



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 05:08 PM EDT

PDB ID : 6W1U  
Title : RT XFEL structure of Photosystem II 400 microseconds after the second illumination at 2.09 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 : 2.09 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.35.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

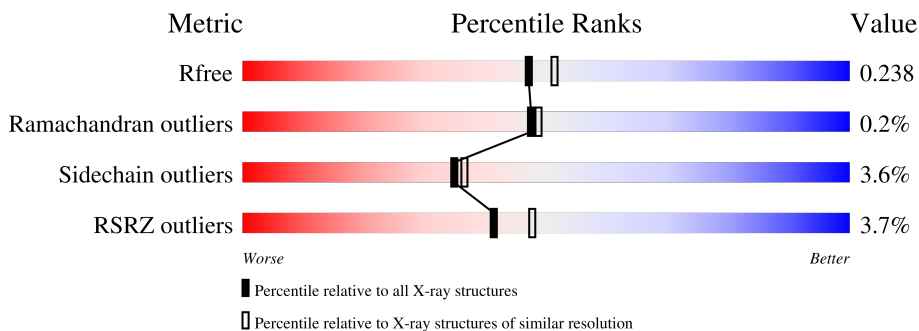
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.09 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	 95%
1	a	344	 92% 5%
2	B	510	 97%

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Refmac : 5.8.0158  
 CCP4 : 7.0.044 (Gargrove)  
 Ideal geometry (proteins) : Engh & Huber (2001)  
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
 Validation Pipeline (wwPDB-VP) : 2.35.1

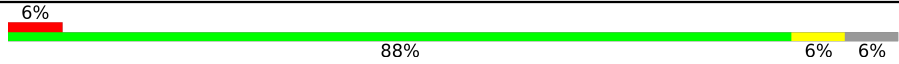

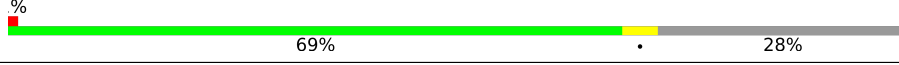



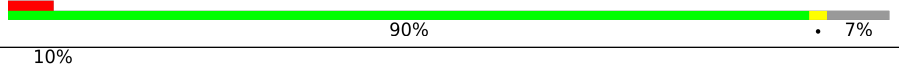
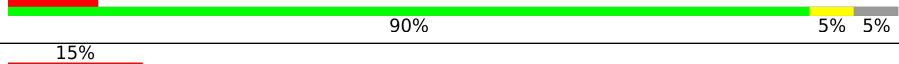


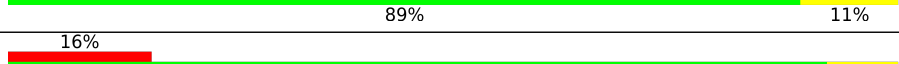
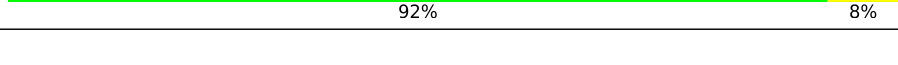


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Mol	Chain	Length	Quality of chain
2	b	510	3% 96% ..
3	C	461	% 94% ..
3	c	461	2% 95% ..
4	D	352	96% ..
4	d	352	94% ..
5	E	84	4% 93% 5% .
5	e	84	5% 94% ..
6	F	45	2% 76% 24%
6	f	45	73% 24%
7	H	66	95% ..
7	h	66	8% 89% 6% 5%
8	I	38	5% 87% 8% 5%
8	i	38	8% 92% 5%
9	J	40	8% 90% 10%
9	j	40	10% 88% 10%
10	K	46	4% 74% 7% 20%
10	k	46	2% 72% 9% 20%
11	L	37	3% 97% .
11	l	37	8% 89% 8% .
12	M	36	92% 8%
12	m	36	81% 8% 11%
13	O	272	6% 84% 6% 10%
13	o	272	5% 86% 10%
14	R	41	32% 71% 12% 17%
14	r	41	56% 63% 12% 24%

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Mol	Chain	Length	Quality of chain
15	T	32	
15	t	32	
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	405	X	-	-	-
22	CLA	B	602	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	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	B	617	X	-	-	-
22	CLA	C	503	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	D	402	X	-	-	-
22	CLA	a	402	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	a	411	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	609	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	c	503	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
22	CLA	c	514	X	-	-	-
22	CLA	c	515	X	-	-	-
22	CLA	d	402	X	-	-	-
22	CLA	d	403	X	-	-	-
22	CLA	h	101	X	-	-	-

## 2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 105950 atoms, of which 52556 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	
			Total	C	H	N	O				S
1	A	334	6031	2014	2942	509	547	19	0	60	0
1	a	334	6019	2011	2933	509	547	19	0	60	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	B	505	7864	2631	3859	666	695	13	0	5	0
2	b	505	7800	2610	3822	665	690	13	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
3	C	442	6876	2283	3397	580	602	14	0	10	0
3	c	451	7021	2324	3468	596	619	14	0	10	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
5	E	82	1316	436	650	107	123	0	1	0
5	e	82	1311	434	647	108	122	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
6	F	34	556	187	281	45	42	1	0	0	0
6	f	34	556	187	281	45	42	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
7	H	65	1042	341	532	82	85	2	0	0	0
7	h	63	1016	333	518	80	83	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
8	I	36	607	200	311	46	49	1	0	0	0
8	i	36	607	200	311	46	49	1	0	0	0

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	
			Total	C	H	N	O				S
9	J	36	525	174	268	40	42	1	0	0	0
9	j	36	525	174	268	40	42	1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
11	L	37	Total 620	C 202	H 316	N 48	O 53	S 1	0	0	0
11	l	36	Total 600	C 197	H 304	N 47	O 52		0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
12	M	33	Total 525	C 171	H 269	N 37	O 47	S 1	0	0	0
12	m	32	Total 518	C 168	H 267	N 36	O 46	S 1	0	0	0

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	
			Total	C	H	N	O				S
13	O	244	Total 3698	C 1168	H 1828	N 313	O 385	S 4	0	1	0
13	o	244	Total 3718	C 1170	H 1844	N 317	O 383	S 4	0	0	0

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

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

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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	0
			519	181	261	36	39	2			
15	t	30	Total	C	H	N	O	S	0	0	0
			512	180	256	36	38	2			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	U	97	Total	C	H	N	O	0	0	0
			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	0
			2132	675	1068	177	208	4			
17	v	137	Total	C	H	N	O	S	0	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	
			Total	C	H	N	O				S
19	Y	27	Total 413	C 128	H 217	N 35	O 30	S 3	0	0	0
19	y	30	Total 459	C 144	H 241	N 35	O 36	S 3	0	0	0

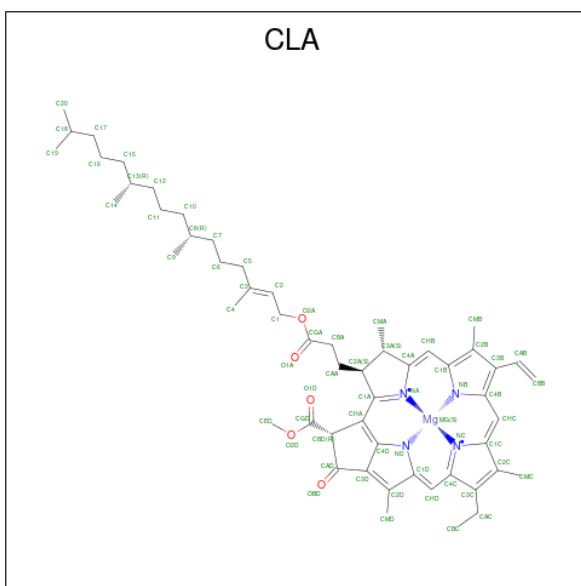
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

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

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

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

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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
			117	49	58	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	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	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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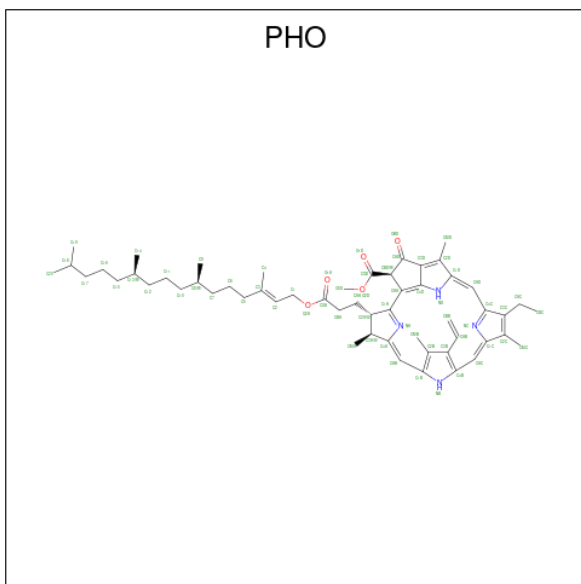
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total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

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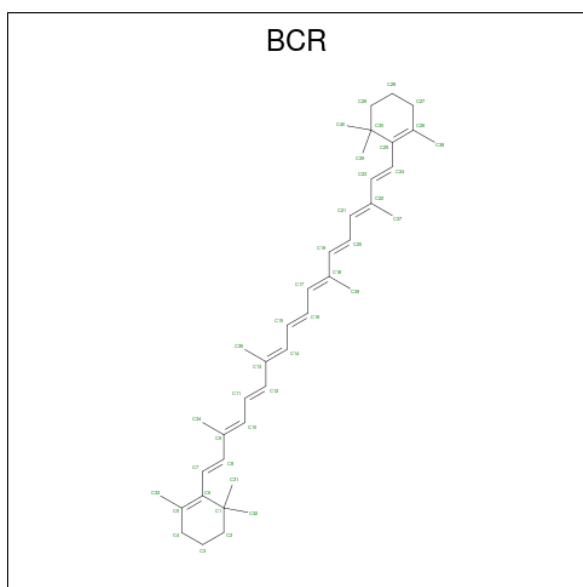
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	h	1	Total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

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



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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	A	1	Total	C	H	0	0
			96	40	56		
24	B	1	Total	C	H	0	0
			96	40	56		
24	B	1	Total	C	H	0	0
			96	40	56		
24	B	1	Total	C	H	0	0
			96	40	56		
24	C	1	Total	C	H	0	0
			96	40	56		
24	D	1	Total	C	H	0	0
			96	40	56		
24	H	1	Total	C	H	0	0
			96	40	56		
24	K	1	Total	C	H	0	0
			96	40	56		
24	T	1	Total	C	H	0	0
			96	40	56		
24	Y	1	Total	C	H	0	0
			96	40	56		
24	Z	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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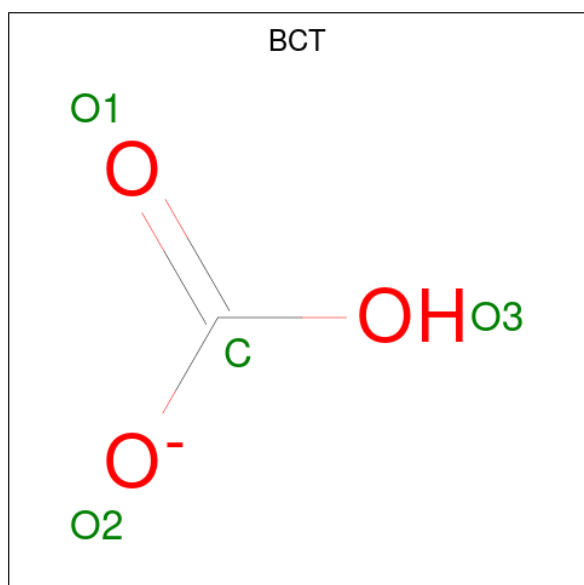
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	b	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	d	1	Total	C	H	0	0
			96	40	56		
24	t	1	Total	C	H	0	0
			96	40	56		
24	x	1	Total	C	H	0	0
			96	40	56		
24	y	1	Total	C	H	0	0
			96	40	56		

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

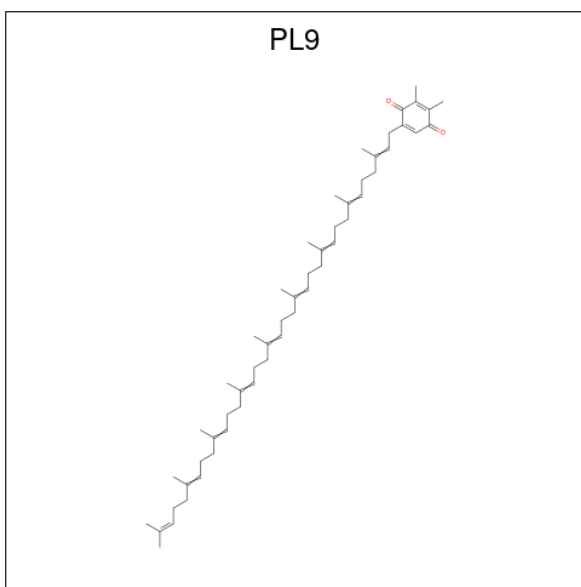
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	2	Total	Cl	0	0
			2	2		
25	a	2	Total	Cl	0	0
			2	2		

- Molecule 26 is BICARBONATE ION (three-letter code: BCT) (formula: CHO<sub>3</sub>).



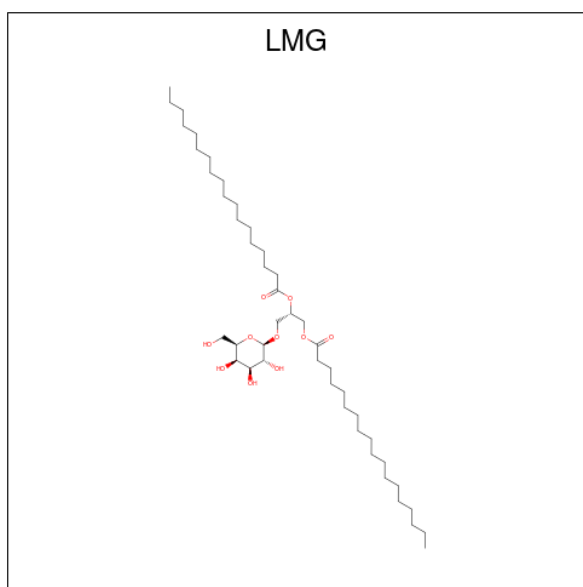
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	H	O	0	0
			5	1	1	3		
26	a	1	Total	C	H	O	0	0
			5	1	1	3		

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



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

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

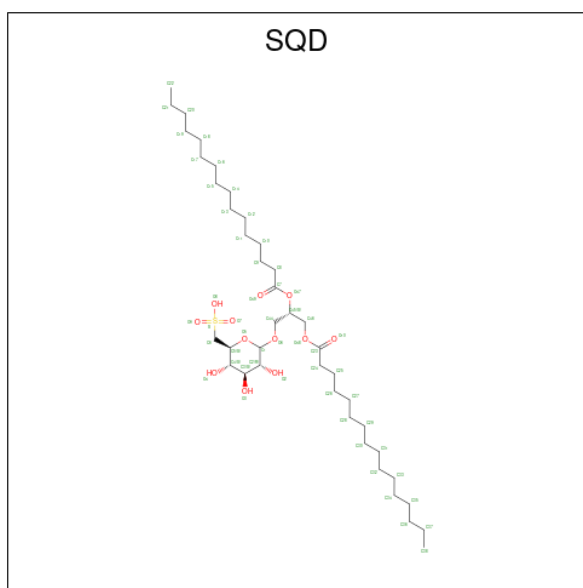


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
28	A	1	Total	C	H	O	0	0
			114	38	66	10		
28	B	1	Total	C	H	O	0	0
			141	45	86	10		
28	C	1	Total	C	H	O	0	0
			111	38	63	10		
28	D	1	Total	C	H	O	0	0
			121	41	70	10		
28	D	1	Total	C	H	O	0	0
			78	27	45	6		
28	D	1	Total	C	H	O	0	0
			68	24	40	4		
28	M	1	Total	C	H	O	0	0
			121	41	70	10		
28	b	1	Total	C	H	O	0	0
			122	41	71	10		
28	b	1	Total	C	H	O	0	0
			141	45	86	10		
28	c	1	Total	C	H	O	0	0
			80	27	43	10		
28	c	1	Total	C	H	O	0	0
			116	38	68	10		
28	c	1	Total	C	H	O	0	0
			117	39	68	10		
28	d	1	Total	C	H	O	0	0
			102	34	58	10		

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

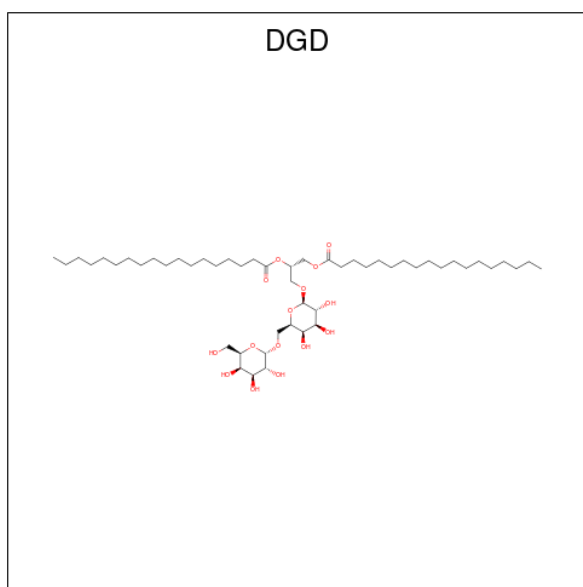


L]-SN-GLYCEROL (three-letter code: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



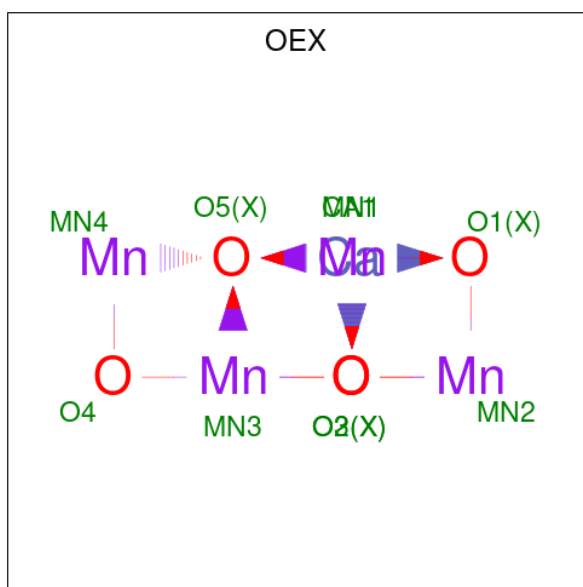
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
29	A	1	Total	C	H	O		0	0
			104	35	65	4			
29	B	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
29	D	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
29	a	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
29	a	1	Total	C	H	O		0	0
			92	31	56	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
			87	28	46	12	1		

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



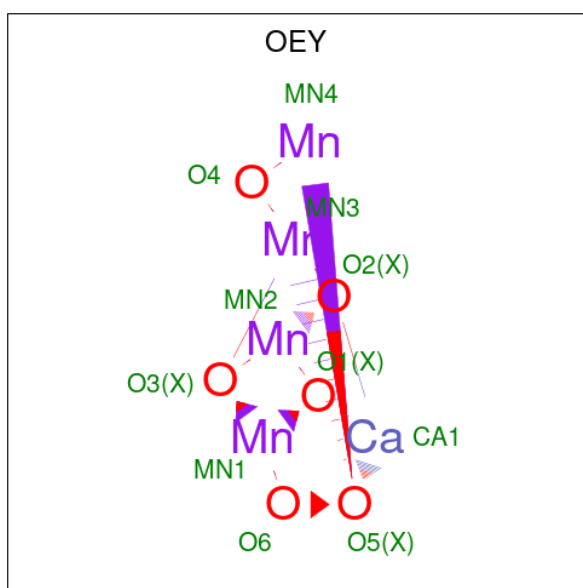
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
30	A	1	Total 159	C 51	H 93	O 15	0	0
30	C	1	Total 143	C 47	H 81	O 15	0	0
30	C	1	Total 140	C 47	H 78	O 15	0	0
30	C	1	Total 143	C 47	H 81	O 15	0	0
30	H	1	Total 142	C 47	H 80	O 15	0	0
30	c	1	Total 140	C 47	H 78	O 15	0	0
30	c	1	Total 141	C 47	H 79	O 15	0	0
30	c	1	Total 140	C 47	H 78	O 15	0	0
30	h	1	Total 140	C 47	H 78	O 15	0	0

- Molecule 31 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



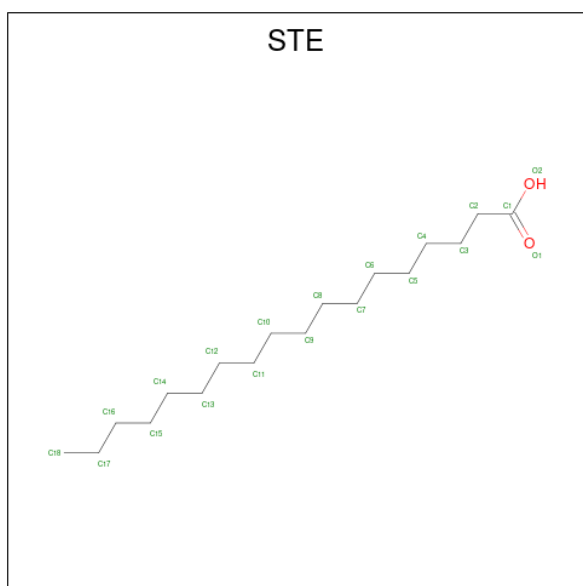
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Ca	Mn	O		
31	A	1	10	1	4	5	0	1
31	a	1	10	1	4	5	0	1

- Molecule 32 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula:  $\text{CaMn}_4\text{O}_6$ ).



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

- Molecule 33 is STEARIC ACID (three-letter code: STE) (formula:  $C_{18}H_{36}O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	B	1	Total	C	H	O	0	0
			28	10	16	2		
33	B	1	Total	C	H	O	0	0
			43	15	26	2		
33	B	1	Total	C	H	O	0	0
			34	12	20	2		
33	B	1	Total	C	H	O	0	0
			28	10	16	2		
33	B	1	Total	C	H	O	0	0
			46	16	28	2		
33	B	1	Total	C	H		0	0
			47	16	31			
33	B	1	Total	C	H		0	0
			41	15	26			
33	C	1	Total	C	H	O	0	0
			28	10	16	2		
33	C	1	Total	C	H		0	0
			47	16	31			
33	C	1	Total	C	H	O	0	0
			28	10	16	2		
33	E	1	Total	C	H	O	0	0
			28	10	16	2		
33	H	1	Total	C	H		0	0
			53	18	35			
33	I	1	Total	C	H		0	0
			41	15	26			

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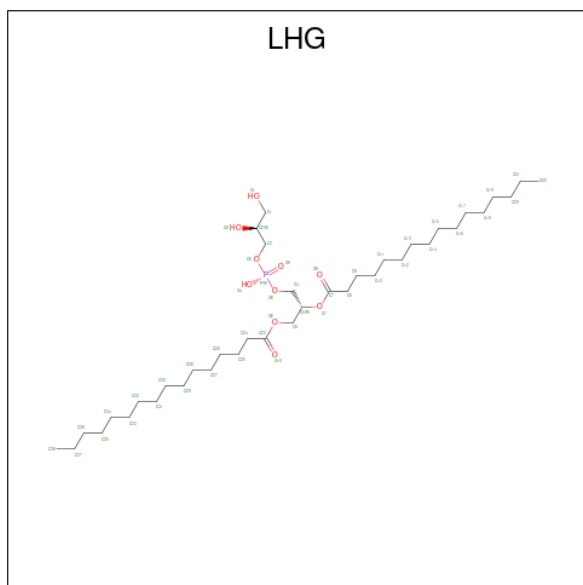
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	J	1	Total	C	H	O	0	0
			28	10	16	2		
33	L	1	Total	C	H	O	0	0
			28	10	16	2		
33	M	1	Total	C	H	O	0	0
			37	13	22	2		
33	M	1	Total	C	H		0	0
			26	10	16			
33	T	1	Total	C	H		0	0
			44	15	29			
33	X	1	Total	C	H	O	0	0
			55	18	35	2		
33	Z	1	Total	C	H		0	0
			20	8	12			
33	a	1	Total	C	H		0	0
			26	10	16			
33	a	1	Total	C	H	O	0	0
			28	10	16	2		
33	b	1	Total	C	H		0	0
			47	16	31			
33	b	1	Total	C	H	O	0	0
			55	18	35	2		
33	b	1	Total	C	H	O	0	0
			40	14	24	2		
33	b	1	Total	C	H	O	0	0
			55	18	35	2		
33	b	1	Total	C	H		0	0
			26	10	16			
33	c	1	Total	C	H	O	0	0
			28	10	16	2		
33	c	1	Total	C	H	O	0	0
			55	18	35	2		
33	d	1	Total	C	H	O	0	0
			43	15	26	2		
33	d	1	Total	C	H	O	0	0
			55	18	35	2		
33	d	1	Total	C	H	O	0	0
			55	18	35	2		
33	h	1	Total	C	H		0	0
			41	14	27			
33	j	1	Total	C	H	O	0	0
			28	10	16	2		

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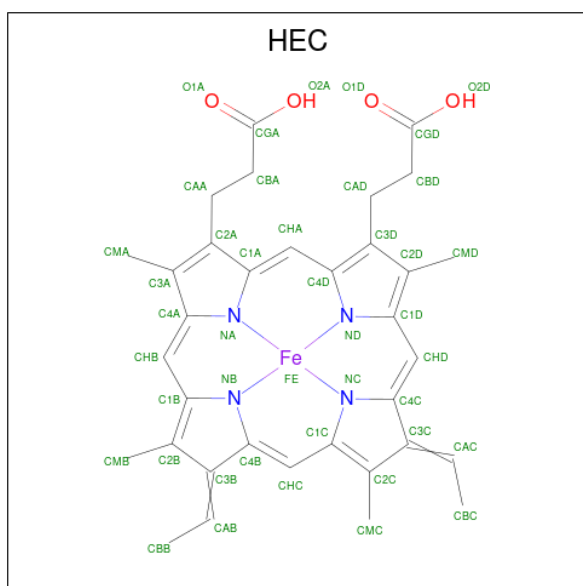
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	1	1	Total	C	H	0	0
			53	18	35		

- Molecule 34 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Fe	H	N			O
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	e	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	153	Total	O	0	8
			153	153		
36	B	216	Total	O	0	0
			216	216		
36	C	179	Total	O	0	0
			179	179		
36	D	131	Total	O	0	0
			131	131		
36	E	39	Total	O	0	0
			39	39		
36	F	7	Total	O	0	0
			7	7		
36	H	23	Total	O	0	0
			23	23		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	I	17	Total O 17 17	0	0
36	J	19	Total O 19 19	0	0
36	K	16	Total O 16 16	0	0
36	L	9	Total O 9 9	0	0
36	M	7	Total O 7 7	0	0
36	O	101	Total O 101 101	0	0
36	R	6	Total O 6 6	0	0
36	T	10	Total O 10 10	0	0
36	U	43	Total O 43 43	0	0
36	V	62	Total O 62 62	0	0
36	X	11	Total O 11 11	0	0
36	Y	5	Total O 5 5	0	0
36	Z	10	Total O 10 10	0	0
36	a	137	Total O 137 137	0	8
36	b	186	Total O 186 186	0	0
36	c	179	Total O 179 179	0	0
36	d	110	Total O 110 110	0	0
36	e	29	Total O 29 29	0	0
36	f	7	Total O 7 7	0	0
36	h	31	Total O 31 31	0	0
36	i	8	Total O 8 8	0	0

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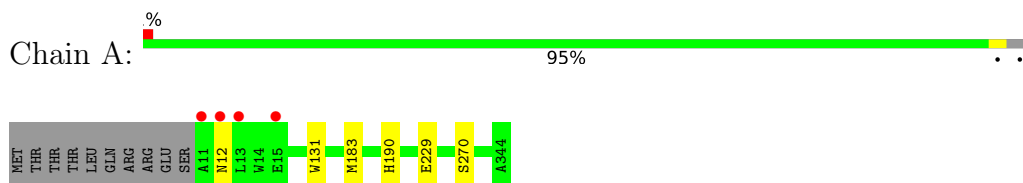
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
36	j	16	Total 16	O 16	0	0
36	k	7	Total 7	O 7	0	0
36	l	9	Total 9	O 9	0	0
36	m	7	Total 7	O 7	0	0
36	o	106	Total 106	O 106	0	0
36	r	6	Total 6	O 6	0	0
36	t	6	Total 6	O 6	0	0
36	u	56	Total 56	O 56	0	0
36	v	75	Total 75	O 75	0	0
36	x	12	Total 12	O 12	0	0
36	y	4	Total 4	O 4	0	0
36	z	11	Total 11	O 11	0	0

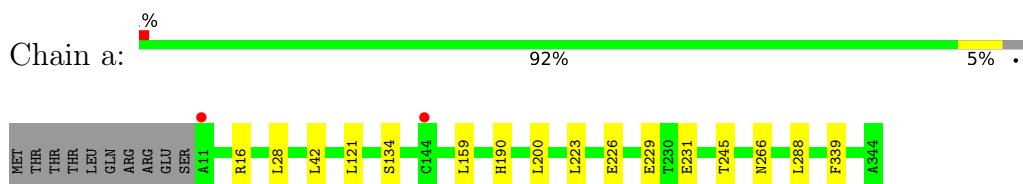
### 3 Residue-property plots [i](#)

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

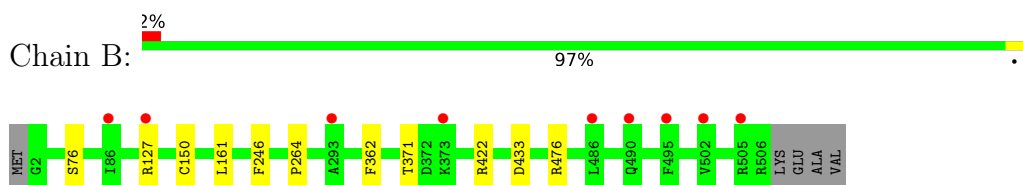
- Molecule 1: Photosystem II protein D1 1



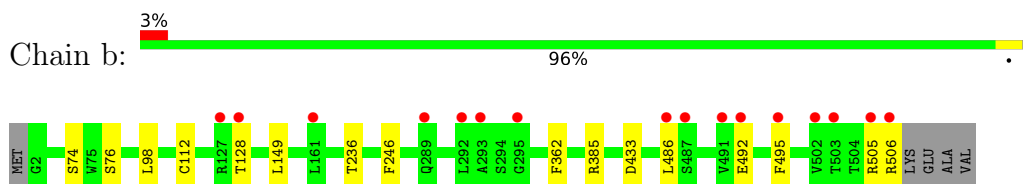
- Molecule 1: Photosystem II protein D1 1



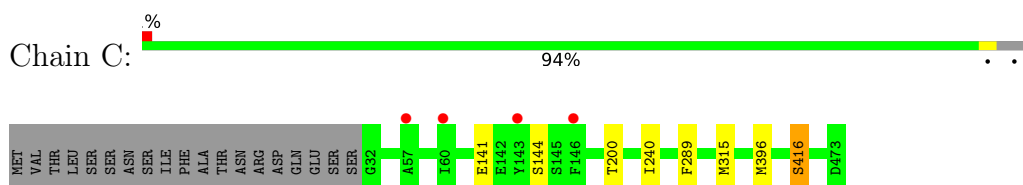
- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein



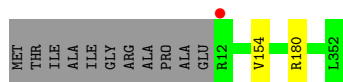
- Molecule 3: Photosystem II CP43 reaction center protein



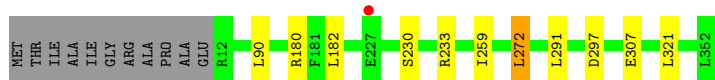
- Molecule 3: Photosystem II CP43 reaction center protein



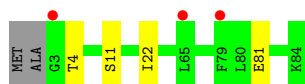
● Molecule 4: Photosystem II D2 protein



● Molecule 4: Photosystem II D2 protein



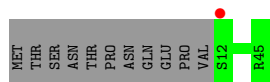
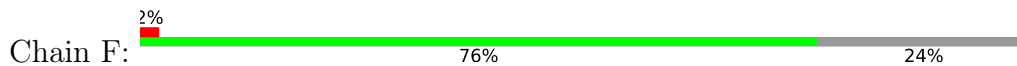
● Molecule 5: Cytochrome b559 subunit alpha



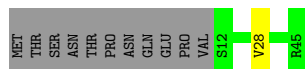
● Molecule 5: Cytochrome b559 subunit alpha



● Molecule 6: Cytochrome b559 subunit beta



● Molecule 6: Cytochrome b559 subunit beta




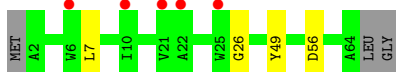
- Molecule 7: Photosystem II reaction center protein H

Chain H:  95%




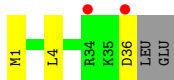
- Molecule 7: Photosystem II reaction center protein H

Chain h:  8% 89% 6% 5%




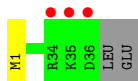
- Molecule 8: Photosystem II reaction center protein I

Chain I:  5% 87% 8% 5%




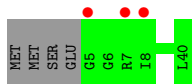
- Molecule 8: Photosystem II reaction center protein I

Chain i:  8% 92% 5% 5%




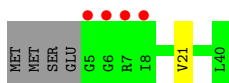
- Molecule 9: Photosystem II reaction center protein J

Chain J:  8% 90% 10%




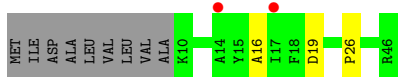
- Molecule 9: Photosystem II reaction center protein J

Chain j:  10% 88% 10% 10%

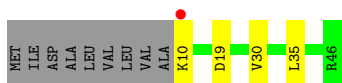


- Molecule 10: Photosystem II reaction center protein K

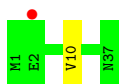
Chain K:  4% 74% 7% 20%



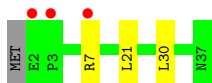
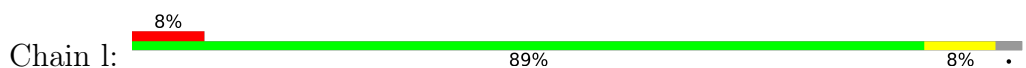
- Molecule 10: Photosystem II reaction center protein K



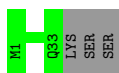
- Molecule 11: Photosystem II reaction center protein L



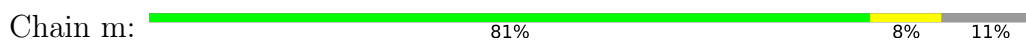
- Molecule 11: Photosystem II reaction center protein L



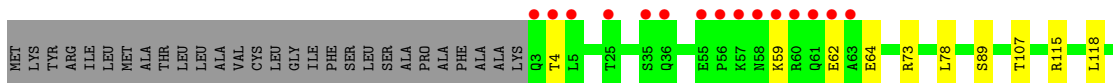
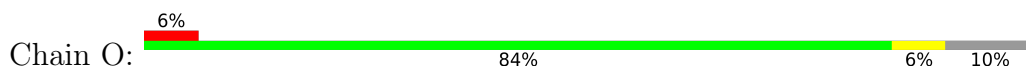
- Molecule 12: Photosystem II reaction center protein M



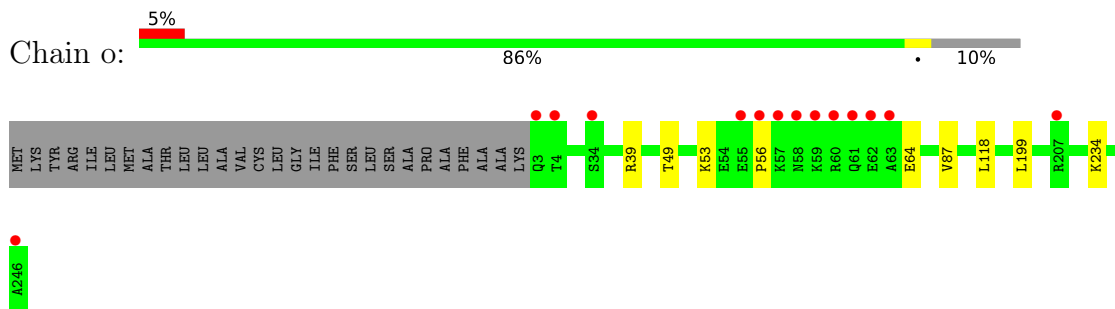
- Molecule 12: Photosystem II reaction center protein M



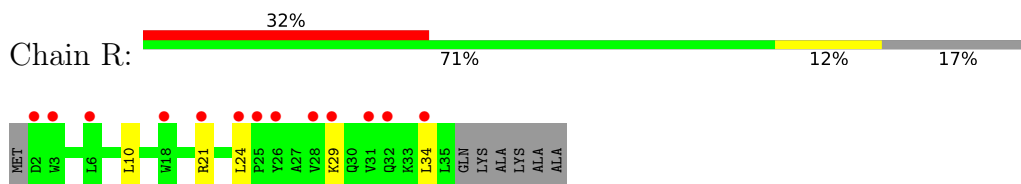
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



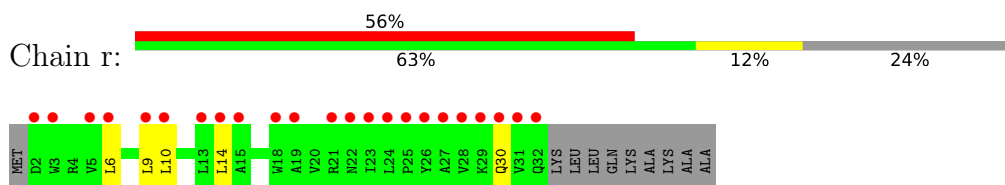
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



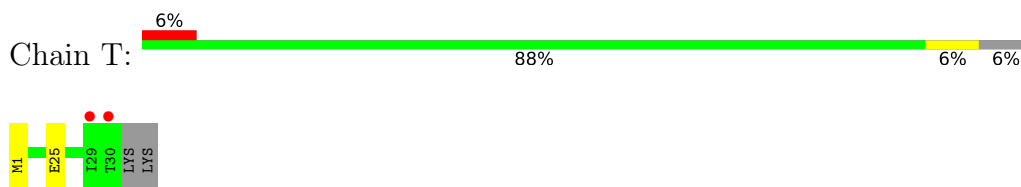
- Molecule 14: Photosystem II protein Y



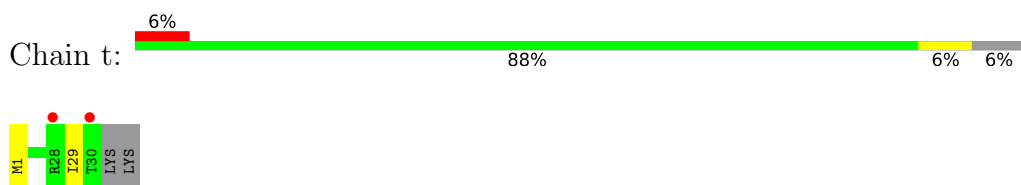
- Molecule 14: Photosystem II protein Y



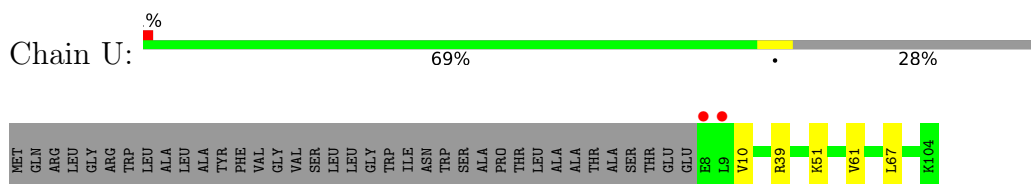
- Molecule 15: Photosystem II reaction center protein T



- Molecule 15: Photosystem II reaction center protein T

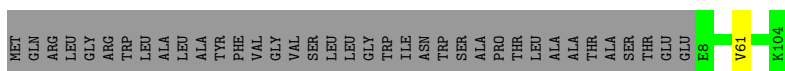


- Molecule 16: Photosystem II 12 kDa extrinsic protein




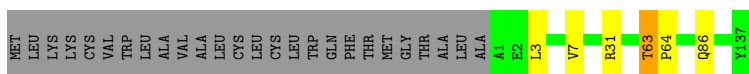
- Molecule 16: Photosystem II 12 kDa extrinsic protein

Chain u:  72% 28%




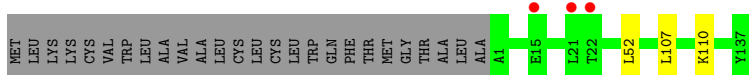
- Molecule 17: Cytochrome c-550

Chain V:  80% 16%




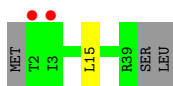
- Molecule 17: Cytochrome c-550

Chain v:  82% 16%




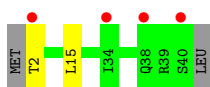
- Molecule 18: Photosystem II reaction center X protein

Chain X:  90% 7%



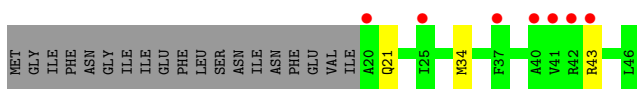
- Molecule 18: Photosystem II reaction center X protein

Chain x:  90% 5% 5%



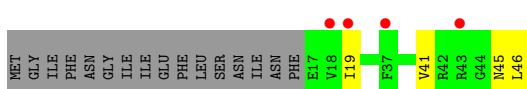
- Molecule 19: Photosystem II reaction center protein Ycf12

Chain Y:  52% 7% 41%

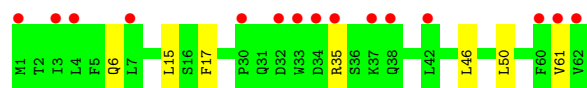
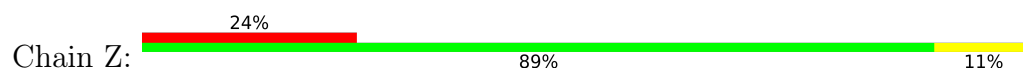


- Molecule 19: Photosystem II reaction center protein Ycf12

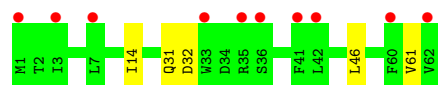
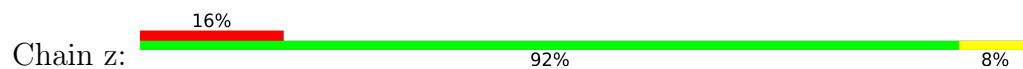
Chain y:  57% 9% 9% 35%



- 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, $\alpha$ , $\beta$ , $\gamma$	116.97Å 221.71Å 308.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.65 – 2.09 33.65 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.7 (33.65-2.09) 86.0 (33.65-2.09)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.72 (at 2.08Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.180 , 0.239 0.180 , 0.238	Depositor DCC
$R_{free}$ test set	4171 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.3	Xtrriage
Anisotropy	0.258	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 68.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	105950	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

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

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality i

### 5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.61	0/3187	0.70	3/4342 (0.1%)
1	a	0.62	0/3184	0.81	6/4338 (0.1%)
2	B	0.65	1/4161 (0.0%)	0.69	2/5669 (0.0%)
2	b	0.65	2/4118 (0.0%)	0.69	2/5611 (0.0%)
3	C	0.61	0/3621	0.68	1/4930 (0.0%)
3	c	0.58	0/3693	0.68	1/5026 (0.0%)
4	D	0.68	0/2820	0.70	0/3840
4	d	0.65	0/2829	0.73	3/3852 (0.1%)
5	E	0.60	0/688	0.61	0/940
5	e	0.53	0/683	0.64	0/932
6	F	0.58	0/284	0.52	0/387
6	f	0.50	0/284	0.58	0/387
7	H	0.63	0/523	0.74	0/713
7	h	0.54	0/511	0.69	0/697
8	I	0.63	0/293	0.67	0/396
8	i	0.64	0/293	0.69	0/396
9	J	0.61	0/263	0.63	0/356
9	j	0.55	0/263	0.69	0/356
10	K	0.57	0/303	0.64	0/416
10	k	0.51	0/303	0.69	0/416
11	L	0.63	0/311	0.70	0/422
11	l	0.68	0/303	0.66	0/412
12	M	0.61	0/249	0.63	0/341
12	m	0.85	1/244 (0.4%)	0.72	0/334
13	O	0.62	0/1904	0.75	3/2585 (0.1%)
13	o	0.63	0/1905	0.75	0/2583
14	R	0.46	0/277	0.53	0/380
14	r	0.40	0/245	0.51	0/336
15	T	0.72	0/257	0.77	0/349
15	t	0.67	0/255	0.65	0/346
16	U	0.58	0/785	0.70	0/1064
16	u	0.64	0/785	0.72	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	V	0.61	0/1085	0.70	1/1473 (0.1%)
17	v	0.60	0/1085	0.69	0/1473
18	X	0.59	0/284	0.69	0/384
18	x	0.47	0/289	0.60	0/391
19	Y	0.47	0/197	0.54	0/264
19	y	0.42	0/219	0.58	0/294
20	Z	0.46	0/490	0.59	0/669
20	z	0.46	0/488	0.57	0/666
All	All	0.62	4/43961 (0.0%)	0.70	22/59830 (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
1	a	0	1
17	V	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	m	26	TYR	CD1-CE1	-6.90	1.28	1.39
2	B	150	CYS	CB-SG	-6.66	1.71	1.82
2	b	112	CYS	CB-SG	-5.61	1.72	1.81
2	b	486	LEU	C-N	5.06	1.45	1.34

All (22) 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	-6.58	106.13	120.60
2	b	385	ARG	NE-CZ-NH2	-6.18	117.21	120.30
4	d	272	LEU	CB-CG-CD1	-5.90	100.97	111.00
4	d	297	ASP	CB-CG-OD1	5.67	123.40	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	165	LEU	CA-CB-CG	5.65	128.29	115.30
13	O	73	ARG	NE-CZ-NH2	-5.59	117.50	120.30
3	C	396	MET	CG-SD-CE	-5.32	91.69	100.20
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
2	B	433	ASP	CB-CG-OD1	5.30	123.07	118.30
2	B	422	ARG	NE-CZ-NH1	-5.20	117.70	120.30
2	b	433	ASP	CB-CG-OD1	5.18	122.96	118.30
1	A	131	TRP	CA-CB-CG	-5.17	103.88	113.70
4	d	272	LEU	CA-CB-CG	5.16	127.17	115.30
13	O	115	ARG	NE-CZ-NH1	5.14	122.87	120.30
13	O	158	ASP	CB-CG-OD1	5.10	122.89	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	190[A]	HIS	Mainchain
17	V	63	THR	Peptide
1	a	339[B]	PHE	Peptide

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	391/344 (114%)	385 (98%)	6 (2%)	0	100	100
1	a	391/344 (114%)	381 (97%)	10 (3%)	0	100	100
2	B	508/510 (100%)	501 (99%)	7 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	503/510 (99%)	491 (98%)	12 (2%)	0	100	100
3	C	450/461 (98%)	440 (98%)	8 (2%)	2 (0%)	34	32
3	c	459/461 (100%)	445 (97%)	13 (3%)	1 (0%)	47	49
4	D	339/352 (96%)	330 (97%)	9 (3%)	0	100	100
4	d	340/352 (97%)	331 (97%)	9 (3%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	55 (87%)	8 (13%)	0	100	100
7	h	61/66 (92%)	56 (92%)	4 (7%)	1 (2%)	9	5
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	32 (94%)	2 (6%)	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%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	227 (93%)	14 (6%)	2 (1%)	19	15
13	o	242/272 (89%)	233 (96%)	8 (3%)	1 (0%)	34	32
14	R	32/41 (78%)	29 (91%)	2 (6%)	1 (3%)	4	1
14	r	27/41 (66%)	27 (100%)	0	0	100	100
15	T	28/32 (88%)	28 (100%)	0	0	100	100
15	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
16	U	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
16	u	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
17	V	135/163 (83%)	127 (94%)	7 (5%)	1 (1%)	22	18
17	v	135/163 (83%)	128 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100	100
18	x	37/41 (90%)	35 (95%)	2 (5%)	0	100	100
19	Y	25/46 (54%)	22 (88%)	2 (8%)	1 (4%)	3	1
19	y	28/46 (61%)	25 (89%)	2 (7%)	1 (4%)	3	1
20	Z	60/62 (97%)	55 (92%)	5 (8%)	0	100	100
20	z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	9	4
All	All	5372/5700 (94%)	5201 (97%)	158 (3%)	13 (0%)	47	49

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
13	O	59	LYS
17	V	64	PRO
3	c	416	SER
14	R	34	LEU
13	O	62	GLU
19	Y	43	ARG
19	y	41	VAL
20	z	61	VAL
10	K	16	ALA
3	C	144	SER
7	h	26	GLY
13	o	56	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	320/280 (114%)	317 (99%)	3 (1%)	78	84
1	a	319/280 (114%)	305 (96%)	14 (4%)	28	28
2	B	408/407 (100%)	400 (98%)	8 (2%)	55	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	402/407 (99%)	390 (97%)	12 (3%)	41	44
3	C	353/362 (98%)	347 (98%)	6 (2%)	60	67
3	c	361/362 (100%)	350 (97%)	11 (3%)	41	44
4	D	277/283 (98%)	275 (99%)	2 (1%)	84	88
4	d	278/283 (98%)	268 (96%)	10 (4%)	35	36
5	E	72/73 (99%)	67 (93%)	5 (7%)	15	12
5	e	71/73 (97%)	68 (96%)	3 (4%)	30	30
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	27 (96%)	1 (4%)	35	36
7	H	54/55 (98%)	52 (96%)	2 (4%)	34	35
7	h	53/55 (96%)	50 (94%)	3 (6%)	20	18
8	I	32/34 (94%)	30 (94%)	2 (6%)	18	15
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	23 (96%)	1 (4%)	30	30
10	K	30/37 (81%)	28 (93%)	2 (7%)	16	13
10	k	30/37 (81%)	26 (87%)	4 (13%)	4	2
11	L	35/35 (100%)	34 (97%)	1 (3%)	42	46
11	l	34/35 (97%)	31 (91%)	3 (9%)	10	6
12	M	28/32 (88%)	28 (100%)	0	100	100
12	m	28/32 (88%)	27 (96%)	1 (4%)	35	36
13	O	206/228 (90%)	196 (95%)	10 (5%)	25	23
13	o	207/228 (91%)	199 (96%)	8 (4%)	32	33
14	R	28/33 (85%)	24 (86%)	4 (14%)	3	1
14	r	23/33 (70%)	18 (78%)	5 (22%)	1	0
15	T	26/28 (93%)	25 (96%)	1 (4%)	33	34
15	t	25/28 (89%)	24 (96%)	1 (4%)	31	32
16	U	84/112 (75%)	79 (94%)	5 (6%)	19	16
16	u	84/112 (75%)	83 (99%)	1 (1%)	71	77
17	V	117/138 (85%)	113 (97%)	4 (3%)	37	39
17	v	117/138 (85%)	114 (97%)	3 (3%)	46	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	X	31/34 (91%)	30 (97%)	1 (3%)	39	41
18	x	31/34 (91%)	29 (94%)	2 (6%)	17	14
19	Y	19/37 (51%)	17 (90%)	2 (10%)	7	4
19	y	22/37 (60%)	19 (86%)	3 (14%)	3	2
20	Z	52/52 (100%)	45 (86%)	7 (14%)	4	2
20	z	51/52 (98%)	47 (92%)	4 (8%)	12	9
All	All	4444/4654 (96%)	4289 (96%)	155 (4%)	35	38

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	229	GLU
1	A	270	SER
2	B	76	SER
2	B	127	ARG
2	B	161	LEU
2	B	246	PHE
2	B	264	PRO
2	B	362	PHE
2	B	371	THR
2	B	476	ARG
3	C	141	GLU
3	C	200	THR
3	C	240	ILE
3	C	289	PHE
3	C	315	MET
3	C	416	SER
4	D	154	VAL
4	D	180	ARG
5	E	4	THR
5	E	11	SER
5	E	22[A]	ILE
5	E	22[B]	ILE
5	E	81	GLU
7	H	41	PHE
7	H	49	TYR
8	I	4	LEU
8	I	36	ASP
10	K	19	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	K	26	PRO
11	L	10	VAL
13	O	4	THR
13	O	64	GLU
13	O	78	LEU
13	O	89	SER
13	O	107	THR
13	O	118	LEU
13	O	135	SER
13	O	145	GLU
13	O	198	SER
13	O	214	THR
14	R	10	LEU
14	R	21	ARG
14	R	24	LEU
14	R	29	LYS
15	T	25	GLU
16	U	10	VAL
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	31	ARG
17	V	86	GLN
18	X	15	LEU
19	Y	21	GLN
19	Y	34	MET
20	Z	6	GLN
20	Z	15	LEU
20	Z	17	PHE
20	Z	35	ARG
20	Z	46	LEU
20	Z	50	LEU
20	Z	61	VAL
1	a	16	ARG
1	a	28	LEU
1	a	42	LEU
1	a	121	LEU
1	a	134	SER
1	a	159	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	a	200	LEU
1	a	223	LEU
1	a	226	GLU
1	a	229	GLU
1	a	231	GLU
1	a	245	THR
1	a	266	ASN
1	a	288	LEU
2	b	74	SER
2	b	76	SER
2	b	98	LEU
2	b	128	THR
2	b	149	LEU
2	b	236	THR
2	b	246	PHE
2	b	362	PHE
2	b	492	GLU
2	b	495	PHE
2	b	505	ARG
2	b	506	ARG
3	c	24	THR
3	c	26	ARG
3	c	72	LEU
3	c	99	VAL
3	c	124	VAL
3	c	125	LEU
3	c	144	SER
3	c	165	LEU
3	c	240	ILE
3	c	396	MET
3	c	416	SER
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	272	LEU
4	d	291	LEU
4	d	307	GLU
4	d	321	LEU
5	e	61	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	e	65	LEU
5	e	83	LEU
6	f	28	VAL
7	h	7	LEU
7	h	49	TYR
7	h	56	ASP
9	j	21	VAL
10	k	10	LYS
10	k	19	ASP
10	k	30	VAL
10	k	35	LEU
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
13	o	39	ARG
13	o	49	THR
13	o	53	LYS
13	o	64	GLU
13	o	87	VAL
13	o	118	LEU
13	o	199	LEU
13	o	234	LYS
14	r	6	LEU
14	r	9	LEU
14	r	10	LEU
14	r	14	LEU
14	r	30	GLN
15	t	29	ILE
16	u	61	VAL
17	v	52	LEU
17	v	107	LEU
17	v	110	LYS
18	x	2	THR
18	x	15	LEU
19	y	19	ILE
19	y	45	ASN
19	y	46	LEU
20	z	14	ILE
20	z	31	GLN
20	z	32	ASP
20	z	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	409	GLN
3	C	327	ASN
11	L	8	GLN
13	O	88	ASN
13	O	132	ASN
14	R	22	ASN
17	V	86	GLN
18	X	38	GLN
19	Y	21	GLN
20	Z	6	GLN
1	a	234	ASN
1	a	266	ASN
2	b	179	GLN
3	c	28	GLN
3	c	378	ASN
5	e	82	GLN
7	h	59	ASN
13	o	132	ASN
18	x	33	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	FME	M	1	12	8,9,10	0.86	0	7,9,11	0.93	0
12	FME	m	1	12	8,9,10	1.04	1 (12%)	7,9,11	1.23	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	FME	i	1	8	8,9,10	0.88	0	7,9,11	1.50	2 (28%)
15	FME	T	1	15	8,9,10	1.02	0	7,9,11	1.46	1 (14%)
8	FME	I	1	8	8,9,10	1.14	1 (12%)	7,9,11	1.46	2 (28%)
15	FME	t	1	15	8,9,10	1.20	1 (12%)	7,9,11	1.05	0

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-2.98	1.42	1.46
8	I	1	FME	CA-N	-2.83	1.42	1.46
12	m	1	FME	CA-N	-2.21	1.43	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	CA-N-CN	-2.75	118.60	122.82
15	T	1	FME	O1-CN-N	-2.61	118.39	125.27
8	I	1	FME	CA-N-CN	-2.18	119.46	122.82
8	i	1	FME	C-CA-N	2.04	113.41	109.73
8	I	1	FME	CE-SD-CG	-2.03	93.43	100.40
12	m	1	FME	CA-N-CN	-2.02	119.72	122.82

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	t	1	FME	CB-CG-SD-CE

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

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 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	B	620	-	41,41,41	1.09	3 (7%)	56,56,56	1.34	7 (12%)
22	CLA	A	402	-	65,73,73	1.54	10 (15%)	76,113,113	1.51	12 (15%)
28	LMG	c	522	-	37,37,55	1.33	6 (16%)	45,45,63	1.26	6 (13%)
33	STE	c	501	-	11,11,19	0.81	0	11,11,19	0.93	0
22	CLA	A	411	36	65,73,73	1.58	9 (13%)	76,113,113	1.29	9 (11%)
22	CLA	C	503	-	65,73,73	1.50	7 (10%)	76,113,113	1.63	10 (13%)
27	PL9	D	405	-	55,55,55	1.68	10 (18%)	68,69,69	1.73	16 (23%)
28	LMG	C	519	-	48,48,55	1.14	4 (8%)	56,56,63	1.36	6 (10%)
22	CLA	b	606	36	65,73,73	1.42	8 (12%)	76,113,113	1.57	10 (13%)
22	CLA	C	504	-	65,73,73	1.77	8 (12%)	76,113,113	1.74	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	BCT	a	409	21	2,3,3	1.20	0	2,3,3	2.70	1 (50%)
33	STE	B	621	-	16,16,19	0.61	0	16,16,19	1.32	2 (12%)
24	BCR	c	518	-	41,41,41	1.02	2 (4%)	56,56,56	1.32	7 (12%)
29	SQD	a	413	-	35,35,54	1.23	2 (5%)	37,37,65	1.49	6 (16%)
22	CLA	C	509	-	65,73,73	1.52	10 (15%)	76,113,113	1.76	14 (18%)
22	CLA	A	403	36	65,73,73	1.55	8 (12%)	76,113,113	1.38	10 (13%)
22	CLA	B	603	-	65,73,73	1.54	8 (12%)	76,113,113	1.55	11 (14%)
30	DGD	c	521	-	63,63,67	1.09	5 (7%)	77,77,81	1.38	10 (12%)
22	CLA	B	613	-	65,73,73	1.51	6 (9%)	76,113,113	1.60	9 (11%)
29	SQD	A	414	-	38,38,54	1.07	3 (7%)	40,40,65	1.39	3 (7%)
22	CLA	B	616	-	65,73,73	1.60	10 (15%)	76,113,113	1.40	10 (13%)
33	STE	B	625	-	11,11,19	0.96	0	11,11,19	1.07	0
22	CLA	b	608	-	65,73,73	1.62	9 (13%)	76,113,113	1.44	12 (15%)
33	STE	a	414	-	9,9,19	0.51	0	8,8,19	0.43	0
33	STE	J	101	-	11,11,19	0.72	0	11,11,19	1.12	1 (9%)
24	BCR	c	516	-	41,41,41	1.05	2 (4%)	56,56,56	1.27	9 (16%)
22	CLA	B	605	-	65,73,73	1.60	9 (13%)	76,113,113	1.82	10 (13%)
28	LMG	A	412	-	48,48,55	1.03	2 (4%)	56,56,63	1.44	8 (14%)
22	CLA	h	101	36	65,73,73	1.60	9 (13%)	76,113,113	1.72	8 (10%)
22	CLA	d	402	-	65,73,73	1.70	8 (12%)	76,113,113	1.38	13 (17%)
34	LHG	d	406	-	48,48,48	1.00	3 (6%)	51,54,54	1.37	6 (11%)
22	CLA	b	605	-	65,73,73	1.90	12 (18%)	76,113,113	1.89	19 (25%)
33	STE	C	522	-	11,11,19	0.72	0	11,11,19	1.34	2 (18%)
22	CLA	c	505	-	65,73,73	1.65	9 (13%)	76,113,113	1.48	9 (11%)
22	CLA	B	606	-	65,73,73	1.35	6 (9%)	76,113,113	1.39	9 (11%)
28	LMG	M	101	-	51,51,55	0.94	3 (5%)	59,59,63	1.40	11 (18%)
22	CLA	B	607	-	65,73,73	1.65	12 (18%)	76,113,113	1.36	10 (13%)
35	HEC	V	201	17	32,50,50	1.99	3 (9%)	24,82,82	2.22	6 (25%)
28	LMG	D	410	-	31,31,55	1.12	3 (9%)	33,33,63	1.15	1 (3%)
28	LMG	b	623	-	55,55,55	0.93	1 (1%)	63,63,63	1.49	9 (14%)
29	SQD	B	623	-	53,54,54	0.98	3 (5%)	62,65,65	1.82	10 (16%)
33	STE	d	410	-	16,16,19	0.56	0	16,16,19	1.38	2 (12%)
24	BCR	C	515	-	41,41,41	1.27	4 (9%)	56,56,56	1.32	7 (12%)
34	LHG	B	622	-	48,48,48	1.03	3 (6%)	51,54,54	1.08	2 (3%)
23	PHO	d	401	-	51,69,69	1.07	2 (3%)	47,99,99	1.33	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	BCR	Y	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.25	7 (12%)
33	STE	b	626	-	9,9,19	0.55	0	8,8,19	0.43	0
22	CLA	b	604	-	65,73,73	1.37	6 (9%)	76,113,113	1.68	15 (19%)
33	STE	b	622	-	19,19,19	0.67	0	19,19,19	1.11	1 (5%)
34	LHG	e	102	-	41,41,48	1.04	4 (9%)	44,47,54	1.37	5 (11%)
22	CLA	a	405	-	65,73,73	1.68	12 (18%)	76,113,113	1.48	9 (11%)
33	STE	B	601	-	11,11,19	0.62	0	11,11,19	1.30	2 (18%)
22	CLA	C	508	36	65,73,73	1.56	5 (7%)	76,113,113	1.69	14 (18%)
33	STE	d	411	-	19,19,19	0.72	0	19,19,19	0.98	2 (10%)
24	BCR	d	404	-	41,41,41	1.13	2 (4%)	56,56,56	1.19	6 (10%)
22	CLA	b	602	-	65,73,73	1.48	10 (15%)	76,113,113	1.72	18 (23%)
33	STE	M	103	-	9,9,19	0.43	0	8,8,19	0.58	0
22	CLA	c	509	36	65,73,73	1.39	7 (10%)	76,113,113	1.47	10 (13%)
22	CLA	D	402	-	65,73,73	1.46	6 (9%)	76,113,113	1.46	8 (10%)
33	STE	B	626	-	17,17,19	0.65	0	17,17,19	1.08	0
22	CLA	c	503	-	65,73,73	1.36	8 (12%)	76,113,113	1.65	13 (17%)
22	CLA	c	513	3	65,73,73	1.51	7 (10%)	76,113,113	1.47	7 (9%)
28	LMG	B	629	-	55,55,55	1.47	6 (10%)	63,63,63	1.47	7 (11%)
22	CLA	b	609	36	65,73,73	1.48	10 (15%)	76,113,113	1.58	14 (18%)
22	CLA	b	603	-	65,73,73	1.43	7 (10%)	76,113,113	1.68	14 (18%)
33	STE	b	625	-	19,19,19	0.78	0	19,19,19	0.73	0
24	BCR	b	618	-	41,41,41	1.10	2 (4%)	56,56,56	1.34	8 (14%)
24	BCR	b	617	-	41,41,41	1.26	4 (9%)	56,56,56	1.28	8 (14%)
22	CLA	b	612	-	65,73,73	1.44	12 (18%)	76,113,113	1.58	15 (19%)
22	CLA	D	403	-	65,73,73	1.70	12 (18%)	76,113,113	1.36	9 (11%)
33	STE	b	624	-	15,15,19	0.84	0	15,15,19	0.81	0
22	CLA	a	402	-	65,73,73	1.58	6 (9%)	76,113,113	1.58	14 (18%)
22	CLA	C	514	-	65,73,73	1.62	7 (10%)	76,113,113	1.29	9 (11%)
28	LMG	c	525	-	49,49,55	1.00	5 (10%)	57,57,63	1.34	5 (8%)
24	BCR	T	101	-	41,41,41	1.04	4 (9%)	56,56,56	1.37	6 (10%)
33	STE	l	102	-	17,17,19	0.36	0	16,16,19	0.87	0
22	CLA	b	607	-	65,73,73	1.61	10 (15%)	76,113,113	1.45	14 (18%)
24	BCR	D	404	-	41,41,41	1.14	2 (4%)	56,56,56	1.23	4 (7%)
22	CLA	B	617	-	60,68,73	1.55	9 (15%)	70,107,113	1.89	18 (25%)
30	DGD	H	102	-	63,63,67	1.39	11 (17%)	77,77,81	1.46	15 (19%)
33	STE	a	415	-	11,11,19	0.81	0	11,11,19	1.13	1 (9%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	a	403	36	65,73,73	1.56	7 (10%)	76,113,113	1.34	7 (9%)
22	CLA	b	611	-	65,73,73	1.36	8 (12%)	76,113,113	1.46	12 (15%)
33	STE	B	627	-	15,15,19	0.49	0	14,14,19	0.70	0
22	CLA	c	515	-	65,73,73	1.58	8 (12%)	76,113,113	1.23	6 (7%)
27	PL9	a	410	-	55,55,55	1.09	5 (9%)	68,69,69	1.57	12 (17%)
22	CLA	c	511	-	65,73,73	1.65	7 (10%)	76,113,113	1.57	9 (11%)
34	LHG	d	408	-	38,38,48	0.78	1 (2%)	41,44,54	1.08	3 (7%)
22	CLA	b	615	-	60,68,73	1.55	12 (20%)	70,107,113	1.66	10 (14%)
34	LHG	l	101	-	48,48,48	0.74	1 (2%)	51,54,54	1.13	4 (7%)
29	SQD	A	413	-	51,52,54	0.93	4 (7%)	60,63,65	1.96	11 (18%)
22	CLA	C	505	36	59,67,73	1.65	6 (10%)	68,105,113	1.54	9 (13%)
23	PHO	A	404	-	51,69,69	1.05	4 (7%)	47,99,99	1.33	5 (10%)
29	SQD	f	101	-	40,41,54	1.10	5 (12%)	49,52,65	2.02	13 (26%)
33	STE	c	523	-	19,19,19	0.80	0	19,19,19	0.82	0
29	SQD	b	619	-	48,49,54	0.96	2 (4%)	57,60,65	2.09	14 (24%)
32	OEY	A	417[B]	36,3,1	0,16,16	-	-	-	-	-
33	STE	B	628	-	14,14,19	0.41	0	13,13,19	0.87	0
28	LMG	c	524	-	48,48,55	1.12	3 (6%)	56,56,63	1.33	7 (12%)
33	STE	X	101	-	19,19,19	0.66	0	19,19,19	1.31	3 (15%)
35	HEC	v	201	17	32,50,50	2.19	3 (9%)	24,82,82	2.07	7 (29%)
29	SQD	a	412	-	53,54,54	0.99	4 (7%)	62,65,65	1.86	11 (17%)
24	BCR	x	101	-	41,41,41	1.08	4 (9%)	56,56,56	1.38	10 (17%)
22	CLA	B	611	36	65,73,73	1.66	9 (13%)	76,113,113	1.72	11 (14%)
22	CLA	c	508	-	65,73,73	1.59	8 (12%)	76,113,113	1.47	11 (14%)
33	STE	T	102	-	14,14,19	0.45	0	13,13,19	0.68	0
22	CLA	C	510	-	65,73,73	1.42	9 (13%)	76,113,113	1.56	7 (9%)
33	STE	M	102	-	14,14,19	0.84	0	14,14,19	0.99	1 (7%)
22	CLA	a	411	36	65,73,73	1.95	8 (12%)	76,113,113	1.34	6 (7%)
24	BCR	t	101	-	41,41,41	0.93	1 (2%)	56,56,56	1.35	5 (8%)
33	STE	C	520	-	11,11,19	0.86	0	11,11,19	1.02	0
33	STE	L	101	-	11,11,19	0.77	0	11,11,19	1.50	2 (18%)
24	BCR	K	101	-	41,41,41	0.99	2 (4%)	56,56,56	1.18	6 (10%)
24	BCR	y	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.09	2 (3%)
33	STE	d	412	-	19,19,19	0.62	0	19,19,19	1.03	2 (10%)
22	CLA	B	612	-	65,73,73	1.58	9 (13%)	76,113,113	1.53	13 (17%)
28	LMG	D	411	-	26,26,55	0.73	1 (3%)	26,26,63	1.21	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	c	514	-	65,73,73	1.55	10 (15%)	76,113,113	1.48	9 (11%)
22	CLA	d	403	-	65,73,73	1.75	10 (15%)	76,113,113	1.51	11 (14%)
26	BCT	A	409	21	2,3,3	1.14	0	2,3,3	3.35	1 (50%)
34	LHG	d	407	-	48,48,48	1.01	3 (6%)	51,54,54	1.24	5 (9%)
33	STE	j	101	-	11,11,19	0.83	0	11,11,19	1.33	1 (9%)
22	CLA	B	602	36	65,73,73	1.67	9 (13%)	76,113,113	1.87	11 (14%)
33	STE	h	103	-	13,13,19	0.42	0	12,12,19	0.63	0
22	CLA	b	601	-	65,73,73	1.44	10 (15%)	76,113,113	1.69	11 (14%)
34	LHG	D	412	-	48,48,48	0.92	2 (4%)	51,54,54	1.43	8 (15%)
22	CLA	c	512	-	65,73,73	1.48	6 (9%)	76,113,113	1.30	8 (10%)
35	HEC	e	101	6,5	32,50,50	2.35	5 (15%)	24,82,82	2.34	5 (20%)
29	SQD	D	407	-	35,36,54	0.97	1 (2%)	42,45,65	2.31	13 (30%)
24	BCR	Z	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.35	8 (14%)
22	CLA	B	610	-	65,73,73	1.54	12 (18%)	76,113,113	1.45	13 (17%)
30	DGD	C	516	-	63,63,67	1.16	6 (9%)	77,77,81	1.41	19 (24%)
24	BCR	B	618	-	41,41,41	1.10	2 (4%)	56,56,56	1.21	7 (12%)
32	OEY	a	417[B]	36,3,1	0,16,16	-	-	-	-	-
34	LHG	D	409	-	46,46,48	0.99	2 (4%)	49,52,54	1.32	2 (4%)
22	CLA	c	506	36	60,68,73	1.58	7 (11%)	70,107,113	1.51	14 (20%)
33	STE	I	101	-	14,14,19	0.48	0	13,13,19	0.61	0
28	LMG	b	621	-	51,51,55	0.98	3 (5%)	59,59,63	1.46	10 (16%)
35	HEC	F	101	6,5	32,50,50	2.23	4 (12%)	24,82,82	2.41	7 (29%)
23	PHO	D	401	-	51,69,69	1.05	4 (7%)	47,99,99	1.29	7 (14%)
24	BCR	A	406	-	41,41,41	1.05	2 (4%)	56,56,56	1.49	8 (14%)
22	CLA	c	510	-	64,72,73	1.68	8 (12%)	74,111,113	1.44	11 (14%)
30	DGD	C	517	-	63,63,67	1.32	8 (12%)	77,77,81	1.35	10 (12%)
22	CLA	C	507	-	65,73,73	1.65	10 (15%)	76,113,113	1.24	5 (6%)
33	STE	H	103	-	17,17,19	0.48	0	16,16,19	0.63	0
22	CLA	b	614	-	65,73,73	1.56	10 (15%)	76,113,113	1.59	13 (17%)
22	CLA	B	604	-	65,73,73	1.44	8 (12%)	76,113,113	1.43	14 (18%)
22	CLA	c	507	-	65,73,73	1.46	8 (12%)	76,113,113	1.25	6 (7%)
34	LHG	E	101	-	48,48,48	0.95	4 (8%)	51,54,54	1.19	5 (9%)
28	LMG	d	409	-	44,44,55	0.99	3 (6%)	52,52,63	1.40	7 (13%)
22	CLA	B	615	-	65,73,73	1.77	10 (15%)	76,113,113	1.46	13 (17%)
22	CLA	A	405	-	54,62,73	1.59	6 (11%)	62,99,113	1.47	11 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	BCR	B	619	-	41,41,41	1.01	2 (4%)	56,56,56	1.40	10 (17%)
31	OEX	a	416[A]	36,3,1	0,15,15	-	-	-	-	-
30	DGD	h	102	-	63,63,67	1.15	7 (11%)	77,77,81	1.51	16 (20%)
22	CLA	C	512	3	65,73,73	1.91	10 (15%)	76,113,113	1.42	7 (9%)
22	CLA	B	609	-	65,73,73	1.31	9 (13%)	76,113,113	1.60	11 (14%)
23	PHO	a	404	-	51,69,69	0.99	3 (5%)	47,99,99	1.37	8 (17%)
30	DGD	c	519	-	63,63,67	1.37	8 (12%)	77,77,81	1.42	15 (19%)
22	CLA	b	613	-	65,73,73	1.53	8 (12%)	76,113,113	1.36	12 (15%)
33	STE	Z	102	-	7,7,19	0.30	0	6,6,19	0.75	0
24	BCR	c	517	-	41,41,41	1.10	2 (4%)	56,56,56	1.34	6 (10%)
33	STE	E	102	-	11,11,19	0.85	0	11,11,19	1.23	1 (9%)
27	PL9	d	405	-	55,55,55	1.59	7 (12%)	68,69,69	1.66	15 (22%)
24	BCR	a	406	-	41,41,41	1.07	2 (4%)	56,56,56	1.44	9 (16%)
28	LMG	D	406	-	51,51,55	0.88	3 (5%)	59,59,63	1.48	9 (15%)
34	LHG	D	408	-	48,48,48	1.09	4 (8%)	51,54,54	1.21	5 (9%)
22	CLA	C	506	-	65,73,73	1.55	7 (10%)	76,113,113	1.25	7 (9%)
30	DGD	A	415	-	67,67,67	1.41	9 (13%)	81,81,81	1.44	13 (16%)
22	CLA	C	502	-	65,73,73	1.72	10 (15%)	76,113,113	1.47	5 (6%)
24	BCR	H	101	-	41,41,41	1.08	1 (2%)	56,56,56	1.49	10 (17%)
24	BCR	b	616	-	41,41,41	1.18	5 (12%)	56,56,56	1.44	12 (21%)
22	CLA	c	504	-	65,73,73	1.66	9 (13%)	76,113,113	1.47	10 (13%)
22	CLA	C	511	-	65,73,73	1.46	9 (13%)	76,113,113	1.33	6 (7%)
27	PL9	A	410	-	55,55,55	1.15	5 (9%)	68,69,69	1.72	14 (20%)
22	CLA	b	610	-	65,73,73	1.33	6 (9%)	76,113,113	1.57	13 (17%)
33	STE	C	521	-	15,15,19	0.46	0	14,14,19	0.67	0
22	CLA	C	513	-	65,73,73	1.55	11 (16%)	76,113,113	1.39	11 (14%)
30	DGD	C	518	-	63,63,67	0.94	5 (7%)	77,77,81	1.31	7 (9%)
22	CLA	B	608	36	65,73,73	1.65	11 (16%)	76,113,113	1.56	8 (10%)
30	DGD	c	520	-	63,63,67	1.05	4 (6%)	77,77,81	1.43	10 (12%)
22	CLA	B	614	-	65,73,73	1.69	10 (15%)	76,113,113	1.37	12 (15%)
31	OEX	A	416[A]	36,3,1	0,15,15	-	-	-	-	-
33	STE	b	620	-	15,15,19	0.44	0	14,14,19	0.71	0
33	STE	B	624	-	13,13,19	0.66	0	13,13,19	1.40	2 (15%)

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	B	620	-	-	4/29/63/63	0/2/2/2
22	CLA	A	402	-	1/1/20/20	3/37/115/115	-
28	LMG	c	522	-	-	9/31/51/70	0/1/1/1
33	STE	c	501	-	-	5/9/9/17	-
22	CLA	C	503	-	1/1/20/20	10/37/115/115	-
22	CLA	A	411	36	-	11/37/115/115	-
27	PL9	D	405	-	-	9/53/73/73	0/1/1/1
28	LMG	C	519	-	-	19/43/63/70	0/1/1/1
22	CLA	b	606	36	1/1/20/20	12/37/115/115	-
22	CLA	C	504	-	-	4/37/115/115	-
33	STE	B	621	-	-	6/14/14/17	-
24	BCR	c	518	-	-	11/29/63/63	0/2/2/2
29	SQD	a	413	-	-	21/37/37/69	-
22	CLA	C	509	-	-	6/37/115/115	-
22	CLA	A	403	36	1/1/20/20	10/37/115/115	-
22	CLA	B	603	-	-	5/37/115/115	-
30	DGD	c	521	-	-	13/51/91/95	0/2/2/2
22	CLA	B	613	-	1/1/20/20	9/37/115/115	-
29	SQD	A	414	-	-	14/39/39/69	-
22	CLA	B	616	-	1/1/20/20	8/37/115/115	-
33	STE	B	625	-	-	5/9/9/17	-
22	CLA	b	608	-	-	6/37/115/115	-
33	STE	a	414	-	-	3/7/7/17	-
33	STE	J	101	-	-	3/9/9/17	-
24	BCR	c	516	-	-	13/29/63/63	0/2/2/2
22	CLA	B	605	-	1/1/20/20	12/37/115/115	-
28	LMG	A	412	-	-	13/43/63/70	0/1/1/1
22	CLA	h	101	36	1/1/20/20	18/37/115/115	-
22	CLA	d	402	-	1/1/20/20	8/37/115/115	-
34	LHG	d	406	-	-	22/53/53/53	-
22	CLA	b	605	-	1/1/20/20	11/37/115/115	-
33	STE	C	522	-	-	3/9/9/17	-
22	CLA	c	505	-	-	4/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	606	-	1/1/20/20	9/37/115/115	-
28	LMG	M	101	-	-	19/46/66/70	0/1/1/1
22	CLA	B	607	-	1/1/20/20	10/37/115/115	-
35	HEC	V	201	17	-	2/10/54/54	-
28	LMG	D	410	-	-	15/33/33/70	-
28	LMG	b	623	-	-	21/50/70/70	0/1/1/1
29	SQD	B	623	-	-	21/49/69/69	0/1/1/1
33	STE	d	410	-	-	9/14/14/17	-
24	BCR	C	515	-	-	3/29/63/63	0/2/2/2
34	LHG	B	622	-	-	20/53/53/53	-
23	PHO	d	401	-	-	7/37/103/103	0/5/6/6
24	BCR	Y	101	-	-	10/29/63/63	0/2/2/2
33	STE	b	626	-	-	5/7/7/17	-
22	CLA	b	604	-	1/1/20/20	10/37/115/115	-
33	STE	b	622	-	-	11/17/17/17	-
34	LHG	e	102	-	-	25/46/46/53	-
22	CLA	a	405	-	1/1/20/20	7/37/115/115	-
33	STE	B	601	-	-	1/9/9/17	-
22	CLA	C	508	36	1/1/20/20	8/37/115/115	-
33	STE	d	411	-	-	12/17/17/17	-
24	BCR	d	404	-	-	4/29/63/63	0/2/2/2
22	CLA	b	602	-	1/1/20/20	8/37/115/115	-
33	STE	M	103	-	-	2/7/7/17	-
22	CLA	c	509	36	1/1/20/20	7/37/115/115	-
22	CLA	D	402	-	1/1/20/20	5/37/115/115	-
33	STE	B	626	-	-	8/15/15/17	-
22	CLA	c	503	-	1/1/20/20	5/37/115/115	-
22	CLA	c	513	3	1/1/20/20	11/37/115/115	-
28	LMG	B	629	-	-	29/50/70/70	0/1/1/1
22	CLA	b	609	36	1/1/20/20	5/37/115/115	-
22	CLA	b	603	-	1/1/20/20	6/37/115/115	-
33	STE	b	625	-	-	6/17/17/17	-
24	BCR	b	618	-	-	4/29/63/63	0/2/2/2
24	BCR	b	617	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	612	-	1/1/20/20	4/37/115/115	-
22	CLA	D	403	-	-	8/37/115/115	-
33	STE	b	624	-	-	9/13/13/17	-
22	CLA	a	402	-	1/1/20/20	7/37/115/115	-
22	CLA	C	514	-	-	12/37/115/115	-
28	LMG	c	525	-	-	18/44/64/70	0/1/1/1
24	BCR	T	101	-	-	6/29/63/63	0/2/2/2
33	STE	l	102	-	-	7/15/15/17	-
22	CLA	b	607	-	1/1/20/20	10/37/115/115	-
24	BCR	D	404	-	-	5/29/63/63	0/2/2/2
22	CLA	B	617	-	1/1/19/20	6/31/109/115	-
30	DGD	H	102	-	-	20/51/91/95	0/2/2/2
33	STE	a	415	-	-	3/9/9/17	-
22	CLA	a	403	36	-	14/37/115/115	-
22	CLA	b	611	-	1/1/20/20	6/37/115/115	-
33	STE	B	627	-	-	6/13/13/17	-
22	CLA	c	515	-	1/1/20/20	8/37/115/115	-
27	PL9	a	410	-	-	17/53/73/73	0/1/1/1
22	CLA	c	511	-	1/1/20/20	9/37/115/115	-
34	LHG	d	408	-	-	15/43/43/53	-
22	CLA	b	615	-	1/1/19/20	9/31/109/115	-
34	LHG	l	101	-	-	20/53/53/53	-
29	SQD	A	413	-	-	17/47/67/69	0/1/1/1
22	CLA	C	505	36	1/1/18/20	9/30/108/115	-
23	PHO	A	404	-	-	4/37/103/103	0/5/6/6
29	SQD	f	101	-	-	13/36/56/69	0/1/1/1
33	STE	c	523	-	-	10/17/17/17	-
29	SQD	b	619	-	-	19/44/64/69	0/1/1/1
33	STE	B	628	-	-	7/12/12/17	-
28	LMG	c	524	-	-	23/43/63/70	0/1/1/1
33	STE	X	101	-	-	9/17/17/17	-
35	HEC	v	201	17	-	2/10/54/54	-
29	SQD	a	412	-	-	30/49/69/69	0/1/1/1
24	BCR	x	101	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	611	36	1/1/20/20	6/37/115/115	-
22	CLA	c	508	-	1/1/20/20	18/37/115/115	-
33	STE	T	102	-	-	7/12/12/17	-
22	CLA	C	510	-	1/1/20/20	8/37/115/115	-
33	STE	M	102	-	-	6/12/12/17	-
22	CLA	a	411	36	1/1/20/20	4/37/115/115	-
24	BCR	t	101	-	-	4/29/63/63	0/2/2/2
33	STE	C	520	-	-	3/9/9/17	-
33	STE	L	101	-	-	5/9/9/17	-
24	BCR	K	101	-	-	5/29/63/63	0/2/2/2
24	BCR	y	101	-	-	11/29/63/63	0/2/2/2
33	STE	d	412	-	-	7/17/17/17	-
22	CLA	B	612	-	1/1/20/20	12/37/115/115	-
28	LMG	D	411	-	-	10/22/22/70	-
22	CLA	c	514	-	1/1/20/20	21/37/115/115	-
22	CLA	d	403	-	1/1/20/20	7/37/115/115	-
34	LHG	d	407	-	-	19/53/53/53	-
33	STE	j	101	-	-	4/9/9/17	-
22	CLA	B	602	36	1/1/20/20	17/37/115/115	-
33	STE	h	103	-	-	5/11/11/17	-
22	CLA	b	601	-	1/1/20/20	8/37/115/115	-
34	LHG	D	412	-	-	17/53/53/53	-
22	CLA	c	512	-	1/1/20/20	12/37/115/115	-
35	HEC	e	101	6,5	-	4/10/54/54	-
29	SQD	D	407	-	-	10/28/48/69	0/1/1/1
24	BCR	Z	101	-	-	15/29/63/63	0/2/2/2
22	CLA	B	610	-	-	7/37/115/115	-
30	DGD	C	516	-	-	18/51/91/95	0/2/2/2
24	BCR	B	618	-	-	8/29/63/63	0/2/2/2
34	LHG	D	409	-	-	25/51/51/53	-
22	CLA	c	506	36	1/1/19/20	9/31/109/115	-
33	STE	I	101	-	-	4/12/12/17	-
28	LMG	b	621	-	-	21/46/66/70	0/1/1/1
35	HEC	F	101	6,5	-	2/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PHO	D	401	-	-	1/37/103/103	0/5/6/6
24	BCR	A	406	-	-	4/29/63/63	0/2/2/2
22	CLA	c	510	-	-	12/36/114/115	-
30	DGD	C	517	-	-	18/51/91/95	0/2/2/2
22	CLA	C	507	-	1/1/20/20	14/37/115/115	-
33	STE	H	103	-	-	8/15/15/17	-
22	CLA	b	614	-	1/1/20/20	11/37/115/115	-
22	CLA	B	604	-	1/1/20/20	9/37/115/115	-
22	CLA	c	507	-	1/1/20/20	5/37/115/115	-
34	LHG	E	101	-	-	29/53/53/53	-
28	LMG	d	409	-	-	12/39/59/70	0/1/1/1
22	CLA	B	615	-	1/1/20/20	14/37/115/115	-
22	CLA	A	405	-	1/1/17/20	6/24/102/115	-
24	BCR	B	619	-	-	9/29/63/63	0/2/2/2
30	DGD	h	102	-	-	14/51/91/95	0/2/2/2
22	CLA	C	512	3	1/1/20/20	11/37/115/115	-
22	CLA	B	609	-	-	2/37/115/115	-
23	PHO	a	404	-	-	5/37/103/103	0/5/6/6
30	DGD	c	519	-	-	24/51/91/95	0/2/2/2
22	CLA	b	613	-	1/1/20/20	19/37/115/115	-
33	STE	Z	102	-	-	2/5/5/17	-
24	BCR	c	517	-	-	9/29/63/63	0/2/2/2
33	STE	E	102	-	-	3/9/9/17	-
27	PL9	d	405	-	-	13/53/73/73	0/1/1/1
24	BCR	a	406	-	-	8/29/63/63	0/2/2/2
28	LMG	D	406	-	-	17/46/66/70	0/1/1/1
34	LHG	D	408	-	-	22/53/53/53	-
22	CLA	C	506	-	1/1/20/20	13/37/115/115	-
30	DGD	A	415	-	-	21/55/95/95	0/2/2/2
22	CLA	C	502	-	-	3/37/115/115	-
24	BCR	H	101	-	-	2/29/63/63	0/2/2/2
24	BCR	b	616	-	-	6/29/63/63	0/2/2/2
22	CLA	c	504	-	-	7/37/115/115	-
22	CLA	C	511	-	1/1/20/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PL9	A	410	-	-	19/53/73/73	0/1/1/1
22	CLA	b	610	-	-	8/37/115/115	-
33	STE	C	521	-	-	5/13/13/17	-
22	CLA	C	513	-	1/1/20/20	16/37/115/115	-
30	DGD	C	518	-	-	15/51/91/95	0/2/2/2
22	CLA	B	608	36	1/1/20/20	10/37/115/115	-
30	DGD	c	520	-	-	19/51/91/95	0/2/2/2
22	CLA	B	614	-	1/1/20/20	10/37/115/115	-
33	STE	b	620	-	-	6/13/13/17	-
33	STE	B	624	-	-	3/11/11/17	-

All (873) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	e	101	HEC	C2B-C3B	-9.06	1.31	1.40
22	a	411	CLA	MG-NA	8.98	2.27	2.06
22	C	512	CLA	MG-NA	8.92	2.27	2.06
22	b	605	CLA	MG-NA	8.78	2.27	2.06
22	B	611	CLA	C4B-NB	8.22	1.42	1.35
22	C	505	CLA	C4B-NB	8.21	1.42	1.35
22	B	614	CLA	C4B-NB	7.93	1.42	1.35
22	B	615	CLA	C4B-NB	7.83	1.42	1.35
22	b	613	CLA	C4B-NB	7.82	1.42	1.35
22	C	504	CLA	C4B-NB	7.79	1.42	1.35
22	B	602	CLA	C4B-NB	7.78	1.42	1.35
22	c	511	CLA	C4B-NB	7.77	1.42	1.35
22	a	411	CLA	C4B-NB	7.77	1.42	1.35
22	C	514	CLA	C4B-NB	7.68	1.42	1.35
22	c	504	CLA	C4B-NB	7.66	1.42	1.35
22	d	403	CLA	C4B-NB	7.62	1.42	1.35
22	B	613	CLA	C4B-NB	7.51	1.41	1.35
22	C	507	CLA	C4B-NB	7.43	1.41	1.35
22	C	512	CLA	C4B-NB	7.42	1.41	1.35
22	c	514	CLA	C4B-NB	7.41	1.41	1.35
22	c	506	CLA	C4B-NB	7.40	1.41	1.35
22	A	411	CLA	C4B-NB	7.38	1.41	1.35
22	C	506	CLA	C4B-NB	7.30	1.41	1.35
35	v	201	HEC	C2B-C3B	-7.29	1.33	1.40
22	A	403	CLA	C4B-NB	7.27	1.41	1.35
22	B	605	CLA	MG-NA	7.25	2.23	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	608	CLA	C4B-NB	7.25	1.41	1.35
22	d	402	CLA	C4B-NB	7.24	1.41	1.35
22	A	402	CLA	C4B-NB	7.23	1.41	1.35
22	B	603	CLA	C4B-NB	7.17	1.41	1.35
22	C	502	CLA	C4B-NB	7.17	1.41	1.35
22	C	504	CLA	MG-NA	7.15	2.23	2.06
22	B	616	CLA	C4B-NB	7.15	1.41	1.35
22	b	607	CLA	C4B-NB	7.12	1.41	1.35
22	C	508	CLA	C4B-NB	7.06	1.41	1.35
22	b	603	CLA	C4B-NB	7.05	1.41	1.35
35	F	101	HEC	C2B-C3B	-7.01	1.33	1.40
22	A	405	CLA	C4B-NB	6.90	1.41	1.35
22	C	509	CLA	C4B-NB	6.88	1.41	1.35
22	c	505	CLA	C4B-NB	6.87	1.41	1.35
22	c	515	CLA	C4B-NB	6.87	1.41	1.35
22	B	610	CLA	C4B-NB	6.86	1.41	1.35
22	a	402	CLA	C4B-NB	6.85	1.41	1.35
22	C	511	CLA	C4B-NB	6.83	1.41	1.35
22	b	601	CLA	C4B-NB	6.79	1.41	1.35
22	h	101	CLA	C4B-NB	6.76	1.41	1.35
22	a	405	CLA	C4B-NB	6.71	1.41	1.35
22	B	612	CLA	MG-NA	6.71	2.22	2.06
22	c	508	CLA	MG-ND	-6.68	1.92	2.05
22	c	510	CLA	C4B-NB	6.47	1.41	1.35
22	D	403	CLA	C4B-NB	6.45	1.41	1.35
22	C	508	CLA	MG-NA	6.39	2.21	2.06
35	F	101	HEC	C3C-C2C	-6.37	1.34	1.40
22	C	513	CLA	C4B-NB	6.37	1.40	1.35
22	B	608	CLA	C4B-NB	6.36	1.40	1.35
22	D	402	CLA	C4B-NB	6.36	1.40	1.35
22	c	503	CLA	C4B-NB	6.35	1.40	1.35
22	c	509	CLA	C4B-NB	6.34	1.40	1.35
22	B	607	CLA	MG-NA	6.34	2.21	2.06
28	B	629	LMG	C4-C5	6.26	1.66	1.53
22	a	403	CLA	C4B-NB	6.23	1.40	1.35
35	V	201	HEC	C2B-C3B	-6.21	1.34	1.40
35	V	201	HEC	C3C-C2C	-6.21	1.34	1.40
22	b	611	CLA	C4B-NB	6.18	1.40	1.35
22	c	512	CLA	C4B-NB	6.16	1.40	1.35
22	c	513	CLA	C4B-NB	6.11	1.40	1.35
22	d	403	CLA	MG-ND	-6.10	1.93	2.05
22	B	604	CLA	MG-NA	6.10	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	505	CLA	MG-NC	6.09	2.20	2.06
27	d	405	PL9	C6-C1	-6.03	1.37	1.48
22	b	614	CLA	MG-NA	6.02	2.20	2.06
22	c	508	CLA	C4B-NB	5.99	1.40	1.35
22	d	402	CLA	MG-ND	-5.97	1.94	2.05
27	D	405	PL9	C7-C3	-5.88	1.45	1.51
22	C	510	CLA	C4B-NB	5.87	1.40	1.35
22	C	502	CLA	MG-NA	5.79	2.20	2.06
22	b	614	CLA	C4B-NB	5.79	1.40	1.35
22	c	507	CLA	C4B-NB	5.74	1.40	1.35
22	D	403	CLA	MG-ND	-5.68	1.94	2.05
22	b	606	CLA	C4B-NB	5.58	1.40	1.35
22	b	610	CLA	C4B-NB	5.55	1.40	1.35
22	h	101	CLA	MG-NA	5.53	2.19	2.06
35	v	201	HEC	C3C-C2C	-5.52	1.35	1.40
22	C	514	CLA	MG-NA	5.51	2.19	2.06
22	b	612	CLA	C4B-NB	5.49	1.40	1.35
22	b	604	CLA	C4B-NB	5.45	1.40	1.35
22	a	403	CLA	MG-NC	5.45	2.19	2.06
22	b	605	CLA	C4B-NB	5.45	1.40	1.35
22	b	602	CLA	C4B-NB	5.26	1.39	1.35
22	B	615	CLA	MG-ND	-5.26	1.95	2.05
22	c	513	CLA	MG-NA	5.24	2.18	2.06
22	B	617	CLA	C4B-NB	5.20	1.39	1.35
22	B	607	CLA	C4B-NB	5.11	1.39	1.35
22	c	510	CLA	MG-NA	5.10	2.18	2.06
22	c	504	CLA	MG-NA	5.05	2.18	2.06
27	d	405	PL9	C3-C4	-5.04	1.41	1.49
22	B	606	CLA	C4B-NB	5.03	1.39	1.35
35	e	101	HEC	C3C-C2C	-5.01	1.35	1.40
22	c	515	CLA	MG-ND	-5.01	1.95	2.05
22	B	612	CLA	C4B-NB	4.98	1.39	1.35
22	D	403	CLA	C1D-ND	4.88	1.43	1.37
22	c	512	CLA	MG-NA	4.84	2.17	2.06
22	b	605	CLA	C1D-ND	4.84	1.43	1.37
22	B	617	CLA	MG-NA	4.82	2.17	2.06
22	C	503	CLA	MG-ND	4.81	2.15	2.05
22	b	615	CLA	MG-ND	-4.79	1.96	2.05
22	A	411	CLA	MG-NA	4.78	2.17	2.06
35	F	101	HEC	C3D-C2D	4.77	1.51	1.37
22	b	609	CLA	C4B-NB	4.76	1.39	1.35
22	C	503	CLA	C4D-ND	-4.73	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	519	DGD	C4D-C3D	4.73	1.64	1.52
22	B	609	CLA	C4B-NB	4.73	1.39	1.35
22	C	507	CLA	MG-NA	4.71	2.17	2.06
24	H	101	BCR	C30-C25	-4.70	1.47	1.53
24	C	515	BCR	C1-C6	-4.70	1.47	1.53
22	c	511	CLA	MG-NC	4.70	2.17	2.06
34	B	622	LHG	O7-C5	-4.69	1.34	1.46
35	v	201	HEC	C3D-C2D	4.69	1.51	1.37
34	D	408	LHG	O8-C6	-4.68	1.34	1.45
35	e	101	HEC	C3D-C2D	4.66	1.51	1.37
22	c	510	CLA	C4D-ND	-4.64	1.31	1.37
22	c	507	CLA	C4D-ND	-4.63	1.31	1.37
22	a	405	CLA	C1D-ND	4.62	1.43	1.37
22	a	402	CLA	MG-NA	4.61	2.17	2.06
35	V	201	HEC	C3D-C2D	4.61	1.51	1.37
27	A	410	PL9	C7-C3	-4.57	1.46	1.51
22	C	503	CLA	C4B-NB	4.56	1.39	1.35
22	c	510	CLA	C1D-ND	4.54	1.43	1.37
24	Y	101	BCR	C30-C25	-4.53	1.47	1.53
22	B	605	CLA	C4B-NB	4.51	1.39	1.35
22	D	402	CLA	C1D-ND	4.49	1.43	1.37
22	A	405	CLA	MG-ND	-4.47	1.96	2.05
22	d	403	CLA	C1D-ND	4.45	1.43	1.37
22	a	405	CLA	MG-NA	4.41	2.16	2.06
22	B	606	CLA	C4D-ND	-4.41	1.31	1.37
22	B	615	CLA	C4D-ND	-4.40	1.31	1.37
22	b	612	CLA	MG-NA	4.39	2.16	2.06
30	A	415	DGD	C3G-C2G	4.39	1.64	1.50
22	A	402	CLA	C1D-ND	4.39	1.43	1.37
22	b	609	CLA	MG-NC	4.36	2.16	2.06
22	b	609	CLA	C1D-ND	4.35	1.43	1.37
22	B	614	CLA	MG-NC	4.35	2.16	2.06
22	B	613	CLA	C4D-ND	-4.33	1.31	1.37
22	b	602	CLA	MG-NA	4.31	2.16	2.06
22	b	605	CLA	C1B-NB	4.30	1.39	1.35
22	b	615	CLA	C1D-ND	4.28	1.43	1.37
22	b	607	CLA	MG-ND	4.28	2.14	2.05
22	C	505	CLA	MG-NA	4.26	2.16	2.06
22	B	602	CLA	C1D-ND	4.26	1.43	1.37
30	H	102	DGD	C4E-C5E	4.24	1.62	1.53
22	c	511	CLA	C1D-ND	4.23	1.43	1.37
24	D	404	BCR	C30-C25	-4.22	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	629	LMG	C4-C3	4.19	1.63	1.52
22	b	606	CLA	MG-NA	4.19	2.16	2.06
22	B	608	CLA	MG-ND	-4.15	1.97	2.05
22	a	403	CLA	C4D-ND	-4.13	1.32	1.37
22	a	411	CLA	MG-ND	-4.11	1.97	2.05
22	C	507	CLA	MG-ND	-4.10	1.97	2.05
22	b	608	CLA	MG-NA	4.09	2.16	2.06
22	C	506	CLA	MG-NA	4.08	2.16	2.06
22	c	503	CLA	C4D-ND	-4.07	1.32	1.37
22	B	616	CLA	C1D-ND	4.05	1.42	1.37
24	b	616	BCR	C1-C6	-4.05	1.48	1.53
22	B	616	CLA	C4D-ND	-4.05	1.32	1.37
22	b	608	CLA	C4D-ND	-4.04	1.32	1.37
27	D	405	PL9	C52-C5	-4.04	1.42	1.50
22	a	402	CLA	C4D-ND	-4.02	1.32	1.37
28	C	519	LMG	C4-C5	4.01	1.61	1.53
22	c	509	CLA	C1D-ND	3.98	1.42	1.37
22	a	411	CLA	C1D-ND	3.97	1.42	1.37
22	B	602	CLA	MG-NA	3.97	2.15	2.06
22	B	608	CLA	C4D-ND	-3.97	1.32	1.37
22	C	512	CLA	C1D-ND	3.92	1.42	1.37
30	C	517	DGD	O5D-C1E	3.91	1.46	1.40
22	c	506	CLA	MG-ND	-3.89	1.98	2.05
22	A	411	CLA	C1D-ND	3.88	1.42	1.37
22	C	503	CLA	MG-NA	3.87	2.15	2.06
22	c	511	CLA	C4D-ND	-3.86	1.32	1.37
27	D	405	PL9	C6-C1	-3.85	1.41	1.48
22	B	615	CLA	MG-NA	3.85	2.15	2.06
22	c	505	CLA	C4D-ND	-3.85	1.32	1.37
22	C	509	CLA	MG-NA	3.85	2.15	2.06
22	B	603	CLA	C1D-ND	3.84	1.42	1.37
22	D	403	CLA	MG-NA	3.83	2.15	2.06
27	D	405	PL9	C41-C39	-3.83	1.43	1.51
22	B	611	CLA	C3B-C2B	-3.82	1.35	1.40
22	A	403	CLA	C4D-ND	-3.81	1.32	1.37
22	a	405	CLA	C4D-ND	-3.80	1.32	1.37
22	b	615	CLA	C4B-NB	3.80	1.38	1.35
22	C	513	CLA	C4D-ND	-3.80	1.32	1.37
22	b	613	CLA	C4D-ND	-3.79	1.32	1.37
22	C	502	CLA	C4D-ND	-3.78	1.32	1.37
22	B	607	CLA	C3B-C2B	-3.78	1.35	1.40
22	B	614	CLA	MG-ND	-3.78	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	517	BCR	C1-C6	-3.77	1.48	1.53
22	C	506	CLA	CHC-C1C	3.76	1.44	1.35
24	c	516	BCR	C1-C6	-3.74	1.48	1.53
22	c	510	CLA	CHC-C1C	3.73	1.44	1.35
22	D	402	CLA	MG-ND	-3.73	1.98	2.05
24	x	101	BCR	C30-C25	-3.72	1.48	1.53
24	d	404	BCR	C1-C6	-3.69	1.48	1.53
30	c	521	DGD	O2G-C2G	-3.66	1.37	1.46
30	C	517	DGD	C4D-C3D	3.66	1.61	1.52
22	b	609	CLA	C3B-C2B	-3.66	1.35	1.40
24	A	406	BCR	C1-C6	-3.65	1.48	1.53
22	C	502	CLA	CHC-C1C	3.65	1.44	1.35
22	c	506	CLA	C4D-ND	-3.64	1.32	1.37
22	B	612	CLA	MG-ND	-3.64	1.98	2.05
22	d	402	CLA	MG-NA	3.61	2.14	2.06
22	C	513	CLA	MG-NA	3.60	2.14	2.06
22	b	611	CLA	C4D-ND	-3.60	1.32	1.37
29	a	413	SQD	O47-C7	3.60	1.44	1.34
24	b	617	BCR	C30-C25	-3.59	1.48	1.53
29	B	623	SQD	O47-C7	3.59	1.44	1.34
22	C	510	CLA	C1D-ND	3.59	1.42	1.37
22	h	101	CLA	C1D-ND	3.58	1.42	1.37
22	c	505	CLA	C1D-ND	3.57	1.42	1.37
22	a	405	CLA	MG-NC	-3.57	1.97	2.06
22	B	609	CLA	C4D-ND	-3.56	1.32	1.37
30	c	519	DGD	O5D-C6D	3.56	1.50	1.43
22	c	515	CLA	C1D-ND	3.55	1.42	1.37
22	C	502	CLA	C1D-ND	3.55	1.42	1.37
22	c	515	CLA	C4D-ND	-3.53	1.32	1.37
22	B	608	CLA	C1D-ND	3.53	1.42	1.37
22	B	614	CLA	MG-NA	3.52	2.14	2.06
29	a	413	SQD	O48-C23	3.51	1.43	1.33
22	b	604	CLA	C4D-ND	-3.51	1.32	1.37
23	D	401	PHO	CAC-C3C	-3.49	1.46	1.52
22	B	604	CLA	C4B-NB	3.48	1.38	1.35
22	A	405	CLA	C4D-ND	-3.48	1.32	1.37
27	a	410	PL9	C6-C1	-3.48	1.42	1.48
24	B	618	BCR	C1-C6	-3.47	1.49	1.53
22	C	505	CLA	CHC-C1C	3.47	1.43	1.35
30	A	415	DGD	C4D-C3D	3.47	1.61	1.52
34	D	412	LHG	O7-C5	-3.47	1.37	1.46
29	A	414	SQD	O48-C23	3.46	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	614	CLA	CHC-C1C	3.46	1.43	1.35
34	d	407	LHG	O7-C5	-3.46	1.37	1.46
24	b	618	BCR	C1-C6	-3.45	1.49	1.53
27	d	405	PL9	C53-C6	-3.44	1.43	1.50
27	d	405	PL9	C46-C44	-3.44	1.44	1.51
22	C	504	CLA	CHC-C1C	3.44	1.43	1.35
22	a	402	CLA	C1D-ND	3.43	1.42	1.37
22	C	511	CLA	C4D-ND	-3.43	1.33	1.37
22	b	609	CLA	C4D-ND	-3.43	1.33	1.37
22	C	506	CLA	C4D-ND	-3.42	1.33	1.37
22	b	604	CLA	CHC-C1C	3.41	1.43	1.35
22	h	101	CLA	CHC-C1C	3.41	1.43	1.35
22	b	607	CLA	CHC-C1C	3.40	1.43	1.35
23	d	401	PHO	CAC-C3C	-3.40	1.46	1.52
28	A	412	LMG	O1-C7	-3.38	1.37	1.43
22	a	402	CLA	CHC-C1C	3.38	1.43	1.35
22	C	514	CLA	C1D-ND	3.37	1.41	1.37
24	Z	101	BCR	C30-C25	-3.37	1.49	1.53
22	c	514	CLA	CHC-C1C	3.37	1.43	1.35
28	c	524	LMG	C3-C2	3.36	1.60	1.52
22	b	615	CLA	C4D-ND	-3.36	1.33	1.37
22	B	617	CLA	C4D-ND	-3.35	1.33	1.37
24	y	101	BCR	C30-C25	-3.35	1.49	1.53
22	B	611	CLA	C1D-ND	3.35	1.41	1.37
22	b	613	CLA	CHC-C1C	3.35	1.43	1.35
27	D	405	PL9	C11-C9	-3.35	1.44	1.51
22	B	607	CLA	C4D-ND	-3.34	1.33	1.37
22	C	511	CLA	C1D-ND	3.34	1.41	1.37
29	a	412	SQD	O48-C23	3.34	1.43	1.33
22	B	608	CLA	MG-NC	3.33	2.14	2.06
29	b	619	SQD	O48-C23	3.31	1.43	1.33
22	c	514	CLA	C1D-ND	3.31	1.41	1.37
22	C	510	CLA	C4D-ND	-3.31	1.33	1.37
22	C	514	CLA	C4D-ND	-3.30	1.33	1.37
22	B	616	CLA	CHC-C1C	3.30	1.43	1.35
22	c	507	CLA	CHC-C1C	3.30	1.43	1.35
22	C	513	CLA	C1D-ND	3.29	1.41	1.37
30	C	517	DGD	O3E-C3E	-3.29	1.35	1.43
22	c	504	CLA	CHC-C1C	3.29	1.43	1.35
22	B	612	CLA	C1D-ND	3.29	1.41	1.37
30	c	520	DGD	O3G-C3G	-3.27	1.37	1.43
29	A	414	SQD	O47-C7	3.27	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	615	CLA	C1D-ND	3.26	1.41	1.37
22	c	509	CLA	C4D-ND	-3.25	1.33	1.37
22	B	605	CLA	C1D-ND	3.24	1.41	1.37
24	d	404	BCR	C30-C25	-3.24	1.49	1.53
22	c	513	CLA	CHC-C1C	3.24	1.43	1.35
22	C	511	CLA	CHC-C1C	3.23	1.43	1.35
22	B	606	CLA	CHC-C1C	3.23	1.43	1.35
22	b	608	CLA	C1D-ND	3.23	1.41	1.37
22	b	615	CLA	C3B-CAB	-3.22	1.41	1.47
22	b	608	CLA	CMB-C2B	-3.22	1.45	1.51
24	y	101	BCR	C1-C6	-3.21	1.49	1.53
22	c	515	CLA	CHC-C1C	3.21	1.43	1.35
22	C	512	CLA	C4D-ND	-3.21	1.33	1.37
30	C	517	DGD	C6E-C5E	3.20	1.62	1.51
22	a	403	CLA	C1D-ND	3.20	1.41	1.37
22	d	402	CLA	C1D-ND	3.20	1.41	1.37
22	B	605	CLA	C4D-ND	-3.19	1.33	1.37
24	b	617	BCR	C1-C6	-3.19	1.49	1.53
22	b	601	CLA	C4D-ND	-3.19	1.33	1.37
29	f	101	SQD	O47-C7	3.19	1.43	1.34
22	B	604	CLA	C3B-CAB	-3.18	1.41	1.47
24	B	618	BCR	C30-C25	-3.18	1.49	1.53
22	c	504	CLA	C1D-ND	3.17	1.41	1.37
22	B	603	CLA	CHC-C1C	3.17	1.43	1.35
30	A	415	DGD	C4E-C5E	3.17	1.59	1.53
22	b	603	CLA	C4D-ND	-3.17	1.33	1.37
34	D	409	LHG	P-O6	3.17	1.72	1.59
22	B	604	CLA	CHC-C1C	3.17	1.43	1.35
22	b	601	CLA	C1D-ND	3.16	1.41	1.37
22	c	514	CLA	MG-NC	3.15	2.13	2.06
22	c	504	CLA	CMD-C2D	-3.15	1.44	1.50
22	C	512	CLA	CHC-C1C	3.15	1.43	1.35
22	C	503	CLA	CHC-C1C	3.14	1.43	1.35
22	B	611	CLA	CMB-C2B	-3.14	1.45	1.51
28	D	410	LMG	C9-C8	3.14	1.60	1.50
22	B	610	CLA	C3B-CAB	-3.14	1.41	1.47
22	a	411	CLA	CMB-C2B	-3.14	1.45	1.51
28	b	623	LMG	C3-C2	3.14	1.60	1.52
22	C	507	CLA	C1D-ND	3.14	1.41	1.37
28	D	410	LMG	C7-C8	3.13	1.58	1.51
22	B	607	CLA	C1D-ND	3.13	1.41	1.37
22	C	505	CLA	C1D-ND	3.13	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	512	CLA	MG-ND	-3.13	1.99	2.05
22	B	614	CLA	CHC-C1C	3.12	1.43	1.35
22	b	614	CLA	C4D-ND	-3.12	1.33	1.37
22	B	603	CLA	MG-NA	3.12	2.13	2.06
22	B	603	CLA	C4D-ND	-3.12	1.33	1.37
28	c	522	LMG	O1-C1	3.12	1.45	1.40
22	b	610	CLA	C1D-ND	3.11	1.41	1.37
22	b	606	CLA	C1D-ND	3.11	1.41	1.37
22	B	602	CLA	MG-NC	3.11	2.13	2.06
29	D	407	SQD	O48-C23	3.11	1.42	1.33
22	B	607	CLA	CHC-C1C	3.10	1.42	1.35
22	C	509	CLA	CHC-C1C	3.10	1.42	1.35
34	d	406	LHG	O7-C5	-3.10	1.38	1.46
22	B	611	CLA	MG-NC	3.10	2.13	2.06
28	B	629	LMG	O8-C9	-3.09	1.38	1.45
22	a	403	CLA	CHC-C1C	3.09	1.42	1.35
22	c	513	CLA	C4D-ND	-3.09	1.33	1.37
22	b	602	CLA	C1D-ND	3.09	1.41	1.37
22	B	617	CLA	CMC-C2C	-3.09	1.44	1.50
24	Y	101	BCR	C1-C6	-3.08	1.49	1.53
30	C	518	DGD	O2G-C2G	-3.08	1.38	1.46
34	e	102	LHG	P-O6	3.07	1.71	1.59
22	B	610	CLA	C1D-ND	3.07	1.41	1.37
22	C	507	CLA	CHC-C1C	3.06	1.42	1.35
30	C	516	DGD	O2E-C2E	-3.06	1.35	1.43
28	c	522	LMG	C1-C2	3.06	1.61	1.52
30	C	516	DGD	C4D-C3D	3.05	1.60	1.52
34	d	407	LHG	C1-C2	-3.05	1.39	1.51
28	c	522	LMG	C3-C2	3.05	1.60	1.52
30	A	415	DGD	C1E-C2E	3.05	1.61	1.52
22	B	615	CLA	CHC-C1C	3.04	1.42	1.35
22	b	612	CLA	MG-NC	-3.04	1.99	2.06
24	K	101	BCR	C30-C25	-3.03	1.49	1.53
22	c	506	CLA	MG-NA	-3.03	1.99	2.06
30	h	102	DGD	C4E-C5E	3.02	1.59	1.53
22	c	508	CLA	CHC-C1C	3.02	1.42	1.35
22	B	611	CLA	CHC-C1C	3.02	1.42	1.35
28	b	621	LMG	C4-C3	3.02	1.60	1.52
24	B	620	BCR	C1-C6	-3.02	1.49	1.53
22	B	604	CLA	C4D-ND	-3.01	1.33	1.37
24	B	620	BCR	C30-C25	-3.01	1.49	1.53
22	b	602	CLA	MG-NC	3.00	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	606	CLA	CHD-C1D	-3.00	1.32	1.38
28	c	525	LMG	O7-C8	-3.00	1.39	1.46
24	B	619	BCR	C30-C25	-3.00	1.49	1.53
22	C	513	CLA	CHC-C1C	2.99	1.42	1.35
22	A	403	CLA	MG-NC	2.99	2.13	2.06
22	b	603	CLA	CHC-C1C	2.99	1.42	1.35
22	d	403	CLA	CMD-C2D	-2.99	1.44	1.50
22	A	403	CLA	C1D-ND	2.98	1.41	1.37
22	c	507	CLA	CMB-C2B	-2.98	1.45	1.51
22	A	403	CLA	CHC-C1C	2.98	1.42	1.35
27	D	405	PL9	C36-C34	-2.98	1.45	1.51
22	b	612	CLA	C4D-ND	-2.98	1.33	1.37
22	B	609	CLA	C1D-ND	2.98	1.41	1.37
22	c	512	CLA	C4D-ND	-2.98	1.33	1.37
22	C	504	CLA	C4D-ND	-2.98	1.33	1.37
22	B	610	CLA	C3B-C2B	-2.97	1.36	1.40
22	C	514	CLA	CHC-C1C	2.97	1.42	1.35
22	b	613	CLA	CMC-C2C	-2.97	1.44	1.50
22	B	602	CLA	C3B-C2B	-2.97	1.36	1.40
24	Z	101	BCR	C1-C6	-2.96	1.49	1.53
30	H	102	DGD	O5D-C1E	2.96	1.45	1.40
22	C	511	CLA	CMC-C2C	-2.96	1.44	1.50
30	c	519	DGD	O3G-C1D	-2.96	1.35	1.40
22	B	613	CLA	C1D-ND	2.96	1.41	1.37
22	C	508	CLA	C1D-ND	2.96	1.41	1.37
22	C	504	CLA	C1D-ND	2.95	1.41	1.37
22	b	607	CLA	C4D-ND	-2.95	1.33	1.37
22	C	510	CLA	CHC-C1C	2.95	1.42	1.35
30	A	415	DGD	C3D-C2D	2.95	1.59	1.52
23	D	401	PHO	CMB-C2B	-2.95	1.44	1.51
22	b	611	CLA	CHC-C1C	2.95	1.42	1.35
22	B	617	CLA	CHC-C1C	2.95	1.42	1.35
22	c	504	CLA	C4D-ND	-2.95	1.33	1.37
22	b	603	CLA	C1D-ND	2.95	1.41	1.37
22	d	402	CLA	CMB-C2B	-2.94	1.45	1.51
29	a	412	SQD	O47-C7	2.94	1.42	1.34
34	E	101	LHG	P-O6	2.94	1.71	1.59
22	c	512	CLA	CHC-C1C	2.94	1.42	1.35
22	b	607	CLA	C3B-C2B	-2.94	1.36	1.40
29	b	619	SQD	O47-C7	2.93	1.42	1.34
30	c	521	DGD	O3D-C3D	-2.93	1.36	1.43
30	A	415	DGD	C4D-C5D	2.93	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	604	CLA	MG-ND	2.93	2.11	2.05
22	C	513	CLA	CMB-C2B	-2.93	1.45	1.51
28	c	525	LMG	C4-C5	2.92	1.59	1.53
22	a	411	CLA	CHC-C1C	2.92	1.42	1.35
22	c	508	CLA	CMD-C2D	-2.92	1.44	1.50
22	a	405	CLA	CMC-C2C	-2.91	1.44	1.50
28	A	412	LMG	C4-C3	2.91	1.59	1.52
22	b	615	CLA	CMB-C2B	-2.91	1.45	1.51
34	d	407	LHG	O8-C6	-2.90	1.38	1.45
24	c	518	BCR	C1-C6	-2.90	1.49	1.53
22	d	403	CLA	CMB-C2B	-2.90	1.45	1.51
22	b	607	CLA	CMB-C2B	-2.89	1.45	1.51
29	A	414	SQD	O47-C45	-2.89	1.42	1.47
29	B	623	SQD	O48-C23	2.89	1.41	1.33
34	E	101	LHG	C24-C23	2.89	1.59	1.50
22	b	614	CLA	CMD-C2D	-2.88	1.44	1.50
22	c	511	CLA	CMB-C2B	-2.88	1.45	1.51
22	B	609	CLA	CMD-C2D	-2.88	1.44	1.50
24	b	618	BCR	C30-C25	-2.87	1.49	1.53
22	B	614	CLA	C1D-ND	2.87	1.41	1.37
28	C	519	LMG	O7-C8	-2.86	1.39	1.46
22	c	507	CLA	C1B-NB	2.86	1.37	1.35
22	B	610	CLA	CMD-C2D	-2.85	1.44	1.50
22	b	604	CLA	C1D-ND	2.85	1.41	1.37
22	c	514	CLA	C4D-ND	-2.85	1.33	1.37
24	b	616	BCR	C30-C25	-2.85	1.49	1.53
22	a	402	CLA	CMB-C2B	-2.85	1.45	1.51
22	B	617	CLA	C3B-CAB	-2.84	1.42	1.47
28	c	524	LMG	C4-C3	2.84	1.59	1.52
34	d	406	LHG	C24-C23	2.84	1.59	1.50
29	f	101	SQD	O48-C23	2.84	1.41	1.33
22	c	512	CLA	CMB-C2B	-2.84	1.45	1.51
22	B	614	CLA	CMD-C2D	-2.83	1.44	1.50
22	C	506	CLA	C1D-ND	2.83	1.41	1.37
22	c	514	CLA	C3B-C2B	-2.83	1.36	1.40
24	c	518	BCR	C30-C25	-2.83	1.49	1.53
22	B	608	CLA	CHC-C1C	2.82	1.42	1.35
22	c	514	CLA	CMB-C2B	-2.82	1.45	1.51
30	c	520	DGD	O2G-C2G	-2.82	1.39	1.46
22	C	502	CLA	C3B-C2B	-2.82	1.36	1.40
30	A	415	DGD	O2G-C1B	2.82	1.42	1.34
22	b	608	CLA	C3B-CAB	-2.82	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	610	CLA	CHC-C1C	2.82	1.42	1.35
22	c	510	CLA	C3B-C2B	-2.82	1.36	1.40
24	C	515	BCR	C30-C25	-2.81	1.49	1.53
22	A	411	CLA	C4D-ND	-2.81	1.33	1.37
22	D	402	CLA	CHC-C1C	2.81	1.42	1.35
22	B	605	CLA	C1B-NB	2.81	1.37	1.35
28	c	522	LMG	C4-C5	2.80	1.58	1.53
34	e	102	LHG	O8-C23	2.80	1.41	1.33
22	B	616	CLA	CMB-C2B	-2.80	1.45	1.51
30	H	102	DGD	O6E-C1E	2.80	1.49	1.41
22	b	604	CLA	CMD-C2D	-2.80	1.44	1.50
22	B	608	CLA	CMB-C2B	-2.79	1.45	1.51
22	c	515	CLA	CMB-C2B	-2.79	1.45	1.51
24	C	515	BCR	C36-C18	-2.79	1.45	1.50
22	c	506	CLA	CAC-C3C	-2.79	1.44	1.51
30	C	516	DGD	C2A-C1A	-2.78	1.42	1.50
22	A	402	CLA	C4D-ND	-2.77	1.33	1.37
22	B	613	CLA	MG-NA	2.77	2.12	2.06
22	c	505	CLA	CHC-C1C	2.77	1.42	1.35
22	B	612	CLA	CMB-C2B	-2.77	1.45	1.51
22	c	507	CLA	MG-NC	2.77	2.12	2.06
22	C	512	CLA	CMB-C2B	-2.76	1.45	1.51
22	B	611	CLA	MG-ND	2.76	2.11	2.05
22	B	615	CLA	C3B-C2B	-2.76	1.36	1.40
22	d	402	CLA	C3B-C2B	-2.75	1.36	1.40
30	H	102	DGD	C3D-C2D	2.74	1.59	1.52
22	B	608	CLA	C3B-CAB	-2.74	1.42	1.47
22	b	602	CLA	CMD-C2D	-2.73	1.45	1.50
22	b	606	CLA	CHC-C1C	2.73	1.42	1.35
22	c	513	CLA	C1D-ND	2.73	1.41	1.37
24	T	101	BCR	C1-C6	-2.72	1.50	1.53
22	b	607	CLA	CMD-C2D	-2.72	1.45	1.50
22	b	603	CLA	CMC-C2C	-2.72	1.45	1.50
34	E	101	LHG	O7-C5	-2.71	1.39	1.46
22	c	511	CLA	MG-ND	2.70	2.11	2.05
22	b	601	CLA	CHC-C1C	2.70	1.41	1.35
22	B	603	CLA	CMB-C2B	-2.70	1.46	1.51
22	b	602	CLA	CHC-C1C	2.70	1.41	1.35
22	C	514	CLA	CMB-C2B	-2.70	1.46	1.51
30	c	521	DGD	C1D-C2D	2.69	1.60	1.52
22	c	509	CLA	C3B-C2B	-2.69	1.36	1.40
22	B	605	CLA	CHC-C1C	2.69	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	614	CLA	C3B-C2B	-2.68	1.36	1.40
30	H	102	DGD	O1G-C1G	-2.68	1.39	1.45
22	B	617	CLA	C3B-C2B	-2.68	1.36	1.40
22	B	602	CLA	CHC-C1C	2.67	1.41	1.35
24	a	406	BCR	C1-C6	-2.67	1.50	1.53
30	h	102	DGD	O2G-C1B	2.67	1.41	1.34
22	D	402	CLA	C4D-ND	-2.66	1.34	1.37
22	b	612	CLA	C1D-ND	2.65	1.41	1.37
22	d	403	CLA	CMC-C2C	-2.65	1.45	1.50
22	b	605	CLA	C4D-ND	-2.65	1.34	1.37
22	B	612	CLA	C3B-C2B	-2.65	1.36	1.40
30	C	518	DGD	O3G-C3G	-2.64	1.38	1.43
23	A	404	PHO	CMC-C2C	-2.64	1.45	1.51
22	B	612	CLA	MG-NC	-2.64	2.00	2.06
22	d	402	CLA	CMD-C2D	-2.63	1.45	1.50
27	a	410	PL9	C30-C29	-2.63	1.43	1.50
34	D	409	LHG	O3-C3	-2.63	1.34	1.44
22	B	610	CLA	MG-NA	2.62	2.12	2.06
22	B	615	CLA	CMB-C2B	-2.62	1.46	1.51
22	C	506	CLA	CMC-C2C	-2.62	1.45	1.50
22	B	606	CLA	C3B-C2B	-2.62	1.36	1.40
22	c	509	CLA	CMB-C2B	-2.62	1.46	1.51
22	B	615	CLA	CMC-C2C	-2.61	1.45	1.50
22	C	505	CLA	CMD-C2D	-2.61	1.45	1.50
24	T	101	BCR	C30-C25	-2.61	1.50	1.53
22	b	605	CLA	MG-ND	-2.61	2.00	2.05
22	b	610	CLA	CMD-C2D	-2.61	1.45	1.50
22	D	403	CLA	CMB-C2B	-2.61	1.46	1.51
22	B	614	CLA	C4D-ND	-2.60	1.34	1.37
22	b	611	CLA	MG-NA	2.60	2.12	2.06
22	c	506	CLA	CHC-C1C	2.59	1.41	1.35
22	C	502	CLA	CMD-C2D	-2.59	1.45	1.50
22	B	610	CLA	C4D-ND	-2.59	1.34	1.37
22	b	605	CLA	MG-NC	2.59	2.12	2.06
22	b	612	CLA	CMD-C2D	-2.58	1.45	1.50
22	C	513	CLA	CAA-C2A	-2.58	1.49	1.54
30	H	102	DGD	C1G-C2G	2.58	1.58	1.50
27	a	410	PL9	C3-C4	-2.57	1.45	1.49
22	C	504	CLA	CMB-C2B	-2.57	1.46	1.51
30	H	102	DGD	C6E-C5E	2.57	1.60	1.51
22	b	604	CLA	C3B-C2B	-2.56	1.36	1.40
22	C	508	CLA	CHC-C1C	2.56	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	403	CLA	CMB-C2B	-2.55	1.46	1.51
24	c	516	BCR	C30-C25	-2.55	1.50	1.53
22	A	405	CLA	CMD-C2D	-2.55	1.45	1.50
30	H	102	DGD	O3E-C3E	-2.55	1.37	1.43
24	b	617	BCR	C38-C26	-2.55	1.46	1.50
27	A	410	PL9	C3-C4	-2.55	1.45	1.49
27	d	405	PL9	C25-C24	-2.55	1.44	1.50
22	C	512	CLA	C3B-C2B	-2.55	1.36	1.40
23	D	401	PHO	C3B-C2B	-2.54	1.36	1.40
22	C	510	CLA	CMD-C2D	-2.54	1.45	1.50
24	c	517	BCR	C30-C25	-2.54	1.50	1.53
22	b	608	CLA	CAC-C3C	-2.54	1.44	1.51
22	B	617	CLA	C1D-ND	2.54	1.40	1.37
22	C	504	CLA	CMD-C2D	-2.54	1.45	1.50
22	C	513	CLA	CMD-C2D	-2.54	1.45	1.50
22	b	613	CLA	C1D-ND	2.53	1.40	1.37
22	A	411	CLA	CMB-C2B	-2.52	1.46	1.51
22	C	509	CLA	C1D-C2D	2.52	1.50	1.45
22	B	607	CLA	C3B-CAB	-2.52	1.42	1.47
22	b	605	CLA	C3B-C2B	-2.52	1.36	1.40
30	C	517	DGD	O3D-C3D	-2.51	1.37	1.43
22	C	509	CLA	CMB-C2B	-2.51	1.46	1.51
22	B	615	CLA	C3B-CAB	-2.51	1.42	1.47
22	C	509	CLA	CMD-C2D	-2.51	1.45	1.50
22	b	601	CLA	CMB-C2B	-2.50	1.46	1.51
24	T	101	BCR	C38-C26	-2.50	1.46	1.50
22	b	615	CLA	C3B-C2B	-2.50	1.36	1.40
22	a	403	CLA	CMB-C2B	-2.50	1.46	1.51
30	H	102	DGD	C4D-C5D	2.49	1.58	1.53
22	b	608	CLA	C3B-C2B	-2.49	1.36	1.40
22	D	403	CLA	C4B-CHC	-2.49	1.34	1.41
22	b	606	CLA	MG-ND	-2.49	2.00	2.05
22	c	511	CLA	CHC-C1C	2.48	1.41	1.35
28	d	409	LMG	O1-C7	-2.48	1.39	1.43
34	B	622	LHG	O8-C6	-2.48	1.39	1.45
22	b	605	CLA	CHC-C1C	2.48	1.41	1.35
22	c	503	CLA	CAC-C3C	-2.48	1.44	1.51
22	b	605	CLA	CMD-C2D	-2.47	1.45	1.50
22	A	402	CLA	MG-ND	-2.47	2.00	2.05
22	c	508	CLA	C4D-ND	-2.47	1.34	1.37
23	a	404	PHO	C3B-C2B	-2.47	1.36	1.40
22	b	612	CLA	CMB-C2B	-2.47	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	508	CLA	CAC-C3C	-2.47	1.44	1.51
23	A	404	PHO	C3B-CAB	-2.47	1.42	1.47
22	b	609	CLA	CMB-C2B	-2.46	1.46	1.51
28	C	519	LMG	C4-C3	2.45	1.58	1.52
22	c	510	CLA	CMB-C2B	-2.45	1.46	1.51
22	B	612	CLA	CHC-C1C	2.45	1.41	1.35
22	b	611	CLA	CMC-C2C	-2.45	1.45	1.50
30	c	519	DGD	C3E-C2E	2.44	1.58	1.52
22	D	403	CLA	CMC-C2C	-2.44	1.45	1.50
22	D	403	CLA	C3B-C2B	-2.44	1.37	1.40
28	D	410	LMG	O8-C28	2.44	1.40	1.33
22	h	101	CLA	C4D-ND	-2.43	1.34	1.37
30	h	102	DGD	O1G-C1G	-2.43	1.39	1.45
22	d	402	CLA	CMC-C2C	-2.43	1.45	1.50
35	e	101	HEC	C4B-C3B	2.43	1.47	1.43
22	C	510	CLA	CMC-C2C	-2.43	1.45	1.50
22	b	615	CLA	CMC-C2C	-2.43	1.45	1.50
22	a	405	CLA	C1B-NB	2.42	1.37	1.35
22	b	608	CLA	CHC-C1C	2.42	1.41	1.35
22	C	507	CLA	C3B-C2B	-2.42	1.37	1.40
22	C	513	CLA	C3B-C2B	-2.41	1.37	1.40
22	b	606	CLA	C4D-ND	-2.41	1.34	1.37
22	A	411	CLA	CAC-C3C	-2.41	1.44	1.51
22	b	605	CLA	C4B-CHC	-2.41	1.34	1.41
22	c	503	CLA	CHC-C1C	2.41	1.41	1.35
22	b	601	CLA	CAC-C3C	-2.41	1.44	1.51
22	c	508	CLA	C1D-ND	2.41	1.40	1.37
22	B	613	CLA	CHC-C1C	2.41	1.41	1.35
28	D	406	LMG	C6-C5	2.41	1.59	1.51
22	C	503	CLA	C3B-C2B	-2.41	1.37	1.40
29	A	413	SQD	O48-C23	2.41	1.40	1.33
28	b	621	LMG	O6-C1	2.40	1.48	1.41
22	B	605	CLA	O2D-CGD	2.40	1.39	1.33
22	a	405	CLA	C3B-CAB	-2.40	1.43	1.47
22	D	403	CLA	CMD-C2D	-2.40	1.45	1.50
28	M	101	LMG	C9-C8	2.40	1.58	1.50
22	B	616	CLA	MG-NA	2.40	2.12	2.06
29	f	101	SQD	O3-C3	-2.40	1.37	1.43
22	b	611	CLA	CMD-C2D	-2.40	1.45	1.50
22	b	607	CLA	C3B-CAB	-2.40	1.43	1.47
24	D	404	BCR	C1-C6	-2.40	1.50	1.53
22	A	402	CLA	C1D-C2D	2.39	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D	406	LMG	C4-C3	2.39	1.58	1.52
22	B	602	CLA	CMB-C2B	-2.39	1.46	1.51
34	D	412	LHG	C24-C23	2.39	1.57	1.50
22	C	507	CLA	CMA-C3A	-2.39	1.48	1.53
22	c	504	CLA	C1B-NB	2.39	1.37	1.35
22	b	611	CLA	CMB-C2B	-2.39	1.46	1.51
22	c	503	CLA	C1D-ND	2.38	1.40	1.37
29	A	413	SQD	O2-C2	-2.38	1.37	1.43
22	B	608	CLA	CMC-C2C	-2.38	1.45	1.50
34	D	408	LHG	C4-C5	2.38	1.58	1.50
30	A	415	DGD	C3E-C2E	2.38	1.58	1.52
22	A	403	CLA	C4B-CHC	-2.38	1.34	1.41
22	B	608	CLA	MG-NA	2.38	2.11	2.06
28	C	519	LMG	O8-C9	-2.38	1.39	1.45
22	d	403	CLA	MG-NC	2.38	2.11	2.06
22	A	411	CLA	C3B-C2B	-2.38	1.37	1.40
23	a	404	PHO	O2D-CGD	2.37	1.39	1.33
22	B	616	CLA	C3B-CAB	-2.37	1.43	1.47
30	h	102	DGD	C4D-C3D	2.36	1.58	1.52
22	b	609	CLA	C3B-CAB	-2.36	1.43	1.47
22	B	616	CLA	C4B-CHC	-2.36	1.34	1.41
24	T	101	BCR	C27-C26	-2.36	1.46	1.51
30	H	102	DGD	C1E-C2E	2.35	1.59	1.52
30	C	517	DGD	C1E-C2E	2.35	1.59	1.52
22	C	507	CLA	CAC-C3C	-2.34	1.45	1.51
22	a	403	CLA	C3B-CAB	-2.34	1.43	1.47
30	C	516	DGD	O6E-C1E	2.34	1.47	1.41
22	b	602	CLA	C4D-ND	-2.34	1.34	1.37
30	C	516	DGD	C3D-C2D	2.34	1.58	1.52
28	c	522	LMG	O2-C2	-2.34	1.37	1.43
29	A	413	SQD	O47-C7	2.33	1.40	1.34
28	c	525	LMG	C1-C2	2.33	1.59	1.52
22	A	402	CLA	CHC-C1C	2.33	1.40	1.35
27	D	405	PL9	C46-C44	-2.33	1.46	1.51
24	b	616	BCR	C4-C5	-2.32	1.46	1.51
30	A	415	DGD	O1G-C1G	-2.32	1.39	1.45
22	C	505	CLA	CMB-C2B	-2.32	1.46	1.51
22	c	505	CLA	CMB-C2B	-2.31	1.46	1.51
35	F	101	HEC	CAD-C3D	2.31	1.55	1.52
28	B	629	LMG	O8-C28	2.31	1.40	1.33
22	b	601	CLA	C4B-CHC	-2.31	1.34	1.41
22	c	514	CLA	C3D-C4D	2.31	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	607	CLA	CMD-C2D	-2.30	1.45	1.50
30	h	102	DGD	O2D-C2D	-2.30	1.37	1.43
22	b	607	CLA	C1D-ND	2.30	1.40	1.37
22	c	504	CLA	CMC-C2C	-2.30	1.45	1.50
22	A	405	CLA	CMB-C2B	-2.30	1.46	1.51
22	C	509	CLA	C1B-NB	2.29	1.37	1.35
22	c	505	CLA	CMC-C2C	-2.29	1.45	1.50
22	B	617	CLA	CMB-C2B	-2.29	1.46	1.51
22	A	411	CLA	CHC-C1C	2.29	1.40	1.35
22	b	614	CLA	MG-ND	-2.29	2.01	2.05
22	h	101	CLA	CMC-C2C	-2.29	1.46	1.50
27	A	410	PL9	C7-C8	-2.29	1.47	1.50
22	B	616	CLA	C3D-C4D	2.28	1.49	1.44
22	D	402	CLA	CAA-C2A	-2.28	1.49	1.54
22	B	606	CLA	CMD-C2D	-2.28	1.46	1.50
30	c	519	DGD	C1D-C2D	2.28	1.59	1.52
22	C	511	CLA	CMD-C2D	-2.28	1.46	1.50
27	d	405	PL9	C16-C14	-2.28	1.46	1.51
22	a	405	CLA	CMB-C2B	-2.27	1.46	1.51
22	C	513	CLA	CMC-C2C	-2.27	1.46	1.50
22	B	604	CLA	CMD-C2D	-2.27	1.46	1.50
22	h	101	CLA	O2A-CGA	2.27	1.40	1.33
22	b	612	CLA	MG-ND	-2.27	2.01	2.05
22	C	509	CLA	MG-ND	2.27	2.10	2.05
22	c	503	CLA	CMB-C2B	-2.27	1.46	1.51
22	A	405	CLA	CHC-C1C	2.27	1.40	1.35
28	c	524	LMG	C1-C2	2.26	1.59	1.52
22	C	503	CLA	CMB-C2B	-2.26	1.46	1.51
22	B	607	CLA	C1B-NB	2.26	1.37	1.35
22	d	403	CLA	C4B-CHC	-2.26	1.34	1.41
27	D	405	PL9	C3-C4	-2.26	1.45	1.49
22	A	402	CLA	C3B-C2B	-2.25	1.37	1.40
22	a	405	CLA	C4B-CHC	-2.25	1.34	1.41
22	C	512	CLA	CMC-C2C	-2.25	1.46	1.50
29	f	101	SQD	O2-C2	-2.25	1.37	1.43
22	B	609	CLA	CMB-C2B	-2.25	1.47	1.51
22	C	502	CLA	CMC-C2C	-2.25	1.46	1.50
22	C	508	CLA	C3B-CAB	-2.24	1.43	1.47
22	c	515	CLA	MG-NA	-2.24	2.00	2.06
22	C	511	CLA	CMB-C2B	-2.24	1.47	1.51
22	C	509	CLA	C4D-ND	-2.24	1.34	1.37
22	b	612	CLA	C3C-C2C	2.24	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	614	CLA	CMB-C2B	-2.24	1.47	1.51
22	b	607	CLA	C1B-NB	2.24	1.37	1.35
28	B	629	LMG	O7-C10	2.23	1.40	1.34
22	A	402	CLA	CMB-C2B	-2.23	1.47	1.51
22	C	506	CLA	C3B-CAB	-2.22	1.43	1.47
27	D	405	PL9	C26-C24	-2.22	1.46	1.51
22	c	509	CLA	CHC-C1C	2.22	1.40	1.35
23	a	404	PHO	CBD-CGD	-2.22	1.49	1.52
22	b	614	CLA	C3B-C2B	-2.22	1.37	1.40
34	d	408	LHG	P-O6	2.22	1.68	1.59
22	A	402	CLA	O2D-CED	-2.22	1.40	1.45
22	B	602	CLA	CMC-C2C	-2.22	1.46	1.50
29	f	101	SQD	O4-C4	-2.22	1.37	1.43
23	A	404	PHO	CAC-C3C	-2.21	1.48	1.52
22	B	609	CLA	CHC-C1C	2.21	1.40	1.35
24	B	620	BCR	C38-C26	-2.21	1.47	1.50
30	C	518	DGD	O1G-C1G	-2.21	1.40	1.45
28	d	409	LMG	O7-C8	-2.21	1.41	1.46
22	B	610	CLA	CMB-C2B	-2.21	1.47	1.51
30	C	517	DGD	O5D-C6D	-2.20	1.39	1.43
29	a	412	SQD	O3-C3	-2.20	1.37	1.43
22	B	614	CLA	CMB-C2B	-2.20	1.47	1.51
22	c	506	CLA	CMD-C2D	-2.20	1.46	1.50
34	D	408	LHG	C3-C2	2.20	1.59	1.51
24	a	406	BCR	C38-C26	-2.20	1.47	1.50
22	D	403	CLA	C4D-ND	-2.20	1.34	1.37
22	c	503	CLA	CMD-C2D	-2.20	1.46	1.50
22	a	411	CLA	C4D-ND	-2.20	1.34	1.37
22	b	613	CLA	C3B-C2B	-2.20	1.37	1.40
35	e	101	HEC	C4D-CHA	-2.19	1.34	1.41
24	K	101	BCR	C1-C6	-2.19	1.50	1.53
22	b	610	CLA	MG-NA	2.19	2.11	2.06
22	B	607	CLA	C4B-CHC	-2.19	1.34	1.41
22	c	504	CLA	C3B-CAB	-2.19	1.43	1.47
30	c	519	DGD	C3G-C2G	2.19	1.57	1.50
22	b	602	CLA	CMB-C2B	-2.19	1.47	1.51
22	B	610	CLA	CHC-C1C	2.19	1.40	1.35
30	h	102	DGD	C1E-C2E	2.18	1.58	1.52
28	c	522	LMG	C7-C8	2.18	1.57	1.50
24	b	616	BCR	C33-C5	-2.18	1.47	1.50
30	C	517	DGD	O2G-C2G	-2.18	1.41	1.46
22	b	606	CLA	CMC-C2C	-2.18	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	507	CLA	CMB-C2B	-2.18	1.47	1.51
24	x	101	BCR	C33-C5	-2.18	1.47	1.50
27	d	405	PL9	C51-C49	-2.17	1.44	1.50
22	B	612	CLA	CMD-C2D	-2.17	1.46	1.50
22	b	615	CLA	C3D-C4D	2.17	1.49	1.44
22	D	403	CLA	C3D-C4D	2.17	1.49	1.44
28	B	629	LMG	C7-C8	2.17	1.57	1.50
22	b	609	CLA	CHC-C1C	2.17	1.40	1.35
28	M	101	LMG	O6-C1	2.17	1.47	1.41
22	c	505	CLA	C3B-C2B	-2.16	1.37	1.40
22	a	405	CLA	CAC-C3C	-2.16	1.45	1.51
22	B	609	CLA	C1D-C2D	2.16	1.49	1.45
30	c	520	DGD	C4D-C5D	2.16	1.57	1.53
24	x	101	BCR	C36-C18	-2.16	1.46	1.50
22	B	607	CLA	MG-NC	-2.16	2.01	2.06
34	l	101	LHG	P-O6	2.15	1.68	1.59
22	c	513	CLA	CMB-C2B	-2.15	1.47	1.51
27	a	410	PL9	C25-C24	-2.15	1.45	1.50
22	B	602	CLA	MG-ND	-2.15	2.01	2.05
22	c	503	CLA	C4B-CHC	-2.15	1.35	1.41
29	a	412	SQD	O4-C4	-2.15	1.37	1.43
22	b	612	CLA	C4B-CHC	-2.14	1.35	1.41
22	B	607	CLA	CMB-C2B	-2.14	1.47	1.51
22	B	616	CLA	C3B-C2B	-2.14	1.37	1.40
30	C	518	DGD	C6E-C5E	2.14	1.59	1.51
22	d	403	CLA	C4D-ND	-2.14	1.34	1.37
22	b	615	CLA	C4B-CHC	-2.14	1.35	1.41
22	b	614	CLA	CMC-C2C	-2.14	1.46	1.50
22	B	611	CLA	C4D-ND	-2.14	1.34	1.37
30	h	102	DGD	C4E-C3E	2.14	1.57	1.52
22	B	606	CLA	CMC-C2C	-2.13	1.46	1.50
22	b	615	CLA	CHC-C1C	2.13	1.40	1.35
24	C	515	BCR	C27-C26	-2.13	1.46	1.51
22	C	502	CLA	MG-NC	2.13	2.11	2.06
22	b	601	CLA	CMD-C2D	-2.13	1.46	1.50
22	c	515	CLA	CMC-C2C	-2.13	1.46	1.50
22	b	605	CLA	CAC-C3C	-2.13	1.45	1.51
28	D	411	LMG	O8-C28	2.13	1.37	1.30
22	C	511	CLA	MG-NC	2.13	2.11	2.06
27	D	405	PL9	C31-C29	-2.13	1.46	1.51
22	B	610	CLA	MG-ND	2.13	2.10	2.05
22	d	403	CLA	O1D-CGD	2.13	1.26	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	t	101	BCR	C30-C25	-2.13	1.50	1.53
22	c	505	CLA	C3D-C4D	2.13	1.49	1.44
22	c	507	CLA	C3B-C2B	-2.13	1.37	1.40
24	b	616	BCR	C38-C26	-2.13	1.47	1.50
29	B	623	SQD	O2-C2	-2.12	1.38	1.43
22	b	602	CLA	C1A-CHA	-2.12	1.34	1.43
22	B	605	CLA	MG-NC	2.12	2.11	2.06
28	c	525	LMG	O1-C7	-2.11	1.39	1.43
22	B	603	CLA	C3C-C2C	2.11	1.41	1.36
28	D	406	LMG	O2-C2	-2.11	1.38	1.43
22	A	411	CLA	CMD-C2D	-2.11	1.46	1.50
30	H	102	DGD	C6D-C5D	2.11	1.58	1.51
22	B	604	CLA	C3B-C2B	-2.11	1.37	1.40
22	b	613	CLA	C3B-CAB	-2.11	1.43	1.47
22	D	403	CLA	C3B-CAB	-2.11	1.43	1.47
22	C	504	CLA	CMC-C2C	-2.11	1.46	1.50
24	x	101	BCR	C1-C6	-2.11	1.50	1.53
30	C	516	DGD	C4D-C5D	2.11	1.57	1.53
27	A	410	PL9	C37-C38	2.10	1.57	1.50
22	b	612	CLA	CMC-C2C	-2.10	1.46	1.50
22	B	605	CLA	MG-ND	-2.10	2.01	2.05
22	c	513	CLA	C1D-C2D	2.10	1.49	1.45
28	d	409	LMG	C4-C5	2.10	1.57	1.53
22	b	610	CLA	C4D-ND	-2.09	1.34	1.37
22	C	510	CLA	O2D-CGD	2.09	1.38	1.33
27	a	410	PL9	C10-C9	-2.09	1.45	1.50
30	C	518	DGD	C4D-C3D	2.09	1.57	1.52
34	D	408	LHG	O7-C5	-2.09	1.41	1.46
34	d	406	LHG	C4-C5	2.09	1.57	1.50
30	c	520	DGD	O2E-C2E	-2.09	1.38	1.43
22	h	101	CLA	CMB-C2B	-2.08	1.47	1.51
22	b	609	CLA	C4B-CHC	-2.08	1.35	1.41
22	c	510	CLA	CMC-C2C	-2.08	1.46	1.50
24	A	406	BCR	C33-C5	-2.08	1.47	1.50
22	c	514	CLA	C3B-CAB	-2.07	1.43	1.47
22	b	613	CLA	CMB-C2B	-2.07	1.47	1.51
34	E	101	LHG	O8-C23	2.07	1.39	1.33
22	B	603	CLA	C1D-C2D	2.07	1.49	1.45
22	B	608	CLA	C1B-NB	2.07	1.37	1.35
22	B	611	CLA	C1B-NB	2.07	1.37	1.35
34	e	102	LHG	C4-C5	2.07	1.57	1.50
22	B	609	CLA	MG-NC	-2.07	2.01	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	612	CLA	CHC-C1C	2.06	1.40	1.35
22	C	514	CLA	C3B-CAB	-2.06	1.43	1.47
22	a	405	CLA	CHC-C1C	2.06	1.40	1.35
22	b	601	CLA	C3B-C2B	-2.06	1.37	1.40
23	d	401	PHO	CMD-C2D	-2.05	1.46	1.51
30	c	521	DGD	C6D-C5D	2.05	1.58	1.51
28	b	621	LMG	C6-C5	2.05	1.58	1.51
29	A	413	SQD	O3-C3	-2.05	1.38	1.43
22	B	613	CLA	C3D-C4D	2.05	1.48	1.44
22	C	502	CLA	CAA-C2A	2.05	1.57	1.54
22	a	411	CLA	C1B-NB	2.04	1.37	1.35
22	A	402	CLA	C3C-C2C	2.04	1.41	1.36
22	b	603	CLA	CAC-C3C	-2.04	1.45	1.51
30	c	519	DGD	O1A-C1A	2.04	1.28	1.22
22	b	603	CLA	MG-ND	-2.04	2.01	2.05
22	c	507	CLA	CMC-C2C	-2.04	1.46	1.50
22	c	509	CLA	C3D-C4D	2.04	1.48	1.44
22	b	614	CLA	C3B-CAB	-2.04	1.43	1.47
28	M	101	LMG	O4-C4	-2.04	1.38	1.43
23	D	401	PHO	C3B-CAB	-2.03	1.43	1.47
22	b	615	CLA	CMD-C2D	-2.03	1.46	1.50
23	A	404	PHO	C3B-C2B	-2.03	1.37	1.40
30	c	519	DGD	O1G-C1A	2.03	1.39	1.33
22	b	611	CLA	C1D-ND	2.03	1.40	1.37
22	b	601	CLA	CMC-C2C	-2.03	1.46	1.50
22	C	513	CLA	C1A-CHA	-2.03	1.34	1.43
27	A	410	PL9	C25-C24	-2.02	1.45	1.50
22	A	403	CLA	MG-NA	-2.02	2.01	2.06
22	C	511	CLA	CAA-C2A	-2.02	1.50	1.54
24	b	617	BCR	C36-C18	-2.02	1.46	1.50
30	c	521	DGD	O4E-C4E	-2.02	1.38	1.43
22	C	510	CLA	O2A-CGA	2.02	1.39	1.33
22	B	610	CLA	O2D-CGD	2.02	1.38	1.33
22	c	514	CLA	CMC-C2C	-2.02	1.46	1.50
22	B	609	CLA	CMC-C2C	-2.02	1.46	1.50
22	C	512	CLA	CMD-C2D	-2.01	1.46	1.50
24	B	619	BCR	C1-C6	-2.01	1.51	1.53
22	B	610	CLA	CMC-C2C	-2.01	1.46	1.50
22	C	510	CLA	CMB-C2B	-2.01	1.47	1.51
34	e	102	LHG	O7-C5	-2.01	1.41	1.46
22	C	507	CLA	C3D-C4D	2.01	1.48	1.44
34	B	622	LHG	C4-C5	2.01	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	512	CLA	C3B-C2B	-2.01	1.37	1.40
22	b	602	CLA	CMC-C2C	-2.01	1.46	1.50
22	b	609	CLA	C1B-NB	2.01	1.37	1.35
28	c	525	LMG	O6-C5	-2.01	1.39	1.44
22	c	508	CLA	MG-NC	2.01	2.11	2.06
22	C	509	CLA	C1D-ND	2.00	1.40	1.37
22	h	101	CLA	C1D-C2D	2.00	1.49	1.45

