



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 12:40 PM EDT

PDB ID : 7RF8  
Title : RT XFEL structure of the two-flash state of Photosystem II (2F, S3-rich) at 2.09 Angstrom resolution  
Authors : Hussein, R.; Ibrahim, M.; Bhowmick, A.; Simon, P.S.; Chatterjee, R.; Lassalle, L.; Doyle, M.D.; Bogacz, I.; Kim, I.-S.; Cheah, M.H.; Gul, S.; de Lichtenberg, C.; Chernev, P.; Pham, C.C.; Young, I.D.; Carbajo, S.; Fuller, F.D.; Alonso-Mori, R.; Batyuk, A.; Sutherlin, K.D.; Brewster, A.S.; Bolotovskii, R.; Mendez, D.; Holton, J.M.; Moriarty, N.W.; Adams, P.D.; Bergmann, U.; Sauter, N.K.; Dobbek, H.; Messinger, J.; Zouni, A.; Kern, J.; Yachandra, V.K.; Yano, J.  
Deposited on : 2021-07-13  
Resolution : 2.09 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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)  
Refmac : 5.8.0158

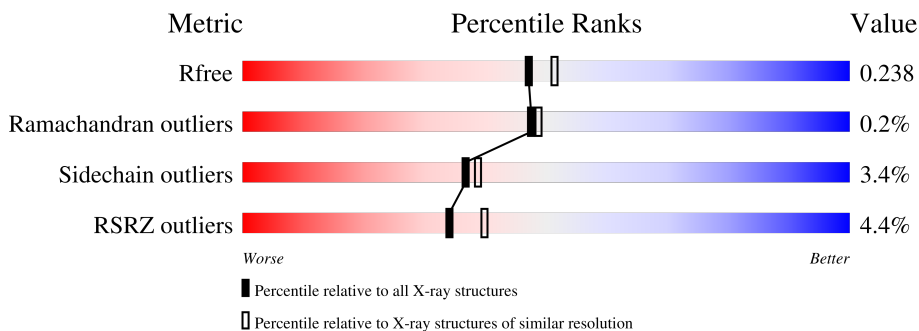
# 1 Overall quality at a glance

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	 93%
2	B	510	 97%
2	b	510	 97%

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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

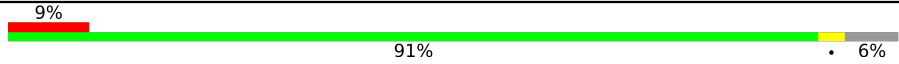

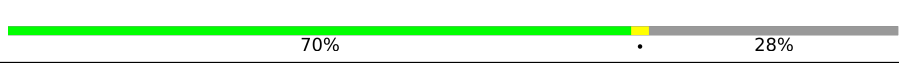


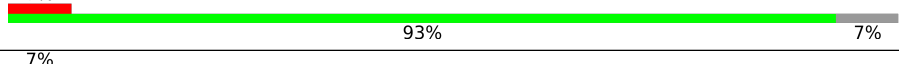
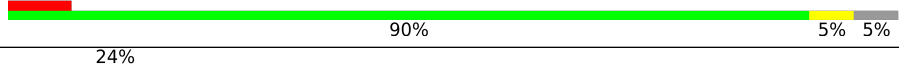

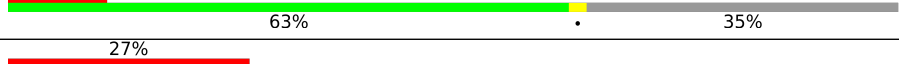

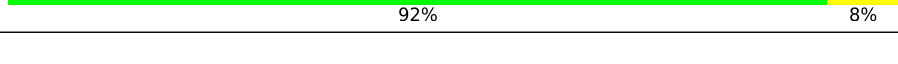


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Mol	Chain	Length	Quality of chain
3	C	461	2% 94%
3	c	461	3% 95%
4	D	352	% 96%
4	d	352	94%
5	E	84	7% 95%
5	e	84	6% 95%
6	F	45	4% 76% 24%
6	f	45	4% 67% 9% 24%
7	H	66	3% 92% 6%
7	h	66	5% 89% 6% 5%
8	I	38	5% 87% 8% 5%
8	i	38	5% 89% 5% 5%
9	J	40	10% 90% 10%
9	j	40	12% 88% 10%
10	K	46	2% 76% 20%
10	k	46	76% 20%
11	L	37	95% 5%
11	l	37	8% 89% 8%
12	M	36	89% 8%
12	m	36	78% 11% 11%
13	O	272	6% 86% 10%
13	o	272	6% 86% 10%
14	R	41	41% 61% 7% 32%
14	r	41	63% 63% 5% 32%
15	T	32	6% 88% 6% 6%

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Mol	Chain	Length	Quality of chain
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	405	X	-	-	-
22	CLA	A	410	X	-	-	-
22	CLA	B	601	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	C	501	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	502	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	a	402	X	-	-	-
22	CLA	a	404	X	-	-	-
22	CLA	b	601	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	c	501	X	-	-	-
22	CLA	c	502	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
22	CLA	d	404	X	-	-	-

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
22	CLA	d	405	X	-	-	-

## 2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 105937 atoms, of which 52685 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	6098	2030	2985	513	551	19	0	66	0
1	a	334	6086	2027	2976	513	551	19	0	66	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	7878	2631	3873	666	695	13	0	5	0
2	b	505	7814	2610	3836	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	6941	2302	3432	586	607	14	0	14	0
3	c	451	7086	2343	3503	602	624	14	0	14	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	5368	1809	2637	446	464	12	0	2	0
4	d	341	5380	1813	2643	446	466	12	0	3	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
6	F	34	Total	C	H	N	O	S	0	0	0
			557	187	282	45	42	1			
6	f	34	Total	C	H	N	O	S	0	0	0
			557	187	282	45	42	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
9	J	36	Total	C	H	N	O	S	0	0	0
			525	174	268	40	42	1			
9	j	36	Total	C	H	N	O	S	0	0	0
			525	174	268	40	42	1			

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
13	O	244	Total	C	H	N	O	S	0	1	0
			3700	1168	1830	313	385	4			
13	o	244	Total	C	H	N	O	S	0	0	0
			3720	1170	1846	317	383	4			

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

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

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

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

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	
			Total	C	H	N	O				S
16	U	97	Total 1547	C 491	H 773	N 129	O 154	S	0	0	0
16	u	97	Total 1547	C 491	H 773	N 129	O 154	S	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
17	V	137	Total 2135	C 675	H 1071	N 177	O 208	S 4	0	0	0
17	v	137	Total 2135	C 675	H 1071	N 177	O 208	S 4	0	0	0

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

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

- 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



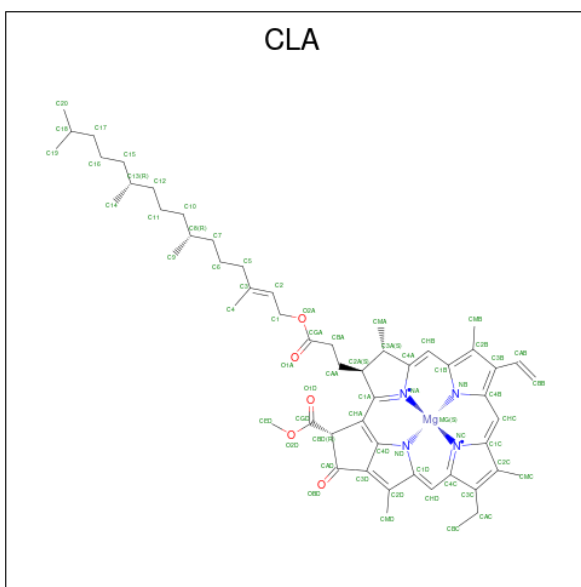
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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>).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
22	C	1	Total	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	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		

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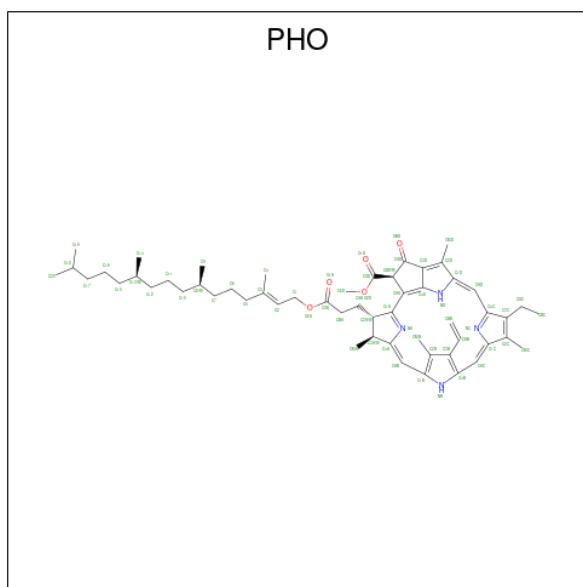
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total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

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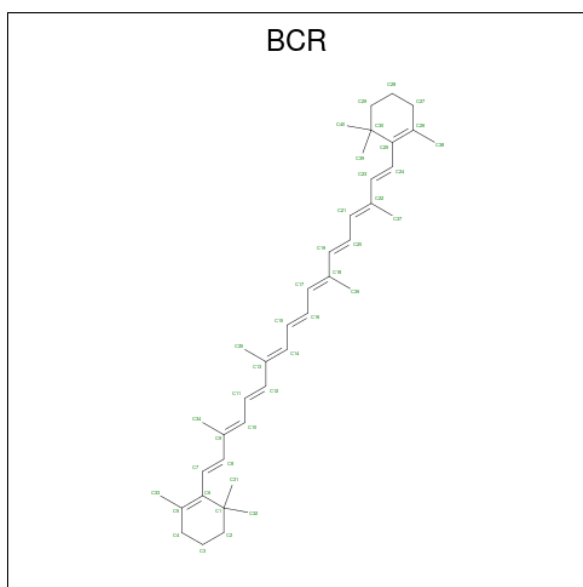
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	Mg	N			O
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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



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

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



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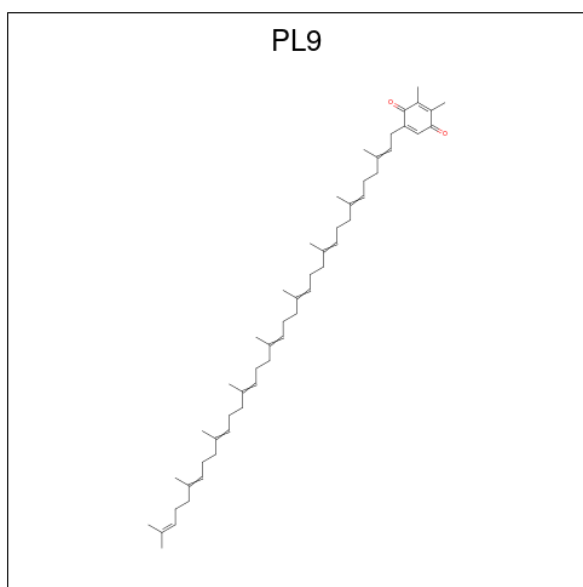
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	b	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	d	1	Total	C	H	0	0
			96	40	56		
24	h	1	Total	C	H	0	0
			96	40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

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

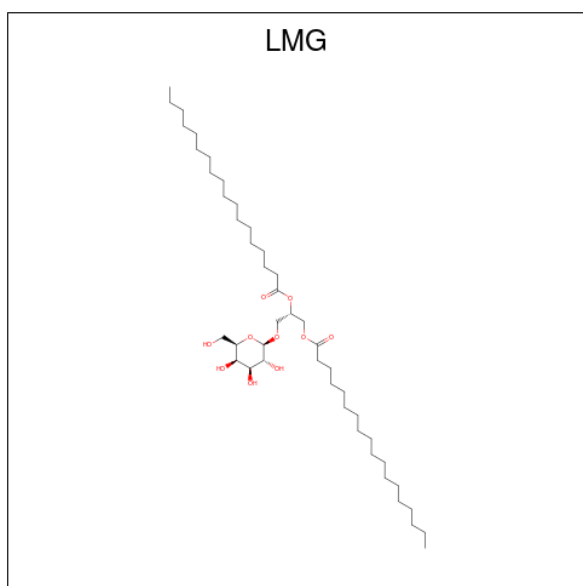
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	2	Total	Cl	0	0
			2	2		
25	a	2	Total	Cl	0	0
			2	2		

- Molecule 26 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: C<sub>53</sub>H<sub>80</sub>O<sub>2</sub>).



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

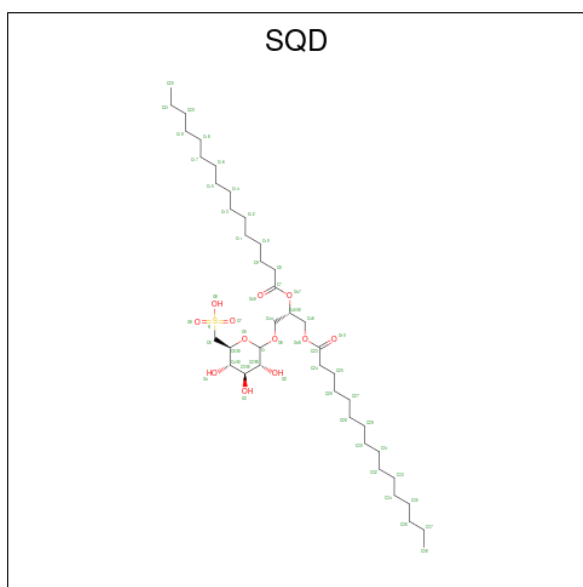
- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).





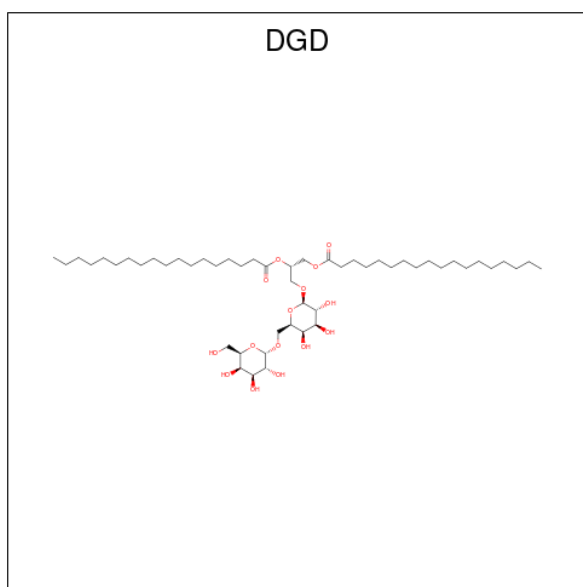
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	H	O	0	0
			114	38	66	10		
27	B	1	Total	C	H	O	0	0
			68	24	40	4		
27	C	1	Total	C	H	O	0	0
			114	38	66	10		
27	D	1	Total	C	H	O	0	0
			123	41	72	10		
27	D	1	Total	C	H	O	0	0
			78	27	45	6		
27	M	1	Total	C	H	O	0	0
			123	41	72	10		
27	b	1	Total	C	H	O	0	0
			123	41	72	10		
27	b	1	Total	C	H	O	0	0
			141	45	86	10		
27	c	1	Total	C	H	O	0	0
			81	27	44	10		
27	c	1	Total	C	H	O	0	0
			117	38	69	10		
27	c	1	Total	C	H	O	0	0
			117	39	68	10		
27	d	1	Total	C	H	O	0	0
			57	21	34	2		
27	d	1	Total	C	H	O	0	0
			102	34	58	10		

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



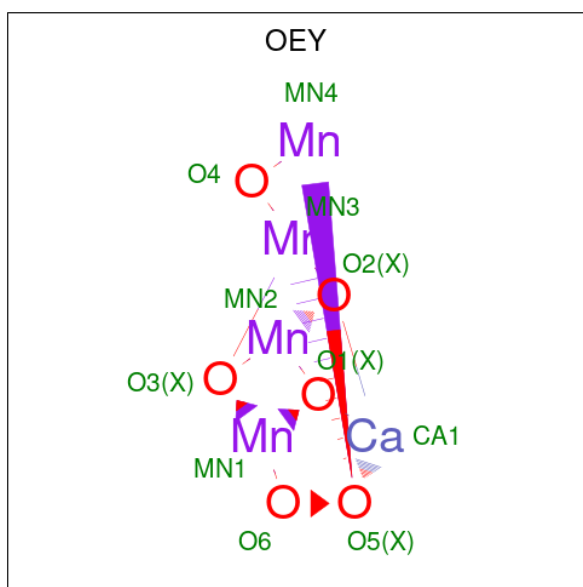
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	S		
28	A	1	123	39	71	12	1	0	0
28	A	1	104	35	65	4		0	0
28	B	1	132	41	78	12	1	0	0
28	F	1	82	25	46	10	1	0	0
28	L	1	114	36	65	12	1	0	0
28	a	1	132	41	78	12	1	0	0
28	a	1	92	31	56	5		0	0
28	f	1	89	28	48	12	1	0	0

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



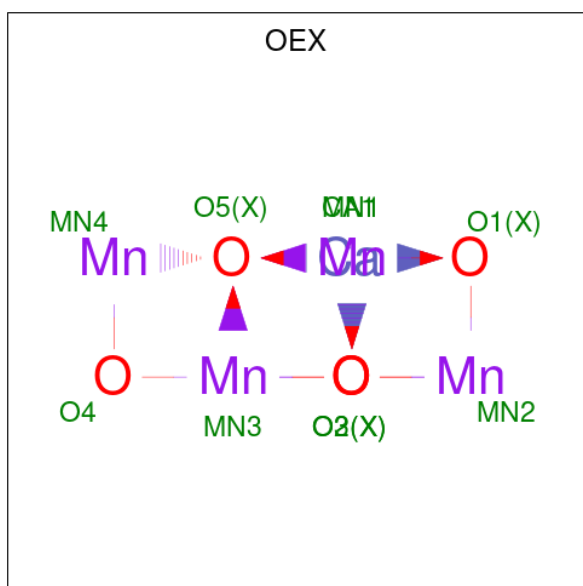
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
29	A	1	Total 162	C 51	H 96	O 15	0	0
29	C	1	Total 144	C 47	H 82	O 15	0	0
29	C	1	Total 144	C 47	H 82	O 15	0	0
29	C	1	Total 144	C 47	H 82	O 15	0	0
29	H	1	Total 144	C 47	H 82	O 15	0	0
29	a	1	Total 119	C 39	H 75	O 5	0	0
29	c	1	Total 144	C 47	H 82	O 15	0	0
29	c	1	Total 144	C 47	H 82	O 15	0	0
29	c	1	Total 144	C 47	H 82	O 15	0	0
29	h	1	Total 144	C 47	H 82	O 15	0	0

- Molecule 30 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula:  $\text{CaMn}_4\text{O}_6$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 31 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ) (labeled as "Ligand of Interest" by depositor).



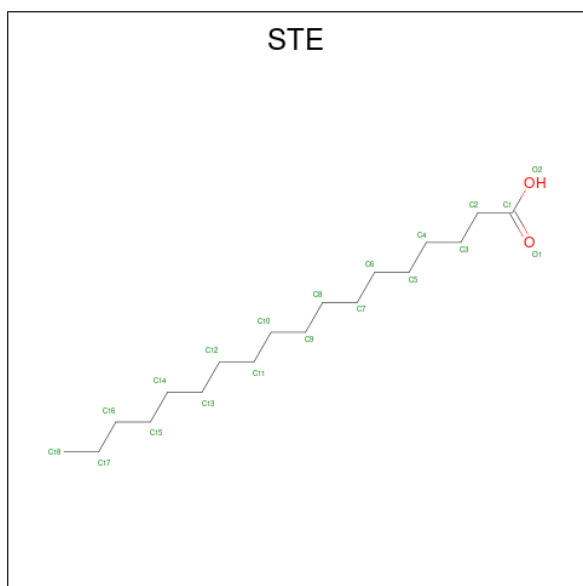
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Ca	Mn	O		
31	A	1	10	1	4	5	0	1

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

- Molecule 32 is STEARIC ACID (three-letter code: STE) (formula: C<sub>18</sub>H<sub>36</sub>O<sub>2</sub>).



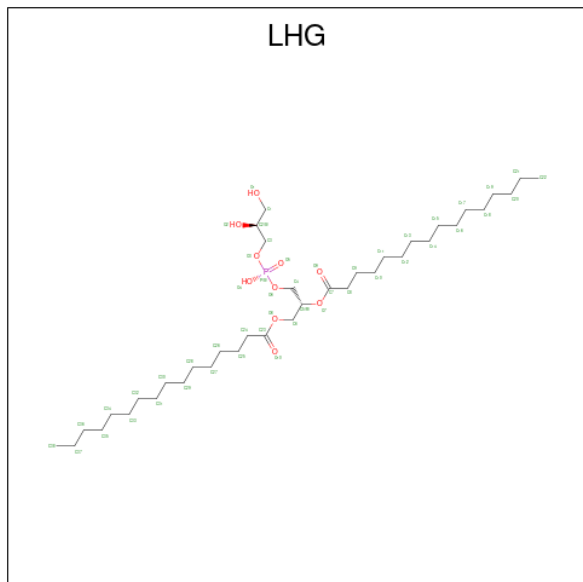
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
32	B	1	43	15	26	2	0	0
32	B	1	28	10	16	2	0	0
32	B	1	46	16	28	2	0	0
32	B	1	47	16	31		0	0
32	B	1	28	10	16	2	0	0
32	C	1	28	10	16	2	0	0
32	C	1	47	16	31		0	0
32	C	1	28	10	16	2	0	0
32	D	1	55	18	35	2	0	0
32	E	1	28	10	16	2	0	0

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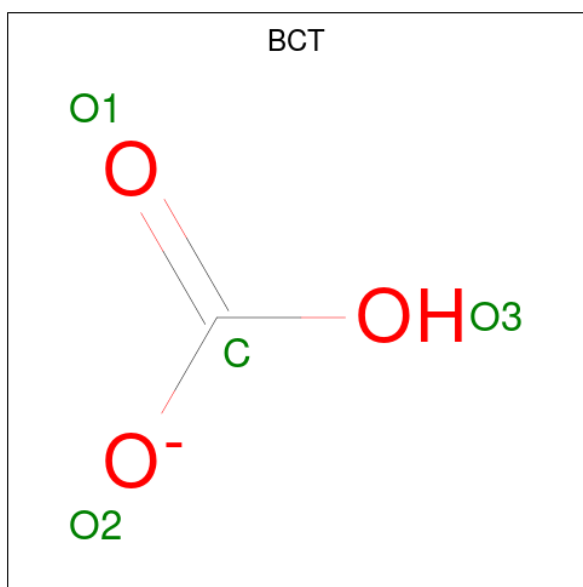
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	H	1	Total C H 53 18 35	0	0
32	I	1	Total C H 41 15 26	0	0
32	J	1	Total C H O 28 10 16 2	0	0
32	M	1	Total C H O 37 13 22 2	0	0
32	M	1	Total C H 26 10 16	0	0
32	T	1	Total C H 47 16 31	0	0
32	T	1	Total C H 44 15 29	0	0
32	a	1	Total C H 26 10 16	0	0
32	a	1	Total C H O 28 10 16 2	0	0
32	b	1	Total C H O 55 18 35 2	0	0
32	b	1	Total C H O 40 14 24 2	0	0
32	b	1	Total C H O 55 18 35 2	0	0
32	b	1	Total C H 26 10 16	0	0
32	c	1	Total C H O 55 18 35 2	0	0
32	c	1	Total C H O 28 10 16 2	0	0
32	d	1	Total C H O 43 15 26 2	0	0
32	j	1	Total C H O 28 10 16 2	0	0
32	l	1	Total C H 53 18 35	0	0
32	m	1	Total C H O 28 10 16 2	0	0
32	t	1	Total C H O 34 12 20 2	0	0
32	x	1	Total C H O 55 18 35 2	0	0

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



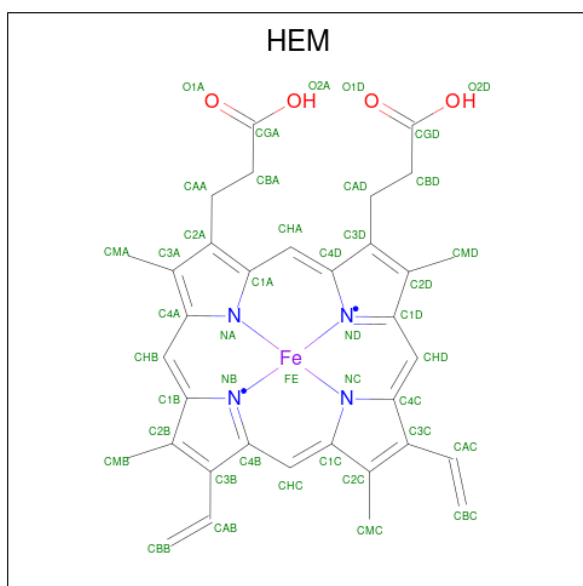
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	P		
33	B	1	Total 123	C 38	H 74	O 10	P 1	0	0
33	D	1	Total 123	C 38	H 74	O 10	P 1	0	0
33	D	1	Total 114	C 36	H 67	O 10	P 1	0	0
33	E	1	Total 123	C 38	H 74	O 10	P 1	0	0
33	L	1	Total 123	C 38	H 74	O 10	P 1	0	0
33	d	1	Total 123	C 38	H 74	O 10	P 1	0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

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



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

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



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	H	42	Total O 42 42	0	0
37	I	12	Total O 12 12	0	0
37	J	13	Total O 13 13	0	0
37	K	4	Total O 4 4	0	0
37	L	9	Total O 9 9	0	0
37	M	9	Total O 9 9	0	0
37	O	99	Total O 99 99	0	0
37	R	4	Total O 4 4	0	0
37	T	9	Total O 9 9	0	0
37	U	33	Total O 33 33	0	0
37	V	64	Total O 64 64	0	0
37	X	14	Total O 14 14	0	0
37	Y	4	Total O 4 4	0	0
37	Z	3	Total O 3 3	0	0
37	a	118	Total O 118 118	0	8
37	b	191	Total O 191 191	0	0
37	c	157	Total O 157 157	0	0
37	d	105	Total O 105 105	0	0
37	e	17	Total O 17 17	0	0
37	f	6	Total O 6 6	0	0
37	h	30	Total O 30 30	0	0

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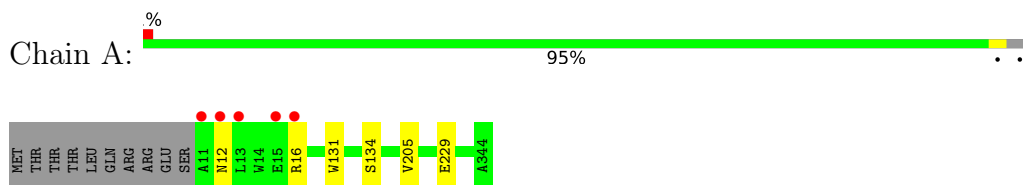
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	i	21	Total 21	O 21	0	0
37	j	6	Total 6	O 6	0	0
37	k	4	Total 4	O 4	0	0
37	l	12	Total 12	O 12	0	0
37	m	5	Total 5	O 5	0	0
37	o	93	Total 93	O 93	0	0
37	r	5	Total 5	O 5	0	0
37	t	8	Total 8	O 8	0	0
37	u	65	Total 65	O 65	0	0
37	v	59	Total 59	O 59	0	0
37	x	9	Total 9	O 9	0	0
37	y	4	Total 4	O 4	0	0

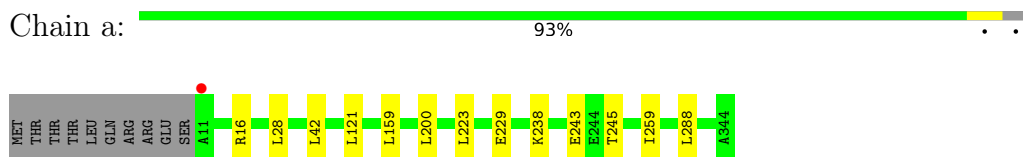
### 3 Residue-property plots [i](#)

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

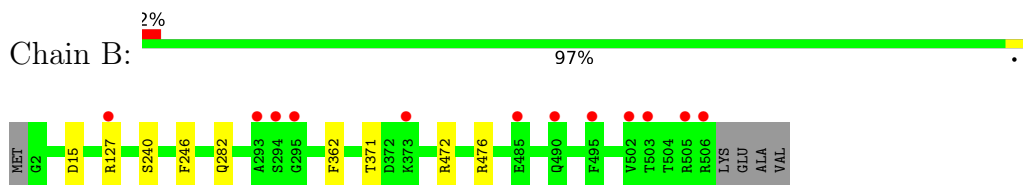
- Molecule 1: Photosystem II protein D1 1



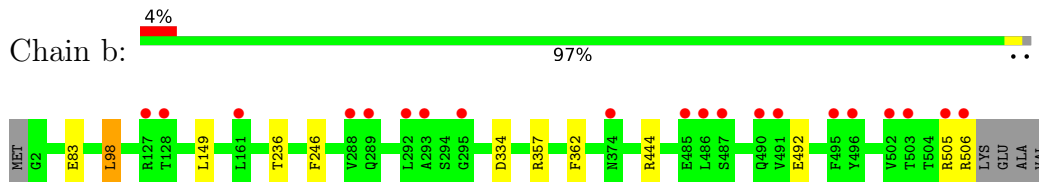
- Molecule 1: Photosystem II protein D1 1



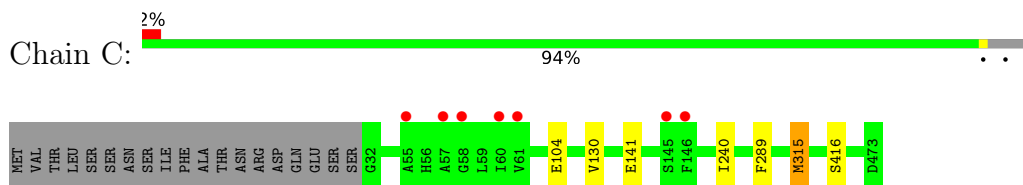
- Molecule 2: Photosystem II CP47 reaction center protein



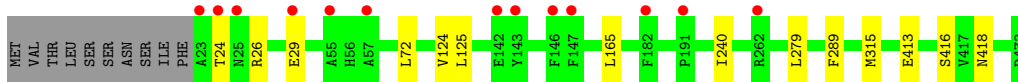
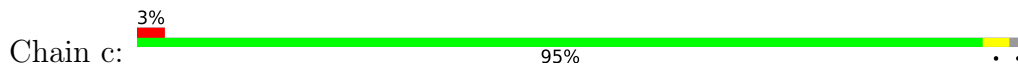
- Molecule 2: Photosystem II CP47 reaction center protein



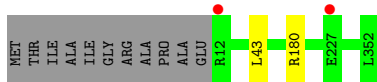
- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein



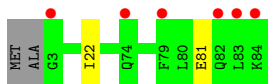
- Molecule 4: Photosystem II D2 protein



- Molecule 4: Photosystem II D2 protein



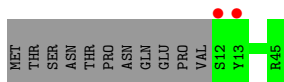
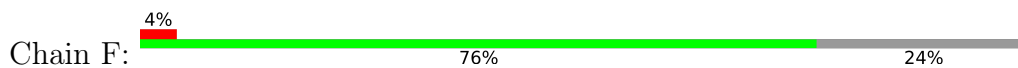
- Molecule 5: Cytochrome b559 subunit alpha



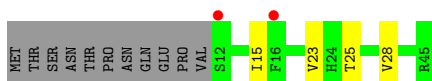
- Molecule 5: Cytochrome b559 subunit alpha



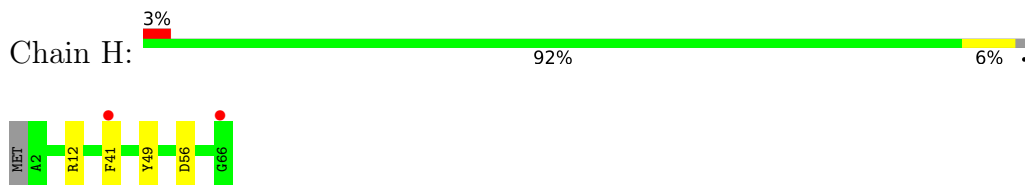
- Molecule 6: Cytochrome b559 subunit beta



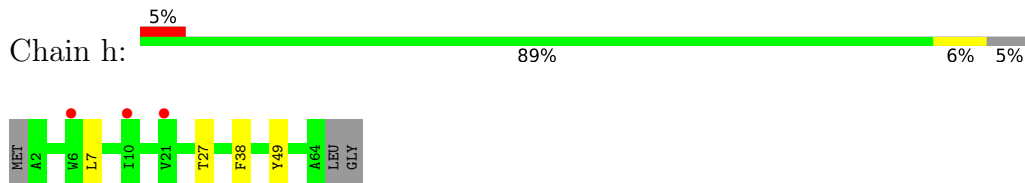
- Molecule 6: Cytochrome b559 subunit beta



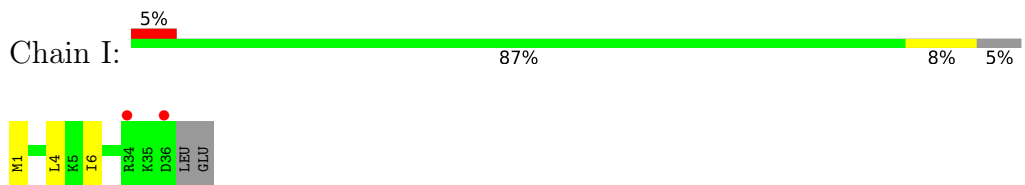
- Molecule 7: Photosystem II reaction center protein H



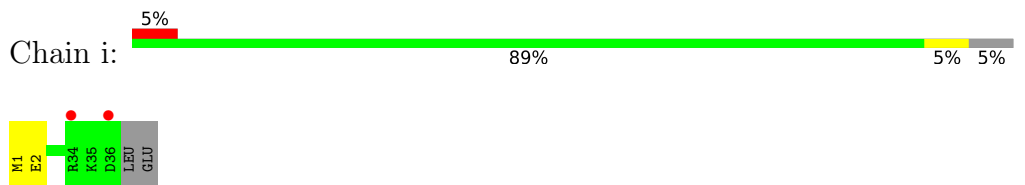
- Molecule 7: Photosystem II reaction center protein H



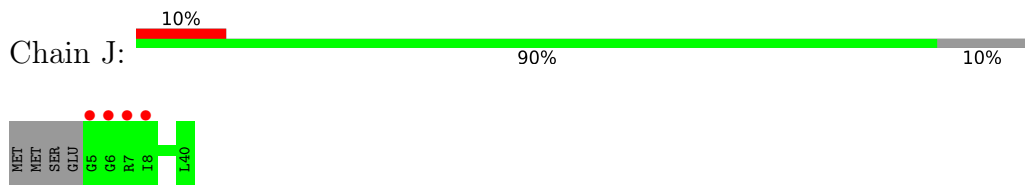
- Molecule 8: Photosystem II reaction center protein I



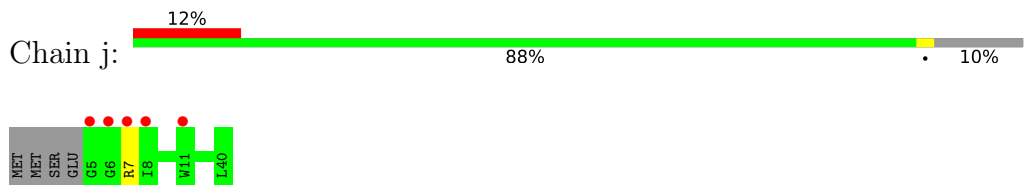
- Molecule 8: Photosystem II reaction center protein I



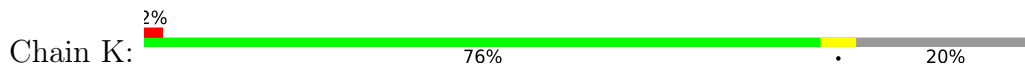
- Molecule 9: Photosystem II reaction center protein J

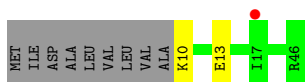


- Molecule 9: Photosystem II reaction center protein J

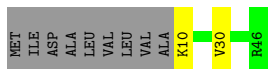


- Molecule 10: Photosystem II reaction center protein K





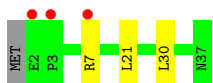
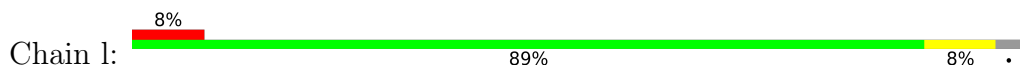
- Molecule 10: Photosystem II reaction center protein K



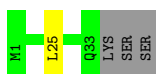
- Molecule 11: Photosystem II reaction center protein L



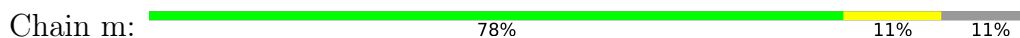
- Molecule 11: Photosystem II reaction center protein L



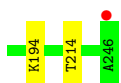
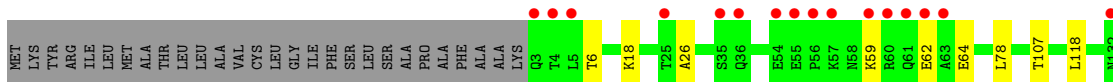
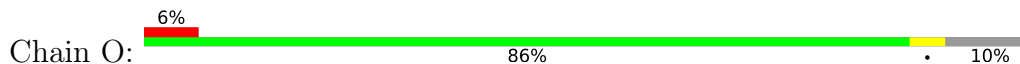
- Molecule 12: Photosystem II reaction center protein M



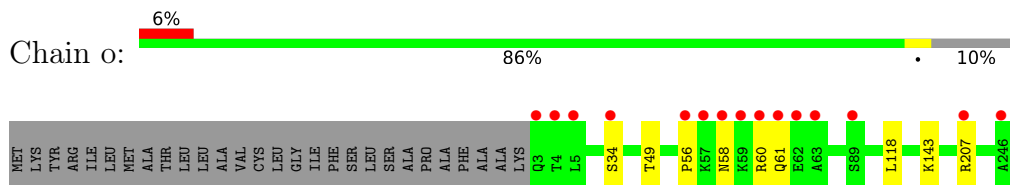
- Molecule 12: Photosystem II reaction center protein M



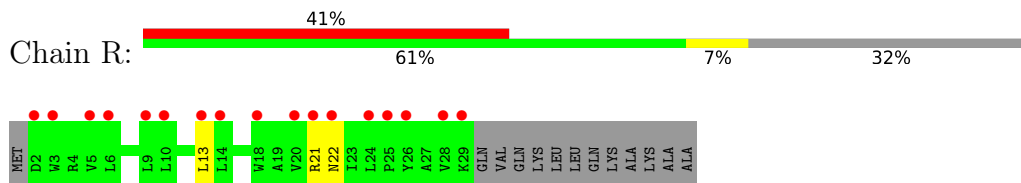
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



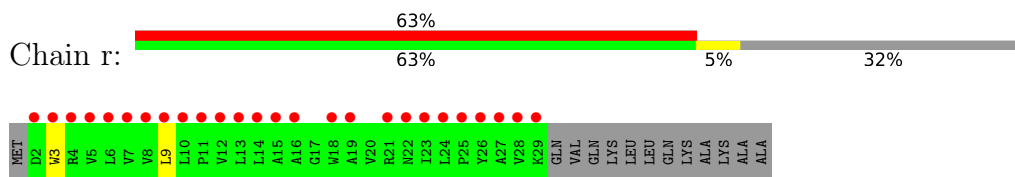
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



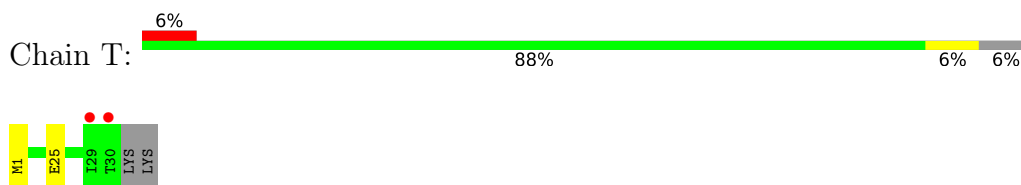
- Molecule 14: Photosystem II protein Y



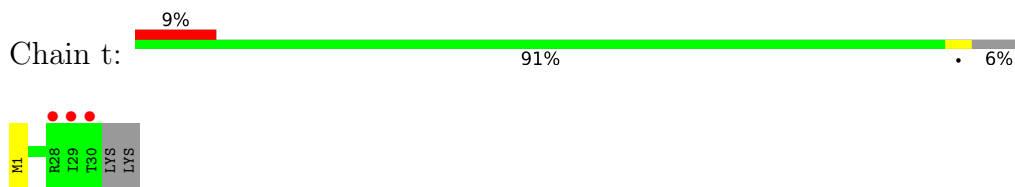
- Molecule 14: Photosystem II protein Y



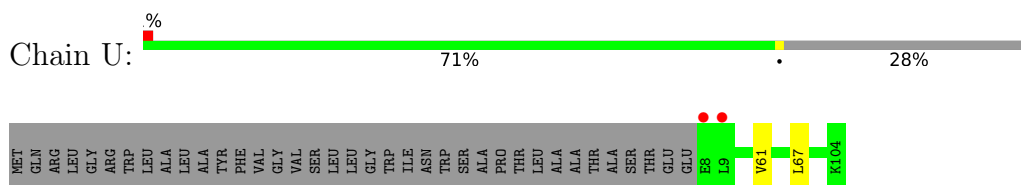
- Molecule 15: Photosystem II reaction center protein T



- Molecule 15: Photosystem II reaction center protein T



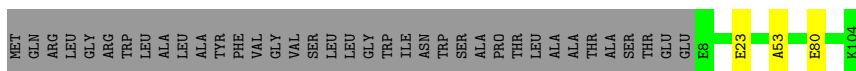
- Molecule 16: Photosystem II 12 kDa extrinsic protein



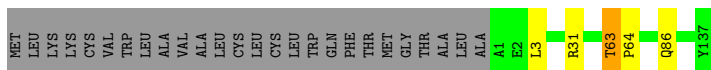
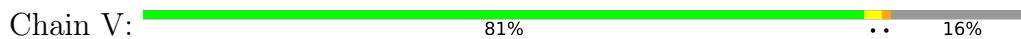
- Molecule 16: Photosystem II 12 kDa extrinsic protein



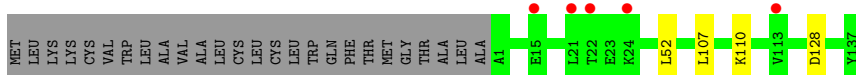
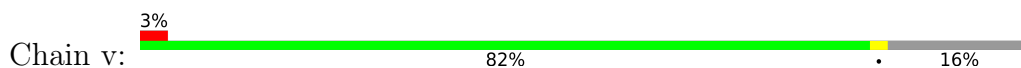




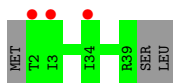
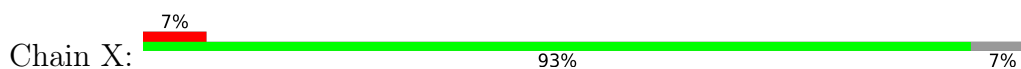
• Molecule 17: Cytochrome c-550



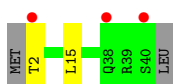
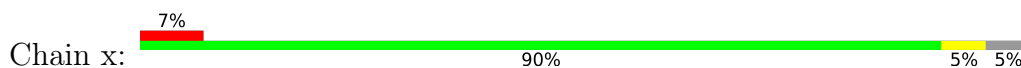
• Molecule 17: Cytochrome c-550



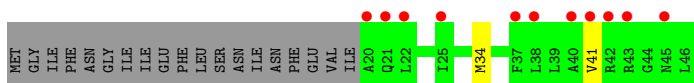
• Molecule 18: Photosystem II reaction center X protein



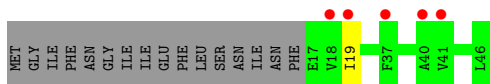
• Molecule 18: Photosystem II reaction center X protein



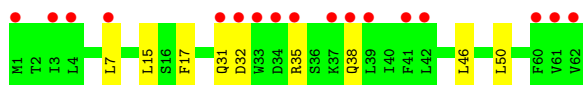
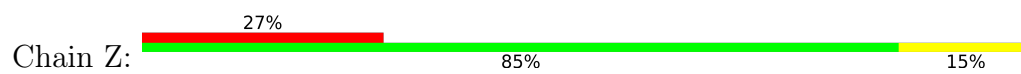
• Molecule 19: Photosystem II reaction center protein Ycf12



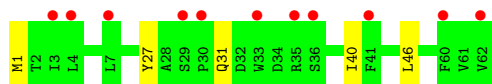
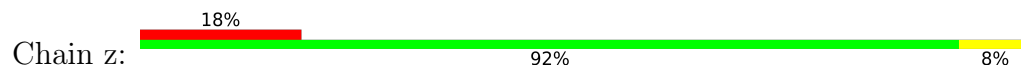
• Molecule 19: Photosystem II reaction center protein Ycf12



• Molecule 20: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II reaction center protein Z



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.96Å 221.65Å 307.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.65 – 2.09 33.65 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.3 (33.65-2.09) 85.3 (33.65-2.09)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.51 (at 2.08Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.181 , 0.239 0.181 , 0.238	Depositor DCC
$R_{free}$ test set	4165 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.1	Xtrriage
Anisotropy	0.219	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 69.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	105937	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: CL, BCR, LMG, OEY, BCT, STE, PL9, LHG, OEX, FE2, DGD, CLA, PHO, HEC, SQD, HEM, FME

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	0/3227	0.66	1/4397 (0.0%)
1	a	0.59	0/3224	0.65	0/4393
2	B	0.63	0/4161	0.68	1/5669 (0.0%)
2	b	0.60	0/4118	0.66	2/5611 (0.0%)
3	C	0.60	0/3647	0.65	1/4965 (0.0%)
3	c	0.56	0/3719	0.65	0/5061
4	D	0.65	0/2825	0.66	0/3847
4	d	0.60	0/2834	0.68	0/3859
5	E	0.58	0/688	0.62	0/940
5	e	0.53	0/683	0.63	0/932
6	F	0.56	0/284	0.58	0/387
6	f	0.53	0/284	0.66	0/387
7	H	0.69	1/523 (0.2%)	0.70	0/713
7	h	0.66	0/511	0.74	0/697
8	I	0.62	0/293	0.67	0/396
8	i	0.78	0/293	0.71	0/396
9	J	0.60	0/263	0.67	0/356
9	j	0.57	0/263	0.68	0/356
10	K	0.57	0/303	0.64	0/416
10	k	0.54	0/303	0.65	0/416
11	L	0.72	0/311	0.73	0/422
11	l	0.71	0/303	0.76	0/412
12	M	0.68	0/249	0.69	0/341
12	m	0.80	0/244	0.70	0/334
13	O	0.67	0/1904	0.77	0/2585
13	o	0.67	0/1905	0.75	0/2583
14	R	0.45	0/227	0.59	0/313
14	r	0.42	0/227	0.60	0/313
15	T	0.78	0/257	0.68	0/349
15	t	0.76	0/255	0.71	0/346
16	U	0.62	0/785	0.71	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	u	0.68	0/785	0.74	0/1064
17	V	0.63	0/1085	0.75	1/1473 (0.1%)
17	v	0.60	0/1085	0.68	0/1473
18	X	0.56	0/284	0.64	0/384
18	x	0.46	0/289	0.58	0/391
19	Y	0.46	0/197	0.63	0/264
19	y	0.41	0/219	0.57	0/294
20	Z	0.51	0/490	0.61	0/669
20	z	0.45	0/488	0.53	0/666
All	All	0.61	1/44035 (0.0%)	0.67	6/59934 (0.0%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	41	PHE	CB-CG	-5.10	1.42	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	98	LEU	CA-CB-CG	5.97	129.04	115.30
17	V	63	THR	C-N-CD	-5.92	107.59	120.60
2	B	15	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	A	131	TRP	CA-CB-CG	-5.18	103.86	113.70
2	b	334	ASP	CB-CG-OD1	5.09	122.89	118.30
3	C	315	MET	CG-SD-CE	-5.02	92.17	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	V	63	THR	Peptide

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	397/344 (115%)	390 (98%)	7 (2%)	0	100	100
1	a	397/344 (115%)	388 (98%)	8 (2%)	1 (0%)	41	41
2	B	508/510 (100%)	500 (98%)	8 (2%)	0	100	100
2	b	503/510 (99%)	492 (98%)	11 (2%)	0	100	100
3	C	454/461 (98%)	440 (97%)	13 (3%)	1 (0%)	47	49
3	c	463/461 (100%)	448 (97%)	14 (3%)	1 (0%)	47	49
4	D	340/352 (97%)	331 (97%)	9 (3%)	0	100	100
4	d	341/352 (97%)	332 (97%)	9 (3%)	0	100	100
5	E	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
5	e	80/84 (95%)	77 (96%)	3 (4%)	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	31 (97%)	1 (3%)	0	100	100
7	H	63/66 (96%)	59 (94%)	3 (5%)	1 (2%)	9	5
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
10	k	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	227 (93%)	13 (5%)	3 (1%)	13	8
13	o	242/272 (89%)	231 (96%)	8 (3%)	3 (1%)	13	8
14	R	26/41 (63%)	26 (100%)	0	0	100	100
14	r	26/41 (63%)	26 (100%)	0	0	100	100
15	T	28/32 (88%)	28 (100%)	0	0	100	100
15	t	28/32 (88%)	28 (100%)	0	0	100	100
16	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
16	u	95/134 (71%)	90 (95%)	4 (4%)	1 (1%)	14	9
17	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	22	18
17	v	135/163 (83%)	132 (98%)	3 (2%)	0	100	100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Y	25/46 (54%)	23 (92%)	2 (8%)	0	100	100
19	y	28/46 (61%)	26 (93%)	2 (7%)	0	100	100
20	Z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
20	z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
All	All	5387/5700 (94%)	5225 (97%)	150 (3%)	12 (0%)	47	49

All (12) 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
13	O	62	GLU
16	u	53	ALA
13	o	61	GLN
13	O	26	ALA
13	o	58	ASN
7	H	12	ARG
1	a	259	ILE

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Mol	Chain	Res	Type
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	324/280 (116%)	319 (98%)	5 (2%)	65	71
1	a	323/280 (115%)	310 (96%)	13 (4%)	31	32
2	B	408/407 (100%)	400 (98%)	8 (2%)	55	60
2	b	402/407 (99%)	391 (97%)	11 (3%)	44	48
3	C	356/362 (98%)	350 (98%)	6 (2%)	60	67
3	c	364/362 (101%)	350 (96%)	14 (4%)	33	34
4	D	277/283 (98%)	275 (99%)	2 (1%)	84	88
4	d	278/283 (98%)	269 (97%)	9 (3%)	39	41
5	E	72/73 (99%)	69 (96%)	3 (4%)	30	30
5	e	71/73 (97%)	69 (97%)	2 (3%)	43	47
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	24 (86%)	4 (14%)	3	1
7	H	54/55 (98%)	52 (96%)	2 (4%)	34	35
7	h	53/55 (96%)	49 (92%)	4 (8%)	13	10
8	I	32/34 (94%)	30 (94%)	2 (6%)	18	15
8	i	32/34 (94%)	31 (97%)	1 (3%)	40	43
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%)	28 (93%)	2 (7%)	16	13
11	L	35/35 (100%)	33 (94%)	2 (6%)	20	18
11	l	34/35 (97%)	31 (91%)	3 (9%)	10	6
12	M	28/32 (88%)	27 (96%)	1 (4%)	35	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	m	28/32 (88%)	25 (89%)	3 (11%)	6	3
13	O	206/228 (90%)	198 (96%)	8 (4%)	32	33
13	o	207/228 (91%)	201 (97%)	6 (3%)	42	46
14	R	22/33 (67%)	19 (86%)	3 (14%)	3	2
14	r	22/33 (67%)	20 (91%)	2 (9%)	9	6
15	T	26/28 (93%)	25 (96%)	1 (4%)	33	34
15	t	25/28 (89%)	25 (100%)	0	100	100
16	U	84/112 (75%)	82 (98%)	2 (2%)	49	53
16	u	84/112 (75%)	82 (98%)	2 (2%)	49	53
17	V	117/138 (85%)	114 (97%)	3 (3%)	46	50
17	v	117/138 (85%)	113 (97%)	4 (3%)	37	39
18	X	31/34 (91%)	31 (100%)	0	100	100
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%)	21 (96%)	1 (4%)	27	27
20	Z	52/52 (100%)	43 (83%)	9 (17%)	2	1
20	z	51/52 (98%)	46 (90%)	5 (10%)	8	5
All	All	4451/4654 (96%)	4301 (97%)	150 (3%)	37	39

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

Mol	Chain	Res	Type
1	A	12	ASN
1	A	16	ARG
1	A	134	SER
1	A	205	VAL
1	A	229	GLU
2	B	127	ARG
2	B	240	SER
2	B	246	PHE
2	B	282	GLN
2	B	362	PHE
2	B	371	THR
2	B	472	ARG
2	B	476	ARG
3	C	104	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	130	VAL
3	C	141	GLU
3	C	240	ILE
3	C	289	PHE
3	C	315	MET
4	D	43	LEU
4	D	180	ARG
5	E	22[A]	ILE
5	E	22[B]	ILE
5	E	81	GLU
7	H	49	TYR
7	H	56	ASP
8	I	4	LEU
8	I	6	ILE
10	K	10	LYS
10	K	13	GLU
11	L	9	PRO
11	L	10	VAL
12	M	25	LEU
13	O	6	THR
13	O	18	LYS
13	O	64	GLU
13	O	78	LEU
13	O	107	THR
13	O	118	LEU
13	O	194	LYS
13	O	214	THR
14	R	13	LEU
14	R	21	ARG
14	R	22	ASN
15	T	25	GLU
16	U	61	VAL
16	U	67	LEU
17	V	3	LEU
17	V	31	ARG
17	V	86	GLN
19	Y	34	MET
19	Y	41	VAL
20	Z	7	LEU
20	Z	15	LEU
20	Z	17	PHE
20	Z	31	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
20	Z	32	ASP
20	Z	35	ARG
20	Z	38	GLN
20	Z	46	LEU
20	Z	50	LEU
1	a	16	ARG
1	a	28	LEU
1	a	42	LEU
1	a	121	LEU
1	a	159[A]	LEU
1	a	159[B]	LEU
1	a	200	LEU
1	a	223	LEU
1	a	229	GLU
1	a	238	LYS
1	a	243	GLU
1	a	245	THR
1	a	288	LEU
2	b	83	GLU
2	b	98	LEU
2	b	149	LEU
2	b	236	THR
2	b	246	PHE
2	b	357	ARG
2	b	362	PHE
2	b	444	ARG
2	b	492	GLU
2	b	505	ARG
2	b	506	ARG
3	c	24	THR
3	c	26	ARG
3	c	29	GLU
3	c	72	LEU
3	c	124	VAL
3	c	125	LEU
3	c	165	LEU
3	c	240	ILE
3	c	279	LEU
3	c	289	PHE
3	c	315	MET
3	c	413[A]	GLU
3	c	413[B]	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	c	418	ASN
4	d	180	ARG
4	d	182	LEU
4	d	230	SER
4	d	233	ARG
4	d	259	ILE
4	d	291	LEU
4	d	293	LEU
4	d	307	GLU
4	d	321	LEU
5	e	4	THR
5	e	66	VAL
6	f	15	ILE
6	f	23	VAL
6	f	25	THR
6	f	28	VAL
7	h	7	LEU
7	h	27	THR
7	h	38	PHE
7	h	49	TYR
8	i	2	GLU
9	j	7	ARG
10	k	10	LYS
10	k	30	VAL
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
12	m	2	GLU
12	m	13	LEU
12	m	16	LEU
13	o	34	SER
13	o	49	THR
13	o	60	ARG
13	o	118	LEU
13	o	143	LYS
13	o	207	ARG
14	r	3	TRP
14	r	9	LEU
16	u	23	GLU
16	u	80	GLU
17	v	52	LEU
17	v	107	LEU

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Mol	Chain	Res	Type
17	v	110	LYS
17	v	128	ASP
18	x	2	THR
18	x	15	LEU
19	y	19	ILE
20	z	1	MET
20	z	27	TYR
20	z	31	GLN
20	z	40	ILE
20	z	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	61	HIS
7	H	59	ASN
13	O	36	GLN
13	O	88	ASN
17	V	86	GLN
20	Z	38	GLN
2	b	179	GLN
2	b	490	GLN
5	e	74	GLN
13	o	61	GLN
20	z	31	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
8	FME	I	1	8	8,9,10	0.95	0	7,9,11	1.30	1 (14%)
15	FME	T	1	15	8,9,10	1.13	1 (12%)	7,9,11	1.09	0
12	FME	M	1	12	8,9,10	0.87	0	7,9,11	1.03	0
8	FME	i	1	8	8,9,10	0.98	0	7,9,11	1.53	1 (14%)
12	FME	m	1	12	8,9,10	1.05	1 (12%)	7,9,11	1.12	0
15	FME	t	1	15	8,9,10	1.68	1 (12%)	7,9,11	0.80	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
8	FME	I	1	8	-	1/7/9/11	-
15	FME	T	1	15	-	1/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
8	FME	i	1	8	-	4/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
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	-4.20	1.40	1.46
12	m	1	FME	CA-N	-2.22	1.43	1.46
15	T	1	FME	CA-N	-2.17	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	C-CA-N	2.62	114.46	109.73
8	I	1	FME	CA-N-CN	-2.47	119.02	122.82

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 188 ligands modelled in this entry, 6 are monoatomic - leaving 182 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	c	505	-	65,73,73	1.38	8 (12%)	76,113,113	1.36	8 (10%)
22	CLA	C	512	-	65,73,73	1.65	12 (18%)	76,113,113	1.40	10 (13%)
22	CLA	C	503	-	65,73,73	1.83	9 (13%)	76,113,113	1.54	13 (17%)
22	CLA	b	615	-	65,73,73	1.66	13 (20%)	76,113,113	1.43	10 (13%)
30	OEY	A	415[B]	37,3,1	0,16,16	-	-	-	-	-
24	BCR	t	101	-	41,41,41	1.15	4 (9%)	56,56,56	1.46	10 (17%)
32	STE	T	102	-	15,15,19	0.50	0	14,14,19	0.70	0
36	HEC	V	201	17	32,50,50	2.10	3 (9%)	24,82,82	1.98	5 (20%)
24	BCR	A	406	-	41,41,41	1.18	2 (4%)	56,56,56	1.46	10 (17%)
27	LMG	b	620	-	51,51,55	1.13	6 (11%)	59,59,63	1.51	11 (18%)
22	CLA	B	601	37	65,73,73	1.78	9 (13%)	76,113,113	1.47	7 (9%)
22	CLA	b	614	-	65,73,73	1.75	9 (13%)	76,113,113	1.41	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	B	607	37	65,73,73	1.63	12 (18%)	76,113,113	1.58	8 (10%)
32	STE	B	627	-	11,11,19	1.03	1 (9%)	11,11,19	0.72	0
29	DGD	c	518	-	63,63,67	1.32	9 (14%)	77,77,81	1.53	10 (12%)
32	STE	b	624	-	19,19,19	0.83	0	19,19,19	0.88	1 (5%)
27	LMG	C	519	-	48,48,55	1.18	7 (14%)	56,56,63	1.43	7 (12%)
22	CLA	A	410	37	65,73,73	1.48	6 (9%)	76,113,113	1.35	7 (9%)
22	CLA	B	605	-	65,73,73	1.49	11 (16%)	76,113,113	1.35	6 (7%)
33	LHG	B	622	-	48,48,48	1.01	4 (8%)	51,54,54	1.40	6 (11%)
22	CLA	B	614	-	65,73,73	1.73	11 (16%)	76,113,113	1.29	11 (14%)
22	CLA	C	509	-	65,73,73	1.58	12 (18%)	76,113,113	1.56	12 (15%)
24	BCR	b	617	-	41,41,41	1.05	3 (7%)	56,56,56	1.45	10 (17%)
27	LMG	A	411	-	48,48,55	0.99	3 (6%)	56,56,63	1.32	7 (12%)
28	SQD	B	623	-	53,54,54	1.00	3 (5%)	62,65,65	1.86	11 (17%)
32	STE	I	101	-	14,14,19	0.60	0	13,13,19	0.39	0
26	PL9	d	407	-	55,55,55	1.39	6 (10%)	68,69,69	1.85	18 (26%)
22	CLA	B	616	-	60,68,73	1.54	9 (15%)	70,107,113	1.82	11 (15%)
31	OEX	a	416[A]	37,3,1	0,15,15	-	-	-	-	-
32	STE	c	521	-	19,19,19	0.77	1 (5%)	19,19,19	0.94	0
23	PHO	d	401	-	51,69,69	1.06	4 (7%)	47,99,99	1.27	5 (10%)
22	CLA	c	501	-	65,73,73	1.47	9 (13%)	76,113,113	1.52	10 (13%)
22	CLA	b	601	37	65,73,73	1.59	8 (12%)	76,113,113	1.62	7 (9%)
27	LMG	D	407	-	51,51,55	1.18	4 (7%)	59,59,63	1.34	9 (15%)
22	CLA	C	511	3	65,73,73	1.60	9 (13%)	76,113,113	1.36	7 (9%)
22	CLA	c	509	-	65,73,73	1.57	8 (12%)	76,113,113	1.79	10 (13%)
24	BCR	K	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.39	7 (12%)
35	HEM	f	101	6,5	41,50,50	1.50	5 (12%)	45,82,82	1.53	7 (15%)
22	CLA	A	402	-	65,73,73	1.48	7 (10%)	76,113,113	1.49	11 (14%)
22	CLA	B	613	-	65,73,73	1.56	9 (13%)	76,113,113	1.56	11 (14%)
28	SQD	a	411	-	35,35,54	1.10	2 (5%)	37,37,65	1.18	5 (13%)
29	DGD	c	519	-	63,63,67	1.38	10 (15%)	77,77,81	1.44	12 (15%)
22	CLA	d	405	-	65,73,73	1.46	10 (15%)	76,113,113	1.34	6 (7%)
33	LHG	D	409	-	46,46,48	1.09	3 (6%)	49,52,54	1.12	3 (6%)
22	CLA	B	612	-	65,73,73	1.44	9 (13%)	76,113,113	1.51	9 (11%)
27	LMG	c	520	-	37,37,55	1.26	6 (16%)	45,45,63	1.31	6 (13%)
24	BCR	B	619	-	41,41,41	1.10	3 (7%)	56,56,56	1.38	5 (8%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	BCR	C	514	-	41,41,41	1.20	4 (9%)	56,56,56	1.33	5 (8%)
32	STE	d	413	-	16,16,19	0.74	0	16,16,19	1.12	1 (6%)
22	CLA	b	603	-	65,73,73	1.54	12 (18%)	76,113,113	1.56	9 (11%)
33	LHG	d	410	-	38,38,48	0.88	3 (7%)	41,44,54	1.12	3 (7%)
22	CLA	b	606	-	65,73,73	1.46	8 (12%)	76,113,113	1.71	9 (11%)
22	CLA	c	502	-	65,73,73	1.54	10 (15%)	76,113,113	1.47	11 (14%)
24	BCR	H	101	-	41,41,41	1.13	1 (2%)	56,56,56	1.28	8 (14%)
22	CLA	C	501	-	65,73,73	1.64	11 (16%)	76,113,113	1.58	10 (13%)
29	DGD	C	516	-	63,63,67	1.36	11 (17%)	77,77,81	1.40	10 (12%)
27	LMG	b	622	-	55,55,55	1.03	7 (12%)	63,63,63	1.44	7 (11%)
22	CLA	b	607	37	65,73,73	1.64	11 (16%)	76,113,113	1.29	8 (10%)
32	STE	M	103	-	9,9,19	0.50	0	8,8,19	0.60	0
32	STE	l	102	-	17,17,19	0.44	0	16,16,19	0.81	0
24	BCR	B	618	-	41,41,41	1.23	4 (9%)	56,56,56	1.18	7 (12%)
22	CLA	c	510	-	65,73,73	1.45	12 (18%)	76,113,113	1.52	9 (11%)
24	BCR	C	515	-	41,41,41	1.16	4 (9%)	56,56,56	1.13	3 (5%)
32	STE	a	414	-	11,11,19	0.76	0	11,11,19	1.13	1 (9%)
22	CLA	b	609	-	65,73,73	1.52	10 (15%)	76,113,113	1.42	8 (10%)
26	PL9	a	409	-	55,55,55	0.93	2 (3%)	68,69,69	1.69	18 (26%)
29	DGD	a	412	-	43,43,67	1.13	3 (6%)	45,45,81	1.45	7 (15%)
29	DGD	c	517	-	63,63,67	1.09	7 (11%)	77,77,81	1.35	7 (9%)
22	CLA	C	504	37	59,67,73	1.51	6 (10%)	68,105,113	1.33	7 (10%)
30	OEY	a	415[B]	37,3,1	0,16,16	-	-	-	-	-
32	STE	J	101	-	11,11,19	0.67	0	11,11,19	1.40	1 (9%)
33	LHG	e	101	-	41,41,48	0.86	1 (2%)	44,47,54	1.26	4 (9%)
28	SQD	L	101	-	48,49,54	1.00	3 (6%)	57,60,65	2.31	17 (29%)
24	BCR	c	515	-	41,41,41	1.22	3 (7%)	56,56,56	1.42	10 (17%)
32	STE	c	524	-	11,11,19	0.73	0	11,11,19	1.20	1 (9%)
22	CLA	C	510	-	65,73,73	1.44	7 (10%)	76,113,113	1.37	9 (11%)
29	DGD	h	102	-	63,63,67	1.29	11 (17%)	77,77,81	1.54	13 (16%)
34	BCT	D	402	21	2,3,3	1.03	0	2,3,3	3.62	2 (100%)
24	BCR	a	405	-	41,41,41	1.17	5 (12%)	56,56,56	1.42	8 (14%)
32	STE	B	624	-	11,11,19	0.84	0	11,11,19	0.97	1 (9%)
22	CLA	b	605	-	65,73,73	1.46	9 (13%)	76,113,113	1.51	16 (21%)
23	PHO	A	404	-	51,69,69	1.09	4 (7%)	47,99,99	1.50	11 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	DGD	A	414	-	67,67,67	1.38	7 (10%)	81,81,81	1.50	12 (14%)
22	CLA	B	602	-	65,73,73	1.61	9 (13%)	76,113,113	1.68	12 (15%)
33	LHG	l	101	-	48,48,48	0.85	1 (2%)	51,54,54	1.15	5 (9%)
24	BCR	B	617	-	41,41,41	1.17	3 (7%)	56,56,56	1.25	6 (10%)
33	LHG	d	409	-	48,48,48	0.74	1 (2%)	51,54,54	1.13	4 (7%)
29	DGD	C	517	-	63,63,67	1.39	7 (11%)	77,77,81	1.58	14 (18%)
28	SQD	a	410	-	53,54,54	0.95	4 (7%)	62,65,65	2.05	13 (20%)
26	PL9	D	406	-	55,55,55	1.46	6 (10%)	68,69,69	1.63	13 (19%)
29	DGD	C	518	-	63,63,67	1.15	9 (14%)	77,77,81	1.36	10 (12%)
32	STE	T	103	-	14,14,19	0.42	0	13,13,19	0.89	0
36	HEC	v	201	17	32,50,50	2.22	6 (18%)	24,82,82	1.58	4 (16%)
22	CLA	b	610	37	65,73,73	1.41	10 (15%)	76,113,113	1.44	15 (19%)
22	CLA	b	608	-	65,73,73	1.39	9 (13%)	76,113,113	1.57	12 (15%)
22	CLA	c	506	-	65,73,73	1.50	12 (18%)	76,113,113	1.41	9 (11%)
28	SQD	A	412	-	51,52,54	1.02	3 (5%)	60,63,65	2.11	12 (20%)
32	STE	m	101	-	11,11,19	0.68	0	11,11,19	1.67	3 (27%)
33	LHG	d	408	-	48,48,48	1.03	3 (6%)	51,54,54	1.45	8 (15%)
22	CLA	a	402	-	65,73,73	1.60	9 (13%)	76,113,113	1.47	11 (14%)
22	CLA	A	403	37	65,73,73	1.64	10 (15%)	76,113,113	1.28	9 (11%)
22	CLA	d	403	-	65,73,73	1.46	8 (12%)	76,113,113	1.30	7 (9%)
23	PHO	D	401	-	51,69,69	1.09	6 (11%)	47,99,99	1.38	8 (17%)
31	OEX	A	416[A]	37,3,1	0,15,15	-	-	-	-	-
32	STE	C	522	-	11,11,19	0.57	0	11,11,19	1.66	3 (27%)
32	STE	B	625	-	17,17,19	0.63	0	17,17,19	0.99	0
24	BCR	D	405	-	41,41,41	1.16	2 (4%)	56,56,56	1.13	5 (8%)
24	BCR	c	514	-	41,41,41	1.22	2 (4%)	56,56,56	1.33	8 (14%)
27	LMG	B	621	-	26,26,55	0.93	1 (3%)	26,26,63	1.14	1 (3%)
32	STE	B	626	-	15,15,19	0.46	0	14,14,19	0.73	0
22	CLA	b	612	-	65,73,73	1.38	8 (12%)	76,113,113	1.54	11 (14%)
22	CLA	C	505	-	65,73,73	1.62	9 (13%)	76,113,113	1.37	6 (7%)
22	CLA	D	403	-	65,73,73	1.58	9 (13%)	76,113,113	1.37	10 (13%)
32	STE	C	521	-	15,15,19	0.54	0	14,14,19	0.51	0
32	STE	D	411	-	19,19,19	0.66	1 (5%)	19,19,19	1.06	0
27	LMG	d	412	-	44,44,55	1.21	6 (13%)	52,52,63	1.39	8 (15%)
35	HEM	E	101	6,5	41,50,50	1.53	5 (12%)	45,82,82	1.33	7 (15%)
33	LHG	L	102	-	48,48,48	1.00	2 (4%)	51,54,54	1.23	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	b	611	-	65,73,73	1.48	11 (16%)	76,113,113	1.50	8 (10%)
27	LMG	M	101	-	51,51,55	1.10	5 (9%)	59,59,63	1.41	7 (11%)
32	STE	x	101	-	19,19,19	0.79	0	19,19,19	0.66	0
32	STE	b	623	-	15,15,19	0.92	1 (6%)	15,15,19	0.93	1 (6%)
22	CLA	c	513	-	65,73,73	1.58	8 (12%)	76,113,113	1.43	10 (13%)
22	CLA	c	507	37	65,73,73	1.48	10 (15%)	76,113,113	1.23	9 (11%)
28	SQD	F	101	-	35,36,54	1.02	3 (8%)	42,45,65	1.95	9 (21%)
22	CLA	b	613	-	65,73,73	1.68	9 (13%)	76,113,113	1.54	13 (17%)
22	CLA	c	511	3	65,73,73	1.74	8 (12%)	76,113,113	1.53	7 (9%)
22	CLA	B	609	-	65,73,73	1.32	8 (12%)	76,113,113	1.31	9 (11%)
22	CLA	C	502	-	65,73,73	1.46	8 (12%)	76,113,113	1.20	4 (5%)
24	BCR	T	101	-	41,41,41	1.28	4 (9%)	56,56,56	1.25	6 (10%)
24	BCR	b	619	-	41,41,41	1.19	2 (4%)	56,56,56	1.43	11 (19%)
32	STE	M	102	-	14,14,19	0.82	0	14,14,19	1.06	0
22	CLA	B	606	-	65,73,73	1.57	9 (13%)	76,113,113	1.43	13 (17%)
22	CLA	B	610	37	65,73,73	1.49	7 (10%)	76,113,113	1.53	11 (14%)
23	PHO	d	402	-	51,69,69	1.06	4 (7%)	47,99,99	1.51	7 (14%)
32	STE	b	625	-	9,9,19	0.59	0	8,8,19	0.46	0
22	CLA	B	615	-	65,73,73	1.78	9 (13%)	76,113,113	1.51	10 (13%)
33	LHG	D	408	-	48,48,48	0.97	5 (10%)	51,54,54	1.28	5 (9%)
22	CLA	b	616	-	60,68,73	1.40	8 (13%)	70,107,113	1.74	10 (14%)
22	CLA	C	513	-	65,73,73	1.50	8 (12%)	76,113,113	1.57	9 (11%)
32	STE	t	102	-	13,13,19	0.68	0	13,13,19	1.16	1 (7%)
27	LMG	d	411	-	21,21,55	0.78	0	20,20,63	1.22	1 (5%)
22	CLA	C	507	37	65,73,73	1.34	6 (9%)	76,113,113	1.71	11 (14%)
32	STE	j	101	-	11,11,19	0.81	0	11,11,19	1.64	3 (27%)
22	CLA	b	602	-	65,73,73	1.44	9 (13%)	76,113,113	1.57	12 (15%)
24	BCR	b	618	-	41,41,41	1.31	4 (9%)	56,56,56	1.24	4 (7%)
22	CLA	A	405	-	54,62,73	1.82	10 (18%)	62,99,113	1.69	12 (19%)
22	CLA	B	611	-	65,73,73	1.29	7 (10%)	76,113,113	1.52	14 (18%)
22	CLA	b	604	-	65,73,73	1.60	8 (12%)	76,113,113	1.63	12 (15%)
24	BCR	d	406	-	41,41,41	1.14	2 (4%)	56,56,56	1.28	5 (8%)
27	LMG	c	523	-	49,49,55	1.03	4 (8%)	57,57,63	1.27	6 (10%)
22	CLA	B	608	-	65,73,73	1.50	9 (13%)	76,113,113	1.69	11 (14%)
32	STE	C	520	-	11,11,19	0.72	0	11,11,19	1.55	2 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	BCR	Y	101	-	41,41,41	0.99	2 (4%)	56,56,56	1.21	4 (7%)
27	LMG	c	522	-	48,48,55	1.19	5 (10%)	56,56,63	1.37	8 (14%)
27	LMG	D	410	-	31,31,55	1.14	3 (9%)	33,33,63	1.09	2 (6%)
22	CLA	c	503	-	65,73,73	1.46	10 (15%)	76,113,113	1.49	8 (10%)
22	CLA	a	403	37	65,73,73	1.61	7 (10%)	76,113,113	1.61	13 (17%)
34	BCT	a	408	21	2,3,3	1.30	0	2,3,3	3.41	2 (100%)
22	CLA	C	506	-	65,73,73	1.63	11 (16%)	76,113,113	1.43	7 (9%)
22	CLA	B	603	-	65,73,73	1.54	14 (21%)	76,113,113	1.54	16 (21%)
24	BCR	h	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.31	9 (16%)
26	PL9	A	409	-	55,55,55	1.15	3 (5%)	68,69,69	1.62	14 (20%)
22	CLA	c	504	37	60,68,73	1.69	7 (11%)	70,107,113	1.49	5 (7%)
22	CLA	C	508	-	65,73,73	1.67	11 (16%)	76,113,113	1.52	7 (9%)
32	STE	B	620	-	16,16,19	0.69	0	16,16,19	1.06	0
32	STE	H	103	-	17,17,19	0.56	0	16,16,19	0.59	0
24	BCR	c	516	-	41,41,41	1.09	2 (4%)	56,56,56	1.17	6 (10%)
29	DGD	H	102	-	63,63,67	1.39	9 (14%)	77,77,81	1.43	8 (10%)
22	CLA	D	404	-	65,73,73	1.48	10 (15%)	76,113,113	1.60	6 (7%)
24	BCR	k	101	-	41,41,41	1.08	3 (7%)	56,56,56	1.12	3 (5%)
28	SQD	f	102	-	40,41,54	1.19	5 (12%)	49,52,65	1.83	11 (22%)
28	SQD	A	413	-	38,38,54	1.03	3 (7%)	40,40,65	1.46	6 (15%)
32	STE	a	413	-	9,9,19	0.64	0	8,8,19	0.41	0
33	LHG	E	102	-	48,48,48	0.86	3 (6%)	51,54,54	1.18	3 (5%)
22	CLA	c	508	-	64,72,73	1.59	9 (14%)	74,111,113	1.59	12 (16%)
22	CLA	c	512	-	65,73,73	1.53	11 (16%)	76,113,113	1.49	10 (13%)
22	CLA	d	404	37	65,73,73	1.63	7 (10%)	76,113,113	1.59	10 (13%)
32	STE	b	621	-	19,19,19	0.69	0	19,19,19	0.91	0
22	CLA	B	604	-	65,73,73	1.44	6 (9%)	76,113,113	1.82	13 (17%)
22	CLA	a	404	-	65,73,73	1.59	11 (16%)	76,113,113	1.32	8 (10%)
32	STE	E	103	-	11,11,19	0.95	0	11,11,19	0.85	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
22	CLA	c	505	-	1/1/20/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	512	-	1/1/20/20	14/37/115/115	-
22	CLA	C	503	-	1/1/20/20	7/37/115/115	-
22	CLA	b	615	-	1/1/20/20	11/37/115/115	-
24	BCR	t	101	-	-	11/29/63/63	0/2/2/2
32	STE	T	102	-	-	5/13/13/17	-
36	HEC	V	201	17	-	2/10/54/54	-
24	BCR	A	406	-	-	5/29/63/63	0/2/2/2
27	LMG	b	620	-	-	14/46/66/70	0/1/1/1
22	CLA	B	601	37	1/1/20/20	18/37/115/115	-
22	CLA	b	614	-	1/1/20/20	17/37/115/115	-
22	CLA	B	607	37	1/1/20/20	13/37/115/115	-
32	STE	B	627	-	-	4/9/9/17	-
29	DGD	c	518	-	-	23/51/91/95	0/2/2/2
32	STE	b	624	-	-	8/17/17/17	-
27	LMG	C	519	-	-	19/43/63/70	0/1/1/1
22	CLA	A	410	37	1/1/20/20	11/37/115/115	-
22	CLA	B	605	-	1/1/20/20	10/37/115/115	-
33	LHG	B	622	-	-	18/53/53/53	-
22	CLA	B	614	-	1/1/20/20	14/37/115/115	-
22	CLA	C	509	-	1/1/20/20	14/37/115/115	-
24	BCR	b	617	-	-	8/29/63/63	0/2/2/2
27	LMG	A	411	-	-	23/43/63/70	0/1/1/1
28	SQD	B	623	-	-	26/49/69/69	0/1/1/1
32	STE	I	101	-	-	8/12/12/17	-
26	PL9	d	407	-	-	12/53/73/73	0/1/1/1
22	CLA	B	616	-	1/1/19/20	12/31/109/115	-
32	STE	c	521	-	-	10/17/17/17	-
23	PHO	d	401	-	-	4/37/103/103	0/5/6/6
22	CLA	c	501	-	1/1/20/20	5/37/115/115	-
22	CLA	b	601	37	1/1/20/20	14/37/115/115	-
27	LMG	D	407	-	-	17/46/66/70	0/1/1/1
22	CLA	C	511	3	1/1/20/20	6/37/115/115	-
22	CLA	c	509	-	1/1/20/20	11/37/115/115	-
24	BCR	K	101	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HEM	f	101	6,5	-	4/12/54/54	-
22	CLA	A	402	-	1/1/20/20	5/37/115/115	-
22	CLA	B	613	-	1/1/20/20	12/37/115/115	-
28	SQD	a	411	-	-	17/37/37/69	-
29	DGD	c	519	-	-	19/51/91/95	0/2/2/2
22	CLA	d	405	-	1/1/20/20	10/37/115/115	-
33	LHG	D	409	-	-	16/51/51/53	-
22	CLA	B	612	-	1/1/20/20	12/37/115/115	-
27	LMG	c	520	-	-	8/31/51/70	0/1/1/1
24	BCR	B	619	-	-	1/29/63/63	0/2/2/2
24	BCR	C	514	-	-	7/29/63/63	0/2/2/2
32	STE	d	413	-	-	11/14/14/17	-
22	CLA	b	603	-	1/1/20/20	4/37/115/115	-
33	LHG	d	410	-	-	14/43/43/53	-
22	CLA	b	606	-	1/1/20/20	15/37/115/115	-
22	CLA	c	502	-	1/1/20/20	12/37/115/115	-
24	BCR	H	101	-	-	7/29/63/63	0/2/2/2
22	CLA	C	501	-	1/1/20/20	4/37/115/115	-
29	DGD	C	516	-	-	22/51/91/95	0/2/2/2
27	LMG	b	622	-	-	29/50/70/70	0/1/1/1
22	CLA	b	607	37	1/1/20/20	17/37/115/115	-
32	STE	M	103	-	-	2/7/7/17	-
32	STE	l	102	-	-	9/15/15/17	-
24	BCR	B	618	-	-	5/29/63/63	0/2/2/2
22	CLA	c	510	-	1/1/20/20	16/37/115/115	-
24	BCR	C	515	-	-	14/29/63/63	0/2/2/2
32	STE	a	414	-	-	7/9/9/17	-
22	CLA	b	609	-	1/1/20/20	9/37/115/115	-
26	PL9	a	409	-	-	18/53/73/73	0/1/1/1
29	DGD	a	412	-	-	27/45/45/95	-
29	DGD	c	517	-	-	27/51/91/95	0/2/2/2
22	CLA	C	504	37	1/1/18/20	8/30/108/115	-
32	STE	J	101	-	-	2/9/9/17	-
33	LHG	e	101	-	-	22/46/46/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	SQD	L	101	-	-	22/44/64/69	0/1/1/1
24	BCR	c	515	-	-	4/29/63/63	0/2/2/2
32	STE	c	524	-	-	5/9/9/17	-
22	CLA	C	510	-	1/1/20/20	10/37/115/115	-
29	DGD	h	102	-	-	15/51/91/95	0/2/2/2
24	BCR	a	405	-	-	4/29/63/63	0/2/2/2
32	STE	B	624	-	-	6/9/9/17	-
22	CLA	b	605	-	1/1/20/20	10/37/115/115	-
23	PHO	A	404	-	-	4/37/103/103	0/5/6/6
29	DGD	A	414	-	-	25/55/95/95	0/2/2/2
22	CLA	B	602	-	-	9/37/115/115	-
33	LHG	l	101	-	-	28/53/53/53	-
24	BCR	B	617	-	-	4/29/63/63	0/2/2/2
33	LHG	d	409	-	-	17/53/53/53	-
29	DGD	C	517	-	-	19/51/91/95	0/2/2/2
28	SQD	a	410	-	-	19/49/69/69	0/1/1/1
26	PL9	D	406	-	-	8/53/73/73	0/1/1/1
29	DGD	C	518	-	-	12/51/91/95	0/2/2/2
32	STE	T	103	-	-	7/12/12/17	-
36	HEC	v	201	17	-	2/10/54/54	-
22	CLA	b	610	37	1/1/20/20	3/37/115/115	-
22	CLA	b	608	-	1/1/20/20	9/37/115/115	-
22	CLA	c	506	-	1/1/20/20	16/37/115/115	-
28	SQD	A	412	-	-	15/47/67/69	0/1/1/1
32	STE	m	101	-	-	5/9/9/17	-
33	LHG	d	408	-	-	25/53/53/53	-
22	CLA	a	402	-	1/1/20/20	7/37/115/115	-
22	CLA	A	403	37	-	11/37/115/115	-
22	CLA	d	403	-	-	10/37/115/115	-
23	PHO	D	401	-	-	1/37/103/103	0/5/6/6
32	STE	C	522	-	-	5/9/9/17	-
32	STE	B	625	-	-	11/15/15/17	-
24	BCR	D	405	-	-	6/29/63/63	0/2/2/2
24	BCR	c	514	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	B	621	-	-	14/22/22/70	-
32	STE	B	626	-	-	6/13/13/17	-
22	CLA	b	612	-	1/1/20/20	8/37/115/115	-
22	CLA	C	505	-	1/1/20/20	19/37/115/115	-
22	CLA	D	403	-	1/1/20/20	5/37/115/115	-
32	STE	C	521	-	-	5/13/13/17	-
32	STE	D	411	-	-	12/17/17/17	-
27	LMG	d	412	-	-	11/39/59/70	0/1/1/1
35	HEM	E	101	6,5	-	2/12/54/54	-
33	LHG	L	102	-	-	20/53/53/53	-
22	CLA	b	611	-	1/1/20/20	7/37/115/115	-
27	LMG	M	101	-	-	23/46/66/70	0/1/1/1
32	STE	x	101	-	-	9/17/17/17	-
32	STE	b	623	-	-	6/13/13/17	-
22	CLA	c	513	-	1/1/20/20	6/37/115/115	-
22	CLA	c	507	37	1/1/20/20	8/37/115/115	-
28	SQD	F	101	-	-	10/28/48/69	0/1/1/1
22	CLA	b	613	-	1/1/20/20	5/37/115/115	-
22	CLA	c	511	3	1/1/20/20	11/37/115/115	-
22	CLA	B	609	-	-	5/37/115/115	-
22	CLA	C	502	-	1/1/20/20	11/37/115/115	-
24	BCR	T	101	-	-	10/29/63/63	0/2/2/2
24	BCR	b	619	-	-	5/29/63/63	0/2/2/2
32	STE	M	102	-	-	4/12/12/17	-
22	CLA	B	606	-	1/1/20/20	13/37/115/115	-
22	CLA	B	610	37	1/1/20/20	7/37/115/115	-
23	PHO	d	402	-	-	8/37/103/103	0/5/6/6
32	STE	b	625	-	-	5/7/7/17	-
22	CLA	B	615	-	1/1/20/20	7/37/115/115	-
33	LHG	D	408	-	-	26/53/53/53	-
22	CLA	b	616	-	1/1/19/20	7/31/109/115	-
22	CLA	C	513	-	1/1/20/20	17/37/115/115	-
32	STE	t	102	-	-	4/11/11/17	-
27	LMG	d	411	-	-	10/17/17/70	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	507	37	1/1/20/20	5/37/115/115	-
32	STE	j	101	-	-	3/9/9/17	-
22	CLA	b	602	-	-	11/37/115/115	-
24	BCR	b	618	-	-	7/29/63/63	0/2/2/2
22	CLA	A	405	-	1/1/17/20	3/24/102/115	-
22	CLA	B	611	-	1/1/20/20	8/37/115/115	-
22	CLA	b	604	-	1/1/20/20	9/37/115/115	-
24	BCR	d	406	-	-	7/29/63/63	0/2/2/2
27	LMG	c	523	-	-	23/44/64/70	0/1/1/1
22	CLA	B	608	-	1/1/20/20	3/37/115/115	-
32	STE	C	520	-	-	5/9/9/17	-
24	BCR	Y	101	-	-	8/29/63/63	0/2/2/2
27	LMG	c	522	-	-	24/43/63/70	0/1/1/1
27	LMG	D	410	-	-	17/33/33/70	-
22	CLA	c	503	-	1/1/20/20	9/37/115/115	-
22	CLA	a	403	37	-	13/37/115/115	-
22	CLA	C	506	-	1/1/20/20	12/37/115/115	-
22	CLA	B	603	-	1/1/20/20	12/37/115/115	-
24	BCR	h	101	-	-	10/29/63/63	0/2/2/2
26	PL9	A	409	-	-	21/53/73/73	0/1/1/1
22	CLA	c	504	37	1/1/19/20	5/31/109/115	-
22	CLA	C	508	-	-	9/37/115/115	-
32	STE	B	620	-	-	8/14/14/17	-
32	STE	H	103	-	-	6/15/15/17	-
24	BCR	c	516	-	-	4/29/63/63	0/2/2/2
29	DGD	H	102	-	-	22/51/91/95	0/2/2/2
22	CLA	D	404	-	-	9/37/115/115	-
24	BCR	k	101	-	-	10/29/63/63	0/2/2/2
28	SQD	f	102	-	-	11/36/56/69	0/1/1/1
28	SQD	A	413	-	-	13/39/39/69	-
32	STE	a	413	-	-	3/7/7/17	-
33	LHG	E	102	-	-	24/53/53/53	-
22	CLA	c	512	-	1/1/20/20	21/37/115/115	-
22	CLA	d	404	37	1/1/20/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	508	-	-	7/36/114/115	-
32	STE	b	621	-	-	12/17/17/17	-
22	CLA	B	604	-	1/1/20/20	14/37/115/115	-
22	CLA	a	404	-	1/1/20/20	9/37/115/115	-
32	STE	E	103	-	-	6/9/9/17	-

All (957) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	614	CLA	C4B-NB	9.27	1.43	1.35
22	B	615	CLA	C4B-NB	8.98	1.43	1.35
22	b	604	CLA	C4B-NB	8.35	1.42	1.35
22	B	602	CLA	C4B-NB	8.13	1.42	1.35
22	c	504	CLA	C4B-NB	7.81	1.42	1.35
22	c	511	CLA	C4B-NB	7.76	1.42	1.35
22	C	503	CLA	C4B-NB	7.71	1.42	1.35
22	C	501	CLA	C4B-NB	7.52	1.41	1.35
22	c	509	CLA	C4B-NB	7.34	1.41	1.35
36	V	201	HEC	C2B-C3B	-7.33	1.33	1.40
22	B	614	CLA	C4B-NB	7.23	1.41	1.35
22	B	601	CLA	C4B-NB	7.21	1.41	1.35
22	b	609	CLA	C4B-NB	7.19	1.41	1.35
22	c	513	CLA	C4B-NB	7.16	1.41	1.35
22	c	502	CLA	C4B-NB	7.15	1.41	1.35
36	v	201	HEC	C2B-C3B	-7.14	1.33	1.40
22	C	513	CLA	C4B-NB	7.10	1.41	1.35
22	c	512	CLA	C4B-NB	7.09	1.41	1.35
22	c	508	CLA	C4B-NB	6.97	1.41	1.35
22	b	601	CLA	C4B-NB	6.95	1.41	1.35
22	d	404	CLA	C4B-NB	6.86	1.41	1.35
22	b	615	CLA	C4B-NB	6.76	1.41	1.35
22	C	504	CLA	C4B-NB	6.68	1.41	1.35
22	c	501	CLA	C4B-NB	6.62	1.41	1.35
22	C	510	CLA	C4B-NB	6.62	1.41	1.35
22	B	613	CLA	C4B-NB	6.62	1.41	1.35
22	A	410	CLA	C4B-NB	6.61	1.41	1.35
22	B	606	CLA	C4B-NB	6.56	1.41	1.35
22	C	508	CLA	C4B-NB	6.56	1.41	1.35
22	b	602	CLA	C4B-NB	6.56	1.41	1.35
22	B	610	CLA	C4B-NB	6.56	1.41	1.35
22	D	403	CLA	C4B-NB	6.54	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	505	CLA	C4B-NB	6.52	1.41	1.35
22	b	605	CLA	C4B-NB	6.52	1.41	1.35
22	B	601	CLA	MG-NA	6.52	2.21	2.06
22	A	405	CLA	C4B-NB	6.50	1.41	1.35
22	C	503	CLA	MG-NA	6.50	2.21	2.06
22	d	405	CLA	C4B-NB	6.49	1.41	1.35
22	C	511	CLA	C4B-NB	6.38	1.40	1.35
22	b	613	CLA	C4B-NB	6.36	1.40	1.35
22	c	511	CLA	MG-NA	6.35	2.21	2.06
22	a	403	CLA	C4B-NB	6.23	1.40	1.35
22	C	509	CLA	C4B-NB	6.16	1.40	1.35
22	c	503	CLA	C4B-NB	6.16	1.40	1.35
22	C	502	CLA	C4B-NB	6.14	1.40	1.35
22	a	402	CLA	C4B-NB	6.14	1.40	1.35
22	A	402	CLA	C4B-NB	6.12	1.40	1.35
22	b	608	CLA	C4B-NB	6.08	1.40	1.35
22	A	405	CLA	MG-ND	-6.06	1.93	2.05
22	C	505	CLA	MG-NA	6.05	2.20	2.06
22	C	506	CLA	C4B-NB	6.04	1.40	1.35
22	a	404	CLA	C4B-NB	6.03	1.40	1.35
22	C	506	CLA	MG-ND	-6.02	1.93	2.05
22	b	607	CLA	C4B-NB	5.95	1.40	1.35
26	D	406	PL9	C6-C1	-5.94	1.37	1.48
22	A	403	CLA	C4B-NB	5.92	1.40	1.35
22	c	505	CLA	C4B-NB	5.92	1.40	1.35
22	d	404	CLA	MG-NA	5.89	2.20	2.06
22	b	612	CLA	MG-ND	-5.89	1.94	2.05
22	b	611	CLA	C4B-NB	5.88	1.40	1.35
22	B	616	CLA	MG-NA	5.82	2.20	2.06
22	b	603	CLA	C4B-NB	5.80	1.40	1.35
22	B	608	CLA	C4B-NB	5.77	1.40	1.35
22	C	507	CLA	C4B-NB	5.76	1.40	1.35
22	B	605	CLA	C4B-NB	5.75	1.40	1.35
22	b	613	CLA	MG-NA	5.73	2.19	2.06
22	C	512	CLA	C4B-NB	5.68	1.40	1.35
22	C	511	CLA	MG-NA	5.62	2.19	2.06
22	c	506	CLA	C4B-NB	5.57	1.40	1.35
22	b	616	CLA	C4B-NB	5.54	1.40	1.35
35	E	101	HEM	C3C-C2C	-5.54	1.32	1.40
36	V	201	HEC	C3C-C2C	-5.54	1.35	1.40
22	D	404	CLA	C4B-NB	5.53	1.40	1.35
22	c	507	CLA	C4B-NB	5.48	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	615	CLA	MG-ND	-5.31	1.95	2.05
22	C	512	CLA	MG-NA	5.30	2.18	2.06
22	b	610	CLA	C4B-NB	5.25	1.39	1.35
22	B	604	CLA	MG-NC	5.25	2.18	2.06
22	B	616	CLA	C4B-NB	5.21	1.39	1.35
22	B	609	CLA	C4B-NB	5.18	1.39	1.35
36	v	201	HEC	C3C-C2C	-5.17	1.35	1.40
22	B	615	CLA	MG-NA	5.14	2.18	2.06
22	b	611	CLA	MG-NA	5.13	2.18	2.06
22	c	506	CLA	MG-ND	-5.13	1.95	2.05
22	C	508	CLA	MG-NA	5.08	2.18	2.06
22	a	403	CLA	MG-ND	-5.06	1.95	2.05
29	H	102	DGD	O5D-C1E	5.06	1.48	1.40
22	c	509	CLA	MG-ND	5.01	2.15	2.05
22	B	604	CLA	C4B-NB	5.00	1.39	1.35
22	B	612	CLA	C4B-NB	4.99	1.39	1.35
22	A	402	CLA	MG-NA	4.90	2.17	2.06
22	c	513	CLA	MG-ND	-4.86	1.96	2.05
22	C	503	CLA	MG-ND	4.85	2.15	2.05
36	v	201	HEC	C3D-C2D	4.84	1.52	1.37
24	b	618	BCR	C30-C25	-4.81	1.47	1.53
22	b	607	CLA	MG-NA	4.80	2.17	2.06
22	b	604	CLA	C4D-ND	-4.79	1.31	1.37
22	B	607	CLA	C1D-ND	4.77	1.43	1.37
22	b	606	CLA	MG-NA	4.75	2.17	2.06
22	B	603	CLA	MG-ND	4.69	2.15	2.05
22	B	607	CLA	C4B-NB	4.69	1.39	1.35
22	a	404	CLA	MG-ND	-4.67	1.96	2.05
24	B	618	BCR	C30-C25	-4.67	1.47	1.53
22	c	510	CLA	C4B-NB	4.67	1.39	1.35
22	d	403	CLA	C4B-NB	4.67	1.39	1.35
22	C	501	CLA	MG-ND	-4.63	1.96	2.05
22	b	605	CLA	C4D-ND	-4.62	1.31	1.37
22	c	504	CLA	MG-ND	-4.61	1.96	2.05
22	B	614	CLA	MG-ND	-4.60	1.96	2.05
26	D	406	PL9	C52-C5	-4.60	1.41	1.50
22	c	505	CLA	C4D-ND	-4.58	1.31	1.37
22	b	606	CLA	C4B-NB	4.56	1.39	1.35
29	C	517	DGD	C4D-C3D	4.55	1.63	1.52
29	A	414	DGD	O5D-C6D	-4.54	1.35	1.43
22	a	402	CLA	C1D-ND	4.48	1.43	1.37
22	B	610	CLA	C3B-C2B	-4.48	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	611	CLA	C4B-NB	4.47	1.39	1.35
22	D	404	CLA	MG-NA	4.41	2.16	2.06
22	c	508	CLA	C4D-ND	-4.40	1.31	1.37
22	b	601	CLA	MG-NA	4.38	2.16	2.06
22	B	607	CLA	MG-NA	4.35	2.16	2.06
29	C	517	DGD	O3G-C3G	-4.35	1.35	1.43
29	c	519	DGD	C6D-C5D	4.34	1.65	1.51
22	a	403	CLA	C1D-ND	4.34	1.43	1.37
27	D	407	LMG	C4-C5	4.31	1.62	1.53
22	C	512	CLA	MG-ND	-4.31	1.97	2.05
22	A	403	CLA	C1D-ND	4.31	1.43	1.37
22	B	613	CLA	C4D-ND	-4.25	1.31	1.37
22	b	602	CLA	C4D-ND	-4.25	1.31	1.37
22	c	507	CLA	C4D-ND	-4.24	1.31	1.37
29	A	414	DGD	C3E-C2E	4.22	1.63	1.52
22	B	603	CLA	C4D-ND	-4.20	1.31	1.37
29	a	412	DGD	O1G-C1A	4.20	1.45	1.33
26	d	407	PL9	C6-C1	-4.17	1.41	1.48
22	b	601	CLA	C1D-ND	4.16	1.42	1.37
24	T	101	BCR	C1-C6	-4.15	1.48	1.53
28	B	623	SQD	O47-C7	4.15	1.46	1.34
22	B	607	CLA	C4D-ND	-4.15	1.32	1.37
22	A	405	CLA	MG-NA	-4.12	1.96	2.06
22	d	403	CLA	C1D-ND	4.12	1.42	1.37
26	d	407	PL9	C3-C4	-4.12	1.42	1.49
22	C	513	CLA	C1D-ND	4.09	1.42	1.37
22	c	502	CLA	C1D-ND	4.09	1.42	1.37
35	f	101	HEM	C3C-C2C	-4.08	1.34	1.40
22	a	402	CLA	MG-NC	4.08	2.15	2.06
24	C	514	BCR	C1-C6	-4.07	1.48	1.53
22	D	403	CLA	MG-NA	4.07	2.15	2.06
22	D	403	CLA	C4D-ND	-4.05	1.32	1.37
22	d	403	CLA	C4D-ND	-4.02	1.32	1.37
22	C	511	CLA	MG-NC	-4.02	1.96	2.06
24	b	619	BCR	C30-C25	-4.00	1.48	1.53
22	b	606	CLA	C4D-ND	-3.99	1.32	1.37
36	V	201	HEC	C3D-C2D	3.99	1.49	1.37
22	b	607	CLA	C3B-C2B	-3.98	1.34	1.40
22	B	608	CLA	MG-NA	3.98	2.15	2.06
22	B	610	CLA	CMB-C2B	-3.97	1.43	1.51
22	C	509	CLA	MG-ND	3.97	2.13	2.05
24	T	101	BCR	C30-C25	-3.96	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	603	CLA	C4B-NB	3.94	1.38	1.35
22	b	610	CLA	C1D-ND	3.93	1.42	1.37
27	D	410	LMG	C7-C8	3.92	1.60	1.51
22	B	613	CLA	MG-NA	3.90	2.15	2.06
22	B	601	CLA	C3B-C2B	-3.87	1.35	1.40
22	b	610	CLA	C4D-ND	-3.86	1.32	1.37
22	B	607	CLA	C1B-NB	3.85	1.38	1.35
22	B	614	CLA	C4D-ND	-3.85	1.32	1.37
22	b	603	CLA	C1D-ND	3.85	1.42	1.37
22	b	607	CLA	MG-ND	-3.84	1.98	2.05
22	B	614	CLA	C1D-ND	3.83	1.42	1.37
24	c	514	BCR	C1-C6	-3.83	1.48	1.53
28	L	101	SQD	O48-C23	3.81	1.44	1.33
22	b	609	CLA	MG-ND	-3.80	1.98	2.05
22	B	606	CLA	MG-NA	3.79	2.15	2.06
24	H	101	BCR	C30-C25	-3.78	1.48	1.53
22	c	501	CLA	C4D-ND	-3.78	1.32	1.37
22	b	614	CLA	C1D-ND	3.77	1.42	1.37
24	A	406	BCR	C1-C6	-3.77	1.48	1.53
22	C	506	CLA	C1D-ND	3.77	1.42	1.37
27	C	519	LMG	C4-C5	3.75	1.60	1.53
22	b	613	CLA	C1D-ND	3.74	1.42	1.37
23	d	402	PHO	CAC-C3C	-3.74	1.45	1.52
27	c	523	LMG	C4-C5	3.74	1.60	1.53
29	c	519	DGD	C4E-C5E	-3.73	1.45	1.53
22	c	504	CLA	C4D-ND	-3.72	1.32	1.37
33	B	622	LHG	O7-C5	-3.71	1.37	1.46
22	A	405	CLA	C4D-ND	-3.71	1.32	1.37
29	c	518	DGD	O3E-C3E	-3.71	1.34	1.43
29	c	519	DGD	O6D-C5D	-3.71	1.35	1.44
22	c	511	CLA	CHC-C1C	3.70	1.44	1.35
24	K	101	BCR	C30-C25	-3.69	1.48	1.53
22	A	403	CLA	C3B-C2B	-3.69	1.35	1.40
29	C	516	DGD	O2E-C2E	-3.69	1.34	1.43
22	a	403	CLA	C4D-ND	-3.69	1.32	1.37
22	d	404	CLA	C1D-ND	3.68	1.42	1.37
22	A	403	CLA	C4D-ND	-3.67	1.32	1.37
24	D	405	BCR	C30-C25	-3.66	1.48	1.53
22	c	503	CLA	C4D-ND	-3.63	1.32	1.37
22	B	606	CLA	C3B-C2B	-3.63	1.35	1.40
22	b	615	CLA	MG-NA	3.62	2.14	2.06
33	D	409	LHG	O8-C6	-3.62	1.36	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	601	CLA	MG-ND	-3.62	1.98	2.05
29	C	516	DGD	O3E-C3E	-3.61	1.34	1.43
22	A	410	CLA	C4D-ND	-3.61	1.32	1.37
22	B	615	CLA	C4D-ND	-3.61	1.32	1.37
28	a	411	SQD	O47-C7	3.61	1.44	1.34
22	B	610	CLA	CHC-C1C	3.60	1.44	1.35
22	B	612	CLA	C4D-ND	-3.60	1.32	1.37
22	B	612	CLA	C1D-ND	3.60	1.42	1.37
22	C	508	CLA	C1B-NB	3.60	1.38	1.35
24	c	515	BCR	C1-C6	-3.59	1.48	1.53
22	B	601	CLA	C1D-ND	3.57	1.42	1.37
24	c	514	BCR	C30-C25	-3.57	1.48	1.53
22	d	403	CLA	MG-NA	3.55	2.14	2.06
26	d	407	PL9	C46-C44	-3.55	1.43	1.51
22	D	404	CLA	C1D-ND	3.55	1.42	1.37
27	c	522	LMG	O1-C1	3.54	1.46	1.40
22	c	507	CLA	C3B-C2B	-3.54	1.35	1.40
22	c	508	CLA	MG-ND	3.53	2.12	2.05
28	A	413	SQD	O48-C23	3.52	1.43	1.33
22	b	608	CLA	CHC-C1C	3.52	1.44	1.35
22	c	510	CLA	C4D-ND	-3.52	1.32	1.37
29	a	412	DGD	O2G-C1B	3.51	1.44	1.34
22	C	509	CLA	MG-NA	3.51	2.14	2.06
22	C	510	CLA	MG-NA	3.51	2.14	2.06
22	B	611	CLA	CHC-C1C	3.51	1.44	1.35
22	C	505	CLA	CHC-C1C	3.51	1.44	1.35
26	A	409	PL9	C7-C3	-3.51	1.47	1.51
22	A	403	CLA	MG-NA	3.49	2.14	2.06
22	C	508	CLA	C1D-ND	3.49	1.42	1.37
22	c	513	CLA	C4D-ND	-3.49	1.32	1.37
22	c	510	CLA	C1D-ND	3.49	1.42	1.37
22	A	405	CLA	C1D-ND	3.47	1.42	1.37
22	C	504	CLA	C4D-ND	-3.47	1.32	1.37
22	b	613	CLA	MG-ND	-3.47	1.98	2.05
24	D	405	BCR	C1-C6	-3.47	1.49	1.53
24	B	617	BCR	C1-C6	-3.47	1.49	1.53
22	A	410	CLA	CHC-C1C	3.45	1.43	1.35
22	A	410	CLA	C1D-ND	3.45	1.42	1.37
22	b	603	CLA	C4D-ND	-3.45	1.33	1.37
29	A	414	DGD	C4E-C5E	3.44	1.60	1.53
28	f	102	SQD	O47-C7	3.44	1.44	1.34
22	b	614	CLA	MG-ND	-3.43	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	619	BCR	C1-C6	-3.42	1.49	1.53
22	A	403	CLA	MG-ND	-3.42	1.99	2.05
22	b	604	CLA	C1D-ND	3.42	1.42	1.37
22	B	602	CLA	C4D-ND	-3.41	1.33	1.37
24	d	406	BCR	C30-C25	-3.40	1.49	1.53
28	f	102	SQD	O48-C23	3.40	1.43	1.33
22	B	612	CLA	MG-ND	-3.40	1.99	2.05
22	c	511	CLA	C1D-ND	3.40	1.42	1.37
24	b	618	BCR	C1-C6	-3.39	1.49	1.53
27	b	620	LMG	C4-C3	3.38	1.60	1.52
22	c	502	CLA	C4D-ND	-3.38	1.33	1.37
22	d	405	CLA	C1D-ND	3.37	1.41	1.37
22	C	512	CLA	CHC-C1C	3.37	1.43	1.35
29	h	102	DGD	C4D-C3D	3.37	1.60	1.52
22	c	512	CLA	C1D-ND	3.36	1.41	1.37
22	C	503	CLA	C4D-ND	-3.36	1.33	1.37
22	c	504	CLA	MG-NC	3.36	2.14	2.06
22	b	615	CLA	CMB-C2B	-3.35	1.44	1.51
22	b	604	CLA	CHC-C1C	3.35	1.43	1.35
29	H	102	DGD	C4D-C5D	3.34	1.60	1.53
22	b	610	CLA	C3B-C2B	-3.34	1.35	1.40
22	B	609	CLA	C1D-ND	3.34	1.41	1.37
22	B	605	CLA	C4D-ND	-3.33	1.33	1.37
22	C	503	CLA	C1D-ND	3.33	1.41	1.37
28	a	411	SQD	O48-C23	3.33	1.43	1.33
33	L	102	LHG	O8-C23	3.32	1.43	1.33
22	B	616	CLA	C1D-ND	3.32	1.41	1.37
24	C	515	BCR	C30-C25	-3.32	1.49	1.53
26	D	406	PL9	C11-C9	-3.31	1.44	1.51
29	c	518	DGD	O2E-C2E	-3.30	1.35	1.43
22	c	507	CLA	C1D-ND	3.29	1.41	1.37
35	f	101	HEM	C3C-CAC	3.29	1.54	1.47
29	A	414	DGD	C6E-C5E	3.29	1.62	1.51
29	C	517	DGD	O3D-C3D	-3.28	1.35	1.43
22	B	603	CLA	CMC-C2C	-3.28	1.43	1.50
22	B	606	CLA	C1D-ND	3.28	1.41	1.37
22	c	513	CLA	C1D-ND	3.28	1.41	1.37
22	c	510	CLA	CMB-C2B	-3.28	1.44	1.51
29	A	414	DGD	C4D-C5D	3.28	1.59	1.53
22	C	509	CLA	C1D-ND	3.27	1.41	1.37
22	B	615	CLA	C1D-ND	3.27	1.41	1.37
22	C	502	CLA	C3B-C2B	-3.26	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	515	BCR	C30-C25	-3.26	1.49	1.53
22	b	601	CLA	CHC-C1C	3.26	1.43	1.35
29	h	102	DGD	O2G-C2G	-3.25	1.38	1.46
22	C	505	CLA	C1D-ND	3.25	1.41	1.37
22	B	603	CLA	CHC-C1C	3.24	1.43	1.35
22	A	402	CLA	CHC-C1C	3.23	1.43	1.35
22	c	501	CLA	C1D-ND	3.22	1.41	1.37
22	C	505	CLA	C4D-ND	-3.22	1.33	1.37
24	c	516	BCR	C30-C25	-3.22	1.49	1.53
22	c	509	CLA	C1D-ND	3.22	1.41	1.37
24	h	101	BCR	C30-C25	-3.22	1.49	1.53
22	C	501	CLA	C4D-ND	-3.22	1.33	1.37
22	b	613	CLA	CMB-C2B	-3.22	1.44	1.51
22	a	402	CLA	MG-ND	-3.21	1.99	2.05
23	d	401	PHO	O2D-CGD	3.21	1.41	1.33
22	B	606	CLA	CHC-C1C	3.21	1.43	1.35
22	B	602	CLA	CHC-C1C	3.20	1.43	1.35
22	C	513	CLA	C4D-ND	-3.20	1.33	1.37
29	h	102	DGD	O2D-C2D	-3.19	1.35	1.43
22	c	503	CLA	C1D-ND	3.19	1.41	1.37
28	L	101	SQD	O47-C7	3.19	1.43	1.34
22	c	505	CLA	CHC-C1C	3.19	1.43	1.35
22	B	608	CLA	C1D-ND	3.18	1.41	1.37
22	B	614	CLA	C3B-C2B	-3.17	1.36	1.40
22	B	609	CLA	CMD-C2D	-3.17	1.44	1.50
22	d	404	CLA	CMB-C2B	-3.17	1.45	1.51
24	b	617	BCR	C1-C6	-3.17	1.49	1.53
27	b	620	LMG	C4-C5	3.17	1.59	1.53
22	b	605	CLA	CHC-C1C	3.17	1.43	1.35
22	b	614	CLA	MG-NA	3.16	2.13	2.06
27	A	411	LMG	C4-C3	3.16	1.60	1.52
22	c	509	CLA	C4D-ND	-3.15	1.33	1.37
22	c	506	CLA	C4D-ND	-3.15	1.33	1.37
22	B	615	CLA	CHC-C1C	3.15	1.43	1.35
23	D	401	PHO	CHA-CBD	-3.15	1.48	1.52
22	a	402	CLA	C4D-ND	-3.14	1.33	1.37
24	B	617	BCR	C30-C25	-3.14	1.49	1.53
22	B	605	CLA	C1C-NC	-3.14	1.33	1.37
29	H	102	DGD	O2D-C2D	-3.14	1.35	1.43
29	C	518	DGD	O2G-C2G	-3.14	1.38	1.46
29	A	414	DGD	C1E-C2E	3.14	1.61	1.52
22	c	504	CLA	CHC-C1C	3.13	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	412	SQD	O2-C2	-3.12	1.35	1.43
22	B	613	CLA	MG-ND	-3.12	1.99	2.05
22	B	601	CLA	CMB-C2B	-3.12	1.45	1.51
22	B	614	CLA	CHC-C1C	3.12	1.43	1.35
22	B	603	CLA	C3B-C2B	-3.12	1.36	1.40
22	C	502	CLA	C4D-ND	-3.11	1.33	1.37
29	c	517	DGD	C4E-C3E	3.11	1.60	1.52
22	C	512	CLA	C4D-ND	-3.11	1.33	1.37
22	b	612	CLA	CMB-C2B	-3.10	1.45	1.51
22	b	613	CLA	C4D-ND	-3.09	1.33	1.37
22	C	510	CLA	CHC-C1C	3.09	1.42	1.35
22	C	507	CLA	CHC-C1C	3.09	1.42	1.35
22	B	611	CLA	C4D-ND	-3.08	1.33	1.37
22	a	404	CLA	C3B-C2B	-3.08	1.36	1.40
27	d	412	LMG	O1-C7	-3.08	1.38	1.43
22	C	512	CLA	MG-NC	-3.08	1.99	2.06
22	B	609	CLA	C3B-C2B	-3.08	1.36	1.40
22	b	616	CLA	C1D-ND	3.07	1.41	1.37
22	B	604	CLA	C4D-ND	-3.07	1.33	1.37
22	B	606	CLA	C4D-ND	-3.07	1.33	1.37
22	b	616	CLA	C4D-ND	-3.06	1.33	1.37
26	d	407	PL9	C53-C6	-3.06	1.44	1.50
22	b	612	CLA	C4B-NB	3.06	1.37	1.35
22	c	512	CLA	MG-NA	3.06	2.13	2.06
22	B	606	CLA	MG-ND	3.05	2.11	2.05
22	c	508	CLA	CHC-C1C	3.05	1.42	1.35
22	c	513	CLA	CHC-C1C	3.05	1.42	1.35
22	B	602	CLA	C1D-ND	3.05	1.41	1.37
27	c	520	LMG	O1-C1	3.05	1.45	1.40
22	C	508	CLA	CHC-C1C	3.05	1.42	1.35
22	b	606	CLA	CHC-C1C	3.05	1.42	1.35
22	B	601	CLA	CHC-C1C	3.04	1.42	1.35
22	D	403	CLA	C1D-ND	3.04	1.41	1.37
29	c	518	DGD	C1E-C2E	3.04	1.61	1.52
22	D	403	CLA	CMD-C2D	-3.03	1.44	1.50
22	B	605	CLA	C3B-C2B	-3.03	1.36	1.40
22	B	608	CLA	C4D-ND	-3.03	1.33	1.37
22	C	508	CLA	C4D-ND	-3.03	1.33	1.37
22	B	611	CLA	C1D-ND	3.03	1.41	1.37
22	B	605	CLA	CHC-C1C	3.02	1.42	1.35
22	b	614	CLA	CMC-C2C	-3.02	1.44	1.50
24	Y	101	BCR	C1-C6	-3.02	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	511	CLA	CMB-C2B	-3.02	1.45	1.51
22	B	615	CLA	CMB-C2B	-3.02	1.45	1.51
22	b	606	CLA	C1D-ND	3.01	1.41	1.37
27	c	520	LMG	C4-C5	3.01	1.59	1.53
29	c	518	DGD	C4D-C3D	3.01	1.60	1.52
22	d	403	CLA	CMB-C2B	-3.01	1.45	1.51
27	D	407	LMG	O2-C2	-3.01	1.35	1.43
26	a	409	PL9	C53-C6	-3.01	1.44	1.50
22	B	614	CLA	C3B-CAB	-3.00	1.41	1.47
29	A	414	DGD	O5D-C1E	3.00	1.45	1.40
22	A	402	CLA	C1D-ND	3.00	1.41	1.37
33	D	408	LHG	P-O3	3.00	1.71	1.59
27	c	522	LMG	C3-C2	3.00	1.60	1.52
22	b	607	CLA	C1D-ND	3.00	1.41	1.37
22	C	504	CLA	CHC-C1C	3.00	1.42	1.35
27	B	621	LMG	O7-C10	3.00	1.40	1.30
22	b	608	CLA	CMB-C2B	-3.00	1.45	1.51
33	D	409	LHG	P-O6	3.00	1.71	1.59
22	c	503	CLA	MG-NA	3.00	2.13	2.06
22	C	503	CLA	CHC-C1C	2.99	1.42	1.35
22	c	512	CLA	CHC-C1C	2.99	1.42	1.35
28	A	413	SQD	O47-C45	-2.99	1.42	1.47
22	B	604	CLA	CHC-C1C	2.99	1.42	1.35
24	k	101	BCR	C30-C25	-2.98	1.49	1.53
22	b	615	CLA	C4D-ND	-2.98	1.33	1.37
22	C	508	CLA	MG-ND	-2.98	1.99	2.05
22	b	615	CLA	CMD-C2D	-2.97	1.44	1.50
33	E	102	LHG	P-O6	2.97	1.71	1.59
22	a	402	CLA	MG-NA	2.97	2.13	2.06
22	C	510	CLA	C4D-ND	-2.97	1.33	1.37
22	a	404	CLA	CMC-C2C	-2.97	1.44	1.50
24	b	619	BCR	C1-C6	-2.97	1.49	1.53
27	d	412	LMG	C4-C5	2.96	1.59	1.53
22	C	506	CLA	C1B-NB	-2.96	1.32	1.35
22	D	404	CLA	CMC-C2C	-2.96	1.44	1.50
22	b	612	CLA	C1D-ND	2.96	1.41	1.37
22	C	504	CLA	C1D-ND	2.96	1.41	1.37
33	d	408	LHG	O7-C5	-2.95	1.39	1.46
28	F	101	SQD	O48-C23	2.95	1.42	1.33
22	B	606	CLA	C3B-CAB	-2.95	1.41	1.47
33	d	408	LHG	C24-C23	2.95	1.59	1.50
22	C	507	CLA	C3B-C2B	-2.94	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	d	404	CLA	C4D-ND	-2.94	1.33	1.37
28	B	623	SQD	O48-C23	2.94	1.41	1.33
29	C	516	DGD	C4D-C3D	2.93	1.59	1.52
22	C	513	CLA	CHC-C1C	2.93	1.42	1.35
22	d	403	CLA	CHC-C1C	2.93	1.42	1.35
22	B	612	CLA	C1B-NB	2.93	1.37	1.35
22	b	607	CLA	CMD-C2D	-2.93	1.44	1.50
35	E	101	HEM	CAB-C3B	2.92	1.55	1.47
27	M	101	LMG	O4-C4	-2.92	1.36	1.43
22	C	509	CLA	CHC-C1C	2.92	1.42	1.35
33	B	622	LHG	C24-C23	2.91	1.59	1.50
22	c	505	CLA	C3B-C2B	-2.91	1.36	1.40
22	c	501	CLA	C3B-C2B	-2.91	1.36	1.40
22	a	402	CLA	CMB-C2B	-2.91	1.45	1.51
24	d	406	BCR	C1-C6	-2.90	1.49	1.53
29	C	517	DGD	O5D-C6D	-2.90	1.38	1.43
22	C	511	CLA	C4D-ND	-2.90	1.33	1.37
22	C	512	CLA	C1D-ND	2.89	1.41	1.37
22	B	611	CLA	CMD-C2D	-2.89	1.44	1.50
22	C	507	CLA	MG-NA	2.89	2.13	2.06
24	b	617	BCR	C30-C25	-2.89	1.49	1.53
22	B	608	CLA	CMD-C2D	-2.89	1.44	1.50
22	B	602	CLA	CMB-C2B	-2.88	1.45	1.51
22	a	404	CLA	CMB-C2B	-2.88	1.45	1.51
22	B	607	CLA	MG-NC	2.88	2.13	2.06
22	b	608	CLA	C4D-ND	-2.87	1.33	1.37
29	C	516	DGD	C4E-C3E	2.87	1.59	1.52
28	A	413	SQD	O47-C7	2.87	1.42	1.34
22	d	405	CLA	C4D-ND	-2.87	1.33	1.37
22	C	502	CLA	CHC-C1C	2.87	1.42	1.35
28	A	412	SQD	O48-C23	2.87	1.41	1.33
22	b	611	CLA	CMD-C2D	-2.87	1.44	1.50
22	C	509	CLA	C4D-ND	-2.86	1.33	1.37
27	b	620	LMG	O6-C1	2.86	1.49	1.41
22	c	513	CLA	MG-NC	2.86	2.13	2.06
26	A	409	PL9	C21-C19	2.86	1.57	1.51
29	h	102	DGD	C4E-C5E	2.86	1.59	1.53
22	a	403	CLA	CHC-C1C	2.86	1.42	1.35
22	D	404	CLA	CMB-C2B	-2.86	1.45	1.51
22	A	403	CLA	CMD-C2D	-2.85	1.44	1.50
22	B	612	CLA	MG-NA	2.85	2.13	2.06
22	b	614	CLA	C4D-ND	-2.85	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	605	CLA	CMC-C2C	-2.84	1.44	1.50
28	f	102	SQD	O2-C2	-2.84	1.36	1.43
22	a	402	CLA	CHC-C1C	2.84	1.42	1.35
22	C	501	CLA	MG-NA	2.84	2.13	2.06
35	f	101	HEM	C3B-C2B	-2.84	1.31	1.37
22	C	506	CLA	CHC-C1C	2.84	1.42	1.35
22	b	602	CLA	CHC-C1C	2.83	1.42	1.35
29	c	518	DGD	O3D-C3D	-2.83	1.36	1.43
27	d	412	LMG	O8-C9	-2.82	1.38	1.45
27	M	101	LMG	O7-C8	-2.82	1.39	1.46
22	b	613	CLA	CAA-C2A	-2.82	1.48	1.54
22	b	611	CLA	CHC-C1C	2.81	1.42	1.35
22	B	614	CLA	MG-NA	2.81	2.12	2.06
22	d	405	CLA	CMB-C2B	-2.81	1.45	1.51
22	B	614	CLA	CMB-C2B	-2.81	1.45	1.51
22	a	404	CLA	C1C-NC	-2.80	1.33	1.37
22	c	501	CLA	CMB-C2B	-2.80	1.45	1.51
29	c	518	DGD	C6E-C5E	2.80	1.61	1.51
22	c	506	CLA	C1D-ND	2.80	1.41	1.37
22	C	511	CLA	CHC-C1C	2.79	1.42	1.35
22	c	507	CLA	MG-NA	2.77	2.12	2.06
22	B	613	CLA	CMD-C2D	-2.77	1.44	1.50
22	B	605	CLA	MG-ND	-2.77	2.00	2.05
27	c	522	LMG	C4-C3	2.77	1.59	1.52
22	c	508	CLA	CMB-C2B	-2.77	1.45	1.51
22	c	502	CLA	CMD-C2D	-2.76	1.44	1.50
22	c	507	CLA	C3B-CAB	-2.74	1.42	1.47
24	K	101	BCR	C1-C6	-2.74	1.50	1.53
22	b	607	CLA	CHC-C1C	2.74	1.42	1.35
22	C	501	CLA	C1D-ND	2.74	1.41	1.37
22	C	513	CLA	CMC-C2C	-2.73	1.45	1.50
22	C	503	CLA	CMB-C2B	-2.73	1.46	1.51
22	a	403	CLA	CMB-C2B	-2.73	1.46	1.51
23	D	401	PHO	CAC-C3C	-2.73	1.47	1.52
22	b	609	CLA	C1D-ND	2.73	1.41	1.37
22	c	502	CLA	CMB-C2B	-2.73	1.46	1.51
28	F	101	SQD	O2-C2	-2.73	1.36	1.43
22	B	609	CLA	C4D-ND	-2.73	1.33	1.37
28	a	410	SQD	O2-C2	-2.72	1.36	1.43
33	L	102	LHG	P-O6	2.72	1.70	1.59
22	c	512	CLA	CMB-C2B	-2.72	1.46	1.51
22	c	511	CLA	C4D-ND	-2.72	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	508	CLA	C1D-ND	2.72	1.41	1.37
29	c	519	DGD	O2G-C2G	-2.72	1.39	1.46
22	A	402	CLA	C4D-ND	-2.72	1.34	1.37
22	C	507	CLA	C1D-ND	2.72	1.41	1.37
22	A	403	CLA	CHC-C1C	2.72	1.41	1.35
22	C	509	CLA	CMB-C2B	-2.71	1.46	1.51
22	D	403	CLA	C1C-NC	-2.70	1.33	1.37
27	c	520	LMG	C3-C2	2.70	1.59	1.52
24	a	405	BCR	C30-C25	-2.70	1.50	1.53
22	D	403	CLA	CHC-C1C	2.70	1.41	1.35
22	c	512	CLA	C3B-C2B	-2.70	1.36	1.40
22	b	602	CLA	C1D-ND	2.70	1.41	1.37
22	c	512	CLA	C4D-ND	-2.69	1.34	1.37
22	b	615	CLA	CHC-C1C	2.69	1.41	1.35
29	C	518	DGD	O6D-C5D	-2.69	1.37	1.44
22	c	501	CLA	CHC-C1C	2.69	1.41	1.35
29	c	518	DGD	O5D-C1E	2.69	1.44	1.40
22	b	603	CLA	CMB-C2B	-2.69	1.46	1.51
33	l	101	LHG	P-O6	2.68	1.70	1.59
22	b	603	CLA	C3B-CAB	-2.68	1.42	1.47
22	c	510	CLA	CHC-C1C	2.68	1.41	1.35
22	C	506	CLA	C3B-C2B	-2.68	1.36	1.40
22	b	607	CLA	CMB-C2B	-2.68	1.46	1.51
27	b	622	LMG	C7-C8	2.67	1.58	1.50
22	B	612	CLA	CHC-C1C	2.67	1.41	1.35
22	b	609	CLA	CMB-C2B	-2.67	1.46	1.51
22	B	609	CLA	C3B-CAB	-2.67	1.42	1.47
22	B	604	CLA	C1D-ND	2.66	1.41	1.37
24	C	514	BCR	C36-C18	-2.66	1.45	1.50
22	b	615	CLA	C3B-C2B	-2.66	1.36	1.40
23	d	402	PHO	CMC-C2C	-2.66	1.45	1.51
22	c	513	CLA	CMB-C2B	-2.66	1.46	1.51
22	B	607	CLA	CAC-C3C	-2.65	1.44	1.51
27	C	519	LMG	O1-C7	-2.65	1.38	1.43
22	c	503	CLA	CMB-C2B	-2.65	1.46	1.51
22	B	607	CLA	CHC-C1C	2.65	1.41	1.35
22	d	405	CLA	CHC-C1C	2.65	1.41	1.35
22	c	506	CLA	CMC-C2C	-2.65	1.45	1.50
22	a	402	CLA	CMC-C2C	-2.64	1.45	1.50
22	B	606	CLA	CMB-C2B	-2.64	1.46	1.51
33	d	410	LHG	P-O6	2.64	1.70	1.59
29	c	518	DGD	O3G-C1D	-2.64	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	403	CLA	CAA-C2A	-2.64	1.49	1.54
22	c	507	CLA	CMB-C2B	-2.63	1.46	1.51
22	a	404	CLA	C4D-ND	-2.63	1.34	1.37
22	b	603	CLA	MG-NA	2.63	2.12	2.06
22	a	404	CLA	C4B-CHC	-2.63	1.33	1.41
28	a	410	SQD	O48-C23	2.62	1.41	1.33
23	A	404	PHO	CMC-C2C	-2.62	1.45	1.51
22	c	502	CLA	C3B-C2B	-2.62	1.36	1.40
22	c	509	CLA	MG-NC	2.61	2.12	2.06
22	D	404	CLA	CMD-C2D	-2.61	1.45	1.50
29	c	519	DGD	O5D-C1E	2.61	1.44	1.40
22	B	603	CLA	C3B-CAB	-2.61	1.42	1.47
22	C	510	CLA	C1D-ND	2.61	1.41	1.37
27	c	522	LMG	C9-C8	2.61	1.58	1.50
22	B	608	CLA	CHC-C1C	2.61	1.41	1.35
22	b	614	CLA	CMB-C2B	-2.60	1.46	1.51
22	b	602	CLA	CMD-C2D	-2.60	1.45	1.50
27	M	101	LMG	C4-C5	2.60	1.58	1.53
22	B	616	CLA	C3B-CAB	-2.60	1.42	1.47
22	C	509	CLA	MG-NC	-2.59	2.00	2.06
22	B	608	CLA	CMB-C2B	-2.59	1.46	1.51
22	c	506	CLA	CHC-C1C	2.59	1.41	1.35
24	t	101	BCR	C27-C26	-2.58	1.45	1.51
22	C	506	CLA	MG-NA	2.58	2.12	2.06
22	c	509	CLA	CHC-C1C	2.58	1.41	1.35
24	Y	101	BCR	C30-C25	-2.58	1.50	1.53
22	b	611	CLA	C3B-C2B	-2.58	1.36	1.40
22	c	509	CLA	CMB-C2B	-2.57	1.46	1.51
22	C	502	CLA	MG-NA	2.57	2.12	2.06
22	c	502	CLA	C4B-CHC	-2.57	1.33	1.41
22	B	610	CLA	C3B-CAB	-2.57	1.42	1.47
22	A	405	CLA	CMD-C2D	-2.57	1.45	1.50
24	B	617	BCR	C33-C5	-2.57	1.46	1.50
22	C	506	CLA	CMC-C2C	-2.57	1.45	1.50
23	D	401	PHO	CMC-C2C	-2.57	1.45	1.51
22	C	512	CLA	CMB-C2B	-2.57	1.46	1.51
22	c	510	CLA	MG-ND	-2.57	2.00	2.05
22	c	510	CLA	MG-NC	2.56	2.12	2.06
29	c	519	DGD	C1D-C2D	2.56	1.59	1.52
22	b	609	CLA	C4D-ND	-2.56	1.34	1.37
28	a	410	SQD	O47-C7	2.56	1.41	1.34
22	c	503	CLA	CHC-C1C	2.56	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	407	LMG	O1-C1	2.56	1.44	1.40
22	a	403	CLA	CMC-C2C	-2.56	1.45	1.50
22	c	508	CLA	CMC-C2C	-2.56	1.45	1.50
27	b	620	LMG	O7-C8	-2.56	1.40	1.46
22	b	604	CLA	CMB-C2B	-2.55	1.46	1.51
22	C	505	CLA	MG-NC	-2.55	2.00	2.06
29	H	102	DGD	C3E-C2E	2.55	1.58	1.52
23	A	404	PHO	CHA-CBD	-2.55	1.49	1.52
27	c	523	LMG	O1-C7	-2.55	1.39	1.43
35	E	101	HEM	C3C-CAC	2.55	1.53	1.47
24	A	406	BCR	C33-C5	-2.54	1.46	1.50
29	C	516	DGD	C2B-C1B	-2.54	1.43	1.50
22	c	510	CLA	CMD-C2D	-2.54	1.45	1.50
24	k	101	BCR	C1-C6	-2.54	1.50	1.53
22	c	504	CLA	CMD-C2D	-2.54	1.45	1.50
22	C	513	CLA	MG-NA	2.54	2.12	2.06
22	C	506	CLA	C4D-ND	-2.53	1.34	1.37
22	c	506	CLA	CMD-C2D	-2.53	1.45	1.50
22	B	602	CLA	CMD-C2D	-2.53	1.45	1.50
23	A	404	PHO	CAC-C3C	-2.53	1.47	1.52
22	C	507	CLA	CMB-C2B	-2.53	1.46	1.51
22	b	614	CLA	CHC-C1C	2.52	1.41	1.35
22	B	613	CLA	CHC-C1C	2.52	1.41	1.35
22	C	502	CLA	CMB-C2B	-2.52	1.46	1.51
24	T	101	BCR	C38-C26	-2.52	1.46	1.50
27	b	622	LMG	C3-C2	2.52	1.58	1.52
27	M	101	LMG	C9-C8	2.51	1.58	1.50
22	B	611	CLA	CMB-C2B	-2.51	1.46	1.51
22	b	612	CLA	C4D-ND	-2.51	1.34	1.37
27	C	519	LMG	O8-C9	-2.51	1.39	1.45
22	C	509	CLA	CMD-C2D	-2.51	1.45	1.50
22	B	612	CLA	CMC-C2C	-2.51	1.45	1.50
22	b	605	CLA	MG-ND	2.51	2.10	2.05
28	A	412	SQD	O47-C7	2.51	1.41	1.34
22	B	603	CLA	CMB-C2B	-2.50	1.46	1.51
22	b	605	CLA	CMD-C2D	-2.50	1.45	1.50
22	b	601	CLA	O2A-CGA	2.50	1.40	1.33
28	a	410	SQD	O4-C4	-2.50	1.37	1.43
22	b	613	CLA	CMD-C2D	-2.49	1.45	1.50
22	c	502	CLA	CHC-C1C	2.49	1.41	1.35
22	B	605	CLA	CMD-C2D	-2.49	1.45	1.50
33	e	101	LHG	P-O6	2.49	1.69	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	v	201	HEC	CAD-C3D	2.49	1.55	1.52
27	c	520	LMG	O7-C10	2.49	1.40	1.35
33	B	622	LHG	P-O6	2.49	1.69	1.59
29	H	102	DGD	C1E-C2E	2.49	1.59	1.52
28	L	101	SQD	O2-C2	-2.49	1.37	1.43
24	C	514	BCR	C33-C5	-2.49	1.46	1.50
29	c	517	DGD	C4D-C3D	2.48	1.58	1.52
22	c	508	CLA	CMD-C2D	-2.48	1.45	1.50
22	b	615	CLA	C1D-ND	2.48	1.40	1.37
24	t	101	BCR	C30-C25	-2.47	1.50	1.53
22	B	613	CLA	C1D-ND	2.47	1.40	1.37
22	C	513	CLA	CMB-C2B	-2.47	1.46	1.51
22	d	405	CLA	MG-ND	-2.46	2.00	2.05
22	b	613	CLA	CMC-C2C	-2.46	1.45	1.50
22	b	606	CLA	C3B-C2B	-2.46	1.37	1.40
24	c	516	BCR	C1-C6	-2.46	1.50	1.53
29	C	517	DGD	C4D-C5D	2.46	1.58	1.53
29	a	412	DGD	C1G-C2G	2.46	1.58	1.50
22	b	616	CLA	C3B-CAB	-2.45	1.42	1.47
23	d	401	PHO	C3B-C2B	-2.45	1.37	1.40
22	C	502	CLA	MG-ND	-2.45	2.00	2.05
22	b	606	CLA	MG-ND	2.45	2.10	2.05
22	b	609	CLA	CMD-C2D	-2.45	1.45	1.50
22	b	603	CLA	C4B-CHC	-2.44	1.34	1.41
24	b	617	BCR	C33-C5	-2.44	1.46	1.50
22	a	404	CLA	O1D-CGD	2.44	1.27	1.21
24	C	515	BCR	C27-C26	-2.44	1.46	1.51
22	b	604	CLA	CMC-C2C	-2.44	1.45	1.50
27	D	410	LMG	C9-C8	2.43	1.58	1.50
28	f	102	SQD	O3-C3	-2.43	1.37	1.43
22	b	607	CLA	C4D-ND	-2.43	1.34	1.37
27	d	412	LMG	O3-C3	-2.43	1.37	1.43
29	C	518	DGD	O1G-C1G	-2.42	1.39	1.45
22	B	603	CLA	MG-NC	-2.42	2.00	2.06
22	a	404	CLA	CMD-C2D	-2.42	1.45	1.50
22	B	609	CLA	C4B-CHC	-2.42	1.34	1.41
22	c	510	CLA	C3B-C2B	-2.42	1.37	1.40
23	D	401	PHO	CMB-C2B	-2.42	1.45	1.51
29	H	102	DGD	C1G-C2G	2.41	1.58	1.50
24	B	619	BCR	C30-C25	-2.41	1.50	1.53
29	C	516	DGD	C2A-C1A	-2.41	1.43	1.50
22	B	607	CLA	CMC-C2C	-2.41	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	405	BCR	C1-C6	-2.41	1.50	1.53
22	B	603	CLA	MG-NA	2.41	2.12	2.06
22	C	502	CLA	C1D-ND	2.41	1.40	1.37
22	B	605	CLA	O2D-CED	-2.40	1.39	1.45
22	B	603	CLA	CMA-C3A	-2.40	1.48	1.53
22	b	602	CLA	MG-NC	-2.40	2.00	2.06
22	b	602	CLA	C4B-CHC	-2.40	1.34	1.41
22	C	501	CLA	CHC-C1C	2.39	1.41	1.35
22	b	610	CLA	CMB-C2B	-2.39	1.46	1.51
29	c	519	DGD	C2A-C1A	-2.39	1.43	1.50
26	d	407	PL9	C41-C39	-2.39	1.46	1.51
22	B	615	CLA	C3B-C2B	-2.39	1.37	1.40
22	d	404	CLA	CHC-C1C	2.39	1.41	1.35
22	b	610	CLA	CMD-C2D	-2.39	1.45	1.50
28	F	101	SQD	O3-C3	-2.39	1.37	1.43
29	h	102	DGD	C1E-C2E	2.38	1.59	1.52
22	B	615	CLA	CAC-C3C	-2.38	1.45	1.51
22	B	616	CLA	C4D-ND	-2.38	1.34	1.37
22	b	612	CLA	CMC-C2C	-2.38	1.45	1.50
22	B	605	CLA	CMB-C2B	-2.38	1.46	1.51
29	c	519	DGD	O4E-C4E	-2.38	1.37	1.43
22	b	616	CLA	CMB-C2B	-2.38	1.46	1.51
22	b	611	CLA	MG-NC	-2.37	2.00	2.06
22	B	616	CLA	CMD-C2D	-2.37	1.45	1.50
22	B	602	CLA	MG-NA	2.37	2.11	2.06
22	c	506	CLA	C4B-CHC	-2.37	1.34	1.41
29	C	516	DGD	O1G-C1G	-2.37	1.39	1.45
29	h	102	DGD	C2A-C1A	-2.37	1.43	1.50
22	c	505	CLA	C3B-CAB	-2.37	1.43	1.47
29	C	516	DGD	O2G-C2G	-2.36	1.40	1.46
29	C	518	DGD	O4D-C4D	-2.36	1.37	1.43
22	c	502	CLA	CMC-C2C	-2.36	1.45	1.50
22	C	505	CLA	C1B-NB	2.35	1.37	1.35
22	C	511	CLA	C4B-CHC	-2.35	1.34	1.41
29	h	102	DGD	C4E-C3E	2.35	1.58	1.52
22	A	405	CLA	C3B-CAB	-2.35	1.43	1.47
29	c	517	DGD	O2G-C2G	-2.35	1.40	1.46
22	C	508	CLA	CMB-C2B	-2.35	1.46	1.51
29	h	102	DGD	O4D-C4D	-2.34	1.37	1.43
22	D	403	CLA	CMB-C2B	-2.34	1.46	1.51
33	D	408	LHG	P-O4	-2.34	1.44	1.55
29	C	517	DGD	O2G-C2G	-2.34	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	b	623	STE	C2-C1	2.34	1.56	1.50
22	b	609	CLA	C3B-CAB	-2.34	1.43	1.47
22	b	601	CLA	C4D-ND	-2.34	1.34	1.37
22	C	512	CLA	CMD-C2D	-2.34	1.45	1.50
22	C	501	CLA	C1C-NC	-2.33	1.34	1.37
22	B	602	CLA	CMC-C2C	-2.33	1.45	1.50
24	c	515	BCR	C33-C5	-2.33	1.47	1.50
22	B	607	CLA	C3B-C2B	-2.33	1.37	1.40
22	C	501	CLA	CMC-C2C	-2.33	1.45	1.50
33	D	408	LHG	O8-C6	-2.33	1.39	1.45
22	C	506	CLA	C3B-CAB	-2.32	1.43	1.47
22	c	501	CLA	CMC-C2C	-2.32	1.45	1.50
22	b	601	CLA	CMB-C2B	-2.32	1.46	1.51
27	b	620	LMG	O1-C7	-2.31	1.39	1.43
22	c	505	CLA	C1D-ND	2.31	1.40	1.37
26	D	406	PL9	C7-C3	-2.31	1.48	1.51
22	c	511	CLA	CMB-C2B	-2.31	1.46	1.51
24	B	618	BCR	C33-C5	-2.31	1.47	1.50
22	C	503	CLA	C3B-C2B	-2.30	1.37	1.40
22	b	605	CLA	CMB-C2B	-2.30	1.46	1.51
22	c	503	CLA	O2D-CGD	2.30	1.38	1.33
35	f	101	HEM	CAB-C3B	2.30	1.53	1.47
22	c	506	CLA	C3B-CAB	-2.30	1.43	1.47
33	D	409	LHG	C3-C2	2.30	1.59	1.51
22	B	612	CLA	C4B-CHC	-2.30	1.34	1.41
22	b	611	CLA	CMC-C2C	-2.30	1.45	1.50
22	b	603	CLA	CHC-C1C	2.30	1.40	1.35
27	A	411	LMG	C4-C5	2.30	1.57	1.53
22	B	608	CLA	C3B-CAB	-2.30	1.43	1.47
22	d	405	CLA	O2D-CGD	2.30	1.38	1.33
27	d	412	LMG	O7-C8	-2.29	1.40	1.46
32	B	627	STE	O1-C1	2.29	1.29	1.22
22	B	603	CLA	CMD-C2D	-2.29	1.45	1.50
23	d	402	PHO	CMD-C2D	-2.29	1.46	1.51
22	c	506	CLA	CMB-C2B	-2.29	1.46	1.51
27	b	622	LMG	C1-C2	2.28	1.59	1.52
22	d	403	CLA	CMD-C2D	-2.28	1.46	1.50
22	A	403	CLA	CMB-C2B	-2.28	1.46	1.51
22	c	501	CLA	C4B-CHC	-2.28	1.34	1.41
22	C	501	CLA	C3B-C2B	-2.28	1.37	1.40
22	c	506	CLA	CAC-C3C	-2.28	1.45	1.51
29	C	518	DGD	O3G-C3G	-2.28	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	518	DGD	O6D-C5D	-2.28	1.38	1.44
22	B	615	CLA	C3B-CAB	-2.27	1.43	1.47
22	b	609	CLA	CHC-C1C	2.27	1.40	1.35
22	c	512	CLA	CMC-C2C	-2.27	1.46	1.50
22	b	612	CLA	CHC-C1C	2.27	1.40	1.35
33	E	102	LHG	O8-C23	2.27	1.40	1.33
29	C	517	DGD	C1E-C2E	2.27	1.59	1.52
22	D	404	CLA	C1C-NC	-2.26	1.34	1.37
22	B	616	CLA	CMC-C2C	-2.26	1.46	1.50
24	b	618	BCR	C33-C5	-2.26	1.47	1.50
24	B	618	BCR	C36-C18	-2.26	1.46	1.50
22	C	501	CLA	CMD-C2D	-2.26	1.46	1.50
22	b	602	CLA	CAC-C3C	-2.25	1.45	1.51
22	C	503	CLA	C3B-CAB	-2.25	1.43	1.47
22	b	607	CLA	C3B-CAB	-2.25	1.43	1.47
22	b	607	CLA	CMC-C2C	-2.25	1.46	1.50
22	b	615	CLA	CMC-C2C	-2.25	1.46	1.50
29	h	102	DGD	O2E-C2E	-2.25	1.37	1.43
22	b	610	CLA	C4B-CHC	-2.25	1.34	1.41
22	c	510	CLA	CMC-C2C	-2.25	1.46	1.50
24	a	405	BCR	C21-C22	-2.25	1.32	1.35
29	H	102	DGD	C6D-C5D	2.25	1.58	1.51
22	c	503	CLA	CMC-C2C	-2.25	1.46	1.50
22	A	403	CLA	CAA-C2A	-2.25	1.49	1.54
22	c	505	CLA	CMC-C2C	-2.25	1.46	1.50
26	D	406	PL9	C21-C19	-2.25	1.46	1.51
33	d	410	LHG	O8-C23	2.24	1.39	1.33
22	B	604	CLA	C3B-C2B	-2.24	1.37	1.40
27	d	412	LMG	C7-C8	2.24	1.57	1.50
29	h	102	DGD	O5D-C6D	-2.24	1.39	1.43
27	c	522	LMG	C1-C2	2.24	1.58	1.52
22	c	507	CLA	CMC-C2C	-2.24	1.46	1.50
24	t	101	BCR	C1-C6	-2.23	1.50	1.53
24	T	101	BCR	C27-C26	-2.23	1.46	1.51
22	B	602	CLA	MG-ND	-2.23	2.01	2.05
22	B	601	CLA	CMC-C2C	-2.23	1.46	1.50
22	B	611	CLA	MG-NA	2.23	2.11	2.06
22	b	616	CLA	CHC-C1C	2.23	1.40	1.35
22	d	404	CLA	C3B-CAB	-2.23	1.43	1.47
33	D	408	LHG	P-O6	2.23	1.68	1.59
36	v	201	HEC	C1D-CHD	-2.23	1.34	1.41
22	A	405	CLA	C4B-CHC	-2.22	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	c	520	LMG	C1-C2	2.22	1.58	1.52
22	c	512	CLA	C1D-C2D	2.22	1.49	1.45
22	c	511	CLA	C3B-CAB	-2.22	1.43	1.47
22	b	605	CLA	MG-NA	2.22	2.11	2.06
24	C	515	BCR	C1-C6	-2.22	1.50	1.53
22	C	501	CLA	CMB-C2B	-2.22	1.47	1.51
27	b	622	LMG	O1-C7	-2.22	1.39	1.43
24	k	101	BCR	C36-C18	-2.22	1.46	1.50
22	B	607	CLA	CMD-C2D	-2.22	1.46	1.50
33	D	408	LHG	C8-C7	-2.22	1.44	1.50
22	D	404	CLA	C4D-ND	-2.21	1.34	1.37
27	C	519	LMG	O1-C1	2.21	1.44	1.40
27	b	620	LMG	C1-C2	2.21	1.58	1.52
22	B	616	CLA	CHC-C1C	2.20	1.40	1.35
29	C	516	DGD	O5D-C6D	-2.20	1.39	1.43
22	C	504	CLA	MG-ND	-2.20	2.01	2.05
24	B	618	BCR	C1-C6	-2.20	1.50	1.53
22	A	405	CLA	CMB-C2B	-2.19	1.47	1.51
23	A	404	PHO	CMD-C2D	-2.19	1.46	1.51
23	d	401	PHO	CBD-CGD	-2.19	1.49	1.52
22	D	404	CLA	C4B-CHC	-2.19	1.34	1.41
22	C	512	CLA	C3B-C2B	-2.19	1.37	1.40
24	a	405	BCR	C35-C13	-2.19	1.46	1.50
22	b	610	CLA	C3D-C4D	2.18	1.49	1.44
22	b	611	CLA	C4D-ND	-2.18	1.34	1.37
22	b	611	CLA	CMB-C2B	-2.18	1.47	1.51
22	b	608	CLA	C3B-C2B	-2.18	1.37	1.40
22	A	402	CLA	CMB-C2B	-2.18	1.47	1.51
22	c	506	CLA	C3B-C2B	-2.18	1.37	1.40
22	b	608	CLA	C3C-C2C	2.18	1.41	1.36
27	M	101	LMG	C4-C3	2.18	1.57	1.52
22	b	603	CLA	C3B-C2B	-2.17	1.37	1.40
22	c	504	CLA	CMB-C2B	-2.17	1.47	1.51
22	C	508	CLA	C1D-C2D	2.17	1.49	1.45
24	t	101	BCR	C38-C26	-2.17	1.47	1.50
27	C	519	LMG	C6-C5	2.16	1.59	1.51
22	C	504	CLA	CAC-C3C	-2.16	1.45	1.51
29	c	517	DGD	O3G-C3G	-2.16	1.39	1.43
24	C	514	BCR	C30-C25	-2.16	1.50	1.53
22	B	608	CLA	C3B-C2B	-2.16	1.37	1.40
22	B	613	CLA	C5-C3	-2.16	1.46	1.51
22	D	404	CLA	CHC-C1C	2.16	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	506	CLA	C3D-C4D	2.16	1.49	1.44
22	C	509	CLA	O2D-CGD	2.15	1.38	1.33
22	B	616	CLA	C3B-C2B	-2.15	1.37	1.40
23	D	401	PHO	C3B-C2B	-2.15	1.37	1.40
22	b	609	CLA	C4B-CHC	-2.15	1.35	1.41
22	d	405	CLA	CMD-C2D	-2.15	1.46	1.50
22	C	509	CLA	O2A-CGA	2.14	1.39	1.33
29	h	102	DGD	O2G-C1B	2.14	1.40	1.34
23	d	402	PHO	C3B-CAB	-2.14	1.43	1.47
29	c	517	DGD	O3E-C3E	-2.14	1.37	1.43
27	b	622	LMG	O6-C1	2.14	1.47	1.41
22	C	510	CLA	CMD-C2D	-2.14	1.46	1.50
27	C	519	LMG	C1-C2	2.13	1.58	1.52
22	c	511	CLA	CMC-C2C	-2.13	1.46	1.50
29	c	519	DGD	O3G-C1D	2.13	1.43	1.40
22	B	601	CLA	CMD-C2D	-2.13	1.46	1.50
24	a	405	BCR	C38-C26	-2.13	1.47	1.50
22	b	609	CLA	C3B-C2B	-2.13	1.37	1.40
22	b	615	CLA	C3B-CAB	-2.13	1.43	1.47
22	b	614	CLA	O2D-CED	-2.12	1.40	1.45
27	c	523	LMG	O6-C5	-2.12	1.39	1.44
22	B	610	CLA	C4D-ND	-2.11	1.34	1.37
24	C	515	BCR	C38-C26	-2.11	1.47	1.50
22	c	513	CLA	CMD-C2D	-2.11	1.46	1.50
35	f	101	HEM	CAA-C2A	2.11	1.55	1.52
22	b	606	CLA	CMD-C2D	-2.11	1.46	1.50
22	b	603	CLA	MG-NC	-2.11	2.01	2.06
33	E	102	LHG	C24-C23	2.11	1.56	1.50
22	b	611	CLA	C1D-ND	2.10	1.40	1.37
22	b	608	CLA	MG-NA	2.10	2.11	2.06
22	b	602	CLA	C1A-CHA	-2.10	1.34	1.43
29	C	518	DGD	C2A-C1A	-2.10	1.44	1.50
22	b	608	CLA	C1D-ND	2.10	1.40	1.37
22	b	603	CLA	CMD-C2D	-2.10	1.46	1.50
22	b	615	CLA	C4B-CHC	-2.10	1.35	1.41
22	a	404	CLA	C3B-CAB	-2.10	1.43	1.47
22	b	616	CLA	O2D-CED	-2.09	1.40	1.45
22	C	508	CLA	C3D-C4D	2.09	1.48	1.44
33	d	410	LHG	C6-C5	2.09	1.57	1.50
22	B	610	CLA	C1A-CHA	-2.09	1.34	1.43
22	b	604	CLA	C3B-CAB	-2.09	1.43	1.47
22	A	410	CLA	C1D-C2D	2.09	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	516	DGD	O5D-C1E	2.09	1.43	1.40
22	c	501	CLA	CMD-C2D	-2.09	1.46	1.50
22	C	505	CLA	C3B-CAB	-2.09	1.43	1.47
29	H	102	DGD	O1G-C1G	-2.08	1.40	1.45
22	c	509	CLA	C4B-CHC	-2.08	1.35	1.41
22	b	615	CLA	MG-NC	-2.08	2.01	2.06
22	d	405	CLA	C3B-CAB	-2.08	1.43	1.47
22	C	512	CLA	C5-C3	-2.08	1.47	1.51
22	c	507	CLA	CHC-C1C	2.08	1.40	1.35
27	D	407	LMG	C7-C8	2.08	1.57	1.50
27	C	519	LMG	O7-C8	-2.08	1.41	1.46
22	b	610	CLA	CMC-C2C	-2.08	1.46	1.50
22	b	611	CLA	C4B-CHC	-2.08	1.35	1.41
22	C	511	CLA	C1D-ND	2.08	1.40	1.37
27	A	411	LMG	C1-C2	2.08	1.58	1.52
22	b	605	CLA	C4B-CHC	-2.08	1.35	1.41
29	C	518	DGD	C3B-C2B	-2.08	1.44	1.52
22	c	502	CLA	C3B-CAB	-2.07	1.43	1.47
22	A	402	CLA	CMD-C2D	-2.07	1.46	1.50
33	d	408	LHG	O6-C4	-2.07	1.36	1.44
22	b	603	CLA	C3D-C4D	2.07	1.48	1.44
33	d	409	LHG	O6-C4	-2.07	1.36	1.44
22	b	608	CLA	C3B-CAB	-2.07	1.43	1.47
27	b	622	LMG	O1-C1	2.07	1.43	1.40
22	c	503	CLA	C3B-C2B	-2.07	1.37	1.40
27	b	622	LMG	C4-C5	2.07	1.57	1.53
22	A	410	CLA	CMC-C2C	-2.07	1.46	1.50
22	c	503	CLA	CMD-C2D	-2.06	1.46	1.50
22	C	510	CLA	CMC-C2C	-2.06	1.46	1.50
22	C	505	CLA	C4B-CHC	-2.06	1.35	1.41
33	B	622	LHG	P-O4	-2.06	1.45	1.55
22	B	614	CLA	C3C-C2C	2.06	1.41	1.36
36	v	201	HEC	O1D-CGD	2.06	1.29	1.22
22	C	512	CLA	C1D-C2D	2.06	1.49	1.45
22	d	405	CLA	O1D-CGD	2.05	1.26	1.21
22	C	508	CLA	CAC-C3C	-2.05	1.45	1.51
24	b	618	BCR	C36-C18	-2.05	1.46	1.50
29	C	518	DGD	O5D-C1E	2.05	1.43	1.40
29	C	516	DGD	C3E-C2E	2.05	1.57	1.52
22	B	603	CLA	C1A-CHA	-2.05	1.34	1.43
22	b	612	CLA	CMD-C2D	-2.05	1.46	1.50
29	c	517	DGD	O5D-C1E	2.05	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	509	CLA	O2D-CED	-2.05	1.40	1.45
22	c	505	CLA	CMB-C2B	-2.04	1.47	1.51
22	C	513	CLA	C4B-CHC	-2.04	1.35	1.41
29	C	518	DGD	O4E-C4E	-2.04	1.38	1.43
28	B	623	SQD	O2-C2	-2.04	1.38	1.43
22	c	510	CLA	CAA-C2A	-2.04	1.50	1.54
26	d	407	PL9	C43-C44	-2.04	1.28	1.33
35	E	101	HEM	CHC-C4B	-2.04	1.35	1.41
22	c	508	CLA	C4B-CHC	-2.04	1.35	1.41
27	D	410	LMG	O8-C28	2.04	1.39	1.33
32	D	411	STE	O1-C1	2.03	1.28	1.22
23	d	401	PHO	C1C-NC	-2.03	1.32	1.38
22	B	603	CLA	O2D-CGD	2.03	1.38	1.33
29	c	519	DGD	O2D-C2D	-2.03	1.38	1.43
22	b	601	CLA	C3B-CAB	-2.03	1.43	1.47
22	d	403	CLA	C4B-CHC	-2.03	1.35	1.41
27	c	520	LMG	C7-C8	2.02	1.56	1.50
32	c	521	STE	C2-C1	2.02	1.55	1.50
22	B	609	CLA	CHC-C1C	2.02	1.40	1.35
23	D	401	PHO	CMD-C2D	-2.02	1.46	1.51
22	B	605	CLA	C4B-CHC	-2.02	1.35	1.41
22	c	507	CLA	C4B-CHC	-2.02	1.35	1.41
22	B	614	CLA	C1A-CHA	-2.01	1.34	1.43
26	A	409	PL9	C41-C39	2.01	1.55	1.51
26	D	406	PL9	C3-C4	-2.01	1.46	1.49
22	c	512	CLA	CMD-C2D	-2.01	1.46	1.50
26	a	409	PL9	C25-C24	-2.01	1.45	1.50
22	c	512	CLA	C3D-C4D	2.01	1.48	1.44
24	B	619	BCR	C31-C1	-2.01	1.49	1.53
35	E	101	HEM	C3D-C2D	-2.01	1.32	1.36
22	b	610	CLA	C3B-CAB	-2.01	1.43	1.47
22	c	510	CLA	C5-C3	-2.01	1.47	1.51
22	b	605	CLA	MG-NC	-2.01	2.01	2.06
29	c	517	DGD	O6E-C1E	-2.01	1.36	1.41
27	c	523	LMG	C1-C2	2.01	1.58	1.52
22	C	511	CLA	CMC-C2C	-2.01	1.46	1.50
22	b	616	CLA	CMD-C2D	-2.01	1.46	1.50
29	H	102	DGD	O3E-C3E	-2.01	1.38	1.43
22	A	405	CLA	CAC-C3C	-2.00	1.46	1.51
22	B	607	CLA	C3B-CAB	-2.00	1.43	1.47
28	f	102	SQD	O4-C4	-2.00	1.38	1.43
22	B	613	CLA	CMC-C2C	-2.00	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	604	CLA	C3B-C2B	-2.00	1.37	1.40

