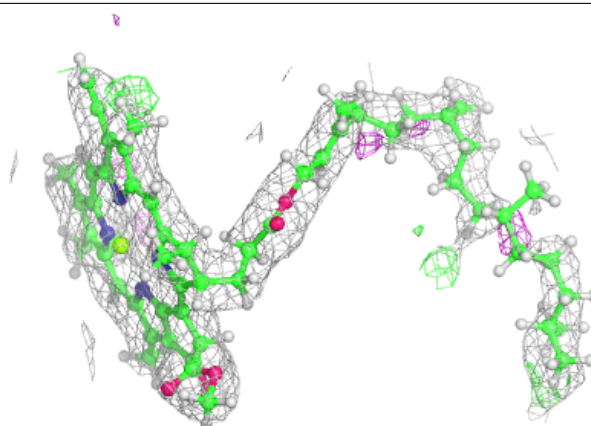
**Electron density around DGD C 518:**

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

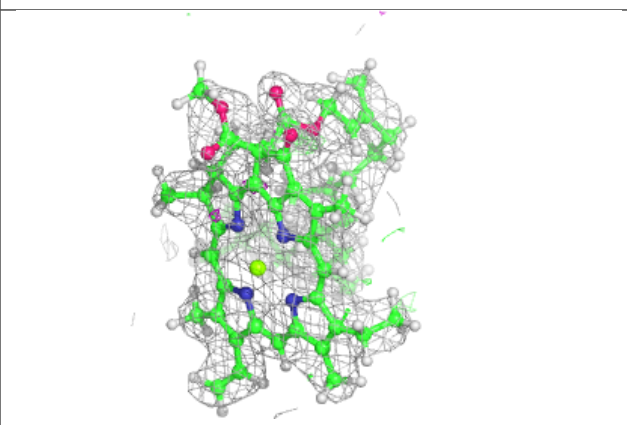
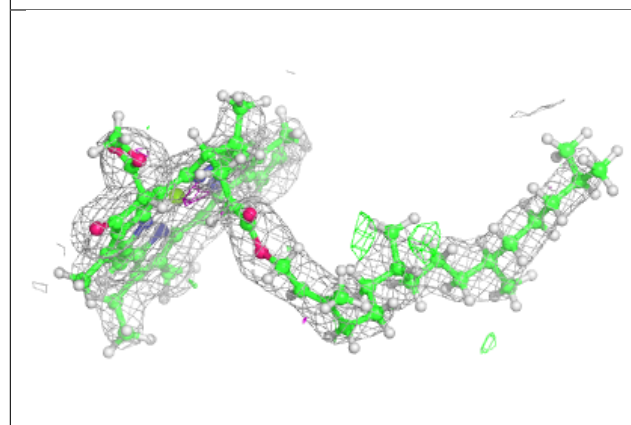
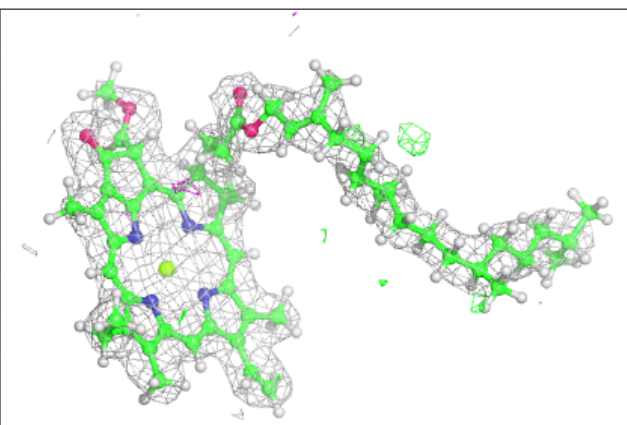


Electron density around CLA b 606:

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

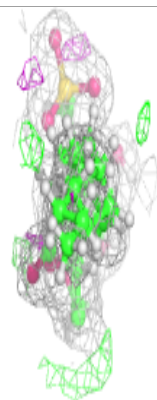
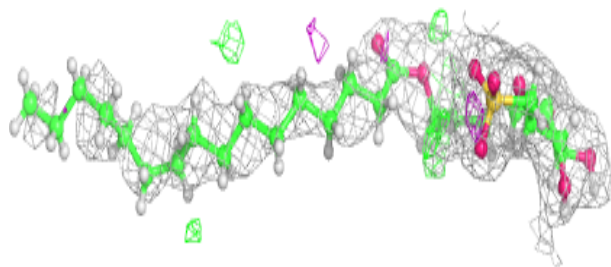
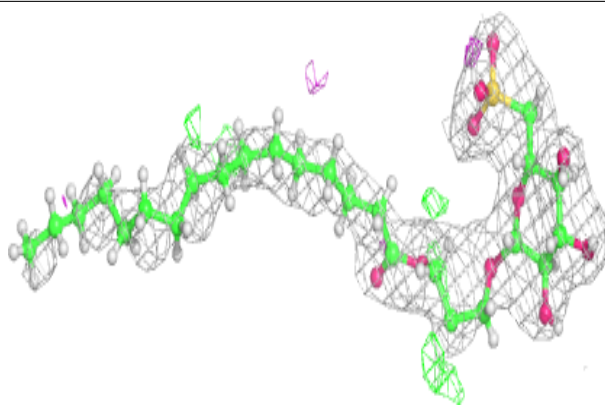
**Electron density around CLA C 511:**

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

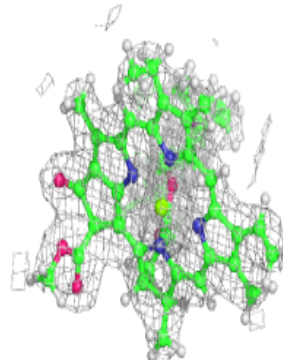
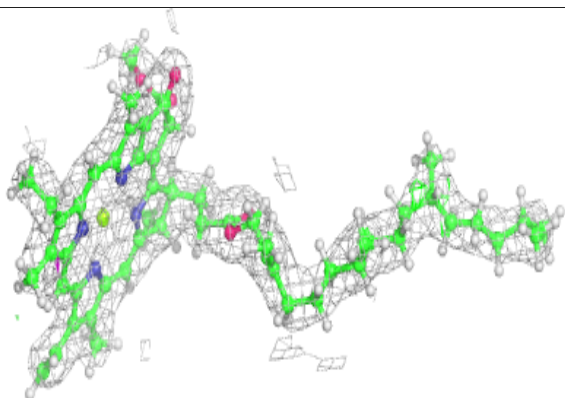
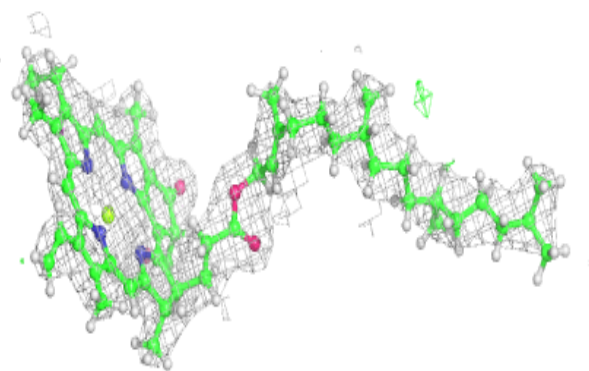


Electron density around SQD D 408:

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

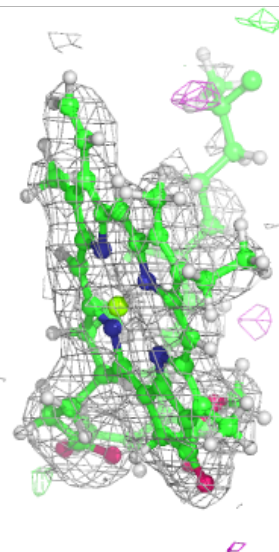
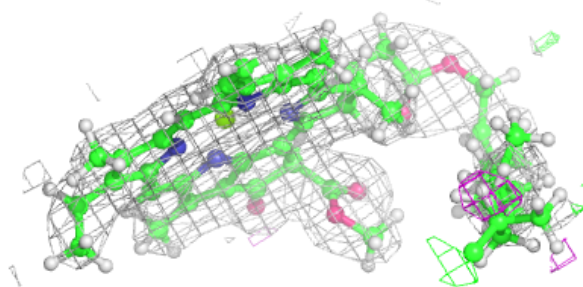
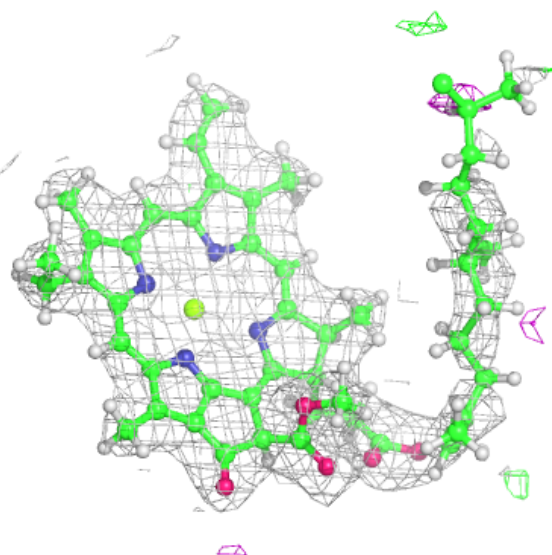
**Electron density around CLA C 502:**

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



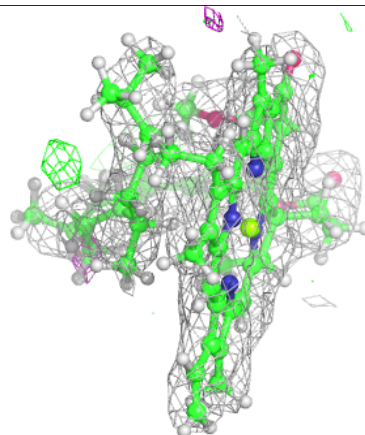
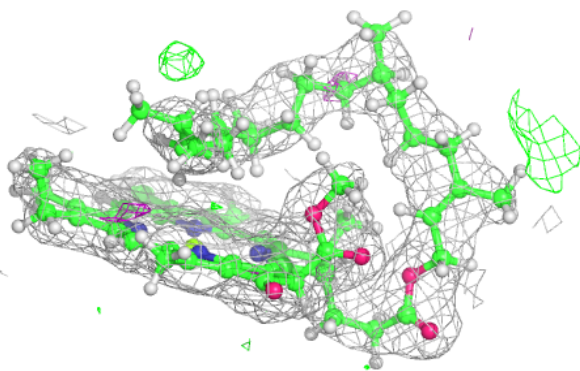
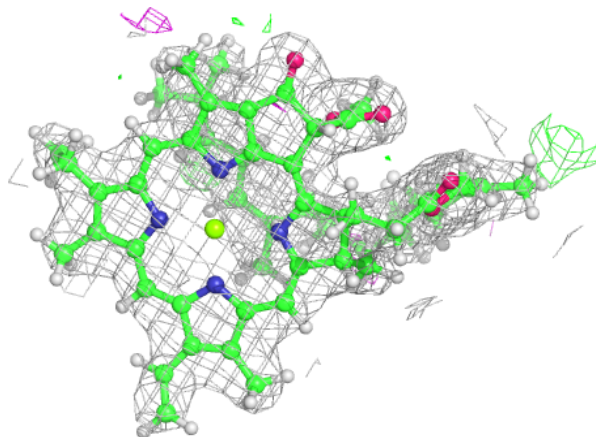
Electron density around CLA B 616:

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

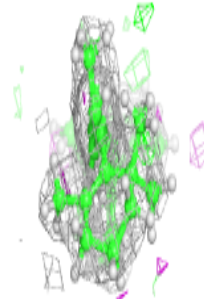
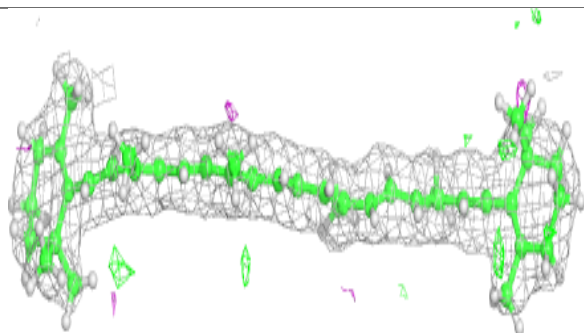
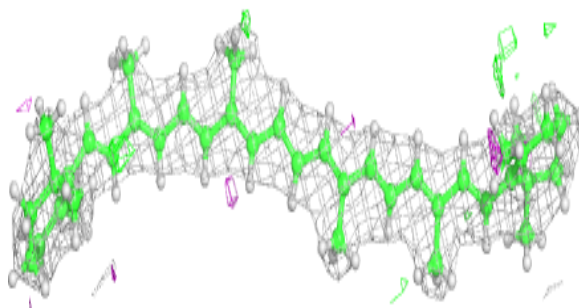


Electron density around CLA c 510:

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

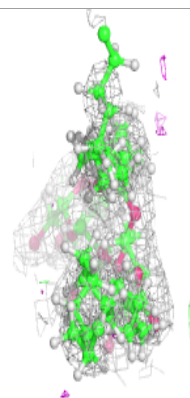
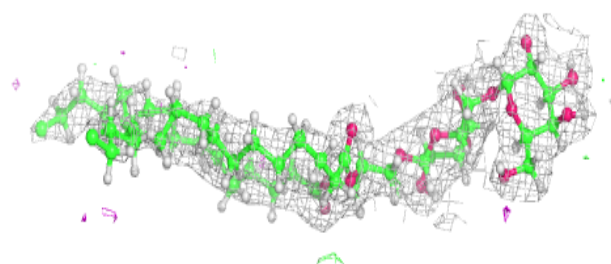
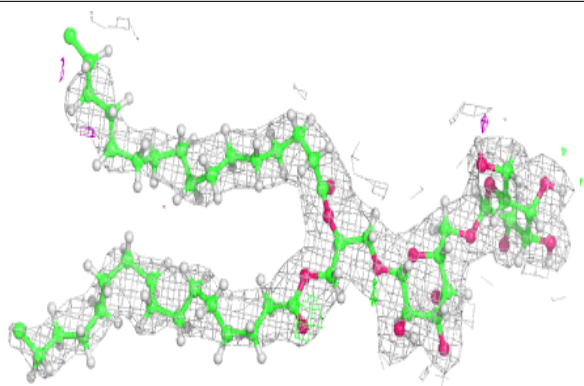
**Electron density around BCR C 515:**

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



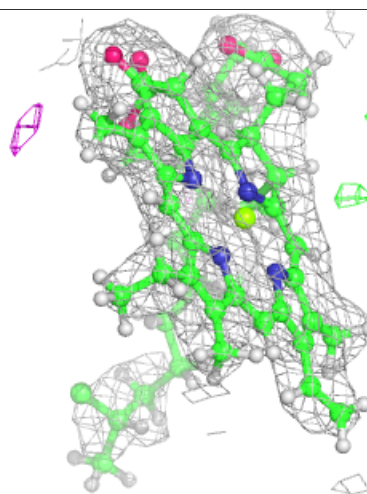
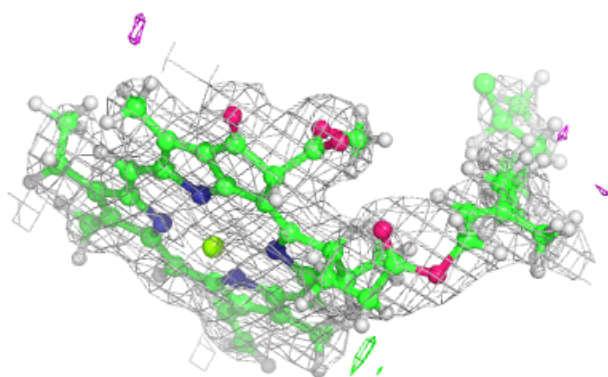
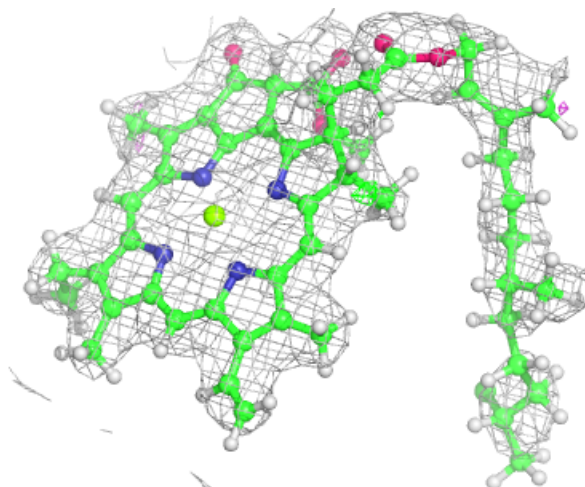
Electron density around DGD C 519:

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



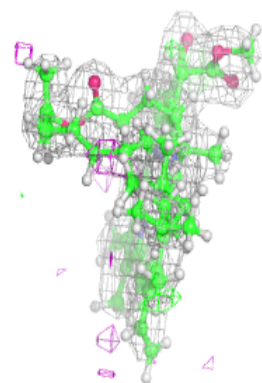
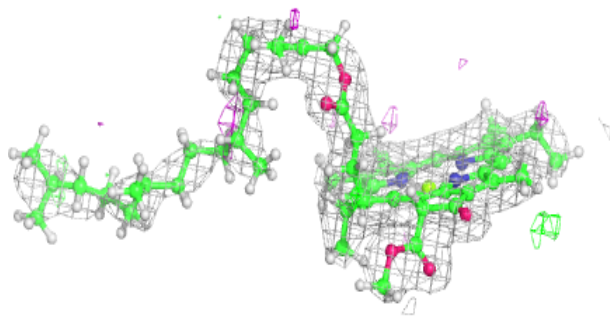
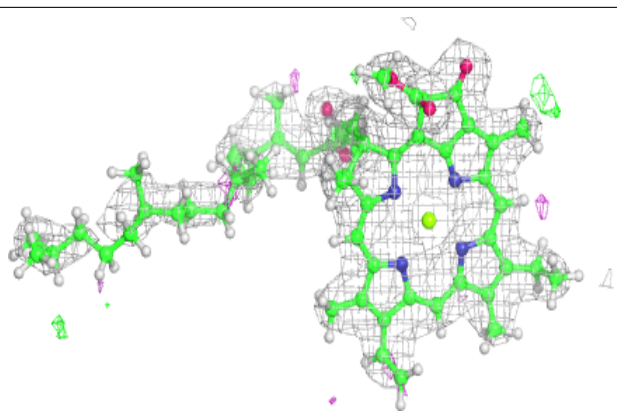
Electron density around CLA b 616:

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

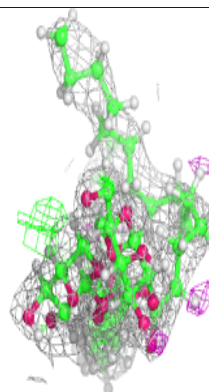
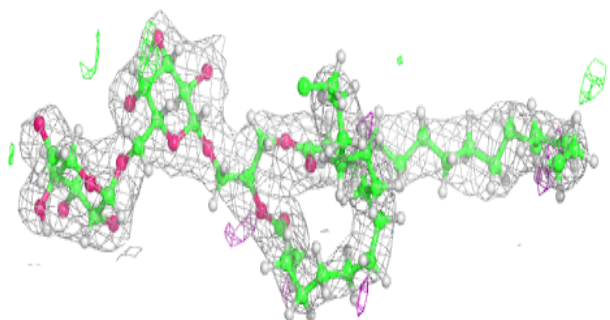
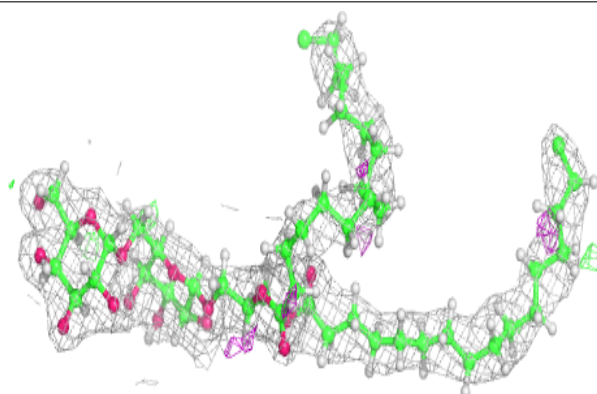


Electron density around CLA d 401:

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

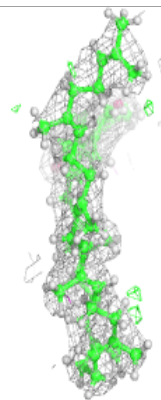
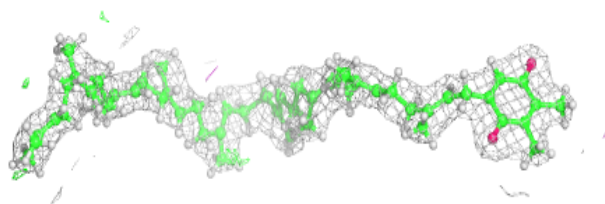
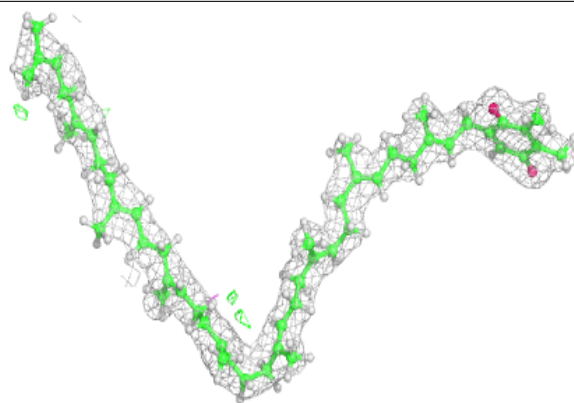
**Electron density around DGD h 101:**

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



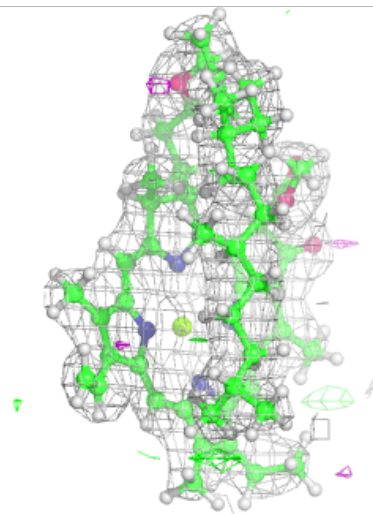
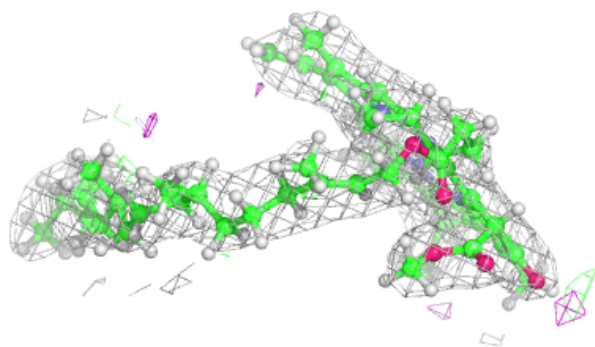
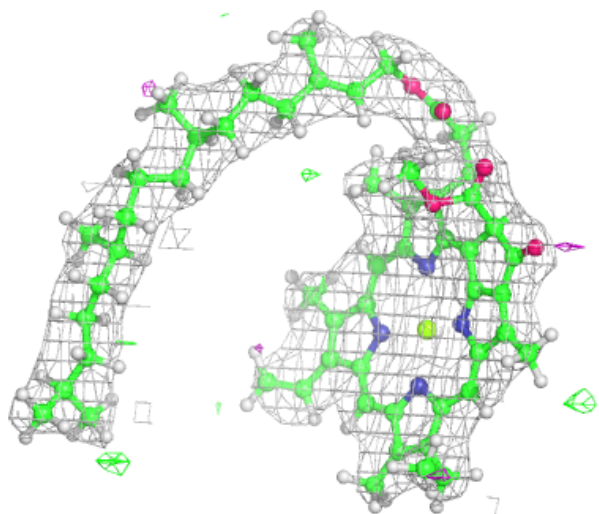
Electron density around PL9 D 406:

