



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2024 – 01:30 PM JST

PDB ID : 8IRA  
Title : XFEL structure of cyanobacterial photosystem II following one flash (1F) with a 200-microsecond delay  
Authors : Li, H.; Suga, M.; Shen, J.R.  
Deposited on : 2023-03-17  
Resolution : 2.20 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 : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

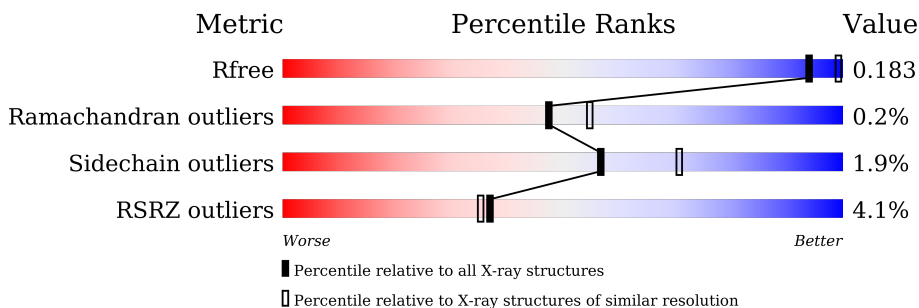
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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.



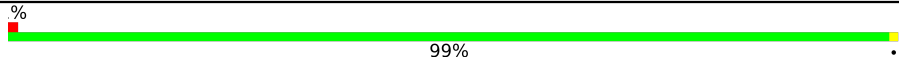
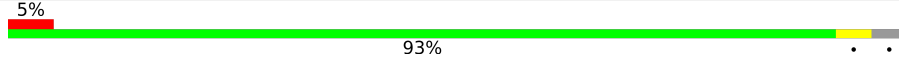
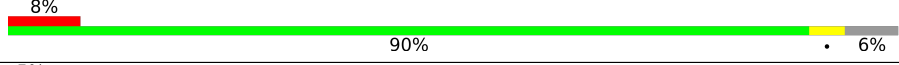

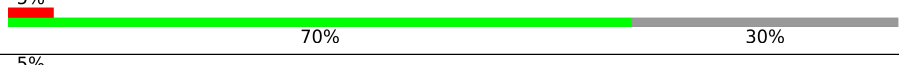
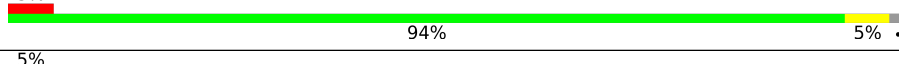
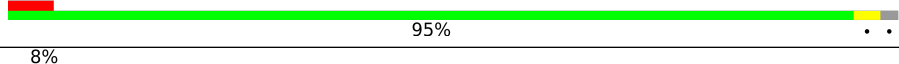
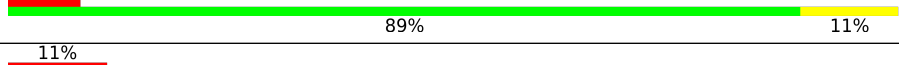
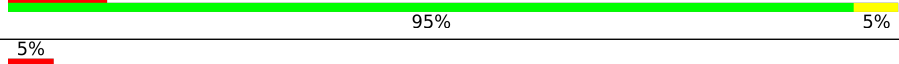
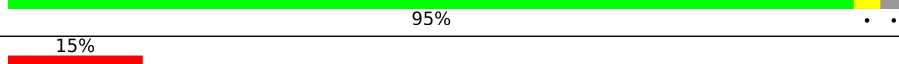
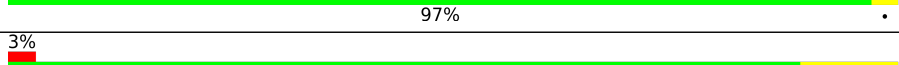
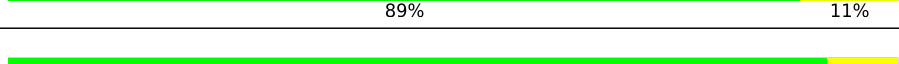
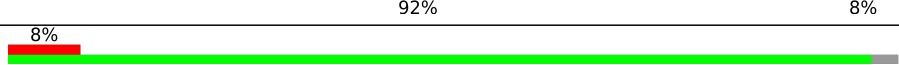
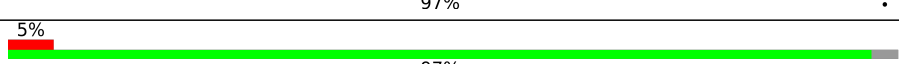
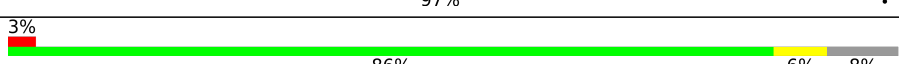
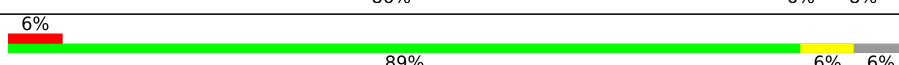
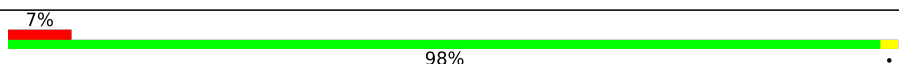
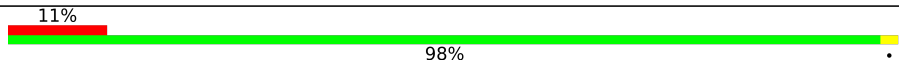
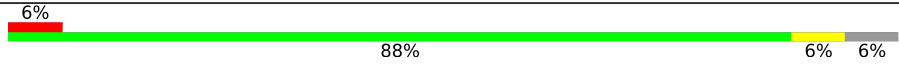
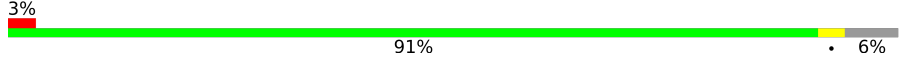
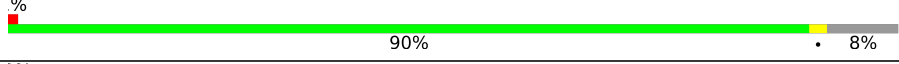
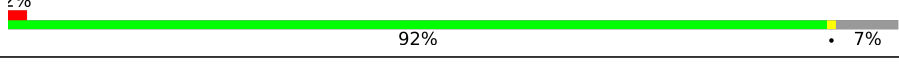
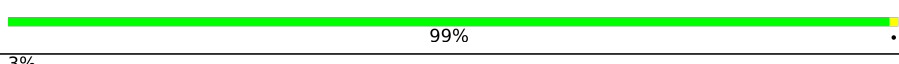
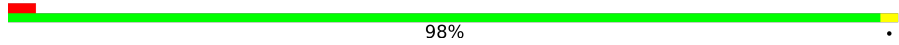

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4898 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	 2% 97% ..
1	a	344	 % 97% ..
2	B	505	 2% 99% .
2	b	505	 5% 98% .
3	C	455	 2% 98% ..
3	c	455	 3% 99% .
4	D	342	 % 99% .

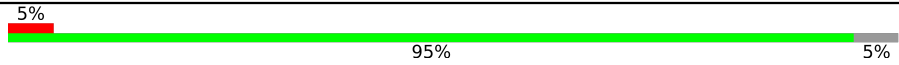
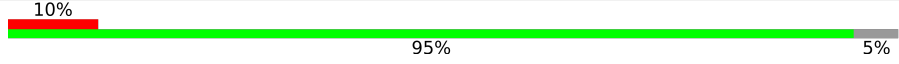
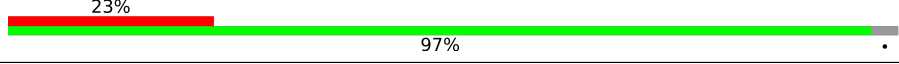
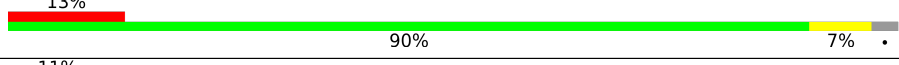
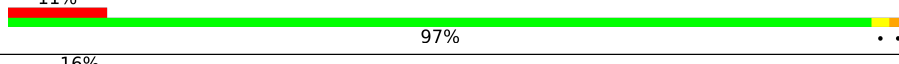
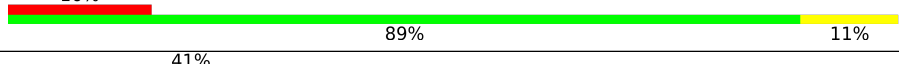
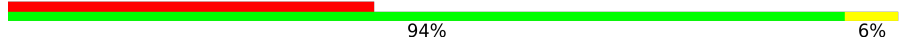
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Mol	Chain	Length	Quality of chain
4	d	342	 99%
5	E	84	 93%
5	e	84	 90% 6%
6	F	44	 77% 23%
6	f	44	 70% 30%
7	H	65	 94% 5%
7	h	65	 95%
8	I	38	 89% 11%
8	i	38	 95% 5%
9	J	39	 95%
9	j	39	 97%
10	K	37	 89% 11%
10	k	37	 92% 8%
11	L	37	 97%
11	l	37	 97%
12	M	36	 86% 6% 8%
12	m	36	 89% 6% 6%
13	O	244	 98%
13	o	244	 98%
14	T	32	 88% 6% 6%
14	t	32	 91% 6%
15	U	104	 90% 8%
15	u	104	 92% 7%
16	V	137	 99%
16	v	137	 98%

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Mol	Chain	Length	Quality of chain
17	X	40	
17	x	40	
18	Y	30	
18	y	30	
19	Z	62	
19	z	62	
20	R	34	

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
23	CLA	A	404[A]	X	-	-	-
23	CLA	A	404[B]	X	-	-	-
23	CLA	A	405[B]	X	-	-	-
23	CLA	A	408	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	D	402[A]	X	-	-	-
23	CLA	D	402[B]	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	a	404[A]	X	-	-	-
23	CLA	a	404[B]	X	-	-	-
23	CLA	a	407	X	-	-	-
23	CLA	b	601	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
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23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	c	501	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
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23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	d	402[A]	X	-	-	-
23	CLA	d	402[B]	X	-	-	-
23	CLA	d	403[A]	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	d	403[B]	X	-	-	-
23	CLA	d	404	X	-	-	-
27	GOL	D	412	-	X	-	-
27	GOL	a	417	-	-	-	X
27	GOL	l	801[A]	-	-	-	X
27	GOL	l	801[B]	-	-	-	X
31	LMT	F	101	-	-	-	X
31	LMT	e	101	-	-	-	X
34	HTG	b	623	-	-	-	X

## 2 Entry composition i

There are 41 unique types of molecules in this entry. The entry contains 62674 atoms, of which 0 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	334	4338	2836	717	760	25	0	222	0
1	a	334	4318	2821	715	757	25	0	220	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	conflict	UNP P51765
a	279	PRO	ARG	conflict	UNP P51765

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	504	4166	2735	694	724	13	0	22	0
2	b	504	4134	2718	687	716	13	0	19	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	451	4272	2796	715	743	18	0	99	0
3	c	455	4316	2827	720	751	18	0	101	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	expression tag	UNP D0VWR7
C	20	SER	-	expression tag	UNP D0VWR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	expression tag	UNP D0VWR7
C	22	PHE	-	expression tag	UNP D0VWR7
c	19	ASN	-	expression tag	UNP D0VWR7
c	20	SER	-	expression tag	UNP D0VWR7
c	21	ILE	-	expression tag	UNP D0VWR7
c	22	PHE	-	expression tag	UNP D0VWR7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	115	0
			3625	2390	597	623	15			
4	d	341	Total	C	N	O	S	0	119	0
			3658	2412	605	626	15			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	0	0
			662	432	107	123			
5	e	79	Total	C	N	O	0	2	0
			670	439	110	121			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	31	Total	C	N	O	S	0	1	0
			261	179	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	0	0
			506	339	81	84	2			
7	h	64	Total	C	N	O	S	0	1	0
			517	345	85	85	2			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total	C	N	O	S	0	0	0
			314	211	48	54	1			
8	i	38	Total	C	N	O	S	0	0	0
			314	211	48	54	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	39	Total	C	N	O	S	0	0	0
			277	185	43	48	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	N	O	0	0	0
			293	204	43	46			
10	k	37	Total	C	N	O	0	0	0
			293	204	43	46			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	conflict	UNP P19054
K	39	TRP	VAL	conflict	UNP P19054
k	33	LEU	PHE	conflict	UNP P19054
k	39	TRP	VAL	conflict	UNP P19054

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	36	Total	C	N	O	0	2	0
			311	207	49	55			
11	l	36	Total	C	N	O	0	2	0
			311	207	49	55			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			268	179	39	49	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	2	0
			286	190	43	52	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	conflict	UNP P12312
m	8	LEU	PHE	conflict	UNP P12312

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	10	0
			1958	1221	335	398	4			
13	o	243	Total	C	N	O	S	0	8	0
			1933	1207	330	392	4			

- Molecule 14 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	6	0
			311	213	48	48	2			
14	t	30	Total	C	N	O	S	0	5	0
			302	208	47	45	2			

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	96	Total	C	N	O	0	4	0
			800	508	133	159			
15	u	97	Total	C	N	O	0	5	0
			815	519	135	161			

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	6	0
			1120	711	185	220	4			
16	v	137	Total	C	N	O	S	0	6	0
			1117	712	185	216	4			

- Molecule 17 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	38	Total	C	N	O	0	1	0
			289	194	46	49			
17	x	38	Total	C	N	O	0	0	0
			281	188	45	48			

- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			
18	y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
19	z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

- Molecule 20 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	0	0	0
			273	186	47	40			

- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total	Fe	0	1
			2	2		
21	a	1	Total	Fe	0	1
			2	2		

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

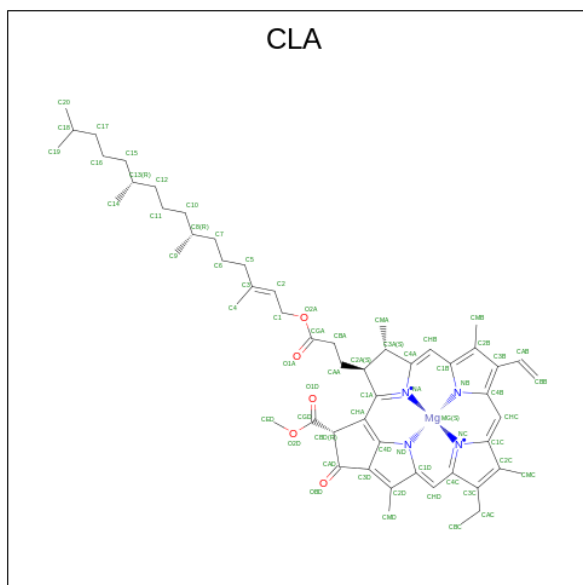
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	2
			4	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	a	2	Total Cl 4 4	0	2

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
23	A	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	A	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	A	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
23	B	1	65	55	1	4	5	0	0
23	B	1	65	55	1	4	5	0	0
23	B	1	65	55	1	4	5	0	0
23	B	1	65	55	1	4	5	0	0
23	B	1	65	55	1	4	5	0	0
23	B	1	65	55	1	4	5	0	0
23	B	1	65	55	1	4	5	0	0
23	B	1	65	55	1	4	5	0	0
23	B	1	65	55	1	4	5	0	0
23	B	1	65	55	1	4	5	0	0
23	B	1	65	55	1	4	5	0	0
23	B	1	65	55	1	4	5	0	0
23	C	1	65	55	1	4	5	0	0
23	C	1	65	55	1	4	5	0	0
23	C	1	65	55	1	4	5	0	0
23	C	1	65	55	1	4	5	0	0
23	C	1	65	55	1	4	5	0	0
23	C	1	65	55	1	4	5	0	0
23	C	1	65	55	1	4	5	0	0
23	C	1	65	55	1	4	5	0	0
23	C	1	65	55	1	4	5	0	0
23	C	1	65	55	1	4	5	0	0
23	C	1	65	55	1	4	5	0	0
23	C	1	65	55	1	4	5	0	0

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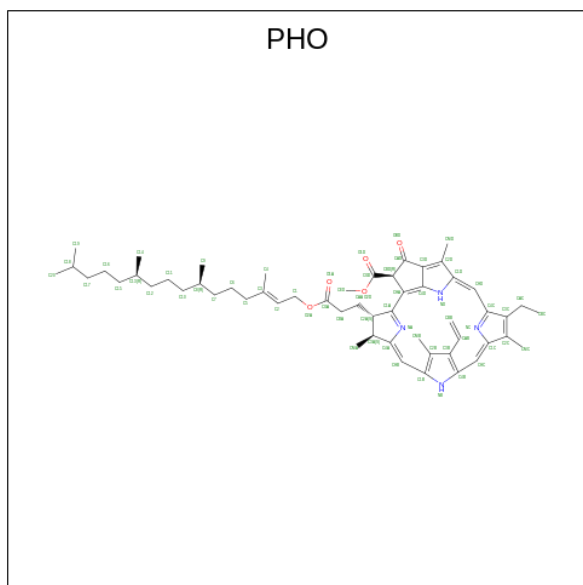
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	D	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	a	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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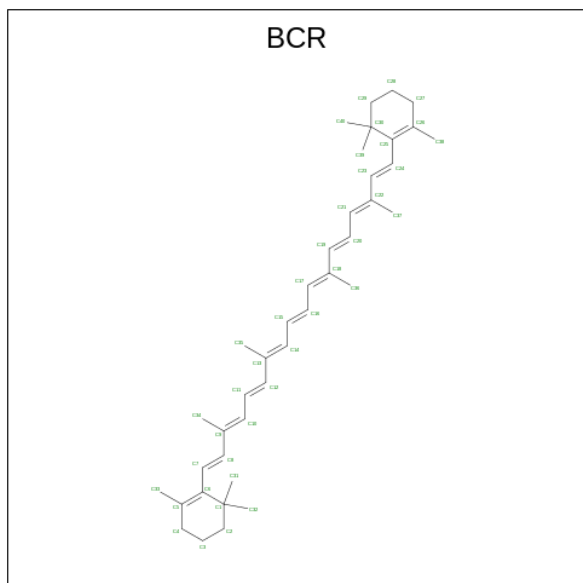
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	d	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	1
			128	110	8	10		

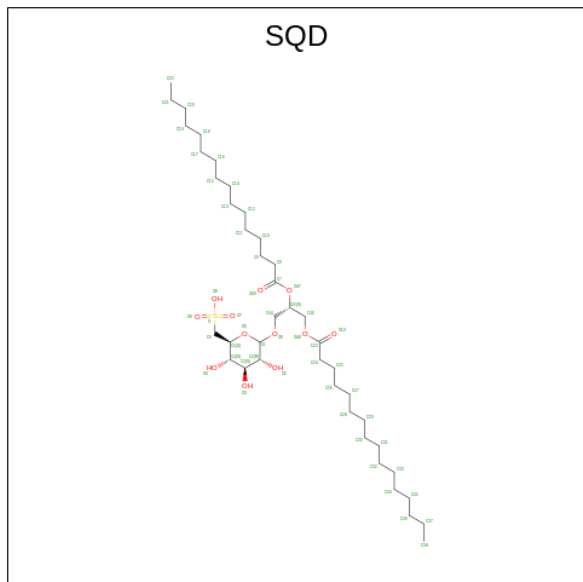
- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).





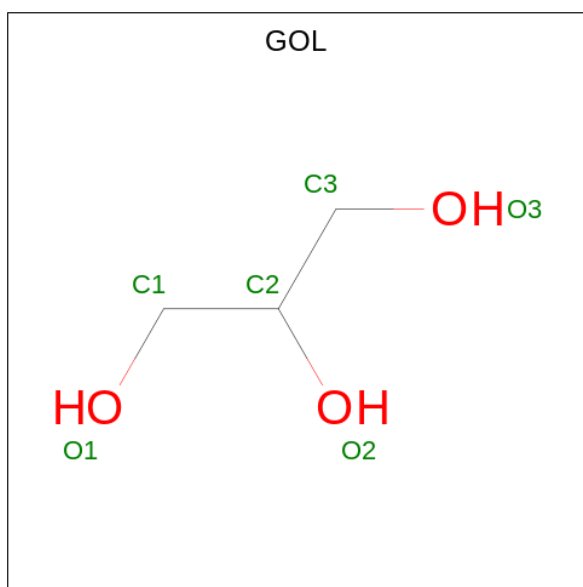
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total C 40 40	0	0
25	a	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	d	1	Total C 40 40	0	0
25	h	1	Total C 40 40	0	0
25	k	1	Total C 40 40	0	0
25	t	1	Total C 40 40	0	0
25	y	1	Total C 40 40	0	0

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
26	A	1	Total 108	C 82	O 24	S 2	0	1
26	A	1	Total 54	C 41	O 12	S 1	0	0
26	B	1	Total 54	C 41	O 12	S 1	0	0
26	F	1	Total 43	C 30	O 12	S 1	0	0
26	a	1	Total 108	C 82	O 24	S 2	0	1
26	a	1	Total 54	C 41	O 12	S 1	0	0
26	b	1	Total 54	C 41	O 12	S 1	0	0
26	f	1	Total 43	C 30	O 12	S 1	0	0

- Molecule 27 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



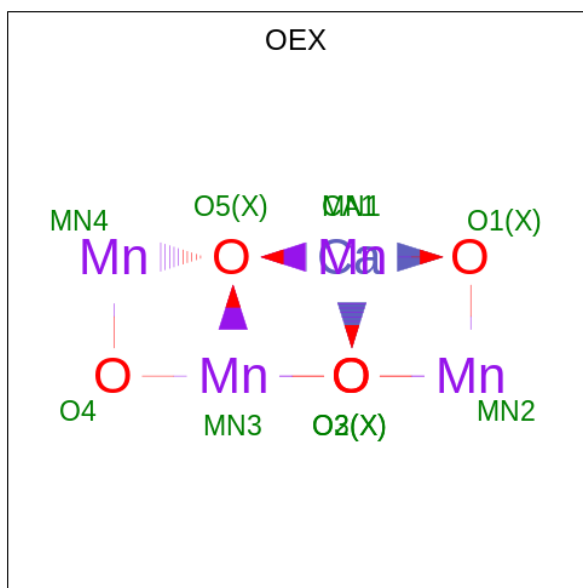
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 6 3 3	0	0
27	A	1	Total C O 6 3 3	0	0
27	B	1	Total C O 6 3 3	0	0
27	B	1	Total C O 6 3 3	0	0
27	B	1	Total C O 6 3 3	0	0
27	C	1	Total C O 12 6 6	0	1
27	D	1	Total C O 6 3 3	0	0
27	O	1	Total C O 6 3 3	0	0
27	O	1	Total C O 6 3 3	0	0
27	V	1	Total C O 12 6 6	0	1
27	a	1	Total C O 6 3 3	0	0
27	a	1	Total C O 6 3 3	0	0
27	b	1	Total C O 6 3 3	0	0
27	b	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	c	1	Total	C	O	0	1
			12	6	6		
27	c	1	Total	C	O	0	0
			6	3	3		
27	d	1	Total	C	O	0	0
			6	3	3		
27	l	1	Total	C	O	0	1
			12	6	6		
27	o	1	Total	C	O	0	0
			6	3	3		
27	o	1	Total	C	O	0	0
			6	3	3		
27	v	1	Total	C	O	0	1
			12	6	6		

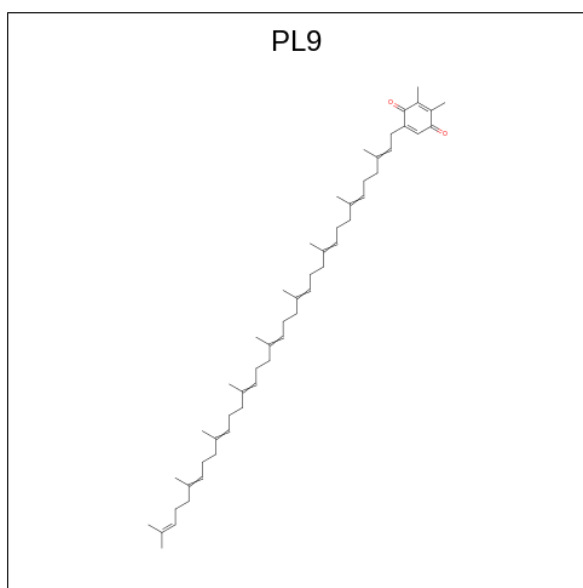
- Molecule 28 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	Ca	Mn	O	0	1
			20	2	8	10		
28	a	1	Total	Ca	Mn	O	0	1
			20	2	8	10		

- Molecule 29 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>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	1
			110	106	4		
29	D	1	Total	C	O	0	1
			110	106	4		
29	a	1	Total	C	O	0	1
			110	106	4		
29	d	1	Total	C	O	0	1
			110	106	4		

- Molecule 30 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

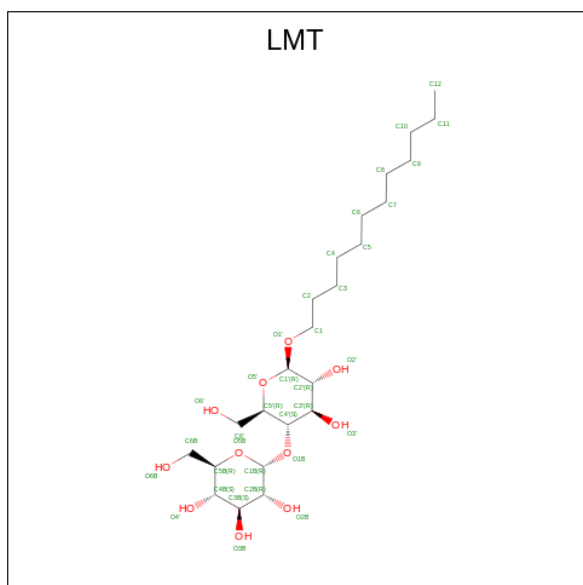
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			28	23	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	I	1	Total	C	O	0	0
			40	35	5		
30	J	1	Total	C		0	0
			10	10			
30	K	1	Total	C	O	0	1
			68	58	10		
30	M	1	Total	C		0	0
			10	10			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	X	1	Total	C	O	0	0
			18	16	2		
30	a	1	Total	C	O	0	0
			30	25	5		
30	b	1	Total	C	O	0	0
			33	28	5		
30	c	1	Total	C	O	0	1
			64	54	10		
30	d	2	Total	C	O	0	0
			53	47	6		
30	i	1	Total	C	O	0	0
			40	35	5		
30	j	1	Total	C		0	0
			10	10			
30	m	1	Total	C		0	0
			10	10			
30	x	1	Total	C	O	0	0
			18	16	2		

- Molecule 31 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



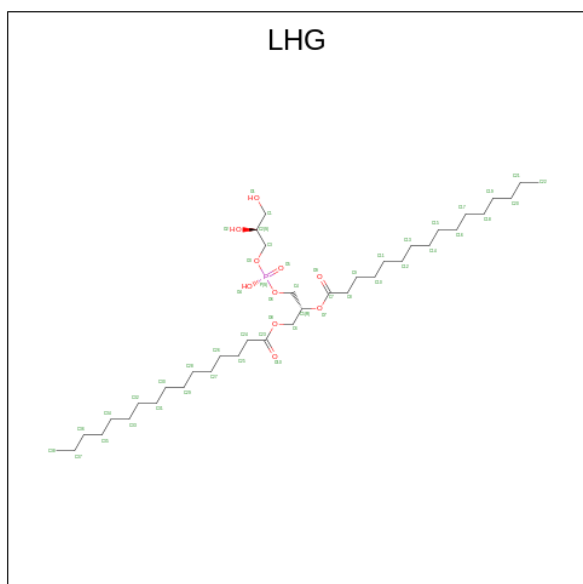
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			35	24	11		
31	A	1	Total	C	O	0	0
			35	24	11		

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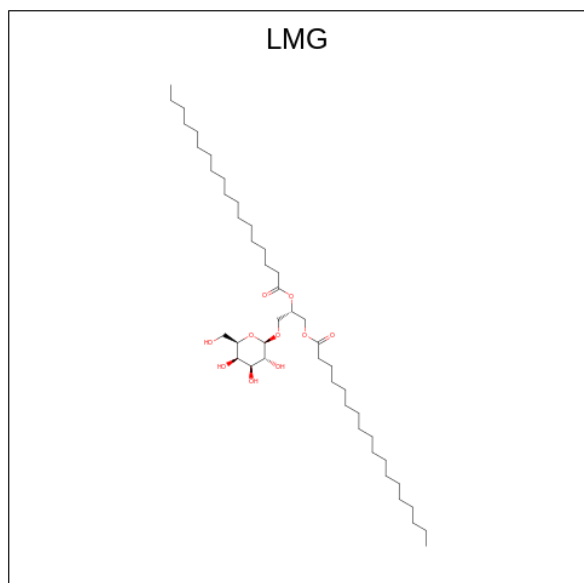
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			25	19	6		
31	F	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total	C	O	0	0
			35	24	11		
31	T	1	Total	C	O	0	0
			35	24	11		
31	a	1	Total	C	O	0	0
			35	24	11		
31	b	1	Total	C	O	0	0
			25	19	6		
31	b	1	Total	C	O	0	0
			25	19	6		
31	e	1	Total	C	O	0	0
			35	24	11		
31	m	1	Total	C	O	0	0
			35	24	11		
31	t	1	Total	C	O	0	0
			26	19	7		

- Molecule 32 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	O	P		
32	A	1	98	76	20	2	0	1
32	D	1	98	76	20	2	0	1
32	D	1	98	76	20	2	0	1
32	E	1	84	62	20	2	0	1
32	L	1	98	76	20	2	0	1
32	a	1	84	62	20	2	0	1
32	b	1	98	76	20	2	0	1
32	d	1	98	76	20	2	0	1
32	d	1	98	76	20	2	0	1
32	d	1	98	76	20	2	0	1

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
33	B	1	51	41	10	0	0

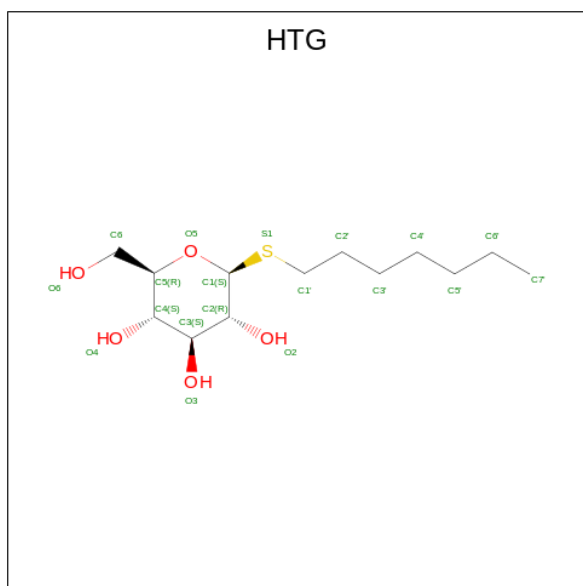
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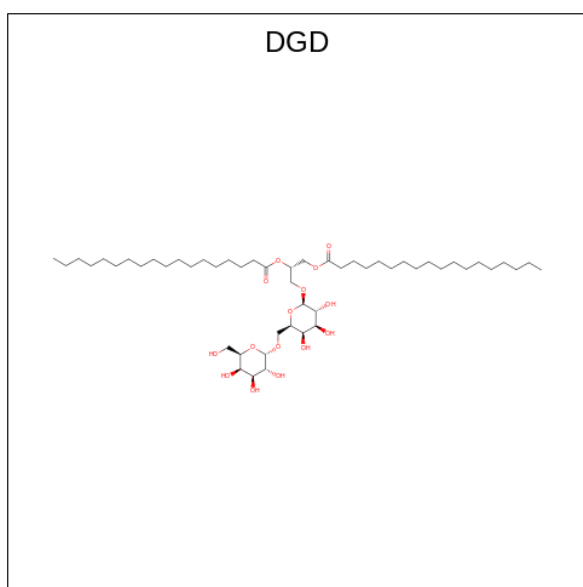
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	D	1	Total	C	O	0	0
			51	41	10		
33	a	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	d	1	Total	C	O	0	0
			51	41	10		
33	m	1	Total	C	O	0	0
			51	41	10		
33	Z	1	Total	C	O	0	0
			37	27	10		
33	z	1	Total	C	O	0	0
			39	29	10		

- Molecule 34 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula:  $C_{13}H_{26}O_5S$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	B	1	Total C O S 19 13 5 1	0	0
34	B	1	Total C O S 19 13 5 1	0	0
34	B	1	Total C O S 19 13 5 1	0	0
34	C	1	Total C O S 19 13 5 1	0	0
34	D	1	Total C O S 16 10 5 1	0	0
34	V	1	Total C O 11 6 5	0	0
34	b	1	Total C O S 19 13 5 1	0	0
34	b	1	Total C O S 19 13 5 1	0	0
34	b	1	Total C O S 19 13 5 1	0	0
34	c	1	Total C O S 19 13 5 1	0	0
34	d	1	Total C O S 16 10 5 1	0	0

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).

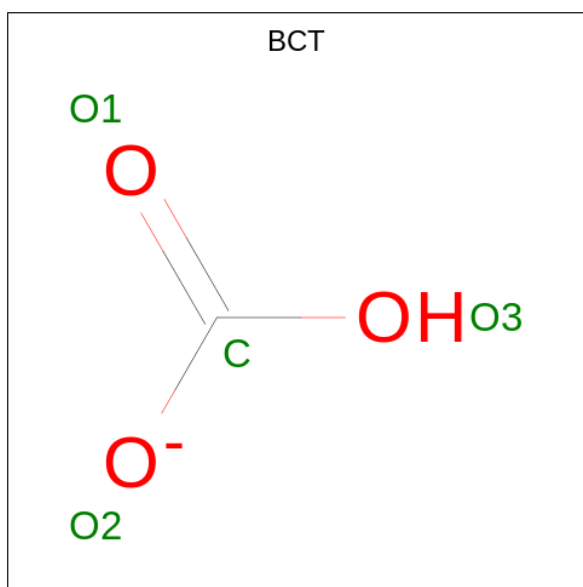


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	C	1	Total C O 124 94 30	0	1
35	C	1	Total C O 124 94 30	0	1
35	C	1	Total C O 62 47 15	0	0
35	H	1	Total C O 62 47 15	0	0
35	c	1	Total C O 124 94 30	0	1
35	c	1	Total C O 124 94 30	0	1
35	c	1	Total C O 62 47 15	0	0
35	h	1	Total C O 62 47 15	0	0

- Molecule 36 is CALCIUM ION (three-letter code: CA) (formula: Ca).

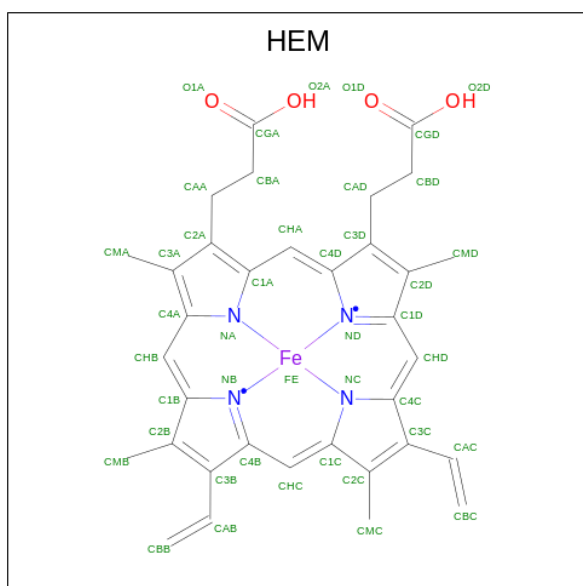
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	C	1	Total Ca 1 1	0	0
36	F	1	Total Ca 1 1	0	0
36	O	1	Total Ca 1 1	0	0
36	c	2	Total Ca 2 2	0	0
36	f	1	Total Ca 1 1	0	0
36	o	1	Total Ca 1 1	0	0

- Molecule 37 is BICARBONATE ION (three-letter code: BCT) (formula: CHO<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	D	1	Total	C	O	0	1
			8	2	6		
37	d	1	Total	C	O	0	1
			8	2	6		

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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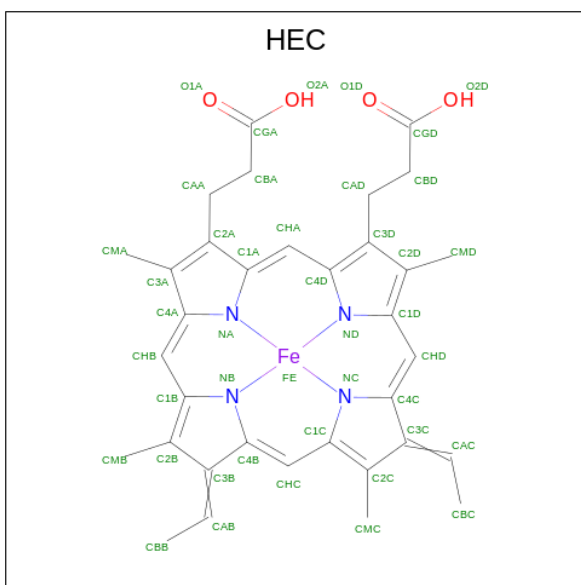
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
38	f	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 39 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	J	1	Total	Mg	0	0
			1	1		
39	j	1	Total	Mg	0	0
			1	1		

- Molecule 40 is HEME C (three-letter code: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
40	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
40	v	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	142	Total	O	0	86
			227	227		
41	B	187	Total	O	0	2
			189	189		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	C	169	Total O 206 206	0	38
41	D	120	Total O 155 155	0	35
41	E	17	Total O 17 17	0	0
41	F	4	Total O 4 4	0	0
41	H	22	Total O 22 22	0	0
41	I	4	Total O 4 4	0	0
41	J	6	Total O 6 6	0	0
41	K	5	Total O 5 5	0	0
41	L	9	Total O 10 10	0	1
41	M	6	Total O 6 6	0	0
41	O	104	Total O 108 108	0	4
41	T	11	Total O 14 14	0	3
41	U	47	Total O 49 49	0	2
41	V	79	Total O 80 80	0	1
41	X	7	Total O 7 7	0	0
41	a	131	Total O 211 211	0	81
41	b	201	Total O 204 204	0	3
41	c	160	Total O 193 193	0	34
41	d	117	Total O 149 149	0	32
41	e	8	Total O 8 8	0	0
41	f	3	Total O 3 3	0	0

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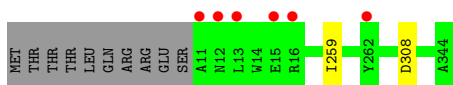
*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	h	17	Total O 17 17	0	0
41	i	2	Total O 2 2	0	0
41	j	1	Total O 1 1	0	0
41	k	3	Total O 3 3	0	0
41	l	8	Total O 10 10	0	2
41	m	13	Total O 13 13	0	0
41	o	99	Total O 103 103	0	4
41	t	8	Total O 11 11	0	3
41	u	51	Total O 52 52	0	1
41	v	56	Total O 58 58	0	2
41	x	6	Total O 6 6	0	0
41	y	2	Total O 2 2	0	0

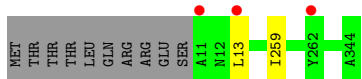
### 3 Residue-property plots [i](#)

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



- Molecule 1: Photosystem II protein D1



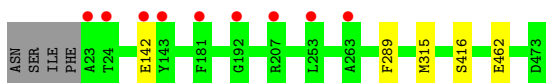
- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein

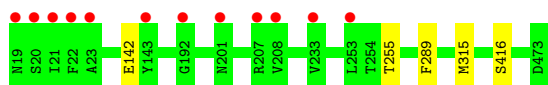


- Molecule 3: Photosystem II CP43 reaction center protein

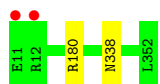


- Molecule 3: Photosystem II CP43 reaction center protein





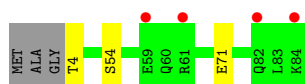
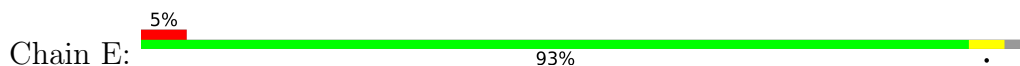
- Molecule 4: Photosystem II D2 protein



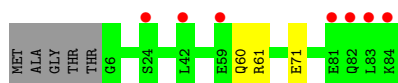
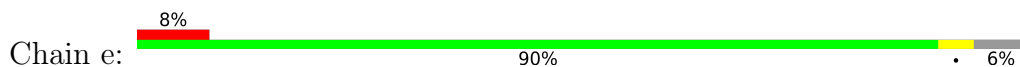
- Molecule 4: Photosystem II D2 protein



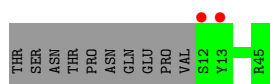
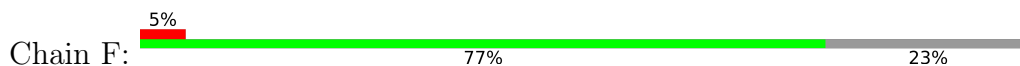
- Molecule 5: Cytochrome b559 subunit alpha



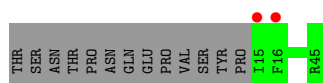
- Molecule 5: Cytochrome b559 subunit alpha



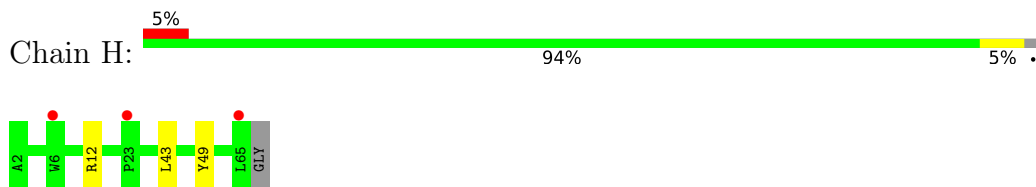
- Molecule 6: Cytochrome b559 subunit beta



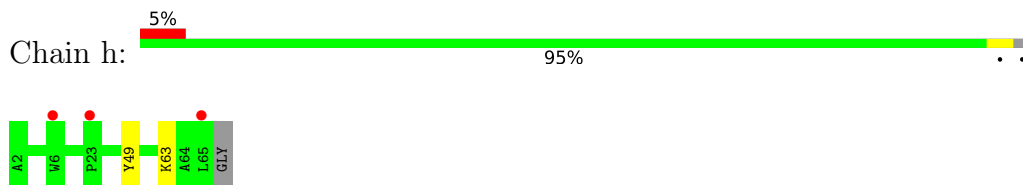
- Molecule 6: Cytochrome b559 subunit beta



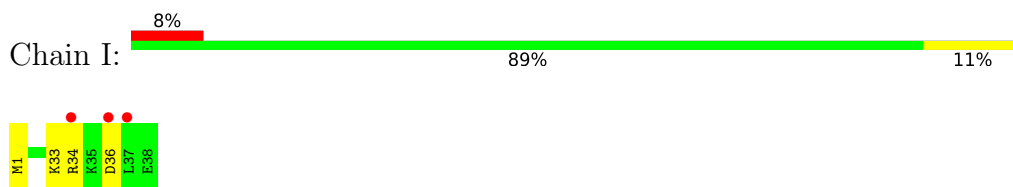
- Molecule 7: Photosystem II reaction center protein H



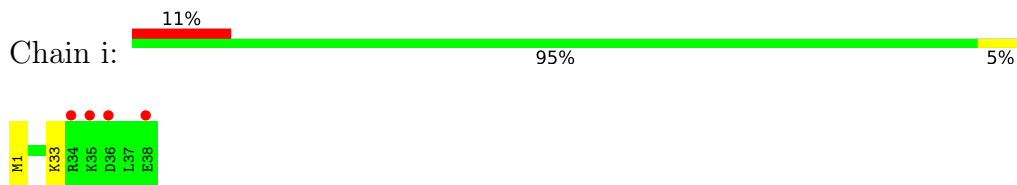
- Molecule 7: Photosystem II reaction center protein H



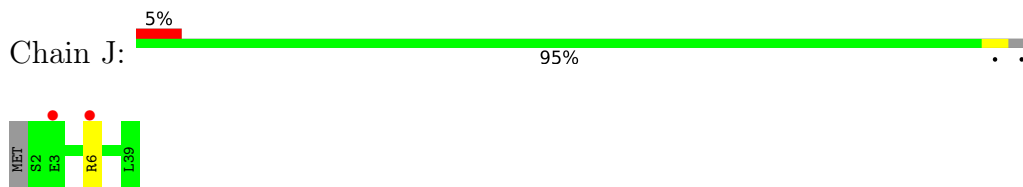
- Molecule 8: Photosystem II reaction center protein I



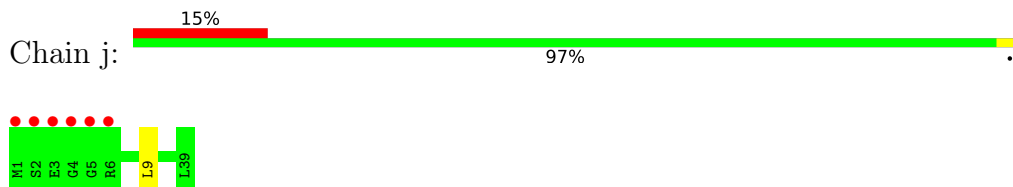
- Molecule 8: Photosystem II reaction center protein I



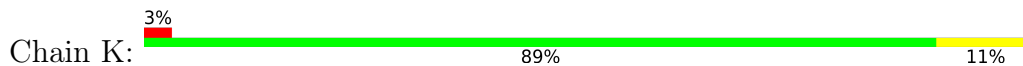
- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J

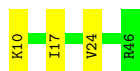


- Molecule 10: Photosystem II reaction center protein K

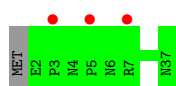




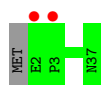
- Molecule 10: Photosystem II reaction center protein K



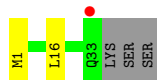
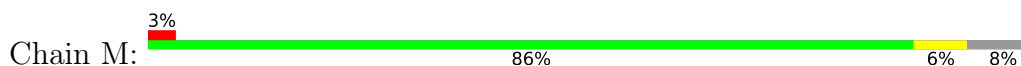
- Molecule 11: Photosystem II reaction center protein L



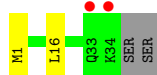
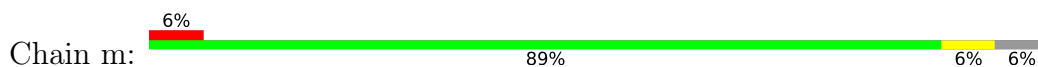
- Molecule 11: Photosystem II reaction center protein L



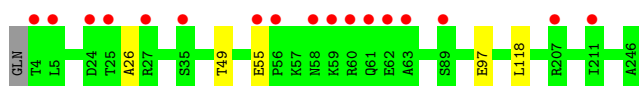
- Molecule 12: Photosystem II reaction center protein M



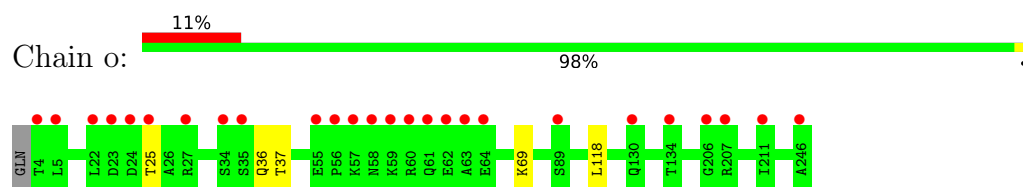
- Molecule 12: Photosystem II reaction center protein M



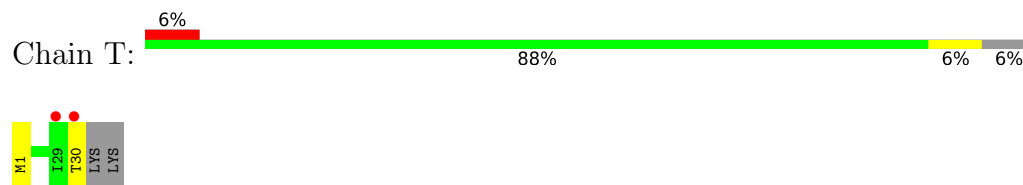
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



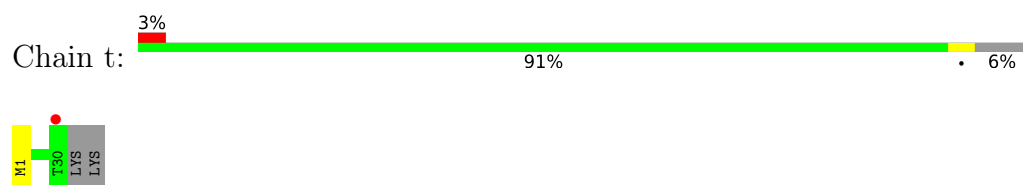
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



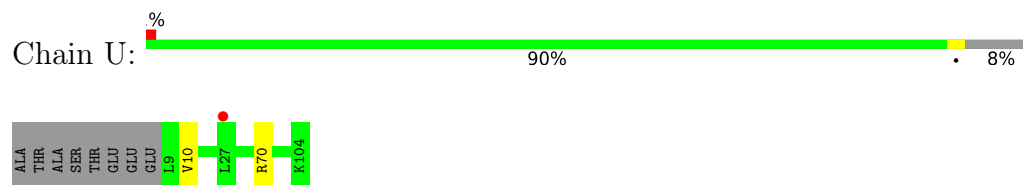
- Molecule 14: Photosystem II reaction center protein T



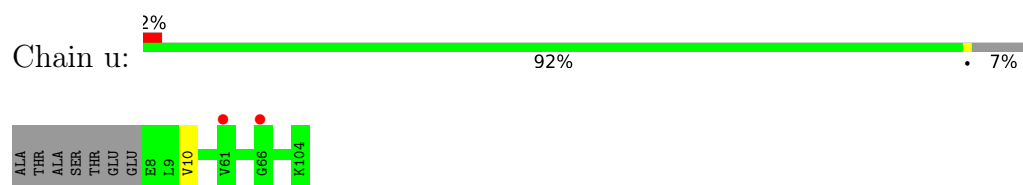
- Molecule 14: Photosystem II reaction center protein T



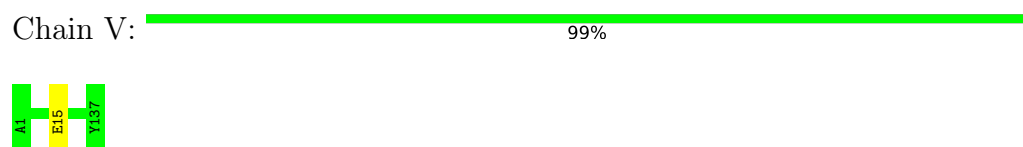
- Molecule 15: Photosystem II 12 kDa extrinsic protein



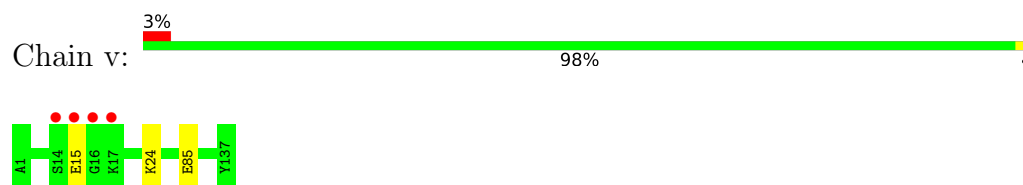
- Molecule 15: Photosystem II 12 kDa extrinsic protein



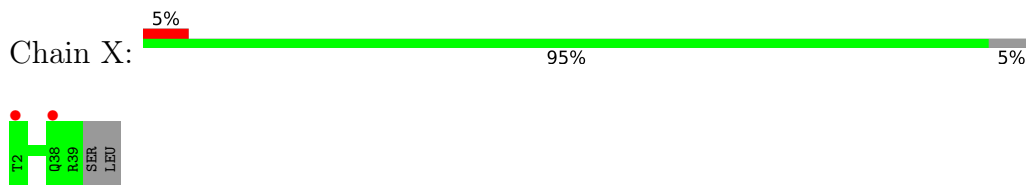
- Molecule 16: Cytochrome c-550



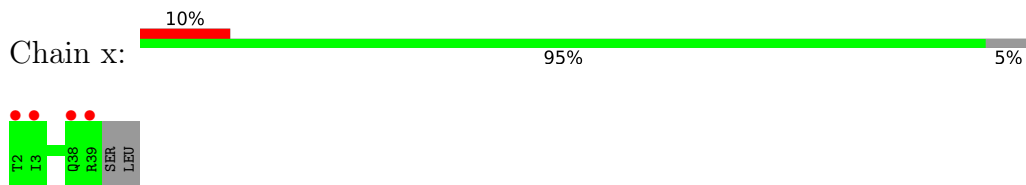
- Molecule 16: Cytochrome c-550



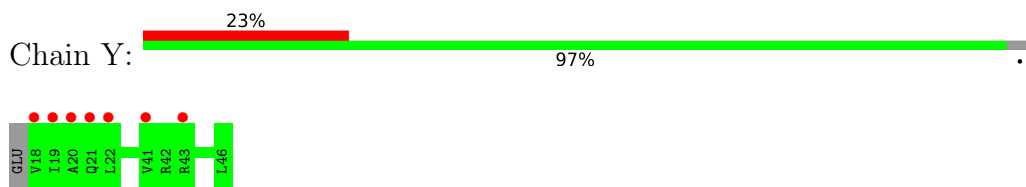
- Molecule 17: Photosystem II reaction center protein X



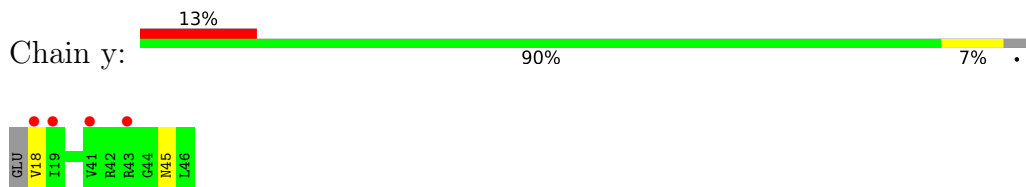
- Molecule 17: Photosystem II reaction center protein X



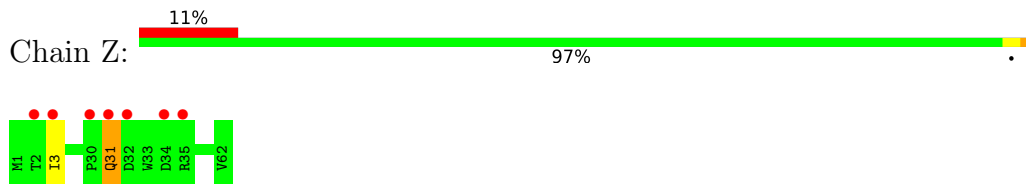
- Molecule 18: Photosystem II reaction center protein Ycf12



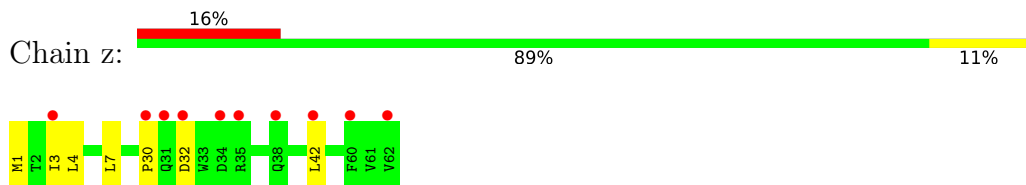
- Molecule 18: Photosystem II reaction center protein Ycf12



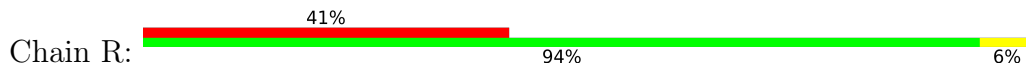
- Molecule 19: Photosystem II reaction center protein Z

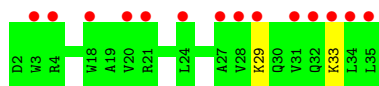


- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.75Å 231.60Å 288.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.20 19.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.98-2.20) 99.9 (19.98-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 2.19Å)	Xtrriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, $R_{free}$	0.142 , 0.178 0.153 , 0.183	Depositor DCC
$R_{free}$ test set	21144 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.0	Xtrriage
Anisotropy	0.485	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 81.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	62674	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% 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

### 5.1 Standard geometry

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

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	0.43	0/4478	0.58	1/6098 (0.0%)
1	a	0.42	0/4457	0.57	0/6069
2	B	0.43	0/4314	0.58	0/5879
2	b	0.41	0/4285	0.57	0/5841
3	C	0.40	0/4416	0.55	0/6013
3	c	0.41	0/4467	0.54	0/6082
4	D	0.46	0/3746	0.60	0/5102
4	d	0.44	0/3780	0.58	0/5147
5	E	0.40	0/681	0.57	0/928
5	e	0.38	0/690	0.54	0/939
6	F	0.40	0/284	0.54	0/387
6	f	0.36	0/269	0.50	0/365
7	H	0.39	0/519	0.58	0/708
7	h	0.36	0/530	0.58	0/722
8	I	0.38	0/311	0.51	0/419
8	i	0.39	0/311	0.56	0/419
9	J	0.38	0/278	0.52	0/376
9	j	0.36	0/283	0.54	0/383
10	K	0.37	0/303	0.51	0/416
10	k	0.38	0/303	0.51	0/416
11	L	0.42	0/318	0.56	0/433
11	l	0.44	0/318	0.54	0/433
12	M	0.45	0/261	0.53	0/357
12	m	0.40	0/279	0.52	0/380
13	O	0.41	0/1991	0.64	0/2698
13	o	0.40	0/1966	0.63	0/2665
14	T	0.46	0/310	0.60	0/419
14	t	0.48	0/301	0.58	0/406
15	U	0.44	0/811	0.62	0/1095
15	u	0.44	0/826	0.61	0/1116
16	V	0.40	0/1142	0.57	0/1545



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	v	0.37	0/1139	0.54	0/1542
17	X	0.32	0/292	0.50	0/395
17	x	0.34	0/284	0.49	0/384
18	Y	0.32	0/216	0.54	0/289
18	y	0.30	0/216	0.49	0/289
19	Z	0.32	0/490	0.45	0/669
19	z	0.32	0/490	0.42	0/669
20	R	0.32	0/279	0.52	0/383
All	All	0.41	0/50634	0.57	1/68876 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	308	ASP	CB-CG-OD1	5.49	123.24	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	553/344 (161%)	544 (98%)	7 (1%)	2 (0%)	34	37
1	a	551/344 (160%)	540 (98%)	9 (2%)	2 (0%)	34	37
2	B	524/505 (104%)	517 (99%)	7 (1%)	0	100	100
2	b	521/505 (103%)	507 (97%)	14 (3%)	0	100	100

*Continued on next page...*

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	548/455 (120%)	540 (98%)	7 (1%)	1 (0%)	47	55
3	c	554/455 (122%)	545 (98%)	8 (1%)	1 (0%)	47	55
4	D	454/342 (133%)	439 (97%)	15 (3%)	0	100	100
4	d	457/342 (134%)	446 (98%)	11 (2%)	0	100	100
5	E	79/84 (94%)	78 (99%)	1 (1%)	0	100	100
5	e	79/84 (94%)	79 (100%)	0	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	62/65 (95%)	62 (100%)	0	0	100	100
7	h	63/65 (97%)	60 (95%)	2 (3%)	1 (2%)	9	7
8	I	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	5	2
8	i	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	37 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
13	O	251/244 (103%)	242 (96%)	8 (3%)	1 (0%)	34	37
13	o	249/244 (102%)	244 (98%)	5 (2%)	0	100	100
14	T	33/32 (103%)	33 (100%)	0	0	100	100
14	t	32/32 (100%)	32 (100%)	0	0	100	100
15	U	97/104 (93%)	93 (96%)	4 (4%)	0	100	100
15	u	99/104 (95%)	94 (95%)	5 (5%)	0	100	100
16	V	140/137 (102%)	136 (97%)	4 (3%)	0	100	100
16	v	140/137 (102%)	135 (96%)	5 (4%)	0	100	100
17	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
17	x	36/40 (90%)	36 (100%)	0	0	100	100
18	Y	27/30 (90%)	24 (89%)	3 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	y	27/30 (90%)	27 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9	6
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	9	6
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	6180/5384 (115%)	6042 (98%)	127 (2%)	11 (0%)	47	55

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	I	36	ASP
3	C	416	SER
13	O	26	ALA
3	c	416	SER
19	Z	31	GLN
19	z	30	PRO
7	h	63	LYS
1	a	259[A]	ILE
1	a	259[B]	ILE
1	A	259[A]	ILE
1	A	259[B]	ILE

### 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	444/279 (159%)	444 (100%)	0	100	100
1	a	442/279 (158%)	441 (100%)	1 (0%)	93	97
2	B	423/403 (105%)	418 (99%)	5 (1%)	71	83
2	b	420/403 (104%)	410 (98%)	10 (2%)	49	62
3	C	431/356 (121%)	426 (99%)	5 (1%)	71	83
3	c	437/356 (123%)	432 (99%)	5 (1%)	73	85
4	D	368/277 (133%)	366 (100%)	2 (0%)	88	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	d	372/277 (134%)	368 (99%)	4 (1%)	73	85
5	E	72/73 (99%)	69 (96%)	3 (4%)	30	38
5	e	72/73 (99%)	69 (96%)	3 (4%)	30	38
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	26/38 (68%)	26 (100%)	0	100	100
7	H	54/54 (100%)	51 (94%)	3 (6%)	21	25
7	h	55/54 (102%)	54 (98%)	1 (2%)	59	72
8	I	34/34 (100%)	32 (94%)	2 (6%)	19	23
8	i	34/34 (100%)	33 (97%)	1 (3%)	42	54
9	J	26/27 (96%)	25 (96%)	1 (4%)	33	42
9	j	26/27 (96%)	25 (96%)	1 (4%)	33	42
10	K	30/30 (100%)	26 (87%)	4 (13%)	4	3
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	7
11	L	36/35 (103%)	36 (100%)	0	100	100
11	l	36/35 (103%)	36 (100%)	0	100	100
12	M	30/32 (94%)	28 (93%)	2 (7%)	16	18
12	m	32/32 (100%)	30 (94%)	2 (6%)	18	20
13	O	216/207 (104%)	212 (98%)	4 (2%)	57	71
13	o	213/207 (103%)	208 (98%)	5 (2%)	50	63
14	T	32/28 (114%)	30 (94%)	2 (6%)	18	20
14	t	31/28 (111%)	31 (100%)	0	100	100
15	U	86/89 (97%)	84 (98%)	2 (2%)	50	63
15	u	88/89 (99%)	86 (98%)	2 (2%)	50	63
16	V	123/117 (105%)	122 (99%)	1 (1%)	81	90
16	v	123/117 (105%)	120 (98%)	3 (2%)	49	62
17	X	32/33 (97%)	32 (100%)	0	100	100
17	x	31/33 (94%)	31 (100%)	0	100	100
18	Y	22/23 (96%)	22 (100%)	0	100	100
18	y	22/23 (96%)	20 (91%)	2 (9%)	9	9
19	Z	52/52 (100%)	50 (96%)	2 (4%)	33	42
19	z	52/52 (100%)	46 (88%)	6 (12%)	5	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	R	29/29 (100%)	27 (93%)	2 (7%)	15	16
All	All	5110/4403 (116%)	5021 (98%)	89 (2%)	57	74

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	294	SER
2	B	362	PHE
2	B	389	LYS
2	B	419	SER
2	B	472	ARG
3	C	142	GLU
3	C	289	PHE
3	C	315[A]	MET
3	C	315[B]	MET
3	C	462	GLU
4	D	180	ARG
4	D	338	ASN
5	E	4	THR
5	E	54	SER
5	E	71	GLU
7	H	12	ARG
7	H	43	LEU
7	H	49	TYR
8	I	33	LYS
8	I	34	ARG
9	J	6	ARG
10	K	10	LYS
10	K	17	ILE
10	K	19	ASP
10	K	27	VAL
12	M	16[A]	LEU
12	M	16[B]	LEU
13	O	49	THR
13	O	55	GLU
13	O	97	GLU
13	O	118	LEU
14	T	30[A]	THR
14	T	30[B]	THR
15	U	10	VAL
15	U	70	ARG
16	V	15	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	a	13	LEU
2	b	127	ARG
2	b	128	THR
2	b	161	LEU
2	b	223	GLN
2	b	298	LEU
2	b	362	PHE
2	b	472	ARG
2	b	486[A]	LEU
2	b	486[B]	LEU
2	b	505	ARG
3	c	142	GLU
3	c	255	THR
3	c	289	PHE
3	c	315[A]	MET
3	c	315[B]	MET
4	d	26	ARG
4	d	180	ARG
4	d	259[A]	ILE
4	d	259[B]	ILE
5	e	60	GLN
5	e	61	ARG
5	e	71	GLU
7	h	49	TYR
8	i	33	LYS
9	j	9	LEU
10	k	10	LYS
10	k	17	ILE
10	k	24	VAL
12	m	16[A]	LEU
12	m	16[B]	LEU
13	o	25	THR
13	o	36	GLN
13	o	37	THR
13	o	69	LYS
13	o	118	LEU
15	u	10[A]	VAL
15	u	10[B]	VAL
16	v	15	GLU
16	v	24	LYS
16	v	85	GLU
18	y	18	VAL

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Mol	Chain	Res	Type
18	y	45	ASN
19	Z	3	ILE
19	Z	31	GLN
20	R	29	LYS
20	R	33	LYS
19	z	1	MET
19	z	3	ILE
19	z	4	LEU
19	z	7	LEU
19	z	32	ASP
19	z	42	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
5	E	60	GLN
13	o	58	ASN
16	v	86	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	0.66	0	7,9,11	1.16	1 (14%)
14	FME	T	1	14	8,9,10	0.63	0	7,9,11	1.31	1 (14%)
12	FME	m	1	12	8,9,10	0.58	0	7,9,11	1.51	2 (28%)

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	0.58	0	7,9,11	1.16	1 (14%)
12	FME	M	1	12	8,9,10	0.64	0	7,9,11	1.18	1 (14%)
14	FME	t	1	14	8,9,10	0.71	0	7,9,11	1.53	2 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	i	1	8	-	0/7/9/11	-
14	FME	T	1	14	-	2/7/9/11	-
12	FME	m	1	12	-	2/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
14	FME	t	1	14	-	0/7/9/11	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	m	1	FME	O1-CN-N	-2.55	118.54	125.27
14	t	1	FME	O-C-CA	-2.40	118.48	124.78
14	T	1	FME	CG-CB-CA	2.39	119.60	112.95
12	m	1	FME	CA-N-CN	-2.26	119.34	122.82
14	t	1	FME	CA-N-CN	-2.22	119.40	122.82
8	I	1	FME	O-C-CA	-2.10	119.28	124.78
8	i	1	FME	O-C-CA	-2.04	119.44	124.78
12	M	1	FME	O-C-CA	-2.02	119.49	124.78

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	O1-CN-N-CA
14	T	1	FME	C-CA-CB-CG
12	m	1	FME	O1-CN-N-CA
12	m	1	FME	O-C-CA-CB
14	T	1	FME	N-CA-CB-CG



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 274 ligands modelled in this entry, 21 are monoatomic and 20 are unknown - leaving 233 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
25	BCR	d	405	-	41,41,41	1.13	2 (4%)	56,56,56	1.98	15 (26%)
23	CLA	C	505	41	65,73,73	2.01	17 (26%)	76,113,113	2.76	26 (34%)
32	LHG	D	406[A]	-	48,48,48	0.86	2 (4%)	51,54,54	0.99	3 (5%)
27	GOL	c	525[B]	-	5,5,5	1.04	0	5,5,5	0.87	0
31	LMT	b	621	-	25,25,36	0.98	1 (4%)	30,30,47	1.20	2 (6%)
25	BCR	A	409	-	41,41,41	1.01	1 (2%)	56,56,56	1.43	8 (14%)
23	CLA	B	606	-	65,73,73	1.96	16 (24%)	76,113,113	2.97	28 (36%)
23	CLA	B	616	-	65,73,73	2.02	16 (24%)	76,113,113	2.88	27 (35%)
29	PL9	d	406[B]	-	55,55,55	0.68	1 (1%)	68,69,69	1.62	17 (25%)
27	GOL	l	801[B]	-	5,5,5	0.88	0	5,5,5	0.97	0
33	LMG	Z	101	-	37,37,55	1.01	2 (5%)	45,45,63	1.44	6 (13%)
34	HTG	d	411	-	16,16,19	0.96	1 (6%)	20,21,24	1.55	1 (5%)
23	CLA	B	603	-	65,73,73	2.03	17 (26%)	76,113,113	2.92	29 (38%)
27	GOL	d	413	-	5,5,5	1.07	0	5,5,5	0.97	0
32	LHG	A	419[A]	-	48,48,48	0.84	2 (4%)	51,54,54	1.31	6 (11%)
26	SQD	a	410	-	53,54,54	1.05	4 (7%)	62,65,65	1.21	8 (12%)
35	DGD	C	518[B]	-	63,63,67	0.87	2 (3%)	77,77,81	1.07	5 (6%)
23	CLA	a	404[A]	-	65,73,73	1.99	15 (23%)	76,113,113	2.87	32 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	HTG	c	521	-	19,19,19	0.93	1 (5%)	23,24,24	1.51	1 (4%)
32	LHG	d	407[A]	-	48,48,48	0.86	2 (4%)	51,54,54	1.08	4 (7%)
27	GOL	a	417	-	5,5,5	0.99	0	5,5,5	1.03	0
32	LHG	D	406[B]	-	48,48,48	0.87	2 (4%)	51,54,54	0.93	3 (5%)
33	LMG	c	520	-	51,51,55	1.00	2 (3%)	59,59,63	1.36	6 (10%)
23	CLA	b	611	-	65,73,73	1.99	16 (24%)	76,113,113	2.87	29 (38%)
33	LMG	B	621	-	51,51,55	0.91	2 (3%)	59,59,63	1.32	5 (8%)
23	CLA	B	615	-	65,73,73	2.06	16 (24%)	76,113,113	2.79	28 (36%)
23	CLA	d	402[A]	41	65,73,73	2.00	14 (21%)	76,113,113	2.75	26 (34%)
31	LMT	B	630	-	36,36,36	1.02	3 (8%)	47,47,47	1.15	5 (10%)
23	CLA	A	404[B]	-	65,73,73	2.05	16 (24%)	76,113,113	2.81	31 (40%)
23	CLA	A	408	-	65,73,73	2.04	16 (24%)	76,113,113	2.86	32 (42%)
33	LMG	z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.08	3 (6%)
33	LMG	a	415	-	51,51,55	0.92	2 (3%)	59,59,63	1.22	5 (8%)
23	CLA	b	610	41	65,73,73	2.04	16 (24%)	76,113,113	2.81	31 (40%)
23	CLA	a	404[B]	-	65,73,73	2.02	16 (24%)	76,113,113	2.82	33 (43%)
23	CLA	c	501	-	65,73,73	2.00	17 (26%)	76,113,113	2.87	26 (34%)
38	HEM	E	102	5,6	41,50,50	1.29	4 (9%)	45,82,82	2.09	14 (31%)
37	BCT	d	401[A]	21	2,3,3	0.57	0	2,3,3	1.58	1 (50%)
23	CLA	C	507	-	65,73,73	2.05	17 (26%)	76,113,113	2.75	30 (39%)
35	DGD	c	517[A]	-	63,63,67	0.84	2 (3%)	77,77,81	0.97	5 (6%)
31	LMT	m	103	-	36,36,36	1.10	3 (8%)	47,47,47	1.12	3 (6%)
23	CLA	C	508	41	65,73,73	2.01	16 (24%)	76,113,113	2.77	27 (35%)
40	HEC	v	201	16	32,50,50	2.05	3 (9%)	24,82,82	1.99	6 (25%)
31	LMT	t	101	-	26,26,36	0.93	2 (7%)	31,31,47	1.35	2 (6%)
23	CLA	B	609	-	65,73,73	2.02	16 (24%)	76,113,113	2.81	25 (32%)
23	CLA	d	402[B]	41	65,73,73	2.07	16 (24%)	76,113,113	2.76	30 (39%)
26	SQD	a	409[A]	-	53,54,54	0.95	3 (5%)	62,65,65	1.77	13 (20%)
34	HTG	b	625	-	19,19,19	1.03	2 (10%)	23,24,24	1.58	3 (13%)
23	CLA	C	503	-	65,73,73	2.04	16 (24%)	76,113,113	2.71	26 (34%)
25	BCR	C	516	-	41,41,41	1.03	1 (2%)	56,56,56	1.46	8 (14%)
33	LMG	C	520	-	51,51,55	0.93	2 (3%)	59,59,63	1.18	6 (10%)
32	LHG	d	408[B]	-	48,48,48	0.93	2 (4%)	51,54,54	1.01	3 (5%)
25	BCR	c	514	-	41,41,41	1.00	1 (2%)	56,56,56	1.68	13 (23%)
23	CLA	D	402[A]	-	65,73,73	1.99	16 (24%)	76,113,113	2.87	29 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	C	513	-	65,73,73	2.03	15 (23%)	76,113,113	2.79	30 (39%)
32	LHG	a	419[A]	-	41,41,48	1.04	2 (4%)	44,47,54	0.92	2 (4%)
23	CLA	b	616	-	65,73,73	2.01	16 (24%)	76,113,113	2.89	28 (36%)
27	GOL	V	203[A]	-	5,5,5	1.22	0	5,5,5	0.91	0
23	CLA	D	403	-	65,73,73	2.07	15 (23%)	76,113,113	2.72	29 (38%)
25	BCR	Y	101	-	41,41,41	0.99	1 (2%)	56,56,56	1.78	13 (23%)
23	CLA	c	507	41	65,73,73	2.02	15 (23%)	76,113,113	2.87	28 (36%)
26	SQD	A	410[A]	-	53,54,54	0.93	3 (5%)	62,65,65	1.81	10 (16%)
23	CLA	c	509	-	65,73,73	2.02	15 (23%)	76,113,113	2.81	29 (38%)
37	BCT	d	401[B]	21	2,3,3	0.61	0	2,3,3	1.23	0
23	CLA	c	508	-	65,73,73	2.14	16 (24%)	76,113,113	2.71	26 (34%)
27	GOL	c	526	-	5,5,5	1.01	0	5,5,5	0.99	0
35	DGD	c	517[B]	-	63,63,67	0.86	2 (3%)	77,77,81	0.97	5 (6%)
25	BCR	C	515	-	41,41,41	1.05	1 (2%)	56,56,56	1.36	6 (10%)
26	SQD	A	412	-	53,54,54	1.03	3 (5%)	62,65,65	1.22	7 (11%)
26	SQD	a	409[B]	-	53,54,54	0.97	3 (5%)	62,65,65	1.64	12 (19%)
27	GOL	b	624	-	5,5,5	1.22	1 (20%)	5,5,5	0.81	0
25	BCR	a	408	-	41,41,41	1.04	1 (2%)	56,56,56	1.29	7 (12%)
31	LMT	B	628	-	36,36,36	1.19	4 (11%)	47,47,47	1.37	6 (12%)
23	CLA	C	510	-	65,73,73	2.08	16 (24%)	76,113,113	2.78	28 (36%)
23	CLA	c	505	-	65,73,73	2.01	16 (24%)	76,113,113	2.72	25 (32%)
26	SQD	B	620	-	53,54,54	1.07	4 (7%)	62,65,65	1.76	11 (17%)
33	LMG	D	411	39	51,51,55	0.84	2 (3%)	59,59,63	0.99	4 (6%)
37	BCT	D	401[A]	21	2,3,3	0.54	0	2,3,3	1.81	1 (50%)
23	CLA	c	506	-	65,73,73	2.05	16 (24%)	76,113,113	2.75	28 (36%)
32	LHG	a	419[B]	-	41,41,48	1.03	2 (4%)	44,47,54	0.92	2 (4%)
25	BCR	B	618	-	41,41,41	1.00	1 (2%)	56,56,56	1.31	7 (12%)
25	BCR	b	619	-	41,41,41	1.07	1 (2%)	56,56,56	1.36	6 (10%)
23	CLA	c	512	-	65,73,73	2.08	16 (24%)	76,113,113	2.74	29 (38%)
27	GOL	V	203[B]	-	5,5,5	1.10	0	5,5,5	0.89	0
35	DGD	c	516[A]	-	63,63,67	0.85	2 (3%)	77,77,81	1.12	6 (7%)
23	CLA	B	605	-	65,73,73	1.96	16 (24%)	76,113,113	2.89	26 (34%)
25	BCR	K	102	-	41,41,41	1.02	1 (2%)	56,56,56	1.41	10 (17%)
23	CLA	b	615	-	65,73,73	2.00	16 (24%)	76,113,113	2.76	27 (35%)
34	HTG	B	625	-	19,19,19	0.97	2 (10%)	23,24,24	1.12	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	BCR	c	515	-	41,41,41	1.04	1 (2%)	56,56,56	1.45	13 (23%)
23	CLA	B	602	-	65,73,73	2.10	17 (26%)	76,113,113	2.81	31 (40%)
24	PHO	a	406[A]	-	51,69,69	1.83	8 (15%)	47,99,99	1.71	10 (21%)
31	LMT	T	101	-	36,36,36	1.05	3 (8%)	47,47,47	1.04	2 (4%)
29	PL9	A	414[A]	-	55,55,55	0.68	2 (3%)	68,69,69	2.08	25 (36%)
35	DGD	h	102	-	63,63,67	0.87	3 (4%)	77,77,81	1.07	6 (7%)
23	CLA	b	601	41	65,73,73	2.13	16 (24%)	76,113,113	2.73	27 (35%)
23	CLA	b	609	-	65,73,73	2.04	16 (24%)	76,113,113	2.80	30 (39%)
23	CLA	d	404	-	65,73,73	2.04	15 (23%)	76,113,113	2.84	27 (35%)
23	CLA	B	601	41	65,73,73	2.09	16 (24%)	76,113,113	2.78	26 (34%)
37	BCT	D	401[B]	21	2,3,3	0.63	0	2,3,3	1.06	0
29	PL9	a	412[A]	-	55,55,55	0.65	2 (3%)	68,69,69	2.00	22 (32%)
31	LMT	A	417	-	36,36,36	0.96	3 (8%)	47,47,47	0.99	1 (2%)
31	LMT	b	627	-	25,25,36	0.89	1 (4%)	30,30,47	1.09	2 (6%)
32	LHG	A	419[B]	-	48,48,48	0.87	2 (4%)	51,54,54	1.17	5 (9%)
23	CLA	b	613	-	65,73,73	1.98	16 (24%)	76,113,113	2.76	29 (38%)
23	CLA	C	506	-	65,73,73	1.99	16 (24%)	76,113,113	2.72	29 (38%)
24	PHO	A	416[A]	-	51,69,69	1.87	8 (15%)	47,99,99	1.93	12 (25%)
25	BCR	k	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.51	13 (23%)
27	GOL	o	302	-	5,5,5	1.00	0	5,5,5	1.00	0
24	PHO	A	407[A]	-	51,69,69	1.78	8 (15%)	47,99,99	1.77	11 (23%)
32	LHG	d	407[B]	-	48,48,48	0.88	2 (4%)	51,54,54	0.99	3 (5%)
25	BCR	B	617	-	41,41,41	1.05	1 (2%)	56,56,56	1.32	6 (10%)
25	BCR	D	404	-	41,41,41	1.11	1 (2%)	56,56,56	1.80	17 (30%)
34	HTG	C	522	-	19,19,19	0.86	1 (5%)	23,24,24	1.36	2 (8%)
23	CLA	b	604	-	65,73,73	2.02	15 (23%)	76,113,113	2.75	25 (32%)
23	CLA	B	608	-	65,73,73	1.97	16 (24%)	76,113,113	2.77	32 (42%)
26	SQD	b	620	-	53,54,54	1.04	3 (5%)	62,65,65	1.68	11 (17%)
29	PL9	A	414[B]	-	55,55,55	0.65	2 (3%)	68,69,69	1.98	25 (36%)
27	GOL	o	303	-	5,5,5	1.07	1 (20%)	5,5,5	1.08	0
27	GOL	O	302	-	5,5,5	0.91	0	5,5,5	0.87	0
23	CLA	d	403[A]	-	65,73,73	1.94	17 (26%)	76,113,113	2.79	29 (38%)
27	GOL	v	202[A]	-	5,5,5	1.27	0	5,5,5	0.72	0
29	PL9	a	412[B]	-	55,55,55	0.64	2 (3%)	68,69,69	1.96	22 (32%)
24	PHO	A	416[B]	-	51,69,69	1.90	7 (13%)	47,99,99	1.84	10 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	BCR	y	101	-	41,41,41	1.09	1 (2%)	56,56,56	1.63	12 (21%)
23	CLA	b	602	-	65,73,73	2.07	16 (24%)	76,113,113	2.84	33 (43%)
24	PHO	A	407[B]	-	51,69,69	1.80	8 (15%)	47,99,99	1.80	10 (21%)
34	HTG	b	623	-	19,19,19	1.01	1 (5%)	23,24,24	1.78	2 (8%)
23	CLA	C	502	-	65,73,73	1.99	16 (24%)	76,113,113	2.76	28 (36%)
23	CLA	C	514	-	65,73,73	2.06	16 (24%)	76,113,113	2.79	28 (36%)
35	DGD	C	517[A]	-	63,63,67	0.81	2 (3%)	77,77,81	1.21	8 (10%)
23	CLA	b	608	-	65,73,73	2.02	15 (23%)	76,113,113	2.78	32 (42%)
40	HEC	V	201	16	32,50,50	1.97	4 (12%)	24,82,82	2.18	7 (29%)
28	OEX	a	411[A]	3,41,1	0,15,15	-	-	-	-	-
29	PL9	D	405[A]	-	55,55,55	0.62	2 (3%)	68,69,69	1.64	18 (26%)
31	LMT	F	101	-	36,36,36	1.07	1 (2%)	47,47,47	1.06	2 (4%)
23	CLA	d	403[B]	-	65,73,73	1.96	17 (26%)	76,113,113	2.83	25 (32%)
27	GOL	v	202[B]	-	5,5,5	1.13	0	5,5,5	0.87	0
23	CLA	B	611	-	65,73,73	2.68	18 (27%)	76,113,113	3.09	28 (36%)
25	BCR	t	102	-	41,41,41	1.00	1 (2%)	56,56,56	1.55	11 (19%)
27	GOL	C	523[A]	-	5,5,5	1.18	0	5,5,5	0.83	0
23	CLA	D	402[B]	-	65,73,73	2.02	16 (24%)	76,113,113	2.84	30 (39%)
31	LMT	e	101	-	36,36,36	1.03	4 (11%)	47,47,47	0.98	1 (2%)
34	HTG	B	622	-	19,19,19	1.07	2 (10%)	23,24,24	1.59	5 (21%)
23	CLA	A	405[A]	41	65,73,73	1.90	16 (24%)	76,113,113	2.85	30 (39%)
32	LHG	D	407[A]	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	4 (7%)
26	SQD	F	102	-	42,43,54	1.19	4 (9%)	51,54,65	2.18	14 (27%)
26	SQD	A	410[B]	-	53,54,54	0.93	3 (5%)	62,65,65	1.79	11 (17%)
25	BCR	T	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.68	15 (26%)
35	DGD	C	517[B]	-	63,63,67	0.84	2 (3%)	77,77,81	1.11	7 (9%)
28	OEX	a	411[B]	3,41,1	0,15,15	-	-	-	-	-
24	PHO	a	414[A]	-	51,69,69	1.86	9 (17%)	47,99,99	1.99	13 (27%)
29	PL9	D	405[B]	-	55,55,55	0.63	2 (3%)	68,69,69	1.68	17 (25%)
23	CLA	c	513	-	65,73,73	2.10	16 (24%)	76,113,113	2.78	26 (34%)
27	GOL	A	411	-	5,5,5	1.13	0	5,5,5	0.74	0
31	LMT	a	416	-	36,36,36	1.01	1 (2%)	47,47,47	1.03	1 (2%)
32	LHG	L	101[A]	-	48,48,48	0.89	2 (4%)	51,54,54	1.15	3 (5%)
34	HTG	D	410	-	16,16,19	1.04	1 (6%)	20,21,24	1.46	1 (5%)
23	CLA	C	509	-	65,73,73	2.11	16 (24%)	76,113,113	2.78	27 (35%)
38	HEM	f	101	5,6	41,50,50	1.29	5 (12%)	45,82,82	1.81	10 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	GOL	C	523[B]	-	5,5,5	1.07	0	5,5,5	0.91	0
35	DGD	c	516[B]	-	63,63,67	0.86	2 (3%)	77,77,81	1.01	3 (3%)
23	CLA	a	405[A]	41	65,73,73	1.94	16 (24%)	76,113,113	2.81	27 (35%)
23	CLA	A	405[B]	41	65,73,73	2.04	16 (24%)	76,113,113	2.78	29 (38%)
32	LHG	D	407[B]	-	48,48,48	0.92	2 (4%)	51,54,54	0.97	3 (5%)
33	LMG	m	101	-	51,51,55	0.87	2 (3%)	59,59,63	1.24	6 (10%)
27	GOL	A	418	-	5,5,5	1.62	2 (40%)	5,5,5	0.97	1 (20%)
35	DGD	C	519	-	63,63,67	0.86	3 (4%)	77,77,81	0.98	3 (3%)
23	CLA	B	607	41	65,73,73	1.98	17 (26%)	76,113,113	2.93	31 (40%)
23	CLA	B	610	41	65,73,73	2.05	17 (26%)	76,113,113	2.87	27 (35%)
23	CLA	a	407	-	65,73,73	1.97	15 (23%)	76,113,113	3.01	30 (39%)
23	CLA	b	605	-	65,73,73	1.93	15 (23%)	76,113,113	2.94	27 (35%)
24	PHO	a	414[B]	-	51,69,69	1.88	8 (15%)	47,99,99	1.90	12 (25%)
24	PHO	a	406[B]	-	51,69,69	1.84	8 (15%)	47,99,99	1.77	9 (19%)
23	CLA	b	614	-	65,73,73	2.00	16 (24%)	76,113,113	2.85	30 (39%)
32	LHG	L	101[B]	-	48,48,48	0.92	2 (4%)	51,54,54	1.09	4 (7%)
25	BCR	h	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.44	11 (19%)
32	LHG	E	101[A]	-	41,41,48	1.06	2 (4%)	44,47,54	1.11	3 (6%)
34	HTG	B	623	-	19,19,19	0.81	1 (5%)	23,24,24	1.46	3 (13%)
33	LMG	C	501	-	51,51,55	0.92	2 (3%)	59,59,63	1.53	7 (11%)
23	CLA	B	614	-	65,73,73	2.03	18 (27%)	76,113,113	2.89	30 (39%)
23	CLA	a	405[B]	41	65,73,73	2.00	16 (24%)	76,113,113	2.79	28 (36%)
23	CLA	b	606	-	65,73,73	1.98	15 (23%)	76,113,113	2.85	29 (38%)
27	GOL	B	624	-	5,5,5	0.75	0	5,5,5	1.10	1 (20%)
33	LMG	C	521	-	51,51,55	1.07	3 (5%)	59,59,63	1.33	6 (10%)
23	CLA	A	404[A]	-	65,73,73	2.02	16 (24%)	76,113,113	2.77	32 (42%)
23	CLA	b	612	-	65,73,73	2.01	16 (24%)	76,113,113	2.80	29 (38%)
27	GOL	a	418	-	5,5,5	1.23	1 (20%)	5,5,5	1.03	0
23	CLA	B	604	-	65,73,73	1.99	18 (27%)	76,113,113	2.63	27 (35%)
23	CLA	B	613	-	65,73,73	2.04	16 (24%)	76,113,113	2.74	29 (38%)
32	LHG	d	414[A]	-	48,48,48	0.89	2 (4%)	51,54,54	1.12	4 (7%)
23	CLA	A	406[A]	41	65,73,73	1.96	16 (24%)	76,113,113	2.81	29 (38%)
33	LMG	d	412	39	51,51,55	0.88	2 (3%)	59,59,63	1.13	5 (8%)
23	CLA	c	502	-	65,73,73	2.02	13 (20%)	76,113,113	2.70	25 (32%)
32	LHG	E	101[B]	-	41,41,48	1.06	2 (4%)	44,47,54	1.09	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	GOL	B	627	-	5,5,5	1.00	0	5,5,5	1.06	1 (20%)
23	CLA	b	603	-	65,73,73	2.04	14 (21%)	76,113,113	2.92	29 (38%)
23	CLA	b	607	41	65,73,73	1.97	17 (26%)	76,113,113	2.75	27 (35%)
23	CLA	c	504	41	65,73,73	2.09	17 (26%)	76,113,113	2.79	29 (38%)
23	CLA	C	504	-	65,73,73	1.94	16 (24%)	76,113,113	2.89	26 (34%)
34	HTG	b	622	-	19,19,19	1.16	2 (10%)	23,24,24	1.96	7 (30%)
28	OEX	A	413[A]	3,41,1	0,15,15	-	-	-	-	-
32	LHG	b	629[A]	-	48,48,48	0.85	3 (6%)	51,54,54	1.03	4 (7%)
31	LMT	B	631	-	25,25,36	0.88	2 (8%)	30,30,47	1.15	3 (10%)
32	LHG	d	408[A]	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	3 (5%)
32	LHG	d	414[B]	-	48,48,48	0.91	2 (4%)	51,54,54	1.07	5 (9%)
23	CLA	A	406[B]	41	65,73,73	2.02	16 (24%)	76,113,113	2.79	28 (36%)
35	DGD	H	102	-	63,63,67	0.85	3 (4%)	77,77,81	1.04	6 (7%)
27	GOL	O	303	-	5,5,5	0.98	0	5,5,5	1.11	1 (20%)
35	DGD	c	518	-	63,63,67	0.86	3 (4%)	77,77,81	1.04	4 (5%)
27	GOL	D	412	-	5,5,5	1.42	2 (40%)	5,5,5	0.81	0
23	CLA	B	612	-	65,73,73	2.07	19 (29%)	76,113,113	2.84	29 (38%)
25	BCR	H	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.48	9 (16%)
27	GOL	B	629	-	5,5,5	0.99	0	5,5,5	1.00	0
27	GOL	c	525[A]	-	5,5,5	0.94	0	5,5,5	0.95	0
33	LMG	c	519	-	51,51,55	0.93	2 (3%)	59,59,63	1.10	4 (6%)
28	OEX	A	413[B]	3,41,1	0,15,15	-	-	-	-	-
23	CLA	c	503	-	65,73,73	1.99	16 (24%)	76,113,113	2.81	26 (34%)
26	SQD	f	102	-	42,43,54	1.18	3 (7%)	51,54,65	1.55	11 (21%)
27	GOL	b	628	-	5,5,5	0.54	0	5,5,5	1.35	1 (20%)
32	LHG	b	629[B]	-	48,48,48	0.88	2 (4%)	51,54,54	1.02	3 (5%)
31	LMT	A	420	-	36,36,36	1.04	2 (5%)	47,47,47	1.15	4 (8%)
23	CLA	C	511	-	65,73,73	2.05	16 (24%)	76,113,113	2.88	30 (39%)
29	PL9	d	406[A]	-	55,55,55	0.65	1 (1%)	68,69,69	1.63	17 (25%)
27	GOL	l	801[A]	-	5,5,5	0.96	0	5,5,5	0.97	0
25	BCR	B	619	-	41,41,41	1.11	2 (4%)	56,56,56	1.31	8 (14%)
23	CLA	C	512	3	65,73,73	2.06	16 (24%)	76,113,113	2.68	25 (32%)
25	BCR	b	618	-	41,41,41	1.01	1 (2%)	56,56,56	1.16	6 (10%)
25	BCR	b	617	-	41,41,41	1.04	1 (2%)	56,56,56	1.37	6 (10%)
23	CLA	c	510	-	65,73,73	2.05	16 (24%)	76,113,113	2.78	30 (39%)
34	HTG	V	202	-	11,11,19	0.29	0	15,15,24	1.17	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	LMT	M	101	-	36,36,36	1.12	3 (8%)	47,47,47	1.17	4 (8%)
35	DGD	C	518[A]	-	63,63,67	0.89	3 (4%)	77,77,81	1.02	5 (6%)
23	CLA	c	511	3	65,73,73	2.10	16 (24%)	76,113,113	2.77	30 (39%)

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
25	BCR	d	405	-	-	5/29/63/63	0/2/2/2
23	CLA	C	505	41	1/1/15/20	6/37/115/115	-
32	LHG	D	406[A]	-	-	16/53/53/53	-
27	GOL	c	525[B]	-	-	0/4/4/4	-
31	LMT	b	621	-	-	8/17/37/61	0/1/1/2
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
23	CLA	B	606	-	1/1/15/20	9/37/115/115	-
23	CLA	B	616	-	1/1/15/20	8/37/115/115	-
29	PL9	d	406[B]	-	-	6/53/73/73	0/1/1/1
27	GOL	l	801[B]	-	-	3/4/4/4	-
33	LMG	Z	101	-	-	10/31/51/70	0/1/1/1
34	HTG	d	411	-	-	1/7/27/30	0/1/1/1
23	CLA	B	603	-	1/1/15/20	8/37/115/115	-
27	GOL	d	413	-	-	3/4/4/4	-
32	LHG	A	419[A]	-	-	10/53/53/53	-
26	SQD	a	410	-	-	14/49/69/69	0/1/1/1
35	DGD	C	518[B]	-	-	13/51/91/95	0/2/2/2
23	CLA	a	404[A]	-	1/1/15/20	3/37/115/115	-
34	HTG	c	521	-	-	2/10/30/30	0/1/1/1
32	LHG	d	407[A]	-	-	13/53/53/53	-
27	GOL	a	417	-	-	2/4/4/4	-
32	LHG	D	406[B]	-	-	16/53/53/53	-
33	LMG	c	520	-	-	10/46/66/70	0/1/1/1
23	CLA	b	611	-	1/1/15/20	2/37/115/115	-
33	LMG	B	621	-	-	19/46/66/70	0/1/1/1
23	CLA	B	615	-	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	d	402[A]	41	1/1/15/20	8/37/115/115	-
31	LMT	B	630	-	-	12/21/61/61	0/2/2/2
23	CLA	A	404[B]	-	1/1/15/20	4/37/115/115	-
23	CLA	A	408	-	1/1/15/20	9/37/115/115	-
33	LMG	z	101	-	-	9/34/54/70	0/1/1/1
33	LMG	a	415	-	-	12/46/66/70	0/1/1/1
23	CLA	b	610	41	1/1/15/20	5/37/115/115	-
23	CLA	a	404[B]	-	1/1/15/20	2/37/115/115	-
23	CLA	c	501	-	1/1/15/20	4/37/115/115	-
38	HEM	E	102	5,6	-	2/12/54/54	-
23	CLA	C	507	-	1/1/15/20	12/37/115/115	-
35	DGD	c	517[A]	-	-	17/51/91/95	0/2/2/2
31	LMT	m	103	-	-	4/21/61/61	0/2/2/2
23	CLA	C	508	41	1/1/15/20	4/37/115/115	-
40	HEC	v	201	16	-	2/10/54/54	-
31	LMT	t	101	-	-	8/17/38/61	0/1/1/2
23	CLA	B	609	-	1/1/15/20	2/37/115/115	-
23	CLA	d	402[B]	41	1/1/15/20	6/37/115/115	-
26	SQD	a	409[A]	-	-	10/49/69/69	0/1/1/1
34	HTG	b	625	-	-	3/10/30/30	0/1/1/1
23	CLA	C	503	-	-	10/37/115/115	-
25	BCR	C	516	-	-	2/29/63/63	0/2/2/2
33	LMG	C	520	-	-	9/46/66/70	0/1/1/1
32	LHG	d	408[B]	-	-	13/53/53/53	-
25	BCR	c	514	-	-	2/29/63/63	0/2/2/2
23	CLA	D	402[A]	-	1/1/15/20	0/37/115/115	-
23	CLA	C	513	-	1/1/15/20	9/37/115/115	-
32	LHG	a	419[A]	-	-	16/46/46/53	-
23	CLA	b	616	-	1/1/15/20	9/37/115/115	-
27	GOL	V	203[A]	-	-	2/4/4/4	-
23	CLA	D	403	-	1/1/15/20	14/37/115/115	-
25	BCR	Y	101	-	-	6/29/63/63	0/2/2/2
23	CLA	c	507	41	1/1/15/20	7/37/115/115	-
26	SQD	A	410[A]	-	-	12/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	509	-	1/1/15/20	14/37/115/115	-
23	CLA	c	508	-	1/1/15/20	5/37/115/115	-
27	GOL	c	526	-	-	4/4/4/4	-
35	DGD	c	517[B]	-	-	17/51/91/95	0/2/2/2
25	BCR	C	515	-	-	2/29/63/63	0/2/2/2
26	SQD	A	412	-	-	14/49/69/69	0/1/1/1
26	SQD	a	409[B]	-	-	9/49/69/69	0/1/1/1
27	GOL	b	624	-	-	2/4/4/4	-
25	BCR	a	408	-	-	1/29/63/63	0/2/2/2
31	LMT	B	628	-	-	12/21/61/61	0/2/2/2
23	CLA	C	510	-	1/1/15/20	4/37/115/115	-
23	CLA	c	505	-	1/1/15/20	7/37/115/115	-
26	SQD	B	620	-	-	13/49/69/69	0/1/1/1
33	LMG	D	411	39	-	9/46/66/70	0/1/1/1
23	CLA	c	506	-	1/1/15/20	8/37/115/115	-
32	LHG	a	419[B]	-	-	16/46/46/53	-
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
25	BCR	b	619	-	-	3/29/63/63	0/2/2/2
23	CLA	c	512	-	1/1/15/20	13/37/115/115	-
27	GOL	V	203[B]	-	-	2/4/4/4	-
35	DGD	c	516[A]	-	-	20/51/91/95	0/2/2/2
23	CLA	B	605	-	1/1/15/20	6/37/115/115	-
25	BCR	K	102	-	-	1/29/63/63	0/2/2/2
23	CLA	b	615	-	1/1/15/20	7/37/115/115	-
34	HTG	B	625	-	-	3/10/30/30	0/1/1/1
25	BCR	c	515	-	-	0/29/63/63	0/2/2/2
23	CLA	B	602	-	1/1/15/20	7/37/115/115	-
24	PHO	a	406[A]	-	-	6/37/103/103	0/5/6/6
31	LMT	T	101	-	-	10/21/61/61	0/2/2/2
29	PL9	A	414[A]	-	-	15/53/73/73	0/1/1/1
35	DGD	h	102	-	-	16/51/91/95	0/2/2/2
23	CLA	b	601	41	1/1/15/20	19/37/115/115	-
23	CLA	b	609	-	1/1/15/20	3/37/115/115	-
23	CLA	d	404	-	1/1/15/20	8/37/115/115	-
23	CLA	B	601	41	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PL9	a	412[A]	-	-	14/53/73/73	0/1/1/1
31	LMT	A	417	-	-	7/21/61/61	0/2/2/2
31	LMT	b	627	-	-	11/17/37/61	0/1/1/2
32	LHG	A	419[B]	-	-	13/53/53/53	-
23	CLA	b	613	-	1/1/15/20	4/37/115/115	-
23	CLA	C	506	-	1/1/15/20	7/37/115/115	-
24	PHO	A	416[A]	-	-	1/37/103/103	0/5/6/6
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
27	GOL	o	302	-	-	2/4/4/4	-
24	PHO	A	407[A]	-	-	4/37/103/103	0/5/6/6
32	LHG	d	407[B]	-	-	11/53/53/53	-
25	BCR	B	617	-	-	2/29/63/63	0/2/2/2
25	BCR	D	404	-	-	4/29/63/63	0/2/2/2
34	HTG	C	522	-	-	0/10/30/30	0/1/1/1
23	CLA	b	604	-	1/1/15/20	10/37/115/115	-
23	CLA	B	608	-	-	4/37/115/115	-
26	SQD	b	620	-	-	19/49/69/69	0/1/1/1
29	PL9	A	414[B]	-	-	18/53/73/73	0/1/1/1
27	GOL	o	303	-	-	3/4/4/4	-
27	GOL	O	302	-	-	2/4/4/4	-
23	CLA	d	403[A]	-	1/1/15/20	2/37/115/115	-
27	GOL	v	202[A]	-	-	1/4/4/4	-
29	PL9	a	412[B]	-	-	15/53/73/73	0/1/1/1
24	PHO	A	416[B]	-	-	3/37/103/103	0/5/6/6
25	BCR	y	101	-	-	6/29/63/63	0/2/2/2
23	CLA	b	602	-	1/1/15/20	4/37/115/115	-
24	PHO	A	407[B]	-	-	2/37/103/103	0/5/6/6
34	HTG	b	623	-	-	5/10/30/30	0/1/1/1
23	CLA	C	502	-	1/1/15/20	5/37/115/115	-
23	CLA	C	514	-	1/1/15/20	7/37/115/115	-
35	DGD	C	517[A]	-	-	11/51/91/95	0/2/2/2
23	CLA	b	608	-	-	5/37/115/115	-
40	HEC	V	201	16	-	2/10/54/54	-
29	PL9	D	405[A]	-	-	8/53/73/73	0/1/1/1
31	LMT	F	101	-	-	8/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	d	403[B]	-	1/1/15/20	4/37/115/115	-
27	GOL	v	202[B]	-	-	2/4/4/4	-
23	CLA	B	611	-	1/1/15/20	2/37/115/115	-
25	BCR	t	102	-	-	1/29/63/63	0/2/2/2
27	GOL	C	523[A]	-	-	0/4/4/4	-
23	CLA	D	402[B]	-	1/1/15/20	0/37/115/115	-
31	LMT	e	101	-	-	15/21/61/61	0/2/2/2
34	HTG	B	622	-	-	4/10/30/30	0/1/1/1
23	CLA	A	405[A]	41	-	4/37/115/115	-
32	LHG	D	407[A]	-	-	14/53/53/53	-
26	SQD	F	102	-	-	14/38/58/69	0/1/1/1
26	SQD	A	410[B]	-	-	10/49/69/69	0/1/1/1
25	BCR	T	102	-	-	1/29/63/63	0/2/2/2
35	DGD	C	517[B]	-	-	14/51/91/95	0/2/2/2
24	PHO	a	414[A]	-	-	2/37/103/103	0/5/6/6
29	PL9	D	405[B]	-	-	8/53/73/73	0/1/1/1
23	CLA	c	513	-	1/1/15/20	10/37/115/115	-
27	GOL	A	411	-	-	2/4/4/4	-
31	LMT	a	416	-	-	10/21/61/61	0/2/2/2
32	LHG	L	101[A]	-	-	19/53/53/53	-
34	HTG	D	410	-	-	3/7/27/30	0/1/1/1
23	CLA	C	509	-	1/1/15/20	3/37/115/115	-
38	HEM	f	101	5,6	-	6/12/54/54	-
27	GOL	C	523[B]	-	-	0/4/4/4	-
35	DGD	c	516[B]	-	-	21/51/91/95	0/2/2/2
23	CLA	a	405[A]	41	-	5/37/115/115	-
23	CLA	A	405[B]	41	1/1/15/20	5/37/115/115	-
32	LHG	D	407[B]	-	-	13/53/53/53	-
33	LMG	m	101	-	-	10/46/66/70	0/1/1/1
27	GOL	A	418	-	-	1/4/4/4	-
35	DGD	C	519	-	-	16/51/91/95	0/2/2/2
23	CLA	B	607	41	1/1/15/20	3/37/115/115	-
23	CLA	B	610	41	1/1/15/20	7/37/115/115	-
23	CLA	a	407	-	1/1/15/20	10/37/115/115	-
23	CLA	b	605	-	1/1/15/20	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PHO	a	414[B]	-	-	1/37/103/103	0/5/6/6
24	PHO	a	406[B]	-	-	6/37/103/103	0/5/6/6
23	CLA	b	614	-	1/1/15/20	15/37/115/115	-
32	LHG	L	101[B]	-	-	18/53/53/53	-
25	BCR	h	101	-	-	1/29/63/63	0/2/2/2
32	LHG	E	101[A]	-	-	22/46/46/53	-
34	HTG	B	623	-	-	4/10/30/30	0/1/1/1
33	LMG	C	501	-	-	13/46/66/70	0/1/1/1
23	CLA	B	614	-	1/1/15/20	14/37/115/115	-
23	CLA	a	405[B]	41	-	6/37/115/115	-
23	CLA	b	606	-	1/1/15/20	11/37/115/115	-
27	GOL	B	624	-	-	2/4/4/4	-
33	LMG	C	521	-	-	13/46/66/70	0/1/1/1
23	CLA	A	404[A]	-	1/1/15/20	5/37/115/115	-
23	CLA	b	612	-	1/1/15/20	3/37/115/115	-
27	GOL	a	418	-	-	0/4/4/4	-
23	CLA	B	604	-	1/1/15/20	4/37/115/115	-
23	CLA	B	613	-	1/1/15/20	8/37/115/115	-
32	LHG	d	414[A]	-	-	13/53/53/53	-
23	CLA	A	406[A]	41	-	5/37/115/115	-
33	LMG	d	412	39	-	11/46/66/70	0/1/1/1
23	CLA	c	502	-	1/1/15/20	6/37/115/115	-
32	LHG	E	101[B]	-	-	23/46/46/53	-
27	GOL	B	627	-	-	1/4/4/4	-
23	CLA	b	603	-	1/1/15/20	4/37/115/115	-
23	CLA	b	607	41	1/1/15/20	3/37/115/115	-
23	CLA	c	504	41	1/1/15/20	6/37/115/115	-
23	CLA	C	504	-	-	2/37/115/115	-
34	HTG	b	622	-	-	5/10/30/30	0/1/1/1
32	LHG	b	629[A]	-	-	20/53/53/53	-
31	LMT	B	631	-	-	11/17/37/61	0/1/1/2
32	LHG	d	408[A]	-	-	11/53/53/53	-
32	LHG	d	414[B]	-	-	12/53/53/53	-
23	CLA	A	406[B]	41	-	6/37/115/115	-
35	DGD	H	102	-	-	9/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	GOL	O	303	-	-	2/4/4/4	-
35	DGD	c	518	-	-	10/51/91/95	0/2/2/2
27	GOL	D	412	-	-	4/4/4/4	-
23	CLA	B	612	-	1/1/15/20	6/37/115/115	-
25	BCR	H	101	-	-	2/29/63/63	0/2/2/2
27	GOL	B	629	-	-	4/4/4/4	-
27	GOL	c	525[A]	-	-	0/4/4/4	-
33	LMG	c	519	-	-	12/46/66/70	0/1/1/1
23	CLA	c	503	-	1/1/15/20	2/37/115/115	-
26	SQD	f	102	-	-	10/38/58/69	0/1/1/1
27	GOL	b	628	-	-	0/4/4/4	-
32	LHG	b	629[B]	-	-	18/53/53/53	-
31	LMT	A	420	-	-	15/21/61/61	0/2/2/2
23	CLA	C	511	-	1/1/15/20	12/37/115/115	-
29	PL9	d	406[A]	-	-	6/53/73/73	0/1/1/1
27	GOL	l	801[A]	-	-	2/4/4/4	-
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
23	CLA	C	512	3	1/1/15/20	3/37/115/115	-
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
23	CLA	c	510	-	1/1/15/20	12/37/115/115	-
34	HTG	V	202	-	-	0/2/19/30	0/1/1/1
31	LMT	M	101	-	-	4/21/61/61	0/2/2/2
35	DGD	C	518[A]	-	-	15/51/91/95	0/2/2/2
23	CLA	c	511	3	1/1/15/20	3/37/115/115	-