All (1284) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	509	CLA	C4A-NA-C1A	9.93	111.17	106.71
22	c	511	CLA	C4A-NA-C1A	9.44	110.95	106.71
22	B	616	CLA	C4A-NA-C1A	9.36	110.91	106.71
22	C	507	CLA	C4A-NA-C1A	9.33	110.90	106.71
28	L	101	SQD	O6-C1-C2	9.25	122.74	108.30
22	B	607	CLA	C4A-NA-C1A	8.87	110.69	106.71
22	C	501	CLA	C4A-NA-C1A	8.76	110.64	106.71
22	B	601	CLA	C4A-NA-C1A	8.51	110.53	106.71
22	b	601	CLA	C4A-NA-C1A	8.43	110.50	106.71
28	a	410	SQD	O6-C1-C2	8.37	121.37	108.30
22	B	604	CLA	C4A-NA-C1A	8.33	110.45	106.71
28	A	412	SQD	O6-C1-C2	8.04	120.86	108.30
22	B	615	CLA	C4A-NA-C1A	7.77	110.20	106.71
22	b	606	CLA	C4A-NA-C1A	7.54	110.09	106.71
22	C	506	CLA	C4A-NA-C1A	7.13	109.91	106.71
22	c	503	CLA	C4A-NA-C1A	7.12	109.91	106.71
22	b	604	CLA	C4A-NA-C1A	7.00	109.85	106.71
22	C	513	CLA	C4A-NA-C1A	6.77	109.75	106.71
28	B	623	SQD	O6-C1-C2	6.74	118.82	108.30
28	L	101	SQD	O7-S-C6	6.67	114.86	106.94
22	b	616	CLA	CMB-C2B-C1B	-6.58	118.36	128.46
26	D	406	PL9	C7-C3-C4	6.36	122.04	116.88
22	d	404	CLA	C4A-NA-C1A	6.35	109.56	106.71
22	c	508	CLA	C4A-NA-C1A	6.35	109.56	106.71
22	c	512	CLA	C4A-NA-C1A	6.32	109.55	106.71
22	D	404	CLA	C4A-NA-C1A	6.31	109.54	106.71
22	C	508	CLA	C4A-NA-C1A	6.26	109.52	106.71
22	C	503	CLA	C4A-NA-C1A	6.25	109.52	106.71
22	B	602	CLA	C4A-NA-C1A	6.15	109.47	106.71
22	b	616	CLA	CMB-C2B-C3B	6.10	136.09	124.68
28	A	412	SQD	O8-S-C6	6.08	115.43	105.74
22	D	404	CLA	CMB-C2B-C1B	-5.97	119.28	128.46
22	b	612	CLA	CMB-C2B-C1B	-5.89	119.41	128.46
22	c	501	CLA	C4A-NA-C1A	5.85	109.33	106.71
22	B	608	CLA	O2D-CGD-O1D	-5.71	112.67	123.84
22	B	602	CLA	CMB-C2B-C1B	-5.67	119.75	128.46
28	F	101	SQD	O9-S-C6	5.64	113.65	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	504	CLA	C4A-NA-C1A	5.57	109.21	106.71
28	A	412	SQD	O7-S-C6	5.57	113.55	106.94
22	b	613	CLA	C4A-NA-C1A	5.56	109.21	106.71
22	A	402	CLA	C4A-NA-C1A	5.55	109.20	106.71
22	C	509	CLA	CMB-C2B-C1B	-5.54	119.94	128.46
22	b	608	CLA	CMB-C2B-C1B	-5.44	120.10	128.46
22	a	403	CLA	CMB-C2B-C1B	-5.44	120.11	128.46
26	d	407	PL9	C7-C3-C4	5.37	121.24	116.88
22	C	511	CLA	C4A-NA-C1A	5.34	109.11	106.71
22	c	510	CLA	C4A-NA-C1A	5.33	109.10	106.71
22	B	608	CLA	C4A-NA-C1A	5.32	109.10	106.71
28	B	623	SQD	O7-S-C6	5.31	113.25	106.94
28	f	102	SQD	O7-S-C6	5.29	113.22	106.94
22	c	505	CLA	C4A-NA-C1A	5.23	109.06	106.71
26	d	407	PL9	C40-C39-C41	5.22	124.06	115.27
28	F	101	SQD	O8-S-C6	5.18	114.00	105.74
22	b	615	CLA	C4A-NA-C1A	5.17	109.03	106.71
22	B	612	CLA	CMB-C2B-C3B	5.17	134.35	124.68
22	d	405	CLA	CMB-C2B-C1B	-5.17	120.52	128.46
22	b	603	CLA	C4A-NA-C1A	5.16	109.02	106.71
26	a	409	PL9	C7-C3-C4	5.15	121.07	116.88
22	c	504	CLA	CMB-C2B-C1B	-5.15	120.54	128.46
22	c	501	CLA	O2D-CGD-O1D	-5.14	113.80	123.84
22	c	513	CLA	CMB-C2B-C1B	-5.13	120.57	128.46
22	C	509	CLA	C4A-NA-C1A	5.10	109.00	106.71
22	B	608	CLA	CMB-C2B-C1B	-5.09	120.64	128.46
22	B	613	CLA	CMB-C2B-C1B	-5.08	120.65	128.46
22	a	403	CLA	C4A-NA-C1A	5.07	108.99	106.71
22	b	606	CLA	CMB-C2B-C1B	-5.07	120.67	128.46
22	B	606	CLA	C4A-NA-C1A	5.06	108.98	106.71
22	C	505	CLA	C4A-NA-C1A	5.02	108.96	106.71
22	B	610	CLA	O2D-CGD-O1D	-5.01	114.04	123.84
22	c	506	CLA	C4A-NA-C1A	4.99	108.95	106.71
22	A	405	CLA	CMB-C2B-C1B	-4.99	120.79	128.46
28	a	410	SQD	C1-O5-C5	-4.98	103.90	113.69
22	B	612	CLA	C4A-NA-C1A	4.96	108.94	106.71
22	b	609	CLA	CMB-C2B-C1B	-4.94	120.86	128.46
22	a	402	CLA	CMB-C2B-C1B	-4.93	120.89	128.46
22	a	402	CLA	C4A-NA-C1A	4.92	108.92	106.71
26	A	409	PL9	C7-C3-C4	4.91	120.87	116.88
22	c	508	CLA	CMB-C2B-C1B	-4.88	120.96	128.46
22	b	603	CLA	CHD-C1D-ND	-4.88	119.97	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	509	CLA	CMB-C2B-C3B	4.88	133.82	124.68
22	b	611	CLA	C4A-NA-C1A	4.86	108.89	106.71
22	B	604	CLA	CMB-C2B-C1B	-4.85	121.01	128.46
22	B	612	CLA	CMB-C2B-C1B	-4.81	121.07	128.46
22	C	508	CLA	CMB-C2B-C1B	-4.80	121.09	128.46
22	d	405	CLA	CMB-C2B-C3B	4.77	133.60	124.68
22	D	404	CLA	O2D-CGD-O1D	-4.75	114.56	123.84
22	c	502	CLA	C4A-NA-C1A	4.74	108.84	106.71
22	B	602	CLA	CMB-C2B-C3B	4.73	133.54	124.68
22	D	404	CLA	CMB-C2B-C3B	4.73	133.53	124.68
22	b	615	CLA	CMB-C2B-C1B	-4.71	121.22	128.46
22	c	510	CLA	CMB-C2B-C1B	-4.68	121.28	128.46
26	A	409	PL9	C20-C19-C21	4.66	123.12	115.27
22	B	605	CLA	C4A-NA-C1A	4.65	108.80	106.71
29	H	102	DGD	O3G-C3G-C2G	-4.63	99.72	110.90
36	V	201	HEC	CMC-C2C-C1C	-4.63	121.35	128.46
22	b	602	CLA	CMB-C2B-C1B	-4.62	121.36	128.46
34	D	402	BCT	O2-C-O1	4.62	131.53	119.55
22	c	513	CLA	C4A-NA-C1A	4.59	108.77	106.71
24	C	514	BCR	C36-C18-C17	-4.58	116.50	122.92
22	C	510	CLA	C4A-NA-C1A	4.58	108.77	106.71
29	A	414	DGD	C4E-C3E-C2E	-4.57	102.85	110.82
28	a	410	SQD	O7-S-C6	4.57	112.36	106.94
22	A	402	CLA	CMB-C2B-C1B	-4.55	121.47	128.46
28	F	101	SQD	O6-C1-C2	4.55	115.40	108.30
22	b	602	CLA	C4A-NA-C1A	4.54	108.75	106.71
22	b	608	CLA	CMB-C2B-C3B	4.51	133.11	124.68
22	C	513	CLA	C4-C3-C5	4.49	122.82	115.27
29	C	517	DGD	O5D-C6D-C5D	-4.47	100.77	109.05
33	L	102	LHG	O4-P-O5	4.47	134.32	112.24
22	b	608	CLA	C4A-NA-C1A	4.46	108.71	106.71
22	b	613	CLA	CMB-C2B-C1B	-4.46	121.61	128.46
24	b	618	BCR	C36-C18-C17	-4.46	116.68	122.92
22	B	602	CLA	O2D-CGD-CBD	4.46	119.19	111.27
22	d	403	CLA	CMB-C2B-C1B	-4.45	121.62	128.46
22	B	613	CLA	CMB-C2B-C3B	4.44	132.99	124.68
22	D	403	CLA	C4A-NA-C1A	4.44	108.70	106.71
22	b	614	CLA	C4A-NA-C1A	4.44	108.70	106.71
28	B	623	SQD	O47-C7-C8	4.44	121.07	111.50
27	b	622	LMG	C1-O6-C5	-4.43	105.00	113.69
22	C	511	CLA	CMB-C2B-C1B	-4.40	121.69	128.46
29	h	102	DGD	O3G-C3G-C2G	-4.39	100.31	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	510	CLA	CMB-C2B-C1B	-4.39	121.72	128.46
22	c	510	CLA	O2D-CGD-O1D	-4.39	115.26	123.84
22	b	612	CLA	CMB-C2B-C3B	4.39	132.88	124.68
22	b	616	CLA	C4A-NA-C1A	4.36	108.67	106.71
22	c	506	CLA	CMB-C2B-C1B	-4.35	121.78	128.46
22	A	410	CLA	CMB-C2B-C3B	4.35	132.82	124.68
28	A	412	SQD	C1-C2-C3	-4.34	100.95	110.00
36	V	201	HEC	CBD-CAD-C3D	-4.34	105.22	112.62
23	A	404	PHO	CMB-C2B-C3B	4.33	132.78	124.68
22	B	611	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
22	B	608	CLA	CMB-C2B-C3B	4.33	132.78	124.68
22	c	509	CLA	CMB-C2B-C1B	-4.30	121.86	128.46
22	A	405	CLA	CMB-C2B-C3B	4.29	132.70	124.68
33	d	408	LHG	O8-C23-O10	-4.29	112.77	123.59
28	L	101	SQD	O9-S-C6	4.28	112.02	106.94
29	a	412	DGD	O3G-C3G-C2G	-4.27	100.46	111.78
22	B	609	CLA	C4A-NA-C1A	4.26	108.62	106.71
33	e	101	LHG	O4-P-O5	4.26	133.31	112.24
22	b	602	CLA	CMB-C2B-C3B	4.26	132.64	124.68
22	c	504	CLA	CMB-C2B-C3B	4.26	132.64	124.68
22	a	403	CLA	CMB-C2B-C3B	4.25	132.64	124.68
22	C	507	CLA	O2D-CGD-O1D	-4.24	115.55	123.84
35	f	101	HEM	CBA-CAA-C2A	-4.23	105.39	112.62
23	d	402	PHO	O2D-CGD-O1D	-4.23	115.56	123.84
29	C	517	DGD	O3G-C3G-C2G	-4.22	100.72	110.90
22	b	611	CLA	O2D-CGD-O1D	-4.22	115.60	123.84
22	b	606	CLA	CMB-C2B-C3B	4.21	132.55	124.68
22	B	608	CLA	O2D-CGD-CBD	4.20	118.74	111.27
22	c	508	CLA	CMB-C2B-C3B	4.20	132.53	124.68
32	m	101	STE	O2-C1-C2	4.19	127.49	114.03
22	a	402	CLA	CMB-C2B-C3B	4.17	132.47	124.68
24	b	617	BCR	C2-C1-C6	4.17	116.89	110.48
22	c	513	CLA	CMB-C2B-C3B	4.16	132.46	124.68
22	A	410	CLA	CMB-C2B-C1B	-4.15	122.08	128.46
22	B	610	CLA	C4A-NA-C1A	4.15	108.57	106.71
22	c	512	CLA	C1-C2-C3	-4.15	118.87	126.04
22	C	510	CLA	CMB-C2B-C3B	4.15	132.44	124.68
22	b	606	CLA	O2D-CGD-O1D	-4.13	115.76	123.84
22	d	403	CLA	CMB-C2B-C3B	4.13	132.41	124.68
22	A	402	CLA	CMB-C2B-C3B	4.13	132.41	124.68
22	A	410	CLA	C4A-NA-C1A	4.12	108.56	106.71
22	c	503	CLA	CMB-C2B-C1B	-4.12	122.14	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	503	CLA	CHD-C1D-ND	-4.11	120.68	124.45
33	E	102	LHG	O4-P-O5	4.10	132.50	112.24
22	c	510	CLA	CMB-C2B-C3B	4.09	132.34	124.68
24	B	619	BCR	C2-C1-C6	4.09	116.77	110.48
33	B	622	LHG	O4-P-O5	4.08	132.43	112.24
22	A	405	CLA	O2D-CGD-O1D	-4.08	115.87	123.84
22	B	604	CLA	CMB-C2B-C3B	4.07	132.30	124.68
29	c	519	DGD	O3G-C3G-C2G	-4.07	101.08	110.90
33	d	408	LHG	O4-P-O5	4.06	132.31	112.24
22	b	604	CLA	CHB-C4A-NA	4.06	130.12	124.51
22	B	616	CLA	CMB-C2B-C3B	4.06	132.27	124.68
22	C	512	CLA	C4A-NA-C1A	4.06	108.53	106.71
22	C	505	CLA	CMB-C2B-C1B	-4.06	122.23	128.46
22	b	616	CLA	CHD-C1D-ND	-4.05	120.73	124.45
22	b	605	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
22	C	508	CLA	CHD-C1D-ND	-4.05	120.73	124.45
33	d	410	LHG	O4-P-O5	4.04	132.22	112.24
34	a	408	BCT	O2-C-O1	4.04	130.02	119.55
23	A	404	PHO	O2D-CGD-CBD	4.04	116.11	111.00
22	c	509	CLA	O2A-CGA-O1A	-4.00	113.49	123.59
22	B	605	CLA	O1D-CGD-CBD	4.00	132.66	124.48
22	B	611	CLA	O2D-CGD-O1D	-3.99	116.03	123.84
22	b	601	CLA	CHB-C4A-NA	3.99	130.03	124.51
22	C	506	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
22	B	616	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
22	b	614	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
26	d	407	PL9	C42-C43-C44	-3.97	118.09	127.66
22	b	605	CLA	C4-C3-C5	3.97	121.94	115.27
23	d	402	PHO	O1D-CGD-CBD	3.95	131.32	124.74
22	d	404	CLA	O2D-CGD-CBD	3.95	118.29	111.27
27	d	411	LMG	O7-C10-O9	-3.95	113.46	123.30
28	A	413	SQD	C45-O47-C7	3.94	122.95	117.88
29	c	518	DGD	O3G-C3G-C2G	-3.94	101.39	110.90
22	c	502	CLA	CHD-C1D-ND	-3.94	120.83	124.45
22	b	609	CLA	CMB-C2B-C3B	3.94	132.05	124.68
22	B	613	CLA	C1-C2-C3	-3.93	119.25	126.04
28	a	410	SQD	C1-C2-C3	-3.92	101.83	110.00
22	b	607	CLA	C4A-NA-C1A	3.92	108.47	106.71
29	C	518	DGD	O3G-C3G-C2G	-3.92	101.45	110.90
28	L	101	SQD	O48-C23-C24	3.92	124.20	111.91
32	j	101	STE	O2-C1-C2	3.90	126.58	114.03
22	B	611	CLA	CMB-C2B-C3B	3.90	131.98	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	d	404	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
22	B	604	CLA	O2D-CGD-O1D	-3.89	116.24	123.84
33	D	408	LHG	O4-P-O5	3.87	131.37	112.24
22	C	502	CLA	C4A-NA-C1A	3.86	108.44	106.71
22	b	612	CLA	O2D-CGD-O1D	-3.85	116.30	123.84
22	B	607	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
22	c	502	CLA	O2D-CGD-O1D	-3.84	116.32	123.84
22	b	602	CLA	CHB-C4A-NA	3.84	129.82	124.51
22	c	502	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
22	B	610	CLA	CHB-C4A-NA	3.83	129.81	124.51
28	A	412	SQD	O9-S-O7	-3.82	100.73	113.95
28	f	102	SQD	O6-C1-C2	3.81	114.25	108.30
22	A	405	CLA	CHD-C1D-ND	-3.81	120.96	124.45
22	B	604	CLA	C2D-C1D-ND	-3.80	107.30	110.10
23	D	401	PHO	CMB-C2B-C3B	3.80	131.79	124.68
22	C	508	CLA	CMB-C2B-C3B	3.80	131.78	124.68
33	d	409	LHG	O4-P-O5	3.80	131.00	112.24
28	A	412	SQD	O47-C7-O49	-3.79	114.54	123.70
22	B	613	CLA	C4A-NA-C1A	3.79	108.41	106.71
22	C	504	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
29	h	102	DGD	O3E-C3E-C2E	-3.76	101.65	110.35
22	b	610	CLA	CAC-C3C-C4C	3.76	129.69	124.81
26	A	409	PL9	C36-C34-C33	-3.75	113.53	121.12
29	C	516	DGD	O3G-C3G-C2G	-3.74	101.87	110.90
22	c	506	CLA	CMB-C2B-C3B	3.73	131.67	124.68
28	f	102	SQD	O9-S-O7	-3.72	101.07	113.95
22	A	405	CLA	C1B-CHB-C4A	-3.70	122.79	130.12
22	b	616	CLA	O2D-CGD-O1D	-3.70	116.61	123.84
22	c	509	CLA	CMB-C2B-C3B	3.69	131.59	124.68
22	b	610	CLA	C1B-CHB-C4A	-3.69	122.80	130.12
28	A	413	SQD	O48-C23-C24	3.69	123.48	111.91
26	a	409	PL9	C35-C34-C36	3.68	121.47	115.27
24	b	619	BCR	C36-C18-C17	-3.68	117.77	122.92
33	D	409	LHG	O4-P-O5	3.67	130.39	112.24
22	B	605	CLA	O2D-CGD-O1D	-3.67	116.67	123.84
24	T	101	BCR	C27-C26-C25	3.67	128.06	122.73
26	d	407	PL9	C36-C34-C33	-3.66	113.71	121.12
22	b	604	CLA	C1-C2-C3	-3.65	119.73	126.04
22	b	603	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
36	V	201	HEC	CMC-C2C-C3C	3.64	130.10	125.82
33	B	622	LHG	O8-C23-C24	3.64	123.33	111.91
22	B	603	CLA	CHD-C1D-ND	-3.61	121.13	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	l	101	LHG	O4-P-O5	3.60	130.04	112.24
29	C	518	DGD	O3G-C1D-C2D	-3.60	102.69	108.30
28	f	102	SQD	O5-C5-C4	3.59	116.22	109.69
22	b	603	CLA	O2D-CGD-O1D	-3.59	116.82	123.84
36	v	201	HEC	CMC-C2C-C1C	-3.58	122.95	128.46
28	a	410	SQD	O9-S-O7	-3.58	101.57	113.95
29	C	516	DGD	O1G-C1A-C2A	-3.57	100.71	111.91
22	C	505	CLA	CMB-C2B-C3B	3.56	131.34	124.68
22	C	512	CLA	CHD-C1D-ND	-3.56	121.18	124.45
22	D	403	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
29	A	414	DGD	O3G-C3G-C2G	-3.56	102.32	110.90
26	a	409	PL9	C7-C3-C2	-3.55	118.63	123.30
22	A	402	CLA	CHB-C4A-NA	3.55	129.42	124.51
22	b	607	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
24	A	406	BCR	C37-C22-C21	-3.54	117.96	122.92
22	C	506	CLA	CMB-C2B-C3B	3.54	131.31	124.68
36	v	201	HEC	CMB-C2B-C1B	-3.54	123.03	128.46
22	C	504	CLA	C4-C3-C5	3.53	121.21	115.27
24	a	405	BCR	C39-C30-C25	-3.53	104.57	110.30
22	B	602	CLA	O2D-CGD-O1D	-3.53	116.95	123.84
22	c	508	CLA	CHB-C4A-NA	3.52	129.38	124.51
22	a	404	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
22	b	611	CLA	CHD-C1D-ND	-3.52	121.22	124.45
29	C	517	DGD	O2D-C2D-C1D	-3.51	101.51	110.05
22	B	604	CLA	CHB-C4A-NA	3.51	129.37	124.51
24	B	617	BCR	C2-C1-C6	3.51	115.88	110.48
28	B	623	SQD	C3-C4-C5	3.51	116.50	110.24
23	d	402	PHO	CMC-C2C-C3C	3.50	131.54	124.94
22	c	501	CLA	O2D-CGD-CBD	3.50	117.48	111.27
28	B	623	SQD	O8-S-C6	3.49	111.31	105.74
22	B	603	CLA	C4-C3-C5	3.49	121.14	115.27
24	d	406	BCR	C38-C26-C25	-3.48	120.62	124.53
22	D	403	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
22	C	512	CLA	CHB-C4A-NA	3.48	129.32	124.51
22	a	404	CLA	C4A-NA-C1A	3.48	108.27	106.71
22	c	502	CLA	C1B-CHB-C4A	-3.47	123.24	130.12
22	b	602	CLA	O2D-CGD-CBD	3.46	117.42	111.27
33	d	408	LHG	O8-C23-C24	3.46	122.77	111.91
22	b	613	CLA	CMB-C2B-C3B	3.46	131.15	124.68
24	T	101	BCR	C7-C8-C9	-3.45	121.02	126.23
22	B	610	CLA	C1B-CHB-C4A	-3.45	123.28	130.12
28	a	410	SQD	C3-C4-C5	3.45	116.39	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	401	PHO	CMB-C2B-C3B	3.45	131.13	124.68
22	b	604	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
22	B	610	CLA	O2D-CGD-CBD	3.44	117.38	111.27
22	c	509	CLA	CHD-C1D-ND	-3.44	121.29	124.45
27	b	620	LMG	O1-C1-C2	-3.44	102.94	108.30
28	A	413	SQD	O47-C7-C8	3.43	118.90	111.50
24	K	101	BCR	C15-C16-C17	-3.43	116.44	123.47
22	b	616	CLA	C1B-CHB-C4A	-3.42	123.33	130.12
29	c	517	DGD	O3G-C3G-C2G	-3.42	102.65	110.90
28	B	623	SQD	O48-C23-C24	3.42	122.63	111.91
28	B	623	SQD	O9-S-O7	-3.41	102.13	113.95
22	d	404	CLA	O2D-CGD-O1D	-3.41	117.18	123.84
22	b	604	CLA	C11-C12-C13	-3.40	104.91	115.92
29	C	517	DGD	O4D-C4D-C3D	3.40	118.21	110.35
22	C	503	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
22	C	507	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
28	L	101	SQD	C1-C2-C3	-3.39	102.93	110.00
27	C	519	LMG	O2-C2-C1	-3.39	101.81	110.05
22	c	513	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
32	C	520	STE	C3-C2-C1	-3.39	105.92	114.47
29	H	102	DGD	C3E-C4E-C5E	-3.38	104.20	110.24
28	A	412	SQD	C1-O5-C5	-3.38	107.05	113.69
22	B	610	CLA	CHD-C1D-ND	-3.38	121.34	124.45
22	c	512	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
22	C	513	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
28	L	101	SQD	O5-C1-C2	-3.38	103.19	110.35
22	B	607	CLA	CMB-C2B-C3B	3.37	130.98	124.68
27	b	620	LMG	O1-C7-C8	-3.36	102.79	110.90
29	C	517	DGD	C3D-C4D-C5D	-3.36	104.24	110.24
27	C	519	LMG	O1-C1-C2	-3.36	103.06	108.30
22	B	612	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
22	b	603	CLA	CMB-C2B-C3B	3.35	130.94	124.68
22	B	614	CLA	C1B-CHB-C4A	-3.34	123.49	130.12
29	c	517	DGD	O3G-C1D-C2D	-3.34	103.08	108.30
29	c	518	DGD	C3D-C4D-C5D	-3.34	104.28	110.24
26	d	407	PL9	C37-C38-C39	-3.33	119.64	127.66
22	C	511	CLA	CMB-C2B-C3B	3.33	130.90	124.68
26	a	409	PL9	C36-C34-C33	-3.33	114.39	121.12
29	c	518	DGD	O2D-C2D-C1D	-3.32	101.97	110.05
24	c	515	BCR	C2-C1-C6	3.32	115.59	110.48
22	b	613	CLA	C1-C2-C3	-3.32	120.31	126.04
22	B	615	CLA	CHB-C4A-NA	3.31	129.09	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	d	403	CLA	C4A-NA-C1A	3.31	108.19	106.71
27	b	620	LMG	O3-C3-C2	-3.31	102.70	110.35
22	B	613	CLA	CAC-C3C-C4C	3.30	129.10	124.81
28	a	410	SQD	O48-C23-C24	3.30	122.26	111.91
26	a	409	PL9	C40-C39-C41	3.30	120.82	115.27
22	a	404	CLA	CHB-C4A-NA	3.30	129.07	124.51
22	b	612	CLA	C1B-CHB-C4A	-3.29	123.61	130.12
22	b	608	CLA	CHB-C4A-NA	3.28	129.05	124.51
22	c	508	CLA	CHD-C1D-ND	-3.28	121.44	124.45
27	d	412	LMG	O2-C2-C1	-3.28	102.08	110.05
29	C	516	DGD	O3E-C3E-C2E	-3.28	102.78	110.35
22	B	616	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
26	A	409	PL9	C40-C39-C38	-3.27	115.30	123.68
24	b	617	BCR	C38-C26-C25	-3.27	120.86	124.53
22	c	502	CLA	CMB-C2B-C3B	3.26	130.79	124.68
22	C	507	CLA	CHB-C4A-NA	3.26	129.02	124.51
35	f	101	HEM	C3B-C2B-C1B	3.26	108.90	106.49
28	a	410	SQD	O9-S-C6	3.26	110.81	106.94
24	b	619	BCR	C12-C13-C14	-3.25	113.95	118.94
27	D	407	LMG	C3-C4-C5	-3.25	104.44	110.24
22	c	501	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
22	A	410	CLA	CHB-C4A-NA	3.24	128.99	124.51
23	D	401	PHO	O1D-CGD-CBD	3.24	130.13	124.74
22	b	601	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
22	C	507	CLA	CMB-C2B-C3B	3.23	130.72	124.68
22	B	606	CLA	CMB-C2B-C1B	-3.23	123.51	128.46
22	C	501	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
27	c	523	LMG	C1-O6-C5	-3.22	107.37	113.69
22	B	612	CLA	C11-C12-C13	-3.22	105.52	115.92
27	M	101	LMG	C1-O6-C5	-3.22	107.38	113.69
28	L	101	SQD	C3-C4-C5	3.22	115.97	110.24
29	A	414	DGD	O5D-C6D-C5D	-3.20	103.12	109.05
22	b	611	CLA	O2D-CGD-CBD	3.20	116.95	111.27
22	b	614	CLA	CHD-C1D-ND	-3.20	121.52	124.45
22	c	507	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
22	B	602	CLA	CHB-C4A-NA	3.19	128.93	124.51
22	a	403	CLA	CHB-C4A-NA	3.19	128.93	124.51
24	Y	101	BCR	C37-C22-C21	-3.19	118.45	122.92
22	a	403	CLA	C1B-CHB-C4A	-3.19	123.80	130.12
24	c	515	BCR	C15-C16-C17	-3.18	116.95	123.47
22	B	610	CLA	O2A-CGA-O1A	-3.18	115.56	123.59
24	K	101	BCR	C11-C10-C9	-3.18	122.77	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	614	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
27	b	622	LMG	C3-C4-C5	-3.18	104.56	110.24
28	L	101	SQD	O9-S-O7	-3.18	102.94	113.95
22	b	616	CLA	CHB-C4A-NA	3.18	128.91	124.51
22	C	513	CLA	CHD-C1D-ND	-3.18	121.53	124.45
24	C	514	BCR	C2-C1-C6	3.18	115.37	110.48
22	c	503	CLA	CMB-C2B-C3B	3.18	130.62	124.68
22	b	612	CLA	O1D-CGD-CBD	3.17	130.97	124.48
24	a	405	BCR	C40-C30-C25	3.17	115.44	110.30
22	A	403	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
22	B	611	CLA	O2D-CGD-CBD	3.16	116.88	111.27
22	C	509	CLA	CHB-C4A-NA	3.16	128.88	124.51
22	b	603	CLA	C1B-CHB-C4A	-3.16	123.87	130.12
22	B	614	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
22	C	513	CLA	O2A-CGA-O1A	-3.16	115.63	123.59
22	D	404	CLA	O2D-CGD-CBD	3.15	116.87	111.27
27	M	101	LMG	C1-C2-C3	-3.15	103.43	110.00
23	d	402	PHO	C1-C2-C3	-3.15	120.60	126.04
24	c	515	BCR	C36-C18-C17	-3.15	118.52	122.92
22	b	614	CLA	C1B-CHB-C4A	-3.14	123.89	130.12
22	b	610	CLA	CMB-C2B-C3B	3.14	130.55	124.68
22	a	403	CLA	CAC-C3C-C4C	3.13	128.87	124.81
22	b	611	CLA	CMB-C2B-C1B	-3.13	123.66	128.46
22	A	405	CLA	O2D-CGD-CBD	3.12	116.82	111.27
32	C	522	STE	C4-C3-C2	-3.12	101.97	113.19
22	B	615	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
24	d	406	BCR	C27-C26-C25	3.12	127.26	122.73
22	b	610	CLA	CHB-C4A-NA	3.12	128.82	124.51
22	b	615	CLA	CMB-C2B-C3B	3.12	130.51	124.68
24	a	405	BCR	C2-C1-C6	3.11	115.27	110.48
22	C	508	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
26	d	407	PL9	C22-C23-C24	-3.10	120.19	127.66
36	V	201	HEC	C1D-C2D-C3D	-3.10	104.84	107.00
22	b	602	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
28	L	101	SQD	O5-C5-C4	3.09	115.31	109.69
27	d	412	LMG	C3-C4-C5	-3.09	104.72	110.24
24	d	406	BCR	C16-C15-C14	-3.09	117.14	123.47
27	b	622	LMG	O2-C2-C1	-3.09	102.54	110.05
22	b	605	CLA	CMB-C2B-C3B	3.09	130.46	124.68
35	f	101	HEM	CBD-CAD-C3D	-3.09	104.05	112.63
28	A	412	SQD	O47-C7-C8	3.09	118.15	111.50
22	B	603	CLA	CHD-C4C-NC	3.08	129.06	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	F	101	SQD	O48-C23-O10	-3.08	115.82	123.59
22	B	602	CLA	C16-C15-C13	-3.08	105.97	115.92
22	c	512	CLA	CHB-C4A-NA	3.07	128.76	124.51
22	B	606	CLA	C6-C5-C3	-3.06	105.42	113.45
26	A	409	PL9	C22-C23-C24	-3.06	120.29	127.66
22	b	615	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
22	b	601	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
22	C	513	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
23	d	401	PHO	OBD-CAD-CBD	-3.05	121.35	125.82
22	C	512	CLA	CMB-C2B-C1B	-3.04	123.78	128.46
22	D	403	CLA	O2D-CGD-CBD	3.04	116.68	111.27
24	t	101	BCR	C1-C6-C5	-3.04	118.33	122.61
22	C	510	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
24	D	405	BCR	C2-C1-C6	3.03	115.14	110.48
22	b	613	CLA	O2D-CGD-CBD	3.02	116.64	111.27
35	E	101	HEM	CBD-CAD-C3D	-3.02	104.25	112.63
22	B	601	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
24	C	514	BCR	C37-C22-C21	-3.01	118.70	122.92
22	C	504	CLA	CHD-C1D-ND	-3.01	121.69	124.45
22	B	607	CLA	C4-C3-C5	3.01	120.34	115.27
22	B	616	CLA	CAA-CBA-CGA	-3.01	104.45	113.25
22	b	607	CLA	CMB-C2B-C3B	3.01	130.31	124.68
28	a	410	SQD	O8-S-C6	3.01	110.53	105.74
22	d	405	CLA	C1B-CHB-C4A	-3.01	124.16	130.12
28	f	102	SQD	C45-O47-C7	3.01	125.19	117.79
24	b	618	BCR	C8-C7-C6	-3.00	118.76	127.20
26	a	409	PL9	C20-C19-C21	3.00	120.32	115.27
22	B	603	CLA	CMB-C2B-C3B	3.00	130.29	124.68
22	D	403	CLA	C1B-CHB-C4A	-3.00	124.18	130.12
28	F	101	SQD	C44-O6-C1	2.99	118.81	113.84
22	b	606	CLA	CHB-C4A-NA	2.99	128.65	124.51
29	C	517	DGD	O5D-C1E-C2E	2.99	112.98	108.30
27	C	519	LMG	O1-C7-C8	-2.99	103.68	110.90
22	c	512	CLA	CHD-C1D-ND	-2.99	121.71	124.45
28	f	102	SQD	C1-C2-C3	-2.99	103.77	110.00
22	A	410	CLA	CHD-C1D-ND	-2.99	121.71	124.45
22	C	511	CLA	CHD-C1D-ND	-2.98	121.71	124.45
22	B	613	CLA	O2A-CGA-O1A	-2.98	116.08	123.59
33	D	408	LHG	C18-C17-C16	-2.97	99.32	114.42
22	C	513	CLA	CMB-C2B-C3B	2.97	130.24	124.68
22	c	505	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
26	D	406	PL9	C12-C13-C14	-2.97	120.51	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	518	DGD	CDB-CCB-CBB	-2.97	99.35	114.42
22	A	405	CLA	C2C-C1C-NC	2.97	112.75	109.97
22	b	602	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
33	D	408	LHG	O8-C23-O10	-2.97	116.10	123.59
22	A	402	CLA	O1D-CGD-CBD	2.97	130.55	124.48
22	c	509	CLA	CHB-C4A-NA	2.97	128.61	124.51
28	A	412	SQD	O48-C23-O10	-2.97	116.11	123.59
29	c	518	DGD	O4D-C4D-C3D	2.97	117.20	110.35
28	L	101	SQD	O2-C2-C1	2.96	117.23	110.05
26	a	409	PL9	C22-C23-C24	-2.95	120.55	127.66
24	C	514	BCR	C15-C16-C17	-2.95	117.42	123.47
29	h	102	DGD	C4D-C3D-C2D	-2.95	105.67	110.82
32	J	101	STE	C3-C2-C1	-2.95	107.04	114.47
22	B	603	CLA	C5-C3-C2	-2.94	115.16	121.12
28	a	411	SQD	O48-C23-O10	-2.94	116.17	123.59
22	C	506	CLA	O1D-CGD-CBD	2.93	130.48	124.48
36	V	201	HEC	CMB-C2B-C1B	-2.93	123.96	128.46
29	a	412	DGD	C5B-C4B-C3B	-2.93	99.56	114.42
22	b	601	CLA	CHD-C1D-ND	-2.93	121.77	124.45
27	c	522	LMG	O1-C1-C2	-2.93	103.74	108.30
22	b	604	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
22	b	610	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
28	a	410	SQD	O47-C7-O49	-2.92	116.65	123.70
33	E	102	LHG	O8-C23-C24	2.92	121.06	111.91
22	C	501	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
27	b	622	LMG	O7-C10-O9	-2.91	116.66	123.70
22	C	504	CLA	O2A-CGA-O1A	-2.91	116.25	123.59
22	a	404	CLA	CMB-C2B-C3B	2.91	130.12	124.68
28	F	101	SQD	O48-C23-C24	2.91	121.03	111.91
26	D	406	PL9	C7-C8-C9	-2.91	121.95	126.79
22	d	404	CLA	CMB-C2B-C3B	2.91	130.11	124.68
28	L	101	SQD	O8-S-O7	-2.90	104.18	111.27
24	h	101	BCR	C15-C16-C17	-2.90	117.53	123.47
22	c	511	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
22	b	609	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
23	d	402	PHO	CMB-C2B-C3B	2.90	130.11	124.68
22	C	509	CLA	CHD-C1D-ND	-2.90	121.79	124.45
22	A	403	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
22	b	610	CLA	CHD-C1D-ND	-2.90	121.79	124.45
24	c	515	BCR	C27-C26-C25	2.90	126.94	122.73
22	c	506	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
29	h	102	DGD	O2D-C2D-C1D	-2.89	103.02	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	505	CLA	CHB-C4A-NA	2.89	128.51	124.51
27	b	622	LMG	O8-C28-O10	-2.89	116.30	123.59
24	H	101	BCR	C16-C15-C14	-2.89	117.56	123.47
22	b	605	CLA	C2D-C1D-ND	-2.88	107.98	110.10
29	H	102	DGD	C1D-C2D-C3D	-2.88	103.99	110.00
22	c	507	CLA	C4A-NA-C1A	2.88	108.00	106.71
27	d	412	LMG	O6-C1-O1	-2.88	103.15	109.97
28	L	101	SQD	O8-S-C6	2.88	110.33	105.74
22	c	510	CLA	O1D-CGD-CBD	2.88	130.37	124.48
22	b	602	CLA	C11-C12-C13	-2.87	106.63	115.92
22	B	601	CLA	C4-C3-C5	2.87	120.10	115.27
22	b	605	CLA	CHD-C1D-ND	-2.86	121.82	124.45
22	B	611	CLA	C1-C2-C3	-2.86	121.10	126.04
22	c	506	CLA	CHB-C4A-NA	2.86	128.46	124.51
22	b	601	CLA	CMB-C2B-C3B	2.85	130.01	124.68
22	B	614	CLA	C4-C3-C5	2.85	120.06	115.27
22	A	403	CLA	CMB-C2B-C3B	2.85	130.00	124.68
24	K	101	BCR	C38-C26-C25	-2.84	121.33	124.53
22	B	603	CLA	C2D-C1D-ND	-2.84	108.01	110.10
22	A	402	CLA	C7-C6-C5	-2.83	105.66	113.36
22	a	402	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
22	D	404	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
22	a	402	CLA	O1D-CGD-CBD	2.83	130.27	124.48
22	C	507	CLA	O1D-CGD-CBD	2.82	130.26	124.48
22	C	502	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
22	b	609	CLA	CHB-C4A-NA	2.81	128.40	124.51
24	a	405	BCR	C37-C22-C21	-2.81	118.99	122.92
22	c	501	CLA	CHD-C1D-ND	-2.81	121.88	124.45
22	B	613	CLA	C4-C3-C5	2.80	119.99	115.27
24	B	619	BCR	C29-C30-C25	2.80	114.80	110.48
29	a	412	DGD	C1G-C2G-C3G	-2.80	105.25	111.80
24	c	516	BCR	C2-C1-C6	2.80	114.79	110.48
22	b	604	CLA	CMB-C2B-C3B	2.80	129.91	124.68
24	B	618	BCR	C2-C1-C6	2.80	114.79	110.48
22	b	613	CLA	CHB-C4A-NA	2.80	128.38	124.51
22	c	509	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
22	C	513	CLA	CHB-C4A-NA	2.79	128.37	124.51
22	b	608	CLA	O2D-CGD-CBD	2.79	116.22	111.27
24	b	619	BCR	C38-C26-C25	-2.79	121.40	124.53
22	B	609	CLA	CMB-C2B-C3B	2.79	129.89	124.68
29	H	102	DGD	O2D-C2D-C1D	-2.78	103.28	110.05
22	D	403	CLA	CHB-C4A-NA	2.78	128.36	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	609	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
33	d	410	LHG	O8-C23-C24	2.78	120.63	111.91
27	c	520	LMG	C9-C8-C7	-2.78	105.22	111.79
24	A	406	BCR	C15-C16-C17	-2.78	117.79	123.47
22	C	504	CLA	CMB-C2B-C3B	2.78	129.87	124.68
29	H	102	DGD	C1E-O6E-C5E	2.77	119.13	113.69
22	C	508	CLA	O2D-CGD-CBD	2.77	116.19	111.27
22	b	602	CLA	C1-C2-C3	-2.77	121.26	126.04
24	k	101	BCR	C27-C26-C25	2.77	126.75	122.73
26	D	406	PL9	C20-C19-C21	2.77	119.92	115.27
28	f	102	SQD	O47-C7-C8	2.76	118.51	110.80
22	B	609	CLA	C2C-C1C-NC	2.76	112.56	109.97
28	A	412	SQD	O5-C1-O6	2.76	116.52	109.97
28	L	101	SQD	O10-C23-C24	-2.76	112.97	123.73
22	a	402	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
24	Y	101	BCR	C27-C26-C25	2.76	126.73	122.73
22	C	510	CLA	CHD-C1D-ND	-2.76	121.92	124.45
22	c	511	CLA	CMB-C2B-C1B	-2.76	124.23	128.46
22	B	603	CLA	C4A-NA-C1A	2.76	107.94	106.71
22	B	609	CLA	CMB-C2B-C1B	-2.76	124.23	128.46
22	d	404	CLA	CHB-C4A-NA	2.76	128.32	124.51
26	D	406	PL9	C30-C29-C31	-2.75	110.64	115.27
24	A	406	BCR	C27-C26-C25	2.75	126.73	122.73
22	b	610	CLA	CAA-CBA-CGA	-2.75	105.21	113.25
22	c	503	CLA	CHD-C1D-ND	-2.75	121.93	124.45
32	d	413	STE	O2-C1-C2	2.75	122.87	114.03
22	b	615	CLA	CHB-C4A-NA	2.75	128.31	124.51
27	c	522	LMG	O7-C10-O9	-2.75	117.06	123.70
22	b	608	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
24	D	405	BCR	C27-C26-C25	2.74	126.72	122.73
32	m	101	STE	O1-C1-C2	-2.74	114.27	123.08
28	a	411	SQD	O49-C7-C8	-2.74	113.03	123.73
22	C	510	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
26	D	406	PL9	C7-C3-C2	-2.74	119.70	123.30
24	b	619	BCR	C37-C22-C21	-2.74	119.09	122.92
24	c	515	BCR	C38-C26-C25	-2.73	121.46	124.53
29	c	518	DGD	O6D-C1D-O3G	-2.73	103.52	109.97
22	b	605	CLA	O2A-CGA-O1A	-2.73	116.71	123.59
22	B	614	CLA	CHB-C4A-NA	2.72	128.28	124.51
24	c	514	BCR	C15-C14-C13	-2.72	123.43	127.31
22	c	513	CLA	CHB-C4A-NA	2.72	128.27	124.51
22	b	614	CLA	CMB-C2B-C3B	2.72	129.76	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	414	DGD	C3E-C4E-C5E	-2.71	105.40	110.24
22	B	611	CLA	C4A-NA-C1A	2.71	107.92	106.71
27	b	620	LMG	O7-C10-O9	-2.71	117.15	123.70
22	b	609	CLA	O1D-CGD-CBD	2.71	130.03	124.48
24	c	514	BCR	C15-C16-C17	-2.71	117.92	123.47
24	t	101	BCR	C36-C18-C19	2.71	122.35	118.08
22	B	604	CLA	C1D-ND-C4D	2.71	108.26	106.33
26	D	406	PL9	C22-C23-C24	-2.71	121.14	127.66
27	D	407	LMG	O3-C3-C2	-2.70	104.10	110.35
22	A	403	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
22	B	611	CLA	CHD-C1D-ND	-2.70	121.97	124.45
22	c	508	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
22	b	612	CLA	CHB-C4A-NA	2.70	128.25	124.51
22	b	614	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
27	b	620	LMG	C38-C37-C36	-2.70	100.72	114.42
29	h	102	DGD	O2E-C2E-C3E	-2.70	104.11	110.35
22	A	402	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
32	b	624	STE	C3-C2-C1	-2.69	107.69	114.47
26	a	409	PL9	O2-C1-C2	-2.69	115.61	121.78
29	C	516	DGD	O6D-C1D-O3G	-2.69	103.60	109.97
27	M	101	LMG	C38-C37-C36	-2.69	100.77	114.42
27	d	412	LMG	O1-C1-C2	-2.69	104.10	108.30
27	c	523	LMG	O6-C1-O1	-2.69	103.61	109.97
22	c	507	CLA	C1B-CHB-C4A	-2.69	124.80	130.12
22	c	501	CLA	CHB-C4A-NA	2.68	128.22	124.51
24	B	618	BCR	C3-C4-C5	-2.68	109.29	114.08
22	c	504	CLA	O2A-CGA-O1A	-2.68	116.83	123.59
22	c	508	CLA	C2D-C1D-ND	-2.68	108.13	110.10
22	B	610	CLA	CMA-C3A-C4A	-2.68	104.58	111.77
26	d	407	PL9	C7-C8-C9	-2.67	122.34	126.79
22	c	507	CLA	O2A-CGA-O1A	-2.67	116.85	123.59
24	H	101	BCR	C37-C22-C21	-2.67	119.18	122.92
22	C	503	CLA	C7-C6-C5	-2.67	106.10	113.36
33	d	410	LHG	C26-C25-C24	2.67	122.79	113.19
22	C	501	CLA	O2A-CGA-O1A	-2.67	116.86	123.59
22	C	509	CLA	C1-C2-C3	-2.66	121.43	126.04
22	d	404	CLA	CMC-C2C-C1C	2.66	129.09	125.04
22	b	608	CLA	C11-C10-C8	-2.66	107.32	115.92
22	C	503	CLA	CMB-C2B-C3B	2.66	129.66	124.68
22	b	605	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
22	b	615	CLA	C1B-CHB-C4A	-2.66	124.86	130.12
26	A	409	PL9	C7-C3-C2	-2.65	119.81	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	514	BCR	C2-C1-C6	2.65	114.57	110.48
24	b	617	BCR	C37-C22-C21	-2.65	119.21	122.92
23	D	401	PHO	C1-C2-C3	-2.65	121.46	126.04
36	v	201	HEC	CBD-CAD-C3D	-2.65	108.10	112.62
22	b	614	CLA	CAC-C3C-C4C	2.65	128.25	124.81
22	c	505	CLA	O2D-CGD-CBD	2.65	115.97	111.27
26	d	407	PL9	C50-C49-C48	-2.64	115.00	122.65
22	b	612	CLA	C1-C2-C3	-2.64	121.47	126.04
24	C	515	BCR	C37-C22-C21	-2.64	119.22	122.92
22	B	615	CLA	O2D-CGD-CBD	2.64	115.96	111.27
22	B	614	CLA	CHD-C1D-ND	-2.64	122.03	124.45
22	D	403	CLA	CMB-C2B-C3B	2.64	129.62	124.68
22	C	502	CLA	CHD-C1D-ND	-2.64	122.03	124.45
22	B	615	CLA	CHD-C1D-ND	-2.64	122.03	124.45
33	l	101	LHG	O8-C23-O10	-2.64	116.94	123.59
22	a	403	CLA	CED-O2D-CGD	-2.63	109.98	115.94
34	a	408	BCT	O3-C-O1	-2.63	112.71	119.55
22	B	605	CLA	CHD-C1D-ND	-2.63	122.03	124.45
29	C	517	DGD	C1D-O6D-C5D	-2.63	108.52	113.69
22	B	611	CLA	CHD-C4C-NC	2.63	128.35	124.20
29	A	414	DGD	CDB-CCB-CBB	-2.63	101.08	114.42
27	D	407	LMG	O6-C1-O1	-2.63	103.75	109.97
33	B	622	LHG	O8-C23-O10	-2.63	116.96	123.59
22	c	502	CLA	O1D-CGD-CBD	2.63	129.86	124.48
27	b	622	LMG	O6-C5-C6	2.63	112.97	106.44
24	a	405	BCR	C37-C22-C23	2.63	122.22	118.08
22	b	605	CLA	C4A-NA-C1A	2.62	107.89	106.71
32	C	520	STE	O2-C1-C2	2.62	122.45	114.03
33	D	408	LHG	C20-C19-C18	-2.62	101.12	114.42
22	C	512	CLA	C1-C2-C3	-2.62	121.51	126.04
22	b	602	CLA	C2D-C1D-ND	-2.62	108.17	110.10
26	d	407	PL9	C7-C3-C2	-2.62	119.86	123.30
23	A	404	PHO	C1B-NB-C4B	2.62	112.46	107.09
22	C	511	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
22	b	613	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
24	H	101	BCR	C2-C1-C6	2.61	114.50	110.48
22	C	503	CLA	C4D-CHA-C1A	2.61	124.42	121.25
24	k	101	BCR	C38-C26-C25	-2.61	121.60	124.53
28	F	101	SQD	C1-C2-C3	-2.61	104.57	110.00
22	c	503	CLA	C4-C3-C5	2.61	119.65	115.27
22	a	402	CLA	CHB-C4A-NA	2.60	128.11	124.51
24	b	617	BCR	C36-C18-C17	-2.60	119.28	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	610	CLA	C1-C2-C3	-2.60	121.54	126.04
27	b	620	LMG	O6-C1-O1	-2.60	103.82	109.97
22	c	511	CLA	O2D-CGD-CBD	2.59	115.88	111.27
26	d	407	PL9	C20-C19-C21	2.59	119.63	115.27
29	c	519	DGD	C6D-O5D-C1E	2.59	118.80	113.74
22	B	604	CLA	C11-C10-C8	-2.59	107.55	115.92
24	c	514	BCR	C36-C18-C17	-2.59	119.30	122.92
22	c	508	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
24	K	101	BCR	C7-C8-C9	-2.58	122.33	126.23
22	B	609	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
22	B	606	CLA	CMB-C2B-C3B	2.58	129.50	124.68
22	b	605	CLA	O1D-CGD-CBD	2.58	129.75	124.48
23	D	401	PHO	O2D-CGD-O1D	-2.57	118.81	123.84
29	C	517	DGD	C6D-O5D-C1E	2.57	118.76	113.74
22	B	613	CLA	CHB-C4A-NA	2.57	128.06	124.51
22	c	513	CLA	CAC-C3C-C4C	2.56	128.14	124.81
26	a	409	PL9	C37-C38-C39	-2.56	121.49	127.66
22	B	611	CLA	CHB-C4A-NA	2.56	128.06	124.51
22	b	615	CLA	CHC-C1C-NC	2.56	128.09	124.20
33	e	101	LHG	O8-C23-C24	2.56	119.94	111.91
27	D	407	LMG	O4-C4-C5	2.56	115.65	109.30
23	D	401	PHO	C1A-C2A-C3A	-2.56	100.41	102.84
22	C	511	CLA	CHB-C4A-NA	2.55	128.04	124.51
26	a	409	PL9	C11-C12-C13	-2.55	103.49	111.88
26	D	406	PL9	C36-C34-C33	-2.55	115.95	121.12
22	B	606	CLA	C4-C3-C5	2.55	119.56	115.27
26	A	409	PL9	C31-C32-C33	-2.55	103.50	111.88
22	B	604	CLA	CGD-CBD-CAD	-2.55	102.48	110.73
22	c	510	CLA	C2D-C1D-ND	-2.55	108.23	110.10
29	c	518	DGD	C1D-C2D-C3D	-2.55	104.69	110.00
24	B	618	BCR	C37-C22-C21	-2.54	119.36	122.92
22	b	612	CLA	C11-C12-C13	-2.54	107.71	115.92
27	D	407	LMG	C38-C37-C36	-2.54	101.53	114.42
29	C	516	DGD	C3G-C2G-C1G	-2.53	105.80	111.79
22	C	512	CLA	CMB-C2B-C3B	2.53	129.41	124.68
22	d	403	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
28	B	623	SQD	O5-C5-C4	2.53	114.28	109.69
22	b	607	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
22	c	501	CLA	O2A-CGA-O1A	-2.53	117.22	123.59
22	B	603	CLA	CHD-C1D-C2D	2.53	130.78	125.48
27	M	101	LMG	O8-C28-O10	-2.52	117.22	123.59
22	b	608	CLA	C3B-C4B-NB	-2.52	105.95	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	414	DGD	C1D-C2D-C3D	-2.52	104.75	110.00
24	h	101	BCR	C36-C18-C17	-2.52	119.39	122.92
22	c	510	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
29	c	519	DGD	O6D-C1D-O3G	-2.52	104.01	109.97
22	b	608	CLA	C1B-CHB-C4A	-2.52	125.14	130.12
33	D	409	LHG	O8-C6-C5	-2.51	101.11	108.43
28	A	412	SQD	O5-C1-C2	-2.51	105.03	110.35
22	B	612	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	B	612	CLA	O1D-CGD-CBD	2.51	129.62	124.48
22	c	513	CLA	C11-C12-C13	-2.51	107.81	115.92
29	A	414	DGD	C5B-C4B-C3B	-2.51	101.70	114.42
22	a	404	CLA	C3D-C4D-ND	2.50	114.29	110.24
23	A	404	PHO	C1A-C2A-C3A	-2.50	100.46	102.84
22	B	602	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
24	b	619	BCR	C2-C1-C6	2.50	114.33	110.48
27	A	411	LMG	O1-C7-C8	-2.50	104.86	110.90
24	h	101	BCR	C37-C22-C21	-2.50	119.42	122.92
24	c	516	BCR	C27-C26-C25	2.50	126.36	122.73
26	d	407	PL9	C8-C7-C3	2.50	119.04	111.98
28	A	413	SQD	O48-C46-C45	2.50	115.57	108.38
28	a	410	SQD	O47-C7-C8	2.50	116.88	111.50
22	C	501	CLA	O2D-CGD-CBD	2.50	115.70	111.27
22	B	616	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
24	d	406	BCR	C24-C23-C22	-2.49	122.47	126.23
22	c	506	CLA	CBC-CAC-C3C	-2.49	105.56	112.43
22	B	601	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
22	B	606	CLA	CHD-C4C-NC	2.49	128.13	124.20
22	b	608	CLA	CHD-C1D-ND	-2.49	122.17	124.45
22	B	615	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
35	E	101	HEM	CAD-CBD-CGD	2.49	118.96	113.60
22	a	403	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
27	c	522	LMG	C9-C8-C7	-2.49	105.91	111.79
22	c	503	CLA	C5-C3-C2	-2.49	116.08	121.12
24	T	101	BCR	C37-C22-C21	-2.49	119.44	122.92
28	a	411	SQD	O48-C23-C24	2.48	119.70	111.91
22	B	611	CLA	C5-C3-C2	2.48	126.14	121.12
28	f	102	SQD	O5-C1-O6	2.48	115.84	109.97
22	C	501	CLA	CHD-C1D-ND	-2.48	122.18	124.45
29	h	102	DGD	C1D-O6D-C5D	-2.48	108.83	113.69
22	c	512	CLA	CMB-C2B-C1B	-2.48	124.66	128.46
22	B	609	CLA	O2A-CGA-O1A	-2.47	117.35	123.59
29	C	517	DGD	CDB-CCB-CBB	-2.47	101.87	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	h	102	DGD	C4E-C3E-C2E	-2.47	106.51	110.82
33	d	409	LHG	C18-C17-C16	-2.47	101.87	114.42
22	B	611	CLA	C14-C13-C15	-2.47	102.35	111.29
24	T	101	BCR	C38-C26-C27	-2.47	108.87	113.62
22	b	613	CLA	CHA-C1A-NA	-2.46	120.75	126.40
22	C	512	CLA	C1B-CHB-C4A	-2.46	125.23	130.12
24	A	406	BCR	C16-C15-C14	-2.46	118.43	123.47
22	B	603	CLA	CMB-C2B-C1B	-2.46	124.68	128.46
22	b	610	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
24	t	101	BCR	C19-C18-C17	-2.46	115.17	118.94
27	c	522	LMG	O3-C3-C2	-2.46	104.66	110.35
22	C	501	CLA	C1B-CHB-C4A	-2.45	125.25	130.12
22	b	606	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
24	B	618	BCR	C15-C16-C17	-2.45	118.45	123.47
22	A	410	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
35	E	101	HEM	O2D-CGD-CBD	2.45	121.91	114.03
22	c	507	CLA	CMB-C2B-C3B	2.45	129.27	124.68
22	B	612	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
22	B	603	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	A	403	CLA	CED-O2D-CGD	-2.45	110.41	115.94
26	A	409	PL9	O1-C4-C3	-2.45	118.03	120.72
36	v	201	HEC	C1D-C2D-C3D	-2.44	105.30	107.00
23	D	401	PHO	CMC-C2C-C3C	2.44	129.55	124.94
22	c	505	CLA	CMB-C2B-C1B	-2.44	124.71	128.46
26	a	409	PL9	C27-C28-C29	-2.44	121.79	127.66
29	C	518	DGD	C3G-C2G-C1G	-2.44	106.02	111.79
22	b	603	CLA	CHD-C1D-C2D	2.44	130.59	125.48
28	A	413	SQD	O47-C45-C44	2.44	113.50	107.93
22	C	509	CLA	CED-O2D-CGD	2.43	121.44	115.94
28	f	102	SQD	O48-C23-C24	2.43	119.54	111.91
24	b	618	BCR	C27-C26-C25	2.43	126.26	122.73
24	h	101	BCR	C27-C26-C25	2.43	126.26	122.73
23	D	401	PHO	C1B-NB-C4B	2.43	112.08	107.09
22	b	614	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
22	c	506	CLA	C2D-C1D-ND	-2.43	108.31	110.10
27	A	411	LMG	O3-C3-C2	-2.43	104.74	110.35
22	d	403	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
23	d	402	PHO	O2A-CGA-O1A	-2.43	117.47	123.59
27	M	101	LMG	O7-C10-O9	-2.42	117.84	123.70
24	b	619	BCR	C36-C18-C19	2.42	121.90	118.08
22	B	614	CLA	C4A-NA-C1A	2.42	107.80	106.71
22	c	509	CLA	C11-C10-C8	-2.42	108.09	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	514	BCR	C20-C21-C22	-2.42	123.85	127.31
22	C	509	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
28	B	623	SQD	O48-C23-O10	-2.42	117.49	123.59
35	E	101	HEM	CHC-C4B-NB	2.42	127.06	124.43
24	b	617	BCR	C29-C30-C25	2.42	114.20	110.48
27	c	523	LMG	C9-C8-C7	-2.42	106.07	111.79
24	B	617	BCR	C38-C26-C25	-2.42	121.81	124.53
27	c	523	LMG	O1-C7-C8	-2.42	105.07	110.90
22	c	510	CLA	CHB-C4A-NA	2.41	127.85	124.51
23	A	404	PHO	CMA-C3A-C2A	-2.41	104.28	113.99
22	d	403	CLA	CHD-C1D-ND	-2.41	122.24	124.45
22	c	507	CLA	CMB-C2B-C1B	-2.41	124.76	128.46
26	D	406	PL9	C42-C43-C44	-2.41	121.86	127.66
22	B	615	CLA	CMB-C2B-C1B	-2.41	124.76	128.46
24	c	516	BCR	C24-C23-C22	-2.41	122.59	126.23
26	D	406	PL9	C35-C34-C36	2.41	119.32	115.27
27	c	522	LMG	C6-C5-C4	-2.41	107.36	113.00
22	b	614	CLA	CHB-C4A-NA	2.41	127.84	124.51
22	A	403	CLA	C4A-NA-C1A	2.41	107.79	106.71
24	A	406	BCR	C11-C10-C9	-2.41	123.88	127.31
24	t	101	BCR	C28-C27-C26	-2.40	109.78	114.08
35	E	101	HEM	CBA-CAA-C2A	-2.40	108.52	112.62
22	d	404	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
23	A	404	PHO	CMC-C2C-C3C	2.40	129.47	124.94
22	b	613	CLA	C16-C15-C13	-2.40	108.16	115.92
33	d	409	LHG	O8-C23-C24	2.40	119.43	111.91
24	B	617	BCR	C3-C4-C5	-2.40	109.80	114.08
22	c	504	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
29	c	519	DGD	CDB-CCB-CBB	-2.40	102.26	114.42
29	a	412	DGD	C7B-C6B-C5B	-2.40	102.26	114.42
22	B	608	CLA	CHD-C1D-ND	-2.39	122.25	124.45
27	c	522	LMG	O2-C2-C1	-2.39	104.23	110.05
24	K	101	BCR	C36-C18-C17	-2.39	119.57	122.92
27	b	620	LMG	C1-O6-C5	-2.39	109.00	113.69
22	a	403	CLA	O2D-CGD-CBD	2.39	115.51	111.27
24	c	515	BCR	C7-C8-C9	-2.39	122.63	126.23
22	B	613	CLA	CHA-C1A-NA	-2.39	120.93	126.40
22	B	614	CLA	O1D-CGD-CBD	2.39	129.37	124.48
22	B	604	CLA	O2D-CGD-CBD	2.38	115.50	111.27
29	c	519	DGD	O5D-C6D-C5D	-2.38	104.64	109.05
28	a	410	SQD	O8-S-O9	-2.38	105.45	111.27
22	a	402	CLA	CAC-C3C-C4C	2.38	127.90	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	516	BCR	C38-C26-C25	-2.38	121.85	124.53
27	C	519	LMG	C6-C5-C4	-2.38	107.43	113.00
22	B	609	CLA	CAC-C3C-C4C	2.38	127.90	124.81
33	B	622	LHG	C18-C17-C16	-2.38	102.34	114.42
27	b	620	LMG	C9-C8-C7	-2.38	106.16	111.79
24	b	617	BCR	C23-C22-C21	-2.38	115.29	118.94
26	A	409	PL9	C12-C13-C14	-2.38	121.94	127.66
22	B	608	CLA	C3C-C4C-NC	-2.38	107.91	110.57
22	C	505	CLA	C1B-CHB-C4A	-2.37	125.41	130.12
22	B	605	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
24	a	405	BCR	C29-C30-C25	2.37	114.13	110.48
26	a	409	PL9	C40-C39-C38	-2.37	117.59	123.68
29	H	102	DGD	CAB-C9B-C8B	-2.37	102.39	114.42
28	L	101	SQD	O47-C45-C46	2.37	116.98	108.40
29	c	518	DGD	CDB-CCB-CBB	-2.37	102.39	114.42
33	l	101	LHG	O10-C23-C24	-2.37	114.49	123.73
22	a	404	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
22	b	602	CLA	CHD-C1D-ND	-2.37	122.28	124.45
23	A	404	PHO	C16-C17-C18	-2.36	104.84	115.98
27	C	519	LMG	C38-C37-C36	-2.36	102.42	114.42
33	L	102	LHG	O8-C23-O10	-2.36	117.63	123.59
24	B	619	BCR	C1-C6-C5	-2.36	119.29	122.61
24	B	619	BCR	C37-C22-C21	-2.36	119.62	122.92
22	A	405	CLA	CHB-C4A-NA	2.36	127.77	124.51
22	c	508	CLA	CHD-C1D-C2D	2.36	130.43	125.48
22	A	402	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
22	B	604	CLA	C6-C7-C8	-2.36	108.30	115.92
28	f	102	SQD	O5-C1-C2	-2.36	105.36	110.35
24	c	515	BCR	C8-C9-C10	2.35	122.55	118.94
22	C	512	CLA	CAA-CBA-CGA	-2.35	106.38	113.25
29	H	102	DGD	C3G-C2G-C1G	-2.35	106.23	111.79
29	C	518	DGD	C4D-C3D-C2D	-2.35	106.72	110.82
22	B	616	CLA	O1D-CGD-CBD	2.35	129.29	124.48
22	b	604	CLA	O1D-CGD-CBD	2.35	129.28	124.48
29	c	519	DGD	C6B-C5B-C4B	-2.35	102.52	114.42
24	b	617	BCR	C27-C26-C25	2.35	126.14	122.73
22	b	609	CLA	CHD-C1D-ND	-2.34	122.30	124.45
22	B	610	CLA	C11-C10-C8	-2.34	108.34	115.92
22	B	616	CLA	C2D-C1D-ND	-2.34	108.38	110.10
24	t	101	BCR	C15-C16-C17	-2.34	118.68	123.47
32	b	623	STE	O2-C1-C2	2.34	121.54	114.03
22	c	508	CLA	C1-C2-C3	-2.34	122.00	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	c	523	LMG	O8-C28-O10	-2.34	117.70	123.59
24	t	101	BCR	C16-C17-C18	-2.34	123.98	127.31
23	d	402	PHO	C1B-NB-C4B	2.33	111.89	107.09
26	a	409	PL9	C25-C24-C26	2.33	119.20	115.27
22	C	512	CLA	O2D-CGD-O1D	-2.33	119.27	123.84
22	C	507	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
22	c	511	CLA	CHB-C4A-NA	2.33	127.73	124.51
22	B	602	CLA	C11-C12-C13	-2.32	108.40	115.92
22	B	602	CLA	O2A-CGA-O1A	-2.32	117.72	123.59
33	l	101	LHG	C20-C19-C18	-2.32	102.62	114.42
29	C	517	DGD	C1D-C2D-C3D	-2.32	105.16	110.00
24	A	406	BCR	C38-C26-C25	-2.32	121.92	124.53
28	a	411	SQD	O47-C7-C8	2.32	116.50	111.50
28	B	623	SQD	C1-C2-C3	-2.32	105.17	110.00
22	b	607	CLA	CED-O2D-CGD	2.32	121.18	115.94
22	a	402	CLA	C4-C3-C5	2.32	119.17	115.27
29	C	517	DGD	CAB-C9B-C8B	-2.31	102.68	114.42
22	B	614	CLA	CMB-C2B-C3B	2.31	129.00	124.68
32	j	101	STE	O2-C1-O1	-2.31	117.54	123.30
24	D	405	BCR	C7-C8-C9	-2.31	122.74	126.23
24	c	515	BCR	C37-C22-C21	-2.31	119.69	122.92
29	A	414	DGD	O6D-C1D-O3G	-2.31	104.51	109.97
22	b	605	CLA	CHD-C4C-NC	2.31	127.84	124.20
22	b	616	CLA	CGD-CBD-CAD	-2.31	103.26	110.73
24	h	101	BCR	C37-C22-C23	2.31	121.71	118.08
29	h	102	DGD	CDB-CCB-CBB	-2.31	102.72	114.42
22	b	612	CLA	CAC-C3C-C4C	2.30	127.80	124.81
26	a	409	PL9	C7-C8-C9	-2.30	122.96	126.79
22	C	504	CLA	CHA-C1A-NA	-2.30	121.13	126.40
35	f	101	HEM	CHB-C1B-NB	2.30	127.22	124.38
22	C	510	CLA	O2D-CGD-CBD	2.30	115.36	111.27
29	C	516	DGD	C4E-C3E-C2E	-2.30	106.81	110.82
22	B	607	CLA	C2A-C1A-CHA	2.30	127.88	123.86
22	b	606	CLA	O1D-CGD-CBD	2.30	129.18	124.48
22	C	505	CLA	O2A-CGA-O1A	-2.30	117.80	123.59
24	c	515	BCR	C37-C22-C23	2.30	121.69	118.08
22	c	505	CLA	CMB-C2B-C3B	2.30	128.97	124.68
24	B	619	BCR	C15-C16-C17	-2.30	118.77	123.47
22	b	610	CLA	O2A-CGA-O1A	-2.30	117.80	123.59
29	C	516	DGD	O5D-C6D-C5D	-2.29	104.80	109.05
24	t	101	BCR	C4-C5-C6	2.29	126.06	122.73
29	C	517	DGD	C7B-C6B-C5B	-2.29	102.79	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	611	CLA	CHB-C4A-NA	2.29	127.68	124.51
22	B	616	CLA	C2C-C1C-NC	2.29	112.12	109.97
22	b	607	CLA	CHB-C4A-NA	2.29	127.68	124.51
29	A	414	DGD	C3G-C2G-C1G	-2.29	106.38	111.79
24	b	619	BCR	C16-C15-C14	-2.29	118.79	123.47
22	b	612	CLA	CED-O2D-CGD	-2.28	110.77	115.94
29	h	102	DGD	O3E-C3E-C4E	2.28	115.63	110.35
22	b	614	CLA	O2D-CGD-CBD	2.28	115.32	111.27
22	d	405	CLA	CHD-C1D-ND	-2.28	122.36	124.45
22	C	512	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
22	b	603	CLA	O2D-CGD-CBD	2.28	115.32	111.27
27	A	411	LMG	C12-C11-C10	-2.28	105.33	113.62
23	A	404	PHO	C1-C2-C3	-2.28	122.10	126.04
33	d	408	LHG	C11-C10-C9	-2.28	102.86	114.42
22	C	501	CLA	CMB-C2B-C3B	2.28	128.94	124.68
29	a	412	DGD	CFB-CEB-CDB	-2.28	102.87	114.42
22	c	513	CLA	O2A-CGA-O1A	-2.28	117.85	123.59
32	C	522	STE	O1-C1-C2	-2.27	115.78	123.08
22	C	507	CLA	C4-C3-C5	2.27	119.09	115.27
22	B	611	CLA	C9-C8-C10	-2.27	103.06	111.29
35	f	101	HEM	CMC-C2C-C3C	2.27	128.93	124.68
22	c	502	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
29	C	516	DGD	C9B-C8B-C7B	-2.27	102.90	114.42
29	H	102	DGD	CDB-CCB-CBB	-2.27	102.90	114.42
22	b	613	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
26	D	406	PL9	C32-C33-C34	-2.27	122.20	127.66
22	b	615	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
22	c	506	CLA	C1-O2A-CGA	2.27	122.39	116.44
22	C	509	CLA	C2A-C3A-C4A	2.27	105.53	101.87
29	c	519	DGD	O1G-C1G-C2G	-2.27	101.84	108.43
29	A	414	DGD	C6E-C5E-C4E	2.27	118.31	113.00
22	B	607	CLA	O2A-C1-C2	-2.26	102.69	108.64
24	h	101	BCR	C2-C1-C6	2.26	113.97	110.48
33	d	408	LHG	C5-O7-C7	-2.26	112.22	117.79
23	A	404	PHO	O2D-CGD-O1D	-2.26	119.41	123.84
22	B	606	CLA	CGD-CBD-CAD	-2.26	103.41	110.73
26	A	409	PL9	C20-C19-C18	-2.26	117.88	123.68
22	c	507	CLA	CHA-C1A-NA	-2.26	121.23	126.40
26	d	407	PL9	C41-C39-C38	-2.26	116.55	121.12
22	c	513	CLA	O1D-CGD-CBD	2.26	129.10	124.48
29	h	102	DGD	C7B-C6B-C5B	-2.26	102.97	114.42
22	C	507	CLA	CHD-C1D-ND	-2.26	122.38	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	518	DGD	CBB-CAB-C9B	-2.26	102.98	114.42
22	B	606	CLA	O2D-CGD-CBD	2.25	115.28	111.27
24	b	619	BCR	C15-C16-C17	-2.25	118.86	123.47
22	b	612	CLA	C4A-NA-C1A	2.25	107.72	106.71
22	B	616	CLA	CHA-C4D-ND	2.25	137.21	132.50
22	c	502	CLA	CHB-C4A-NA	2.25	127.63	124.51
22	A	402	CLA	C6-C5-C3	2.25	119.36	113.45
22	A	402	CLA	CAA-CBA-CGA	-2.25	106.67	113.25
22	c	510	CLA	C1-C2-C3	-2.25	122.15	126.04
22	B	603	CLA	OBD-CAD-C3D	2.25	133.94	128.52
22	b	608	CLA	C4-C3-C5	2.25	119.06	115.27
22	B	603	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
28	a	411	SQD	O6-C44-C45	-2.25	105.82	111.78
22	d	403	CLA	C1C-C2C-C3C	-2.25	104.59	106.96
22	b	605	CLA	CHD-C1D-C2D	2.25	130.19	125.48
24	H	101	BCR	C29-C30-C25	2.24	113.94	110.48
22	D	403	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
22	B	608	CLA	C11-C12-C13	-2.24	108.67	115.92
22	b	605	CLA	C16-C15-C13	-2.24	108.67	115.92
24	H	101	BCR	C27-C26-C25	2.24	125.99	122.73
22	A	405	CLA	C4A-NA-C1A	2.24	107.71	106.71
22	C	508	CLA	CHD-C4C-NC	2.24	127.74	124.20
32	j	101	STE	O1-C1-C2	-2.24	115.88	123.08
22	b	606	CLA	CHD-C4C-NC	2.24	127.73	124.20
22	D	403	CLA	C4-C3-C5	2.24	119.04	115.27
22	B	605	CLA	C2D-C1D-ND	-2.24	108.45	110.10
22	c	503	CLA	C11-C12-C13	-2.24	108.69	115.92
24	A	406	BCR	C36-C18-C17	-2.24	119.79	122.92
22	b	605	CLA	CHA-C1A-NA	-2.24	121.28	126.40
27	M	101	LMG	O3-C3-C2	-2.23	105.18	110.35
33	e	101	LHG	C11-C10-C9	-2.23	103.08	114.42
22	B	613	CLA	O2A-C1-C2	-2.23	102.77	108.64
22	b	614	CLA	C4-C3-C5	2.23	119.03	115.27
28	A	413	SQD	O48-C23-O10	-2.23	117.96	123.59
24	Y	101	BCR	C15-C16-C17	-2.23	118.91	123.47
29	a	412	DGD	CDB-CCB-CBB	-2.23	103.10	114.42
29	c	517	DGD	C4E-C3E-C2E	-2.23	106.94	110.82
22	B	614	CLA	CHD-C4C-NC	2.23	127.71	124.20
22	c	501	CLA	CMB-C2B-C3B	2.23	128.84	124.68
26	a	409	PL9	O1-C4-C3	-2.22	118.27	120.72
29	c	519	DGD	O5D-C1E-C2E	2.22	111.77	108.30
29	c	517	DGD	C4A-C3A-C2A	-2.22	105.20	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	B	622	LHG	C20-C19-C18	-2.22	103.14	114.42
22	B	608	CLA	CHB-C4A-NA	2.22	127.58	124.51
24	a	405	BCR	C27-C26-C25	2.22	125.96	122.73
22	c	513	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
23	d	401	PHO	C1-C2-C3	-2.22	122.20	126.04
22	B	613	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
22	B	609	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
32	B	624	STE	C4-C3-C2	-2.22	105.21	113.19
34	D	402	BCT	O3-C-O1	-2.22	113.79	119.55
24	T	101	BCR	C4-C5-C6	2.22	125.95	122.73
22	b	602	CLA	CHC-C1C-NC	2.22	127.57	124.20
22	B	615	CLA	C2A-C3A-C4A	2.22	105.45	101.87
28	F	101	SQD	O9-S-O7	-2.22	106.28	113.95
26	A	409	PL9	C41-C39-C38	-2.22	116.63	121.12
22	B	606	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
22	b	610	CLA	C11-C12-C13	-2.22	108.75	115.92
29	c	519	DGD	O2D-C2D-C1D	-2.22	104.66	110.05
22	a	403	CLA	CMA-C3A-C4A	-2.22	105.82	111.77
24	B	618	BCR	C38-C26-C25	-2.21	122.04	124.53
22	C	503	CLA	O2A-C1-C2	-2.21	102.82	108.64
22	b	611	CLA	CHD-C1D-C2D	2.21	130.12	125.48
24	C	515	BCR	C27-C26-C25	2.21	125.94	122.73
28	a	410	SQD	O48-C23-O10	-2.21	118.01	123.59
22	C	506	CLA	CHB-C4A-NA	2.21	127.57	124.51
22	b	601	CLA	C3C-C4C-NC	-2.21	108.09	110.57
27	c	520	LMG	C6-C5-C4	-2.21	107.83	113.00
29	c	517	DGD	O2G-C1B-C2B	-2.21	106.74	111.50
24	c	516	BCR	C15-C16-C17	-2.21	118.95	123.47
22	c	507	CLA	C2C-C1C-NC	2.21	112.04	109.97
22	d	404	CLA	C1C-C2C-C3C	-2.21	104.64	106.96
22	A	402	CLA	CHD-C1D-ND	-2.21	122.43	124.45
29	c	519	DGD	C8B-C7B-C6B	-2.21	103.23	114.42
27	d	412	LMG	C40-C39-C38	-2.21	103.23	114.42
22	b	611	CLA	CMB-C2B-C3B	2.20	128.80	124.68
22	C	503	CLA	CHD-C4C-NC	2.20	127.68	124.20
32	C	522	STE	C6-C5-C4	-2.20	103.24	114.42
33	E	102	LHG	C18-C17-C16	-2.20	103.25	114.42
24	K	101	BCR	C2-C1-C6	2.20	113.87	110.48
27	d	412	LMG	C7-O1-C1	-2.20	109.44	113.74
35	f	101	HEM	CAB-C3B-C2B	-2.20	121.36	128.60
27	D	407	LMG	O1-C1-C2	-2.20	104.87	108.30
24	c	515	BCR	C34-C9-C10	-2.20	119.85	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	507	CLA	O1D-CGD-CBD	2.20	128.98	124.48
29	A	414	DGD	C8B-C7B-C6B	-2.19	103.29	114.42
27	c	520	LMG	C40-C39-C38	-2.19	103.30	114.42
27	c	522	LMG	O6-C1-O1	-2.19	104.79	109.97
22	C	503	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
22	c	506	CLA	C4-C3-C2	-2.19	118.06	123.68
24	b	617	BCR	C8-C7-C6	-2.19	121.06	127.20
22	b	613	CLA	C2A-C1A-CHA	2.19	127.68	123.86
24	b	617	BCR	C24-C23-C22	-2.19	122.93	126.23
28	L	101	SQD	O47-C7-C8	2.19	116.21	111.50
26	D	406	PL9	C37-C38-C39	-2.18	122.40	127.66
24	t	101	BCR	C27-C26-C25	2.18	125.90	122.73
22	B	604	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
22	D	403	CLA	C1-C2-C3	-2.18	122.27	126.04
22	b	605	CLA	C1-C2-C3	-2.18	122.27	126.04
23	A	404	PHO	C5-C3-C2	2.18	125.53	121.12
22	c	503	CLA	CHB-C4A-NA	2.18	127.52	124.51
29	C	518	DGD	C7B-C6B-C5B	-2.18	103.37	114.42
23	d	401	PHO	CMA-C3A-C4A	-2.18	109.61	114.38
24	c	514	BCR	C37-C22-C21	-2.18	119.87	122.92
22	C	501	CLA	OBD-CAD-C3D	2.18	133.76	128.52
22	B	602	CLA	CHD-C1D-ND	-2.18	122.45	124.45
24	c	514	BCR	C33-C5-C6	-2.17	122.09	124.53
32	a	414	STE	C3-C2-C1	-2.17	109.00	114.47
27	b	620	LMG	O8-C28-O10	-2.17	118.11	123.59
22	b	613	CLA	C2C-C1C-NC	2.17	112.01	109.97
28	L	101	SQD	C44-O6-C1	2.17	117.98	113.74
22	b	609	CLA	CHA-C1A-NA	-2.17	121.43	126.40
22	B	615	CLA	C6-C7-C8	-2.17	108.92	115.92
22	B	607	CLA	C1B-CHB-C4A	-2.17	125.83	130.12
24	T	101	BCR	C1-C6-C5	-2.17	119.56	122.61
24	D	405	BCR	C3-C4-C5	-2.16	110.21	114.08
29	C	518	DGD	O3E-C3E-C2E	-2.16	105.34	110.35
24	b	619	BCR	C29-C30-C25	2.16	113.81	110.48
22	A	405	CLA	C1C-C2C-C3C	-2.16	104.68	106.96
27	D	407	LMG	O1-C7-C8	-2.16	105.68	110.90
22	B	611	CLA	C7-C6-C5	-2.16	107.49	113.36
22	B	610	CLA	CMB-C2B-C1B	-2.16	125.14	128.46
22	b	607	CLA	O1A-CGA-CBA	2.16	132.16	123.73
29	h	102	DGD	O6E-C1E-O5D	-2.16	104.86	109.97
29	h	102	DGD	C1D-C2D-C3D	-2.16	105.50	110.00
27	c	520	LMG	O6-C1-O1	-2.16	104.86	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	407	PL9	C27-C28-C29	-2.16	122.47	127.66
29	C	517	DGD	O6D-C1D-O3G	-2.16	104.87	109.97
24	B	617	BCR	C37-C22-C23	2.16	121.47	118.08
29	C	516	DGD	CDB-CCB-CBB	-2.16	103.48	114.42
33	e	101	LHG	O8-C23-O10	-2.15	118.16	123.59
22	C	505	CLA	C6-C7-C8	-2.15	108.96	115.92
26	a	409	PL9	C31-C32-C33	-2.15	104.81	111.88
26	d	407	PL9	C12-C13-C14	-2.15	122.48	127.66
24	b	619	BCR	C27-C26-C25	2.15	125.86	122.73
22	b	610	CLA	O1D-CGD-CBD	2.15	128.88	124.48
22	B	601	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
22	C	509	CLA	CHD-C4C-NC	2.15	127.59	124.20
22	B	604	CLA	C2A-C3A-C4A	2.15	105.34	101.87
27	B	621	LMG	O7-C10-O9	-2.15	117.95	123.30
28	f	102	SQD	O47-C7-O49	-2.15	118.51	123.70
24	A	406	BCR	C34-C9-C8	-2.14	114.70	118.08
22	c	512	CLA	C3C-C4C-NC	-2.14	108.17	110.57
24	t	101	BCR	C38-C26-C27	-2.14	109.50	113.62
22	C	513	CLA	O1D-CGD-CBD	2.14	128.86	124.48
24	c	514	BCR	C27-C26-C25	2.14	125.84	122.73
24	H	101	BCR	C16-C17-C18	-2.14	124.26	127.31
22	B	607	CLA	CHA-C1A-NA	-2.14	121.50	126.40
24	h	101	BCR	C36-C18-C19	2.14	121.45	118.08
22	c	511	CLA	O1A-CGA-CBA	2.14	132.07	123.73
22	c	512	CLA	CMB-C2B-C3B	2.14	128.68	124.68
27	d	412	LMG	O3-C3-C2	-2.14	105.41	110.35
23	d	401	PHO	O2A-CGA-O1A	-2.14	118.20	123.59
22	C	509	CLA	C11-C12-C13	-2.14	109.02	115.92
24	b	619	BCR	C11-C10-C9	-2.13	124.27	127.31
26	A	409	PL9	C36-C37-C38	-2.13	104.87	111.88
24	b	617	BCR	C11-C10-C9	-2.13	124.27	127.31
22	C	506	CLA	C1-C2-C3	-2.13	122.36	126.04
22	c	509	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
22	a	403	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
35	f	101	HEM	CHC-C4B-C3B	2.13	127.83	124.57
33	B	622	LHG	C11-C10-C9	-2.12	103.64	114.42
22	c	512	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
22	B	606	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
22	b	610	CLA	C2C-C1C-NC	2.12	111.96	109.97
22	c	502	CLA	C1-C2-C3	-2.12	122.37	126.04
33	l	101	LHG	O8-C23-C24	2.12	118.57	111.91
22	C	502	CLA	CHA-C1A-NA	-2.12	121.54	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	603	CLA	C11-C12-C13	-2.12	109.06	115.92
22	B	603	CLA	CHD-C4C-C3C	-2.12	121.72	124.84
22	A	410	CLA	CED-O2D-CGD	-2.12	111.14	115.94
22	B	609	CLA	CAA-CBA-CGA	-2.12	107.06	113.25
33	d	408	LHG	O8-C6-C5	-2.12	102.27	108.43
28	L	101	SQD	C45-O47-C7	2.12	123.01	117.79
22	C	510	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
26	d	407	PL9	C32-C33-C34	-2.12	122.56	127.66
27	C	519	LMG	O7-C10-O9	-2.12	118.58	123.70
27	A	411	LMG	O6-C1-O1	-2.12	104.96	109.97
27	b	620	LMG	C22-C21-C20	-2.11	103.69	114.42
24	A	406	BCR	C2-C1-C6	2.11	113.73	110.48
24	h	101	BCR	C7-C8-C9	-2.11	123.04	126.23
26	D	406	PL9	C50-C49-C48	-2.11	116.54	122.65
22	a	402	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
22	A	405	CLA	C4-C3-C5	2.11	118.82	115.27
29	c	517	DGD	CDB-CCB-CBB	-2.11	103.71	114.42
22	B	612	CLA	C1B-CHB-C4A	-2.11	125.94	130.12
22	b	604	CLA	CHC-C1C-NC	2.11	127.40	124.20
22	B	608	CLA	C1C-C2C-C3C	-2.11	104.74	106.96
22	b	608	CLA	C1-C2-C3	-2.10	122.40	126.04
22	c	511	CLA	C11-C12-C13	-2.10	109.12	115.92
24	t	101	BCR	C7-C8-C9	-2.10	123.06	126.23
22	B	606	CLA	C1B-CHB-C4A	-2.10	125.95	130.12
22	B	606	CLA	CHB-C4A-NA	2.10	127.42	124.51
24	C	515	BCR	C3-C4-C5	-2.10	110.32	114.08
22	b	606	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
24	B	618	BCR	C7-C8-C9	-2.10	123.06	126.23
22	C	503	CLA	C3A-C2A-C1A	2.10	104.49	101.34
22	b	610	CLA	CBC-CAC-C3C	2.10	118.22	112.43
22	b	616	CLA	O1D-CGD-CBD	2.10	128.78	124.48
32	c	524	STE	O2-C1-C2	2.10	120.78	114.03
28	A	412	SQD	C3-C4-C5	2.10	113.98	110.24
24	B	617	BCR	C15-C16-C17	-2.10	119.17	123.47
22	b	610	CLA	CHC-C1C-C2C	-2.10	120.92	126.72
22	b	615	CLA	O2D-CGD-CBD	2.10	115.00	111.27
24	a	405	BCR	C36-C18-C17	-2.10	119.98	122.92
22	c	502	CLA	CHD-C1D-C2D	2.10	129.88	125.48
26	a	409	PL9	O2-C1-C6	2.10	124.22	120.59
22	c	505	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
26	d	407	PL9	C31-C29-C28	2.10	125.36	121.12
24	k	101	BCR	C36-C18-C17	-2.09	119.99	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	505	CLA	C3B-C4B-NB	-2.09	106.50	109.21
29	c	518	DGD	C3G-O3G-C1D	2.09	117.83	113.74
27	c	522	LMG	C3-C4-C5	-2.09	106.51	110.24
32	t	102	STE	O2-C1-C2	2.09	120.75	114.03
33	d	408	LHG	C18-C17-C16	-2.09	103.81	114.42
24	H	101	BCR	C38-C26-C25	-2.09	122.18	124.53
27	D	410	LMG	C38-C37-C36	-2.09	103.81	114.42
22	b	604	CLA	C4D-C3D-CAD	-2.09	105.63	108.10
22	C	503	CLA	C1-C2-C3	2.09	129.66	126.04
22	B	603	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
22	c	501	CLA	CHC-C1C-NC	2.09	127.37	124.20
29	c	519	DGD	O1G-C1A-O1A	-2.09	118.32	123.59
24	K	101	BCR	C31-C1-C6	2.09	113.69	110.30
29	C	517	DGD	O6E-C1E-O5D	-2.09	105.03	109.97
33	d	408	LHG	C20-C19-C18	-2.09	103.84	114.42
22	a	404	CLA	CHA-C1A-NA	-2.08	121.62	126.40
28	B	623	SQD	C25-C24-C23	-2.08	106.04	113.62
24	B	617	BCR	C29-C30-C25	2.08	113.69	110.48
22	C	507	CLA	C2A-C1A-CHA	2.08	127.50	123.86
22	d	405	CLA	CHA-C1A-NA	-2.08	121.64	126.40
22	B	611	CLA	C4-C3-C2	-2.08	118.34	123.68
22	b	616	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
35	E	101	HEM	CHB-C1B-NB	2.08	126.95	124.38
22	d	404	CLA	C2D-C1D-ND	-2.08	108.57	110.10
22	b	605	CLA	O1A-CGA-CBA	2.07	131.82	123.73
22	a	403	CLA	CHA-C1A-NA	-2.07	121.66	126.40
22	b	615	CLA	CHC-C1C-C2C	-2.07	121.00	126.72
22	b	604	CLA	C6-C7-C8	-2.07	109.23	115.92
29	C	518	DGD	O5D-C6D-C5D	-2.07	105.22	109.05
29	a	412	DGD	CBB-CAB-C9B	-2.07	103.92	114.42
22	A	403	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
24	d	406	BCR	C2-C1-C6	2.06	113.66	110.48
24	H	101	BCR	C36-C18-C17	-2.06	120.03	122.92
27	D	410	LMG	O8-C28-O10	-2.06	118.39	123.59
27	C	519	LMG	C40-C39-C38	-2.06	103.97	114.42
22	b	613	CLA	C1B-CHB-C4A	-2.06	126.04	130.12
29	c	518	DGD	O5D-C1E-C2E	2.06	111.52	108.30
24	D	405	BCR	C24-C23-C22	-2.06	123.12	126.23
22	a	402	CLA	CHA-C4D-ND	2.06	136.80	132.50
24	B	618	BCR	C27-C26-C25	2.06	125.72	122.73
22	C	504	CLA	C11-C10-C8	-2.06	109.27	115.92
22	B	606	CLA	CHD-C4C-C3C	-2.06	121.82	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	407	LMG	O2-C2-C3	-2.06	105.60	110.35
22	a	403	CLA	CHC-C1C-NC	2.05	127.32	124.20
22	C	503	CLA	CHA-C1A-NA	-2.05	121.69	126.40
29	c	517	DGD	O6D-C1D-O3G	-2.05	105.11	109.97
22	B	603	CLA	C3B-C4B-NB	-2.05	106.56	109.21
22	c	501	CLA	O1D-CGD-CBD	2.05	128.68	124.48
22	B	614	CLA	C1-C2-C3	-2.05	122.49	126.04
27	c	520	LMG	O2-C2-C1	-2.05	105.06	110.05
29	C	518	DGD	C6D-O5D-C1E	2.05	117.75	113.74
27	M	101	LMG	C22-C21-C20	-2.05	104.01	114.42
22	C	506	CLA	O2D-CGD-O1D	-2.05	119.83	123.84
22	C	501	CLA	C2D-C1D-ND	-2.05	108.59	110.10
22	a	404	CLA	CAC-C3C-C4C	2.05	127.47	124.81
29	h	102	DGD	C3E-C4E-C5E	-2.05	106.58	110.24
22	B	608	CLA	CHA-C1A-NA	-2.05	121.71	126.40
33	D	409	LHG	O8-C23-O10	-2.05	118.42	123.59
27	b	622	LMG	C40-C39-C38	-2.05	104.03	114.42
24	Y	101	BCR	C16-C15-C14	-2.05	119.28	123.47
22	b	604	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
22	B	601	CLA	CHA-C4D-ND	2.04	136.78	132.50
22	C	503	CLA	C5-C3-C2	-2.04	116.98	121.12
22	A	403	CLA	C1-O2A-CGA	2.04	121.80	116.44
22	C	509	CLA	C1-O2A-CGA	2.04	121.80	116.44
24	C	514	BCR	C7-C8-C9	-2.04	123.15	126.23
22	b	605	CLA	C4-C3-C2	-2.04	118.44	123.68
22	c	509	CLA	C16-C15-C13	-2.04	109.33	115.92
22	d	405	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
22	B	610	CLA	C1-C2-C3	-2.04	122.52	126.04
26	A	409	PL9	C11-C9-C8	-2.04	117.00	121.12
27	d	412	LMG	C1-C2-C3	-2.03	105.76	110.00
33	D	408	LHG	C11-C10-C9	-2.03	104.10	114.42
22	C	510	CLA	C7-C6-C5	-2.03	107.83	113.36
24	b	618	BCR	C15-C16-C17	-2.03	119.31	123.47
22	A	403	CLA	CHA-C1A-NA	-2.03	121.74	126.40
22	c	508	CLA	C7-C6-C5	-2.03	107.84	113.36
27	b	620	LMG	C33-C32-C31	-2.03	104.11	114.42
22	c	512	CLA	O1D-CGD-CBD	2.03	128.64	124.48
22	b	607	CLA	CHA-C1A-NA	-2.03	121.75	126.40
26	d	407	PL9	C31-C32-C33	-2.03	105.21	111.88
22	c	508	CLA	CHD-C4C-NC	2.03	127.40	124.20
27	A	411	LMG	C9-C8-C7	-2.03	106.99	111.79
32	m	101	STE	O2-C1-O1	-2.03	118.24	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	507	CLA	C1B-CHB-C4A	-2.03	126.10	130.12
29	c	518	DGD	CCB-CBB-CAB	-2.03	104.14	114.42
26	A	409	PL9	O2-C1-C2	-2.03	117.14	121.78
27	D	407	LMG	O2-C2-C1	-2.03	105.13	110.05
22	b	614	CLA	O2A-C1-C2	-2.02	103.31	108.64
29	C	516	DGD	CAB-C9B-C8B	-2.02	104.15	114.42
22	C	511	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
28	F	101	SQD	O8-S-O9	-2.02	106.33	111.27
22	B	603	CLA	C3C-C4C-NC	-2.02	108.30	110.57
23	D	401	PHO	CMD-C2D-C3D	2.02	128.46	124.68
26	a	409	PL9	C32-C33-C34	-2.02	122.79	127.66
27	c	520	LMG	O8-C28-O10	-2.02	118.50	123.59
35	E	101	HEM	CHD-C1D-ND	2.02	126.62	124.43
24	c	516	BCR	C16-C15-C14	-2.02	119.35	123.47
22	B	601	CLA	O2D-CGD-CBD	2.01	114.84	111.27
33	d	409	LHG	O7-C7-C8	-2.01	107.16	111.50
22	B	602	CLA	C2D-C1D-ND	-2.01	108.62	110.10
26	d	407	PL9	O1-C4-C3	-2.01	118.50	120.72
29	A	414	DGD	C3G-O3G-C1D	2.01	117.67	113.74
24	h	101	BCR	C15-C14-C13	-2.01	124.44	127.31
27	c	523	LMG	C12-C11-C10	-2.01	106.31	113.62
27	A	411	LMG	C1-O6-C5	-2.01	109.75	113.69
24	A	406	BCR	C7-C8-C9	-2.01	123.20	126.23
27	A	411	LMG	C38-C37-C36	-2.01	104.24	114.42
22	A	405	CLA	C1D-ND-C4D	-2.01	104.91	106.33
22	B	615	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
22	B	616	CLA	CHB-C4A-NA	2.00	127.28	124.51
23	A	404	PHO	OBD-CAD-CBD	-2.00	122.89	125.82
29	c	519	DGD	O3G-C1D-C2D	-2.00	105.18	108.30

All (61) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	402	CLA	ND
22	A	405	CLA	ND
22	A	410	CLA	ND
22	B	601	CLA	ND
22	B	603	CLA	ND
22	B	604	CLA	ND
22	B	605	CLA	ND
22	B	606	CLA	ND
22	B	607	CLA	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
22	B	608	CLA	ND
22	B	610	CLA	ND
22	B	611	CLA	ND
22	B	612	CLA	ND
22	B	613	CLA	ND
22	B	614	CLA	ND
22	B	615	CLA	ND
22	B	616	CLA	ND
22	C	501	CLA	ND
22	C	502	CLA	ND
22	C	503	CLA	ND
22	C	504	CLA	ND
22	C	505	CLA	ND
22	C	506	CLA	ND
22	C	507	CLA	ND
22	C	509	CLA	ND
22	C	510	CLA	ND
22	C	511	CLA	ND
22	C	512	CLA	ND
22	C	513	CLA	ND
22	D	403	CLA	ND
22	a	402	CLA	ND
22	a	404	CLA	ND
22	b	601	CLA	ND
22	b	603	CLA	ND
22	b	604	CLA	ND
22	b	605	CLA	ND
22	b	606	CLA	ND
22	b	607	CLA	ND
22	b	608	CLA	ND
22	b	609	CLA	ND
22	b	610	CLA	ND
22	b	611	CLA	ND
22	b	612	CLA	ND
22	b	613	CLA	ND
22	b	614	CLA	ND
22	b	615	CLA	ND
22	b	616	CLA	ND
22	c	501	CLA	ND
22	c	502	CLA	ND
22	c	503	CLA	ND
22	c	504	CLA	ND

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Mol	Chain	Res	Type	Atom
22	c	505	CLA	ND
22	c	506	CLA	ND
22	c	507	CLA	ND
22	c	509	CLA	ND
22	c	510	CLA	ND
22	c	511	CLA	ND
22	c	512	CLA	ND
22	c	513	CLA	ND
22	d	404	CLA	ND
22	d	405	CLA	ND