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



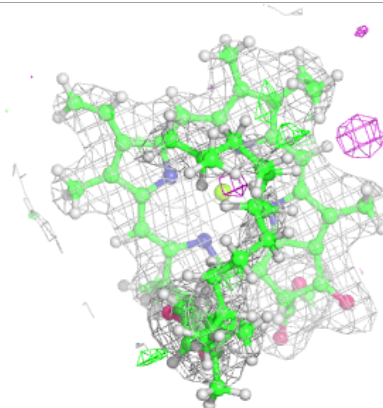
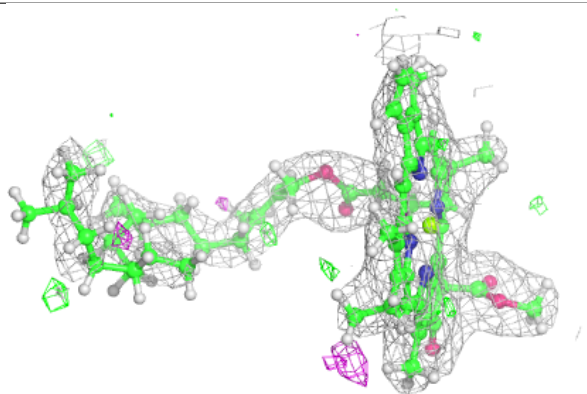
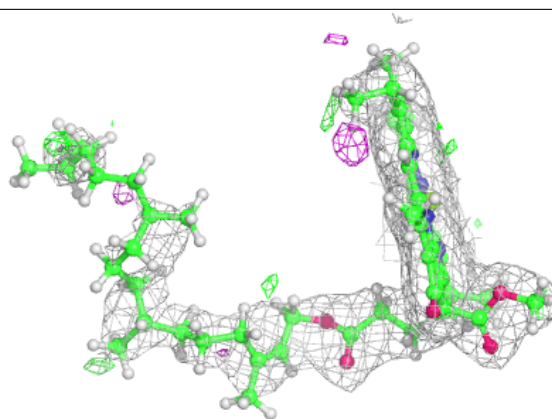
Electron density around CLA C 507:

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

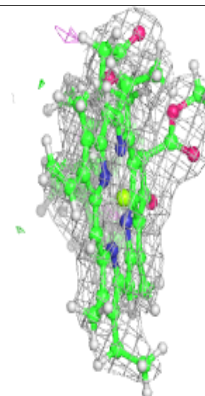
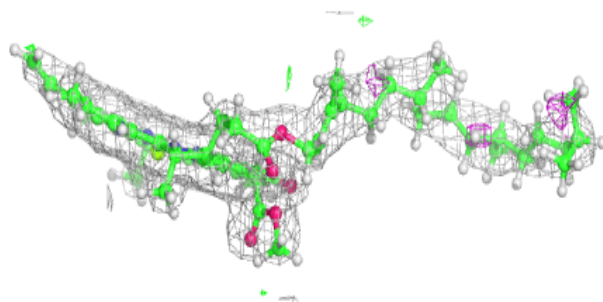
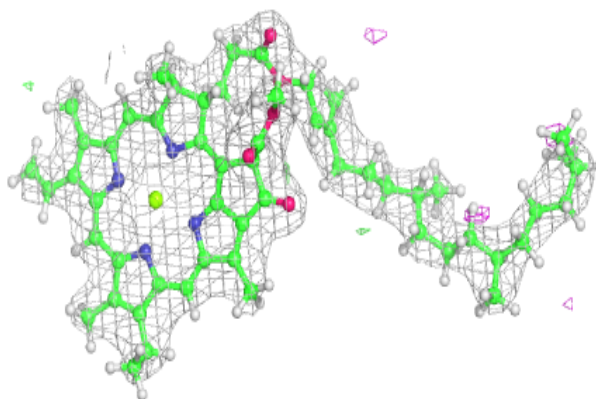


Electron density around CLA c 506:

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

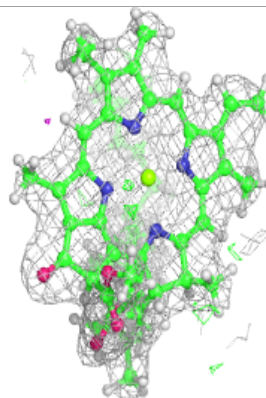
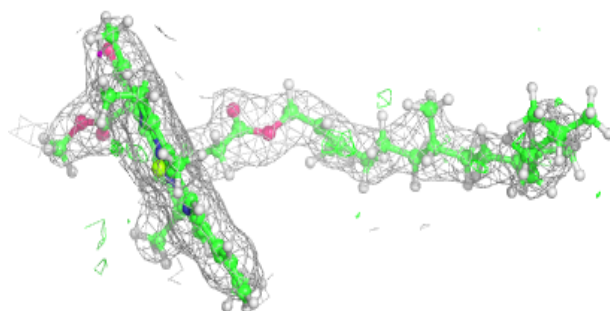
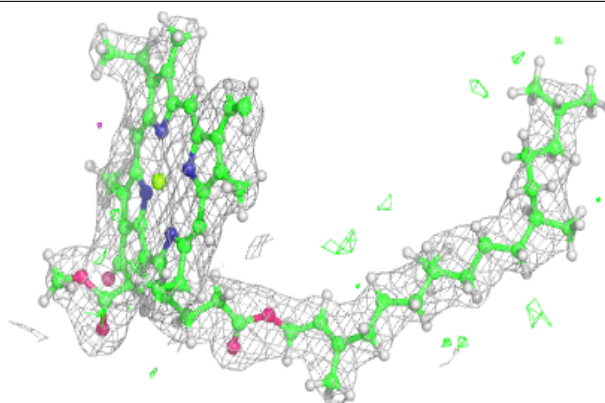
**Electron density around CLA b 602:**

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

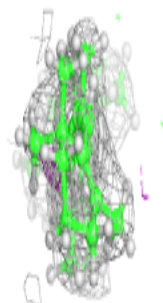
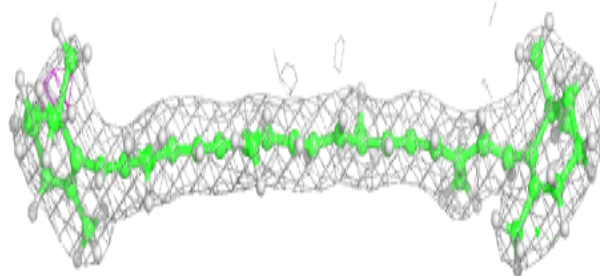
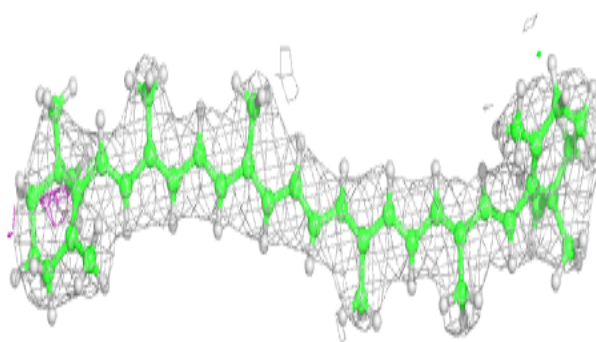


Electron density around CLA b 609:

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

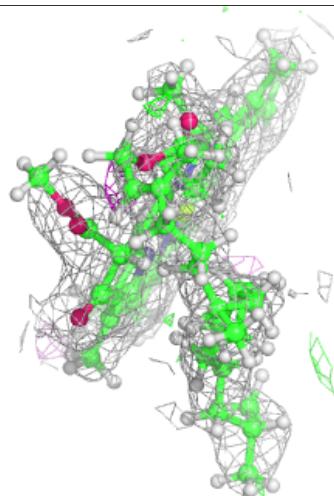
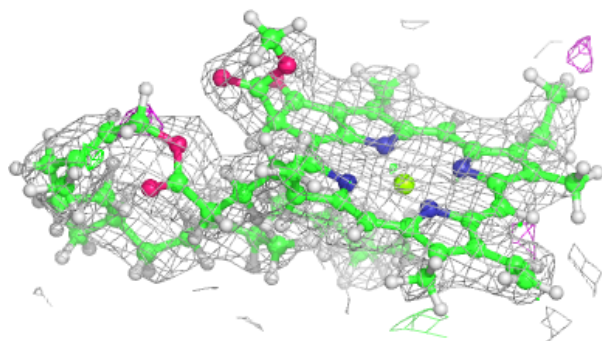
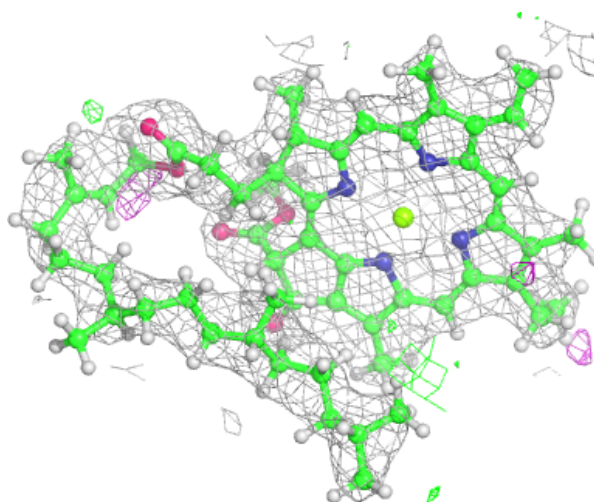
**Electron density around BCR b 618:**

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



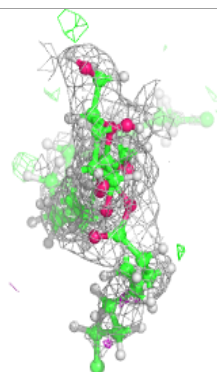
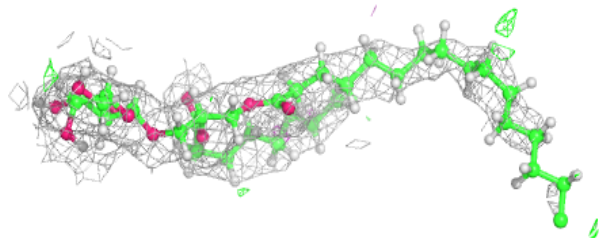
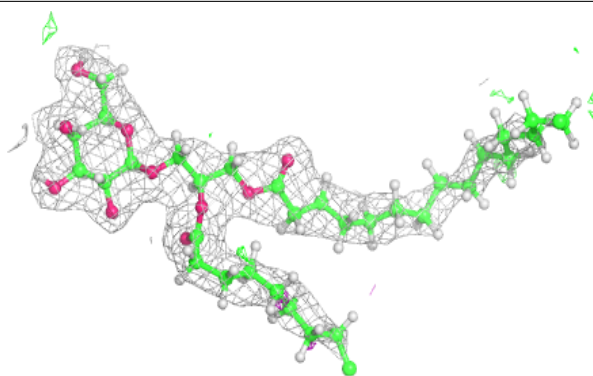
Electron density around CLA c 509:

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

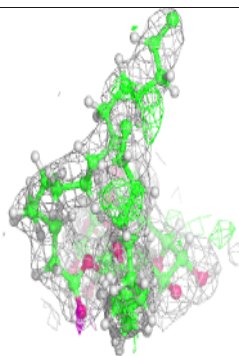
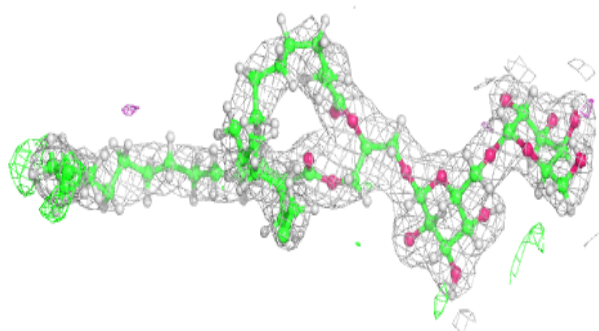
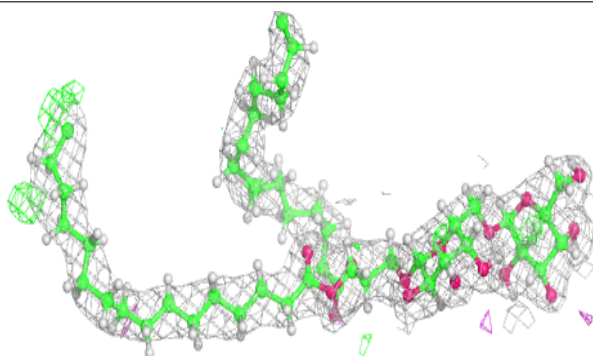


Electron density around LMG d 410:

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

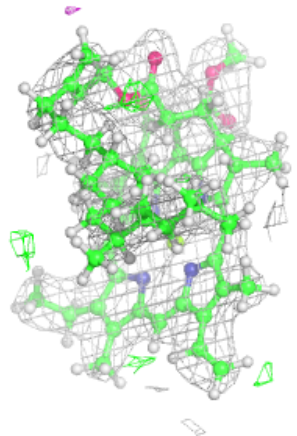
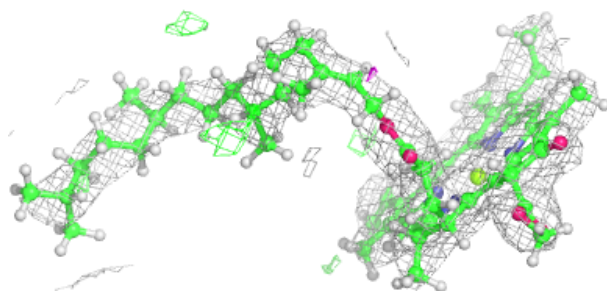
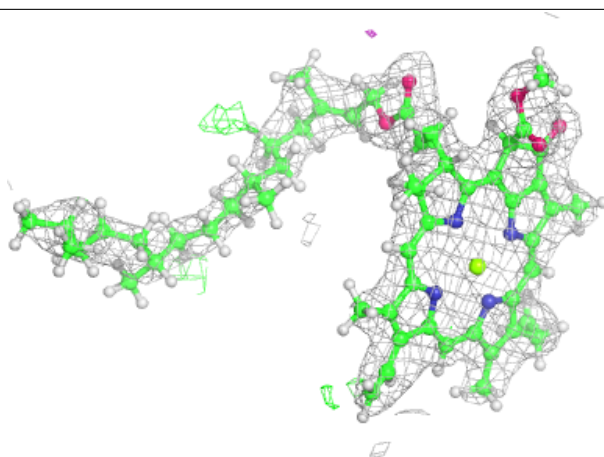
**Electron density around DGD H 102:**

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



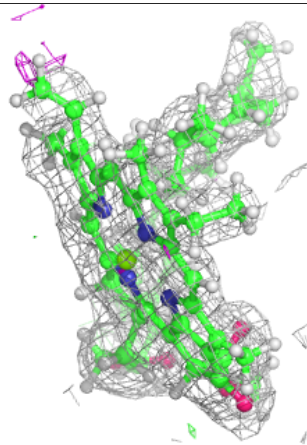
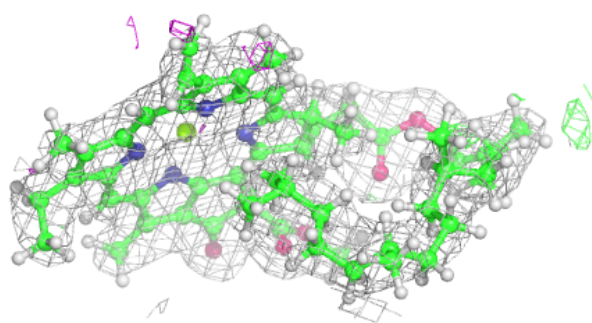
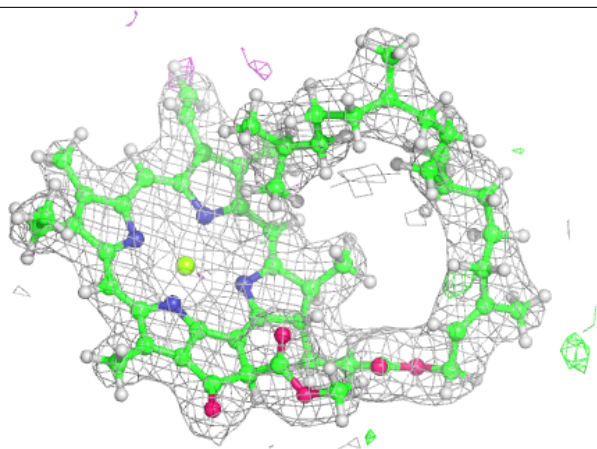
Electron density around CLA c 511:

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



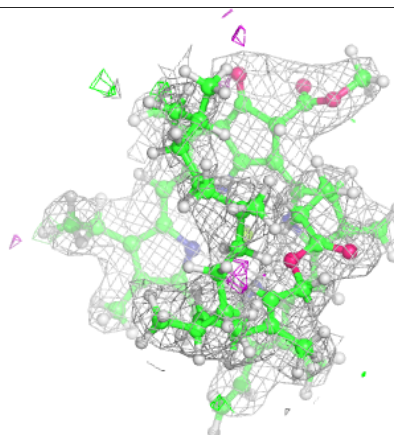
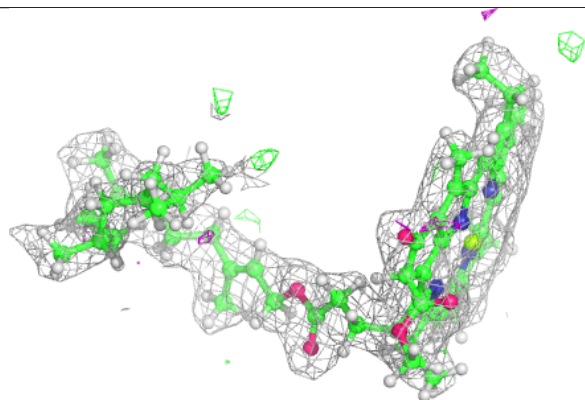
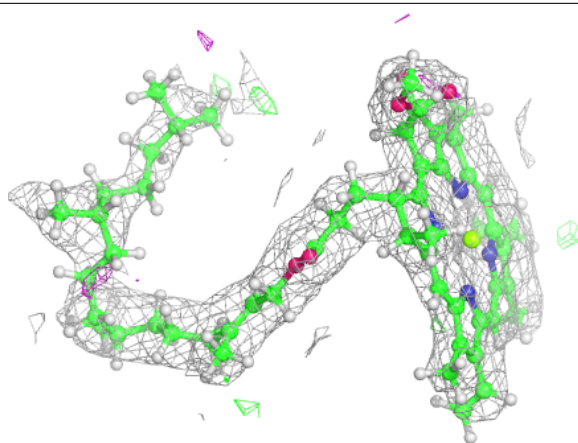
Electron density around CLA B 615:

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

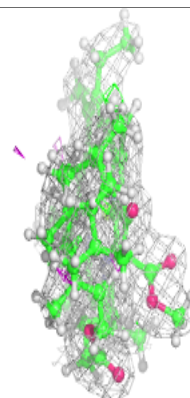
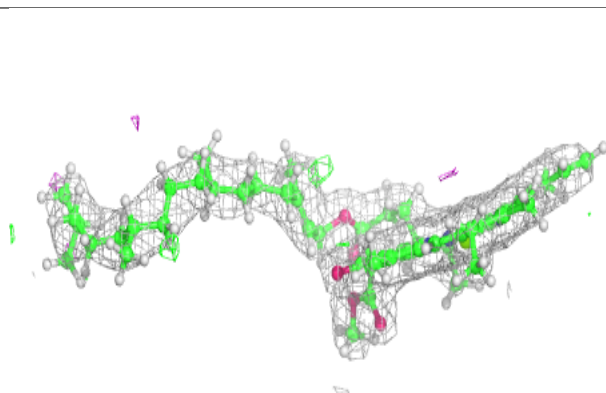
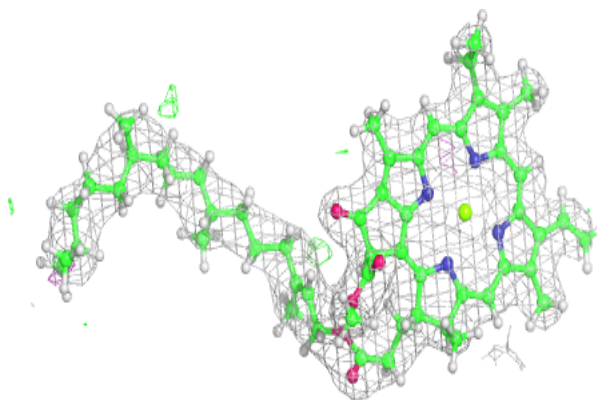


Electron density around CLA B 606:

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

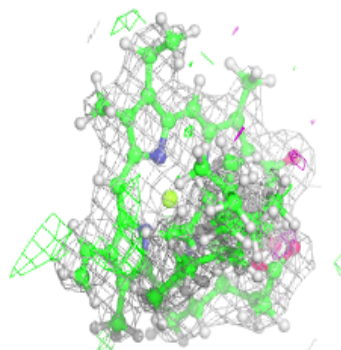
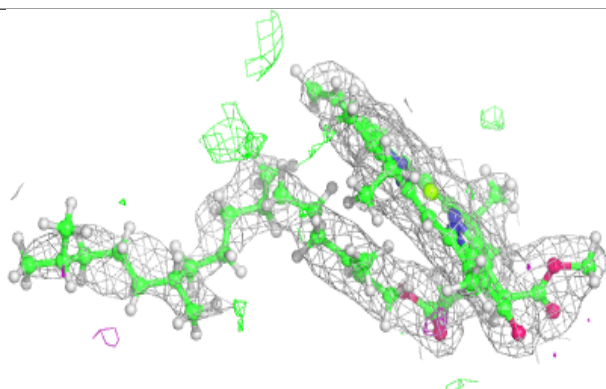
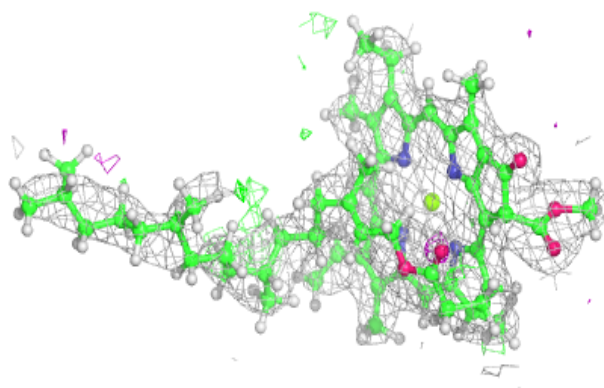
**Electron density around CLA B 602:**