All (1550) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	611	CLA	C3B-C2B	10.57	1.55	1.40
23	B	611	CLA	CMB-C2B	7.01	1.66	1.51
23	B	612	CLA	C3B-C2B	6.95	1.50	1.40
23	C	509	CLA	C3B-C2B	6.92	1.50	1.40
23	C	512	CLA	C3B-C2B	6.86	1.49	1.40
23	B	608	CLA	C3B-C2B	6.66	1.49	1.40
23	B	616	CLA	C3B-C2B	6.57	1.49	1.40
23	b	608	CLA	C3B-C2B	6.51	1.49	1.40
23	B	611	CLA	C1D-ND	6.50	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	603	CLA	C3B-C2B	6.47	1.49	1.40
23	c	502	CLA	C3B-C2B	6.46	1.49	1.40
24	A	416[B]	PHO	C3B-C2B	6.45	1.49	1.40
23	B	603	CLA	C3B-C2B	6.44	1.49	1.40
23	C	510	CLA	C3B-C2B	6.43	1.49	1.40
23	c	504	CLA	C3B-C2B	6.40	1.49	1.40
23	A	408	CLA	C3B-C2B	6.40	1.49	1.40
24	a	406[A]	PHO	C3B-C2B	6.36	1.49	1.40
23	c	511	CLA	C3B-C2B	6.36	1.49	1.40
23	B	613	CLA	C3B-C2B	6.36	1.49	1.40
23	B	607	CLA	C3B-C2B	6.30	1.49	1.40
23	C	503	CLA	C3B-C2B	6.28	1.49	1.40
23	C	514	CLA	C3B-C2B	6.26	1.49	1.40
23	a	404[A]	CLA	C3B-C2B	6.26	1.49	1.40
23	A	404[A]	CLA	C3B-C2B	6.26	1.49	1.40
23	b	601	CLA	C3B-C2B	6.25	1.49	1.40
23	a	404[B]	CLA	C3B-C2B	6.19	1.49	1.40
40	v	201	HEC	C2B-C3B	-6.19	1.34	1.40
24	A	407[A]	PHO	C3B-C2B	6.19	1.49	1.40
23	b	604	CLA	C3B-C2B	6.18	1.48	1.40
23	b	616	CLA	C3B-C2B	6.16	1.48	1.40
23	C	505	CLA	C3B-C2B	6.16	1.48	1.40
23	A	404[B]	CLA	C3B-C2B	6.15	1.48	1.40
23	b	612	CLA	C3B-C2B	6.14	1.48	1.40
24	A	416[A]	PHO	C3B-C2B	6.12	1.48	1.40
23	b	610	CLA	C3B-C2B	6.11	1.48	1.40
24	a	406[B]	PHO	C3B-C2B	6.07	1.48	1.40
23	B	611	CLA	CHC-C1C	6.06	1.50	1.35
23	C	507	CLA	C3B-C2B	5.99	1.48	1.40
23	a	407	CLA	C3B-C2B	5.98	1.48	1.40
23	c	508	CLA	C3B-C2B	5.98	1.48	1.40
23	c	510	CLA	C3B-C2B	5.97	1.48	1.40
24	a	414[B]	PHO	C3B-C2B	5.95	1.48	1.40
23	D	402[B]	CLA	C3B-C2B	5.95	1.48	1.40
23	B	610	CLA	C3C-C2C	5.95	1.49	1.36
23	b	611	CLA	C3B-C2B	5.94	1.48	1.40
23	D	402[A]	CLA	C3B-C2B	5.94	1.48	1.40
23	b	613	CLA	C3B-C2B	5.94	1.48	1.40
23	c	506	CLA	C3B-C2B	5.93	1.48	1.40
23	C	511	CLA	C3B-C2B	5.92	1.48	1.40
23	b	614	CLA	C3B-C2B	5.91	1.48	1.40
24	a	414[A]	PHO	C3B-C2B	5.90	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	602	CLA	C3B-C2B	5.90	1.48	1.40
24	A	407[B]	PHO	C3B-C2B	5.88	1.48	1.40
23	b	607	CLA	C3B-C2B	5.86	1.48	1.40
23	B	601	CLA	C3B-C2B	5.82	1.48	1.40
23	c	509	CLA	C3B-C2B	5.81	1.48	1.40
23	C	511	CLA	C1D-ND	5.81	1.44	1.37
23	B	604	CLA	C3B-C2B	5.81	1.48	1.40
23	B	611	CLA	C3C-C2C	5.81	1.49	1.36
23	c	513	CLA	C3B-C2B	5.73	1.48	1.40
23	d	403[B]	CLA	C3B-C2B	5.70	1.48	1.40
23	d	402[B]	CLA	C3C-C2C	5.69	1.48	1.36
23	D	403	CLA	C3C-C2C	5.68	1.48	1.36
23	b	609	CLA	C3B-C2B	5.68	1.48	1.40
23	d	404	CLA	C3B-C2B	5.65	1.48	1.40
23	d	403[A]	CLA	C3B-C2B	5.65	1.48	1.40
23	C	502	CLA	C3B-C2B	5.60	1.48	1.40
23	c	513	CLA	C1D-ND	5.58	1.44	1.37
23	C	509	CLA	C3C-C2C	5.58	1.48	1.36
23	C	513	CLA	C3B-C2B	5.57	1.48	1.40
23	c	512	CLA	C3C-C2C	5.55	1.48	1.36
23	B	606	CLA	C3B-C2B	5.55	1.48	1.40
23	B	602	CLA	C1D-ND	5.55	1.44	1.37
24	a	406[B]	PHO	C3D-C2D	5.54	1.49	1.39
23	c	508	CLA	C3C-C2C	5.53	1.48	1.36
23	C	504	CLA	C3C-C2C	5.53	1.48	1.36
23	b	606	CLA	C3B-C2B	5.52	1.48	1.40
23	c	512	CLA	C3B-C2B	5.52	1.48	1.40
23	B	616	CLA	C3C-C2C	5.52	1.48	1.36
23	d	404	CLA	C3C-C2C	5.51	1.48	1.36
23	b	607	CLA	C3C-C2C	5.50	1.48	1.36
23	c	509	CLA	C3C-C2C	5.50	1.48	1.36
23	B	614	CLA	C3B-C2B	5.49	1.48	1.40
23	C	513	CLA	CHC-C1C	5.49	1.49	1.35
23	a	405[B]	CLA	C3B-C2B	5.49	1.48	1.40
23	C	508	CLA	C3B-C2B	5.46	1.47	1.40
23	A	404[A]	CLA	C3C-C2C	5.45	1.48	1.36
24	a	414[B]	PHO	C3D-C2D	5.45	1.49	1.39
23	c	512	CLA	CHC-C1C	5.44	1.48	1.35
23	c	505	CLA	C3C-C2C	5.44	1.48	1.36
23	B	612	CLA	CHC-C1C	5.43	1.48	1.35
23	C	511	CLA	C3C-C2C	5.43	1.48	1.36
23	b	601	CLA	C1D-ND	5.43	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	508	CLA	C3C-C2C	5.42	1.48	1.36
23	A	406[B]	CLA	C3C-C2C	5.42	1.48	1.36
23	B	609	CLA	C3B-C2B	5.42	1.47	1.40
23	b	603	CLA	C3C-C2C	5.42	1.48	1.36
23	b	606	CLA	C3C-C2C	5.42	1.48	1.36
23	A	404[B]	CLA	C3C-C2C	5.41	1.48	1.36
24	a	406[A]	PHO	C3D-C2D	5.41	1.49	1.39
23	C	513	CLA	C3C-C2C	5.41	1.48	1.36
23	C	510	CLA	C3C-C2C	5.40	1.48	1.36
40	v	201	HEC	C3D-C2D	5.40	1.53	1.37
23	b	615	CLA	C3C-C2C	5.39	1.48	1.36
24	A	416[B]	PHO	C3D-C2D	5.39	1.49	1.39
23	c	513	CLA	C3C-C2C	5.39	1.48	1.36
23	B	610	CLA	C1D-ND	5.39	1.44	1.37
23	D	403	CLA	C1D-ND	5.39	1.44	1.37
23	D	402[B]	CLA	C3C-C2C	5.39	1.48	1.36
23	b	610	CLA	C3C-C2C	5.38	1.48	1.36
40	V	201	HEC	C2B-C3B	-5.37	1.35	1.40
23	b	602	CLA	CHC-C1C	5.37	1.48	1.35
23	d	404	CLA	C1D-ND	5.37	1.44	1.37
23	c	508	CLA	C1D-ND	5.37	1.44	1.37
23	C	503	CLA	C1D-ND	5.37	1.44	1.37
23	A	405[B]	CLA	C3B-C2B	5.36	1.47	1.40
23	c	501	CLA	C3B-C2B	5.36	1.47	1.40
23	c	503	CLA	C3C-C2C	5.35	1.48	1.36
23	d	402[A]	CLA	C3C-C2C	5.35	1.48	1.36
23	c	508	CLA	CHC-C1C	5.35	1.48	1.35
23	b	614	CLA	CHC-C1C	5.34	1.48	1.35
23	B	609	CLA	CHC-C1C	5.34	1.48	1.35
23	A	406[B]	CLA	CHC-C1C	5.34	1.48	1.35
23	b	602	CLA	C3C-C2C	5.34	1.48	1.36
23	B	613	CLA	O2D-CGD	5.34	1.46	1.33
23	a	405[A]	CLA	C3C-C2C	5.34	1.48	1.36
23	b	601	CLA	C3C-C2C	5.33	1.48	1.36
23	B	601	CLA	CHC-C1C	5.33	1.48	1.35
23	c	504	CLA	C3C-C2C	5.32	1.48	1.36
23	c	505	CLA	CHC-C1C	5.32	1.48	1.35
23	d	402[B]	CLA	C3B-C2B	5.31	1.47	1.40
23	B	603	CLA	C1D-ND	5.31	1.44	1.37
23	d	402[B]	CLA	O2D-CGD	5.30	1.46	1.33
23	b	614	CLA	C3C-C2C	5.28	1.48	1.36
24	a	414[A]	PHO	C3D-C2D	5.28	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	613	CLA	CHC-C1C	5.28	1.48	1.35
23	c	510	CLA	C1D-ND	5.27	1.44	1.37
23	b	612	CLA	C3C-C2C	5.27	1.47	1.36
23	c	502	CLA	C3C-C2C	5.27	1.47	1.36
23	c	509	CLA	O2D-CGD	5.27	1.46	1.33
23	b	605	CLA	C3B-C2B	5.27	1.47	1.40
23	d	404	CLA	CHC-C1C	5.26	1.48	1.35
23	c	512	CLA	C1D-ND	5.26	1.44	1.37
23	b	605	CLA	C3C-C2C	5.26	1.47	1.36
23	B	601	CLA	C3C-C2C	5.25	1.47	1.36
23	C	509	CLA	O2D-CGD	5.25	1.46	1.33
24	A	416[A]	PHO	C3D-C2D	5.25	1.48	1.39
23	b	610	CLA	CHC-C1C	5.25	1.48	1.35
23	a	407	CLA	CHC-C1C	5.24	1.48	1.35
23	C	504	CLA	C3B-C2B	5.24	1.47	1.40
23	B	613	CLA	CHC-C1C	5.24	1.48	1.35
23	c	506	CLA	C1D-ND	5.23	1.44	1.37
23	d	403[A]	CLA	C3C-C2C	5.23	1.47	1.36
23	a	405[A]	CLA	C3B-C2B	5.22	1.47	1.40
23	d	402[B]	CLA	C1D-ND	5.22	1.44	1.37
23	B	615	CLA	CHC-C1C	5.22	1.48	1.35
23	D	402[A]	CLA	C3C-C2C	5.22	1.47	1.36
23	d	403[B]	CLA	C3C-C2C	5.22	1.47	1.36
23	a	404[A]	CLA	C3C-C2C	5.22	1.47	1.36
23	C	514	CLA	C3C-C2C	5.21	1.47	1.36
23	a	407	CLA	C3C-C2C	5.20	1.47	1.36
23	C	502	CLA	CHC-C1C	5.20	1.48	1.35
23	B	609	CLA	C3C-C2C	5.20	1.47	1.36
23	B	606	CLA	CHC-C1C	5.20	1.48	1.35
23	A	405[B]	CLA	CHC-C1C	5.20	1.48	1.35
23	c	510	CLA	C3C-C2C	5.19	1.47	1.36
23	B	605	CLA	C3C-C2C	5.19	1.47	1.36
23	a	405[B]	CLA	CHC-C1C	5.19	1.48	1.35
23	c	508	CLA	O2D-CGD	5.18	1.45	1.33
23	a	405[B]	CLA	C3C-C2C	5.18	1.47	1.36
23	c	504	CLA	O2D-CGD	5.18	1.45	1.33
23	A	405[A]	CLA	C3B-C2B	5.18	1.47	1.40
23	A	408	CLA	C3C-C2C	5.18	1.47	1.36
23	B	604	CLA	C3C-C2C	5.18	1.47	1.36
23	c	507	CLA	C3B-C2B	5.18	1.47	1.40
23	B	606	CLA	C3C-C2C	5.17	1.47	1.36
23	B	614	CLA	C3C-C2C	5.17	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	609	CLA	CHC-C1C	5.17	1.48	1.35
23	c	501	CLA	C3C-C2C	5.17	1.47	1.36
23	c	503	CLA	CHC-C1C	5.17	1.48	1.35
25	C	515	BCR	C23-C22	-5.16	1.34	1.45
23	b	606	CLA	CHC-C1C	5.16	1.48	1.35
23	c	501	CLA	CHC-C1C	5.16	1.48	1.35
23	A	406[B]	CLA	C3B-C2B	5.16	1.47	1.40
23	C	512	CLA	O2D-CGD	5.16	1.45	1.33
23	d	402[A]	CLA	C1D-ND	5.16	1.44	1.37
23	c	505	CLA	C3B-C2B	5.16	1.47	1.40
24	a	414[B]	PHO	OBD-CAD	5.15	1.29	1.22
23	B	601	CLA	C1D-ND	5.15	1.44	1.37
23	b	609	CLA	O2D-CGD	5.15	1.45	1.33
23	D	403	CLA	CHC-C1C	5.15	1.48	1.35
23	B	601	CLA	O2D-CGD	5.15	1.45	1.33
23	B	605	CLA	C1D-ND	5.15	1.44	1.37
23	c	510	CLA	O2D-CGD	5.15	1.45	1.33
23	c	503	CLA	C1D-ND	5.15	1.44	1.37
23	C	512	CLA	CHC-C1C	5.14	1.48	1.35
23	b	603	CLA	O2D-CGD	5.14	1.45	1.33
23	B	603	CLA	C3C-C2C	5.14	1.47	1.36
23	B	602	CLA	CHC-C1C	5.14	1.48	1.35
23	C	506	CLA	CHC-C1C	5.13	1.48	1.35
23	B	612	CLA	C3C-C2C	5.13	1.47	1.36
23	A	406[A]	CLA	CHC-C1C	5.12	1.48	1.35
23	a	404[B]	CLA	C3C-C2C	5.12	1.47	1.36
23	c	507	CLA	CHC-C1C	5.12	1.48	1.35
23	C	504	CLA	CHC-C1C	5.12	1.48	1.35
23	b	611	CLA	C3C-C2C	5.11	1.47	1.36
23	B	601	CLA	O2A-CGA	5.11	1.48	1.33
23	B	610	CLA	CHC-C1C	5.11	1.48	1.35
23	c	511	CLA	C3C-C2C	5.10	1.47	1.36
23	c	511	CLA	C1D-ND	5.10	1.44	1.37
25	k	101	BCR	C23-C22	-5.10	1.35	1.45
23	C	506	CLA	C3B-C2B	5.10	1.47	1.40
23	b	603	CLA	CHC-C1C	5.09	1.48	1.35
23	a	404[B]	CLA	C1D-ND	5.09	1.44	1.37
23	C	507	CLA	C3C-C2C	5.09	1.47	1.36
24	a	414[B]	PHO	O2D-CGD	5.09	1.45	1.33
23	c	504	CLA	CHC-C1C	5.08	1.48	1.35
23	A	405[B]	CLA	C3C-C2C	5.08	1.47	1.36
23	B	615	CLA	C1D-ND	5.08	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	508	CLA	CHC-C1C	5.08	1.48	1.35
23	B	615	CLA	O2D-CGD	5.08	1.45	1.33
23	b	616	CLA	C1D-ND	5.07	1.44	1.37
23	C	505	CLA	C3C-C2C	5.07	1.47	1.36
24	A	416[B]	PHO	O2D-CGD	5.07	1.45	1.33
23	c	501	CLA	C1D-ND	5.06	1.44	1.37
23	b	615	CLA	C3B-C2B	5.06	1.47	1.40
23	c	507	CLA	C1D-ND	5.06	1.44	1.37
23	b	616	CLA	C3C-C2C	5.06	1.47	1.36
23	c	506	CLA	C3C-C2C	5.06	1.47	1.36
23	A	406[A]	CLA	C3C-C2C	5.05	1.47	1.36
23	B	602	CLA	C3C-C2C	5.05	1.47	1.36
23	C	502	CLA	C3C-C2C	5.05	1.47	1.36
23	a	407	CLA	O2D-CGD	5.05	1.45	1.33
23	B	608	CLA	C3C-C2C	5.04	1.47	1.36
23	b	604	CLA	CHC-C1C	5.04	1.47	1.35
23	b	616	CLA	CHC-C1C	5.04	1.47	1.35
23	c	511	CLA	CHC-C1C	5.04	1.47	1.35
23	B	613	CLA	C3C-C2C	5.04	1.47	1.36
23	A	404[B]	CLA	CHC-C1C	5.04	1.47	1.35
24	a	406[A]	PHO	O2D-CGD	5.03	1.45	1.33
23	B	610	CLA	C3B-C2B	5.02	1.47	1.40
23	c	513	CLA	CHC-C1C	5.02	1.47	1.35
24	A	416[B]	PHO	OBD-CAD	5.02	1.29	1.22
25	d	405	BCR	C23-C22	-5.02	1.35	1.45
23	c	503	CLA	C3B-C2B	5.02	1.47	1.40
24	A	407[B]	PHO	O2D-CGD	5.01	1.45	1.33
23	C	507	CLA	O2D-CGD	5.01	1.45	1.33
23	a	405[A]	CLA	CHC-C1C	5.01	1.47	1.35
23	d	402[A]	CLA	C3B-C2B	5.01	1.47	1.40
23	A	405[B]	CLA	C1D-ND	5.01	1.43	1.37
23	b	602	CLA	C1D-ND	5.00	1.43	1.37
23	C	506	CLA	C1D-ND	5.00	1.43	1.37
23	B	614	CLA	C1D-ND	5.00	1.43	1.37
23	b	605	CLA	O2D-CGD	5.00	1.45	1.33
23	C	513	CLA	C1D-ND	5.00	1.43	1.37
23	C	514	CLA	C1D-ND	5.00	1.43	1.37
23	B	615	CLA	C3B-C2B	4.99	1.47	1.40
23	A	405[A]	CLA	CHC-C1C	4.99	1.47	1.35
23	B	615	CLA	C3C-C2C	4.99	1.47	1.36
24	A	407[B]	PHO	C3D-C2D	4.99	1.48	1.39
23	b	602	CLA	C3B-C2B	4.99	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	508	CLA	C1D-ND	4.98	1.43	1.37
23	b	615	CLA	CHC-C1C	4.98	1.47	1.35
23	d	402[A]	CLA	O2D-CGD	4.98	1.45	1.33
23	c	507	CLA	C3C-C2C	4.97	1.47	1.36
23	c	513	CLA	O2D-CGD	4.97	1.45	1.33
23	D	403	CLA	C3B-C2B	4.96	1.47	1.40
23	B	604	CLA	O2D-CGD	4.96	1.45	1.33
23	b	608	CLA	C3C-C2C	4.96	1.47	1.36
25	B	619	BCR	C23-C22	-4.96	1.35	1.45
23	A	404[B]	CLA	O2D-CGD	4.96	1.45	1.33
23	C	514	CLA	CHC-C1C	4.96	1.47	1.35
23	B	605	CLA	CHC-C1C	4.95	1.47	1.35
23	b	601	CLA	CHC-C1C	4.95	1.47	1.35
23	A	405[B]	CLA	O2D-CGD	4.95	1.45	1.33
24	a	414[A]	PHO	O2D-CGD	4.95	1.45	1.33
23	b	611	CLA	CHC-C1C	4.95	1.47	1.35
24	a	406[B]	PHO	O2D-CGD	4.94	1.45	1.33
23	b	609	CLA	C3C-C2C	4.94	1.47	1.36
24	a	406[B]	PHO	OBD-CAD	4.94	1.29	1.22
23	b	613	CLA	C3C-C2C	4.94	1.47	1.36
23	A	406[B]	CLA	O2D-CGD	4.94	1.45	1.33
23	b	612	CLA	CHC-C1C	4.94	1.47	1.35
40	V	201	HEC	C3D-C2D	4.93	1.52	1.37
23	b	604	CLA	C3C-C2C	4.93	1.47	1.36
23	B	616	CLA	CHC-C1C	4.93	1.47	1.35
23	D	402[B]	CLA	O2D-CGD	4.93	1.45	1.33
23	c	506	CLA	CHC-C1C	4.93	1.47	1.35
23	A	406[A]	CLA	C3B-C2B	4.93	1.47	1.40
23	C	503	CLA	C3C-C2C	4.93	1.47	1.36
23	D	403	CLA	O2D-CGD	4.93	1.45	1.33
23	C	514	CLA	O2D-CGD	4.92	1.45	1.33
23	C	511	CLA	CHC-C1C	4.92	1.47	1.35
23	b	602	CLA	O2D-CGD	4.92	1.45	1.33
23	A	404[B]	CLA	C1D-ND	4.91	1.43	1.37
40	V	201	HEC	C3C-C2C	-4.91	1.35	1.40
23	B	604	CLA	CHC-C1C	4.91	1.47	1.35
24	A	416[A]	PHO	O2D-CGD	4.91	1.45	1.33
23	b	610	CLA	O2D-CGD	4.91	1.45	1.33
23	b	614	CLA	O2D-CGD	4.90	1.45	1.33
23	b	614	CLA	C1D-ND	4.90	1.43	1.37
23	C	505	CLA	O2D-CGD	4.90	1.45	1.33
24	A	407[A]	PHO	O2D-CGD	4.90	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	406[A]	CLA	O2D-CGD	4.90	1.45	1.33
23	c	511	CLA	O2D-CGD	4.90	1.45	1.33
23	b	604	CLA	C1D-ND	4.90	1.43	1.37
23	B	607	CLA	C3C-C2C	4.89	1.47	1.36
23	B	611	CLA	O2D-CGD	4.89	1.45	1.33
23	b	608	CLA	CHC-C1C	4.89	1.47	1.35
40	v	201	HEC	C3C-C2C	-4.89	1.35	1.40
25	y	101	BCR	C23-C22	-4.88	1.35	1.45
24	A	407[A]	PHO	C3D-C2D	4.88	1.48	1.39
23	d	402[A]	CLA	CHC-C1C	4.87	1.47	1.35
23	C	502	CLA	C1D-ND	4.87	1.43	1.37
23	c	506	CLA	O2D-CGD	4.87	1.45	1.33
23	c	504	CLA	C1D-ND	4.87	1.43	1.37
23	d	402[B]	CLA	CHC-C1C	4.87	1.47	1.35
23	A	405[A]	CLA	C3C-C2C	4.87	1.47	1.36
23	C	503	CLA	CHC-C1C	4.86	1.47	1.35
25	D	404	BCR	C23-C22	-4.86	1.35	1.45
23	B	606	CLA	C1D-ND	4.86	1.43	1.37
23	C	503	CLA	O2D-CGD	4.85	1.45	1.33
23	C	506	CLA	C3C-C2C	4.85	1.47	1.36
23	D	402[B]	CLA	CHC-C1C	4.85	1.47	1.35
24	a	414[A]	PHO	OBD-CAD	4.84	1.29	1.22
23	a	404[A]	CLA	CHC-C1C	4.84	1.47	1.35
23	C	510	CLA	O2D-CGD	4.84	1.45	1.33
23	b	607	CLA	CHC-C1C	4.83	1.47	1.35
25	c	515	BCR	C23-C22	-4.83	1.35	1.45
23	b	605	CLA	CHC-C1C	4.83	1.47	1.35
26	F	102	SQD	O47-C7	4.82	1.47	1.34
23	C	509	CLA	CHC-C1C	4.82	1.47	1.35
23	B	609	CLA	O2D-CGD	4.81	1.44	1.33
23	b	601	CLA	O2D-CGD	4.80	1.44	1.33
23	D	402[A]	CLA	O2D-CGD	4.80	1.44	1.33
23	A	404[A]	CLA	CHC-C1C	4.80	1.47	1.35
23	C	505	CLA	CHC-C1C	4.80	1.47	1.35
23	B	603	CLA	CHC-C1C	4.79	1.47	1.35
23	C	510	CLA	CHC-C1C	4.79	1.47	1.35
23	a	405[B]	CLA	C1D-ND	4.79	1.43	1.37
23	a	404[B]	CLA	CHC-C1C	4.79	1.47	1.35
23	B	614	CLA	O2D-CGD	4.78	1.44	1.33
23	C	511	CLA	O2D-CGD	4.78	1.44	1.33
23	B	607	CLA	CHC-C1C	4.77	1.47	1.35
23	b	602	CLA	CHD-C1D	4.77	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	615	CLA	CHD-C1D	4.77	1.47	1.38
23	b	611	CLA	O2D-CGD	4.77	1.44	1.33
23	C	509	CLA	C1D-ND	4.77	1.43	1.37
23	d	403[B]	CLA	O2D-CGD	4.77	1.44	1.33
23	b	615	CLA	O2D-CGD	4.77	1.44	1.33
23	b	605	CLA	C1D-ND	4.76	1.43	1.37
23	c	510	CLA	CHC-C1C	4.75	1.47	1.35
23	b	601	CLA	O2A-CGA	4.75	1.47	1.33
23	D	402[A]	CLA	CHC-C1C	4.75	1.47	1.35
23	a	405[B]	CLA	O2D-CGD	4.74	1.44	1.33
23	b	613	CLA	O2D-CGD	4.74	1.44	1.33
23	C	506	CLA	O2D-CGD	4.73	1.44	1.33
25	K	102	BCR	C23-C22	-4.73	1.35	1.45
23	A	404[A]	CLA	O2D-CGD	4.73	1.44	1.33
23	c	502	CLA	O2D-CGD	4.73	1.44	1.33
25	C	516	BCR	C23-C22	-4.73	1.35	1.45
23	B	616	CLA	O2D-CGD	4.73	1.44	1.33
23	B	605	CLA	O2D-CGD	4.73	1.44	1.33
23	B	613	CLA	C1D-ND	4.72	1.43	1.37
23	A	408	CLA	O2D-CGD	4.72	1.44	1.33
23	c	502	CLA	CHC-C1C	4.72	1.47	1.35
23	c	502	CLA	C1D-ND	4.72	1.43	1.37
23	b	609	CLA	C1D-ND	4.71	1.43	1.37
23	A	408	CLA	CHC-C1C	4.71	1.47	1.35
23	b	606	CLA	C1D-ND	4.71	1.43	1.37
23	b	616	CLA	O2D-CGD	4.71	1.44	1.33
23	c	507	CLA	O2D-CGD	4.69	1.44	1.33
23	B	614	CLA	CHC-C1C	4.69	1.47	1.35
23	C	505	CLA	C1D-ND	4.69	1.43	1.37
23	b	613	CLA	C1D-ND	4.68	1.43	1.37
25	B	617	BCR	C23-C22	-4.68	1.35	1.45
23	b	615	CLA	C1D-ND	4.67	1.43	1.37
23	d	403[A]	CLA	O2D-CGD	4.66	1.44	1.33
23	d	403[A]	CLA	CHC-C1C	4.66	1.46	1.35
33	c	520	LMG	O7-C10	4.65	1.47	1.34
23	c	512	CLA	O2D-CGD	4.64	1.44	1.33
25	b	619	BCR	C23-C22	-4.64	1.36	1.45
25	T	102	BCR	C23-C22	-4.64	1.36	1.45
23	b	608	CLA	O2D-CGD	4.63	1.44	1.33
25	A	409	BCR	C23-C22	-4.63	1.36	1.45
23	b	606	CLA	O2D-CGD	4.63	1.44	1.33
23	b	612	CLA	O2D-CGD	4.62	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	404[A]	CLA	C1D-ND	4.62	1.43	1.37
23	B	602	CLA	O2D-CGD	4.61	1.44	1.33
23	B	610	CLA	O2D-CGD	4.61	1.44	1.33
23	c	509	CLA	C1D-ND	4.61	1.43	1.37
23	C	512	CLA	C3C-C2C	4.61	1.46	1.36
33	C	521	LMG	O7-C10	4.60	1.47	1.34
25	H	101	BCR	C23-C22	-4.60	1.36	1.45
23	b	603	CLA	C1D-ND	4.60	1.43	1.37
23	a	404[B]	CLA	O2D-CGD	4.59	1.44	1.33
23	C	510	CLA	C1D-ND	4.59	1.43	1.37
23	d	403[B]	CLA	CHC-C1C	4.58	1.46	1.35
26	B	620	SQD	O47-C7	4.58	1.47	1.34
23	b	611	CLA	C1D-ND	4.58	1.43	1.37
23	c	505	CLA	O2D-CGD	4.57	1.44	1.33
25	b	617	BCR	C23-C22	-4.56	1.36	1.45
25	t	102	BCR	C23-C22	-4.56	1.36	1.45
23	b	610	CLA	C1D-ND	4.55	1.43	1.37
23	a	404[A]	CLA	O2D-CGD	4.54	1.44	1.33
23	B	606	CLA	O2D-CGD	4.53	1.44	1.33
23	C	507	CLA	CHC-C1C	4.53	1.46	1.35
25	c	514	BCR	C23-C22	-4.53	1.36	1.45
23	C	513	CLA	O2D-CGD	4.53	1.44	1.33
23	A	406[B]	CLA	C1D-ND	4.53	1.43	1.37
26	f	102	SQD	O47-C7	4.52	1.47	1.34
23	b	607	CLA	O2D-CGD	4.52	1.44	1.33
23	C	507	CLA	CHD-C1D	4.51	1.47	1.38
23	D	402[B]	CLA	C1D-ND	4.50	1.43	1.37
23	c	513	CLA	CHD-C1D	4.50	1.47	1.38
23	b	601	CLA	CHD-C1D	4.50	1.47	1.38
23	a	405[A]	CLA	O2D-CGD	4.50	1.44	1.33
33	C	521	LMG	O8-C28	4.49	1.46	1.33
23	B	603	CLA	O2D-CGD	4.49	1.44	1.33
23	C	507	CLA	C1D-ND	4.48	1.43	1.37
23	D	403	CLA	CHD-C1D	4.48	1.47	1.38
32	E	101[B]	LHG	O8-C23	4.48	1.46	1.33
23	c	509	CLA	CHC-C1C	4.48	1.46	1.35
32	E	101[A]	LHG	O8-C23	4.48	1.46	1.33
23	B	605	CLA	C3B-C2B	4.47	1.46	1.40
26	A	412	SQD	O48-C23	4.47	1.46	1.33
23	B	608	CLA	C1D-ND	4.47	1.43	1.37
23	b	611	CLA	O2A-CGA	4.47	1.46	1.33
23	B	604	CLA	CHD-C1D	4.47	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	612	CLA	C1D-ND	4.47	1.43	1.37
23	C	504	CLA	C1D-ND	4.46	1.43	1.37
24	A	407[B]	PHO	OBD-CAD	4.46	1.28	1.22
23	c	512	CLA	O2A-CGA	4.45	1.46	1.33
23	C	502	CLA	CHD-C1D	4.44	1.47	1.38
23	A	408	CLA	C1D-ND	4.44	1.43	1.37
23	c	511	CLA	CHD-C1D	4.44	1.47	1.38
23	B	608	CLA	CHC-C1C	4.44	1.46	1.35
25	b	618	BCR	C23-C22	-4.44	1.36	1.45
23	B	609	CLA	C1D-ND	4.44	1.43	1.37
25	Y	101	BCR	C23-C22	-4.43	1.36	1.45
25	a	408	BCR	C23-C22	-4.43	1.36	1.45
25	h	101	BCR	C23-C22	-4.43	1.36	1.45
33	z	101	LMG	O8-C28	4.42	1.46	1.33
23	C	512	CLA	C1D-ND	4.41	1.43	1.37
23	c	505	CLA	C1D-ND	4.41	1.43	1.37
23	B	602	CLA	CHD-C1D	4.41	1.46	1.38
23	B	609	CLA	CHD-C1D	4.40	1.46	1.38
23	B	608	CLA	CHD-C1D	4.40	1.46	1.38
33	B	621	LMG	O8-C28	4.40	1.46	1.33
23	b	609	CLA	CHD-C1D	4.40	1.46	1.38
32	a	419[A]	LHG	O8-C23	4.39	1.46	1.33
23	C	504	CLA	O2D-CGD	4.38	1.43	1.33
26	b	620	SQD	O47-C7	4.38	1.46	1.34
23	d	402[A]	CLA	C3D-C2D	4.38	1.51	1.39
23	C	508	CLA	O2A-CGA	4.37	1.46	1.33
23	C	508	CLA	O2D-CGD	4.37	1.43	1.33
23	c	508	CLA	O2A-CGA	4.37	1.46	1.33
23	c	508	CLA	CHD-C1D	4.37	1.46	1.38
26	a	410	SQD	O48-C23	4.36	1.46	1.33
24	a	406[A]	PHO	OBD-CAD	4.36	1.28	1.22
23	a	407	CLA	O2A-CGA	4.35	1.46	1.33
23	A	408	CLA	O2A-CGA	4.35	1.46	1.33
23	A	405[A]	CLA	O2D-CGD	4.35	1.43	1.33
23	c	513	CLA	O2A-CGA	4.34	1.46	1.33
23	C	506	CLA	CHD-C1D	4.34	1.46	1.38
32	a	419[B]	LHG	O8-C23	4.34	1.46	1.33
23	a	404[B]	CLA	CHD-C1D	4.33	1.46	1.38
23	d	404	CLA	O2D-CGD	4.32	1.43	1.33
24	A	416[A]	PHO	OBD-CAD	4.31	1.28	1.22
32	d	408[A]	LHG	O8-C23	4.31	1.45	1.33
23	c	512	CLA	CHD-C1D	4.31	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	C	520	LMG	O8-C28	4.30	1.45	1.33
23	B	611	CLA	CHD-C1D	4.30	1.46	1.38
23	C	502	CLA	O2A-CGA	4.29	1.45	1.33
23	d	402[B]	CLA	C3D-C2D	4.29	1.50	1.39
23	D	402[B]	CLA	O2A-CGA	4.28	1.45	1.33
23	B	615	CLA	C3D-C2D	4.27	1.50	1.39
23	A	404[B]	CLA	CHD-C1D	4.27	1.46	1.38
33	c	519	LMG	O7-C10	4.27	1.46	1.34
23	b	608	CLA	C1D-ND	4.27	1.43	1.37
23	D	402[A]	CLA	C1D-ND	4.27	1.43	1.37
23	a	405[B]	CLA	O2A-CGA	4.27	1.45	1.33
23	B	607	CLA	O2D-CGD	4.27	1.43	1.33
23	b	604	CLA	O2D-CGD	4.26	1.43	1.33
23	B	616	CLA	C1D-ND	4.26	1.43	1.37
32	d	408[B]	LHG	O8-C23	4.26	1.45	1.33
23	B	609	CLA	O2A-CGA	4.26	1.45	1.33
23	c	506	CLA	O2A-CGA	4.26	1.45	1.33
23	C	514	CLA	CHD-C1D	4.25	1.46	1.38
23	d	404	CLA	O2A-CGA	4.25	1.45	1.33
23	d	402[B]	CLA	CHD-C1D	4.25	1.46	1.38
26	B	620	SQD	O48-C23	4.25	1.45	1.33
23	C	510	CLA	CHD-C1D	4.25	1.46	1.38
26	f	102	SQD	O48-C23	4.25	1.45	1.33
23	C	509	CLA	O2A-CGA	4.24	1.45	1.33
23	d	404	CLA	CHD-C1D	4.24	1.46	1.38
23	A	405[B]	CLA	O2A-CGA	4.24	1.45	1.33
23	C	508	CLA	CHD-C1D	4.24	1.46	1.38
23	C	514	CLA	O2A-CGA	4.24	1.45	1.33
23	A	406[B]	CLA	CHD-C1D	4.23	1.46	1.38
26	b	620	SQD	O48-C23	4.23	1.45	1.33
33	c	520	LMG	O8-C28	4.22	1.45	1.33
23	A	404[A]	CLA	C1D-ND	4.22	1.43	1.37
23	D	402[A]	CLA	O2A-CGA	4.22	1.45	1.33
23	c	506	CLA	CHD-C1D	4.22	1.46	1.38
23	C	509	CLA	OBD-CAD	4.22	1.29	1.22
23	c	511	CLA	O2A-CGA	4.21	1.45	1.33
33	Z	101	LMG	O7-C10	4.21	1.46	1.34
23	b	610	CLA	CHD-C1D	4.19	1.46	1.38
23	C	513	CLA	CHD-C1D	4.19	1.46	1.38
23	c	503	CLA	CHD-C1D	4.19	1.46	1.38
33	m	101	LMG	O8-C28	4.19	1.45	1.33
23	c	507	CLA	CHD-C1D	4.19	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	E	101[A]	LHG	O7-C7	4.19	1.46	1.34
23	c	502	CLA	CHD-C1D	4.18	1.46	1.38
23	A	406[A]	CLA	CHD-C1D	4.18	1.46	1.38
23	b	602	CLA	CHD-C4C	4.18	1.48	1.39
23	c	503	CLA	O2D-CGD	4.17	1.43	1.33
23	c	505	CLA	CHD-C1D	4.17	1.46	1.38
32	E	101[B]	LHG	O7-C7	4.16	1.46	1.34
23	b	608	CLA	CHD-C1D	4.16	1.46	1.38
23	b	608	CLA	O2A-CGA	4.16	1.45	1.33
23	b	603	CLA	CHD-C1D	4.16	1.46	1.38
25	B	618	BCR	C23-C22	-4.16	1.37	1.45
23	b	615	CLA	CHD-C1D	4.16	1.46	1.38
23	a	404[B]	CLA	CHD-C4C	4.15	1.48	1.39
23	b	604	CLA	CHD-C1D	4.15	1.46	1.38
35	c	518	DGD	O1G-C1A	4.15	1.45	1.33
23	c	504	CLA	CHD-C1D	4.15	1.46	1.38
23	a	405[A]	CLA	C1D-ND	4.15	1.42	1.37
23	b	601	CLA	CHD-C4C	4.15	1.48	1.39
33	c	519	LMG	O8-C28	4.15	1.45	1.33
23	d	403[B]	CLA	C1D-ND	4.15	1.42	1.37
23	C	512	CLA	O2A-CGA	4.14	1.45	1.33
24	A	407[A]	PHO	OBD-CAD	4.14	1.28	1.22
32	a	419[B]	LHG	O7-C7	4.14	1.46	1.34
23	b	609	CLA	OBD-CAD	4.13	1.29	1.22
23	A	408	CLA	CHD-C4C	4.13	1.48	1.39
32	a	419[A]	LHG	O7-C7	4.13	1.46	1.34
33	a	415	LMG	O7-C10	4.13	1.46	1.34
23	B	606	CLA	CHD-C1D	4.12	1.46	1.38
23	a	405[A]	CLA	O2A-CGA	4.12	1.45	1.33
23	A	406[B]	CLA	O2A-CGA	4.12	1.45	1.33
35	c	517[B]	DGD	O1G-C1A	4.12	1.45	1.33
23	B	601	CLA	CHD-C1D	4.12	1.46	1.38
23	B	611	CLA	O2A-CGA	4.11	1.45	1.33
23	A	405[B]	CLA	CHD-C1D	4.11	1.46	1.38
23	C	503	CLA	CHD-C1D	4.11	1.46	1.38
23	b	601	CLA	C3D-C2D	4.11	1.50	1.39
32	D	407[B]	LHG	O8-C23	4.11	1.45	1.33
23	d	403[B]	CLA	O2A-CGA	4.10	1.45	1.33
35	c	516[B]	DGD	O2G-C1B	4.10	1.45	1.34
23	c	508	CLA	C3D-C2D	4.10	1.50	1.39
23	C	507	CLA	CHD-C4C	4.10	1.48	1.39
23	d	402[B]	CLA	O2A-CGA	4.09	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	509	CLA	C3D-C2D	4.09	1.50	1.39
23	B	610	CLA	OBD-CAD	4.09	1.29	1.22
23	B	614	CLA	O2A-CGA	4.09	1.45	1.33
35	c	516[A]	DGD	O2G-C1B	4.09	1.45	1.34
33	z	101	LMG	O7-C10	4.09	1.45	1.34
23	b	614	CLA	CHD-C1D	4.09	1.46	1.38
35	h	102	DGD	O2G-C1B	4.09	1.45	1.34
35	C	517[B]	DGD	O2G-C1B	4.09	1.45	1.34
23	C	511	CLA	CHD-C4C	4.08	1.48	1.39
23	d	402[A]	CLA	O2A-CGA	4.08	1.45	1.33
23	B	602	CLA	O2A-CGA	4.08	1.45	1.33
23	b	615	CLA	O2A-CGA	4.08	1.45	1.33
23	C	513	CLA	O2A-CGA	4.08	1.45	1.33
26	a	409[B]	SQD	O48-C23	4.07	1.45	1.33
26	a	409[A]	SQD	O47-C7	4.07	1.45	1.34
23	B	613	CLA	C3D-C2D	4.07	1.50	1.39
24	A	416[B]	PHO	O2A-CGA	4.06	1.45	1.33
23	C	510	CLA	C3D-C2D	4.06	1.50	1.39
35	C	517[A]	DGD	O2G-C1B	4.06	1.45	1.34
26	a	409[B]	SQD	O47-C7	4.06	1.45	1.34
32	L	101[B]	LHG	O8-C23	4.06	1.45	1.33
23	c	507	CLA	O2A-CGA	4.05	1.45	1.33
23	A	405[A]	CLA	C3D-C2D	4.05	1.50	1.39
23	d	403[A]	CLA	O2A-CGA	4.05	1.45	1.33
33	C	501	LMG	O7-C10	4.04	1.45	1.34
23	a	407	CLA	C1D-ND	4.04	1.42	1.37
23	b	606	CLA	CHD-C1D	4.04	1.46	1.38
23	C	503	CLA	C3D-C2D	4.04	1.50	1.39
24	A	416[A]	PHO	C3C-C2C	4.04	1.49	1.37
23	A	404[A]	CLA	CHD-C1D	4.03	1.46	1.38
26	a	410	SQD	O47-C7	4.03	1.45	1.34
23	c	504	CLA	C3D-C2D	4.03	1.50	1.39
26	A	412	SQD	O47-C7	4.03	1.45	1.34
23	c	506	CLA	CHD-C4C	4.03	1.48	1.39
33	a	415	LMG	O8-C28	4.02	1.45	1.33
23	b	613	CLA	C3D-C2D	4.02	1.50	1.39
23	A	406[A]	CLA	C1D-ND	4.02	1.42	1.37
23	c	501	CLA	O2D-CGD	4.02	1.43	1.33
23	c	502	CLA	O2A-CGA	4.01	1.45	1.33
23	A	405[B]	CLA	C3D-C2D	4.01	1.50	1.39
23	C	502	CLA	O2D-CGD	4.01	1.43	1.33
23	B	610	CLA	CHD-C1D	4.01	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	O2A-CGA	4.01	1.45	1.33
23	B	608	CLA	O2D-CGD	4.01	1.43	1.33
23	c	503	CLA	CHD-C4C	4.00	1.48	1.39
23	B	615	CLA	CHD-C4C	4.00	1.48	1.39
23	A	408	CLA	CHD-C1D	4.00	1.46	1.38
23	b	612	CLA	OBD-CAD	4.00	1.29	1.22
23	c	501	CLA	CHD-C1D	4.00	1.46	1.38
23	B	612	CLA	O2D-CGD	4.00	1.42	1.33
33	C	501	LMG	O8-C28	3.99	1.45	1.33
32	d	414[B]	LHG	O8-C23	3.99	1.45	1.33
23	b	616	CLA	O2A-CGA	3.99	1.45	1.33
23	C	512	CLA	CHD-C1D	3.99	1.46	1.38
23	a	404[A]	CLA	CHD-C1D	3.99	1.46	1.38
23	A	404[B]	CLA	CHD-C4C	3.99	1.48	1.39
23	B	615	CLA	O2A-CGA	3.99	1.45	1.33
23	b	615	CLA	CHD-C4C	3.99	1.48	1.39
23	d	402[B]	CLA	CHD-C4C	3.99	1.48	1.39
32	D	407[A]	LHG	O7-C7	3.98	1.45	1.34
23	c	513	CLA	CHD-C4C	3.98	1.48	1.39
26	a	409[A]	SQD	O48-C23	3.98	1.45	1.33
23	c	512	CLA	CHD-C4C	3.98	1.48	1.39
23	c	512	CLA	C3D-C2D	3.98	1.50	1.39
23	B	615	CLA	OBD-CAD	3.97	1.29	1.22
23	c	503	CLA	O2A-CGA	3.97	1.45	1.33
24	a	414[A]	PHO	C3C-C2C	3.97	1.49	1.37
23	D	402[B]	CLA	CHD-C1D	3.97	1.46	1.38
23	c	507	CLA	CHD-C4C	3.96	1.48	1.39
24	A	416[B]	PHO	C3C-C2C	3.96	1.49	1.37
23	c	504	CLA	O2A-CGA	3.96	1.44	1.33
35	C	518[B]	DGD	O1G-C1A	3.96	1.44	1.33
24	a	414[B]	PHO	C3C-C2C	3.96	1.49	1.37
23	c	508	CLA	OBD-CAD	3.96	1.29	1.22
23	a	404[A]	CLA	CHD-C4C	3.96	1.48	1.39
23	b	607	CLA	CHD-C1D	3.96	1.46	1.38
23	c	511	CLA	OBD-CAD	3.96	1.29	1.22
32	L	101[B]	LHG	O7-C7	3.95	1.45	1.34
33	d	412	LMG	O8-C28	3.95	1.44	1.33
23	c	506	CLA	C3D-C2D	3.95	1.49	1.39
26	A	410[B]	SQD	O48-C23	3.95	1.44	1.33
23	c	507	CLA	OBD-CAD	3.94	1.29	1.22
23	C	505	CLA	C3D-C2D	3.94	1.49	1.39
23	B	602	CLA	C3D-C2D	3.94	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	405[B]	CLA	C3D-C2D	3.94	1.49	1.39
23	B	602	CLA	CHD-C4C	3.94	1.48	1.39
23	D	403	CLA	C3D-C2D	3.94	1.49	1.39
23	B	614	CLA	CHD-C4C	3.93	1.48	1.39
23	b	607	CLA	C1D-ND	3.93	1.42	1.37
26	F	102	SQD	O48-C23	3.92	1.44	1.33
35	C	519	DGD	O1G-C1A	3.92	1.44	1.33
23	D	402[A]	CLA	CHD-C1D	3.92	1.46	1.38
23	C	503	CLA	O2A-CGA	3.92	1.44	1.33
23	B	609	CLA	C3D-C2D	3.92	1.49	1.39
23	A	406[B]	CLA	C3D-C2D	3.91	1.49	1.39
23	B	616	CLA	C3D-C2D	3.91	1.49	1.39
23	C	514	CLA	C3D-C2D	3.91	1.49	1.39
23	c	501	CLA	C3D-C2D	3.91	1.49	1.39
23	B	616	CLA	O2A-CGA	3.91	1.44	1.33
23	b	615	CLA	C3D-C2D	3.91	1.49	1.39
23	C	511	CLA	O2A-CGA	3.91	1.44	1.33
23	c	502	CLA	C3D-C2D	3.91	1.49	1.39
33	C	520	LMG	O7-C10	3.91	1.45	1.34
23	B	611	CLA	OBD-CAD	3.91	1.29	1.22
23	C	507	CLA	C3D-C2D	3.91	1.49	1.39
32	D	407[A]	LHG	O8-C23	3.90	1.44	1.33
23	B	613	CLA	OBD-CAD	3.90	1.29	1.22
23	c	501	CLA	CHD-C4C	3.90	1.48	1.39
23	b	606	CLA	O2A-CGA	3.90	1.44	1.33
23	c	508	CLA	CHD-C4C	3.90	1.48	1.39
23	c	509	CLA	CHD-C1D	3.90	1.46	1.38
23	A	408	CLA	C3D-C2D	3.90	1.49	1.39
23	a	405[A]	CLA	C3D-C2D	3.90	1.49	1.39
23	D	402[A]	CLA	CHD-C4C	3.89	1.48	1.39
23	c	510	CLA	O2A-CGA	3.89	1.44	1.33
23	c	502	CLA	CHD-C4C	3.89	1.48	1.39
23	A	405[A]	CLA	C1D-ND	3.89	1.42	1.37
23	B	604	CLA	C1D-ND	3.88	1.42	1.37
23	c	513	CLA	C3D-C2D	3.88	1.49	1.39
23	C	504	CLA	CHD-C4C	3.88	1.48	1.39
23	C	504	CLA	O2A-CGA	3.87	1.44	1.33
23	B	605	CLA	O2A-CGA	3.87	1.44	1.33
24	a	414[B]	PHO	O2A-CGA	3.87	1.44	1.33
23	c	510	CLA	CHD-C1D	3.87	1.45	1.38
23	c	509	CLA	O2A-CGA	3.86	1.44	1.33
23	A	406[B]	CLA	CHD-C4C	3.86	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	506	CLA	CHD-C4C	3.86	1.48	1.39
24	A	407[B]	PHO	O2A-CGA	3.86	1.44	1.33
24	A	416[A]	PHO	O2A-CGA	3.86	1.44	1.33
23	D	402[B]	CLA	CHD-C4C	3.86	1.48	1.39
35	c	516[B]	DGD	O1G-C1A	3.85	1.44	1.33
33	B	621	LMG	O7-C10	3.85	1.45	1.34
35	C	518[B]	DGD	O2G-C1B	3.85	1.45	1.34
23	C	510	CLA	CHD-C4C	3.85	1.48	1.39
23	C	513	CLA	C3D-C2D	3.85	1.49	1.39
23	C	514	CLA	CHD-C4C	3.85	1.48	1.39
23	B	603	CLA	C3D-C2D	3.85	1.49	1.39
35	C	518[A]	DGD	O2G-C1B	3.85	1.45	1.34
26	A	410[A]	SQD	O48-C23	3.85	1.44	1.33
23	b	608	CLA	C3D-C2D	3.85	1.49	1.39
32	b	629[B]	LHG	O7-C7	3.84	1.45	1.34
35	H	102	DGD	O1G-C1A	3.84	1.44	1.33
23	b	616	CLA	CHD-C1D	3.84	1.45	1.38
32	d	407[B]	LHG	O7-C7	3.84	1.45	1.34
32	L	101[A]	LHG	O8-C23	3.84	1.44	1.33
23	C	510	CLA	O2A-CGA	3.84	1.44	1.33
23	C	504	CLA	CHD-C1D	3.84	1.45	1.38
23	A	406[A]	CLA	C3D-C2D	3.84	1.49	1.39
35	c	517[A]	DGD	O1G-C1A	3.83	1.44	1.33
23	b	607	CLA	C3D-C2D	3.83	1.49	1.39
23	A	405[A]	CLA	O2A-CGA	3.83	1.44	1.33
23	b	604	CLA	C3D-C2D	3.83	1.49	1.39
23	b	602	CLA	O2A-CGA	3.83	1.44	1.33
24	a	414[A]	PHO	O2A-CGA	3.83	1.44	1.33
23	c	507	CLA	C3D-C2D	3.83	1.49	1.39
23	c	511	CLA	C3D-C2D	3.83	1.49	1.39
23	c	505	CLA	C3D-C2D	3.82	1.49	1.39
23	c	501	CLA	O2A-CGA	3.82	1.44	1.33
23	B	611	CLA	C3D-C2D	3.82	1.49	1.39
32	L	101[A]	LHG	O7-C7	3.82	1.45	1.34
32	D	406[B]	LHG	O7-C7	3.82	1.45	1.34
23	C	512	CLA	C3D-C2D	3.82	1.49	1.39
23	b	605	CLA	CHD-C4C	3.81	1.47	1.39
32	D	407[B]	LHG	O7-C7	3.81	1.45	1.34
23	A	405[B]	CLA	CHD-C4C	3.81	1.47	1.39
32	b	629[B]	LHG	O8-C23	3.81	1.44	1.33
23	d	403[A]	CLA	CHD-C1D	3.81	1.45	1.38
35	C	517[B]	DGD	O1G-C1A	3.81	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	605	CLA	CHD-C4C	3.81	1.47	1.39
23	b	611	CLA	CHD-C1D	3.80	1.45	1.38
23	c	510	CLA	C3D-C2D	3.80	1.49	1.39
23	d	404	CLA	C3D-C2D	3.80	1.49	1.39
23	b	613	CLA	O2A-CGA	3.80	1.44	1.33
23	C	510	CLA	OBD-CAD	3.80	1.29	1.22
33	d	412	LMG	O7-C10	3.80	1.45	1.34
23	B	611	CLA	C1C-C2C	3.80	1.51	1.44
23	A	406[A]	CLA	O2A-CGA	3.80	1.44	1.33
23	d	402[A]	CLA	CHD-C1D	3.80	1.45	1.38
23	c	510	CLA	CHD-C4C	3.80	1.47	1.39
23	a	405[B]	CLA	CHD-C1D	3.80	1.45	1.38
23	B	608	CLA	C3D-C2D	3.79	1.49	1.39
23	B	601	CLA	CHD-C4C	3.79	1.47	1.39
24	A	416[A]	PHO	CHA-CBD	-3.79	1.47	1.52
23	c	505	CLA	CHD-C4C	3.78	1.47	1.39
23	b	609	CLA	CHD-C4C	3.78	1.47	1.39
35	c	517[B]	DGD	O2G-C1B	3.78	1.45	1.34
23	C	509	CLA	CHD-C1D	3.78	1.45	1.38
23	B	605	CLA	C3D-C2D	3.78	1.49	1.39
32	d	408[B]	LHG	O7-C7	3.78	1.45	1.34
23	B	607	CLA	CHD-C1D	3.78	1.45	1.38
23	B	610	CLA	CHD-C4C	3.78	1.47	1.39
23	b	608	CLA	OBD-CAD	3.78	1.29	1.22
23	B	610	CLA	C3D-C2D	3.78	1.49	1.39
23	b	604	CLA	CHD-C4C	3.78	1.47	1.39
23	C	512	CLA	CHD-C4C	3.77	1.47	1.39
23	d	402[A]	CLA	OBD-CAD	3.77	1.29	1.22
24	A	407[B]	PHO	C3C-C2C	3.77	1.48	1.37
23	b	610	CLA	CHD-C4C	3.77	1.47	1.39
23	c	505	CLA	OBD-CAD	3.77	1.29	1.22
23	B	604	CLA	OBD-CAD	3.76	1.29	1.22
23	d	402[B]	CLA	OBD-CAD	3.76	1.29	1.22
23	c	511	CLA	CHD-C4C	3.76	1.47	1.39
35	h	102	DGD	O1G-C1A	3.76	1.44	1.33
34	B	622	HTG	C1'-S1	-3.75	1.76	1.81
23	b	612	CLA	CHD-C1D	3.75	1.45	1.38
23	A	406[B]	CLA	OBD-CAD	3.75	1.28	1.22
23	b	610	CLA	C3D-C2D	3.75	1.49	1.39
32	d	414[A]	LHG	O8-C23	3.75	1.44	1.33
23	a	405[B]	CLA	OBD-CAD	3.75	1.28	1.22
23	C	502	CLA	CHD-C4C	3.74	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	604	CLA	CHD-C4C	3.74	1.47	1.39
23	d	404	CLA	OBD-CAD	3.74	1.28	1.22
23	B	604	CLA	O2A-CGA	3.74	1.44	1.33
23	b	602	CLA	C3D-C2D	3.74	1.49	1.39
23	A	406[A]	CLA	OBD-CAD	3.74	1.28	1.22
23	b	605	CLA	CHD-C1D	3.73	1.45	1.38
23	D	403	CLA	CHD-C4C	3.73	1.47	1.39
23	A	404[A]	CLA	CHD-C4C	3.73	1.47	1.39
23	b	614	CLA	CHD-C4C	3.73	1.47	1.39
23	C	513	CLA	CHD-C4C	3.72	1.47	1.39
32	d	407[A]	LHG	O7-C7	3.72	1.44	1.34
33	m	101	LMG	O7-C10	3.72	1.44	1.34
23	A	405[A]	CLA	CHD-C1D	3.72	1.45	1.38
23	B	612	CLA	CHD-C1D	3.72	1.45	1.38
23	b	603	CLA	CHD-C4C	3.71	1.47	1.39
35	C	518[A]	DGD	O1G-C1A	3.71	1.44	1.33
23	c	512	CLA	OBD-CAD	3.71	1.28	1.22
23	b	615	CLA	OBD-CAD	3.71	1.28	1.22
23	B	612	CLA	O2A-CGA	3.71	1.44	1.33
23	B	607	CLA	CHD-C4C	3.71	1.47	1.39
32	d	407[B]	LHG	O8-C23	3.71	1.44	1.33
23	c	504	CLA	CHD-C4C	3.71	1.47	1.39
23	d	403[B]	CLA	CHD-C4C	3.70	1.47	1.39
23	B	607	CLA	C1D-ND	3.70	1.42	1.37
23	B	609	CLA	CHD-C4C	3.70	1.47	1.39
32	A	419[B]	LHG	O7-C7	3.70	1.44	1.34
23	D	403	CLA	O2A-CGA	3.70	1.44	1.33
34	b	622	HTG	C1'-S1	-3.70	1.76	1.81
23	C	511	CLA	CHD-C1D	3.69	1.45	1.38
32	A	419[B]	LHG	O8-C23	3.69	1.44	1.33
23	c	505	CLA	O2A-CGA	3.69	1.44	1.33
35	C	519	DGD	O2G-C1B	3.69	1.44	1.34
23	b	601	CLA	OBD-CAD	3.69	1.28	1.22
23	b	603	CLA	O2A-CGA	3.69	1.44	1.33
24	A	407[A]	PHO	C3C-C2C	3.68	1.48	1.37
26	A	410[A]	SQD	O47-C7	3.68	1.44	1.34
23	a	405[A]	CLA	OBD-CAD	3.68	1.28	1.22
23	b	605	CLA	C3D-C2D	3.68	1.49	1.39
23	b	616	CLA	C3D-C2D	3.68	1.49	1.39
23	B	603	CLA	CHD-C4C	3.67	1.47	1.39
23	B	603	CLA	O2A-CGA	3.67	1.44	1.33
32	d	414[B]	LHG	O7-C7	3.67	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	505	CLA	CHD-C4C	3.67	1.47	1.39
23	C	503	CLA	CHD-C4C	3.67	1.47	1.39
23	A	406[A]	CLA	CHD-C4C	3.67	1.47	1.39
33	D	411	LMG	O8-C28	3.66	1.44	1.33
23	B	603	CLA	OBD-CAD	3.66	1.28	1.22
23	a	404[A]	CLA	C3D-C2D	3.66	1.49	1.39
23	a	404[B]	CLA	OBD-CAD	3.66	1.28	1.22
23	C	502	CLA	C3D-C2D	3.66	1.49	1.39
32	d	408[A]	LHG	O7-C7	3.66	1.44	1.34
23	C	505	CLA	CHD-C1D	3.66	1.45	1.38
23	a	404[B]	CLA	O2A-CGA	3.66	1.44	1.33
23	B	603	CLA	CHD-C1D	3.65	1.45	1.38
23	b	614	CLA	C3D-C2D	3.65	1.49	1.39
23	B	613	CLA	CHD-C1D	3.64	1.45	1.38
24	a	406[B]	PHO	C3C-C2C	3.64	1.48	1.37
23	b	607	CLA	CHD-C4C	3.64	1.47	1.39
24	A	407[A]	PHO	O2A-CGA	3.64	1.44	1.33
23	A	404[B]	CLA	C3D-C2D	3.64	1.49	1.39
23	B	601	CLA	C3D-C2D	3.64	1.49	1.39
23	C	506	CLA	O2A-CGA	3.64	1.44	1.33
23	B	612	CLA	C1D-ND	3.64	1.42	1.37
23	b	604	CLA	OBD-CAD	3.63	1.28	1.22
23	A	404[A]	CLA	C3D-C2D	3.63	1.49	1.39
23	B	605	CLA	CHD-C1D	3.63	1.45	1.38
23	B	611	CLA	C4B-NB	-3.63	1.32	1.35
23	C	507	CLA	OBD-CAD	3.63	1.28	1.22
23	b	602	CLA	OBD-CAD	3.63	1.28	1.22
23	b	613	CLA	CHD-C1D	3.63	1.45	1.38
24	a	406[A]	PHO	C3C-C2C	3.62	1.48	1.37
23	C	508	CLA	C3D-C2D	3.62	1.49	1.39
23	a	404[B]	CLA	C3D-C2D	3.62	1.49	1.39
35	c	516[A]	DGD	O1G-C1A	3.62	1.43	1.33
23	c	509	CLA	CHD-C4C	3.62	1.47	1.39
23	d	403[B]	CLA	CHD-C1D	3.62	1.45	1.38
23	b	608	CLA	CHD-C4C	3.62	1.47	1.39
23	d	402[A]	CLA	CHD-C4C	3.62	1.47	1.39
32	b	629[A]	LHG	O7-C7	3.62	1.44	1.34
23	a	404[A]	CLA	OBD-CAD	3.61	1.28	1.22
23	c	509	CLA	C3D-C2D	3.61	1.49	1.39
23	D	403	CLA	OBD-CAD	3.61	1.28	1.22
23	B	606	CLA	C3D-C2D	3.60	1.49	1.39
23	b	606	CLA	C3D-C2D	3.60	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	D	406[A]	LHG	O7-C7	3.60	1.44	1.34
23	b	609	CLA	O2A-CGA	3.60	1.43	1.33
23	C	511	CLA	C3D-C2D	3.60	1.48	1.39
23	b	616	CLA	CHD-C4C	3.60	1.47	1.39
23	B	606	CLA	O2A-CGA	3.59	1.43	1.33
34	b	623	HTG	C1'-S1	-3.59	1.76	1.81
26	A	410[B]	SQD	O47-C7	3.59	1.44	1.34
32	D	406[B]	LHG	O8-C23	3.59	1.43	1.33
23	b	611	CLA	C3D-C2D	3.59	1.48	1.39
23	B	611	CLA	CHD-C4C	3.58	1.47	1.39
23	B	607	CLA	OBD-CAD	3.58	1.28	1.22
23	a	405[A]	CLA	CHD-C4C	3.58	1.47	1.39
23	b	612	CLA	C3D-C2D	3.58	1.48	1.39
23	C	506	CLA	C3D-C2D	3.58	1.48	1.39
23	A	404[B]	CLA	O2A-CGA	3.57	1.43	1.33
23	d	403[A]	CLA	CHD-C4C	3.57	1.47	1.39
23	b	611	CLA	CHD-C4C	3.57	1.47	1.39
23	C	508	CLA	CHD-C4C	3.56	1.47	1.39
23	a	407	CLA	CHD-C1D	3.56	1.45	1.38
23	A	405[A]	CLA	CHD-C4C	3.56	1.47	1.39
23	B	616	CLA	CHD-C1D	3.55	1.45	1.38
24	a	406[B]	PHO	O2A-CGA	3.55	1.43	1.33
23	b	609	CLA	C3D-C2D	3.55	1.48	1.39
35	c	518	DGD	O2G-C1B	3.55	1.44	1.34
35	C	517[A]	DGD	O1G-C1A	3.55	1.43	1.33
23	d	403[A]	CLA	C3D-C2D	3.55	1.48	1.39
23	B	614	CLA	CHD-C1D	3.55	1.45	1.38
23	b	614	CLA	O2A-CGA	3.55	1.43	1.33
23	a	405[B]	CLA	CHD-C4C	3.55	1.47	1.39
23	b	606	CLA	CHD-C4C	3.54	1.47	1.39
23	D	402[B]	CLA	C3D-C2D	3.54	1.48	1.39
23	A	405[B]	CLA	OBD-CAD	3.54	1.28	1.22
23	a	405[A]	CLA	CHD-C1D	3.54	1.45	1.38
23	b	603	CLA	OBD-CAD	3.54	1.28	1.22
38	E	102	HEM	C1B-NB	-3.54	1.34	1.40
23	C	513	CLA	OBD-CAD	3.54	1.28	1.22
35	c	517[A]	DGD	O2G-C1B	3.53	1.44	1.34
23	B	612	CLA	C3D-C2D	3.53	1.48	1.39
32	d	407[A]	LHG	O8-C23	3.53	1.43	1.33
23	C	514	CLA	OBD-CAD	3.53	1.28	1.22
32	D	406[A]	LHG	O8-C23	3.53	1.43	1.33
23	d	403[B]	CLA	C3D-C2D	3.52	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	D	411	LMG	O7-C10	3.52	1.44	1.34
23	b	610	CLA	OBD-CAD	3.52	1.28	1.22
32	A	419[A]	LHG	O8-C23	3.52	1.43	1.33
23	b	603	CLA	C3D-C2D	3.52	1.48	1.39
38	f	101	HEM	C4D-ND	-3.52	1.34	1.40
23	b	612	CLA	O2A-CGA	3.51	1.43	1.33
32	d	414[A]	LHG	O7-C7	3.50	1.44	1.34
32	A	419[A]	LHG	O7-C7	3.49	1.44	1.34
23	B	608	CLA	CHD-C4C	3.49	1.47	1.39
32	b	629[A]	LHG	O8-C23	3.49	1.43	1.33
23	D	402[B]	CLA	OBD-CAD	3.49	1.28	1.22
23	c	502	CLA	OBD-CAD	3.48	1.28	1.22
23	c	509	CLA	OBD-CAD	3.48	1.28	1.22
23	b	607	CLA	O2A-CGA	3.47	1.43	1.33
23	B	607	CLA	O2A-CGA	3.47	1.43	1.33
23	c	506	CLA	OBD-CAD	3.46	1.28	1.22
23	c	503	CLA	C3D-C2D	3.46	1.48	1.39
23	B	613	CLA	CHD-C4C	3.45	1.47	1.39
23	C	503	CLA	OBD-CAD	3.45	1.28	1.22
23	B	601	CLA	OBD-CAD	3.44	1.28	1.22
23	B	608	CLA	O2A-CGA	3.44	1.43	1.33
23	D	402[A]	CLA	C3D-C2D	3.43	1.48	1.39
23	B	610	CLA	O2A-CGA	3.43	1.43	1.33
23	C	509	CLA	CHD-C4C	3.42	1.47	1.39
23	B	606	CLA	CHD-C4C	3.42	1.47	1.39
23	C	504	CLA	C3D-C2D	3.42	1.48	1.39
23	d	404	CLA	CHD-C4C	3.42	1.47	1.39
23	C	505	CLA	O2A-CGA	3.42	1.43	1.33
23	d	403[A]	CLA	OBD-CAD	3.41	1.28	1.22
23	b	616	CLA	OBD-CAD	3.41	1.28	1.22
23	C	505	CLA	OBD-CAD	3.41	1.28	1.22
23	B	602	CLA	OBD-CAD	3.40	1.28	1.22
23	c	513	CLA	OBD-CAD	3.40	1.28	1.22
23	B	614	CLA	C4B-NB	-3.39	1.32	1.35
24	a	406[A]	PHO	O2A-CGA	3.39	1.43	1.33
23	b	604	CLA	O2A-CGA	3.39	1.43	1.33
38	f	101	HEM	C1B-NB	-3.39	1.34	1.40
23	b	605	CLA	O2A-CGA	3.38	1.43	1.33
23	B	612	CLA	CHD-C4C	3.38	1.46	1.39
23	B	611	CLA	C4B-CHC	3.38	1.50	1.41
35	H	102	DGD	O2G-C1B	3.37	1.43	1.34
23	B	614	CLA	C3D-C2D	3.36	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	403[B]	CLA	OBD-CAD	3.36	1.28	1.22
23	A	404[A]	CLA	OBD-CAD	3.34	1.28	1.22
23	c	510	CLA	OBD-CAD	3.33	1.28	1.22
23	a	407	CLA	CHD-C4C	3.33	1.46	1.39
23	B	613	CLA	O2A-CGA	3.31	1.43	1.33
23	b	606	CLA	OBD-CAD	3.31	1.28	1.22
23	C	504	CLA	OBD-CAD	3.30	1.28	1.22
23	B	609	CLA	OBD-CAD	3.29	1.28	1.22
23	B	602	CLA	C1C-C2C	3.28	1.50	1.44
23	d	403[A]	CLA	C1D-ND	3.27	1.41	1.37
34	B	625	HTG	C1'-S1	-3.27	1.77	1.81
23	D	402[A]	CLA	OBD-CAD	3.26	1.28	1.22
23	b	613	CLA	CHD-C4C	3.26	1.46	1.39
23	B	612	CLA	C1C-C2C	3.26	1.50	1.44
23	C	511	CLA	OBD-CAD	3.24	1.28	1.22
23	b	605	CLA	OBD-CAD	3.24	1.28	1.22
23	B	612	CLA	C1B-NB	-3.24	1.32	1.35
23	B	606	CLA	OBD-CAD	3.24	1.28	1.22
23	B	607	CLA	C3D-C2D	3.22	1.47	1.39
23	A	404[B]	CLA	OBD-CAD	3.22	1.28	1.22
23	B	616	CLA	OBD-CAD	3.21	1.28	1.22
34	D	410	HTG	C1'-S1	-3.20	1.77	1.81
23	b	612	CLA	CHD-C4C	3.20	1.46	1.39
23	A	404[A]	CLA	O2A-CGA	3.19	1.42	1.33
23	C	506	CLA	OBD-CAD	3.19	1.28	1.22
38	E	102	HEM	C4D-ND	-3.18	1.34	1.40
23	C	502	CLA	OBD-CAD	3.18	1.28	1.22
34	d	411	HTG	C1'-S1	-3.18	1.77	1.81
23	b	610	CLA	O2A-CGA	3.17	1.42	1.33
23	B	616	CLA	CHD-C4C	3.16	1.46	1.39
34	c	521	HTG	C1'-S1	-3.15	1.77	1.81
23	B	608	CLA	OBD-CAD	3.14	1.27	1.22
23	c	501	CLA	OBD-CAD	3.13	1.27	1.22
34	b	625	HTG	C1'-S1	-3.12	1.77	1.81
23	C	508	CLA	OBD-CAD	3.12	1.27	1.22
23	A	405[A]	CLA	OBD-CAD	3.12	1.27	1.22
24	A	407[B]	PHO	CHA-CBD	-3.12	1.48	1.52
24	A	416[B]	PHO	CHA-CBD	-3.12	1.48	1.52
23	B	612	CLA	OBD-CAD	3.11	1.27	1.22
23	B	614	CLA	OBD-CAD	3.10	1.27	1.22
23	a	404[A]	CLA	O2A-CGA	3.07	1.42	1.33
23	D	403	CLA	C1C-C2C	3.06	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	504	CLA	OBD-CAD	3.05	1.27	1.22
23	C	512	CLA	OBD-CAD	3.04	1.27	1.22
23	b	611	CLA	OBD-CAD	3.03	1.27	1.22
23	B	605	CLA	OBD-CAD	3.03	1.27	1.22
23	A	408	CLA	OBD-CAD	3.03	1.27	1.22
23	C	512	CLA	C4D-CHA	3.02	1.49	1.38
23	B	607	CLA	C1B-NB	-3.02	1.32	1.35
23	a	407	CLA	C1C-C2C	3.02	1.50	1.44
23	B	604	CLA	C3D-C2D	3.00	1.47	1.39
23	B	612	CLA	C1B-CHB	2.99	1.49	1.41
23	a	407	CLA	C3D-C2D	2.99	1.47	1.39
23	C	513	CLA	C1C-C2C	2.98	1.50	1.44
23	a	407	CLA	OBD-CAD	2.97	1.27	1.22
23	b	602	CLA	C1C-C2C	2.97	1.50	1.44
23	c	509	CLA	C1B-NB	-2.97	1.32	1.35
23	A	404[A]	CLA	C4C-C3C	2.96	1.50	1.45
23	B	605	CLA	C4B-CHC	2.96	1.49	1.41
23	b	612	CLA	C1C-C2C	2.95	1.50	1.44
23	c	510	CLA	C1C-C2C	2.94	1.50	1.44
23	c	503	CLA	C1C-C2C	2.94	1.50	1.44
23	b	614	CLA	OBD-CAD	2.93	1.27	1.22
23	A	405[B]	CLA	C1C-C2C	2.92	1.50	1.44
23	B	606	CLA	C1C-C2C	2.92	1.50	1.44
34	b	625	HTG	C1-S1	-2.92	1.76	1.80
23	b	604	CLA	C4B-CHC	2.90	1.49	1.41
23	A	408	CLA	C4D-CHA	2.89	1.48	1.38
23	C	505	CLA	C4D-CHA	2.89	1.48	1.38
23	B	614	CLA	C1B-CHB	2.88	1.49	1.41
23	B	615	CLA	C1C-C2C	2.87	1.50	1.44
23	d	404	CLA	C1C-C2C	2.87	1.50	1.44
23	c	505	CLA	C4C-C3C	2.86	1.50	1.45
26	a	409[B]	SQD	C6-S	-2.86	1.66	1.77
35	H	102	DGD	O5D-C1E	2.85	1.45	1.40
34	C	522	HTG	C1'-S1	-2.85	1.77	1.81
23	c	501	CLA	C1C-C2C	2.85	1.50	1.44
23	C	508	CLA	C4D-CHA	2.85	1.48	1.38
27	A	418	GOL	O2-C2	-2.85	1.34	1.43
23	c	508	CLA	C1C-C2C	2.84	1.50	1.44
23	C	512	CLA	C1C-C2C	2.83	1.50	1.44
23	B	614	CLA	C3D-C4D	-2.83	1.37	1.44
24	A	407[A]	PHO	CBD-CGD	-2.83	1.48	1.52
23	B	604	CLA	C4D-CHA	2.82	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	C1C-C2C	2.82	1.50	1.44
23	B	609	CLA	C1C-C2C	2.81	1.50	1.44
23	C	513	CLA	C4B-CHC	2.80	1.48	1.41
23	a	405[B]	CLA	C1C-C2C	2.79	1.50	1.44
23	b	602	CLA	C4B-CHC	2.79	1.48	1.41
23	B	607	CLA	C4D-CHA	2.79	1.48	1.38
23	b	612	CLA	C1B-CHB	2.79	1.48	1.41
23	C	506	CLA	C4D-CHA	2.78	1.48	1.38
23	c	505	CLA	C1C-C2C	2.77	1.49	1.44
23	b	613	CLA	OBD-CAD	2.77	1.27	1.22
23	C	510	CLA	C4B-NB	-2.77	1.32	1.35
29	A	414[A]	PL9	C6-C5	2.76	1.49	1.35
23	B	612	CLA	C4D-CHA	2.76	1.48	1.38
23	b	616	CLA	C1C-C2C	2.76	1.49	1.44
23	b	604	CLA	C4D-CHA	2.76	1.48	1.38
29	A	414[B]	PL9	C6-C5	2.76	1.49	1.35
23	c	511	CLA	C1C-C2C	2.75	1.49	1.44
29	a	412[A]	PL9	C6-C5	2.75	1.49	1.35
23	c	503	CLA	OBD-CAD	2.75	1.27	1.22
23	b	610	CLA	C1B-CHB	2.75	1.48	1.41
23	d	403[A]	CLA	C1B-CHB	2.75	1.48	1.41
23	B	607	CLA	C1C-C2C	2.75	1.49	1.44
24	a	414[B]	PHO	CHA-CBD	-2.74	1.49	1.52
23	c	503	CLA	C4B-CHC	2.74	1.48	1.41
23	b	604	CLA	C1C-C2C	2.74	1.49	1.44
23	B	615	CLA	C4D-CHA	2.74	1.48	1.38
26	a	409[A]	SQD	C6-S	-2.73	1.67	1.77
33	Z	101	LMG	O8-C28	2.73	1.46	1.33
26	A	410[A]	SQD	C6-S	-2.73	1.67	1.77
23	C	506	CLA	C1C-C2C	2.73	1.49	1.44
23	c	504	CLA	C1C-C2C	2.73	1.49	1.44
23	A	406[A]	CLA	C4D-CHA	2.72	1.48	1.38
23	a	405[A]	CLA	C1C-C2C	2.72	1.49	1.44
23	b	613	CLA	C4D-CHA	2.72	1.48	1.38
23	B	605	CLA	C3D-C4D	-2.72	1.38	1.44
38	f	101	HEM	FE-NB	2.72	2.10	1.96
23	B	601	CLA	C4B-CHC	2.72	1.48	1.41
29	a	412[B]	PL9	C6-C5	2.72	1.49	1.35
23	B	611	CLA	C1B-CHB	2.72	1.48	1.41
23	b	610	CLA	C4D-CHA	2.72	1.48	1.38
23	c	508	CLA	C4C-C3C	2.72	1.49	1.45
23	C	503	CLA	C1C-C2C	2.72	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	402[A]	CLA	C4D-CHA	2.71	1.48	1.38
23	d	404	CLA	C4B-CHC	2.71	1.48	1.41
23	D	403	CLA	C4C-C3C	2.71	1.49	1.45
23	B	610	CLA	C1B-CHB	2.71	1.48	1.41
23	c	510	CLA	C4D-CHA	2.71	1.48	1.38
23	c	507	CLA	C1C-C2C	2.70	1.49	1.44
23	D	402[A]	CLA	C1B-CHB	2.70	1.48	1.41
23	B	611	CLA	C4D-CHA	2.70	1.48	1.38
23	B	601	CLA	C1C-C2C	2.70	1.49	1.44
23	C	507	CLA	C4C-C3C	2.70	1.49	1.45
23	C	502	CLA	C4D-CHA	2.70	1.48	1.38
23	c	512	CLA	C4D-CHA	2.70	1.48	1.38
23	C	505	CLA	C1C-C2C	2.69	1.49	1.44
23	c	505	CLA	C4B-CHC	2.69	1.48	1.41
23	b	608	CLA	C4D-CHA	2.69	1.47	1.38
23	A	405[A]	CLA	C4D-CHA	2.68	1.47	1.38
23	b	609	CLA	C4D-CHA	2.68	1.47	1.38
23	d	403[B]	CLA	C1B-CHB	2.68	1.48	1.41
23	C	506	CLA	C1B-CHB	2.68	1.48	1.41
23	c	507	CLA	C4D-CHA	2.68	1.47	1.38
23	b	607	CLA	C4D-CHA	2.68	1.47	1.38
23	B	614	CLA	C4D-CHA	2.67	1.47	1.38
23	C	512	CLA	C1B-CHB	2.67	1.48	1.41
23	b	610	CLA	C1C-C2C	2.67	1.49	1.44
23	c	503	CLA	C1B-CHB	2.67	1.48	1.41
23	b	614	CLA	C3D-C4D	-2.67	1.38	1.44
23	B	602	CLA	C3D-C4D	-2.67	1.38	1.44
23	b	609	CLA	C1B-CHB	2.67	1.48	1.41
23	A	404[B]	CLA	C4C-C3C	2.66	1.49	1.45
23	C	502	CLA	C4B-CHC	2.66	1.48	1.41
23	c	510	CLA	C1B-CHB	2.66	1.48	1.41
23	b	611	CLA	C4C-C3C	2.66	1.49	1.45
26	f	102	SQD	C6-S	-2.66	1.67	1.77
23	b	614	CLA	C4B-CHC	2.66	1.48	1.41
23	c	511	CLA	C1B-CHB	2.66	1.48	1.41
26	A	410[B]	SQD	C6-S	-2.65	1.67	1.77
26	A	412	SQD	C6-S	-2.65	1.67	1.77
38	E	102	HEM	FE-NB	2.65	2.10	1.96
23	D	403	CLA	C4B-CHC	2.65	1.48	1.41
23	b	607	CLA	OBD-CAD	2.65	1.27	1.22
23	C	505	CLA	C1B-CHB	2.65	1.48	1.41
23	c	511	CLA	C4D-CHA	2.64	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	501	CLA	C1B-CHB	2.63	1.48	1.41
23	c	501	CLA	C4D-CHA	2.63	1.47	1.38
23	b	610	CLA	C4B-CHC	2.63	1.48	1.41
23	a	405[B]	CLA	C4D-CHA	2.63	1.47	1.38
23	b	610	CLA	C4C-C3C	2.63	1.49	1.45
40	V	201	HEC	C3C-C4C	2.63	1.47	1.43
23	b	615	CLA	C4D-CHA	2.63	1.47	1.38
23	b	606	CLA	C4D-CHA	2.63	1.47	1.38
23	B	602	CLA	C1B-CHB	2.62	1.48	1.41
23	B	609	CLA	C4B-CHC	2.62	1.48	1.41
23	a	405[A]	CLA	C4D-CHA	2.62	1.47	1.38
23	B	610	CLA	C4D-CHA	2.62	1.47	1.38
23	C	503	CLA	C4B-CHC	2.62	1.48	1.41
23	c	504	CLA	C4D-CHA	2.62	1.47	1.38
23	A	405[B]	CLA	C4D-CHA	2.62	1.47	1.38
23	d	402[B]	CLA	C4D-CHA	2.61	1.47	1.38
23	B	608	CLA	C4D-CHA	2.61	1.47	1.38
23	C	507	CLA	C4D-CHA	2.61	1.47	1.38
26	a	410	SQD	C6-S	-2.61	1.67	1.77
23	b	603	CLA	C1C-C2C	2.61	1.49	1.44
23	D	403	CLA	C1B-CHB	2.61	1.48	1.41
35	C	519	DGD	O2G-C2G	-2.60	1.40	1.46
23	B	607	CLA	C1B-CHB	2.60	1.48	1.41
23	C	506	CLA	C4C-C3C	2.60	1.49	1.45
23	B	613	CLA	C4D-CHA	2.60	1.47	1.38
23	b	607	CLA	C1C-C2C	2.60	1.49	1.44
23	B	607	CLA	C4B-CHC	2.60	1.48	1.41
23	c	506	CLA	C1B-CHB	2.60	1.48	1.41
23	c	509	CLA	C1B-CHB	2.60	1.48	1.41
31	t	101	LMT	O3'-C3'	-2.59	1.36	1.43
23	b	602	CLA	C4C-C3C	2.59	1.49	1.45
23	b	611	CLA	C4D-CHA	2.59	1.47	1.38
23	B	611	CLA	C1B-NB	2.59	1.37	1.35
23	B	616	CLA	C1B-CHB	2.59	1.48	1.41
23	C	502	CLA	C1C-C2C	2.59	1.49	1.44
23	c	503	CLA	C4D-CHA	2.59	1.47	1.38
23	B	602	CLA	C4D-CHA	2.59	1.47	1.38
23	c	501	CLA	C3D-C4D	-2.59	1.38	1.44
23	B	606	CLA	C4D-CHA	2.58	1.47	1.38
34	b	622	HTG	O5-C1	2.58	1.46	1.42
23	A	408	CLA	C3D-C4D	-2.58	1.38	1.44
23	c	513	CLA	C1C-C2C	2.58	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	514	CLA	C4D-CHA	2.58	1.47	1.38
23	b	605	CLA	C1B-CHB	2.57	1.48	1.41
23	c	508	CLA	C4D-CHA	2.57	1.47	1.38
23	A	404[A]	CLA	C4D-CHA	2.57	1.47	1.38
23	B	604	CLA	C1B-CHB	2.57	1.48	1.41
31	M	101	LMT	O2B-C2B	-2.57	1.36	1.43
23	B	605	CLA	C4D-CHA	2.57	1.47	1.38
23	B	609	CLA	C4D-CHA	2.57	1.47	1.38
23	c	502	CLA	C4D-CHA	2.56	1.47	1.38
23	c	509	CLA	C4D-CHA	2.56	1.47	1.38
23	c	505	CLA	C1B-CHB	2.56	1.48	1.41
23	A	405[B]	CLA	C4B-CHC	2.56	1.48	1.41
23	c	508	CLA	C1B-CHB	2.56	1.48	1.41
23	d	403[A]	CLA	C4C-C3C	2.56	1.49	1.45
23	c	505	CLA	C4D-CHA	2.55	1.47	1.38
23	d	403[B]	CLA	C4D-CHA	2.55	1.47	1.38
23	B	603	CLA	C1B-CHB	2.55	1.48	1.41
23	c	508	CLA	C4B-CHC	2.55	1.48	1.41
23	C	511	CLA	C1C-C2C	2.55	1.49	1.44
23	B	615	CLA	C1B-CHB	2.55	1.48	1.41
23	a	404[B]	CLA	C4D-CHA	2.55	1.47	1.38
23	b	603	CLA	C4B-CHC	2.55	1.48	1.41
24	a	414[A]	PHO	C3A-C2A	-2.55	1.52	1.54
23	C	510	CLA	C1C-C2C	2.54	1.49	1.44
23	C	510	CLA	C4D-CHA	2.54	1.47	1.38
23	C	504	CLA	C4B-CHC	2.54	1.48	1.41
23	B	606	CLA	C1B-CHB	2.54	1.48	1.41
23	d	403[B]	CLA	C4C-C3C	2.54	1.49	1.45
23	c	507	CLA	C4B-CHC	2.54	1.48	1.41
23	B	605	CLA	C1B-CHB	2.54	1.48	1.41
23	b	613	CLA	C4C-C3C	2.54	1.49	1.45
23	A	404[B]	CLA	C4D-CHA	2.54	1.47	1.38
26	b	620	SQD	C6-S	-2.53	1.68	1.77
23	C	514	CLA	C1B-CHB	2.53	1.48	1.41
23	C	508	CLA	C1C-C2C	2.53	1.49	1.44
23	a	407	CLA	C4B-CHC	2.53	1.48	1.41
23	c	513	CLA	C1B-CHB	2.53	1.48	1.41
29	D	405[B]	PL9	C6-C5	2.53	1.48	1.35
23	b	613	CLA	C1C-C2C	2.53	1.49	1.44
31	A	420	LMT	O3'-C3'	-2.53	1.37	1.43
31	B	628	LMT	C3'-C2'	2.52	1.58	1.52
33	C	521	LMG	O1-C1	2.52	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	511	CLA	C4D-CHA	2.52	1.47	1.38
23	b	611	CLA	C1B-CHB	2.52	1.48	1.41
23	A	406[B]	CLA	C4D-CHA	2.52	1.47	1.38
23	D	402[B]	CLA	C4D-CHA	2.52	1.47	1.38
23	c	512	CLA	C4B-CHC	2.52	1.48	1.41
23	b	601	CLA	C4D-CHA	2.52	1.47	1.38
23	b	611	CLA	C1C-C2C	2.51	1.49	1.44
23	C	506	CLA	C4B-CHC	2.51	1.48	1.41
24	a	406[A]	PHO	CHA-CBD	-2.51	1.49	1.52
23	B	613	CLA	C1B-CHB	2.51	1.48	1.41
23	b	612	CLA	C4B-CHC	2.51	1.48	1.41
23	B	606	CLA	C4B-CHC	2.51	1.48	1.41
23	c	501	CLA	C4B-CHC	2.51	1.48	1.41
23	b	615	CLA	C4B-CHC	2.51	1.48	1.41
23	b	606	CLA	C1C-C2C	2.51	1.49	1.44
23	B	602	CLA	C4B-CHC	2.51	1.48	1.41
23	C	513	CLA	C4D-CHA	2.50	1.47	1.38
23	c	503	CLA	C3D-C4D	-2.50	1.38	1.44
23	B	603	CLA	C4B-CHC	2.50	1.47	1.41
23	A	404[A]	CLA	C1C-C2C	2.49	1.49	1.44
23	a	404[A]	CLA	C4C-C3C	2.49	1.49	1.45
23	A	406[B]	CLA	C1C-C2C	2.49	1.49	1.44
23	A	406[A]	CLA	C4B-CHC	2.49	1.47	1.41
29	d	406[B]	PL9	C6-C5	2.49	1.48	1.35
23	b	601	CLA	C1C-C2C	2.49	1.49	1.44
23	c	510	CLA	C4C-C3C	2.49	1.49	1.45
23	B	601	CLA	C4D-CHA	2.49	1.47	1.38
23	B	616	CLA	C4D-CHA	2.49	1.47	1.38
23	b	613	CLA	C1B-CHB	2.48	1.47	1.41
31	e	101	LMT	O3'-C3'	-2.48	1.37	1.43
23	A	405[A]	CLA	C1B-CHB	2.48	1.47	1.41
23	a	404[B]	CLA	C4C-C3C	2.48	1.49	1.45
23	b	606	CLA	C3D-C4D	-2.48	1.38	1.44
23	C	509	CLA	C4D-CHA	2.48	1.47	1.38
23	B	616	CLA	C4B-CHC	2.48	1.47	1.41
23	a	404[A]	CLA	C4D-CHA	2.48	1.47	1.38
23	d	402[A]	CLA	C4D-CHA	2.48	1.47	1.38
23	b	605	CLA	C4D-CHA	2.48	1.47	1.38
26	B	620	SQD	C6-S	-2.47	1.68	1.77
23	C	511	CLA	C3D-C4D	-2.47	1.38	1.44
23	c	513	CLA	C4D-CHA	2.47	1.47	1.38
23	B	603	CLA	C4D-CHA	2.47	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	502	CLA	C1B-CHB	2.46	1.47	1.41
23	b	608	CLA	C1B-CHB	2.46	1.47	1.41
23	b	616	CLA	C4D-CHA	2.46	1.47	1.38
23	a	405[A]	CLA	C1B-CHB	2.46	1.47	1.41
23	C	514	CLA	C1C-C2C	2.46	1.49	1.44
23	C	503	CLA	C1B-CHB	2.46	1.47	1.41
23	B	611	CLA	C3D-C4D	-2.46	1.38	1.44
23	b	616	CLA	C4B-CHC	2.45	1.47	1.41
23	c	512	CLA	C1C-C2C	2.45	1.49	1.44
23	c	507	CLA	C1B-CHB	2.45	1.47	1.41
23	B	602	CLA	C4C-C3C	2.45	1.49	1.45
23	b	613	CLA	C4B-CHC	2.45	1.47	1.41
23	b	612	CLA	C4D-CHA	2.45	1.47	1.38
23	c	506	CLA	C4C-C3C	2.45	1.49	1.45
23	B	608	CLA	C1C-NC	-2.45	1.34	1.37
23	C	504	CLA	C1C-C2C	2.44	1.49	1.44
34	B	623	HTG	C1'-S1	-2.44	1.78	1.81
23	d	403[A]	CLA	C1B-NB	-2.44	1.33	1.35
23	b	603	CLA	C4D-CHA	2.44	1.47	1.38
23	a	405[A]	CLA	C3D-C4D	-2.44	1.38	1.44
23	b	609	CLA	C4B-CHC	2.44	1.47	1.41
23	b	602	CLA	C3D-C4D	-2.44	1.38	1.44
23	d	404	CLA	C4D-CHA	2.43	1.47	1.38
23	a	407	CLA	C4D-CHA	2.43	1.47	1.38
23	B	612	CLA	C4C-C3C	2.43	1.49	1.45
23	b	615	CLA	C1B-CHB	2.43	1.47	1.41
23	D	402[B]	CLA	C1B-CHB	2.43	1.47	1.41
23	A	406[B]	CLA	C4B-CHC	2.43	1.47	1.41
31	m	103	LMT	C3'-C2'	2.42	1.58	1.52
23	B	610	CLA	C3D-C4D	-2.42	1.38	1.44
23	b	607	CLA	C4B-CHC	2.42	1.47	1.41
23	B	612	CLA	C4B-NB	-2.42	1.33	1.35
23	b	604	CLA	C1B-CHB	2.42	1.47	1.41
23	D	402[B]	CLA	C3D-C4D	-2.42	1.38	1.44
24	A	407[A]	PHO	CHA-CBD	-2.42	1.49	1.52
23	b	614	CLA	C1B-CHB	2.42	1.47	1.41
31	b	621	LMT	C3'-C2'	2.42	1.58	1.52
31	B	628	LMT	O3'-C3'	-2.42	1.37	1.43
23	B	605	CLA	C1C-C2C	2.41	1.49	1.44
27	a	418	GOL	C1-C2	2.41	1.61	1.51
23	b	611	CLA	C4B-CHC	2.41	1.47	1.41
23	A	405[A]	CLA	C1C-C2C	2.41	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	512	CLA	C4B-CHC	2.41	1.47	1.41
23	C	513	CLA	C3D-C4D	-2.41	1.38	1.44
23	A	406[A]	CLA	C1C-C2C	2.41	1.49	1.44
23	a	404[A]	CLA	C1B-CHB	2.41	1.47	1.41
23	c	506	CLA	C4D-CHA	2.41	1.47	1.38
34	B	625	HTG	C1-S1	-2.41	1.77	1.80
23	c	510	CLA	C4B-CHC	2.41	1.47	1.41
23	C	504	CLA	C4D-CHA	2.41	1.47	1.38
23	c	504	CLA	C4C-C3C	2.41	1.49	1.45
23	c	513	CLA	C4C-C3C	2.40	1.49	1.45
23	b	614	CLA	C1C-C2C	2.40	1.49	1.44
23	C	504	CLA	C1B-CHB	2.40	1.47	1.41
31	m	103	LMT	O2B-C2B	-2.40	1.37	1.43
23	b	609	CLA	C1C-C2C	2.40	1.49	1.44
31	F	101	LMT	O3'-C3'	-2.40	1.37	1.43
23	b	608	CLA	C3D-C4D	-2.40	1.38	1.44
23	C	509	CLA	C1B-CHB	2.40	1.47	1.41
23	d	403[B]	CLA	C1C-C2C	2.40	1.49	1.44
23	a	405[B]	CLA	C1B-CHB	2.40	1.47	1.41
31	B	630	LMT	O2'-C2'	-2.40	1.37	1.43
23	d	404	CLA	C1B-CHB	2.39	1.47	1.41
23	D	402[A]	CLA	C3D-C4D	-2.39	1.38	1.44
23	B	610	CLA	C1C-C2C	2.39	1.49	1.44
31	B	630	LMT	O2B-C2B	-2.39	1.37	1.43
31	A	420	LMT	O2'-C2'	-2.39	1.37	1.43
23	b	609	CLA	C1C-NC	-2.39	1.34	1.37
23	c	509	CLA	C4C-C3C	2.39	1.49	1.45
23	C	512	CLA	C4C-C3C	2.39	1.49	1.45
31	T	101	LMT	O3'-C3'	-2.39	1.37	1.43
23	a	404[B]	CLA	C1B-CHB	2.39	1.47	1.41
23	C	511	CLA	C1B-CHB	2.38	1.47	1.41
23	b	615	CLA	C4C-C3C	2.38	1.49	1.45
23	B	610	CLA	C4C-C3C	2.38	1.49	1.45
23	B	608	CLA	C1B-CHB	2.38	1.47	1.41
23	d	403[A]	CLA	C4D-CHA	2.38	1.46	1.38
38	f	101	HEM	C1D-ND	-2.38	1.33	1.38
23	C	508	CLA	C4B-CHC	2.38	1.47	1.41
31	a	416	LMT	O3'-C3'	-2.37	1.37	1.43
31	B	631	LMT	O3'-C3'	-2.37	1.37	1.43
23	b	601	CLA	C4C-C3C	2.37	1.49	1.45
31	M	101	LMT	O3'-C3'	-2.37	1.37	1.43
23	c	506	CLA	C4B-CHC	2.37	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	609	CLA	C1B-CHB	2.37	1.47	1.41
23	A	408	CLA	C4B-CHC	2.36	1.47	1.41
23	B	606	CLA	C3D-C4D	-2.36	1.38	1.44
23	A	405[B]	CLA	C1B-CHB	2.36	1.47	1.41
23	c	512	CLA	C1B-CHB	2.36	1.47	1.41
23	D	402[B]	CLA	C4C-C3C	2.36	1.49	1.45
23	b	610	CLA	C3D-C4D	-2.36	1.38	1.44
23	b	601	CLA	C4B-CHC	2.36	1.47	1.41
27	b	624	GOL	C3-C2	2.36	1.61	1.51
23	b	615	CLA	C3D-C4D	-2.36	1.38	1.44
23	b	613	CLA	C1B-NB	-2.36	1.33	1.35
26	F	102	SQD	C6-S	-2.36	1.68	1.77
23	C	505	CLA	C4B-CHC	2.36	1.47	1.41
23	c	504	CLA	C1C-NC	-2.36	1.34	1.37
23	b	602	CLA	C4D-CHA	2.36	1.46	1.38
23	C	507	CLA	C1C-C2C	2.36	1.49	1.44
25	B	619	BCR	C30-C25	-2.35	1.50	1.53
29	d	406[A]	PL9	C6-C5	2.35	1.47	1.35
23	C	507	CLA	C3D-C4D	-2.35	1.38	1.44
24	a	414[A]	PHO	CHA-CBD	-2.35	1.49	1.52
31	M	101	LMT	O2'-C2'	-2.35	1.37	1.43
23	D	402[B]	CLA	C1C-C2C	2.35	1.49	1.44
23	B	608	CLA	C3D-C4D	-2.35	1.38	1.44
23	B	616	CLA	C1C-NC	-2.35	1.34	1.37
23	C	503	CLA	C4D-CHA	2.35	1.46	1.38
23	b	606	CLA	C4B-CHC	2.35	1.47	1.41
23	b	607	CLA	C1B-CHB	2.35	1.47	1.41
24	A	416[A]	PHO	C3A-C2A	-2.34	1.52	1.54
31	A	417	LMT	O2'-C2'	-2.34	1.37	1.43
23	A	405[A]	CLA	C3D-C4D	-2.34	1.38	1.44
23	C	510	CLA	C4C-C3C	2.34	1.49	1.45
31	t	101	LMT	O2'-C2'	-2.34	1.37	1.43
23	B	610	CLA	C4B-CHC	2.34	1.47	1.41
29	D	405[A]	PL9	C6-C5	2.34	1.47	1.35
23	A	404[B]	CLA	C1C-C2C	2.34	1.49	1.44
23	C	502	CLA	C3D-C4D	-2.34	1.38	1.44
23	b	614	CLA	C4D-CHA	2.34	1.46	1.38
23	B	609	CLA	C3D-C4D	-2.33	1.38	1.44
23	b	616	CLA	C1B-CHB	2.33	1.47	1.41
23	C	511	CLA	C4C-C3C	2.33	1.49	1.45
23	B	601	CLA	C1B-CHB	2.33	1.47	1.41
24	a	406[A]	PHO	CBD-CGD	-2.33	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	407	CLA	C1B-CHB	2.33	1.47	1.41
23	b	605	CLA	C4B-CHC	2.33	1.47	1.41
23	B	604	CLA	C3D-C4D	-2.33	1.38	1.44
24	a	406[B]	PHO	CHA-CBD	-2.32	1.49	1.52
23	A	404[B]	CLA	C1B-CHB	2.32	1.47	1.41
23	b	607	CLA	C4C-C3C	2.32	1.49	1.45
35	c	518	DGD	O2G-C2G	-2.32	1.40	1.46
23	c	507	CLA	C3D-C4D	-2.32	1.38	1.44
23	b	605	CLA	C1C-C2C	2.32	1.49	1.44
23	A	406[B]	CLA	C4C-C3C	2.31	1.49	1.45
23	C	514	CLA	C3D-C4D	-2.31	1.39	1.44
23	a	404[B]	CLA	C4B-CHC	2.31	1.47	1.41
23	B	603	CLA	C1C-C2C	2.31	1.49	1.44
23	d	403[B]	CLA	C3D-C4D	-2.31	1.39	1.44
23	d	403[A]	CLA	C1C-C2C	2.30	1.49	1.44
23	d	403[A]	CLA	C3D-C4D	-2.30	1.39	1.44
23	C	503	CLA	C3D-C4D	-2.30	1.39	1.44
23	A	405[A]	CLA	C4B-CHC	2.30	1.47	1.41
23	C	505	CLA	C3D-C4D	-2.30	1.39	1.44
23	A	404[A]	CLA	C1B-CHB	2.30	1.47	1.41
23	B	608	CLA	C4C-C3C	2.30	1.49	1.45
23	C	508	CLA	C4C-C3C	2.30	1.49	1.45
23	d	403[B]	CLA	C4B-CHC	2.29	1.47	1.41
23	b	603	CLA	C1B-CHB	2.29	1.47	1.41
23	A	404[B]	CLA	C4B-CHC	2.29	1.47	1.41
23	C	504	CLA	C3D-C4D	-2.29	1.39	1.44
23	b	607	CLA	C3D-C4D	-2.29	1.39	1.44
23	B	604	CLA	C4C-C3C	2.29	1.49	1.45
23	C	510	CLA	C1B-CHB	2.29	1.47	1.41
26	F	102	SQD	O6-C1	2.28	1.44	1.40
23	a	405[B]	CLA	C4B-CHC	2.28	1.47	1.41
23	c	501	CLA	C4C-C3C	2.28	1.49	1.45
23	b	606	CLA	C1B-CHB	2.27	1.47	1.41
23	A	408	CLA	C1B-NB	-2.27	1.33	1.35
23	b	616	CLA	C3D-C4D	-2.27	1.39	1.44
23	c	504	CLA	C4B-CHC	2.27	1.47	1.41
23	C	507	CLA	C4B-NB	-2.27	1.33	1.35
23	C	507	CLA	C1B-CHB	2.26	1.47	1.41
23	C	508	CLA	C1B-CHB	2.26	1.47	1.41
31	m	103	LMT	O3'-C3'	-2.26	1.37	1.43
23	A	404[B]	CLA	C3D-C4D	-2.26	1.39	1.44
23	c	509	CLA	C4B-NB	-2.26	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	603	CLA	C4C-C3C	2.26	1.48	1.45
23	B	613	CLA	C4B-CHC	2.26	1.47	1.41
23	c	513	CLA	C3D-C4D	-2.26	1.39	1.44
23	b	609	CLA	C3D-C4D	-2.25	1.39	1.44
31	B	630	LMT	O3'-C3'	-2.25	1.37	1.43
23	B	612	CLA	C4B-CHC	2.25	1.47	1.41
23	a	404[A]	CLA	C1C-C2C	2.25	1.48	1.44
24	A	407[B]	PHO	CBD-CGD	-2.25	1.49	1.52
23	d	402[B]	CLA	C1B-CHB	2.25	1.47	1.41
23	c	510	CLA	C3D-C4D	-2.25	1.39	1.44
23	D	403	CLA	C4D-CHA	2.25	1.46	1.38
23	A	406[A]	CLA	C3D-C4D	-2.24	1.39	1.44
23	b	612	CLA	C3D-C4D	-2.24	1.39	1.44
23	B	613	CLA	C4C-C3C	2.24	1.48	1.45
23	D	402[A]	CLA	C1B-NB	-2.24	1.33	1.35
31	A	417	LMT	O3'-C3'	-2.24	1.37	1.43
23	d	402[A]	CLA	C1B-CHB	2.24	1.47	1.41
23	C	502	CLA	C4C-C3C	2.24	1.48	1.45
23	B	614	CLA	C1C-C2C	2.24	1.48	1.44
23	c	512	CLA	C3D-C4D	-2.23	1.39	1.44
23	c	511	CLA	C4B-CHC	2.23	1.47	1.41
23	C	506	CLA	C3D-C4D	-2.23	1.39	1.44
23	c	504	CLA	C3D-C4D	-2.23	1.39	1.44
23	c	511	CLA	C4C-C3C	2.23	1.48	1.45
23	d	402[A]	CLA	C4B-CHC	2.23	1.47	1.41
24	a	414[B]	PHO	C3A-C2A	-2.23	1.52	1.54
23	c	512	CLA	C4C-C3C	2.23	1.48	1.45
23	B	614	CLA	C4C-C3C	2.23	1.48	1.45
23	B	603	CLA	C1B-NB	-2.23	1.33	1.35
23	b	605	CLA	C3D-C4D	-2.22	1.39	1.44
23	B	612	CLA	C4D-ND	2.22	1.40	1.37
25	d	405	BCR	C30-C25	-2.22	1.50	1.53
23	A	408	CLA	C1C-C2C	2.22	1.48	1.44
23	c	513	CLA	C4B-CHC	2.22	1.47	1.41
23	c	511	CLA	MG-NA	2.21	2.11	2.06
23	C	507	CLA	C1D-C2D	2.21	1.49	1.45
27	D	412	GOL	O2-C2	-2.21	1.36	1.43
23	B	604	CLA	C4B-CHC	2.21	1.47	1.41
23	d	402[B]	CLA	C1C-NC	-2.21	1.34	1.37
35	C	518[A]	DGD	O5D-C1E	2.21	1.44	1.40
23	D	402[A]	CLA	C4C-C3C	2.21	1.48	1.45
23	b	608	CLA	C1C-C2C	2.20	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	607	CLA	C1B-NB	-2.20	1.33	1.35
29	D	405[B]	PL9	C2-C3	2.20	1.40	1.34
38	f	101	HEM	CHB-C1B	2.20	1.40	1.35
23	a	407	CLA	C4C-C3C	2.20	1.48	1.45
23	A	406[A]	CLA	C1B-CHB	2.20	1.47	1.41
23	B	615	CLA	C4B-CHC	2.20	1.47	1.41
23	C	512	CLA	C3D-C4D	-2.20	1.39	1.44
23	C	513	CLA	C1B-CHB	2.19	1.47	1.41
29	a	412[A]	PL9	C2-C3	2.19	1.40	1.34
23	d	403[A]	CLA	C4B-CHC	2.19	1.47	1.41
23	B	602	CLA	C1B-NB	-2.19	1.33	1.35
23	b	615	CLA	C1B-NB	-2.19	1.33	1.35
23	B	615	CLA	MG-NA	2.19	2.11	2.06
23	C	505	CLA	C4C-C3C	2.19	1.48	1.45
23	C	502	CLA	C1B-CHB	2.18	1.47	1.41
31	B	628	LMT	O5'-C5'	-2.18	1.39	1.44
23	A	404[A]	CLA	C4B-NB	-2.18	1.33	1.35
23	C	510	CLA	C4B-CHC	2.18	1.47	1.41
23	B	613	CLA	C1C-C2C	2.18	1.48	1.44
23	b	601	CLA	C1B-CHB	2.18	1.47	1.41
31	T	101	LMT	O3B-C3B	-2.18	1.37	1.43
23	c	506	CLA	C3D-C4D	-2.18	1.39	1.44
35	h	102	DGD	O5D-C1E	2.17	1.43	1.40
23	d	403[B]	CLA	C1B-NB	-2.17	1.33	1.35
23	a	405[B]	CLA	C3D-C4D	-2.17	1.39	1.44
23	A	406[A]	CLA	C1B-NB	-2.17	1.33	1.35
23	A	408	CLA	C4C-C3C	2.17	1.48	1.45
34	B	622	HTG	O5-C1	2.16	1.45	1.42
23	C	503	CLA	C4C-C3C	2.16	1.48	1.45
23	c	502	CLA	C4B-CHC	2.16	1.47	1.41
23	C	504	CLA	C4C-C3C	2.16	1.48	1.45
23	b	611	CLA	C3D-C4D	-2.16	1.39	1.44
23	B	601	CLA	C3D-C4D	-2.15	1.39	1.44
23	C	514	CLA	C4B-CHC	2.15	1.47	1.41
23	A	405[A]	CLA	C1B-NB	-2.15	1.33	1.35
23	C	509	CLA	C1C-C2C	2.15	1.48	1.44
23	A	406[B]	CLA	C1B-CHB	2.15	1.47	1.41
23	B	614	CLA	C4B-CHC	2.15	1.47	1.41
23	c	506	CLA	C1C-C2C	2.14	1.48	1.44
23	c	504	CLA	C1B-CHB	2.14	1.47	1.41
23	B	604	CLA	C1C-C2C	2.14	1.48	1.44
23	a	404[A]	CLA	C4B-CHC	2.14	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	e	101	LMT	O2'-C2'	-2.14	1.37	1.43
23	c	503	CLA	C4C-C3C	2.14	1.48	1.45
23	B	612	CLA	C3D-C4D	-2.14	1.39	1.44
31	B	628	LMT	O4'-C4B	-2.14	1.37	1.43
23	C	509	CLA	C4C-C3C	2.13	1.48	1.45
29	A	414[A]	PL9	C2-C1	-2.12	1.39	1.44
31	B	631	LMT	O2'-C2'	-2.12	1.38	1.43
23	D	402[A]	CLA	C4B-CHC	2.12	1.46	1.41
31	e	101	LMT	O2B-C2B	-2.12	1.38	1.43
23	D	402[B]	CLA	C4B-CHC	2.12	1.46	1.41
23	d	402[A]	CLA	C1C-C2C	2.12	1.48	1.44
23	d	402[B]	CLA	C3D-C4D	-2.11	1.39	1.44
23	C	511	CLA	C4B-CHC	2.11	1.46	1.41
29	a	412[B]	PL9	C2-C3	2.11	1.40	1.34
23	B	616	CLA	C3D-C4D	-2.11	1.39	1.44
23	d	404	CLA	C3D-C4D	-2.11	1.39	1.44
23	B	607	CLA	C3D-C4D	-2.11	1.39	1.44
23	b	602	CLA	C1B-CHB	2.11	1.46	1.41
27	A	418	GOL	C3-C2	2.10	1.60	1.51
23	C	509	CLA	C4B-CHC	2.10	1.46	1.41
23	a	405[B]	CLA	C4C-C3C	2.10	1.48	1.45
23	c	501	CLA	C1C-NC	-2.10	1.34	1.37
23	B	610	CLA	C1B-NB	-2.10	1.33	1.35
23	B	604	CLA	C1A-CHA	2.10	1.51	1.43
23	B	605	CLA	C4C-C3C	2.10	1.48	1.45
26	a	410	SQD	O6-C1	2.10	1.43	1.40
23	A	405[B]	CLA	C3D-C4D	-2.10	1.39	1.44
23	B	606	CLA	C4C-C3C	2.09	1.48	1.45
38	E	102	HEM	CHB-C1B	2.09	1.40	1.35
23	a	405[A]	CLA	C4C-C3C	2.08	1.48	1.45
24	a	406[B]	PHO	CBD-CGD	-2.08	1.49	1.52
23	a	404[B]	CLA	C3D-C4D	-2.08	1.39	1.44
23	B	608	CLA	C1C-C2C	2.07	1.48	1.44
23	B	615	CLA	C3D-C4D	-2.07	1.39	1.44
23	C	514	CLA	C1C-NC	-2.07	1.34	1.37
23	b	608	CLA	C4B-CHC	2.07	1.46	1.41
23	a	404[B]	CLA	C1C-C2C	2.07	1.48	1.44
27	D	412	GOL	C3-C2	2.06	1.60	1.51
31	b	627	LMT	O3'-C3'	-2.06	1.38	1.43
23	B	601	CLA	C4C-C3C	2.06	1.48	1.45
23	A	406[B]	CLA	C3D-C4D	-2.06	1.39	1.44
23	b	601	CLA	C1D-C2D	2.06	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	508	CLA	C3D-C4D	-2.06	1.39	1.44
23	C	508	CLA	C3D-C4D	-2.05	1.39	1.44
23	b	616	CLA	C1C-NC	-2.05	1.34	1.37
23	d	402[B]	CLA	C4B-CHC	2.05	1.46	1.41
31	A	417	LMT	O2B-C2B	-2.05	1.38	1.43
26	B	620	SQD	O6-C1	2.05	1.43	1.40
27	o	303	GOL	C1-C2	2.05	1.60	1.51
23	c	505	CLA	C3D-C4D	-2.04	1.39	1.44
23	a	405[A]	CLA	C4B-CHC	2.04	1.46	1.41
23	C	505	CLA	C1B-NB	-2.04	1.33	1.35
23	B	609	CLA	C4C-C3C	2.04	1.48	1.45
23	C	509	CLA	C1C-NC	-2.04	1.34	1.37
29	D	405[A]	PL9	C2-C3	2.04	1.40	1.34
23	B	607	CLA	C4C-C3C	2.03	1.48	1.45
31	e	101	LMT	O3B-C3B	-2.03	1.38	1.43
32	b	629[A]	LHG	O7-C5	-2.02	1.41	1.46
23	B	614	CLA	C1C-NC	-2.02	1.34	1.37
23	d	402[B]	CLA	C1C-C2C	2.02	1.48	1.44
23	B	604	CLA	MG-NA	2.02	2.11	2.06
23	A	405[B]	CLA	C1B-NB	-2.02	1.33	1.35
31	T	101	LMT	O2'-C2'	-2.02	1.38	1.43
23	A	404[A]	CLA	C3D-C4D	-2.02	1.39	1.44
29	A	414[B]	PL9	C2-C3	2.02	1.39	1.34
23	b	614	CLA	C4C-C3C	2.01	1.48	1.45
23	B	613	CLA	C1A-CHA	2.01	1.51	1.43
23	B	603	CLA	C3D-C4D	-2.00	1.39	1.44
24	a	414[A]	PHO	CBD-CGD	-2.00	1.49	1.52
23	b	604	CLA	C1A-CHA	2.00	1.51	1.43
23	b	612	CLA	C4C-C3C	2.00	1.48	1.45