All (1378) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	602	CLA	C4A-NA-C1A	11.54	111.89	106.71
22	B	605	CLA	C4A-NA-C1A	10.81	111.56	106.71
22	b	605	CLA	C4A-NA-C1A	9.82	111.12	106.71
22	h	101	CLA	C4A-NA-C1A	9.80	111.11	106.71
22	C	504	CLA	C4A-NA-C1A	9.67	111.05	106.71
29	D	407	SQD	O6-C1-C2	9.00	122.35	108.30
29	b	619	SQD	O6-C1-C2	8.94	122.27	108.30
22	C	508	CLA	C4A-NA-C1A	8.77	110.65	106.71
22	C	509	CLA	C4A-NA-C1A	8.55	110.55	106.71
22	b	606	CLA	C4A-NA-C1A	8.20	110.39	106.71
29	a	412	SQD	O6-C1-C2	8.07	120.90	108.30
29	A	413	SQD	O6-C1-C2	7.83	120.53	108.30
22	B	617	CLA	C4A-NA-C1A	7.79	110.21	106.71
22	C	503	CLA	C4A-NA-C1A	7.55	110.10	106.71
22	b	601	CLA	C4A-NA-C1A	7.50	110.08	106.71
22	b	603	CLA	C4A-NA-C1A	7.44	110.05	106.71
35	e	101	HEC	CBD-CAD-C3D	-7.43	99.94	112.62
22	c	513	CLA	C4A-NA-C1A	7.32	110.00	106.71
22	c	505	CLA	C4A-NA-C1A	7.30	109.99	106.71
29	B	623	SQD	O6-C1-C2	7.30	119.70	108.30
22	a	405	CLA	C4A-NA-C1A	7.29	109.98	106.71
29	f	101	SQD	O7-S-C6	7.24	115.54	106.94
22	C	512	CLA	C4A-NA-C1A	7.16	109.92	106.71
22	c	511	CLA	C4A-NA-C1A	7.14	109.91	106.71
22	C	510	CLA	C4A-NA-C1A	6.91	109.81	106.71
22	B	608	CLA	C4A-NA-C1A	6.83	109.78	106.71
22	c	504	CLA	C4A-NA-C1A	6.68	109.71	106.71
22	C	511	CLA	C4A-NA-C1A	6.53	109.64	106.71
22	c	514	CLA	C4A-NA-C1A	6.39	109.58	106.71
22	b	614	CLA	C4A-NA-C1A	6.38	109.57	106.71
22	B	611	CLA	C4A-NA-C1A	6.30	109.54	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	610	CLA	C4A-NA-C1A	6.25	109.52	106.71
22	B	611	CLA	O2D-CGD-O1D	-6.23	111.67	123.84
22	C	502	CLA	C4A-NA-C1A	6.15	109.47	106.71
35	F	101	HEC	CBA-CAA-C2A	-6.14	102.26	112.60
29	D	407	SQD	O9-S-C6	6.07	114.16	106.94
22	b	615	CLA	C4A-NA-C1A	6.07	109.43	106.71
22	B	613	CLA	C4A-NA-C1A	6.04	109.42	106.71
22	a	411	CLA	C4A-NA-C1A	6.01	109.41	106.71
27	D	405	PL9	C7-C3-C4	6.00	121.76	116.88
22	c	510	CLA	C4A-NA-C1A	5.89	109.35	106.71
22	c	503	CLA	O2D-CGD-O1D	-5.85	112.40	123.84
35	v	201	HEC	CBD-CAD-C3D	-5.80	102.72	112.62
22	b	609	CLA	C4A-NA-C1A	5.79	109.31	106.71
27	A	410	PL9	C7-C3-C4	5.76	121.56	116.88
22	B	603	CLA	O2D-CGD-CBD	5.73	121.45	111.27
22	A	411	CLA	C4A-NA-C1A	5.67	109.25	106.71
22	D	402	CLA	C4A-NA-C1A	5.66	109.25	106.71
22	B	607	CLA	C4A-NA-C1A	5.65	109.25	106.71
35	e	101	HEC	CBA-CAA-C2A	-5.63	103.12	112.60
35	F	101	HEC	CBD-CAD-C3D	-5.62	103.03	112.62
27	a	410	PL9	C7-C3-C4	5.60	121.43	116.88
22	c	509	CLA	C4A-NA-C1A	5.54	109.20	106.71
22	c	503	CLA	C4A-NA-C1A	5.54	109.20	106.71
22	B	612	CLA	C4A-NA-C1A	5.49	109.18	106.71
22	a	402	CLA	CMB-C2B-C1B	-5.46	120.07	128.46
22	B	608	CLA	CMB-C2B-C1B	-5.33	120.27	128.46
22	b	615	CLA	O2D-CGD-O1D	-5.33	113.42	123.84
22	d	403	CLA	CMB-C2B-C1B	-5.33	120.28	128.46
22	B	603	CLA	O2D-CGD-O1D	-5.24	113.60	123.84
29	b	619	SQD	O7-S-C6	5.17	113.08	106.94
35	V	201	HEC	CBD-CAD-C3D	-5.15	103.82	112.62
22	B	615	CLA	C4A-NA-C1A	5.15	109.02	106.71
22	C	505	CLA	C4A-NA-C1A	5.15	109.02	106.71
22	b	604	CLA	C4A-NA-C1A	5.13	109.01	106.71
28	b	623	LMG	C1-O6-C5	-5.12	103.64	113.69
22	b	612	CLA	C1-C2-C3	-5.09	117.25	126.04
22	C	514	CLA	C4A-NA-C1A	5.06	108.98	106.71
29	f	101	SQD	O6-C1-C2	5.03	116.16	108.30
29	B	623	SQD	O7-S-C6	4.96	112.83	106.94
35	V	201	HEC	CMC-C2C-C1C	-4.93	120.88	128.46
22	b	602	CLA	CMB-C2B-C1B	-4.93	120.89	128.46
22	b	614	CLA	CMB-C2B-C1B	-4.90	120.93	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	d	405	PL9	C7-C3-C4	4.90	120.86	116.88
22	C	505	CLA	CMB-C2B-C1B	-4.90	120.94	128.46
29	a	412	SQD	O7-S-C6	4.88	112.74	106.94
22	A	403	CLA	CMB-C2B-C1B	-4.84	121.02	128.46
29	A	414	SQD	C45-O47-C7	4.78	124.03	117.88
22	C	507	CLA	C4A-NA-C1A	4.78	108.86	106.71
22	a	402	CLA	C4A-NA-C1A	4.77	108.85	106.71
22	c	512	CLA	C4A-NA-C1A	4.77	108.85	106.71
22	C	502	CLA	O2D-CGD-O1D	-4.76	114.54	123.84
22	c	503	CLA	O2D-CGD-CBD	4.70	119.63	111.27
22	b	602	CLA	O2D-CGD-O1D	-4.70	114.65	123.84
22	b	613	CLA	CHD-C1D-ND	-4.70	120.14	124.45
29	a	413	SQD	O48-C23-O10	-4.69	111.75	123.59
34	D	409	LHG	O4-P-O5	4.68	135.35	112.24
22	d	403	CLA	CMB-C2B-C3B	4.66	133.39	124.68
22	b	610	CLA	O2D-CGD-CBD	4.64	119.52	111.27
29	a	412	SQD	O9-S-C6	4.60	112.41	106.94
22	C	503	CLA	CHD-C1D-ND	-4.60	120.23	124.45
22	B	609	CLA	CMB-C2B-C1B	-4.60	121.40	128.46
22	b	610	CLA	O2D-CGD-O1D	-4.58	114.88	123.84
29	A	413	SQD	C1-C2-C3	-4.58	100.45	110.00
22	b	608	CLA	CMB-C2B-C1B	-4.57	121.44	128.46
24	A	406	BCR	C35-C13-C14	-4.56	116.53	122.92
22	D	403	CLA	C4A-NA-C1A	4.56	108.75	106.71
22	C	509	CLA	CMB-C2B-C1B	-4.55	121.48	128.46
22	B	609	CLA	CHD-C1D-ND	-4.54	120.28	124.45
22	c	506	CLA	CMB-C2B-C1B	-4.52	121.51	128.46
22	B	608	CLA	CMB-C2B-C3B	4.50	133.09	124.68
22	h	101	CLA	O2D-CGD-O1D	-4.47	115.10	123.84
29	A	413	SQD	O47-C7-C8	4.46	121.11	111.50
29	D	407	SQD	O8-S-C6	4.44	112.81	105.74
23	A	404	PHO	CMB-C2B-C3B	4.43	132.96	124.68
22	B	605	CLA	CMB-C2B-C1B	-4.42	121.68	128.46
35	V	201	HEC	C1D-C2D-C3D	-4.40	103.93	107.00
22	b	602	CLA	CMB-C2B-C3B	4.39	132.90	124.68
30	c	521	DGD	O3G-C3G-C2G	-4.38	100.32	110.90
22	c	507	CLA	CMB-C2B-C1B	-4.37	121.74	128.46
30	C	517	DGD	O3G-C3G-C2G	-4.37	100.35	110.90
22	C	513	CLA	CMB-C2B-C1B	-4.36	121.76	128.46
30	C	518	DGD	O3G-C3G-C2G	-4.34	100.44	110.90
26	A	409	BCT	O2-C-O1	4.32	130.76	119.55
22	B	616	CLA	C4A-NA-C1A	4.32	108.65	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	402	CLA	CMB-C2B-C3B	4.31	132.75	124.68
22	A	403	CLA	CMB-C2B-C3B	4.30	132.72	124.68
22	B	606	CLA	CHD-C1D-ND	-4.30	120.50	124.45
22	a	403	CLA	CMB-C2B-C1B	-4.29	121.87	128.46
29	A	413	SQD	O7-S-C6	4.27	112.01	106.94
22	C	509	CLA	O2D-CGD-O1D	-4.26	115.51	123.84
22	c	515	CLA	CMB-C2B-C1B	-4.25	121.93	128.46
22	B	603	CLA	CMB-C2B-C1B	-4.25	121.93	128.46
28	B	629	LMG	C1-C2-C3	-4.24	101.16	110.00
30	H	102	DGD	O3G-C3G-C2G	-4.24	100.67	110.90
35	F	101	HEC	CMC-C2C-C1C	-4.24	121.95	128.46
28	B	629	LMG	C1-O6-C5	-4.24	105.38	113.69
22	A	405	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
29	a	413	SQD	O47-C7-C8	4.22	120.59	111.50
22	b	609	CLA	O2D-CGD-O1D	-4.20	115.62	123.84
29	f	101	SQD	O9-S-O7	-4.19	99.44	113.95
29	B	623	SQD	O47-C7-C8	4.19	120.53	111.50
22	b	610	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
22	A	402	CLA	CHD-C1D-ND	-4.19	120.61	124.45
29	A	413	SQD	C1-O5-C5	-4.16	105.51	113.69
29	b	619	SQD	C1-C2-C3	-4.14	101.38	110.00
22	b	603	CLA	CMB-C2B-C1B	-4.14	122.11	128.46
24	H	101	BCR	C16-C15-C14	-4.13	115.01	123.47
34	E	101	LHG	O4-P-O5	4.12	132.62	112.24
22	B	609	CLA	O2D-CGD-O1D	-4.12	115.78	123.84
22	A	402	CLA	C4A-NA-C1A	4.09	108.55	106.71
22	b	601	CLA	O2D-CGD-CBD	4.07	118.51	111.27
22	b	602	CLA	C4A-NA-C1A	4.07	108.54	106.71
22	B	612	CLA	O2D-CGD-O1D	-4.07	115.89	123.84
34	e	102	LHG	O4-P-O5	4.06	132.32	112.24
22	b	601	CLA	O2D-CGD-O1D	-4.05	115.92	123.84
22	C	504	CLA	C7-C6-C5	-4.05	102.37	113.36
34	D	412	LHG	O4-P-O5	4.04	132.24	112.24
22	C	510	CLA	CHB-C4A-NA	4.04	130.10	124.51
22	D	403	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
22	b	612	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
22	b	614	CLA	CMB-C2B-C3B	4.01	132.19	124.68
22	b	615	CLA	CHB-C4A-NA	4.01	130.06	124.51
28	d	409	LMG	O1-C1-C2	-4.01	102.05	108.30
34	l	101	LHG	O4-P-O5	4.00	131.99	112.24
35	v	201	HEC	C1D-C2D-C3D	-3.99	104.22	107.00
22	B	604	CLA	CMB-C2B-C3B	3.98	132.13	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	511	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
27	A	410	PL9	C7-C3-C2	-3.97	118.08	123.30
22	a	411	CLA	CMB-C2B-C1B	-3.97	122.37	128.46
22	B	611	CLA	C1B-CHB-C4A	-3.97	122.26	130.12
34	D	412	LHG	O8-C23-C24	3.96	124.35	111.91
34	B	622	LHG	O4-P-O5	3.96	131.81	112.24
23	a	404	PHO	OBD-CAD-CBD	-3.95	120.02	125.82
22	B	602	CLA	CAA-CBA-CGA	-3.92	101.81	113.25
22	b	608	CLA	CHD-C1D-ND	-3.91	120.86	124.45
22	b	613	CLA	C4A-NA-C1A	3.91	108.47	106.71
22	b	615	CLA	CMB-C2B-C3B	3.91	131.99	124.68
29	A	413	SQD	O9-S-O7	-3.89	100.47	113.95
34	d	406	LHG	O8-C23-C24	3.88	124.09	111.91
22	c	514	CLA	C1-C2-C3	-3.88	119.33	126.04
22	D	402	CLA	CED-O2D-CGD	3.87	124.70	115.94
22	B	615	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
22	b	604	CLA	O2D-CGD-O1D	-3.86	116.28	123.84
22	c	511	CLA	O2A-CGA-O1A	-3.84	113.89	123.59
22	B	613	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
22	b	605	CLA	C2D-C1D-ND	-3.84	107.28	110.10
35	v	201	HEC	CMB-C2B-C1B	-3.83	122.57	128.46
22	b	601	CLA	CMB-C2B-C1B	-3.82	122.60	128.46
24	t	101	BCR	C3-C4-C5	-3.81	107.27	114.08
22	B	609	CLA	CMB-C2B-C3B	3.80	131.80	124.68
22	a	403	CLA	CMB-C2B-C3B	3.80	131.79	124.68
27	a	410	PL9	C35-C34-C36	3.80	121.67	115.27
22	c	506	CLA	CMB-C2B-C3B	3.80	131.79	124.68
22	c	508	CLA	C4-C3-C5	3.79	121.64	115.27
27	d	405	PL9	C37-C38-C39	-3.79	118.54	127.66
34	d	406	LHG	O4-P-O5	3.78	130.95	112.24
22	B	603	CLA	CMB-C2B-C3B	3.78	131.75	124.68
22	d	403	CLA	C1B-CHB-C4A	-3.77	122.66	130.12
22	B	602	CLA	CAA-C2A-C3A	-3.76	102.49	112.78
29	a	412	SQD	O9-S-O7	-3.75	100.98	113.95
22	b	612	CLA	O2D-CGD-O1D	-3.74	116.53	123.84
29	A	413	SQD	O9-S-C6	3.73	111.38	106.94
22	B	611	CLA	O2A-CGA-O1A	-3.73	114.17	123.59
22	B	609	CLA	O2D-CGD-CBD	3.73	117.89	111.27
22	c	509	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
28	b	623	LMG	O2-C2-C1	-3.71	101.02	110.05
22	b	604	CLA	C4-C3-C5	3.71	121.52	115.27
22	B	608	CLA	CED-O2D-CGD	3.71	124.33	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	D	402	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
23	d	401	PHO	O1D-CGD-CBD	3.71	130.91	124.74
22	c	508	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
30	c	520	DGD	O3G-C3G-C2G	-3.70	101.97	110.90
22	b	604	CLA	C2D-C1D-ND	-3.69	107.38	110.10
22	b	603	CLA	CHD-C1D-ND	-3.69	121.07	124.45
22	b	611	CLA	C4A-NA-C1A	3.68	108.36	106.71
22	b	605	CLA	CMB-C2B-C3B	3.67	131.55	124.68
35	F	101	HEC	CMB-C2B-C1B	-3.67	122.82	128.46
34	d	408	LHG	O4-P-O5	3.67	130.39	112.24
22	b	615	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
34	D	408	LHG	O4-P-O5	3.66	130.34	112.24
27	d	405	PL9	C40-C39-C41	3.66	121.43	115.27
22	C	506	CLA	O2D-CGD-O1D	-3.66	116.69	123.84
30	A	415	DGD	O5D-C1E-C2E	3.66	114.01	108.30
22	B	612	CLA	O2D-CGD-CBD	3.66	117.76	111.27
22	b	608	CLA	CMB-C2B-C3B	3.65	131.51	124.68
22	B	614	CLA	C1-C2-C3	-3.65	119.73	126.04
24	x	101	BCR	C37-C22-C21	-3.65	117.81	122.92
22	C	504	CLA	CHD-C1D-ND	-3.65	121.10	124.45
22	b	603	CLA	C1-C2-C3	-3.64	119.74	126.04
27	a	410	PL9	C7-C3-C2	-3.64	118.51	123.30
30	h	102	DGD	O3G-C3G-C2G	-3.62	102.16	110.90
34	d	407	LHG	O4-P-O5	3.62	130.13	112.24
22	B	614	CLA	C4A-NA-C1A	3.62	108.33	106.71
30	A	415	DGD	C4E-C3E-C2E	-3.61	104.52	110.82
34	e	102	LHG	O8-C23-C24	3.61	123.24	111.91
22	b	607	CLA	C1B-CHB-C4A	-3.61	122.97	130.12
22	c	515	CLA	CMB-C2B-C3B	3.60	131.41	124.68
22	c	513	CLA	CHD-C1D-ND	-3.60	121.15	124.45
22	B	613	CLA	CMB-C2B-C3B	3.59	131.40	124.68
22	d	402	CLA	C4A-NA-C1A	3.59	108.32	106.71
24	C	515	BCR	C36-C18-C17	-3.58	117.90	122.92
22	b	610	CLA	CMB-C2B-C3B	3.58	131.38	124.68
22	B	616	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
22	C	510	CLA	CMB-C2B-C3B	3.57	131.36	124.68
22	A	405	CLA	CMB-C2B-C3B	3.57	131.36	124.68
22	B	611	CLA	O2D-CGD-CBD	3.57	117.61	111.27
22	c	504	CLA	O2D-CGD-O1D	-3.57	116.87	123.84
22	C	502	CLA	O2D-CGD-CBD	3.56	117.60	111.27
22	b	606	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
22	C	503	CLA	O2D-CGD-O1D	-3.55	116.89	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	605	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
22	h	101	CLA	CHD-C1D-ND	-3.54	121.20	124.45
28	b	621	LMG	O3-C3-C2	-3.54	102.17	110.35
24	C	515	BCR	C15-C16-C17	-3.53	116.24	123.47
22	C	510	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
22	c	508	CLA	CBC-CAC-C3C	-3.53	102.70	112.43
34	d	406	LHG	O8-C23-O10	-3.52	114.72	123.59
24	b	616	BCR	C2-C1-C6	3.51	115.89	110.48
22	B	617	CLA	C2D-C1D-ND	-3.51	107.52	110.10
22	d	402	CLA	C1B-CHB-C4A	-3.51	123.17	130.12
22	A	402	CLA	CMB-C2B-C3B	3.51	131.24	124.68
22	B	613	CLA	CHD-C1D-ND	-3.50	121.23	124.45
30	c	520	DGD	O2D-C2D-C1D	-3.50	101.54	110.05
30	h	102	DGD	C1D-C2D-C3D	-3.49	102.72	110.00
24	c	517	BCR	C35-C13-C14	-3.49	118.03	122.92
24	c	518	BCR	C16-C15-C14	-3.49	116.33	123.47
22	B	609	CLA	C4A-NA-C1A	3.49	108.27	106.71
22	D	402	CLA	CMB-C2B-C3B	3.49	131.20	124.68
22	A	402	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
22	B	617	CLA	O2A-C1-C2	3.48	117.78	108.64
27	D	405	PL9	C22-C23-C24	-3.48	119.28	127.66
29	f	101	SQD	O47-C7-C8	3.48	120.50	110.80
30	C	516	DGD	O3G-C3G-C2G	-3.48	102.50	110.90
22	b	609	CLA	CAC-C3C-C4C	3.48	129.32	124.81
24	T	101	BCR	C7-C8-C9	-3.48	120.98	126.23
28	A	412	LMG	O6-C1-O1	-3.47	101.75	109.97
22	B	611	CLA	CHD-C1D-ND	-3.47	121.27	124.45
22	A	403	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
22	a	402	CLA	CAC-C3C-C4C	3.47	129.31	124.81
22	B	617	CLA	C1D-ND-C4D	3.45	108.79	106.33
33	L	101	STE	O2-C1-C2	3.45	125.10	114.03
22	B	615	CLA	O2D-CGD-O1D	-3.45	117.10	123.84
23	D	401	PHO	O2D-CGD-O1D	-3.44	117.12	123.84
22	c	511	CLA	CMB-C2B-C3B	3.44	131.10	124.68
22	B	617	CLA	C1-O2A-CGA	3.43	125.46	116.44
24	Z	101	BCR	C33-C5-C6	-3.43	120.67	124.53
22	B	612	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
24	D	404	BCR	C24-C23-C22	-3.42	121.06	126.23
28	b	621	LMG	O1-C1-C2	-3.41	102.97	108.30
22	C	505	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
22	B	607	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
29	b	619	SQD	O8-S-C6	3.39	111.14	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	617	CLA	O2D-CGD-O1D	-3.39	117.22	123.84
22	h	101	CLA	CHB-C4A-NA	3.38	129.19	124.51
22	B	613	CLA	CHB-C4A-NA	3.38	129.19	124.51
22	C	513	CLA	CMB-C2B-C3B	3.38	131.00	124.68
22	C	506	CLA	CAC-C3C-C4C	3.38	129.19	124.81
22	D	402	CLA	C1B-CHB-C4A	-3.37	123.44	130.12
35	V	201	HEC	CMB-C2B-C1B	-3.37	123.28	128.46
22	C	509	CLA	C2D-C1D-ND	-3.37	107.62	110.10
22	d	403	CLA	CAC-C3C-C4C	3.37	129.18	124.81
22	c	506	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
27	D	405	PL9	C7-C3-C2	-3.36	118.88	123.30
22	c	507	CLA	CMB-C2B-C3B	3.36	130.96	124.68
22	C	502	CLA	C2D-C1D-ND	-3.35	107.63	110.10
29	A	414	SQD	O48-C23-C24	3.35	122.43	111.91
22	B	603	CLA	CHB-C4A-NA	3.34	129.14	124.51
22	B	605	CLA	CMB-C2B-C3B	3.34	130.94	124.68
22	B	613	CLA	O2A-CGA-O1A	-3.34	115.16	123.59
23	d	401	PHO	CMB-C2B-C3B	3.34	130.93	124.68
28	D	406	LMG	O1-C7-C8	-3.34	102.84	110.90
22	b	610	CLA	CHB-C4A-NA	3.34	129.13	124.51
24	Y	101	BCR	C27-C26-C25	3.34	127.58	122.73
24	Z	101	BCR	C11-C10-C9	-3.33	122.55	127.31
22	c	508	CLA	C4A-NA-C1A	3.33	108.20	106.71
22	B	602	CLA	O2D-CGD-O1D	-3.33	117.34	123.84
22	b	612	CLA	CED-O2D-CGD	3.32	123.45	115.94
22	C	509	CLA	CMB-C2B-C3B	3.32	130.90	124.68
22	B	614	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
22	C	503	CLA	O1D-CGD-CBD	3.32	131.28	124.48
27	D	405	PL9	C42-C43-C44	-3.32	119.67	127.66
35	V	201	HEC	CBA-CAA-C2A	-3.31	107.03	112.60
22	B	604	CLA	C4A-NA-C1A	3.31	108.19	106.71
30	H	102	DGD	O2D-C2D-C1D	-3.30	102.03	110.05
27	d	405	PL9	C22-C23-C24	-3.30	119.72	127.66
22	a	402	CLA	C1B-CHB-C4A	-3.29	123.59	130.12
22	A	402	CLA	C1D-ND-C4D	-3.29	104.00	106.33
22	c	514	CLA	O2A-CGA-O1A	-3.29	115.29	123.59
22	D	403	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
22	C	505	CLA	C4-C3-C5	3.29	120.80	115.27
26	a	409	BCT	O2-C-O1	3.28	128.06	119.55
22	B	606	CLA	CHB-C4A-NA	3.28	129.05	124.51
22	c	505	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
22	b	613	CLA	CMB-C2B-C1B	-3.27	123.43	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	605	CLA	O2D-CGD-CBD	3.27	117.08	111.27
22	b	605	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
22	c	505	CLA	C7-C6-C5	-3.27	104.48	113.36
22	B	604	CLA	C2D-C1D-ND	-3.26	107.70	110.10
22	C	504	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
22	b	607	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
22	b	611	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
24	x	101	BCR	C33-C5-C6	-3.26	120.87	124.53
27	A	410	PL9	C22-C23-C24	-3.26	119.82	127.66
22	c	514	CLA	CHB-C4A-NA	3.25	129.01	124.51
22	D	403	CLA	CMB-C2B-C3B	3.25	130.77	124.68
22	C	503	CLA	C4D-CHA-C1A	3.25	125.21	121.25
27	A	410	PL9	O2-C1-C6	3.25	126.22	120.59
22	C	513	CLA	O2D-CGD-CBD	3.25	117.04	111.27
22	A	402	CLA	CHB-C4A-NA	3.25	129.00	124.51
29	f	101	SQD	C1-C2-C3	-3.25	103.24	110.00
22	b	601	CLA	CMB-C2B-C3B	3.24	130.75	124.68
27	D	405	PL9	C37-C38-C39	-3.24	119.85	127.66
22	a	403	CLA	C1B-CHB-C4A	-3.24	123.70	130.12
33	j	101	STE	O2-C1-C2	3.24	124.43	114.03
29	a	412	SQD	O48-C23-C24	3.23	122.05	111.91
30	C	517	DGD	O6D-C1D-O3G	-3.23	102.32	109.97
29	a	412	SQD	C1-C2-C3	-3.23	103.28	110.00
22	b	606	CLA	CHD-C1D-ND	-3.23	121.49	124.45
29	D	407	SQD	C1-C2-C3	-3.22	103.29	110.00
22	b	604	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
22	C	511	CLA	CHB-C4A-NA	3.22	128.96	124.51
22	h	101	CLA	O2D-CGD-CBD	3.22	116.98	111.27
22	b	602	CLA	C7-C6-C5	-3.21	104.63	113.36
22	B	617	CLA	CMB-C2B-C3B	3.21	130.69	124.68
30	C	517	DGD	O2D-C2D-C1D	-3.21	102.25	110.05
29	B	623	SQD	C1-O5-C5	-3.21	107.39	113.69
22	c	515	CLA	CHD-C1D-ND	-3.20	121.51	124.45
22	b	609	CLA	C1B-CHB-C4A	-3.20	123.78	130.12
22	c	512	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
24	T	101	BCR	C35-C13-C14	-3.20	118.44	122.92
22	c	514	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
24	B	620	BCR	C2-C1-C6	3.19	115.39	110.48
22	d	402	CLA	O2A-CGA-O1A	-3.19	115.55	123.59
22	c	511	CLA	C1B-CHB-C4A	-3.19	123.81	130.12
29	a	412	SQD	C1-O5-C5	-3.18	107.44	113.69
22	b	611	CLA	C1B-CHB-C4A	-3.18	123.81	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	H	101	BCR	C35-C13-C14	-3.18	118.47	122.92
24	c	518	BCR	C11-C10-C9	-3.18	122.78	127.31
24	B	619	BCR	C40-C30-C25	3.17	115.45	110.30
22	c	504	CLA	C1B-CHB-C4A	-3.17	123.84	130.12
22	c	508	CLA	CMB-C2B-C3B	3.17	130.60	124.68
34	D	412	LHG	O3-P-O5	-3.16	96.70	109.07
23	d	401	PHO	CMC-C2C-C3C	3.16	130.91	124.94
22	c	503	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
22	c	510	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
22	b	607	CLA	C4A-NA-C1A	3.16	108.13	106.71
34	D	409	LHG	O8-C23-C24	3.16	121.82	111.91
22	b	602	CLA	C2D-C1D-ND	-3.16	107.78	110.10
22	B	606	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
22	B	617	CLA	C5-C3-C2	3.16	127.50	121.12
22	b	609	CLA	C2C-C1C-NC	3.15	112.92	109.97
29	b	619	SQD	O47-C7-C8	3.14	118.28	111.50
22	A	411	CLA	C2C-C1C-NC	3.14	112.91	109.97
24	t	101	BCR	C7-C8-C9	-3.13	121.50	126.23
27	d	405	PL9	C36-C34-C33	-3.13	114.79	121.12
22	C	505	CLA	CMB-C2B-C3B	3.13	130.53	124.68
22	c	509	CLA	O2A-CGA-O1A	-3.12	115.71	123.59
22	a	403	CLA	C4A-NA-C1A	3.12	108.11	106.71
22	b	613	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
22	B	604	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
29	D	407	SQD	O5-C1-C2	-3.11	103.76	110.35
22	a	405	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
22	C	508	CLA	C1-C2-C3	-3.11	120.66	126.04
24	a	406	BCR	C27-C26-C25	3.11	127.25	122.73
22	b	607	CLA	O2A-CGA-O1A	-3.10	115.76	123.59
22	b	612	CLA	C4A-NA-C1A	3.10	108.10	106.71
22	C	504	CLA	O2A-C1-C2	-3.09	100.50	108.64
22	C	508	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
28	b	623	LMG	O1-C1-C2	-3.09	103.48	108.30
22	b	612	CLA	CMB-C2B-C3B	3.08	130.45	124.68
22	C	513	CLA	C4A-NA-C1A	3.08	108.09	106.71
22	C	514	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
29	a	413	SQD	O48-C23-C24	3.08	121.57	111.91
22	b	612	CLA	CHB-C4A-NA	3.08	128.77	124.51
28	C	519	LMG	O1-C7-C8	-3.08	103.48	110.90
22	c	512	CLA	CMB-C2B-C1B	-3.08	123.74	128.46
30	C	518	DGD	O6D-C1D-O3G	-3.07	102.70	109.97
27	D	405	PL9	C7-C8-C9	-3.07	121.68	126.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	603	CLA	CMB-C2B-C3B	3.07	130.42	124.68
22	b	608	CLA	C4A-NA-C1A	3.07	108.08	106.71
22	d	402	CLA	CMB-C2B-C1B	-3.07	123.75	128.46
22	C	507	CLA	CMB-C2B-C1B	-3.05	123.77	128.46
22	C	508	CLA	CHD-C1D-ND	-3.05	121.66	124.45
22	B	611	CLA	O1D-CGD-CBD	3.05	130.72	124.48
22	b	607	CLA	CHD-C1D-ND	-3.04	121.66	124.45
22	b	606	CLA	C6-C7-C8	-3.04	106.09	115.92
22	b	601	CLA	CHB-C4A-NA	3.04	128.72	124.51
22	b	604	CLA	O1D-CGD-CBD	3.04	130.71	124.48
22	b	611	CLA	CMB-C2B-C3B	3.04	130.36	124.68
22	b	611	CLA	C11-C12-C13	-3.04	106.10	115.92
28	c	525	LMG	O6-C1-O1	-3.03	102.79	109.97
22	C	508	CLA	C4-C3-C5	3.03	120.37	115.27
28	A	412	LMG	C1-O6-C5	-3.03	107.73	113.69
22	b	606	CLA	C1D-ND-C4D	-3.03	104.18	106.33
22	B	616	CLA	CHB-C4A-NA	3.02	128.69	124.51
24	b	617	BCR	C15-C14-C13	-3.02	123.00	127.31
22	d	403	CLA	O2A-CGA-O1A	-3.02	115.96	123.59
22	b	610	CLA	CHD-C1D-ND	-3.02	121.68	124.45
22	B	610	CLA	CMB-C2B-C1B	-3.02	123.83	128.46
29	b	619	SQD	O9-S-O7	-3.01	103.52	113.95
22	c	509	CLA	CMB-C2B-C3B	3.01	130.31	124.68
23	a	404	PHO	CMC-C2C-C3C	3.01	130.62	124.94
22	B	616	CLA	CHD-C1D-ND	-3.00	121.70	124.45
22	b	605	CLA	CGD-CBD-CAD	-3.00	101.02	110.73
22	A	403	CLA	CED-O2D-CGD	-3.00	109.16	115.94
30	c	520	DGD	C3G-O3G-C1D	2.99	119.59	113.74
30	c	520	DGD	O3G-C1D-C2D	-2.99	103.63	108.30
22	c	510	CLA	CHD-C1D-ND	-2.99	121.70	124.45
22	a	405	CLA	C1B-CHB-C4A	-2.99	124.19	130.12
22	b	611	CLA	O2A-CGA-O1A	-2.99	116.05	123.59
22	C	509	CLA	CHD-C1D-ND	-2.99	121.71	124.45
27	a	410	PL9	C22-C23-C24	-2.99	120.47	127.66
22	C	514	CLA	O2A-CGA-O1A	-2.99	116.05	123.59
23	D	401	PHO	CMC-C2C-C3C	2.99	130.57	124.94
29	B	623	SQD	O48-C23-C24	2.99	121.28	111.91
22	B	605	CLA	C11-C12-C13	-2.98	106.28	115.92
22	c	513	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
22	h	101	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
30	c	521	DGD	C3D-C4D-C5D	-2.98	104.93	110.24
27	a	410	PL9	C20-C19-C21	2.98	120.28	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	401	PHO	O1D-CGD-CBD	2.98	129.70	124.74
24	B	620	BCR	C29-C30-C25	2.98	115.06	110.48
24	a	406	BCR	C30-C25-C26	-2.97	118.43	122.61
22	c	504	CLA	CMB-C2B-C3B	2.97	130.23	124.68
22	c	504	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
35	v	201	HEC	CMC-C2C-C1C	-2.96	123.92	128.46
35	F	101	HEC	CMB-C2B-C3B	2.96	129.30	125.82
29	b	619	SQD	O5-C5-C4	2.95	115.06	109.69
27	A	410	PL9	O2-C1-C2	-2.95	115.02	121.78
22	B	604	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
24	a	406	BCR	C29-C30-C25	2.94	115.01	110.48
22	c	503	CLA	CMB-C2B-C3B	2.94	130.18	124.68
30	c	519	DGD	O2G-C1B-O1B	-2.94	116.60	123.70
24	H	101	BCR	C27-C26-C25	2.94	127.00	122.73
24	x	101	BCR	C27-C26-C25	2.94	127.00	122.73
34	D	408	LHG	O8-C23-O10	-2.93	116.19	123.59
22	b	605	CLA	C1C-C2C-C3C	-2.93	103.87	106.96
30	A	415	DGD	O2D-C2D-C1D	-2.93	102.94	110.05
22	A	402	CLA	O1D-CGD-CBD	2.92	130.47	124.48
22	B	616	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
30	h	102	DGD	C3D-C4D-C5D	-2.92	105.03	110.24
22	b	609	CLA	C1-C2-C3	-2.92	120.99	126.04
22	C	510	CLA	C1-C2-C3	-2.92	120.99	126.04
22	b	604	CLA	CMB-C2B-C3B	2.92	130.14	124.68
22	c	509	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
28	b	623	LMG	C3-C4-C5	-2.91	105.04	110.24
22	C	511	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
22	a	411	CLA	CMB-C2B-C3B	2.91	130.13	124.68
28	b	621	LMG	C38-C37-C36	-2.91	99.66	114.42
22	c	513	CLA	CHB-C4A-NA	2.91	128.53	124.51
22	B	606	CLA	C7-C6-C5	-2.91	105.47	113.36
28	D	406	LMG	C3-C4-C5	-2.91	105.06	110.24
22	c	515	CLA	CHB-C4A-NA	2.90	128.53	124.51
22	b	615	CLA	O2D-CGD-CBD	2.90	116.43	111.27
24	y	101	BCR	C33-C5-C6	-2.90	121.27	124.53
34	D	408	LHG	O8-C23-C24	2.90	121.00	111.91
29	a	413	SQD	O49-C7-C8	-2.90	112.43	123.73
22	B	614	CLA	OBD-CAD-C3D	2.90	135.49	128.52
24	H	101	BCR	C2-C1-C6	2.89	114.94	110.48
29	D	407	SQD	O48-C23-C24	2.89	120.99	111.91
22	b	606	CLA	CMB-C2B-C3B	2.89	130.09	124.68
29	D	407	SQD	C1-O5-C5	-2.89	108.02	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	616	BCR	C3-C4-C5	-2.89	108.92	114.08
22	a	403	CLA	CHB-C4A-NA	2.89	128.50	124.51
28	d	409	LMG	O6-C1-O1	-2.88	103.15	109.97
30	c	519	DGD	O6E-C5E-C4E	2.88	114.93	109.69
22	C	505	CLA	CHD-C1D-ND	-2.88	121.81	124.45
28	B	629	LMG	O6-C1-C2	-2.88	104.26	110.35
24	T	101	BCR	C28-C27-C26	-2.88	108.94	114.08
22	b	607	CLA	CMB-C2B-C3B	2.88	130.06	124.68
30	C	516	DGD	O1G-C1A-C2A	-2.87	102.88	111.91
24	b	617	BCR	C30-C25-C26	-2.87	118.56	122.61
23	a	404	PHO	CMB-C2B-C3B	2.87	130.06	124.68
28	b	621	LMG	O7-C10-O9	-2.87	116.76	123.70
22	B	617	CLA	CMB-C2B-C1B	-2.87	124.05	128.46
24	Z	101	BCR	C24-C23-C22	-2.87	121.90	126.23
22	A	402	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
24	b	617	BCR	C27-C26-C25	2.86	126.89	122.73
24	Y	101	BCR	C30-C25-C26	-2.86	118.58	122.61
30	c	519	DGD	O6D-C1D-O3G	-2.86	103.20	109.97
24	A	406	BCR	C38-C26-C25	-2.86	121.32	124.53
30	A	415	DGD	C3G-C2G-C1G	-2.86	105.03	111.79
22	c	512	CLA	CHD-C1D-ND	-2.86	121.83	124.45
29	B	623	SQD	O8-S-C6	2.85	110.28	105.74
24	b	618	BCR	C2-C1-C6	2.85	114.87	110.48
22	C	509	CLA	C1D-ND-C4D	2.85	108.36	106.33
22	B	617	CLA	CHB-C4A-NA	2.84	128.44	124.51
28	d	409	LMG	O2-C2-C1	-2.84	103.15	110.05
22	b	613	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
22	A	402	CLA	CMD-C2D-C1D	2.83	129.71	124.71
33	d	410	STE	O2-C1-C2	2.83	123.13	114.03
28	b	621	LMG	C1-O6-C5	-2.83	108.13	113.69
22	C	507	CLA	CHB-C4A-NA	2.83	128.42	124.51
22	B	613	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
24	T	101	BCR	C27-C26-C25	2.83	126.83	122.73
29	A	413	SQD	O47-C7-O49	-2.82	116.88	123.70
24	c	516	BCR	C11-C10-C9	-2.82	123.28	127.31
34	d	407	LHG	C20-C19-C18	-2.82	100.11	114.42
22	C	507	CLA	CHA-C1A-NA	-2.82	119.95	126.40
27	A	410	PL9	C35-C34-C36	2.82	120.01	115.27
22	B	604	CLA	O2A-CGA-O1A	-2.81	116.49	123.59
22	b	605	CLA	O1D-CGD-CBD	2.81	130.24	124.48
22	C	514	CLA	CMB-C2B-C3B	2.81	129.94	124.68
22	B	613	CLA	C11-C12-C13	-2.81	106.84	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	404	BCR	C24-C23-C22	-2.81	121.99	126.23
22	B	602	CLA	CHB-C4A-NA	2.81	128.39	124.51
22	C	513	CLA	C1-C2-C3	-2.80	121.19	126.04
27	A	410	PL9	C36-C34-C33	-2.80	115.45	121.12
22	A	405	CLA	O2D-CGD-CBD	2.80	116.25	111.27
22	B	614	CLA	CHA-C1A-NA	-2.80	119.98	126.40
22	B	604	CLA	O2D-CGD-CBD	2.80	116.24	111.27
22	B	615	CLA	CHB-C4A-NA	2.80	128.38	124.51
22	B	617	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
22	b	613	CLA	CMB-C2B-C3B	2.80	129.91	124.68
22	b	608	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
29	B	623	SQD	O5-C5-C4	2.79	114.77	109.69
22	b	604	CLA	C1D-ND-C4D	2.79	108.32	106.33
28	c	524	LMG	O7-C10-O9	-2.79	116.96	123.70
22	C	512	CLA	C2D-C1D-ND	-2.79	108.05	110.10
27	A	410	PL9	C30-C29-C31	-2.78	110.59	115.27
27	d	405	PL9	C7-C3-C2	-2.78	119.64	123.30
22	B	614	CLA	CMB-C2B-C3B	2.78	129.88	124.68
23	D	401	PHO	CMB-C2B-C3B	2.78	129.88	124.68
22	b	601	CLA	CAC-C3C-C4C	2.78	128.42	124.81
22	b	606	CLA	C2D-C1D-ND	2.78	112.15	110.10
22	B	605	CLA	O2A-CGA-O1A	-2.78	116.58	123.59
29	b	619	SQD	O2-C2-C1	2.78	116.79	110.05
22	b	611	CLA	CHB-C4A-NA	2.78	128.35	124.51
30	h	102	DGD	O3E-C3E-C2E	-2.77	103.94	110.35
24	b	616	BCR	C36-C18-C17	-2.77	119.04	122.92
24	c	516	BCR	C33-C5-C6	-2.77	121.42	124.53
22	B	612	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
22	b	615	CLA	O1D-CGD-CBD	2.77	130.15	124.48
22	B	615	CLA	CMD-C2D-C3D	2.76	133.97	127.61
22	b	605	CLA	C1D-ND-C4D	2.76	108.30	106.33
33	X	101	STE	C3-C2-C1	-2.76	107.51	114.47
22	B	615	CLA	CHA-C1A-NA	-2.76	120.07	126.40
29	B	623	SQD	O9-S-O7	-2.76	104.39	113.95
22	b	615	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
30	c	521	DGD	O6D-C1D-O3G	-2.76	103.44	109.97
30	h	102	DGD	O6E-C5E-C6E	-2.76	99.57	106.44
22	a	405	CLA	CHD-C1D-ND	-2.76	121.92	124.45
28	M	101	LMG	C1-C2-C3	-2.76	104.26	110.00
22	a	403	CLA	O2D-CGD-CBD	2.76	116.17	111.27
27	A	410	PL9	C27-C28-C29	-2.75	121.03	127.66
24	B	618	BCR	C15-C16-C17	-2.75	117.85	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	406	LMG	O6-C1-O1	-2.75	103.47	109.97
22	C	513	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
24	c	518	BCR	C37-C22-C21	-2.74	119.08	122.92
24	c	518	BCR	C27-C26-C25	2.74	126.72	122.73
30	A	415	DGD	O1G-C1A-O1A	-2.74	116.67	123.59
22	c	503	CLA	CED-O2D-CGD	-2.74	109.73	115.94
24	b	616	BCR	C8-C7-C6	-2.74	119.50	127.20
22	c	506	CLA	O2D-CGD-CBD	2.74	116.14	111.27
27	D	405	PL9	C12-C13-C14	-2.74	121.06	127.66
22	b	604	CLA	C1-C2-C3	-2.73	121.33	126.04
22	B	608	CLA	O2A-C1-C2	-2.73	101.47	108.64
24	b	616	BCR	C15-C14-C13	-2.73	123.42	127.31
35	e	101	HEC	CMC-C2C-C1C	-2.72	124.28	128.46
28	C	519	LMG	O1-C1-C2	-2.72	104.06	108.30
22	c	506	CLA	C7-C6-C5	-2.72	105.98	113.36
22	b	614	CLA	CHB-C4A-NA	2.72	128.27	124.51
22	b	602	CLA	C4-C3-C5	2.72	119.84	115.27
30	c	520	DGD	O5D-C6D-C5D	-2.71	104.03	109.05
22	b	601	CLA	C2D-C1D-ND	-2.71	108.11	110.10
22	C	506	CLA	O1D-CGD-CBD	2.71	130.03	124.48
33	B	624	STE	C3-C2-C1	-2.71	107.64	114.47
22	b	612	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
22	b	601	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
22	B	608	CLA	O2A-CGA-O1A	-2.70	116.77	123.59
22	c	506	CLA	C1B-CHB-C4A	-2.70	124.76	130.12
22	a	405	CLA	C4-C3-C5	2.70	119.81	115.27
30	C	516	DGD	CDB-CCB-CBB	-2.70	100.72	114.42
27	D	405	PL9	C32-C33-C34	-2.70	121.17	127.66
28	A	412	LMG	O8-C28-O10	-2.70	116.79	123.59
22	C	508	CLA	CMB-C2B-C1B	-2.69	124.32	128.46
22	C	506	CLA	CMB-C2B-C1B	-2.69	124.32	128.46
34	d	406	LHG	C11-C10-C9	-2.69	100.75	114.42
22	c	508	CLA	CMC-C2C-C1C	2.69	129.13	125.04
22	B	602	CLA	C2A-C1A-CHA	2.69	128.56	123.86
22	B	609	CLA	CHD-C4C-NC	2.69	128.44	124.20
24	t	101	BCR	C35-C13-C14	-2.69	119.16	122.92
29	B	623	SQD	C3-C4-C5	2.69	115.03	110.24
30	C	516	DGD	C3G-C2G-C1G	-2.69	105.43	111.79
30	c	519	DGD	C4D-C3D-C2D	-2.69	106.13	110.82
30	H	102	DGD	C3D-C4D-C5D	-2.69	105.44	110.24
30	C	517	DGD	O5D-C6D-C5D	-2.69	104.07	109.05
22	B	615	CLA	C4-C3-C5	2.69	119.79	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	602	CLA	C5-C3-C2	-2.68	115.69	121.12
22	B	612	CLA	C7-C6-C5	-2.68	106.07	113.36
28	c	524	LMG	O3-C3-C2	-2.68	104.15	110.35
22	b	613	CLA	CHB-C4A-NA	2.68	128.22	124.51
22	C	511	CLA	CMB-C2B-C1B	-2.68	124.34	128.46
22	D	403	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
24	b	616	BCR	C11-C10-C9	-2.68	123.49	127.31
22	c	510	CLA	CMB-C2B-C1B	-2.68	124.35	128.46
22	B	610	CLA	CHD-C1D-ND	-2.67	122.00	124.45
33	E	102	STE	O2-C1-C2	2.67	122.61	114.03
22	b	604	CLA	CHC-C1C-NC	2.67	128.25	124.20
22	D	403	CLA	O2A-CGA-O1A	-2.67	116.85	123.59
22	b	610	CLA	C7-C6-C5	-2.67	106.11	113.36
28	B	629	LMG	O6-C5-C4	2.67	114.54	109.69
30	c	519	DGD	CDB-CCB-CBB	-2.67	100.88	114.42
22	b	612	CLA	O2A-CGA-O1A	-2.66	116.87	123.59
22	A	403	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
22	b	614	CLA	C3B-C4B-NB	-2.66	105.77	109.21
28	c	525	LMG	C1-O6-C5	-2.66	108.47	113.69
22	C	510	CLA	C2A-C1A-CHA	2.66	128.50	123.86
33	b	622	STE	O2-C1-C2	2.65	122.56	114.03
22	d	403	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
22	C	508	CLA	CMB-C2B-C3B	2.65	129.64	124.68
24	Z	101	BCR	C28-C27-C26	-2.65	109.34	114.08
29	b	619	SQD	O48-C23-C24	2.65	120.22	111.91
22	B	617	CLA	C1-C2-C3	2.65	130.62	126.04
22	b	604	CLA	CHD-C1D-ND	-2.65	122.02	124.45
29	D	407	SQD	O8-S-O9	-2.65	104.80	111.27
22	B	602	CLA	C1-C2-C3	-2.65	121.47	126.04
30	C	517	DGD	C1D-C2D-C3D	-2.65	104.49	110.00
24	b	618	BCR	C15-C16-C17	-2.64	118.06	123.47
22	B	605	CLA	CHB-C4A-NA	2.64	128.17	124.51
30	H	102	DGD	C3E-C4E-C5E	-2.64	105.53	110.24
27	D	405	PL9	C50-C49-C48	-2.64	115.01	122.65
22	b	602	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
22	c	504	CLA	CHD-C1D-ND	-2.64	122.03	124.45
22	B	604	CLA	CHB-C4A-NA	2.63	128.15	124.51
30	h	102	DGD	C3G-C2G-C1G	-2.63	105.56	111.79
24	x	101	BCR	C2-C1-C6	2.63	114.53	110.48
22	C	512	CLA	CHA-C4D-ND	2.63	137.99	132.50
33	d	411	STE	O2-C1-O1	-2.63	116.75	123.30
22	c	503	CLA	CHB-C4A-NA	2.63	128.14	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	612	CLA	CHD-C4C-NC	2.62	128.34	124.20
22	C	503	CLA	C1D-ND-C4D	2.62	108.20	106.33
24	b	618	BCR	C29-C30-C25	2.62	114.51	110.48
22	B	609	CLA	CHB-C4A-NA	2.62	128.13	124.51
23	d	401	PHO	C6-C7-C8	-2.61	107.47	115.92
22	B	607	CLA	CMB-C2B-C1B	-2.61	124.45	128.46
24	A	406	BCR	C27-C26-C25	2.61	126.52	122.73
28	D	406	LMG	O3-C3-C2	-2.61	104.32	110.35
28	c	524	LMG	C1-O6-C5	-2.61	108.57	113.69
30	H	102	DGD	C1D-C2D-C3D	-2.61	104.57	110.00
28	b	623	LMG	O6-C5-C6	2.60	112.91	106.44
22	B	615	CLA	CMB-C2B-C3B	2.60	129.55	124.68
22	d	402	CLA	CMB-C2B-C3B	2.60	129.54	124.68
22	b	602	CLA	CMD-C2D-C1D	2.60	129.29	124.71
22	c	506	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
22	B	611	CLA	CHB-C4A-NA	2.60	128.10	124.51
24	T	101	BCR	C38-C26-C27	-2.59	108.63	113.62
29	b	619	SQD	C3-C4-C5	2.59	114.87	110.24
22	b	602	CLA	O2A-C1-C2	-2.59	101.82	108.64
22	B	609	CLA	C1D-ND-C4D	-2.59	104.50	106.33
24	B	618	BCR	C2-C1-C6	2.59	114.47	110.48
22	b	602	CLA	O2D-CGD-CBD	2.59	115.87	111.27
24	B	619	BCR	C29-C30-C25	2.59	114.47	110.48
22	B	612	CLA	C2C-C1C-NC	2.59	112.40	109.97
22	C	509	CLA	CHB-C4A-NA	2.59	128.09	124.51
22	B	616	CLA	C5-C3-C2	-2.59	115.89	121.12
22	B	616	CLA	CMB-C2B-C3B	2.58	129.51	124.68
35	v	201	HEC	CBA-CAA-C2A	-2.58	108.25	112.60
22	B	610	CLA	CMB-C2B-C3B	2.58	129.51	124.68
22	b	613	CLA	O2D-CGD-CBD	2.58	115.86	111.27
22	B	610	CLA	O2D-CGD-CBD	2.58	115.85	111.27
24	c	517	BCR	C11-C10-C9	-2.58	123.63	127.31
29	f	101	SQD	O48-C23-O10	-2.58	117.08	123.59
22	B	608	CLA	CHD-C1D-ND	-2.58	122.08	124.45
22	d	402	CLA	C4-C3-C5	2.58	119.61	115.27
24	d	404	BCR	C33-C5-C6	-2.58	121.63	124.53
24	c	517	BCR	C27-C26-C25	2.58	126.47	122.73
30	H	102	DGD	O2G-C1B-O1B	-2.58	117.47	123.70
22	c	515	CLA	C1B-CHB-C4A	-2.58	125.02	130.12
22	B	617	CLA	O1D-CGD-CBD	2.58	129.75	124.48
24	d	404	BCR	C16-C15-C14	-2.57	118.20	123.47
22	B	607	CLA	C6-C5-C3	-2.57	106.70	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	506	CLA	CHB-C4A-NA	2.57	128.07	124.51
22	D	403	CLA	O1D-CGD-CBD	2.57	129.75	124.48
30	c	521	DGD	O5D-C6D-C5D	-2.57	104.29	109.05
30	c	519	DGD	O6D-C1D-C2D	2.57	115.78	110.35
34	e	102	LHG	C20-C19-C18	-2.57	101.40	114.42
22	A	405	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
28	c	525	LMG	O7-C10-O9	-2.57	117.50	123.70
29	a	413	SQD	C45-O47-C7	2.57	124.11	117.79
24	B	619	BCR	C15-C14-C13	-2.56	123.65	127.31
24	Y	101	BCR	C39-C30-C25	-2.56	106.14	110.30
22	c	505	CLA	CMB-C2B-C3B	2.56	129.46	124.68
22	c	508	CLA	C4-C3-C2	-2.55	117.12	123.68
24	c	517	BCR	C15-C16-C17	-2.55	118.24	123.47
22	c	510	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
24	b	618	BCR	C32-C1-C6	-2.55	106.16	110.30
22	b	609	CLA	O2D-CGD-CBD	2.55	115.80	111.27
22	B	602	CLA	O2D-CGD-CBD	2.55	115.79	111.27
22	C	513	CLA	CHB-C4A-NA	2.55	128.03	124.51
22	C	504	CLA	C1B-CHB-C4A	-2.55	125.08	130.12
24	B	619	BCR	C39-C30-C25	-2.55	106.17	110.30
33	C	522	STE	C3-C2-C1	-2.54	108.06	114.47
22	C	512	CLA	CMB-C2B-C1B	-2.54	124.55	128.46
24	b	616	BCR	C35-C13-C12	2.54	122.08	118.08
33	B	601	STE	O2-C1-C2	2.54	122.19	114.03
30	C	516	DGD	O2G-C1B-C2B	-2.54	106.02	111.50
22	c	509	CLA	CHD-C1D-ND	-2.54	122.12	124.45
23	a	404	PHO	O2A-CGA-O1A	-2.54	117.18	123.59
22	C	514	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
23	a	404	PHO	CMD-C2D-C3D	2.54	129.42	124.68
24	a	406	BCR	C7-C8-C9	-2.54	122.40	126.23
22	a	411	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
22	d	402	CLA	CHB-C4A-NA	2.53	128.01	124.51
24	b	617	BCR	C31-C1-C6	2.53	114.40	110.30
22	b	615	CLA	CHD-C1D-ND	-2.53	122.13	124.45
24	A	406	BCR	C15-C14-C13	-2.53	123.70	127.31
22	B	602	CLA	C4-C3-C5	2.53	119.52	115.27
22	C	512	CLA	C4-C3-C5	2.53	119.52	115.27
29	b	619	SQD	O5-C1-C2	-2.53	105.00	110.35
27	a	410	PL9	C36-C34-C33	-2.52	116.01	121.12
22	b	605	CLA	C2A-C1A-CHA	2.52	128.27	123.86
22	b	610	CLA	CED-O2D-CGD	-2.52	110.24	115.94
24	C	515	BCR	C33-C5-C6	-2.52	121.70	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	406	LMG	C1-C2-C3	-2.52	104.76	110.00
30	C	518	DGD	O3E-C3E-C2E	-2.51	104.54	110.35
27	a	410	PL9	C7-C8-C9	-2.51	122.61	126.79
22	C	506	CLA	CMB-C2B-C3B	2.51	129.38	124.68
30	c	519	DGD	O5E-C6E-C5E	-2.51	102.67	111.29
33	B	621	STE	C3-C2-C1	-2.51	108.14	114.47
22	c	505	CLA	C3A-C2A-C1A	2.51	105.10	101.34
34	E	101	LHG	O8-C23-C24	2.51	119.79	111.91
28	c	524	LMG	O2-C2-C1	-2.51	103.95	110.05
22	b	614	CLA	C1-O2A-CGA	2.51	123.02	116.44
22	b	603	CLA	C2A-C1A-CHA	2.51	128.24	123.86
22	c	506	CLA	CHD-C4C-NC	2.51	128.15	124.20
24	D	404	BCR	C27-C26-C25	2.51	126.37	122.73
28	A	412	LMG	C38-C37-C36	-2.50	101.71	114.42
22	C	508	CLA	CHB-C4A-NA	2.50	127.97	124.51
24	a	406	BCR	C38-C26-C27	-2.50	108.81	113.62
22	a	402	CLA	C7-C6-C5	-2.50	106.57	113.36
22	B	604	CLA	C3B-C4B-NB	-2.50	105.98	109.21
22	c	509	CLA	C2C-C1C-NC	2.50	112.31	109.97
22	B	616	CLA	C14-C13-C15	-2.50	102.25	111.29
28	d	409	LMG	C9-C8-C7	-2.50	105.88	111.79
30	C	516	DGD	C3D-C4D-C5D	-2.50	105.79	110.24
27	d	405	PL9	C15-C14-C13	-2.49	117.28	123.68
24	c	517	BCR	C34-C9-C10	-2.49	119.43	122.92
22	C	508	CLA	C2A-C1A-CHA	2.49	128.22	123.86
33	d	411	STE	O2-C1-C2	2.49	122.03	114.03
24	B	619	BCR	C11-C10-C9	-2.49	123.76	127.31
28	c	525	LMG	C40-C39-C38	-2.49	101.79	114.42
22	b	602	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
22	d	403	CLA	O1D-CGD-CBD	2.48	129.57	124.48
28	B	629	LMG	O5-C6-C5	-2.48	102.77	111.29
34	D	412	LHG	O8-C23-O10	-2.48	117.33	123.59
22	c	510	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
28	c	522	LMG	O7-C10-O9	-2.48	118.03	122.96
30	H	102	DGD	C7B-C6B-C5B	-2.48	101.83	114.42
22	A	405	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
22	B	602	CLA	C3A-C2A-C1A	2.48	105.05	101.34
22	b	614	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
22	B	617	CLA	CHD-C1D-ND	-2.48	122.18	124.45
22	b	607	CLA	CHB-C4A-NA	2.47	127.93	124.51
22	C	509	CLA	CHD-C1D-C2D	2.47	130.67	125.48
24	c	518	BCR	C8-C7-C6	-2.47	120.25	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	609	CLA	C11-C12-C13	-2.47	107.93	115.92
24	b	616	BCR	C29-C30-C25	2.47	114.29	110.48
22	C	502	CLA	O2A-CGA-O1A	-2.47	117.36	123.59
27	A	410	PL9	C40-C39-C41	2.47	119.43	115.27
30	H	102	DGD	C1E-O6E-C5E	2.46	118.53	113.69
22	c	514	CLA	CHD-C1D-ND	-2.46	122.19	124.45
23	A	404	PHO	O2A-CGA-O1A	-2.46	117.38	123.59
22	D	402	CLA	CHB-C4A-NA	2.46	127.92	124.51
22	B	606	CLA	CHD-C4C-C3C	-2.46	121.22	124.84
33	C	522	STE	C4-C3-C2	-2.46	104.34	113.19
34	d	408	LHG	O8-C23-O10	-2.46	117.38	123.59
29	f	101	SQD	O5-C1-O6	2.46	115.80	109.97
22	B	615	CLA	C2A-C1A-CHA	2.46	128.16	123.86
22	C	508	CLA	C4-C3-C2	-2.46	117.38	123.68
22	C	504	CLA	CMB-C2B-C3B	2.46	129.27	124.68
24	B	619	BCR	C7-C8-C9	-2.46	122.52	126.23
22	c	503	CLA	C2C-C1C-NC	2.46	112.27	109.97
22	c	507	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
33	L	101	STE	O1-C1-C2	-2.45	115.21	123.08
33	B	624	STE	O2-C1-C2	2.45	121.90	114.03
22	B	614	CLA	O1D-CGD-CBD	2.45	129.50	124.48
30	C	516	DGD	O6D-C1D-O3G	-2.45	104.18	109.97
22	B	610	CLA	C2C-C1C-NC	2.45	112.27	109.97
22	b	612	CLA	CHD-C1D-ND	-2.45	122.21	124.45
22	c	506	CLA	CMC-C2C-C1C	2.44	128.76	125.04
24	x	101	BCR	C38-C26-C25	-2.44	121.79	124.53
22	C	504	CLA	O1D-CGD-CBD	2.44	129.47	124.48
28	c	522	LMG	O6-C1-O1	-2.44	104.21	109.97
22	b	604	CLA	CHD-C1D-C2D	2.43	130.59	125.48
22	C	508	CLA	C1C-C2C-C3C	-2.43	104.40	106.96
30	c	519	DGD	O1G-C1A-C2A	-2.43	104.28	111.91
34	B	622	LHG	C27-C26-C25	-2.43	102.09	114.42
22	A	405	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
28	B	629	LMG	C9-C8-C7	-2.43	106.05	111.79
22	B	613	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
22	b	609	CLA	CHB-C4A-NA	2.43	127.87	124.51
27	D	405	PL9	C41-C39-C38	-2.42	116.21	121.12
24	t	101	BCR	C15-C16-C17	-2.42	118.51	123.47
29	D	407	SQD	C44-O6-C1	2.42	117.85	113.84
29	b	619	SQD	C45-O47-C7	2.42	123.75	117.79
30	c	519	DGD	O3G-C3G-C2G	-2.42	105.06	110.90
22	c	509	CLA	O2D-CGD-O1D	-2.42	119.11	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	609	CLA	C6-C7-C8	-2.42	108.11	115.92
22	a	405	CLA	CMB-C2B-C3B	2.41	129.20	124.68
23	a	404	PHO	CMA-C3A-C4A	-2.41	109.09	114.38
24	A	406	BCR	C24-C23-C22	-2.41	122.59	126.23
22	B	607	CLA	CHB-C4A-NA	2.41	127.85	124.51
30	h	102	DGD	C4D-C3D-C2D	-2.41	106.61	110.82
22	c	512	CLA	CMB-C2B-C3B	2.41	129.19	124.68
33	X	101	STE	C12-C11-C10	-2.41	102.18	114.42
22	A	403	CLA	CHB-C4A-NA	2.41	127.84	124.51
22	B	607	CLA	O2D-CGD-CBD	2.41	115.55	111.27
29	f	101	SQD	C1-O5-C5	-2.41	108.96	113.69
22	B	609	CLA	C3D-C4D-ND	2.41	114.13	110.24
28	B	629	LMG	O7-C10-O9	-2.41	117.89	123.70
22	b	602	CLA	CHD-C1D-ND	-2.40	122.24	124.45
24	H	101	BCR	C29-C30-C25	2.40	114.18	110.48
24	T	101	BCR	C39-C30-C25	2.40	114.20	110.30
24	a	406	BCR	C15-C16-C17	-2.40	118.55	123.47
22	b	608	CLA	CED-O2D-CGD	2.40	121.37	115.94
22	b	607	CLA	CHC-C1C-NC	2.40	127.84	124.20
22	A	403	CLA	C4A-NA-C1A	2.40	107.78	106.71
24	B	620	BCR	C28-C27-C26	-2.40	109.80	114.08
28	C	519	LMG	O2-C2-C1	-2.40	104.22	110.05
29	f	101	SQD	O5-C5-C4	2.40	114.05	109.69
30	H	102	DGD	O6D-C1D-O3G	-2.40	104.30	109.97
24	b	616	BCR	C15-C16-C17	-2.40	118.57	123.47
22	b	602	CLA	O1D-CGD-CBD	2.40	129.39	124.48
28	b	623	LMG	O5-C6-C5	-2.40	103.07	111.29
24	B	618	BCR	C27-C26-C25	2.39	126.21	122.73
22	C	504	CLA	C1-O2A-CGA	2.39	122.73	116.44
22	c	513	CLA	CMB-C2B-C3B	2.39	129.16	124.68
23	d	401	PHO	O2D-CGD-O1D	-2.39	119.16	123.84
22	B	603	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
22	c	508	CLA	CHD-C1D-ND	-2.39	122.26	124.45
22	A	405	CLA	C2C-C1C-NC	2.39	112.21	109.97
35	F	101	HEC	CMC-C2C-C3C	-2.39	123.01	125.82
22	b	607	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
34	D	408	LHG	C29-C28-C27	-2.39	102.30	114.42
22	a	405	CLA	O2D-CGD-CBD	2.39	115.51	111.27
22	A	402	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
24	H	101	BCR	C38-C26-C25	-2.39	121.85	124.53
22	c	514	CLA	O1D-CGD-CBD	2.39	129.37	124.48
30	C	516	DGD	C7B-C6B-C5B	-2.38	102.32	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	614	CLA	CHD-C1D-ND	-2.38	122.27	124.45
22	B	616	CLA	C6-C7-C8	-2.38	108.22	115.92
34	e	102	LHG	C11-C10-C9	-2.38	102.33	114.42
24	K	101	BCR	C3-C4-C5	-2.38	109.83	114.08
22	b	611	CLA	CMC-C2C-C1C	-2.38	121.42	125.04
22	b	603	CLA	C6-C7-C8	-2.38	108.23	115.92
24	Z	101	BCR	C35-C13-C14	-2.38	119.59	122.92
30	H	102	DGD	O3E-C3E-C2E	-2.37	104.86	110.35
22	C	514	CLA	CHD-C1D-ND	-2.37	122.27	124.45
24	b	616	BCR	C24-C23-C22	-2.37	122.65	126.23
28	d	409	LMG	O3-C3-C2	-2.37	104.87	110.35
22	c	503	CLA	CBC-CAC-C3C	-2.37	105.90	112.43
27	A	410	PL9	C15-C14-C16	-2.37	111.29	115.27
30	c	519	DGD	O2D-C2D-C1D	-2.37	104.30	110.05
22	A	411	CLA	CHB-C4A-NA	2.37	127.78	124.51
22	c	511	CLA	CHB-C4A-NA	2.37	127.78	124.51
22	c	512	CLA	CHB-C4A-NA	2.37	127.78	124.51
22	A	411	CLA	C1C-C2C-C3C	-2.37	104.47	106.96
22	c	506	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
22	c	505	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
22	c	511	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
34	D	412	LHG	C20-C19-C18	-2.36	102.42	114.42
23	d	401	PHO	C1-C2-C3	-2.36	121.95	126.04
24	A	406	BCR	C35-C13-C12	2.36	121.80	118.08
27	d	405	PL9	C12-C13-C14	-2.36	121.97	127.66
22	D	402	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
24	b	616	BCR	C38-C26-C25	-2.36	121.88	124.53
22	b	605	CLA	C2C-C1C-NC	2.36	112.18	109.97
34	e	102	LHG	C15-C14-C13	-2.36	102.46	114.42
22	h	101	CLA	CMB-C2B-C3B	2.36	129.09	124.68
22	c	511	CLA	O1D-CGD-CBD	2.36	129.31	124.48
29	A	414	SQD	O48-C23-O10	-2.36	117.64	123.59
22	b	605	CLA	CHB-C4A-NA	2.36	127.77	124.51
22	D	403	CLA	O2A-C1-C2	-2.36	102.44	108.64
30	c	520	DGD	O3D-C3D-C4D	-2.35	104.91	110.35
22	d	402	CLA	CMA-C3A-C4A	-2.35	105.45	111.77
22	A	411	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
27	d	405	PL9	C31-C32-C33	-2.35	104.17	111.88
24	d	404	BCR	C2-C1-C6	2.35	114.09	110.48
27	D	405	PL9	C36-C34-C33	-2.35	116.37	121.12
22	B	604	CLA	CAC-C3C-C4C	2.34	127.85	124.81
22	a	402	CLA	C3A-C2A-C1A	2.34	104.85	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	d	403	CLA	CHD-C4C-C3C	2.34	128.28	124.84
22	b	609	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
28	A	412	LMG	C1-C2-C3	-2.34	105.12	110.00
24	a	406	BCR	C2-C1-C6	2.34	114.08	110.48
28	A	412	LMG	C35-C34-C33	-2.34	102.55	114.42
24	x	101	BCR	C36-C18-C17	-2.34	119.65	122.92
22	d	403	CLA	C1-C2-C3	-2.33	122.01	126.04
24	c	517	BCR	C36-C18-C17	-2.33	119.65	122.92
28	D	410	LMG	O8-C28-O10	-2.33	117.71	123.59
28	D	406	LMG	O2-C2-C1	-2.33	104.38	110.05
22	b	608	CLA	C1C-C2C-C3C	-2.33	104.51	106.96
22	B	617	CLA	CAC-C3C-C4C	2.33	127.83	124.81
22	b	603	CLA	C4D-CHA-C1A	2.33	124.08	121.25
34	l	101	LHG	C11-C10-C9	-2.33	102.61	114.42
29	b	619	SQD	O47-C45-C46	2.33	116.83	108.40
22	A	405	CLA	C1D-ND-C4D	-2.33	104.68	106.33
28	b	621	LMG	O1-C7-C8	-2.33	105.29	110.90
28	C	519	LMG	O3-C3-C2	-2.33	104.97	110.35
34	d	407	LHG	O7-C7-C8	-2.32	106.49	111.50
27	a	410	PL9	C42-C43-C44	-2.32	122.06	127.66
22	c	505	CLA	C11-C12-C13	-2.32	108.41	115.92
22	d	402	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
22	C	504	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
27	d	405	PL9	C20-C19-C21	2.32	119.17	115.27
30	C	517	DGD	CDB-CCB-CBB	-2.32	102.67	114.42
22	c	515	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
28	C	519	LMG	C38-C37-C36	-2.32	102.67	114.42
24	H	101	BCR	C37-C22-C21	-2.32	119.68	122.92
22	c	508	CLA	CHB-C4A-NA	2.31	127.71	124.51
22	h	101	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
22	d	402	CLA	C6-C7-C8	-2.31	108.45	115.92
22	a	403	CLA	CAC-C3C-C4C	2.31	127.81	124.81
22	C	509	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
30	c	520	DGD	O6D-C1D-O3G	-2.31	104.51	109.97
22	C	503	CLA	C4D-C3D-CAD	-2.31	105.38	108.10
22	b	611	CLA	O2A-C1-C2	-2.31	102.57	108.64
27	A	410	PL9	C20-C19-C21	2.31	119.15	115.27
35	e	101	HEC	C1D-C2D-C3D	-2.30	105.39	107.00
28	D	411	LMG	O8-C28-O10	-2.30	117.56	123.30
24	b	618	BCR	C31-C1-C6	2.30	114.03	110.30
22	B	606	CLA	CHD-C4C-NC	2.30	127.83	124.20
22	b	612	CLA	CHA-C1A-NA	-2.30	121.13	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	M	101	LMG	C4-C3-C2	-2.30	106.81	110.82
24	d	404	BCR	C38-C26-C25	-2.30	121.95	124.53
22	B	617	CLA	CHD-C1D-C2D	2.30	130.30	125.48
22	C	505	CLA	C6-C5-C3	2.30	119.48	113.45
22	b	610	CLA	CHA-C1A-NA	-2.30	121.14	126.40
22	b	612	CLA	O1D-CGD-CBD	2.29	129.17	124.48
24	K	101	BCR	C7-C8-C9	-2.29	122.77	126.23
22	C	513	CLA	CAA-CBA-CGA	-2.29	106.56	113.25
22	C	512	CLA	C1D-ND-C4D	2.29	107.96	106.33
34	d	406	LHG	C27-C26-C25	-2.29	102.80	114.42
29	D	407	SQD	O5-C5-C4	2.29	113.85	109.69
22	c	503	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
29	b	619	SQD	O48-C23-O10	-2.29	117.82	123.59
22	C	509	CLA	O1D-CGD-CBD	2.29	129.16	124.48
22	B	603	CLA	C1-C2-C3	-2.29	122.09	126.04
34	d	407	LHG	C18-C17-C16	-2.29	102.82	114.42
28	M	101	LMG	C1-O6-C5	-2.28	109.20	113.69
28	D	406	LMG	O1-C1-C2	-2.28	104.74	108.30
22	b	601	CLA	CHC-C1C-NC	2.28	127.67	124.20
24	B	620	BCR	C30-C25-C26	-2.28	119.40	122.61
22	c	503	CLA	CHD-C1D-ND	-2.28	122.36	124.45
30	C	516	DGD	C9B-C8B-C7B	-2.28	102.84	114.42
28	b	621	LMG	C9-C8-C7	-2.28	106.39	111.79
27	d	405	PL9	C42-C43-C44	-2.28	122.18	127.66
22	c	505	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
22	c	504	CLA	C1-C2-C3	-2.27	122.11	126.04
34	D	412	LHG	C11-C10-C9	-2.27	102.88	114.42
22	C	514	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
34	d	407	LHG	C11-C10-C9	-2.27	102.89	114.42
22	C	503	CLA	CHD-C4C-NC	2.27	127.78	124.20
30	C	516	DGD	C6B-C5B-C4B	-2.27	102.89	114.42
28	c	524	LMG	C3-C4-C5	-2.27	106.19	110.24
22	B	606	CLA	C3D-C4D-ND	2.27	113.91	110.24
30	c	519	DGD	O3E-C3E-C2E	-2.27	105.11	110.35
30	c	521	DGD	CAB-C9B-C8B	-2.27	102.92	114.42
22	b	610	CLA	C4A-NA-C1A	2.27	107.72	106.71
24	Y	101	BCR	C38-C26-C27	-2.27	109.26	113.62
24	t	101	BCR	C29-C30-C25	2.26	113.97	110.48
30	C	516	DGD	CCB-CBB-CAB	-2.26	102.94	114.42
22	B	603	CLA	CHD-C1D-ND	-2.26	122.38	124.45
22	B	612	CLA	CHD-C1D-ND	-2.26	122.38	124.45
24	b	618	BCR	C36-C18-C17	-2.26	119.76	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	F	101	HEC	O2D-CGD-CBD	2.26	121.28	114.03
30	C	516	DGD	O3E-C3E-C2E	-2.26	105.13	110.35
22	b	611	CLA	CMD-C2D-C3D	2.26	132.81	127.61
30	C	518	DGD	CDB-CCB-CBB	-2.26	102.97	114.42
22	C	504	CLA	C6-C7-C8	-2.25	108.63	115.92
22	C	514	CLA	O1D-CGD-CBD	2.25	129.10	124.48
22	a	402	CLA	C2D-C1D-ND	-2.25	108.44	110.10
33	J	101	STE	C4-C3-C2	-2.25	105.09	113.19
22	c	507	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
22	c	509	CLA	C1C-C2C-C3C	-2.25	104.59	106.96
22	a	402	CLA	CGD-CBD-CAD	-2.25	103.44	110.73
24	a	406	BCR	C11-C10-C9	-2.25	124.10	127.31
22	B	610	CLA	CHA-C1A-NA	-2.25	121.24	126.40
24	B	620	BCR	C1-C6-C5	-2.25	119.44	122.61
30	c	521	DGD	C1D-C2D-C3D	-2.25	105.31	110.00
22	B	616	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
22	B	615	CLA	C4D-C3D-CAD	-2.25	105.44	108.10
29	f	101	SQD	O9-S-C6	2.25	109.61	106.94
24	B	619	BCR	C2-C1-C6	2.25	113.94	110.48
22	c	514	CLA	O2A-C1-C2	-2.25	102.73	108.64
28	b	623	LMG	C40-C39-C38	-2.25	103.03	114.42
24	c	516	BCR	C12-C13-C14	-2.25	115.50	118.94
22	b	607	CLA	O2D-CGD-CBD	2.24	115.26	111.27
28	c	525	LMG	C38-C37-C36	-2.24	103.03	114.42
29	A	413	SQD	O5-C1-O6	2.24	115.29	109.97
30	c	519	DGD	C3D-C4D-C5D	-2.24	106.23	110.24
22	a	411	CLA	O2D-CGD-CBD	2.24	115.26	111.27
22	d	403	CLA	C2D-C1D-ND	-2.24	108.45	110.10
28	b	621	LMG	O2-C2-C1	-2.24	104.60	110.05
22	B	607	CLA	CMB-C2B-C3B	2.24	128.87	124.68
24	K	101	BCR	C29-C30-C25	2.24	113.93	110.48
30	c	521	DGD	O3E-C3E-C2E	-2.24	105.17	110.35
24	Z	101	BCR	C36-C18-C17	-2.24	119.79	122.92
30	C	517	DGD	O3D-C3D-C4D	-2.24	105.18	110.35
24	b	617	BCR	C8-C7-C6	-2.23	120.92	127.20
28	C	519	LMG	C40-C39-C38	-2.23	103.09	114.42
22	B	611	CLA	C3A-C2A-C1A	2.23	104.68	101.34
30	A	415	DGD	CDB-CCB-CBB	-2.23	103.09	114.42
22	B	614	CLA	O2D-CGD-CBD	-2.23	107.30	111.27
29	a	412	SQD	O47-C7-C8	2.23	116.31	111.50
22	c	513	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
24	x	101	BCR	C8-C9-C10	2.23	122.36	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	603	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
27	D	405	PL9	C8-C7-C3	2.23	118.28	111.98
22	B	603	CLA	C2D-C1D-ND	-2.23	108.46	110.10
30	H	102	DGD	CCB-CBB-CAB	-2.23	103.12	114.42
28	b	621	LMG	O8-C28-O10	-2.23	117.97	123.59
30	h	102	DGD	C7B-C6B-C5B	-2.23	103.12	114.42
24	y	101	BCR	C27-C26-C25	2.23	125.96	122.73
24	B	619	BCR	C15-C16-C17	-2.22	118.92	123.47
22	a	402	CLA	CHB-C4A-NA	2.22	127.59	124.51
24	K	101	BCR	C15-C16-C17	-2.22	118.92	123.47
34	l	101	LHG	O8-C23-C24	2.22	118.89	111.91
22	B	604	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
28	D	406	LMG	O8-C28-O10	-2.22	117.98	123.59
29	f	101	SQD	C46-C45-C44	-2.22	106.54	111.79
30	C	518	DGD	O3D-C3D-C4D	-2.22	105.22	110.35
27	A	410	PL9	C12-C13-C14	-2.22	122.31	127.66
22	c	508	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
22	A	405	CLA	CHA-C1A-NA	-2.22	121.32	126.40
22	b	610	CLA	C11-C10-C8	-2.22	108.75	115.92
22	B	612	CLA	CMB-C2B-C3B	2.22	128.83	124.68
24	b	618	BCR	C33-C5-C6	-2.22	122.04	124.53
28	M	101	LMG	O6-C1-O1	-2.22	104.72	109.97
22	c	503	CLA	C1C-C2C-C3C	-2.22	104.63	106.96
35	v	201	HEC	CMB-C2B-C3B	2.22	128.43	125.82
34	l	101	LHG	O8-C23-O10	-2.22	118.00	123.59
22	B	607	CLA	C2A-C1A-CHA	2.21	127.73	123.86
22	B	610	CLA	C2A-C3A-C4A	2.21	105.44	101.87
24	B	618	BCR	C11-C10-C9	-2.21	124.15	127.31
22	a	411	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
22	b	602	CLA	CMA-C3A-C4A	2.21	117.72	111.77
22	a	402	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
22	C	509	CLA	O2D-CGD-CBD	2.21	115.19	111.27
29	D	407	SQD	O2-C2-C1	2.21	115.41	110.05
22	c	510	CLA	C7-C6-C5	-2.21	107.36	113.36
22	b	609	CLA	C2A-C1A-CHA	2.21	127.72	123.86
22	B	612	CLA	CHD-C4C-C3C	-2.21	121.60	124.84
24	c	516	BCR	C28-C27-C26	-2.20	110.14	114.08
28	b	621	LMG	C36-C35-C34	-2.20	103.24	114.42
30	C	516	DGD	CBB-CAB-C9B	-2.20	103.25	114.42
22	B	614	CLA	CMA-C3A-C4A	-2.20	105.86	111.77
29	D	407	SQD	O48-C23-O10	-2.20	118.04	123.59
22	B	610	CLA	CHB-C4A-NA	2.20	127.55	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	411	CLA	C2A-C1A-CHA	2.20	127.70	123.86
22	c	504	CLA	O2D-CGD-CBD	2.20	115.17	111.27
22	b	605	CLA	CHA-C1A-NA	-2.20	121.36	126.40
22	B	605	CLA	C1-O2A-CGA	-2.19	110.69	116.44
22	B	614	CLA	C2A-C1A-CHA	2.19	127.70	123.86
28	c	522	LMG	C40-C39-C38	-2.19	103.28	114.42
33	B	621	STE	C6-C5-C4	-2.19	103.28	114.42
30	C	516	DGD	C6D-O5D-C1E	2.19	118.02	113.74
22	b	602	CLA	CHA-C4D-ND	2.19	137.08	132.50
34	E	101	LHG	C20-C19-C18	-2.19	103.31	114.42
24	c	516	BCR	C7-C8-C9	-2.19	122.93	126.23
28	c	524	LMG	O6-C1-O1	-2.19	104.79	109.97
28	M	101	LMG	C22-C21-C20	-2.19	103.31	114.42
22	d	402	CLA	C6-C5-C3	2.19	119.19	113.45
30	A	415	DGD	O6D-C1D-O3G	-2.19	104.80	109.97
35	e	101	HEC	O1A-CGA-CBA	-2.19	116.06	123.08
24	x	101	BCR	C35-C13-C14	-2.18	119.86	122.92
28	c	524	LMG	O1-C1-C2	-2.18	104.90	108.30
22	C	513	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
22	b	603	CLA	CHD-C4C-NC	2.18	127.64	124.20
29	B	623	SQD	C1-C2-C3	-2.18	105.46	110.00
22	c	505	CLA	CMA-C3A-C4A	2.18	117.63	111.77
27	a	410	PL9	C11-C12-C13	-2.18	104.72	111.88
30	c	520	DGD	C1D-O6D-C5D	-2.18	109.41	113.69
23	D	401	PHO	OBD-CAD-CBD	-2.18	122.63	125.82
22	b	606	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
24	B	618	BCR	C8-C7-C6	-2.18	121.09	127.20
24	B	618	BCR	C33-C5-C6	-2.18	122.08	124.53
22	c	513	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
27	d	405	PL9	C35-C34-C36	2.17	118.93	115.27
22	b	611	CLA	CMD-C2D-C1D	-2.17	120.88	124.71
28	D	411	LMG	O7-C10-O9	-2.17	117.88	123.30
27	d	405	PL9	C7-C8-C9	-2.17	123.17	126.79
22	b	613	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
28	d	409	LMG	C38-C37-C36	-2.17	103.39	114.42
28	c	522	LMG	O2-C2-C1	-2.17	104.77	110.05
22	A	403	CLA	O1D-CGD-CBD	2.17	128.93	124.48
22	B	615	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
34	E	101	LHG	C11-C10-C9	-2.17	103.40	114.42
22	d	403	CLA	CHA-C1A-NA	-2.17	121.43	126.40
30	h	102	DGD	C1E-O6E-C5E	2.17	117.95	113.69
22	c	506	CLA	CHD-C1D-ND	-2.17	122.46	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	H	101	BCR	C16-C17-C18	-2.17	124.22	127.31
22	C	505	CLA	O1A-CGA-CBA	2.17	132.19	123.73
22	b	614	CLA	C16-C15-C13	-2.17	108.91	115.92
28	M	101	LMG	C37-C36-C35	-2.17	103.42	114.42
22	b	603	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
22	b	607	CLA	C2D-C1D-ND	-2.17	108.51	110.10
27	d	405	PL9	C46-C47-C48	-2.16	104.77	111.88
30	A	415	DGD	O6E-C5E-C4E	2.16	113.62	109.69
22	B	607	CLA	CHA-C1A-NA	-2.16	121.44	126.40
24	c	518	BCR	C15-C16-C17	-2.16	119.04	123.47
22	b	608	CLA	CHD-C4C-NC	2.16	127.61	124.20
28	A	412	LMG	O1-C7-C8	-2.16	105.69	110.90
28	M	101	LMG	O3-C3-C2	-2.16	105.35	110.35
34	D	408	LHG	C27-C26-C25	-2.16	103.46	114.42
22	C	511	CLA	CMB-C2B-C3B	2.16	128.72	124.68
22	C	505	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
22	b	603	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
22	a	402	CLA	CHA-C4D-ND	2.16	137.01	132.50
30	h	102	DGD	C4E-C3E-C2E	-2.16	107.06	110.82
30	C	516	DGD	O2D-C2D-C1D	-2.16	104.80	110.05
22	b	605	CLA	C7-C6-C5	-2.16	107.50	113.36
30	c	521	DGD	O2D-C2D-C1D	-2.16	104.81	110.05
22	C	506	CLA	CGD-CBD-CAD	-2.15	103.75	110.73
24	D	404	BCR	C3-C4-C5	-2.15	110.23	114.08
22	b	604	CLA	CBC-CAC-C3C	-2.15	106.50	112.43
22	C	512	CLA	CHA-C1A-NA	-2.15	121.47	126.40
22	C	508	CLA	O2D-CGD-CBD	2.15	115.09	111.27
22	b	614	CLA	C14-C13-C15	-2.15	103.50	111.29
23	a	404	PHO	C1-C2-C3	-2.15	122.32	126.04
22	B	605	CLA	OBD-CAD-C3D	2.15	133.69	128.52
27	a	410	PL9	C31-C29-C28	2.15	125.47	121.12
22	A	403	CLA	CHD-C1D-ND	-2.15	122.48	124.45
24	C	515	BCR	C15-C14-C13	-2.15	124.25	127.31
24	Y	101	BCR	C16-C15-C14	-2.15	119.08	123.47
27	a	410	PL9	C27-C28-C29	-2.15	122.49	127.66
28	b	623	LMG	C38-C37-C36	-2.14	103.54	114.42
22	c	510	CLA	CHB-C4A-NA	2.14	127.48	124.51
33	B	601	STE	O1-C1-C2	-2.14	116.20	123.08
24	Z	101	BCR	C2-C1-C6	2.14	113.78	110.48
22	C	503	CLA	CMB-C2B-C1B	-2.14	125.17	128.46
22	A	411	CLA	CHA-C1A-NA	-2.14	121.49	126.40
22	A	411	CLA	CMB-C2B-C1B	-2.14	125.17	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	516	BCR	C35-C13-C14	-2.14	119.92	122.92
22	b	608	CLA	CHB-C4A-NA	2.14	127.47	124.51
29	A	413	SQD	O48-C23-O10	-2.14	118.19	123.59
22	b	602	CLA	CHD-C1D-C2D	2.14	129.97	125.48
22	c	509	CLA	CHB-C4A-NA	2.14	127.47	124.51
28	M	101	LMG	C38-C37-C36	-2.14	103.58	114.42
22	a	405	CLA	CMB-C2B-C1B	-2.14	125.18	128.46
22	D	402	CLA	C1D-CHD-C4C	-2.14	121.45	126.06
22	c	508	CLA	CHA-C1A-NA	-2.13	121.51	126.40
22	b	613	CLA	C1-C2-C3	-2.13	122.35	126.04
23	a	404	PHO	C7-C6-C5	-2.13	107.56	113.36
22	b	603	CLA	OBD-CAD-C3D	2.13	133.66	128.52
29	a	412	SQD	C9-C8-C7	-2.13	105.86	113.62
27	A	410	PL9	C32-C33-C34	-2.13	122.52	127.66
24	x	101	BCR	C15-C16-C17	-2.13	119.11	123.47
22	b	603	CLA	CHA-C1A-NA	-2.13	121.52	126.40
22	C	510	CLA	CHA-C1A-NA	-2.13	121.52	126.40
22	B	610	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
24	C	515	BCR	C32-C1-C6	-2.13	106.85	110.30
28	M	101	LMG	C40-C39-C38	-2.13	103.63	114.42
28	M	101	LMG	O8-C28-O10	-2.13	118.23	123.59
22	b	615	CLA	CED-O2D-CGD	-2.13	111.13	115.94
22	C	508	CLA	C2C-C1C-NC	2.13	111.96	109.97
22	B	615	CLA	C1B-CHB-C4A	-2.12	125.91	130.12
29	D	407	SQD	O9-S-O7	-2.12	106.60	113.95
24	b	617	BCR	C15-C16-C17	-2.12	119.12	123.47
22	A	402	CLA	CAA-CBA-CGA	-2.12	107.05	113.25
22	b	609	CLA	CAA-CBA-CGA	-2.12	107.06	113.25
30	c	520	DGD	C4E-C3E-C2E	-2.12	107.12	110.82
22	C	503	CLA	CHD-C1D-C2D	2.12	129.93	125.48
24	c	516	BCR	C27-C26-C25	2.12	125.81	122.73
22	C	506	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
22	B	604	CLA	CHD-C1D-ND	-2.12	122.51	124.45
27	D	405	PL9	C20-C19-C21	2.12	118.83	115.27
24	D	404	BCR	C30-C25-C26	-2.12	119.63	122.61
29	a	412	SQD	O8-S-C6	2.12	109.11	105.74
22	A	405	CLA	C1B-CHB-C4A	-2.12	125.93	130.12
22	d	402	CLA	O1D-CGD-CBD	2.12	128.81	124.48
22	B	606	CLA	CHD-C1D-C2D	2.11	129.91	125.48
22	c	504	CLA	C4D-CHA-C1A	2.11	123.82	121.25
23	D	401	PHO	O2A-CGA-O1A	-2.11	118.27	123.59
22	c	512	CLA	O1D-CGD-CBD	2.11	128.79	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	617	BCR	C39-C30-C25	2.11	113.72	110.30
30	c	519	DGD	C4E-C3E-C2E	-2.11	107.15	110.82
30	C	516	DGD	C4E-C3E-C2E	-2.10	107.15	110.82
22	c	503	CLA	C2D-C1D-ND	-2.10	108.55	110.10
29	a	412	SQD	C45-O47-C7	2.10	122.97	117.79
22	B	606	CLA	O1D-CGD-CBD	2.10	128.79	124.48
22	a	405	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
30	A	415	DGD	O4D-C4D-C3D	2.10	115.21	110.35
30	c	520	DGD	C3E-C4E-C5E	-2.10	106.49	110.24
22	b	614	CLA	O2D-CGD-CBD	2.10	115.00	111.27
22	b	614	CLA	CHD-C4C-C3C	-2.10	121.75	124.84
22	B	610	CLA	CMC-C2C-C1C	2.10	128.24	125.04
23	A	404	PHO	CMC-C2C-C3C	2.10	128.90	124.94
22	b	605	CLA	CHA-C4D-ND	2.10	136.89	132.50
30	c	521	DGD	CDB-CCB-CBB	-2.10	103.78	114.42
30	C	517	DGD	C7B-C6B-C5B	-2.10	103.78	114.42
33	d	412	STE	O2-C1-C2	2.10	120.77	114.03
24	B	618	BCR	C3-C4-C5	-2.10	110.33	114.08
34	d	408	LHG	C26-C25-C24	2.10	120.72	113.19
30	h	102	DGD	O6D-C1D-O3G	-2.10	105.01	109.97
22	B	607	CLA	C1B-CHB-C4A	-2.10	125.97	130.12
22	b	605	CLA	CHC-C1C-C2C	-2.09	120.93	126.72
33	d	410	STE	C3-C2-C1	-2.09	109.19	114.47
24	B	620	BCR	C2-C3-C4	-2.09	106.70	111.38
24	c	518	BCR	C38-C26-C25	-2.09	122.18	124.53
22	C	509	CLA	C5-C3-C2	-2.09	116.89	121.12
22	b	614	CLA	CHD-C4C-NC	2.09	127.50	124.20
22	c	506	CLA	C4A-NA-C1A	2.09	107.64	106.71
22	c	507	CLA	C4C-C3C-C2C	-2.09	103.85	106.90
22	B	614	CLA	CED-O2D-CGD	2.09	120.66	115.94
30	H	102	DGD	C4D-C3D-C2D	-2.09	107.18	110.82
24	K	101	BCR	C38-C26-C25	-2.09	122.19	124.53
22	b	605	CLA	C3C-C4C-NC	-2.08	108.23	110.57
22	D	403	CLA	CHA-C1A-NA	-2.08	121.63	126.40
28	d	409	LMG	C3-C4-C5	-2.08	106.53	110.24
24	B	619	BCR	C40-C30-C29	-2.08	100.58	108.91
22	b	607	CLA	C3B-C4B-NB	-2.08	106.52	109.21
22	C	514	CLA	CHB-C4A-NA	2.08	127.39	124.51
22	a	402	CLA	O1D-CGD-CBD	2.08	128.74	124.48
22	B	608	CLA	C6-C5-C3	-2.08	108.00	113.45
28	D	406	LMG	C38-C37-C36	-2.08	103.87	114.42
22	b	609	CLA	CHA-C1A-NA	-2.08	121.64	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	612	CLA	C7-C6-C5	-2.08	107.72	113.36
24	d	404	BCR	C27-C26-C25	2.08	125.75	122.73
23	A	404	PHO	O2D-CGD-O1D	-2.08	119.78	123.84
28	b	623	LMG	O7-C10-O9	-2.08	118.68	123.70
30	H	102	DGD	CAB-C9B-C8B	-2.08	103.89	114.42
22	c	510	CLA	CHD-C4C-NC	2.08	127.47	124.20
33	M	102	STE	C3-C2-C1	-2.07	109.24	114.47
22	c	504	CLA	C2D-C1D-ND	-2.07	108.58	110.10
22	B	615	CLA	O1D-CGD-CBD	2.07	128.73	124.48
22	B	605	CLA	C1B-CHB-C4A	-2.07	126.01	130.12
22	b	610	CLA	C2D-C1D-ND	-2.07	108.58	110.10
28	c	522	LMG	C1-O6-C5	-2.07	109.62	113.69
23	A	404	PHO	O2A-C1-C2	2.07	114.08	108.64
22	b	607	CLA	C11-C10-C8	-2.07	109.22	115.92
22	b	612	CLA	C16-C15-C13	-2.07	109.22	115.92
22	B	614	CLA	CAC-C3C-C4C	2.07	127.50	124.81
27	D	405	PL9	C11-C12-C13	-2.07	105.08	111.88
24	b	616	BCR	C27-C26-C25	2.07	125.74	122.73
22	C	511	CLA	CHA-C1A-NA	-2.07	121.66	126.40
30	h	102	DGD	O6E-C1E-O5D	-2.07	105.07	109.97
24	A	406	BCR	C37-C22-C21	-2.07	120.02	122.92
22	c	511	CLA	C3A-C2A-C1A	2.07	104.44	101.34
30	C	516	DGD	O6E-C5E-C4E	2.07	113.45	109.69
24	H	101	BCR	C35-C13-C12	2.07	121.33	118.08
24	C	515	BCR	C10-C11-C12	-2.07	116.77	123.22
22	B	610	CLA	CHD-C4C-NC	2.07	127.46	124.20
24	H	101	BCR	C36-C18-C17	-2.06	120.03	122.92
24	Y	101	BCR	C15-C16-C17	-2.06	119.25	123.47
30	C	516	DGD	C5B-C4B-C3B	-2.06	103.95	114.42
22	c	510	CLA	CAC-C3C-C4C	-2.06	122.14	124.81
22	c	510	CLA	O2D-CGD-CBD	2.06	114.93	111.27
22	b	605	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
24	A	406	BCR	C33-C5-C6	-2.06	122.22	124.53
22	B	612	CLA	C17-C16-C15	-2.06	103.78	113.24
22	C	509	CLA	C3A-C2A-C1A	2.06	104.42	101.34
22	b	606	CLA	CHB-C4A-NA	2.06	127.36	124.51
33	X	101	STE	C10-C9-C8	-2.06	103.99	114.42
22	B	612	CLA	CHB-C4A-NA	2.06	127.35	124.51
22	b	604	CLA	C4-C3-C2	-2.06	118.41	123.68
30	C	517	DGD	O3G-C1D-C2D	-2.05	105.10	108.30
22	B	604	CLA	CHD-C1D-C2D	2.05	129.79	125.48
22	B	602	CLA	C1B-CHB-C4A	-2.05	126.05	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	515	BCR	C27-C26-C25	2.05	125.71	122.73
22	A	411	CLA	CMB-C2B-C3B	2.05	128.52	124.68
22	c	512	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
22	b	603	CLA	CHB-C4A-NA	2.05	127.35	124.51
22	b	608	CLA	CHD-C1D-C2D	2.05	129.78	125.48
28	c	522	LMG	C3-C4-C5	-2.05	106.58	110.24
24	Y	101	BCR	C8-C7-C6	-2.05	121.45	127.20
22	C	513	CLA	CMA-C3A-C2A	-2.05	105.57	113.83
22	B	604	CLA	O1A-CGA-CBA	2.05	131.72	123.73
22	d	402	CLA	C1-C2-C3	-2.05	122.50	126.04
30	c	519	DGD	CBB-CAB-C9B	-2.05	104.04	114.42
33	a	415	STE	O2-C1-C2	2.04	120.60	114.03
22	C	507	CLA	O1D-CGD-CBD	2.04	128.66	124.48
29	f	101	SQD	O5-C1-C2	-2.04	106.03	110.35
33	d	412	STE	O2-C1-O1	-2.04	118.21	123.30
30	h	102	DGD	C3E-C4E-C5E	-2.04	106.60	110.24
24	b	618	BCR	C16-C15-C14	-2.04	119.29	123.47
22	b	601	CLA	CHD-C1D-ND	-2.04	122.58	124.45
22	B	611	CLA	C4D-CHA-C1A	2.04	123.73	121.25
24	B	620	BCR	C38-C26-C25	-2.04	122.24	124.53
22	b	613	CLA	CHD-C1D-C2D	2.04	129.75	125.48
30	A	415	DGD	O5E-C6E-C5E	-2.04	104.30	111.29
27	d	405	PL9	C47-C48-C49	-2.04	120.79	127.75
22	B	611	CLA	O1A-CGA-CBA	2.04	131.67	123.73
30	C	516	DGD	C4A-C3A-C2A	-2.04	105.87	113.19
22	a	402	CLA	CAC-C3C-C2C	-2.04	124.05	127.53
22	c	506	CLA	O1A-CGA-CBA	2.03	131.67	123.73
30	A	415	DGD	O3G-C3G-C2G	-2.03	105.99	110.90
22	b	613	CLA	CMD-C2D-C1D	2.03	128.29	124.71
22	b	608	CLA	O1D-CGD-CBD	2.03	128.64	124.48
30	H	102	DGD	C1D-O6D-C5D	-2.03	109.70	113.69
30	c	521	DGD	C6B-C5B-C4B	-2.03	104.12	114.42
23	D	401	PHO	CBA-CAA-C2A	-2.03	107.88	113.81
22	b	610	CLA	CHD-C1D-C2D	2.03	129.74	125.48
28	D	411	LMG	C36-C35-C34	-2.03	104.12	114.42
22	b	606	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
30	c	519	DGD	C3G-C2G-C1G	-2.03	106.99	111.79
30	C	518	DGD	C6B-C5B-C4B	-2.03	104.13	114.42
28	A	412	LMG	C3-C4-C5	-2.03	106.62	110.24
22	C	508	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
22	B	603	CLA	C4A-NA-C1A	2.03	107.62	106.71
28	M	101	LMG	C33-C32-C31	-2.03	104.14	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	507	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
29	a	413	SQD	C46-O48-C23	2.03	124.62	117.12
22	B	617	CLA	CAA-CBA-CGA	-2.02	107.34	113.25
22	B	617	CLA	C4-C3-C2	-2.02	118.49	123.68
34	d	406	LHG	C20-C19-C18	-2.02	104.16	114.42
22	A	403	CLA	O1A-CGA-CBA	2.02	131.62	123.73
22	b	611	CLA	CMC-C2C-C3C	2.02	131.61	126.12
34	D	412	LHG	C27-C26-C25	-2.02	104.17	114.42
22	b	607	CLA	CHD-C1D-C2D	2.02	129.71	125.48
35	v	201	HEC	CMA-C3A-C2A	2.02	128.75	124.94
24	B	619	BCR	C27-C26-C25	2.02	125.66	122.73
30	h	102	DGD	O5D-C6D-C5D	-2.02	105.31	109.05
22	b	608	CLA	C3C-C4C-NC	-2.02	108.31	110.57
22	A	402	CLA	CED-O2D-CGD	2.02	120.50	115.94
22	B	610	CLA	C1B-CHB-C4A	-2.02	126.12	130.12
24	b	617	BCR	C38-C26-C27	-2.02	109.74	113.62
24	K	101	BCR	C37-C22-C21	-2.02	120.10	122.92
29	f	101	SQD	C45-O47-C7	2.02	122.75	117.79
34	D	412	LHG	C18-C17-C16	-2.02	104.19	114.42
30	C	517	DGD	CBB-CAB-C9B	-2.01	104.20	114.42
24	c	516	BCR	C20-C21-C22	-2.01	124.44	127.31
22	C	513	CLA	C11-C12-C13	-2.01	109.41	115.92
35	V	201	HEC	O1A-CGA-CBA	-2.01	116.61	123.08
30	h	102	DGD	C1D-O6D-C5D	-2.01	109.74	113.69
22	A	405	CLA	CHB-C4A-NA	2.01	127.30	124.51
24	c	516	BCR	C15-C16-C17	-2.01	119.35	123.47
22	b	612	CLA	C2C-C1C-NC	2.01	111.86	109.97
22	b	604	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
34	E	101	LHG	O8-C23-O10	-2.01	118.52	123.59
30	A	415	DGD	CBB-CAB-C9B	-2.01	104.24	114.42
30	h	102	DGD	C4B-C3B-C2B	-2.01	105.98	113.19
29	A	413	SQD	O8-S-O9	2.01	116.18	111.27
27	a	410	PL9	C21-C19-C18	-2.01	117.06	121.12
24	a	406	BCR	C37-C22-C21	-2.00	120.11	122.92
30	A	415	DGD	CAB-C9B-C8B	-2.00	104.25	114.42
27	D	405	PL9	C35-C34-C36	2.00	118.64	115.27
30	H	102	DGD	CBB-CAB-C9B	-2.00	104.25	114.42
22	c	514	CLA	CMB-C2B-C1B	-2.00	125.39	128.46
22	b	605	CLA	C1B-CHB-C4A	-2.00	126.15	130.12
30	C	518	DGD	C5B-C4B-C3B	-2.00	104.26	114.42
24	x	101	BCR	C35-C13-C12	2.00	121.23	118.08
23	d	401	PHO	CMA-C3A-C2A	-2.00	105.93	113.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	609	CLA	C2D-C1D-ND	-2.00	108.63	110.10
24	Z	101	BCR	C7-C8-C9	-2.00	123.21	126.23
27	D	405	PL9	C11-C9-C8	-2.00	117.07	121.12

All (55) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	402	CLA	ND
22	A	403	CLA	ND
22	A	405	CLA	ND
22	B	602	CLA	ND
22	B	604	CLA	ND
22	B	605	CLA	ND
22	B	606	CLA	ND
22	B	607	CLA	ND
22	B	608	CLA	ND
22	B	611	CLA	ND
22	B	612	CLA	ND
22	B	613	CLA	ND
22	B	614	CLA	ND
22	B	615	CLA	ND
22	B	616	CLA	ND
22	B	617	CLA	ND
22	C	503	CLA	ND
22	C	505	CLA	ND
22	C	506	CLA	ND
22	C	507	CLA	ND
22	C	508	CLA	ND
22	C	510	CLA	ND
22	C	511	CLA	ND
22	C	512	CLA	ND
22	C	513	CLA	ND
22	D	402	CLA	ND
22	a	402	CLA	ND
22	a	405	CLA	ND
22	a	411	CLA	ND
22	b	601	CLA	ND
22	b	602	CLA	ND
22	b	603	CLA	ND
22	b	604	CLA	ND
22	b	605	CLA	ND
22	b	606	CLA	ND

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Mol	Chain	Res	Type	Atom
22	b	607	CLA	ND
22	b	609	CLA	ND
22	b	611	CLA	ND
22	b	612	CLA	ND
22	b	613	CLA	ND
22	b	614	CLA	ND
22	b	615	CLA	ND
22	c	503	CLA	ND
22	c	506	CLA	ND
22	c	507	CLA	ND
22	c	508	CLA	ND
22	c	509	CLA	ND
22	c	511	CLA	ND
22	c	512	CLA	ND
22	c	513	CLA	ND
22	c	514	CLA	ND
22	c	515	CLA	ND
22	d	402	CLA	ND
22	d	403	CLA	ND
22	h	101	CLA	ND