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

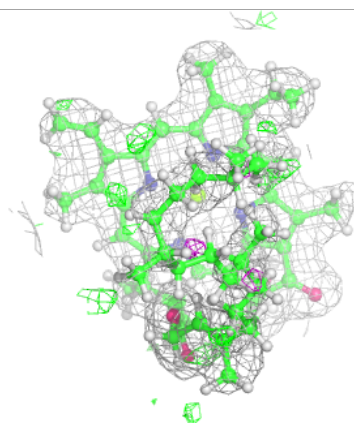
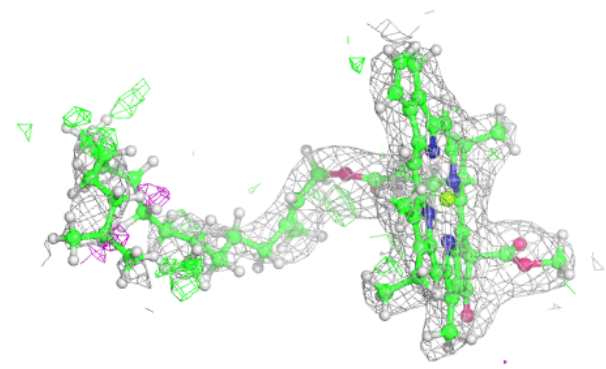
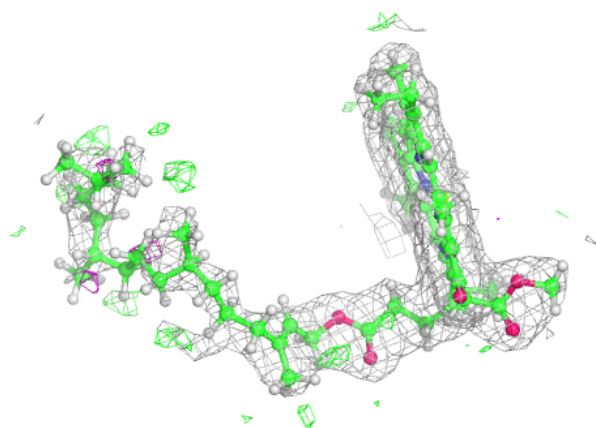


Electron density around CLA C 505:

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

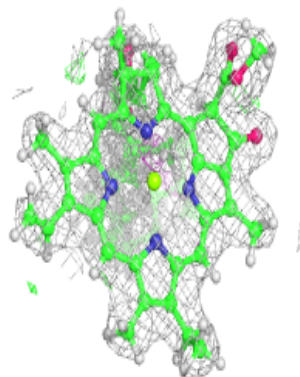
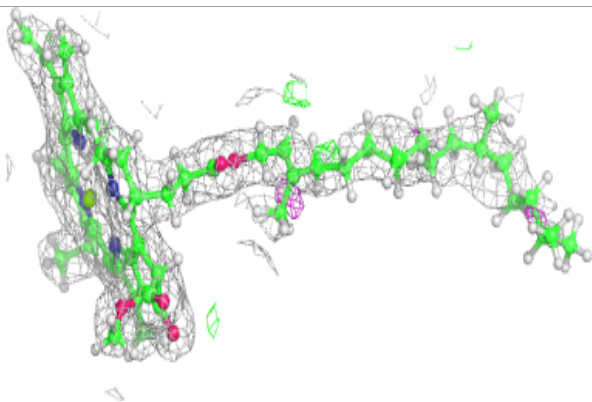
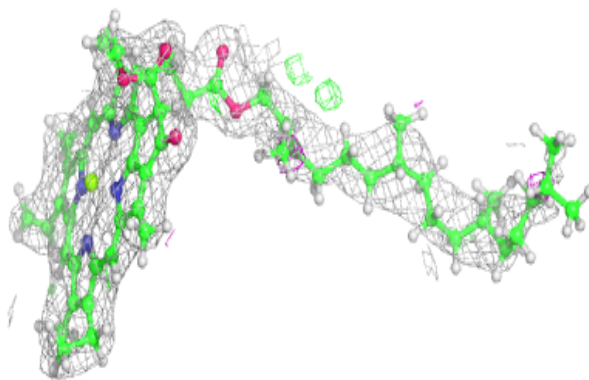
**Electron density around CLA C 506:**

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

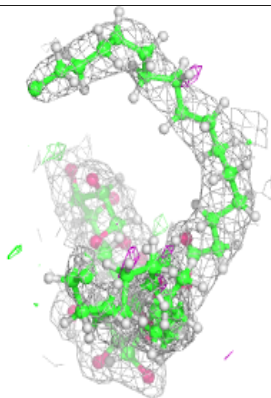
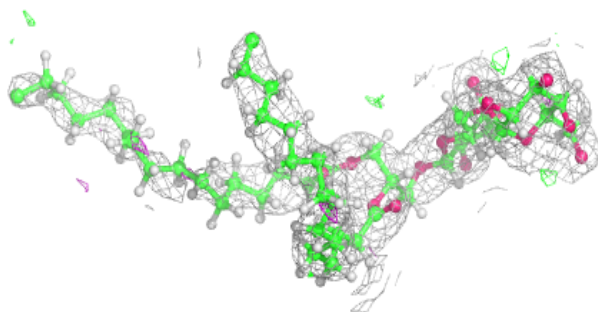
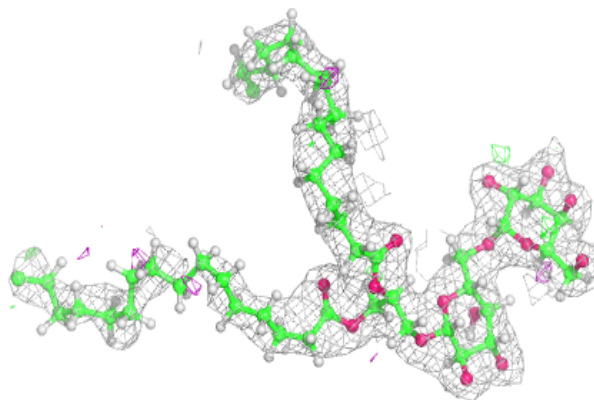


Electron density around CLA B 604:

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

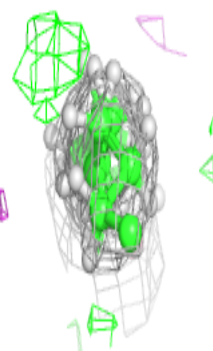
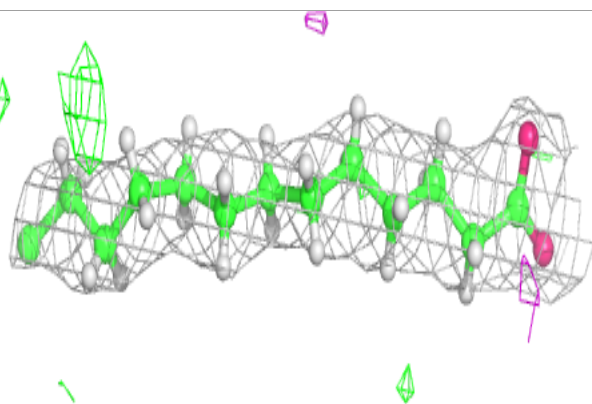
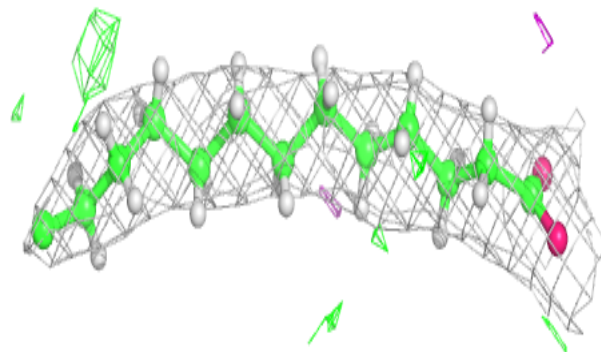
**Electron density around DGD c 518:**

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



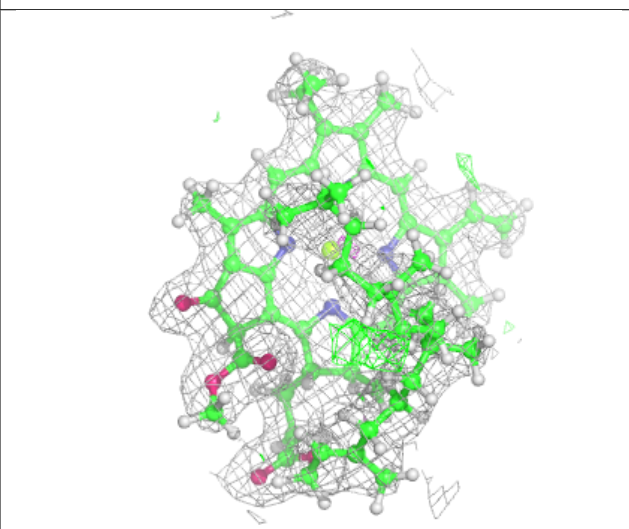
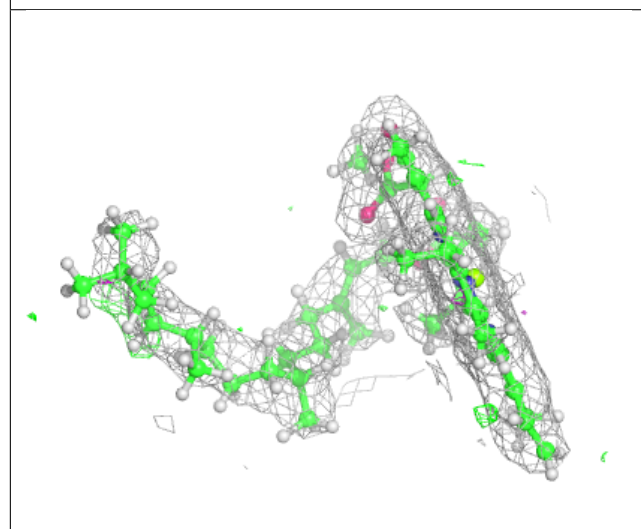
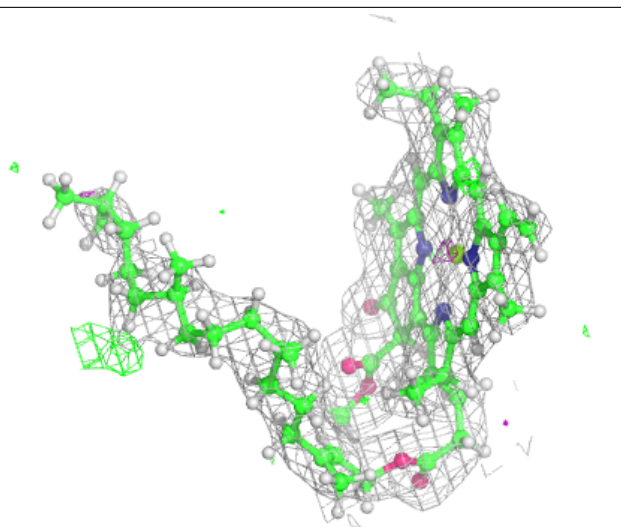
Electron density around STE M 102:

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



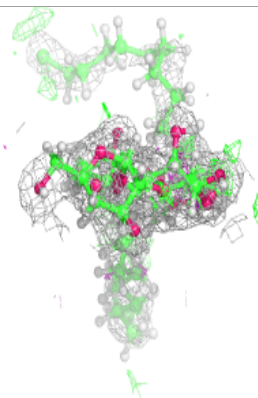
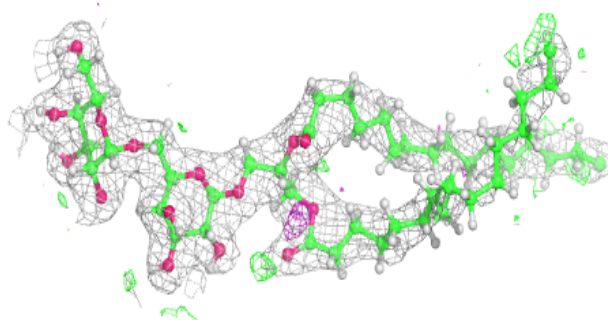
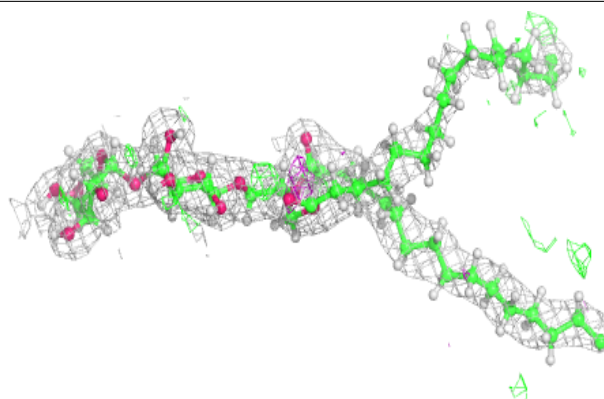
Electron density around CLA B 613:

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

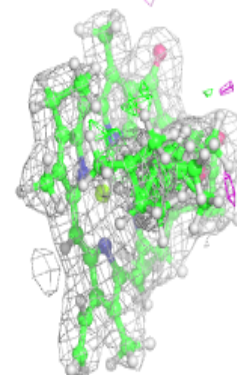
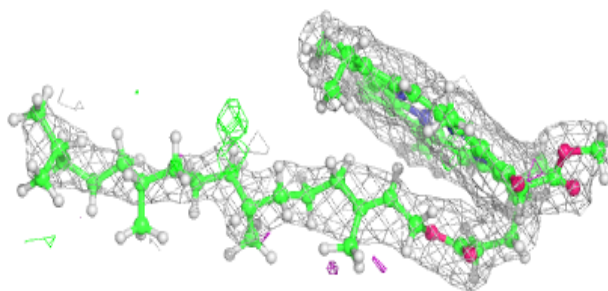
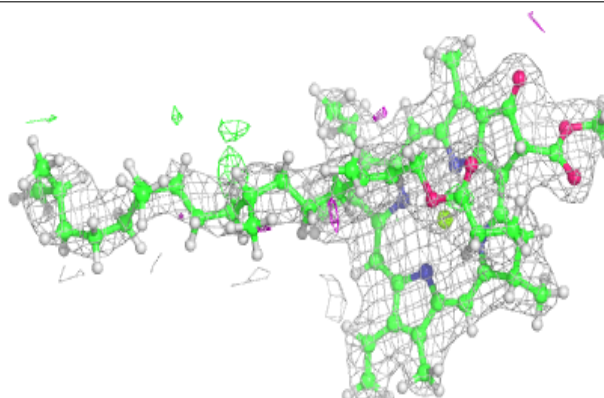


Electron density around DGD C 517:

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

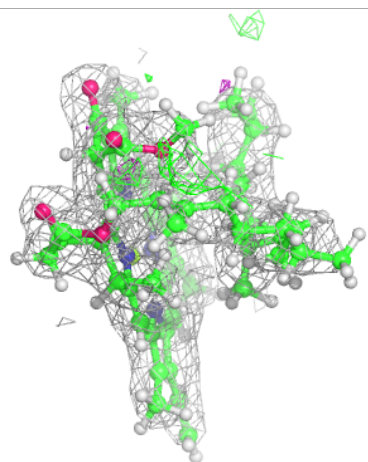
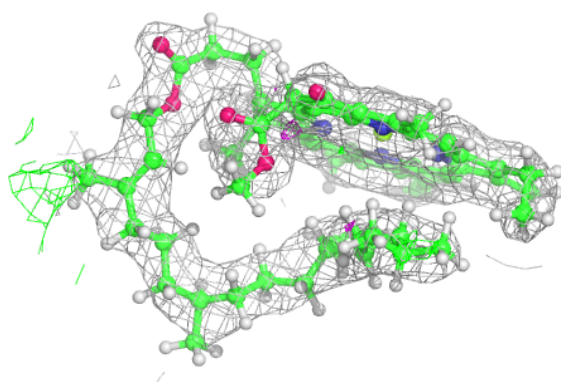
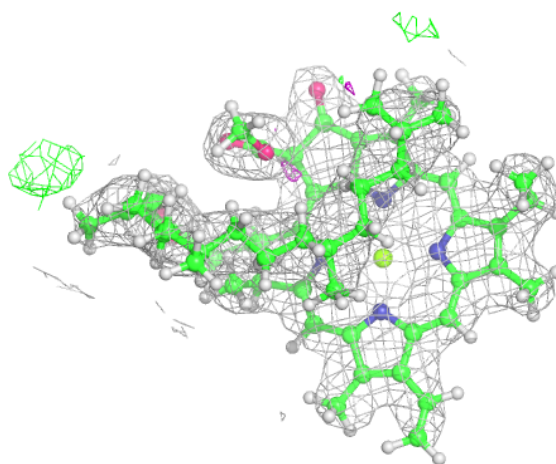
**Electron density around CLA B 614:**

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



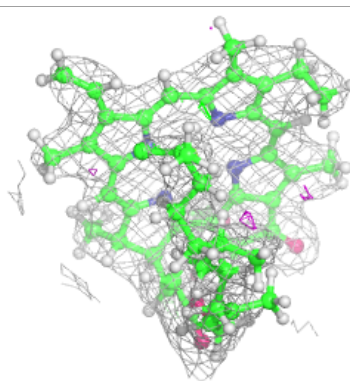
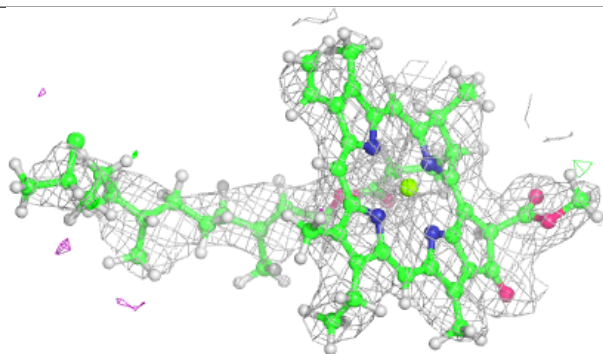
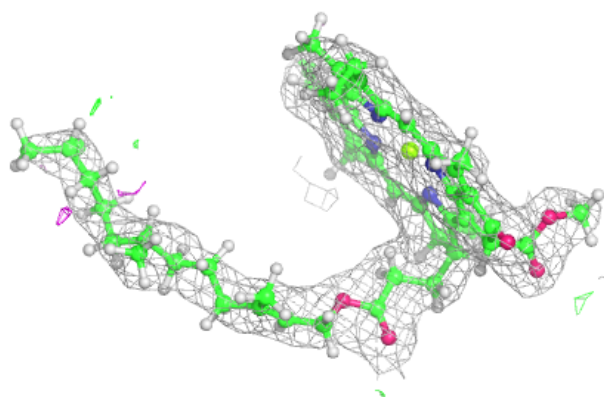
Electron density around CLA C 510:

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

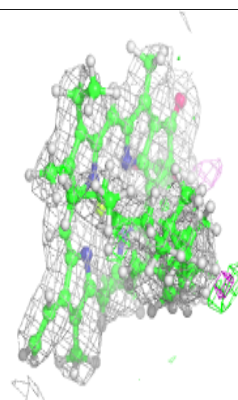
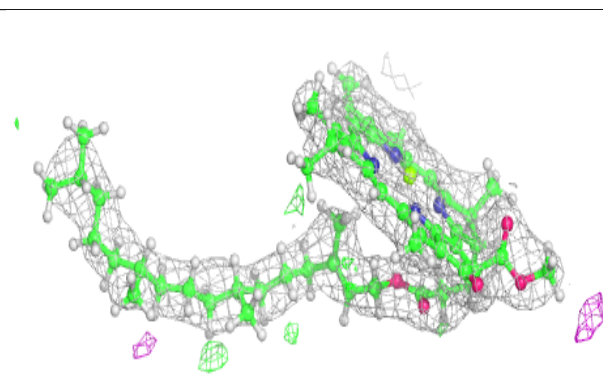
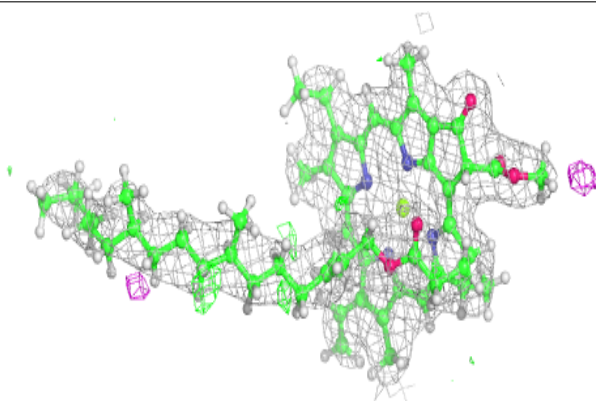


Electron density around CLA c 504:

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

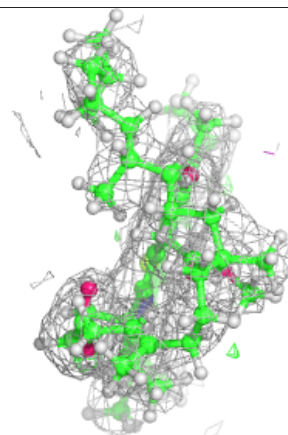
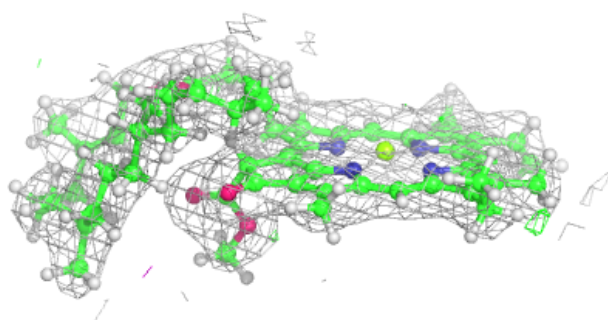
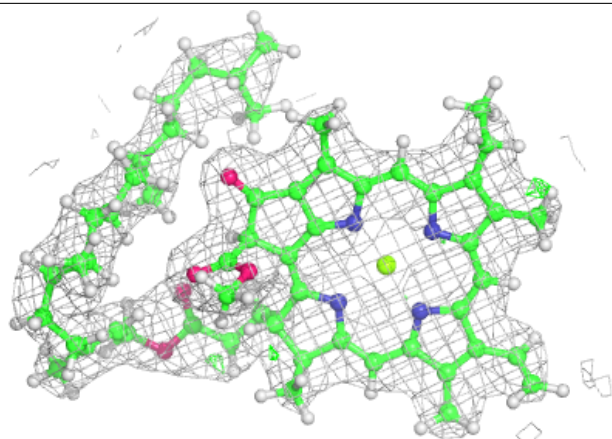
**Electron density around CLA b 608:**