All (3102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	407	CLA	C1D-ND-C4D	-11.35	98.27	106.33
23	B	611	CLA	C1D-ND-C4D	-11.17	98.40	106.33
23	a	407	CLA	C2D-C1D-ND	10.70	117.99	110.10
23	B	612	CLA	C1D-ND-C4D	-10.60	98.81	106.33
23	C	504	CLA	C1D-ND-C4D	-10.32	99.00	106.33
23	b	605	CLA	C1D-ND-C4D	-10.07	99.18	106.33
23	b	603	CLA	C1D-ND-C4D	-10.03	99.21	106.33
23	A	406[B]	CLA	C1D-ND-C4D	-9.98	99.25	106.33
23	a	405[B]	CLA	C1D-ND-C4D	-9.86	99.33	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	503	CLA	C1D-ND-C4D	-9.85	99.34	106.33
23	d	404	CLA	C1D-ND-C4D	-9.83	99.35	106.33
23	c	511	CLA	C1D-ND-C4D	-9.75	99.41	106.33
23	a	405[A]	CLA	C1D-ND-C4D	-9.69	99.45	106.33
23	B	606	CLA	C1D-ND-C4D	-9.66	99.47	106.33
23	B	607	CLA	C1D-ND-C4D	-9.64	99.49	106.33
23	B	601	CLA	C1D-ND-C4D	-9.61	99.51	106.33
23	C	514	CLA	C1D-ND-C4D	-9.60	99.52	106.33
23	d	403[B]	CLA	C1D-ND-C4D	-9.58	99.53	106.33
23	C	511	CLA	C1D-ND-C4D	-9.49	99.59	106.33
23	B	609	CLA	C1D-ND-C4D	-9.49	99.59	106.33
23	B	611	CLA	C2D-C1D-ND	9.46	117.08	110.10
23	c	509	CLA	C1D-ND-C4D	-9.45	99.62	106.33
23	B	605	CLA	C1D-ND-C4D	-9.43	99.63	106.33
23	c	501	CLA	C1D-ND-C4D	-9.42	99.64	106.33
23	A	406[A]	CLA	C1D-ND-C4D	-9.41	99.65	106.33
23	B	616	CLA	C1D-ND-C4D	-9.37	99.68	106.33
23	a	404[B]	CLA	C1D-ND-C4D	-9.36	99.68	106.33
23	b	611	CLA	C1D-ND-C4D	-9.36	99.69	106.33
23	B	612	CLA	C2D-C1D-ND	9.35	116.99	110.10
23	B	603	CLA	C1D-ND-C4D	-9.34	99.70	106.33
23	c	513	CLA	C1D-ND-C4D	-9.34	99.70	106.33
23	b	615	CLA	C1D-ND-C4D	-9.27	99.75	106.33
23	C	504	CLA	C2D-C1D-ND	9.26	116.92	110.10
23	B	614	CLA	C1D-ND-C4D	-9.24	99.77	106.33
23	C	502	CLA	C1D-ND-C4D	-9.24	99.77	106.33
23	b	612	CLA	C1D-ND-C4D	-9.22	99.78	106.33
23	b	609	CLA	C1D-ND-C4D	-9.20	99.80	106.33
23	B	607	CLA	C2D-C1D-ND	9.18	116.87	110.10
23	B	610	CLA	C1D-ND-C4D	-9.18	99.82	106.33
23	A	405[B]	CLA	C1D-ND-C4D	-9.17	99.82	106.33
23	B	615	CLA	C1D-ND-C4D	-9.15	99.83	106.33
23	D	402[A]	CLA	C1D-ND-C4D	-9.14	99.84	106.33
23	B	606	CLA	C2D-C1D-ND	9.14	116.84	110.10
23	A	408	CLA	C1D-ND-C4D	-9.12	99.86	106.33
23	b	614	CLA	C1D-ND-C4D	-9.11	99.86	106.33
23	C	510	CLA	C1D-ND-C4D	-9.11	99.87	106.33
23	c	505	CLA	C1D-ND-C4D	-9.10	99.87	106.33
23	B	616	CLA	C2D-C1D-ND	9.09	116.81	110.10
23	c	504	CLA	C1D-ND-C4D	-9.09	99.88	106.33
23	A	405[A]	CLA	C2D-C1D-ND	9.08	116.79	110.10
23	b	616	CLA	C1D-ND-C4D	-9.07	99.89	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	405[A]	CLA	C1D-ND-C4D	-9.06	99.90	106.33
23	b	611	CLA	C2D-C1D-ND	9.03	116.76	110.10
23	d	403[A]	CLA	C1D-ND-C4D	-9.03	99.92	106.33
23	C	505	CLA	C2D-C1D-ND	9.00	116.74	110.10
23	b	608	CLA	C1D-ND-C4D	-8.99	99.95	106.33
23	C	506	CLA	C1D-ND-C4D	-8.99	99.95	106.33
23	D	402[B]	CLA	C1D-ND-C4D	-8.98	99.95	106.33
23	b	602	CLA	C1D-ND-C4D	-8.98	99.95	106.33
23	a	404[A]	CLA	C1D-ND-C4D	-8.97	99.96	106.33
23	b	605	CLA	C2D-C1D-ND	8.92	116.68	110.10
23	B	608	CLA	C1D-ND-C4D	-8.90	100.01	106.33
23	c	506	CLA	C1D-ND-C4D	-8.87	100.04	106.33
23	B	613	CLA	C2D-C1D-ND	8.87	116.64	110.10
23	a	405[B]	CLA	C2D-C1D-ND	8.86	116.64	110.10
23	C	505	CLA	C1D-ND-C4D	-8.85	100.05	106.33
23	C	509	CLA	C1D-ND-C4D	-8.84	100.06	106.33
23	c	502	CLA	C1D-ND-C4D	-8.83	100.06	106.33
23	a	405[A]	CLA	C2D-C1D-ND	8.81	116.60	110.10
23	b	613	CLA	C2D-C1D-ND	8.81	116.60	110.10
23	c	507	CLA	C1D-ND-C4D	-8.80	100.08	106.33
23	b	610	CLA	C1D-ND-C4D	-8.79	100.09	106.33
23	b	606	CLA	C1D-ND-C4D	-8.77	100.10	106.33
23	A	408	CLA	C2D-C1D-ND	8.75	116.55	110.10
23	b	614	CLA	C2D-C1D-ND	8.74	116.55	110.10
23	A	406[B]	CLA	C2D-C1D-ND	8.74	116.55	110.10
23	B	613	CLA	C1D-ND-C4D	-8.72	100.14	106.33
23	b	601	CLA	C1D-ND-C4D	-8.71	100.15	106.33
23	b	607	CLA	C1D-ND-C4D	-8.71	100.15	106.33
23	D	403	CLA	C1D-ND-C4D	-8.70	100.15	106.33
23	C	513	CLA	C1D-ND-C4D	-8.70	100.16	106.33
23	c	503	CLA	C2D-C1D-ND	8.69	116.51	110.10
23	B	602	CLA	C1D-ND-C4D	-8.69	100.16	106.33
23	d	402[B]	CLA	C1D-ND-C4D	-8.68	100.17	106.33
23	c	512	CLA	C1D-ND-C4D	-8.68	100.17	106.33
23	d	404	CLA	C2D-C1D-ND	8.67	116.49	110.10
23	d	402[A]	CLA	C1D-ND-C4D	-8.67	100.18	106.33
23	A	404[B]	CLA	C1D-ND-C4D	-8.65	100.19	106.33
23	c	508	CLA	C1D-ND-C4D	-8.64	100.20	106.33
23	C	512	CLA	C1D-ND-C4D	-8.64	100.20	106.33
23	C	507	CLA	C1D-ND-C4D	-8.63	100.20	106.33
23	A	406[A]	CLA	C2D-C1D-ND	8.61	116.45	110.10
23	C	508	CLA	C1D-ND-C4D	-8.61	100.22	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	509	CLA	C2D-C1D-ND	8.60	116.44	110.10
23	B	609	CLA	C2D-C1D-ND	8.59	116.43	110.10
23	B	603	CLA	C2D-C1D-ND	8.56	116.41	110.10
23	C	509	CLA	C2D-C1D-ND	8.54	116.40	110.10
23	B	615	CLA	C2D-C1D-ND	8.53	116.39	110.10
23	d	402[A]	CLA	C2D-C1D-ND	8.52	116.39	110.10
23	c	511	CLA	C2D-C1D-ND	8.49	116.36	110.10
23	D	402[A]	CLA	C2D-C1D-ND	8.48	116.35	110.10
23	c	508	CLA	C2D-C1D-ND	8.47	116.35	110.10
23	c	502	CLA	C2D-C1D-ND	8.47	116.34	110.10
23	C	514	CLA	C2D-C1D-ND	8.43	116.32	110.10
23	C	503	CLA	C1D-ND-C4D	-8.43	100.35	106.33
23	b	603	CLA	C2D-C1D-ND	8.42	116.31	110.10
23	B	610	CLA	C2D-C1D-ND	8.40	116.29	110.10
23	b	616	CLA	C2D-C1D-ND	8.36	116.26	110.10
23	B	601	CLA	C2D-C1D-ND	8.33	116.24	110.10
23	B	605	CLA	C2D-C1D-ND	8.33	116.24	110.10
23	b	613	CLA	C1D-ND-C4D	-8.31	100.43	106.33
23	B	614	CLA	C2D-C1D-ND	8.31	116.22	110.10
23	C	510	CLA	C2D-C1D-ND	8.29	116.21	110.10
23	b	615	CLA	C2D-C1D-ND	8.27	116.20	110.10
23	b	607	CLA	C2D-C1D-ND	8.25	116.19	110.10
23	A	405[B]	CLA	C2D-C1D-ND	8.25	116.19	110.10
23	c	504	CLA	C2D-C1D-ND	8.25	116.18	110.10
23	c	501	CLA	C2D-C1D-ND	8.24	116.18	110.10
23	C	512	CLA	C2D-C1D-ND	8.22	116.16	110.10
23	B	608	CLA	C2D-C1D-ND	8.20	116.14	110.10
23	b	604	CLA	C1D-ND-C4D	-8.17	100.53	106.33
23	b	610	CLA	C2D-C1D-ND	8.16	116.11	110.10
23	b	602	CLA	C4A-NA-C1A	-8.14	103.05	106.71
23	d	403[B]	CLA	C2D-C1D-ND	8.14	116.10	110.10
23	C	511	CLA	C2D-C1D-ND	8.09	116.06	110.10
23	d	402[B]	CLA	C2D-C1D-ND	8.07	116.05	110.10
23	c	510	CLA	C1D-ND-C4D	-8.04	100.62	106.33
23	a	404[A]	CLA	C2D-C1D-ND	8.03	116.02	110.10
23	b	612	CLA	C2D-C1D-ND	8.02	116.01	110.10
23	D	402[B]	CLA	C2D-C1D-ND	8.00	116.00	110.10
23	c	506	CLA	C2D-C1D-ND	7.98	115.99	110.10
23	D	403	CLA	C2D-C1D-ND	7.97	115.98	110.10
23	b	608	CLA	C2D-C1D-ND	7.96	115.97	110.10
23	c	505	CLA	C2D-C1D-ND	7.96	115.97	110.10
23	C	502	CLA	C2D-C1D-ND	7.94	115.95	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	403[A]	CLA	C2D-C1D-ND	7.92	115.94	110.10
23	C	508	CLA	C2D-C1D-ND	7.91	115.94	110.10
24	a	406[B]	PHO	O2D-CGD-CBD	7.89	121.00	111.00
23	c	513	CLA	C2D-C1D-ND	7.89	115.92	110.10
23	b	606	CLA	C2D-C1D-ND	7.82	115.87	110.10
23	b	609	CLA	C2D-C1D-ND	7.81	115.86	110.10
23	b	604	CLA	C2D-C1D-ND	7.77	115.83	110.10
23	c	507	CLA	C2D-C1D-ND	7.77	115.83	110.10
23	C	511	CLA	CMD-C2D-C1D	7.73	138.34	124.71
23	C	503	CLA	C2D-C1D-ND	7.72	115.80	110.10
23	A	404[A]	CLA	C1D-ND-C4D	-7.69	100.87	106.33
23	B	604	CLA	C1D-ND-C4D	-7.68	100.88	106.33
24	A	407[B]	PHO	O2D-CGD-CBD	7.68	120.73	111.00
23	C	513	CLA	C2D-C1D-ND	7.60	115.70	110.10
23	c	512	CLA	C2D-C1D-ND	7.55	115.67	110.10
23	B	611	CLA	CHD-C4C-C3C	-7.55	113.74	124.84
23	A	404[A]	CLA	C2D-C1D-ND	7.53	115.66	110.10
23	a	404[B]	CLA	C2D-C1D-ND	7.52	115.65	110.10
23	B	616	CLA	O2D-CGD-CBD	7.48	124.55	111.27
23	c	501	CLA	CMD-C2D-C1D	7.47	137.88	124.71
23	B	602	CLA	C2D-C1D-ND	7.47	115.61	110.10
23	c	510	CLA	C2D-C1D-ND	7.45	115.59	110.10
23	B	615	CLA	C4A-NA-C1A	-7.43	103.37	106.71
23	C	506	CLA	C2D-C1D-ND	7.41	115.56	110.10
24	A	416[A]	PHO	O2D-CGD-CBD	7.38	120.34	111.00
23	b	601	CLA	C2D-C1D-ND	7.33	115.50	110.10
23	C	507	CLA	C2D-C1D-ND	7.29	115.48	110.10
23	b	606	CLA	C4A-NA-C1A	-7.28	103.43	106.71
26	F	102	SQD	O6-C1-C2	7.27	119.65	108.30
24	a	414[A]	PHO	O2D-CGD-CBD	7.21	120.13	111.00
34	b	623	HTG	C1'-S1-C1	7.19	113.55	100.09
23	B	606	CLA	CMD-C2D-C1D	7.18	137.36	124.71
23	A	404[B]	CLA	C4A-NA-C1A	-7.16	103.48	106.71
24	a	406[A]	PHO	O2D-CGD-CBD	7.16	120.07	111.00
23	b	602	CLA	C2D-C1D-ND	7.13	115.36	110.10
23	C	513	CLA	C4A-NA-C1A	-7.12	103.50	106.71
23	c	507	CLA	CMD-C2D-C1D	7.12	137.25	124.71
23	a	407	CLA	CHD-C4C-C3C	-7.10	114.41	124.84
23	c	501	CLA	CHD-C1D-ND	-7.10	117.93	124.45
23	c	507	CLA	O2D-CGD-CBD	7.09	123.86	111.27
24	A	416[B]	PHO	O2D-CGD-CBD	7.08	119.97	111.00
23	A	404[B]	CLA	C2D-C1D-ND	7.08	115.32	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	616	CLA	O2D-CGD-CBD	7.06	123.81	111.27
23	B	609	CLA	C4A-NA-C1A	-7.05	103.54	106.71
23	B	603	CLA	O2D-CGD-CBD	7.05	123.79	111.27
24	a	414[B]	PHO	O2D-CGD-CBD	7.05	119.92	111.00
23	d	404	CLA	CMD-C2D-C1D	7.03	137.10	124.71
23	C	504	CLA	C4A-NA-C1A	-7.01	103.56	106.71
23	B	605	CLA	CHD-C4C-C3C	-6.92	114.66	124.84
24	A	407[A]	PHO	O2D-CGD-CBD	6.91	119.75	111.00
23	B	614	CLA	CMD-C2D-C1D	6.90	136.88	124.71
23	B	606	CLA	CHD-C1D-ND	-6.90	118.12	124.45
23	B	616	CLA	CHD-C4C-C3C	-6.86	114.76	124.84
23	b	603	CLA	C4A-NA-C1A	-6.83	103.64	106.71
23	c	507	CLA	CHD-C1D-ND	-6.83	118.18	124.45
23	b	616	CLA	CHD-C4C-C3C	-6.82	114.82	124.84
23	A	406[B]	CLA	CHD-C1D-ND	-6.81	118.20	124.45
23	C	513	CLA	CHD-C4C-C3C	-6.74	114.93	124.84
23	b	605	CLA	CHD-C4C-C3C	-6.74	114.93	124.84
23	b	606	CLA	CMD-C2D-C1D	6.70	136.52	124.71
23	D	402[B]	CLA	CMD-C2D-C1D	6.70	136.51	124.71
23	b	612	CLA	CHD-C4C-C3C	-6.67	115.04	124.84
23	B	605	CLA	CMD-C2D-C1D	6.66	136.45	124.71
23	d	404	CLA	CHD-C1D-ND	-6.66	118.33	124.45
23	B	604	CLA	C2D-C1D-ND	6.66	115.01	110.10
23	b	606	CLA	CHD-C4C-C3C	-6.66	115.05	124.84
23	b	601	CLA	C4A-NA-C1A	-6.66	103.71	106.71
23	C	504	CLA	CHD-C4C-C3C	-6.65	115.06	124.84
23	c	513	CLA	CMD-C2D-C1D	6.62	136.38	124.71
23	A	404[A]	CLA	CMD-C2D-C1D	6.62	136.38	124.71
23	B	609	CLA	CHD-C1D-ND	-6.61	118.38	124.45
23	C	507	CLA	C2C-C1C-NC	6.61	116.16	109.97
23	b	615	CLA	C4A-NA-C1A	-6.60	103.74	106.71
23	c	504	CLA	CHD-C1D-ND	-6.57	118.42	124.45
23	d	403[B]	CLA	C2C-C1C-NC	6.57	116.13	109.97
23	B	611	CLA	CMD-C2D-C1D	6.57	136.29	124.71
23	B	610	CLA	O2D-CGD-CBD	6.57	122.94	111.27
23	C	504	CLA	CMD-C2D-C1D	6.56	136.28	124.71
23	B	604	CLA	C2C-C1C-NC	6.55	116.11	109.97
23	D	402[A]	CLA	C4A-NA-C1A	-6.52	103.77	106.71
23	d	403[A]	CLA	C2C-C1C-NC	6.51	116.07	109.97
23	b	601	CLA	O2D-CGD-CBD	6.51	122.83	111.27
23	c	506	CLA	CMD-C2D-C1D	6.50	136.17	124.71
23	c	502	CLA	C2C-C1C-NC	6.49	116.05	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	503	CLA	C4A-NA-C1A	-6.49	103.79	106.71
23	C	508	CLA	CMD-C2D-C1D	6.49	136.14	124.71
23	c	503	CLA	CHD-C4C-C3C	-6.47	115.33	124.84
23	b	609	CLA	CHD-C4C-C3C	-6.47	115.34	124.84
23	D	402[A]	CLA	CMD-C2D-C1D	6.46	136.10	124.71
23	B	612	CLA	CHD-C4C-C3C	-6.44	115.37	124.84
23	B	606	CLA	CHD-C4C-C3C	-6.43	115.39	124.84
23	B	601	CLA	CHD-C4C-C3C	-6.43	115.39	124.84
23	C	502	CLA	C4A-NA-C1A	-6.42	103.82	106.71
23	C	507	CLA	CHD-C1D-ND	-6.41	118.56	124.45
23	b	610	CLA	CHD-C4C-C3C	-6.41	115.42	124.84
23	A	404[B]	CLA	CMD-C2D-C1D	6.41	136.01	124.71
23	D	403	CLA	C4A-NA-C1A	-6.41	103.83	106.71
23	c	510	CLA	CMD-C2D-C1D	6.40	136.00	124.71
23	C	509	CLA	C2C-C1C-NC	6.39	115.96	109.97
23	C	514	CLA	CHD-C1D-ND	-6.39	118.58	124.45
23	B	609	CLA	CHD-C4C-C3C	-6.38	115.46	124.84
23	b	613	CLA	CHD-C4C-C3C	-6.35	115.51	124.84
23	b	616	CLA	C4A-NA-C1A	-6.34	103.85	106.71
23	a	405[A]	CLA	CHD-C4C-C3C	-6.34	115.52	124.84
23	b	611	CLA	CMD-C2D-C1D	6.34	135.88	124.71
23	B	606	CLA	C4A-NA-C1A	-6.33	103.86	106.71
23	D	402[B]	CLA	C4A-NA-C1A	-6.33	103.86	106.71
23	B	601	CLA	CMD-C2D-C1D	6.33	135.88	124.71
23	b	602	CLA	CMD-C2D-C1D	6.33	135.87	124.71
23	b	603	CLA	CHD-C4C-C3C	-6.33	115.54	124.84
34	c	521	HTG	C1'-S1-C1	6.32	111.91	100.09
23	c	503	CLA	CMD-C2D-C1D	6.31	135.83	124.71
23	B	615	CLA	CHD-C4C-C3C	-6.31	115.57	124.84
23	D	402[B]	CLA	CHD-C1D-ND	-6.31	118.66	124.45
23	c	511	CLA	CHD-C4C-C3C	-6.31	115.57	124.84
23	a	405[A]	CLA	CHD-C1D-ND	-6.31	118.66	124.45
23	C	509	CLA	CHD-C4C-C3C	-6.29	115.59	124.84
23	A	405[B]	CLA	CHD-C4C-C3C	-6.28	115.61	124.84
23	b	605	CLA	CMD-C2D-C1D	6.27	135.77	124.71
23	b	601	CLA	CMD-C2D-C1D	6.27	135.77	124.71
23	C	505	CLA	C2C-C1C-NC	6.27	115.85	109.97
23	D	402[A]	CLA	C2C-C1C-NC	6.26	115.84	109.97
26	F	102	SQD	O47-C7-C8	6.26	124.99	111.50
23	d	403[B]	CLA	CHD-C1D-ND	-6.26	118.70	124.45
23	a	404[A]	CLA	C2C-C1C-NC	6.26	115.83	109.97
23	A	408	CLA	CMD-C2D-C1D	6.25	135.73	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	611	CLA	CHD-C4C-C3C	-6.25	115.66	124.84
23	d	402[B]	CLA	CHD-C4C-C3C	-6.25	115.66	124.84
23	b	614	CLA	CMD-C2D-C1D	6.23	135.69	124.71
23	a	405[B]	CLA	CHD-C1D-ND	-6.22	118.74	124.45
23	B	609	CLA	CMD-C2D-C1D	6.22	135.67	124.71
23	c	512	CLA	C4A-NA-C1A	-6.22	103.91	106.71
23	d	402[A]	CLA	CHD-C4C-C3C	-6.22	115.70	124.84
23	c	506	CLA	CHD-C1D-ND	-6.21	118.75	124.45
23	C	504	CLA	CHD-C1D-ND	-6.21	118.75	124.45
23	b	614	CLA	CHD-C4C-C3C	-6.20	115.72	124.84
23	a	404[B]	CLA	C2C-C1C-NC	6.20	115.78	109.97
23	d	404	CLA	CHD-C4C-C3C	-6.20	115.73	124.84
23	a	404[A]	CLA	C4A-NA-C1A	-6.19	103.92	106.71
23	A	404[B]	CLA	CHD-C1D-ND	-6.19	118.77	124.45
23	c	510	CLA	CHD-C4C-C3C	-6.19	115.74	124.84
23	B	602	CLA	CHD-C4C-C3C	-6.19	115.75	124.84
23	b	609	CLA	C4A-NA-C1A	-6.19	103.92	106.71
23	B	607	CLA	CHD-C1D-ND	-6.19	118.77	124.45
23	C	506	CLA	CMD-C2D-C1D	6.18	135.60	124.71
40	V	201	HEC	CBD-CAD-C3D	-6.18	102.08	112.62
23	b	609	CLA	CMD-C2D-C1D	6.17	135.59	124.71
23	b	613	CLA	C2C-C1C-NC	6.17	115.75	109.97
23	C	507	CLA	CMD-C2D-C1D	6.17	135.58	124.71
23	b	614	CLA	O2D-CGD-CBD	6.16	122.22	111.27
23	D	402[A]	CLA	CHD-C1D-ND	-6.16	118.79	124.45
23	B	610	CLA	CMD-C2D-C1D	6.16	135.57	124.71
23	b	605	CLA	CHD-C1D-ND	-6.15	118.80	124.45
23	a	405[B]	CLA	CHD-C4C-C3C	-6.15	115.80	124.84
23	C	508	CLA	O2D-CGD-CBD	6.15	122.20	111.27
23	C	508	CLA	CHD-C4C-C3C	-6.15	115.80	124.84
23	B	603	CLA	CHD-C4C-C3C	-6.15	115.80	124.84
23	c	512	CLA	CMD-C2D-C1D	6.14	135.53	124.71
23	b	606	CLA	CHD-C1D-ND	-6.14	118.81	124.45
23	B	602	CLA	CMD-C2D-C1D	6.13	135.51	124.71
23	d	403[B]	CLA	CMD-C2D-C1D	6.13	135.51	124.71
23	b	607	CLA	C2C-C1C-NC	6.12	115.71	109.97
23	a	404[B]	CLA	CMD-C2D-C1D	6.11	135.47	124.71
23	c	513	CLA	CHD-C1D-ND	-6.10	118.85	124.45
23	b	615	CLA	CMD-C2D-C1D	6.09	135.45	124.71
23	A	404[A]	CLA	C2C-C1C-NC	6.08	115.67	109.97
23	C	512	CLA	CHD-C4C-C3C	-6.08	115.90	124.84
26	A	410[B]	SQD	O6-C1-C2	6.08	117.79	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	610	CLA	CHD-C4C-C3C	-6.08	115.91	124.84
23	c	504	CLA	CMD-C2D-C1D	6.08	135.42	124.71
23	d	403[B]	CLA	CHD-C4C-C3C	-6.07	115.92	124.84
23	D	402[B]	CLA	C2C-C1C-NC	6.07	115.66	109.97
26	B	620	SQD	O6-C1-C2	6.06	117.77	108.30
23	C	511	CLA	CHD-C1D-ND	-6.06	118.89	124.45
23	c	505	CLA	O2D-CGD-CBD	6.06	122.03	111.27
23	b	602	CLA	CHD-C1D-ND	-6.05	118.90	124.45
23	b	611	CLA	C2C-C1C-NC	6.04	115.63	109.97
26	A	410[A]	SQD	O6-C1-C2	6.03	117.72	108.30
23	C	502	CLA	CMD-C2D-C1D	6.03	135.34	124.71
23	d	403[A]	CLA	C4A-NA-C1A	-6.03	104.00	106.71
23	b	604	CLA	C2C-C1C-NC	6.02	115.61	109.97
23	c	508	CLA	CHD-C4C-C3C	-6.01	116.00	124.84
23	C	505	CLA	CMD-C2D-C1D	6.01	135.31	124.71
23	A	408	CLA	CHD-C4C-C3C	-6.00	116.01	124.84
23	c	501	CLA	CHD-C4C-C3C	-6.00	116.01	124.84
23	b	616	CLA	CMD-C2D-C1D	6.00	135.29	124.71
23	c	505	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
23	B	601	CLA	O2D-CGD-CBD	5.99	121.91	111.27
23	A	406[A]	CLA	CHD-C4C-C3C	-5.98	116.05	124.84
23	C	506	CLA	CHD-C4C-C3C	-5.98	116.05	124.84
23	c	502	CLA	CHD-C4C-C3C	-5.98	116.05	124.84
23	B	605	CLA	CHD-C1D-ND	-5.97	118.97	124.45
23	b	604	CLA	O2D-CGD-CBD	5.97	121.88	111.27
23	B	607	CLA	C2C-C1C-NC	5.96	115.56	109.97
23	C	503	CLA	CHD-C4C-C3C	-5.95	116.09	124.84
23	A	408	CLA	CHD-C1D-ND	-5.94	119.00	124.45
23	b	607	CLA	CHD-C1D-ND	-5.94	119.00	124.45
34	D	410	HTG	C1'-S1-C1	5.93	111.19	100.09
23	c	512	CLA	O2D-CGD-CBD	5.93	121.80	111.27
23	B	602	CLA	C4A-NA-C1A	-5.93	104.04	106.71
23	C	511	CLA	CHD-C4C-C3C	-5.92	116.14	124.84
23	c	504	CLA	CHD-C4C-C3C	-5.92	116.14	124.84
23	A	406[B]	CLA	CMD-C2D-C1D	5.91	135.14	124.71
23	B	601	CLA	CHD-C1D-ND	-5.91	119.02	124.45
23	C	510	CLA	C4A-NA-C1A	-5.91	104.05	106.71
23	C	502	CLA	O2D-CGD-CBD	5.90	121.74	111.27
23	C	514	CLA	CMD-C2D-C1D	5.89	135.10	124.71
23	A	405[A]	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
29	A	414[A]	PL9	C7-C8-C9	-5.89	116.99	126.79
23	d	402[B]	CLA	C2C-C1C-NC	5.89	115.49	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	404[A]	CLA	C4A-NA-C1A	-5.89	104.06	106.71
23	A	406[A]	CLA	CHD-C1D-ND	-5.88	119.05	124.45
23	c	509	CLA	C2C-C1C-NC	5.88	115.48	109.97
23	b	611	CLA	CHD-C1D-ND	-5.87	119.06	124.45
23	b	611	CLA	O2D-CGD-CBD	5.87	121.70	111.27
23	c	510	CLA	C4A-NA-C1A	-5.87	104.07	106.71
23	D	403	CLA	CHD-C4C-C3C	-5.87	116.22	124.84
23	B	616	CLA	C3C-C4C-NC	5.86	117.15	110.57
23	b	604	CLA	CMD-C2D-C1D	5.86	135.04	124.71
23	B	614	CLA	O2D-CGD-CBD	5.86	121.68	111.27
23	c	507	CLA	CHD-C4C-C3C	-5.84	116.26	124.84
23	B	607	CLA	CMD-C2D-C1D	5.83	135.00	124.71
23	C	505	CLA	CHD-C1D-ND	-5.82	119.10	124.45
23	A	405[B]	CLA	CHD-C1D-ND	-5.82	119.11	124.45
23	B	612	CLA	CHD-C1D-ND	-5.82	119.11	124.45
23	b	603	CLA	CMD-C2D-C1D	5.81	134.96	124.71
23	A	404[A]	CLA	CHD-C1D-ND	-5.81	119.11	124.45
23	c	509	CLA	C1-C2-C3	-5.81	115.99	126.04
23	b	601	CLA	CHD-C1D-ND	-5.81	119.11	124.45
23	d	402[B]	CLA	CMD-C2D-C1D	5.81	134.95	124.71
23	c	506	CLA	C2C-C1C-NC	5.80	115.41	109.97
23	C	512	CLA	CMD-C2D-C1D	5.80	134.94	124.71
23	B	606	CLA	O2D-CGD-CBD	5.80	121.58	111.27
23	A	404[B]	CLA	C2C-C1C-NC	5.80	115.40	109.97
23	c	504	CLA	C4A-NA-C1A	-5.79	104.10	106.71
23	B	614	CLA	CHD-C4C-C3C	-5.79	116.33	124.84
23	C	506	CLA	C2C-C1C-NC	5.78	115.39	109.97
23	C	503	CLA	C2C-C1C-NC	5.77	115.38	109.97
23	c	509	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
23	b	601	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
23	B	607	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
23	C	514	CLA	CHD-C4C-C3C	-5.76	116.37	124.84
23	C	505	CLA	CHD-C4C-C3C	-5.76	116.37	124.84
23	b	603	CLA	CHD-C1D-ND	-5.76	119.16	124.45
23	C	510	CLA	CHD-C1D-ND	-5.76	119.16	124.45
23	B	608	CLA	CHD-C4C-C3C	-5.76	116.38	124.84
23	C	513	CLA	CMD-C2D-C1D	5.76	134.86	124.71
23	B	614	CLA	C2C-C1C-NC	5.75	115.36	109.97
23	a	404[A]	CLA	CMD-C2D-C1D	5.75	134.84	124.71
23	d	402[A]	CLA	C4A-NA-C1A	-5.75	104.12	106.71
23	c	508	CLA	C2C-C1C-NC	5.74	115.35	109.97
23	c	511	CLA	CMD-C2D-C1D	5.74	134.83	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	605	CLA	C4A-NA-C1A	-5.74	104.13	106.71
23	D	403	CLA	CMD-C2D-C1D	5.74	134.82	124.71
23	A	408	CLA	C4A-NA-C1A	-5.73	104.13	106.71
23	c	509	CLA	CMD-C2D-C1D	5.73	134.81	124.71
23	C	502	CLA	CHD-C4C-C3C	-5.73	116.42	124.84
23	b	608	CLA	C2C-C1C-NC	5.72	115.33	109.97
23	A	406[A]	CLA	C4A-NA-C1A	-5.72	104.13	106.71
23	b	615	CLA	C2C-C1C-NC	5.72	115.33	109.97
23	A	406[B]	CLA	C4A-NA-C1A	-5.72	104.14	106.71
23	B	603	CLA	CHD-C1D-ND	-5.72	119.20	124.45
23	b	615	CLA	CHD-C4C-C3C	-5.71	116.44	124.84
23	b	604	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
23	c	506	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
23	b	608	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
23	A	408	CLA	C2C-C1C-NC	5.70	115.31	109.97
23	B	602	CLA	O2D-CGD-CBD	5.69	121.39	111.27
23	B	604	CLA	CMD-C2D-C1D	5.69	134.73	124.71
23	b	607	CLA	CMD-C2D-C1D	5.68	134.73	124.71
23	C	503	CLA	CMD-C2D-C1D	5.68	134.72	124.71
23	A	406[B]	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
23	b	610	CLA	CMD-C2D-C1D	5.67	134.71	124.71
23	B	604	CLA	CHD-C4C-C3C	-5.67	116.50	124.84
23	B	611	CLA	CMB-C2B-C1B	5.67	137.18	128.46
23	c	512	CLA	CHD-C4C-C3C	-5.66	116.51	124.84
38	E	102	HEM	CAD-CBD-CGD	5.66	125.79	113.60
23	b	604	CLA	CHD-C1D-ND	-5.66	119.25	124.45
23	c	511	CLA	CHD-C1D-ND	-5.66	119.25	124.45
23	C	508	CLA	C2C-C1C-NC	5.65	115.27	109.97
23	c	513	CLA	CHD-C4C-C3C	-5.65	116.54	124.84
25	Y	101	BCR	C33-C5-C6	-5.65	118.19	124.53
23	B	613	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
23	B	608	CLA	C2C-C1C-NC	5.64	115.25	109.97
23	B	603	CLA	CMD-C2D-C1D	5.64	134.65	124.71
23	d	403[A]	CLA	CMD-C2D-C1D	5.64	134.65	124.71
23	C	508	CLA	CHD-C1D-ND	-5.63	119.28	124.45
23	c	508	CLA	CMD-C2D-C1D	5.63	134.64	124.71
23	c	501	CLA	O2D-CGD-CBD	5.63	121.28	111.27
34	d	411	HTG	C1'-S1-C1	5.62	110.60	100.09
23	C	510	CLA	CHD-C4C-C3C	-5.62	116.58	124.84
23	C	510	CLA	C2C-C1C-NC	5.62	115.23	109.97
23	B	615	CLA	CHD-C1D-ND	-5.61	119.29	124.45
23	B	613	CLA	C2C-C1C-NC	5.61	115.23	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402[A]	CLA	C2C-C1C-NC	5.61	115.22	109.97
23	B	611	CLA	C3D-C2D-C1D	-5.60	98.19	105.83
23	a	404[B]	CLA	CHD-C1D-ND	-5.60	119.31	124.45
23	d	402[B]	CLA	CHD-C1D-ND	-5.59	119.31	124.45
23	A	405[B]	CLA	CMD-C2D-C1D	5.59	134.57	124.71
23	B	604	CLA	O2D-CGD-CBD	5.59	121.19	111.27
26	a	409[A]	SQD	O6-C1-C2	5.58	117.02	108.30
23	c	512	CLA	CHD-C1D-ND	-5.58	119.33	124.45
23	C	511	CLA	O2D-CGD-CBD	5.58	121.18	111.27
23	A	405[A]	CLA	C2C-C1C-NC	5.58	115.19	109.97
26	A	410[A]	SQD	C1-O5-C5	-5.56	102.77	113.69
23	c	503	CLA	CHD-C1D-ND	-5.56	119.34	124.45
23	b	605	CLA	O2D-CGD-CBD	5.56	121.15	111.27
23	d	403[A]	CLA	CHD-C1D-ND	-5.56	119.35	124.45
23	a	405[A]	CLA	C4A-NA-C1A	-5.55	104.21	106.71
23	d	403[A]	CLA	CHD-C4C-C3C	-5.55	116.69	124.84
23	D	402[B]	CLA	CHD-C4C-C3C	-5.54	116.69	124.84
23	D	402[A]	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
23	A	405[A]	CLA	CHD-C1D-ND	-5.53	119.37	124.45
23	B	615	CLA	CMD-C2D-C1D	5.53	134.45	124.71
23	c	507	CLA	C4A-NA-C1A	-5.53	104.22	106.71
23	C	502	CLA	CHD-C1D-ND	-5.52	119.38	124.45
23	B	613	CLA	C1-C2-C3	-5.52	116.50	126.04
23	b	615	CLA	CHD-C1D-ND	-5.51	119.39	124.45
23	B	611	CLA	O2D-CGD-CBD	5.51	121.05	111.27
25	D	404	BCR	C7-C8-C9	-5.50	117.92	126.23
23	b	607	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
23	b	605	CLA	C2C-C1C-NC	5.50	115.12	109.97
23	c	510	CLA	C2C-C1C-NC	5.50	115.12	109.97
23	b	609	CLA	CHD-C1D-ND	-5.49	119.41	124.45
23	a	405[B]	CLA	CMD-C2D-C1D	5.49	134.38	124.71
23	b	602	CLA	CHD-C4C-C3C	-5.48	116.79	124.84
23	C	508	CLA	C4A-NA-C1A	-5.47	104.25	106.71
23	c	513	CLA	C2C-C1C-NC	5.47	115.09	109.97
23	b	605	CLA	C4A-NA-C1A	-5.46	104.25	106.71
23	C	505	CLA	C3D-C2D-C1D	-5.46	98.39	105.83
23	B	614	CLA	CHD-C1D-ND	-5.45	119.44	124.45
26	b	620	SQD	O6-C1-C2	5.45	116.82	108.30
23	a	407	CLA	C3D-C2D-C1D	-5.45	98.40	105.83
23	b	610	CLA	O2D-CGD-CBD	5.44	120.94	111.27
26	F	102	SQD	C1-O5-C5	-5.44	103.00	113.69
23	B	606	CLA	C3D-C2D-C1D	-5.44	98.41	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402[A]	CLA	CHD-C1D-ND	-5.44	119.46	124.45
23	b	611	CLA	C3D-C2D-C1D	-5.44	98.41	105.83
23	b	612	CLA	CMD-C2D-C1D	5.43	134.29	124.71
23	A	404[B]	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
25	t	102	BCR	C33-C5-C6	-5.41	118.46	124.53
23	c	505	CLA	C4A-NA-C1A	-5.40	104.28	106.71
23	d	404	CLA	O2D-CGD-CBD	5.39	120.85	111.27
23	c	505	CLA	C2C-C1C-NC	5.39	115.02	109.97
23	b	613	CLA	C3C-C4C-NC	5.39	116.61	110.57
23	a	404[A]	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
23	B	610	CLA	CHD-C1D-ND	-5.38	119.51	124.45
23	C	510	CLA	CMD-C2D-C1D	5.38	134.20	124.71
23	b	612	CLA	C3C-C4C-NC	5.37	116.59	110.57
24	a	414[A]	PHO	C1-C2-C3	-5.37	116.76	126.04
23	C	511	CLA	C2C-C1C-NC	5.36	115.00	109.97
23	A	408	CLA	C3D-C2D-C1D	-5.36	98.52	105.83
23	B	607	CLA	C4A-NA-C1A	-5.36	104.30	106.71
23	A	405[A]	CLA	O2D-CGD-CBD	5.35	120.78	111.27
23	a	405[B]	CLA	C4A-NA-C1A	-5.35	104.30	106.71
23	b	613	CLA	CMD-C2D-C1D	5.34	134.13	124.71
23	b	614	CLA	CHD-C1D-ND	-5.34	119.55	124.45
23	a	405[A]	CLA	CMD-C2D-C1D	5.34	134.12	124.71
23	C	513	CLA	O2D-CGD-CBD	5.34	120.75	111.27
23	A	406[A]	CLA	C2C-C1C-NC	5.33	114.97	109.97
23	b	614	CLA	C3D-C2D-C1D	-5.33	98.56	105.83
23	b	613	CLA	C4A-NA-C1A	-5.32	104.31	106.71
23	C	503	CLA	CHD-C1D-ND	-5.32	119.56	124.45
23	c	507	CLA	C2C-C1C-NC	5.32	114.96	109.97
23	B	611	CLA	CHD-C1D-ND	-5.31	119.57	124.45
23	b	612	CLA	C2C-C1C-NC	5.31	114.95	109.97
23	b	608	CLA	C4A-NA-C1A	-5.31	104.32	106.71
23	B	603	CLA	C2C-C1C-NC	5.31	114.94	109.97
23	C	514	CLA	C2C-C1C-NC	5.30	114.94	109.97
23	b	604	CLA	C4A-NA-C1A	-5.30	104.32	106.71
23	B	612	CLA	C3C-C4C-NC	5.30	116.51	110.57
23	a	404[A]	CLA	CHD-C1D-ND	-5.29	119.59	124.45
23	b	602	CLA	O2D-CGD-CBD	5.27	120.64	111.27
23	B	614	CLA	C3D-C2D-C1D	-5.27	98.64	105.83
23	C	509	CLA	CMD-C2D-C1D	5.27	133.99	124.71
23	a	404[B]	CLA	CHD-C4C-C3C	-5.26	117.11	124.84
23	C	503	CLA	O2D-CGD-CBD	5.26	120.62	111.27
23	C	506	CLA	O2D-CGD-CBD	5.26	120.61	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	409[B]	SQD	O6-C1-C2	5.26	116.51	108.30
23	B	610	CLA	C2C-C1C-NC	5.26	114.90	109.97
23	c	505	CLA	CMD-C2D-C1D	5.25	133.97	124.71
34	B	623	HTG	C1'-S1-C1	5.25	109.91	100.09
23	D	403	CLA	CHD-C1D-ND	-5.25	119.63	124.45
26	A	410[A]	SQD	C1-C2-C3	-5.25	99.07	110.00
23	C	503	CLA	C4A-NA-C1A	-5.24	104.35	106.71
26	B	620	SQD	O47-C7-C8	5.24	122.79	111.50
23	A	405[B]	CLA	C2C-C1C-NC	5.23	114.88	109.97
23	a	407	CLA	C2C-C1C-NC	5.22	114.86	109.97
23	B	613	CLA	CHD-C1D-ND	-5.22	119.66	124.45
23	c	501	CLA	C4A-NA-C1A	-5.21	104.36	106.71
26	a	409[A]	SQD	O47-C7-C8	5.21	122.73	111.50
23	B	604	CLA	C3C-C4C-NC	5.21	116.41	110.57
33	C	501	LMG	C7-O1-C1	-5.20	103.58	113.74
23	b	608	CLA	CHD-C1D-ND	-5.20	119.68	124.45
23	c	509	CLA	CHD-C1D-ND	-5.19	119.68	124.45
23	A	405[A]	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
23	d	402[A]	CLA	CMD-C2D-C1D	5.19	133.85	124.71
23	b	616	CLA	CHD-C1D-ND	-5.18	119.69	124.45
23	B	605	CLA	C3D-C2D-C1D	-5.18	98.77	105.83
23	B	608	CLA	CHD-C1D-ND	-5.17	119.70	124.45
23	C	512	CLA	C2C-C1C-NC	5.17	114.81	109.97
23	a	407	CLA	C3C-C4C-NC	5.17	116.36	110.57
23	c	503	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
23	c	504	CLA	C2C-C1C-NC	5.15	114.80	109.97
34	C	522	HTG	C1'-S1-C1	5.15	109.73	100.09
23	c	508	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
23	c	505	CLA	CHD-C1D-ND	-5.15	119.72	124.45
23	b	606	CLA	O2D-CGD-CBD	5.15	120.41	111.27
23	b	610	CLA	C2C-C1C-NC	5.14	114.79	109.97
23	b	605	CLA	C3D-C2D-C1D	-5.14	98.81	105.83
23	b	607	CLA	C3C-C4C-NC	5.12	116.32	110.57
23	c	511	CLA	C2C-C1C-NC	5.12	114.77	109.97
23	D	402[A]	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
23	A	406[A]	CLA	CMD-C2D-C1D	5.12	133.74	124.71
23	B	610	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
23	B	612	CLA	CMD-C2D-C1D	5.11	133.71	124.71
23	c	513	CLA	C4A-NA-C1A	-5.11	104.41	106.71
23	B	602	CLA	C2C-C1C-NC	5.11	114.76	109.97
23	B	603	CLA	C4A-NA-C1A	-5.10	104.41	106.71
23	b	613	CLA	C3D-C2D-C1D	-5.10	98.87	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	608	CLA	CMD-C2D-C1D	5.10	133.69	124.71
23	B	602	CLA	CHD-C1D-ND	-5.09	119.78	124.45
38	f	101	HEM	CHC-C4B-NB	5.09	129.96	124.43
23	b	610	CLA	C4A-NA-C1A	-5.09	104.42	106.71
26	b	620	SQD	O47-C7-C8	5.09	122.46	111.50
23	a	407	CLA	CHD-C1D-ND	-5.08	119.78	124.45
23	C	511	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
23	a	407	CLA	CMD-C2D-C1D	5.08	133.67	124.71
29	A	414[B]	PL9	C7-C8-C9	-5.08	118.34	126.79
23	B	614	CLA	C4A-NA-C1A	-5.08	104.42	106.71
23	b	603	CLA	O2D-CGD-CBD	5.06	120.27	111.27
23	B	616	CLA	C2C-C1C-NC	5.06	114.71	109.97
23	c	501	CLA	O2D-CGD-O1D	-5.06	113.95	123.84
23	d	402[B]	CLA	O2D-CGD-CBD	5.05	120.24	111.27
23	b	607	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
23	B	605	CLA	C2C-C1C-NC	5.04	114.70	109.97
23	a	407	CLA	O2D-CGD-CBD	5.04	120.22	111.27
23	c	501	CLA	C3D-C2D-C1D	-5.04	98.96	105.83
23	C	509	CLA	C3C-C4C-NC	5.03	116.22	110.57
23	c	504	CLA	O2D-CGD-CBD	5.03	120.21	111.27
23	c	505	CLA	C3C-C4C-NC	5.03	116.21	110.57
23	B	616	CLA	C4A-NA-C1A	-5.03	104.44	106.71
23	c	502	CLA	O2D-CGD-CBD	5.03	120.20	111.27
23	C	506	CLA	CHD-C1D-ND	-5.02	119.84	124.45
25	d	405	BCR	C7-C8-C9	-5.01	118.66	126.23
23	b	604	CLA	C1-C2-C3	-5.01	117.39	126.04
23	C	504	CLA	C3D-C2D-C1D	-5.00	99.00	105.83
23	B	613	CLA	CMD-C2D-C1D	5.00	133.53	124.71
23	B	607	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
23	B	608	CLA	CMD-C2D-C1D	5.00	133.52	124.71
23	C	507	CLA	CHD-C4C-C3C	-5.00	117.49	124.84
23	B	615	CLA	C2C-C1C-NC	4.99	114.65	109.97
23	B	605	CLA	O2D-CGD-CBD	4.99	120.14	111.27
23	C	513	CLA	CHD-C1D-ND	-4.99	119.87	124.45
23	B	613	CLA	C3D-C2D-C1D	-4.99	99.03	105.83
23	c	508	CLA	CHD-C1D-ND	-4.98	119.87	124.45
23	b	616	CLA	C3D-C2D-C1D	-4.97	99.04	105.83
23	a	404[B]	CLA	C4A-NA-C1A	-4.97	104.47	106.71
23	B	607	CLA	O2D-CGD-CBD	4.97	120.10	111.27
23	B	612	CLA	O2D-CGD-CBD	4.96	120.09	111.27
23	b	614	CLA	C4A-NA-C1A	-4.96	104.47	106.71
23	C	512	CLA	CHD-C1D-ND	-4.96	119.90	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	610	CLA	C3C-C4C-NC	4.95	116.13	110.57
23	B	609	CLA	C2C-C1C-NC	4.95	114.61	109.97
25	d	405	BCR	C15-C14-C13	-4.94	120.25	127.31
23	c	506	CLA	C4A-NA-C1A	-4.94	104.48	106.71
23	C	506	CLA	C4A-NA-C1A	-4.94	104.48	106.71
23	A	406[B]	CLA	C3D-C4D-ND	4.94	118.23	110.24
23	a	405[A]	CLA	C2C-C1C-NC	4.94	114.60	109.97
26	f	102	SQD	O47-C7-C8	4.94	122.14	111.50
23	B	608	CLA	O2D-CGD-CBD	4.93	120.03	111.27
23	b	613	CLA	CHD-C1D-ND	-4.93	119.93	124.45
23	d	404	CLA	C3D-C2D-C1D	-4.92	99.11	105.83
23	b	609	CLA	C2C-C1C-NC	4.92	114.58	109.97
23	c	502	CLA	C1C-C2C-C3C	-4.92	101.79	106.96
23	B	603	CLA	C3D-C2D-C1D	-4.92	99.12	105.83
23	a	405[A]	CLA	C3D-C2D-C1D	-4.91	99.12	105.83
23	B	616	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
23	C	509	CLA	CHD-C1D-ND	-4.91	119.94	124.45
23	d	404	CLA	C4A-NA-C1A	-4.91	104.50	106.71
23	b	603	CLA	C2C-C1C-NC	4.91	114.57	109.97
23	C	509	CLA	O2D-CGD-CBD	4.91	119.99	111.27
23	B	606	CLA	C2C-C1C-NC	4.90	114.56	109.97
23	C	507	CLA	C1C-C2C-C3C	-4.90	101.81	106.96
23	c	503	CLA	C2C-C1C-NC	4.90	114.56	109.97
23	d	402[A]	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
23	c	506	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
23	B	611	CLA	C3C-C4C-NC	4.88	116.05	110.57
23	c	508	CLA	C4A-NA-C1A	-4.88	104.51	106.71
23	B	609	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
23	b	601	CLA	C2C-C1C-NC	4.86	114.53	109.97
23	c	504	CLA	C3D-C2D-C1D	-4.86	99.21	105.83
23	B	607	CLA	C1C-C2C-C3C	-4.85	101.85	106.96
23	A	405[A]	CLA	C4A-NA-C1A	-4.85	104.53	106.71
33	d	412	LMG	O7-C10-C11	4.84	121.94	111.50
23	A	404[A]	CLA	CHD-C4C-C3C	-4.84	117.73	124.84
23	b	609	CLA	O2D-CGD-CBD	4.83	119.85	111.27
38	E	102	HEM	CBA-CAA-C2A	-4.83	104.38	112.62
23	a	405[B]	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
23	D	402[B]	CLA	C3D-C2D-C1D	-4.81	99.26	105.83
23	c	501	CLA	C2C-C1C-NC	4.80	114.47	109.97
23	C	506	CLA	C3C-C4C-NC	4.80	115.95	110.57
23	c	509	CLA	O2D-CGD-CBD	4.80	119.79	111.27
23	b	609	CLA	C3C-C4C-NC	4.79	115.94	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	509	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
23	b	607	CLA	C4A-NA-C1A	-4.79	104.55	106.71
23	C	512	CLA	C4A-NA-C1A	-4.79	104.55	106.71
23	d	402[B]	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
23	C	508	CLA	C3D-C2D-C1D	-4.78	99.30	105.83
23	b	610	CLA	C1-C2-C3	-4.78	117.77	126.04
23	B	615	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
23	C	505	CLA	C3C-C4C-NC	4.78	115.93	110.57
23	B	608	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
23	b	614	CLA	C2C-C1C-NC	4.77	114.44	109.97
23	A	405[B]	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
26	a	409[B]	SQD	O47-C7-C8	4.77	121.78	111.50
23	b	606	CLA	C2C-C1C-NC	4.76	114.44	109.97
23	b	606	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
24	A	416[B]	PHO	C1-C2-C3	-4.76	117.81	126.04
23	C	514	CLA	C3D-C2D-C1D	-4.76	99.34	105.83
23	B	611	CLA	CMC-C2C-C1C	4.76	132.29	125.04
23	c	502	CLA	C3D-C2D-C1D	-4.76	99.34	105.83
23	d	403[B]	CLA	C4A-NA-C1A	-4.76	104.57	106.71
23	A	405[B]	CLA	O2D-CGD-CBD	4.76	119.72	111.27
23	C	502	CLA	C2C-C1C-NC	4.75	114.43	109.97
25	H	101	BCR	C38-C26-C25	-4.75	119.20	124.53
23	c	510	CLA	CHD-C1D-ND	-4.75	120.09	124.45
23	D	403	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
23	b	604	CLA	C3C-C4C-NC	4.74	115.89	110.57
23	C	503	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
23	A	406[A]	CLA	O2D-CGD-CBD	4.74	119.69	111.27
23	A	406[B]	CLA	C3D-C2D-C1D	-4.74	99.37	105.83
23	b	615	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
23	C	512	CLA	O2D-CGD-CBD	4.73	119.67	111.27
23	b	610	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
24	a	414[B]	PHO	C1-C2-C3	-4.72	117.88	126.04
23	A	405[A]	CLA	C1C-C2C-C3C	-4.71	102.00	106.96
23	A	404[A]	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
23	a	405[B]	CLA	O2D-CGD-CBD	4.71	119.63	111.27
23	c	513	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
23	A	406[B]	CLA	C2C-C1C-NC	4.70	114.37	109.97
40	v	201	HEC	CMC-C2C-C1C	-4.70	121.25	128.46
23	D	403	CLA	O2D-CGD-CBD	4.70	119.61	111.27
23	b	605	CLA	O2D-CGD-O1D	-4.69	114.66	123.84
23	c	503	CLA	O2D-CGD-CBD	4.69	119.61	111.27
23	C	512	CLA	C3D-C2D-C1D	-4.69	99.43	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	602	CLA	C3D-C2D-C1D	-4.69	99.44	105.83
23	a	405[A]	CLA	C3D-C4D-ND	4.68	117.81	110.24
23	B	601	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
23	B	611	CLA	C3D-C4D-ND	4.67	117.79	110.24
23	d	403[A]	CLA	C3C-C4C-NC	4.67	115.80	110.57
23	B	606	CLA	C3C-C4C-NC	4.66	115.80	110.57
23	b	603	CLA	C3D-C4D-ND	4.66	117.78	110.24
23	B	610	CLA	C4A-NA-C1A	-4.66	104.61	106.71
23	B	609	CLA	C3C-C4C-NC	4.66	115.80	110.57
23	C	514	CLA	O2D-CGD-CBD	4.65	119.53	111.27
23	B	601	CLA	C2C-C1C-NC	4.65	114.33	109.97
23	c	508	CLA	C3C-C4C-NC	4.65	115.79	110.57
23	C	504	CLA	O2D-CGD-CBD	4.65	119.53	111.27
23	c	503	CLA	C3C-C4C-NC	4.65	115.79	110.57
23	b	612	CLA	O2D-CGD-CBD	4.65	119.53	111.27
23	C	510	CLA	O2D-CGD-CBD	4.64	119.51	111.27
23	c	507	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
33	B	621	LMG	O7-C10-C11	4.63	121.48	111.50
23	b	605	CLA	C3D-C4D-ND	4.63	117.73	110.24
23	A	406[A]	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
23	B	608	CLA	C3C-C4C-NC	4.62	115.76	110.57
34	b	622	HTG	C1-O5-C5	4.62	121.10	112.58
26	A	410[B]	SQD	C1-O5-C5	-4.61	104.63	113.69
23	D	403	CLA	C2C-C1C-NC	4.61	114.29	109.97
38	E	102	HEM	CHC-C4B-NB	4.61	129.44	124.43
23	b	602	CLA	C2C-C1C-NC	4.61	114.29	109.97
23	c	513	CLA	O2D-CGD-CBD	4.61	119.45	111.27
29	a	412[A]	PL9	C7-C8-C9	-4.60	119.13	126.79
23	B	608	CLA	C4A-NA-C1A	-4.60	104.64	106.71
23	C	502	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
23	C	504	CLA	C3C-C4C-NC	4.59	115.72	110.57
23	a	405[B]	CLA	C3D-C4D-ND	4.59	117.67	110.24
23	b	608	CLA	C1C-C2C-C3C	-4.59	102.13	106.96
26	b	620	SQD	C1-O5-C5	-4.58	104.69	113.69
23	a	404[A]	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
23	c	510	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
23	d	403[B]	CLA	C1C-C2C-C3C	-4.58	102.14	106.96
23	a	405[A]	CLA	O2D-CGD-CBD	4.58	119.40	111.27
23	c	509	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
23	b	616	CLA	C3C-C4C-NC	4.57	115.70	110.57
23	C	507	CLA	C4A-NA-C1A	-4.57	104.65	106.71
25	y	101	BCR	C33-C5-C6	-4.57	119.40	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	502	CLA	C4A-NA-C1A	-4.57	104.65	106.71
23	C	505	CLA	O2D-CGD-CBD	4.57	119.38	111.27
23	b	612	CLA	CHD-C1D-ND	-4.56	120.26	124.45
23	c	502	CLA	CHD-C1D-ND	-4.56	120.26	124.45
23	C	504	CLA	C2C-C1C-NC	4.56	114.24	109.97
23	b	609	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
26	A	410[B]	SQD	C1-C2-C3	-4.56	100.51	110.00
23	B	604	CLA	C1-C2-C3	-4.56	118.17	126.04
23	D	402[A]	CLA	O2D-CGD-CBD	4.55	119.36	111.27
23	B	612	CLA	C2C-C1C-NC	4.55	114.24	109.97
23	A	406[A]	CLA	C3D-C4D-ND	4.55	117.61	110.24
23	C	508	CLA	C3C-C4C-NC	4.55	115.67	110.57
23	A	405[A]	CLA	CMD-C2D-C1D	4.55	132.73	124.71
23	b	604	CLA	C1C-C2C-C3C	-4.55	102.18	106.96
23	b	602	CLA	C3D-C4D-ND	4.55	117.59	110.24
23	b	603	CLA	C1D-CHD-C4C	-4.54	116.26	126.06
23	b	605	CLA	C3C-C4C-NC	4.54	115.66	110.57
23	d	403[B]	CLA	C3D-C4D-ND	4.53	117.57	110.24
24	A	416[A]	PHO	C1-C2-C3	-4.53	118.22	126.04
23	b	608	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
23	B	612	CLA	C3D-C4D-ND	4.52	117.55	110.24
23	b	607	CLA	O2D-CGD-CBD	4.52	119.30	111.27
23	c	511	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
31	t	101	LMT	C3'-C4'-C5'	-4.52	100.57	110.93
23	c	512	CLA	C3D-C2D-C1D	-4.52	99.67	105.83
23	B	601	CLA	C4A-NA-C1A	-4.52	104.68	106.71
23	B	613	CLA	C3C-C4C-NC	4.51	115.63	110.57
23	C	513	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
23	C	503	CLA	C3C-C4C-NC	4.51	115.62	110.57
23	C	514	CLA	C4A-NA-C1A	-4.50	104.68	106.71
23	B	610	CLA	O2A-CGA-CBA	4.50	126.03	111.91
23	c	508	CLA	O2D-CGD-CBD	4.50	119.26	111.27
23	b	604	CLA	C3D-C2D-C1D	-4.50	99.70	105.83
23	d	402[A]	CLA	C1C-C2C-C3C	-4.49	102.24	106.96
23	b	611	CLA	C3C-C4C-NC	4.48	115.60	110.57
23	C	507	CLA	C3D-C4D-ND	4.48	117.49	110.24
23	C	512	CLA	C3C-C4C-NC	4.48	115.60	110.57
23	C	507	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
23	B	603	CLA	O2D-CGD-O1D	-4.48	115.08	123.84
23	B	609	CLA	C3D-C4D-ND	4.48	117.48	110.24
23	a	405[B]	CLA	C2C-C1C-NC	4.48	114.17	109.97
23	a	404[B]	CLA	C3D-C4D-ND	4.48	117.48	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	402[B]	CLA	O2D-CGD-CBD	4.48	119.22	111.27
23	c	510	CLA	C3C-C4C-NC	4.47	115.59	110.57
23	d	402[B]	CLA	C1C-C2C-C3C	-4.47	102.26	106.96
23	b	613	CLA	C1-C2-C3	-4.47	118.31	126.04
23	c	510	CLA	C1-C2-C3	-4.46	118.32	126.04
23	c	510	CLA	O2D-CGD-CBD	4.46	119.20	111.27
26	A	410[B]	SQD	O9-S-C6	4.46	112.24	106.94
23	D	402[B]	CLA	C3C-C4C-NC	4.46	115.57	110.57
23	B	616	CLA	O2D-CGD-O1D	-4.46	115.12	123.84
23	B	615	CLA	C3C-C4C-NC	4.46	115.57	110.57
23	B	607	CLA	C3C-C4C-NC	4.45	115.57	110.57
23	C	507	CLA	O2D-CGD-CBD	4.45	119.18	111.27
23	c	511	CLA	C3D-C4D-ND	4.45	117.43	110.24
23	d	403[A]	CLA	C1C-C2C-C3C	-4.45	102.28	106.96
23	a	407	CLA	C3D-C4D-ND	4.44	117.42	110.24
23	b	610	CLA	CHD-C1D-ND	-4.44	120.37	124.45
23	d	403[A]	CLA	C3D-C4D-ND	4.44	117.42	110.24
23	c	507	CLA	CMC-C2C-C1C	4.44	131.80	125.04
23	d	403[B]	CLA	C3C-C4C-NC	4.44	115.55	110.57
23	c	511	CLA	O2D-CGD-CBD	4.44	119.15	111.27
23	b	608	CLA	C3D-C4D-ND	4.43	117.41	110.24
23	C	505	CLA	C1C-C2C-C3C	-4.43	102.30	106.96
23	C	504	CLA	C3D-C4D-ND	4.43	117.40	110.24
23	b	603	CLA	C3C-C4C-NC	4.43	115.54	110.57
23	C	513	CLA	C3C-C4C-NC	4.42	115.53	110.57
25	c	514	BCR	C11-C10-C9	-4.42	121.01	127.31
23	b	601	CLA	C3D-C4D-ND	4.41	117.37	110.24
23	D	403	CLA	C3C-C4C-NC	4.41	115.52	110.57
23	B	611	CLA	C4A-NA-C1A	-4.41	104.72	106.71
23	B	602	CLA	C3C-C4C-NC	4.40	115.51	110.57
23	b	615	CLA	C3D-C4D-ND	4.40	117.36	110.24
23	C	502	CLA	O2D-CGD-O1D	-4.40	115.23	123.84
23	b	608	CLA	O2D-CGD-CBD	4.40	119.09	111.27
23	d	404	CLA	C3D-C4D-ND	4.40	117.35	110.24
33	C	501	LMG	O7-C10-C11	4.39	120.97	111.50
29	a	412[B]	PL9	C7-C3-C4	4.39	120.45	116.88
23	B	601	CLA	C3C-C4C-NC	4.39	115.50	110.57
23	d	402[A]	CLA	O2D-CGD-CBD	4.39	119.07	111.27
23	C	510	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
23	B	612	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
33	c	520	LMG	O6-C5-C4	4.38	117.65	109.69
23	B	603	CLA	C3C-C4C-NC	4.38	115.48	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	412[A]	PL9	C7-C3-C4	4.38	120.44	116.88
23	C	514	CLA	C3D-C4D-ND	4.38	117.32	110.24
26	f	102	SQD	C1-O5-C5	4.38	122.28	113.69
23	b	602	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
23	c	511	CLA	C3C-C4C-NC	4.37	115.47	110.57
23	c	507	CLA	C1C-C2C-C3C	-4.36	102.37	106.96
25	C	516	BCR	C7-C8-C9	-4.36	119.65	126.23
23	B	605	CLA	C3C-C4C-NC	4.36	115.46	110.57
23	c	501	CLA	C3D-C4D-ND	4.35	117.28	110.24
23	c	505	CLA	C3D-C4D-ND	4.35	117.28	110.24
23	b	601	CLA	C3D-C2D-C1D	-4.35	99.90	105.83
23	c	513	CLA	C1D-CHD-C4C	-4.34	116.69	126.06
23	c	513	CLA	C3D-C4D-ND	4.34	117.26	110.24
23	B	616	CLA	CMD-C2D-C1D	4.34	132.36	124.71
23	b	607	CLA	C3D-C4D-ND	4.33	117.25	110.24
40	v	201	HEC	CBD-CAD-C3D	-4.33	105.23	112.62
23	c	503	CLA	C1D-CHD-C4C	-4.33	116.71	126.06
25	T	102	BCR	C15-C16-C17	-4.33	114.60	123.47
23	C	510	CLA	C3D-C4D-ND	4.33	117.24	110.24
23	b	616	CLA	C1D-CHD-C4C	-4.32	116.73	126.06
32	E	101[A]	LHG	O7-C7-C8	4.32	120.82	111.50
23	A	404[A]	CLA	C1C-C2C-C3C	-4.32	102.41	106.96
23	A	405[B]	CLA	C1C-C2C-C3C	-4.32	102.41	106.96
29	a	412[B]	PL9	C32-C33-C34	-4.32	117.27	127.66
33	a	415	LMG	O7-C10-C11	4.32	120.81	111.50
23	A	408	CLA	C3C-C4C-NC	4.32	115.41	110.57
23	C	510	CLA	C1-C2-C3	-4.32	118.58	126.04
23	D	402[A]	CLA	C3C-C4C-NC	4.31	115.41	110.57
23	A	405[B]	CLA	C3D-C4D-ND	4.31	117.22	110.24
23	c	511	CLA	C4A-NA-C1A	-4.31	104.77	106.71
23	C	513	CLA	C2C-C1C-NC	4.31	114.01	109.97
23	d	403[B]	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
23	c	504	CLA	C3D-C4D-ND	4.30	117.20	110.24
23	B	605	CLA	C3D-C4D-ND	4.30	117.20	110.24
23	B	615	CLA	C3D-C4D-ND	4.30	117.20	110.24
23	b	612	CLA	C4A-NA-C1A	-4.30	104.77	106.71
23	B	610	CLA	C3C-C4C-NC	4.30	115.39	110.57
29	A	414[A]	PL9	C32-C33-C34	-4.30	117.31	127.66
23	b	609	CLA	C3D-C4D-ND	4.30	117.19	110.24
23	D	402[B]	CLA	C1-C2-C3	-4.29	118.62	126.04
29	d	406[B]	PL9	C7-C8-C9	-4.29	119.65	126.79
23	c	506	CLA	C3D-C4D-ND	4.29	117.18	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	414[B]	PL9	C32-C33-C34	-4.29	117.33	127.66
23	a	404[A]	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
23	b	606	CLA	C3C-C4C-NC	4.29	115.38	110.57
23	C	508	CLA	C1D-CHD-C4C	-4.28	116.83	126.06
23	C	502	CLA	C3D-C4D-ND	4.27	117.14	110.24
23	A	404[B]	CLA	C1C-C2C-C3C	-4.27	102.47	106.96
23	B	601	CLA	C3D-C4D-ND	4.26	117.14	110.24
23	c	513	CLA	C3C-C4C-NC	4.26	115.34	110.57
23	C	510	CLA	C3C-C4C-NC	4.25	115.34	110.57
23	a	405[A]	CLA	C3C-C4C-NC	4.25	115.34	110.57
23	C	513	CLA	C1D-CHD-C4C	-4.25	116.89	126.06
23	c	501	CLA	C3C-C4C-NC	4.25	115.33	110.57
38	E	102	HEM	C1B-NB-C4B	4.25	109.46	105.07
23	C	514	CLA	C3C-C4C-NC	4.25	115.33	110.57
23	B	604	CLA	C4A-NA-C1A	-4.24	104.80	106.71
23	c	502	CLA	CMD-C2D-C1D	4.24	132.19	124.71
23	d	402[B]	CLA	C3D-C4D-ND	4.24	117.10	110.24
34	b	622	HTG	C1'-S1-C1	4.24	108.02	100.09
23	A	404[B]	CLA	C3D-C4D-ND	4.24	117.09	110.24
23	b	616	CLA	C2C-C1C-NC	4.24	113.94	109.97
23	C	506	CLA	C3D-C2D-C1D	-4.23	100.05	105.83
23	d	404	CLA	C2C-C1C-NC	4.23	113.94	109.97
23	a	404[B]	CLA	C1D-CHD-C4C	-4.23	116.93	126.06
23	C	506	CLA	C3D-C4D-ND	4.23	117.08	110.24
23	A	404[B]	CLA	C3D-C2D-C1D	-4.23	100.06	105.83
23	b	603	CLA	C3D-C2D-C1D	-4.23	100.06	105.83
26	A	410[B]	SQD	C44-O6-C1	-4.23	105.48	113.74
23	C	511	CLA	C3D-C4D-ND	4.22	117.07	110.24
29	a	412[B]	PL9	C7-C8-C9	-4.22	119.76	126.79
23	C	509	CLA	C4A-NA-C1A	-4.22	104.81	106.71
23	B	603	CLA	C3D-C4D-ND	4.22	117.06	110.24
23	c	502	CLA	C1D-CHD-C4C	-4.22	116.96	126.06
23	a	404[A]	CLA	C3D-C4D-ND	4.22	117.06	110.24
33	Z	101	LMG	O7-C10-C11	4.22	120.59	111.50
23	B	616	CLA	C3D-C4D-ND	4.21	117.06	110.24
23	c	503	CLA	C3D-C4D-ND	4.21	117.05	110.24
23	d	404	CLA	C3C-C4C-NC	4.21	115.29	110.57
23	b	606	CLA	C1D-CHD-C4C	-4.21	116.98	126.06
23	b	608	CLA	CMC-C2C-C1C	4.21	131.44	125.04
23	a	404[A]	CLA	C1D-CHD-C4C	-4.21	116.98	126.06
23	c	504	CLA	C3C-C4C-NC	4.21	115.29	110.57
25	d	405	BCR	C40-C30-C25	-4.20	103.49	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	505	CLA	C3D-C2D-C1D	-4.20	100.10	105.83
23	c	512	CLA	C2C-C1C-NC	4.19	113.90	109.97
26	a	409[A]	SQD	C1-C2-C3	-4.19	101.27	110.00
23	a	405[B]	CLA	C3C-C4C-NC	4.18	115.26	110.57
23	b	611	CLA	C3D-C4D-ND	4.18	117.00	110.24
23	b	607	CLA	C1C-C2C-C3C	-4.18	102.56	106.96
23	c	509	CLA	C3D-C4D-ND	4.18	116.99	110.24
23	a	404[A]	CLA	CAA-C2A-C3A	-4.18	101.34	112.78
23	b	602	CLA	C3C-C4C-NC	4.17	115.25	110.57
23	b	616	CLA	O2D-CGD-O1D	-4.17	115.68	123.84
23	d	403[B]	CLA	O2D-CGD-CBD	4.17	118.68	111.27
23	c	506	CLA	C1-C2-C3	-4.17	118.83	126.04
23	B	615	CLA	C1D-CHD-C4C	-4.17	117.07	126.06
23	B	611	CLA	C1D-CHD-C4C	-4.16	117.07	126.06
23	a	404[B]	CLA	C1C-C2C-C3C	-4.16	102.58	106.96
23	a	407	CLA	C1D-CHD-C4C	-4.16	117.08	126.06
23	C	509	CLA	C3D-C4D-ND	4.16	116.97	110.24
23	A	406[A]	CLA	C1C-C2C-C3C	-4.16	102.59	106.96
23	b	607	CLA	C3B-C4B-NB	4.16	114.58	109.21
24	A	407[B]	PHO	C1A-C2A-C3A	-4.16	98.89	102.84
25	b	617	BCR	C33-C5-C6	-4.15	119.86	124.53
23	B	616	CLA	C4C-C3C-C2C	-4.15	100.84	106.90
23	B	602	CLA	CMC-C2C-C1C	4.15	131.36	125.04
29	D	405[B]	PL9	C42-C43-C44	-4.15	117.67	127.66
23	c	502	CLA	C3D-C4D-ND	4.15	116.95	110.24
23	A	405[B]	CLA	C4A-NA-C1A	-4.14	104.84	106.71
23	B	608	CLA	C3D-C4D-ND	4.14	116.94	110.24
23	D	402[A]	CLA	C1C-C2C-C3C	-4.14	102.60	106.96
23	A	408	CLA	C3D-C4D-ND	4.14	116.93	110.24
23	D	402[B]	CLA	C3D-C4D-ND	4.14	116.93	110.24
23	c	509	CLA	C1C-C2C-C3C	-4.13	102.61	106.96
23	A	404[B]	CLA	C1D-CHD-C4C	-4.13	117.14	126.06
33	C	501	LMG	O1-C1-C2	4.13	114.75	108.30
23	b	611	CLA	C1C-C2C-C3C	-4.13	102.61	106.96
25	Y	101	BCR	C16-C17-C18	-4.13	121.42	127.31
23	a	404[B]	CLA	C3D-C2D-C1D	-4.13	100.20	105.83
23	d	402[B]	CLA	C1D-CHD-C4C	-4.12	117.16	126.06
23	B	607	CLA	C3D-C4D-ND	4.12	116.91	110.24
23	C	513	CLA	C3D-C4D-ND	4.12	116.91	110.24
35	C	518[B]	DGD	O2G-C1B-C2B	4.12	120.38	111.50
23	d	402[A]	CLA	C3D-C4D-ND	4.12	116.90	110.24
23	c	509	CLA	C3B-C4B-NB	4.12	114.53	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	414[A]	PL9	C7-C3-C2	-4.12	117.89	123.30
23	d	403[A]	CLA	O2D-CGD-CBD	4.11	118.58	111.27
32	E	101[B]	LHG	O7-C7-C8	4.11	120.37	111.50
23	D	402[B]	CLA	C1C-C2C-C3C	-4.11	102.63	106.96
23	d	403[A]	CLA	C3D-C2D-C1D	-4.11	100.22	105.83
26	F	102	SQD	O8-S-C6	4.11	112.28	105.74
23	A	404[A]	CLA	C3B-C4B-NB	4.11	114.52	109.21
23	C	503	CLA	C1C-C2C-C3C	-4.11	102.64	106.96
23	B	616	CLA	CHD-C1D-ND	-4.11	120.68	124.45
23	B	602	CLA	C3D-C4D-ND	4.11	116.88	110.24
34	b	625	HTG	C1-O5-C5	4.10	120.15	112.58
23	b	612	CLA	C3D-C2D-C1D	-4.10	100.23	105.83
23	B	613	CLA	O2D-CGD-CBD	4.10	118.56	111.27
23	B	606	CLA	O2D-CGD-O1D	-4.10	115.81	123.84
23	C	511	CLA	C4A-NA-C1A	-4.10	104.86	106.71
23	A	405[A]	CLA	C3D-C4D-ND	4.10	116.87	110.24
23	B	614	CLA	C1D-CHD-C4C	-4.09	117.23	126.06
23	b	614	CLA	O2D-CGD-O1D	-4.09	115.84	123.84
23	b	615	CLA	C3C-C4C-NC	4.08	115.15	110.57
23	A	406[B]	CLA	O2D-CGD-CBD	4.08	118.52	111.27
23	D	403	CLA	C3D-C4D-ND	4.08	116.84	110.24
33	C	521	LMG	O6-C5-C4	4.08	117.10	109.69
23	A	404[A]	CLA	CAA-C2A-C3A	-4.08	101.61	112.78
23	A	405[A]	CLA	CAA-C2A-C3A	-4.08	101.61	112.78
35	C	517[A]	DGD	O2G-C1B-C2B	4.08	120.29	111.50
23	A	404[B]	CLA	CAA-C2A-C3A	-4.08	101.61	112.78
25	b	617	BCR	C7-C8-C9	-4.08	120.08	126.23
33	c	520	LMG	O7-C10-C11	4.08	120.28	111.50
26	a	409[A]	SQD	C1-O5-C5	-4.07	105.69	113.69
33	C	521	LMG	O7-C10-C11	4.07	120.28	111.50
23	B	610	CLA	C3D-C4D-ND	4.07	116.82	110.24
23	D	402[A]	CLA	C3D-C4D-ND	4.07	116.82	110.24
23	c	512	CLA	C3D-C4D-ND	4.07	116.81	110.24
23	B	610	CLA	CAA-C2A-C3A	-4.06	101.65	112.78
23	A	406[A]	CLA	C3C-C4C-NC	4.06	115.13	110.57
23	d	402[A]	CLA	C3C-C4C-NC	4.06	115.12	110.57
23	B	604	CLA	C1D-CHD-C4C	-4.05	117.32	126.06
23	B	606	CLA	C3D-C4D-ND	4.05	116.79	110.24
23	b	610	CLA	O2A-CGA-CBA	4.05	124.61	111.91
23	b	612	CLA	C3D-C4D-ND	4.05	116.79	110.24
23	b	610	CLA	C3D-C4D-ND	4.05	116.78	110.24
23	B	605	CLA	C1D-CHD-C4C	-4.05	117.33	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	404[B]	CLA	C3B-C4B-NB	4.04	114.44	109.21
23	C	509	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
23	B	613	CLA	C4A-NA-C1A	-4.03	104.89	106.71
23	C	503	CLA	O2D-CGD-O1D	-4.03	115.95	123.84
25	B	618	BCR	C29-C30-C25	4.03	116.69	110.48
23	C	507	CLA	C3B-C4B-NB	4.03	114.42	109.21
23	c	505	CLA	O2D-CGD-O1D	-4.02	115.97	123.84
23	d	402[A]	CLA	C1D-CHD-C4C	-4.01	117.41	126.06
23	c	512	CLA	C1-C2-C3	-4.01	119.11	126.04
23	c	508	CLA	C3D-C4D-ND	4.01	116.72	110.24
23	C	509	CLA	C3B-C4B-NB	4.00	114.38	109.21
23	b	610	CLA	C1D-CHD-C4C	-4.00	117.43	126.06
23	b	616	CLA	C3D-C4D-ND	4.00	116.70	110.24
23	C	503	CLA	C3D-C4D-ND	4.00	116.70	110.24
23	c	510	CLA	C1D-CHD-C4C	-3.99	117.44	126.06
23	B	604	CLA	C1C-C2C-C3C	-3.99	102.76	106.96
23	C	512	CLA	C1D-CHD-C4C	-3.99	117.44	126.06
33	c	520	LMG	C3-C4-C5	3.99	117.35	110.24
23	c	506	CLA	O2D-CGD-CBD	3.98	118.35	111.27
23	b	612	CLA	CMC-C2C-C1C	3.98	131.10	125.04
25	d	405	BCR	C29-C30-C25	3.97	116.59	110.48
23	c	507	CLA	C3D-C4D-ND	3.96	116.65	110.24
25	d	405	BCR	C16-C17-C18	-3.96	121.66	127.31
23	c	509	CLA	C1D-CHD-C4C	-3.96	117.52	126.06
23	d	402[B]	CLA	C3C-C4C-NC	3.96	115.01	110.57
23	C	504	CLA	C1D-CHD-C4C	-3.95	117.53	126.06
23	a	404[A]	CLA	C3C-C4C-NC	3.95	115.00	110.57
23	d	402[B]	CLA	C4A-NA-C1A	-3.95	104.93	106.71
26	B	620	SQD	C3-C4-C5	3.95	117.28	110.24
33	C	520	LMG	O7-C10-C11	3.95	120.01	111.50
23	B	610	CLA	C1C-C2C-C3C	-3.95	102.81	106.96
23	a	404[A]	CLA	C3B-C4B-NB	3.95	114.31	109.21
23	b	615	CLA	C1D-CHD-C4C	-3.95	117.54	126.06
23	A	404[A]	CLA	C3C-C4C-NC	3.95	115.00	110.57
23	b	601	CLA	C1D-CHD-C4C	-3.95	117.55	126.06
23	B	611	CLA	CMB-C2B-C3B	3.95	132.06	124.68
23	C	511	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
23	A	408	CLA	O2D-CGD-CBD	3.94	118.28	111.27
23	B	603	CLA	C1D-CHD-C4C	-3.94	117.55	126.06
23	C	511	CLA	C1D-CHD-C4C	-3.94	117.56	126.06
23	C	502	CLA	C3C-C4C-NC	3.94	114.99	110.57
29	d	406[A]	PL9	C42-C43-C44	-3.93	118.19	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	404[B]	CLA	CAA-C2A-C3A	-3.93	102.02	112.78
23	B	605	CLA	C4-C3-C5	3.93	121.88	115.27
23	D	402[A]	CLA	C1-C2-C3	-3.93	119.25	126.04
23	a	405[A]	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
23	b	611	CLA	C3B-C4B-NB	3.93	114.29	109.21
23	A	408	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
23	C	502	CLA	C1D-CHD-C4C	-3.93	117.59	126.06
23	b	606	CLA	C3D-C4D-ND	3.92	116.58	110.24
23	C	510	CLA	C1C-C2C-C3C	-3.92	102.83	106.96
35	C	517[B]	DGD	O2G-C1B-C2B	3.92	119.95	111.50
23	C	512	CLA	C3D-C4D-ND	3.92	116.58	110.24
23	b	605	CLA	C1D-CHD-C4C	-3.92	117.61	126.06
23	A	408	CLA	C3B-C4B-NB	3.92	114.27	109.21
23	C	509	CLA	C1-C2-C3	-3.92	119.27	126.04
23	B	601	CLA	C1D-CHD-C4C	-3.92	117.61	126.06
23	b	612	CLA	C3B-C4B-NB	3.92	114.27	109.21
23	A	405[B]	CLA	C3C-C4C-NC	3.91	114.96	110.57
26	a	409[A]	SQD	C44-O6-C1	-3.91	106.09	113.74
40	V	201	HEC	C1D-C2D-C3D	-3.91	104.28	107.00
29	A	414[A]	PL9	C7-C3-C4	3.91	120.05	116.88
23	c	511	CLA	C1D-CHD-C4C	-3.91	117.63	126.06
23	B	602	CLA	O2D-CGD-O1D	-3.91	116.20	123.84
23	B	614	CLA	C1-C2-C3	-3.90	119.29	126.04
31	B	628	LMT	C1'-O5'-C5'	-3.90	106.02	113.69
23	b	614	CLA	C3C-C4C-NC	3.90	114.95	110.57
23	b	614	CLA	C3D-C4D-ND	3.90	116.55	110.24
29	a	412[A]	PL9	C32-C33-C34	-3.89	118.28	127.66
23	B	602	CLA	C1D-CHD-C4C	-3.89	117.66	126.06
23	d	403[B]	CLA	C3B-C4B-NB	3.89	114.24	109.21
29	A	414[B]	PL9	C37-C38-C39	-3.89	118.30	127.66
23	b	613	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
23	C	511	CLA	C3B-C4B-NB	3.89	114.24	109.21
23	b	616	CLA	O2A-CGA-CBA	3.89	124.11	111.91
23	b	614	CLA	C1D-CHD-C4C	-3.88	117.68	126.06
32	A	419[A]	LHG	O8-C23-O10	-3.88	113.79	123.59
35	c	516[A]	DGD	O2G-C1B-C2B	3.88	119.87	111.50
23	A	405[A]	CLA	CMC-C2C-C1C	3.88	130.95	125.04
23	A	405[B]	CLA	C1D-CHD-C4C	-3.88	117.69	126.06
23	b	612	CLA	CAC-C3C-C4C	3.88	129.84	124.81
26	A	412	SQD	O47-C7-C8	3.87	119.85	111.50
23	B	609	CLA	O2D-CGD-CBD	3.87	118.15	111.27
24	a	414[B]	PHO	C4-C3-C5	3.87	121.78	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406[B]	CLA	C3C-C4C-NC	3.87	114.91	110.57
23	B	613	CLA	C3D-C4D-ND	3.87	116.50	110.24
23	b	606	CLA	C4-C3-C5	3.87	121.78	115.27
23	d	402[A]	CLA	CAA-C2A-C3A	-3.87	102.19	112.78
23	c	506	CLA	C3C-C4C-NC	3.87	114.91	110.57
24	A	407[A]	PHO	C1A-C2A-C3A	-3.87	99.16	102.84
23	B	616	CLA	C3B-C4B-NB	3.87	114.21	109.21
33	m	101	LMG	O7-C10-C11	3.87	119.83	111.50
23	B	613	CLA	C1C-C2C-C3C	-3.86	102.89	106.96
23	c	504	CLA	C1-O2A-CGA	3.86	126.58	116.44
23	A	404[B]	CLA	O2D-CGD-CBD	3.86	118.13	111.27
23	B	607	CLA	O2D-CGD-O1D	-3.86	116.29	123.84
23	a	407	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
23	A	405[A]	CLA	C3C-C4C-NC	3.85	114.89	110.57
23	c	513	CLA	C3B-C4B-NB	3.85	114.19	109.21
23	c	506	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
23	c	507	CLA	C3C-C4C-NC	3.85	114.88	110.57
25	T	102	BCR	C16-C17-C18	-3.84	121.82	127.31
23	c	508	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
23	B	614	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
23	b	606	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
23	b	601	CLA	C3C-C4C-NC	3.84	114.88	110.57
29	a	412[A]	PL9	C7-C3-C2	-3.84	118.25	123.30
23	b	603	CLA	O2D-CGD-O1D	-3.83	116.35	123.84
23	B	616	CLA	C1D-CHD-C4C	-3.83	117.79	126.06
23	B	614	CLA	O2D-CGD-O1D	-3.83	116.35	123.84
23	C	506	CLA	C1D-CHD-C4C	-3.83	117.80	126.06
23	c	502	CLA	C3C-C4C-NC	3.83	114.86	110.57
23	b	604	CLA	C3D-C4D-ND	3.82	116.42	110.24
23	C	505	CLA	C3D-C4D-ND	3.82	116.42	110.24
23	C	508	CLA	C3D-C4D-ND	3.82	116.41	110.24
25	H	101	BCR	C16-C17-C18	-3.81	121.87	127.31
23	A	405[B]	CLA	CAA-C2A-C3A	-3.81	102.34	112.78
23	B	611	CLA	CHD-C4C-NC	3.81	130.20	124.20
33	Z	101	LMG	C1-C2-C3	3.80	117.92	110.00
32	A	419[A]	LHG	O7-C7-C8	3.80	119.69	111.50
24	A	416[A]	PHO	C1A-C2A-C3A	-3.80	99.22	102.84
33	c	519	LMG	O7-C10-C11	3.79	119.68	111.50
23	b	611	CLA	C4A-NA-C1A	-3.79	105.00	106.71
23	C	511	CLA	C1-C2-C3	-3.79	119.49	126.04
23	C	514	CLA	C1C-C2C-C3C	-3.79	102.98	106.96
23	C	513	CLA	C1-C2-C3	-3.78	119.50	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	512	CLA	C1D-CHD-C4C	-3.78	117.90	126.06
23	D	403	CLA	C1D-CHD-C4C	-3.78	117.91	126.06
26	A	410[A]	SQD	C44-O6-C1	-3.78	106.36	113.74
23	C	514	CLA	C3B-C4B-NB	3.78	114.09	109.21
23	b	608	CLA	C3B-C4B-NB	3.78	114.09	109.21
23	A	405[A]	CLA	CBC-CAC-C3C	-3.77	102.04	112.43
23	b	609	CLA	C1-C2-C3	-3.77	119.52	126.04
26	A	410[B]	SQD	O47-C7-C8	3.77	119.63	111.50
34	B	622	HTG	C1'-S1-C1	3.77	107.13	100.09
40	v	201	HEC	CMB-C2B-C1B	-3.77	122.68	128.46
23	c	502	CLA	O2D-CGD-O1D	-3.76	116.48	123.84
23	B	613	CLA	C3B-C4B-NB	3.76	114.08	109.21
35	c	517[B]	DGD	O2G-C1B-C2B	3.76	119.60	111.50
24	a	414[A]	PHO	C4-C3-C5	3.76	121.59	115.27
26	a	410	SQD	O47-C7-C8	3.75	119.58	111.50
23	B	614	CLA	C3D-C4D-ND	3.75	116.30	110.24
23	c	507	CLA	O2D-CGD-O1D	-3.75	116.51	123.84
23	c	506	CLA	C3B-C4B-NB	3.75	114.05	109.21
26	A	410[A]	SQD	O47-C7-C8	3.74	119.56	111.50
23	B	606	CLA	C1D-CHD-C4C	-3.74	117.99	126.06
23	b	609	CLA	C1D-CHD-C4C	-3.74	117.99	126.06
29	a	412[A]	PL9	C15-C14-C16	3.74	121.56	115.27
23	b	612	CLA	C4-C3-C5	3.74	121.56	115.27
23	B	604	CLA	C3D-C2D-C1D	-3.74	100.73	105.83
23	b	608	CLA	C3C-C4C-NC	3.74	114.76	110.57
23	c	509	CLA	C3C-C4C-NC	3.74	114.76	110.57
23	b	603	CLA	CAA-C2A-C3A	-3.73	102.56	112.78
23	A	406[A]	CLA	C1D-CHD-C4C	-3.73	118.01	126.06
23	B	608	CLA	CAC-C3C-C4C	3.72	129.64	124.81
23	C	513	CLA	C4-C3-C5	3.72	121.53	115.27
23	C	508	CLA	C1C-C2C-C3C	-3.72	103.04	106.96
23	A	404[A]	CLA	C3D-C4D-ND	3.72	116.25	110.24
23	A	404[B]	CLA	C3C-C4C-NC	3.72	114.74	110.57
23	B	612	CLA	C4C-C3C-C2C	-3.72	101.48	106.90
23	b	613	CLA	O2D-CGD-CBD	3.72	117.87	111.27
23	B	614	CLA	C3C-C4C-NC	3.72	114.74	110.57
23	B	608	CLA	O2D-CGD-O1D	-3.71	116.58	123.84
23	b	608	CLA	C1D-CHD-C4C	-3.71	118.06	126.06
23	B	607	CLA	CBC-CAC-C3C	-3.71	102.21	112.43
23	b	610	CLA	C4C-C3C-C2C	-3.71	101.50	106.90
23	b	613	CLA	C3B-C4B-NB	3.70	114.00	109.21
23	d	402[B]	CLA	C3B-C4B-NB	3.70	114.00	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	C	518[A]	DGD	O2G-C1B-C2B	3.69	119.46	111.50
23	B	606	CLA	C1C-C2C-C3C	-3.69	103.07	106.96
23	b	615	CLA	C1C-C2C-C3C	-3.69	103.07	106.96
29	A	414[B]	PL9	C7-C3-C2	-3.68	118.45	123.30
23	c	504	CLA	C1C-C2C-C3C	-3.68	103.08	106.96
23	C	505	CLA	C3B-C4B-NB	3.68	113.97	109.21
32	L	101[A]	LHG	O7-C7-C8	3.68	119.43	111.50
32	d	414[B]	LHG	O7-C7-C8	3.68	119.43	111.50
23	C	512	CLA	CAC-C3C-C4C	3.68	129.58	124.81
29	a	412[B]	PL9	C7-C3-C2	-3.68	118.47	123.30
23	B	610	CLA	O2D-CGD-O1D	-3.67	116.66	123.84
23	c	510	CLA	C1C-C2C-C3C	-3.67	103.09	106.96
23	B	612	CLA	O2D-CGD-O1D	-3.67	116.66	123.84
23	B	614	CLA	C3B-C4B-NB	3.67	113.96	109.21
38	f	101	HEM	C1B-NB-C4B	3.67	108.86	105.07
29	A	414[A]	PL9	C37-C38-C39	-3.67	118.82	127.66
23	a	404[A]	CLA	O2A-CGA-O1A	-3.67	114.34	123.59
25	T	102	BCR	C11-C10-C9	-3.66	122.09	127.31
23	c	508	CLA	C1D-CHD-C4C	-3.66	118.17	126.06
23	b	614	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
38	f	101	HEM	CHD-C1D-ND	3.65	128.40	124.43
23	b	612	CLA	C1D-CHD-C4C	-3.65	118.18	126.06
23	a	404[A]	CLA	CMB-C2B-C3B	3.65	131.51	124.68
23	B	608	CLA	C3B-C4B-NB	3.65	113.92	109.21
29	a	412[B]	PL9	C15-C14-C16	3.65	121.40	115.27
23	a	404[B]	CLA	O2D-CGD-CBD	3.64	117.74	111.27
23	b	605	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
25	b	619	BCR	C24-C23-C22	-3.64	120.74	126.23
23	c	504	CLA	C1D-CHD-C4C	-3.64	118.21	126.06
23	a	407	CLA	CMC-C2C-C1C	3.64	130.58	125.04
23	B	610	CLA	C1D-CHD-C4C	-3.63	118.22	126.06
23	B	611	CLA	C4C-C3C-C2C	-3.63	101.60	106.90
23	B	603	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
26	a	409[A]	SQD	O9-S-C6	3.63	111.25	106.94
23	b	604	CLA	C3B-C4B-NB	3.63	113.90	109.21
23	B	609	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
23	c	501	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
23	D	402[A]	CLA	C3B-C4B-NB	3.62	113.89	109.21
23	c	510	CLA	C3B-C4B-NB	3.62	113.89	109.21
23	C	514	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
23	C	511	CLA	C3C-C4C-NC	3.62	114.63	110.57
23	A	405[A]	CLA	C1D-CHD-C4C	-3.62	118.25	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	404[B]	CLA	C3C-C4C-NC	3.62	114.63	110.57
23	A	406[B]	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
23	B	612	CLA	CMC-C2C-C1C	3.62	130.55	125.04
23	C	506	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
25	c	515	BCR	C7-C8-C9	-3.61	120.77	126.23
23	A	404[B]	CLA	C3B-C4B-NB	3.61	113.88	109.21
23	B	615	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
26	F	102	SQD	O7-S-C6	3.61	111.23	106.94
23	b	608	CLA	C1-C2-C3	-3.61	119.81	126.04
25	b	619	BCR	C11-C10-C9	-3.60	122.17	127.31
23	B	605	CLA	CHD-C4C-NC	3.60	129.88	124.20
23	c	505	CLA	CAC-C3C-C4C	3.60	129.48	124.81
23	c	511	CLA	C3B-C4B-NB	3.60	113.86	109.21
32	L	101[B]	LHG	O7-C7-C8	3.59	119.24	111.50
23	b	606	CLA	O2D-CGD-O1D	-3.59	116.82	123.84
25	B	617	BCR	C7-C8-C9	-3.59	120.81	126.23
23	A	405[A]	CLA	O2D-CGD-O1D	-3.58	116.83	123.84
23	c	510	CLA	C3D-C4D-ND	3.58	116.04	110.24
23	B	615	CLA	O2D-CGD-CBD	3.58	117.64	111.27
23	b	609	CLA	C4C-C3C-C2C	-3.58	101.67	106.90
32	A	419[B]	LHG	O7-C7-C8	3.58	119.22	111.50
23	d	403[A]	CLA	C3B-C4B-NB	3.58	113.84	109.21
23	B	608	CLA	C4C-C3C-C2C	-3.58	101.69	106.90
23	d	403[B]	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
23	B	607	CLA	C3B-C4B-NB	3.58	113.83	109.21
26	a	409[B]	SQD	C1-O5-C5	-3.57	106.67	113.69
23	C	506	CLA	C1-C2-C3	-3.57	119.86	126.04
23	B	603	CLA	CAA-C2A-C3A	-3.57	103.00	112.78
23	A	408	CLA	C1D-CHD-C4C	-3.57	118.35	126.06
23	B	602	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
23	B	612	CLA	CAC-C3C-C4C	3.57	129.44	124.81
23	b	612	CLA	C4C-C3C-C2C	-3.57	101.69	106.90
25	B	617	BCR	C33-C5-C6	-3.57	120.52	124.53
23	c	505	CLA	C4C-C3C-C2C	-3.57	101.70	106.90
33	B	621	LMG	O8-C28-C29	3.56	123.09	111.91
25	d	405	BCR	C38-C26-C25	-3.56	120.53	124.53
32	d	408[B]	LHG	O7-C7-C8	3.56	119.18	111.50
23	B	607	CLA	CMC-C2C-C1C	3.56	130.46	125.04
29	d	406[B]	PL9	C42-C43-C44	-3.56	119.09	127.66
23	d	403[A]	CLA	C1-C2-C3	-3.56	119.89	126.04
23	b	613	CLA	C3D-C4D-ND	3.56	115.99	110.24
25	y	101	BCR	C38-C26-C25	-3.56	120.53	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	604	CLA	C3B-C4B-NB	3.55	113.80	109.21
23	B	603	CLA	C3B-C4B-NB	3.55	113.80	109.21
23	b	614	CLA	C3B-C4B-NB	3.55	113.80	109.21
23	c	510	CLA	CMC-C2C-C1C	3.55	130.44	125.04
29	d	406[A]	PL9	C40-C39-C41	3.55	121.23	115.27
23	d	402[B]	CLA	CAA-C2A-C3A	-3.54	103.07	112.78
23	b	602	CLA	O2D-CGD-O1D	-3.54	116.91	123.84
29	a	412[A]	PL9	C27-C28-C29	-3.54	119.13	127.66
33	a	415	LMG	C7-O1-C1	-3.54	106.82	113.74
23	b	601	CLA	O2D-CGD-O1D	-3.54	116.91	123.84
23	b	602	CLA	C1-C2-C3	-3.54	119.92	126.04
23	B	602	CLA	C3B-C4B-NB	3.54	113.78	109.21
23	c	512	CLA	C3C-C4C-NC	3.54	114.54	110.57
23	c	513	CLA	C1C-C2C-C3C	-3.54	103.24	106.96
23	B	610	CLA	O2A-CGA-O1A	-3.53	114.68	123.59
23	A	404[A]	CLA	O2D-CGD-CBD	3.53	117.54	111.27
23	b	603	CLA	C3B-C4B-NB	3.53	113.77	109.21
26	B	620	SQD	O7-S-C6	3.53	111.13	106.94
23	B	608	CLA	C1D-CHD-C4C	-3.53	118.45	126.06
25	Y	101	BCR	C15-C14-C13	-3.53	122.28	127.31
25	C	515	BCR	C33-C5-C6	-3.52	120.58	124.53
29	A	414[A]	PL9	C22-C23-C24	-3.52	119.19	127.66
23	a	404[B]	CLA	CMB-C2B-C3B	3.52	131.26	124.68
23	B	604	CLA	C3D-C4D-ND	3.51	115.92	110.24
23	b	608	CLA	CMB-C2B-C3B	3.51	131.25	124.68
23	D	402[B]	CLA	C3B-C4B-NB	3.51	113.75	109.21
29	A	414[A]	PL9	C15-C14-C16	3.51	121.18	115.27
34	V	202	HTG	C1-O5-C5	3.51	116.95	112.19
34	b	625	HTG	O5-C5-C4	3.51	116.07	109.69
23	c	503	CLA	O2D-CGD-O1D	-3.51	116.98	123.84
23	A	404[A]	CLA	C1D-CHD-C4C	-3.51	118.49	126.06
23	c	511	CLA	O2D-CGD-O1D	-3.51	116.98	123.84
23	b	612	CLA	O2D-CGD-O1D	-3.51	116.98	123.84
23	C	512	CLA	CMC-C2C-C1C	3.51	130.38	125.04
23	A	408	CLA	CAA-C2A-C3A	-3.50	103.19	112.78
23	C	503	CLA	C1-C2-C3	-3.50	119.98	126.04
24	A	416[B]	PHO	C1A-C2A-C3A	-3.50	99.51	102.84
29	D	405[A]	PL9	C53-C6-C1	3.50	122.15	114.99
23	a	405[A]	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
23	a	405[B]	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
29	a	412[A]	PL9	C30-C29-C31	3.48	121.13	115.27
23	B	613	CLA	C4-C3-C5	3.48	121.13	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	404[A]	CLA	O2A-CGA-CBA	3.48	122.83	111.91
23	C	509	CLA	C1D-CHD-C4C	-3.48	118.56	126.06
29	D	405[A]	PL9	C42-C43-C44	-3.47	119.29	127.66
23	b	608	CLA	CAC-C3C-C4C	3.47	129.32	124.81
23	a	404[A]	CLA	O2D-CGD-CBD	3.47	117.43	111.27
23	B	605	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
23	c	504	CLA	C3B-C4B-NB	3.47	113.69	109.21
33	C	521	LMG	C3-C4-C5	3.47	116.42	110.24
23	C	510	CLA	C3B-C4B-NB	3.47	113.69	109.21
23	A	406[A]	CLA	O2A-CGA-O1A	-3.46	114.85	123.59
38	E	102	HEM	CBD-CAD-C3D	-3.46	103.01	112.63
23	d	403[A]	CLA	O2A-CGA-CBA	3.46	122.77	111.91
33	Z	101	LMG	O6-C1-C2	3.45	117.66	110.35
23	c	506	CLA	C1D-CHD-C4C	-3.45	118.61	126.06
23	a	405[B]	CLA	C1D-CHD-C4C	-3.45	118.62	126.06
23	b	602	CLA	CAA-C2A-C3A	-3.45	103.34	112.78
25	A	409	BCR	C24-C23-C22	-3.44	121.03	126.23
23	b	615	CLA	C3B-C4B-NB	3.44	113.66	109.21
23	C	508	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
23	b	603	CLA	C2A-C1A-CHA	-3.44	117.84	123.86
23	C	503	CLA	C1D-CHD-C4C	-3.44	118.64	126.06
25	c	514	BCR	C15-C14-C13	-3.44	122.40	127.31
23	b	602	CLA	C1D-CHD-C4C	-3.44	118.64	126.06
23	B	604	CLA	CHD-C1D-ND	-3.44	121.30	124.45
23	d	404	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
23	C	509	CLA	C4C-C3C-C2C	-3.43	101.89	106.90
32	b	629[B]	LHG	O7-C7-C8	3.43	118.90	111.50
29	D	405[B]	PL9	C53-C6-C1	3.43	122.00	114.99
23	B	612	CLA	C4A-NA-C1A	-3.43	105.17	106.71
23	c	508	CLA	C3B-C4B-NB	3.43	113.64	109.21
26	F	102	SQD	C44-O6-C1	-3.42	107.05	113.74
25	K	102	BCR	C7-C8-C9	-3.42	121.06	126.23
29	A	414[B]	PL9	C7-C3-C4	3.42	119.66	116.88
26	B	620	SQD	C1-O5-C5	-3.42	106.97	113.69
23	C	504	CLA	C4-C3-C5	3.42	121.02	115.27
23	B	615	CLA	CMC-C2C-C1C	3.42	130.25	125.04
23	C	504	CLA	C4C-C3C-C2C	-3.42	101.92	106.90
23	c	511	CLA	C1C-C2C-C3C	-3.42	103.37	106.96
23	a	404[A]	CLA	O2A-CGA-CBA	3.41	122.61	111.91
29	a	412[A]	PL9	C35-C34-C36	3.41	121.01	115.27
23	b	606	CLA	CHD-C4C-NC	3.41	129.57	124.20
23	c	512	CLA	O2D-CGD-O1D	-3.41	117.18	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	607	CLA	C4-C3-C5	3.41	121.00	115.27
23	b	613	CLA	C4C-C3C-C2C	-3.40	101.94	106.90
23	b	611	CLA	C1D-CHD-C4C	-3.40	118.72	126.06
23	b	612	CLA	C1C-C2C-C3C	-3.40	103.39	106.96
23	b	616	CLA	C4C-C3C-C2C	-3.39	101.95	106.90
40	V	201	HEC	CMB-C2B-C1B	-3.39	123.25	128.46
23	C	507	CLA	C3C-C4C-NC	3.39	114.37	110.57
23	A	406[A]	CLA	C3B-C4B-NB	3.39	113.59	109.21
29	D	405[A]	PL9	C25-C24-C26	3.39	120.97	115.27
23	C	513	CLA	CHD-C4C-NC	3.39	129.54	124.20
23	b	614	CLA	C1-C2-C3	-3.38	120.19	126.04
23	b	603	CLA	C1C-C2C-C3C	-3.38	103.40	106.96
29	a	412[B]	PL9	C27-C28-C29	-3.38	119.52	127.66
32	A	419[B]	LHG	O8-C23-O10	-3.38	115.06	123.59
23	b	612	CLA	C2A-C1A-CHA	-3.38	117.95	123.86
23	B	612	CLA	CMB-C2B-C3B	3.38	131.00	124.68
23	C	505	CLA	C1D-CHD-C4C	-3.38	118.77	126.06
23	b	601	CLA	C1C-C2C-C3C	-3.38	103.41	106.96
23	c	510	CLA	C4-C3-C5	3.38	120.95	115.27
35	c	517[A]	DGD	O2G-C1B-C2B	3.37	118.77	111.50
23	C	510	CLA	C1D-CHD-C4C	-3.37	118.79	126.06
23	c	507	CLA	C4-C3-C5	3.37	120.94	115.27
23	a	404[B]	CLA	CHC-C1C-C2C	-3.37	117.40	126.72
25	C	515	BCR	C7-C8-C9	-3.37	121.15	126.23
26	a	409[B]	SQD	C44-O6-C1	-3.37	107.16	113.74
23	b	611	CLA	C1-C2-C3	-3.37	120.22	126.04
23	b	613	CLA	C1D-CHD-C4C	-3.37	118.80	126.06
23	B	606	CLA	CMC-C2C-C1C	3.36	130.16	125.04
23	b	610	CLA	O2A-CGA-O1A	-3.36	115.10	123.59
23	c	512	CLA	C4-C3-C5	3.36	120.93	115.27
23	c	503	CLA	CMC-C2C-C1C	3.36	130.16	125.04
25	k	101	BCR	C7-C8-C9	-3.36	121.16	126.23
33	z	101	LMG	O7-C10-C11	3.36	118.74	111.50
25	T	102	BCR	C12-C13-C14	-3.36	113.79	118.94
23	C	505	CLA	C4A-NA-C1A	-3.35	105.20	106.71
23	b	612	CLA	C1-C2-C3	-3.35	120.24	126.04
24	A	416[A]	PHO	CMC-C2C-C3C	3.35	131.26	124.94
23	b	616	CLA	CHD-C4C-NC	3.35	129.48	124.20
23	a	407	CLA	C4A-NA-C1A	-3.35	105.20	106.71
23	C	506	CLA	CAC-C3C-C4C	3.35	129.15	124.81
23	B	611	CLA	CHB-C4A-NA	3.34	129.14	124.51
23	C	507	CLA	C1D-CHD-C4C	-3.34	118.85	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	409[B]	SQD	O9-S-C6	3.34	110.91	106.94
25	D	404	BCR	C29-C30-C25	3.34	115.62	110.48
23	B	604	CLA	C4C-C3C-C2C	-3.34	102.03	106.90
23	b	615	CLA	O2D-CGD-CBD	3.34	117.19	111.27
23	d	403[A]	CLA	C1D-CHD-C4C	-3.33	118.87	126.06
23	B	605	CLA	C1C-C2C-C3C	-3.33	103.46	106.96
26	F	102	SQD	C1-C2-C3	-3.33	103.07	110.00
23	b	609	CLA	CAC-C3C-C4C	3.33	129.12	124.81
23	A	405[A]	CLA	C3B-C4B-NB	3.33	113.51	109.21
23	B	616	CLA	CAC-C3C-C4C	3.32	129.12	124.81
38	f	101	HEM	CAD-CBD-CGD	3.32	120.75	113.60
23	A	405[B]	CLA	CHD-C4C-NC	3.32	129.43	124.20
23	B	611	CLA	C2A-C1A-CHA	-3.32	118.06	123.86
24	A	407[A]	PHO	CMA-C3A-C4A	-3.32	107.11	114.38
23	B	615	CLA	C3B-C4B-NB	3.32	113.50	109.21
29	A	414[B]	PL9	C15-C14-C16	3.32	120.85	115.27
23	B	603	CLA	CAC-C3C-C4C	3.31	129.11	124.81
29	a	412[B]	PL9	C37-C38-C39	-3.31	119.68	127.66
23	c	503	CLA	C1C-C2C-C3C	-3.31	103.47	106.96
23	C	502	CLA	CAC-C3C-C4C	3.31	129.11	124.81
23	c	509	CLA	CHC-C1C-C2C	-3.31	117.57	126.72
23	c	502	CLA	C3B-C4B-NB	3.31	113.48	109.21
25	C	516	BCR	C33-C5-C6	-3.30	120.82	124.53
23	A	406[B]	CLA	CAA-C2A-C3A	-3.30	103.73	112.78
23	a	404[B]	CLA	CAC-C3C-C4C	3.30	129.09	124.81
23	B	614	CLA	CAC-C3C-C4C	3.30	129.09	124.81
23	B	614	CLA	CMC-C2C-C1C	3.30	130.06	125.04
23	c	502	CLA	CHC-C1C-C2C	-3.30	117.60	126.72
25	y	101	BCR	C24-C23-C22	-3.30	121.25	126.23
23	a	407	CLA	CAA-C2A-C3A	-3.30	103.75	112.78
32	d	414[A]	LHG	O8-C23-O10	-3.30	115.27	123.59
23	b	605	CLA	CHD-C4C-NC	3.30	129.40	124.20
25	h	101	BCR	C38-C26-C25	-3.29	120.83	124.53
23	D	403	CLA	C4C-C3C-C2C	-3.29	102.10	106.90
23	C	512	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
32	d	408[A]	LHG	O7-C7-C8	3.29	118.59	111.50
25	y	101	BCR	C15-C14-C13	-3.29	122.61	127.31
23	C	511	CLA	C4-C3-C5	3.29	120.81	115.27
23	A	405[B]	CLA	CMC-C2C-C1C	3.29	130.05	125.04
23	B	601	CLA	C1C-C2C-C3C	-3.29	103.50	106.96
23	C	507	CLA	CBC-CAC-C3C	-3.29	103.37	112.43
23	c	505	CLA	C1D-CHD-C4C	-3.29	118.97	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	608	CLA	C1-C2-C3	-3.28	120.36	126.04
23	C	507	CLA	C1-C2-C3	-3.28	120.36	126.04
23	d	404	CLA	C1D-CHD-C4C	-3.28	118.98	126.06
23	B	602	CLA	CAA-C2A-C3A	-3.28	103.80	112.78
23	b	607	CLA	C4C-C3C-C2C	-3.28	102.12	106.90
29	A	414[B]	PL9	C22-C23-C24	-3.28	119.76	127.66
23	b	604	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
23	c	511	CLA	CMC-C2C-C1C	3.28	130.03	125.04
23	B	607	CLA	O2A-CGA-O1A	-3.28	115.32	123.59
23	B	608	CLA	C1C-C2C-C3C	-3.27	103.51	106.96
23	d	404	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
25	c	514	BCR	C37-C22-C21	-3.27	118.34	122.92
35	h	102	DGD	O2G-C1B-C2B	3.27	118.55	111.50
29	a	412[B]	PL9	C30-C29-C31	3.27	120.77	115.27
23	c	505	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
25	K	102	BCR	C38-C26-C25	-3.27	120.86	124.53
23	B	613	CLA	O2A-CGA-O1A	-3.27	115.34	123.59
23	A	406[B]	CLA	C1D-CHD-C4C	-3.27	119.01	126.06
23	c	501	CLA	C1-C2-C3	-3.27	120.40	126.04
23	b	604	CLA	CMC-C2C-C1C	3.26	130.01	125.04
40	V	201	HEC	CMC-C2C-C1C	-3.26	123.45	128.46
23	C	505	CLA	C1-O2A-CGA	3.26	125.01	116.44
23	c	510	CLA	CAC-C3C-C4C	3.26	129.04	124.81
23	c	507	CLA	C1D-CHD-C4C	-3.26	119.02	126.06
23	b	616	CLA	O2A-CGA-O1A	-3.26	115.36	123.59
23	C	507	CLA	CHC-C1C-C2C	-3.26	117.71	126.72
23	c	508	CLA	C1-C2-C3	-3.26	120.41	126.04
23	B	601	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
23	C	508	CLA	C4C-C3C-C2C	-3.26	102.15	106.90
23	D	403	CLA	C1C-C2C-C3C	-3.26	103.53	106.96
23	d	402[B]	CLA	CHD-C4C-NC	3.26	129.33	124.20
23	d	402[A]	CLA	C3B-C4B-NB	3.25	113.42	109.21
23	b	614	CLA	CHD-C4C-NC	3.25	129.33	124.20
23	B	601	CLA	C4C-C3C-C2C	-3.25	102.16	106.90
23	A	404[A]	CLA	CMB-C2B-C3B	3.25	130.75	124.68
32	d	414[A]	LHG	O7-C7-C8	3.25	118.50	111.50
23	C	510	CLA	CMB-C2B-C3B	3.24	130.75	124.68
23	A	408	CLA	C1-C2-C3	-3.24	120.43	126.04
26	B	620	SQD	O9-S-C6	3.24	110.79	106.94
23	C	504	CLA	C1-C2-C3	-3.24	120.44	126.04
23	C	513	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
23	C	506	CLA	CMC-C2C-C1C	3.24	129.97	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	502	CLA	CBC-CAC-C3C	-3.24	103.50	112.43
25	k	101	BCR	C29-C30-C25	3.24	115.46	110.48
23	A	405[B]	CLA	C3B-C4B-NB	3.23	113.39	109.21
23	C	512	CLA	C1C-C2C-C3C	-3.23	103.56	106.96
29	d	406[B]	PL9	C10-C9-C11	3.23	120.70	115.27
34	B	622	HTG	O5-C1-C2	3.23	114.37	110.31
23	a	405[B]	CLA	CMC-C2C-C1C	3.23	129.95	125.04
32	d	414[B]	LHG	O8-C23-C24	3.22	122.03	111.91
23	b	611	CLA	CHC-C1C-C2C	-3.22	117.80	126.72
23	B	609	CLA	C1D-CHD-C4C	-3.22	119.11	126.06
23	c	512	CLA	C1C-C2C-C3C	-3.22	103.57	106.96
35	c	516[B]	DGD	O2G-C1B-C2B	3.22	118.44	111.50
33	C	520	LMG	O8-C28-C29	3.22	122.02	111.91
24	a	414[A]	PHO	C4A-C3A-C2A	-3.22	99.77	102.84
23	b	614	CLA	CMC-C2C-C1C	3.22	129.94	125.04
23	c	506	CLA	CHC-C1C-C2C	-3.22	117.82	126.72
25	D	404	BCR	C38-C26-C25	-3.22	120.92	124.53
32	d	414[A]	LHG	O8-C23-C24	3.22	122.00	111.91
23	C	503	CLA	CAC-C3C-C4C	3.21	128.98	124.81
23	c	507	CLA	CBC-CAC-C3C	-3.21	103.58	112.43
23	A	404[B]	CLA	O2A-CGA-CBA	3.21	121.97	111.91
23	c	504	CLA	C4C-C3C-C2C	-3.21	102.22	106.90
23	B	602	CLA	CAC-C3C-C4C	3.21	128.97	124.81
34	b	622	HTG	O5-C5-C4	3.21	115.52	109.69
23	B	615	CLA	C11-C10-C8	-3.21	105.56	115.92
23	c	506	CLA	CAC-C3C-C4C	3.21	128.97	124.81
23	d	403[B]	CLA	C1-C2-C3	-3.20	120.50	126.04
29	D	405[B]	PL9	C10-C9-C11	3.20	120.66	115.27
23	C	506	CLA	C3B-C4B-NB	3.20	113.35	109.21
23	a	404[A]	CLA	CHC-C1C-C2C	-3.20	117.86	126.72
23	D	403	CLA	CAC-C3C-C4C	3.20	128.96	124.81
23	a	405[A]	CLA	C3B-C4B-NB	3.20	113.34	109.21
23	A	404[B]	CLA	CMB-C2B-C3B	3.20	130.66	124.68
23	d	403[B]	CLA	C4-C3-C5	3.20	120.65	115.27
26	A	412	SQD	O8-S-C6	3.19	110.83	105.74
23	B	612	CLA	C1D-CHD-C4C	-3.19	119.17	126.06
26	b	620	SQD	C3-C4-C5	3.19	115.94	110.24
23	b	613	CLA	O2A-CGA-O1A	-3.19	115.53	123.59
23	a	404[A]	CLA	CAA-C2A-C1A	-3.19	101.52	111.97
23	C	502	CLA	C1C-C2C-C3C	-3.19	103.60	106.96
23	C	506	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
23	a	407	CLA	CHD-C4C-NC	3.19	129.23	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	511	CLA	CHD-C4C-NC	3.19	129.23	124.20
25	D	404	BCR	C37-C22-C23	3.19	123.10	118.08
23	b	602	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
23	c	513	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
23	c	503	CLA	C1-C2-C3	-3.19	120.53	126.04
29	a	412[A]	PL9	C17-C18-C19	-3.19	119.99	127.66
23	C	509	CLA	CHC-C1C-C2C	-3.19	117.91	126.72
23	b	616	CLA	C3B-C4B-NB	3.18	113.33	109.21
26	b	620	SQD	O7-S-C6	3.18	110.72	106.94
23	C	504	CLA	CHD-C4C-NC	3.18	129.22	124.20
23	b	602	CLA	CAC-C3C-C4C	3.18	128.94	124.81
23	B	616	CLA	CMB-C2B-C3B	3.18	130.63	124.68
23	b	612	CLA	O2A-CGA-O1A	-3.18	115.57	123.59
23	b	603	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
23	A	406[A]	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
29	A	414[B]	PL9	C20-C19-C21	3.18	120.62	115.27
23	a	407	CLA	C3B-C4B-NB	3.18	113.32	109.21
23	c	512	CLA	O2A-CGA-CBA	3.18	121.88	111.91
29	A	414[A]	PL9	C27-C28-C29	-3.18	120.01	127.66
23	C	503	CLA	C3B-C4B-NB	3.17	113.31	109.21
23	c	508	CLA	C4C-C3C-C2C	-3.17	102.27	106.90
23	C	511	CLA	O2D-CGD-O1D	-3.17	117.63	123.84
23	d	404	CLA	C4-C3-C5	3.17	120.61	115.27
33	C	521	LMG	O8-C28-C29	3.17	121.86	111.91
29	a	412[A]	PL9	C25-C24-C26	3.17	120.61	115.27
23	A	404[A]	CLA	O2A-CGA-O1A	-3.17	115.59	123.59
23	b	611	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
23	D	402[A]	CLA	C1D-CHD-C4C	-3.17	119.22	126.06
29	a	412[B]	PL9	C25-C24-C26	3.17	120.60	115.27
23	C	512	CLA	C1-O2A-CGA	3.17	124.75	116.44
23	A	405[B]	CLA	CBC-CAC-C3C	-3.17	103.70	112.43
25	D	404	BCR	C28-C27-C26	-3.17	108.42	114.08
23	B	613	CLA	O2A-CGA-CBA	3.16	121.83	111.91
24	a	406[B]	PHO	CMA-C3A-C4A	-3.16	107.45	114.38
34	b	622	HTG	O2-C2-C1	3.16	116.07	110.27
40	V	201	HEC	CBA-CAA-C2A	-3.16	107.28	112.60
23	B	606	CLA	O2A-CGA-O1A	-3.16	115.62	123.59
23	B	605	CLA	O2A-CGA-O1A	-3.16	115.62	123.59
38	f	101	HEM	CHA-C4D-ND	3.16	128.28	124.38
40	v	201	HEC	C1D-C2D-C3D	-3.16	104.80	107.00
23	B	611	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
23	a	404[B]	CLA	O2A-CGA-CBA	3.16	121.81	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	610	CLA	C4C-C3C-C2C	-3.16	102.30	106.90
23	a	407	CLA	C4C-C3C-C2C	-3.16	102.30	106.90
24	A	416[A]	PHO	C4-C3-C5	3.15	120.58	115.27
23	c	503	CLA	C4C-C3C-C2C	-3.15	102.30	106.90
23	d	402[A]	CLA	CHD-C4C-NC	3.15	129.17	124.20
32	A	419[A]	LHG	C5-O7-C7	-3.15	110.03	117.79
23	C	511	CLA	CHC-C1C-C2C	-3.15	118.01	126.72
38	E	102	HEM	CHD-C1D-ND	3.15	127.85	124.43
25	d	405	BCR	C10-C11-C12	-3.15	113.39	123.22
32	A	419[A]	LHG	O8-C23-C24	3.15	121.79	111.91
29	D	405[A]	PL9	C17-C18-C19	-3.15	120.08	127.66
31	B	628	LMT	C4B-C3B-C2B	3.14	116.31	110.82
23	b	605	CLA	C2A-C1A-CHA	-3.14	118.36	123.86
23	B	609	CLA	CMC-C2C-C1C	3.14	129.82	125.04
23	C	503	CLA	CMC-C2C-C1C	3.14	129.82	125.04
23	b	609	CLA	C3B-C4B-NB	3.14	113.27	109.21
31	b	627	LMT	C3'-C4'-C5'	-3.14	103.73	110.93
23	d	402[B]	CLA	CHC-C1C-C2C	-3.14	118.04	126.72
26	a	409[B]	SQD	C1-C2-C3	-3.14	103.46	110.00
23	b	615	CLA	C4-C3-C5	3.13	120.54	115.27
23	C	512	CLA	C4C-C3C-C2C	-3.13	102.33	106.90
23	B	603	CLA	O2A-CGA-O1A	-3.13	115.69	123.59
23	D	403	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
23	C	512	CLA	C3B-C4B-NB	3.13	113.26	109.21
23	a	405[A]	CLA	CHD-C4C-NC	3.13	129.13	124.20
23	D	402[B]	CLA	C1D-CHD-C4C	-3.13	119.31	126.06
23	d	403[B]	CLA	CHC-C1C-C2C	-3.13	118.07	126.72
25	c	514	BCR	C16-C17-C18	-3.13	122.85	127.31
23	a	405[A]	CLA	C1-C2-C3	-3.13	120.64	126.04
23	d	403[A]	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
23	b	615	CLA	CHC-C1C-C2C	-3.12	118.08	126.72
23	c	511	CLA	C4-C3-C5	3.12	120.52	115.27
29	D	405[A]	PL9	C51-C49-C50	3.12	121.49	114.60
23	B	601	CLA	CHD-C4C-NC	3.12	129.11	124.20
23	C	510	CLA	CMC-C2C-C1C	3.11	129.78	125.04
23	a	407	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
23	B	610	CLA	C3B-C4B-NB	3.11	113.23	109.21
25	D	404	BCR	C10-C11-C12	-3.11	113.52	123.22
29	D	405[A]	PL9	C10-C9-C11	3.11	120.50	115.27
23	c	509	CLA	O2A-CGA-CBA	3.11	121.66	111.91
23	c	501	CLA	C3B-C4B-NB	3.11	113.22	109.21
23	c	501	CLA	C4C-C3C-C2C	-3.11	102.37	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	605	CLA	C4C-C3C-C2C	-3.10	102.37	106.90
23	c	511	CLA	C4C-C3C-C2C	-3.10	102.37	106.90
23	b	601	CLA	CMB-C2B-C3B	3.10	130.48	124.68
23	B	610	CLA	CAA-CBA-CGA	-3.10	104.19	113.25
23	C	507	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
29	D	405[B]	PL9	C25-C24-C26	3.10	120.49	115.27
23	a	405[B]	CLA	C3B-C4B-NB	3.10	113.22	109.21
35	h	102	DGD	O1G-C1A-O1A	-3.10	115.77	123.59
23	b	604	CLA	C1D-CHD-C4C	-3.10	119.37	126.06
23	c	502	CLA	CHD-C4C-NC	3.10	129.09	124.20
29	A	414[A]	PL9	C10-C9-C11	3.10	120.48	115.27
32	D	407[B]	LHG	O7-C7-C8	3.10	118.17	111.50
29	A	414[B]	PL9	C27-C28-C29	-3.09	120.21	127.66
23	C	514	CLA	C1-C2-C3	-3.09	120.69	126.04
26	f	102	SQD	O5-C1-C2	3.09	116.90	110.35
32	b	629[A]	LHG	O7-C7-C8	3.09	118.16	111.50
23	D	402[B]	CLA	O2A-CGA-CBA	3.09	121.60	111.91
23	B	603	CLA	C4C-C3C-C2C	-3.09	102.40	106.90
23	a	405[B]	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
24	A	407[B]	PHO	CMA-C3A-C4A	-3.08	107.62	114.38
23	d	403[B]	CLA	O2A-CGA-CBA	3.08	121.58	111.91
24	a	414[A]	PHO	CMB-C2B-C3B	3.08	130.44	124.68
29	a	412[A]	PL9	C10-C9-C11	3.08	120.45	115.27
33	c	520	LMG	C9-C8-C7	-3.08	104.51	111.79
23	b	602	CLA	C1C-C2C-C3C	-3.08	103.72	106.96
38	f	101	HEM	C4D-ND-C1D	3.07	108.25	105.07
23	C	509	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
25	K	102	BCR	C24-C23-C22	-3.07	121.59	126.23
23	a	404[A]	CLA	C1-C2-C3	-3.07	120.73	126.04
25	k	101	BCR	C20-C21-C22	-3.07	122.93	127.31
23	B	608	CLA	CMB-C2B-C3B	3.06	130.41	124.68
23	b	616	CLA	CBC-CAC-C3C	-3.06	103.99	112.43
23	A	406[B]	CLA	C3B-C4B-NB	3.06	113.17	109.21
23	c	511	CLA	CAC-C3C-C4C	3.06	128.78	124.81
26	b	620	SQD	O8-S-C6	3.06	110.61	105.74
25	H	101	BCR	C24-C23-C22	-3.05	121.62	126.23
23	b	602	CLA	CMC-C2C-C1C	3.05	129.69	125.04
29	d	406[A]	PL9	C10-C9-C11	3.05	120.41	115.27
23	b	601	CLA	C4-C3-C5	3.05	120.41	115.27
23	a	404[A]	CLA	C4-C3-C5	3.05	120.41	115.27
23	C	504	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
23	D	402[A]	CLA	O2A-CGA-CBA	3.05	121.48	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	405[A]	CLA	CMC-C2C-C1C	3.05	129.68	125.04
23	d	402[B]	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
23	d	403[A]	CLA	C2A-C1A-CHA	-3.05	118.53	123.86
25	h	101	BCR	C7-C8-C9	-3.04	121.63	126.23
23	b	607	CLA	CHC-C1C-C2C	-3.04	118.30	126.72
23	d	403[A]	CLA	C4C-C3C-C2C	-3.04	102.46	106.90
23	C	513	CLA	O2A-CGA-CBA	3.04	121.45	111.91
23	C	510	CLA	CAC-C3C-C4C	3.04	128.75	124.81
23	B	612	CLA	C1C-C2C-C3C	-3.04	103.76	106.96
29	A	414[A]	PL9	C20-C19-C21	3.04	120.38	115.27
23	C	513	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
29	A	414[B]	PL9	C17-C18-C19	-3.04	120.35	127.66
32	d	407[B]	LHG	O7-C7-C8	3.04	118.04	111.50
33	m	101	LMG	O8-C28-C29	3.03	121.43	111.91
23	B	613	CLA	C4C-C3C-C2C	-3.03	102.47	106.90
23	c	509	CLA	C4A-NA-C1A	-3.03	105.34	106.71
23	c	509	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
23	B	612	CLA	C11-C12-C13	-3.03	106.12	115.92
23	A	404[B]	CLA	CHC-C1C-C2C	-3.03	118.34	126.72
23	B	608	CLA	CHC-C1C-C2C	-3.03	118.34	126.72
25	t	102	BCR	C15-C16-C17	-3.03	117.27	123.47
29	D	405[B]	PL9	C27-C28-C29	-3.03	120.36	127.66
23	c	501	CLA	C1D-CHD-C4C	-3.03	119.52	126.06
23	d	403[A]	CLA	O2A-CGA-O1A	-3.03	115.94	123.59
23	A	406[A]	CLA	O2A-CGA-CBA	3.03	121.42	111.91
23	d	404	CLA	CHD-C4C-NC	3.03	128.98	124.20
23	b	615	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
23	A	404[A]	CLA	C1-C2-C3	-3.03	120.81	126.04
23	C	510	CLA	C4C-C3C-C2C	-3.03	102.49	106.90
23	b	613	CLA	CHC-C1C-C2C	-3.03	118.35	126.72
23	a	404[B]	CLA	CAA-C2A-C1A	-3.02	102.07	111.97
23	d	403[A]	CLA	C4-C3-C5	3.02	120.36	115.27
23	B	614	CLA	O2A-CGA-CBA	3.02	121.39	111.91
23	d	404	CLA	C4C-C3C-C2C	-3.02	102.49	106.90
29	d	406[A]	PL9	C37-C38-C39	-3.02	120.38	127.66
23	C	510	CLA	C16-C15-C13	-3.02	106.15	115.92
29	a	412[B]	PL9	C35-C34-C36	3.02	120.35	115.27
23	B	603	CLA	CMB-C2B-C3B	3.02	130.33	124.68
23	c	513	CLA	CAC-C3C-C4C	3.02	128.73	124.81
26	a	409[B]	SQD	C45-O47-C7	-3.02	110.36	117.79
23	B	603	CLA	CHC-C1C-C2C	-3.02	118.38	126.72
23	c	511	CLA	CHD-C4C-NC	3.02	128.96	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	408	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
23	A	404[A]	CLA	CAA-C2A-C1A	-3.01	102.09	111.97
35	h	102	DGD	O1G-C1A-C2A	3.01	121.36	111.91
25	b	619	BCR	C38-C26-C25	-3.01	121.14	124.53
29	a	412[A]	PL9	C42-C43-C44	-3.01	120.41	127.66
23	b	603	CLA	CMA-C3A-C2A	-3.01	101.68	113.83
23	c	503	CLA	C3B-C4B-NB	3.01	113.10	109.21
23	c	512	CLA	CHD-C4C-NC	3.01	128.95	124.20
23	C	513	CLA	CMC-C2C-C1C	3.01	129.62	125.04
29	d	406[B]	PL9	C37-C38-C39	-3.01	120.41	127.66
32	d	407[A]	LHG	O7-C7-C8	3.01	117.99	111.50
23	A	408	CLA	O2A-CGA-CBA	3.01	121.35	111.91
23	c	505	CLA	C3B-C4B-NB	3.01	113.10	109.21
23	D	402[A]	CLA	CAC-C3C-C4C	3.01	128.71	124.81
23	B	615	CLA	C4-C3-C5	3.01	120.33	115.27
23	a	405[B]	CLA	CHD-C4C-NC	3.01	128.94	124.20
23	B	608	CLA	O2A-CGA-O1A	-3.01	116.00	123.59
23	B	613	CLA	CMB-C2B-C3B	3.00	130.30	124.68
23	b	605	CLA	C4C-C3C-C2C	-3.00	102.52	106.90
23	b	607	CLA	C1D-CHD-C4C	-3.00	119.58	126.06
23	B	614	CLA	CMB-C2B-C3B	3.00	130.29	124.68
24	a	414[B]	PHO	C4A-C3A-C2A	-3.00	99.99	102.84
23	A	404[A]	CLA	CHC-C1C-C2C	-3.00	118.43	126.72
23	B	605	CLA	CMC-C2C-C1C	3.00	129.60	125.04
29	A	414[B]	PL9	C30-C29-C31	3.00	120.31	115.27
23	A	405[A]	CLA	CHD-C4C-NC	3.00	128.93	124.20
23	b	603	CLA	CHD-C4C-NC	3.00	128.93	124.20
26	a	409[A]	SQD	C45-O47-C7	-3.00	110.42	117.79
26	a	410	SQD	O48-C23-C24	2.99	121.31	111.91
23	D	402[B]	CLA	C4C-C3C-C2C	-2.99	102.53	106.90
25	C	516	BCR	C11-C10-C9	-2.99	123.04	127.31
23	B	605	CLA	C1-C2-C3	-2.99	120.87	126.04
23	B	604	CLA	CHC-C1C-C2C	-2.99	118.44	126.72
26	B	620	SQD	O48-C23-C24	2.99	121.30	111.91
23	B	613	CLA	C1D-CHD-C4C	-2.99	119.60	126.06
23	c	513	CLA	O2A-CGA-CBA	2.99	121.29	111.91
23	b	612	CLA	O2A-CGA-CBA	2.99	121.29	111.91
31	A	417	LMT	O5B-C5B-C4B	2.99	115.12	109.69
23	B	607	CLA	C1D-CHD-C4C	-2.99	119.62	126.06
23	b	611	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
23	C	502	CLA	C3B-C4B-NB	2.98	113.07	109.21
32	D	407[A]	LHG	O8-C23-C24	2.98	121.27	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	410	SQD	O7-S-C6	2.98	110.48	106.94
25	A	409	BCR	C40-C30-C25	-2.98	105.46	110.30
32	a	419[B]	LHG	O7-C7-C8	2.98	117.93	111.50
29	a	412[B]	PL9	C42-C43-C44	-2.98	120.48	127.66
23	B	614	CLA	CHD-C4C-NC	2.98	128.90	124.20
26	a	409[B]	SQD	O8-S-C6	2.98	110.49	105.74
23	b	609	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
23	b	610	CLA	C1C-C2C-C3C	-2.98	103.82	106.96
25	Y	101	BCR	C36-C18-C19	2.98	122.77	118.08
25	A	409	BCR	C15-C14-C13	-2.98	123.06	127.31
32	d	414[B]	LHG	O8-C23-O10	-2.98	116.08	123.59
23	B	614	CLA	O2A-CGA-O1A	-2.97	116.09	123.59
32	E	101[A]	LHG	O8-C23-C24	2.97	121.23	111.91
23	c	509	CLA	CHD-C4C-NC	2.97	128.88	124.20
23	b	601	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
23	b	606	CLA	C3B-C4B-NB	2.97	113.05	109.21
23	C	512	CLA	CMB-C2B-C3B	2.97	130.23	124.68
23	C	509	CLA	CMB-C2B-C3B	2.97	130.23	124.68
23	C	506	CLA	C4-C3-C5	2.96	120.25	115.27
23	B	611	CLA	C3B-C4B-NB	2.96	113.04	109.21
23	d	402[A]	CLA	CHC-C1C-C2C	-2.96	118.53	126.72
23	c	510	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
23	D	403	CLA	C3B-C4B-NB	2.96	113.04	109.21
23	c	503	CLA	CHD-C4C-NC	2.96	128.87	124.20
23	B	615	CLA	CHD-C4C-NC	2.96	128.86	124.20
24	A	407[A]	PHO	O1D-CGD-CBD	-2.96	119.81	124.74
26	f	102	SQD	C4-C3-C2	-2.96	105.66	110.82
29	a	412[B]	PL9	C22-C23-C24	-2.96	120.54	127.66
23	c	507	CLA	CHD-C4C-NC	2.95	128.85	124.20
23	a	407	CLA	C4-C3-C5	2.95	120.23	115.27
23	B	603	CLA	O2A-CGA-CBA	2.95	121.16	111.91
23	b	605	CLA	CHC-C1C-C2C	-2.95	118.56	126.72
26	A	410[A]	SQD	O9-S-C6	2.95	110.44	106.94
35	C	517[B]	DGD	O6D-C1D-O3G	-2.95	103.00	109.97
23	c	508	CLA	O2A-CGA-CBA	2.94	121.15	111.91
23	A	406[B]	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
29	a	412[B]	PL9	C17-C18-C19	-2.94	120.57	127.66
29	A	414[A]	PL9	C30-C29-C31	2.94	120.22	115.27
23	C	514	CLA	CMC-C2C-C1C	2.94	129.51	125.04
23	C	505	CLA	CHC-C1C-C2C	-2.94	118.59	126.72
23	a	407	CLA	O2A-CGA-CBA	2.94	121.12	111.91
32	a	419[A]	LHG	O7-C7-C8	2.94	117.83	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	608	CLA	CHC-C1C-C2C	-2.94	118.60	126.72
23	B	604	CLA	CAC-C3C-C4C	2.93	128.62	124.81
23	A	406[A]	CLA	CHD-C4C-NC	2.93	128.83	124.20
29	A	414[A]	PL9	C17-C18-C19	-2.93	120.59	127.66
23	B	606	CLA	C3B-C4B-NB	2.93	113.00	109.21
23	b	610	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
32	D	406[A]	LHG	O8-C23-O10	-2.93	116.19	123.59
23	A	404[B]	CLA	C2A-C1A-CHA	-2.93	118.73	123.86
29	d	406[A]	PL9	C22-C23-C24	-2.93	120.60	127.66
32	E	101[B]	LHG	O8-C23-C24	2.93	121.11	111.91
23	b	609	CLA	CBC-CAC-C3C	-2.93	104.35	112.43
25	A	409	BCR	C38-C26-C25	-2.93	121.24	124.53
25	b	617	BCR	C29-C30-C25	2.93	114.99	110.48
23	B	616	CLA	C1C-C2C-C3C	-2.93	103.88	106.96
23	b	606	CLA	CAA-C2A-C3A	-2.93	104.75	112.78
24	A	416[B]	PHO	O2D-CGD-O1D	-2.93	118.11	123.84
23	B	609	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
23	D	403	CLA	C4-C3-C5	2.93	120.19	115.27
32	A	419[B]	LHG	C5-O7-C7	-2.93	110.58	117.79
23	C	502	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
29	d	406[A]	PL9	C27-C28-C29	-2.93	120.61	127.66
23	A	404[A]	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
23	A	408	CLA	CHC-C1C-C2C	-2.92	118.64	126.72
23	c	510	CLA	O2A-CGA-CBA	2.92	121.08	111.91
23	d	402[A]	CLA	CBC-CAC-C3C	-2.92	104.38	112.43
23	A	406[A]	CLA	CAA-C2A-C3A	-2.92	104.78	112.78
23	a	405[B]	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
23	C	514	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
29	d	406[A]	PL9	C53-C6-C1	2.92	120.95	114.99
23	B	606	CLA	CHD-C4C-NC	2.92	128.80	124.20
29	d	406[B]	PL9	C40-C39-C41	2.92	120.17	115.27
29	a	412[A]	PL9	C22-C23-C24	-2.92	120.64	127.66
23	D	402[B]	CLA	CHC-C1C-C2C	-2.91	118.66	126.72
23	B	613	CLA	CMC-C2C-C1C	2.91	129.47	125.04
23	d	404	CLA	CAA-C2A-C3A	-2.91	104.81	112.78
26	A	410[A]	SQD	O48-C23-C24	2.91	121.04	111.91
26	A	412	SQD	O48-C23-C24	2.91	121.03	111.91
23	b	608	CLA	CBC-CAC-C3C	-2.91	104.41	112.43
32	D	407[A]	LHG	O8-C23-O10	-2.91	116.25	123.59
23	B	607	CLA	CAA-C2A-C3A	-2.91	104.81	112.78
23	C	507	CLA	C4-C3-C5	2.91	120.16	115.27
23	B	609	CLA	CBC-CAC-C3C	-2.91	104.42	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	405[A]	CLA	C4-C3-C5	2.91	120.16	115.27
25	Y	101	BCR	C36-C18-C17	-2.90	118.85	122.92
23	A	406[B]	CLA	O2A-CGA-O1A	-2.90	116.26	123.59
23	b	608	CLA	CHD-C4C-NC	2.90	128.78	124.20
23	a	404[A]	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
23	a	405[A]	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
23	d	403[B]	CLA	CAA-C2A-C3A	-2.90	104.83	112.78
29	a	412[B]	PL9	C10-C9-C11	2.90	120.15	115.27
23	b	610	CLA	CAA-C2A-C3A	-2.90	104.84	112.78
23	d	402[A]	CLA	CMA-C3A-C2A	-2.90	102.14	113.83
23	b	613	CLA	O2A-CGA-CBA	2.90	121.00	111.91
23	b	601	CLA	CHD-C4C-NC	2.90	128.77	124.20
23	b	603	CLA	C4-C3-C5	2.90	120.14	115.27
31	A	420	LMT	O5B-C5B-C4B	2.90	114.95	109.69
23	A	406[B]	CLA	O2A-CGA-CBA	2.89	120.98	111.91
23	A	405[A]	CLA	CHC-C1C-C2C	-2.89	118.72	126.72
23	D	402[A]	CLA	CHC-C1C-C2C	-2.89	118.72	126.72
33	C	501	LMG	C6-C5-C4	2.89	119.78	113.00
23	D	402[A]	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
23	C	504	CLA	O2A-CGA-O1A	-2.89	116.31	123.59
32	A	419[B]	LHG	O8-C23-C24	2.89	120.96	111.91
23	D	402[B]	CLA	CAC-C3C-C4C	2.88	128.55	124.81
23	B	609	CLA	CHD-C4C-NC	2.88	128.75	124.20
23	A	405[B]	CLA	C4-C3-C5	2.88	120.12	115.27
29	A	414[B]	PL9	C10-C9-C11	2.88	120.12	115.27
23	b	611	CLA	CHD-C4C-NC	2.88	128.75	124.20
25	B	619	BCR	C24-C23-C22	-2.88	121.88	126.23
23	B	602	CLA	CHD-C4C-NC	2.88	128.74	124.20
23	b	616	CLA	CAC-C3C-C4C	2.88	128.54	124.81
25	A	409	BCR	C16-C17-C18	-2.88	123.20	127.31
23	C	503	CLA	CHC-C1C-C2C	-2.88	118.77	126.72
24	A	416[B]	PHO	C4-C3-C5	2.88	120.11	115.27
23	B	615	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
25	C	515	BCR	C15-C14-C13	-2.87	123.21	127.31
23	a	404[B]	CLA	O2A-CGA-O1A	-2.87	116.34	123.59
23	b	602	CLA	CMA-C3A-C4A	-2.87	104.05	111.77
23	C	507	CLA	CMC-C2C-C1C	2.87	129.41	125.04
24	a	406[A]	PHO	O2A-CGA-CBA	2.87	120.92	111.91
23	D	402[A]	CLA	O2A-CGA-O1A	-2.87	116.35	123.59
23	b	614	CLA	CBC-CAC-C3C	-2.87	104.52	112.43
23	B	602	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
31	b	621	LMT	C1'-O5'-C5'	-2.87	108.06	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	606	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
24	a	406[B]	PHO	O1D-CGD-CBD	-2.87	119.97	124.74
23	B	604	CLA	O2A-CGA-O1A	-2.87	116.36	123.59
25	C	516	BCR	C29-C30-C25	2.87	114.89	110.48
23	b	614	CLA	O2A-CGA-O1A	-2.87	116.36	123.59
23	c	502	CLA	CMC-C2C-C1C	2.86	129.40	125.04
23	b	609	CLA	CHD-C4C-NC	2.86	128.72	124.20
29	a	412[A]	PL9	C37-C38-C39	-2.86	120.77	127.66
38	f	101	HEM	CBD-CAD-C3D	-2.86	104.67	112.63
23	B	603	CLA	C4-C3-C5	2.86	120.09	115.27
24	a	406[B]	PHO	C1A-C2A-C3A	-2.86	100.12	102.84
23	b	615	CLA	C11-C10-C8	-2.86	106.67	115.92
23	C	506	CLA	CHC-C1C-C2C	-2.86	118.81	126.72
23	B	606	CLA	O2A-CGA-CBA	2.86	120.88	111.91
23	B	603	CLA	CHD-C4C-NC	2.86	128.71	124.20
23	B	616	CLA	C1-O2A-CGA	2.86	123.94	116.44
23	b	605	CLA	C3B-C4B-NB	2.86	112.90	109.21
25	D	404	BCR	C15-C14-C13	-2.85	123.24	127.31
23	B	601	CLA	C3B-C4B-NB	2.85	112.90	109.21
23	c	509	CLA	C4-C3-C5	2.85	120.07	115.27
23	b	609	CLA	C1C-C2C-C3C	-2.85	103.96	106.96
23	B	603	CLA	CMC-C2C-C1C	2.85	129.38	125.04
23	B	610	CLA	CHD-C4C-NC	2.85	128.70	124.20
23	c	505	CLA	CHC-C1C-C2C	-2.85	118.83	126.72
23	C	504	CLA	C1C-C2C-C3C	-2.85	103.96	106.96
23	c	508	CLA	CHC-C1C-C2C	-2.85	118.83	126.72
24	a	406[A]	PHO	C1A-C2A-C3A	-2.85	100.13	102.84
23	b	614	CLA	CHC-C1C-C2C	-2.85	118.83	126.72
23	C	514	CLA	CBC-CAC-C3C	-2.85	104.57	112.43
23	c	506	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
23	C	505	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
32	b	629[A]	LHG	O8-C23-C24	2.85	120.84	111.91
25	D	404	BCR	C40-C30-C25	-2.85	105.68	110.30
23	c	505	CLA	CMC-C2C-C1C	2.85	129.37	125.04
23	b	607	CLA	C4-C3-C5	2.85	120.06	115.27
23	B	615	CLA	C6-C7-C8	-2.84	106.73	115.92
23	b	604	CLA	CHC-C1C-C2C	-2.84	118.86	126.72
23	c	509	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
24	a	406[A]	PHO	O1D-CGD-CBD	-2.84	120.01	124.74
23	B	609	CLA	C3B-C4B-NB	2.84	112.88	109.21
23	d	403[B]	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
23	c	510	CLA	CMB-C2B-C3B	2.84	129.99	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	502	CLA	CMC-C2C-C1C	2.84	129.36	125.04
25	D	404	BCR	C16-C17-C18	-2.84	123.26	127.31
23	b	601	CLA	CAC-C3C-C4C	2.83	128.49	124.81
23	B	614	CLA	CHC-C1C-C2C	-2.83	118.88	126.72
23	c	513	CLA	CHC-C1C-C2C	-2.83	118.88	126.72
23	b	601	CLA	CHC-C1C-C2C	-2.83	118.88	126.72
25	h	101	BCR	C36-C18-C17	-2.83	118.95	122.92
23	C	510	CLA	O2A-CGA-CBA	2.83	120.80	111.91
23	c	510	CLA	CHD-C4C-NC	2.83	128.67	124.20
33	Z	101	LMG	C4-C3-C2	2.83	115.77	110.82
29	A	414[B]	PL9	C40-C39-C41	2.83	120.03	115.27
23	C	505	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
24	A	407[B]	PHO	O1D-CGD-CBD	-2.83	120.03	124.74
23	c	513	CLA	CAA-C2A-C3A	-2.83	105.04	112.78
23	b	607	CLA	CAA-C2A-C3A	-2.83	105.04	112.78
26	A	410[B]	SQD	O48-C23-C24	2.82	120.77	111.91
23	b	607	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
23	B	613	CLA	CAC-C3C-C4C	2.82	128.47	124.81
33	c	519	LMG	O1-C7-C8	-2.82	104.09	110.90
23	c	501	CLA	CHD-C4C-NC	2.82	128.65	124.20
26	B	620	SQD	C4-C3-C2	2.82	115.75	110.82
23	b	616	CLA	C1C-C2C-C3C	-2.82	103.99	106.96
25	T	102	BCR	C35-C13-C12	2.82	122.52	118.08
23	C	505	CLA	CMC-C2C-C1C	2.82	129.33	125.04
23	B	610	CLA	CHC-C1C-C2C	-2.82	118.92	126.72
23	C	514	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
23	B	612	CLA	C3B-C4B-NB	2.82	112.85	109.21
23	c	506	CLA	CHD-C4C-NC	2.82	128.64	124.20
32	D	407[B]	LHG	O8-C23-C24	2.82	120.74	111.91
35	c	516[A]	DGD	O3G-C3G-C2G	-2.82	104.11	110.90
33	z	101	LMG	O8-C28-C29	2.81	120.74	111.91
23	C	512	CLA	C4-C3-C5	2.81	120.00	115.27
23	b	605	CLA	O2A-CGA-O1A	-2.81	116.49	123.59
25	d	405	BCR	C21-C20-C19	-2.81	114.44	123.22
23	A	408	CLA	CMB-C2B-C3B	2.81	129.94	124.68
23	b	610	CLA	C3B-C4B-NB	2.81	112.84	109.21
24	a	414[A]	PHO	CMC-C2C-C3C	2.81	130.23	124.94
23	b	602	CLA	C2A-C1A-CHA	-2.81	118.95	123.86
33	c	519	LMG	O8-C28-C29	2.80	120.71	111.91
23	C	511	CLA	O2A-CGA-CBA	2.80	120.71	111.91
23	d	403[A]	CLA	CHC-C1C-C2C	-2.80	118.97	126.72
23	a	404[B]	CLA	C4-C3-C5	2.80	119.99	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	T	102	BCR	C33-C5-C6	-2.80	121.38	124.53
23	C	508	CLA	CHC-C1C-C2C	-2.80	118.97	126.72
23	b	606	CLA	CHC-C1C-C2C	-2.80	118.97	126.72
23	A	404[B]	CLA	CAA-C2A-C1A	-2.80	102.80	111.97
23	B	607	CLA	C2A-C1A-CHA	-2.80	118.97	123.86
23	b	610	CLA	C4-C3-C5	2.80	119.98	115.27
23	c	511	CLA	O2A-CGA-CBA	2.80	120.69	111.91
23	A	406[A]	CLA	CHC-C1C-C2C	-2.80	118.99	126.72
35	C	517[A]	DGD	O3G-C3G-C2G	-2.79	104.16	110.90
23	c	512	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
35	C	517[B]	DGD	C2G-O2G-C1B	-2.79	110.92	117.79
24	A	407[A]	PHO	CMC-C2C-C3C	2.79	130.21	124.94
23	C	511	CLA	CMB-C2B-C3B	2.79	129.90	124.68
23	c	512	CLA	CAC-C3C-C4C	2.79	128.43	124.81
25	k	101	BCR	C38-C26-C25	-2.79	121.39	124.53
23	b	615	CLA	O2A-CGA-O1A	-2.79	116.55	123.59
38	E	102	HEM	CHB-C1B-NB	2.79	127.83	124.38
23	a	405[B]	CLA	CAA-C2A-C3A	-2.79	105.14	112.78
23	C	511	CLA	O2A-CGA-O1A	-2.79	116.56	123.59
23	a	405[B]	CLA	C4-C3-C5	2.79	119.96	115.27
23	A	406[B]	CLA	CHD-C4C-NC	2.79	128.59	124.20
23	C	502	CLA	CHD-C4C-NC	2.79	128.59	124.20
32	D	407[A]	LHG	O7-C7-C8	2.79	117.50	111.50
23	c	510	CLA	O2A-CGA-O1A	-2.79	116.56	123.59
23	C	511	CLA	CAC-C3C-C4C	2.79	128.42	124.81
31	B	628	LMT	C2'-C3'-C4'	2.78	116.04	109.68
25	Y	101	BCR	C38-C26-C25	-2.78	121.40	124.53
25	A	409	BCR	C31-C1-C6	-2.78	105.79	110.30
23	c	509	CLA	O2A-C1-C2	2.78	115.95	108.64
26	a	409[A]	SQD	O47-C7-O49	-2.78	116.98	123.70
23	C	514	CLA	C2A-C1A-CHA	-2.78	119.00	123.86
29	D	405[B]	PL9	C51-C49-C50	2.78	120.74	114.60
26	f	102	SQD	O8-S-C6	2.78	110.17	105.74
23	A	404[A]	CLA	CAA-CBA-CGA	-2.78	105.14	113.25
23	A	408	CLA	CHD-C4C-NC	2.77	128.57	124.20
23	B	614	CLA	C4C-C3C-C2C	-2.77	102.85	106.90
23	C	510	CLA	O2A-CGA-O1A	-2.77	116.60	123.59
23	c	504	CLA	CHD-C4C-NC	2.77	128.57	124.20
23	b	608	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
24	a	414[B]	PHO	CMB-C2B-C3B	2.77	129.86	124.68
23	A	405[B]	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
23	c	507	CLA	C3B-C4B-NB	2.77	112.78	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	504	CLA	CHC-C1C-C2C	-2.77	119.07	126.72
23	B	609	CLA	O2A-CGA-CBA	2.76	120.58	111.91
31	M	101	LMT	C1'-O5'-C5'	-2.76	108.26	113.69
23	C	514	CLA	CAC-C3C-C4C	2.76	128.40	124.81
25	D	404	BCR	C3-C4-C5	-2.76	109.14	114.08
23	B	614	CLA	C2A-C1A-CHA	-2.76	119.03	123.86
29	a	412[A]	PL9	C53-C6-C1	2.76	120.64	114.99
23	B	602	CLA	C2A-C1A-CHA	-2.76	119.04	123.86
23	D	402[B]	CLA	O2A-CGA-O1A	-2.76	116.63	123.59
23	D	403	CLA	CHC-C1C-C2C	-2.76	119.09	126.72
26	a	410	SQD	C3-C4-C5	2.76	115.16	110.24
31	a	416	LMT	C3'-C4'-C5'	-2.76	104.61	110.93
23	c	501	CLA	CHC-C1C-C2C	-2.76	119.10	126.72
23	c	510	CLA	CHC-C1C-C2C	-2.76	119.10	126.72
23	b	609	CLA	CHC-C1C-C2C	-2.75	119.10	126.72
25	C	515	BCR	C38-C26-C25	-2.75	121.44	124.53
23	a	405[B]	CLA	C1-C2-C3	-2.75	121.28	126.04
23	d	404	CLA	C2A-C1A-CHA	-2.75	119.05	123.86
23	C	507	CLA	CAC-C3C-C4C	2.75	128.38	124.81
23	b	601	CLA	C3B-C4B-NB	2.75	112.77	109.21
25	b	618	BCR	C15-C14-C13	-2.75	123.39	127.31
29	A	414[A]	PL9	C40-C39-C41	2.75	119.90	115.27
23	d	403[B]	CLA	CHD-C4C-NC	2.75	128.53	124.20
23	B	601	CLA	O2A-CGA-CBA	2.75	120.53	111.91
35	c	518	DGD	O2G-C1B-C2B	2.75	117.42	111.50
23	C	508	CLA	CHD-C4C-NC	2.75	128.53	124.20
23	b	609	CLA	O2A-CGA-O1A	-2.74	116.67	123.59
23	a	404[B]	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
29	D	405[B]	PL9	C17-C18-C19	-2.74	121.07	127.66
23	d	402[B]	CLA	C4C-C3C-C2C	-2.74	102.91	106.90
23	A	405[B]	CLA	CHC-C1C-C2C	-2.74	119.15	126.72
23	c	501	CLA	CMC-C2C-C1C	2.74	129.21	125.04
25	a	408	BCR	C38-C26-C25	-2.74	121.45	124.53
23	A	406[B]	CLA	CHC-C1C-C2C	-2.74	119.15	126.72
23	A	408	CLA	CBC-CAC-C3C	-2.74	104.89	112.43
29	A	414[A]	PL9	C10-C9-C8	-2.74	116.66	123.68
25	k	101	BCR	C39-C30-C25	-2.73	105.86	110.30
23	A	404[A]	CLA	CAC-C3C-C4C	2.73	128.36	124.81
33	C	501	LMG	O6-C1-O1	-2.73	103.50	109.97
25	d	405	BCR	C33-C5-C6	-2.73	121.46	124.53
23	a	404[B]	CLA	C1-C2-C3	-2.73	121.32	126.04
23	A	406[A]	CLA	CBC-CAC-C3C	-2.73	104.90	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	a	415	LMG	C8-O7-C10	-2.73	111.07	117.79
29	D	405[B]	PL9	C7-C8-C9	-2.73	122.25	126.79
35	C	517[A]	DGD	C2G-O2G-C1B	-2.73	111.07	117.79
23	C	513	CLA	O2A-CGA-O1A	-2.73	116.71	123.59
32	D	406[B]	LHG	O7-C7-C8	2.73	117.38	111.50
23	C	514	CLA	CHC-C1C-C2C	-2.73	119.18	126.72
33	c	520	LMG	O8-C28-C29	2.73	120.47	111.91
23	c	512	CLA	CHC-C1C-C2C	-2.73	119.18	126.72
25	B	617	BCR	C16-C17-C18	-2.73	123.42	127.31
32	d	408[A]	LHG	O8-C23-C24	2.73	120.46	111.91
23	C	512	CLA	CHD-C4C-NC	2.73	128.50	124.20
23	D	402[B]	CLA	CAA-C2A-C3A	-2.72	105.32	112.78
23	c	504	CLA	C2A-C1A-CHA	-2.72	119.10	123.86
23	d	402[A]	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
29	D	405[A]	PL9	C42-C41-C39	-2.72	104.03	112.98
25	c	514	BCR	C20-C21-C22	-2.72	123.43	127.31
23	D	402[A]	CLA	CAA-C2A-C3A	-2.72	105.33	112.78
35	c	518	DGD	O3G-C1D-C2D	-2.72	104.06	108.30
26	f	102	SQD	O48-C23-C24	2.72	120.44	111.91
23	c	507	CLA	O2A-CGA-CBA	2.72	120.44	111.91
32	A	419[A]	LHG	O7-C7-O9	-2.72	117.13	123.70
23	B	601	CLA	CMC-C2C-C1C	2.72	129.18	125.04
26	F	102	SQD	O48-C23-C24	2.71	120.42	111.91
29	d	406[A]	PL9	C36-C34-C33	-2.71	115.63	121.12
23	d	402[B]	CLA	O2A-CGA-CBA	2.71	120.41	111.91
25	y	101	BCR	C10-C11-C12	-2.71	114.76	123.22
35	C	519	DGD	O1G-C1A-C2A	2.71	120.41	111.91
23	a	405[A]	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
25	c	515	BCR	C15-C14-C13	-2.71	123.44	127.31
25	c	514	BCR	C28-C27-C26	-2.71	109.24	114.08
24	a	406[A]	PHO	CMA-C3A-C4A	-2.71	108.45	114.38
23	b	607	CLA	CAC-C3C-C4C	2.71	128.32	124.81
29	D	405[B]	PL9	C45-C44-C46	2.71	119.82	115.27
23	A	406[A]	CLA	C2A-C1A-CHA	-2.71	119.13	123.86
23	A	404[A]	CLA	C2A-C1A-CHA	-2.70	119.13	123.86
23	d	404	CLA	CBC-CAC-C3C	-2.70	104.98	112.43
23	C	511	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
23	a	404[B]	CLA	CMA-C3A-C4A	-2.70	104.51	111.77
23	B	612	CLA	C2A-C1A-CHA	-2.70	119.14	123.86
23	C	507	CLA	C2A-C1A-CHA	-2.70	119.14	123.86
23	b	603	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
23	B	611	CLA	C1-C2-C3	-2.70	121.37	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	502	CLA	CHC-C1C-C2C	-2.70	119.25	126.72
23	b	610	CLA	CHD-C4C-NC	2.70	128.46	124.20
35	C	518[A]	DGD	O1G-C1A-O1A	-2.70	116.78	123.59
23	D	402[A]	CLA	CMC-C2C-C1C	2.70	129.15	125.04
23	b	603	CLA	CMB-C2B-C3B	2.70	129.72	124.68
25	h	101	BCR	C33-C5-C6	-2.69	121.50	124.53
23	A	404[B]	CLA	C1-C2-C3	-2.69	121.39	126.04
23	b	613	CLA	C4-C3-C5	2.69	119.80	115.27
25	d	405	BCR	C28-C27-C26	-2.69	109.27	114.08
23	B	616	CLA	C2A-C1A-CHA	-2.69	119.15	123.86
23	B	613	CLA	CHC-C1C-C2C	-2.69	119.28	126.72
23	c	511	CLA	CHC-C1C-C2C	-2.69	119.28	126.72
31	M	101	LMT	C3'-C4'-C5'	-2.69	104.76	110.93
25	t	102	BCR	C21-C20-C19	-2.69	114.83	123.22
24	A	407[B]	PHO	CMC-C2C-C3C	2.69	130.01	124.94
25	h	101	BCR	C16-C17-C18	-2.69	123.47	127.31
23	a	404[A]	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
23	a	405[A]	CLA	CHC-C1C-C2C	-2.69	119.29	126.72
23	C	514	CLA	O2A-CGA-CBA	2.68	120.33	111.91
23	C	510	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
23	b	608	CLA	C11-C12-C13	-2.68	107.24	115.92
23	b	606	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
25	H	101	BCR	C31-C1-C6	-2.68	105.95	110.30
23	c	501	CLA	CAC-C3C-C4C	2.68	128.29	124.81
23	A	406[A]	CLA	CMC-C2C-C1C	2.68	129.12	125.04
23	B	608	CLA	CMC-C2C-C1C	2.68	129.12	125.04
35	H	102	DGD	O1G-C1A-C2A	2.68	120.32	111.91
23	c	508	CLA	CAA-C2A-C3A	-2.68	105.44	112.78
23	A	405[A]	CLA	CAC-C3C-C4C	2.68	128.29	124.81
23	A	405[B]	CLA	C1-C2-C3	-2.68	121.41	126.04
23	c	512	CLA	CMC-C2C-C1C	2.68	129.12	125.04
23	A	408	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
23	a	404[B]	CLA	C2A-C1A-CHA	-2.68	119.17	123.86
29	a	412[B]	PL9	C40-C39-C41	2.68	119.78	115.27
23	D	403	CLA	CAA-C2A-C3A	-2.68	105.44	112.78
23	c	506	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
23	b	614	CLA	C4C-C3C-C2C	-2.68	103.00	106.90
23	c	513	CLA	C2A-C1A-CHA	-2.68	119.18	123.86
25	k	101	BCR	C24-C23-C22	-2.68	122.19	126.23
32	a	419[A]	LHG	O8-C23-C24	2.68	120.30	111.91
24	a	414[A]	PHO	CBA-CAA-C2A	-2.68	105.99	113.81
23	b	606	CLA	C1-C2-C3	-2.68	121.42	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	503	CLA	C4C-C3C-C2C	-2.68	103.00	106.90
35	c	516[A]	DGD	C3G-C2G-C1G	-2.68	105.46	111.79
29	D	405[A]	PL9	C37-C38-C39	-2.67	121.22	127.66
23	D	402[B]	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
23	A	406[A]	CLA	C1-C2-C3	-2.67	121.42	126.04
23	A	404[B]	CLA	C4C-C3C-C2C	-2.67	103.00	106.90
33	C	501	LMG	C8-O7-C10	-2.67	111.22	117.79
23	C	503	CLA	C4-C3-C5	2.67	119.76	115.27
23	C	508	CLA	C3B-C4B-NB	2.67	112.66	109.21
24	a	414[B]	PHO	CBA-CAA-C2A	-2.67	106.01	113.81
26	a	410	SQD	C1-O5-C5	2.67	118.93	113.69
23	c	504	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
23	b	615	CLA	CHD-C4C-NC	2.67	128.41	124.20
25	T	102	BCR	C15-C14-C13	2.67	131.12	127.31
23	b	610	CLA	CMA-C3A-C4A	-2.66	104.61	111.77
23	C	510	CLA	CHC-C1C-C2C	-2.66	119.35	126.72
29	A	414[B]	PL9	C12-C13-C14	-2.66	121.25	127.66
23	A	408	CLA	CMC-C2C-C1C	2.66	129.09	125.04
23	C	509	CLA	O2A-CGA-CBA	2.66	120.25	111.91
23	b	616	CLA	CHC-C1C-C2C	-2.66	119.37	126.72
29	D	405[B]	PL9	C37-C38-C39	-2.66	121.26	127.66
23	a	405[A]	CLA	CAA-C2A-C3A	-2.66	105.50	112.78
23	C	507	CLA	CMB-C2B-C3B	2.66	129.65	124.68
23	d	404	CLA	C3B-C4B-NB	2.66	112.64	109.21
23	B	608	CLA	CHB-C4A-NA	2.66	128.19	124.51
23	b	614	CLA	C2A-C1A-CHA	-2.65	119.22	123.86
26	A	410[A]	SQD	O48-C23-O10	-2.65	116.89	123.59
23	B	609	CLA	CHC-C1C-C2C	-2.65	119.38	126.72
23	B	608	CLA	CMA-C3A-C4A	-2.65	104.64	111.77
31	B	630	LMT	O1'-C1'-C2'	2.65	112.44	108.30
23	a	404[A]	CLA	CAC-C3C-C4C	2.65	128.25	124.81
23	C	514	CLA	CMB-C2B-C3B	2.65	129.64	124.68
32	b	629[B]	LHG	O8-C23-C24	2.65	120.22	111.91
23	c	512	CLA	C3B-C4B-NB	2.65	112.64	109.21
25	B	619	BCR	C29-C30-C25	2.65	114.56	110.48
29	D	405[A]	PL9	C40-C39-C41	2.65	119.72	115.27
23	B	604	CLA	C6-C5-C3	-2.65	106.51	113.45
31	B	631	LMT	C3'-C4'-C5'	-2.65	104.86	110.93
23	b	611	CLA	CMB-C2B-C3B	2.65	129.63	124.68
23	c	504	CLA	CMB-C2B-C3B	2.65	129.63	124.68
23	C	513	CLA	CBC-CAC-C3C	-2.65	105.14	112.43
23	c	501	CLA	O2A-CGA-O1A	-2.64	116.92	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	610	CLA	CAA-CBA-CGA	-2.64	105.53	113.25
23	b	612	CLA	CHD-C4C-NC	2.64	128.37	124.20
23	c	509	CLA	CMB-C2B-C3B	2.64	129.62	124.68
23	B	608	CLA	C11-C12-C13	-2.64	107.39	115.92
23	A	406[A]	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
23	b	601	CLA	C1-O2A-CGA	2.64	123.36	116.44
23	C	509	CLA	CAC-C3C-C4C	2.64	128.23	124.81
23	B	605	CLA	C2A-C1A-CHA	-2.64	119.25	123.86
23	A	404[B]	CLA	O2A-CGA-O1A	-2.63	116.94	123.59
23	A	406[A]	CLA	C4-C3-C5	2.63	119.70	115.27
23	b	615	CLA	O2A-CGA-CBA	2.63	120.17	111.91
23	b	605	CLA	C4-C3-C5	2.63	119.70	115.27
23	A	404[B]	CLA	CHD-C4C-NC	2.63	128.35	124.20
24	A	416[A]	PHO	O2D-CGD-O1D	-2.63	118.69	123.84
23	b	606	CLA	CMC-C2C-C1C	2.63	129.05	125.04
24	a	406[B]	PHO	O2A-CGA-O1A	-2.63	116.95	123.59
33	D	411	LMG	O8-C28-O10	-2.63	116.95	123.59
23	B	616	CLA	O2A-CGA-CBA	2.63	120.16	111.91
23	B	615	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
23	D	402[B]	CLA	C2A-C1A-CHA	-2.63	119.26	123.86
25	t	102	BCR	C11-C10-C9	-2.63	123.56	127.31
23	b	616	CLA	CMC-C2C-C1C	2.63	129.04	125.04
33	C	520	LMG	O1-C1-C2	-2.63	104.20	108.30
23	A	406[B]	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
26	F	102	SQD	O8-S-O7	-2.62	104.87	111.27
23	D	402[A]	CLA	CMB-C2B-C3B	2.62	129.58	124.68
23	d	403[A]	CLA	CAA-C2A-C3A	-2.62	105.61	112.78
23	B	609	CLA	O2A-CGA-O1A	-2.62	116.99	123.59
34	B	622	HTG	C1-O5-C5	2.62	117.40	112.58
29	A	414[A]	PL9	C53-C6-C1	2.61	120.33	114.99
31	B	628	LMT	O1'-C1'-C2'	2.61	112.38	108.30
32	D	406[A]	LHG	O8-C23-C24	2.61	120.09	111.91
32	D	406[A]	LHG	O7-C7-C8	2.61	117.12	111.50
29	d	406[B]	PL9	C22-C23-C24	-2.61	121.38	127.66
23	c	502	CLA	CMB-C2B-C3B	2.60	129.55	124.68
23	c	508	CLA	CAC-C3C-C4C	2.60	128.19	124.81
23	A	406[B]	CLA	C2A-C1A-CHA	-2.60	119.31	123.86
38	E	102	HEM	CHA-C4D-ND	2.60	127.59	124.38
23	b	603	CLA	CHC-C1C-C2C	-2.60	119.53	126.72
23	C	514	CLA	CHD-C4C-NC	2.60	128.30	124.20
32	L	101[A]	LHG	O8-C23-C24	2.60	120.06	111.91
31	m	103	LMT	C3B-C4B-C5B	-2.60	105.61	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	d	408[B]	LHG	O8-C23-C24	2.60	120.05	111.91
25	Y	101	BCR	C24-C23-C22	-2.60	122.31	126.23
23	C	508	CLA	C1-C2-C3	-2.60	121.55	126.04
23	c	505	CLA	C1-C2-C3	-2.60	121.55	126.04
23	b	603	CLA	O2A-CGA-CBA	2.60	120.05	111.91
23	B	601	CLA	C1-O2A-CGA	2.59	123.25	116.44
23	B	613	CLA	CMA-C3A-C4A	-2.59	104.80	111.77
34	b	622	HTG	O2-C2-C3	-2.59	104.35	110.35
23	d	402[A]	CLA	O2A-CGA-CBA	2.59	120.05	111.91
23	A	405[A]	CLA	OBD-CAD-C3D	-2.59	122.28	128.52
23	B	614	CLA	OBD-CAD-C3D	-2.59	122.28	128.52
23	b	611	CLA	O2A-CGA-CBA	2.59	120.04	111.91
23	a	407	CLA	CMA-C3A-C2A	-2.59	103.38	113.83
29	A	414[B]	PL9	C42-C43-C44	-2.59	121.42	127.66
23	c	505	CLA	O2A-CGA-CBA	2.59	120.03	111.91
24	a	406[B]	PHO	O2A-CGA-CBA	2.59	120.03	111.91
23	b	613	CLA	CMB-C2B-C3B	2.59	129.52	124.68
32	L	101[B]	LHG	O8-C23-C24	2.59	120.03	111.91
23	b	612	CLA	C4D-CHA-C1A	-2.59	118.10	121.25
23	C	503	CLA	CHD-C4C-NC	2.59	128.28	124.20
23	a	404[A]	CLA	C2A-C1A-CHA	-2.59	119.34	123.86
32	a	419[B]	LHG	O8-C23-C24	2.59	120.02	111.91
23	C	502	CLA	CBC-CAC-C3C	-2.59	105.30	112.43
23	B	612	CLA	O2A-CGA-CBA	2.59	120.02	111.91
35	H	102	DGD	O1G-C1A-O1A	-2.58	117.07	123.59
33	C	520	LMG	O8-C28-O10	-2.58	117.07	123.59
35	c	518	DGD	O1G-C1A-C2A	2.58	120.02	111.91
29	a	412[B]	PL9	C20-C19-C21	2.58	119.62	115.27
23	A	405[B]	CLA	C2A-C1A-CHA	-2.58	119.34	123.86
23	c	509	CLA	C1-O2A-CGA	2.58	123.22	116.44
29	d	406[A]	PL9	C36-C37-C38	-2.58	103.40	111.88
33	B	621	LMG	O8-C28-O10	-2.58	117.08	123.59
23	C	505	CLA	C4-C3-C5	2.58	119.61	115.27
23	D	403	CLA	CHD-C4C-NC	2.58	128.26	124.20
23	a	404[B]	CLA	CHD-C4C-NC	2.58	128.26	124.20
23	c	502	CLA	C1-C2-C3	-2.58	121.59	126.04
25	K	102	BCR	C33-C5-C6	-2.58	121.64	124.53
23	A	408	CLA	CAC-C3C-C4C	2.57	128.15	124.81
23	b	612	CLA	CMB-C2B-C3B	2.57	129.49	124.68
23	b	609	CLA	O2A-CGA-CBA	2.57	119.97	111.91
23	D	403	CLA	O2A-CGA-O1A	-2.57	117.11	123.59
23	a	404[A]	CLA	CMA-C3A-C4A	-2.57	104.87	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	604	CLA	C4C-C3C-C2C	-2.57	103.15	106.90
23	B	615	CLA	CHC-C1C-C2C	-2.57	119.62	126.72
23	b	604	CLA	CAC-C3C-C4C	2.57	128.14	124.81
31	T	101	LMT	C3'-C4'-C5'	-2.56	105.05	110.93
23	D	402[A]	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
23	b	606	CLA	CBC-CAC-C3C	-2.56	105.37	112.43
23	D	402[A]	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
32	D	407[B]	LHG	O8-C23-O10	-2.56	117.13	123.59
35	c	516[A]	DGD	O1G-C1A-O1A	-2.56	117.13	123.59
34	B	625	HTG	C1'-S1-C1	2.56	104.88	100.09
23	D	402[B]	CLA	C4-C3-C5	2.56	119.57	115.27
23	B	606	CLA	CHC-C1C-C2C	-2.56	119.65	126.72
38	f	101	HEM	CHB-C1B-NB	2.56	127.54	124.38
34	b	622	HTG	O5-C1-C2	2.56	113.53	110.31
23	b	610	CLA	CHC-C1C-C2C	-2.56	119.65	126.72
23	B	604	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
23	a	407	CLA	CMB-C2B-C3B	2.55	129.46	124.68
23	a	405[B]	CLA	O2A-CGA-CBA	2.55	119.92	111.91
23	c	502	CLA	O2A-CGA-CBA	2.55	119.92	111.91
31	A	420	LMT	O5'-C5'-C6'	2.55	112.78	106.44
23	B	611	CLA	O2A-CGA-O1A	-2.55	117.15	123.59
31	m	103	LMT	C1'-O5'-C5'	-2.55	108.68	113.69
23	c	506	CLA	C4-C3-C5	2.55	119.56	115.27
23	d	403[B]	CLA	CMB-C2B-C3B	2.55	129.45	124.68
23	C	503	CLA	C2A-C1A-CHA	-2.55	119.40	123.86
23	a	405[B]	CLA	CAC-C3C-C4C	2.55	128.12	124.81
23	D	402[B]	CLA	CMC-C2C-C1C	2.55	128.92	125.04
23	c	503	CLA	CAC-C3C-C4C	2.55	128.12	124.81
23	C	505	CLA	CBC-CAC-C3C	-2.55	105.41	112.43
23	A	405[B]	CLA	CED-O2D-CGD	2.55	121.70	115.94
26	F	102	SQD	O47-C7-O49	-2.55	117.55	123.70
23	c	513	CLA	C1-C2-C3	-2.55	121.64	126.04
23	B	609	CLA	O2D-CGD-O1D	-2.54	118.86	123.84
25	B	618	BCR	C2-C1-C6	2.54	114.40	110.48
23	D	403	CLA	C2A-C1A-CHA	-2.54	119.41	123.86
23	C	504	CLA	CMC-C2C-C1C	2.54	128.91	125.04
40	v	201	HEC	CMB-C2B-C3B	2.54	128.81	125.82
23	c	507	CLA	CAC-C3C-C4C	2.54	128.11	124.81
23	A	405[A]	CLA	CMA-C3A-C2A	-2.54	103.58	113.83
23	c	508	CLA	CHD-C4C-NC	2.54	128.21	124.20
23	B	608	CLA	CBC-CAC-C3C	-2.54	105.43	112.43
23	C	505	CLA	CAC-C3C-C4C	2.54	128.10	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	414[A]	PHO	O1D-CGD-CBD	-2.54	120.51	124.74
23	c	508	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
35	C	518[B]	DGD	O1G-C1A-C2A	2.54	119.87	111.91
31	m	103	LMT	C3'-C4'-C5'	-2.54	105.11	110.93
33	D	411	LMG	O8-C28-C29	2.53	119.86	111.91
31	F	101	LMT	C1'-O5'-C5'	-2.53	108.71	113.69
23	C	514	CLA	CAA-C2A-C3A	-2.53	105.84	112.78
23	d	402[B]	CLA	O2A-CGA-O1A	-2.53	117.20	123.59
23	B	606	CLA	C4-C3-C5	2.53	119.53	115.27
23	B	606	CLA	C2A-C1A-CHA	-2.53	119.43	123.86
29	A	414[A]	PL9	C35-C34-C36	2.53	119.53	115.27
23	D	403	CLA	CMA-C3A-C2A	-2.53	103.62	113.83
23	C	509	CLA	CHD-C4C-NC	2.53	128.19	124.20
23	B	604	CLA	C11-C12-C13	-2.53	107.74	115.92
23	A	405[A]	CLA	C2A-C1A-CHA	-2.53	119.44	123.86
23	b	605	CLA	CMC-C2C-C1C	2.53	128.89	125.04
25	b	618	BCR	C37-C22-C21	-2.53	119.38	122.92
23	C	507	CLA	O2A-CGA-O1A	-2.53	117.21	123.59
23	c	511	CLA	CBC-CAC-C3C	-2.53	105.46	112.43
23	C	508	CLA	C4-C3-C5	2.53	119.52	115.27
26	f	102	SQD	O47-C7-O49	-2.53	117.60	123.70
23	C	508	CLA	O2A-CGA-CBA	2.53	119.83	111.91
23	C	507	CLA	CAA-C2A-C3A	-2.52	105.87	112.78
23	b	611	CLA	O2A-CGA-O1A	-2.52	117.22	123.59
25	B	619	BCR	C21-C20-C19	-2.52	115.34	123.22
23	a	405[A]	CLA	C2A-C1A-CHA	-2.52	119.45	123.86
23	c	507	CLA	C1-C2-C3	-2.52	121.68	126.04
23	A	406[A]	CLA	CMA-C3A-C2A	-2.52	103.66	113.83
23	b	606	CLA	CMB-C2B-C3B	2.52	129.39	124.68
23	c	507	CLA	O2A-CGA-O1A	-2.52	117.23	123.59
35	C	518[B]	DGD	O1G-C1A-O1A	-2.52	117.24	123.59
26	f	102	SQD	O5-C5-C4	2.52	114.26	109.69
23	d	403[A]	CLA	CMB-C2B-C3B	2.52	129.39	124.68
26	a	409[B]	SQD	O47-C7-O49	-2.51	117.63	123.70
25	H	101	BCR	C10-C11-C12	-2.51	115.37	123.22
29	a	412[A]	PL9	C47-C48-C49	-2.51	119.16	127.75
23	a	405[B]	CLA	C2A-C1A-CHA	-2.51	119.46	123.86
23	C	510	CLA	C11-C12-C13	-2.51	107.80	115.92
23	d	402[A]	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
23	a	404[B]	CLA	CMC-C2C-C1C	2.51	128.86	125.04
24	A	407[A]	PHO	O2A-CGA-CBA	2.51	119.78	111.91
24	A	407[A]	PHO	CMB-C2B-C3B	2.51	129.37	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	k	101	BCR	C15-C14-C13	-2.51	123.73	127.31
24	a	414[B]	PHO	O2D-CGD-O1D	-2.51	118.93	123.84
23	a	405[A]	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
23	B	602	CLA	C11-C12-C13	-2.51	107.82	115.92
23	c	506	CLA	CMC-C2C-C1C	2.51	128.86	125.04
23	c	509	CLA	CAC-C3C-C4C	2.51	128.06	124.81
23	A	404[B]	CLA	CAA-CBA-CGA	-2.51	105.93	113.25
25	B	619	BCR	C7-C8-C9	-2.51	122.45	126.23
25	B	618	BCR	C15-C14-C13	-2.50	123.73	127.31
29	D	405[B]	PL9	C40-C39-C41	2.50	119.48	115.27
23	B	607	CLA	CHC-C1C-C2C	-2.50	119.80	126.72
23	B	605	CLA	C3B-C4B-NB	2.50	112.44	109.21
23	A	408	CLA	CMA-C3A-C2A	-2.50	103.74	113.83
23	D	403	CLA	O2A-CGA-CBA	2.50	119.75	111.91
23	c	503	CLA	C2A-C1A-CHA	-2.50	119.49	123.86
25	T	102	BCR	C2-C1-C6	2.50	114.33	110.48
23	C	504	CLA	CHC-C1C-C2C	-2.50	119.81	126.72
27	b	628	GOL	C3-C2-C1	-2.50	102.00	111.70
23	b	614	CLA	O2A-CGA-CBA	2.50	119.74	111.91
40	v	201	HEC	CBA-CAA-C2A	-2.50	108.40	112.60
23	a	404[A]	CLA	CMC-C2C-C1C	2.50	128.84	125.04
23	C	504	CLA	C2A-C1A-CHA	-2.50	119.49	123.86
23	B	607	CLA	CMB-C2B-C3B	2.49	129.35	124.68
23	B	611	CLA	C2C-C1C-NC	2.49	112.31	109.97
23	c	508	CLA	CMC-C2C-C1C	2.49	128.84	125.04
25	A	409	BCR	C33-C5-C6	-2.49	121.73	124.53
29	d	406[B]	PL9	C36-C37-C38	-2.49	103.69	111.88
29	a	412[B]	PL9	C53-C6-C1	2.49	120.08	114.99
23	A	404[B]	CLA	CAC-C3C-C4C	2.49	128.04	124.81
25	h	101	BCR	C37-C22-C21	-2.49	119.43	122.92
29	a	412[B]	PL9	C47-C48-C49	-2.49	119.24	127.75
23	C	507	CLA	CHD-C4C-NC	2.49	128.13	124.20
25	c	515	BCR	C21-C20-C19	-2.49	115.45	123.22
24	A	416[B]	PHO	CMB-C2B-C3B	2.49	129.34	124.68
23	B	601	CLA	CHC-C1C-C2C	-2.49	119.84	126.72
23	a	405[A]	CLA	O2A-CGA-CBA	2.49	119.72	111.91
23	a	405[B]	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
40	V	201	HEC	CMB-C2B-C3B	2.49	128.75	125.82
25	H	101	BCR	C36-C18-C17	-2.49	119.44	122.92
23	b	602	CLA	C11-C12-C13	-2.49	107.88	115.92
23	a	404[B]	CLA	C4C-C3C-C2C	-2.49	103.28	106.90
24	a	406[A]	PHO	CMB-C2B-C3B	2.48	129.33	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	614	CLA	CAC-C3C-C4C	2.48	128.03	124.81
23	B	604	CLA	C6-C7-C8	-2.48	107.89	115.92
23	C	506	CLA	O2A-CGA-O1A	-2.48	117.32	123.59
23	C	504	CLA	O2A-CGA-CBA	2.48	119.70	111.91
23	a	405[B]	CLA	CHC-C1C-C2C	-2.48	119.85	126.72
23	c	513	CLA	CHD-C4C-NC	2.48	128.12	124.20
25	H	101	BCR	C7-C8-C9	-2.48	122.48	126.23
25	c	515	BCR	C37-C22-C23	2.48	121.99	118.08
31	B	630	LMT	O5'-C5'-C6'	2.48	112.60	106.44
23	d	403[B]	CLA	C2A-C1A-CHA	-2.48	119.52	123.86
35	C	517[A]	DGD	O5D-C6D-C5D	-2.48	104.46	109.05
29	d	406[A]	PL9	C17-C18-C19	-2.48	121.69	127.66
23	B	612	CLA	CHD-C4C-NC	2.48	128.11	124.20
23	B	616	CLA	CHC-C1C-C2C	-2.48	119.86	126.72
23	C	505	CLA	CMB-C2B-C3B	2.48	129.31	124.68
29	d	406[B]	PL9	C27-C28-C29	-2.48	121.70	127.66
23	d	403[B]	CLA	O2A-CGA-O1A	-2.48	117.34	123.59
24	A	407[A]	PHO	O2A-CGA-O1A	-2.48	117.34	123.59
23	A	404[B]	CLA	CMC-C2C-C1C	2.47	128.81	125.04
23	B	604	CLA	CMC-C2C-C1C	2.47	128.81	125.04
23	A	404[A]	CLA	CMA-C3A-C2A	-2.47	103.85	113.83
23	b	609	CLA	CMC-C2C-C1C	2.47	128.80	125.04
23	b	612	CLA	CHC-C1C-C2C	-2.47	119.88	126.72
25	D	404	BCR	C37-C22-C21	-2.47	119.46	122.92
32	d	407[B]	LHG	O8-C23-C24	2.47	119.66	111.91
23	B	603	CLA	C2A-C1A-CHA	-2.47	119.54	123.86
23	A	404[B]	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
35	c	517[B]	DGD	C2G-O2G-C1B	-2.47	111.71	117.79
23	B	605	CLA	CHC-C1C-C2C	-2.47	119.89	126.72
23	B	616	CLA	CHD-C4C-NC	2.47	128.09	124.20
23	B	601	CLA	CAC-C3C-C4C	2.46	128.00	124.81
32	d	407[A]	LHG	O8-C23-O10	-2.46	117.38	123.59
25	k	101	BCR	C3-C4-C5	-2.46	109.68	114.08
23	C	514	CLA	C4-C3-C5	2.46	119.41	115.27
26	B	620	SQD	O5-C1-C2	-2.46	105.14	110.35
23	c	505	CLA	C4-C3-C5	2.46	119.41	115.27
26	a	409[A]	SQD	O7-S-C6	2.46	109.86	106.94
34	B	622	HTG	C2'-C1'-S1	-2.46	104.46	112.40
23	C	508	CLA	CBC-CAC-C3C	-2.46	105.66	112.43
33	B	621	LMG	O1-C7-C8	-2.46	104.97	110.90
23	C	510	CLA	CHD-C4C-NC	2.46	128.08	124.20
23	b	612	CLA	OBD-CAD-C3D	-2.46	122.61	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	406[B]	PHO	O2D-CGD-O1D	-2.46	119.03	123.84
29	a	412[B]	PL9	C45-C44-C46	2.46	119.40	115.27
25	a	408	BCR	C33-C5-C6	-2.45	121.77	124.53
23	c	513	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
23	B	607	CLA	CHD-C4C-NC	2.45	128.07	124.20
23	d	402[A]	CLA	C4C-C3C-C2C	-2.45	103.32	106.90
31	T	101	LMT	C1'-O5'-C5'	-2.45	108.88	113.69
23	c	510	CLA	C4-C3-C2	-2.45	117.39	123.68
23	A	404[B]	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
32	D	406[B]	LHG	O8-C23-O10	-2.45	117.41	123.59
25	y	101	BCR	C40-C30-C25	-2.45	106.33	110.30
23	A	405[A]	CLA	CMA-C3A-C4A	-2.45	105.19	111.77
23	B	608	CLA	O2A-CGA-CBA	2.45	119.59	111.91
29	a	412[A]	PL9	C40-C39-C41	2.45	119.39	115.27
23	C	506	CLA	CMB-C2B-C1B	2.45	132.22	128.46
23	C	511	CLA	CMC-C2C-C1C	2.45	128.76	125.04
25	d	405	BCR	C36-C18-C17	-2.45	119.50	122.92
29	D	405[A]	PL9	C27-C28-C29	-2.44	121.77	127.66
29	a	412[A]	PL9	C20-C19-C21	2.44	119.38	115.27
23	c	506	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
23	b	603	CLA	O2A-CGA-O1A	-2.44	117.42	123.59
26	B	620	SQD	O48-C23-O10	-2.44	117.42	123.59
23	B	612	CLA	O2A-CGA-O1A	-2.44	117.43	123.59
23	d	402[B]	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
35	c	517[B]	DGD	O1G-C1A-C2A	2.44	119.57	111.91
23	C	502	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
23	B	602	CLA	CHC-C1C-C2C	-2.44	119.97	126.72
33	C	520	LMG	C8-O7-C10	-2.44	111.78	117.79
23	d	402[B]	CLA	CAC-C3C-C2C	2.44	131.70	127.53
23	d	403[B]	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
26	a	409[B]	SQD	O48-C23-C24	2.44	119.56	111.91
23	C	511	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
23	A	405[A]	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
26	A	412	SQD	C4-C3-C2	-2.44	106.57	110.82
23	a	404[A]	CLA	CHD-C4C-NC	2.44	128.05	124.20
38	E	102	HEM	C4B-C3B-C2B	-2.44	105.18	107.11
23	A	404[B]	CLA	C4-C3-C5	2.44	119.37	115.27
24	A	407[B]	PHO	O2A-CGA-CBA	2.44	119.56	111.91
34	b	623	HTG	O5-C1-C2	2.44	113.38	110.31
38	E	102	HEM	O2D-CGD-CBD	2.44	121.86	114.03
23	b	608	CLA	O2A-CGA-CBA	2.44	119.55	111.91
23	C	506	CLA	O2A-CGA-CBA	2.44	119.55	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	615	CLA	CMB-C2B-C1B	2.44	132.21	128.46
23	b	613	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
23	B	607	CLA	C4C-C3C-C2C	-2.43	103.35	106.90
23	B	613	CLA	CHB-C4A-NA	2.43	127.88	124.51
24	a	406[A]	PHO	O2A-CGA-O1A	-2.43	117.46	123.59
33	D	411	LMG	O7-C10-C11	2.43	116.73	111.50
31	A	420	LMT	O1'-C1'-C2'	2.43	112.09	108.30
29	d	406[B]	PL9	C53-C6-C1	2.43	119.95	114.99
23	b	610	CLA	CMC-C2C-C1C	2.43	128.73	125.04
23	B	614	CLA	CBC-CAC-C3C	-2.43	105.74	112.43
25	d	405	BCR	C39-C30-C25	-2.43	106.36	110.30
29	D	405[B]	PL9	C22-C23-C24	-2.42	121.82	127.66
29	d	406[A]	PL9	C47-C48-C49	-2.42	119.47	127.75
25	T	102	BCR	C3-C4-C5	-2.42	109.75	114.08
33	C	521	LMG	C9-C8-C7	-2.42	106.06	111.79
29	d	406[B]	PL9	C17-C18-C19	-2.42	121.84	127.66
25	K	102	BCR	C39-C30-C25	-2.42	106.38	110.30
26	a	409[A]	SQD	O8-S-C6	2.41	109.59	105.74
23	C	509	CLA	O2A-CGA-O1A	-2.41	117.50	123.59
34	B	625	HTG	O5-C5-C4	2.41	114.08	109.69
29	A	414[A]	PL9	C35-C34-C33	-2.41	117.49	123.68
23	C	504	CLA	C3B-C4B-NB	2.41	112.33	109.21
23	C	507	CLA	O2A-CGA-CBA	2.41	119.47	111.91
25	H	101	BCR	C16-C15-C14	-2.41	118.54	123.47
23	A	408	CLA	C4-C3-C5	2.41	119.32	115.27
23	A	404[A]	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
23	c	505	CLA	O2A-CGA-O1A	-2.41	117.52	123.59
23	b	601	CLA	C2A-C1A-CHA	-2.41	119.65	123.86
25	c	515	BCR	C37-C22-C21	-2.41	119.55	122.92
23	c	508	CLA	C4-C3-C5	2.41	119.32	115.27
23	b	611	CLA	CMC-C2C-C1C	2.41	128.70	125.04
23	c	507	CLA	CHC-C1C-C2C	-2.41	120.07	126.72
23	C	513	CLA	O2D-CGD-O1D	-2.41	119.14	123.84
29	A	414[A]	PL9	C42-C43-C44	-2.41	121.87	127.66
23	B	604	CLA	O2A-CGA-CBA	2.41	119.45	111.91
24	A	416[B]	PHO	O2A-CGA-CBA	2.40	119.45	111.91
23	b	610	CLA	CAC-C3C-C4C	2.40	127.93	124.81
23	C	506	CLA	CHD-C4C-NC	2.40	127.99	124.20
23	d	404	CLA	CHC-C1C-C2C	-2.40	120.07	126.72
23	A	406[B]	CLA	CBC-CAC-C3C	-2.40	105.81	112.43
23	c	501	CLA	O2A-CGA-CBA	2.40	119.45	111.91
23	B	603	CLA	CMA-C3A-C2A	-2.40	104.14	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	615	CLA	CED-O2D-CGD	2.40	121.37	115.94
23	d	404	CLA	CMC-C2C-C1C	2.40	128.69	125.04
23	B	606	CLA	C7-C6-C5	-2.40	106.84	113.36
25	a	408	BCR	C37-C22-C21	-2.40	119.56	122.92
26	A	410[B]	SQD	O8-S-C6	2.40	109.56	105.74
23	c	506	CLA	CAA-C2A-C3A	-2.40	106.22	112.78
23	B	602	CLA	CMA-C3A-C4A	-2.40	105.33	111.77
29	D	405[B]	PL9	C20-C19-C21	2.40	119.30	115.27
23	B	602	CLA	CAA-CBA-CGA	-2.40	106.25	113.25
35	C	517[B]	DGD	O3G-C3G-C2G	-2.39	105.12	110.90
23	b	606	CLA	O2A-CGA-O1A	-2.39	117.55	123.59
23	b	611	CLA	C2A-C1A-CHA	-2.39	119.68	123.86
26	F	102	SQD	O5-C1-O6	2.39	115.64	109.97
23	c	501	CLA	C4-C3-C5	2.39	119.29	115.27
23	c	507	CLA	O1D-CGD-CBD	-2.39	119.60	124.48
23	c	513	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
25	Y	101	BCR	C34-C9-C8	2.39	121.84	118.08
25	Y	101	BCR	C10-C11-C12	-2.39	115.77	123.22
26	b	620	SQD	C1-C2-C3	-2.38	105.03	110.00
23	B	608	CLA	CAA-C2A-C3A	-2.38	106.25	112.78
25	B	618	BCR	C38-C26-C25	-2.38	121.85	124.53
25	c	514	BCR	C34-C9-C10	-2.38	119.58	122.92
23	A	405[B]	CLA	C4C-C3C-C2C	-2.38	103.42	106.90
32	d	407[B]	LHG	O8-C23-O10	-2.38	117.58	123.59
23	b	613	CLA	CAC-C3C-C4C	2.38	127.90	124.81
23	b	602	CLA	CHD-C4C-NC	2.38	127.95	124.20
32	L	101[A]	LHG	O8-C23-O10	-2.38	117.59	123.59
23	c	509	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
25	c	514	BCR	C38-C26-C25	-2.38	121.86	124.53
23	b	603	CLA	C7-C6-C5	-2.38	106.90	113.36
23	B	613	CLA	CBC-CAC-C3C	-2.38	105.88	112.43
23	C	512	CLA	CHC-C1C-C2C	-2.38	120.15	126.72
23	C	513	CLA	CHC-C1C-C2C	-2.38	120.15	126.72
23	C	502	CLA	O2A-CGA-CBA	2.38	119.36	111.91
29	a	412[A]	PL9	C10-C9-C8	-2.38	117.58	123.68
23	c	511	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
29	d	406[A]	PL9	C7-C8-C9	-2.38	122.84	126.79
29	D	405[A]	PL9	C45-C44-C46	2.38	119.27	115.27
29	d	406[B]	PL9	C45-C44-C46	2.38	119.27	115.27
25	a	408	BCR	C29-C30-C25	2.37	114.14	110.48
29	A	414[B]	PL9	C45-C44-C46	2.37	119.26	115.27
23	B	610	CLA	CMA-C3A-C2A	-2.37	104.26	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	515	BCR	C38-C26-C25	-2.37	121.86	124.53
23	b	605	CLA	CAC-C3C-C4C	2.37	127.89	124.81
23	b	601	CLA	CMC-C2C-C1C	2.37	128.65	125.04
23	B	602	CLA	CMB-C2B-C3B	2.37	129.11	124.68
23	c	504	CLA	CAC-C3C-C4C	2.37	127.88	124.81
25	B	618	BCR	C37-C22-C21	-2.37	119.61	122.92
31	B	631	LMT	O1'-C1'-C2'	2.37	112.00	108.30
23	C	511	CLA	CBC-CAC-C3C	-2.37	105.91	112.43
23	c	506	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
25	C	516	BCR	C32-C1-C6	-2.37	106.46	110.30
33	m	101	LMG	C8-O7-C10	-2.36	111.97	117.79
23	b	607	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
23	B	612	CLA	C1-C2-C3	-2.36	121.96	126.04
23	C	504	CLA	CAC-C3C-C4C	2.36	127.87	124.81
23	c	511	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
23	A	406[B]	CLA	C4-C3-C5	2.36	119.24	115.27
35	c	516[B]	DGD	C3G-C2G-C1G	-2.36	106.21	111.79
23	B	610	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
29	D	405[A]	PL9	C22-C23-C24	-2.36	121.98	127.66
23	B	615	CLA	CAC-C3C-C4C	2.36	127.87	124.81
25	C	515	BCR	C24-C23-C22	-2.36	122.67	126.23
26	B	620	SQD	C44-O6-C1	-2.36	109.14	113.74
23	a	407	CLA	O2A-CGA-O1A	-2.36	117.65	123.59
23	B	611	CLA	C1C-C2C-C3C	-2.36	104.48	106.96
23	b	616	CLA	C4-C3-C5	2.36	119.23	115.27
25	b	617	BCR	C32-C1-C6	-2.36	106.48	110.30
35	C	518[B]	DGD	C2G-O2G-C1B	-2.35	111.99	117.79
23	b	602	CLA	CHC-C1C-C2C	-2.35	120.21	126.72
24	A	407[B]	PHO	O2D-CGD-O1D	-2.35	119.24	123.84
24	A	416[A]	PHO	CMA-C3A-C4A	-2.35	109.23	114.38
29	d	406[B]	PL9	C20-C19-C21	2.35	119.23	115.27
23	b	611	CLA	C7-C6-C5	-2.35	106.98	113.36
23	D	402[B]	CLA	CBC-CAC-C3C	-2.35	105.95	112.43
29	A	414[A]	PL9	C45-C44-C46	2.35	119.22	115.27
25	t	102	BCR	C28-C27-C26	-2.35	109.88	114.08
35	C	518[A]	DGD	O6E-C5E-C6E	2.35	112.28	106.44
32	A	419[B]	LHG	O7-C7-O9	-2.35	118.03	123.70
25	Y	101	BCR	C37-C22-C23	2.35	121.78	118.08
29	a	412[A]	PL9	C45-C44-C46	2.35	119.22	115.27
23	c	508	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
35	H	102	DGD	O2G-C1B-C2B	2.35	116.56	111.50
23	d	402[A]	CLA	O2A-CGA-O1A	-2.35	117.67	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	F	101	LMT	C3B-C4B-C5B	-2.35	106.05	110.24
23	C	513	CLA	C3B-C4B-NB	2.35	112.24	109.21
25	T	102	BCR	C21-C20-C19	-2.35	115.90	123.22
23	C	506	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
23	d	402[B]	CLA	CBC-CAC-C3C	-2.34	105.97	112.43
35	C	519	DGD	O2G-C1B-C2B	2.34	116.55	111.50
31	B	628	LMT	C1B-C2B-C3B	2.34	114.88	110.00
38	E	102	HEM	O2A-CGA-CBA	2.34	121.55	114.03
23	C	507	CLA	CGD-CBD-CAD	-2.34	103.16	110.73
23	c	512	CLA	CHB-C4A-NA	2.34	127.75	124.51
23	C	505	CLA	CAA-C2A-C3A	-2.34	106.37	112.78
25	c	515	BCR	C32-C1-C6	-2.34	106.51	110.30
24	a	406[A]	PHO	CMC-C2C-C3C	2.34	129.35	124.94
23	B	611	CLA	CAC-C3C-C4C	2.34	127.84	124.81
25	h	101	BCR	C16-C15-C14	-2.33	118.69	123.47
23	C	509	CLA	C2A-C1A-CHA	-2.33	119.78	123.86
23	c	504	CLA	CMC-C2C-C1C	2.33	128.59	125.04
29	A	414[B]	PL9	C53-C6-C1	2.33	119.76	114.99
25	B	617	BCR	C31-C1-C6	-2.33	106.52	110.30
26	A	410[B]	SQD	O9-S-O7	-2.33	105.88	113.95
23	b	613	CLA	CHD-C4C-NC	2.33	127.88	124.20
23	D	402[A]	CLA	CHD-C4C-NC	2.33	127.88	124.20
23	d	402[A]	CLA	C1-O2A-CGA	2.33	122.56	116.44
26	A	412	SQD	O6-C44-C45	-2.33	105.28	110.90
23	B	614	CLA	C4-C3-C5	2.33	119.19	115.27
29	A	414[B]	PL9	C10-C9-C8	-2.33	117.70	123.68
29	a	412[A]	PL9	C35-C34-C33	-2.33	117.70	123.68
35	C	518[A]	DGD	O1G-C1A-C2A	2.33	119.21	111.91
35	c	517[A]	DGD	O1G-C1A-C2A	2.33	119.21	111.91
25	a	408	BCR	C7-C8-C9	-2.33	122.72	126.23
25	Y	101	BCR	C28-C27-C26	-2.33	109.92	114.08
25	k	101	BCR	C2-C1-C6	2.33	114.06	110.48
23	c	501	CLA	CBC-CAC-C3C	-2.33	106.02	112.43
32	d	407[A]	LHG	O8-C23-C24	2.33	119.21	111.91
23	B	608	CLA	CHD-C4C-NC	2.33	127.87	124.20
23	B	611	CLA	C11-C12-C13	-2.32	108.41	115.92
24	a	414[B]	PHO	CMC-C2C-C3C	2.32	129.32	124.94
35	c	516[A]	DGD	C2G-O2G-C1B	-2.32	112.07	117.79
32	D	406[B]	LHG	O8-C23-C24	2.32	119.20	111.91
24	a	406[B]	PHO	C1-C2-C3	-2.32	122.03	126.04
33	c	520	LMG	O8-C28-O10	-2.32	117.73	123.59
23	c	504	CLA	O2A-CGA-O1A	-2.32	117.74	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	407	CLA	CAC-C3C-C4C	2.32	127.82	124.81
23	a	405[A]	CLA	C4-C3-C5	2.32	119.17	115.27
29	A	414[B]	PL9	C35-C34-C36	2.32	119.17	115.27
23	A	404[A]	CLA	CMA-C3A-C4A	-2.32	105.54	111.77
23	c	510	CLA	C11-C10-C8	-2.32	108.43	115.92
25	b	618	BCR	C8-C7-C6	-2.32	120.69	127.20
23	b	602	CLA	C3B-C4B-NB	2.32	112.20	109.21
26	a	409[A]	SQD	O48-C23-C24	2.32	119.17	111.91
23	a	407	CLA	CHC-C1C-C2C	-2.32	120.32	126.72
25	A	409	BCR	C37-C22-C21	-2.32	119.68	122.92
23	b	602	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
23	c	507	CLA	CMB-C2B-C1B	2.31	132.02	128.46
23	b	608	CLA	C11-C10-C8	-2.31	108.44	115.92
23	a	407	CLA	C2A-C1A-CHA	-2.31	119.82	123.86
25	h	101	BCR	C34-C9-C8	2.31	121.72	118.08
23	b	614	CLA	CAA-C2A-C3A	-2.31	106.45	112.78
29	A	414[A]	PL9	C37-C36-C34	-2.31	105.38	112.98
25	K	102	BCR	C20-C21-C22	-2.31	124.01	127.31
23	C	505	CLA	OBD-CAD-C3D	-2.31	122.97	128.52
23	c	507	CLA	C4C-C3C-C2C	-2.31	103.53	106.90
40	V	201	HEC	CAD-CBD-CGD	-2.31	107.30	113.76
23	a	404[A]	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
23	B	616	CLA	CBC-CAC-C3C	-2.30	106.08	112.43
25	B	619	BCR	C38-C26-C25	-2.30	121.94	124.53
23	b	613	CLA	CED-O2D-CGD	2.30	121.15	115.94
25	k	101	BCR	C34-C9-C8	2.30	121.71	118.08
23	d	403[A]	CLA	CMC-C2C-C1C	2.30	128.55	125.04
23	B	607	CLA	O2A-CGA-CBA	2.30	119.14	111.91
33	d	412	LMG	O7-C10-O9	-2.30	118.14	123.70
25	Y	101	BCR	C15-C16-C17	-2.30	118.76	123.47
25	t	102	BCR	C1-C6-C7	2.30	122.29	115.78
23	b	615	CLA	C6-C7-C8	-2.30	108.48	115.92
25	h	101	BCR	C24-C23-C22	-2.30	122.76	126.23
23	b	608	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
29	A	414[A]	PL9	C2-C3-C4	2.30	121.97	118.80
23	a	407	CLA	CHB-C4A-NA	2.30	127.69	124.51
26	F	102	SQD	O48-C23-O10	-2.30	117.78	123.59
25	t	102	BCR	C10-C11-C12	-2.30	116.04	123.22
23	A	404[A]	CLA	CMC-C2C-C1C	2.30	128.54	125.04
23	b	608	CLA	CAA-C2A-C3A	-2.30	106.48	112.78
25	k	101	BCR	C11-C10-C9	-2.30	124.03	127.31
23	b	604	CLA	C6-C5-C3	-2.30	107.43	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	414[B]	PL9	C47-C48-C49	-2.30	119.90	127.75
25	B	618	BCR	C37-C22-C23	2.30	121.69	118.08
23	B	602	CLA	C1-C2-C3	-2.30	122.07	126.04
29	D	405[B]	PL9	C12-C13-C14	-2.30	122.13	127.66
25	a	408	BCR	C40-C30-C25	-2.30	106.58	110.30
23	D	402[B]	CLA	CED-O2D-CGD	2.30	121.13	115.94
23	b	607	CLA	O2A-CGA-O1A	-2.29	117.80	123.59
23	b	608	CLA	C2A-C1A-CHA	-2.29	119.85	123.86
25	B	618	BCR	C11-C10-C9	-2.29	124.04	127.31
23	B	602	CLA	CMA-C3A-C2A	-2.29	104.58	113.83
23	c	511	CLA	CMB-C2B-C3B	2.29	128.97	124.68
23	C	502	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
23	B	613	CLA	CHD-C4C-NC	2.29	127.81	124.20
29	A	414[A]	PL9	C47-C48-C49	-2.29	119.92	127.75
24	a	414[A]	PHO	O2D-CGD-O1D	-2.29	119.36	123.84
23	D	403	CLA	CMC-C2C-C1C	2.29	128.53	125.04
25	y	101	BCR	C21-C20-C19	-2.29	116.07	123.22
31	B	630	LMT	O5'-C5'-C4'	2.29	114.58	109.75
26	A	412	SQD	C1-C2-C3	-2.29	105.23	110.00
23	c	513	CLA	C4-C3-C5	2.29	119.12	115.27
32	d	408[A]	LHG	O8-C23-O10	-2.29	117.82	123.59
23	a	405[A]	CLA	CBC-CAC-C3C	-2.29	106.12	112.43
23	d	402[B]	CLA	CHB-C4A-NA	2.29	127.67	124.51
23	c	503	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
23	B	609	CLA	CAC-C3C-C4C	2.28	127.77	124.81
23	A	408	CLA	CHB-C4A-NA	2.28	127.67	124.51
23	b	609	CLA	C4-C3-C5	2.28	119.11	115.27
25	d	405	BCR	C40-C30-C39	2.28	115.54	108.53
33	Z	101	LMG	C9-C8-C7	-2.28	106.39	111.79
23	C	511	CLA	CHB-C4A-NA	2.28	127.67	124.51
25	y	101	BCR	C16-C15-C14	-2.28	118.80	123.47
29	A	414[B]	PL9	C51-C49-C50	2.28	119.64	114.60
23	b	605	CLA	C1-C2-C3	-2.28	122.11	126.04
25	c	514	BCR	C36-C18-C17	-2.28	119.74	122.92
23	B	612	CLA	C7-C6-C5	-2.28	107.18	113.36
29	A	414[B]	PL9	C25-C24-C26	2.27	119.10	115.27
23	b	615	CLA	CAC-C3C-C4C	2.27	127.76	124.81
23	a	404[A]	CLA	CMA-C3A-C2A	-2.27	104.66	113.83
23	b	602	CLA	C4-C3-C5	2.27	119.09	115.27
25	t	102	BCR	C20-C21-C22	-2.27	124.07	127.31
29	d	406[A]	PL9	C31-C32-C33	-2.27	104.42	111.88
23	b	611	CLA	OBD-CAD-C3D	-2.27	123.06	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	617	BCR	C11-C10-C9	-2.27	124.07	127.31
23	c	506	CLA	O2A-CGA-CBA	2.27	119.03	111.91
23	B	605	CLA	CBC-CAC-C3C	-2.27	106.18	112.43
23	B	606	CLA	CAC-C3C-C4C	2.27	127.75	124.81
26	F	102	SQD	O5-C1-C2	-2.27	105.55	110.35
26	a	410	SQD	O48-C23-O10	-2.27	117.87	123.59
23	C	508	CLA	C6-C7-C8	-2.27	108.59	115.92
33	c	519	LMG	C8-O7-C10	-2.27	112.21	117.79
24	A	416[A]	PHO	O1D-CGD-CBD	-2.27	120.96	124.74
23	C	507	CLA	CHB-C4A-NA	2.27	127.65	124.51
23	b	601	CLA	O2A-CGA-CBA	2.27	119.02	111.91
31	A	420	LMT	O5'-C5'-C4'	2.27	114.53	109.75
23	C	507	CLA	C4C-C3C-C2C	-2.27	103.59	106.90
23	B	612	CLA	CHC-C1C-C2C	-2.27	120.45	126.72
23	C	510	CLA	C2A-C1A-CHA	-2.26	119.90	123.86
23	B	615	CLA	C2A-C1A-CHA	-2.26	119.90	123.86
23	a	404[B]	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
23	b	608	CLA	C4C-C3C-C2C	-2.26	103.60	106.90
23	C	512	CLA	O2A-CGA-CBA	2.26	119.01	111.91
23	C	509	CLA	C4-C3-C5	2.26	119.08	115.27
32	d	414[A]	LHG	O7-C7-O9	-2.26	118.24	123.70
25	c	514	BCR	C33-C5-C6	-2.26	121.99	124.53
23	D	402[A]	CLA	C4-C3-C5	2.26	119.07	115.27
32	d	407[A]	LHG	C6-C5-C4	-2.26	106.44	111.79
23	c	503	CLA	CHC-C1C-C2C	-2.26	120.47	126.72
23	c	505	CLA	CHD-C4C-NC	2.26	127.76	124.20
23	b	607	CLA	CBC-CAC-C3C	-2.26	106.21	112.43
32	b	629[A]	LHG	O8-C23-O10	-2.26	117.90	123.59
25	b	618	BCR	C37-C22-C23	2.26	121.63	118.08
24	a	414[A]	PHO	C4-C3-C2	-2.26	117.89	123.68
29	A	414[B]	PL9	C37-C36-C34	-2.26	105.56	112.98
24	A	407[B]	PHO	C1-C2-C3	-2.26	122.14	126.04
23	B	607	CLA	CED-O2D-CGD	2.26	121.04	115.94
23	D	403	CLA	CMA-C3A-C4A	-2.25	105.71	111.77
25	c	515	BCR	C16-C17-C18	-2.25	124.09	127.31
23	b	603	CLA	CBC-CAC-C3C	-2.25	106.22	112.43
23	B	604	CLA	C4-C3-C5	2.25	119.06	115.27
23	c	502	CLA	C4C-C3C-C2C	-2.25	103.62	106.90
35	c	518	DGD	O3G-C3G-C2G	-2.25	105.47	110.90
29	D	405[A]	PL9	C20-C19-C21	2.25	119.05	115.27
23	C	503	CLA	CBC-CAC-C3C	-2.25	106.23	112.43
24	A	416[A]	PHO	CMB-C2B-C3B	2.25	128.88	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	404	CLA	O2A-CGA-CBA	2.25	118.96	111.91
26	a	410	SQD	O5-C5-C4	2.25	113.78	109.69
32	d	414[B]	LHG	C5-O7-C7	-2.25	112.26	117.79
23	C	503	CLA	O2A-CGA-CBA	2.25	118.96	111.91
25	c	515	BCR	C11-C10-C9	-2.24	124.11	127.31
23	a	407	CLA	CBC-CAC-C3C	-2.24	106.25	112.43
23	c	505	CLA	CMA-C3A-C4A	-2.24	105.75	111.77
29	A	414[B]	PL9	C2-C3-C4	2.24	121.89	118.80
38	E	102	HEM	C4D-ND-C1D	2.24	107.39	105.07
24	a	414[A]	PHO	CED-O2D-CGD	2.24	121.00	115.94
26	f	102	SQD	O7-S-C6	2.24	109.60	106.94
23	B	606	CLA	CBC-CAC-C3C	-2.24	106.26	112.43
25	K	102	BCR	C2-C1-C6	2.24	113.93	110.48
23	D	402[B]	CLA	CHD-C4C-NC	2.24	127.73	124.20
23	B	609	CLA	C2A-C1A-CHA	-2.24	119.95	123.86
23	d	402[B]	CLA	CAA-CBA-CGA	2.24	119.79	113.25
32	d	414[B]	LHG	O7-C7-O9	-2.24	118.30	123.70
23	B	601	CLA	CMB-C2B-C3B	2.24	128.86	124.68
25	D	404	BCR	C21-C20-C19	-2.24	116.24	123.22
23	B	612	CLA	C4-C3-C5	2.24	119.03	115.27
23	b	608	CLA	CMA-C3A-C4A	-2.23	105.77	111.77
23	B	608	CLA	CMA-C3A-C2A	-2.23	104.82	113.83
25	c	515	BCR	C2-C1-C6	2.23	113.92	110.48
35	H	102	DGD	C3E-C4E-C5E	-2.23	106.25	110.24
23	C	502	CLA	C4-C3-C5	2.23	119.03	115.27
23	A	405[B]	CLA	CHB-C4A-NA	2.23	127.60	124.51
29	D	405[A]	PL9	C36-C37-C38	-2.23	104.54	111.88
23	b	604	CLA	O2A-CGA-CBA	2.23	118.91	111.91
23	C	513	CLA	C2A-C1A-CHA	-2.23	119.96	123.86
26	F	102	SQD	C46-C45-C44	-2.23	106.51	111.79
31	B	631	LMT	O5'-C5'-C4'	2.23	114.46	109.75
32	L	101[B]	LHG	O8-C23-O10	-2.23	117.96	123.59
23	d	402[B]	CLA	CMA-C3A-C2A	-2.23	104.84	113.83
31	M	101	LMT	C3B-C4B-C5B	-2.23	106.26	110.24
23	a	404[B]	CLA	CHB-C4A-NA	2.23	127.59	124.51
23	d	404	CLA	CMA-C3A-C2A	-2.23	104.84	113.83
26	a	409[B]	SQD	C3-C4-C5	2.23	114.21	110.24
23	c	504	CLA	C1-C2-C3	-2.23	122.19	126.04
25	c	514	BCR	C36-C18-C19	2.23	121.58	118.08
23	a	404[A]	CLA	C7-C6-C5	-2.22	107.32	113.36
26	f	102	SQD	O48-C23-O10	-2.22	117.98	123.59
23	d	403[A]	CLA	C1B-CHB-C4A	-2.22	125.72	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	410[A]	SQD	O8-S-C6	2.22	109.28	105.74
23	B	616	CLA	CMC-C2C-C1C	2.22	128.42	125.04
25	C	515	BCR	C16-C17-C18	-2.22	124.14	127.31
25	T	102	BCR	C39-C30-C25	-2.22	106.70	110.30
23	c	511	CLA	C11-C10-C8	-2.22	108.75	115.92
23	C	505	CLA	CHD-C4C-NC	2.22	127.70	124.20
23	A	405[A]	CLA	CHB-C4A-NA	2.22	127.58	124.51
23	C	513	CLA	CMA-C3A-C4A	-2.22	105.81	111.77
26	b	620	SQD	O48-C23-C24	2.22	118.87	111.91
23	B	605	CLA	O2A-CGA-CBA	2.22	118.86	111.91
23	B	601	CLA	CHB-C4A-NA	2.22	127.58	124.51
24	A	407[B]	PHO	C4-C3-C5	2.22	119.00	115.27
35	C	517[A]	DGD	C3G-C2G-C1G	-2.22	106.55	111.79
35	c	517[A]	DGD	O4E-C4E-C3E	-2.22	105.23	110.35
23	b	614	CLA	CMA-C3A-C2A	-2.21	104.90	113.83
23	c	504	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
23	B	604	CLA	O1D-CGD-CBD	-2.21	119.96	124.48
23	b	613	CLA	CMC-C2C-C1C	2.21	128.41	125.04
23	b	616	CLA	C1-C2-C3	-2.21	122.22	126.04
31	e	101	LMT	O1'-C1'-C2'	2.21	111.75	108.30
23	c	509	CLA	C2A-C1A-CHA	-2.21	120.00	123.86
31	B	630	LMT	C3B-C4B-C5B	-2.21	106.31	110.24
29	D	405[B]	PL9	C42-C41-C39	-2.20	105.72	112.98
23	D	403	CLA	CED-O2D-CGD	2.20	120.92	115.94
25	y	101	BCR	C34-C9-C10	-2.20	119.84	122.92
38	E	102	HEM	C3C-C4C-NC	-2.20	106.78	110.94
29	a	412[B]	PL9	C10-C9-C8	-2.20	118.03	123.68
24	A	407[A]	PHO	C1-C2-C3	-2.20	122.24	126.04
23	a	405[A]	CLA	CAC-C3C-C4C	2.20	127.67	124.81
23	C	506	CLA	CBC-CAC-C3C	-2.20	106.36	112.43
33	a	415	LMG	O8-C28-C29	2.20	118.81	111.91
33	d	412	LMG	O8-C28-C29	2.20	118.81	111.91
23	d	402[B]	CLA	C4-C3-C5	2.20	118.97	115.27
29	D	405[B]	PL9	C30-C29-C31	2.20	118.97	115.27
23	B	615	CLA	CHA-C1A-NA	-2.20	121.36	126.40
29	A	414[A]	PL9	C51-C49-C50	2.20	119.46	114.60
26	A	410[B]	SQD	O48-C23-O10	-2.20	118.05	123.59
29	d	406[B]	PL9	C51-C49-C50	2.20	119.45	114.60
23	b	604	CLA	CHD-C4C-NC	2.20	127.66	124.20
23	b	615	CLA	CHA-C1A-NA	-2.20	121.37	126.40
24	A	416[A]	PHO	O2A-CGA-CBA	2.20	118.80	111.91
23	b	613	CLA	C2A-C1A-CHA	-2.19	120.02	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	501	CLA	C2A-C1A-CHA	-2.19	120.02	123.86
35	H	102	DGD	O6E-C5E-C6E	2.19	111.89	106.44
31	b	621	LMT	C2'-C3'-C4'	2.19	114.69	109.68
23	C	510	CLA	C4-C3-C5	2.19	118.96	115.27
23	A	406[B]	CLA	CMC-C2C-C1C	2.19	128.38	125.04
23	B	613	CLA	C4-C3-C2	-2.19	118.06	123.68
35	C	519	DGD	O3G-C3G-C2G	-2.19	105.62	110.90
23	B	603	CLA	C7-C6-C5	-2.19	107.42	113.36
23	C	513	CLA	C4-C3-C2	-2.19	118.06	123.68
25	c	515	BCR	C33-C5-C6	-2.19	122.07	124.53
23	A	408	CLA	OBD-CAD-C3D	-2.19	123.26	128.52
23	c	503	CLA	C4-C3-C5	2.19	118.95	115.27
23	B	616	CLA	C4-C3-C2	-2.19	118.07	123.68
23	B	614	CLA	CAA-C2A-C3A	-2.19	106.79	112.78
23	D	402[A]	CLA	CED-O2D-CGD	2.19	120.88	115.94
26	a	409[A]	SQD	O9-S-O7	-2.18	106.39	113.95
25	K	102	BCR	C37-C22-C21	-2.18	119.87	122.92
25	k	101	BCR	C36-C18-C19	2.18	121.52	118.08
26	A	412	SQD	O48-C23-O10	-2.18	118.09	123.59
23	c	503	CLA	O2A-CGA-CBA	2.18	118.75	111.91
26	f	102	SQD	C44-O6-C1	-2.18	109.48	113.74
25	C	516	BCR	C3-C4-C5	-2.18	110.19	114.08
23	B	605	CLA	OBD-CAD-C3D	-2.18	123.28	128.52
29	d	406[A]	PL9	C51-C49-C50	2.18	119.42	114.60
23	d	403[A]	CLA	CAC-C3C-C4C	2.18	127.64	124.81
25	b	617	BCR	C8-C7-C6	-2.18	121.09	127.20
33	C	501	LMG	O8-C28-C29	2.18	118.74	111.91
35	c	517[A]	DGD	C2G-O2G-C1B	-2.18	112.43	117.79
25	K	102	BCR	C3-C4-C5	-2.18	110.19	114.08
23	B	608	CLA	C11-C10-C8	-2.17	108.89	115.92
38	E	102	HEM	CMD-C2D-C1D	2.17	128.35	125.04
23	B	610	CLA	CHB-C4A-NA	2.17	127.52	124.51
25	D	404	BCR	C31-C1-C6	-2.17	106.77	110.30
25	D	404	BCR	C15-C16-C17	-2.17	119.03	123.47
25	k	101	BCR	C10-C11-C12	-2.17	116.44	123.22
26	a	410	SQD	O8-S-C6	2.17	109.20	105.74
23	b	610	CLA	C4-C3-C2	-2.17	118.11	123.68
31	B	630	LMT	O5B-C5B-C4B	2.17	113.64	109.69
23	B	610	CLA	C4-C3-C5	2.17	118.92	115.27
23	b	611	CLA	CAC-C3C-C4C	2.17	127.62	124.81
24	a	406[A]	PHO	CBA-CAA-C2A	-2.17	107.47	113.81
32	A	419[A]	LHG	O4-P-O5	2.17	122.95	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	619	BCR	C34-C9-C10	-2.17	119.89	122.92
23	b	611	CLA	CBC-CAC-C3C	-2.17	106.46	112.43
23	a	405[B]	CLA	CMB-C2B-C3B	2.17	128.73	124.68
29	d	406[B]	PL9	C12-C13-C14	-2.17	122.44	127.66
23	A	408	CLA	C11-C12-C13	-2.17	108.92	115.92
23	B	602	CLA	C4-C3-C5	2.17	118.91	115.27
23	B	609	CLA	C16-C15-C13	-2.16	108.92	115.92
23	B	601	CLA	C2A-C1A-CHA	-2.16	120.08	123.86
24	A	416[B]	PHO	CMC-C2C-C3C	2.16	129.02	124.94
25	C	516	BCR	C39-C30-C25	-2.16	106.79	110.30
23	A	405[A]	CLA	C4C-C3C-C2C	-2.16	103.75	106.90
23	b	602	CLA	C11-C10-C8	-2.16	108.93	115.92
23	c	513	CLA	CMC-C2C-C1C	2.16	128.33	125.04
33	Z	101	LMG	C1-O6-C5	2.16	117.93	113.69
25	T	102	BCR	C1-C6-C7	2.16	121.89	115.78
24	a	414[B]	PHO	O1D-CGD-CBD	-2.16	121.14	124.74
23	d	404	CLA	CMB-C2B-C3B	2.16	128.72	124.68
23	b	611	CLA	CHB-C4A-NA	2.16	127.50	124.51
23	b	614	CLA	C4-C3-C5	2.16	118.90	115.27
23	B	610	CLA	CMC-C2C-C1C	2.16	128.33	125.04
26	A	410[A]	SQD	O9-S-O7	-2.16	106.48	113.95
23	c	508	CLA	C2A-C1A-CHA	-2.16	120.09	123.86
25	t	102	BCR	C7-C6-C5	-2.16	116.24	121.46
34	b	622	HTG	C6-C5-C4	-2.15	107.96	113.00
23	c	512	CLA	CMB-C2B-C3B	2.15	128.71	124.68
26	b	620	SQD	O5-C1-C2	-2.15	105.79	110.35
23	b	615	CLA	C2A-C1A-CHA	-2.15	120.10	123.86
23	C	513	CLA	CMB-C2B-C3B	2.15	128.70	124.68
35	C	518[A]	DGD	C2G-O2G-C1B	-2.15	112.50	117.79
23	C	514	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
23	b	608	CLA	C4-C3-C5	2.15	118.88	115.27
35	c	516[A]	DGD	O6D-C1D-O3G	-2.15	104.89	109.97
23	c	502	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
29	d	406[A]	PL9	C35-C34-C36	2.15	118.88	115.27
23	C	513	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
23	c	509	CLA	C4-C3-C2	-2.15	118.17	123.68
23	a	404[B]	CLA	C7-C6-C5	-2.15	107.53	113.36
23	b	609	CLA	C16-C15-C13	-2.14	108.99	115.92
29	a	412[B]	PL9	C51-C49-C50	2.14	119.34	114.60
25	B	617	BCR	C15-C14-C13	-2.14	124.25	127.31
25	T	102	BCR	C7-C8-C9	-2.14	123.00	126.23
23	C	502	CLA	C1-O2A-CGA	2.14	122.06	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	C	517[B]	DGD	O1G-C1A-O1A	-2.14	118.19	123.59
35	C	518[B]	DGD	O2G-C1B-O1B	-2.14	118.53	123.70
29	A	414[A]	PL9	C25-C24-C26	2.14	118.87	115.27
23	b	606	CLA	C2A-C1A-CHA	-2.14	120.12	123.86
23	b	603	CLA	CMC-C2C-C1C	2.14	128.30	125.04
33	C	520	LMG	O7-C10-O9	-2.14	118.53	123.70
25	t	102	BCR	C7-C8-C9	-2.14	123.00	126.23
25	B	617	BCR	C11-C10-C9	-2.14	124.26	127.31
23	C	506	CLA	CHA-C1A-NA	-2.14	121.50	126.40
23	d	404	CLA	CHB-C4A-NA	2.14	127.47	124.51
23	b	604	CLA	C4-C3-C5	2.14	118.86	115.27
23	C	502	CLA	OBD-CAD-C3D	-2.14	123.38	128.52
23	c	510	CLA	OBD-CAD-C3D	-2.14	123.38	128.52
24	A	407[A]	PHO	CBA-CAA-C2A	-2.14	107.57	113.81
29	D	405[B]	PL9	C47-C48-C49	-2.13	120.46	127.75
26	b	620	SQD	O9-S-C6	2.13	109.47	106.94
25	D	404	BCR	C29-C28-C27	-2.13	106.61	111.38
23	C	503	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
23	c	512	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
23	C	506	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
33	m	101	LMG	O8-C28-O10	-2.13	118.22	123.59
23	C	512	CLA	CBC-CAC-C3C	-2.13	106.57	112.43
35	C	517[A]	DGD	O1G-C1A-O1A	-2.13	118.22	123.59
23	C	511	CLA	C4-C3-C2	-2.13	118.22	123.68
35	c	517[A]	DGD	O1G-C1A-O1A	-2.13	118.23	123.59
24	A	407[B]	PHO	O2A-CGA-O1A	-2.13	118.23	123.59
23	A	406[B]	CLA	CAC-C3C-C4C	2.12	127.57	124.81
31	t	101	LMT	C1-O1'-C1'	2.12	117.36	113.84
24	a	414[A]	PHO	C1A-C2A-C3A	-2.12	100.82	102.84
35	C	517[A]	DGD	O6D-C1D-O3G	-2.12	104.95	109.97
23	A	405[A]	CLA	O2A-CGA-CBA	2.12	118.56	111.91
23	a	405[B]	CLA	CBC-CAC-C3C	-2.12	106.59	112.43
25	b	619	BCR	C28-C27-C26	-2.12	110.29	114.08
33	m	101	LMG	C3-C4-C5	2.12	114.02	110.24
25	h	101	BCR	C36-C18-C19	2.12	121.42	118.08
29	A	414[A]	PL9	C12-C13-C14	-2.12	122.56	127.66
34	B	622	HTG	O2-C2-C3	-2.12	105.45	110.35
23	B	608	CLA	C4-C3-C5	2.12	118.83	115.27
23	A	404[B]	CLA	CMA-C3A-C2A	-2.12	105.30	113.83
25	B	619	BCR	C34-C9-C8	2.11	121.41	118.08
34	B	623	HTG	C1-C2-C3	2.11	114.76	110.59
29	a	412[B]	PL9	C35-C34-C33	-2.11	118.26	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	609	CLA	C7-C6-C5	-2.11	107.62	113.36
23	c	506	CLA	CMB-C2B-C3B	2.11	128.63	124.68
34	C	522	HTG	C1-O5-C5	2.11	116.47	112.58
23	C	511	CLA	CMD-C2D-C3D	-2.11	122.76	127.61
33	a	415	LMG	O6-C5-C4	2.11	113.53	109.69
23	b	606	CLA	O2A-CGA-CBA	2.11	118.53	111.91
25	d	405	BCR	C29-C28-C27	-2.11	106.67	111.38
25	d	405	BCR	C38-C26-C27	2.11	117.67	113.62
26	b	620	SQD	O47-C7-O49	-2.11	118.61	123.70
23	b	605	CLA	CHB-C4A-NA	2.11	127.43	124.51
23	b	609	CLA	CHA-C1A-NA	-2.11	121.57	126.40
32	b	629[B]	LHG	O8-C23-O10	-2.11	118.28	123.59
25	t	102	BCR	C16-C15-C14	2.11	127.79	123.47
23	A	405[B]	CLA	CAC-C3C-C4C	2.11	127.54	124.81
24	A	416[A]	PHO	C6-C5-C3	-2.11	107.94	113.45
35	C	517[B]	DGD	C3G-C2G-C1G	-2.10	106.82	111.79
23	c	507	CLA	C2A-C1A-CHA	-2.10	120.18	123.86
23	a	407	CLA	OBD-CAD-C3D	-2.10	123.46	128.52
23	b	615	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
29	d	406[A]	PL9	C12-C13-C14	-2.10	122.60	127.66
23	b	616	CLA	C11-C12-C13	-2.10	109.13	115.92
32	b	629[A]	LHG	O7-C7-O9	-2.10	118.63	123.70
23	C	506	CLA	C11-C10-C8	-2.10	109.14	115.92
31	M	101	LMT	O5B-C5B-C6B	2.10	111.65	106.44
23	b	604	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
23	c	510	CLA	CED-O2D-CGD	2.10	120.68	115.94
32	d	408[B]	LHG	O8-C23-O10	-2.09	118.31	123.59
35	h	102	DGD	O4D-C4D-C3D	-2.09	105.51	110.35
23	b	606	CLA	OBD-CAD-C3D	-2.09	123.48	128.52
26	A	410[B]	SQD	O47-C7-O49	-2.09	118.64	123.70
32	E	101[A]	LHG	O7-C7-O9	-2.09	118.64	123.70
23	d	402[B]	CLA	C1-C2-C3	-2.09	122.42	126.04
23	b	601	CLA	CAA-C2A-C3A	-2.09	107.05	112.78
23	c	502	CLA	CAC-C3C-C4C	2.09	127.53	124.81
24	a	414[B]	PHO	O2A-CGA-CBA	2.09	118.47	111.91
23	A	408	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
23	B	607	CLA	OBD-CAD-C3D	-2.09	123.49	128.52
23	b	612	CLA	CMA-C3A-C2A	-2.09	105.40	113.83
25	c	515	BCR	C29-C30-C25	2.09	113.70	110.48
23	C	508	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
23	A	406[B]	CLA	CHB-C4A-NA	2.09	127.40	124.51
23	A	404[A]	CLA	C7-C6-C5	-2.09	107.69	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	414[B]	PHO	C7-C6-C5	-2.09	107.69	113.36
23	b	613	CLA	C16-C15-C13	-2.09	109.18	115.92
23	b	602	CLA	CAA-CBA-CGA	-2.09	107.16	113.25
23	d	403[A]	CLA	CHD-C4C-NC	2.08	127.49	124.20
33	z	101	LMG	C8-O7-C10	-2.08	112.67	117.79
23	B	615	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
27	O	303	GOL	C3-C2-C1	-2.08	103.61	111.70
23	C	508	CLA	CAC-C3C-C4C	2.08	127.51	124.81
25	h	101	BCR	C11-C10-C9	-2.08	124.34	127.31
23	b	602	CLA	CMA-C3A-C2A	-2.08	105.44	113.83
29	A	414[B]	PL9	C35-C34-C33	-2.08	118.35	123.68
23	A	405[B]	CLA	CMA-C3A-C2A	-2.08	105.45	113.83
23	b	610	CLA	CHB-C4A-NA	2.08	127.38	124.51
23	B	611	CLA	OBD-CAD-C3D	-2.08	123.53	128.52
34	B	623	HTG	O5-C1-C2	2.07	112.92	110.31
26	a	409[B]	SQD	O9-S-O7	-2.07	106.77	113.95
23	c	511	CLA	CMA-C3A-C4A	2.07	117.35	111.77
27	A	418	GOL	C3-C2-C1	-2.07	103.64	111.70
23	B	611	CLA	O2A-CGA-CBA	2.07	118.41	111.91
33	m	101	LMG	O1-C7-C8	-2.07	105.90	110.90
25	H	101	BCR	C33-C5-C6	-2.07	122.20	124.53
23	D	402[B]	CLA	CMB-C2B-C3B	2.07	128.55	124.68
23	C	502	CLA	C11-C12-C13	-2.07	109.23	115.92
23	b	601	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
23	B	606	CLA	OBD-CAD-C3D	-2.07	123.54	128.52
23	A	404[A]	CLA	C4-C3-C5	2.07	118.75	115.27
29	D	405[A]	PL9	C12-C13-C14	-2.07	122.68	127.66
23	D	402[B]	CLA	OBD-CAD-C3D	-2.07	123.54	128.52
33	D	411	LMG	O1-C1-C2	-2.07	105.07	108.30
23	b	607	CLA	CAA-CBA-CGA	2.07	119.30	113.25
35	H	102	DGD	O3G-C3G-C2G	-2.07	105.91	110.90
25	b	618	BCR	C33-C5-C6	-2.07	122.21	124.53
23	b	607	CLA	CMB-C2B-C3B	2.07	128.55	124.68
25	c	514	BCR	C37-C22-C23	2.07	121.33	118.08
25	D	404	BCR	C20-C21-C22	-2.07	124.36	127.31
23	c	512	CLA	CBC-CAC-C3C	-2.07	106.73	112.43
29	D	405[A]	PL9	C30-C29-C31	2.07	118.75	115.27
29	a	412[A]	PL9	C51-C49-C50	2.07	119.17	114.60
25	B	619	BCR	C10-C11-C12	-2.06	116.77	123.22
23	b	610	CLA	C2A-C1A-CHA	-2.06	120.25	123.86
29	D	405[A]	PL9	C25-C24-C23	-2.06	118.38	123.68
23	c	509	CLA	CBC-CAC-C3C	-2.06	106.74	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	614	CLA	CMA-C3A-C2A	-2.06	105.51	113.83
38	f	101	HEM	CMD-C2D-C1D	2.06	128.18	125.04
35	C	517[B]	DGD	O1G-C1A-C2A	2.06	118.38	111.91
23	b	616	CLA	CHA-C1A-NA	-2.06	121.68	126.40
24	a	414[B]	PHO	C4-C3-C2	-2.06	118.39	123.68
31	B	628	LMT	O1B-C4'-C5'	-2.06	103.81	109.45
23	b	607	CLA	C1-C2-C3	-2.06	122.49	126.04
32	E	101[B]	LHG	O7-C7-O9	-2.06	118.73	123.70
23	C	508	CLA	CHA-C1A-NA	-2.06	121.69	126.40
23	b	608	CLA	CMA-C3A-C2A	-2.06	105.54	113.83
24	a	406[B]	PHO	C4-C3-C5	2.06	118.73	115.27
32	L	101[B]	LHG	O4-P-O5	2.05	122.40	112.24
23	D	403	CLA	CMB-C2B-C1B	2.05	131.62	128.46
23	b	607	CLA	C1-O2A-CGA	2.05	121.83	116.44
35	C	517[A]	DGD	C3E-C4E-C5E	2.05	113.90	110.24
23	b	606	CLA	C1-O2A-CGA	2.05	121.83	116.44
23	A	406[A]	CLA	CMA-C3A-C4A	-2.05	106.26	111.77
23	A	404[A]	CLA	CHB-C4A-NA	2.05	127.34	124.51
23	B	613	CLA	C7-C6-C5	-2.05	107.80	113.36
25	K	102	BCR	C11-C10-C9	-2.05	124.39	127.31
23	b	605	CLA	OBD-CAD-C3D	-2.05	123.59	128.52
27	B	627	GOL	C3-C2-C1	-2.05	103.75	111.70
23	b	602	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
25	y	101	BCR	C11-C10-C9	-2.05	124.39	127.31
33	B	621	LMG	C12-C11-C10	-2.05	106.18	113.62
35	c	517[B]	DGD	O2G-C1B-O1B	-2.05	118.76	123.70
29	d	406[B]	PL9	C7-C3-C4	2.05	118.54	116.88
23	A	406[B]	CLA	C1-C2-C3	-2.04	122.51	126.04
23	b	609	CLA	CMA-C3A-C4A	-2.04	106.28	111.77
29	d	406[B]	PL9	C35-C34-C36	2.04	118.71	115.27
23	c	503	CLA	OBD-CAD-C3D	-2.04	123.60	128.52
32	D	407[A]	LHG	O4-P-O5	2.04	122.34	112.24
29	d	406[B]	PL9	C25-C24-C26	2.04	118.71	115.27
23	B	606	CLA	CAA-C2A-C3A	-2.04	107.18	112.78
24	A	407[A]	PHO	C4-C3-C5	2.04	118.70	115.27
25	a	408	BCR	C8-C7-C6	-2.04	121.47	127.20
25	c	514	BCR	C29-C30-C25	2.04	113.62	110.48
25	y	101	BCR	C1-C6-C7	2.04	121.55	115.78
25	D	404	BCR	C30-C25-C24	2.04	121.55	115.78
23	c	512	CLA	CMA-C3A-C4A	-2.04	106.29	111.77
23	B	612	CLA	CMA-C3A-C2A	-2.04	105.61	113.83
23	c	504	CLA	CBC-CAC-C3C	-2.04	106.81	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	607	CLA	CAA-CBA-CGA	2.04	119.21	113.25
23	d	402[B]	CLA	CED-O2D-CGD	2.04	120.55	115.94
23	C	508	CLA	CMC-C2C-C1C	2.04	128.14	125.04
23	c	511	CLA	C1-C2-C3	-2.04	122.52	126.04
23	b	613	CLA	CMA-C3A-C4A	-2.04	106.30	111.77
23	c	512	CLA	CHA-C1A-NA	-2.03	121.74	126.40
23	B	616	CLA	O1D-CGD-CBD	-2.03	120.32	124.48
27	B	624	GOL	C3-C2-C1	-2.03	103.81	111.70
25	T	102	BCR	C36-C18-C17	-2.03	120.08	122.92
23	C	513	CLA	CHB-C4A-NA	2.03	127.32	124.51
25	T	102	BCR	C7-C6-C5	-2.03	116.54	121.46
33	d	412	LMG	O8-C28-O10	-2.03	118.47	123.59
23	d	402[A]	CLA	CAC-C3C-C2C	2.03	131.00	127.53
26	a	409[A]	SQD	O48-C23-O10	-2.03	118.47	123.59
25	b	618	BCR	C29-C30-C25	2.03	113.60	110.48
23	A	408	CLA	CMA-C3A-C4A	-2.03	106.32	111.77
23	C	509	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
25	b	619	BCR	C16-C15-C14	-2.03	119.32	123.47
23	b	602	CLA	CHB-C4A-NA	2.03	127.32	124.51
23	c	511	CLA	C1-O2A-CGA	2.03	121.76	116.44
23	c	510	CLA	C2A-C1A-CHA	-2.03	120.32	123.86
29	d	406[A]	PL9	C45-C44-C46	2.03	118.68	115.27
25	y	101	BCR	C32-C1-C6	-2.03	107.01	110.30
23	b	609	CLA	CGD-CBD-CAD	-2.02	104.17	110.73
23	c	510	CLA	CAA-C2A-C3A	-2.02	107.23	112.78
23	c	506	CLA	C1-O2A-CGA	2.02	121.75	116.44
23	B	607	CLA	C11-C10-C8	-2.02	109.38	115.92
33	d	412	LMG	C7-O1-C1	-2.02	109.79	113.74
23	b	602	CLA	O2A-CGA-CBA	2.02	118.25	111.91
23	b	614	CLA	OBD-CAD-C3D	-2.02	123.65	128.52
23	b	614	CLA	CMB-C2B-C3B	2.02	128.46	124.68
35	c	516[B]	DGD	O3G-C3G-C2G	-2.02	106.02	110.90
24	a	414[A]	PHO	O2A-CGA-CBA	2.02	118.25	111.91
23	B	601	CLA	C4-C3-C5	2.02	118.67	115.27
23	c	504	CLA	C4-C3-C5	2.02	118.67	115.27
23	A	406[A]	CLA	CHB-C4A-NA	2.02	127.30	124.51
35	c	517[B]	DGD	O1G-C1A-O1A	-2.02	118.50	123.59
35	h	102	DGD	O3G-C1D-C2D	2.02	111.45	108.30
23	A	405[B]	CLA	O2A-CGA-CBA	2.02	118.24	111.91
34	b	625	HTG	C1-C2-C3	-2.02	106.61	110.59
23	B	602	CLA	CHB-C4A-NA	2.02	127.30	124.51
35	h	102	DGD	C3B-C2B-C1B	-2.02	106.29	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	619	BCR	C2-C1-C6	2.02	113.58	110.48
33	C	521	LMG	O1-C1-C2	2.02	111.45	108.30
24	A	416[A]	PHO	CED-O2D-CGD	2.01	120.49	115.94
25	C	516	BCR	C2-C1-C6	2.01	113.58	110.48
23	d	403[A]	CLA	CBC-CAC-C3C	-2.01	106.88	112.43
23	a	404[B]	CLA	CMA-C3A-C2A	-2.01	105.71	113.83
24	a	406[A]	PHO	O2D-CGD-O1D	-2.01	119.90	123.84
38	f	101	HEM	C3C-C4C-NC	-2.01	107.14	110.94
23	b	610	CLA	CMA-C3A-C2A	-2.01	105.71	113.83
23	b	605	CLA	C1-O2A-CGA	2.01	121.72	116.44
23	b	616	CLA	C2A-C1A-CHA	-2.01	120.34	123.86
23	B	603	CLA	C5-C3-C2	-2.01	117.05	121.12
23	b	615	CLA	C1-C2-C3	-2.01	122.56	126.04
37	D	401[A]	BCT	O2-C-O1	2.01	124.76	119.55
24	A	416[B]	PHO	CMA-C3A-C4A	-2.01	109.97	114.38
23	B	607	CLA	O2A-C1-C2	-2.01	103.35	108.64
23	D	402[A]	CLA	CBC-CAC-C3C	-2.01	106.89	112.43
37	d	401[A]	BCT	O2-C-O1	2.01	124.76	119.55
31	b	627	LMT	O1'-C1'-C2'	2.01	111.44	108.30
25	c	515	BCR	C20-C21-C22	-2.01	124.44	127.31
29	D	405[A]	PL9	O2-C1-C6	-2.01	117.11	120.59
23	C	504	CLA	CBC-CAC-C3C	-2.01	106.90	112.43
25	Y	101	BCR	C1-C6-C7	2.01	121.46	115.78
23	c	504	CLA	O2A-CGA-CBA	2.01	118.20	111.91
24	A	416[B]	PHO	CED-O2D-CGD	2.00	120.47	115.94
23	C	509	CLA	CMC-C2C-C1C	2.00	128.09	125.04
23	B	602	CLA	OBD-CAD-C3D	-2.00	123.70	128.52