All (1923) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	405	CLA	C4-C3-C5-C6
22	A	410	CLA	CHA-CBD-CGD-O1D
22	A	410	CLA	CHA-CBD-CGD-O2D
22	B	601	CLA	CHA-CBD-CGD-O1D
22	B	601	CLA	CHA-CBD-CGD-O2D
22	B	601	CLA	CAD-CBD-CGD-O1D
22	B	603	CLA	C4-C3-C5-C6
22	B	607	CLA	C14-C13-C15-C16
22	B	614	CLA	CAD-CBD-CGD-O1D
22	B	614	CLA	CAD-CBD-CGD-O2D
22	C	502	CLA	CHA-CBD-CGD-O1D
22	C	504	CLA	CHA-CBD-CGD-O1D
22	C	504	CLA	C2-C3-C5-C6
22	C	504	CLA	C4-C3-C5-C6
22	C	508	CLA	CHA-CBD-CGD-O1D
22	C	508	CLA	C12-C13-C15-C16
22	C	513	CLA	C6-C7-C8-C9
22	a	403	CLA	CHA-CBD-CGD-O1D
22	b	601	CLA	O2A-C1-C2-C3
22	b	614	CLA	CHA-CBD-CGD-O1D
22	b	614	CLA	CHA-CBD-CGD-O2D
22	b	614	CLA	CAD-CBD-CGD-O1D
22	b	614	CLA	C2-C3-C5-C6
22	c	508	CLA	CHA-CBD-CGD-O1D
22	c	509	CLA	C6-C7-C8-C9
22	c	509	CLA	C11-C12-C13-C14
24	A	406	BCR	C17-C18-C19-C20
24	B	618	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
24	C	514	BCR	C20-C21-C22-C37
24	C	515	BCR	C1-C6-C7-C8
24	C	515	BCR	C17-C18-C19-C20
24	C	515	BCR	C36-C18-C19-C20
24	C	515	BCR	C37-C22-C23-C24
24	D	405	BCR	C37-C22-C23-C24
24	D	405	BCR	C22-C23-C24-C25
24	D	405	BCR	C23-C24-C25-C26
24	D	405	BCR	C23-C24-C25-C30
24	H	101	BCR	C11-C12-C13-C35
24	K	101	BCR	C7-C8-C9-C34
24	T	101	BCR	C1-C6-C7-C8
24	T	101	BCR	C7-C8-C9-C10
24	T	101	BCR	C36-C18-C19-C20
24	T	101	BCR	C20-C21-C22-C37
24	Y	101	BCR	C1-C6-C7-C8
24	Y	101	BCR	C5-C6-C7-C8
24	Y	101	BCR	C21-C22-C23-C24
24	a	405	BCR	C36-C18-C19-C20
24	b	617	BCR	C1-C6-C7-C8
24	b	617	BCR	C7-C8-C9-C34
24	b	617	BCR	C20-C21-C22-C37
24	b	618	BCR	C36-C18-C19-C20
24	b	619	BCR	C11-C12-C13-C35
24	b	619	BCR	C37-C22-C23-C24
24	c	514	BCR	C35-C13-C14-C15
24	c	514	BCR	C16-C17-C18-C36
24	d	406	BCR	C7-C8-C9-C34
24	d	406	BCR	C21-C22-C23-C24
24	k	101	BCR	C7-C8-C9-C10
24	k	101	BCR	C7-C8-C9-C34
24	k	101	BCR	C17-C18-C19-C20
24	t	101	BCR	C7-C8-C9-C34
24	t	101	BCR	C11-C10-C9-C34
24	t	101	BCR	C36-C18-C19-C20
24	t	101	BCR	C20-C21-C22-C37
26	A	409	PL9	C12-C13-C14-C15
26	A	409	PL9	C12-C13-C14-C16
26	A	409	PL9	C20-C19-C21-C22
26	A	409	PL9	C22-C23-C24-C25
26	A	409	PL9	C22-C23-C24-C26
26	A	409	PL9	C24-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
26	A	409	PL9	C37-C38-C39-C40
26	A	409	PL9	C43-C44-C46-C47
26	D	406	PL9	C32-C33-C34-C36
26	a	409	PL9	C22-C23-C24-C25
26	a	409	PL9	C22-C23-C24-C26
26	a	409	PL9	C24-C26-C27-C28
26	a	409	PL9	C32-C33-C34-C36
26	a	409	PL9	C42-C43-C44-C46
26	d	407	PL9	C40-C39-C41-C42
26	d	407	PL9	C42-C43-C44-C45
27	A	411	LMG	O6-C1-O1-C7
27	A	411	LMG	O1-C7-C8-O7
27	A	411	LMG	O9-C10-O7-C8
27	c	522	LMG	O7-C8-C9-O8
27	c	522	LMG	O9-C10-O7-C8
27	c	523	LMG	O6-C1-O1-C7
28	B	623	SQD	O5-C1-O6-C44
28	B	623	SQD	O49-C7-O47-C45
28	L	101	SQD	C8-C7-O47-C45
28	L	101	SQD	O10-C23-O48-C46
28	L	101	SQD	C24-C23-O48-C46
28	a	411	SQD	C8-C7-O47-C45
28	f	102	SQD	C2-C1-O6-C44
28	f	102	SQD	O5-C1-O6-C44
29	A	414	DGD	O1B-C1B-O2G-C2G
29	C	517	DGD	C2E-C1E-O5D-C6D
33	B	622	LHG	O1-C1-C2-C3
33	B	622	LHG	C3-O3-P-O5
33	B	622	LHG	C3-O3-P-O6
33	D	408	LHG	C1-C2-C3-O3
33	D	408	LHG	C3-O3-P-O5
33	D	408	LHG	C4-O6-P-O4
33	D	409	LHG	C4-O6-P-O4
33	E	102	LHG	C3-O3-P-O5
33	L	102	LHG	C3-O3-P-O4
33	L	102	LHG	C4-O6-P-O4
33	d	408	LHG	O1-C1-C2-C3
33	d	408	LHG	C4-O6-P-O5
33	d	409	LHG	O1-C1-C2-C3
33	d	409	LHG	C3-O3-P-O4
33	d	409	LHG	C4-O6-P-O4
33	e	101	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
33	e	101	LHG	O1-C1-C2-C3
33	e	101	LHG	C3-O3-P-O4
33	e	101	LHG	O10-C23-O8-C6
33	l	101	LHG	C3-O3-P-O4
33	l	101	LHG	C4-O6-P-O4
22	b	614	CLA	O1D-CGD-O2D-CED
22	D	404	CLA	CBD-CGD-O2D-CED
22	b	614	CLA	CBD-CGD-O2D-CED
23	d	402	PHO	CBD-CGD-O2D-CED
22	B	601	CLA	O1A-CGA-O2A-C1
28	f	102	SQD	O10-C23-O48-C46
33	E	102	LHG	O10-C23-O8-C6
22	B	601	CLA	CBA-CGA-O2A-C1
33	e	101	LHG	C24-C23-O8-C6
26	d	407	PL9	C47-C48-C49-C50
26	d	407	PL9	C47-C48-C49-C51
22	c	509	CLA	CBD-CGD-O2D-CED
22	c	511	CLA	CBD-CGD-O2D-CED
22	c	512	CLA	CBD-CGD-O2D-CED
22	c	513	CLA	CBD-CGD-O2D-CED
27	M	101	LMG	O10-C28-O8-C9
28	F	101	SQD	O10-C23-O48-C46
28	a	411	SQD	O10-C23-O48-C46
22	b	601	CLA	CBD-CGD-O2D-CED
27	b	622	LMG	O9-C10-O7-C8
28	f	102	SQD	O49-C7-O47-C45
22	b	614	CLA	C3-C5-C6-C7
28	a	411	SQD	C24-C23-O48-C46
27	A	411	LMG	C11-C10-O7-C8
27	C	519	LMG	C11-C10-O7-C8
27	D	410	LMG	C11-C10-O7-C8
28	B	623	SQD	C8-C7-O47-C45
29	A	414	DGD	C2B-C1B-O2G-C2G
22	D	404	CLA	O1D-CGD-O2D-CED
22	b	614	CLA	C4-C3-C5-C6
26	a	409	PL9	C20-C19-C21-C22
26	a	409	PL9	C35-C34-C36-C37
22	A	405	CLA	C2-C3-C5-C6
26	A	409	PL9	C38-C39-C41-C42
26	a	409	PL9	C33-C34-C36-C37
26	d	407	PL9	C38-C39-C41-C42
22	c	510	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	B	606	CLA	C2A-CAA-CBA-CGA
22	B	616	CLA	C3-C5-C6-C7
22	C	513	CLA	C3-C5-C6-C7
22	b	606	CLA	C3-C5-C6-C7
22	c	510	CLA	C3-C5-C6-C7
27	c	523	LMG	C29-C28-O8-C9
28	B	623	SQD	C24-C23-O48-C46
28	f	102	SQD	C24-C23-O48-C46
33	E	102	LHG	C24-C23-O8-C6
27	A	411	LMG	O6-C5-C6-O5
26	D	406	PL9	C47-C48-C49-C51
26	A	409	PL9	C32-C33-C34-C36
26	A	409	PL9	C37-C38-C39-C41
23	d	402	PHO	O1D-CGD-O2D-CED
22	D	403	CLA	CBD-CGD-O2D-CED
33	D	408	LHG	O2-C2-C3-O3
33	e	101	LHG	O2-C2-C3-O3
22	B	605	CLA	C3-C5-C6-C7
22	a	404	CLA	CBA-CGA-O2A-C1
28	F	101	SQD	C24-C23-O48-C46
29	c	519	DGD	O1A-C1A-O1G-C1G
28	f	102	SQD	C8-C7-O47-C45
22	B	603	CLA	CBD-CGD-O2D-CED
22	B	610	CLA	CBD-CGD-O2D-CED
22	C	511	CLA	CBD-CGD-O2D-CED
27	A	411	LMG	C4-C5-C6-O5
27	D	410	LMG	O9-C10-O7-C8
27	c	523	LMG	O10-C28-O8-C9
32	b	625	STE	C3-C4-C5-C6
26	a	409	PL9	C47-C48-C49-C51
22	C	513	CLA	C4-C3-C5-C6
26	A	409	PL9	C45-C44-C46-C47
22	B	603	CLA	C2-C3-C5-C6
22	C	513	CLA	C2-C3-C5-C6
26	A	409	PL9	C18-C19-C21-C22
28	B	623	SQD	O10-C23-O48-C46
29	C	517	DGD	O6E-C1E-O5D-C6D
26	A	409	PL9	C19-C21-C22-C23
26	a	409	PL9	C44-C46-C47-C48
26	d	407	PL9	C44-C46-C47-C48
32	B	624	STE	C4-C5-C6-C7
33	l	101	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
22	a	404	CLA	O1A-CGA-O2A-C1
27	b	622	LMG	C11-C10-O7-C8
27	c	522	LMG	C4-C5-C6-O5
26	A	409	PL9	C32-C33-C34-C35
26	D	406	PL9	C37-C38-C39-C40
33	d	408	LHG	C1-C2-C3-O3
26	d	407	PL9	C42-C43-C44-C46
22	B	604	CLA	C3-C5-C6-C7
22	C	513	CLA	CBA-CGA-O2A-C1
27	C	519	LMG	C29-C28-O8-C9
27	M	101	LMG	C29-C28-O8-C9
22	C	509	CLA	C5-C6-C7-C8
22	b	603	CLA	C5-C6-C7-C8
22	b	615	CLA	C5-C6-C7-C8
26	D	406	PL9	C47-C48-C49-C50
26	a	409	PL9	C47-C48-C49-C50
28	F	101	SQD	C44-C45-C46-O48
28	a	410	SQD	C11-C12-C13-C14
29	H	102	DGD	C4E-C5E-C6E-O5E
33	d	408	LHG	O2-C2-C3-O3
29	c	518	DGD	C1A-C2A-C3A-C4A
32	D	411	STE	C1-C2-C3-C4
27	c	523	LMG	C2-C1-O1-C7
28	B	623	SQD	C2-C1-O6-C44
28	a	410	SQD	O6-C44-C45-O47
33	B	622	LHG	C28-C29-C30-C31
26	a	409	PL9	C38-C39-C41-C42
22	B	606	CLA	C11-C10-C8-C9
22	B	611	CLA	C11-C12-C13-C14
22	B	613	CLA	C11-C12-C13-C14
22	B	614	CLA	C14-C13-C15-C16
22	B	616	CLA	C11-C10-C8-C9
22	C	503	CLA	C11-C10-C8-C9
22	C	509	CLA	C11-C10-C8-C9
22	C	512	CLA	C6-C7-C8-C9
22	C	512	CLA	C11-C10-C8-C9
22	b	601	CLA	C14-C13-C15-C16
22	b	605	CLA	C11-C10-C8-C9
22	b	606	CLA	C14-C13-C15-C16
22	b	607	CLA	C11-C10-C8-C9
22	b	614	CLA	C6-C7-C8-C9
22	b	616	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	c	502	CLA	C6-C7-C8-C9
22	c	511	CLA	C11-C10-C8-C9
22	c	511	CLA	C14-C13-C15-C16
22	c	512	CLA	C6-C7-C8-C9
22	c	512	CLA	O1D-CGD-O2D-CED
22	C	509	CLA	CBD-CGD-O2D-CED
22	B	603	CLA	C8-C10-C11-C12
22	C	506	CLA	C13-C15-C16-C17
22	c	505	CLA	C5-C6-C7-C8
24	C	514	BCR	C36-C18-C19-C20
24	Y	101	BCR	C37-C22-C23-C24
24	d	406	BCR	C37-C22-C23-C24
28	L	101	SQD	O49-C7-O47-C45
28	a	411	SQD	O49-C7-O47-C45
27	c	520	LMG	C4-C5-C6-O5
27	c	523	LMG	C4-C5-C6-O5
27	d	412	LMG	C28-C29-C30-C31
28	A	413	SQD	C7-C8-C9-C10
33	e	101	LHG	C23-C24-C25-C26
22	B	603	CLA	C15-C16-C17-C18
22	C	509	CLA	C8-C10-C11-C12
22	c	510	CLA	C10-C11-C12-C13
22	c	511	CLA	O1D-CGD-O2D-CED
27	c	522	LMG	O6-C5-C6-O5
29	H	102	DGD	O6E-C5E-C6E-O5E
22	A	410	CLA	C13-C15-C16-C17
22	C	510	CLA	C13-C15-C16-C17
22	C	513	CLA	C5-C6-C7-C8
22	C	513	CLA	C8-C10-C11-C12
22	a	404	CLA	C5-C6-C7-C8
22	b	602	CLA	C13-C15-C16-C17
22	b	605	CLA	C5-C6-C7-C8
28	L	101	SQD	C23-C24-C25-C26
32	d	413	STE	C1-C2-C3-C4
33	d	408	LHG	C23-C24-C25-C26
23	d	401	PHO	CBD-CGD-O2D-CED
22	B	601	CLA	C5-C6-C7-C8
22	B	607	CLA	C5-C6-C7-C8
22	C	503	CLA	C5-C6-C7-C8
22	C	506	CLA	C8-C10-C11-C12
22	b	611	CLA	C8-C10-C11-C12
22	c	503	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	c	503	CLA	C8-C10-C11-C12
22	c	506	CLA	C8-C10-C11-C12
22	c	509	CLA	C10-C11-C12-C13
27	D	410	LMG	C10-C11-C12-C13
28	a	410	SQD	C23-C24-C25-C26
29	C	516	DGD	C1B-C2B-C3B-C4B
29	H	102	DGD	C1A-C2A-C3A-C4A
29	a	412	DGD	C1A-C2A-C3A-C4A
32	B	620	STE	C1-C2-C3-C4
33	d	408	LHG	C7-C8-C9-C10
22	A	410	CLA	C15-C16-C17-C18
22	B	614	CLA	C13-C15-C16-C17
22	b	603	CLA	C13-C15-C16-C17
32	T	102	STE	C5-C6-C7-C8
22	c	513	CLA	O1D-CGD-O2D-CED
22	c	506	CLA	C2-C1-O2A-CGA
22	b	605	CLA	C10-C11-C12-C13
22	b	615	CLA	C10-C11-C12-C13
22	b	616	CLA	C5-C6-C7-C8
22	C	505	CLA	C2C-C3C-CAC-CBC
29	A	414	DGD	O6E-C5E-C6E-O5E
22	A	410	CLA	C11-C12-C13-C15
22	C	505	CLA	C11-C10-C8-C7
22	C	512	CLA	C6-C7-C8-C10
22	C	513	CLA	C12-C13-C15-C16
22	b	606	CLA	C6-C7-C8-C10
22	b	606	CLA	C11-C10-C8-C7
22	b	615	CLA	C11-C12-C13-C15
22	d	405	CLA	C12-C13-C15-C16
22	C	509	CLA	C3-C5-C6-C7
22	b	606	CLA	C2A-CAA-CBA-CGA
22	b	601	CLA	O1D-CGD-O2D-CED
22	c	509	CLA	O1D-CGD-O2D-CED
22	b	608	CLA	C5-C6-C7-C8
22	c	510	CLA	C15-C16-C17-C18
22	C	513	CLA	O1A-CGA-O2A-C1
27	b	622	LMG	O10-C28-O8-C9
29	C	518	DGD	O1A-C1A-O1G-C1G
29	a	412	DGD	O1A-C1A-O1G-C1G
28	L	101	SQD	O5-C1-O6-C44
22	B	601	CLA	C15-C16-C17-C18
26	A	409	PL9	C34-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
24	C	514	BCR	C18-C19-C20-C21
24	C	515	BCR	C18-C19-C20-C21
24	H	101	BCR	C10-C11-C12-C13
24	c	514	BCR	C18-C19-C20-C21
24	d	406	BCR	C10-C11-C12-C13
24	t	101	BCR	C10-C11-C12-C13
33	B	622	LHG	O2-C2-C3-O3
22	b	602	CLA	C3-C5-C6-C7
22	B	607	CLA	C10-C11-C12-C13
22	B	611	CLA	C8-C10-C11-C12
22	B	613	CLA	C8-C10-C11-C12
22	C	513	CLA	C15-C16-C17-C18
29	A	414	DGD	C4E-C5E-C6E-O5E
22	B	604	CLA	C13-C15-C16-C17
22	B	605	CLA	C13-C15-C16-C17
22	B	607	CLA	C13-C15-C16-C17
22	B	615	CLA	C5-C6-C7-C8
22	C	513	CLA	C13-C15-C16-C17
22	D	404	CLA	C10-C11-C12-C13
22	b	601	CLA	C10-C11-C12-C13
22	b	607	CLA	C8-C10-C11-C12
22	b	613	CLA	C13-C15-C16-C17
22	c	511	CLA	C13-C15-C16-C17
22	c	511	CLA	C15-C16-C17-C18
22	c	512	CLA	C13-C15-C16-C17
33	d	410	LHG	C24-C25-C26-C27
22	c	506	CLA	O1A-CGA-O2A-C1
22	c	506	CLA	C13-C15-C16-C17
22	d	405	CLA	C5-C6-C7-C8
33	D	408	LHG	C3-O3-P-O6
33	d	408	LHG	C3-O3-P-O6
33	d	409	LHG	C3-O3-P-O6
33	e	101	LHG	C3-O3-P-O6
33	l	101	LHG	C4-O6-P-O3
22	c	506	CLA	CBA-CGA-O2A-C1
27	c	522	LMG	C29-C28-O8-C9
22	b	614	CLA	C8-C10-C11-C12
27	b	622	LMG	C28-C29-C30-C31
29	c	519	DGD	C1A-C2A-C3A-C4A
33	B	622	LHG	C1-C2-C3-O3
33	E	102	LHG	C1-C2-C3-O3
33	e	101	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
22	b	607	CLA	C10-C11-C12-C13
22	B	608	CLA	C3-C5-C6-C7
22	B	601	CLA	C10-C11-C12-C13
22	C	512	CLA	C13-C15-C16-C17
22	c	510	CLA	C8-C10-C11-C12
27	M	101	LMG	C28-C29-C30-C31
27	D	410	LMG	C14-C15-C16-C17
27	b	620	LMG	C39-C40-C41-C42
32	l	102	STE	C3-C4-C5-C6
33	d	409	LHG	C12-C13-C14-C15
24	C	515	BCR	C20-C21-C22-C37
24	K	101	BCR	C16-C17-C18-C36
24	T	101	BCR	C11-C10-C9-C34
24	T	101	BCR	C35-C13-C14-C15
24	Y	101	BCR	C16-C17-C18-C36
24	a	405	BCR	C35-C13-C14-C15
24	b	618	BCR	C20-C21-C22-C37
24	b	619	BCR	C35-C13-C14-C15
24	b	619	BCR	C20-C21-C22-C37
24	c	515	BCR	C16-C17-C18-C36
24	h	101	BCR	C35-C13-C14-C15
24	h	101	BCR	C20-C21-C22-C37
24	k	101	BCR	C35-C13-C14-C15
24	k	101	BCR	C16-C17-C18-C36
24	t	101	BCR	C35-C13-C14-C15
27	B	621	LMG	C33-C34-C35-C36
27	c	522	LMG	C30-C31-C32-C33
28	A	413	SQD	C12-C13-C14-C15
28	a	411	SQD	C18-C19-C20-C21
29	C	516	DGD	C5B-C6B-C7B-C8B
29	C	518	DGD	C2B-C3B-C4B-C5B
29	a	412	DGD	C6A-C7A-C8A-C9A
32	B	626	STE	C5-C6-C7-C8
33	D	409	LHG	C34-C35-C36-C37
33	L	102	LHG	C27-C28-C29-C30
33	d	408	LHG	C32-C33-C34-C35
33	d	409	LHG	C29-C30-C31-C32
33	d	410	LHG	C33-C34-C35-C36
33	e	101	LHG	C27-C28-C29-C30
33	l	101	LHG	C28-C29-C30-C31
22	a	403	CLA	C16-C17-C18-C20
22	b	607	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
27	B	621	LMG	C32-C33-C34-C35
27	C	519	LMG	C17-C18-C19-C20
27	M	101	LMG	C38-C39-C40-C41
27	b	622	LMG	C16-C17-C18-C19
27	b	622	LMG	C23-C24-C25-C26
27	c	522	LMG	C36-C37-C38-C39
27	d	411	LMG	C34-C35-C36-C37
28	A	412	SQD	C16-C17-C18-C19
29	H	102	DGD	C8B-C9B-CAB-CBB
29	c	518	DGD	CCA-CDA-CEA-CFA
32	H	103	STE	C11-C12-C13-C14
32	I	101	STE	C4-C5-C6-C7
32	I	101	STE	C10-C11-C12-C13
32	T	103	STE	C5-C6-C7-C8
32	a	414	STE	C5-C6-C7-C8
32	x	101	STE	C2-C3-C4-C5
32	x	101	STE	C12-C13-C14-C15
28	L	101	SQD	C46-C45-O47-C7
22	D	403	CLA	O1D-CGD-O2D-CED
27	M	101	LMG	C15-C16-C17-C18
28	B	623	SQD	C11-C12-C13-C14
28	a	410	SQD	C17-C18-C19-C20
28	a	411	SQD	C10-C11-C12-C13
29	C	517	DGD	C9A-CAA-CBA-CCA
29	C	517	DGD	C6B-C7B-C8B-C9B
29	a	412	DGD	C3A-C4A-C5A-C6A
29	c	518	DGD	C8A-C9A-CAA-CBA
29	c	519	DGD	CCA-CDA-CEA-CFA
32	H	103	STE	C5-C6-C7-C8
32	x	101	STE	C3-C4-C5-C6
22	c	510	CLA	O1D-CGD-O2D-CED
27	M	101	LMG	C12-C13-C14-C15
27	M	101	LMG	C14-C15-C16-C17
27	c	523	LMG	C12-C13-C14-C15
27	c	523	LMG	C34-C35-C36-C37
29	C	518	DGD	C8A-C9A-CAA-CBA
29	c	517	DGD	C7A-C8A-C9A-CAA
32	B	620	STE	C6-C7-C8-C9
32	B	627	STE	C5-C6-C7-C8
33	d	409	LHG	C32-C33-C34-C35
22	D	404	CLA	C13-C15-C16-C17
28	A	412	SQD	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
28	a	411	SQD	C11-C10-C9-C8
33	B	622	LHG	C26-C27-C28-C29
33	D	408	LHG	C10-C11-C12-C13
33	e	101	LHG	C14-C15-C16-C17
33	l	101	LHG	C24-C25-C26-C27
24	C	514	BCR	C16-C17-C18-C19
24	C	514	BCR	C20-C21-C22-C23
24	C	515	BCR	C12-C13-C14-C15
24	K	101	BCR	C16-C17-C18-C19
24	b	617	BCR	C12-C13-C14-C15
24	b	618	BCR	C11-C10-C9-C8
24	b	618	BCR	C20-C21-C22-C23
24	c	514	BCR	C12-C13-C14-C15
24	c	514	BCR	C16-C17-C18-C19
24	d	406	BCR	C20-C21-C22-C23
24	h	101	BCR	C11-C10-C9-C8
24	h	101	BCR	C16-C17-C18-C19
24	h	101	BCR	C20-C21-C22-C23
27	C	519	LMG	C2-C1-O1-C7
28	F	101	SQD	C2-C1-O6-C44
29	c	518	DGD	C2E-C1E-O5D-C6D
27	b	620	LMG	C29-C28-O8-C9
29	c	519	DGD	C2A-C1A-O1G-C1G
27	D	407	LMG	C31-C32-C33-C34
27	b	622	LMG	C11-C12-C13-C14
27	c	522	LMG	C33-C34-C35-C36
27	d	411	LMG	C31-C32-C33-C34
28	a	410	SQD	C13-C14-C15-C16
28	a	410	SQD	C34-C35-C36-C37
29	A	414	DGD	C8B-C9B-CAB-CBB
32	B	620	STE	C9-C10-C11-C12
32	B	625	STE	C5-C6-C7-C8
32	c	524	STE	C5-C6-C7-C8
22	c	509	CLA	C8-C10-C11-C12
22	B	602	CLA	C16-C17-C18-C19
22	B	604	CLA	C16-C17-C18-C20
22	C	513	CLA	C16-C17-C18-C19
22	b	607	CLA	C16-C17-C18-C20
22	c	511	CLA	C16-C17-C18-C20
27	c	520	LMG	O6-C5-C6-O5
26	D	406	PL9	C30-C29-C31-C32
27	D	407	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
27	d	411	LMG	C35-C36-C37-C38
28	a	411	SQD	C11-C12-C13-C14
29	h	102	DGD	C5B-C6B-C7B-C8B
29	h	102	DGD	C6B-C7B-C8B-C9B
32	C	520	STE	C3-C4-C5-C6
22	b	609	CLA	C2-C3-C5-C6
22	A	403	CLA	C14-C13-C15-C16
22	A	410	CLA	C11-C12-C13-C14
22	B	606	CLA	C11-C12-C13-C14
22	d	403	CLA	C6-C7-C8-C9
32	x	101	STE	C1-C2-C3-C4
27	c	522	LMG	C31-C32-C33-C34
27	d	411	LMG	C32-C33-C34-C35
28	a	410	SQD	C29-C30-C31-C32
29	A	414	DGD	C2B-C3B-C4B-C5B
29	H	102	DGD	C6B-C7B-C8B-C9B
29	c	517	DGD	C3B-C4B-C5B-C6B
29	c	517	DGD	C4B-C5B-C6B-C7B
29	c	517	DGD	CBB-CCB-CDB-CEB
29	c	518	DGD	C4A-C5A-C6A-C7A
29	c	519	DGD	C9A-CAA-CBA-CCA
32	b	623	STE	C6-C7-C8-C9
33	d	408	LHG	C11-C10-C9-C8
33	d	409	LHG	C34-C35-C36-C37
33	d	410	LHG	C27-C28-C29-C30
22	b	604	CLA	C15-C16-C17-C18
27	C	519	LMG	C13-C14-C15-C16
27	D	410	LMG	C34-C35-C36-C37
27	c	523	LMG	C18-C19-C20-C21
28	F	101	SQD	C25-C26-C27-C28
28	F	101	SQD	C26-C27-C28-C29
29	c	517	DGD	C9B-CAB-CBB-CCB
33	D	409	LHG	C29-C30-C31-C32
33	D	408	LHG	O1-C1-C2-C3
33	d	410	LHG	O1-C1-C2-C3
22	B	616	CLA	C5-C6-C7-C8
22	b	601	CLA	C13-C15-C16-C17
27	M	101	LMG	C37-C38-C39-C40
27	b	620	LMG	C17-C18-C19-C20
29	C	516	DGD	C4B-C5B-C6B-C7B
32	B	624	STE	C2-C3-C4-C5
32	T	102	STE	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
32	c	521	STE	C9-C10-C11-C12
33	E	102	LHG	C17-C18-C19-C20
33	E	102	LHG	C29-C30-C31-C32
33	L	102	LHG	C18-C19-C20-C21
33	e	101	LHG	C16-C17-C18-C19
33	l	101	LHG	C10-C11-C12-C13
27	D	407	LMG	C10-C11-C12-C13
27	A	411	LMG	C14-C15-C16-C17
27	A	411	LMG	C31-C32-C33-C34
27	B	621	LMG	C34-C35-C36-C37
27	C	519	LMG	C31-C32-C33-C34
27	D	407	LMG	C14-C15-C16-C17
27	D	407	LMG	C15-C16-C17-C18
27	c	520	LMG	C38-C39-C40-C41
27	c	522	LMG	C15-C16-C17-C18
27	c	522	LMG	C16-C17-C18-C19
27	d	411	LMG	C38-C39-C40-C41
28	A	413	SQD	C28-C29-C30-C31
28	A	413	SQD	C30-C31-C32-C33
28	B	623	SQD	C33-C34-C35-C36
28	a	410	SQD	C27-C28-C29-C30
28	f	102	SQD	C24-C25-C26-C27
28	f	102	SQD	C29-C30-C31-C32
29	C	516	DGD	C3B-C4B-C5B-C6B
29	H	102	DGD	C6A-C7A-C8A-C9A
29	H	102	DGD	CAB-CBB-CCB-CDB
29	c	517	DGD	C4A-C5A-C6A-C7A
29	c	517	DGD	C6B-C7B-C8B-C9B
29	c	517	DGD	CCB-CDB-CEB-CFB
32	D	411	STE	C4-C5-C6-C7
32	M	102	STE	C9-C10-C11-C12
32	b	621	STE	C3-C4-C5-C6
32	b	621	STE	C6-C7-C8-C9
32	d	413	STE	C10-C11-C12-C13
32	t	102	STE	C11-C10-C9-C8
33	E	102	LHG	C11-C10-C9-C8
33	E	102	LHG	C25-C26-C27-C28
33	E	102	LHG	C27-C28-C29-C30
33	E	102	LHG	C32-C33-C34-C35
33	L	102	LHG	C12-C13-C14-C15
33	d	410	LHG	C26-C27-C28-C29
22	B	602	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
22	a	403	CLA	C16-C17-C18-C19
27	C	519	LMG	O6-C1-O1-C7
27	M	101	LMG	O6-C1-O1-C7
28	F	101	SQD	O5-C1-O6-C44
29	c	518	DGD	O6E-C1E-O5D-C6D
22	b	615	CLA	C15-C16-C17-C18
27	D	407	LMG	C38-C39-C40-C41
27	c	523	LMG	C35-C36-C37-C38
28	B	623	SQD	C16-C17-C18-C19
29	a	412	DGD	C8B-C9B-CAB-CBB
29	c	517	DGD	C8A-C9A-CAA-CBA
32	I	101	STE	C2-C3-C4-C5
32	J	101	STE	C3-C4-C5-C6
32	a	414	STE	C4-C5-C6-C7
32	x	101	STE	C7-C8-C9-C10
27	c	522	LMG	C32-C33-C34-C35
29	A	414	DGD	C2A-C3A-C4A-C5A
29	C	517	DGD	CBA-CCA-CDA-CEA
29	a	412	DGD	CEB-CFB-CGB-CHB
29	c	519	DGD	CBA-CCA-CDA-CEA
32	C	522	STE	C6-C7-C8-C9
32	d	413	STE	C4-C5-C6-C7
32	d	413	STE	C11-C12-C13-C14
32	m	101	STE	C5-C6-C7-C8
32	x	101	STE	C4-C5-C6-C7
33	D	408	LHG	C30-C31-C32-C33
33	l	101	LHG	C16-C17-C18-C19
22	b	615	CLA	C13-C15-C16-C17
22	c	507	CLA	C5-C6-C7-C8
27	D	407	LMG	C32-C33-C34-C35
27	M	101	LMG	C13-C14-C15-C16
29	C	517	DGD	C4B-C5B-C6B-C7B
29	c	517	DGD	CCA-CDA-CEA-CFA
33	D	409	LHG	C13-C14-C15-C16
33	E	102	LHG	C34-C35-C36-C37
33	d	410	LHG	C31-C32-C33-C34
33	l	101	LHG	C33-C34-C35-C36
22	c	512	CLA	CBA-CGA-O2A-C1
29	a	412	DGD	C2A-C1A-O1G-C1G
27	B	621	LMG	C11-C12-C13-C14
28	A	413	SQD	C18-C19-C20-C21
28	L	101	SQD	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
29	C	517	DGD	C5A-C6A-C7A-C8A
22	c	512	CLA	C3A-C2A-CAA-CBA
23	d	402	PHO	C3A-C2A-CAA-CBA
27	M	101	LMG	C33-C34-C35-C36
29	C	518	DGD	C4B-C5B-C6B-C7B
29	c	519	DGD	C8B-C9B-CAB-CBB
29	h	102	DGD	C9A-CAA-CBA-CCA
33	D	409	LHG	C33-C34-C35-C36
22	A	410	CLA	C16-C17-C18-C20
22	b	615	CLA	C16-C17-C18-C20
29	h	102	DGD	C3B-C4B-C5B-C6B
32	E	103	STE	C3-C4-C5-C6
32	c	521	STE	C2-C3-C4-C5
33	B	622	LHG	C12-C13-C14-C15
33	E	102	LHG	C33-C34-C35-C36
28	A	412	SQD	O6-C44-C45-C46
22	d	404	CLA	CBD-CGD-O2D-CED
27	A	411	LMG	C29-C30-C31-C32
27	A	411	LMG	C37-C38-C39-C40
27	b	622	LMG	C18-C19-C20-C21
32	C	521	STE	C7-C8-C9-C10
32	b	624	STE	C4-C5-C6-C7
32	j	101	STE	C4-C5-C6-C7
33	e	101	LHG	C11-C10-C9-C8
24	K	101	BCR	C14-C15-C16-C17
24	k	101	BCR	C14-C15-C16-C17
27	c	522	LMG	C10-C11-C12-C13
29	C	516	DGD	C1A-C2A-C3A-C4A
29	c	518	DGD	C1B-C2B-C3B-C4B
22	d	405	CLA	C10-C11-C12-C13
22	B	607	CLA	C4-C3-C5-C6
22	C	505	CLA	C4-C3-C5-C6
29	A	414	DGD	C2A-C1A-O1G-C1G
23	A	404	PHO	C2-C3-C5-C6
26	a	409	PL9	C18-C19-C21-C22
26	d	407	PL9	C13-C14-C16-C17
26	d	407	PL9	C33-C34-C36-C37
26	d	407	PL9	C43-C44-C46-C47
29	a	412	DGD	C2B-C1B-O2G-C2G
27	b	622	LMG	C12-C13-C14-C15
27	d	411	LMG	C36-C37-C38-C39
32	a	413	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
32	c	521	STE	C11-C12-C13-C14
33	B	622	LHG	O1-C1-C2-O2
33	d	408	LHG	O1-C1-C2-O2
33	d	409	LHG	O1-C1-C2-O2
27	c	522	LMG	C38-C39-C40-C41
27	c	522	LMG	C40-C41-C42-C43
29	a	412	DGD	C8A-C9A-CAA-CBA
29	c	519	DGD	C2A-C3A-C4A-C5A
32	l	102	STE	C7-C8-C9-C10
33	D	409	LHG	C9-C10-C11-C12
33	l	101	LHG	C23-C24-C25-C26
22	B	605	CLA	C16-C17-C18-C20
22	B	609	CLA	C16-C17-C18-C20
22	c	503	CLA	C16-C17-C18-C20
22	a	402	CLA	C15-C16-C17-C18
22	c	503	CLA	C15-C16-C17-C18
33	D	409	LHG	C27-C28-C29-C30
28	B	623	SQD	C18-C19-C20-C21
32	B	625	STE	C2-C3-C4-C5
33	D	409	LHG	C11-C12-C13-C14
33	L	102	LHG	C11-C12-C13-C14
27	c	522	LMG	C13-C14-C15-C16
28	A	412	SQD	C11-C10-C9-C8
29	C	516	DGD	C9B-CAB-CBB-CCB
27	b	622	LMG	C13-C14-C15-C16
27	c	522	LMG	C11-C12-C13-C14
32	B	620	STE	C11-C12-C13-C14
32	T	103	STE	C6-C7-C8-C9
32	l	102	STE	C13-C14-C15-C16
32	x	101	STE	C5-C6-C7-C8
33	l	101	LHG	C11-C12-C13-C14
22	C	509	CLA	C13-C15-C16-C17
27	d	411	LMG	C37-C38-C39-C40
33	D	408	LHG	C29-C30-C31-C32
33	d	410	LHG	C23-C24-C25-C26
24	C	514	BCR	C23-C24-C25-C30
24	C	515	BCR	C5-C6-C7-C8
24	H	101	BCR	C23-C24-C25-C26
24	H	101	BCR	C23-C24-C25-C30
24	T	101	BCR	C5-C6-C7-C8
24	b	617	BCR	C5-C6-C7-C8
24	d	406	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
24	d	406	BCR	C23-C24-C25-C30
24	h	101	BCR	C23-C24-C25-C26
24	k	101	BCR	C1-C6-C7-C8
24	k	101	BCR	C5-C6-C7-C8
24	t	101	BCR	C1-C6-C7-C8
32	B	625	STE	C12-C13-C14-C15
32	b	621	STE	C14-C15-C16-C17
22	B	607	CLA	C8-C10-C11-C12
22	b	616	CLA	C10-C11-C12-C13
22	c	507	CLA	C8-C10-C11-C12
28	f	102	SQD	C28-C29-C30-C31
33	E	102	LHG	C24-C25-C26-C27
22	c	512	CLA	O1A-CGA-O2A-C1
27	c	523	LMG	O6-C5-C6-O5
29	C	516	DGD	O6E-C5E-C6E-O5E
28	L	101	SQD	C7-C8-C9-C10
27	D	410	LMG	C16-C17-C18-C19
22	B	606	CLA	C15-C16-C17-C18
29	H	102	DGD	C8A-C9A-CAA-CBA
29	c	517	DGD	C8B-C9B-CAB-CBB
32	M	102	STE	C11-C10-C9-C8
32	a	413	STE	C2-C3-C4-C5
33	L	102	LHG	C17-C18-C19-C20
22	B	614	CLA	C4-C3-C5-C6
22	b	609	CLA	C4-C3-C5-C6
23	A	404	PHO	C4-C3-C5-C6
26	d	407	PL9	C15-C14-C16-C17
22	A	403	CLA	C12-C13-C15-C16
22	B	604	CLA	C11-C10-C8-C7
22	B	606	CLA	C11-C10-C8-C7
22	B	606	CLA	C11-C12-C13-C15
22	B	611	CLA	C12-C13-C15-C16
22	C	505	CLA	C2-C3-C5-C6
22	C	506	CLA	C6-C7-C8-C10
22	C	513	CLA	C11-C10-C8-C7
22	a	403	CLA	C12-C13-C15-C16
22	b	605	CLA	C11-C10-C8-C7
22	b	607	CLA	C11-C10-C8-C7
22	b	614	CLA	C6-C7-C8-C10
22	b	616	CLA	C11-C10-C8-C7
22	c	508	CLA	C11-C10-C8-C7
22	c	510	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	c	512	CLA	C11-C12-C13-C15
22	d	403	CLA	C6-C7-C8-C10
29	A	414	DGD	CEA-CFA-CGA-CHA
22	B	606	CLA	C5-C6-C7-C8
22	B	606	CLA	C13-C15-C16-C17
22	C	505	CLA	C5-C6-C7-C8
22	C	509	CLA	C10-C11-C12-C13
22	C	513	CLA	C16-C17-C18-C20
22	c	511	CLA	C16-C17-C18-C19
29	c	517	DGD	O1B-C1B-O2G-C2G
29	H	102	DGD	CCB-CDB-CEB-CFB
29	a	412	DGD	C4B-C5B-C6B-C7B
33	L	102	LHG	C30-C31-C32-C33
22	B	603	CLA	C10-C11-C12-C13
22	D	403	CLA	C15-C16-C17-C18
32	I	101	STE	C7-C8-C9-C10
29	c	517	DGD	C5B-C6B-C7B-C8B
29	c	518	DGD	C2A-C3A-C4A-C5A
32	l	102	STE	C4-C5-C6-C7
28	A	412	SQD	C7-C8-C9-C10
32	E	103	STE	C1-C2-C3-C4
22	b	602	CLA	C15-C16-C17-C18
27	D	407	LMG	C36-C37-C38-C39
27	C	519	LMG	C30-C31-C32-C33
29	c	519	DGD	C6A-C7A-C8A-C9A
32	T	103	STE	C9-C10-C11-C12
32	T	103	STE	C11-C12-C13-C14
29	c	517	DGD	O6E-C1E-O5D-C6D
22	c	502	CLA	C13-C15-C16-C17
27	c	522	LMG	C34-C35-C36-C37
28	B	623	SQD	C32-C33-C34-C35
29	H	102	DGD	CBA-CCA-CDA-CEA
29	a	412	DGD	C3B-C4B-C5B-C6B
33	D	409	LHG	C25-C26-C27-C28
27	c	522	LMG	C11-C10-O7-C8
24	T	101	BCR	C18-C19-C20-C21
27	c	520	LMG	C31-C32-C33-C34
29	h	102	DGD	C2B-C3B-C4B-C5B
29	h	102	DGD	CAB-CBB-CCB-CDB
33	L	102	LHG	C32-C33-C34-C35
33	l	101	LHG	C25-C26-C27-C28
22	A	403	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
27	A	411	LMG	C38-C39-C40-C41
27	C	519	LMG	O9-C10-O7-C8
29	a	412	DGD	O1B-C1B-O2G-C2G
27	d	411	LMG	C30-C31-C32-C33
27	M	101	LMG	C2-C1-O1-C7
28	A	412	SQD	O6-C44-C45-O47
28	a	410	SQD	O47-C45-C46-O48
28	B	623	SQD	C12-C13-C14-C15
29	A	414	DGD	CCA-CDA-CEA-CFA
29	H	102	DGD	C5A-C6A-C7A-C8A
33	E	102	LHG	C13-C14-C15-C16
33	L	102	LHG	C13-C14-C15-C16
28	a	410	SQD	C25-C26-C27-C28
22	B	605	CLA	C2-C3-C5-C6
22	B	607	CLA	C2-C3-C5-C6
22	B	614	CLA	C2-C3-C5-C6
22	b	605	CLA	C2-C3-C5-C6
26	A	409	PL9	C4-C3-C7-C8
22	C	505	CLA	C4C-C3C-CAC-CBC
32	B	620	STE	C7-C8-C9-C10
22	B	604	CLA	C11-C10-C8-C9
22	B	605	CLA	C11-C12-C13-C14
22	B	607	CLA	C6-C7-C8-C9
22	B	615	CLA	C11-C12-C13-C14
22	B	616	CLA	C6-C7-C8-C9
22	C	502	CLA	C11-C12-C13-C14
22	C	503	CLA	C14-C13-C15-C16
22	C	505	CLA	C11-C10-C8-C9
22	C	506	CLA	C6-C7-C8-C9
22	C	511	CLA	C6-C7-C8-C9
22	C	513	CLA	C11-C10-C8-C9
22	a	403	CLA	C14-C13-C15-C16
22	b	606	CLA	C6-C7-C8-C9
22	b	606	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	C14-C13-C15-C16
22	c	512	CLA	C11-C12-C13-C14
22	d	405	CLA	C14-C13-C15-C16
22	C	511	CLA	O1D-CGD-O2D-CED
27	A	411	LMG	C16-C17-C18-C19
27	b	622	LMG	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
32	b	621	STE	C5-C6-C7-C8
22	C	510	CLA	C3-C5-C6-C7
22	C	512	CLA	C3-C5-C6-C7
29	A	414	DGD	C5B-C6B-C7B-C8B
27	d	412	LMG	O6-C5-C6-O5
22	B	615	CLA	C13-C15-C16-C17
22	C	505	CLA	C10-C11-C12-C13
27	D	407	LMG	C12-C13-C14-C15
28	L	101	SQD	C29-C30-C31-C32
32	D	411	STE	C14-C15-C16-C17
27	D	410	LMG	O10-C28-O8-C9
22	B	604	CLA	C1A-C2A-CAA-CBA
22	b	601	CLA	C1A-C2A-CAA-CBA
22	c	512	CLA	C1A-C2A-CAA-CBA
22	c	513	CLA	C1A-C2A-CAA-CBA
22	B	605	CLA	C16-C17-C18-C19
22	B	612	CLA	C16-C17-C18-C20
22	b	615	CLA	C16-C17-C18-C19
33	e	101	LHG	O9-C7-O7-C5
28	F	101	SQD	C30-C31-C32-C33
29	c	519	DGD	C8A-C9A-CAA-CBA
32	B	626	STE	C6-C7-C8-C9
32	d	413	STE	C9-C10-C11-C12
22	C	510	CLA	C15-C16-C17-C18
33	l	101	LHG	C3-O3-P-O6
27	c	523	LMG	C15-C16-C17-C18
29	A	414	DGD	CBB-CCB-CDB-CEB
29	C	517	DGD	C4A-C5A-C6A-C7A
32	l	102	STE	C10-C11-C12-C13
22	B	601	CLA	C8-C10-C11-C12
22	C	512	CLA	C8-C10-C11-C12
22	b	609	CLA	C13-C15-C16-C17
33	e	101	LHG	O6-C4-C5-C6
26	D	406	PL9	C32-C33-C34-C35
22	C	509	CLA	O1D-CGD-O2D-CED
28	A	412	SQD	C12-C13-C14-C15
28	A	413	SQD	C32-C33-C34-C35
32	D	411	STE	C6-C7-C8-C9
32	b	621	STE	C1-C2-C3-C4
27	b	622	LMG	C37-C38-C39-C40
29	C	518	DGD	C8B-C9B-CAB-CBB
32	b	623	STE	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
28	B	623	SQD	C45-C46-O48-C23
22	B	604	CLA	C16-C17-C18-C19
27	b	622	LMG	C38-C39-C40-C41
28	a	410	SQD	C24-C25-C26-C27
32	D	411	STE	C7-C8-C9-C10
33	L	102	LHG	C31-C32-C33-C34
29	c	517	DGD	O6D-C5D-C6D-O5D
22	b	604	CLA	C3-C5-C6-C7
28	a	411	SQD	C15-C16-C17-C18
33	D	409	LHG	C30-C31-C32-C33
26	a	409	PL9	C15-C14-C16-C17
27	B	621	LMG	C16-C17-C18-C19
27	B	621	LMG	C31-C32-C33-C34
27	d	412	LMG	C30-C31-C32-C33
29	C	517	DGD	C6A-C7A-C8A-C9A
22	B	605	CLA	C8-C10-C11-C12
22	b	601	CLA	C15-C16-C17-C18
27	M	101	LMG	C35-C36-C37-C38
27	b	622	LMG	C33-C34-C35-C36
27	c	520	LMG	C39-C40-C41-C42
29	a	412	DGD	C4A-C5A-C6A-C7A
32	B	625	STE	C3-C4-C5-C6
33	e	101	LHG	C17-C18-C19-C20
27	C	519	LMG	C14-C15-C16-C17
28	B	623	SQD	C9-C10-C11-C12
32	a	414	STE	C2-C3-C4-C5
32	c	524	STE	C6-C7-C8-C9
32	t	102	STE	C6-C7-C8-C9
32	x	101	STE	C9-C10-C11-C12
27	A	411	LMG	O1-C7-C8-C9
27	M	101	LMG	C7-C8-C9-O8
27	c	522	LMG	C7-C8-C9-O8
27	c	523	LMG	C7-C8-C9-O8
28	B	623	SQD	O6-C44-C45-C46
28	a	410	SQD	C44-C45-C46-O48
28	a	411	SQD	C44-C45-C46-O48
32	C	520	STE	C6-C7-C8-C9
33	D	408	LHG	C11-C12-C13-C14
33	E	102	LHG	C4-C5-C6-O8
22	B	614	CLA	C15-C16-C17-C18
27	d	412	LMG	C36-C37-C38-C39
32	t	102	STE	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
29	C	517	DGD	C2G-C3G-O3G-C1D
29	c	518	DGD	C5D-C6D-O5D-C1E
27	M	101	LMG	C17-C18-C19-C20
27	c	523	LMG	C20-C21-C22-C23
32	M	103	STE	C1-C2-C3-C4
22	a	402	CLA	CBD-CGD-O2D-CED
27	D	410	LMG	C15-C16-C17-C18
28	B	623	SQD	C31-C32-C33-C34
29	c	518	DGD	CBA-CCA-CDA-CEA
32	D	411	STE	C15-C16-C17-C18
32	b	621	STE	C13-C14-C15-C16
29	H	102	DGD	O2G-C1B-C2B-C3B
27	C	519	LMG	O10-C28-O8-C9
29	c	519	DGD	C5B-C6B-C7B-C8B
22	c	506	CLA	C16-C17-C18-C20
33	d	410	LHG	O1-C1-C2-O2
28	A	412	SQD	C27-C28-C29-C30
29	a	412	DGD	CBA-CCA-CDA-CEA
32	C	521	STE	C5-C6-C7-C8
32	m	101	STE	C1-C2-C3-C4
33	D	408	LHG	C18-C19-C20-C21
33	d	409	LHG	C14-C15-C16-C17
29	A	414	DGD	CFB-CGB-CHB-CIB
32	b	625	STE	C7-C8-C9-C10
22	b	606	CLA	C10-C11-C12-C13
24	b	619	BCR	C16-C17-C18-C36
27	b	622	LMG	O6-C5-C6-O5
29	c	517	DGD	O6E-C5E-C6E-O5E
22	C	510	CLA	C4-C3-C5-C6
22	a	404	CLA	C10-C11-C12-C13
22	b	606	CLA	C8-C10-C11-C12
22	b	606	CLA	C15-C16-C17-C18
28	f	102	SQD	C35-C36-C37-C38
29	c	519	DGD	CDA-CEA-CFA-CGA
27	D	410	LMG	C9-C8-O7-C10
29	a	412	DGD	C1G-C2G-O2G-C1B
27	D	407	LMG	O6-C5-C6-O5
28	A	412	SQD	C17-C18-C19-C20
29	A	414	DGD	CFA-CGA-CHA-CIA
32	c	521	STE	C10-C11-C12-C13
33	L	102	LHG	C15-C16-C17-C18
23	d	401	PHO	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	h	102	DGD	O6E-C5E-C6E-O5E
27	b	620	LMG	C37-C38-C39-C40
28	L	101	SQD	C16-C17-C18-C19
32	B	625	STE	C10-C11-C12-C13
32	T	102	STE	C12-C13-C14-C15
32	b	624	STE	C12-C13-C14-C15
33	l	101	LHG	C14-C15-C16-C17
22	B	610	CLA	O1D-CGD-O2D-CED
27	D	410	LMG	C35-C36-C37-C38
29	c	518	DGD	C7B-C8B-C9B-CAB
33	d	409	LHG	C35-C36-C37-C38
33	e	101	LHG	O6-C4-C5-O7
27	d	412	LMG	C37-C38-C39-C40
29	a	412	DGD	CDA-CEA-CFA-CGA
29	a	412	DGD	CEA-CFA-CGA-CHA
32	b	621	STE	C7-C8-C9-C10
33	d	408	LHG	C16-C17-C18-C19
32	c	521	STE	C1-C2-C3-C4
22	b	613	CLA	C10-C11-C12-C13
24	b	618	BCR	C16-C17-C18-C19
27	M	101	LMG	O7-C8-C9-O8
28	B	623	SQD	O6-C44-C45-O47
29	A	414	DGD	O2G-C2G-C3G-O3G
29	C	517	DGD	C3A-C4A-C5A-C6A
33	d	408	LHG	C17-C18-C19-C20
33	B	622	LHG	O9-C7-O7-C5
27	c	520	LMG	C35-C36-C37-C38
32	E	103	STE	C4-C5-C6-C7
33	l	101	LHG	C31-C32-C33-C34
29	c	517	DGD	C4D-C5D-C6D-O5D
22	A	403	CLA	C6-C7-C8-C10
22	A	403	CLA	C11-C10-C8-C7
22	B	602	CLA	C11-C12-C13-C15
22	B	604	CLA	C12-C13-C15-C16
22	B	614	CLA	C12-C13-C15-C16
22	B	615	CLA	C11-C12-C13-C15
22	B	616	CLA	C6-C7-C8-C10
22	C	502	CLA	C11-C12-C13-C15
22	C	503	CLA	C12-C13-C15-C16
22	C	505	CLA	C12-C13-C15-C16
22	C	507	CLA	C11-C10-C8-C7
22	C	510	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	C	511	CLA	C6-C7-C8-C10
22	C	512	CLA	C11-C10-C8-C7
22	b	601	CLA	C12-C13-C15-C16
22	b	604	CLA	C12-C13-C15-C16
22	b	606	CLA	C12-C13-C15-C16
22	b	607	CLA	C6-C7-C8-C10
22	b	608	CLA	C11-C12-C13-C15
22	b	615	CLA	C11-C10-C8-C7
22	c	504	CLA	C11-C10-C8-C7
22	c	505	CLA	C11-C10-C8-C7
22	c	506	CLA	C11-C10-C8-C7
22	c	507	CLA	C11-C10-C8-C7
22	c	509	CLA	C6-C7-C8-C10
28	B	623	SQD	C14-C15-C16-C17
22	A	403	CLA	C6-C7-C8-C9
22	B	602	CLA	C11-C12-C13-C14
22	B	604	CLA	C11-C12-C13-C14
22	B	608	CLA	C6-C7-C8-C9
22	C	507	CLA	C11-C10-C8-C9
22	C	508	CLA	C14-C13-C15-C16
22	D	404	CLA	C6-C7-C8-C9
22	b	602	CLA	C6-C7-C8-C9
22	b	607	CLA	C6-C7-C8-C9
22	b	608	CLA	C11-C12-C13-C14
22	b	609	CLA	C14-C13-C15-C16
22	b	615	CLA	C11-C10-C8-C9
22	c	506	CLA	C11-C10-C8-C9
27	b	620	LMG	C15-C16-C17-C18
27	c	523	LMG	C31-C32-C33-C34
28	L	101	SQD	C18-C19-C20-C21
33	d	408	LHG	C29-C30-C31-C32
22	b	614	CLA	C13-C15-C16-C17
27	b	622	LMG	C24-C25-C26-C27
27	d	412	LMG	C14-C15-C16-C17
29	C	517	DGD	CDA-CEA-CFA-CGA
22	a	403	CLA	CBD-CGD-O2D-CED
22	B	614	CLA	C16-C17-C18-C19
27	A	411	LMG	C30-C31-C32-C33
28	L	101	SQD	C12-C13-C14-C15
27	d	412	LMG	C39-C40-C41-C42
28	a	411	SQD	C14-C15-C16-C17
28	f	102	SQD	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
29	a	412	DGD	CFA-CGA-CHA-CIA
32	a	413	STE	C4-C5-C6-C7
28	A	412	SQD	C8-C7-O47-C45
29	a	412	DGD	C7B-C8B-C9B-CAB
32	T	102	STE	C15-C16-C17-C18
22	B	604	CLA	CBA-CGA-O2A-C1
22	b	607	CLA	C13-C15-C16-C17
22	b	608	CLA	C13-C15-C16-C17
27	b	620	LMG	C31-C32-C33-C34
29	a	412	DGD	C9A-CAA-CBA-CCA
33	d	409	LHG	C11-C12-C13-C14
27	c	523	LMG	C29-C30-C31-C32
27	c	523	LMG	C38-C39-C40-C41
32	H	103	STE	C15-C16-C17-C18
33	D	408	LHG	C15-C16-C17-C18
22	b	612	CLA	C13-C15-C16-C17
27	D	410	LMG	C33-C34-C35-C36
29	C	517	DGD	CCB-CDB-CEB-CFB
29	C	518	DGD	CDA-CEA-CFA-CGA
32	B	625	STE	C13-C14-C15-C16
32	b	624	STE	C14-C15-C16-C17
27	c	523	LMG	C28-C29-C30-C31
32	B	627	STE	C1-C2-C3-C4
27	b	622	LMG	C31-C32-C33-C34
29	c	517	DGD	C5A-C6A-C7A-C8A
22	c	505	CLA	C4-C3-C5-C6
32	b	621	STE	C12-C13-C14-C15
22	b	602	CLA	CBD-CGD-O2D-CED
28	A	413	SQD	C10-C11-C12-C13
29	A	414	DGD	C7B-C8B-C9B-CAB
29	C	517	DGD	C8B-C9B-CAB-CBB
29	a	412	DGD	C5A-C6A-C7A-C8A
33	D	408	LHG	C32-C33-C34-C35
28	a	411	SQD	C31-C32-C33-C34
29	c	518	DGD	CBB-CCB-CDB-CEB
28	A	413	SQD	C23-C24-C25-C26
29	C	518	DGD	CBB-CCB-CDB-CEB
33	d	408	LHG	C15-C16-C17-C18
27	b	620	LMG	C20-C21-C22-C23
29	a	412	DGD	CAB-CBB-CCB-CDB
33	D	408	LHG	C12-C13-C14-C15
27	C	519	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
29	H	102	DGD	CDB-CEB-CFB-CGB
32	t	102	STE	C3-C4-C5-C6
32	E	103	STE	C7-C8-C9-C10
33	d	409	LHG	C33-C34-C35-C36
27	c	520	LMG	C29-C28-O8-C9
29	c	517	DGD	CAB-CBB-CCB-CDB
32	b	621	STE	C2-C3-C4-C5
27	C	519	LMG	O1-C7-C8-C9
27	M	101	LMG	O1-C7-C8-C9
28	a	410	SQD	O6-C44-C45-C46
29	A	414	DGD	C1G-C2G-C3G-O3G
32	x	101	STE	C11-C10-C9-C8
33	e	101	LHG	C28-C29-C30-C31
32	H	103	STE	C13-C14-C15-C16
33	e	101	LHG	C11-C12-C13-C14
27	c	522	LMG	C41-C42-C43-C44
33	d	408	LHG	C14-C15-C16-C17
22	b	605	CLA	C4-C3-C5-C6
22	B	612	CLA	C16-C17-C18-C19
22	c	503	CLA	C16-C17-C18-C19
27	A	411	LMG	C12-C13-C14-C15
28	a	411	SQD	C12-C13-C14-C15
32	D	411	STE	C12-C13-C14-C15
32	j	101	STE	C5-C6-C7-C8
28	a	410	SQD	C15-C16-C17-C18
27	A	411	LMG	C35-C36-C37-C38
22	B	603	CLA	O1D-CGD-O2D-CED
22	c	512	CLA	C2A-CAA-CBA-CGA
22	C	505	CLA	CBD-CGD-O2D-CED
22	B	616	CLA	CBA-CGA-O2A-C1
27	D	410	LMG	C29-C28-O8-C9
33	L	102	LHG	O10-C23-O8-C6
27	b	622	LMG	C10-C11-C12-C13
28	B	623	SQD	C23-C24-C25-C26
28	A	413	SQD	C14-C15-C16-C17
29	a	412	DGD	C6B-C7B-C8B-C9B
29	h	102	DGD	CDB-CEB-CFB-CGB
32	M	102	STE	C10-C11-C12-C13
22	A	402	CLA	C15-C16-C17-C18
22	b	604	CLA	C13-C15-C16-C17
22	B	616	CLA	O1A-CGA-O2A-C1
32	j	101	STE	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
27	c	523	LMG	O7-C8-C9-O8
22	B	612	CLA	CBA-CGA-O2A-C1
27	A	411	LMG	C11-C12-C13-C14
27	M	101	LMG	C39-C40-C41-C42
29	H	102	DGD	C3B-C4B-C5B-C6B
33	E	102	LHG	C10-C11-C12-C13
27	b	620	LMG	C11-C10-O7-C8
22	A	410	CLA	C16-C17-C18-C19
22	B	609	CLA	C16-C17-C18-C19
27	C	519	LMG	C18-C19-C20-C21
28	L	101	SQD	C24-C25-C26-C27
33	l	101	LHG	C17-C18-C19-C20
33	L	102	LHG	O9-C7-O7-C5
29	C	516	DGD	O6D-C5D-C6D-O5D
22	c	505	CLA	C2-C3-C5-C6
28	L	101	SQD	C19-C20-C21-C22
22	B	612	CLA	C10-C11-C12-C13
22	A	403	CLA	C11-C12-C13-C14
22	B	604	CLA	C14-C13-C15-C16
22	B	614	CLA	C6-C7-C8-C9
22	C	505	CLA	C14-C13-C15-C16
22	C	510	CLA	C11-C10-C8-C9
22	b	604	CLA	C14-C13-C15-C16
22	b	615	CLA	C11-C12-C13-C14
22	c	505	CLA	C11-C10-C8-C9
22	c	506	CLA	C14-C13-C15-C16
29	h	102	DGD	C7A-C8A-C9A-CAA
33	d	410	LHG	C35-C36-C37-C38
22	C	501	CLA	CBD-CGD-O2D-CED
29	c	519	DGD	C5A-C6A-C7A-C8A
32	B	626	STE	C4-C5-C6-C7
32	d	413	STE	C12-C13-C14-C15
33	l	101	LHG	C30-C31-C32-C33
22	c	513	CLA	C5-C6-C7-C8
27	c	522	LMG	O10-C28-O8-C9
27	B	621	LMG	C15-C16-C17-C18
27	D	407	LMG	C22-C23-C24-C25
29	A	414	DGD	CDB-CEB-CFB-CGB
33	B	622	LHG	C9-C10-C11-C12
33	D	409	LHG	C11-C10-C9-C8
22	a	402	CLA	C16-C17-C18-C20
24	A	406	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	B	618	BCR	C23-C24-C25-C26
24	B	618	BCR	C23-C24-C25-C30
24	b	618	BCR	C23-C24-C25-C26
24	c	514	BCR	C5-C6-C7-C8
24	c	516	BCR	C23-C24-C25-C26
24	h	101	BCR	C23-C24-C25-C30
27	D	407	LMG	C30-C31-C32-C33
29	A	414	DGD	C8A-C9A-CAA-CBA
24	D	405	BCR	C21-C22-C23-C24
24	H	101	BCR	C7-C8-C9-C10
24	T	101	BCR	C17-C18-C19-C20
22	b	609	CLA	C15-C16-C17-C18
32	b	623	STE	C1-C2-C3-C4
32	c	524	STE	C7-C8-C9-C10
22	b	612	CLA	C16-C17-C18-C20
32	B	625	STE	C4-C5-C6-C7
22	c	508	CLA	C8-C10-C11-C12
29	H	102	DGD	C4B-C5B-C6B-C7B
32	T	103	STE	C13-C14-C15-C16
32	m	101	STE	C3-C4-C5-C6
22	B	613	CLA	C5-C6-C7-C8
22	c	509	CLA	C13-C15-C16-C17
27	D	407	LMG	C39-C40-C41-C42
32	b	624	STE	C5-C6-C7-C8
22	A	403	CLA	C11-C12-C13-C15
22	B	604	CLA	C11-C12-C13-C15
22	B	607	CLA	C12-C13-C15-C16
22	B	608	CLA	C6-C7-C8-C10
22	B	613	CLA	C12-C13-C15-C16
22	C	503	CLA	C11-C10-C8-C7
22	C	509	CLA	C11-C10-C8-C7
22	C	512	CLA	C11-C12-C13-C15
22	C	513	CLA	C6-C7-C8-C10
22	D	404	CLA	C6-C7-C8-C10
22	a	404	CLA	C12-C13-C15-C16
22	b	602	CLA	C6-C7-C8-C10
22	b	605	CLA	C12-C13-C15-C16
22	b	607	CLA	C11-C12-C13-C15
22	b	609	CLA	C12-C13-C15-C16
22	c	506	CLA	C12-C13-C15-C16
22	c	509	CLA	C11-C12-C13-C15
22	c	510	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	c	511	CLA	C12-C13-C15-C16
22	d	405	CLA	C11-C12-C13-C15
28	L	101	SQD	C26-C27-C28-C29
32	C	520	STE	C4-C5-C6-C7
32	I	101	STE	C12-C13-C14-C15
32	T	102	STE	C6-C7-C8-C9
33	d	409	LHG	C15-C16-C17-C18
24	h	101	BCR	C15-C16-C17-C18
22	b	609	CLA	C16-C17-C18-C20
22	c	510	CLA	C5-C6-C7-C8
32	b	625	STE	C1-C2-C3-C4
22	B	611	CLA	C13-C15-C16-C17
24	B	617	BCR	C35-C13-C14-C15
24	B	617	BCR	C20-C21-C22-C37
24	C	515	BCR	C35-C13-C14-C15
24	C	515	BCR	C16-C17-C18-C36
24	H	101	BCR	C11-C10-C9-C34
24	H	101	BCR	C20-C21-C22-C37
24	Y	101	BCR	C20-C21-C22-C37
24	b	617	BCR	C11-C10-C9-C34
24	b	617	BCR	C35-C13-C14-C15
24	c	515	BCR	C20-C21-C22-C37
24	h	101	BCR	C16-C17-C18-C36
28	A	412	SQD	C14-C15-C16-C17
29	a	412	DGD	C9B-CAB-CBB-CCB
29	a	412	DGD	C5B-C6B-C7B-C8B
29	c	519	DGD	CAB-CBB-CCB-CDB
22	c	502	CLA	CBA-CGA-O2A-C1
28	L	101	SQD	C11-C12-C13-C14
33	d	408	LHG	C27-C28-C29-C30
32	C	520	STE	C5-C6-C7-C8
22	C	508	CLA	C5-C6-C7-C8
22	c	506	CLA	C5-C6-C7-C8
22	B	601	CLA	CAD-CBD-CGD-O2D
22	B	603	CLA	CAD-CBD-CGD-O2D
22	B	604	CLA	CAD-CBD-CGD-O2D
22	C	503	CLA	CAD-CBD-CGD-O2D
22	C	512	CLA	CAD-CBD-CGD-O2D
22	a	402	CLA	CAD-CBD-CGD-O2D
22	c	513	CLA	CAD-CBD-CGD-O2D
23	A	404	PHO	CAD-CBD-CGD-O2D
23	d	401	PHO	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	c	502	CLA	C3-C5-C6-C7
33	E	102	LHG	O9-C7-O7-C5
27	c	523	LMG	C13-C14-C15-C16
29	c	519	DGD	C4A-C5A-C6A-C7A
29	c	519	DGD	C7B-C8B-C9B-CAB
22	B	614	CLA	C16-C17-C18-C20
27	c	522	LMG	C42-C43-C44-C45
29	c	518	DGD	O6D-C1D-O3G-C3G
23	D	401	PHO	C2C-C3C-CAC-CBC
33	B	622	LHG	C4-C5-C6-O8
22	C	502	CLA	C3-C5-C6-C7
32	a	414	STE	C6-C7-C8-C9
22	b	610	CLA	C2A-CAA-CBA-CGA
27	C	519	LMG	C15-C16-C17-C18
32	B	626	STE	C3-C4-C5-C6
32	C	521	STE	C4-C5-C6-C7
22	c	505	CLA	C16-C17-C18-C20
22	c	506	CLA	C16-C17-C18-C19
33	E	102	LHG	O2-C2-C3-O3
22	C	502	CLA	CHA-CBD-CGD-O2D
22	C	504	CLA	CHA-CBD-CGD-O2D
22	C	508	CLA	CHA-CBD-CGD-O2D
22	a	403	CLA	CHA-CBD-CGD-O2D
22	b	606	CLA	CHA-CBD-CGD-O1D
22	b	607	CLA	CHA-CBD-CGD-O1D
22	b	607	CLA	CHA-CBD-CGD-O2D
22	b	616	CLA	CHA-CBD-CGD-O1D
22	c	504	CLA	CHA-CBD-CGD-O1D
22	c	504	CLA	CHA-CBD-CGD-O2D
22	c	508	CLA	CHA-CBD-CGD-O2D
22	c	502	CLA	O1D-CGD-O2D-CED
22	c	502	CLA	O1A-CGA-O2A-C1
33	D	409	LHG	O10-C23-O8-C6
27	A	411	LMG	C17-C18-C19-C20
24	t	101	BCR	C20-C21-C22-C23
27	A	411	LMG	C2-C1-O1-C7
29	c	517	DGD	C2E-C1E-O5D-C6D
27	C	519	LMG	O1-C7-C8-O7
27	M	101	LMG	O1-C7-C8-O7
28	a	411	SQD	O47-C45-C46-O48
29	C	516	DGD	O1G-C1G-C2G-O2G
22	B	604	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	B	612	CLA	O1A-CGA-O2A-C1
32	c	524	STE	C2-C3-C4-C5
33	D	408	LHG	O1-C1-C2-O2
32	B	625	STE	C7-C8-C9-C10
32	d	413	STE	C6-C7-C8-C9
33	D	408	LHG	C17-C18-C19-C20
22	C	506	CLA	C4-C3-C5-C6
22	c	512	CLA	C4-C3-C5-C6
33	E	102	LHG	C28-C29-C30-C31
29	H	102	DGD	CDA-CEA-CFA-CGA
32	B	620	STE	C11-C10-C9-C8
22	B	613	CLA	C14-C13-C15-C16
22	C	508	CLA	C11-C10-C8-C9
22	C	512	CLA	C11-C12-C13-C14
22	b	601	CLA	C6-C7-C8-C9
29	C	516	DGD	C4D-C5D-C6D-O5D
27	b	620	LMG	C14-C15-C16-C17
33	L	102	LHG	C19-C20-C21-C22
22	D	403	CLA	C2C-C3C-CAC-CBC
32	M	102	STE	C4-C5-C6-C7
28	A	412	SQD	C29-C30-C31-C32
33	d	410	LHG	C30-C31-C32-C33
22	a	402	CLA	O1D-CGD-O2D-CED
32	l	102	STE	C1-C2-C3-C4
22	C	505	CLA	O1A-CGA-O2A-C1
32	a	414	STE	C1-C2-C3-C4
32	B	620	STE	C4-C5-C6-C7
24	t	101	BCR	C17-C18-C19-C20
27	A	411	LMG	C40-C41-C42-C43
27	b	622	LMG	C19-C20-C21-C22
29	C	518	DGD	C3A-C4A-C5A-C6A
22	B	601	CLA	C1A-C2A-CAA-CBA
22	b	608	CLA	C16-C17-C18-C19
33	d	408	LHG	C18-C19-C20-C21
22	C	509	CLA	C2-C1-O2A-CGA
22	c	502	CLA	CBD-CGD-O2D-CED
22	c	503	CLA	CBA-CGA-O2A-C1
32	I	101	STE	C11-C12-C13-C14
22	B	606	CLA	C10-C11-C12-C13
33	D	408	LHG	C4-O6-P-O3
28	a	410	SQD	C19-C20-C21-C22
32	b	624	STE	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
26	a	409	PL9	C25-C24-C26-C27
33	D	409	LHG	C2-C3-O3-P
33	d	410	LHG	C2-C3-O3-P
22	c	512	CLA	C2-C3-C5-C6
33	d	409	LHG	C17-C18-C19-C20
33	D	408	LHG	C3-O3-P-O4
33	d	408	LHG	C3-O3-P-O5
33	l	101	LHG	C4-O6-P-O5
22	B	610	CLA	C16-C17-C18-C19
22	D	404	CLA	C16-C17-C18-C19
22	b	604	CLA	C16-C17-C18-C19
22	d	404	CLA	C16-C17-C18-C19
29	A	414	DGD	O6D-C1D-O3G-C3G
22	C	505	CLA	CBA-CGA-O2A-C1
33	l	101	LHG	C24-C23-O8-C6
29	C	516	DGD	CCB-CDB-CEB-CFB
32	B	620	STE	C10-C11-C12-C13
33	D	408	LHG	C25-C26-C27-C28
22	A	405	CLA	C6-C7-C8-C9
22	C	504	CLA	C11-C12-C13-C14
33	L	102	LHG	C10-C11-C12-C13
27	c	523	LMG	C39-C40-C41-C42
29	c	518	DGD	CCB-CDB-CEB-CFB
32	H	103	STE	C10-C11-C12-C13
27	C	519	LMG	C16-C17-C18-C19
29	c	517	DGD	CDB-CEB-CFB-CGB
22	C	502	CLA	CAD-CBD-CGD-O1D
22	C	504	CLA	CAD-CBD-CGD-O1D
22	b	607	CLA	CAD-CBD-CGD-O1D
22	c	504	CLA	CAD-CBD-CGD-O1D
22	c	509	CLA	CAA-CBA-CGA-O2A
29	a	412	DGD	CFB-CGB-CHB-CIB
32	J	101	STE	C2-C3-C4-C5
29	A	414	DGD	CBA-CCA-CDA-CEA
29	c	518	DGD	C5B-C6B-C7B-C8B
33	l	101	LHG	C32-C33-C34-C35
22	C	501	CLA	C16-C17-C18-C20
22	B	601	CLA	C3A-C2A-CAA-CBA
22	B	602	CLA	C12-C13-C15-C16
22	B	603	CLA	C12-C13-C15-C16
22	B	613	CLA	C6-C7-C8-C10
22	B	616	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	C	505	CLA	C6-C7-C8-C10
22	C	506	CLA	C12-C13-C15-C16
22	C	508	CLA	C11-C10-C8-C7
22	C	509	CLA	C12-C13-C15-C16
22	C	510	CLA	C11-C10-C8-C7
22	b	602	CLA	C11-C12-C13-C15
22	b	603	CLA	C11-C12-C13-C15
22	b	606	CLA	C11-C12-C13-C15
22	c	505	CLA	C6-C7-C8-C10
22	c	512	CLA	C6-C7-C8-C10
22	c	512	CLA	C12-C13-C15-C16
33	d	410	LHG	C7-C8-C9-C10
35	f	101	HEM	C2A-CAA-CBA-CGA
32	B	624	STE	C7-C8-C9-C10
24	k	101	BCR	C19-C20-C21-C22
28	F	101	SQD	C45-C44-O6-C1
29	C	516	DGD	O1G-C1A-C2A-C3A
27	b	622	LMG	C39-C40-C41-C42
27	c	522	LMG	C29-C30-C31-C32
29	C	518	DGD	C6A-C7A-C8A-C9A
22	a	402	CLA	C16-C17-C18-C19
27	b	622	LMG	C34-C35-C36-C37
32	E	103	STE	C5-C6-C7-C8
32	b	623	STE	C11-C10-C9-C8
33	l	101	LHG	C27-C28-C29-C30
28	L	101	SQD	O47-C45-C46-O48
27	B	621	LMG	C29-C30-C31-C32
32	b	623	STE	C7-C8-C9-C10
28	B	623	SQD	C27-C28-C29-C30
33	d	409	LHG	C31-C32-C33-C34
32	B	625	STE	C6-C7-C8-C9
29	c	518	DGD	C2G-C3G-O3G-C1D
22	B	601	CLA	C16-C17-C18-C20
27	C	519	LMG	C37-C38-C39-C40
29	h	102	DGD	CBA-CCA-CDA-CEA
22	B	609	CLA	C4-C3-C5-C6
27	c	523	LMG	C40-C41-C42-C43
22	B	605	CLA	C10-C11-C12-C13
22	B	613	CLA	C6-C7-C8-C9
22	C	502	CLA	C6-C7-C8-C9
22	a	403	CLA	C6-C7-C8-C9
22	a	404	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	b	605	CLA	C11-C12-C13-C14
22	b	605	CLA	C14-C13-C15-C16
22	b	607	CLA	C11-C12-C13-C14
22	c	507	CLA	C11-C10-C8-C9
22	d	405	CLA	C11-C12-C13-C14
24	K	101	BCR	C6-C7-C8-C9
22	b	604	CLA	C16-C17-C18-C20
22	b	611	CLA	C16-C17-C18-C20
22	b	612	CLA	C16-C17-C18-C19
22	d	404	CLA	C16-C17-C18-C20
29	c	517	DGD	C6A-C7A-C8A-C9A
28	a	410	SQD	C12-C13-C14-C15
29	A	414	DGD	O1A-C1A-O1G-C1G
27	d	412	LMG	C11-C12-C13-C14
32	H	103	STE	C7-C8-C9-C10
33	L	102	LHG	C14-C15-C16-C17
22	C	506	CLA	C16-C17-C18-C20
27	A	411	LMG	C13-C14-C15-C16
32	l	102	STE	C12-C13-C14-C15
33	l	101	LHG	C18-C19-C20-C21
24	c	514	BCR	C17-C18-C19-C20
27	D	410	LMG	C31-C32-C33-C34
32	T	103	STE	C10-C11-C12-C13
33	l	101	LHG	C26-C27-C28-C29
29	H	102	DGD	C9B-CAB-CBB-CCB
27	d	412	LMG	C10-C11-C12-C13
29	H	102	DGD	C3A-C4A-C5A-C6A
33	d	408	LHG	C25-C26-C27-C28
27	A	411	LMG	C9-C8-O7-C10
27	b	622	LMG	C9-C8-O7-C10
28	B	623	SQD	C46-C45-O47-C7
22	B	603	CLA	C2A-CAA-CBA-CGA
22	c	501	CLA	C2A-CAA-CBA-CGA
22	A	402	CLA	C13-C15-C16-C17
22	A	402	CLA	C2-C1-O2A-CGA
22	C	506	CLA	C2-C1-O2A-CGA
22	a	402	CLA	C2-C1-O2A-CGA
22	c	513	CLA	C2-C1-O2A-CGA
22	b	608	CLA	C2C-C3C-CAC-CBC
27	D	407	LMG	C34-C35-C36-C37
32	m	101	STE	C6-C7-C8-C9
32	b	625	STE	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
27	D	410	LMG	C32-C33-C34-C35
32	C	522	STE	C3-C4-C5-C6
33	B	622	LHG	C19-C20-C21-C22
32	l	102	STE	C15-C16-C17-C18
24	A	406	BCR	C1-C6-C7-C8
24	C	514	BCR	C23-C24-C25-C26
24	C	515	BCR	C23-C24-C25-C26
24	C	515	BCR	C23-C24-C25-C30
24	Y	101	BCR	C23-C24-C25-C30
24	b	618	BCR	C23-C24-C25-C30
24	c	514	BCR	C1-C6-C7-C8
24	c	516	BCR	C23-C24-C25-C30
22	C	506	CLA	C2-C3-C5-C6
26	D	406	PL9	C38-C39-C41-C42
22	c	503	CLA	O1A-CGA-O2A-C1
27	b	620	LMG	C12-C13-C14-C15
27	c	523	LMG	C11-C12-C13-C14
28	a	411	SQD	C30-C31-C32-C33
32	D	411	STE	C2-C3-C4-C5
33	d	410	LHG	C25-C26-C27-C28
29	C	518	DGD	C2A-C1A-O1G-C1G
22	A	402	CLA	C4C-C3C-CAC-CBC
32	d	413	STE	C5-C6-C7-C8
22	b	614	CLA	C16-C17-C18-C20
24	B	619	BCR	C11-C10-C9-C8
33	E	102	LHG	O7-C5-C6-O8
33	l	101	LHG	C11-C10-C9-C8
33	d	409	LHG	C4-O6-P-O3
33	d	408	LHG	C33-C34-C35-C36
22	B	615	CLA	C16-C17-C18-C19
23	d	402	PHO	CHA-CBD-CGD-O2D
29	h	102	DGD	C7B-C8B-C9B-CAB
29	C	516	DGD	CDA-CEA-CFA-CGA
32	c	521	STE	C7-C8-C9-C10
29	h	102	DGD	C5A-C6A-C7A-C8A
22	a	403	CLA	O1D-CGD-O2D-CED
22	c	512	CLA	C11-C10-C8-C7
29	c	518	DGD	C5A-C6A-C7A-C8A
32	b	623	STE	C9-C10-C11-C12
29	c	518	DGD	C8B-C9B-CAB-CBB
22	A	403	CLA	C11-C10-C8-C9
22	B	602	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	C	505	CLA	C6-C7-C8-C9
22	C	513	CLA	C14-C13-C15-C16
22	b	602	CLA	C11-C12-C13-C14
22	b	603	CLA	C11-C12-C13-C14
22	c	505	CLA	C6-C7-C8-C9
22	c	510	CLA	C6-C7-C8-C9
32	T	103	STE	C12-C13-C14-C15
22	C	511	CLA	CBA-CGA-O2A-C1
27	D	410	LMG	C29-C30-C31-C32
32	b	625	STE	C5-C6-C7-C8
24	B	618	BCR	C37-C22-C23-C24
24	c	515	BCR	C7-C8-C9-C34
29	c	518	DGD	C3B-C4B-C5B-C6B
33	D	409	LHG	O1-C1-C2-C3
29	C	518	DGD	CBA-CCA-CDA-CEA
28	B	623	SQD	C28-C29-C30-C31
26	a	409	PL9	C13-C14-C16-C17
22	A	403	CLA	C16-C17-C18-C20
22	C	508	CLA	C16-C17-C18-C19
29	C	516	DGD	C2A-C3A-C4A-C5A
35	f	101	HEM	CAD-CBD-CGD-O1D
22	C	505	CLA	C15-C16-C17-C18
22	B	614	CLA	C2A-CAA-CBA-CGA
32	b	624	STE	O1-C1-C2-C3
24	a	405	BCR	C19-C20-C21-C22
22	C	511	CLA	O1A-CGA-O2A-C1
29	H	102	DGD	C2B-C3B-C4B-C5B
32	M	103	STE	C4-C5-C6-C7
33	E	102	LHG	C19-C20-C21-C22
22	A	402	CLA	C2C-C3C-CAC-CBC
27	A	411	LMG	C28-C29-C30-C31
27	b	620	LMG	C33-C34-C35-C36
32	m	101	STE	C4-C5-C6-C7
22	B	616	CLA	C4-C3-C5-C6
22	d	405	CLA	C4-C3-C5-C6
22	c	511	CLA	C8-C10-C11-C12
22	B	609	CLA	C2-C3-C5-C6
22	c	512	CLA	C5-C6-C7-C8
29	h	102	DGD	O2G-C1B-C2B-C3B
22	B	613	CLA	C2-C1-O2A-CGA
22	b	608	CLA	C2-C1-O2A-CGA
22	d	403	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
27	d	412	LMG	C15-C16-C17-C18
32	C	521	STE	C14-C15-C16-C17
22	D	404	CLA	C16-C17-C18-C20
22	c	505	CLA	C16-C17-C18-C19
32	c	521	STE	C3-C4-C5-C6
33	E	102	LHG	C30-C31-C32-C33
22	b	614	CLA	C10-C11-C12-C13
22	b	601	CLA	C2A-CAA-CBA-CGA
27	B	621	LMG	C28-C29-C30-C31
27	b	622	LMG	C29-C30-C31-C32
22	b	609	CLA	C16-C17-C18-C19
32	C	521	STE	C9-C10-C11-C12
32	b	621	STE	O1-C1-C2-C3
32	d	413	STE	O2-C1-C2-C3
36	V	201	HEC	CAD-CBD-CGD-O2D
32	D	411	STE	C11-C12-C13-C14
26	a	409	PL9	C4-C3-C7-C8
33	D	408	LHG	C16-C17-C18-C19
22	C	501	CLA	C14-C13-C15-C16
22	C	509	CLA	C14-C13-C15-C16
24	C	515	BCR	C11-C10-C9-C34
27	D	410	LMG	C7-C8-C9-O8
27	b	622	LMG	O1-C7-C8-C9
29	C	516	DGD	O1G-C1G-C2G-C3G
32	d	413	STE	O1-C1-C2-C3
36	v	201	HEC	CAD-CBD-CGD-O1D
26	d	407	PL9	C32-C33-C34-C36
22	C	512	CLA	O2A-C1-C2-C3
27	b	622	LMG	C29-C28-O8-C9
29	C	516	DGD	O6E-C1E-O5D-C6D
29	C	517	DGD	O6D-C1D-O3G-C3G
22	C	503	CLA	C15-C16-C17-C18
24	h	101	BCR	C7-C8-C9-C34
27	d	411	LMG	O7-C10-C11-C12
35	f	101	HEM	CAD-CBD-CGD-O2D
32	c	521	STE	O1-C1-C2-C3
27	c	523	LMG	C7-C8-O7-C10
22	B	602	CLA	C1A-C2A-CAA-CBA
22	C	512	CLA	C1A-C2A-CAA-CBA
22	c	508	CLA	C1A-C2A-CAA-CBA
22	c	511	CLA	C1A-C2A-CAA-CBA
22	A	410	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	B	613	CLA	C11-C12-C13-C15
22	C	510	CLA	C6-C7-C8-C10
22	a	403	CLA	C6-C7-C8-C10
22	b	605	CLA	C11-C12-C13-C15
22	c	502	CLA	C6-C7-C8-C10
29	c	518	DGD	CDA-CEA-CFA-CGA
32	b	624	STE	O2-C1-C2-C3
35	E	101	HEM	CAD-CBD-CGD-O1D
27	B	621	LMG	C37-C38-C39-C40
33	L	102	LHG	C3-O3-P-O6
22	C	502	CLA	C16-C17-C18-C20
22	b	611	CLA	C16-C17-C18-C19
22	d	403	CLA	C5-C6-C7-C8
32	D	411	STE	C13-C14-C15-C16
33	D	409	LHG	C17-C18-C19-C20
32	E	103	STE	C6-C7-C8-C9
33	B	622	LHG	C29-C30-C31-C32
33	D	408	LHG	C11-C10-C9-C8
29	C	517	DGD	C8A-C9A-CAA-CBA
32	b	621	STE	O2-C1-C2-C3
26	A	409	PL9	C15-C14-C16-C17
22	b	604	CLA	C8-C10-C11-C12
33	d	408	LHG	C31-C32-C33-C34
28	A	412	SQD	C34-C35-C36-C37
22	d	404	CLA	O1D-CGD-O2D-CED
33	B	622	LHG	O7-C5-C6-O8
32	b	624	STE	C1-C2-C3-C4
27	B	621	LMG	O9-C10-C11-C12
24	b	617	BCR	C6-C7-C8-C9
28	A	413	SQD	C16-C17-C18-C19
29	A	414	DGD	O6D-C5D-C6D-O5D
22	d	403	CLA	C16-C17-C18-C19
29	C	518	DGD	C9A-CAA-CBA-CCA
32	a	414	STE	C7-C8-C9-C10
32	c	521	STE	O2-C1-C2-C3
32	c	521	STE	C4-C5-C6-C7
22	b	616	CLA	C2-C1-O2A-CGA
22	c	502	CLA	C2-C1-O2A-CGA
26	A	409	PL9	C13-C14-C16-C17
29	H	102	DGD	O1A-C1A-O1G-C1G
32	B	625	STE	O2-C1-C2-C3
36	V	201	HEC	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	c	506	CLA	C11-C12-C13-C14
36	v	201	HEC	CAD-CBD-CGD-O2D
23	d	402	PHO	C1A-C2A-CAA-CBA
22	b	608	CLA	C4C-C3C-CAC-CBC
29	C	516	DGD	C8A-C9A-CAA-CBA
33	D	409	LHG	C12-C13-C14-C15
22	b	610	CLA	C10-C11-C12-C13
22	C	501	CLA	C2A-CAA-CBA-CGA
24	A	406	BCR	C23-C24-C25-C30
24	B	617	BCR	C1-C6-C7-C8
24	B	617	BCR	C5-C6-C7-C8
24	c	514	BCR	C23-C24-C25-C26
24	c	514	BCR	C23-C24-C25-C30
24	k	101	BCR	C23-C24-C25-C30
27	d	411	LMG	O9-C10-C11-C12
32	B	627	STE	C2-C3-C4-C5
24	B	618	BCR	C19-C20-C21-C22
32	C	522	STE	C7-C8-C9-C10
22	B	605	CLA	C4-C3-C5-C6
22	c	507	CLA	C4-C3-C5-C6
22	B	601	CLA	C16-C17-C18-C19
22	b	614	CLA	C16-C17-C18-C19
22	d	403	CLA	C16-C17-C18-C20
22	b	607	CLA	C5-C6-C7-C8
22	B	602	CLA	C15-C16-C17-C18
22	B	612	CLA	C13-C15-C16-C17
22	C	510	CLA	C8-C10-C11-C12
29	C	516	DGD	C5D-C6D-O5D-C1E
27	b	620	LMG	C18-C19-C20-C21
27	b	622	LMG	C14-C15-C16-C17
22	B	611	CLA	C16-C17-C18-C20
22	d	404	CLA	C2C-C3C-CAC-CBC
29	c	519	DGD	C1B-C2B-C3B-C4B
22	C	512	CLA	C2A-CAA-CBA-CGA
33	D	408	LHG	C35-C36-C37-C38
22	d	405	CLA	C8-C10-C11-C12
22	d	405	CLA	C16-C17-C18-C19
22	c	506	CLA	C4-C3-C5-C6
22	C	505	CLA	O1D-CGD-O2D-CED
26	A	409	PL9	C9-C11-C12-C13
26	A	409	PL9	C44-C46-C47-C48
32	B	626	STE	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	C	502	CLA	C6-C7-C8-C10
22	c	501	CLA	C11-C12-C13-C15
32	B	625	STE	O1-C1-C2-C3
29	H	102	DGD	C7B-C8B-C9B-CAB
24	c	514	BCR	C15-C16-C17-C18
28	B	623	SQD	C19-C20-C21-C22
27	b	622	LMG	O1-C7-C8-O7
28	L	101	SQD	O6-C44-C45-O47
29	c	517	DGD	O1G-C1G-C2G-O2G
32	b	621	STE	C4-C5-C6-C7
27	B	621	LMG	O7-C10-C11-C12
22	b	613	CLA	CAA-CBA-CGA-O2A
33	B	622	LHG	C24-C23-O8-C6
22	B	607	CLA	C15-C16-C17-C18
23	d	402	PHO	C4C-C3C-CAC-CBC
24	a	405	BCR	C11-C10-C9-C34
32	d	413	STE	C11-C10-C9-C8
28	F	101	SQD	C23-C24-C25-C26
33	l	101	LHG	O7-C7-C8-C9
22	C	507	CLA	C4-C3-C5-C6
22	d	403	CLA	C4-C3-C5-C6
26	a	409	PL9	C23-C24-C26-C27
22	B	610	CLA	C16-C17-C18-C20
22	A	410	CLA	C6-C7-C8-C9
22	B	601	CLA	C6-C7-C8-C9
22	B	603	CLA	C14-C13-C15-C16
22	B	610	CLA	C14-C13-C15-C16
22	C	506	CLA	C14-C13-C15-C16
22	C	510	CLA	C6-C7-C8-C9
22	D	403	CLA	C11-C10-C8-C9
22	a	404	CLA	C6-C7-C8-C9
22	b	606	CLA	C11-C12-C13-C14
22	b	607	CLA	C14-C13-C15-C16
22	c	501	CLA	C11-C12-C13-C14
27	D	410	LMG	C11-C12-C13-C14
22	C	512	CLA	C3A-C2A-CAA-CBA
27	b	620	LMG	C32-C33-C34-C35
27	b	620	LMG	O8-C28-C29-C30
32	B	624	STE	O2-C1-C2-C3
35	E	101	HEM	CAD-CBD-CGD-O2D
22	B	605	CLA	CAD-CBD-CGD-O2D
22	B	610	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	B	616	CLA	CAD-CBD-CGD-O2D
22	C	505	CLA	CAD-CBD-CGD-O2D
22	b	601	CLA	CAD-CBD-CGD-O2D
22	b	604	CLA	CAD-CBD-CGD-O2D
22	b	609	CLA	CAD-CBD-CGD-O2D
22	b	610	CLA	CAD-CBD-CGD-O2D
22	b	612	CLA	CAD-CBD-CGD-O2D
22	b	614	CLA	CAD-CBD-CGD-O2D
22	c	503	CLA	CAD-CBD-CGD-O2D
22	c	505	CLA	CAD-CBD-CGD-O2D
22	c	509	CLA	CAD-CBD-CGD-O2D
22	c	512	CLA	CAD-CBD-CGD-O2D
27	M	101	LMG	C9-C8-O7-C10
22	C	506	CLA	C16-C17-C18-C19
33	E	102	LHG	C35-C36-C37-C38
24	C	515	BCR	C15-C16-C17-C18
24	c	516	BCR	C13-C14-C15-C16
28	a	410	SQD	C14-C15-C16-C17
27	M	101	LMG	C36-C37-C38-C39
22	c	508	CLA	O1D-CGD-O2D-CED
33	E	102	LHG	C16-C17-C18-C19
22	C	502	CLA	C4-C3-C5-C6
22	c	510	CLA	C4-C3-C5-C6
32	B	624	STE	O1-C1-C2-C3
32	D	411	STE	O2-C1-C2-C3
33	D	408	LHG	C33-C34-C35-C36
22	B	612	CLA	CAA-CBA-CGA-O2A
22	b	612	CLA	CAA-CBA-CGA-O2A
22	a	403	CLA	C13-C15-C16-C17
23	d	402	PHO	C2C-C3C-CAC-CBC
28	L	101	SQD	C44-C45-C46-O48
29	c	517	DGD	C1G-C2G-C3G-O3G
22	b	601	CLA	CAA-CBA-CGA-O2A
27	D	407	LMG	C13-C14-C15-C16
32	C	520	STE	C1-C2-C3-C4
28	A	413	SQD	C17-C18-C19-C20
22	B	601	CLA	O2A-C1-C2-C3
22	B	616	CLA	O2A-C1-C2-C3
22	C	509	CLA	O2A-C1-C2-C3
22	D	404	CLA	O2A-C1-C2-C3
22	b	613	CLA	O2A-C1-C2-C3
22	d	403	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
23	d	401	PHO	O2A-C1-C2-C3
27	d	412	LMG	C32-C33-C34-C35
32	B	626	STE	C11-C10-C9-C8
35	f	101	HEM	C4B-C3B-CAB-CBB
22	b	602	CLA	C2A-CAA-CBA-CGA
33	L	102	LHG	C9-C10-C11-C12
28	a	410	SQD	O47-C7-C8-C9
33	L	102	LHG	O7-C7-C8-C9
22	B	606	CLA	CHA-CBD-CGD-O1D
22	B	606	CLA	CHA-CBD-CGD-O2D
22	B	607	CLA	CHA-CBD-CGD-O1D
22	B	607	CLA	CHA-CBD-CGD-O2D
22	B	612	CLA	CHA-CBD-CGD-O1D
22	B	614	CLA	CHA-CBD-CGD-O1D
22	B	614	CLA	CHA-CBD-CGD-O2D
22	C	507	CLA	CHA-CBD-CGD-O2D
22	C	509	CLA	CHA-CBD-CGD-O2D
22	b	606	CLA	CHA-CBD-CGD-O2D
22	b	611	CLA	CHA-CBD-CGD-O1D
22	b	611	CLA	CHA-CBD-CGD-O2D
22	b	616	CLA	CHA-CBD-CGD-O2D
22	c	502	CLA	CHA-CBD-CGD-O1D
22	c	507	CLA	CHA-CBD-CGD-O1D
22	c	507	CLA	CHA-CBD-CGD-O2D
22	d	404	CLA	CHA-CBD-CGD-O2D
29	C	517	DGD	C3B-C4B-C5B-C6B
24	c	516	BCR	C11-C10-C9-C8
28	A	412	SQD	O47-C7-C8-C9
29	A	414	DGD	O2G-C1B-C2B-C3B
27	M	101	LMG	C40-C41-C42-C43
22	C	508	CLA	C8-C10-C11-C12
22	B	613	CLA	C16-C17-C18-C19
22	C	507	CLA	C5-C6-C7-C8
32	c	524	STE	C3-C4-C5-C6
22	B	613	CLA	CAA-CBA-CGA-O2A
29	c	517	DGD	O1G-C1A-C2A-C3A
27	B	621	LMG	O10-C28-C29-C30
22	B	601	CLA	C6-C7-C8-C10
22	B	601	CLA	C11-C12-C13-C15
22	B	612	CLA	C11-C10-C8-C7
22	B	615	CLA	C12-C13-C15-C16
22	b	608	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	c	507	CLA	C2-C3-C5-C6
22	c	510	CLA	C2-C3-C5-C6
22	A	403	CLA	C16-C17-C18-C19
29	c	518	DGD	CAB-CBB-CCB-CDB
29	c	517	DGD	C2A-C3A-C4A-C5A
22	B	611	CLA	C6-C7-C8-C9
22	B	612	CLA	C11-C10-C8-C9
22	B	615	CLA	C14-C13-C15-C16
22	a	403	CLA	C11-C10-C8-C9
22	c	512	CLA	C11-C10-C8-C9
22	c	512	CLA	C14-C13-C15-C16
29	a	412	DGD	C7A-C8A-C9A-CAA
32	C	522	STE	C4-C5-C6-C7
27	D	407	LMG	C37-C38-C39-C40
27	D	407	LMG	O10-C28-O8-C9
33	e	101	LHG	C12-C13-C14-C15
22	c	510	CLA	CAA-CBA-CGA-O2A
32	l	102	STE	C9-C10-C11-C12
22	d	403	CLA	C2C-C3C-CAC-CBC
28	a	411	SQD	C29-C30-C31-C32
27	b	622	LMG	C32-C33-C34-C35
33	l	101	LHG	O1-C1-C2-C3
27	c	520	LMG	C36-C37-C38-C39
28	L	101	SQD	C25-C26-C27-C28
33	e	101	LHG	O10-C23-C24-C25
32	B	624	STE	C3-C4-C5-C6
22	b	612	CLA	C1A-C2A-CAA-CBA
22	B	612	CLA	CAA-CBA-CGA-O1A
22	b	602	CLA	O1D-CGD-O2D-CED
29	c	519	DGD	C4B-C5B-C6B-C7B
33	d	408	LHG	C35-C36-C37-C38
27	M	101	LMG	O6-C5-C6-O5
28	A	412	SQD	C23-C24-C25-C26
22	b	613	CLA	CAA-CBA-CGA-O1A
29	c	518	DGD	O1A-C1A-C2A-C3A
29	C	516	DGD	C1G-C2G-C3G-O3G
28	a	410	SQD	C35-C36-C37-C38
29	h	102	DGD	CCA-CDA-CEA-CFA
33	D	408	LHG	C13-C14-C15-C16
22	C	505	CLA	C16-C17-C18-C19
22	c	502	CLA	C16-C17-C18-C19
29	A	414	DGD	O1B-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
22	b	612	CLA	C8-C10-C11-C12
32	B	627	STE	C4-C5-C6-C7
22	d	405	CLA	C2-C3-C5-C6
33	D	408	LHG	O10-C23-O8-C6
32	D	411	STE	O1-C1-C2-C3
22	b	615	CLA	C8-C10-C11-C12
33	D	408	LHG	C4-O6-P-O5
33	l	101	LHG	C3-O3-P-O5
29	c	517	DGD	O1B-C1B-C2B-C3B
29	h	102	DGD	O1B-C1B-C2B-C3B
33	l	101	LHG	O9-C7-C8-C9
32	I	101	STE	C6-C7-C8-C9
27	B	621	LMG	O8-C28-C29-C30
24	A	406	BCR	C23-C24-C25-C26
24	Y	101	BCR	C23-C24-C25-C26
24	t	101	BCR	C5-C6-C7-C8
27	C	519	LMG	C36-C37-C38-C39
28	A	413	SQD	O10-C23-C24-C25
29	C	516	DGD	O1B-C1B-C2B-C3B
28	L	101	SQD	C14-C15-C16-C17
29	c	519	DGD	C2B-C3B-C4B-C5B
23	A	404	PHO	C16-C17-C18-C20
27	b	622	LMG	O10-C28-C29-C30
22	b	611	CLA	C10-C11-C12-C13
22	c	503	CLA	C10-C11-C12-C13
22	d	404	CLA	C4C-C3C-CAC-CBC
29	C	516	DGD	CAA-CBA-CCA-CDA
22	b	602	CLA	C8-C10-C11-C12
22	a	404	CLA	C4-C3-C5-C6
22	C	502	CLA	C2-C3-C5-C6
22	A	410	CLA	C4C-C3C-CAC-CBC
32	I	101	STE	C5-C6-C7-C8
22	B	607	CLA	CAD-CBD-CGD-O1D
22	B	609	CLA	CAD-CBD-CGD-O1D
22	B	612	CLA	CAD-CBD-CGD-O1D
22	C	506	CLA	CAD-CBD-CGD-O1D
22	c	502	CLA	CAD-CBD-CGD-O1D
22	c	506	CLA	CAD-CBD-CGD-O1D
22	c	510	CLA	CAD-CBD-CGD-O1D
22	d	404	CLA	CAD-CBD-CGD-O1D
28	B	623	SQD	O5-C5-C6-S
33	B	622	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
22	b	601	CLA	CAA-CBA-CGA-O1A
22	b	612	CLA	CAA-CBA-CGA-O1A
28	a	411	SQD	O10-C23-C24-C25
33	d	408	LHG	O8-C23-C24-C25
22	c	512	CLA	C15-C16-C17-C18
22	B	606	CLA	C14-C13-C15-C16
22	B	611	CLA	C14-C13-C15-C16
22	C	504	CLA	C11-C10-C8-C9
28	A	413	SQD	O48-C23-C24-C25
29	H	102	DGD	C5B-C6B-C7B-C8B
33	B	622	LHG	C35-C36-C37-C38
22	c	501	CLA	CAA-CBA-CGA-O2A
28	B	623	SQD	O48-C23-C24-C25
33	e	101	LHG	O8-C23-C24-C25
23	d	402	PHO	C5-C6-C7-C8
22	B	602	CLA	C3A-C2A-CAA-CBA
22	B	606	CLA	C12-C13-C15-C16
22	B	611	CLA	C11-C12-C13-C15
22	B	616	CLA	C2-C3-C5-C6
22	C	504	CLA	C11-C10-C8-C7
22	a	403	CLA	C11-C10-C8-C7
22	b	611	CLA	C12-C13-C15-C16
22	b	614	CLA	C11-C12-C13-C15
22	c	506	CLA	C11-C12-C13-C15
22	d	403	CLA	C11-C12-C13-C15
29	C	516	DGD	O2G-C1B-C2B-C3B
24	D	405	BCR	C7-C8-C9-C10
24	T	101	BCR	C21-C22-C23-C24
24	c	515	BCR	C21-C22-C23-C24
24	t	101	BCR	C11-C12-C13-C14
33	d	410	LHG	O10-C23-C24-C25
32	C	522	STE	O2-C1-C2-C3
32	a	414	STE	O2-C1-C2-C3
29	C	517	DGD	C9B-CAB-CBB-CCB
29	C	517	DGD	C2B-C3B-C4B-C5B
22	B	610	CLA	C10-C11-C12-C13
22	B	613	CLA	CAA-CBA-CGA-O1A
22	c	501	CLA	CAA-CBA-CGA-O1A
22	b	607	CLA	CBA-CGA-O2A-C1
26	D	406	PL9	C44-C46-C47-C48
22	B	603	CLA	C13-C15-C16-C17
28	B	623	SQD	O47-C7-C8-C9

*Continued on next page...*

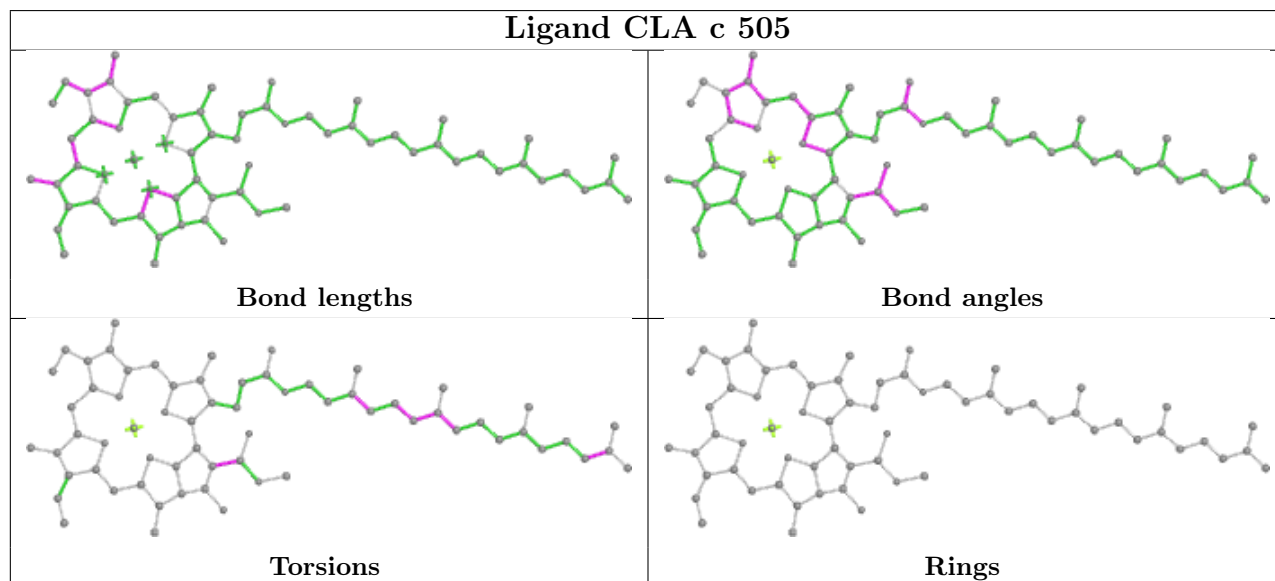
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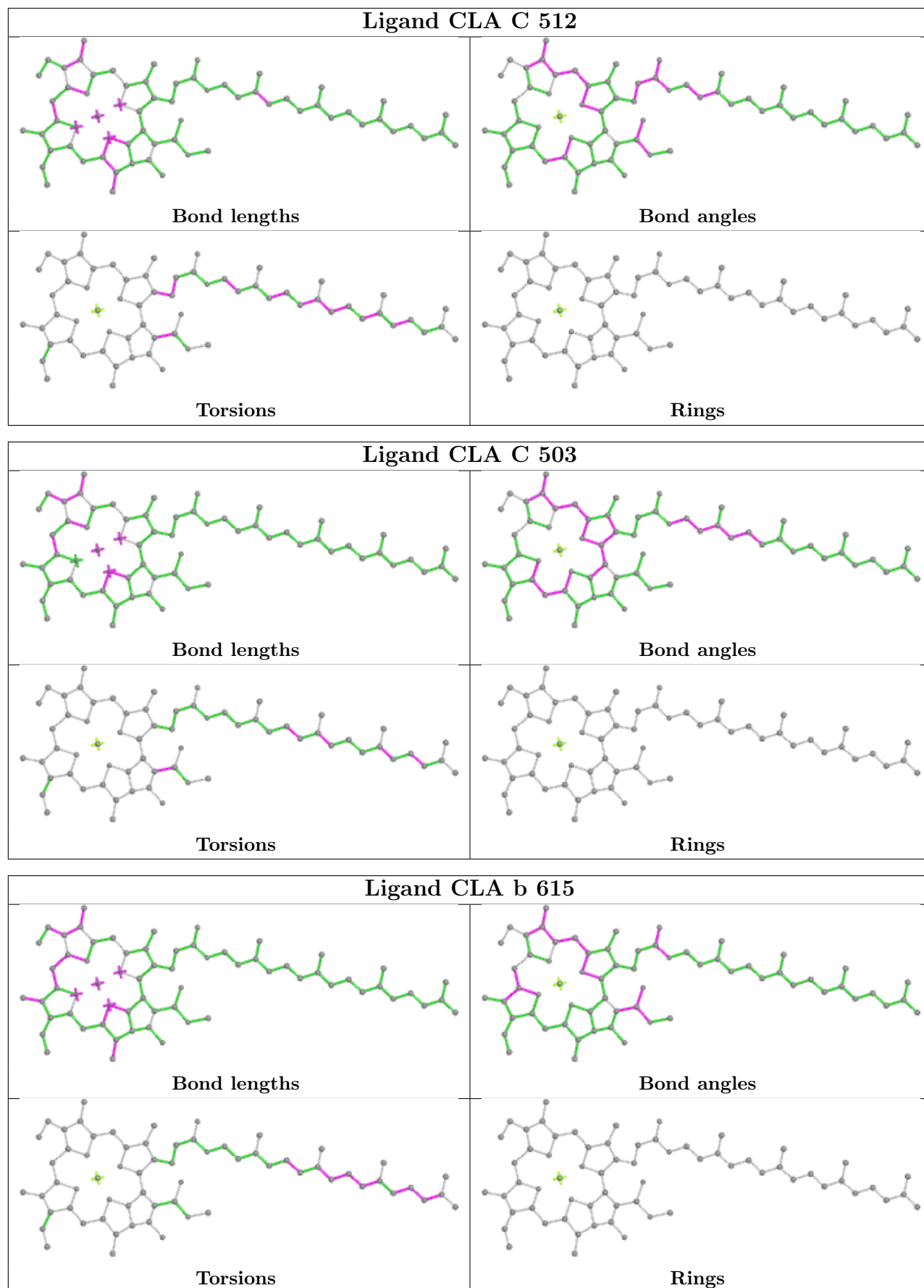
Mol	Chain	Res	Type	Atoms
22	a	404	CLA	C15-C16-C17-C18
33	d	408	LHG	C26-C27-C28-C29
22	c	510	CLA	CAA-CBA-CGA-O1A
29	c	518	DGD	O1B-C1B-C2B-C3B
33	d	408	LHG	C10-C11-C12-C13

There are no ring outliers.

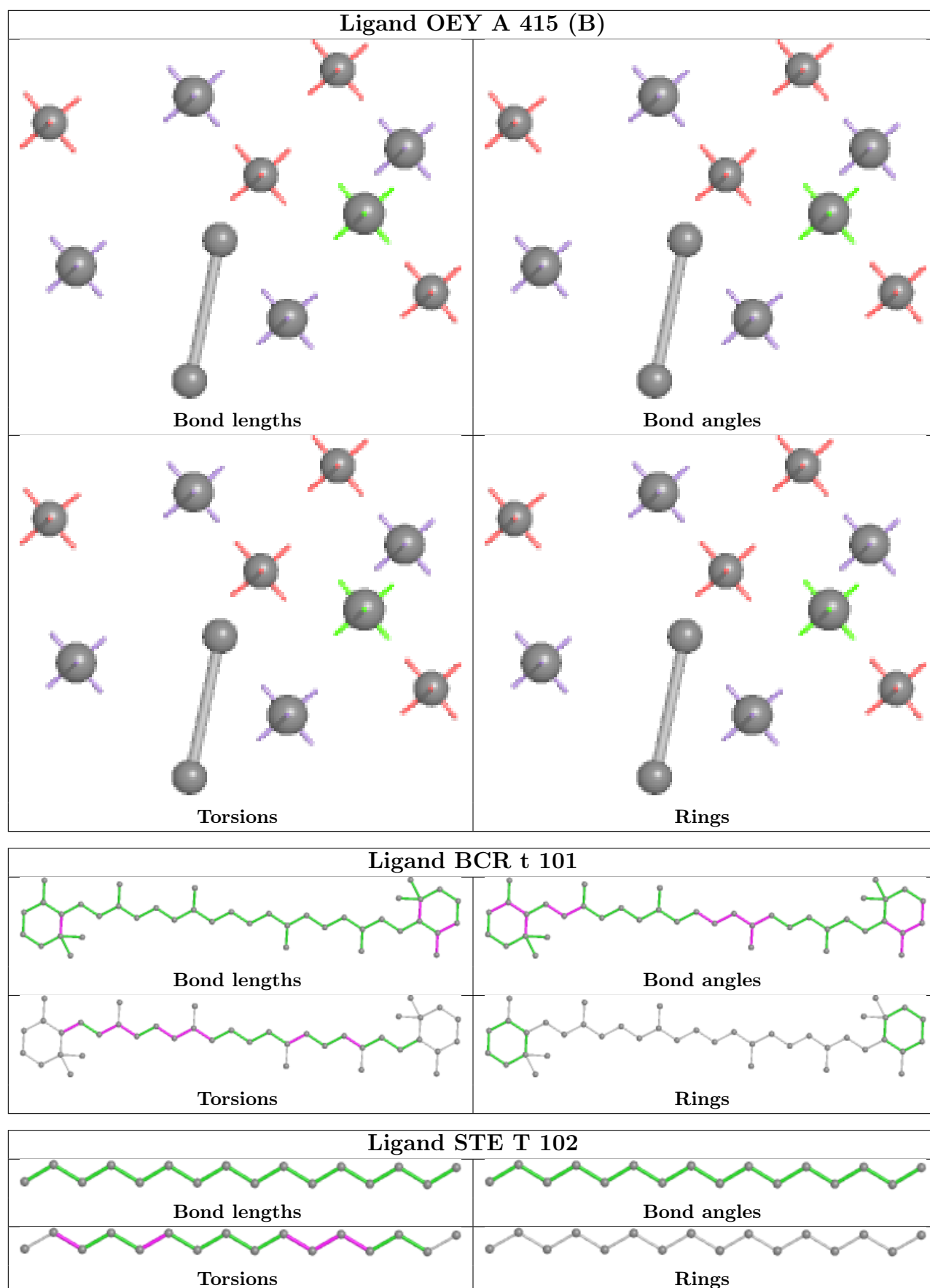
No monomer is involved in short contacts.

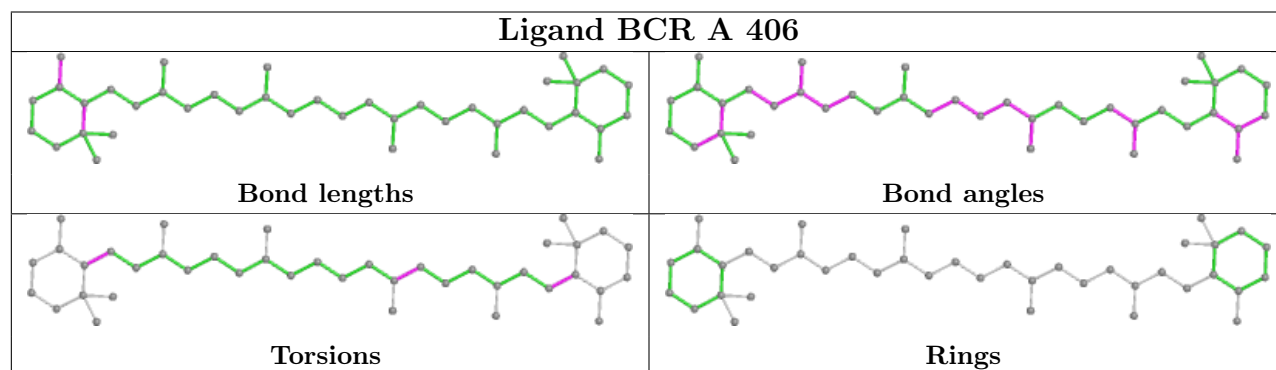
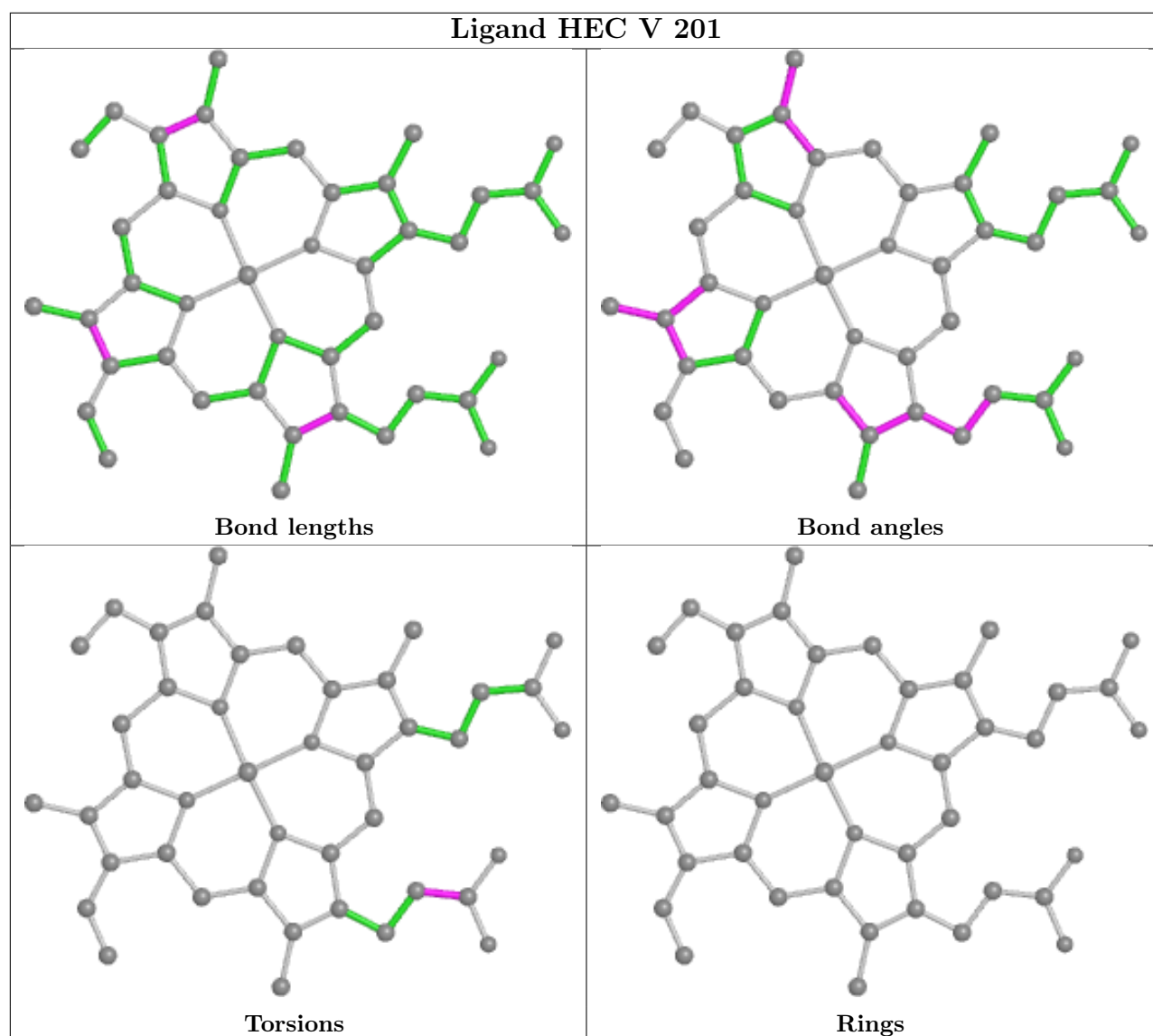
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

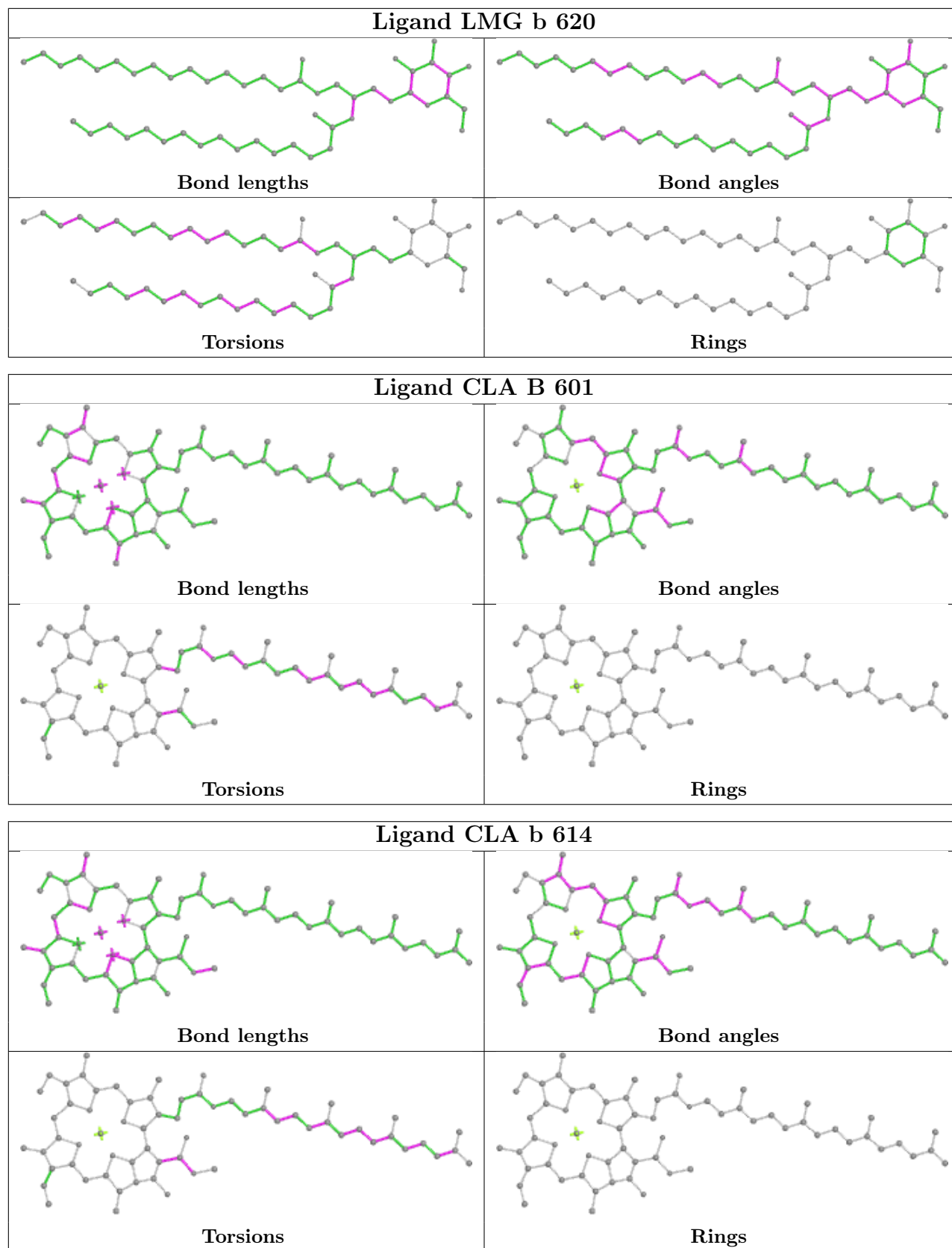


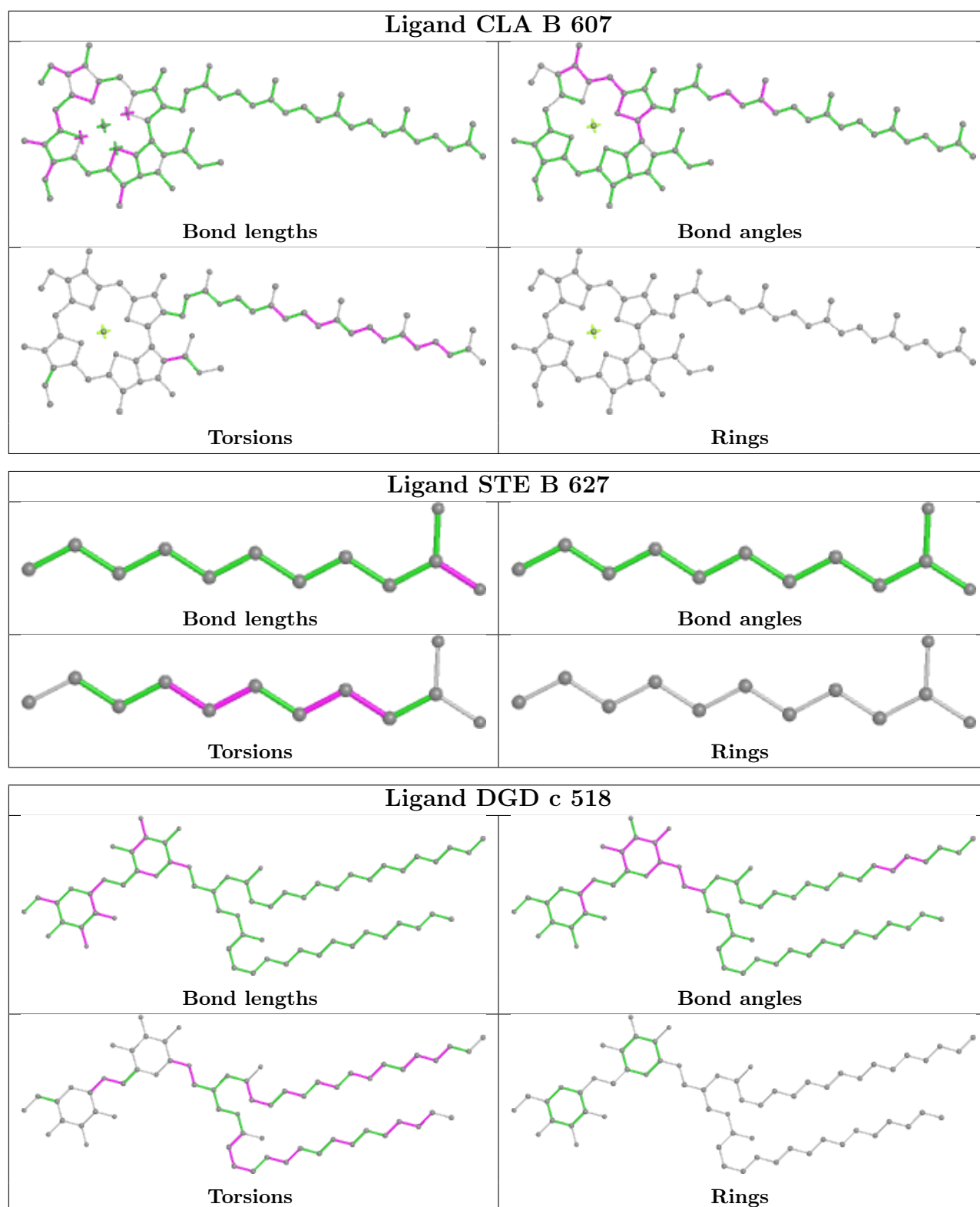


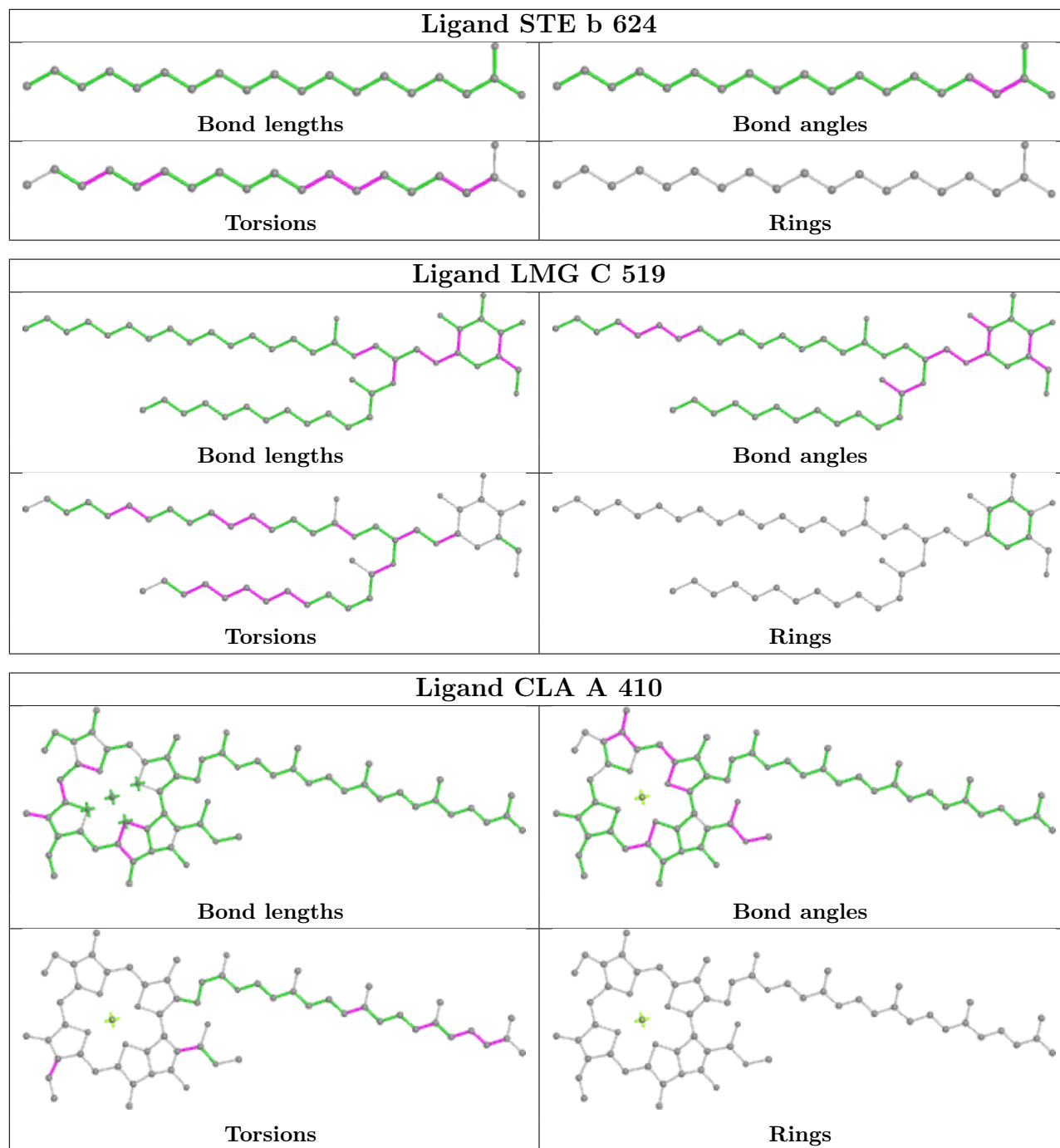


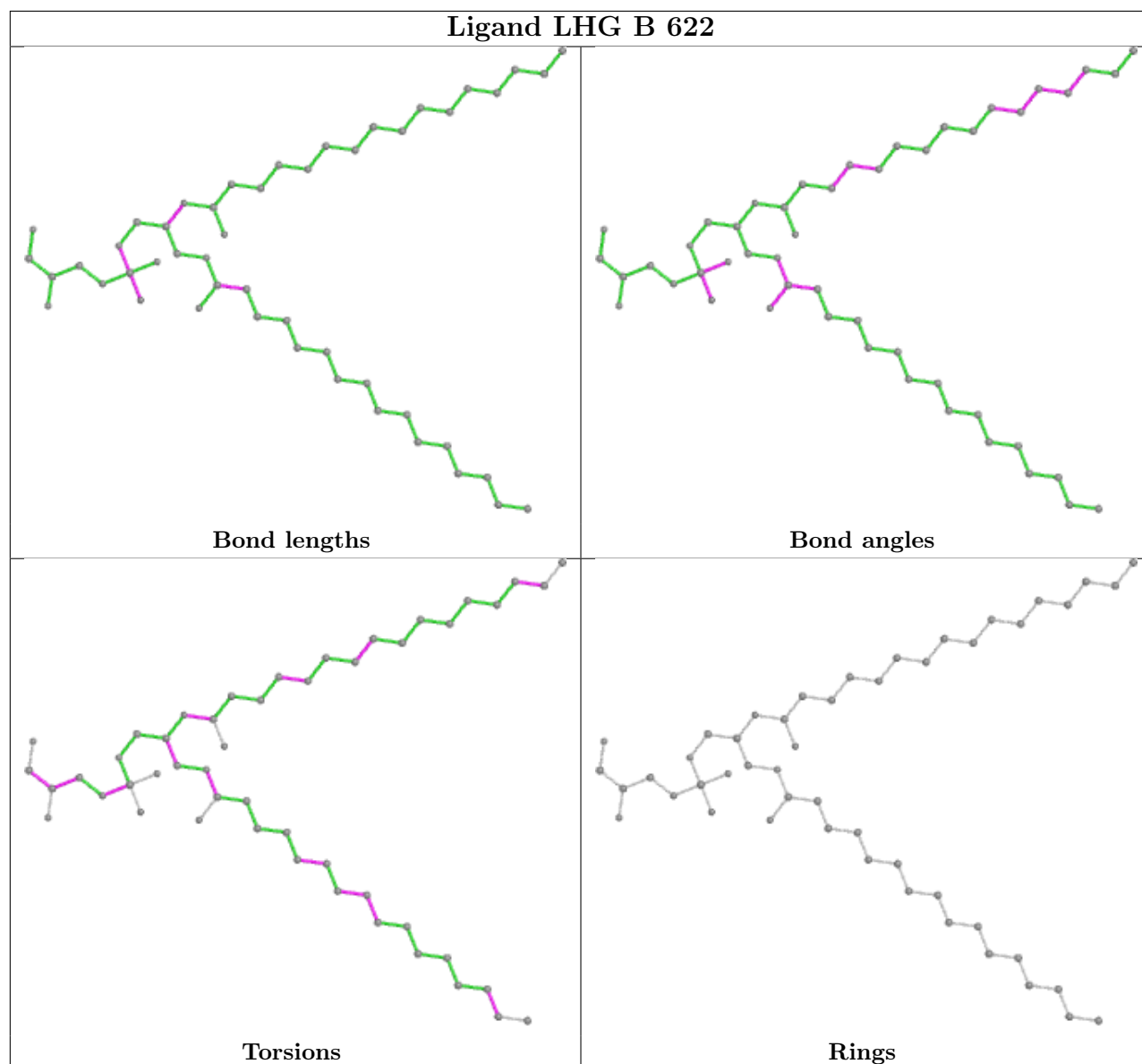
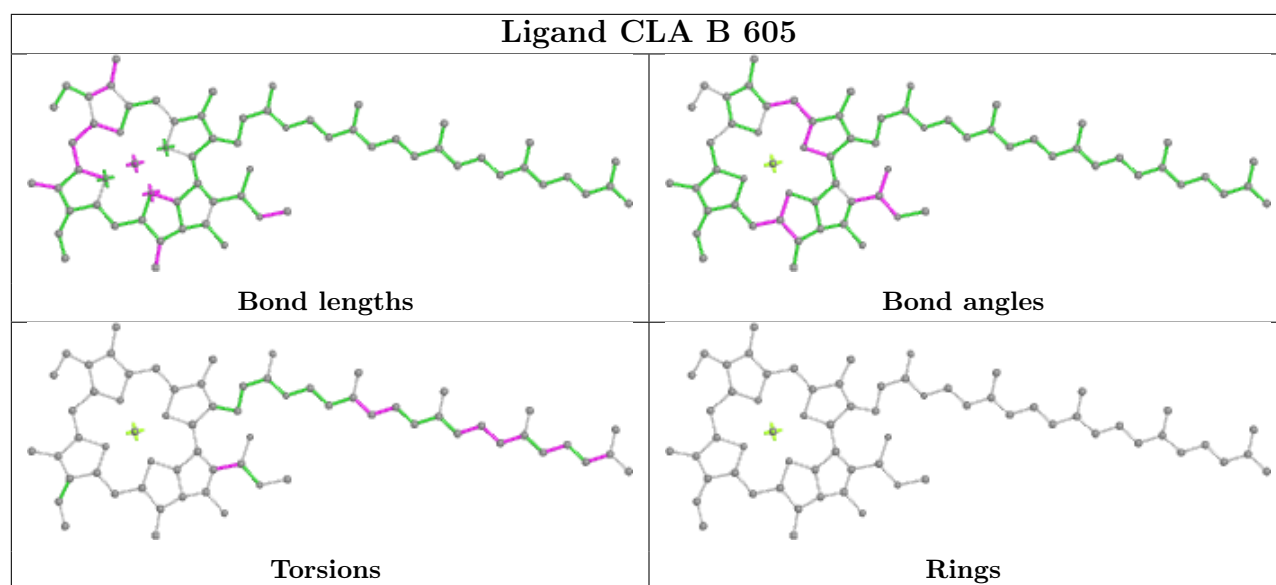