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

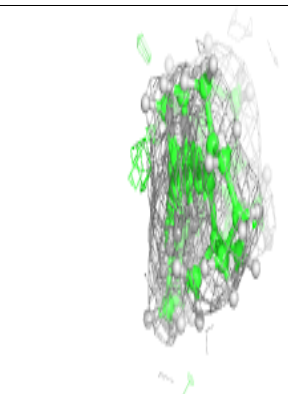
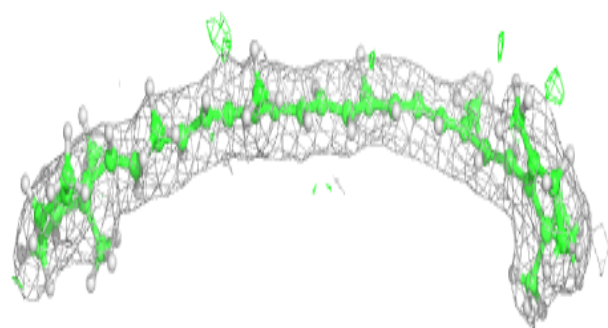
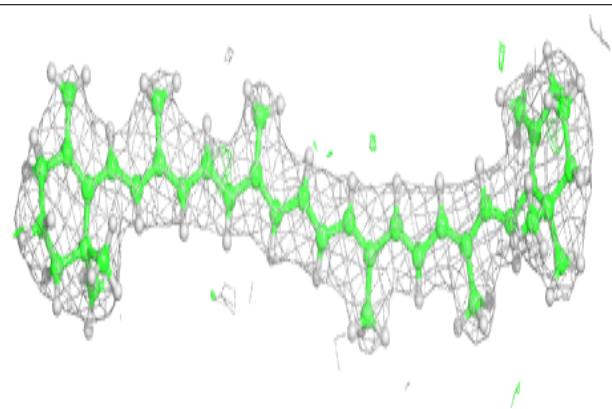


Electron density around CLA b 610:

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

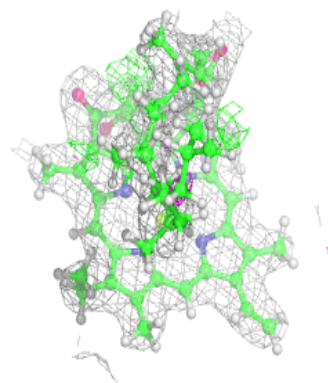
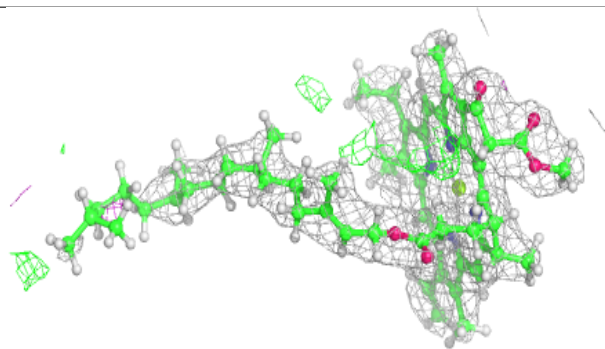
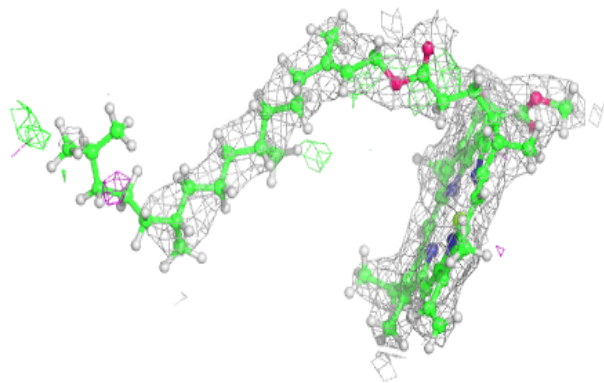
**Electron density around BCR t 101:**

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

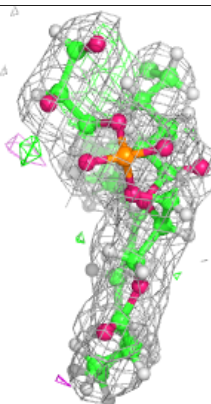
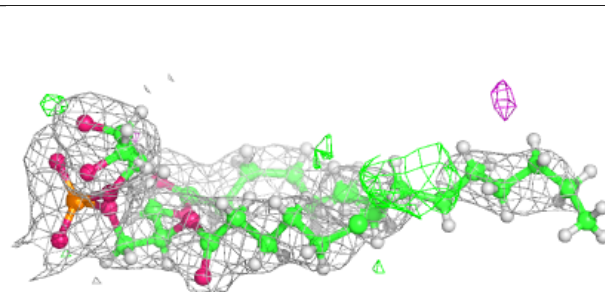
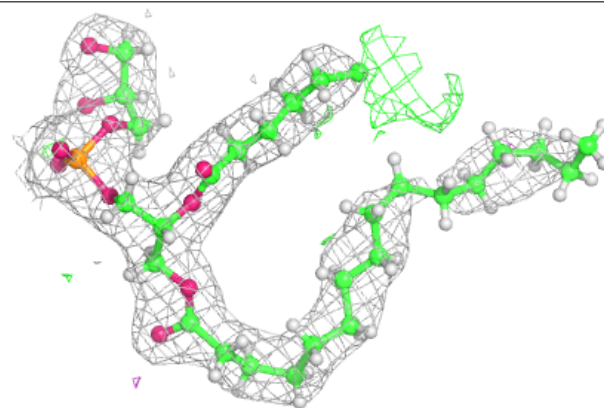


Electron density around CLA C 508:

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

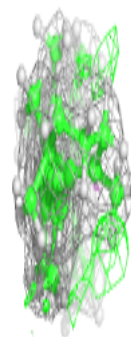
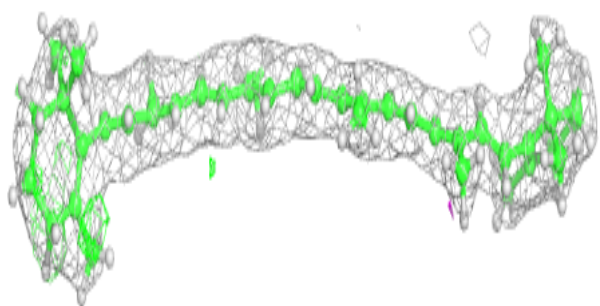
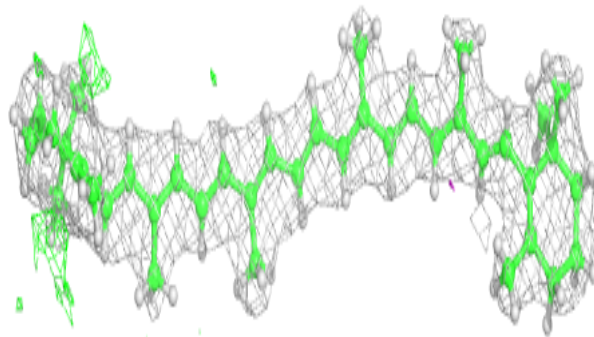
**Electron density around LHG d 409:**

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



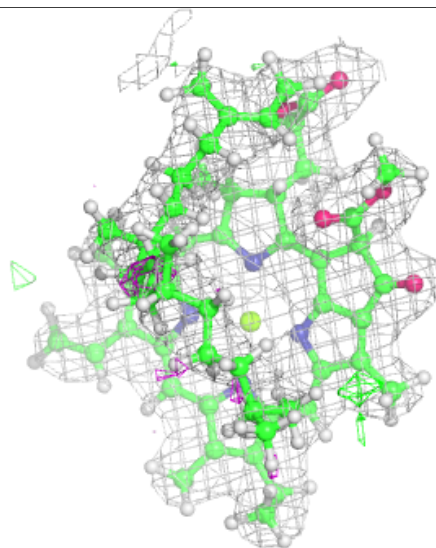
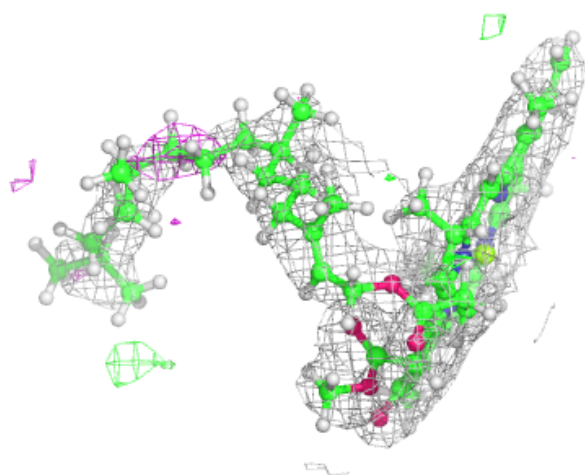
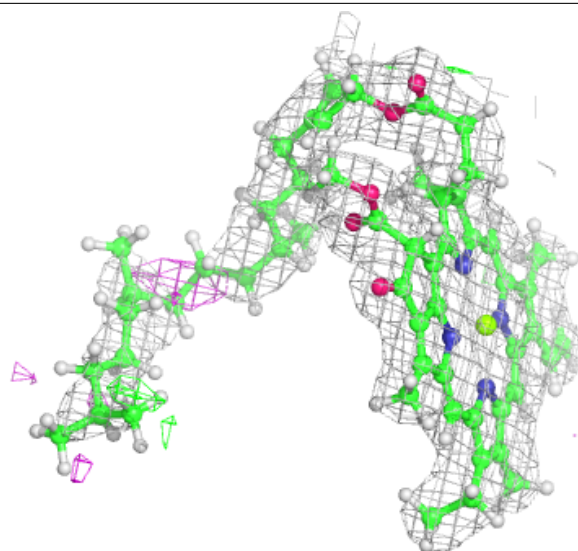
Electron density around BCR b 617:

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



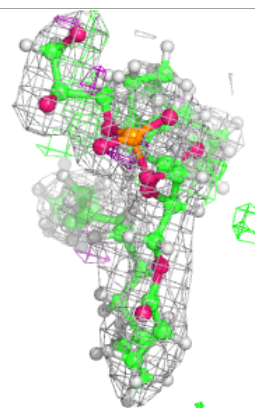
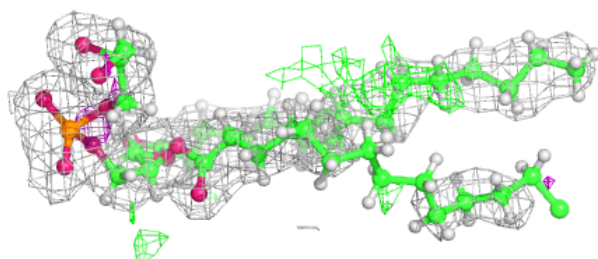
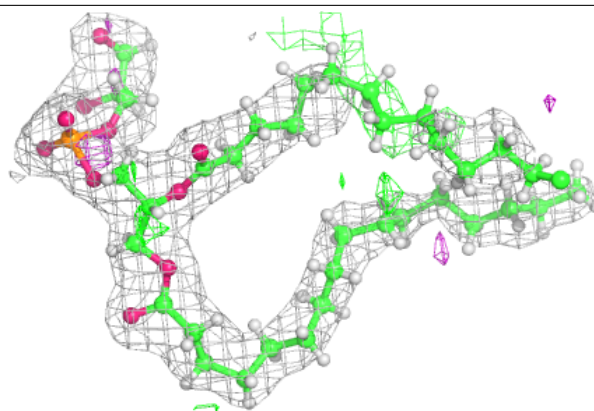
Electron density around CLA b 613:

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

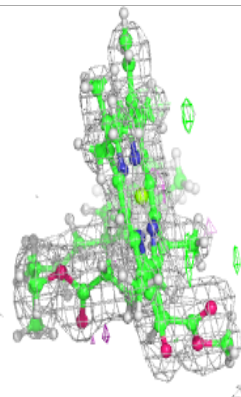
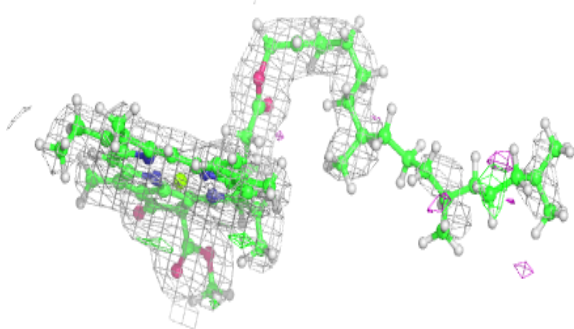
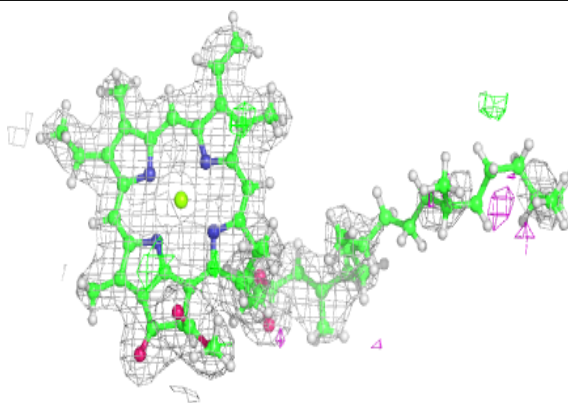


Electron density around LHG A 412:

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

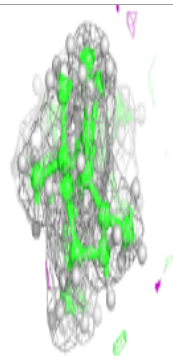
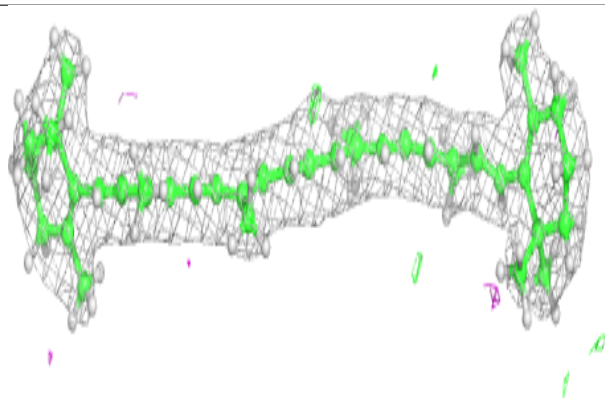
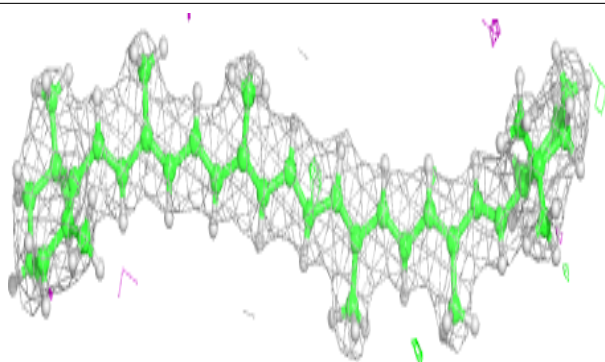
**Electron density around CLA A 403:**

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

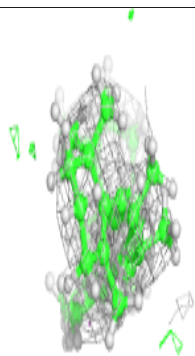
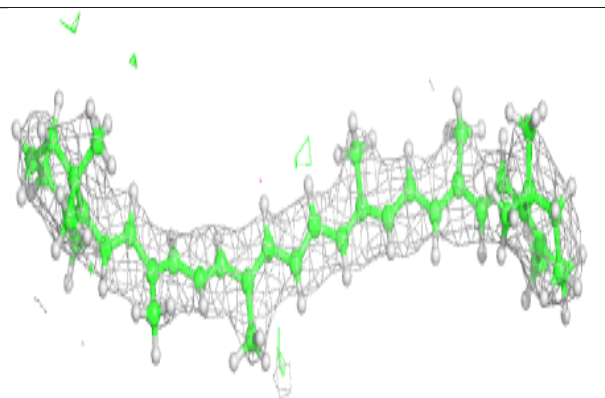
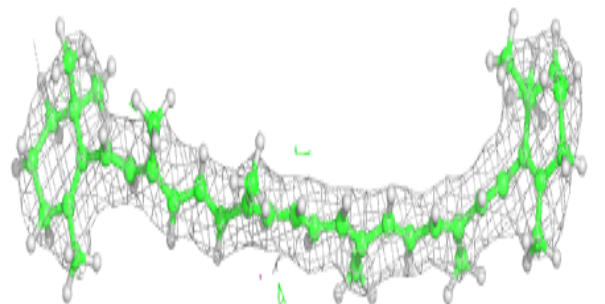


Electron density around BCR a 405:

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

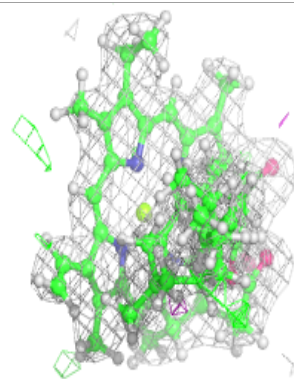
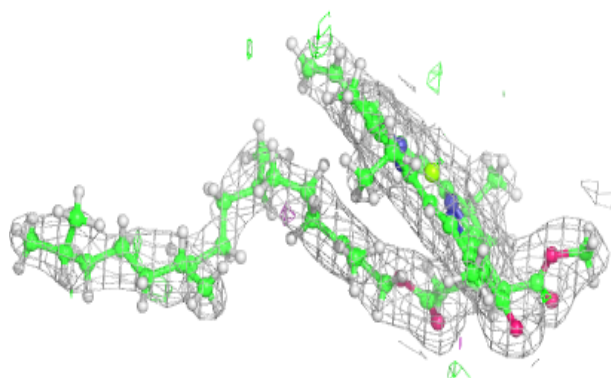
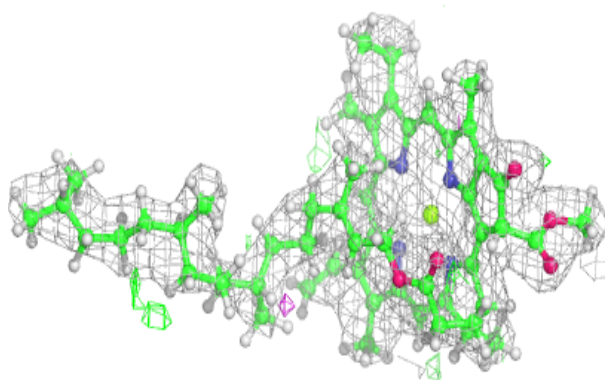
**Electron density around BCR C 516:**

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

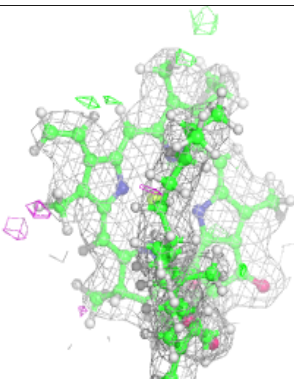
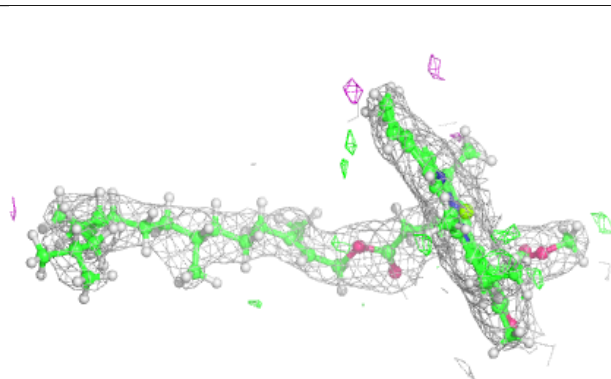
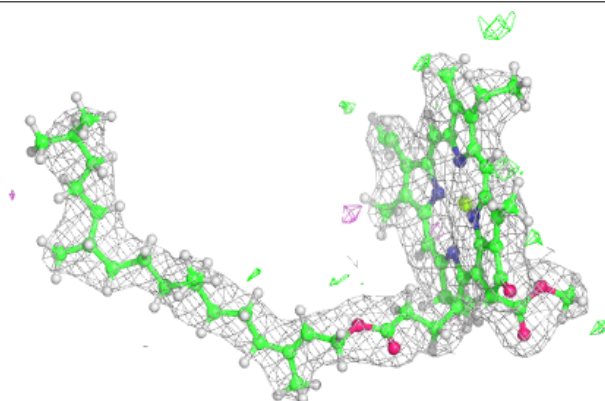


Electron density around CLA c 505:

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

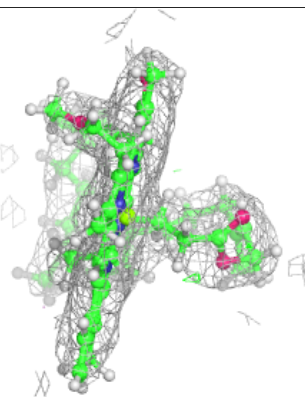
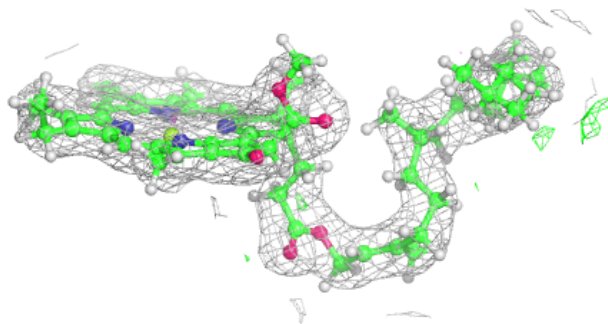
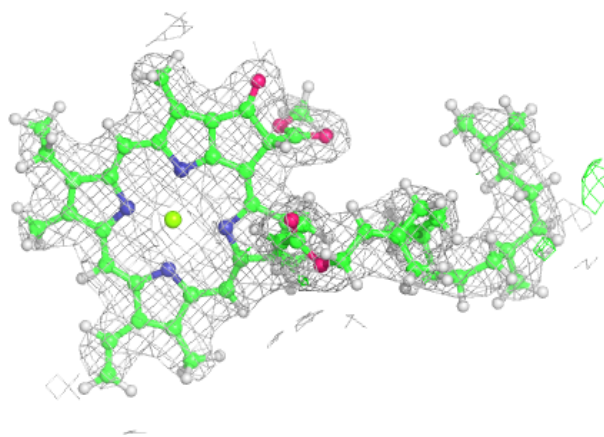
**Electron density around CLA B 609:**

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



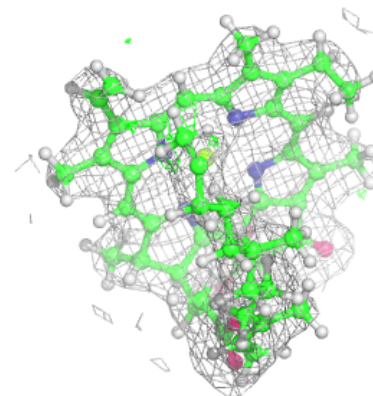
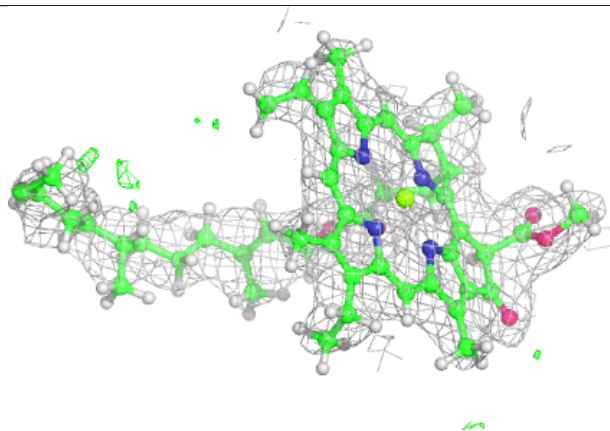
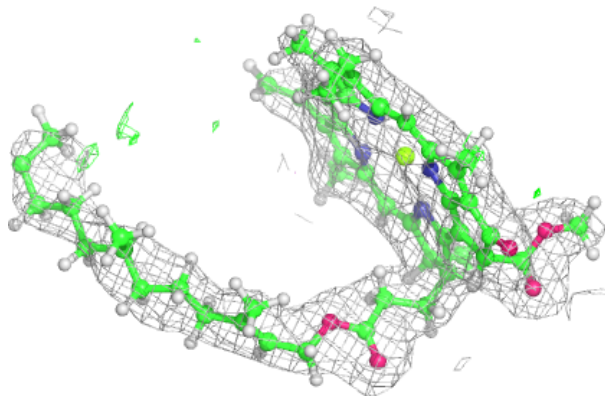
Electron density around CLA b 612:

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

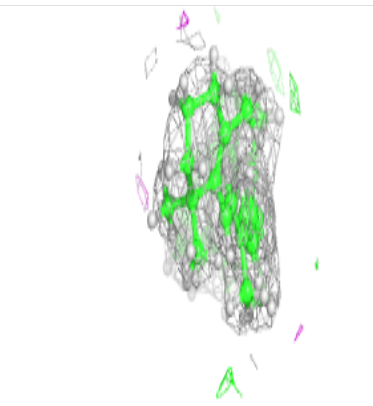
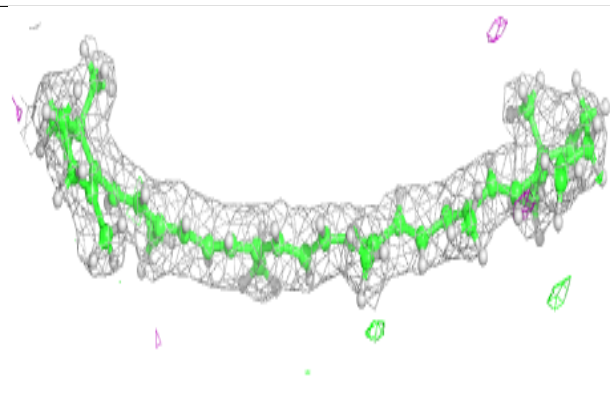
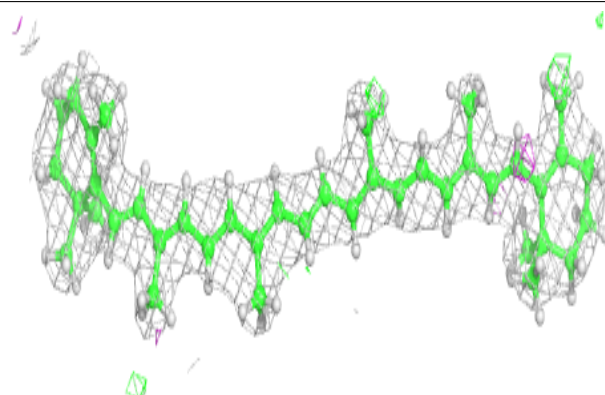


Electron density around CLA C 504:

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

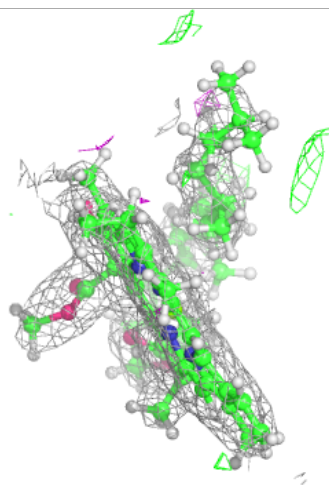
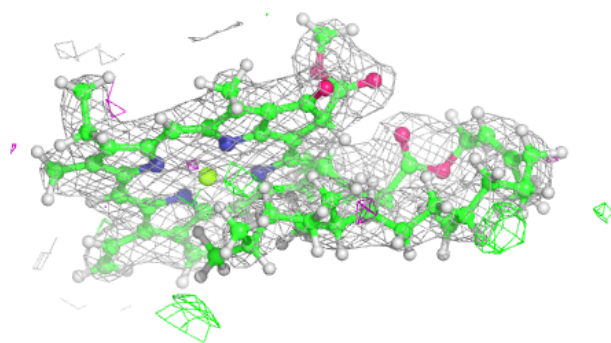
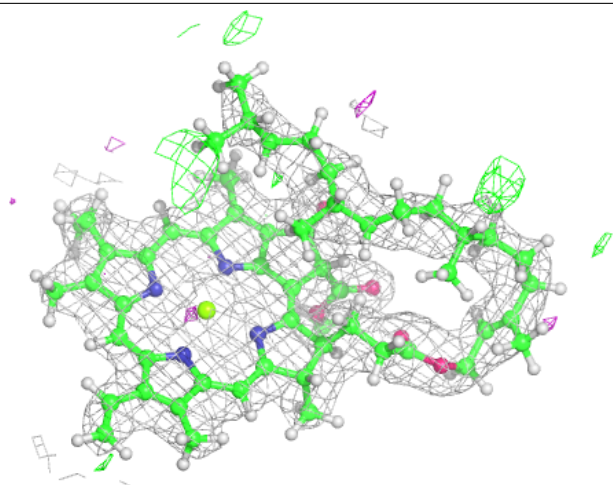
**Electron density around BCR T 101:**

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



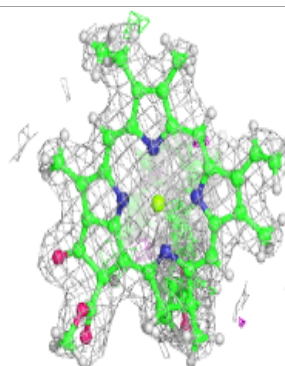
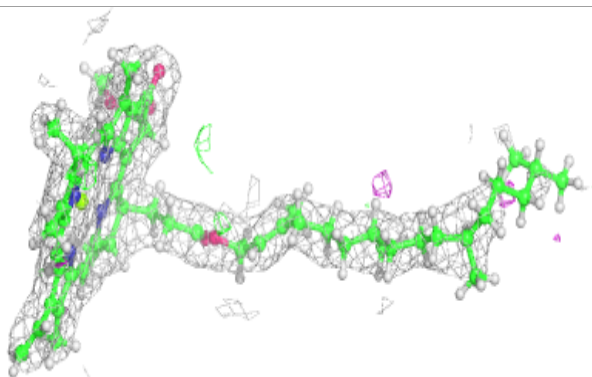
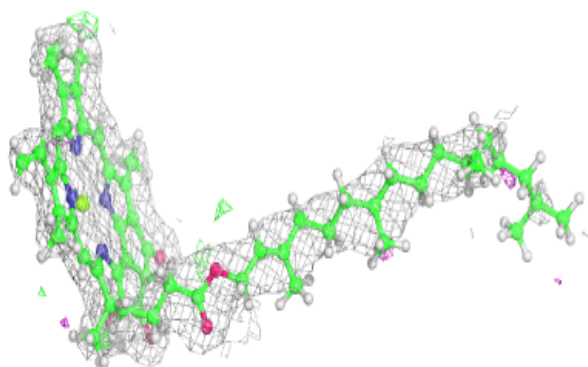
Electron density around CLA C 509:

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

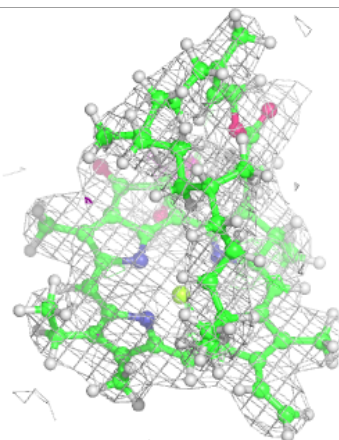
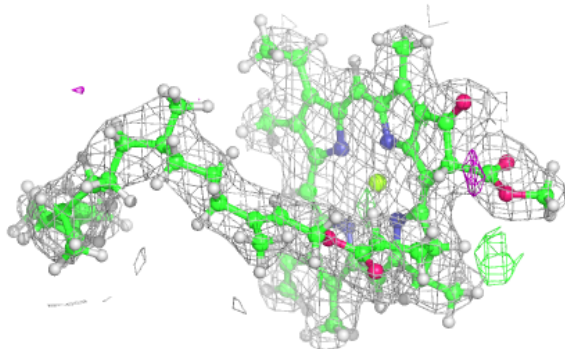
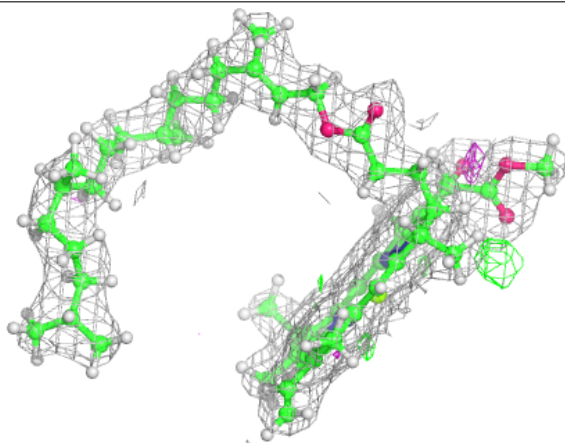


Electron density around CLA b 604:

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

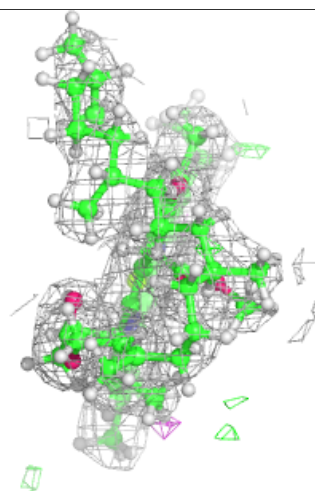
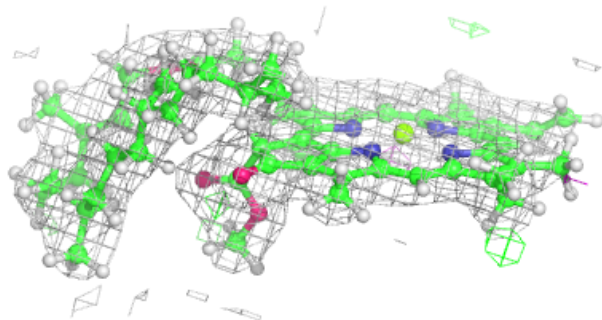
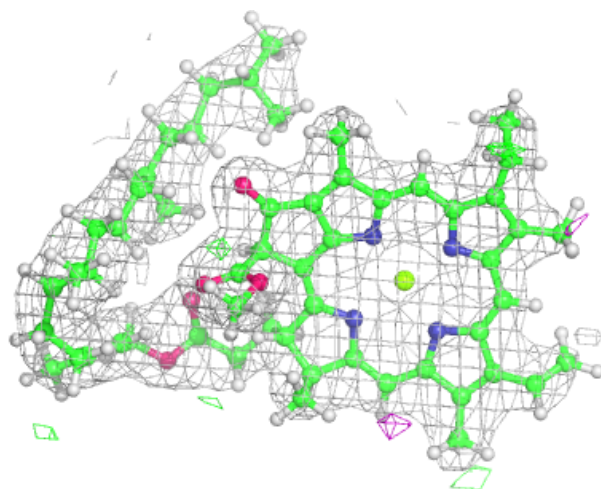
**Electron density around CLA b 611:**

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



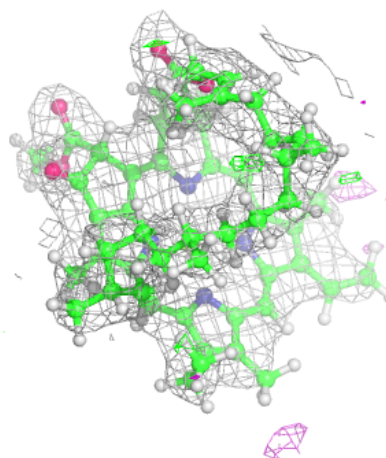
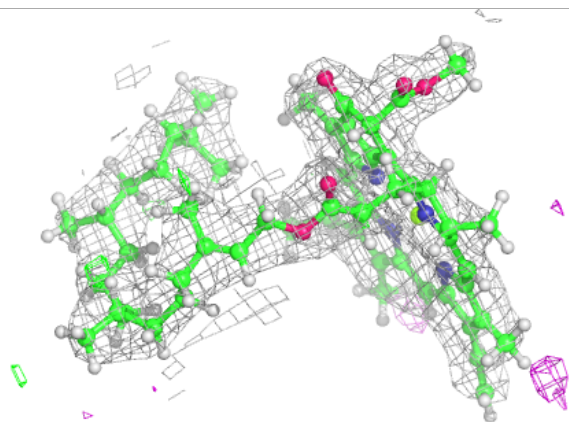
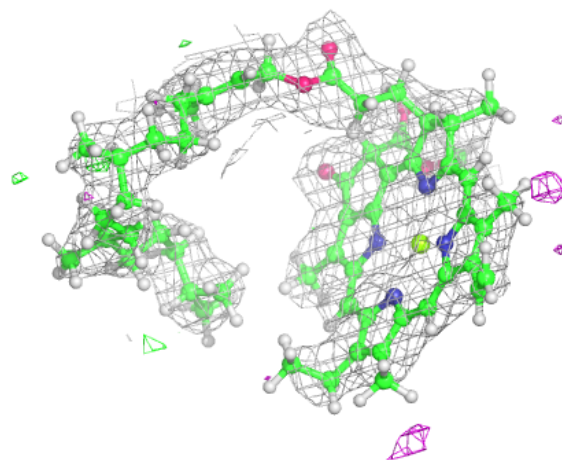
Electron density around CLA B 610:

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



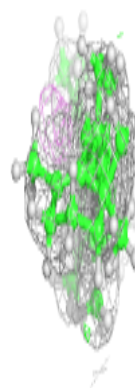
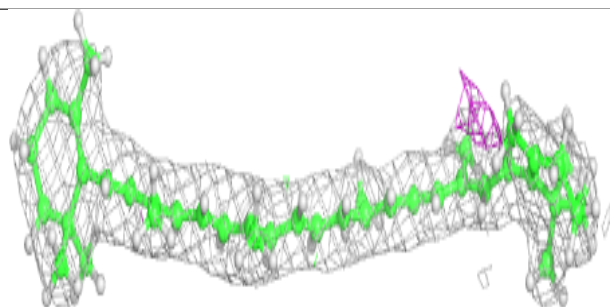
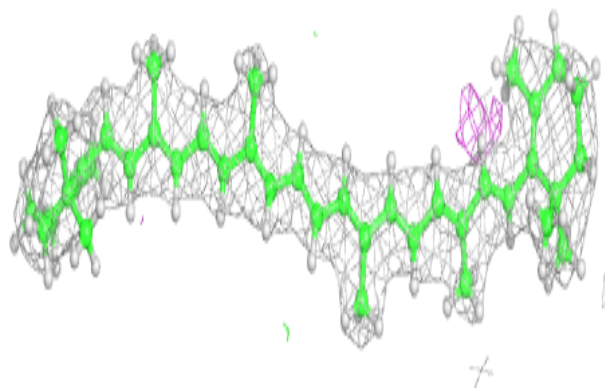
Electron density around CLA c 503:

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

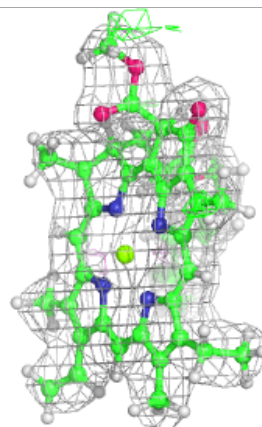
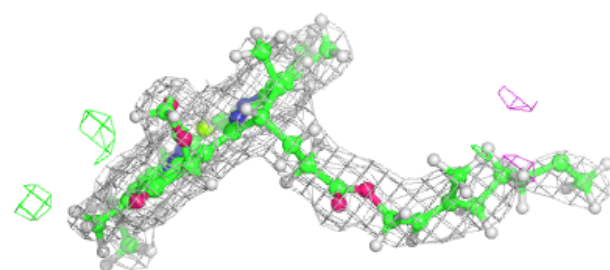
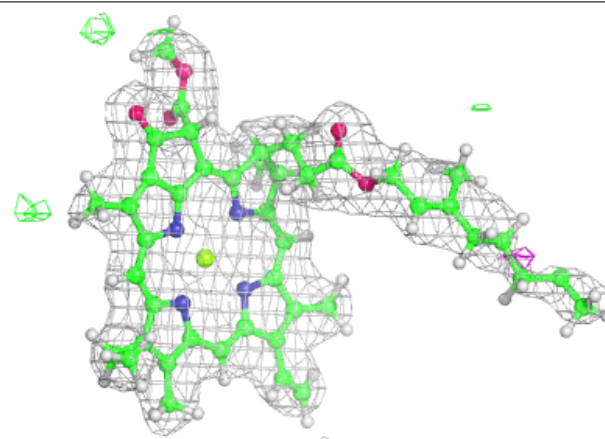


Electron density around BCR B 617:

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

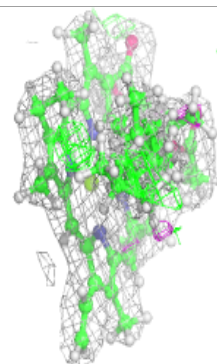
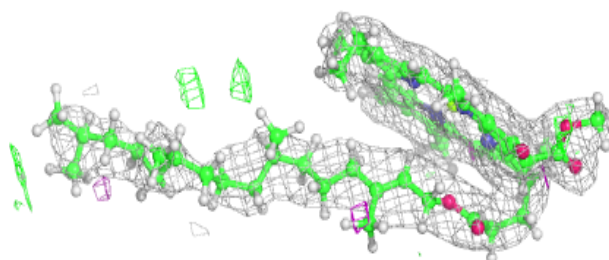
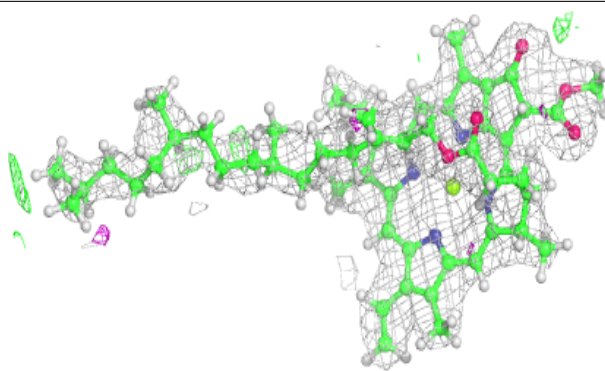
**Electron density around CLA A 406:**

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

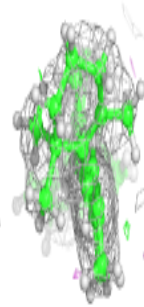
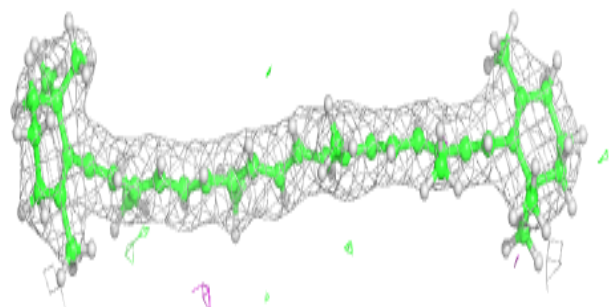
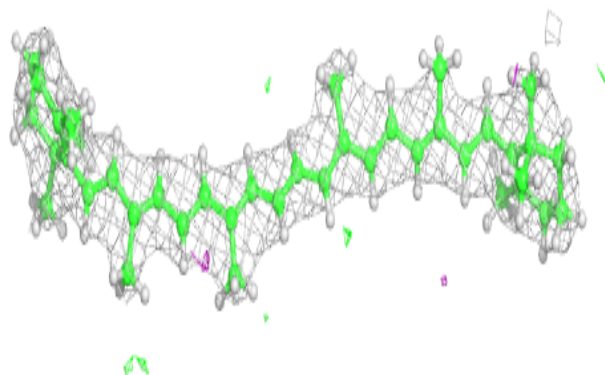


Electron density around CLA b 614:

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

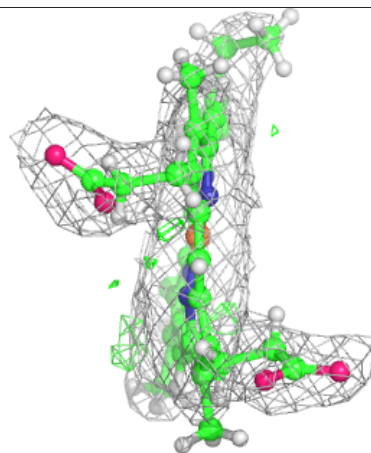
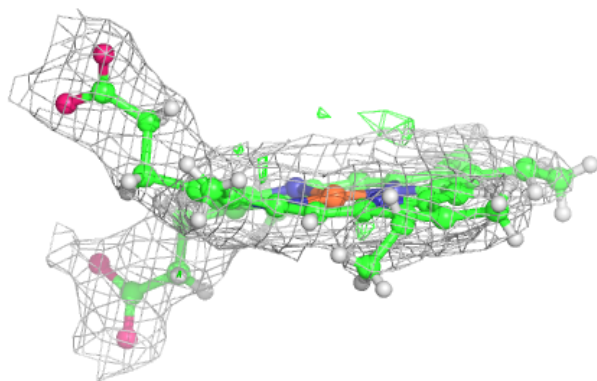
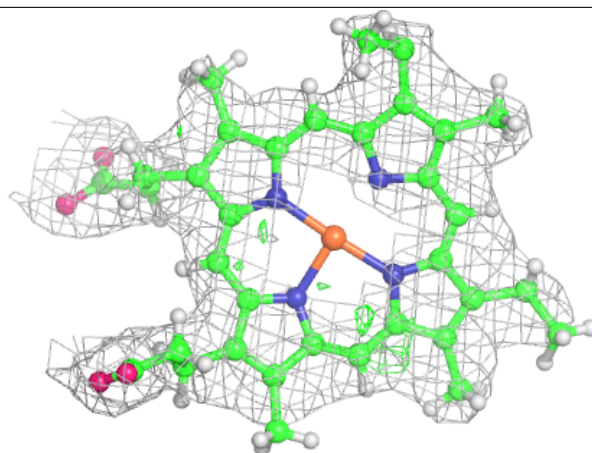
**Electron density around BCR c 515:**

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

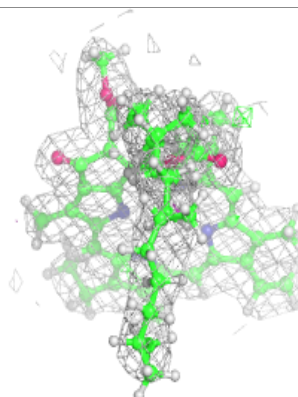
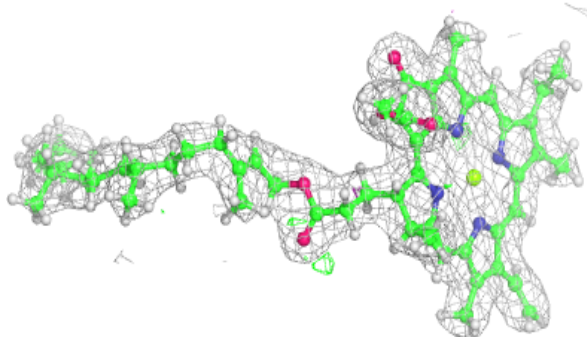
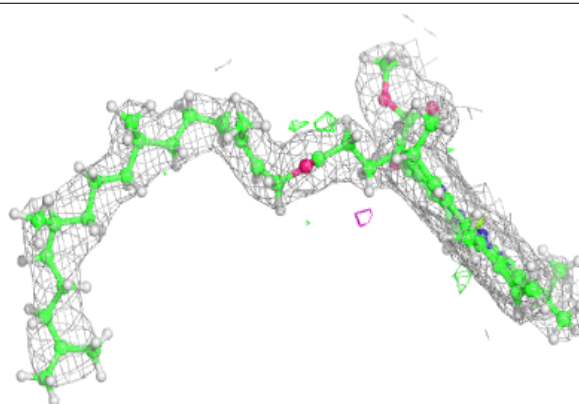