All (69) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404[A]	CLA	ND
23	A	404[B]	CLA	ND
23	A	405[B]	CLA	ND
23	A	408	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND
23	B	604	CLA	ND
23	B	605	CLA	ND
23	B	606	CLA	ND
23	B	607	CLA	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
23	B	609	CLA	ND
23	B	610	CLA	ND
23	B	611	CLA	ND
23	B	612	CLA	ND
23	B	613	CLA	ND
23	B	614	CLA	ND
23	B	615	CLA	ND
23	B	616	CLA	ND
23	C	502	CLA	ND
23	C	505	CLA	ND
23	C	506	CLA	ND
23	C	507	CLA	ND
23	C	508	CLA	ND
23	C	509	CLA	ND
23	C	510	CLA	ND
23	C	511	CLA	ND
23	C	512	CLA	ND
23	C	513	CLA	ND
23	C	514	CLA	ND
23	D	402[A]	CLA	ND
23	D	402[B]	CLA	ND
23	D	403	CLA	ND
23	a	404[A]	CLA	ND
23	a	404[B]	CLA	ND
23	a	407	CLA	ND
23	b	601	CLA	ND
23	b	602	CLA	ND
23	b	603	CLA	ND
23	b	604	CLA	ND
23	b	605	CLA	ND
23	b	606	CLA	ND
23	b	607	CLA	ND
23	b	609	CLA	ND
23	b	610	CLA	ND
23	b	611	CLA	ND
23	b	612	CLA	ND
23	b	613	CLA	ND
23	b	614	CLA	ND
23	b	615	CLA	ND
23	b	616	CLA	ND
23	c	501	CLA	ND
23	c	502	CLA	ND

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Mol	Chain	Res	Type	Atom
23	c	503	CLA	ND
23	c	504	CLA	ND
23	c	505	CLA	ND
23	c	506	CLA	ND
23	c	507	CLA	ND
23	c	508	CLA	ND
23	c	509	CLA	ND
23	c	510	CLA	ND
23	c	511	CLA	ND
23	c	512	CLA	ND
23	c	513	CLA	ND
23	d	402[A]	CLA	ND
23	d	402[B]	CLA	ND
23	d	403[A]	CLA	ND
23	d	403[B]	CLA	ND
23	d	404	CLA	ND

All (1632) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	408	CLA	C4-C3-C5-C6
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	C	507	CLA	C14-C13-C15-C16
23	C	509	CLA	CHA-CBD-CGD-O1D
23	C	509	CLA	CHA-CBD-CGD-O2D
23	a	407	CLA	C4-C3-C5-C6
23	b	601	CLA	C11-C10-C8-C9
23	b	605	CLA	C2-C3-C5-C6
23	b	605	CLA	C4-C3-C5-C6
23	b	606	CLA	CHA-CBD-CGD-O1D
23	b	614	CLA	CHA-CBD-CGD-O1D
23	b	614	CLA	CHA-CBD-CGD-O2D
23	b	614	CLA	CAD-CBD-CGD-O1D
23	b	614	CLA	CAD-CBD-CGD-O2D
23	c	507	CLA	C4-C3-C5-C6
23	c	508	CLA	CHA-CBD-CGD-O1D
23	c	508	CLA	CHA-CBD-CGD-O2D
23	c	509	CLA	C2-C1-O2A-CGA
23	c	509	CLA	C11-C10-C8-C9
23	d	404	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	d	404	CLA	C4-C3-C5-C6
25	B	617	BCR	C1-C6-C7-C8
25	Y	101	BCR	C1-C6-C7-C8
25	Y	101	BCR	C5-C6-C7-C8
25	Y	101	BCR	C21-C22-C23-C24
25	Y	101	BCR	C37-C22-C23-C24
25	y	101	BCR	C1-C6-C7-C8
25	y	101	BCR	C5-C6-C7-C8
26	A	410[A]	SQD	O49-C7-O47-C45
26	A	410[B]	SQD	O49-C7-O47-C45
26	A	412	SQD	O6-C44-C45-O47
26	B	620	SQD	O49-C7-O47-C45
26	F	102	SQD	C2-C1-O6-C44
26	F	102	SQD	O49-C7-O47-C45
26	F	102	SQD	C8-C7-O47-C45
26	a	410	SQD	O6-C44-C45-O47
26	a	410	SQD	C5-C6-S-O7
26	a	410	SQD	C5-C6-S-O8
26	a	410	SQD	C5-C6-S-O9
26	b	620	SQD	C8-C7-O47-C45
26	f	102	SQD	O6-C44-C45-O47
26	f	102	SQD	O49-C7-O47-C45
26	f	102	SQD	C8-C7-O47-C45
27	A	411	GOL	O1-C1-C2-O2
27	A	411	GOL	O1-C1-C2-C3
27	B	624	GOL	C1-C2-C3-O3
27	B	629	GOL	O1-C1-C2-C3
27	D	412	GOL	C1-C2-C3-O3
27	V	203[A]	GOL	C1-C2-C3-O3
27	V	203[B]	GOL	C1-C2-C3-O3
27	b	624	GOL	C1-C2-C3-O3
27	c	526	GOL	C1-C2-C3-O3
27	o	302	GOL	C1-C2-C3-O3
27	o	303	GOL	C1-C2-C3-O3
29	A	414[A]	PL9	C9-C11-C12-C13
29	A	414[A]	PL9	C15-C14-C16-C17
29	A	414[A]	PL9	C14-C16-C17-C18
29	A	414[B]	PL9	C9-C11-C12-C13
29	A	414[B]	PL9	C15-C14-C16-C17
29	A	414[B]	PL9	C14-C16-C17-C18
29	a	412[A]	PL9	C9-C11-C12-C13
29	a	412[A]	PL9	C14-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
29	a	412[A]	PL9	C25-C24-C26-C27
29	a	412[B]	PL9	C9-C11-C12-C13
29	a	412[B]	PL9	C14-C16-C17-C18
31	A	417	LMT	C2'-C1'-O1'-C1
31	A	417	LMT	O5'-C1'-O1'-C1
31	A	420	LMT	O5'-C1'-O1'-C1
31	B	630	LMT	C2'-C1'-O1'-C1
31	B	631	LMT	O5'-C1'-O1'-C1
31	B	631	LMT	C2-C1-O1'-C1'
31	F	101	LMT	C2'-C1'-O1'-C1
31	F	101	LMT	O5'-C1'-O1'-C1
31	T	101	LMT	C2-C1-O1'-C1'
31	b	627	LMT	C2'-C1'-O1'-C1
31	b	627	LMT	O5'-C1'-O1'-C1
31	t	101	LMT	O5'-C1'-O1'-C1
31	t	101	LMT	C2-C1-O1'-C1'
32	D	406[A]	LHG	O2-C2-C3-O3
32	D	406[A]	LHG	C3-O3-P-O4
32	D	406[A]	LHG	C3-O3-P-O5
32	D	406[A]	LHG	C3-O3-P-O6
32	D	406[A]	LHG	C4-O6-P-O4
32	D	406[B]	LHG	C3-O3-P-O4
32	D	406[B]	LHG	C3-O3-P-O5
32	D	406[B]	LHG	C3-O3-P-O6
32	D	406[B]	LHG	C4-O6-P-O4
32	D	406[B]	LHG	C4-O6-P-O5
32	E	101[A]	LHG	C3-O3-P-O4
32	E	101[A]	LHG	C3-O3-P-O5
32	E	101[A]	LHG	O10-C23-O8-C6
32	E	101[A]	LHG	C24-C23-O8-C6
32	E	101[B]	LHG	C3-O3-P-O4
32	E	101[B]	LHG	C3-O3-P-O5
32	E	101[B]	LHG	O10-C23-O8-C6
32	E	101[B]	LHG	C24-C23-O8-C6
32	L	101[A]	LHG	C4-O6-P-O4
32	L	101[A]	LHG	C4-O6-P-O5
32	L	101[B]	LHG	C4-O6-P-O4
32	L	101[B]	LHG	C4-O6-P-O5
32	a	419[A]	LHG	C3-O3-P-O4
32	a	419[A]	LHG	C4-O6-P-O5
32	a	419[A]	LHG	O10-C23-O8-C6
32	a	419[A]	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
32	a	419[B]	LHG	C3-O3-P-O4
32	a	419[B]	LHG	C4-O6-P-O5
32	a	419[B]	LHG	O10-C23-O8-C6
32	a	419[B]	LHG	C24-C23-O8-C6
32	b	629[A]	LHG	C4-O6-P-O3
32	b	629[A]	LHG	C4-O6-P-O4
32	b	629[A]	LHG	C4-O6-P-O5
32	b	629[B]	LHG	C4-O6-P-O4
32	b	629[B]	LHG	C4-O6-P-O5
32	d	407[A]	LHG	C3-O3-P-O5
32	d	407[A]	LHG	C4-O6-P-O4
32	d	407[B]	LHG	C3-O3-P-O4
32	d	407[B]	LHG	C3-O3-P-O5
32	d	407[B]	LHG	C3-O3-P-O6
32	d	407[B]	LHG	C4-O6-P-O4
32	d	414[A]	LHG	C3-O3-P-O5
33	C	521	LMG	C11-C10-O7-C8
33	c	520	LMG	O9-C10-O7-C8
33	c	520	LMG	C11-C10-O7-C8
33	Z	101	LMG	O9-C10-O7-C8
33	Z	101	LMG	C11-C10-O7-C8
33	z	101	LMG	O6-C1-O1-C7
34	B	622	HTG	C2'-C1'-S1-C1
34	B	623	HTG	C2'-C1'-S1-C1
34	b	623	HTG	O5-C1-S1-C1'
31	A	420	LMT	O5B-C1B-O1B-C4'
31	B	630	LMT	C4'-C5'-C6'-O6'
26	b	620	SQD	O49-C7-O47-C45
23	D	403	CLA	C3-C5-C6-C7
23	c	512	CLA	C3-C5-C6-C7
23	d	404	CLA	C3-C5-C6-C7
31	m	103	LMT	C4B-C5B-C6B-O6B
26	A	410[A]	SQD	C8-C7-O47-C45
26	A	410[B]	SQD	C8-C7-O47-C45
26	B	620	SQD	C8-C7-O47-C45
23	C	505	CLA	C4-C3-C5-C6
23	D	403	CLA	C4-C3-C5-C6
29	A	414[B]	PL9	C30-C29-C31-C32
29	a	412[B]	PL9	C25-C24-C26-C27
23	A	408	CLA	C2-C3-C5-C6
23	a	407	CLA	C2-C3-C5-C6
29	A	414[A]	PL9	C18-C19-C21-C22

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Mol	Chain	Res	Type	Atoms
23	B	606	CLA	C2A-CAA-CBA-CGA
23	b	606	CLA	C2A-CAA-CBA-CGA
23	B	614	CLA	C3-C5-C6-C7
23	B	616	CLA	C3-C5-C6-C7
23	b	616	CLA	C3-C5-C6-C7
31	B	630	LMT	O5B-C5B-C6B-O6B
31	a	416	LMT	O5B-C5B-C6B-O6B
31	m	103	LMT	O5B-C5B-C6B-O6B
34	D	410	HTG	O5-C5-C6-O6
31	T	101	LMT	C4B-C5B-C6B-O6B
34	b	625	HTG	S1-C1'-C2'-C3'
31	F	101	LMT	O5'-C5'-C6'-O6'
33	C	521	LMG	O9-C10-O7-C8
31	B	628	LMT	C4'-C5'-C6'-O6'
25	T	102	BCR	C13-C14-C15-C16
31	T	101	LMT	O5'-C5'-C6'-O6'
23	C	502	CLA	CBD-CGD-O2D-CED
23	C	504	CLA	CBD-CGD-O2D-CED
23	c	510	CLA	CBD-CGD-O2D-CED
32	D	406[B]	LHG	O2-C2-C3-O3
32	E	101[A]	LHG	O2-C2-C3-O3
32	d	407[A]	LHG	O2-C2-C3-O3
32	d	407[B]	LHG	O2-C2-C3-O3
23	A	408	CLA	C3-C5-C6-C7
33	C	521	LMG	O6-C5-C6-O5
34	b	625	HTG	O5-C5-C6-O6
33	z	101	LMG	C11-C10-O7-C8
23	D	403	CLA	CBD-CGD-O2D-CED
33	c	520	LMG	C4-C5-C6-O5
31	B	628	LMT	C6-C7-C8-C9
35	C	519	DGD	C6B-C7B-C8B-C9B
31	B	628	LMT	O5'-C5'-C6'-O6'
34	D	410	HTG	S1-C1'-C2'-C3'
31	A	420	LMT	O5'-C5'-C6'-O6'
31	b	621	LMT	O5'-C5'-C6'-O6'
31	b	627	LMT	O5'-C5'-C6'-O6'
31	B	630	LMT	C4B-C5B-C6B-O6B
31	a	416	LMT	C4B-C5B-C6B-O6B
34	D	410	HTG	C4-C5-C6-O6
31	A	420	LMT	O5B-C5B-C6B-O6B
31	B	628	LMT	O5B-C5B-C6B-O6B
23	B	605	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	C	508	CLA	C4-C3-C5-C6
23	b	603	CLA	C4-C3-C5-C6
23	b	614	CLA	C4-C3-C5-C6
29	A	414[A]	PL9	C20-C19-C21-C22
29	A	414[B]	PL9	C20-C19-C21-C22
29	a	412[A]	PL9	C15-C14-C16-C17
29	a	412[A]	PL9	C30-C29-C31-C32
29	a	412[B]	PL9	C15-C14-C16-C17
29	a	412[B]	PL9	C30-C29-C31-C32
31	T	101	LMT	C4'-C5'-C6'-O6'
23	B	605	CLA	C2-C3-C5-C6
23	C	508	CLA	C2-C3-C5-C6
23	D	403	CLA	C2-C3-C5-C6
23	b	603	CLA	C2-C3-C5-C6
23	b	614	CLA	C2-C3-C5-C6
23	c	507	CLA	C2-C3-C5-C6
29	A	414[A]	PL9	C13-C14-C16-C17
29	A	414[B]	PL9	C13-C14-C16-C17
29	A	414[B]	PL9	C18-C19-C21-C22
29	a	412[A]	PL9	C13-C14-C16-C17
29	a	412[A]	PL9	C28-C29-C31-C32
29	a	412[B]	PL9	C13-C14-C16-C17
29	a	412[B]	PL9	C28-C29-C31-C32
31	B	630	LMT	O5'-C5'-C6'-O6'
31	B	631	LMT	O5'-C5'-C6'-O6'
31	T	101	LMT	O5B-C5B-C6B-O6B
31	F	101	LMT	C4'-C5'-C6'-O6'
26	B	620	SQD	O5-C1-O6-C44
31	e	101	LMT	O5'-C1'-O1'-C1
29	D	405[A]	PL9	C39-C41-C42-C43
31	e	101	LMT	C4'-C5'-C6'-O6'
34	b	622	HTG	S1-C1'-C2'-C3'
32	d	407[A]	LHG	C1-C2-C3-O3
33	c	520	LMG	O6-C5-C6-O5
23	c	509	CLA	CBA-CGA-O2A-C1
31	t	101	LMT	O5'-C5'-C6'-O6'
31	A	420	LMT	C4B-C5B-C6B-O6B
33	B	621	LMG	C39-C40-C41-C42
32	D	407[A]	LHG	C33-C34-C35-C36
26	F	102	SQD	C23-C24-C25-C26
31	A	420	LMT	C2'-C1'-O1'-C1
31	B	631	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
31	t	101	LMT	C2'-C1'-O1'-C1
23	C	505	CLA	C2-C3-C5-C6
29	a	412[A]	PL9	C23-C24-C26-C27
29	a	412[B]	PL9	C23-C24-C26-C27
23	B	613	CLA	C11-C12-C13-C14
23	C	503	CLA	C14-C13-C15-C16
23	b	604	CLA	C6-C7-C8-C9
23	b	616	CLA	C6-C7-C8-C9
23	c	504	CLA	C11-C12-C13-C14
25	b	619	BCR	C7-C8-C9-C34
25	d	405	BCR	C7-C8-C9-C34
25	b	619	BCR	C7-C8-C9-C10
31	e	101	LMT	O5B-C5B-C6B-O6B
31	b	621	LMT	C4'-C5'-C6'-O6'
31	b	627	LMT	C4'-C5'-C6'-O6'
23	b	601	CLA	C10-C11-C12-C13
23	c	512	CLA	C15-C16-C17-C18
31	B	628	LMT	C5'-C4'-O1B-C1B
23	a	407	CLA	CBA-CGA-O2A-C1
23	B	602	CLA	C13-C15-C16-C17
23	B	614	CLA	C8-C10-C11-C12
23	b	604	CLA	C8-C10-C11-C12
34	b	623	HTG	C1'-C2'-C3'-C4'
31	A	420	LMT	C5'-C4'-O1B-C1B
31	A	417	LMT	O5B-C5B-C6B-O6B
23	A	408	CLA	C5-C6-C7-C8
23	C	508	CLA	C5-C6-C7-C8
23	b	614	CLA	C8-C10-C11-C12
31	B	628	LMT	C4B-C5B-C6B-O6B
26	B	620	SQD	C30-C31-C32-C33
27	B	624	GOL	O2-C2-C3-O3
27	V	203[A]	GOL	O2-C2-C3-O3
35	c	517[B]	DGD	C1B-C2B-C3B-C4B
31	B	631	LMT	C4'-C5'-C6'-O6'
23	D	403	CLA	C10-C11-C12-C13
23	b	605	CLA	C8-C10-C11-C12
23	b	611	CLA	C15-C16-C17-C18
33	z	101	LMG	O9-C10-O7-C8
23	B	606	CLA	C10-C11-C12-C13
32	E	101[A]	LHG	C23-C24-C25-C26
33	Z	101	LMG	C10-C11-C12-C13
35	c	517[A]	DGD	C1B-C2B-C3B-C4B

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Mol	Chain	Res	Type	Atoms
31	A	420	LMT	O1'-C1-C2-C3
23	A	408	CLA	C12-C13-C15-C16
23	C	511	CLA	C11-C12-C13-C15
23	D	403	CLA	C11-C10-C8-C7
23	b	614	CLA	C12-C13-C15-C16
23	c	509	CLA	C3-C5-C6-C7
23	c	509	CLA	O1A-CGA-O2A-C1
35	C	519	DGD	C2B-C3B-C4B-C5B
33	d	412	LMG	C10-C11-C12-C13
23	B	601	CLA	C5-C6-C7-C8
23	B	601	CLA	C10-C11-C12-C13
23	b	606	CLA	C10-C11-C12-C13
31	A	420	LMT	C4'-C5'-C6'-O6'
23	c	512	CLA	CBD-CGD-O2D-CED
26	F	102	SQD	O5-C1-O6-C44
31	B	630	LMT	O5'-C1'-O1'-C1
31	b	621	LMT	O5'-C1'-O1'-C1
29	A	414[A]	PL9	C44-C46-C47-C48
29	A	414[B]	PL9	C44-C46-C47-C48
29	D	405[B]	PL9	C39-C41-C42-C43
29	d	406[A]	PL9	C39-C41-C42-C43
29	d	406[B]	PL9	C39-C41-C42-C43
26	B	620	SQD	C7-C8-C9-C10
34	B	625	HTG	S1-C1'-C2'-C3'
32	D	407[B]	LHG	C33-C34-C35-C36
23	B	615	CLA	C5-C6-C7-C8
23	C	513	CLA	C10-C11-C12-C13
23	b	604	CLA	C5-C6-C7-C8
23	c	513	CLA	C10-C11-C12-C13
23	a	407	CLA	O1A-CGA-O2A-C1
31	a	416	LMT	O1'-C1-C2-C3
23	B	614	CLA	C10-C11-C12-C13
23	C	503	CLA	C13-C15-C16-C17
23	b	606	CLA	C15-C16-C17-C18
33	c	519	LMG	C4-C5-C6-O5
33	B	621	LMG	C15-C16-C17-C18
23	C	509	CLA	C10-C11-C12-C13
23	a	404[A]	CLA	C15-C16-C17-C18
23	a	404[B]	CLA	C15-C16-C17-C18
32	D	406[B]	LHG	C4-O6-P-O3
32	E	101[A]	LHG	C3-O3-P-O6
32	E	101[A]	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
32	E	101[B]	LHG	C3-O3-P-O6
32	E	101[B]	LHG	C4-O6-P-O3
32	L	101[A]	LHG	C4-O6-P-O3
32	L	101[B]	LHG	C4-O6-P-O3
32	a	419[A]	LHG	C3-O3-P-O6
32	a	419[A]	LHG	C4-O6-P-O3
32	a	419[B]	LHG	C3-O3-P-O6
32	a	419[B]	LHG	C4-O6-P-O3
32	b	629[B]	LHG	C4-O6-P-O3
32	d	407[A]	LHG	C3-O3-P-O6
26	b	620	SQD	C31-C32-C33-C34
34	B	622	HTG	C1'-C2'-C3'-C4'
23	b	606	CLA	C13-C15-C16-C17
31	B	631	LMT	O1'-C1-C2-C3
34	d	411	HTG	S1-C1'-C2'-C3'
26	A	410[A]	SQD	C7-C8-C9-C10
32	E	101[B]	LHG	C23-C24-C25-C26
32	D	406[A]	LHG	C1-C2-C3-O3
32	D	406[B]	LHG	C1-C2-C3-O3
32	d	407[B]	LHG	C1-C2-C3-O3
34	B	625	HTG	O5-C5-C6-O6
31	a	416	LMT	C4'-C5'-C6'-O6'
31	A	417	LMT	O1'-C1-C2-C3
23	C	510	CLA	CBD-CGD-O2D-CED
23	a	407	CLA	C16-C17-C18-C19
23	c	509	CLA	C16-C17-C18-C20
26	A	410[A]	SQD	C15-C16-C17-C18
32	D	406[B]	LHG	C16-C17-C18-C19
32	L	101[A]	LHG	C12-C13-C14-C15
32	L	101[B]	LHG	C12-C13-C14-C15
33	C	521	LMG	C18-C19-C20-C21
26	F	102	SQD	C30-C31-C32-C33
31	A	420	LMT	C3-C4-C5-C6
32	L	101[A]	LHG	C17-C18-C19-C20
32	b	629[B]	LHG	C14-C15-C16-C17
32	d	407[B]	LHG	C34-C35-C36-C37
32	d	414[A]	LHG	C16-C17-C18-C19
33	B	621	LMG	C34-C35-C36-C37
33	D	411	LMG	C19-C20-C21-C22
35	c	516[B]	DGD	C2B-C3B-C4B-C5B
35	c	517[A]	DGD	CAA-CBA-CCA-CDA
23	d	404	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
26	A	410[B]	SQD	C15-C16-C17-C18
31	b	627	LMT	C7-C8-C9-C10
32	d	414[B]	LHG	C16-C17-C18-C19
33	a	415	LMG	C30-C31-C32-C33
34	b	622	HTG	C2'-C3'-C4'-C5'
35	c	517[A]	DGD	C9A-CAA-CBA-CCA
35	c	517[B]	DGD	C9A-CAA-CBA-CCA
35	c	517[B]	DGD	CAA-CBA-CCA-CDA
35	h	102	DGD	C6B-C7B-C8B-C9B
35	C	518[A]	DGD	CCB-CDB-CEB-CFB
35	H	102	DGD	C5B-C6B-C7B-C8B
31	e	101	LMT	O5'-C5'-C6'-O6'
33	a	415	LMG	C34-C35-C36-C37
35	C	518[B]	DGD	CCB-CDB-CEB-CFB
35	c	516[A]	DGD	C2B-C3B-C4B-C5B
32	E	101[B]	LHG	O2-C2-C3-O3
32	a	419[B]	LHG	C26-C27-C28-C29
34	B	623	HTG	C3'-C4'-C5'-C6'
35	C	517[A]	DGD	C4B-C5B-C6B-C7B
35	c	517[B]	DGD	CBA-CCA-CDA-CEA
31	b	621	LMT	C2'-C1'-O1'-C1
31	e	101	LMT	C2'-C1'-O1'-C1
35	C	518[A]	DGD	C2E-C1E-O5D-C6D
35	C	518[B]	DGD	C2E-C1E-O5D-C6D
32	D	407[B]	LHG	C32-C33-C34-C35
33	C	501	LMG	C17-C18-C19-C20
33	C	520	LMG	C16-C17-C18-C19
33	C	521	LMG	C17-C18-C19-C20
35	C	517[A]	DGD	C5B-C6B-C7B-C8B
35	c	516[A]	DGD	C9A-CAA-CBA-CCA
23	B	615	CLA	C16-C17-C18-C19
23	b	614	CLA	C16-C17-C18-C20
23	b	615	CLA	C16-C17-C18-C19
23	c	508	CLA	C16-C17-C18-C19
31	a	416	LMT	O5'-C5'-C6'-O6'
29	A	414[A]	PL9	C45-C44-C46-C47
29	A	414[B]	PL9	C45-C44-C46-C47
26	f	102	SQD	C32-C33-C34-C35
31	t	101	LMT	C4-C5-C6-C7
32	D	406[A]	LHG	C16-C17-C18-C19
32	a	419[A]	LHG	C26-C27-C28-C29
32	b	629[A]	LHG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
33	D	411	LMG	C35-C36-C37-C38
29	d	406[A]	PL9	C13-C14-C16-C17
23	a	405[A]	CLA	C11-C12-C13-C14
23	a	405[B]	CLA	C11-C12-C13-C14
23	b	614	CLA	C11-C12-C13-C14
23	c	502	CLA	C11-C12-C13-C14
23	c	504	CLA	C14-C13-C15-C16
23	c	513	CLA	C6-C7-C8-C9
35	C	517[B]	DGD	O6D-C5D-C6D-O5D
31	e	101	LMT	C4-C5-C6-C7
31	e	101	LMT	C5-C6-C7-C8
32	A	419[B]	LHG	C34-C35-C36-C37
32	D	407[A]	LHG	C32-C33-C34-C35
32	L	101[A]	LHG	C15-C16-C17-C18
23	b	610	CLA	C2A-CAA-CBA-CGA
34	b	625	HTG	C4-C5-C6-O6
26	b	620	SQD	C18-C19-C20-C21
32	A	419[B]	LHG	C12-C13-C14-C15
32	b	629[B]	LHG	C16-C17-C18-C19
32	d	414[A]	LHG	C32-C33-C34-C35
33	C	501	LMG	C12-C13-C14-C15
35	c	516[B]	DGD	C9A-CAA-CBA-CCA
35	c	517[A]	DGD	CBA-CCA-CDA-CEA
35	h	102	DGD	C9A-CAA-CBA-CCA
27	B	629	GOL	C1-C2-C3-O3
27	D	412	GOL	O1-C1-C2-C3
27	O	302	GOL	O1-C1-C2-C3
27	O	303	GOL	O1-C1-C2-C3
27	a	417	GOL	O1-C1-C2-C3
27	d	413	GOL	O1-C1-C2-C3
27	l	801[B]	GOL	O1-C1-C2-C3
27	v	202[B]	GOL	O1-C1-C2-C3
32	A	419[B]	LHG	O1-C1-C2-C3
33	B	621	LMG	O9-C10-O7-C8
23	b	611	CLA	C8-C10-C11-C12
33	B	621	LMG	C11-C10-O7-C8
32	L	101[A]	LHG	C25-C26-C27-C28
32	L	101[B]	LHG	C13-C14-C15-C16
32	L	101[B]	LHG	C25-C26-C27-C28
33	c	519	LMG	C10-C11-C12-C13
26	F	102	SQD	C29-C30-C31-C32
31	B	628	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	B	630	LMT	C2-C3-C4-C5
32	A	419[A]	LHG	C34-C35-C36-C37
32	L	101[B]	LHG	C15-C16-C17-C18
32	d	407[A]	LHG	C11-C10-C9-C8
33	C	501	LMG	C19-C20-C21-C22
33	C	521	LMG	C13-C14-C15-C16
33	C	521	LMG	C19-C20-C21-C22
33	D	411	LMG	C30-C31-C32-C33
33	m	101	LMG	C35-C36-C37-C38
35	c	518	DGD	CBB-CCB-CDB-CEB
23	B	603	CLA	C16-C17-C18-C19
23	B	603	CLA	C16-C17-C18-C20
23	a	407	CLA	C16-C17-C18-C20
23	b	602	CLA	C16-C17-C18-C19
23	b	602	CLA	C16-C17-C18-C20
23	c	509	CLA	C16-C17-C18-C19
35	C	518[B]	DGD	O6E-C1E-O5D-C6D
26	A	410[A]	SQD	C12-C13-C14-C15
35	C	517[B]	DGD	C4B-C5B-C6B-C7B
35	C	517[B]	DGD	C5B-C6B-C7B-C8B
34	b	622	HTG	O5-C5-C6-O6
31	b	627	LMT	C3-C4-C5-C6
32	L	101[A]	LHG	C13-C14-C15-C16
32	d	407[A]	LHG	C34-C35-C36-C37
32	d	408[B]	LHG	C27-C28-C29-C30
32	d	408[A]	LHG	C27-C28-C29-C30
33	c	519	LMG	C31-C32-C33-C34
33	m	101	LMG	C39-C40-C41-C42
31	B	630	LMT	C5-C6-C7-C8
31	B	631	LMT	C11-C10-C9-C8
33	C	501	LMG	C36-C37-C38-C39
23	B	602	CLA	C15-C16-C17-C18
23	C	507	CLA	C5-C6-C7-C8
23	C	511	CLA	C10-C11-C12-C13
31	A	420	LMT	C2-C1-O1'-C1'
31	B	628	LMT	C2-C1-O1'-C1'
31	b	627	LMT	C2-C1-O1'-C1'
33	c	519	LMG	C34-C35-C36-C37
26	F	102	SQD	C24-C25-C26-C27
26	a	410	SQD	C31-C32-C33-C34
32	A	419[A]	LHG	C12-C13-C14-C15
32	b	629[A]	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
33	m	101	LMG	C38-C39-C40-C41
23	C	504	CLA	O1D-CGD-O2D-CED
23	c	510	CLA	O1D-CGD-O2D-CED
31	A	420	LMT	C1-C2-C3-C4
31	B	631	LMT	C3-C4-C5-C6
32	E	101[A]	LHG	C24-C25-C26-C27
33	D	411	LMG	C12-C13-C14-C15
35	H	102	DGD	CCB-CDB-CEB-CFB
35	h	102	DGD	C2B-C3B-C4B-C5B
35	c	516[A]	DGD	O6D-C5D-C6D-O5D
35	c	516[B]	DGD	O6D-C5D-C6D-O5D
31	a	416	LMT	C1-C2-C3-C4
23	C	511	CLA	C4-C3-C5-C6
23	c	505	CLA	C4-C3-C5-C6
29	d	406[A]	PL9	C15-C14-C16-C17
29	d	406[B]	PL9	C15-C14-C16-C17
35	c	516[A]	DGD	C2A-C1A-O1G-C1G
23	C	506	CLA	C2-C3-C5-C6
23	c	505	CLA	C2-C3-C5-C6
24	a	406[B]	PHO	C2-C3-C5-C6
29	A	414[A]	PL9	C12-C11-C9-C8
29	A	414[A]	PL9	C43-C44-C46-C47
29	A	414[B]	PL9	C12-C11-C9-C8
29	A	414[B]	PL9	C28-C29-C31-C32
29	D	405[A]	PL9	C13-C14-C16-C17
29	D	405[B]	PL9	C13-C14-C16-C17
33	m	101	LMG	C11-C10-O7-C8
31	M	101	LMT	C3-C4-C5-C6
33	B	621	LMG	C17-C18-C19-C20
35	h	102	DGD	C7B-C8B-C9B-CAB
27	B	629	GOL	O1-C1-C2-O2
27	D	412	GOL	O1-C1-C2-O2
27	D	412	GOL	O2-C2-C3-O3
27	O	302	GOL	O1-C1-C2-O2
27	V	203[B]	GOL	O2-C2-C3-O3
27	b	624	GOL	O2-C2-C3-O3
27	c	526	GOL	O2-C2-C3-O3
27	o	302	GOL	O2-C2-C3-O3
27	v	202[B]	GOL	O1-C1-C2-O2
23	c	506	CLA	C15-C16-C17-C18
31	t	101	LMT	O1'-C1-C2-C3
32	L	101[B]	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
35	c	516[B]	DGD	C5A-C6A-C7A-C8A
35	c	517[A]	DGD	CBB-CCB-CDB-CEB
23	B	615	CLA	C16-C17-C18-C20
23	b	606	CLA	C16-C17-C18-C20
23	c	508	CLA	C16-C17-C18-C20
23	d	403[B]	CLA	C16-C17-C18-C20
23	d	404	CLA	C16-C17-C18-C19
32	D	407[A]	LHG	C15-C16-C17-C18
33	d	412	LMG	C29-C30-C31-C32
35	c	516[A]	DGD	C5A-C6A-C7A-C8A
23	C	510	CLA	C3-C5-C6-C7
26	f	102	SQD	C25-C26-C27-C28
33	c	519	LMG	C33-C34-C35-C36
26	A	410[B]	SQD	C7-C8-C9-C10
31	b	627	LMT	C5-C6-C7-C8
35	c	516[A]	DGD	CAA-CBA-CCA-CDA
33	m	101	LMG	O9-C10-O7-C8
31	b	621	LMT	C3'-C4'-O1B-C1B
23	C	510	CLA	C2-C1-O2A-CGA
23	b	601	CLA	C2-C1-O2A-CGA
26	b	620	SQD	C27-C28-C29-C30
32	b	629[B]	LHG	C12-C13-C14-C15
32	d	414[A]	LHG	C29-C30-C31-C32
34	b	622	HTG	C3'-C4'-C5'-C6'
23	A	404[B]	CLA	C13-C15-C16-C17
23	B	614	CLA	C5-C6-C7-C8
26	b	620	SQD	C13-C14-C15-C16
35	c	516[A]	DGD	C7A-C8A-C9A-CAA
35	c	517[B]	DGD	C2B-C3B-C4B-C5B
25	B	617	BCR	C5-C6-C7-C8
25	b	617	BCR	C1-C6-C7-C8
25	b	617	BCR	C5-C6-C7-C8
26	B	620	SQD	C11-C10-C9-C8
31	B	631	LMT	C4-C5-C6-C7
35	c	516[B]	DGD	C2A-C1A-O1G-C1G
23	B	603	CLA	C13-C15-C16-C17
26	A	412	SQD	C26-C27-C28-C29
32	E	101[B]	LHG	C24-C25-C26-C27
35	C	517[B]	DGD	C9A-CAA-CBA-CCA
35	H	102	DGD	C9B-CAB-CBB-CCB
35	c	517[A]	DGD	C6A-C7A-C8A-C9A
35	c	516[B]	DGD	CAA-CBA-CCA-CDA

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Mol	Chain	Res	Type	Atoms
23	C	503	CLA	C15-C16-C17-C18
26	A	412	SQD	C17-C18-C19-C20
32	d	414[B]	LHG	C32-C33-C34-C35
23	C	506	CLA	C4-C3-C5-C6
24	a	406[B]	PHO	C4-C3-C5-C6
29	A	414[A]	PL9	C30-C29-C31-C32
29	D	405[A]	PL9	C15-C14-C16-C17
23	B	606	CLA	C11-C10-C8-C7
23	B	613	CLA	C11-C12-C13-C15
23	B	614	CLA	C11-C10-C8-C7
23	C	511	CLA	C2-C3-C5-C6
23	a	405[A]	CLA	C11-C12-C13-C15
23	a	405[B]	CLA	C11-C12-C13-C15
23	b	606	CLA	C11-C10-C8-C7
23	b	606	CLA	C12-C13-C15-C16
23	c	502	CLA	C11-C12-C13-C15
23	c	504	CLA	C12-C13-C15-C16
29	d	406[B]	PL9	C13-C14-C16-C17
23	B	607	CLA	C3-C5-C6-C7
31	B	628	LMT	C3'-C4'-O1B-C1B
33	C	501	LMG	C10-C11-C12-C13
33	a	415	LMG	C10-C11-C12-C13
23	c	512	CLA	CBA-CGA-O2A-C1
32	D	407[A]	LHG	C29-C30-C31-C32
23	B	610	CLA	C2A-CAA-CBA-CGA
31	A	420	LMT	C3'-C4'-O1B-C1B
32	D	406[A]	LHG	C13-C14-C15-C16
31	B	630	LMT	C6-C7-C8-C9
23	B	601	CLA	C15-C16-C17-C18
35	C	517[A]	DGD	C8A-C9A-CAA-CBA
35	c	516[A]	DGD	O1A-C1A-O1G-C1G
35	C	517[B]	DGD	C4D-C5D-C6D-O5D
31	t	101	LMT	C4'-C5'-C6'-O6'
35	C	518[A]	DGD	O6E-C1E-O5D-C6D
35	c	517[B]	DGD	O6E-C1E-O5D-C6D
26	A	412	SQD	C27-C28-C29-C30
26	a	409[A]	SQD	C9-C10-C11-C12
26	a	410	SQD	C25-C26-C27-C28
33	C	520	LMG	C17-C18-C19-C20
26	A	410[B]	SQD	C11-C10-C9-C8
35	C	517[B]	DGD	C8A-C9A-CAA-CBA
33	Z	101	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
26	A	410[A]	SQD	O6-C44-C45-O47
26	A	410[B]	SQD	O6-C44-C45-O47
33	m	101	LMG	C37-C38-C39-C40
23	b	614	CLA	C16-C17-C18-C19
26	B	620	SQD	C34-C35-C36-C37
26	a	409[B]	SQD	C12-C13-C14-C15
32	D	407[B]	LHG	C17-C18-C19-C20
33	z	101	LMG	C19-C20-C21-C22
35	C	517[A]	DGD	C9A-CAA-CBA-CCA
35	c	517[A]	DGD	C2B-C3B-C4B-C5B
23	B	608	CLA	C13-C15-C16-C17
29	D	405[B]	PL9	C15-C14-C16-C17
35	c	517[B]	DGD	C6A-C7A-C8A-C9A
23	B	602	CLA	C11-C12-C13-C14
23	B	606	CLA	C11-C10-C8-C9
23	D	403	CLA	C11-C10-C8-C9
23	D	403	CLA	C14-C13-C15-C16
23	b	606	CLA	C11-C10-C8-C9
35	C	517[A]	DGD	O6E-C5E-C6E-O5E
26	b	620	SQD	C26-C27-C28-C29
31	m	103	LMT	C7-C8-C9-C10
32	b	629[A]	LHG	C13-C14-C15-C16
32	D	407[B]	LHG	C15-C16-C17-C18
33	a	415	LMG	C21-C22-C23-C24
25	y	101	BCR	C37-C22-C23-C24
23	C	502	CLA	O1D-CGD-O2D-CED
23	A	406[B]	CLA	C13-C15-C16-C17
32	d	408[B]	LHG	C29-C30-C31-C32
33	a	415	LMG	C35-C36-C37-C38
31	B	628	LMT	C1-C2-C3-C4
35	c	516[B]	DGD	O1A-C1A-O1G-C1G
23	A	405[A]	CLA	C1A-C2A-CAA-CBA
23	B	611	CLA	C1A-C2A-CAA-CBA
34	b	623	HTG	O5-C5-C6-O6
23	B	610	CLA	C16-C17-C18-C20
23	b	615	CLA	C16-C17-C18-C20
23	d	403[B]	CLA	C16-C17-C18-C19
32	D	407[A]	LHG	C17-C18-C19-C20
35	c	517[B]	DGD	C4A-C5A-C6A-C7A
23	D	403	CLA	O1D-CGD-O2D-CED
23	A	406[A]	CLA	C13-C15-C16-C17
23	b	601	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
23	b	614	CLA	C10-C11-C12-C13
32	d	407[B]	LHG	C4-O6-P-O3
33	d	412	LMG	O6-C5-C6-O5
23	b	607	CLA	C3-C5-C6-C7
31	T	101	LMT	C7-C8-C9-C10
33	z	101	LMG	C10-C11-C12-C13
23	d	402[B]	CLA	C2C-C3C-CAC-CBC
32	b	629[B]	LHG	C27-C28-C29-C30
32	d	414[B]	LHG	C24-C25-C26-C27
31	e	101	LMT	C1-C2-C3-C4
23	A	404[A]	CLA	C13-C15-C16-C17
23	d	403[A]	CLA	C16-C17-C18-C20
26	b	620	SQD	C14-C15-C16-C17
32	d	408[A]	LHG	C25-C26-C27-C28
35	h	102	DGD	C3B-C4B-C5B-C6B
23	C	512	CLA	C8-C10-C11-C12
26	A	410[B]	SQD	C12-C13-C14-C15
32	d	414[B]	LHG	C29-C30-C31-C32
33	C	501	LMG	C13-C14-C15-C16
29	a	412[B]	PL9	C12-C11-C9-C10
23	c	511	CLA	C8-C10-C11-C12
31	A	420	LMT	C4-C5-C6-C7
32	d	408[B]	LHG	C25-C26-C27-C28
35	c	517[A]	DGD	C4A-C5A-C6A-C7A
23	B	610	CLA	C16-C17-C18-C19
26	A	410[A]	SQD	O6-C44-C45-C46
26	A	410[B]	SQD	O6-C44-C45-C46
26	A	412	SQD	O6-C44-C45-C46
26	B	620	SQD	C44-C45-C46-O48
26	a	409[A]	SQD	O6-C44-C45-C46
26	b	620	SQD	C44-C45-C46-O48
26	f	102	SQD	O6-C44-C45-C46
26	f	102	SQD	C44-C45-C46-O48
32	E	101[B]	LHG	C4-C5-C6-O8
33	a	415	LMG	C7-C8-C9-O8
31	b	621	LMT	C11-C10-C9-C8
32	E	101[A]	LHG	C25-C26-C27-C28
35	C	518[B]	DGD	CDA-CEA-CFA-CGA
35	h	102	DGD	CAA-CBA-CCA-CDA
23	c	512	CLA	O1A-CGA-O2A-C1
35	C	518[A]	DGD	C2G-C3G-O3G-C1D
35	C	518[A]	DGD	C5D-C6D-O5D-C1E

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Mol	Chain	Res	Type	Atoms
35	C	518[B]	DGD	C2G-C3G-O3G-C1D
35	c	517[A]	DGD	C2G-C3G-O3G-C1D
35	c	517[A]	DGD	C5D-C6D-O5D-C1E
35	c	517[B]	DGD	C5D-C6D-O5D-C1E
35	C	518[A]	DGD	CDA-CEA-CFA-CGA
31	b	627	LMT	C1-C2-C3-C4
32	D	406[B]	LHG	C12-C13-C14-C15
33	C	520	LMG	C36-C37-C38-C39
33	D	411	LMG	C36-C37-C38-C39
35	c	516[A]	DGD	C4D-C5D-C6D-O5D
35	c	516[B]	DGD	C4D-C5D-C6D-O5D
31	a	416	LMT	C9-C10-C11-C12
33	a	415	LMG	C29-C30-C31-C32
35	C	517[A]	DGD	C3B-C4B-C5B-C6B
23	b	604	CLA	C15-C16-C17-C18
32	E	101[B]	LHG	C25-C26-C27-C28
35	h	102	DGD	CAB-CBB-CCB-CDB
27	B	629	GOL	O2-C2-C3-O3
27	d	413	GOL	O1-C1-C2-O2
27	o	303	GOL	O2-C2-C3-O3
31	a	416	LMT	C2-C3-C4-C5
35	c	518	DGD	CBA-CCA-CDA-CEA
23	C	507	CLA	C15-C16-C17-C18
32	d	414[B]	LHG	C25-C26-C27-C28
34	B	622	HTG	C2'-C3'-C4'-C5'
35	C	519	DGD	CAA-CBA-CCA-CDA
23	A	405[A]	CLA	C15-C16-C17-C18
23	b	610	CLA	C15-C16-C17-C18
33	D	411	LMG	O6-C5-C6-O5
35	C	517[B]	DGD	O6E-C5E-C6E-O5E
35	c	516[A]	DGD	O6E-C5E-C6E-O5E
29	a	412[A]	PL9	C12-C11-C9-C10
35	C	518[B]	DGD	C5B-C6B-C7B-C8B
23	B	612	CLA	C10-C11-C12-C13
23	c	512	CLA	C10-C11-C12-C13
23	d	402[A]	CLA	C2C-C3C-CAC-CBC
32	d	414[A]	LHG	C33-C34-C35-C36
26	b	620	SQD	C46-C45-O47-C7
35	c	516[B]	DGD	O6E-C5E-C6E-O5E
23	B	601	CLA	C2A-CAA-CBA-CGA
23	B	616	CLA	C2-C1-O2A-CGA
26	a	409[B]	SQD	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
32	d	408[A]	LHG	C34-C35-C36-C37
35	H	102	DGD	C7A-C8A-C9A-CAA
26	a	409[A]	SQD	C12-C13-C14-C15
32	D	406[A]	LHG	C12-C13-C14-C15
23	b	601	CLA	C13-C15-C16-C17
33	C	520	LMG	C37-C38-C39-C40
23	C	513	CLA	CBA-CGA-O2A-C1
26	b	620	SQD	C24-C23-O48-C46
32	D	407[B]	LHG	C29-C30-C31-C32
33	d	412	LMG	C35-C36-C37-C38
32	D	406[B]	LHG	C10-C11-C12-C13
35	h	102	DGD	C9B-CAB-CBB-CCB
26	A	412	SQD	C2-C1-O6-C44
35	c	517[B]	DGD	C2E-C1E-O5D-C6D
31	t	101	LMT	C7-C8-C9-C10
32	d	408[B]	LHG	C28-C29-C30-C31
35	h	102	DGD	CBA-CCA-CDA-CEA
35	C	517[A]	DGD	O6D-C5D-C6D-O5D
23	d	403[A]	CLA	C16-C17-C18-C19
32	D	407[B]	LHG	C13-C14-C15-C16
32	d	408[A]	LHG	C29-C30-C31-C32
35	h	102	DGD	CDB-CEB-CFB-CGB
23	A	406[A]	CLA	C12-C13-C15-C16
23	A	406[B]	CLA	C12-C13-C15-C16
23	B	602	CLA	C11-C12-C13-C15
23	B	613	CLA	C11-C10-C8-C7
23	B	614	CLA	C12-C13-C15-C16
23	C	503	CLA	C12-C13-C15-C16
23	C	505	CLA	C12-C13-C15-C16
23	C	514	CLA	C11-C10-C8-C7
23	C	514	CLA	C11-C12-C13-C15
23	D	403	CLA	C12-C13-C15-C16
23	b	601	CLA	C11-C10-C8-C7
23	c	504	CLA	C11-C12-C13-C15
23	c	505	CLA	C11-C12-C13-C15
23	c	506	CLA	C11-C10-C8-C7
23	c	510	CLA	C11-C10-C8-C7
23	c	512	CLA	C12-C13-C15-C16
31	a	416	LMT	C3-C4-C5-C6
33	C	501	LMG	C18-C19-C20-C21
33	C	520	LMG	C34-C35-C36-C37
23	B	602	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	B	614	CLA	C14-C13-C15-C16
23	C	505	CLA	C14-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C14
23	C	514	CLA	C6-C7-C8-C9
23	C	514	CLA	C11-C10-C8-C9
23	a	405[B]	CLA	C6-C7-C8-C9
23	c	505	CLA	C11-C12-C13-C14
23	b	613	CLA	CBD-CGD-O2D-CED
32	d	408[A]	LHG	C28-C29-C30-C31
23	C	511	CLA	CBA-CGA-O2A-C1
32	D	407[B]	LHG	C24-C23-O8-C6
27	B	627	GOL	C1-C2-C3-O3
25	y	101	BCR	C21-C22-C23-C24
26	b	620	SQD	C28-C29-C30-C31
23	c	512	CLA	C13-C15-C16-C17
32	b	629[A]	LHG	C27-C28-C29-C30
33	m	101	LMG	C14-C15-C16-C17
35	C	517[B]	DGD	CCA-CDA-CEA-CFA
23	A	405[B]	CLA	C15-C16-C17-C18
23	B	613	CLA	C13-C15-C16-C17
23	C	514	CLA	CBD-CGD-O2D-CED
23	c	501	CLA	CBD-CGD-O2D-CED
33	C	501	LMG	C11-C12-C13-C14
33	C	521	LMG	C35-C36-C37-C38
35	C	518[A]	DGD	C5B-C6B-C7B-C8B
32	E	101[A]	LHG	O6-C4-C5-C6
32	b	629[A]	LHG	O6-C4-C5-C6
32	D	406[A]	LHG	C10-C11-C12-C13
32	D	407[A]	LHG	C13-C14-C15-C16
32	d	408[A]	LHG	C9-C10-C11-C12
35	C	518[B]	DGD	C1A-C2A-C3A-C4A
26	a	410	SQD	C16-C17-C18-C19
34	b	623	HTG	S1-C1'-C2'-C3'
29	d	406[A]	PL9	C45-C44-C46-C47
23	b	609	CLA	C2-C3-C5-C6
23	C	511	CLA	O1A-CGA-O2A-C1
32	A	419[A]	LHG	C26-C27-C28-C29
32	d	407[A]	LHG	C13-C14-C15-C16
32	L	101[B]	LHG	C24-C25-C26-C27
31	e	101	LMT	C4B-C5B-C6B-O6B
33	c	519	LMG	C28-C29-C30-C31
26	F	102	SQD	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
35	C	517[A]	DGD	C7A-C8A-C9A-CAA
23	c	513	CLA	CBD-CGD-O2D-CED
23	c	506	CLA	C3A-C2A-CAA-CBA
31	M	101	LMT	O1'-C1-C2-C3
31	F	101	LMT	C2-C1-O1'-C1'
31	m	103	LMT	C2-C1-O1'-C1'
34	c	521	HTG	C4'-C5'-C6'-C7'
35	C	519	DGD	CDB-CEB-CFB-CGB
23	B	601	CLA	CBA-CGA-O2A-C1
33	B	621	LMG	C32-C33-C34-C35
35	c	517[A]	DGD	CDA-CEA-CFA-CGA
32	a	419[A]	LHG	C4-C5-C6-O8
32	a	419[B]	LHG	C4-C5-C6-O8
32	L	101[A]	LHG	C24-C25-C26-C27
32	a	419[A]	LHG	C10-C11-C12-C13
32	b	629[A]	LHG	C12-C13-C14-C15
35	H	102	DGD	CCA-CDA-CEA-CFA
24	a	406[A]	PHO	O2A-C1-C2-C3
31	M	101	LMT	O5'-C5'-C6'-O6'
35	C	517[B]	DGD	C7A-C8A-C9A-CAA
23	c	512	CLA	O1D-CGD-O2D-CED
33	Z	101	LMG	C19-C20-C21-C22
35	c	516[B]	DGD	C7A-C8A-C9A-CAA
35	c	517[A]	DGD	C5A-C6A-C7A-C8A
23	c	513	CLA	C4-C3-C5-C6
24	a	406[A]	PHO	C4-C3-C5-C6
23	B	608	CLA	C16-C17-C18-C20
29	D	405[A]	PL9	C43-C44-C46-C47
32	L	101[A]	LHG	C11-C12-C13-C14
32	d	414[B]	LHG	C33-C34-C35-C36
31	F	101	LMT	C4-C5-C6-C7
32	a	419[A]	LHG	C7-C8-C9-C10
32	a	419[B]	LHG	C23-C24-C25-C26
23	C	513	CLA	O1A-CGA-O2A-C1
31	b	621	LMT	C3-C4-C5-C6
33	C	501	LMG	C29-C30-C31-C32
32	E	101[A]	LHG	O6-C4-C5-O7
23	b	601	CLA	CBA-CGA-O2A-C1
33	c	520	LMG	C29-C28-O8-C9
35	C	519	DGD	C8A-C9A-CAA-CBA
26	b	620	SQD	O10-C23-O48-C46
23	A	406[A]	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
32	b	629[A]	LHG	C31-C32-C33-C34
33	B	621	LMG	O8-C28-C29-C30
32	d	408[B]	LHG	C9-C10-C11-C12
35	c	517[B]	DGD	C5A-C6A-C7A-C8A
32	D	407[B]	LHG	O10-C23-O8-C6
26	a	409[A]	SQD	C34-C35-C36-C37
35	c	518	DGD	C2B-C3B-C4B-C5B
26	a	409[A]	SQD	O6-C44-C45-O47
26	a	409[B]	SQD	O6-C44-C45-O47
26	b	620	SQD	O47-C45-C46-O48
26	f	102	SQD	O47-C45-C46-O48
23	c	506	CLA	C13-C15-C16-C17
32	D	407[B]	LHG	C10-C11-C12-C13
35	C	518[A]	DGD	C8B-C9B-CAB-CBB
23	C	507	CLA	C16-C17-C18-C20
32	E	101[A]	LHG	C17-C18-C19-C20
29	a	412[A]	PL9	C24-C26-C27-C28
26	B	620	SQD	C24-C25-C26-C27
31	B	630	LMT	C3-C4-C5-C6
32	D	406[B]	LHG	C13-C14-C15-C16
32	D	407[A]	LHG	C10-C11-C12-C13
23	b	608	CLA	C2-C1-O2A-CGA
23	b	614	CLA	C2-C1-O2A-CGA
23	c	507	CLA	C5-C6-C7-C8
23	B	610	CLA	C14-C13-C15-C16
23	C	513	CLA	C6-C7-C8-C9
23	b	601	CLA	C6-C7-C8-C9
23	c	512	CLA	C6-C7-C8-C9
34	B	625	HTG	C4'-C5'-C6'-C7'
32	b	629[B]	LHG	C13-C14-C15-C16
23	B	601	CLA	C13-C15-C16-C17
35	C	518[A]	DGD	C8A-C9A-CAA-CBA
35	H	102	DGD	CAB-CBB-CCB-CDB
23	A	406[B]	CLA	C16-C17-C18-C20
25	D	404	BCR	C23-C24-C25-C26
25	D	404	BCR	C23-C24-C25-C30
25	H	101	BCR	C23-C24-C25-C26
25	Y	101	BCR	C23-C24-C25-C26
32	d	408[B]	LHG	C34-C35-C36-C37
33	C	520	LMG	C29-C30-C31-C32
32	d	414[A]	LHG	C25-C26-C27-C28
25	D	404	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
25	d	405	BCR	C7-C8-C9-C10
23	C	511	CLA	C13-C15-C16-C17
23	b	615	CLA	C10-C11-C12-C13
32	E	101[B]	LHG	C13-C14-C15-C16
35	c	517[B]	DGD	CBB-CCB-CDB-CEB
23	b	606	CLA	C16-C17-C18-C19
32	A	419[B]	LHG	C26-C27-C28-C29
26	A	412	SQD	C30-C31-C32-C33
23	b	609	CLA	C4-C3-C5-C6
32	D	407[B]	LHG	C27-C28-C29-C30
32	a	419[B]	LHG	C10-C11-C12-C13
23	B	610	CLA	C12-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C15
23	C	507	CLA	C6-C7-C8-C10
23	a	405[B]	CLA	C6-C7-C8-C10
23	a	407	CLA	C11-C10-C8-C7
23	b	601	CLA	C6-C7-C8-C10
23	b	604	CLA	C6-C7-C8-C10
23	c	509	CLA	C6-C7-C8-C10
23	c	509	CLA	C11-C10-C8-C7
24	a	406[A]	PHO	C2-C3-C5-C6
23	B	601	CLA	O1A-CGA-O2A-C1
26	F	102	SQD	C32-C33-C34-C35
23	B	608	CLA	C16-C17-C18-C19
32	L	101[A]	LHG	C11-C10-C9-C8
32	d	414[A]	LHG	C24-C25-C26-C27
33	z	101	LMG	C14-C15-C16-C17
31	A	420	LMT	C5-C6-C7-C8
32	b	629[A]	LHG	C34-C35-C36-C37
35	C	517[A]	DGD	CCA-CDA-CEA-CFA
32	b	629[A]	LHG	C9-C10-C11-C12
34	c	521	HTG	C2'-C1'-S1-C1
32	L	101[B]	LHG	C23-C24-C25-C26
31	e	101	LMT	C9-C10-C11-C12
32	d	408[B]	LHG	C24-C23-O8-C6
23	b	601	CLA	CAA-CBA-CGA-O2A
23	C	510	CLA	O1D-CGD-O2D-CED
31	b	627	LMT	C6-C7-C8-C9
33	c	519	LMG	C29-C30-C31-C32
23	B	606	CLA	C8-C10-C11-C12
23	B	615	CLA	C10-C11-C12-C13
23	B	610	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	C	513	CLA	CAD-CBD-CGD-O2D
23	b	610	CLA	CAD-CBD-CGD-O2D
23	b	616	CLA	CAD-CBD-CGD-O2D
23	c	501	CLA	CAD-CBD-CGD-O2D
23	c	510	CLA	CAD-CBD-CGD-O2D
24	A	407[A]	PHO	CAD-CBD-CGD-O2D
24	A	416[B]	PHO	CAD-CBD-CGD-O2D
24	a	406[A]	PHO	CAD-CBD-CGD-O2D
24	a	406[B]	PHO	CAD-CBD-CGD-O2D
26	B	620	SQD	C46-C45-O47-C7
38	f	101	HEM	C2B-C3B-CAB-CBB
33	C	521	LMG	C4-C5-C6-O5
32	E	101[A]	LHG	C13-C14-C15-C16
23	B	613	CLA	C15-C16-C17-C18
23	b	604	CLA	C10-C11-C12-C13
23	c	509	CLA	C8-C10-C11-C12
26	a	409[A]	SQD	C27-C28-C29-C30
26	A	412	SQD	C24-C23-O48-C46
35	c	518	DGD	C2A-C1A-O1G-C1G
23	c	510	CLA	C4-C3-C5-C6
32	D	406[A]	LHG	C34-C35-C36-C37
32	d	407[B]	LHG	C11-C10-C9-C8
26	A	412	SQD	O5-C1-O6-C44
29	a	412[B]	PL9	C24-C26-C27-C28
26	a	409[B]	SQD	O6-C44-C45-C46
26	a	410	SQD	O6-C44-C45-C46
32	D	407[B]	LHG	C2-C3-O3-P
32	E	101[A]	LHG	C4-C5-C6-O8
33	C	501	LMG	C7-C8-C9-O8
32	d	408[B]	LHG	O10-C23-O8-C6
32	d	407[B]	LHG	C13-C14-C15-C16
32	E	101[B]	LHG	O6-C4-C5-O7
32	b	629[A]	LHG	O6-C4-C5-O7
35	C	518[A]	DGD	C7A-C8A-C9A-CAA
23	B	601	CLA	CHA-CBD-CGD-O1D
23	B	601	CLA	CHA-CBD-CGD-O2D
23	C	503	CLA	CHA-CBD-CGD-O1D
23	C	503	CLA	CHA-CBD-CGD-O2D
23	c	502	CLA	CHA-CBD-CGD-O1D
23	c	502	CLA	CHA-CBD-CGD-O2D
23	c	503	CLA	CHA-CBD-CGD-O1D
26	a	409[B]	SQD	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
23	c	511	CLA	O1A-CGA-O2A-C1
33	c	520	LMG	O10-C28-O8-C9
35	c	518	DGD	O1A-C1A-O1G-C1G
26	F	102	SQD	O47-C45-C46-O48
32	a	419[A]	LHG	O7-C5-C6-O8
33	a	415	LMG	O7-C8-C9-O8
35	h	102	DGD	O1G-C1G-C2G-O2G
23	c	511	CLA	CBA-CGA-O2A-C1
33	C	520	LMG	C31-C32-C33-C34
23	b	602	CLA	C10-C11-C12-C13
35	H	102	DGD	O2G-C1B-C2B-C3B
27	O	303	GOL	O1-C1-C2-O2
27	c	526	GOL	O1-C1-C2-O2
32	A	419[B]	LHG	O1-C1-C2-O2
33	B	621	LMG	C36-C37-C38-C39
35	C	517[B]	DGD	C3B-C4B-C5B-C6B
23	C	513	CLA	C3-C5-C6-C7
29	D	405[A]	PL9	C45-C44-C46-C47
23	b	601	CLA	O1A-CGA-O2A-C1
35	c	517[A]	DGD	C1A-C2A-C3A-C4A
29	A	414[B]	PL9	C4-C3-C7-C8
23	C	511	CLA	C14-C13-C15-C16
23	d	404	CLA	C11-C12-C13-C14
35	C	517[A]	DGD	C4D-C5D-C6D-O5D
33	C	501	LMG	C39-C40-C41-C42
31	b	621	LMT	C7-C8-C9-C10
31	e	101	LMT	C3-C4-C5-C6
23	b	608	CLA	C13-C15-C16-C17
23	a	404[A]	CLA	C2C-C3C-CAC-CBC
33	C	521	LMG	C12-C13-C14-C15
33	Z	101	LMG	C11-C12-C13-C14
35	C	518[B]	DGD	C8B-C9B-CAB-CBB
23	d	402[A]	CLA	C1A-C2A-CAA-CBA
23	A	404[B]	CLA	C16-C17-C18-C19
32	d	408[A]	LHG	C24-C23-O8-C6
31	F	101	LMT	C6-C7-C8-C9
32	A	419[A]	LHG	C32-C33-C34-C35
32	d	414[B]	LHG	C34-C35-C36-C37
25	t	102	BCR	C13-C14-C15-C16
23	c	506	CLA	C10-C11-C12-C13
32	D	406[A]	LHG	C4-O6-P-O3
32	d	414[A]	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
32	L	101[B]	LHG	C27-C28-C29-C30
32	a	419[A]	LHG	C23-C24-C25-C26
26	a	409[A]	SQD	C35-C36-C37-C38
23	b	601	CLA	C4-C3-C5-C6
29	d	406[B]	PL9	C45-C44-C46-C47
32	D	407[A]	LHG	C2-C3-O3-P
32	d	408[A]	LHG	C2-C3-O3-P
32	d	408[B]	LHG	C2-C3-O3-P
29	a	412[B]	PL9	C12-C11-C9-C8
33	c	519	LMG	O6-C5-C6-O5
35	C	519	DGD	CBA-CCA-CDA-CEA
32	D	406[A]	LHG	C4-O6-P-O5
32	E	101[A]	LHG	C4-O6-P-O5
32	E	101[B]	LHG	C4-O6-P-O5
32	a	419[A]	LHG	C4-O6-P-O4
32	a	419[B]	LHG	C4-O6-P-O4
32	d	407[A]	LHG	C3-O3-P-O4
32	d	407[B]	LHG	C4-O6-P-O5
35	c	516[A]	DGD	O6E-C1E-O5D-C6D
23	b	604	CLA	C13-C15-C16-C17
32	E	101[B]	LHG	O6-C4-C5-C6
32	L	101[A]	LHG	O6-C4-C5-C6
32	b	629[B]	LHG	O6-C4-C5-C6
26	A	410[A]	SQD	C18-C19-C20-C21
32	d	414[A]	LHG	C27-C28-C29-C30
35	c	516[A]	DGD	CCB-CDB-CEB-CFB
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	605	CLA	CAD-CBD-CGD-O1D
23	C	503	CLA	CAD-CBD-CGD-O1D
23	C	505	CLA	CAD-CBD-CGD-O1D
23	c	502	CLA	CAD-CBD-CGD-O1D
35	c	517[B]	DGD	C1A-C2A-C3A-C4A
23	B	601	CLA	CAA-CBA-CGA-O2A
32	D	406[B]	LHG	C34-C35-C36-C37
23	b	601	CLA	C3-C5-C6-C7
32	D	407[A]	LHG	C24-C23-O8-C6
32	E	101[A]	LHG	C1-C2-C3-O3
35	h	102	DGD	C6A-C7A-C8A-C9A
23	B	616	CLA	C12-C13-C15-C16
23	C	511	CLA	C12-C13-C15-C16
23	b	601	CLA	C11-C12-C13-C15
23	b	603	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
23	b	608	CLA	C12-C13-C15-C16
23	b	615	CLA	C12-C13-C15-C16
23	b	616	CLA	C6-C7-C8-C10
23	c	505	CLA	C12-C13-C15-C16
23	d	403[B]	CLA	C11-C12-C13-C15
32	d	408[A]	LHG	O10-C23-O8-C6
35	C	518[A]	DGD	C1A-C2A-C3A-C4A
26	A	412	SQD	O10-C23-O48-C46
32	D	407[A]	LHG	O10-C23-O8-C6
32	L	101[B]	LHG	C11-C10-C9-C8
35	c	516[A]	DGD	C8B-C9B-CAB-CBB
26	A	410[A]	SQD	C34-C35-C36-C37
32	D	406[B]	LHG	C26-C27-C28-C29
35	h	102	DGD	O1G-C1G-C2G-C3G
32	E	101[A]	LHG	O7-C5-C6-O8
32	a	419[B]	LHG	O7-C5-C6-O8
32	b	629[B]	LHG	C34-C35-C36-C37
23	d	402[B]	CLA	C4C-C3C-CAC-CBC
26	a	409[A]	SQD	C11-C12-C13-C14
35	C	518[B]	DGD	C5D-C6D-O5D-C1E
35	c	517[B]	DGD	C2G-C3G-O3G-C1D
31	B	628	LMT	C9-C10-C11-C12
35	C	519	DGD	CAB-CBB-CCB-CDB
35	c	517[B]	DGD	C9B-CAB-CBB-CCB
26	a	409[B]	SQD	C35-C36-C37-C38
31	T	101	LMT	C3-C4-C5-C6
23	A	406[A]	CLA	C14-C13-C15-C16
23	A	408	CLA	C14-C13-C15-C16
23	C	507	CLA	C6-C7-C8-C9
23	a	407	CLA	C11-C10-C8-C9
23	b	601	CLA	C11-C12-C13-C14
23	b	615	CLA	C14-C13-C15-C16
23	c	506	CLA	C11-C10-C8-C9
23	c	509	CLA	C6-C7-C8-C9
23	c	510	CLA	C11-C10-C8-C9
32	b	629[B]	LHG	C25-C26-C27-C28
35	C	519	DGD	C6A-C7A-C8A-C9A
33	B	621	LMG	C20-C21-C22-C23
32	a	419[B]	LHG	C7-C8-C9-C10
33	a	415	LMG	O8-C28-C29-C30
27	a	417	GOL	O1-C1-C2-O2
24	a	406[A]	PHO	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
25	D	404	BCR	C37-C22-C23-C24
35	C	517[B]	DGD	C2A-C3A-C4A-C5A
29	a	412[A]	PL9	C12-C11-C9-C8
23	c	509	CLA	C15-C16-C17-C18
23	C	507	CLA	C16-C17-C18-C19
32	d	414[A]	LHG	C34-C35-C36-C37
33	C	521	LMG	C20-C21-C22-C23
35	c	517[B]	DGD	C7B-C8B-C9B-CAB
33	m	101	LMG	C11-C12-C13-C14
35	H	102	DGD	C6A-C7A-C8A-C9A
32	d	408[A]	LHG	C32-C33-C34-C35
34	B	622	HTG	C3'-C4'-C5'-C6'
35	h	102	DGD	CDA-CEA-CFA-CGA
23	A	408	CLA	C2-C1-O2A-CGA
23	B	608	CLA	C2-C1-O2A-CGA
23	B	613	CLA	C2-C1-O2A-CGA
23	C	514	CLA	C2-C1-O2A-CGA
23	b	613	CLA	C2-C1-O2A-CGA
23	c	513	CLA	C2-C1-O2A-CGA
26	A	410[A]	SQD	C16-C17-C18-C19
26	A	412	SQD	C15-C16-C17-C18
34	B	623	HTG	C4'-C5'-C6'-C7'
31	B	631	LMT	C1-C2-C3-C4
26	A	410[B]	SQD	C16-C17-C18-C19
23	B	605	CLA	C5-C6-C7-C8
23	D	403	CLA	O1A-CGA-O2A-C1
32	d	407[A]	LHG	O10-C23-O8-C6
32	L	101[A]	LHG	O6-C4-C5-O7
29	A	414[B]	PL9	C25-C24-C26-C27
31	b	627	LMT	O1'-C1-C2-C3
33	z	101	LMG	C13-C14-C15-C16
23	b	613	CLA	O1D-CGD-O2D-CED
25	H	101	BCR	C23-C24-C25-C30
25	Y	101	BCR	C23-C24-C25-C30
25	y	101	BCR	C23-C24-C25-C26
25	y	101	BCR	C23-C24-C25-C30
23	c	510	CLA	C2-C3-C5-C6
29	A	414[A]	PL9	C28-C29-C31-C32
23	b	616	CLA	O1A-CGA-O2A-C1
33	d	412	LMG	C11-C12-C13-C14
32	D	406[B]	LHG	C11-C10-C9-C8
32	d	407[A]	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
23	d	402[A]	CLA	C4C-C3C-CAC-CBC
26	B	620	SQD	C29-C30-C31-C32
34	b	622	HTG	C1'-C2'-C3'-C4'
35	c	517[A]	DGD	O6E-C1E-O5D-C6D
35	C	517[A]	DGD	C6A-C7A-C8A-C9A
35	c	516[A]	DGD	C2E-C1E-O5D-C6D
35	c	517[A]	DGD	C2E-C1E-O5D-C6D
32	L	101[A]	LHG	C26-C27-C28-C29
26	a	410	SQD	O10-C23-O48-C46
26	B	620	SQD	O47-C45-C46-O48
32	E	101[B]	LHG	O7-C5-C6-O8
32	d	414[B]	LHG	C3-O3-P-O6
32	L	101[A]	LHG	C27-C28-C29-C30
33	C	521	LMG	C10-C11-C12-C13
23	b	601	CLA	C2-C3-C5-C6
23	b	614	CLA	C11-C12-C13-C15
23	c	510	CLA	C12-C13-C15-C16
23	c	510	CLA	O1A-CGA-O2A-C1
26	a	410	SQD	C26-C27-C28-C29
35	C	517[B]	DGD	C6A-C7A-C8A-C9A
23	A	406[B]	CLA	C14-C13-C15-C16
23	B	603	CLA	C11-C12-C13-C14
23	B	614	CLA	C11-C10-C8-C9
23	C	511	CLA	C11-C12-C13-C14
23	b	603	CLA	C11-C10-C8-C9
23	b	608	CLA	C14-C13-C15-C16
23	b	610	CLA	C11-C12-C13-C14
23	b	614	CLA	C14-C13-C15-C16
23	c	505	CLA	C14-C13-C15-C16
23	d	403[B]	CLA	C11-C12-C13-C14
32	A	419[B]	LHG	C32-C33-C34-C35
33	B	621	LMG	O6-C5-C6-O5
23	a	404[A]	CLA	C4C-C3C-CAC-CBC
31	F	101	LMT	C2-C3-C4-C5
23	b	615	CLA	C5-C6-C7-C8
35	c	516[B]	DGD	CAB-CBB-CCB-CDB
32	D	407[A]	LHG	C27-C28-C29-C30
26	a	410	SQD	C24-C23-O48-C46
26	a	410	SQD	C24-C25-C26-C27
31	e	101	LMT	C2-C3-C4-C5
35	c	516[A]	DGD	C4B-C5B-C6B-C7B
35	c	516[B]	DGD	C8B-C9B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
33	B	621	LMG	C37-C38-C39-C40
32	d	414[A]	LHG	C1-C2-C3-O3
27	l	801[B]	GOL	O1-C1-C2-O2
23	b	616	CLA	CBA-CGA-O2A-C1
33	d	412	LMG	C18-C19-C20-C21
32	A	419[B]	LHG	C17-C18-C19-C20
32	d	408[A]	LHG	C33-C34-C35-C36
35	c	518	DGD	O6D-C5D-C6D-O5D
23	D	403	CLA	CBA-CGA-O2A-C1
33	B	621	LMG	O6-C1-O1-C7
35	C	517[B]	DGD	O6E-C1E-O5D-C6D
32	E	101[B]	LHG	C17-C18-C19-C20
33	C	520	LMG	C30-C31-C32-C33
23	C	512	CLA	C3-C5-C6-C7
29	A	414[B]	PL9	C39-C41-C42-C43
26	A	412	SQD	C7-C8-C9-C10
32	b	629[B]	LHG	C28-C29-C30-C31
35	C	518[B]	DGD	C7A-C8A-C9A-CAA
26	b	620	SQD	C30-C31-C32-C33
23	A	408	CLA	C16-C17-C18-C19
38	f	101	HEM	C4B-C3B-CAB-CBB
35	C	518[B]	DGD	C8A-C9A-CAA-CBA
26	A	410[A]	SQD	C11-C10-C9-C8
32	d	414[B]	LHG	C13-C14-C15-C16
33	a	415	LMG	C33-C34-C35-C36
24	a	406[B]	PHO	C8-C10-C11-C12
32	b	629[A]	LHG	C25-C26-C27-C28
35	C	519	DGD	C7A-C8A-C9A-CAA
23	C	507	CLA	C2-C1-O2A-CGA
32	A	419[B]	LHG	C18-C19-C20-C21
32	D	406[A]	LHG	C11-C10-C9-C8
33	c	519	LMG	C32-C33-C34-C35
33	Z	101	LMG	C2-C1-O1-C7
35	C	517[B]	DGD	C2E-C1E-O5D-C6D
23	A	404[B]	CLA	C2A-CAA-CBA-CGA
23	A	405[B]	CLA	C2C-C3C-CAC-CBC
32	a	419[A]	LHG	C24-C25-C26-C27
33	a	415	LMG	C13-C14-C15-C16
23	c	501	CLA	O1D-CGD-O2D-CED
33	d	412	LMG	C19-C20-C21-C22
23	C	507	CLA	C3A-C2A-CAA-CBA
23	c	513	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
33	c	519	LMG	C30-C31-C32-C33
23	c	510	CLA	CBA-CGA-O2A-C1
38	E	102	HEM	CAD-CBD-CGD-O1D
29	A	414[B]	PL9	C12-C11-C9-C10
29	D	405[B]	PL9	C45-C44-C46-C47
29	D	405[B]	PL9	C4-C3-C7-C8
29	a	412[A]	PL9	C4-C3-C7-C8
29	a	412[B]	PL9	C4-C3-C7-C8
23	a	405[A]	CLA	C6-C7-C8-C9
23	a	405[B]	CLA	C14-C13-C15-C16
23	C	502	CLA	C16-C17-C18-C20
26	b	620	SQD	C11-C10-C9-C8
32	d	414[B]	LHG	C27-C28-C29-C30
35	C	519	DGD	C8B-C9B-CAB-CBB
35	c	517[A]	DGD	C7B-C8B-C9B-CAB
23	b	605	CLA	C13-C15-C16-C17
33	z	101	LMG	O7-C10-C11-C12
32	L	101[A]	LHG	C23-C24-C25-C26
35	c	516[B]	DGD	O6E-C1E-O5D-C6D
31	A	417	LMT	C7-C8-C9-C10
23	d	402[A]	CLA	C15-C16-C17-C18
26	A	410[A]	SQD	C13-C14-C15-C16
23	B	604	CLA	C1A-C2A-CAA-CBA
23	a	405[B]	CLA	C1A-C2A-CAA-CBA
23	c	513	CLA	C1A-C2A-CAA-CBA
33	d	412	LMG	C38-C39-C40-C41
23	B	601	CLA	C11-C12-C13-C15
23	B	603	CLA	C11-C12-C13-C15
23	b	615	CLA	C11-C12-C13-C15
29	a	412[B]	PL9	C43-C44-C46-C47
23	A	404[A]	CLA	C2C-C3C-CAC-CBC
23	D	403	CLA	C8-C10-C11-C12
32	A	419[A]	LHG	C18-C19-C20-C21
32	b	629[A]	LHG	C17-C18-C19-C20
26	F	102	SQD	C24-C23-O48-C46
35	h	102	DGD	C4E-C5E-C6E-O5E
35	c	516[B]	DGD	C4B-C5B-C6B-C7B
23	c	507	CLA	C2A-CAA-CBA-CGA
31	M	101	LMT	C2-C3-C4-C5
32	D	406[A]	LHG	C26-C27-C28-C29
32	L	101[B]	LHG	O6-C4-C5-C6
26	A	410[B]	SQD	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
34	b	623	HTG	C4'-C5'-C6'-C7'
32	d	407[A]	LHG	C16-C17-C18-C19
23	C	514	CLA	O1D-CGD-O2D-CED
23	b	616	CLA	C4-C3-C5-C6
29	a	412[B]	PL9	C45-C44-C46-C47
29	d	406[A]	PL9	C43-C44-C46-C47
38	E	102	HEM	CAD-CBD-CGD-O2D
23	B	610	CLA	C13-C15-C16-C17
31	T	101	LMT	C1-C2-C3-C4
26	B	620	SQD	C33-C34-C35-C36
33	C	501	LMG	O7-C8-C9-O8
35	H	102	DGD	O1G-C1G-C2G-O2G
23	B	612	CLA	CBA-CGA-O2A-C1
25	K	102	BCR	C19-C20-C21-C22
40	V	201	HEC	CAD-CBD-CGD-O1D
23	A	406[A]	CLA	C16-C17-C18-C19
29	A	414[A]	PL9	C39-C41-C42-C43
29	a	412[A]	PL9	C45-C44-C46-C47
29	D	405[B]	PL9	C43-C44-C46-C47
29	d	406[B]	PL9	C28-C29-C31-C32
23	d	404	CLA	O1A-CGA-O2A-C1
33	a	415	LMG	C31-C32-C33-C34
35	c	517[B]	DGD	CDA-CEA-CFA-CGA
32	A	419[A]	LHG	C29-C30-C31-C32
32	d	408[B]	LHG	C33-C34-C35-C36
35	c	516[A]	DGD	CAB-CBB-CCB-CDB
35	c	518	DGD	CDA-CEA-CFA-CGA
23	A	406[B]	CLA	C16-C17-C18-C19
26	a	409[B]	SQD	C10-C11-C12-C13
25	C	515	BCR	C23-C24-C25-C30
25	C	516	BCR	C1-C6-C7-C8
25	a	408	BCR	C1-C6-C7-C8
25	c	514	BCR	C23-C24-C25-C30
25	d	405	BCR	C23-C24-C25-C30
25	h	101	BCR	C23-C24-C25-C30
23	B	606	CLA	C15-C16-C17-C18
27	l	801[A]	GOL	O1-C1-C2-C3
27	v	202[A]	GOL	O1-C1-C2-C3
26	F	102	SQD	O10-C23-O48-C46
32	d	408[B]	LHG	C32-C33-C34-C35
35	c	518	DGD	C7B-C8B-C9B-CAB
29	D	405[A]	PL9	C35-C34-C36-C37

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Mol	Chain	Res	Type	Atoms
32	a	419[B]	LHG	C24-C25-C26-C27
33	C	520	LMG	C11-C12-C13-C14
29	a	412[A]	PL9	C43-C44-C46-C47
29	d	406[B]	PL9	C43-C44-C46-C47
23	C	512	CLA	O1A-CGA-O2A-C1
35	c	516[B]	DGD	C5D-C6D-O5D-C1E
33	D	411	LMG	C34-C35-C36-C37
38	f	101	HEM	CAA-CBA-CGA-O2A
40	V	201	HEC	CAD-CBD-CGD-O2D
40	v	201	HEC	CAD-CBD-CGD-O2D
33	C	501	LMG	C20-C21-C22-C23
23	A	404[A]	CLA	C16-C17-C18-C19
32	b	629[B]	LHG	O6-C4-C5-O7
35	c	518	DGD	O6E-C5E-C6E-O5E
32	A	419[A]	LHG	C35-C36-C37-C38
40	v	201	HEC	CAD-CBD-CGD-O1D
23	C	502	CLA	C2A-CAA-CBA-CGA
23	b	604	CLA	C2C-C3C-CAC-CBC
32	b	629[A]	LHG	C10-C11-C12-C13
29	D	405[B]	PL9	C35-C34-C36-C37
23	a	405[A]	CLA	C6-C7-C8-C10
23	b	616	CLA	C2-C3-C5-C6
29	A	414[B]	PL9	C43-C44-C46-C47
23	c	509	CLA	C10-C11-C12-C13
31	B	631	LMT	C6-C7-C8-C9
32	L	101[A]	LHG	C16-C17-C18-C19
27	A	418	GOL	O2-C2-C3-O3
35	c	516[B]	DGD	C2E-C1E-O5D-C6D
23	c	502	CLA	C16-C17-C18-C19
23	B	604	CLA	C2C-C3C-CAC-CBC
26	f	102	SQD	C26-C27-C28-C29
38	f	101	HEM	CAD-CBD-CGD-O1D
32	A	419[B]	LHG	O8-C23-C24-C25
32	A	419[A]	LHG	O8-C23-C24-C25
33	Z	101	LMG	C29-C28-O8-C9
23	B	603	CLA	C4-C3-C5-C6
23	c	504	CLA	C4-C3-C5-C6
29	a	412[B]	PL9	C35-C34-C36-C37
32	L	101[B]	LHG	C32-C33-C34-C35
33	B	621	LMG	C30-C31-C32-C33
35	C	519	DGD	C3B-C4B-C5B-C6B
23	B	612	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	c	513	CLA	C2-C3-C5-C6
29	A	414[B]	PL9	C23-C24-C26-C27
35	c	517[A]	DGD	C9B-CAB-CBB-CCB
23	C	513	CLA	CAA-CBA-CGA-O2A
23	A	408	CLA	C11-C12-C13-C14
23	B	614	CLA	C6-C7-C8-C9
23	B	616	CLA	C6-C7-C8-C9
23	B	616	CLA	C14-C13-C15-C16
23	D	403	CLA	C6-C7-C8-C9
23	a	405[A]	CLA	C14-C13-C15-C16
26	a	409[B]	SQD	C27-C28-C29-C30
33	Z	101	LMG	O7-C10-C11-C12
23	B	603	CLA	CAD-CBD-CGD-O2D
23	B	604	CLA	CAD-CBD-CGD-O2D
23	B	616	CLA	CAD-CBD-CGD-O2D
23	b	604	CLA	CAD-CBD-CGD-O2D
23	c	505	CLA	CAD-CBD-CGD-O2D
23	c	512	CLA	CAD-CBD-CGD-O2D
24	A	407[B]	PHO	CAD-CBD-CGD-O2D
24	a	414[A]	PHO	CAD-CBD-CGD-O2D
23	B	616	CLA	C16-C17-C18-C20
31	B	628	LMT	C7-C8-C9-C10
32	D	407[A]	LHG	C28-C29-C30-C31
32	L	101[B]	LHG	C10-C11-C12-C13
35	C	519	DGD	O1A-C1A-O1G-C1G
32	b	629[A]	LHG	C30-C31-C32-C33
38	f	101	HEM	CAA-CBA-CGA-O1A
32	b	629[B]	LHG	C9-C10-C11-C12
35	c	516[B]	DGD	C1A-C2A-C3A-C4A
32	L	101[A]	LHG	O7-C7-C8-C9
32	a	419[A]	LHG	O8-C23-C24-C25
32	d	408[B]	LHG	C10-C11-C12-C13
29	A	414[A]	PL9	C25-C24-C26-C27
23	b	608	CLA	C16-C17-C18-C20
23	b	616	CLA	C5-C6-C7-C8
23	B	613	CLA	CAA-CBA-CGA-O2A
33	c	519	LMG	O7-C10-C11-C12
33	C	521	LMG	C38-C39-C40-C41
25	d	405	BCR	C21-C22-C23-C24
24	A	407[A]	PHO	C2C-C3C-CAC-CBC
24	A	416[A]	PHO	C2C-C3C-CAC-CBC
24	A	416[B]	PHO	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
24	a	406[A]	PHO	C2C-C3C-CAC-CBC
24	a	406[B]	PHO	C2C-C3C-CAC-CBC
24	a	414[A]	PHO	C2C-C3C-CAC-CBC
24	a	414[B]	PHO	C2C-C3C-CAC-CBC
26	F	102	SQD	C44-C45-C46-O48
33	d	412	LMG	C16-C17-C18-C19
32	b	629[A]	LHG	O7-C7-C8-C9
35	h	102	DGD	O2G-C1B-C2B-C3B
32	A	419[B]	LHG	C35-C36-C37-C38
23	A	404[A]	CLA	C15-C16-C17-C18
23	B	602	CLA	O2A-C1-C2-C3
24	A	407[A]	PHO	O2A-C1-C2-C3
24	A	407[B]	PHO	O2A-C1-C2-C3
24	a	406[B]	PHO	O2A-C1-C2-C3
23	A	404[A]	CLA	C4C-C3C-CAC-CBC
34	B	623	HTG	S1-C1'-C2'-C3'
23	C	511	CLA	C8-C10-C11-C12
32	L	101[B]	LHG	O7-C7-C8-C9
32	b	629[B]	LHG	O7-C7-C8-C9
26	b	620	SQD	C16-C17-C18-C19
26	b	620	SQD	C33-C34-C35-C36
23	A	405[A]	CLA	CHA-CBD-CGD-O1D
23	A	405[A]	CLA	CHA-CBD-CGD-O2D
23	A	405[B]	CLA	CHA-CBD-CGD-O1D
23	A	405[B]	CLA	CHA-CBD-CGD-O2D
23	A	406[B]	CLA	CHA-CBD-CGD-O2D
23	B	606	CLA	CHA-CBD-CGD-O1D
23	B	606	CLA	CHA-CBD-CGD-O2D
23	B	607	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O2D
23	C	505	CLA	CHA-CBD-CGD-O1D
23	b	601	CLA	CHA-CBD-CGD-O1D
23	b	606	CLA	CHA-CBD-CGD-O2D
23	c	507	CLA	CHA-CBD-CGD-O1D
23	c	507	CLA	CHA-CBD-CGD-O2D
23	c	509	CLA	CHA-CBD-CGD-O2D
23	d	402[A]	CLA	CHA-CBD-CGD-O1D
23	d	402[A]	CLA	CHA-CBD-CGD-O2D
23	d	402[B]	CLA	CHA-CBD-CGD-O2D
31	A	417	LMT	C2B-C1B-O1B-C4'
23	B	604	CLA	C4C-C3C-CAC-CBC
32	b	629[B]	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
32	A	419[B]	LHG	C9-C10-C11-C12
35	C	519	DGD	CDA-CEA-CFA-CGA
23	C	503	CLA	C16-C17-C18-C19
35	C	519	DGD	O1G-C1A-C2A-C3A
32	A	419[A]	LHG	C17-C18-C19-C20
32	d	414[A]	LHG	C13-C14-C15-C16
33	c	520	LMG	O1-C7-C8-O7
33	d	412	LMG	C40-C41-C42-C43
33	m	101	LMG	C30-C31-C32-C33
35	C	518[A]	DGD	CAB-CBB-CCB-CDB
31	T	101	LMT	O1'-C1-C2-C3
31	A	417	LMT	C9-C10-C11-C12
23	C	511	CLA	CAA-CBA-CGA-O2A
32	E	101[B]	LHG	O7-C7-C8-C9
33	c	520	LMG	C39-C40-C41-C42
24	A	407[A]	PHO	CHA-CBD-CGD-O1D
24	A	416[B]	PHO	CHA-CBD-CGD-O1D
33	B	621	LMG	C14-C15-C16-C17
33	d	412	LMG	C28-C29-C30-C31
33	B	621	LMG	O10-C28-C29-C30
35	c	518	DGD	C6A-C7A-C8A-C9A
31	e	101	LMT	C2B-C1B-O1B-C4'
23	C	507	CLA	C12-C13-C15-C16
23	b	607	CLA	C12-C13-C15-C16
23	d	402[A]	CLA	C11-C12-C13-C15
29	A	414[A]	PL9	C4-C3-C7-C8
23	c	510	CLA	CAA-CBA-CGA-O2A
32	L	101[B]	LHG	C26-C27-C28-C29
32	d	414[B]	LHG	C18-C19-C20-C21
23	B	601	CLA	C11-C12-C13-C14
23	B	605	CLA	C11-C12-C13-C14
23	B	615	CLA	C14-C13-C15-C16
23	C	506	CLA	C14-C13-C15-C16
23	b	607	CLA	C14-C13-C15-C16
23	c	513	CLA	C14-C13-C15-C16
32	E	101[B]	LHG	C12-C13-C14-C15
23	B	611	CLA	C8-C10-C11-C12
33	B	621	LMG	C21-C22-C23-C24
23	d	404	CLA	CBA-CGA-O2A-C1
31	e	101	LMT	O1'-C1-C2-C3
32	d	414[A]	LHG	C18-C19-C20-C21
38	f	101	HEM	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
29	D	405[B]	PL9	C11-C12-C13-C14
32	b	629[A]	LHG	C24-C25-C26-C27
33	c	520	LMG	C32-C33-C34-C35
32	a	419[B]	LHG	O8-C23-C24-C25
32	A	419[B]	LHG	O10-C23-C24-C25
23	B	606	CLA	C16-C17-C18-C19
27	c	526	GOL	O1-C1-C2-C3
27	d	413	GOL	C1-C2-C3-O3
27	l	801[A]	GOL	C1-C2-C3-O3
27	l	801[B]	GOL	C1-C2-C3-O3
27	o	303	GOL	O1-C1-C2-C3
29	D	405[A]	PL9	C28-C29-C31-C32
23	b	613	CLA	CAA-CBA-CGA-O2A
23	b	612	CLA	C10-C11-C12-C13
23	C	502	CLA	C1A-C2A-CAA-CBA
31	B	630	LMT	C1-C2-C3-C4
26	a	409[B]	SQD	C11-C12-C13-C14
23	B	616	CLA	C16-C17-C18-C19
32	A	419[A]	LHG	O10-C23-C24-C25
33	Z	101	LMG	O9-C10-C11-C12
29	A	414[B]	PL9	C46-C47-C48-C49
23	a	404[B]	CLA	C2-C1-O2A-CGA
23	c	512	CLA	C2-C1-O2A-CGA
23	C	513	CLA	CAA-CBA-CGA-O1A
32	a	419[A]	LHG	O10-C23-C24-C25
32	b	629[A]	LHG	O9-C7-C8-C9
32	D	407[B]	LHG	C28-C29-C30-C31
33	B	621	LMG	O1-C7-C8-C9
23	C	503	CLA	C3-C5-C6-C7
35	c	516[A]	DGD	O2G-C1B-C2B-C3B
23	c	503	CLA	C8-C10-C11-C12
23	c	507	CLA	C8-C10-C11-C12
23	B	603	CLA	C2A-CAA-CBA-CGA
23	B	614	CLA	C2A-CAA-CBA-CGA
33	B	621	LMG	C29-C30-C31-C32
32	a	419[B]	LHG	O10-C23-C24-C25
33	c	519	LMG	O9-C10-C11-C12
23	a	407	CLA	C15-C16-C17-C18
35	C	519	DGD	C9A-CAA-CBA-CCA
32	E	101[A]	LHG	O7-C7-C8-C9
32	A	419[B]	LHG	C11-C12-C13-C14
23	B	613	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
32	b	629[B]	LHG	O9-C7-C8-C9
33	m	101	LMG	C2-C1-O1-C7
31	T	101	LMT	C4-C5-C6-C7
32	b	629[B]	LHG	C31-C32-C33-C34
32	d	407[A]	LHG	C4-O6-P-O5
32	d	414[B]	LHG	C3-O3-P-O5
35	c	516[B]	DGD	CDB-CEB-CFB-CGB
35	C	519	DGD	O1A-C1A-C2A-C3A
31	a	416	LMT	O5'-C1'-O1'-C1
23	A	404[B]	CLA	C15-C16-C17-C18
23	b	610	CLA	C13-C15-C16-C17
26	a	410	SQD	C18-C19-C20-C21
25	C	515	BCR	C23-C24-C25-C26
25	C	516	BCR	C5-C6-C7-C8
25	c	514	BCR	C23-C24-C25-C26
25	d	405	BCR	C23-C24-C25-C26
32	D	406[B]	LHG	C28-C29-C30-C31
32	E	101[B]	LHG	O9-C7-C8-C9
32	L	101[A]	LHG	O9-C7-C8-C9
35	c	516[B]	DGD	C7B-C8B-C9B-CAB
23	C	503	CLA	C16-C17-C18-C20
35	c	516[A]	DGD	C1A-C2A-C3A-C4A
23	C	508	CLA	C2A-CAA-CBA-CGA
23	b	602	CLA	C2A-CAA-CBA-CGA
32	L	101[B]	LHG	O9-C7-C8-C9
23	a	407	CLA	C8-C10-C11-C12
23	B	612	CLA	CAA-CBA-CGA-O2A
32	d	408[B]	LHG	O8-C23-C24-C25
23	b	612	CLA	C8-C10-C11-C12
23	B	615	CLA	C4-C3-C5-C6
29	d	406[A]	PL9	C11-C12-C13-C14
23	B	607	CLA	CAD-CBD-CGD-O1D
23	B	609	CLA	CAD-CBD-CGD-O1D
23	C	507	CLA	CAD-CBD-CGD-O1D
23	b	601	CLA	CAD-CBD-CGD-O1D
23	b	605	CLA	CAD-CBD-CGD-O1D
23	b	609	CLA	CAD-CBD-CGD-O1D
23	c	504	CLA	CAD-CBD-CGD-O1D
23	c	506	CLA	CAD-CBD-CGD-O1D
23	d	402[B]	CLA	CAD-CBD-CGD-O1D
26	f	102	SQD	O5-C5-C6-S
26	a	409[A]	SQD	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	b	612	CLA	CAA-CBA-CGA-O2A
32	E	101[B]	LHG	O8-C23-C24-C25
23	B	612	CLA	C8-C10-C11-C12
23	C	513	CLA	C11-C10-C8-C9
23	c	506	CLA	C6-C7-C8-C9
23	d	402[A]	CLA	C11-C12-C13-C14
23	d	402[B]	CLA	C11-C12-C13-C14
23	c	512	CLA	CAA-CBA-CGA-O2A
32	D	407[A]	LHG	O8-C23-C24-C25
33	z	101	LMG	C20-C21-C22-C23
23	c	510	CLA	CAA-CBA-CGA-O1A
35	c	516[B]	DGD	CBA-CCA-CDA-CEA
32	E	101[B]	LHG	C1-C2-C3-O3
31	B	630	LMT	C7-C8-C9-C10
23	b	604	CLA	C4C-C3C-CAC-CBC
26	a	409[A]	SQD	C19-C20-C21-C22
23	C	507	CLA	C4-C3-C5-C6
29	D	405[A]	PL9	C40-C39-C41-C42
35	c	516[A]	DGD	CBA-CCA-CDA-CEA
23	B	605	CLA	C11-C12-C13-C15
23	B	609	CLA	C2-C3-C5-C6
23	B	615	CLA	C11-C12-C13-C15
23	B	615	CLA	C12-C13-C15-C16
23	C	506	CLA	C12-C13-C15-C16
23	c	508	CLA	C12-C13-C15-C16
23	c	513	CLA	C12-C13-C15-C16
23	d	402[B]	CLA	C11-C12-C13-C15
23	b	601	CLA	CAA-CBA-CGA-O1A
26	A	412	SQD	O48-C23-C24-C25
26	a	410	SQD	O48-C23-C24-C25
32	E	101[A]	LHG	O8-C23-C24-C25
35	C	518[A]	DGD	O2G-C1B-C2B-C3B
35	C	518[B]	DGD	O2G-C1B-C2B-C3B
32	D	406[A]	LHG	C28-C29-C30-C31
26	b	620	SQD	C12-C13-C14-C15
25	b	619	BCR	C21-C22-C23-C24
32	D	407[A]	LHG	O10-C23-C24-C25
35	c	516[A]	DGD	O1B-C1B-C2B-C3B
35	C	518[A]	DGD	C3A-C4A-C5A-C6A
31	e	101	LMT	C2-C1-O1'-C1'
32	D	407[B]	LHG	O8-C23-C24-C25
33	D	411	LMG	O7-C10-C11-C12

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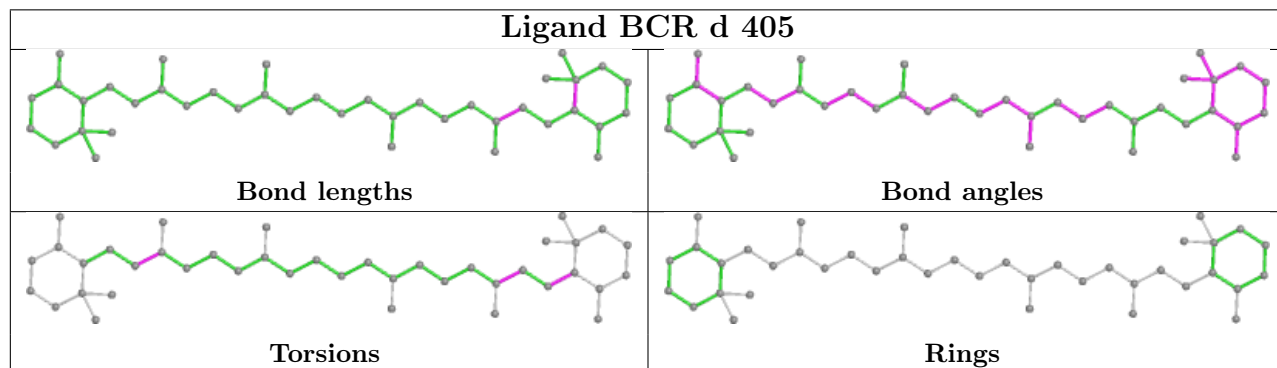
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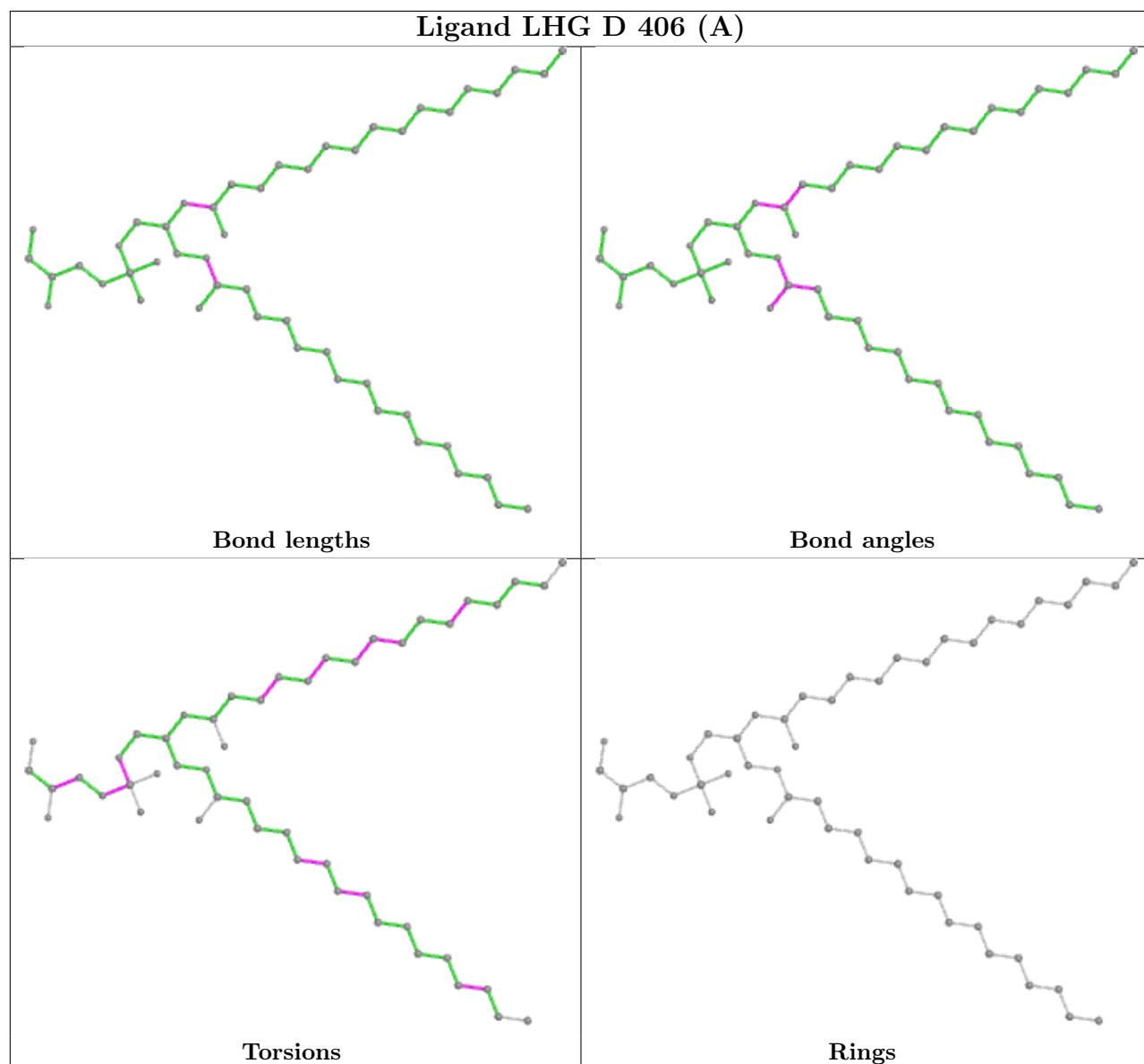
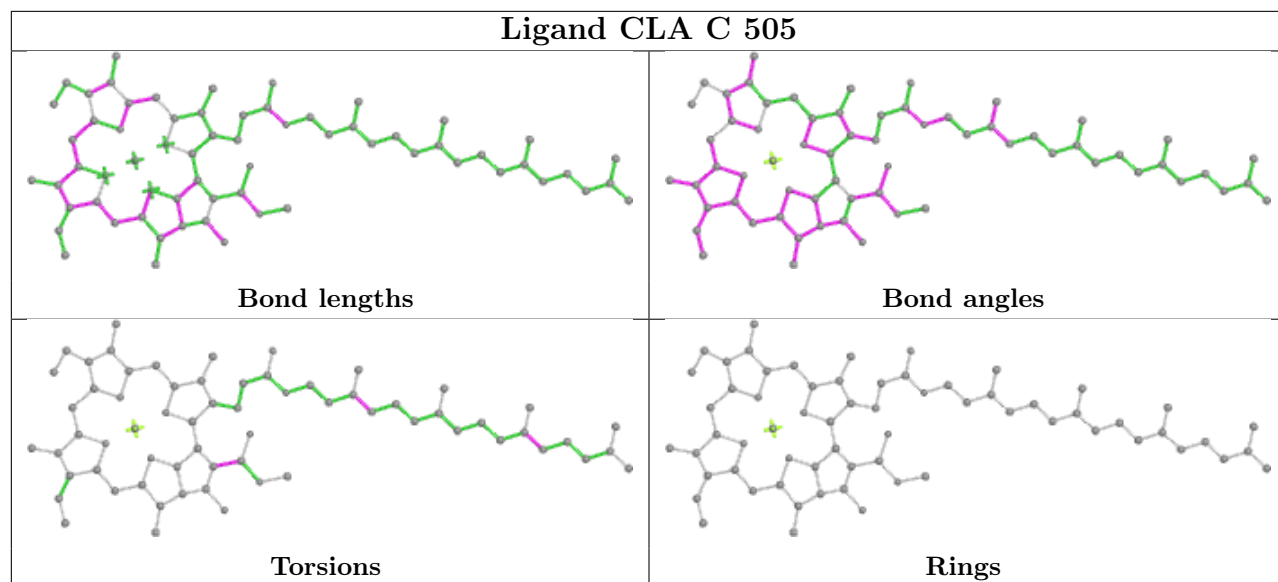
Mol	Chain	Res	Type	Atoms
23	A	405[B]	CLA	C4C-C3C-CAC-CBC
32	E	101[B]	LHG	O10-C23-C24-C25
35	C	518[B]	DGD	O1B-C1B-C2B-C3B
23	B	602	CLA	C8-C10-C11-C12
23	C	506	CLA	CAA-CBA-CGA-O2A
33	c	520	LMG	O7-C10-C11-C12
35	c	516[B]	DGD	O2G-C1B-C2B-C3B
23	B	612	CLA	CAA-CBA-CGA-O1A
32	E	101[A]	LHG	O9-C7-C8-C9
32	E	101[A]	LHG	O10-C23-C24-C25
26	A	412	SQD	O10-C23-C24-C25
33	D	411	LMG	O9-C10-C11-C12
35	C	518[A]	DGD	O1B-C1B-C2B-C3B
23	c	501	CLA	CAA-CBA-CGA-O2A

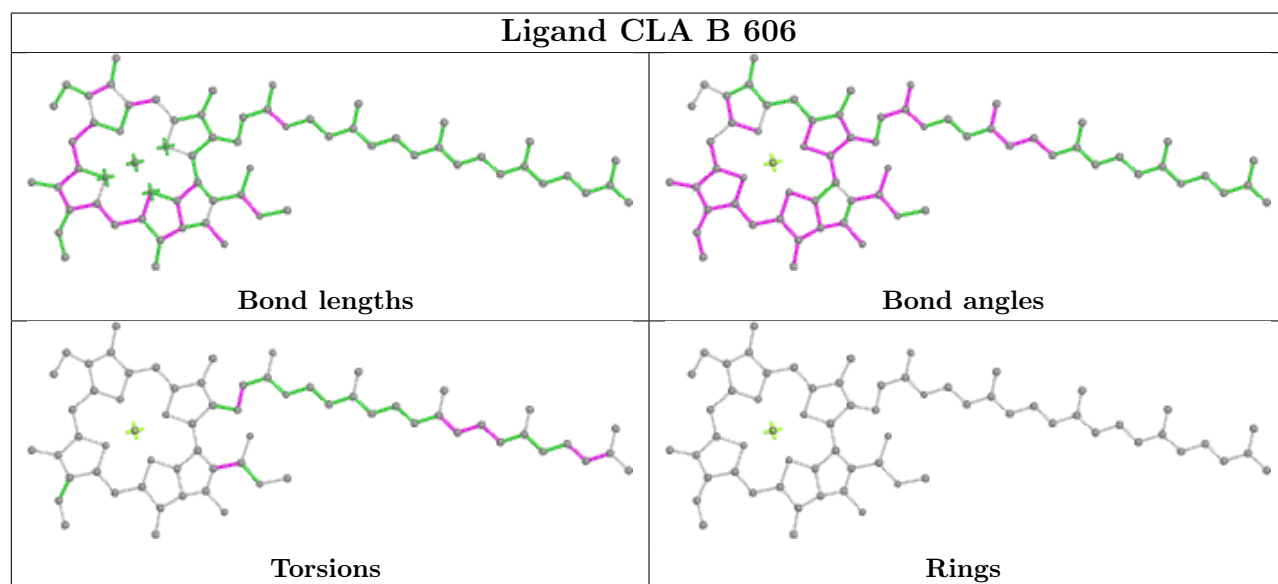
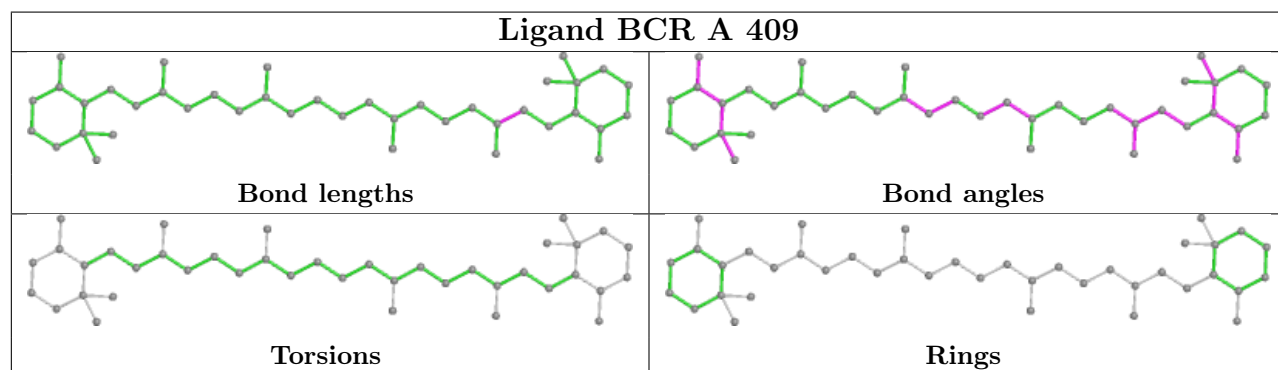
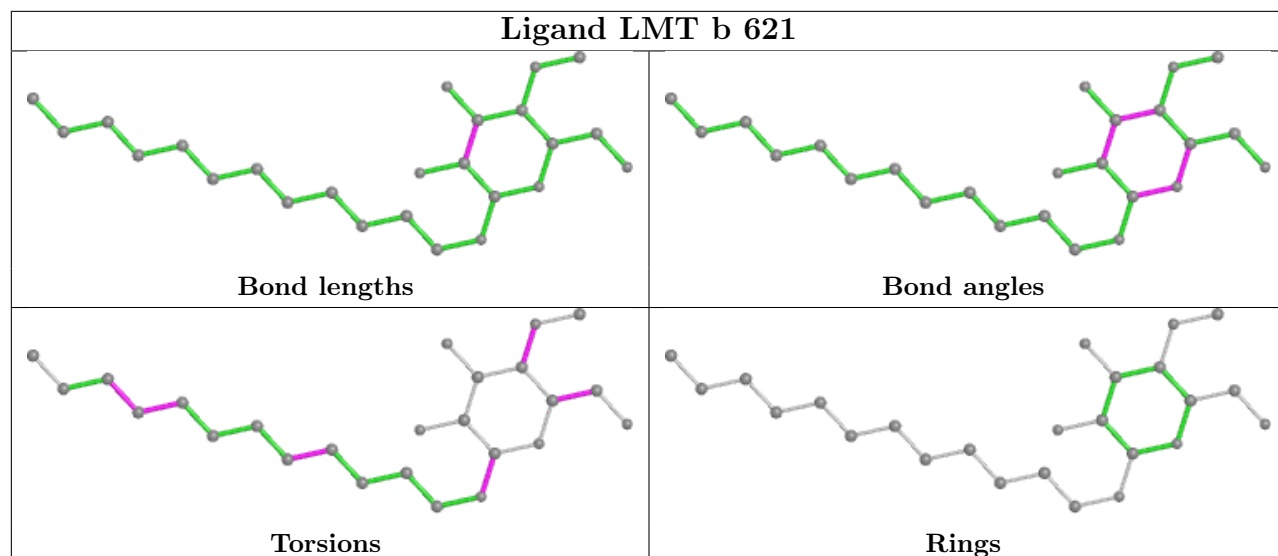
There are no ring outliers.

No monomer is involved in short contacts.