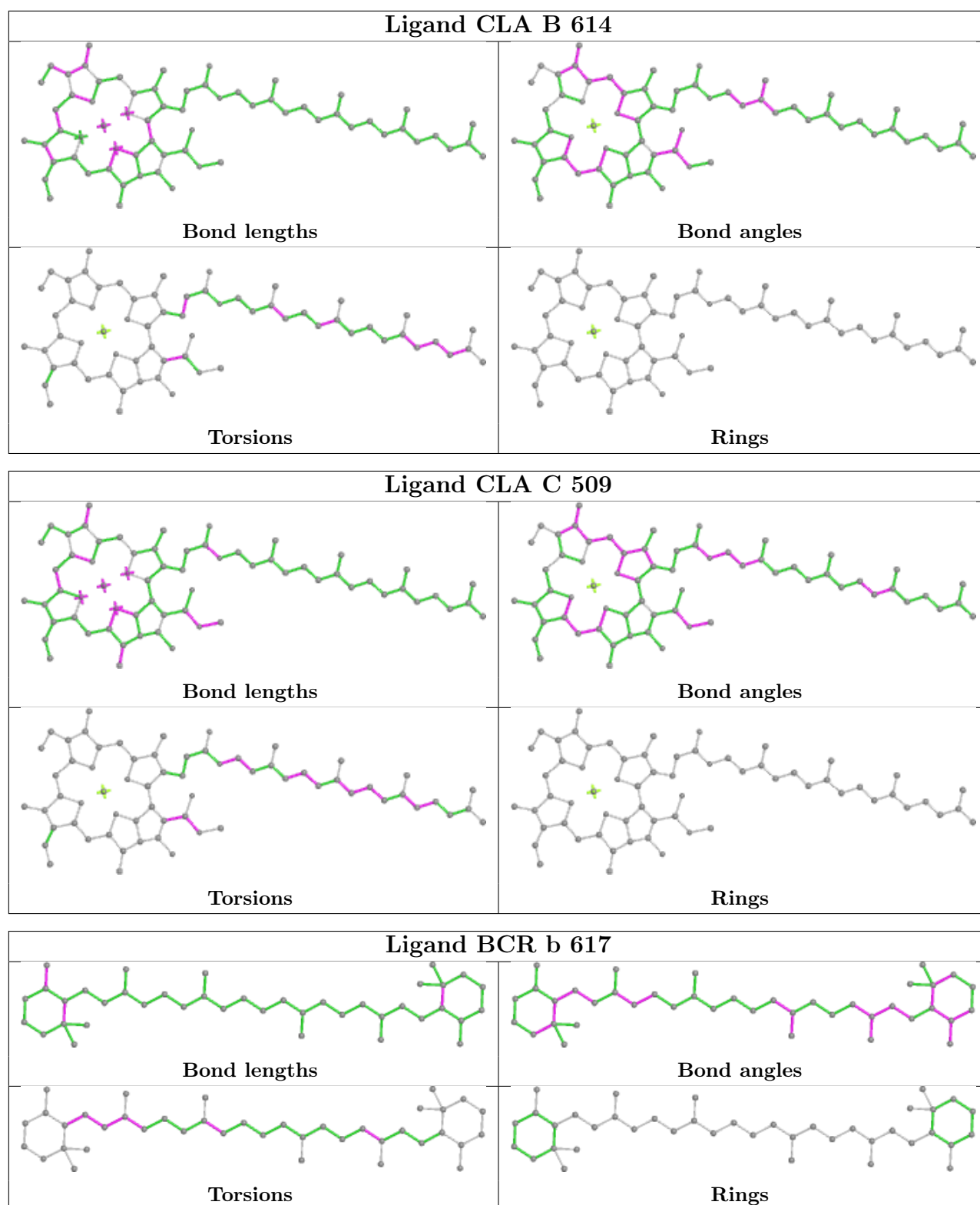


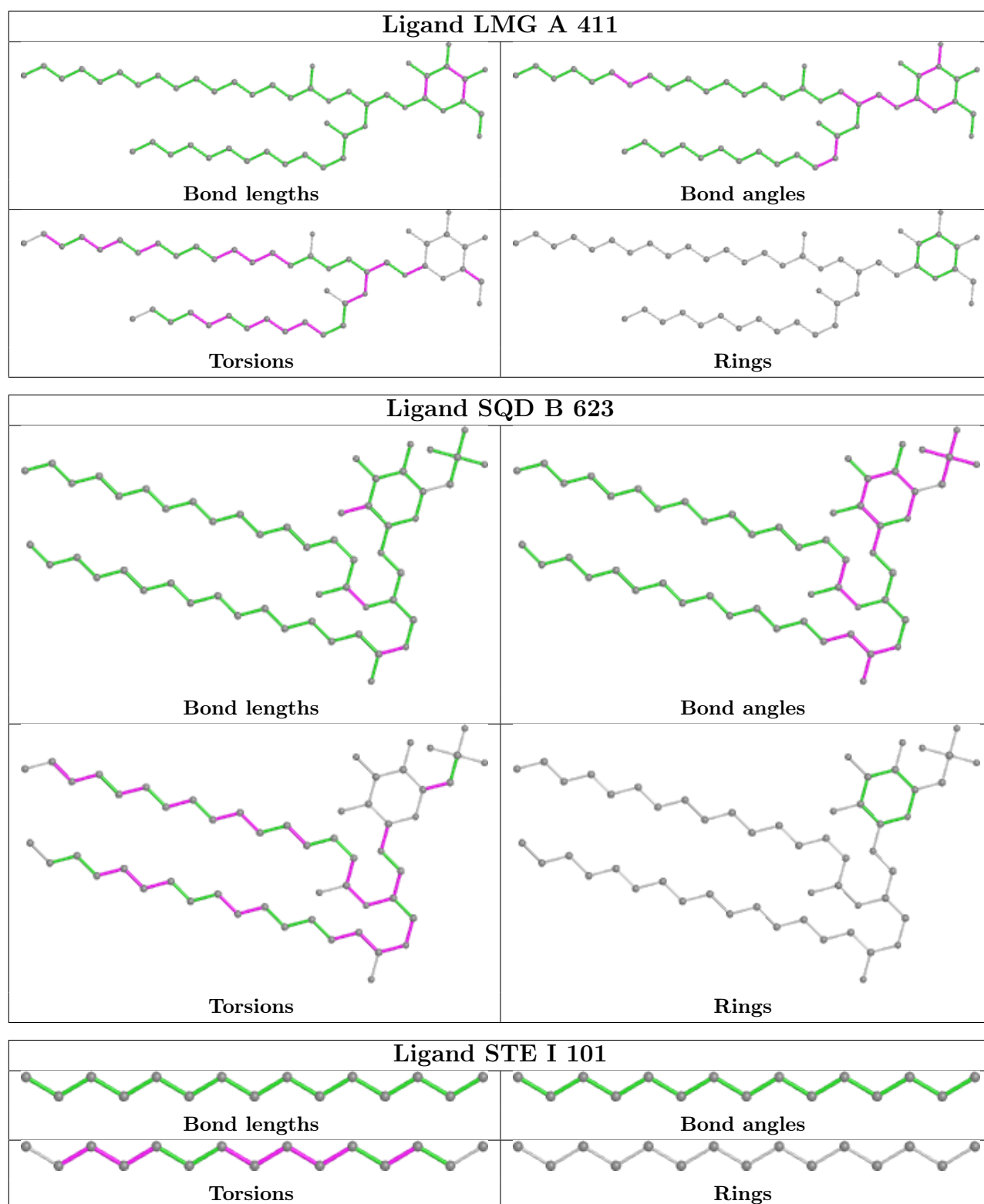




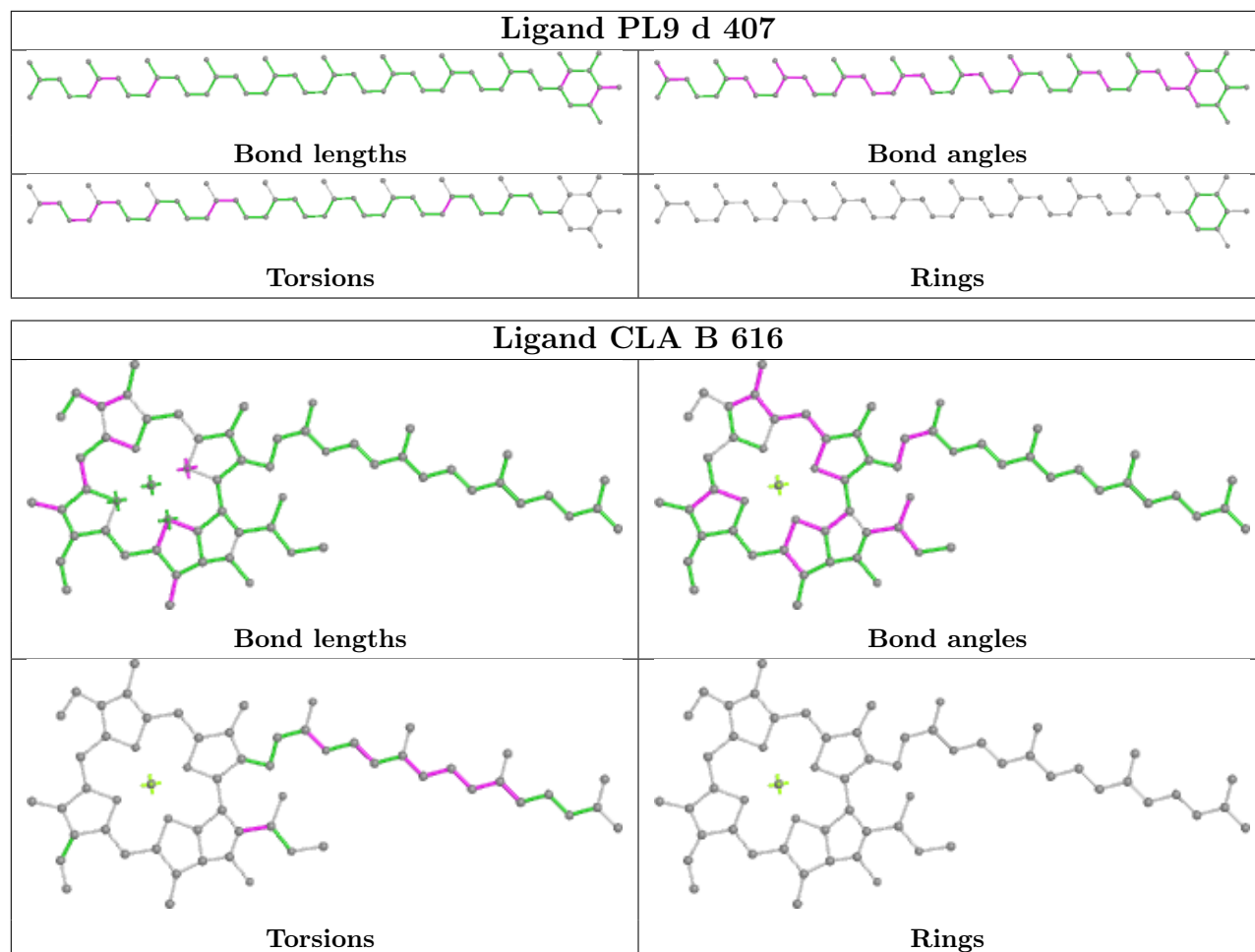


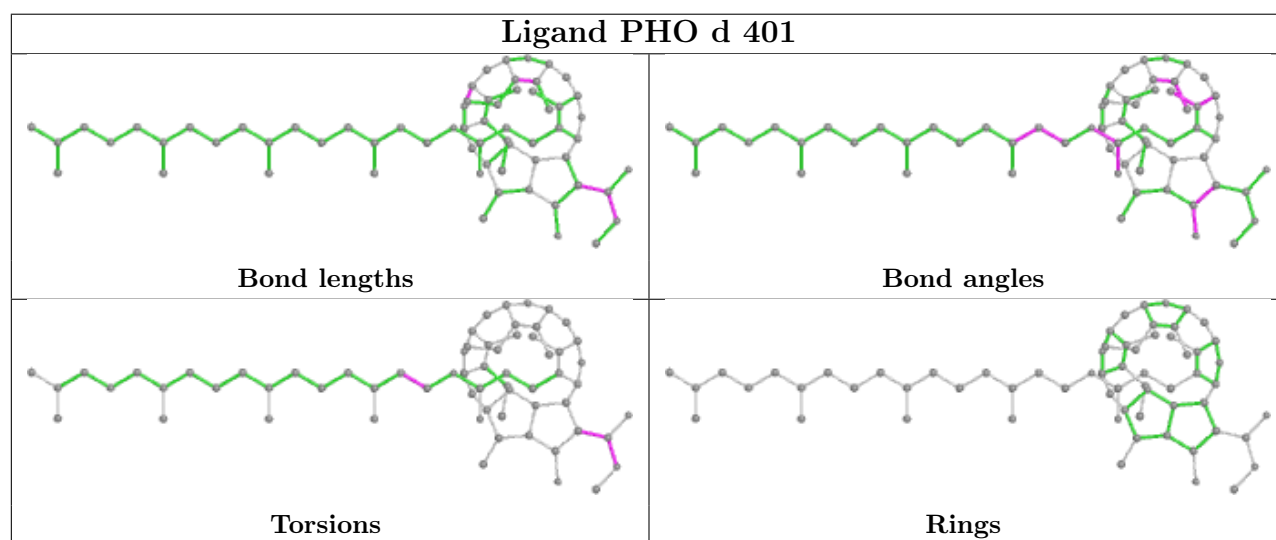
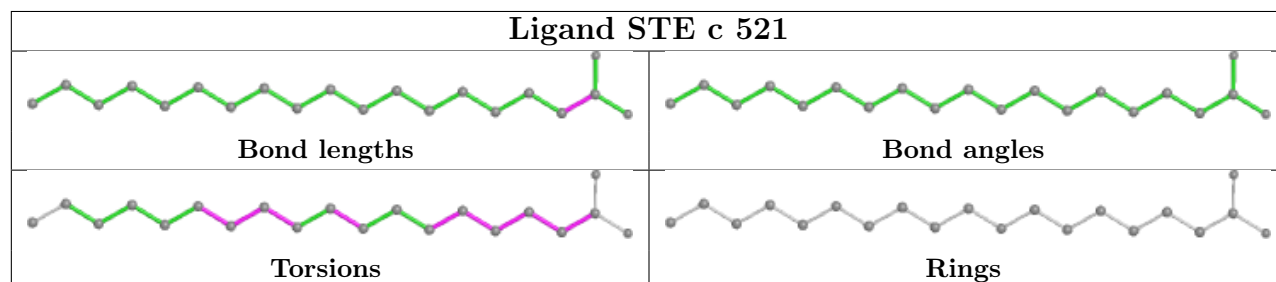
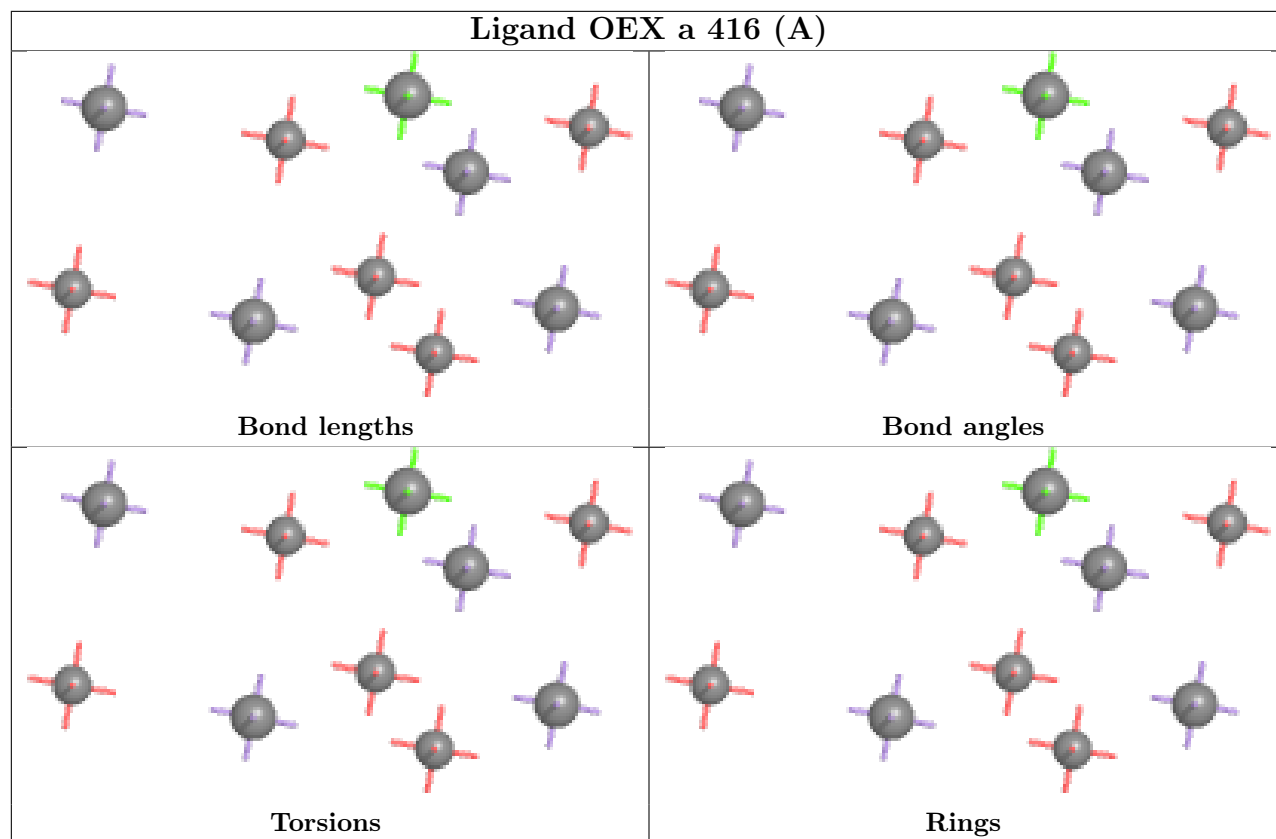


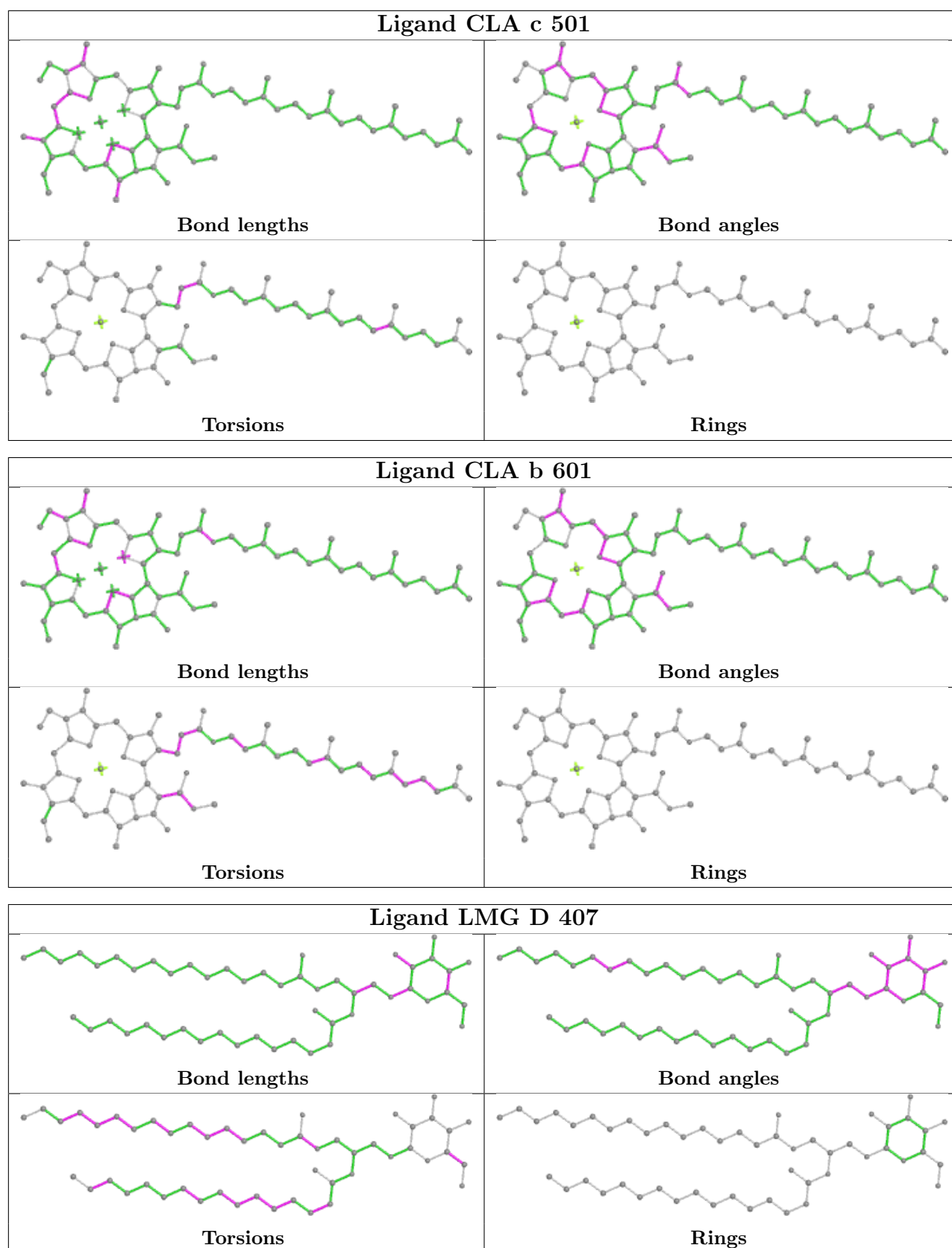


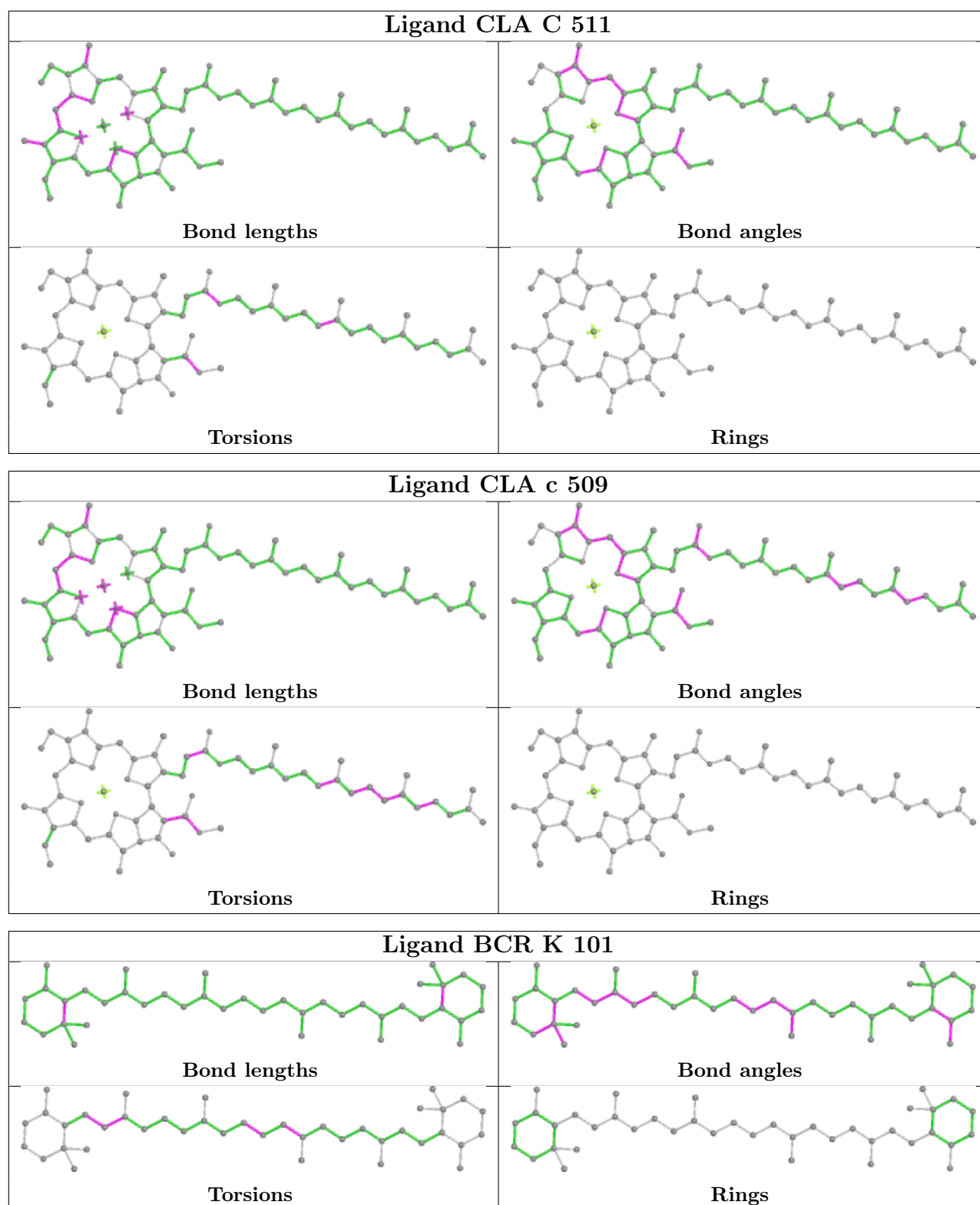


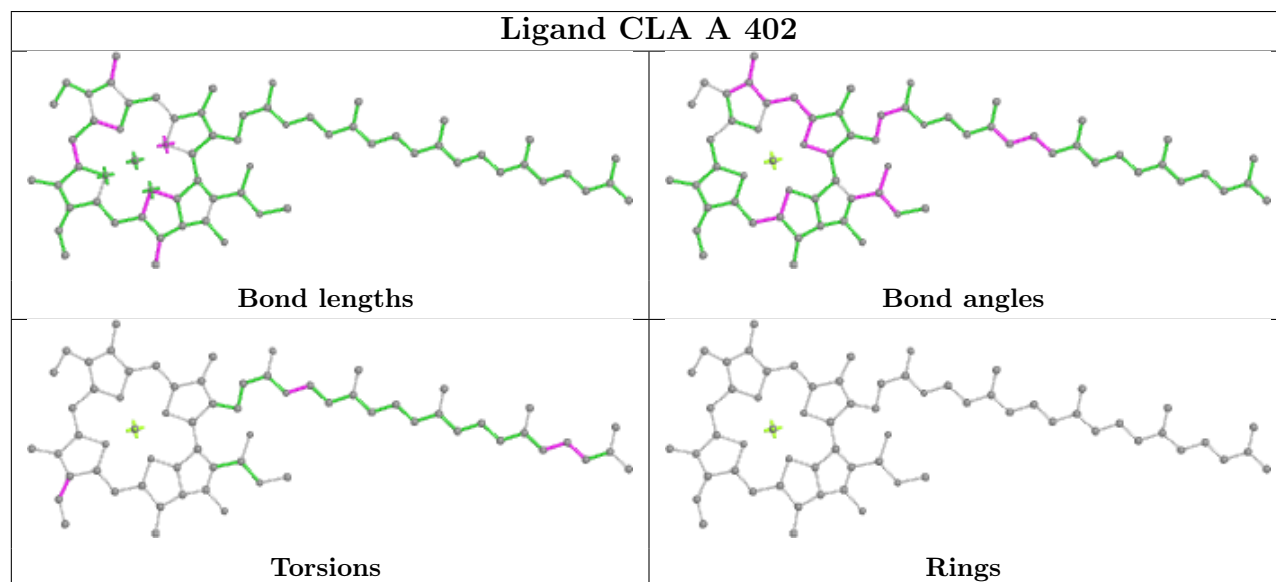
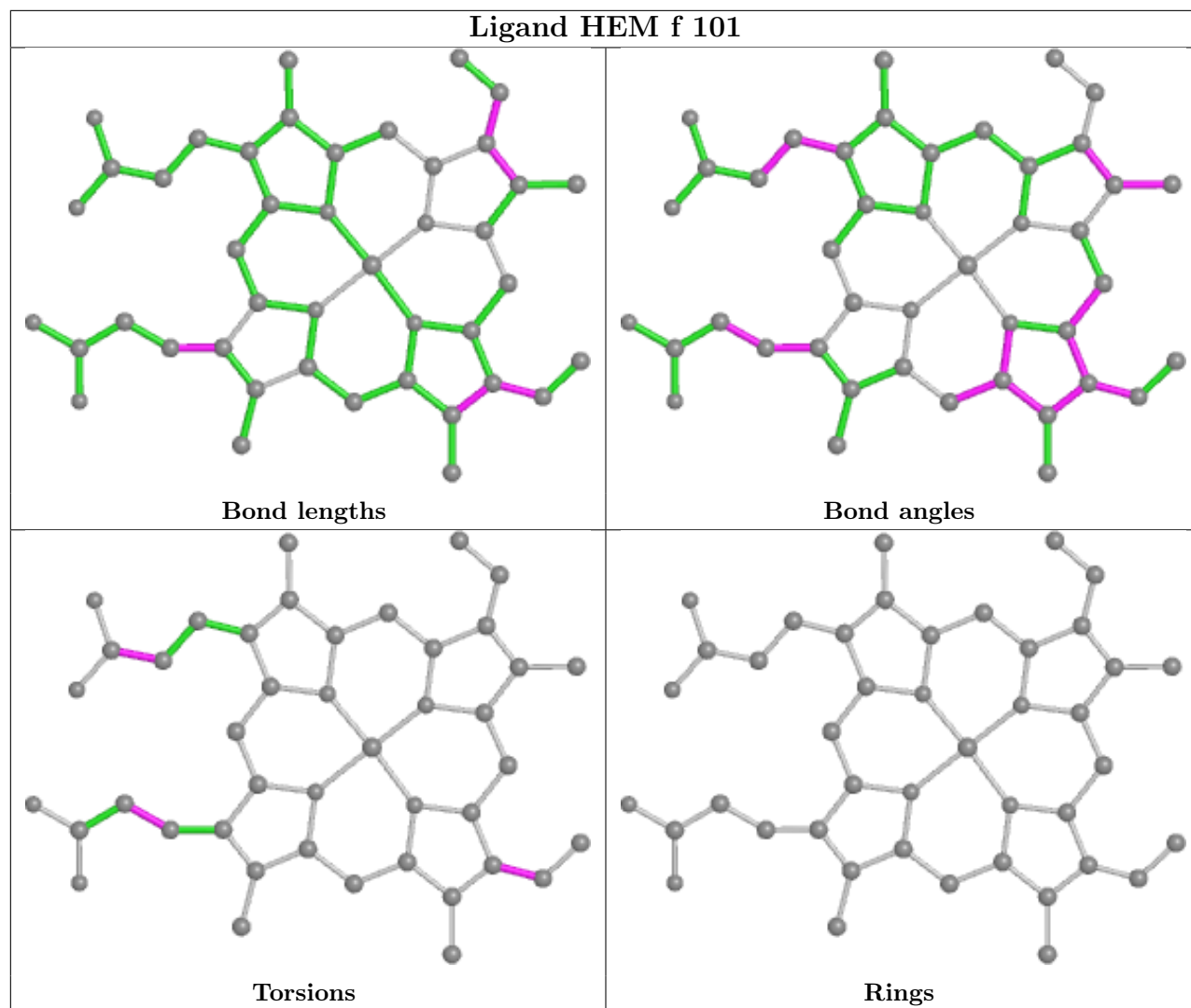


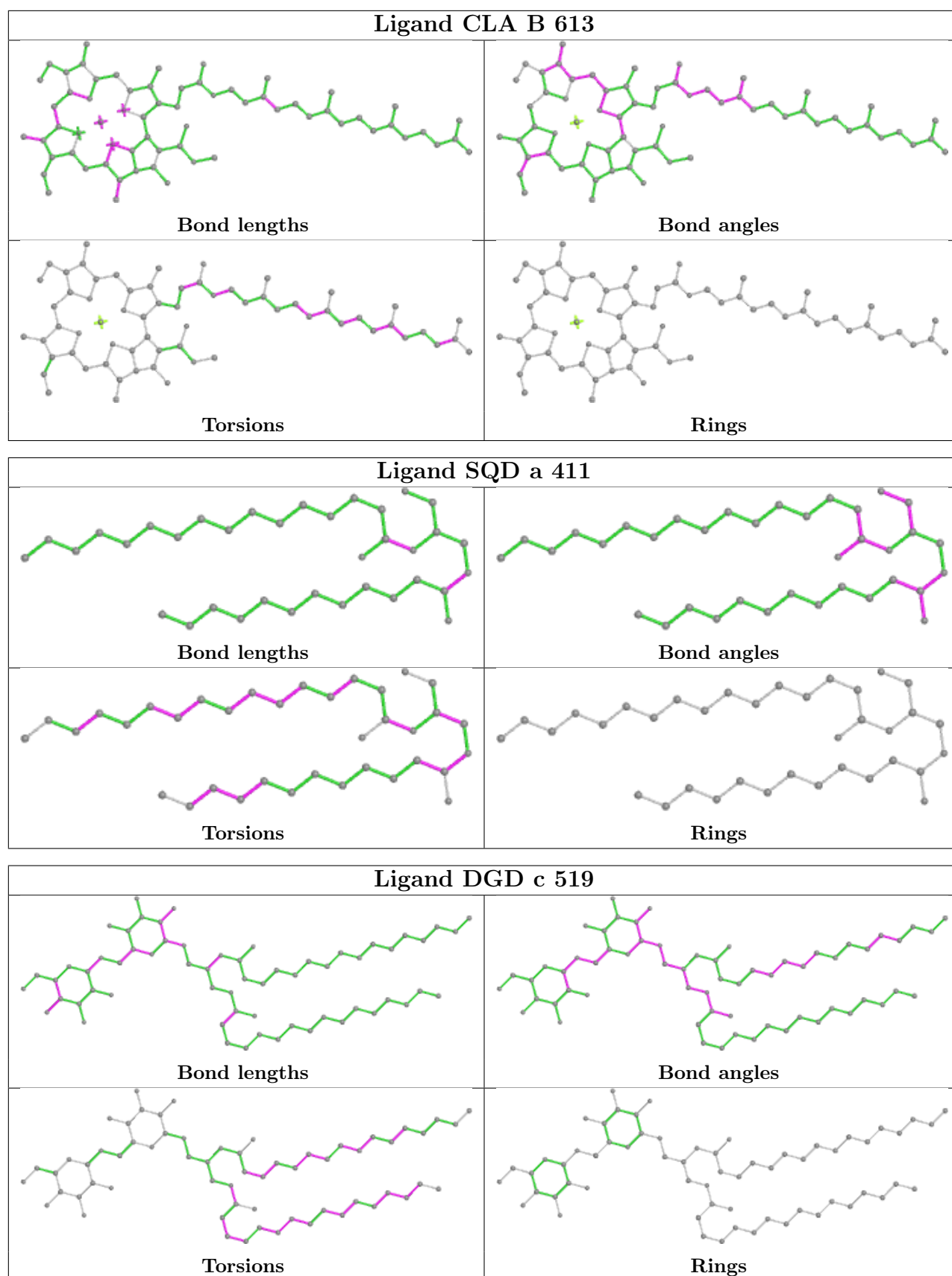


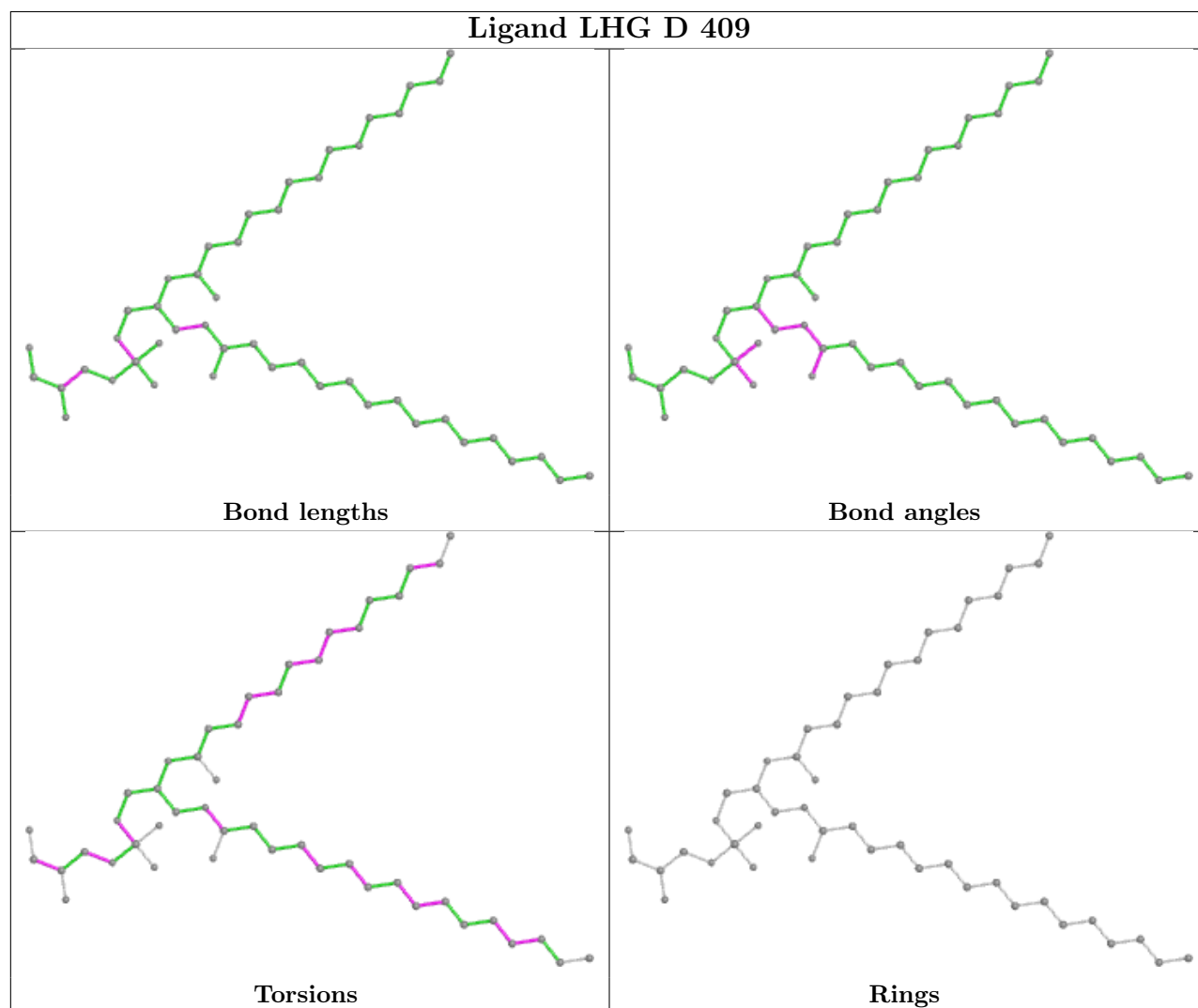
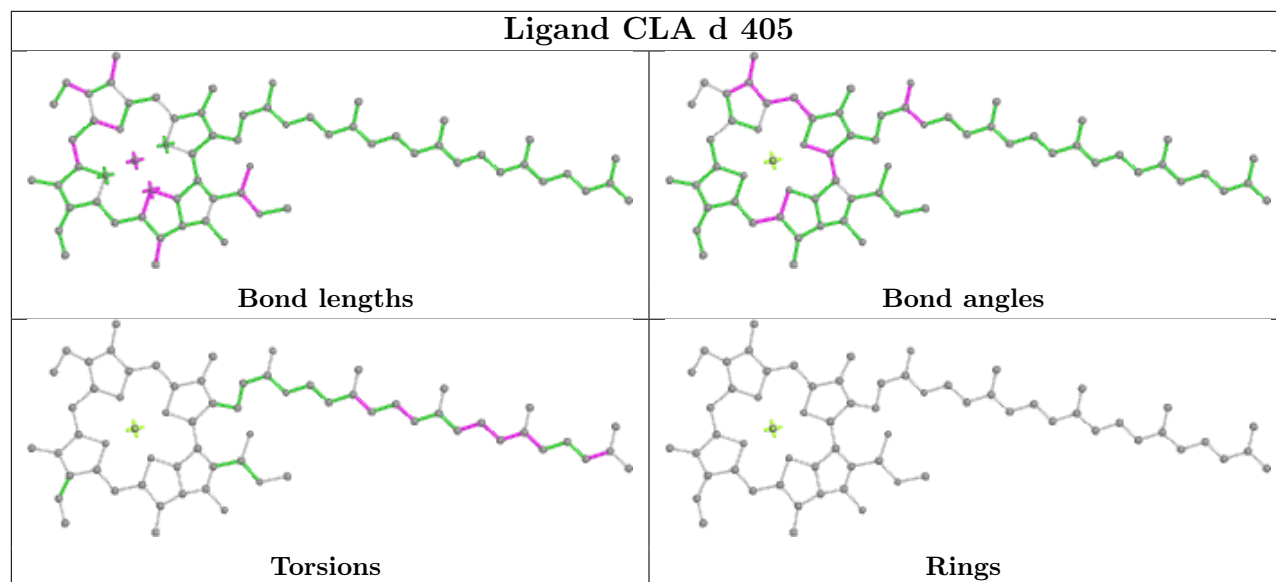


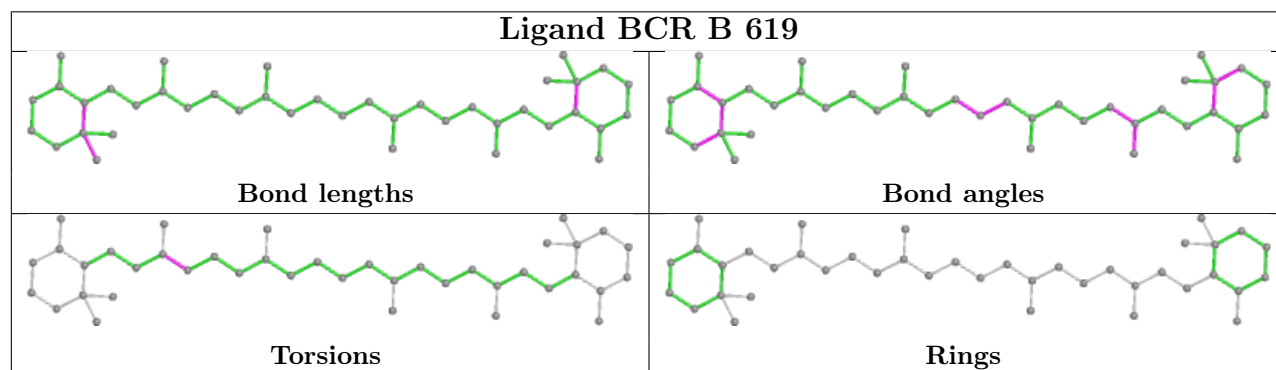
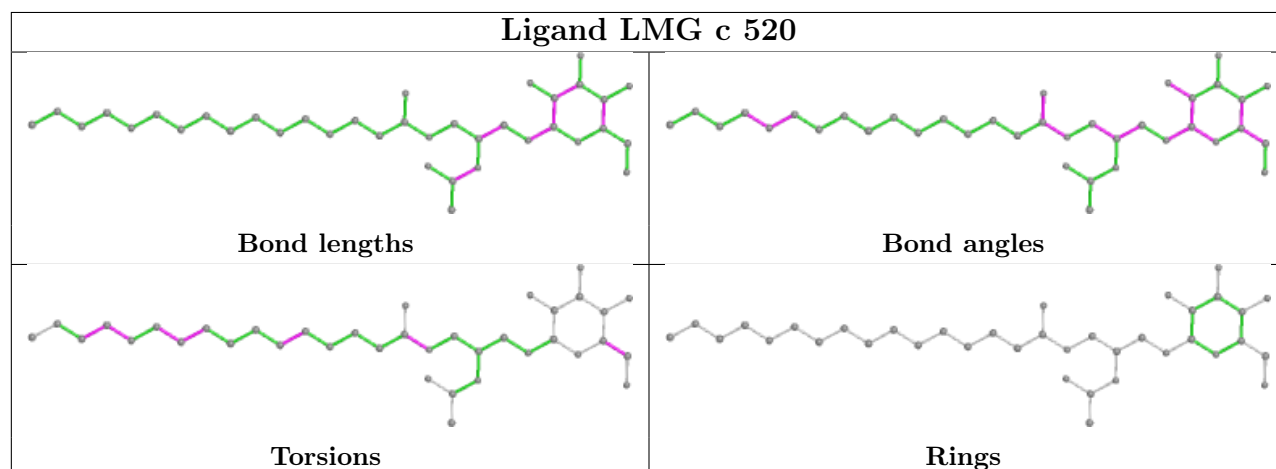
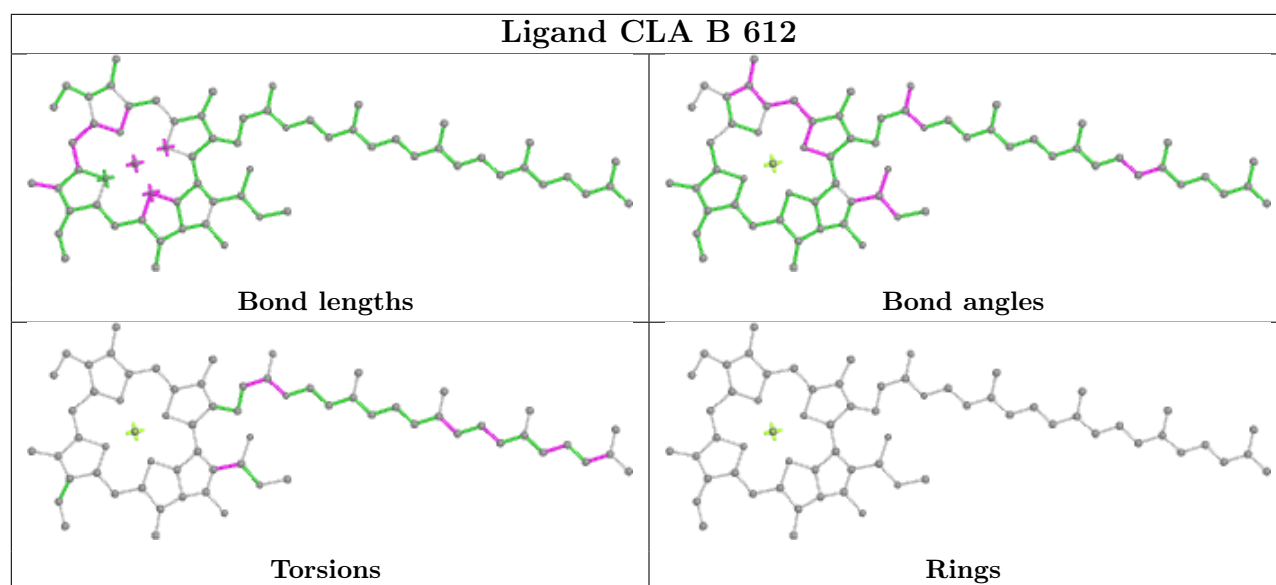




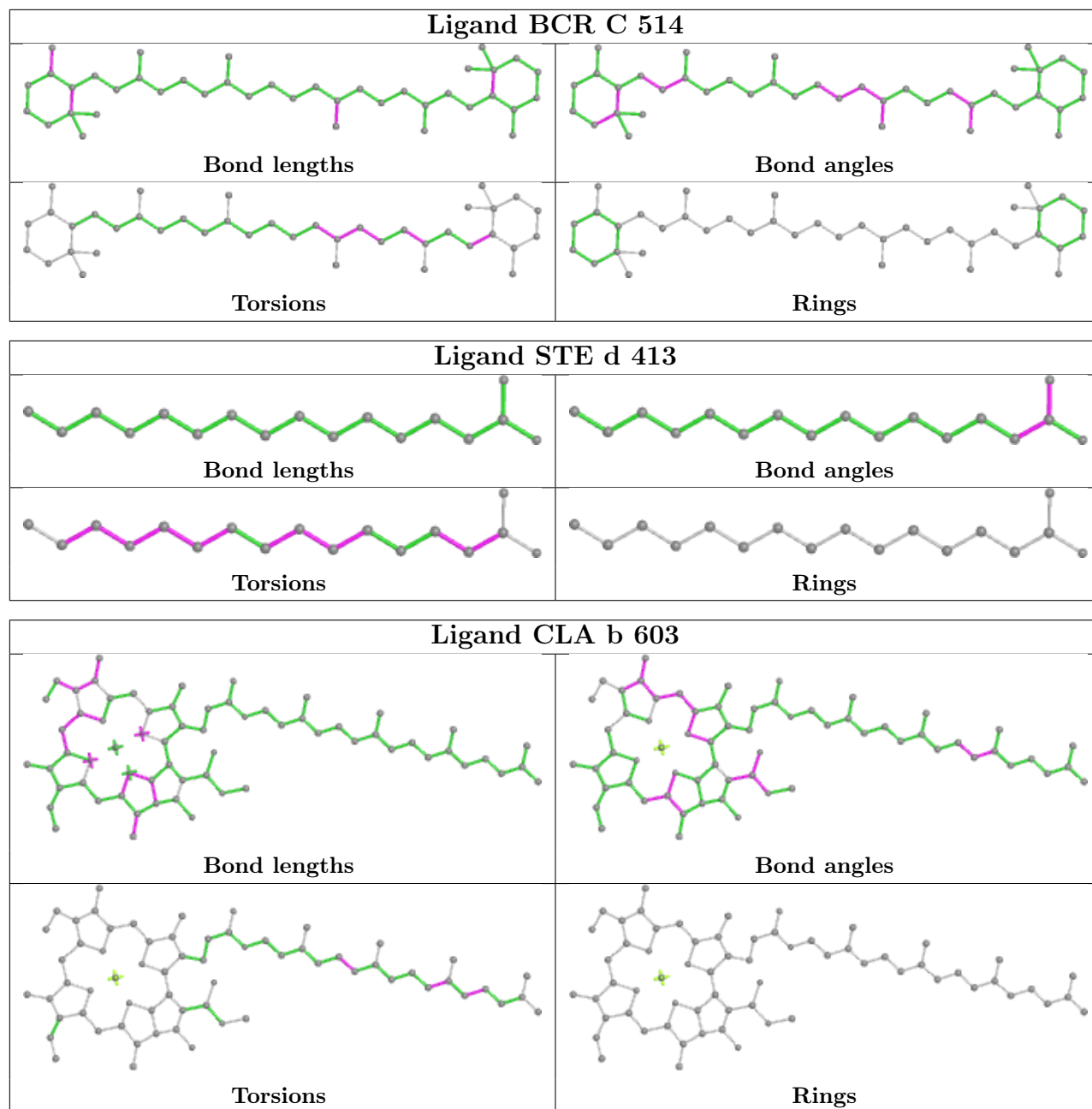


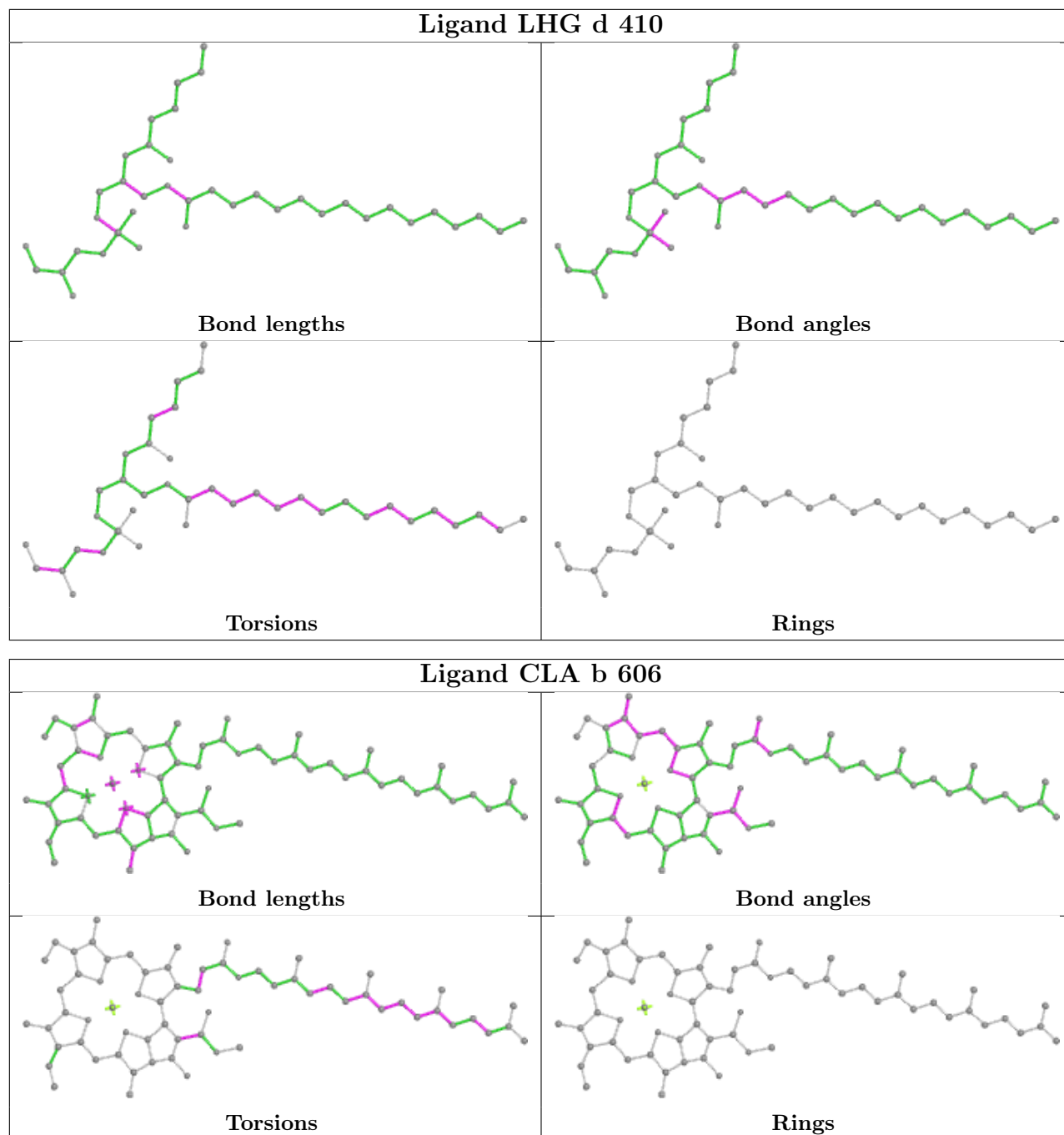


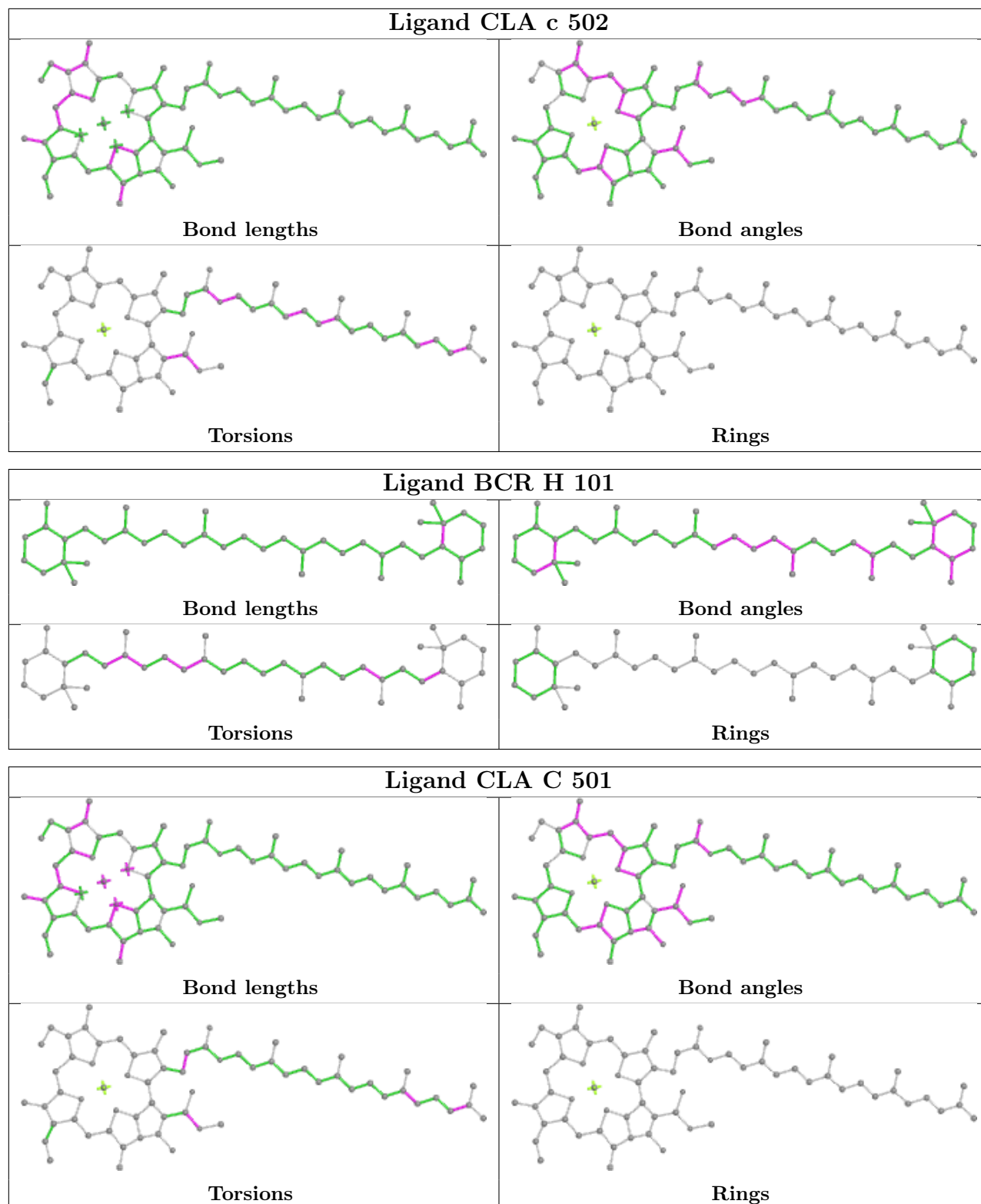


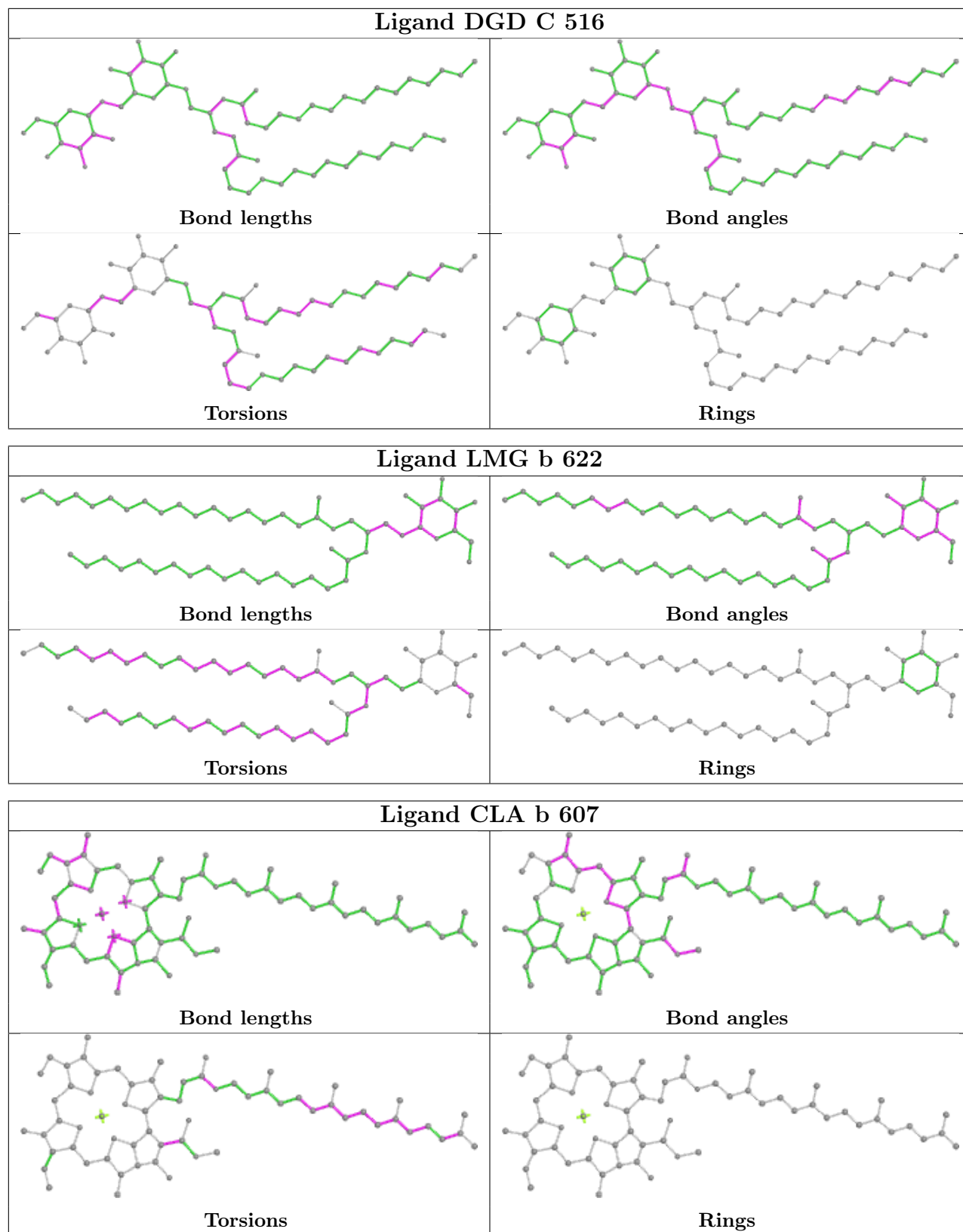


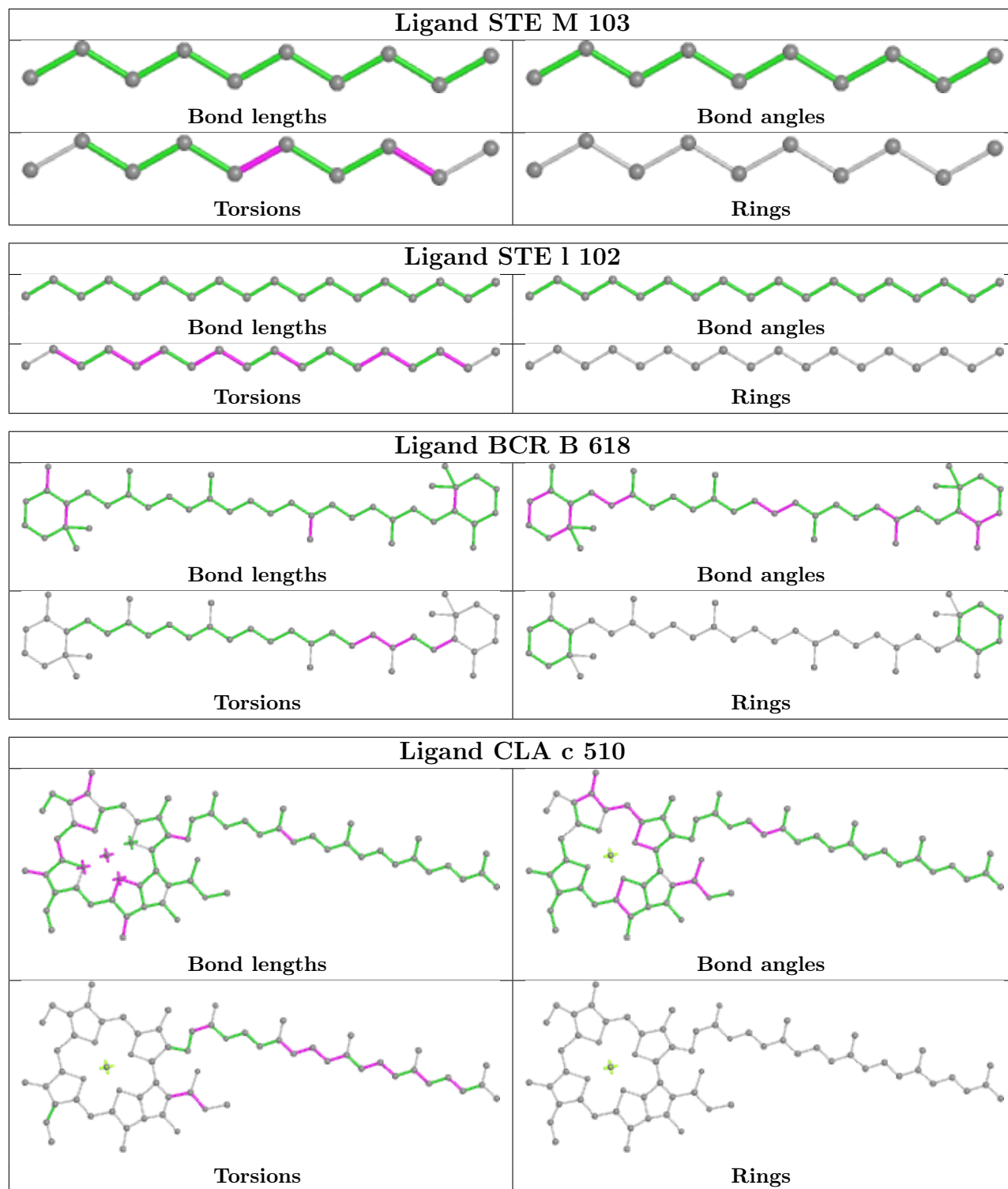


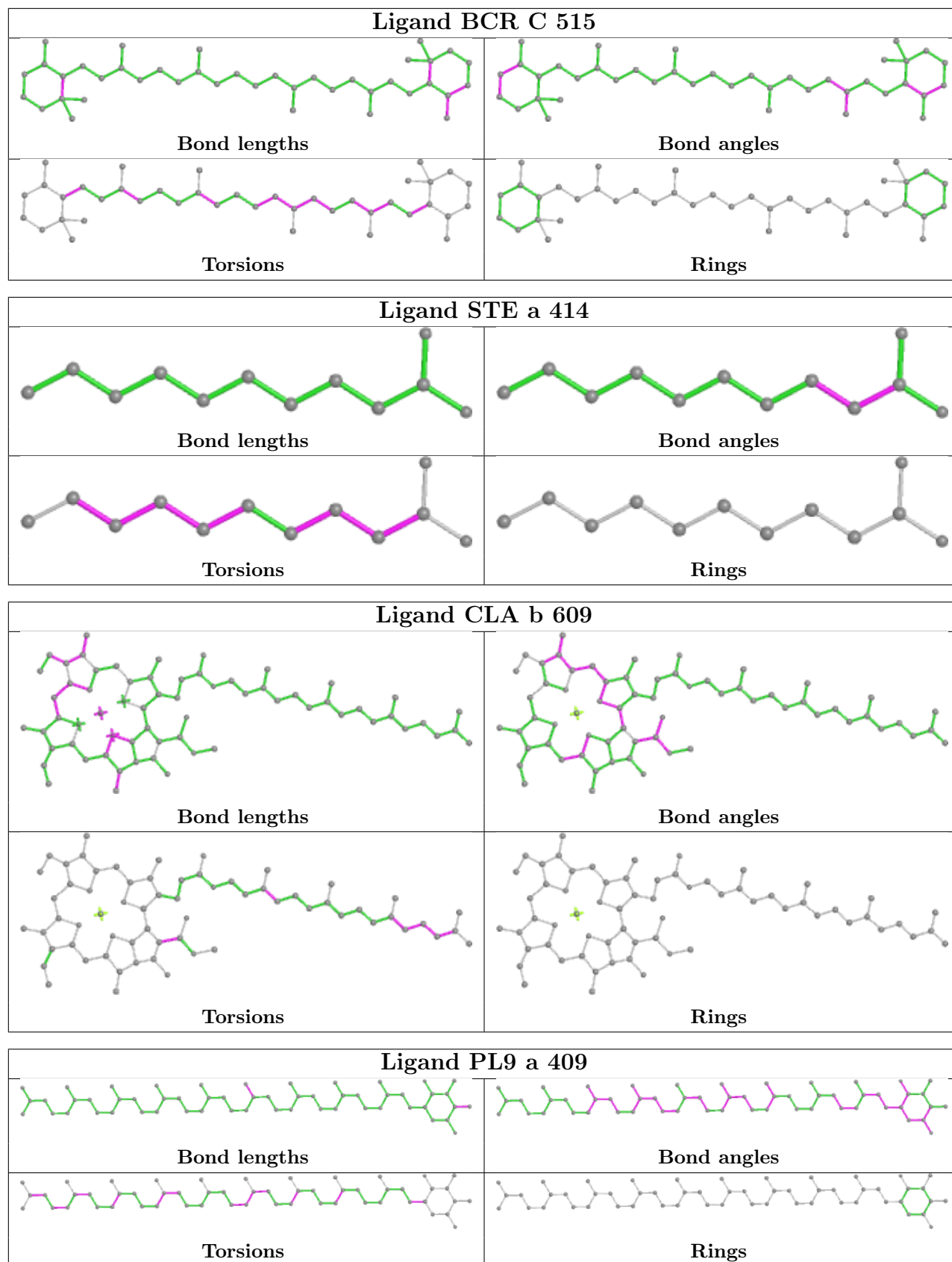


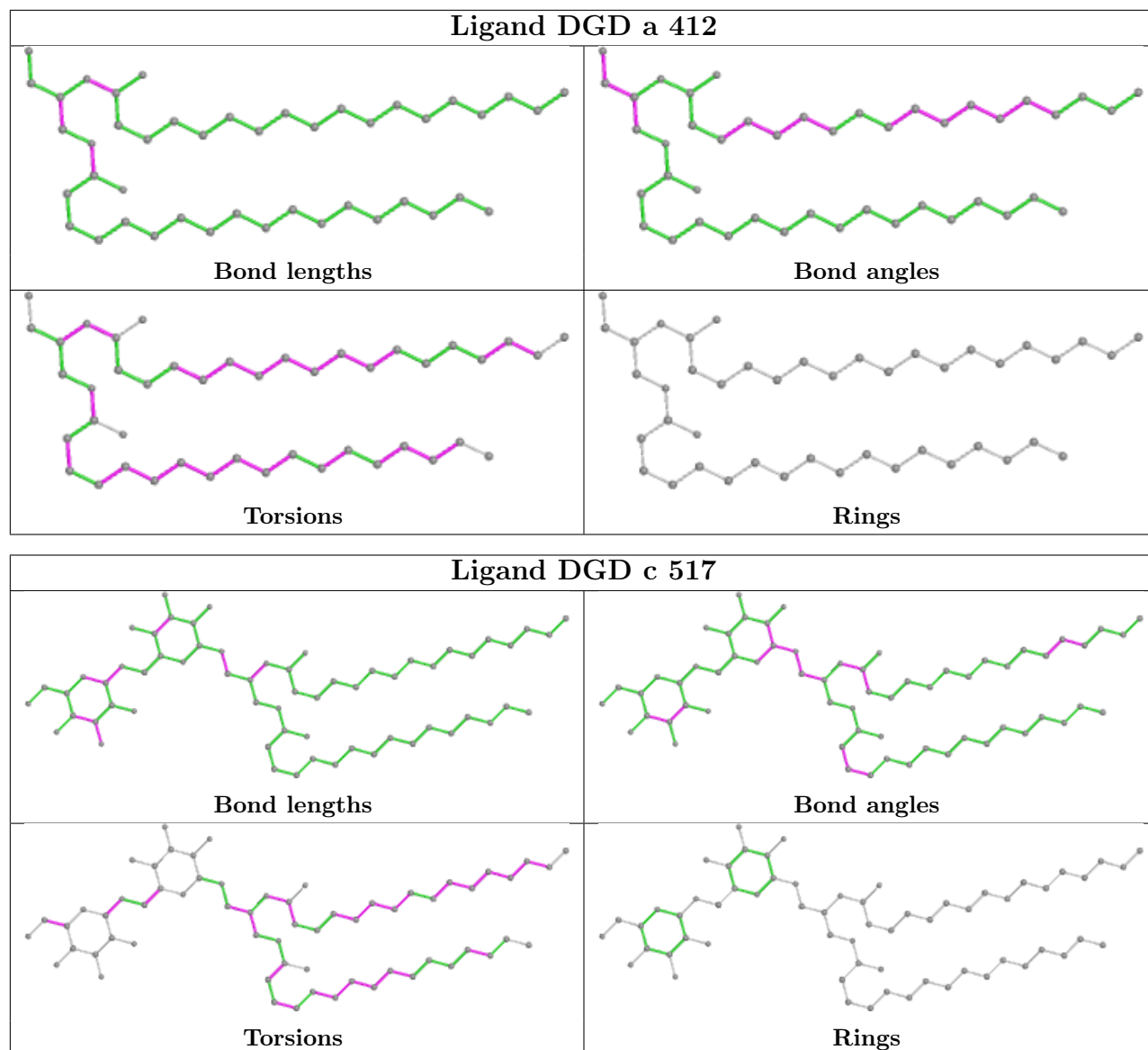


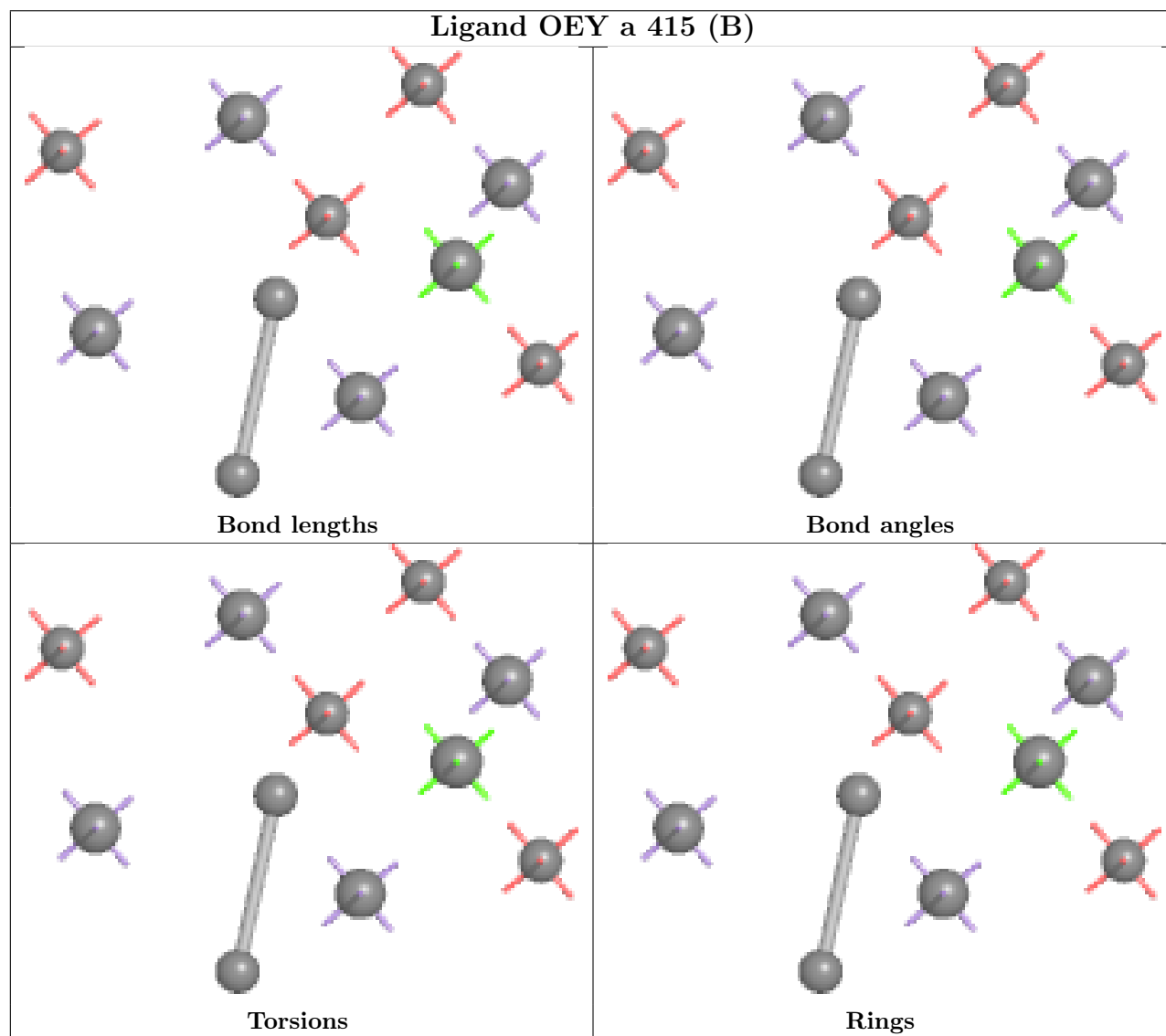
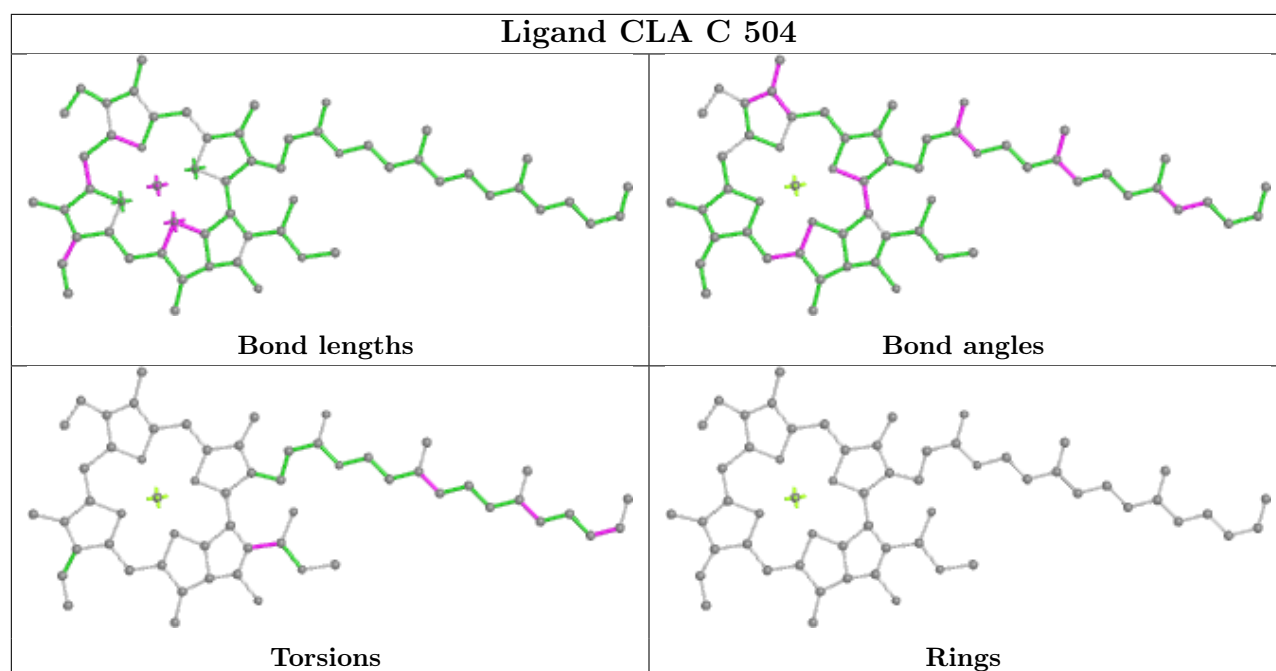




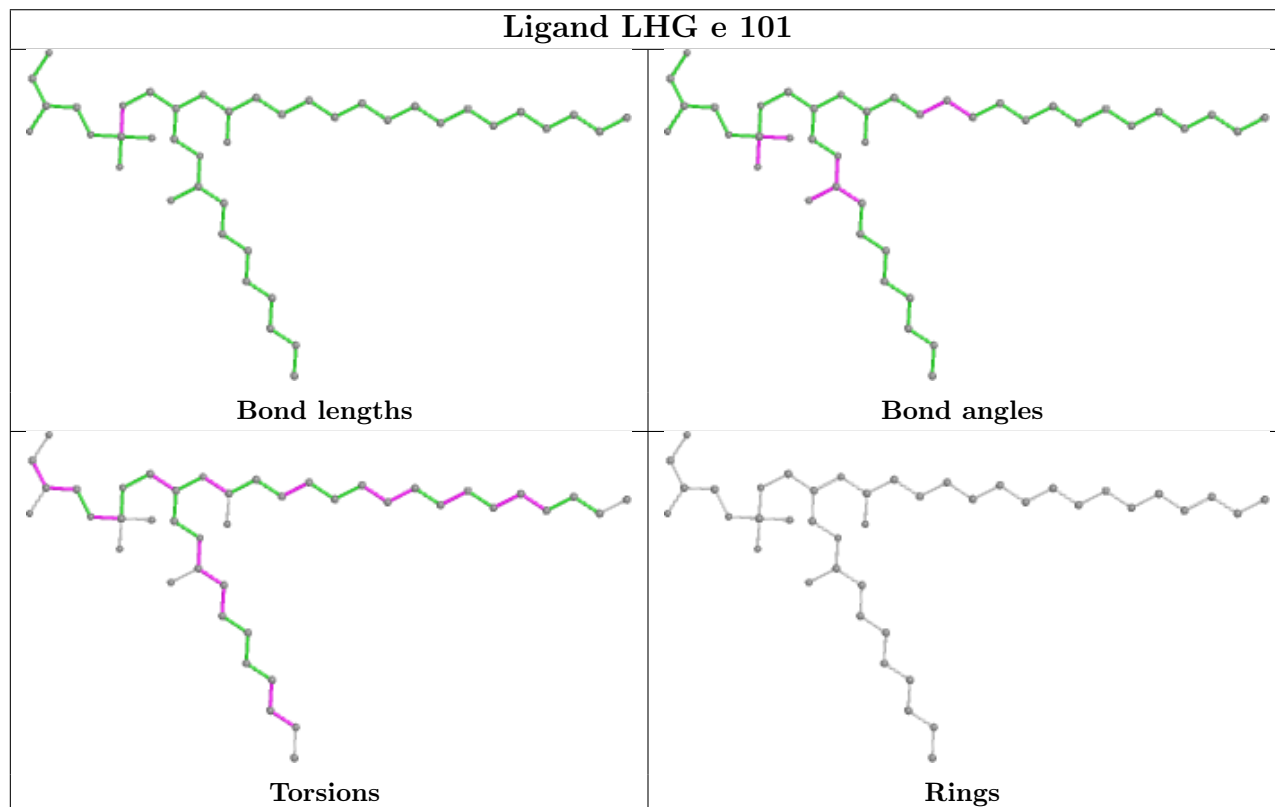
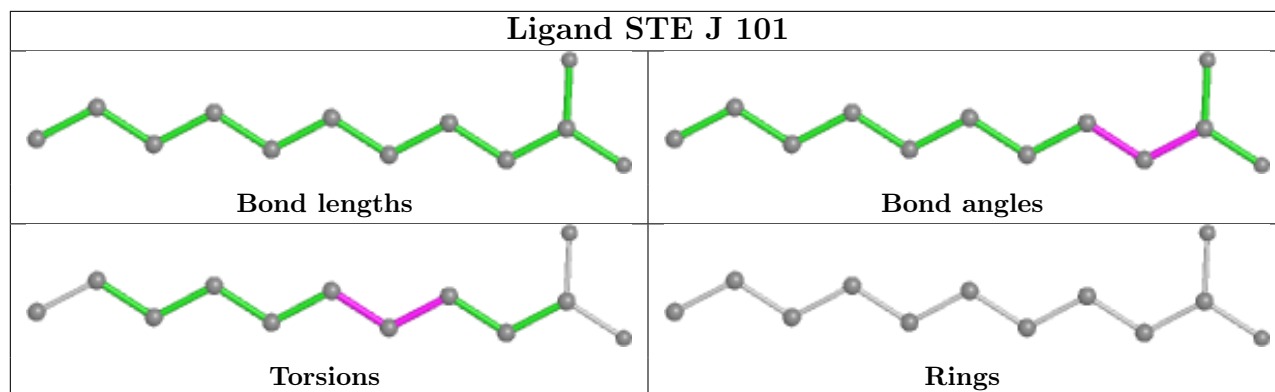


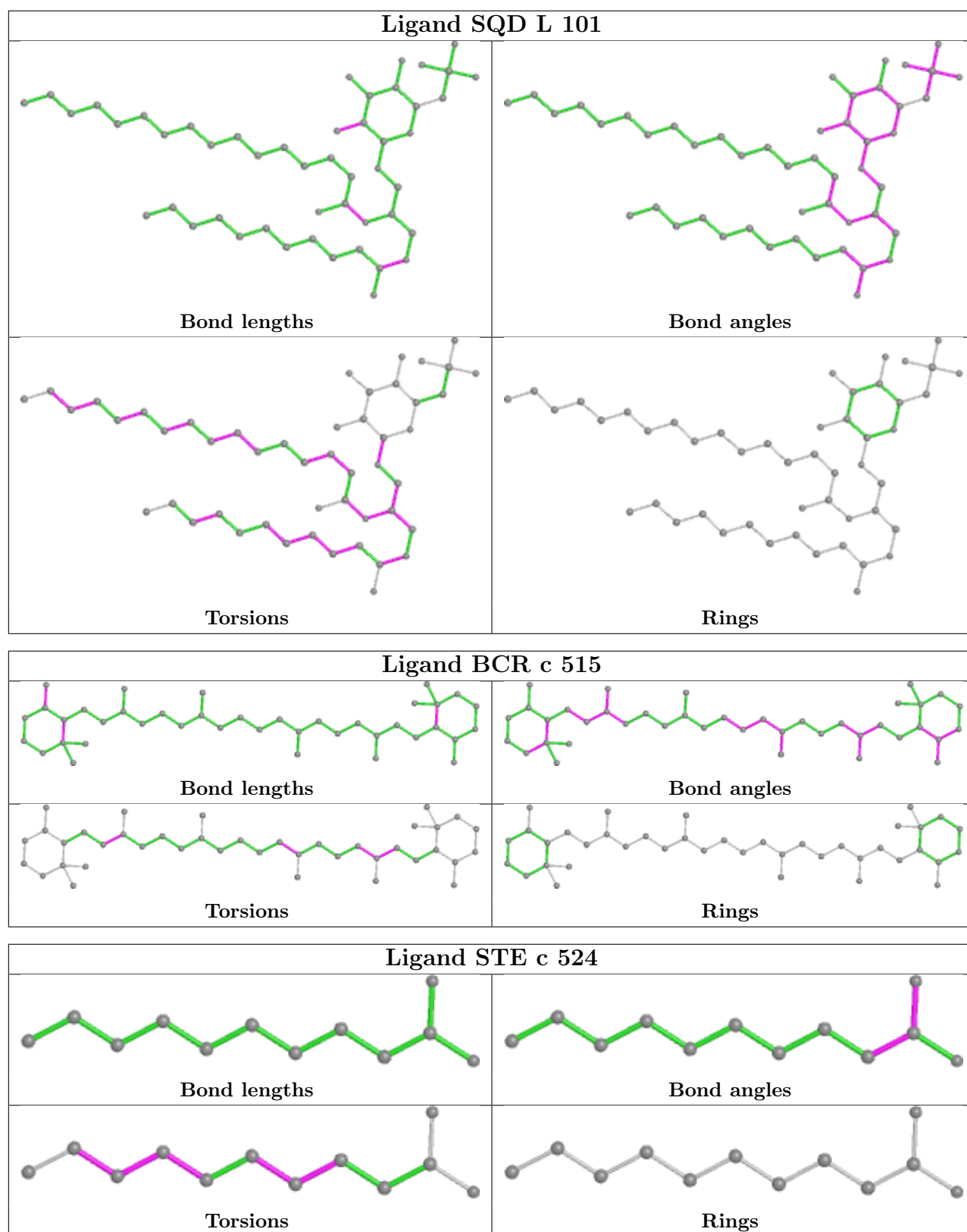


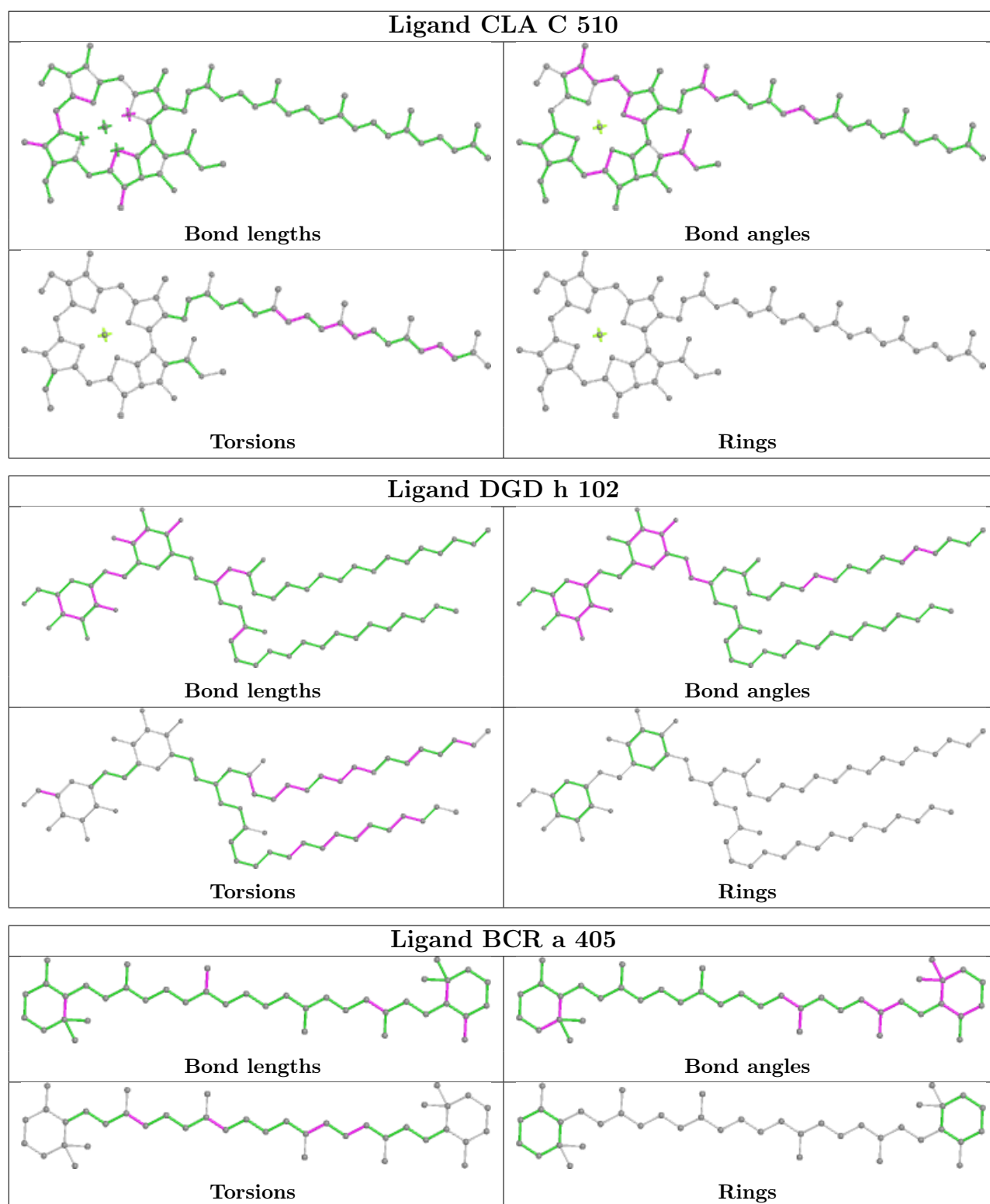


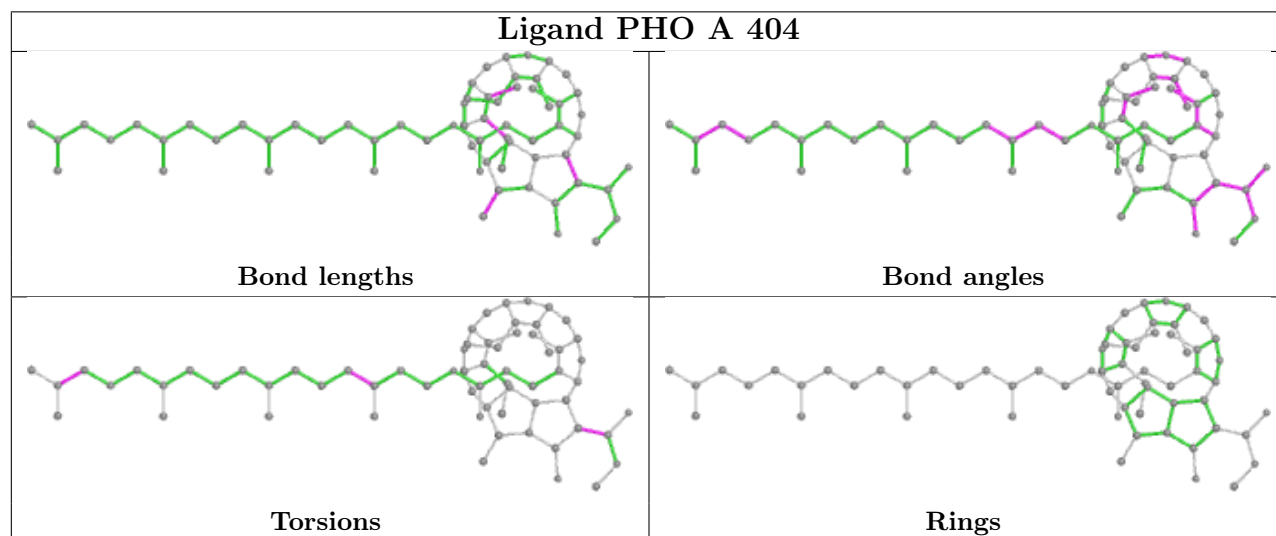
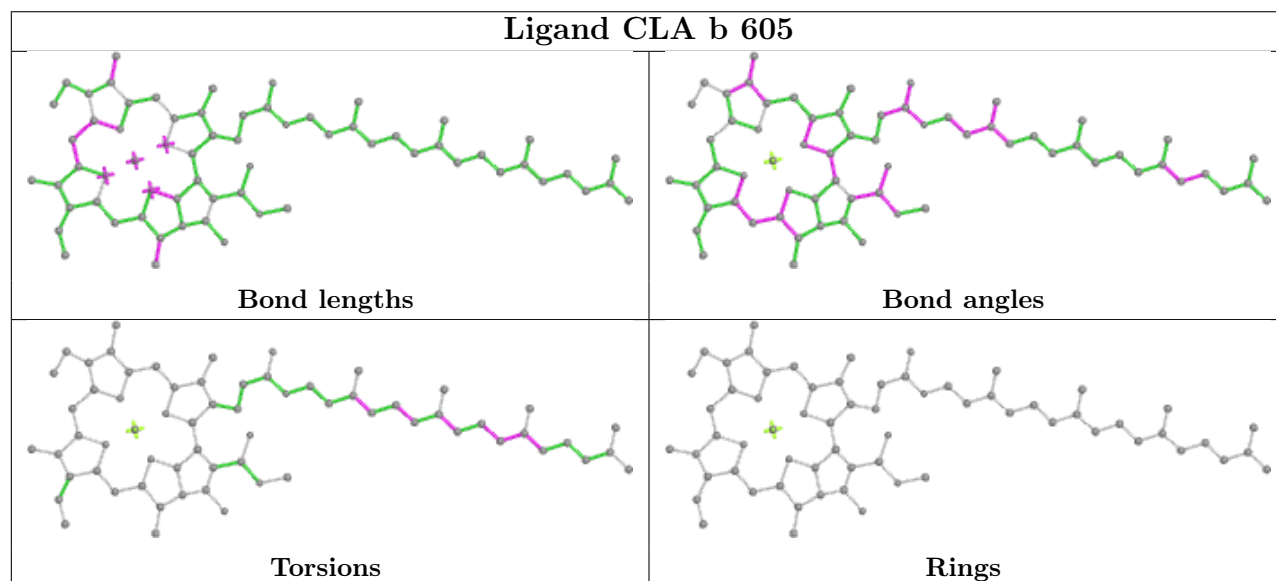
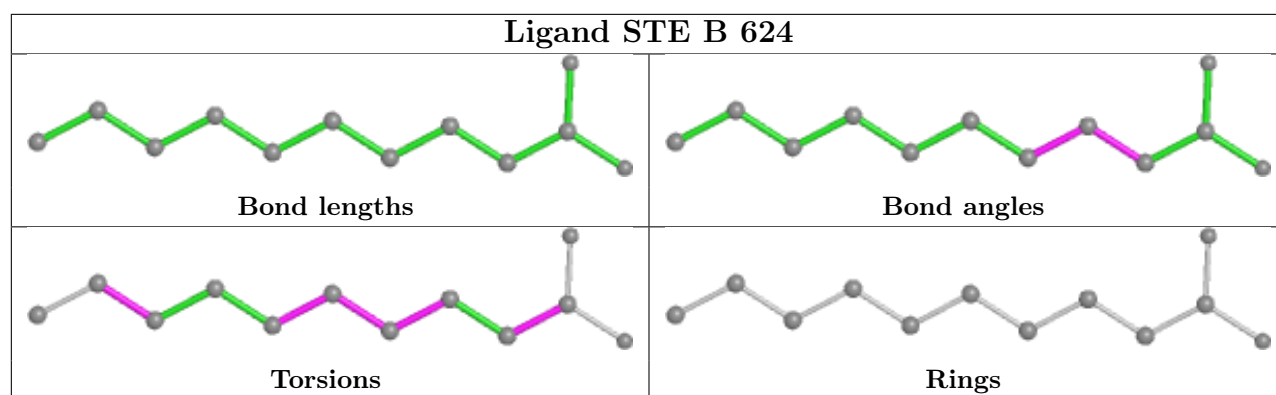


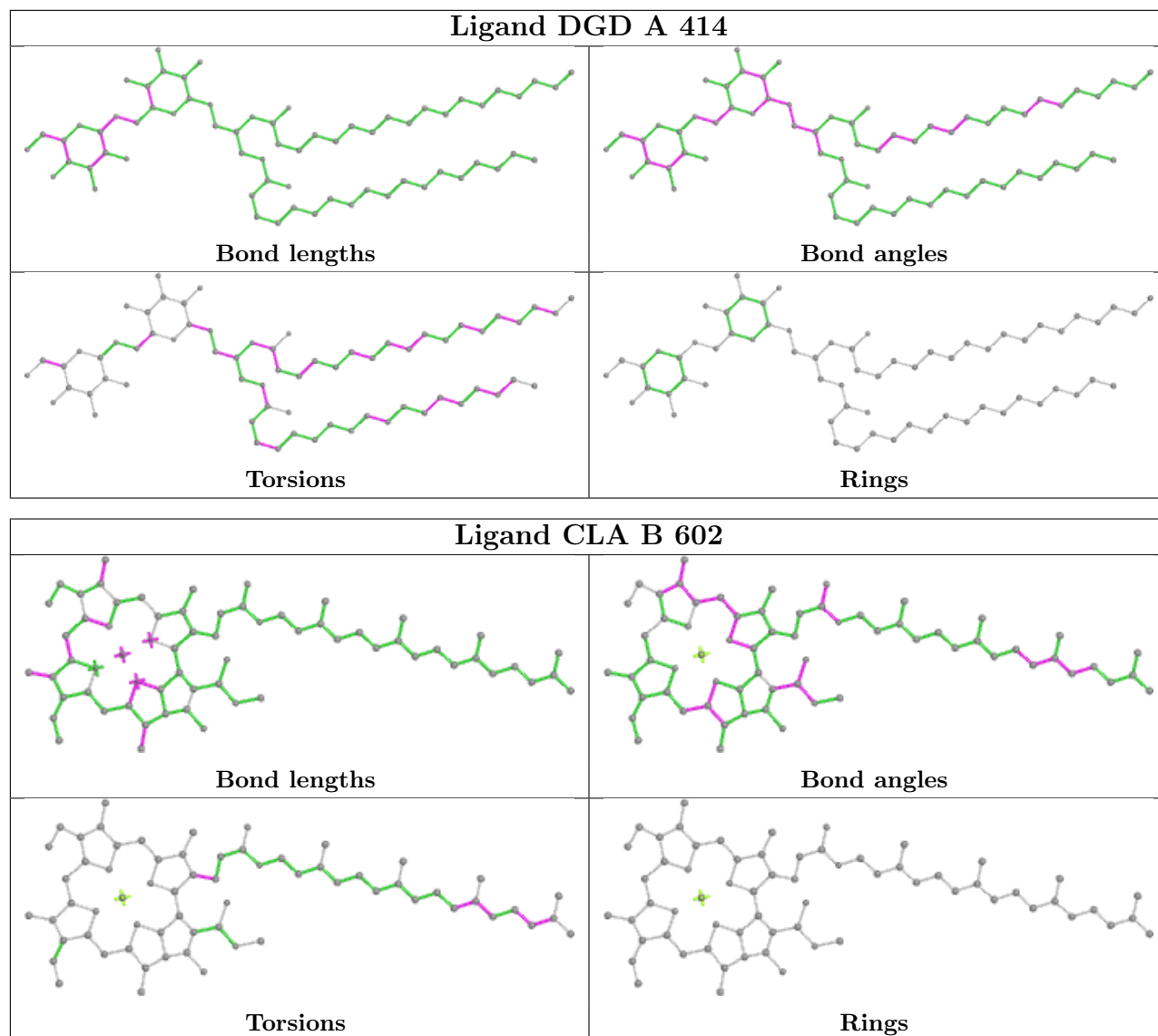


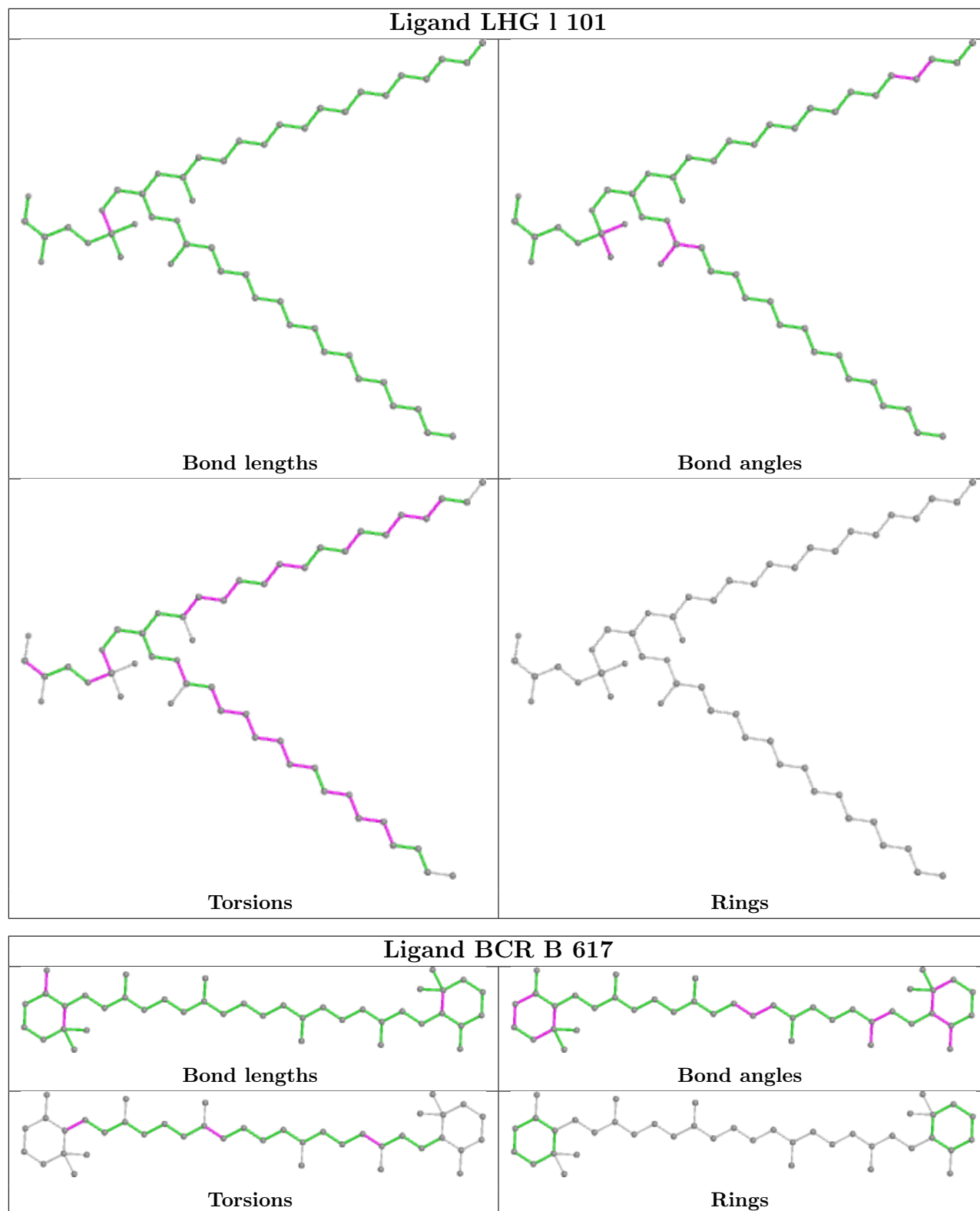


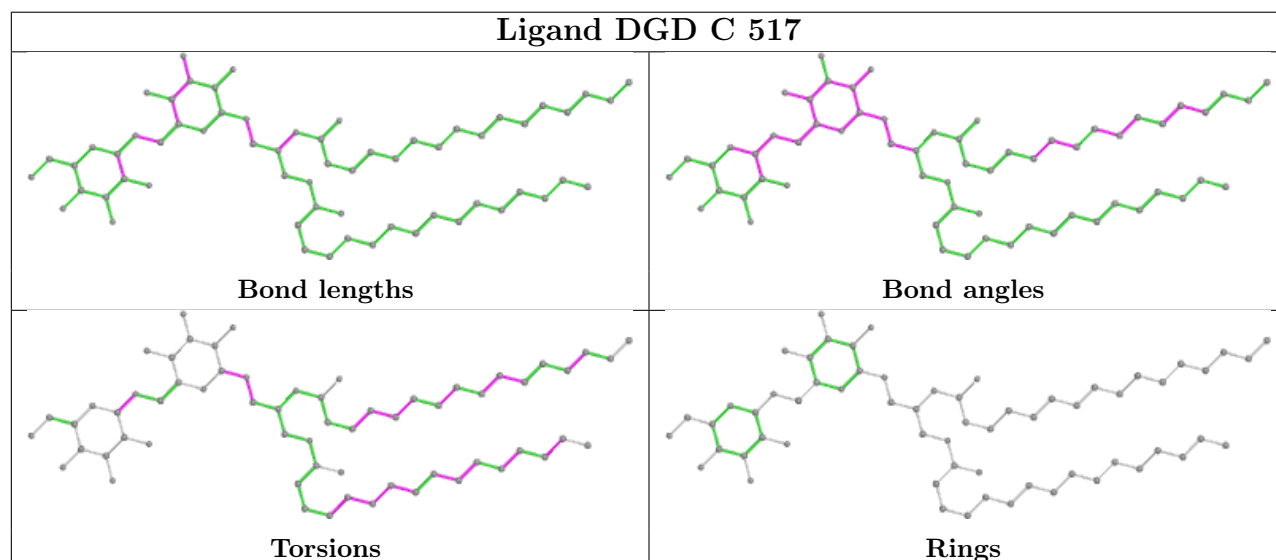
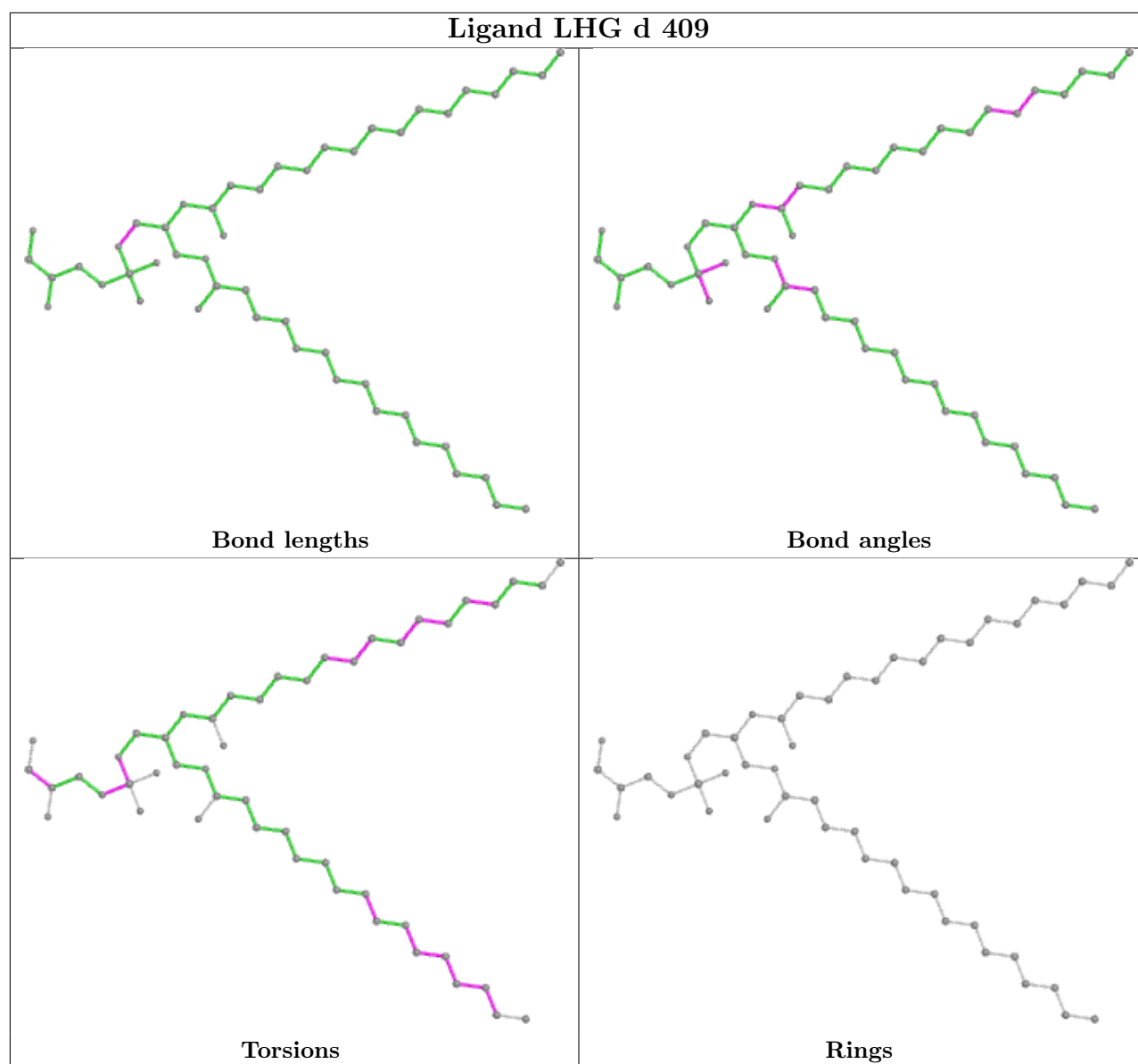


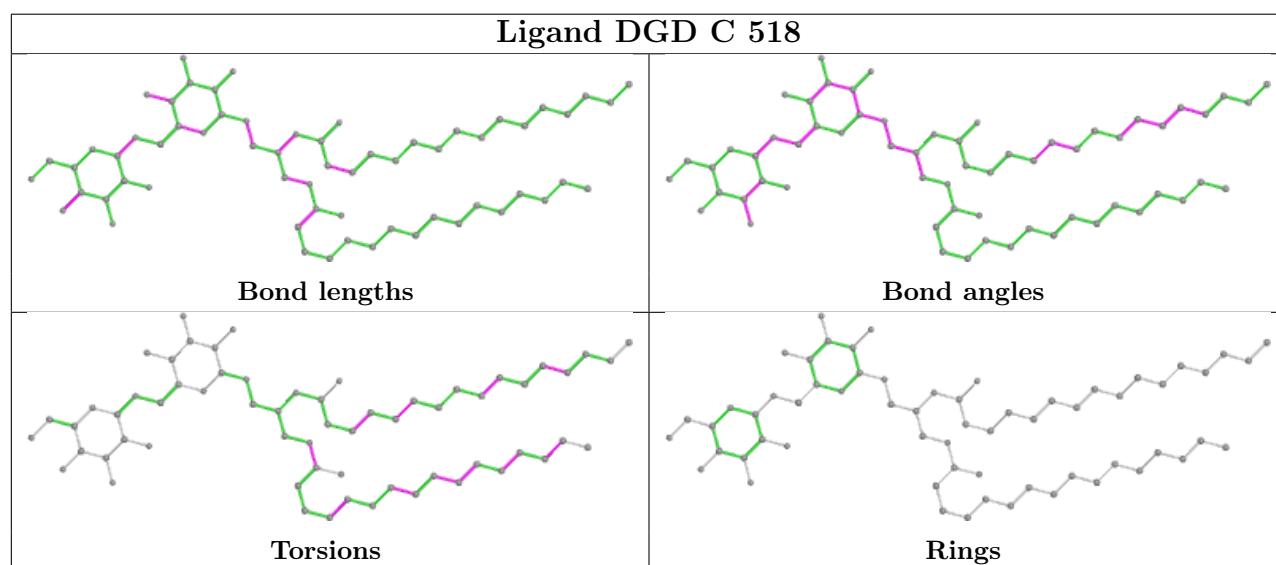
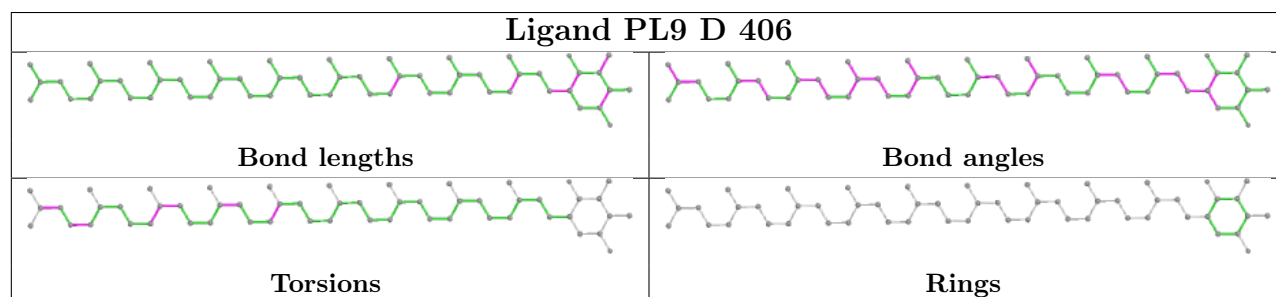
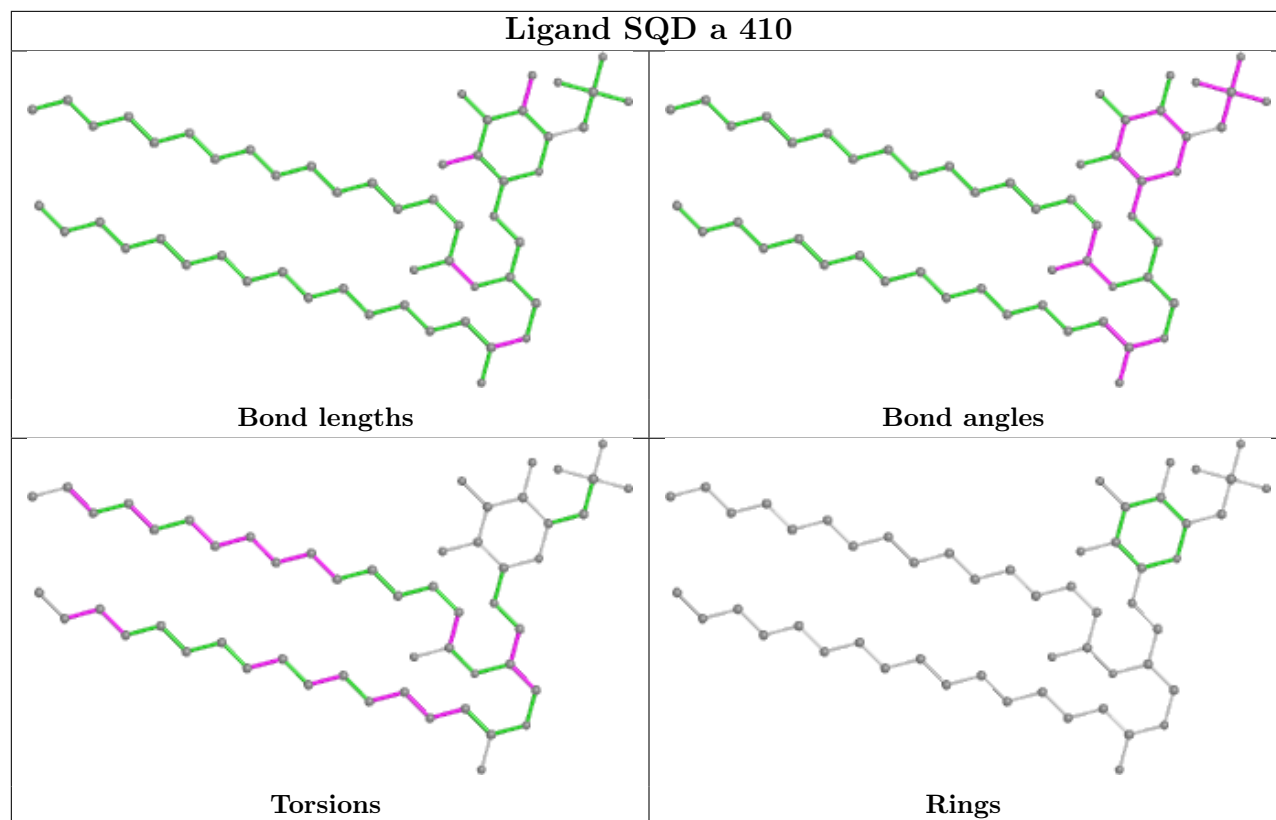




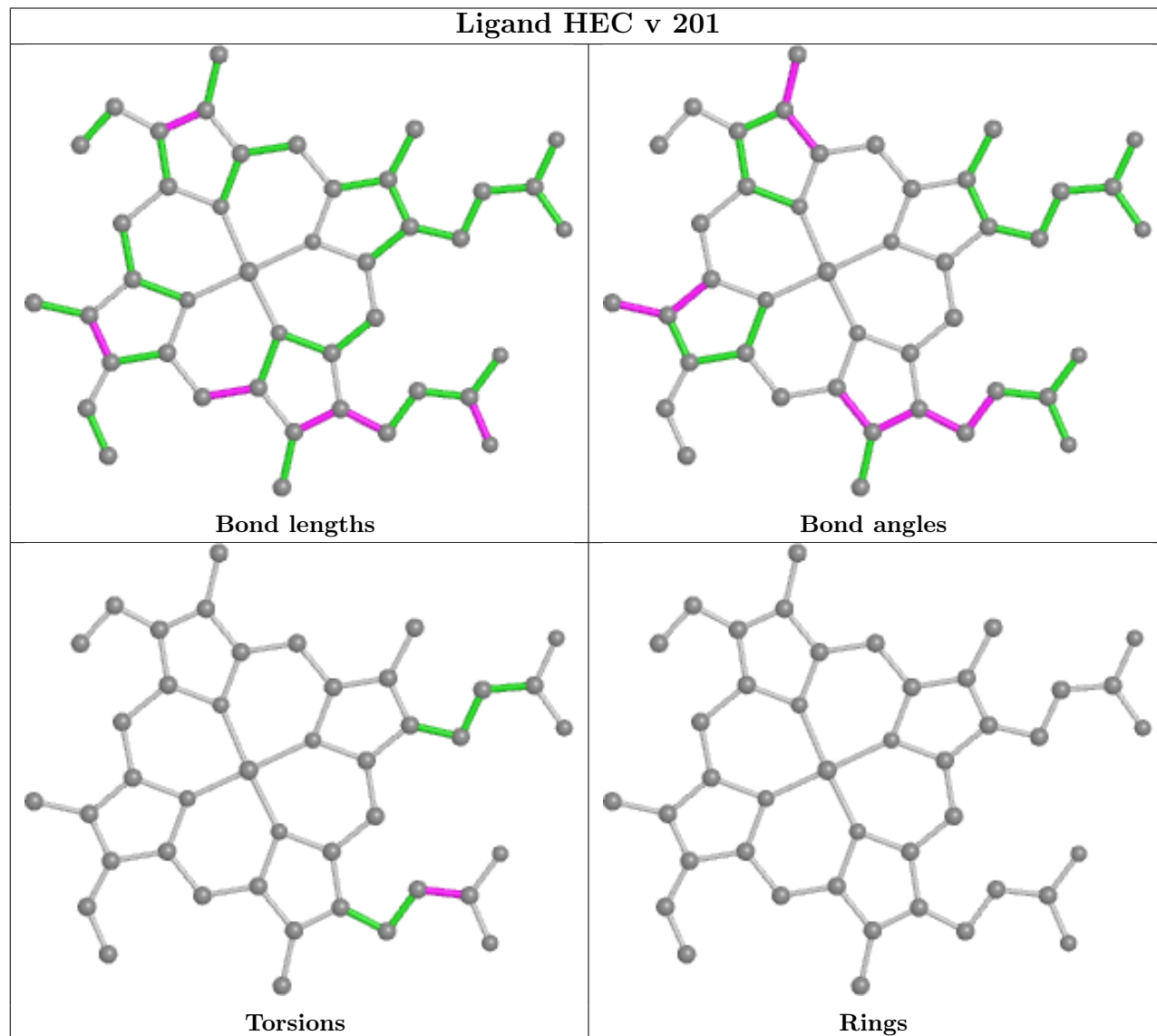
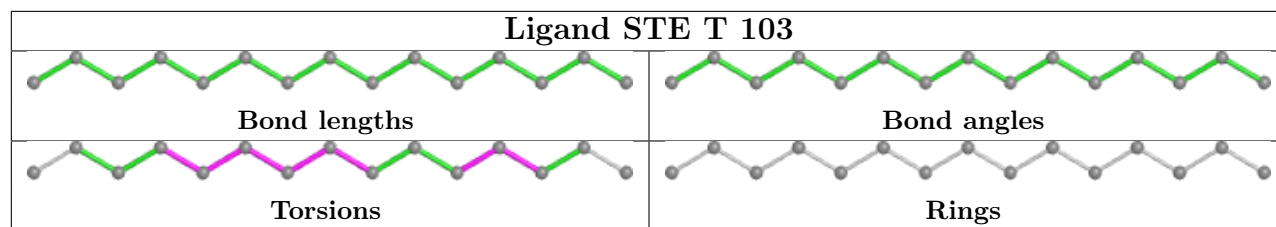