Electron density around HEC F 101:

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

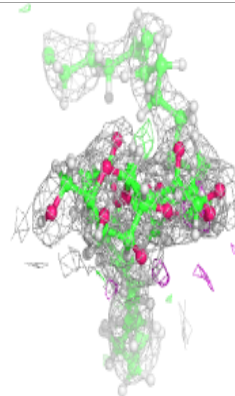
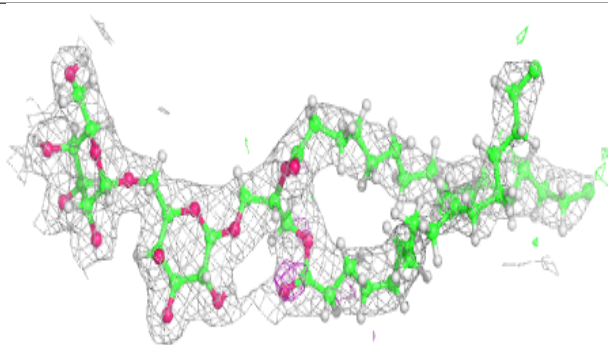
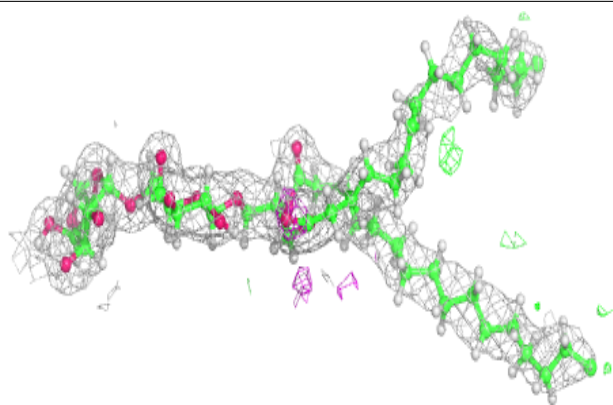
**Electron density around CLA D 402:**

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

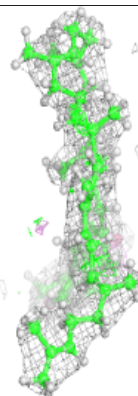
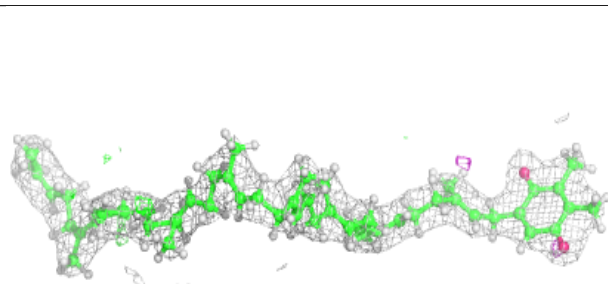
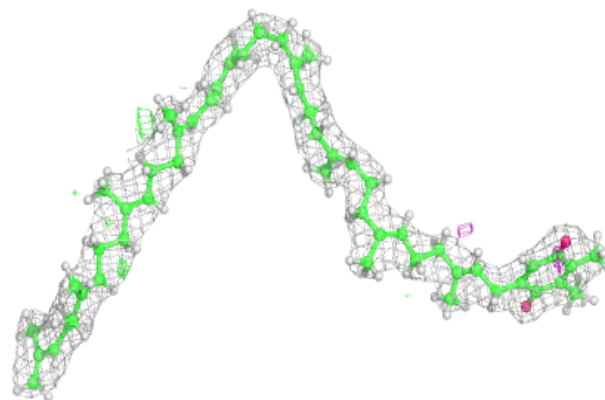


Electron density around DGD c 517:

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

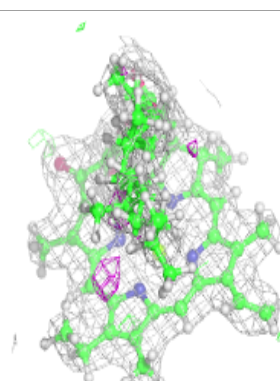
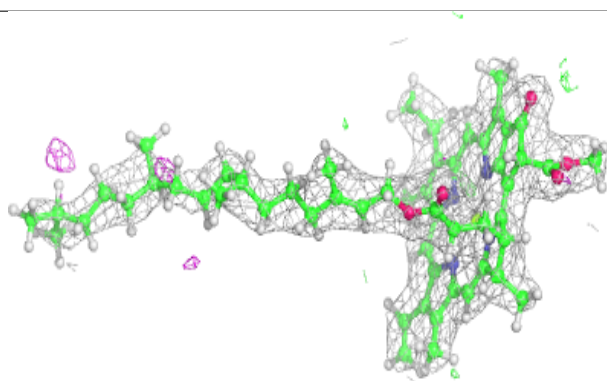
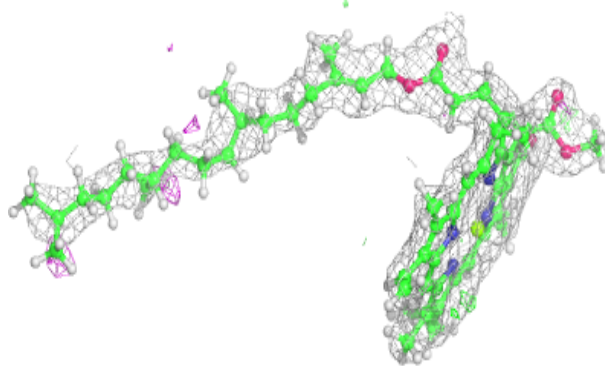
**Electron density around PL9 d 407:**

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

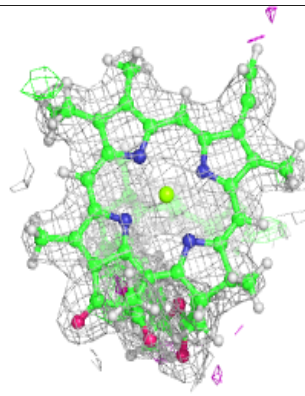
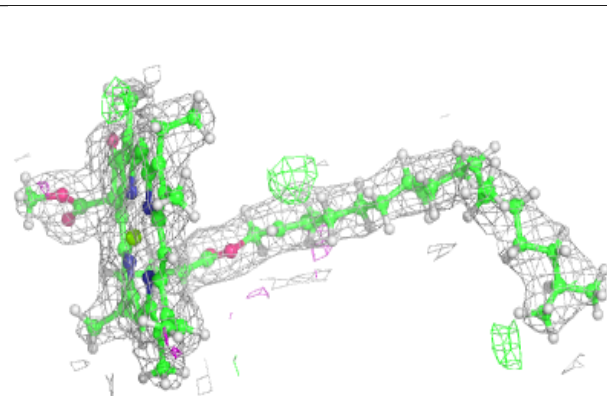
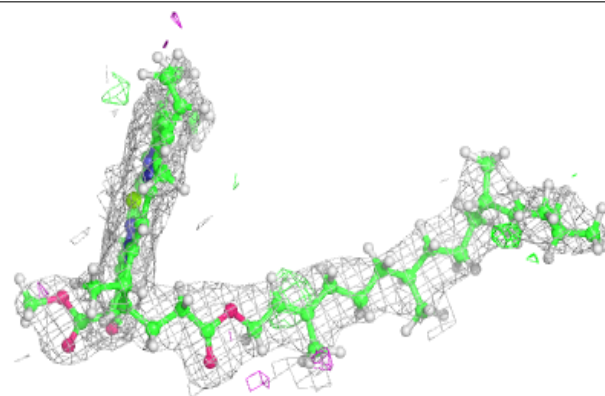


Electron density around CLA b 607:

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

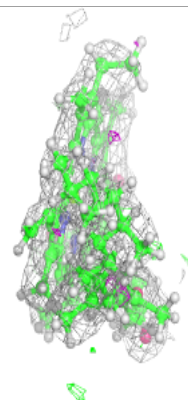
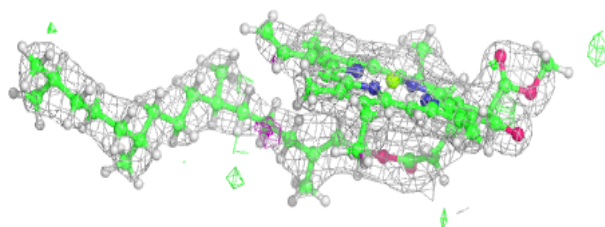
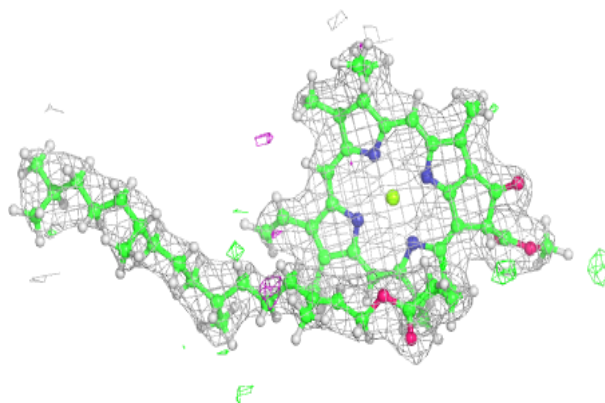
**Electron density around CLA b 605:**

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

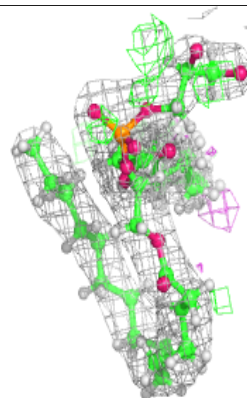
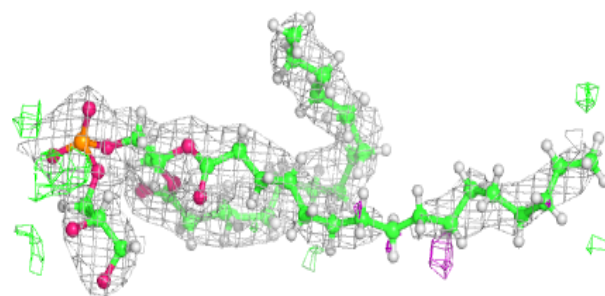
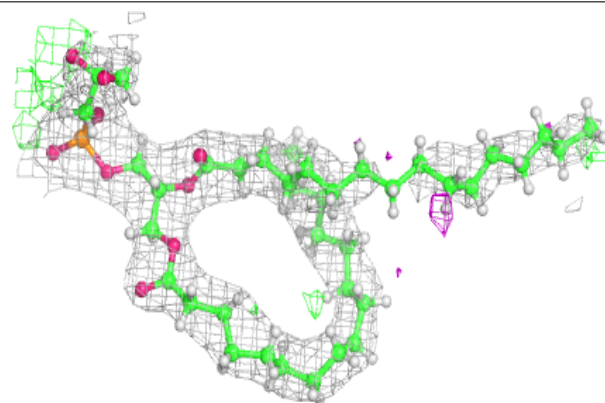


Electron density around CLA c 501:

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

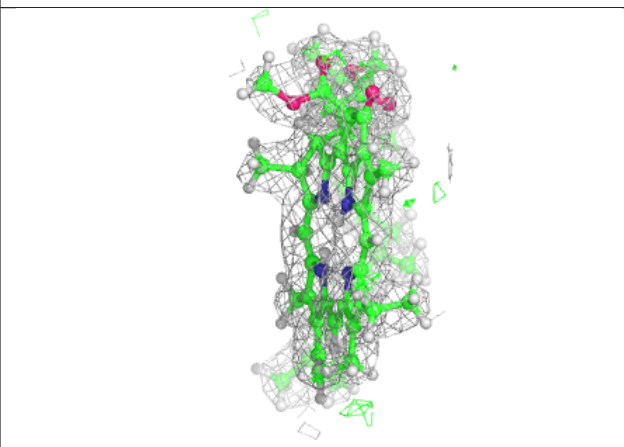
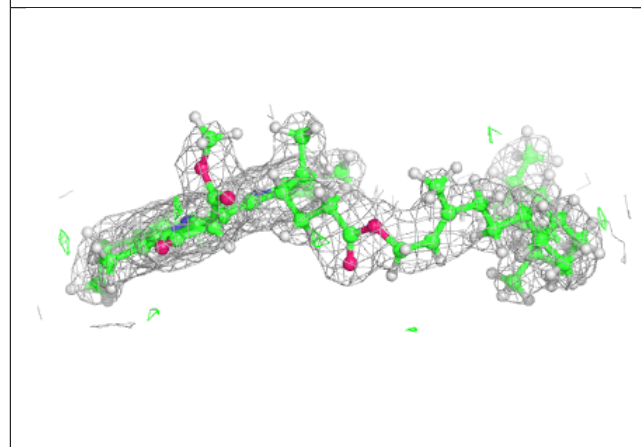
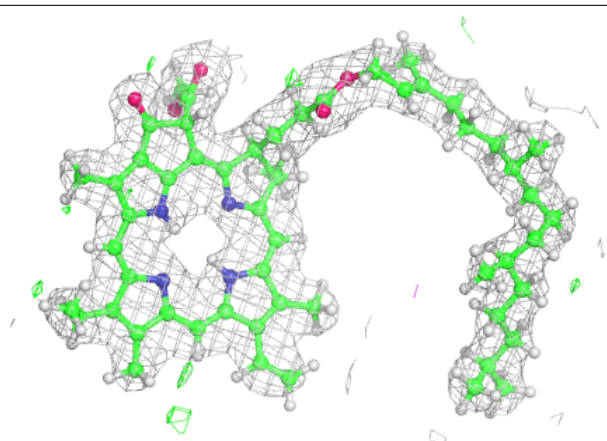
**Electron density around LHG a 410:**

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

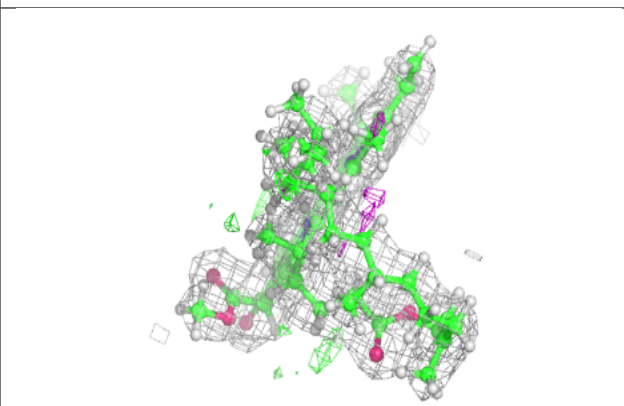
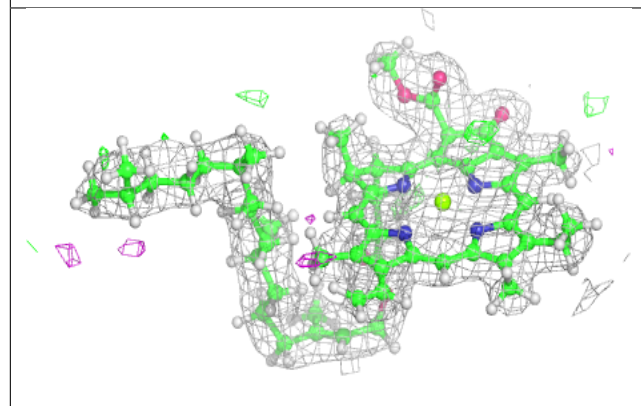
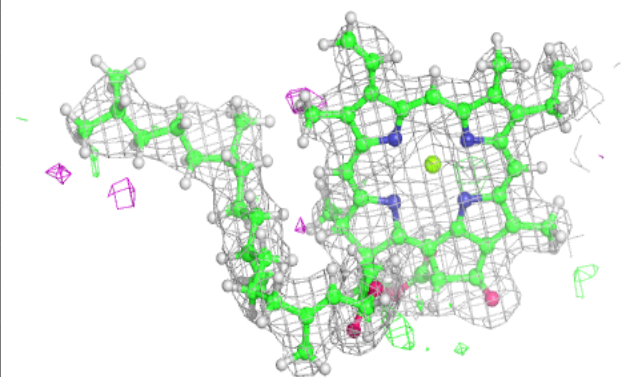


Electron density around PHO a 403:

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

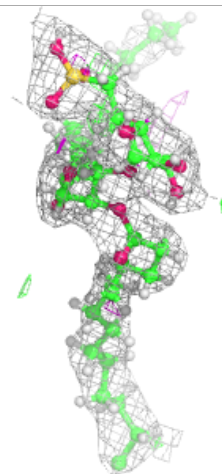
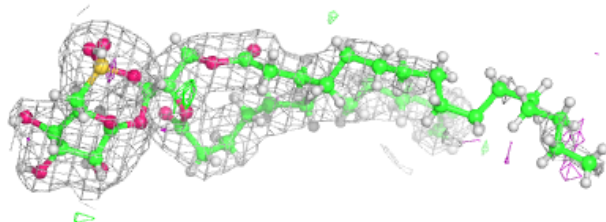
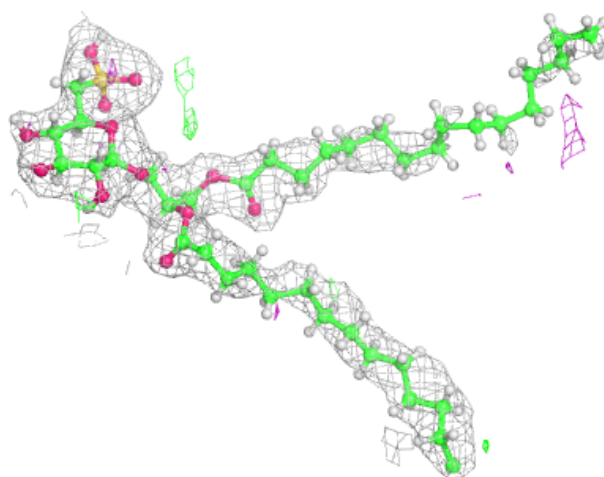
**Electron density around CLA d 404:**

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



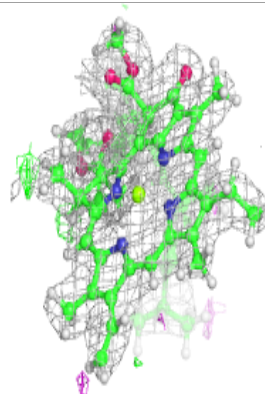
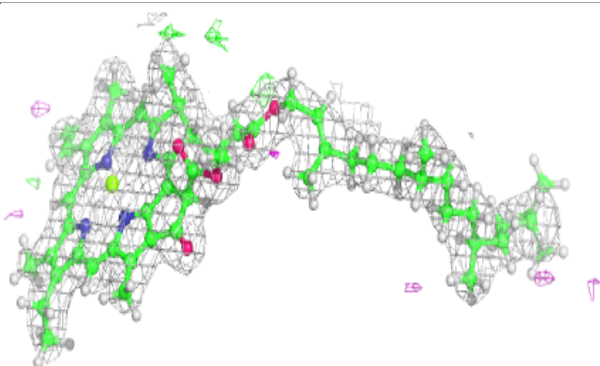
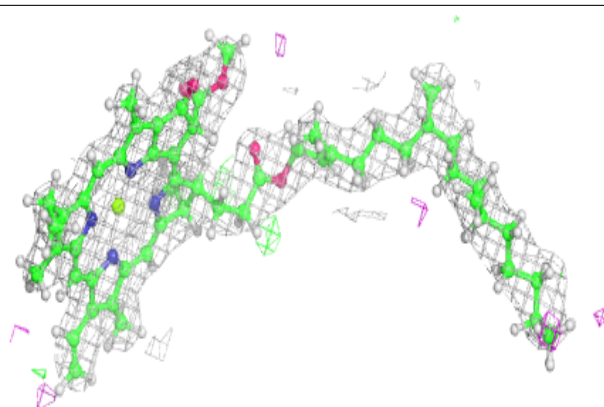
Electron density around SQD A 413:

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

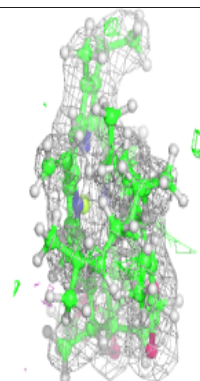
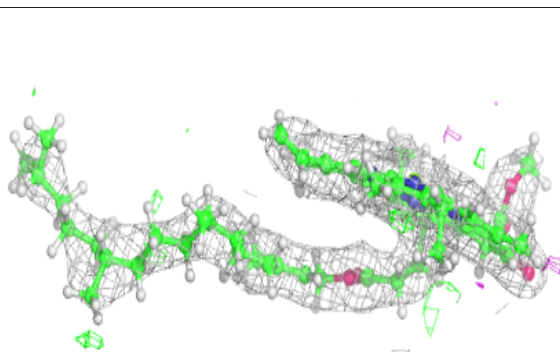
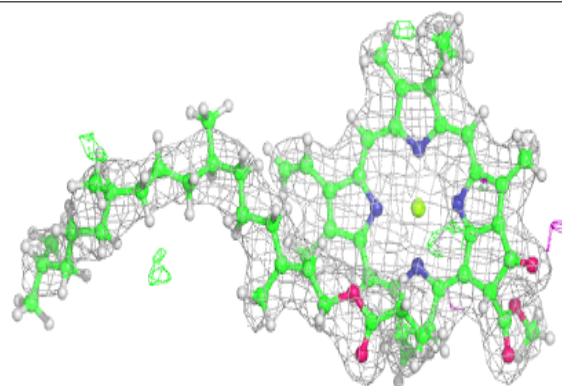


Electron density around CLA a 402:

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

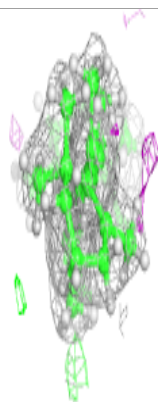
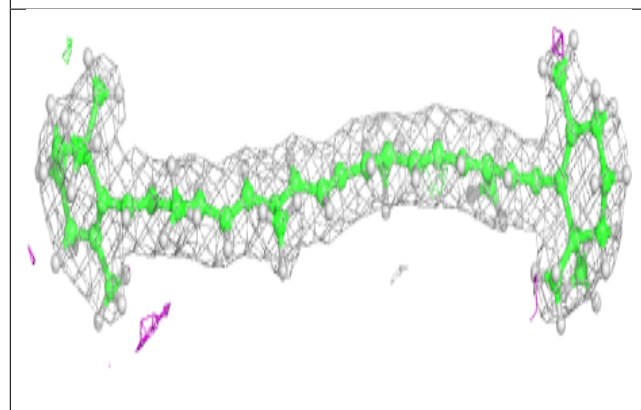
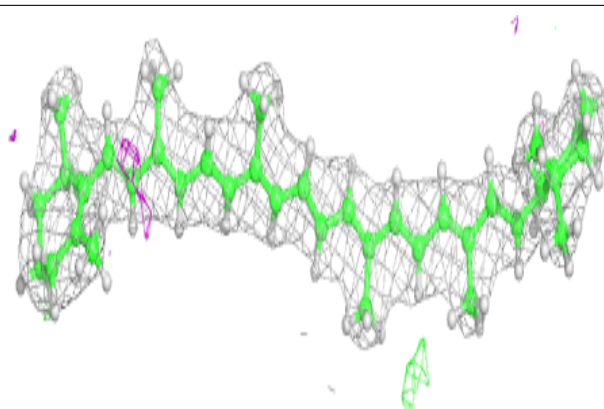
**Electron density around CLA B 603:**