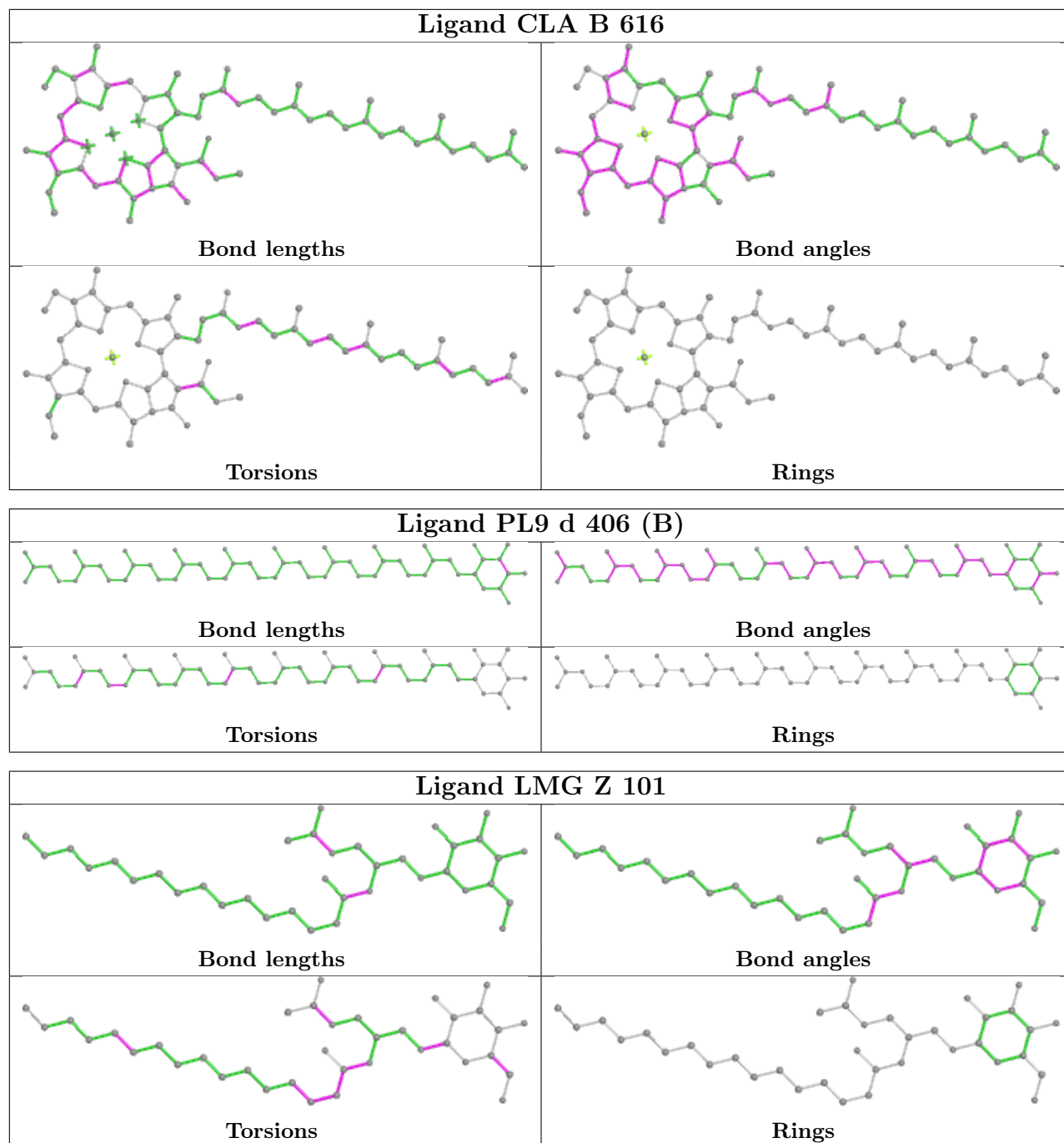
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

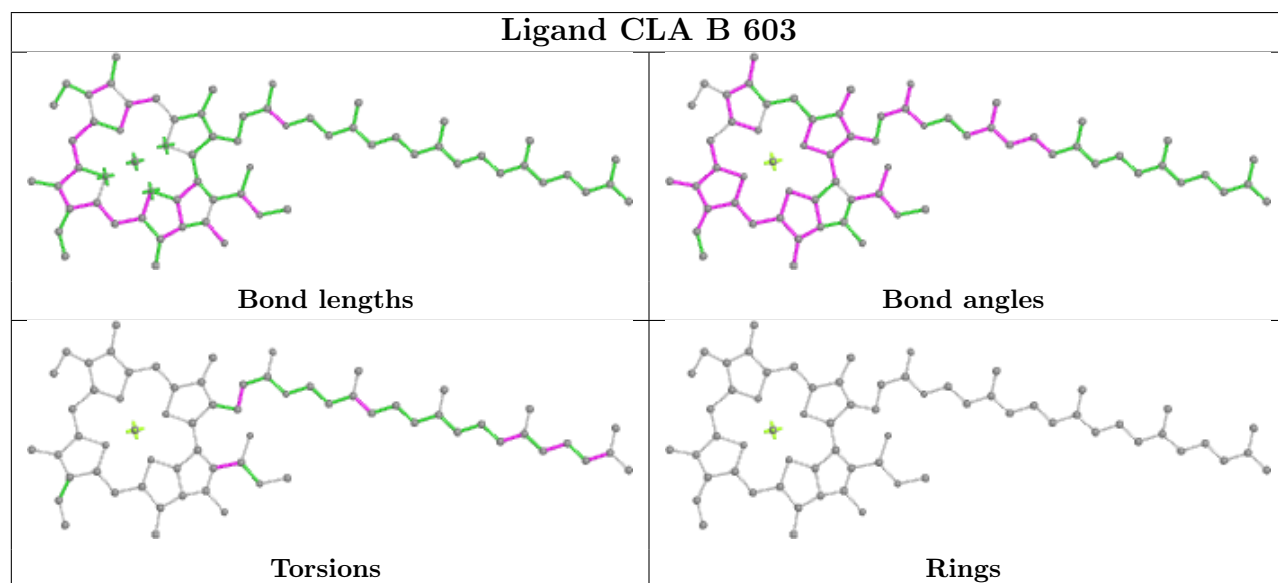
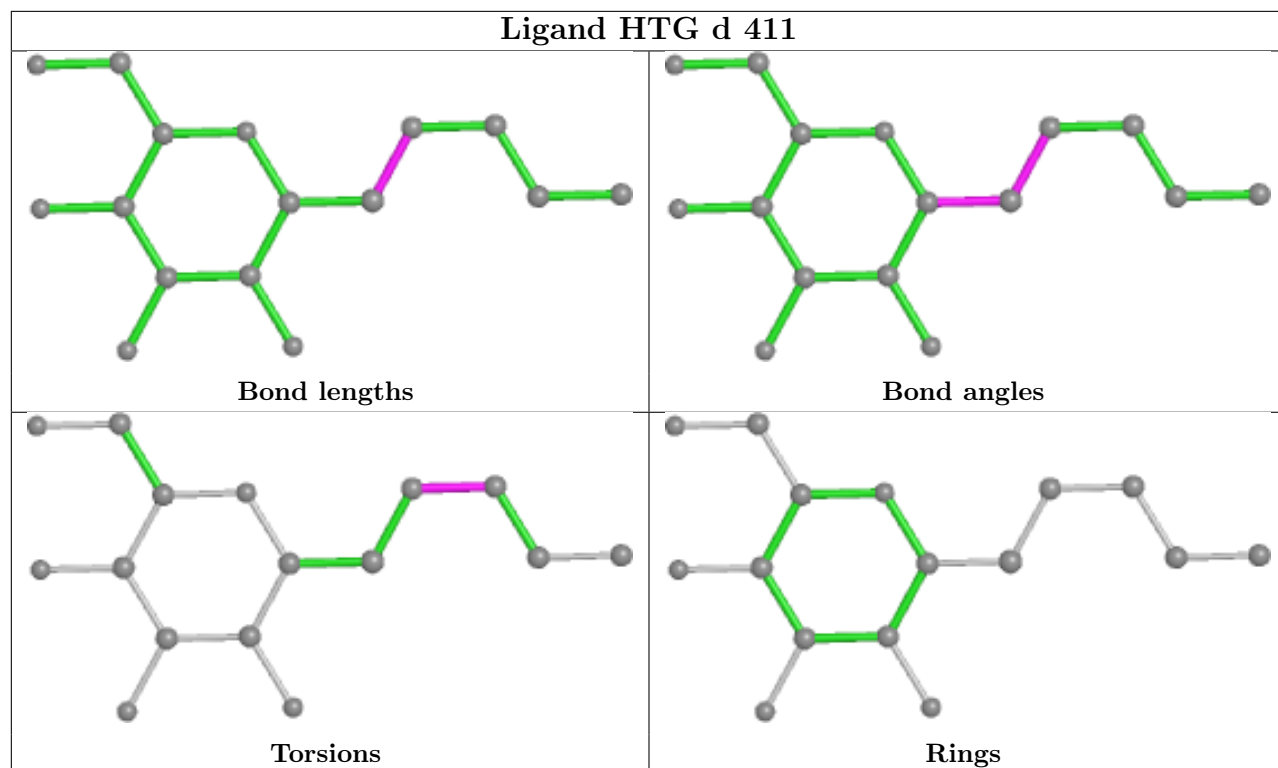


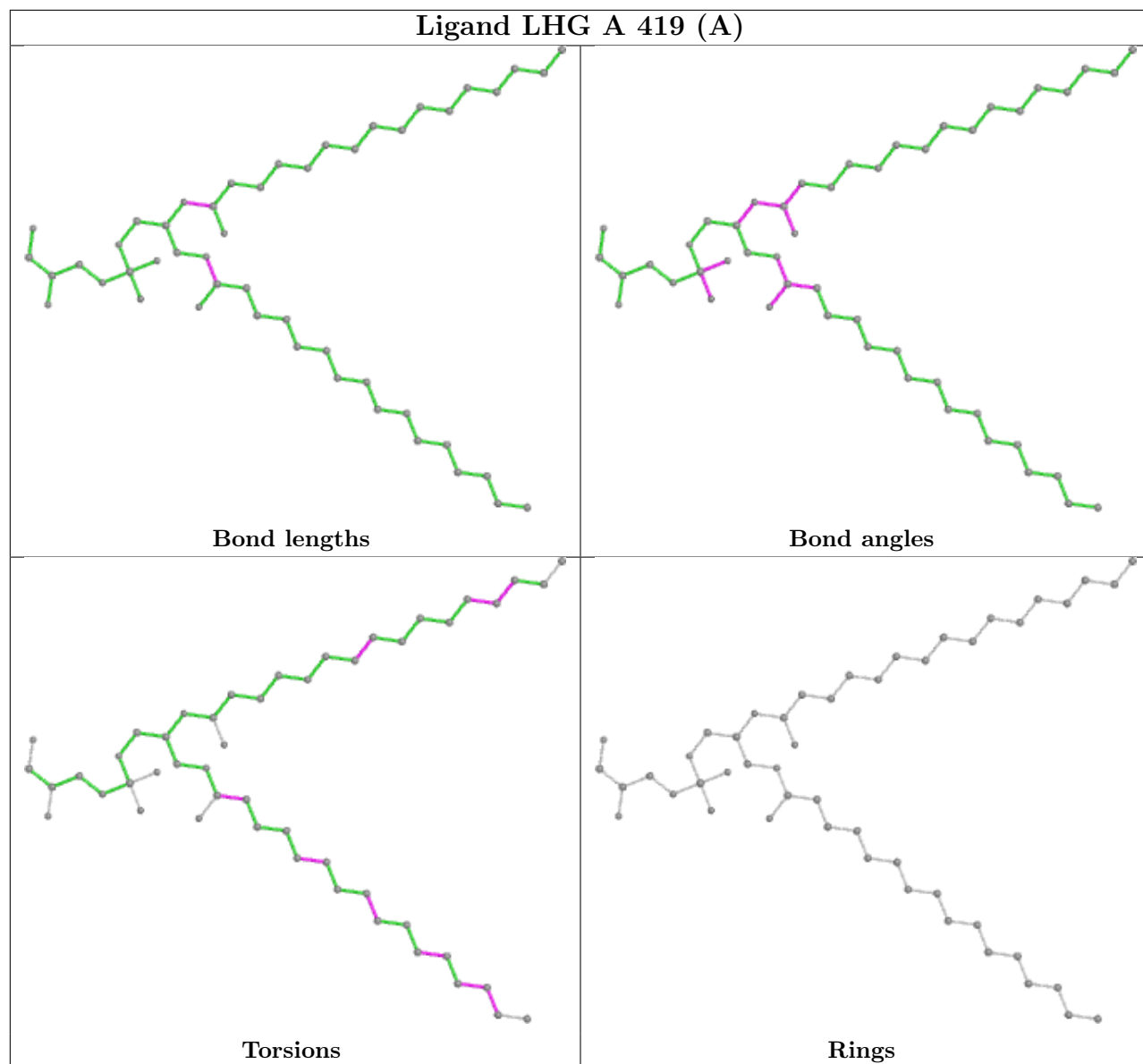


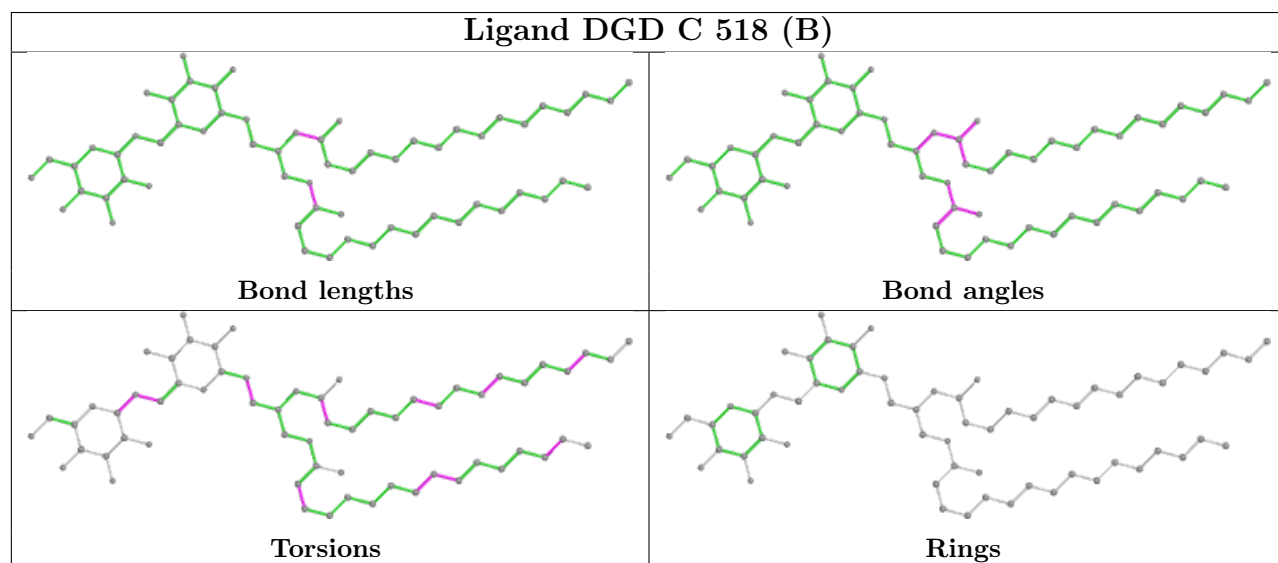
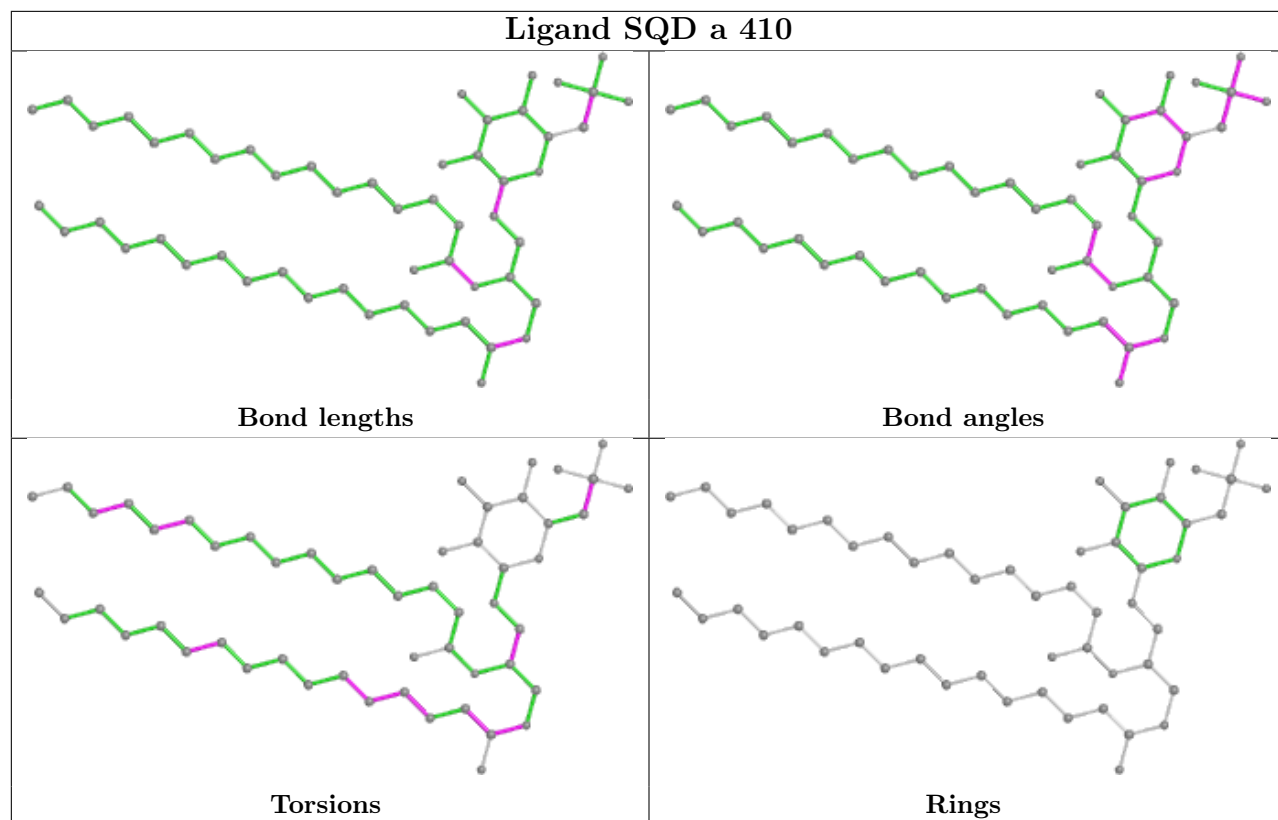


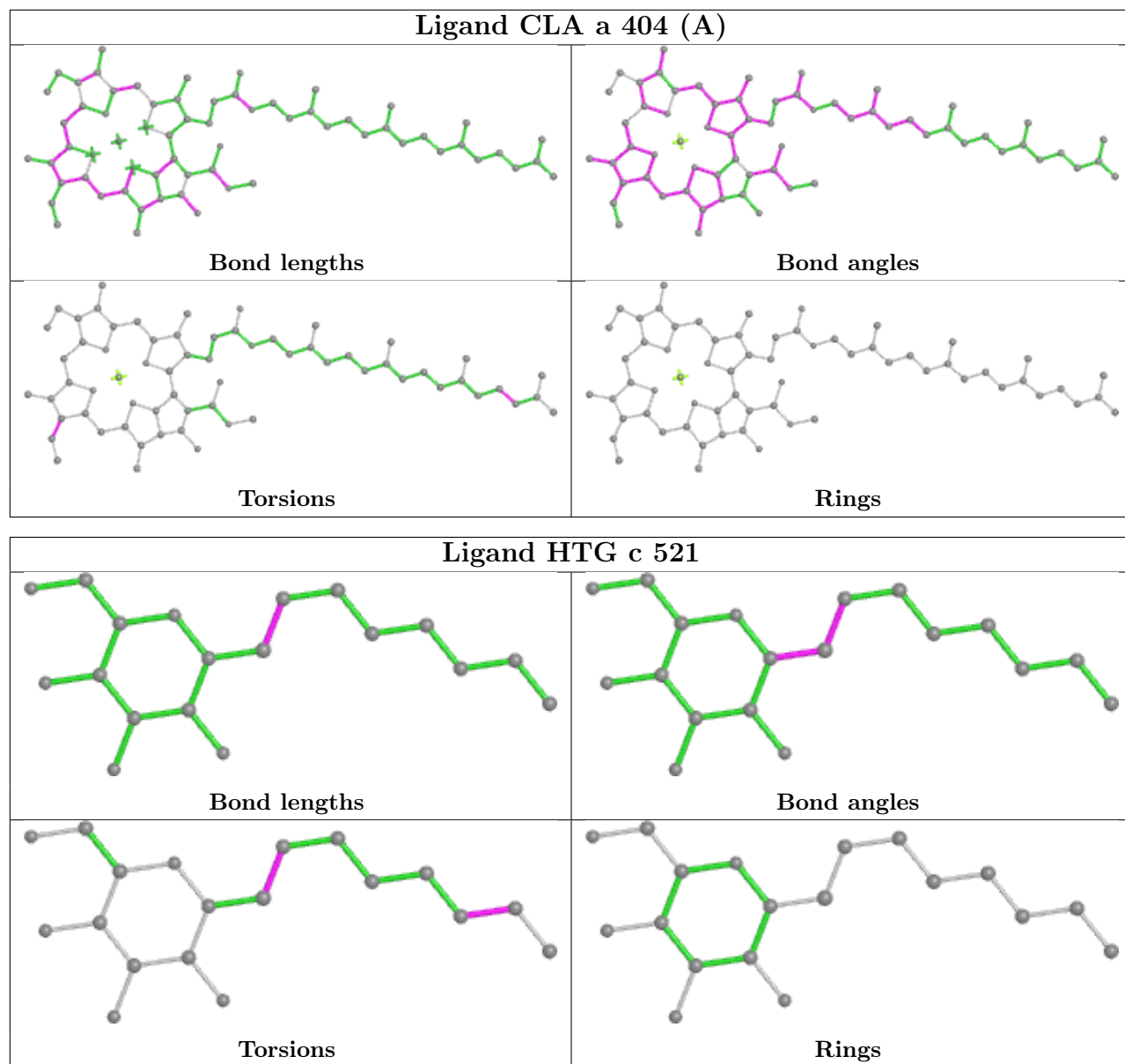


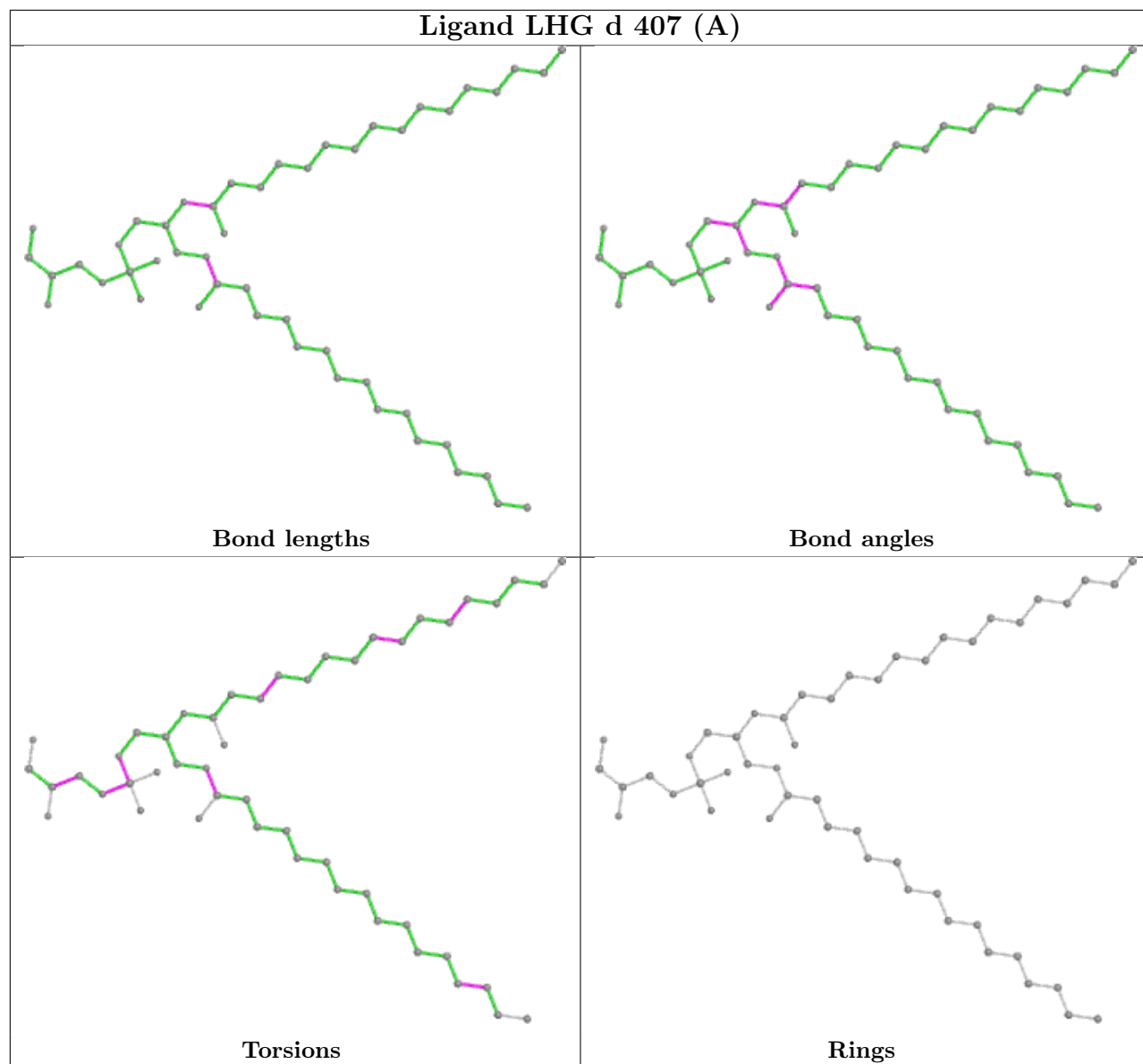


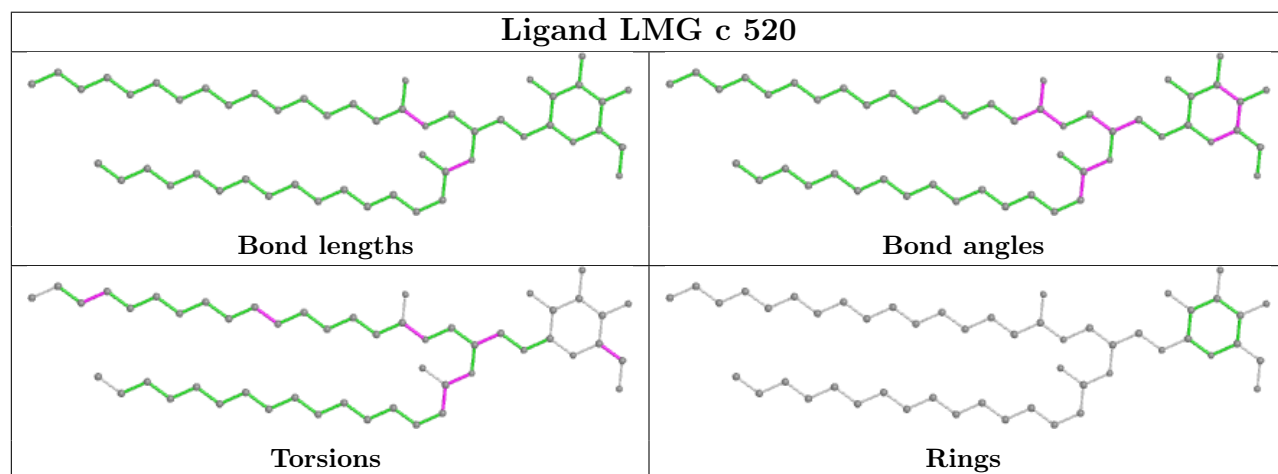
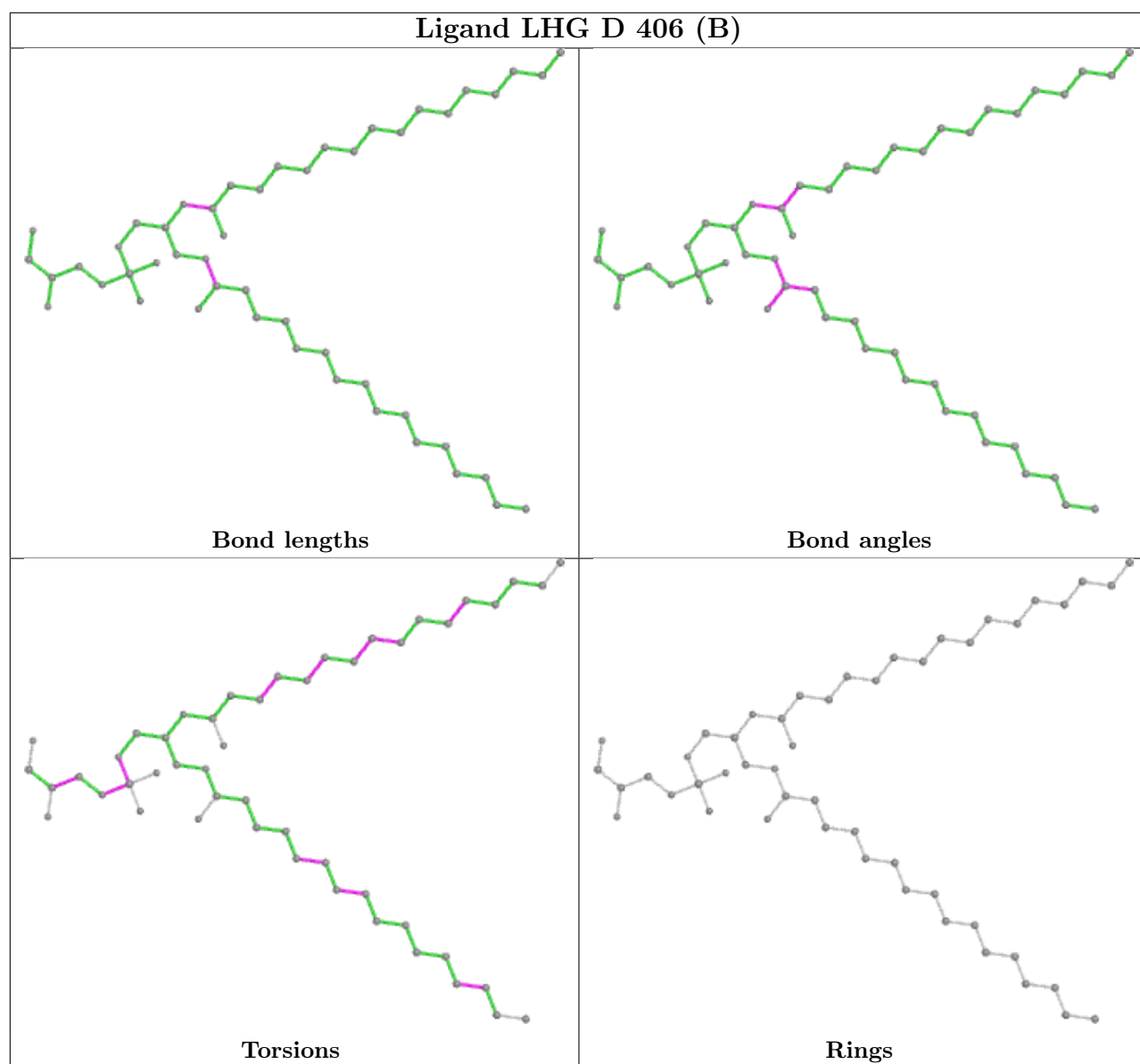


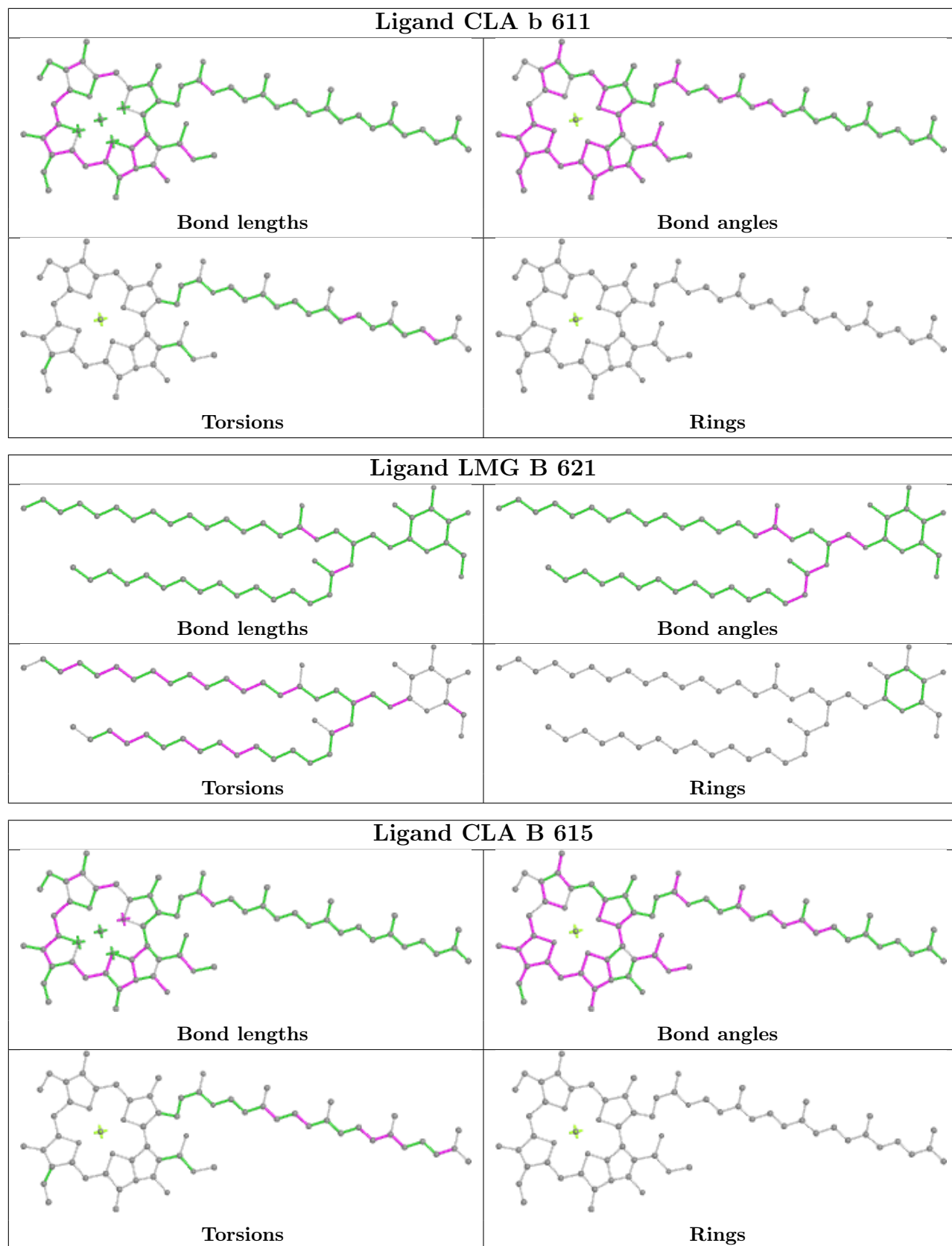




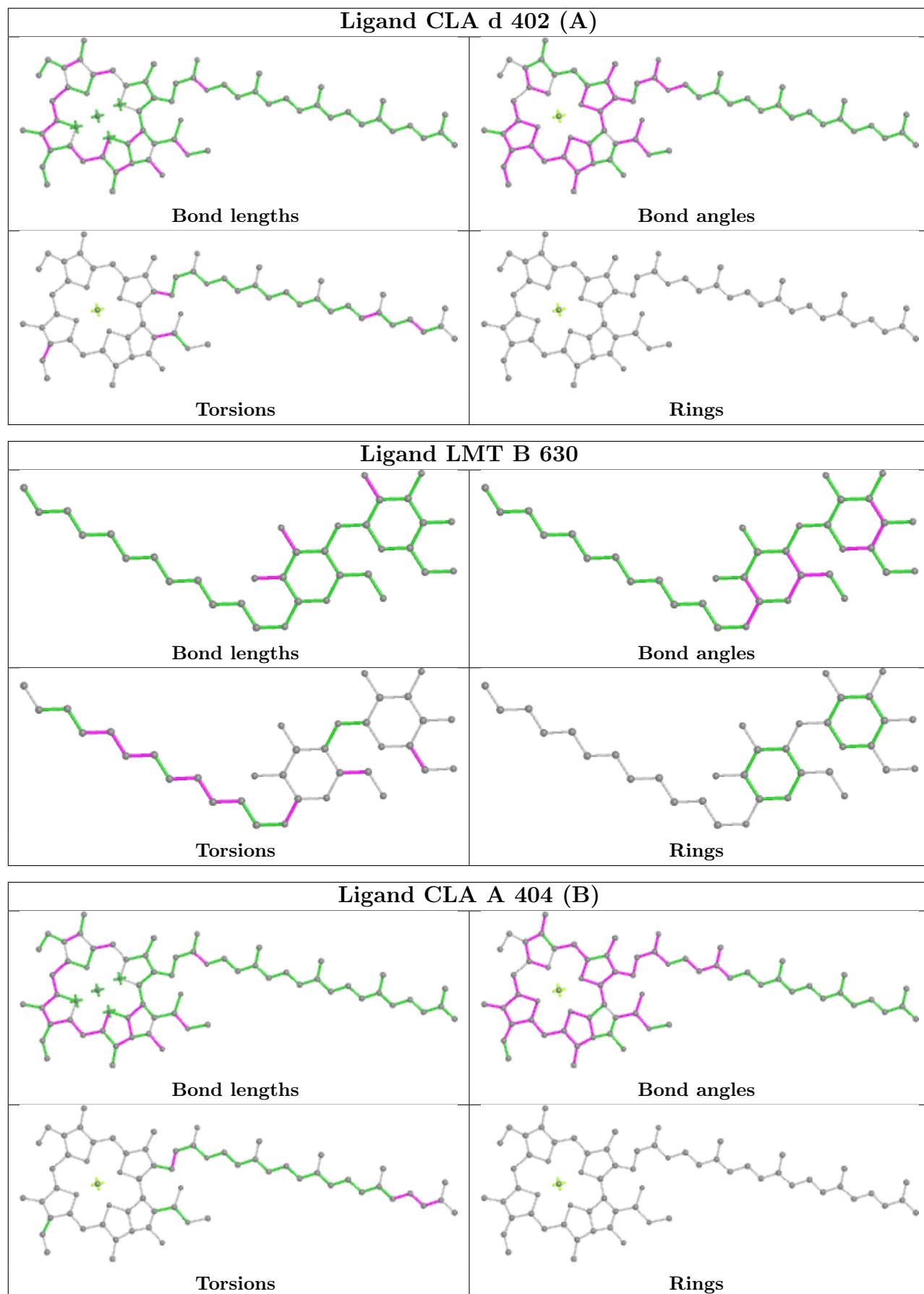


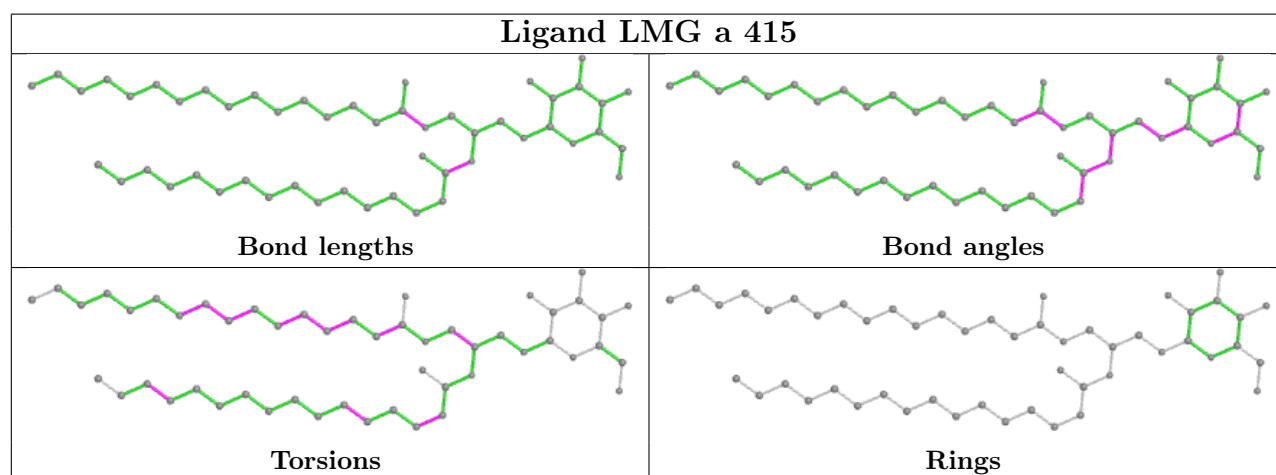
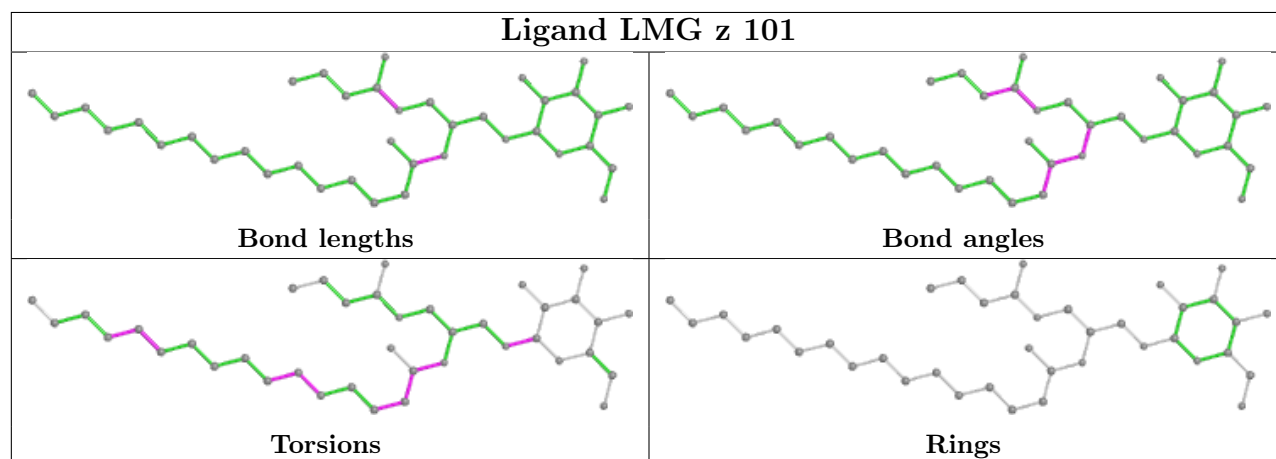
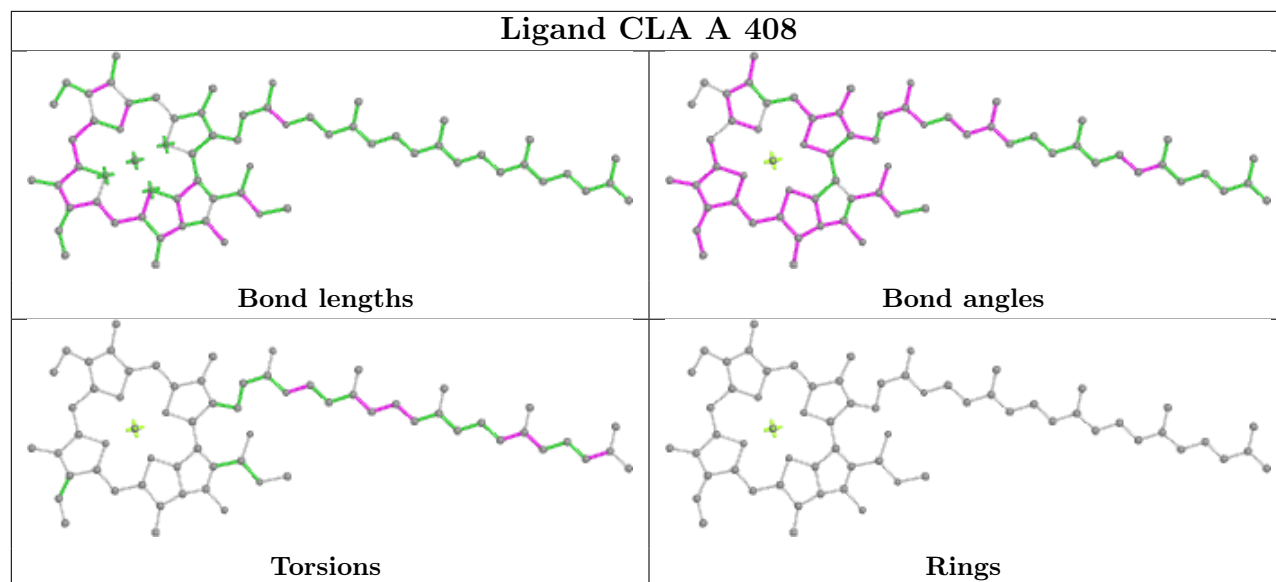


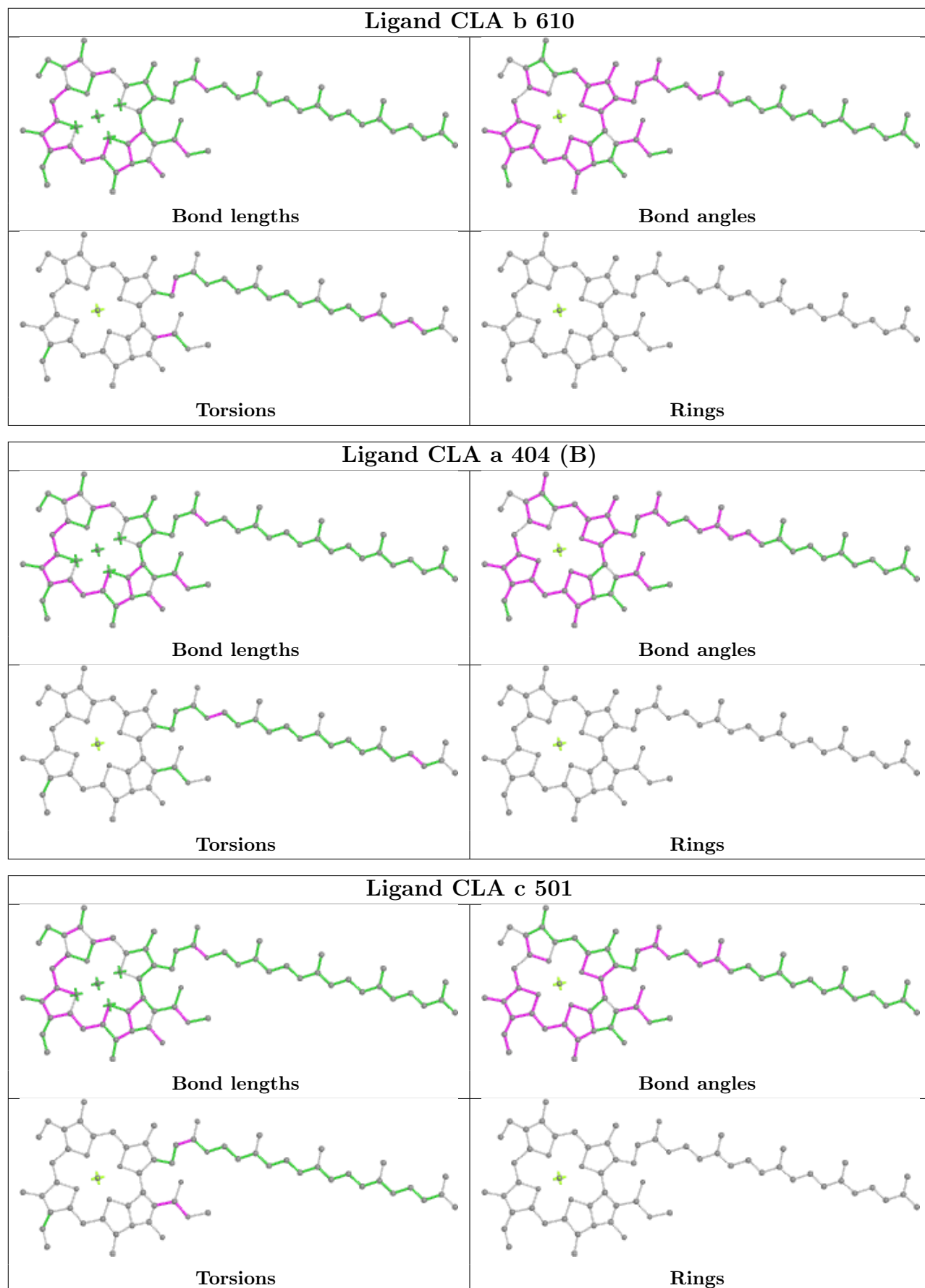


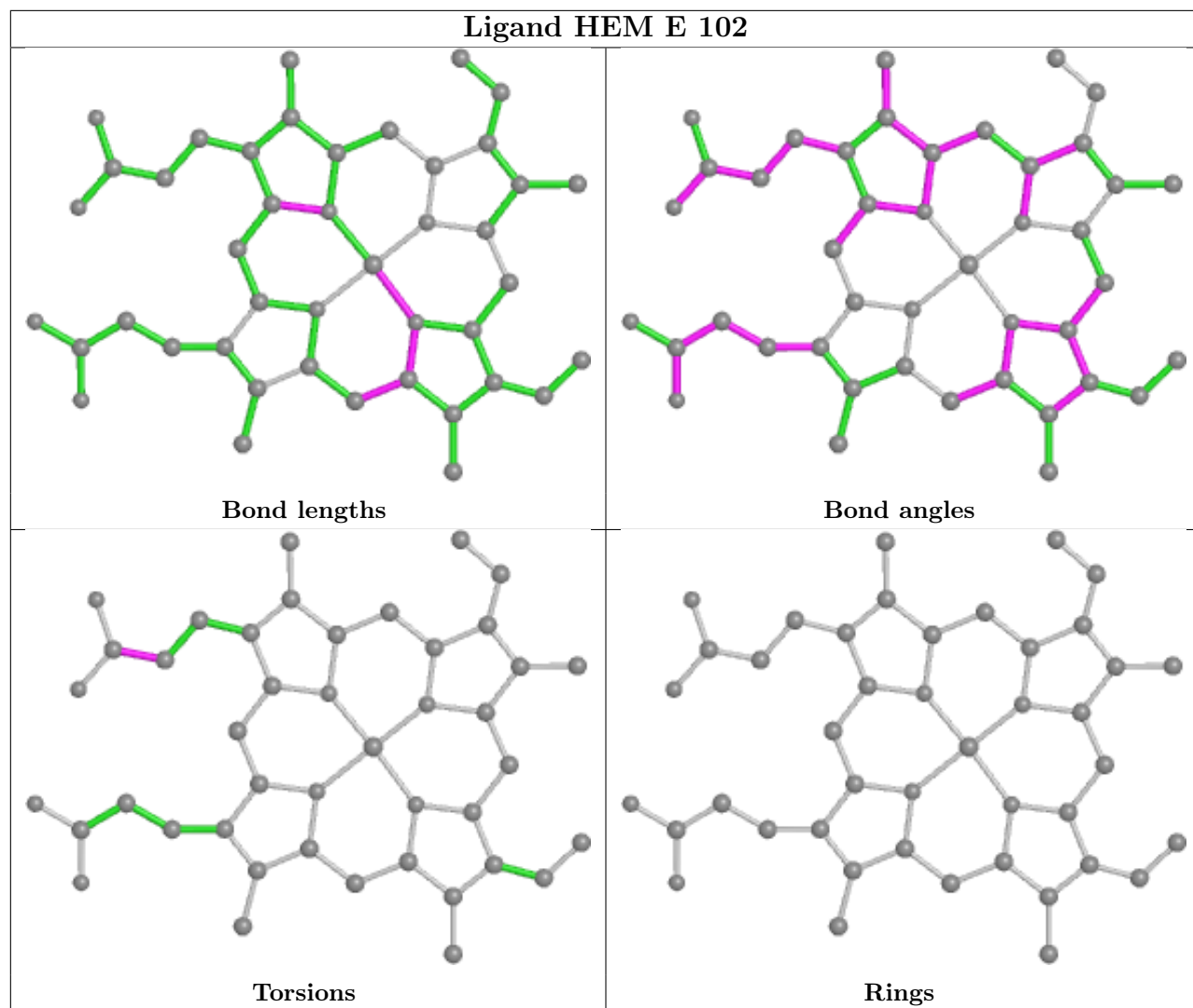


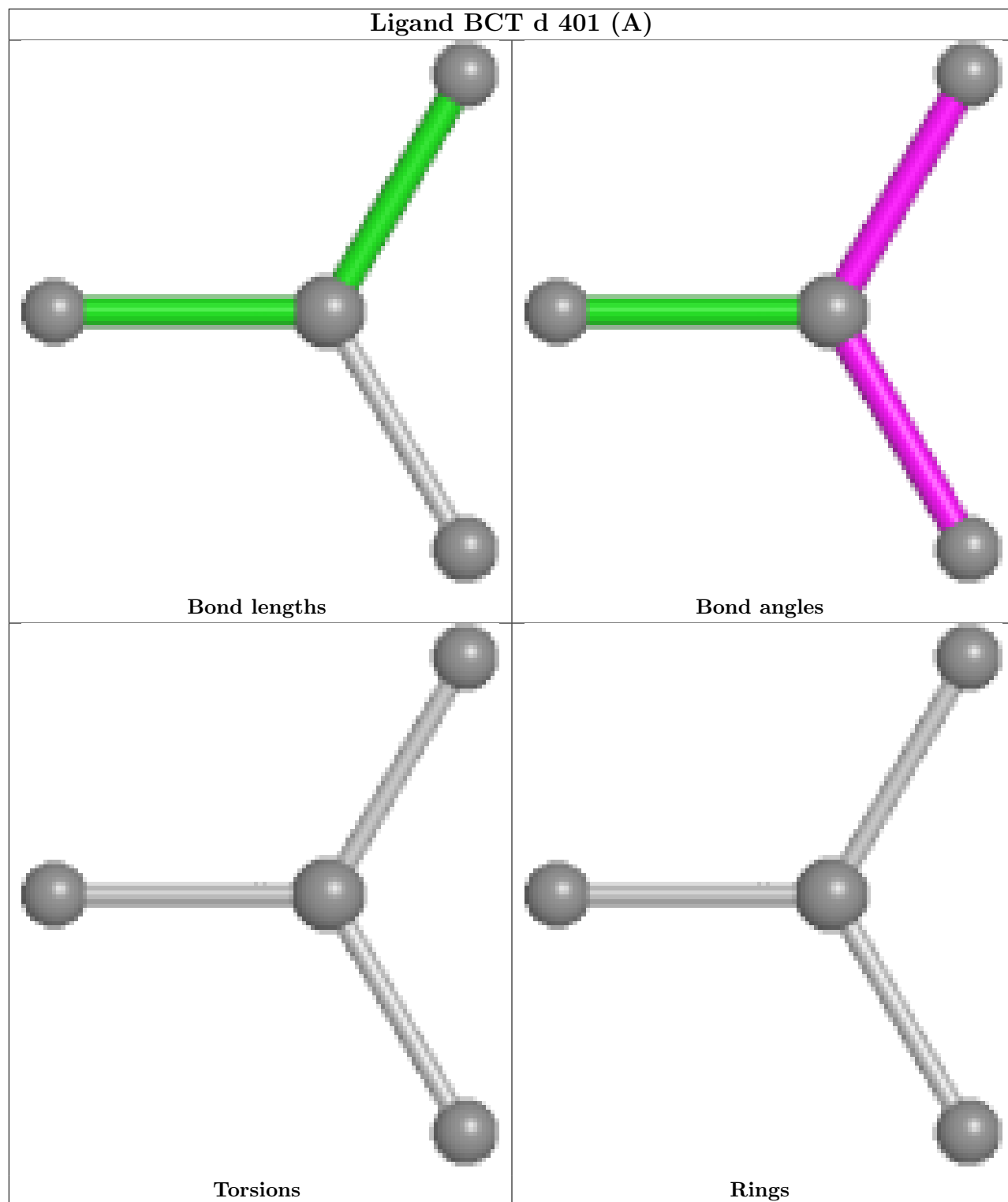


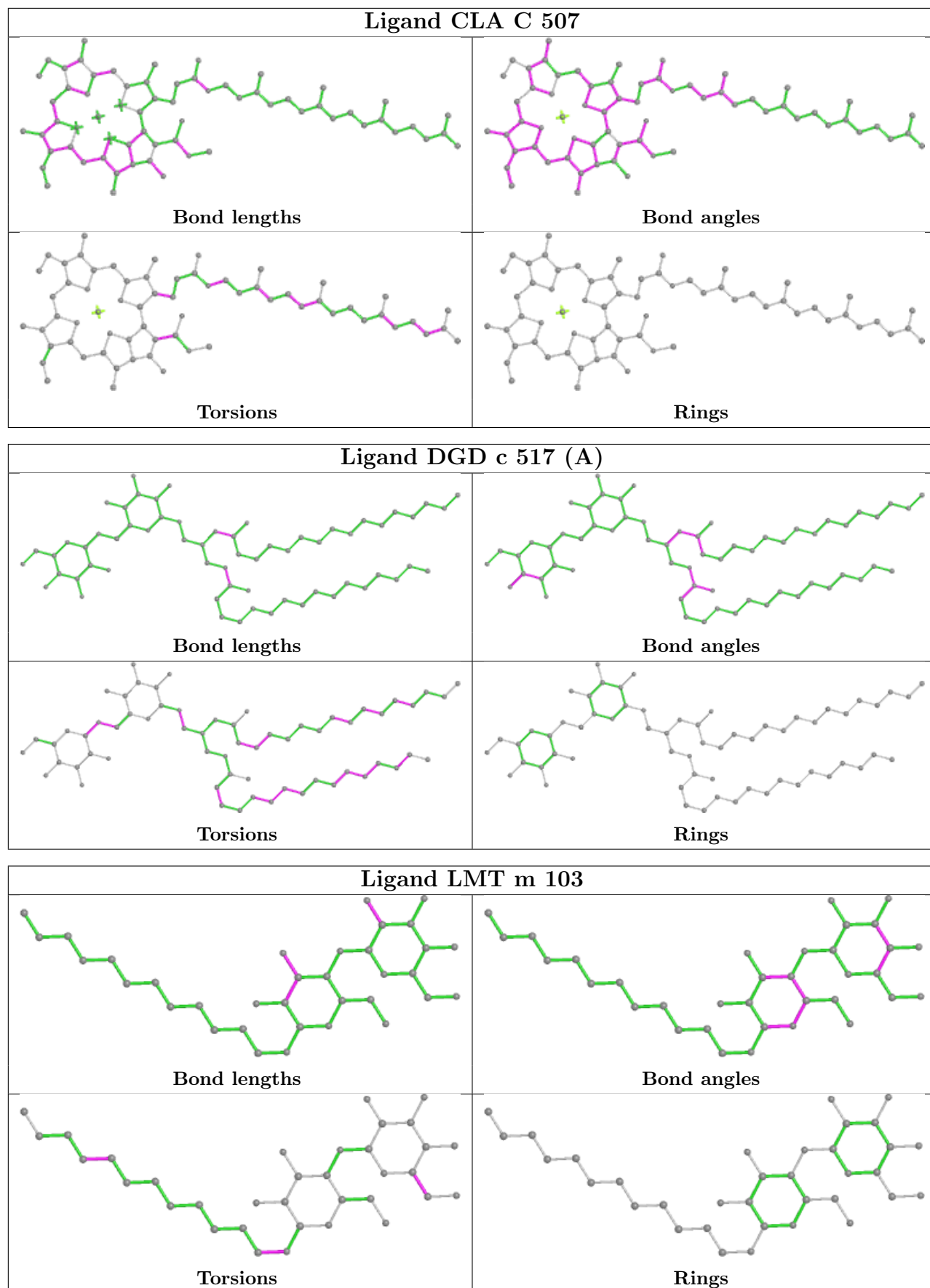


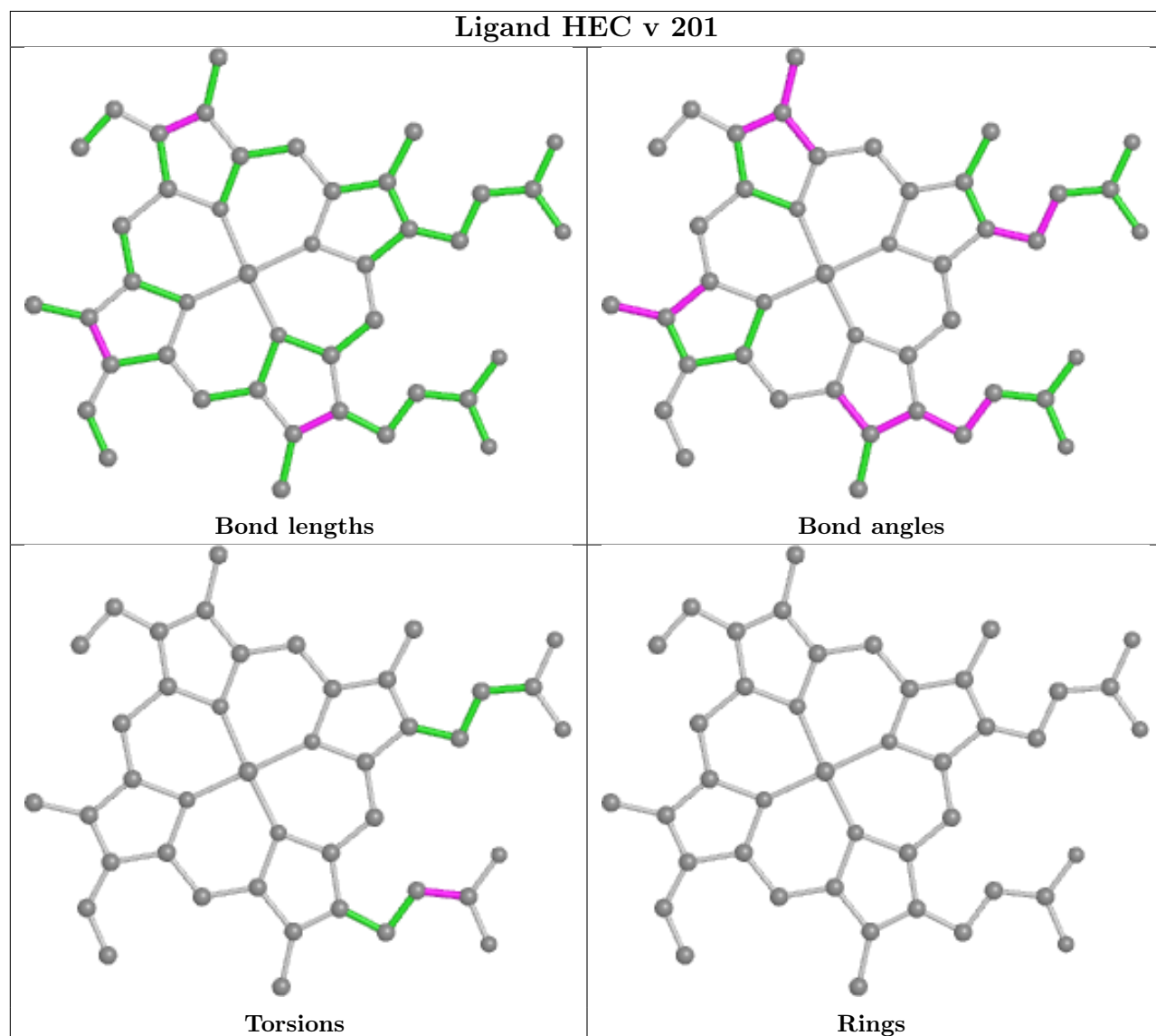
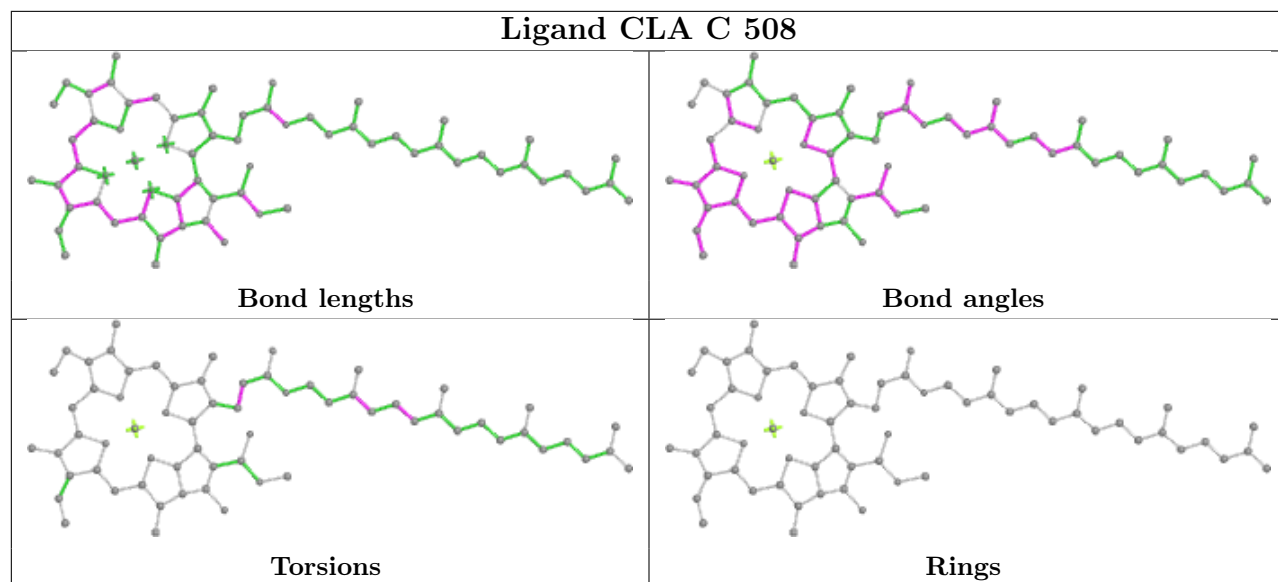


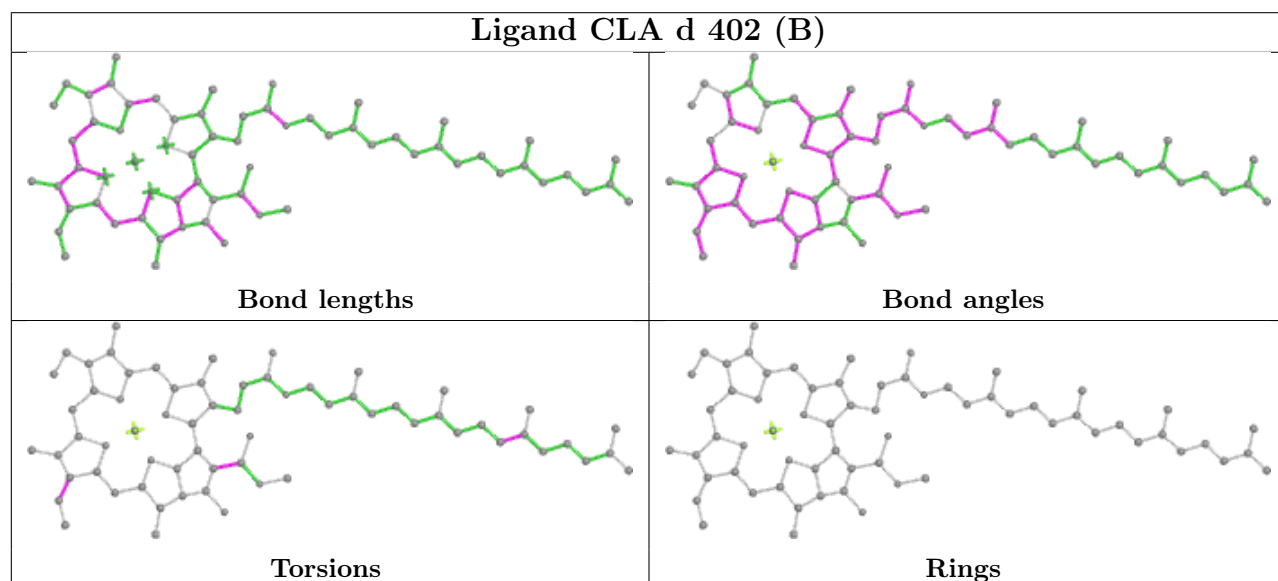
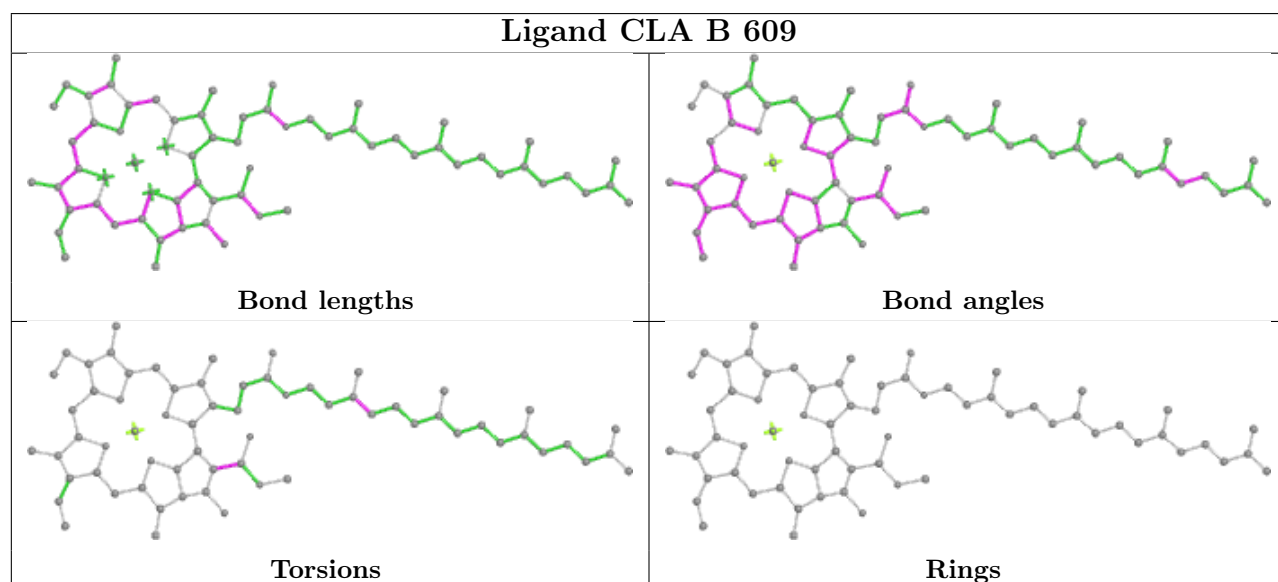
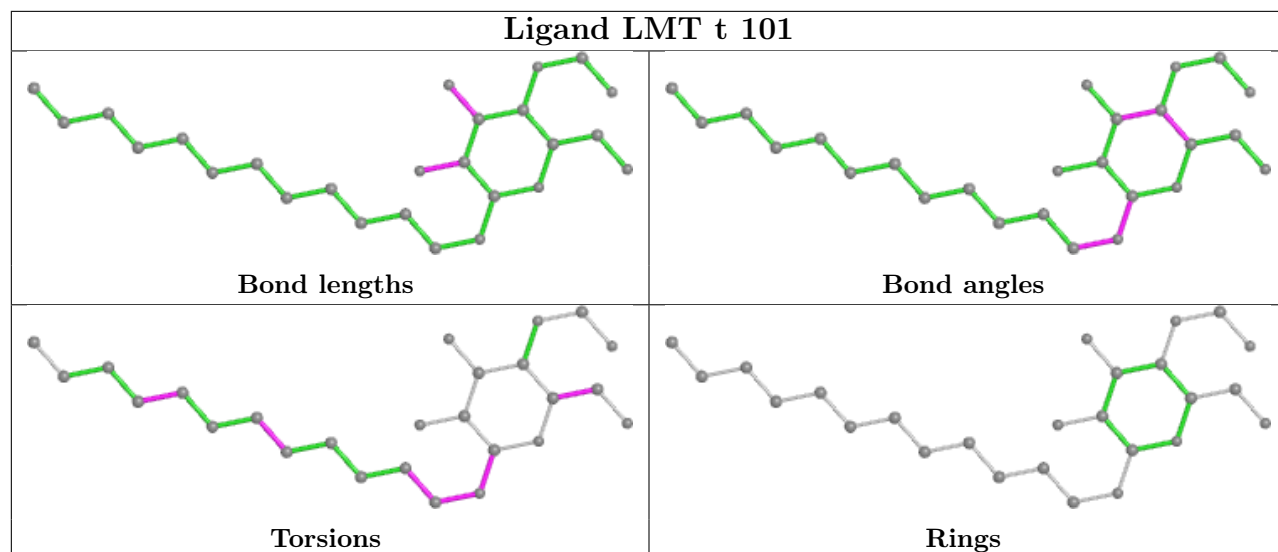




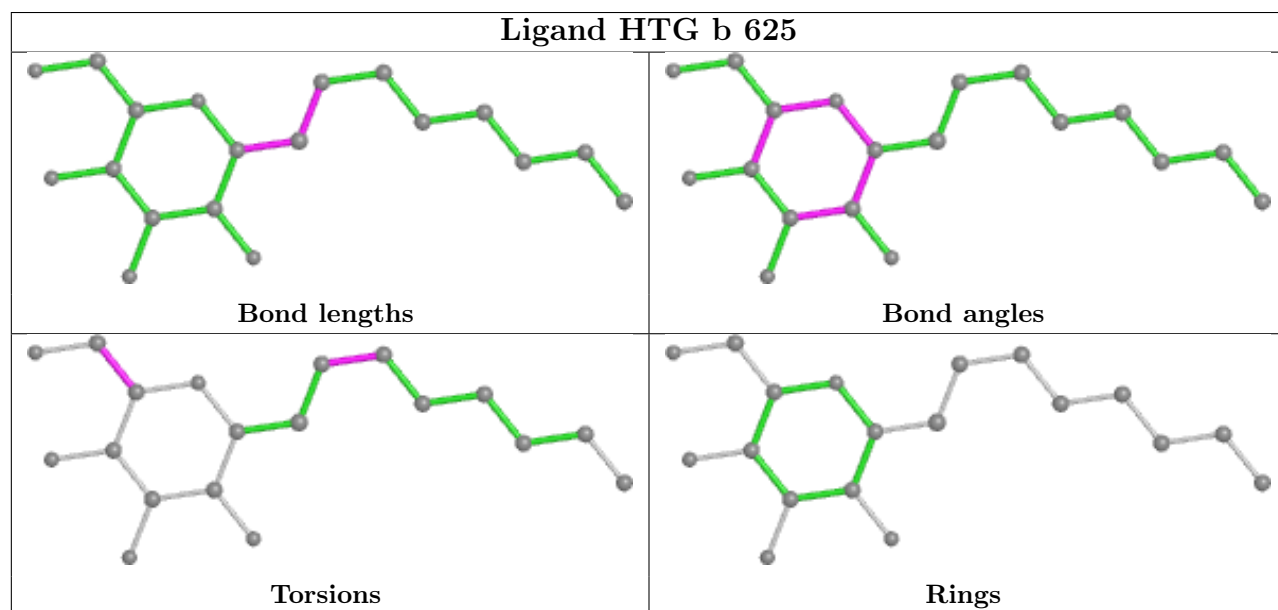
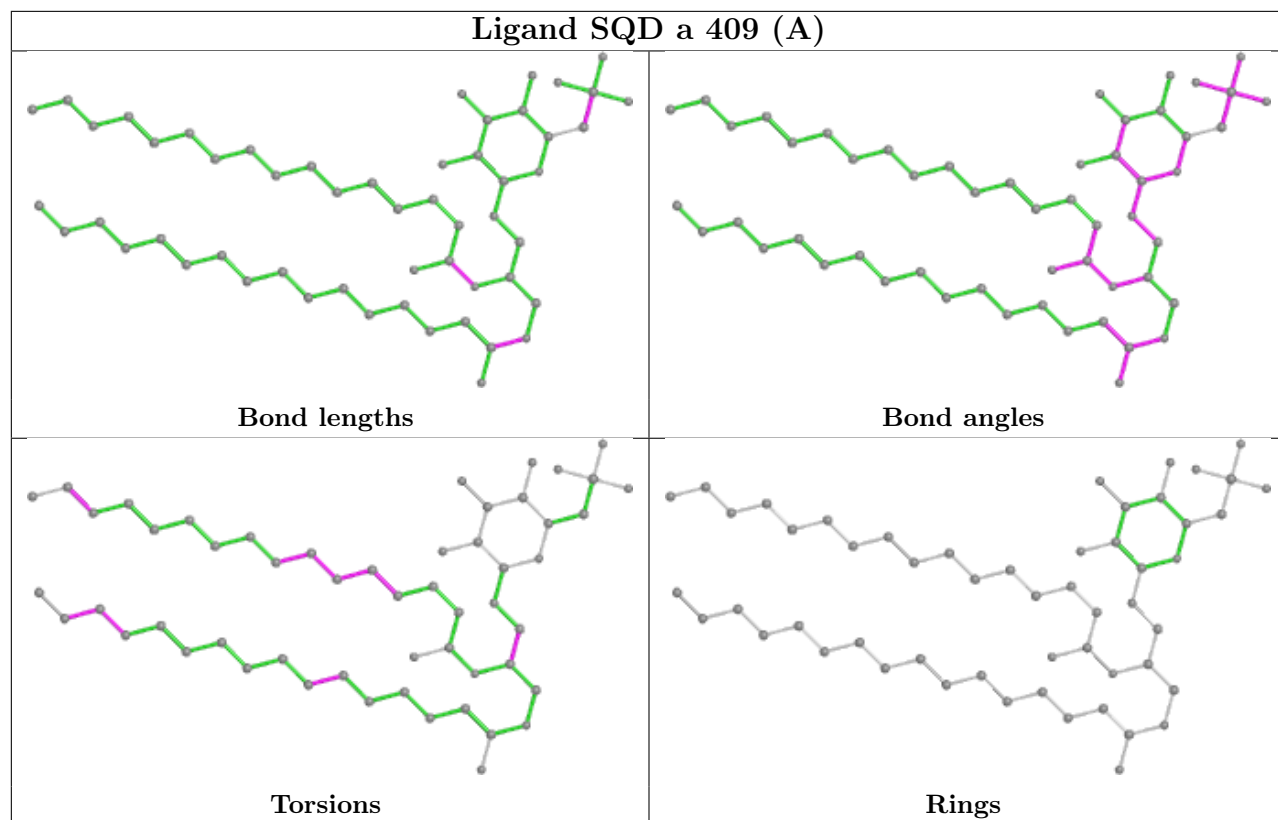


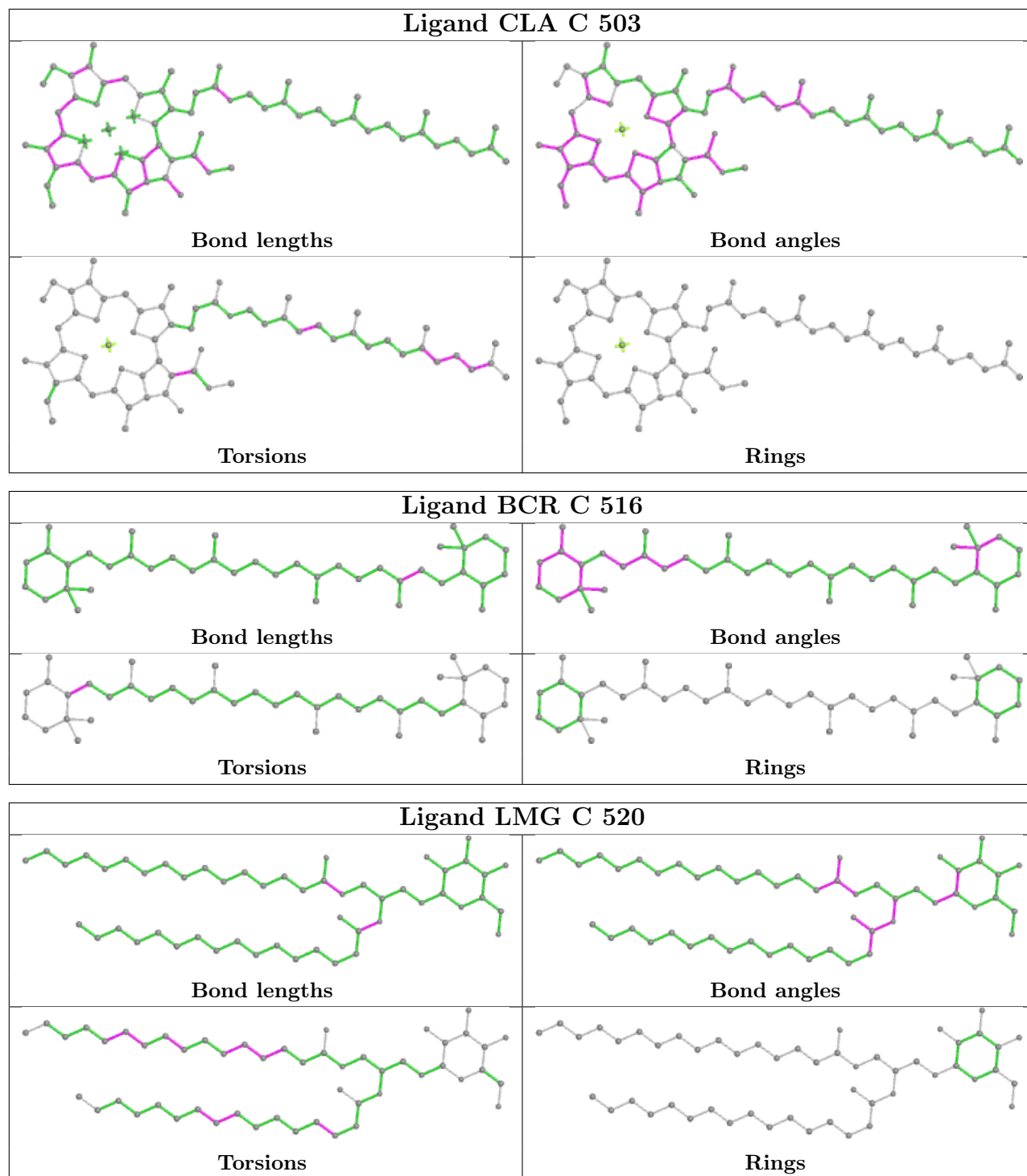


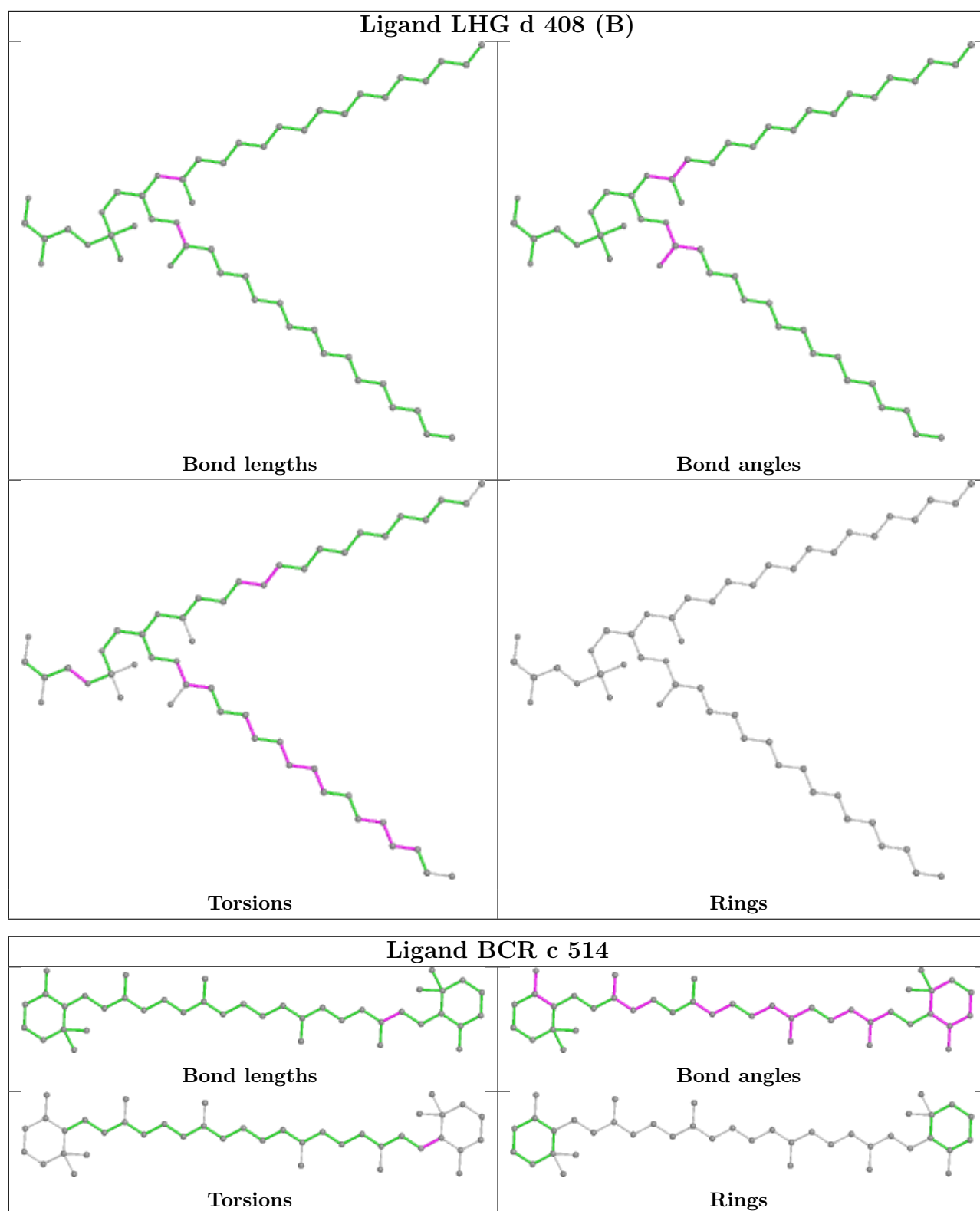


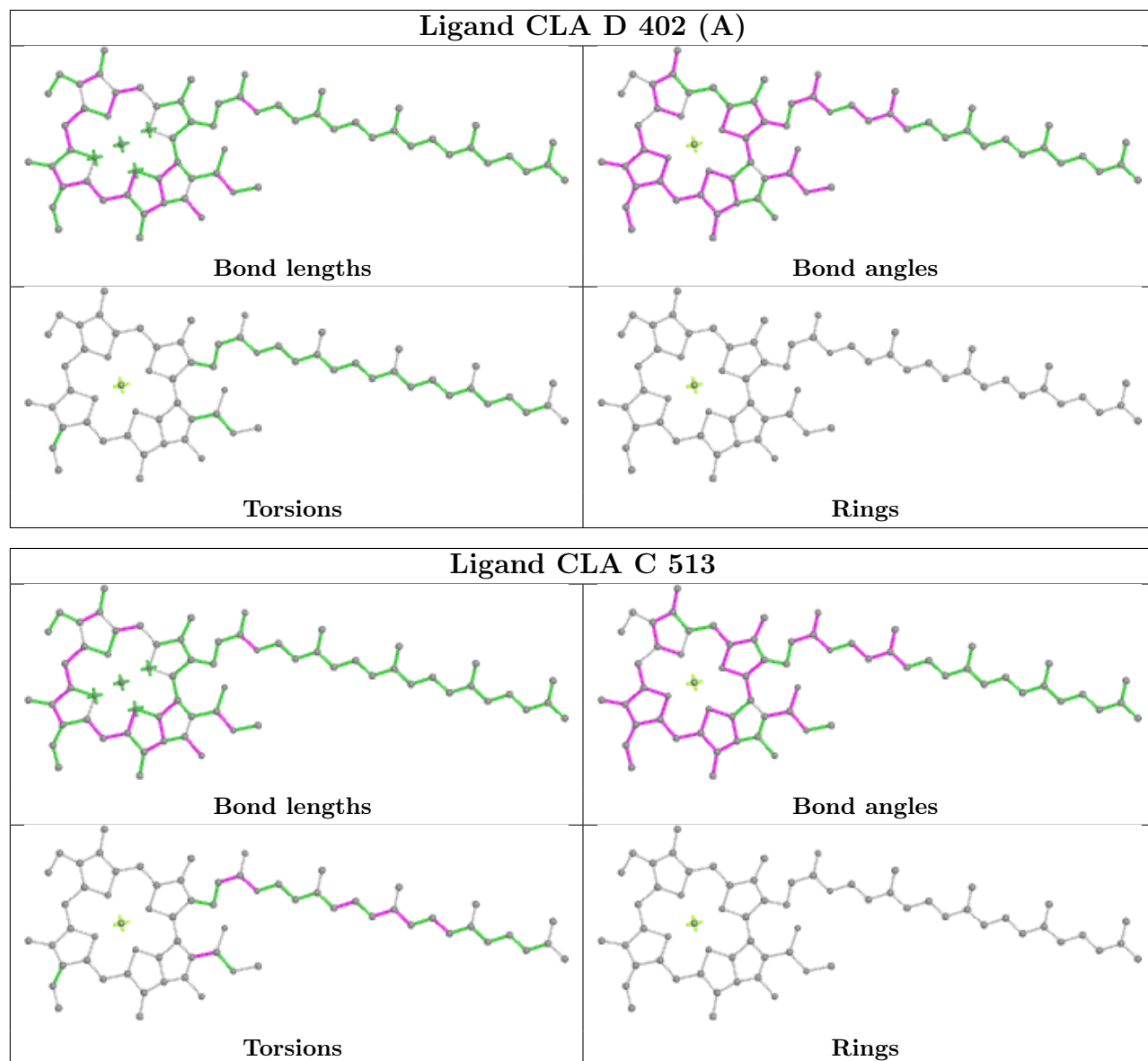


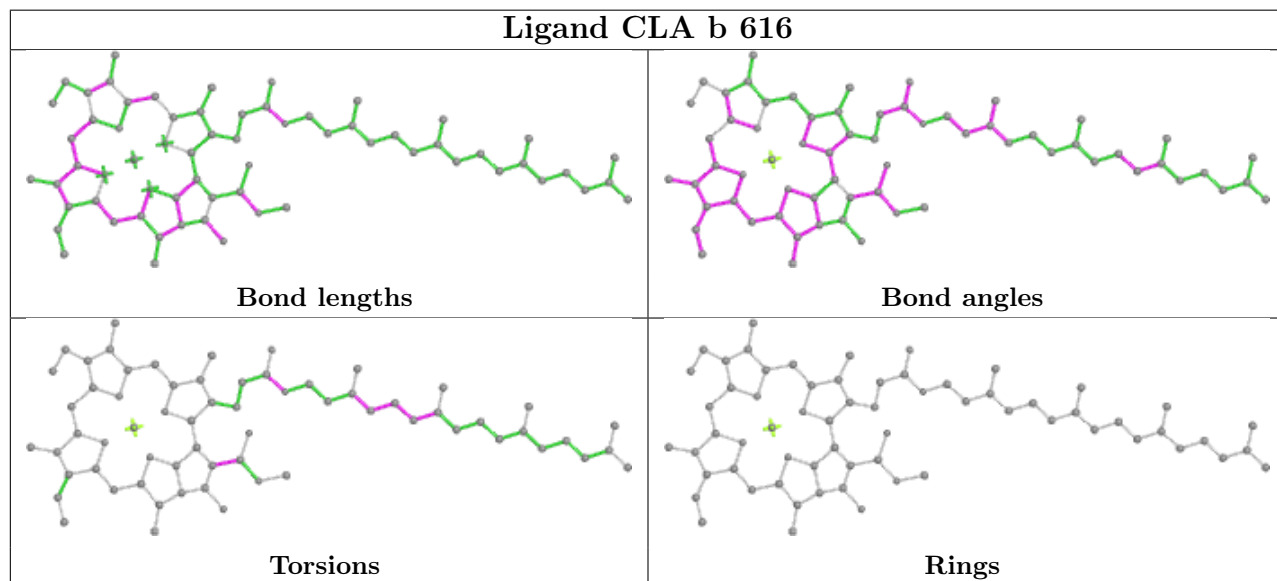
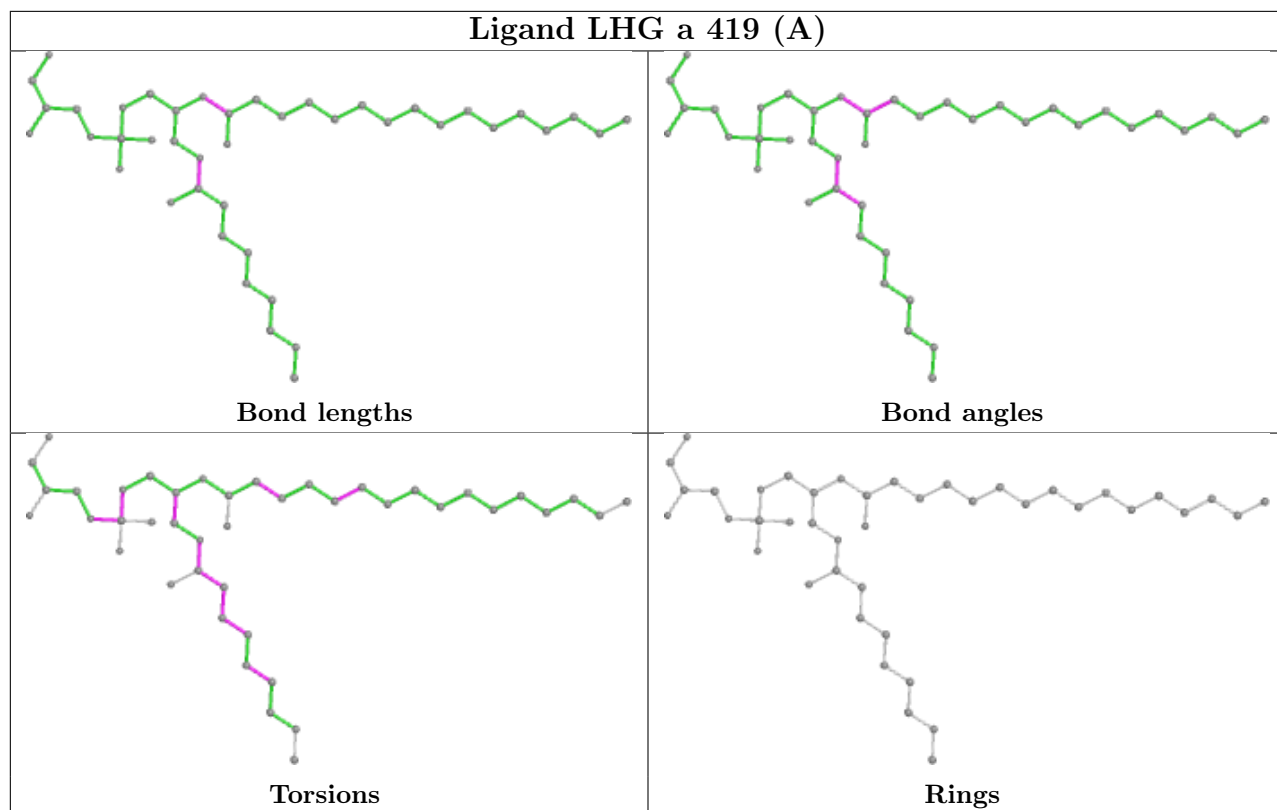


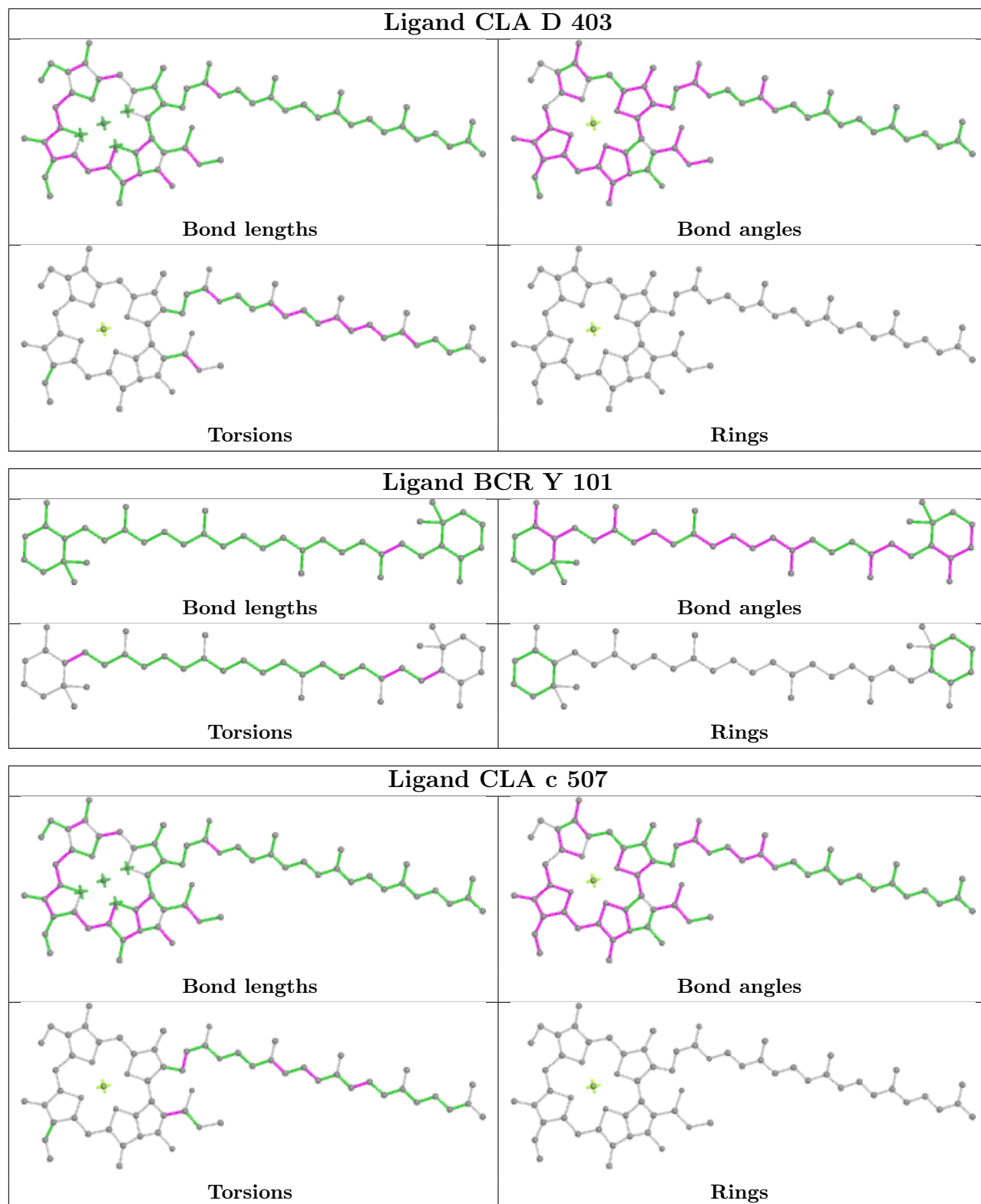


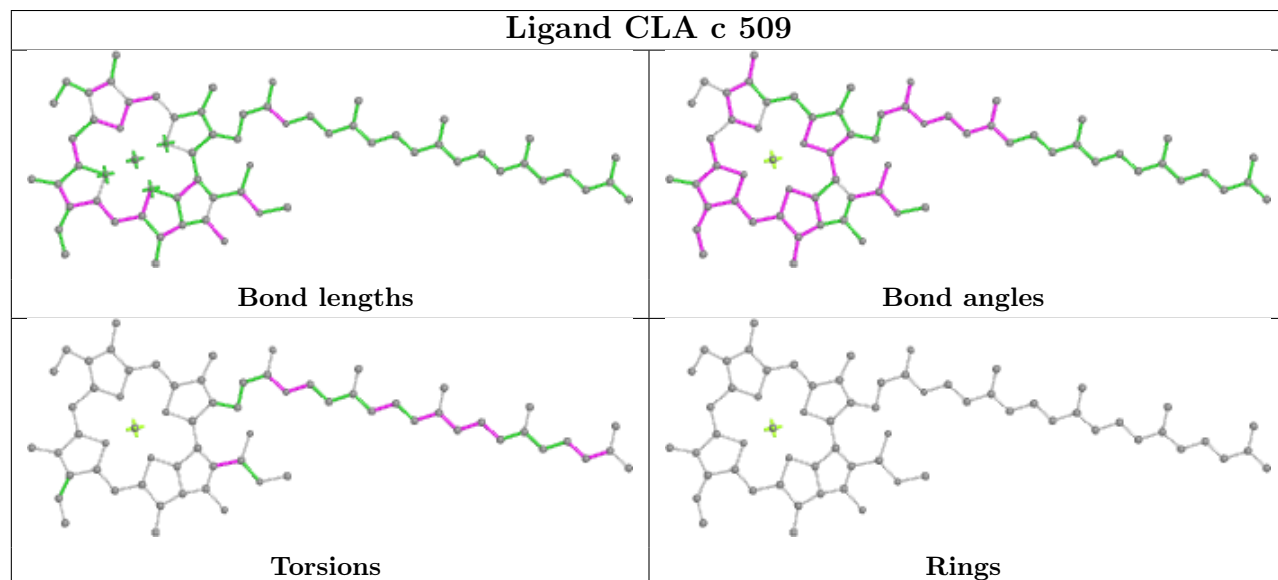
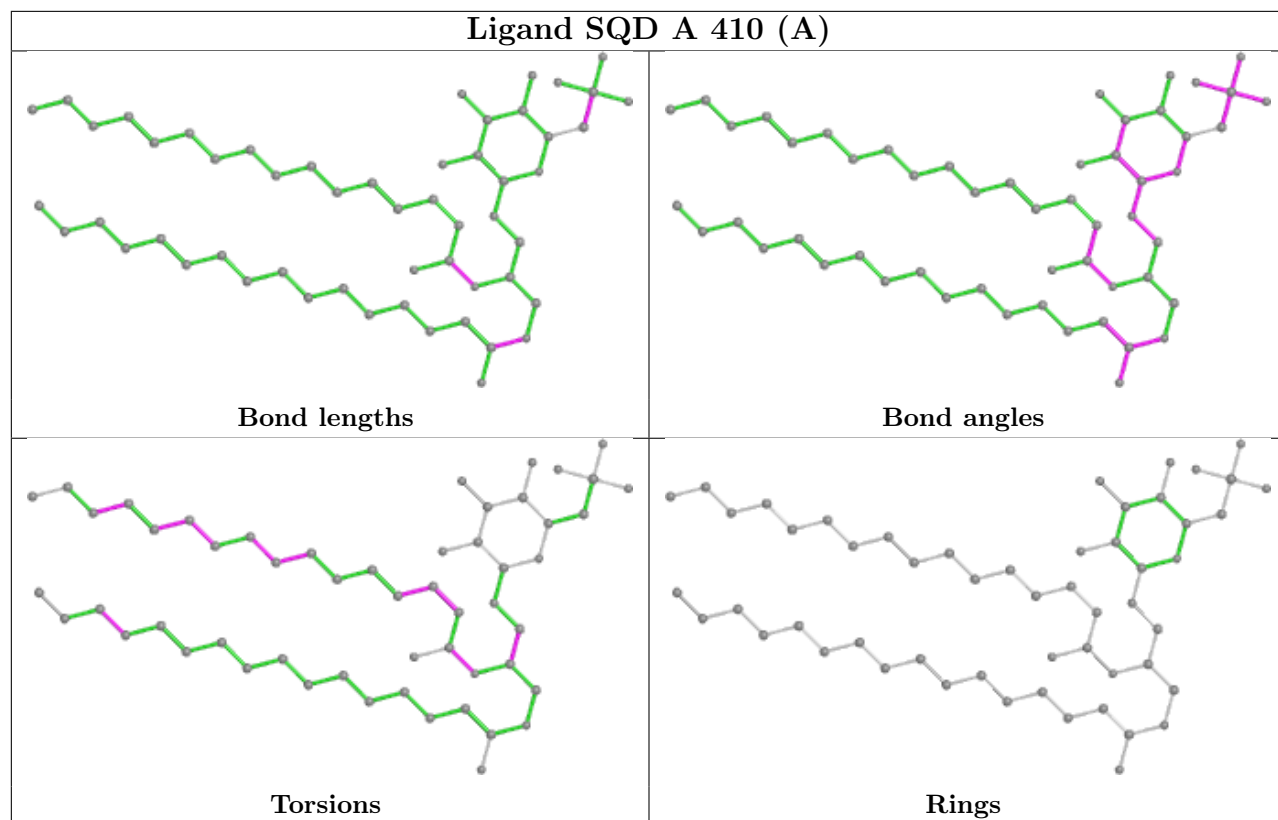


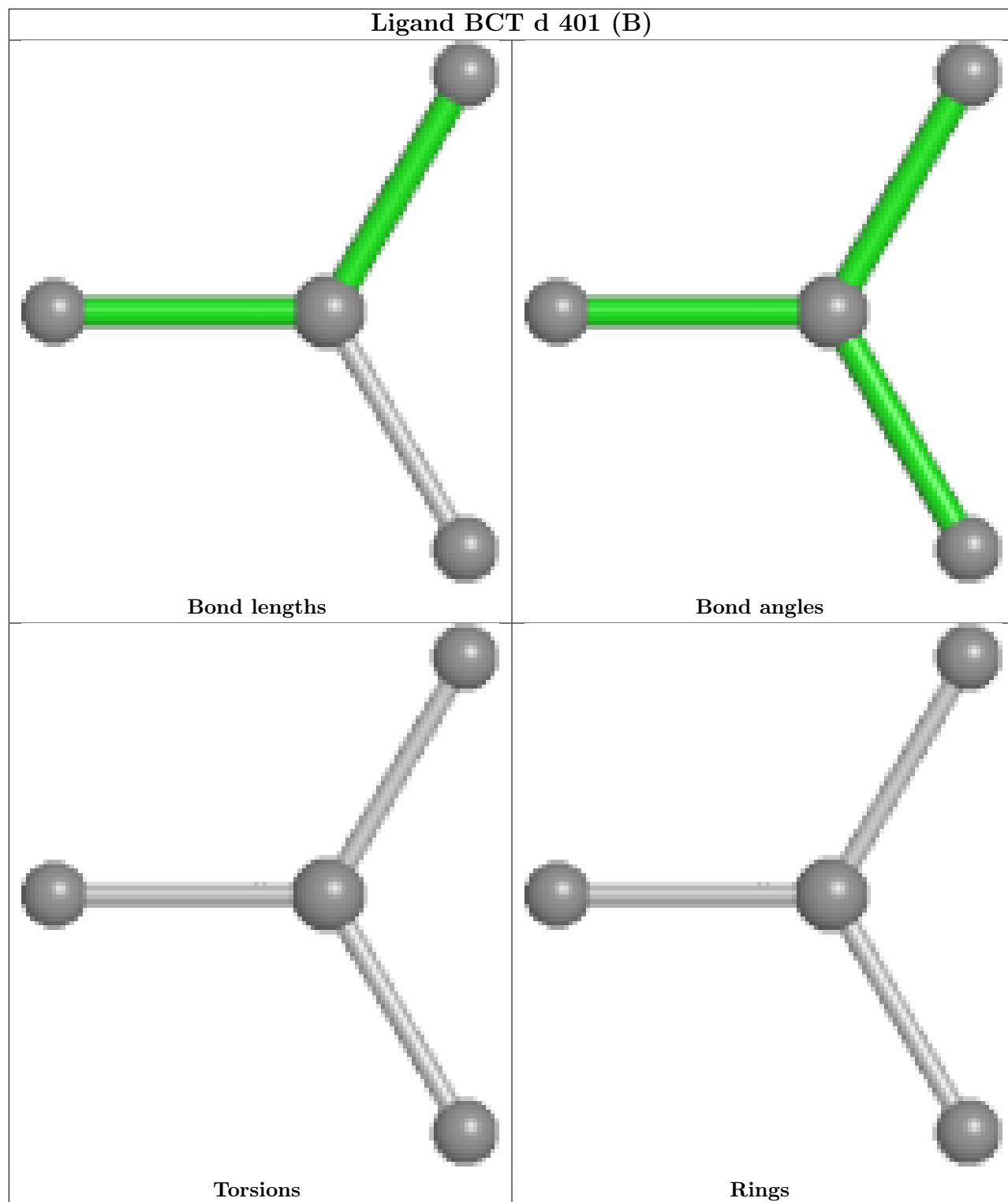




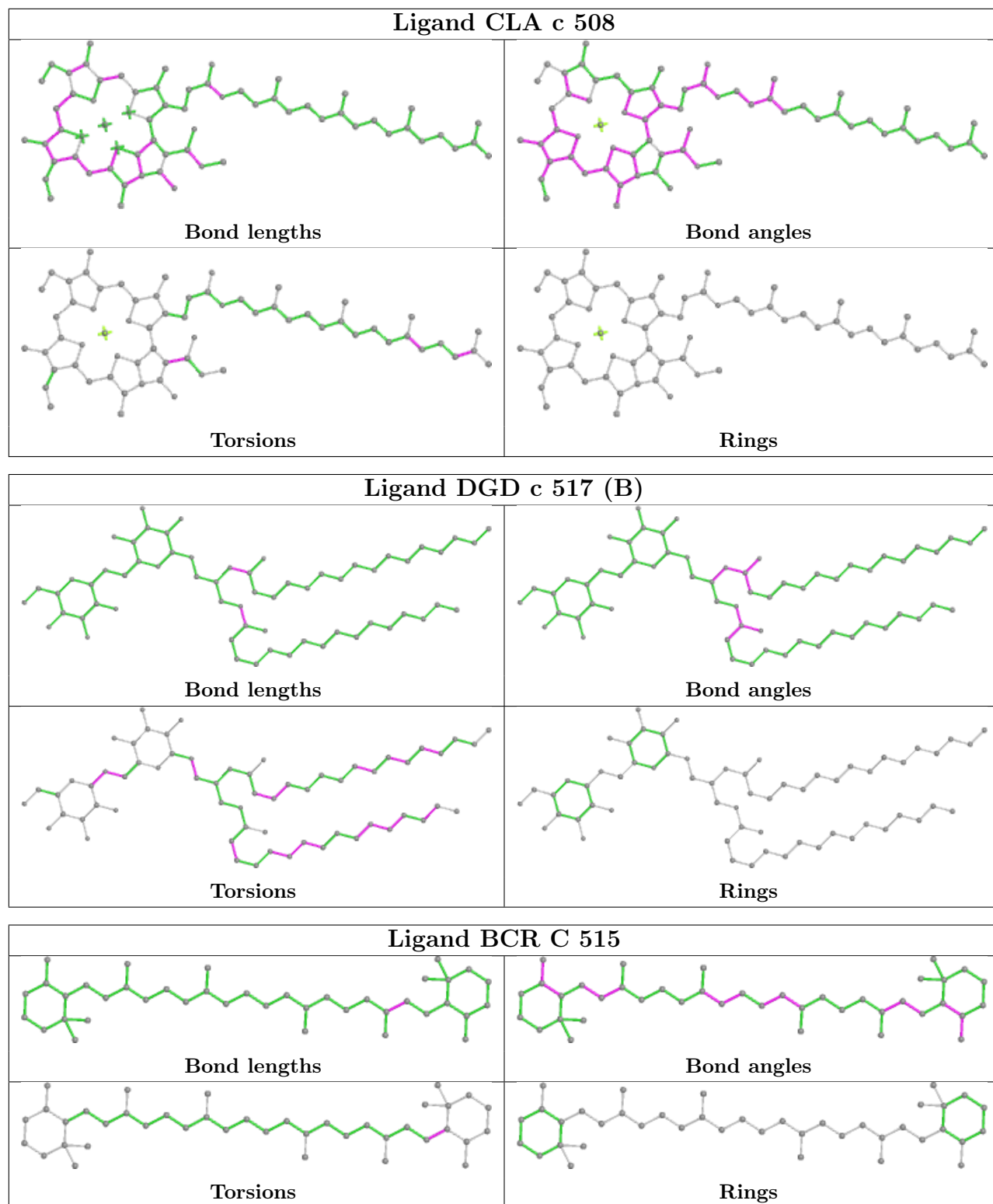


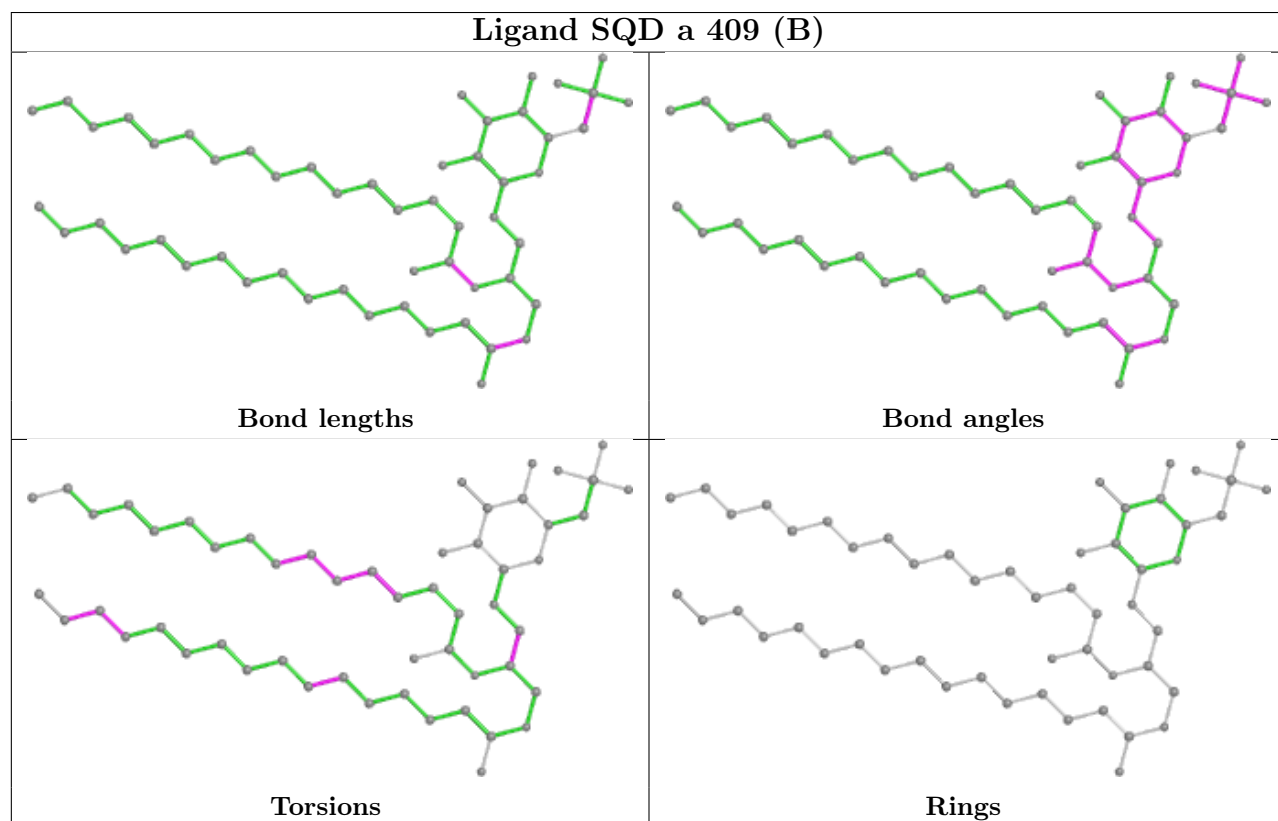
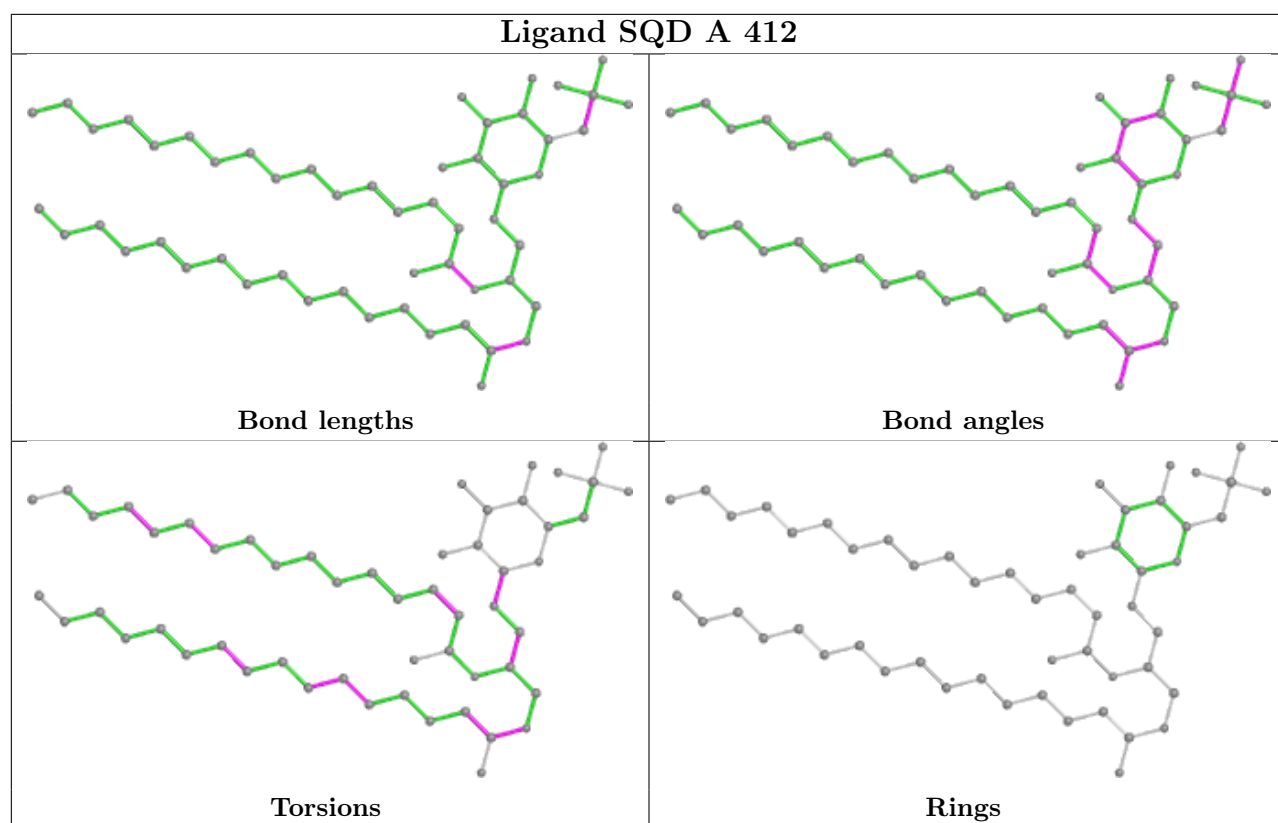


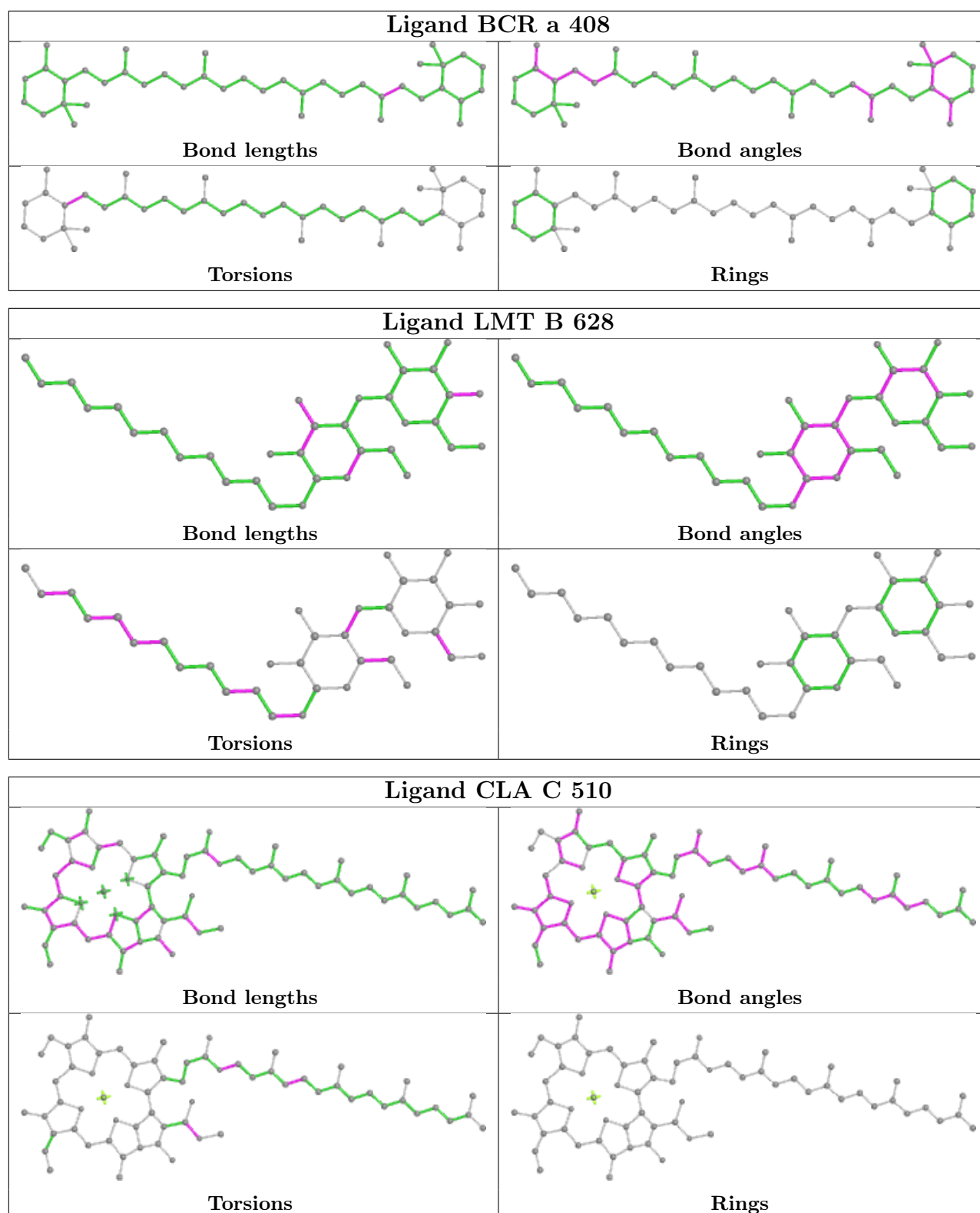


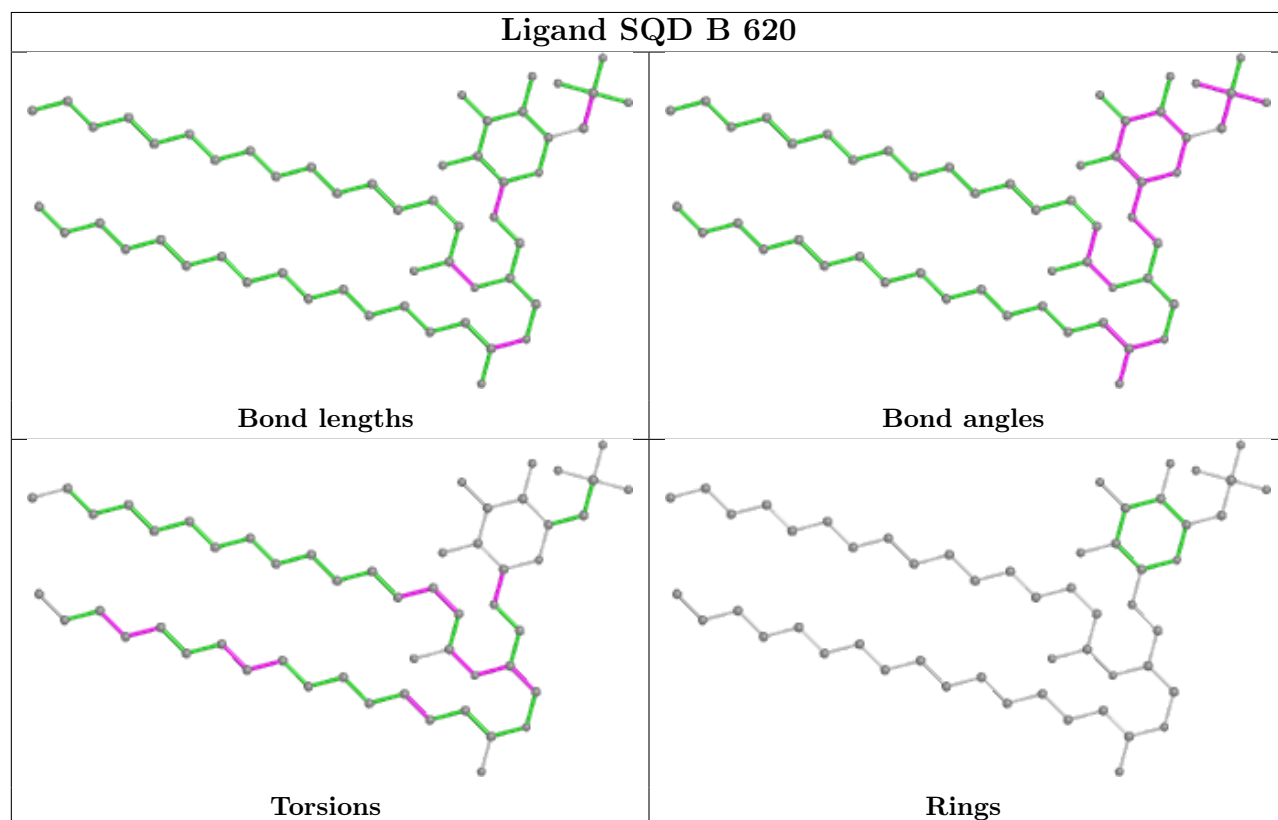
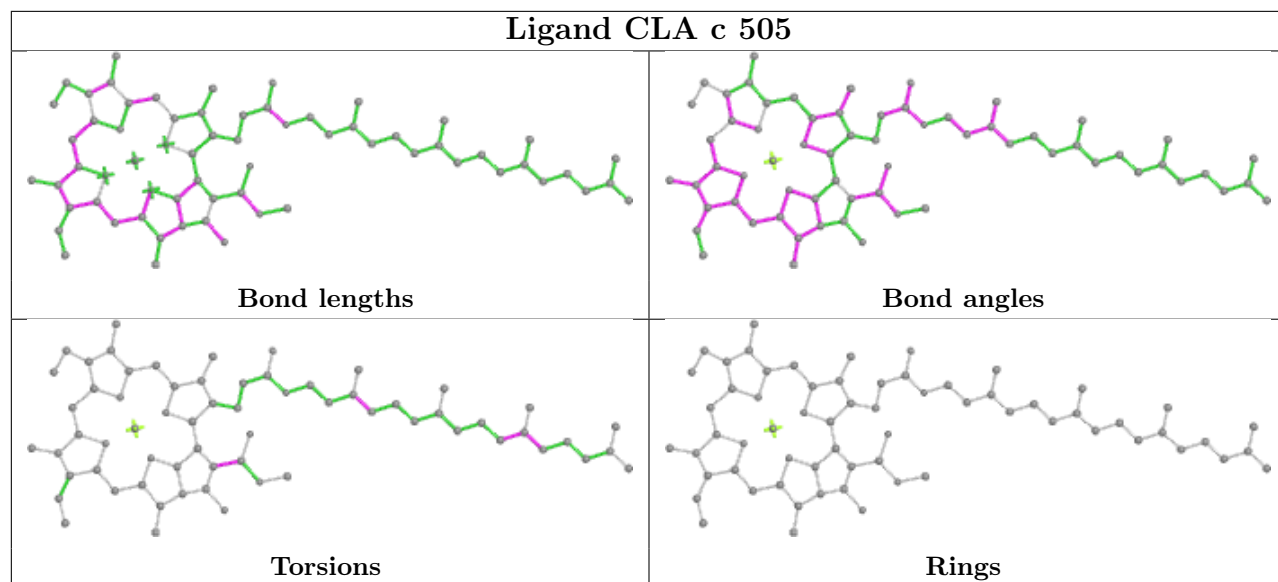


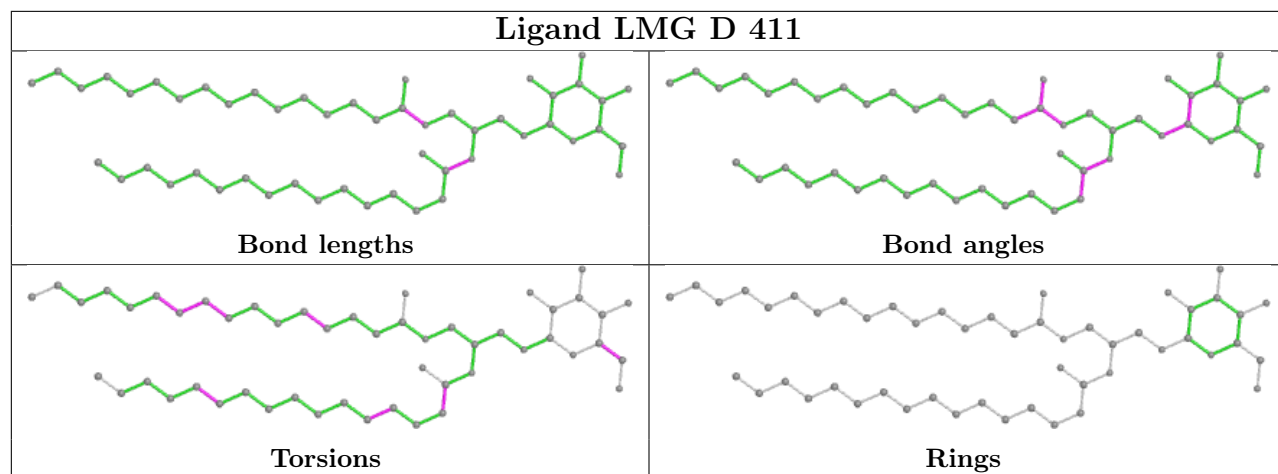


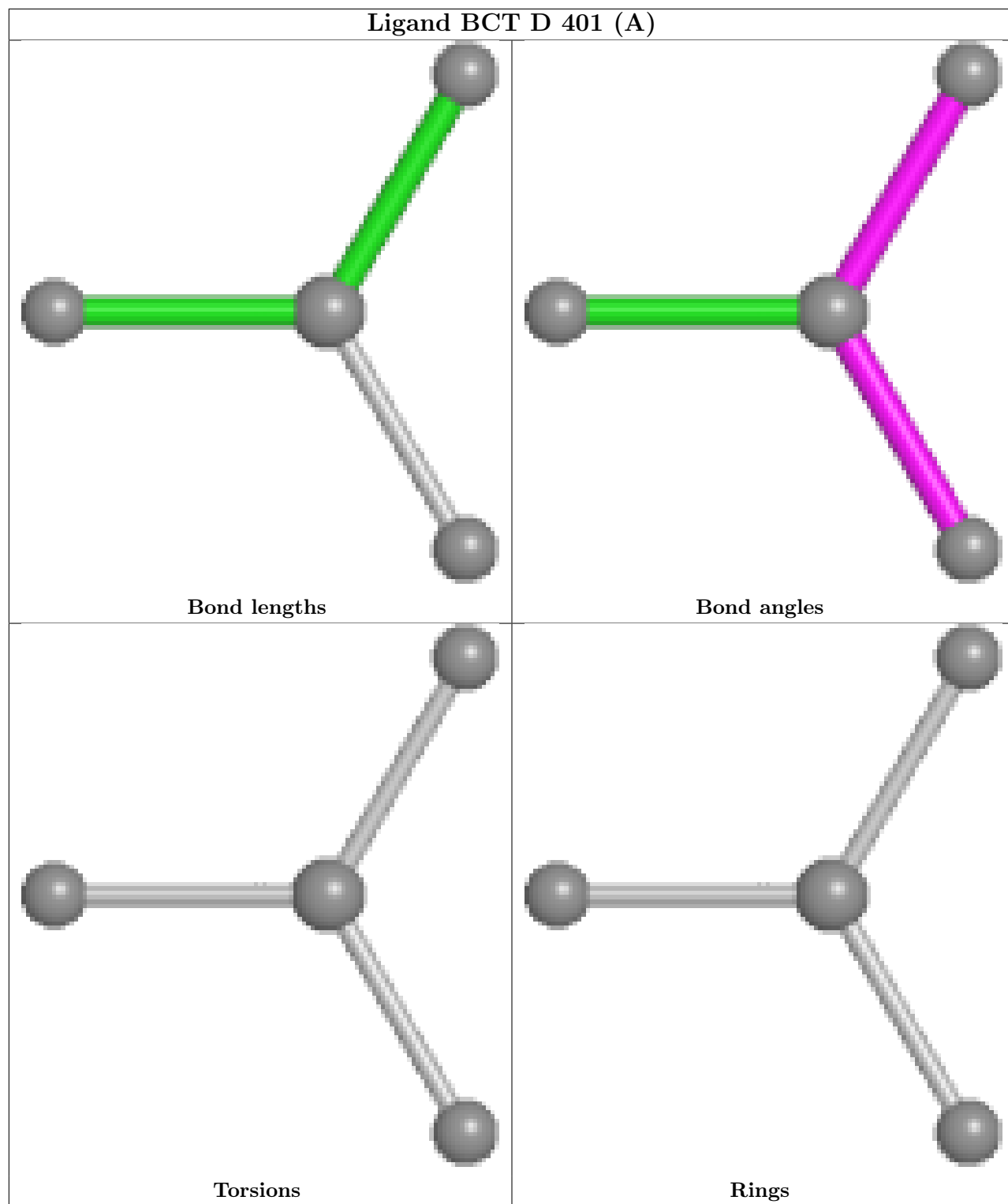


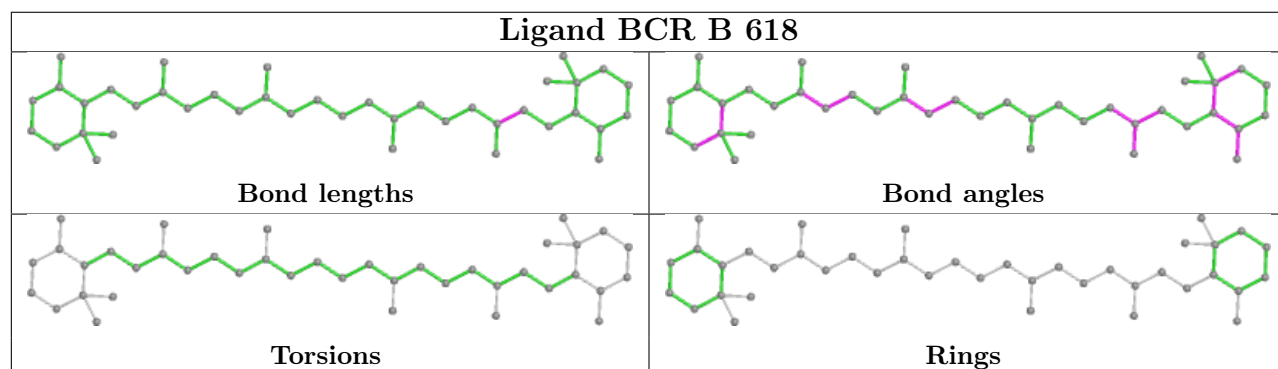
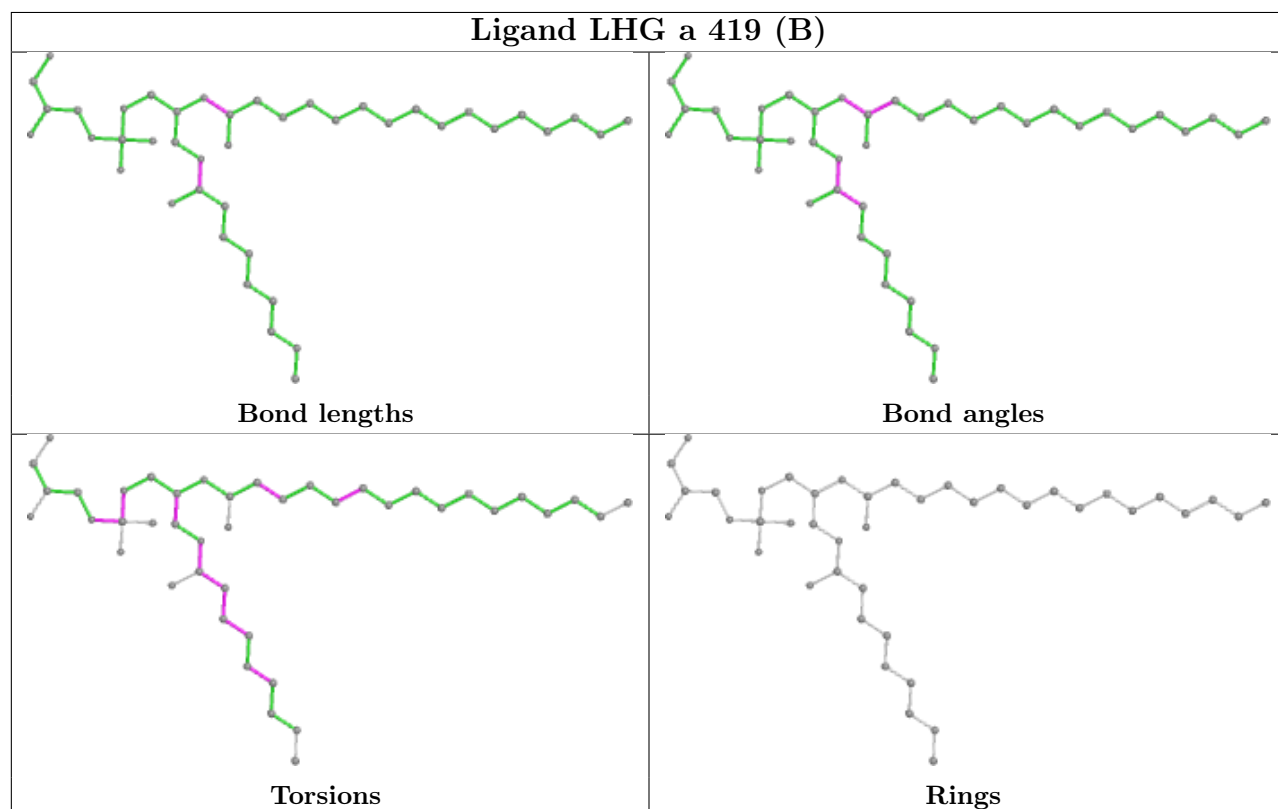
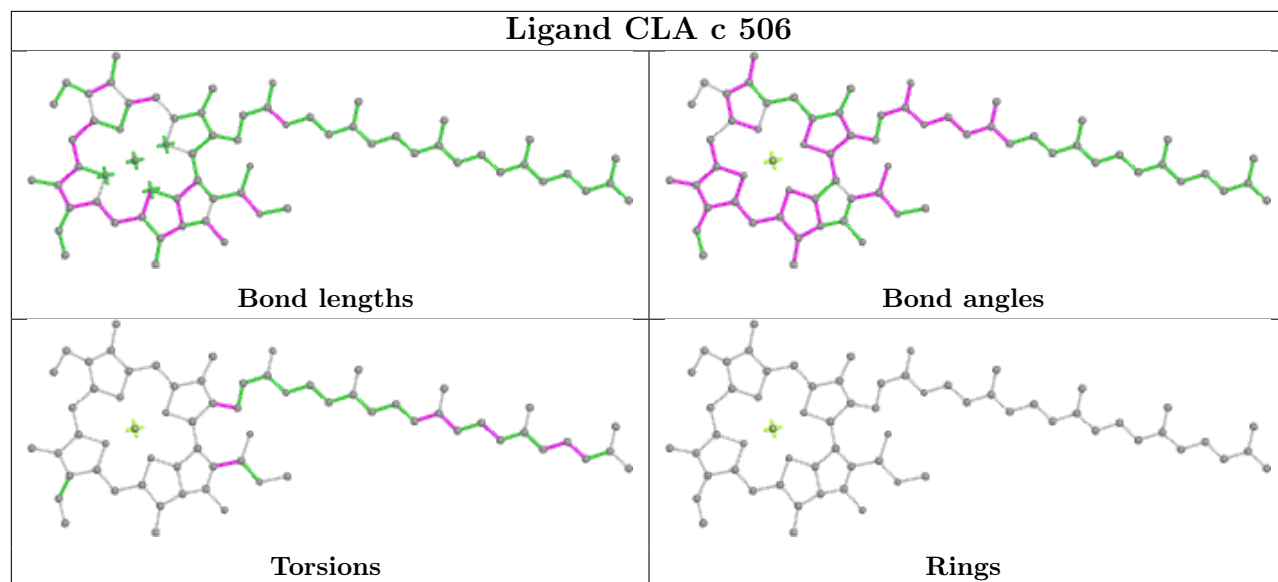


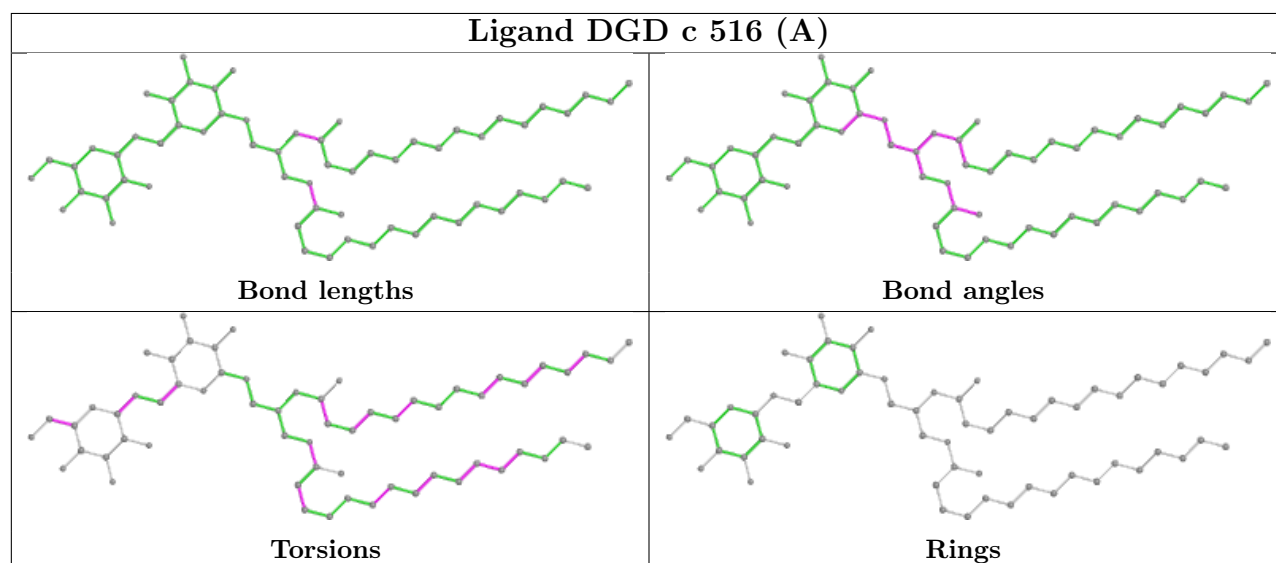
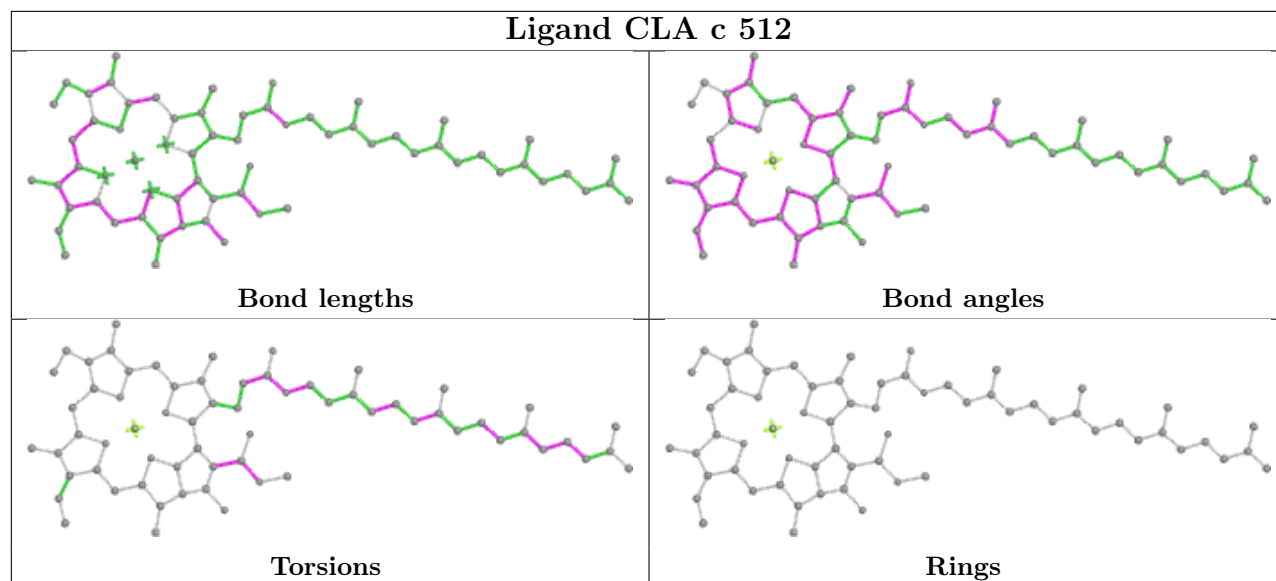
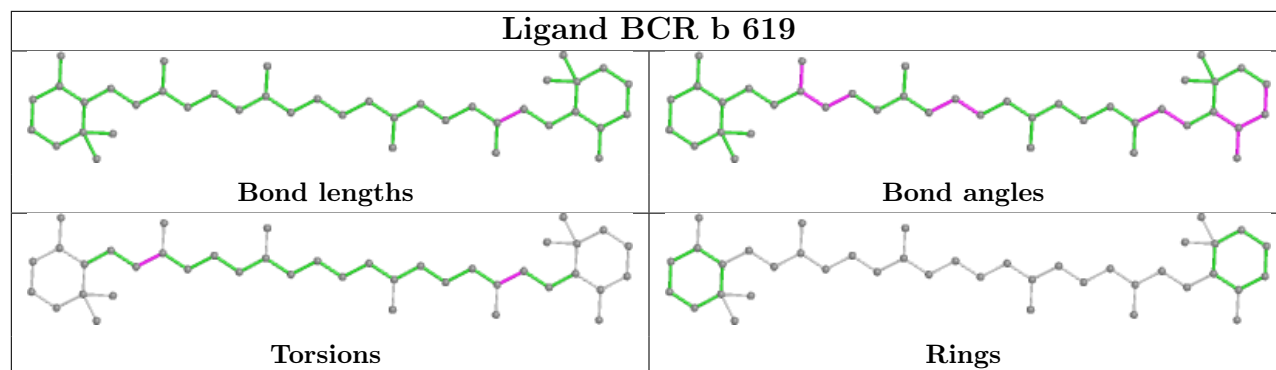