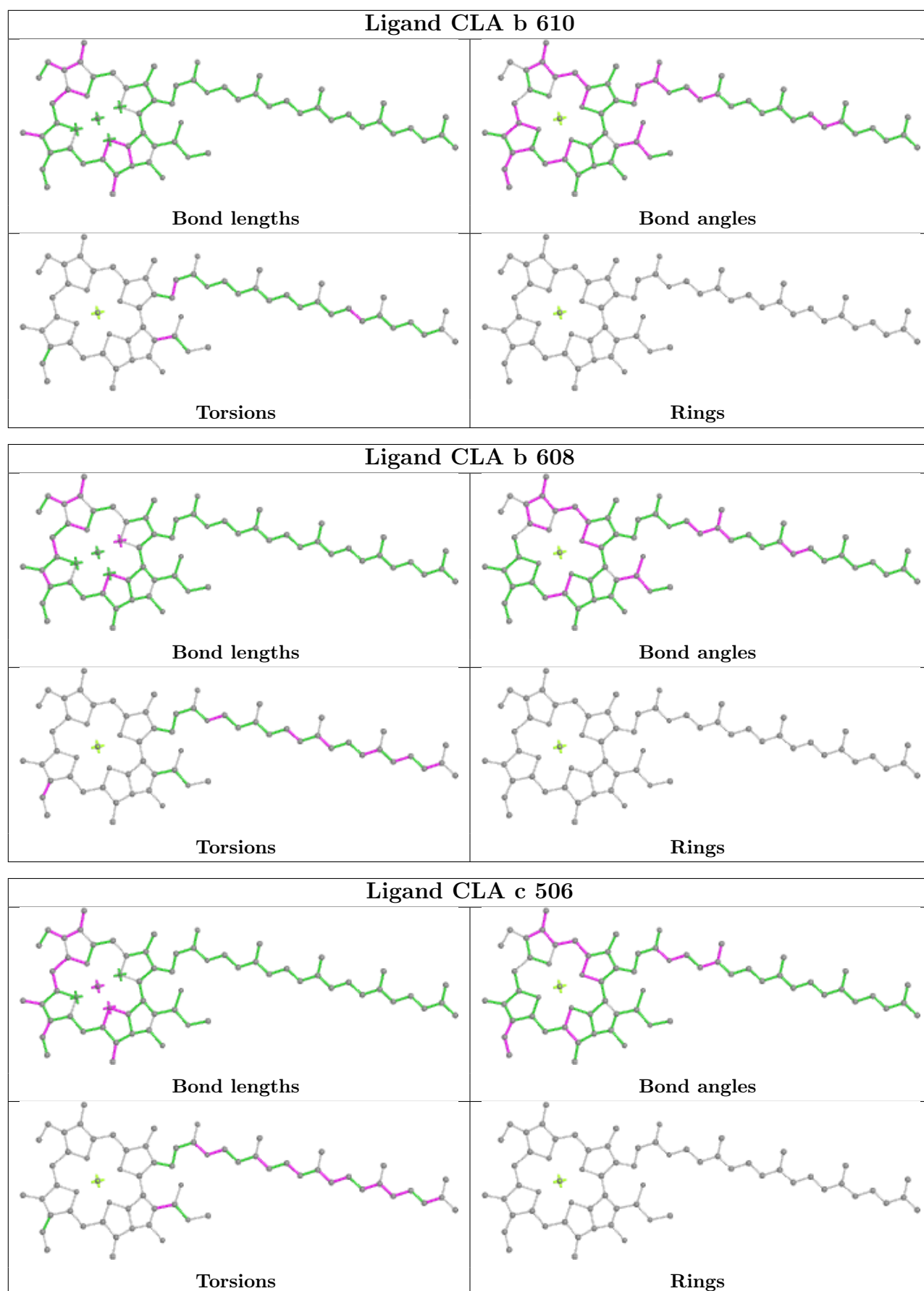


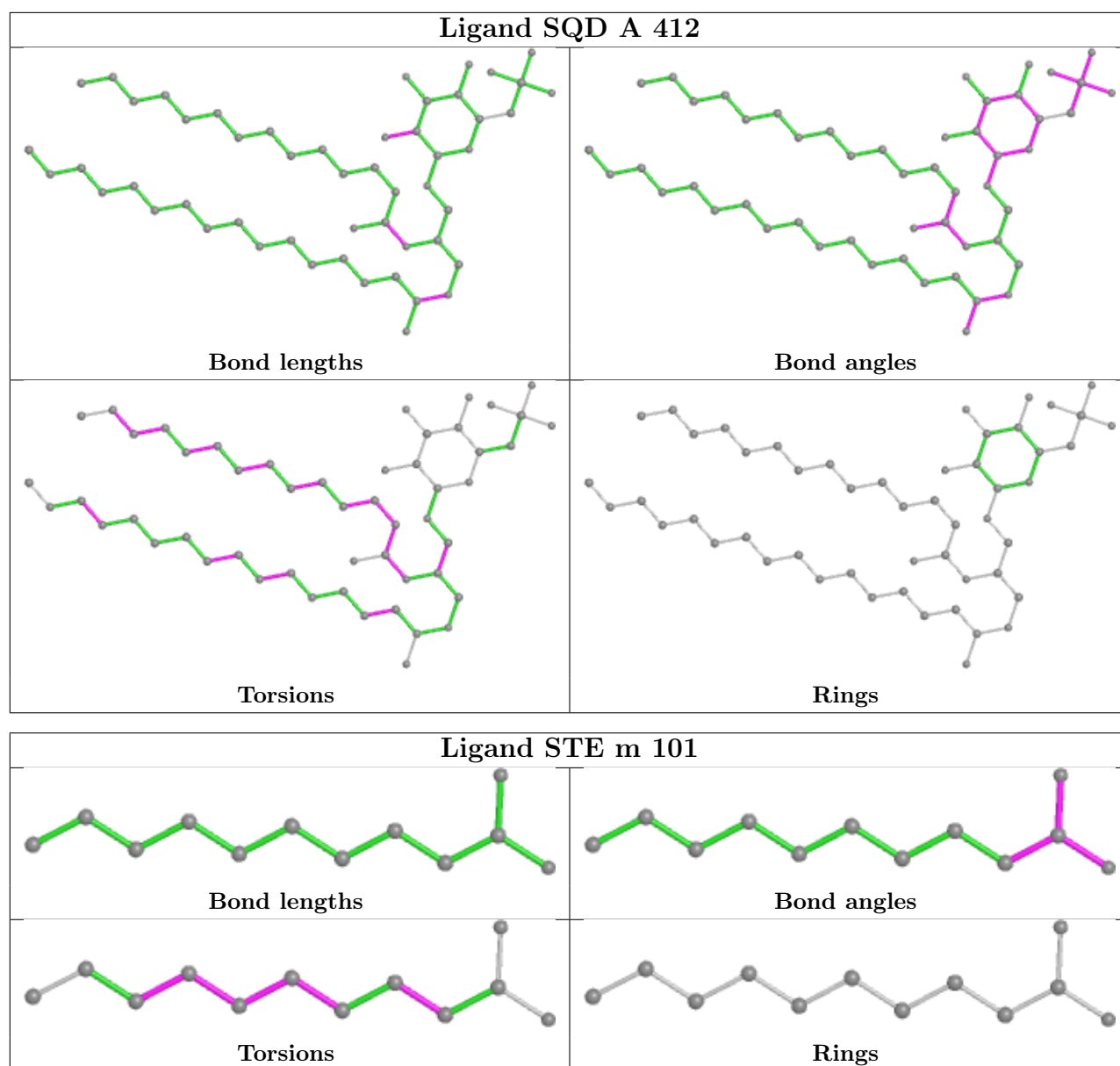


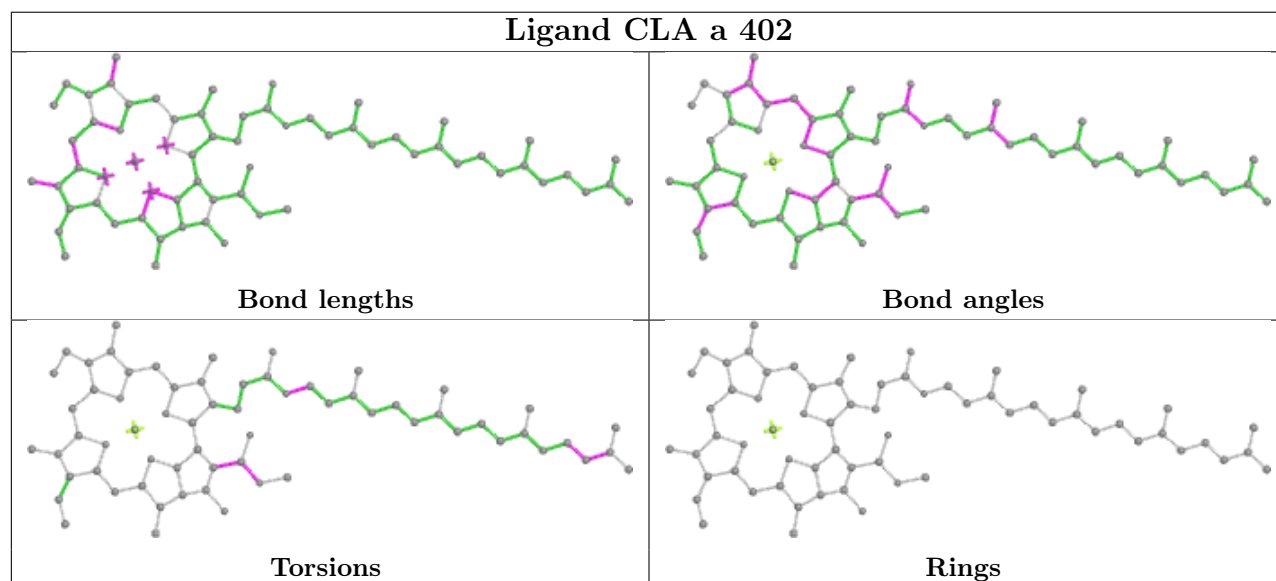
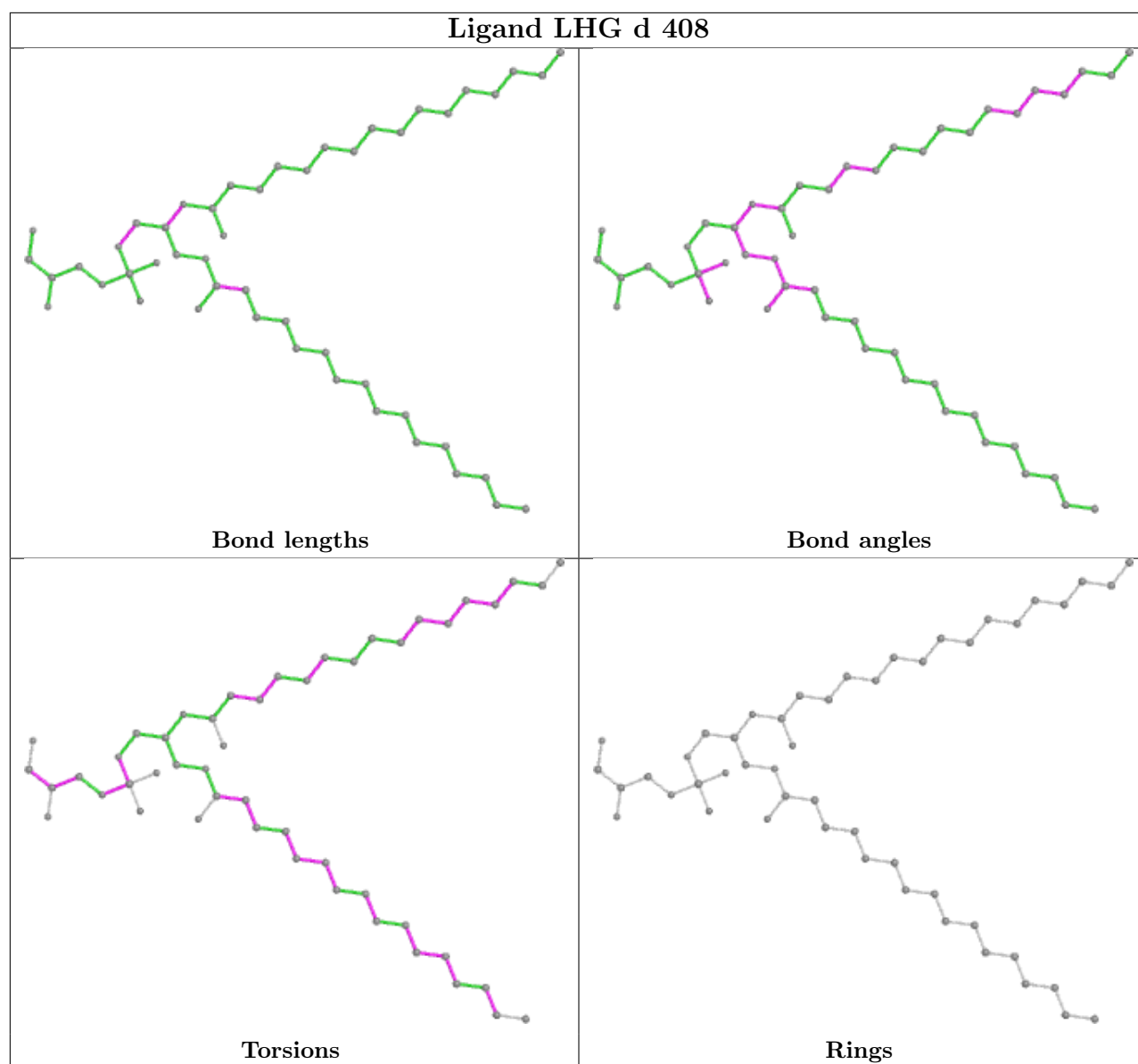


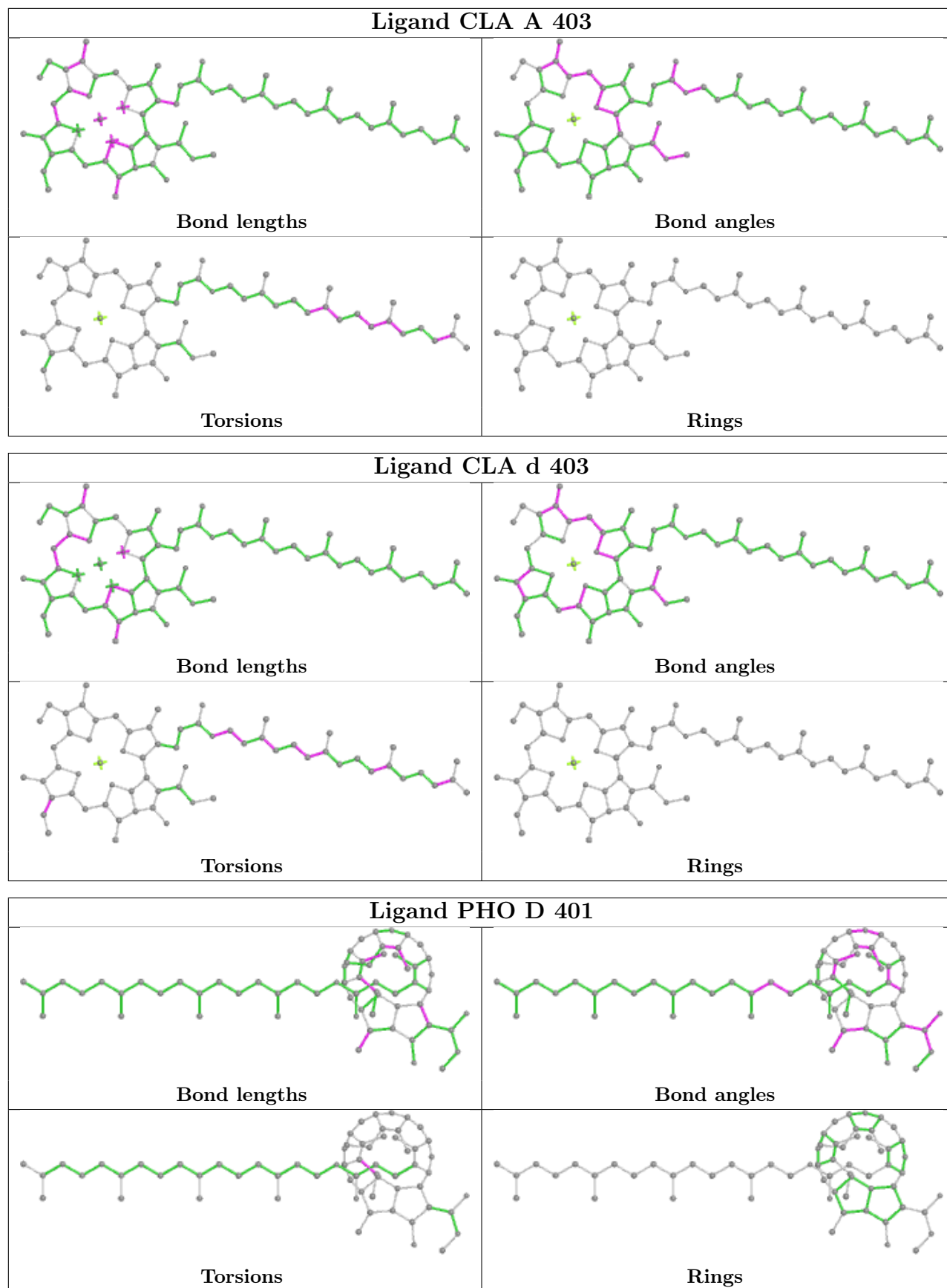


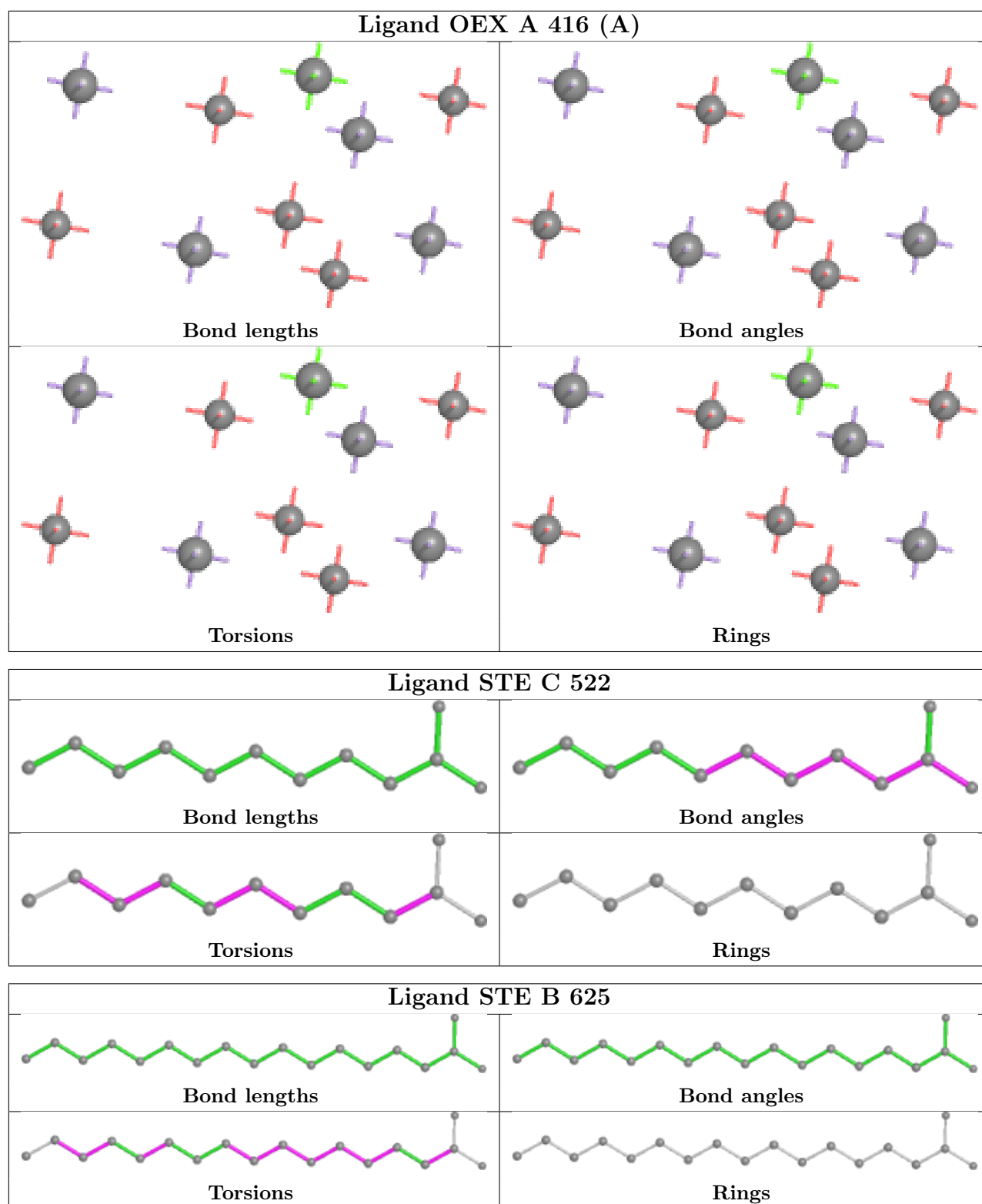


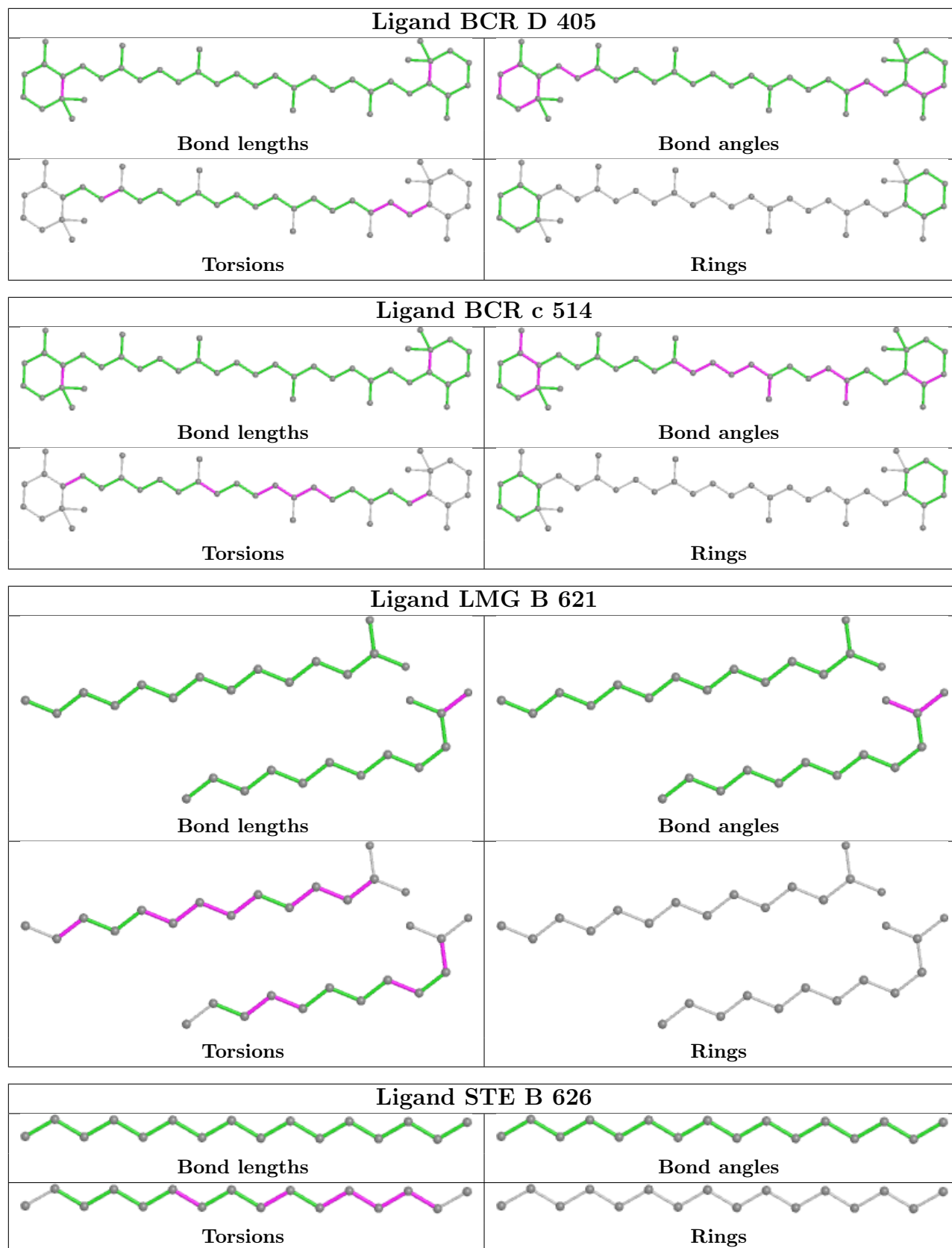


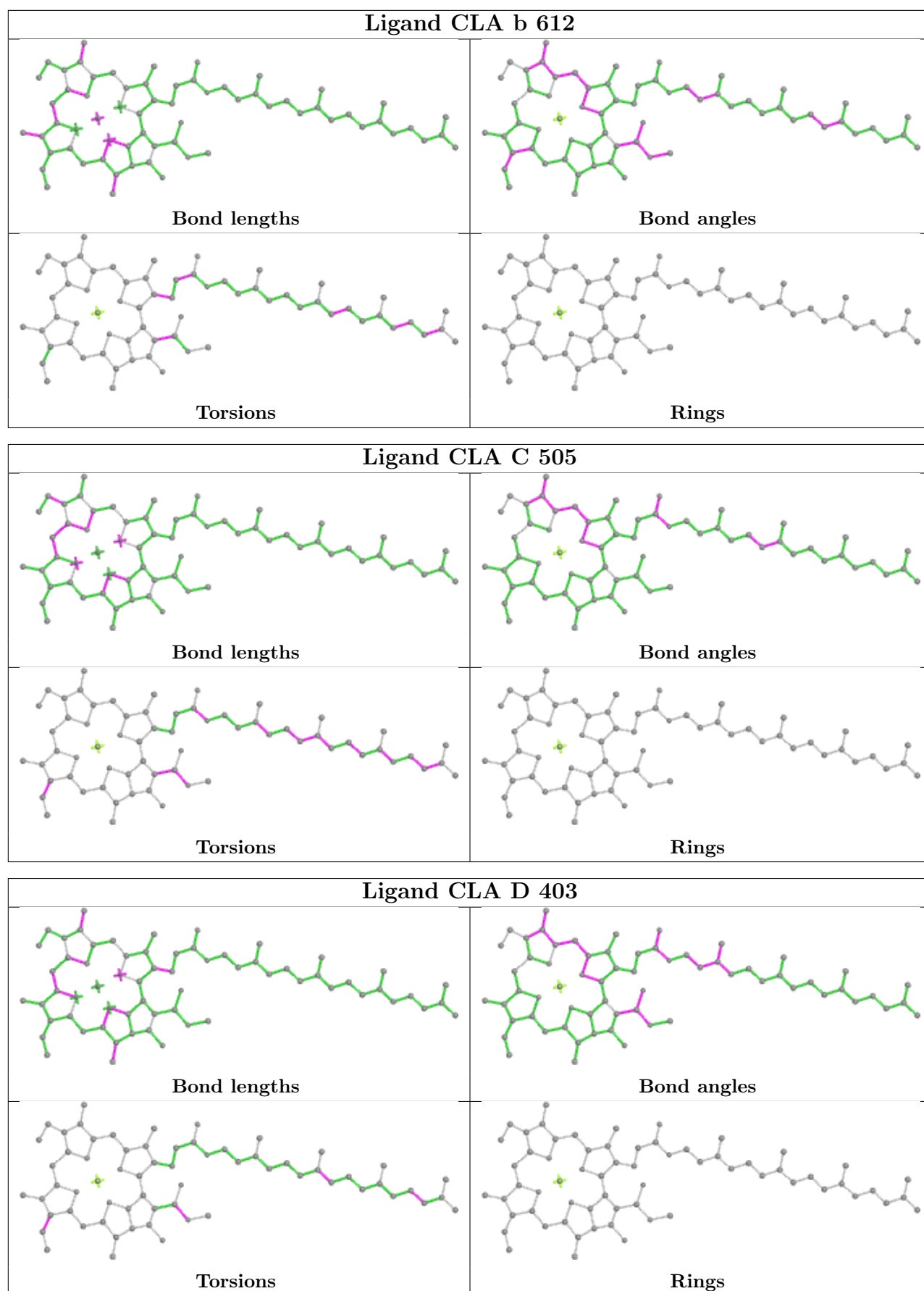




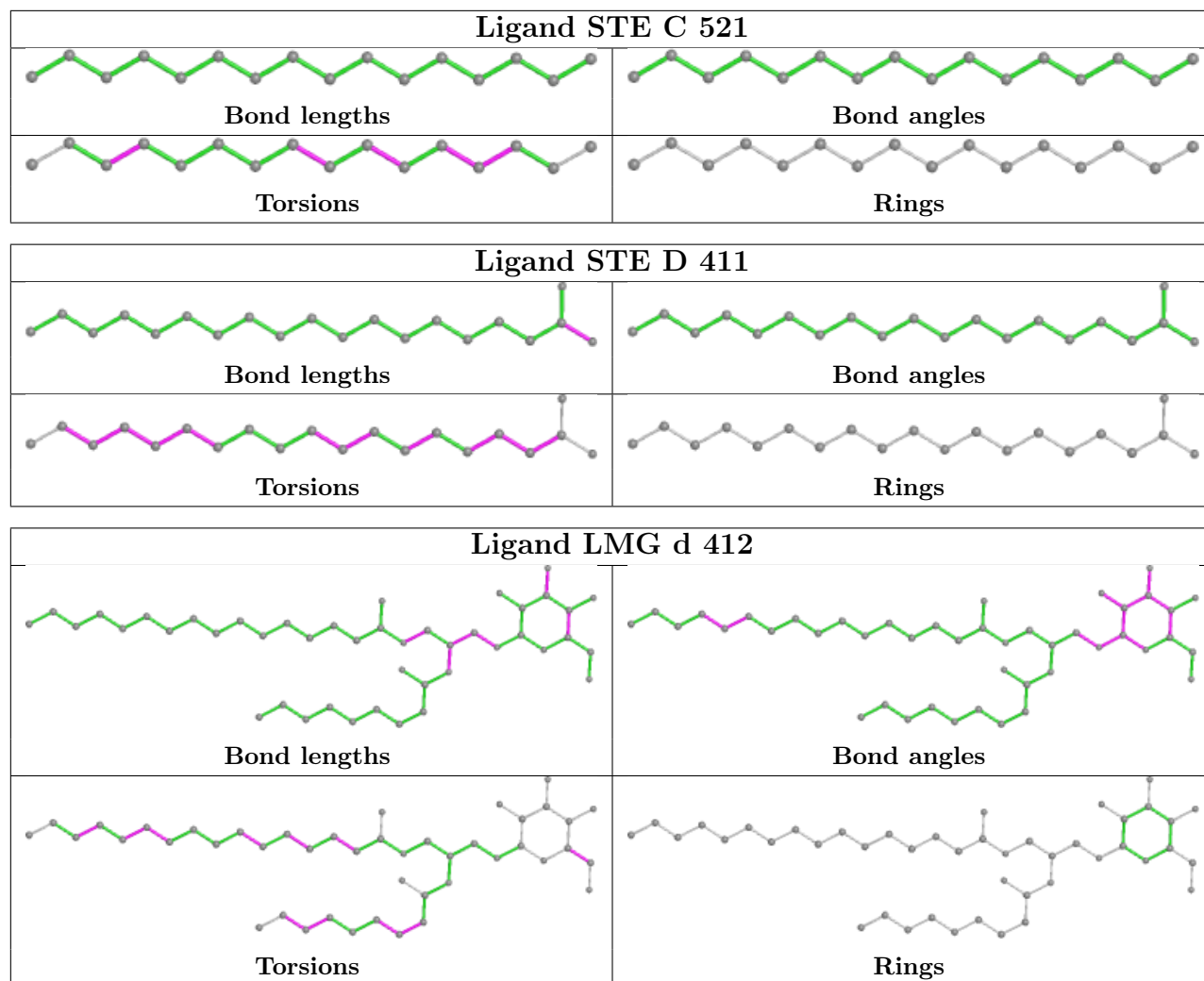


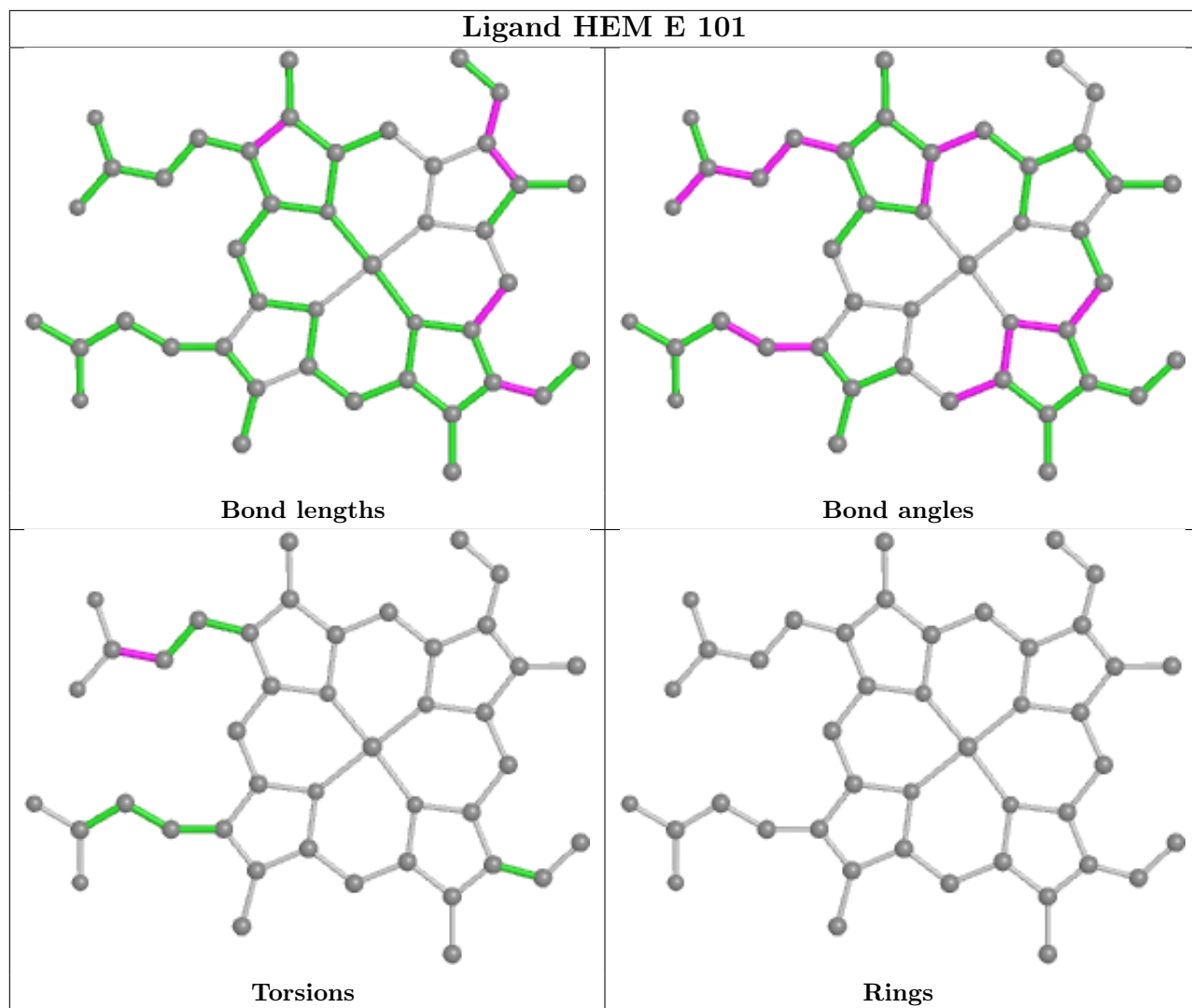


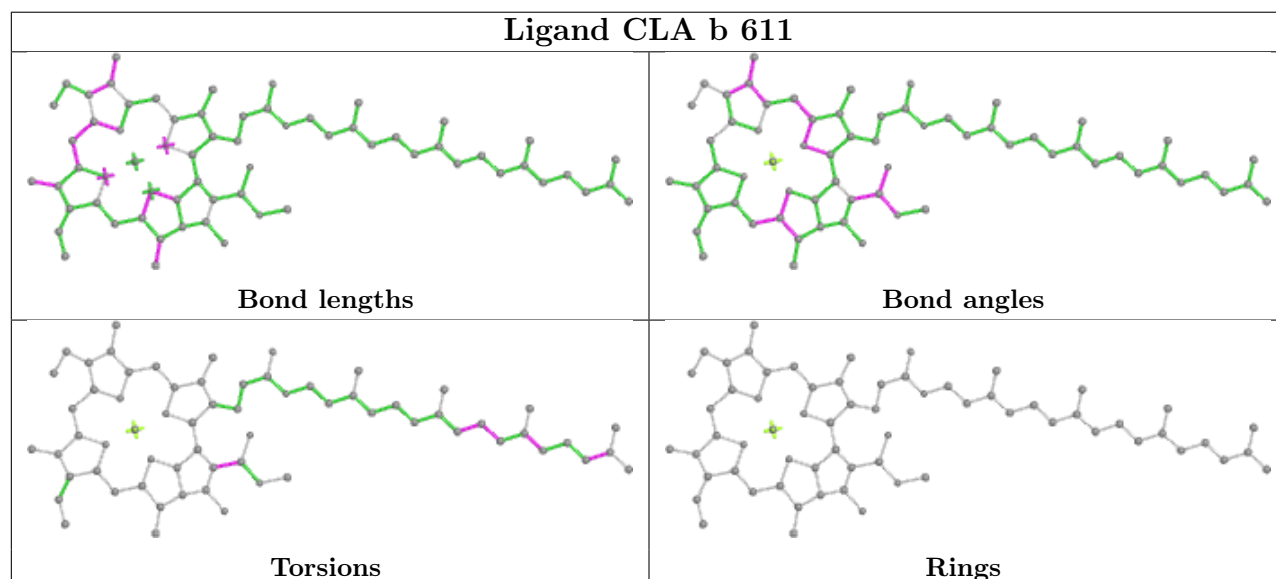
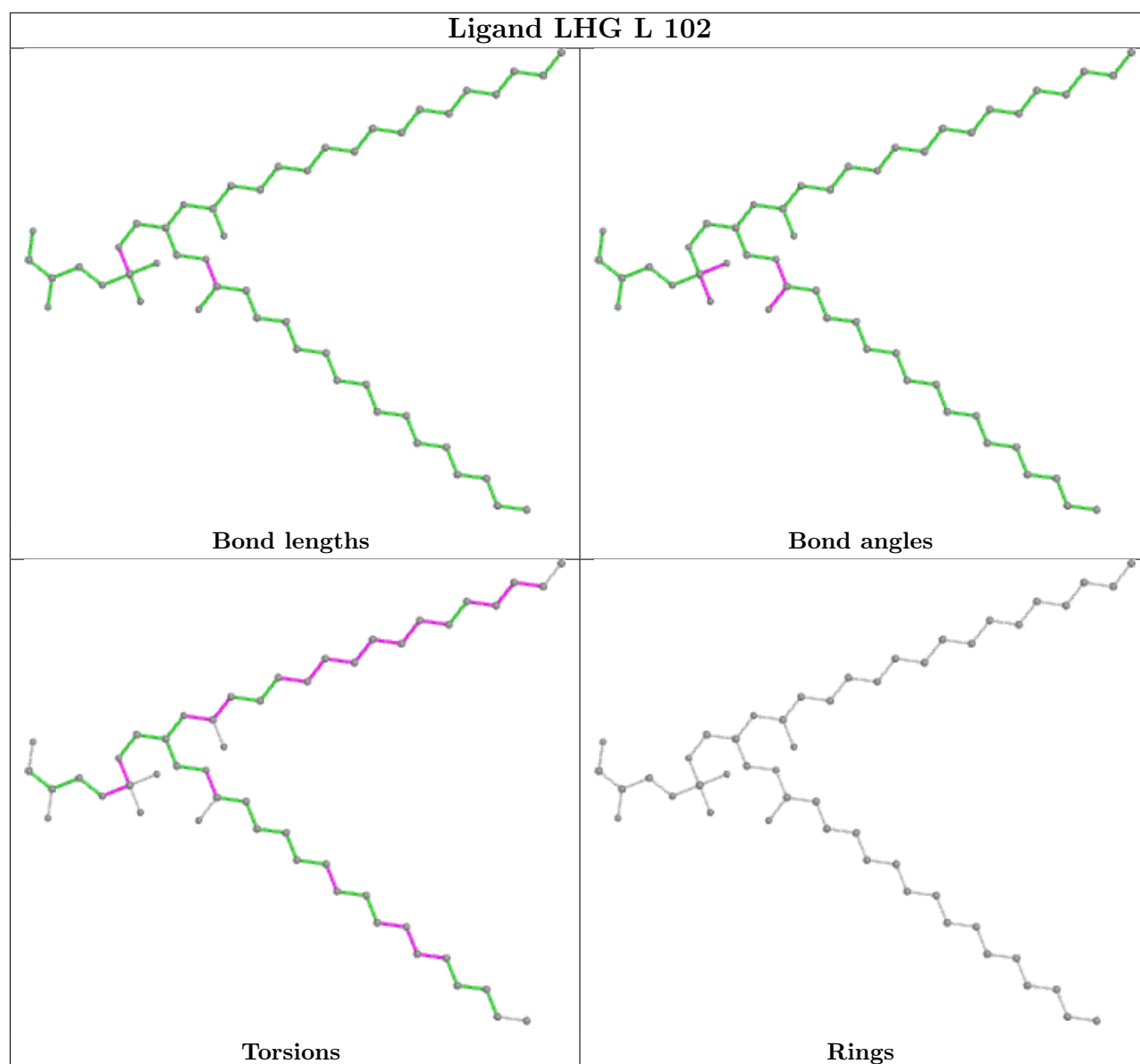


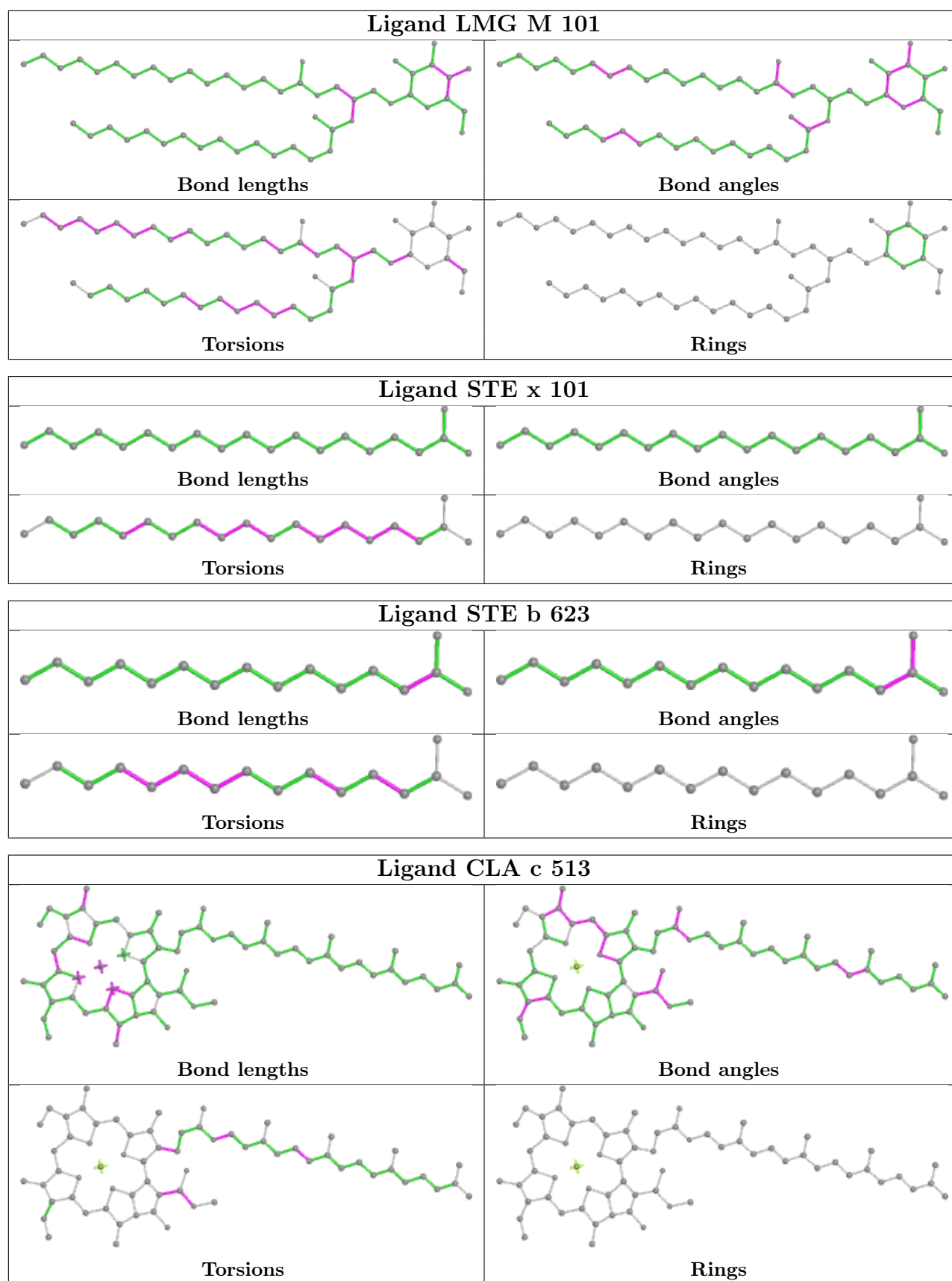


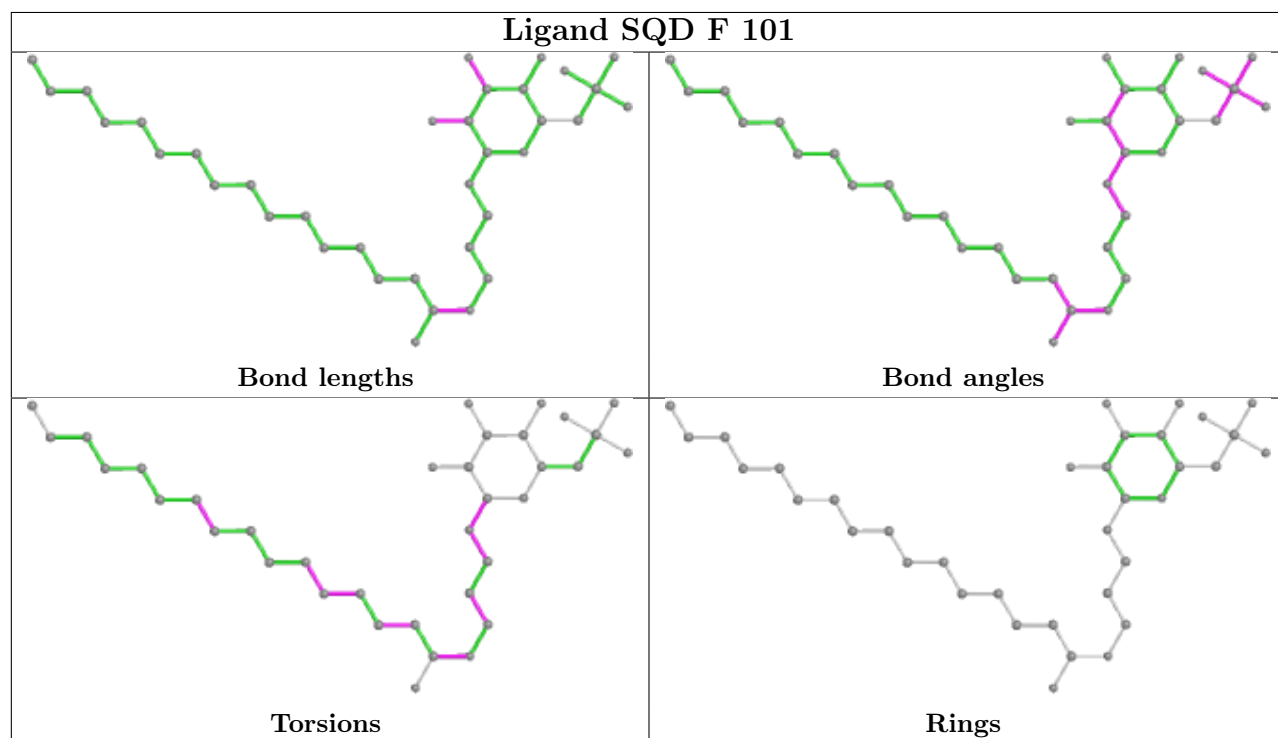
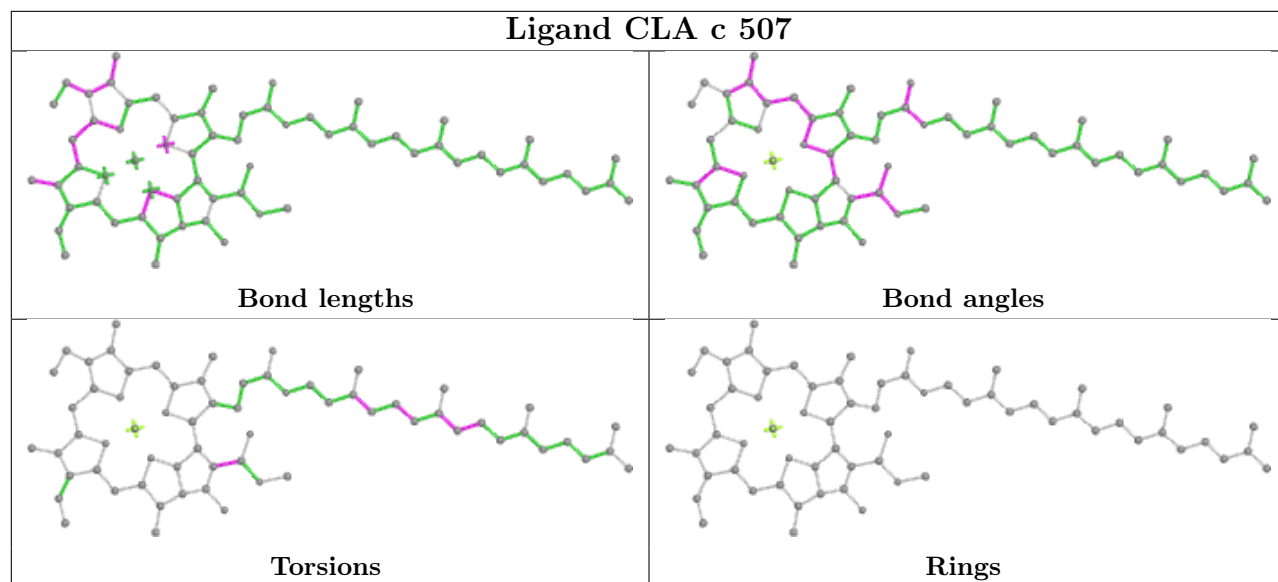


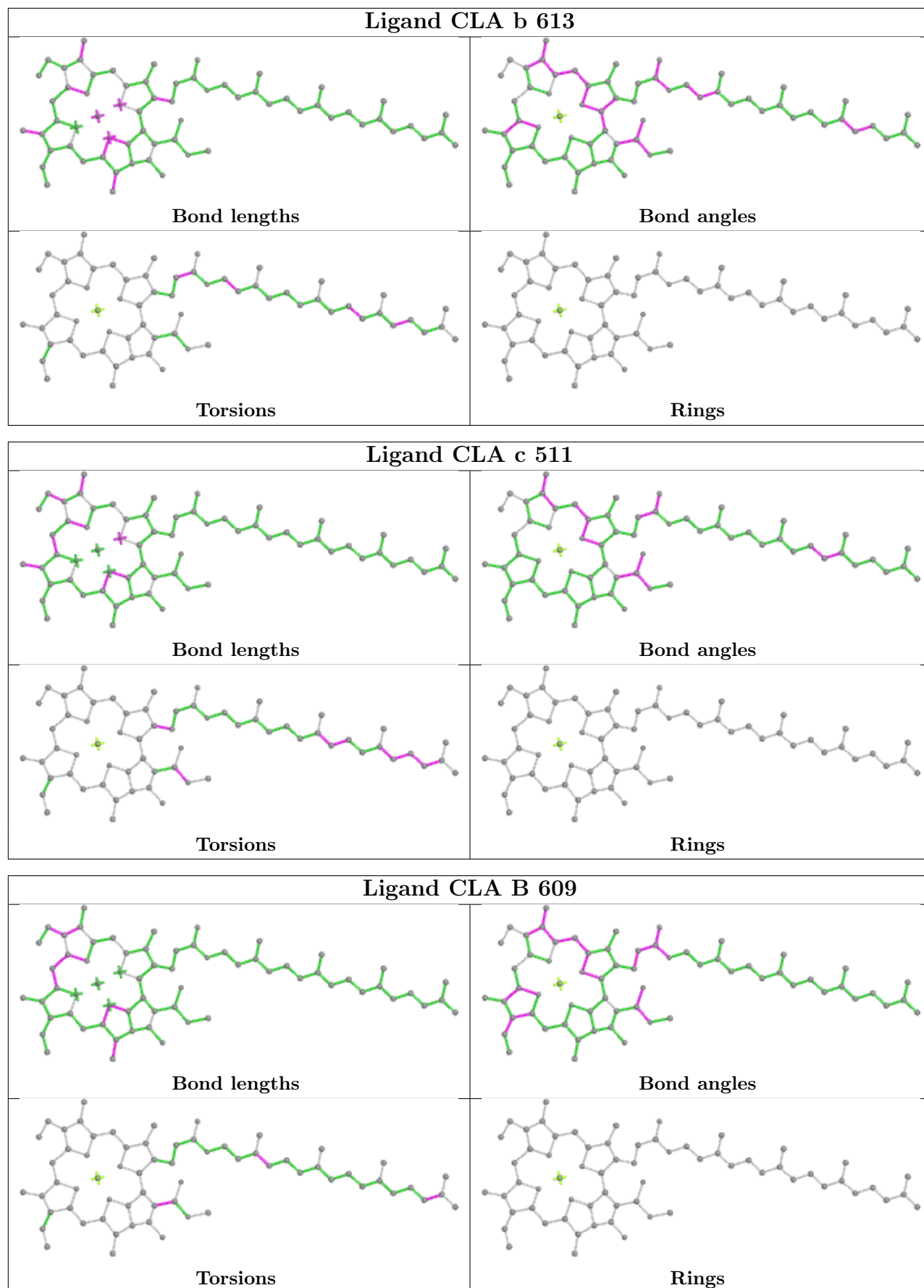


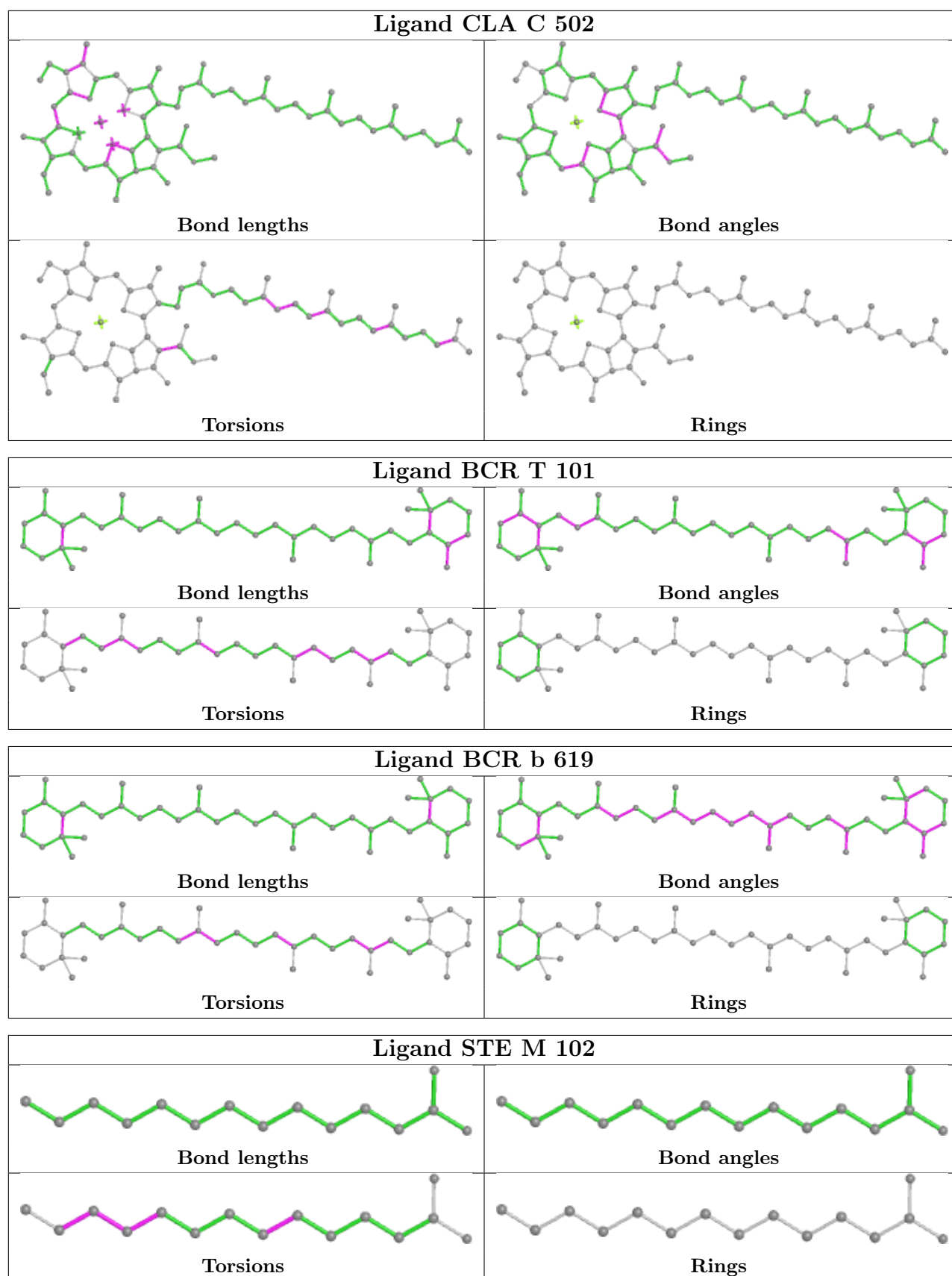


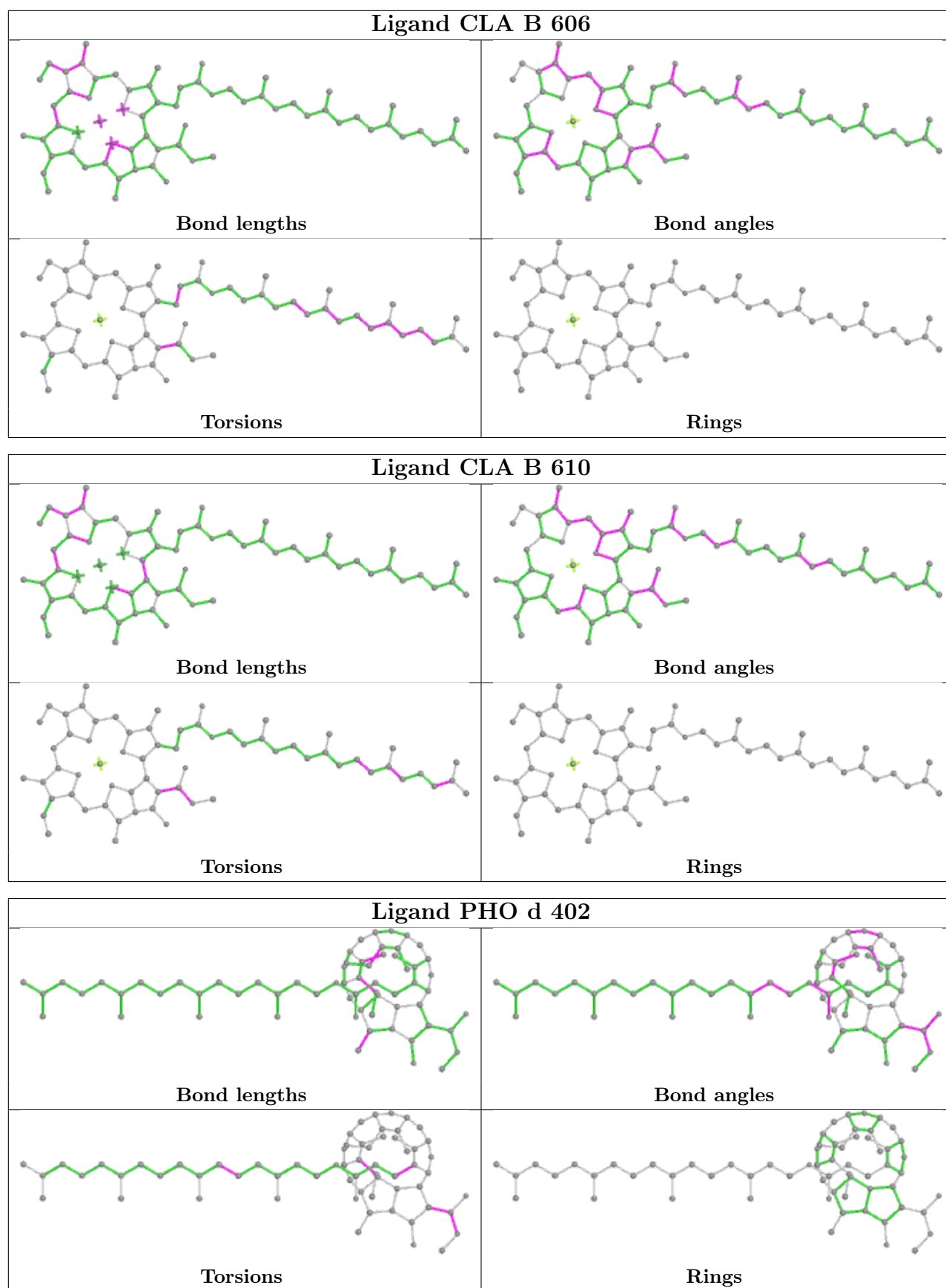




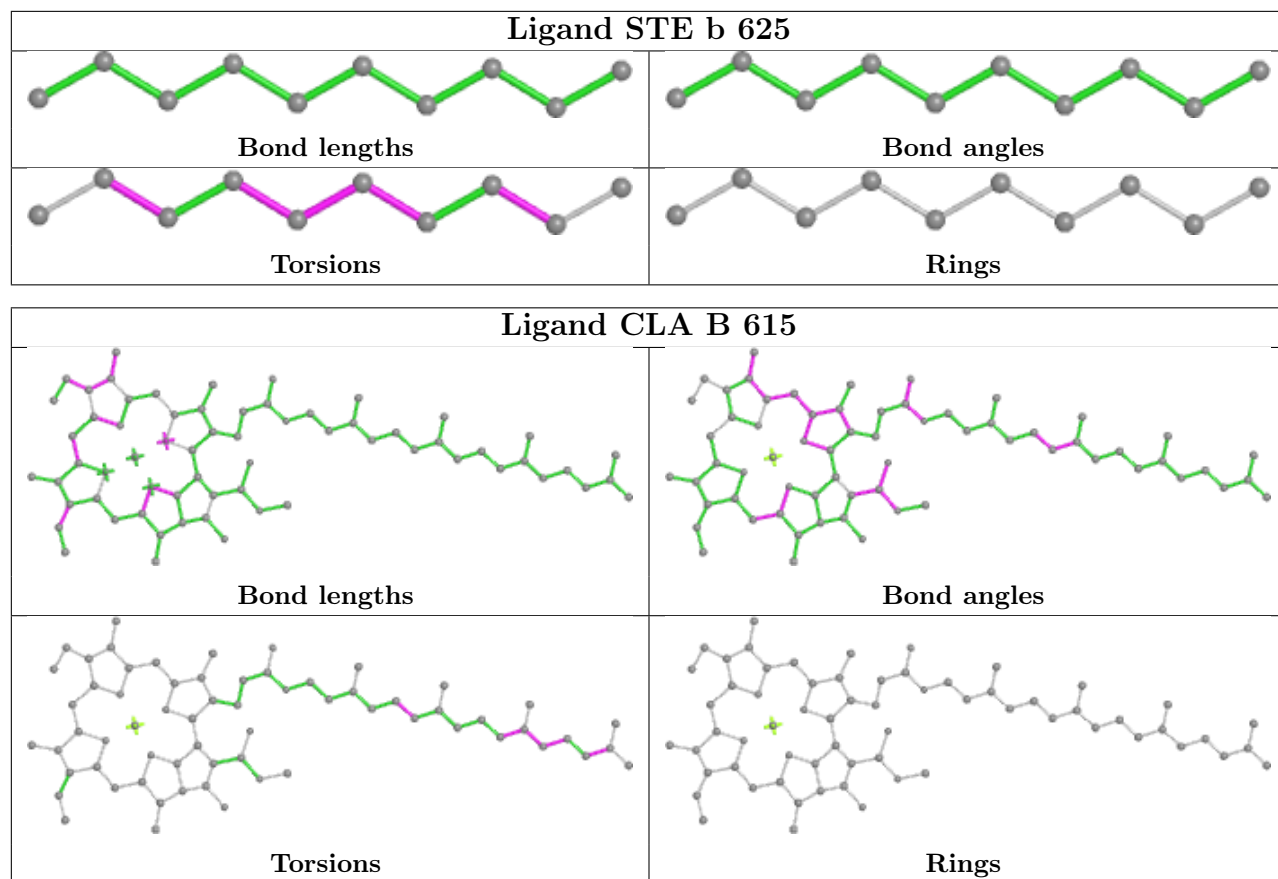


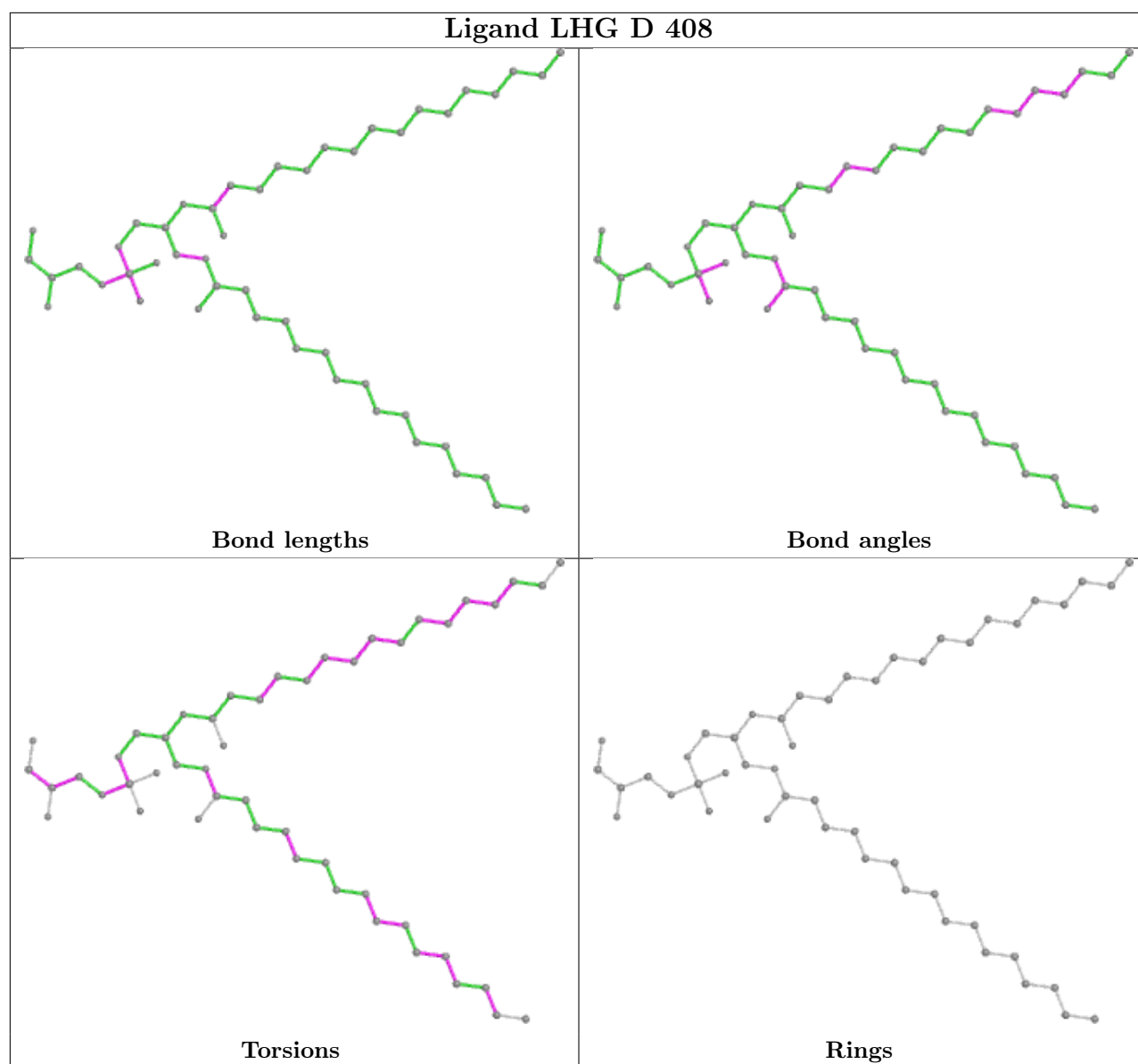


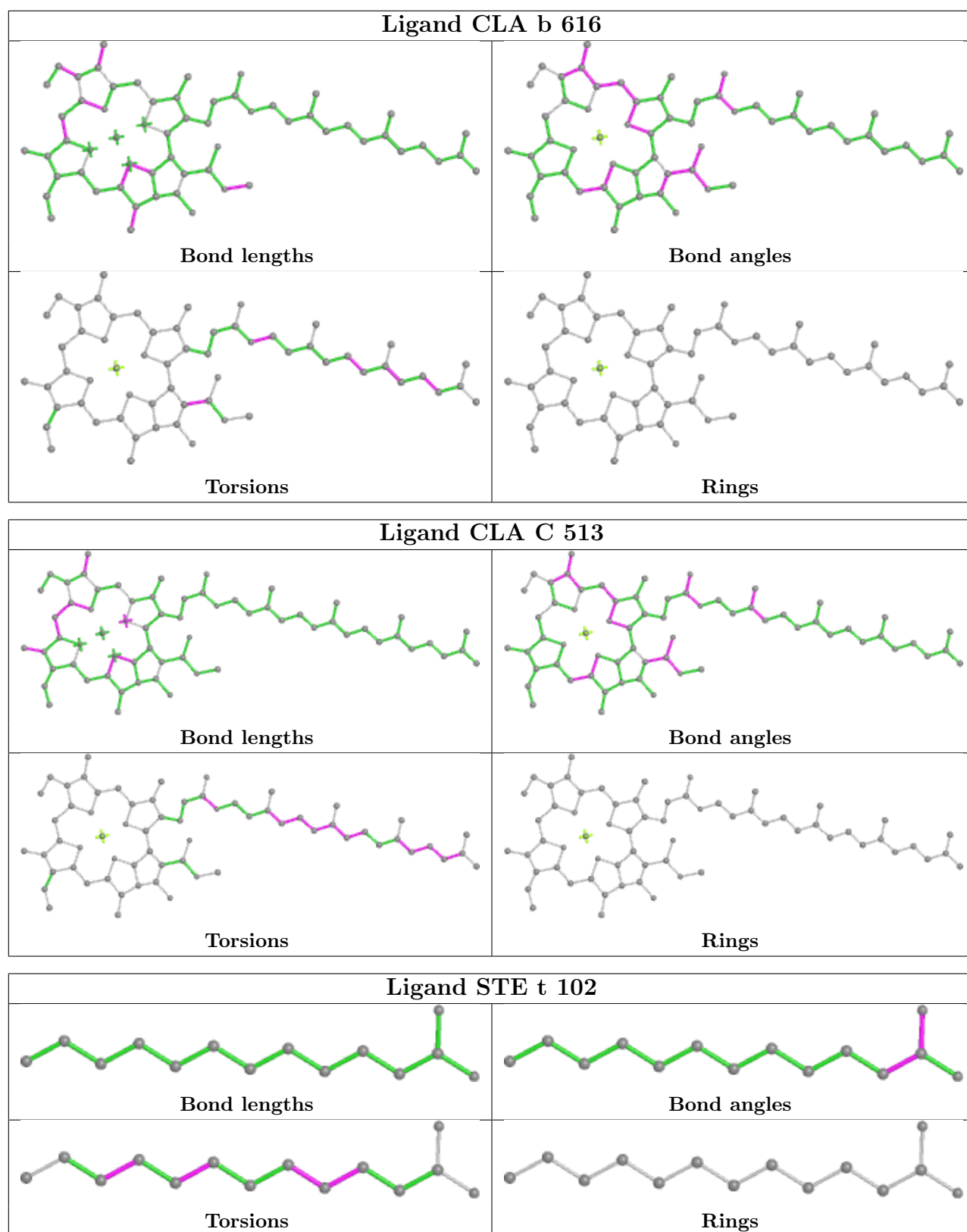


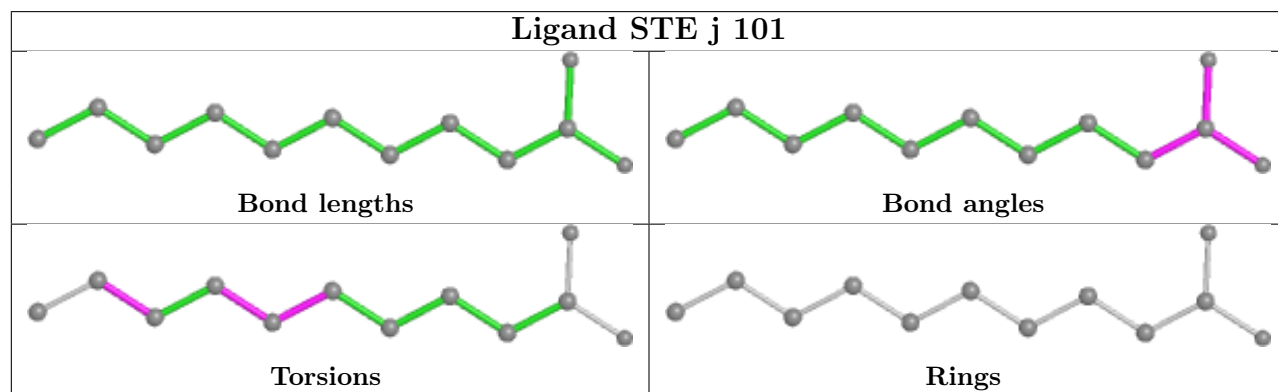
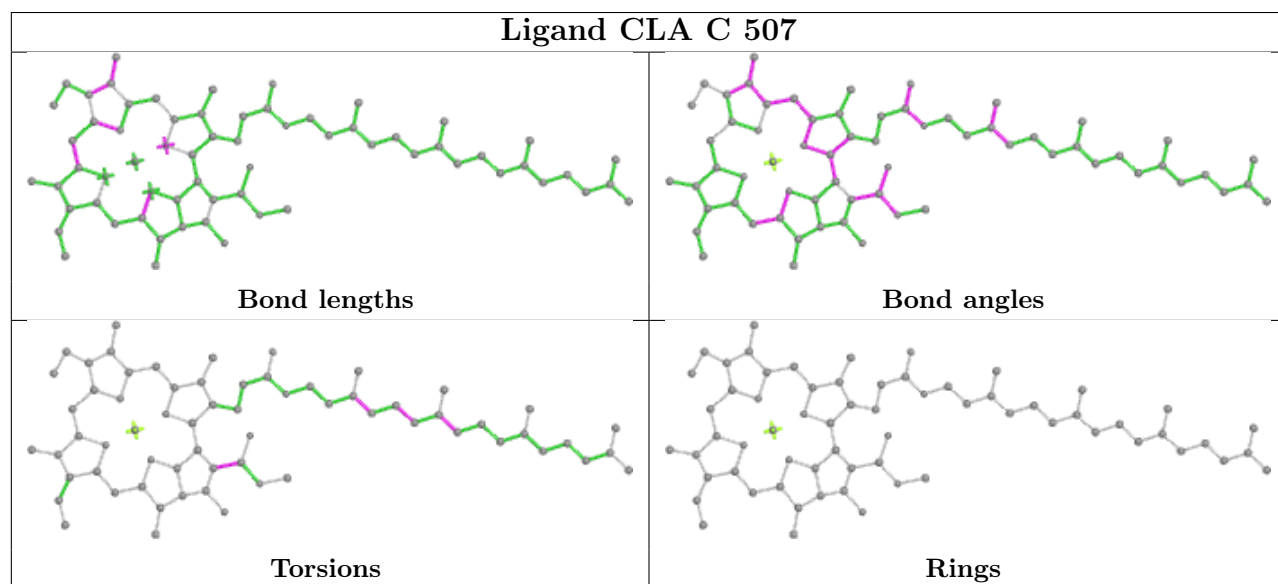
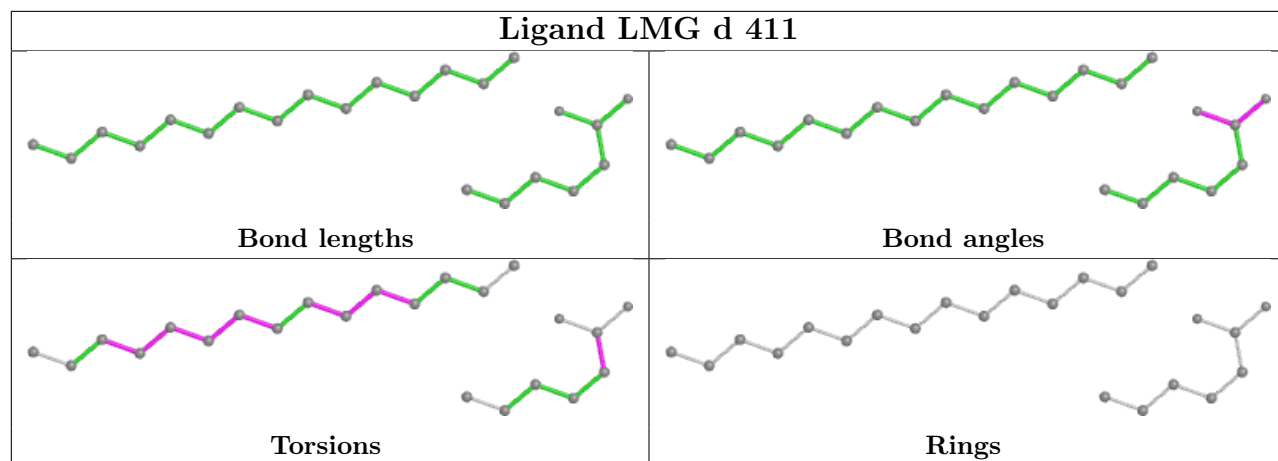


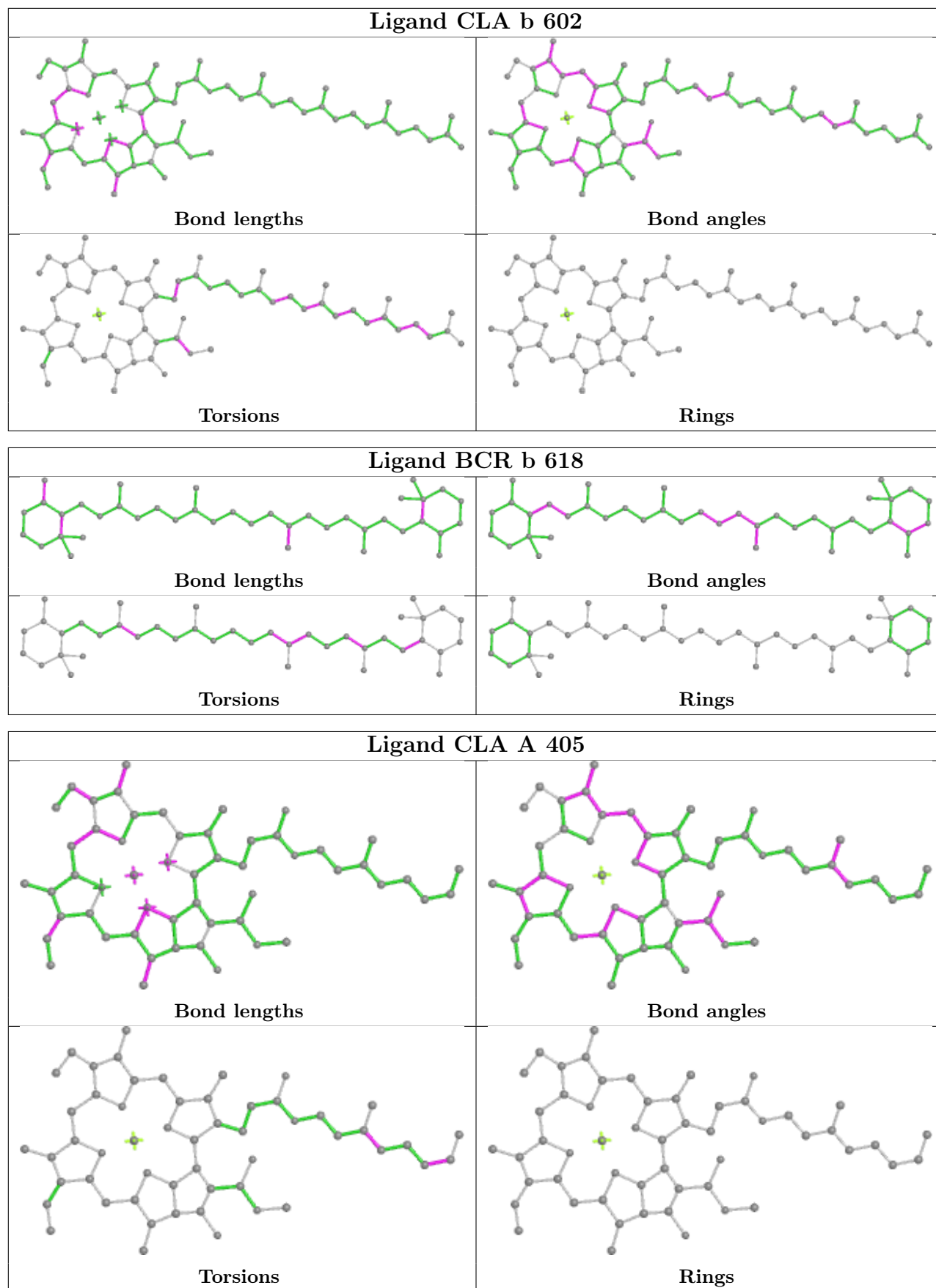


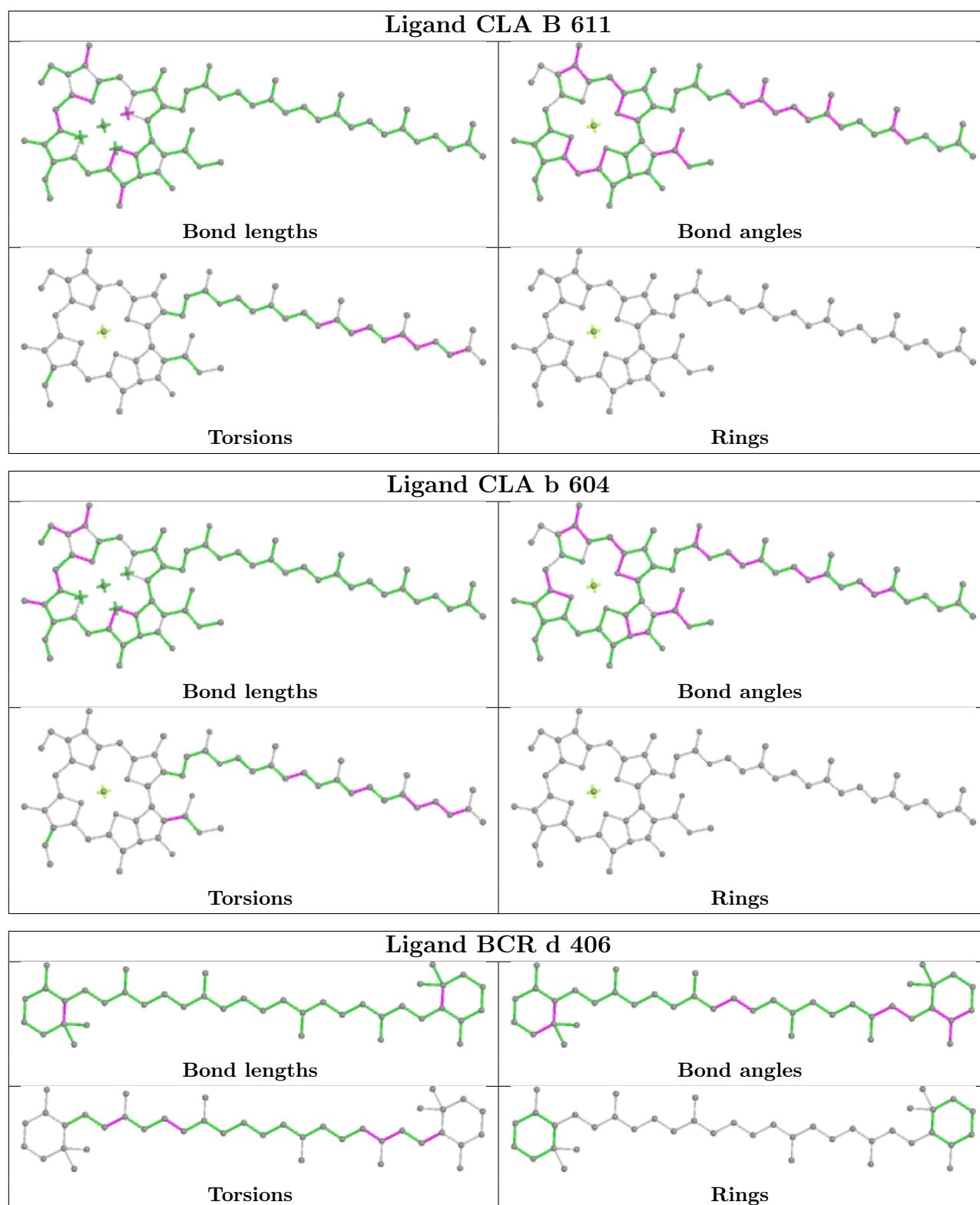


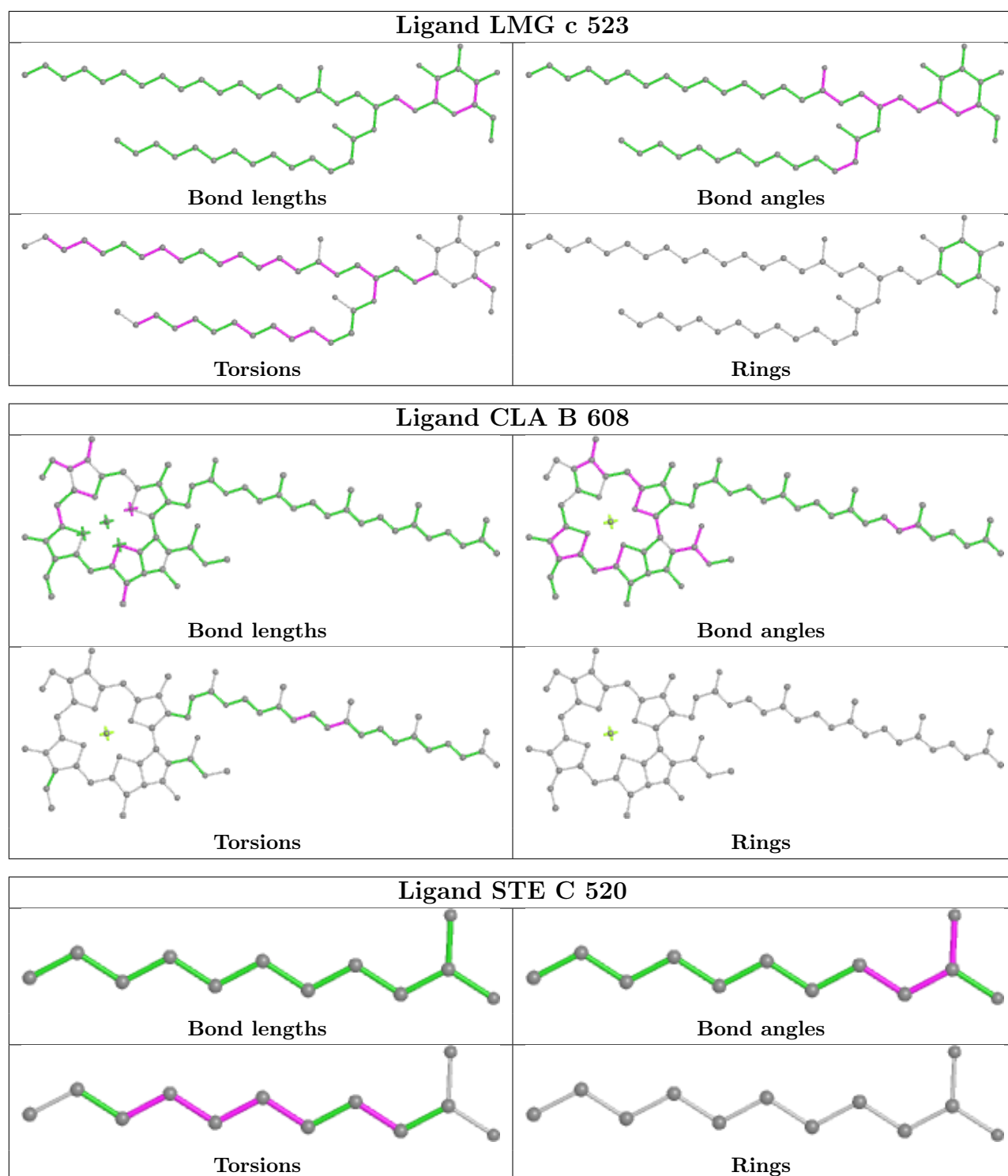


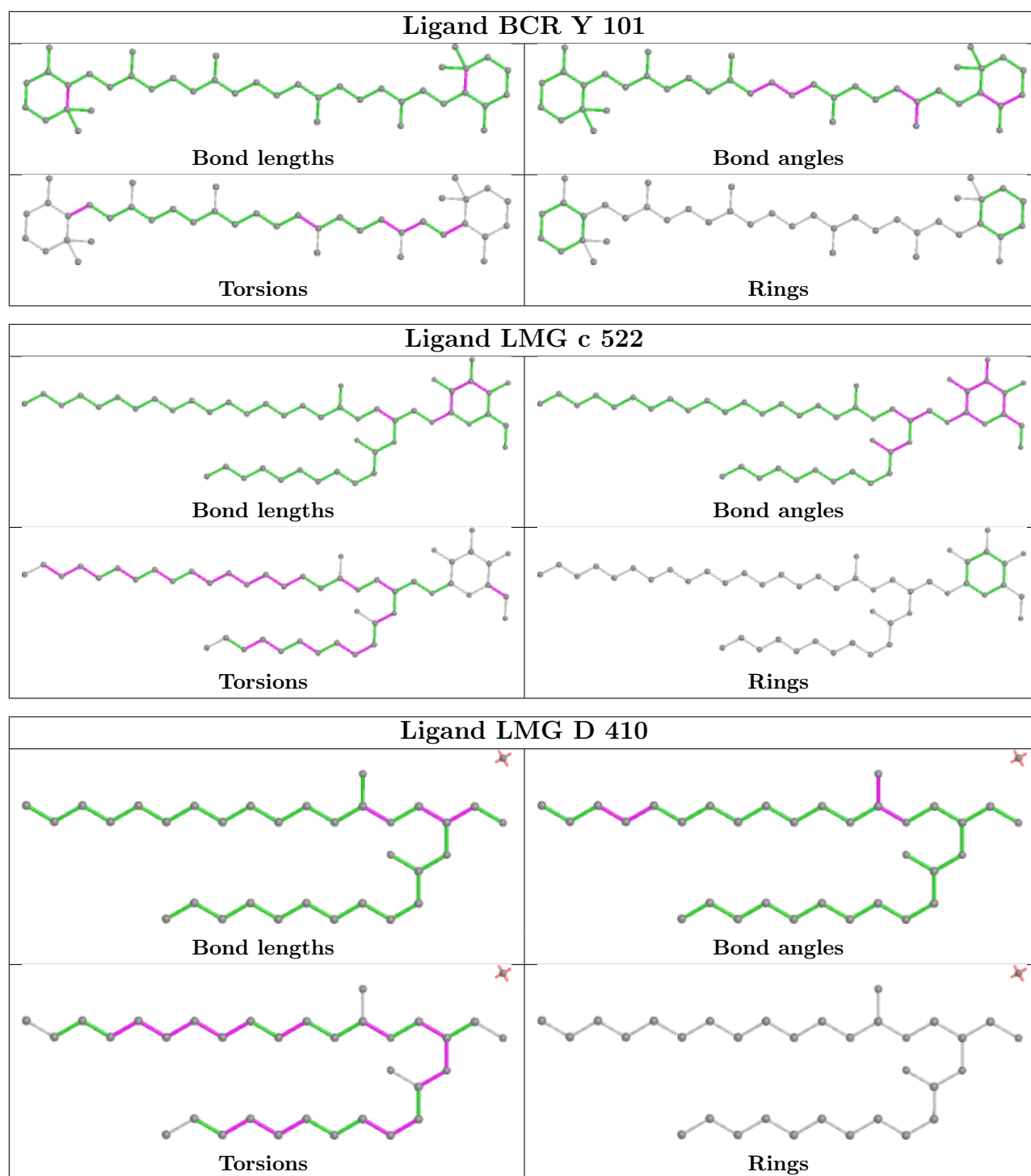




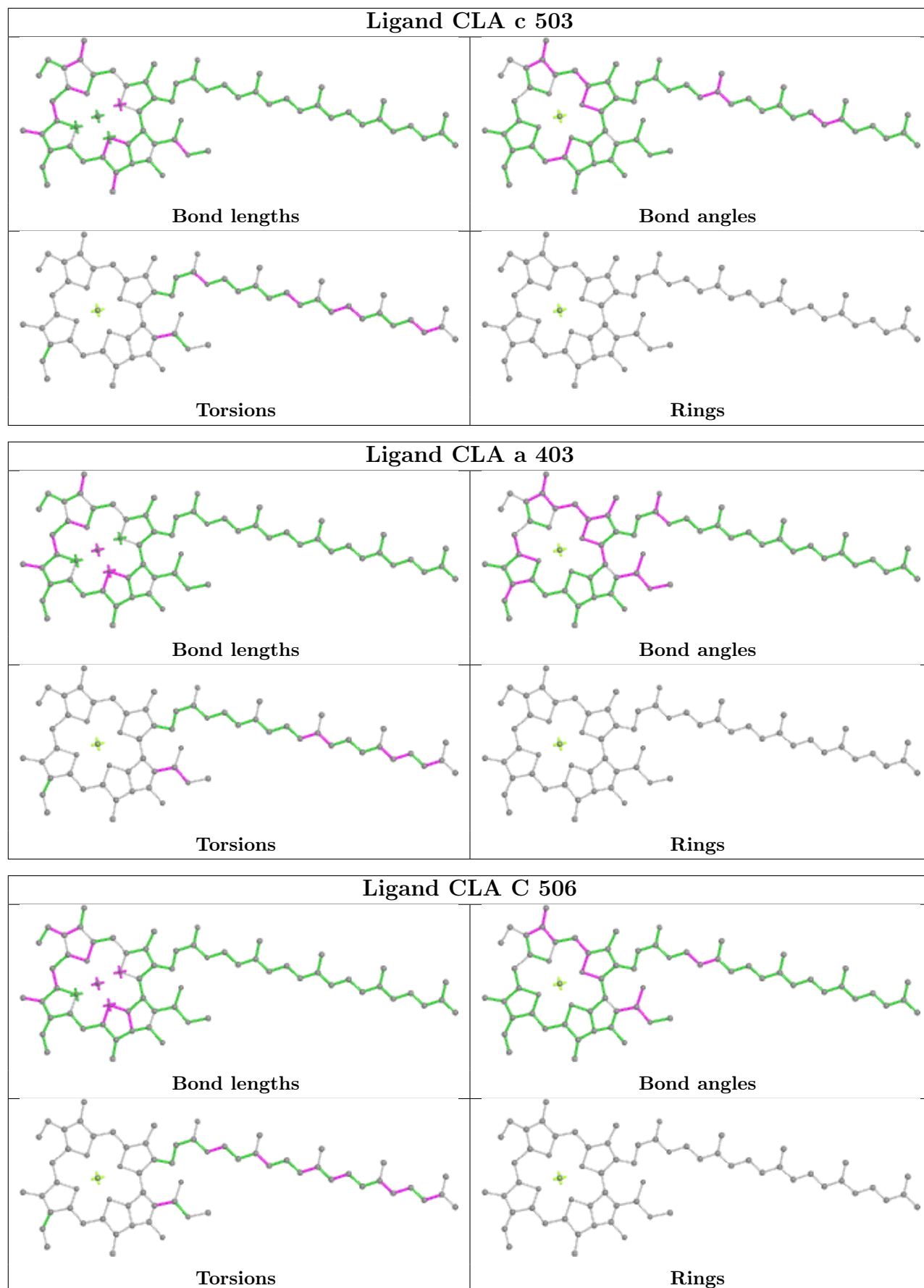


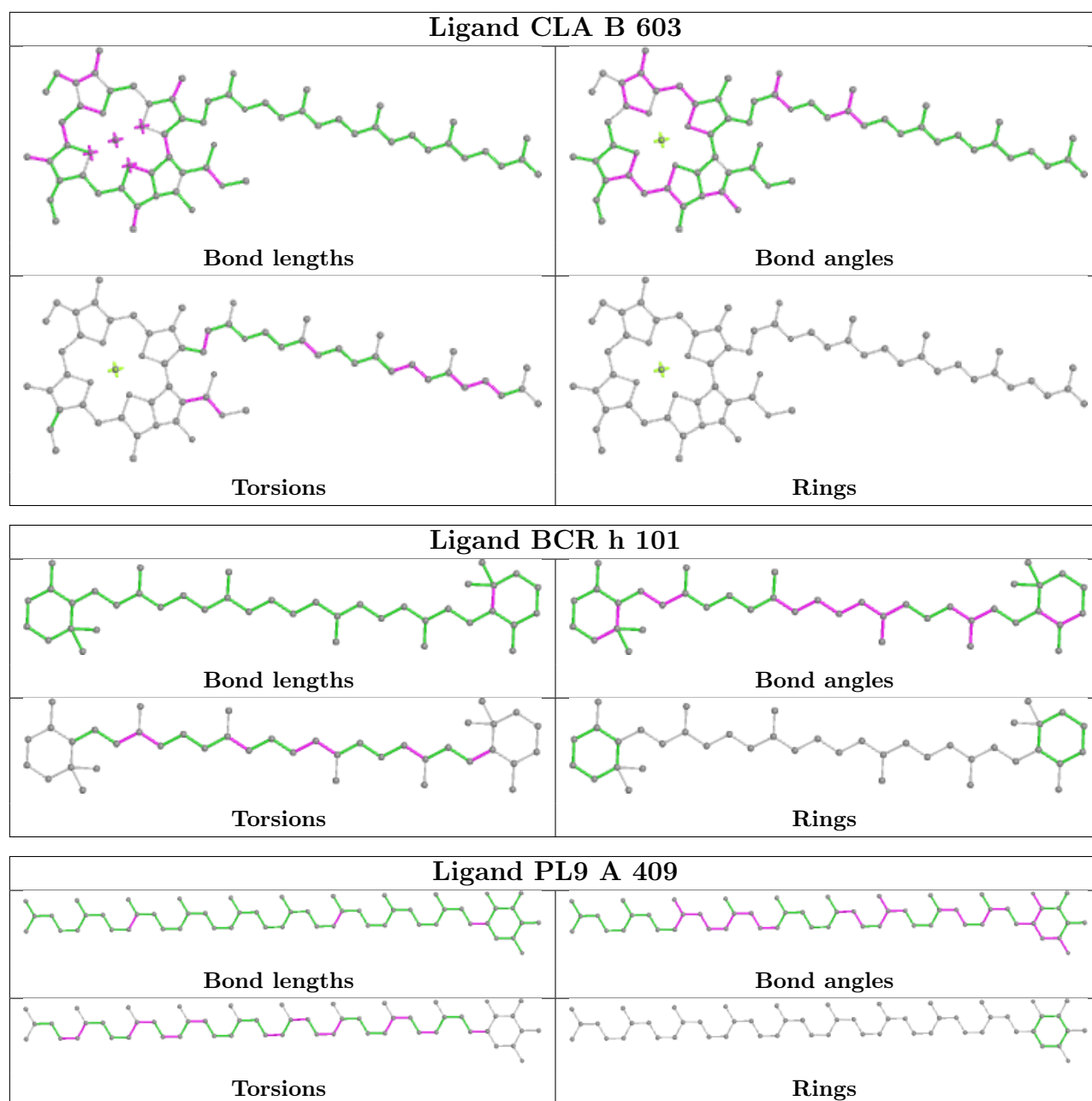


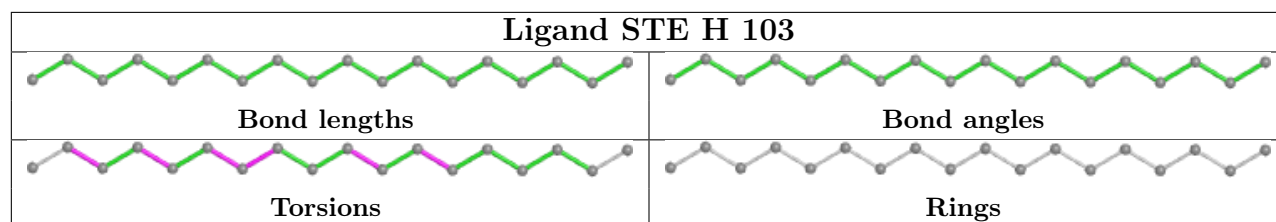
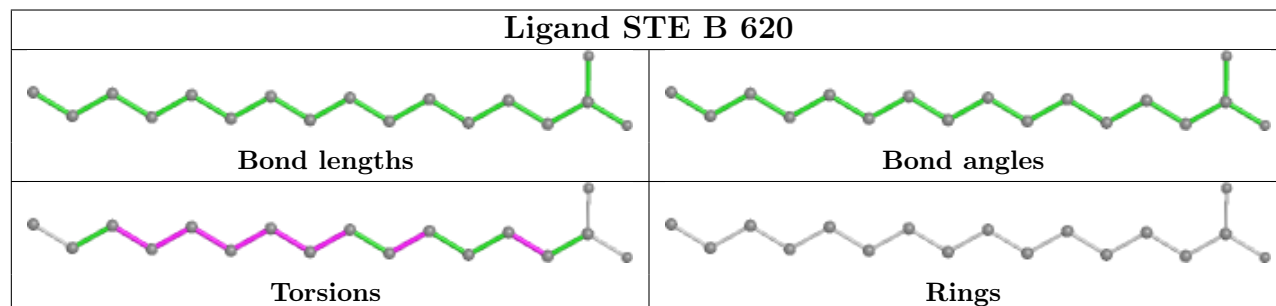
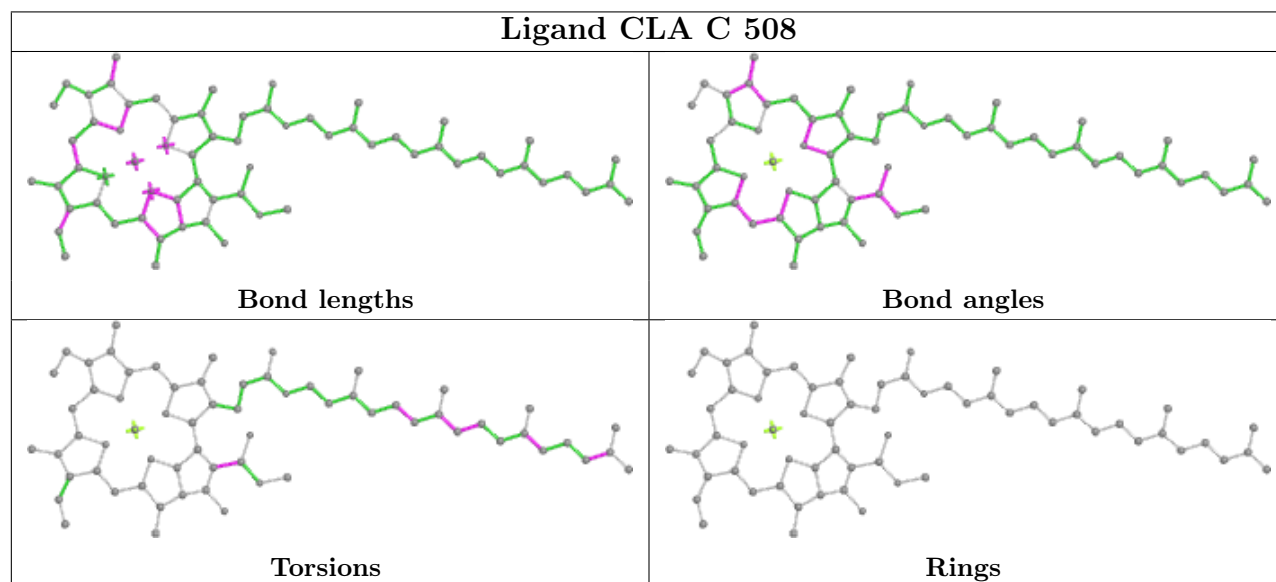
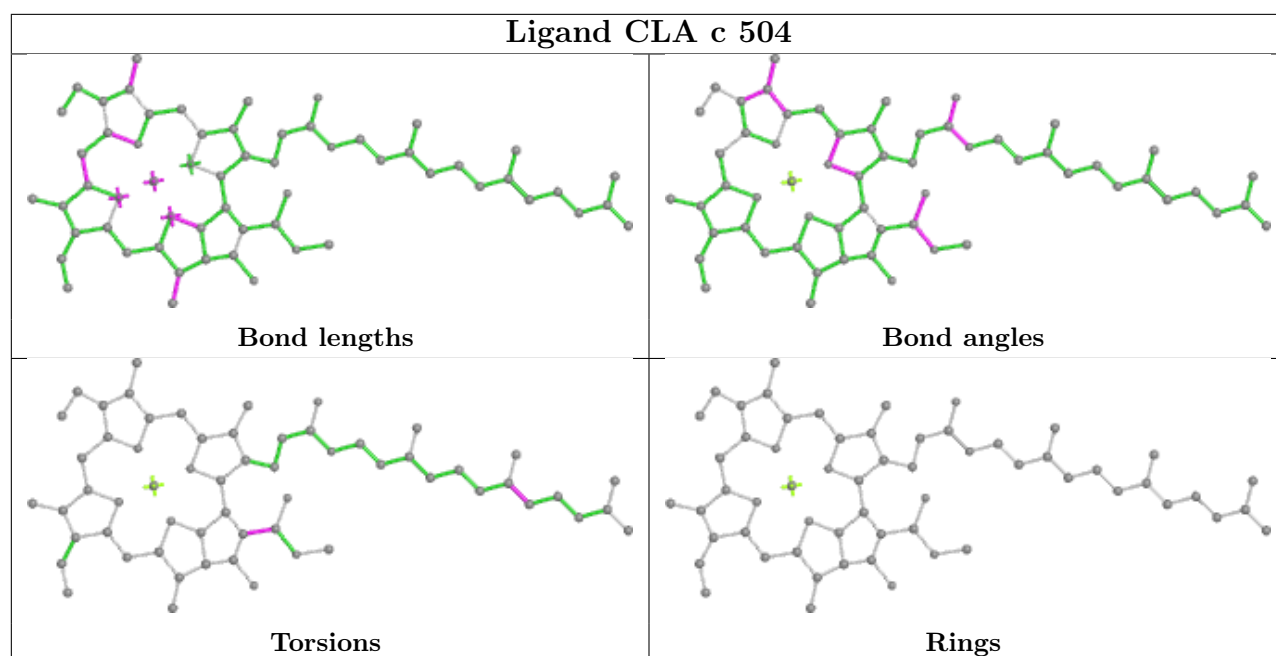


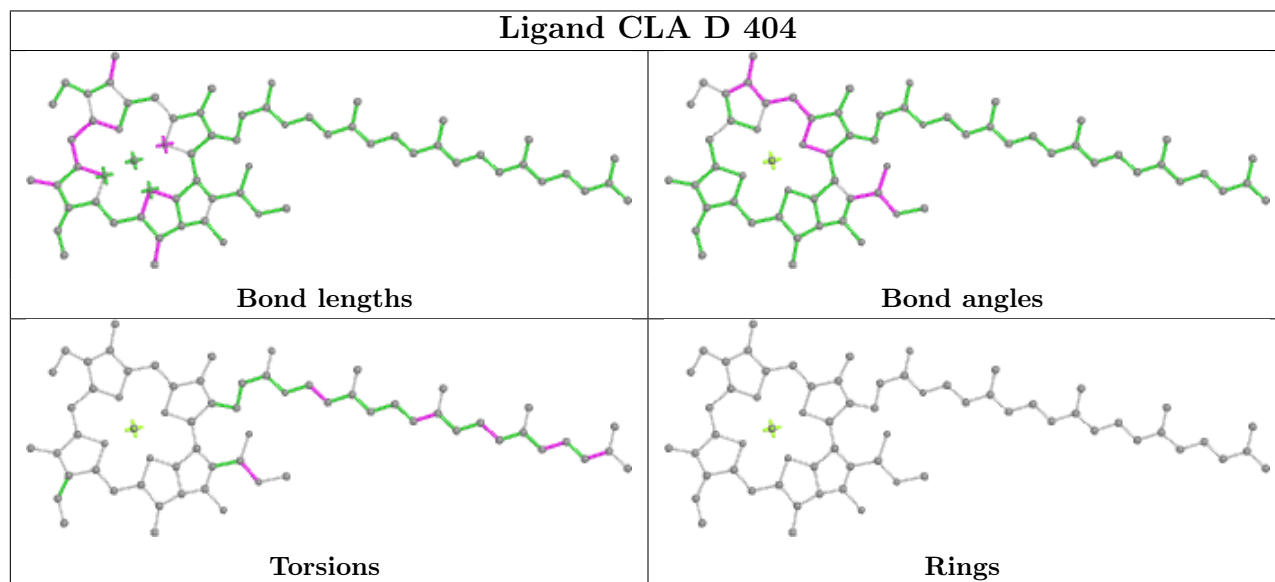
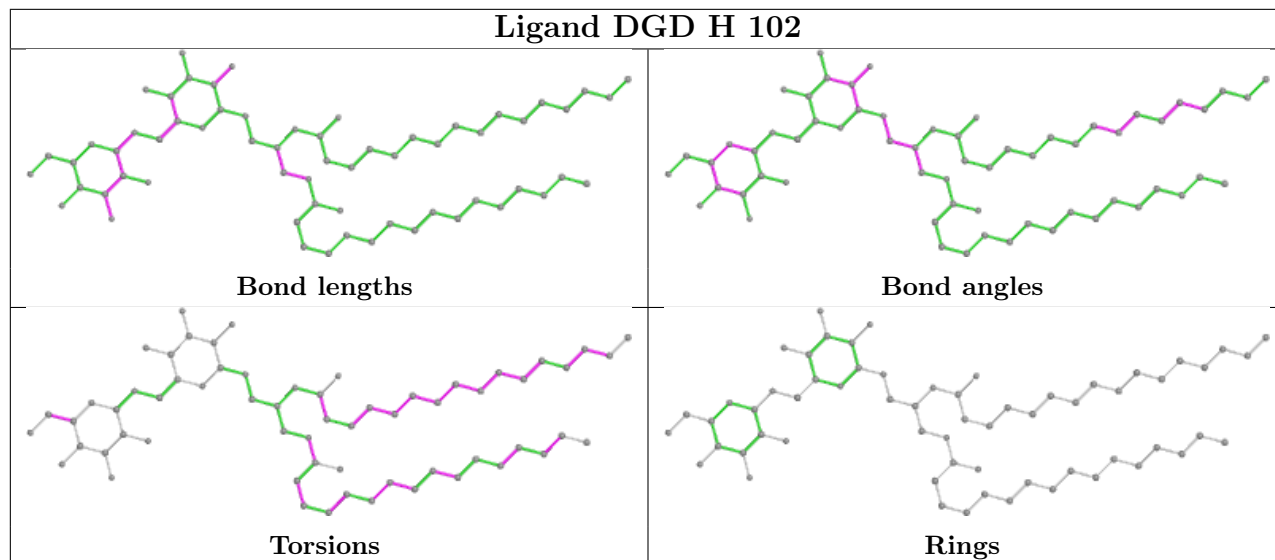
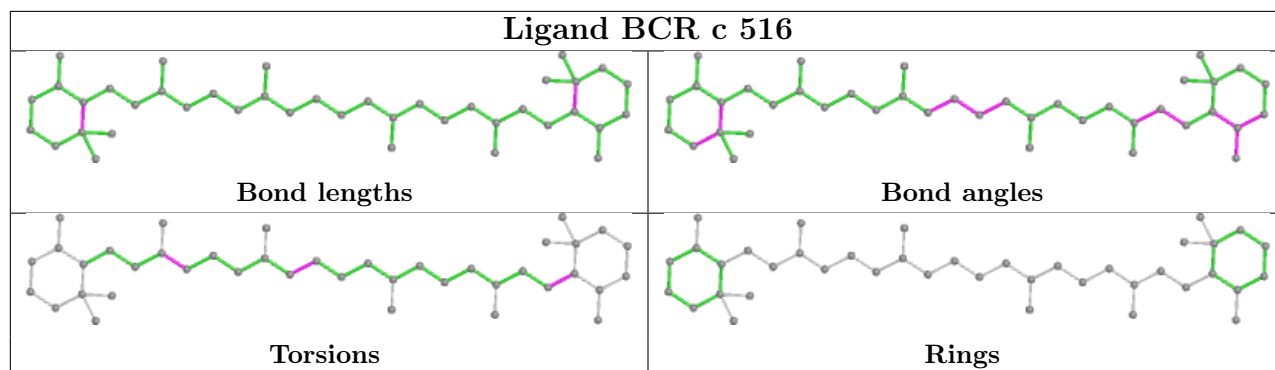


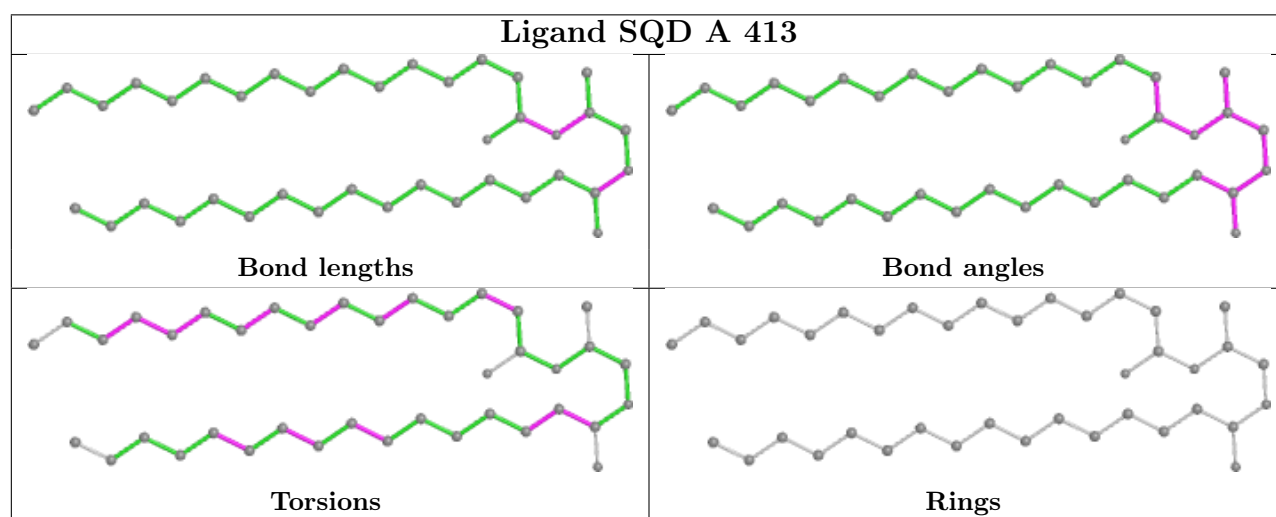
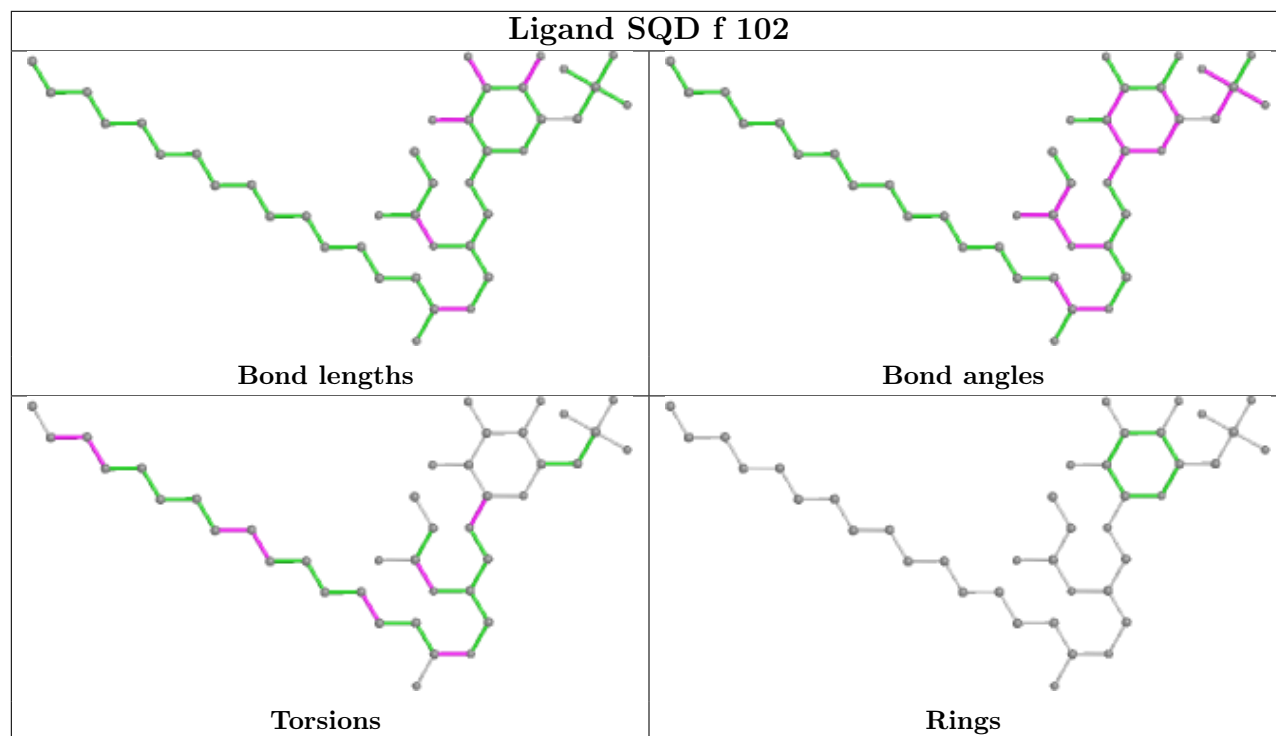
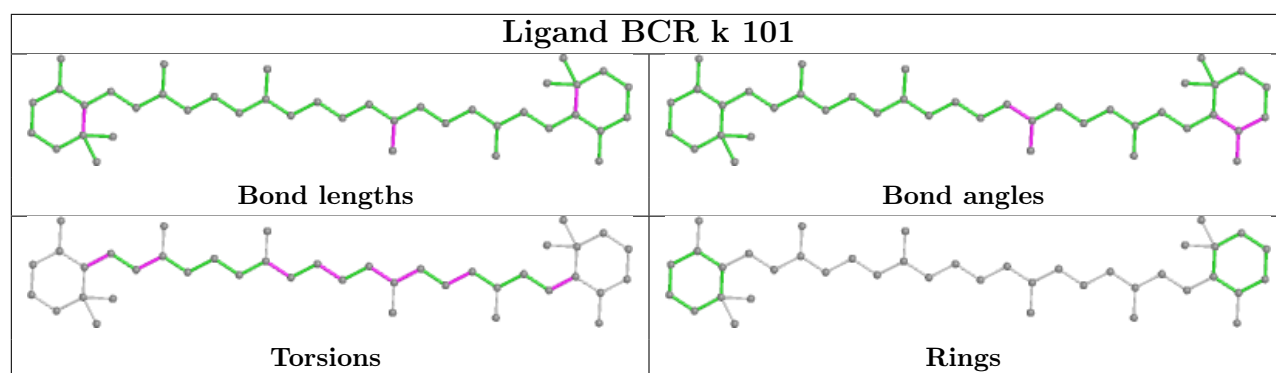


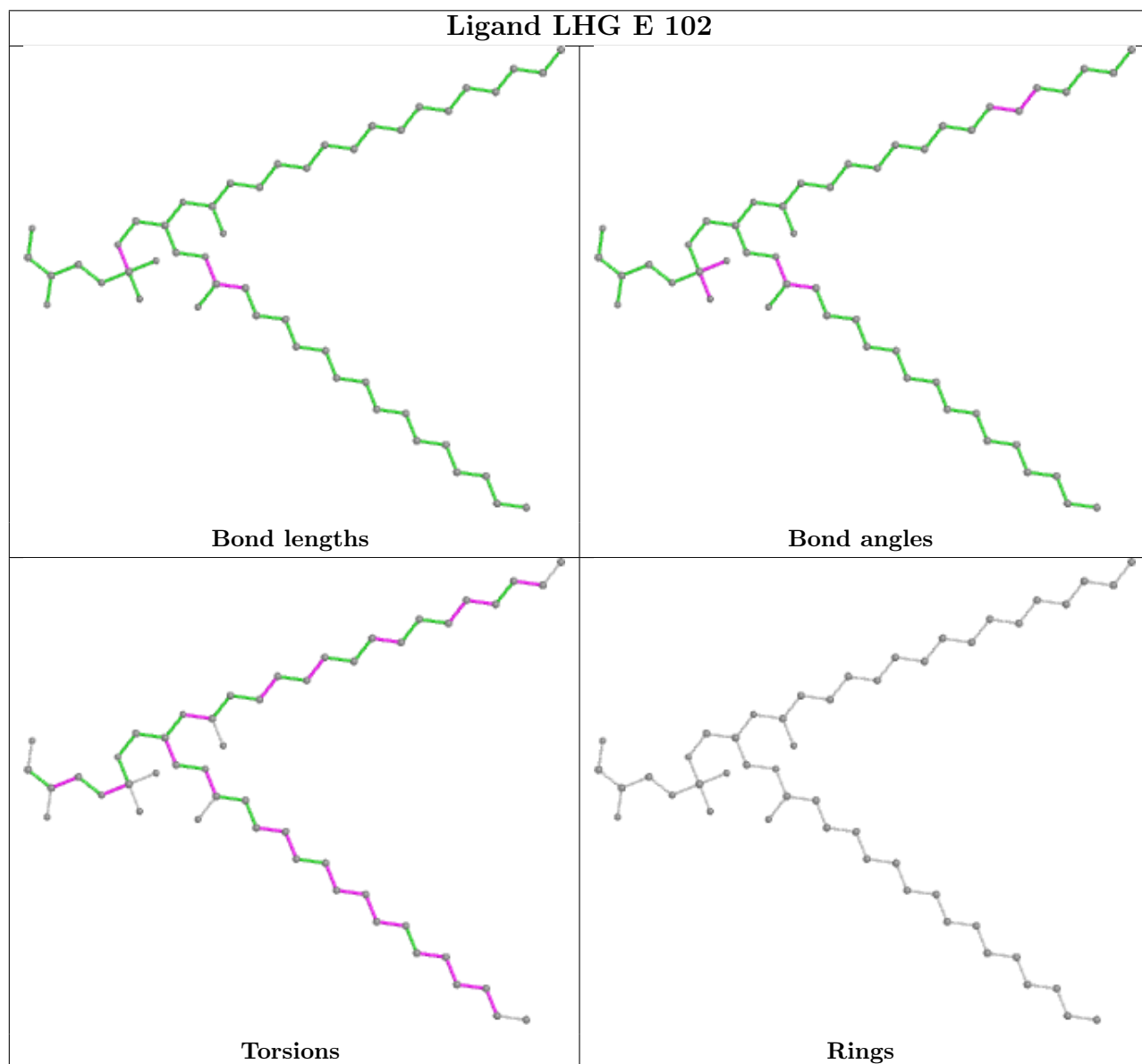
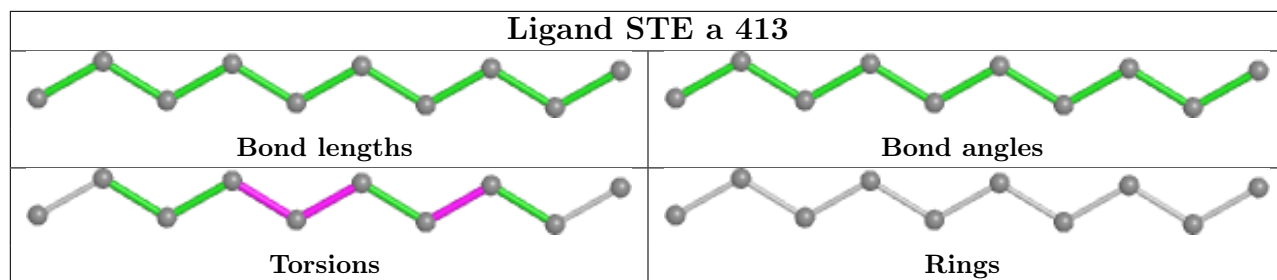


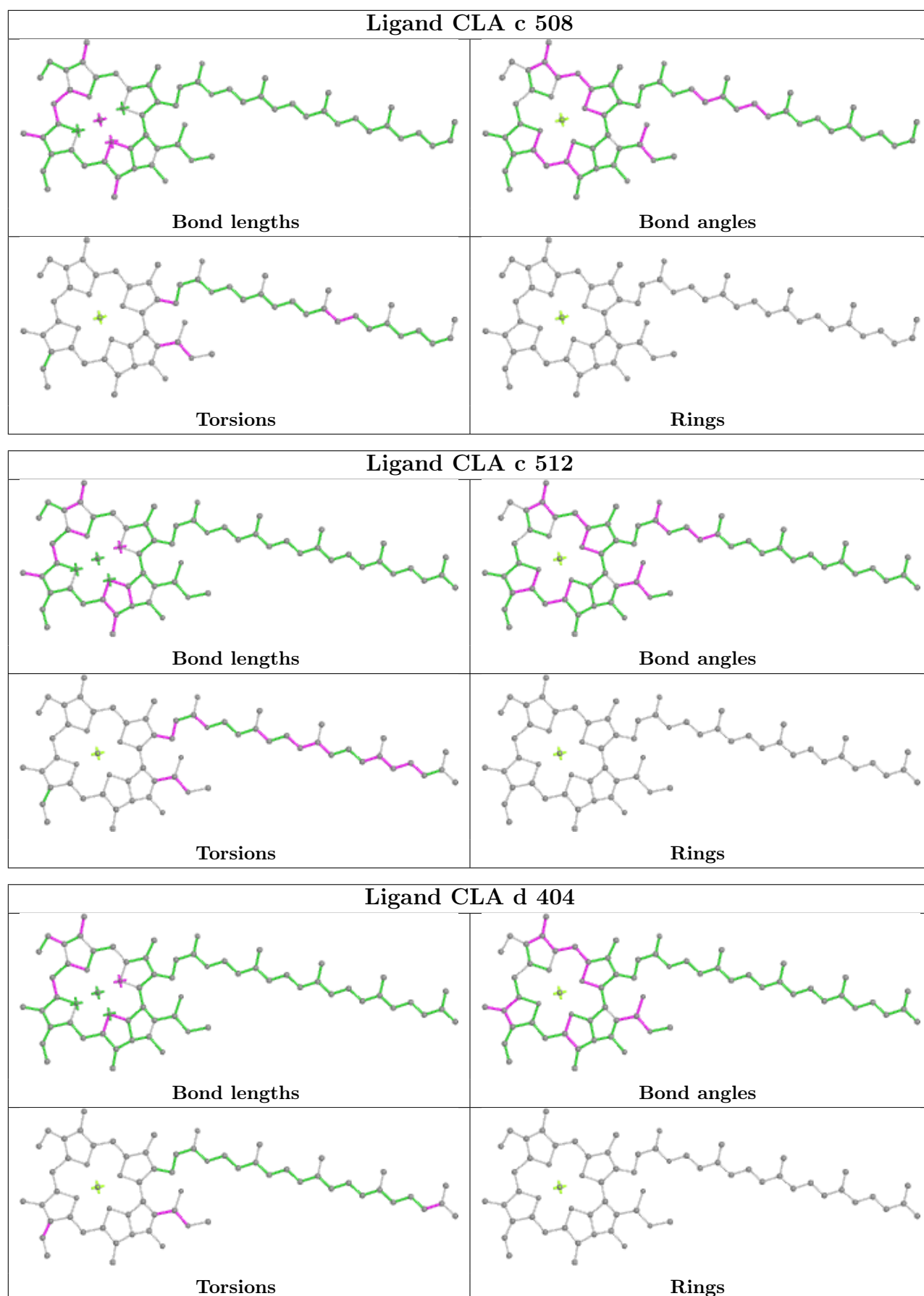


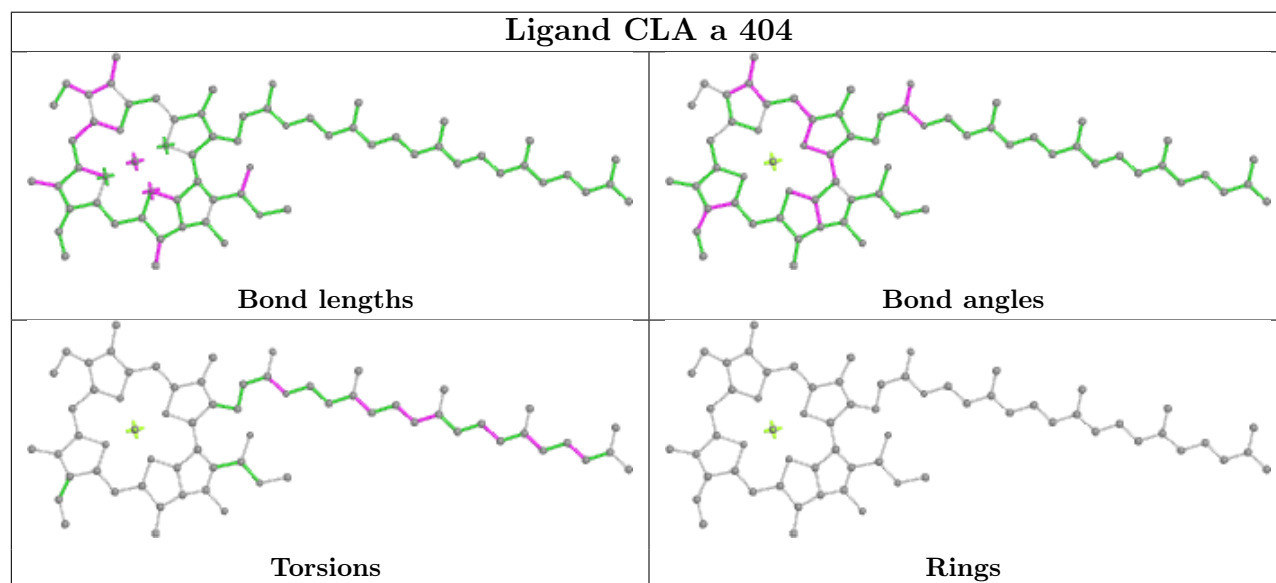
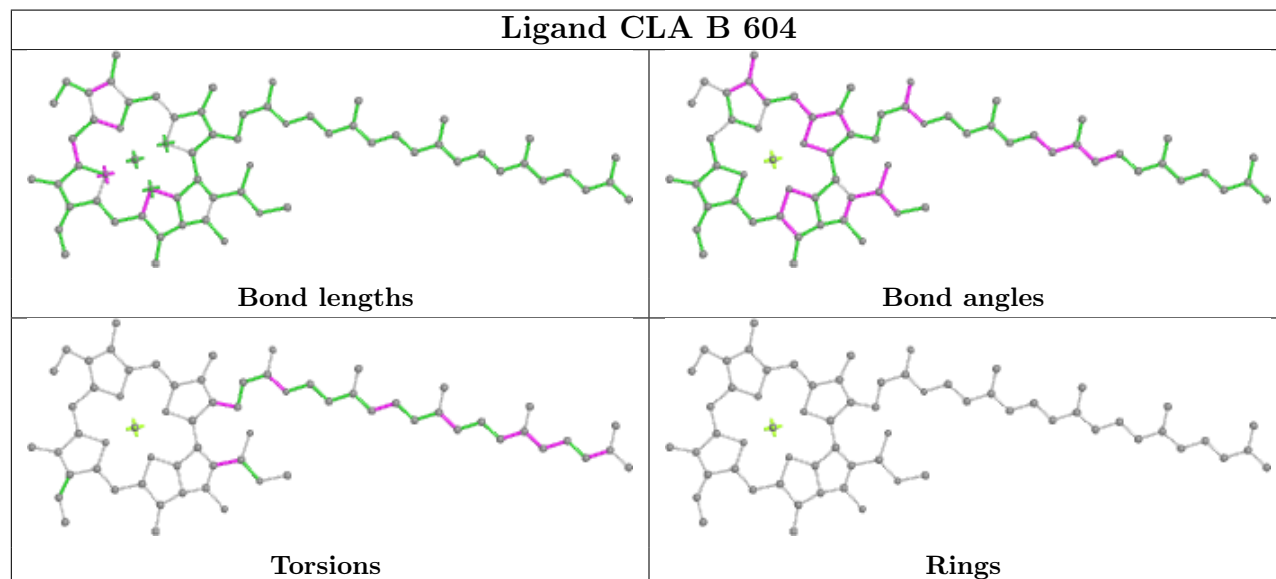
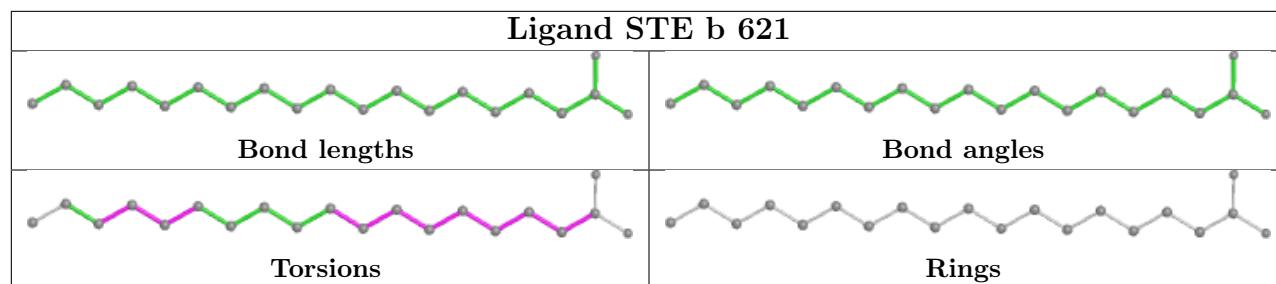