All (1818) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	411	CLA	CHA-CBD-CGD-O1D
22	A	411	CLA	CHA-CBD-CGD-O2D
22	B	607	CLA	CHA-CBD-CGD-O1D
22	B	607	CLA	C11-C12-C13-C14
22	B	615	CLA	CHA-CBD-CGD-O1D
22	B	615	CLA	CHA-CBD-CGD-O2D
22	B	615	CLA	CAD-CBD-CGD-O1D
22	B	615	CLA	CAD-CBD-CGD-O2D
22	C	505	CLA	C2-C3-C5-C6
22	C	505	CLA	C4-C3-C5-C6
22	C	509	CLA	CHA-CBD-CGD-O1D
22	C	513	CLA	C1A-C2A-CAA-CBA
22	C	514	CLA	O2A-C1-C2-C3
22	a	411	CLA	CHA-CBD-CGD-O1D
22	a	411	CLA	CHA-CBD-CGD-O2D
22	b	601	CLA	CHA-CBD-CGD-O1D
22	b	601	CLA	CHA-CBD-CGD-O2D
22	b	604	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	b	605	CLA	CHA-CBD-CGD-O1D
22	b	605	CLA	CHA-CBD-CGD-O2D
22	b	613	CLA	CHA-CBD-CGD-O1D
22	b	613	CLA	CHA-CBD-CGD-O2D
22	b	613	CLA	CBD-CGD-O2D-CED
22	b	615	CLA	C2-C3-C5-C6
22	b	615	CLA	C4-C3-C5-C6
22	c	509	CLA	C2-C3-C5-C6
22	c	509	CLA	C4-C3-C5-C6
22	c	510	CLA	CHA-CBD-CGD-O1D
22	c	510	CLA	CHA-CBD-CGD-O2D
22	c	512	CLA	C12-C13-C15-C16
22	c	513	CLA	C14-C13-C15-C16
24	A	406	BCR	C20-C21-C22-C37
24	B	619	BCR	C11-C10-C9-C34
24	B	619	BCR	C37-C22-C23-C24
24	C	515	BCR	C36-C18-C19-C20
24	C	515	BCR	C20-C21-C22-C37
24	D	404	BCR	C23-C24-C25-C26
24	D	404	BCR	C23-C24-C25-C30
24	K	101	BCR	C17-C18-C19-C20
24	K	101	BCR	C36-C18-C19-C20
24	K	101	BCR	C37-C22-C23-C24
24	T	101	BCR	C18-C19-C20-C21
24	Y	101	BCR	C1-C6-C7-C8
24	Y	101	BCR	C5-C6-C7-C8
24	Y	101	BCR	C11-C12-C13-C35
24	Y	101	BCR	C21-C22-C23-C24
24	Y	101	BCR	C37-C22-C23-C24
24	Z	101	BCR	C11-C12-C13-C35
24	Z	101	BCR	C35-C13-C14-C15
24	Z	101	BCR	C16-C17-C18-C19
24	Z	101	BCR	C16-C17-C18-C36
24	Z	101	BCR	C17-C18-C19-C20
24	Z	101	BCR	C21-C22-C23-C24
24	Z	101	BCR	C23-C24-C25-C30
24	a	406	BCR	C11-C10-C9-C34
24	a	406	BCR	C35-C13-C14-C15
24	a	406	BCR	C20-C21-C22-C37
24	b	616	BCR	C36-C18-C19-C20
24	b	618	BCR	C37-C22-C23-C24
24	c	516	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
24	c	516	BCR	C7-C8-C9-C34
24	c	516	BCR	C11-C12-C13-C35
24	c	516	BCR	C12-C13-C14-C15
24	c	516	BCR	C35-C13-C14-C15
24	c	516	BCR	C18-C19-C20-C21
24	c	517	BCR	C35-C13-C14-C15
24	c	517	BCR	C18-C19-C20-C21
24	c	517	BCR	C20-C21-C22-C37
24	c	518	BCR	C35-C13-C14-C15
24	c	518	BCR	C36-C18-C19-C20
24	c	518	BCR	C37-C22-C23-C24
24	t	101	BCR	C17-C18-C19-C20
24	t	101	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	C36-C18-C19-C20
27	A	410	PL9	C12-C13-C14-C15
27	A	410	PL9	C12-C13-C14-C16
27	A	410	PL9	C17-C18-C19-C21
27	A	410	PL9	C37-C38-C39-C40
27	A	410	PL9	C37-C38-C39-C41
27	D	405	PL9	C32-C33-C34-C35
27	D	405	PL9	C32-C33-C34-C36
27	a	410	PL9	C17-C18-C19-C21
27	a	410	PL9	C22-C23-C24-C25
27	a	410	PL9	C22-C23-C24-C26
27	a	410	PL9	C42-C43-C44-C45
27	d	405	PL9	C32-C33-C34-C36
27	d	405	PL9	C42-C43-C44-C45
27	d	405	PL9	C42-C43-C44-C46
28	A	412	LMG	O9-C10-O7-C8
28	D	410	LMG	O1-C7-C8-C9
28	D	410	LMG	O1-C7-C8-O7
28	D	410	LMG	C11-C10-O7-C8
28	b	623	LMG	O9-C10-O7-C8
28	b	623	LMG	C11-C10-O7-C8
28	c	524	LMG	C11-C10-O7-C8
28	c	525	LMG	O6-C1-O1-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
29	B	623	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
29	D	407	SQD	O5-C1-O6-C44
29	a	412	SQD	O6-C44-C45-O47
29	a	412	SQD	C5-C6-S-O7
29	a	412	SQD	C5-C6-S-O8
29	a	412	SQD	C5-C6-S-O9
29	a	413	SQD	O6-C44-C45-C46
29	a	413	SQD	O6-C44-C45-O47
29	a	413	SQD	C8-C7-O47-C45
29	f	101	SQD	C2-C1-O6-C44
29	f	101	SQD	O5-C1-O6-C44
30	A	415	DGD	C2B-C1B-O2G-C2G
30	A	415	DGD	O1B-C1B-O2G-C2G
34	B	622	LHG	C3-O3-P-O4
34	B	622	LHG	C4-O6-P-O4
34	B	622	LHG	C4-O6-P-O5
34	D	408	LHG	O1-C1-C2-C3
34	D	408	LHG	C1-C2-C3-O3
34	D	408	LHG	O2-C2-C3-O3
34	D	408	LHG	C3-O3-P-O4
34	D	408	LHG	C4-O6-P-O4
34	D	412	LHG	O1-C1-C2-O2
34	D	412	LHG	O1-C1-C2-C3
34	E	101	LHG	O1-C1-C2-C3
34	E	101	LHG	C4-O6-P-O4
34	d	406	LHG	O1-C1-C2-C3
34	d	406	LHG	C4-O6-P-O5
34	d	407	LHG	O1-C1-C2-C3
34	d	407	LHG	C3-O3-P-O4
34	d	407	LHG	C4-O6-P-O3
34	d	407	LHG	C4-O6-P-O4
34	d	407	LHG	C4-O6-P-O5
34	e	102	LHG	C3-O3-P-O5
34	e	102	LHG	O10-C23-O8-C6
34	e	102	LHG	C24-C23-O8-C6
34	l	101	LHG	C4-O6-P-O3
34	l	101	LHG	C4-O6-P-O4
34	l	101	LHG	C4-O6-P-O5
22	b	613	CLA	O1D-CGD-O2D-CED
28	M	101	LMG	O10-C28-O8-C9
28	c	524	LMG	O10-C28-O8-C9
28	c	525	LMG	O10-C28-O8-C9
34	E	101	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
29	D	407	SQD	C24-C23-O48-C46
34	E	101	LHG	C24-C23-O8-C6
22	B	602	CLA	CBD-CGD-O2D-CED
22	b	615	CLA	CBD-CGD-O2D-CED
22	c	510	CLA	CBD-CGD-O2D-CED
29	D	407	SQD	O10-C23-O48-C46
29	a	413	SQD	O10-C23-O48-C46
29	b	619	SQD	O10-C23-O48-C46
22	B	604	CLA	CBD-CGD-O2D-CED
28	D	410	LMG	O9-C10-O7-C8
28	c	524	LMG	O9-C10-O7-C8
29	a	413	SQD	O49-C7-O47-C45
22	A	405	CLA	C3-C5-C6-C7
22	b	601	CLA	C3-C5-C6-C7
22	b	613	CLA	C3-C5-C6-C7
28	c	524	LMG	C29-C28-O8-C9
28	c	525	LMG	C29-C28-O8-C9
29	a	413	SQD	C24-C23-O48-C46
29	b	619	SQD	C24-C23-O48-C46
29	f	101	SQD	C24-C23-O48-C46
28	A	412	LMG	C11-C10-O7-C8
29	B	623	SQD	O10-C23-O48-C46
30	A	415	DGD	O6E-C5E-C6E-O5E
22	A	405	CLA	C4-C3-C5-C6
22	b	602	CLA	C4-C3-C5-C6
22	c	508	CLA	C4-C3-C5-C6
27	A	410	PL9	C20-C19-C21-C22
27	a	410	PL9	C35-C34-C36-C37
22	A	405	CLA	C2-C3-C5-C6
27	d	405	PL9	C38-C39-C41-C42
22	a	402	CLA	CBD-CGD-O2D-CED
22	b	606	CLA	CBD-CGD-O2D-CED
33	C	522	STE	C4-C5-C6-C7
22	B	602	CLA	CBA-CGA-O2A-C1
28	M	101	LMG	C29-C28-O8-C9
28	b	621	LMG	C29-C28-O8-C9
29	B	623	SQD	C24-C23-O48-C46
27	d	405	PL9	C12-C13-C14-C15
22	c	514	CLA	CBD-CGD-O2D-CED
27	a	410	PL9	C42-C43-C44-C46
29	f	101	SQD	O10-C23-O48-C46
28	c	522	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
22	c	503	CLA	CBD-CGD-O2D-CED
22	c	513	CLA	CBD-CGD-O2D-CED
34	d	406	LHG	O2-C2-C3-O3
34	e	102	LHG	O2-C2-C3-O3
22	B	606	CLA	C3-C5-C6-C7
29	b	619	SQD	C8-C7-O47-C45
30	C	516	DGD	C1B-C2B-C3B-C4B
22	C	513	CLA	CBD-CGD-O2D-CED
22	h	101	CLA	CBD-CGD-O2D-CED
28	d	409	LMG	C10-C11-C12-C13
34	B	622	LHG	C7-C8-C9-C10
33	X	101	STE	C13-C14-C15-C16
22	B	602	CLA	O1A-CGA-O2A-C1
27	D	405	PL9	C47-C48-C49-C51
22	B	615	CLA	C4-C3-C5-C6
22	C	508	CLA	C4-C3-C5-C6
30	A	415	DGD	C4E-C5E-C6E-O5E
30	H	102	DGD	C4E-C5E-C6E-O5E
22	B	615	CLA	C2-C3-C5-C6
22	C	508	CLA	C2-C3-C5-C6
22	b	602	CLA	C2-C3-C5-C6
22	b	604	CLA	C2-C3-C5-C6
29	A	413	SQD	C7-C8-C9-C10
22	B	607	CLA	C2A-CAA-CBA-CGA
27	A	410	PL9	C9-C11-C12-C13
27	A	410	PL9	C39-C41-C42-C43
27	a	410	PL9	C19-C21-C22-C23
27	a	410	PL9	C24-C26-C27-C28
27	a	410	PL9	C34-C36-C37-C38
22	B	605	CLA	C3-C5-C6-C7
22	d	402	CLA	C3-C5-C6-C7
23	d	401	PHO	CBD-CGD-O2D-CED
29	A	413	SQD	C11-C12-C13-C14
27	D	405	PL9	C27-C28-C29-C30
27	a	410	PL9	C7-C8-C9-C10
27	a	410	PL9	C17-C18-C19-C20
34	d	406	LHG	C1-C2-C3-O3
34	e	102	LHG	C1-C2-C3-O3
22	B	617	CLA	C3-C5-C6-C7
22	B	602	CLA	O1D-CGD-O2D-CED
22	b	615	CLA	O1D-CGD-O2D-CED
22	c	510	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	c	508	CLA	CBA-CGA-O2A-C1
22	h	101	CLA	CBA-CGA-O2A-C1
28	B	629	LMG	C29-C28-O8-C9
30	A	415	DGD	C2A-C1A-O1G-C1G
22	C	512	CLA	CBD-CGD-O2D-CED
22	b	606	CLA	C10-C11-C12-C13
22	B	603	CLA	C13-C15-C16-C17
22	B	612	CLA	C8-C10-C11-C12
22	B	616	CLA	C5-C6-C7-C8
22	C	507	CLA	C5-C6-C7-C8
22	D	402	CLA	C15-C16-C17-C18
22	b	612	CLA	C15-C16-C17-C18
22	c	511	CLA	C3-C5-C6-C7
33	b	622	STE	C1-C2-C3-C4
29	B	623	SQD	C2-C1-O6-C44
28	c	524	LMG	C4-C5-C6-O5
22	b	613	CLA	C2-C3-C5-C6
27	a	410	PL9	C33-C34-C36-C37
22	A	403	CLA	C14-C13-C15-C16
22	B	602	CLA	C11-C12-C13-C14
22	B	617	CLA	C11-C10-C8-C9
22	C	504	CLA	C11-C10-C8-C9
22	C	508	CLA	C11-C10-C8-C9
22	C	510	CLA	C11-C10-C8-C9
22	C	512	CLA	C11-C10-C8-C9
22	C	513	CLA	C11-C10-C8-C9
22	D	402	CLA	C11-C10-C8-C9
22	D	403	CLA	C11-C12-C13-C14
22	b	606	CLA	C11-C10-C8-C9
22	b	610	CLA	C14-C13-C15-C16
22	b	613	CLA	C6-C7-C8-C9
22	b	615	CLA	C6-C7-C8-C9
22	c	511	CLA	C11-C12-C13-C14
22	h	101	CLA	C14-C13-C15-C16
23	A	404	PHO	C14-C13-C15-C16
22	B	608	CLA	C10-C11-C12-C13
22	C	507	CLA	C13-C15-C16-C17
22	b	605	CLA	C2A-CAA-CBA-CGA
24	T	101	BCR	C36-C18-C19-C20
24	d	404	BCR	C37-C22-C23-C24
28	b	623	LMG	O6-C5-C6-O5
28	d	409	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
33	B	621	STE	C1-C2-C3-C4
33	j	101	STE	C1-C2-C3-C4
34	E	101	LHG	C7-C8-C9-C10
22	B	606	CLA	C8-C10-C11-C12
22	c	508	CLA	C15-C16-C17-C18
30	H	102	DGD	O6E-C5E-C6E-O5E
28	c	522	LMG	C11-C10-O7-C8
22	B	614	CLA	C13-C15-C16-C17
22	B	615	CLA	C8-C10-C11-C12
22	C	510	CLA	C10-C11-C12-C13
22	C	514	CLA	C15-C16-C17-C18
22	c	508	CLA	C13-C15-C16-C17
22	c	514	CLA	C5-C6-C7-C8
28	D	406	LMG	C10-C11-C12-C13
28	D	411	LMG	C28-C29-C30-C31
28	M	101	LMG	C28-C29-C30-C31
33	L	101	STE	C1-C2-C3-C4
34	d	406	LHG	C23-C24-C25-C26
22	B	614	CLA	C8-C10-C11-C12
22	C	503	CLA	C15-C16-C17-C18
22	C	508	CLA	C10-C11-C12-C13
22	C	511	CLA	C15-C16-C17-C18
22	a	402	CLA	C15-C16-C17-C18
22	b	603	CLA	C15-C16-C17-C18
22	b	614	CLA	C10-C11-C12-C13
22	c	505	CLA	C8-C10-C11-C12
22	c	511	CLA	C13-C15-C16-C17
27	d	405	PL9	C32-C33-C34-C35
28	C	519	LMG	C28-C29-C30-C31
28	M	101	LMG	C10-C11-C12-C13
28	c	522	LMG	C28-C29-C30-C31
29	B	623	SQD	C23-C24-C25-C26
30	c	521	DGD	C1A-C2A-C3A-C4A
33	b	624	STE	C1-C2-C3-C4
22	B	602	CLA	C5-C6-C7-C8
22	C	504	CLA	C5-C6-C7-C8
22	b	602	CLA	C5-C6-C7-C8
22	b	608	CLA	C15-C16-C17-C18
22	b	610	CLA	C13-C15-C16-C17
22	c	514	CLA	C13-C15-C16-C17
28	D	410	LMG	C10-C11-C12-C13
28	b	623	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
34	D	409	LHG	C7-C8-C9-C10
29	A	413	SQD	C30-C31-C32-C33
22	c	513	CLA	C15-C16-C17-C18
22	B	604	CLA	O1D-CGD-O2D-CED
22	A	411	CLA	C11-C12-C13-C15
22	B	612	CLA	C12-C13-C15-C16
22	a	403	CLA	C6-C7-C8-C10
22	b	605	CLA	C11-C10-C8-C7
22	h	101	CLA	C11-C12-C13-C15
22	c	508	CLA	O1A-CGA-O2A-C1
28	B	629	LMG	O10-C28-O8-C9
28	D	410	LMG	O10-C28-O8-C9
22	c	514	CLA	C2A-CAA-CBA-CGA
22	B	606	CLA	C13-C15-C16-C17
22	B	608	CLA	C5-C6-C7-C8
22	C	505	CLA	C8-C10-C11-C12
22	C	506	CLA	C10-C11-C12-C13
22	c	514	CLA	C8-C10-C11-C12
22	h	101	CLA	O1A-CGA-O2A-C1
28	C	519	LMG	O10-C28-O8-C9
22	A	402	CLA	C15-C16-C17-C18
22	c	513	CLA	C13-C15-C16-C17
27	A	410	PL9	C29-C31-C32-C33
27	A	410	PL9	C34-C36-C37-C38
27	d	405	PL9	C34-C36-C37-C38
24	B	618	BCR	C10-C11-C12-C13
24	B	620	BCR	C10-C11-C12-C13
24	a	406	BCR	C18-C19-C20-C21
24	d	404	BCR	C10-C11-C12-C13
22	B	603	CLA	C8-C10-C11-C12
22	B	613	CLA	C10-C11-C12-C13
22	B	616	CLA	C13-C15-C16-C17
22	b	603	CLA	C10-C11-C12-C13
22	b	614	CLA	C15-C16-C17-C18
29	a	412	SQD	C7-C8-C9-C10
34	l	101	LHG	C7-C8-C9-C10
22	B	608	CLA	C8-C10-C11-C12
22	B	609	CLA	C13-C15-C16-C17
22	C	510	CLA	C13-C15-C16-C17
22	c	505	CLA	C5-C6-C7-C8
22	c	508	CLA	C8-C10-C11-C12
22	h	101	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
30	A	415	DGD	CEB-CFB-CGB-CHB
22	a	402	CLA	O1D-CGD-O2D-CED
30	c	520	DGD	C4E-C5E-C6E-O5E
28	C	519	LMG	C11-C10-O7-C8
22	B	607	CLA	C15-C16-C17-C18
22	C	509	CLA	C15-C16-C17-C18
22	b	610	CLA	C15-C16-C17-C18
22	c	511	CLA	C8-C10-C11-C12
22	c	512	CLA	C8-C10-C11-C12
22	d	403	CLA	C15-C16-C17-C18
34	B	622	LHG	C4-O6-P-O3
34	D	408	LHG	C3-O3-P-O6
34	D	409	LHG	C3-O3-P-O6
34	d	407	LHG	C3-O3-P-O6
22	C	514	CLA	CBA-CGA-O2A-C1
22	c	514	CLA	CBA-CGA-O2A-C1
28	C	519	LMG	C29-C28-O8-C9
22	b	613	CLA	C4-C3-C5-C6
22	b	601	CLA	C16-C17-C18-C20
22	c	507	CLA	C15-C16-C17-C18
24	B	619	BCR	C14-C15-C16-C17
30	c	520	DGD	O6E-C5E-C6E-O5E
28	c	522	LMG	C36-C37-C38-C39
29	a	413	SQD	C10-C11-C12-C13
30	C	518	DGD	C6A-C7A-C8A-C9A
34	D	412	LHG	C29-C30-C31-C32
34	E	101	LHG	C11-C12-C13-C14
28	B	629	LMG	C11-C10-O7-C8
24	A	406	BCR	C35-C13-C14-C15
24	B	618	BCR	C11-C10-C9-C34
24	B	618	BCR	C35-C13-C14-C15
24	B	618	BCR	C16-C17-C18-C36
24	B	619	BCR	C16-C17-C18-C36
24	B	619	BCR	C20-C21-C22-C37
24	B	620	BCR	C11-C10-C9-C34
24	B	620	BCR	C20-C21-C22-C37
24	D	404	BCR	C20-C21-C22-C37
24	Y	101	BCR	C11-C10-C9-C34
24	Y	101	BCR	C16-C17-C18-C36
24	Z	101	BCR	C20-C21-C22-C37
24	b	616	BCR	C16-C17-C18-C36
24	b	616	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
24	b	617	BCR	C16-C17-C18-C36
24	b	617	BCR	C20-C21-C22-C37
24	b	618	BCR	C35-C13-C14-C15
24	c	518	BCR	C20-C21-C22-C37
24	t	101	BCR	C20-C21-C22-C37
24	x	101	BCR	C11-C10-C9-C34
24	x	101	BCR	C20-C21-C22-C37
28	B	629	LMG	C36-C37-C38-C39
28	D	406	LMG	C21-C22-C23-C24
28	D	411	LMG	C30-C31-C32-C33
28	c	524	LMG	C34-C35-C36-C37
29	a	413	SQD	C11-C10-C9-C8
33	B	624	STE	C11-C10-C9-C8
33	B	627	STE	C11-C12-C13-C14
33	E	102	STE	C3-C4-C5-C6
33	b	620	STE	C6-C7-C8-C9
33	b	622	STE	C7-C8-C9-C10
33	b	625	STE	C12-C13-C14-C15
33	d	410	STE	C5-C6-C7-C8
33	h	103	STE	C9-C10-C11-C12
34	B	622	LHG	C31-C32-C33-C34
34	D	408	LHG	C11-C12-C13-C14
34	D	412	LHG	C12-C13-C14-C15
34	d	406	LHG	C32-C33-C34-C35
34	e	102	LHG	C14-C15-C16-C17
34	l	101	LHG	C17-C18-C19-C20
22	c	512	CLA	C16-C17-C18-C20
22	d	402	CLA	C16-C17-C18-C19
28	C	519	LMG	C32-C33-C34-C35
28	D	406	LMG	C35-C36-C37-C38
28	c	525	LMG	C15-C16-C17-C18
29	A	413	SQD	C13-C14-C15-C16
29	D	407	SQD	C31-C32-C33-C34
30	c	519	DGD	C6B-C7B-C8B-C9B
30	h	102	DGD	C2B-C3B-C4B-C5B
33	b	625	STE	C14-C15-C16-C17
33	c	523	STE	C9-C10-C11-C12
34	D	408	LHG	C10-C11-C12-C13
34	D	412	LHG	C9-C10-C11-C12
29	b	619	SQD	C46-C45-O47-C7
22	c	514	CLA	O1D-CGD-O2D-CED
22	B	604	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	b	612	CLA	C13-C15-C16-C17
22	C	502	CLA	CBD-CGD-O2D-CED
28	B	629	LMG	C12-C13-C14-C15
28	b	623	LMG	C30-C31-C32-C33
29	B	623	SQD	C33-C34-C35-C36
30	A	415	DGD	CBA-CCA-CDA-CEA
30	A	415	DGD	CBB-CCB-CDB-CEB
30	C	517	DGD	C9A-CAA-CBA-CCA
30	H	102	DGD	C7A-C8A-C9A-CAA
30	c	519	DGD	C4B-C5B-C6B-C7B
33	l	102	STE	C14-C15-C16-C17
29	a	412	SQD	C15-C16-C17-C18
30	C	516	DGD	C5A-C6A-C7A-C8A
33	b	620	STE	C7-C8-C9-C10
34	B	622	LHG	C29-C30-C31-C32
34	D	409	LHG	C25-C26-C27-C28
22	b	606	CLA	O1D-CGD-O2D-CED
34	D	409	LHG	O2-C2-C3-O3
28	A	412	LMG	C16-C17-C18-C19
28	b	623	LMG	C32-C33-C34-C35
28	c	524	LMG	C31-C32-C33-C34
29	B	623	SQD	C13-C14-C15-C16
33	H	103	STE	C13-C14-C15-C16
33	d	412	STE	C9-C10-C11-C12
34	E	101	LHG	C34-C35-C36-C37
24	Z	101	BCR	C12-C13-C14-C15
24	a	406	BCR	C20-C21-C22-C23
24	c	516	BCR	C20-C21-C22-C23
24	c	517	BCR	C20-C21-C22-C23
24	c	518	BCR	C16-C17-C18-C19
24	t	101	BCR	C20-C21-C22-C23
24	x	101	BCR	C11-C10-C9-C8
24	y	101	BCR	C20-C21-C22-C23
30	C	517	DGD	C2E-C1E-O5D-C6D
30	c	520	DGD	C2E-C1E-O5D-C6D
28	c	524	LMG	C16-C17-C18-C19
33	d	412	STE	C14-C15-C16-C17
34	D	412	LHG	C18-C19-C20-C21
34	d	407	LHG	C29-C30-C31-C32
22	B	615	CLA	C13-C15-C16-C17
22	C	514	CLA	O1A-CGA-O2A-C1
28	b	621	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
22	B	607	CLA	C16-C17-C18-C19
22	B	612	CLA	C16-C17-C18-C19
22	B	613	CLA	C16-C17-C18-C20
22	c	514	CLA	C16-C17-C18-C19
28	A	412	LMG	C38-C39-C40-C41
28	c	525	LMG	C13-C14-C15-C16
34	B	622	LHG	C17-C18-C19-C20
34	d	406	LHG	C10-C11-C12-C13
22	c	508	CLA	C2-C3-C5-C6
22	C	507	CLA	C6-C7-C8-C9
22	c	507	CLA	C11-C10-C8-C9
22	c	512	CLA	C14-C13-C15-C16
28	A	412	LMG	C28-C29-C30-C31
28	c	524	LMG	C28-C29-C30-C31
34	E	101	LHG	C23-C24-C25-C26
28	A	412	LMG	C12-C13-C14-C15
29	B	623	SQD	C11-C12-C13-C14
29	f	101	SQD	C32-C33-C34-C35
30	C	517	DGD	C7B-C8B-C9B-CAB
33	b	626	STE	C6-C7-C8-C9
33	c	523	STE	C11-C12-C13-C14
34	D	408	LHG	C30-C31-C32-C33
34	e	102	LHG	C16-C17-C18-C19
34	l	101	LHG	C32-C33-C34-C35
22	b	605	CLA	C15-C16-C17-C18
22	c	514	CLA	O1A-CGA-O2A-C1
30	c	521	DGD	O1A-C1A-O1G-C1G
24	b	617	BCR	C37-C22-C23-C24
28	M	101	LMG	C36-C37-C38-C39
33	b	622	STE	C14-C15-C16-C17
33	h	103	STE	C11-C12-C13-C14
34	D	409	LHG	O1-C1-C2-C3
34	d	408	LHG	O1-C1-C2-C3
24	d	404	BCR	C21-C22-C23-C24
28	d	409	LMG	C32-C33-C34-C35
29	f	101	SQD	C29-C30-C31-C32
33	B	627	STE	C4-C5-C6-C7
33	d	410	STE	C10-C11-C12-C13
33	l	102	STE	C10-C11-C12-C13
34	D	408	LHG	C34-C35-C36-C37
28	b	621	LMG	C28-C29-C30-C31
33	B	625	STE	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
34	d	406	LHG	C7-C8-C9-C10
34	d	408	LHG	C23-C24-C25-C26
22	C	513	CLA	O1D-CGD-O2D-CED
28	B	629	LMG	C11-C12-C13-C14
28	D	411	LMG	C14-C15-C16-C17
29	a	412	SQD	C29-C30-C31-C32
29	a	413	SQD	C15-C16-C17-C18
30	A	415	DGD	C6B-C7B-C8B-C9B
30	H	102	DGD	C5B-C6B-C7B-C8B
33	b	626	STE	C2-C3-C4-C5
33	l	102	STE	C4-C5-C6-C7
34	d	407	LHG	C11-C12-C13-C14
34	d	408	LHG	C32-C33-C34-C35
22	C	511	CLA	C16-C17-C18-C19
22	C	511	CLA	C16-C17-C18-C20
22	a	402	CLA	C16-C17-C18-C20
22	c	506	CLA	C11-C12-C13-C14
30	c	520	DGD	O6E-C1E-O5D-C6D
22	C	507	CLA	C8-C10-C11-C12
22	c	511	CLA	C10-C11-C12-C13
22	c	515	CLA	C5-C6-C7-C8
28	B	629	LMG	C16-C17-C18-C19
28	c	525	LMG	C17-C18-C19-C20
28	c	525	LMG	C39-C40-C41-C42
29	a	413	SQD	C11-C12-C13-C14
30	A	415	DGD	C4B-C5B-C6B-C7B
30	c	519	DGD	C3B-C4B-C5B-C6B
30	c	519	DGD	C5B-C6B-C7B-C8B
33	L	101	STE	C4-C5-C6-C7
33	b	625	STE	C4-C5-C6-C7
34	D	409	LHG	C32-C33-C34-C35
28	D	406	LMG	C17-C18-C19-C20
28	D	406	LMG	C39-C40-C41-C42
30	C	517	DGD	C5A-C6A-C7A-C8A
30	C	517	DGD	CBA-CCA-CDA-CEA
30	C	518	DGD	C5A-C6A-C7A-C8A
30	c	521	DGD	C2A-C3A-C4A-C5A
30	h	102	DGD	CBA-CCA-CDA-CEA
33	B	621	STE	C4-C5-C6-C7
33	B	627	STE	C5-C6-C7-C8
33	d	410	STE	C4-C5-C6-C7
34	B	622	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
34	D	408	LHG	C32-C33-C34-C35
34	D	409	LHG	C30-C31-C32-C33
34	d	407	LHG	C12-C13-C14-C15
34	l	101	LHG	C26-C27-C28-C29
28	B	629	LMG	C14-C15-C16-C17
28	b	621	LMG	C33-C34-C35-C36
33	l	102	STE	C9-C10-C11-C12
29	b	619	SQD	C26-C27-C28-C29
33	X	101	STE	C4-C5-C6-C7
34	D	409	LHG	C9-C10-C11-C12
22	C	513	CLA	C3A-C2A-CAA-CBA
22	c	514	CLA	C3A-C2A-CAA-CBA
28	D	411	LMG	C31-C32-C33-C34
28	b	621	LMG	C32-C33-C34-C35
29	A	413	SQD	C16-C17-C18-C19
29	A	413	SQD	C28-C29-C30-C31
30	h	102	DGD	C9A-CAA-CBA-CCA
34	D	408	LHG	C12-C13-C14-C15
34	E	101	LHG	C32-C33-C34-C35
22	B	606	CLA	C16-C17-C18-C19
22	a	402	CLA	C16-C17-C18-C19
22	d	402	CLA	C16-C17-C18-C20
28	M	101	LMG	C16-C17-C18-C19
30	c	520	DGD	C6B-C7B-C8B-C9B
34	d	406	LHG	C34-C35-C36-C37
34	l	101	LHG	C27-C28-C29-C30
28	d	409	LMG	C33-C34-C35-C36
30	c	520	DGD	C5B-C6B-C7B-C8B
34	D	409	LHG	C11-C10-C9-C8
22	C	513	CLA	O2A-C1-C2-C3
30	c	519	DGD	O6D-C5D-C6D-O5D
24	A	406	BCR	C14-C15-C16-C17
24	c	517	BCR	C14-C15-C16-C17
28	D	410	LMG	C28-C29-C30-C31
33	E	102	STE	C1-C2-C3-C4
33	B	626	STE	C9-C10-C11-C12
33	h	103	STE	C7-C8-C9-C10
22	B	610	CLA	C4-C3-C5-C6
22	B	610	CLA	C2-C3-C5-C6
22	c	512	CLA	C2-C3-C5-C6
27	A	410	PL9	C28-C29-C31-C32
27	D	405	PL9	C13-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
27	D	405	PL9	C28-C29-C31-C32
30	c	520	DGD	CBB-CCB-CDB-CEB
33	a	414	STE	C2-C3-C4-C5
33	b	622	STE	C2-C3-C4-C5
34	D	409	LHG	C31-C32-C33-C34
34	E	101	LHG	O1-C1-C2-O2
34	d	406	LHG	O1-C1-C2-O2
34	d	407	LHG	O1-C1-C2-O2
28	D	411	LMG	C32-C33-C34-C35
30	A	415	DGD	C2B-C3B-C4B-C5B
33	C	521	STE	C4-C5-C6-C7
33	M	102	STE	C11-C10-C9-C8
33	T	102	STE	C5-C6-C7-C8
33	b	624	STE	C3-C4-C5-C6
30	C	518	DGD	O1A-C1A-O1G-C1G
22	c	514	CLA	C16-C17-C18-C20
22	C	505	CLA	C11-C12-C13-C14
28	B	629	LMG	C32-C33-C34-C35
28	c	525	LMG	C12-C13-C14-C15
28	c	525	LMG	C30-C31-C32-C33
30	c	521	DGD	C9B-CAB-CBB-CCB
28	C	519	LMG	C18-C19-C20-C21
28	b	623	LMG	C11-C12-C13-C14
28	c	522	LMG	C33-C34-C35-C36
29	D	407	SQD	C30-C31-C32-C33
30	c	520	DGD	CAB-CBB-CCB-CDB
33	c	501	STE	C5-C6-C7-C8
33	d	410	STE	C1-C2-C3-C4
28	D	406	LMG	C30-C31-C32-C33
29	A	414	SQD	C12-C13-C14-C15
33	H	103	STE	C7-C8-C9-C10
33	T	102	STE	C12-C13-C14-C15
34	D	408	LHG	C13-C14-C15-C16
28	b	621	LMG	O9-C10-O7-C8
29	b	619	SQD	O49-C7-O47-C45
22	c	508	CLA	C2-C1-O2A-CGA
28	b	621	LMG	C37-C38-C39-C40
28	b	623	LMG	C16-C17-C18-C19
33	c	523	STE	C2-C3-C4-C5
33	d	411	STE	C3-C4-C5-C6
34	D	409	LHG	C10-C11-C12-C13
22	C	506	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
28	A	412	LMG	C34-C35-C36-C37
28	D	410	LMG	C14-C15-C16-C17
28	b	623	LMG	C34-C35-C36-C37
29	A	413	SQD	C9-C10-C11-C12
33	b	622	STE	C9-C10-C11-C12
33	c	501	STE	C6-C7-C8-C9
34	D	409	LHG	C24-C25-C26-C27
22	D	403	CLA	C16-C17-C18-C19
22	b	601	CLA	C16-C17-C18-C19
22	c	512	CLA	C16-C17-C18-C19
30	c	520	DGD	C1A-C2A-C3A-C4A
24	T	101	BCR	C1-C6-C7-C8
24	Z	101	BCR	C23-C24-C25-C26
24	c	516	BCR	C1-C6-C7-C8
24	c	516	BCR	C5-C6-C7-C8
28	c	524	LMG	O6-C5-C6-O5
34	D	408	LHG	C33-C34-C35-C36
34	d	406	LHG	C31-C32-C33-C34
34	d	406	LHG	C33-C34-C35-C36
22	b	613	CLA	C5-C6-C7-C8
28	c	525	LMG	C33-C34-C35-C36
30	A	415	DGD	CCA-CDA-CEA-CFA
33	b	626	STE	C5-C6-C7-C8
28	B	629	LMG	C30-C31-C32-C33
22	A	411	CLA	C15-C16-C17-C18
22	B	602	CLA	C8-C10-C11-C12
22	B	617	CLA	C5-C6-C7-C8
22	d	403	CLA	C8-C10-C11-C12
28	b	621	LMG	C18-C19-C20-C21
30	A	415	DGD	C4A-C5A-C6A-C7A
33	j	101	STE	C4-C5-C6-C7
22	C	506	CLA	C4-C3-C5-C6
22	C	511	CLA	C4-C3-C5-C6
22	A	403	CLA	C6-C7-C8-C10
22	A	403	CLA	C12-C13-C15-C16
22	C	504	CLA	C11-C10-C8-C7
22	C	506	CLA	C2-C3-C5-C6
22	C	511	CLA	C2-C3-C5-C6
22	b	606	CLA	C11-C10-C8-C7
22	b	610	CLA	C12-C13-C15-C16
22	b	611	CLA	C6-C7-C8-C10
22	b	612	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	b	613	CLA	C6-C7-C8-C10
22	b	614	CLA	C11-C12-C13-C15
22	c	504	CLA	C11-C12-C13-C15
22	c	506	CLA	C11-C10-C8-C7
22	d	403	CLA	C12-C13-C15-C16
22	h	101	CLA	C3-C5-C6-C7
22	A	402	CLA	C2C-C3C-CAC-CBC
22	B	612	CLA	C13-C15-C16-C17
22	c	509	CLA	C5-C6-C7-C8
22	c	513	CLA	C16-C17-C18-C19
34	B	622	LHG	O9-C7-O7-C5
33	b	622	STE	C10-C11-C12-C13
29	a	412	SQD	C32-C33-C34-C35
30	H	102	DGD	C9A-CAA-CBA-CCA
33	T	102	STE	C13-C14-C15-C16
34	l	101	LHG	C29-C30-C31-C32
22	c	513	CLA	O1D-CGD-O2D-CED
33	L	101	STE	C5-C6-C7-C8
33	d	410	STE	C11-C12-C13-C14
34	e	102	LHG	C7-C8-C9-C10
29	B	623	SQD	C35-C36-C37-C38
30	C	516	DGD	CCB-CDB-CEB-CFB
30	H	102	DGD	C7B-C8B-C9B-CAB
33	b	622	STE	C13-C14-C15-C16
34	E	101	LHG	C24-C25-C26-C27
22	h	101	CLA	O1D-CGD-O2D-CED
30	c	521	DGD	C6A-C7A-C8A-C9A
22	B	607	CLA	C16-C17-C18-C20
22	C	503	CLA	C16-C17-C18-C20
22	b	614	CLA	C16-C17-C18-C19
30	C	517	DGD	O6E-C1E-O5D-C6D
22	A	411	CLA	C13-C15-C16-C17
22	B	610	CLA	C15-C16-C17-C18
28	C	519	LMG	C31-C32-C33-C34
28	c	524	LMG	C30-C31-C32-C33
30	c	519	DGD	C4A-C5A-C6A-C7A
33	H	103	STE	C10-C11-C12-C13
34	B	622	LHG	C18-C19-C20-C21
34	d	406	LHG	C16-C17-C18-C19
29	A	414	SQD	C7-C8-C9-C10
22	a	405	CLA	C10-C11-C12-C13
27	D	405	PL9	C47-C48-C49-C50

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Mol	Chain	Res	Type	Atoms
28	D	411	LMG	C16-C17-C18-C19
29	A	414	SQD	C18-C19-C20-C21
30	C	517	DGD	C9B-CAB-CBB-CCB
33	d	411	STE	C10-C11-C12-C13
34	D	409	LHG	C27-C28-C29-C30
34	d	406	LHG	C18-C19-C20-C21
34	d	407	LHG	C17-C18-C19-C20
29	a	412	SQD	O49-C7-O47-C45
34	d	407	LHG	C14-C15-C16-C17
29	D	407	SQD	C2-C1-O6-C44
30	A	415	DGD	O2G-C2G-C3G-O3G
30	c	519	DGD	O6E-C5E-C6E-O5E
30	C	517	DGD	C3A-C4A-C5A-C6A
30	c	519	DGD	C7A-C8A-C9A-CAA
34	D	408	LHG	C9-C10-C11-C12
28	A	412	LMG	C33-C34-C35-C36
29	f	101	SQD	C24-C25-C26-C27
22	c	512	CLA	C4-C3-C5-C6
27	A	410	PL9	C23-C24-C26-C27
27	d	405	PL9	C13-C14-C16-C17
33	B	628	STE	C5-C6-C7-C8
22	A	403	CLA	C6-C7-C8-C9
22	A	411	CLA	C11-C12-C13-C14
22	B	604	CLA	C11-C12-C13-C14
22	B	616	CLA	C11-C12-C13-C14
22	a	405	CLA	C11-C10-C8-C9
22	b	612	CLA	C14-C13-C15-C16
22	c	506	CLA	C11-C10-C8-C9
22	c	512	CLA	C11-C12-C13-C14
22	d	403	CLA	C14-C13-C15-C16
22	h	101	CLA	C11-C12-C13-C14
28	D	406	LMG	C12-C13-C14-C15
29	a	412	SQD	C24-C25-C26-C27
30	h	102	DGD	C5B-C6B-C7B-C8B
33	B	628	STE	C10-C11-C12-C13
28	B	629	LMG	C39-C40-C41-C42
28	b	621	LMG	C31-C32-C33-C34
28	b	623	LMG	C31-C32-C33-C34
29	b	619	SQD	C25-C26-C27-C28
30	C	516	DGD	C9A-CAA-CBA-CCA
30	h	102	DGD	C6B-C7B-C8B-C9B
33	B	627	STE	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
33	H	103	STE	C5-C6-C7-C8
33	Z	102	STE	C11-C12-C13-C14
33	a	414	STE	C4-C5-C6-C7
34	D	408	LHG	C25-C26-C27-C28
28	D	410	LMG	C29-C28-O8-C9
24	y	101	BCR	C7-C8-C9-C34
28	b	623	LMG	C40-C41-C42-C43
29	A	413	SQD	C26-C27-C28-C29
29	a	413	SQD	C9-C10-C11-C12
30	c	520	DGD	C4A-C5A-C6A-C7A
34	B	622	LHG	C14-C15-C16-C17
34	D	412	LHG	C24-C25-C26-C27
34	d	408	LHG	O10-C23-O8-C6
22	c	510	CLA	C1A-C2A-CAA-CBA
22	c	513	CLA	C1A-C2A-CAA-CBA
22	c	514	CLA	C1A-C2A-CAA-CBA
22	B	613	CLA	C16-C17-C18-C19
22	D	403	CLA	C16-C17-C18-C20
22	b	614	CLA	C16-C17-C18-C20
22	c	513	CLA	C16-C17-C18-C20
30	c	519	DGD	O1B-C1B-O2G-C2G
28	b	623	LMG	C17-C18-C19-C20
29	B	623	SQD	C34-C35-C36-C37
29	a	412	SQD	C17-C18-C19-C20
33	E	102	STE	C4-C5-C6-C7
33	M	103	STE	C4-C5-C6-C7
30	h	102	DGD	C7A-C8A-C9A-CAA
34	B	622	LHG	C34-C35-C36-C37
28	d	409	LMG	C14-C15-C16-C17
28	D	406	LMG	C19-C20-C21-C22
29	B	623	SQD	C9-C10-C11-C12
34	D	412	LHG	C27-C28-C29-C30
34	l	101	LHG	C34-C35-C36-C37
30	H	102	DGD	CCA-CDA-CEA-CFA
28	c	524	LMG	C41-C42-C43-C44
29	a	412	SQD	C12-C13-C14-C15
29	f	101	SQD	C31-C32-C33-C34
33	d	412	STE	C11-C12-C13-C14
34	d	406	LHG	C25-C26-C27-C28
28	B	629	LMG	C37-C38-C39-C40
28	C	519	LMG	C30-C31-C32-C33
28	b	623	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
29	B	623	SQD	C18-C19-C20-C21
30	C	516	DGD	C2A-C3A-C4A-C5A
27	D	405	PL9	C30-C29-C31-C32
35	e	101	HEC	C2A-CAA-CBA-CGA
30	A	415	DGD	CCB-CDB-CEB-CFB
33	h	103	STE	C6-C7-C8-C9
34	E	101	LHG	C15-C16-C17-C18
28	M	101	LMG	C29-C30-C31-C32
33	B	601	STE	C2-C3-C4-C5
33	C	520	STE	C2-C3-C4-C5
33	d	410	STE	C9-C10-C11-C12
34	d	407	LHG	C11-C10-C9-C8
29	A	413	SQD	C34-C35-C36-C37
29	a	412	SQD	C25-C26-C27-C28
33	b	620	STE	C10-C11-C12-C13
34	e	102	LHG	C24-C25-C26-C27
22	B	611	CLA	C16-C17-C18-C20
22	h	101	CLA	C16-C17-C18-C20
28	B	629	LMG	O1-C7-C8-C9
29	B	623	SQD	O6-C44-C45-C46
30	A	415	DGD	C1G-C2G-C3G-O3G
30	c	519	DGD	O1G-C1G-C2G-C3G
33	H	103	STE	C3-C4-C5-C6
34	d	408	LHG	C4-C5-C6-O8
22	b	604	CLA	C15-C16-C17-C18
29	A	413	SQD	C17-C18-C19-C20
30	C	517	DGD	CDA-CEA-CFA-CGA
28	B	629	LMG	C8-C7-O1-C1
30	C	517	DGD	C2G-C3G-O3G-C1D
30	C	517	DGD	C5D-C6D-O5D-C1E
30	c	520	DGD	C2G-C3G-O3G-C1D
30	c	520	DGD	C5D-C6D-O5D-C1E
22	C	512	CLA	O1D-CGD-O2D-CED
28	b	623	LMG	C42-C43-C44-C45
29	a	413	SQD	C19-C20-C21-C22
22	c	503	CLA	O1D-CGD-O2D-CED
28	M	101	LMG	C14-C15-C16-C17
30	c	520	DGD	CBA-CCA-CDA-CEA
33	B	628	STE	C11-C10-C9-C8
33	I	101	STE	C1-C2-C3-C4
33	b	622	STE	C5-C6-C7-C8
33	d	410	STE	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
34	d	406	LHG	C27-C28-C29-C30
34	d	407	LHG	C16-C17-C18-C19
28	c	522	LMG	O6-C5-C6-O5
30	C	516	DGD	O6E-C5E-C6E-O5E
33	B	624	STE	C4-C5-C6-C7
33	B	628	STE	C6-C7-C8-C9
33	H	103	STE	C1-C2-C3-C4
22	B	604	CLA	C5-C6-C7-C8
28	d	409	LMG	C38-C39-C40-C41
33	b	626	STE	C1-C2-C3-C4
34	D	408	LHG	O1-C1-C2-O2
28	D	410	LMG	C33-C34-C35-C36
30	c	519	DGD	C3A-C4A-C5A-C6A
22	a	403	CLA	C8-C10-C11-C12
29	A	414	SQD	C19-C20-C21-C22
34	D	412	LHG	C19-C20-C21-C22
34	d	408	LHG	C26-C27-C28-C29
34	D	409	LHG	C35-C36-C37-C38
34	d	406	LHG	C19-C20-C21-C22
22	b	606	CLA	C8-C10-C11-C12
28	D	406	LMG	O6-C5-C6-O5
28	d	409	LMG	O6-C5-C6-O5
30	H	102	DGD	CAA-CBA-CCA-CDA
34	D	409	LHG	C14-C15-C16-C17
34	l	101	LHG	C13-C14-C15-C16
30	h	102	DGD	O6E-C5E-C6E-O5E
22	c	510	CLA	C16-C17-C18-C19
28	M	101	LMG	C12-C13-C14-C15
30	H	102	DGD	C3B-C4B-C5B-C6B
30	h	102	DGD	CDB-CEB-CFB-CGB
33	C	521	STE	C3-C4-C5-C6
28	c	522	LMG	C34-C35-C36-C37
28	D	410	LMG	C9-C8-O7-C10
28	B	629	LMG	O6-C5-C6-O5
29	a	412	SQD	C10-C11-C12-C13
30	c	521	DGD	C5A-C6A-C7A-C8A
28	B	629	LMG	C33-C34-C35-C36
30	h	102	DGD	CAB-CBB-CCB-CDB
23	d	401	PHO	O1D-CGD-O2D-CED
22	c	506	CLA	C5-C6-C7-C8
30	A	415	DGD	CFA-CGA-CHA-CIA
34	B	622	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
29	a	412	SQD	C19-C20-C21-C22
33	X	101	STE	C2-C3-C4-C5
33	d	411	STE	C2-C3-C4-C5
30	c	519	DGD	CDB-CEB-CFB-CGB
28	B	629	LMG	C34-C35-C36-C37
29	a	412	SQD	C35-C36-C37-C38
30	C	517	DGD	C5B-C6B-C7B-C8B
33	I	101	STE	C4-C5-C6-C7
34	e	102	LHG	C13-C14-C15-C16
34	D	412	LHG	C7-C8-C9-C10
34	e	102	LHG	C23-C24-C25-C26
24	B	619	BCR	C11-C10-C9-C8
24	C	515	BCR	C16-C17-C18-C19
24	b	616	BCR	C20-C21-C22-C23
24	c	516	BCR	C16-C17-C18-C19
28	c	525	LMG	C2-C1-O1-C7
34	E	101	LHG	C28-C29-C30-C31
28	c	524	LMG	O1-C7-C8-O7
28	c	525	LMG	O1-C7-C8-O7
29	A	413	SQD	O6-C44-C45-O47
29	b	619	SQD	O47-C45-C46-O48
22	A	405	CLA	C6-C7-C8-C9
30	c	520	DGD	C7A-C8A-C9A-CAA
33	B	627	STE	C3-C4-C5-C6
33	l	102	STE	C2-C3-C4-C5
27	A	410	PL9	C42-C43-C44-C45
27	a	410	PL9	C40-C39-C41-C42
34	D	409	LHG	C26-C27-C28-C29
22	B	604	CLA	C11-C12-C13-C15
22	B	605	CLA	C12-C13-C15-C16
22	B	616	CLA	C11-C10-C8-C7
22	B	616	CLA	C11-C12-C13-C15
22	C	506	CLA	C12-C13-C15-C16
22	C	513	CLA	C11-C12-C13-C15
22	C	514	CLA	C11-C10-C8-C7
22	a	405	CLA	C11-C10-C8-C7
22	b	602	CLA	C11-C12-C13-C15
22	b	606	CLA	C11-C12-C13-C15
22	b	607	CLA	C11-C12-C13-C15
22	b	613	CLA	C11-C12-C13-C15
22	c	507	CLA	C6-C7-C8-C10
22	c	511	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	c	515	CLA	C11-C12-C13-C15
22	h	101	CLA	C12-C13-C15-C16
28	b	621	LMG	C39-C40-C41-C42
34	l	101	LHG	C33-C34-C35-C36
22	A	403	CLA	C11-C12-C13-C14
22	B	605	CLA	C6-C7-C8-C9
22	B	605	CLA	C14-C13-C15-C16
22	B	608	CLA	C11-C10-C8-C9
22	C	506	CLA	C14-C13-C15-C16
22	C	513	CLA	C11-C12-C13-C14
22	a	403	CLA	C6-C7-C8-C9
22	b	603	CLA	C11-C12-C13-C14
22	b	606	CLA	C11-C12-C13-C14
22	b	611	CLA	C6-C7-C8-C9
22	c	504	CLA	C11-C12-C13-C14
22	c	507	CLA	C6-C7-C8-C9
22	c	508	CLA	C11-C12-C13-C14
22	c	511	CLA	C6-C7-C8-C9
22	c	515	CLA	C11-C12-C13-C14
33	B	626	STE	C11-C12-C13-C14
34	l	101	LHG	C15-C16-C17-C18
22	b	607	CLA	CBA-CGA-O2A-C1
22	c	513	CLA	CBA-CGA-O2A-C1
33	L	101	STE	C7-C8-C9-C10
30	c	519	DGD	C4D-C5D-C6D-O5D
34	e	102	LHG	C27-C28-C29-C30
30	A	415	DGD	CAA-CBA-CCA-CDA
34	d	408	LHG	C35-C36-C37-C38
34	e	102	LHG	C11-C10-C9-C8
22	A	405	CLA	CBA-CGA-O2A-C1
22	a	405	CLA	CBA-CGA-O2A-C1
28	b	623	LMG	C4-C5-C6-O5
29	D	407	SQD	C25-C26-C27-C28
30	H	102	DGD	CAB-CBB-CCB-CDB
33	c	523	STE	C7-C8-C9-C10
33	L	101	STE	C3-C4-C5-C6
33	b	625	STE	C11-C10-C9-C8
22	C	503	CLA	C16-C17-C18-C19
22	a	403	CLA	C16-C17-C18-C20
34	d	407	LHG	O6-C4-C5-C6
30	C	518	DGD	CCA-CDA-CEA-CFA
33	M	102	STE	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
33	b	624	STE	C9-C10-C11-C12
34	d	406	LHG	C15-C16-C17-C18
22	c	514	CLA	C4-C3-C5-C6
27	a	410	PL9	C20-C19-C21-C22
22	c	514	CLA	C2-C3-C5-C6
33	d	411	STE	C1-C2-C3-C4
28	D	406	LMG	C36-C37-C38-C39
30	c	521	DGD	C7A-C8A-C9A-CAA
34	B	622	LHG	C19-C20-C21-C22
34	D	412	LHG	C28-C29-C30-C31
22	C	506	CLA	C16-C17-C18-C20
29	a	413	SQD	C31-C32-C33-C34
33	d	412	STE	C1-C2-C3-C4
33	X	101	STE	C11-C10-C9-C8
33	c	523	STE	C4-C5-C6-C7
33	c	523	STE	C12-C13-C14-C15
33	C	521	STE	C12-C13-C14-C15
33	X	101	STE	C10-C11-C12-C13
33	a	415	STE	C6-C7-C8-C9
22	B	611	CLA	C16-C17-C18-C19
33	H	103	STE	C12-C13-C14-C15
22	c	512	CLA	C5-C6-C7-C8
28	c	524	LMG	O1-C7-C8-C9
28	c	524	LMG	C7-C8-C9-O8
28	c	525	LMG	O1-C7-C8-C9
29	a	412	SQD	O6-C44-C45-C46
34	E	101	LHG	C4-C5-C6-O8
28	M	101	LMG	C18-C19-C20-C21
29	a	413	SQD	C14-C15-C16-C17
30	c	521	DGD	C3B-C4B-C5B-C6B
30	A	415	DGD	O1A-C1A-O1G-C1G
28	A	412	LMG	C40-C41-C42-C43
28	C	519	LMG	C15-C16-C17-C18
28	C	519	LMG	C19-C20-C21-C22
34	D	409	LHG	C33-C34-C35-C36
29	a	413	SQD	C18-C19-C20-C21
34	E	101	LHG	C16-C17-C18-C19
34	d	407	LHG	C25-C26-C27-C28
23	A	404	PHO	C4-C3-C5-C6
22	C	506	CLA	C16-C17-C18-C19
22	a	403	CLA	C16-C17-C18-C19
33	d	410	STE	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
28	c	525	LMG	C31-C32-C33-C34
34	D	408	LHG	C4-O6-P-O3
34	E	101	LHG	C4-O6-P-O3
34	e	102	LHG	C4-O6-P-O3
28	b	621	LMG	C38-C39-C40-C41
34	d	408	LHG	O1-C1-C2-O2
28	b	621	LMG	C13-C14-C15-C16
34	d	407	LHG	C32-C33-C34-C35
34	D	412	LHG	O9-C7-O7-C5
33	a	414	STE	C7-C8-C9-C10
33	d	411	STE	C9-C10-C11-C12
27	d	405	PL9	C37-C38-C39-C40
22	c	513	CLA	O1A-CGA-O2A-C1
30	c	519	DGD	C1A-C2A-C3A-C4A
22	B	606	CLA	C16-C17-C18-C20
22	B	614	CLA	C16-C17-C18-C19
22	c	504	CLA	C16-C17-C18-C20
34	e	102	LHG	C10-C11-C12-C13
28	B	629	LMG	O8-C28-C29-C30
30	C	516	DGD	O1G-C1A-C2A-C3A
29	B	623	SQD	C27-C28-C29-C30
33	M	102	STE	C4-C5-C6-C7
33	b	622	STE	C6-C7-C8-C9
28	b	621	LMG	C11-C12-C13-C14
28	M	101	LMG	O7-C8-C9-O8
28	b	621	LMG	O7-C8-C9-O8
29	a	412	SQD	O47-C45-C46-O48
29	a	413	SQD	O47-C45-C46-O48
28	b	621	LMG	C14-C15-C16-C17
30	c	519	DGD	C2A-C3A-C4A-C5A
33	B	628	STE	C2-C3-C4-C5
33	X	101	STE	C3-C4-C5-C6
33	b	624	STE	C11-C10-C9-C8
22	C	513	CLA	C13-C15-C16-C17
22	c	515	CLA	C13-C15-C16-C17
33	C	520	STE	C3-C4-C5-C6
22	C	511	CLA	C10-C11-C12-C13
22	B	606	CLA	C14-C13-C15-C16
22	B	614	CLA	C11-C12-C13-C14
22	B	615	CLA	C11-C10-C8-C9
22	C	509	CLA	C11-C10-C8-C9
22	C	511	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	C	512	CLA	C6-C7-C8-C9
22	C	513	CLA	C14-C13-C15-C16
22	C	514	CLA	C11-C10-C8-C9
22	a	403	CLA	C11-C10-C8-C9
22	b	601	CLA	C11-C10-C8-C9
22	b	602	CLA	C11-C10-C8-C9
22	b	604	CLA	C11-C10-C8-C9
22	b	608	CLA	C14-C13-C15-C16
22	b	614	CLA	C6-C7-C8-C9
22	c	514	CLA	C6-C7-C8-C9
22	c	514	CLA	C11-C12-C13-C14
29	A	414	SQD	C30-C31-C32-C33
28	M	101	LMG	C13-C14-C15-C16
22	B	602	CLA	C15-C16-C17-C18
22	b	615	CLA	C10-C11-C12-C13
34	E	101	LHG	C2-C3-O3-P
34	d	408	LHG	C2-C3-O3-P
29	D	407	SQD	O6-C44-C45-C46
22	A	402	CLA	C4C-C3C-CAC-CBC
22	c	506	CLA	C11-C12-C13-C15
22	h	101	CLA	C16-C17-C18-C19
24	B	618	BCR	C1-C6-C7-C8
24	B	618	BCR	C5-C6-C7-C8
24	K	101	BCR	C23-C24-C25-C26
24	K	101	BCR	C23-C24-C25-C30
24	T	101	BCR	C5-C6-C7-C8
24	Y	101	BCR	C23-C24-C25-C30
24	b	616	BCR	C1-C6-C7-C8
28	b	621	LMG	C16-C17-C18-C19
24	B	619	BCR	C11-C12-C13-C35
28	c	524	LMG	C15-C16-C17-C18
30	C	517	DGD	C6A-C7A-C8A-C9A
24	A	406	BCR	C17-C18-C19-C20
24	B	618	BCR	C11-C12-C13-C14
24	T	101	BCR	C7-C8-C9-C10
24	Y	101	BCR	C11-C12-C13-C14
24	c	518	BCR	C11-C12-C13-C14
33	J	101	STE	C3-C4-C5-C6
22	a	411	CLA	C2C-C3C-CAC-CBC
34	d	408	LHG	C30-C31-C32-C33
33	C	522	STE	C5-C6-C7-C8
33	l	102	STE	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	B	612	CLA	C16-C17-C18-C20
22	B	615	CLA	C15-C16-C17-C18
34	l	101	LHG	O6-C4-C5-C6
28	c	525	LMG	C19-C20-C21-C22
29	B	623	SQD	C30-C31-C32-C33
30	c	520	DGD	C3A-C4A-C5A-C6A
33	c	523	STE	C10-C11-C12-C13
22	A	403	CLA	C11-C12-C13-C15
22	B	602	CLA	C11-C12-C13-C15
22	B	605	CLA	C6-C7-C8-C10
22	B	606	CLA	C12-C13-C15-C16
22	B	607	CLA	C11-C12-C13-C15
22	B	608	CLA	C11-C10-C8-C7
22	B	612	CLA	C6-C7-C8-C10
22	B	617	CLA	C6-C7-C8-C10
22	C	503	CLA	C12-C13-C15-C16
22	C	507	CLA	C6-C7-C8-C10
22	C	509	CLA	C11-C10-C8-C7
22	C	511	CLA	C11-C10-C8-C7
22	C	513	CLA	C12-C13-C15-C16
22	a	403	CLA	C11-C10-C8-C7
22	b	603	CLA	C11-C12-C13-C15
22	b	606	CLA	C6-C7-C8-C10
22	b	608	CLA	C12-C13-C15-C16
22	b	613	CLA	C12-C13-C15-C16
22	c	508	CLA	C11-C12-C13-C15
22	c	513	CLA	C12-C13-C15-C16
22	c	514	CLA	C11-C12-C13-C15
22	c	514	CLA	C12-C13-C15-C16
22	d	402	CLA	C6-C7-C8-C10
24	c	518	BCR	C19-C20-C21-C22
24	y	101	BCR	C19-C20-C21-C22
22	c	504	CLA	C16-C17-C18-C19
30	C	518	DGD	C3A-C4A-C5A-C6A
28	d	409	LMG	C30-C31-C32-C33
22	c	504	CLA	C13-C15-C16-C17
22	B	605	CLA	C2C-C3C-CAC-CBC
30	c	520	DGD	CCA-CDA-CEA-CFA
24	B	618	BCR	C20-C21-C22-C37
24	H	101	BCR	C35-C13-C14-C15
24	y	101	BCR	C16-C17-C18-C36
24	y	101	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
22	A	411	CLA	C16-C17-C18-C19
22	b	606	CLA	C16-C17-C18-C20
22	C	506	CLA	CBA-CGA-O2A-C1
29	a	412	SQD	C24-C23-O48-C46
28	M	101	LMG	C39-C40-C41-C42
30	H	102	DGD	CBA-CCA-CDA-CEA
28	D	410	LMG	C13-C14-C15-C16
34	D	409	LHG	C17-C18-C19-C20
34	E	101	LHG	C19-C20-C21-C22
22	C	512	CLA	C15-C16-C17-C18
29	a	412	SQD	O10-C23-O48-C46
30	C	518	DGD	C9B-CAB-CBB-CCB
33	d	412	STE	C2-C3-C4-C5
22	B	611	CLA	CAD-CBD-CGD-O2D
22	C	514	CLA	CAD-CBD-CGD-O2D
22	b	609	CLA	CAD-CBD-CGD-O2D
22	c	505	CLA	CAD-CBD-CGD-O2D
22	c	515	CLA	CAD-CBD-CGD-O2D
28	B	629	LMG	C9-C8-O7-C10
29	f	101	SQD	C46-C45-O47-C7
33	X	101	STE	C12-C13-C14-C15
33	j	101	STE	C5-C6-C7-C8
24	y	101	BCR	C22-C23-C24-C25
22	B	614	CLA	C16-C17-C18-C20
22	b	611	CLA	C16-C17-C18-C20
30	c	521	DGD	C8B-C9B-CAB-CBB
33	C	521	STE	C7-C8-C9-C10
27	a	410	PL9	C9-C11-C12-C13
28	D	406	LMG	C32-C33-C34-C35
33	l	102	STE	C7-C8-C9-C10
28	b	621	LMG	C7-C8-C9-O8
29	A	413	SQD	O6-C44-C45-C46
29	f	101	SQD	C44-C45-C46-O48
22	d	403	CLA	CBD-CGD-O2D-CED
22	A	405	CLA	O1A-CGA-O2A-C1
22	c	515	CLA	C3-C5-C6-C7
29	b	619	SQD	C28-C29-C30-C31
30	C	518	DGD	CAB-CBB-CCB-CDB
33	I	101	STE	C7-C8-C9-C10
33	h	103	STE	C10-C11-C12-C13
34	e	102	LHG	C28-C29-C30-C31
28	C	519	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
22	B	608	CLA	CHA-CBD-CGD-O1D
22	B	608	CLA	CHA-CBD-CGD-O2D
22	C	503	CLA	CHA-CBD-CGD-O1D
22	C	503	CLA	CHA-CBD-CGD-O2D
22	C	505	CLA	CHA-CBD-CGD-O1D
22	C	509	CLA	CHA-CBD-CGD-O2D
22	c	504	CLA	CHA-CBD-CGD-O1D
22	c	506	CLA	CHA-CBD-CGD-O1D
22	c	506	CLA	CHA-CBD-CGD-O2D
22	c	508	CLA	CHA-CBD-CGD-O1D
22	h	101	CLA	CHA-CBD-CGD-O1D
22	h	101	CLA	CHA-CBD-CGD-O2D
29	f	101	SQD	C28-C29-C30-C31
30	c	520	DGD	C9A-CAA-CBA-CCA
22	a	405	CLA	O1A-CGA-O2A-C1
22	b	607	CLA	O1A-CGA-O2A-C1
28	D	406	LMG	C15-C16-C17-C18
30	C	516	DGD	CBA-CCA-CDA-CEA
24	Z	101	BCR	C11-C10-C9-C8
33	T	102	STE	C6-C7-C8-C9
28	c	524	LMG	O7-C8-C9-O8
29	f	101	SQD	O47-C45-C46-O48
34	E	101	LHG	O7-C5-C6-O8
28	B	629	LMG	C38-C39-C40-C41
28	b	623	LMG	O10-C28-O8-C9
33	X	101	STE	C7-C8-C9-C10
29	a	413	SQD	C28-C29-C30-C31
27	A	410	PL9	C11-C12-C13-C14
28	c	524	LMG	C12-C13-C14-C15
22	C	506	CLA	O1A-CGA-O2A-C1
27	A	410	PL9	C13-C14-C16-C17
27	a	410	PL9	C4-C3-C7-C8
22	a	403	CLA	C14-C13-C15-C16
22	b	613	CLA	C14-C13-C15-C16
22	c	508	CLA	C6-C7-C8-C9
22	c	514	CLA	C14-C13-C15-C16
33	B	621	STE	C7-C8-C9-C10
34	D	412	LHG	C25-C26-C27-C28
34	D	412	LHG	C31-C32-C33-C34
22	b	608	CLA	C13-C15-C16-C17
22	b	610	CLA	C8-C10-C11-C12
28	C	519	LMG	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
30	C	518	DGD	CDB-CEB-CFB-CGB
24	x	101	BCR	C37-C22-C23-C24
29	D	407	SQD	C32-C33-C34-C35
22	c	506	CLA	C8-C10-C11-C12
28	B	629	LMG	C18-C19-C20-C21
30	C	517	DGD	CAB-CBB-CCB-CDB
30	H	102	DGD	C6B-C7B-C8B-C9B
30	c	519	DGD	CBB-CCB-CDB-CEB
34	d	406	LHG	C13-C14-C15-C16
22	B	604	CLA	C16-C17-C18-C19
22	b	607	CLA	C16-C17-C18-C19
34	D	409	LHG	O9-C7-O7-C5
33	C	520	STE	C4-C5-C6-C7
22	B	617	CLA	C2-C1-O2A-CGA
28	B	629	LMG	C23-C24-C25-C26
29	a	413	SQD	C12-C13-C14-C15
33	j	101	STE	C3-C4-C5-C6
22	B	607	CLA	C5-C6-C7-C8
34	D	409	LHG	C2-C3-O3-P
27	A	410	PL9	C43-C44-C46-C47
34	D	409	LHG	C3-O3-P-O5
34	d	408	LHG	C4-O6-P-O4
34	l	101	LHG	C3-O3-P-O4
22	C	514	CLA	C10-C11-C12-C13
28	b	623	LMG	C37-C38-C39-C40
33	a	415	STE	C3-C4-C5-C6
34	D	412	LHG	C30-C31-C32-C33
34	l	101	LHG	C14-C15-C16-C17
22	b	605	CLA	C5-C6-C7-C8
22	C	507	CLA	C3-C5-C6-C7
28	c	522	LMG	C30-C31-C32-C33
34	E	101	LHG	C30-C31-C32-C33
22	C	508	CLA	C16-C17-C18-C20
33	b	620	STE	C3-C4-C5-C6
33	c	523	STE	C3-C4-C5-C6
33	d	410	STE	C6-C7-C8-C9
22	B	608	CLA	CAD-CBD-CGD-O1D
22	C	503	CLA	CAD-CBD-CGD-O1D
22	C	505	CLA	CAD-CBD-CGD-O1D
22	b	613	CLA	CAD-CBD-CGD-O1D
22	c	506	CLA	CAD-CBD-CGD-O1D
22	c	508	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	h	101	CLA	CAD-CBD-CGD-O1D
29	A	414	SQD	C15-C16-C17-C18
22	C	513	CLA	C16-C17-C18-C19
22	A	411	CLA	C12-C13-C15-C16
22	B	605	CLA	C11-C12-C13-C15
22	B	614	CLA	C6-C7-C8-C10
22	C	506	CLA	C6-C7-C8-C10
22	C	508	CLA	C11-C10-C8-C7
22	C	512	CLA	C11-C12-C13-C15
22	C	513	CLA	C11-C10-C8-C7
22	a	403	CLA	C11-C12-C13-C15
22	a	403	CLA	C12-C13-C15-C16
22	b	602	CLA	C11-C10-C8-C7
22	c	503	CLA	C11-C12-C13-C15
22	c	508	CLA	C11-C10-C8-C7
22	c	510	CLA	C12-C13-C15-C16
22	d	403	CLA	C11-C12-C13-C15
23	a	404	PHO	C6-C7-C8-C10
34	d	407	LHG	O6-C4-C5-O7
28	C	519	LMG	C16-C17-C18-C19
29	a	412	SQD	C11-C12-C13-C14
30	h	102	DGD	C7B-C8B-C9B-CAB
33	B	621	STE	C6-C7-C8-C9
24	c	516	BCR	C13-C14-C15-C16
30	h	102	DGD	O2G-C1B-C2B-C3B
30	H	102	DGD	C5A-C6A-C7A-C8A
30	A	415	DGD	C5B-C6B-C7B-C8B
33	d	411	STE	C12-C13-C14-C15
22	C	513	CLA	C2A-CAA-CBA-CGA
28	b	621	LMG	C35-C36-C37-C38
28	c	525	LMG	C35-C36-C37-C38
28	d	409	LMG	C36-C37-C38-C39
28	A	412	LMG	C7-C8-C9-O8
28	M	101	LMG	C7-C8-C9-O8
29	a	413	SQD	C44-C45-C46-O48
30	C	516	DGD	CDB-CEB-CFB-CGB
28	A	412	LMG	O7-C8-C9-O8
28	B	629	LMG	O1-C7-C8-O7
29	b	619	SQD	O6-C44-C45-O47
30	C	516	DGD	O1G-C1G-C2G-O2G
30	c	519	DGD	O1G-C1G-C2G-O2G
34	d	408	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
28	D	410	LMG	C34-C35-C36-C37
30	C	516	DGD	C2B-C3B-C4B-C5B
34	E	101	LHG	C11-C10-C9-C8
33	T	102	STE	C10-C11-C12-C13
30	H	102	DGD	O2G-C1B-C2B-C3B
22	b	614	CLA	C8-C10-C11-C12
30	C	516	DGD	C5B-C6B-C7B-C8B
34	E	101	LHG	C9-C10-C11-C12
22	b	604	CLA	C5-C6-C7-C8
23	A	404	PHO	C2-C3-C5-C6
27	A	410	PL9	C33-C34-C36-C37
28	c	524	LMG	C13-C14-C15-C16
22	B	611	CLA	C8-C10-C11-C12
22	B	612	CLA	C6-C7-C8-C9
22	B	612	CLA	C11-C12-C13-C14
22	B	617	CLA	C6-C7-C8-C9
22	C	503	CLA	C14-C13-C15-C16
22	b	607	CLA	C11-C12-C13-C14
22	b	614	CLA	C11-C12-C13-C14
22	d	402	CLA	C6-C7-C8-C9
24	b	618	BCR	C6-C7-C8-C9
34	B	622	LHG	C32-C33-C34-C35
22	b	606	CLA	C16-C17-C18-C19
33	B	628	STE	C4-C5-C6-C7
34	E	101	LHG	C26-C27-C28-C29
34	D	409	LHG	O1-C1-C2-O2
33	I	101	STE	C11-C10-C9-C8
33	M	103	STE	C5-C6-C7-C8
33	T	102	STE	C14-C15-C16-C17
24	T	101	BCR	C7-C8-C9-C34
24	c	517	BCR	C7-C8-C9-C34
22	D	402	CLA	C2C-C3C-CAC-CBC
30	A	415	DGD	C2A-C3A-C4A-C5A
28	D	406	LMG	C33-C34-C35-C36
29	A	414	SQD	C10-C11-C12-C13
24	Z	101	BCR	C11-C12-C13-C14
22	B	610	CLA	C13-C15-C16-C17
22	d	402	CLA	C2C-C3C-CAC-CBC
33	J	101	STE	C6-C7-C8-C9
28	b	621	LMG	C19-C20-C21-C22
33	c	501	STE	C7-C8-C9-C10
24	c	517	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
33	X	101	STE	C6-C7-C8-C9
33	Z	102	STE	C14-C15-C16-C17
29	a	413	SQD	C24-C25-C26-C27
33	b	625	STE	C2-C3-C4-C5
29	B	623	SQD	C46-C45-O47-C7
29	a	412	SQD	C44-C45-O47-C7
22	c	503	CLA	C2A-CAA-CBA-CGA
34	e	102	LHG	O9-C7-O7-C5
22	B	614	CLA	C2-C1-O2A-CGA
22	a	402	CLA	C2-C1-O2A-CGA
29	A	414	SQD	C32-C33-C34-C35
22	c	511	CLA	CAA-CBA-CGA-O2A
22	C	513	CLA	C3-C5-C6-C7
28	C	519	LMG	C14-C15-C16-C17
33	C	522	STE	C6-C7-C8-C9
28	c	524	LMG	C35-C36-C37-C38
34	l	101	LHG	O6-C4-C5-O7
33	a	415	STE	C4-C5-C6-C7
33	B	625	STE	C6-C7-C8-C9
24	b	616	BCR	C5-C6-C7-C8
24	c	518	BCR	C1-C6-C7-C8
30	c	521	DGD	CBA-CCA-CDA-CEA
28	D	410	LMG	C15-C16-C17-C18
30	c	520	DGD	C4B-C5B-C6B-C7B
30	c	519	DGD	O1G-C1A-C2A-C3A
28	M	101	LMG	C15-C16-C17-C18
28	d	409	LMG	C37-C38-C39-C40
29	A	413	SQD	C31-C32-C33-C34
29	A	414	SQD	C28-C29-C30-C31
22	C	508	CLA	C16-C17-C18-C19
29	b	619	SQD	O5-C1-O6-C44
24	B	619	BCR	C16-C17-C18-C19
24	B	620	BCR	C11-C10-C9-C8
24	c	517	BCR	C12-C13-C14-C15
24	y	101	BCR	C11-C10-C9-C8
34	e	102	LHG	O7-C5-C6-O8
22	c	510	CLA	C8-C10-C11-C12
29	a	412	SQD	C28-C29-C30-C31
30	h	102	DGD	CDA-CEA-CFA-CGA
33	b	626	STE	C4-C5-C6-C7
34	l	101	LHG	C9-C10-C11-C12
34	E	101	LHG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
30	C	518	DGD	O6D-C5D-C6D-O5D
22	a	405	CLA	C15-C16-C17-C18
33	d	411	STE	C11-C12-C13-C14
23	d	401	PHO	CHA-CBD-CGD-O2D
30	C	518	DGD	C9A-CAA-CBA-CCA
29	A	414	SQD	C46-C45-O47-C7
28	C	519	LMG	O1-C7-C8-C9
30	C	516	DGD	O1G-C1G-C2G-C3G
28	D	406	LMG	C34-C35-C36-C37
34	D	412	LHG	C26-C27-C28-C29
22	C	503	CLA	C11-C12-C13-C15
22	c	507	CLA	C11-C10-C8-C7
22	c	508	CLA	C12-C13-C15-C16
27	d	405	PL9	C47-C48-C49-C50
22	B	614	CLA	C6-C7-C8-C9
22	C	503	CLA	C11-C12-C13-C14
22	a	403	CLA	C11-C12-C13-C14
22	b	605	CLA	C11-C10-C8-C9
22	b	606	CLA	C6-C7-C8-C9
22	d	403	CLA	C11-C12-C13-C14
24	Z	101	BCR	C9-C10-C11-C12
24	Z	101	BCR	C15-C16-C17-C18
30	C	516	DGD	C6B-C7B-C8B-C9B
28	C	519	LMG	C37-C38-C39-C40
28	D	406	LMG	C37-C38-C39-C40
33	b	624	STE	C6-C7-C8-C9
30	C	517	DGD	C6B-C7B-C8B-C9B
33	B	628	STE	C7-C8-C9-C10
33	d	412	STE	C3-C4-C5-C6
22	b	610	CLA	C10-C11-C12-C13
33	b	620	STE	C15-C16-C17-C18
29	b	619	SQD	C14-C15-C16-C17
22	C	509	CLA	C16-C17-C18-C19
30	c	521	DGD	C2A-C1A-O1G-C1G
29	a	412	SQD	C9-C10-C11-C12
22	B	615	CLA	CBD-CGD-O2D-CED
35	e	101	HEC	CAD-CBD-CGD-O1D
33	d	411	STE	C15-C16-C17-C18
22	a	405	CLA	C5-C6-C7-C8
28	b	623	LMG	O6-C1-O1-C7
24	y	101	BCR	C9-C10-C11-C12
29	b	619	SQD	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
30	C	516	DGD	C3A-C4A-C5A-C6A
30	c	519	DGD	C6A-C7A-C8A-C9A
33	B	626	STE	C13-C14-C15-C16
23	d	401	PHO	C5-C6-C7-C8
29	b	619	SQD	C29-C30-C31-C32
34	d	408	LHG	C9-C10-C11-C12
35	F	101	HEC	CAD-CBD-CGD-O1D
34	e	102	LHG	O6-C4-C5-O7
24	d	404	BCR	C18-C19-C20-C21
22	b	608	CLA	C3-C5-C6-C7
34	B	622	LHG	C11-C12-C13-C14
34	l	101	LHG	C18-C19-C20-C21
33	d	411	STE	C4-C5-C6-C7
22	B	612	CLA	C2-C3-C5-C6
33	T	102	STE	C15-C16-C17-C18
22	D	402	CLA	C10-C11-C12-C13
22	d	402	CLA	C2-C1-O2A-CGA
30	C	518	DGD	CBA-CCA-CDA-CEA
29	D	407	SQD	C44-C45-C46-O48
28	c	522	LMG	C31-C32-C33-C34
34	d	406	LHG	C17-C18-C19-C20
33	d	412	STE	C15-C16-C17-C18
30	C	518	DGD	C2A-C3A-C4A-C5A
28	B	629	LMG	C21-C22-C23-C24
28	b	623	LMG	C12-C13-C14-C15
30	C	518	DGD	C4B-C5B-C6B-C7B
22	B	602	CLA	C3A-C2A-CAA-CBA
22	B	608	CLA	C3A-C2A-CAA-CBA
33	c	523	STE	O1-C1-C2-C3
22	B	605	CLA	C13-C15-C16-C17
33	B	626	STE	O1-C1-C2-C3
27	A	410	PL9	C4-C3-C7-C8
28	D	411	LMG	C29-C30-C31-C32
28	C	519	LMG	C4-C5-C6-O5
22	B	612	CLA	C14-C13-C15-C16
22	C	512	CLA	C11-C12-C13-C14
22	b	609	CLA	C14-C13-C15-C16
22	c	512	CLA	C11-C10-C8-C9
33	c	523	STE	O2-C1-C2-C3
24	c	516	BCR	C16-C17-C18-C36
34	e	102	LHG	C4-C5-C6-O8
28	D	411	LMG	O8-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
28	M	101	LMG	C11-C12-C13-C14
22	B	605	CLA	O2A-C1-C2-C3
22	h	101	CLA	O2A-C1-C2-C3
30	C	517	DGD	O6D-C1D-O3G-C3G
33	B	626	STE	O2-C1-C2-C3
33	c	501	STE	O1-C1-C2-C3
24	Z	101	BCR	C14-C15-C16-C17
28	d	409	LMG	C12-C13-C14-C15
30	c	519	DGD	CBA-CCA-CDA-CEA
29	a	412	SQD	C46-C45-O47-C7
22	b	613	CLA	C10-C11-C12-C13
22	c	515	CLA	C1A-C2A-CAA-CBA
28	A	412	LMG	C14-C15-C16-C17
30	c	519	DGD	C8A-C9A-CAA-CBA
22	A	403	CLA	C11-C10-C8-C7
22	B	607	CLA	C6-C7-C8-C10
22	C	505	CLA	C11-C10-C8-C7
22	C	507	CLA	C12-C13-C15-C16
22	C	510	CLA	C11-C10-C8-C7
22	b	607	CLA	C11-C10-C8-C7
23	A	404	PHO	C12-C13-C15-C16
30	C	517	DGD	C4A-C5A-C6A-C7A
29	a	412	SQD	C11-C10-C9-C8
22	C	514	CLA	C8-C10-C11-C12
22	B	615	CLA	C16-C17-C18-C19
33	b	620	STE	C12-C13-C14-C15
22	b	613	CLA	C2A-CAA-CBA-CGA
22	C	506	CLA	C15-C16-C17-C18
22	b	611	CLA	C8-C10-C11-C12
30	C	518	DGD	C3B-C4B-C5B-C6B
22	b	607	CLA	C2C-C3C-CAC-CBC
33	B	625	STE	C7-C8-C9-C10
33	H	103	STE	C11-C12-C13-C14
34	e	102	LHG	O6-C4-C5-C6
22	B	610	CLA	C16-C17-C18-C19
22	b	611	CLA	C16-C17-C18-C19
33	C	521	STE	C11-C12-C13-C14
34	D	408	LHG	C29-C30-C31-C32
34	d	406	LHG	C29-C30-C31-C32
22	D	403	CLA	C4-C3-C5-C6
22	D	403	CLA	C13-C15-C16-C17
22	b	615	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
28	c	525	LMG	C28-C29-C30-C31
35	F	101	HEC	CAD-CBD-CGD-O2D
22	D	403	CLA	C3-C5-C6-C7
22	h	101	CLA	C10-C11-C12-C13
33	b	622	STE	O2-C1-C2-C3
28	B	629	LMG	O7-C8-C9-O8
24	c	516	BCR	C9-C10-C11-C12
35	e	101	HEC	CAD-CBD-CGD-O2D
22	b	602	CLA	C13-C15-C16-C17
33	B	627	STE	C7-C8-C9-C10
30	H	102	DGD	CDA-CEA-CFA-CGA
30	C	516	DGD	O6E-C1E-O5D-C6D
28	D	411	LMG	O7-C10-C11-C12
33	B	621	STE	O2-C1-C2-C3
22	A	411	CLA	C4C-C3C-CAC-CBC
33	b	625	STE	C6-C7-C8-C9
22	B	602	CLA	C2-C1-O2A-CGA
22	D	402	CLA	C2-C1-O2A-CGA
34	E	101	LHG	C18-C19-C20-C21
35	V	201	HEC	CAD-CBD-CGD-O2D
34	D	408	LHG	C17-C18-C19-C20
22	B	602	CLA	C6-C7-C8-C9
22	b	604	CLA	C11-C12-C13-C14
29	b	619	SQD	C10-C11-C12-C13
33	B	621	STE	O1-C1-C2-C3
33	c	501	STE	O2-C1-C2-C3
29	A	413	SQD	C10-C11-C12-C13
24	a	406	BCR	C1-C6-C7-C8
24	c	518	BCR	C23-C24-C25-C26
24	c	518	BCR	C23-C24-C25-C30
24	x	101	BCR	C23-C24-C25-C30
22	a	411	CLA	C4C-C3C-CAC-CBC
33	B	624	STE	C7-C8-C9-C10
28	b	623	LMG	C33-C34-C35-C36
24	Y	101	BCR	C13-C14-C15-C16
22	D	403	CLA	C10-C11-C12-C13
28	D	411	LMG	O10-C28-C29-C30
29	f	101	SQD	C35-C36-C37-C38
28	B	629	LMG	C35-C36-C37-C38
28	M	101	LMG	C22-C23-C24-C25
23	D	401	PHO	O1D-CGD-O2D-CED
34	E	101	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
22	B	609	CLA	C16-C17-C18-C19
22	b	601	CLA	C8-C10-C11-C12
22	b	603	CLA	C4-C3-C5-C6
33	M	102	STE	C5-C6-C7-C8
22	B	613	CLA	C11-C10-C8-C7
22	b	604	CLA	C11-C12-C13-C15
22	b	613	CLA	C11-C10-C8-C7
22	b	615	CLA	C6-C7-C8-C10
22	c	508	CLA	C6-C7-C8-C10
27	a	410	PL9	C38-C39-C41-C42
33	B	625	STE	O2-C1-C2-C3
22	B	605	CLA	C4C-C3C-CAC-CBC
29	a	412	SQD	C16-C17-C18-C19
34	d	408	LHG	C11-C10-C9-C8
28	b	623	LMG	C2-C1-O1-C7
22	A	411	CLA	C16-C17-C18-C20
29	b	619	SQD	C19-C20-C21-C22
34	e	102	LHG	C19-C20-C21-C22
28	b	621	LMG	C12-C13-C14-C15
34	D	408	LHG	C14-C15-C16-C17
22	b	604	CLA	C10-C11-C12-C13
33	b	622	STE	O1-C1-C2-C3
33	B	626	STE	C4-C5-C6-C7
22	c	511	CLA	C15-C16-C17-C18
22	B	610	CLA	C16-C17-C18-C20
22	B	615	CLA	C16-C17-C18-C20
28	D	410	LMG	C37-C38-C39-C40
22	C	512	CLA	CBA-CGA-O2A-C1
23	d	401	PHO	C4C-C3C-CAC-CBC
22	B	613	CLA	CAA-CBA-CGA-O2A
28	B	629	LMG	O10-C28-C29-C30
22	C	514	CLA	C4-C3-C5-C6
27	d	405	PL9	C40-C39-C41-C42
28	B	629	LMG	C22-C23-C24-C25
22	A	403	CLA	C11-C10-C8-C9
22	A	411	CLA	C14-C13-C15-C16
22	B	613	CLA	C11-C10-C8-C9
22	b	605	CLA	C14-C13-C15-C16
22	b	613	CLA	C11-C12-C13-C14
22	c	503	CLA	C11-C12-C13-C14
22	c	508	CLA	C11-C10-C8-C9
22	c	510	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	a	404	PHO	C6-C7-C8-C9
30	C	516	DGD	O6D-C5D-C6D-O5D
22	B	602	CLA	CAD-CBD-CGD-O2D
22	B	604	CLA	CAD-CBD-CGD-O2D
22	B	605	CLA	CAD-CBD-CGD-O2D
22	B	606	CLA	CAD-CBD-CGD-O2D
22	C	502	CLA	CAD-CBD-CGD-O2D
22	C	504	CLA	CAD-CBD-CGD-O2D
22	C	511	CLA	CAD-CBD-CGD-O2D
22	C	513	CLA	CAD-CBD-CGD-O2D
22	a	402	CLA	CAD-CBD-CGD-O2D
22	b	603	CLA	CAD-CBD-CGD-O2D
22	c	514	CLA	CAD-CBD-CGD-O2D
29	A	414	SQD	C24-C25-C26-C27
30	H	102	DGD	C4A-C5A-C6A-C7A
28	c	524	LMG	C36-C37-C38-C39
30	H	102	DGD	CCB-CDB-CEB-CFB
30	h	102	DGD	O1B-C1B-C2B-C3B
24	D	404	BCR	C22-C23-C24-C25
22	C	507	CLA	C4-C3-C5-C6
22	B	604	CLA	C16-C17-C18-C20
22	C	514	CLA	C2-C3-C5-C6
22	B	602	CLA	CAA-CBA-CGA-O2A
22	B	614	CLA	CAA-CBA-CGA-O2A
28	d	409	LMG	O7-C10-C11-C12
34	B	622	LHG	O7-C7-C8-C9
34	D	409	LHG	O8-C23-C24-C25
24	a	406	BCR	C21-C22-C23-C24
24	c	517	BCR	C21-C22-C23-C24
22	b	609	CLA	O1D-CGD-O2D-CED
23	a	404	PHO	C2C-C3C-CAC-CBC
23	d	401	PHO	C2C-C3C-CAC-CBC
28	M	101	LMG	O1-C7-C8-C9
29	b	619	SQD	C44-C45-C46-O48
35	v	201	HEC	CAD-CBD-CGD-O2D
22	c	514	CLA	C15-C16-C17-C18
22	B	602	CLA	O2A-C1-C2-C3
22	C	510	CLA	O2A-C1-C2-C3
22	D	403	CLA	O2A-C1-C2-C3
22	d	402	CLA	O2A-C1-C2-C3
23	a	404	PHO	O2A-C1-C2-C3
22	b	609	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
28	D	406	LMG	C38-C39-C40-C41
33	B	626	STE	C7-C8-C9-C10
30	C	517	DGD	C8A-C9A-CAA-CBA
33	M	102	STE	C1-C2-C3-C4
22	A	403	CLA	CHA-CBD-CGD-O1D
22	A	403	CLA	CHA-CBD-CGD-O2D
22	B	603	CLA	CHA-CBD-CGD-O2D
22	B	607	CLA	CHA-CBD-CGD-O2D
22	B	613	CLA	CHA-CBD-CGD-O1D
22	C	505	CLA	CHA-CBD-CGD-O2D
22	C	507	CLA	CHA-CBD-CGD-O1D
22	a	403	CLA	CHA-CBD-CGD-O1D
22	a	403	CLA	CHA-CBD-CGD-O2D
22	b	610	CLA	CHA-CBD-CGD-O1D
22	b	610	CLA	CHA-CBD-CGD-O2D
22	c	505	CLA	CHA-CBD-CGD-O2D
22	c	508	CLA	CHA-CBD-CGD-O2D
22	c	509	CLA	CHA-CBD-CGD-O1D
22	c	509	CLA	CHA-CBD-CGD-O2D
35	V	201	HEC	CAD-CBD-CGD-O1D
29	A	414	SQD	O48-C23-C24-C25
22	b	615	CLA	CBA-CGA-O2A-C1
28	C	519	LMG	C11-C12-C13-C14
33	d	411	STE	C5-C6-C7-C8
28	C	519	LMG	O1-C7-C8-O7
29	A	413	SQD	O47-C45-C46-O48
29	A	414	SQD	C31-C32-C33-C34
30	C	518	DGD	C8A-C9A-CAA-CBA
22	C	514	CLA	C13-C15-C16-C17
33	B	625	STE	O1-C1-C2-C3
28	b	621	LMG	O8-C28-C29-C30
34	E	101	LHG	C10-C11-C12-C13
35	v	201	HEC	CAD-CBD-CGD-O1D
23	d	401	PHO	CHA-CBD-CGD-O1D
30	H	102	DGD	CBB-CCB-CDB-CEB
22	B	606	CLA	C2-C3-C5-C6
22	B	616	CLA	C12-C13-C15-C16
22	C	507	CLA	C2-C3-C5-C6
22	C	512	CLA	C6-C7-C8-C10
22	b	605	CLA	C11-C12-C13-C15
22	b	614	CLA	C12-C13-C15-C16
29	a	412	SQD	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
28	A	412	LMG	O6-C1-O1-C7
29	B	623	SQD	C11-C10-C9-C8
33	B	626	STE	C11-C10-C9-C8
34	e	102	LHG	C17-C18-C19-C20
22	B	605	CLA	C11-C12-C13-C14
22	B	616	CLA	C11-C10-C8-C9
22	C	505	CLA	C11-C10-C8-C9
22	C	506	CLA	C6-C7-C8-C9
22	C	507	CLA	C14-C13-C15-C16
22	C	510	CLA	C11-C12-C13-C14
22	b	601	CLA	C14-C13-C15-C16
22	b	605	CLA	C11-C12-C13-C14
22	b	607	CLA	C11-C10-C8-C9
22	b	614	CLA	C14-C13-C15-C16
22	c	509	CLA	C14-C13-C15-C16
27	A	410	PL9	C44-C46-C47-C48
22	B	611	CLA	C15-C16-C17-C18
33	b	624	STE	C10-C11-C12-C13
29	a	412	SQD	O47-C7-C8-C9
22	B	613	CLA	CAA-CBA-CGA-O1A
29	b	619	SQD	C11-C12-C13-C14
22	C	512	CLA	O1A-CGA-O2A-C1
30	H	102	DGD	CDB-CEB-CFB-CGB
34	d	408	LHG	C24-C25-C26-C27
22	B	602	CLA	C1A-C2A-CAA-CBA
22	B	603	CLA	C1A-C2A-CAA-CBA
22	B	608	CLA	C1A-C2A-CAA-CBA
33	b	624	STE	C7-C8-C9-C10
34	B	622	LHG	C30-C31-C32-C33
30	c	520	DGD	C8B-C9B-CAB-CBB
34	D	412	LHG	C10-C11-C12-C13
28	D	406	LMG	C16-C17-C18-C19
34	D	409	LHG	C28-C29-C30-C31
22	B	602	CLA	CAA-CBA-CGA-O1A
29	A	414	SQD	O10-C23-C24-C25
29	B	623	SQD	O10-C23-C24-C25
30	c	519	DGD	O1B-C1B-C2B-C3B
33	b	624	STE	O1-C1-C2-C3
28	c	524	LMG	C38-C39-C40-C41
30	c	521	DGD	C2B-C3B-C4B-C5B
33	J	101	STE	C5-C6-C7-C8
34	D	408	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
34	E	101	LHG	C4-O6-P-O5
34	e	102	LHG	C4-O6-P-O4
34	e	102	LHG	C4-O6-P-O5
22	B	615	CLA	O1D-CGD-O2D-CED
22	C	502	CLA	O1D-CGD-O2D-CED
34	B	622	LHG	C26-C27-C28-C29
24	H	101	BCR	C23-C24-C25-C26
24	a	406	BCR	C5-C6-C7-C8
24	c	518	BCR	C5-C6-C7-C8
24	x	101	BCR	C23-C24-C25-C26
22	B	614	CLA	CAA-CBA-CGA-O1A
22	b	611	CLA	CAA-CBA-CGA-O2A
29	a	413	SQD	C30-C31-C32-C33
24	D	404	BCR	C18-C19-C20-C21
22	B	611	CLA	C2A-CAA-CBA-CGA
22	h	101	CLA	C2A-CAA-CBA-CGA
22	C	507	CLA	O1D-CGD-O2D-CED
22	B	612	CLA	C4-C3-C5-C6
22	b	607	CLA	C4-C3-C5-C6
22	c	510	CLA	C4-C3-C5-C6
27	D	405	PL9	C46-C47-C48-C49
28	c	524	LMG	C40-C41-C42-C43
22	B	610	CLA	CAD-CBD-CGD-O1D
22	B	613	CLA	CAD-CBD-CGD-O1D
22	C	507	CLA	CAD-CBD-CGD-O1D
22	b	608	CLA	CAD-CBD-CGD-O1D
22	c	504	CLA	CAD-CBD-CGD-O1D
34	D	409	LHG	O10-C23-C24-C25
22	a	403	CLA	C13-C15-C16-C17
22	B	616	CLA	C14-C13-C15-C16
22	b	604	CLA	C14-C13-C15-C16
22	b	614	CLA	C11-C10-C8-C9
22	c	510	CLA	C6-C7-C8-C9
22	c	515	CLA	C6-C7-C8-C9
30	H	102	DGD	C8B-C9B-CAB-CBB
29	b	619	SQD	C23-C24-C25-C26
30	h	102	DGD	C1A-C2A-C3A-C4A
28	B	629	LMG	O7-C10-C11-C12
29	A	413	SQD	O47-C7-C8-C9
30	C	516	DGD	O2G-C1B-C2B-C3B
34	l	101	LHG	O9-C7-C8-C9
34	d	406	LHG	C35-C36-C37-C38

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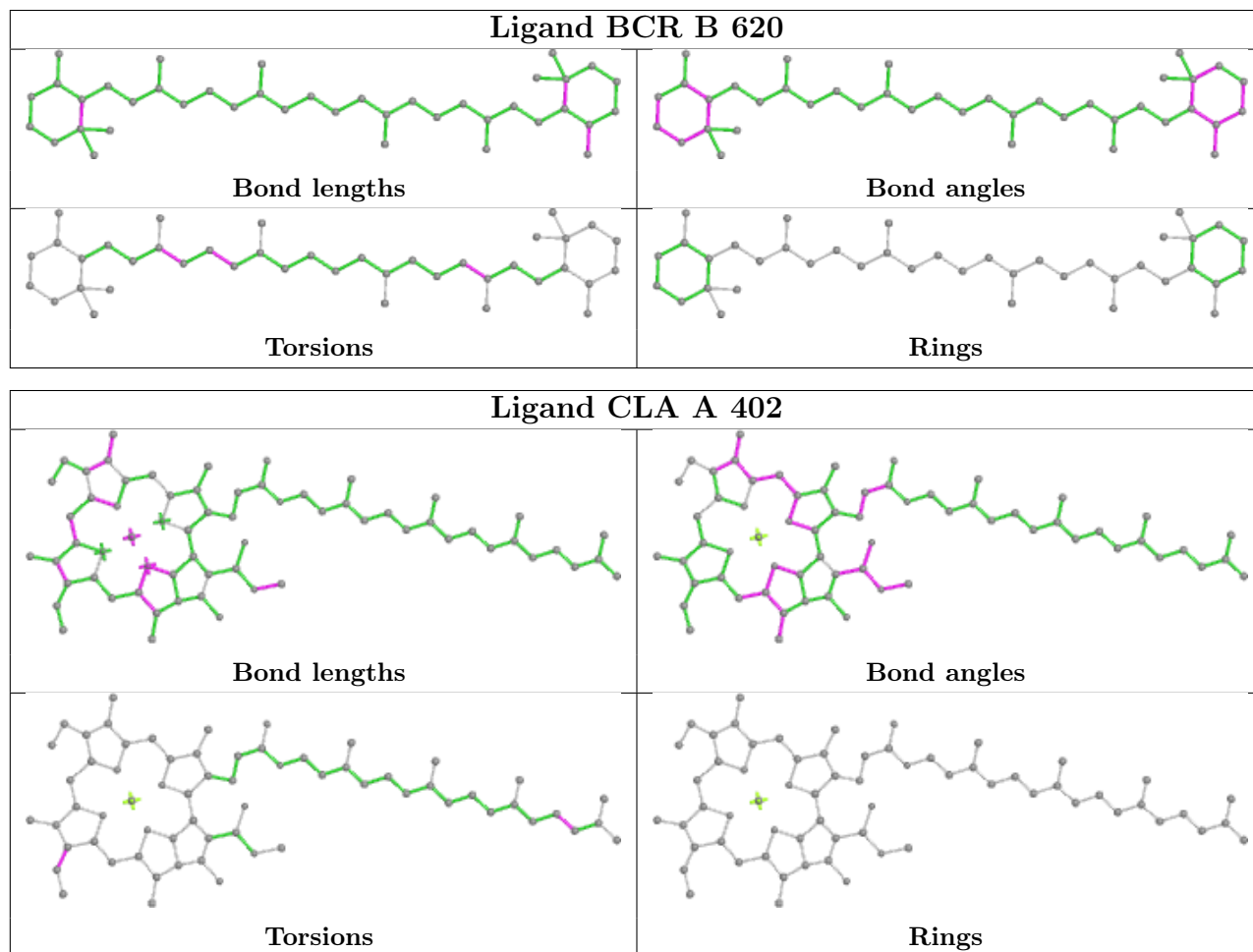
Mol	Chain	Res	Type	Atoms
30	c	521	DGD	O1G-C1A-C2A-C3A
22	C	508	CLA	C5-C6-C7-C8
22	b	613	CLA	C13-C15-C16-C17
27	d	405	PL9	C45-C44-C46-C47
34	d	407	LHG	C26-C27-C28-C29
22	B	603	CLA	C3A-C2A-CAA-CBA
22	B	612	CLA	C11-C10-C8-C7
22	C	510	CLA	C11-C12-C13-C15
22	C	512	CLA	C11-C10-C8-C7
22	b	602	CLA	C6-C7-C8-C10
22	b	604	CLA	C12-C13-C15-C16
22	c	509	CLA	C12-C13-C15-C16
22	c	510	CLA	C6-C7-C8-C10
27	d	405	PL9	C33-C34-C36-C37
29	A	413	SQD	O49-C7-C8-C9
33	d	411	STE	O2-C1-C2-C3
28	M	101	LMG	C34-C35-C36-C37
30	c	519	DGD	O2G-C1B-C2B-C3B
24	B	619	BCR	C7-C8-C9-C10
24	b	618	BCR	C17-C18-C19-C20
22	b	605	CLA	C16-C17-C18-C19
30	c	519	DGD	O6E-C1E-O5D-C6D
22	C	510	CLA	C8-C10-C11-C12
22	b	609	CLA	C15-C16-C17-C18
22	c	512	CLA	CAA-CBA-CGA-O1A
33	M	102	STE	O2-C1-C2-C3
33	d	411	STE	O1-C1-C2-C3
22	C	507	CLA	C15-C16-C17-C18
22	b	607	CLA	C13-C15-C16-C17
28	c	525	LMG	C8-C9-O8-C28
22	c	512	CLA	CAA-CBA-CGA-O2A
35	e	101	HEC	CAA-CBA-CGA-O2A
29	a	412	SQD	O49-C7-C8-C9
23	a	404	PHO	C4-C3-C5-C6
34	E	101	LHG	C14-C15-C16-C17
33	b	624	STE	O2-C1-C2-C3

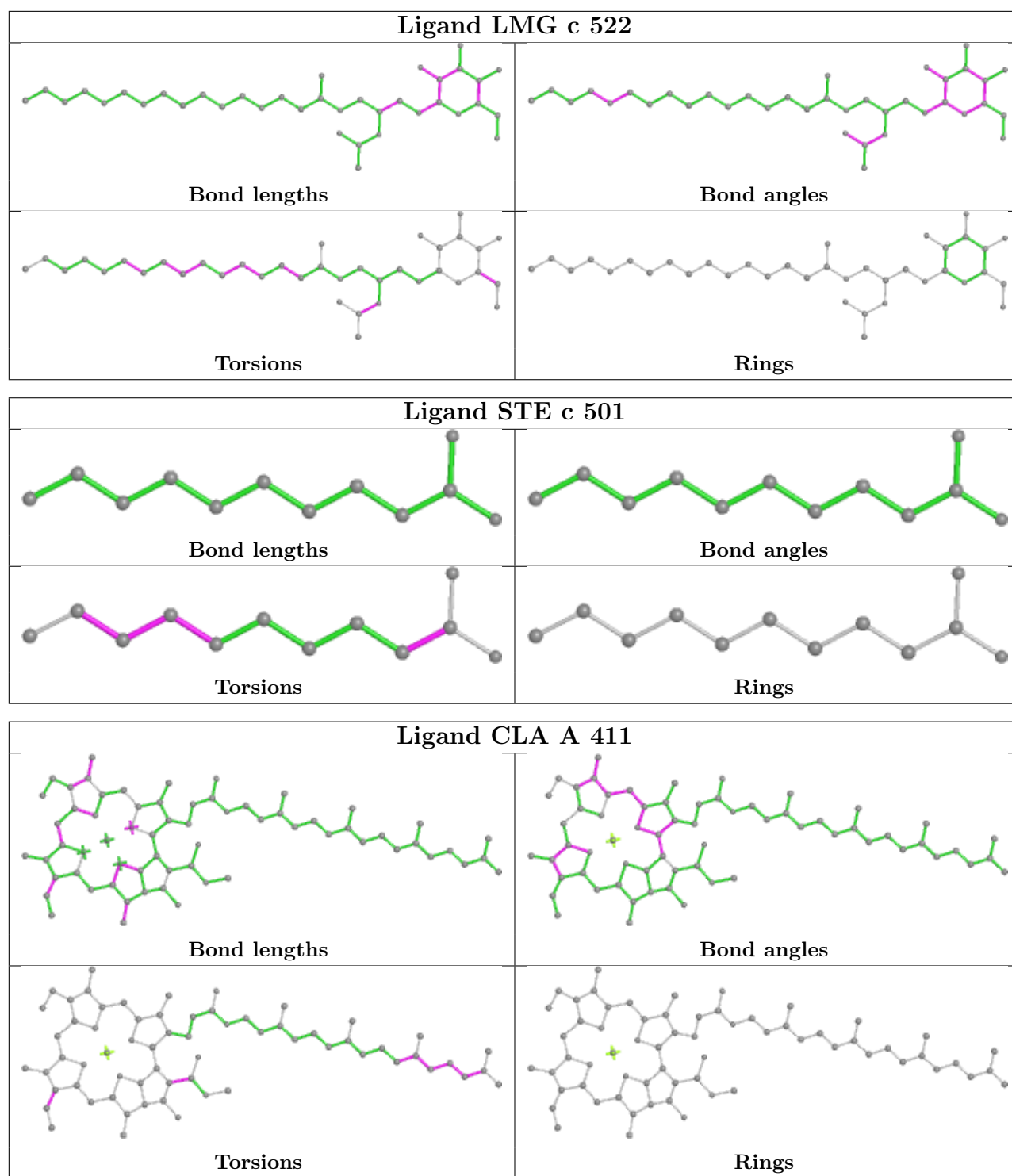
There are no ring outliers.

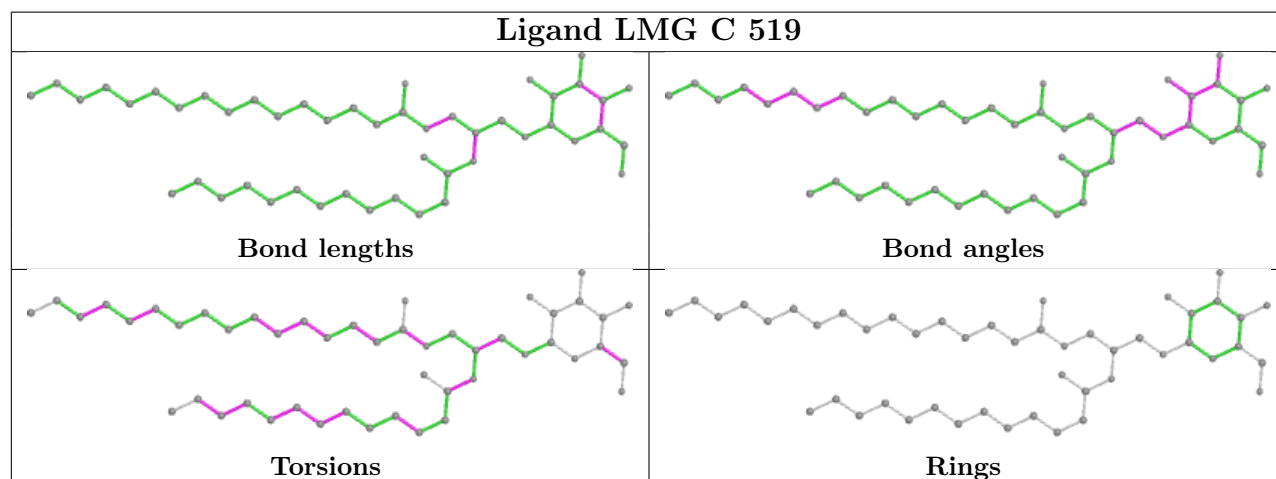
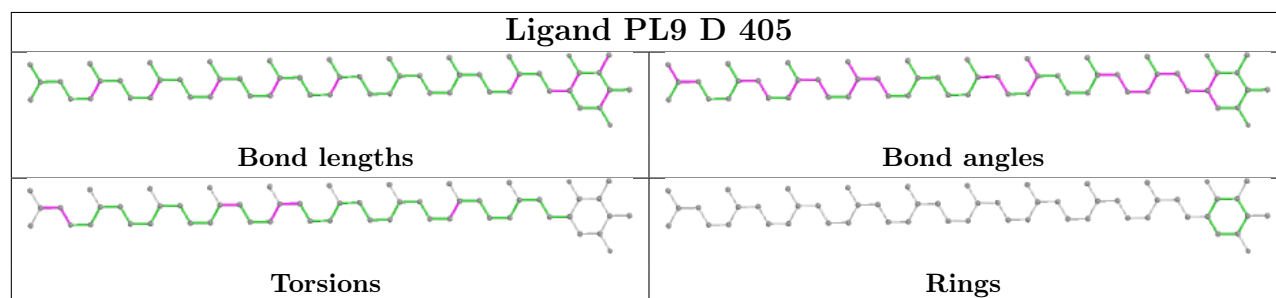
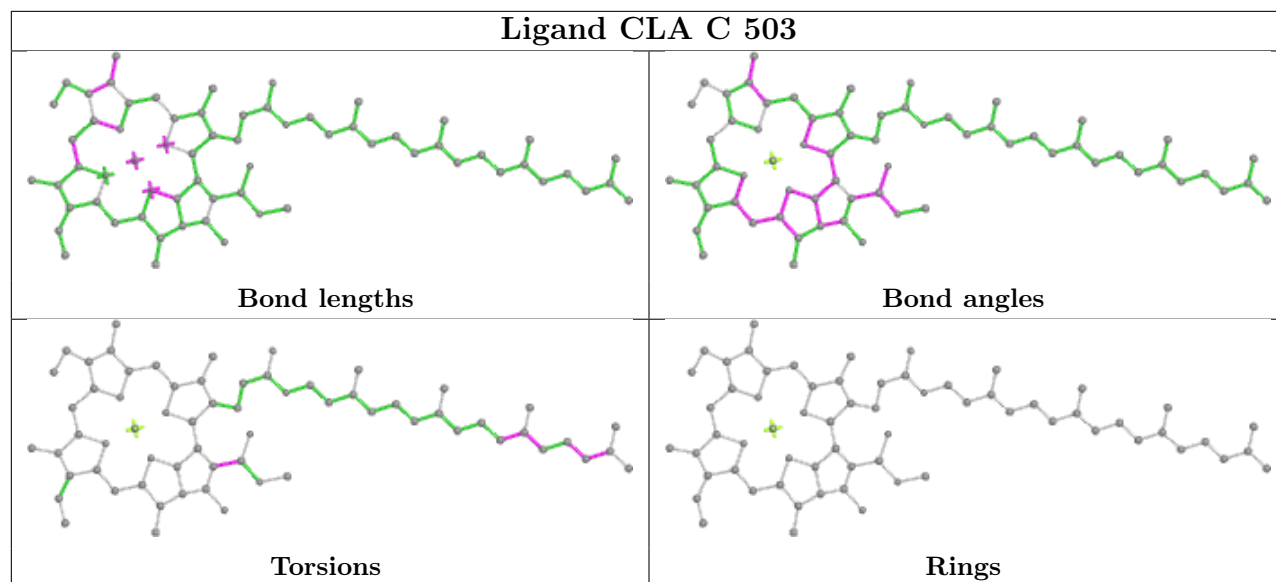
No monomer is involved in short contacts.

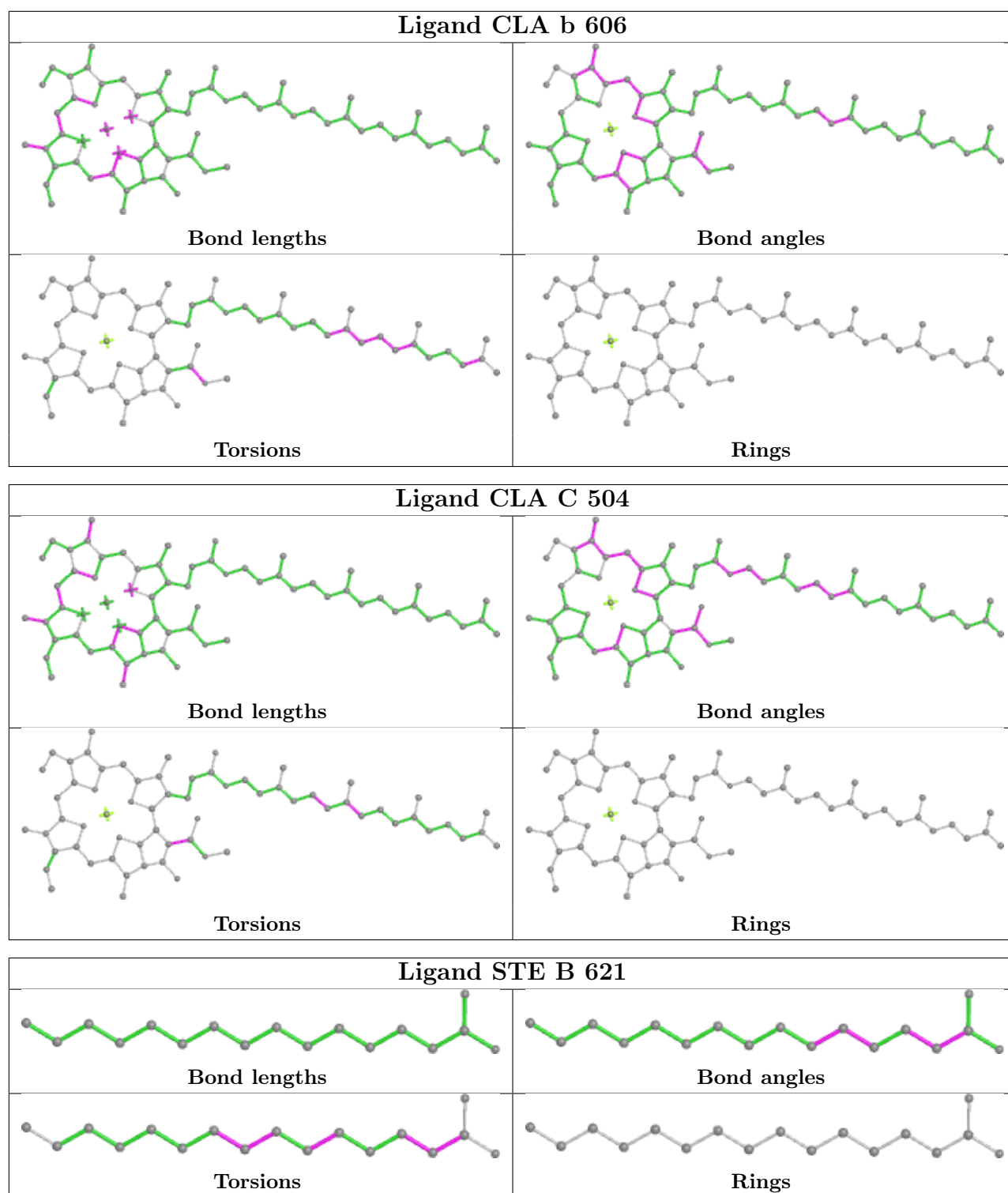
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

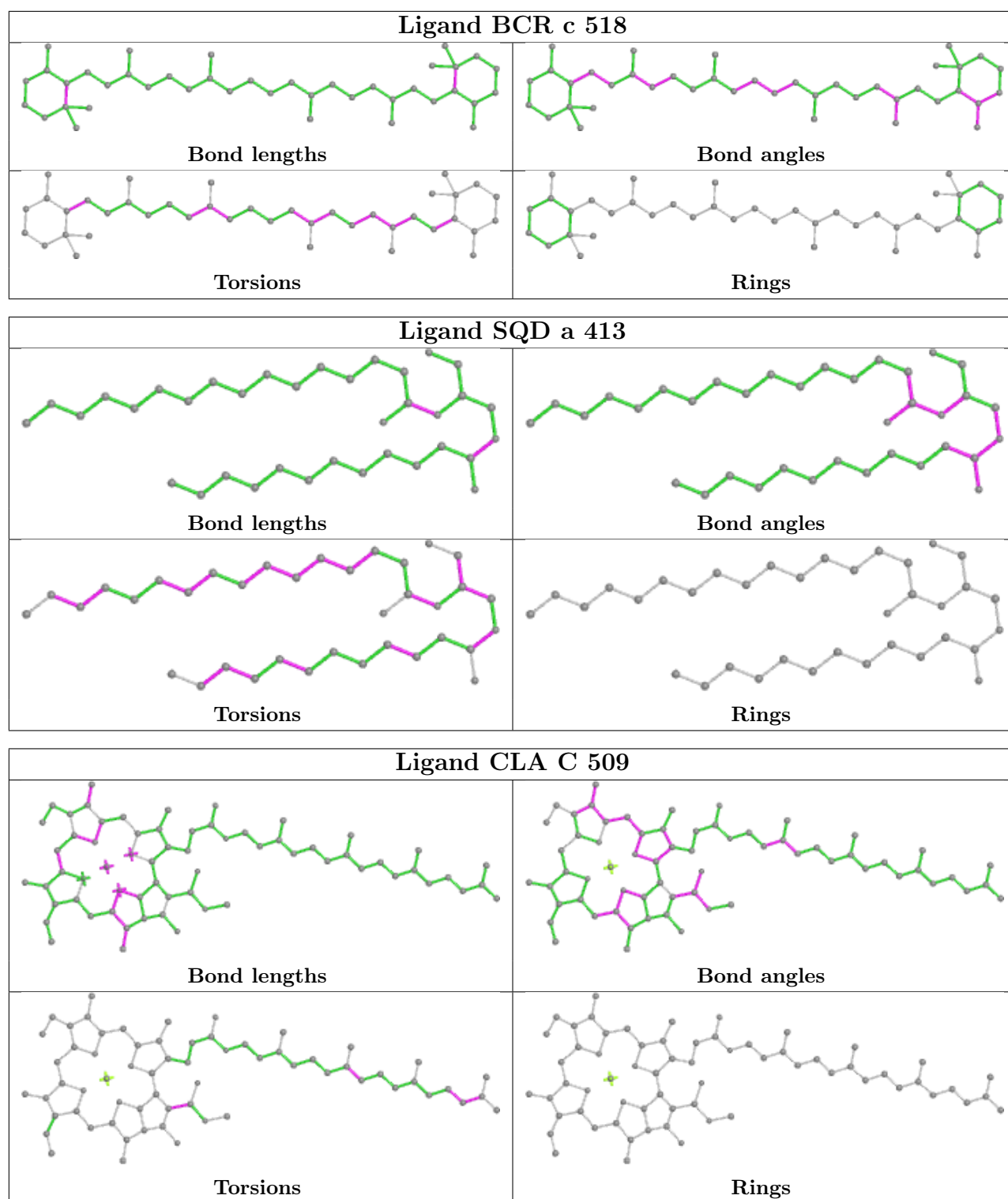
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



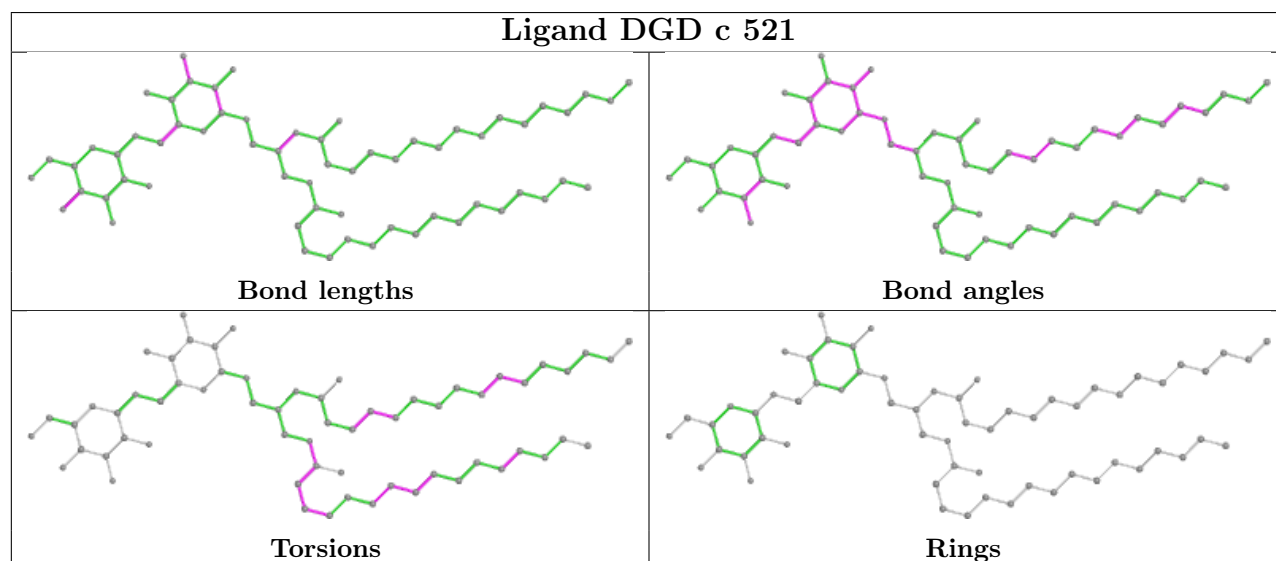
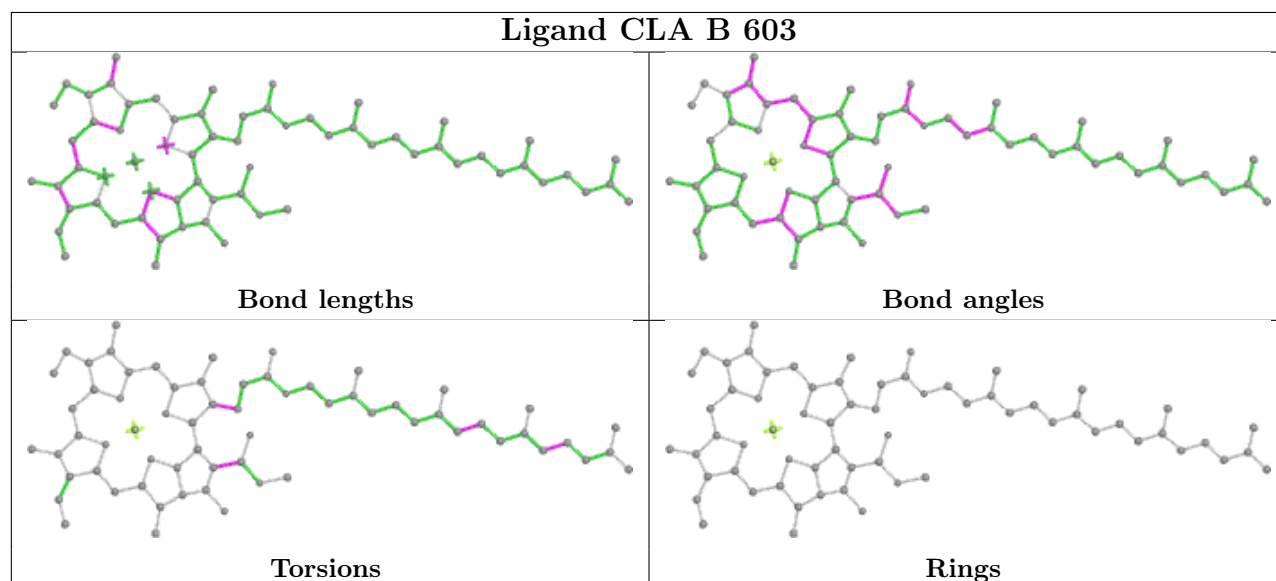
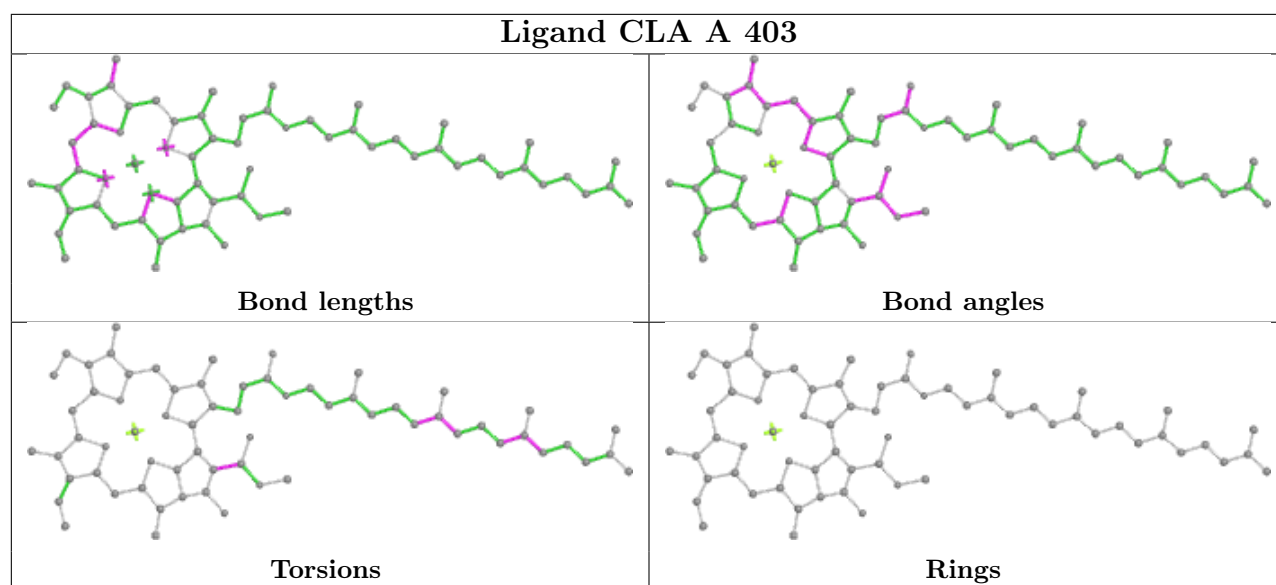


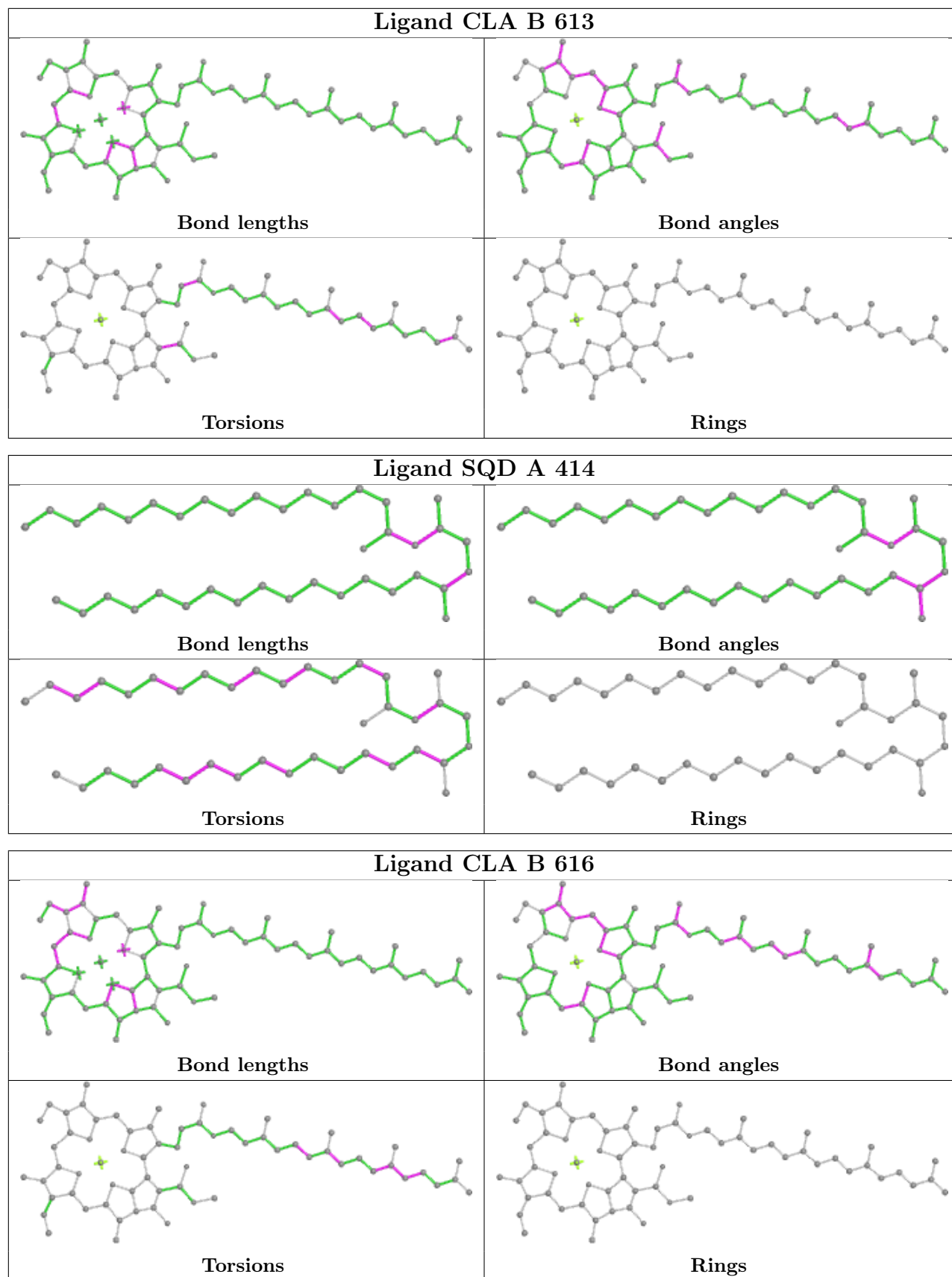


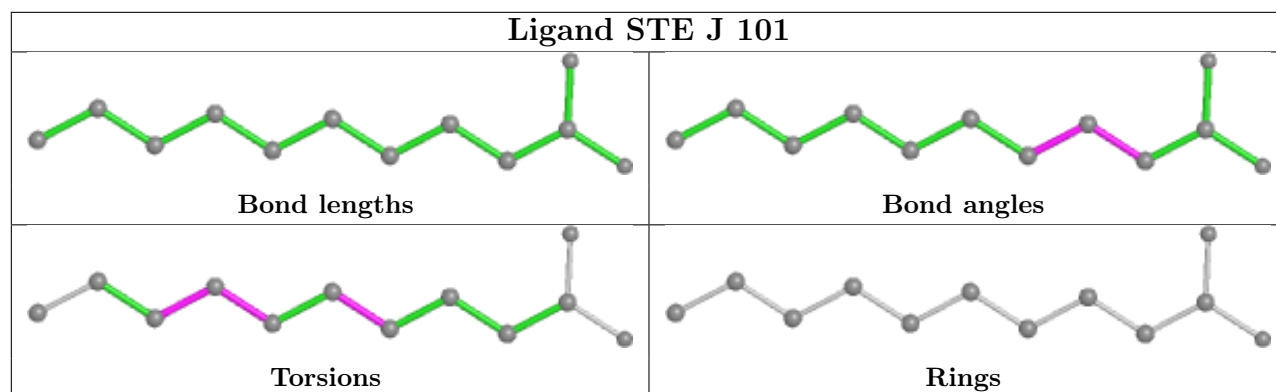
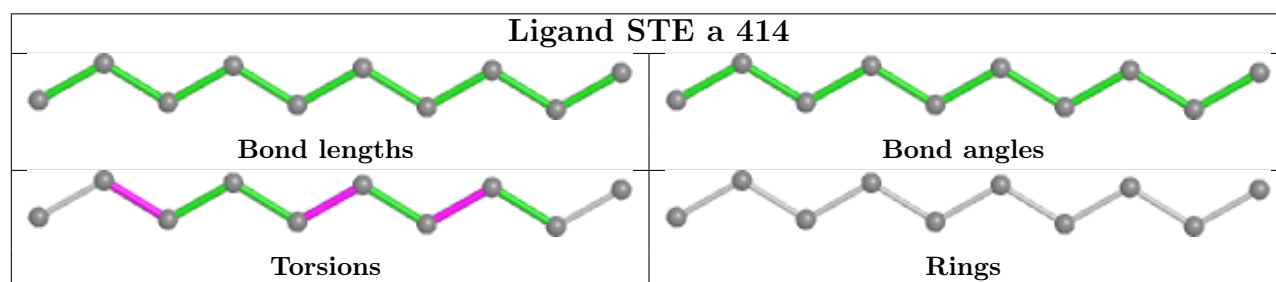
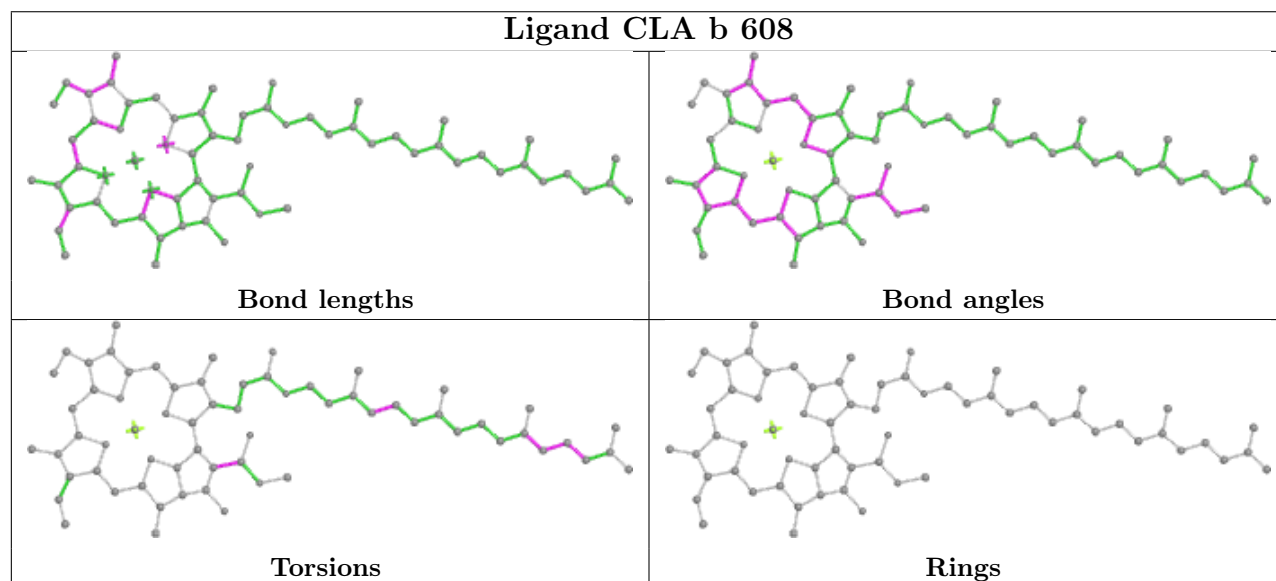
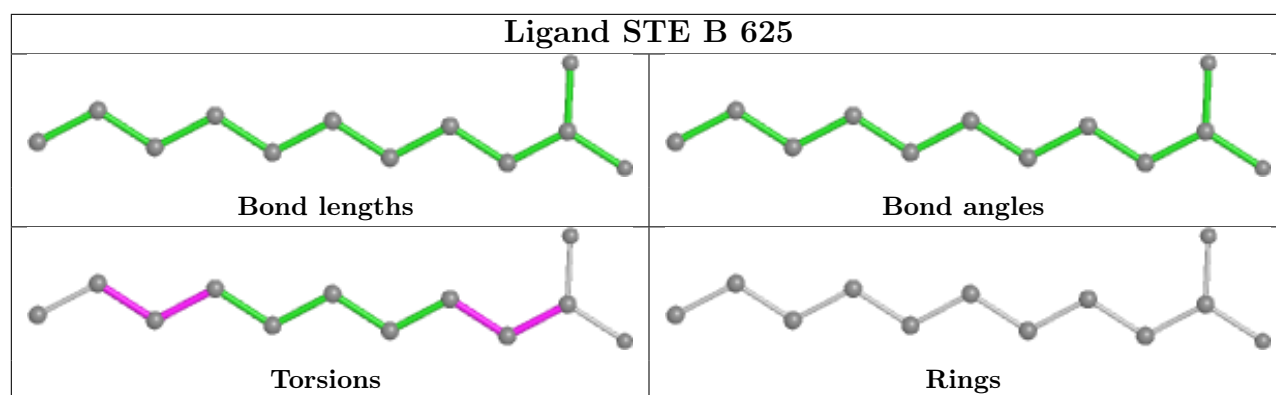


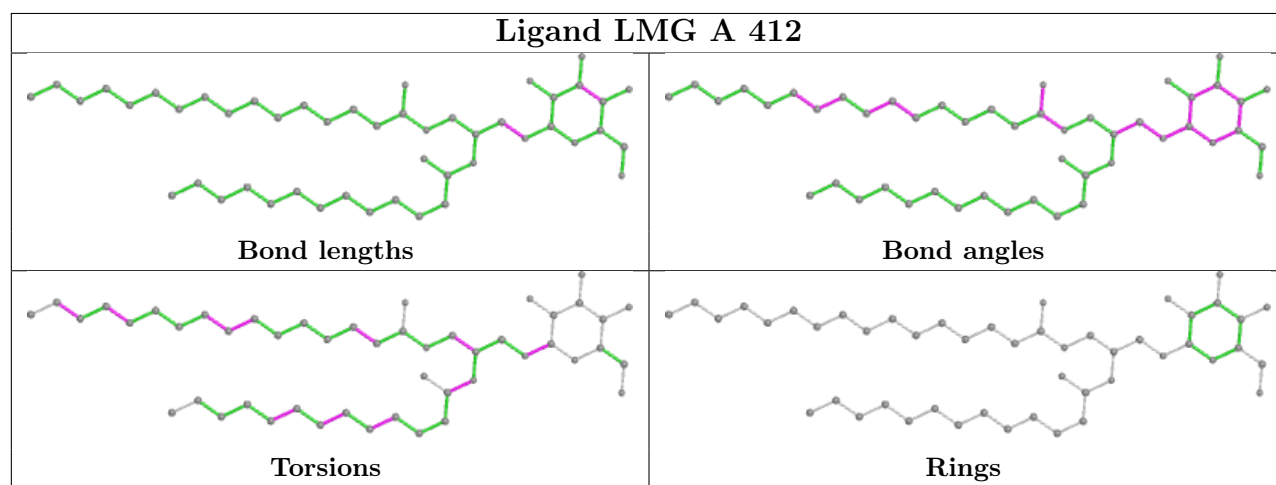
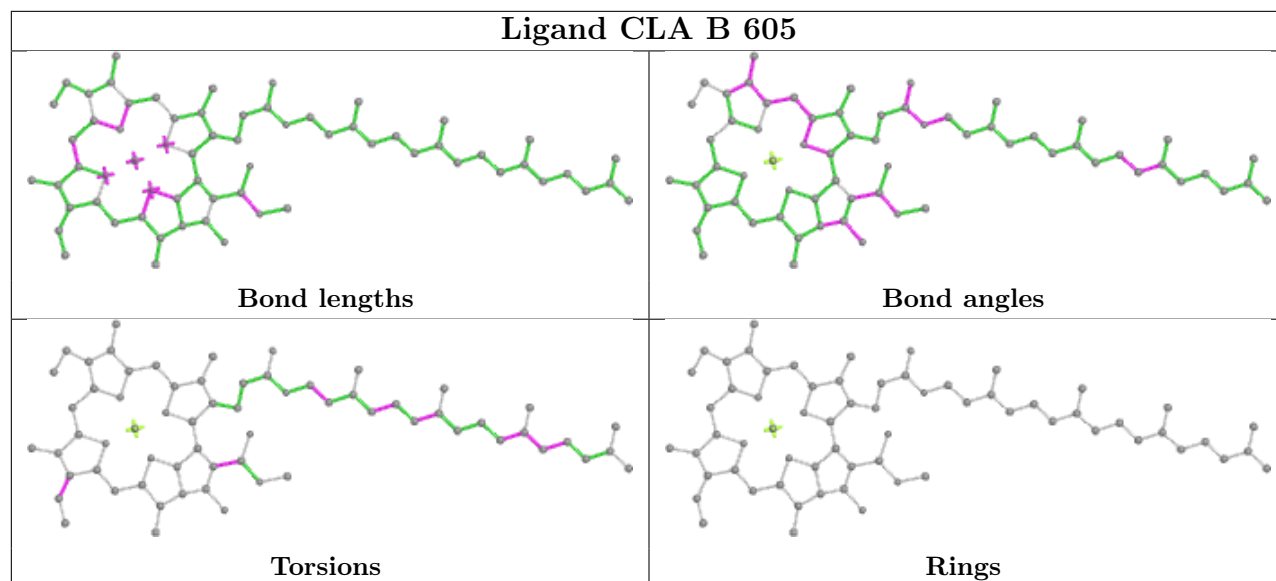
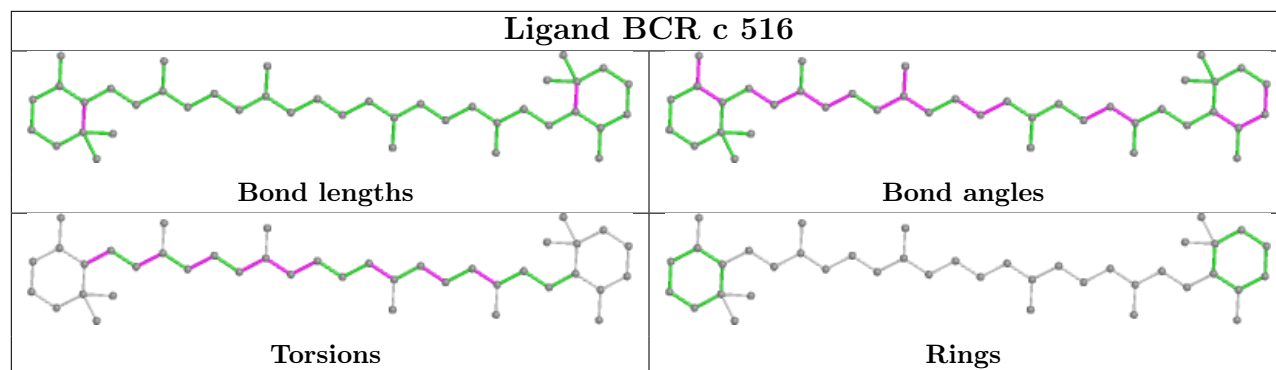