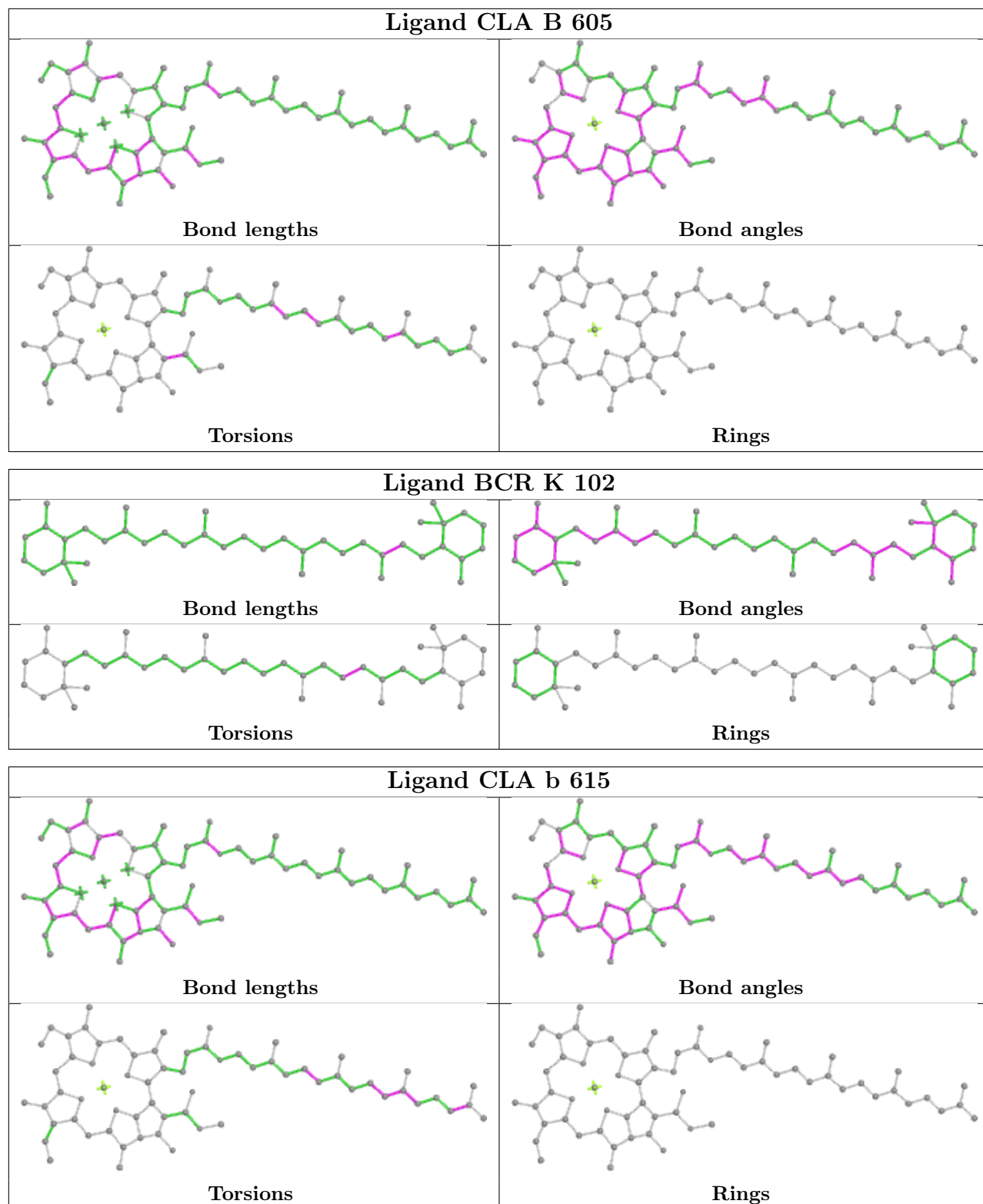


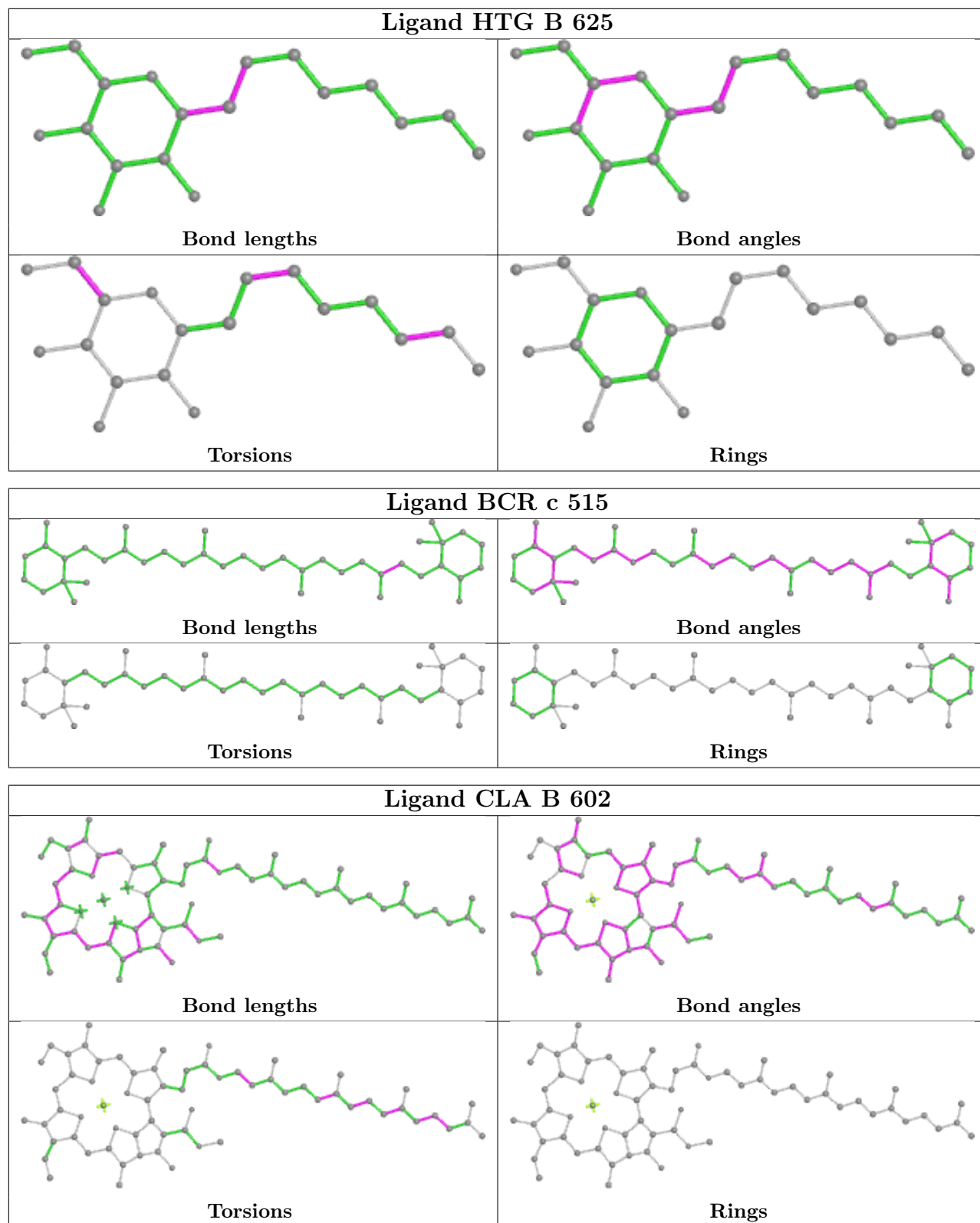


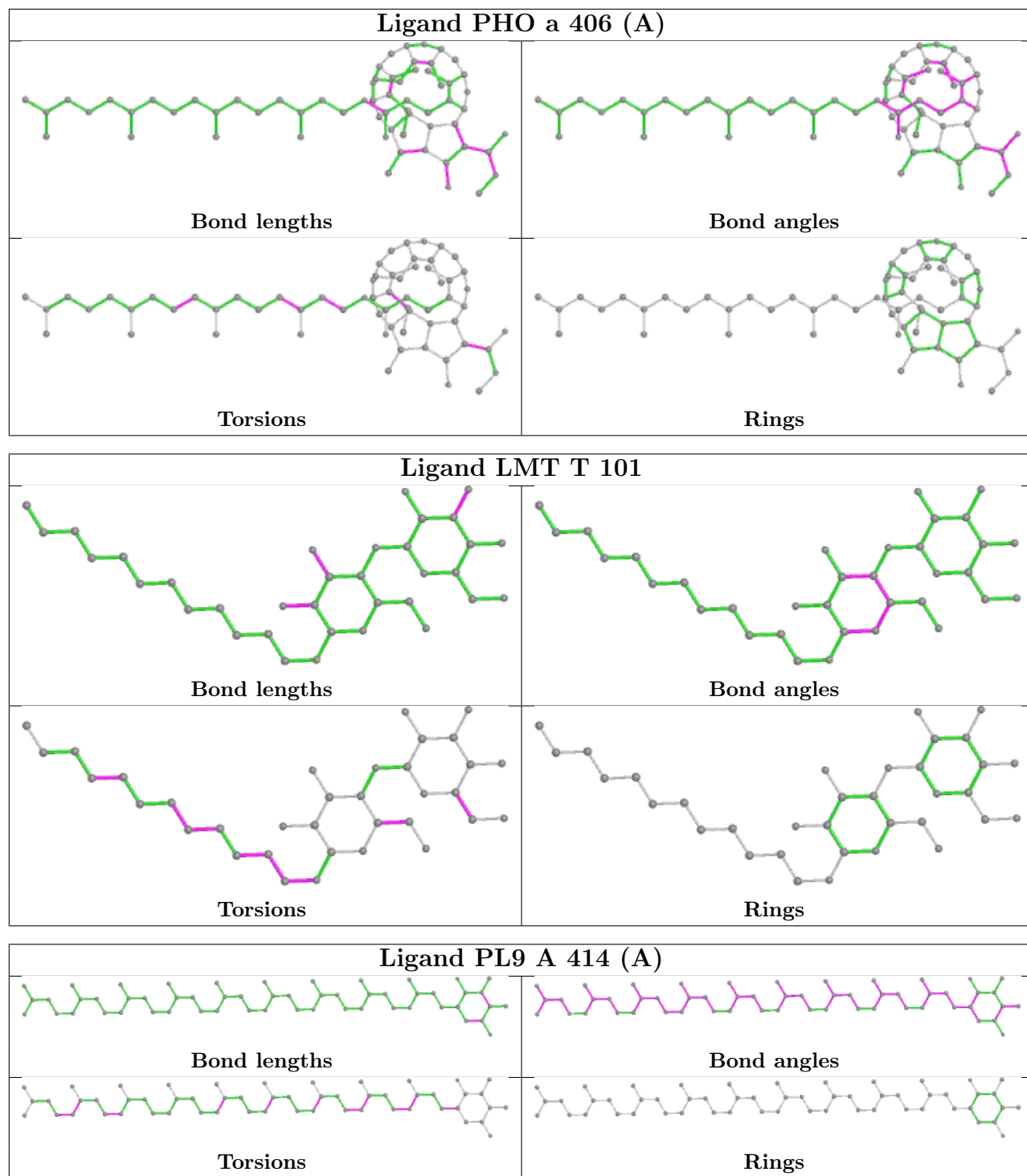


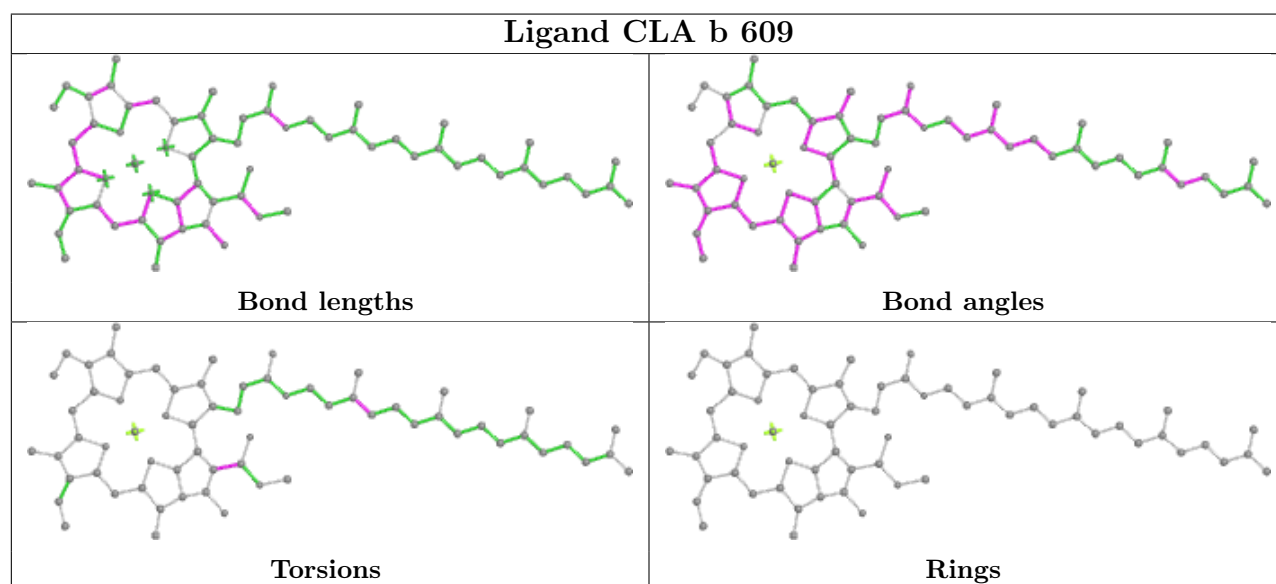
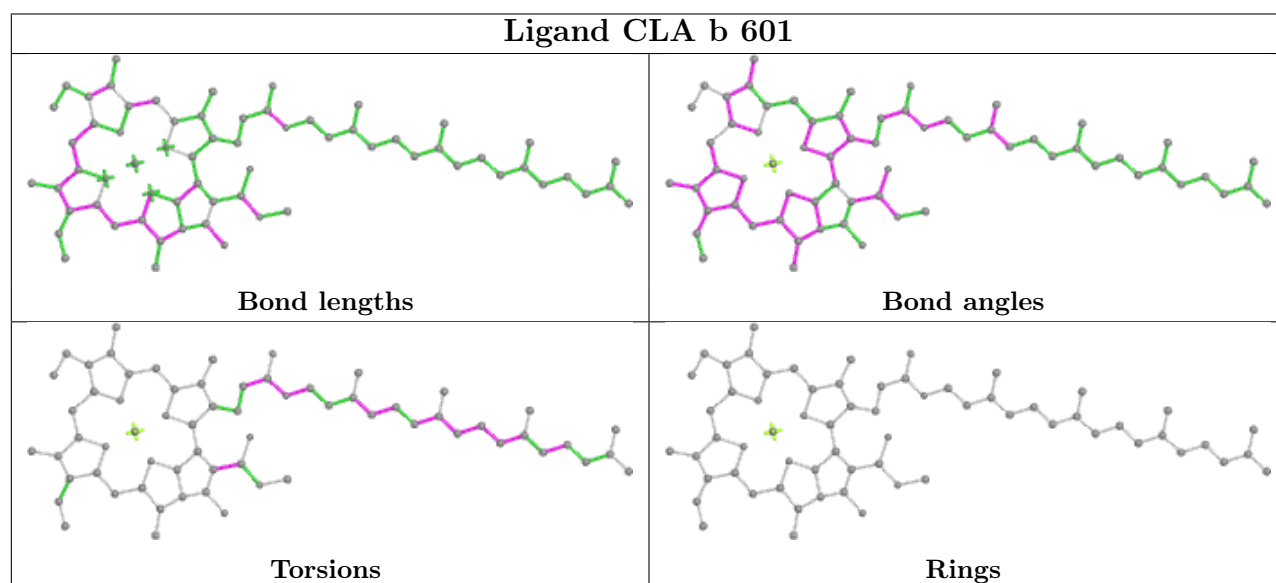
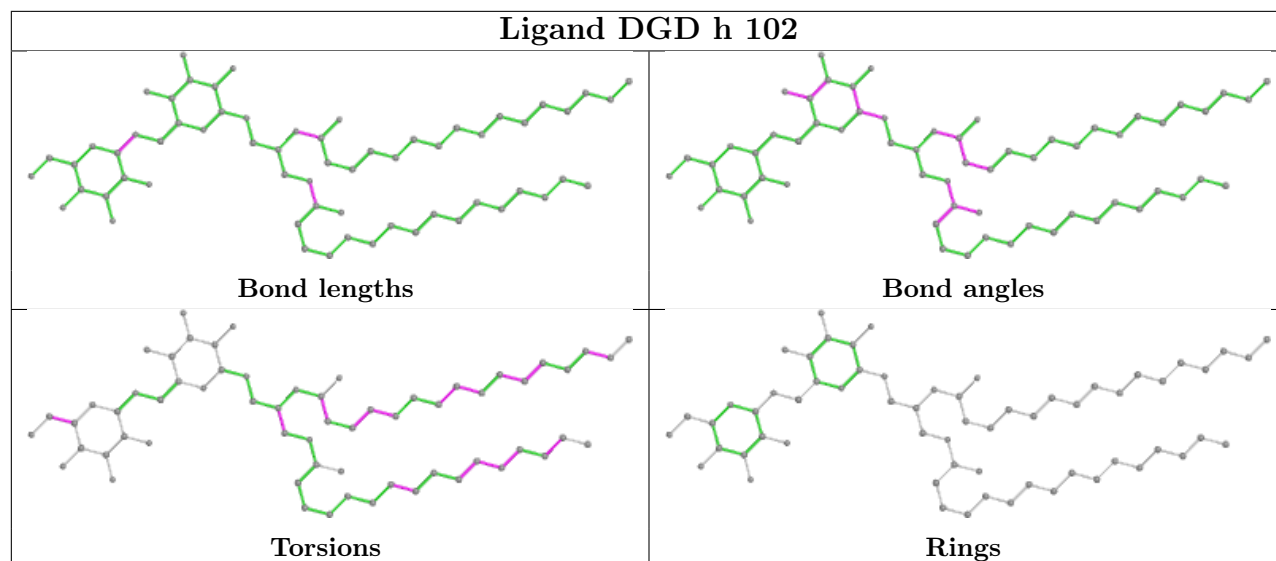


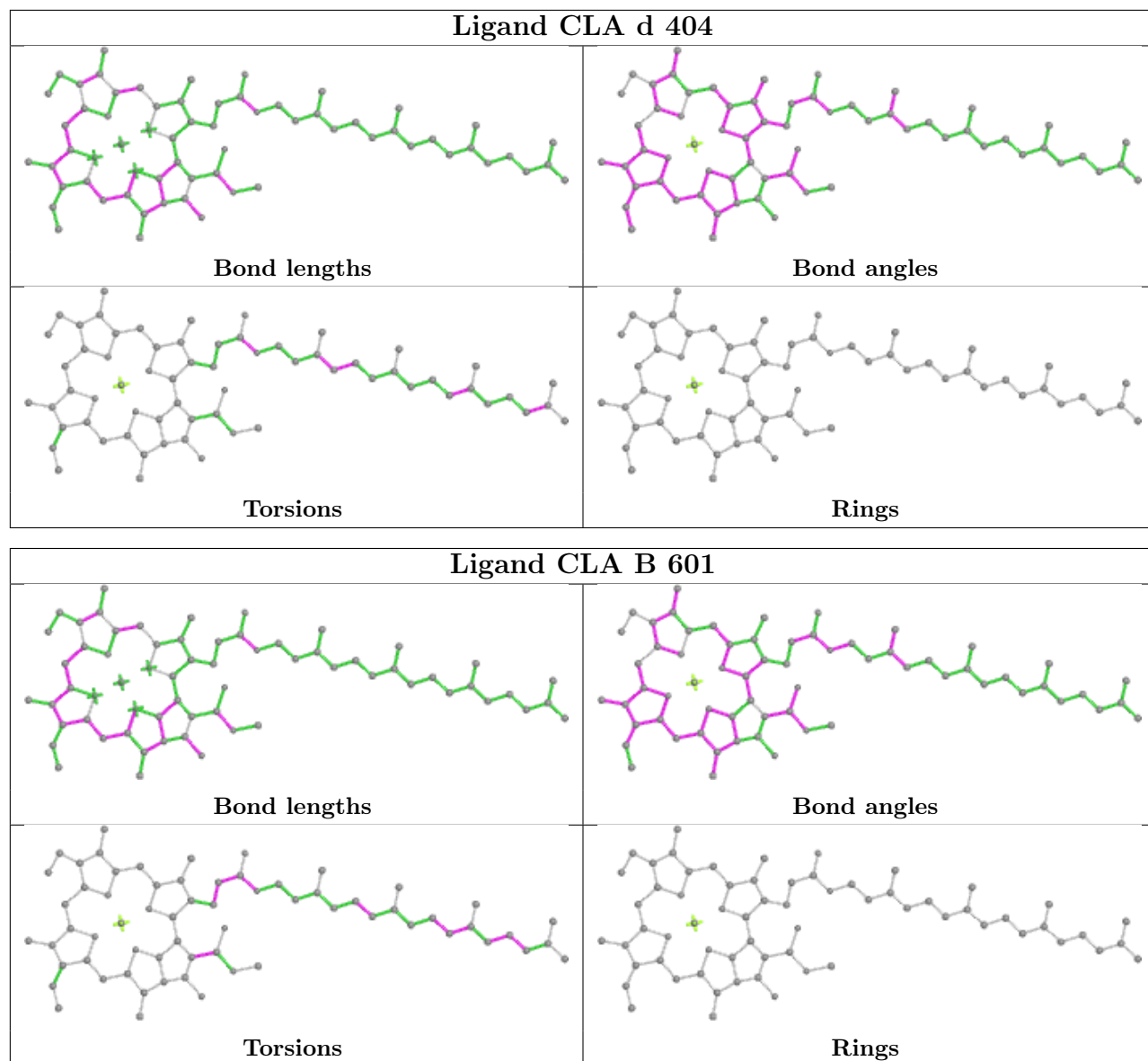


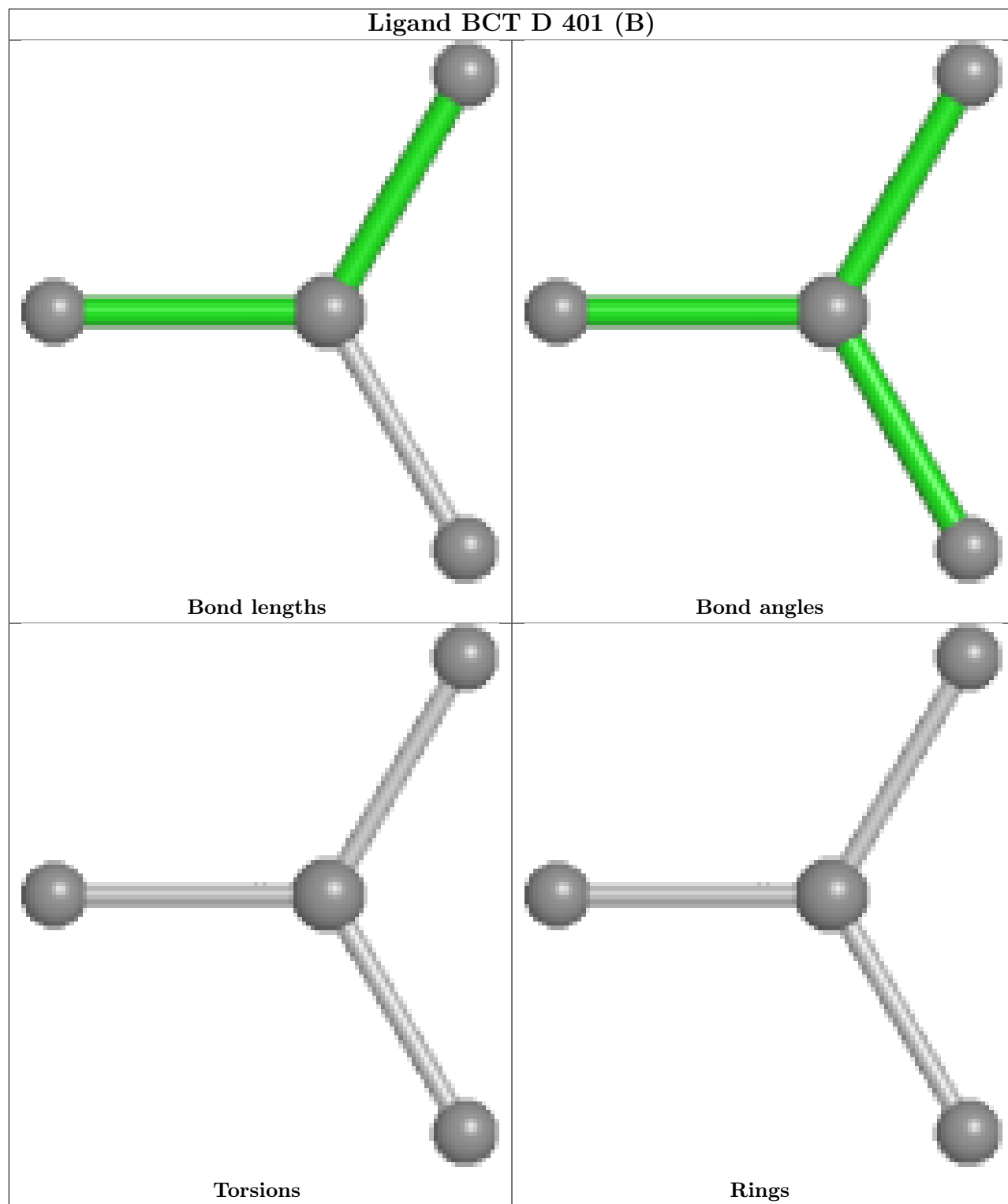


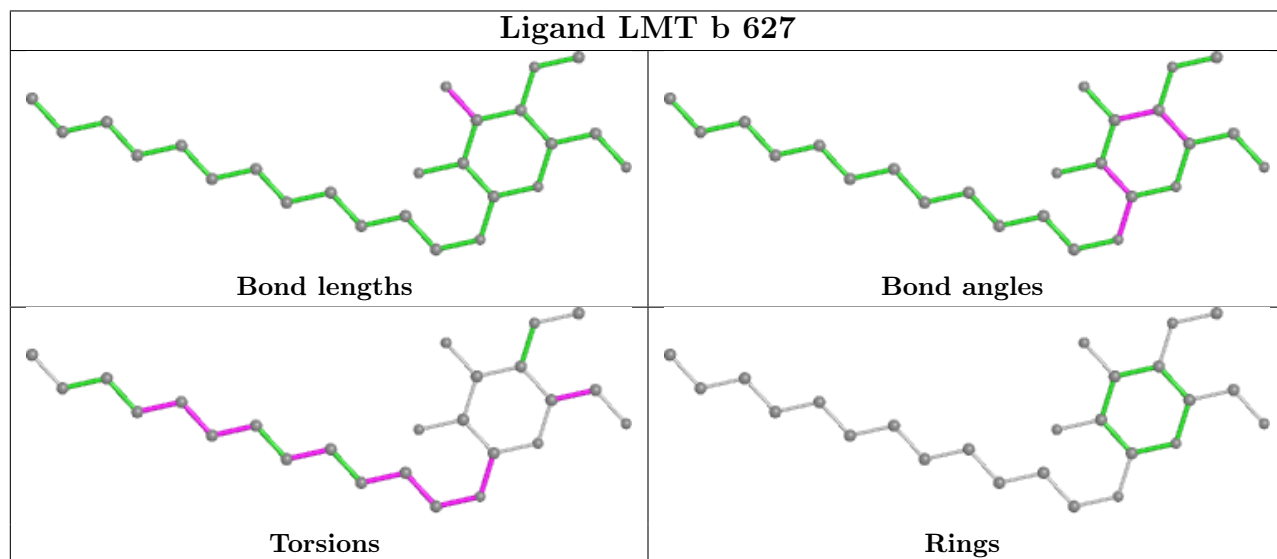
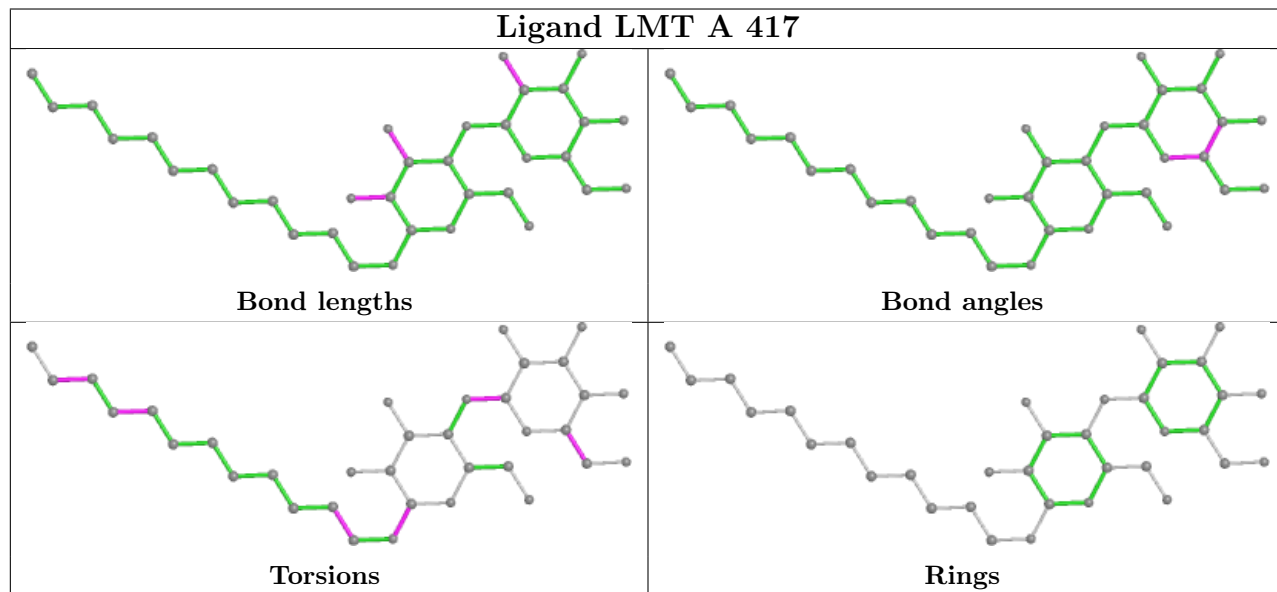
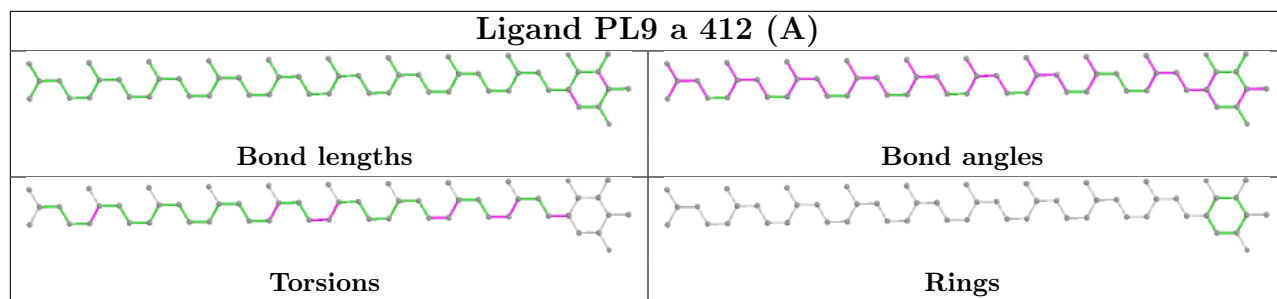


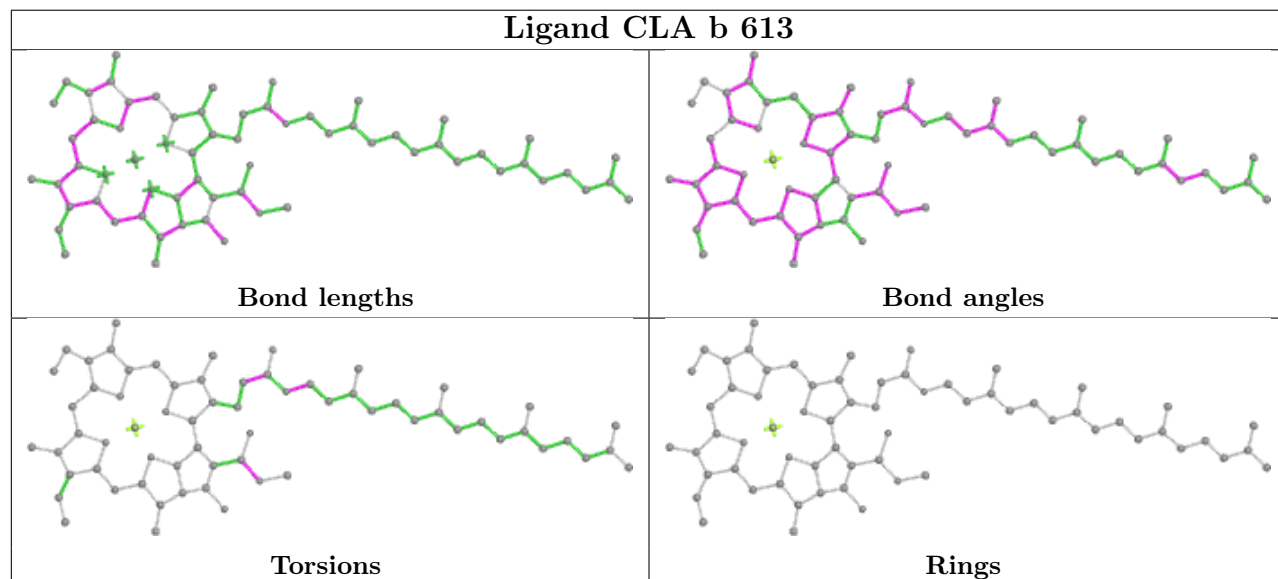
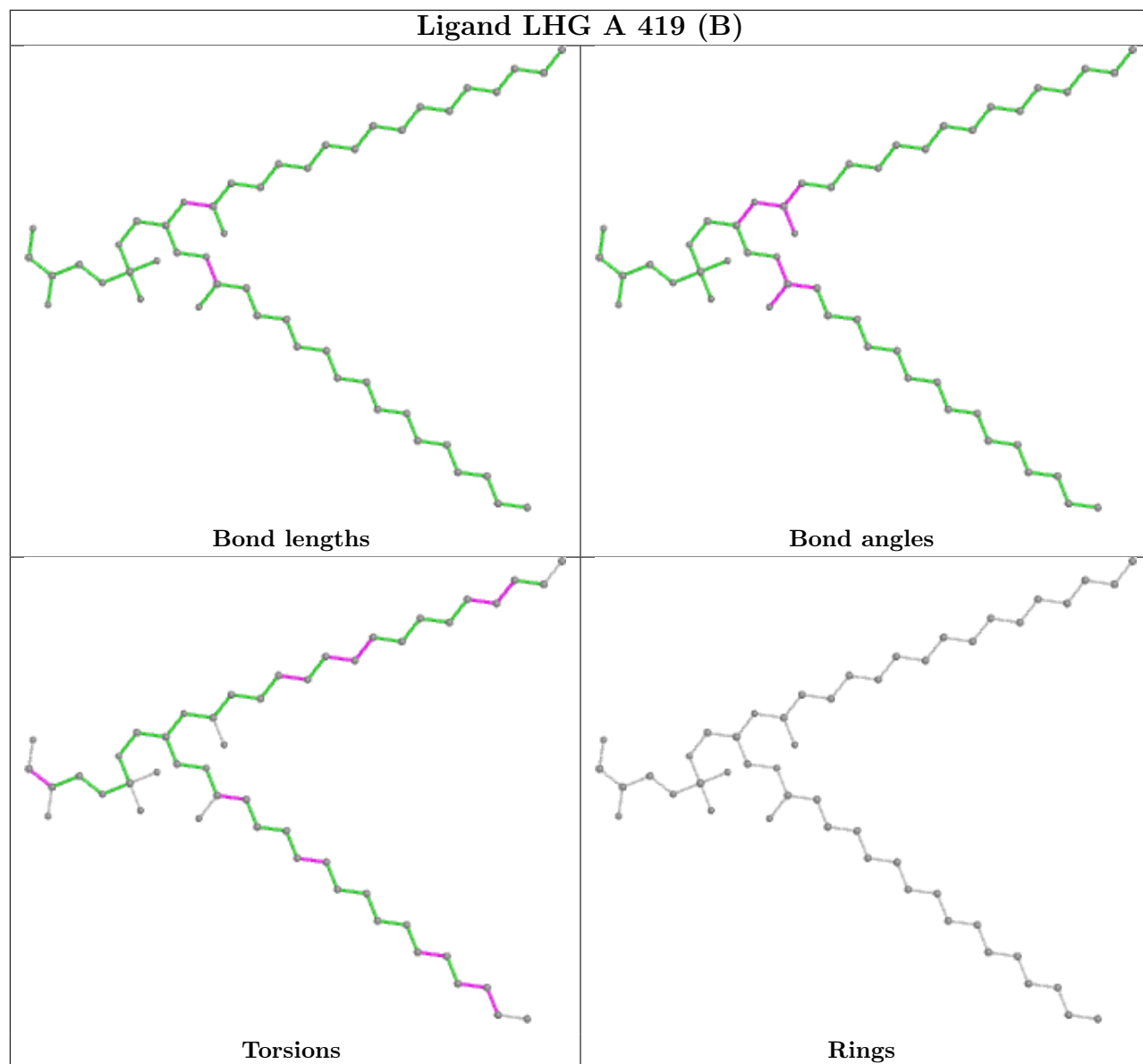




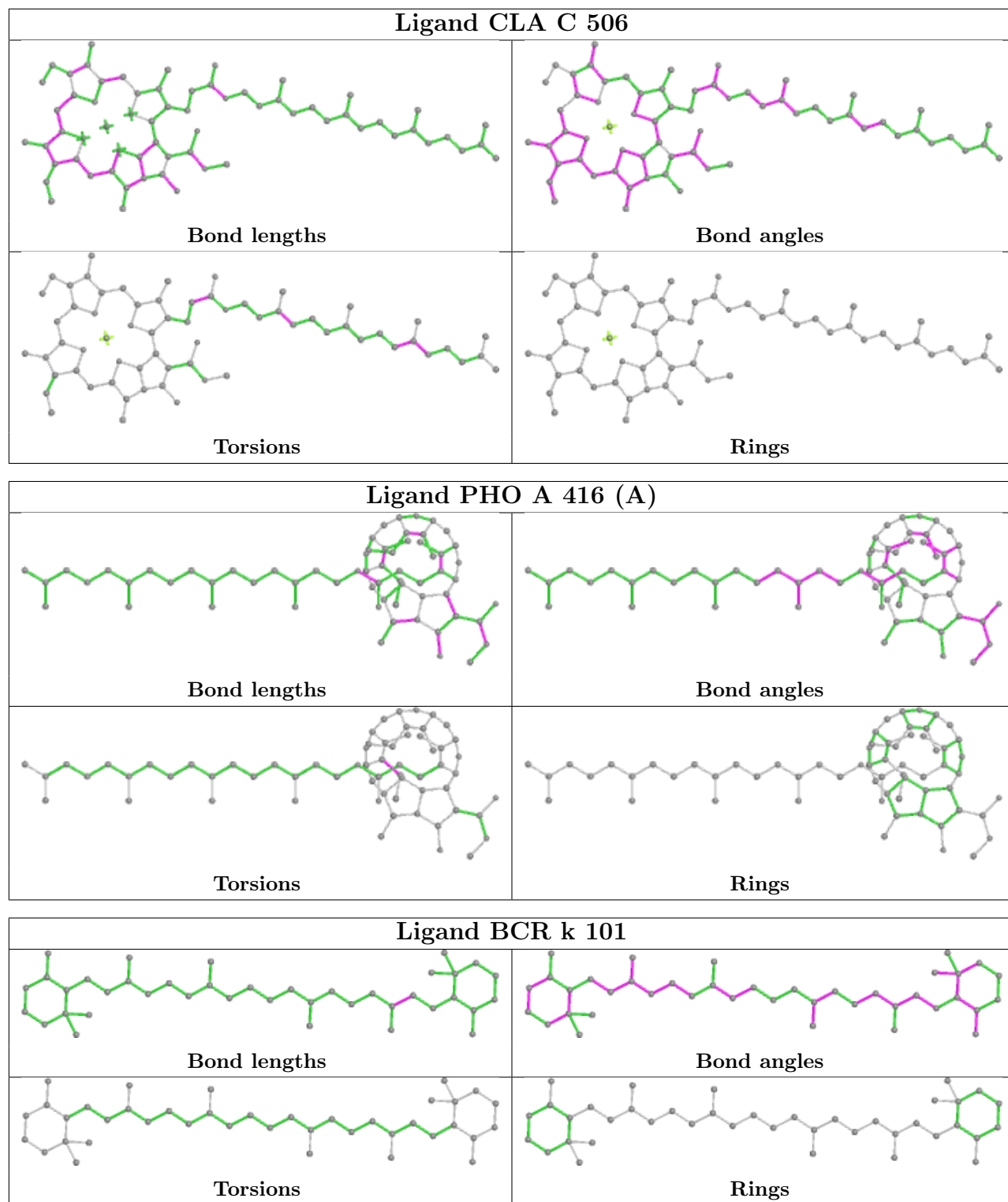


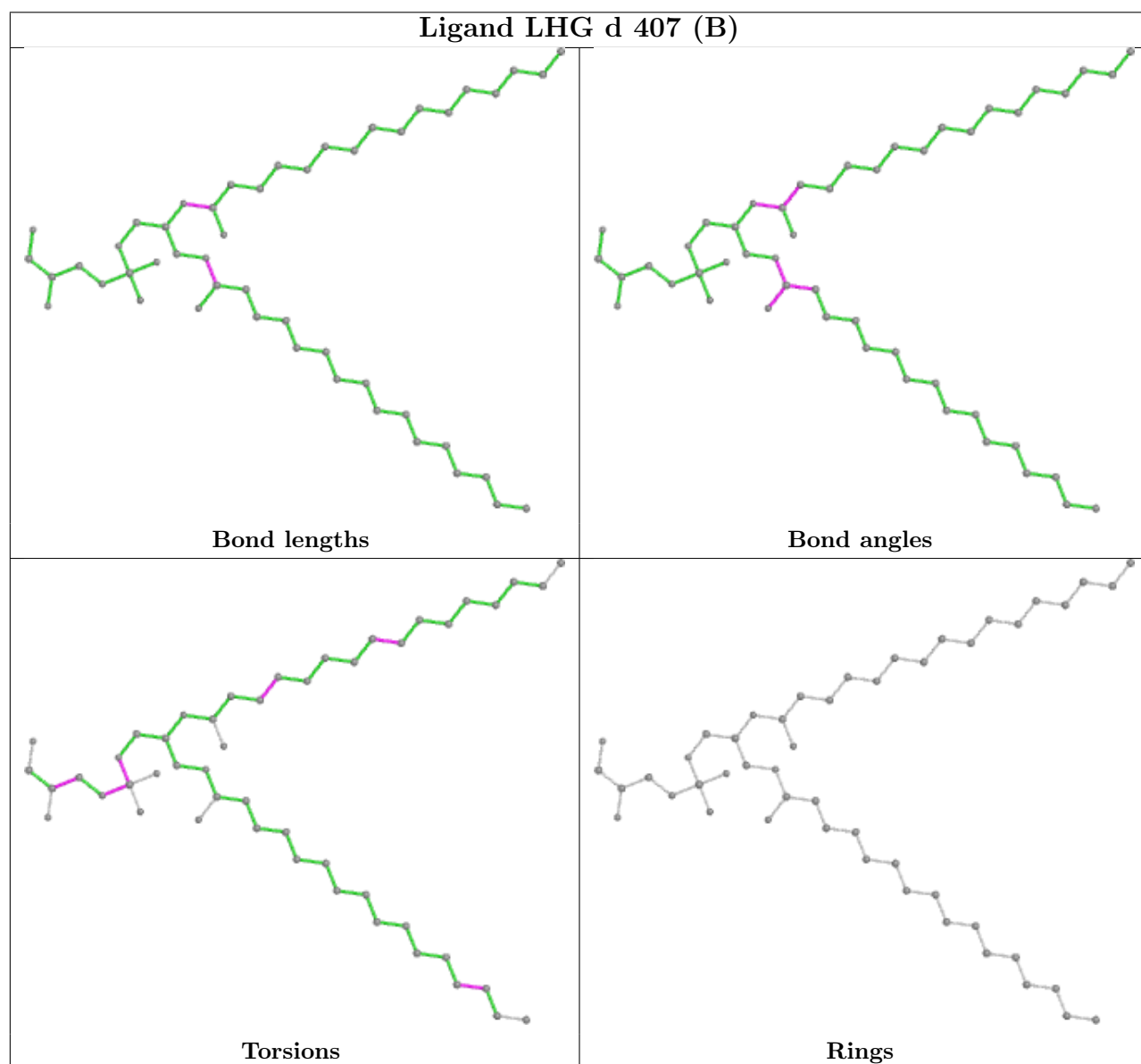
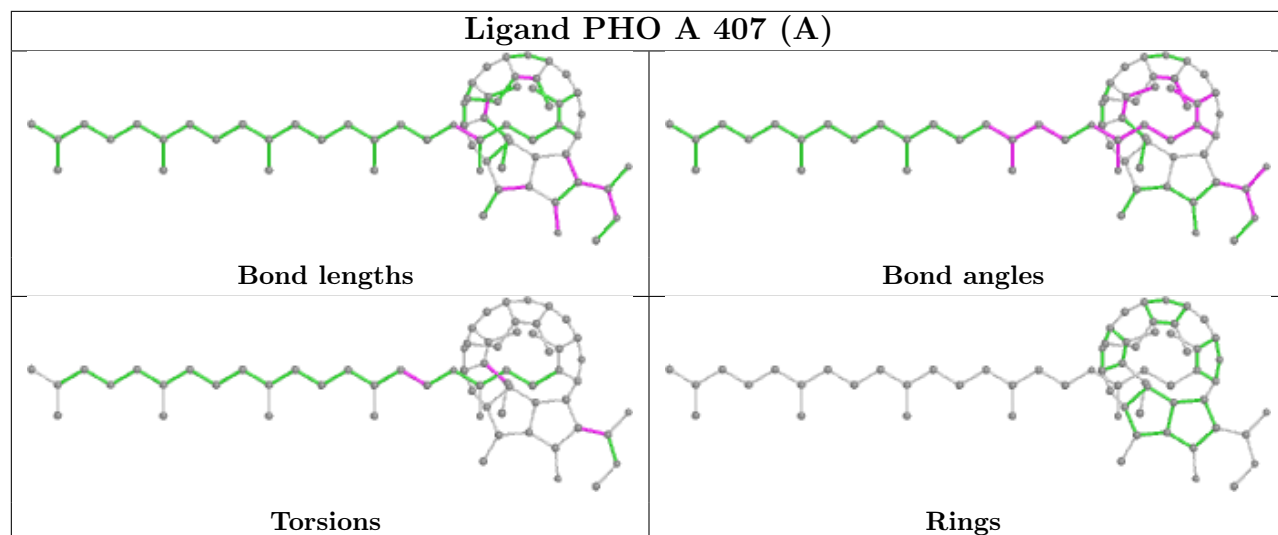


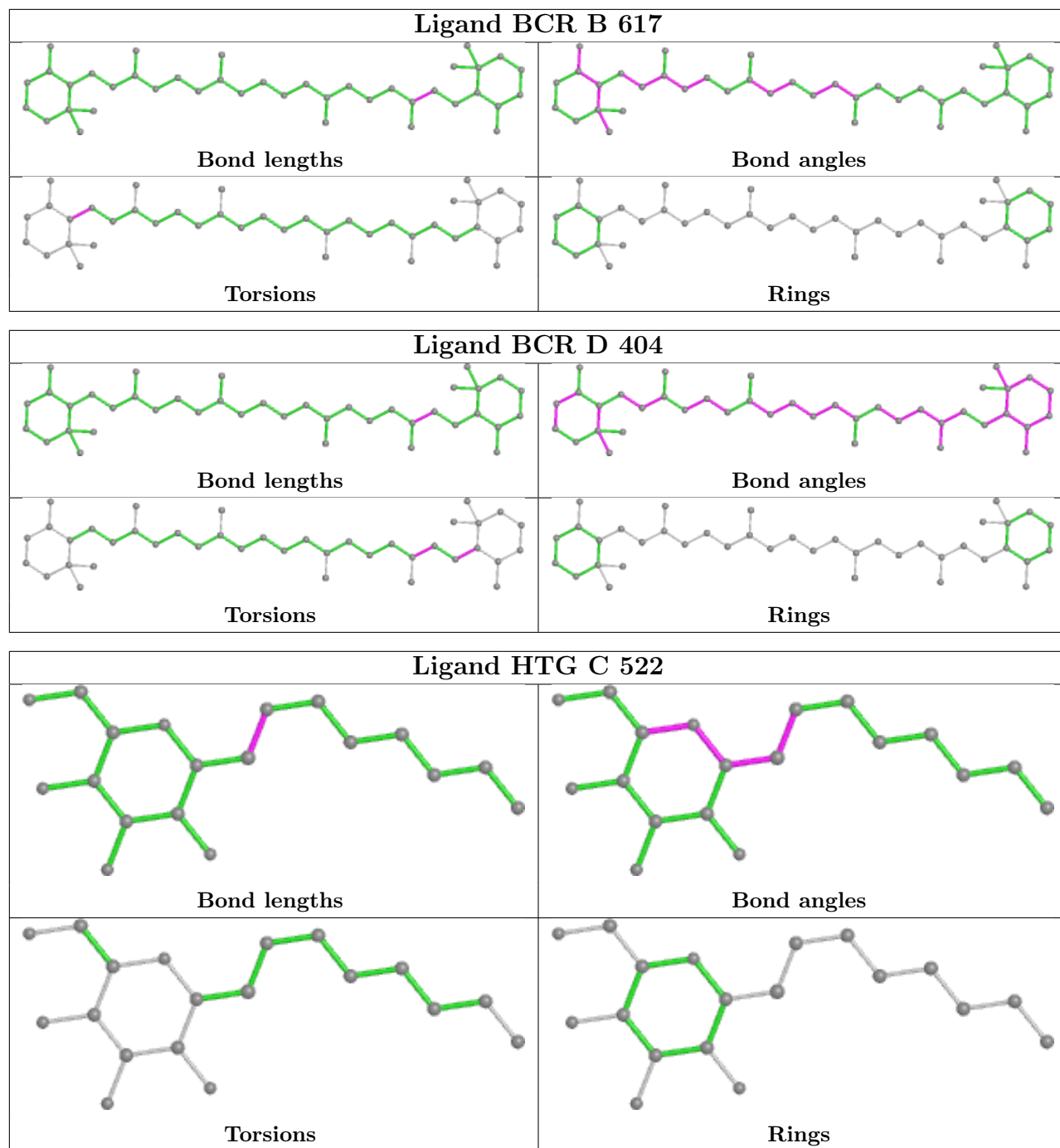


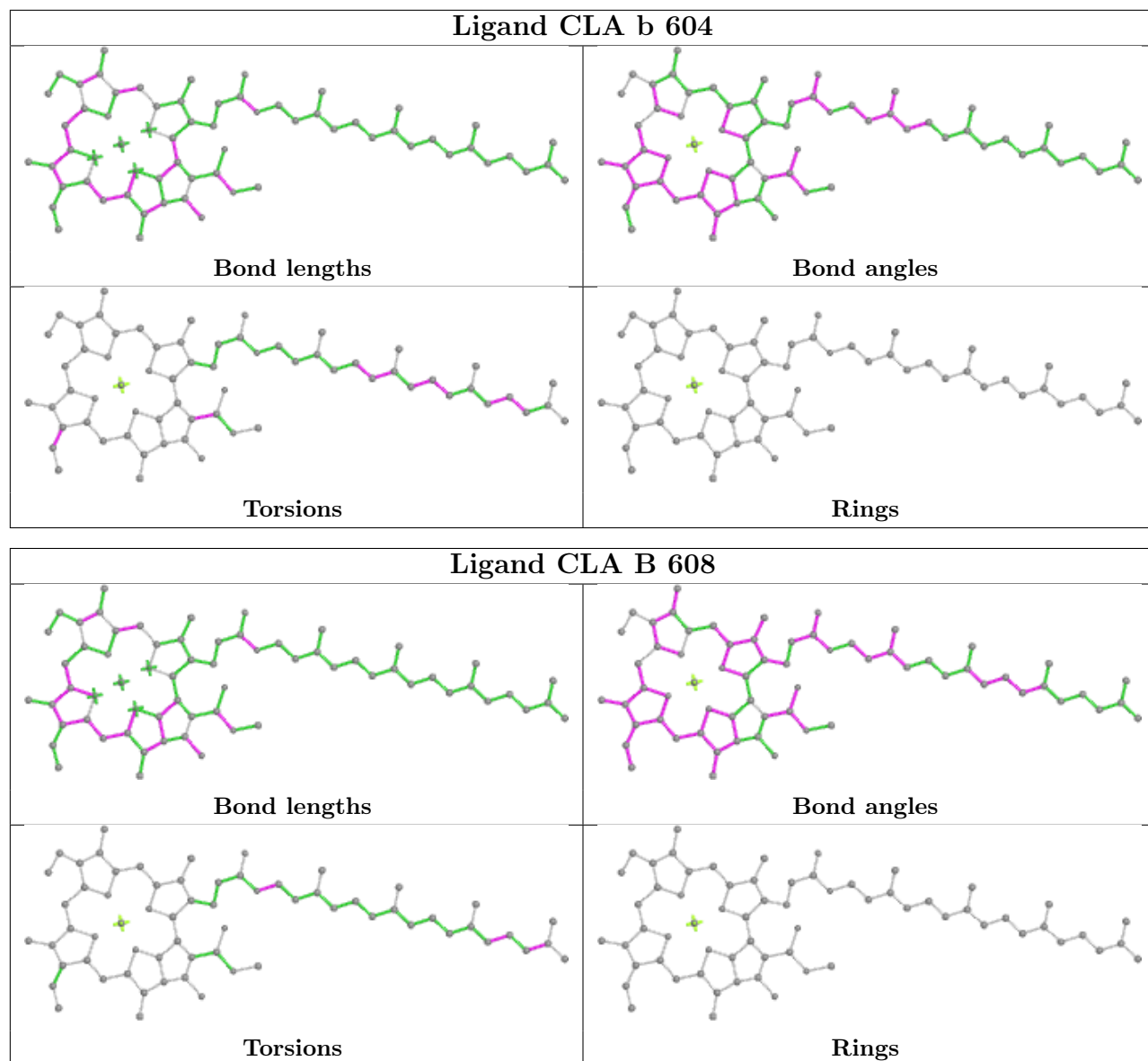


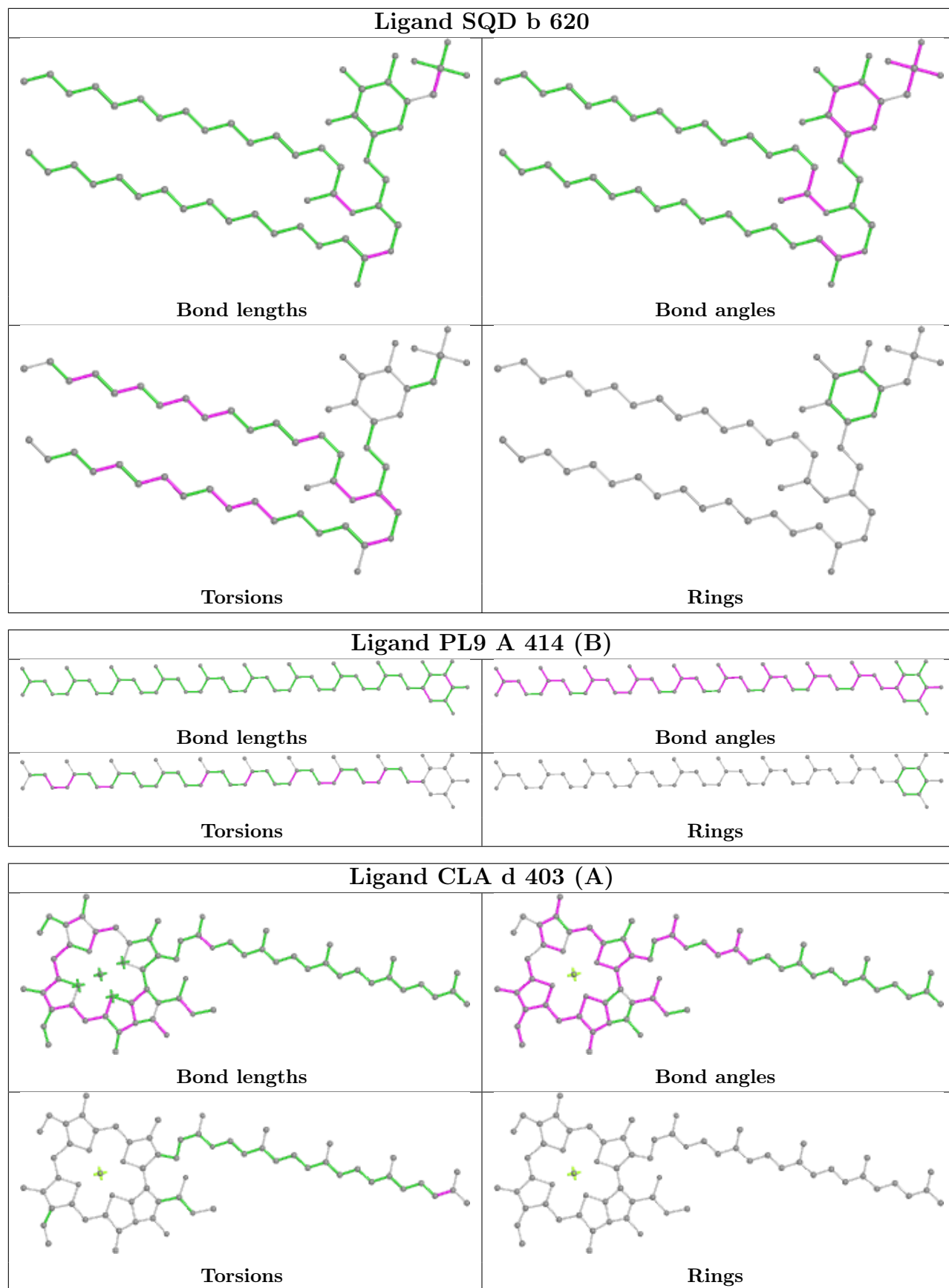


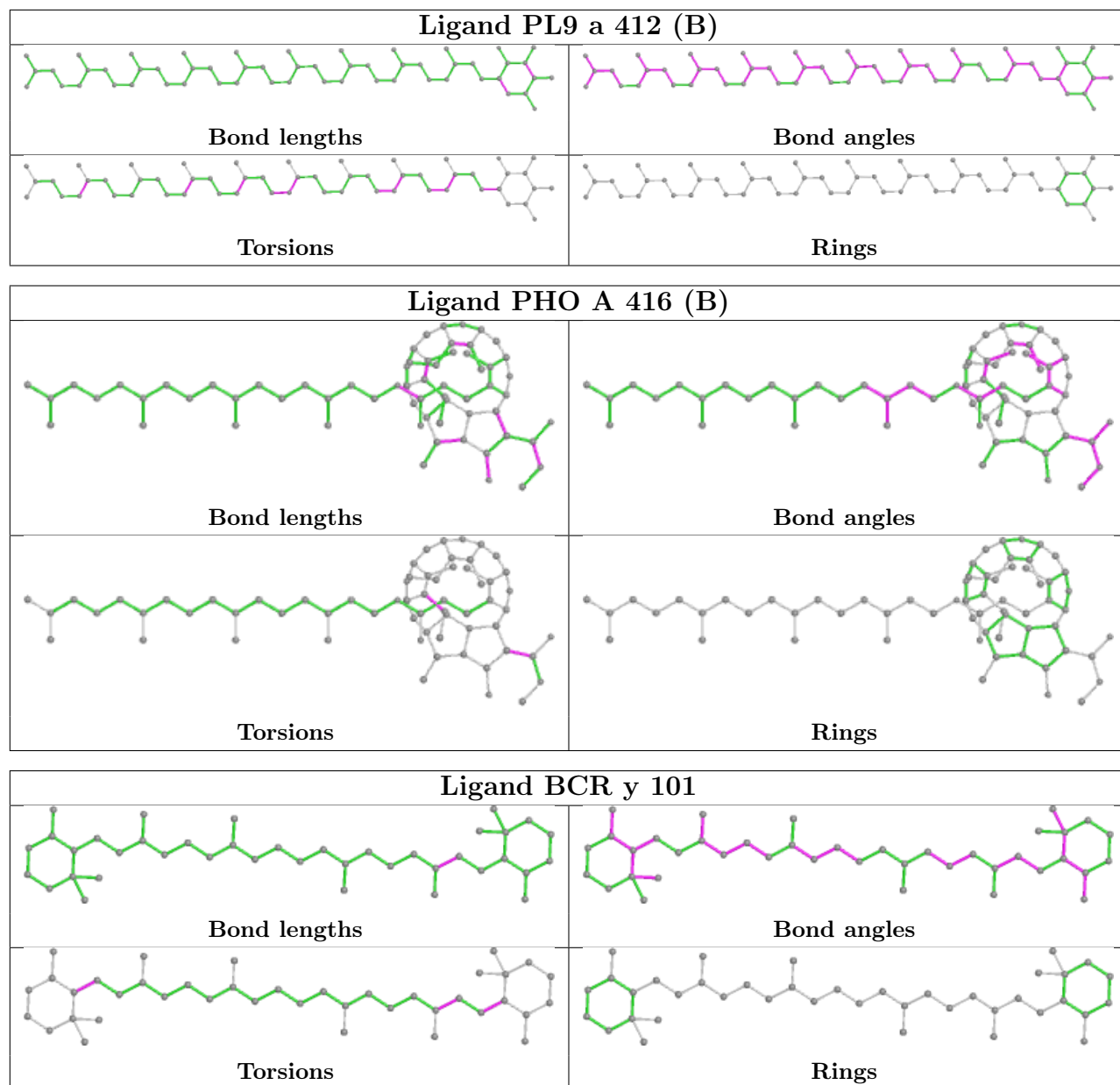


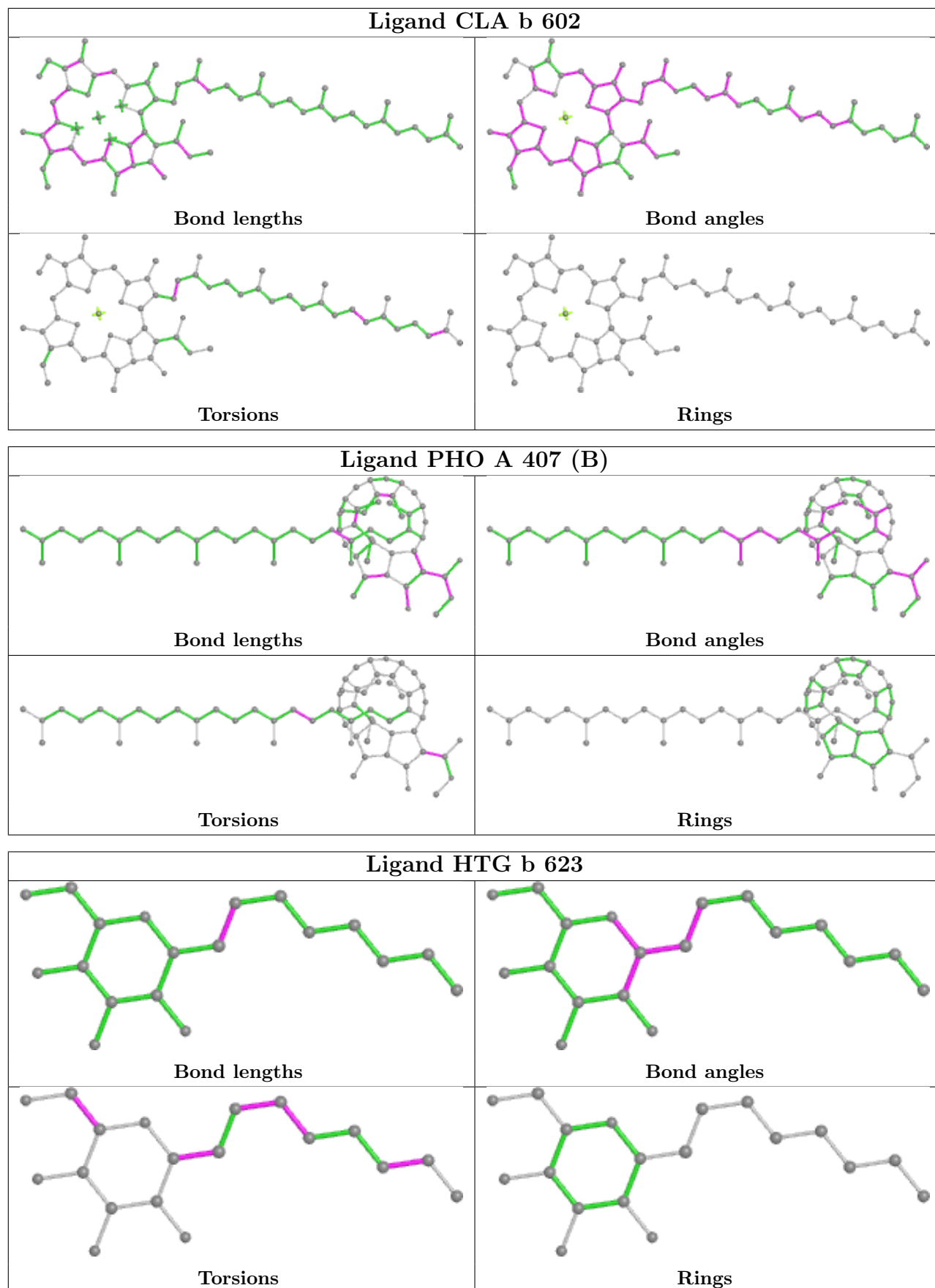


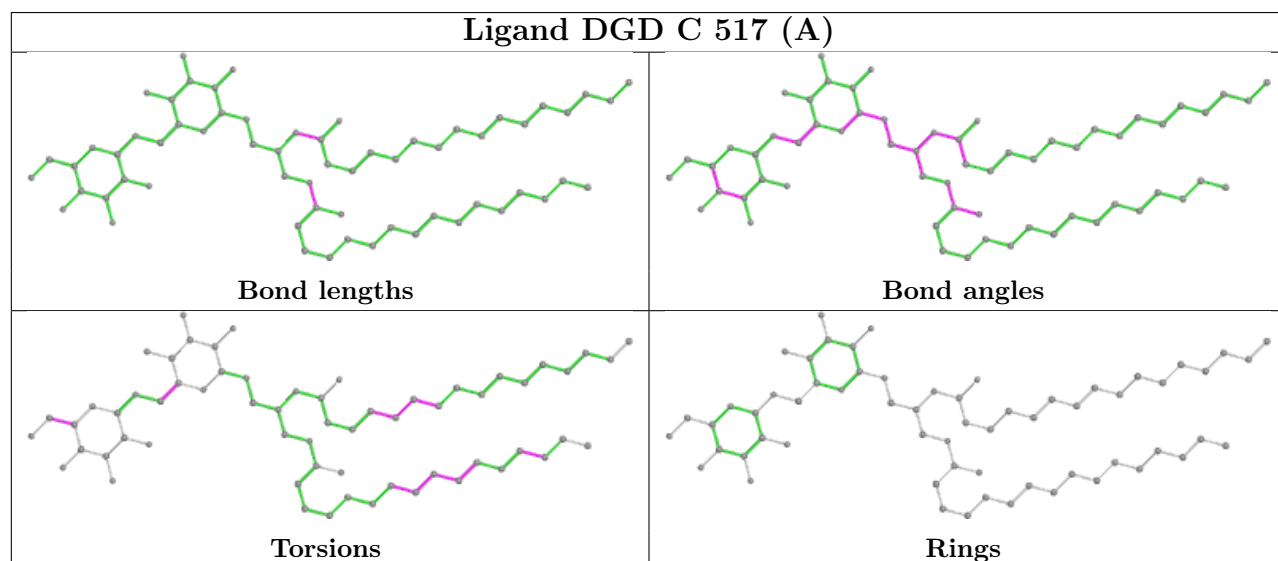
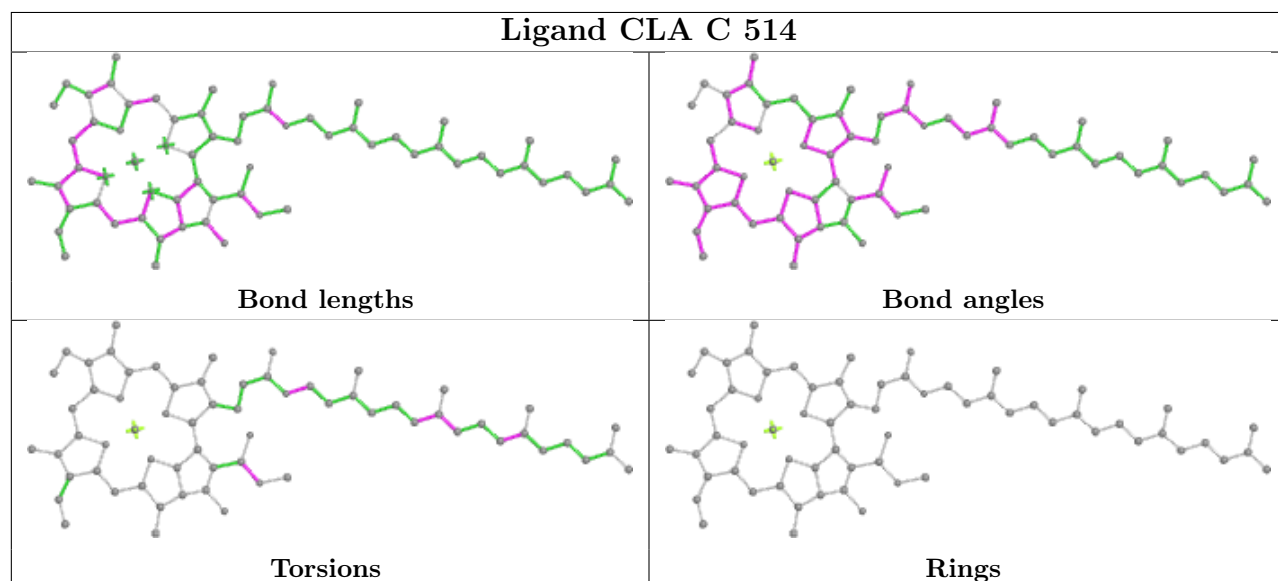
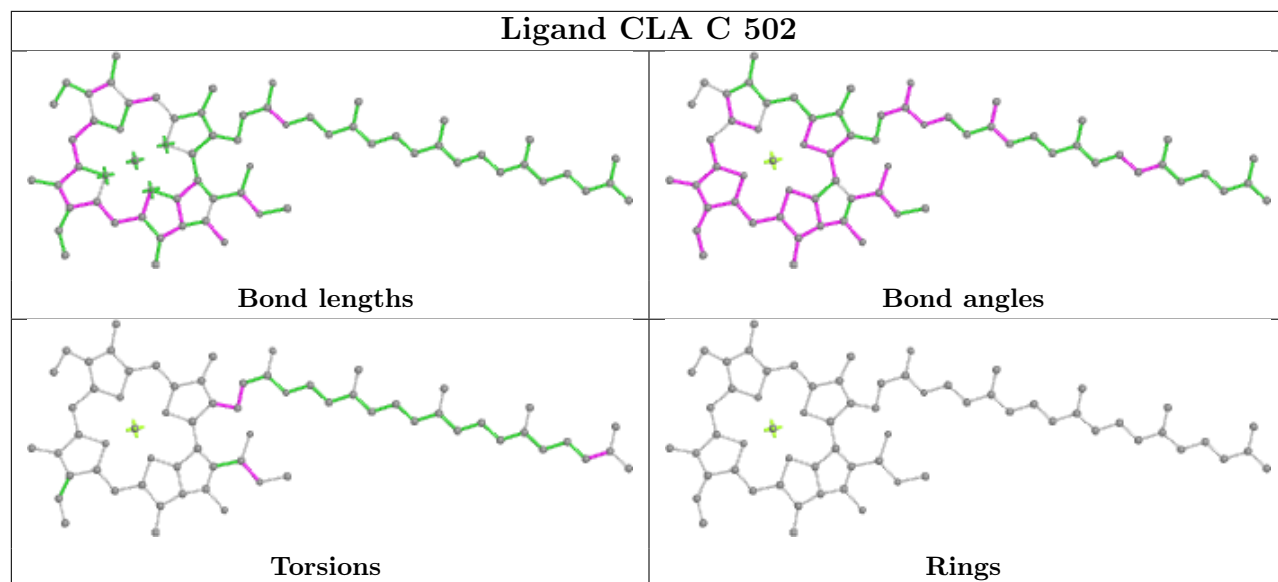




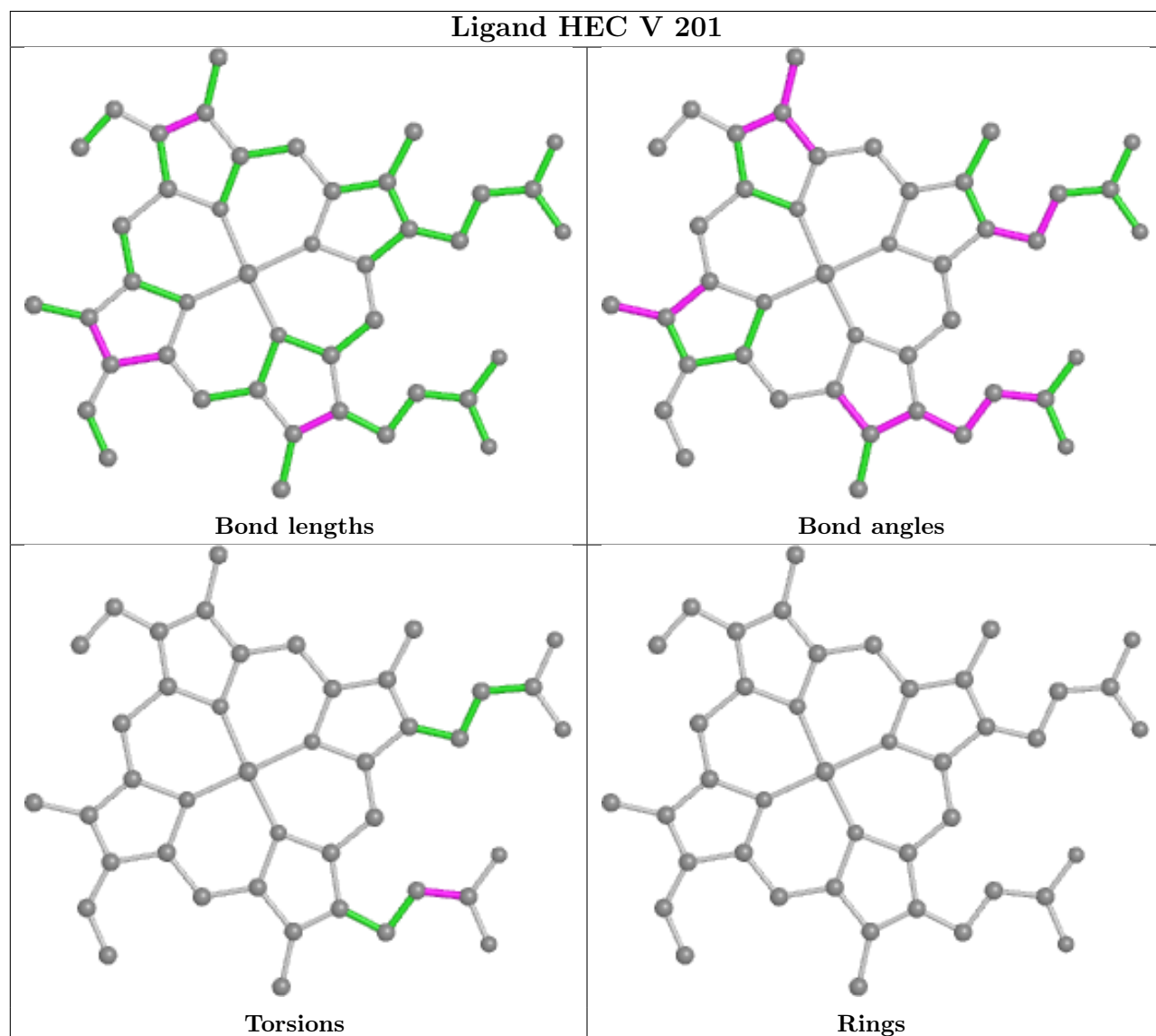
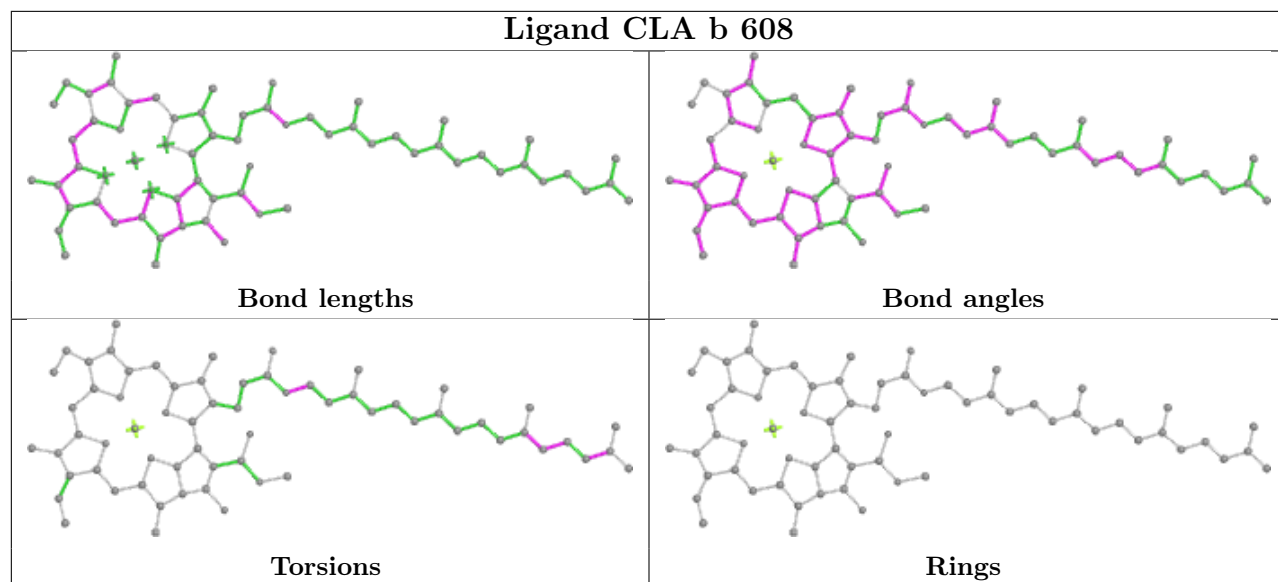


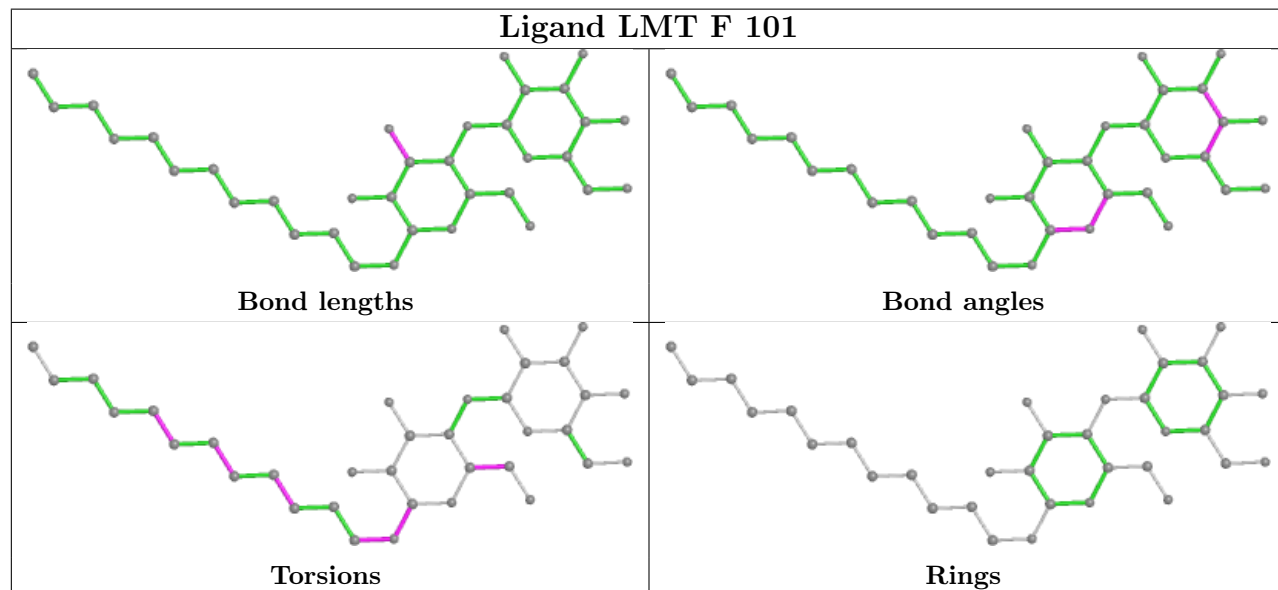
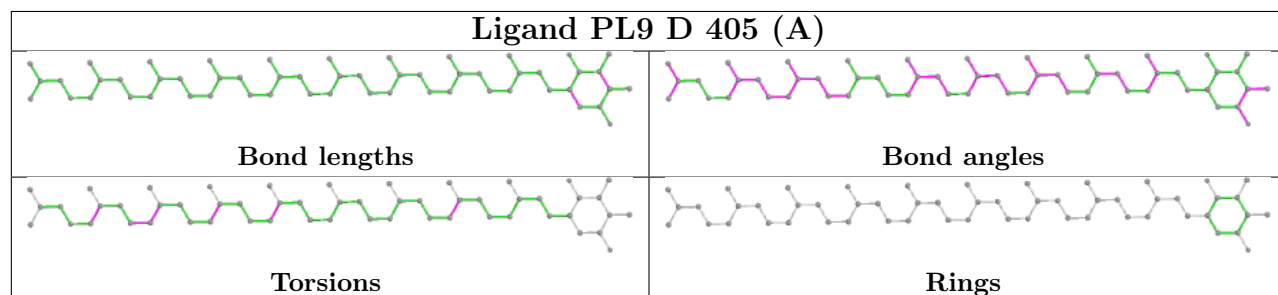
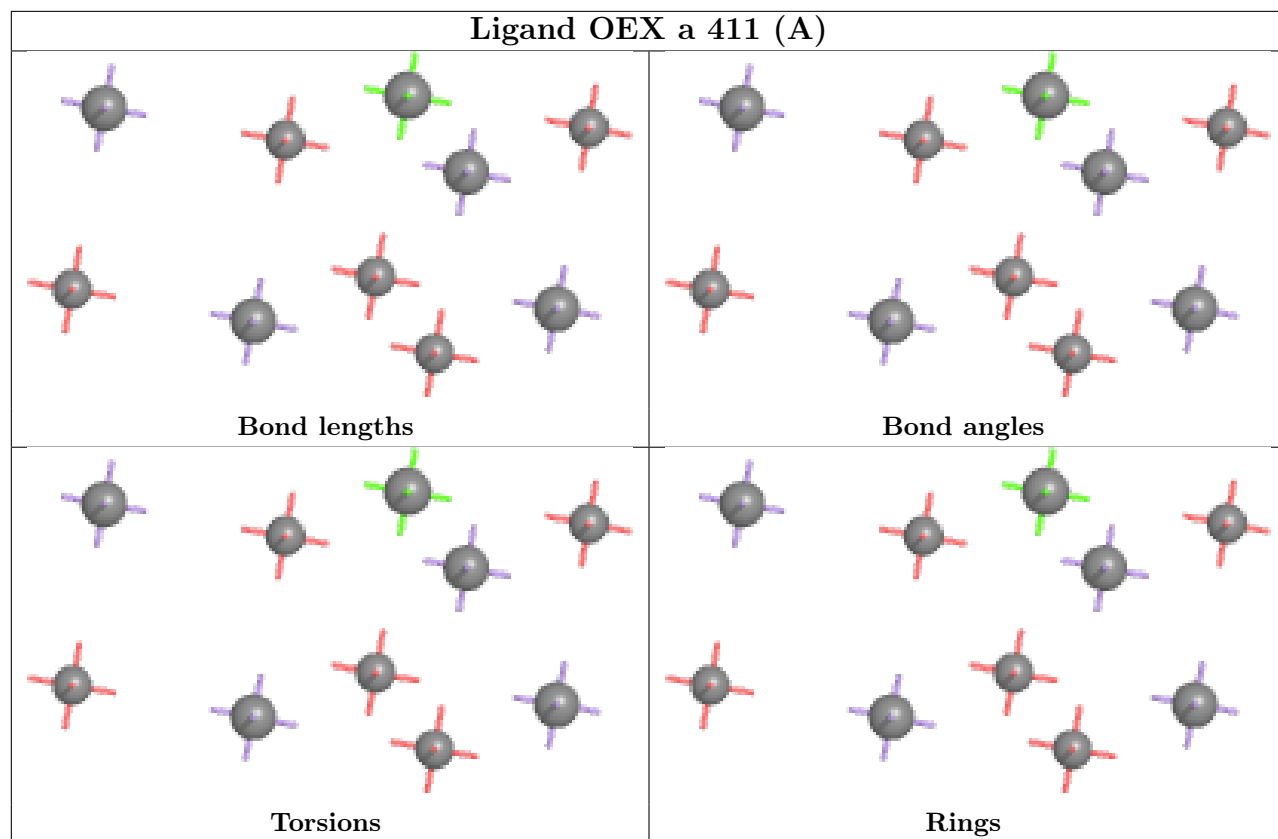


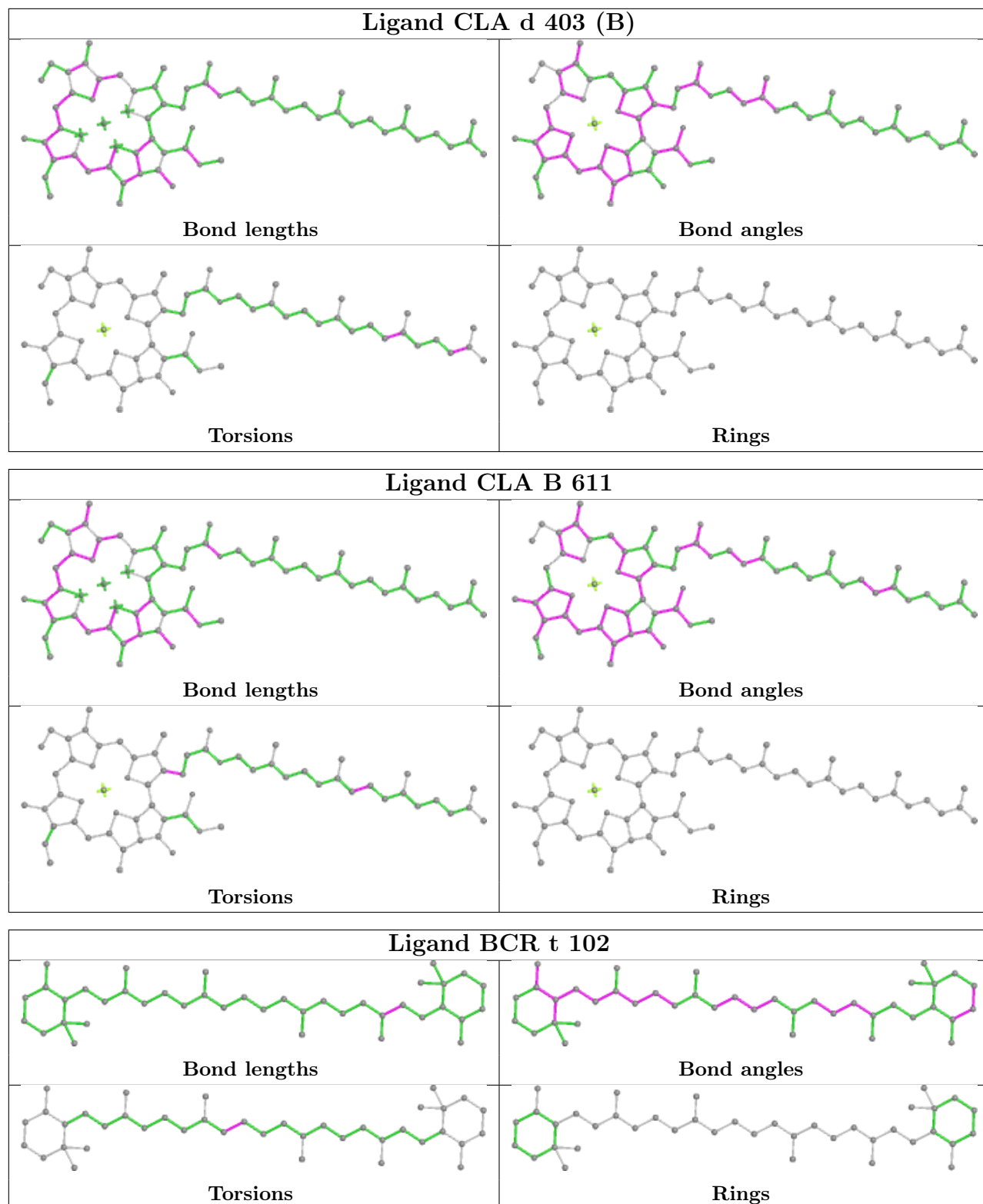


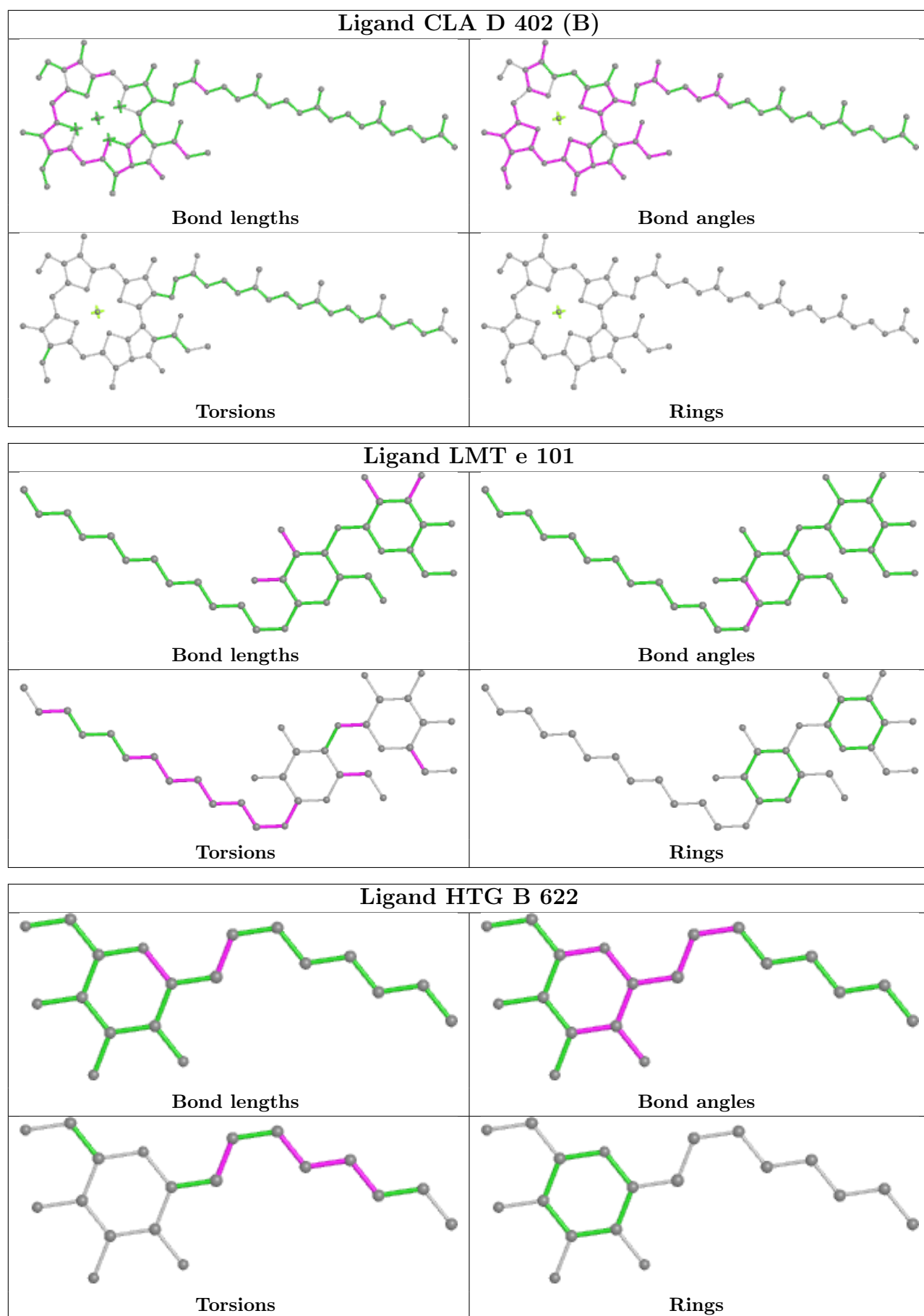


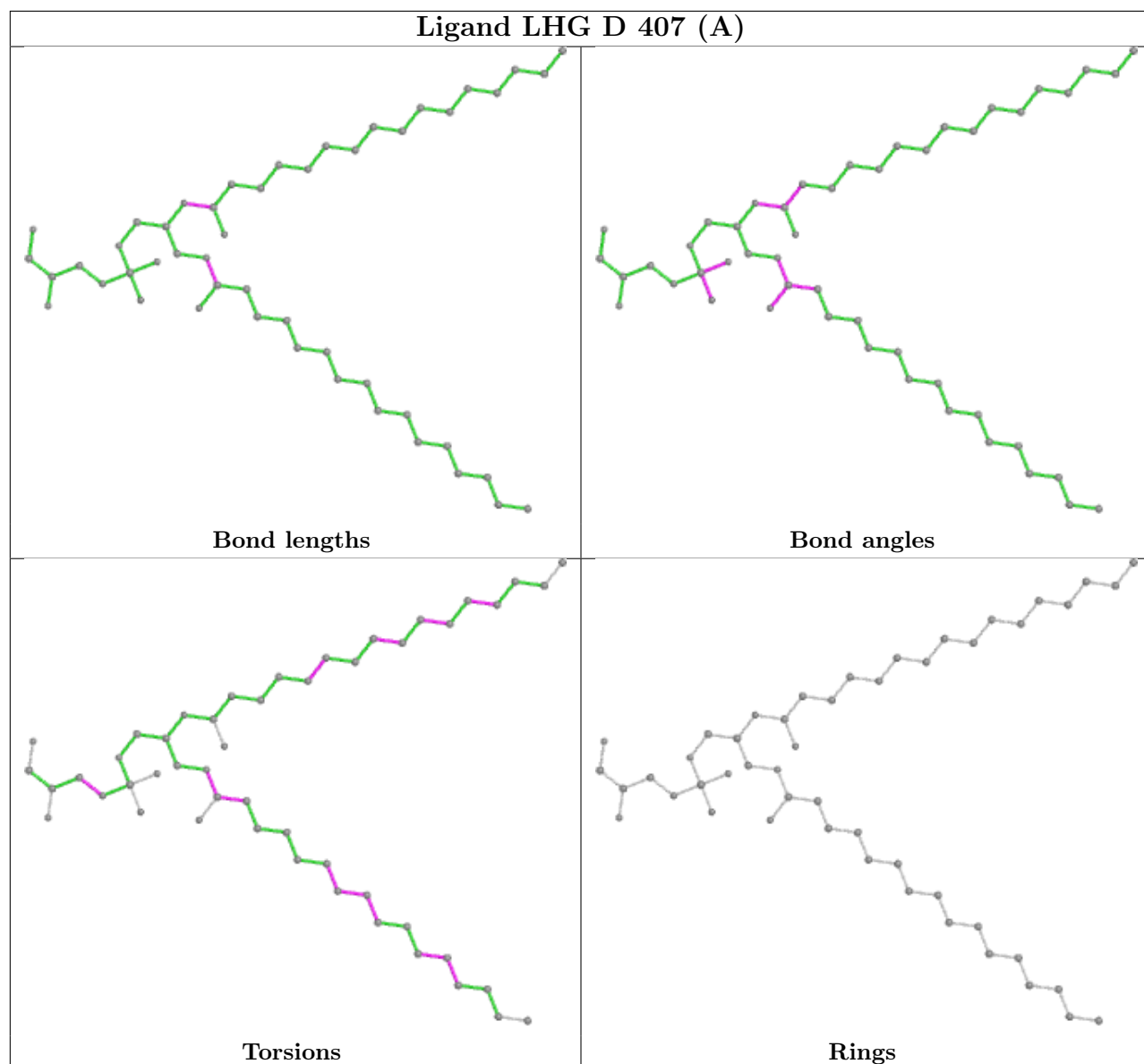
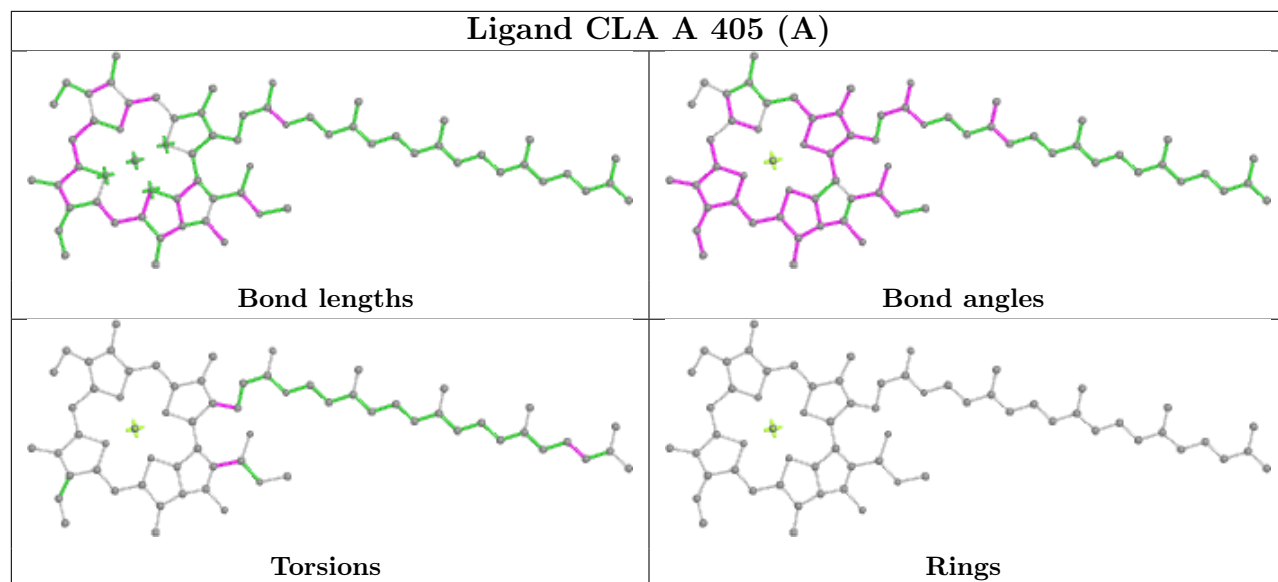


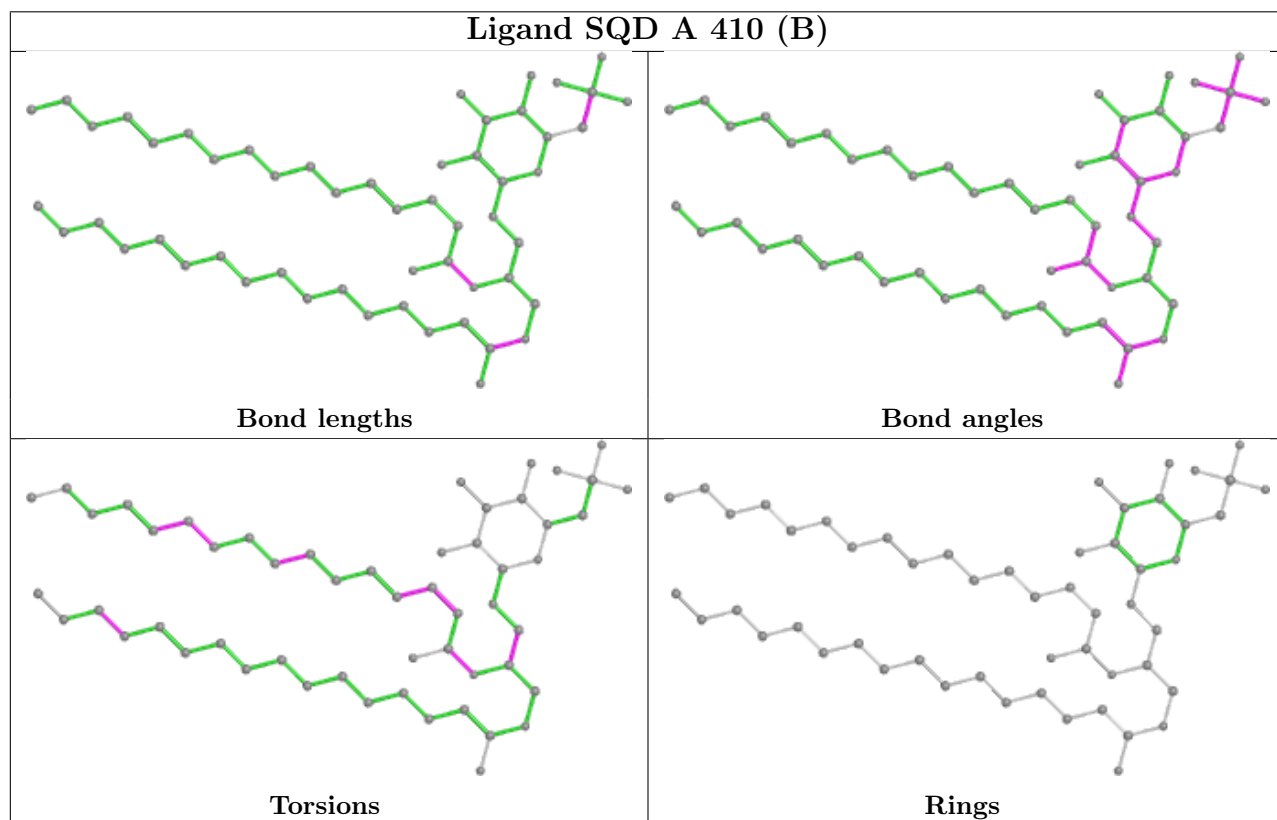
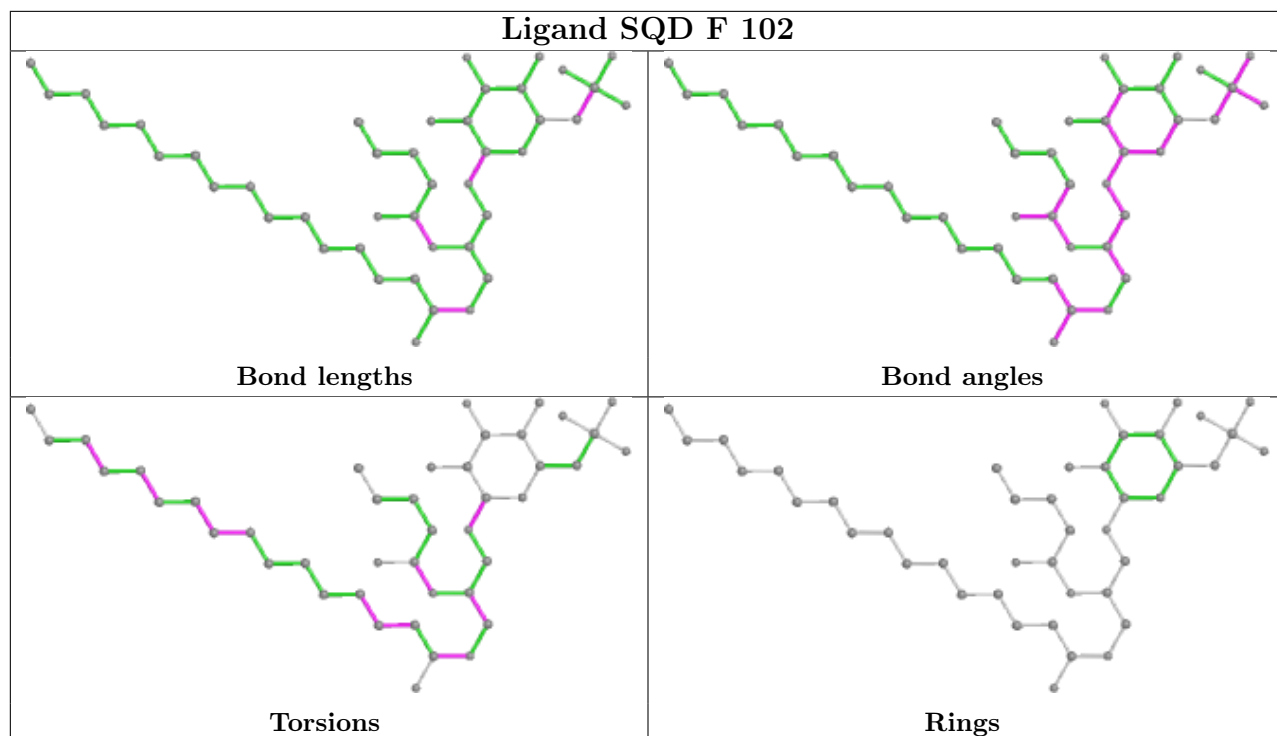


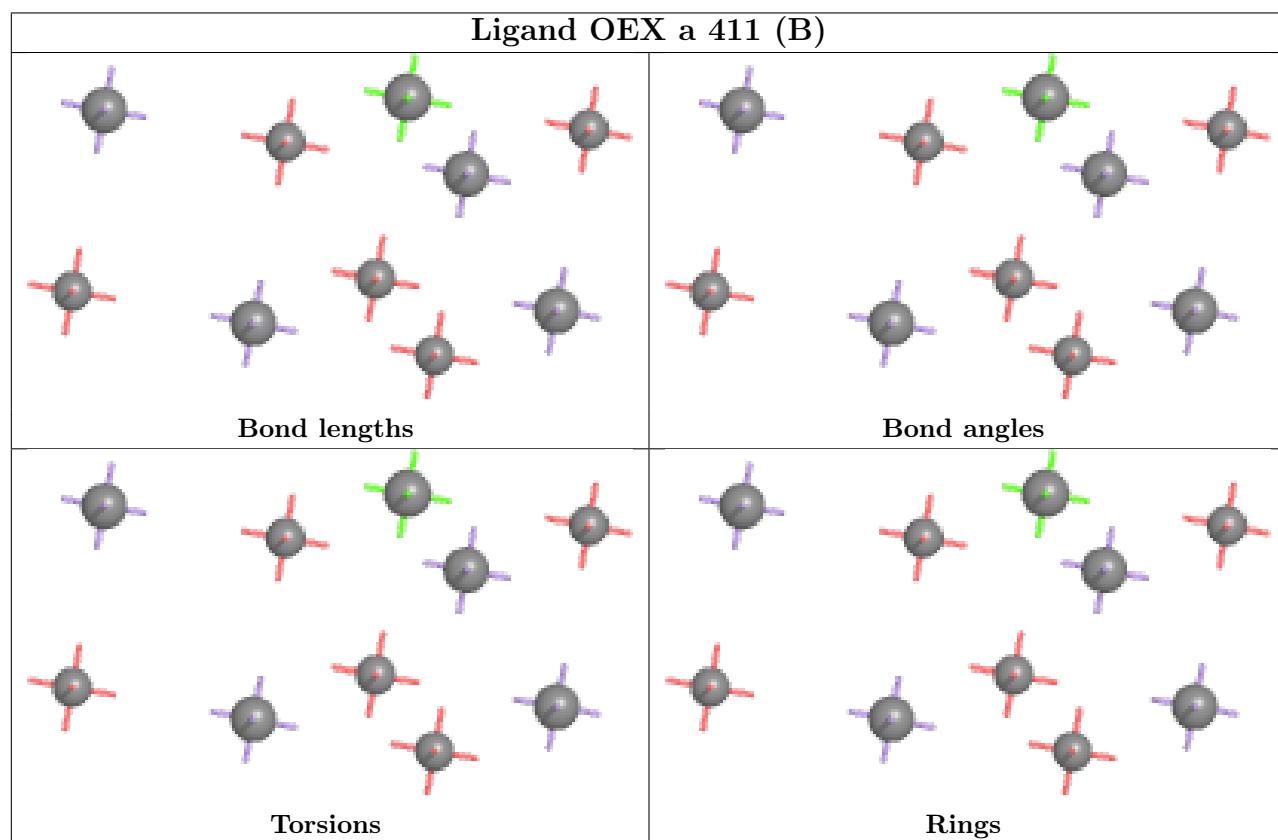
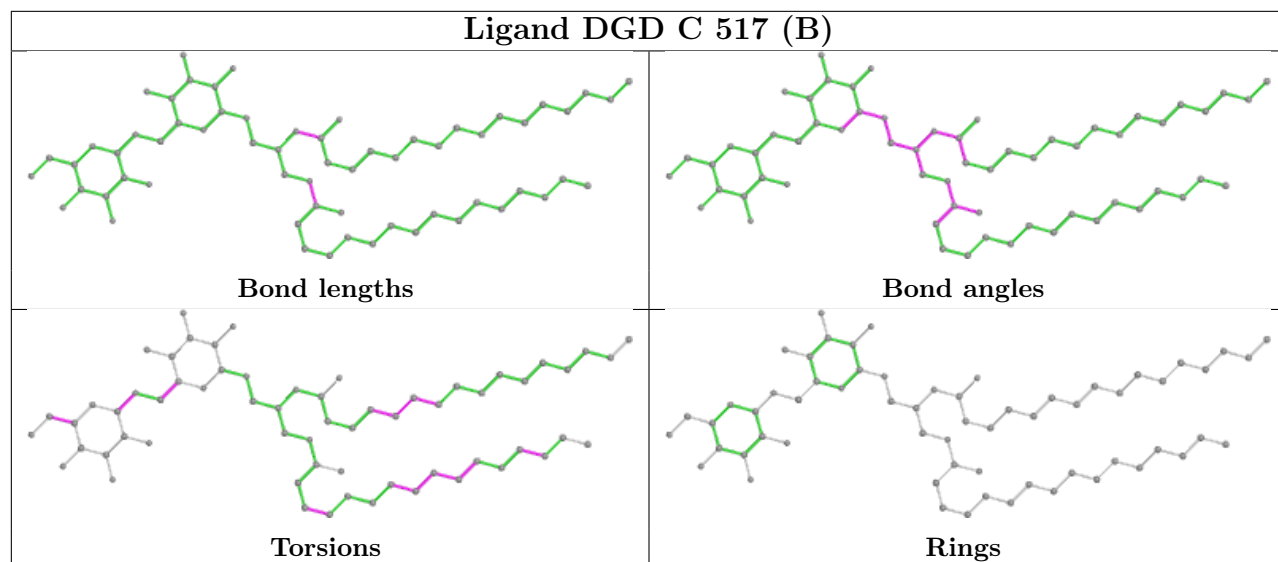
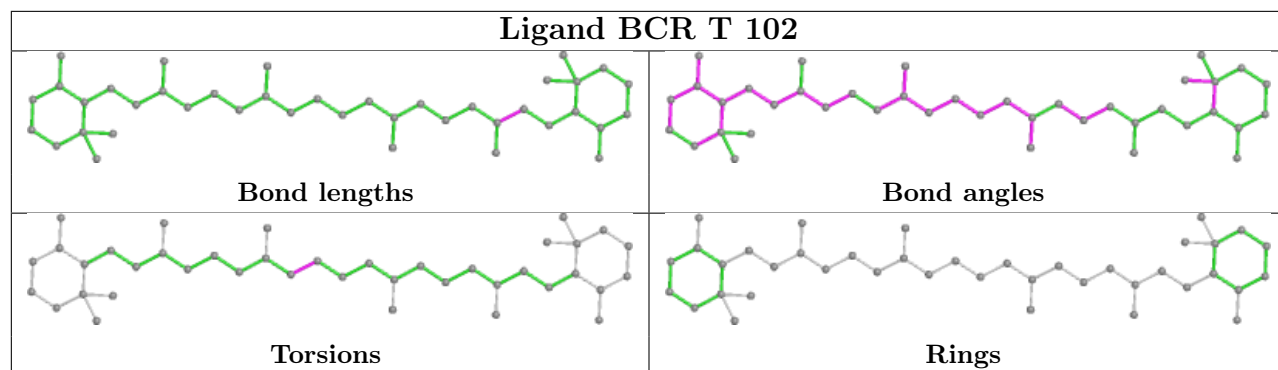


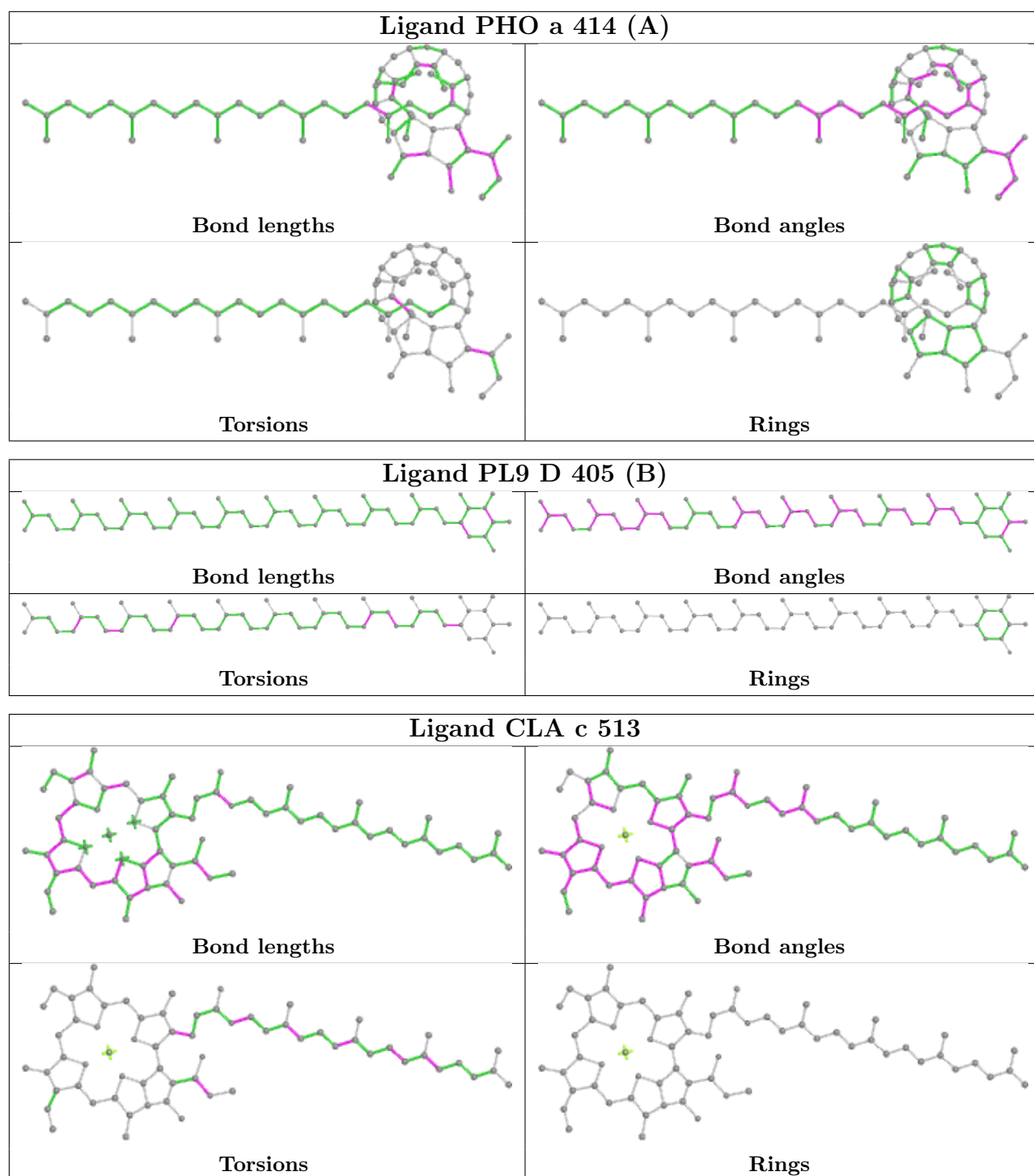




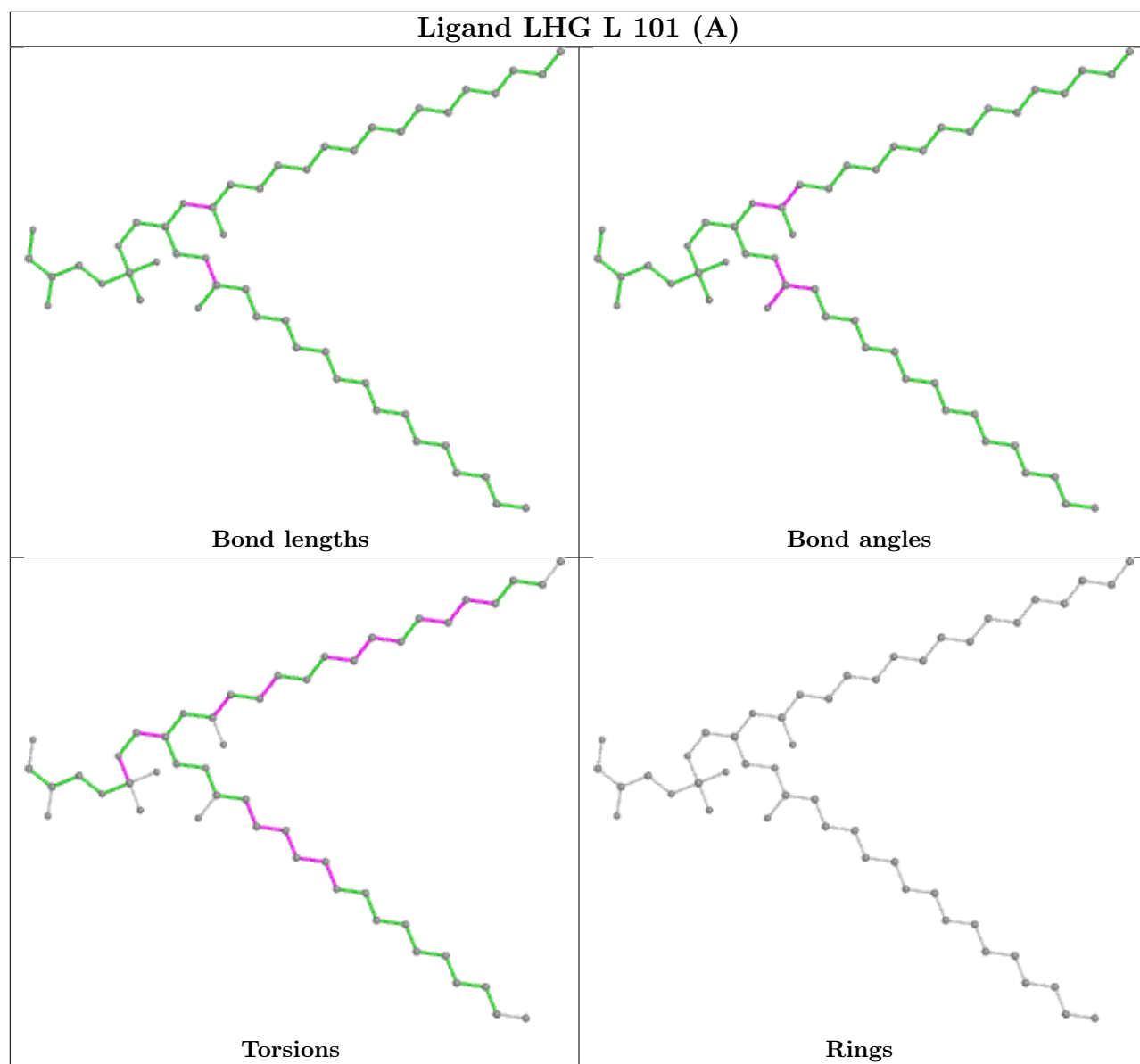
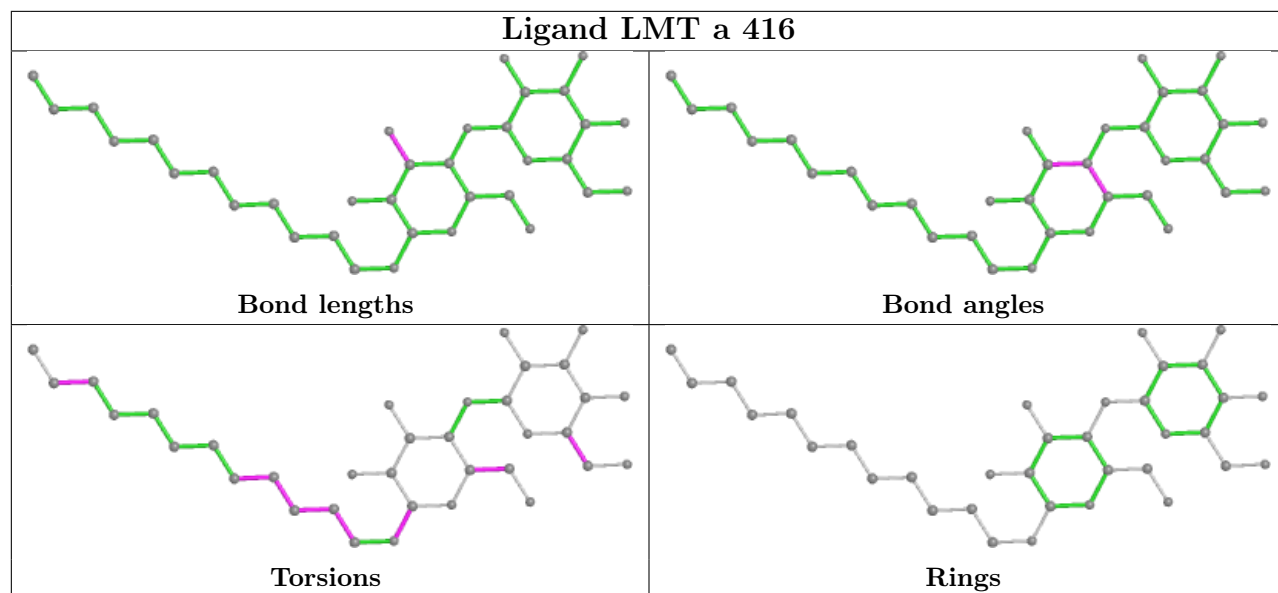


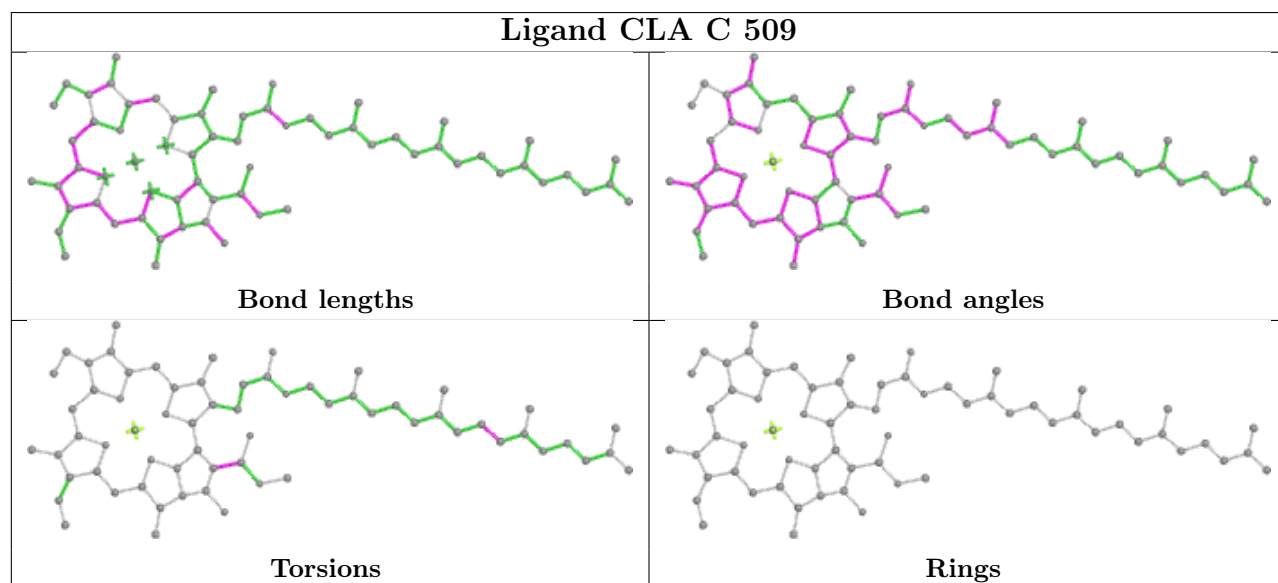
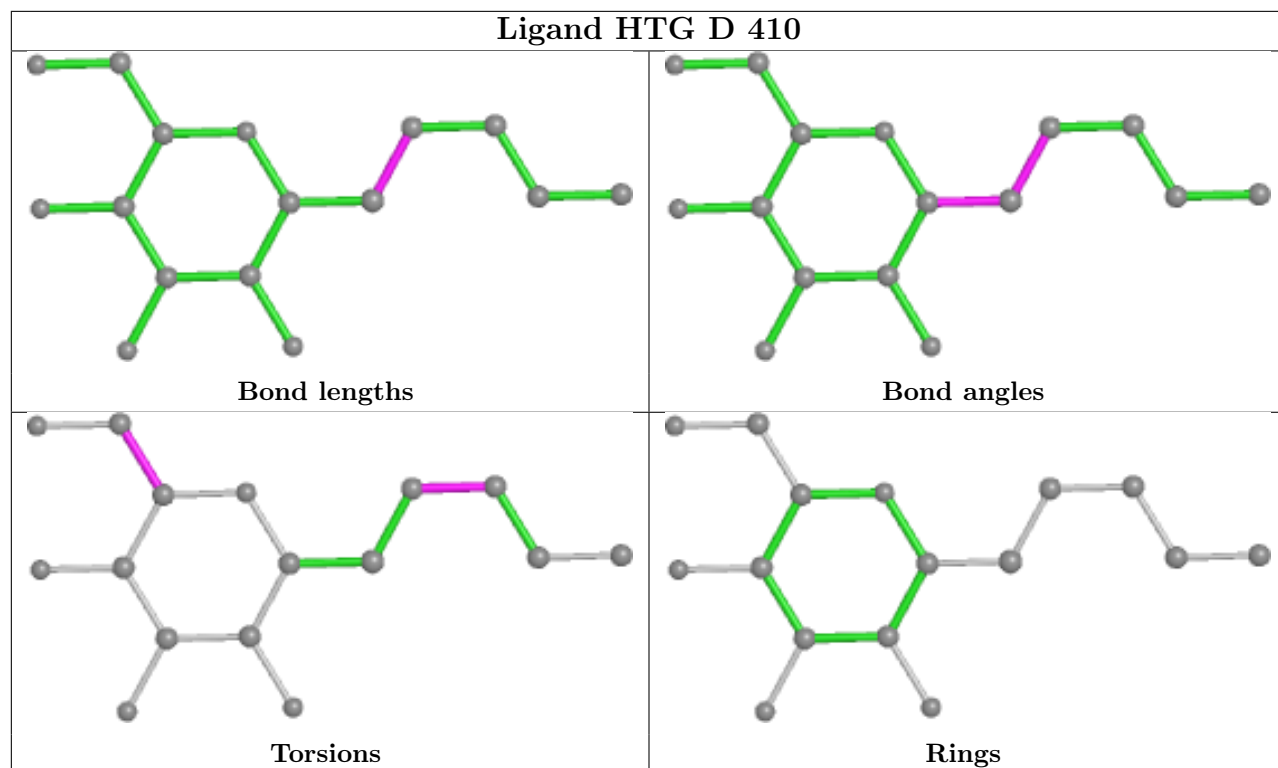


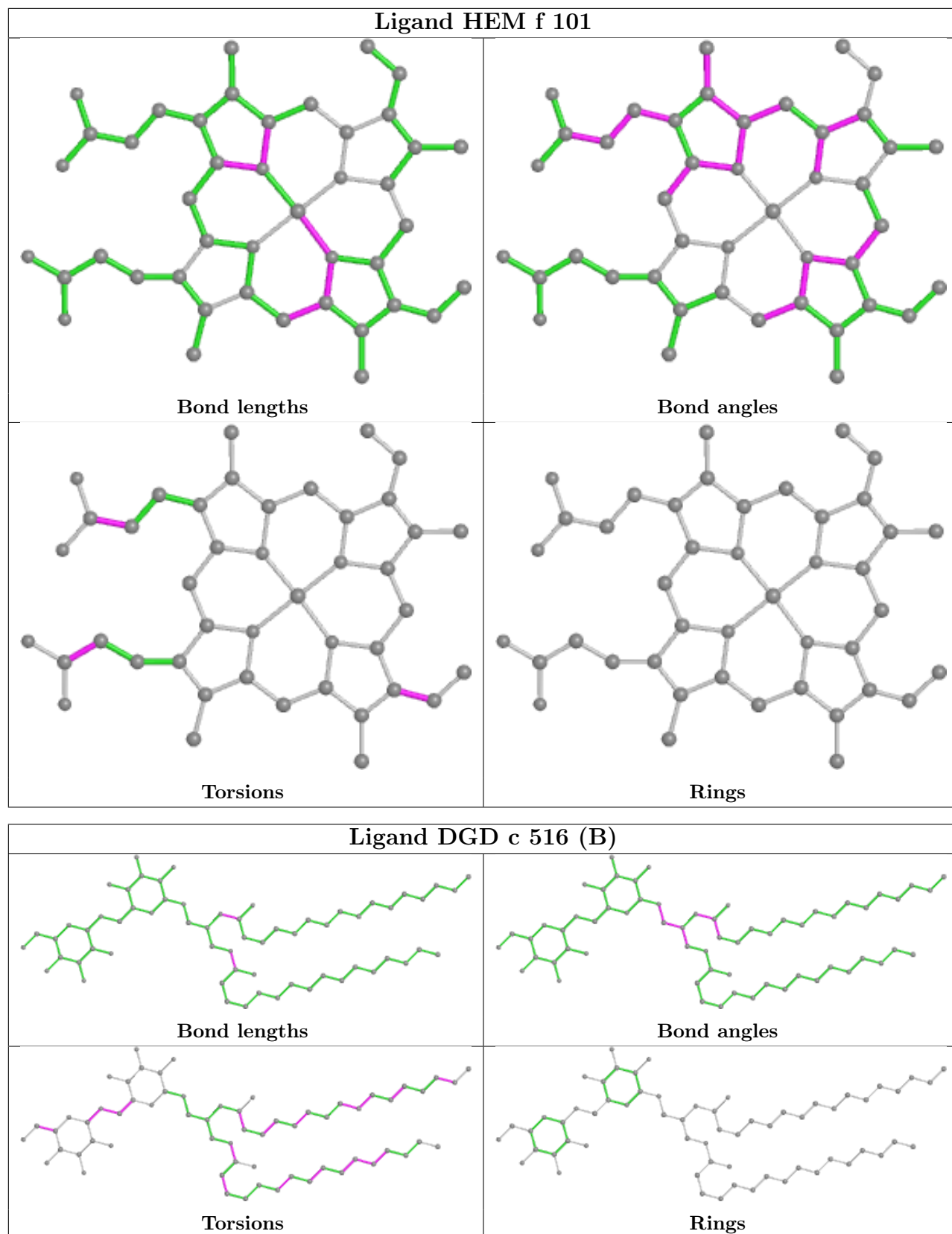


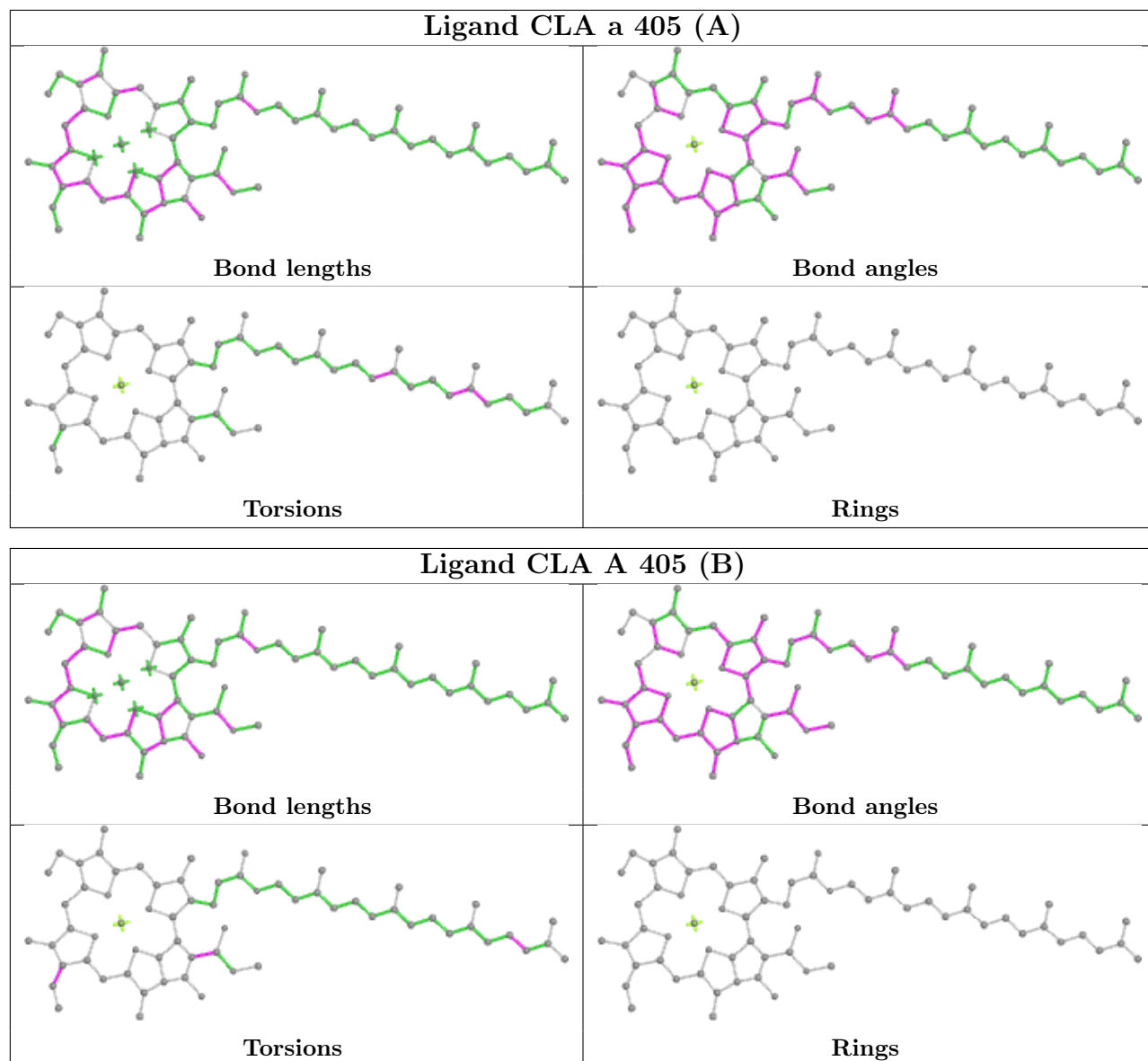


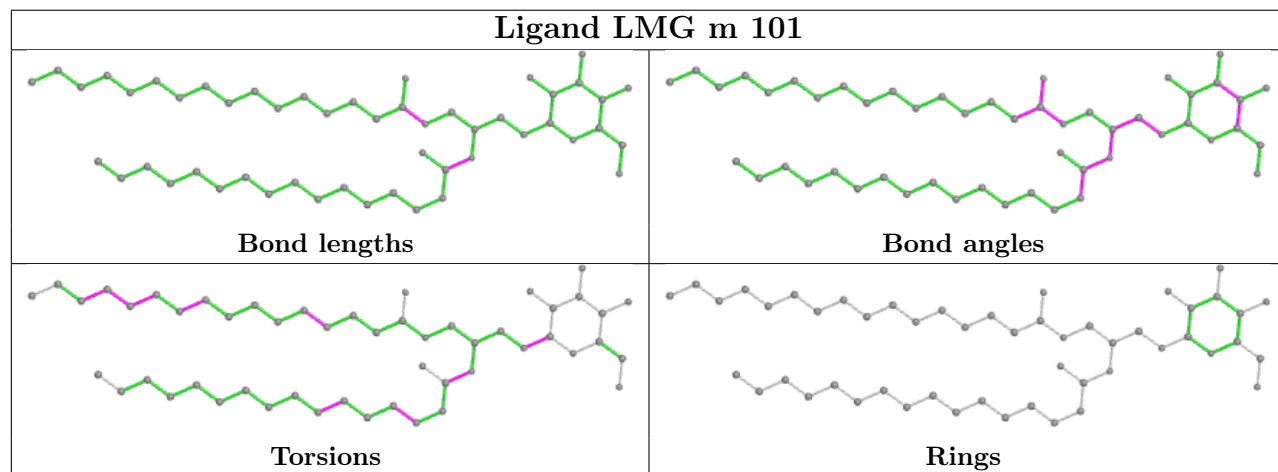
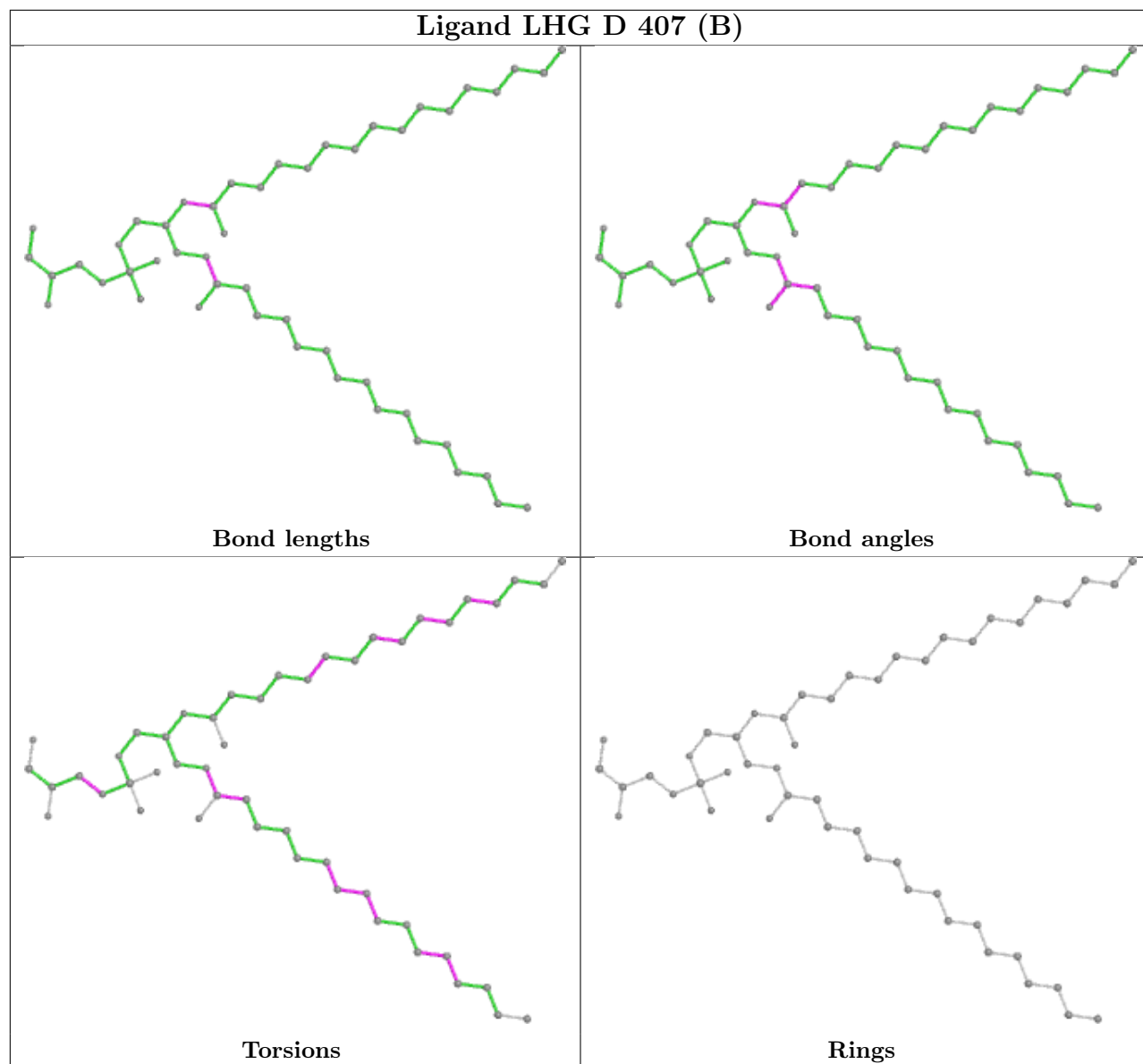