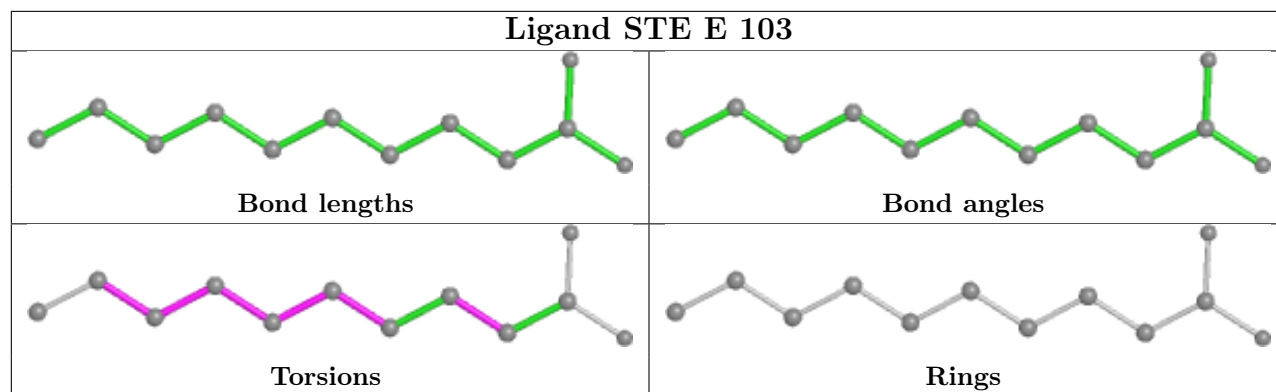












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.26	5 (1%) 73 77	23, 32, 53, 84	0
1	a	334/344 (97%)	-0.29	1 (0%) 94 94	26, 34, 61, 80	0
2	B	505/510 (99%)	-0.27	12 (2%) 59 64	26, 36, 65, 92	0
2	b	505/510 (99%)	-0.07	20 (3%) 38 44	28, 39, 75, 115	0
3	C	442/461 (95%)	-0.18	7 (1%) 72 75	27, 39, 56, 81	0
3	c	451/461 (97%)	-0.05	13 (2%) 51 57	28, 43, 64, 99	0
4	D	341/352 (96%)	-0.22	2 (0%) 89 91	27, 34, 51, 78	0
4	d	341/352 (96%)	-0.20	1 (0%) 94 94	27, 38, 62, 84	0
5	E	82/84 (97%)	0.16	6 (7%) 15 19	37, 55, 73, 86	0
5	e	82/84 (97%)	0.26	5 (6%) 21 26	40, 62, 82, 90	0
6	F	34/45 (75%)	-0.20	2 (5%) 22 27	41, 48, 70, 91	0
6	f	34/45 (75%)	-0.14	2 (5%) 22 27	44, 52, 80, 93	0
7	H	65/66 (98%)	-0.06	2 (3%) 49 55	36, 44, 61, 76	0
7	h	63/66 (95%)	0.30	3 (4%) 30 36	44, 52, 65, 70	0
8	I	35/38 (92%)	-0.15	2 (5%) 23 29	35, 40, 72, 82	0
8	i	35/38 (92%)	-0.12	2 (5%) 23 29	34, 43, 77, 84	0
9	J	36/40 (90%)	0.03	4 (11%) 5 7	37, 52, 78, 91	0
9	j	36/40 (90%)	0.26	5 (13%) 2 3	43, 54, 89, 102	0
10	K	37/46 (80%)	0.22	1 (2%) 54 60	48, 56, 74, 83	0
10	k	37/46 (80%)	0.12	0 100 100	48, 57, 72, 84	0
11	L	37/37 (100%)	-0.38	0 100 100	27, 33, 65, 73	0
11	l	36/37 (97%)	-0.22	3 (8%) 11 14	26, 34, 70, 89	0
12	M	32/36 (88%)	0.04	0 100 100	30, 36, 62, 71	0
12	m	31/36 (86%)	-0.21	0 100 100	27, 37, 53, 69	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	244/272 (89%)	0.03	17 (6%) 16 20	29, 44, 82, 140	0
13	o	244/272 (89%)	-0.02	15 (6%) 21 26	29, 44, 85, 124	0
14	R	28/41 (68%)	2.35	17 (60%) 0 0	65, 78, 90, 100	0
14	r	28/41 (68%)	4.32	26 (92%) 0 0	79, 101, 115, 123	0
15	T	29/32 (90%)	-0.36	2 (6%) 16 21	29, 33, 65, 73	0
15	t	29/32 (90%)	-0.20	3 (10%) 6 8	29, 34, 78, 90	0
16	U	97/134 (72%)	-0.18	2 (2%) 63 68	34, 46, 71, 92	0
16	u	97/134 (72%)	-0.34	0 100 100	33, 42, 60, 84	0
17	V	137/163 (84%)	-0.45	0 100 100	32, 43, 59, 85	0
17	v	137/163 (84%)	-0.08	5 (3%) 42 49	35, 49, 69, 88	0
18	X	38/41 (92%)	0.03	3 (7%) 12 16	43, 53, 75, 84	0
18	x	39/41 (95%)	0.45	3 (7%) 13 17	52, 63, 92, 105	0
19	Y	27/46 (58%)	1.54	11 (40%) 0 0	55, 76, 92, 98	0
19	y	30/46 (65%)	0.54	5 (16%) 1 2	64, 77, 90, 97	0
20	Z	62/62 (100%)	1.01	17 (27%) 0 0	58, 71, 112, 129	0
20	z	62/62 (100%)	0.89	11 (17%) 1 1	63, 73, 116, 123	0
All	All	5293/5700 (92%)	-0.06	235 (4%) 34 40	23, 41, 76, 140	0

All (235) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	8.5
14	r	28	VAL	7.8
14	r	9	LEU	7.3
13	O	56	PRO	7.1
14	r	29	LYS	7.1
9	j	6	GLY	7.0
13	O	60	ARG	7.0
14	r	10	LEU	7.0
14	r	3	TRP	6.4
13	O	3	GLN	6.1
20	Z	33	TRP	5.9
6	F	12	SER	5.8
14	R	3	TRP	5.8
14	r	26	TYR	5.8
14	r	24	LEU	5.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
14	r	14	LEU	5.7
14	R	6	LEU	5.7
2	b	495	PHE	5.4
3	c	24	THR	5.4
20	Z	32	ASP	5.4
13	O	59	LYS	5.3
14	r	18	TRP	5.1
13	o	3	GLN	5.1
14	r	25	PRO	5.1
19	Y	20	ALA	5.1
1	A	13	LEU	5.0
20	Z	61	VAL	5.0
20	Z	34	ASP	4.8
14	r	6	LEU	4.8
14	r	13	LEU	4.8
18	x	2	THR	4.8
18	X	2	THR	4.8
14	R	26	TYR	4.7
20	z	33	TRP	4.7
14	r	15	ALA	4.7
14	r	7	VAL	4.6
19	Y	22	LEU	4.6
5	e	79	PHE	4.4
2	b	506	ARG	4.4
13	O	4	THR	4.3
13	o	4	THR	4.3
19	Y	25	ILE	4.3
15	T	30	THR	4.2
13	o	60	ARG	4.2
3	c	23	ALA	4.1
20	Z	3	ILE	4.1
19	Y	43	ARG	4.0
13	O	62	GLU	4.0
15	t	30	THR	3.9
13	O	5	LEU	3.9
20	Z	41	PHE	3.9
14	r	23	ILE	3.9
14	R	24	LEU	3.8
13	O	246	ALA	3.8
14	R	20	VAL	3.8
3	c	146	PHE	3.8
20	Z	62	VAL	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
19	Y	41	VAL	3.7
14	r	19	ALA	3.7
8	i	36	ASP	3.7
14	r	5	VAL	3.6
14	r	2	ASP	3.6
20	z	41	PHE	3.6
14	r	12	VAL	3.6
2	b	486	LEU	3.6
16	U	8	GLU	3.6
14	R	25	PRO	3.6
13	o	59	LYS	3.5
8	I	36	ASP	3.5
5	E	83	LEU	3.5
13	o	61	GLN	3.5
2	b	505	ARG	3.5
20	Z	35	ARG	3.5
14	R	29	LYS	3.5
13	o	5	LEU	3.5
13	o	57	LYS	3.5
3	C	146	PHE	3.4
2	b	487	SER	3.4
7	h	21	VAL	3.4
11	l	3	PRO	3.4
9	j	7	ARG	3.4
13	o	207	ARG	3.4
19	y	40	ALA	3.4
5	e	61	ARG	3.4
18	x	38	GLN	3.3
13	o	62	GLU	3.3
20	Z	31	GLN	3.3
9	J	6	GLY	3.3
18	x	40	SER	3.3
14	R	21	ARG	3.3
20	z	62	VAL	3.3
5	e	82	GLN	3.2
2	b	127	ARG	3.2
9	J	7	ARG	3.2
19	Y	42	ARG	3.2
14	R	5	VAL	3.2
2	b	490	GLN	3.2
20	z	35	ARG	3.2
13	O	61	GLN	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
20	z	3	ILE	3.2
13	o	56	PRO	3.1
10	K	17	ILE	3.1
18	X	3	ILE	3.1
20	z	36	SER	3.1
7	h	6	TRP	3.1
19	y	41	VAL	3.1
7	H	66	GLY	3.1
14	r	27	ALA	3.1
2	B	506	ARG	3.1
3	c	143	TYR	3.1
2	b	503	THR	3.0
2	b	502	VAL	3.0
13	o	63	ALA	3.0
2	b	289	GLN	3.0
2	B	485	GLU	3.0
2	b	128	THR	3.0
2	b	295	GLY	3.0
5	E	3	GLY	3.0
19	Y	40	ALA	3.0
9	J	5	GLY	2.9
17	v	21	LEU	2.9
20	Z	7	LEU	2.9
3	c	29	GLU	2.9
15	t	29	ILE	2.9
19	Y	37	PHE	2.9
20	z	60	PHE	2.9
6	F	13	TYR	2.9
1	A	11	ALA	2.9
9	j	5	GLY	2.9
3	C	60	ILE	2.8
2	B	293	ALA	2.8
1	a	11	ALA	2.8
20	Z	42	LEU	2.8
14	R	18	TRP	2.8
14	r	16	ALA	2.8
6	f	12	SER	2.8
13	O	57	LYS	2.8
2	b	374	ASN	2.8
2	B	505	ARG	2.8
14	R	28	VAL	2.8
14	R	2	ASP	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	b	161	LEU	2.8
14	R	13	LEU	2.8
14	r	11	PRO	2.7
3	c	262	ARG	2.7
14	r	4	ARG	2.7
9	j	8	ILE	2.7
19	y	19	ILE	2.7
20	Z	60	PHE	2.7
13	o	246	ALA	2.7
7	h	10	ILE	2.7
8	I	34	ARG	2.7
4	D	227	GLU	2.6
14	r	8	VAL	2.6
5	e	74	GLN	2.6
13	O	63	ALA	2.6
2	B	127	ARG	2.6
14	R	9	LEU	2.6
5	E	79	PHE	2.6
19	y	37	PHE	2.6
20	z	4	LEU	2.6
3	C	57	ALA	2.5
20	Z	1	MET	2.5
3	c	55	ALA	2.5
3	c	25	ASN	2.5
19	Y	21	GLN	2.5
2	B	495	PHE	2.5
2	b	293	ALA	2.5
17	v	22	THR	2.5
1	A	15	GLU	2.4
15	T	29	ILE	2.4
3	C	145	SER	2.4
20	z	7	LEU	2.4
3	c	57	ALA	2.4
9	J	8	ILE	2.4
18	X	34	ILE	2.4
8	i	34	ARG	2.4
20	Z	38	GLN	2.4
2	B	503	THR	2.4
3	C	58	GLY	2.3
2	b	292	LEU	2.3
14	R	10	LEU	2.3
13	O	35	SER	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	b	485	GLU	2.3
20	Z	4	LEU	2.3
3	c	147	PHE	2.3
9	j	11	TRP	2.3
15	t	28	ARG	2.3
13	O	132	ASN	2.3
3	c	142	GLU	2.3
19	Y	38	LEU	2.2
17	v	15	GLU	2.2
13	O	36	GLN	2.2
2	B	373	LYS	2.2
14	r	21	ARG	2.2
13	o	34	SER	2.2
2	B	295	GLY	2.2
20	z	29	SER	2.2
11	l	7	ARG	2.2
2	b	288	VAL	2.2
19	Y	45	ASN	2.2
13	O	25	THR	2.2
4	D	12	ARG	2.2
6	f	16	PHE	2.1
3	C	55	ALA	2.1
20	z	30	PRO	2.1
20	Z	39	LEU	2.1
17	v	113	VAL	2.1
3	c	182	PHE	2.1
5	E	74	GLN	2.1
4	d	51	GLY	2.1
2	B	294	SER	2.1
13	o	89	SER	2.1
20	Z	37	LYS	2.1
5	E	82	GLN	2.1
2	b	491	VAL	2.1
14	R	22	ASN	2.1
11	l	2	GLU	2.1
1	A	16	ARG	2.1
2	B	502	VAL	2.1
3	C	61	VAL	2.1
14	r	22	ASN	2.1
2	B	490	GLN	2.0
16	U	9	LEU	2.0
17	v	24	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
7	H	41	PHE	2.0
2	b	496	TYR	2.0
5	e	60	GLN	2.0
3	c	191	PRO	2.0
19	y	18	VAL	2.0
1	A	12	ASN	2.0
13	O	54	GLU	2.0
13	O	55	GLU	2.0
14	R	14	LEU	2.0
5	E	84	LYS	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	0.09	33,48,71,72	0
15	FME	T	1	10/11	0.94	0.10	29,52,69,69	0
12	FME	M	1	10/11	0.95	0.11	44,54,68,76	0
8	FME	I	1	10/11	0.95	0.16	40,52,64,70	0
8	FME	i	1	10/11	0.95	0.19	41,51,64,67	0
12	FME	m	1	10/11	0.96	0.14	33,50,72,82	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
32	STE	E	103	12/20	0.67	0.35	63,80,88,95	0
32	STE	H	103	18/20	0.69	0.31	43,78,89,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
32	STE	b	624	20/20	0.70	0.18	51,69,78,93	0
26	PL9	A	409	55/55	0.74	0.29	44,72,93,105	0
32	STE	c	521	20/20	0.76	0.23	44,63,94,107	0
27	LMG	d	411	23/55	0.77	0.23	42,72,88,92	0
32	STE	B	626	16/20	0.77	0.28	39,72,94,94	0
32	STE	a	413	10/20	0.78	0.20	37,66,75,80	0
32	STE	x	101	20/20	0.78	0.24	49,67,79,79	0
24	BCR	h	101	40/40	0.79	0.16	43,60,79,91	0
27	LMG	c	522	48/55	0.79	0.24	39,82,115,118	0
28	SQD	a	411	36/54	0.80	0.17	32,65,86,91	0
26	PL9	a	409	55/55	0.80	0.24	42,76,96,107	0
32	STE	C	521	16/20	0.80	0.16	38,58,85,88	0
33	LHG	E	102	49/49	0.80	0.23	55,87,113,120	0
29	DGD	A	414	66/66	0.81	0.16	47,67,82,90	0
29	DGD	a	412	44/66	0.81	0.16	35,58,82,91	0
32	STE	B	620	17/20	0.81	0.16	39,59,71,80	0
24	BCR	H	101	40/40	0.81	0.16	38,53,64,74	0
22	CLA	b	601	65/65	0.81	0.17	53,72,92,96	0
27	LMG	D	410	33/55	0.81	0.15	41,58,86,90	0
32	STE	a	414	12/20	0.82	0.23	54,67,77,79	0
22	CLA	C	512	65/65	0.82	0.18	35,61,88,97	0
32	STE	b	625	10/20	0.82	0.25	40,53,63,74	0
32	STE	B	627	12/20	0.82	0.38	53,66,83,86	0
32	STE	I	101	15/20	0.82	0.18	38,59,77,81	0
27	LMG	b	622	55/55	0.82	0.25	53,80,98,112	0
32	STE	b	623	16/20	0.83	0.17	50,68,83,94	0
28	SQD	A	413	39/54	0.83	0.18	43,66,94,100	0
33	LHG	e	101	42/49	0.83	0.23	56,93,112,132	0
22	CLA	c	512	65/65	0.84	0.17	47,64,99,104	0
22	CLA	c	513	65/65	0.85	0.20	49,74,106,110	0
32	STE	b	621	20/20	0.85	0.23	39,58,79,80	0
32	STE	l	102	18/20	0.85	0.17	37,54,88,89	0
32	STE	j	101	12/20	0.86	0.13	48,62,70,79	0
32	STE	T	103	15/20	0.86	0.15	44,60,81,84	0
22	CLA	B	601	65/65	0.86	0.15	35,64,90,100	0
22	CLA	C	513	65/65	0.86	0.19	45,68,103,112	0
32	STE	T	102	16/20	0.86	0.17	41,53,78,79	0
24	BCR	k	101	40/40	0.87	0.13	45,67,78,80	0
24	BCR	Y	101	40/40	0.87	0.12	43,58,76,83	0
32	STE	B	625	18/20	0.87	0.14	41,59,81,88	0
32	STE	c	524	12/20	0.87	0.21	57,73,82,84	0
32	STE	d	413	17/20	0.87	0.17	48,62,75,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
28	SQD	B	623	54/54	0.88	0.15	43,66,97,109	0
27	LMG	A	411	48/55	0.88	0.15	43,65,84,101	0
32	STE	m	101	12/20	0.88	0.15	48,64,76,82	0
24	BCR	c	516	40/40	0.88	0.19	45,60,71,79	0
32	STE	J	101	12/20	0.88	0.12	49,62,72,73	0
32	STE	D	411	20/20	0.88	0.18	38,55,79,84	0
32	STE	C	520	12/20	0.89	0.13	43,57,68,70	0
28	SQD	f	102	41/54	0.89	0.18	63,89,107,109	0
24	BCR	c	514	40/40	0.89	0.15	47,64,79,81	0
22	CLA	c	502	65/65	0.89	0.16	34,49,69,75	0
24	BCR	d	406	40/40	0.89	0.14	40,57,98,114	0
24	BCR	K	101	40/40	0.89	0.14	51,65,74,78	0
28	SQD	L	101	49/54	0.89	0.13	40,61,93,97	0
24	BCR	D	405	40/40	0.89	0.12	35,49,85,89	0
22	CLA	c	508	64/65	0.90	0.15	37,50,94,112	0
22	CLA	c	510	65/65	0.90	0.17	36,53,67,73	0
27	LMG	c	523	49/55	0.90	0.12	35,62,83,99	0
22	CLA	C	502	65/65	0.90	0.14	35,47,60,68	0
32	STE	M	103	10/20	0.90	0.13	36,54,57,61	0
22	CLA	b	615	65/65	0.90	0.14	31,45,61,65	0
22	CLA	d	405	65/65	0.90	0.16	32,53,93,101	0
27	LMG	B	621	28/55	0.90	0.16	37,53,66,72	0
27	LMG	C	519	48/55	0.90	0.15	49,74,93,98	0
32	STE	C	522	12/20	0.90	0.10	34,45,58,64	0
22	CLA	D	404	65/65	0.90	0.14	27,47,106,117	0
22	CLA	b	616	60/65	0.91	0.14	34,48,89,91	0
27	LMG	c	520	37/55	0.91	0.15	43,72,92,96	0
24	BCR	B	619	40/40	0.91	0.10	33,45,59,61	0
24	BCR	C	515	40/40	0.91	0.19	45,60,78,81	0
24	BCR	b	619	40/40	0.91	0.11	35,52,70,70	0
22	CLA	c	503	65/65	0.91	0.16	35,48,61,64	0
32	STE	t	102	14/20	0.91	0.11	35,55,65,68	0
27	LMG	M	101	51/55	0.91	0.11	33,53,76,92	0
27	LMG	b	620	51/55	0.91	0.11	38,57,76,91	0
32	STE	M	102	15/20	0.91	0.14	37,50,66,69	0
22	CLA	C	507	65/65	0.92	0.14	27,45,60,65	0
22	CLA	b	602	65/65	0.92	0.16	31,46,65,71	0
27	LMG	D	407	51/55	0.92	0.16	31,60,86,92	0
22	CLA	c	511	65/65	0.92	0.14	43,60,78,82	0
22	CLA	b	604	65/65	0.92	0.15	24,39,80,93	0
22	CLA	B	616	60/65	0.92	0.15	28,45,84,100	0
29	DGD	h	102	62/66	0.92	0.11	33,53,64,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
22	CLA	C	503	65/65	0.92	0.14	36,47,59,62	0
24	BCR	B	618	40/40	0.92	0.10	28,41,58,61	0
22	CLA	C	506	65/65	0.92	0.12	29,49,89,94	0
22	CLA	a	404	65/65	0.92	0.13	21,40,80,85	0
22	CLA	c	505	65/65	0.92	0.17	28,45,71,75	0
22	CLA	c	507	65/65	0.92	0.14	30,49,61,66	0
22	CLA	B	606	65/65	0.93	0.12	28,41,71,77	0
22	CLA	c	509	65/65	0.93	0.19	37,53,70,75	0
24	BCR	c	515	40/40	0.93	0.11	35,47,58,72	0
22	CLA	B	615	65/65	0.93	0.12	29,42,67,77	0
22	CLA	C	508	65/65	0.93	0.12	32,46,104,115	0
28	SQD	F	101	36/54	0.93	0.17	43,77,93,98	0
22	CLA	b	606	65/65	0.93	0.11	29,45,77,78	0
22	CLA	b	609	65/65	0.93	0.14	32,50,71,77	0
22	CLA	b	614	65/65	0.93	0.14	25,44,78,85	0
26	PL9	D	406	55/55	0.93	0.11	24,38,49,50	0
29	DGD	C	517	62/66	0.93	0.12	41,56,102,121	0
29	DGD	H	102	62/66	0.93	0.11	33,48,61,66	0
24	BCR	B	617	40/40	0.93	0.12	30,45,60,65	0
29	DGD	c	518	62/66	0.93	0.12	35,58,94,103	0
22	CLA	C	511	65/65	0.93	0.12	36,57,71,76	0
22	CLA	A	403	65/65	0.93	0.14	26,40,103,112	0
32	STE	B	624	12/20	0.93	0.10	37,56,70,74	0
24	BCR	C	514	40/40	0.93	0.11	32,43,56,61	0
22	CLA	B	602	65/65	0.93	0.16	27,40,62,65	0
22	CLA	B	604	65/65	0.93	0.13	26,38,75,80	0
22	CLA	a	403	65/65	0.93	0.14	30,45,99,107	0
22	CLA	c	506	65/65	0.93	0.12	36,53,94,101	0
22	CLA	C	505	65/65	0.93	0.16	22,44,72,75	0
24	BCR	b	618	40/40	0.93	0.11	30,44,56,60	0
22	CLA	C	509	65/65	0.94	0.19	32,50,65,74	0
22	CLA	b	608	65/65	0.94	0.14	34,48,64,68	0
27	LMG	d	412	44/55	0.94	0.13	37,58,89,92	0
22	CLA	C	510	65/65	0.94	0.14	34,49,66,74	0
22	CLA	b	611	65/65	0.94	0.15	27,39,57,66	0
22	CLA	b	612	65/65	0.94	0.18	26,39,54,63	0
22	CLA	b	613	65/65	0.94	0.15	26,40,76,83	0
28	SQD	a	410	54/54	0.94	0.14	44,67,96,99	0
23	PHO	d	401	64/64	0.94	0.13	23,35,43,48	0
24	BCR	A	406	40/40	0.94	0.09	28,38,49,52	0
22	CLA	A	402	65/65	0.94	0.10	21,32,46,56	0
29	DGD	C	516	62/66	0.94	0.12	25,48,84,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
22	CLA	A	405	54/65	0.94	0.11	20,34,68,73	0
29	DGD	C	518	62/66	0.94	0.12	33,54,82,91	0
26	PL9	d	407	55/55	0.94	0.11	27,38,45,52	0
22	CLA	B	609	65/65	0.94	0.14	29,42,56,59	0
22	CLA	B	610	65/65	0.94	0.14	23,35,47,51	0
29	DGD	c	519	62/66	0.94	0.14	31,57,86,101	0
22	CLA	C	504	59/65	0.94	0.13	32,47,85,92	0
22	CLA	c	504	60/65	0.94	0.11	35,50,87,88	0
22	CLA	B	611	65/65	0.94	0.15	23,35,50,56	0
22	CLA	B	612	65/65	0.94	0.15	25,36,50,55	0
24	BCR	T	101	40/40	0.94	0.10	29,44,58,62	0
22	CLA	B	613	65/65	0.94	0.14	21,35,71,75	0
24	BCR	a	405	40/40	0.94	0.09	25,36,52,56	0
22	CLA	B	614	65/65	0.94	0.17	26,43,77,92	0
22	CLA	b	610	65/65	0.95	0.18	28,42,53,58	0
22	CLA	C	501	65/65	0.95	0.12	26,41,54,58	0
22	CLA	A	410	65/65	0.95	0.09	20,32,52,58	0
24	BCR	t	101	40/40	0.95	0.09	27,39,55,58	0
28	SQD	A	412	52/54	0.95	0.15	33,66,94,99	0
22	CLA	B	605	65/65	0.95	0.14	24,35,49,54	0
22	CLA	b	603	65/65	0.95	0.14	24,40,71,79	0
22	CLA	D	403	65/65	0.95	0.12	22,32,59,60	0
22	CLA	b	605	65/65	0.95	0.12	24,39,54,60	0
22	CLA	c	501	65/65	0.95	0.13	31,44,54,62	0
22	CLA	d	403	65/65	0.95	0.12	23,40,60,68	0
22	CLA	d	404	65/65	0.95	0.12	24,35,46,50	0
24	BCR	b	617	40/40	0.95	0.10	29,43,52,56	0
22	CLA	B	603	65/65	0.95	0.14	24,38,63,64	0
23	PHO	A	404	64/64	0.95	0.09	20,31,40,48	0
22	CLA	b	607	65/65	0.95	0.14	21,40,65,77	0
33	LHG	B	622	49/49	0.95	0.12	28,48,68,77	0
22	CLA	a	402	65/65	0.95	0.10	24,35,48,62	0
22	CLA	B	607	65/65	0.95	0.11	17,37,68,76	0
33	LHG	l	101	49/49	0.95	0.10	34,48,59,67	0
22	CLA	B	608	65/65	0.96	0.11	22,39,59,65	0
33	LHG	D	409	47/49	0.96	0.11	29,53,82,99	0
29	DGD	c	517	62/66	0.96	0.10	25,46,77,83	0
33	LHG	L	102	49/49	0.96	0.11	30,44,59,74	0
33	LHG	d	408	49/49	0.96	0.12	30,55,77,83	0
33	LHG	d	409	49/49	0.96	0.10	30,49,61,71	0
33	LHG	d	410	39/49	0.96	0.10	34,50,72,74	0
23	PHO	d	402	64/64	0.96	0.10	32,43,54,63	0

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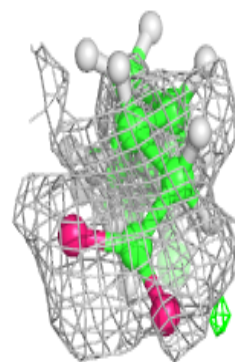
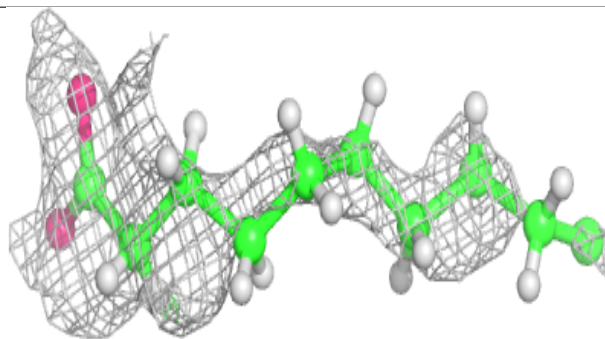
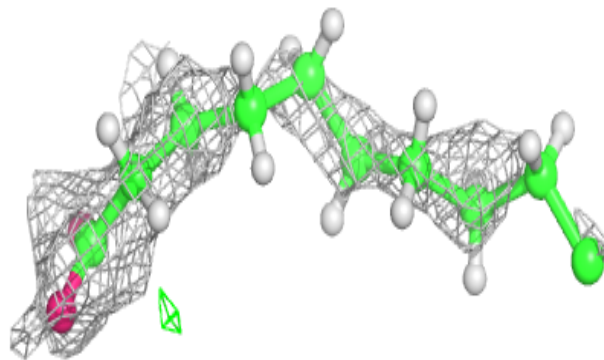
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
23	PHO	D	401	64/64	0.96	0.14	25,37,45,53	0
34	BCT	a	408	4/4	0.96	0.18	35,40,48,58	0
35	HEM	E	101	43/43	0.96	0.12	42,57,75,75	0
35	HEM	f	101	43/43	0.96	0.12	46,64,89,90	0
36	HEC	V	201	43/43	0.96	0.13	24,37,49,51	0
36	HEC	v	201	43/43	0.96	0.13	32,41,52,55	0
34	BCT	D	402	4/4	0.97	0.20	32,33,37,44	0
33	LHG	D	408	49/49	0.97	0.09	26,44,56,63	0
31	OEX	A	416[A]	10/10	0.98	0.13	35,37,41,41	10
25	CL	a	407	1/1	0.98	0.05	33,33,33,33	0
21	FE2	a	401	1/1	0.98	0.06	37,37,37,37	0
30	OEY	A	415[B]	11/11	0.98	0.13	21,26,30,34	11
31	OEX	a	416[A]	10/10	0.99	0.11	32,38,41,41	10
25	CL	A	408	1/1	0.99	0.03	32,32,32,32	0
25	CL	a	406	1/1	0.99	0.04	30,30,30,30	0
21	FE2	A	401	1/1	0.99	0.11	33,33,33,33	0
30	OEY	a	415[B]	11/11	0.99	0.11	25,27,31,37	11
25	CL	A	407	1/1	0.99	0.06	33,33,33,33	0

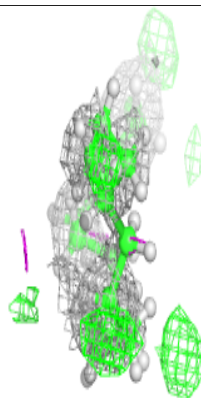
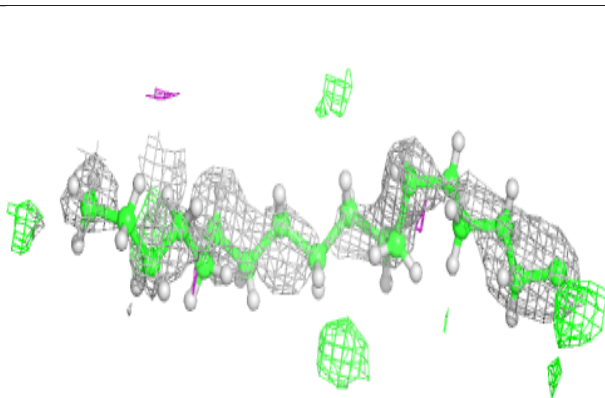
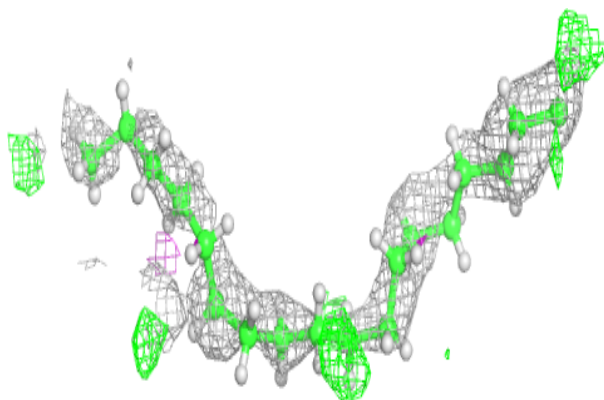
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around STE E 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 H 103:**

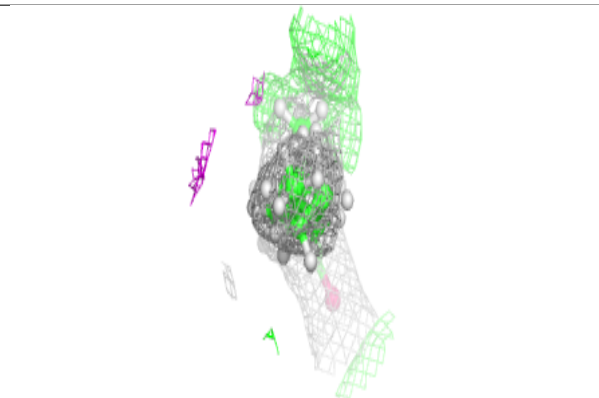
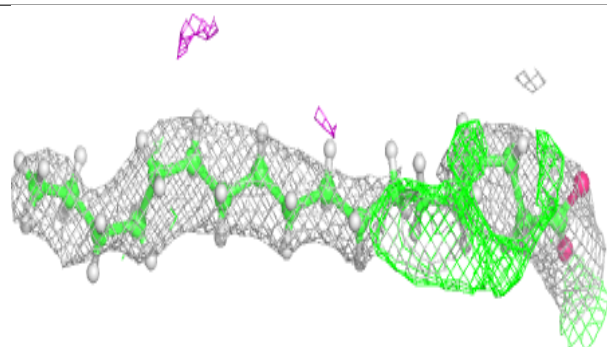
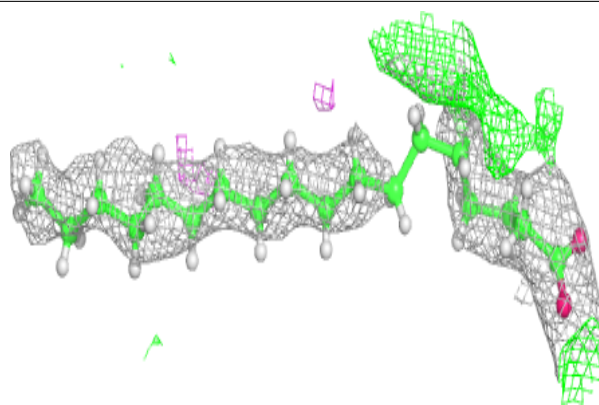
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



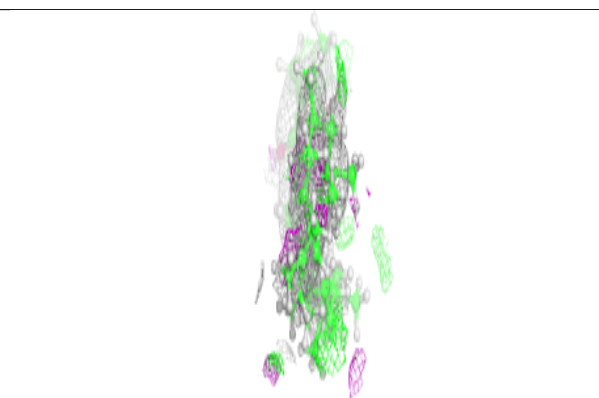
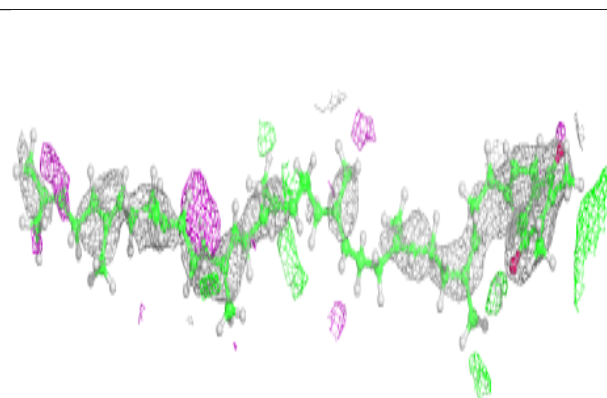
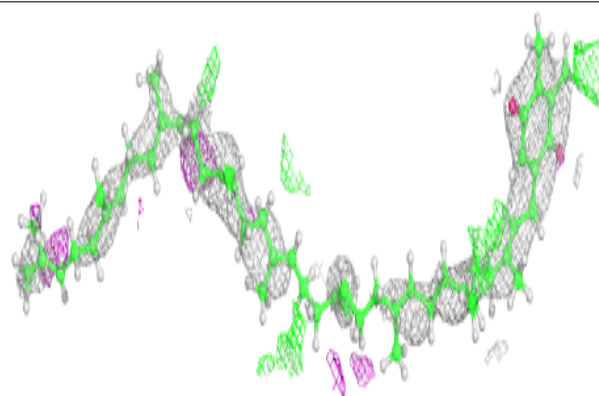


**Electron density around STE b 624:**

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

**Electron density around PL9 A 409:**

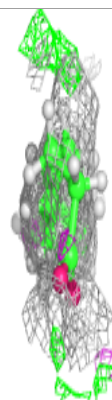
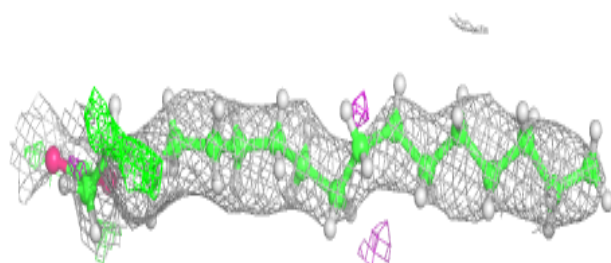
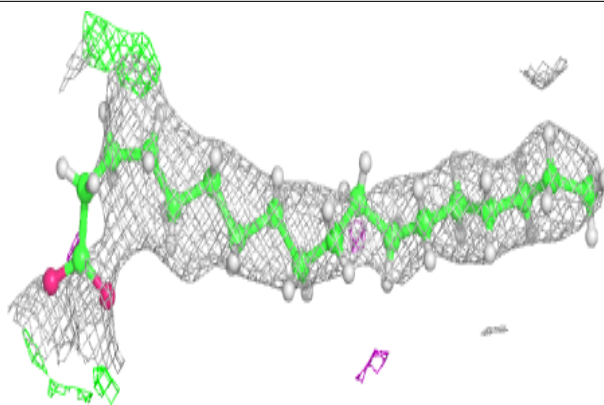
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



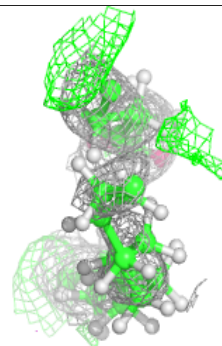
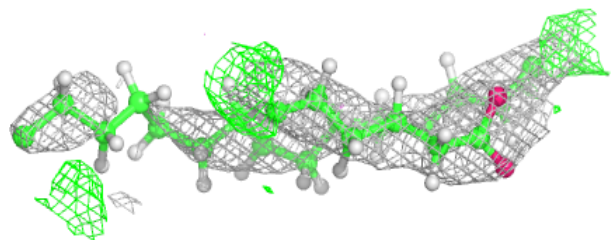
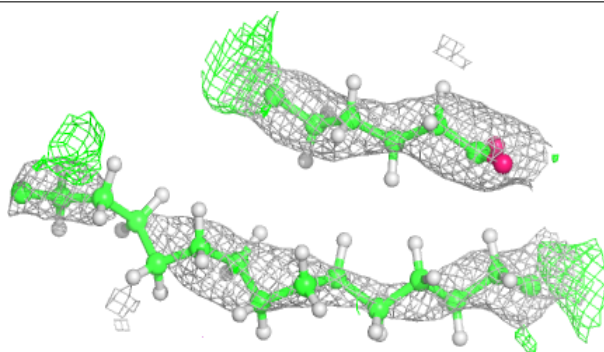


**Electron density around STE c 521:**

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

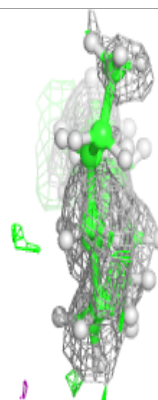
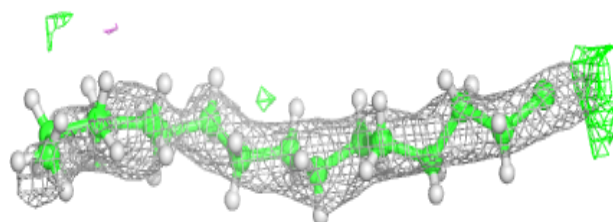
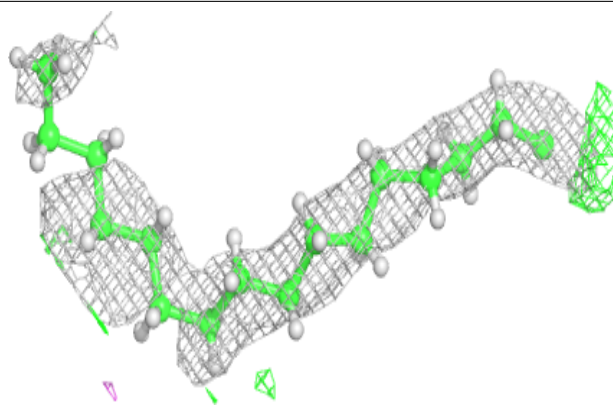
**Electron density around LMG d 411:**

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

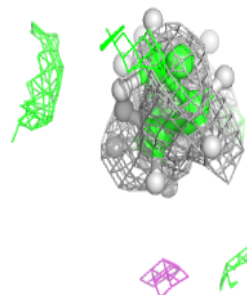
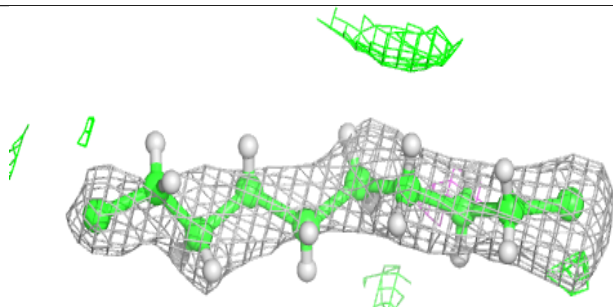
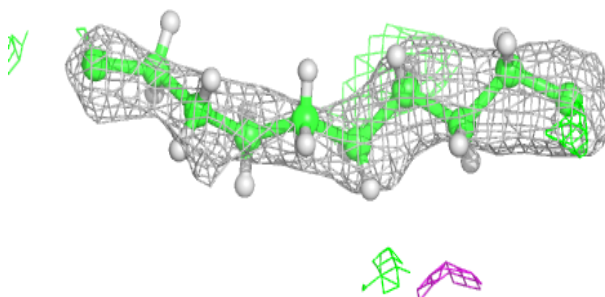


**Electron density around STE B 626:**

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

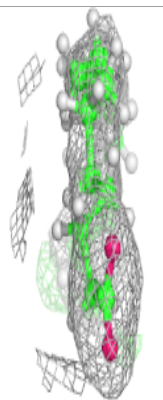
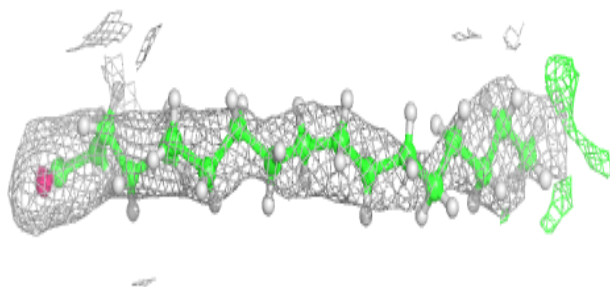
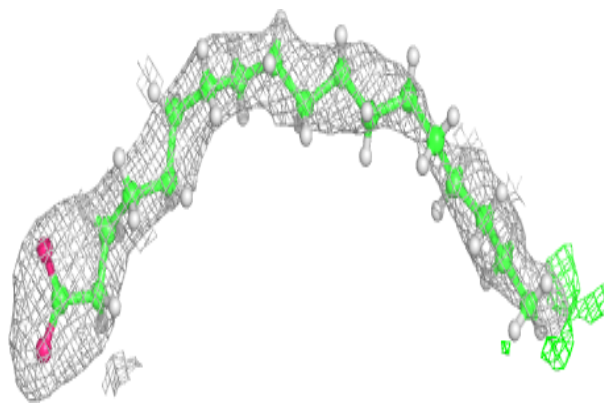
**Electron density around STE a 413:**

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

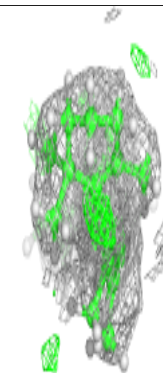
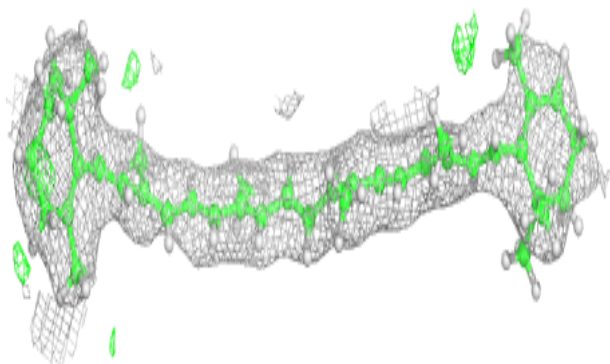
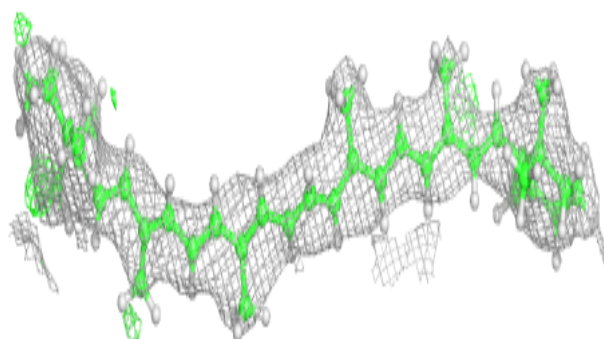


**Electron density around STE x 101:**

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

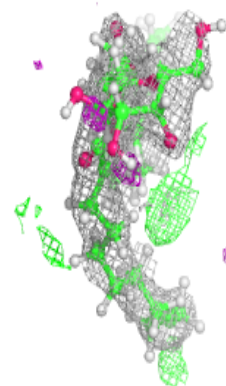
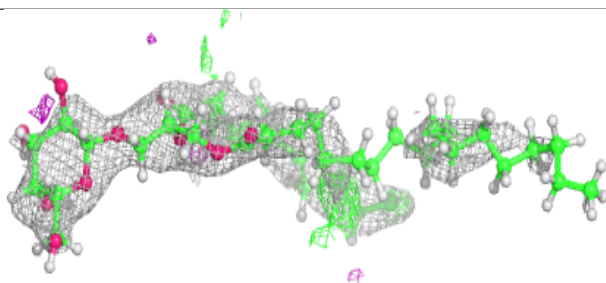
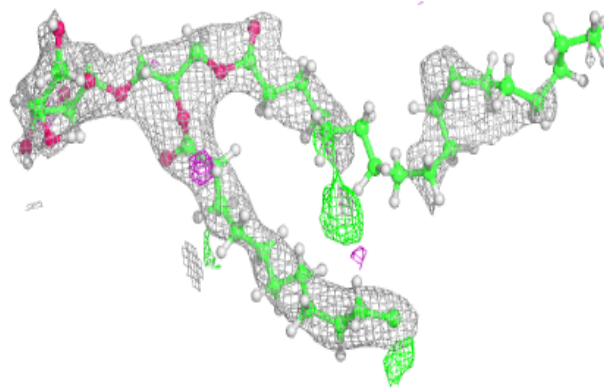
**Electron density around BCR h 101:**

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



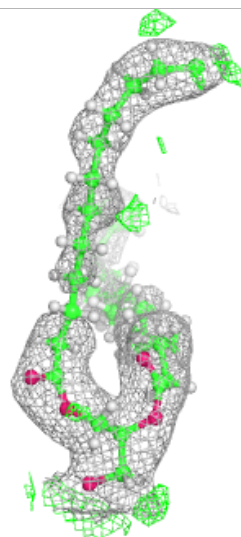
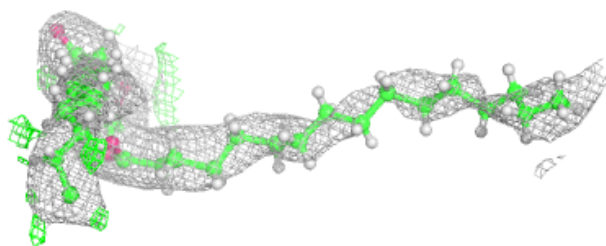
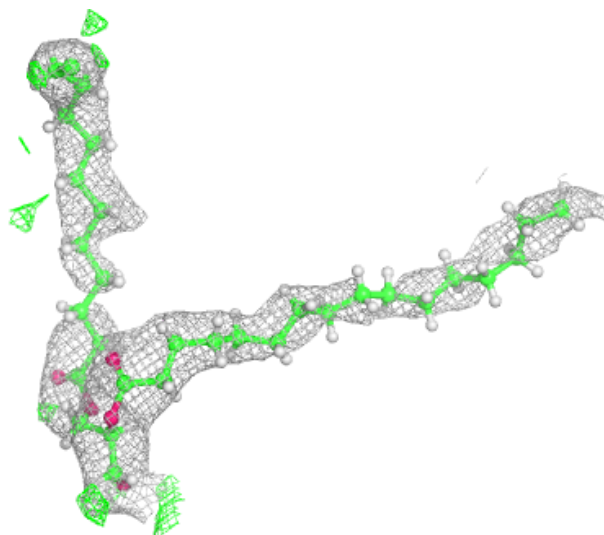
**Electron density around LMG c 522:**

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



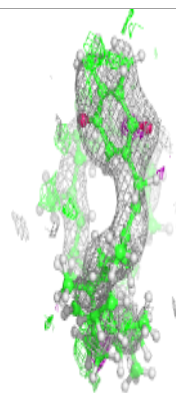
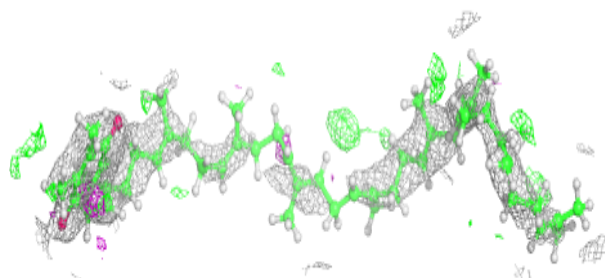
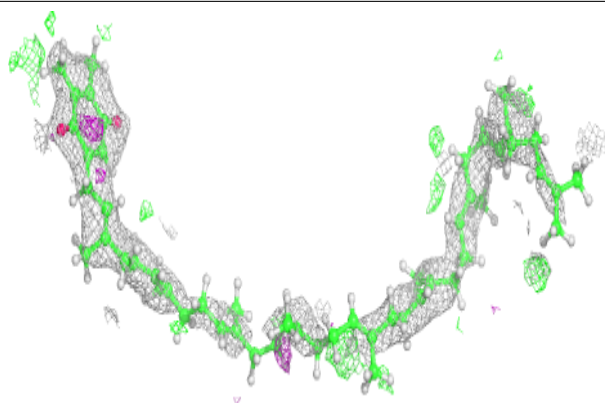
**Electron density around SQD a 411:**

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

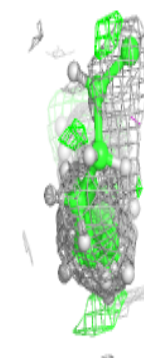
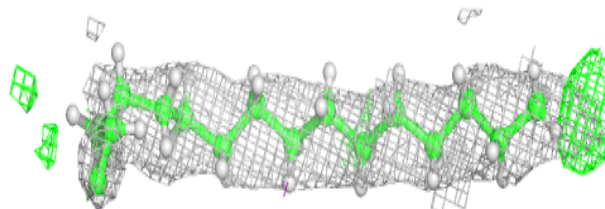
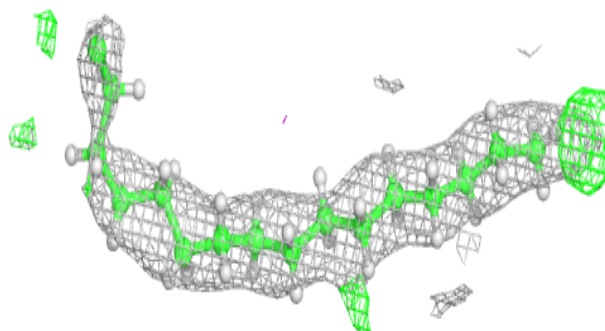


**Electron density around PL9 a 409:**

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

**Electron density around STE C 521:**

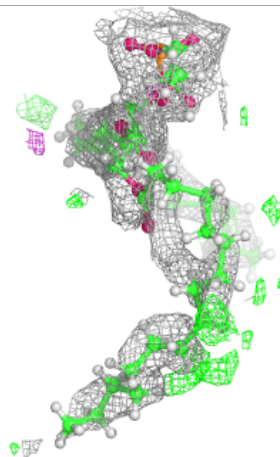
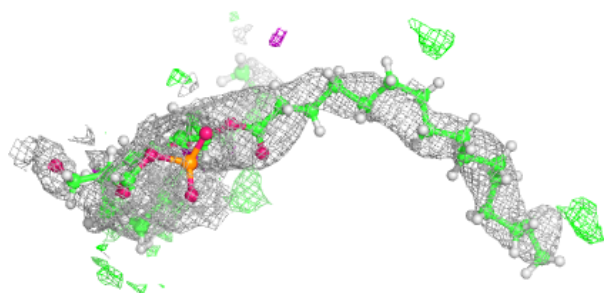
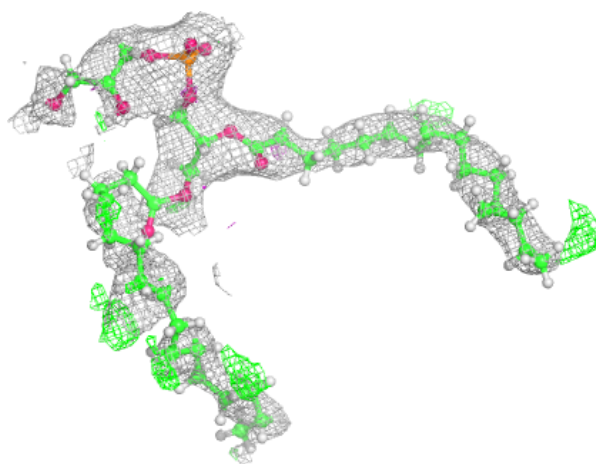
$2mF_o-DF_c$  (at 0.7 rnsd) in gray  
 $mF_o-DF_c$  (at 3 rnsd) in purple (negative)  
and green (positive)





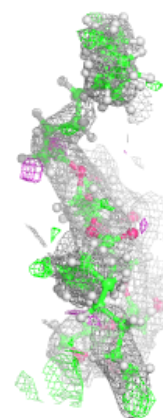
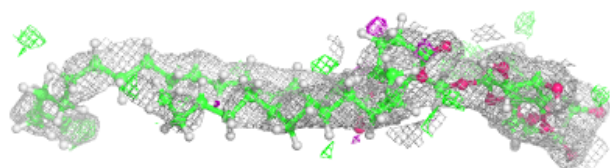
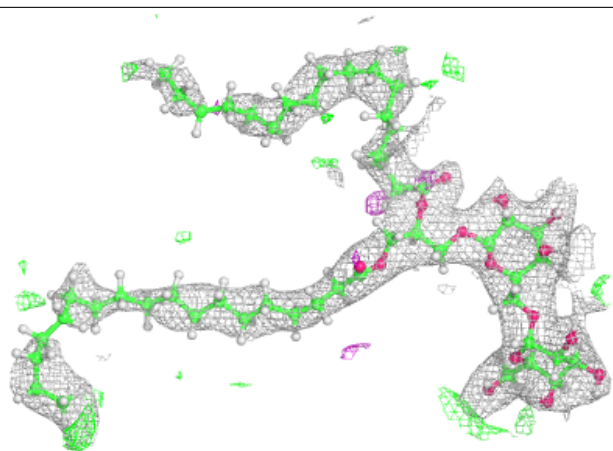
**Electron density around LHG E 102:**

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

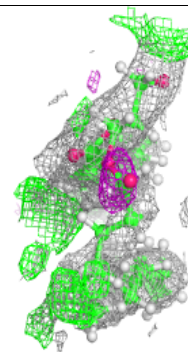
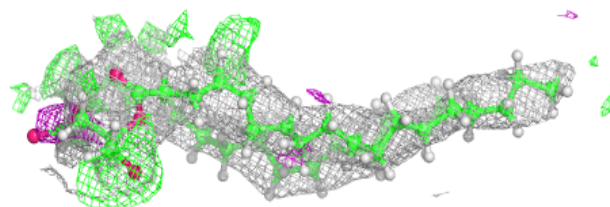
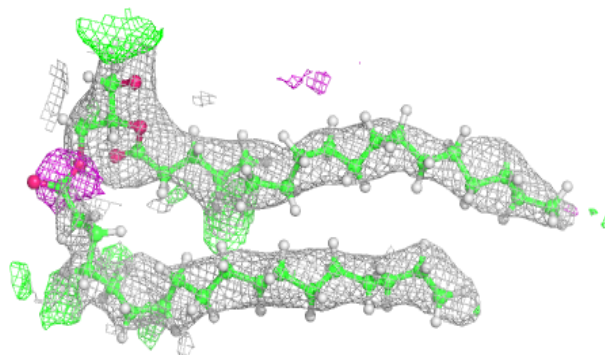


**Electron density around DGD A 414:**

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

**Electron density around DGD a 412:**

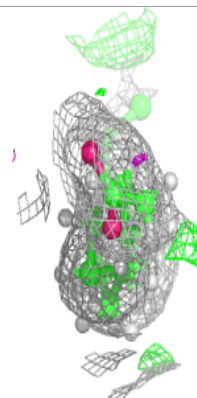
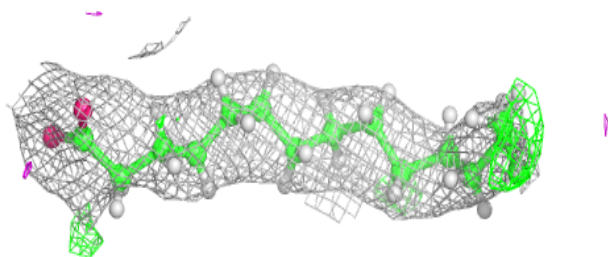
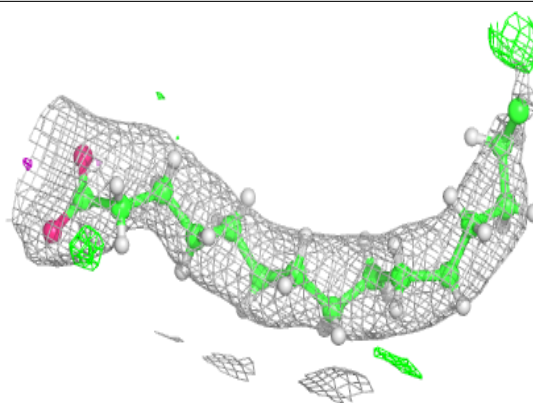
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



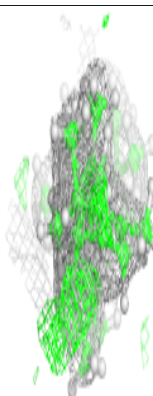
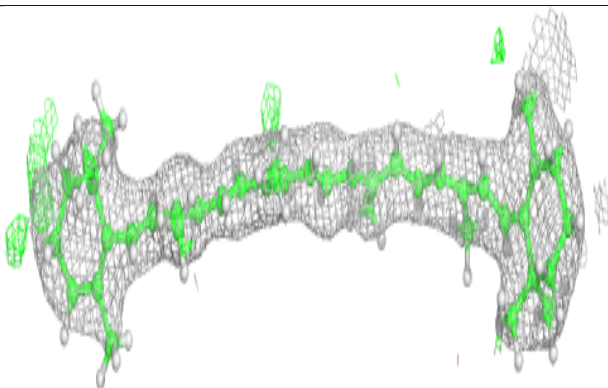
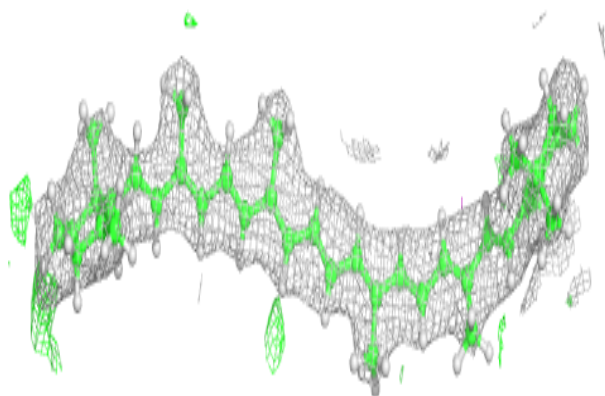


**Electron density around STE B 620:**

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

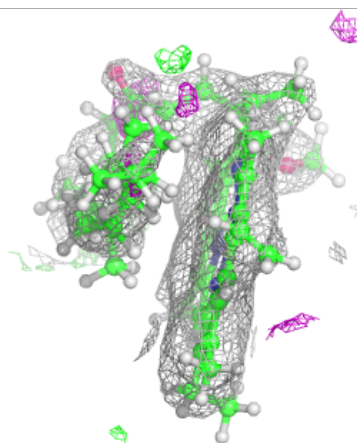
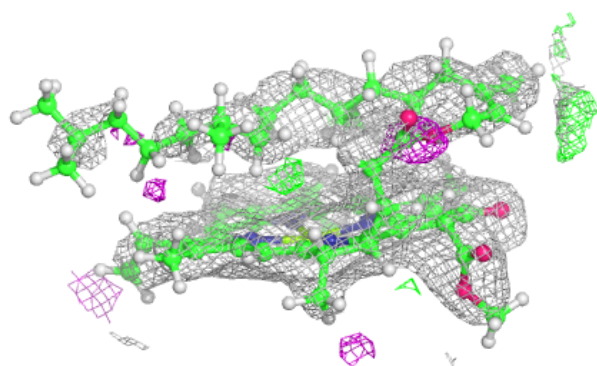
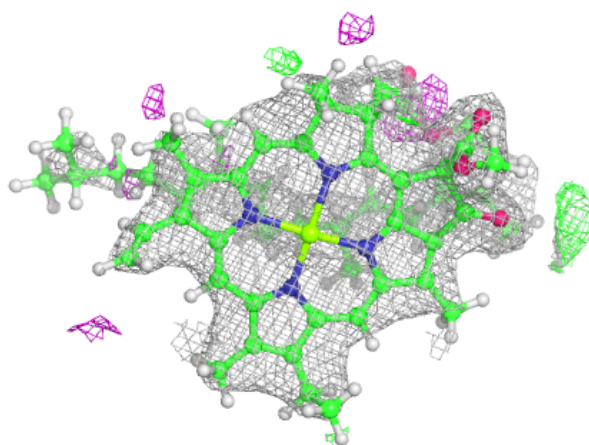
**Electron density around BCR H 101:**

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



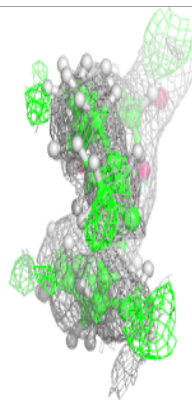
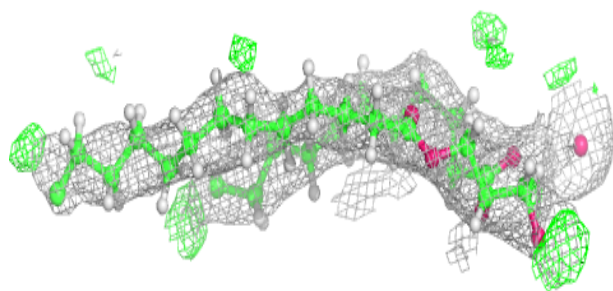
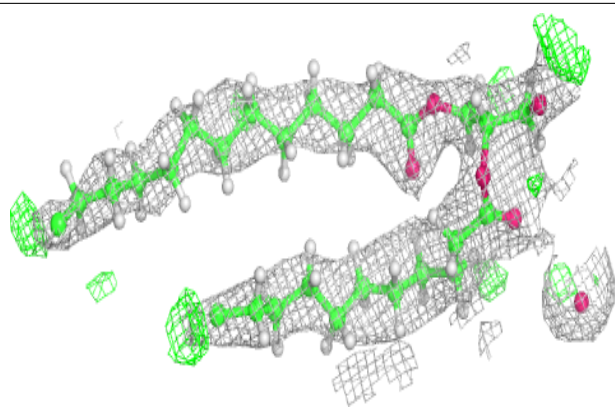
**Electron density around CLA b 601:**

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

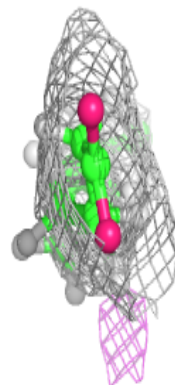
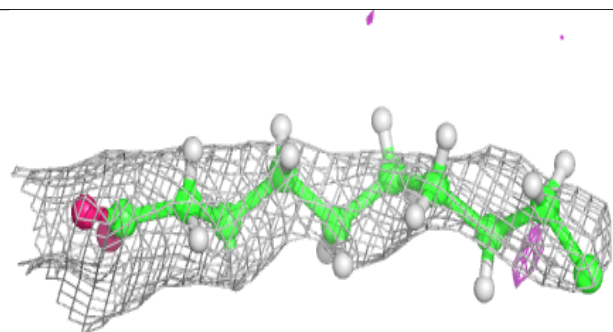
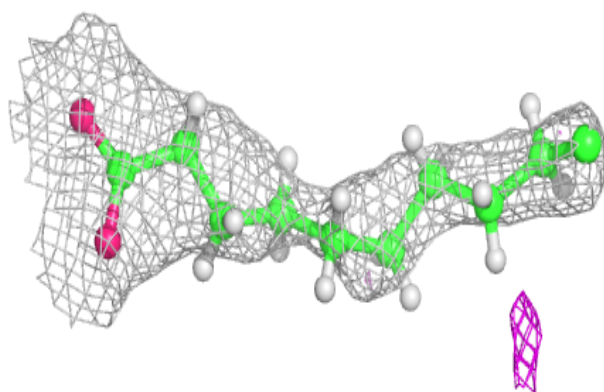


**Electron density around LMG D 410:**

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

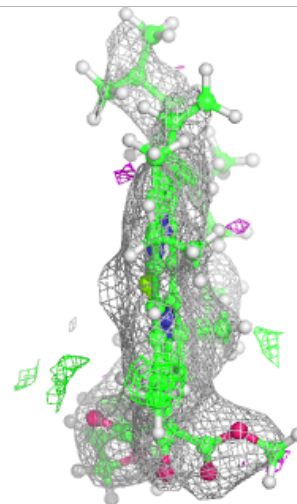
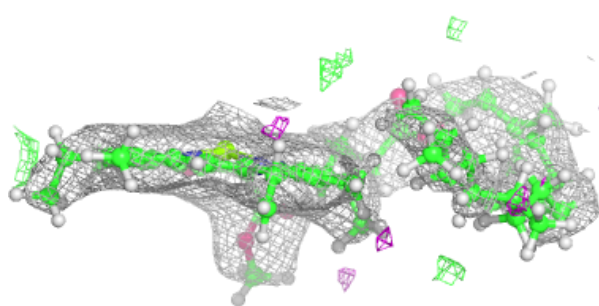
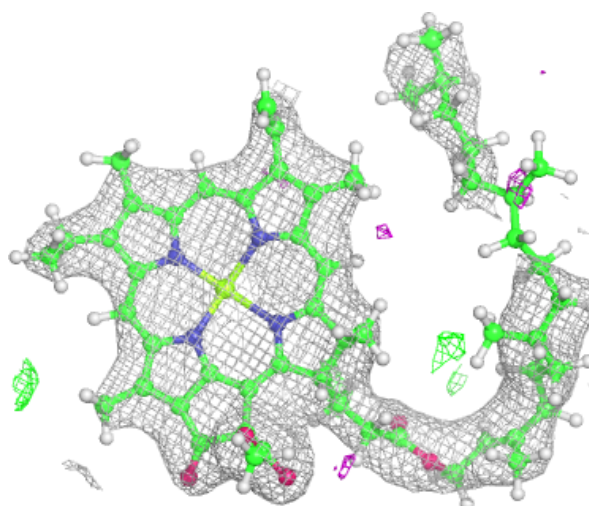
**Electron density around STE a 414:**

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



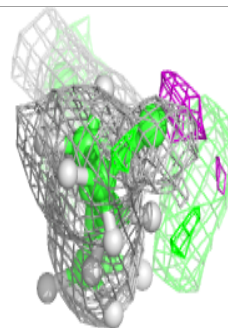
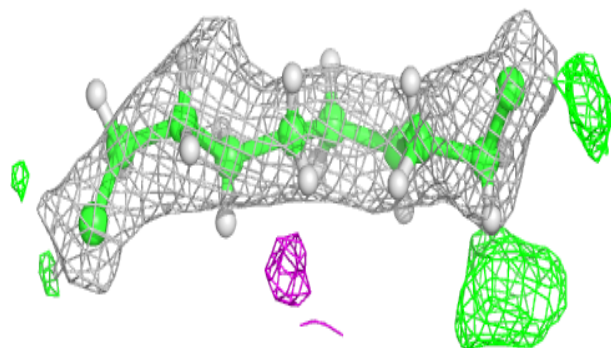
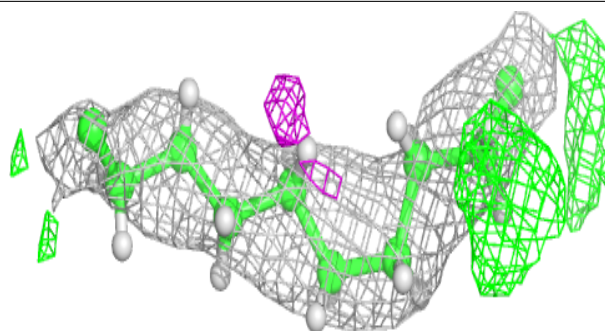
**Electron density around CLA C 512:**

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

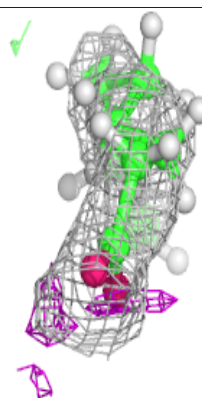
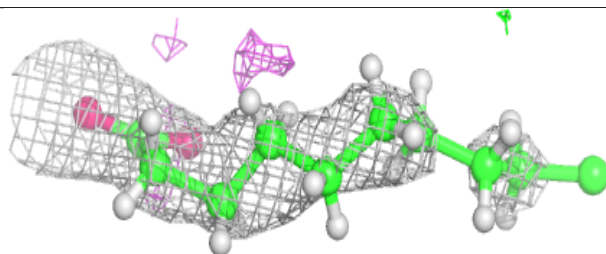
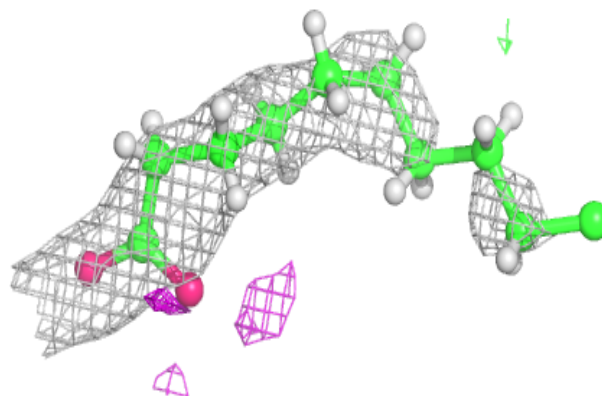


**Electron density around STE b 625:**

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

**Electron density around STE B 627:**

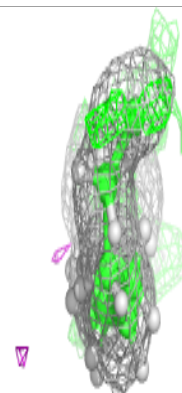
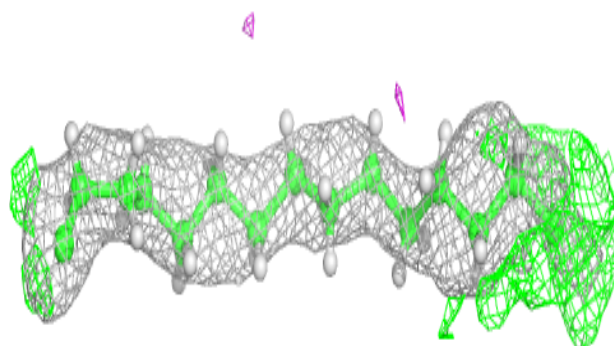
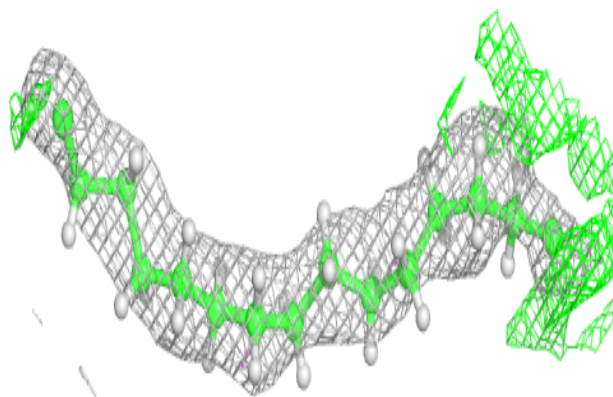
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



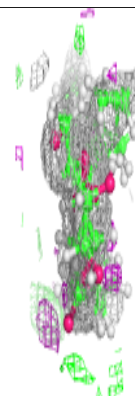
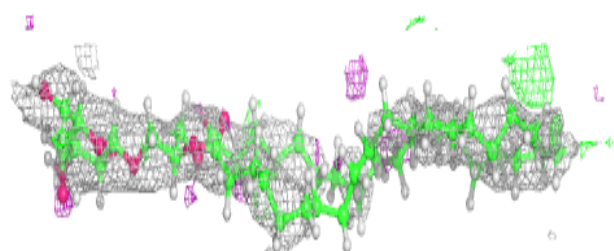
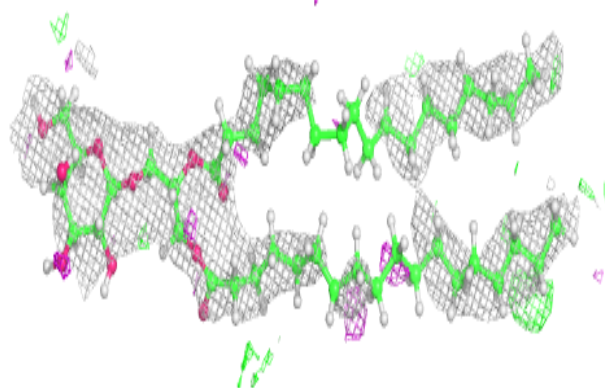


**Electron density around STE I 101:**

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

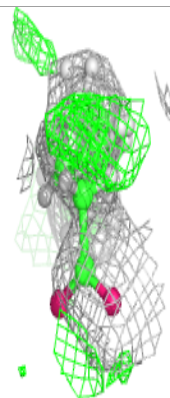
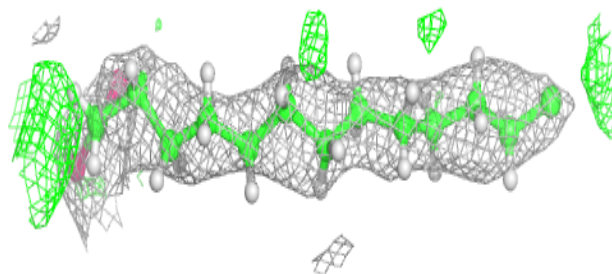
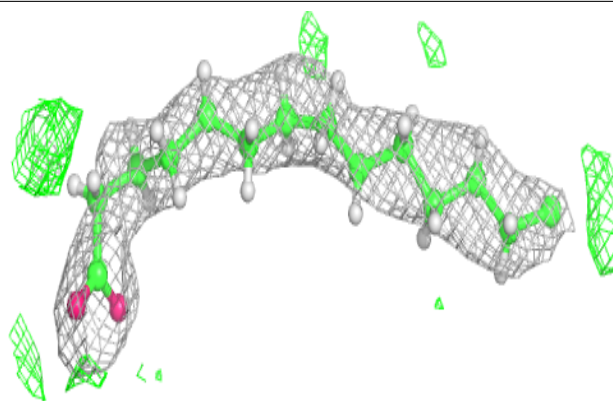
**Electron density around LMG b 622:**

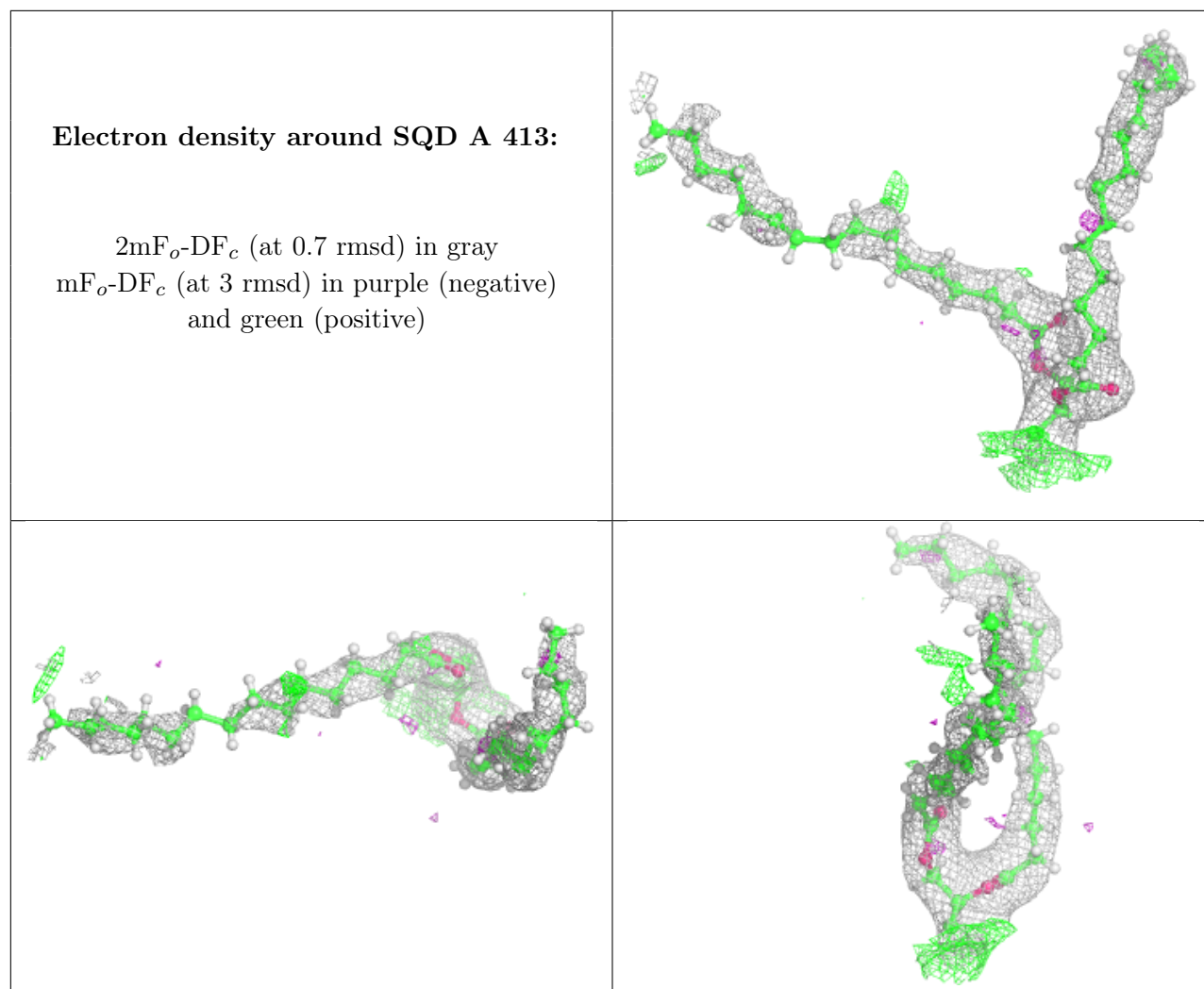
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around STE b 623:**

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

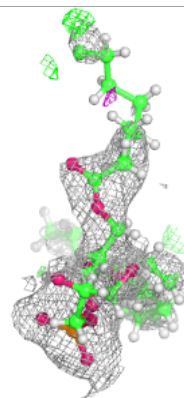
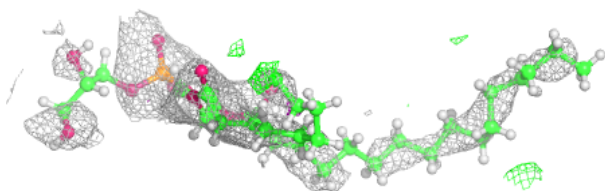
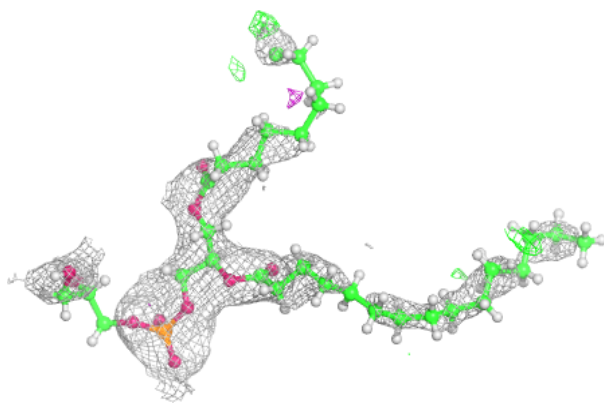






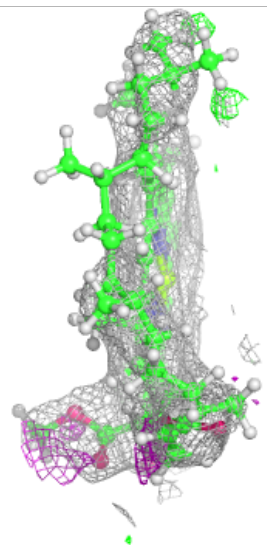
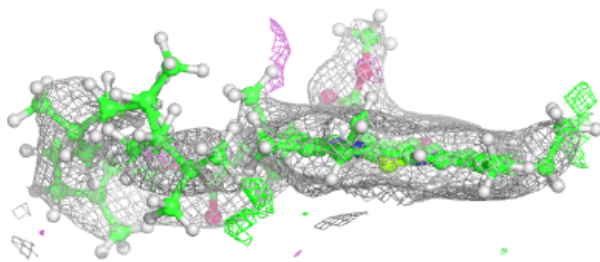
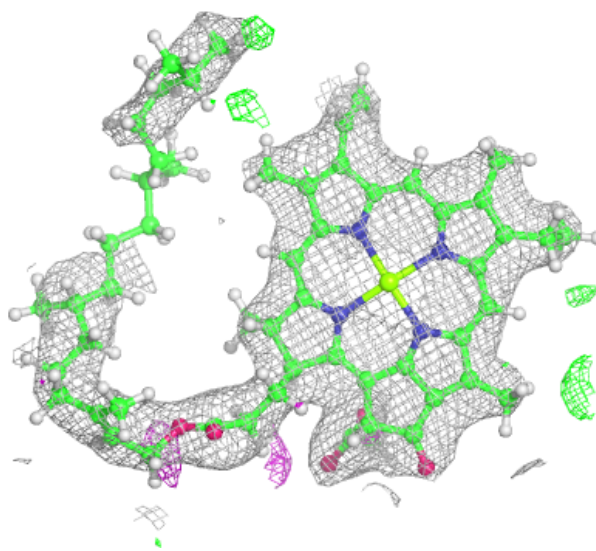
**Electron density around LHG e 101:**

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



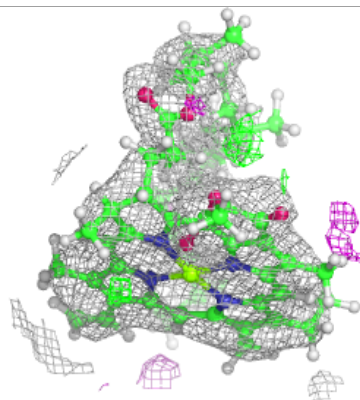
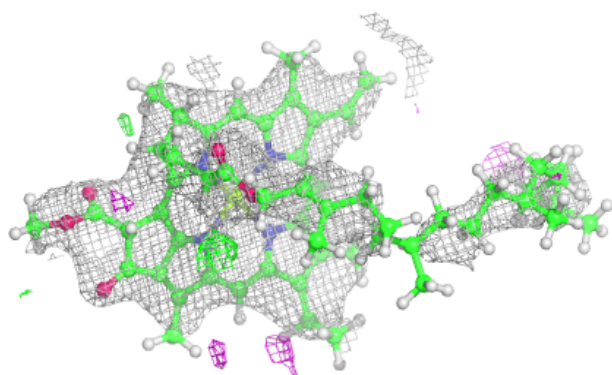
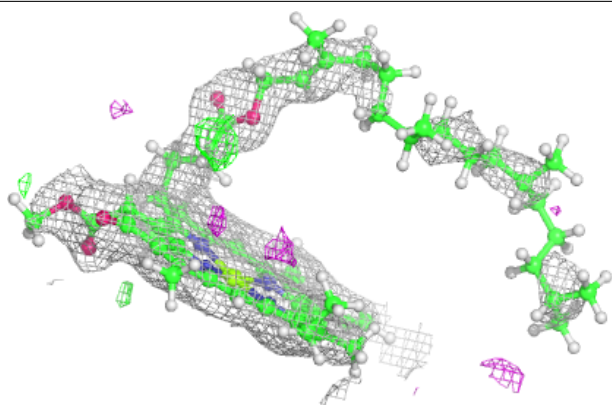
**Electron density around CLA c 512:**

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

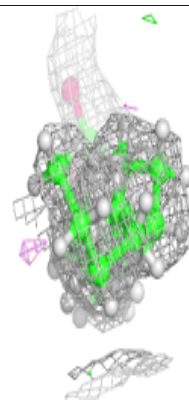
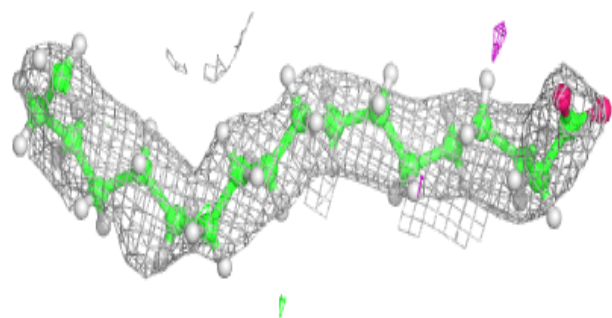
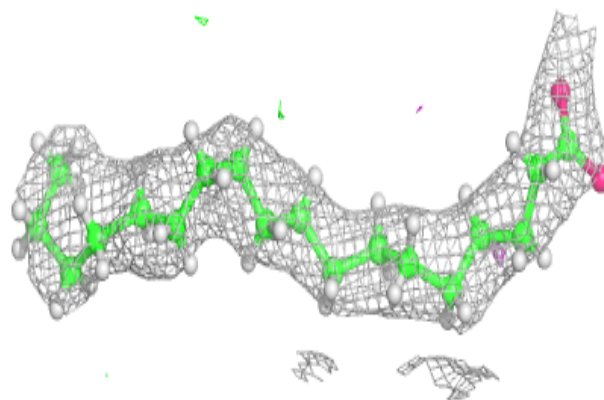


**Electron density around CLA c 513:**

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

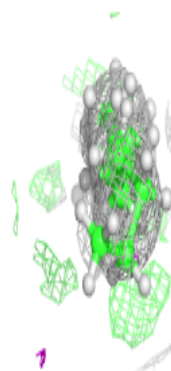
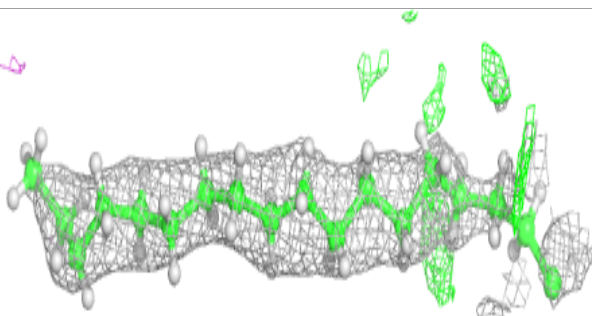
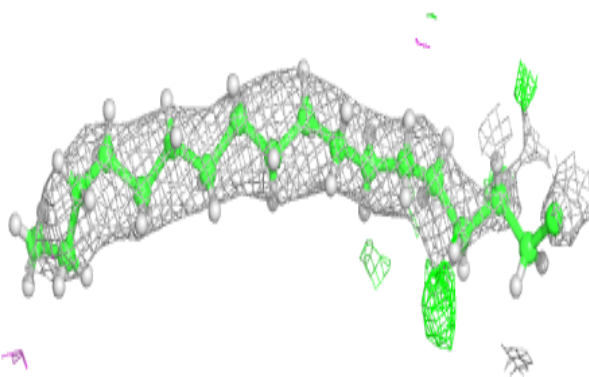
**Electron density around STE b 621:**

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

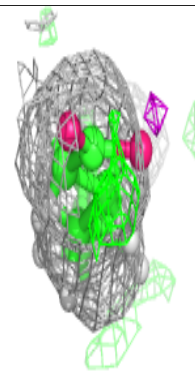
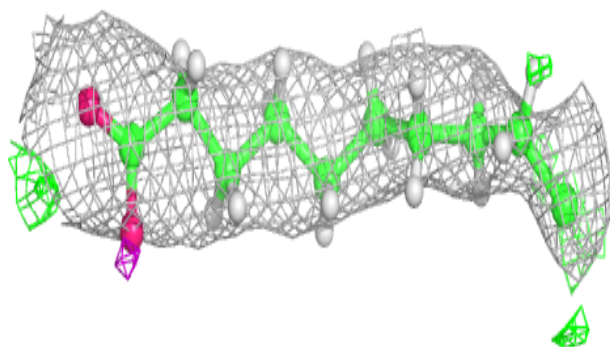
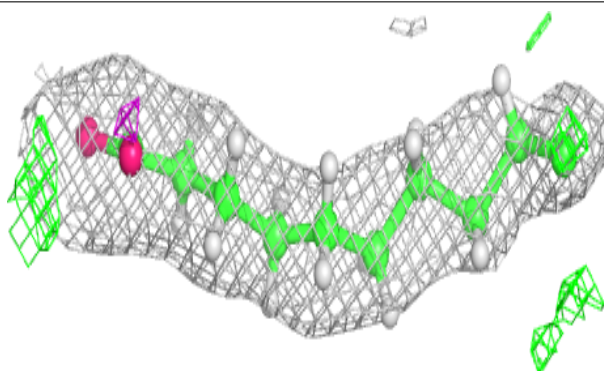


**Electron density around STE I 102:**

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

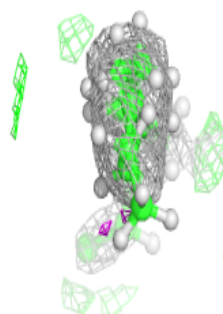
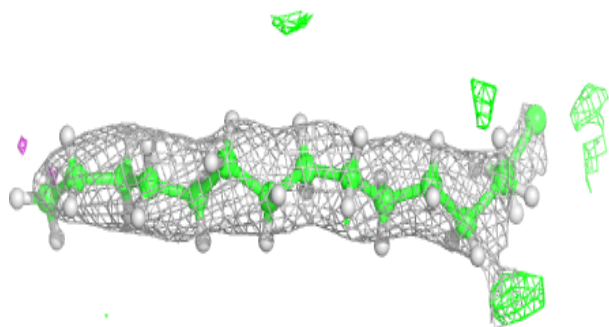
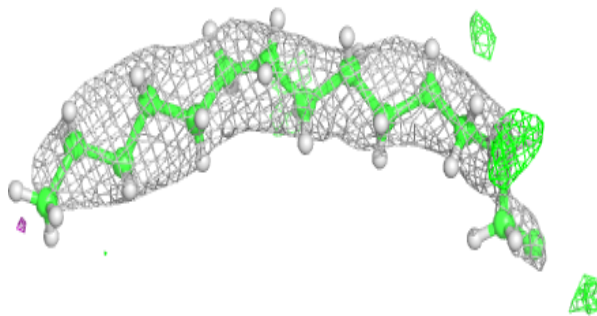
**Electron density around STE j 101:**

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

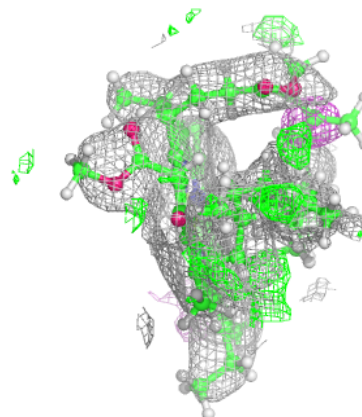
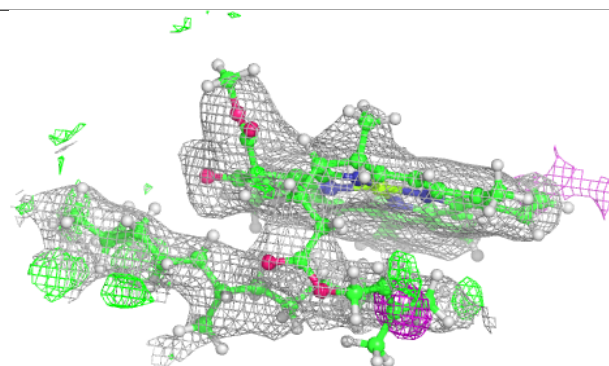
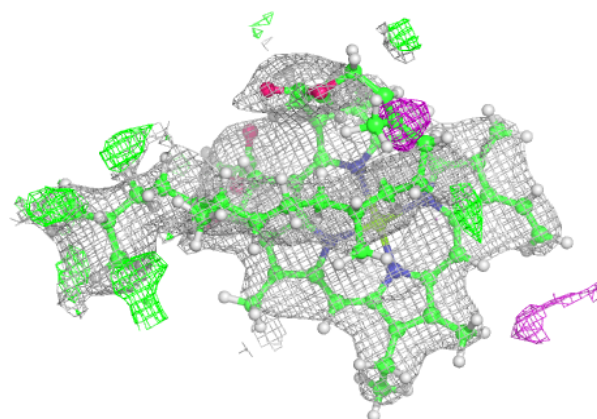


**Electron density around STE T 103:**

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

**Electron density around CLA B 601:**

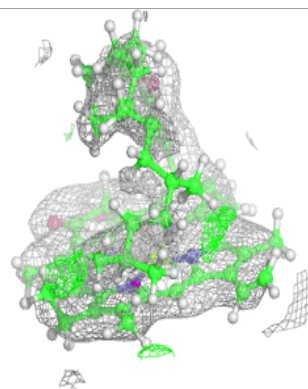
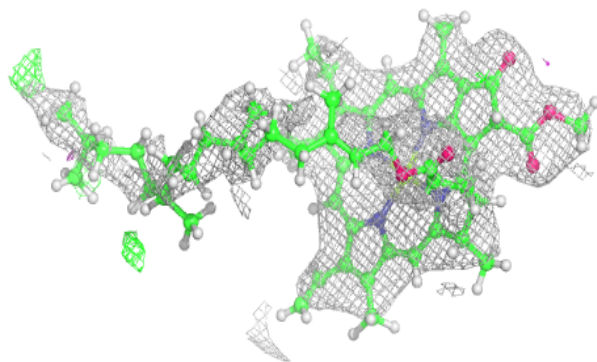
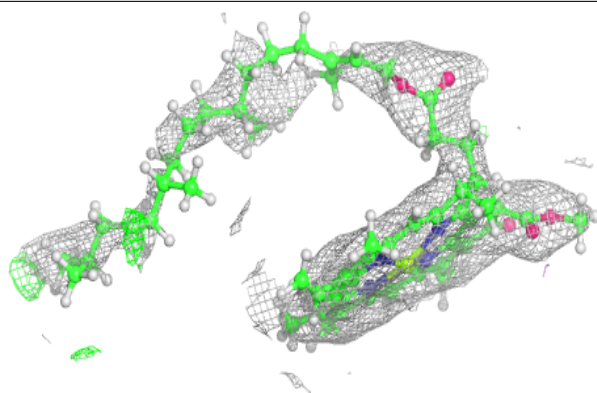
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



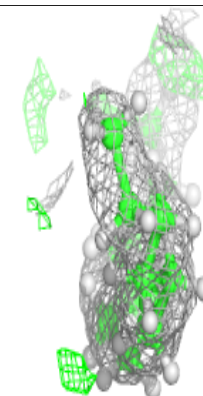
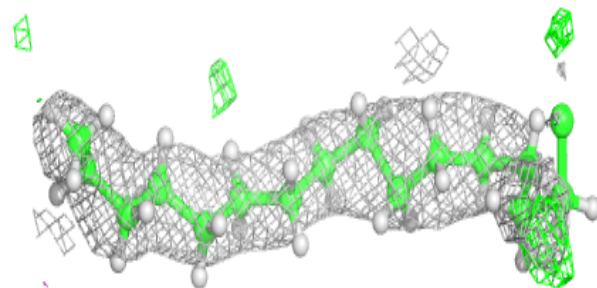
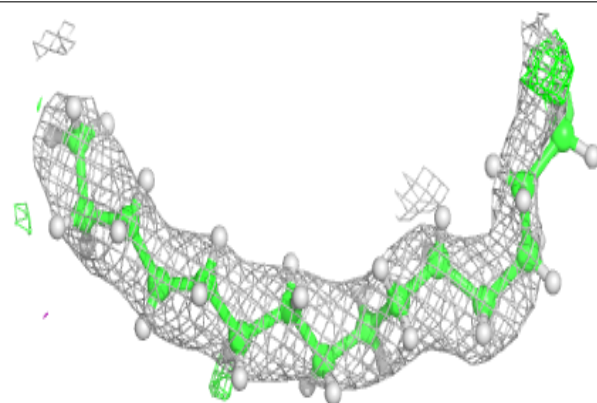


**Electron density around CLA C 513:**

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

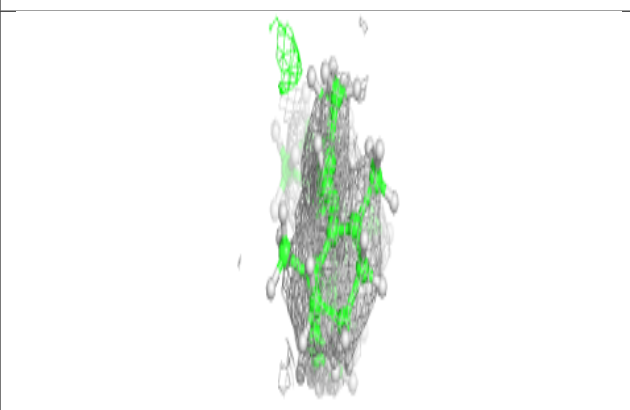
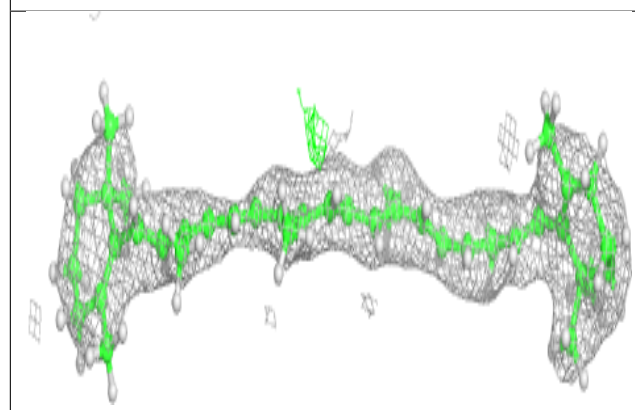
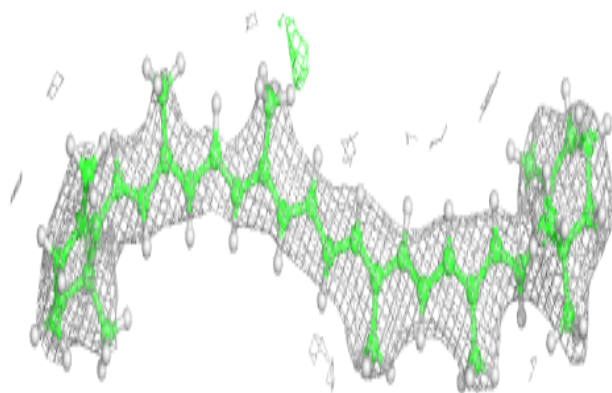
**Electron density around STE T 102:**

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

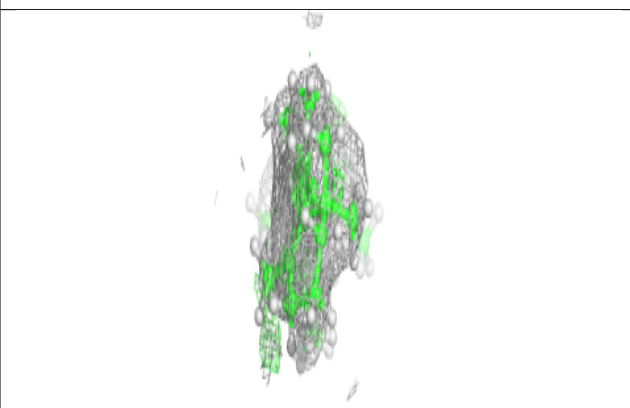
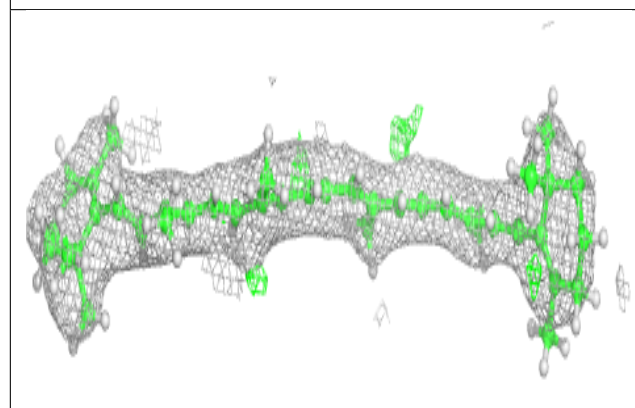
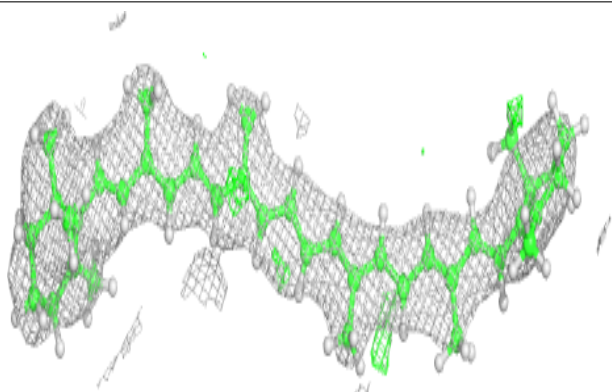


**Electron density around BCR k 101:**

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

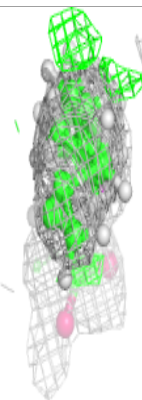
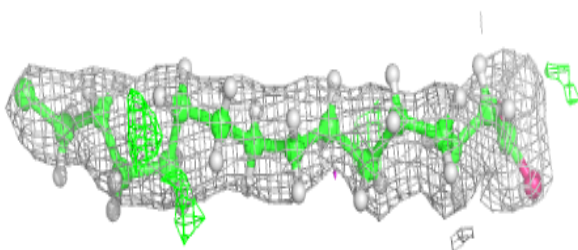
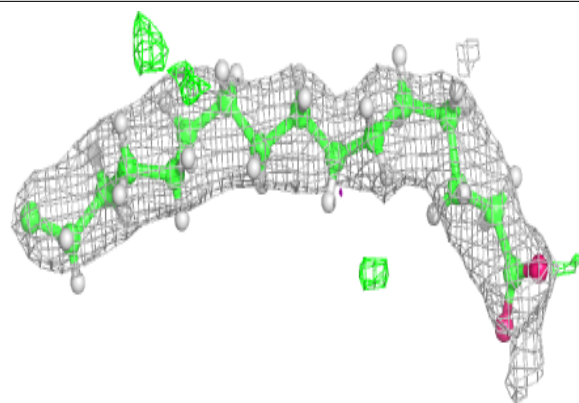
**Electron density around BCR Y 101:**

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

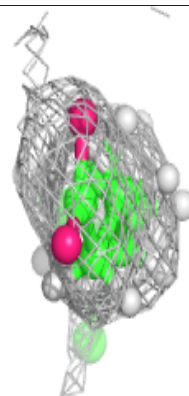
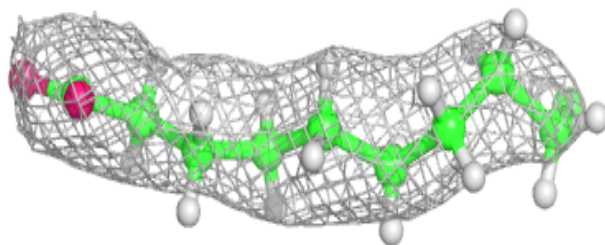
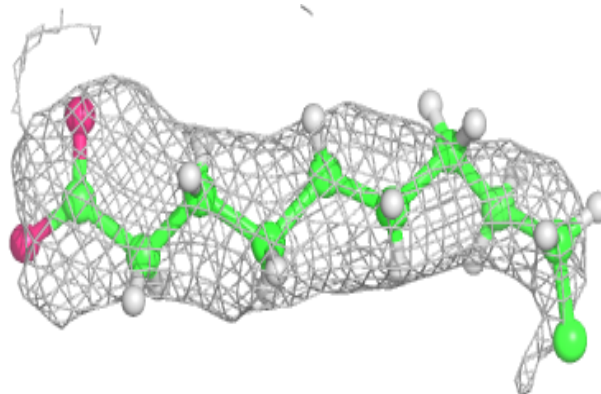


**Electron density around STE B 625:**

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

**Electron density around STE c 524:**

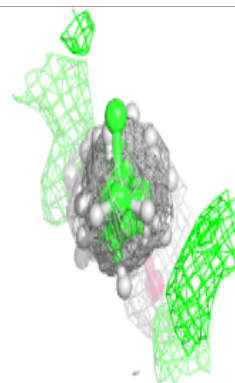
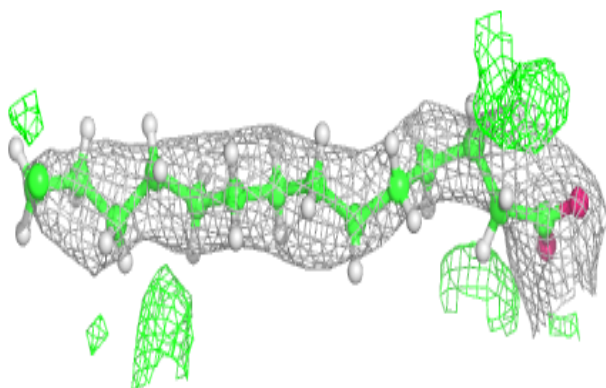
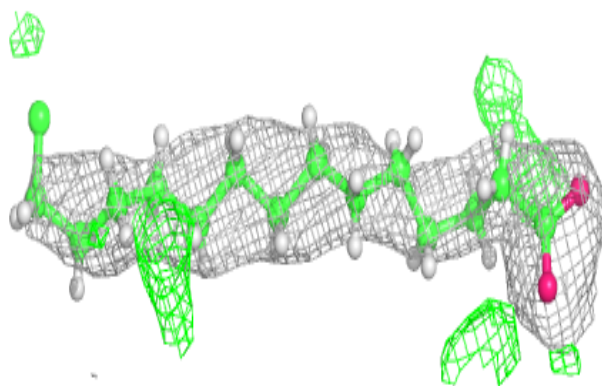
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



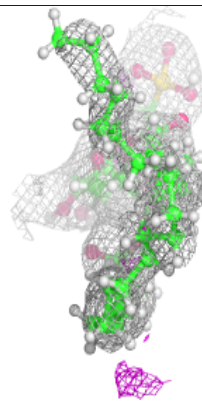
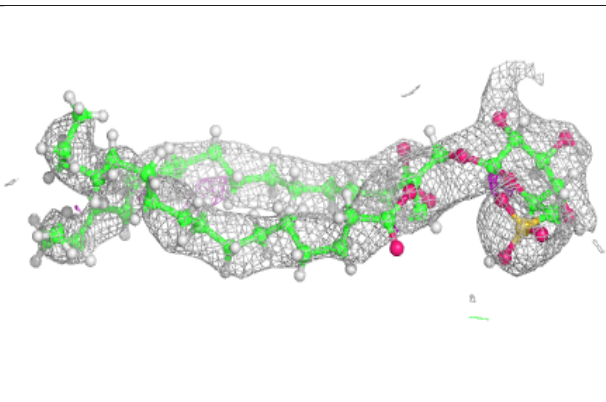
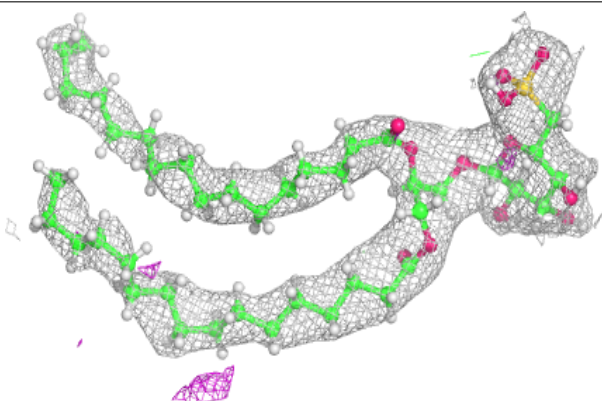


**Electron density around STE d 413:**

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

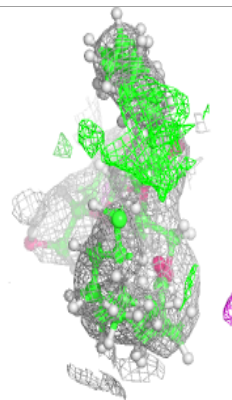
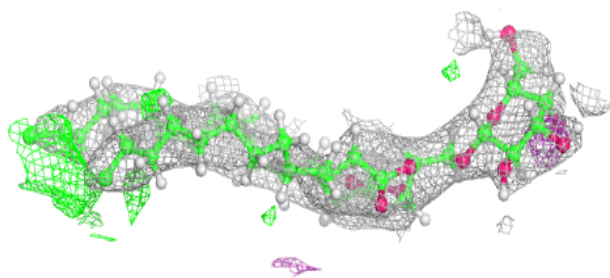
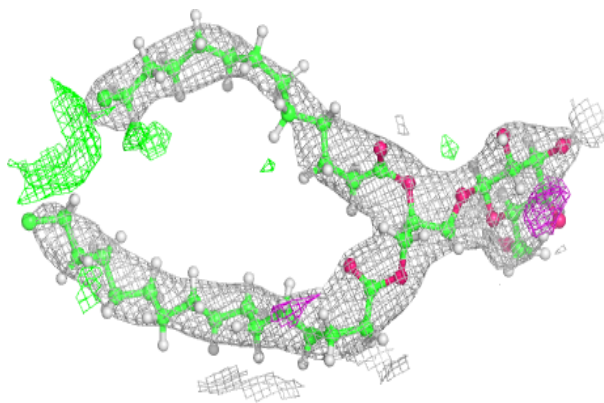
**Electron density around SQD B 623:**

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

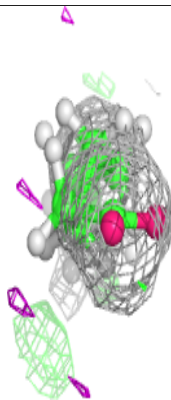
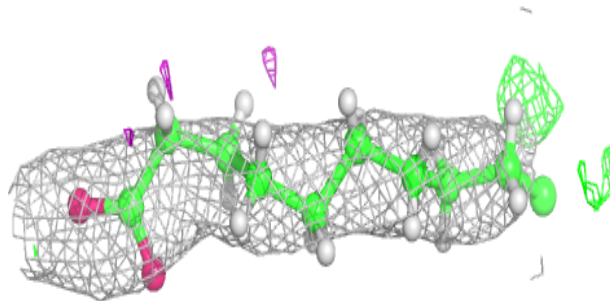
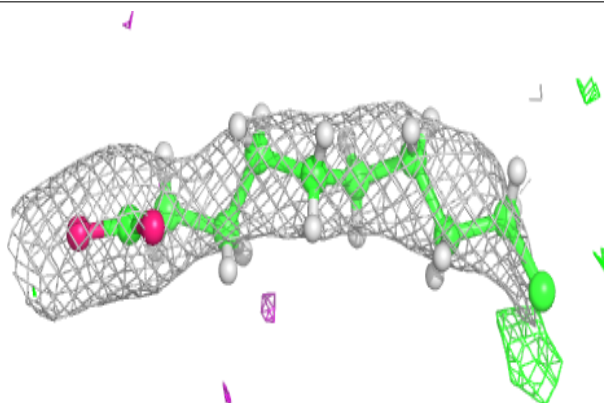


**Electron density around LMG A 411:**

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

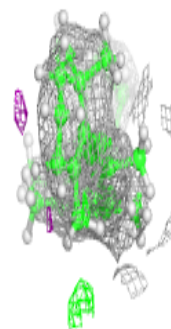
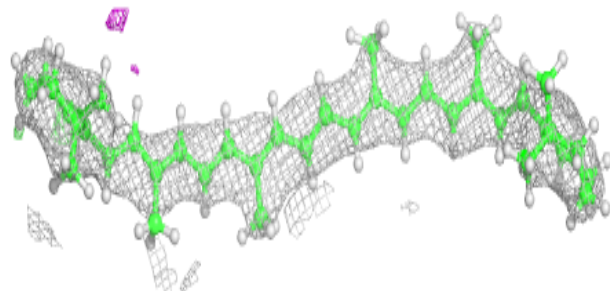
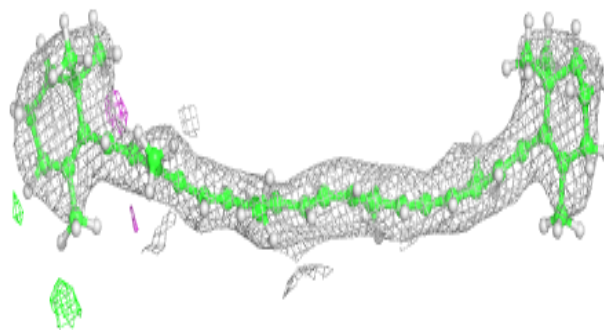
**Electron density around STE m 101:**

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

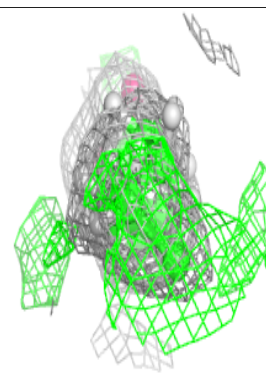
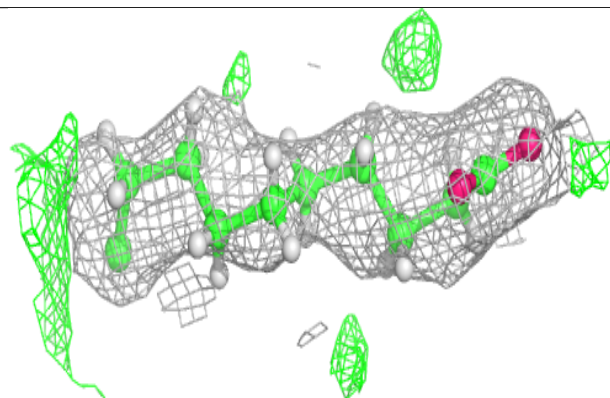
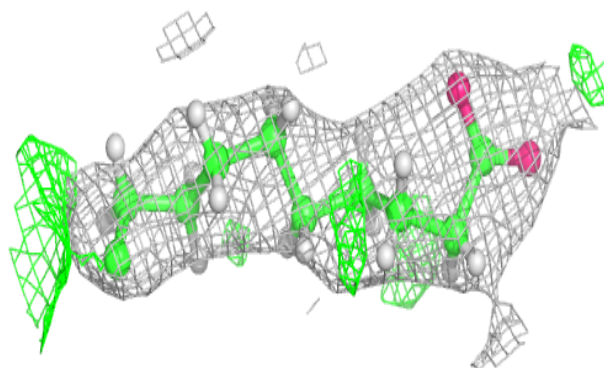


**Electron density around BCR c 516:**

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

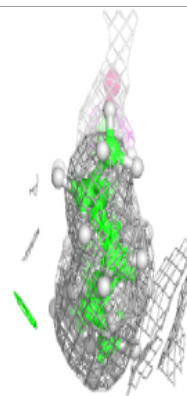
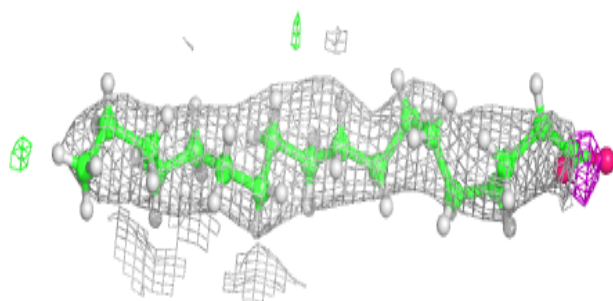
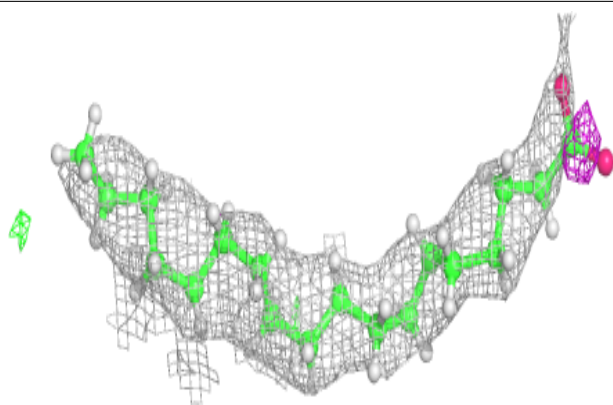
**Electron density around STE J 101:**

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

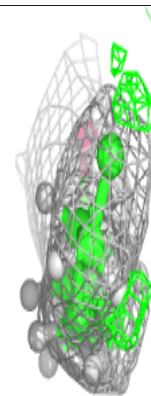
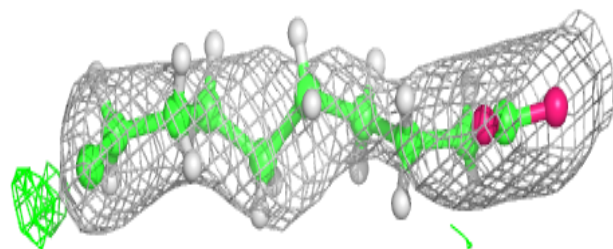
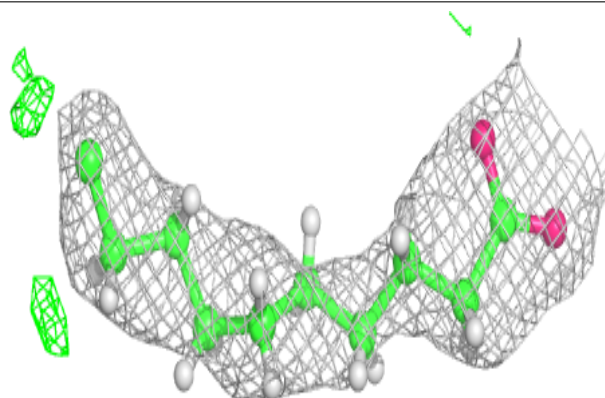


**Electron density around STE D 411:**

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

**Electron density around STE C 520:**

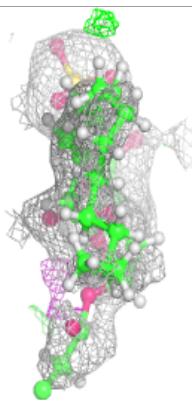
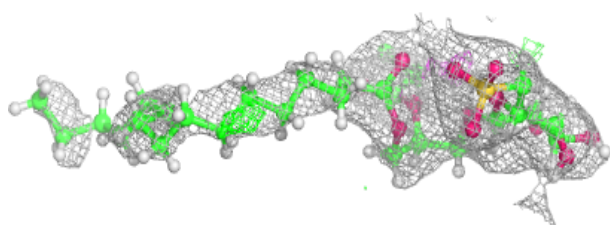
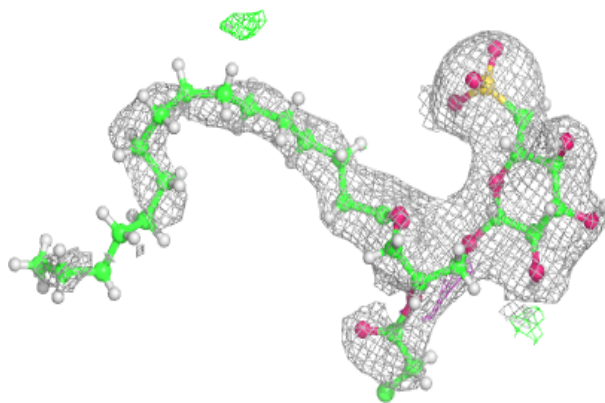
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



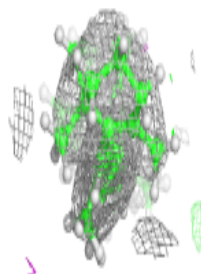
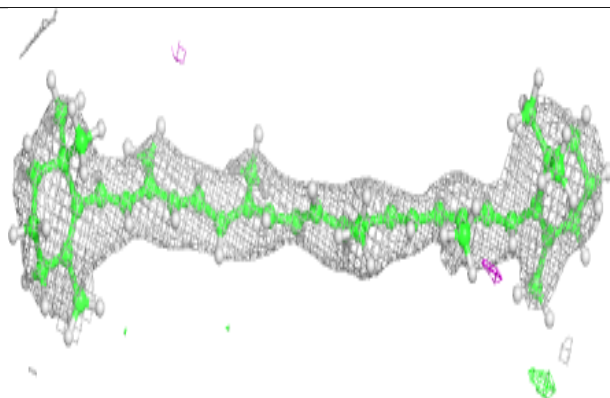
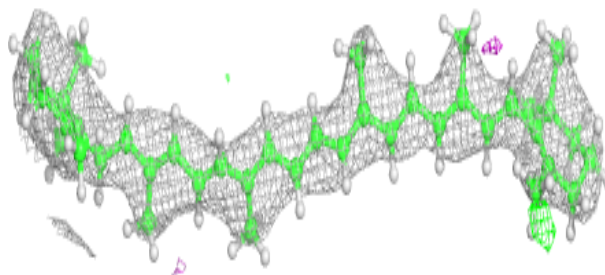


**Electron density around SQD f 102:**

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

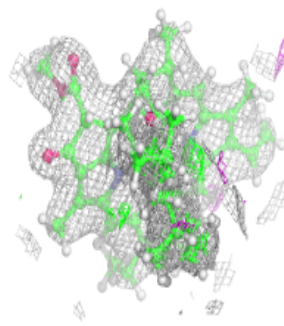
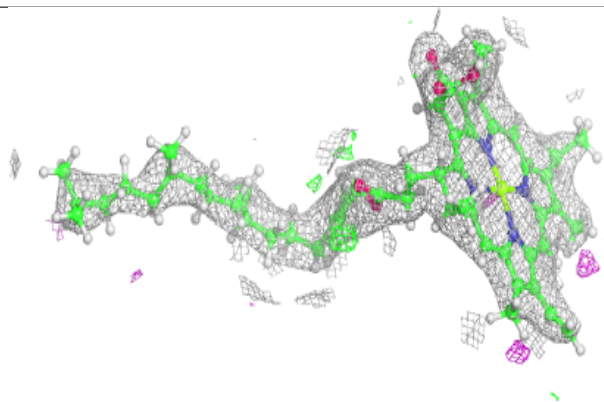
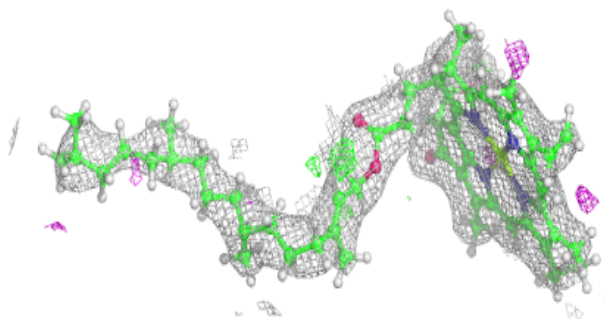
**Electron density around BCR c 514:**

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

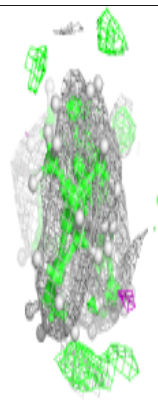
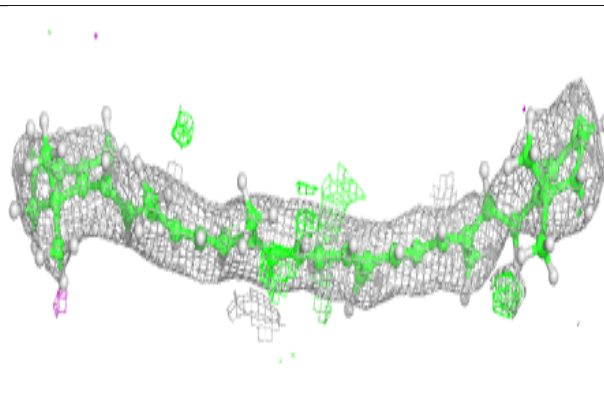
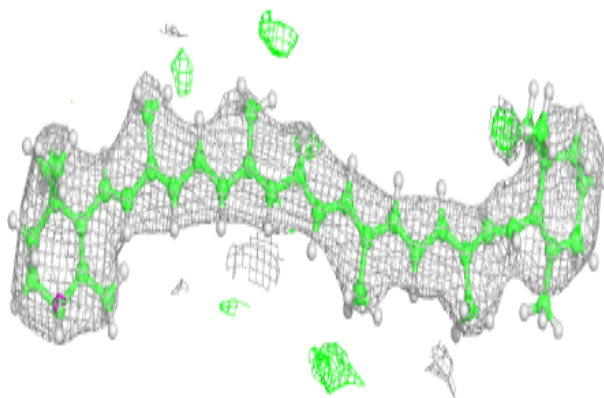


**Electron density around CLA c 502:**

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

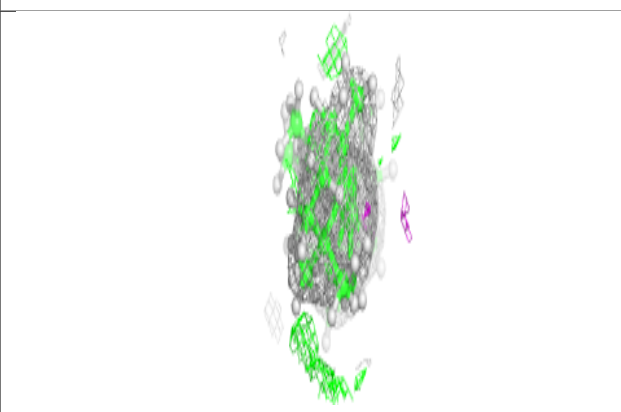
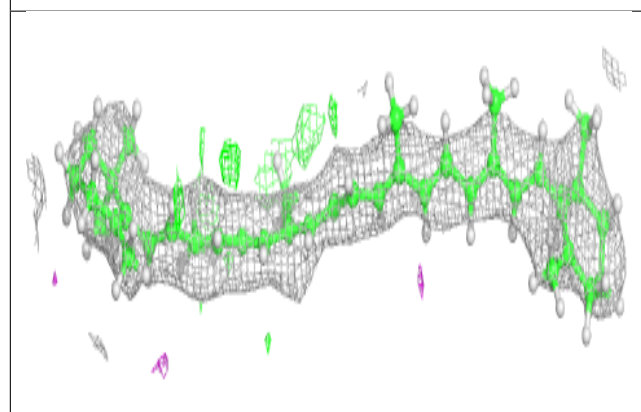
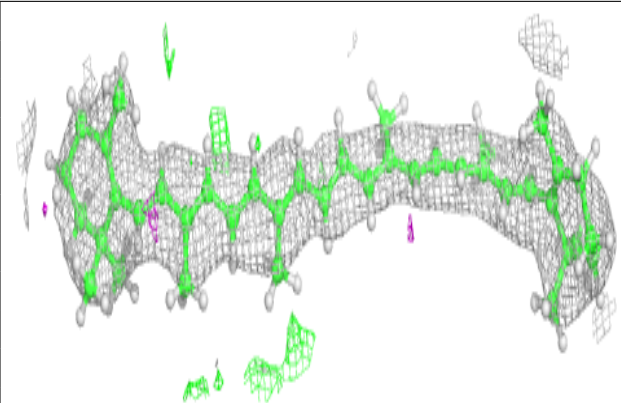
**Electron density around BCR d 406:**