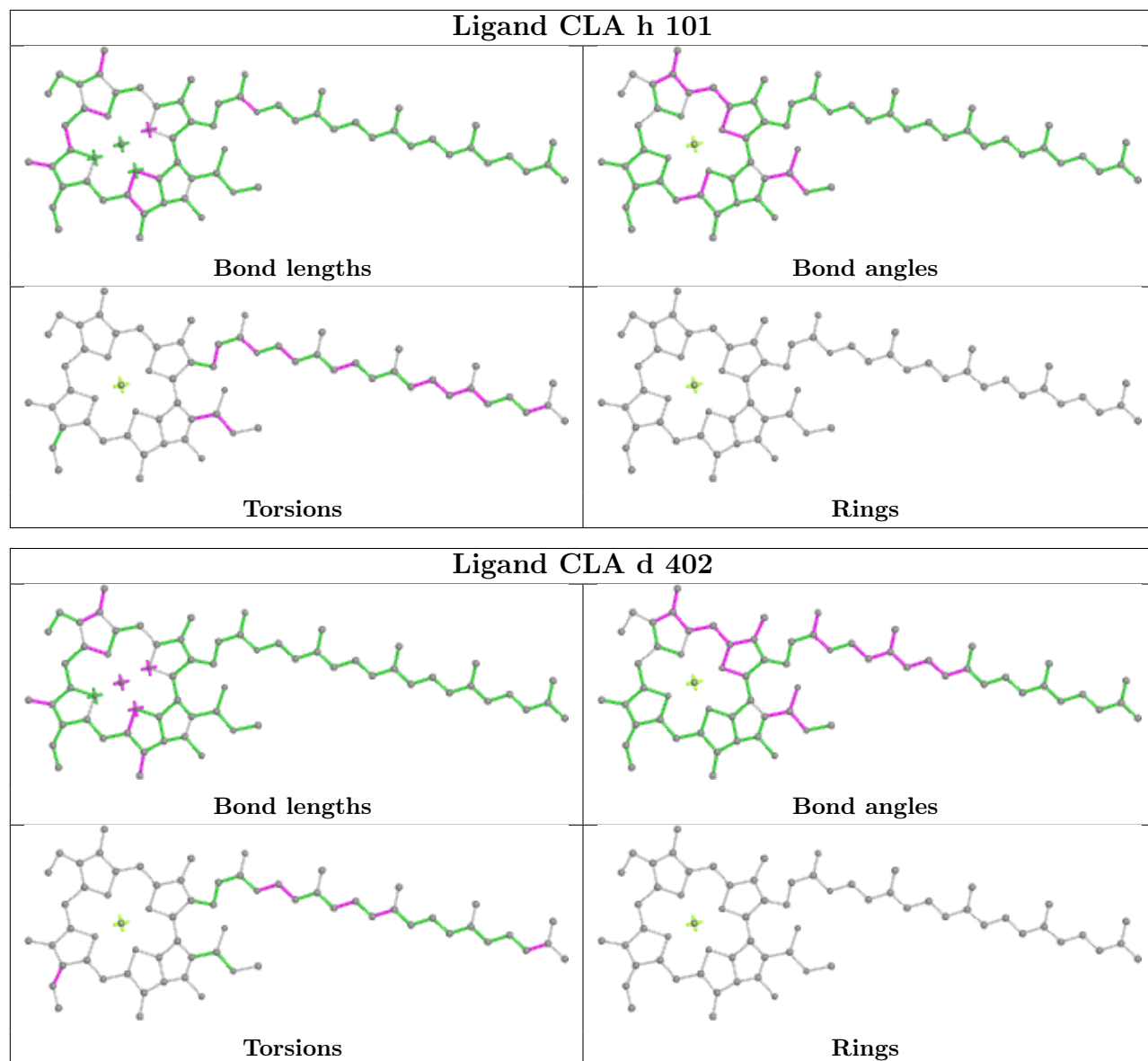


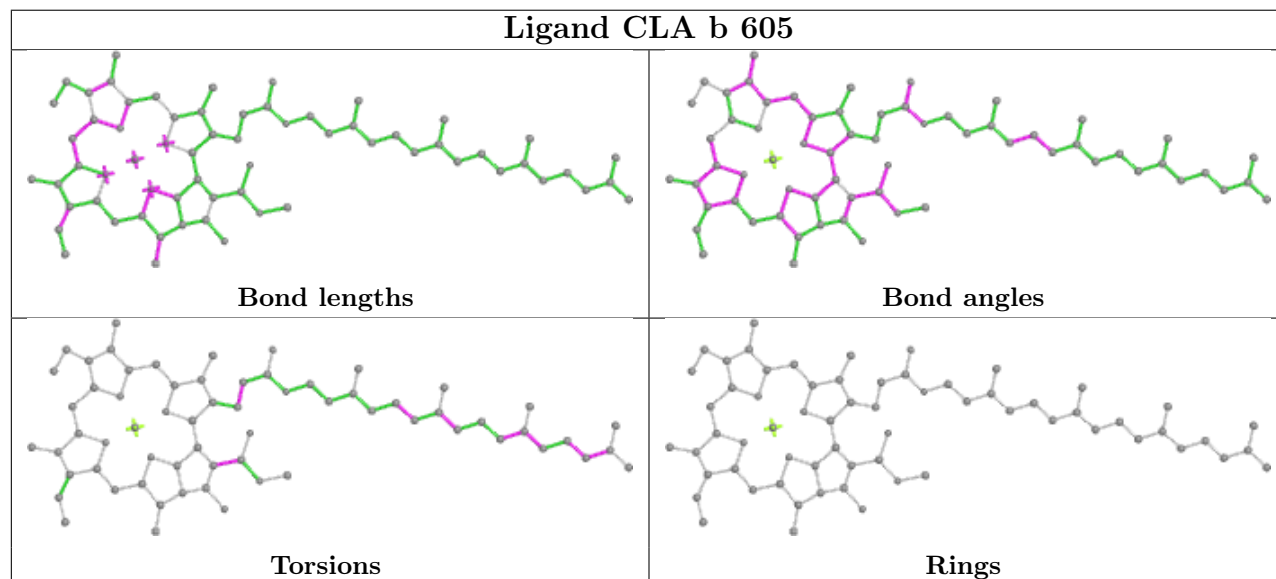
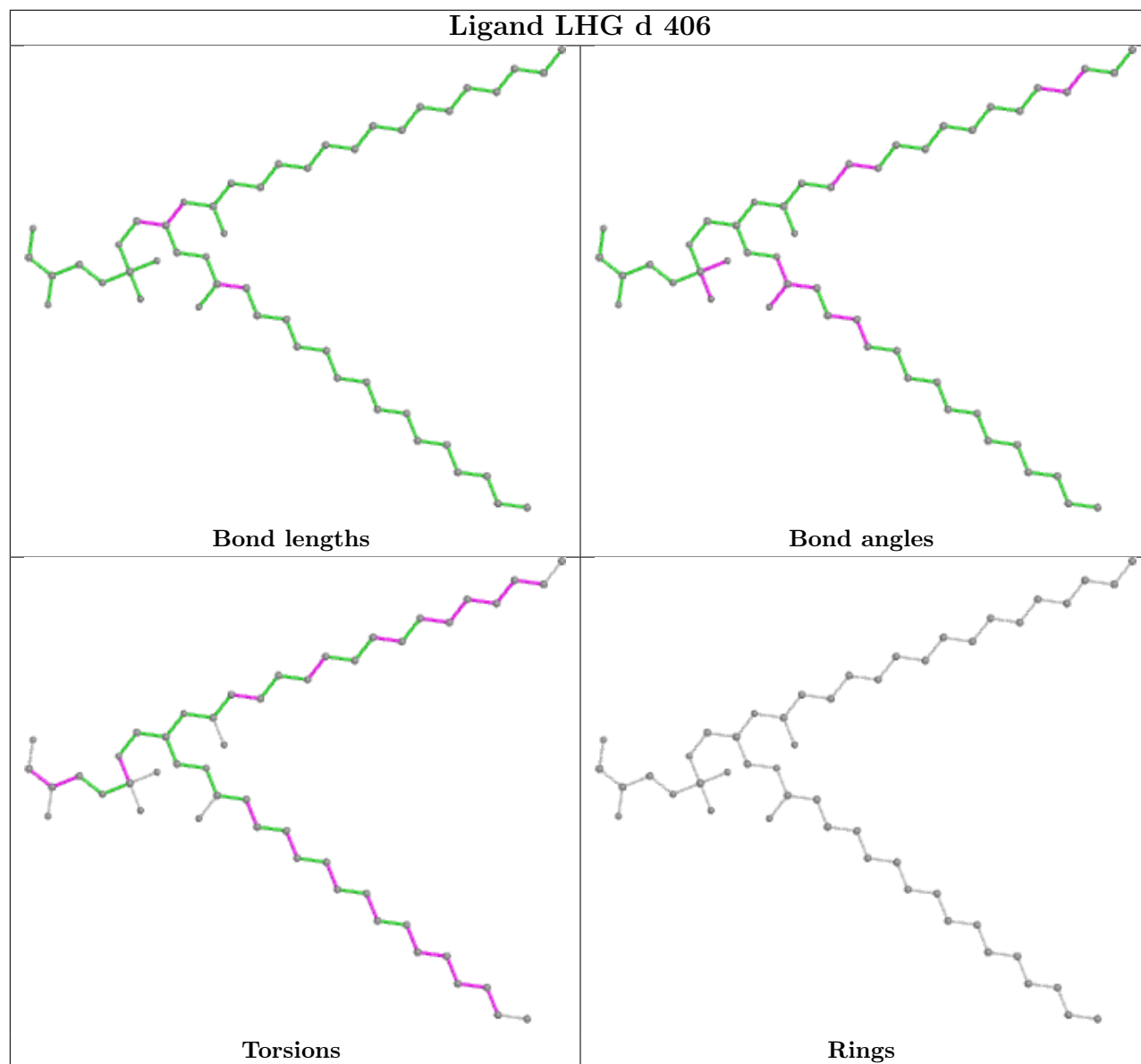


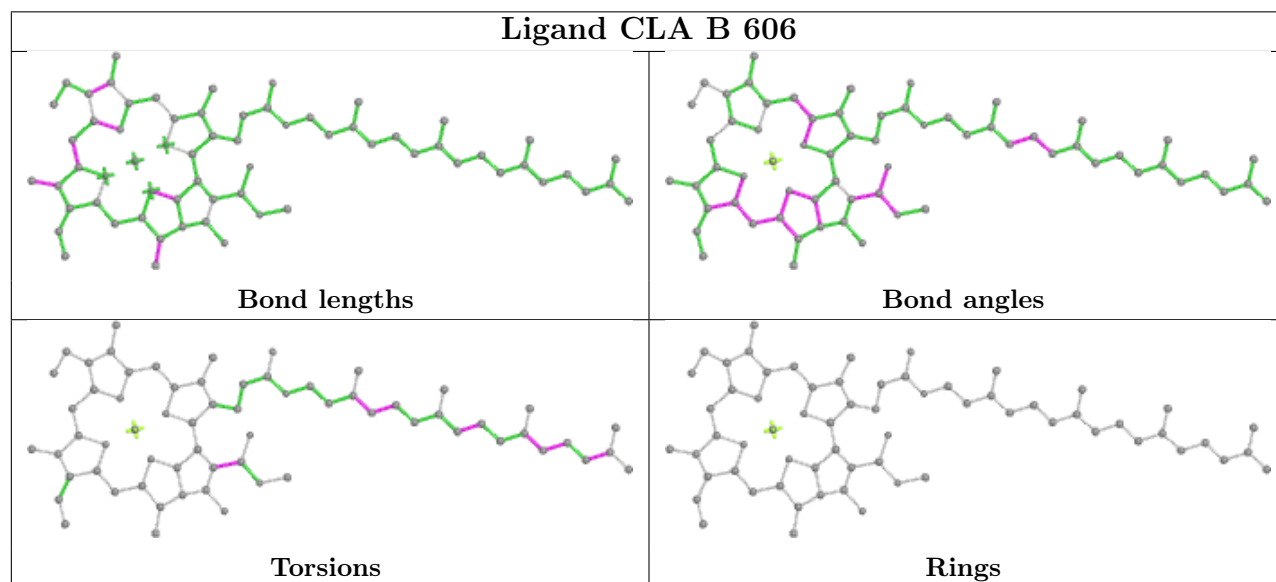
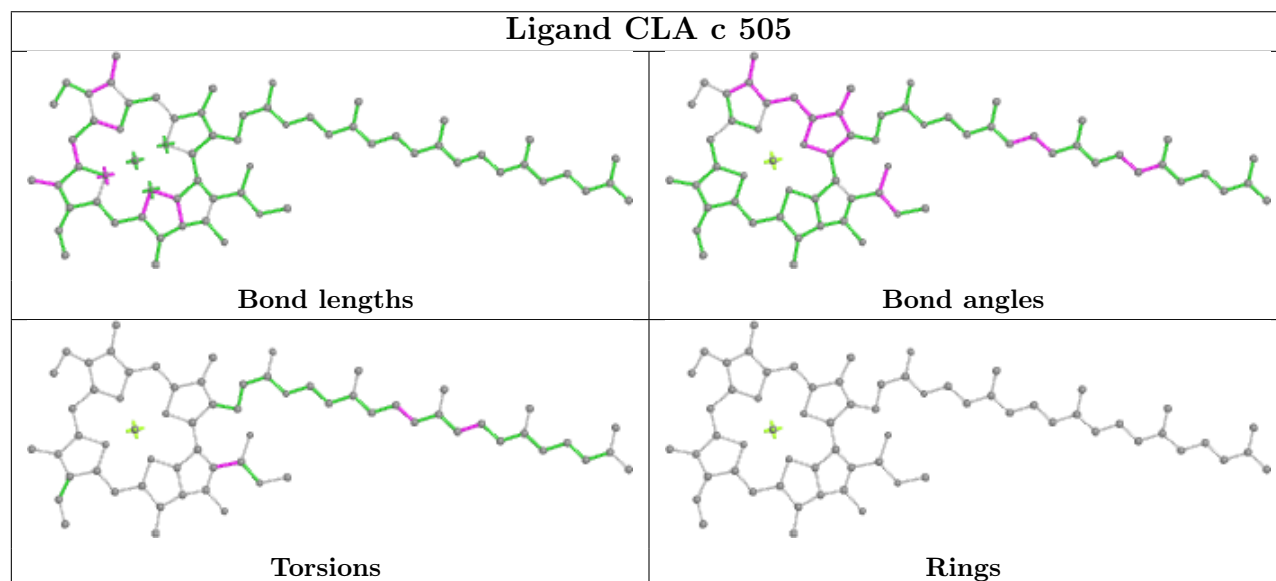
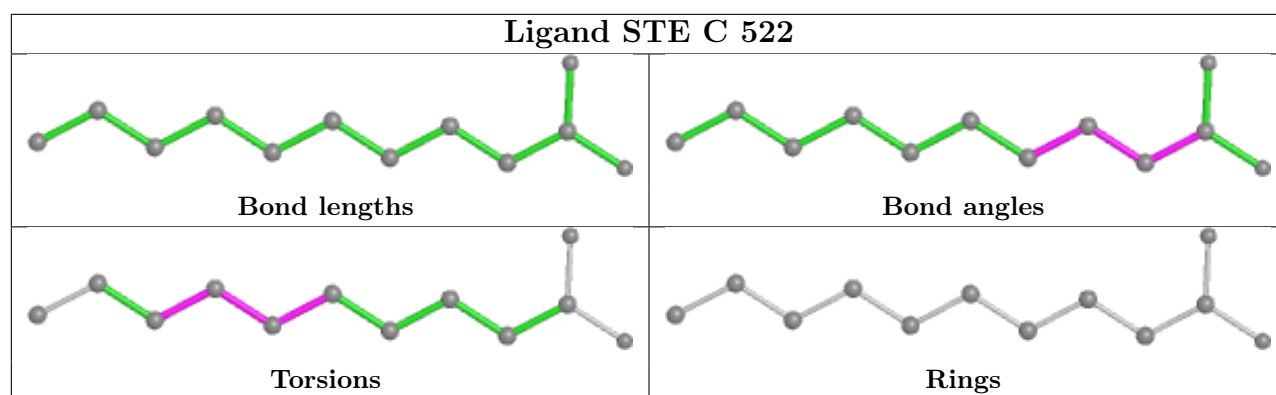


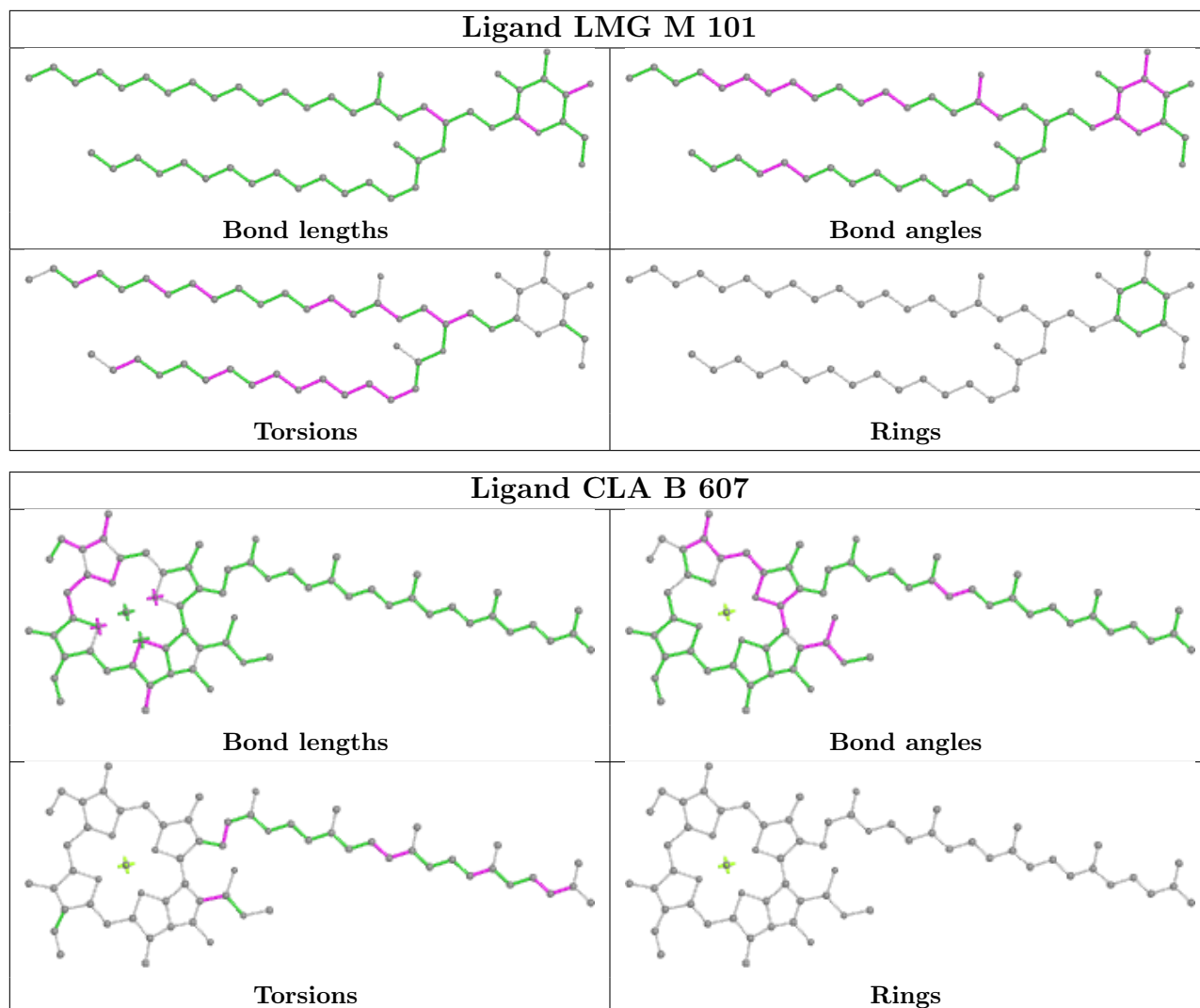




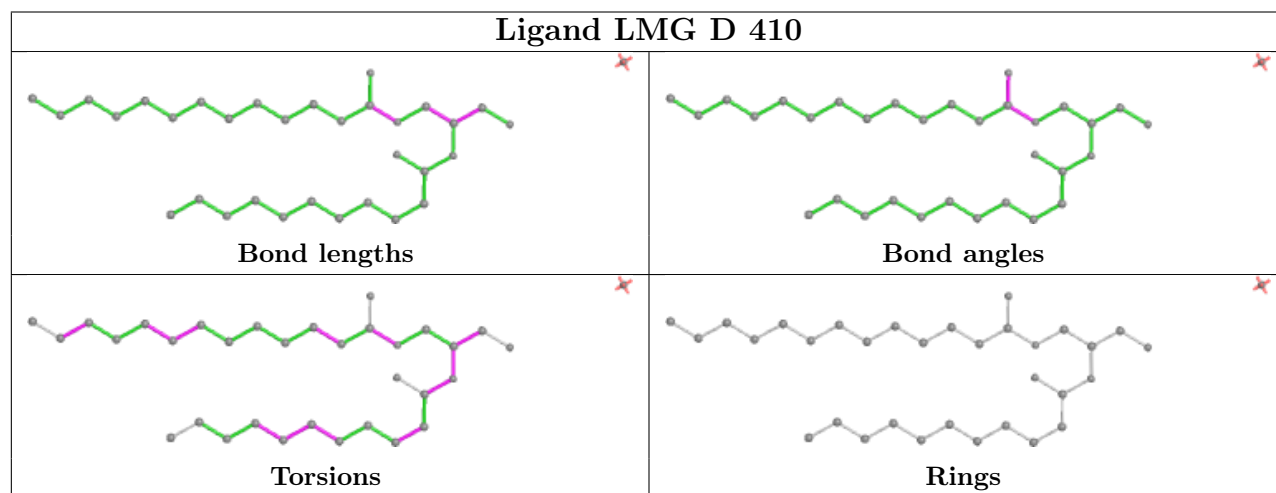
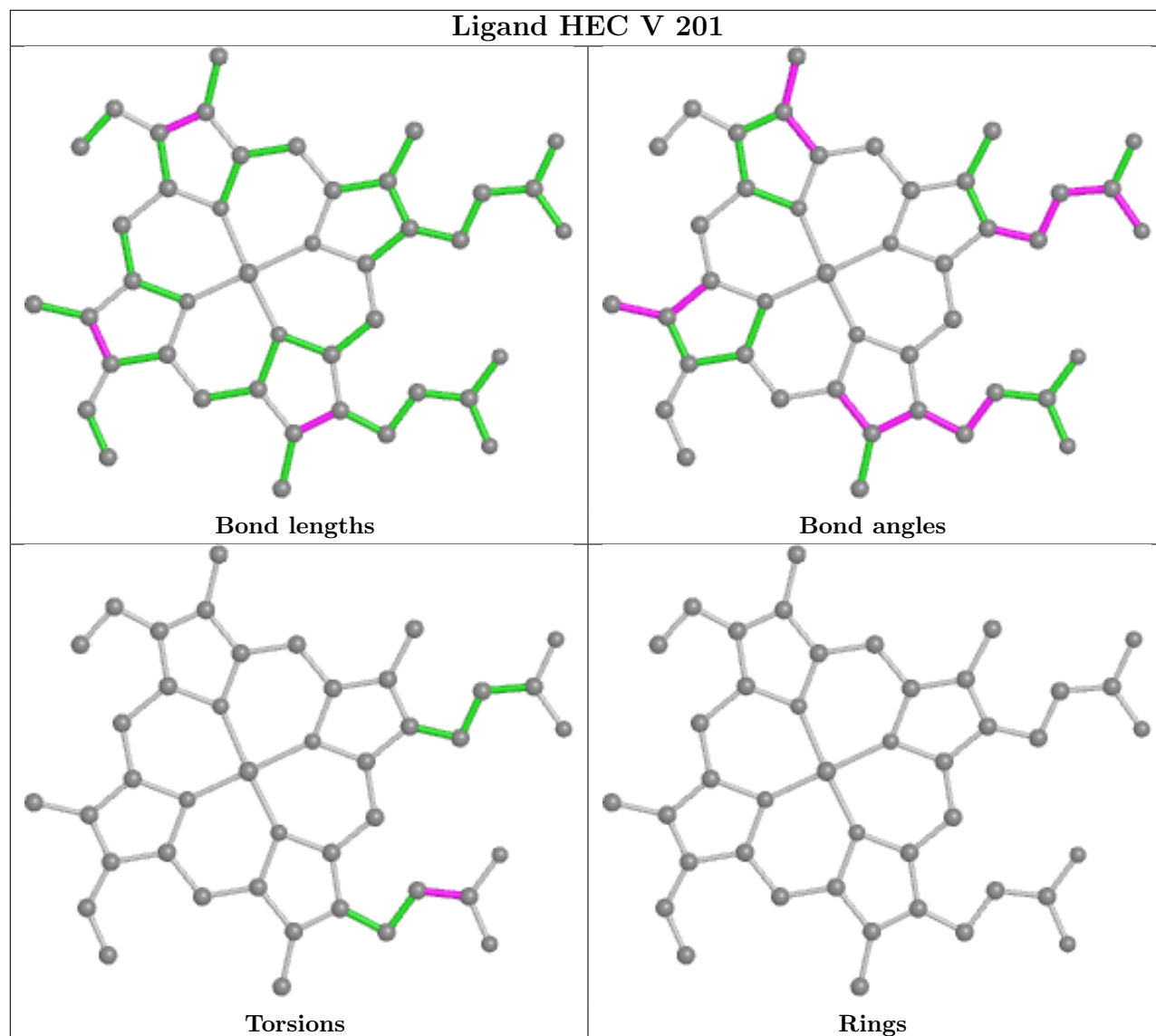


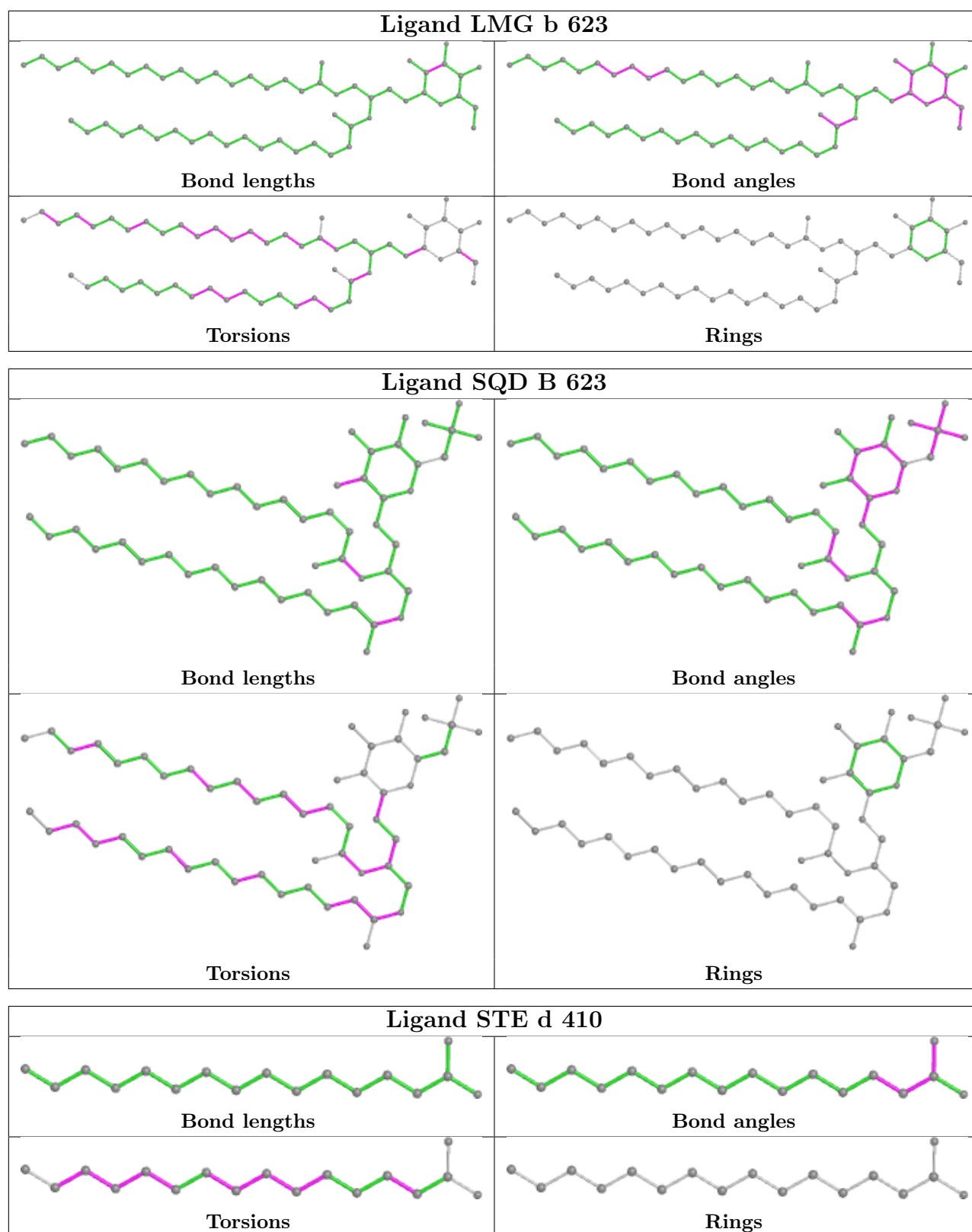


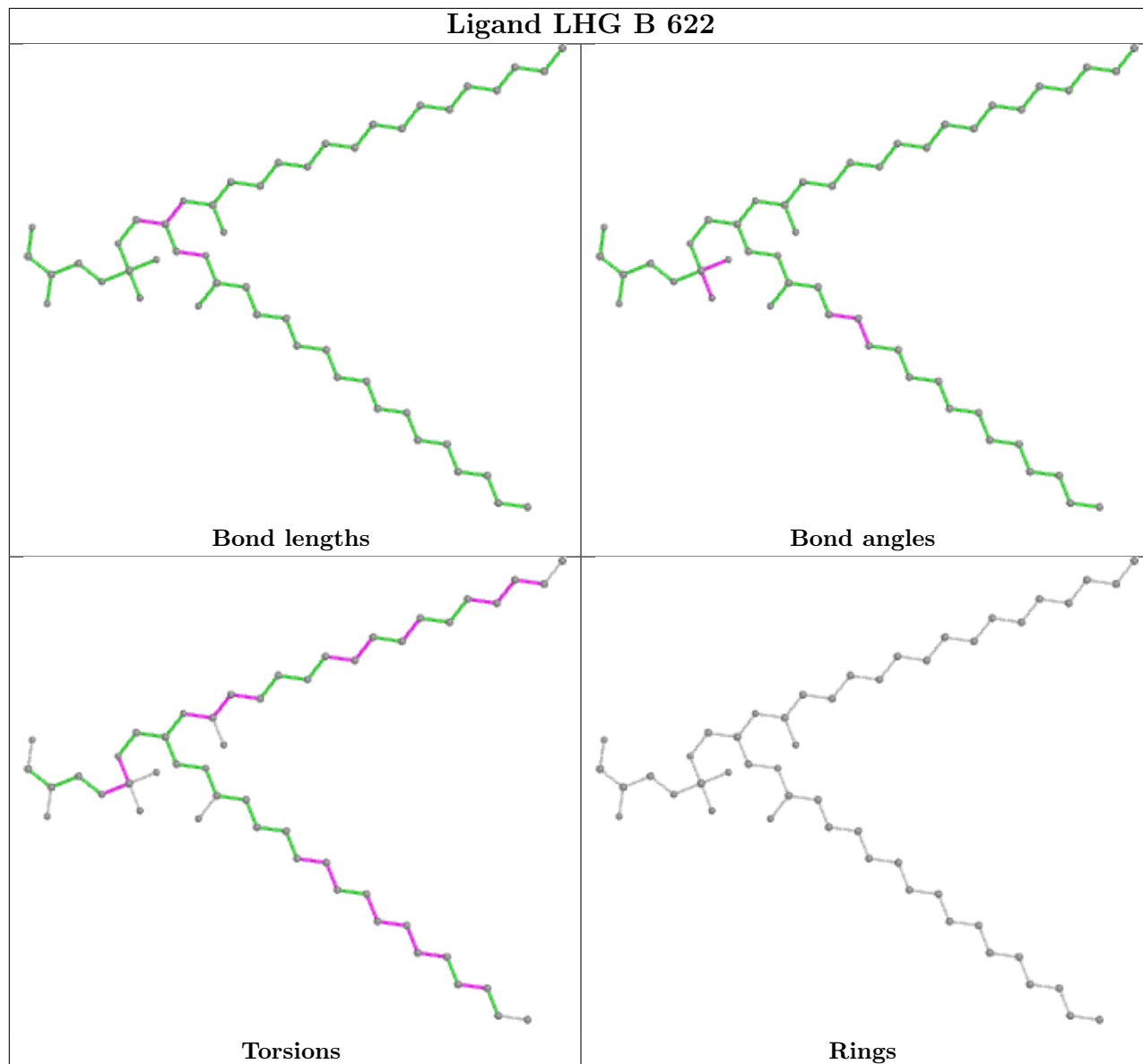
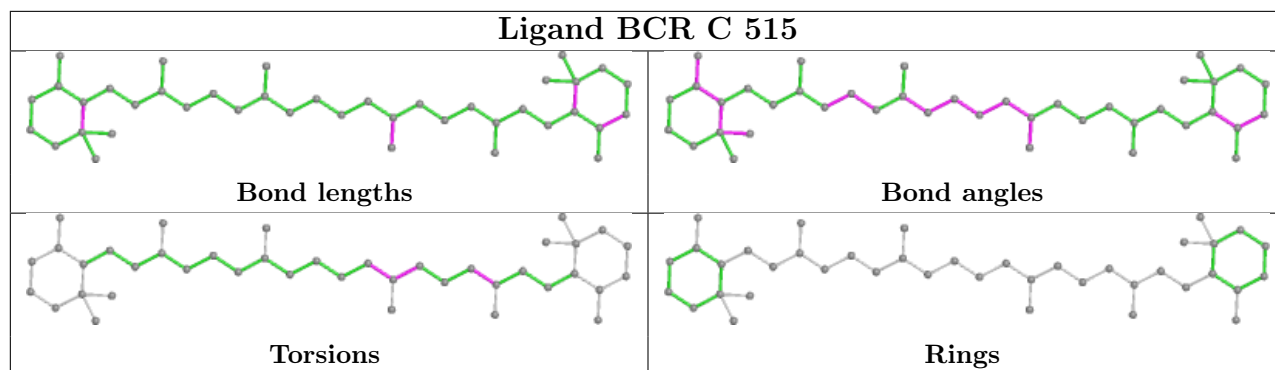


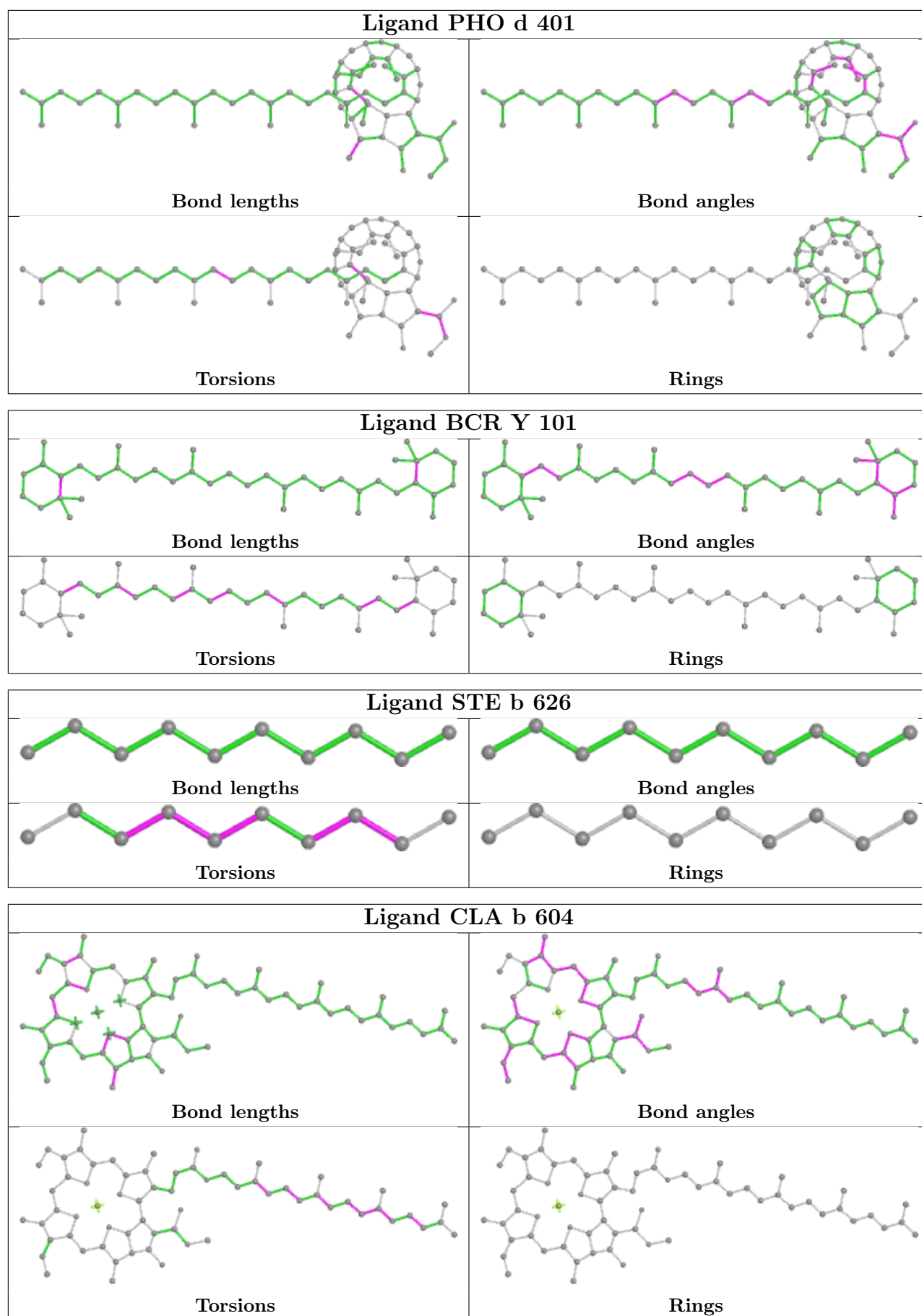


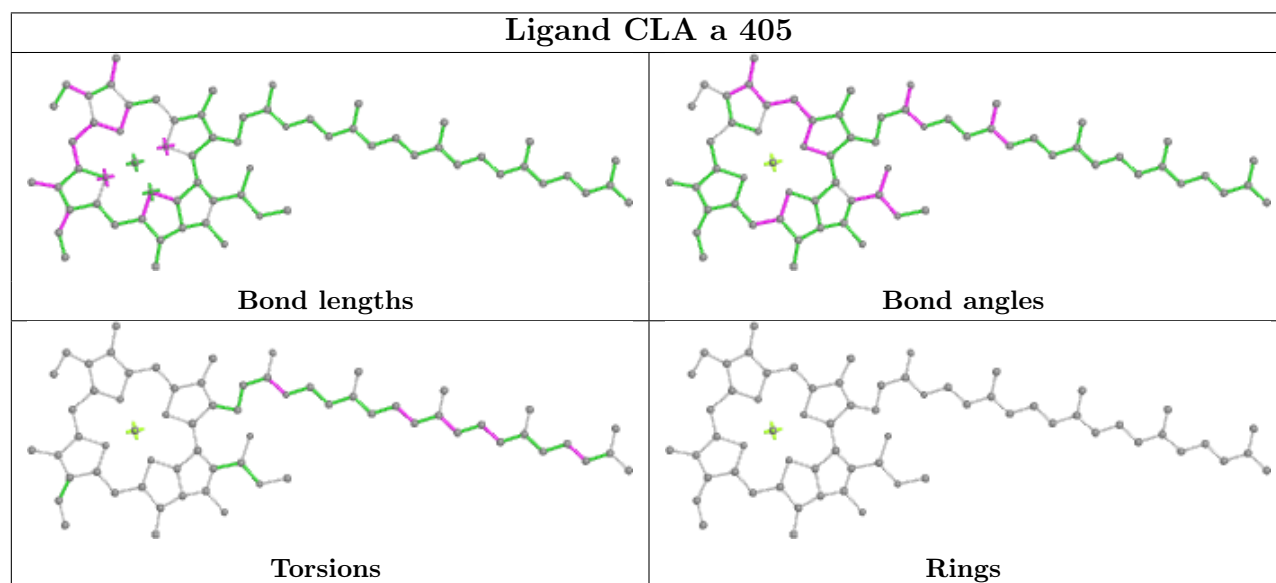
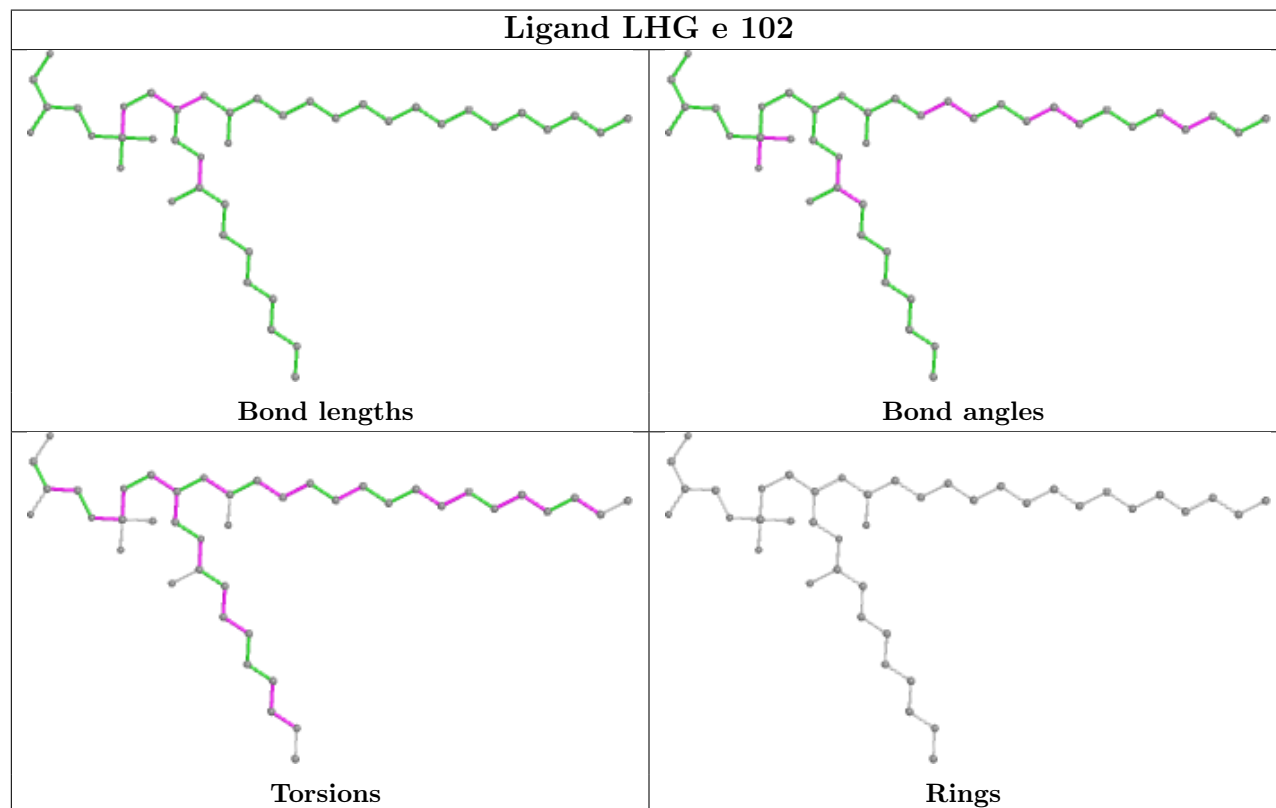
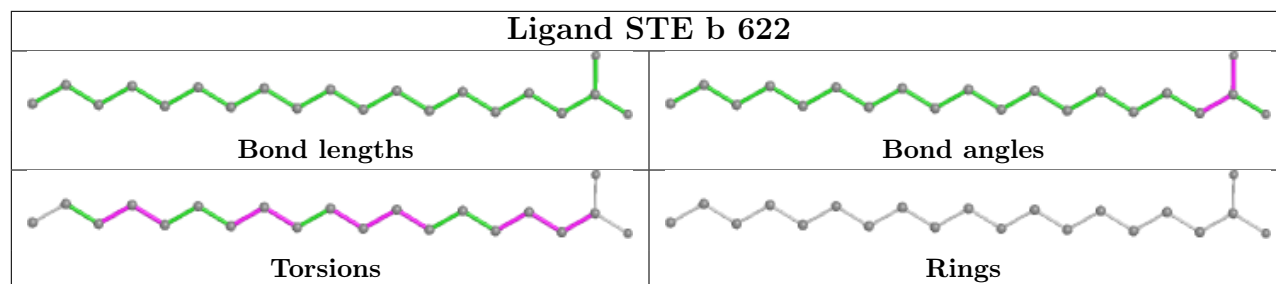


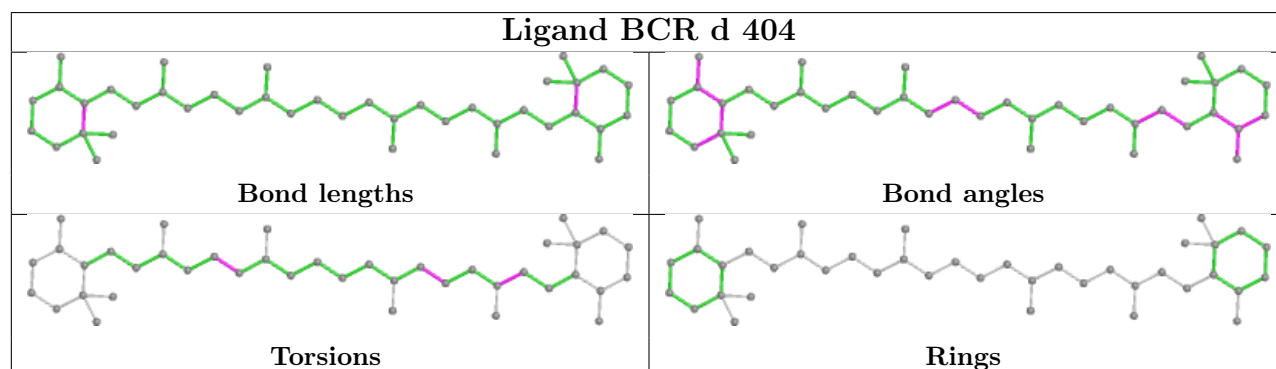
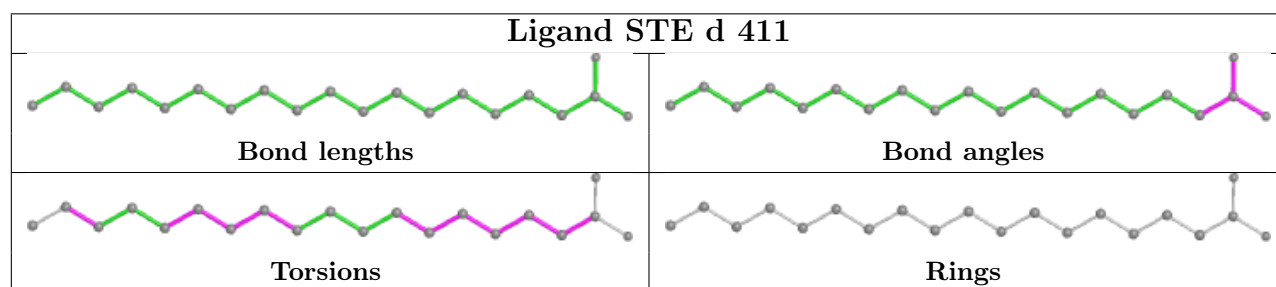
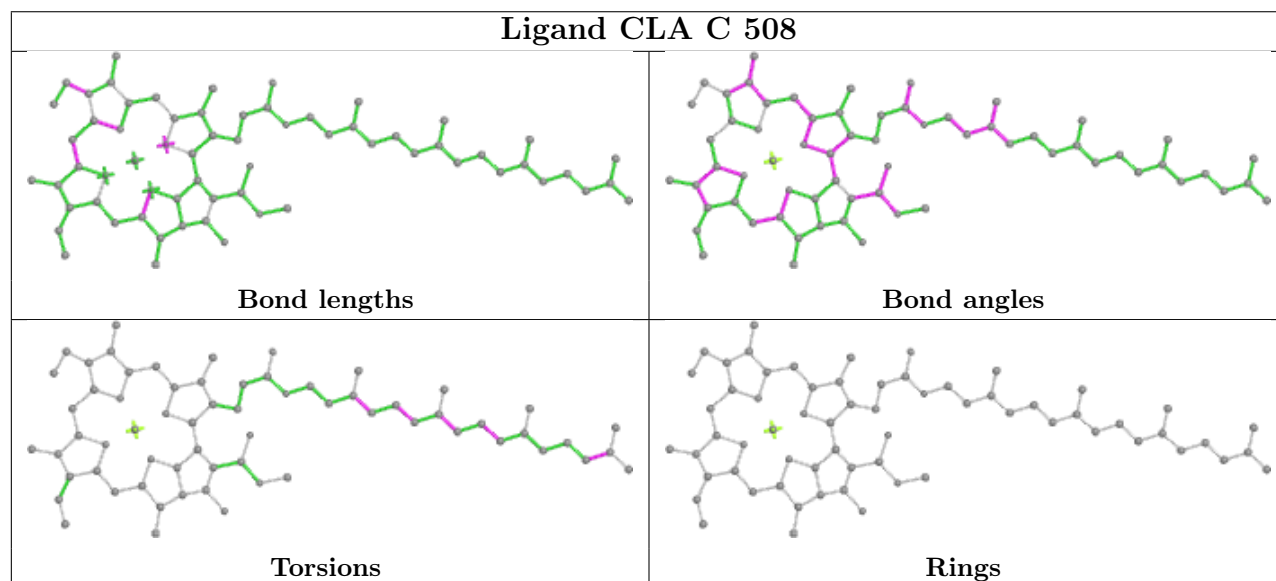
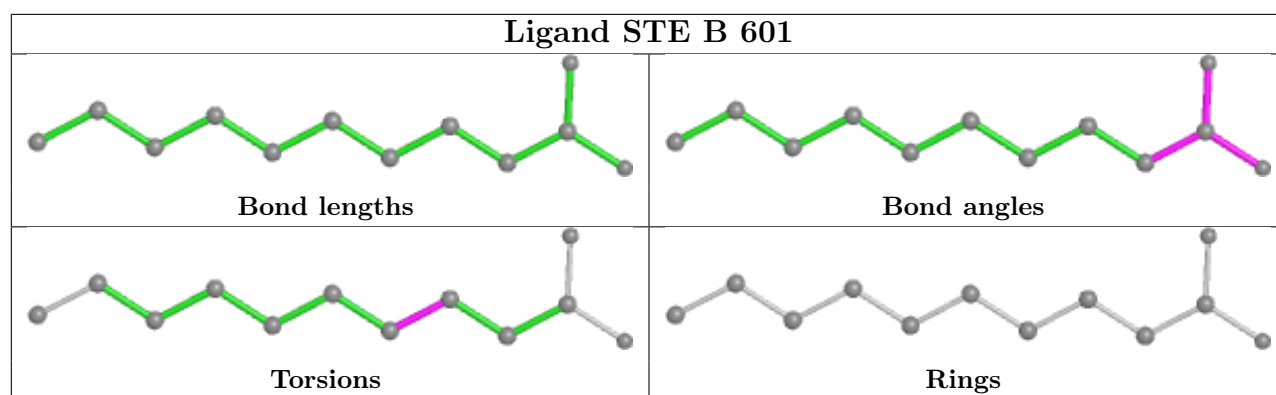


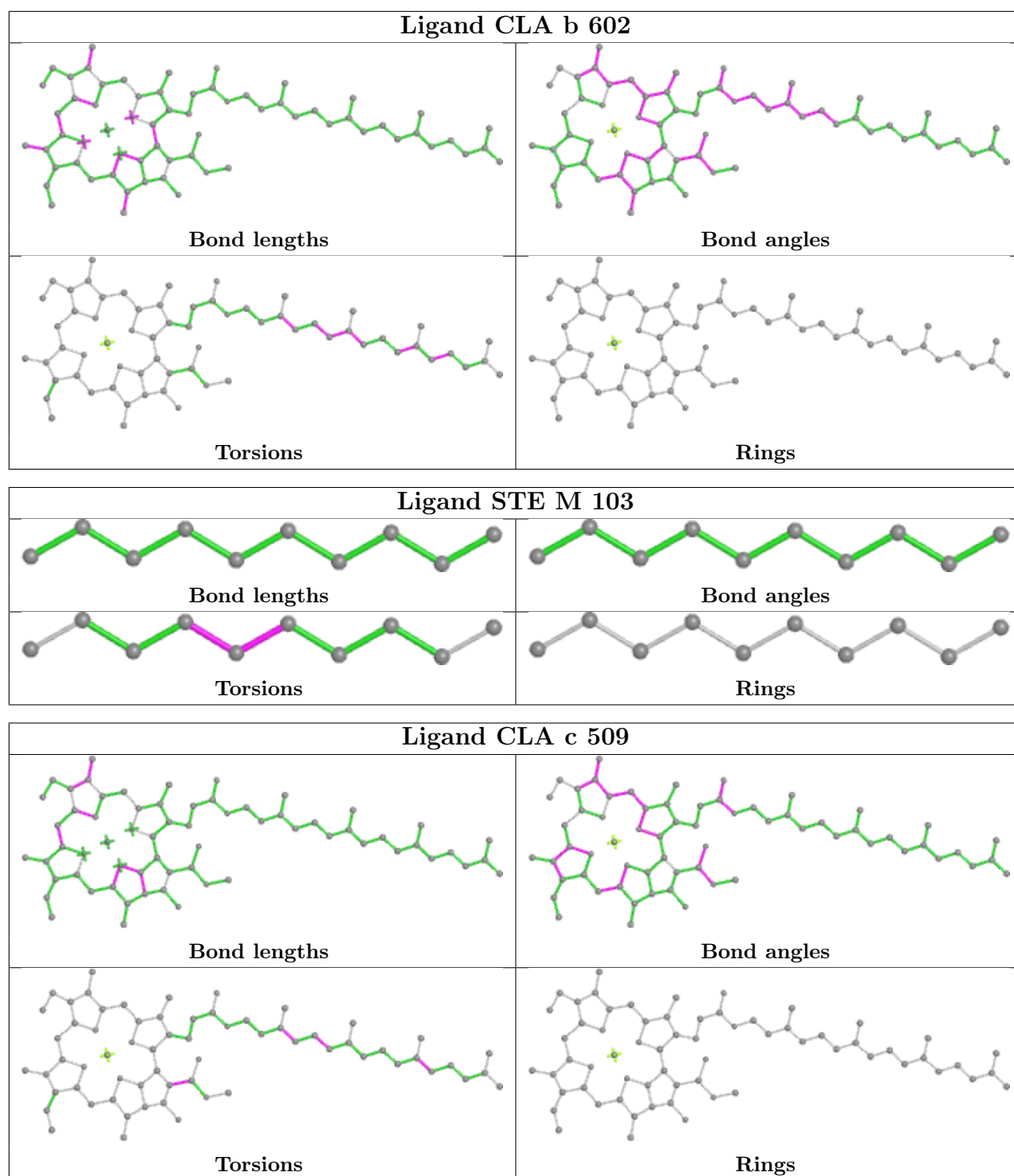


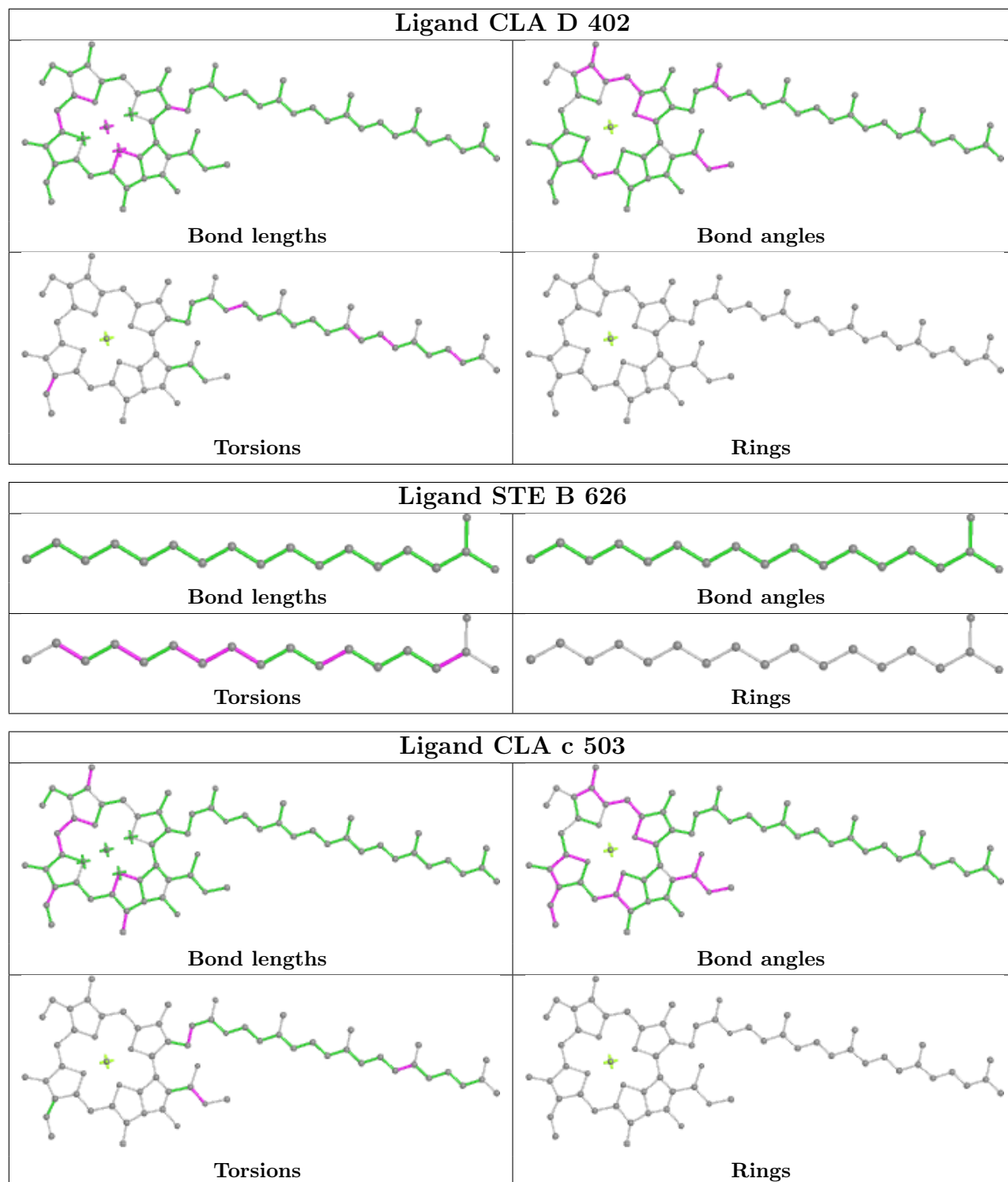




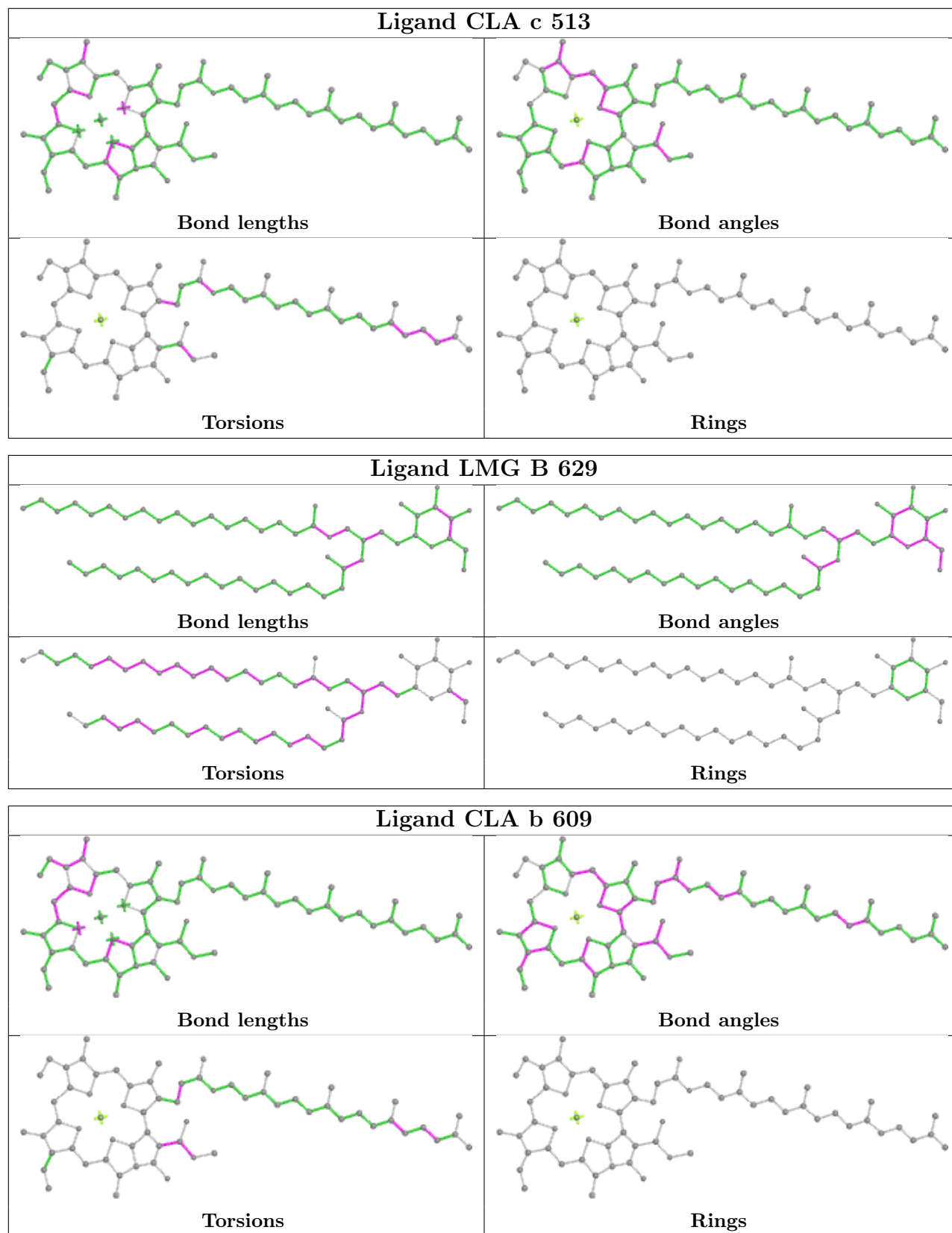


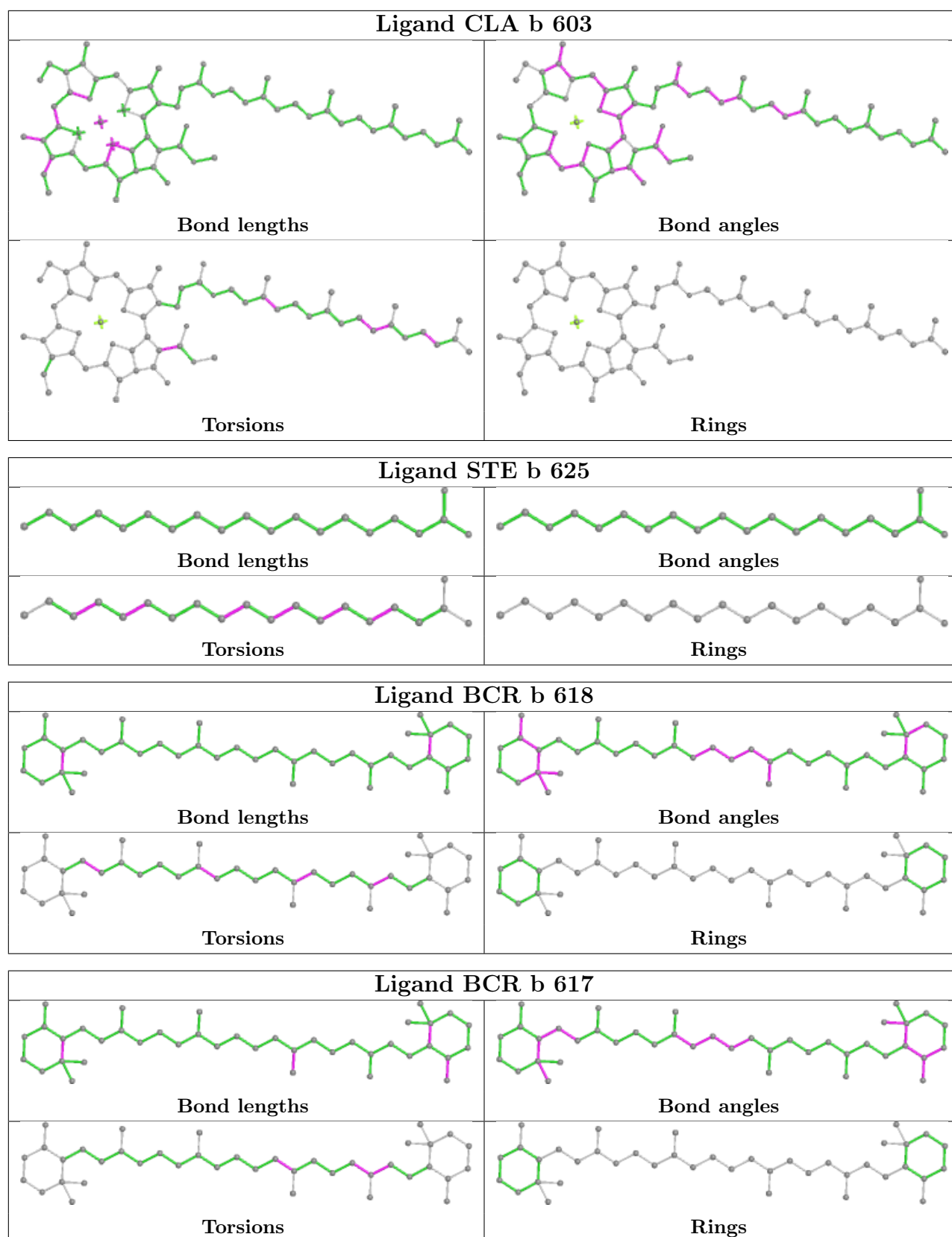


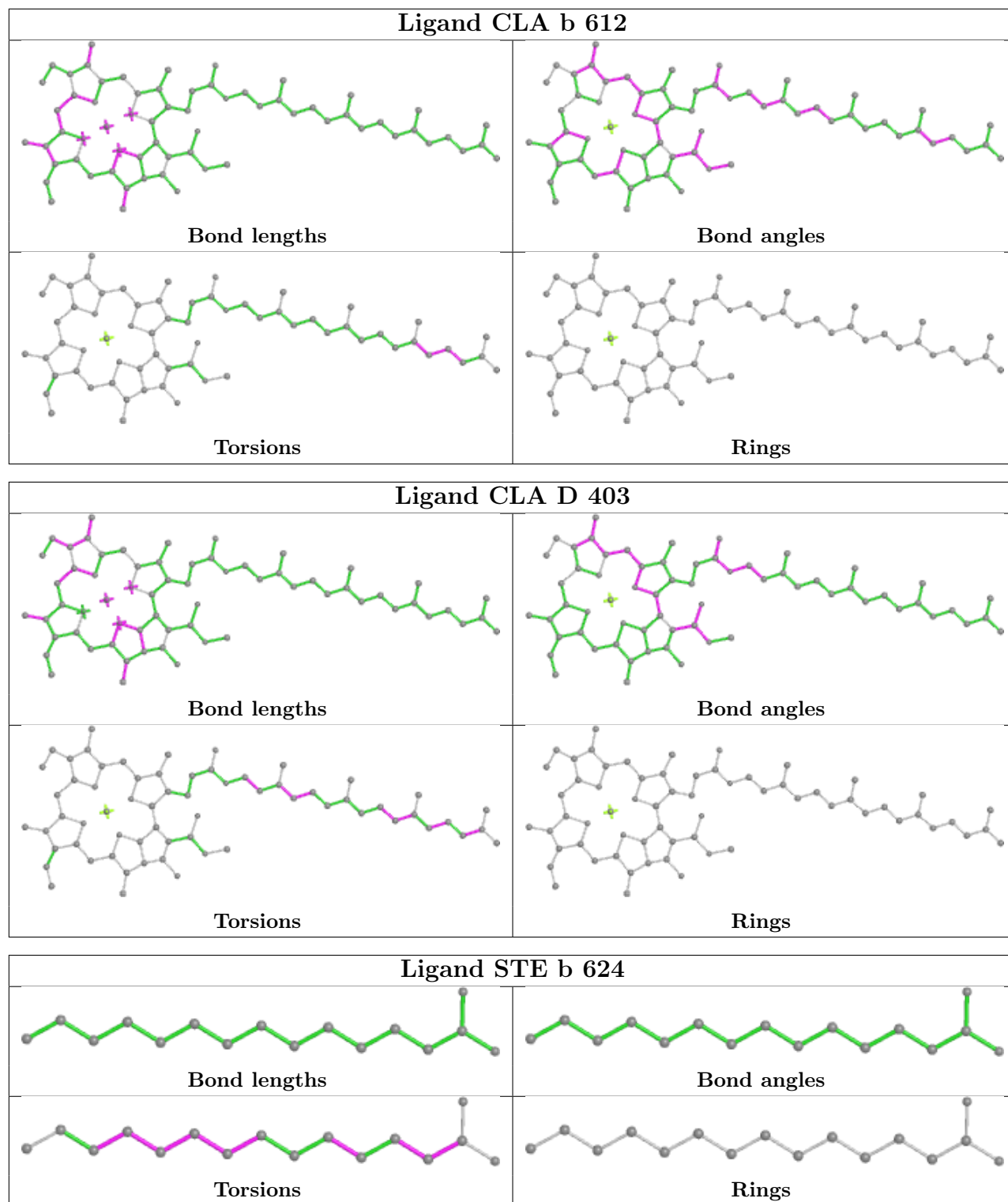


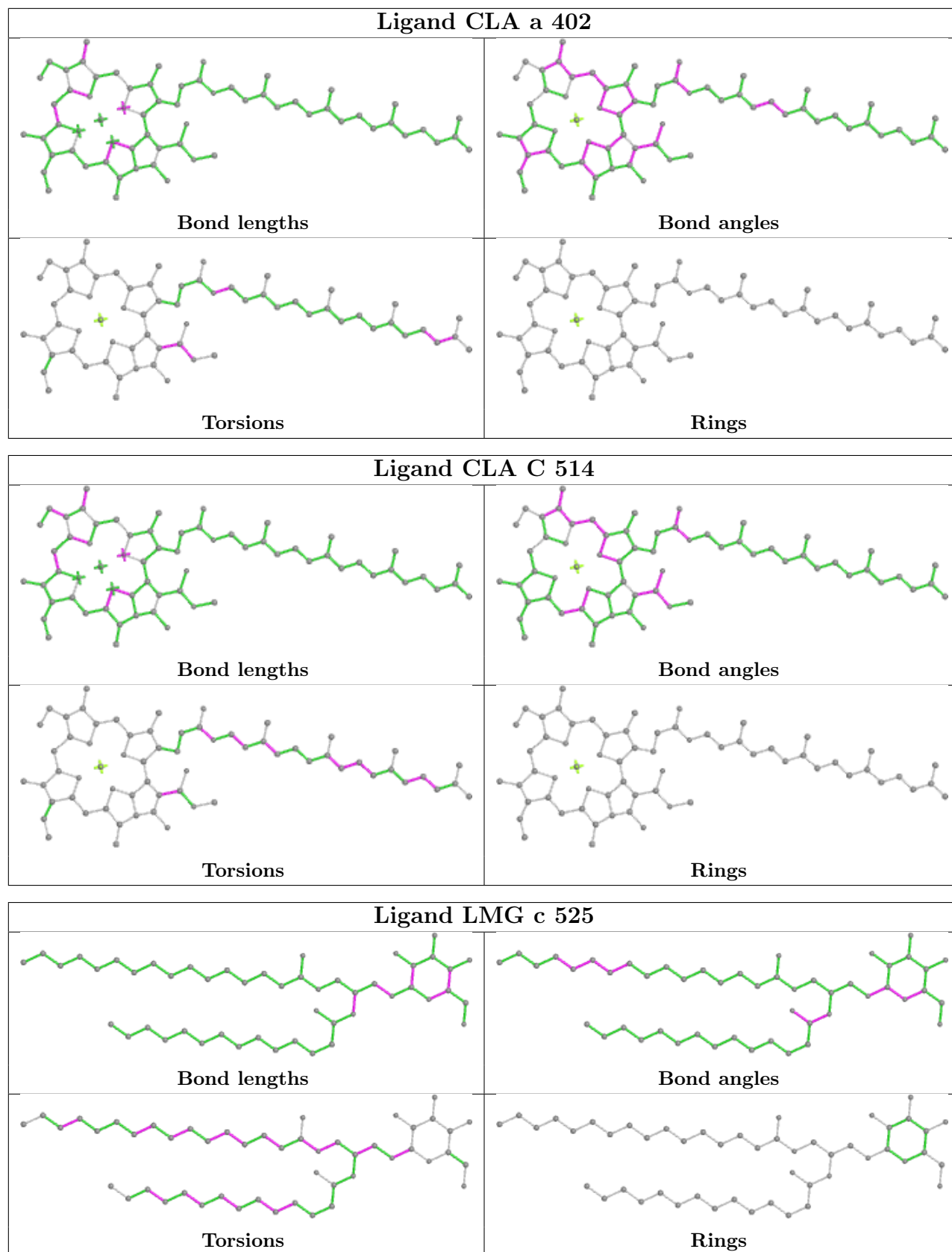


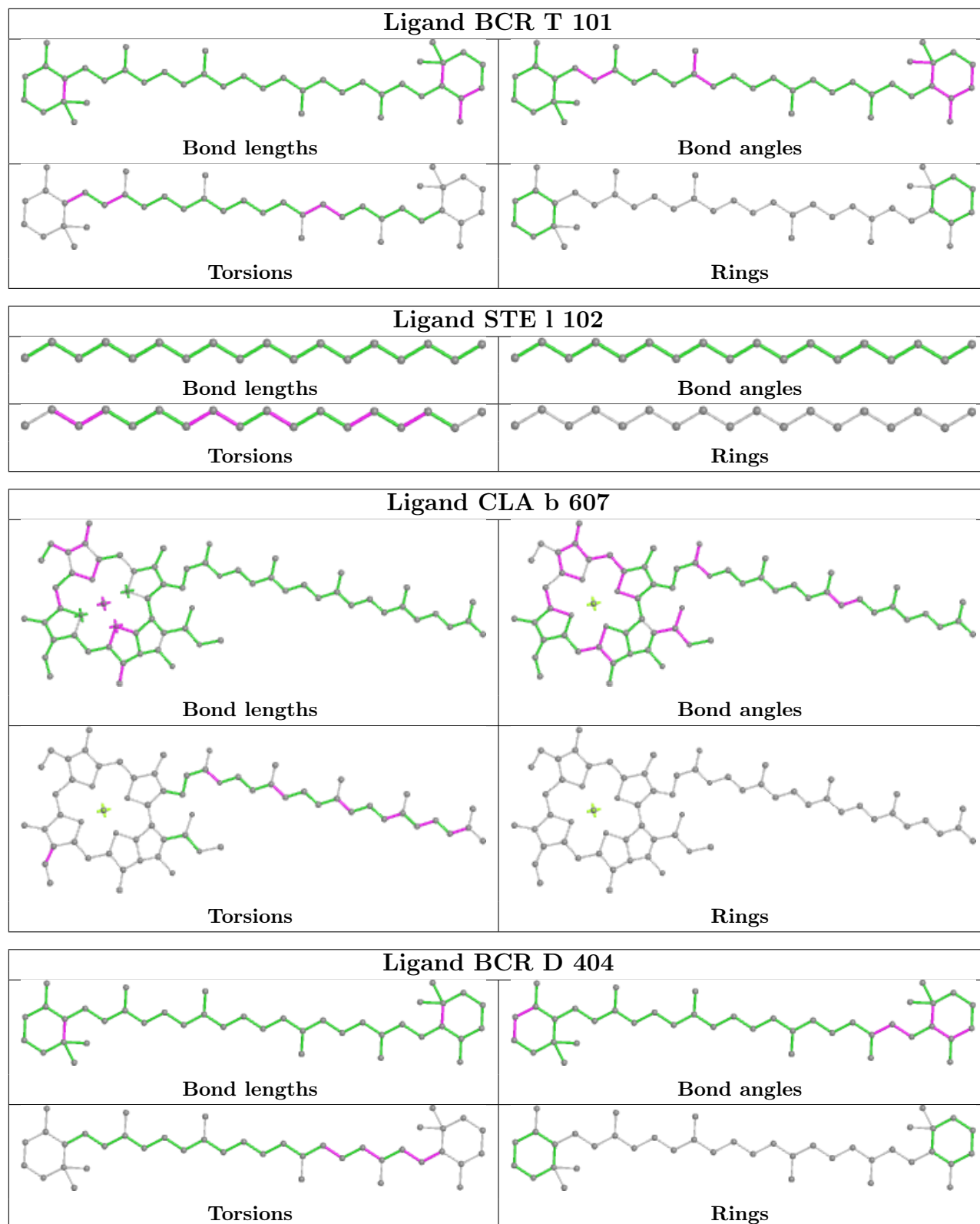


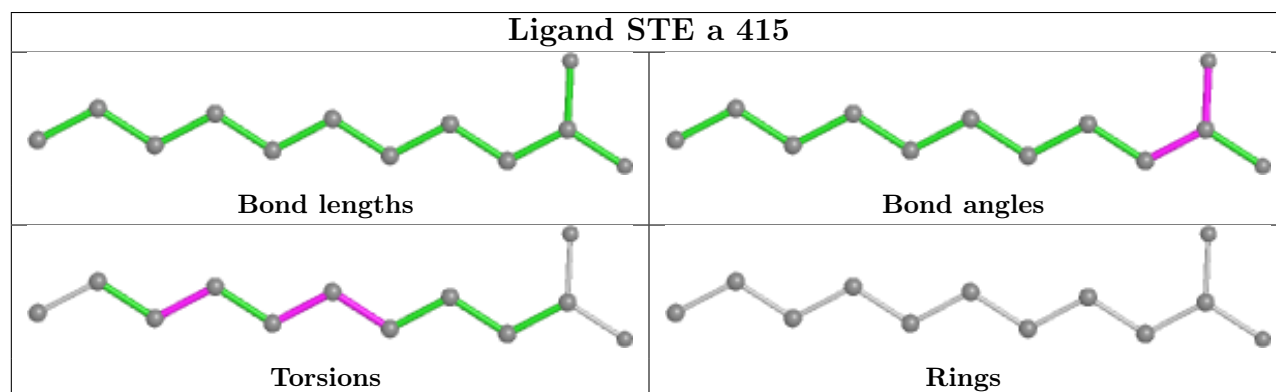
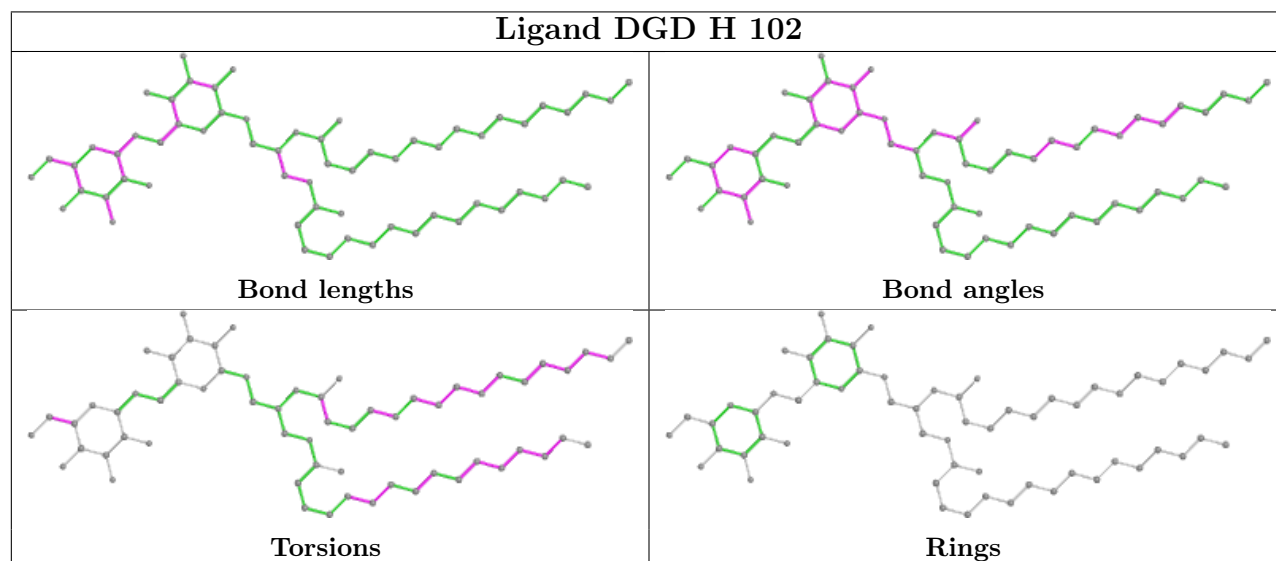
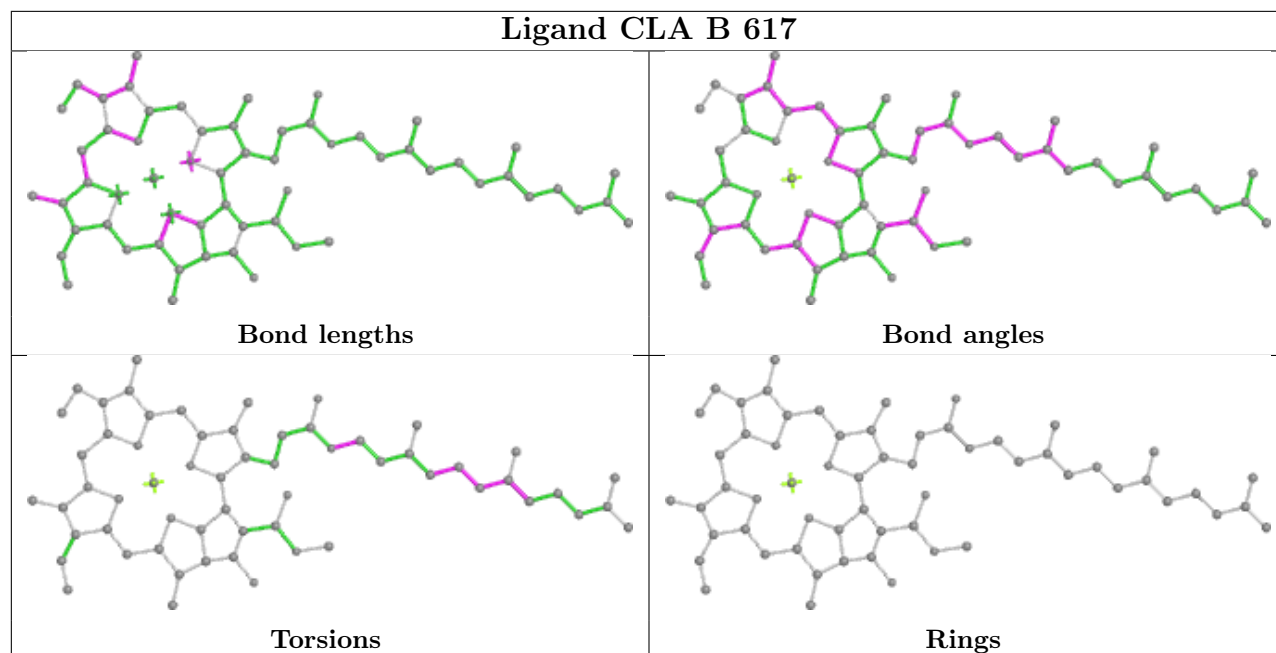


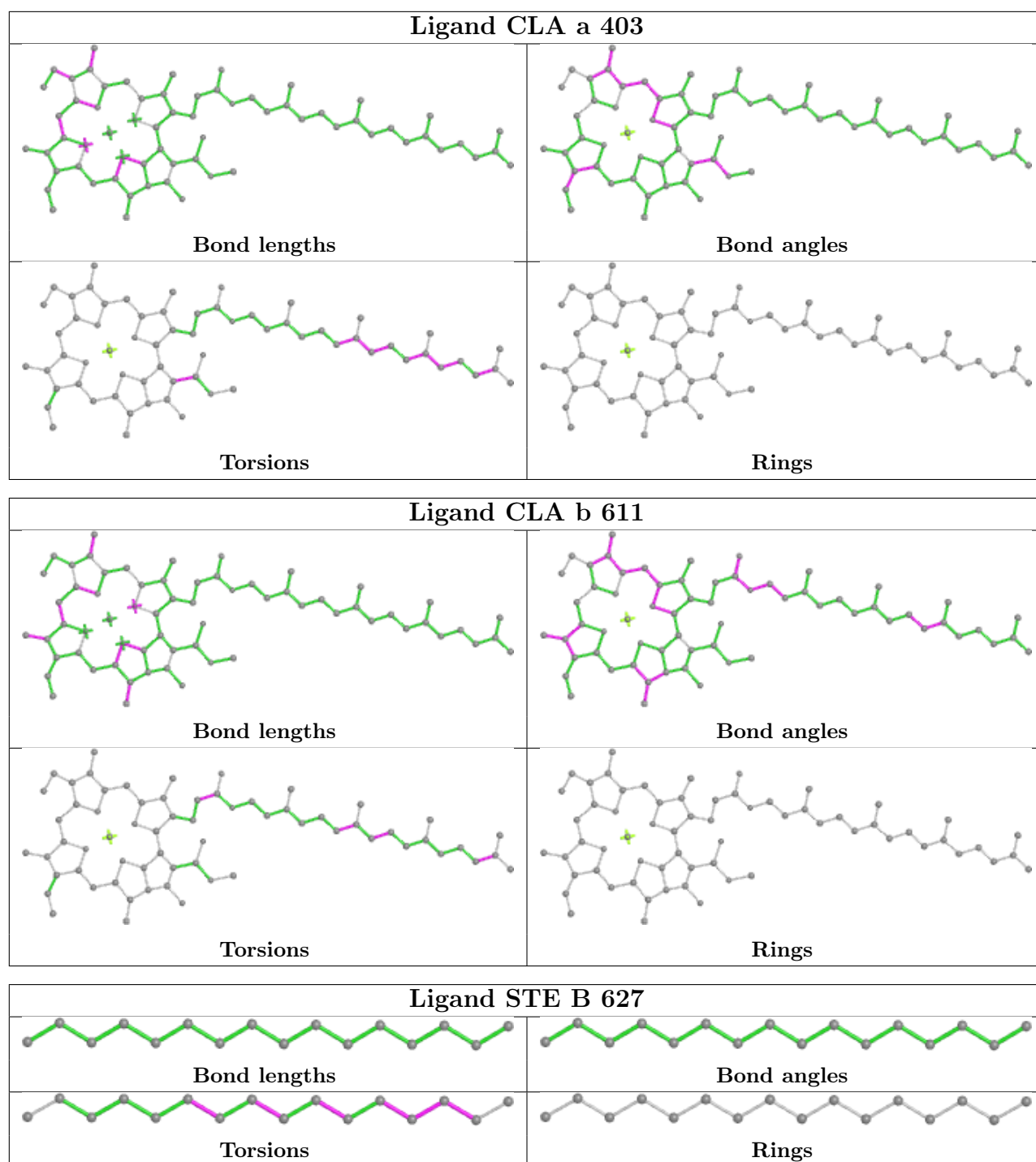


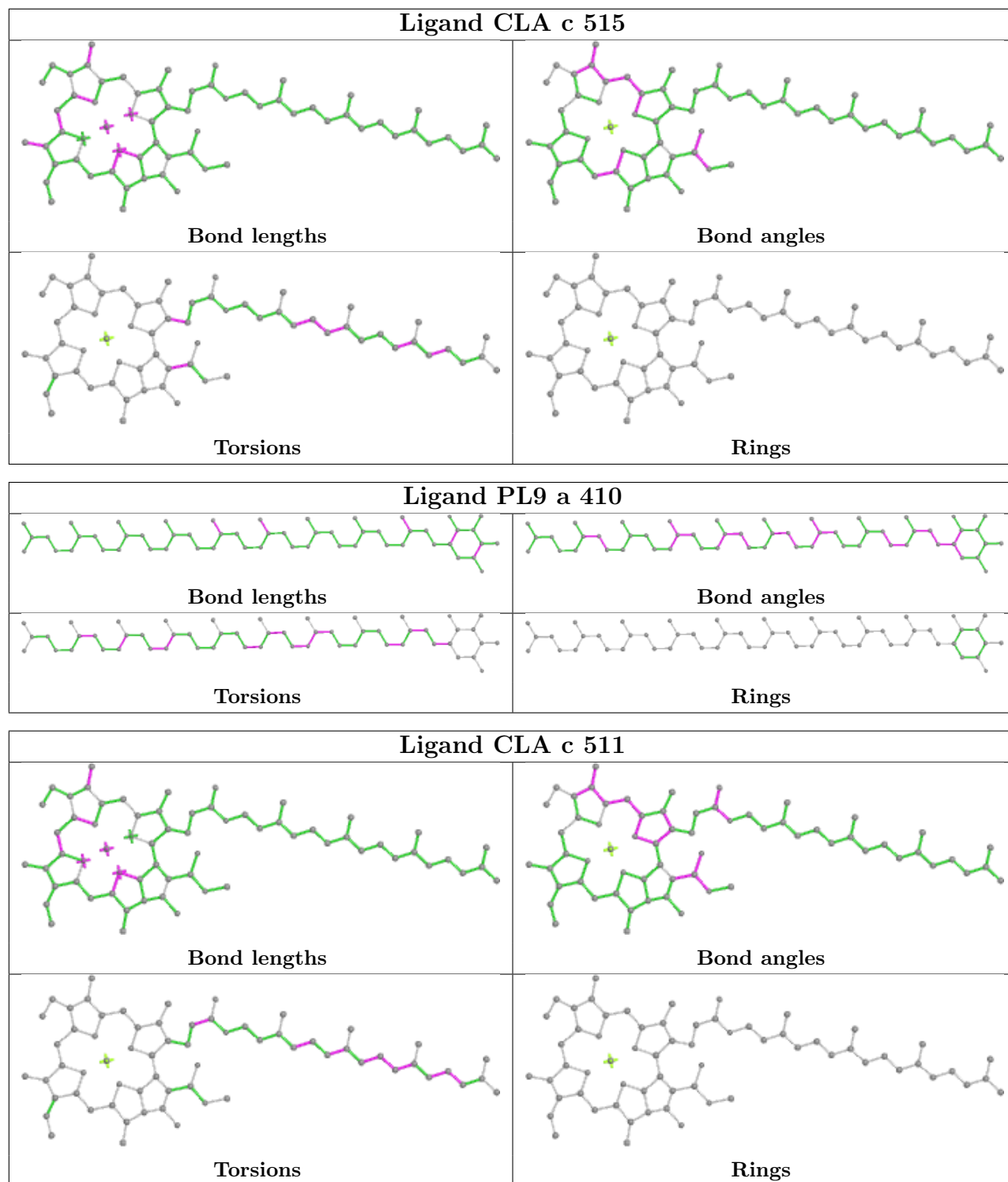




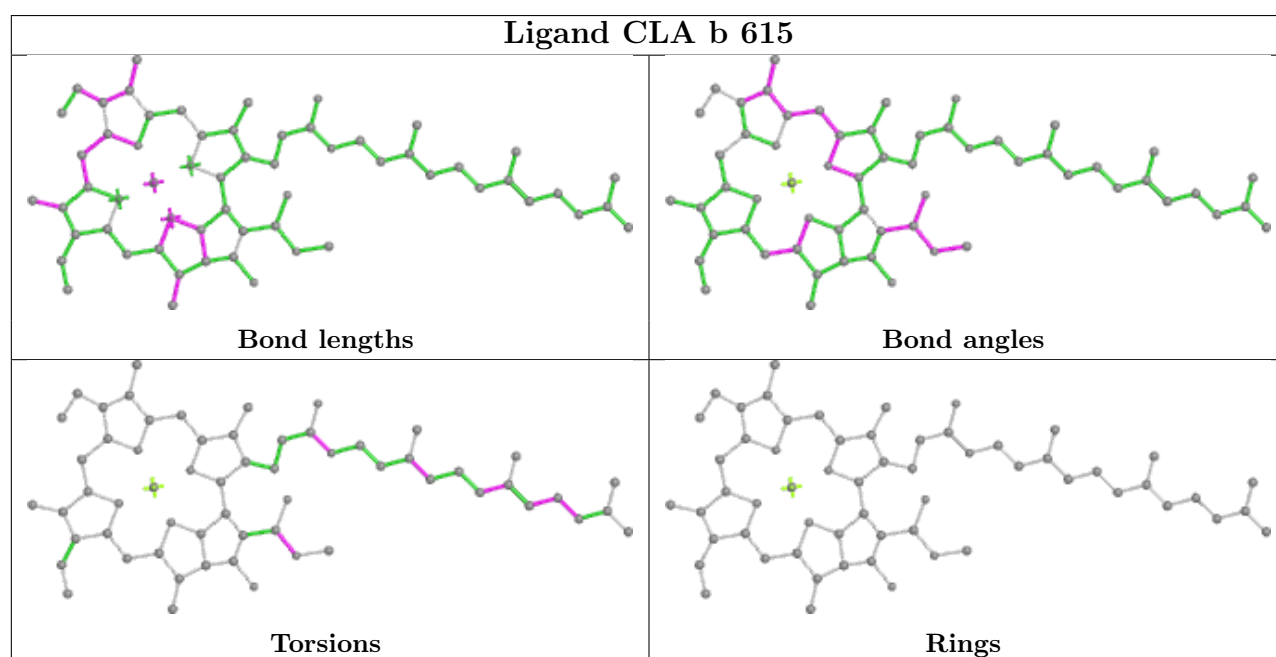
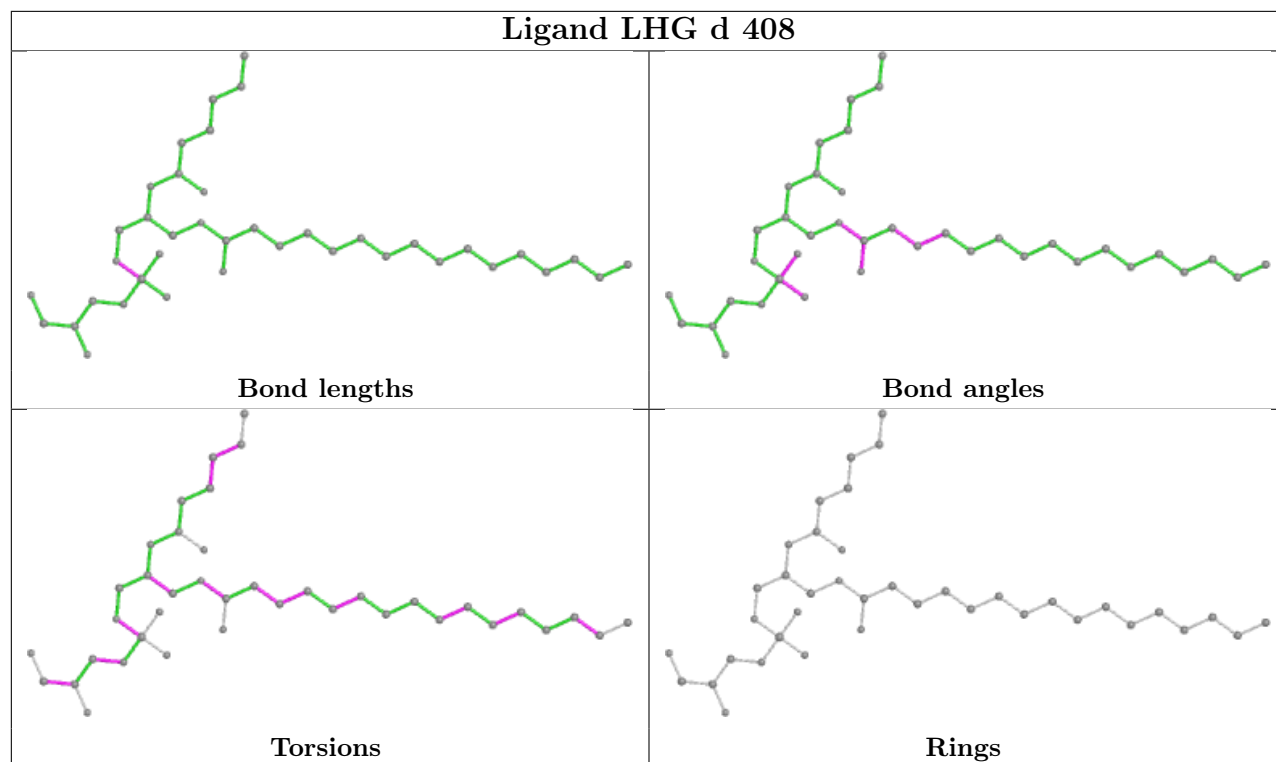


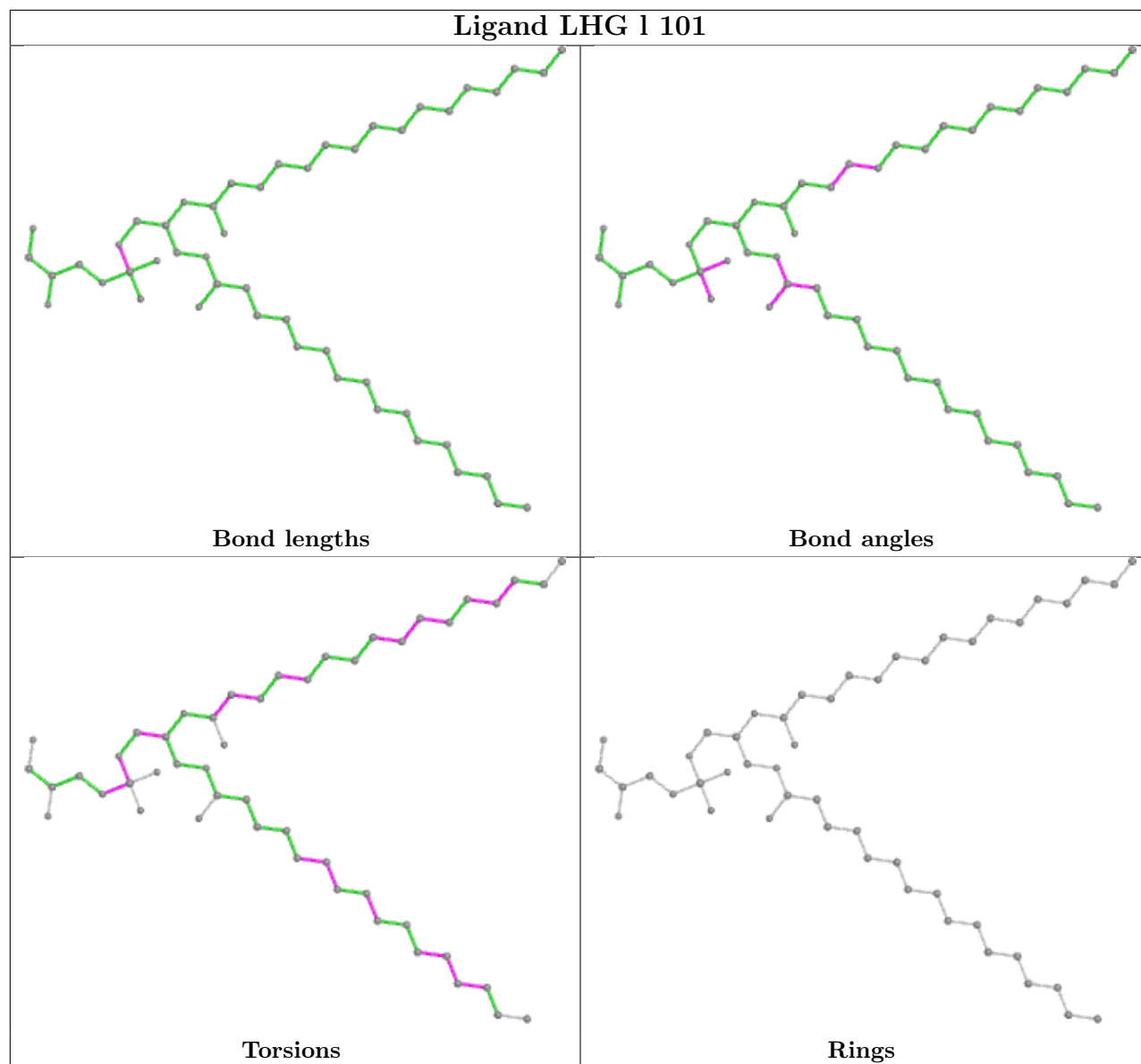


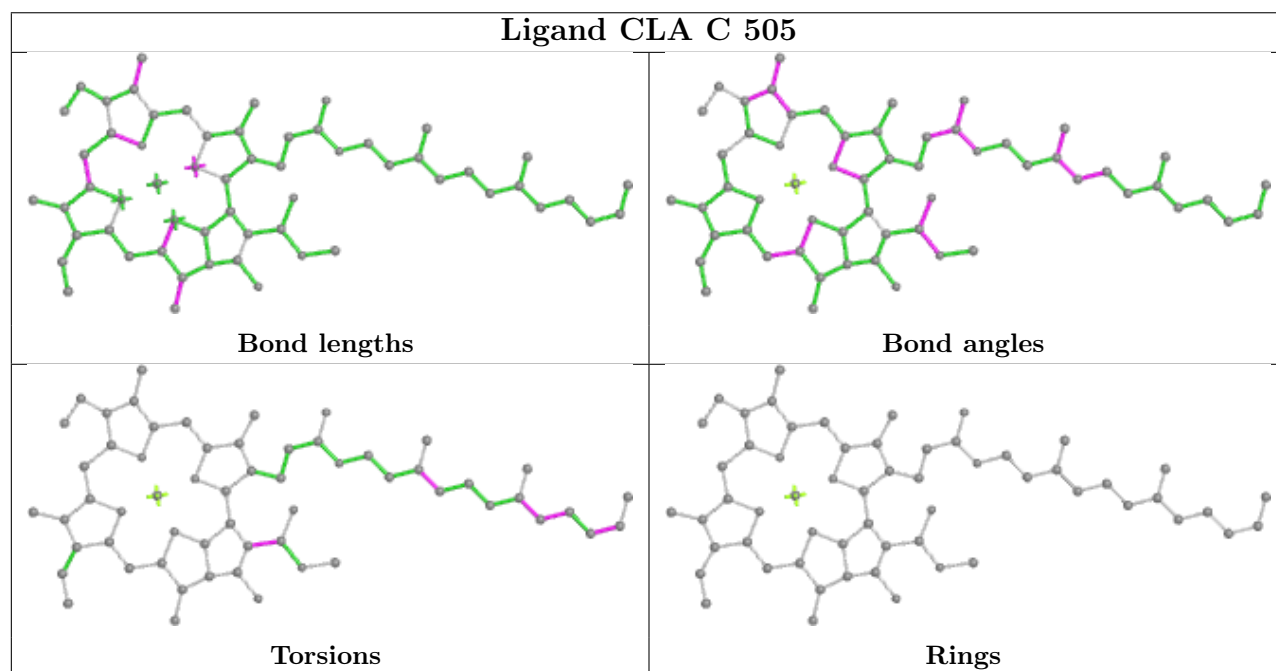
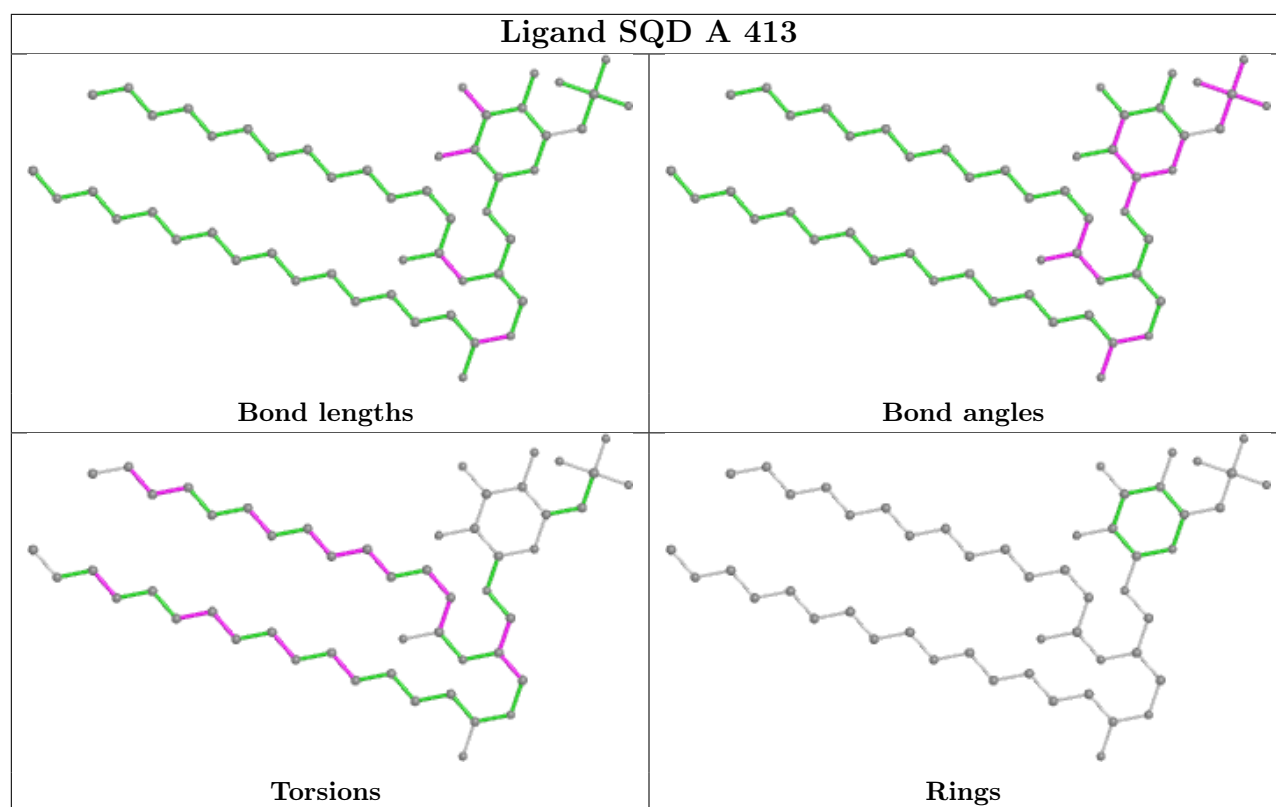


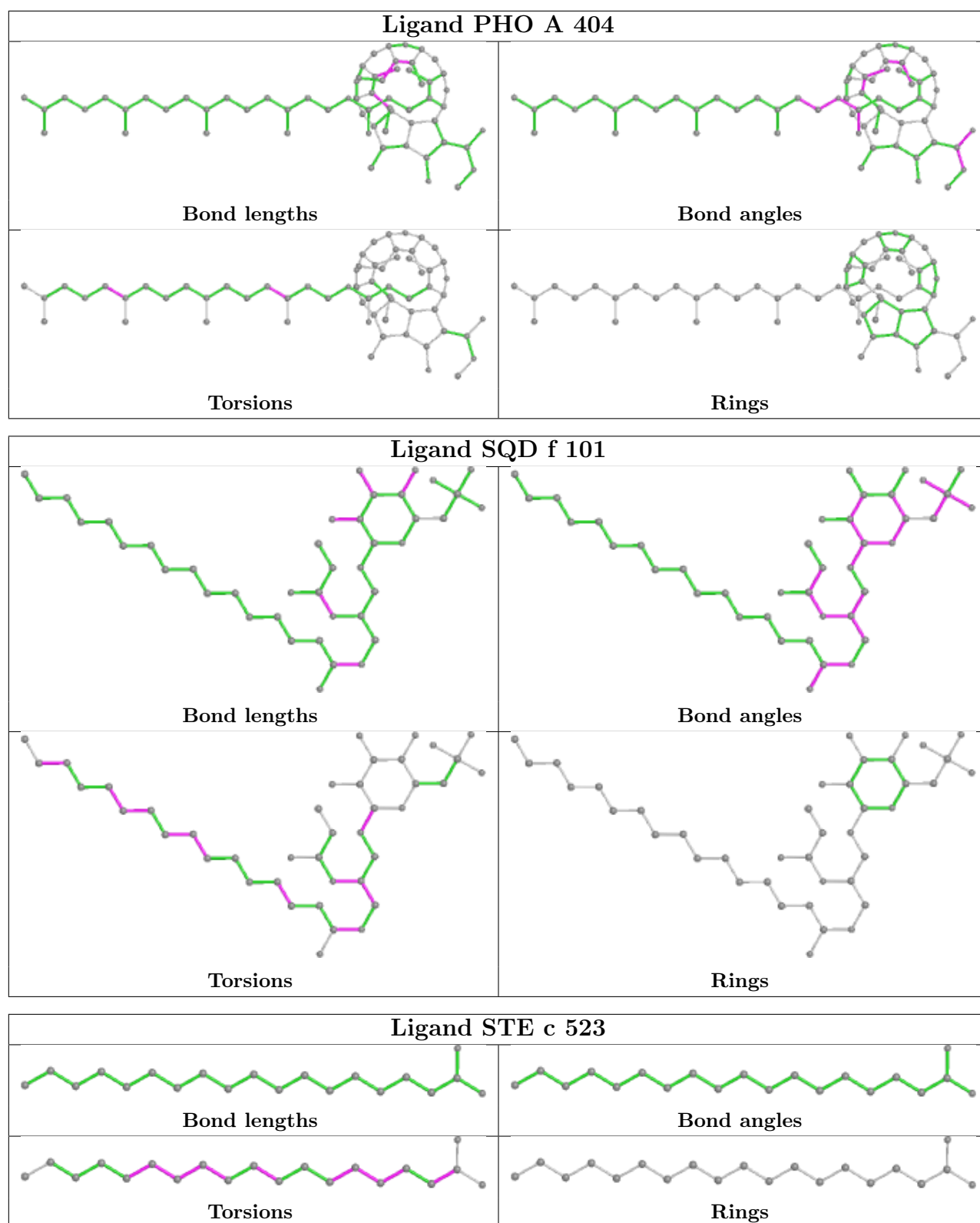


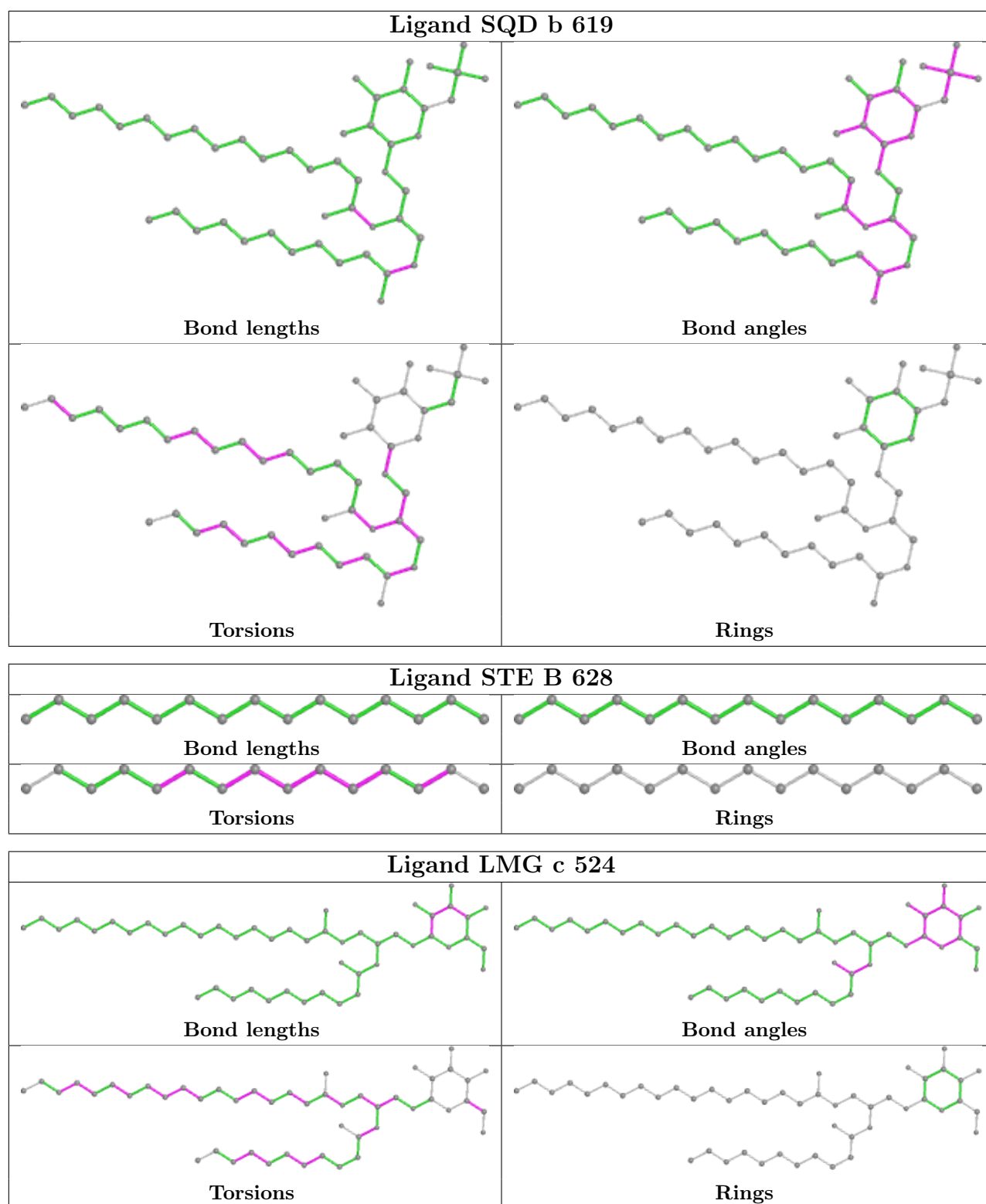


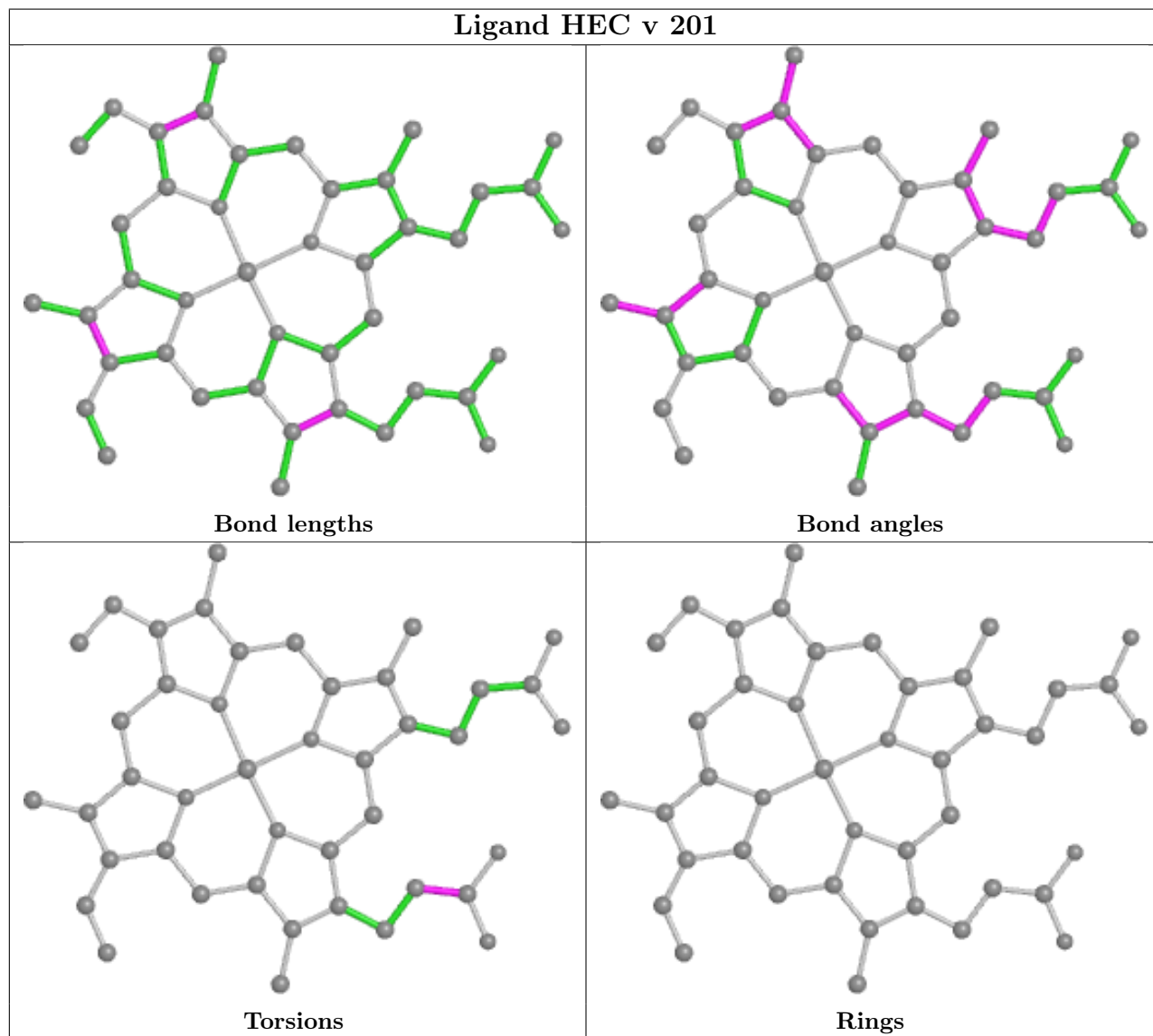
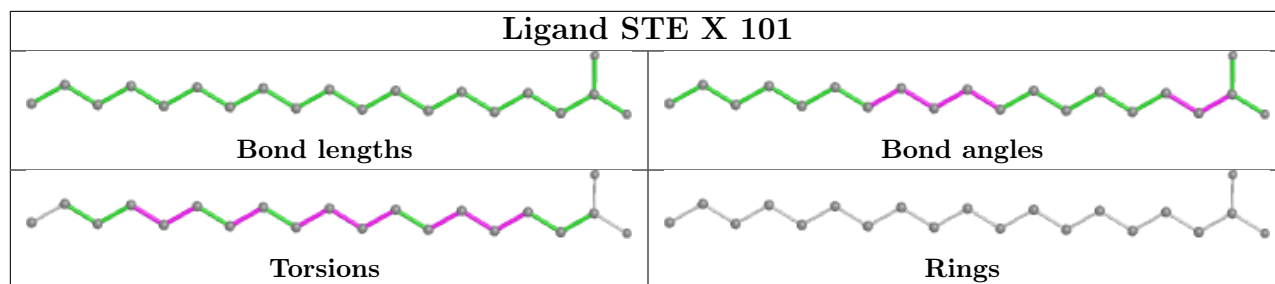