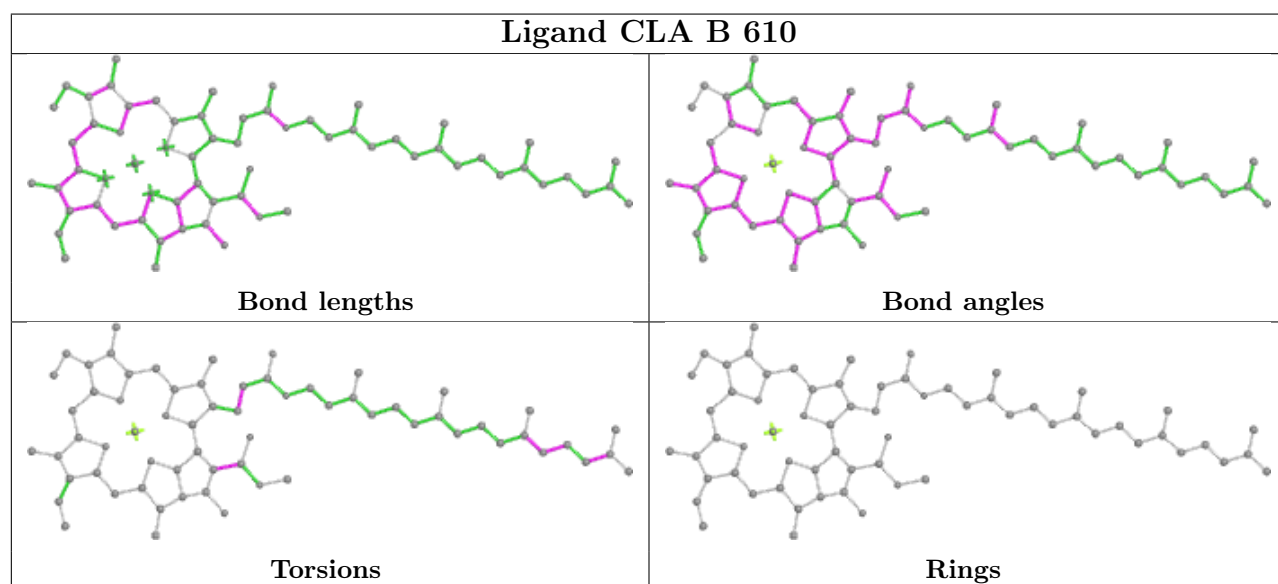
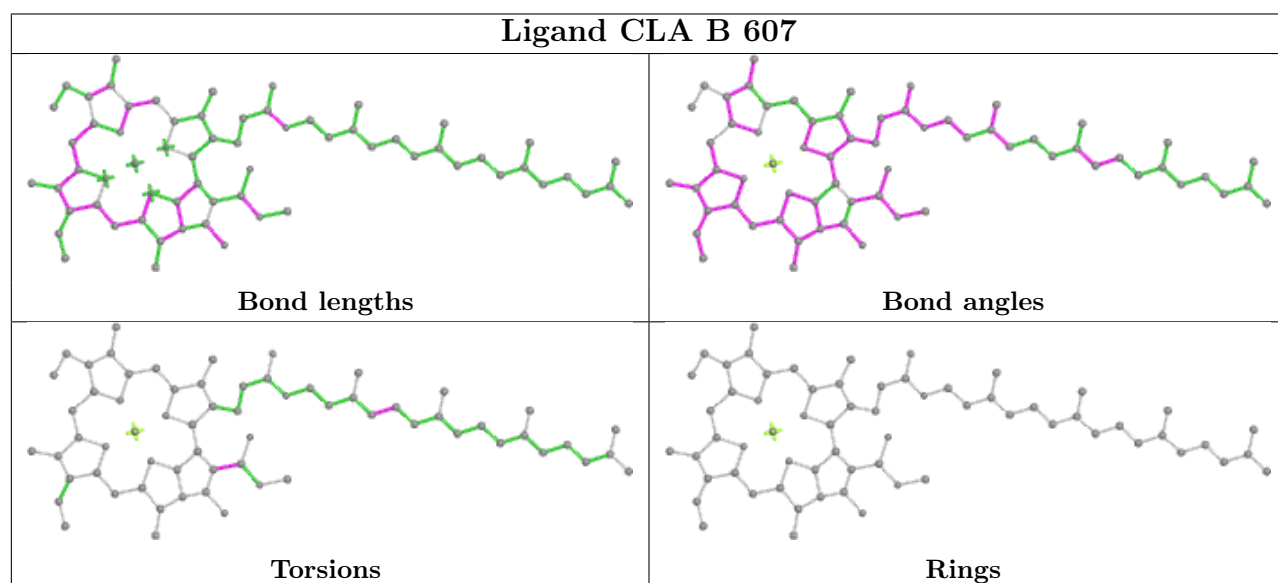
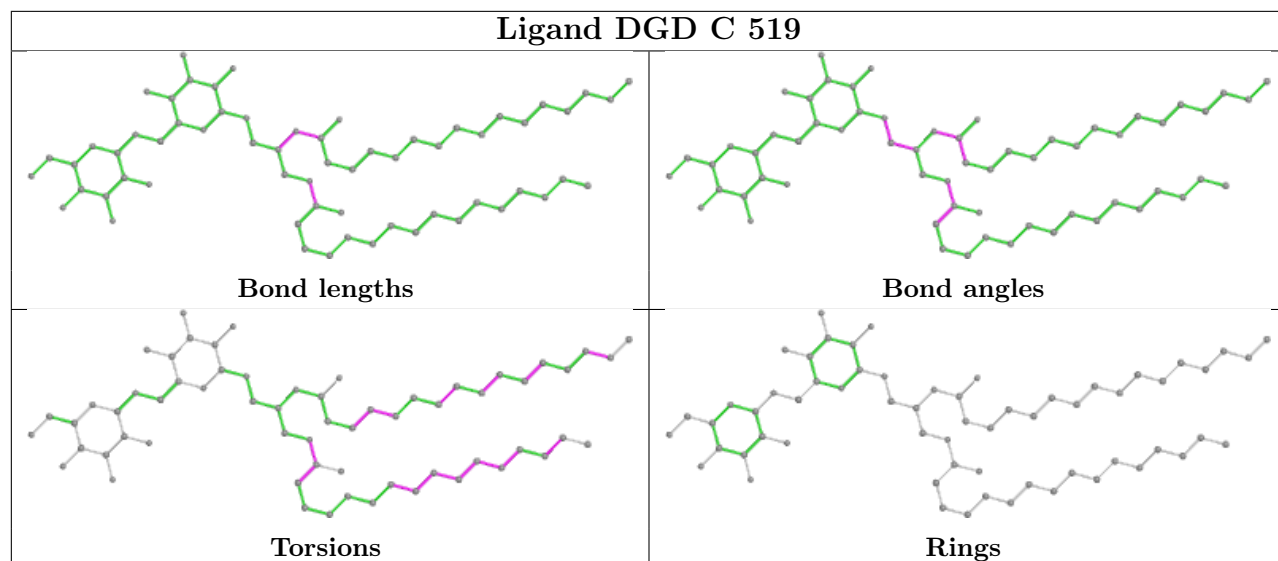


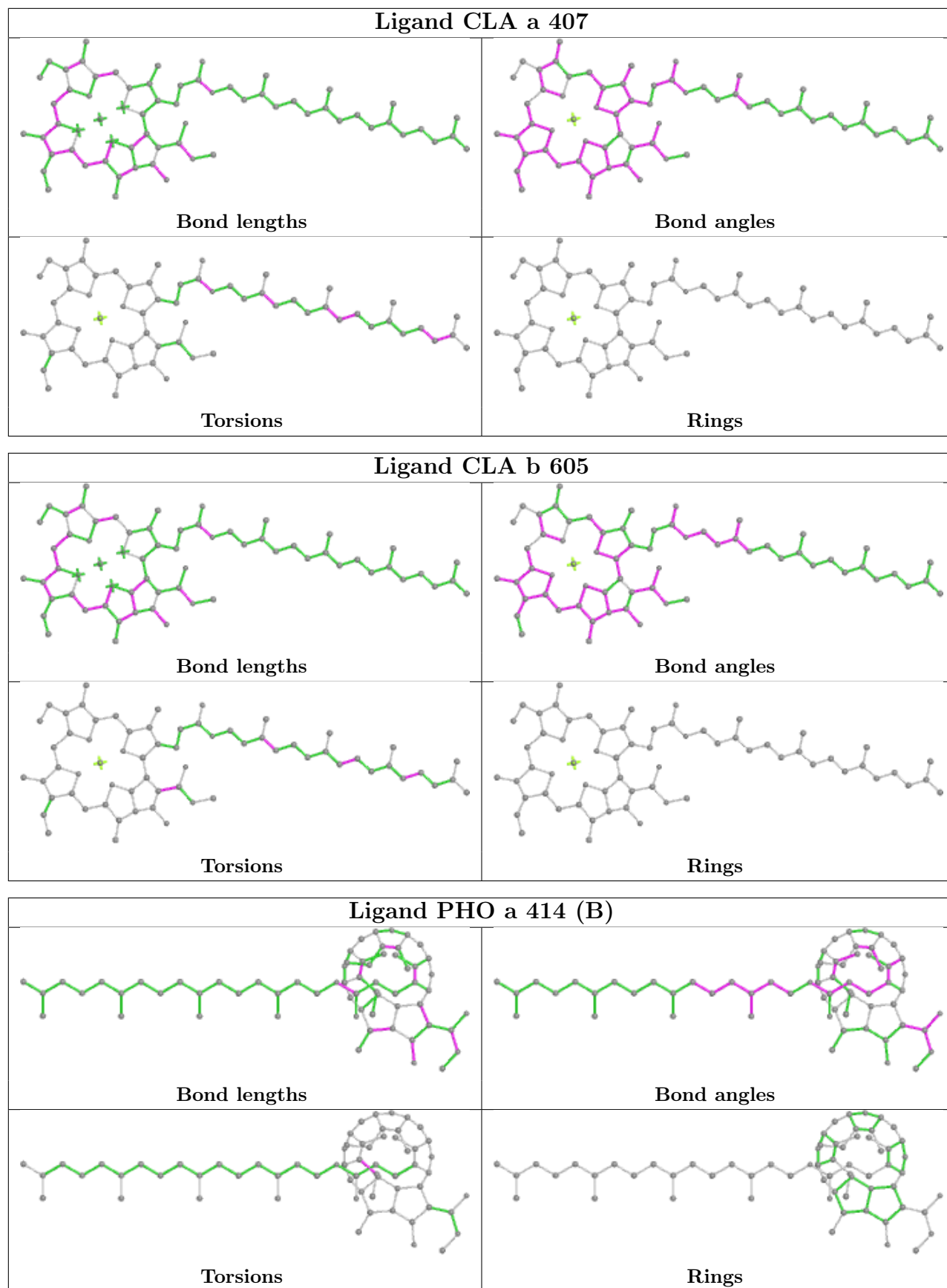


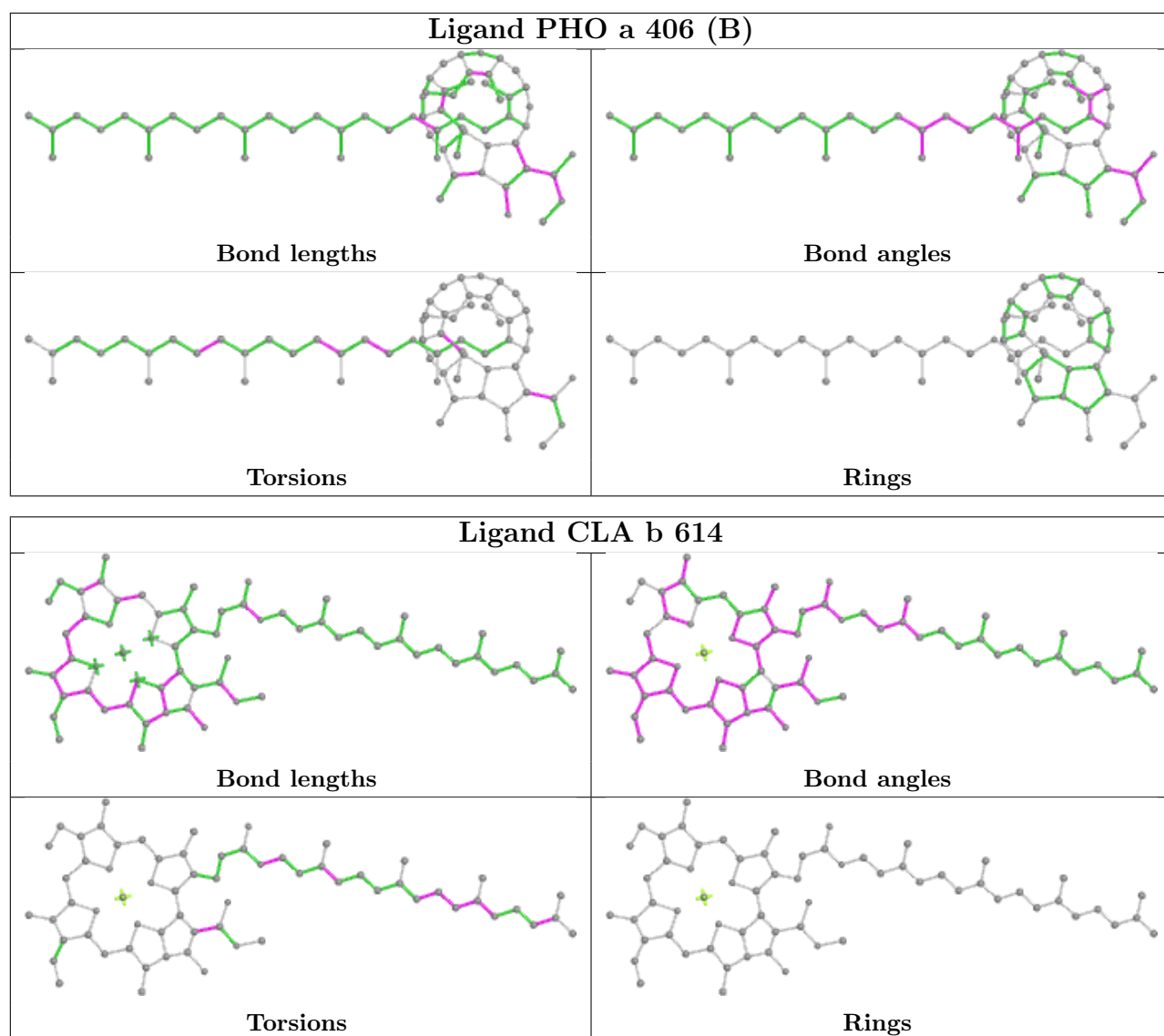




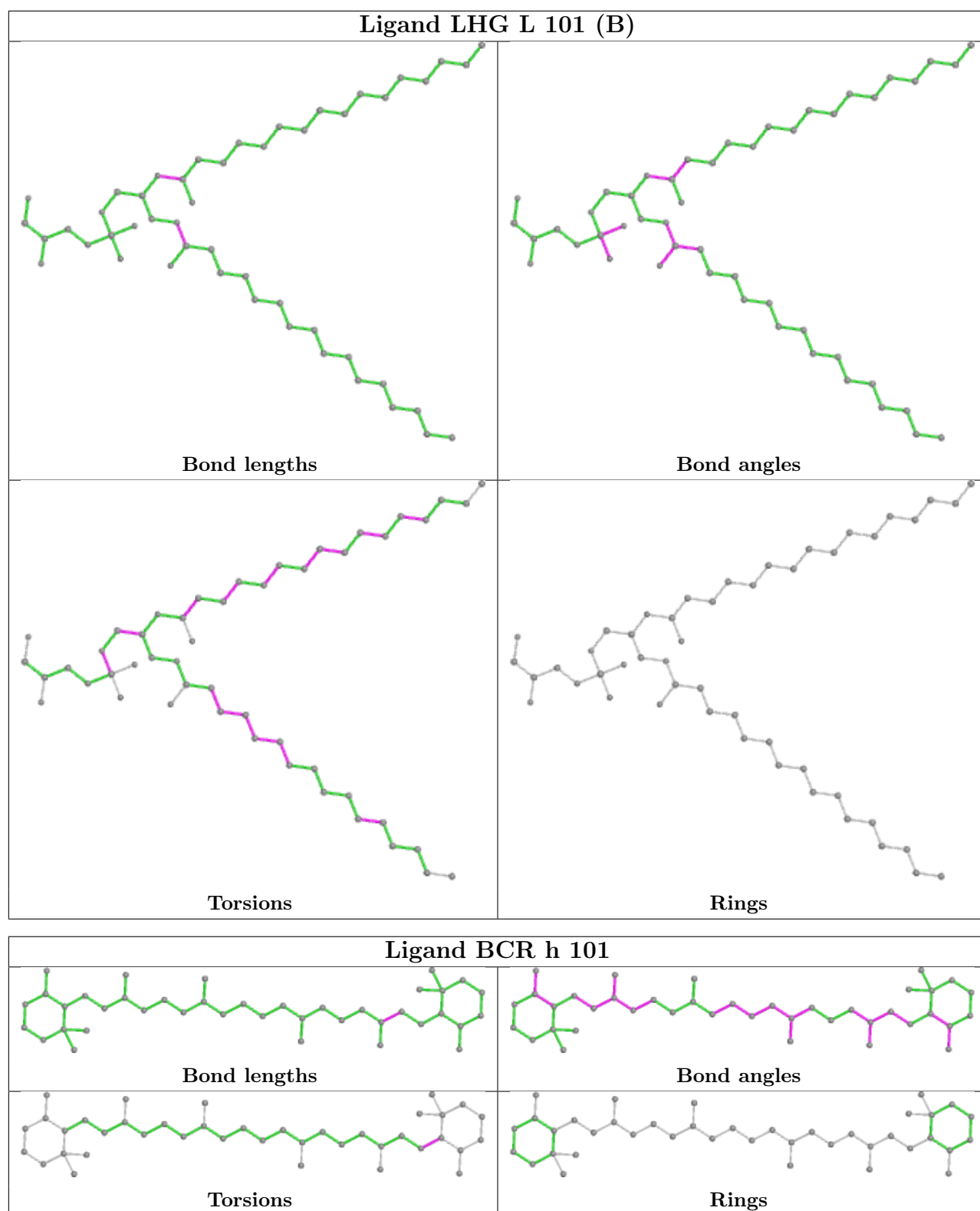


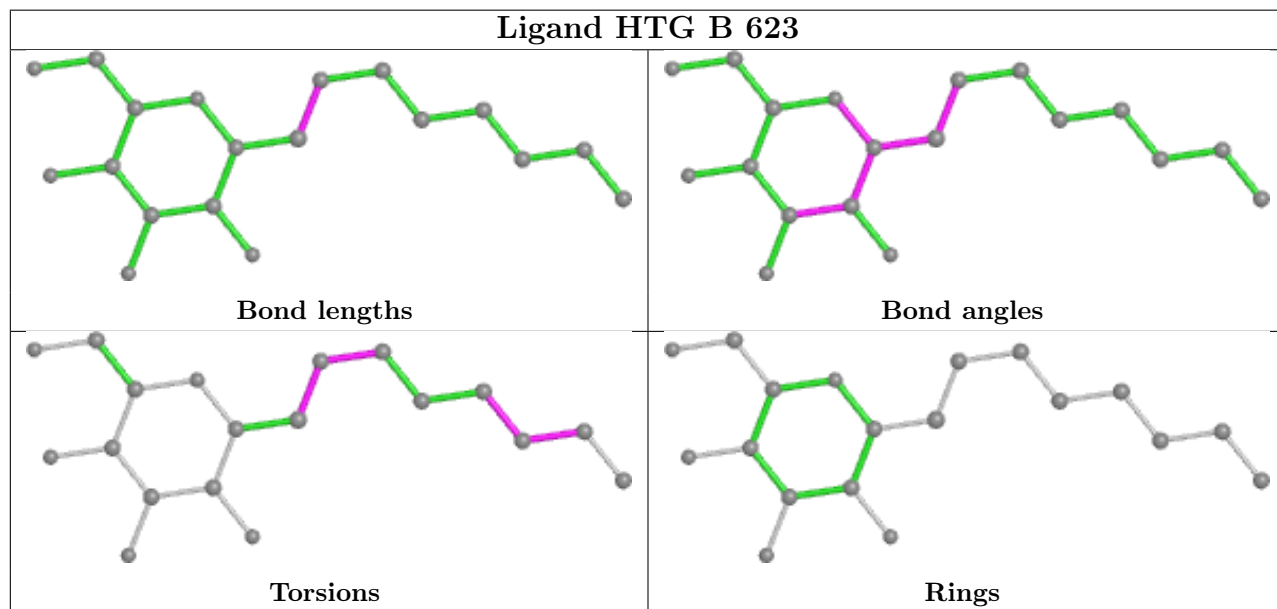
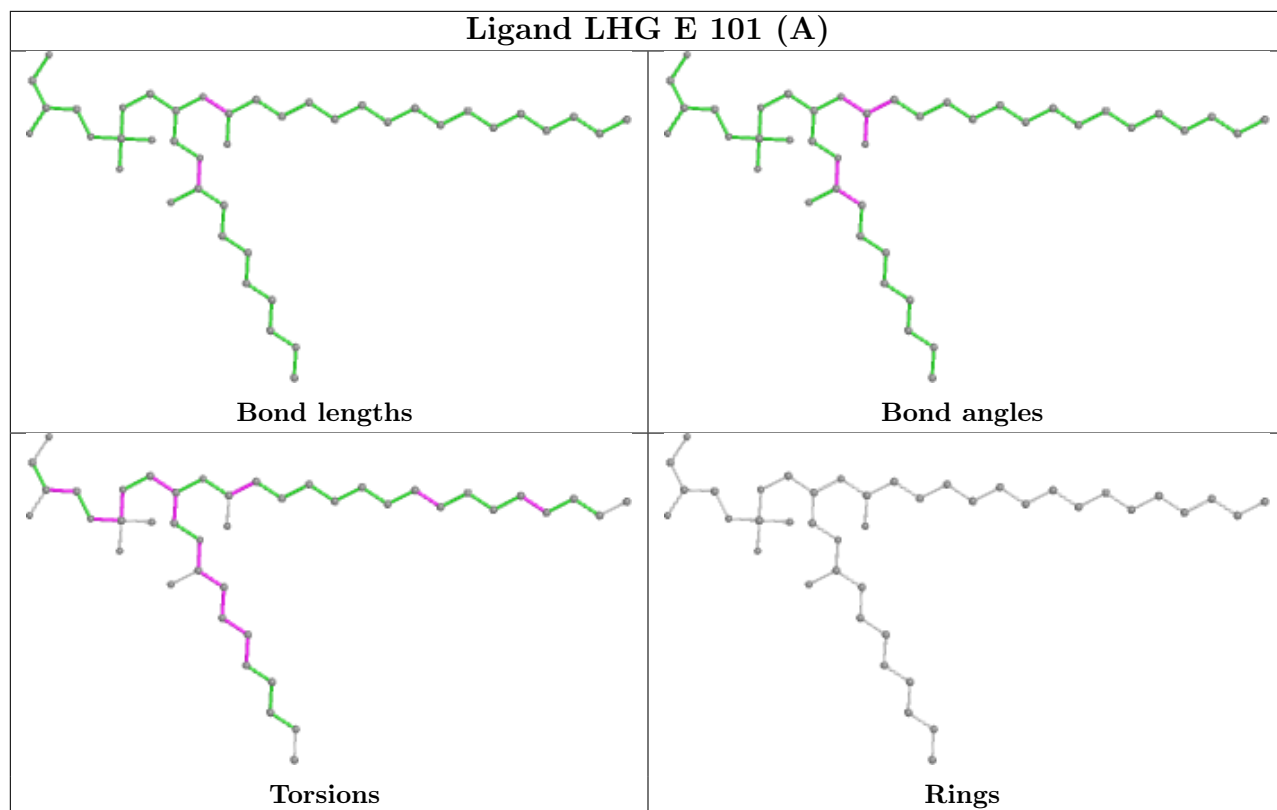


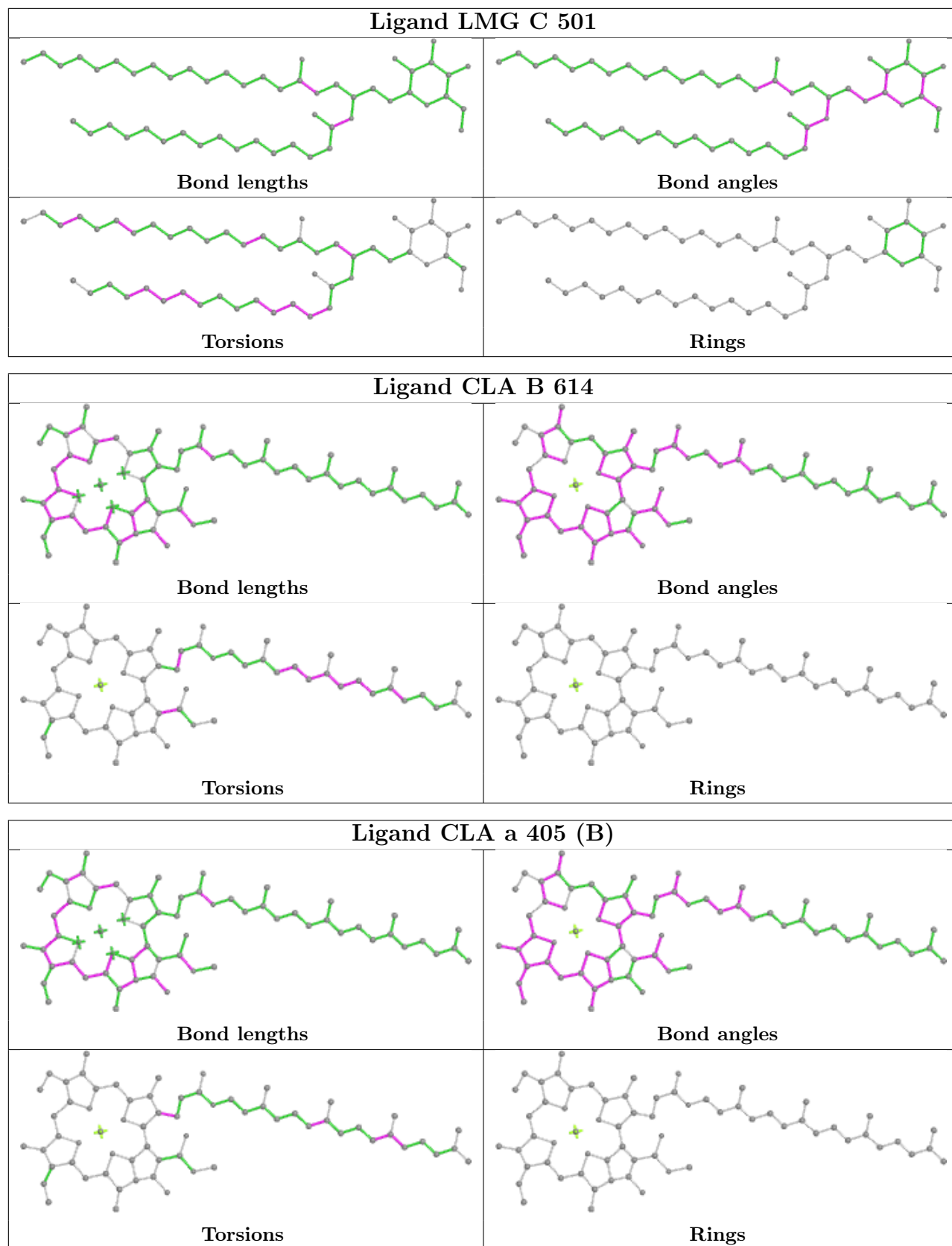


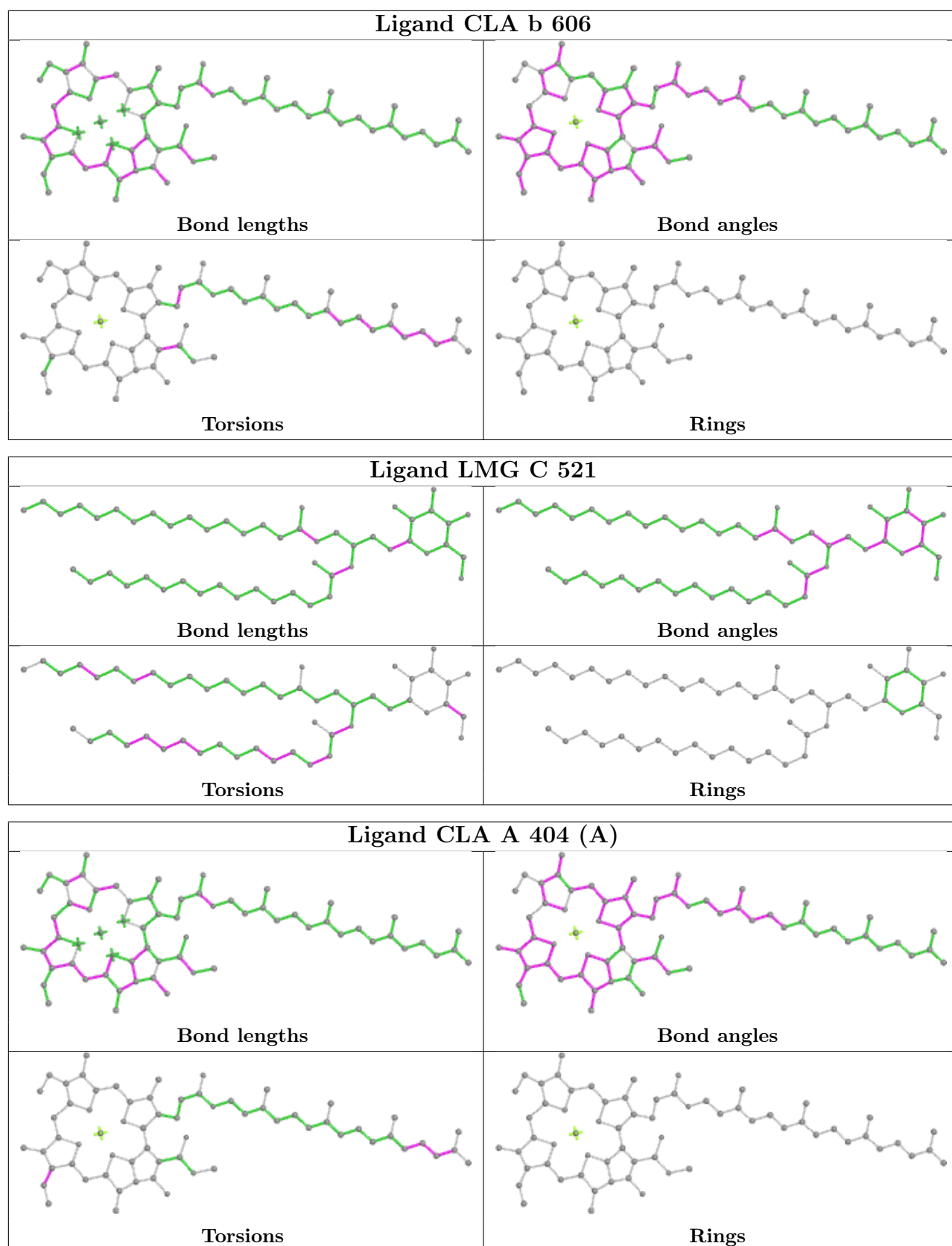


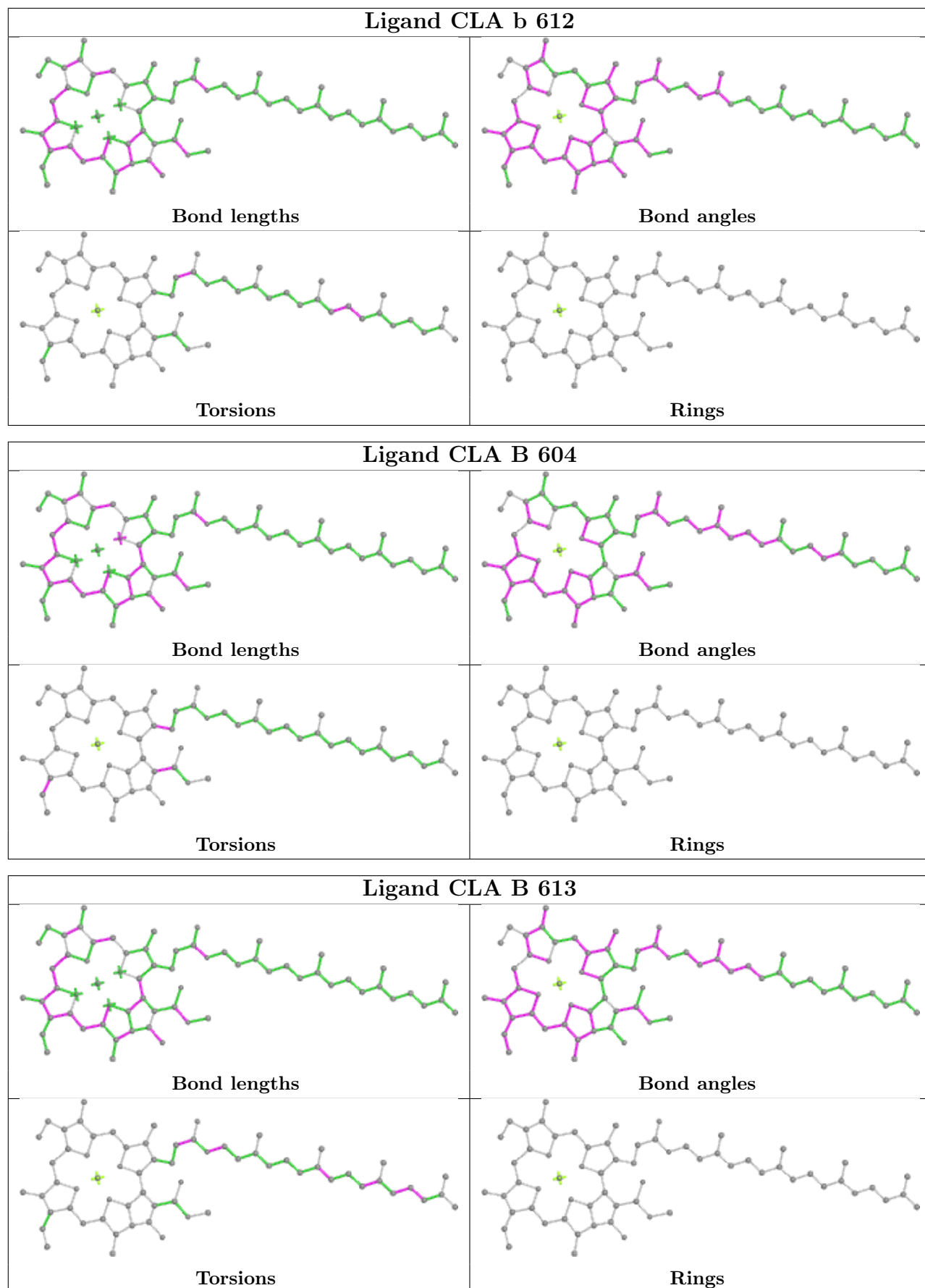


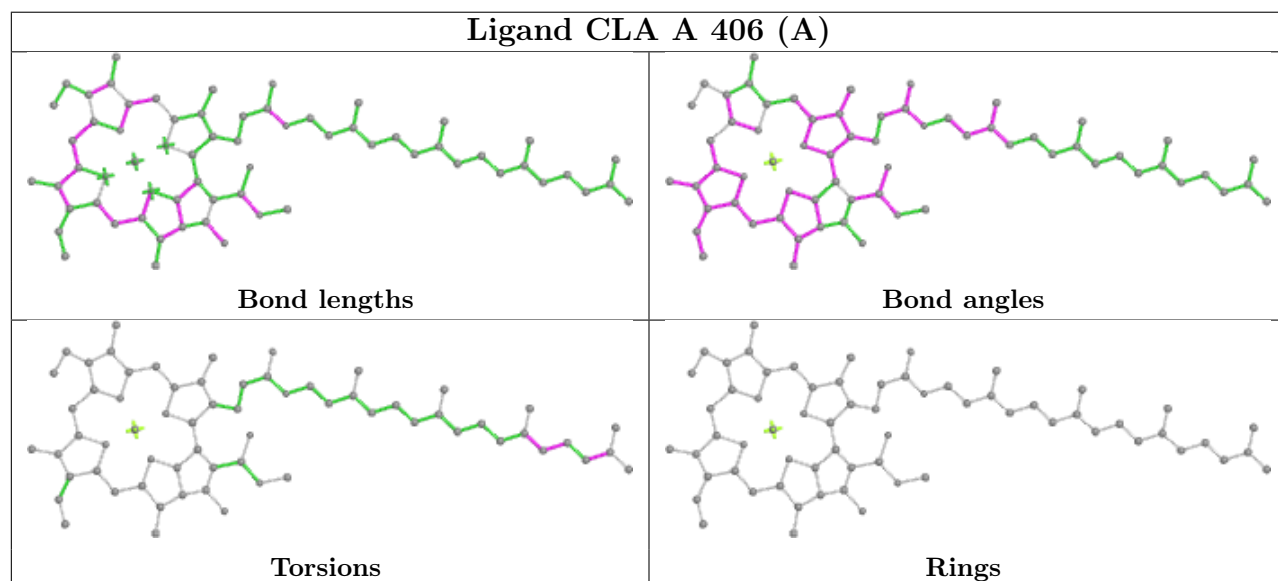
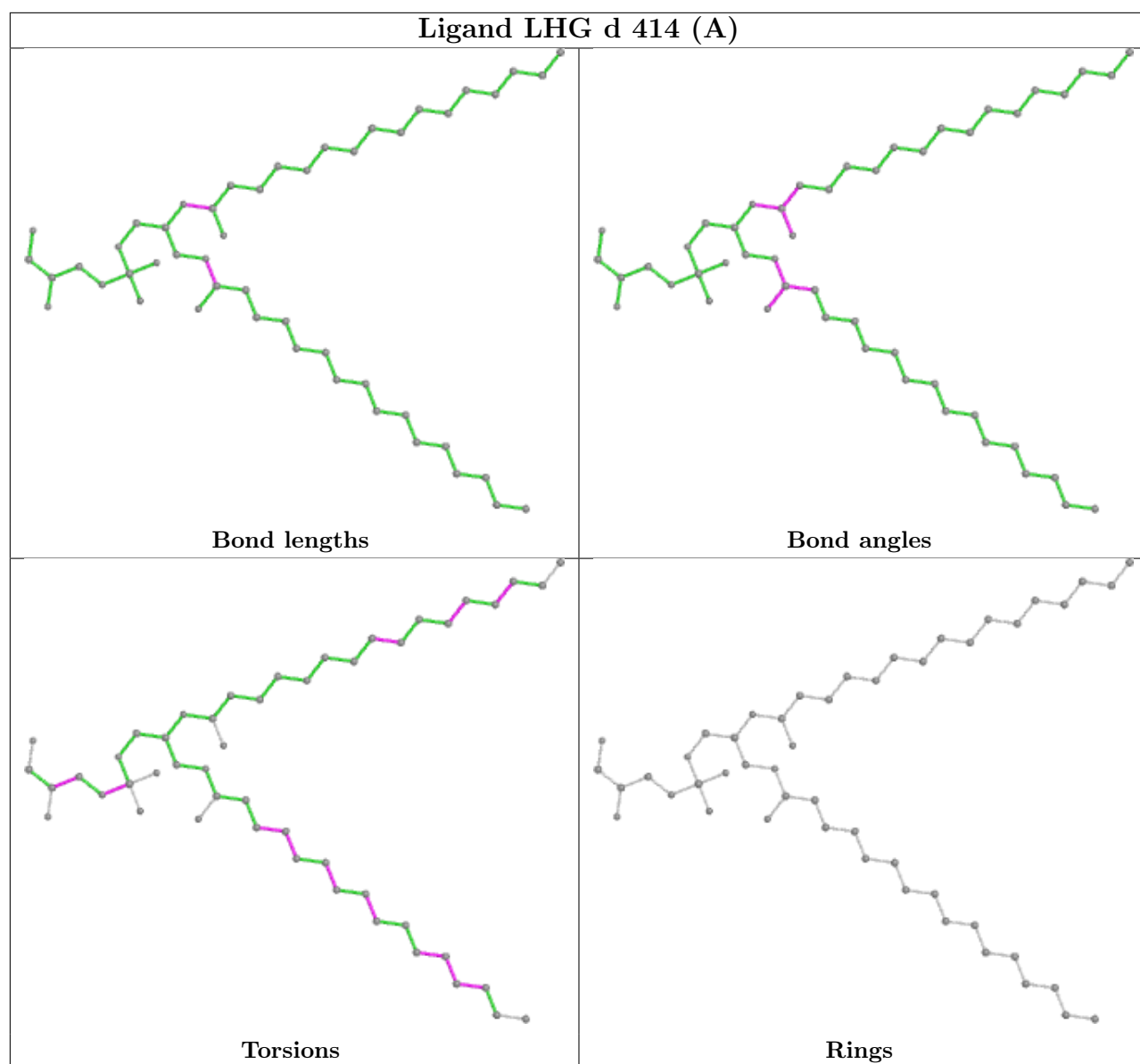


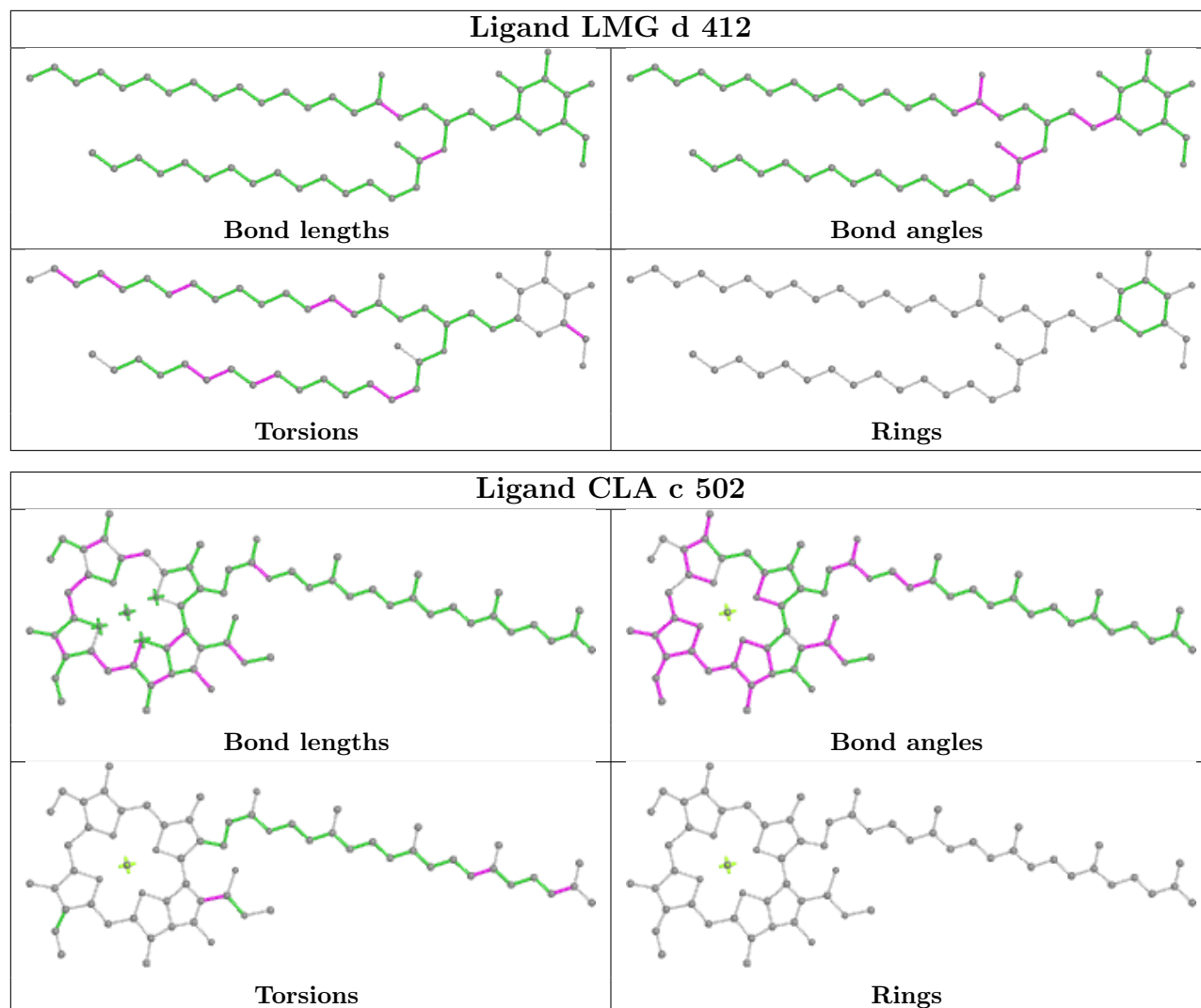


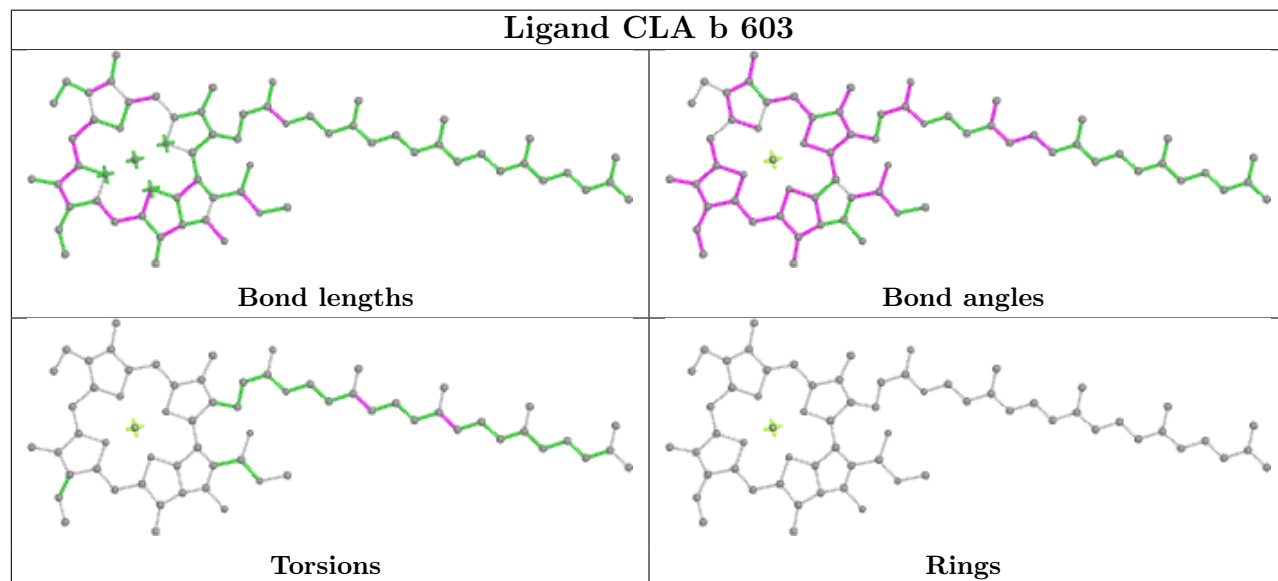
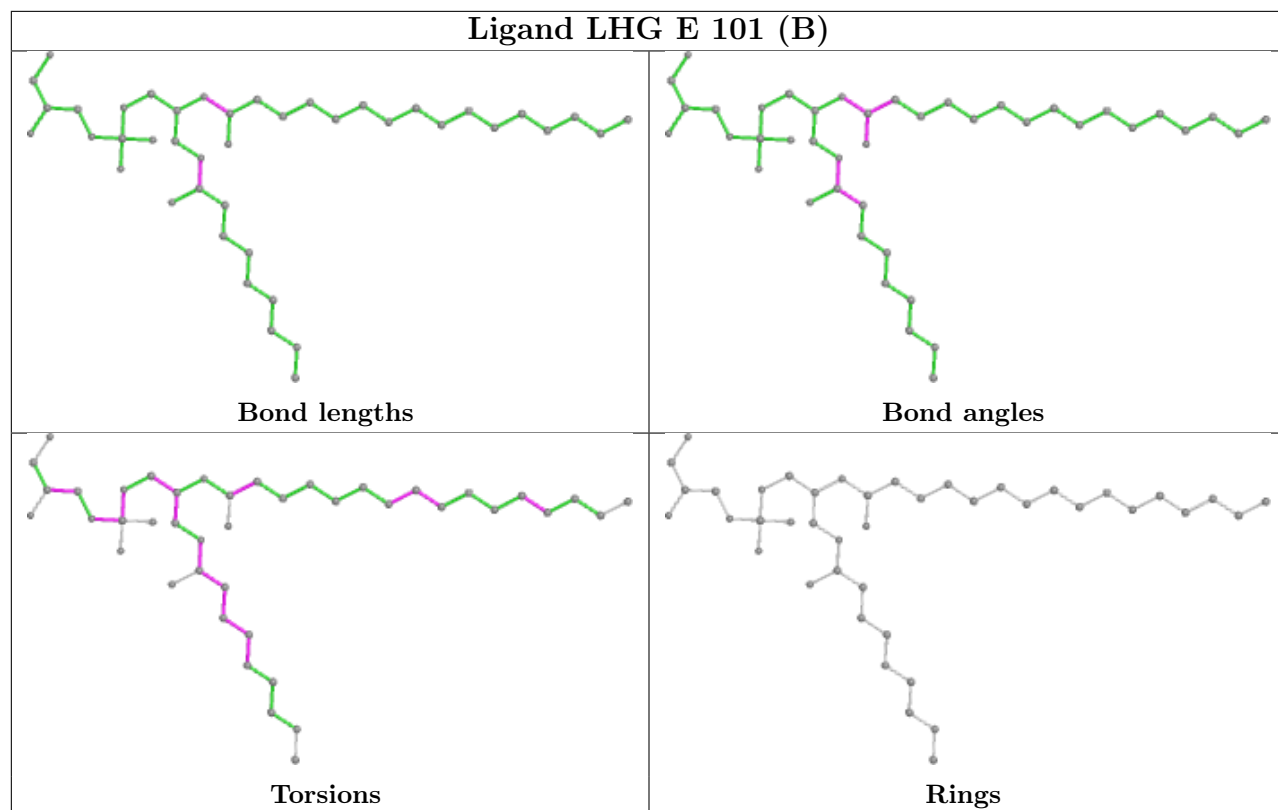




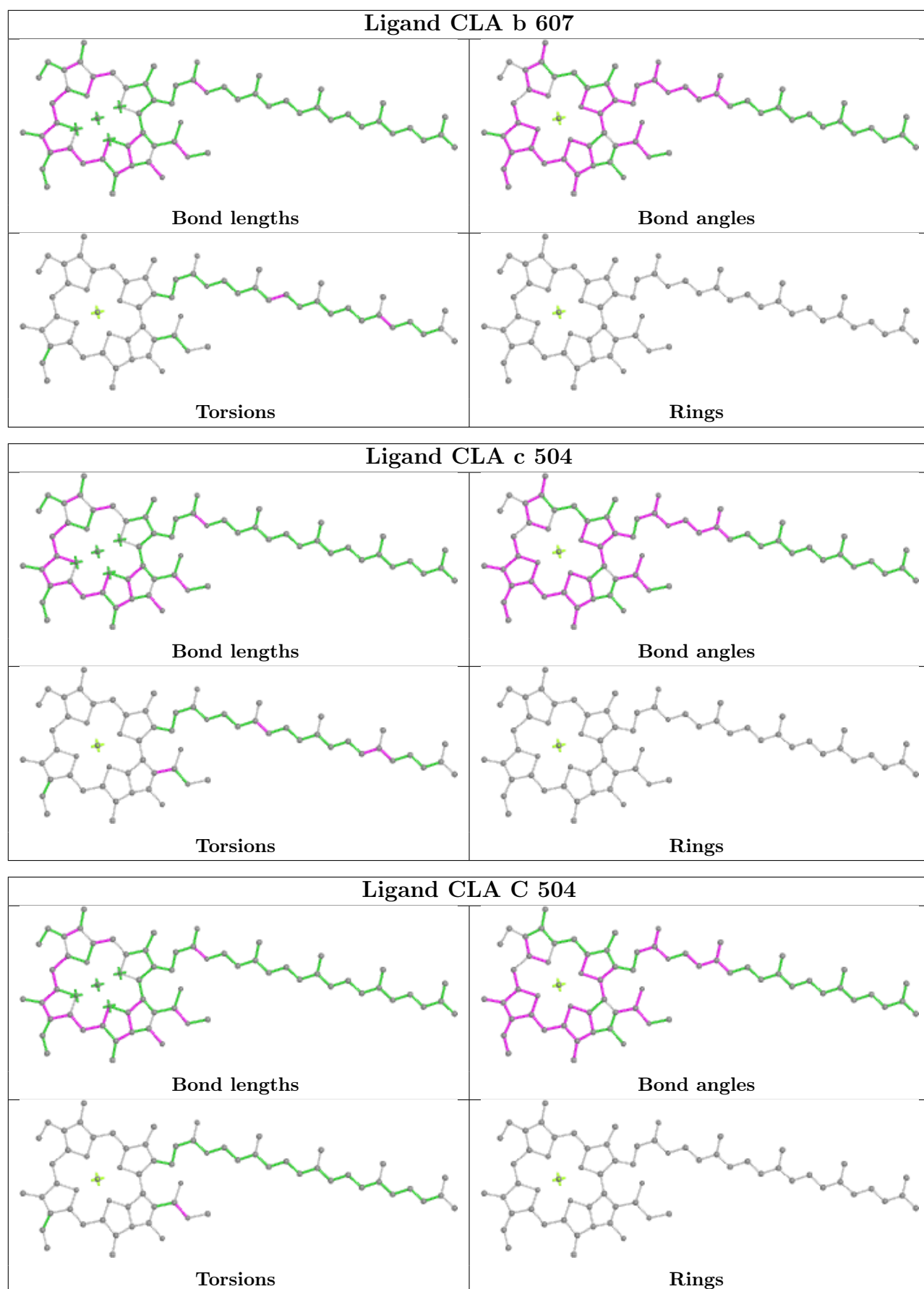


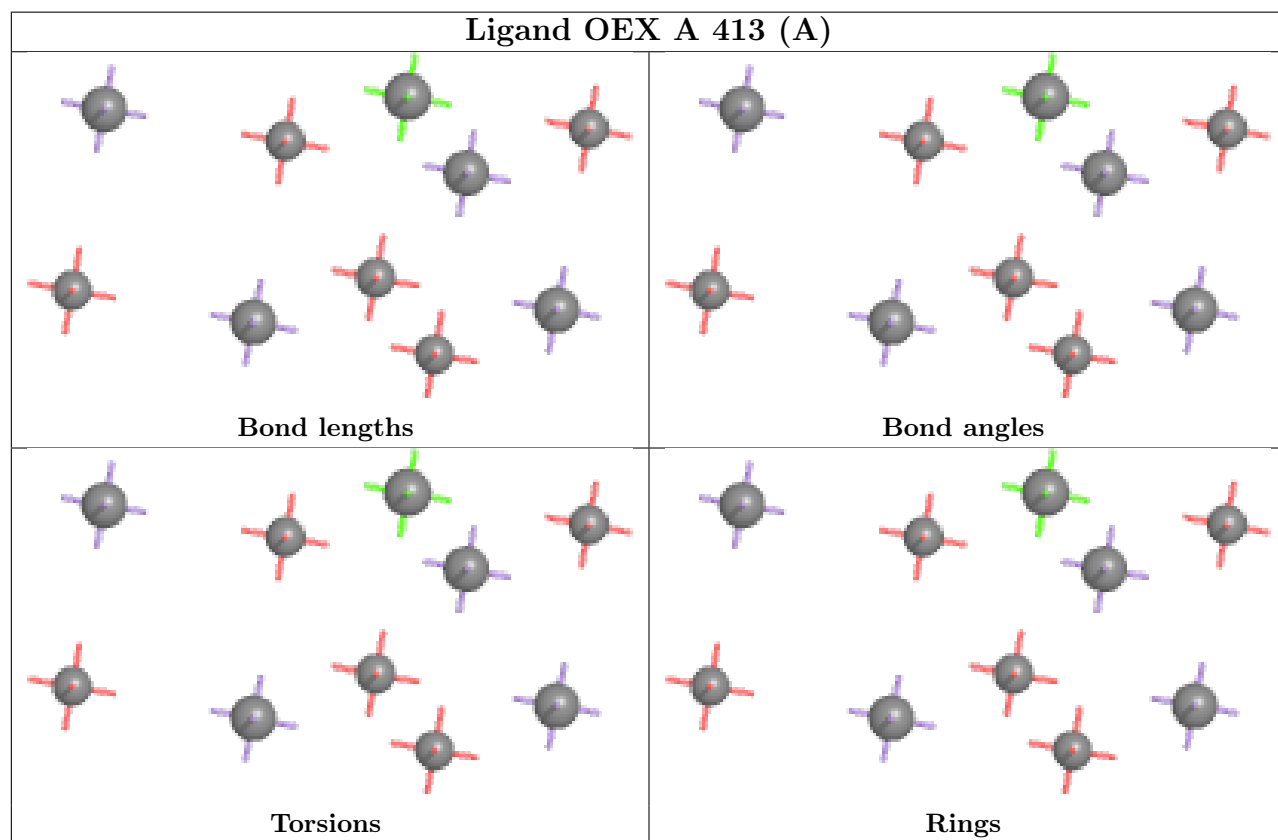
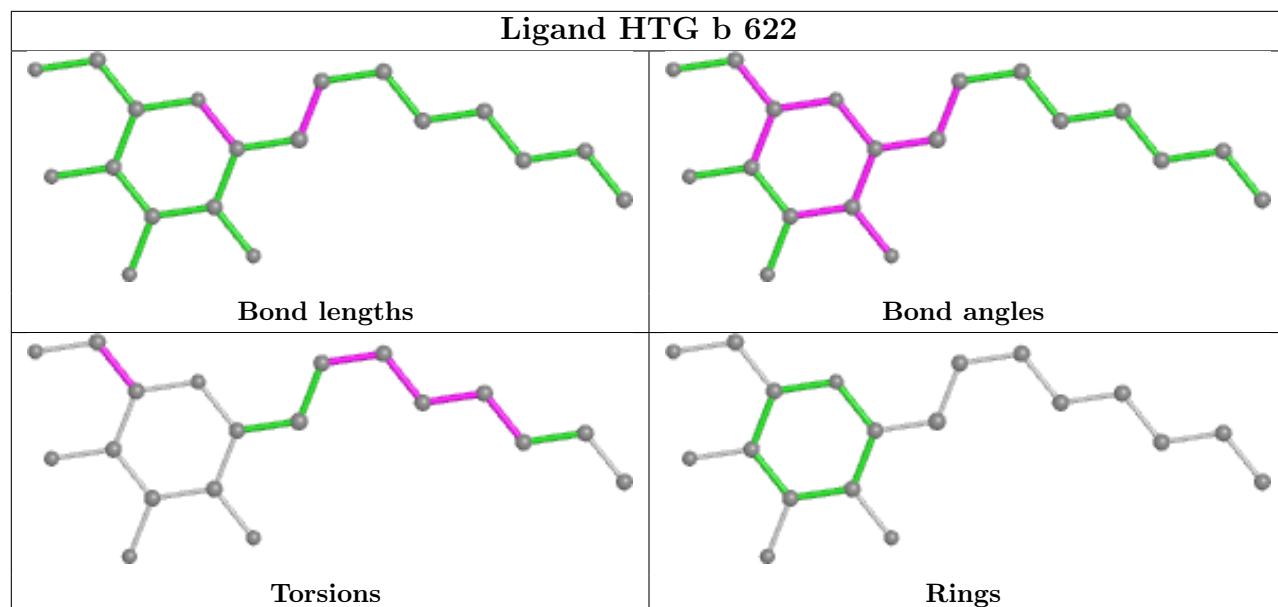


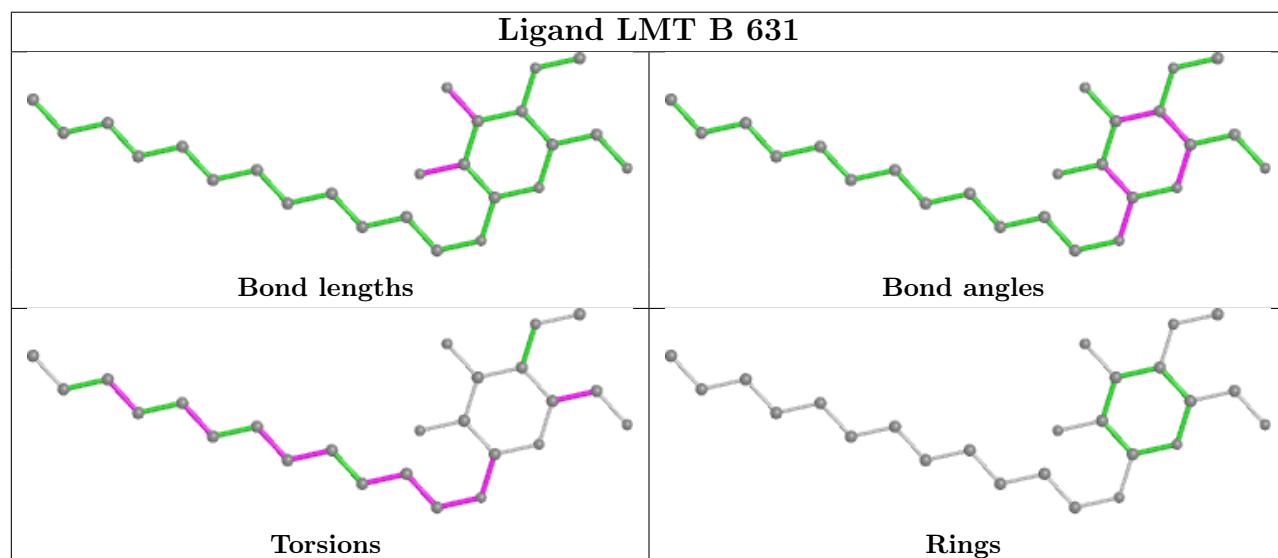
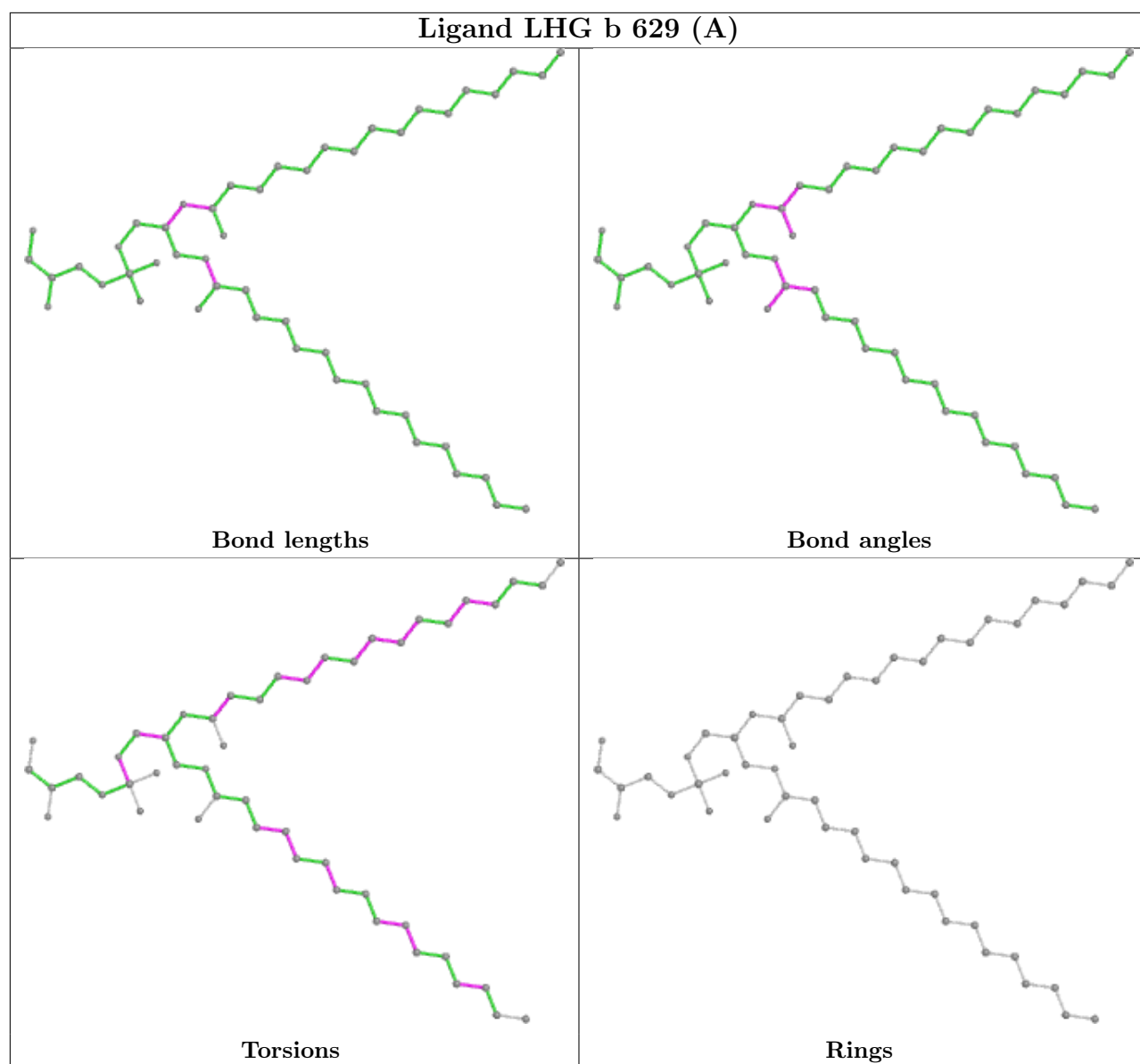


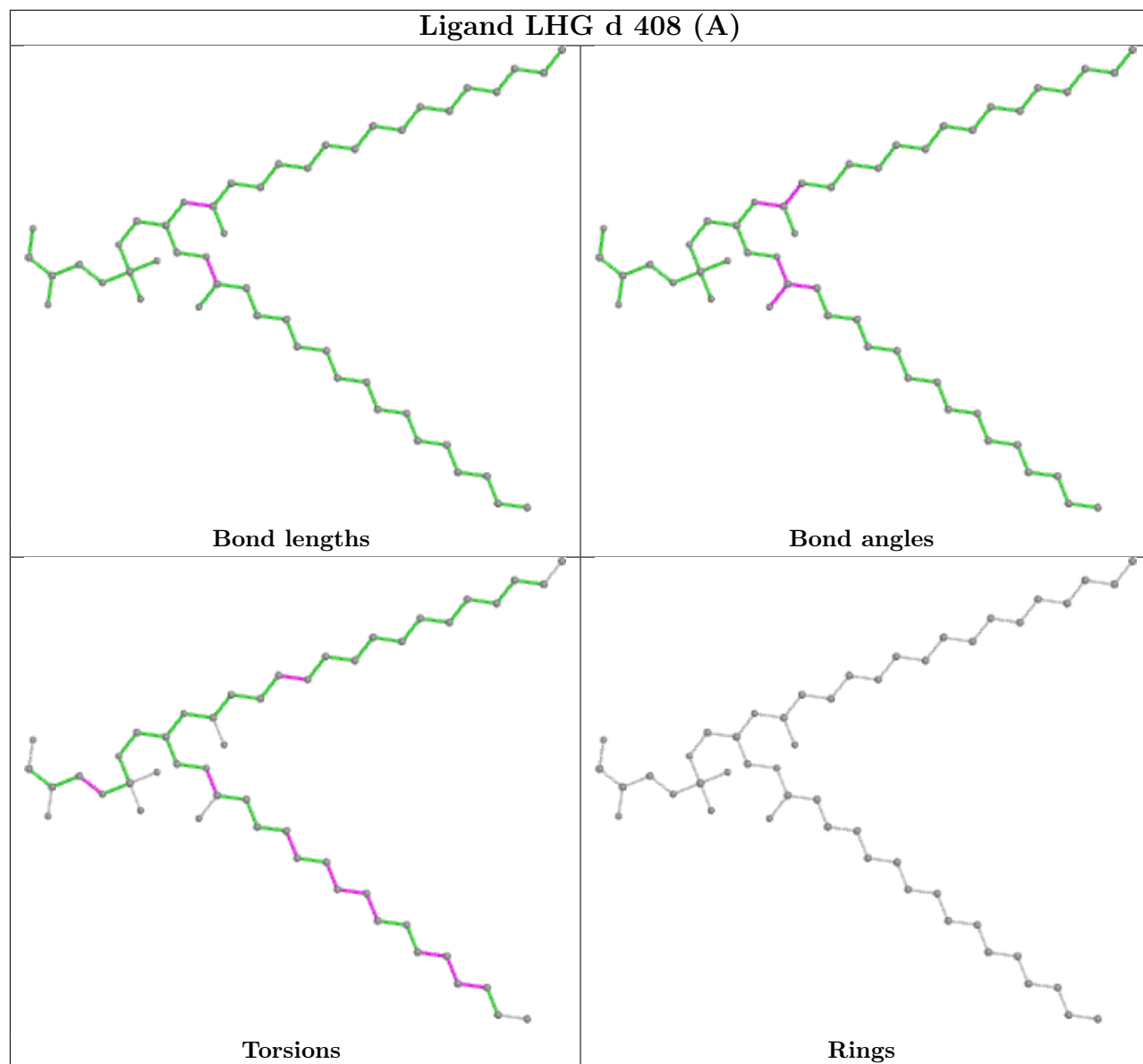


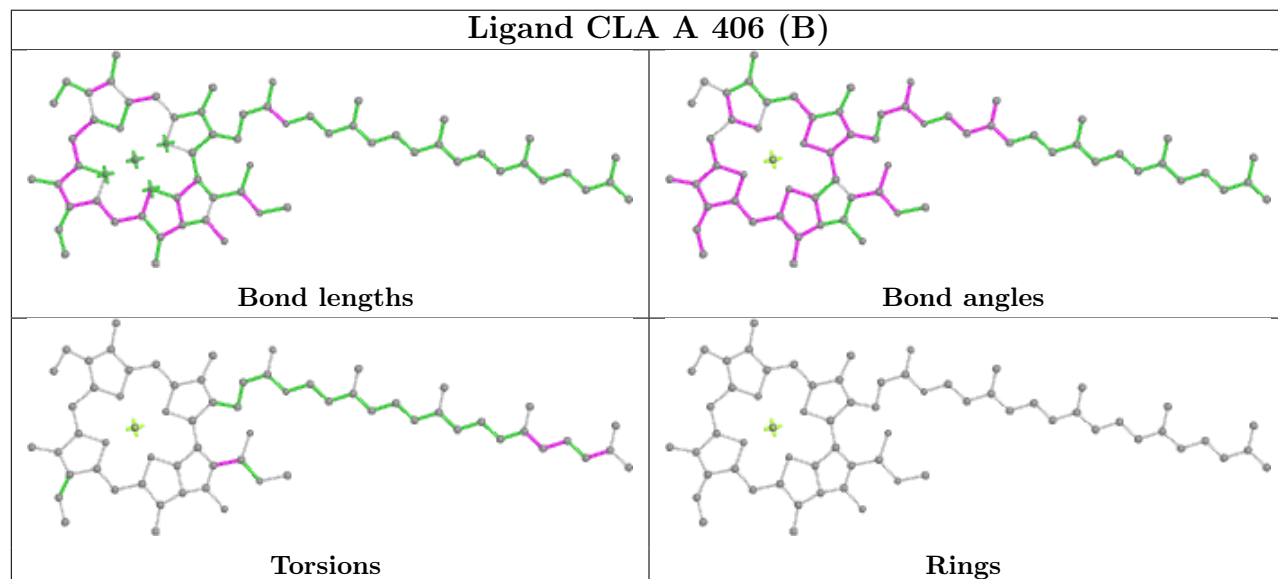
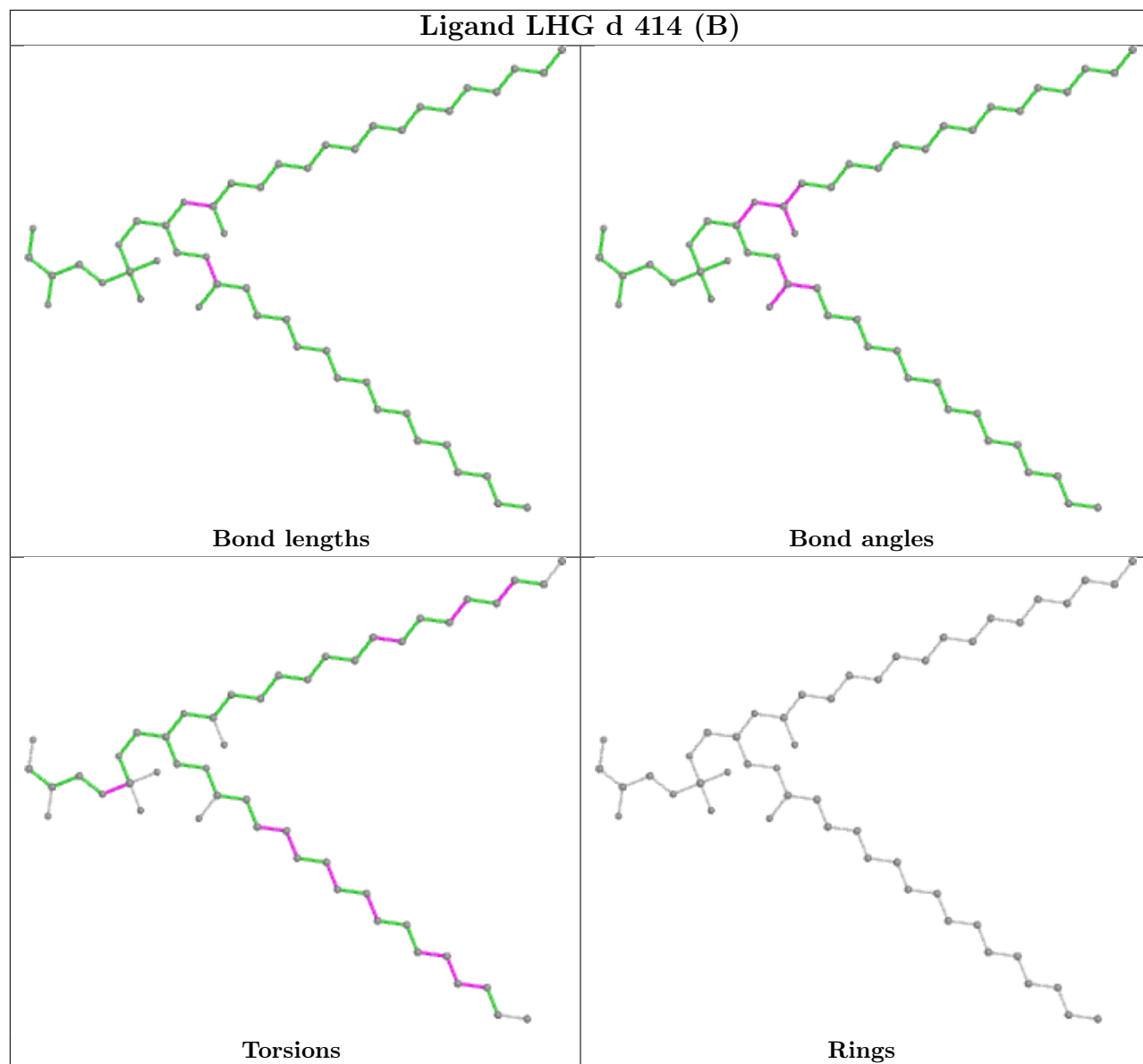


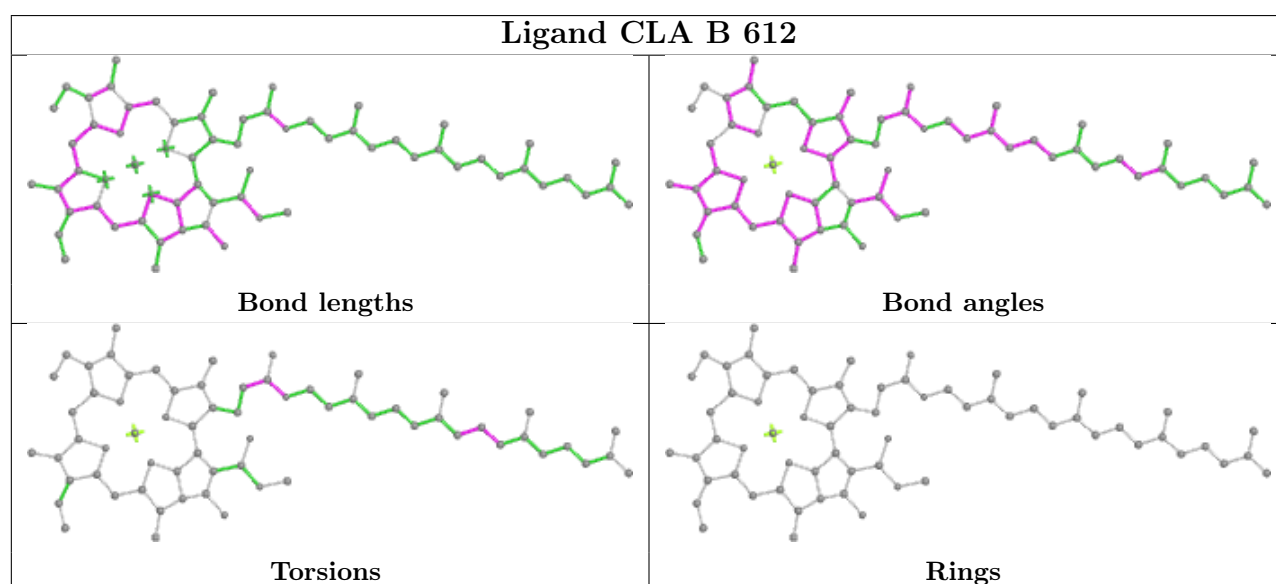
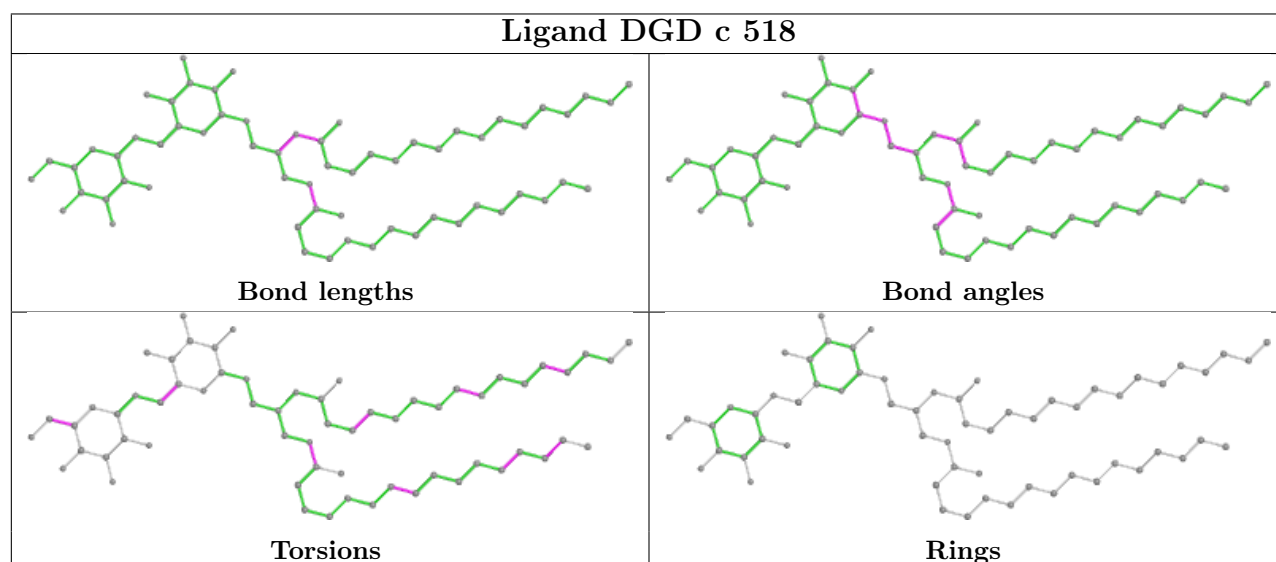
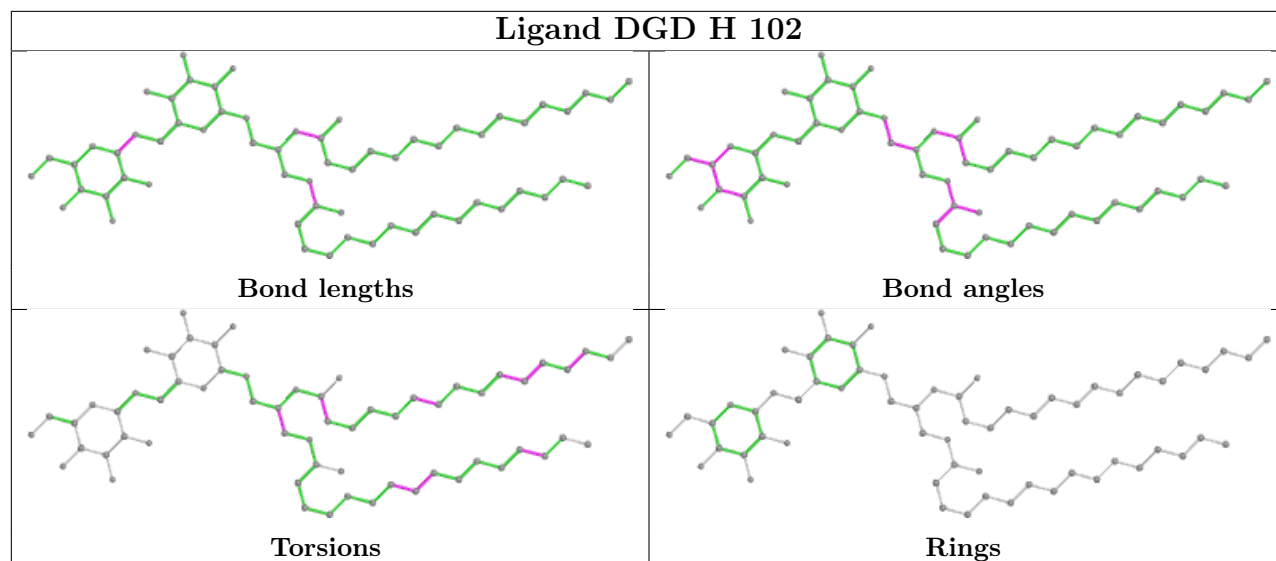


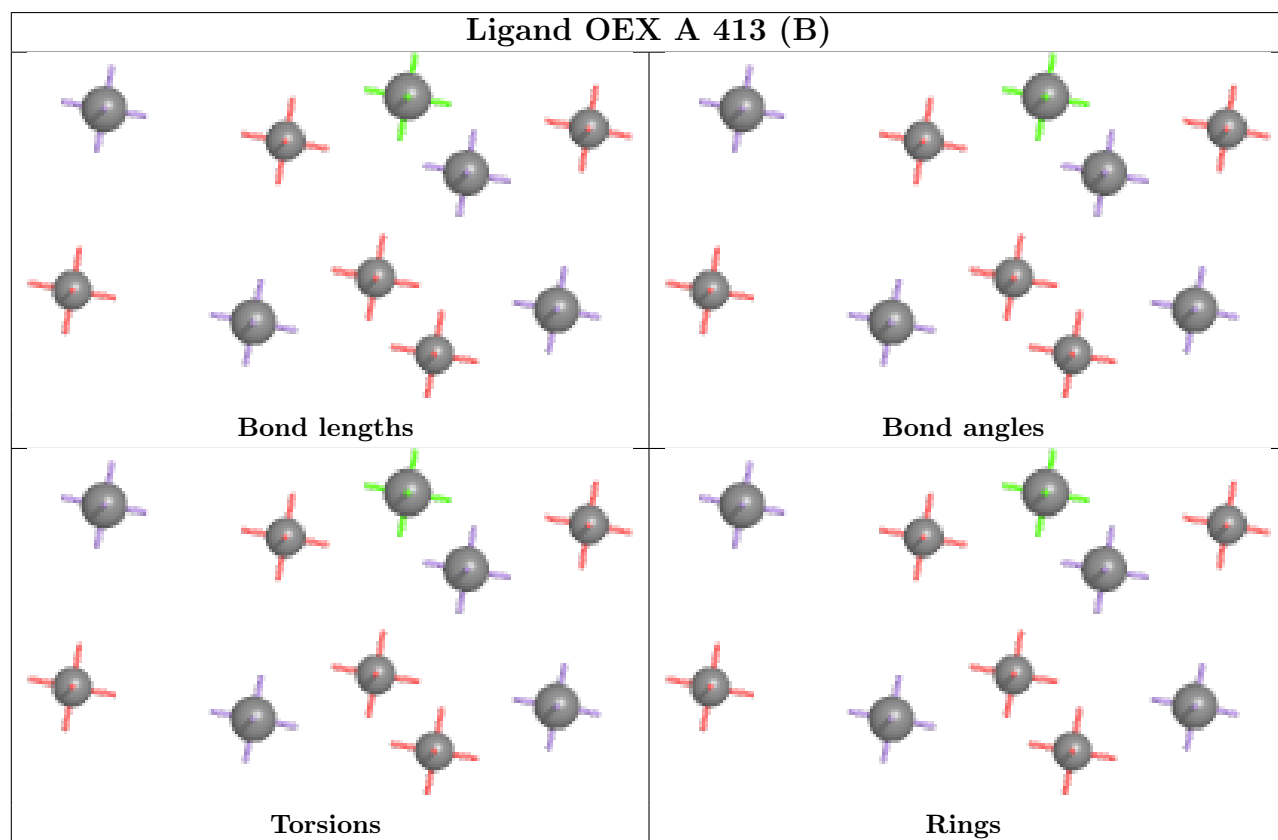
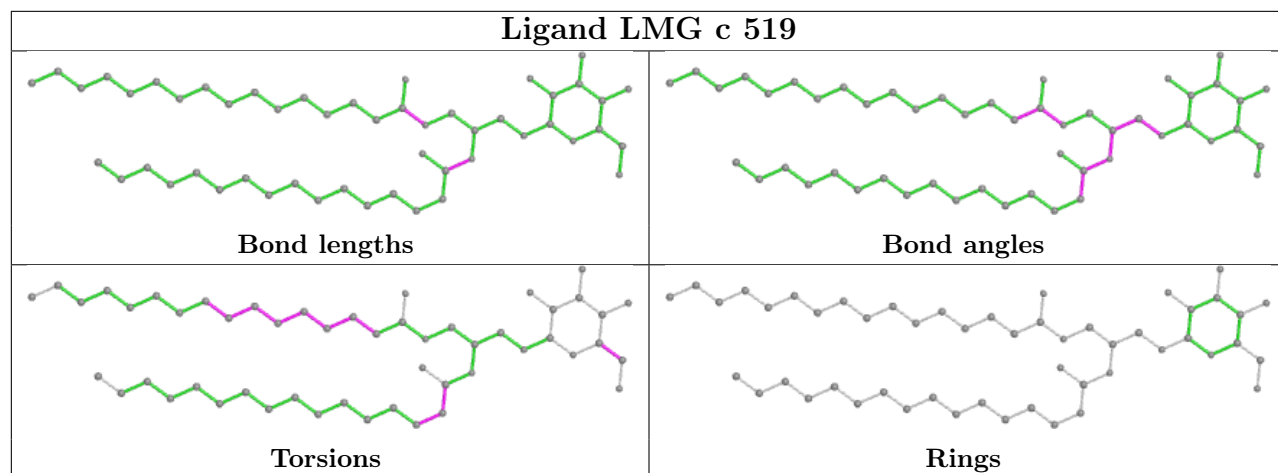
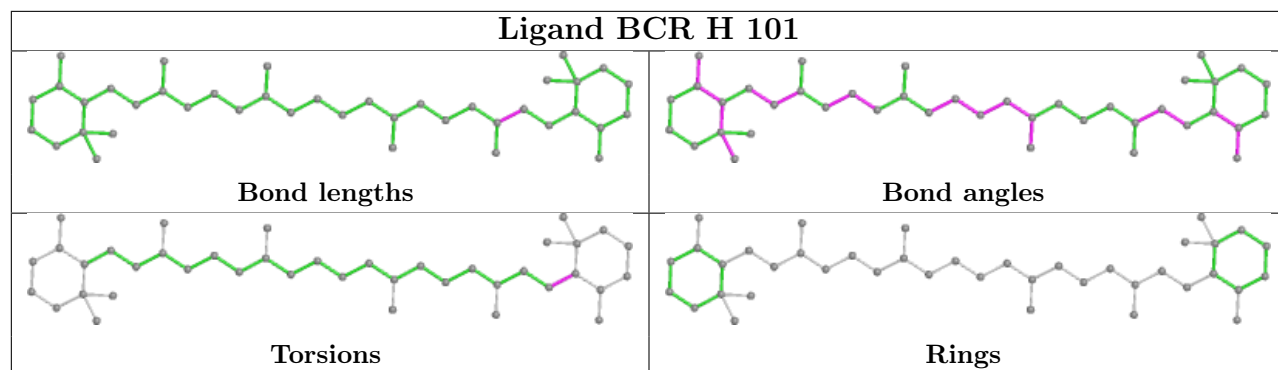


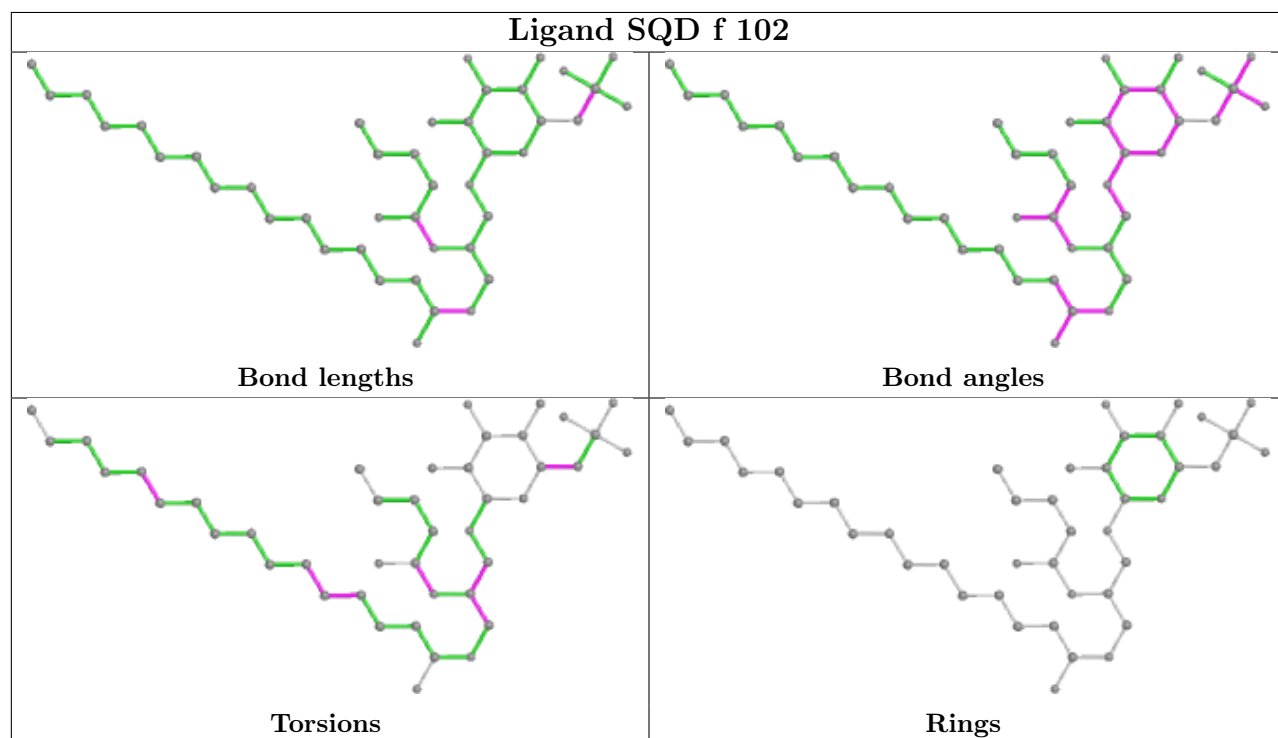
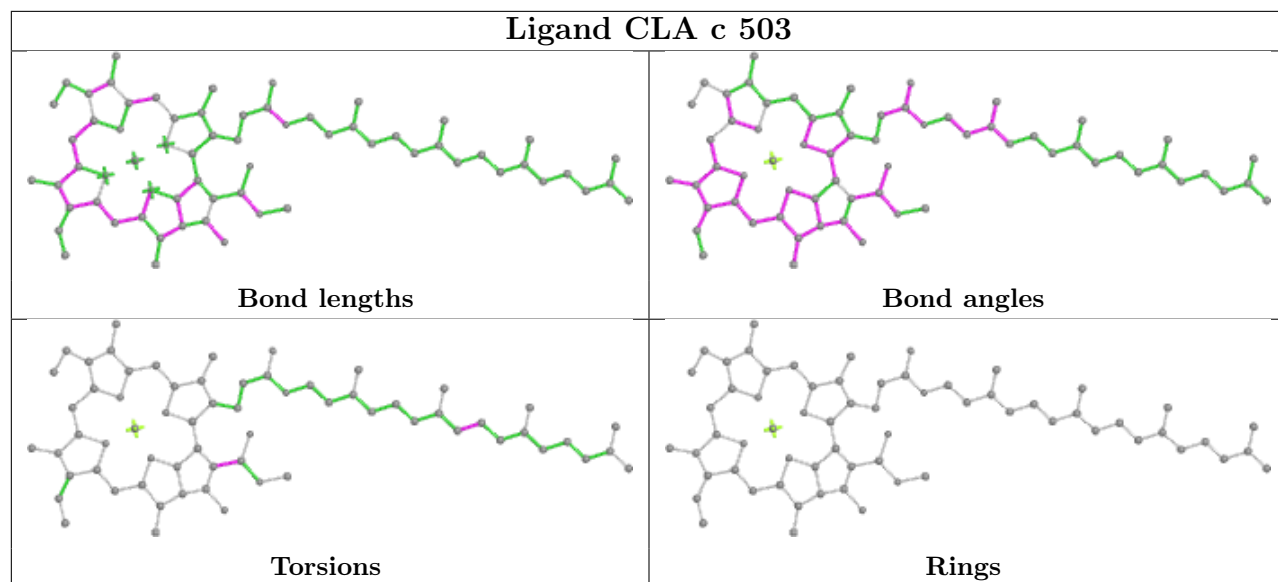




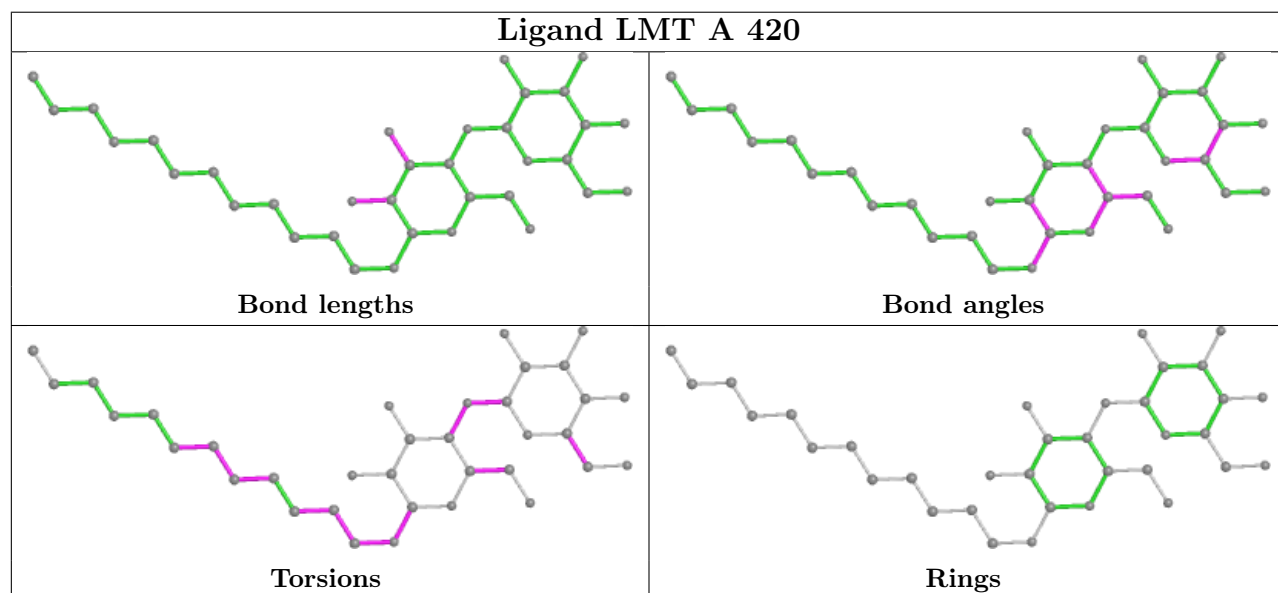
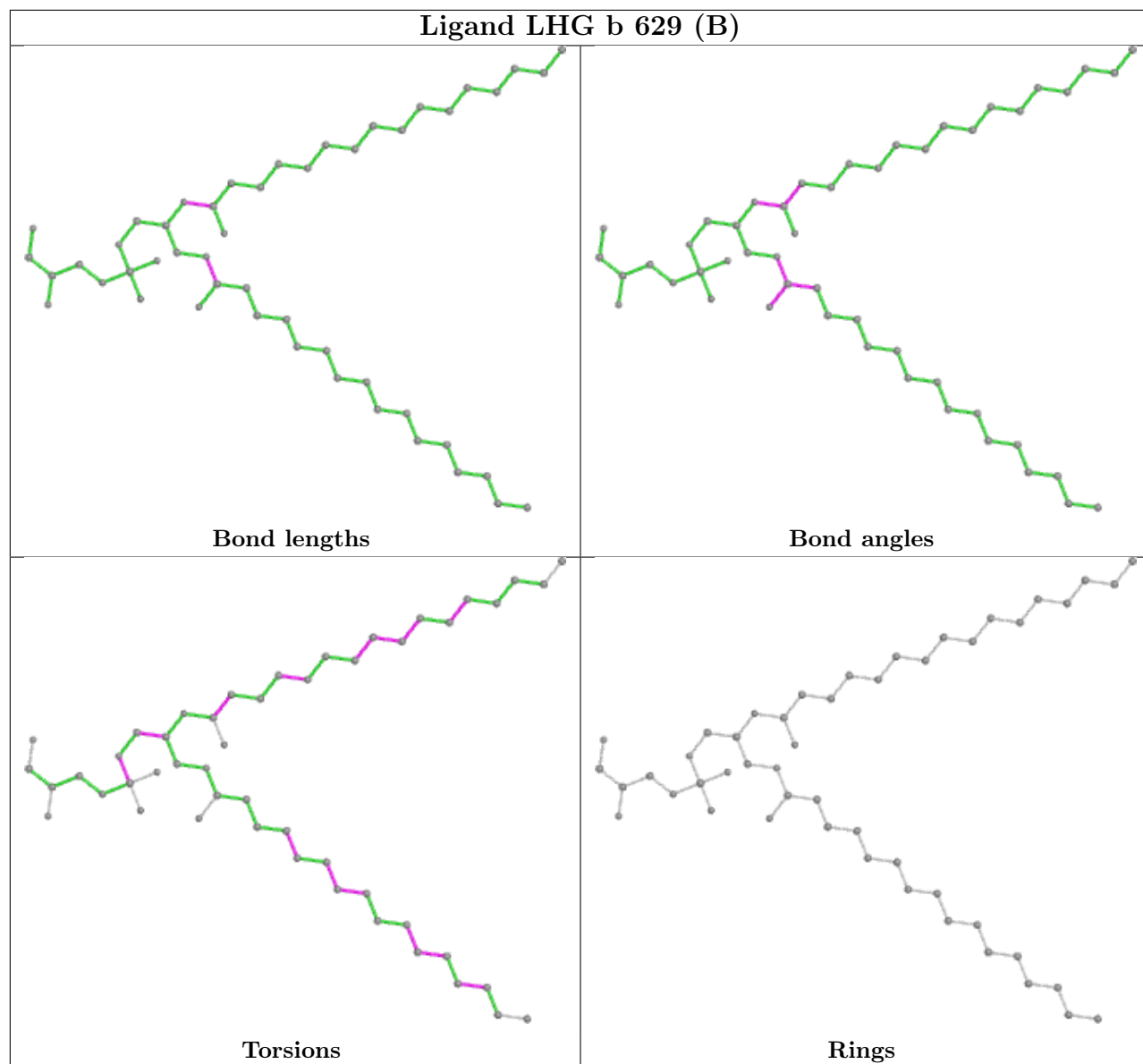


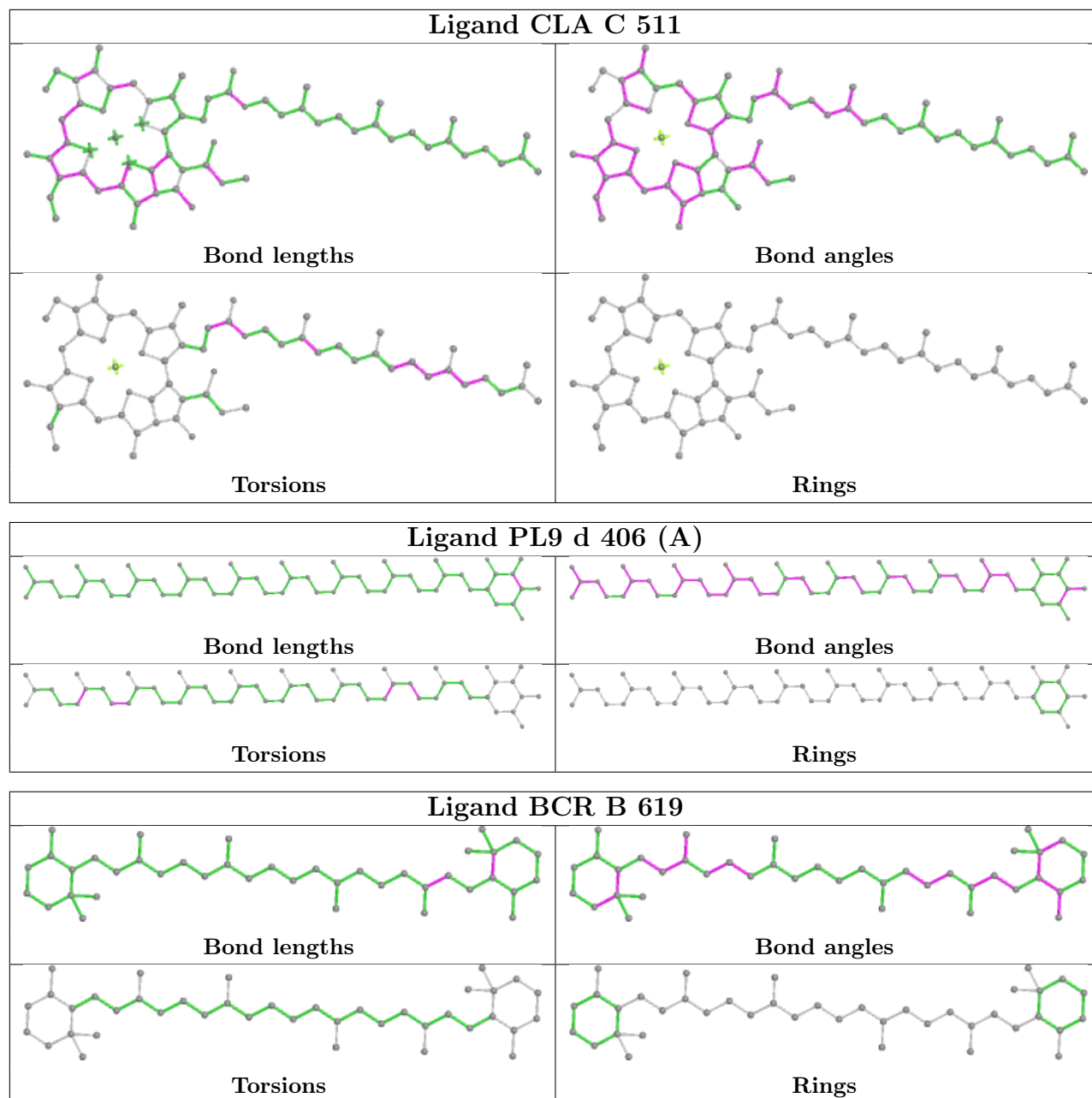


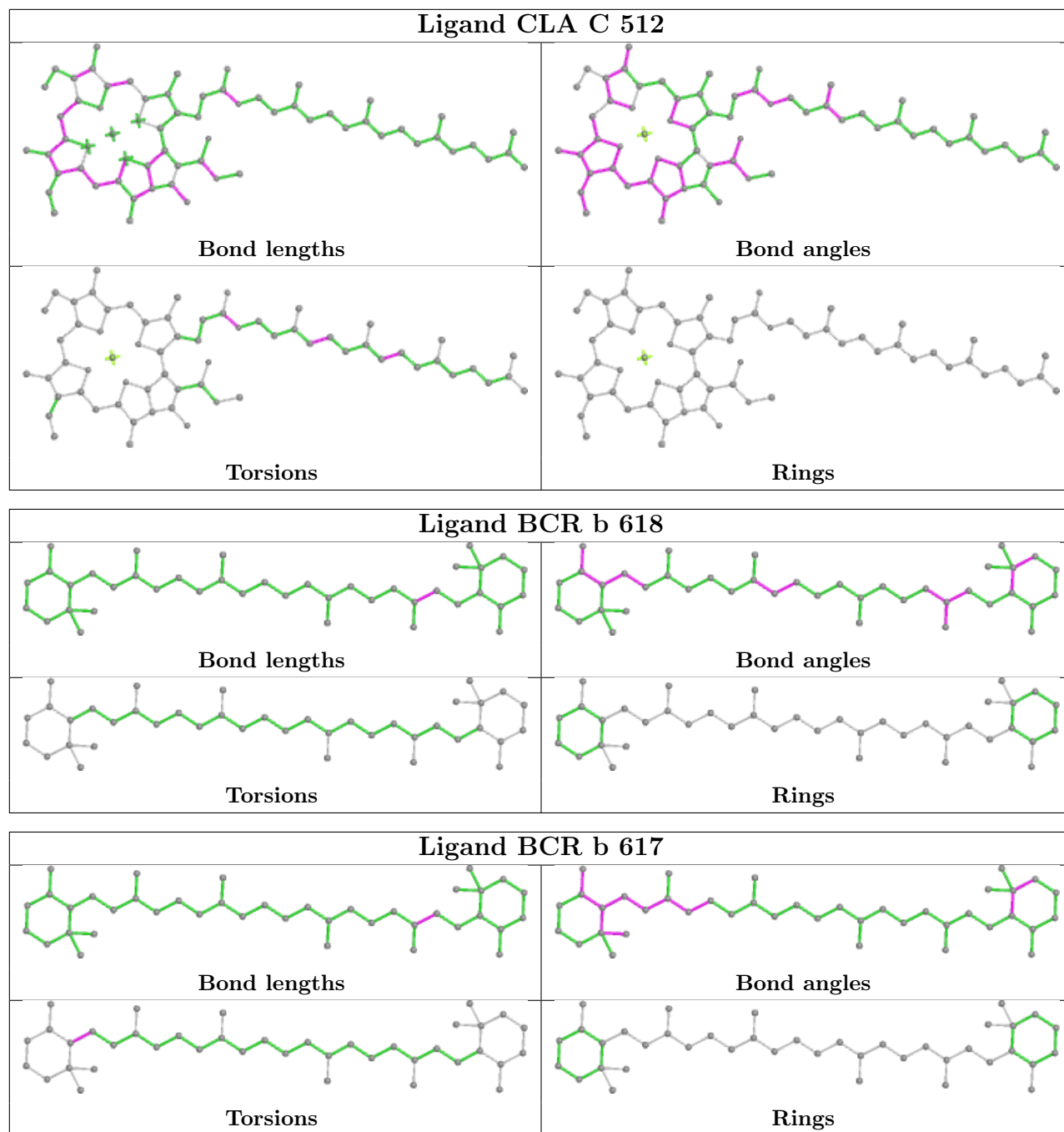


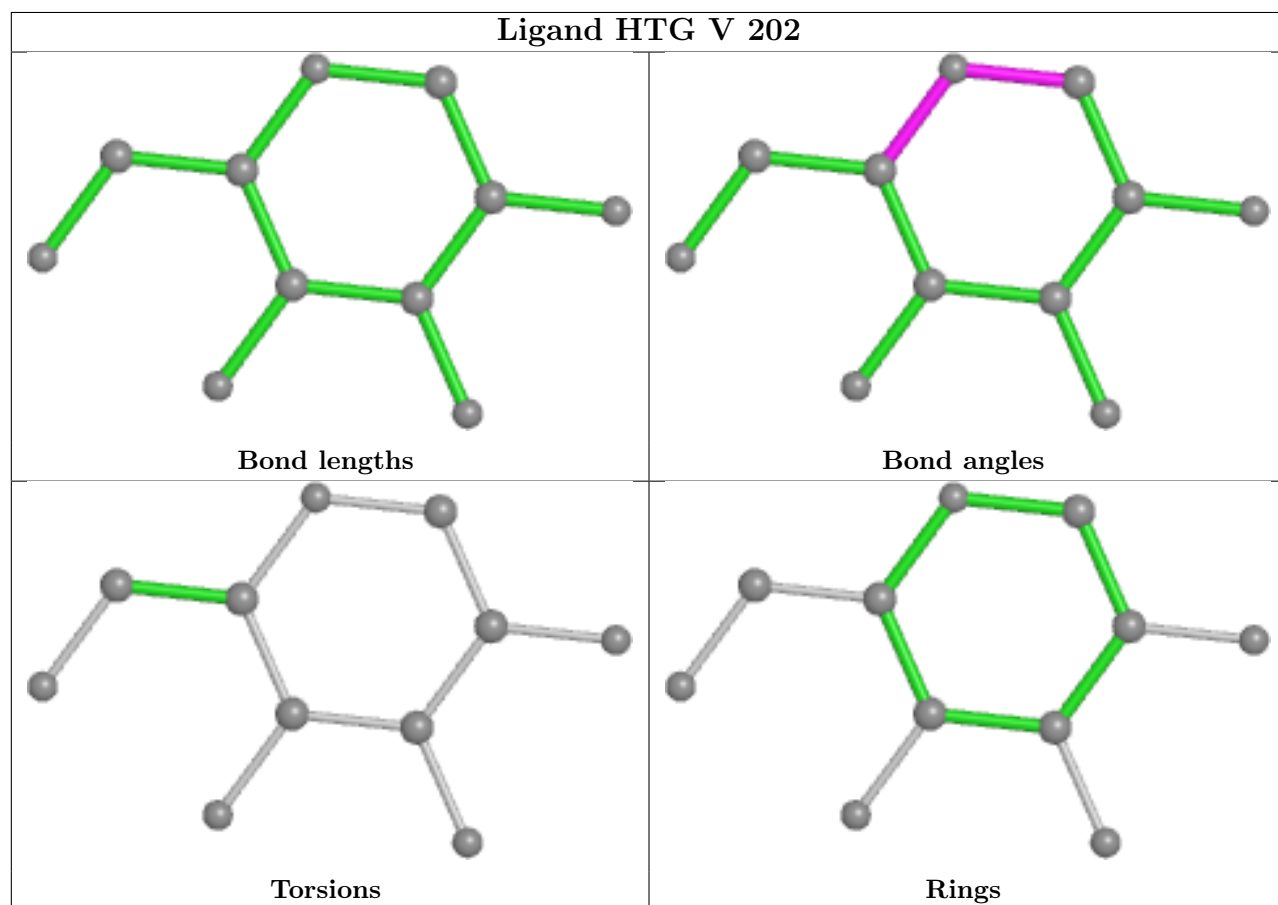
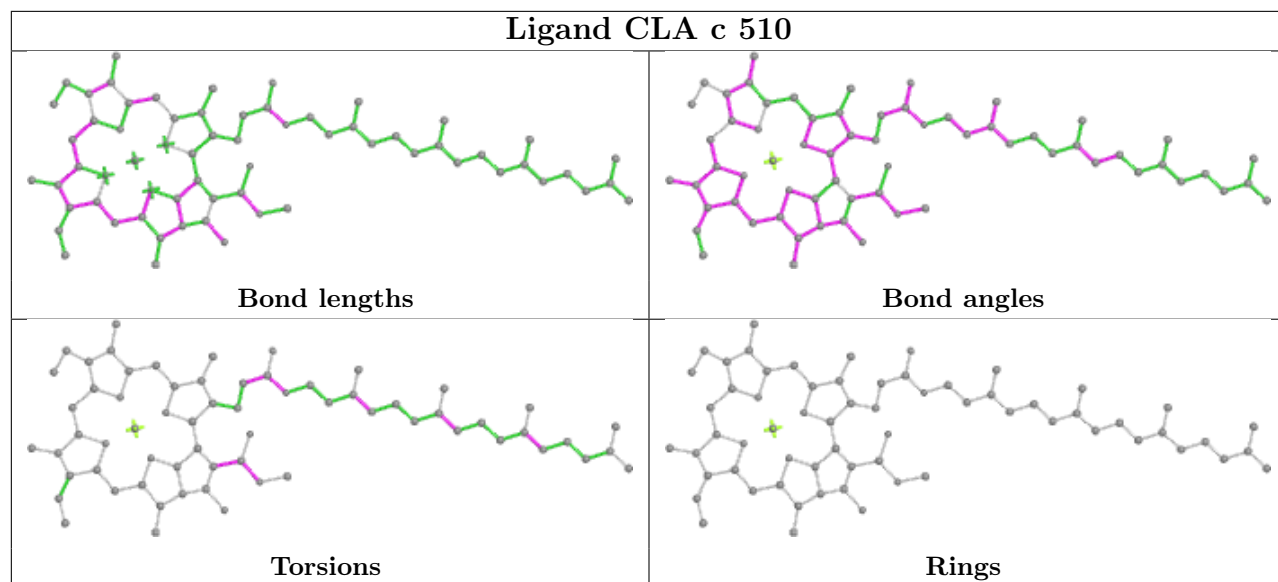


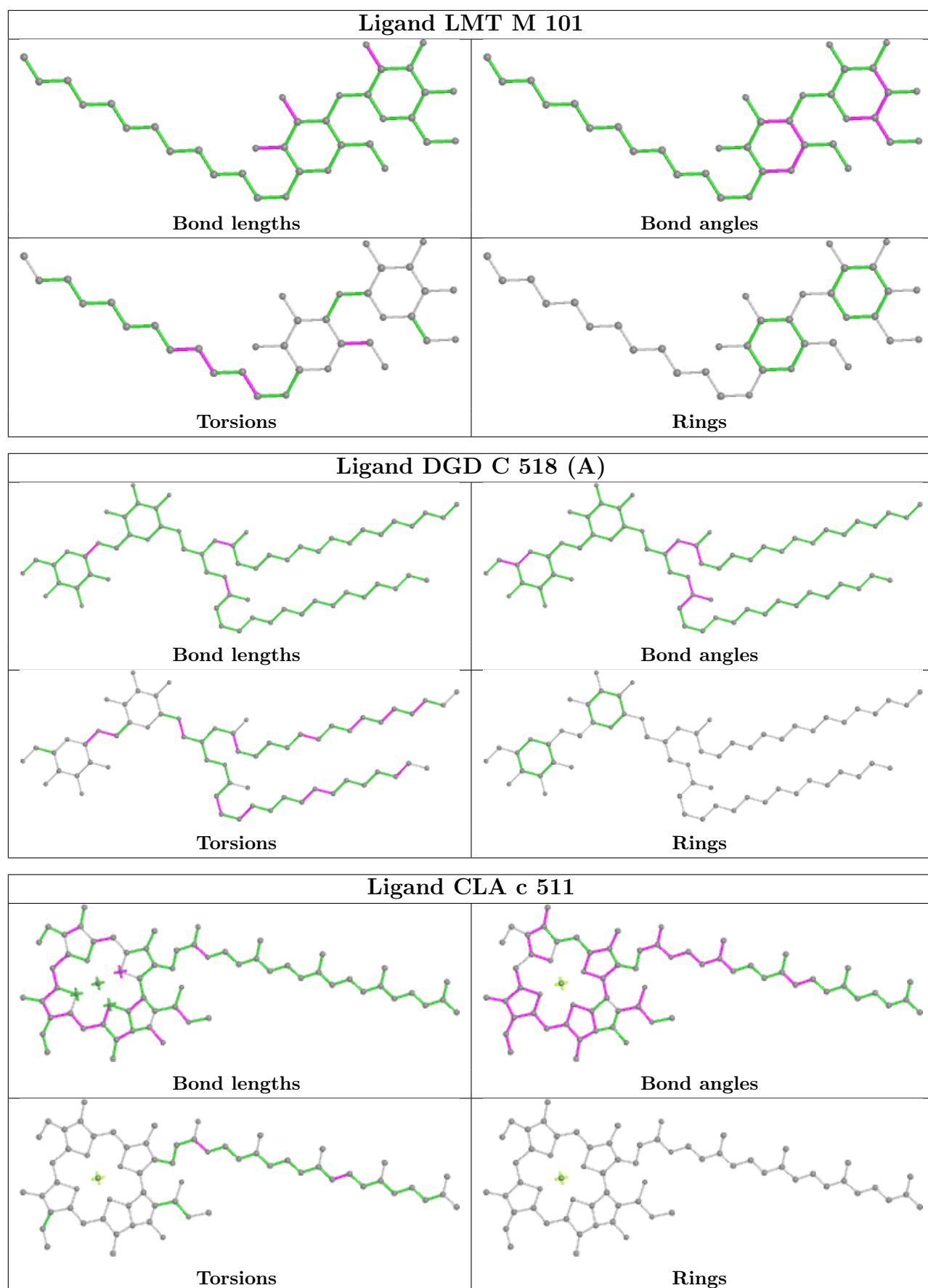












## 5.7 Other polymers [i](#)

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%)	-0.77	6 (1%) 68 66	41, 48, 70, 126	0
1	a	334/344 (97%)	-0.64	3 (0%) 84 83	43, 52, 79, 132	0
2	B	504/505 (99%)	-0.47	11 (2%) 62 59	43, 54, 82, 116	0
2	b	504/505 (99%)	-0.31	26 (5%) 27 26	46, 58, 97, 167	1 (0%)
3	C	451/455 (99%)	-0.56	9 (1%) 65 63	45, 59, 79, 163	0
3	c	455/455 (100%)	-0.40	12 (2%) 56 53	48, 66, 85, 134	2 (0%)
4	D	342/342 (100%)	-0.68	2 (0%) 89 88	41, 50, 67, 141	0
4	d	341/342 (99%)	-0.67	2 (0%) 89 88	44, 54, 76, 133	0
5	E	81/84 (96%)	-0.11	4 (4%) 29 28	53, 70, 102, 166	0
5	e	79/84 (94%)	0.19	7 (8%) 9 8	63, 78, 116, 153	0
6	F	34/44 (77%)	-0.44	2 (5%) 22 21	54, 62, 84, 115	0
6	f	31/44 (70%)	-0.38	2 (6%) 18 17	59, 66, 96, 156	0
7	H	64/65 (98%)	-0.21	3 (4%) 31 30	51, 63, 86, 111	0
7	h	64/65 (98%)	-0.26	3 (4%) 31 30	57, 69, 94, 113	0
8	I	37/38 (97%)	-0.09	3 (8%) 12 10	57, 63, 124, 169	0
8	i	37/38 (97%)	-0.04	4 (10%) 5 5	54, 64, 122, 146	0
9	J	38/39 (97%)	-0.24	2 (5%) 26 25	52, 69, 117, 183	0
9	j	39/39 (100%)	0.13	6 (15%) 2 1	59, 77, 129, 165	0
10	K	37/37 (100%)	-0.58	1 (2%) 54 52	60, 68, 88, 105	0
10	k	37/37 (100%)	-0.48	0 100 100	68, 74, 95, 113	0
11	L	36/37 (97%)	-0.39	3 (8%) 11 10	41, 47, 103, 147	0
11	l	36/37 (97%)	-0.39	2 (5%) 24 23	44, 49, 100, 124	0
12	M	32/36 (88%)	-0.67	1 (3%) 49 47	45, 50, 77, 136	0
12	m	33/36 (91%)	-0.43	2 (6%) 21 20	44, 50, 72, 153	0

*Continued on next page...*

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/244 (99%)	-0.07	17 (6%) 16 15	43, 65, 120, 188	0
13	o	243/244 (99%)	0.05	26 (10%) 6 5	46, 66, 124, 171	0
14	T	29/32 (90%)	-0.63	2 (6%) 16 15	44, 49, 77, 124	0
14	t	29/32 (90%)	-0.70	1 (3%) 45 43	45, 51, 76, 126	0
15	U	96/104 (92%)	-0.42	1 (1%) 82 81	49, 59, 92, 102	0
15	u	97/104 (93%)	-0.37	2 (2%) 63 61	53, 63, 83, 137	0
16	V	137/137 (100%)	-0.56	0 100 100	48, 57, 83, 109	0
16	v	137/137 (100%)	-0.21	4 (2%) 51 49	54, 71, 102, 138	0
17	X	38/40 (95%)	-0.29	2 (5%) 26 25	61, 71, 90, 114	0
17	x	38/40 (95%)	0.18	4 (10%) 6 5	64, 77, 119, 164	0
18	Y	29/30 (96%)	0.94	7 (24%) 0 0	67, 84, 127, 131	0
18	y	29/30 (96%)	0.29	4 (13%) 2 2	75, 92, 112, 119	0
19	Z	62/62 (100%)	0.06	7 (11%) 5 4	67, 80, 132, 162	0
19	z	62/62 (100%)	0.30	10 (16%) 1 1	80, 94, 140, 206	0
20	R	34/34 (100%)	1.90	14 (41%) 0 0	79, 101, 130, 137	0
All	All	5283/5384 (98%)	-0.38	217 (4%) 37 35	41, 59, 100, 206	3 (0%)

All (217) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	c	20	SER	8.0
5	E	84	LYS	7.5
2	b	495	PHE	7.0
1	a	11	ALA	6.4
13	o	4	THR	6.4
3	C	23	ALA	6.4
13	O	60	ARG	6.3
19	Z	32	ASP	6.0
18	Y	18	VAL	5.8
2	b	494	GLY	5.8
18	Y	19	ILE	5.7
12	m	34	LYS	5.5
13	O	62	GLU	5.5
1	A	11	ALA	5.4
13	o	56	PRO	5.4
13	O	56	PRO	5.1
17	x	38	GLN	4.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
19	Z	31	GLN	4.9
17	x	2	THR	4.8
6	F	12	SER	4.8
13	O	4	THR	4.8
2	b	504	THR	4.7
13	O	63	ALA	4.7
5	e	84	LYS	4.7
19	z	31	GLN	4.7
19	Z	3	ILE	4.6
2	b	293	ALA	4.6
20	R	32	GLN	4.6
20	R	35	LEU	4.6
13	o	207	ARG	4.5
3	C	143	TYR	4.5
3	c	21	ILE	4.5
13	o	60	ARG	4.5
13	o	57	LYS	4.4
13	o	62	GLU	4.4
19	z	3	ILE	4.4
9	j	3	GLU	4.4
13	o	63	ALA	4.3
13	O	5	LEU	4.3
12	M	33	GLN	4.3
13	o	59	LYS	4.2
3	C	207	ARG	4.2
7	h	6	TRP	4.2
13	o	58	ASN	4.2
13	o	24	ASP	4.2
4	D	11	GLU	4.1
3	c	19	ASN	4.1
14	T	30[A]	THR	4.1
11	L	3	PRO	4.1
13	O	59	LYS	4.0
18	y	18	VAL	4.0
8	I	36	ASP	4.0
19	z	32	ASP	4.0
3	c	143	TYR	4.0
6	f	15	ILE	3.9
2	b	127	ARG	3.9
13	o	35	SER	3.9
18	Y	21	GLN	3.9
2	b	493[A]	TRP	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
20	R	33	LYS	3.9
4	D	12	ARG	3.8
11	l	3	PRO	3.7
20	R	3	TRP	3.7
20	R	21	ARG	3.7
19	z	60	PHE	3.7
19	z	34	ASP	3.6
2	b	505	ARG	3.6
2	b	489	GLU	3.6
2	b	503	THR	3.6
8	I	34	ARG	3.6
19	z	42	LEU	3.6
2	b	502	VAL	3.5
9	j	5	GLY	3.5
2	B	494	GLY	3.5
5	e	81	GLU	3.5
9	j	1	MET	3.4
1	A	13	LEU	3.4
6	f	16[A]	PHE	3.4
12	m	33	GLN	3.4
1	a	13	LEU	3.4
19	Z	30	PRO	3.3
19	z	38	GLN	3.3
19	Z	34	ASP	3.3
7	H	6	TRP	3.3
3	c	22	PHE	3.3
13	O	61	GLN	3.2
16	v	17	LYS	3.2
20	R	31	VAL	3.2
19	Z	35	ARG	3.2
2	B	295	GLY	3.2
11	l	2	GLU	3.2
13	o	25	THR	3.2
18	Y	20	ALA	3.2
18	y	19	ILE	3.1
1	a	262[A]	TYR	3.1
13	o	23	ASP	3.1
20	R	20	VAL	3.1
8	i	34	ARG	3.1
17	X	2	THR	3.1
18	y	41	VAL	3.1
18	y	43	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
9	j	6	ARG	3.0
3	c	23	ALA	3.0
19	z	62	VAL	3.0
13	o	206	GLY	3.0
13	o	5	LEU	3.0
16	v	15	GLU	3.0
2	b	86	ILE	3.0
17	X	38	GLN	3.0
13	O	25	THR	3.0
3	c	207	ARG	3.0
18	Y	43	ARG	3.0
9	j	4	GLY	2.9
20	R	28	VAL	2.9
18	Y	22	LEU	2.9
20	R	24	LEU	2.9
19	z	30	PRO	2.9
2	b	373	LYS	2.9
13	o	27	ARG	2.9
3	C	24	THR	2.9
3	c	192	GLY	2.9
9	J	3	GLU	2.9
4	d	12	ARG	2.9
6	F	13	TYR	2.9
2	b	294	SER	2.8
8	i	38	GLU	2.8
13	o	61	GLN	2.8
2	b	485	GLU	2.8
19	z	35	ARG	2.8
5	E	59	GLU	2.8
2	B	485	GLU	2.8
20	R	34	LEU	2.8
13	o	134	THR	2.8
2	B	86	ILE	2.8
20	R	4	ARG	2.7
13	o	246	ALA	2.7
11	L	7	ARG	2.7
13	o	22	LEU	2.7
17	x	3	ILE	2.7
2	B	162	PHE	2.7
3	c	233	VAL	2.7
2	b	161	LEU	2.7
2	b	497	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
9	j	2	SER	2.7
2	B	293	ALA	2.7
20	R	29	LYS	2.6
20	R	27	ALA	2.6
2	b	376	VAL	2.5
2	b	488	PRO	2.5
3	c	253	LEU	2.5
13	o	130	GLN	2.5
13	o	64	GLU	2.5
8	i	35	LYS	2.5
1	A	16	ARG	2.5
20	R	18	TRP	2.5
2	b	484[A]	PRO	2.5
7	H	23	PRO	2.5
7	h	23	PRO	2.5
2	b	374	ASN	2.5
5	e	82	GLN	2.5
5	e	59	GLU	2.4
16	v	16	GLY	2.4
13	O	89	SER	2.4
3	C	181	PHE	2.4
11	L	5	PRO	2.4
3	C	142	GLU	2.4
2	b	85	GLY	2.4
14	t	30[A]	THR	2.4
13	o	89	SER	2.4
3	c	201	ASN	2.4
5	E	61	ARG	2.4
1	A	12	ASN	2.4
17	x	39	ARG	2.3
13	O	27	ARG	2.3
13	O	35	SER	2.3
8	I	37	LEU	2.3
2	B	487	SER	2.3
5	E	82	GLN	2.3
13	O	211	ILE	2.3
2	B	128	THR	2.3
2	b	295	GLY	2.3
8	i	36	ASP	2.3
19	Z	2	THR	2.3
4	d	237[A]	PRO	2.3
15	U	27	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
13	O	55	GLU	2.2
2	B	85	GLY	2.2
13	o	211	ILE	2.2
3	C	253	LEU	2.2
1	A	262[A]	TYR	2.2
2	b	89	GLY	2.2
13	o	55	GLU	2.2
7	H	65	LEU	2.2
16	v	14	SER	2.2
5	e	42	LEU	2.2
10	K	13	GLU	2.2
9	J	6	ARG	2.1
7	h	65	LEU	2.1
13	O	207	ARG	2.1
18	Y	41	VAL	2.1
2	B	495	PHE	2.1
2	b	162	PHE	2.1
3	C	263	ALA	2.1
13	O	58	ASN	2.1
2	b	126	PRO	2.1
15	u	66	GLY	2.1
14	T	29[A]	ILE	2.1
5	e	24	SER	2.1
3	C	192	GLY	2.0
13	o	34	SER	2.0
3	c	208	VAL	2.0
15	u	61	VAL	2.0
5	e	83	LEU	2.0
1	A	15	GLU	2.0
13	O	24	ASP	2.0
2	b	496	TYR	2.0
2	B	373	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
8	FME	i	1	10/11	0.93	0.17	53,68,77,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
14	FME	T	1	10/11	0.94	0.10	45,55,64,72	0
8	FME	I	1	10/11	0.96	0.07	58,69,79,82	0
14	FME	t	1	10/11	0.96	0.09	44,51,65,75	0
12	FME	m	1	10/11	0.97	0.12	53,63,88,122	0
12	FME	M	1	10/11	0.97	0.11	52,60,89,108	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
30	UNL	b	626	33/-	0.47	0.36	68,97,161,173	0
30	UNL	I	101	40/-	0.48	0.35	73,111,158,166	0
30	UNL	B	626	33/-	0.49	0.37	54,117,145,149	0
31	LMT	T	101	35/35	0.49	0.31	77,131,185,192	0
30	UNL	j	101	10/-	0.50	0.29	80,93,103,106	0
31	LMT	b	621	25/35	0.55	0.29	84,112,164,173	0
27	GOL	a	417	6/6	0.58	0.54	78,98,110,112	0
30	UNL	i	101	40/-	0.59	0.30	73,110,160,171	0
30	UNL	A	415	28/-	0.60	0.35	93,117,135,155	0
31	LMT	B	630	35/35	0.60	0.36	66,117,148,156	0
30	UNL	K	101[A]	34/-	0.64	0.34	88,115,128,132	34
30	UNL	K	101[B]	34/-	0.64	0.34	88,115,128,133	34
33	LMG	C	521	51/55	0.64	0.30	63,117,164,179	0
30	UNL	c	524[B]	32/-	0.65	0.40	98,113,127,139	32
30	UNL	c	524[A]	32/-	0.65	0.40	98,113,127,139	32
31	LMT	M	101	35/35	0.65	0.26	63,96,120,125	0
31	LMT	A	417	35/35	0.66	0.32	65,116,144,148	0
31	LMT	F	101	35/35	0.68	0.52	102,138,184,189	0
33	LMG	c	520	51/55	0.68	0.28	73,135,172,190	0
34	HTG	D	410	16/19	0.68	0.29	84,104,134,149	0
31	LMT	B	631	25/35	0.69	0.24	63,87,150,170	0
30	UNL	d	410	36/-	0.70	0.20	65,93,136,146	0
34	HTG	b	623	19/19	0.70	0.50	84,135,161,168	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
31	LMT	B	628	35/35	0.71	0.28	67,102,138,150	0
33	LMG	Z	101	37/55	0.71	0.28	72,123,151,171	0
31	LMT	m	103	35/35	0.72	0.25	66,90,109,125	0
30	UNL	x	101	18/-	0.72	0.23	68,84,140,141	0
32	LHG	a	419[B]	42/49	0.73	0.35	94,140,157,165	42
31	LMT	A	420	35/35	0.73	0.36	100,135,156,170	0
32	LHG	a	419[A]	42/49	0.73	0.35	94,140,157,165	42
30	UNL	m	102	10/-	0.74	0.35	73,77,96,102	0
33	LMG	z	101	39/55	0.75	0.26	78,132,153,170	0
31	LMT	e	101	35/35	0.76	0.49	110,151,197,199	0
31	LMT	b	627	25/35	0.77	0.23	59,100,155,167	0
27	GOL	o	302	6/6	0.78	0.30	84,102,112,116	0
31	LMT	a	416	35/35	0.78	0.40	109,138,152,164	0
30	UNL	a	413	30/-	0.79	0.32	93,119,146,161	0
27	GOL	l	801[A]	6/6	0.79	0.87	73,104,107,111	6
27	GOL	l	801[B]	6/6	0.79	0.87	73,105,107,111	6
34	HTG	d	411	16/19	0.79	0.28	89,122,140,154	0
27	GOL	A	411	6/6	0.80	0.18	64,81,85,91	0
30	UNL	X	101	18/-	0.80	0.20	64,73,112,112	0
27	GOL	B	627	6/6	0.80	0.23	71,88,97,112	0
27	GOL	O	302	6/6	0.81	0.21	77,86,99,113	0
30	UNL	M	102	10/-	0.81	0.26	69,78,93,96	0
29	PL9	A	414[A]	55/55	0.82	0.23	74,100,115,120	55
32	LHG	E	101[A]	42/49	0.82	0.24	76,106,118,123	42
32	LHG	E	101[B]	42/49	0.82	0.24	76,106,118,124	42
34	HTG	C	522	19/19	0.82	0.34	112,130,148,148	0
29	PL9	A	414[B]	55/55	0.82	0.23	74,100,115,120	55
30	UNL	J	101	10/-	0.82	0.18	72,81,90,95	0
26	SQD	f	102	43/54	0.82	0.30	90,133,179,195	0
31	LMT	t	101	26/35	0.83	0.18	78,105,148,163	0
27	GOL	b	624	6/6	0.83	0.17	88,95,107,111	0
26	SQD	b	620	54/54	0.83	0.17	65,96,118,130	0
27	GOL	a	418	6/6	0.83	0.42	58,78,84,88	0
29	PL9	a	412[A]	55/55	0.83	0.23	82,109,121,129	55
29	PL9	a	412[B]	55/55	0.83	0.23	82,109,121,129	55
33	LMG	a	415	51/55	0.83	0.17	71,96,115,119	0
27	GOL	c	526	6/6	0.84	0.21	102,111,120,127	0
34	HTG	c	521	19/19	0.84	0.27	105,125,141,151	0
26	SQD	A	412	54/54	0.84	0.17	65,90,140,150	0
33	LMG	C	501	51/55	0.85	0.15	68,90,118,136	0
27	GOL	o	303	6/6	0.85	0.16	82,91,102,110	0
26	SQD	a	410	54/54	0.85	0.19	67,97,136,154	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	HTG	B	622	19/19	0.85	0.18	61,87,121,126	0
34	HTG	B	623	19/19	0.85	0.26	67,93,117,125	0
36	CA	f	103	1/1	0.85	0.06	120,120,120,120	0
27	GOL	A	418	6/6	0.86	0.48	51,82,88,93	0
34	HTG	b	622	19/19	0.86	0.18	58,80,121,125	0
36	CA	F	103	1/1	0.86	0.20	127,127,127,127	0
30	UNL	D	409	40/-	0.86	0.18	67,94,139,151	0
26	SQD	B	620	54/54	0.87	0.15	66,93,135,146	0
23	CLA	c	513	65/65	0.87	0.18	66,93,129,148	0
27	GOL	V	203[A]	6/6	0.87	0.19	60,70,77,77	6
27	GOL	V	203[B]	6/6	0.87	0.19	60,70,77,77	6
27	GOL	d	413	6/6	0.87	0.30	55,75,76,91	0
36	CA	o	301	1/1	0.87	0.07	103,103,103,103	0
25	BCR	K	102	40/40	0.88	0.18	56,65,76,82	0
33	LMG	d	412	51/55	0.88	0.18	54,72,124,155	0
25	BCR	C	515	40/40	0.88	0.13	55,75,91,93	0
33	LMG	D	411	51/55	0.88	0.18	50,72,124,138	0
27	GOL	O	303	6/6	0.88	0.25	82,95,107,108	0
23	CLA	b	601	65/65	0.89	0.17	59,84,128,166	0
23	CLA	b	616	65/65	0.89	0.17	48,62,133,146	0
27	GOL	v	202[A]	6/6	0.89	0.16	65,79,85,86	6
27	GOL	v	202[B]	6/6	0.89	0.16	65,79,85,87	6
25	BCR	h	101	40/40	0.89	0.15	55,70,91,97	0
27	GOL	B	629	6/6	0.89	0.27	74,79,93,97	0
23	CLA	C	514	65/65	0.89	0.14	59,83,115,120	0
27	GOL	D	412	6/6	0.90	0.23	51,68,73,94	0
23	CLA	c	512	65/65	0.90	0.17	60,81,126,140	0
23	CLA	B	616	65/65	0.90	0.18	48,59,132,147	0
23	CLA	d	404	65/65	0.90	0.14	52,67,130,157	0
33	LMG	c	519	51/55	0.90	0.18	62,91,136,161	0
34	HTG	b	625	19/19	0.91	0.11	68,79,97,110	0
33	LMG	C	520	51/55	0.91	0.17	55,85,123,134	0
23	CLA	B	601	65/65	0.91	0.14	57,78,114,156	0
25	BCR	Y	101	40/40	0.91	0.13	54,65,84,92	0
25	BCR	d	405	40/40	0.91	0.12	51,69,109,113	0
26	SQD	F	102	43/54	0.91	0.18	69,107,131,145	0
30	UNL	D	408	17/-	0.92	0.14	62,78,99,122	0
23	CLA	B	606	65/65	0.92	0.14	44,56,114,130	0
23	CLA	C	507	65/65	0.92	0.14	53,71,125,144	0
23	CLA	b	606	65/65	0.92	0.13	43,58,117,132	0
35	DGD	c	517[A]	62/66	0.92	0.12	56,69,123,138	62
35	DGD	c	517[B]	62/66	0.92	0.12	56,69,123,139	62

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	DGD	h	102	62/66	0.92	0.12	52,65,79,82	0
36	CA	C	524	1/1	0.92	0.07	72,72,72,72	0
23	CLA	C	513	65/65	0.92	0.14	54,72,117,136	0
33	LMG	B	621	51/55	0.92	0.12	55,72,95,116	0
23	CLA	c	506	65/65	0.92	0.15	54,72,126,142	0
25	BCR	c	514	40/40	0.93	0.11	71,83,93,98	0
33	LMG	m	101	51/55	0.93	0.13	63,76,98,115	0
35	DGD	c	518	62/66	0.93	0.12	50,67,106,131	0
30	UNL	d	409	17/-	0.93	0.12	69,79,114,116	0
23	CLA	B	609	65/65	0.93	0.16	47,59,72,83	0
34	HTG	V	202	11/19	0.93	0.39	83,111,123,130	0
35	DGD	C	519	62/66	0.93	0.12	45,61,103,122	0
35	DGD	H	102	62/66	0.93	0.12	47,63,75,90	0
25	BCR	H	101	40/40	0.94	0.10	53,68,90,93	0
23	CLA	a	407	65/65	0.94	0.16	42,57,141,161	0
23	CLA	c	507	65/65	0.94	0.12	50,67,85,92	0
25	BCR	b	618	40/40	0.94	0.10	47,57,76,94	0
27	GOL	C	523[A]	6/6	0.94	0.13	59,62,67,72	6
27	GOL	C	523[B]	6/6	0.94	0.13	59,63,67,72	6
35	DGD	C	518[A]	62/66	0.94	0.12	49,63,114,118	62
35	DGD	C	518[B]	62/66	0.94	0.12	49,63,114,118	62
23	CLA	c	511	65/65	0.94	0.12	56,68,87,107	0
23	CLA	A	408	65/65	0.94	0.12	43,54,128,149	0
23	CLA	C	509	65/65	0.94	0.10	47,56,122,147	0
25	BCR	k	101	40/40	0.94	0.14	59,75,85,87	0
23	CLA	b	612	65/65	0.94	0.11	41,54,65,76	0
25	BCR	A	409	40/40	0.94	0.10	40,52,67,71	0
25	BCR	B	618	40/40	0.94	0.09	43,55,73,80	0
25	BCR	B	619	40/40	0.94	0.10	47,60,90,101	0
23	CLA	D	403	65/65	0.94	0.13	47,60,132,138	0
25	BCR	D	404	40/40	0.94	0.09	44,62,108,115	0
32	LHG	b	629[B]	49/49	0.95	0.13	51,60,72,95	49
32	LHG	d	408[A]	49/49	0.95	0.16	52,64,117,134	49
32	LHG	d	408[B]	49/49	0.95	0.16	52,64,117,134	49
23	CLA	C	505	65/65	0.95	0.10	42,58,106,131	0
26	SQD	a	409[A]	54/54	0.95	0.14	61,83,121,123	54
26	SQD	a	409[B]	54/54	0.95	0.14	61,83,121,123	54
23	CLA	B	611	65/65	0.95	0.10	38,46,65,74	0
25	BCR	b	619	40/40	0.95	0.09	48,64,90,95	0
23	CLA	c	508	65/65	0.95	0.12	46,63,133,152	0
23	CLA	b	609	65/65	0.95	0.13	49,65,77,90	0
25	BCR	C	516	40/40	0.95	0.12	51,61,76,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	DGD	c	516[A]	62/66	0.95	0.11	48,64,103,113	62
35	DGD	c	516[B]	62/66	0.95	0.11	47,64,103,114	62
23	CLA	C	508	65/65	0.95	0.11	47,61,83,93	0
25	BCR	t	102	40/40	0.95	0.09	44,59,80,89	0
26	SQD	A	410[A]	54/54	0.95	0.12	57,81,115,119	54
26	SQD	A	410[B]	54/54	0.95	0.12	57,81,115,119	54
23	CLA	C	502	65/65	0.95	0.09	49,60,74,81	0
23	CLA	c	504	65/65	0.95	0.10	53,64,107,142	0
36	CA	O	301	1/1	0.95	0.08	104,104,104,104	0
34	HTG	B	625	19/19	0.95	0.10	68,82,98,105	0
32	LHG	b	629[A]	49/49	0.95	0.13	51,60,72,95	49
32	LHG	d	414[B]	49/49	0.96	0.14	51,69,82,94	49
25	BCR	c	515	40/40	0.96	0.11	57,65,78,86	0
23	CLA	a	405[A]	65/65	0.96	0.10	43,55,126,133	65
23	CLA	a	405[B]	65/65	0.96	0.10	42,55,126,133	65
23	CLA	c	509	65/65	0.96	0.10	46,62,90,101	0
23	CLA	B	603	65/65	0.96	0.11	43,54,73,83	0
25	BCR	y	101	40/40	0.96	0.08	59,71,89,100	0
23	CLA	B	610	65/65	0.96	0.12	42,55,68,84	0
23	CLA	b	602	65/65	0.96	0.12	47,61,80,92	0
23	CLA	b	604	65/65	0.96	0.12	42,52,106,121	0
24	PHO	a	414[A]	64/64	0.96	0.12	44,56,64,72	64
24	PHO	a	414[B]	64/64	0.96	0.12	44,56,64,72	64
23	CLA	b	605	65/65	0.96	0.11	38,52,73,83	0
23	CLA	C	510	65/65	0.96	0.11	50,59,83,94	0
23	CLA	b	607	65/65	0.96	0.08	38,48,81,94	0
29	PL9	D	405[A]	55/55	0.96	0.11	38,50,57,72	55
29	PL9	D	405[B]	55/55	0.96	0.11	38,50,58,72	55
23	CLA	C	511	65/65	0.96	0.09	48,59,81,89	0
23	CLA	b	611	65/65	0.96	0.09	41,51,72,81	0
29	PL9	d	406[A]	55/55	0.96	0.11	41,52,63,72	55
29	PL9	d	406[B]	55/55	0.96	0.11	40,52,63,72	55
23	CLA	C	512	65/65	0.96	0.13	49,64,80,84	0
23	CLA	b	614	65/65	0.96	0.09	42,53,102,117	0
27	GOL	B	624	6/6	0.96	0.19	70,73,86,91	0
35	DGD	C	517[A]	62/66	0.96	0.10	47,57,103,109	62
35	DGD	C	517[B]	62/66	0.96	0.10	47,57,103,109	62
32	LHG	A	419[A]	49/49	0.96	0.13	50,66,89,93	49
32	LHG	A	419[B]	49/49	0.96	0.13	50,66,89,93	49
32	LHG	D	407[A]	49/49	0.96	0.14	49,61,110,113	49
32	LHG	D	407[B]	49/49	0.96	0.14	49,61,110,114	49
23	CLA	b	615	65/65	0.96	0.10	48,59,83,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	BCR	T	102	40/40	0.96	0.08	45,57,73,86	0
23	CLA	C	504	65/65	0.96	0.08	46,62,72,88	0
25	BCR	a	408	40/40	0.96	0.08	45,53,67,69	0
25	BCR	b	617	40/40	0.96	0.09	43,53,64,69	0
23	CLA	c	501	65/65	0.96	0.11	55,67,80,93	0
32	LHG	d	407[A]	49/49	0.96	0.15	49,57,72,79	49
32	LHG	d	407[B]	49/49	0.96	0.15	49,58,72,79	49
23	CLA	B	602	65/65	0.96	0.11	46,56,74,88	0
36	CA	c	522	1/1	0.96	0.13	73,73,73,73	0
23	CLA	B	614	65/65	0.96	0.10	39,50,104,118	0
32	LHG	d	414[A]	49/49	0.96	0.14	51,69,81,93	49
38	HEM	f	101	43/43	0.96	0.13	61,80,114,135	0
23	CLA	b	603	65/65	0.97	0.08	43,56,80,101	0
23	CLA	B	607	65/65	0.97	0.10	38,48,72,85	0
24	PHO	A	416[A]	64/64	0.97	0.10	39,51,56,63	64
24	PHO	A	416[B]	64/64	0.97	0.10	38,51,56,64	64
24	PHO	a	406[A]	64/64	0.97	0.09	43,50,55,60	64
24	PHO	a	406[B]	64/64	0.97	0.09	43,50,56,60	64
23	CLA	A	406[B]	65/65	0.97	0.09	41,48,114,125	65
21	FE2	a	401[A]	1/1	0.97	0.06	55,55,55,55	1
21	FE2	a	401[B]	1/1	0.97	0.06	55,55,55,55	1
25	BCR	B	617	40/40	0.97	0.09	42,55,65,69	0
23	CLA	B	612	65/65	0.97	0.07	38,50,63,72	0
23	CLA	b	610	65/65	0.97	0.09	46,57,68,71	0
23	CLA	B	613	65/65	0.97	0.08	39,48,100,109	0
23	CLA	A	404[A]	65/65	0.97	0.12	37,45,63,71	65
32	LHG	D	406[A]	49/49	0.97	0.14	46,57,70,80	49
32	LHG	D	406[B]	49/49	0.97	0.14	46,57,71,80	49
23	CLA	b	613	65/65	0.97	0.08	43,50,88,108	0
23	CLA	B	615	65/65	0.97	0.10	45,55,78,96	0
23	CLA	D	402[A]	65/65	0.97	0.11	36,45,69,80	65
23	CLA	D	402[B]	65/65	0.97	0.11	36,45,69,80	65
32	LHG	L	101[A]	49/49	0.97	0.12	49,58,71,94	49
32	LHG	L	101[B]	49/49	0.97	0.12	48,58,71,94	49
23	CLA	A	404[B]	65/65	0.97	0.12	37,45,63,71	65
23	CLA	c	502	65/65	0.97	0.09	46,60,92,112	0
23	CLA	c	503	65/65	0.97	0.09	49,70,86,93	0
23	CLA	a	404[A]	65/65	0.97	0.13	41,46,64,77	65
23	CLA	c	505	65/65	0.97	0.09	51,64,92,97	0
23	CLA	a	404[B]	65/65	0.97	0.13	41,46,65,78	65
23	CLA	B	604	65/65	0.97	0.09	37,49,118,134	0
27	GOL	b	628	6/6	0.97	0.21	78,88,92,92	0

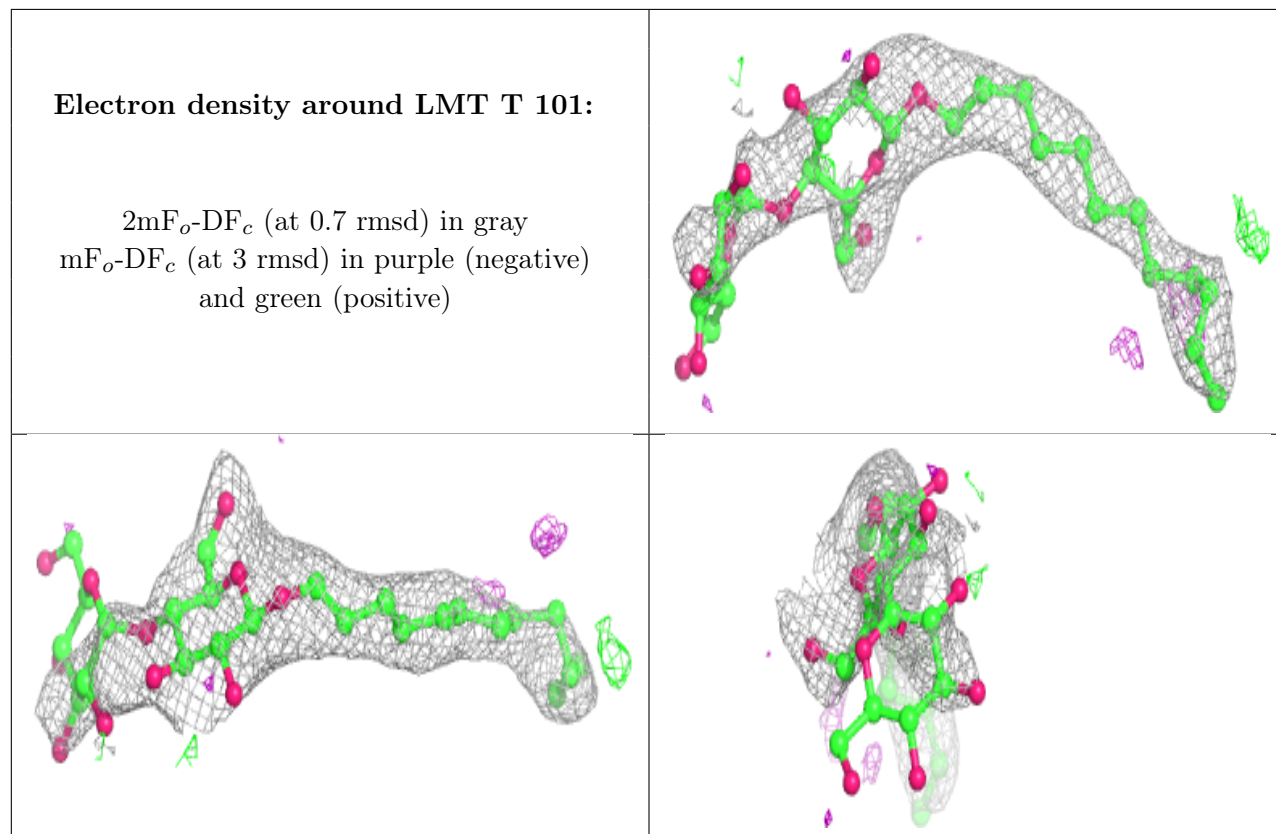
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
27	GOL	c	525[A]	6/6	0.97	0.20	65,72,77,77	6
27	GOL	c	525[B]	6/6	0.97	0.20	65,73,77,78	6
23	CLA	C	503	65/65	0.97	0.08	43,55,84,91	0
23	CLA	B	605	65/65	0.97	0.11	39,49,69,86	0
36	CA	c	523	1/1	0.97	0.06	77,77,77,77	0
23	CLA	c	510	65/65	0.97	0.10	51,62,80,95	0
23	CLA	A	406[A]	65/65	0.97	0.09	41,48,114,125	65
38	HEM	E	102	43/43	0.97	0.11	53,69,82,94	0
23	CLA	C	506	65/65	0.97	0.09	46,60,96,109	0
40	HEC	V	201	43/43	0.97	0.13	40,51,58,62	0
40	HEC	v	201	43/43	0.97	0.12	50,62,67,75	0
22	CL	a	403[B]	1/1	0.98	0.03	54,54,54,54	1
22	CL	a	402[A]	1/1	0.98	0.05	50,50,50,50	1
22	CL	a	402[B]	1/1	0.98	0.05	50,50,50,50	1
23	CLA	d	402[A]	65/65	0.98	0.08	40,46,64,73	65
23	CLA	d	402[B]	65/65	0.98	0.08	40,46,64,73	65
23	CLA	d	403[A]	65/65	0.98	0.11	38,48,76,95	65
23	CLA	d	403[B]	65/65	0.98	0.11	37,48,76,95	65
23	CLA	B	608	65/65	0.98	0.08	40,50,69,83	0
24	PHO	A	407[A]	64/64	0.98	0.09	38,47,53,59	64
24	PHO	A	407[B]	64/64	0.98	0.09	38,47,53,60	64
37	BCT	D	401[A]	4/4	0.98	0.13	54,55,61,68	4
37	BCT	D	401[B]	4/4	0.98	0.13	54,55,62,69	4
37	BCT	d	401[A]	4/4	0.98	0.10	59,61,69,78	4
37	BCT	d	401[B]	4/4	0.98	0.10	60,61,69,80	4
23	CLA	A	405[A]	65/65	0.98	0.09	37,45,58,74	65
23	CLA	b	608	65/65	0.98	0.08	41,57,79,95	0
39	MG	J	102	1/1	0.98	0.03	57,57,57,57	0
39	MG	j	102	1/1	0.98	0.08	62,62,62,62	0
23	CLA	A	405[B]	65/65	0.98	0.09	37,45,58,75	65
22	CL	a	403[A]	1/1	0.98	0.03	54,54,54,54	1
22	CL	A	402[A]	1/1	0.99	0.03	44,44,44,44	1
22	CL	A	402[B]	1/1	0.99	0.03	44,44,44,44	1
28	OEX	A	413[A]	10/10	0.99	0.05	42,44,48,50	10
28	OEX	A	413[B]	10/10	0.99	0.05	42,45,49,50	10
28	OEX	a	411[A]	10/10	0.99	0.06	48,51,52,56	10
28	OEX	a	411[B]	10/10	0.99	0.06	48,50,52,54	10
22	CL	A	403[A]	1/1	0.99	0.08	49,49,49,49	1
22	CL	A	403[B]	1/1	0.99	0.08	49,49,49,49	1
21	FE2	A	401[A]	1/1	0.99	0.06	51,51,51,51	1
21	FE2	A	401[B]	1/1	0.99	0.06	51,51,51,51	1

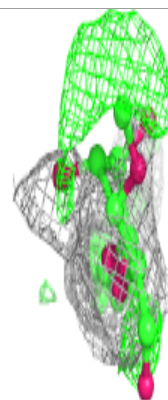
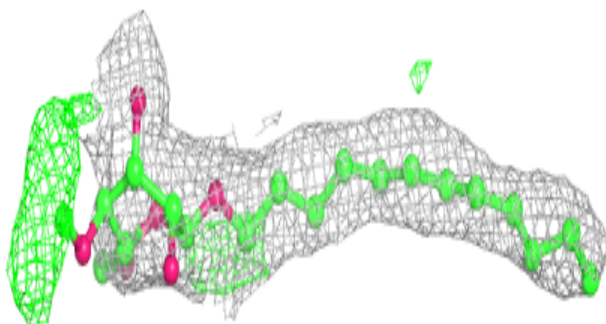
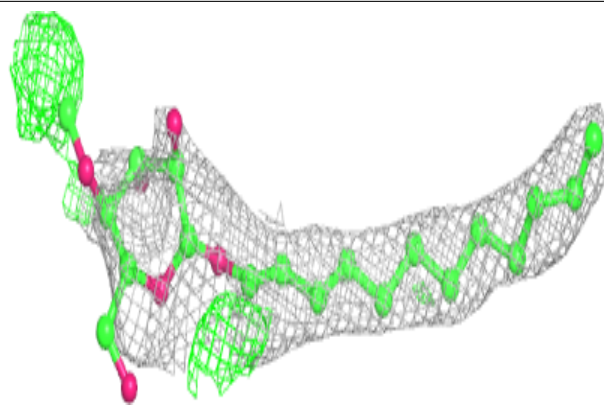
The following is a graphical depiction of the model fit to experimental electron density of all

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.