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

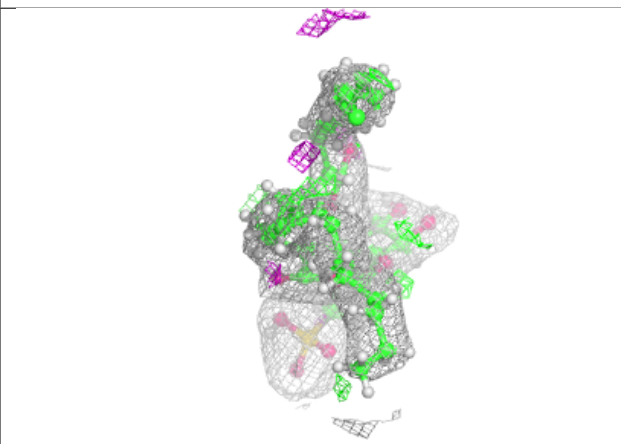
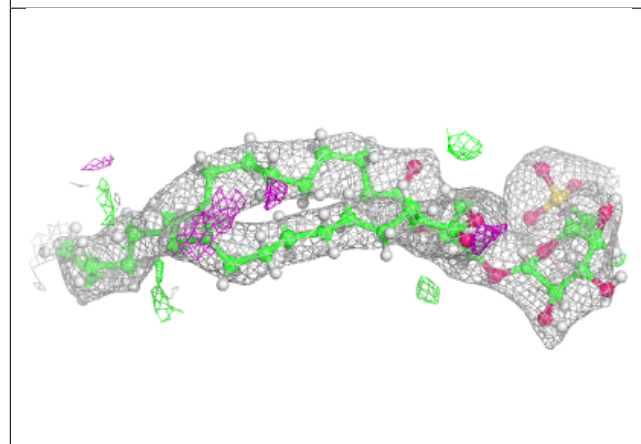
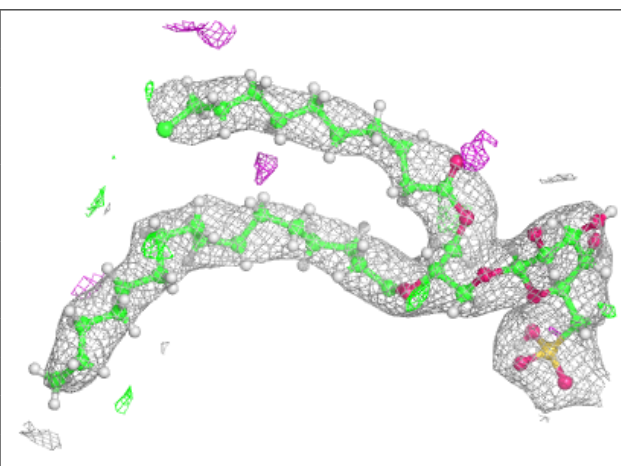


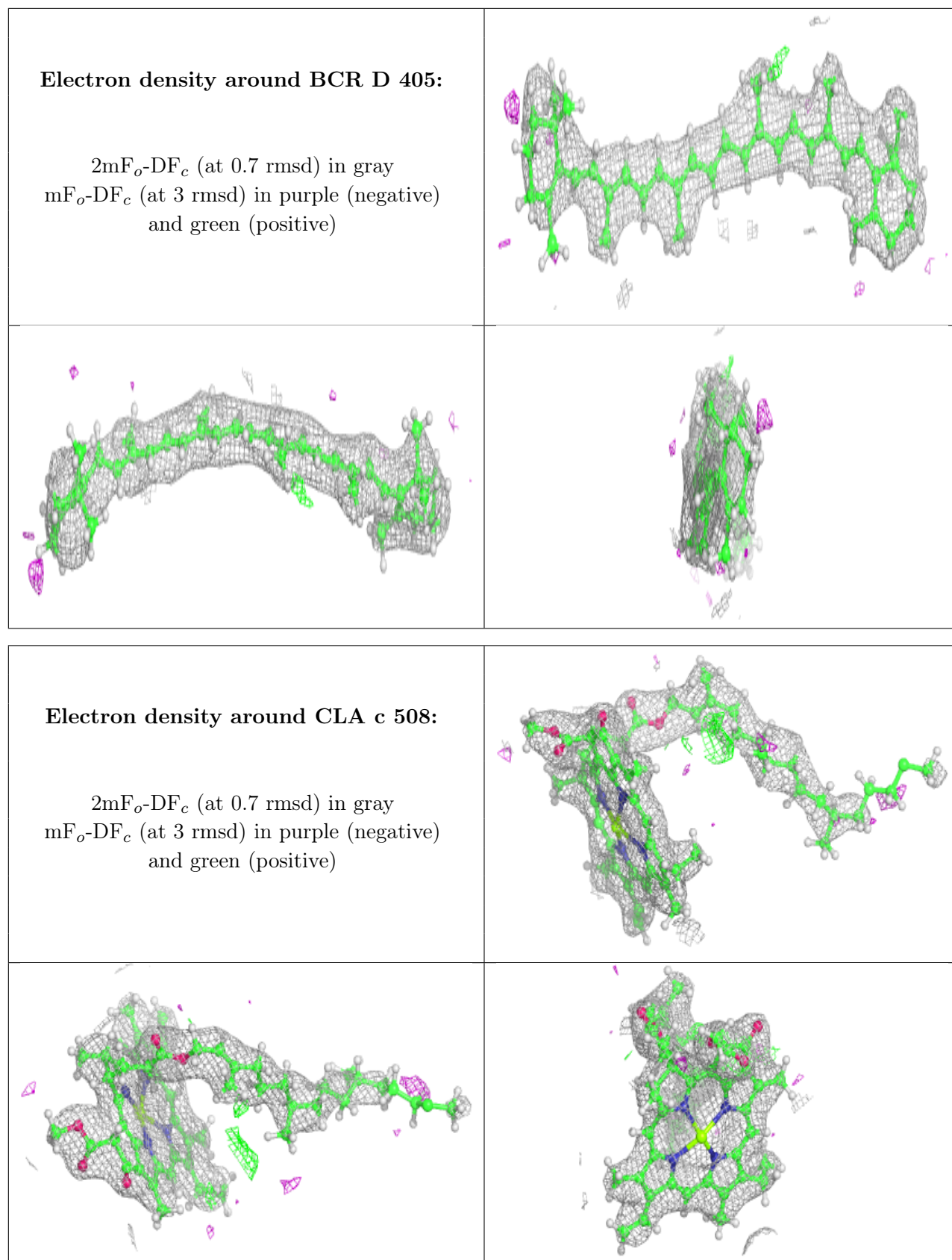
**Electron density around BCR K 101:**

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

**Electron density around SQD L 101:**

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

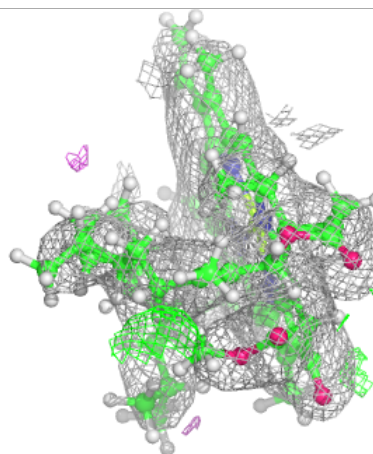
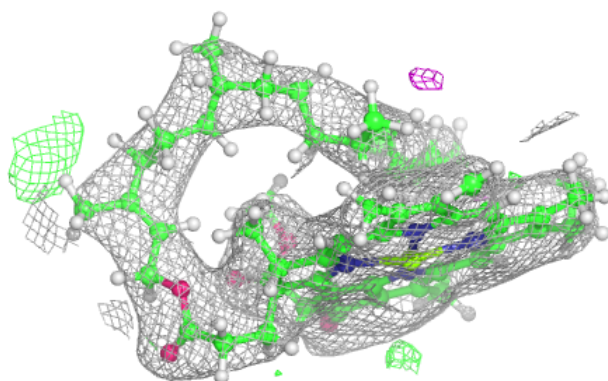
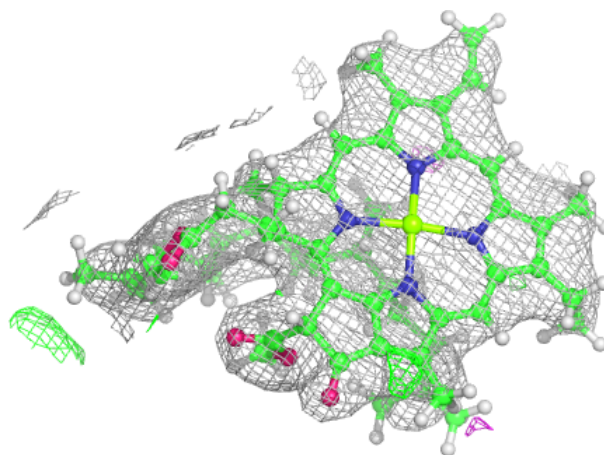






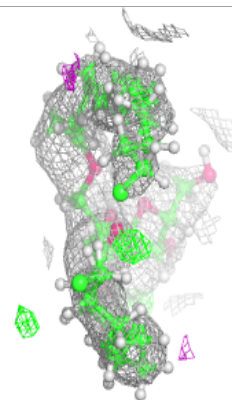
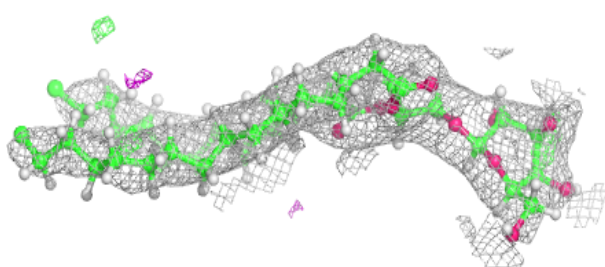
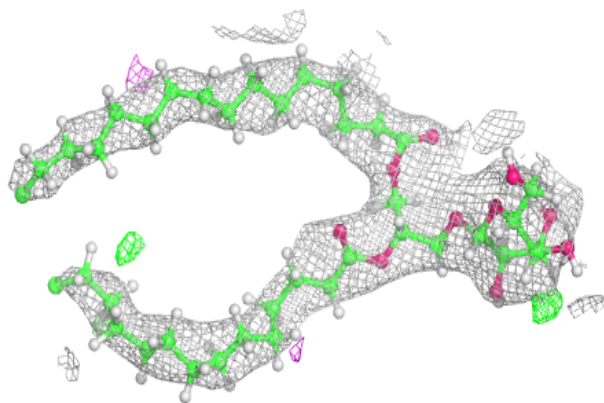
**Electron density around CLA c 510:**

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

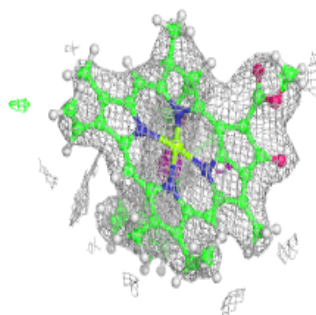
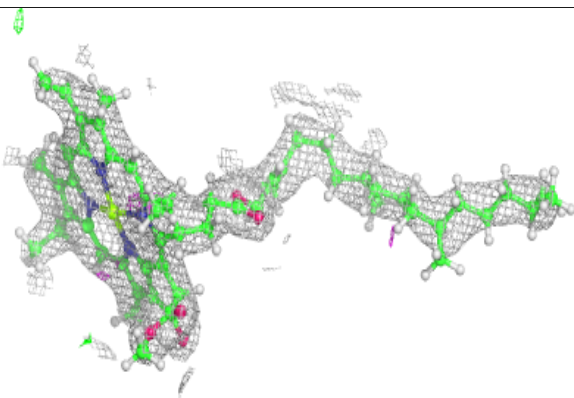
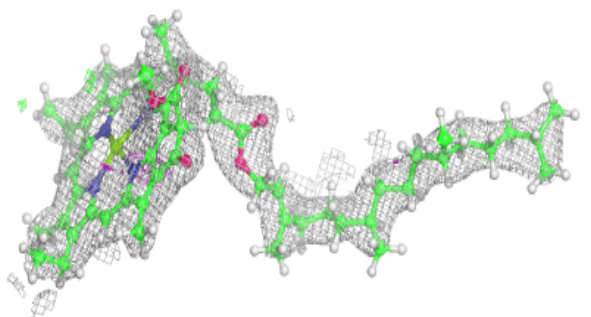


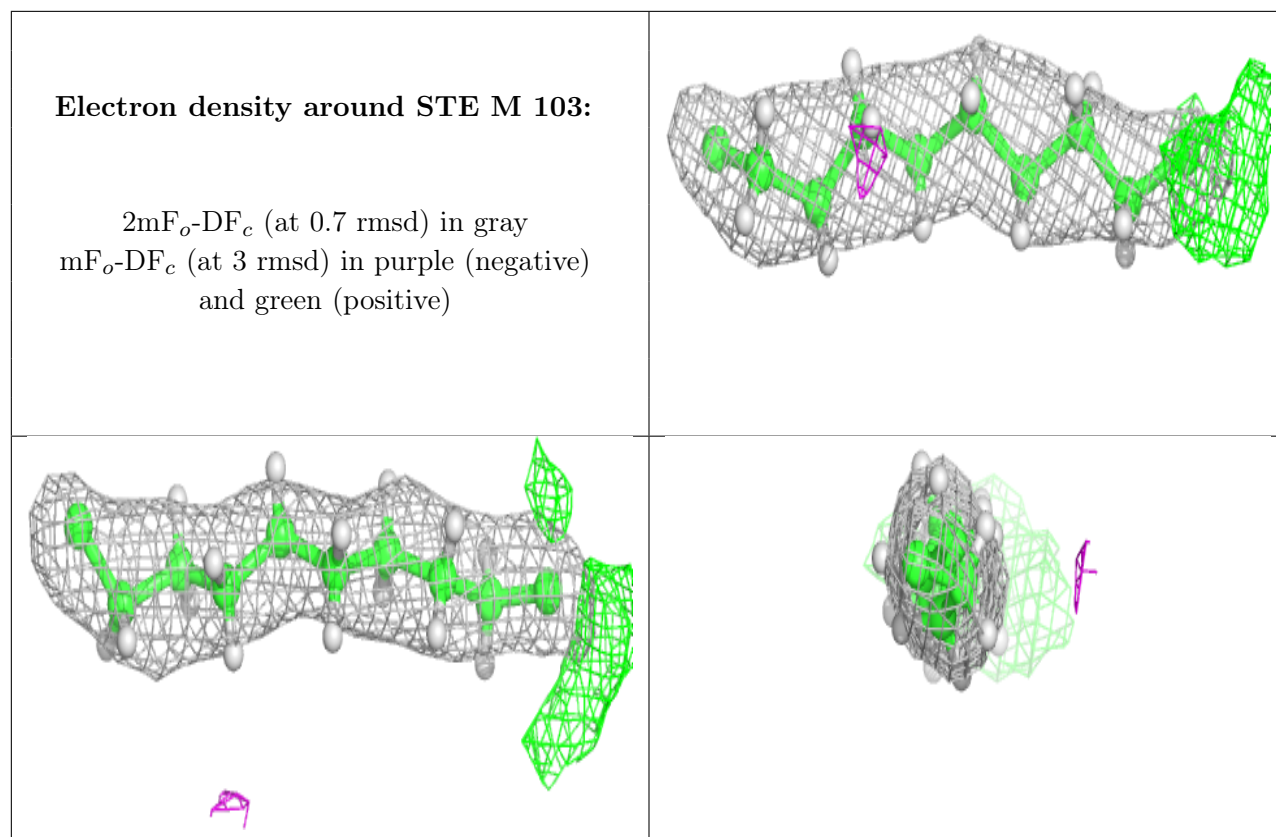
**Electron density around LMG c 523:**

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

**Electron density around CLA C 502:**

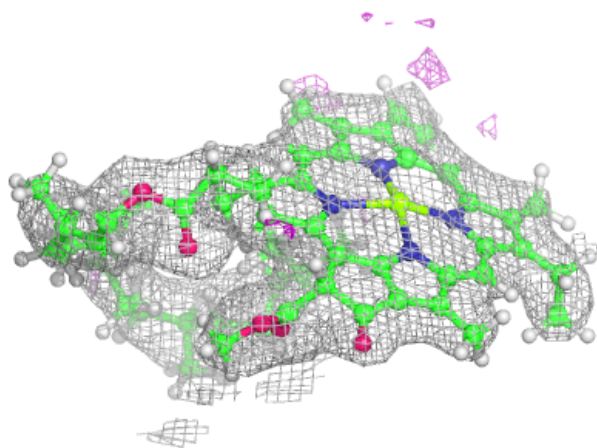
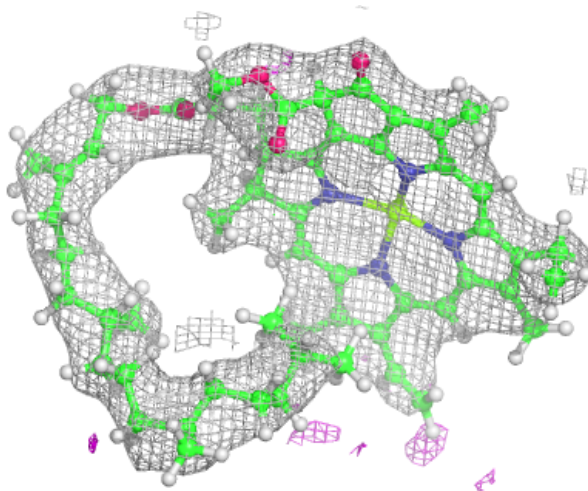
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





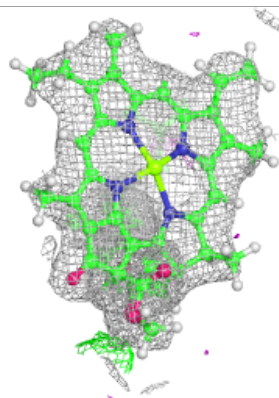
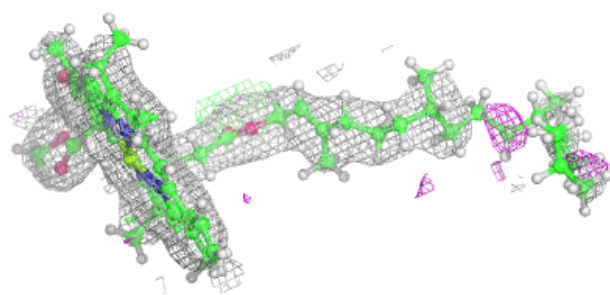
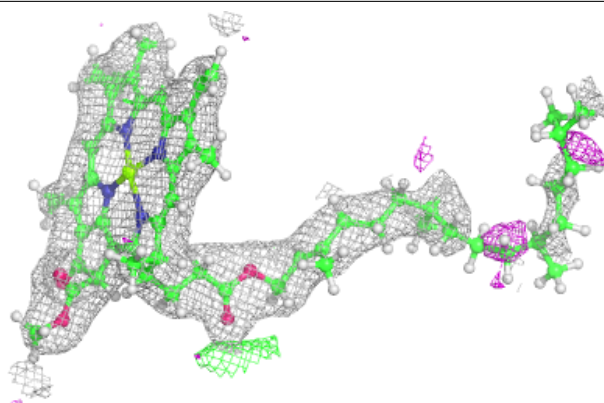
**Electron density around CLA b 615:**

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

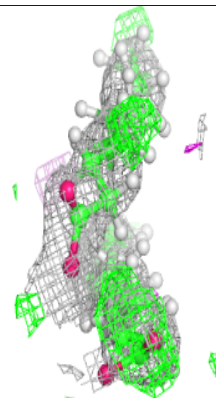
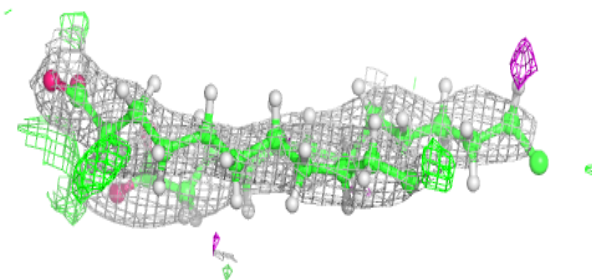
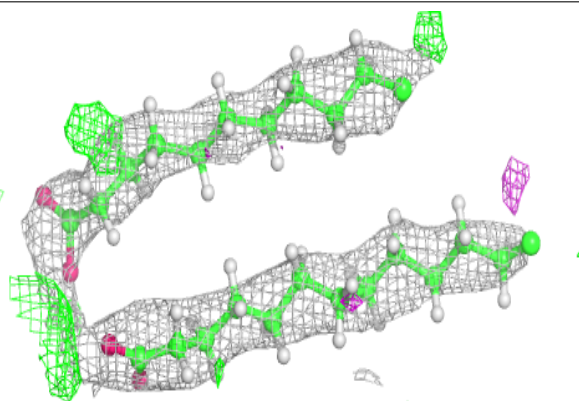


**Electron density around CLA d 405:**

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

**Electron density around LMG B 621:**

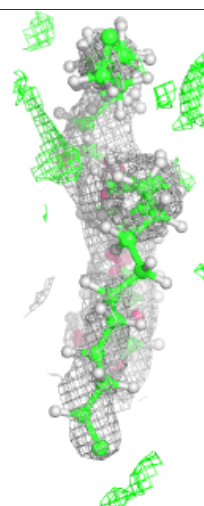
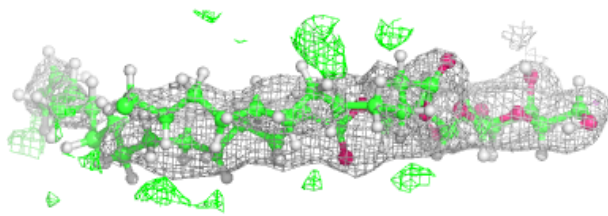
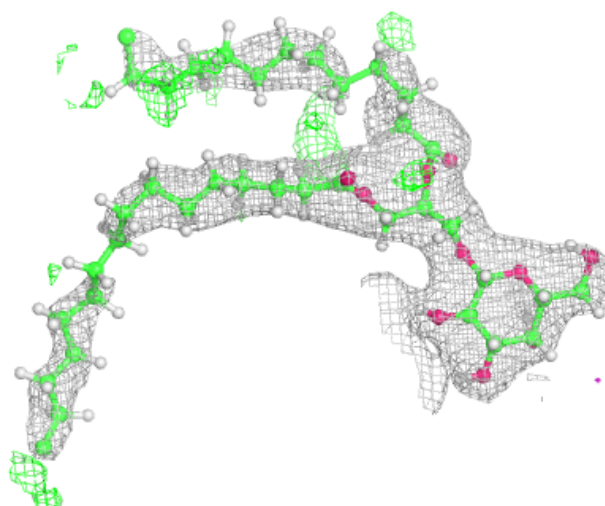
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





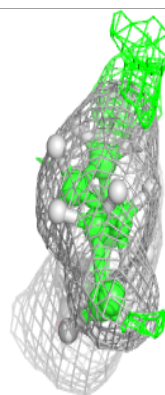
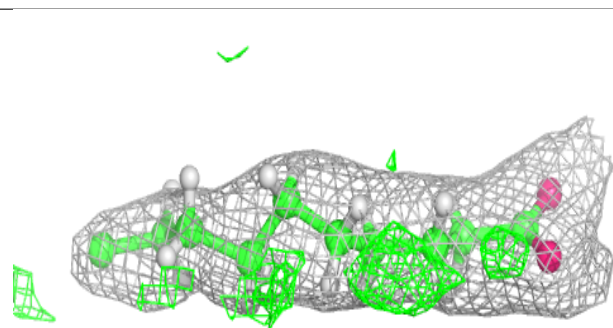
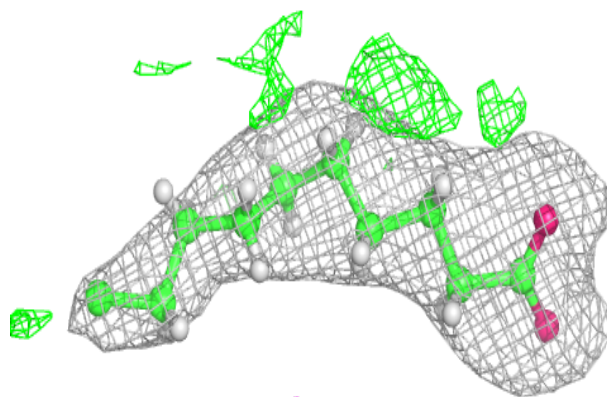
**Electron density around LMG C 519:**

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

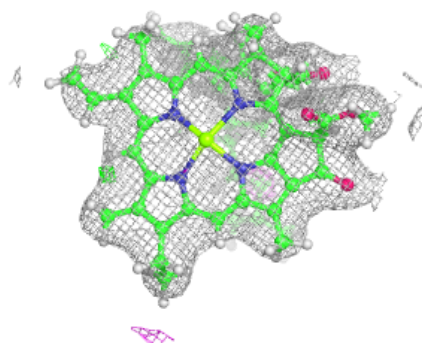
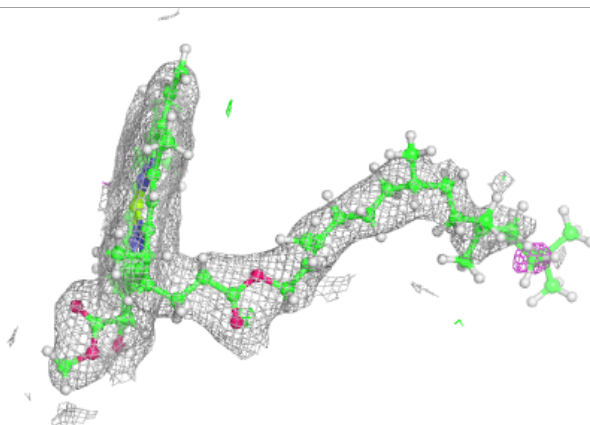
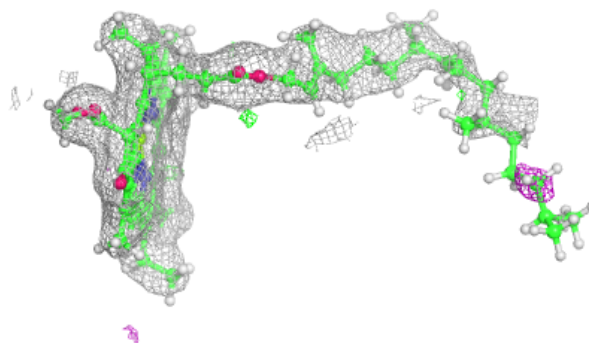


**Electron density around STE C 522:**

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

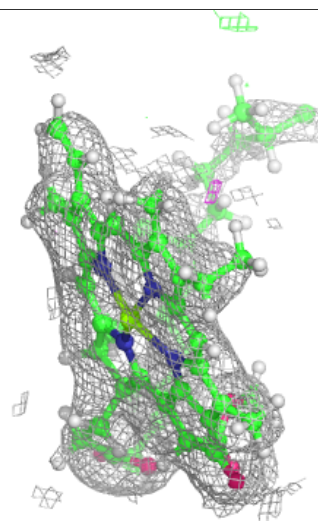
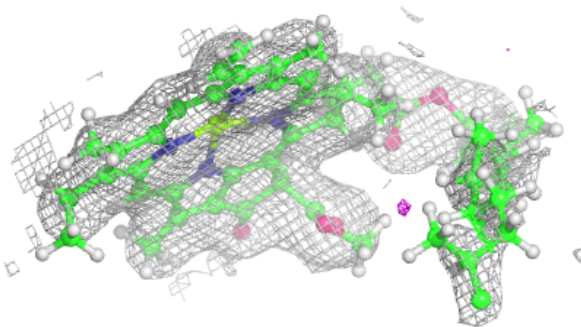
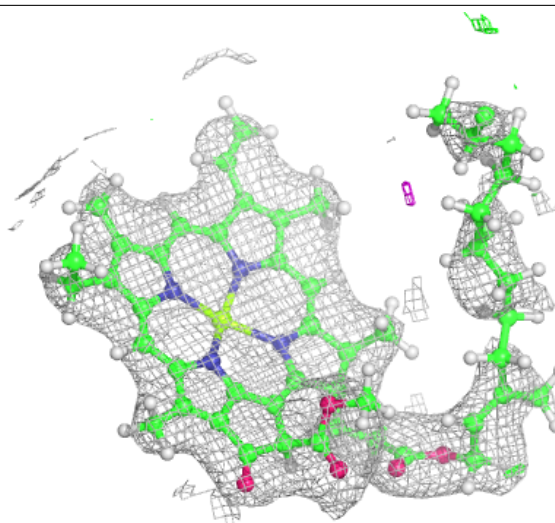
**Electron density around CLA D 404:**

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



**Electron density around CLA b 616:**

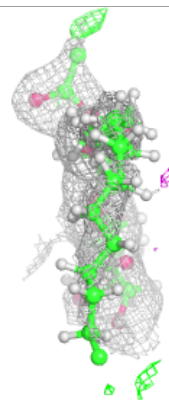
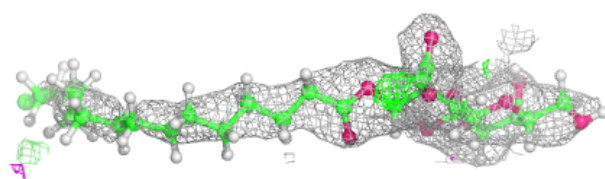
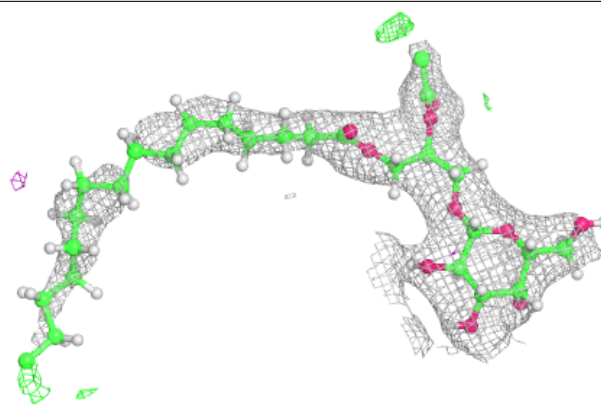
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



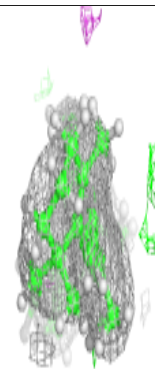
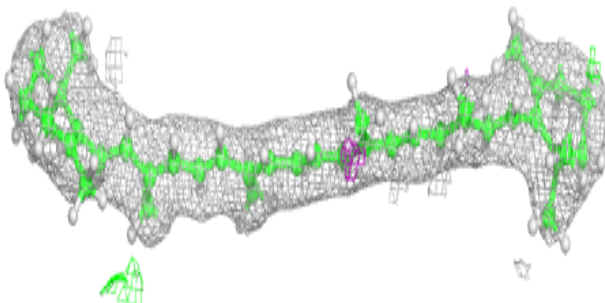
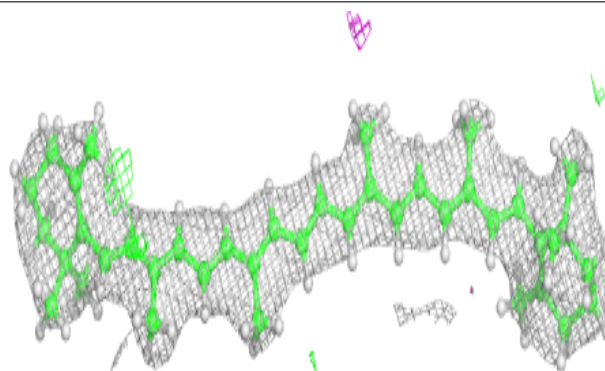


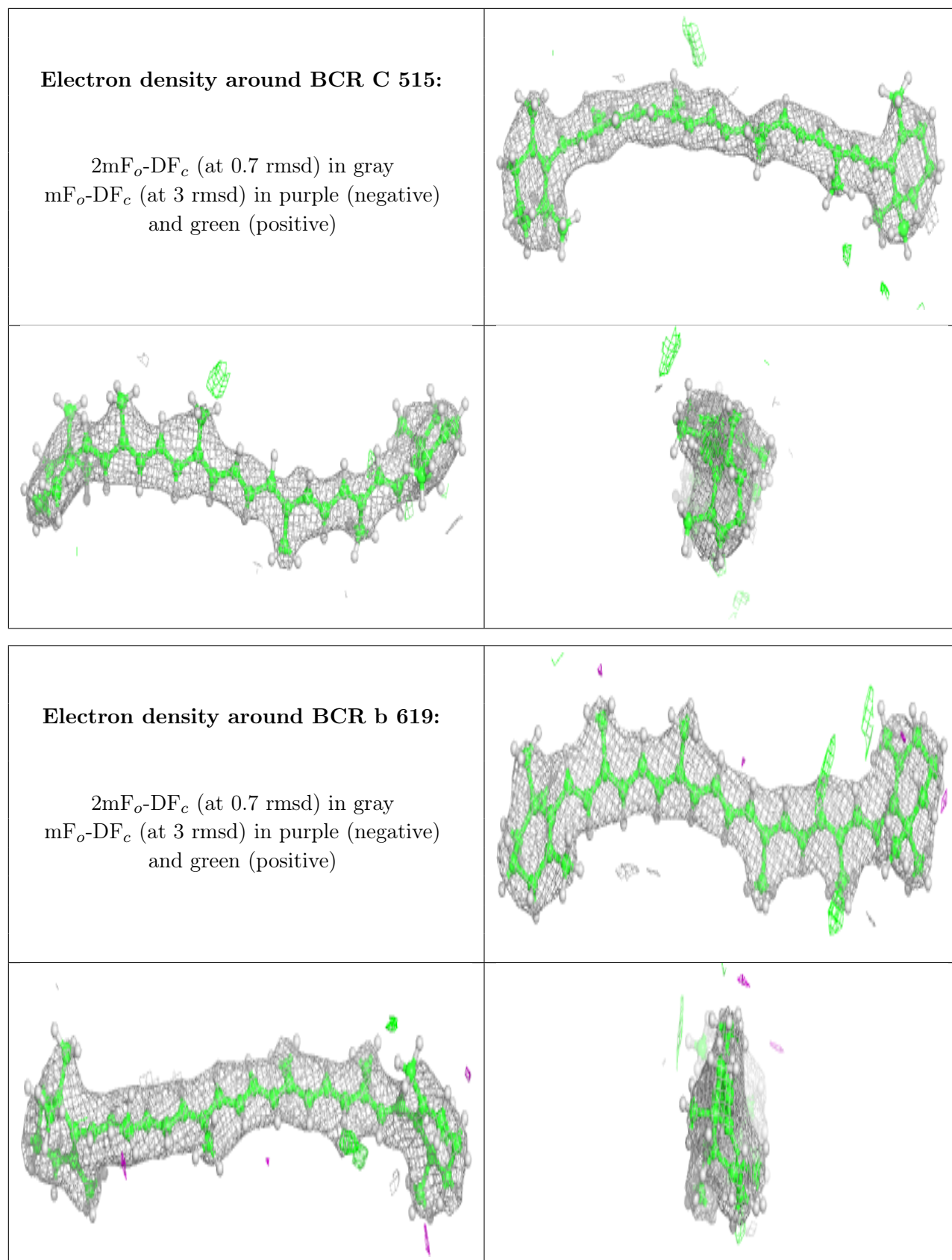
**Electron density around LMG c 520:**

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

**Electron density around BCR B 619:**

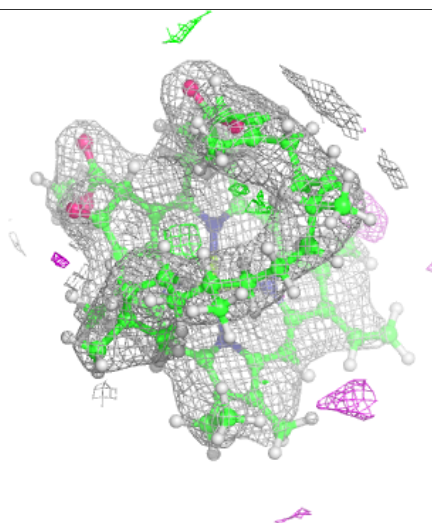
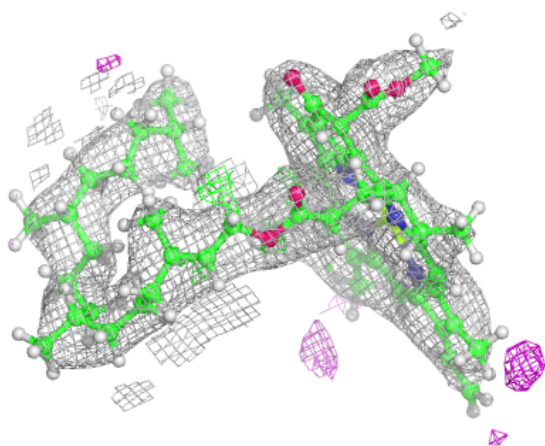
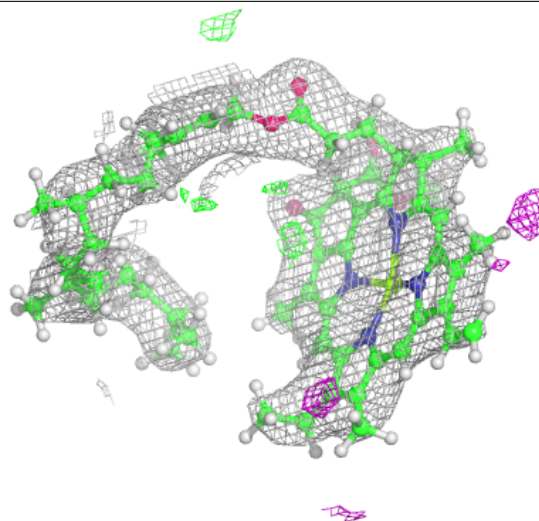
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





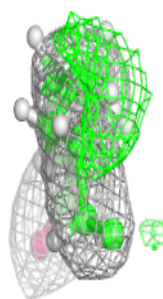
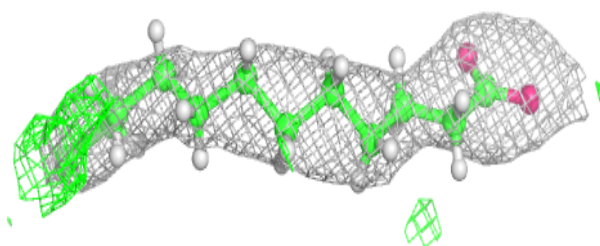
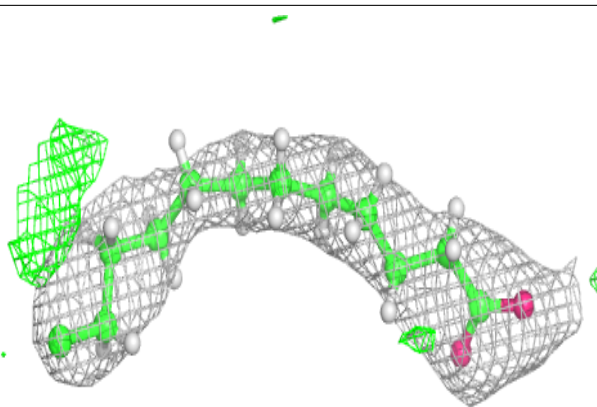
**Electron density around CLA c 503:**

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

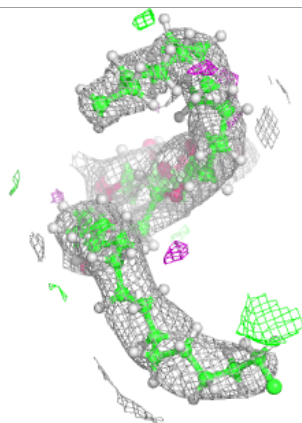
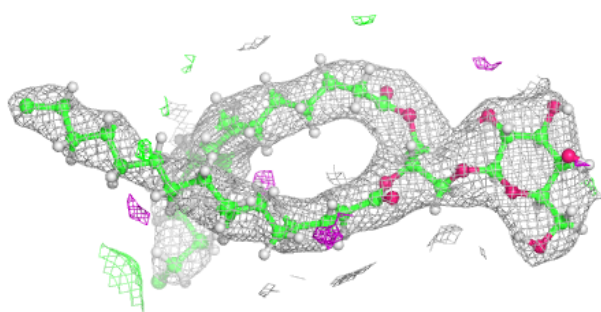
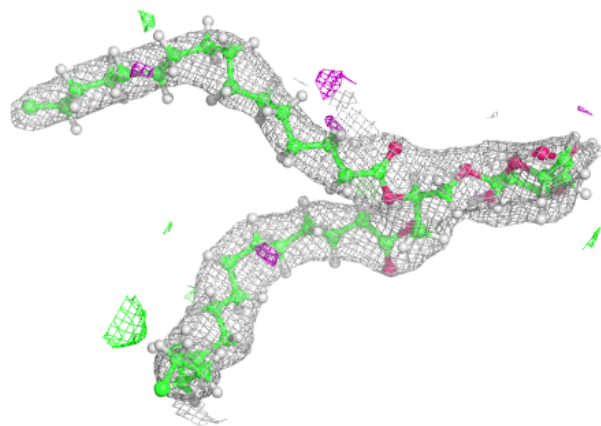


**Electron density around STE t 102:**

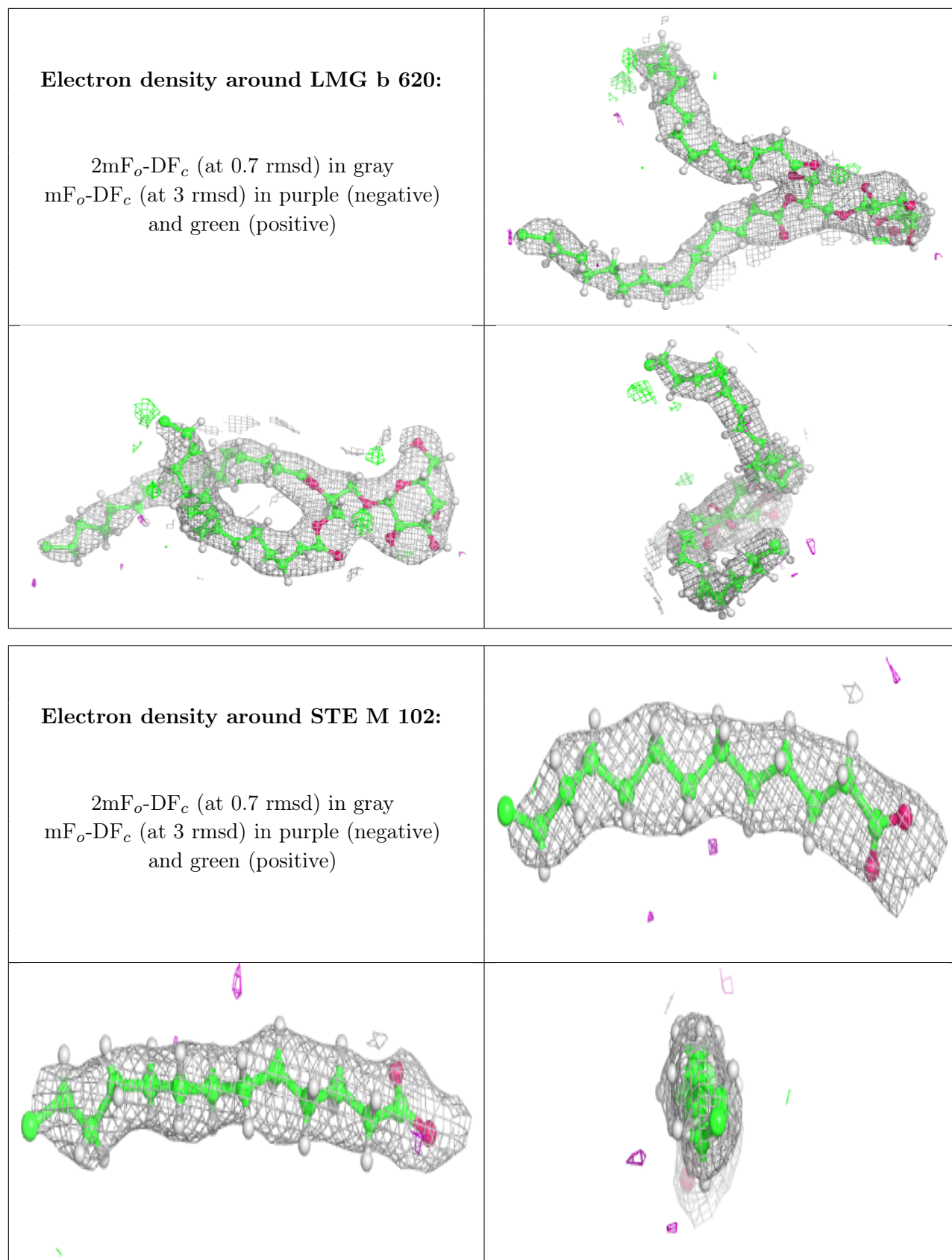
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around LMG M 101:**

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

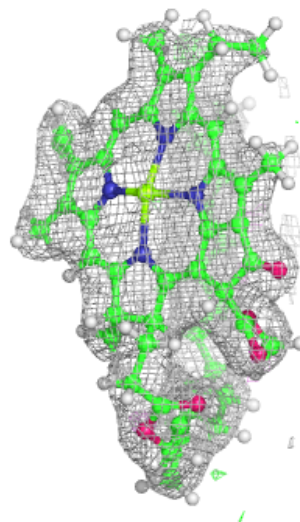
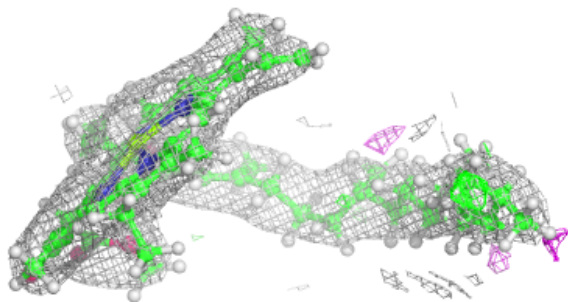
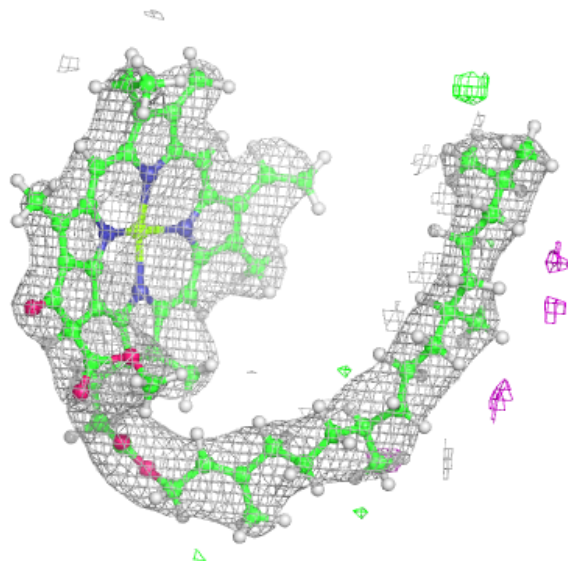






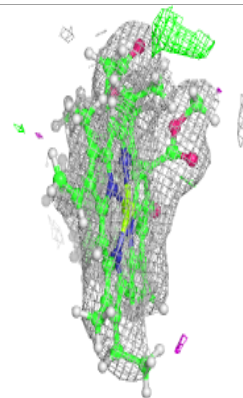
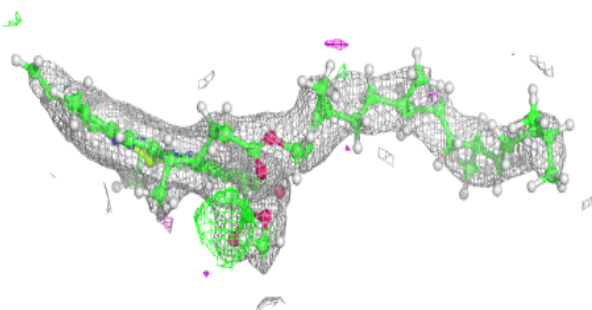
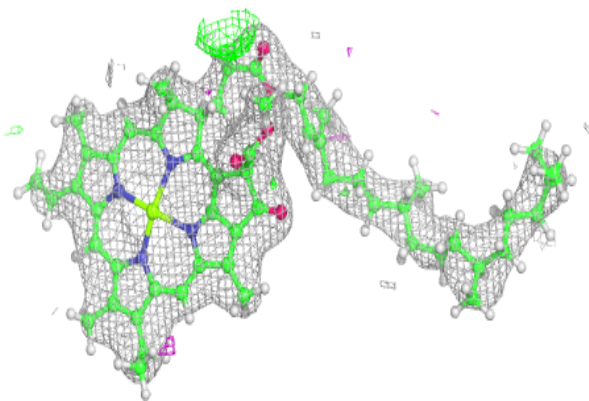
**Electron density around CLA C 507:**

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

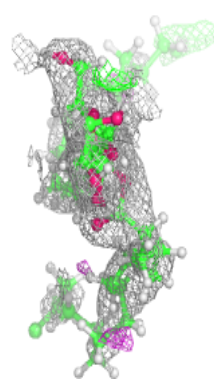
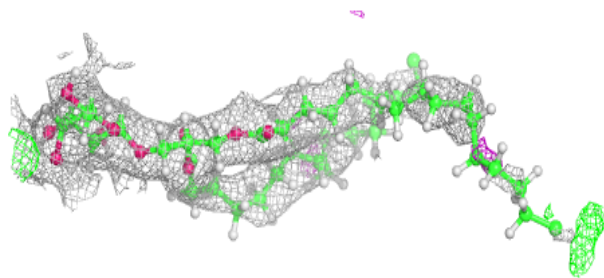
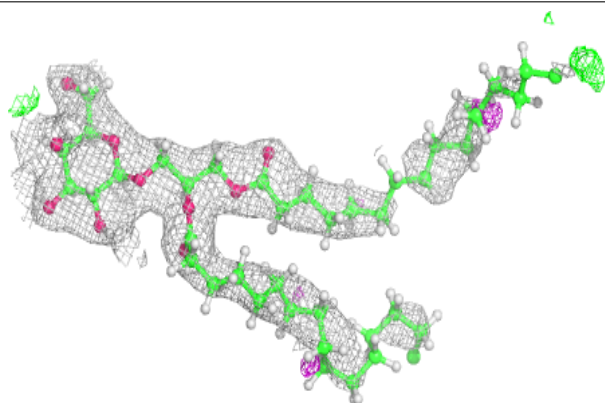


**Electron density around CLA b 602:**

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

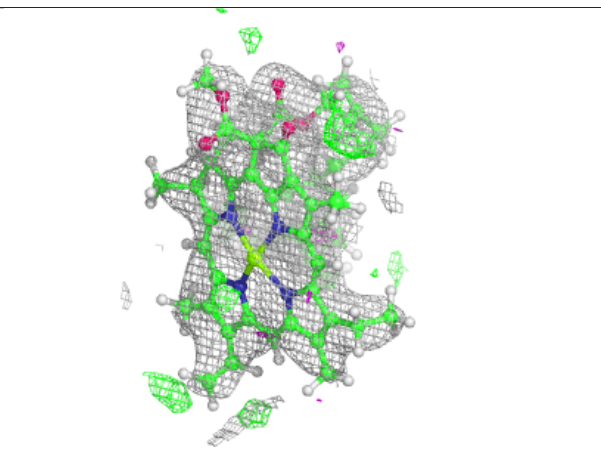
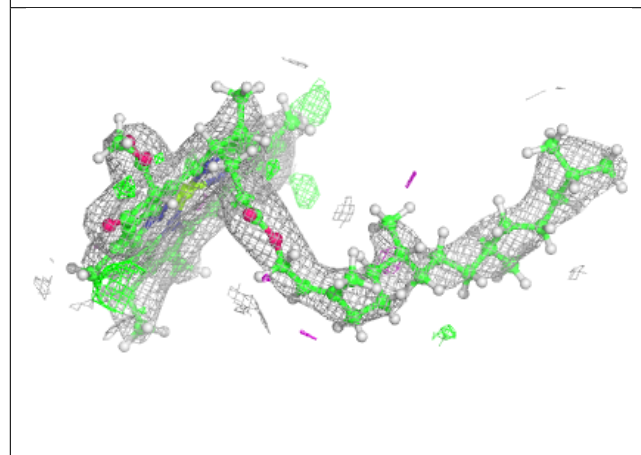
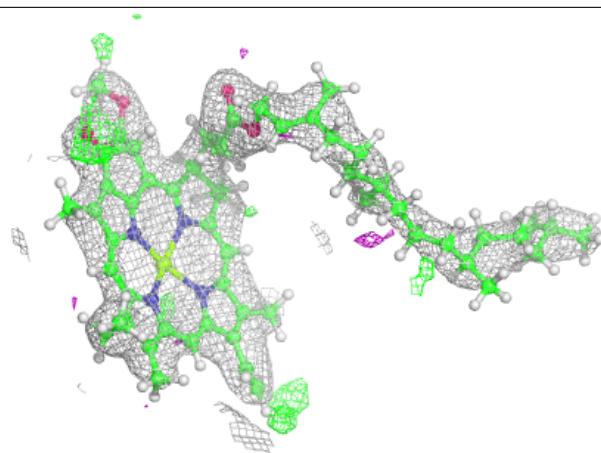
**Electron density around LMG D 407:**

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

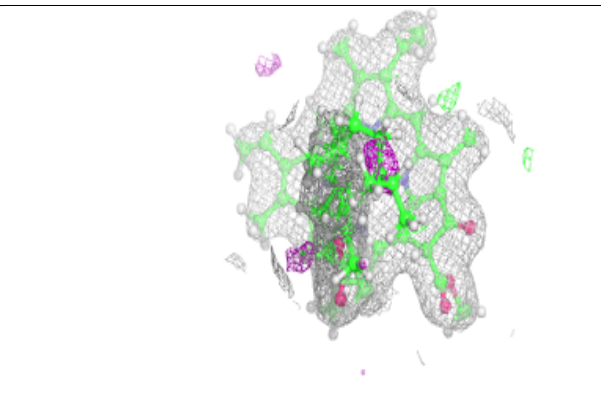
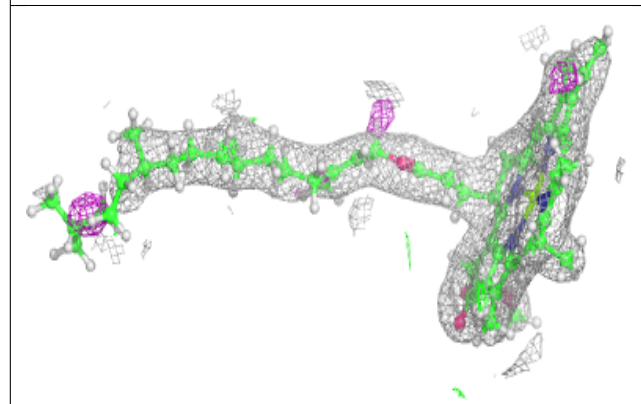
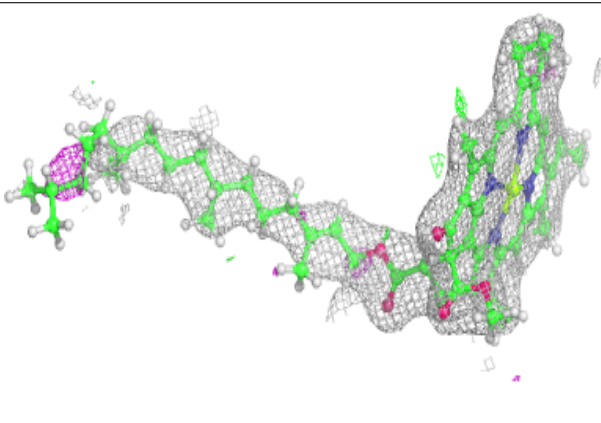


**Electron density around CLA c 511:**

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

**Electron density around CLA b 604:**

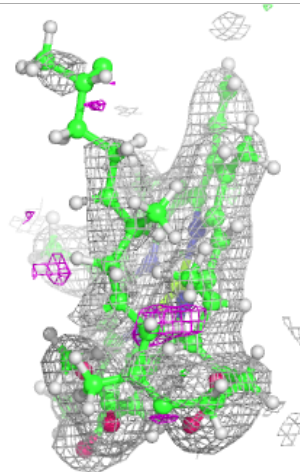
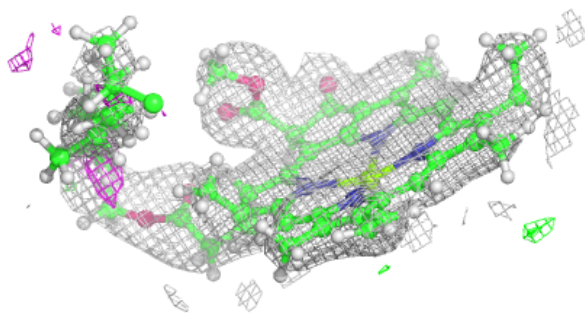
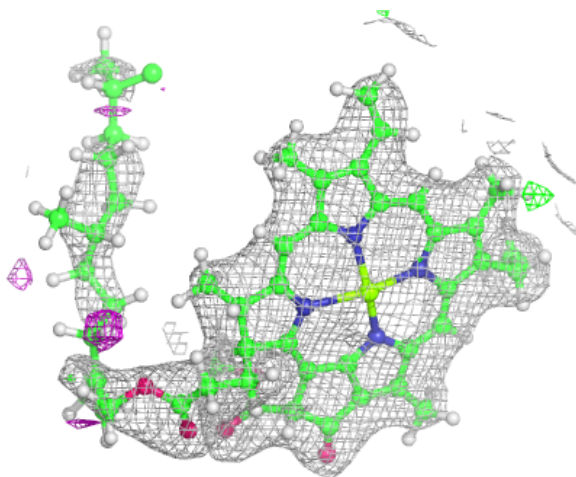
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

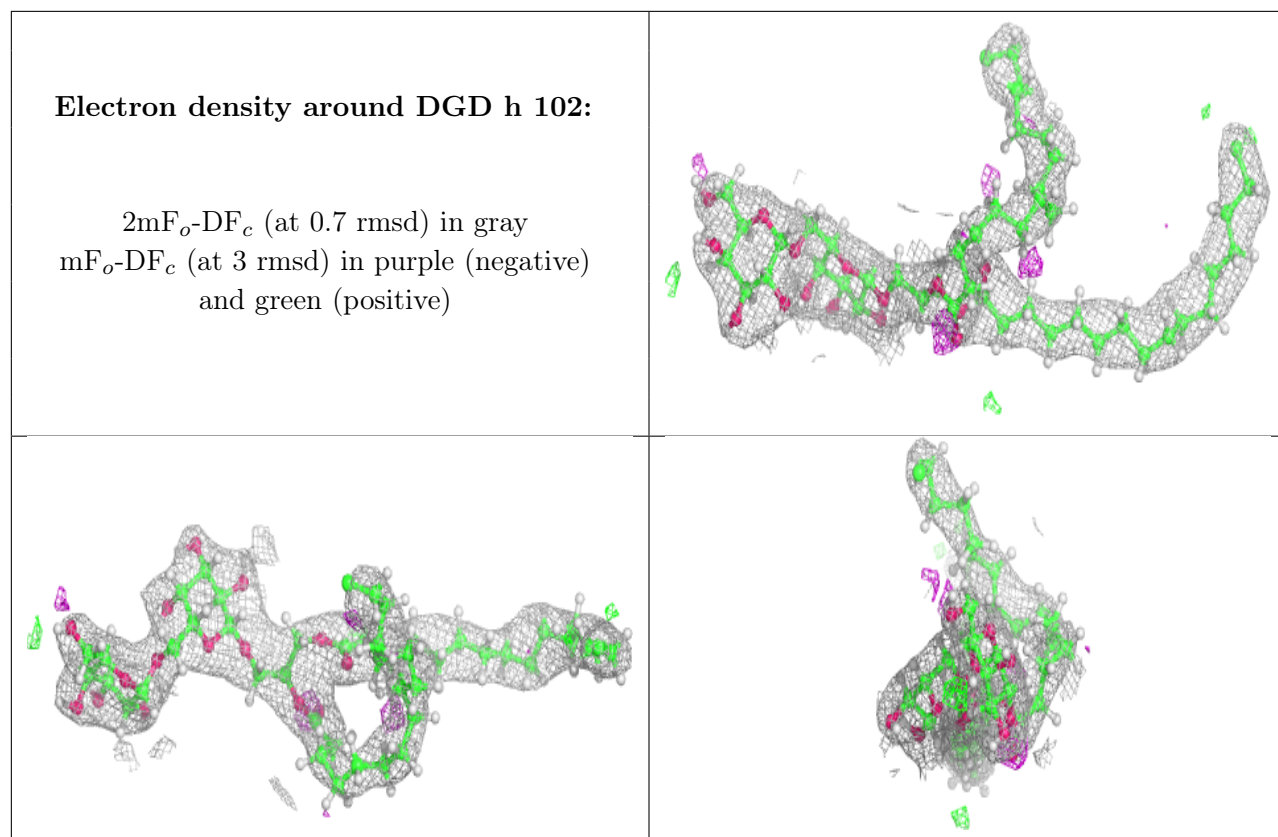




**Electron density around CLA B 616:**

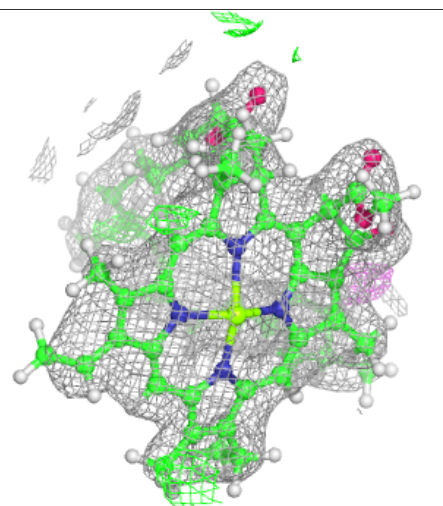
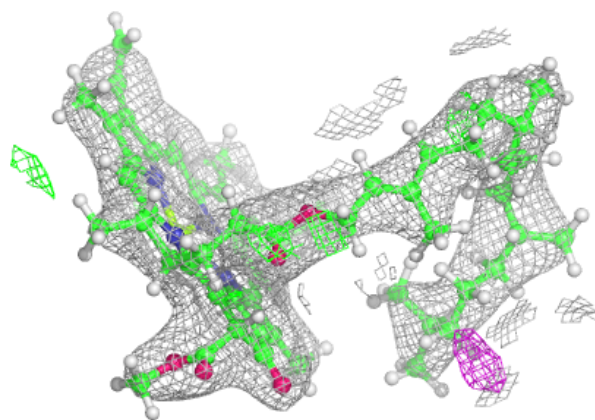
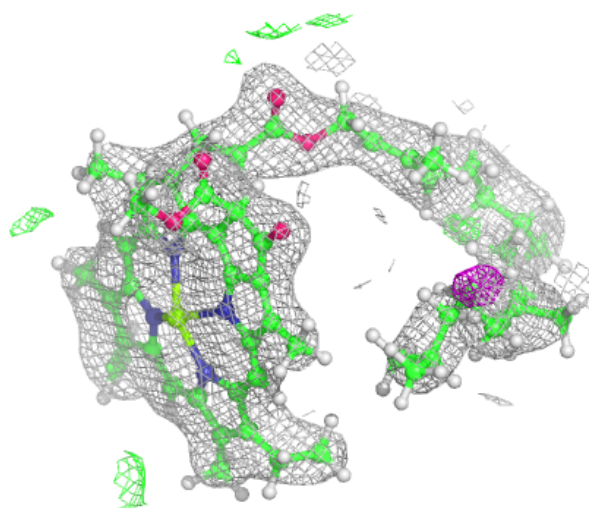
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

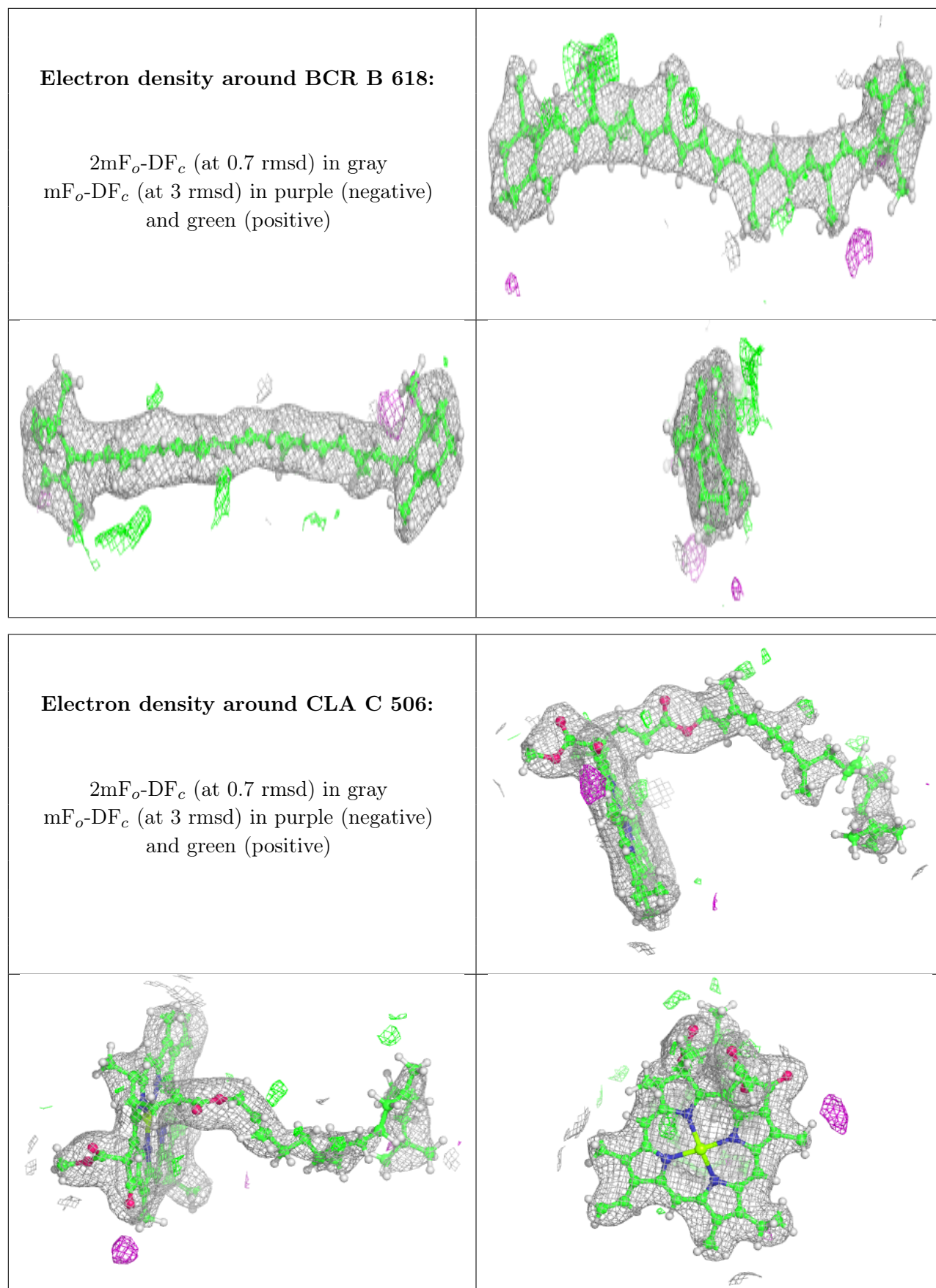




**Electron density around CLA C 503:**

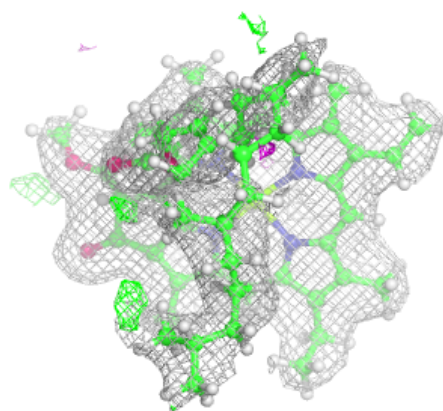
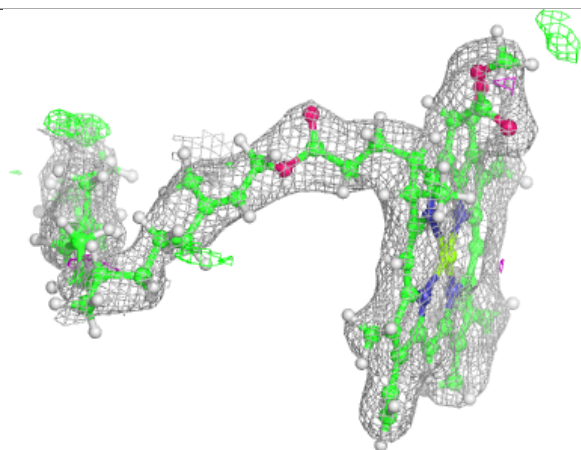
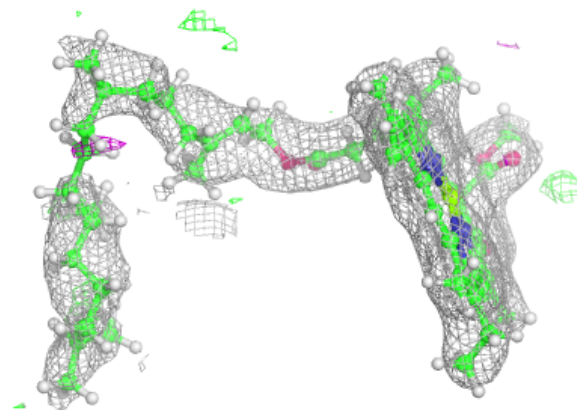
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA a 404:**

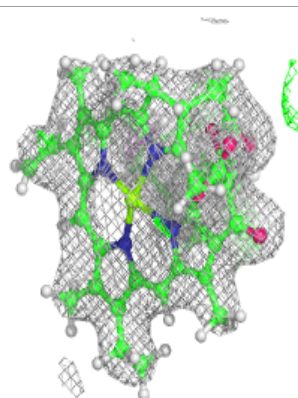
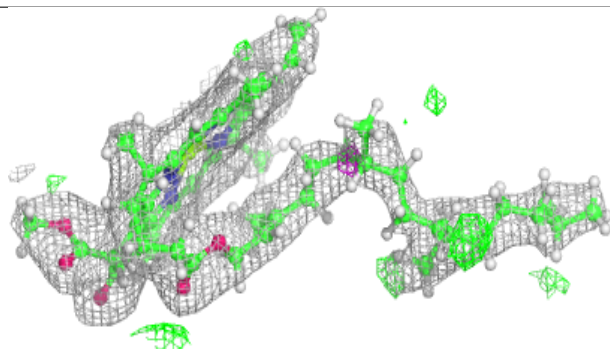
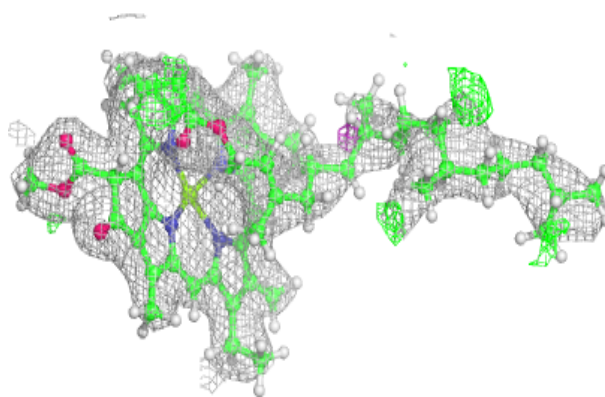
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





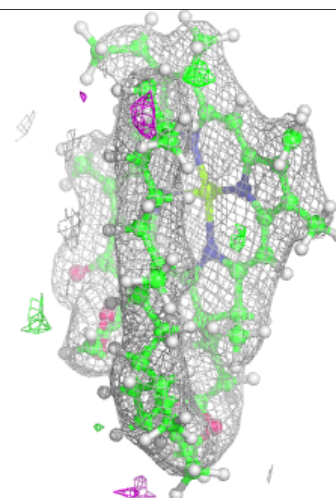
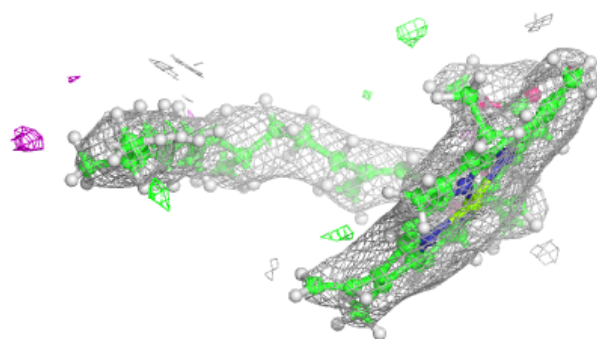
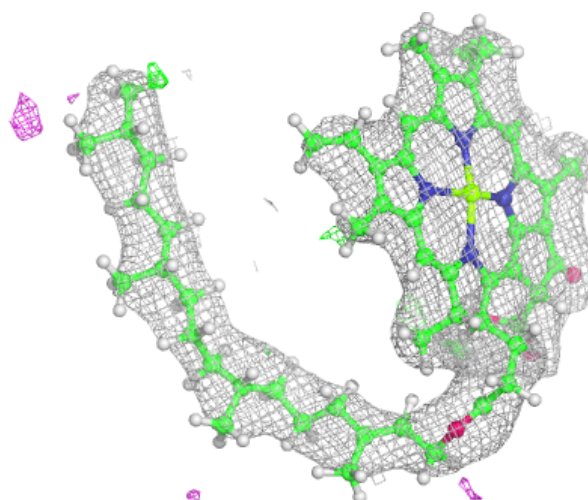
**Electron density around CLA c 505:**

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



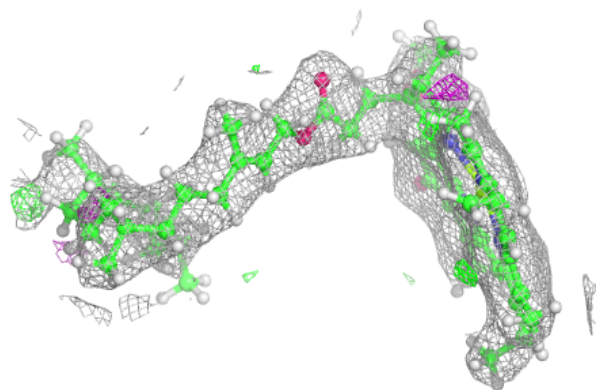
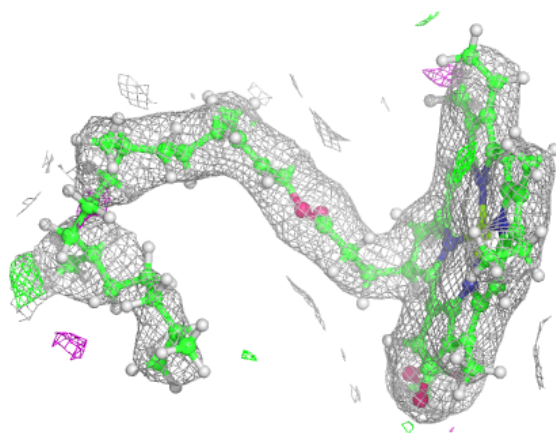
**Electron density around CLA c 507:**

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



**Electron density around CLA B 606:**

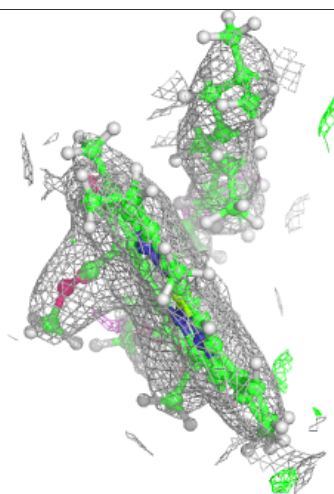
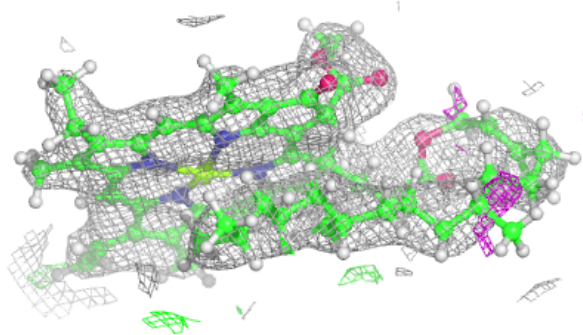
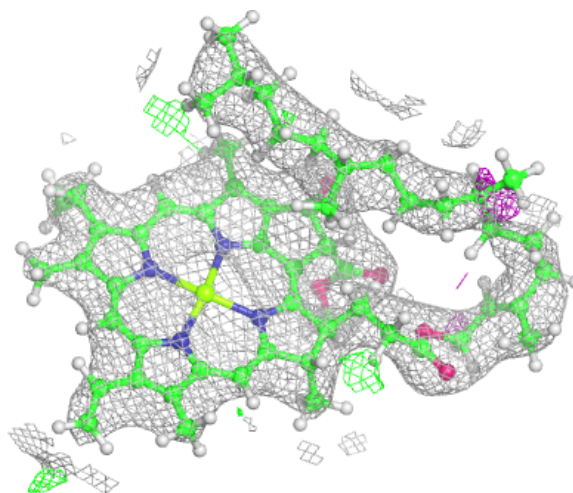
$2mF_o-DF_c$  (at 0.7 rnsd) in gray  
 $mF_o-DF_c$  (at 3 rnsd) in purple (negative)  
and green (positive)





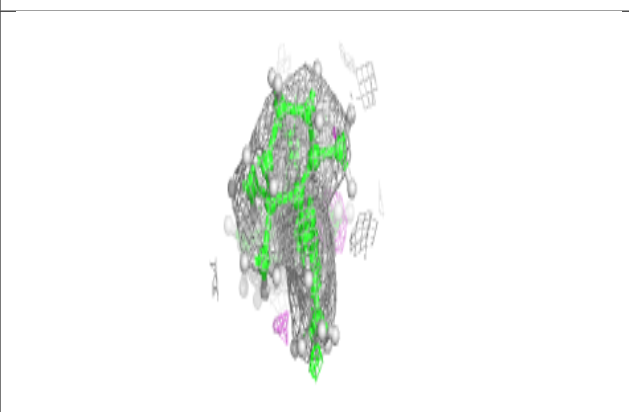
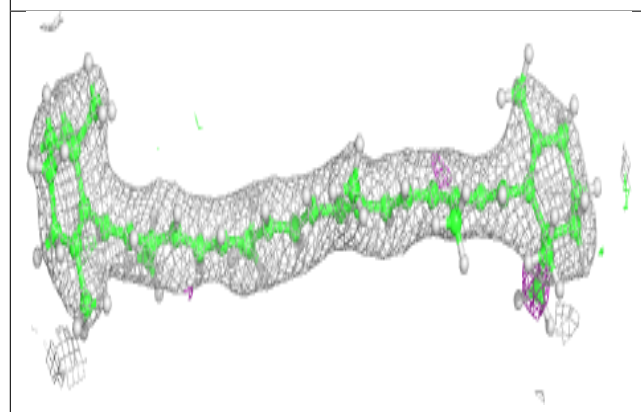
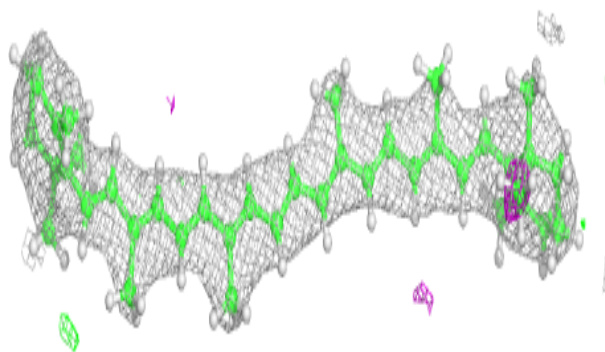
**Electron density around CLA c 509:**

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

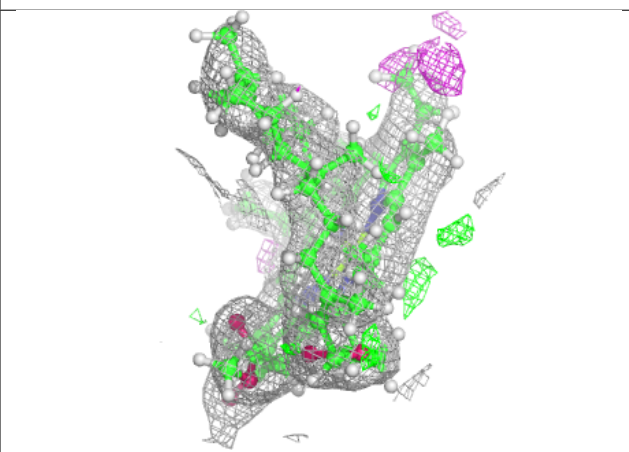
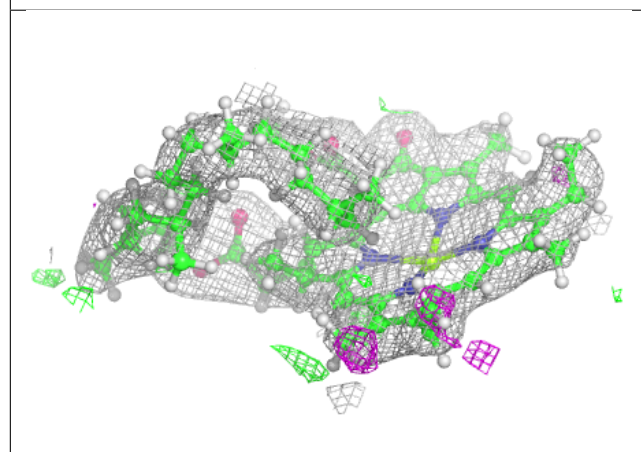
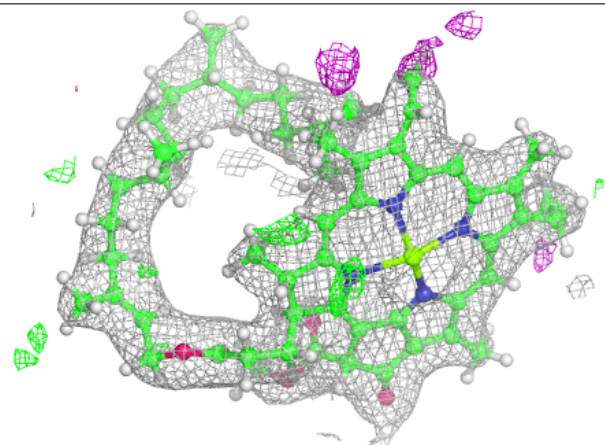


**Electron density around BCR c 515:**

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

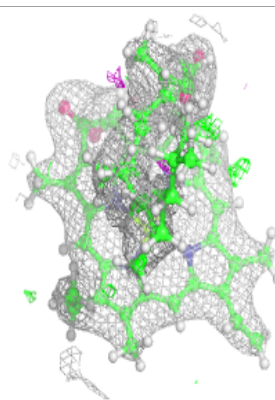
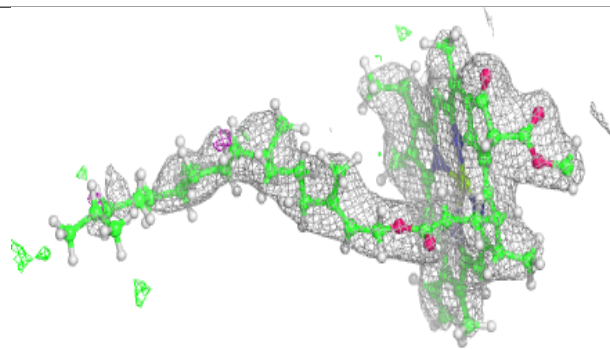
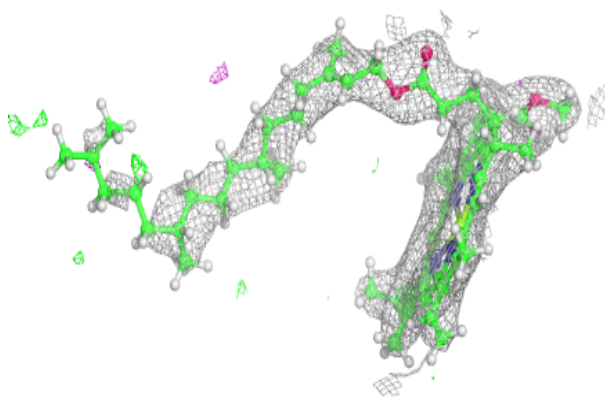
**Electron density around CLA B 615:**

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

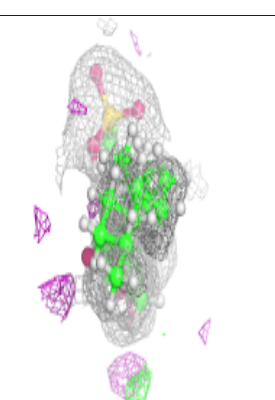
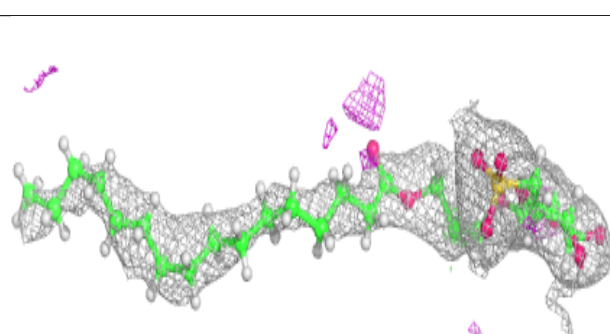
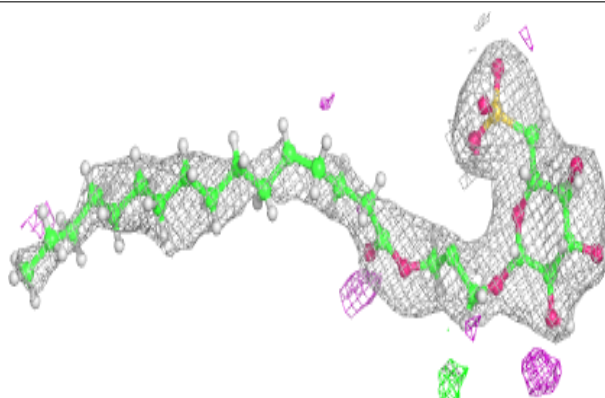


**Electron density around CLA C 508:**

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

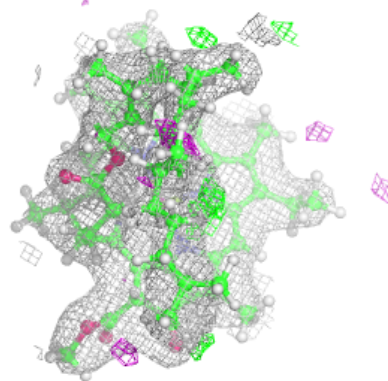
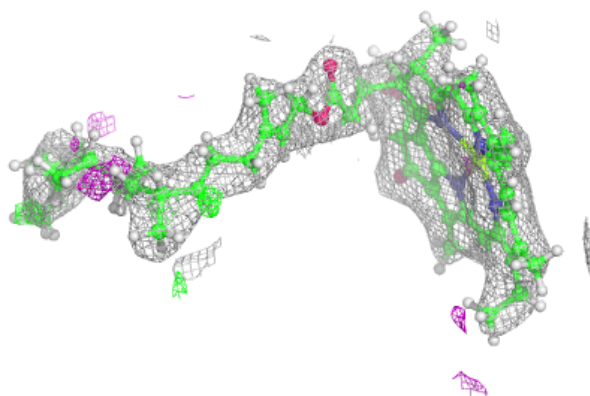
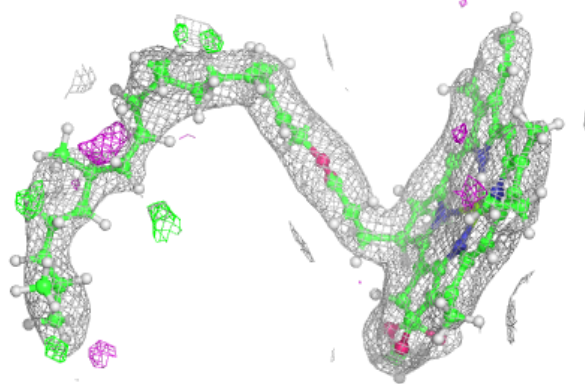
**Electron density around SQD F 101:**

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

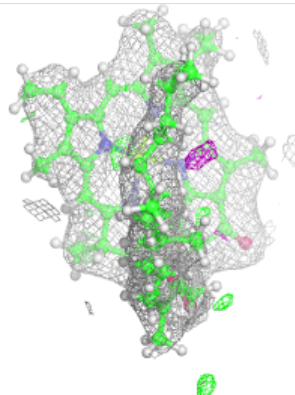
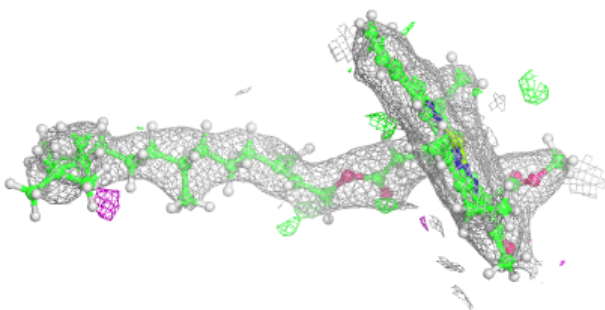
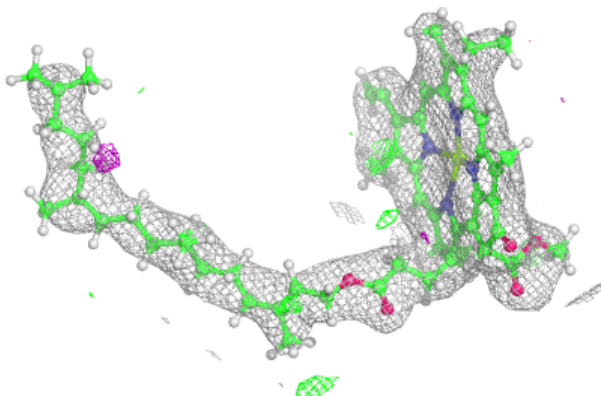


**Electron density around CLA b 606:**

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

**Electron density around CLA b 609:**

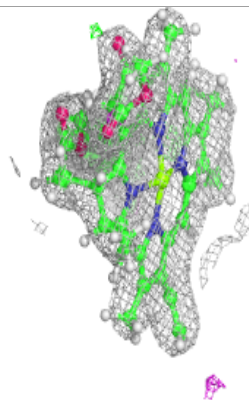
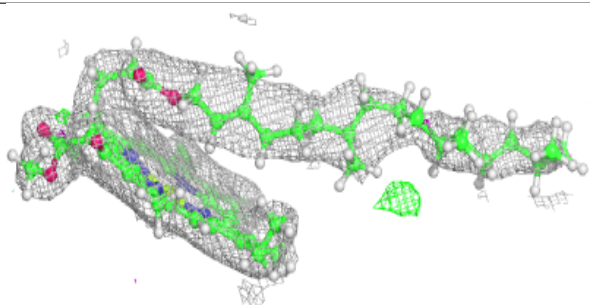
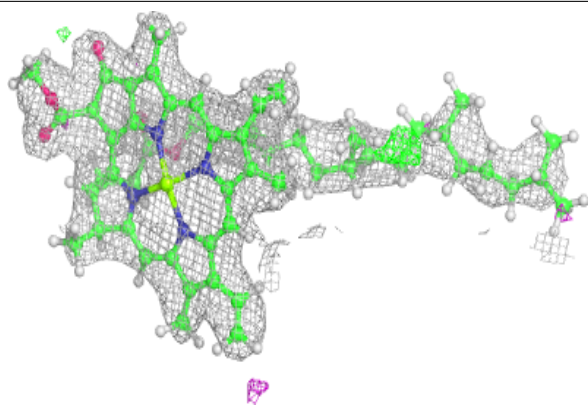
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



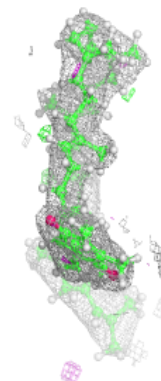
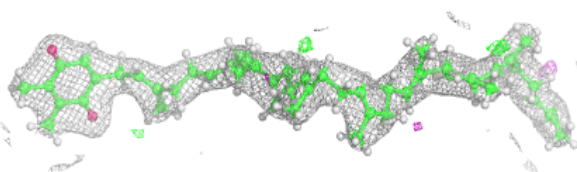
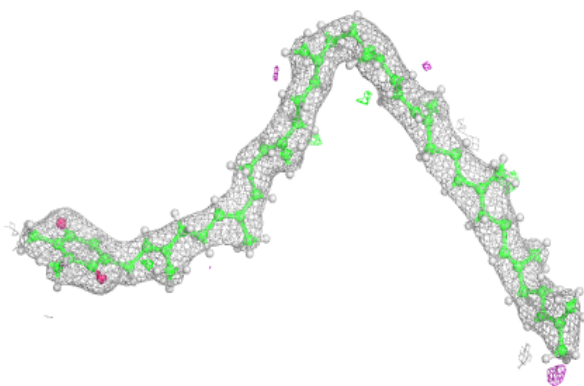


**Electron density around CLA b 614:**

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

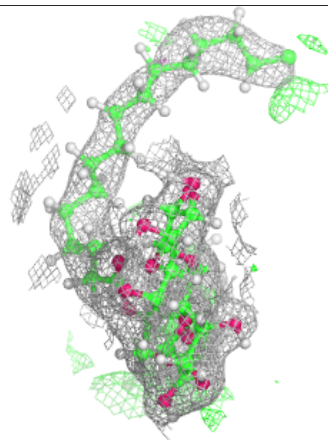
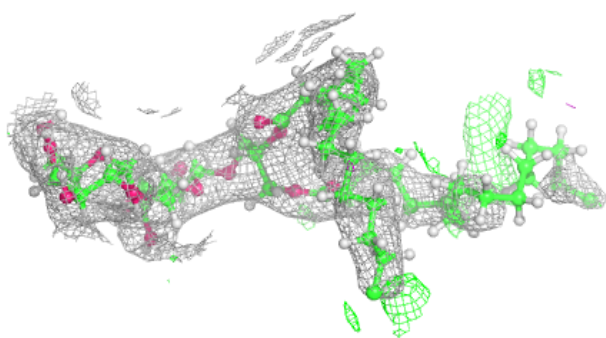
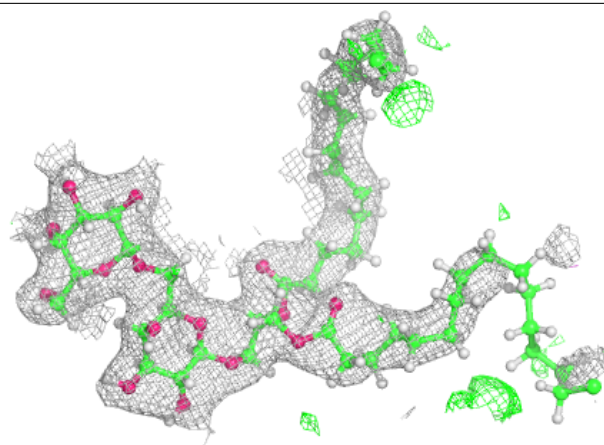
**Electron density around PL9 D 406:**

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

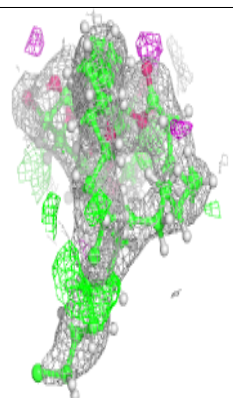
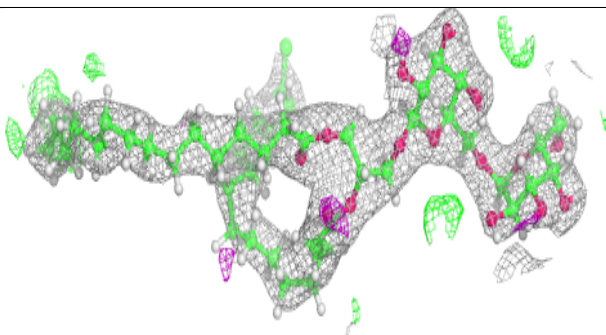
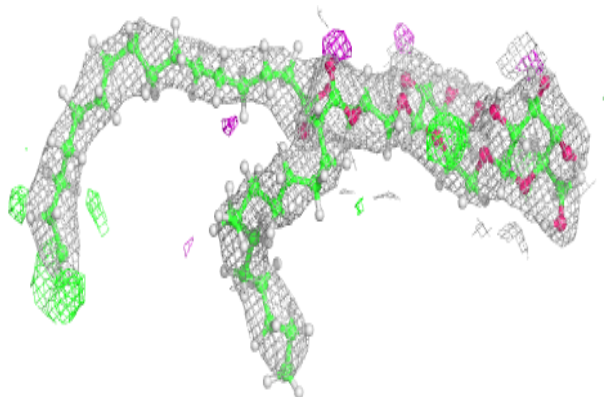


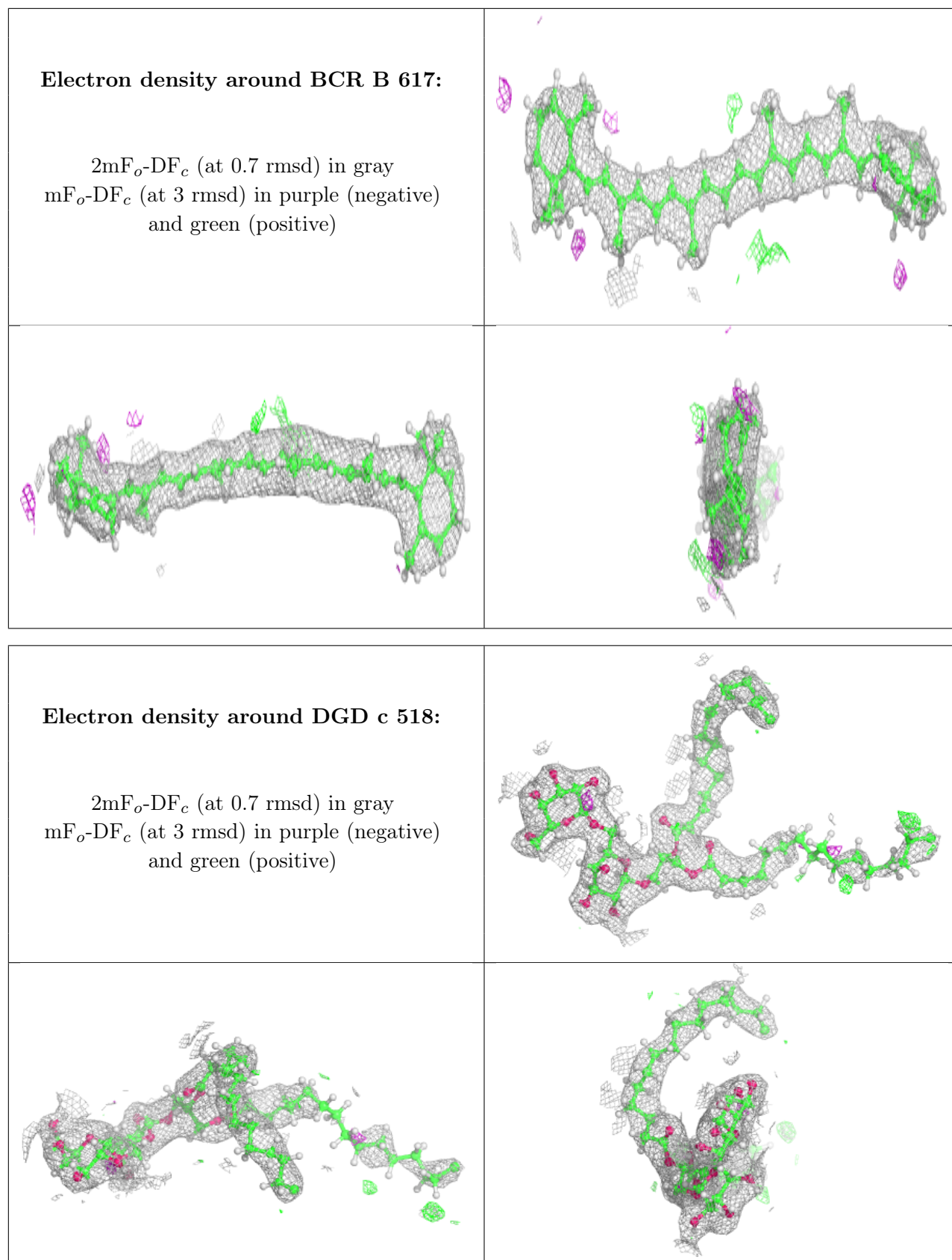
**Electron density around DGD C 517:**

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

**Electron density around DGD H 102:**

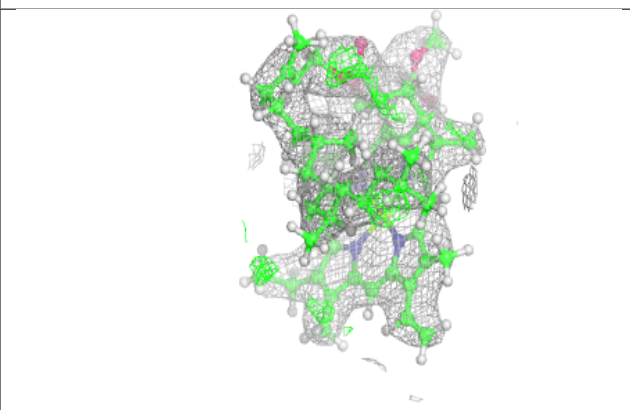
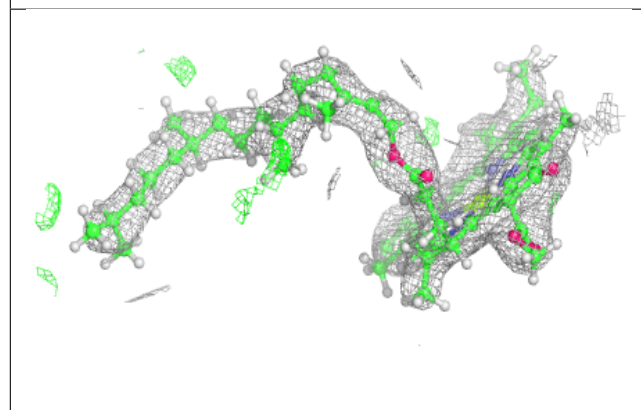
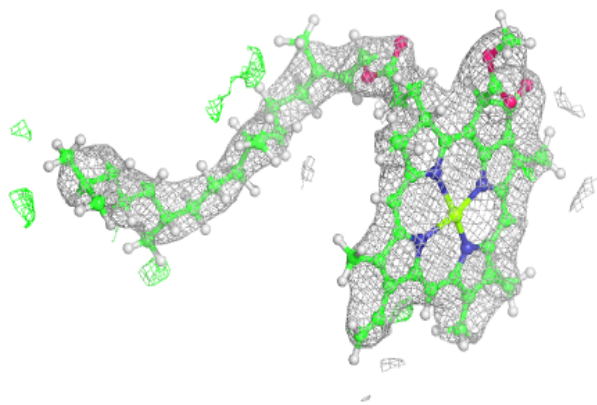
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



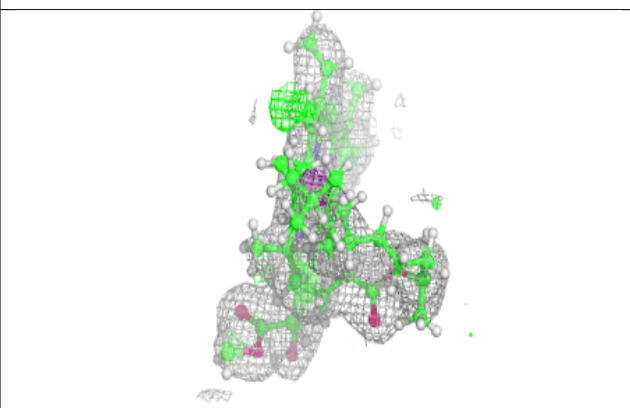
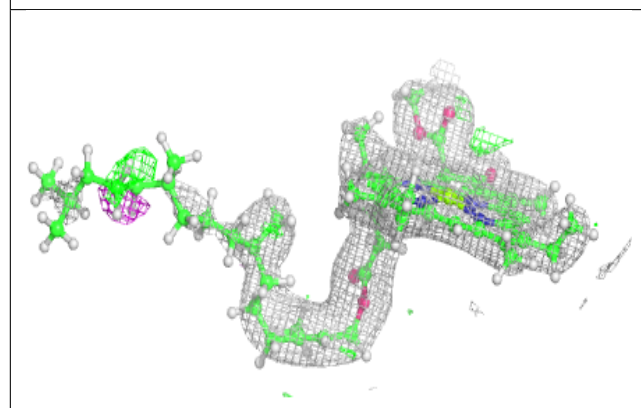
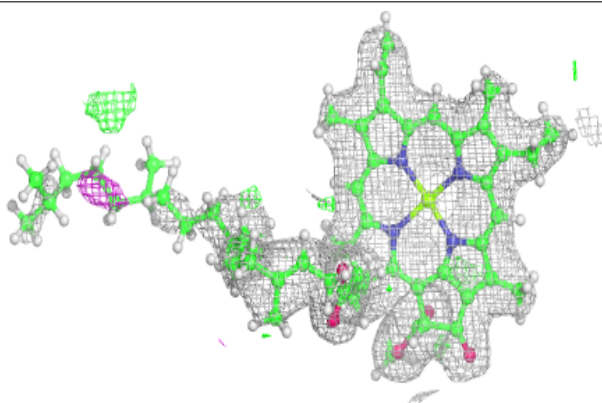


**Electron density around CLA C 511:**

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

**Electron density around CLA A 403:**

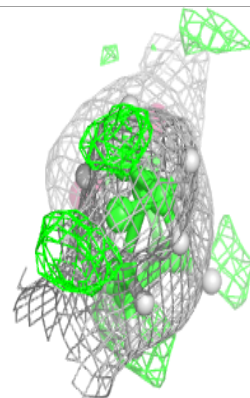
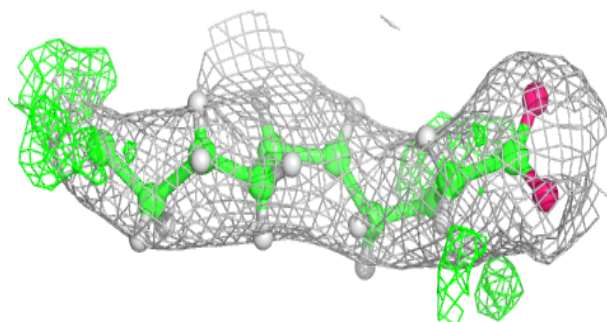
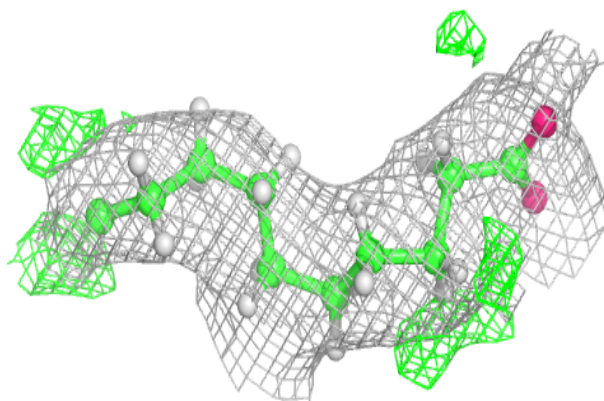
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



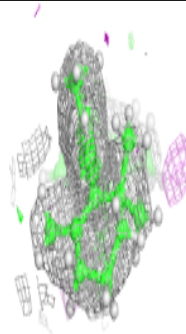
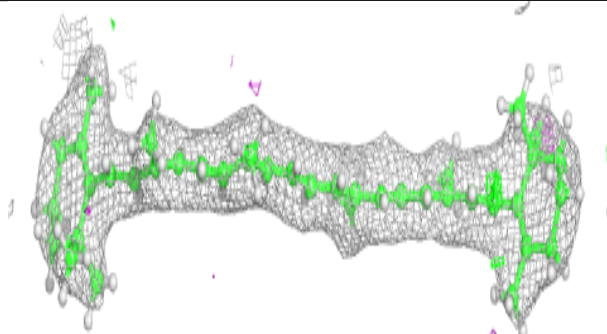
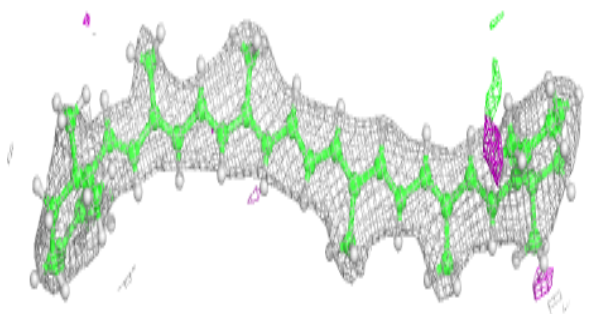


**Electron density around STE B 624:**

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

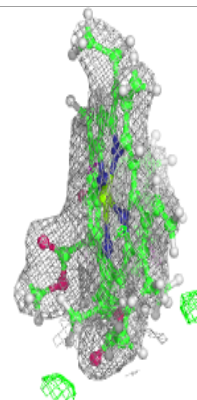
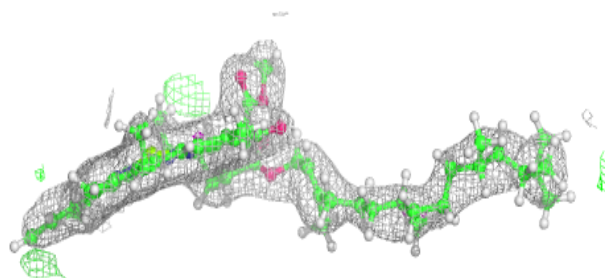
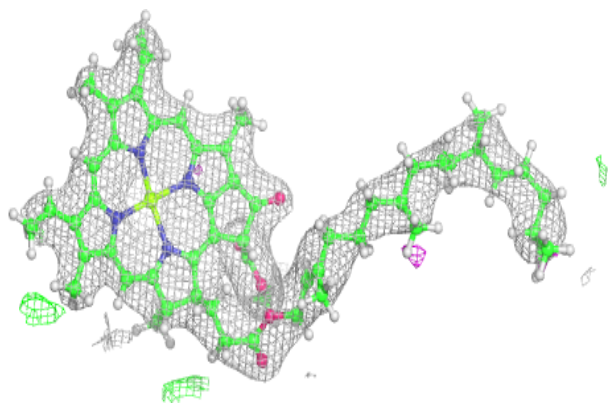
**Electron density around BCR C 514:**

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

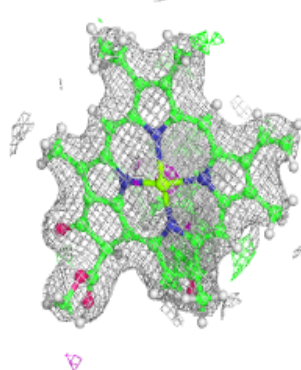
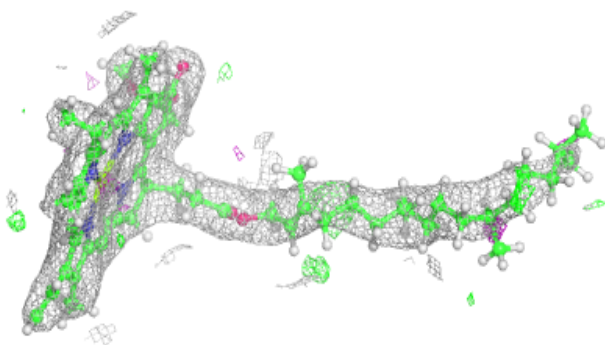
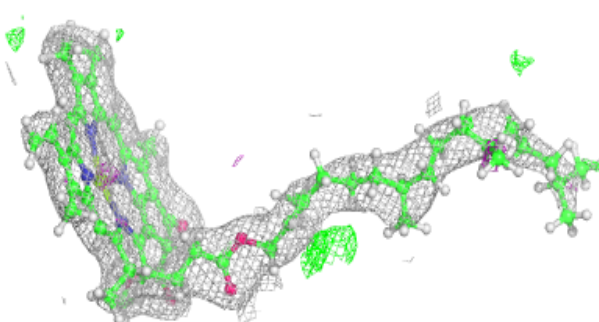


**Electron density around CLA B 602:**

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

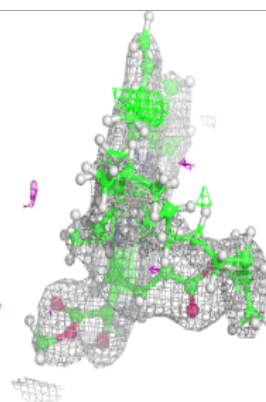
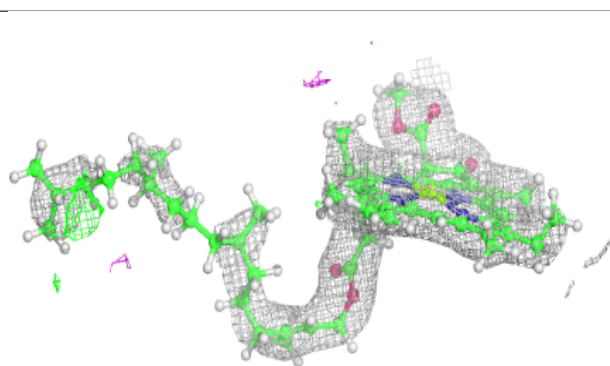
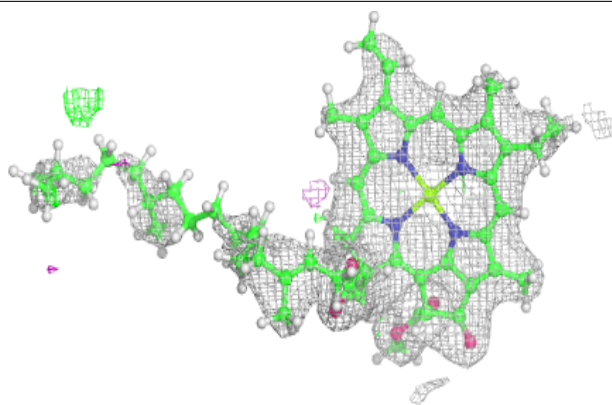
**Electron density around CLA B 604:**

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

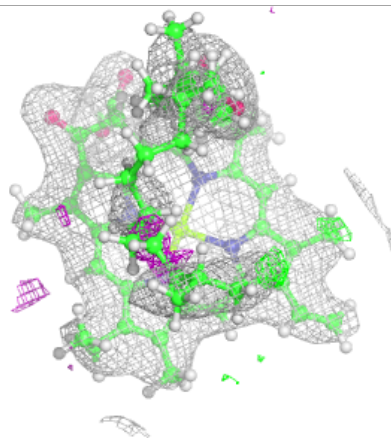
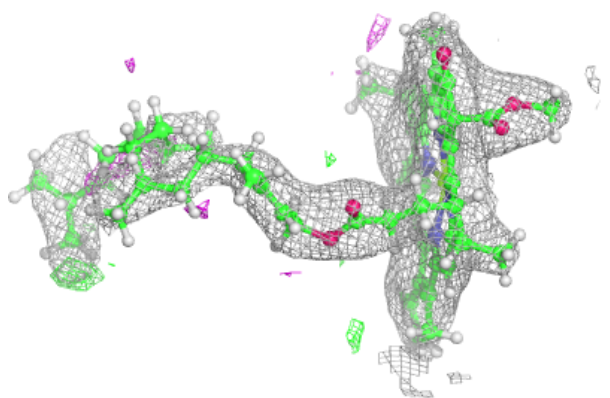
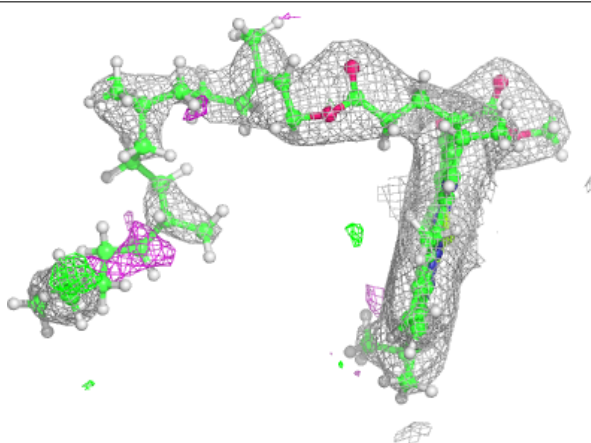


**Electron density around CLA a 403:**

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

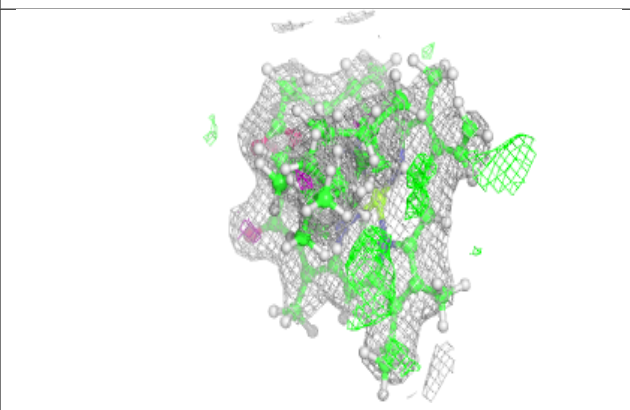
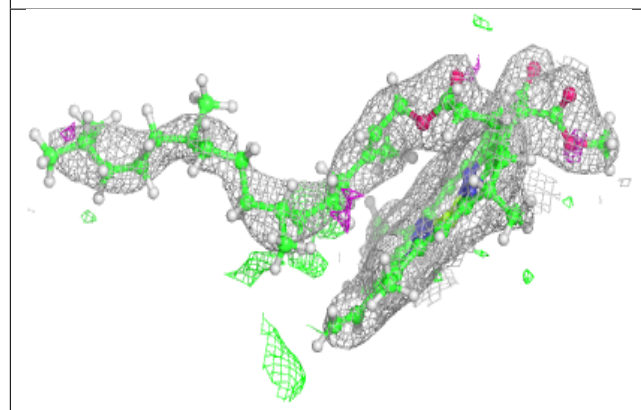
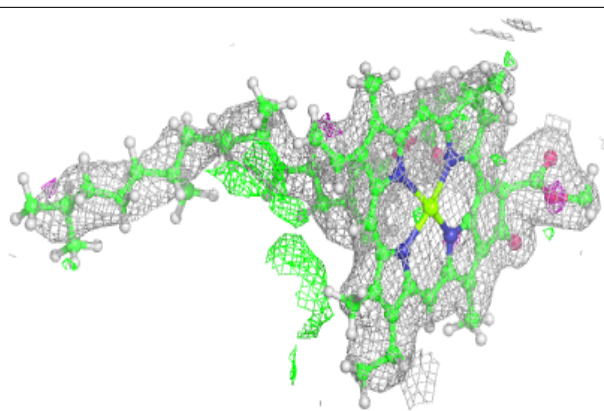
**Electron density around CLA c 506:**

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

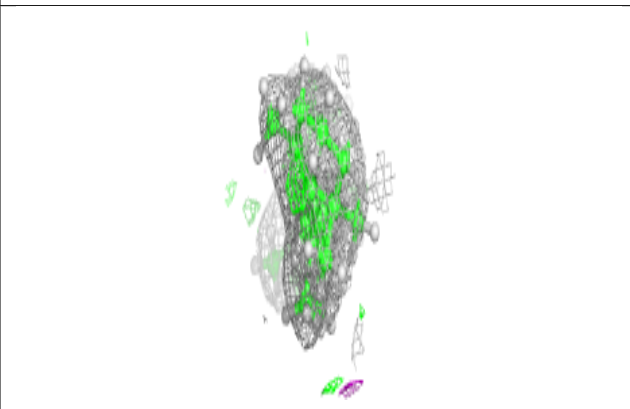
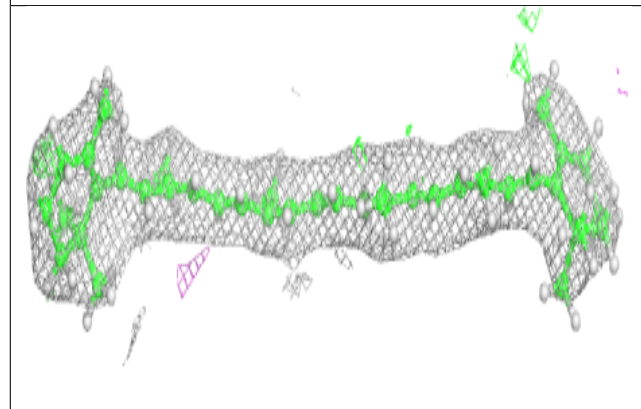
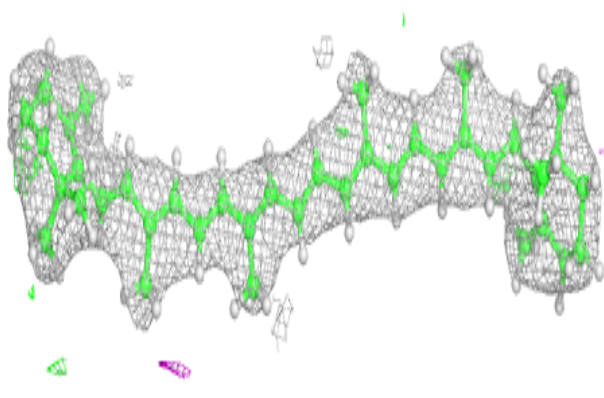


**Electron density around CLA C 505:**

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

**Electron density around BCR b 618:**

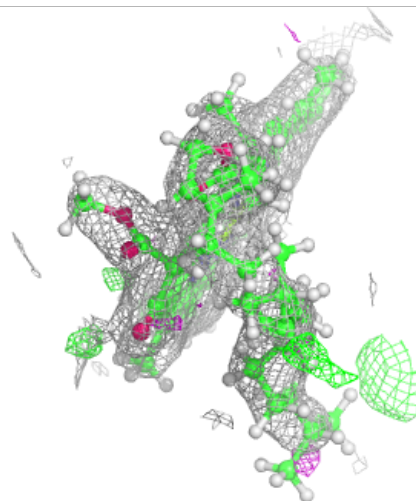
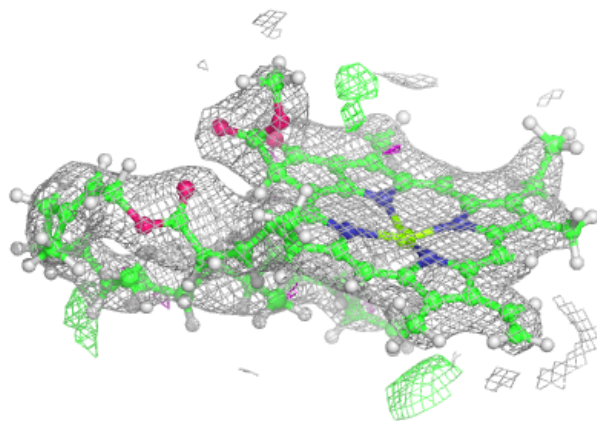
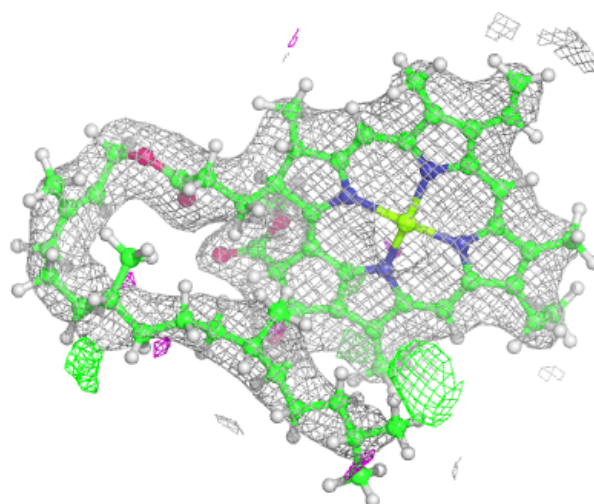
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





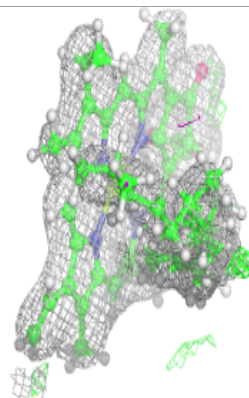
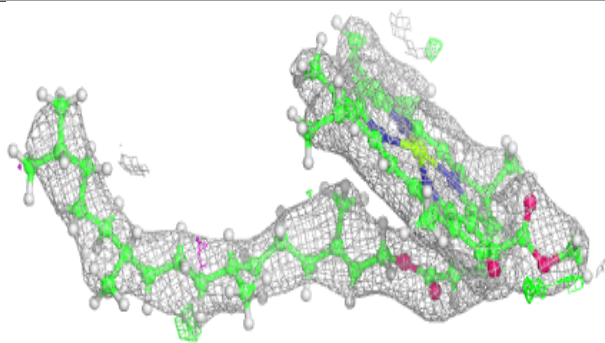
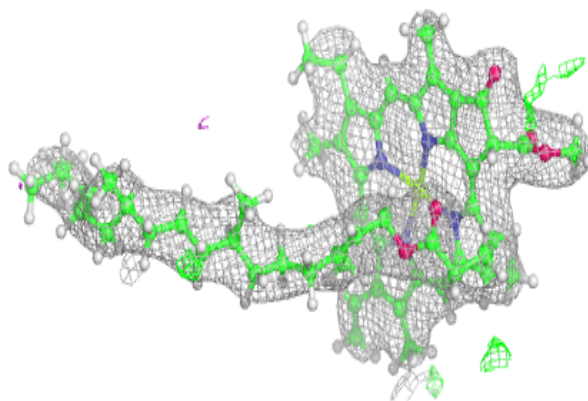
**Electron density around CLA C 509:**

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

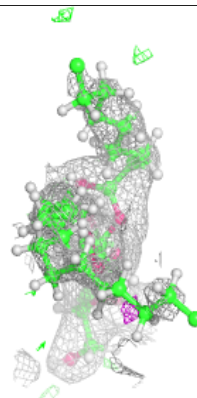
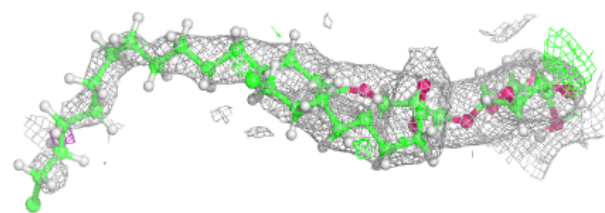
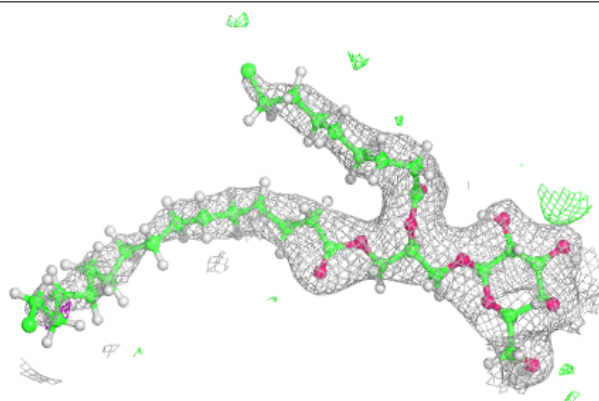


**Electron density around CLA b 608:**

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

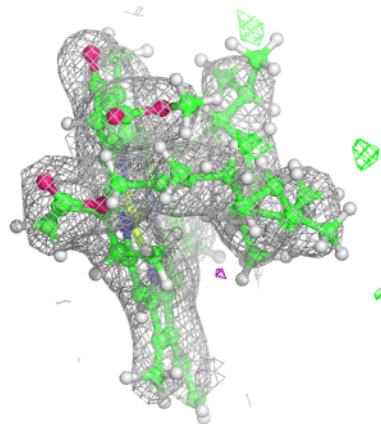
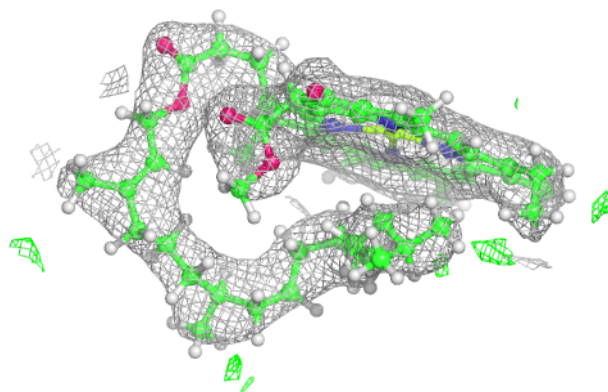
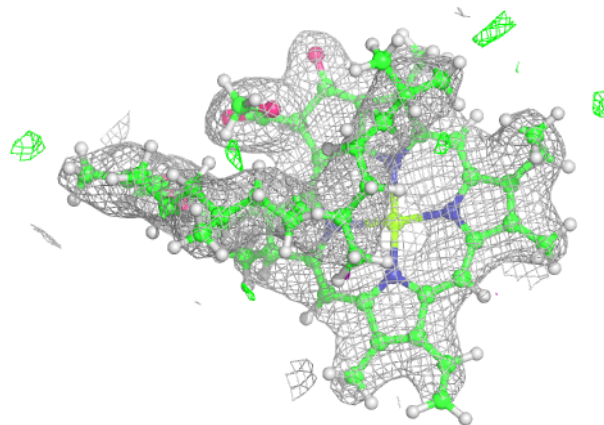
**Electron density around LMG d 412:**