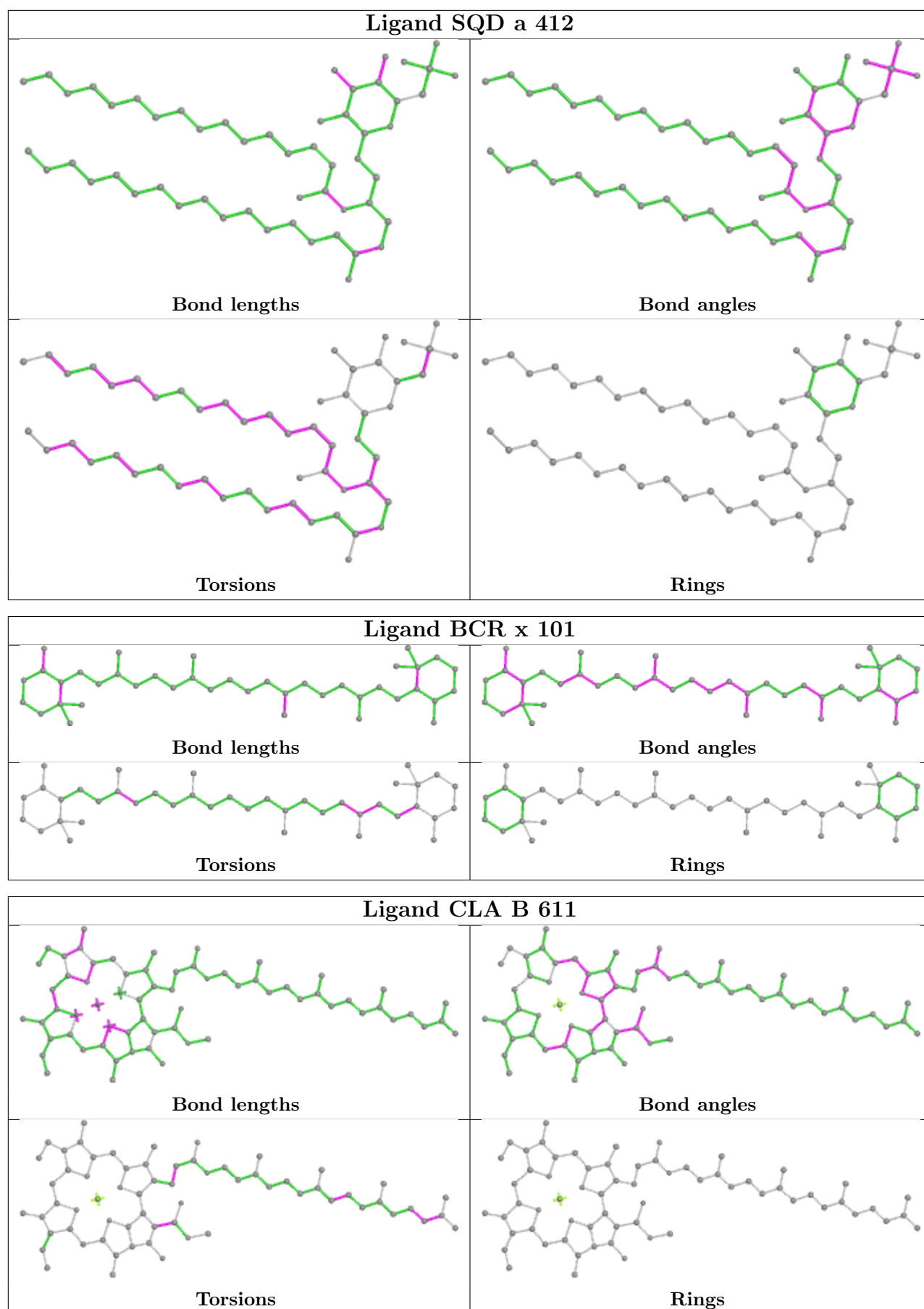


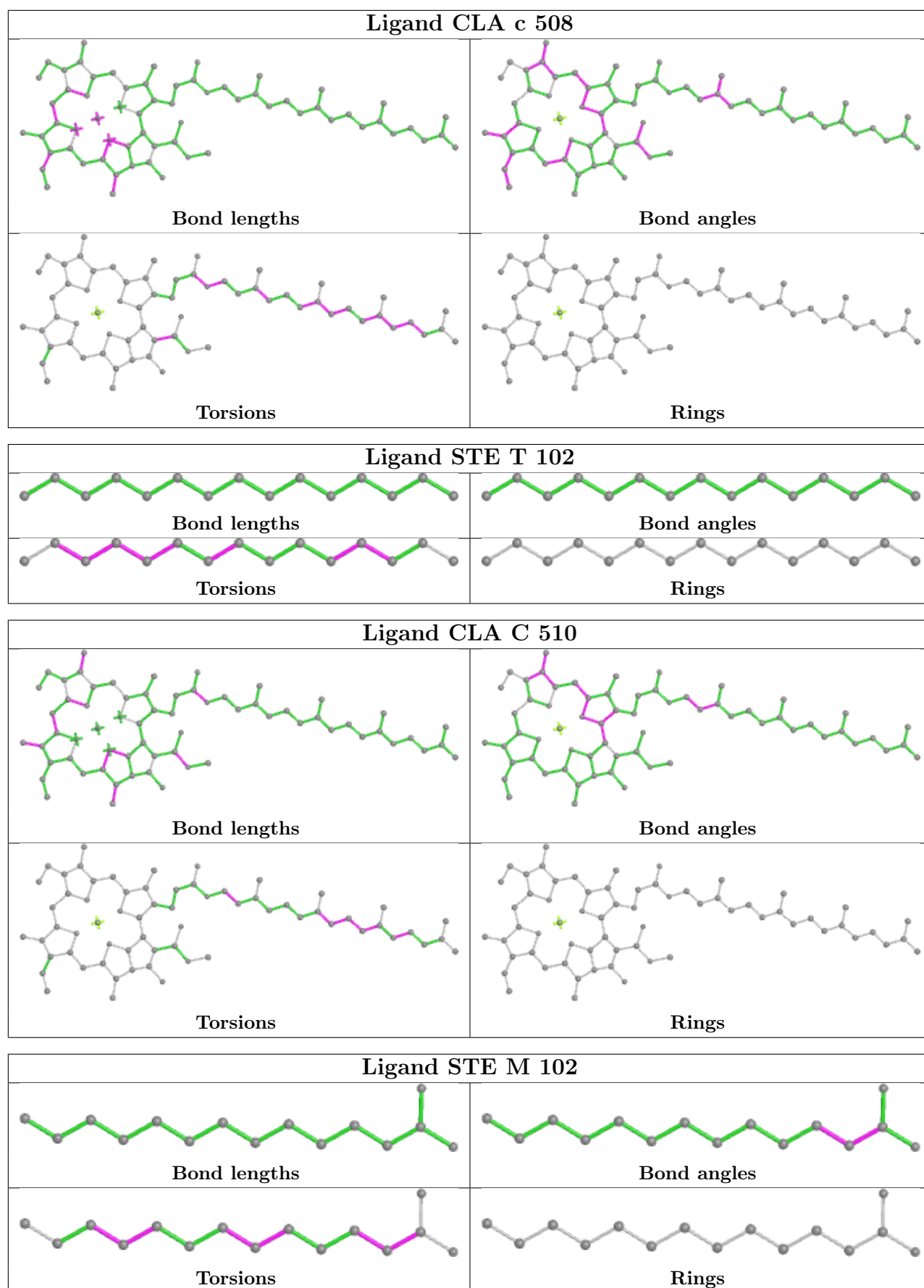




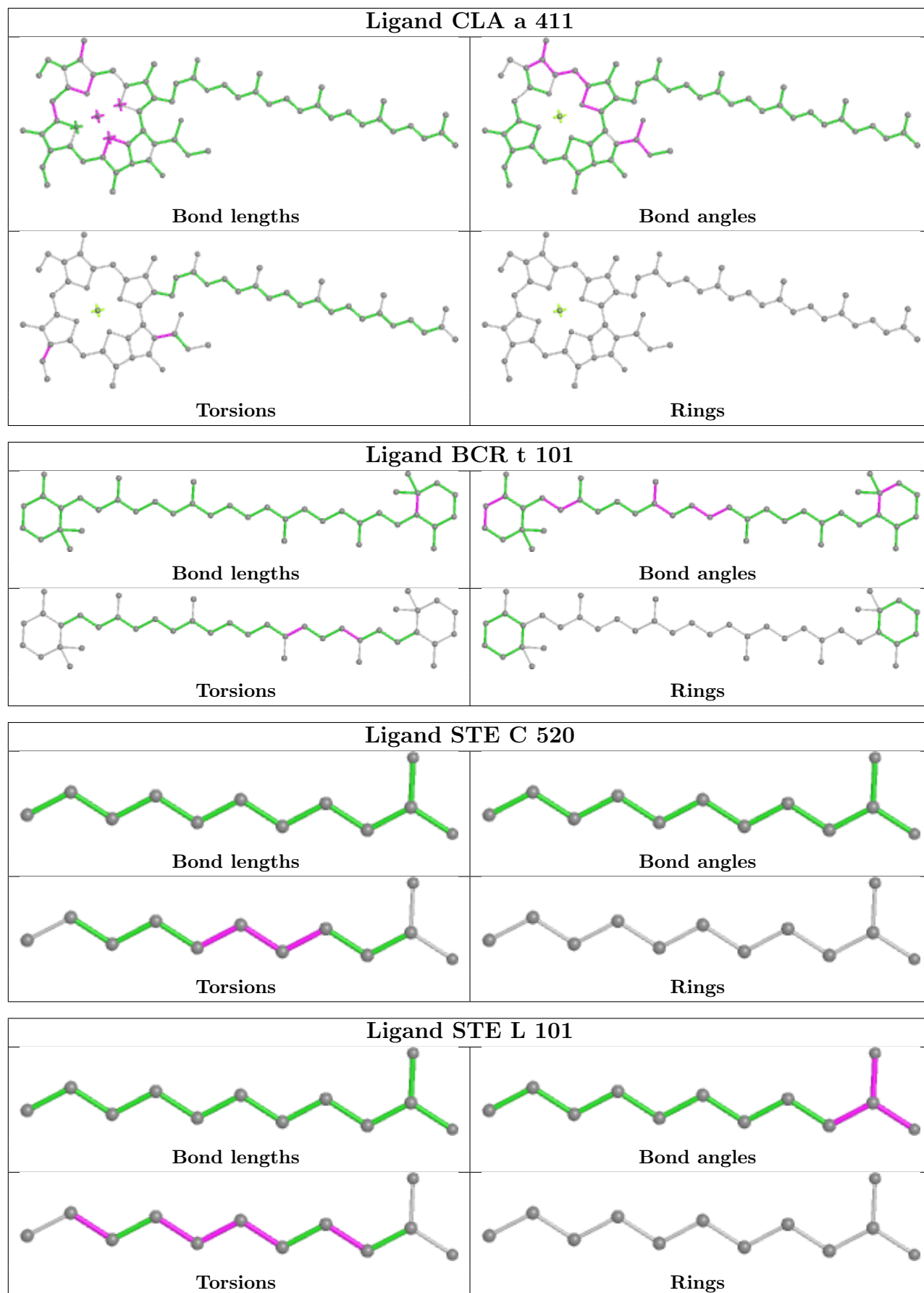


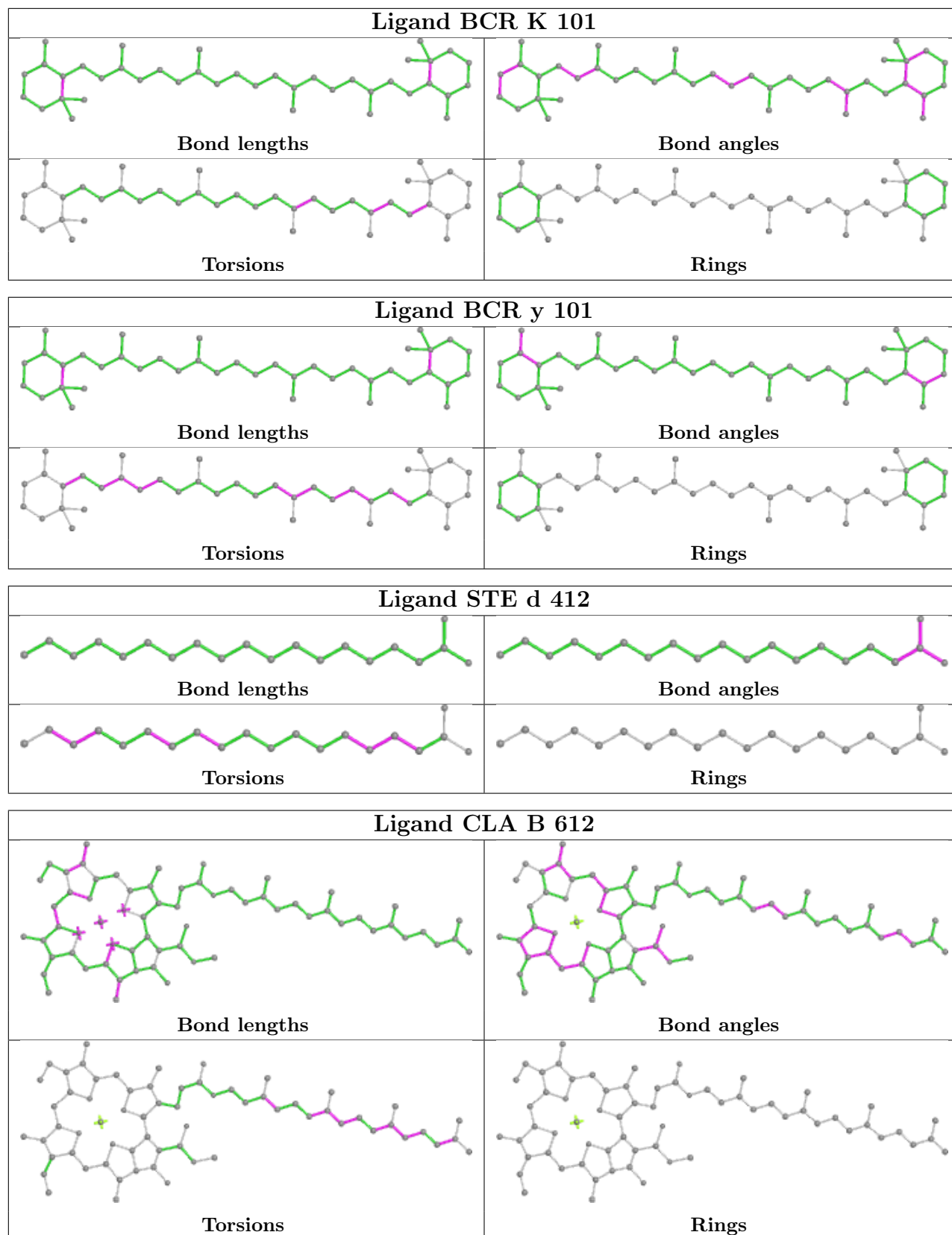


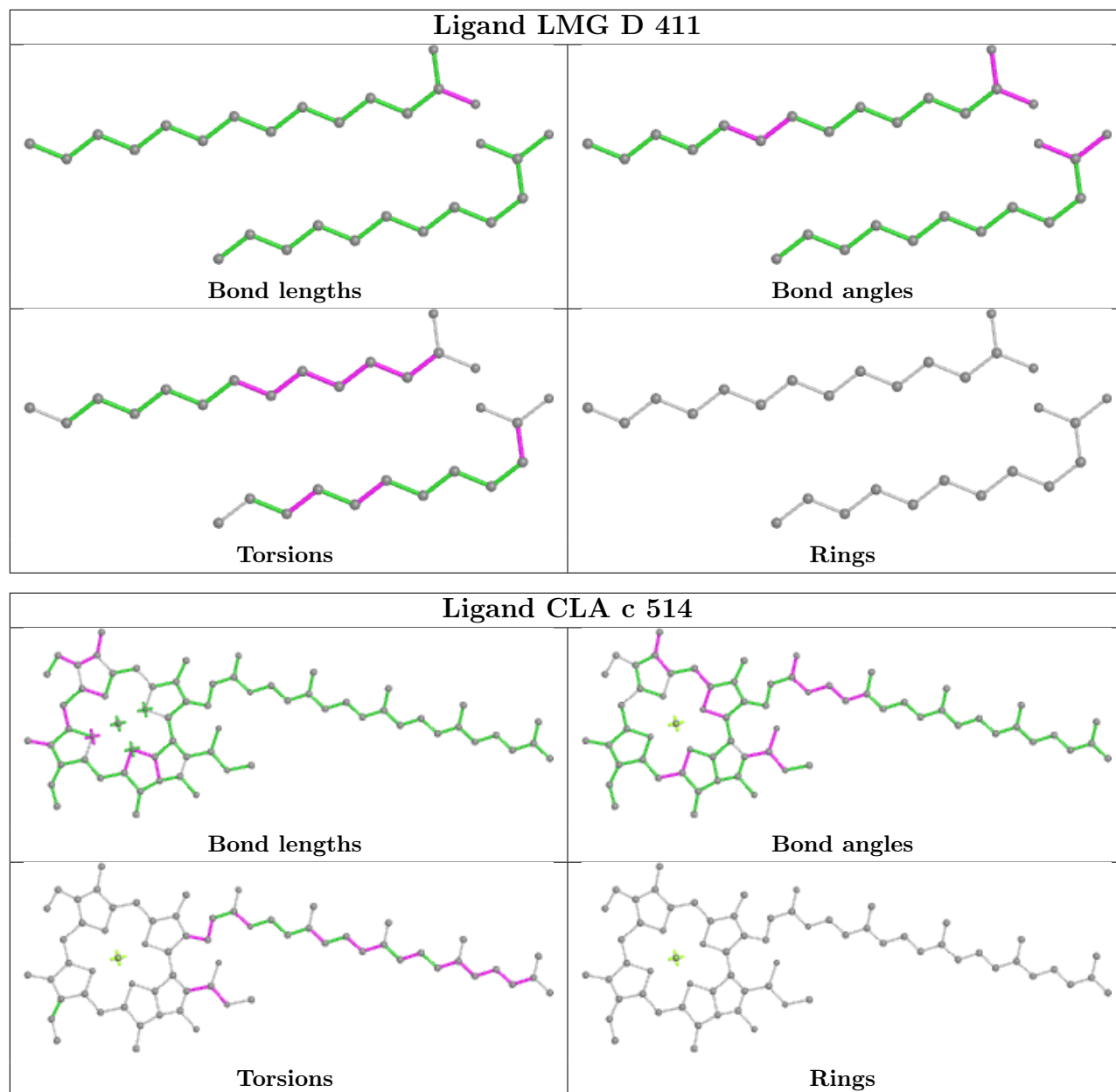


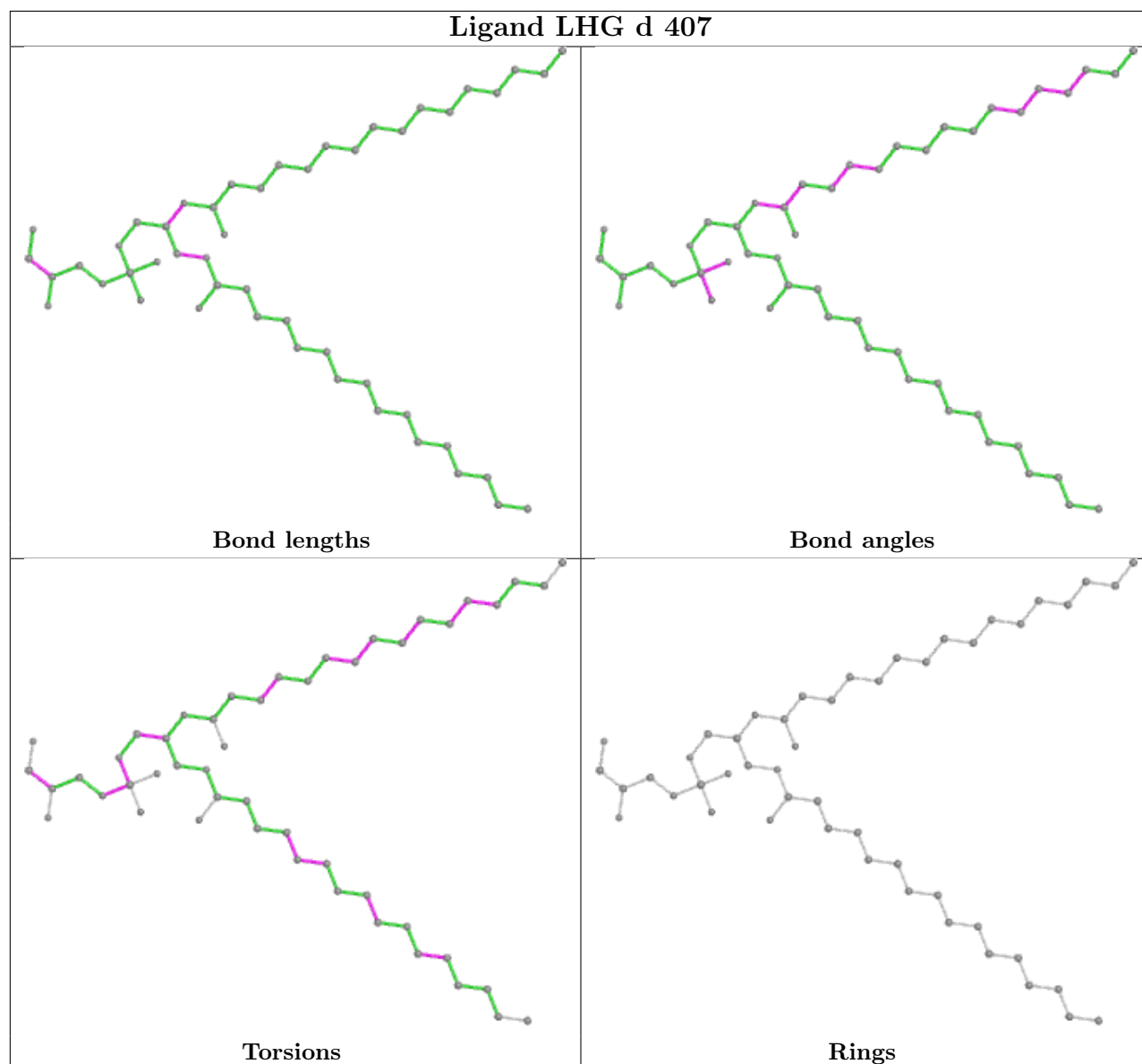
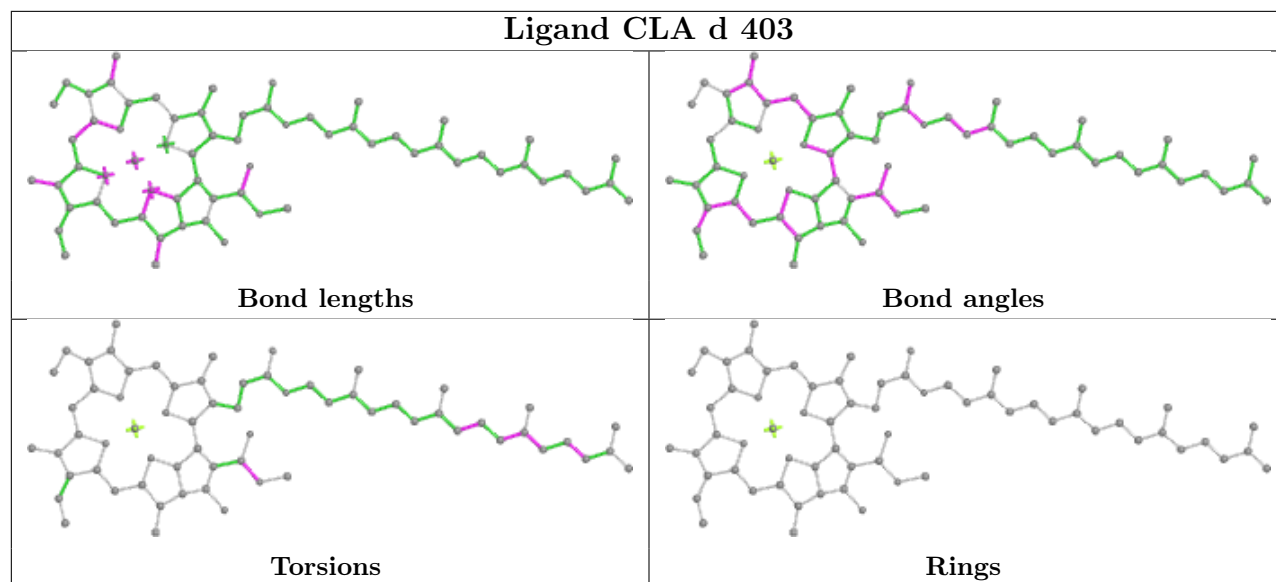


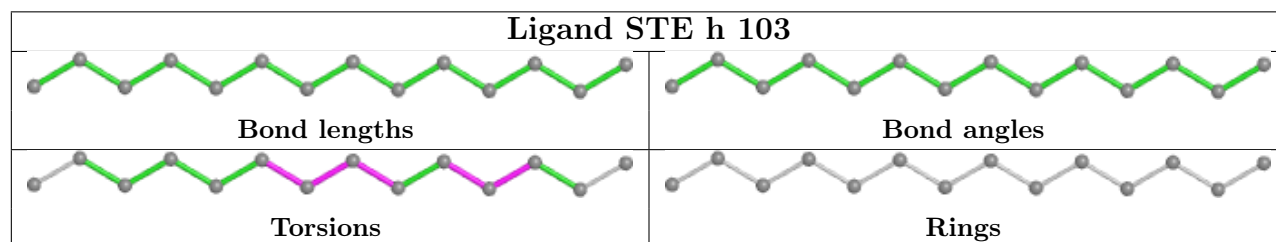
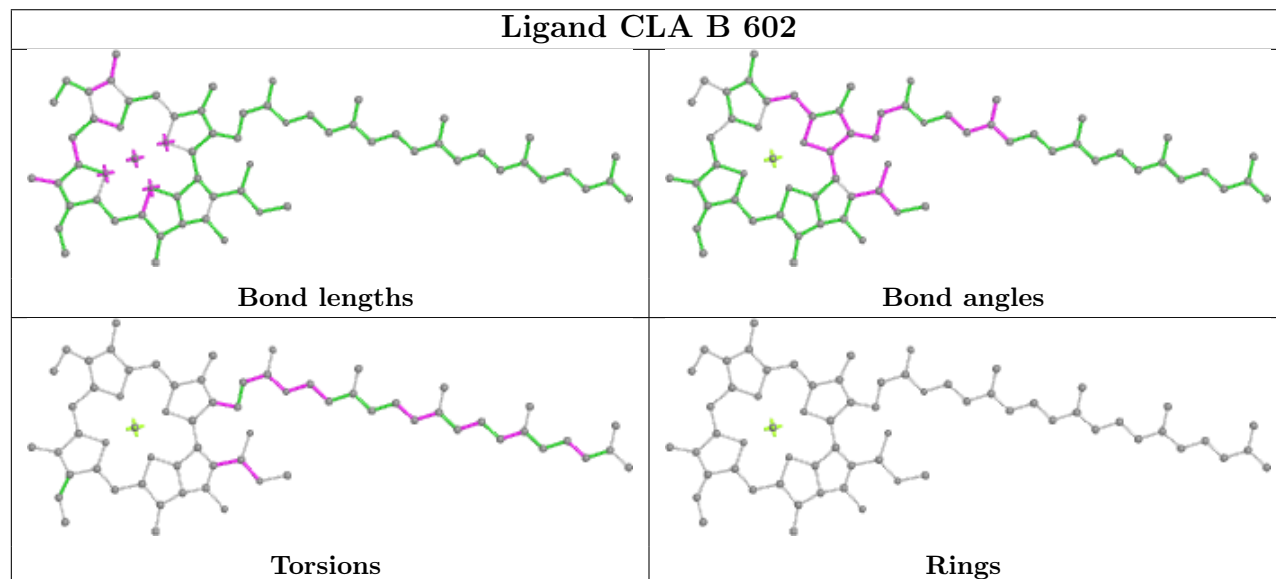
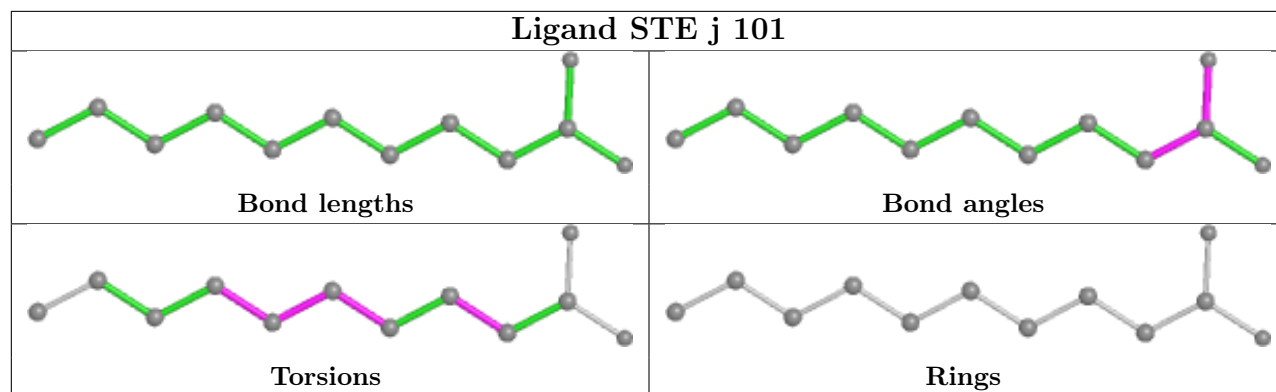


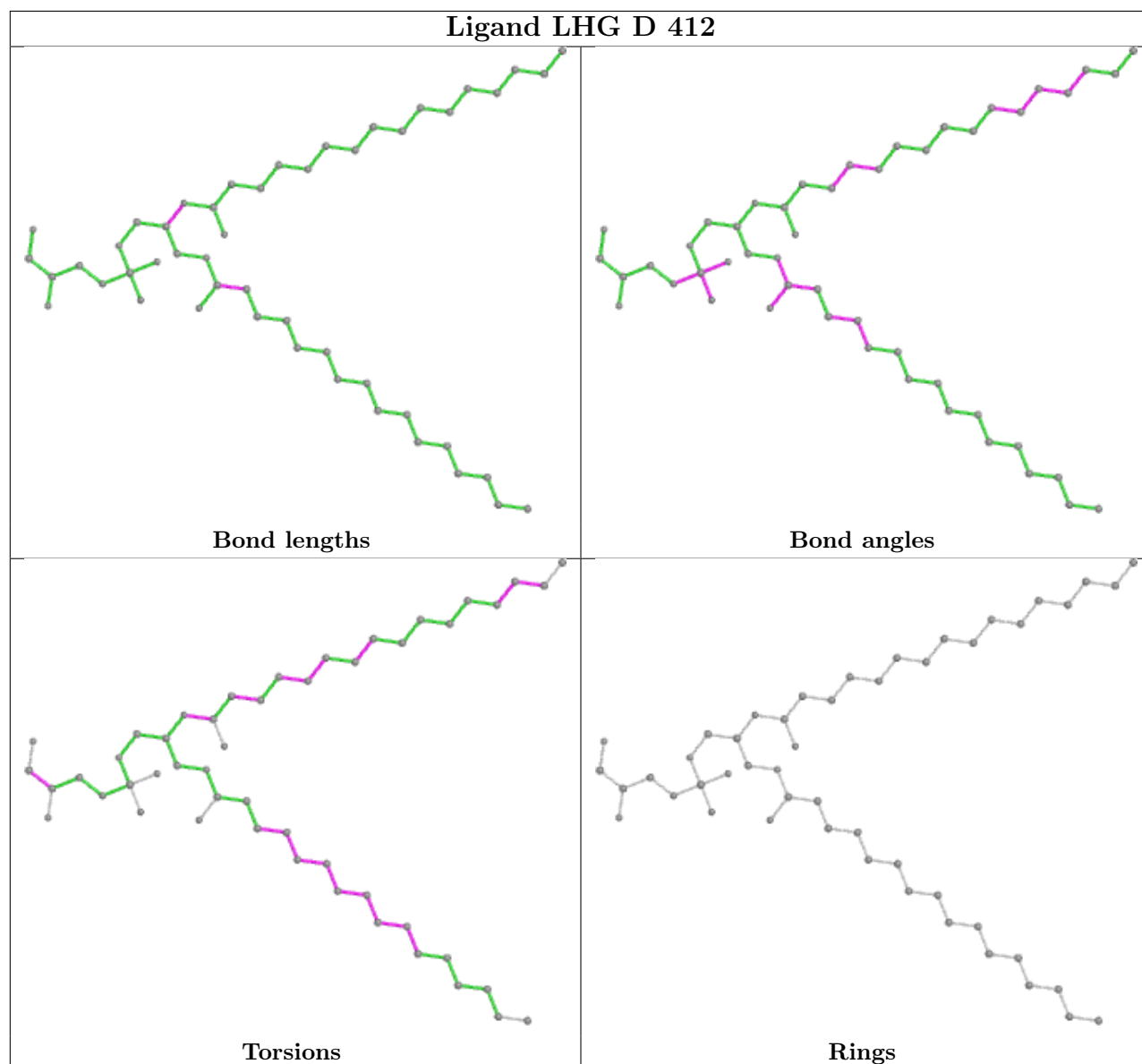
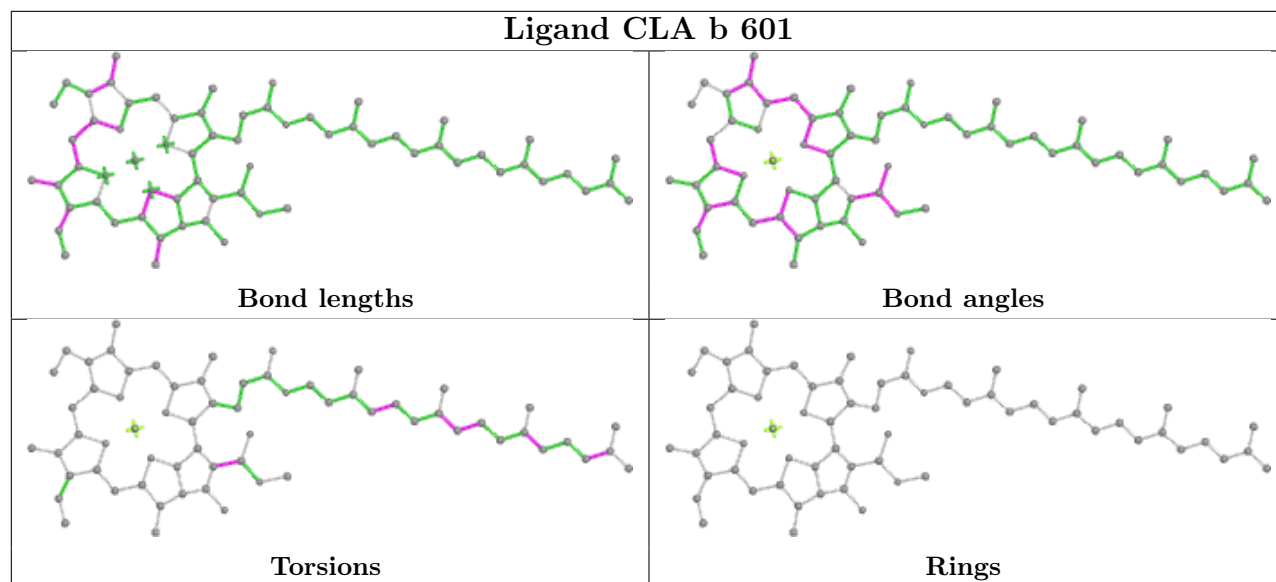


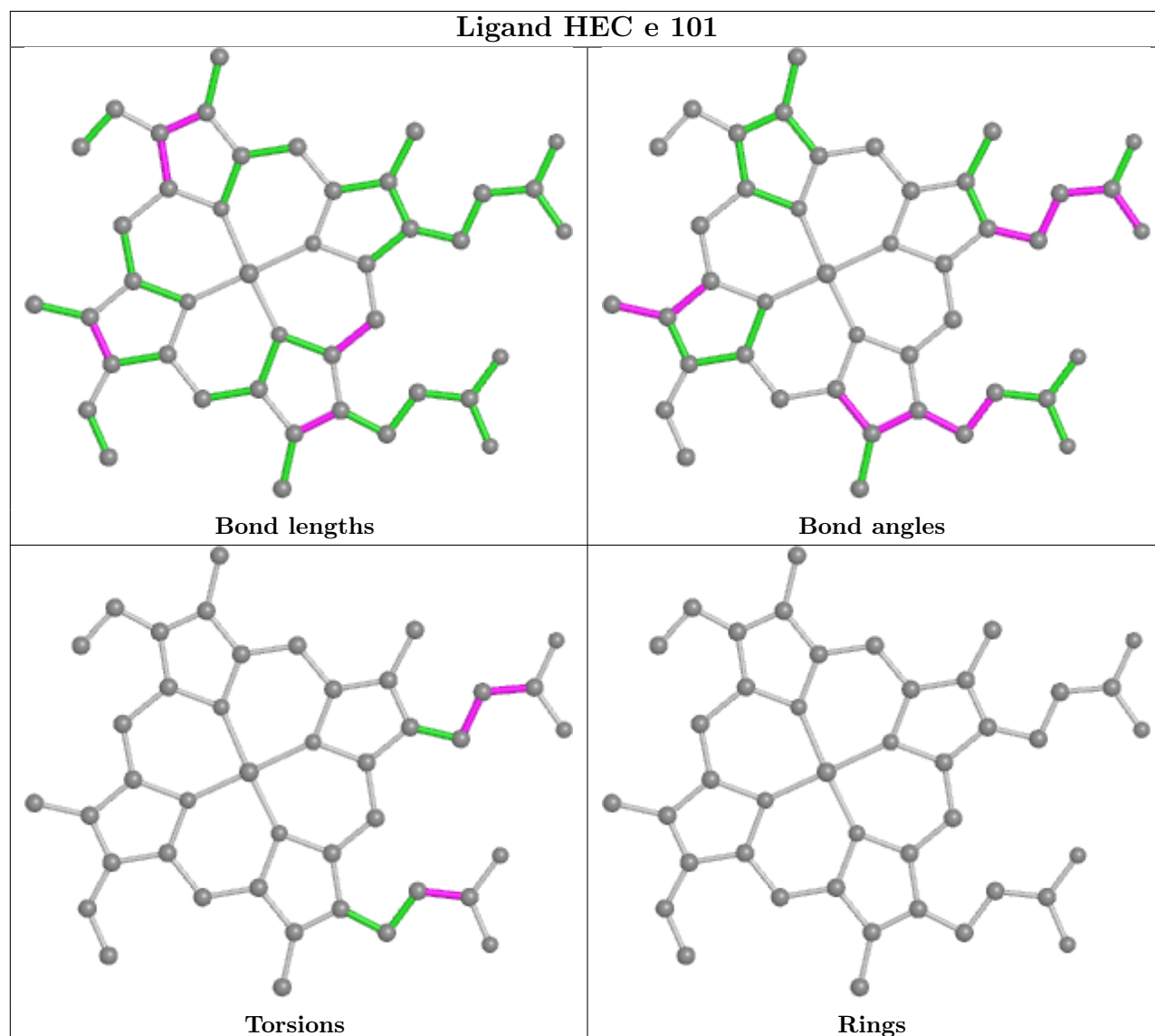
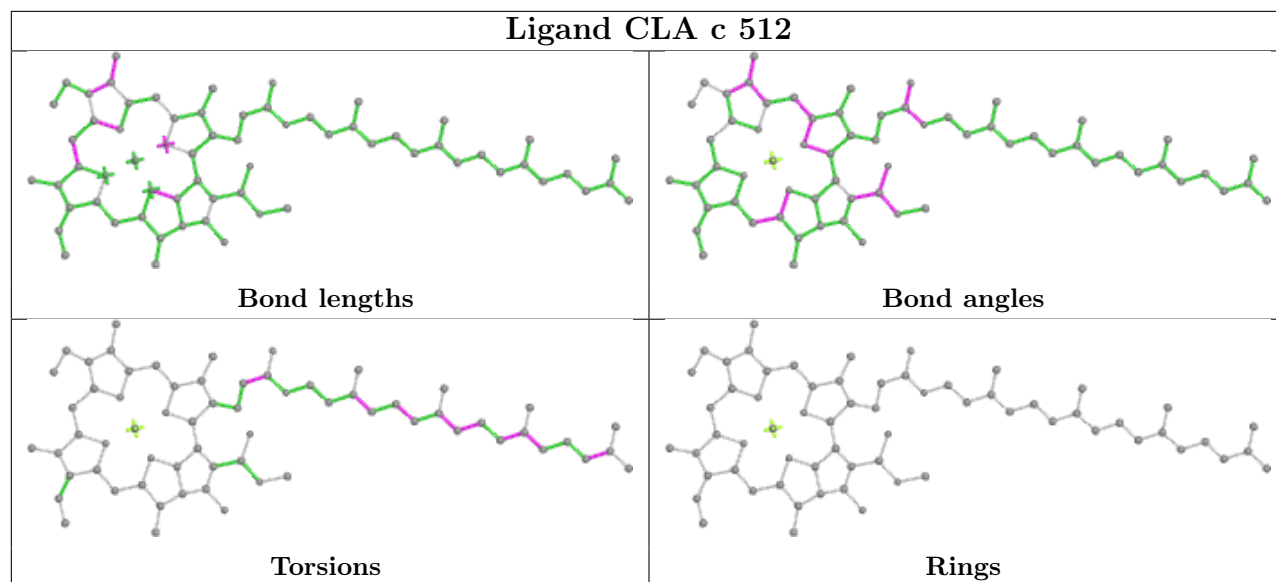


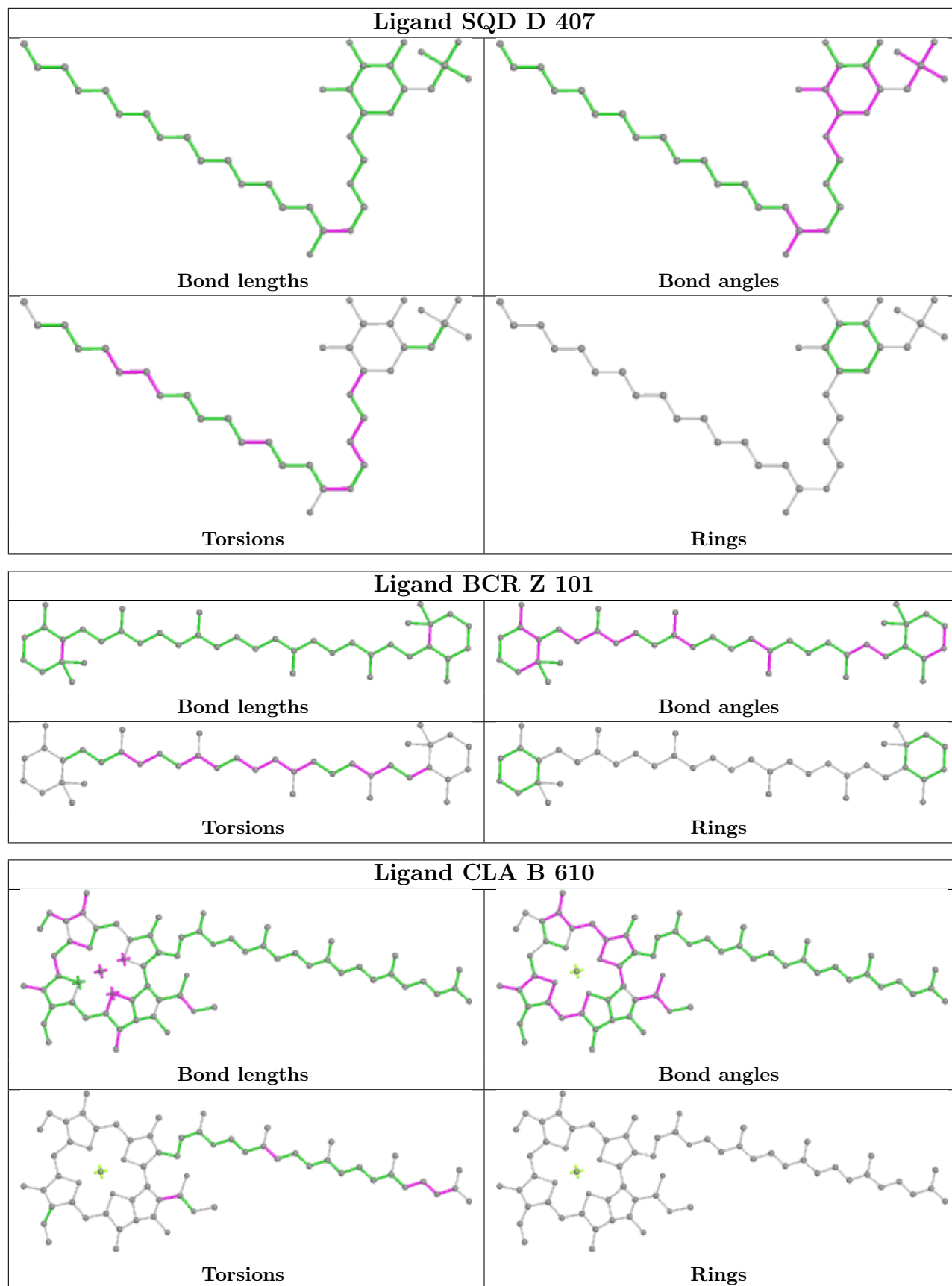




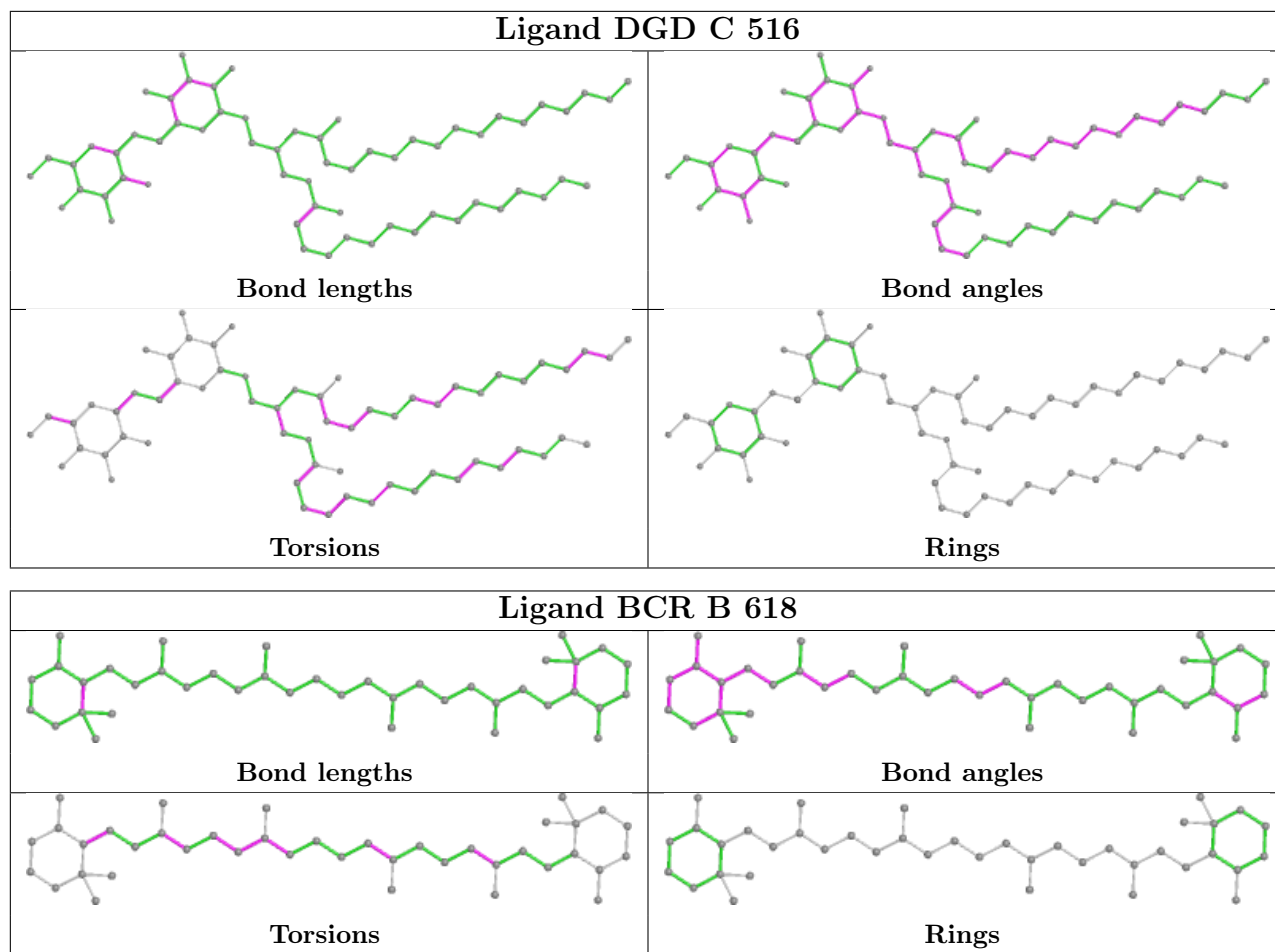


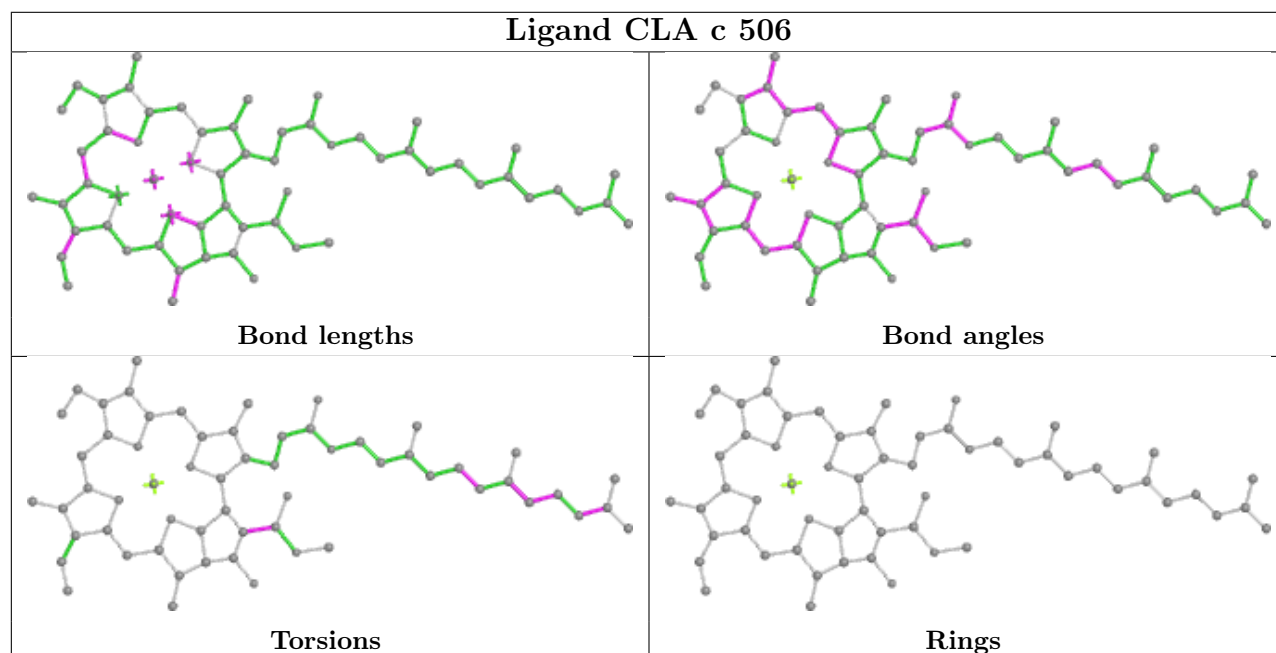
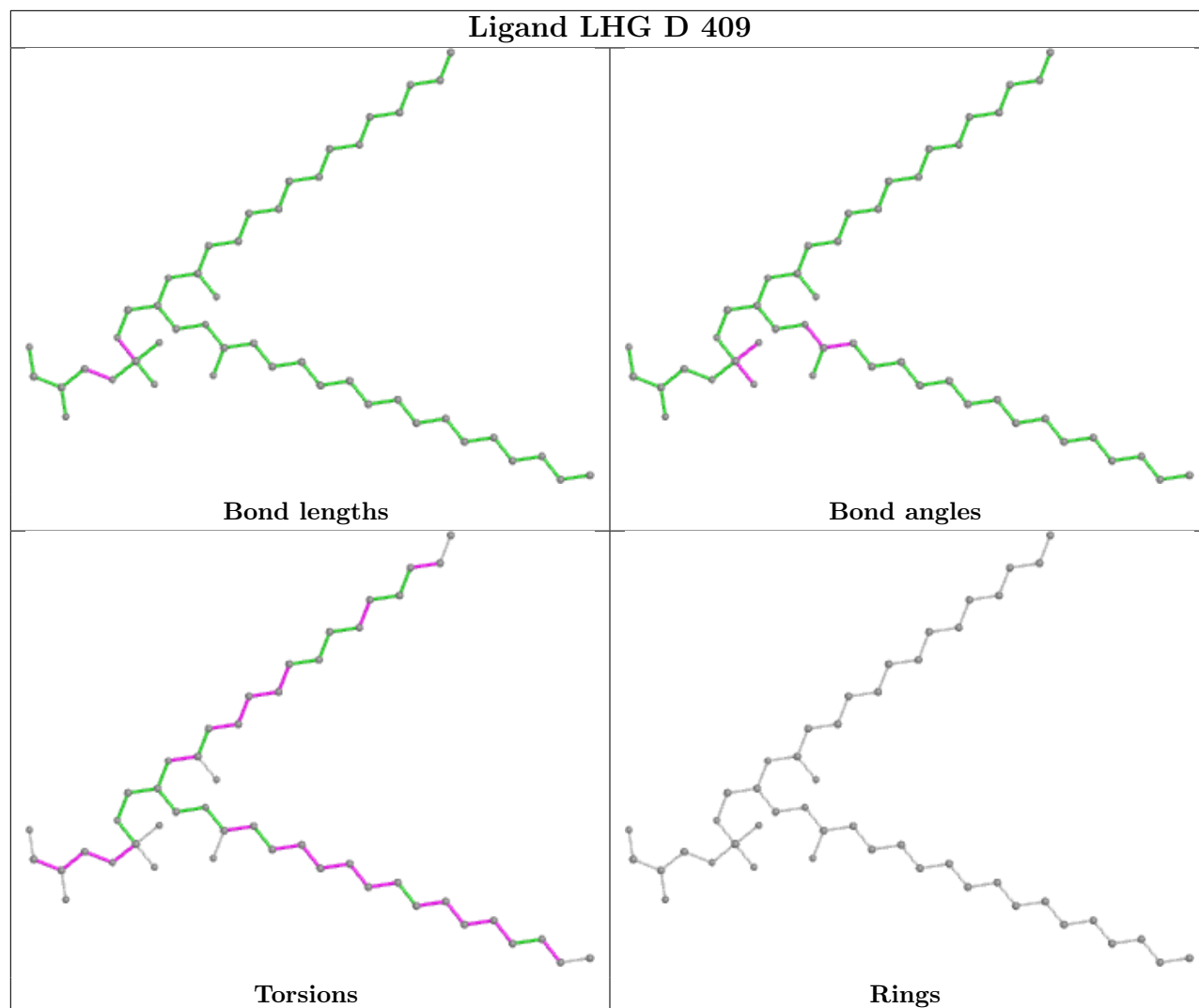


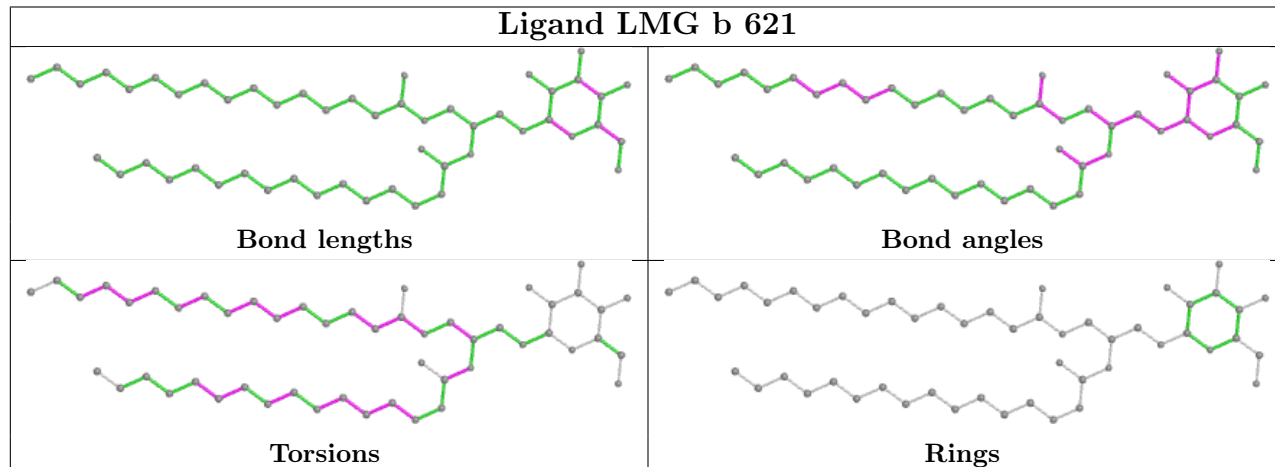
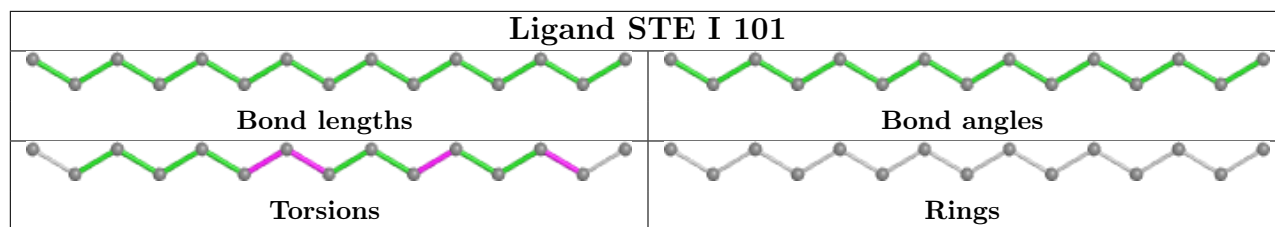


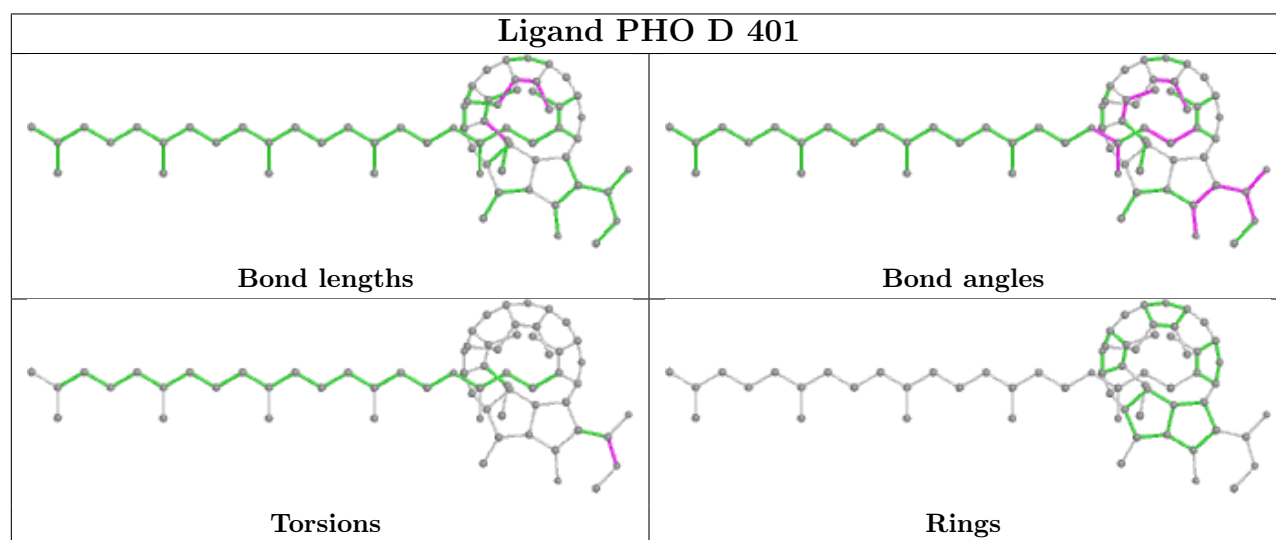
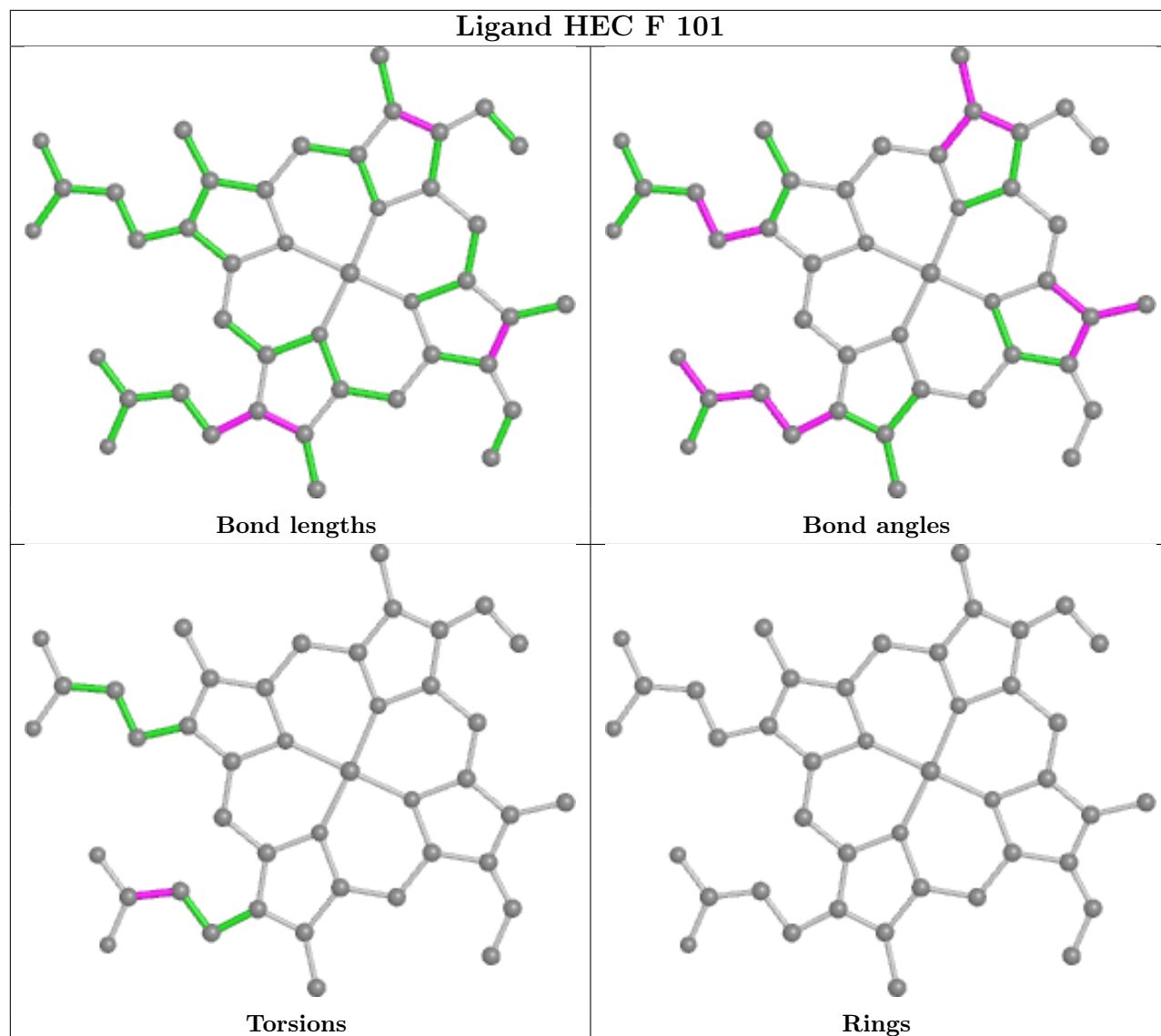


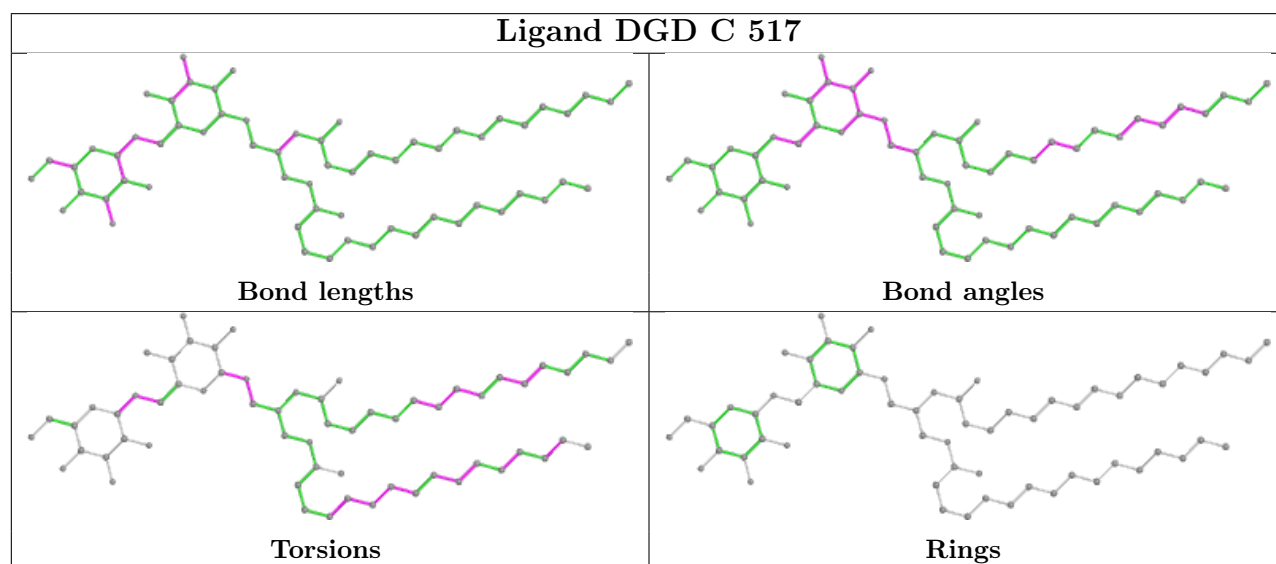
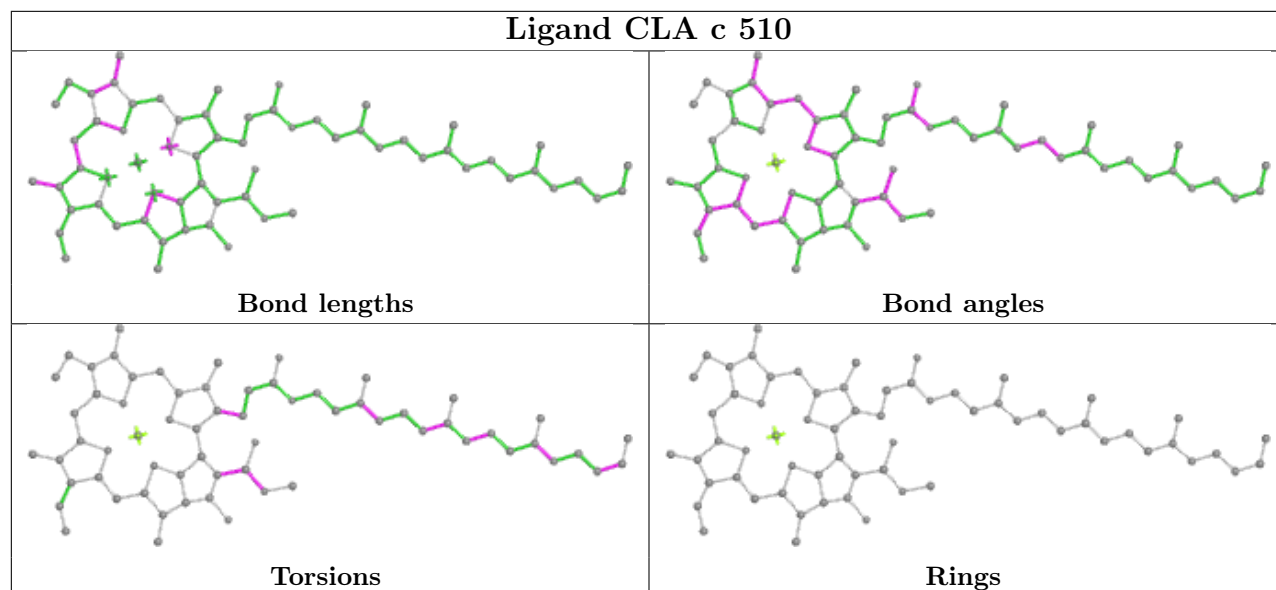
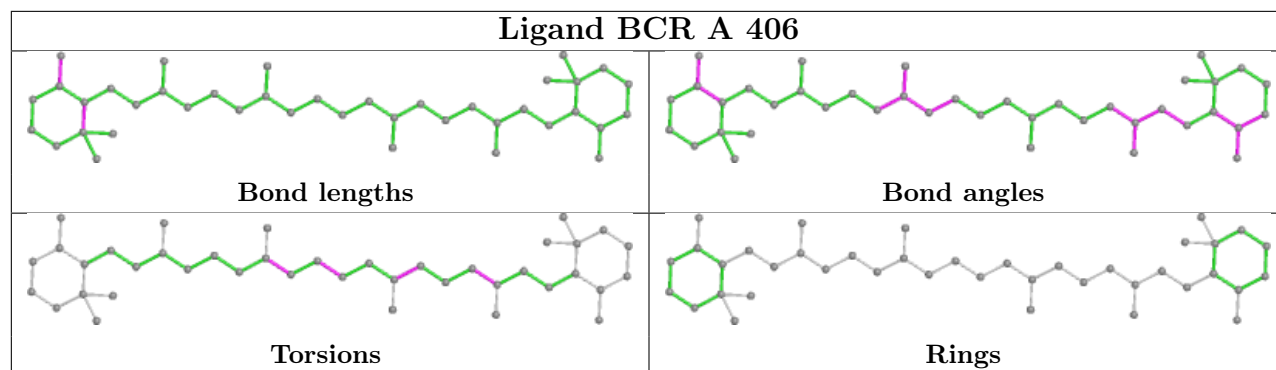


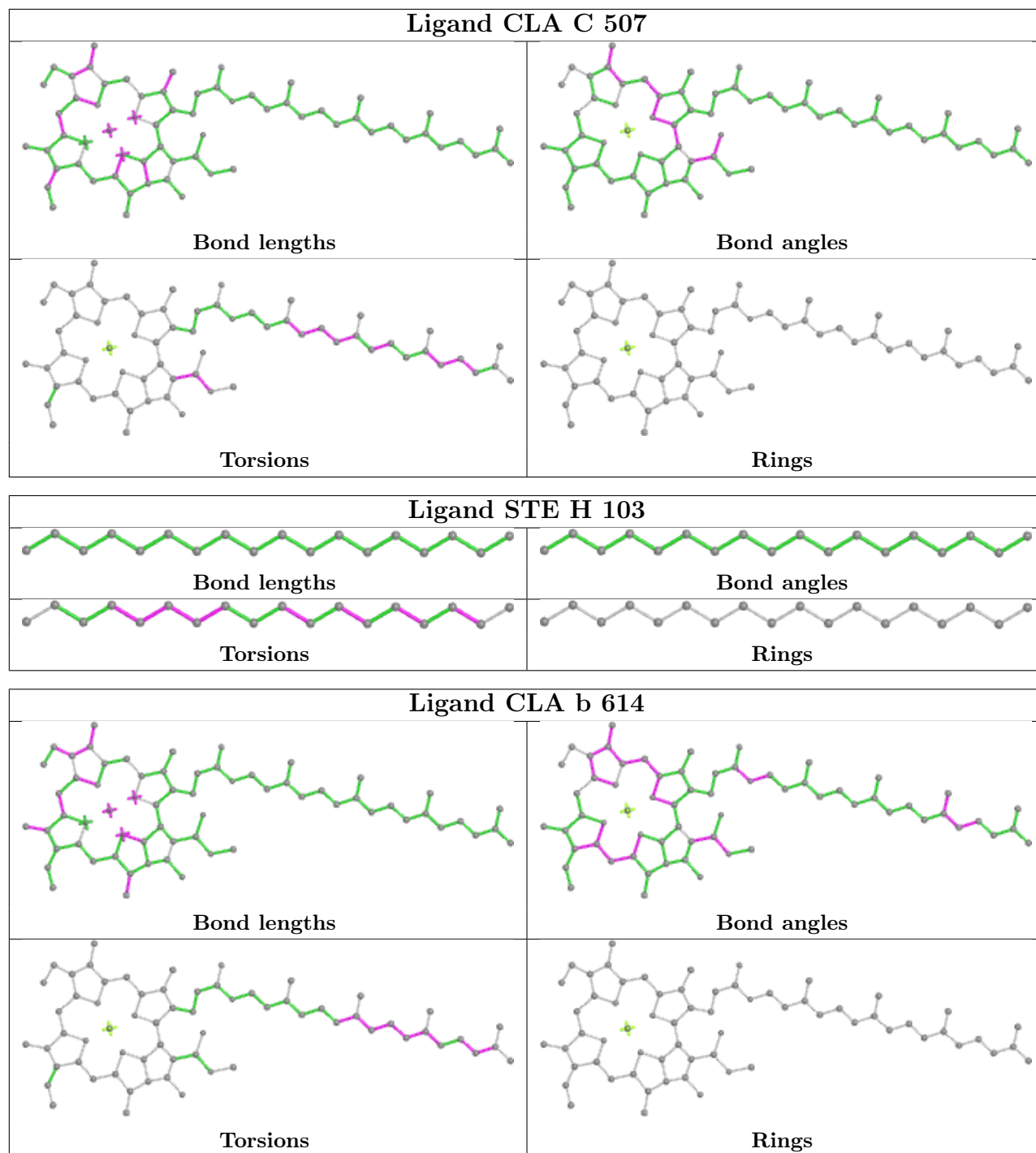


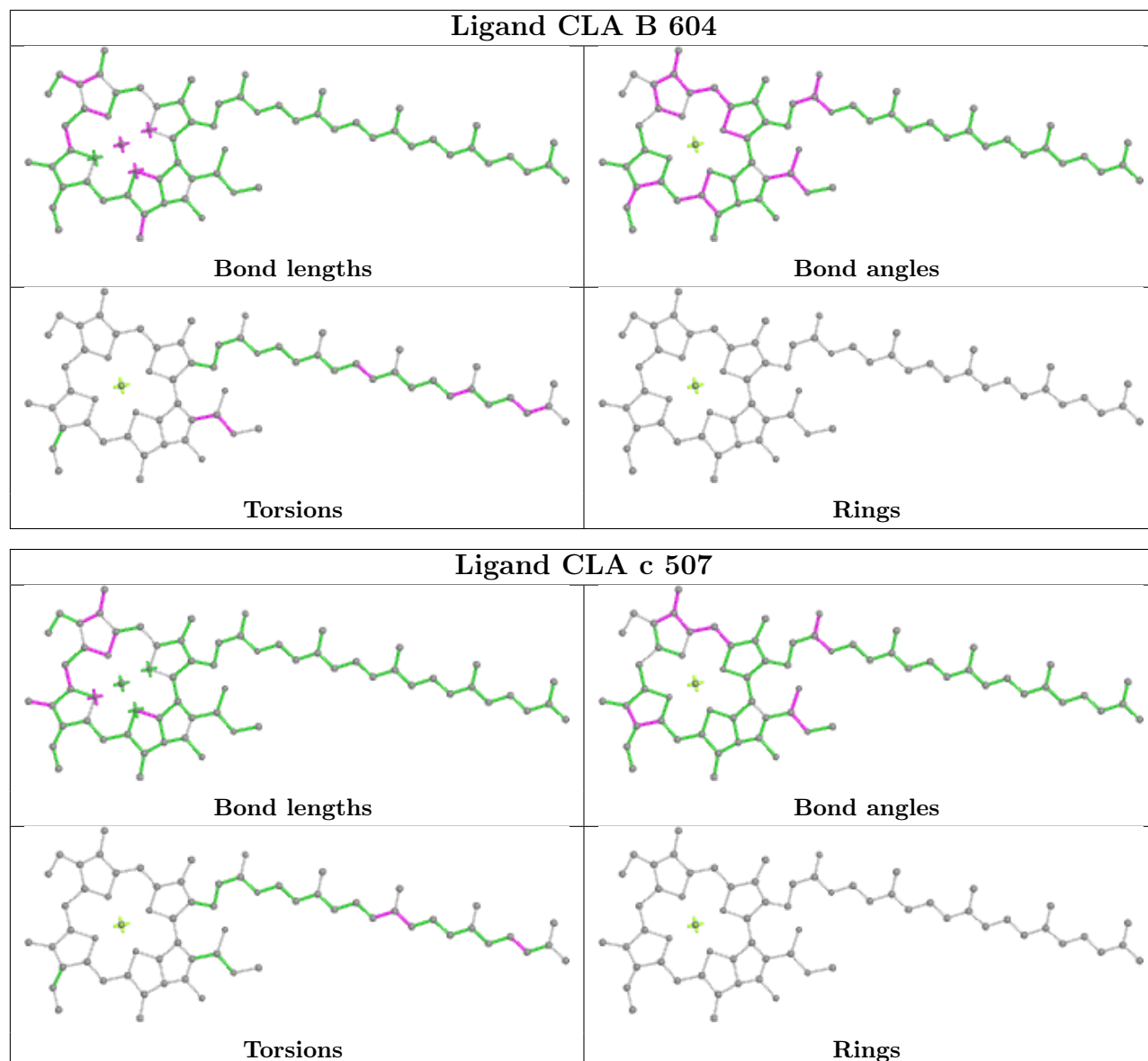


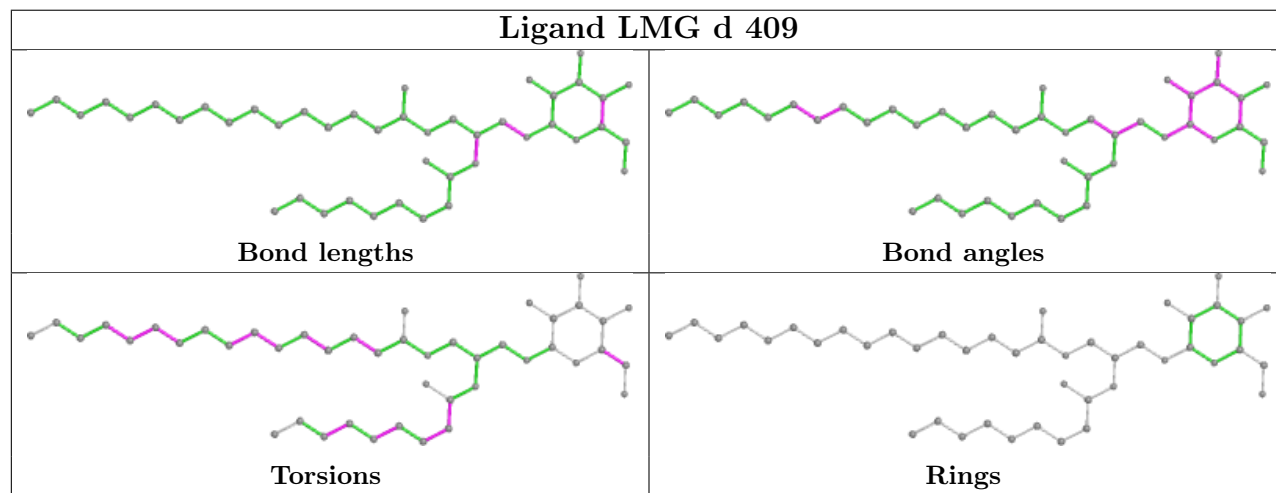
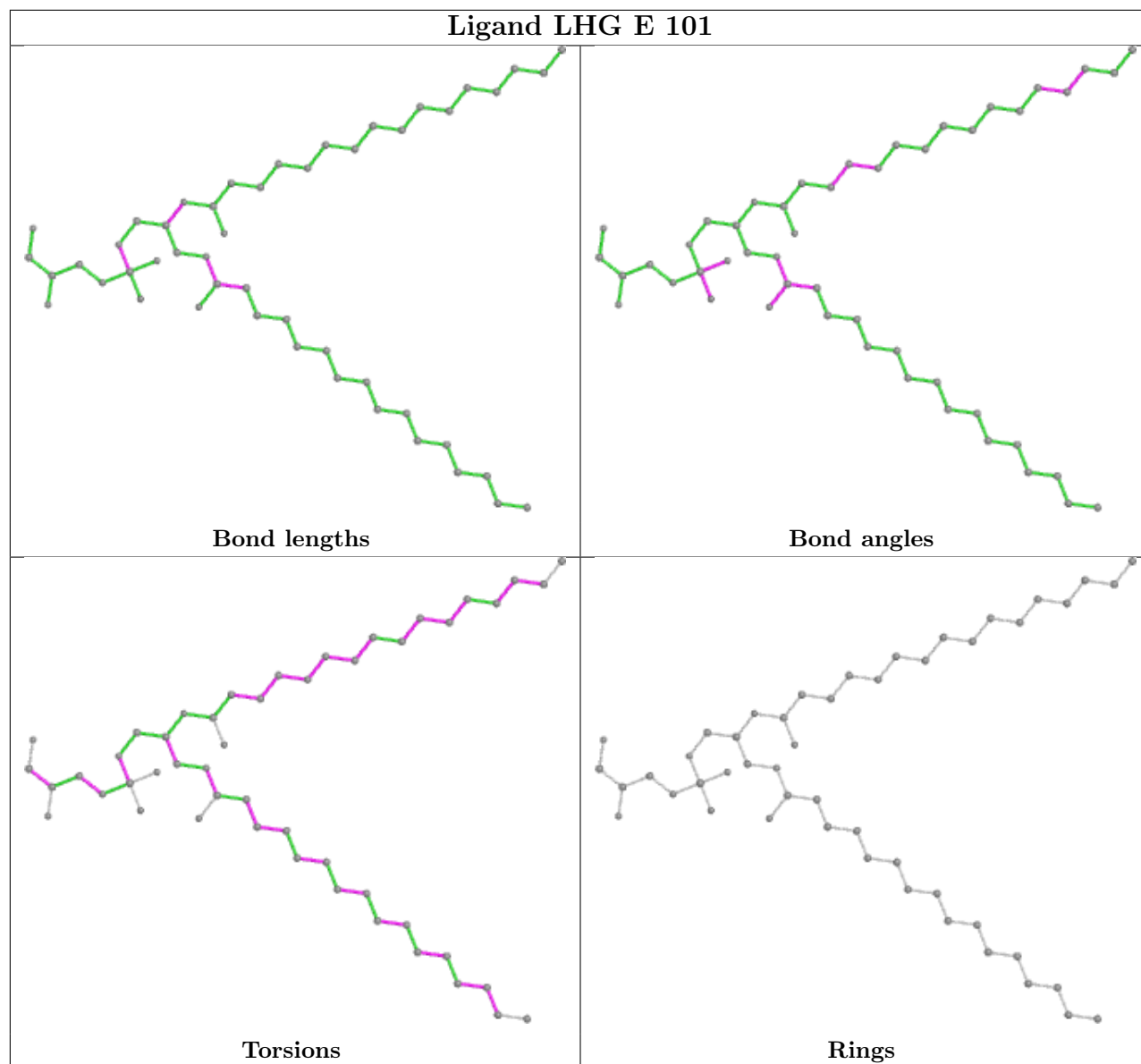




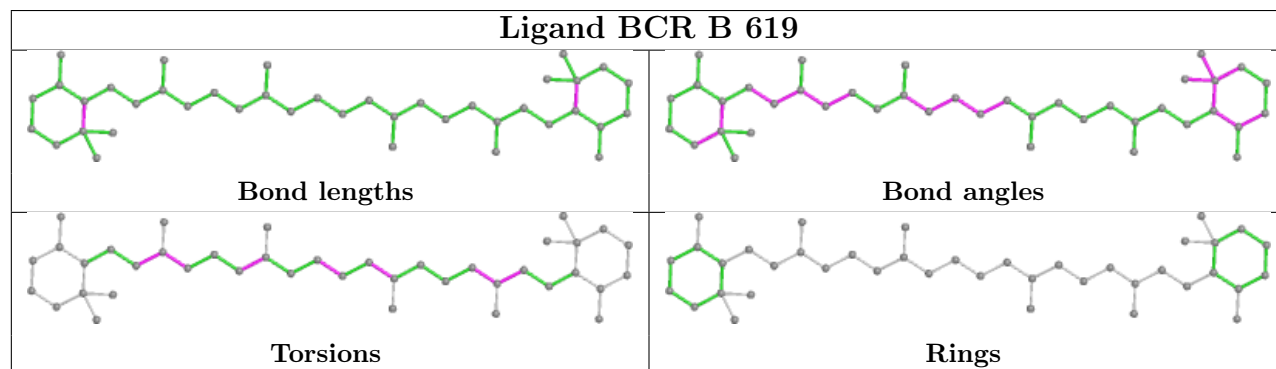
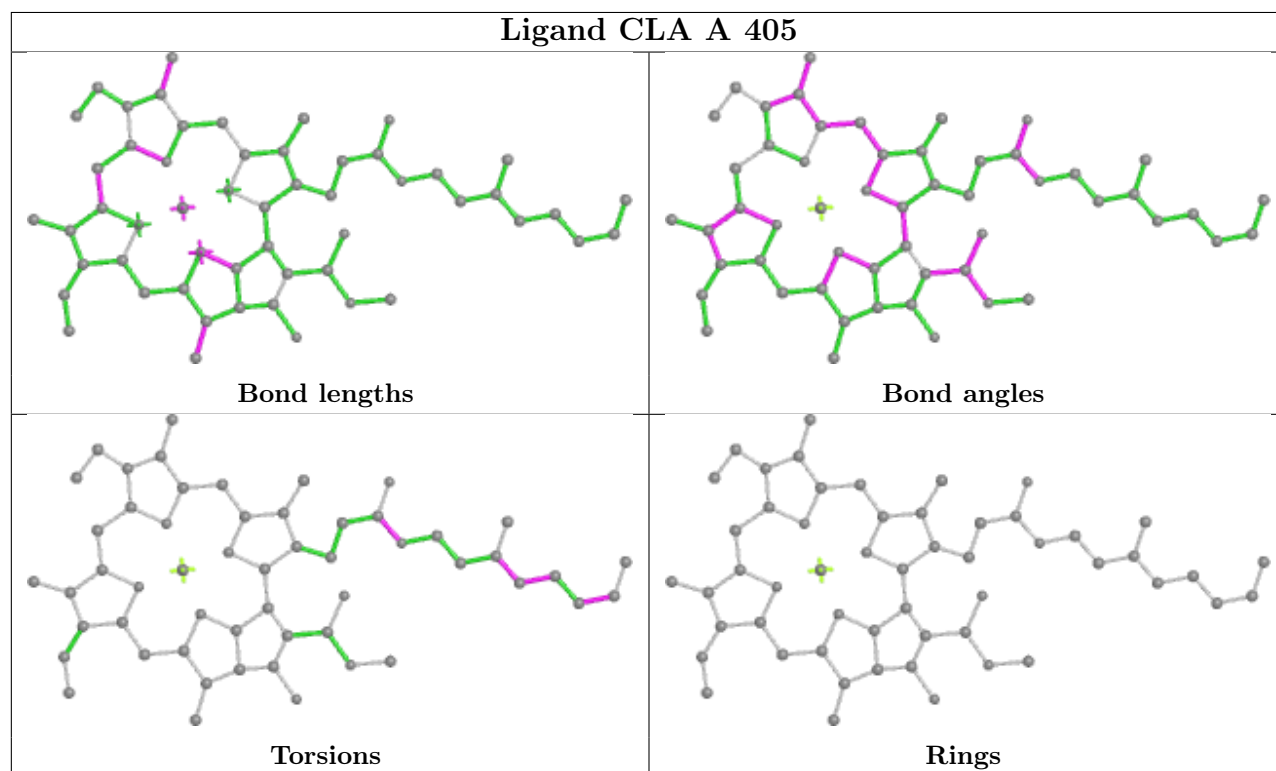
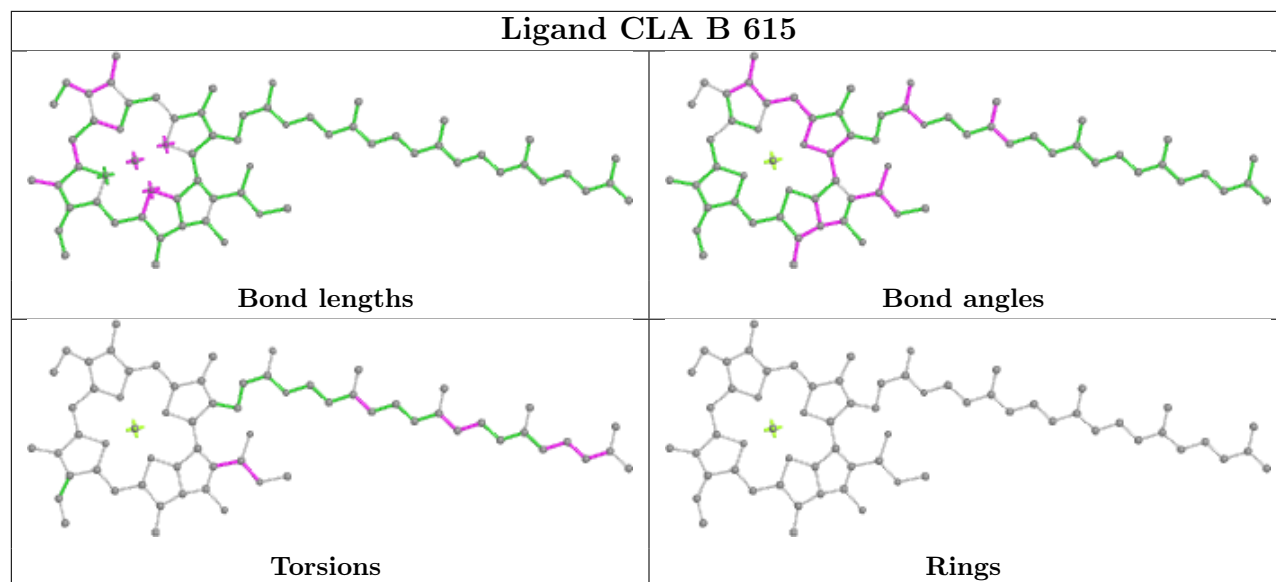


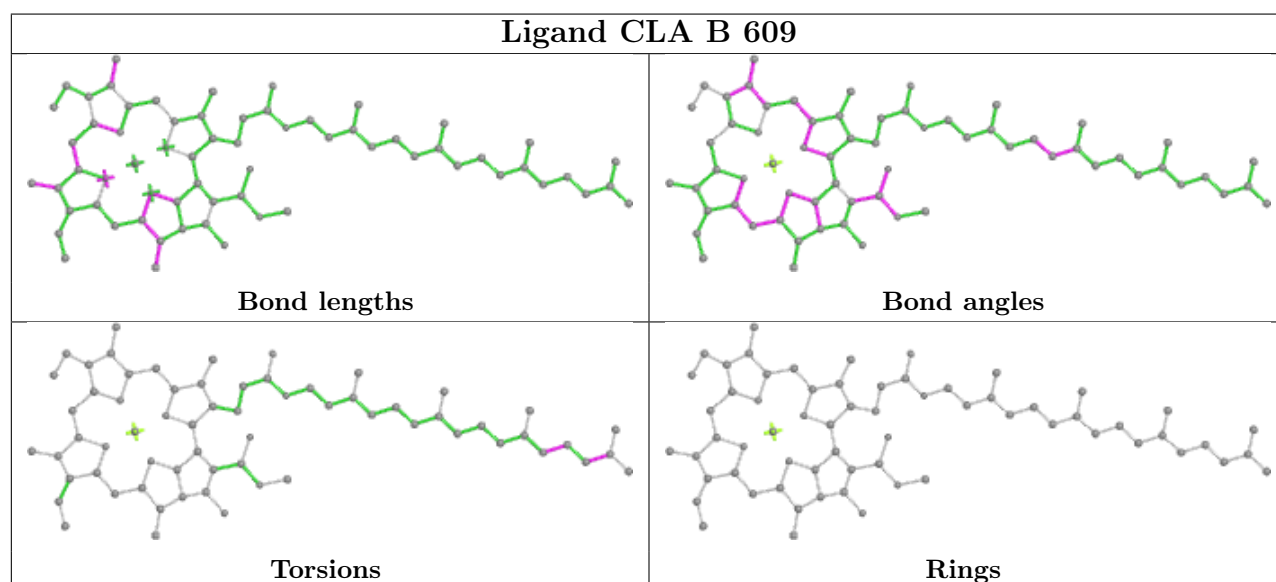
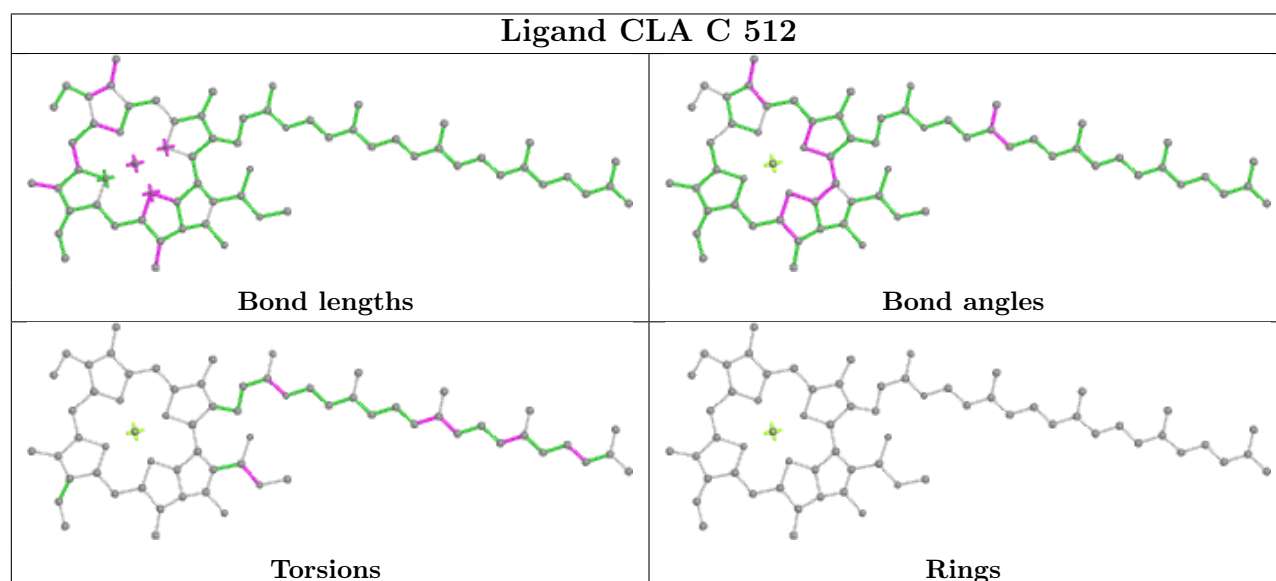
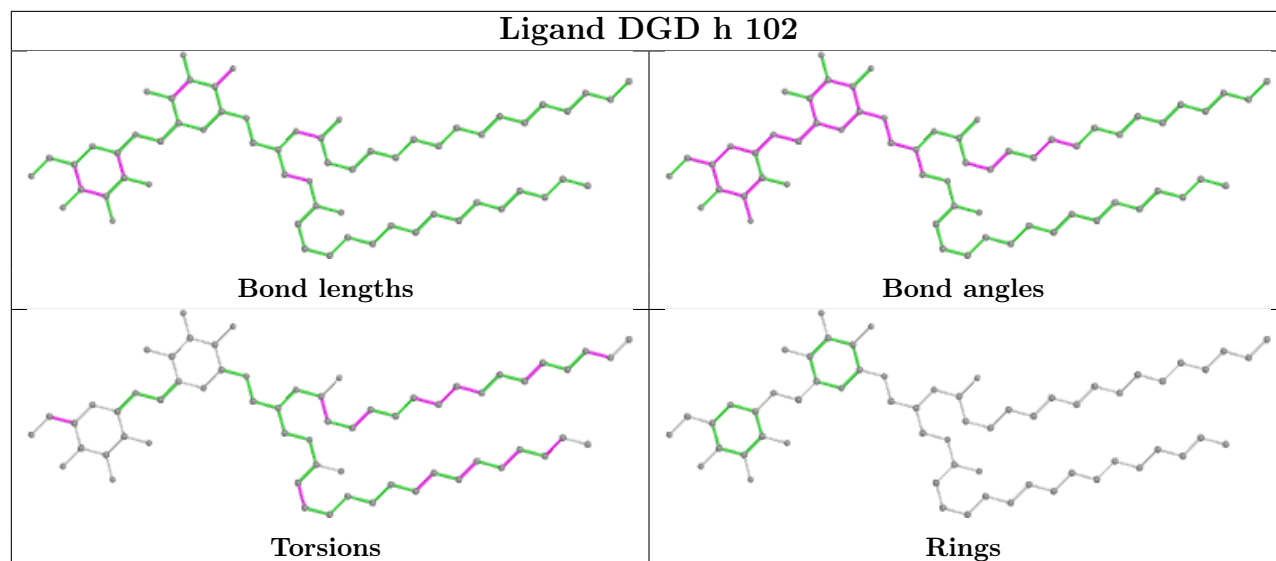


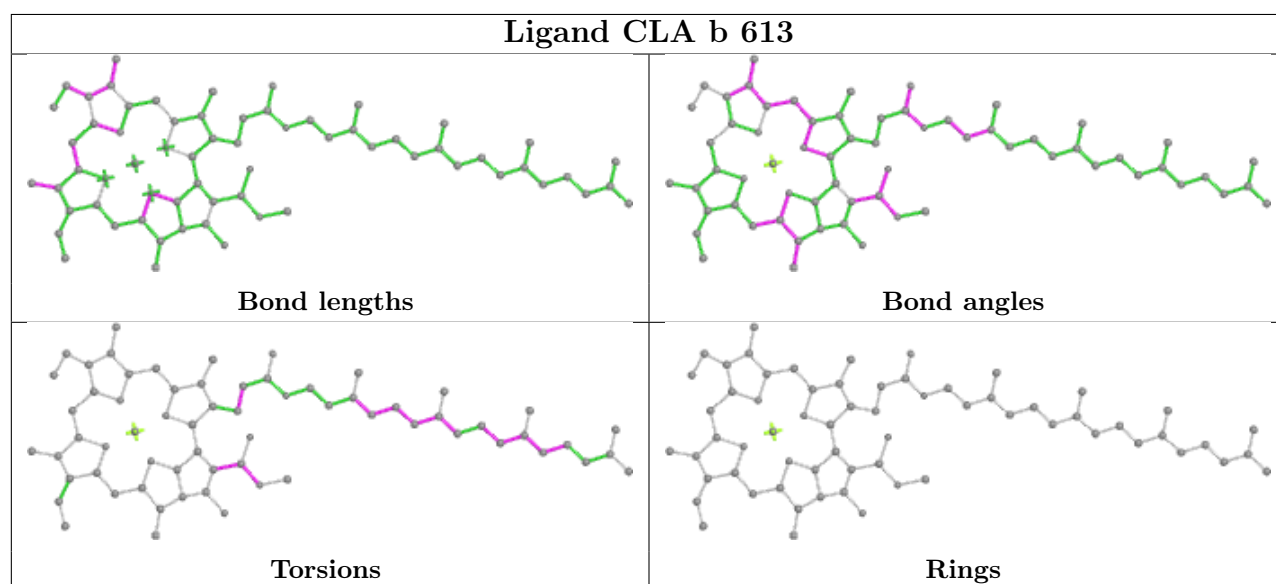
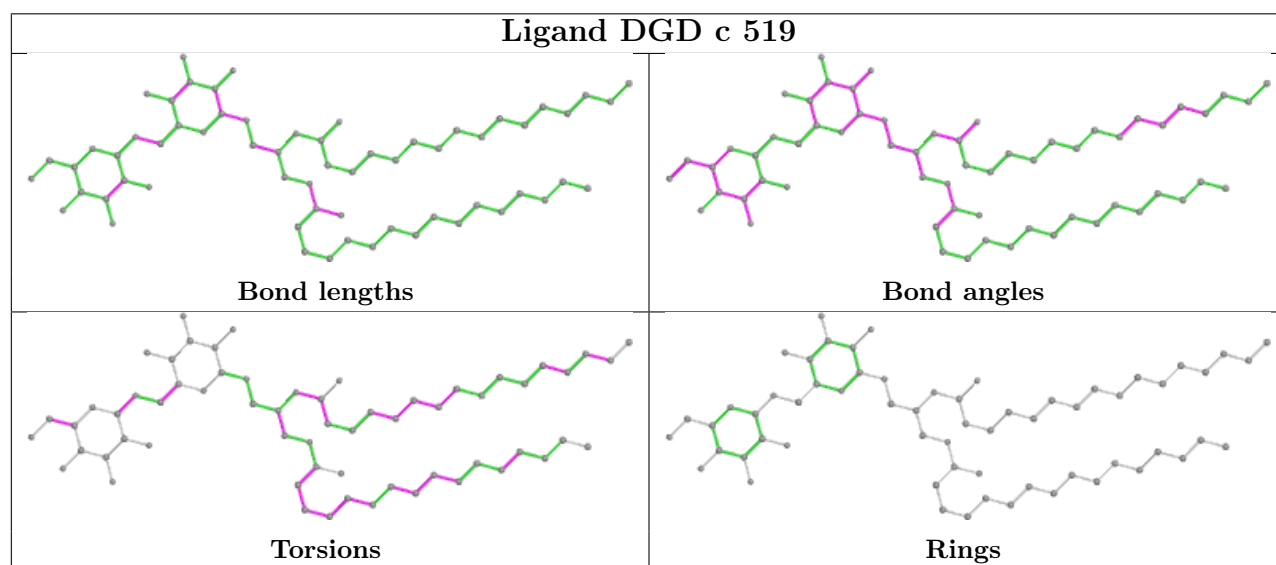
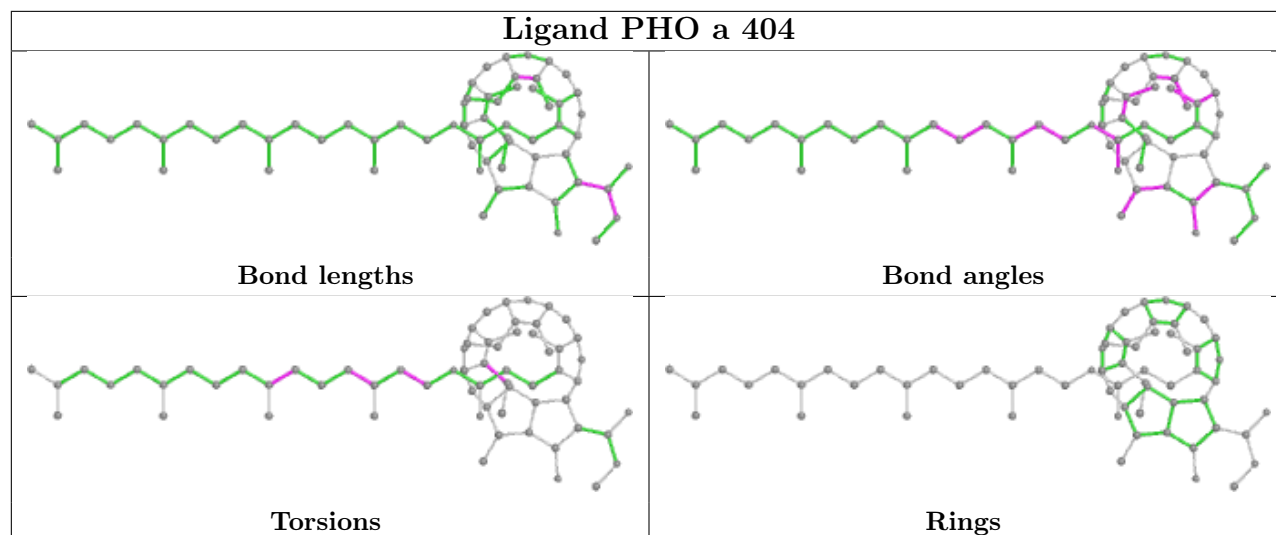


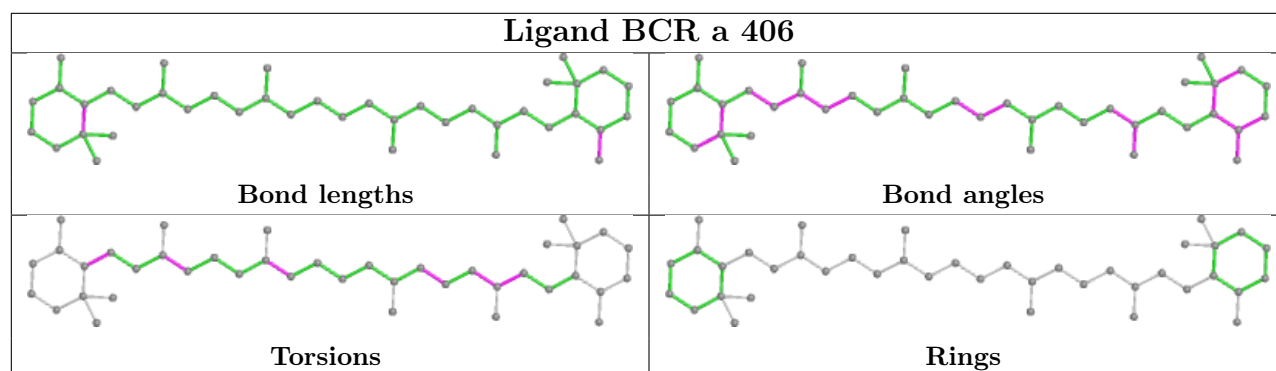
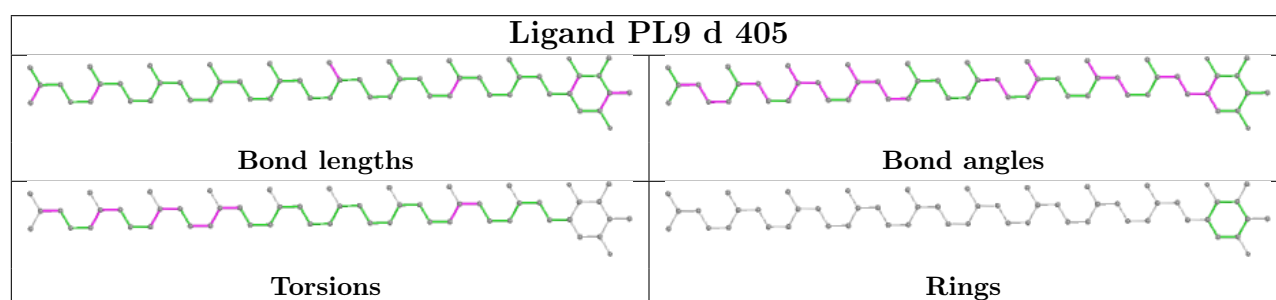
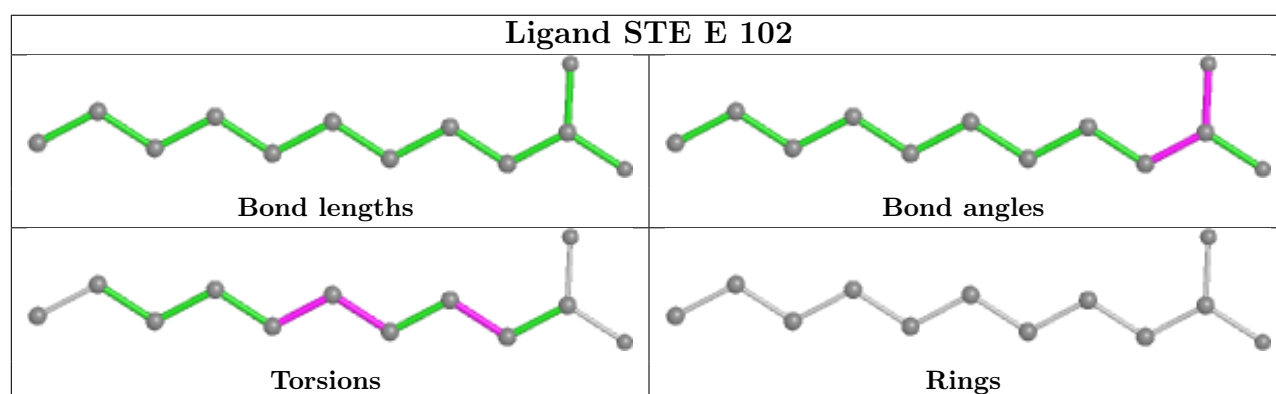
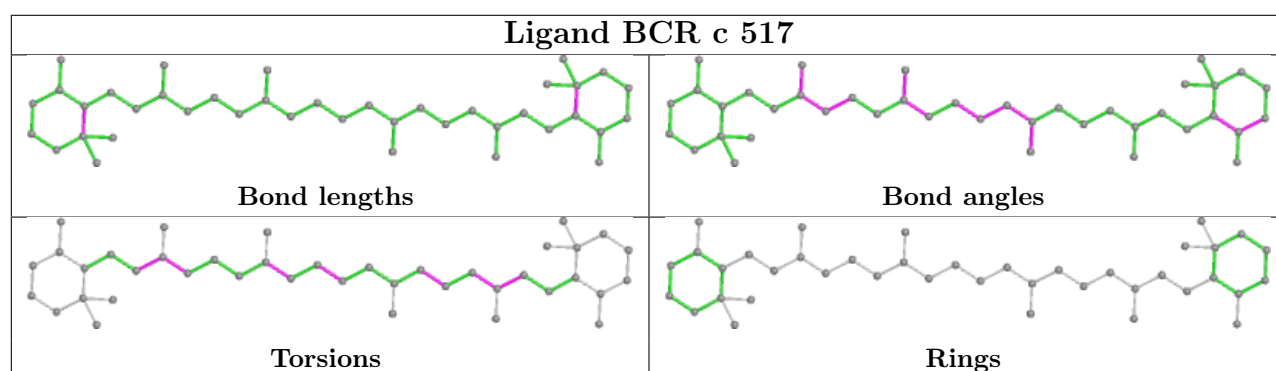
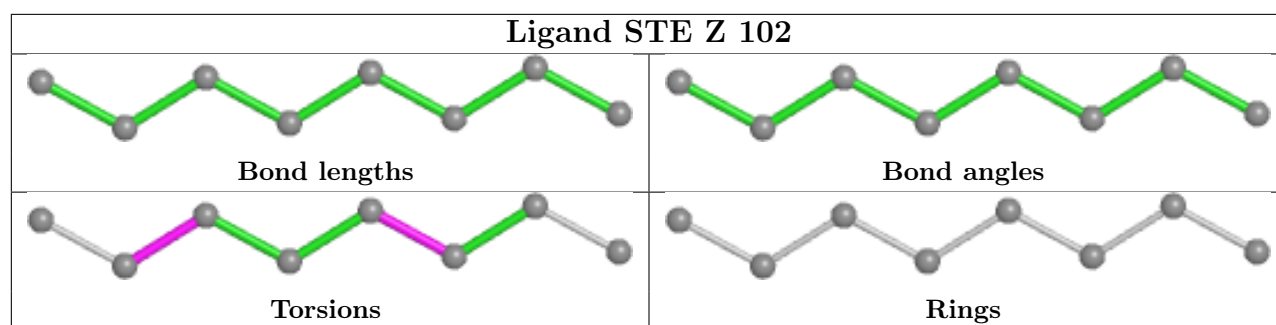


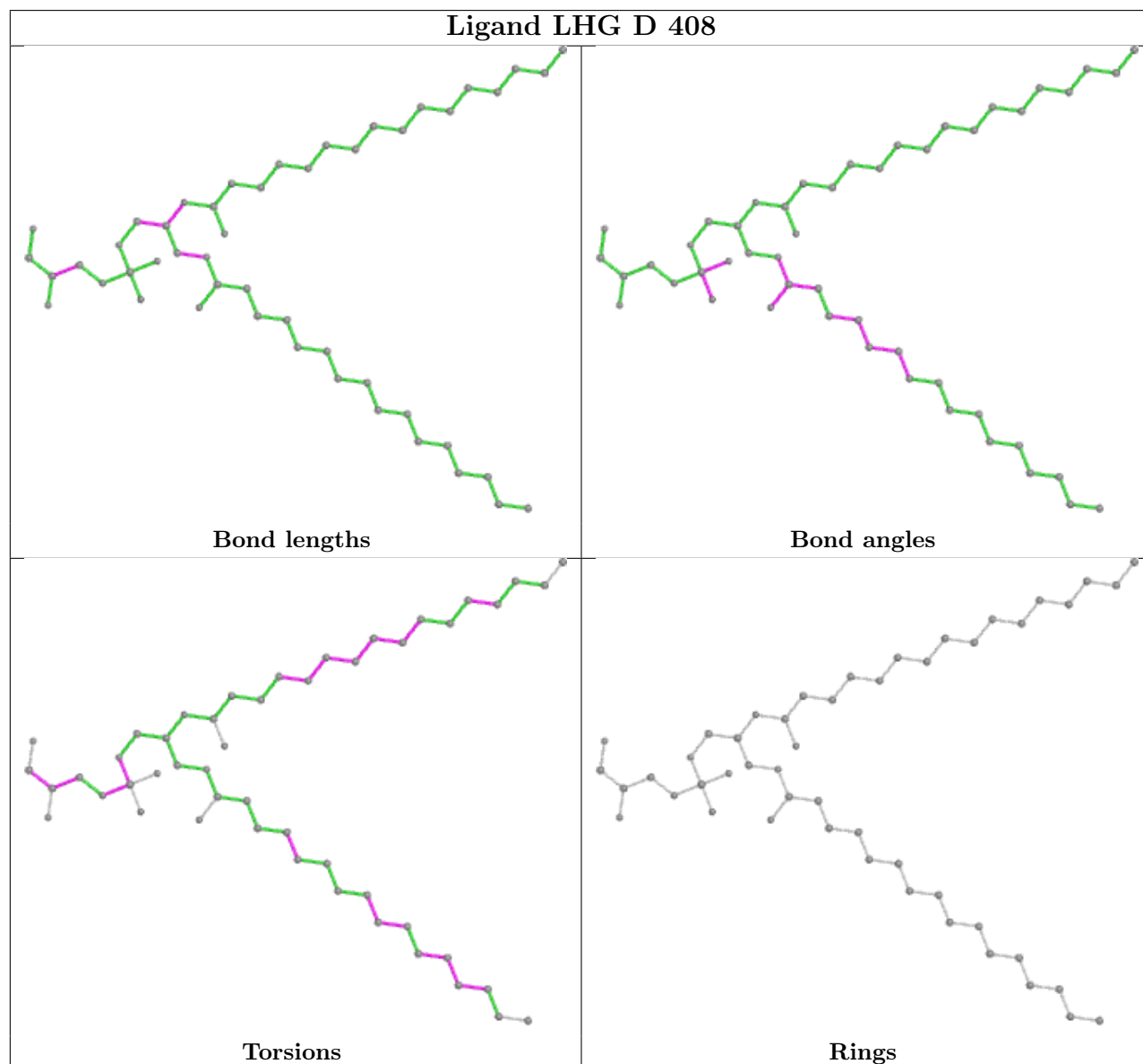
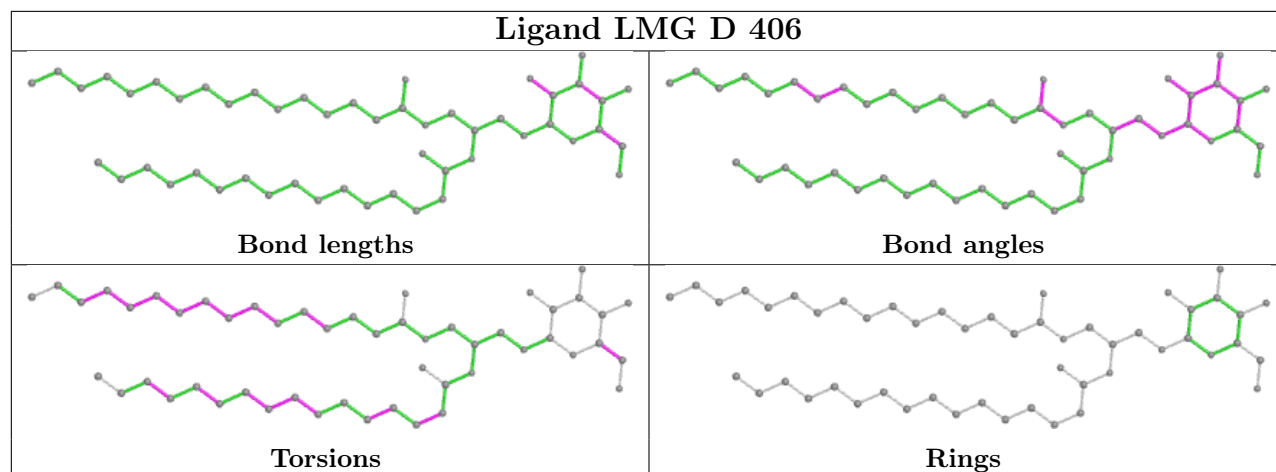


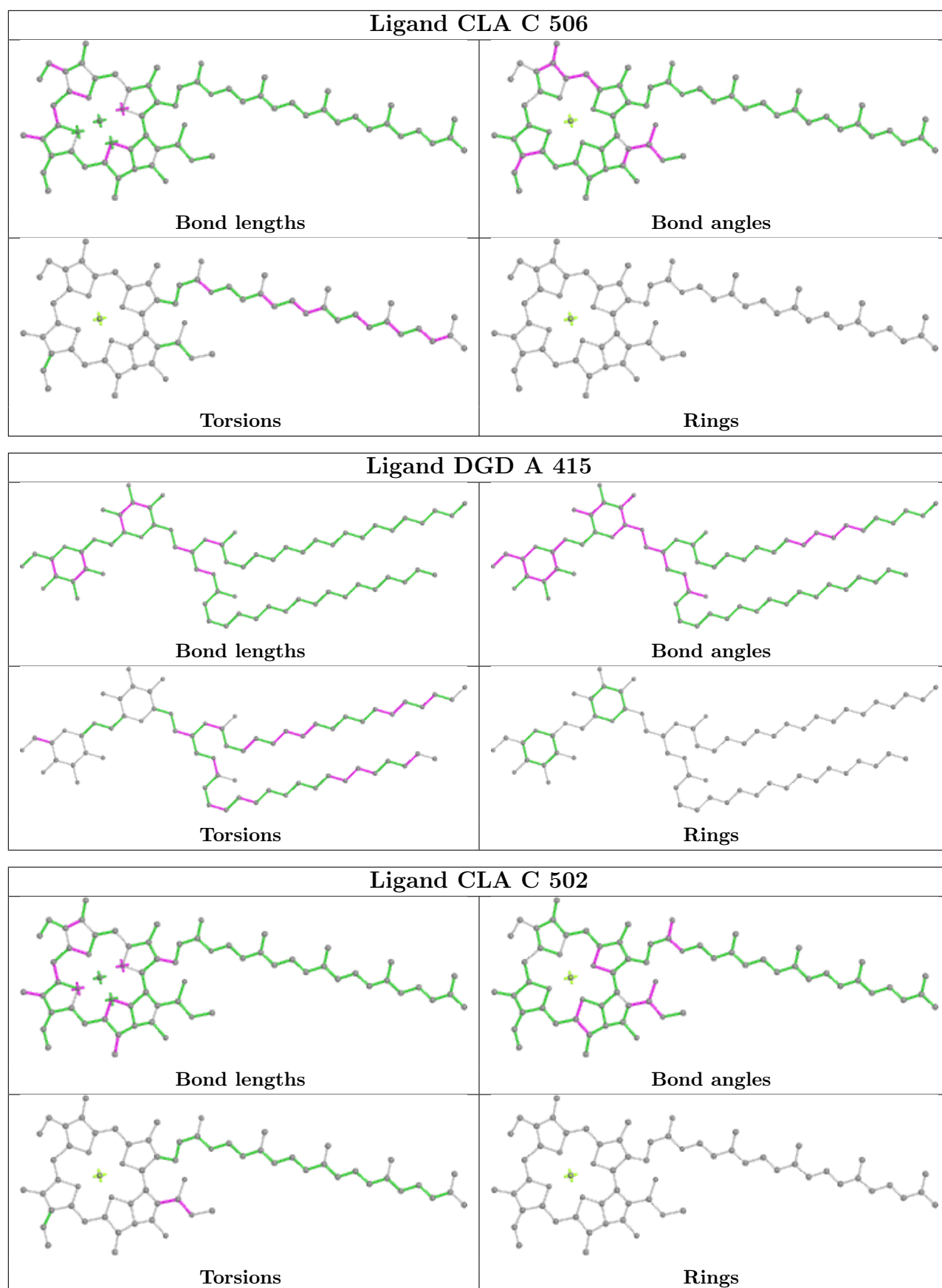


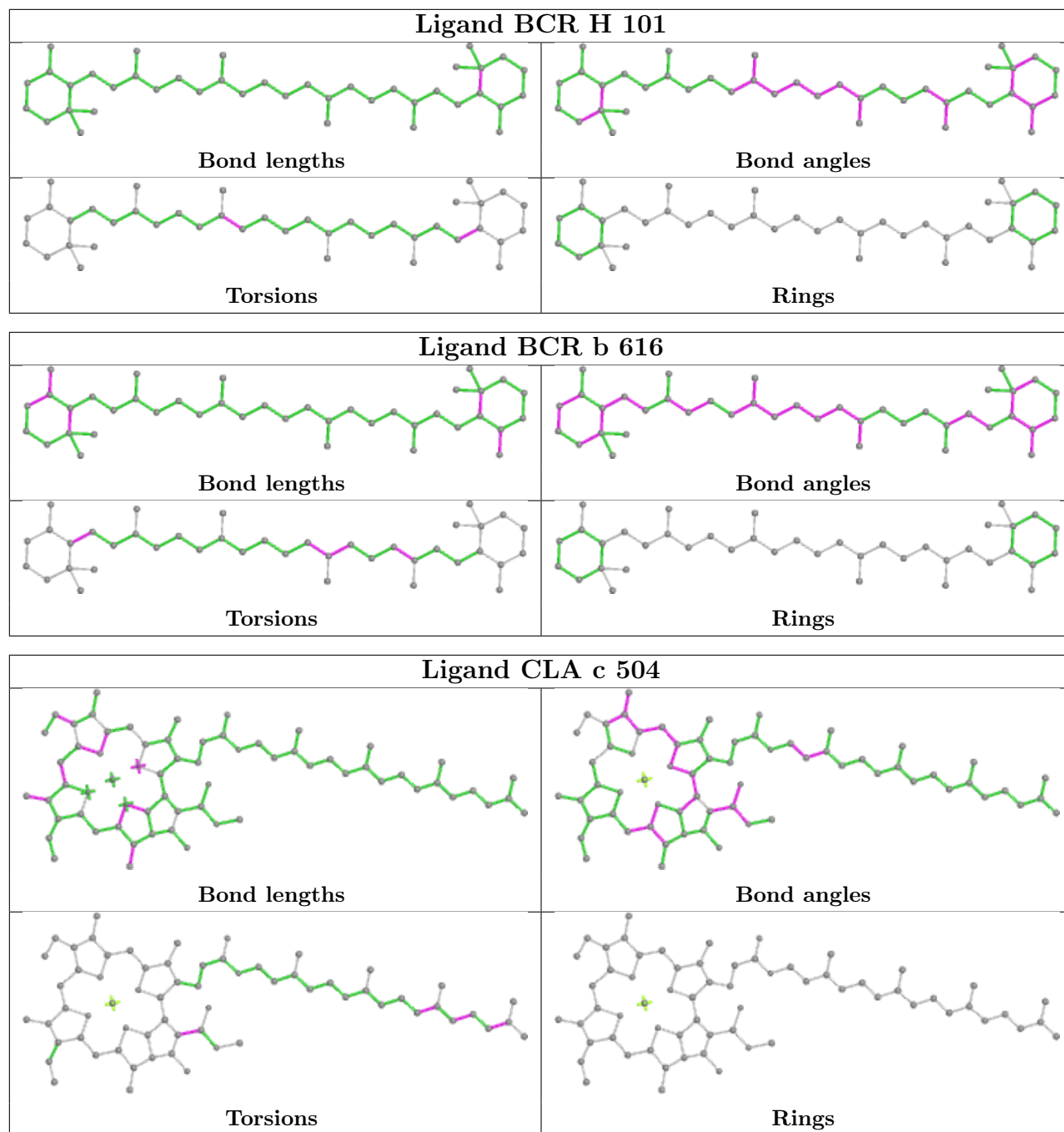


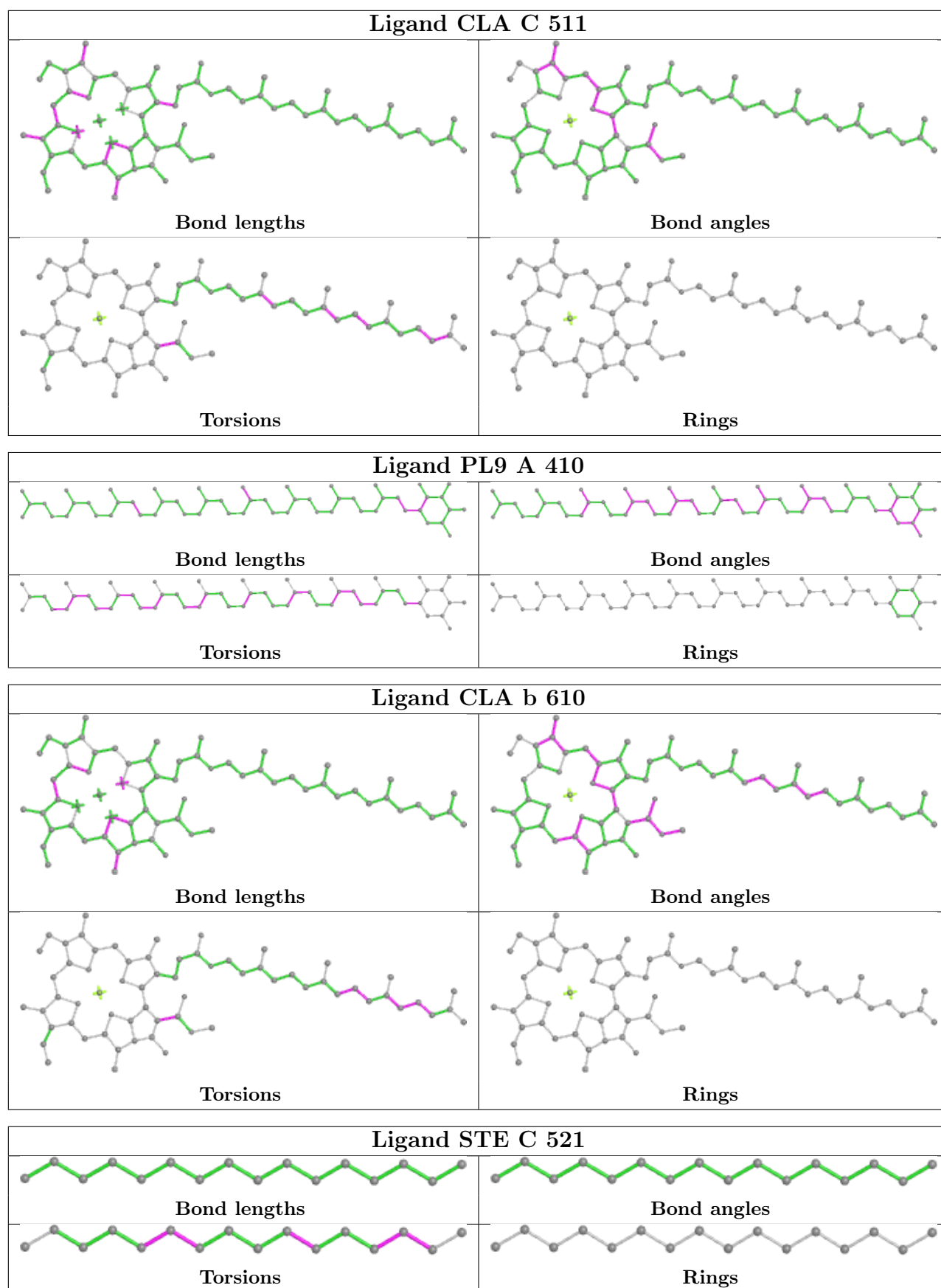




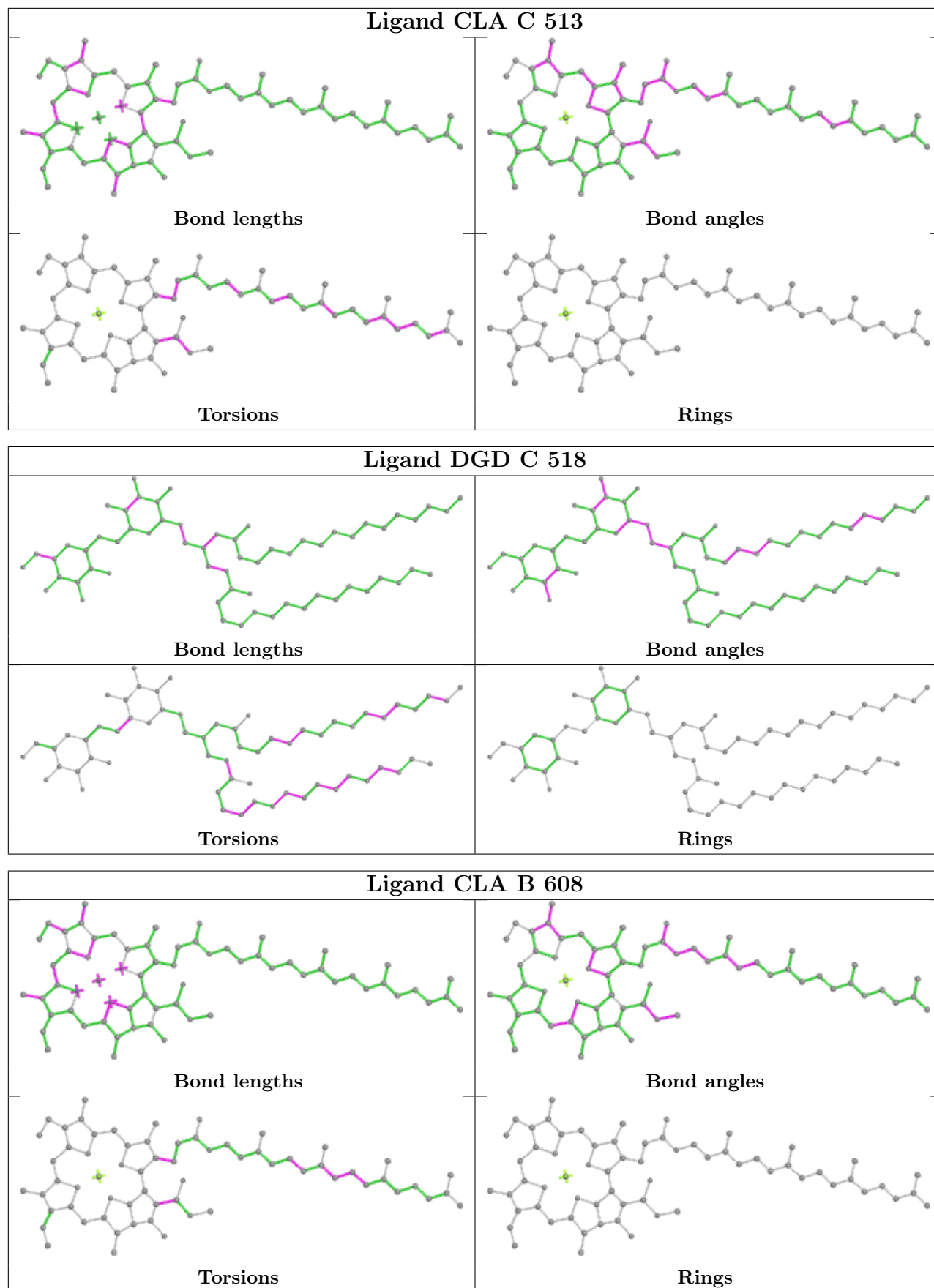


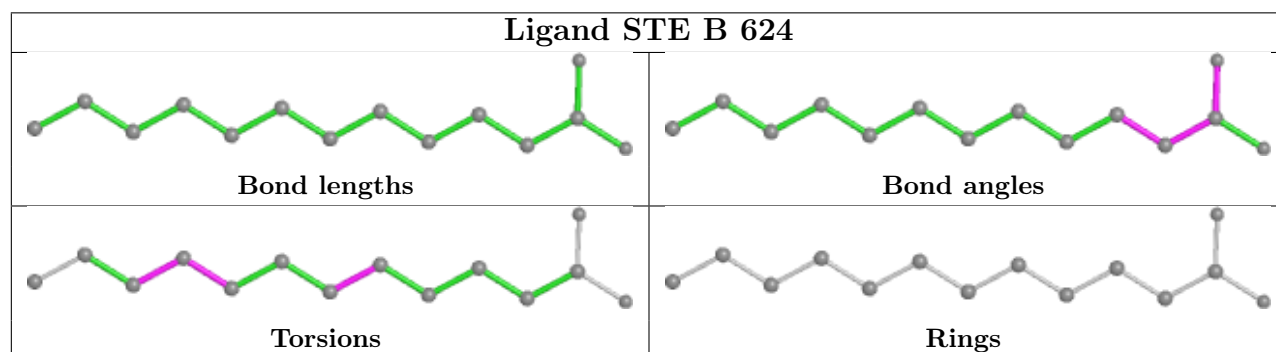
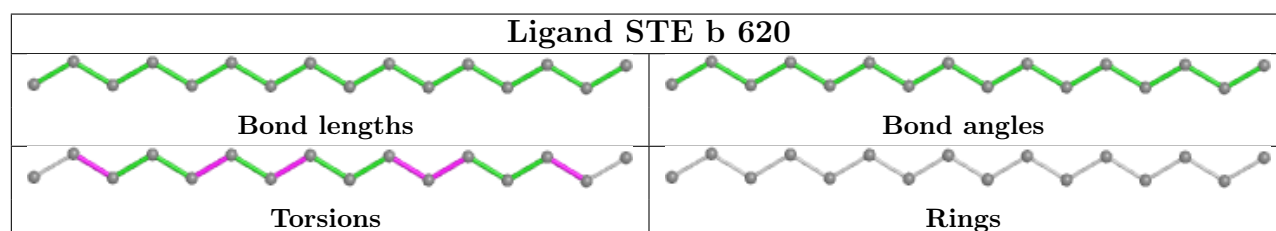
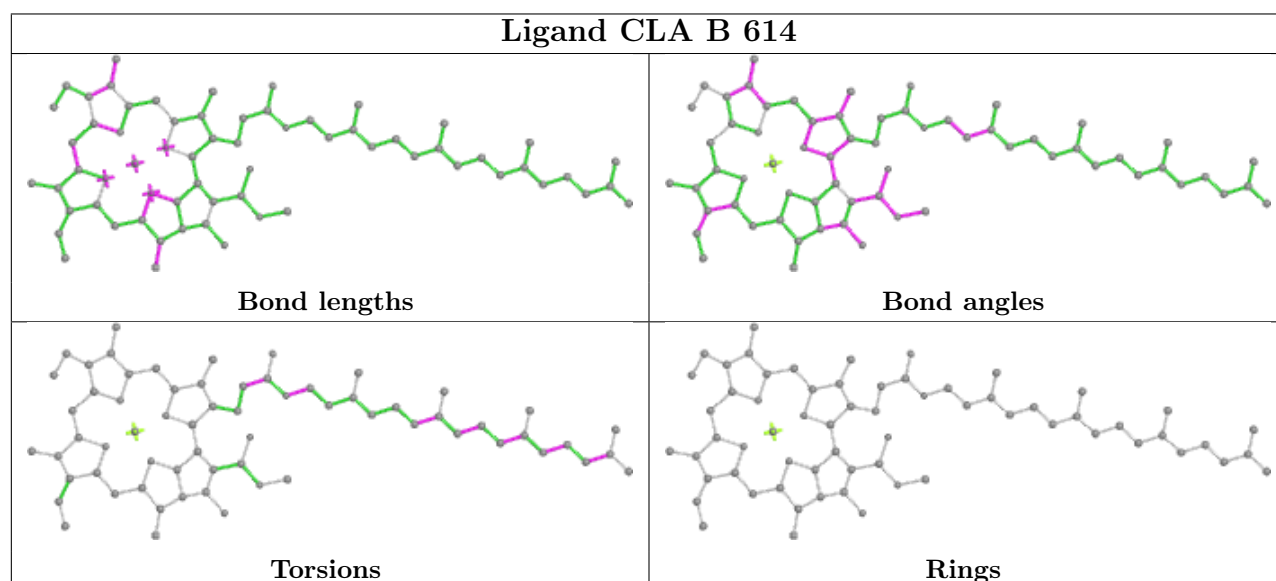
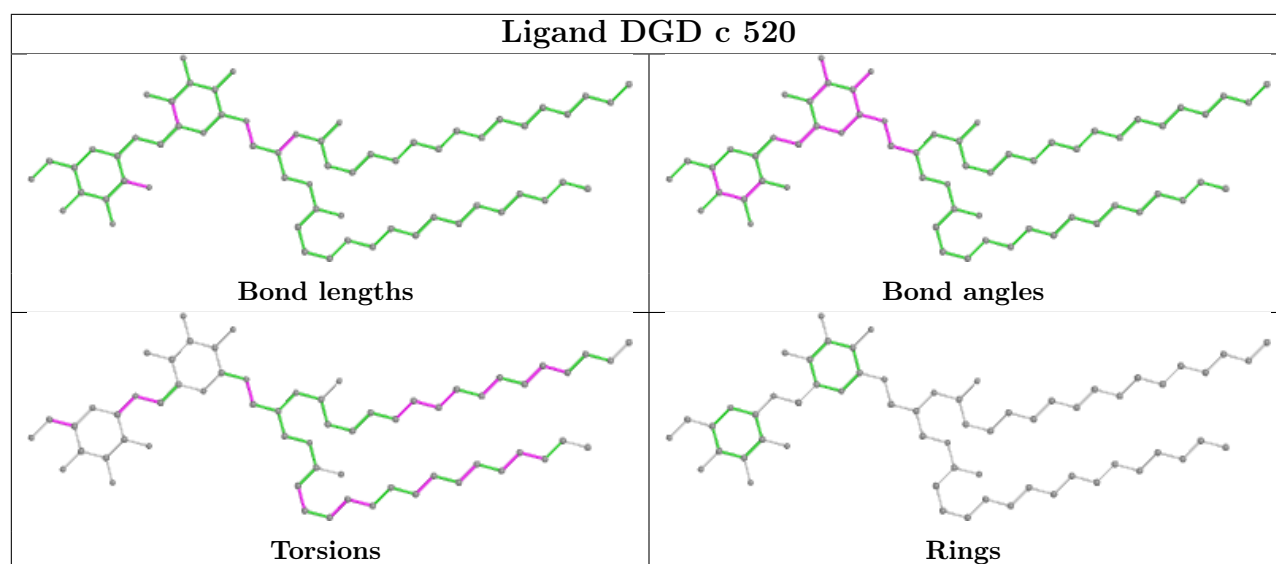