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



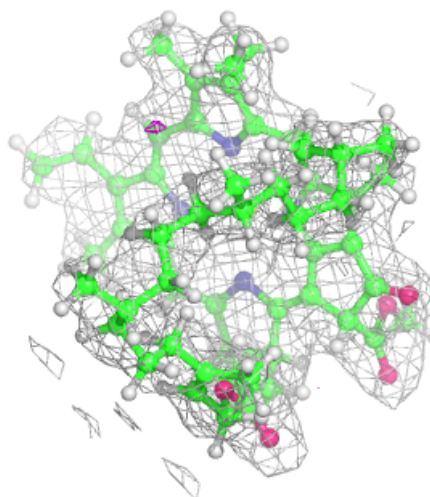
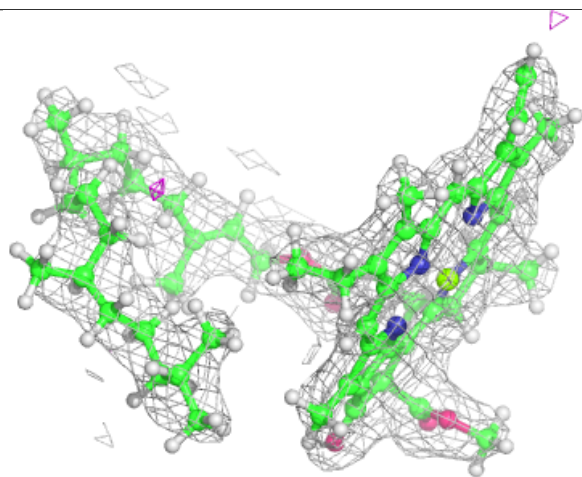
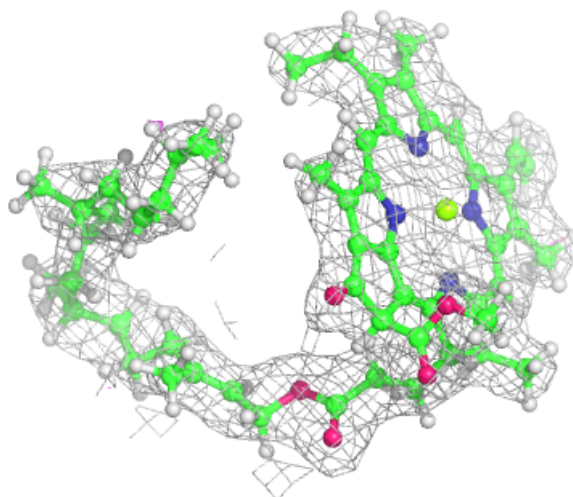
Electron density around BCR A 407:

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



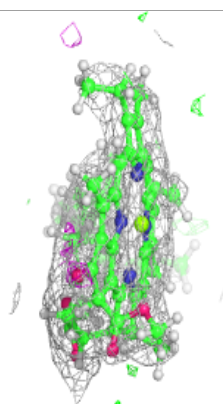
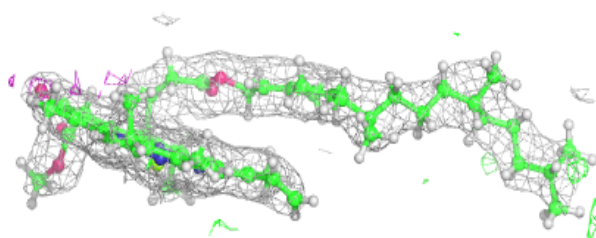
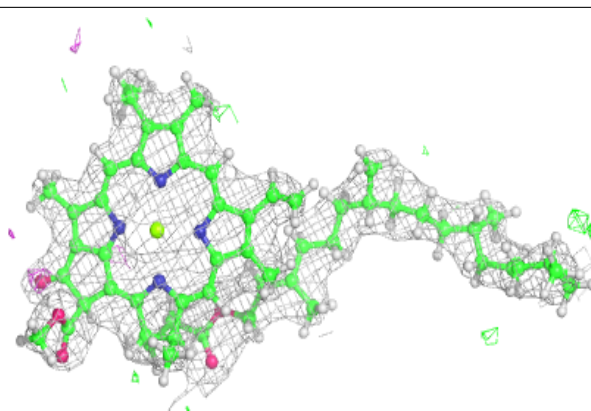
Electron density around CLA C 503:

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

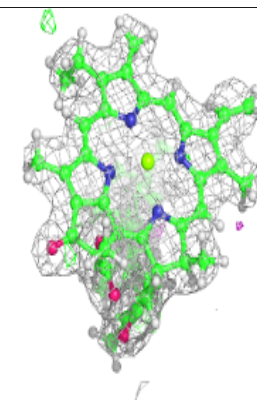
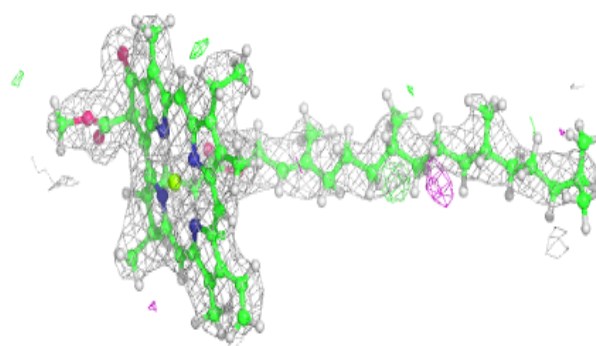
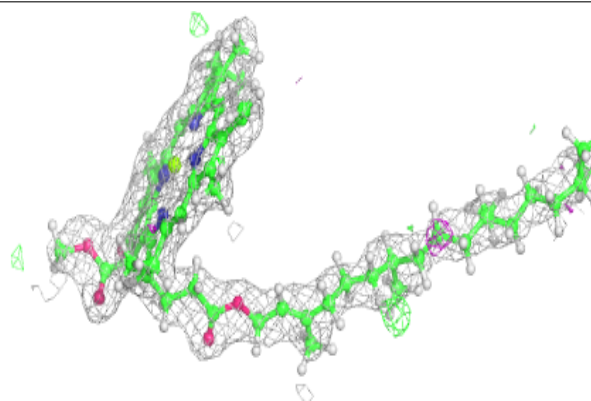


Electron density around CLA b 603:

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

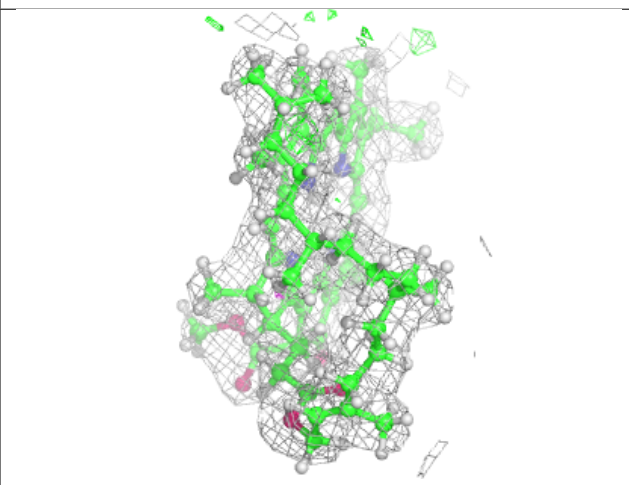
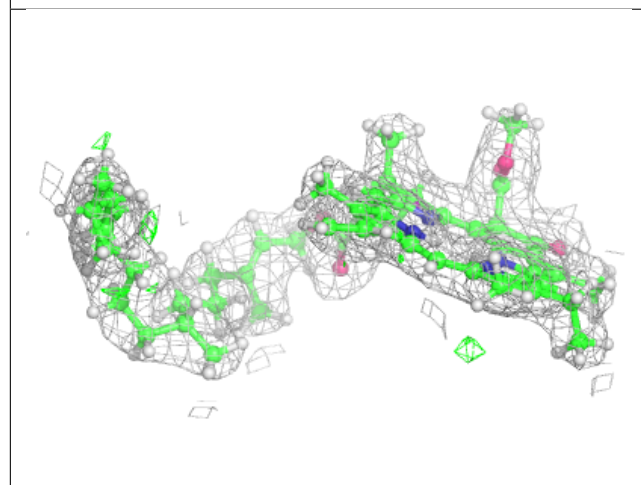
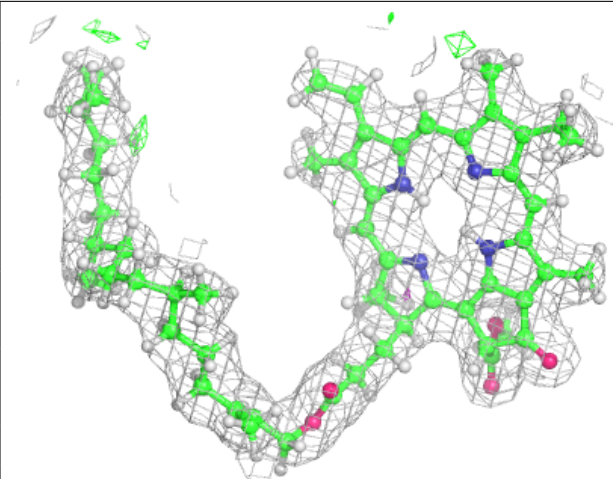
**Electron density around CLA B 607:**

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



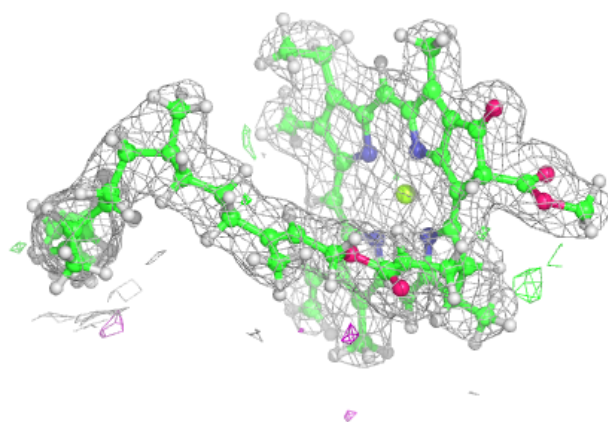
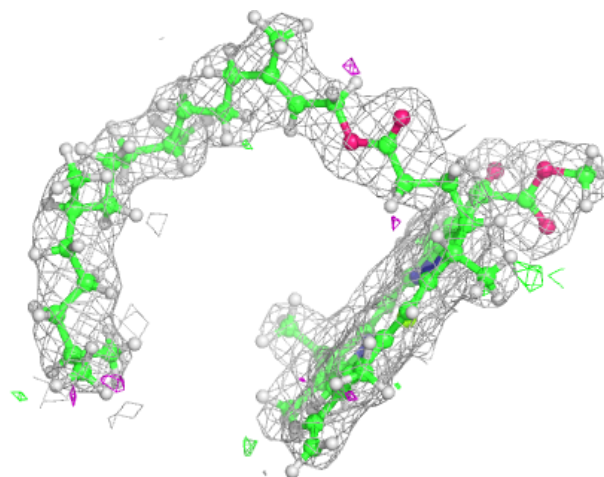
Electron density around PHO A 405:

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



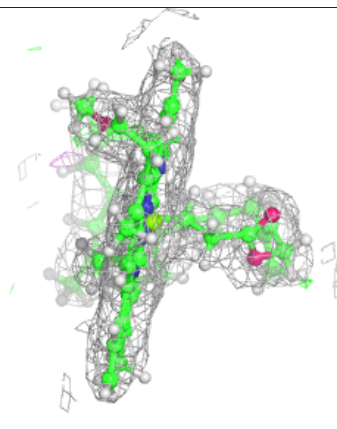
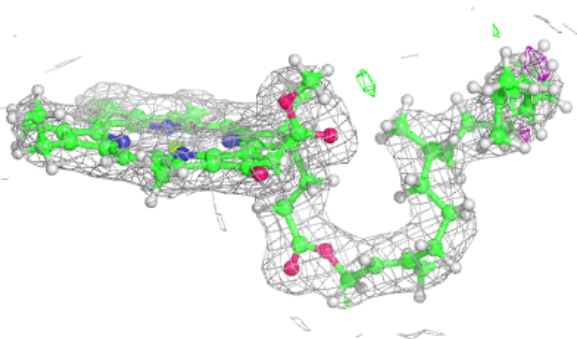
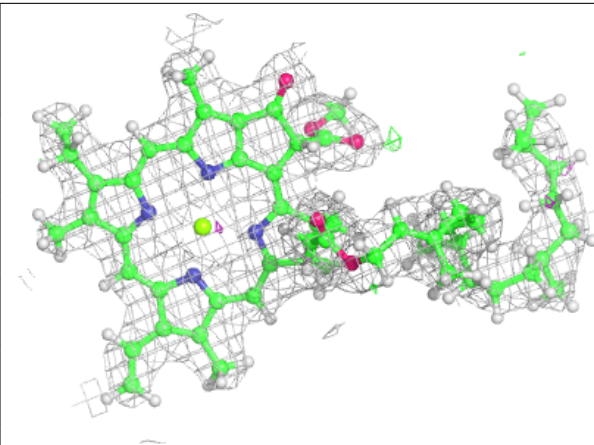
Electron density around CLA B 611:

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

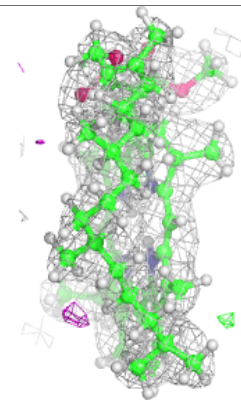
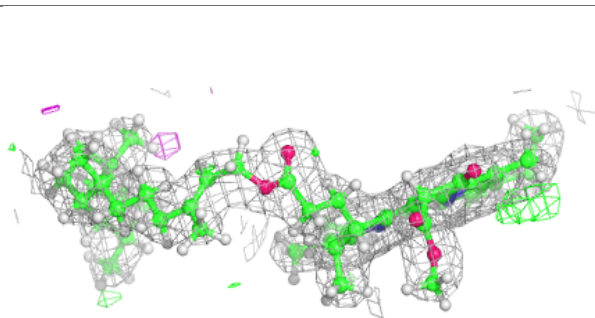
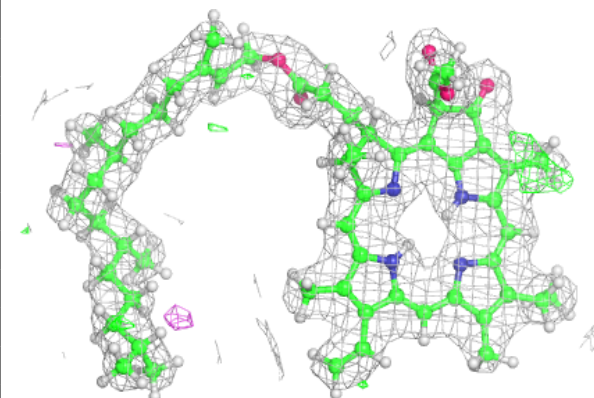


Electron density around CLA B 612:

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

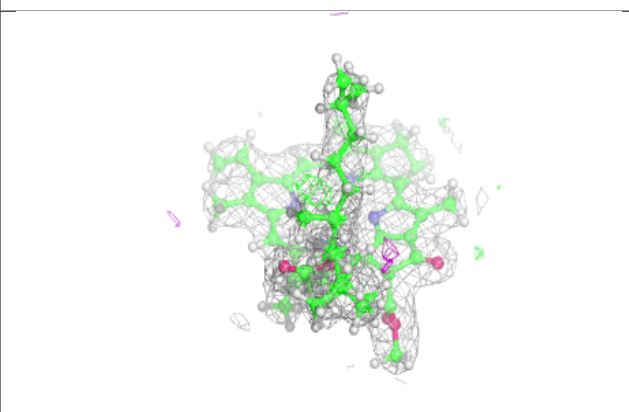
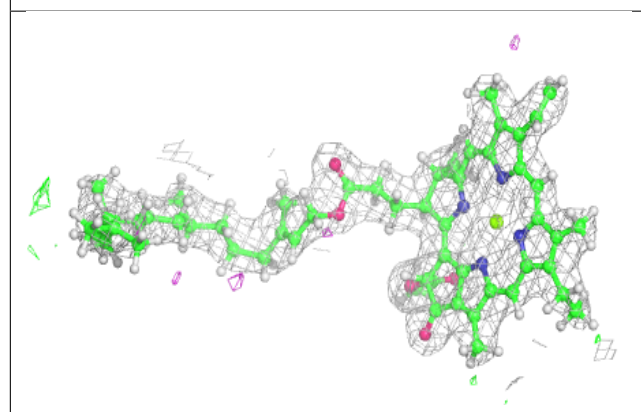
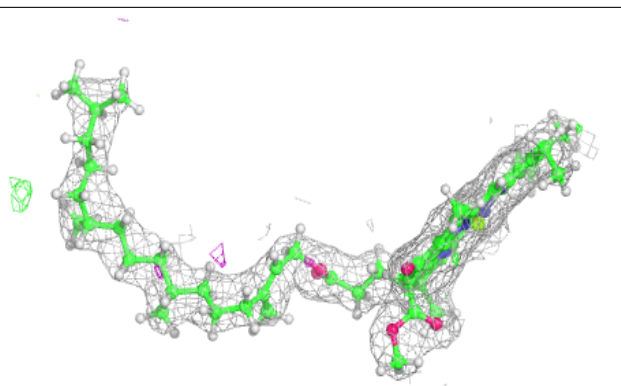
**Electron density around PHO A 404:**

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

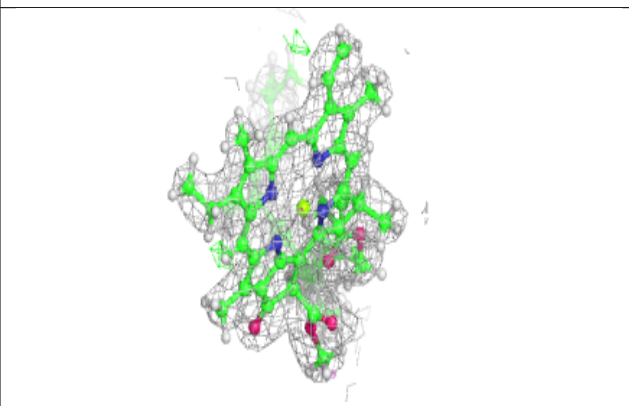
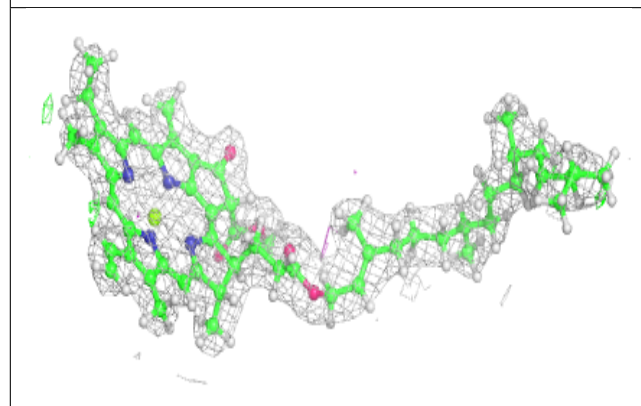
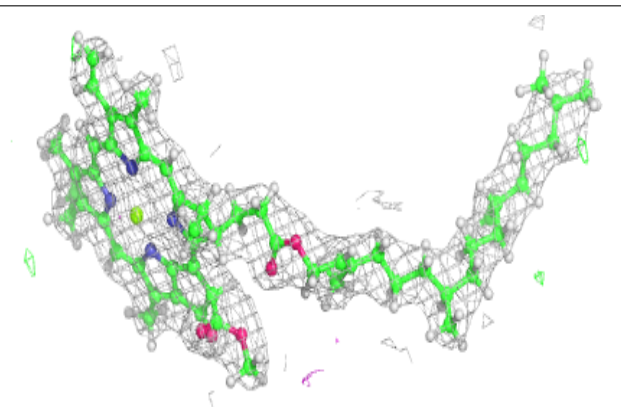


Electron density around CLA d 403:

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

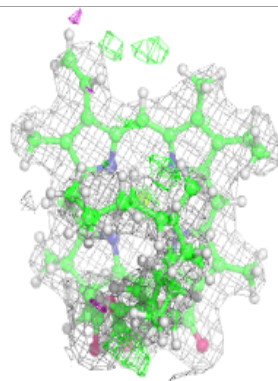
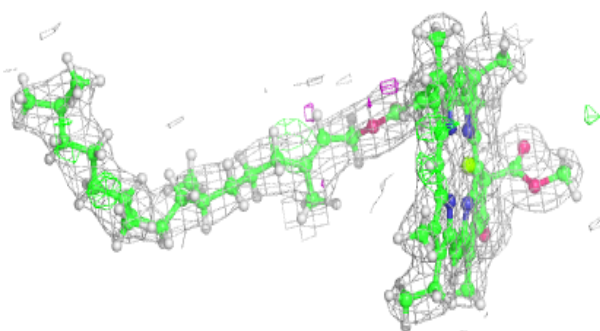
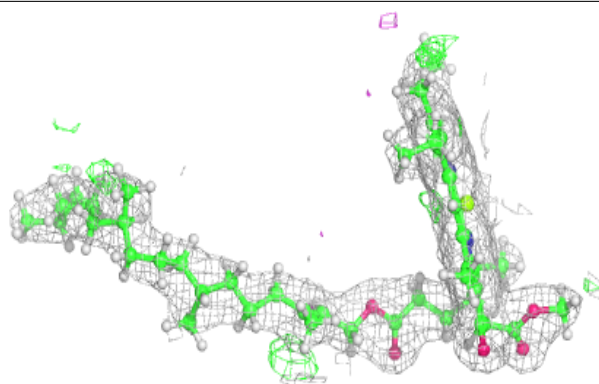
**Electron density around CLA A 402:**