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



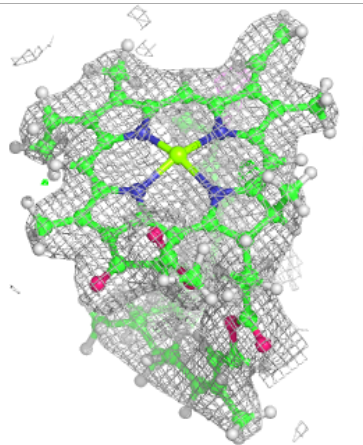
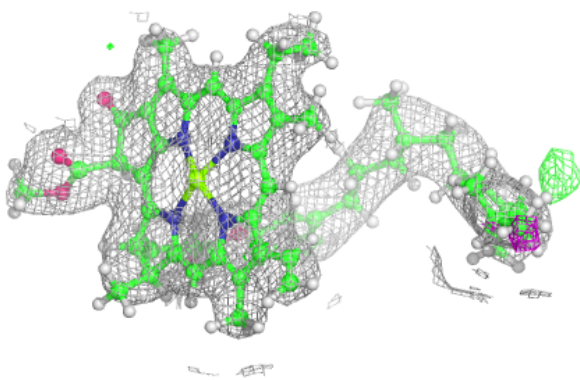
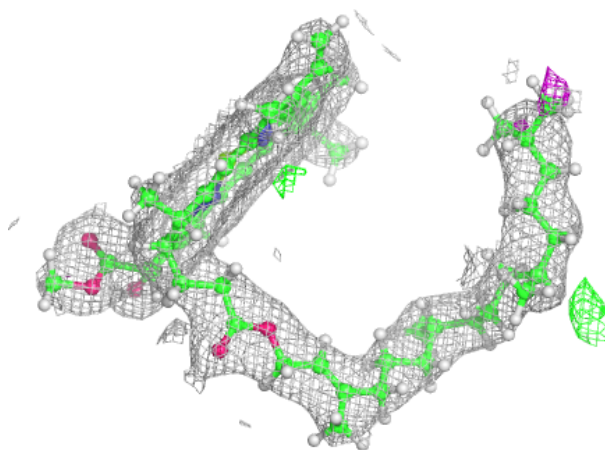
**Electron density around CLA C 510:**

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



**Electron density around CLA b 611:**

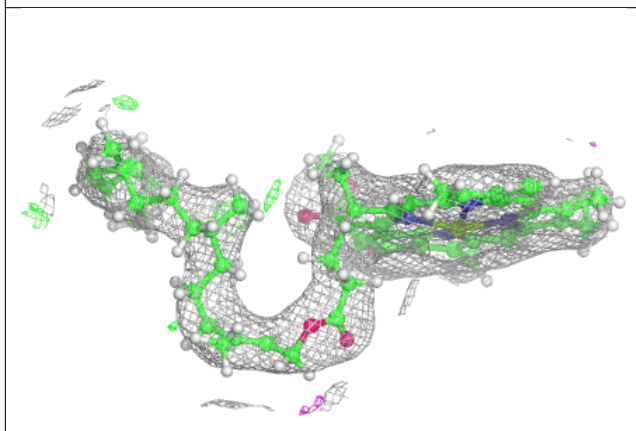
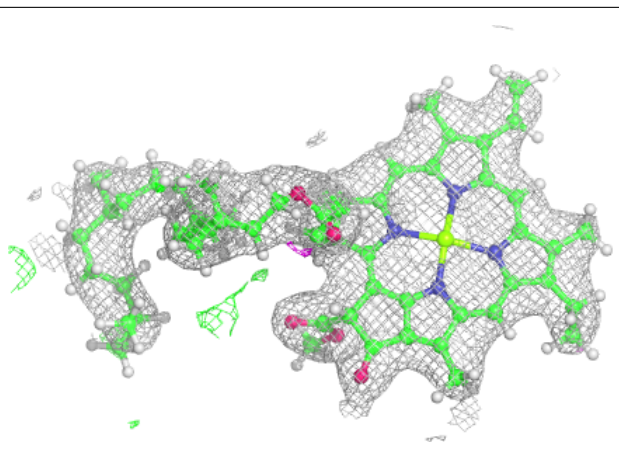
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





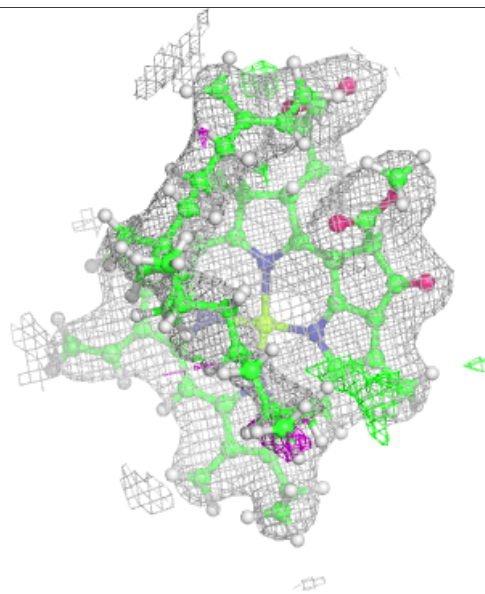
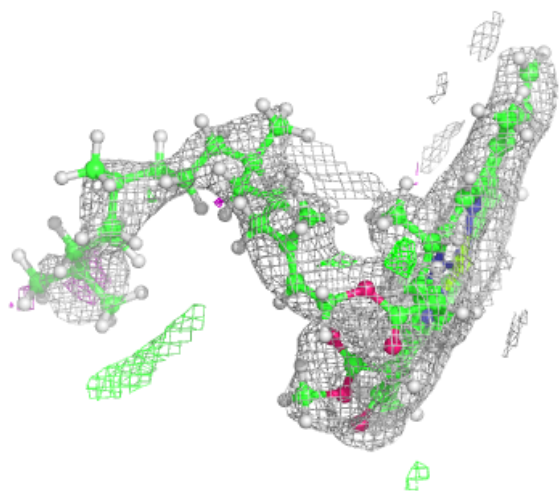
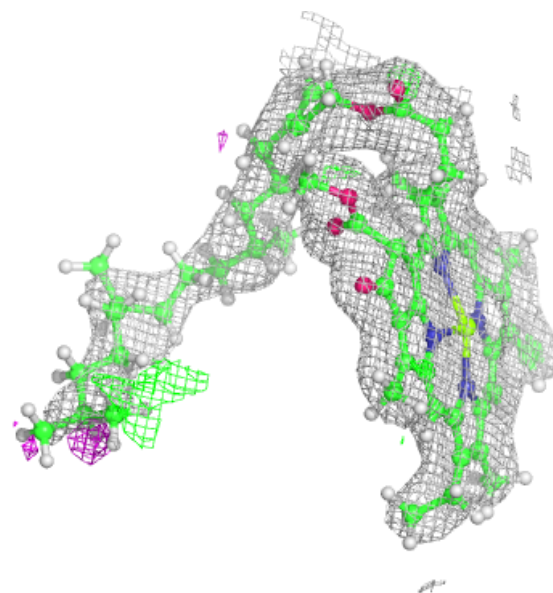
**Electron density around CLA b 612:**

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



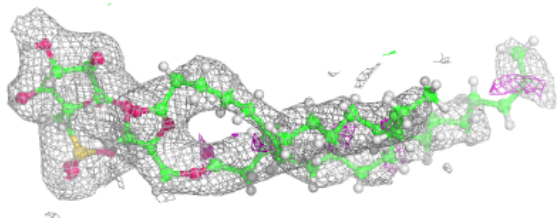
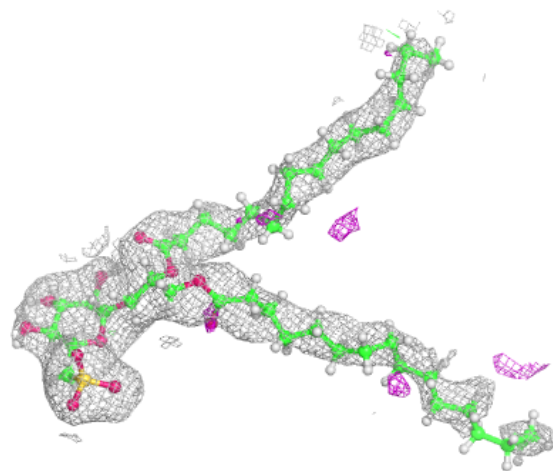
**Electron density around CLA b 613:**

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



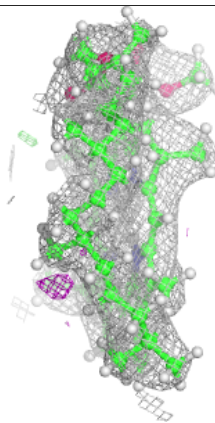
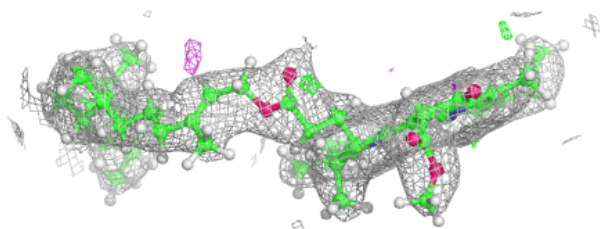
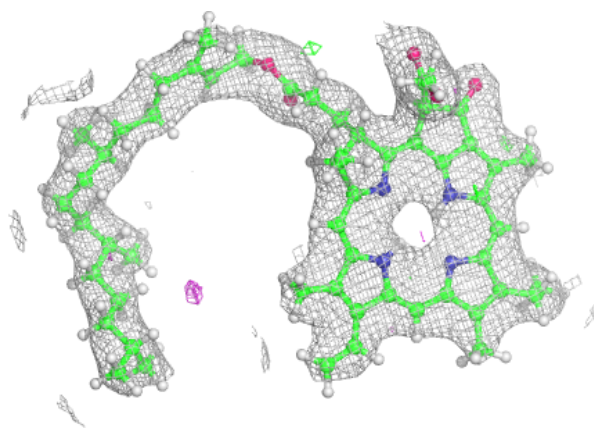
**Electron density around SQD a 410:**

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

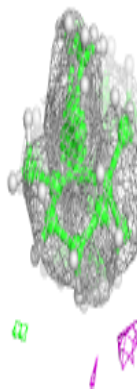
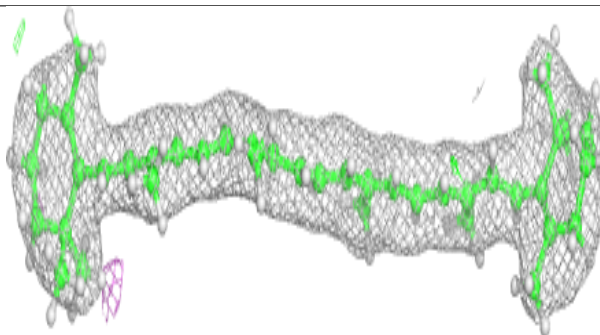
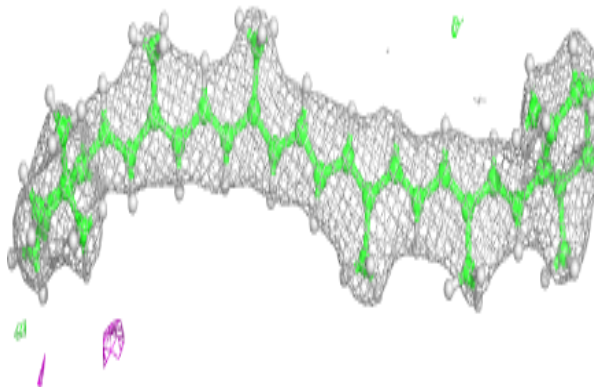


**Electron density around PHO d 401:**

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

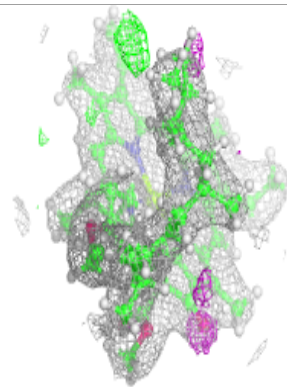
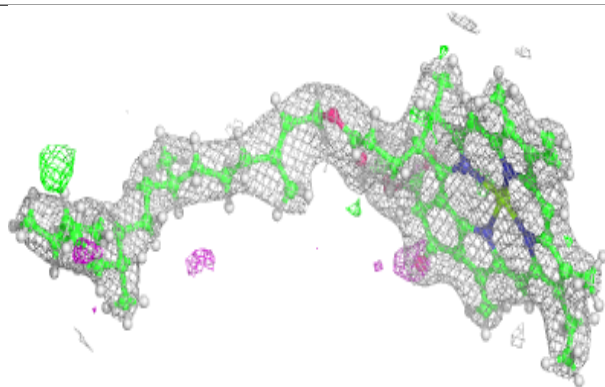
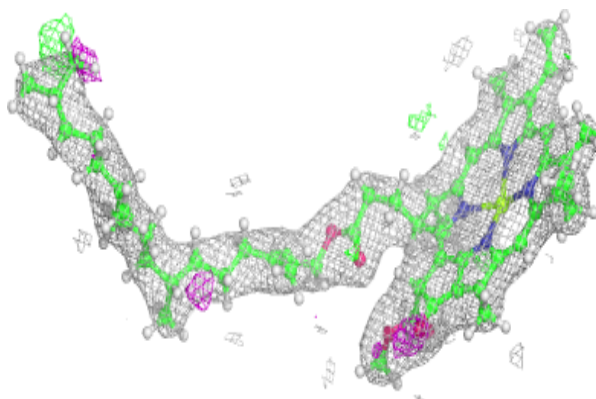
**Electron density around BCR A 406:**

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

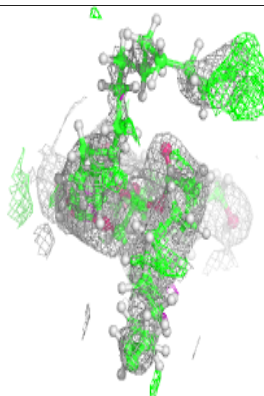
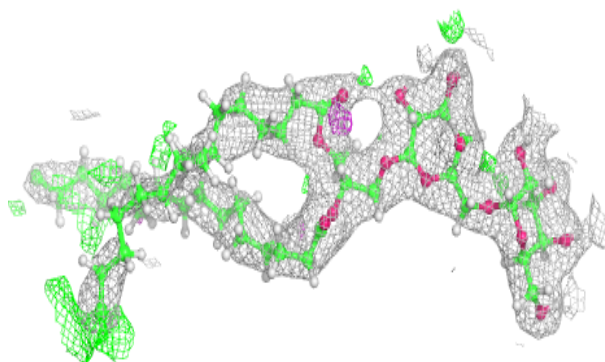
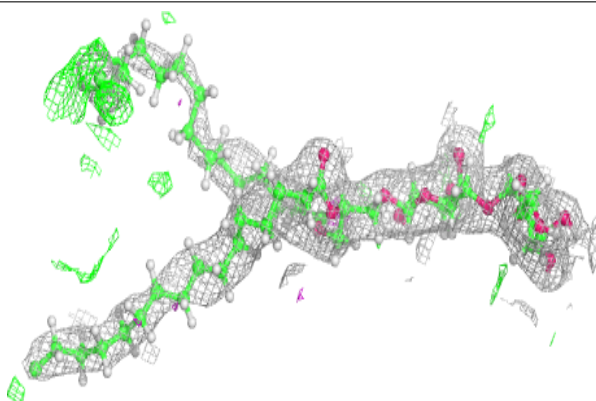


**Electron density around CLA A 402:**

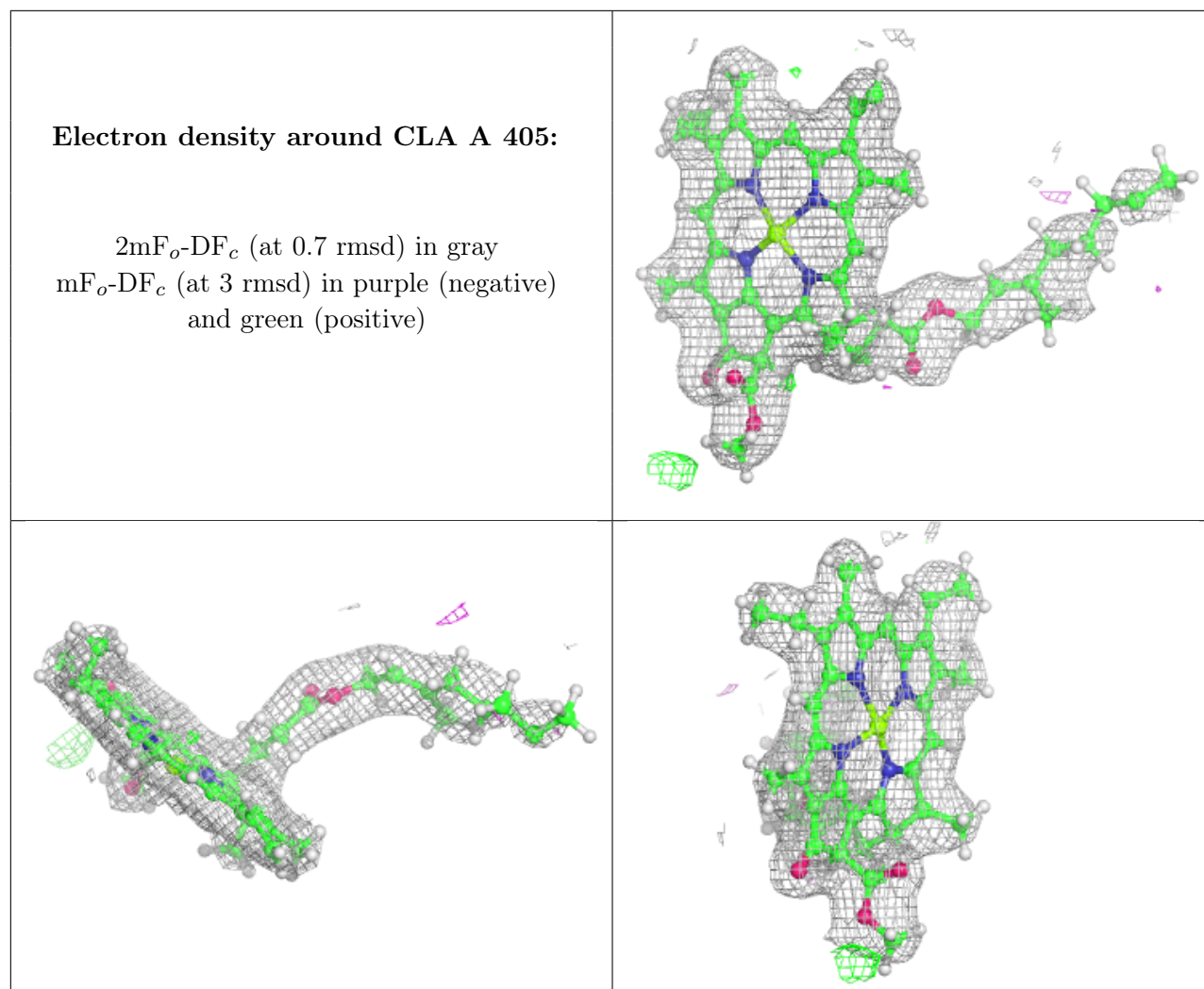
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around DGD C 516:**

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

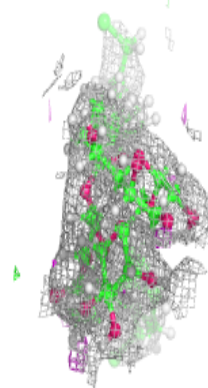
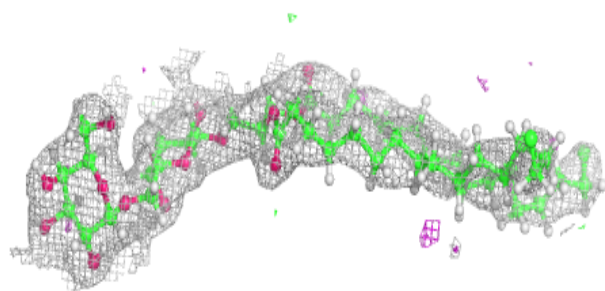
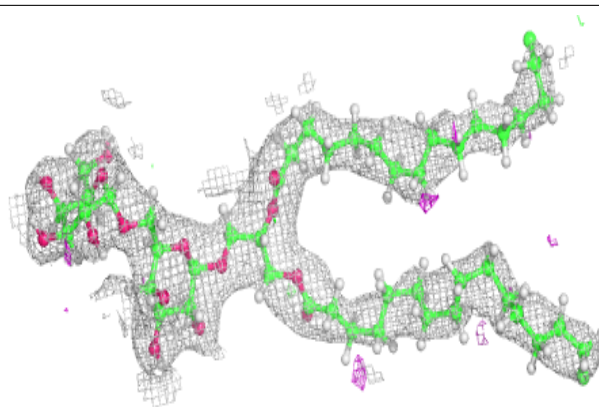




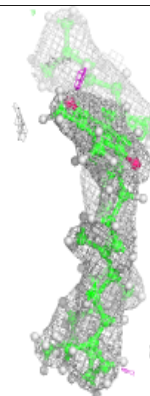
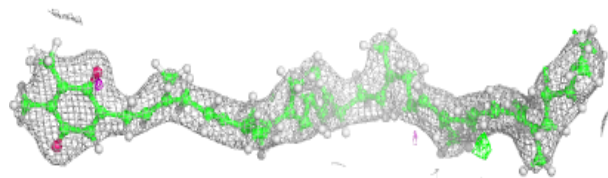
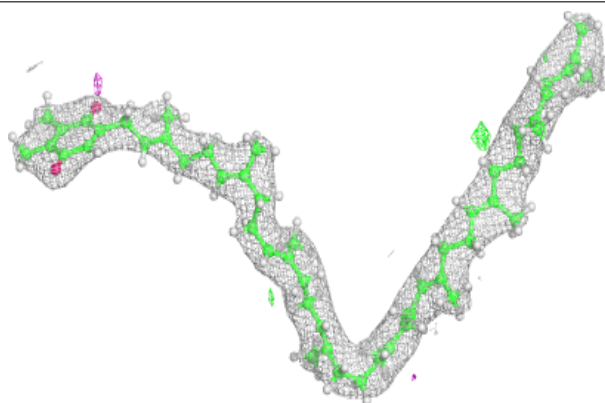


**Electron density around DGD C 518:**

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

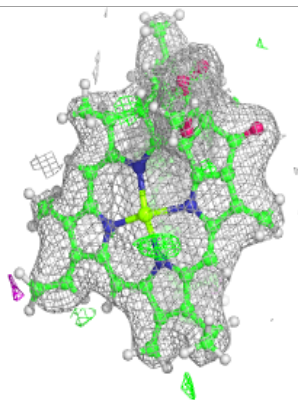
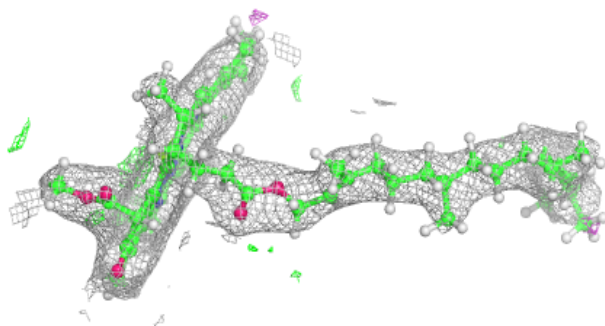
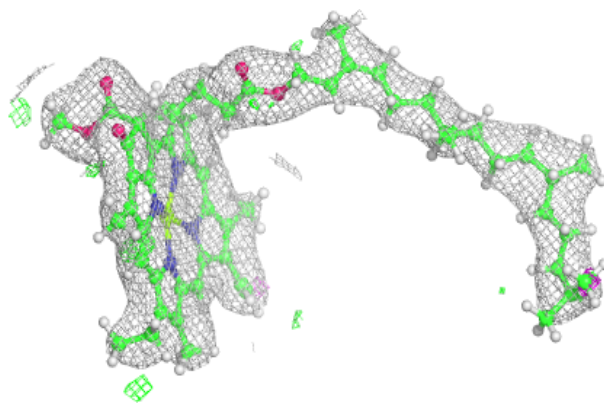
**Electron density around PL9 d 407:**

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

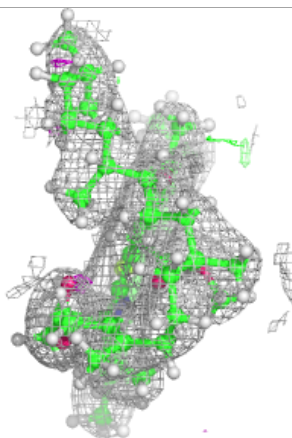
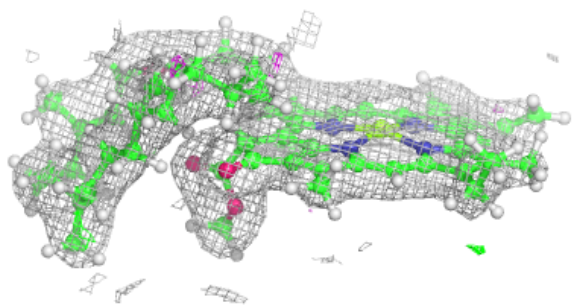
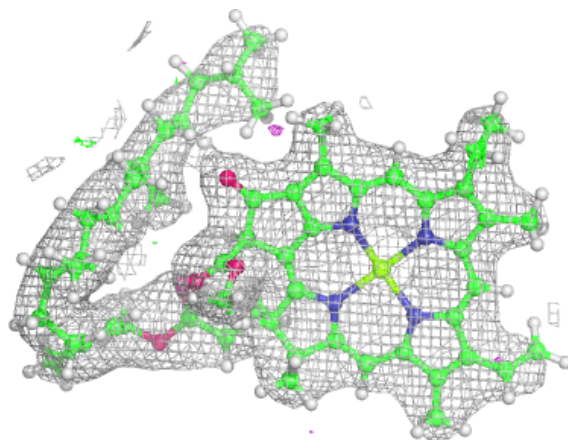


**Electron density around CLA B 609:**

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

**Electron density around CLA B 610:**

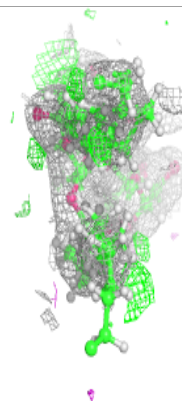
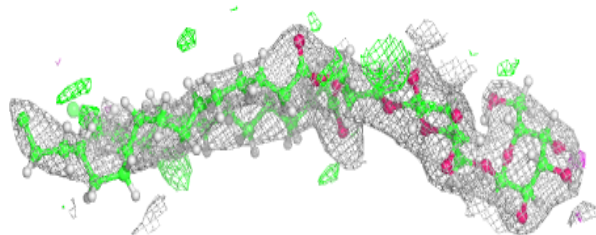
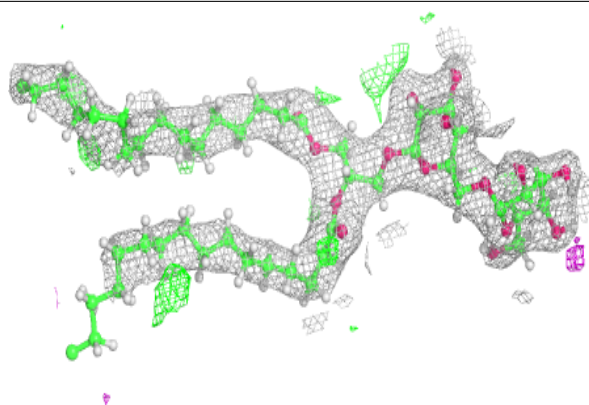
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



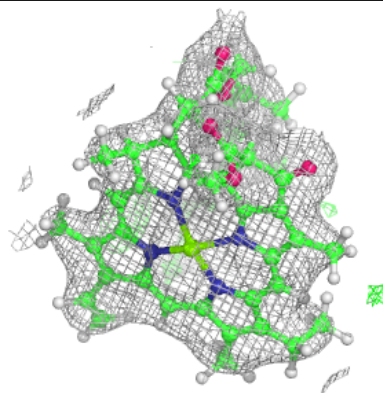
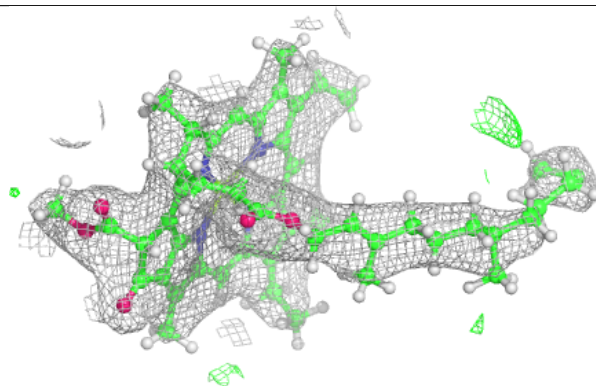
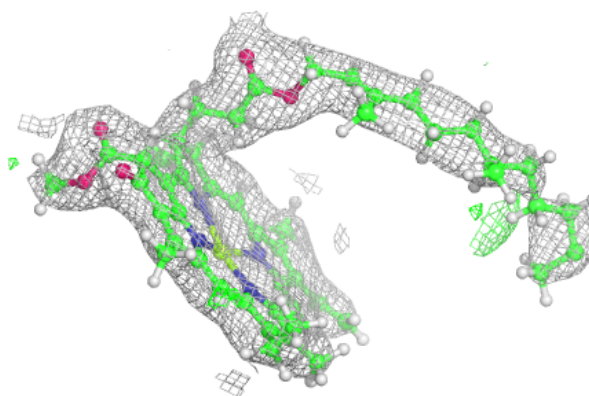


**Electron density around DGD c 519:**

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

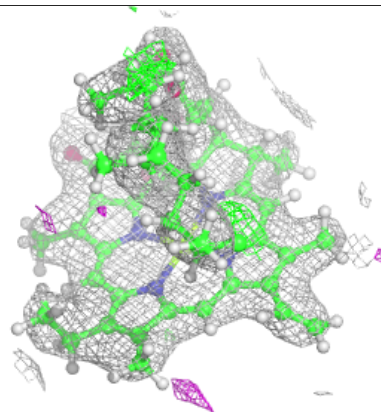
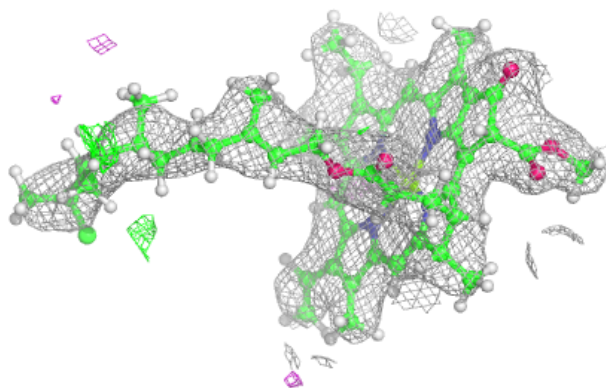
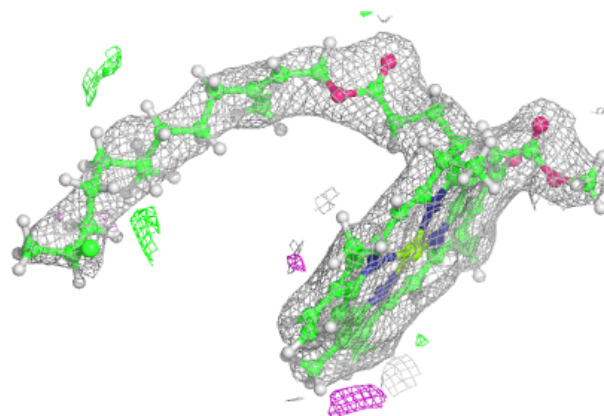
**Electron density around CLA C 504:**

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



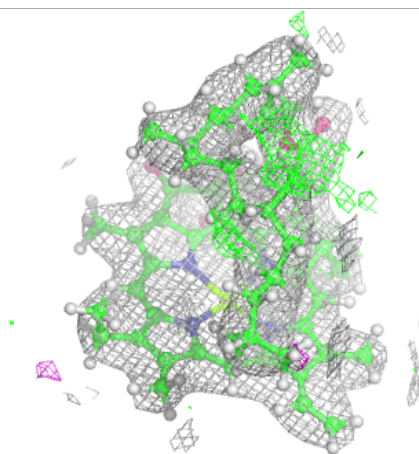
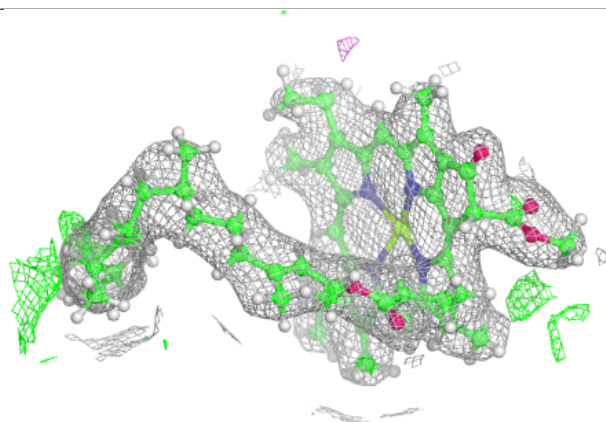
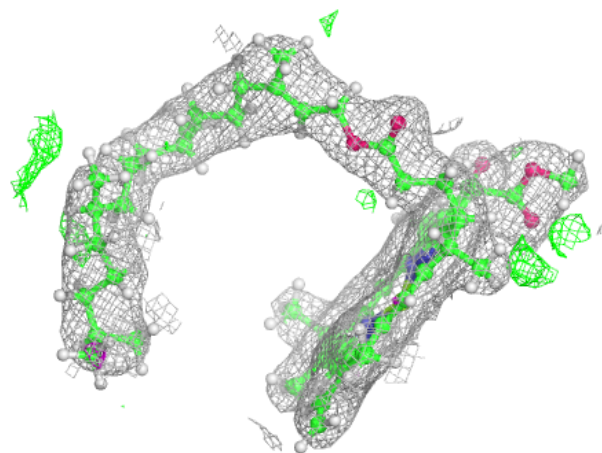
**Electron density around CLA c 504:**

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



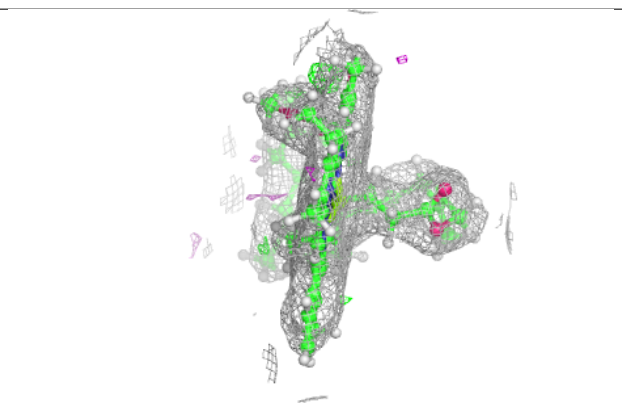
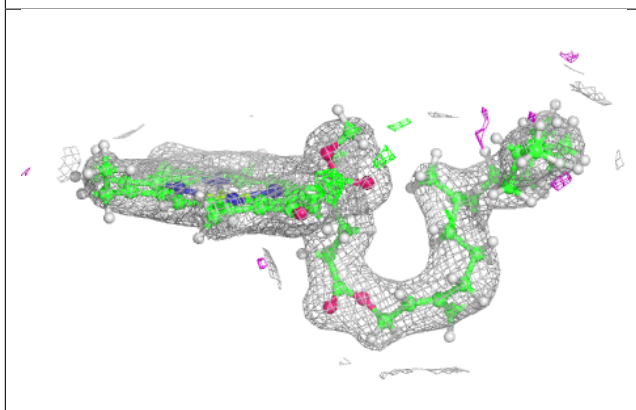
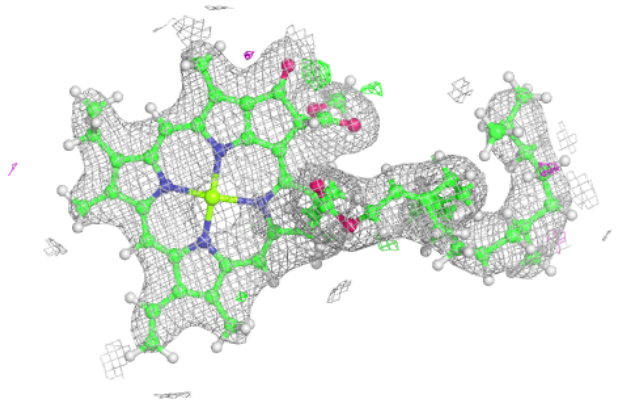
**Electron density around CLA B 611:**

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

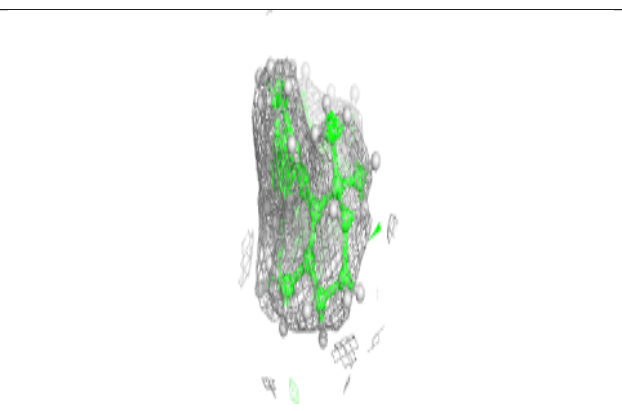
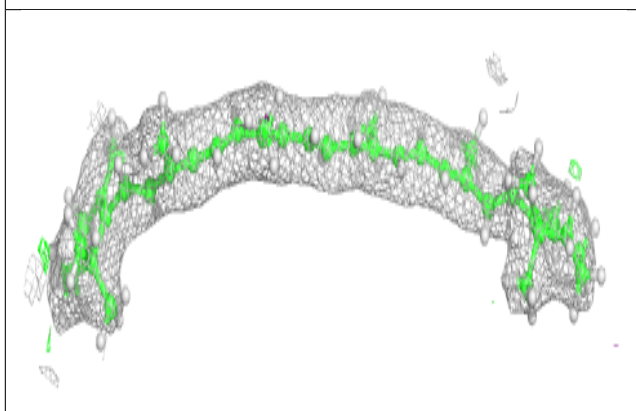
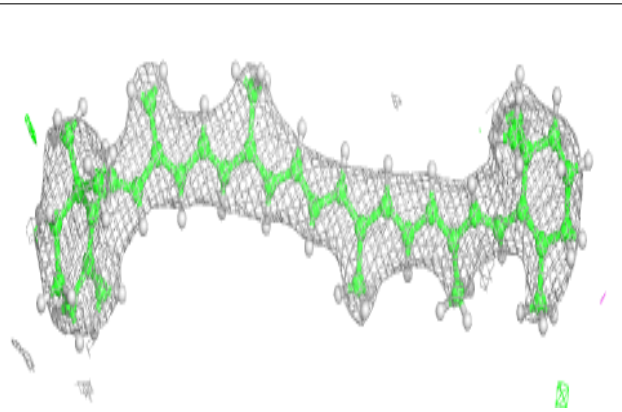


**Electron density around CLA B 612:**

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

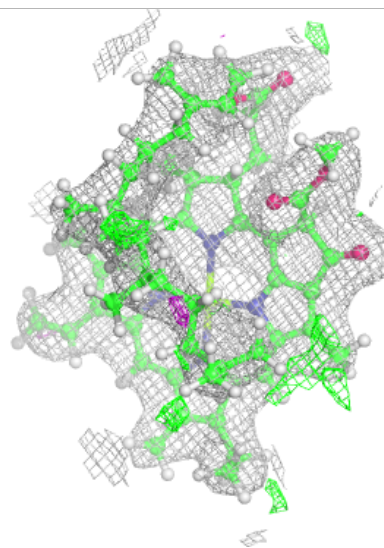
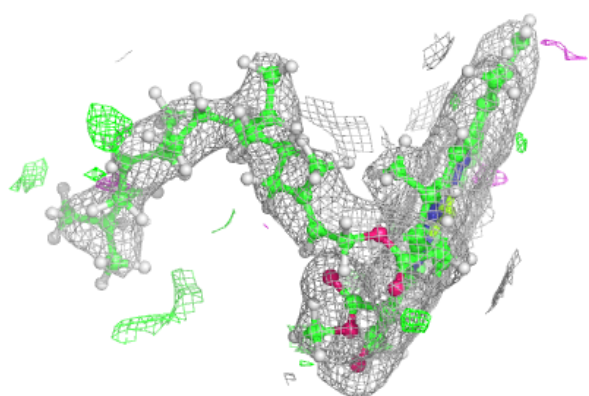
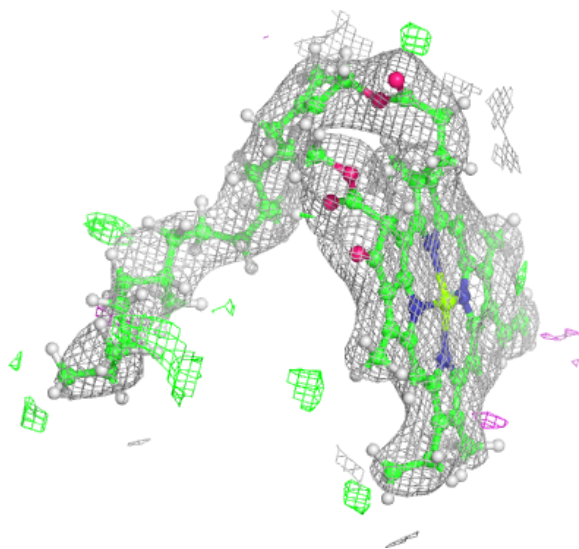
**Electron density around BCR T 101:**

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



**Electron density around CLA B 613:**

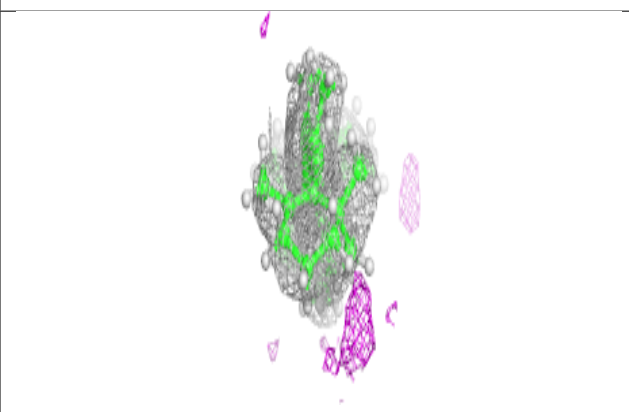
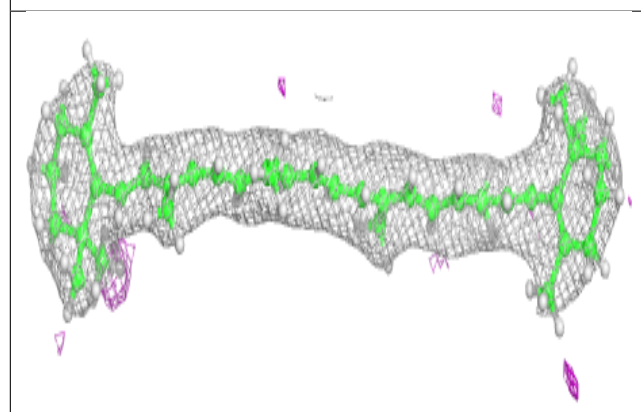
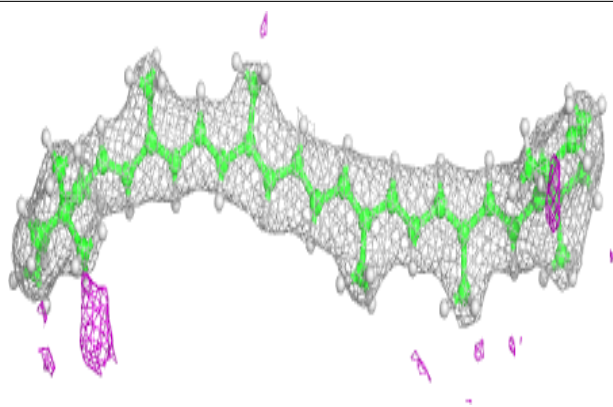
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



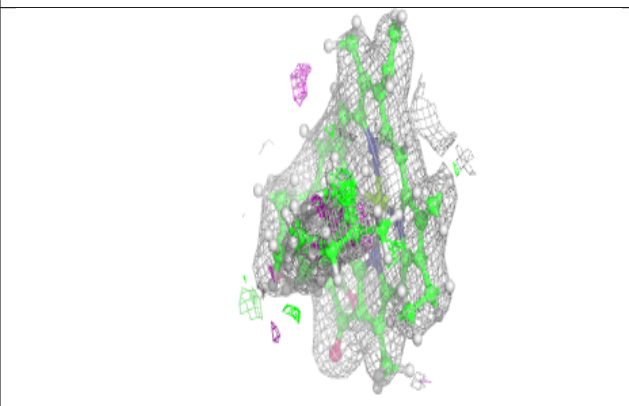
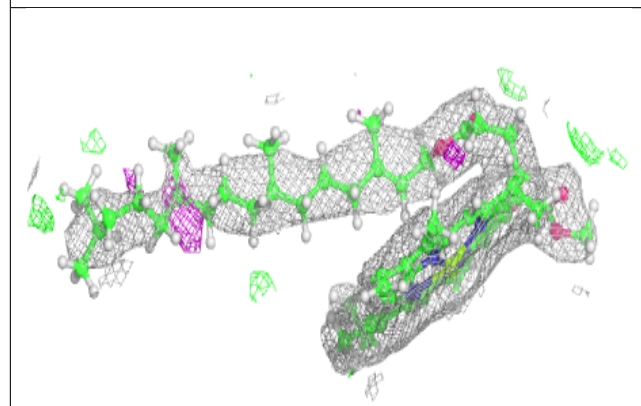
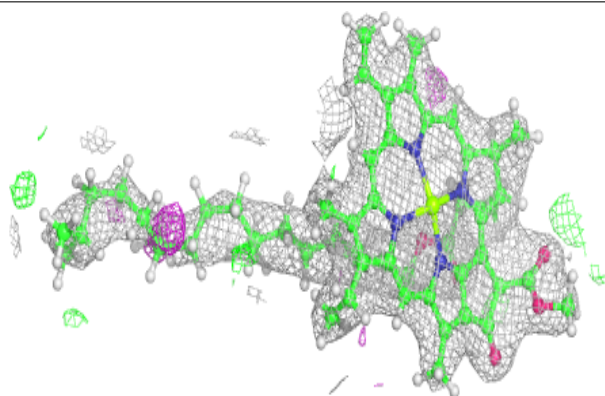


**Electron density around BCR a 405:**

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

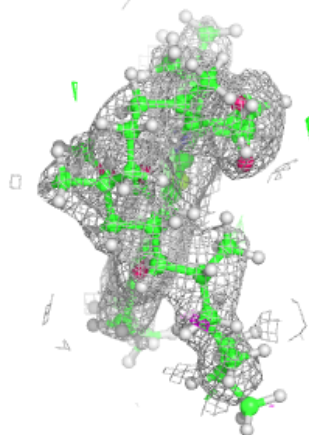
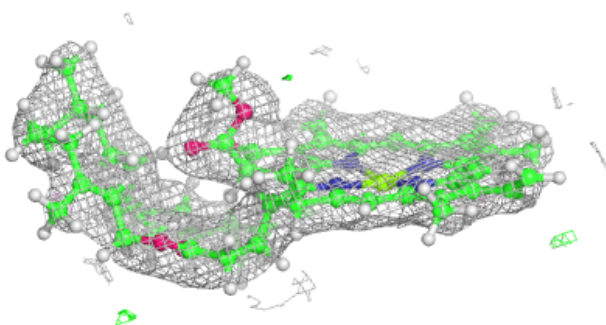
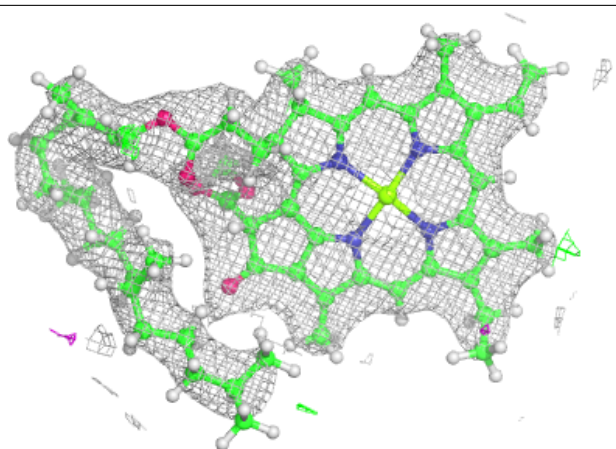
**Electron density around CLA B 614:**

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

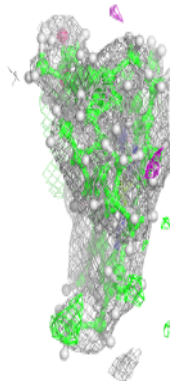
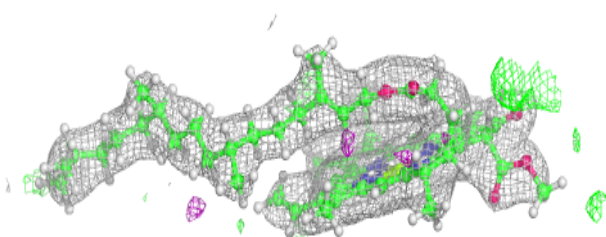
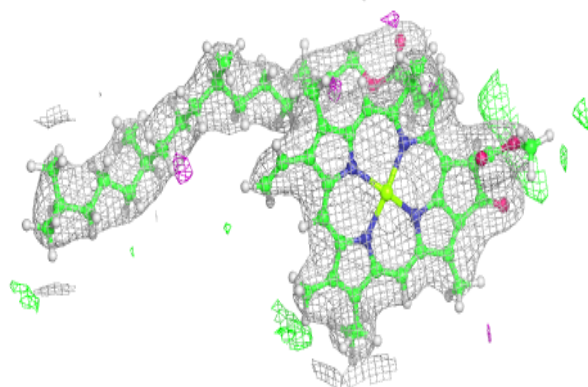


**Electron density around CLA b 610:**

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

**Electron density around CLA C 501:**

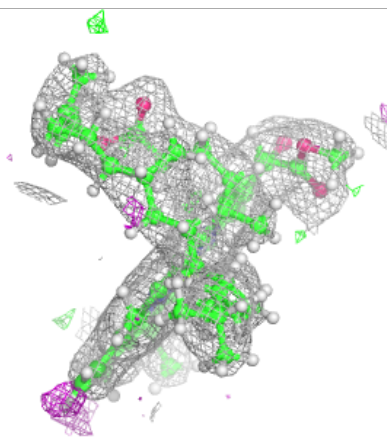
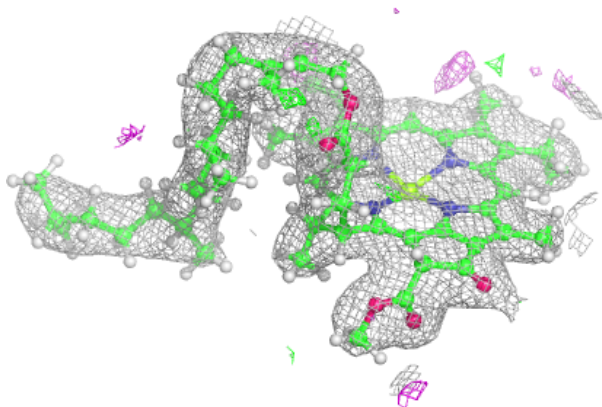
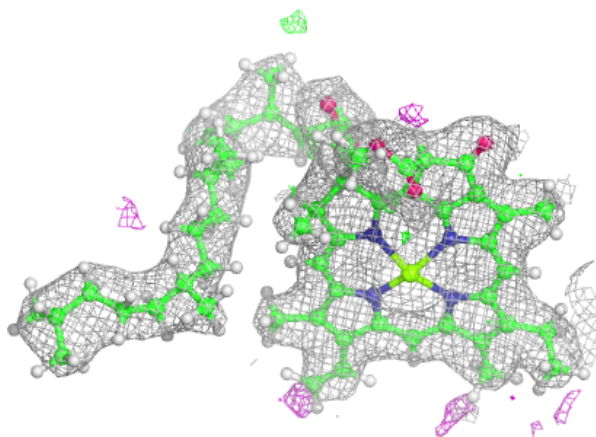
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





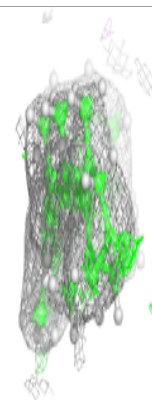
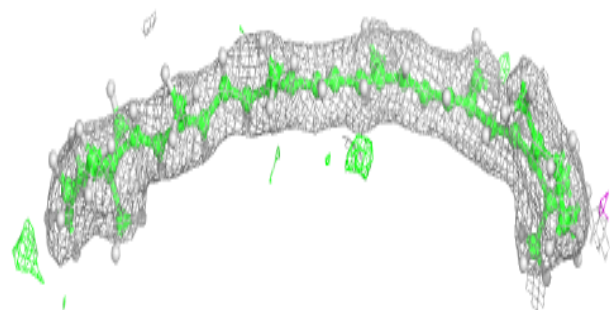
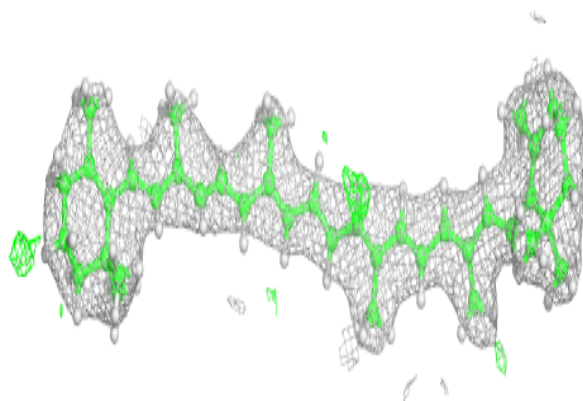
**Electron density around CLA A 410:**

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

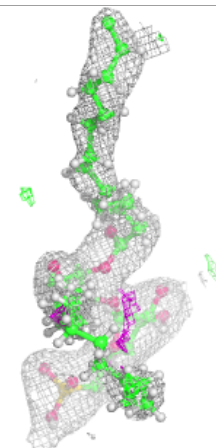
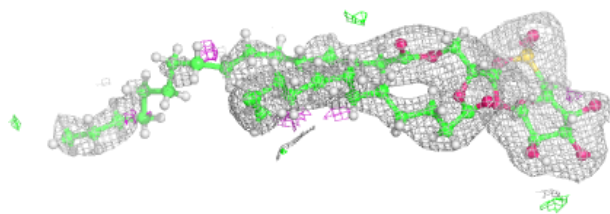
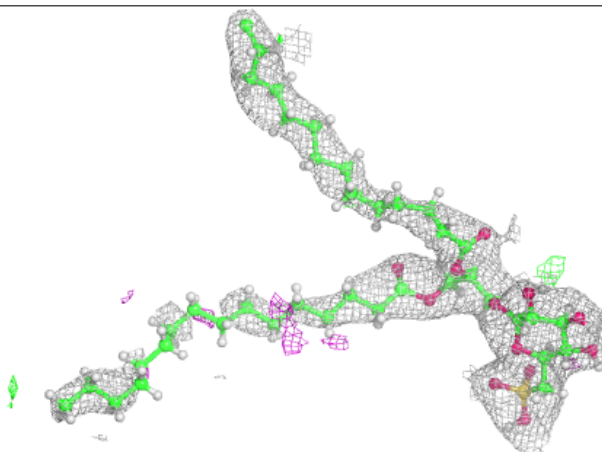


**Electron density around BCR t 101:**

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

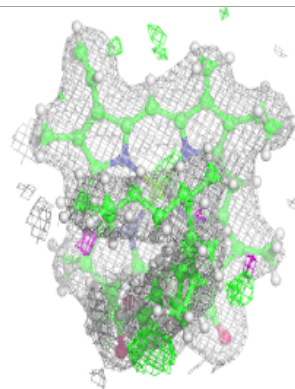
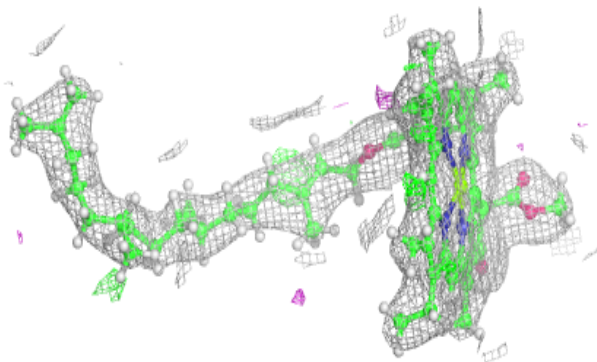
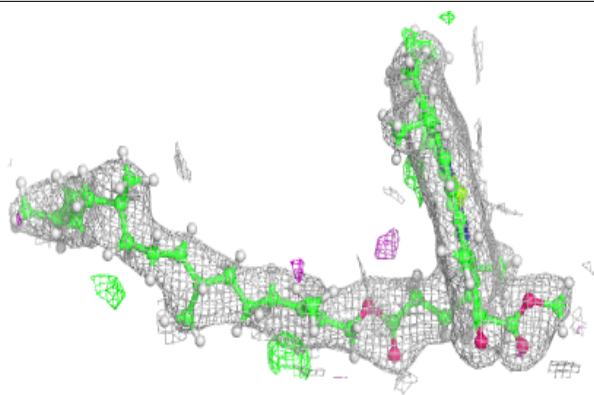
**Electron density around SQD A 412:**

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

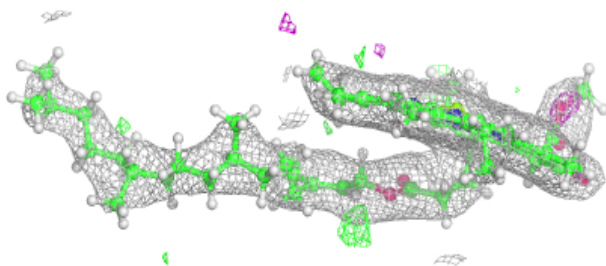
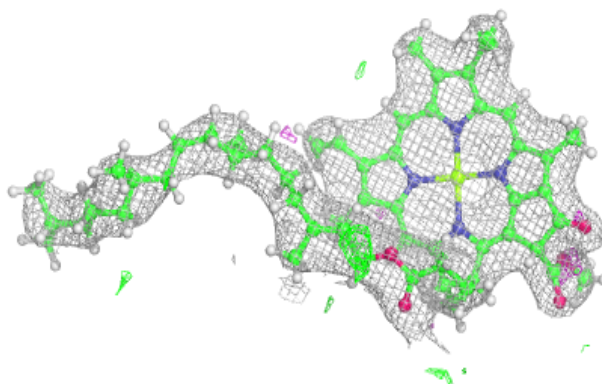


**Electron density around CLA B 605:**

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

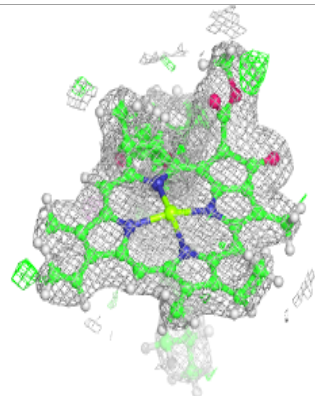
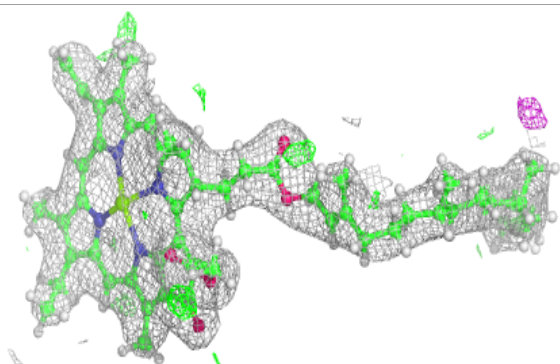
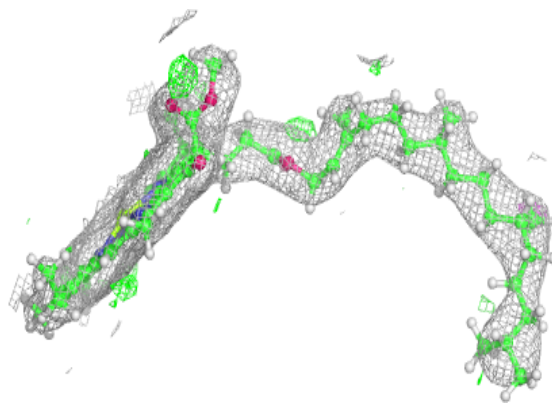
**Electron density around CLA b 603:**

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

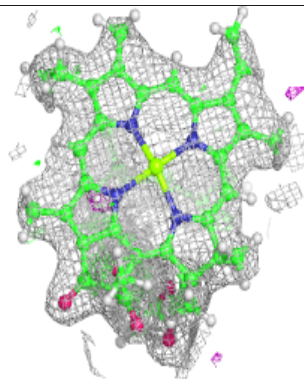
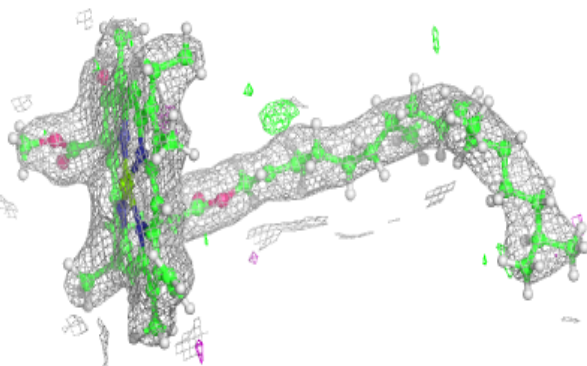
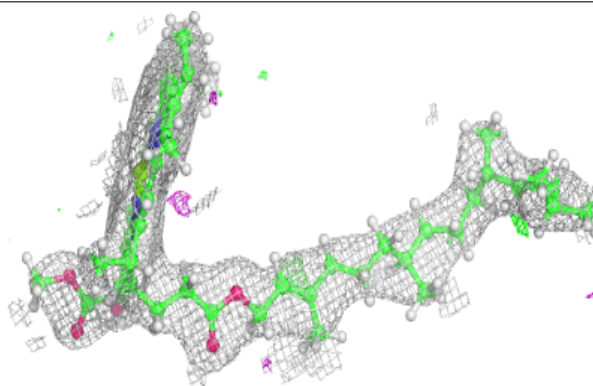


**Electron density around CLA D 403:**

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

**Electron density around CLA b 605:**

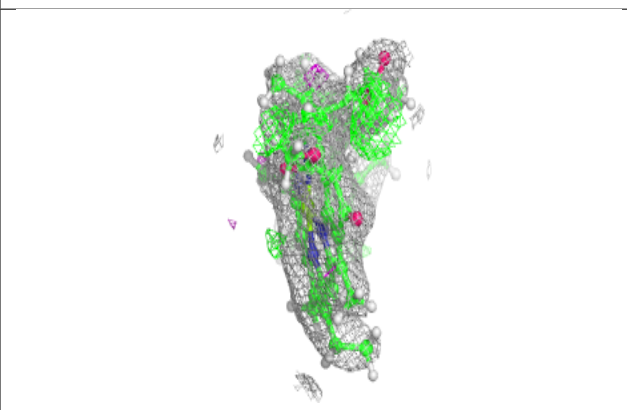
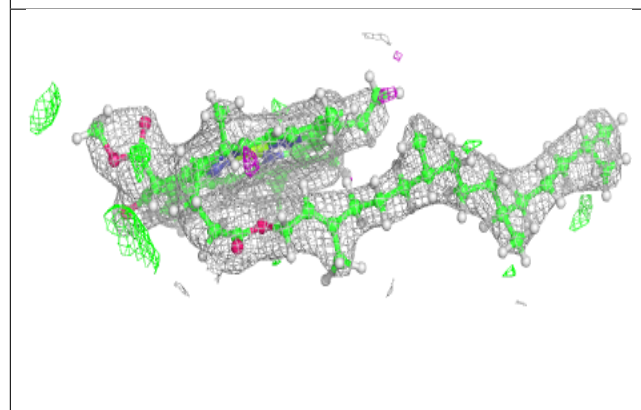
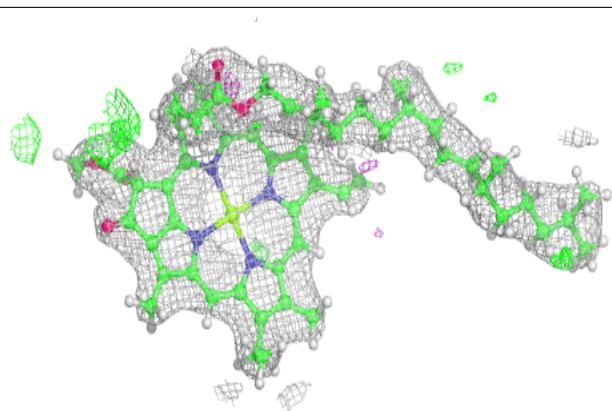
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



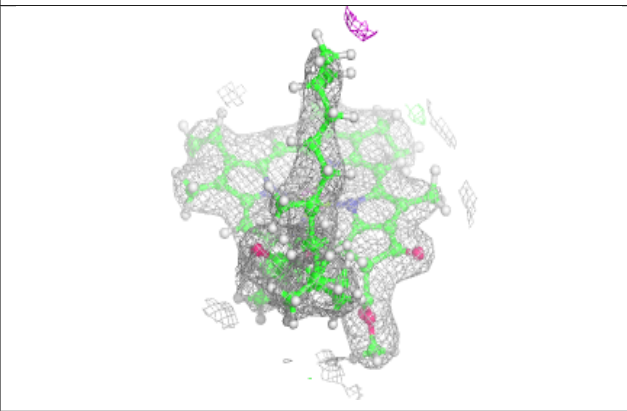
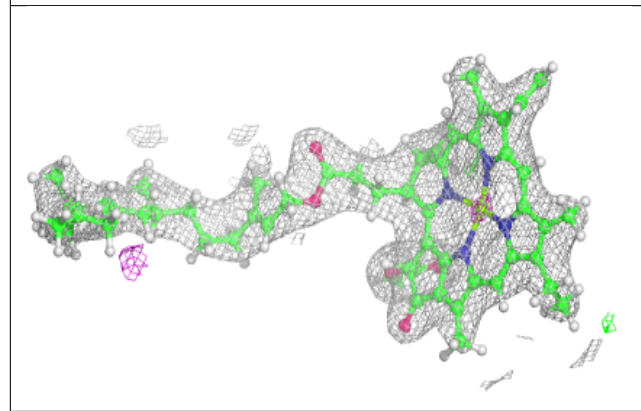
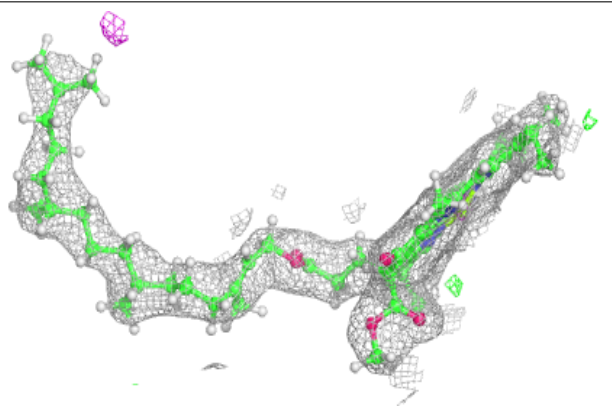


**Electron density around CLA c 501:**

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

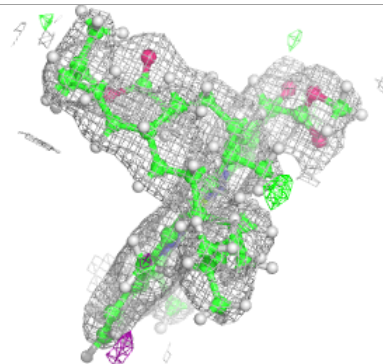
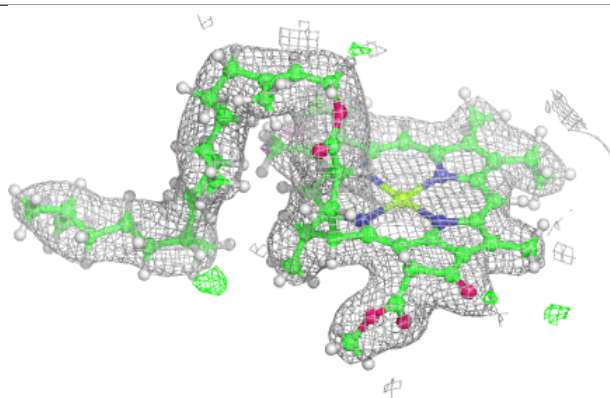
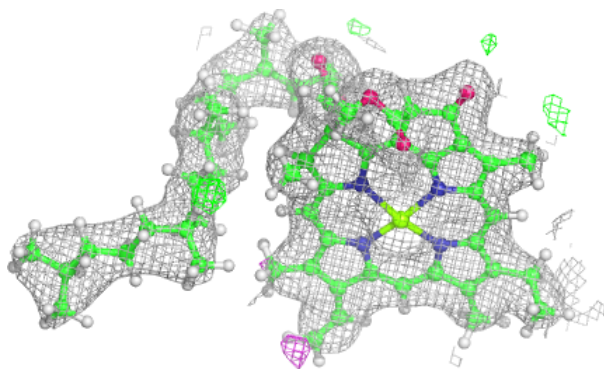
**Electron density around CLA d 403:**

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

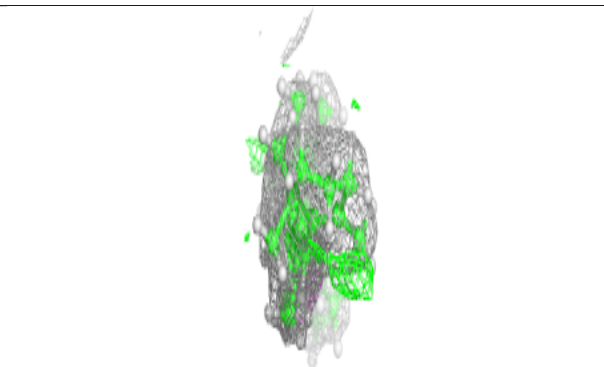
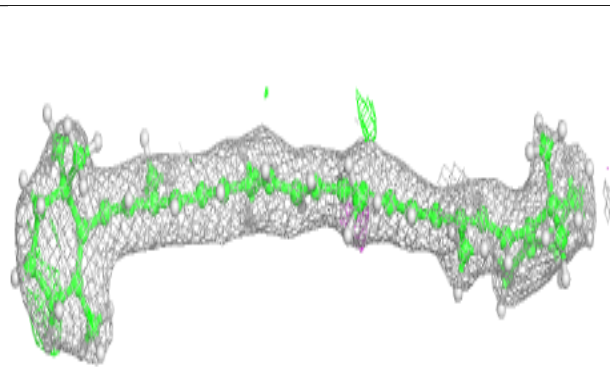
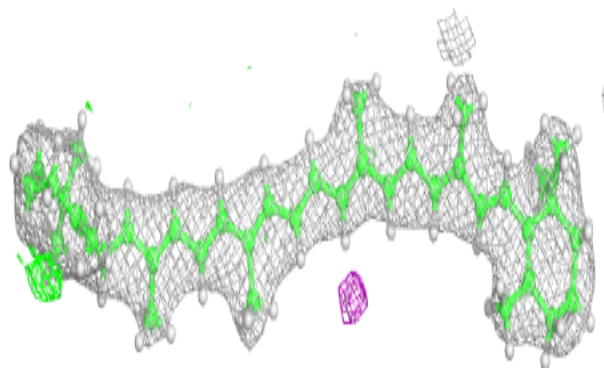


**Electron density around CLA d 404:**

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

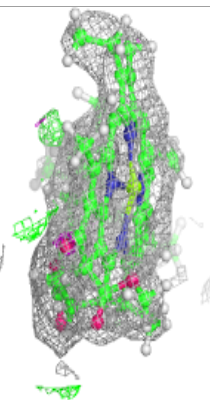
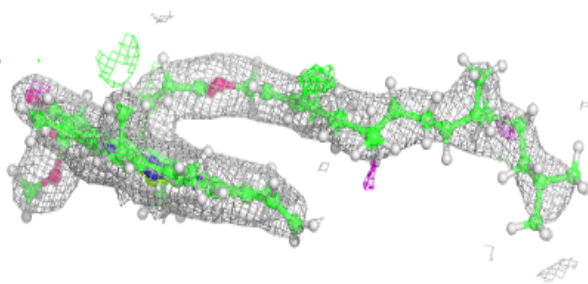
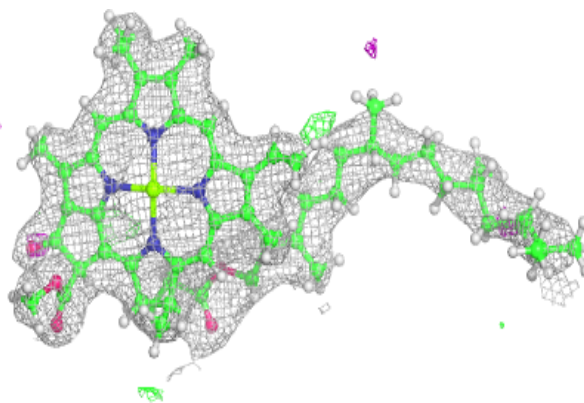
**Electron density around BCR b 617:**

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

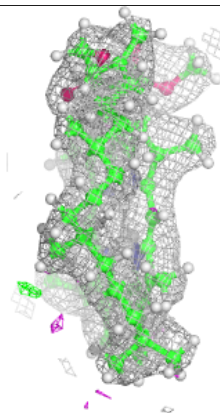
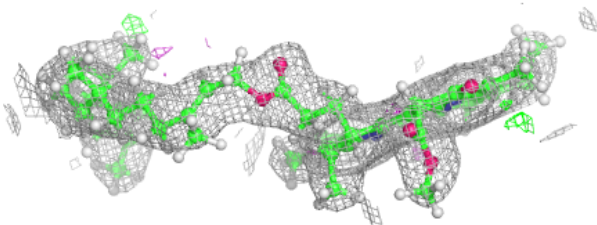
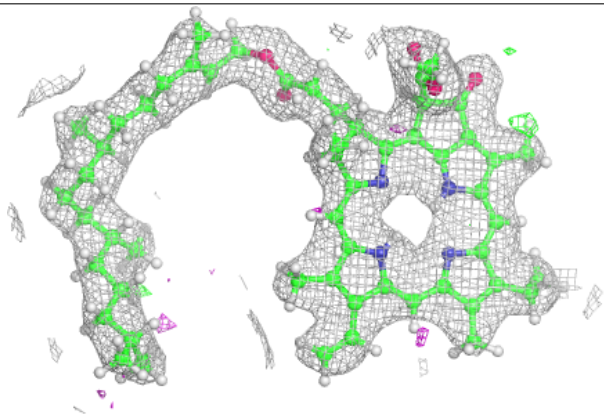


**Electron density around CLA B 603:**

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

**Electron density around PHO A 404:**

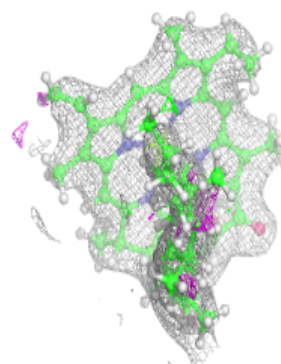
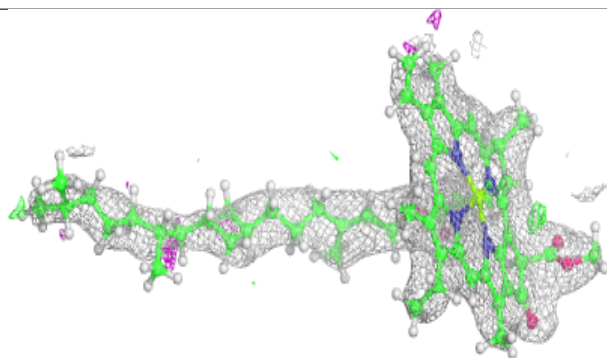
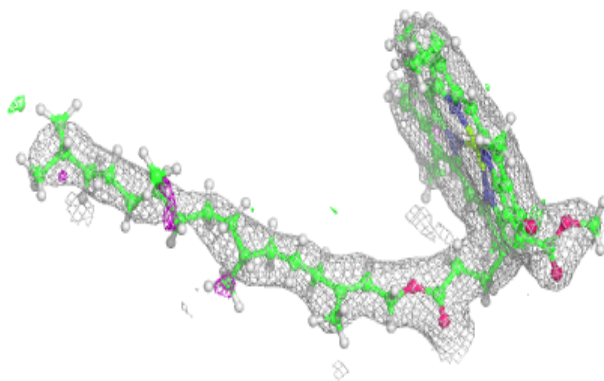
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



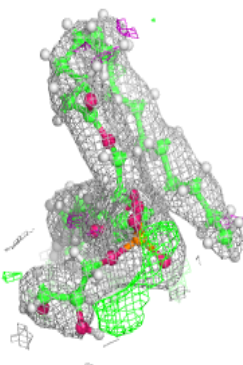
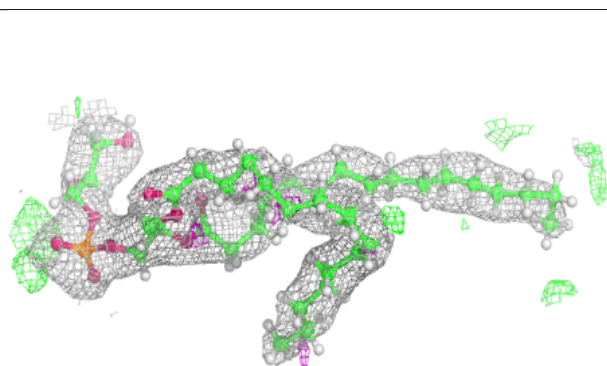
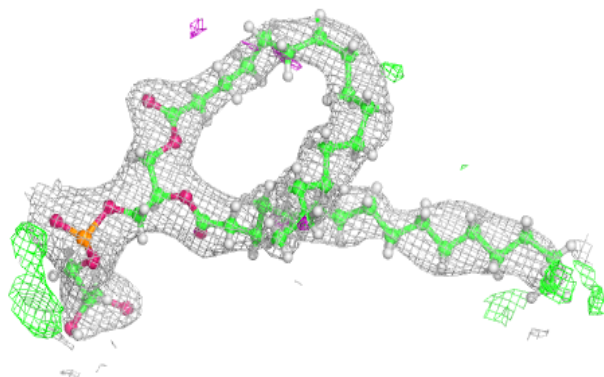


**Electron density around CLA b 607:**

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

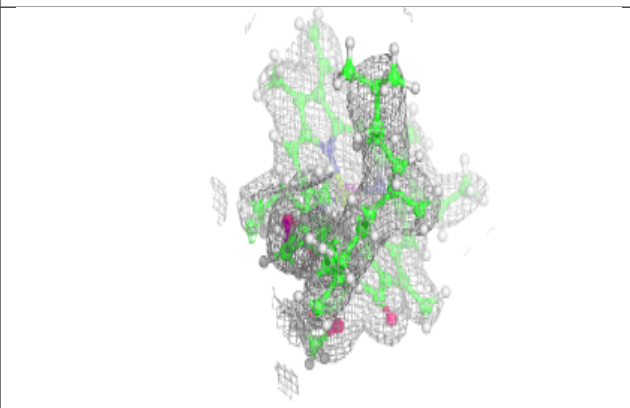
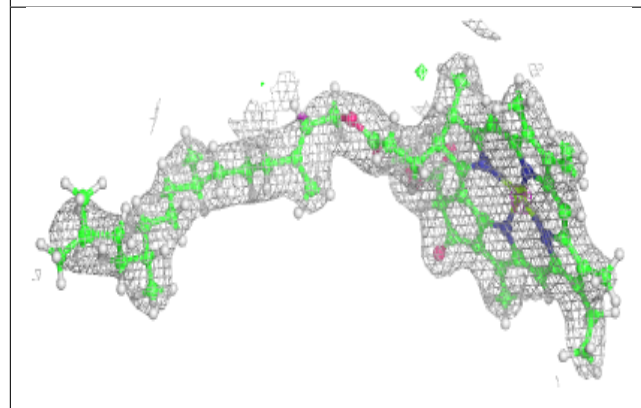
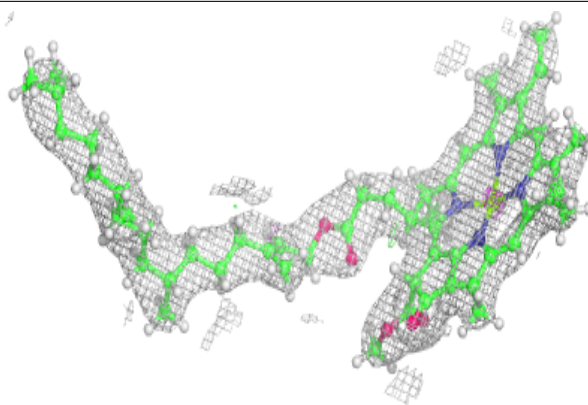
**Electron density around LHG B 622:**

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

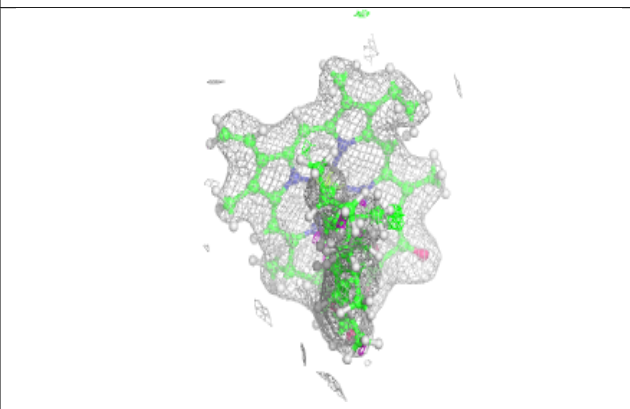
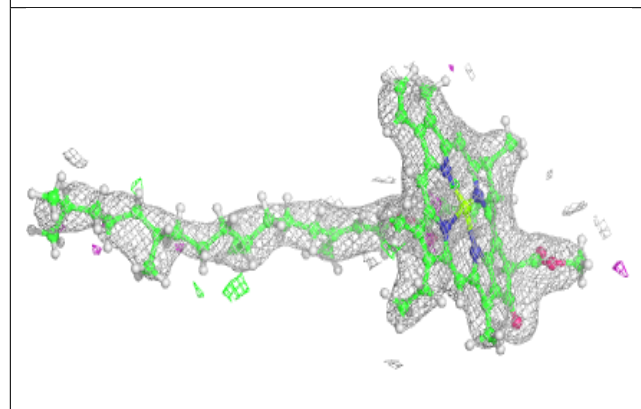
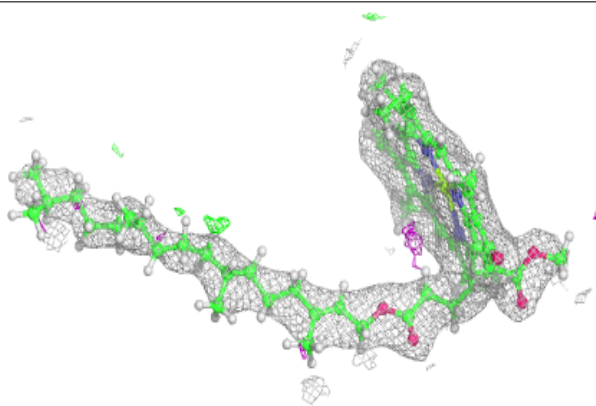


**Electron density around CLA a 402:**

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

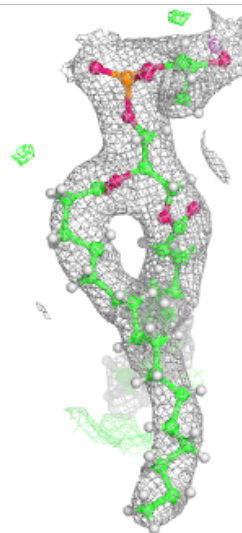
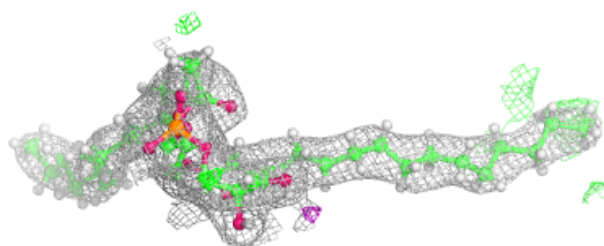
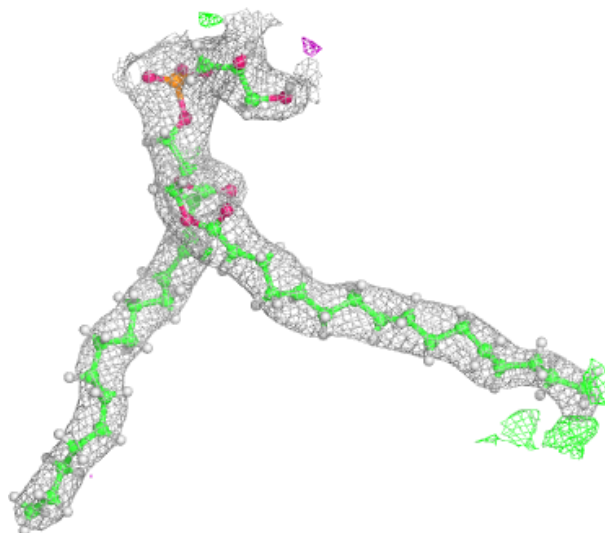
**Electron density around CLA B 607:**

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



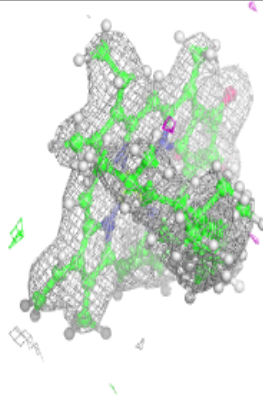
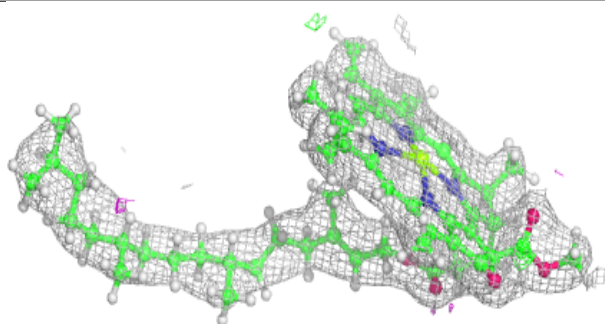
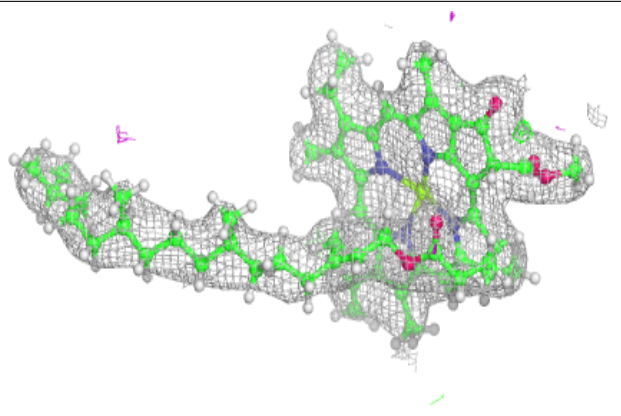
**Electron density around LHG 1 101:**

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

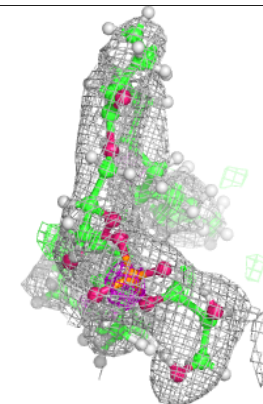
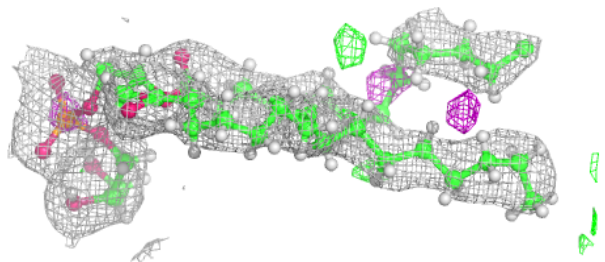
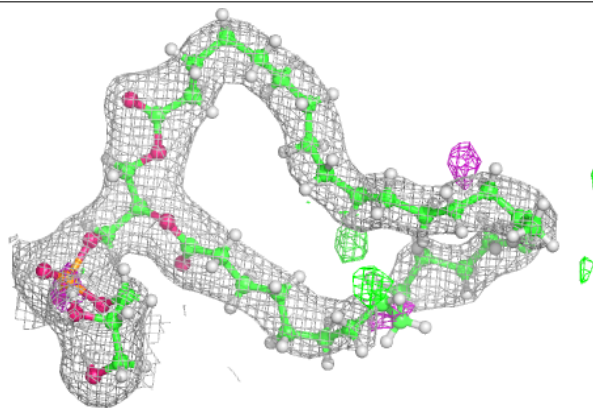


**Electron density around CLA B 608:**

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

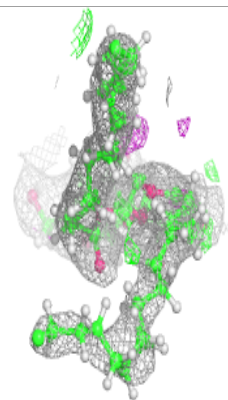
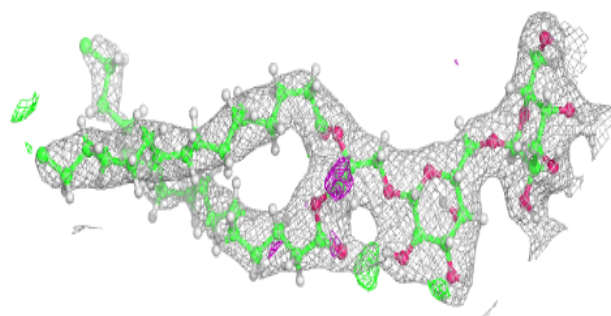
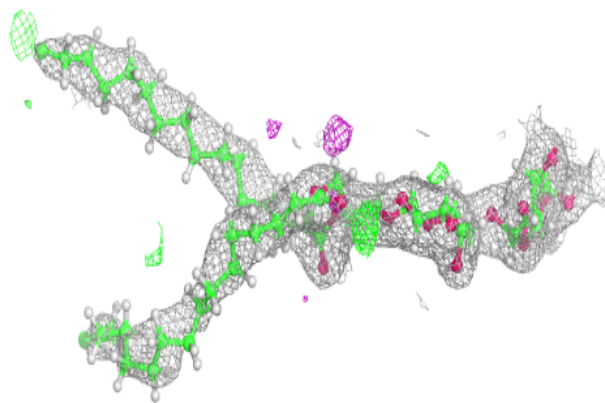
**Electron density around LHG D 409:**

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



**Electron density around DGD c 517:**

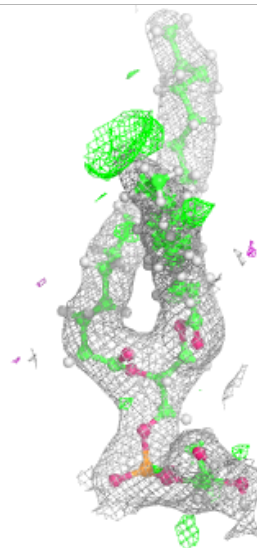
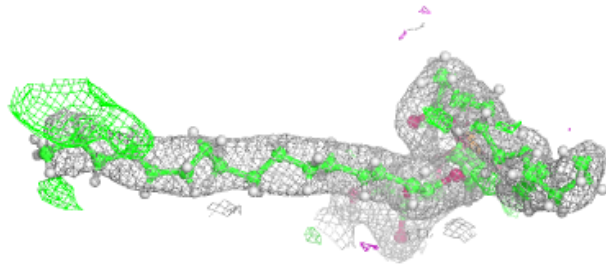
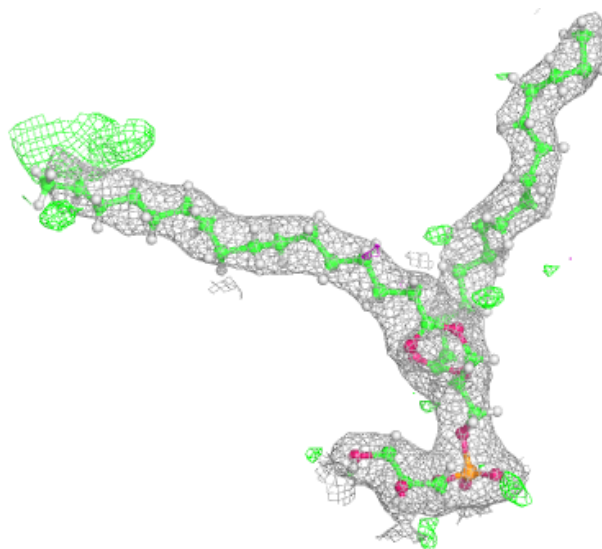
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





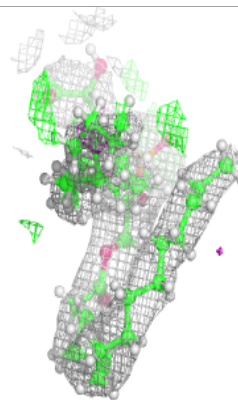
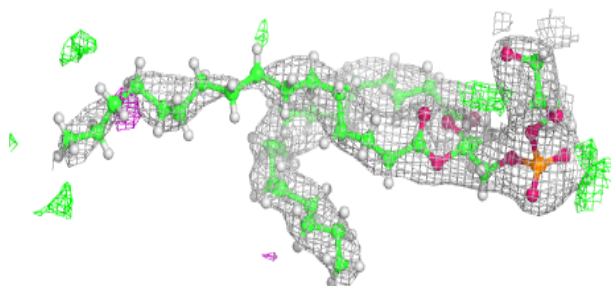
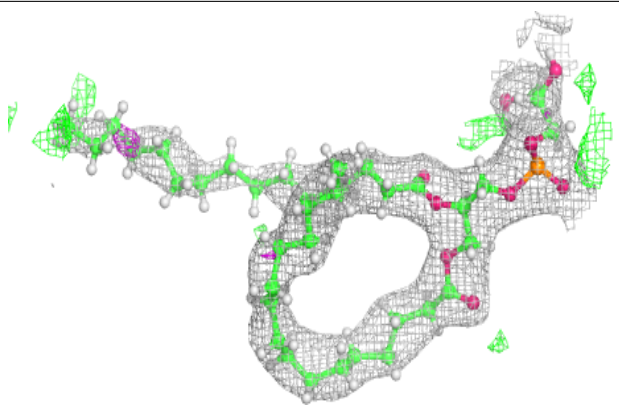
**Electron density around LHG L 102:**

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

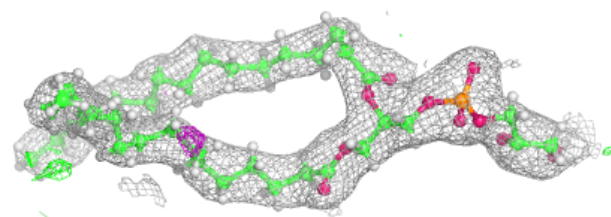
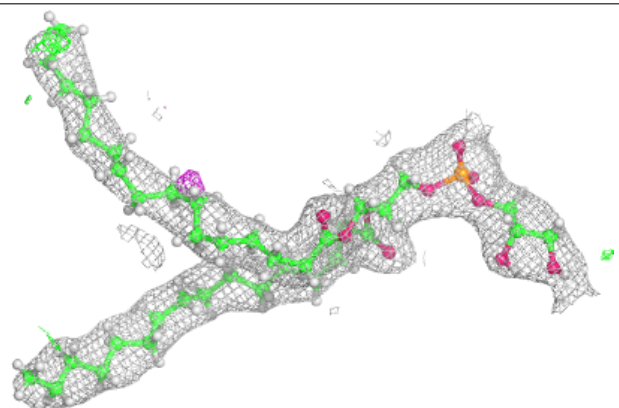


**Electron density around LHG d 408:**

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

**Electron density around LHG d 409:**

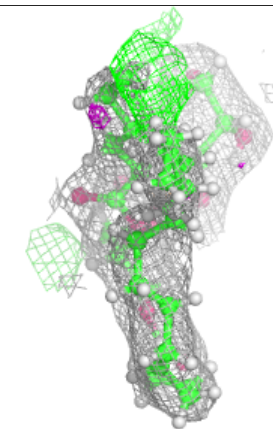
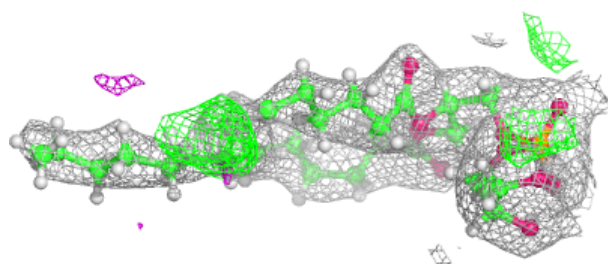
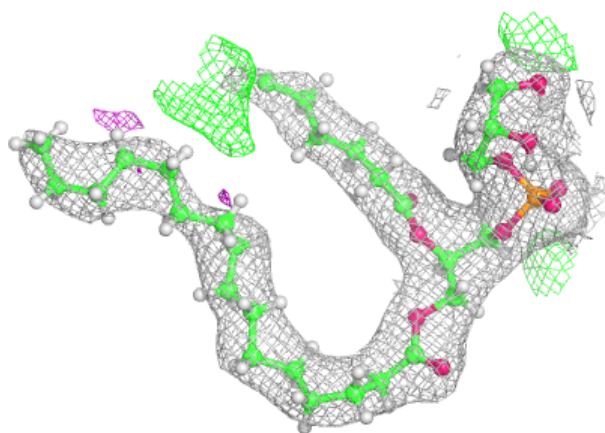
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





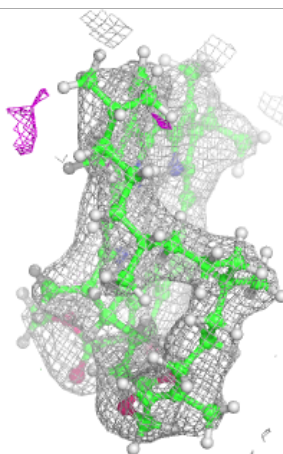
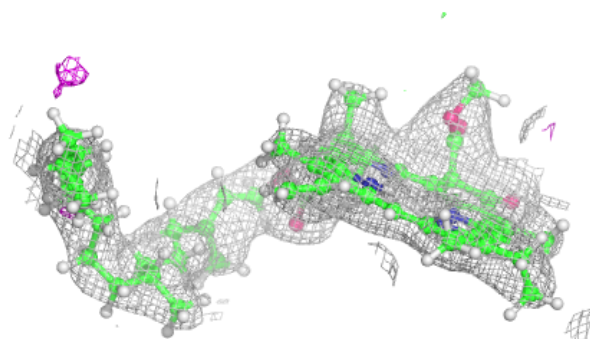
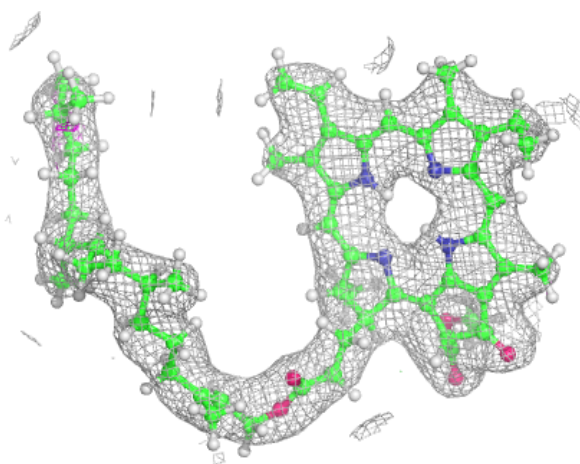
**Electron density around LHG d 410:**

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



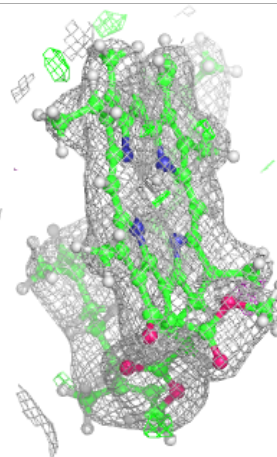
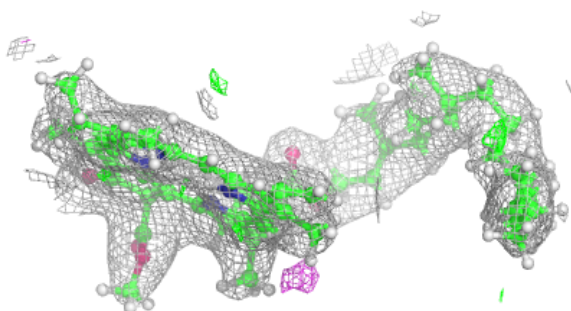
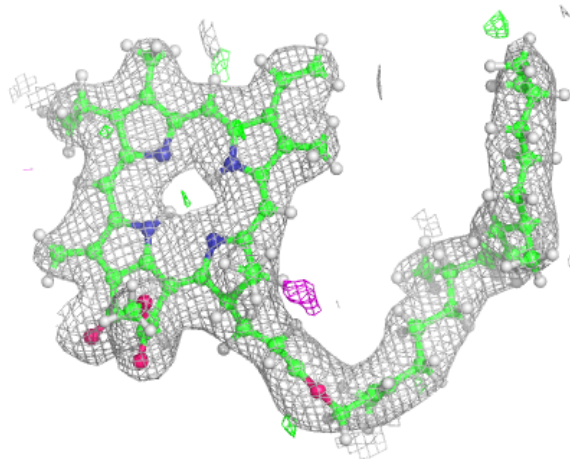
**Electron density around PHO d 402:**

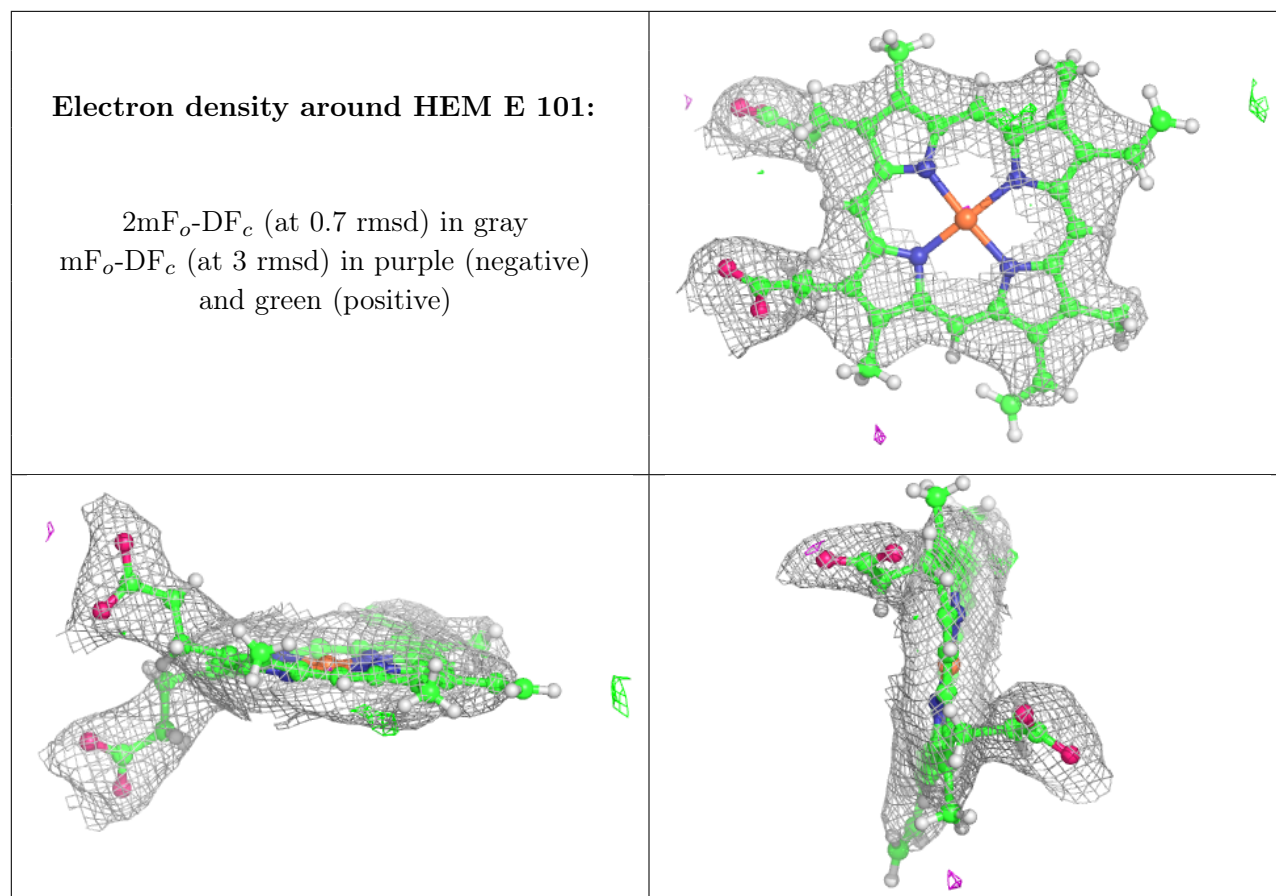
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PHO D 401:**

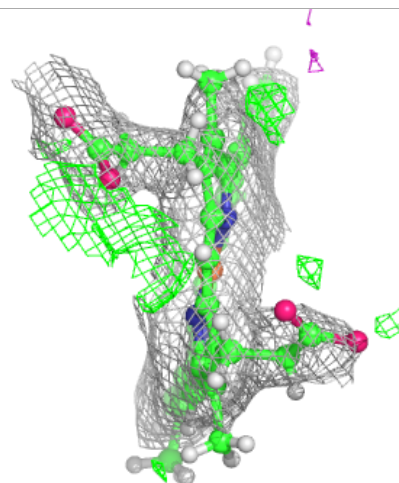
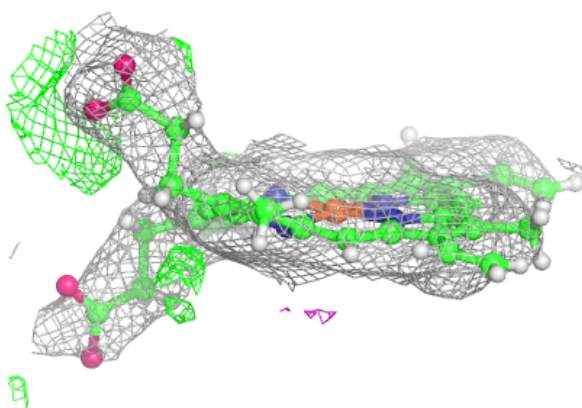
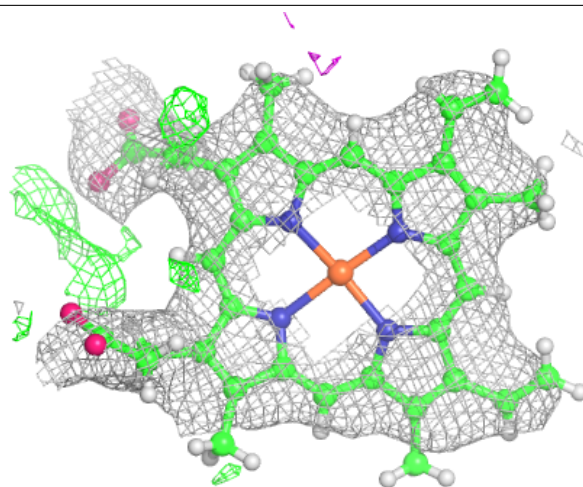
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

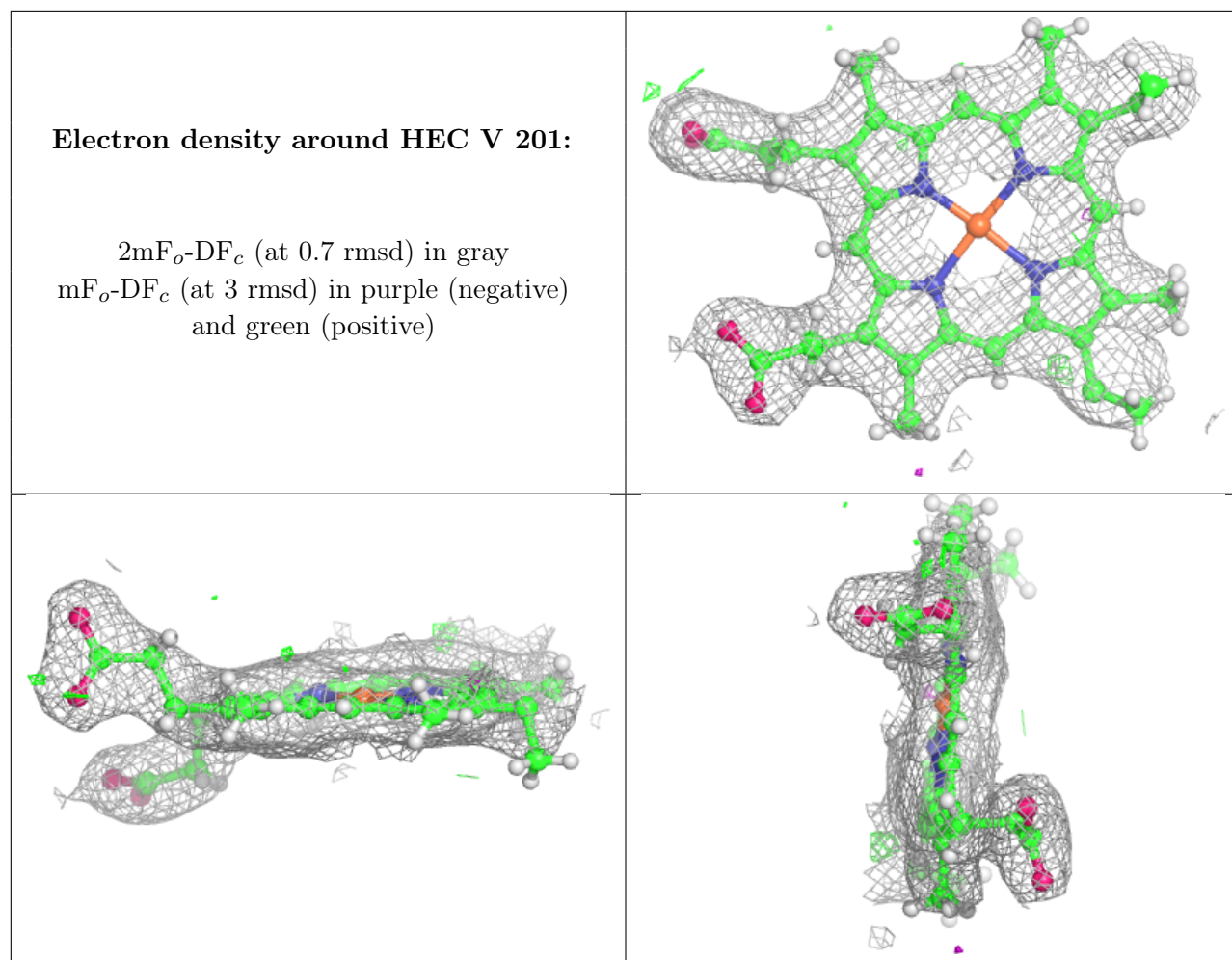




**Electron density around HEM f 101:**

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

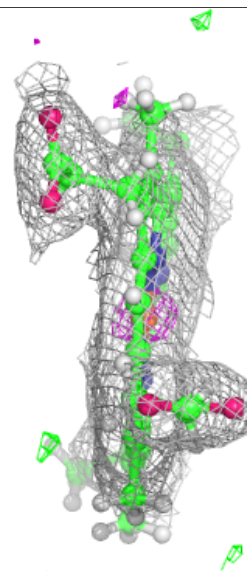
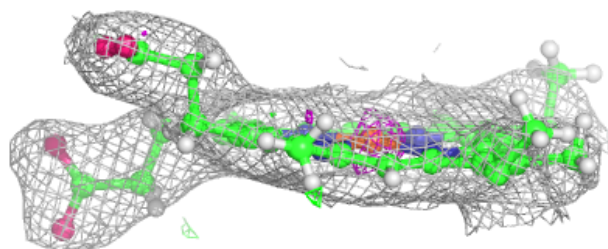
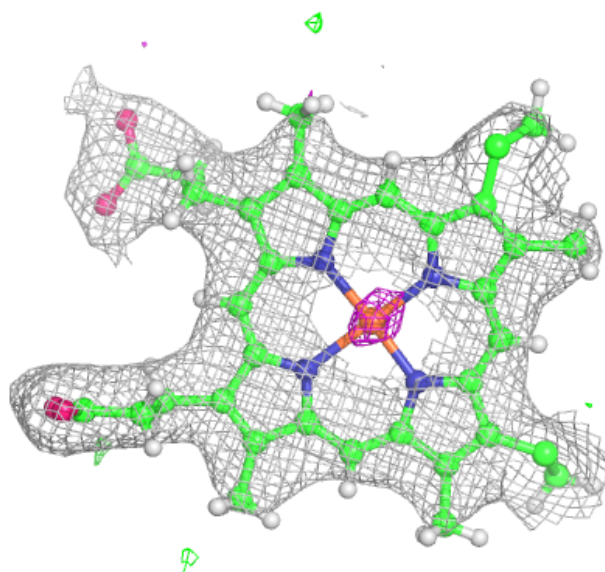




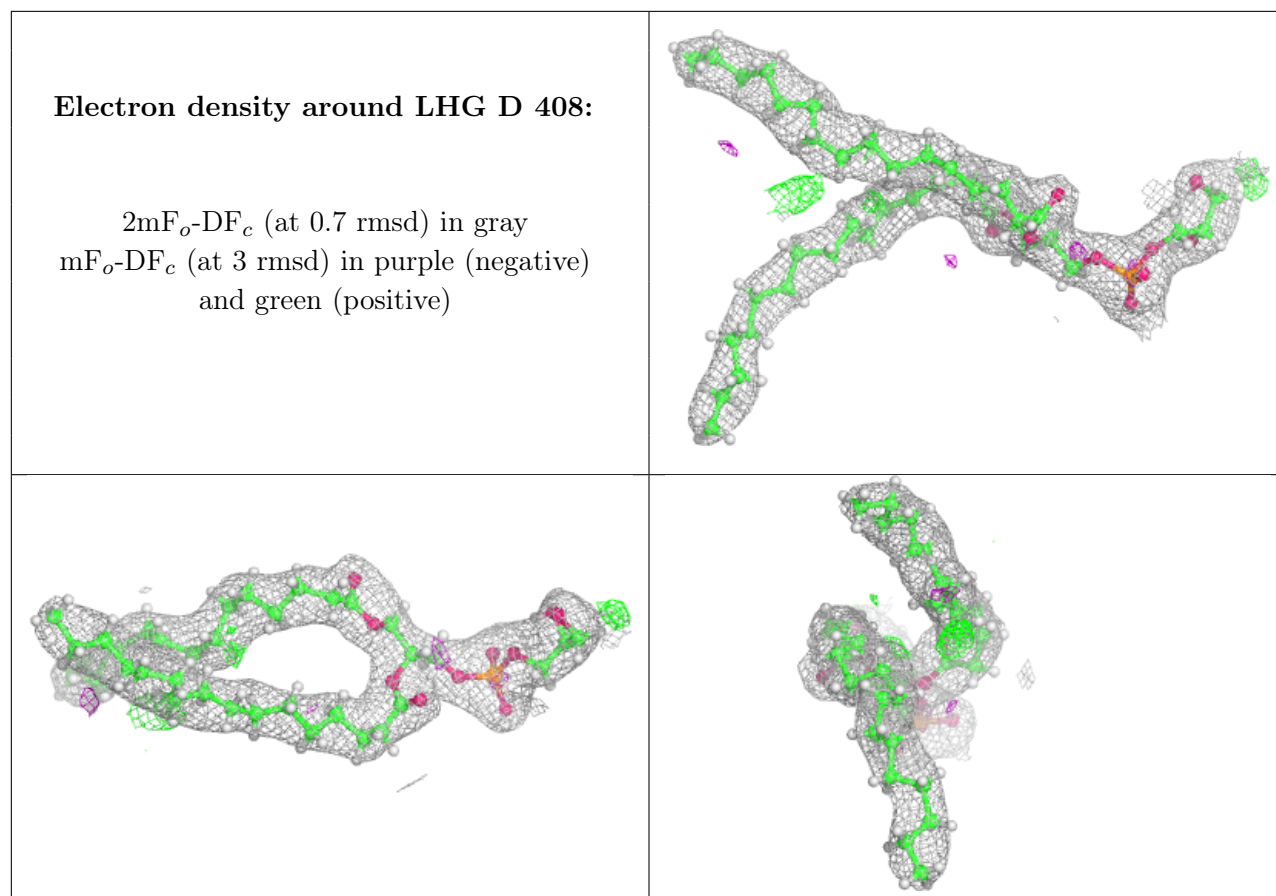


**Electron density around HEC v 201:**

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

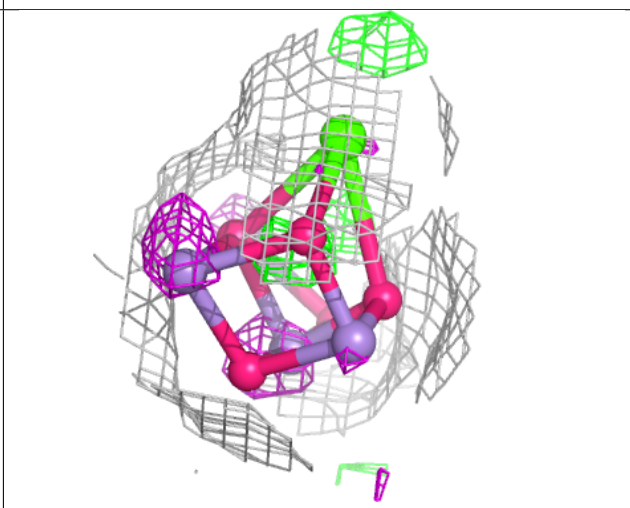
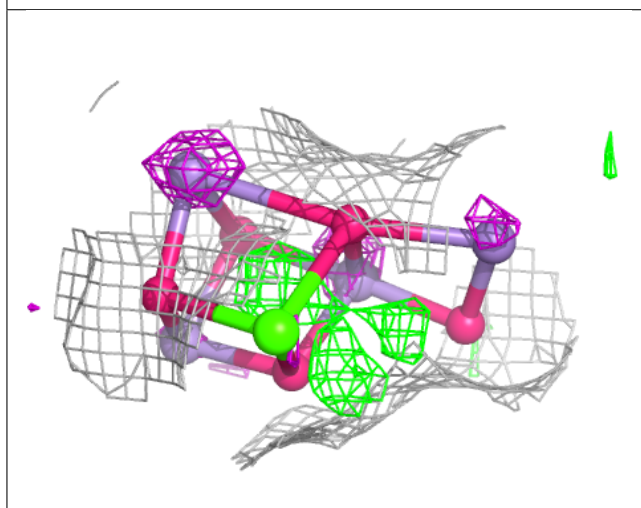
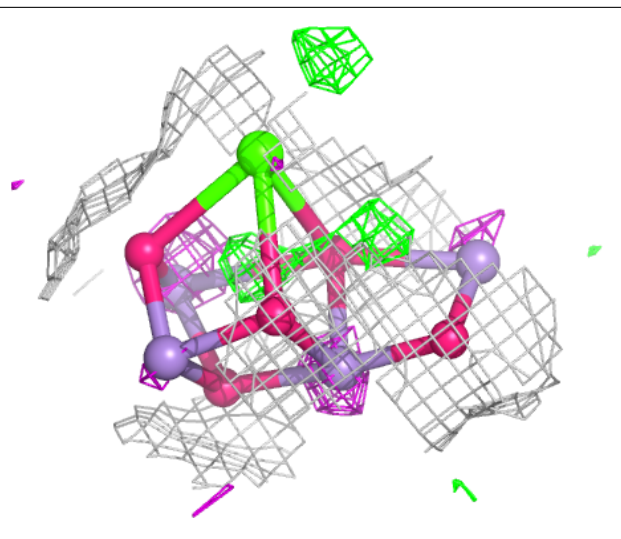






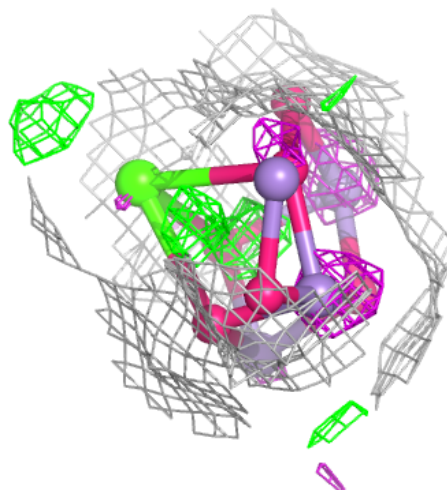
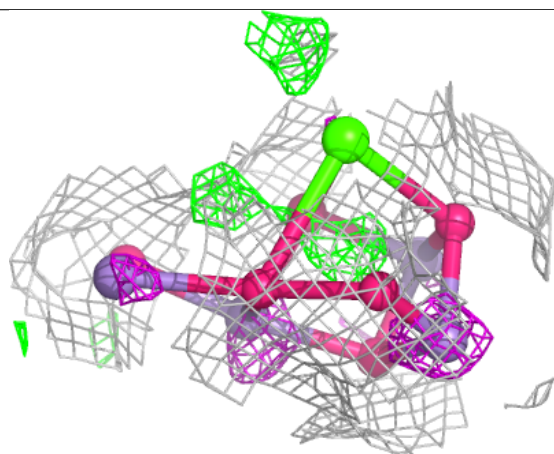
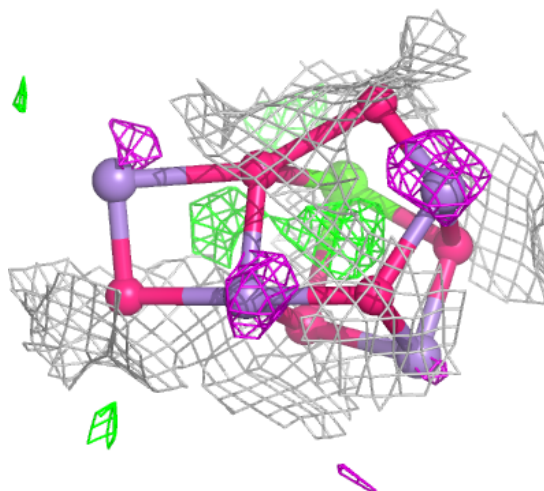
**Electron density around OEX A 416 (A):**

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



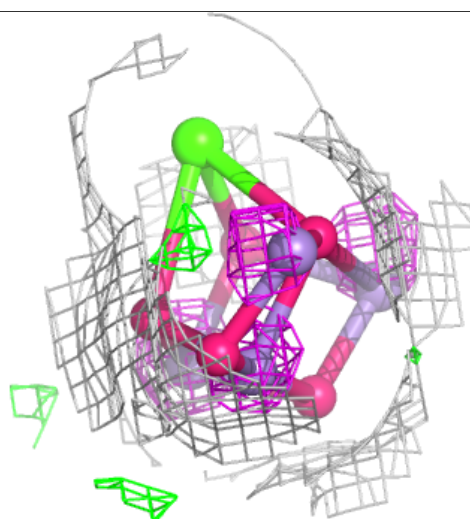
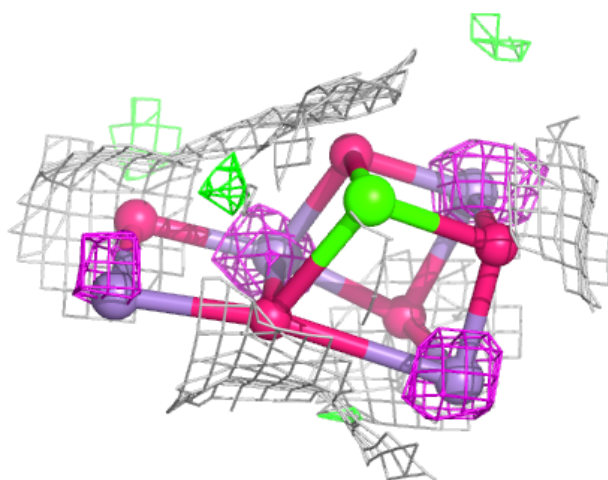
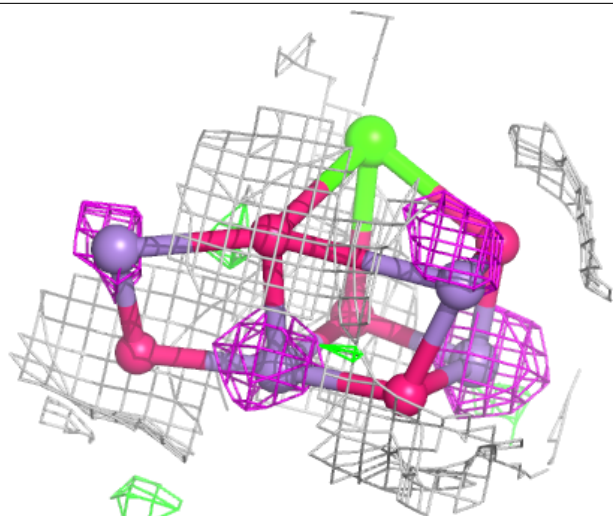
**Electron density around OEY A 415 (B):**

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



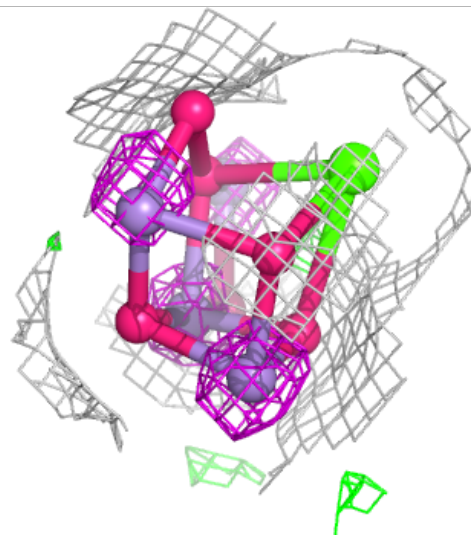
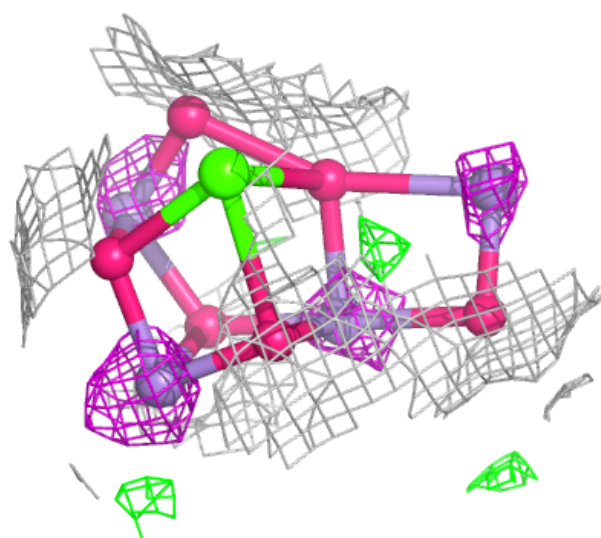
**Electron density around OEX a 416 (A):**

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



**Electron density around OEY a 415 (B):**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.