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
14	r	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r	30:GLN	C	31:VAL	N	3.77

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	334/344 (97%)	-0.37	4 (1%) 79 82	21, 28, 44, 78	0
1	a	334/344 (97%)	-0.39	2 (0%) 89 91	22, 30, 52, 81	0
2	B	505/510 (99%)	-0.39	9 (1%) 68 72	24, 32, 58, 85	0
2	b	505/510 (99%)	-0.19	16 (3%) 47 54	22, 35, 68, 92	0
3	C	442/461 (95%)	-0.28	4 (0%) 84 86	25, 34, 49, 69	0
3	c	451/461 (97%)	-0.22	8 (1%) 68 72	26, 37, 59, 91	0
4	D	341/352 (96%)	-0.34	1 (0%) 94 94	23, 29, 44, 75	0
4	d	341/352 (96%)	-0.32	1 (0%) 94 94	24, 33, 53, 74	0
5	E	82/84 (97%)	-0.03	3 (3%) 41 48	31, 48, 66, 80	0
5	e	82/84 (97%)	0.17	4 (4%) 29 35	37, 54, 72, 78	0
6	F	34/45 (75%)	-0.43	1 (2%) 51 57	33, 39, 57, 79	0
6	f	34/45 (75%)	-0.30	0 100 100	37, 46, 67, 83	0
7	H	65/66 (98%)	-0.09	0 100 100	30, 38, 55, 66	0
7	h	63/66 (95%)	0.26	5 (7%) 12 16	36, 45, 61, 67	0
8	I	35/38 (92%)	-0.18	2 (5%) 23 29	31, 37, 67, 78	0
8	i	35/38 (92%)	-0.12	3 (8%) 10 13	30, 38, 73, 84	0
9	J	36/40 (90%)	-0.03	3 (8%) 11 14	32, 46, 67, 85	0
9	j	36/40 (90%)	0.01	4 (11%) 5 7	33, 47, 82, 90	0
10	K	37/46 (80%)	0.10	2 (5%) 25 31	38, 48, 64, 70	0
10	k	37/46 (80%)	-0.05	1 (2%) 54 60	42, 50, 66, 72	0
11	L	37/37 (100%)	-0.47	1 (2%) 54 60	25, 29, 60, 70	0
11	l	36/37 (97%)	-0.25	3 (8%) 11 14	25, 29, 73, 83	0
12	M	32/36 (88%)	-0.12	0 100 100	27, 33, 60, 69	0
12	m	31/36 (86%)	-0.17	0 100 100	25, 33, 54, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	244/272 (89%)	-0.00	16 (6%) 18 23	24, 41, 79, 128	0
13	o	244/272 (89%)	-0.08	14 (5%) 23 29	26, 39, 77, 117	0
14	R	34/41 (82%)	1.64	13 (38%) 0 0	54, 63, 84, 102	0
14	r	31/41 (75%)	3.41	23 (74%) 0 0	65, 81, 96, 107	0
15	T	29/32 (90%)	-0.42	2 (6%) 16 21	25, 30, 59, 78	0
15	t	29/32 (90%)	-0.22	2 (6%) 16 21	28, 31, 80, 88	0
16	U	97/134 (72%)	-0.28	2 (2%) 63 68	31, 42, 65, 84	0
16	u	97/134 (72%)	-0.45	0 100 100	30, 39, 58, 77	0
17	V	137/163 (84%)	-0.49	0 100 100	30, 39, 54, 78	0
17	v	137/163 (84%)	-0.25	3 (2%) 62 66	31, 44, 64, 80	0
18	X	38/41 (92%)	-0.12	2 (5%) 26 32	35, 46, 67, 74	0
18	x	39/41 (95%)	0.26	4 (10%) 6 8	44, 51, 81, 94	0
19	Y	27/46 (58%)	1.13	7 (25%) 0 0	50, 65, 85, 98	0
19	y	30/46 (65%)	0.37	4 (13%) 3 4	56, 64, 82, 90	0
20	Z	62/62 (100%)	0.84	15 (24%) 0 0	49, 60, 102, 112	0
20	z	62/62 (100%)	0.75	10 (16%) 1 2	52, 65, 100, 110	0
All	All	5302/5700 (93%)	-0.18	194 (3%) 41 48	21, 36, 69, 128	0

All (194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	r	32	GLN	8.5
13	o	58	ASN	8.4
20	Z	33	TRP	7.6
13	o	3	GLN	7.0
14	r	29	LYS	6.5
13	O	56	PRO	6.3
14	r	3	TRP	6.2
1	A	13	LEU	6.1
13	O	3	GLN	5.9
20	z	33	TRP	5.9
14	r	6	LEU	5.7
2	b	495	PHE	5.4
14	r	10	LEU	5.3
13	O	4	THR	5.2
9	j	5	GLY	5.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
14	r	25	PRO	5.2
13	o	57	LYS	5.1
13	O	59	LYS	5.1
14	r	31	VAL	5.1
14	R	3	TRP	5.1
20	Z	3	ILE	5.1
14	R	6	LEU	5.0
13	o	60	ARG	5.0
2	b	127	ARG	4.9
13	O	60	ARG	4.9
20	Z	61	VAL	4.8
14	r	28	VAL	4.7
13	O	61	GLN	4.6
20	Z	62	VAL	4.6
14	r	27	ALA	4.6
13	O	62	GLU	4.5
15	t	30	THR	4.5
20	z	35	ARG	4.5
14	r	9	LEU	4.4
13	o	56	PRO	4.4
5	e	79	PHE	4.4
1	a	11	ALA	4.3
9	J	5	GLY	4.3
13	O	57	LYS	4.3
3	c	143	TYR	4.3
18	X	2	THR	4.2
20	Z	35	ARG	4.2
14	R	32	GLN	4.2
13	o	4	THR	4.1
15	T	30	THR	4.1
14	r	24	LEU	4.1
1	A	11	ALA	4.1
14	r	13	LEU	4.0
7	h	21	VAL	4.0
3	c	24	THR	3.9
20	z	3	ILE	3.9
14	r	15	ALA	3.8
9	j	7	ARG	3.8
3	c	23	ALA	3.8
13	o	61	GLN	3.8
20	z	1	MET	3.7
13	O	5	LEU	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
13	O	63	ALA	3.6
19	Y	20	ALA	3.6
8	I	36	ASP	3.6
3	c	147	PHE	3.6
19	Y	43	ARG	3.6
19	Y	25	ILE	3.6
20	z	7	LEU	3.6
3	C	146	PHE	3.5
14	r	18	TRP	3.5
2	b	486	LEU	3.5
13	O	246	ALA	3.5
3	c	146	PHE	3.5
9	J	7	ARG	3.5
20	Z	42	LEU	3.4
18	x	38	GLN	3.4
14	r	14	LEU	3.3
20	Z	1	MET	3.3
13	o	207	ARG	3.3
8	I	34	ARG	3.3
20	Z	7	LEU	3.3
9	J	8	ILE	3.3
19	y	18	VAL	3.3
20	Z	32	ASP	3.2
18	x	40	SER	3.2
13	O	35	SER	3.2
2	b	487	SER	3.2
20	z	41	PHE	3.2
5	E	3	GLY	3.1
14	r	5	VAL	3.1
19	Y	40	ALA	3.1
13	o	62	GLU	3.1
5	E	79	PHE	3.1
14	R	28	VAL	3.1
20	Z	4	LEU	3.0
14	r	23	ILE	3.0
14	r	26	TYR	3.0
20	Z	34	ASP	3.0
13	O	58	ASN	3.0
14	R	21	ARG	3.0
8	i	36	ASP	2.9
14	r	2	ASP	2.9
2	b	506	ARG	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
5	e	61	ARG	2.9
2	b	505	ARG	2.9
13	O	55	GLU	2.9
20	z	62	VAL	2.9
13	o	63	ALA	2.9
15	t	28	ARG	2.9
20	z	36	SER	2.8
7	h	6	TRP	2.8
1	A	12	ASN	2.8
19	Y	37	PHE	2.8
20	z	60	PHE	2.8
2	b	293	ALA	2.8
2	B	486	LEU	2.8
2	B	502	VAL	2.7
3	c	25	ASN	2.7
7	h	10	ILE	2.7
2	b	491	VAL	2.7
11	l	2	GLU	2.7
11	l	3	PRO	2.6
19	Y	41	VAL	2.6
8	i	35	LYS	2.6
8	i	34	ARG	2.6
6	F	12	SER	2.6
14	R	25	PRO	2.6
13	o	246	ALA	2.6
17	v	15	GLU	2.6
20	Z	30	PRO	2.6
19	y	19	ILE	2.6
20	Z	37	LYS	2.5
3	C	57	ALA	2.5
18	x	34	ILE	2.5
16	U	8	GLU	2.5
2	b	128	THR	2.5
2	B	373	LYS	2.5
9	j	8	ILE	2.5
10	K	17	ILE	2.5
2	B	293	ALA	2.5
2	B	127	ARG	2.4
5	e	83	LEU	2.4
2	b	502	VAL	2.4
2	B	86	ILE	2.4
3	C	143	TYR	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
17	v	21	LEU	2.4
14	r	21	ARG	2.4
2	B	490	GLN	2.3
2	b	289	GLN	2.3
15	T	29	ILE	2.3
14	R	34	LEU	2.3
20	Z	38	GLN	2.3
2	b	295	GLY	2.3
13	o	59	LYS	2.3
7	h	25	TRP	2.3
18	X	3	ILE	2.3
14	R	2	ASP	2.3
2	b	503	THR	2.3
14	R	18	TRP	2.3
14	R	24	LEU	2.3
7	h	22	ALA	2.3
2	b	492	GLU	2.3
13	O	36	GLN	2.2
1	A	15	GLU	2.2
14	R	26	TYR	2.2
2	B	495	PHE	2.2
4	d	227[A]	GLU	2.2
16	U	9	LEU	2.2
20	Z	60	PHE	2.2
9	j	6	GLY	2.2
14	r	19	ALA	2.2
2	b	292	LEU	2.2
20	z	42	LEU	2.2
14	r	22	ASN	2.2
2	B	505	ARG	2.1
10	K	14	ALA	2.1
13	o	55	GLU	2.1
14	R	31	VAL	2.1
13	o	34	SER	2.1
19	y	37	PHE	2.1
3	c	57	ALA	2.1
5	e	84	LYS	2.1
18	x	2	THR	2.1
1	a	144	CYS	2.1
19	Y	42	ARG	2.1
13	O	25	THR	2.1
5	E	65	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
11	l	7	ARG	2.1
14	r	30	GLN	2.1
17	v	22	THR	2.1
3	C	60	ILE	2.0
4	D	12	ARG	2.0
19	y	43	ARG	2.0
10	k	10	LYS	2.0
14	R	29	LYS	2.0
11	L	2	GLU	2.0
3	c	262	ARG	2.0
2	b	161	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
15	FME	T	1	10/11	0.93	0.11	29,40,67,67	0
8	FME	i	1	10/11	0.96	0.17	37,46,63,63	0
15	FME	t	1	10/11	0.96	0.08	27,43,73,73	0
12	FME	m	1	10/11	0.97	0.13	32,49,65,76	0
8	FME	I	1	10/11	0.97	0.15	35,42,57,69	0
12	FME	M	1	10/11	0.97	0.12	42,52,69,73	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
33	STE	L	101	12/20	0.72	0.17	45,61,76,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
33	STE	E	102	12/20	0.74	0.28	42,72,79,86	0
33	STE	b	626	10/20	0.74	0.24	43,58,68,71	0
33	STE	H	103	18/20	0.75	0.25	49,70,84,84	0
33	STE	b	625	20/20	0.78	0.20	47,64,79,85	0
33	STE	a	415	12/20	0.78	0.26	39,68,76,84	0
33	STE	B	627	16/20	0.79	0.23	42,64,79,80	0
29	SQD	a	413	36/54	0.80	0.17	31,61,87,90	0
33	STE	h	103	14/20	0.80	0.23	50,65,88,91	0
30	DGD	A	415	66/66	0.81	0.16	41,62,85,89	0
34	LHG	E	101	49/49	0.81	0.20	46,74,98,118	0
33	STE	c	501	12/20	0.82	0.26	45,66,83,85	0
33	STE	B	626	18/20	0.82	0.14	39,63,82,84	0
28	LMG	c	524	48/55	0.82	0.22	47,71,106,116	0
22	CLA	C	513	65/65	0.83	0.17	33,54,85,98	0
33	STE	c	523	20/20	0.83	0.18	40,59,79,87	0
29	SQD	A	414	39/54	0.83	0.17	38,63,93,102	0
33	STE	j	101	12/20	0.83	0.13	38,54,72,78	0
28	LMG	D	410	33/55	0.83	0.18	33,53,78,93	0
34	LHG	e	102	42/49	0.83	0.23	61,78,99,119	0
33	STE	a	414	10/20	0.84	0.19	34,65,74,75	0
33	STE	d	411	20/20	0.84	0.22	33,57,73,77	0
24	BCR	H	101	40/40	0.84	0.15	22,44,58,70	0
24	BCR	x	101	40/40	0.84	0.13	29,48,66,73	0
33	STE	B	625	12/20	0.84	0.12	42,55,66,66	0
28	LMG	B	629	55/55	0.84	0.15	35,58,81,93	0
28	LMG	b	623	55/55	0.85	0.29	49,77,101,110	0
33	STE	B	628	15/20	0.85	0.14	39,62,75,80	0
22	CLA	h	101	65/65	0.86	0.15	37,64,87,99	0
33	STE	B	601	12/20	0.86	0.38	44,63,83,88	0
33	STE	l	102	18/20	0.86	0.15	33,50,77,89	0
33	STE	b	622	20/20	0.86	0.22	39,58,75,78	0
28	LMG	c	525	49/55	0.86	0.15	35,54,95,112	0
33	STE	C	521	16/20	0.87	0.12	38,51,63,70	0
33	STE	C	522	12/20	0.87	0.09	35,48,54,55	0
24	BCR	y	101	40/40	0.87	0.12	38,59,75,79	0
27	PL9	A	410	55/55	0.87	0.21	35,65,88,95	0
27	PL9	a	410	55/55	0.87	0.19	36,67,87,103	0
33	STE	d	412	20/20	0.87	0.14	39,63,81,82	0
24	BCR	Y	101	40/40	0.87	0.12	34,49,67,72	0
22	CLA	c	514	65/65	0.87	0.15	36,55,95,110	0
33	STE	b	620	16/20	0.87	0.17	35,50,75,81	0
29	SQD	b	619	49/54	0.87	0.15	42,60,97,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	STE	b	624	16/20	0.87	0.14	45,61,80,82	0
29	SQD	B	623	54/54	0.88	0.15	38,58,94,100	0
33	STE	I	101	15/20	0.88	0.15	38,55,74,78	0
33	STE	B	621	17/20	0.88	0.18	35,49,69,71	0
33	STE	T	102	15/20	0.88	0.17	41,57,79,85	0
22	CLA	B	602	65/65	0.88	0.15	30,57,92,101	0
28	LMG	A	412	48/55	0.89	0.14	36,54,79,101	0
22	CLA	C	514	65/65	0.89	0.17	39,62,91,98	0
24	BCR	Z	101	40/40	0.89	0.14	38,56,69,70	0
22	CLA	c	515	65/65	0.89	0.18	39,66,105,110	0
24	BCR	d	404	40/40	0.90	0.12	28,48,86,102	0
33	STE	X	101	20/20	0.90	0.14	27,50,73,76	0
28	LMG	c	522	37/55	0.90	0.16	42,64,82,91	0
22	CLA	c	504	65/65	0.90	0.14	27,42,62,69	0
33	STE	M	102	15/20	0.90	0.13	34,48,62,68	0
33	STE	M	103	10/20	0.90	0.15	33,49,60,63	0
33	STE	C	520	12/20	0.91	0.11	45,56,65,65	0
28	LMG	M	101	51/55	0.91	0.12	26,48,73,85	0
22	CLA	C	503	65/65	0.91	0.14	24,39,61,66	0
24	BCR	B	620	40/40	0.91	0.10	26,41,58,69	0
22	CLA	c	510	64/65	0.91	0.14	30,45,86,105	0
22	CLA	a	405	65/65	0.91	0.13	18,38,79,87	0
22	CLA	b	614	65/65	0.91	0.13	23,39,56,60	0
24	BCR	c	516	40/40	0.91	0.15	43,58,71,73	0
22	CLA	d	403	65/65	0.91	0.15	26,46,89,103	0
24	BCR	c	518	40/40	0.92	0.15	39,51,61,68	0
28	LMG	C	519	48/55	0.92	0.13	34,67,87,93	0
28	LMG	D	406	51/55	0.92	0.16	28,54,88,96	0
24	BCR	C	515	40/40	0.92	0.11	25,41,53,65	0
29	SQD	f	101	41/54	0.92	0.17	47,78,110,116	0
28	LMG	D	411	28/55	0.92	0.13	25,49,62,67	0
24	BCR	D	404	40/40	0.92	0.12	24,42,81,90	0
33	STE	d	410	17/20	0.92	0.10	38,52,60,66	0
28	LMG	b	621	51/55	0.92	0.12	29,51,77,92	0
33	STE	B	624	14/20	0.92	0.09	32,49,66,66	0
22	CLA	B	607	65/65	0.92	0.11	21,35,74,78	0
22	CLA	c	509	65/65	0.92	0.14	27,43,57,64	0
33	STE	Z	102	8/20	0.92	0.14	43,56,67,67	0
22	CLA	D	403	65/65	0.92	0.12	21,42,102,116	0
22	CLA	b	615	60/65	0.92	0.13	26,42,84,93	0
22	CLA	C	506	65/65	0.93	0.17	23,40,69,82	0
22	CLA	C	507	65/65	0.93	0.12	22,40,87,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	CLA	c	512	65/65	0.93	0.15	30,46,62,71	0
29	SQD	a	412	54/54	0.93	0.15	38,64,93,96	0
22	CLA	c	513	65/65	0.93	0.12	38,53,68,75	0
24	BCR	b	617	40/40	0.93	0.11	25,40,55,61	0
24	BCR	b	618	40/40	0.93	0.10	26,44,66,67	0
22	CLA	b	601	65/65	0.93	0.15	25,42,62,70	0
33	STE	J	101	12/20	0.93	0.09	45,60,72,73	0
30	DGD	C	517	62/66	0.93	0.12	27,50,99,120	0
30	DGD	h	102	62/66	0.93	0.11	24,49,65,74	0
22	CLA	b	608	65/65	0.93	0.14	29,43,57,64	0
22	CLA	C	508	65/65	0.93	0.13	21,38,53,59	0
22	CLA	B	616	65/65	0.93	0.12	22,36,61,64	0
22	CLA	B	615	65/65	0.93	0.16	22,35,80,90	0
22	CLA	c	508	65/65	0.93	0.12	27,46,95,106	0
27	PL9	D	405	55/55	0.94	0.10	20,33,48,49	0
22	CLA	c	505	65/65	0.94	0.15	30,43,53,59	0
22	CLA	c	506	60/65	0.94	0.11	29,42,79,84	0
22	CLA	c	507	65/65	0.94	0.15	25,39,67,76	0
30	DGD	c	520	62/66	0.94	0.10	32,50,88,94	0
30	DGD	c	521	62/66	0.94	0.13	28,52,93,108	0
22	CLA	C	509	65/65	0.94	0.12	25,43,98,114	0
24	BCR	K	101	40/40	0.94	0.14	30,48,58,62	0
22	CLA	C	512	65/65	0.94	0.11	27,48,66,70	0
22	CLA	b	605	65/65	0.94	0.11	25,39,73,80	0
22	CLA	c	511	65/65	0.94	0.16	30,45,62,67	0
22	CLA	b	607	65/65	0.94	0.13	23,39,59,62	0
22	CLA	B	617	60/65	0.94	0.13	21,38,87,94	0
24	BCR	c	517	40/40	0.94	0.11	25,43,60,62	0
22	CLA	b	611	65/65	0.94	0.16	21,35,52,56	0
22	CLA	B	605	65/65	0.94	0.11	19,34,72,81	0
28	LMG	d	409	44/55	0.94	0.12	28,50,79,91	0
24	BCR	t	101	40/40	0.94	0.10	23,38,51,53	0
22	CLA	C	504	65/65	0.94	0.14	24,40,54,56	0
29	SQD	D	407	36/54	0.94	0.14	43,66,86,99	0
22	CLA	a	403	65/65	0.94	0.13	24,41,95,107	0
24	BCR	B	619	40/40	0.94	0.09	23,38,49,57	0
22	CLA	B	603	65/65	0.95	0.14	22,37,54,60	0
22	CLA	c	503	65/65	0.95	0.12	22,40,53,61	0
22	CLA	A	405	54/65	0.95	0.10	18,33,61,69	0
24	BCR	T	101	40/40	0.95	0.09	21,38,55,67	0
22	CLA	C	502	65/65	0.95	0.12	20,34,53,55	0
22	CLA	A	411	65/65	0.95	0.10	16,27,54,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	BCR	a	406	40/40	0.95	0.08	19,33,47,52	0
29	SQD	A	413	52/54	0.95	0.14	28,56,88,98	0
24	BCR	b	616	40/40	0.95	0.10	21,41,52,59	0
22	CLA	B	610	65/65	0.95	0.12	23,37,58,69	0
22	CLA	C	505	59/65	0.95	0.12	27,40,78,90	0
22	CLA	B	611	65/65	0.95	0.14	19,33,46,47	0
22	CLA	b	603	65/65	0.95	0.13	17,37,85,98	0
22	CLA	b	604	65/65	0.95	0.12	18,35,50,58	0
22	CLA	B	613	65/65	0.95	0.15	17,33,49,53	0
22	CLA	B	614	65/65	0.95	0.14	18,31,67,71	0
30	DGD	C	516	62/66	0.95	0.11	21,39,75,91	0
22	CLA	A	403	65/65	0.95	0.13	22,36,90,100	0
30	DGD	C	518	62/66	0.95	0.11	26,46,75,85	0
30	DGD	H	102	62/66	0.95	0.10	26,43,58,61	0
22	CLA	b	609	65/65	0.95	0.17	23,39,51,57	0
22	CLA	d	402	65/65	0.95	0.11	18,35,52,67	0
22	CLA	b	610	65/65	0.95	0.13	21,34,53,59	0
22	CLA	C	510	65/65	0.95	0.17	24,43,64,68	0
23	PHO	d	401	64/64	0.95	0.10	26,37,46,48	0
24	BCR	A	406	40/40	0.95	0.08	22,34,47,51	0
24	BCR	B	618	40/40	0.95	0.11	27,39,57,69	0
22	CLA	b	612	65/65	0.95	0.14	19,33,72,90	0
22	CLA	b	613	65/65	0.95	0.12	22,40,81,91	0
34	LHG	d	408	39/49	0.95	0.11	28,45,68,75	0
22	CLA	C	511	65/65	0.95	0.13	26,43,58,66	0
34	LHG	l	101	49/49	0.95	0.10	31,43,60,69	0
22	CLA	B	609	65/65	0.96	0.11	21,36,57,63	0
22	CLA	a	411	65/65	0.96	0.10	19,29,45,50	0
22	CLA	A	402	65/65	0.96	0.09	15,27,42,61	0
22	CLA	b	602	65/65	0.96	0.13	22,36,67,77	0
22	CLA	B	606	65/65	0.96	0.13	21,33,47,52	0
22	CLA	B	612	65/65	0.96	0.14	21,32,51,52	0
22	CLA	D	402	65/65	0.96	0.10	13,30,52,59	0
22	CLA	b	606	65/65	0.96	0.12	19,36,71,78	0
30	DGD	c	519	62/66	0.96	0.10	22,41,74,96	0
22	CLA	B	604	65/65	0.96	0.14	17,34,61,63	0
26	BCT	a	409	4/4	0.96	0.19	26,33,40,48	0
22	CLA	a	402	65/65	0.96	0.10	18,29,47,59	0
22	CLA	B	608	65/65	0.96	0.10	17,34,65,74	0
34	LHG	D	409	47/49	0.96	0.11	27,48,87,104	0
34	LHG	D	412	49/49	0.96	0.12	27,43,71,77	0
23	PHO	A	404	64/64	0.96	0.10	18,28,37,39	0

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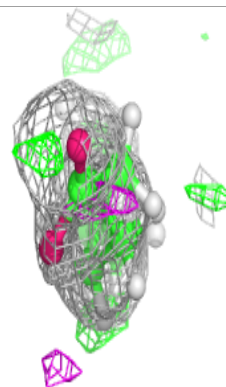
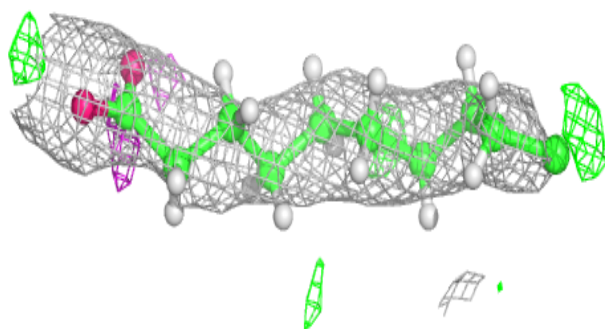
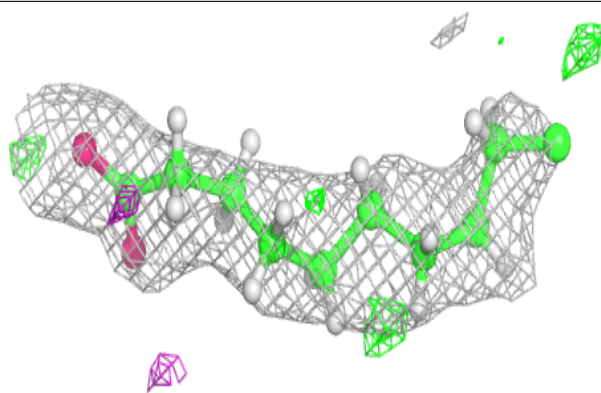
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
34	LHG	d	406	49/49	0.96	0.12	32,48,82,87	0
27	PL9	d	405	55/55	0.96	0.10	19,34,45,46	0
23	PHO	D	401	64/64	0.96	0.12	23,34,44,48	0
23	PHO	a	404	64/64	0.96	0.12	17,31,42,45	0
35	HEC	F	101	43/43	0.96	0.11	26,44,64,66	0
35	HEC	e	101	43/43	0.96	0.12	36,52,72,81	0
34	LHG	d	407	49/49	0.97	0.10	25,42,55,61	0
34	LHG	B	622	49/49	0.97	0.10	25,41,56,64	0
34	LHG	D	408	49/49	0.97	0.10	18,41,53,59	0
35	HEC	v	201	43/43	0.97	0.13	25,37,45,48	0
35	HEC	V	201	43/43	0.98	0.11	21,31,44,53	0
32	OEY	a	417[B]	11/11	0.99	0.11	22,26,28,31	11
26	BCT	A	409	4/4	0.99	0.18	31,33,36,43	0
21	FE2	a	401	1/1	0.99	0.08	34,34,34,34	0
25	CL	A	407	1/1	0.99	0.06	27,27,27,27	0
25	CL	A	408	1/1	0.99	0.02	28,28,28,28	0
25	CL	a	407	1/1	0.99	0.08	28,28,28,28	0
25	CL	a	408	1/1	0.99	0.03	28,28,28,28	0
31	OEX	A	416[A]	10/10	0.99	0.13	25,30,31,31	10
31	OEX	a	416[A]	10/10	0.99	0.11	27,28,30,30	10
32	OEY	A	417[B]	11/11	0.99	0.13	21,27,31,34	11
21	FE2	A	401	1/1	1.00	0.08	26,26,26,26	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.

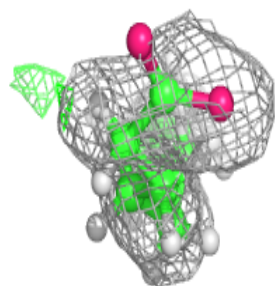
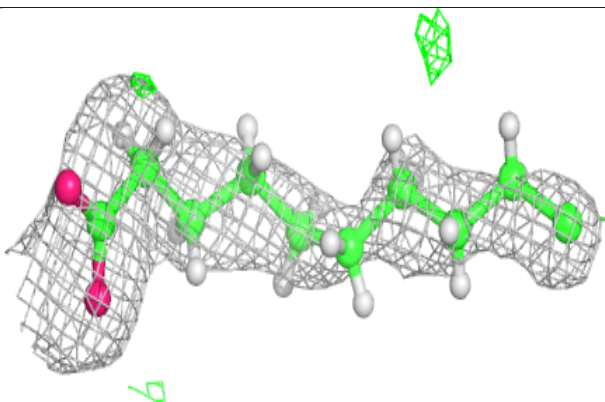
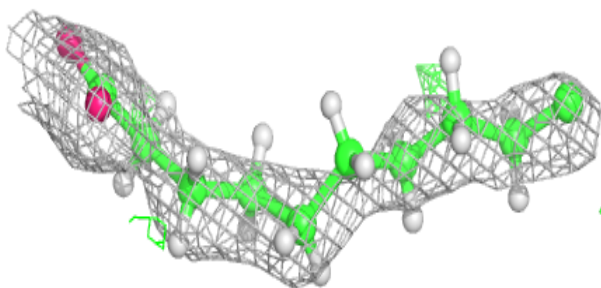


**Electron density around STE L 101:**

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

**Electron density around STE E 102:**

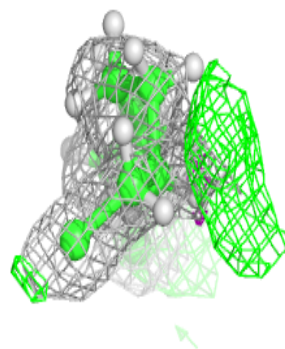
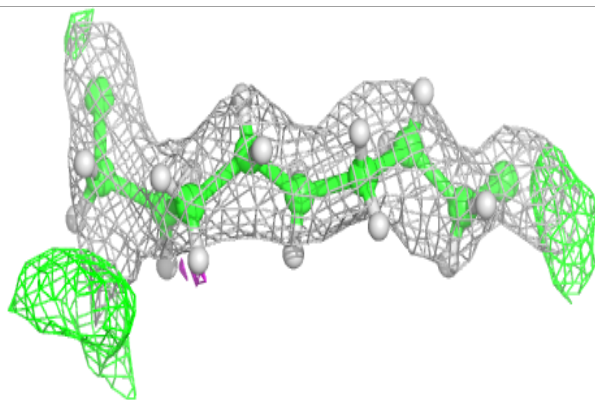
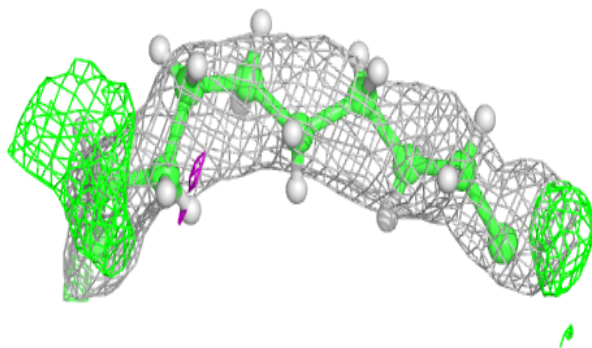
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



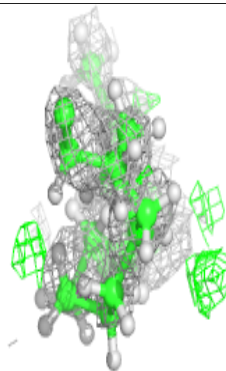
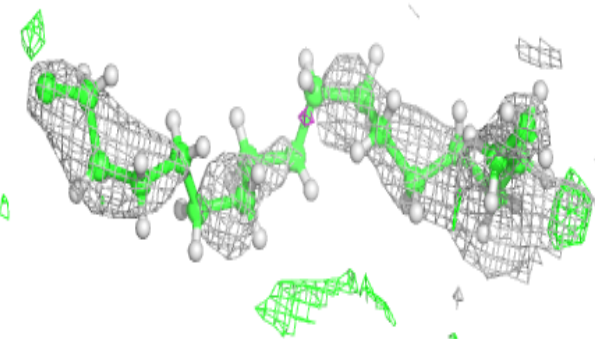
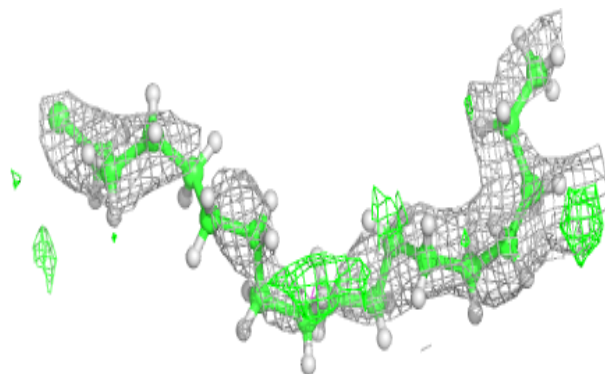


**Electron density around STE b 626:**

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

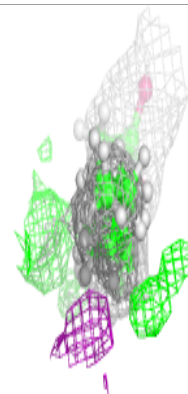
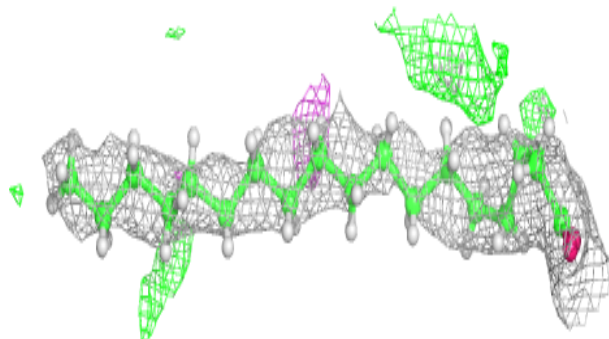
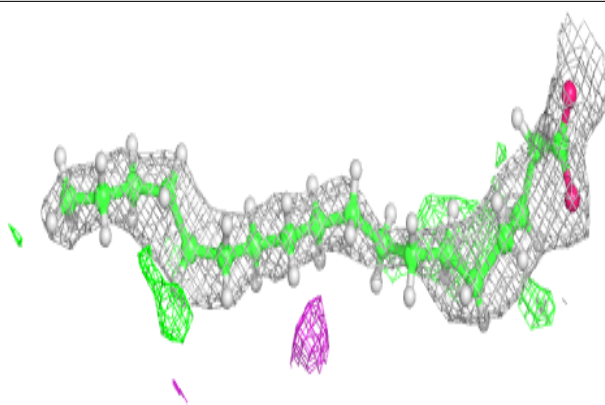
**Electron density around STE H 103:**

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

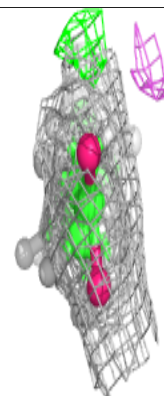
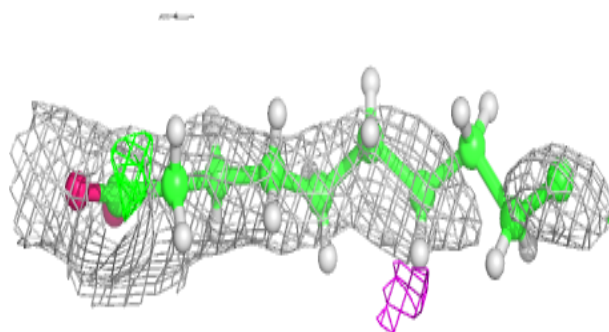
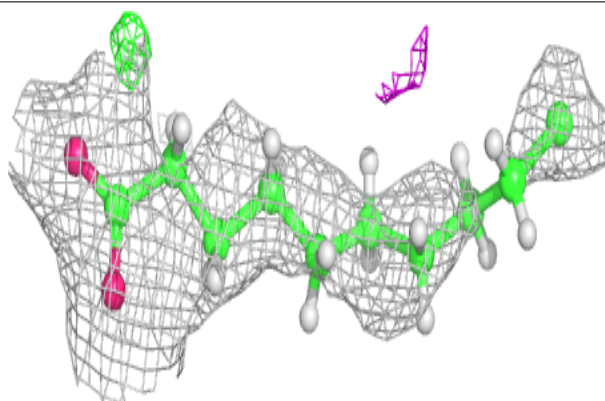


**Electron density around STE b 625:**

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

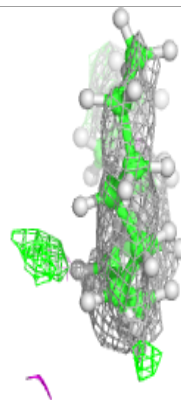
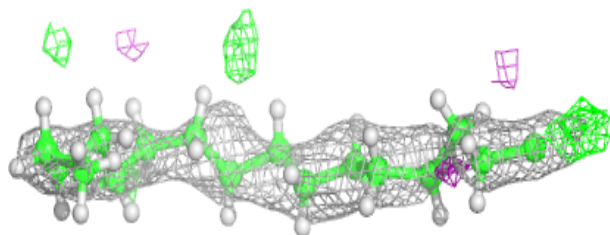
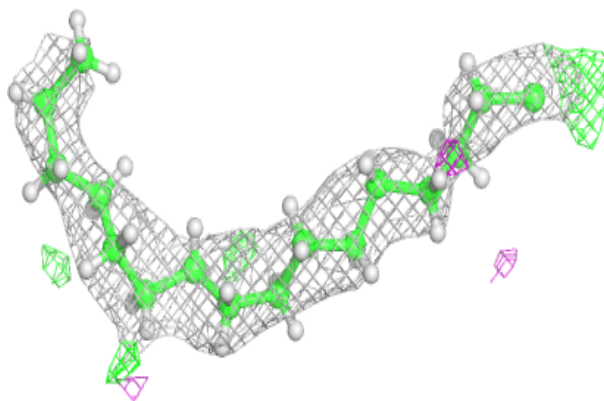
**Electron density around STE a 415:**

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



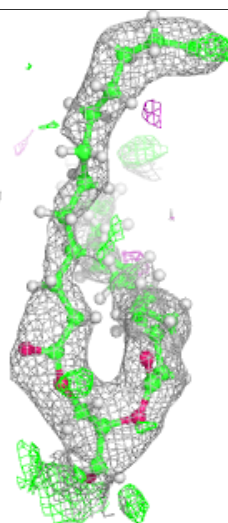
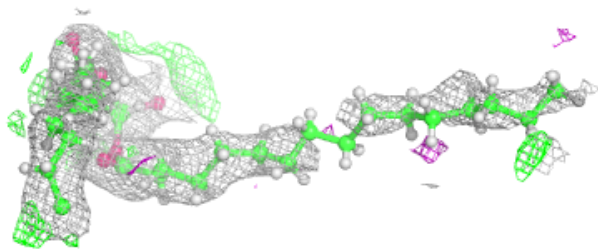
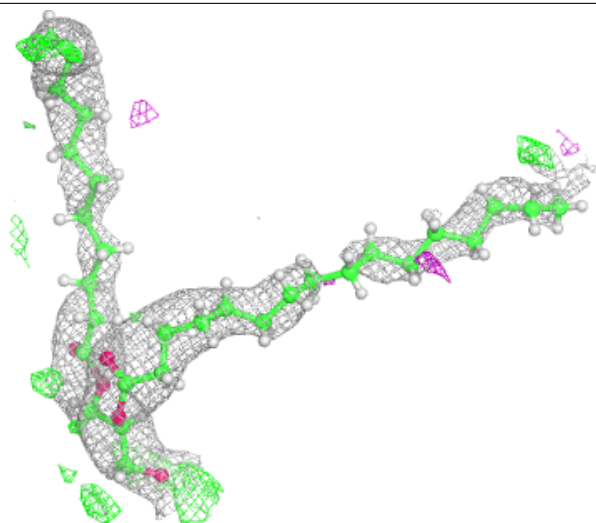
**Electron density around STE B 627:**

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



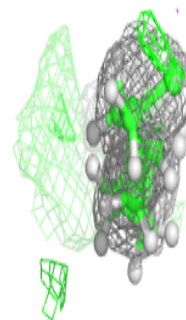
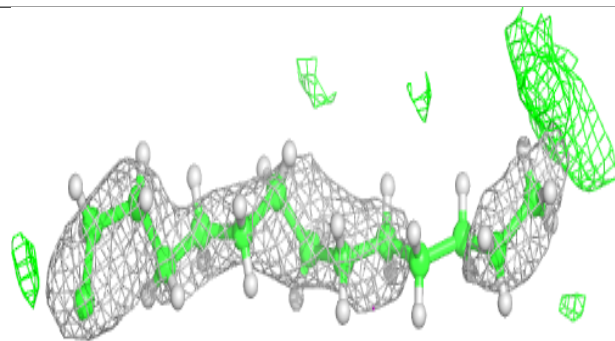
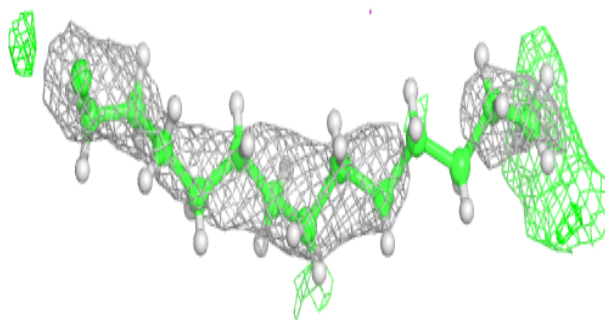
**Electron density around SQD a 413:**

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

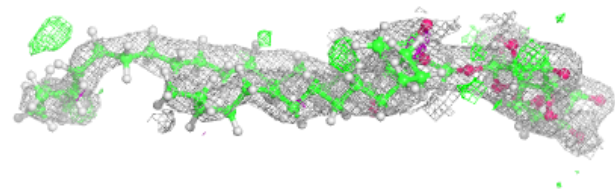
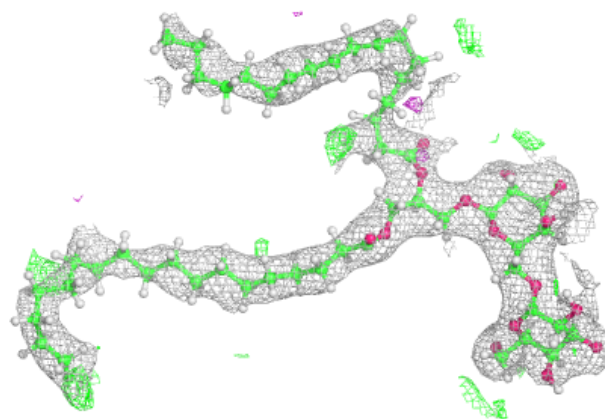


**Electron density around STE h 103:**

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

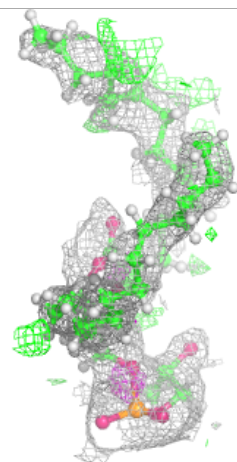
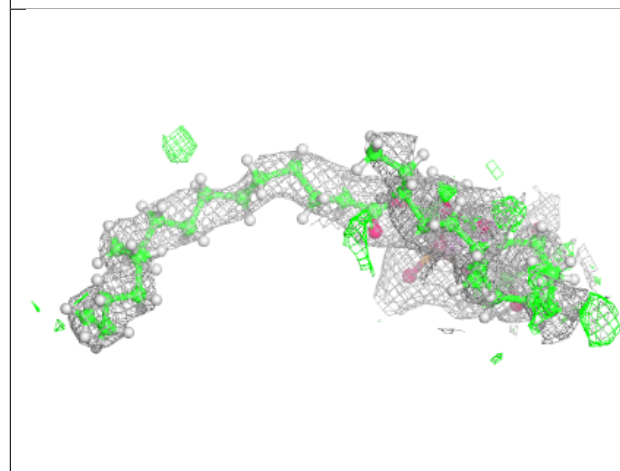
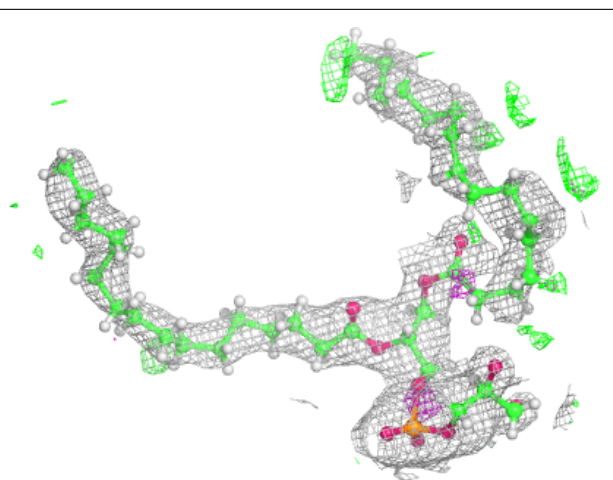
**Electron density around DGD A 415:**

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



**Electron density around LHG E 101:**

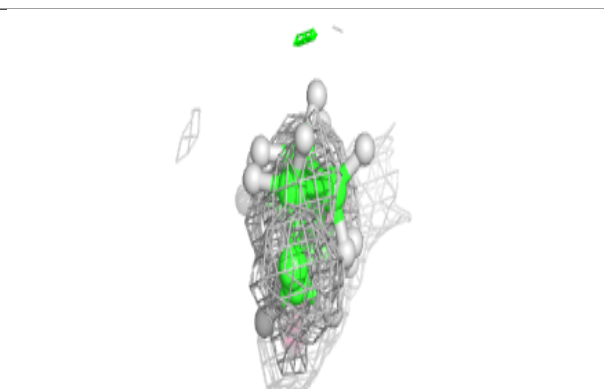
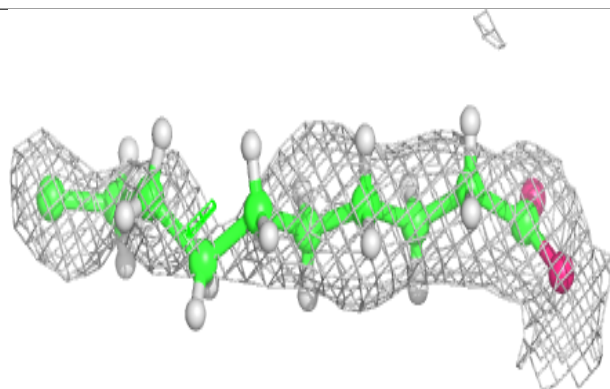
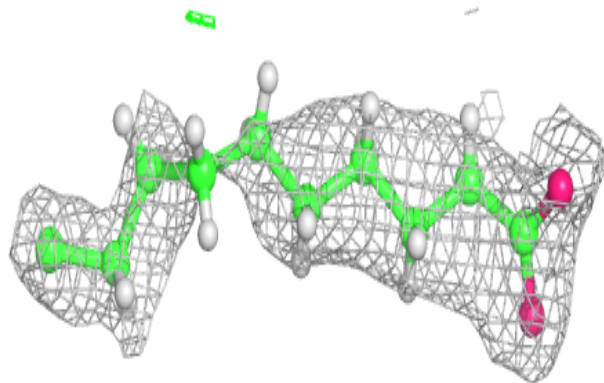
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



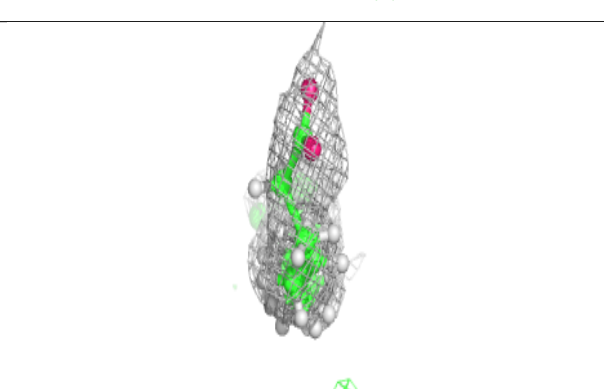
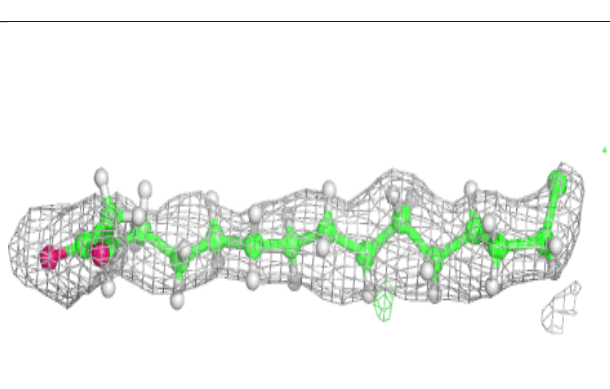
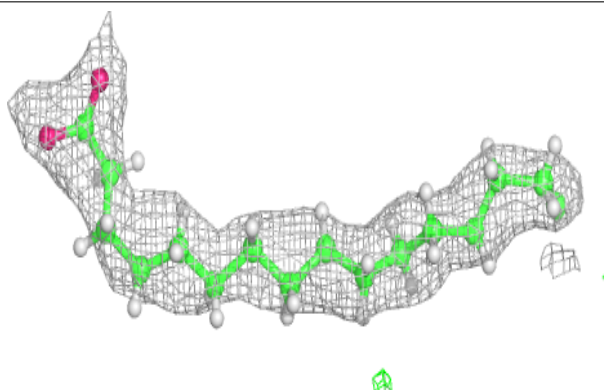


**Electron density around STE c 501:**

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

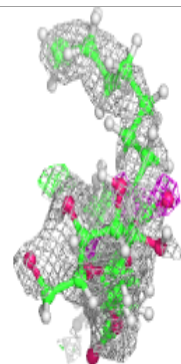
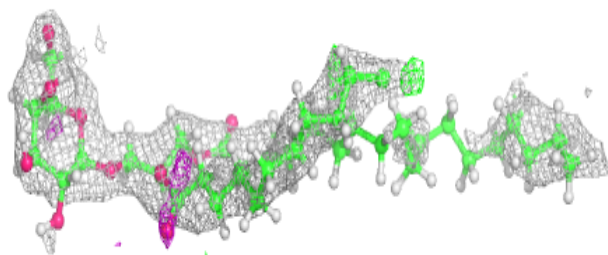
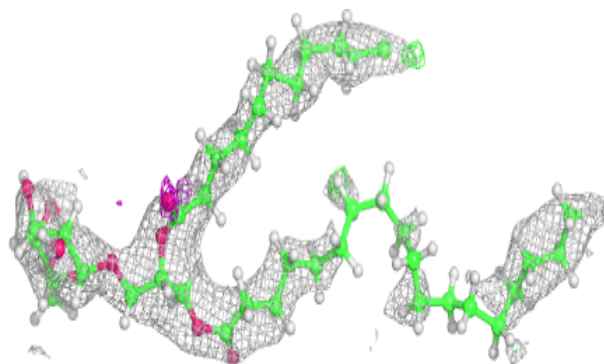
**Electron density around STE B 626:**

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



**Electron density around LMG c 524:**

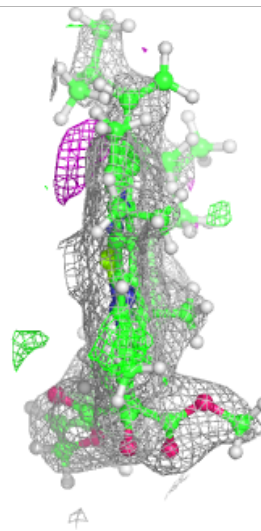
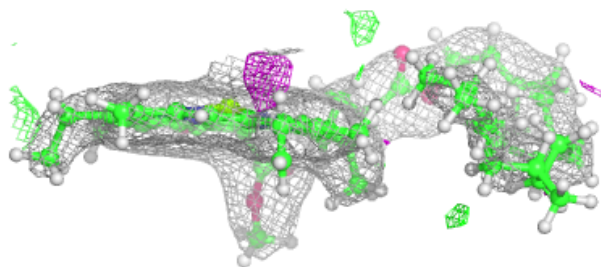
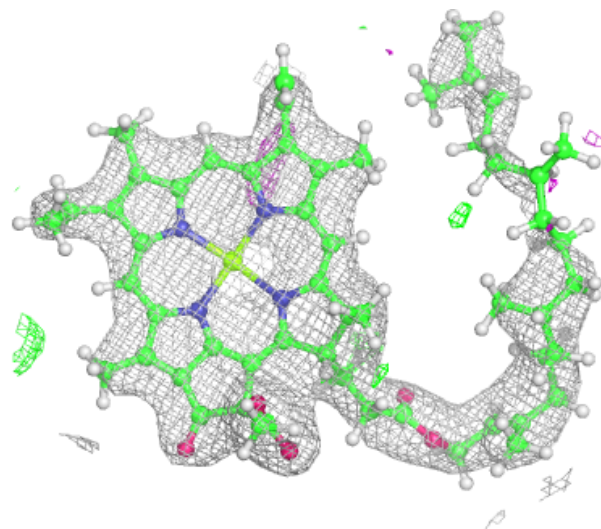
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





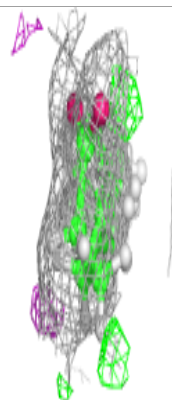
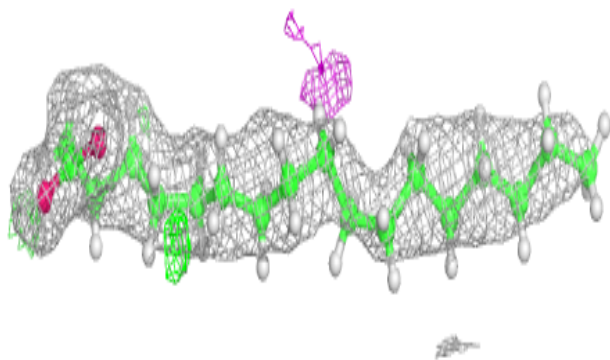
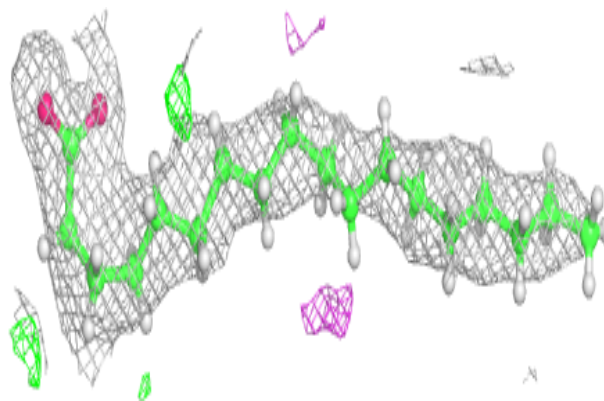
**Electron density around CLA C 513:**

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



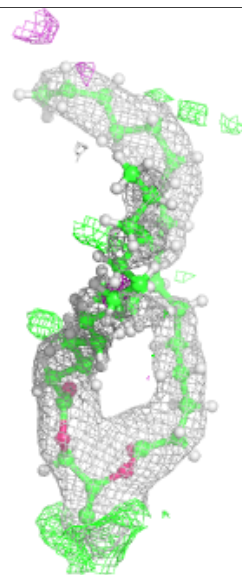
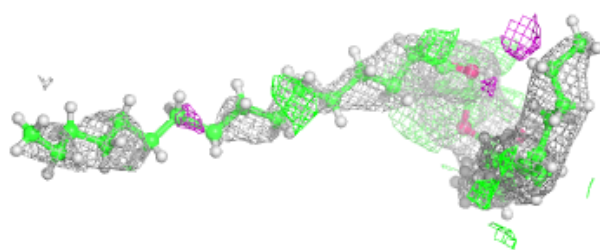
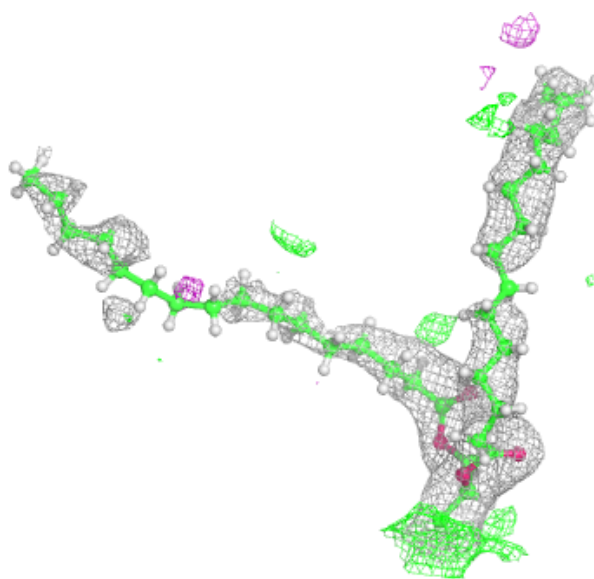
**Electron density around STE c 523:**

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



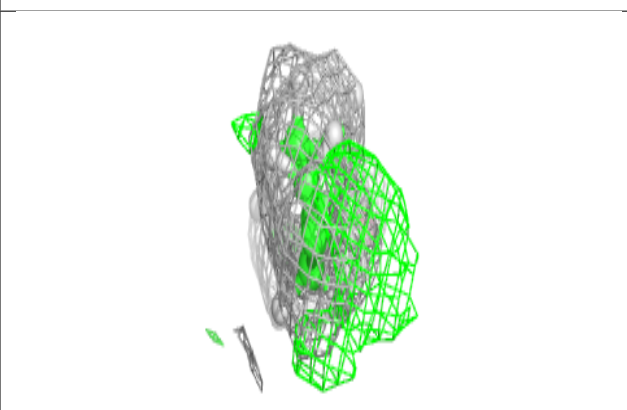
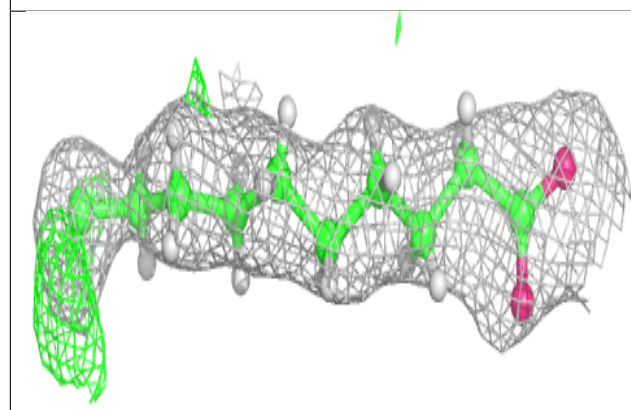
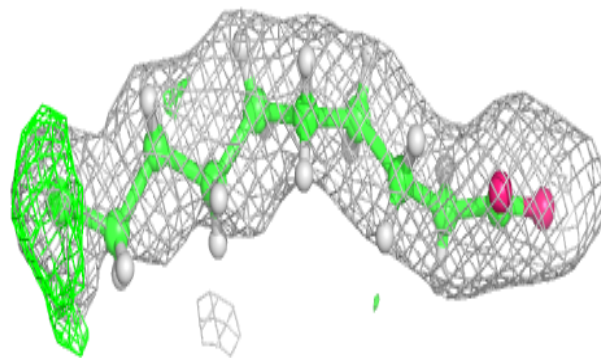
**Electron density around SQD A 414:**

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

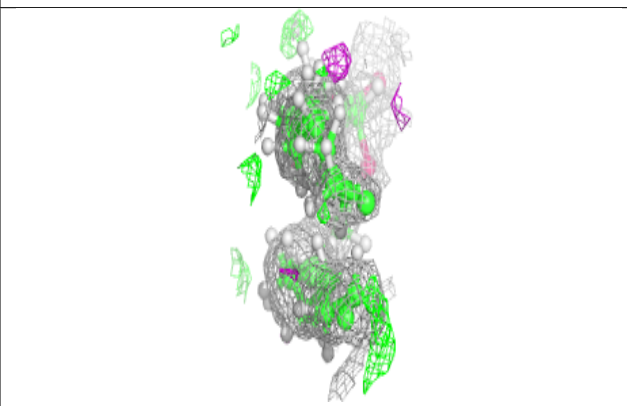
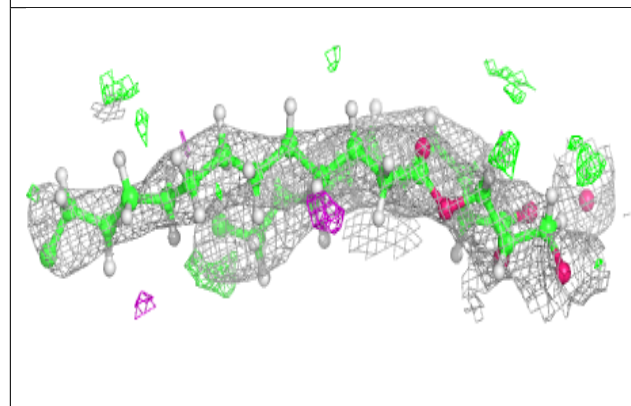
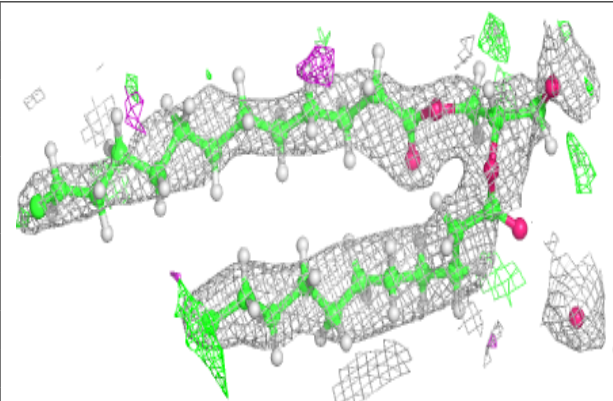


**Electron density around STE j 101:**

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

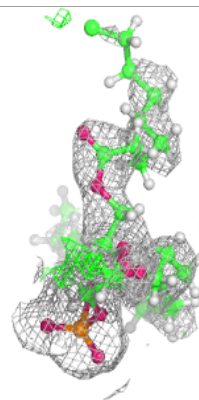
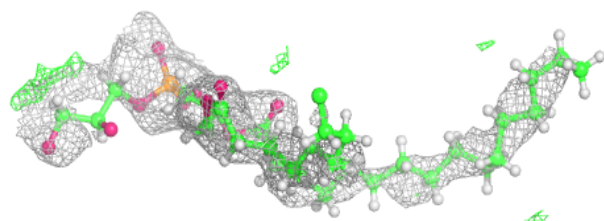
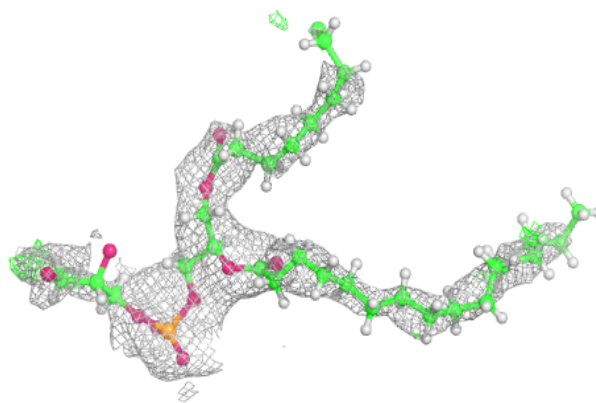
**Electron density around LMG D 410:**

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

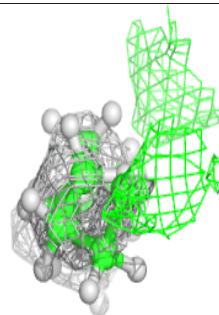
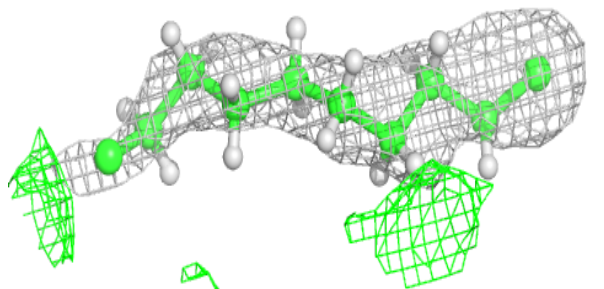
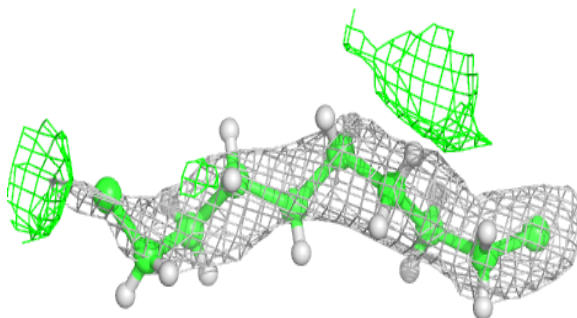


**Electron density around LHG e 102:**

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

**Electron density around STE a 414:**

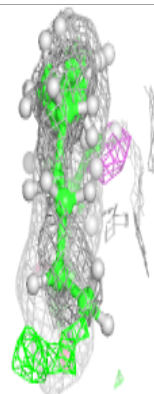
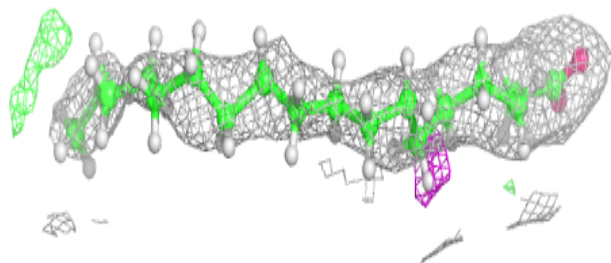
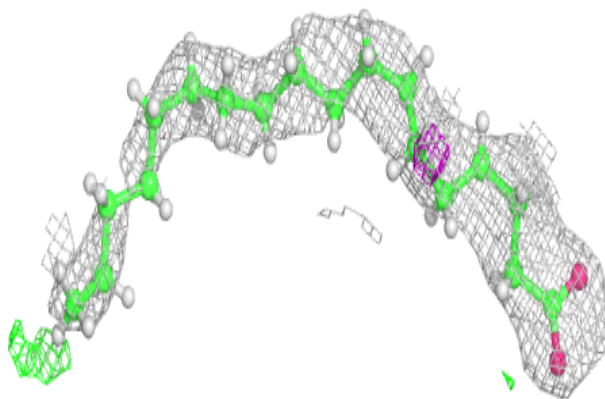
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



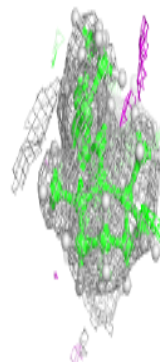
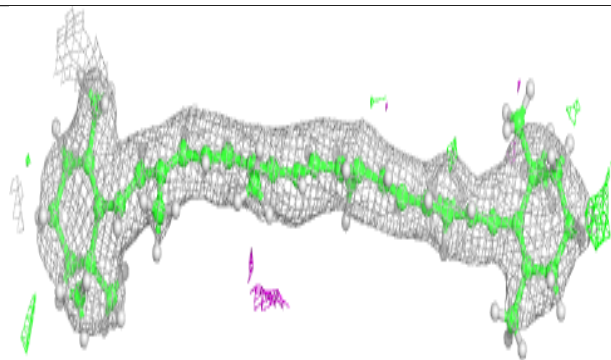
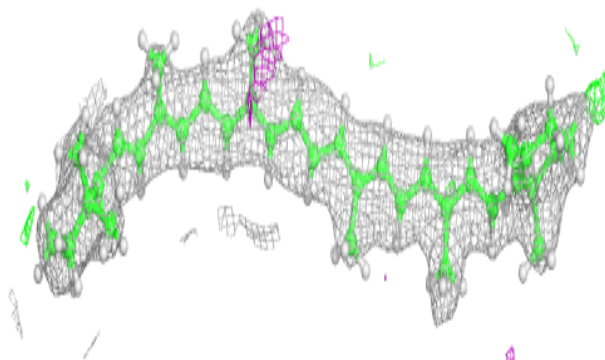


**Electron density around STE d 411:**

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

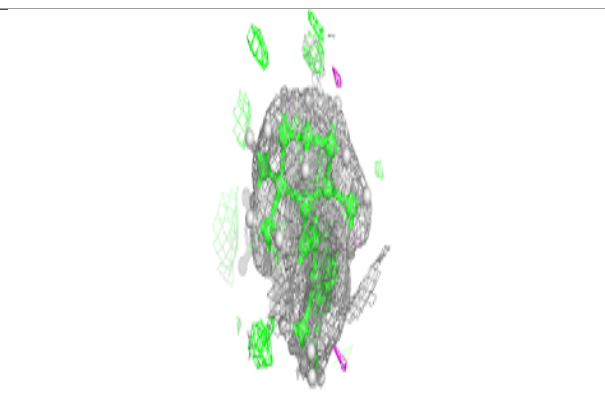
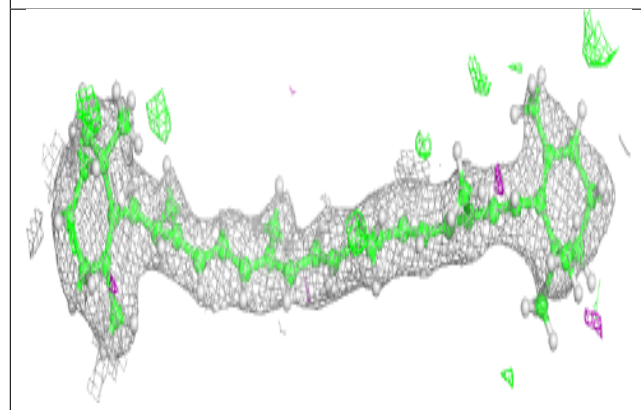
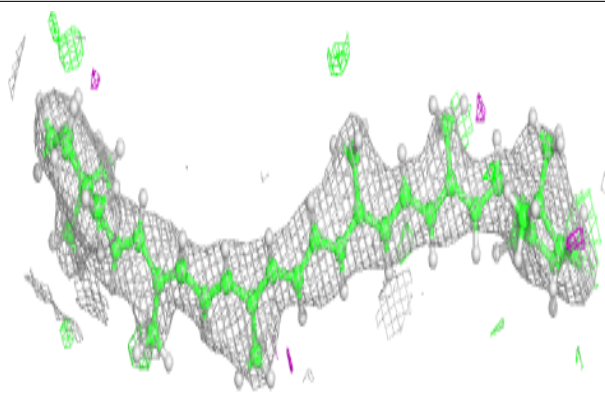
**Electron density around BCR H 101:**

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

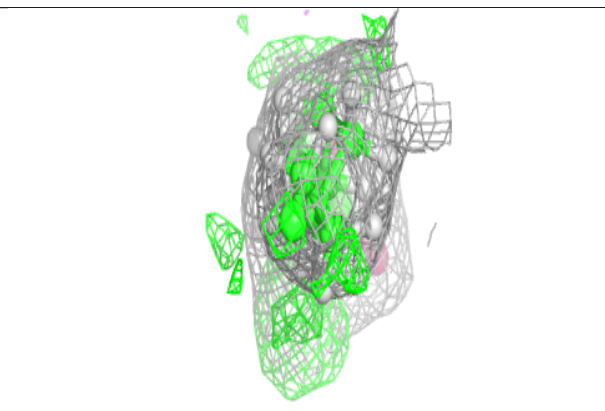
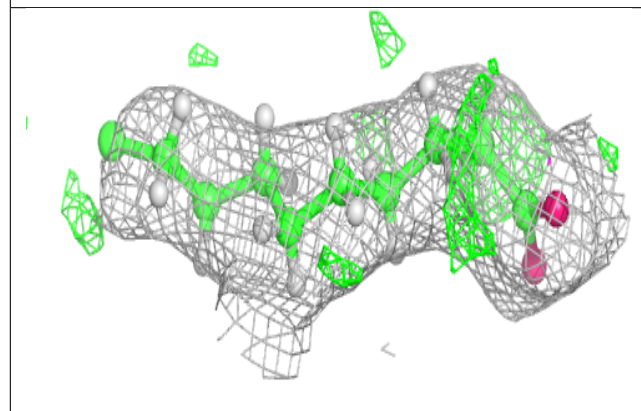
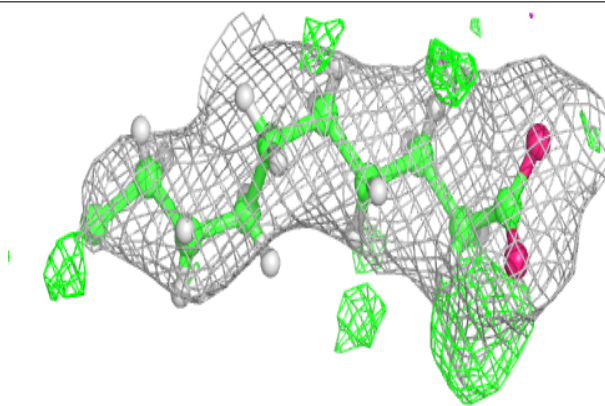


**Electron density around BCR x 101:**

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

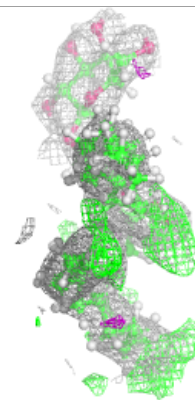
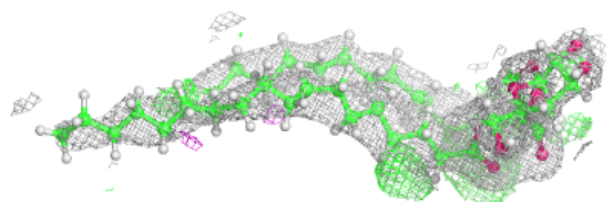
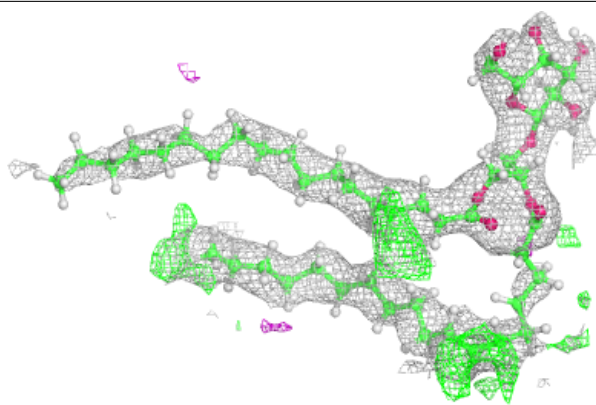
**Electron density around STE B 625:**

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

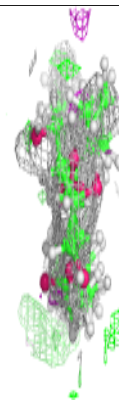
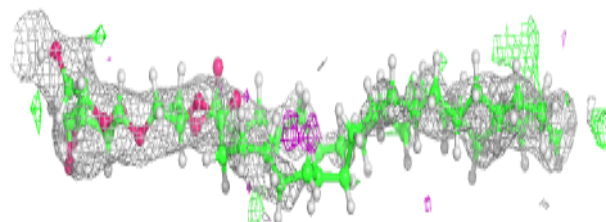
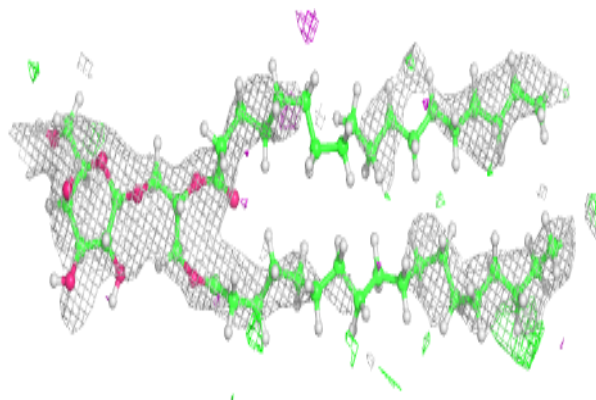


**Electron density around LMG B 629:**

$2mF_o-DF_c$  (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:**

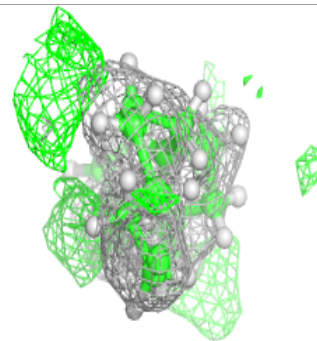
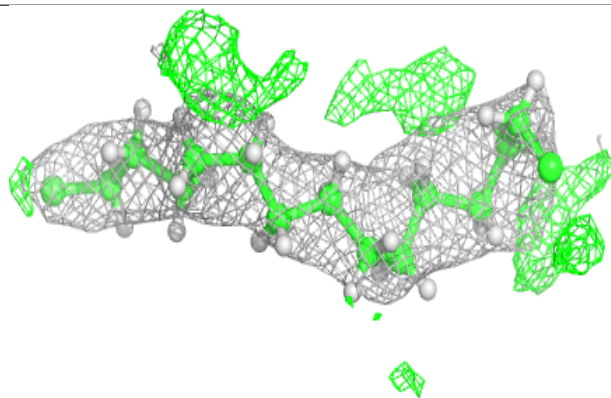
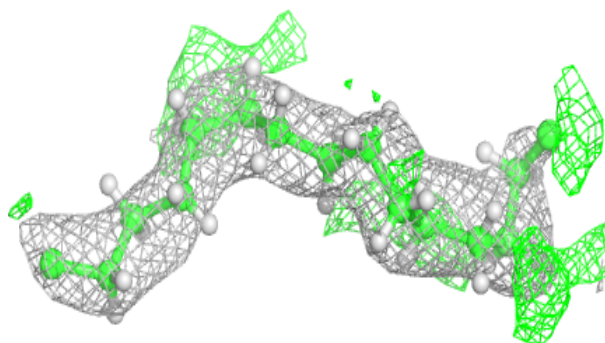
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





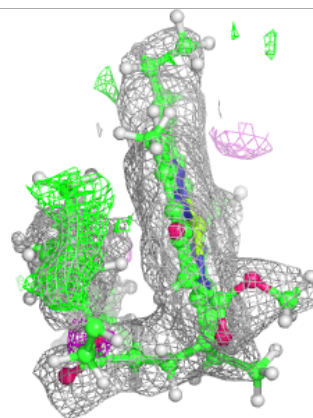
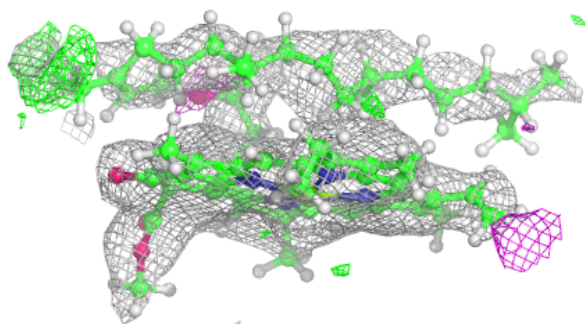
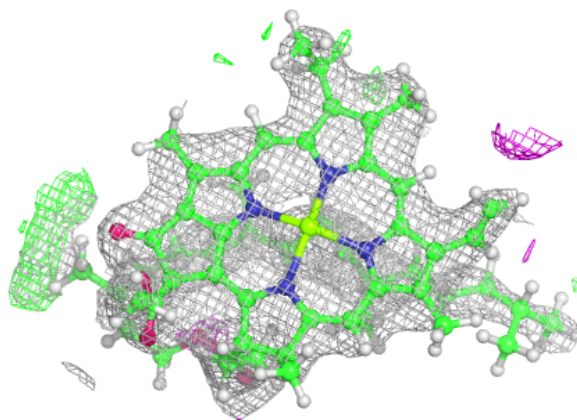
**Electron density around STE B 628:**

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



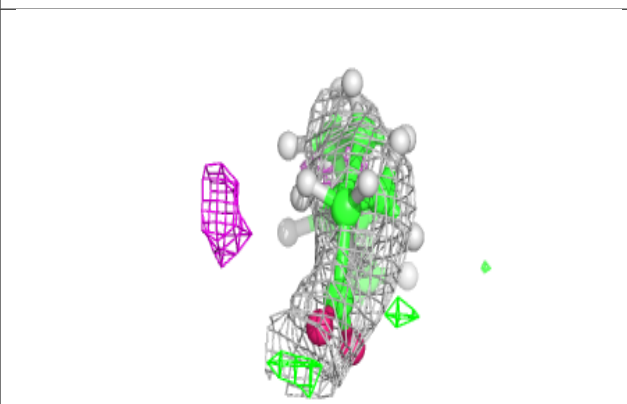
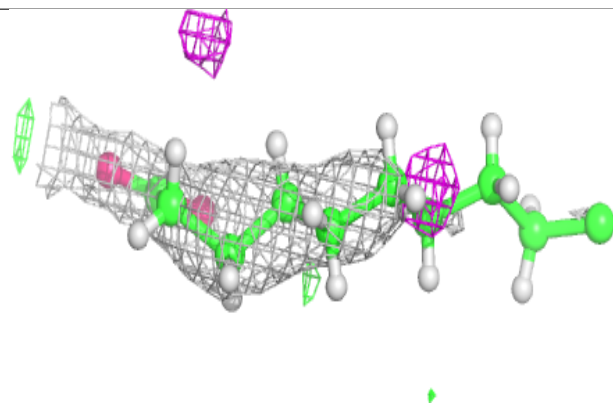
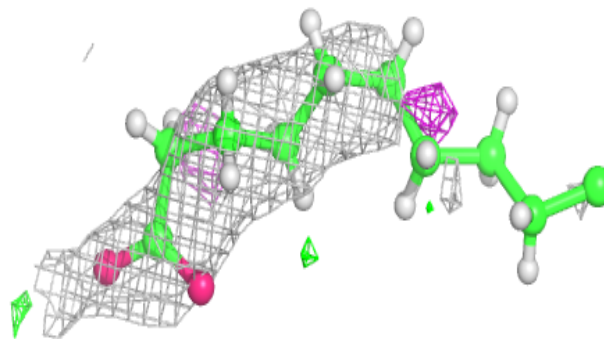
**Electron density around CLA h 101:**

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

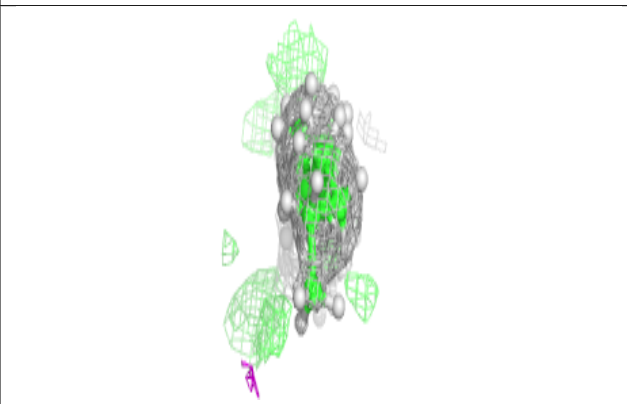
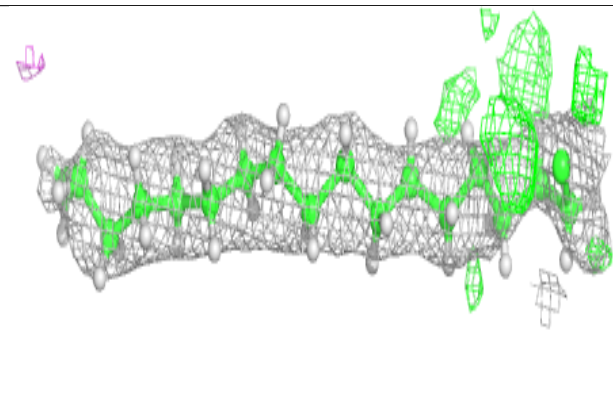
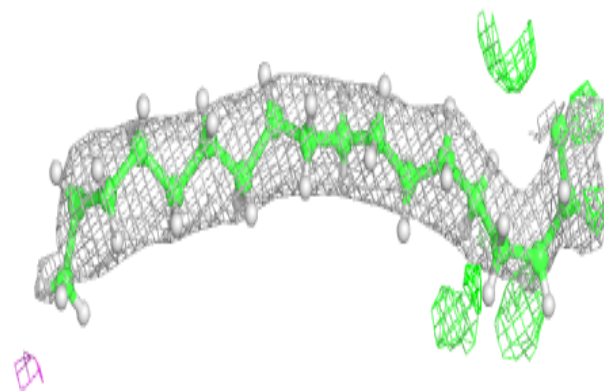


**Electron density around STE B 601:**

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

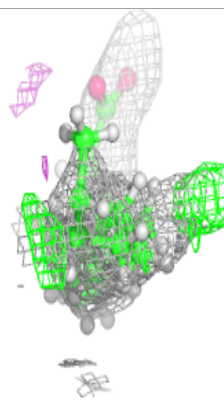
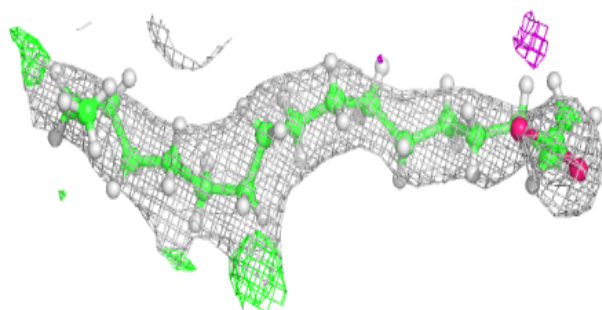
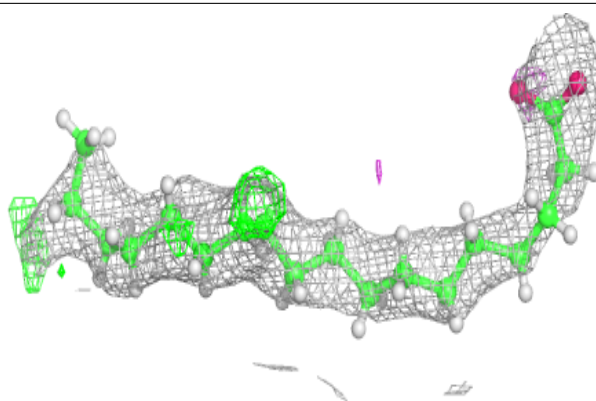
**Electron density around STE I 102:**

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

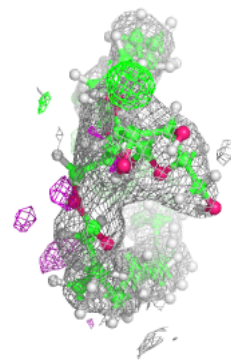
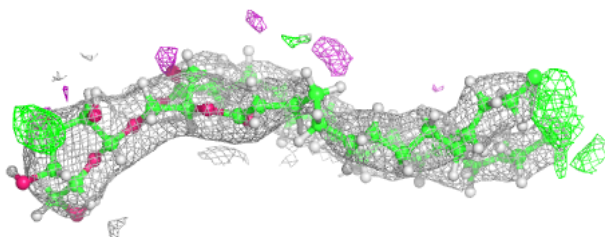
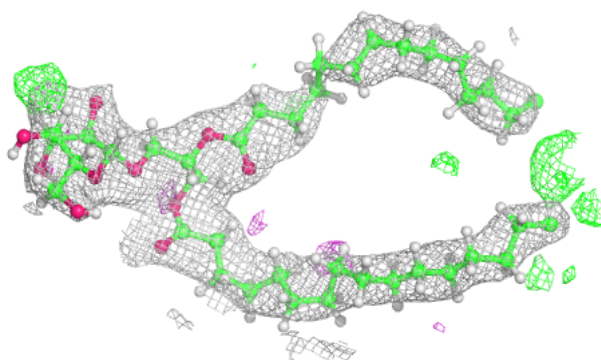


**Electron density around STE b 622:**

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

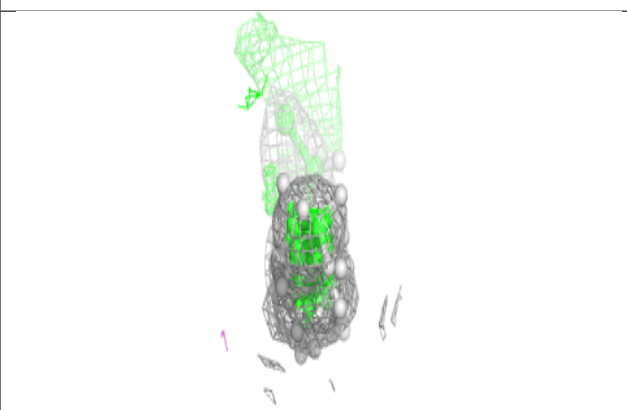
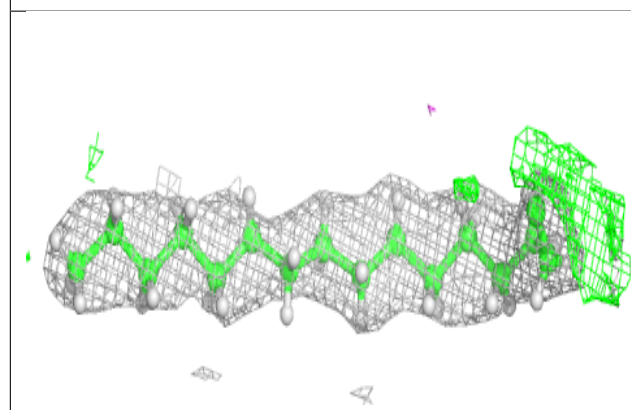
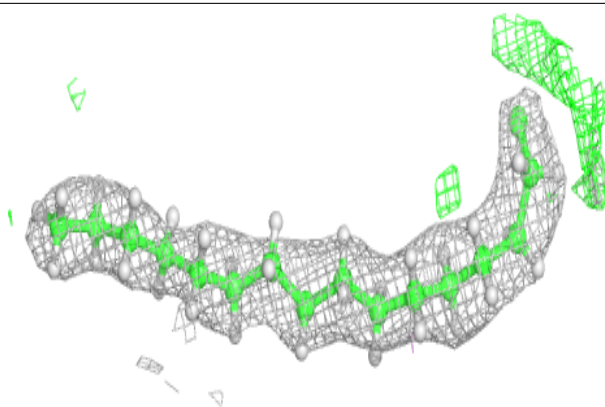
**Electron density around LMG c 525:**

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

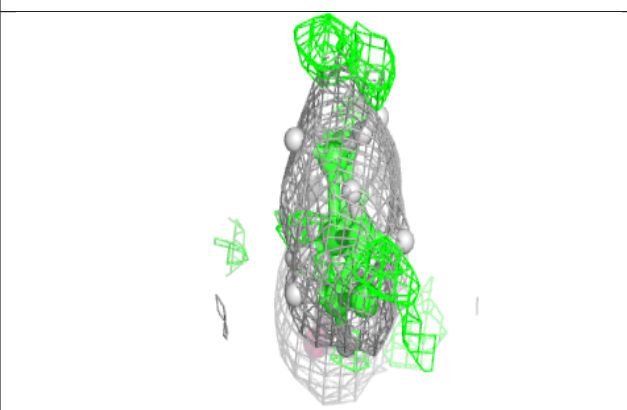
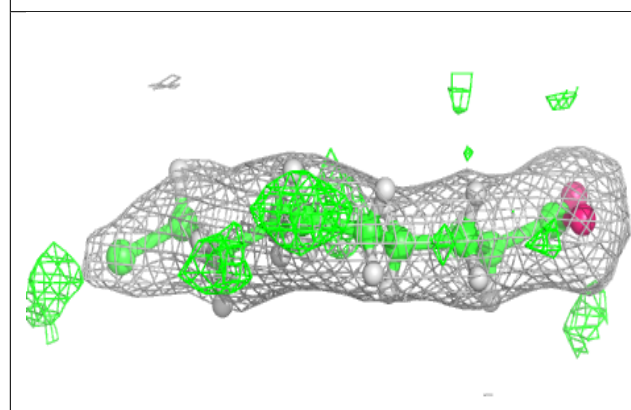
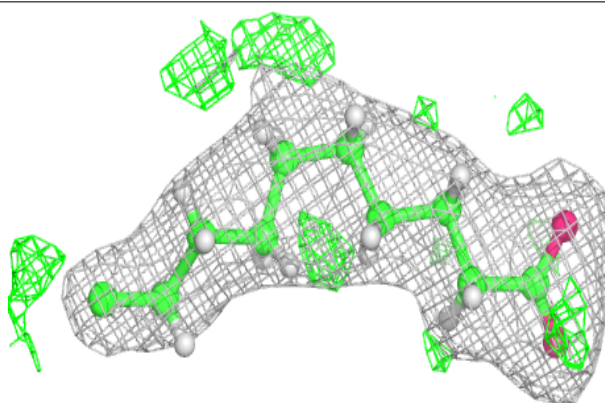


**Electron density around STE C 521:**

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

**Electron density around STE C 522:**

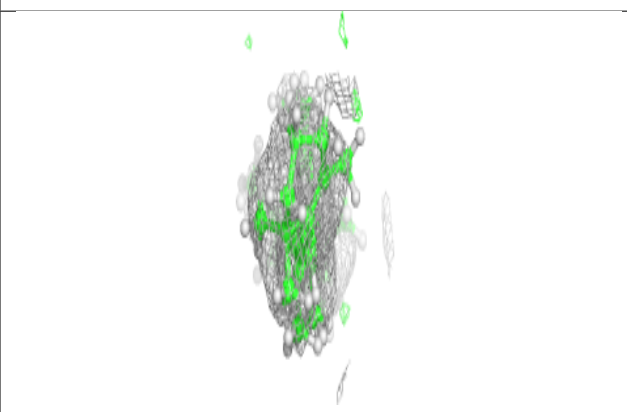
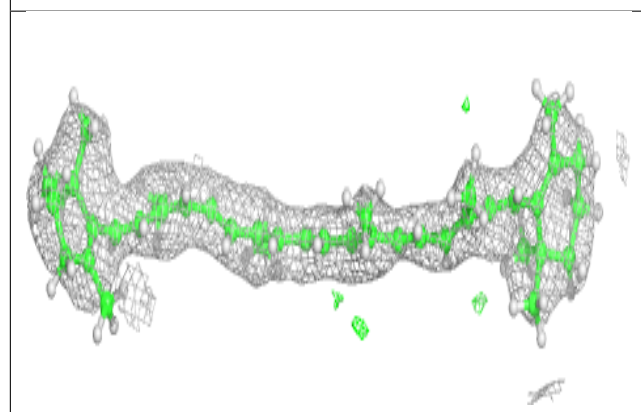
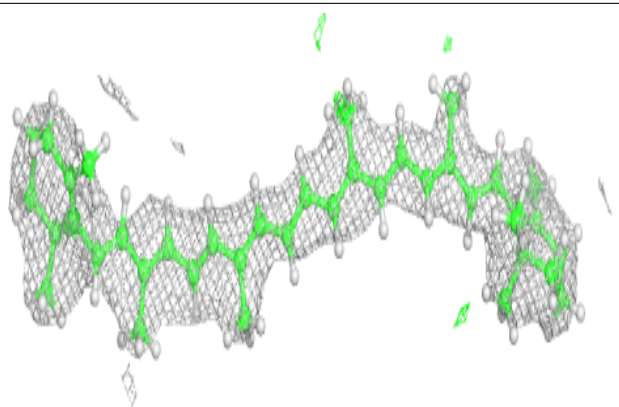
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



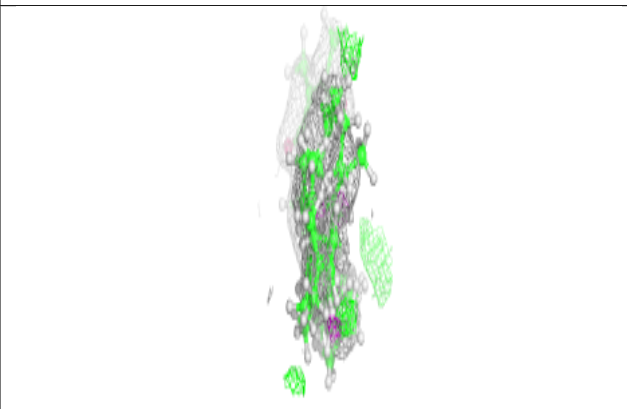
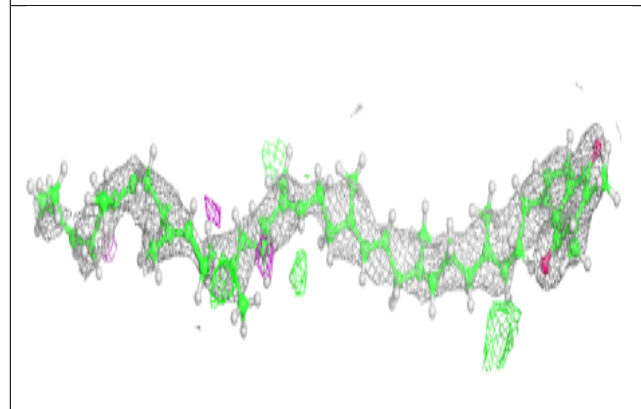
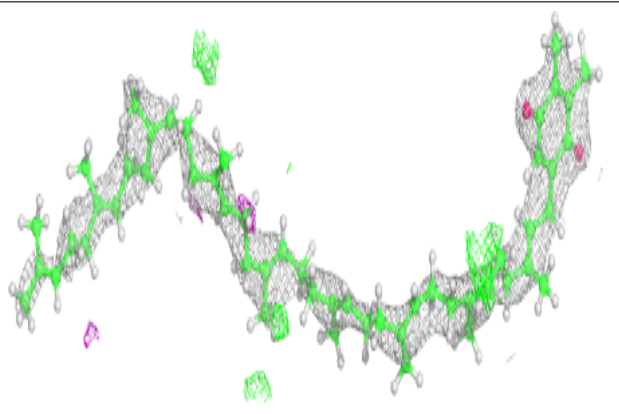


**Electron density around BCR y 101:**

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

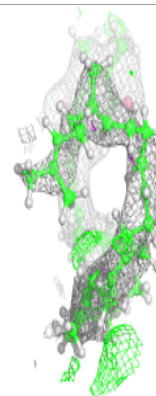
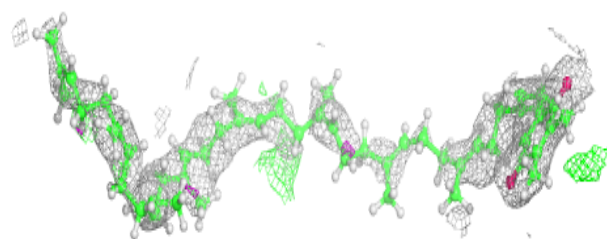
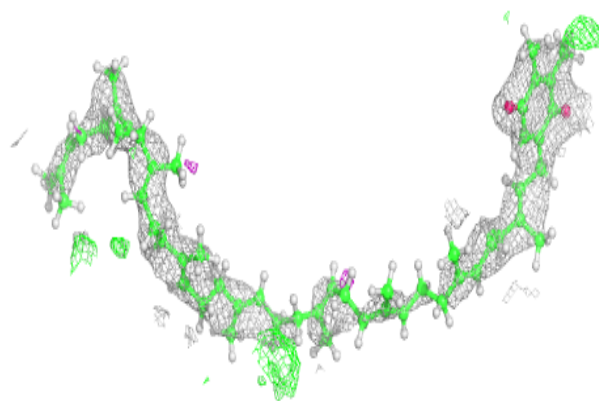
**Electron density around PL9 A 410:**

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

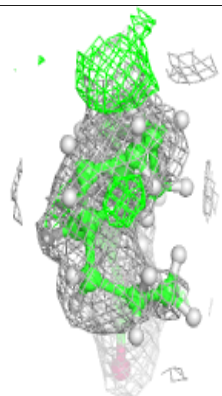
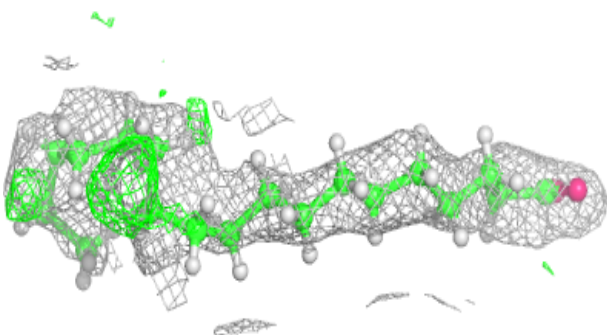
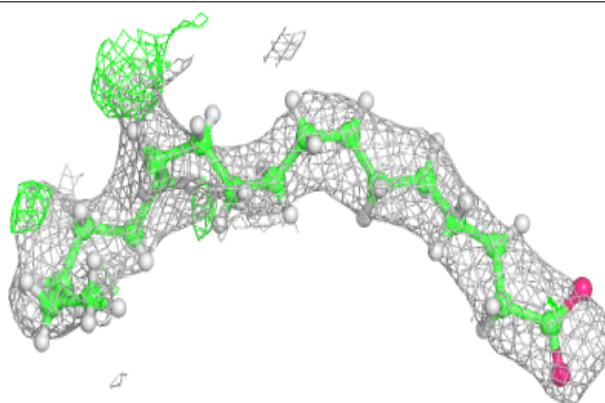


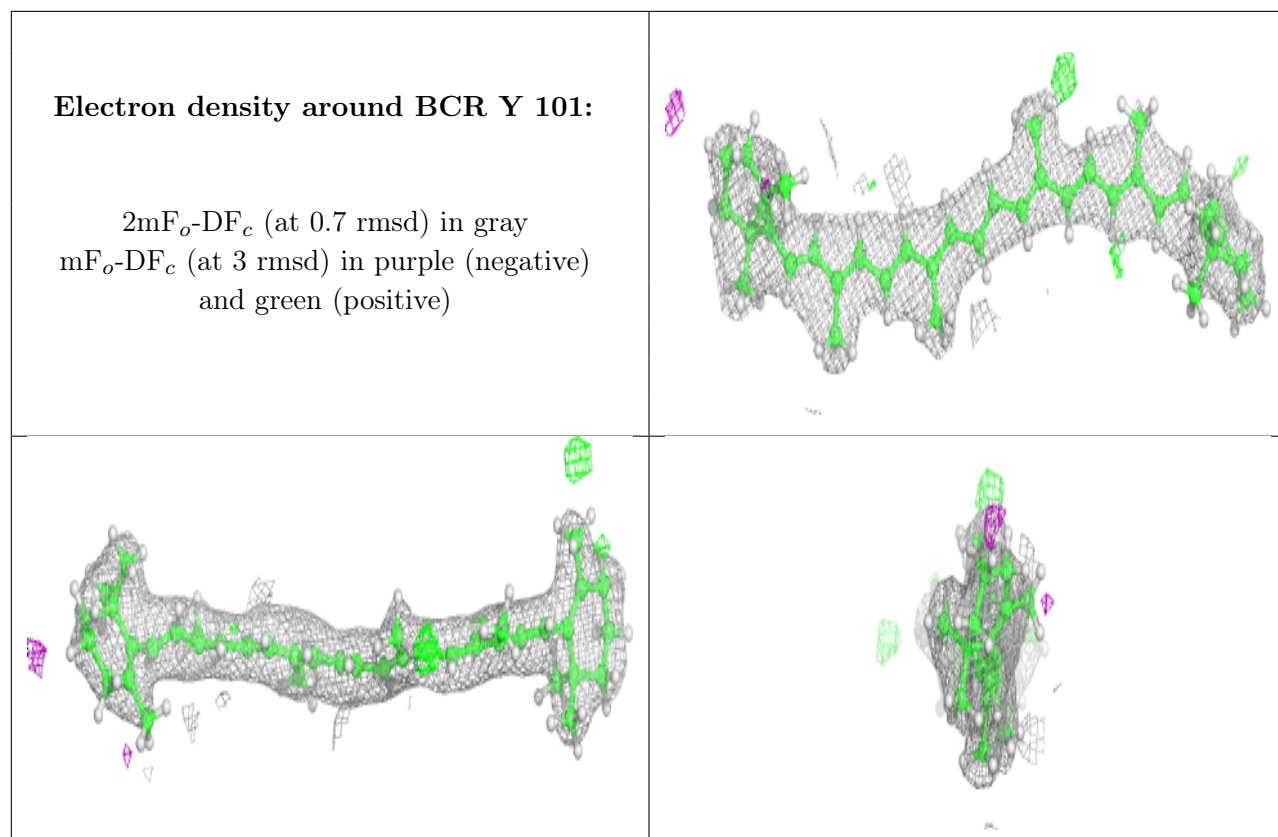
**Electron density around PL9 a 410:**

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

**Electron density around STE d 412:**

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

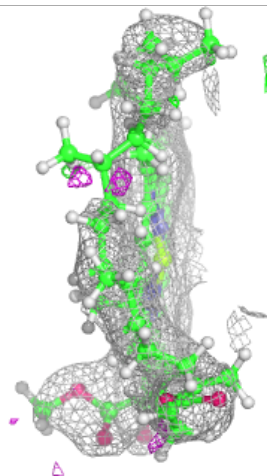
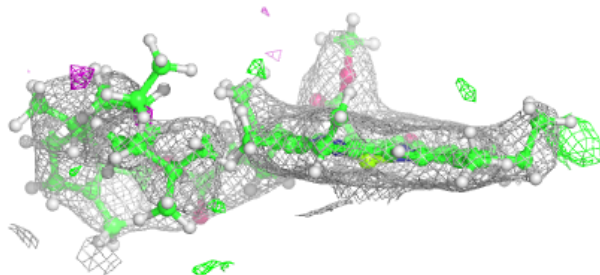
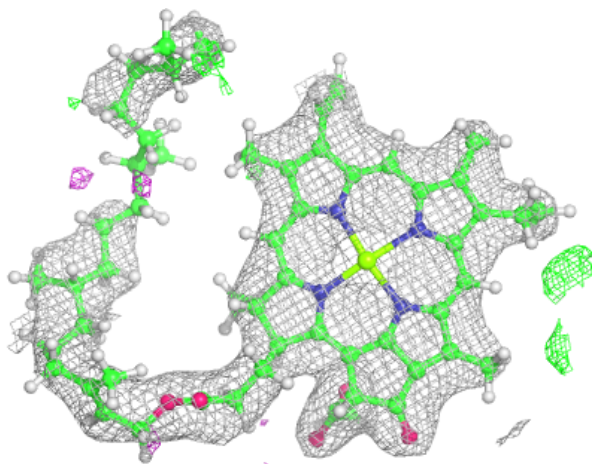






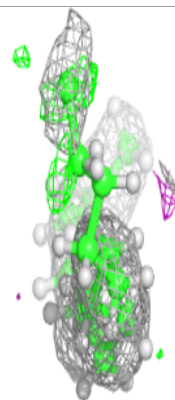
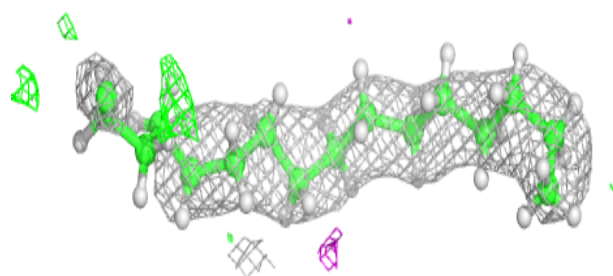
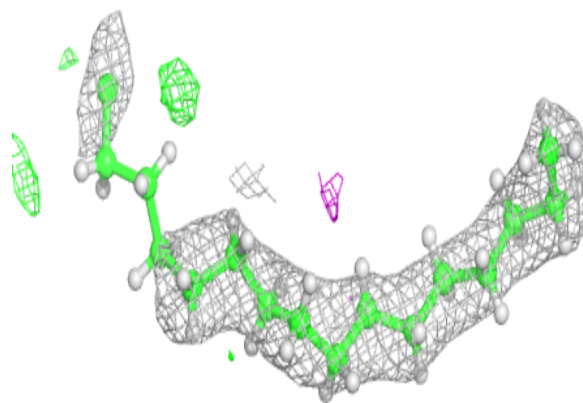
**Electron density around CLA c 514:**

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

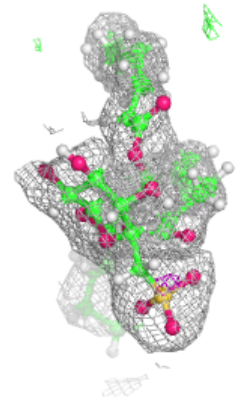
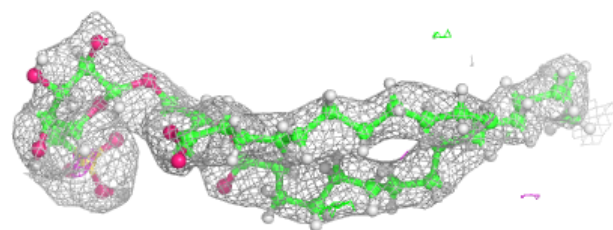
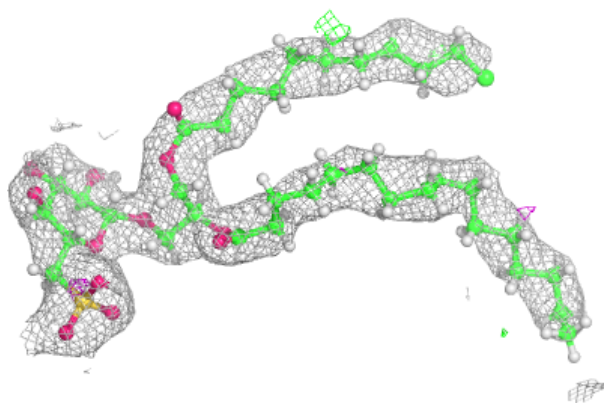


**Electron density around STE b 620:**

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

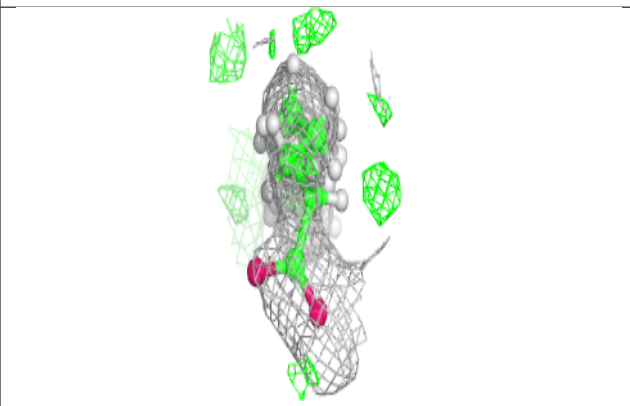
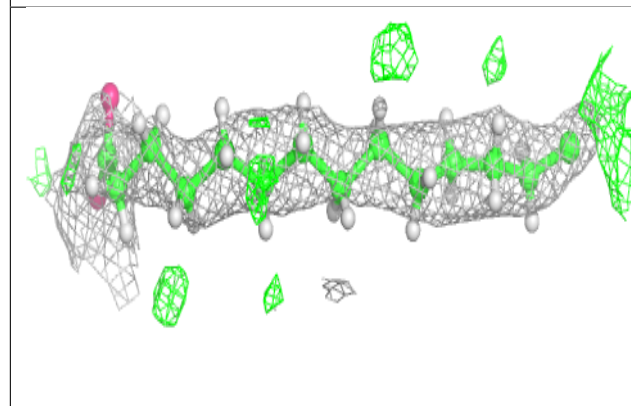
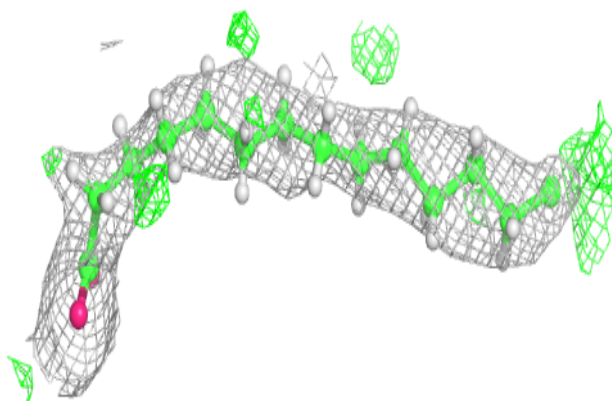
**Electron density around SQD b 619:**

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

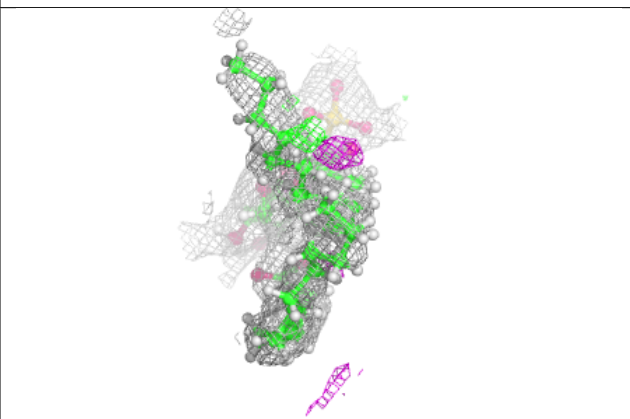
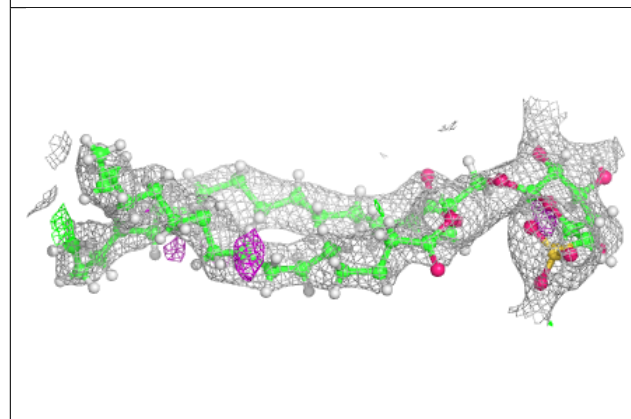
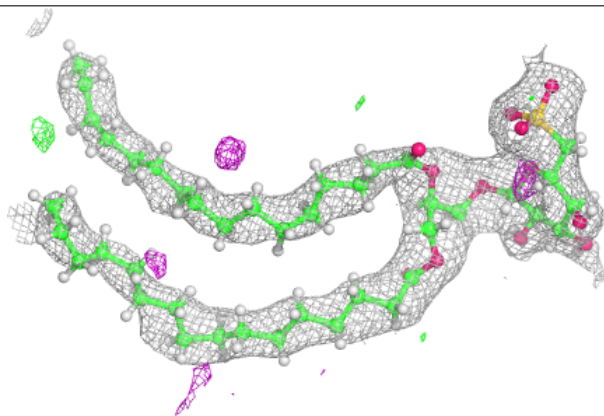


**Electron density around STE b 624:**

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

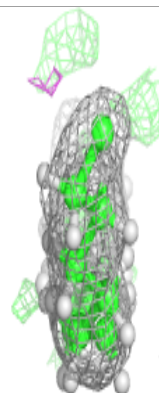
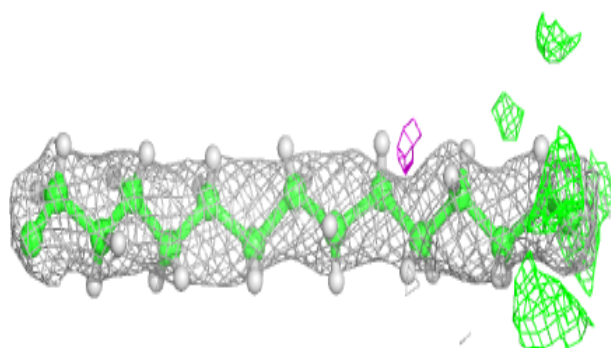
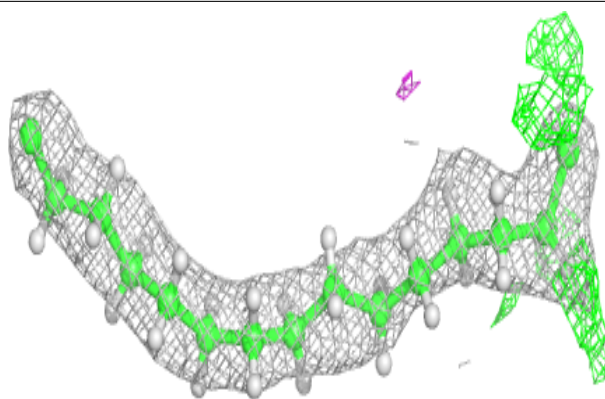
**Electron density around SQD B 623:**

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

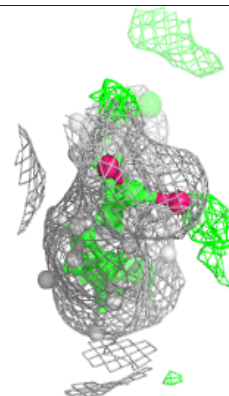
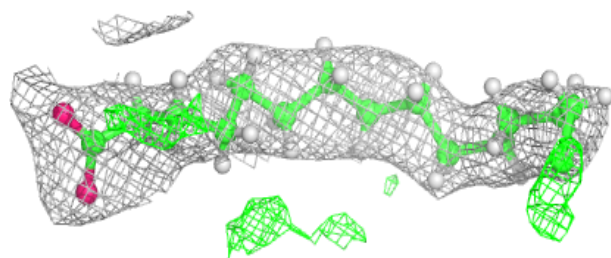
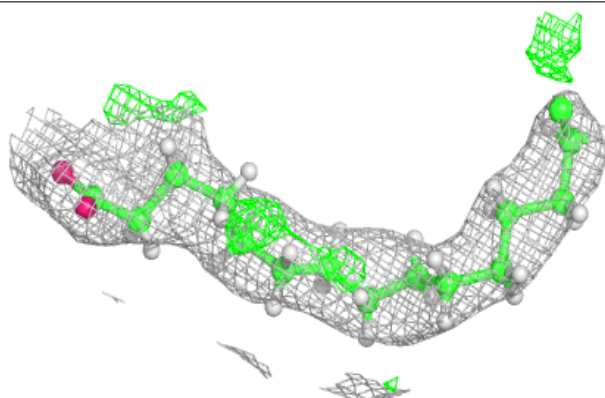


**Electron density around STE I 101:**

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

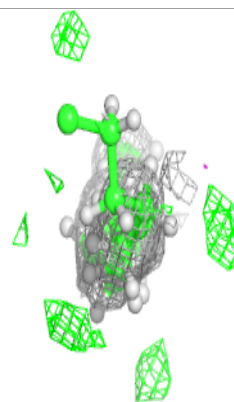
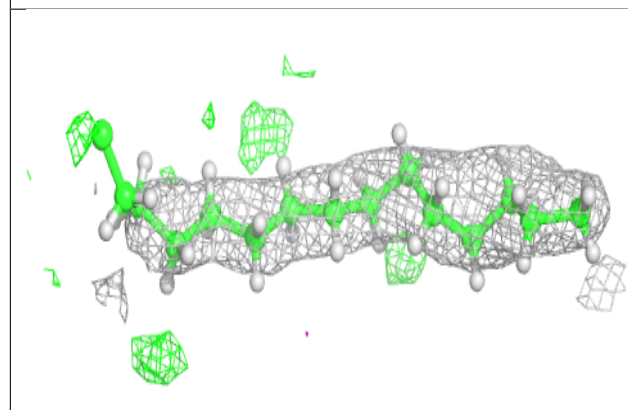
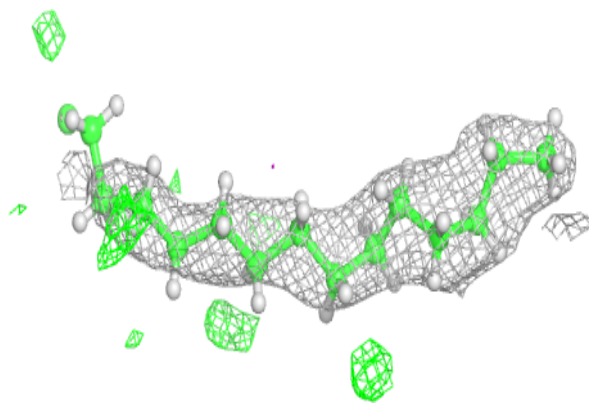
**Electron density around STE B 621:**

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



**Electron density around STE T 102:**

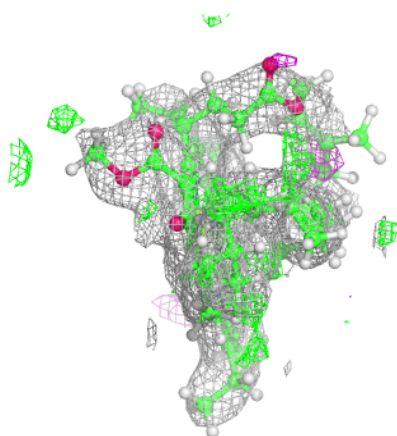
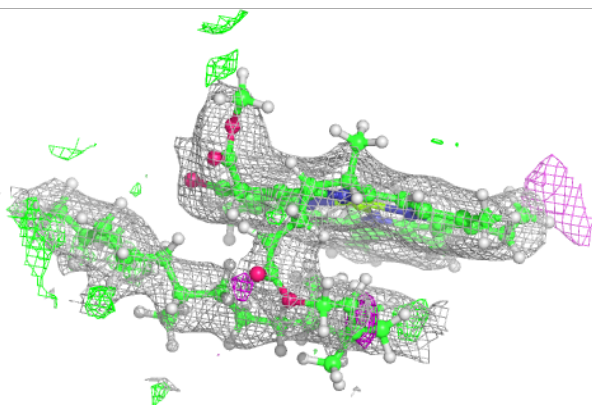
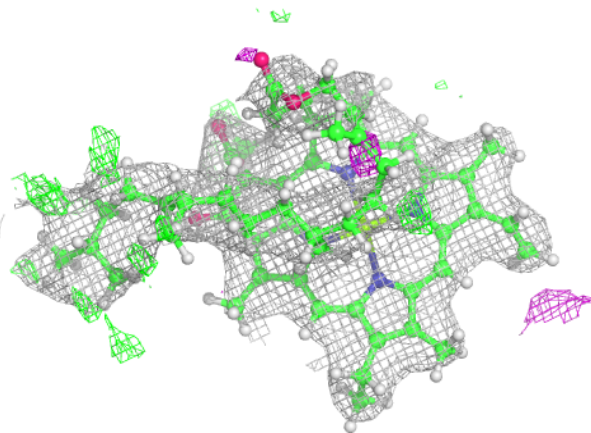
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





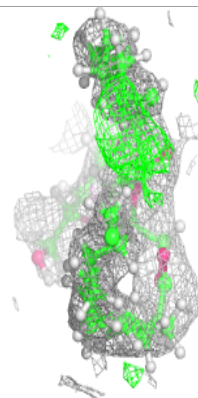
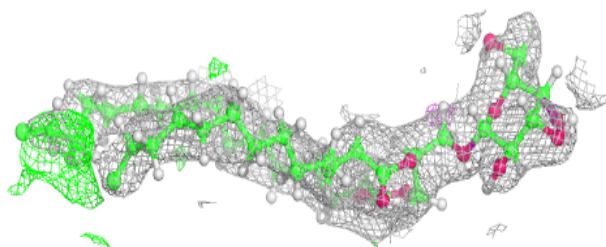
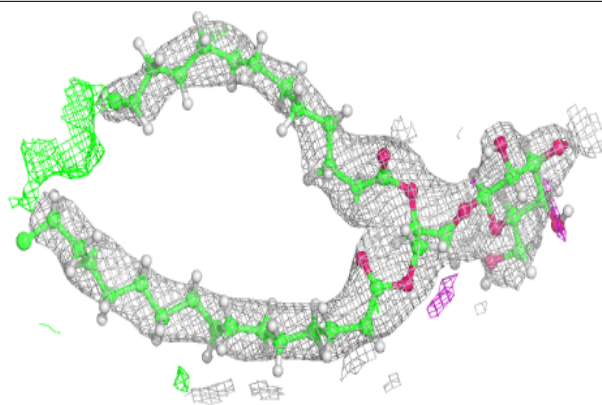
**Electron density around CLA B 602:**

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

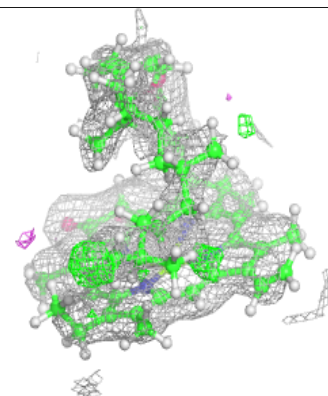
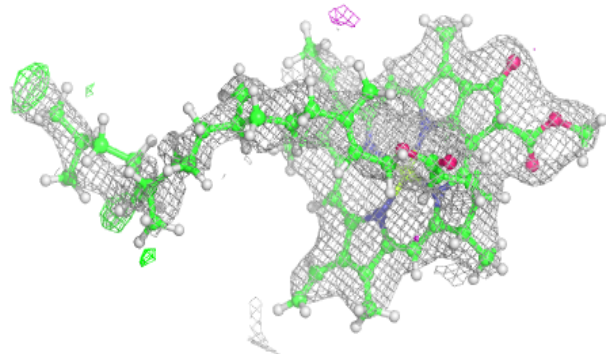
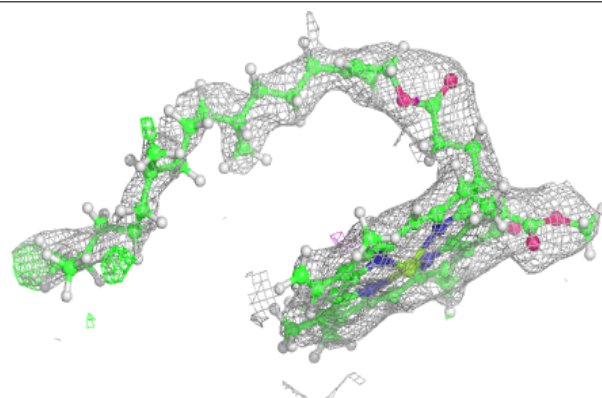


**Electron density around LMG A 412:**

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

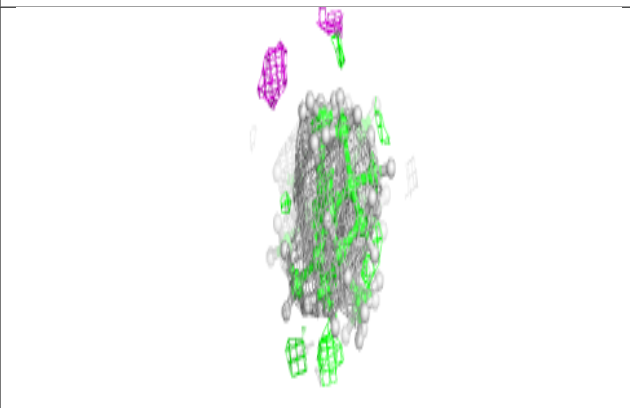
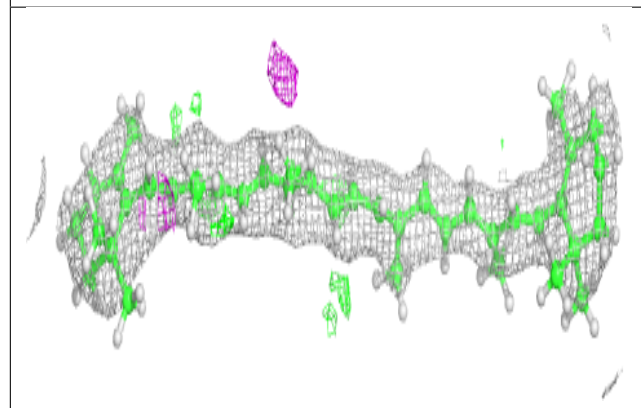
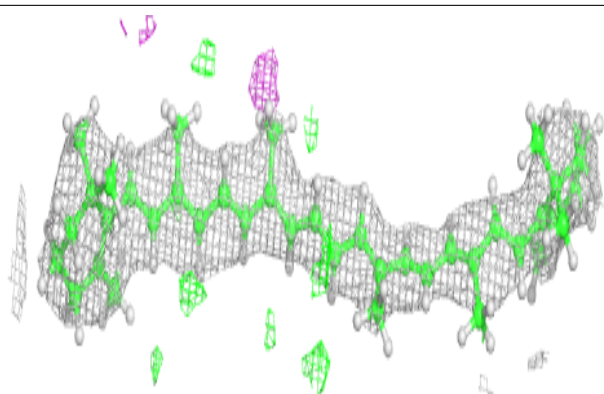
**Electron density around CLA C 514:**