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

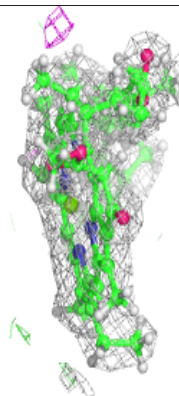
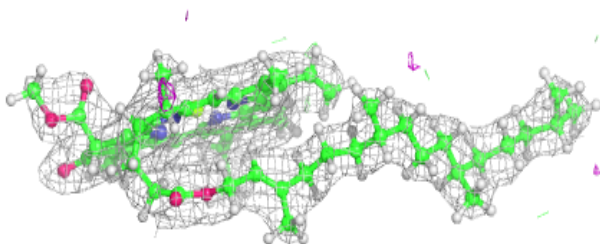
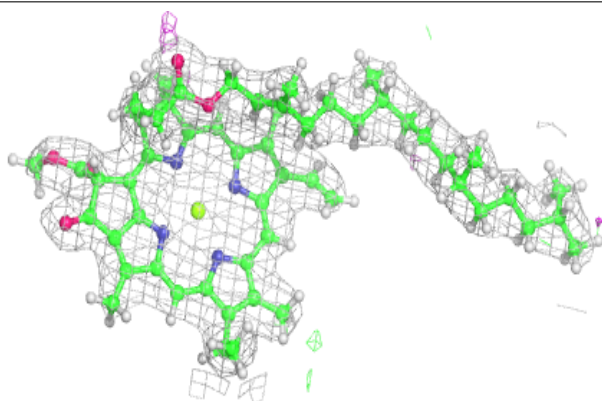


Electron density around CLA B 605:

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

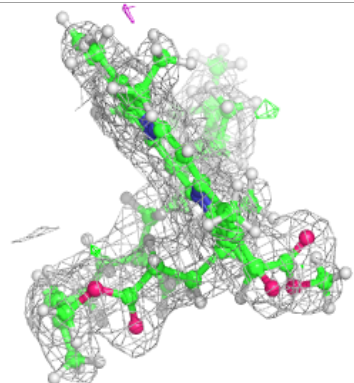
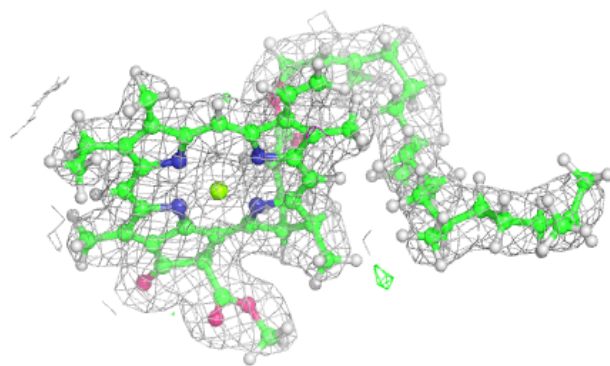
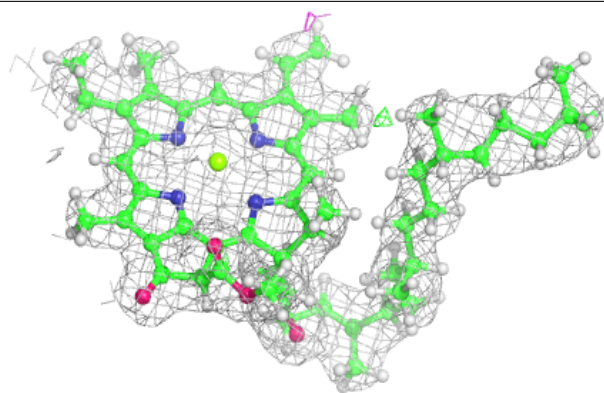
**Electron density around CLA C 501:**

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



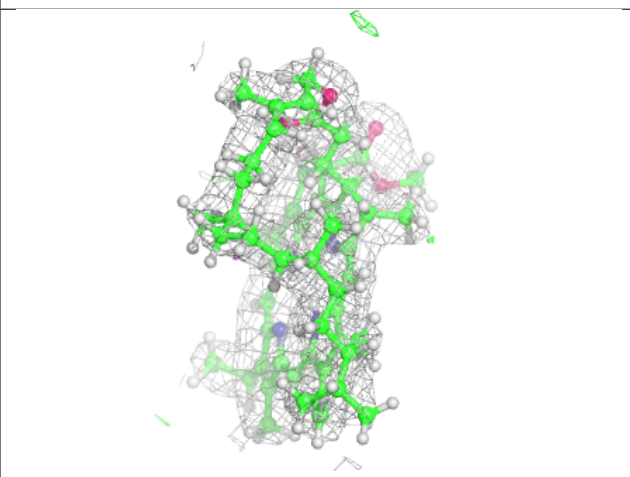
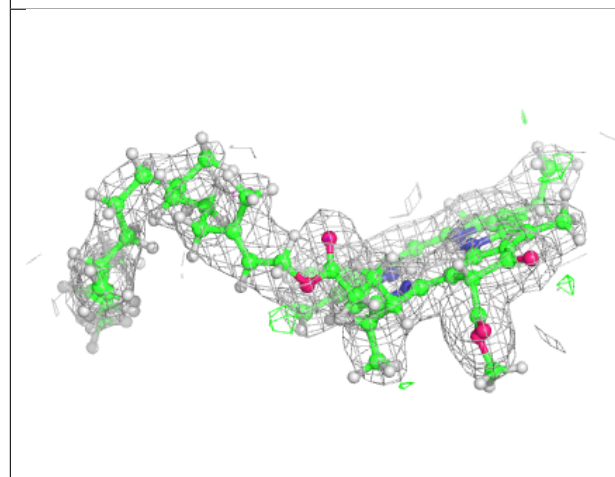
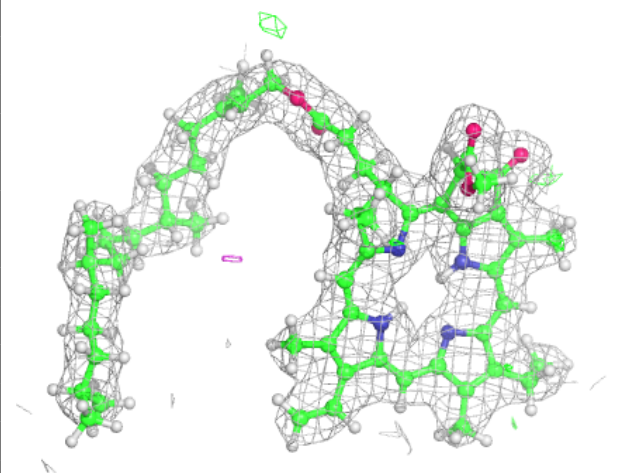
Electron density around CLA D 403:

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



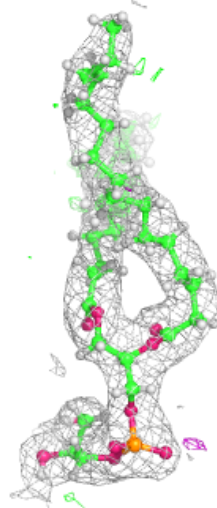
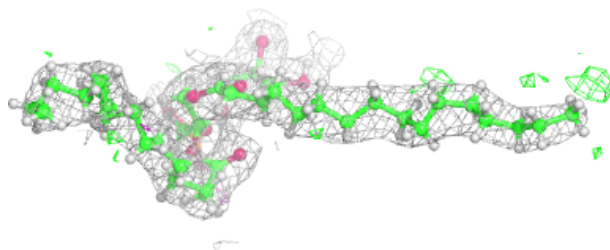
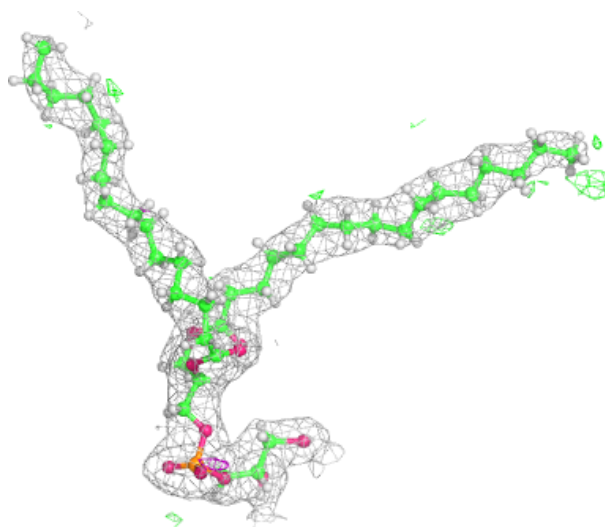
Electron density around PHO d 402:

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



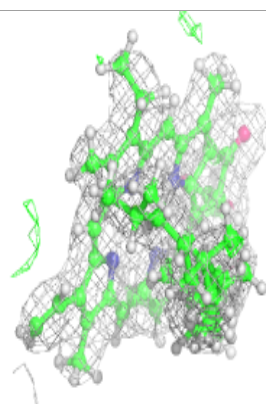
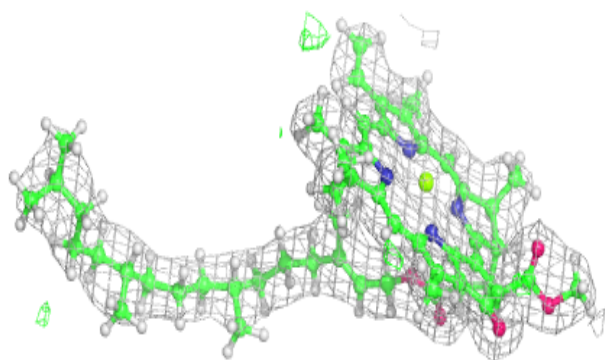
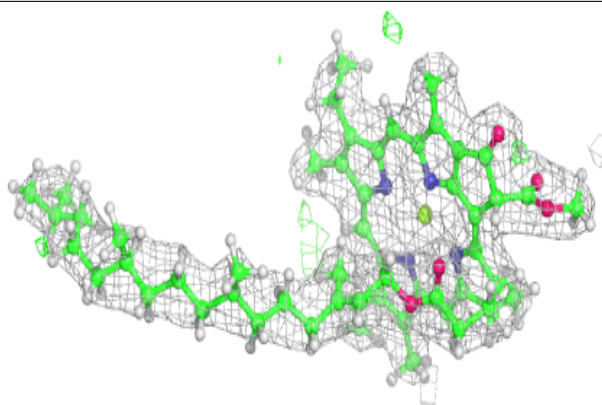
Electron density around LHG B 621:

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

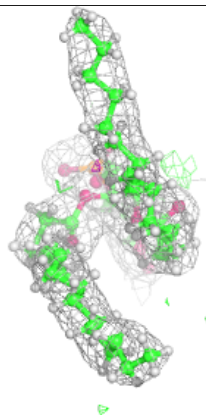
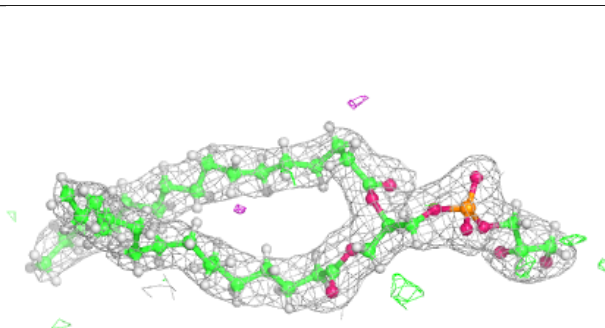
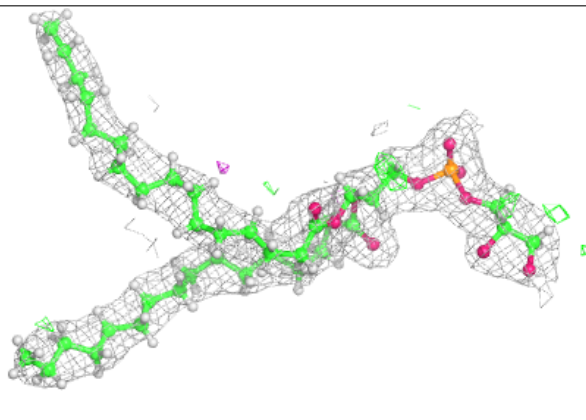


Electron density around CLA B 608:

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

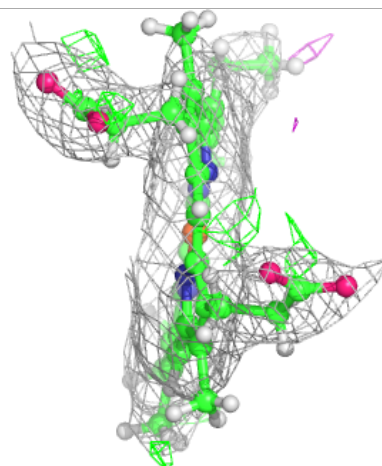
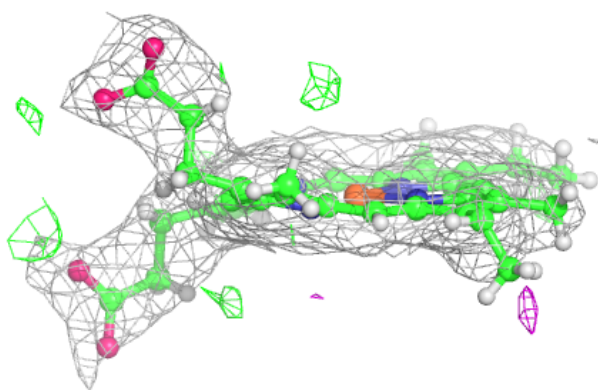
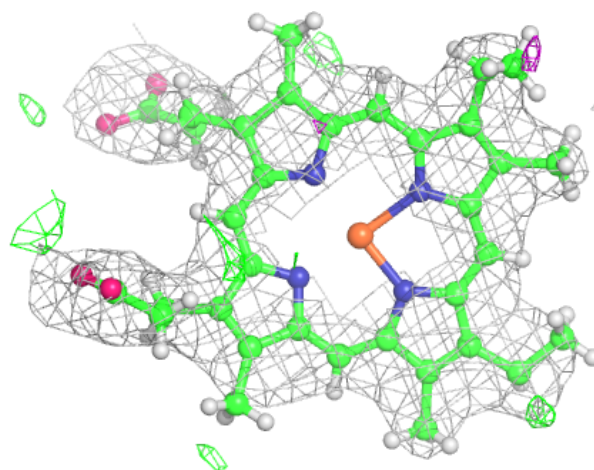
**Electron density around LHG d 408:**

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



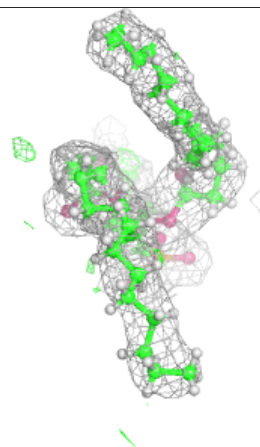
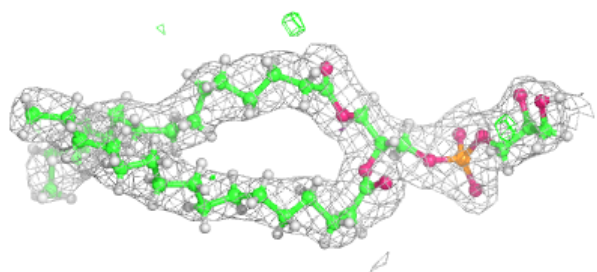
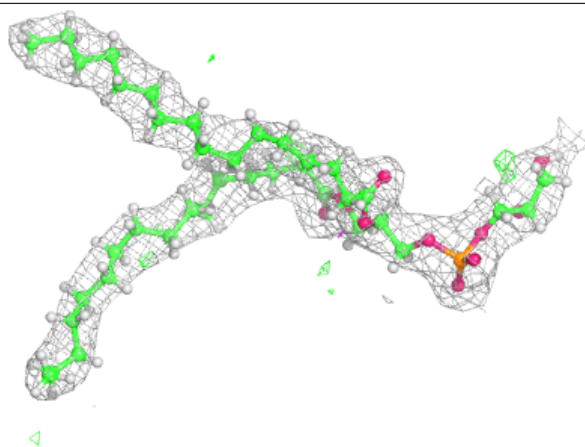
Electron density around HEC f 101:

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



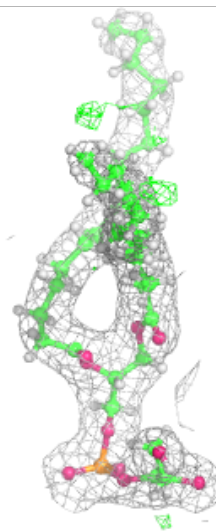
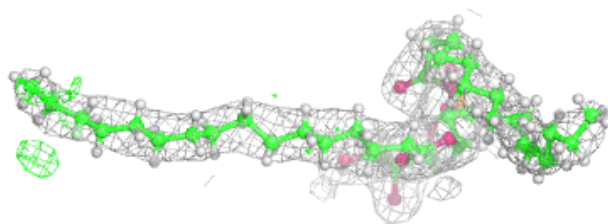
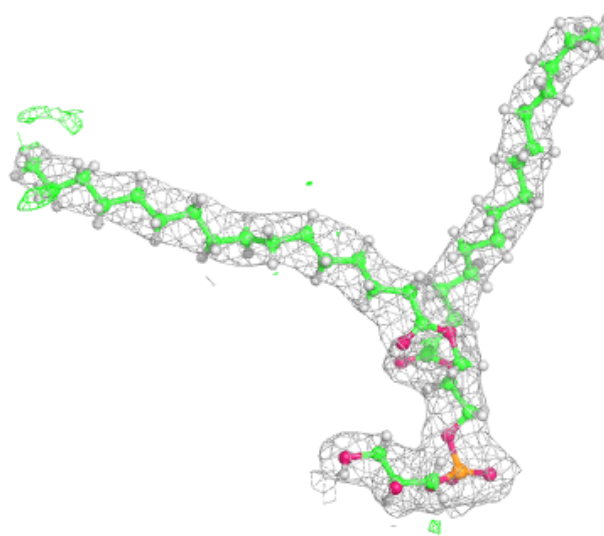
Electron density around LHG D 409:

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



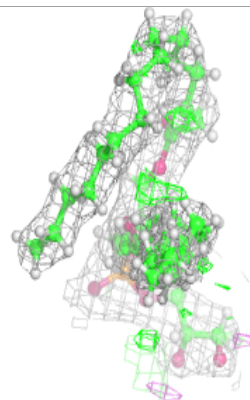
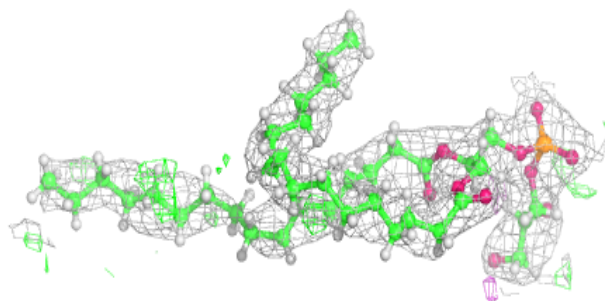
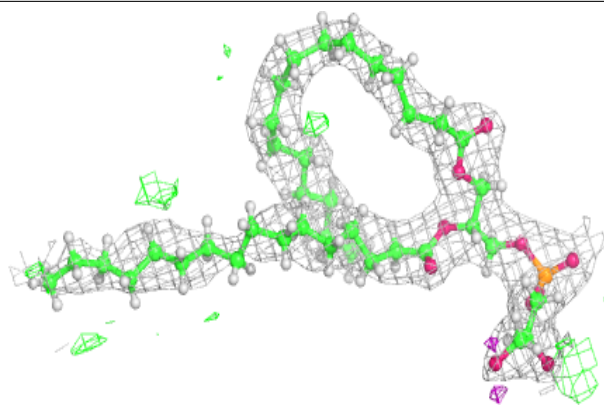
Electron density around LHG 1 101:

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



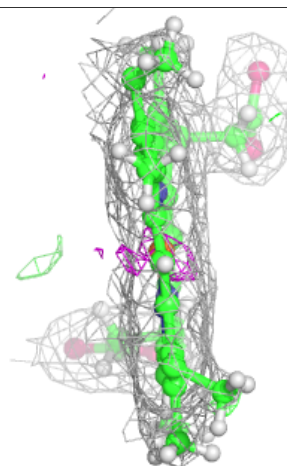
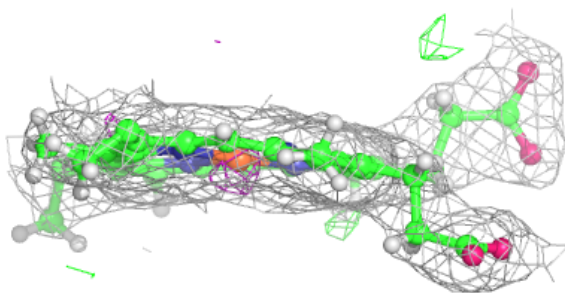
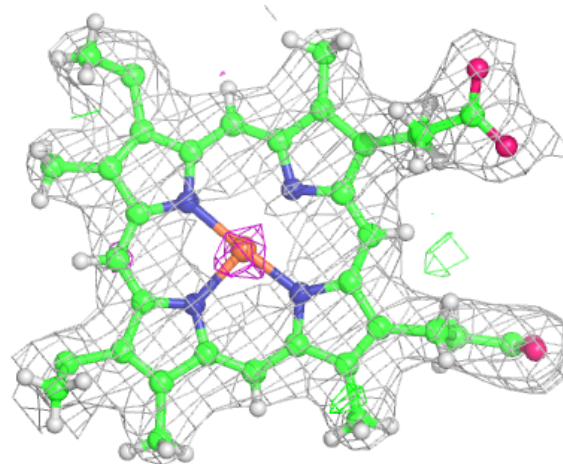
Electron density around LHG B 622:

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



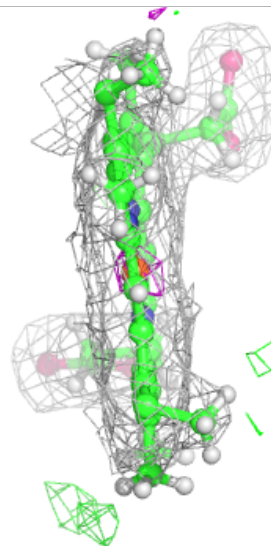
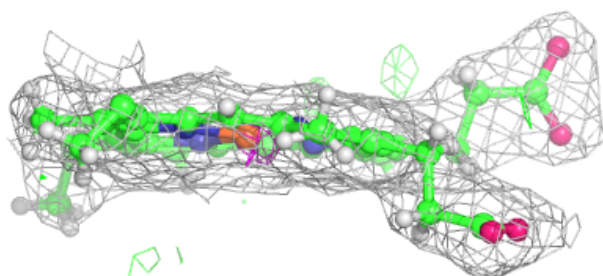
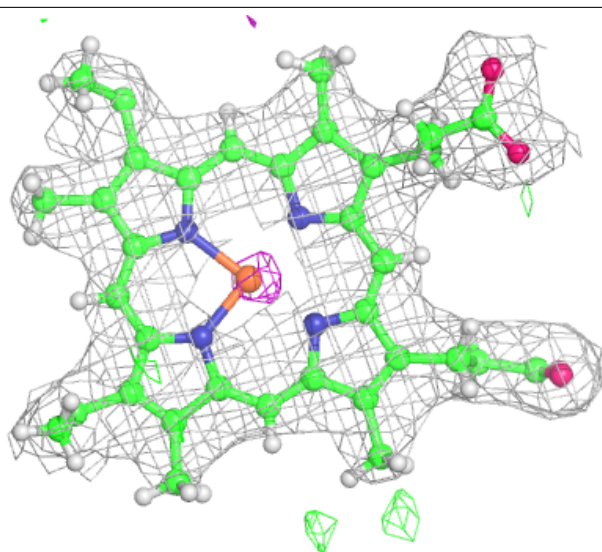
Electron density around HEC V 201:

$2mF_o-DF_c$ (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)



6.5 Other polymers ⓘ

There are no such residues in this entry.