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

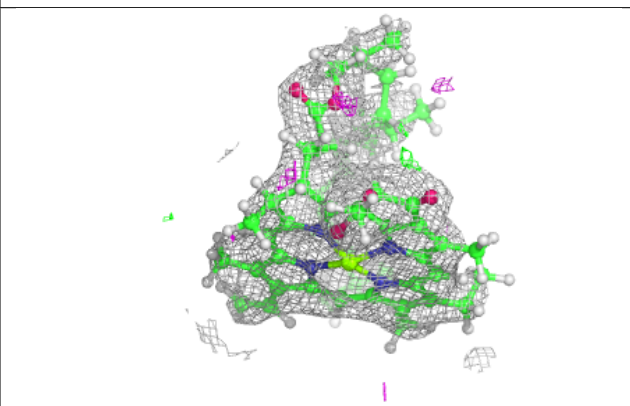
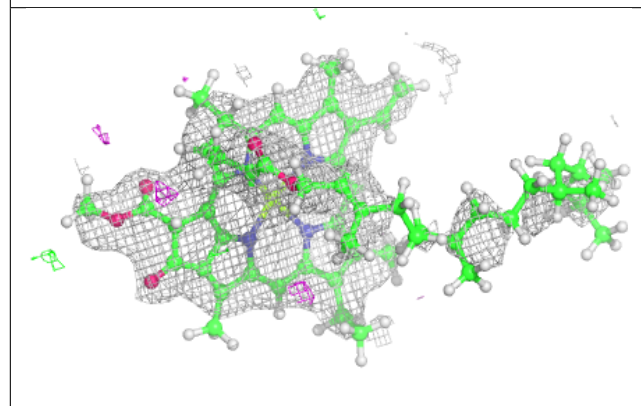
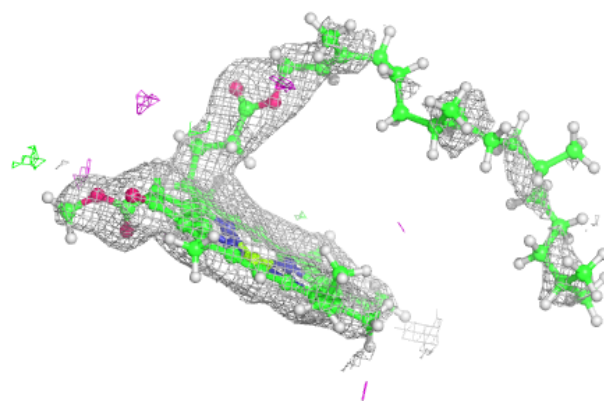


**Electron density around BCR Z 101:**

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

**Electron density around CLA c 515:**

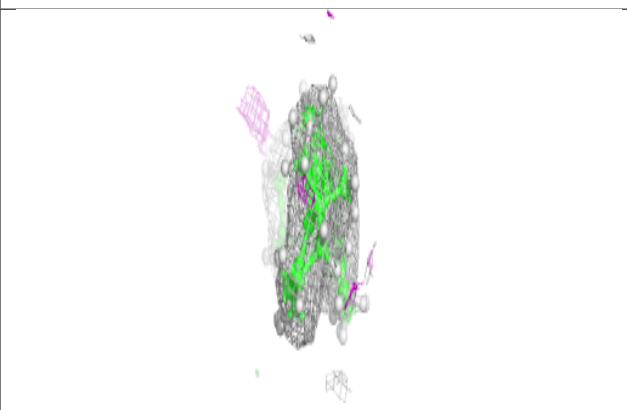
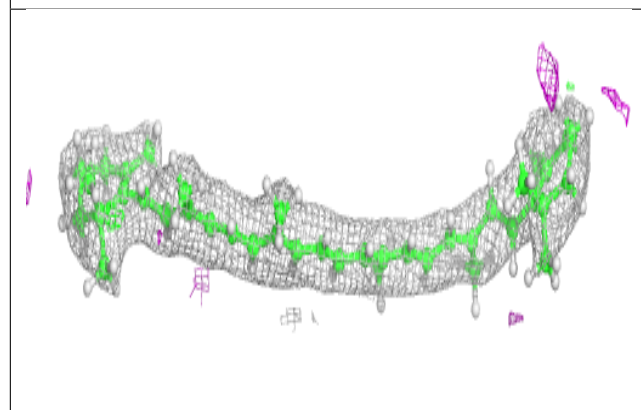
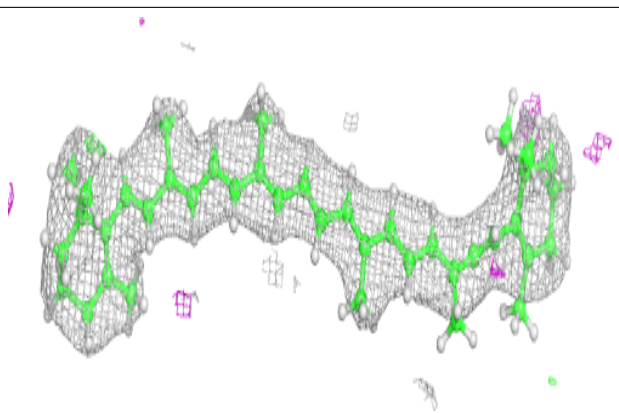
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



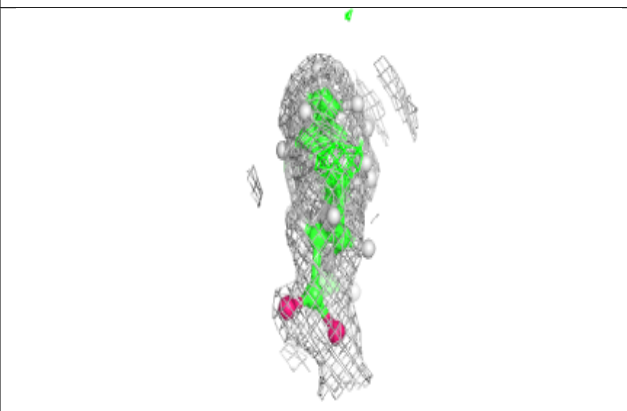
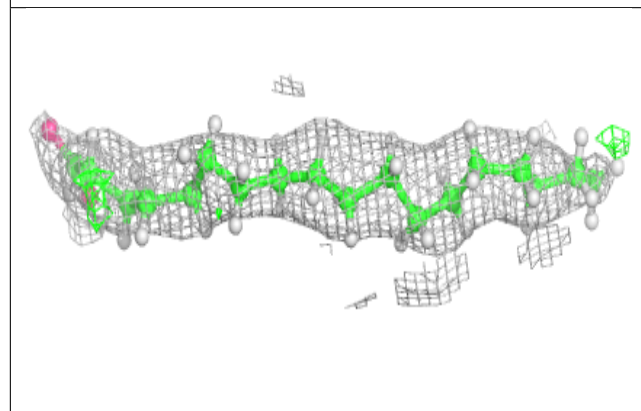
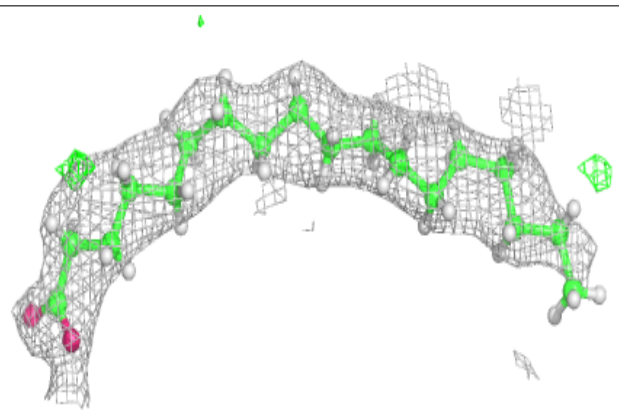


**Electron density around BCR d 404:**

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

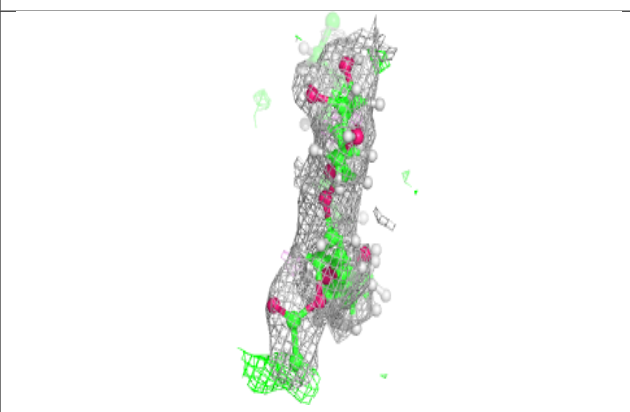
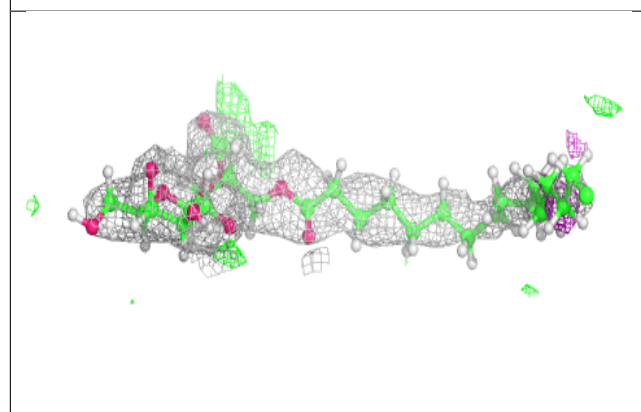
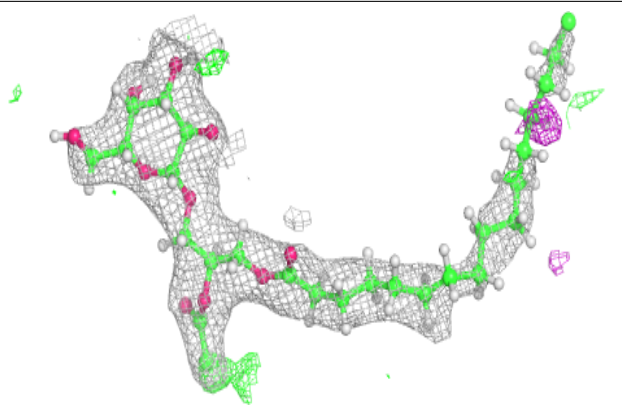
**Electron density around STE X 101:**

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

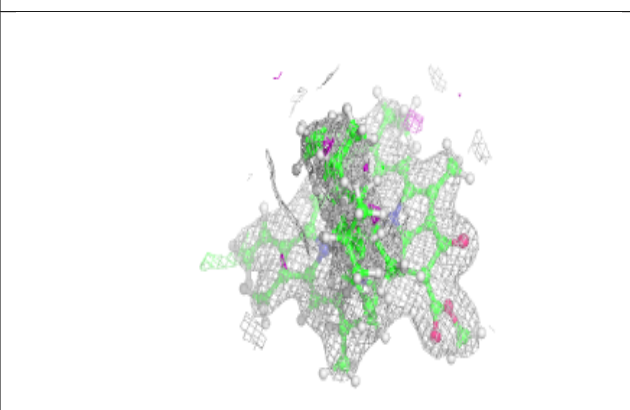
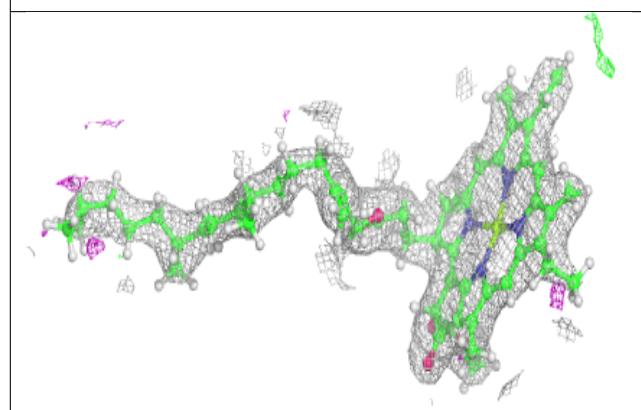
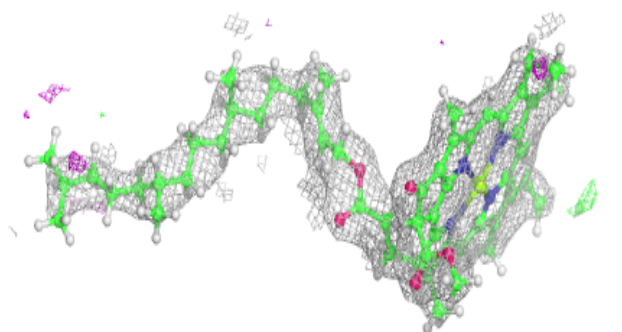


**Electron density around LMG c 522:**

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

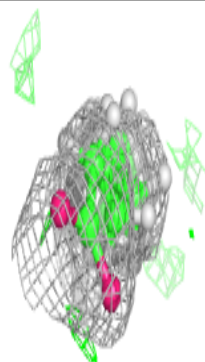
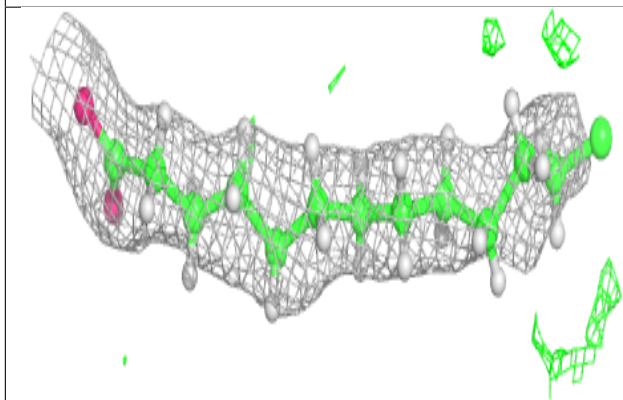
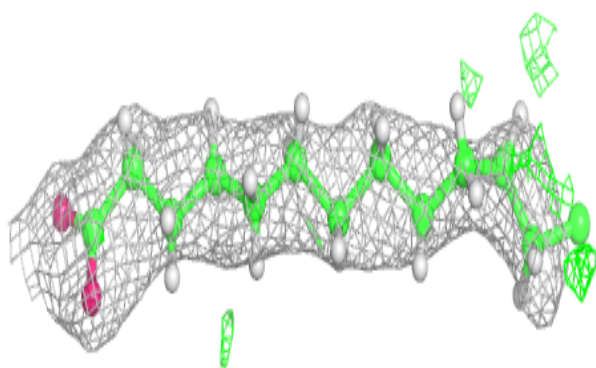
**Electron density around CLA c 504:**

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

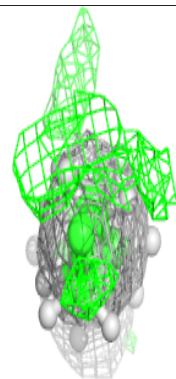
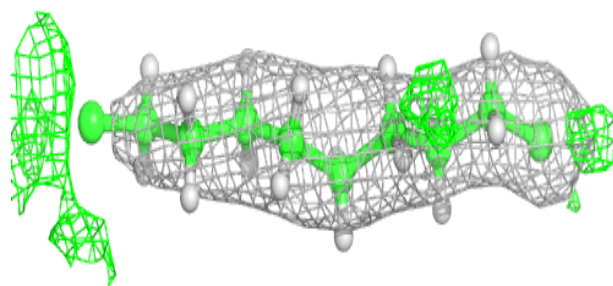
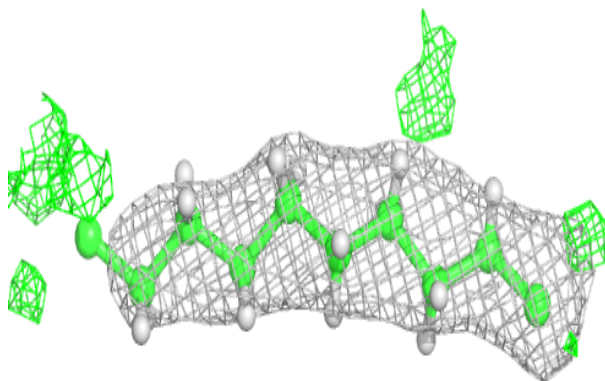


**Electron density around STE M 102:**

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

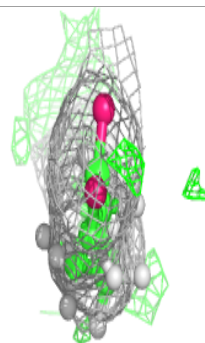
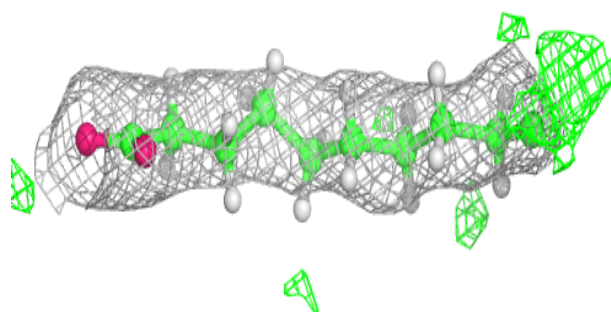
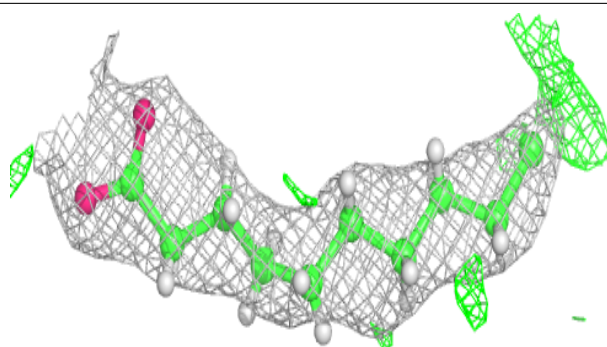
**Electron density around STE M 103:**

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

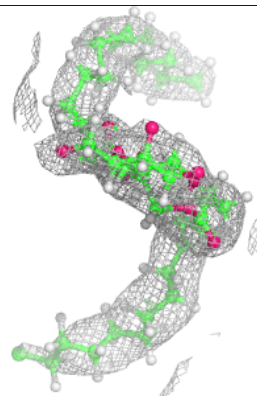
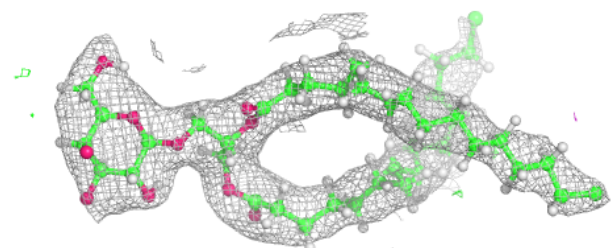
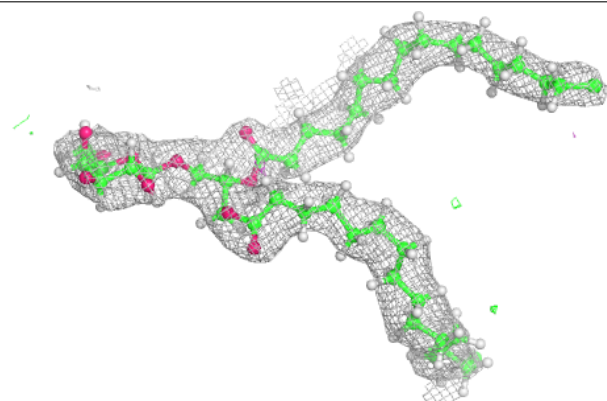


**Electron density around STE C 520:**

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

**Electron density around LMG M 101:**

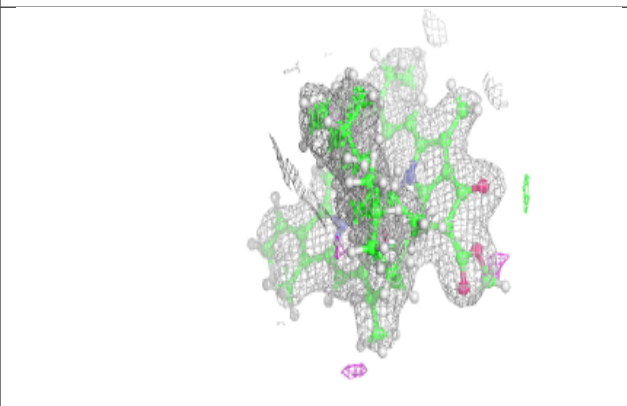
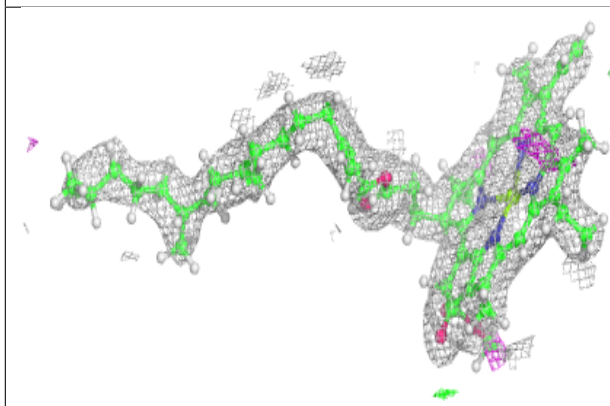
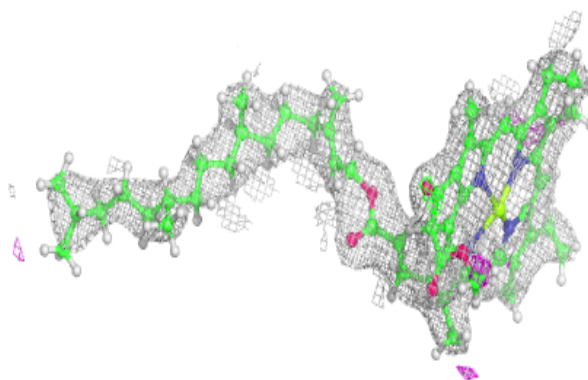
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



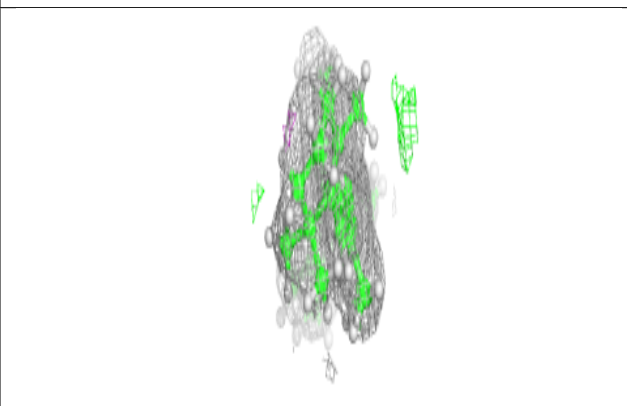
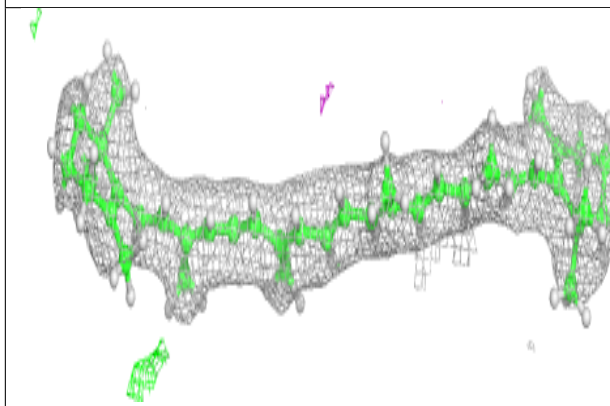
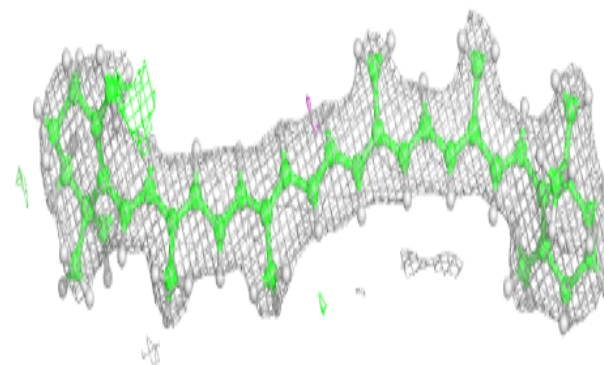


**Electron density around CLA C 503:**

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

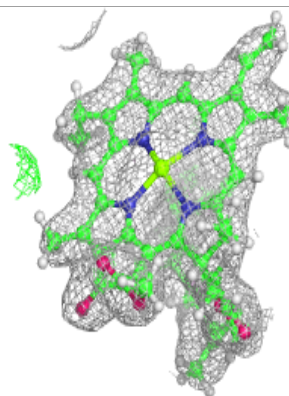
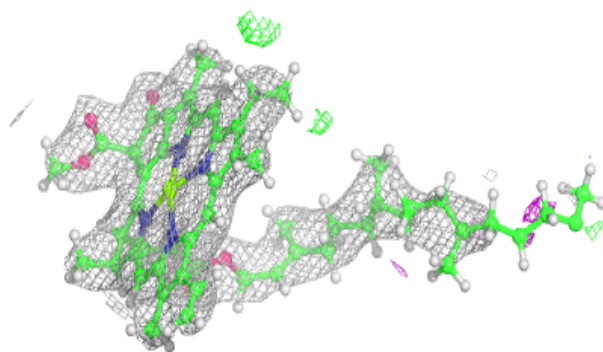
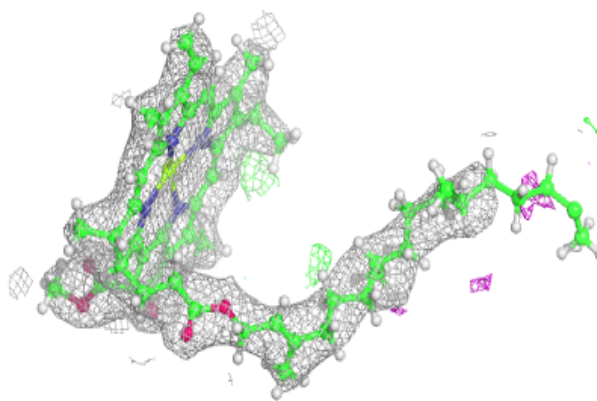
**Electron density around BCR B 620:**

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



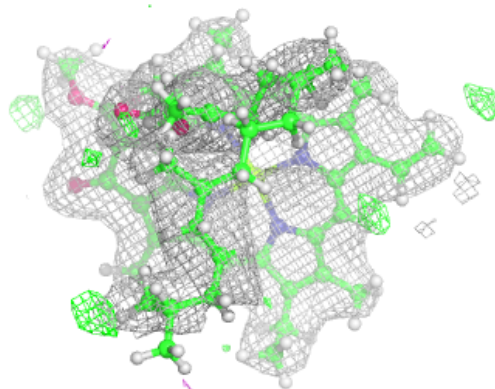
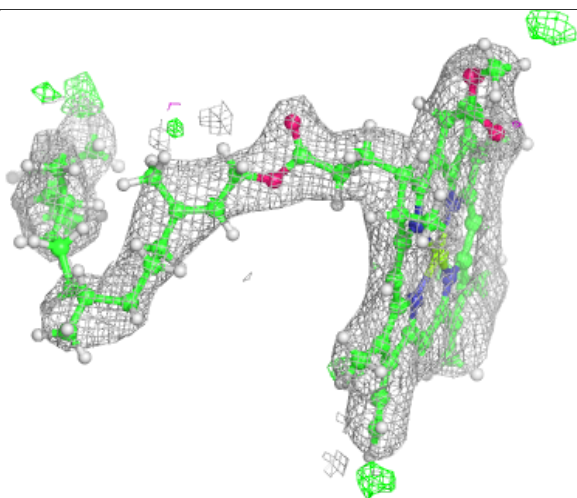
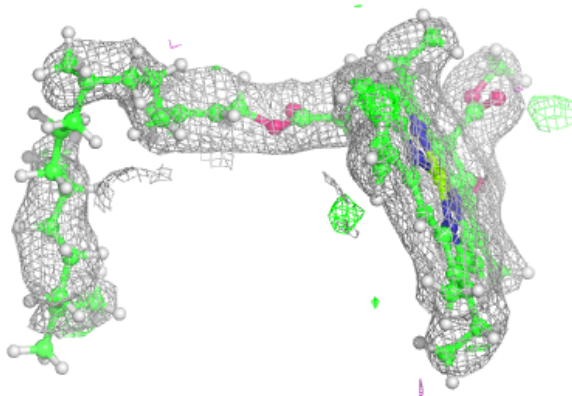
**Electron density around CLA c 510:**

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



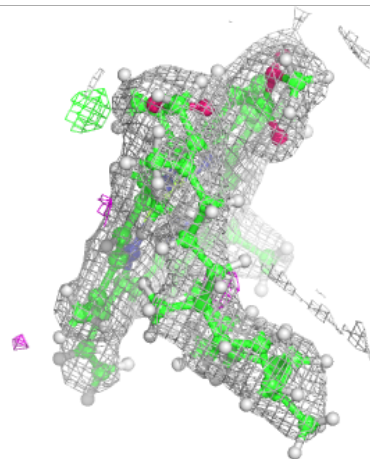
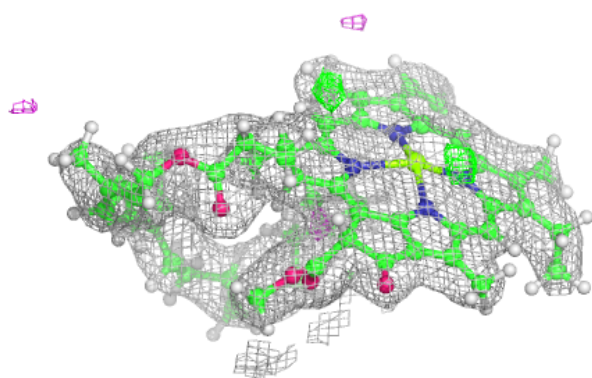
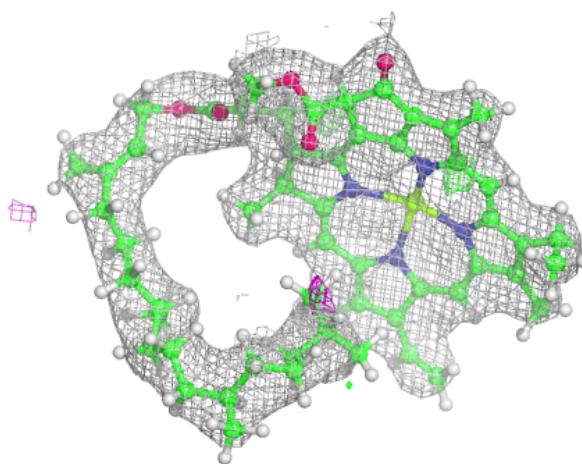
**Electron density around CLA a 405:**

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



**Electron density around CLA b 614:**

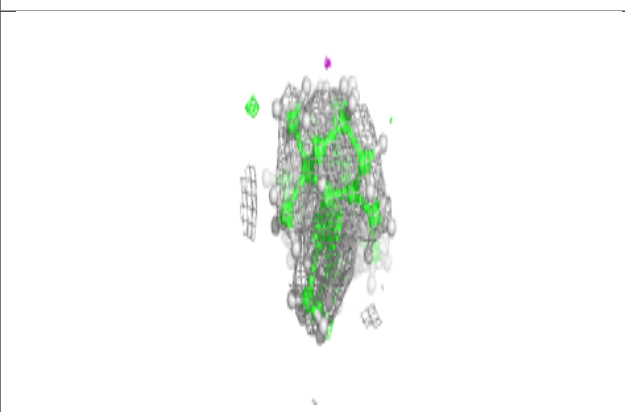
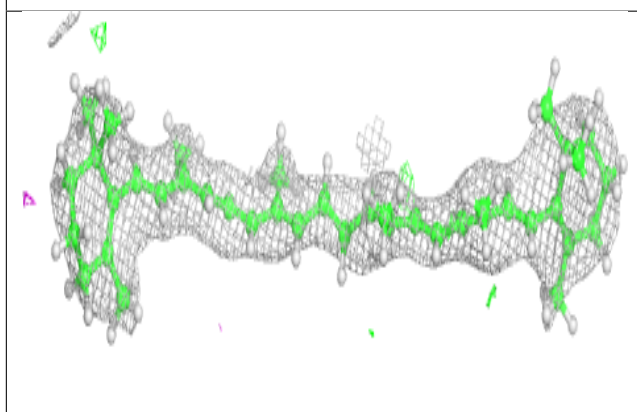
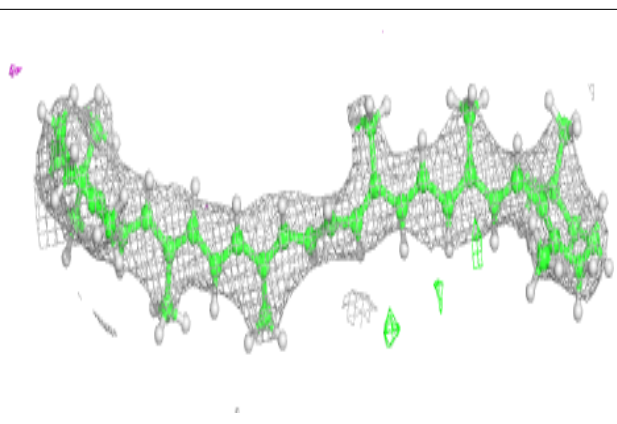
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



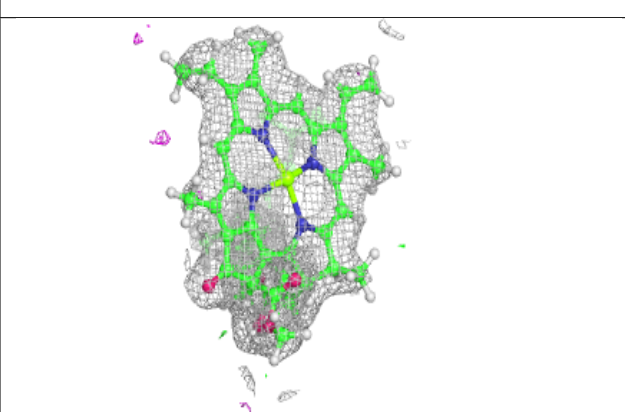
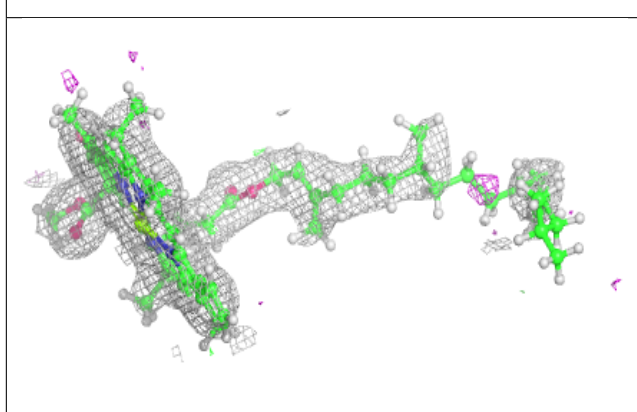
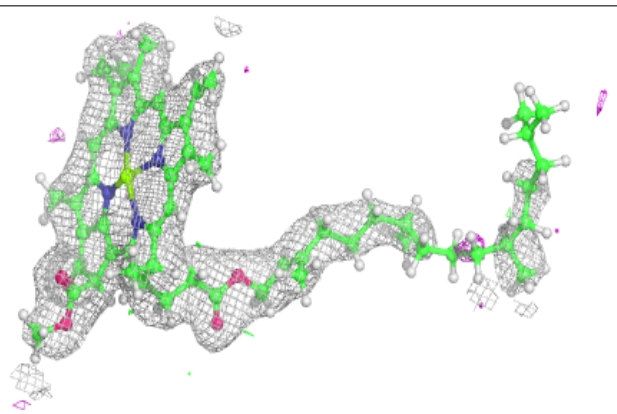


**Electron density around BCR c 516:**

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

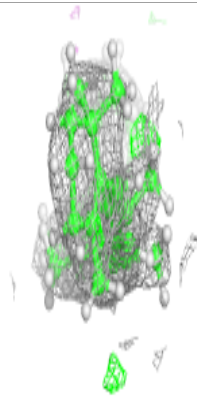
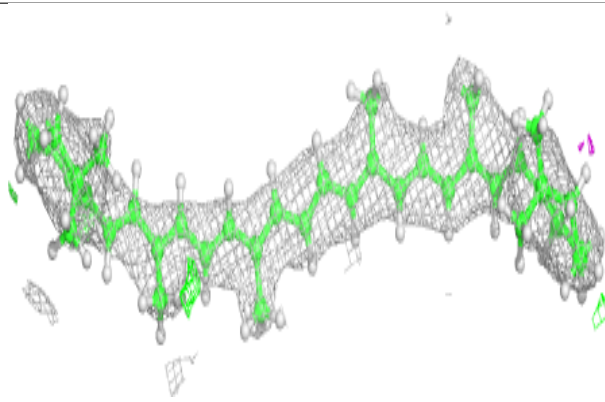
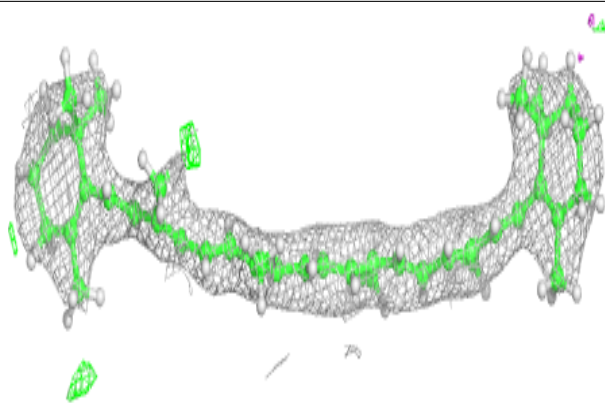
**Electron density around CLA d 403:**

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



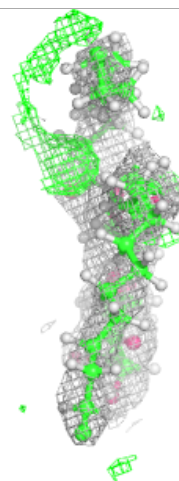
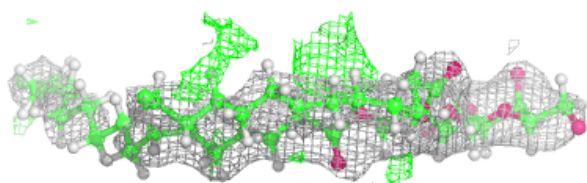
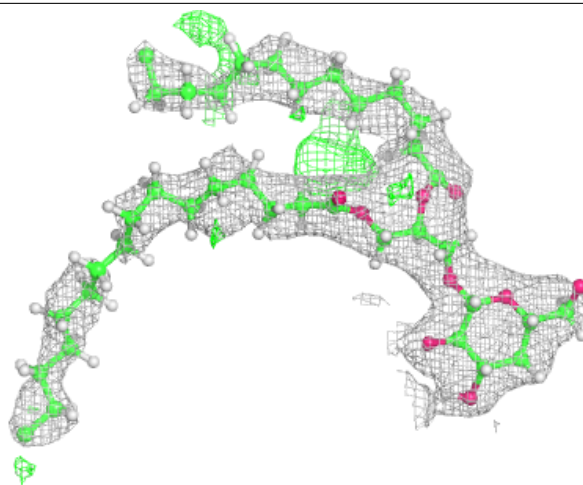
**Electron density around BCR c 518:**

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



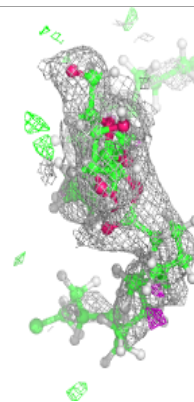
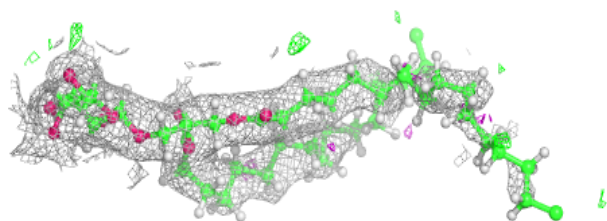
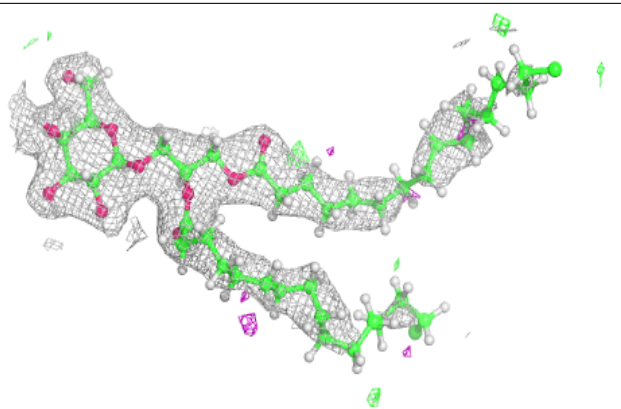
**Electron density around LMG C 519:**

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

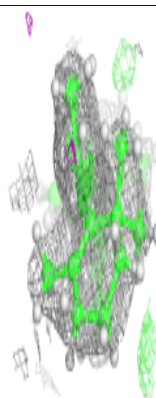
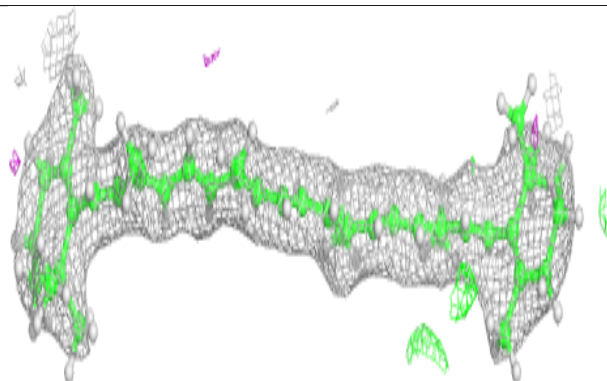
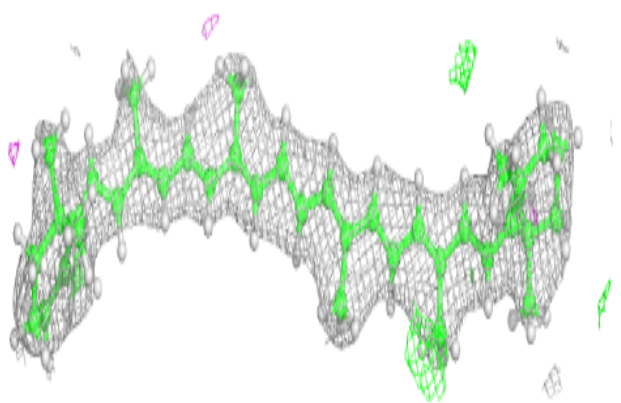


**Electron density around LMG D 406:**

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

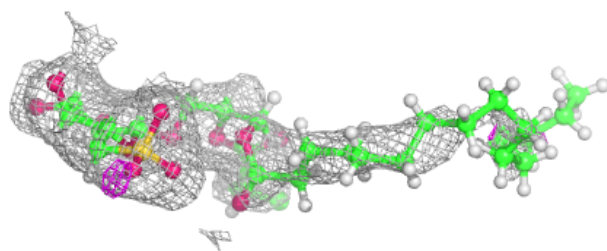
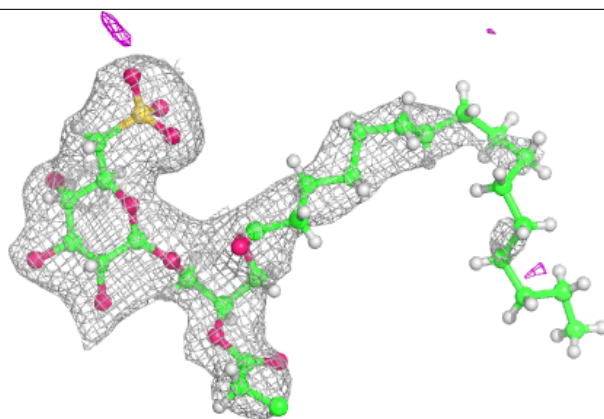
**Electron density around BCR C 515:**

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

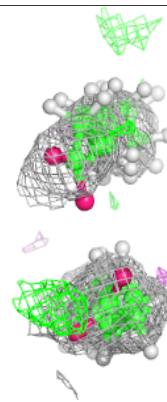
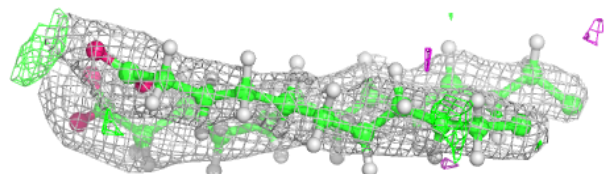
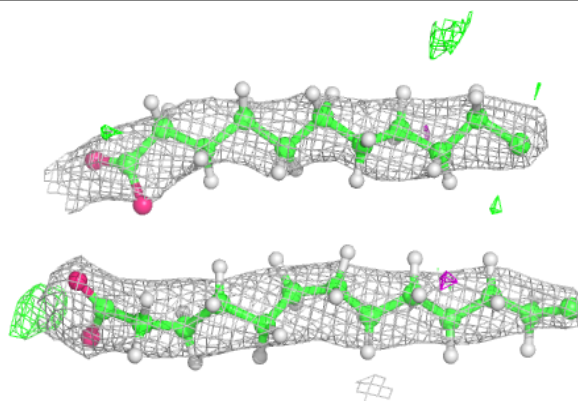


**Electron density around SQD f 101:**

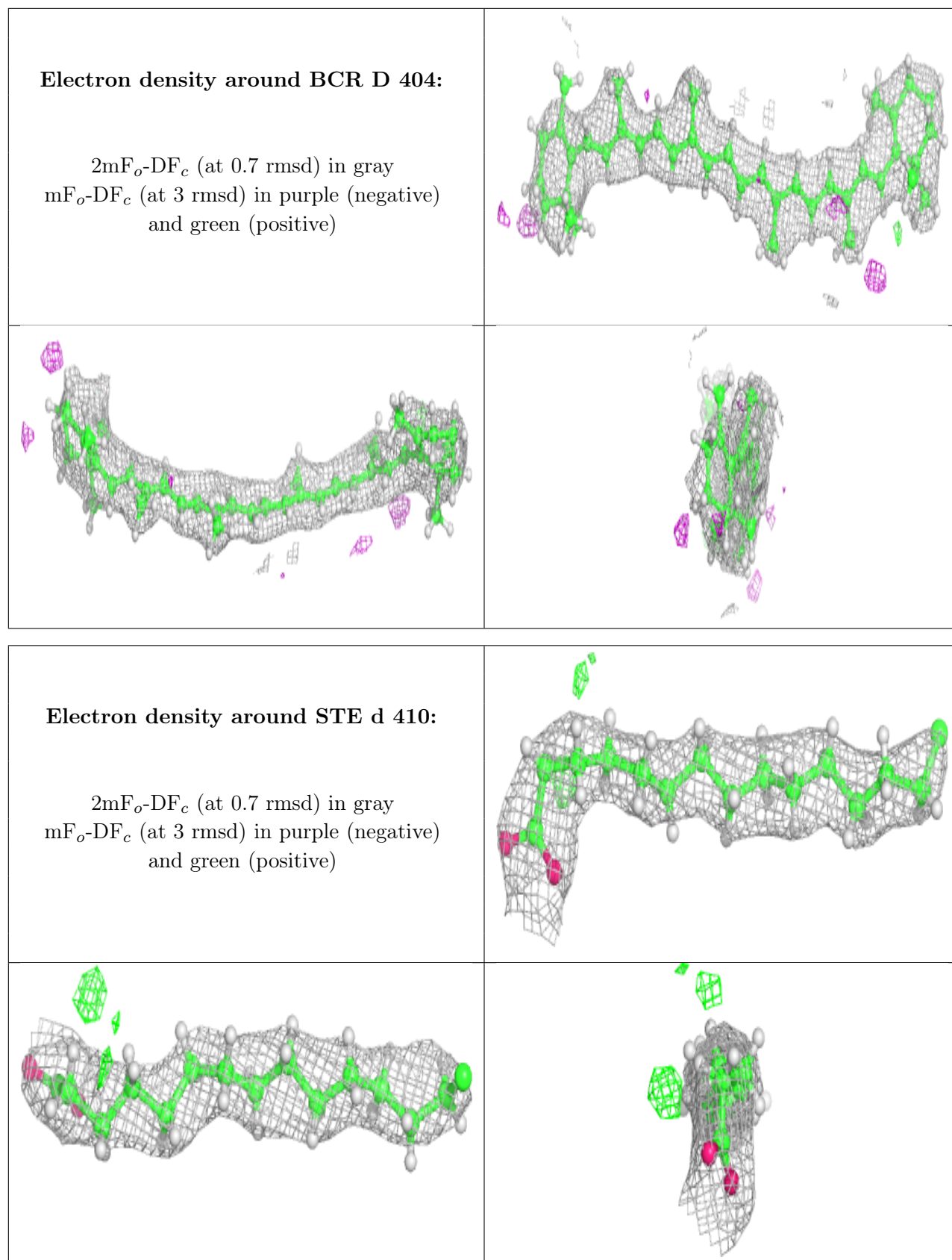
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

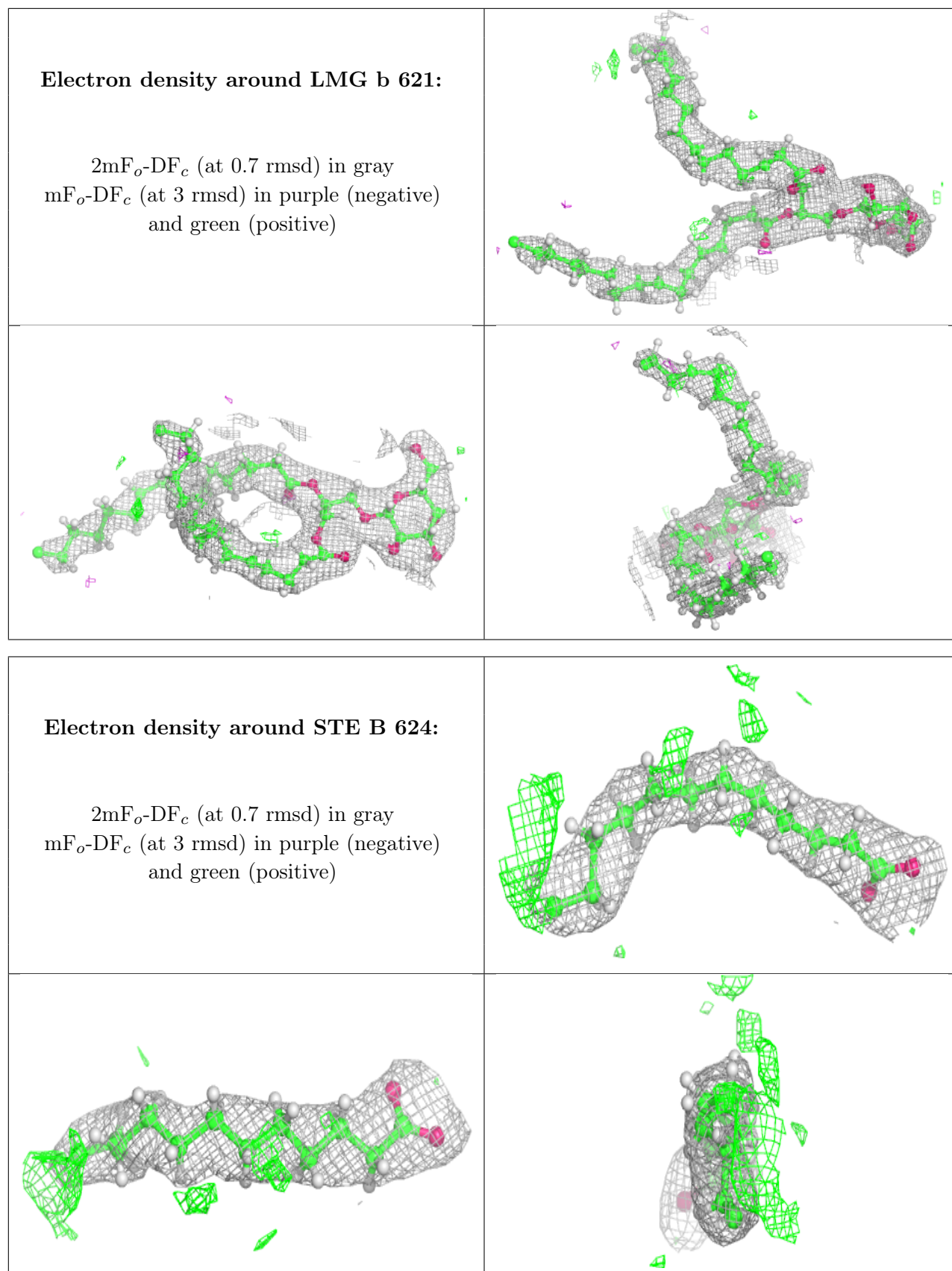
**Electron density around LMG D 411:**

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



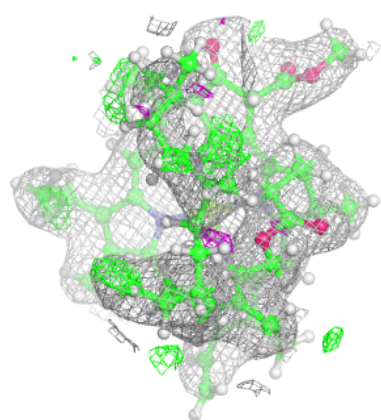
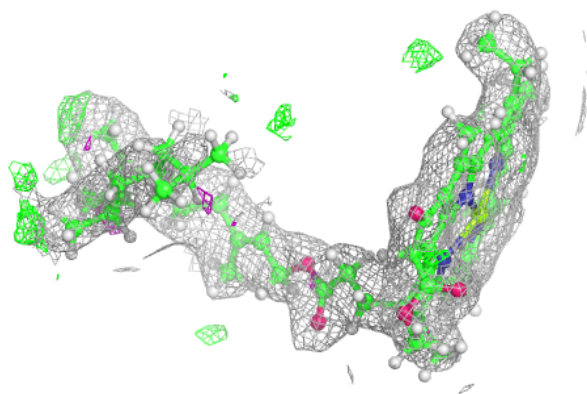
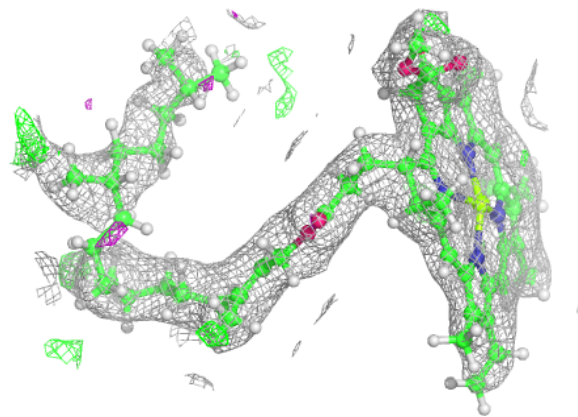






**Electron density around CLA B 607:**

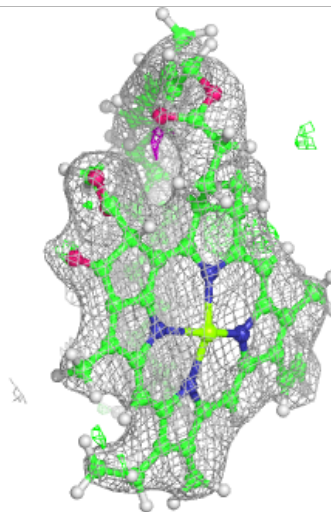
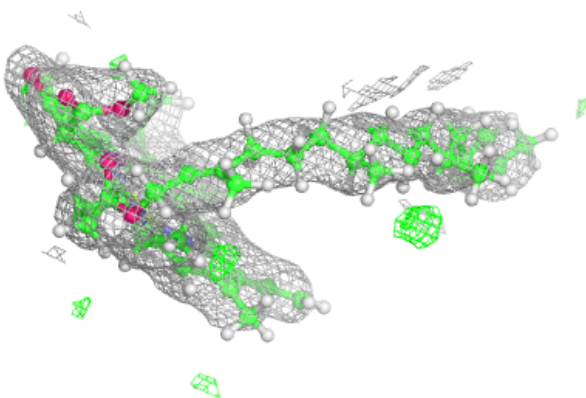
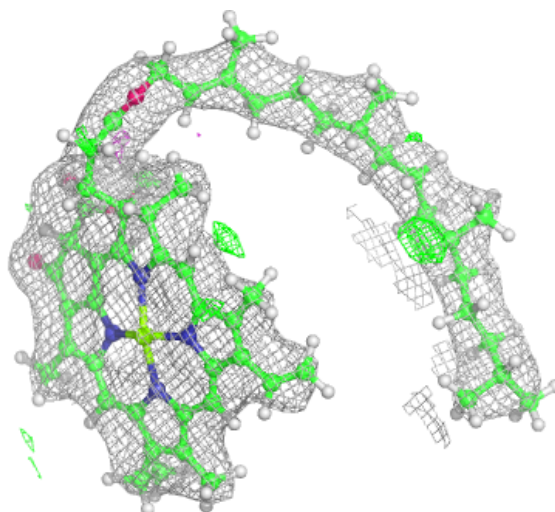
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





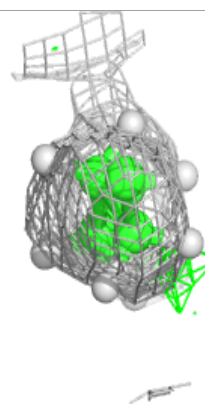
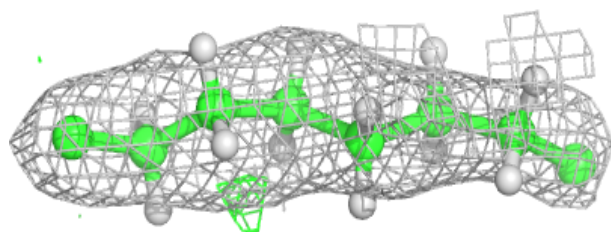
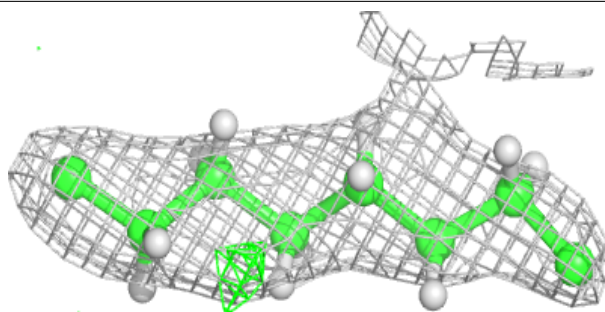
**Electron density around CLA c 509:**

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

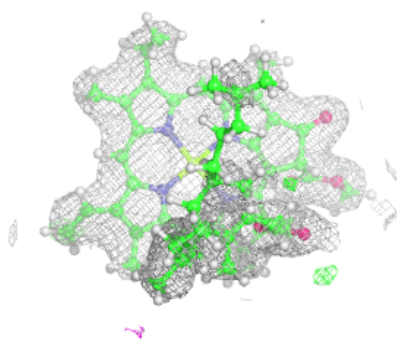
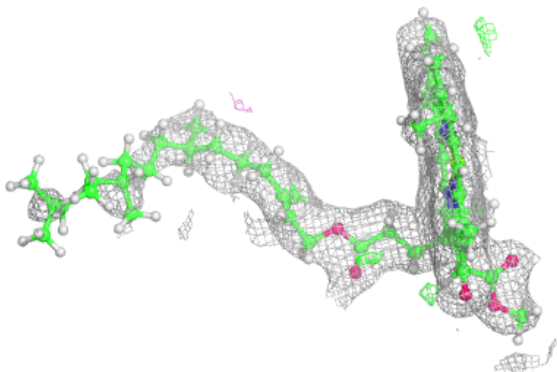
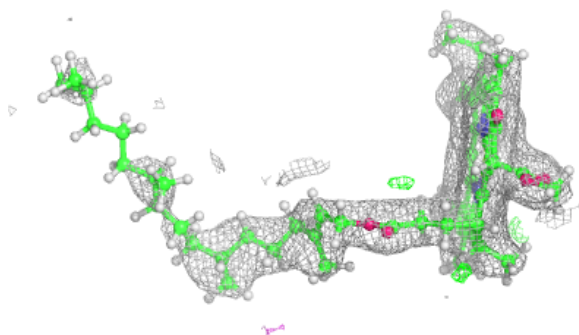


**Electron density around STE Z 102:**

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

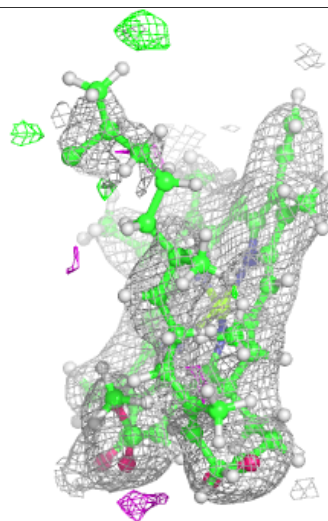
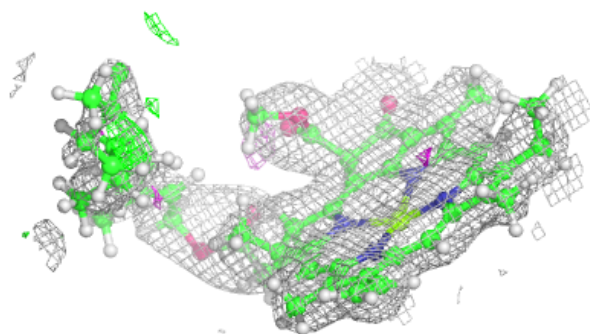
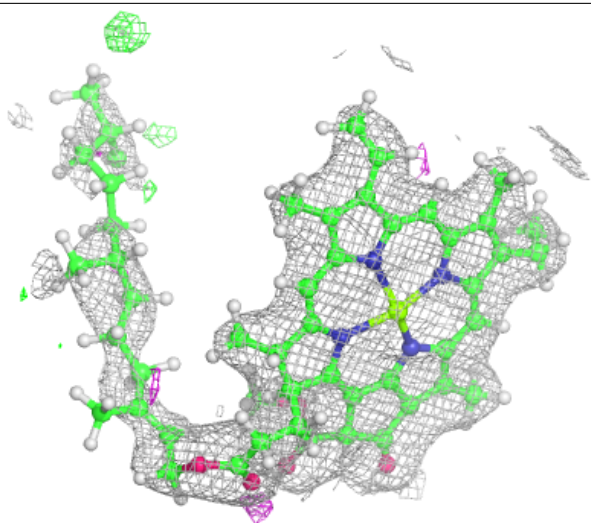
**Electron density around CLA D 403:**

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



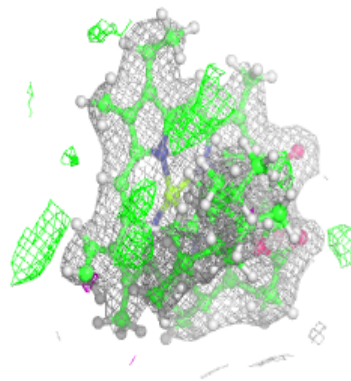
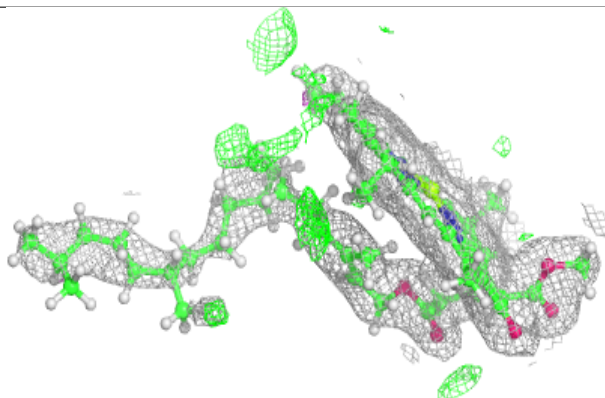
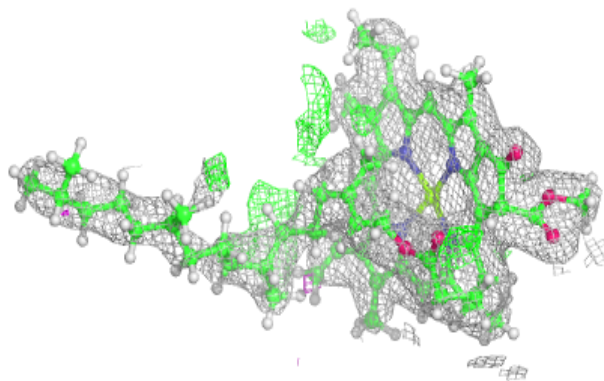
**Electron density around CLA b 615:**

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

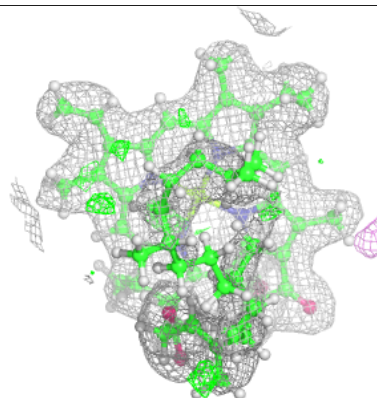
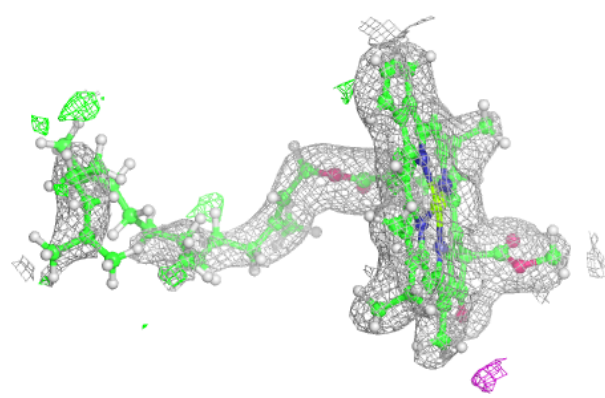
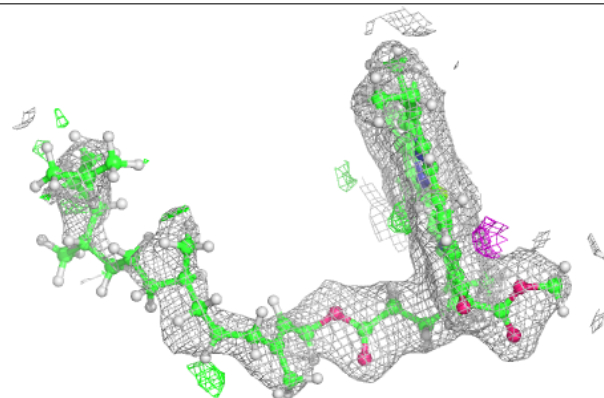


**Electron density around CLA C 506:**

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

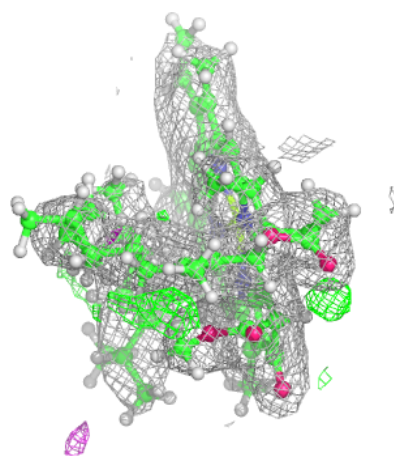
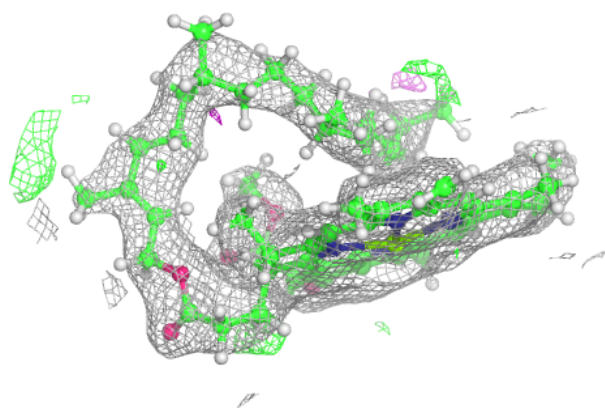
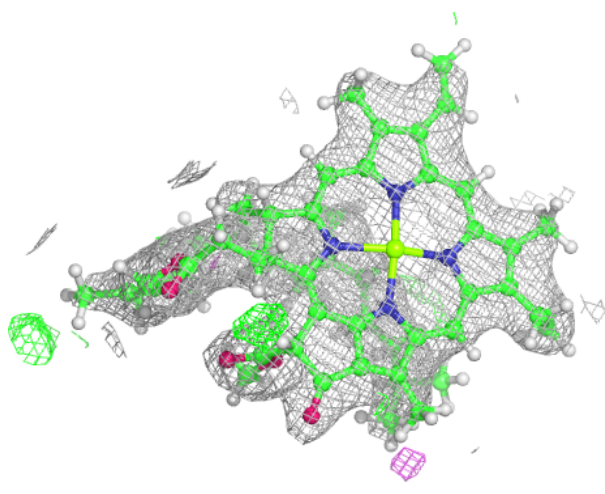
**Electron density around CLA C 507:**

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



**Electron density around CLA c 512:**

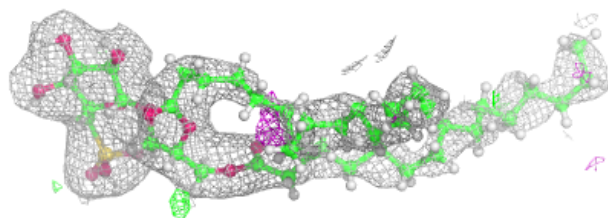
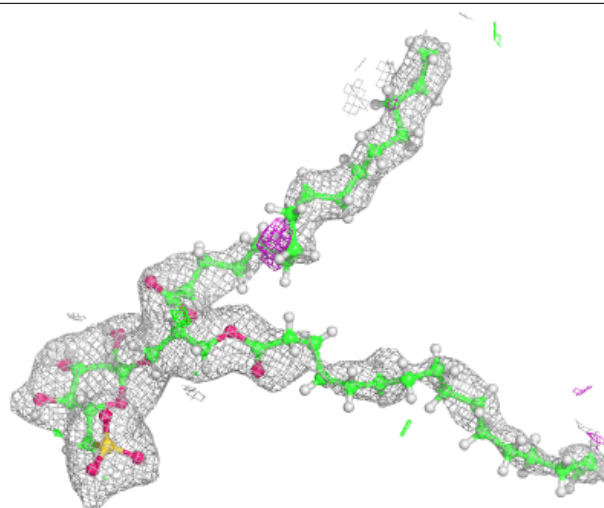
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





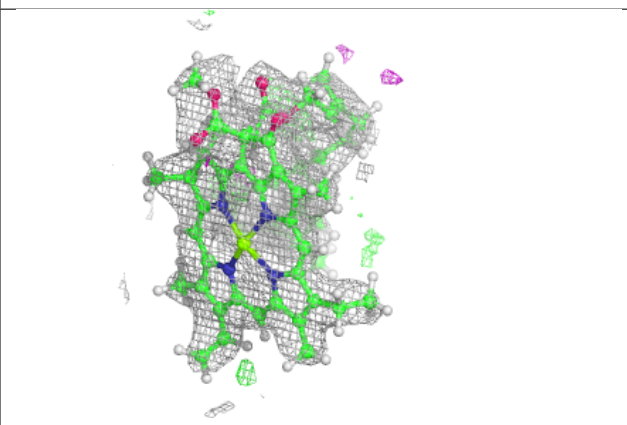
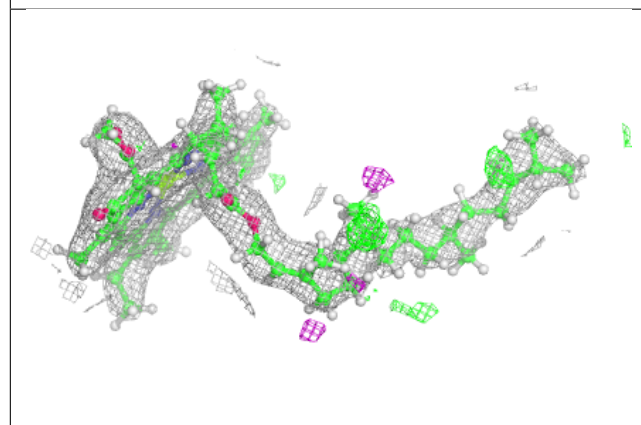
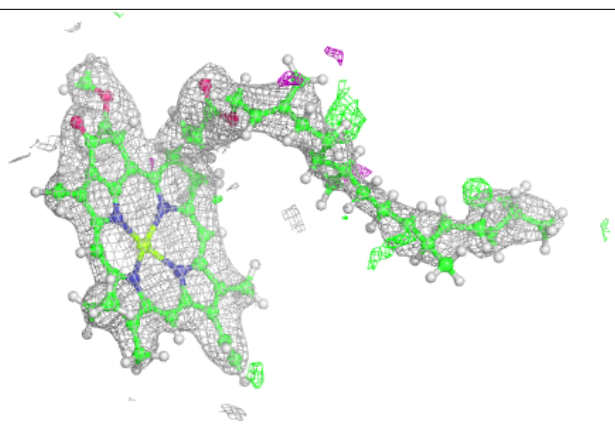
**Electron density around SQD a 412:**

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

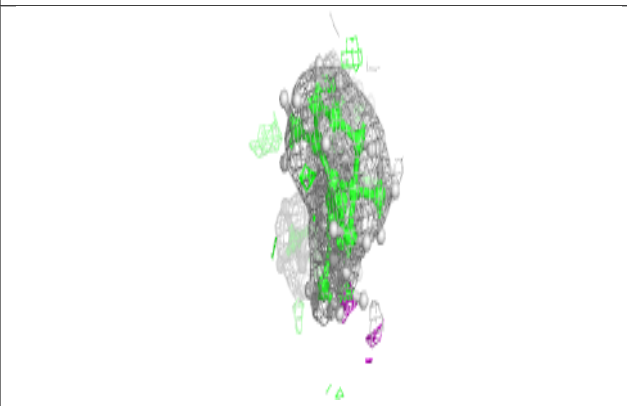
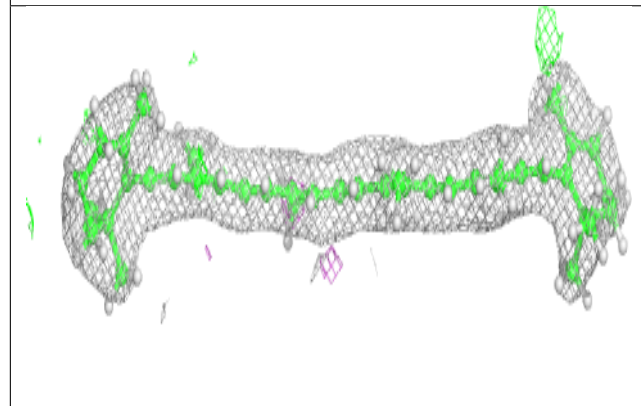
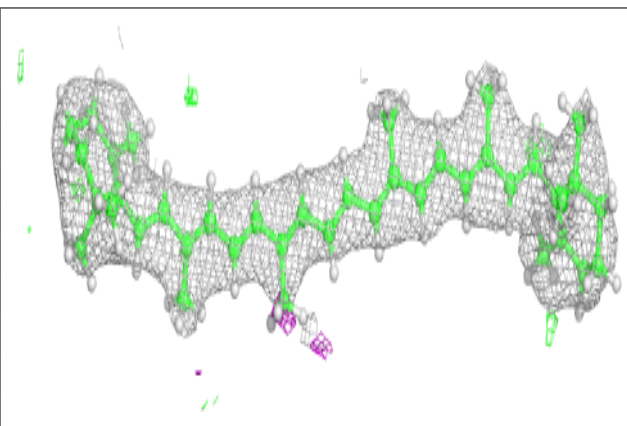


**Electron density around CLA c 513:**

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

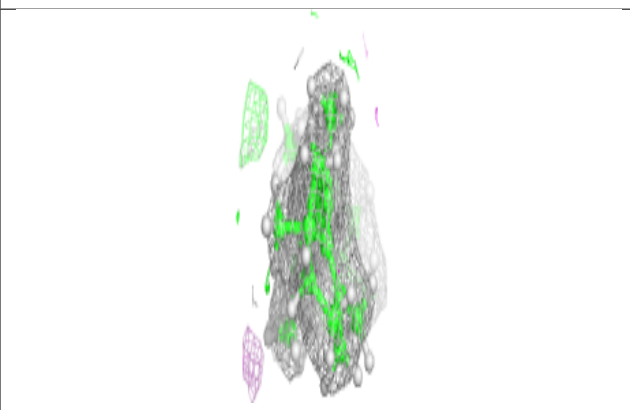
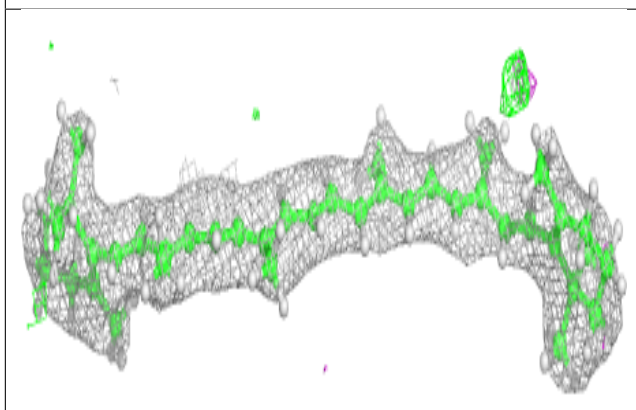
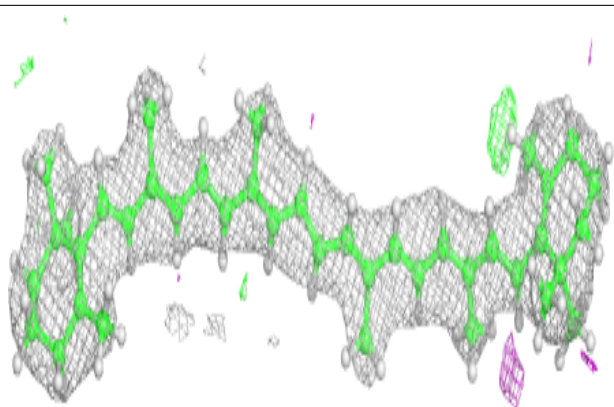
**Electron density around BCR b 617:**

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

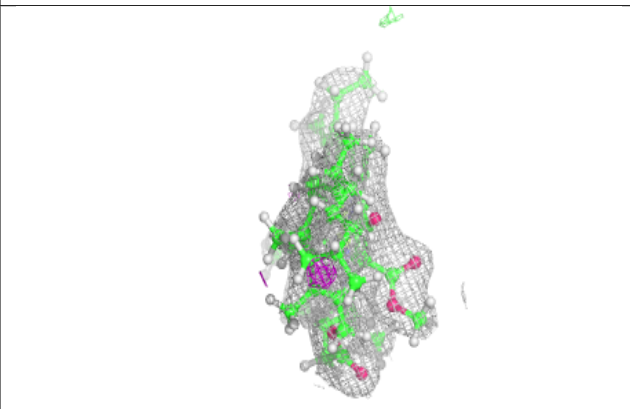
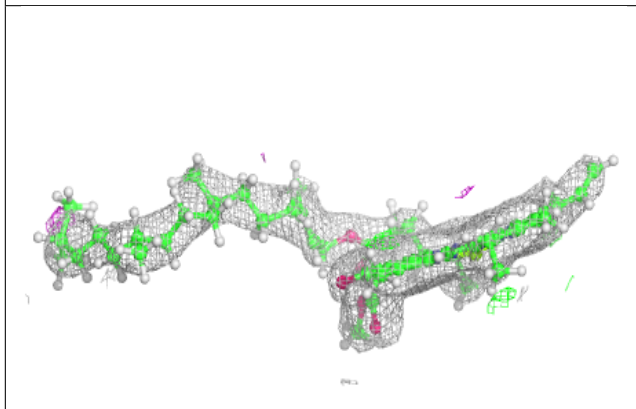
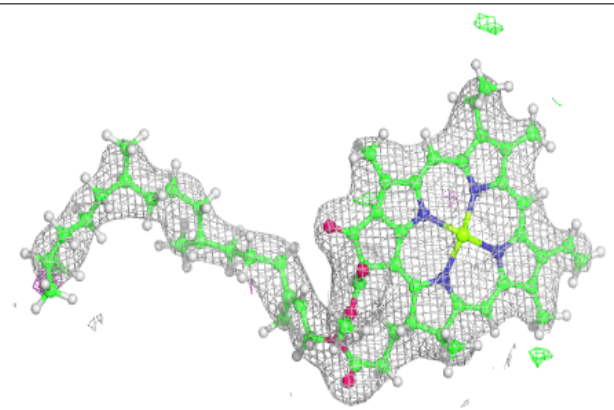


**Electron density around BCR b 618:**

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

**Electron density around CLA b 601:**

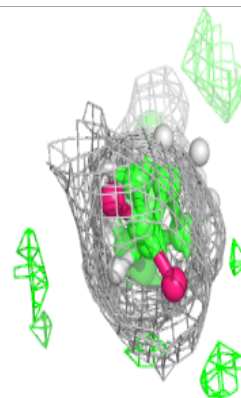
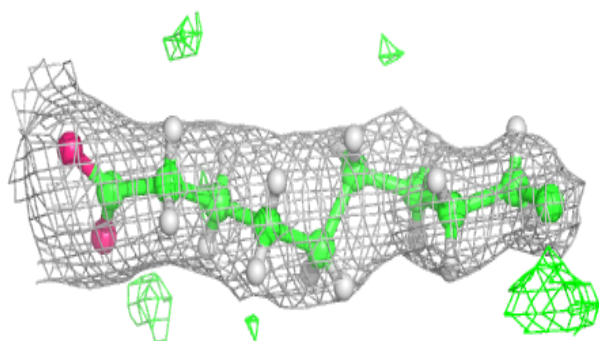
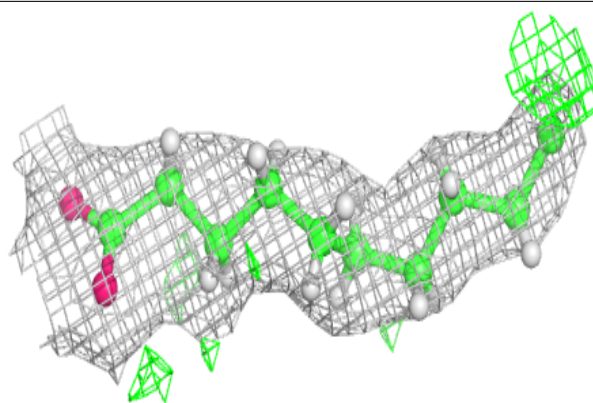
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



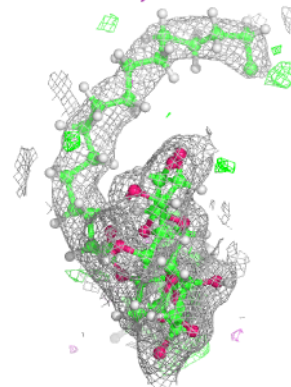
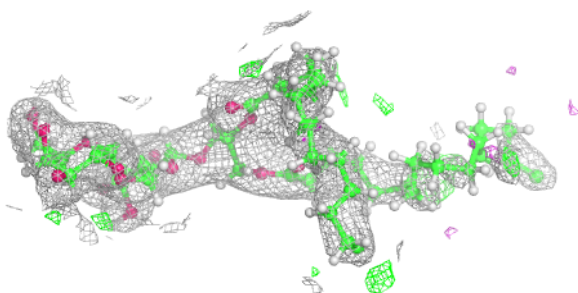
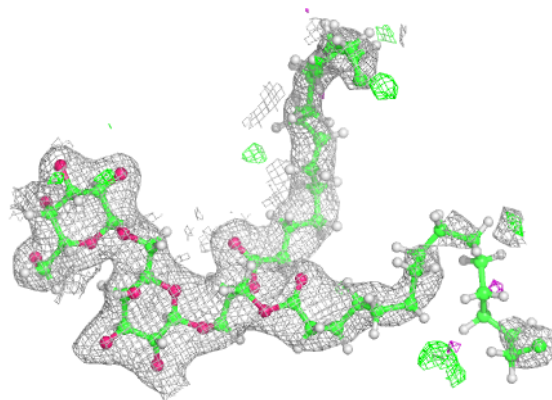


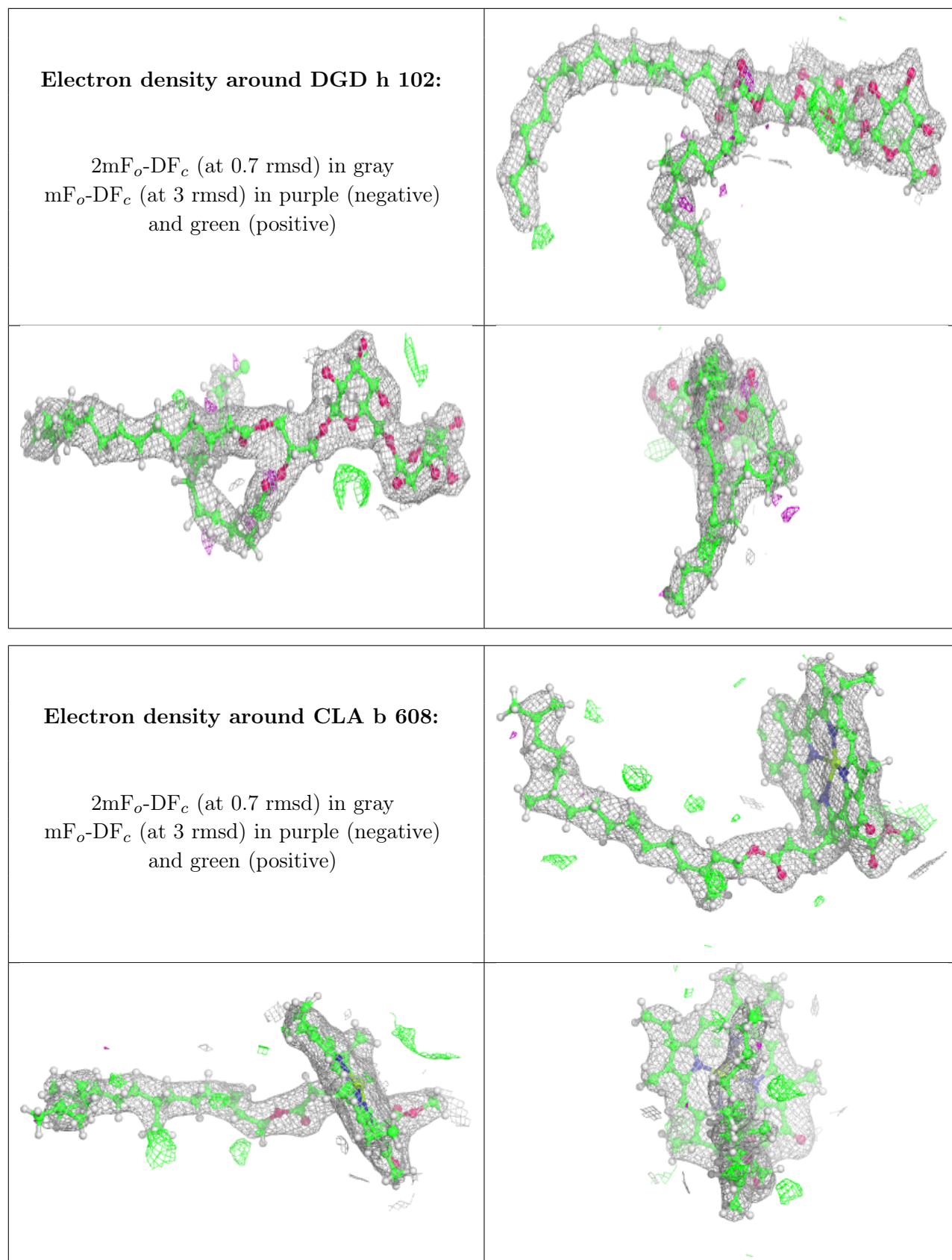
**Electron density around STE J 101:**

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

**Electron density around DGD C 517:**

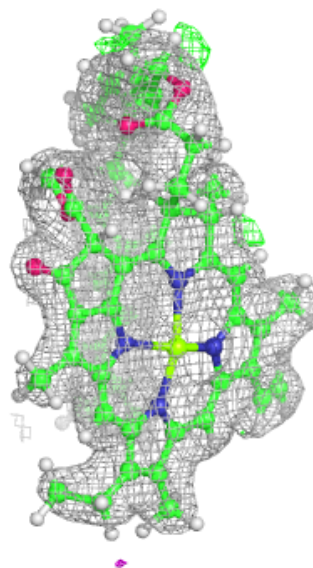
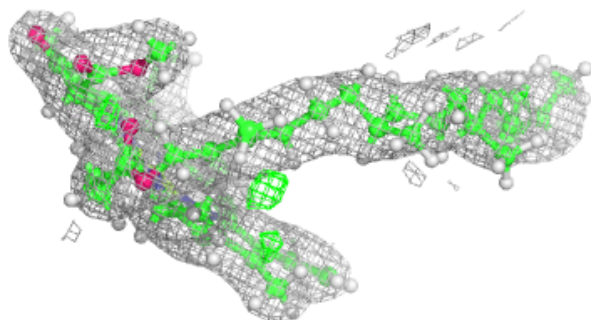
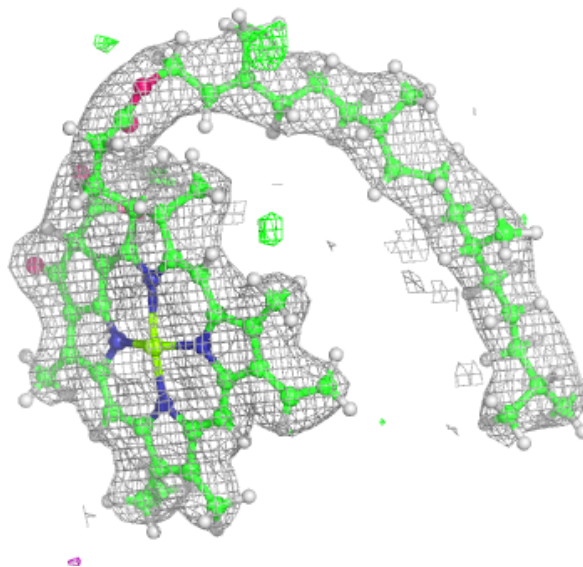
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





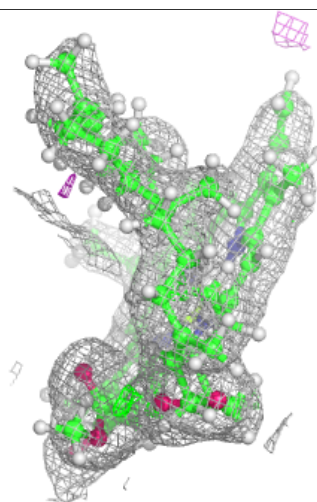
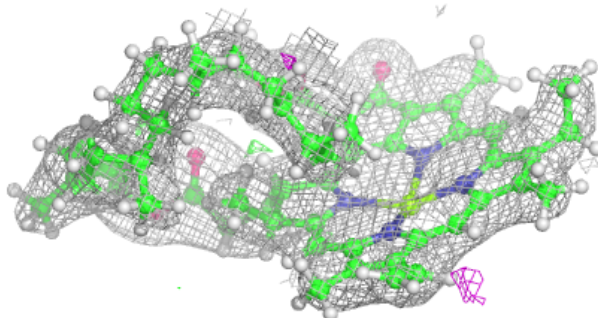
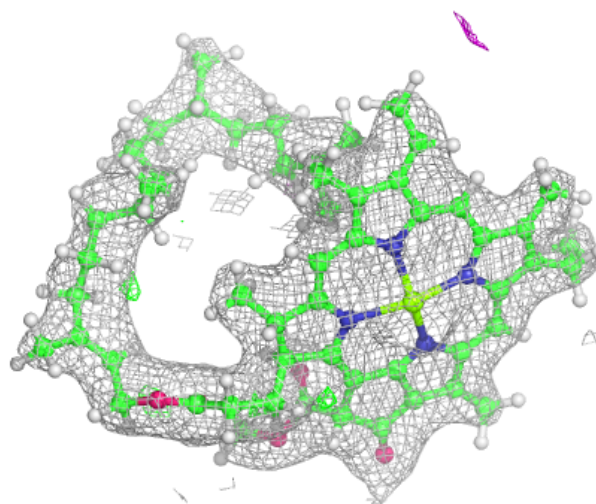
**Electron density around CLA C 508:**

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



**Electron density around CLA B 616:**

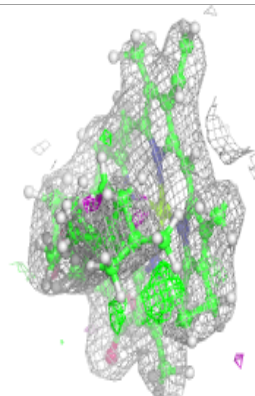
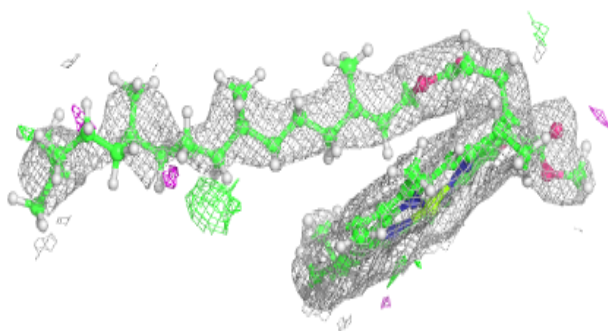
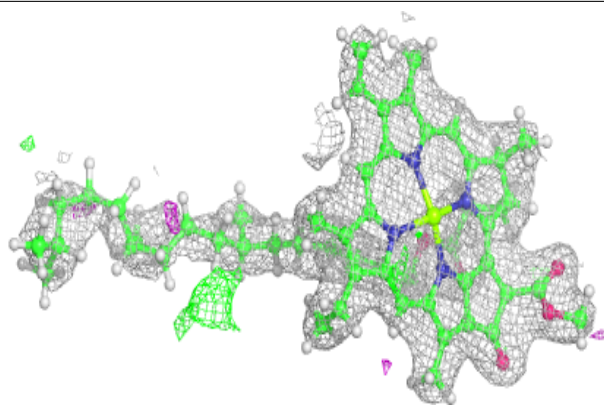
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



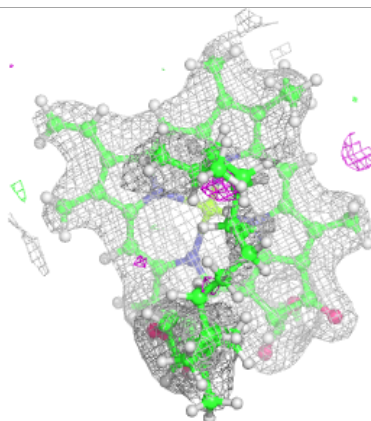
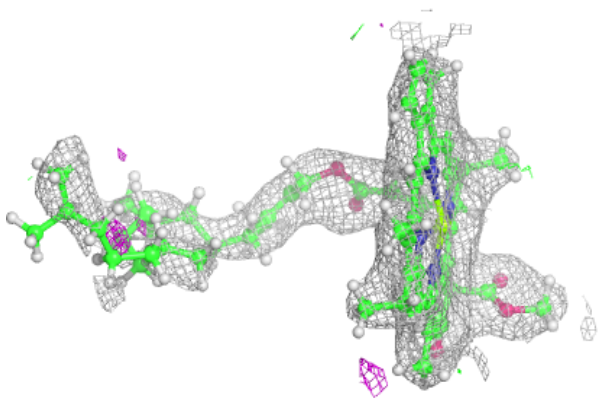
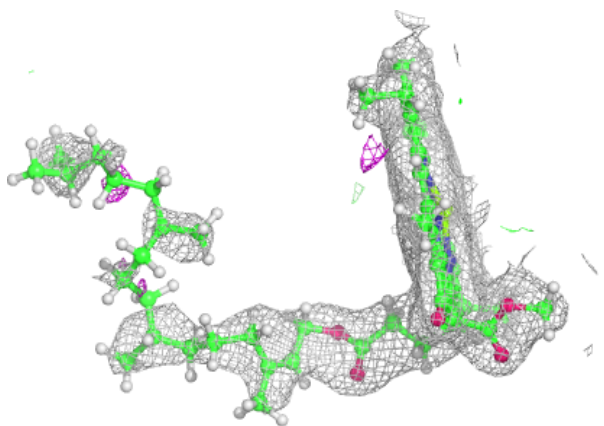


**Electron density around CLA B 615:**

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

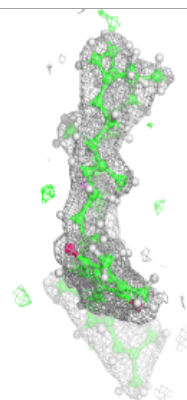
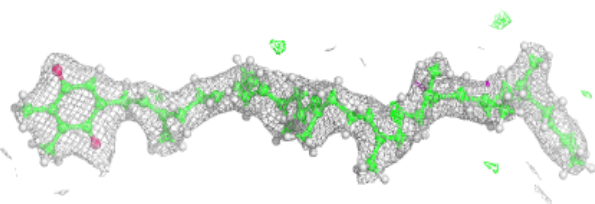
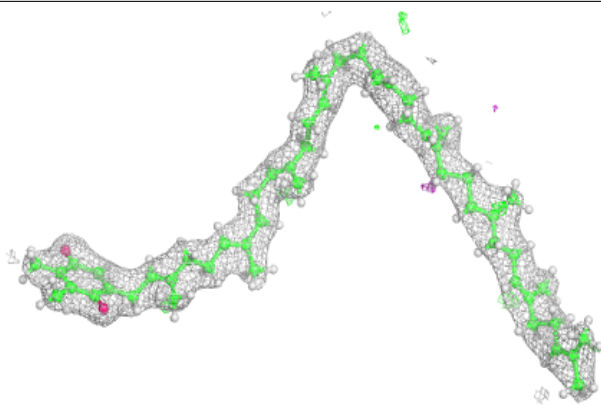
**Electron density around CLA c 508:**

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



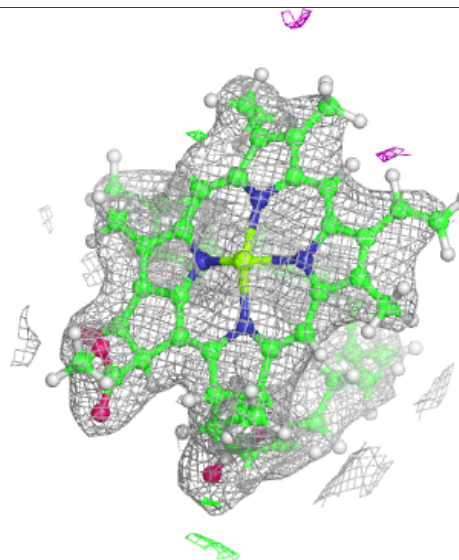
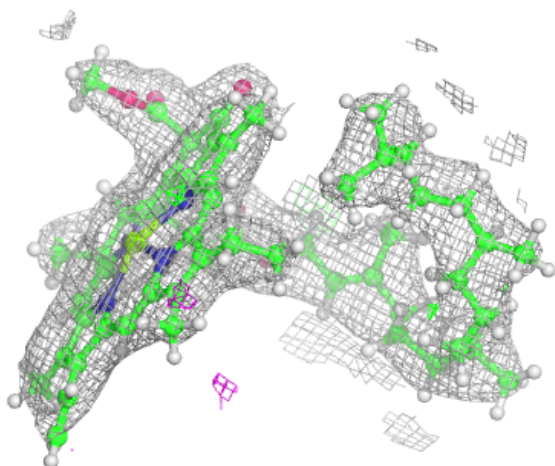
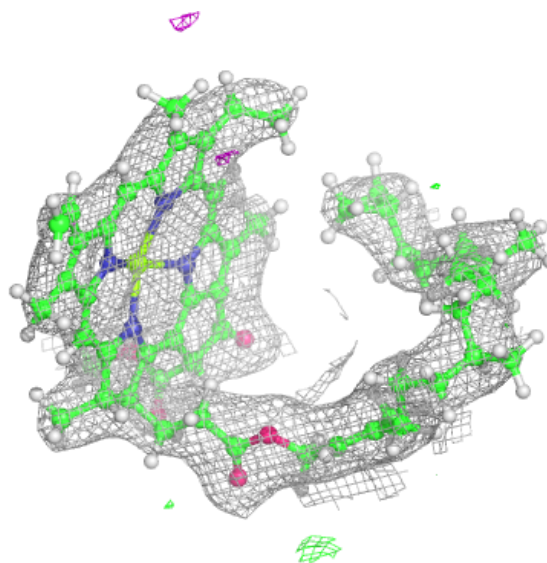
**Electron density around PL9 D 405:**

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



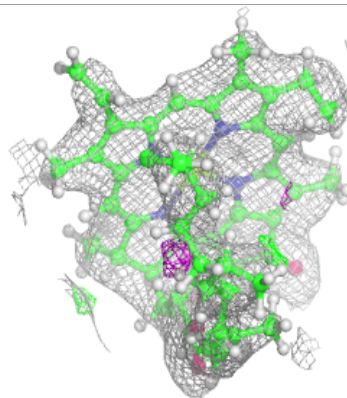
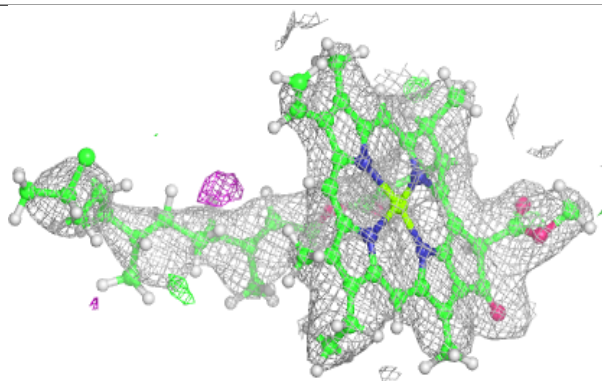
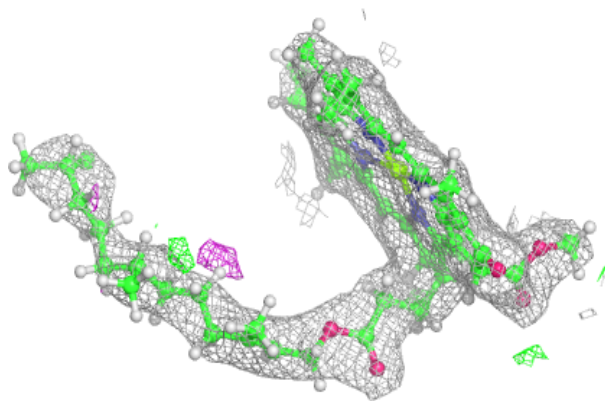
**Electron density around CLA c 505:**

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

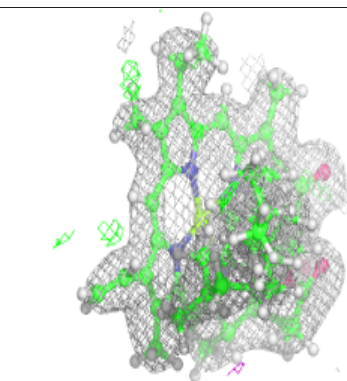
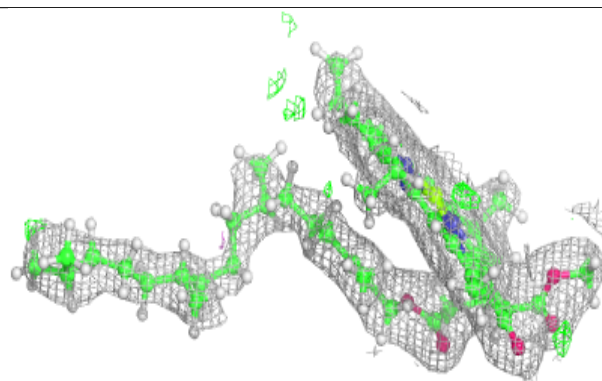
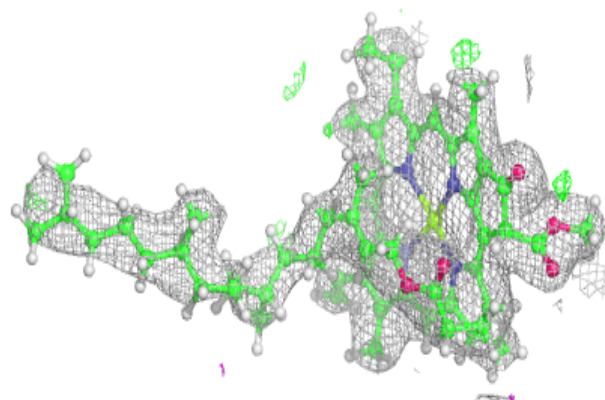


**Electron density around CLA c 506:**

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

**Electron density around CLA c 507:**

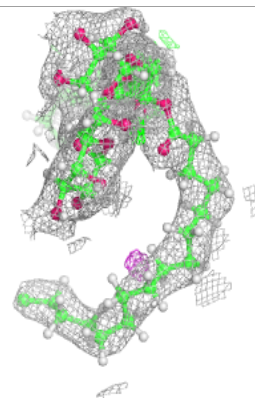
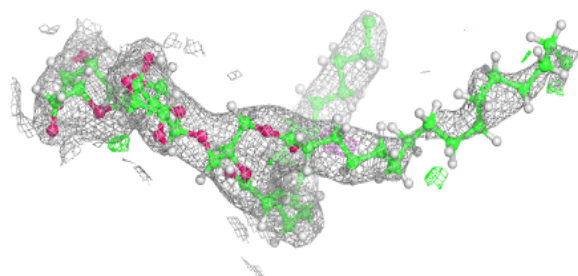
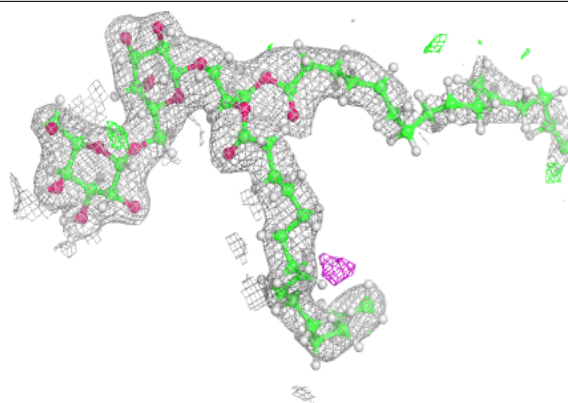
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



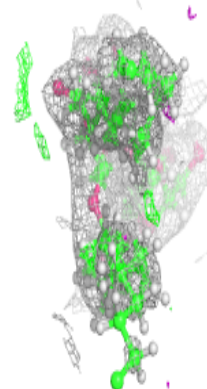
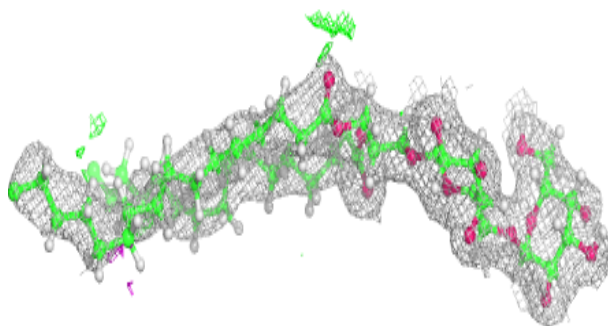
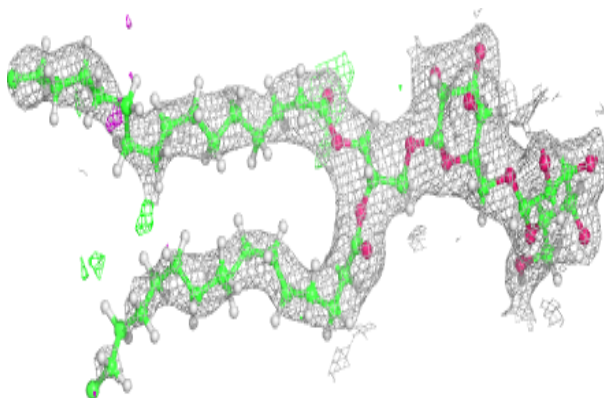


**Electron density around DGD c 520:**

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

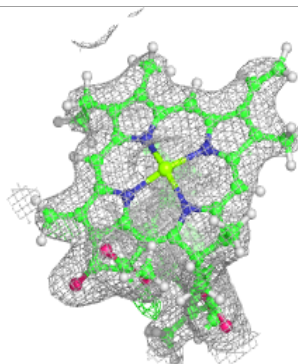
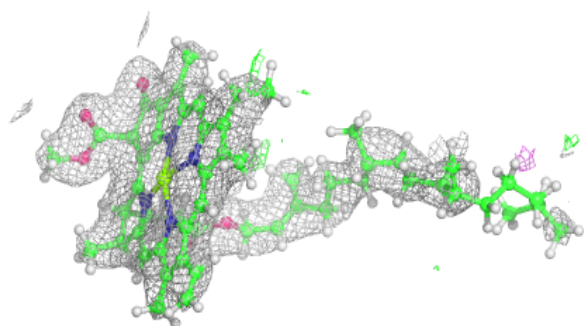
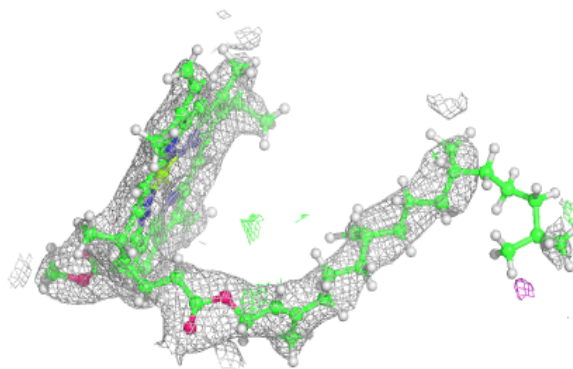
**Electron density around DGD c 521:**

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

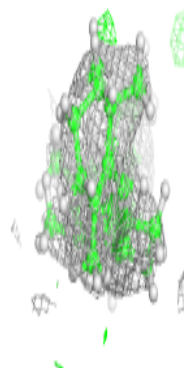
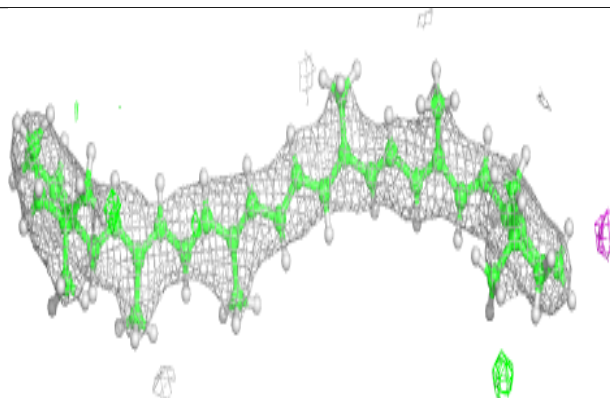
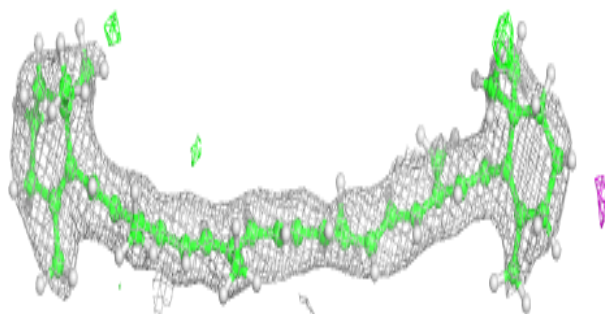


**Electron density around CLA C 509:**

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

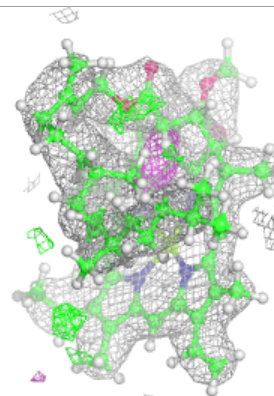
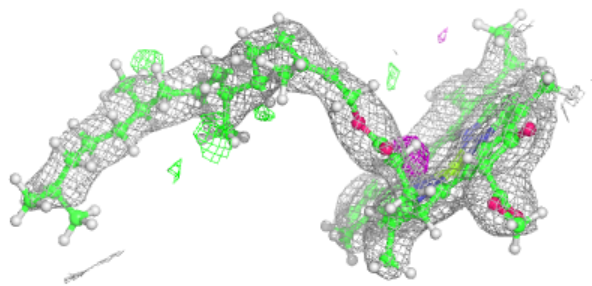
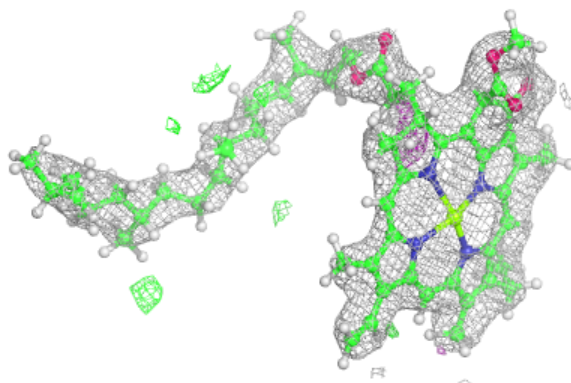
**Electron density around BCR K 101:**

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

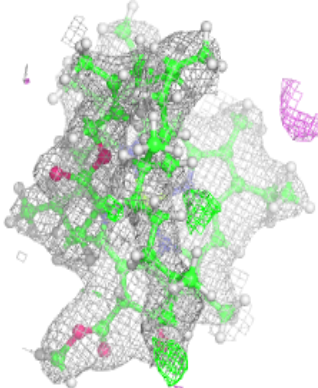
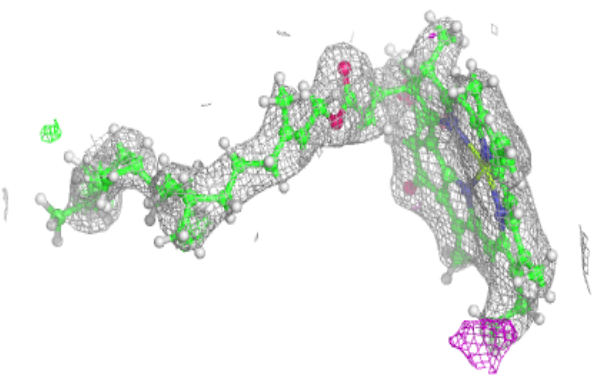
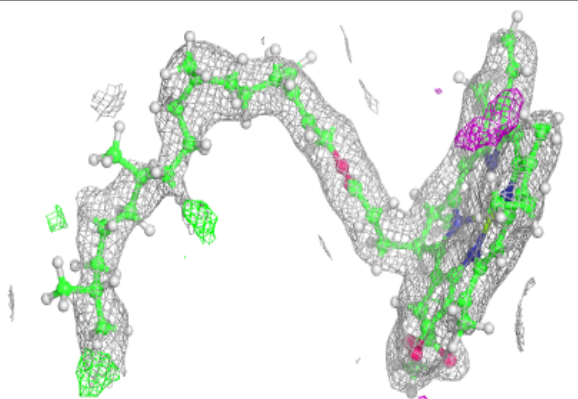


**Electron density around CLA C 512:**

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

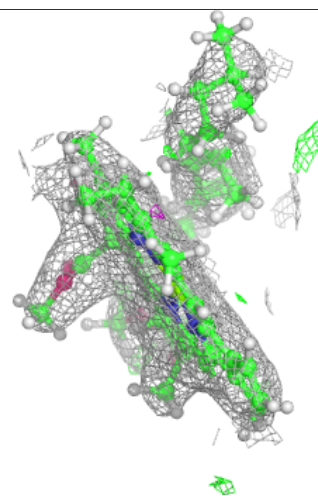
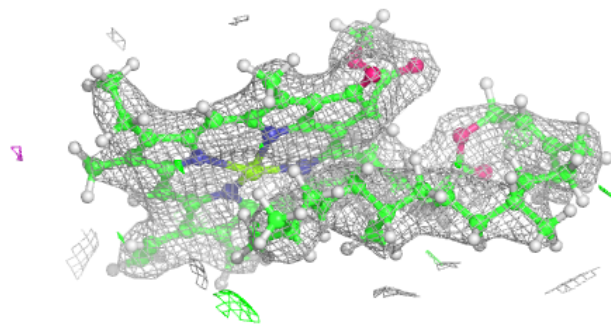
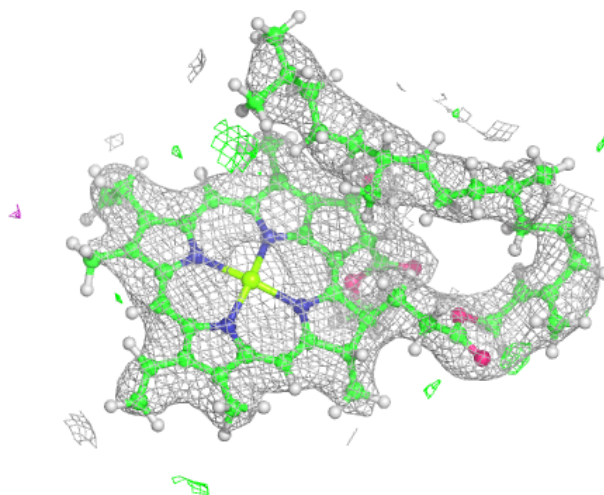
**Electron density around CLA b 605:**

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



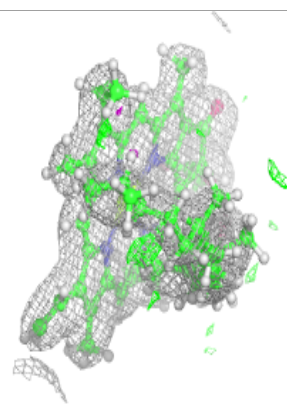
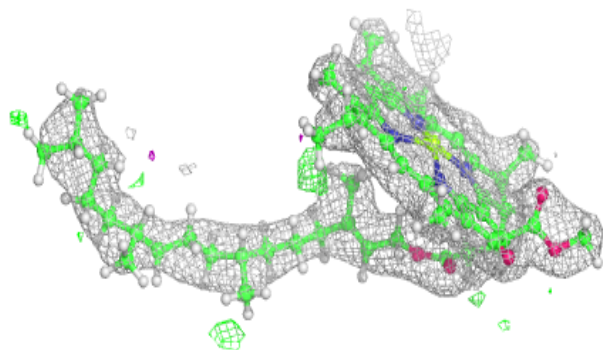
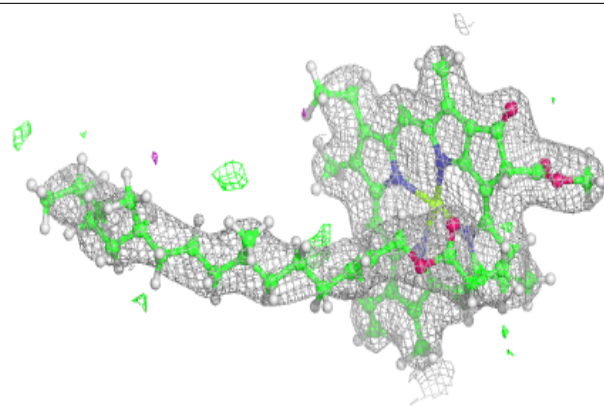
**Electron density around CLA c 511:**

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



**Electron density around CLA b 607:**

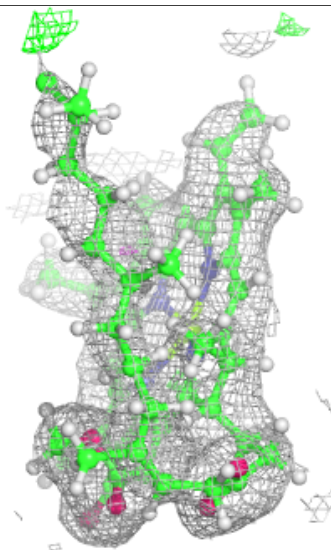
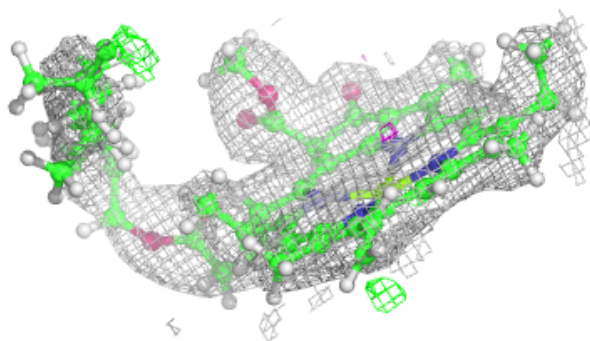
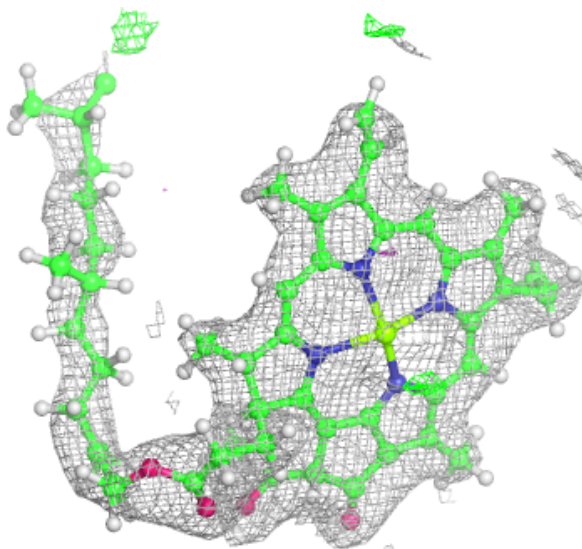
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





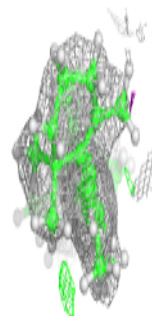
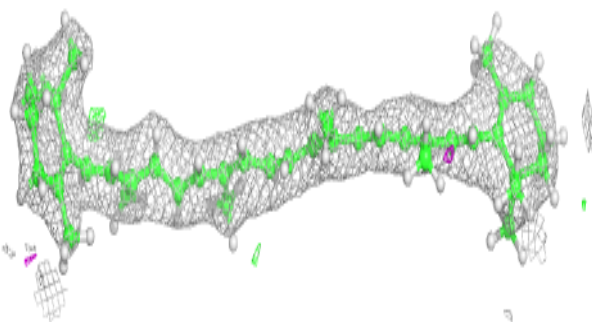
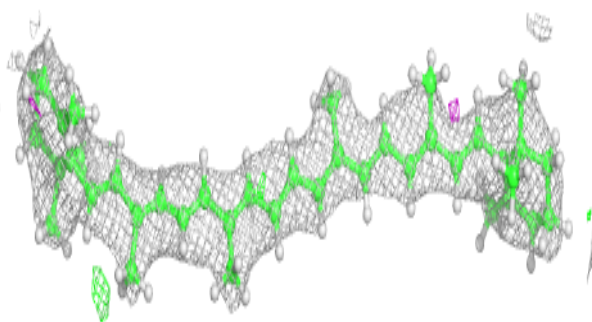
**Electron density around CLA B 617:**

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

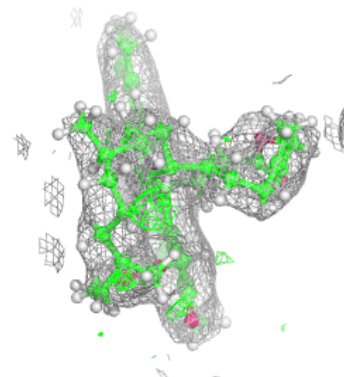
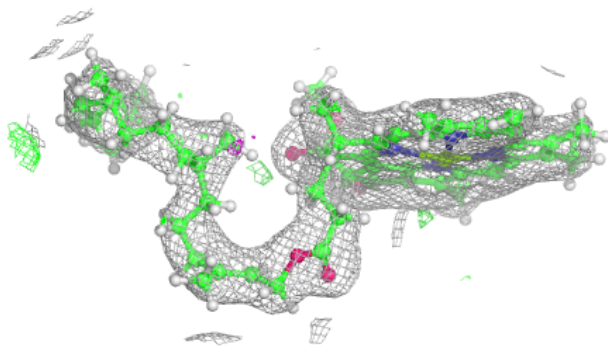
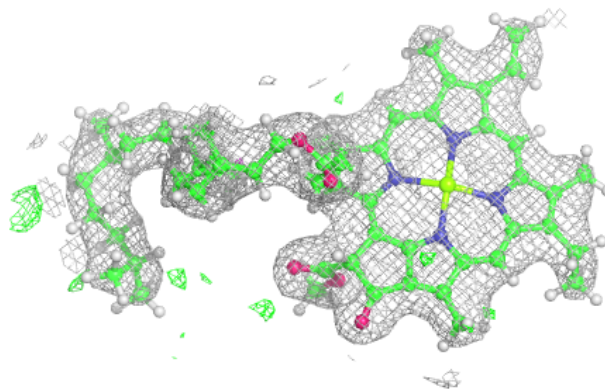


**Electron density around BCR c 517:**

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

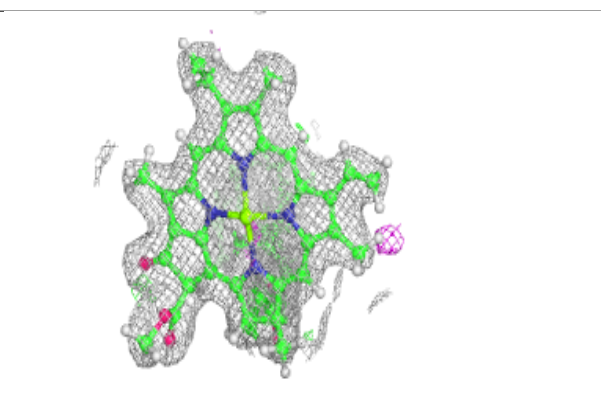
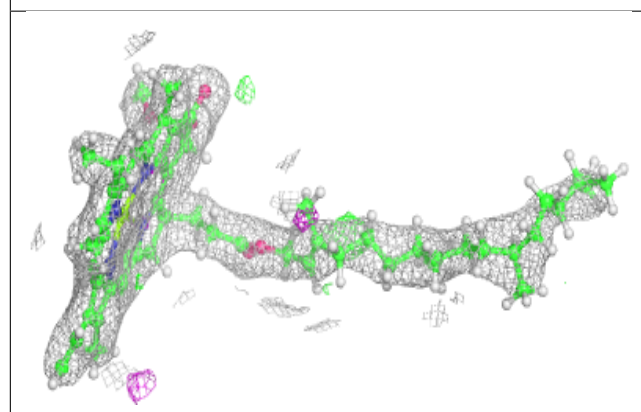
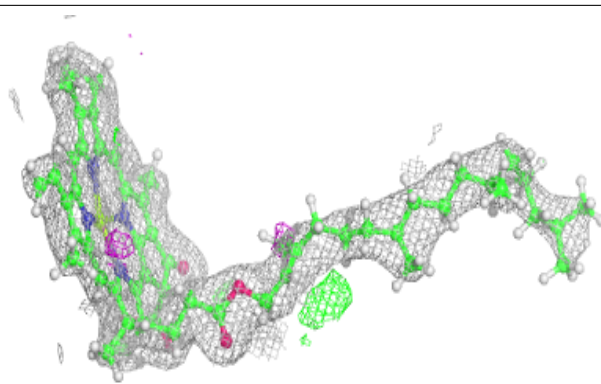
**Electron density around CLA b 611:**

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

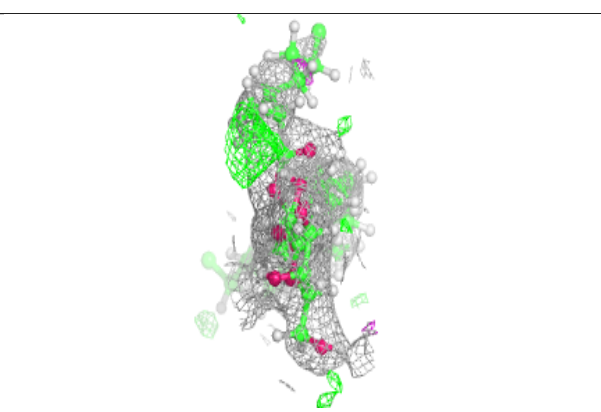
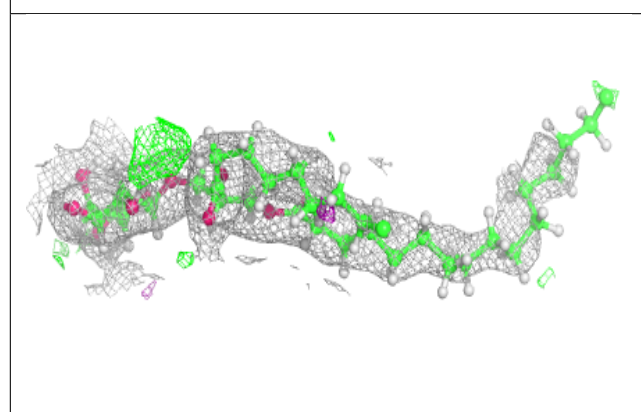
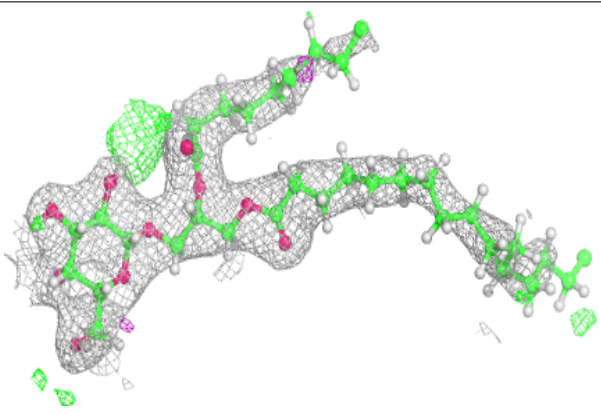


**Electron density around CLA B 605:**

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

**Electron density around LMG d 409:**

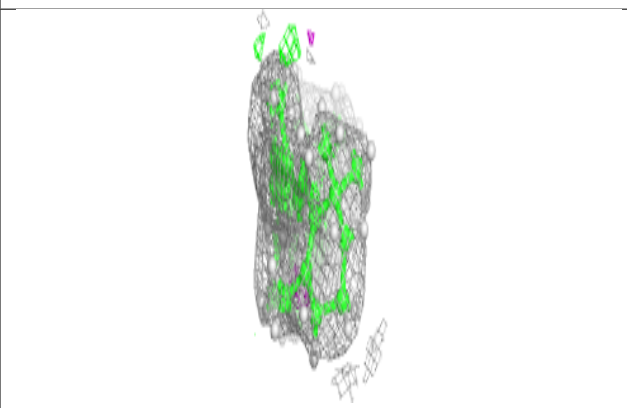
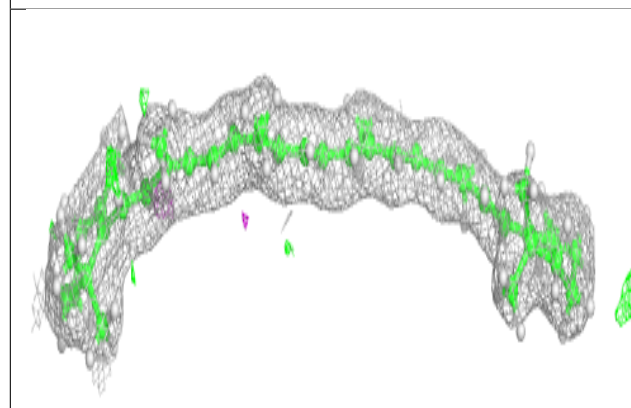
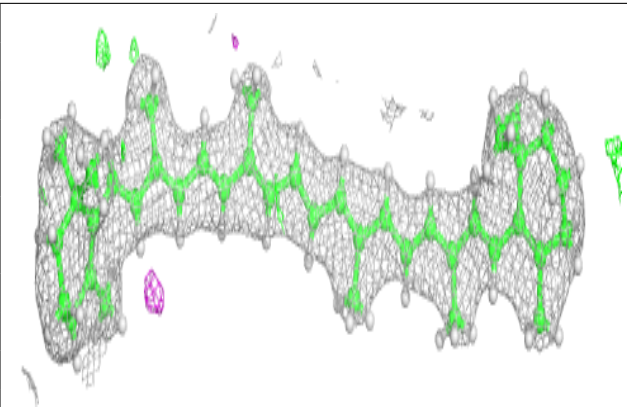
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





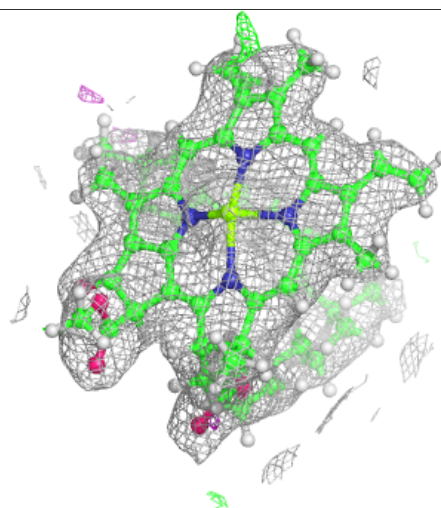
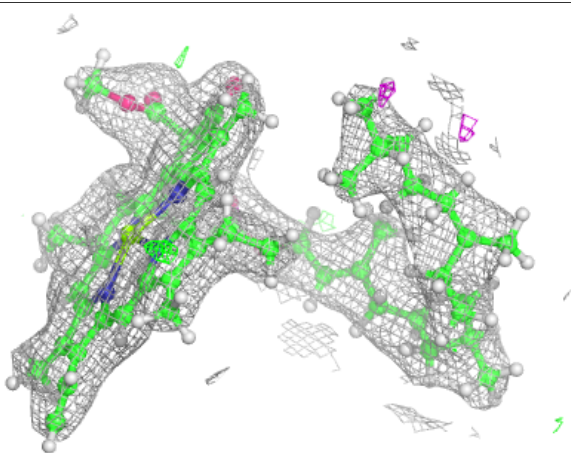
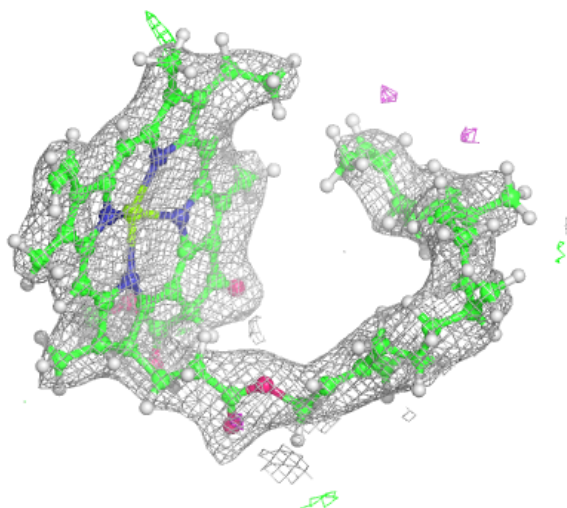
**Electron density around BCR t 101:**

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



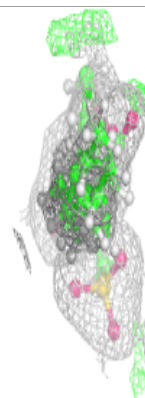
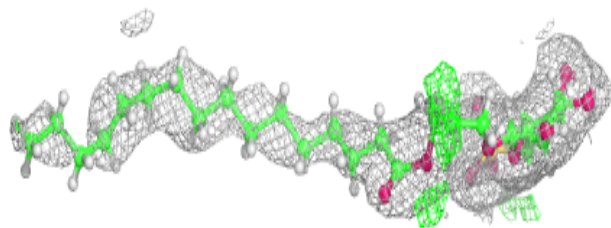
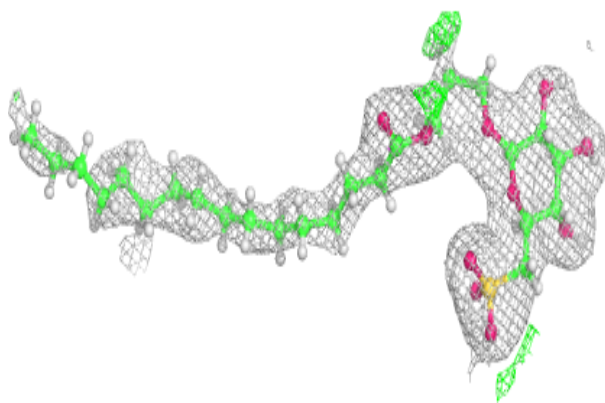
**Electron density around CLA C 504:**

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

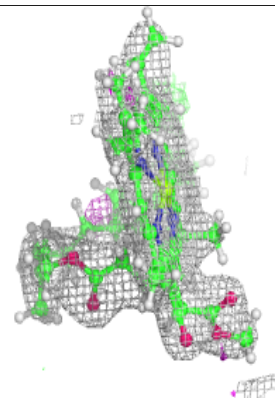
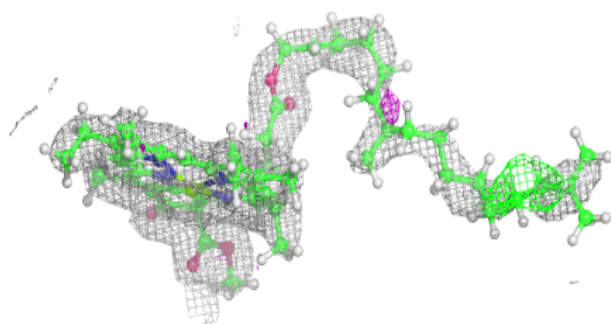
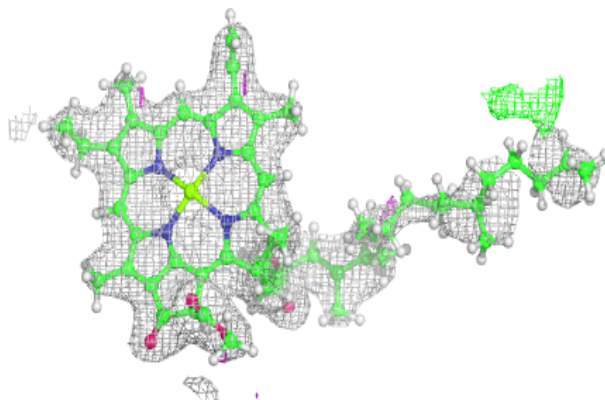


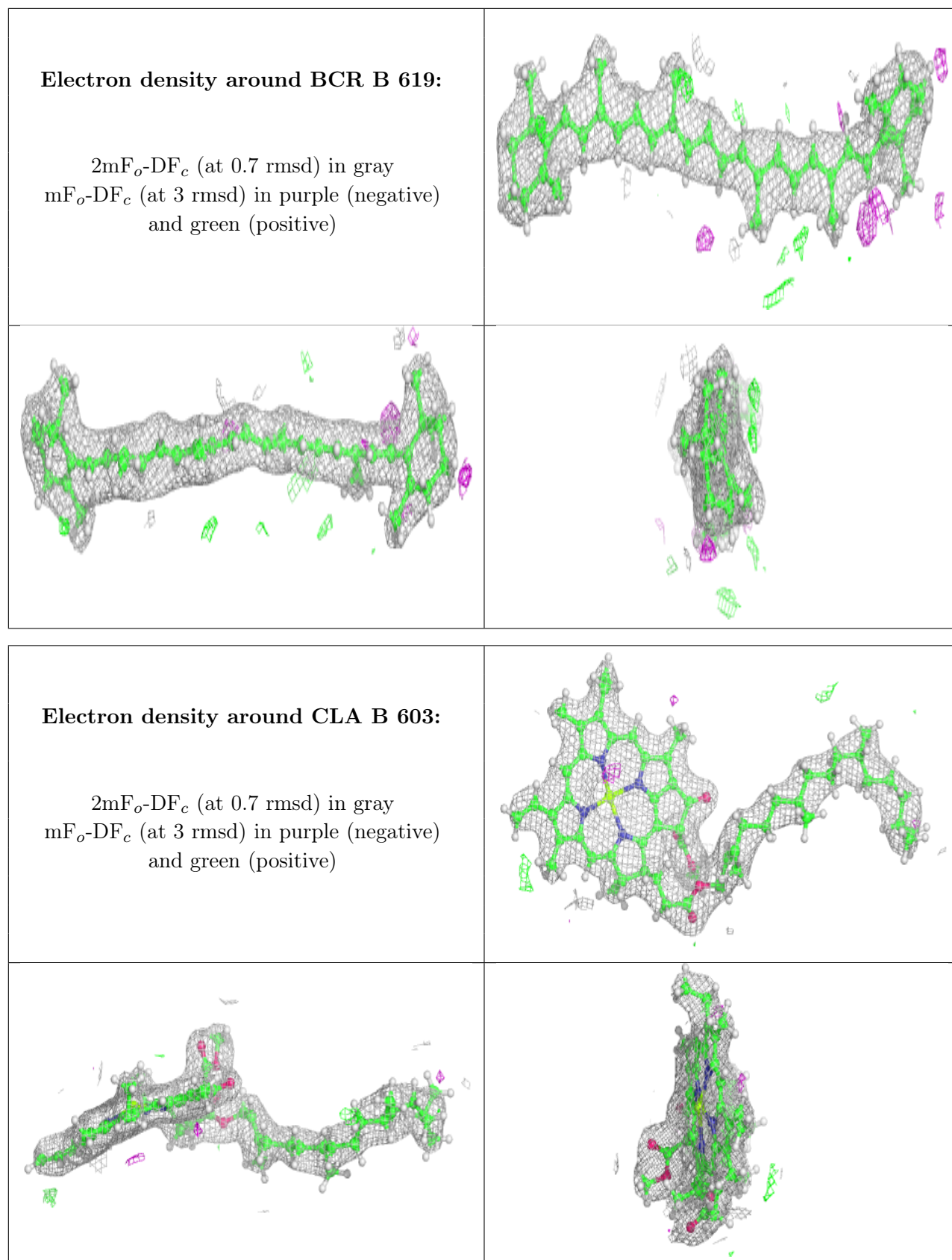
**Electron density around SQD D 407:**

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

**Electron density around CLA a 403:**

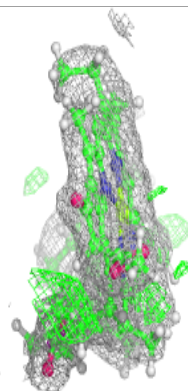
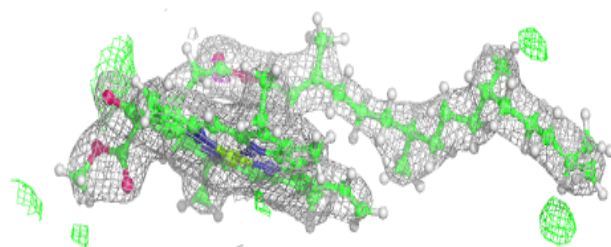
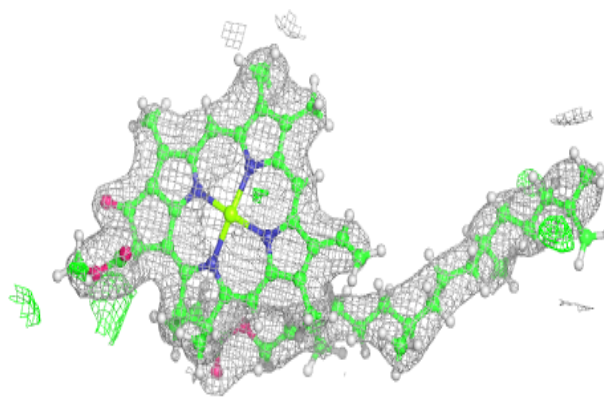
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





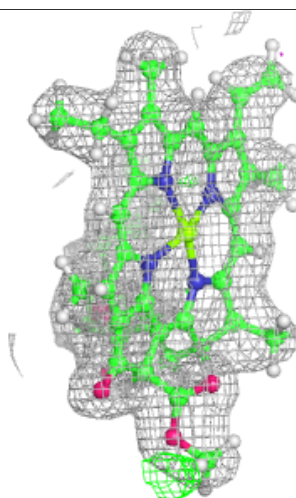
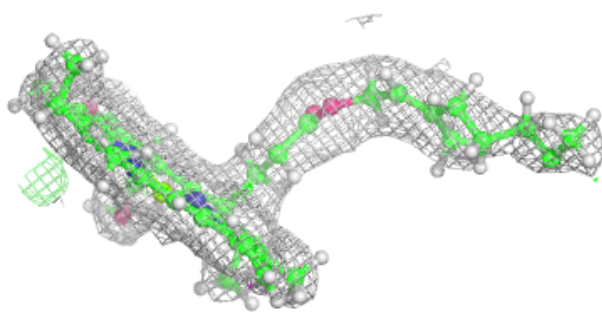
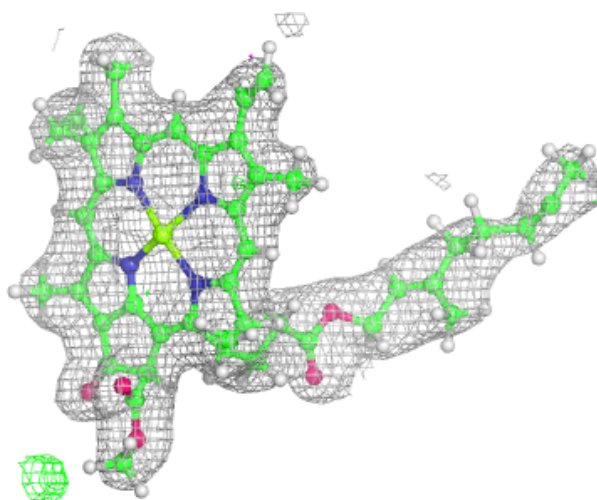
**Electron density around CLA c 503:**

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

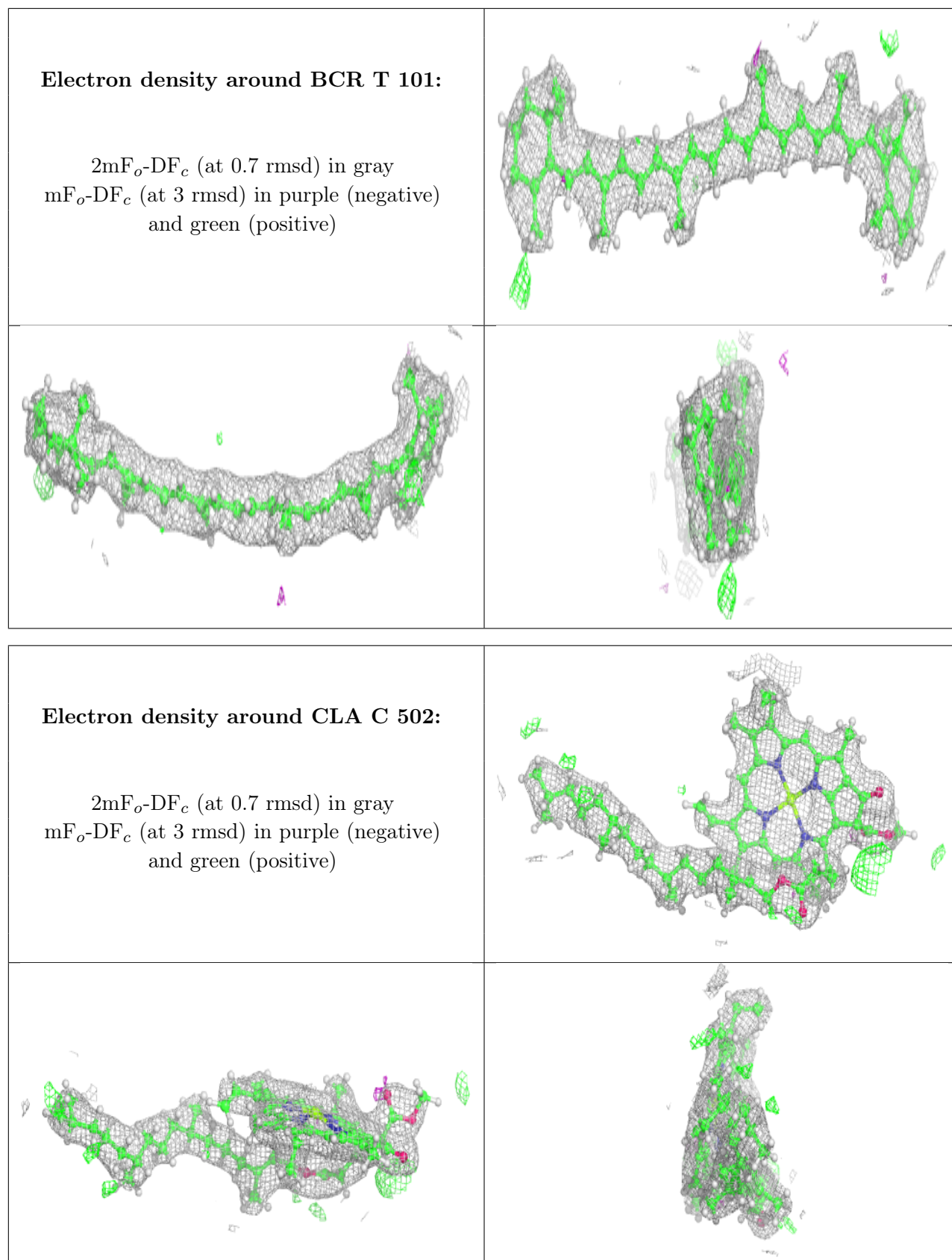


**Electron density around CLA A 405:**

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

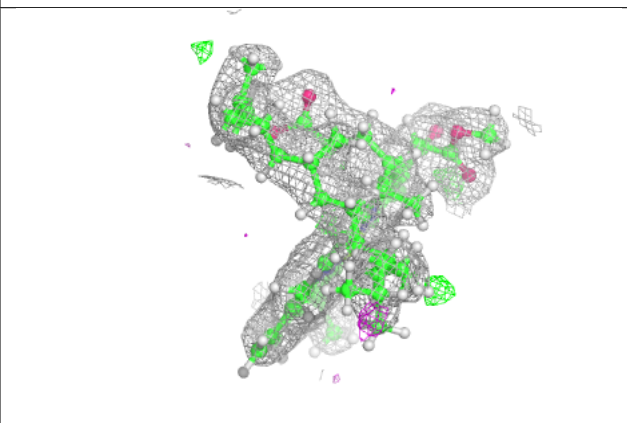
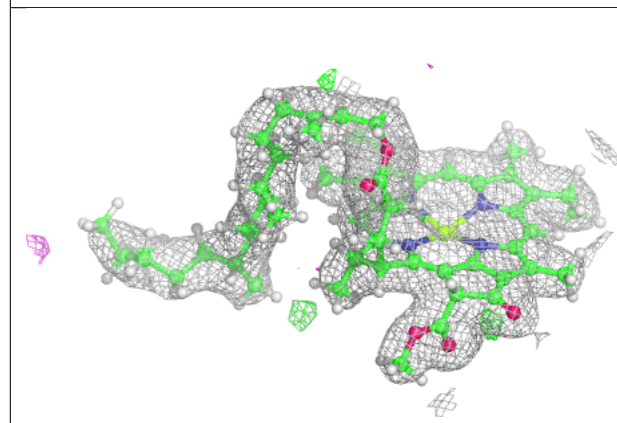
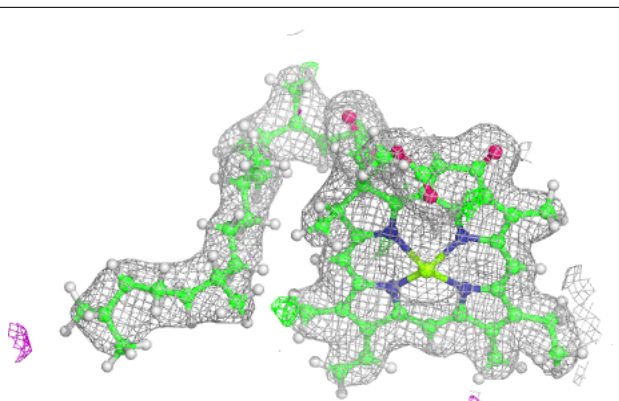




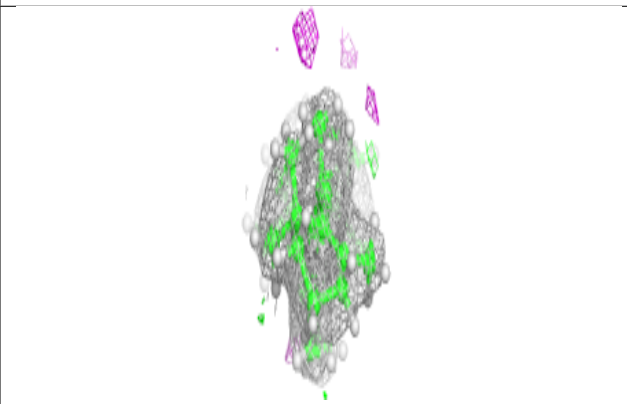
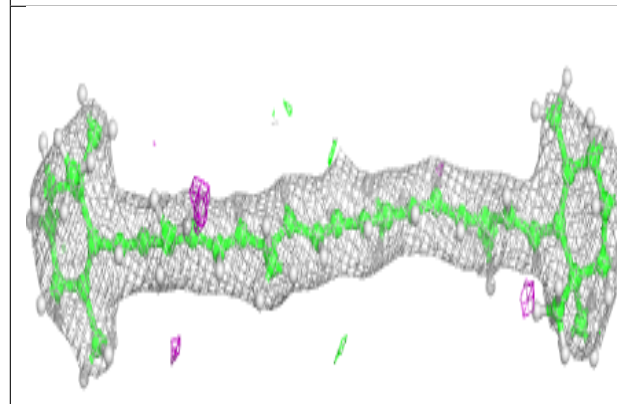
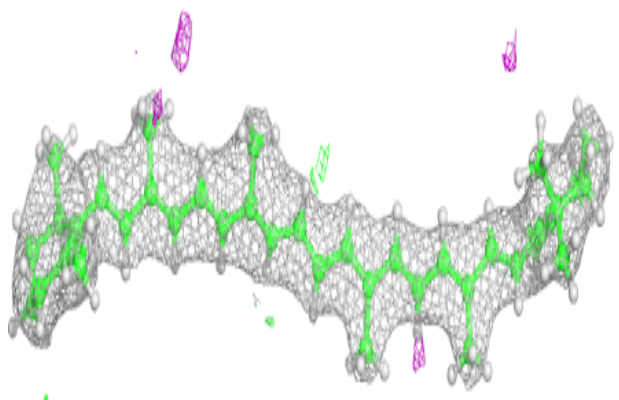


**Electron density around CLA A 411:**

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

**Electron density around BCR a 406:**

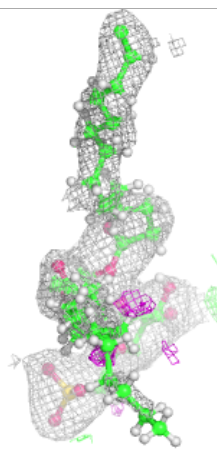
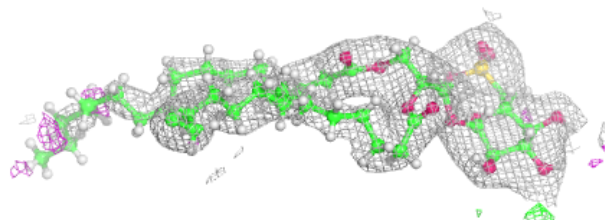
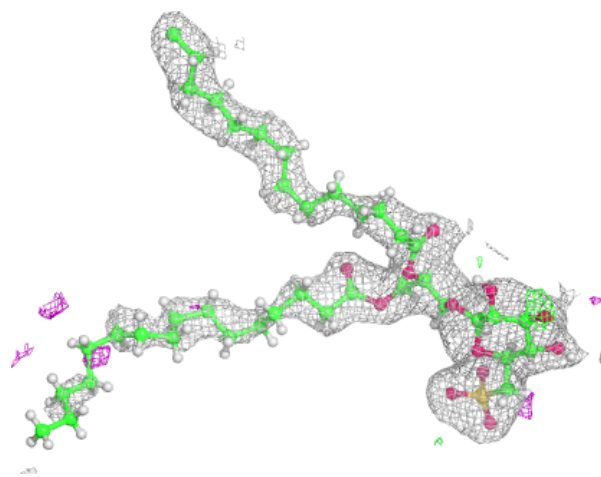
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





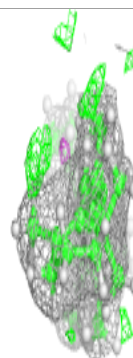
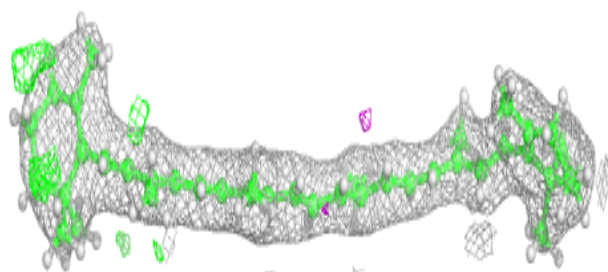
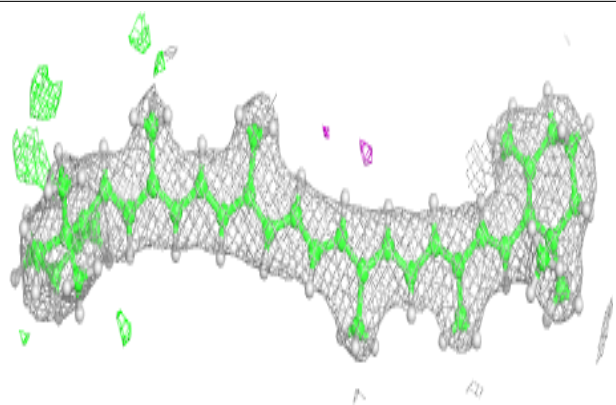
**Electron density around SQD A 413:**

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

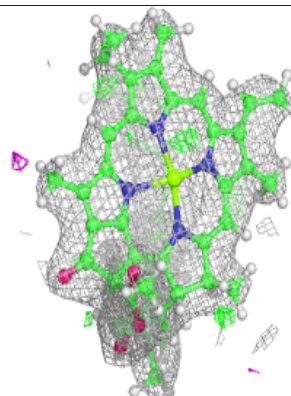
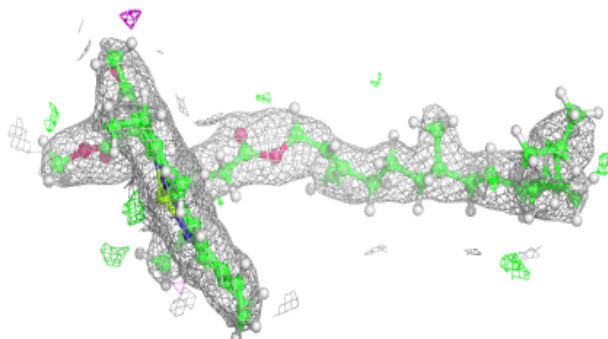
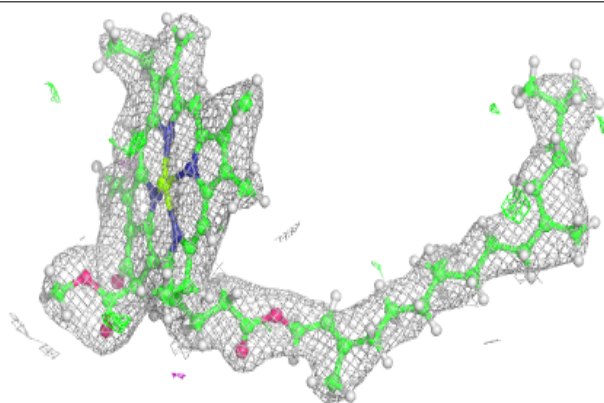


**Electron density around BCR b 616:**

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

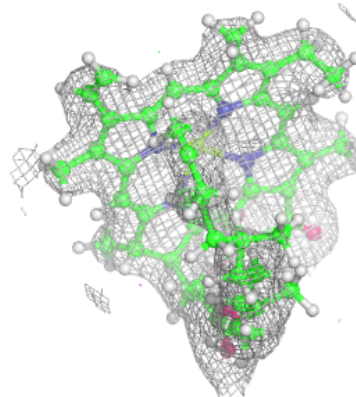
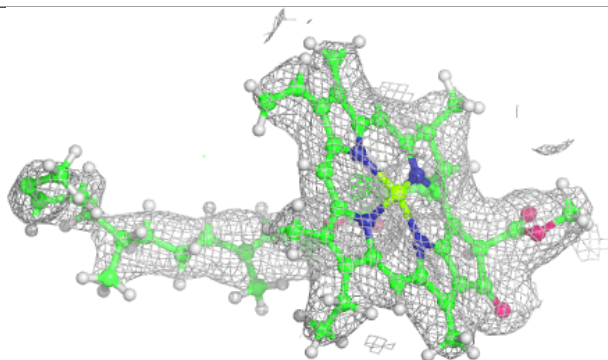
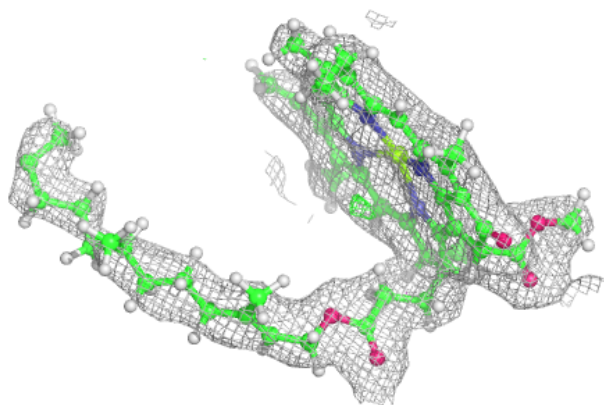
**Electron density around CLA B 610:**

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

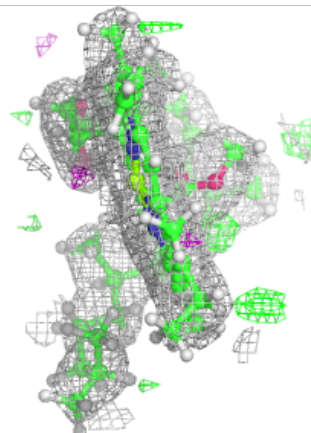
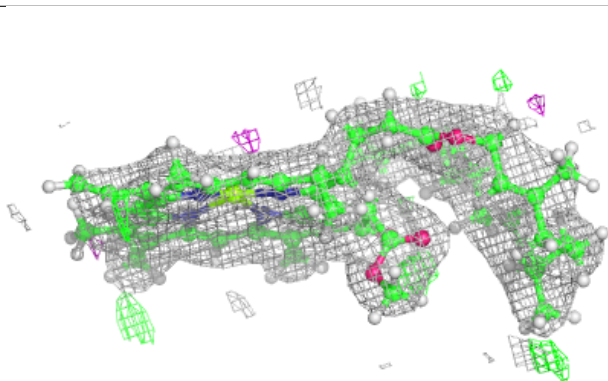
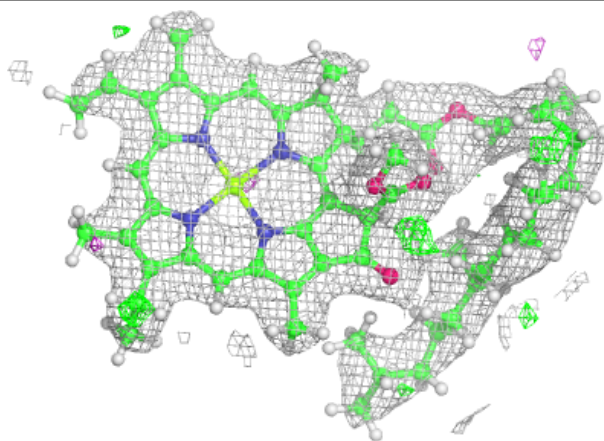


**Electron density around CLA C 505:**

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

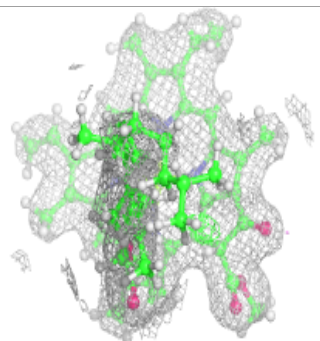
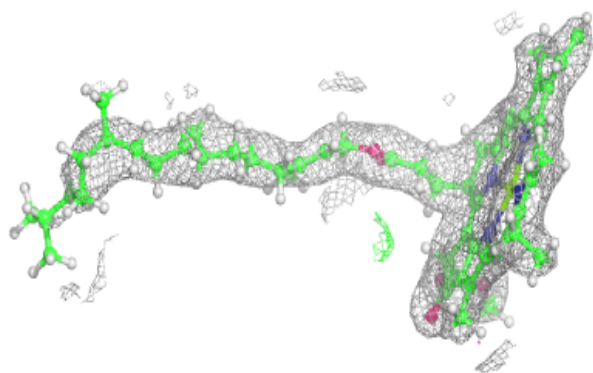
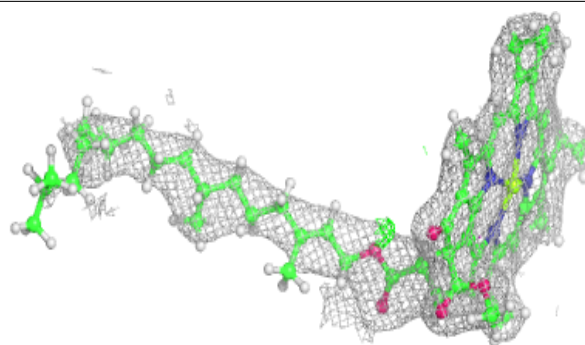
**Electron density around CLA B 611:**

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

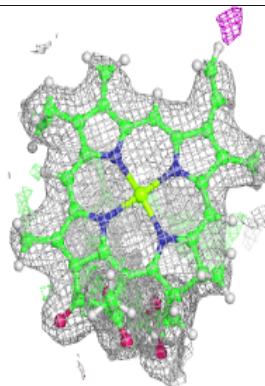
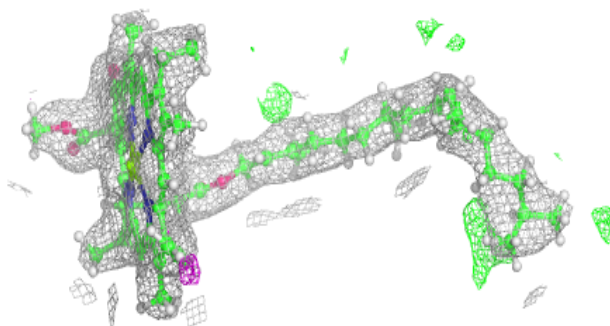
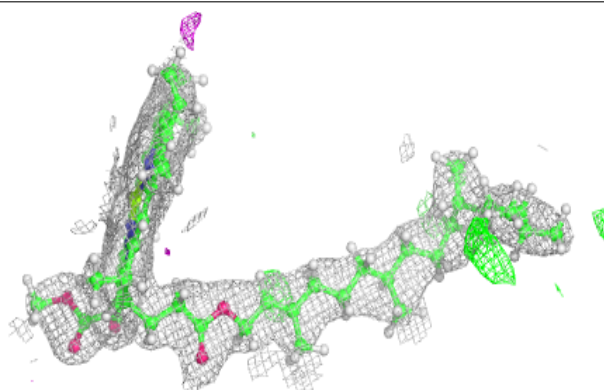


**Electron density around CLA b 603:**

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

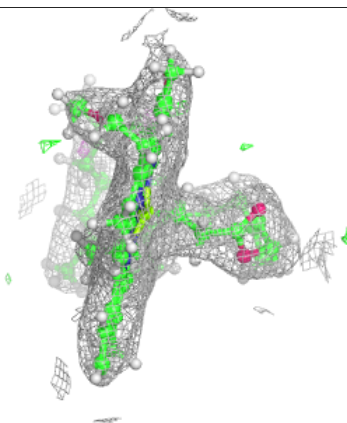
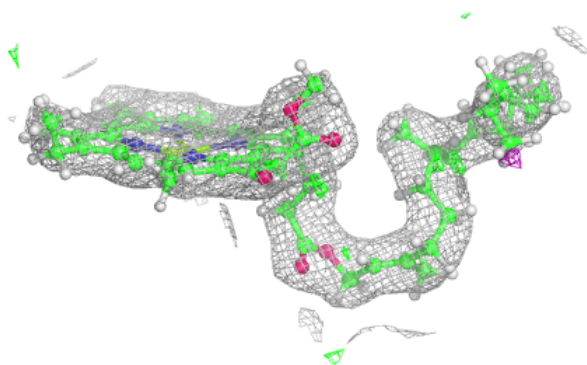
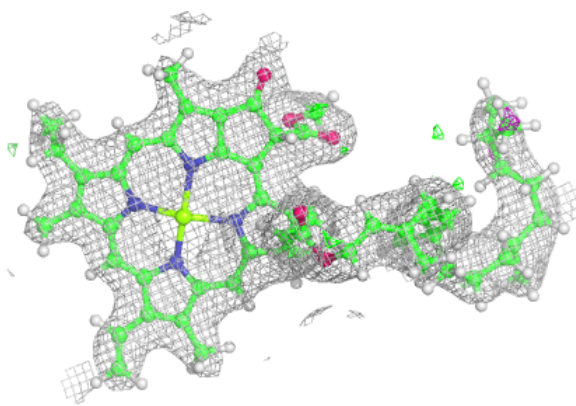
**Electron density around CLA b 604:**

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



**Electron density around CLA B 613:**

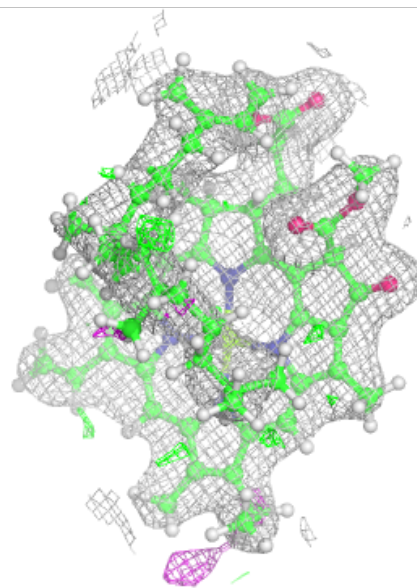
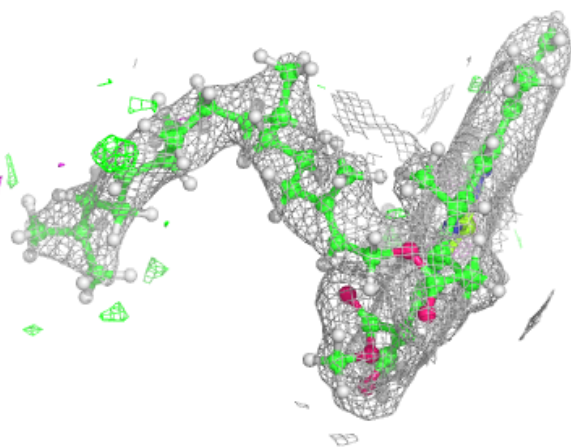
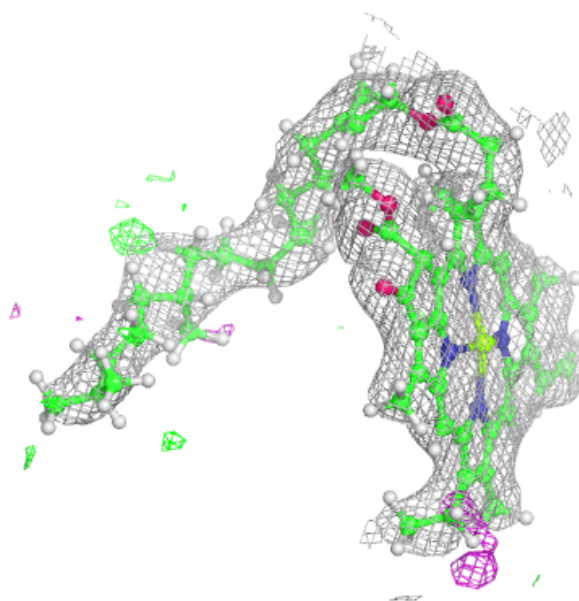
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





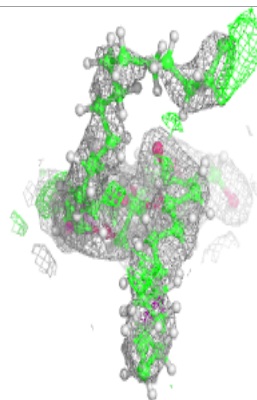
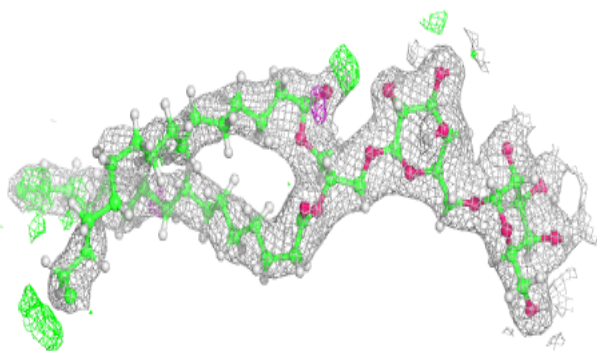
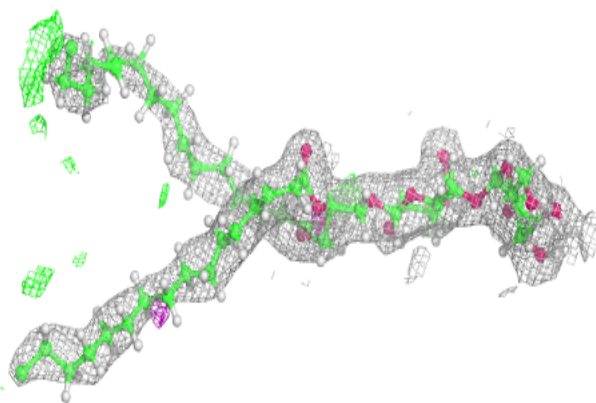
**Electron density around CLA B 614:**

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

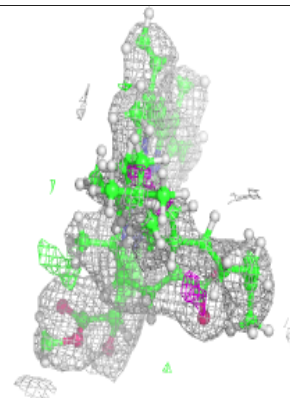
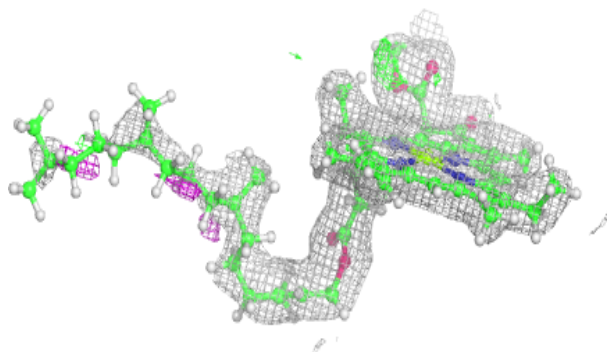
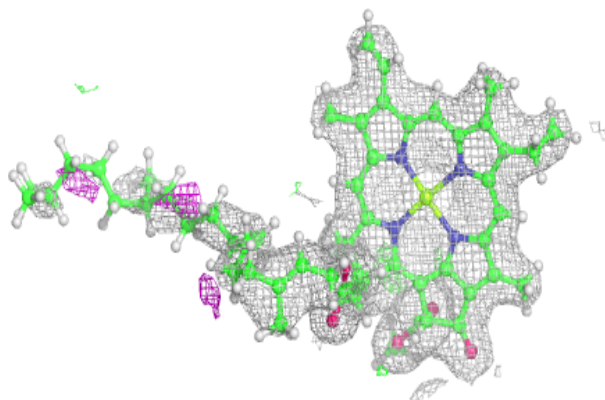


**Electron density around DGD C 516:**

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

**Electron density around CLA A 403:**

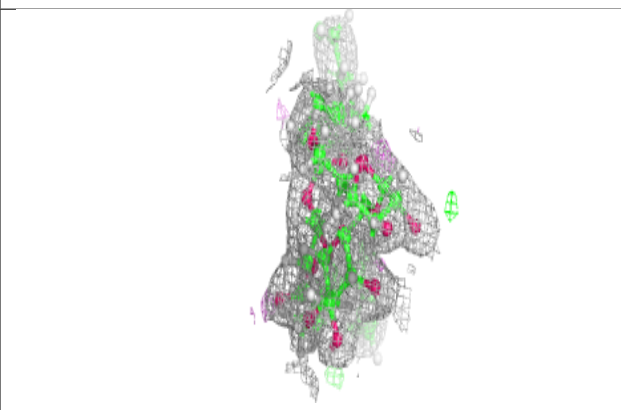
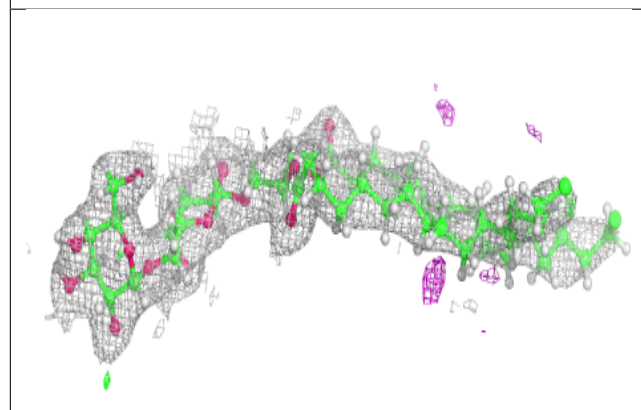
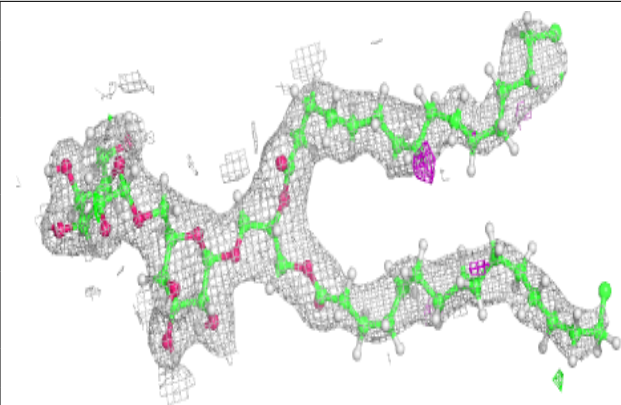
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



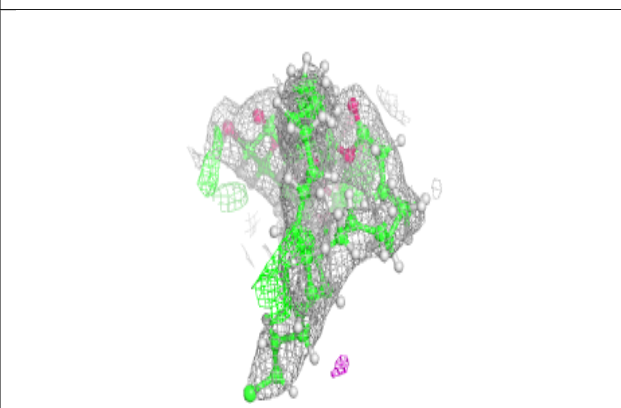
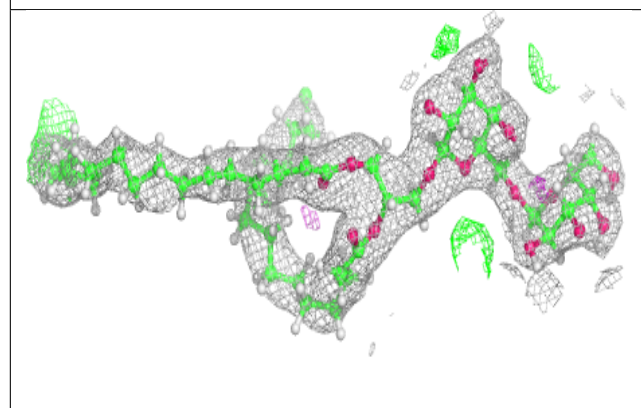
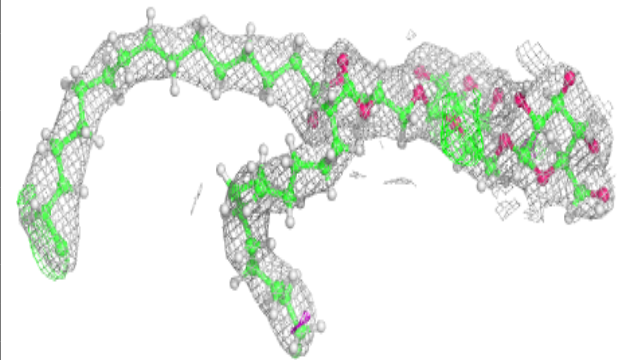


**Electron density around DGD C 518:**

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

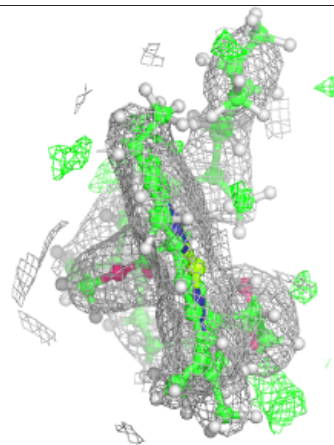
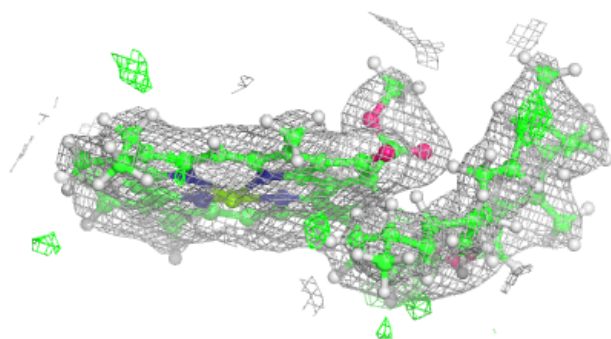
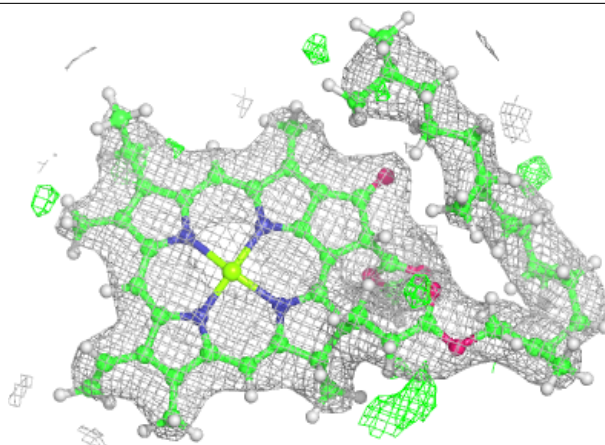
**Electron density around DGD H 102:**

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

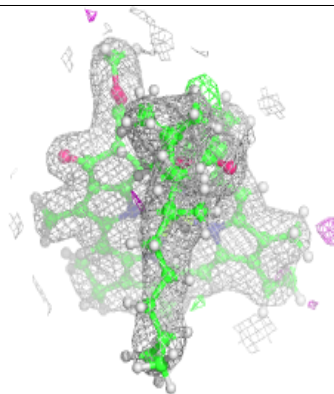
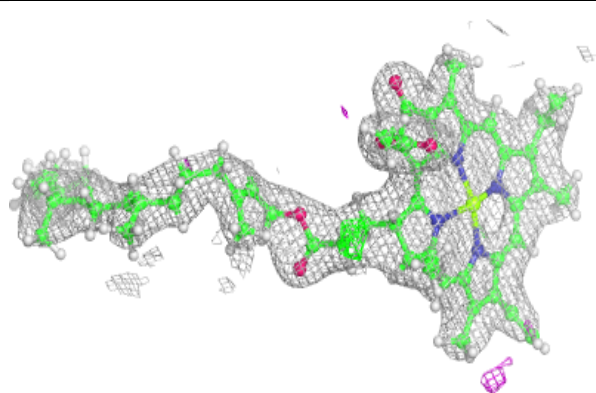
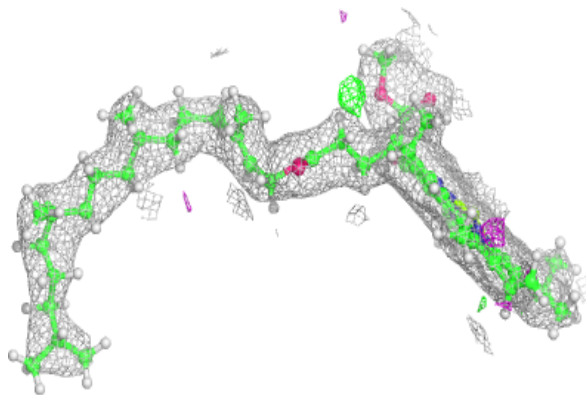


**Electron density around CLA b 609:**

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

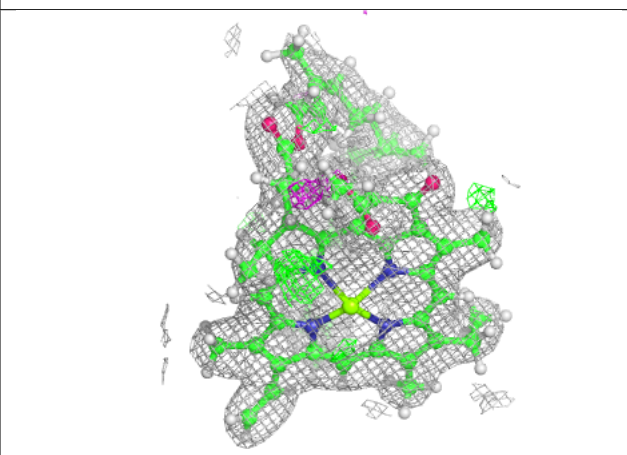
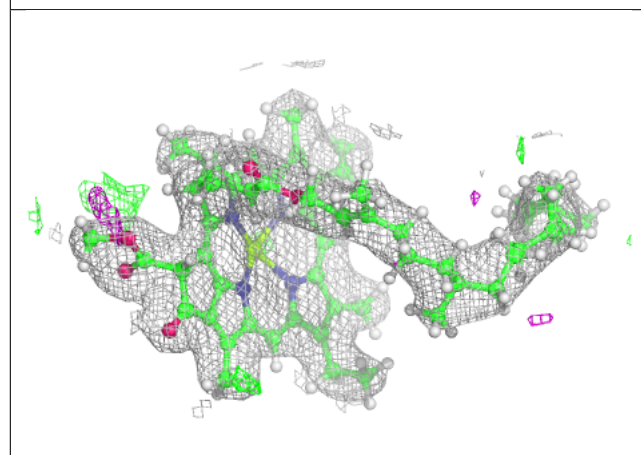
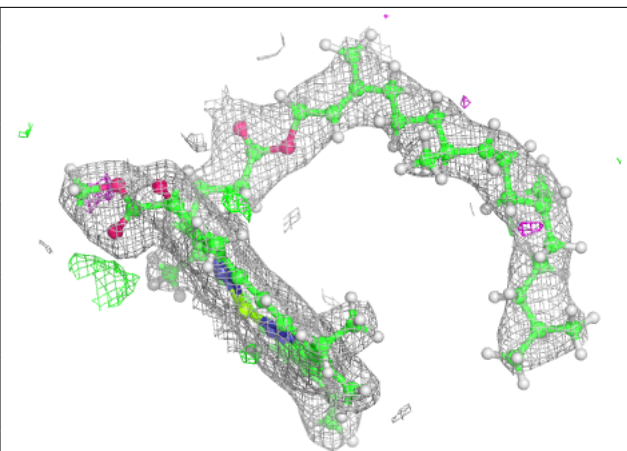
**Electron density around CLA d 402:**

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



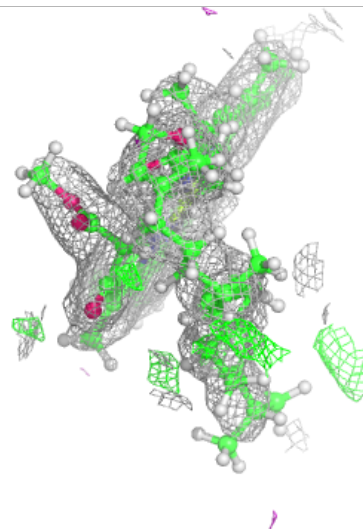
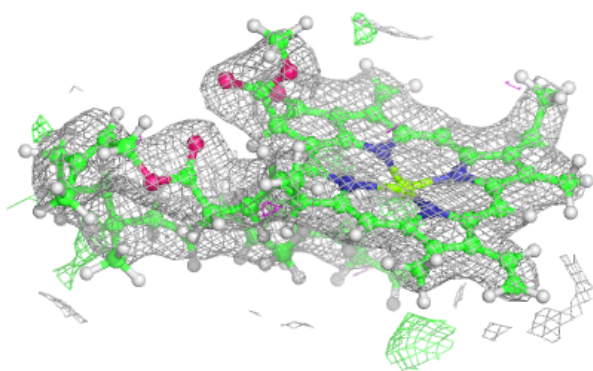
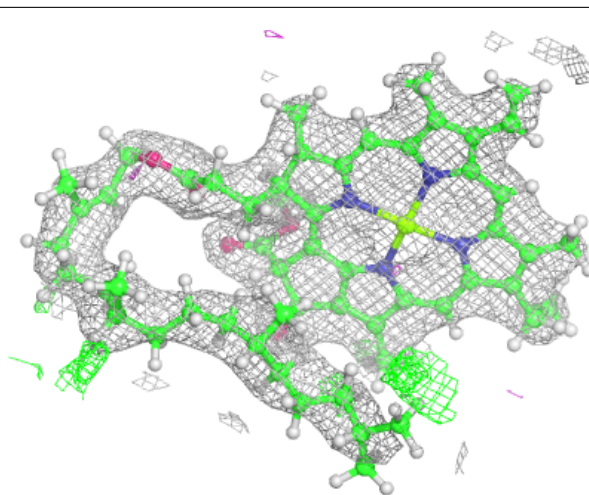
**Electron density around CLA b 610:**

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



**Electron density around CLA C 510:**

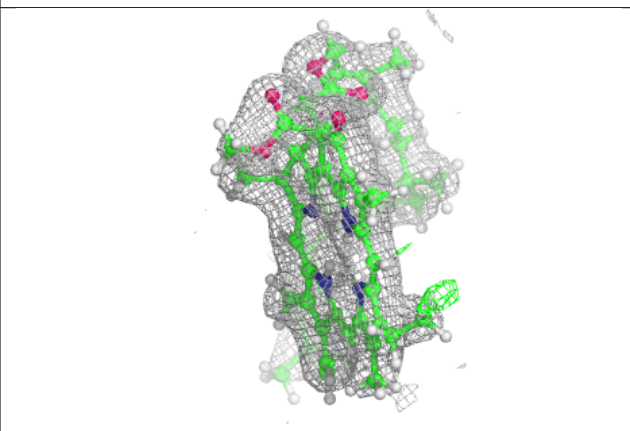
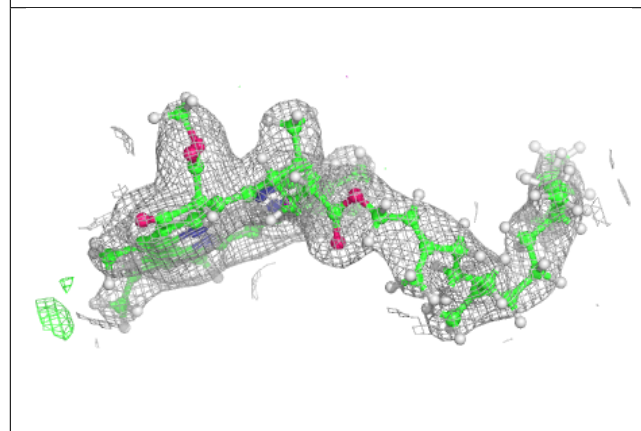
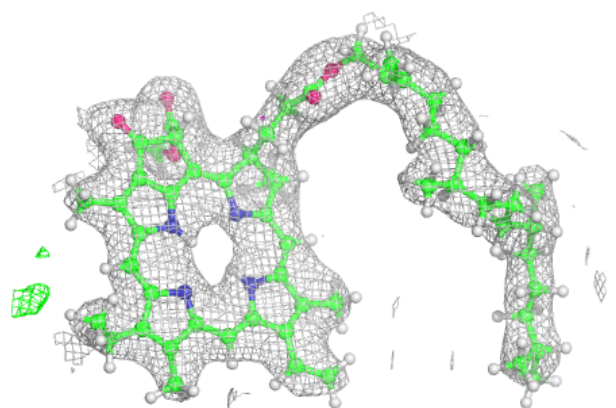
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



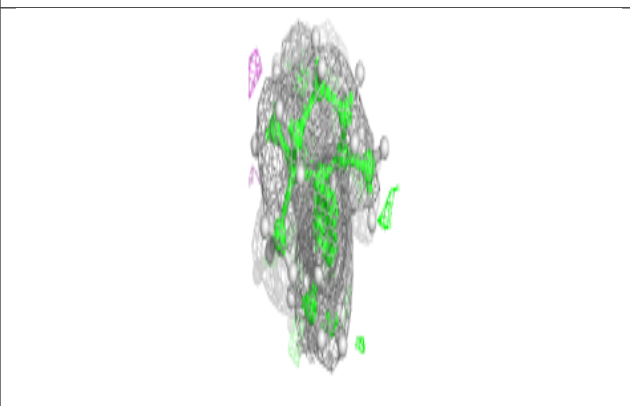
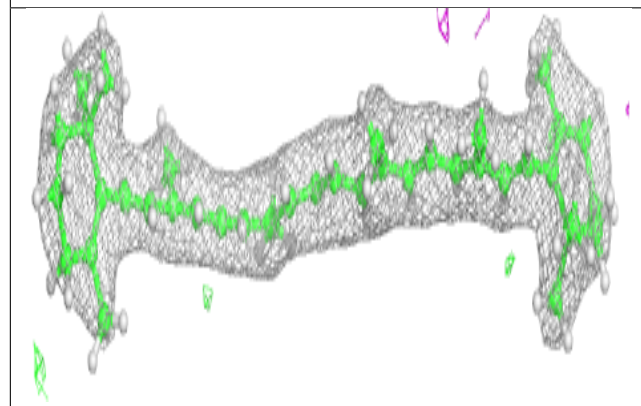
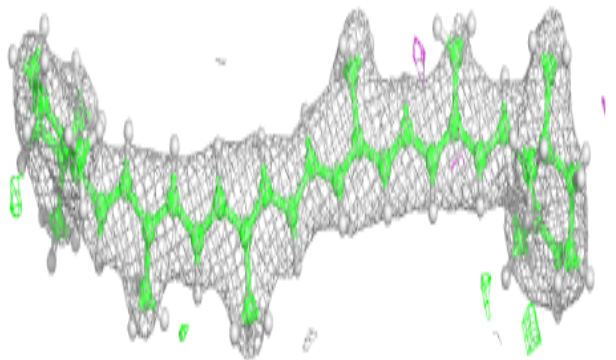


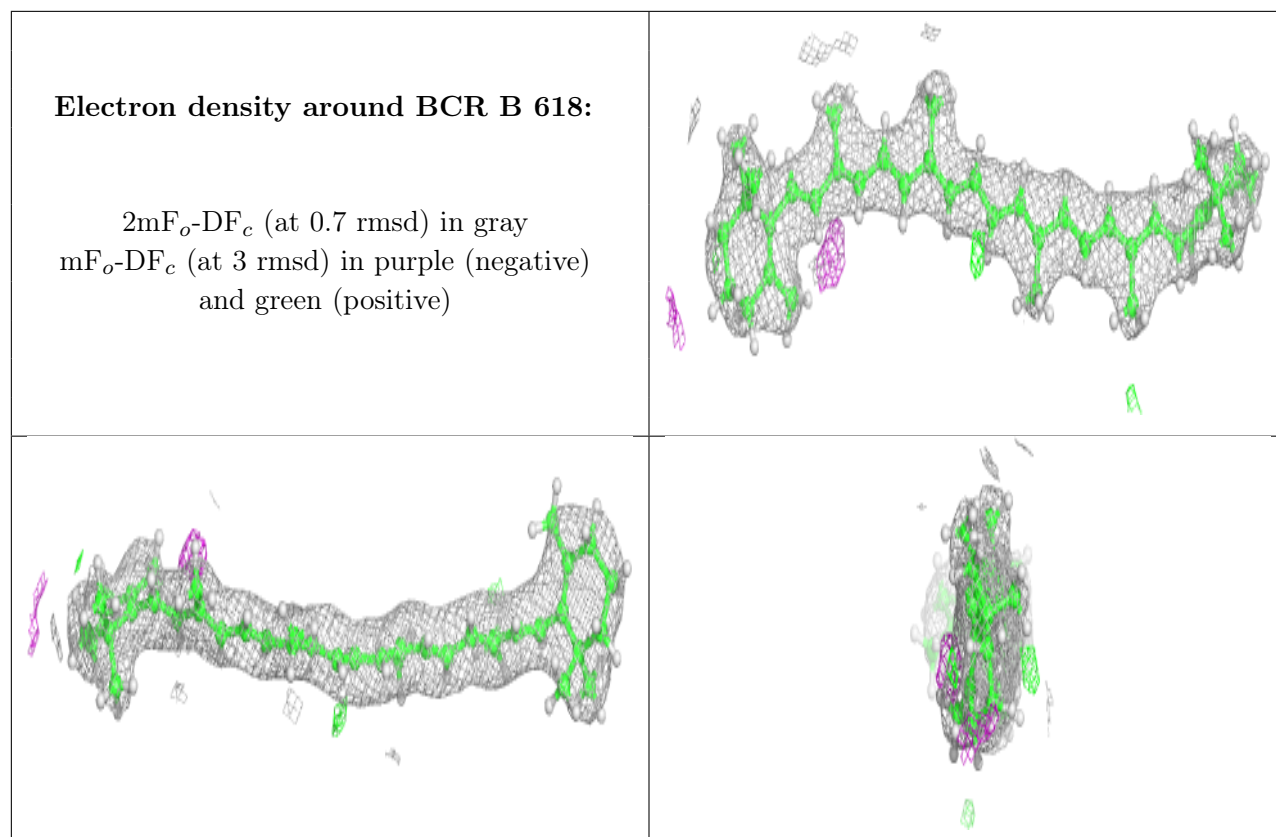
**Electron density around PHO d 401:**

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

**Electron density around BCR A 406:**

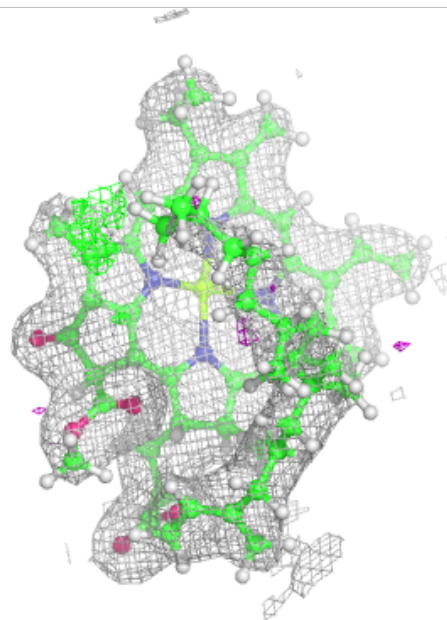
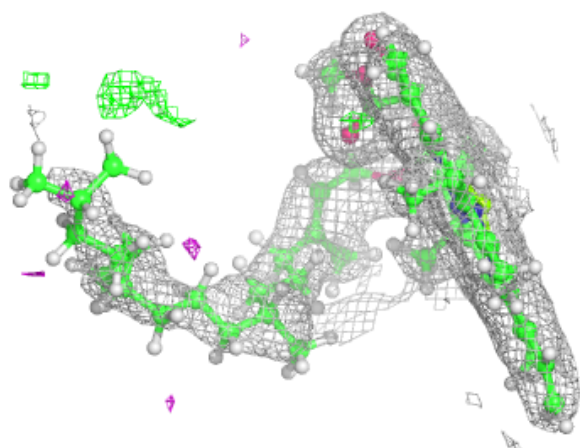
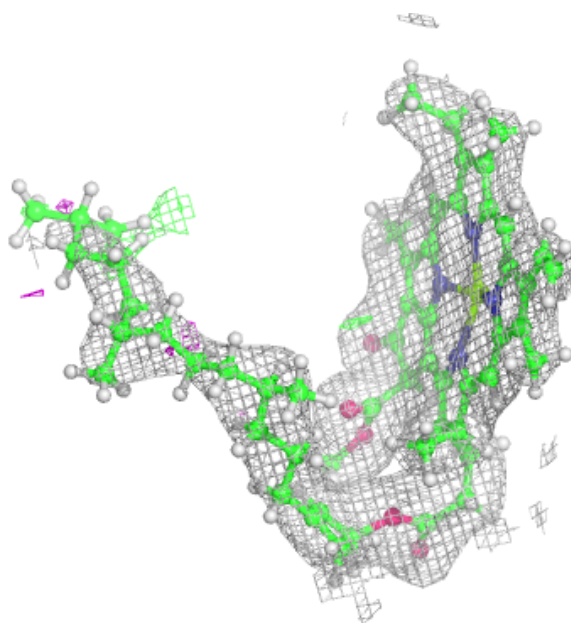
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA b 612:**

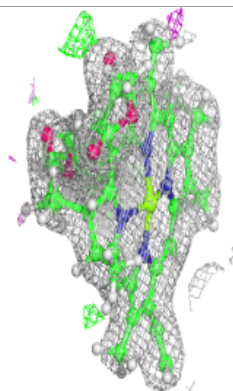
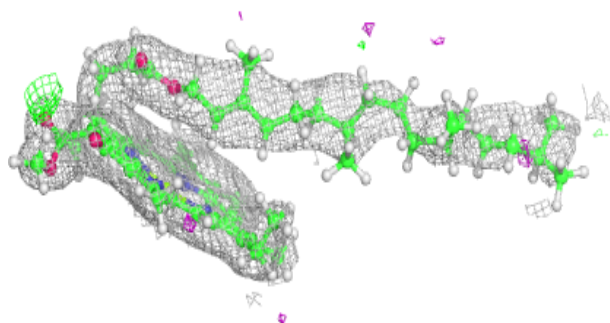
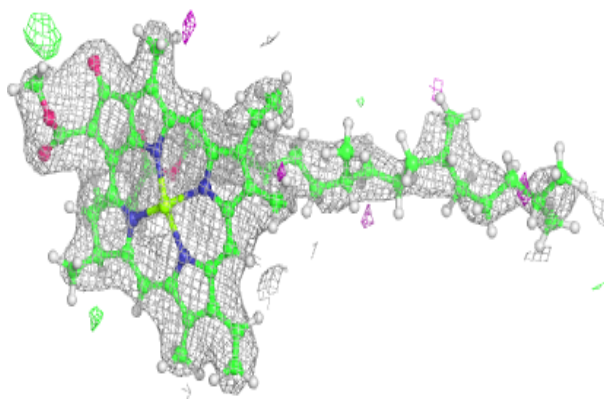
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



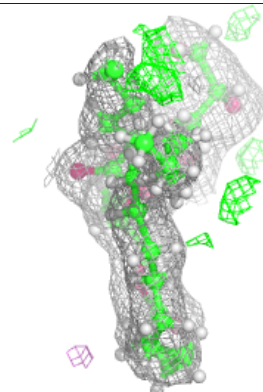
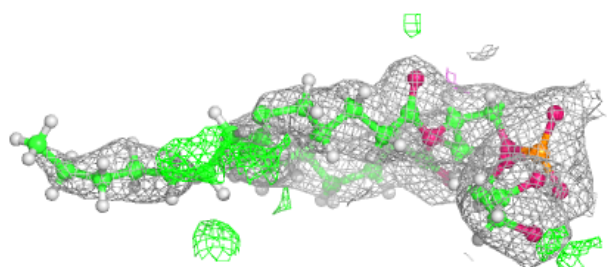
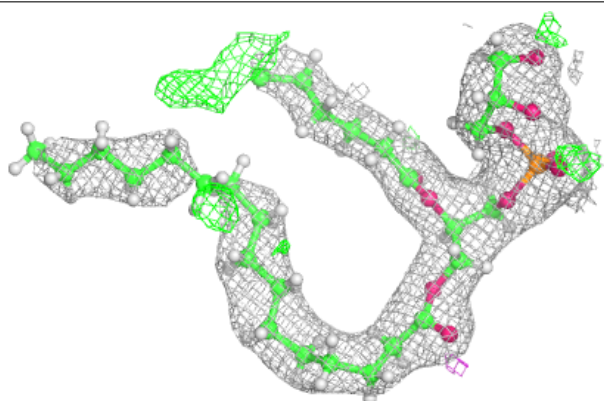


**Electron density around CLA b 613:**

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

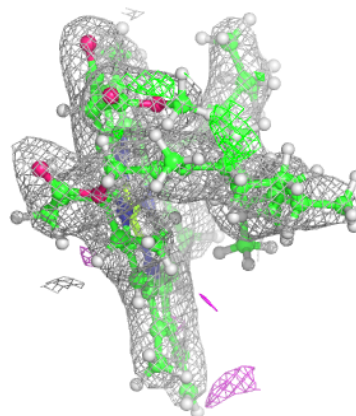
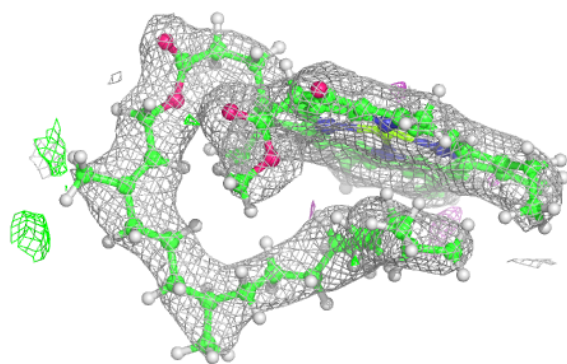
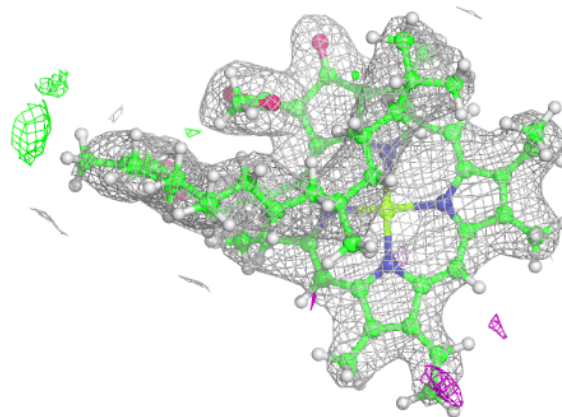
**Electron density around LHG d 408:**

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



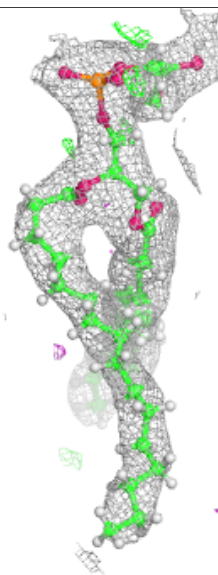
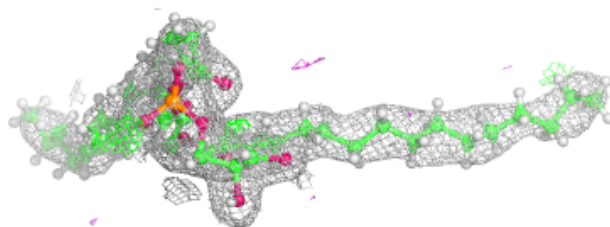
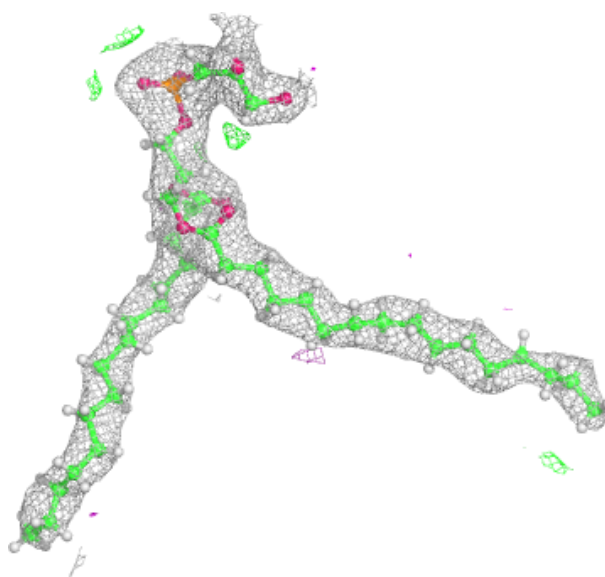
**Electron density around CLA C 511:**

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



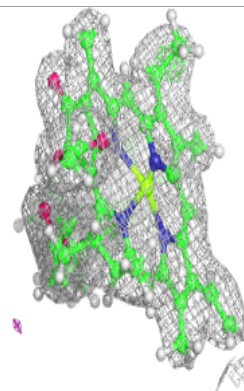
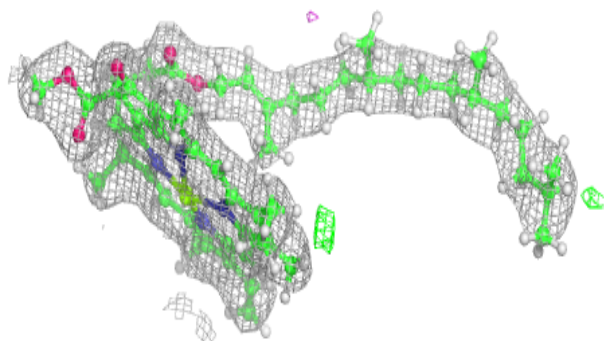
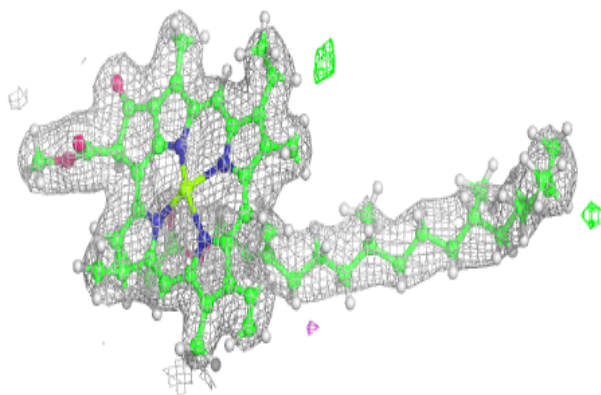
**Electron density around LHG 1 101:**

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

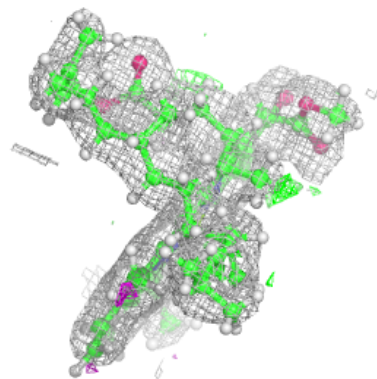
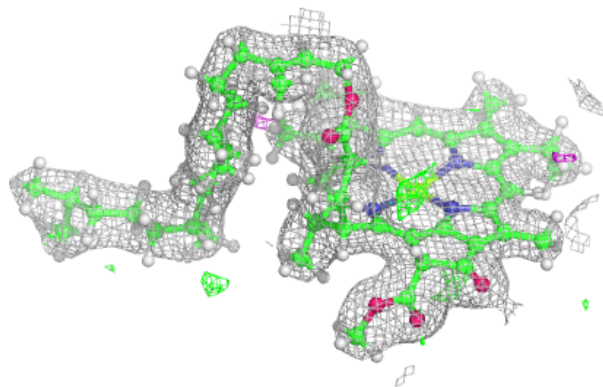
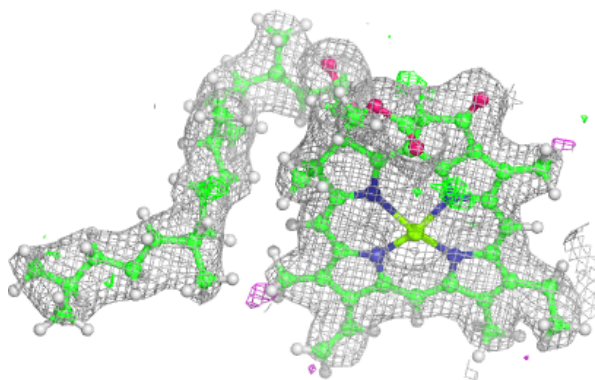


**Electron density around CLA B 609:**

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

**Electron density around CLA a 411:**

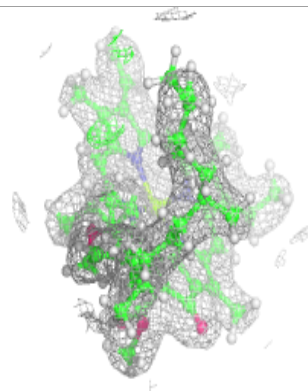
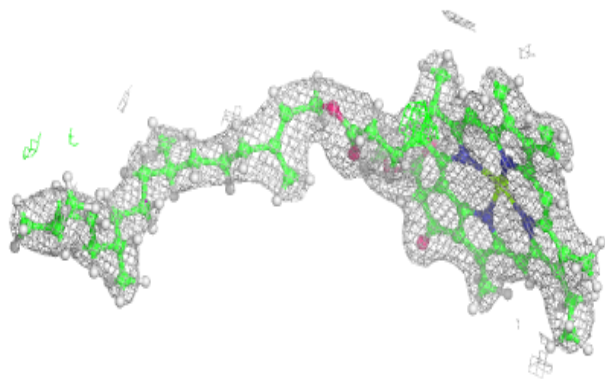
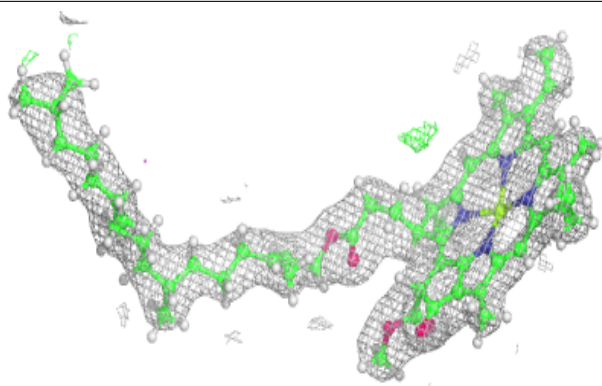
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



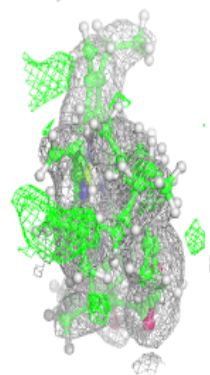
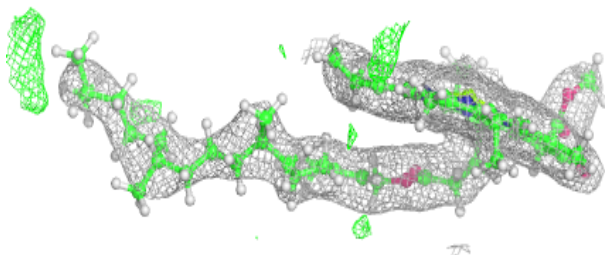
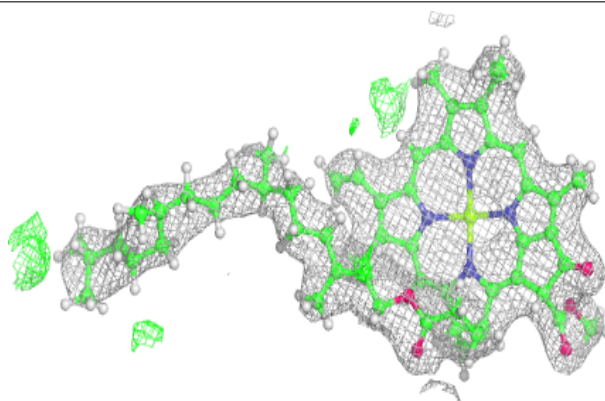


**Electron density around CLA A 402:**

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

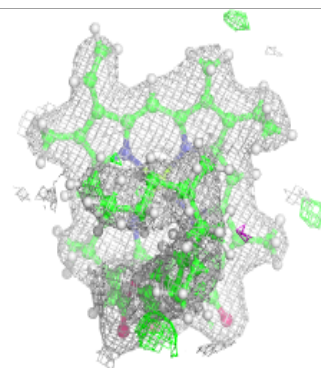
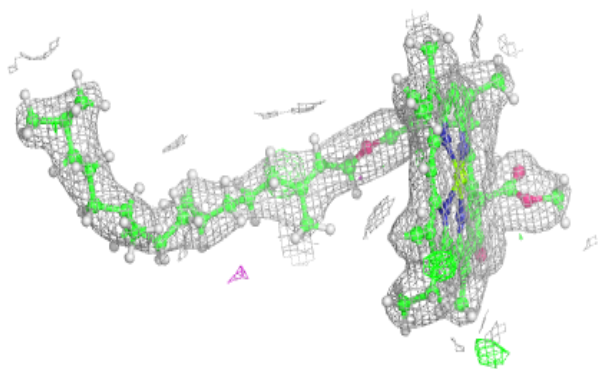
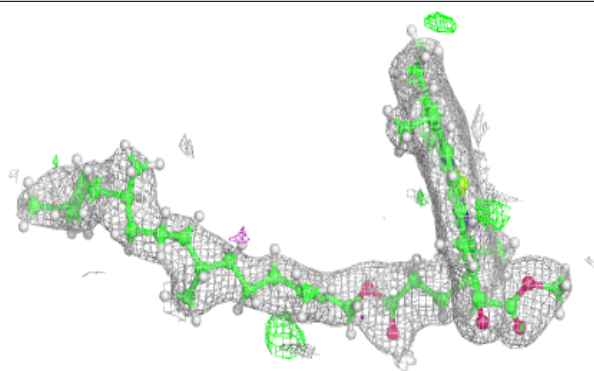
**Electron density around CLA b 602:**

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



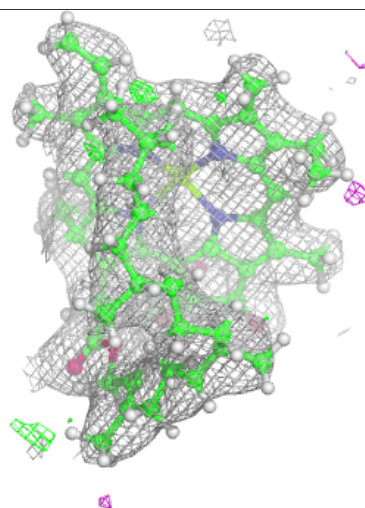
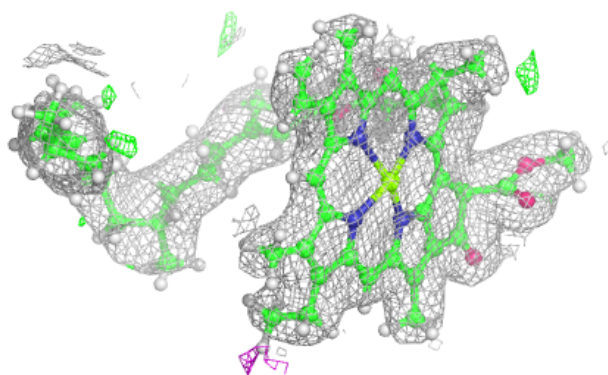
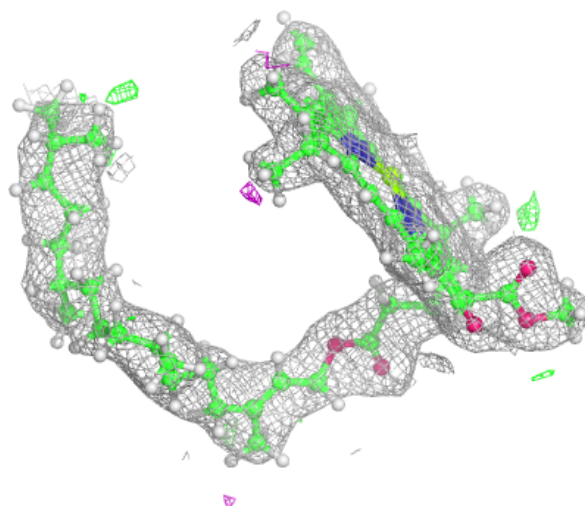
**Electron density around CLA B 606:**

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



**Electron density around CLA B 612:**

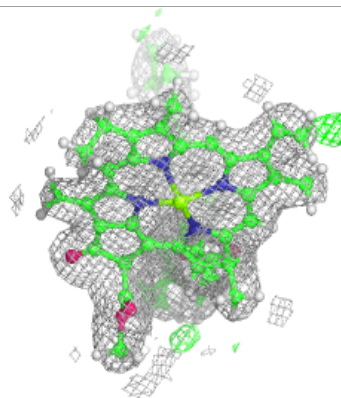
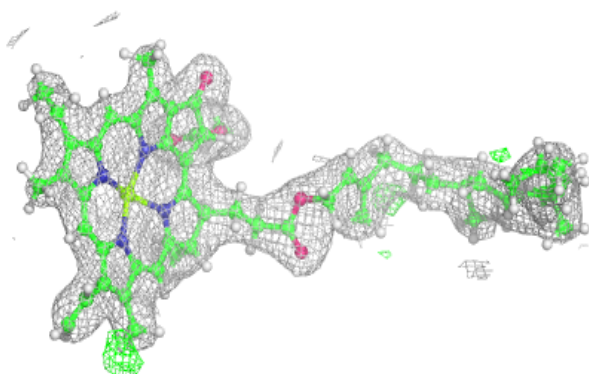
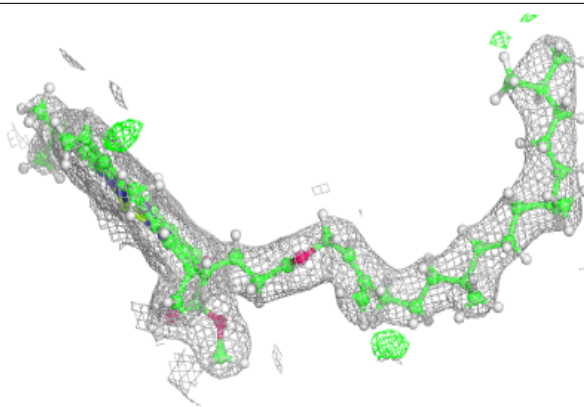
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



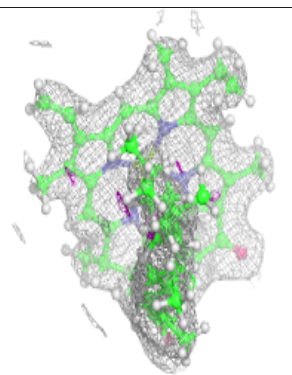
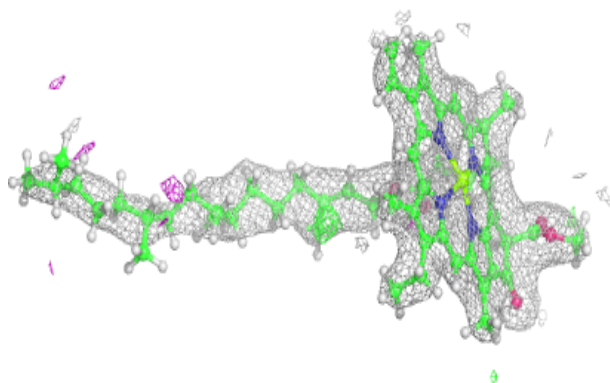
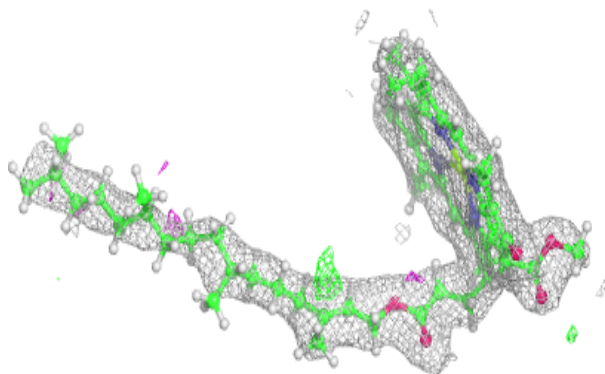


**Electron density around CLA D 402:**

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

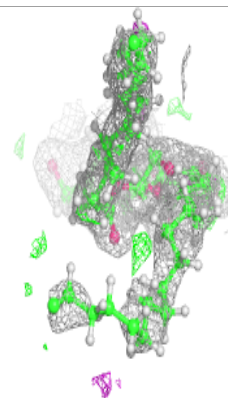
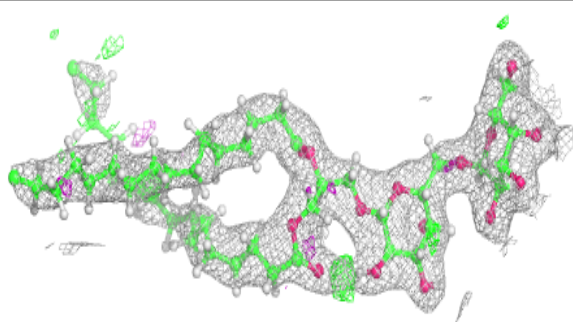
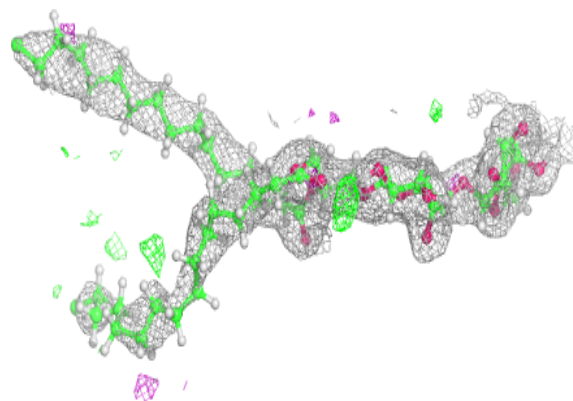
**Electron density around CLA b 606:**

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

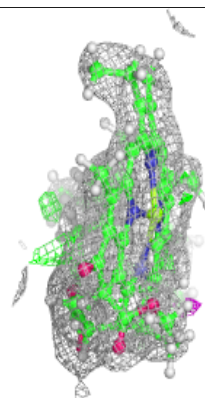
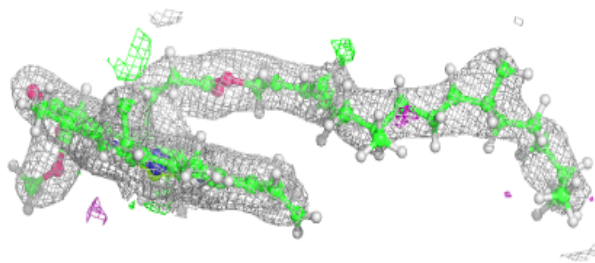
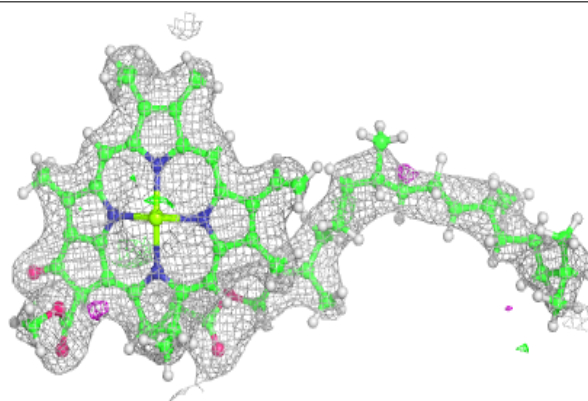


**Electron density around DGD c 519:**

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

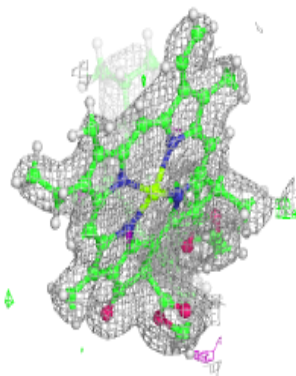
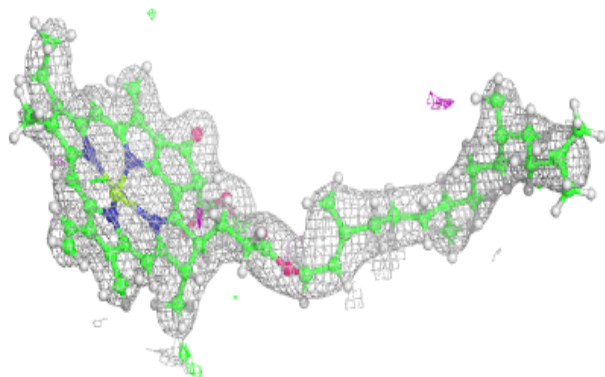
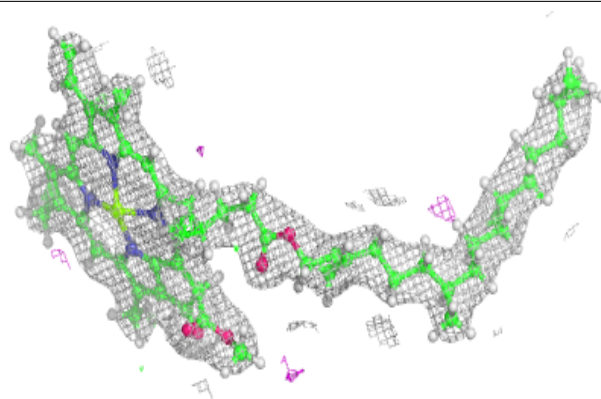
**Electron density around CLA B 604:**

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

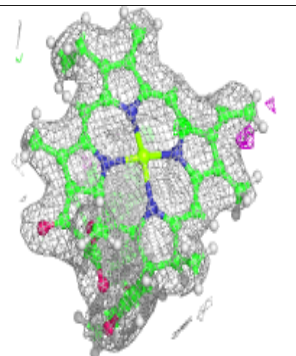
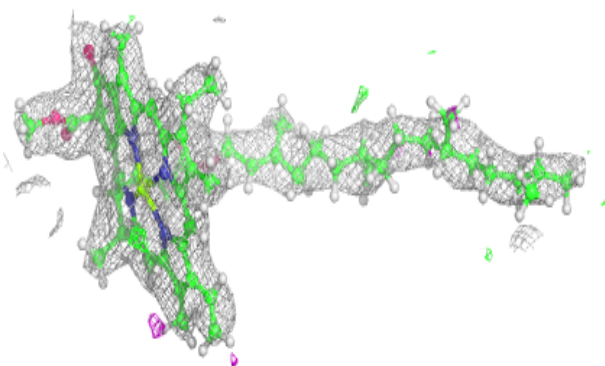
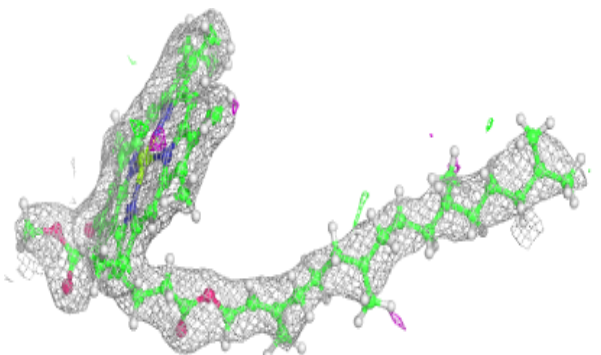


**Electron density around CLA a 402:**

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

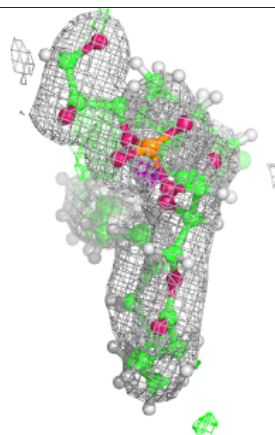
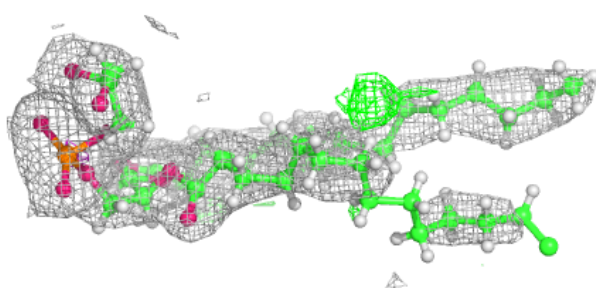
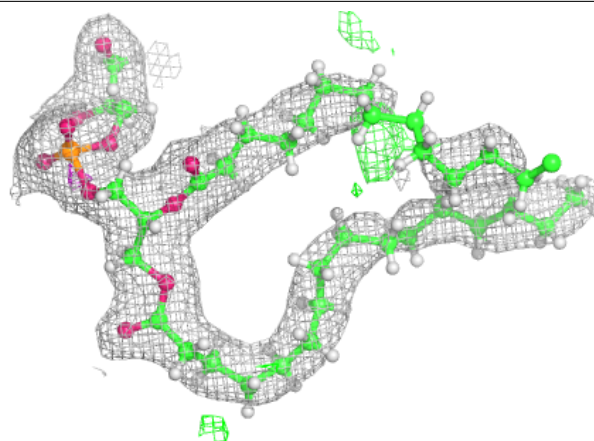
**Electron density around CLA B 608:**

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

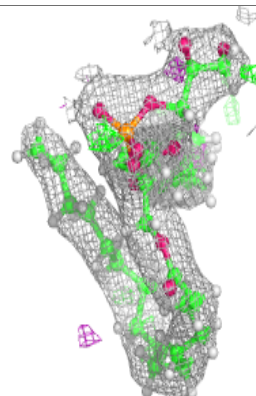
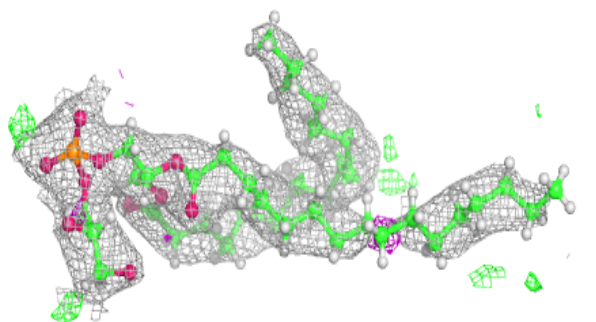
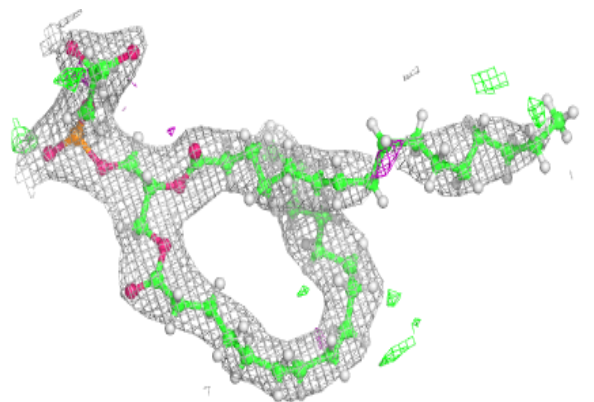


**Electron density around LHG D 409:**

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

**Electron density around LHG D 412:**

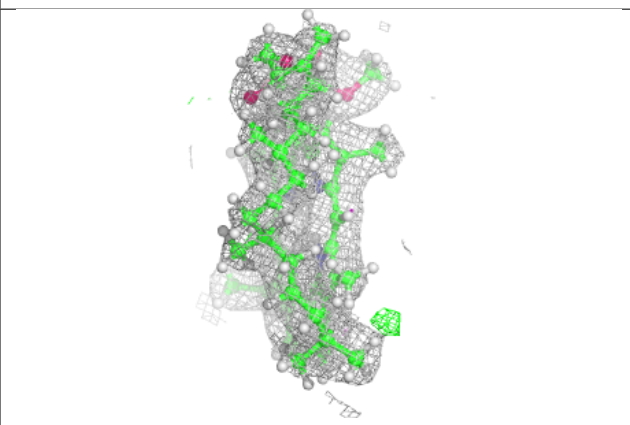
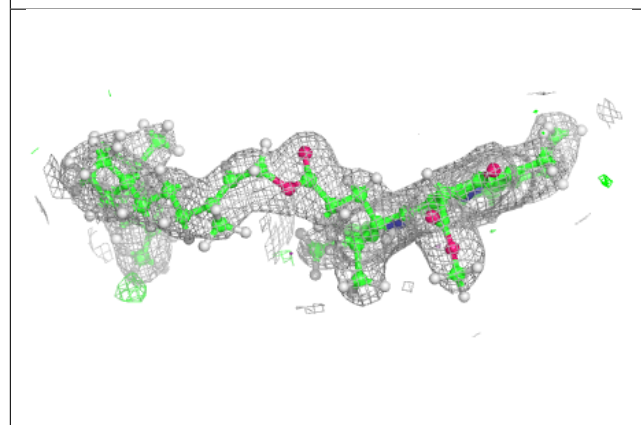
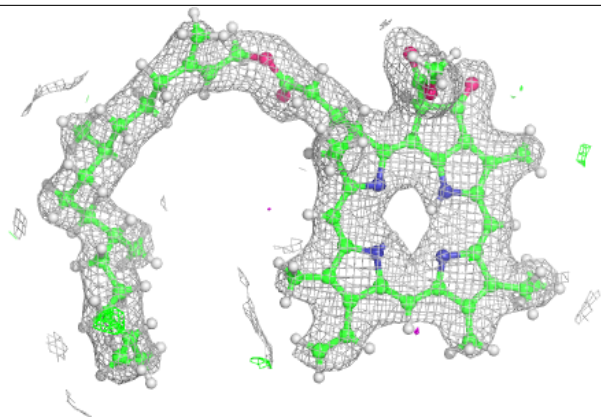
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



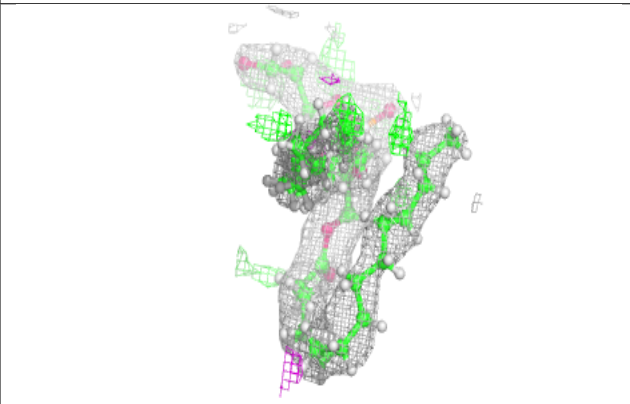
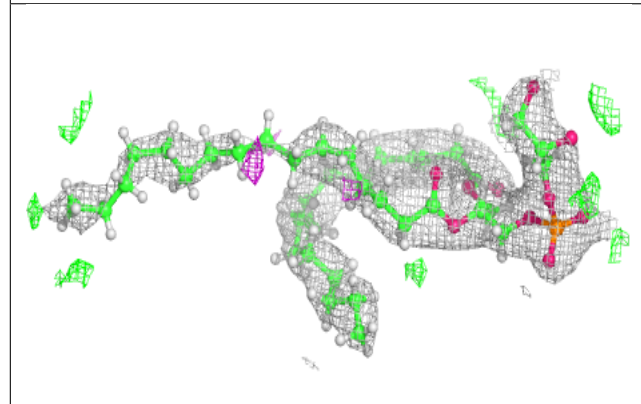
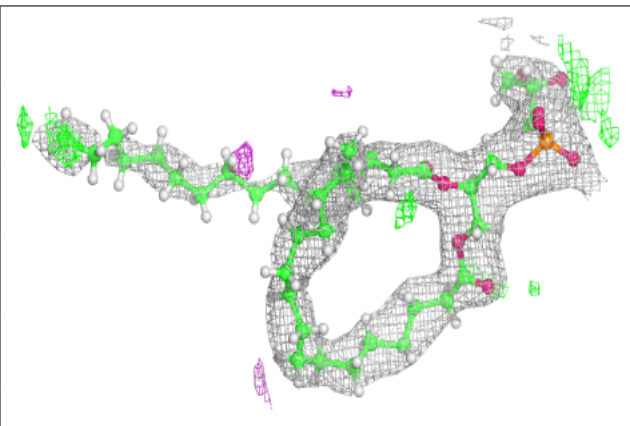


**Electron density around PHO A 404:**

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

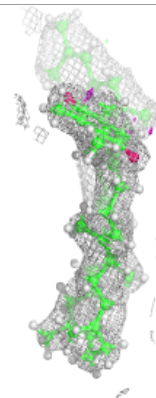
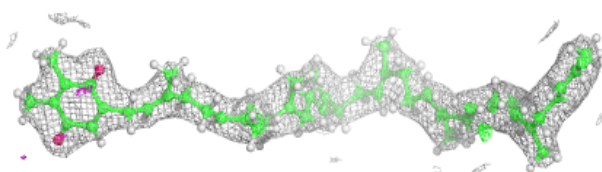
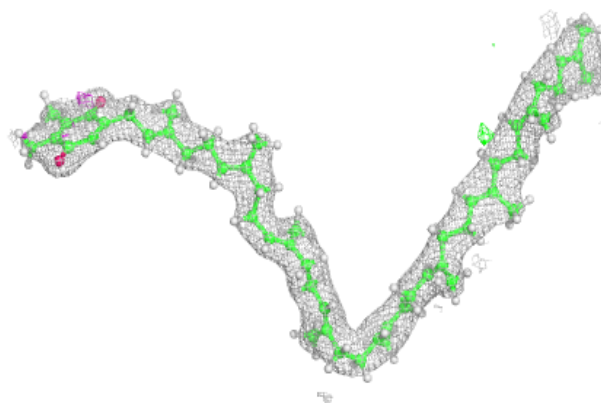
**Electron density around LHG d 406:**

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



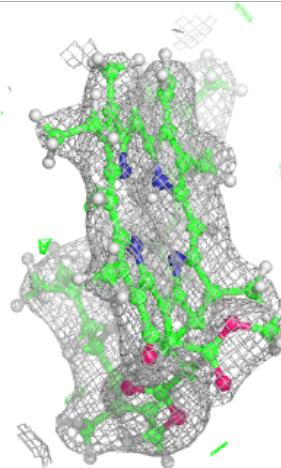
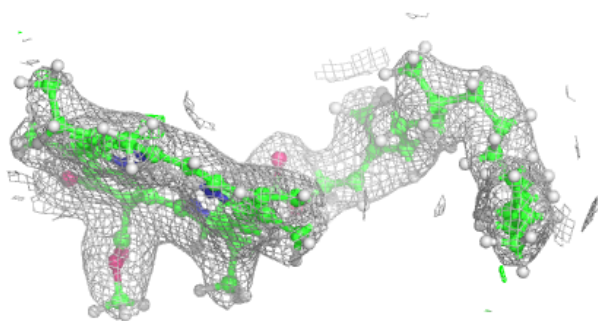
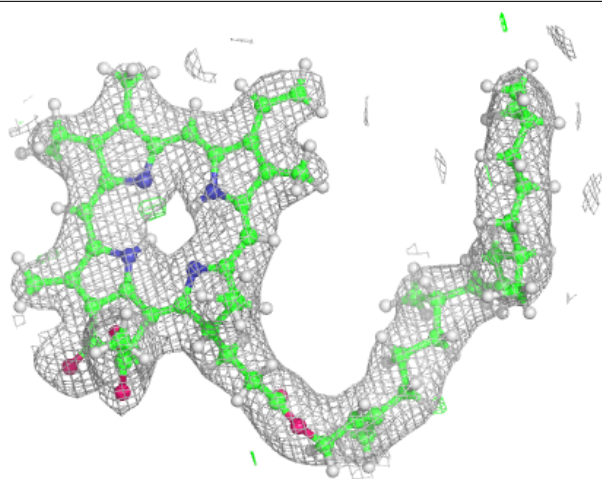
**Electron density around PL9 d 405:**

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



**Electron density around PHO D 401:**

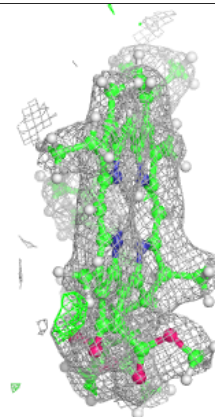
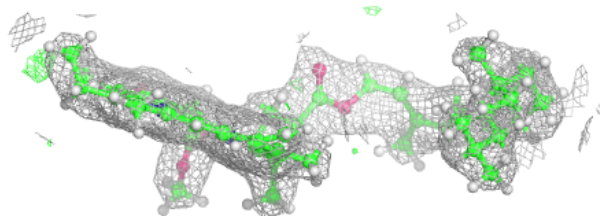
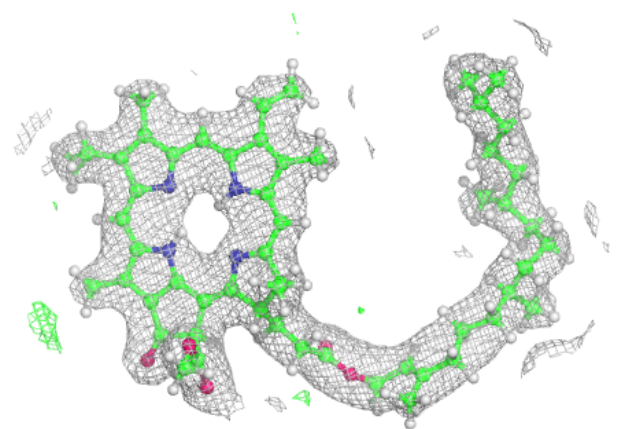
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



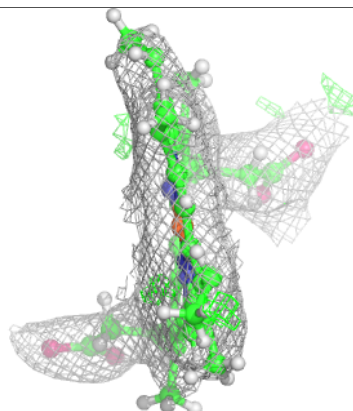
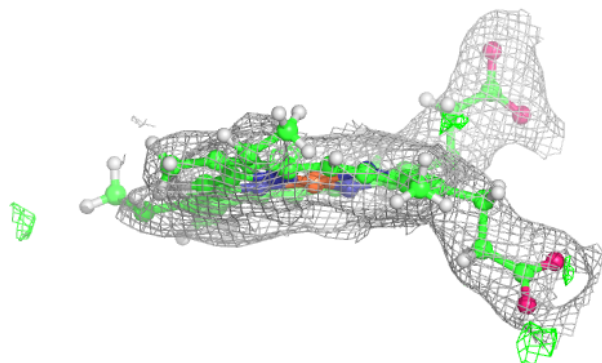
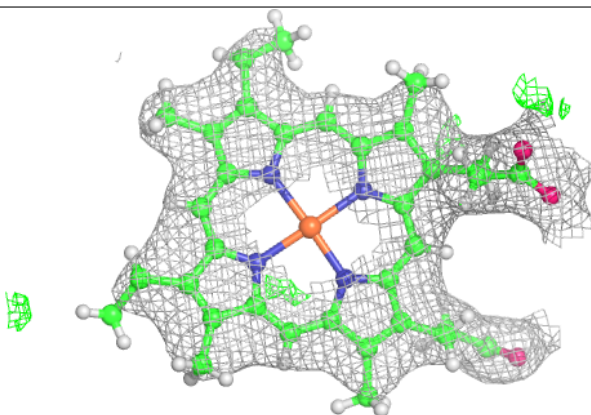


**Electron density around PHO a 404:**

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

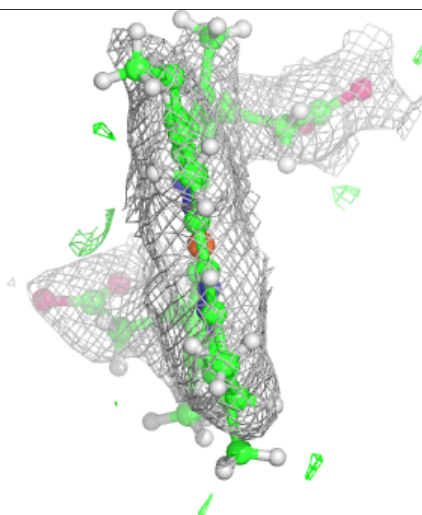
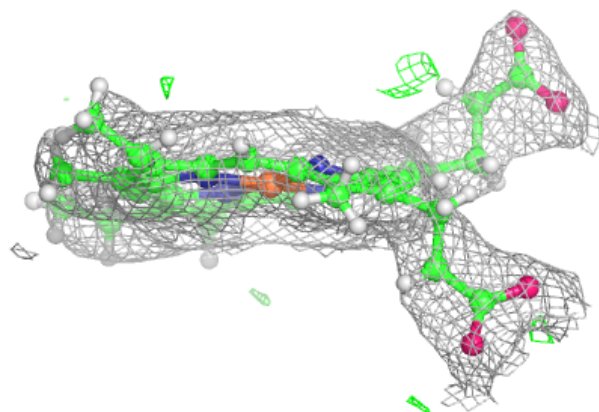
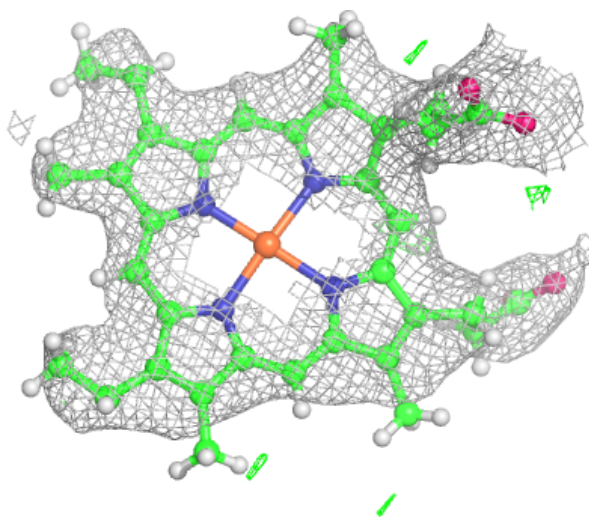
**Electron density around HEC F 101:**

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



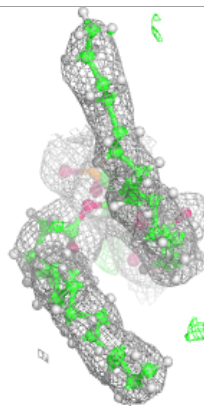
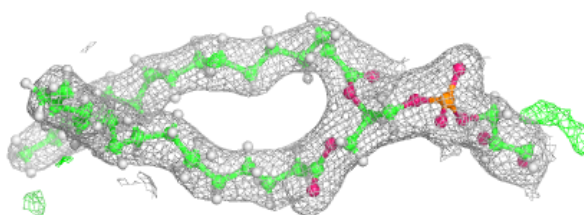
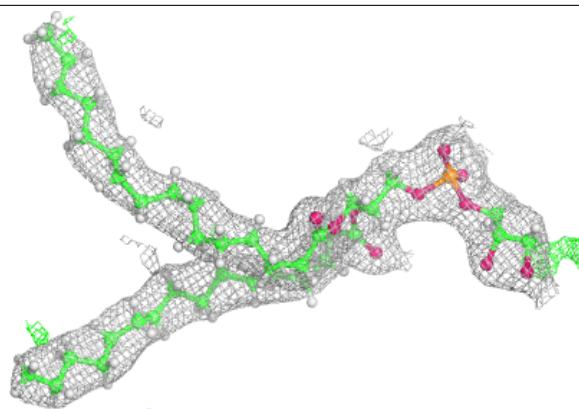
**Electron density around HEC e 101:**

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



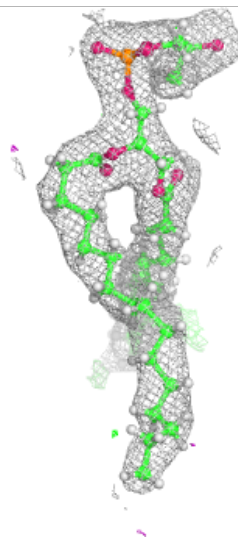
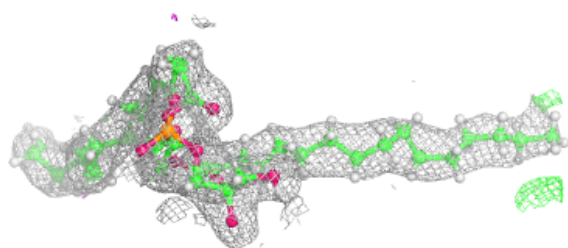
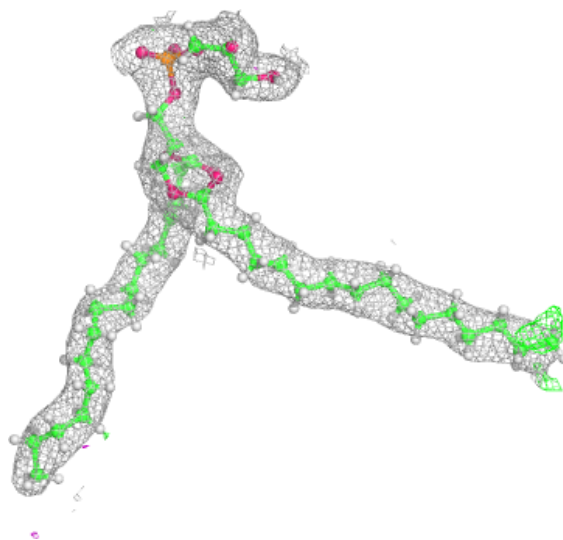
**Electron density around LHG d 407:**

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



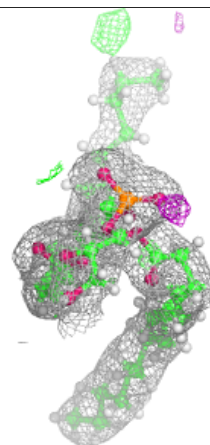
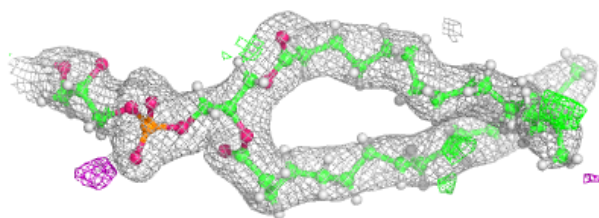
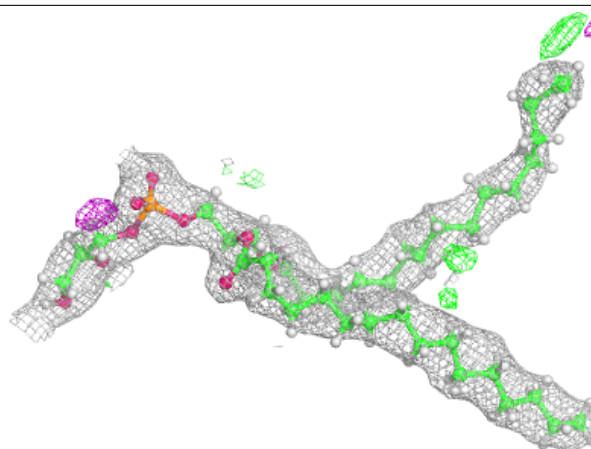
**Electron density around LHG B 622:**

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



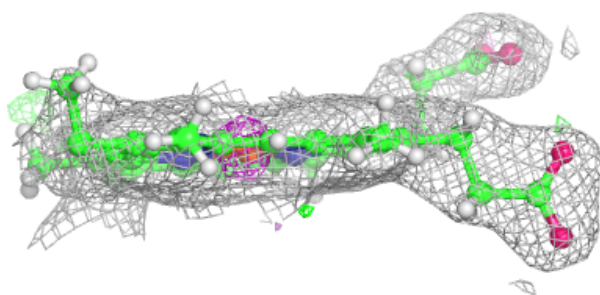
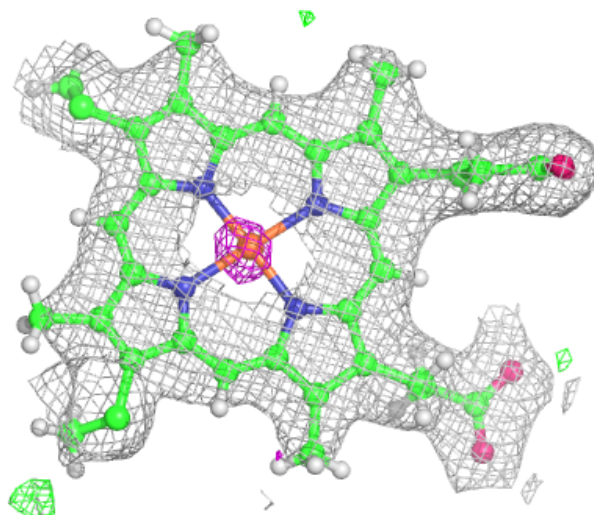
**Electron density around LHG D 408:**

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

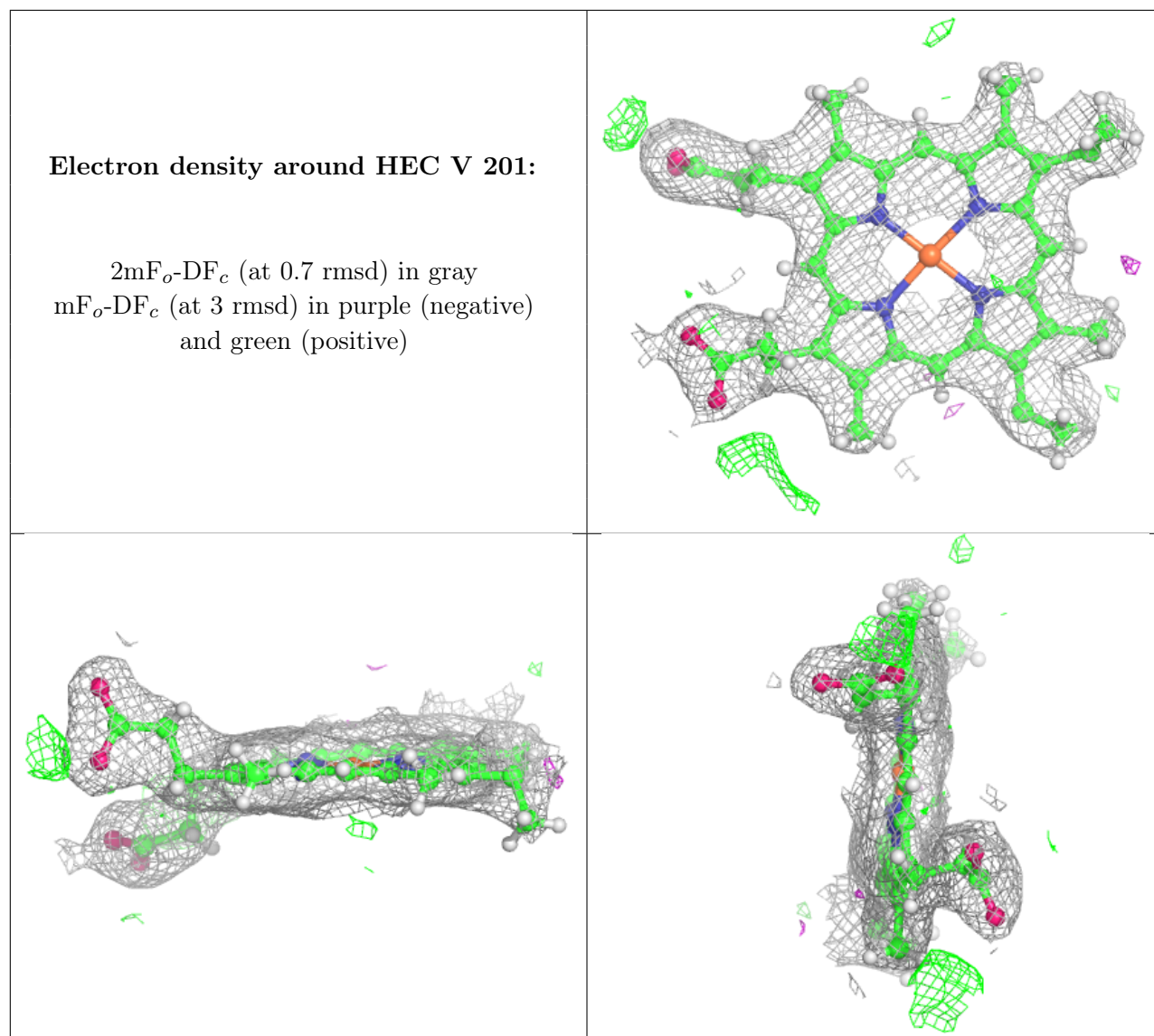


**Electron density around HEC v 201:**

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







## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.