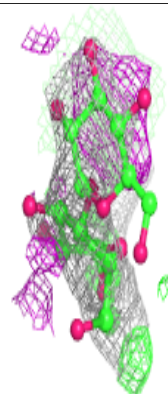
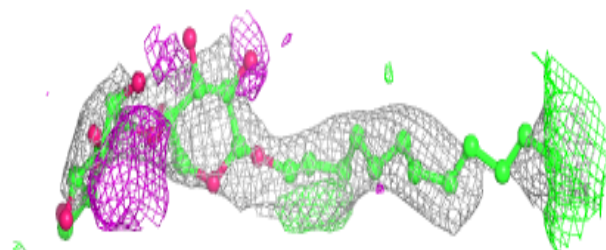
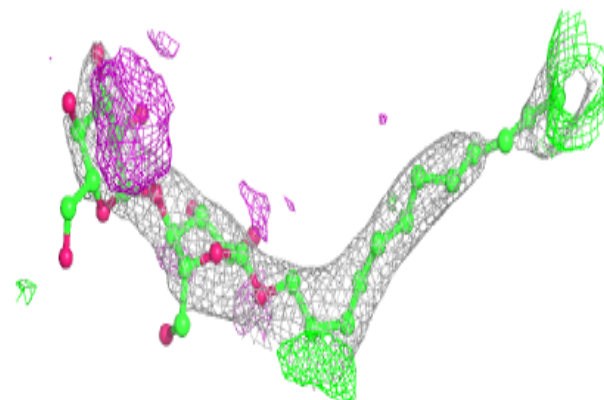


**Electron density around LMT b 621:**

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

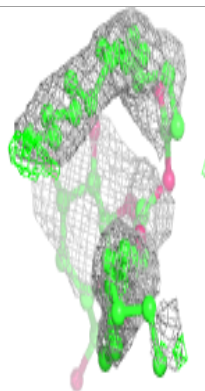
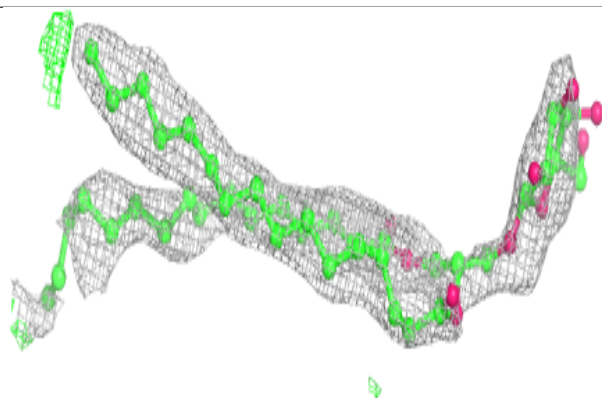
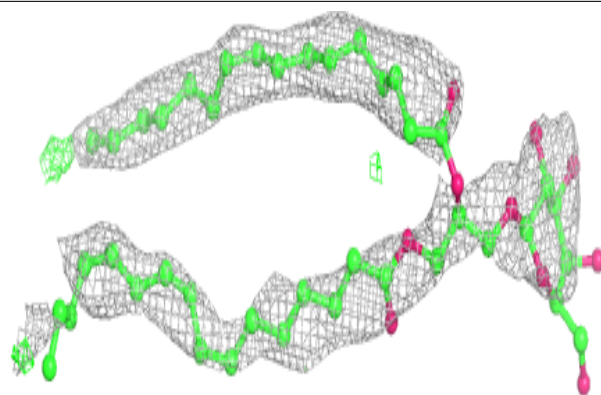
**Electron density around LMT B 630:**

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

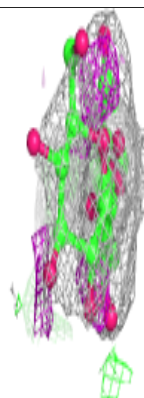
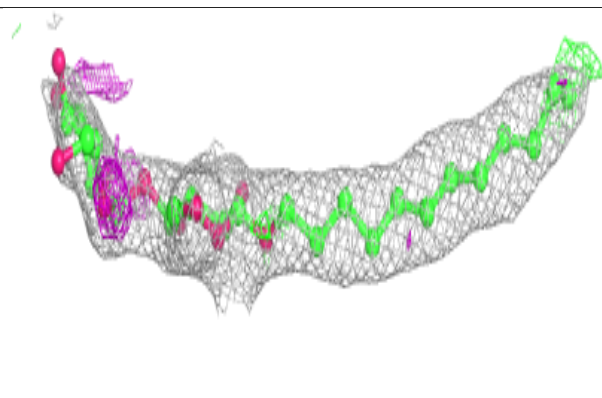
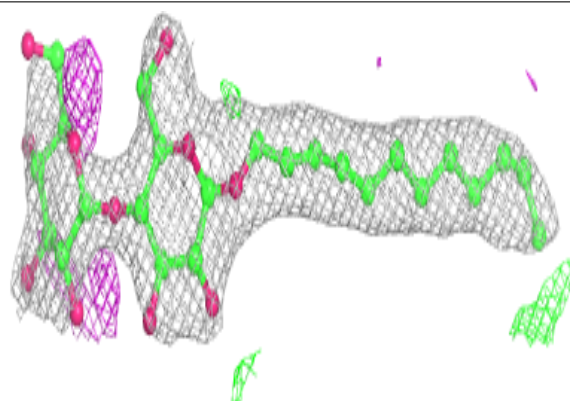


**Electron density around LMG C 521:**

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

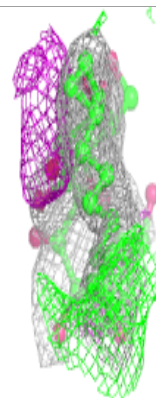
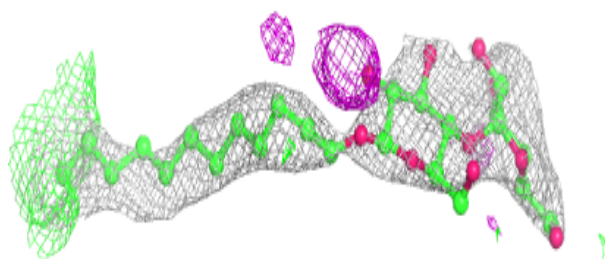
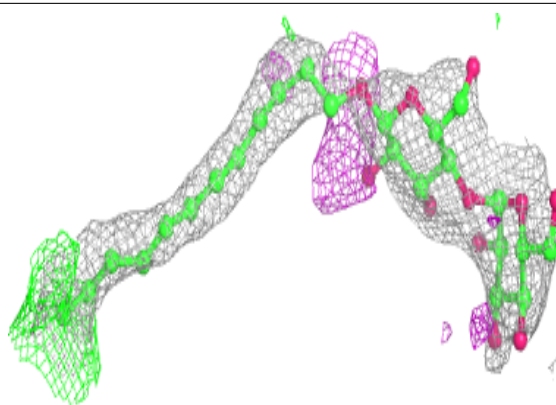
**Electron density around LMT M 101:**

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

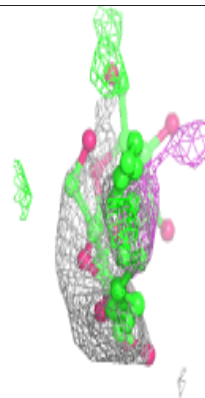
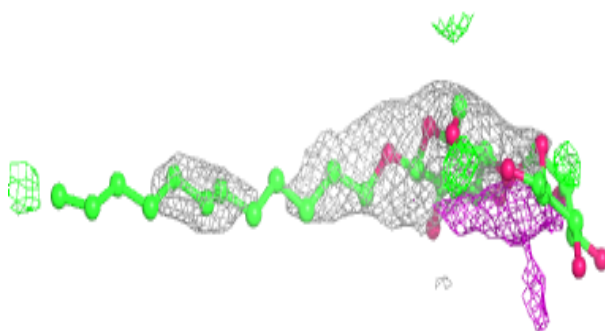
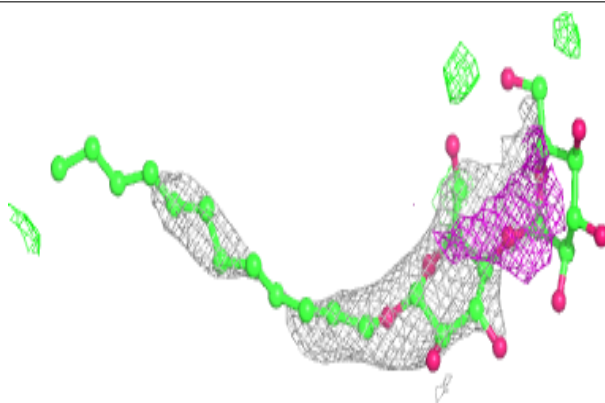


**Electron density around LMT A 417:**

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

**Electron density around LMT F 101:**

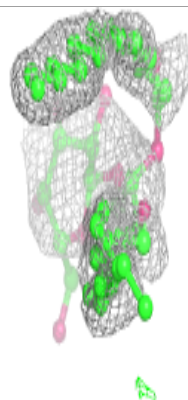
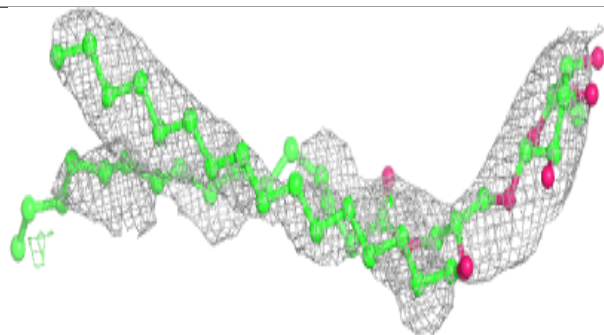
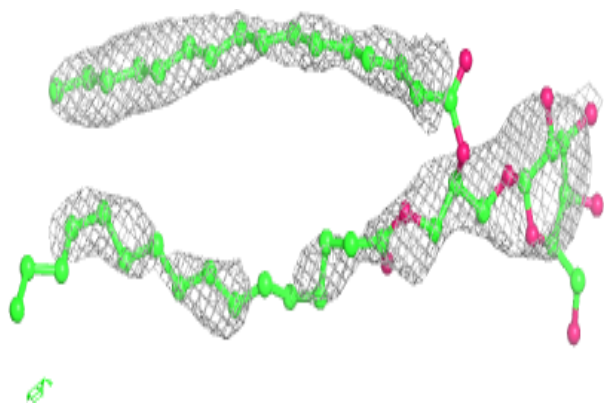
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



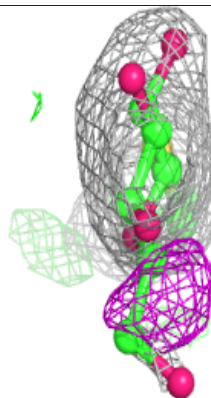
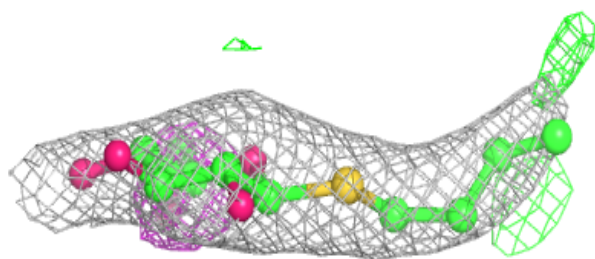
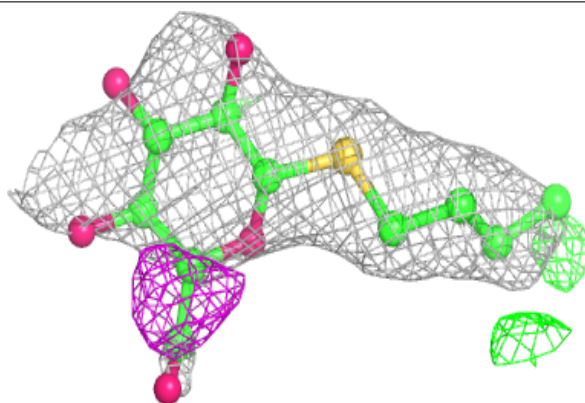


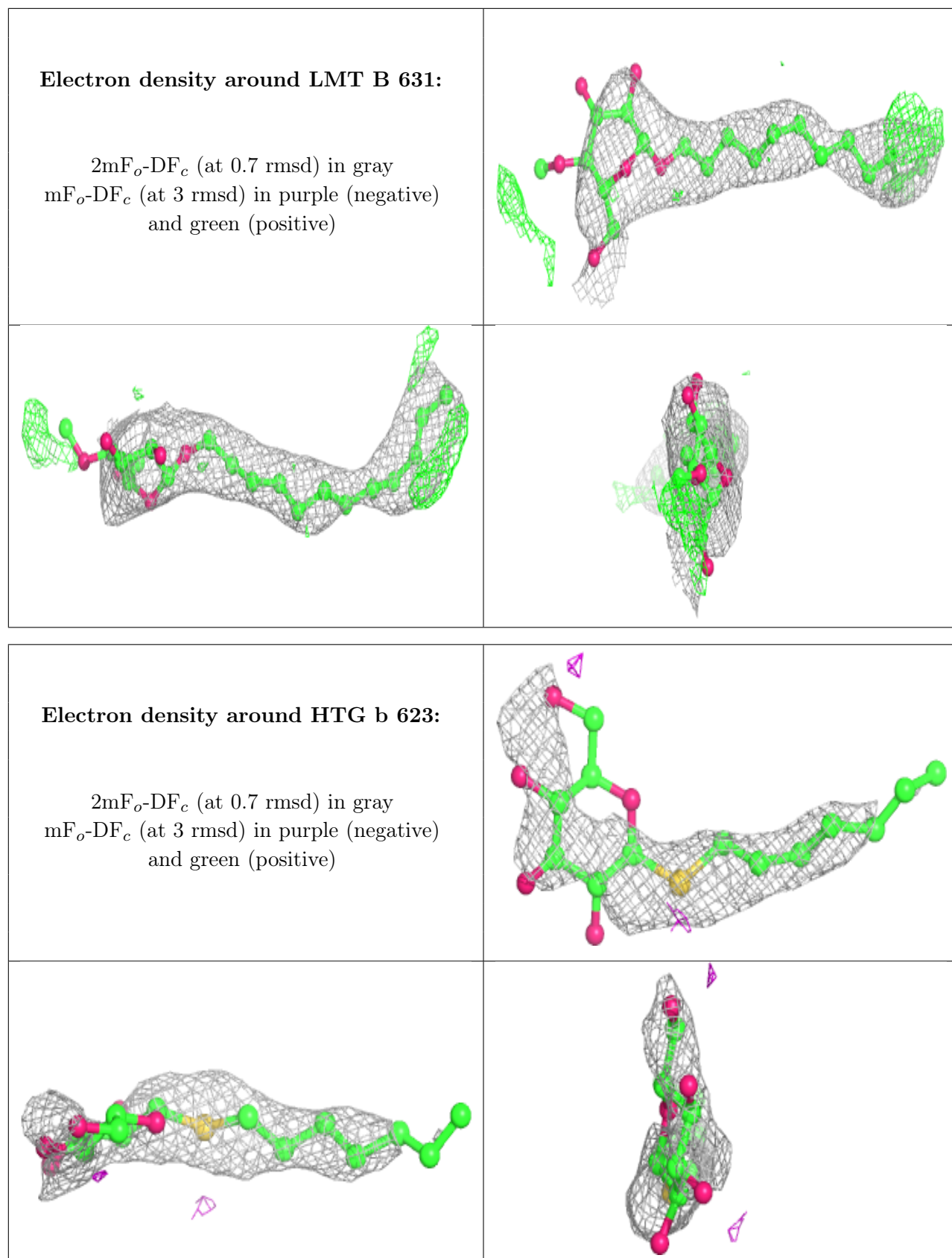
**Electron density around LMG c 520:**

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

**Electron density around HTG D 410:**

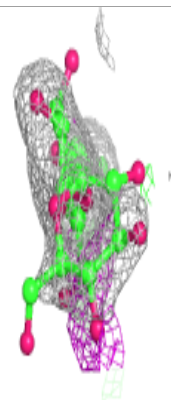
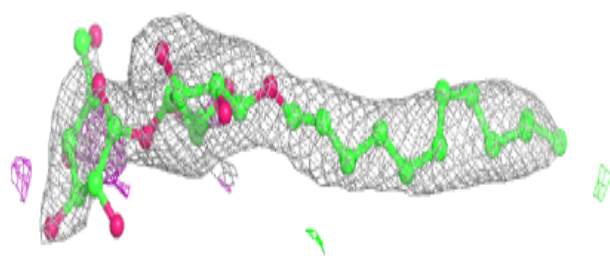
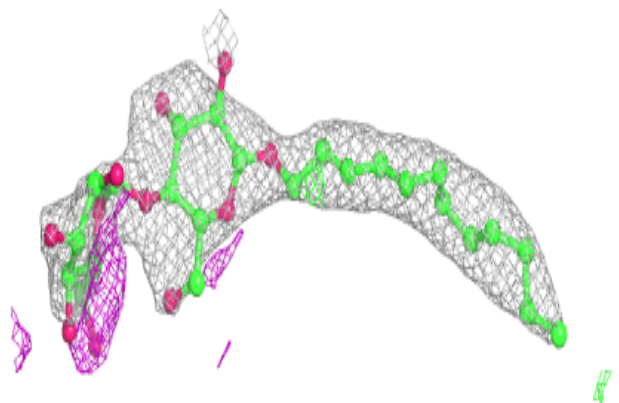
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



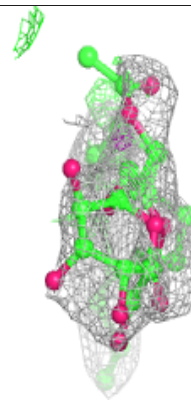
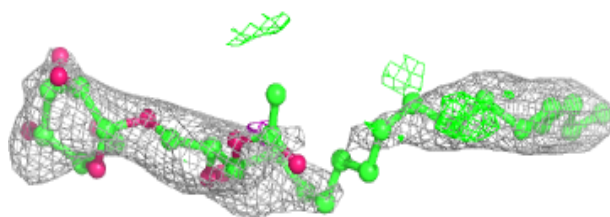
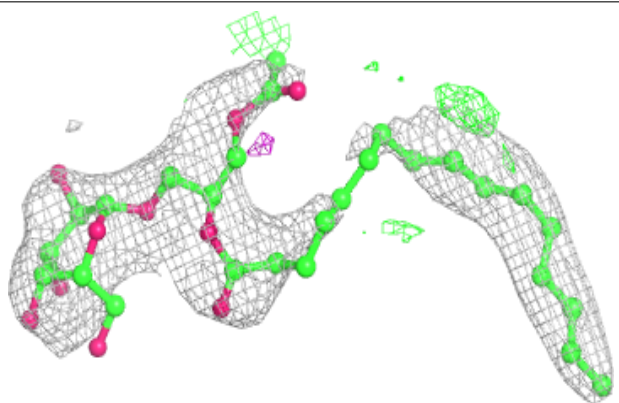


**Electron density around LMT B 628:**

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

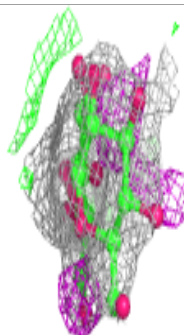
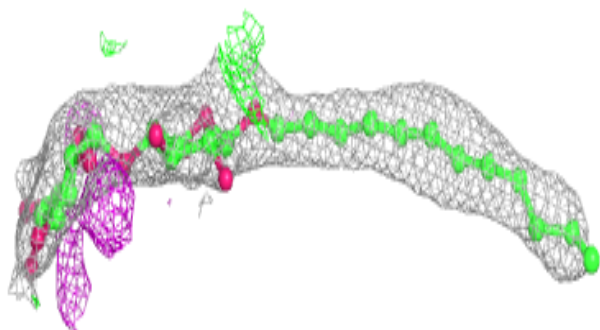
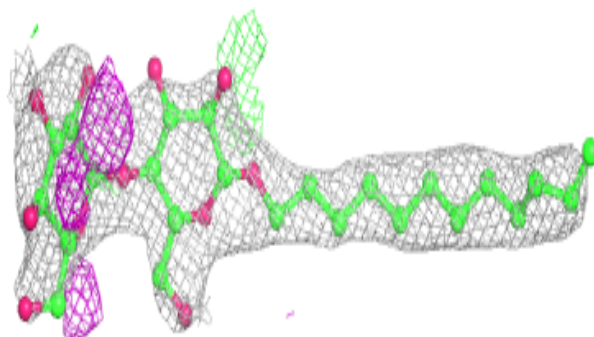
**Electron density around LMG Z 101:**

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

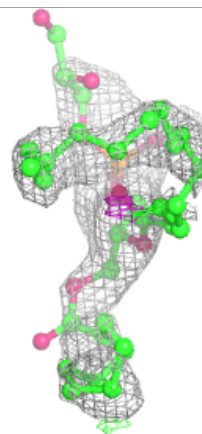
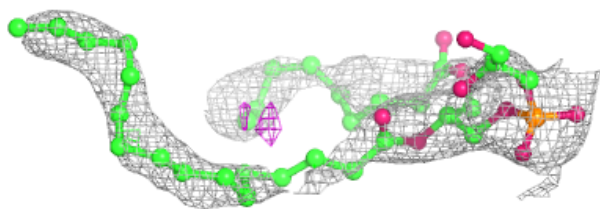
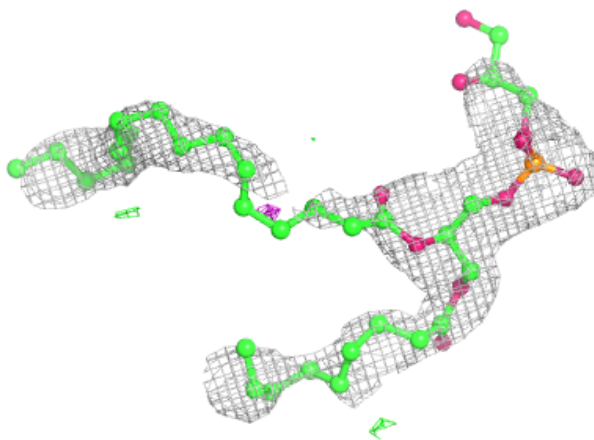


**Electron density around LMT m 103:**

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

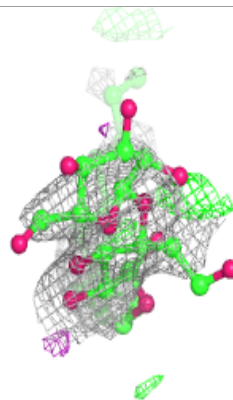
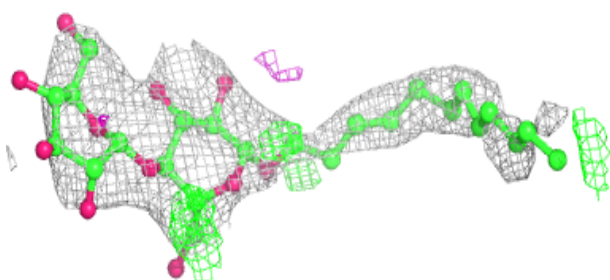
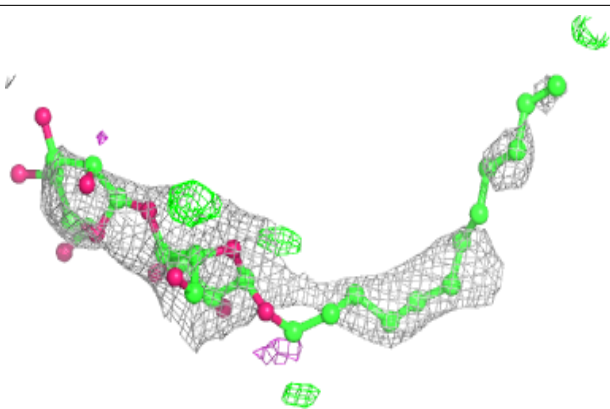
**Electron density around LHG a 419 (B):**

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

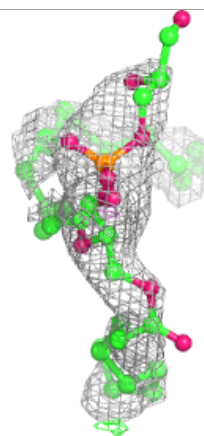
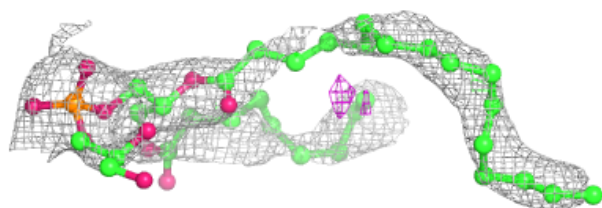
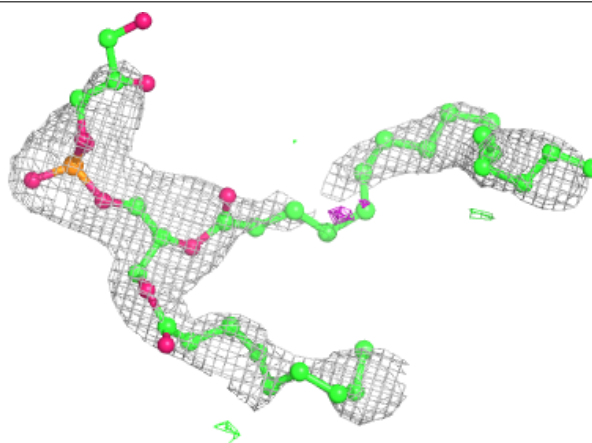


**Electron density around LMT A 420:**

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

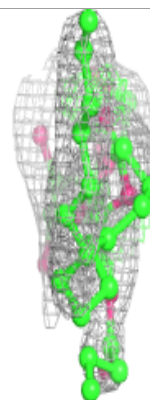
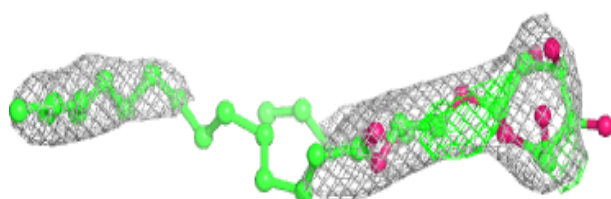
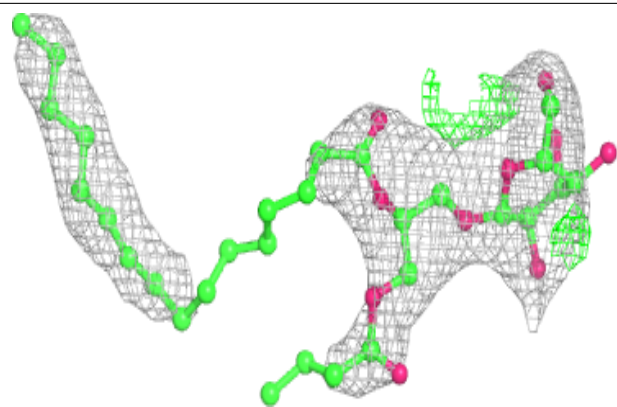
**Electron density around LHG a 419 (A):**

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

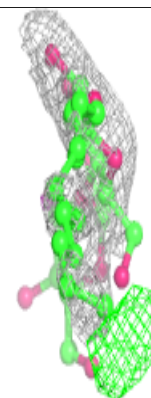
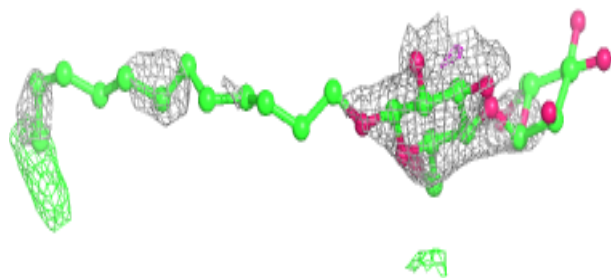
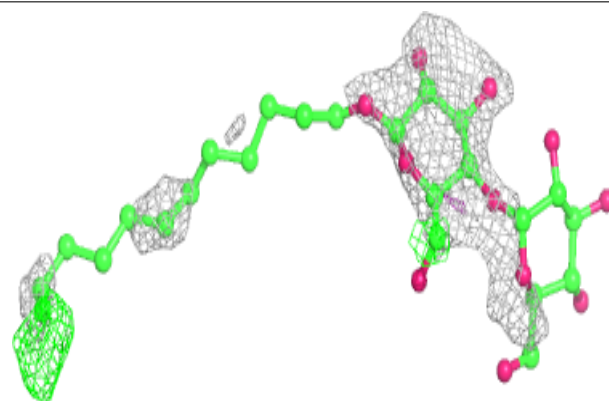


**Electron density around LMG z 101:**

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

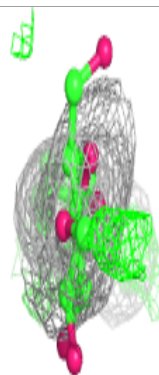
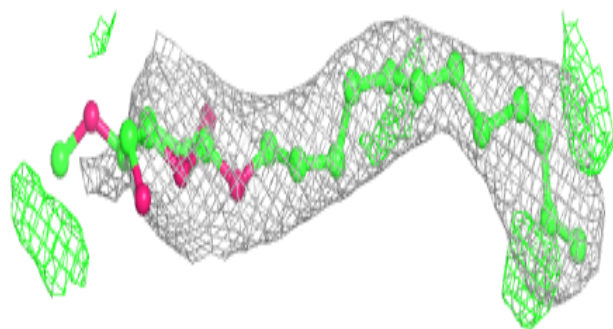
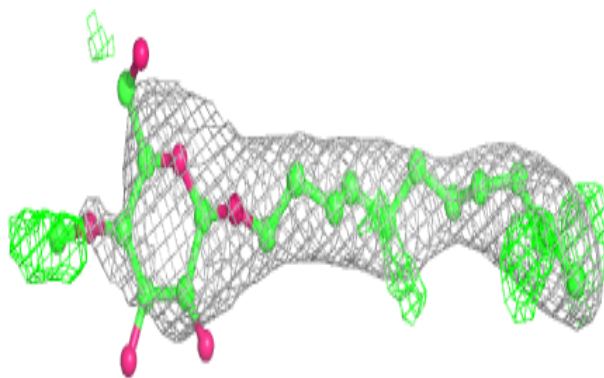
**Electron density around LMT e 101:**

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

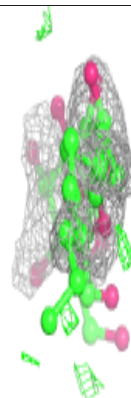
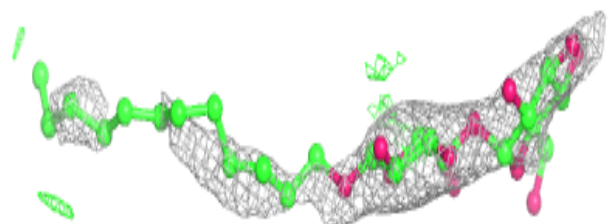
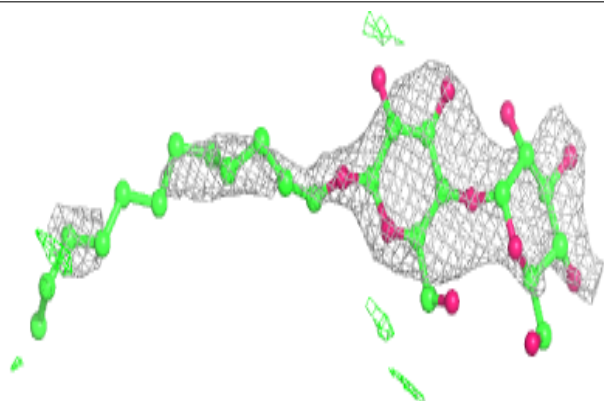


**Electron density around LMT b 627:**

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

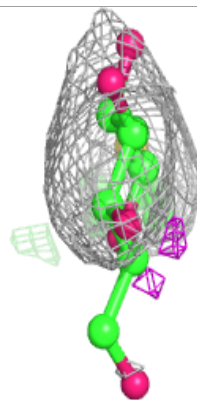
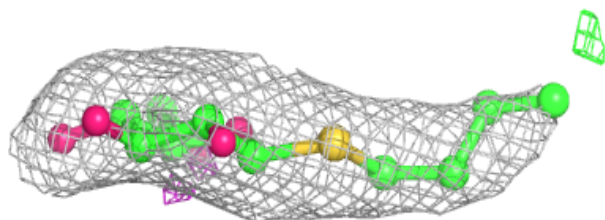
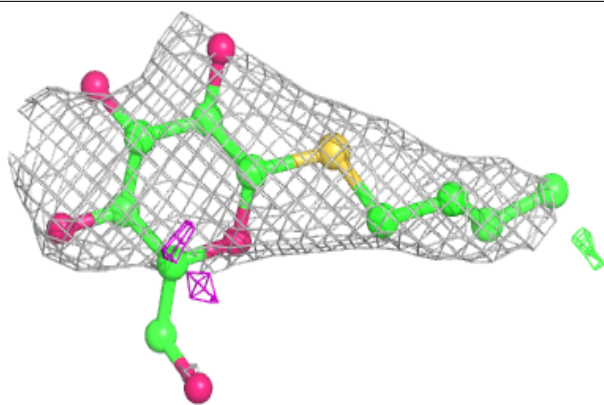
**Electron density around LMT a 416:**

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

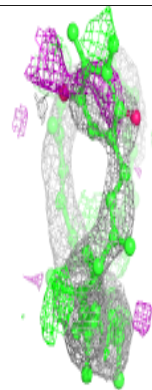
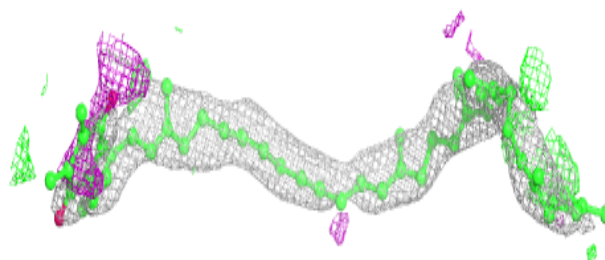
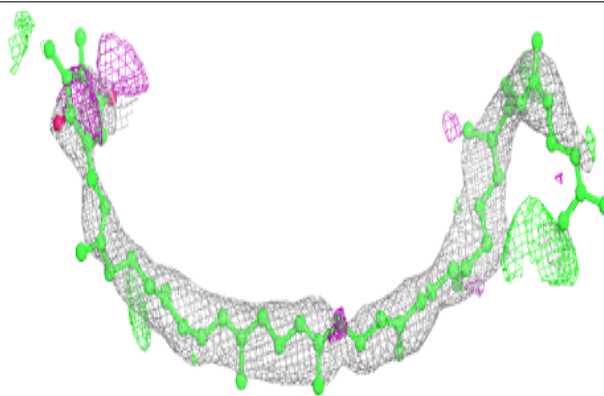


**Electron density around HTG d 411:**

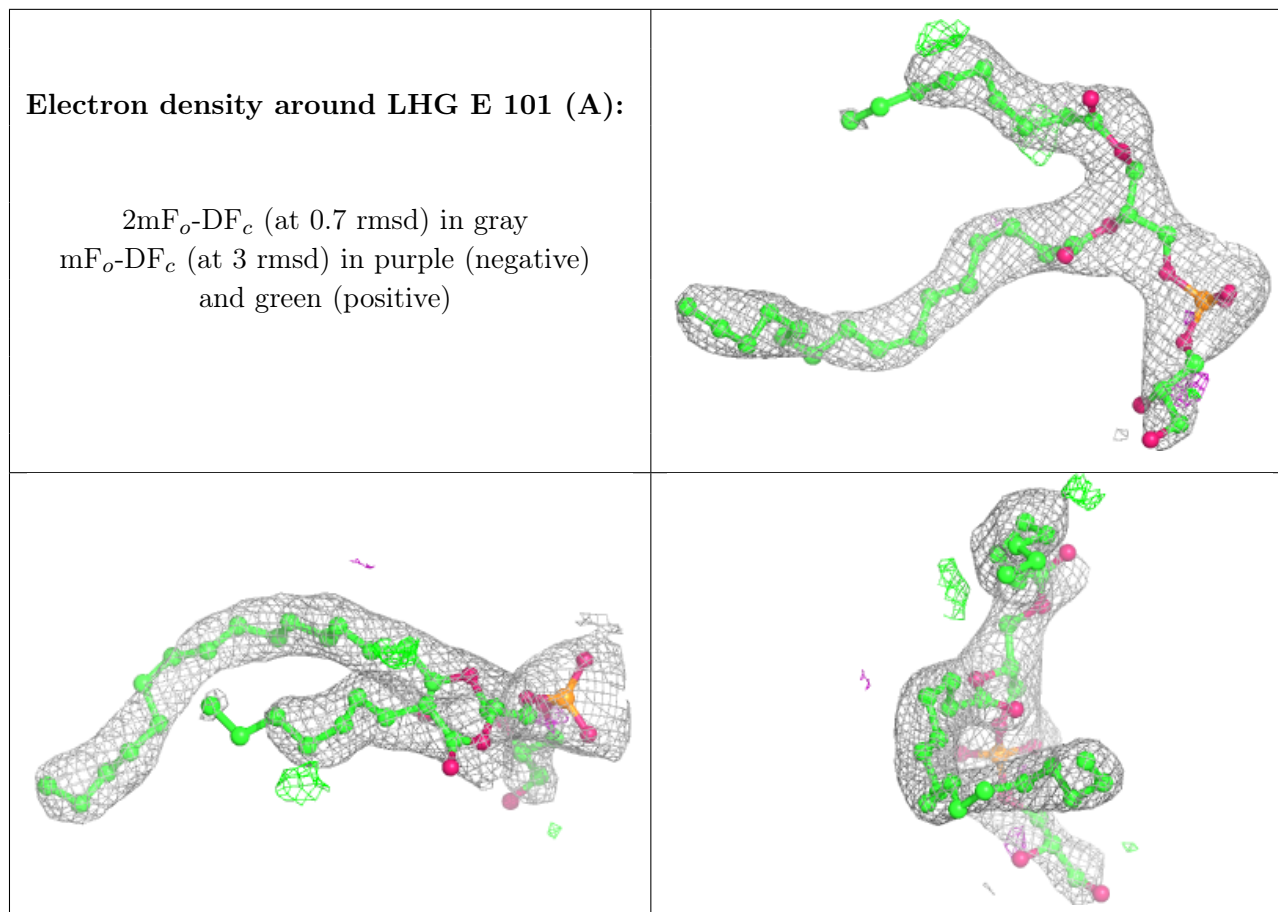
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around PL9 A 414 (A):**

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

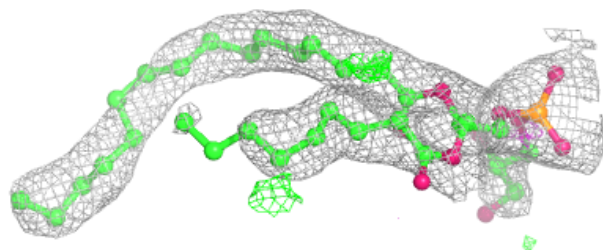
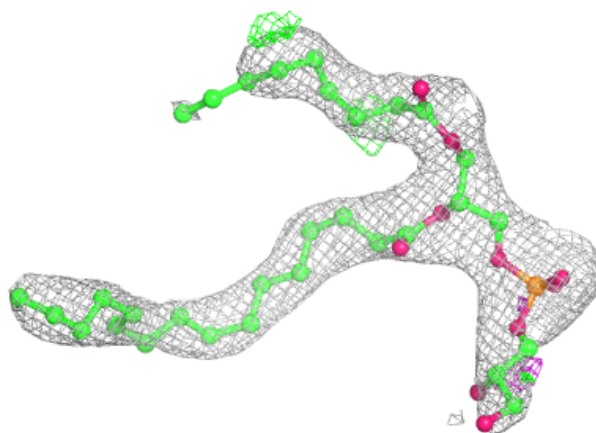




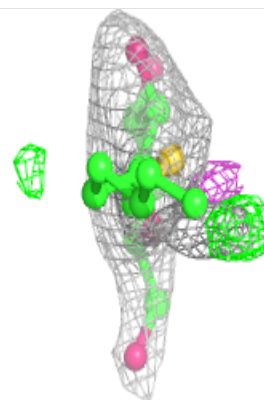
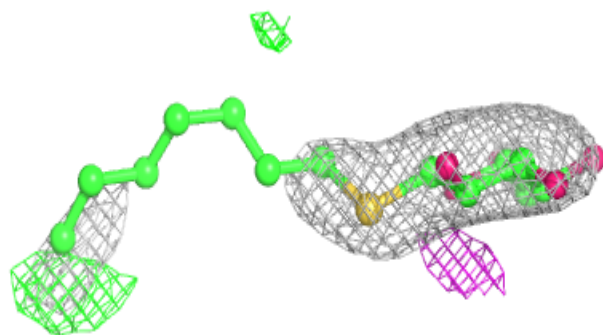
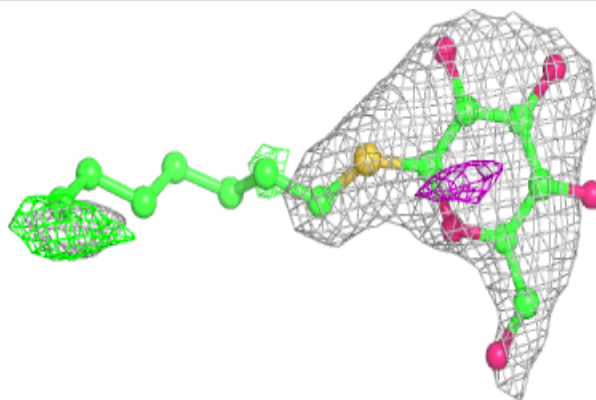


**Electron density around LHG E 101 (B):**

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

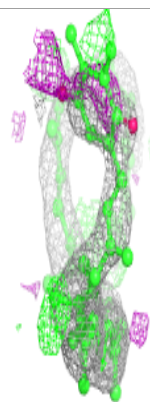
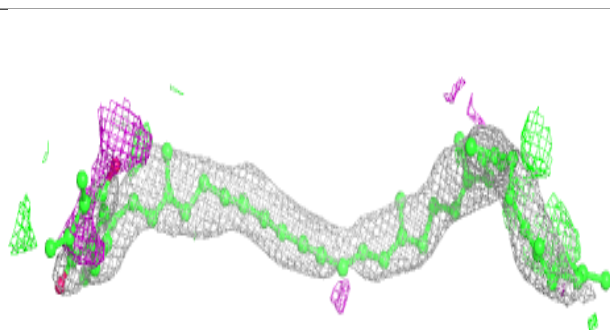
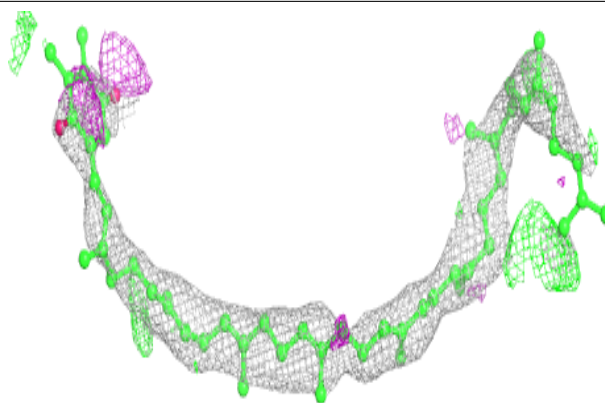
**Electron density around HTG C 522:**

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

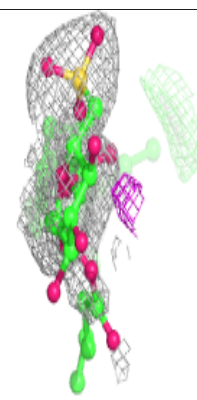
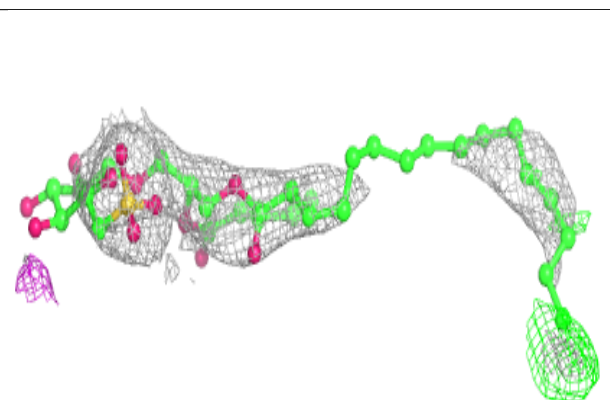
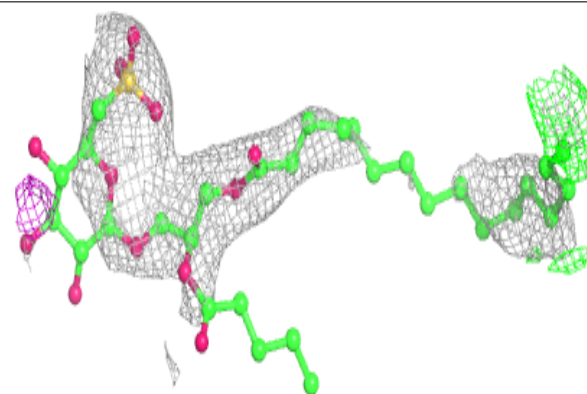


**Electron density around PL9 A 414 (B):**

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

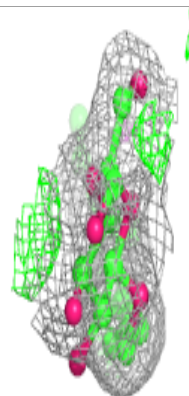
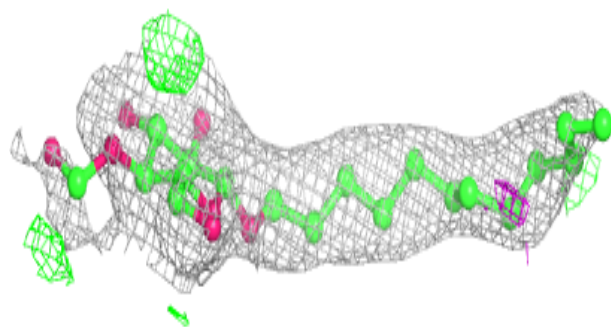
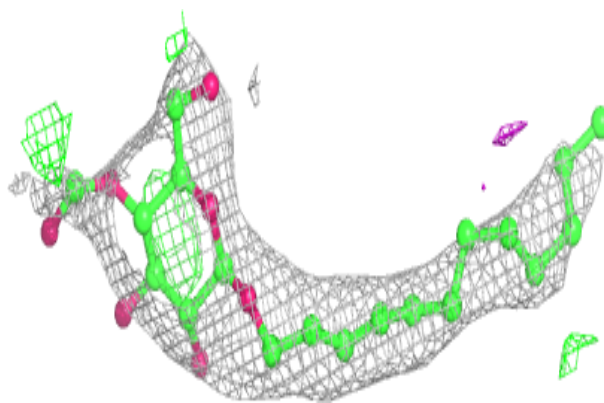
**Electron density around SQD f 102:**

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

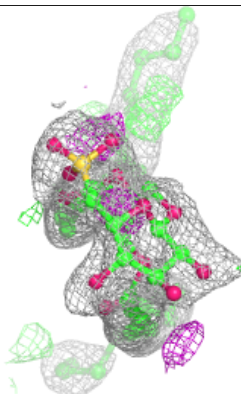
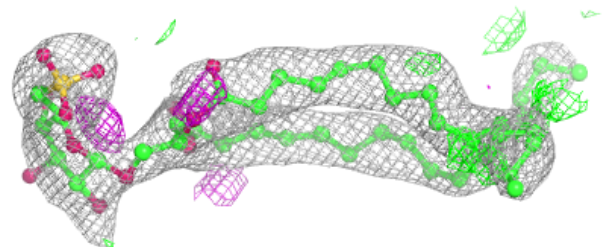
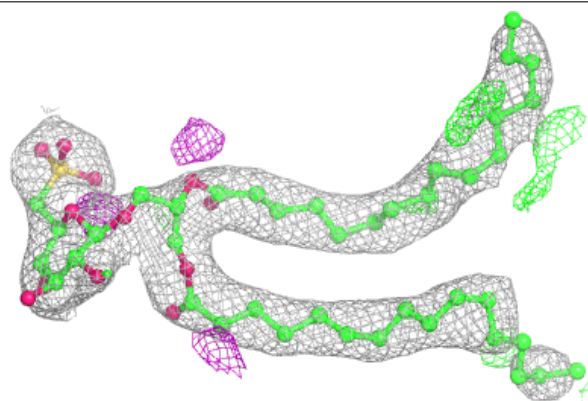


**Electron density around LMT t 101:**

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

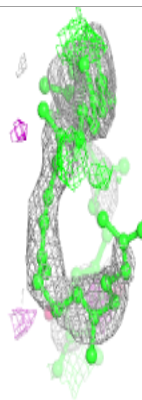
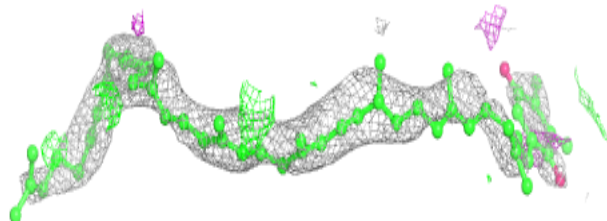
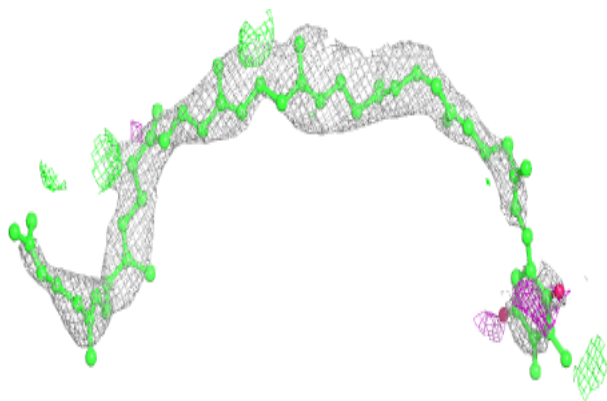
**Electron density around SQD b 620:**

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

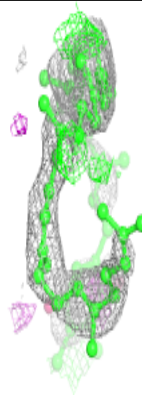
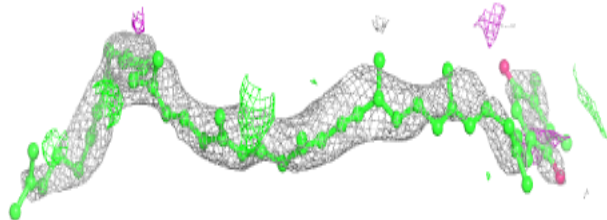
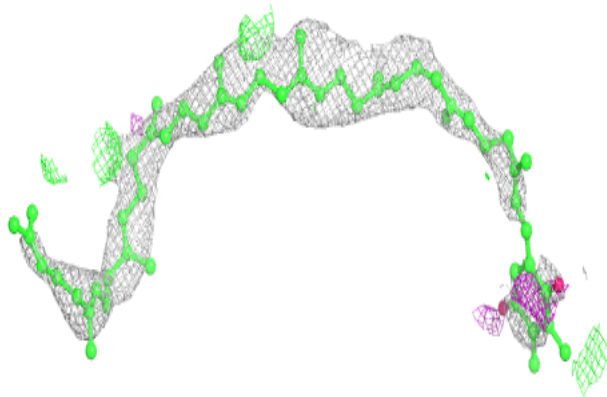


**Electron density around PL9 a 412 (A):**

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

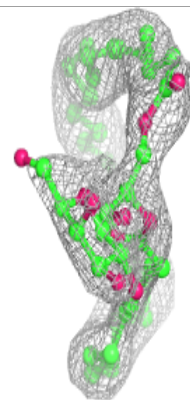
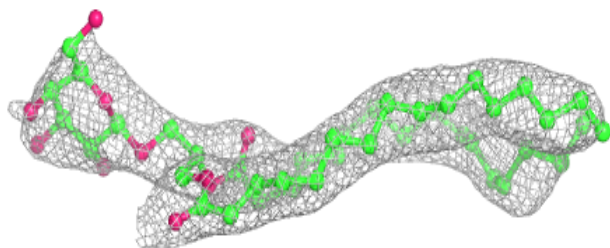
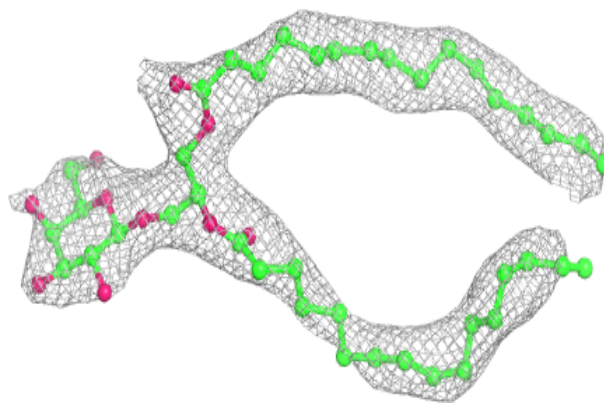
**Electron density around PL9 a 412 (B):**

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

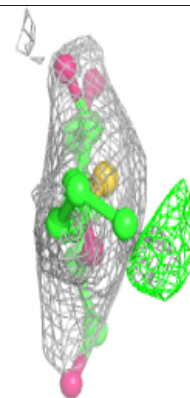
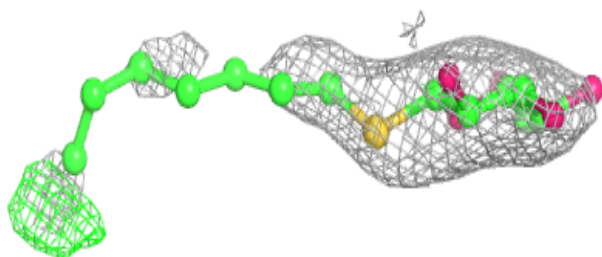
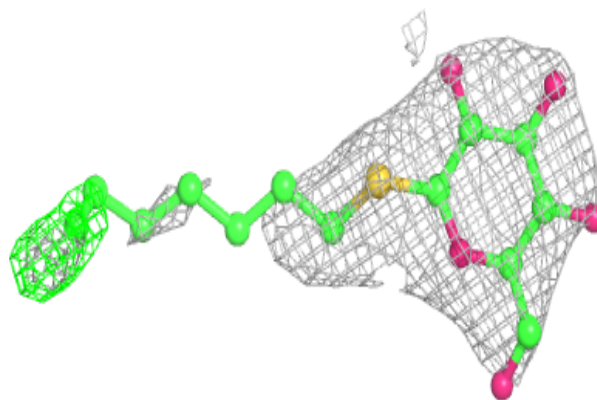


**Electron density around LMG a 415:**

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

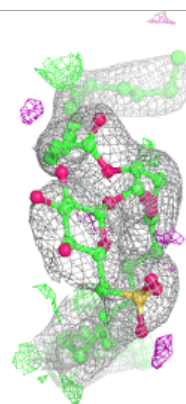
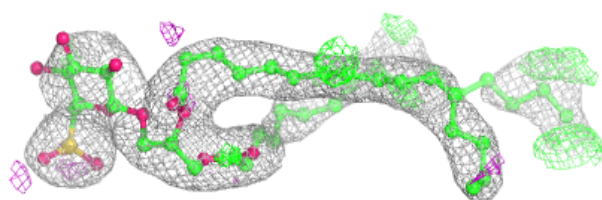
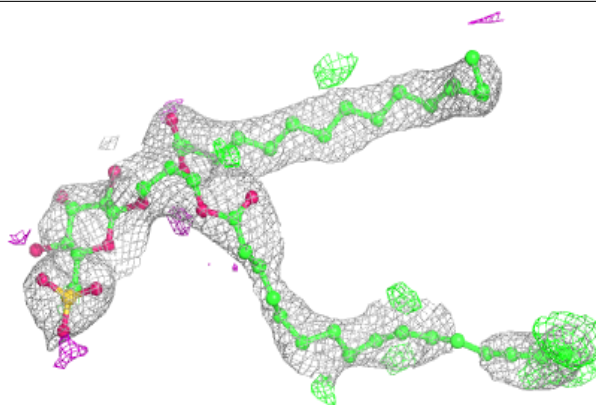
**Electron density around HTG c 521:**

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

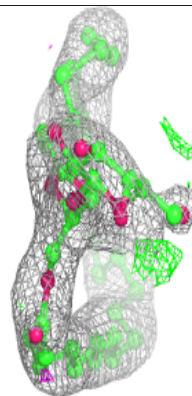
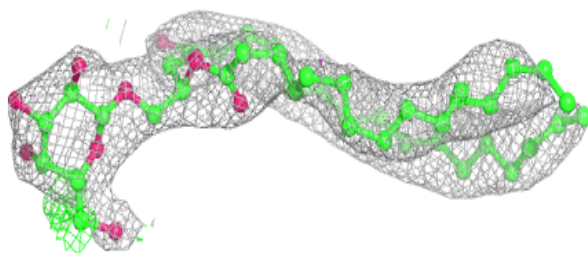
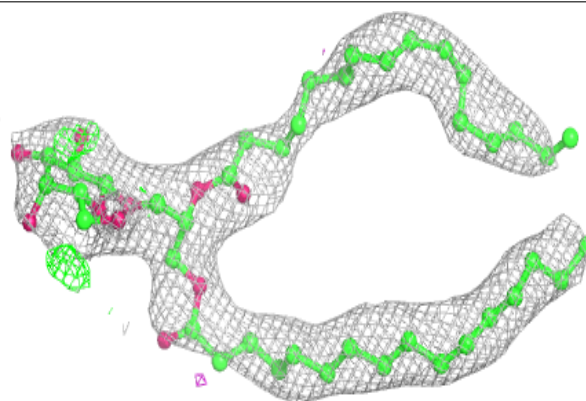


**Electron density around SQD A 412:**

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

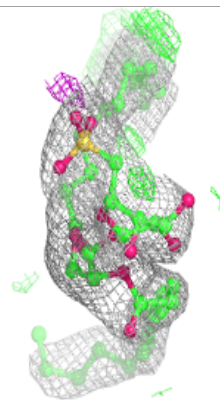
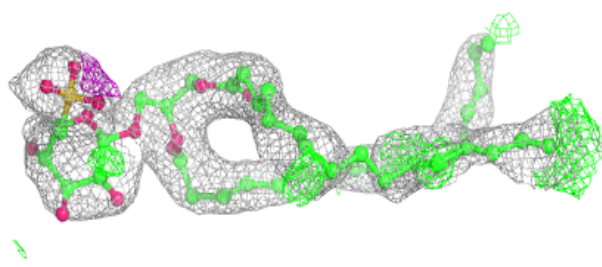
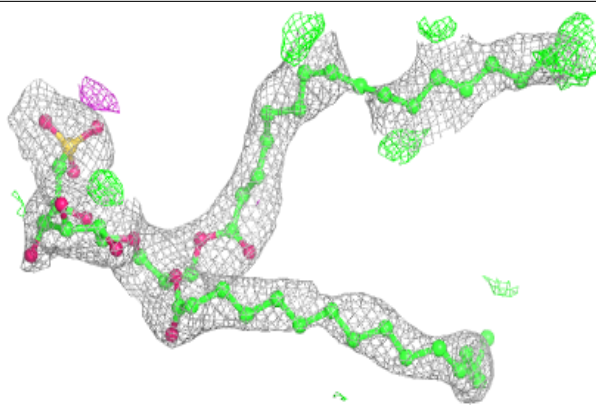
**Electron density around LMG C 501:**

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

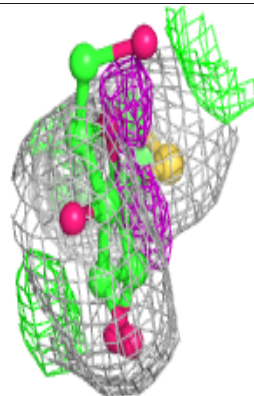
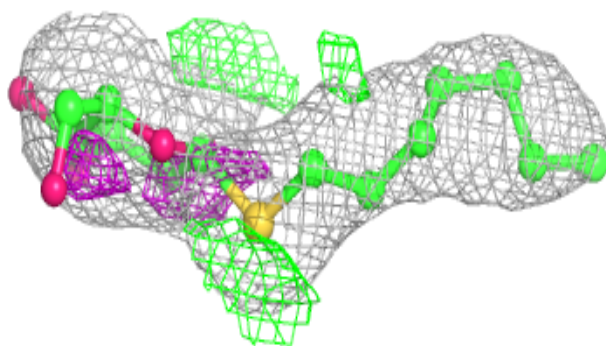
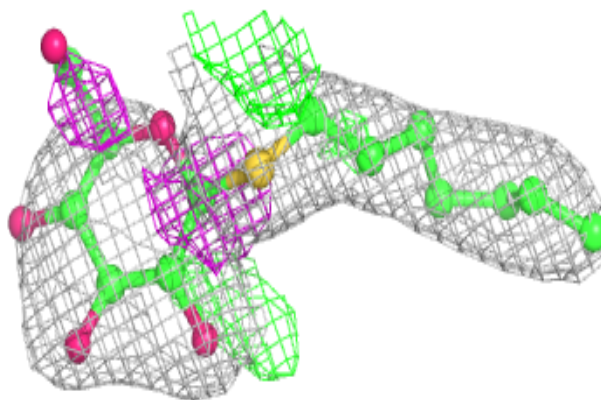


**Electron density around SQD a 410:**

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

**Electron density around HTG B 622:**

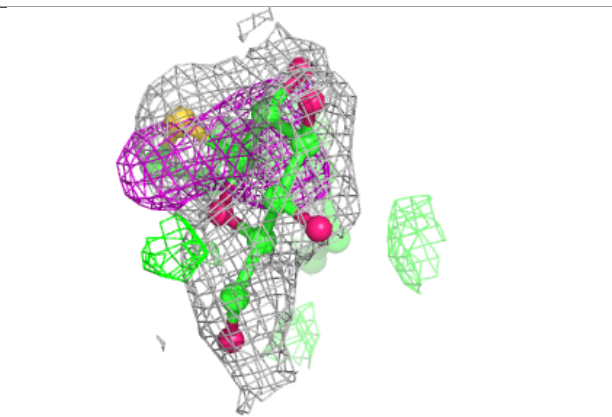
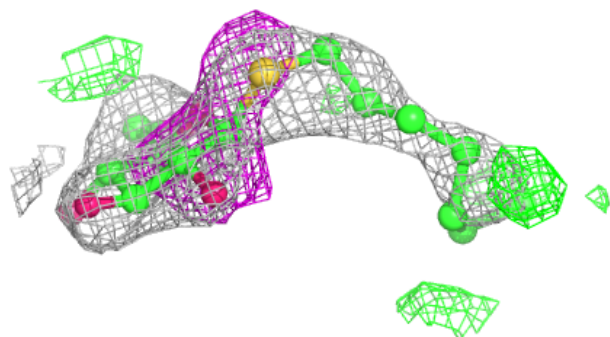
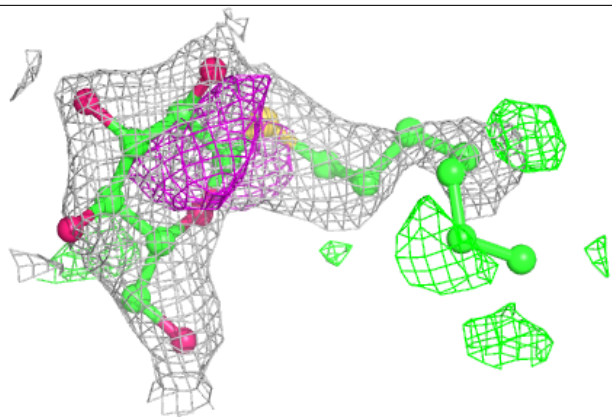
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



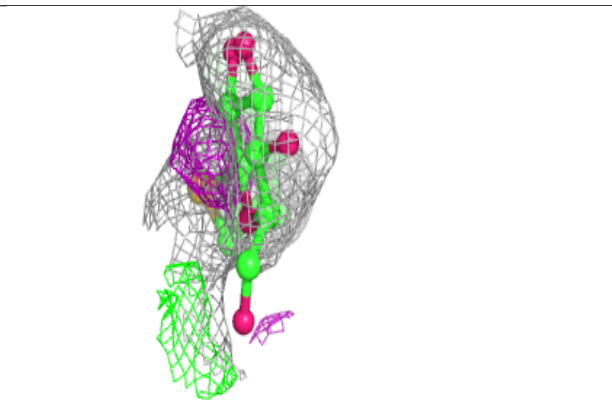
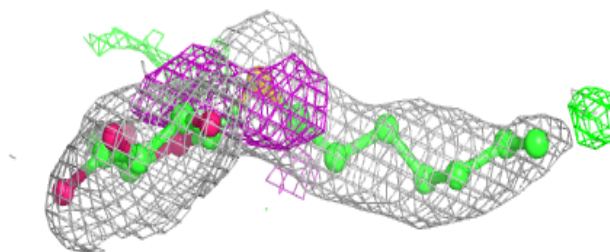
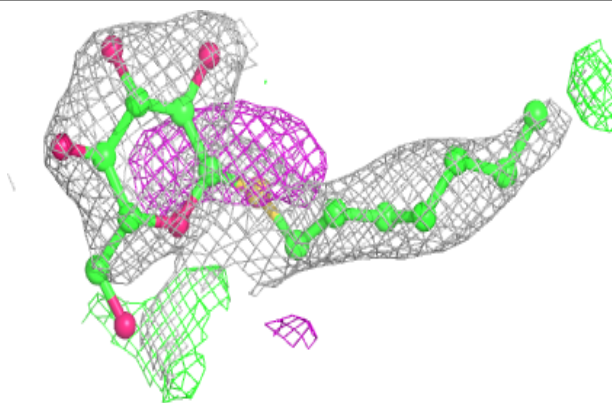


**Electron density around HTG B 623:**

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

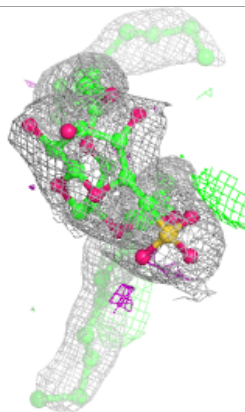
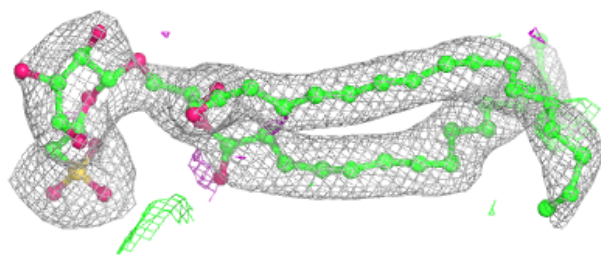
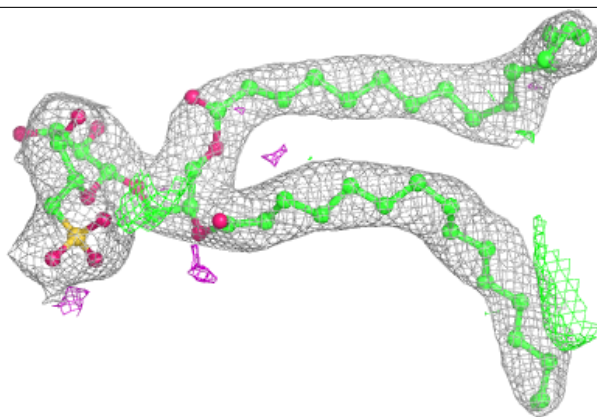
**Electron density around HTG b 622:**

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

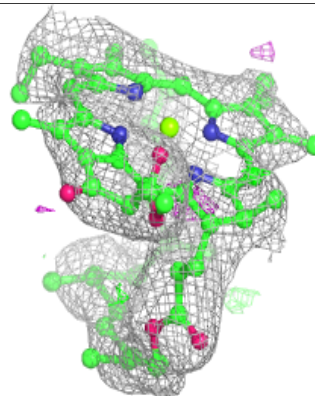
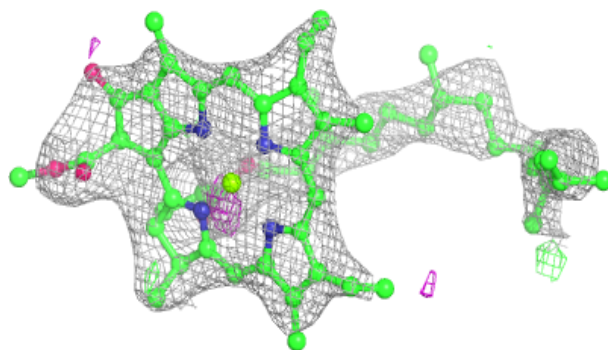
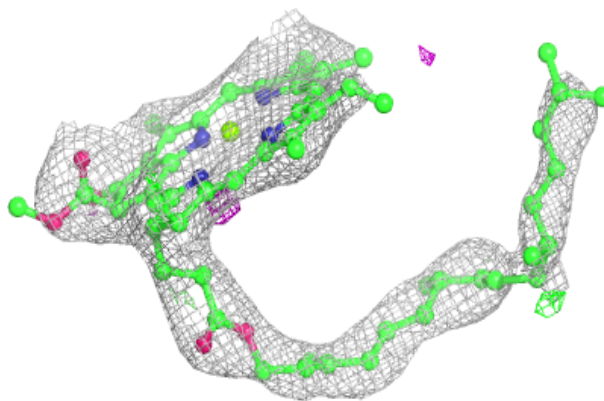


**Electron density around SQD B 620:**

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

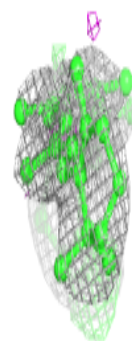
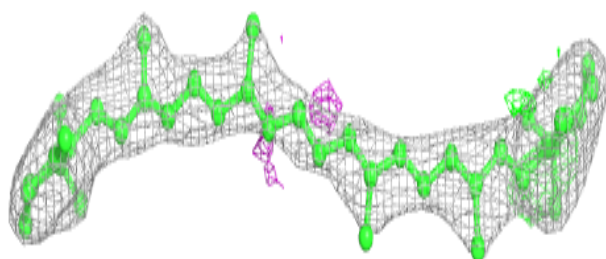
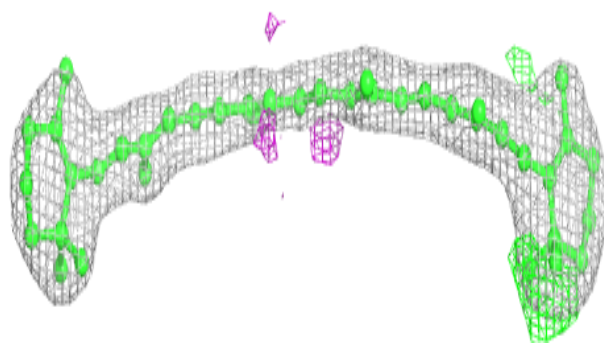
**Electron density around CLA c 513:**

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

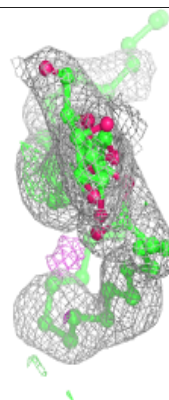
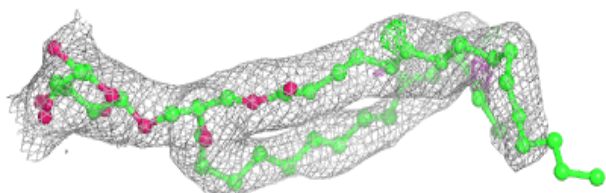
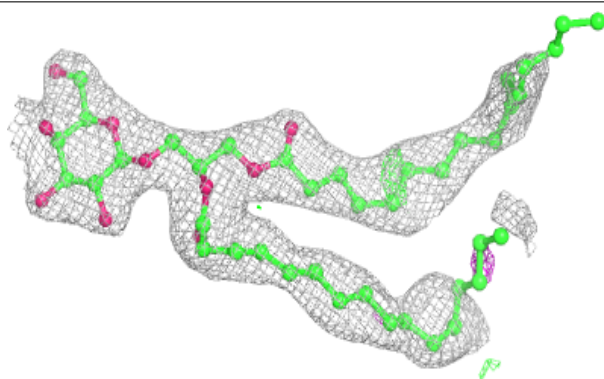


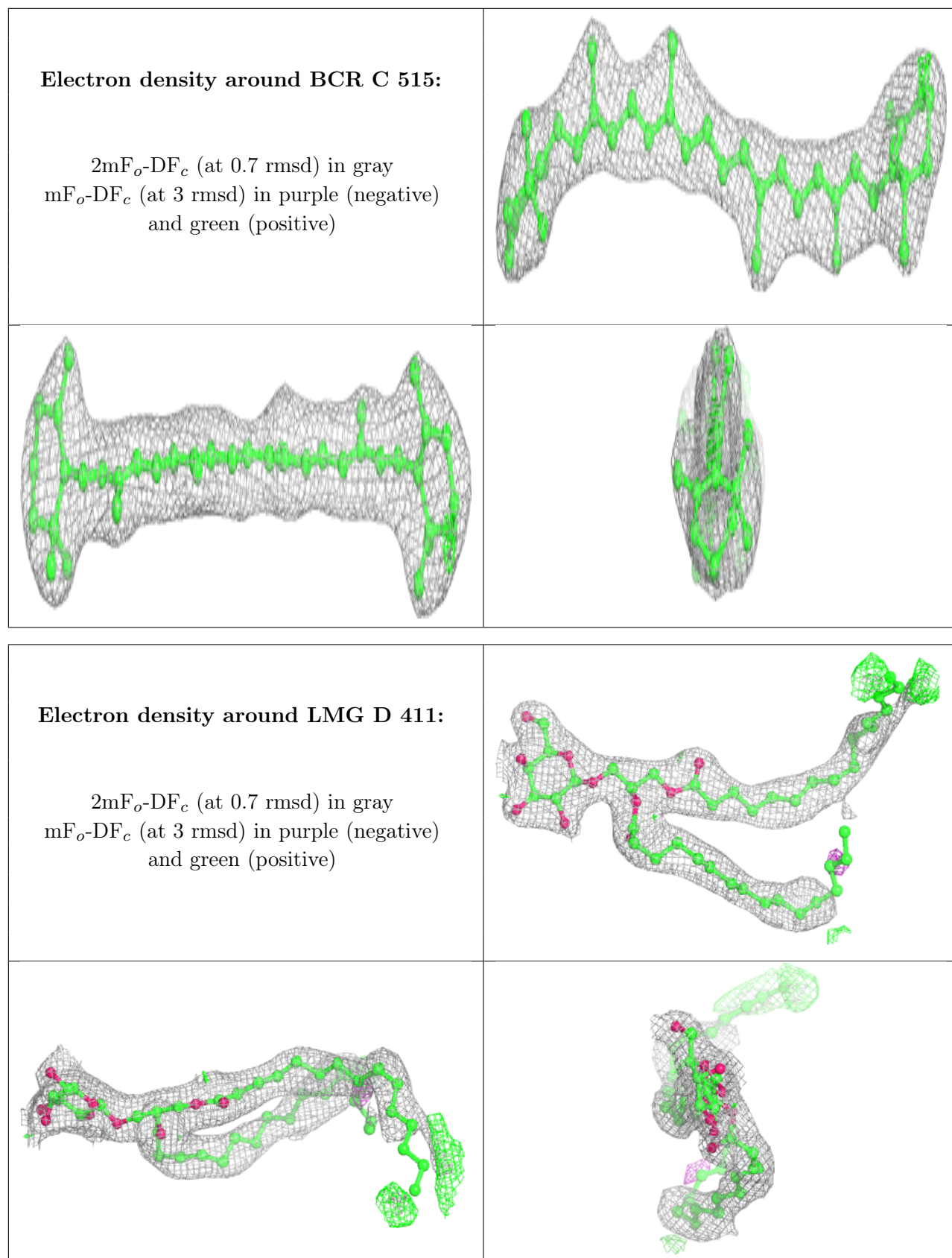
**Electron density around BCR K 102:**

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

**Electron density around LMG d 412:**

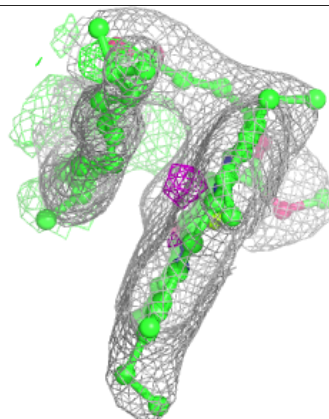
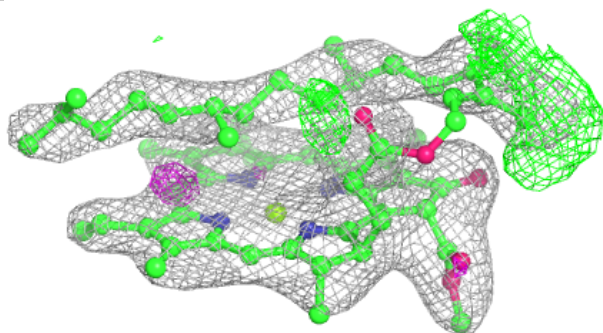
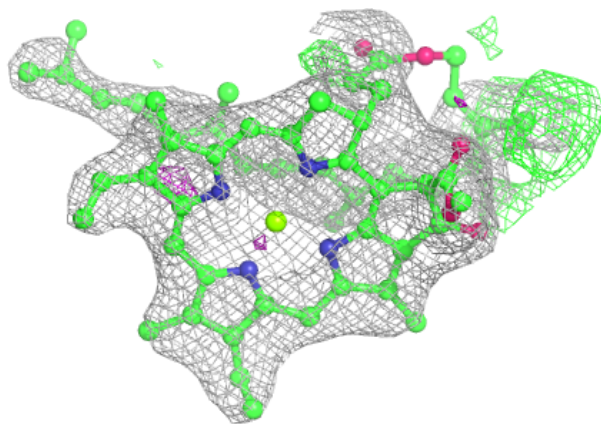
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





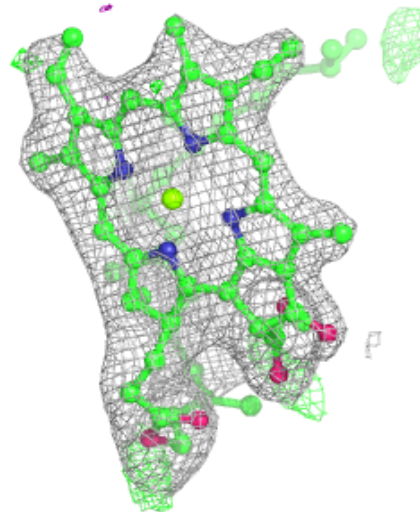
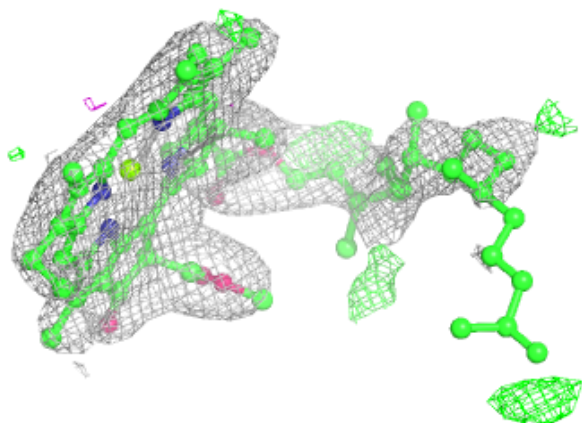
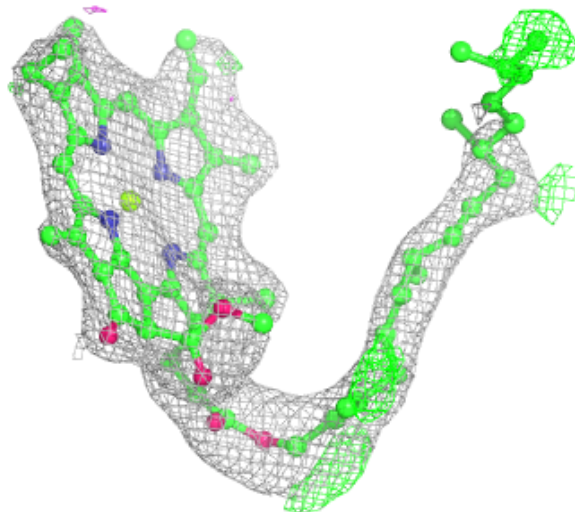
**Electron density around CLA b 601:**

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



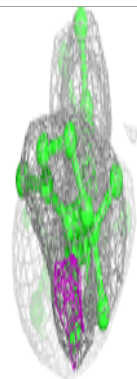
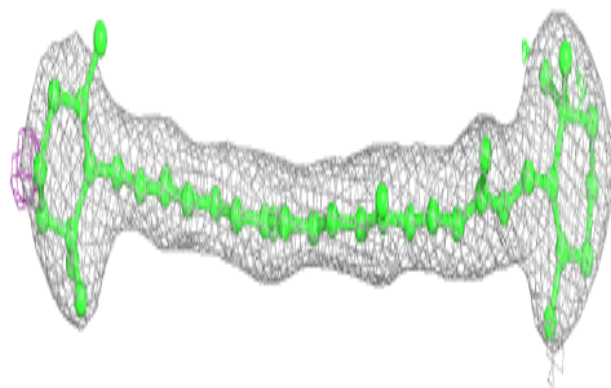
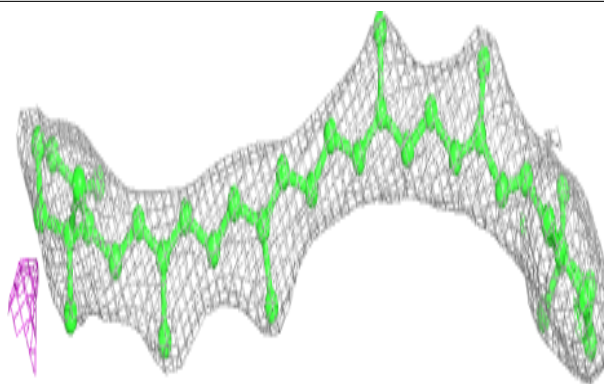
**Electron density around CLA b 616:**

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

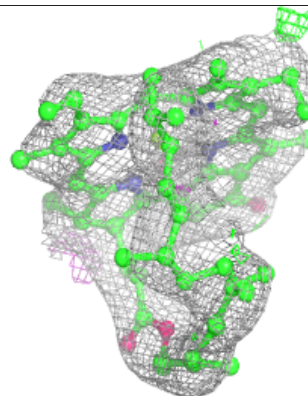
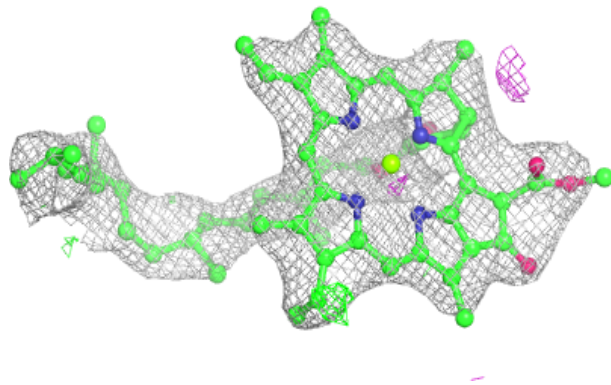
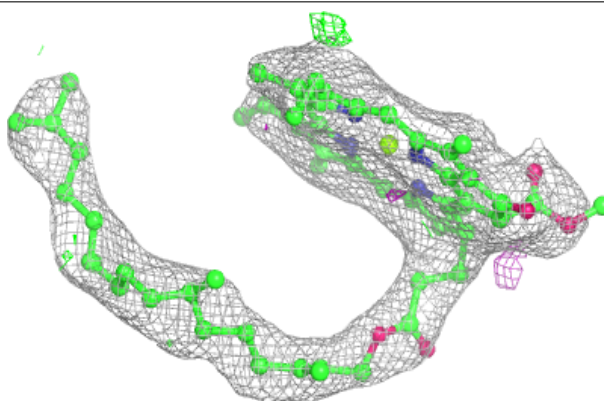


**Electron density around BCR h 101:**

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

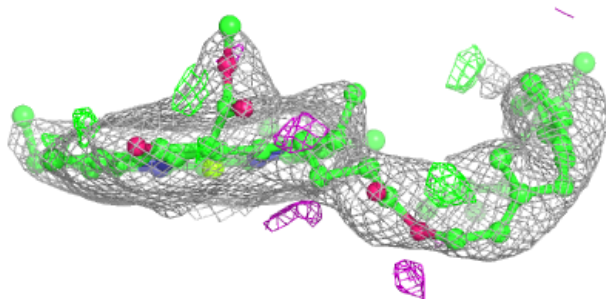
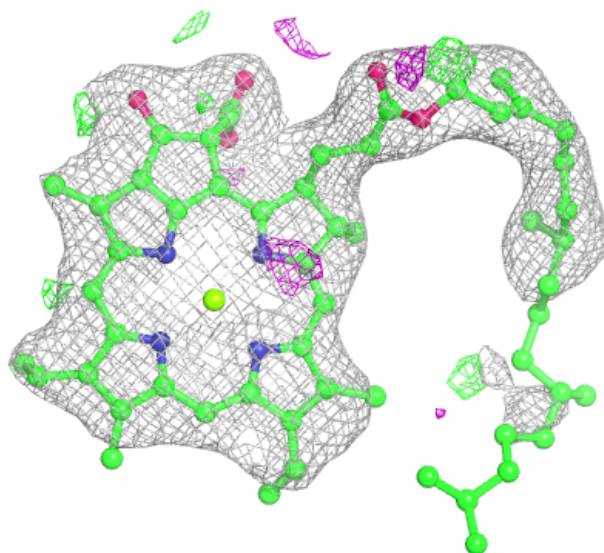
**Electron density around CLA C 514:**

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



**Electron density around CLA c 512:**

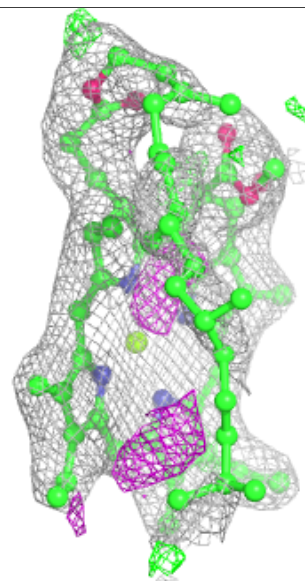
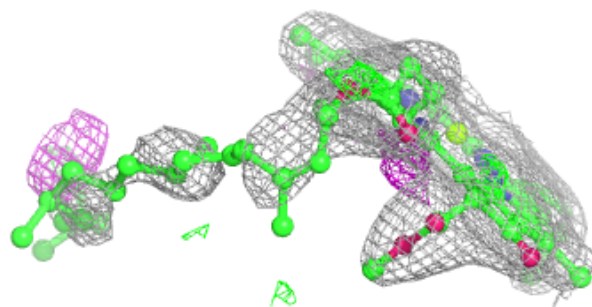
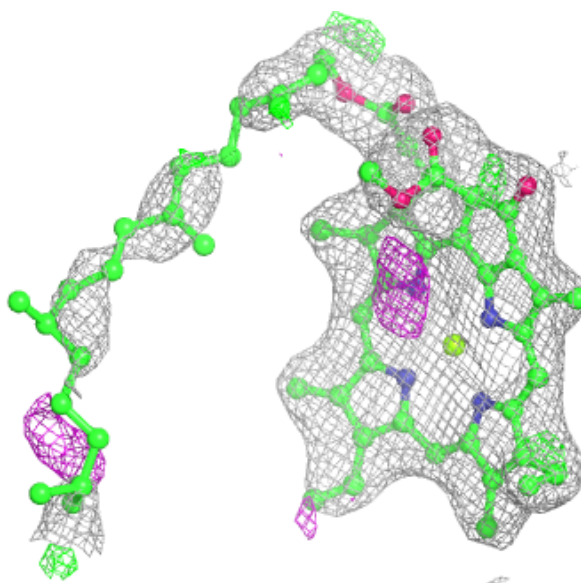
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





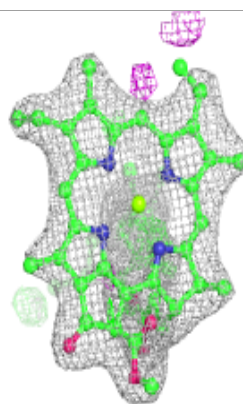
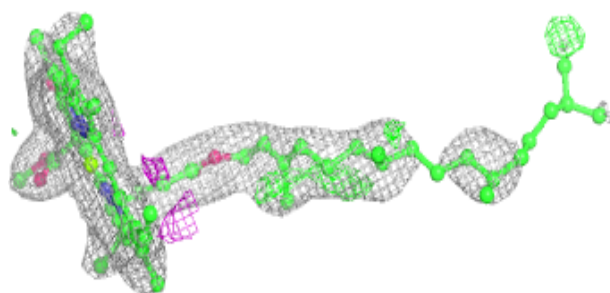
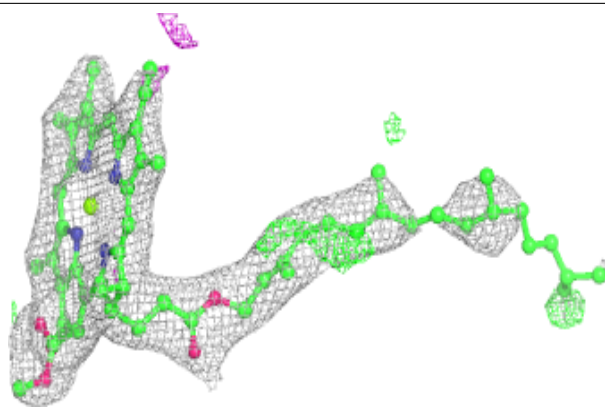
**Electron density around CLA B 616:**

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

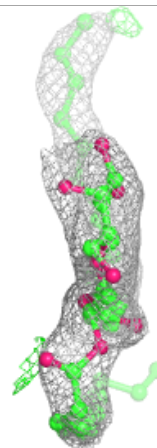
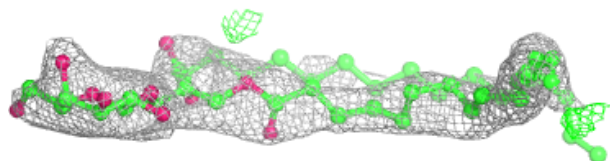
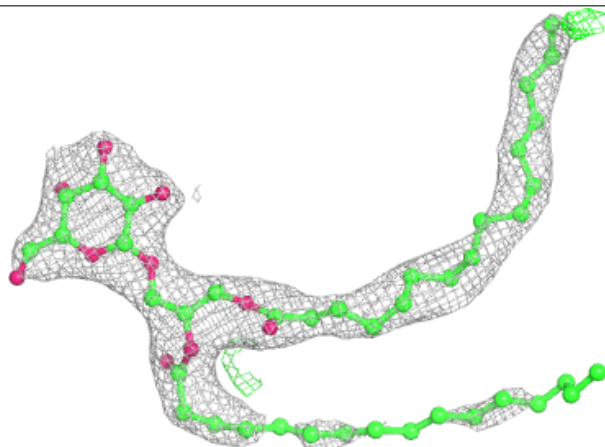


**Electron density around CLA d 404:**

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

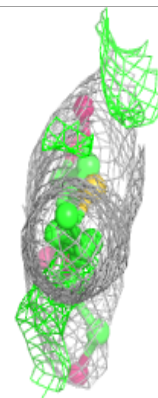
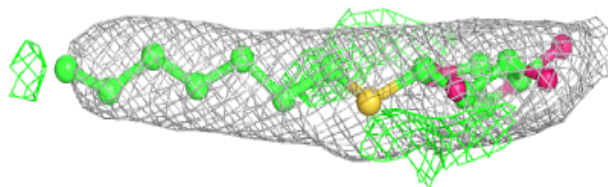
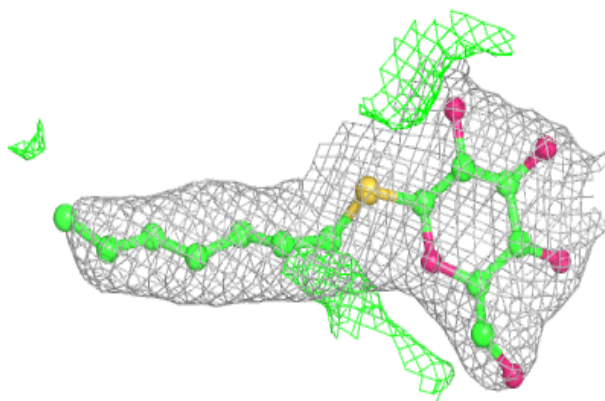
**Electron density around LMG c 519:**

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

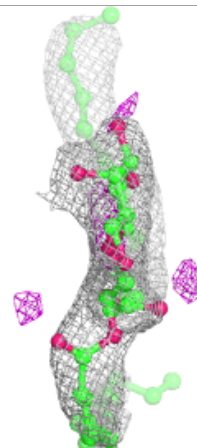
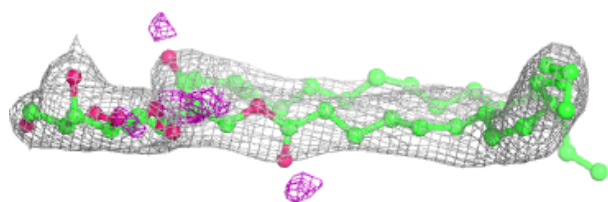
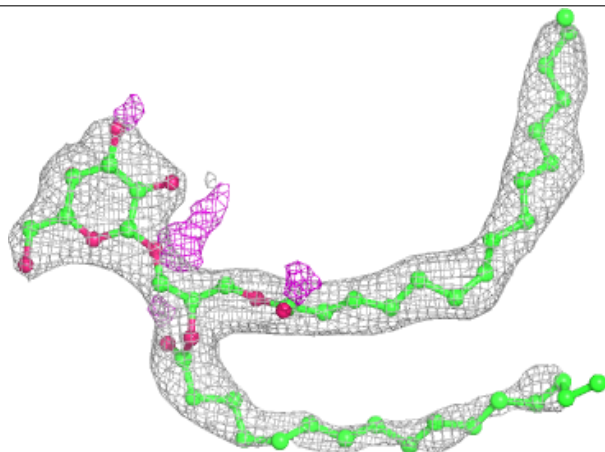


**Electron density around HTG b 625:**

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

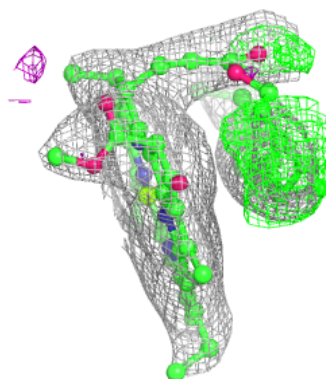
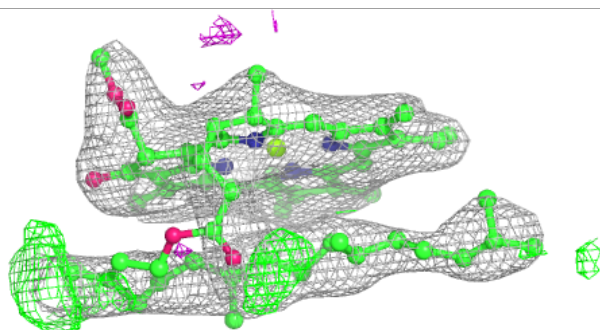
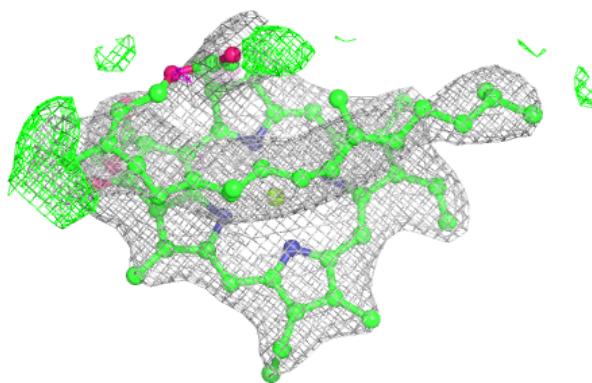
**Electron density around LMG C 520:**

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

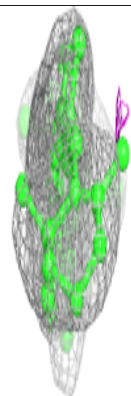
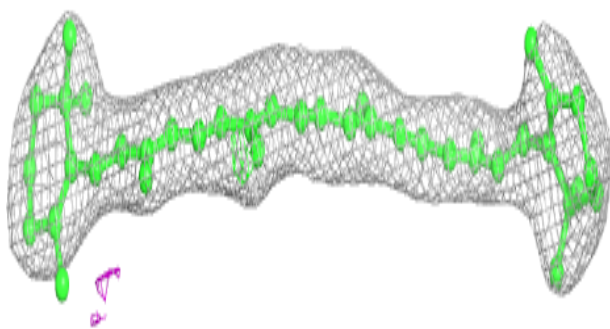
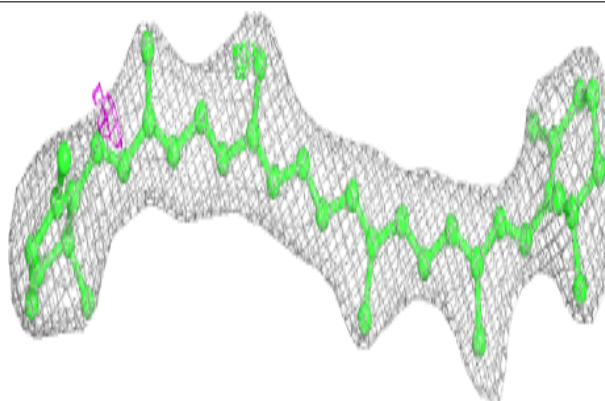


**Electron density around CLA B 601:**

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

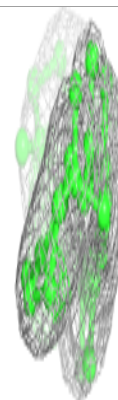
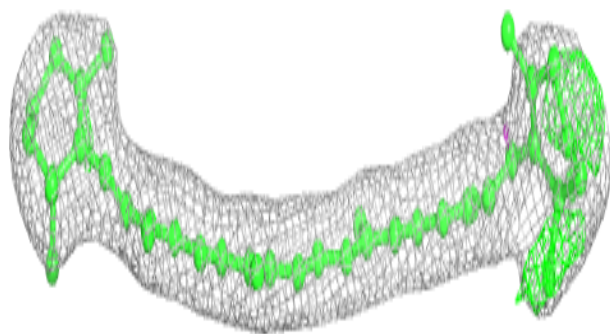
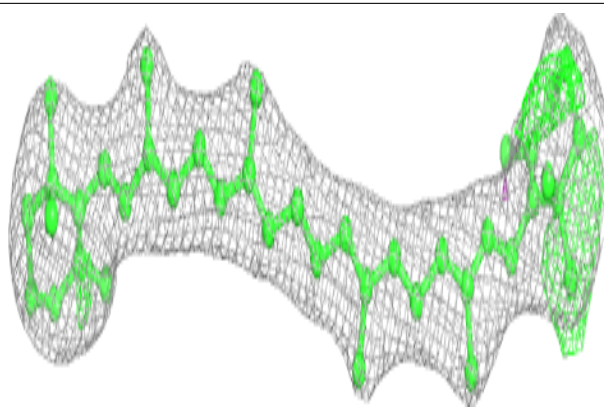
**Electron density around BCR Y 101:**

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

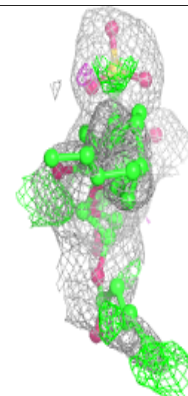
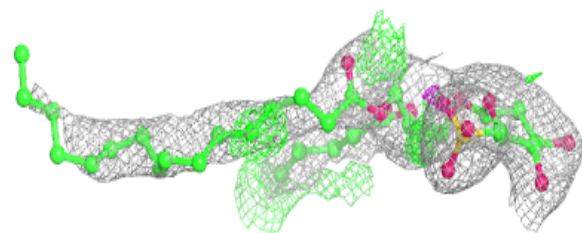
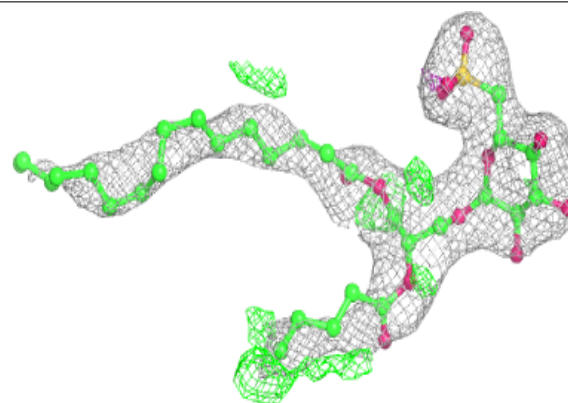


**Electron density around BCR d 405:**

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

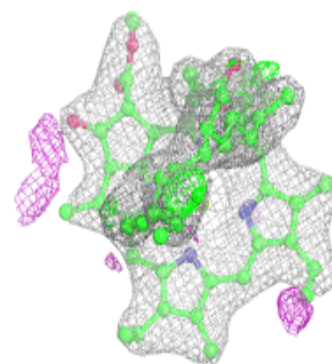
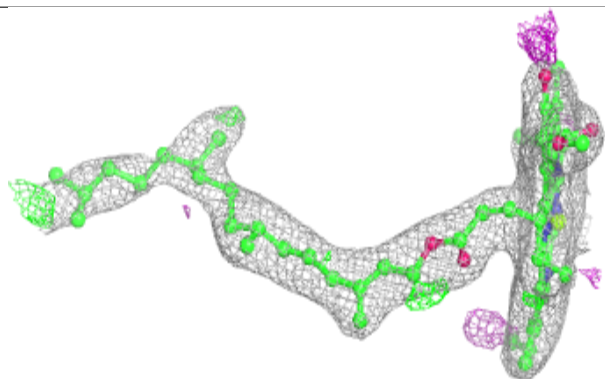
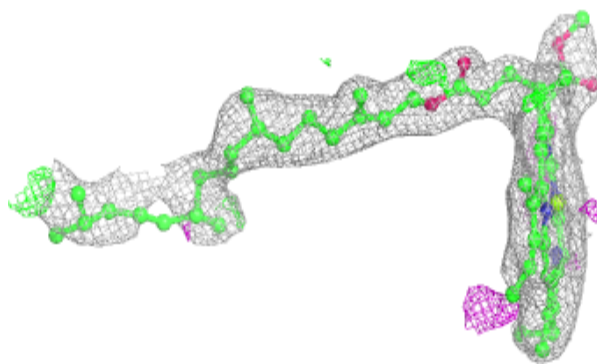
**Electron density around SQD F 102:**

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

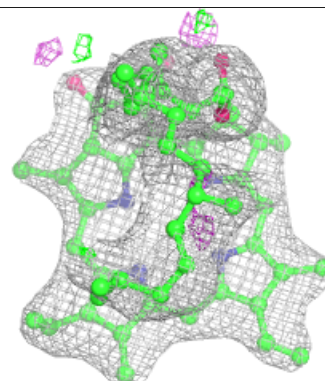
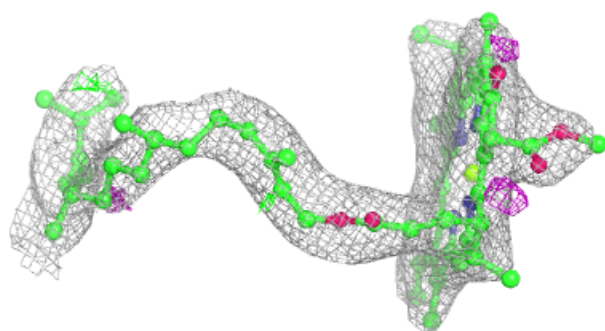
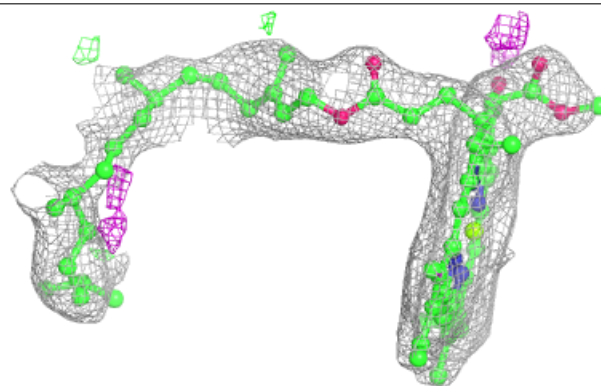


**Electron density around CLA B 606:**

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

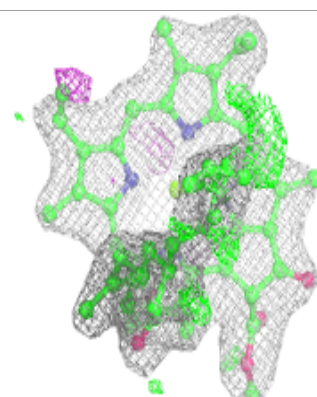
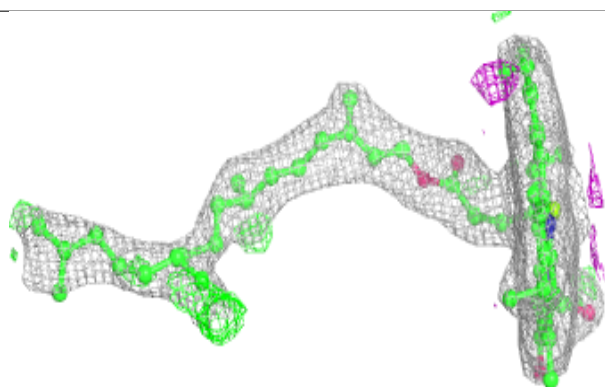
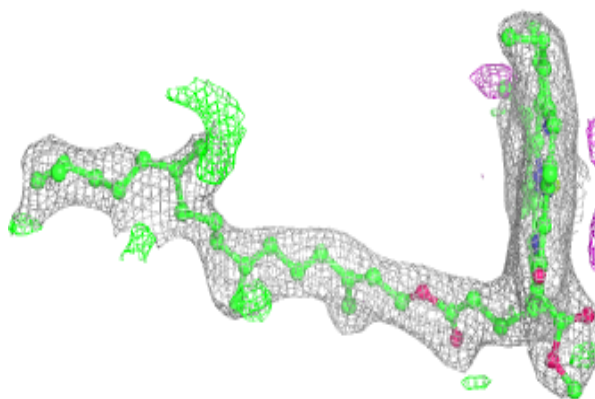
**Electron density around CLA C 507:**

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

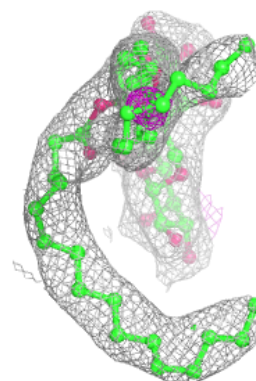
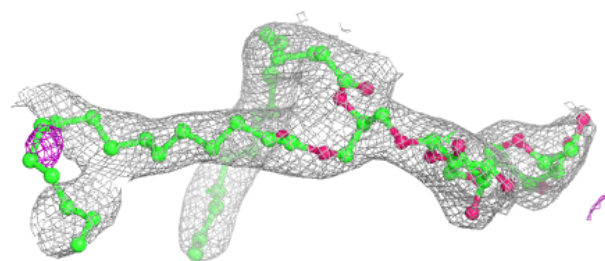
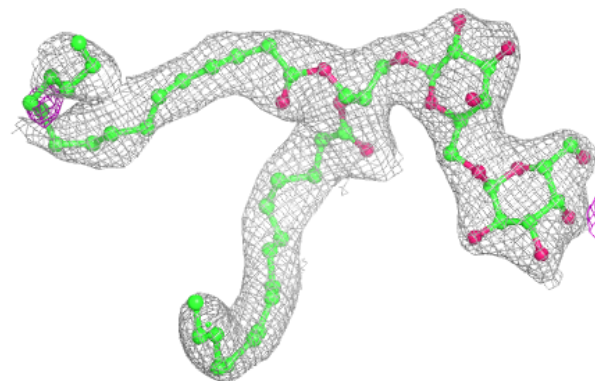


**Electron density around CLA b 606:**

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

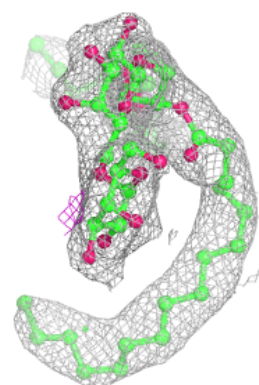
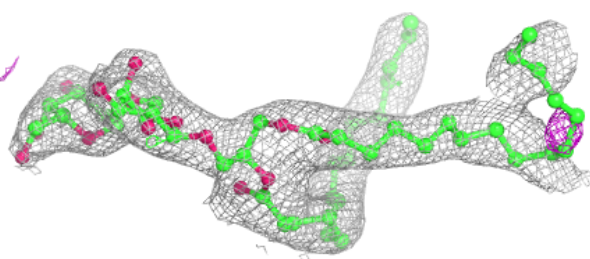
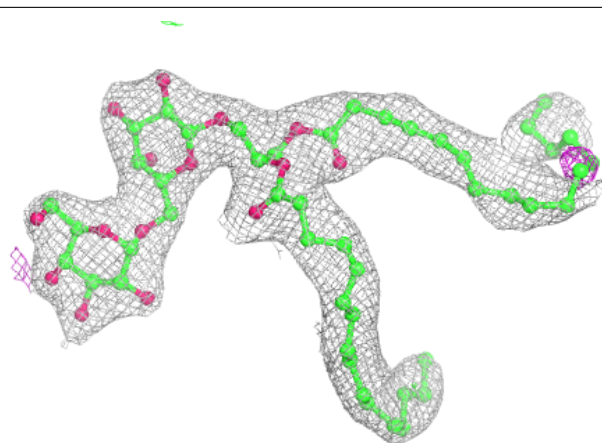
**Electron density around DGD c 517 (A):**

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

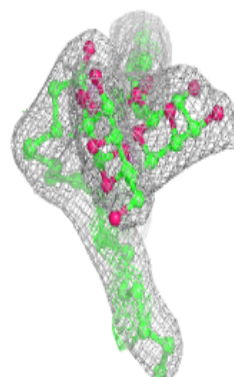
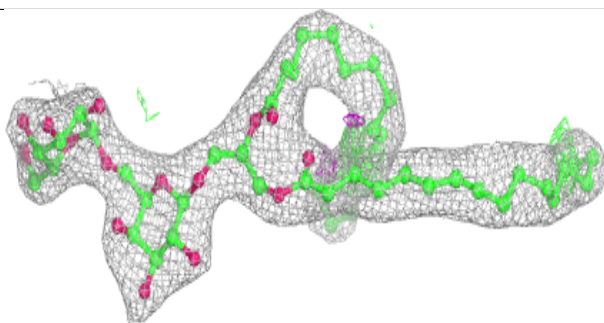
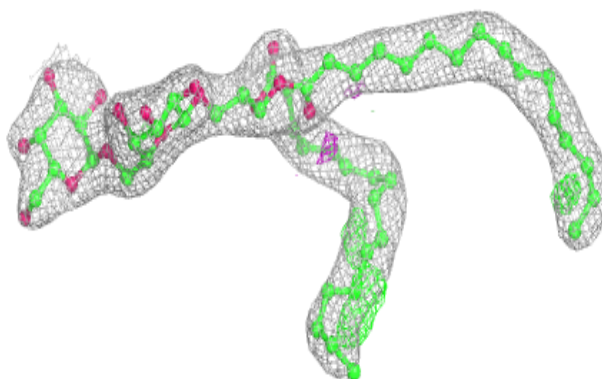


**Electron density around DGD c 517 (B):**

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

**Electron density around DGD h 102:**

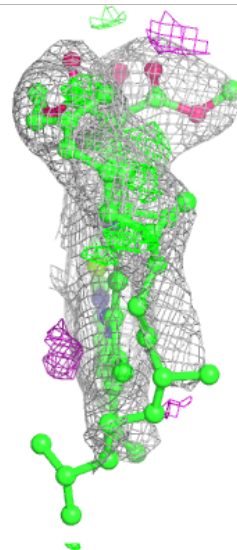
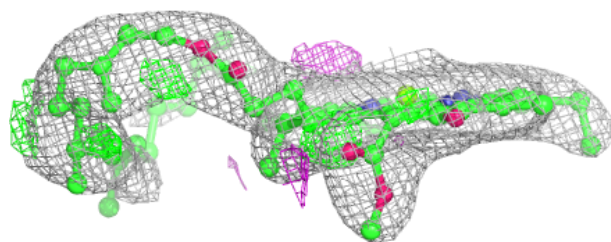
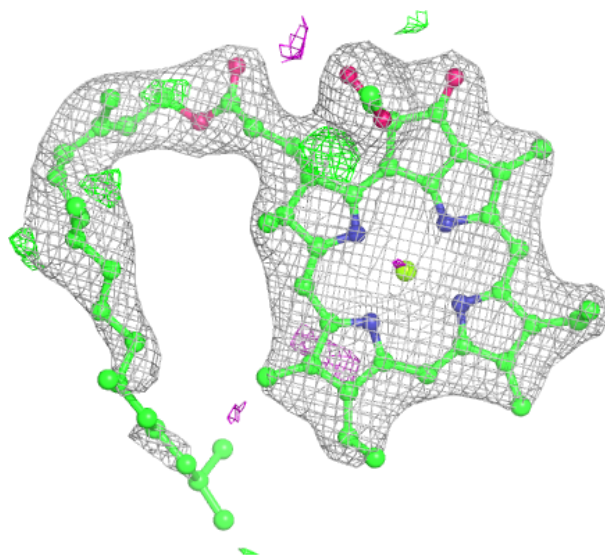
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





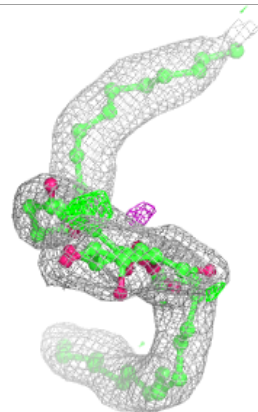
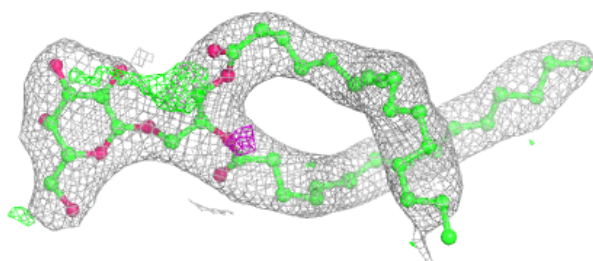
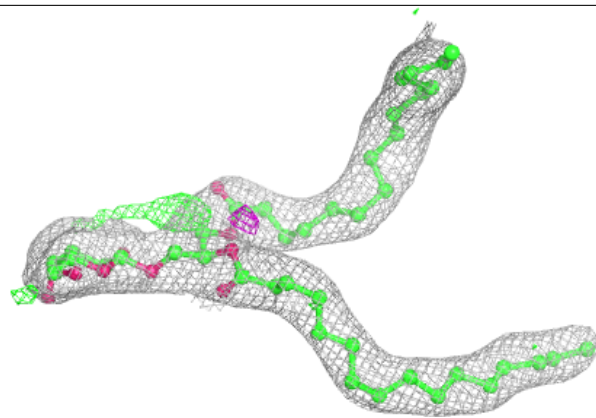
**Electron density around CLA C 513:**

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

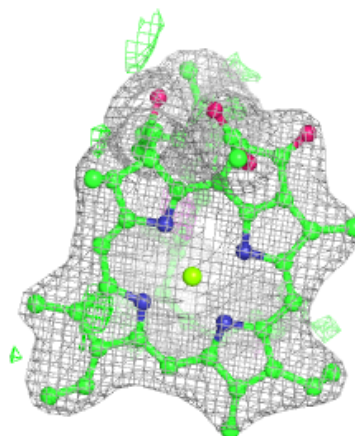
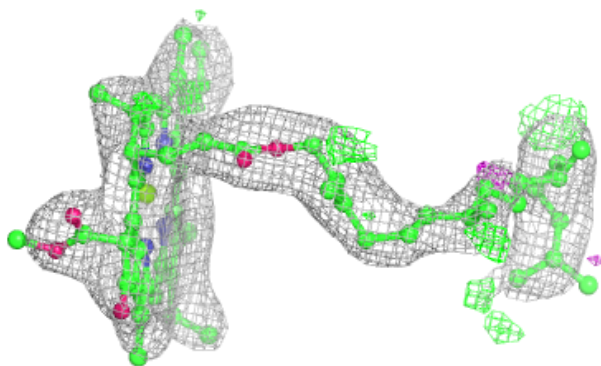
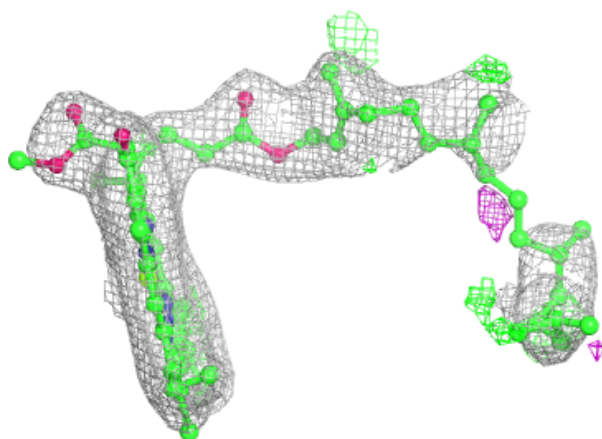


**Electron density around LMG B 621:**

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

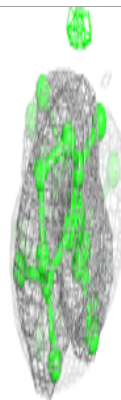
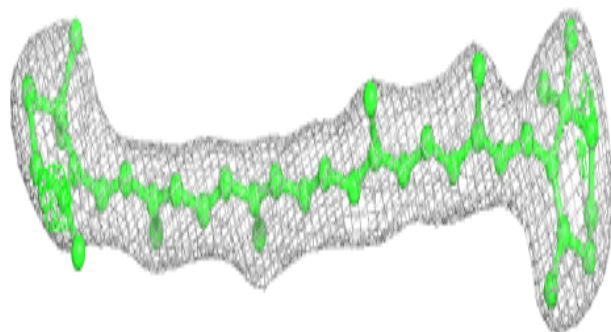
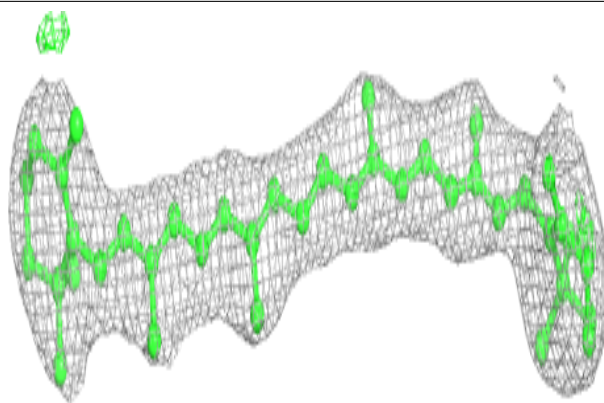
**Electron density around CLA c 506:**

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

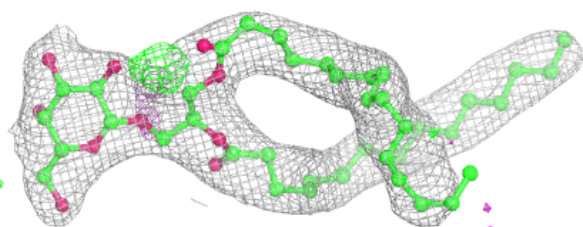
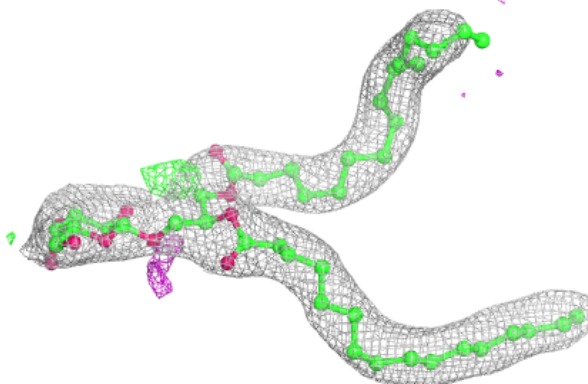


**Electron density around BCR c 514:**

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

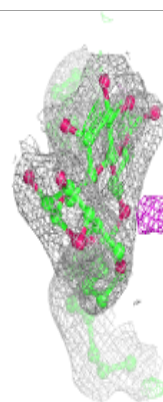
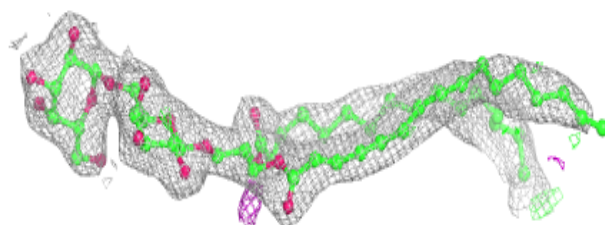
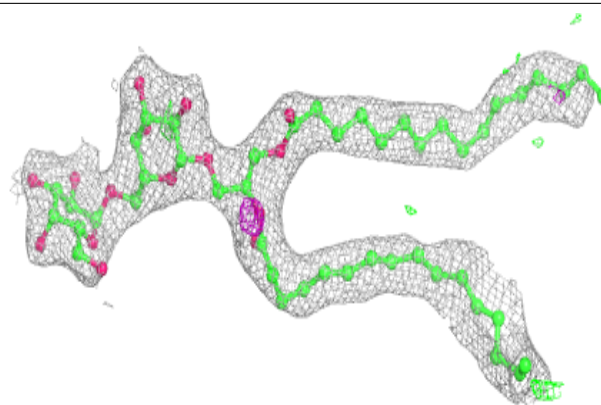
**Electron density around LMG m 101:**

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

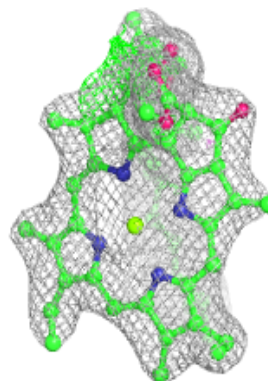
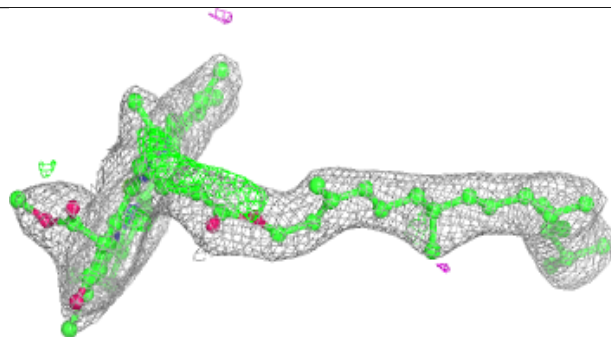
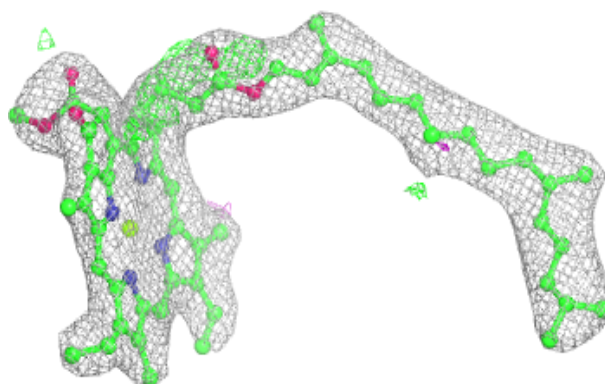


**Electron density around DGD c 518:**

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

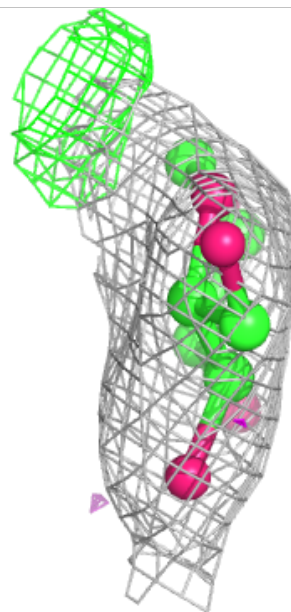
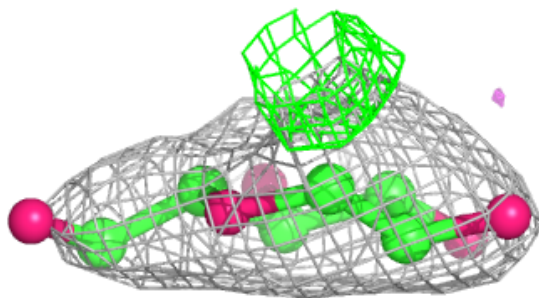
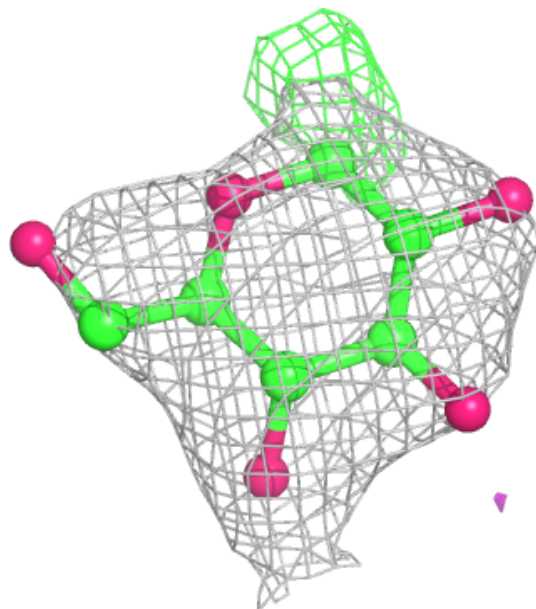
**Electron density around CLA B 609:**

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



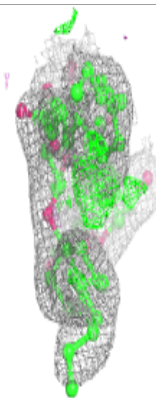
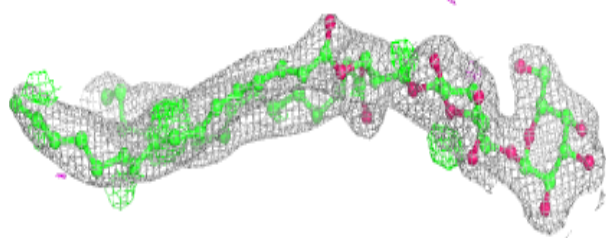
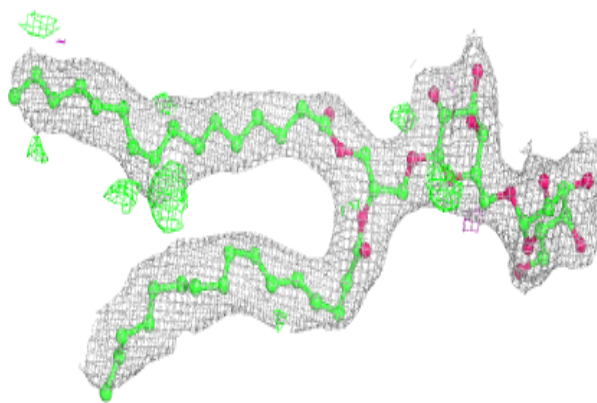
**Electron density around HTG V 202:**

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

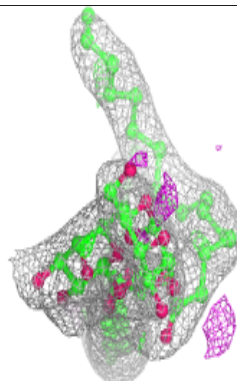
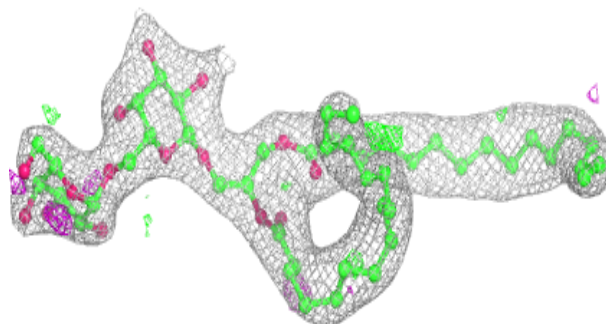
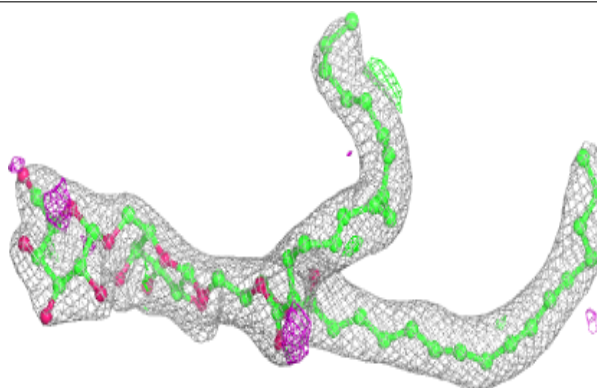


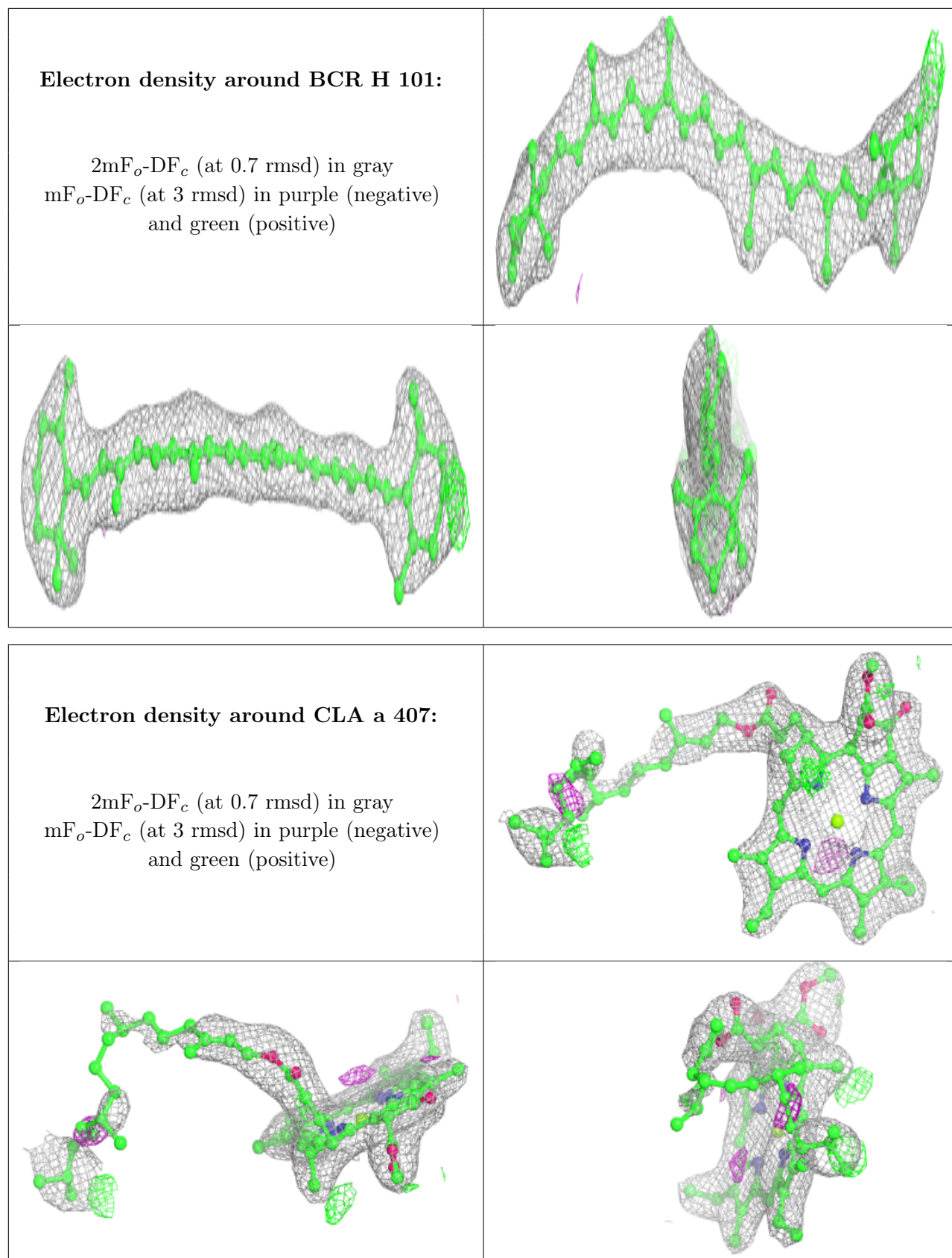
**Electron density around DGD C 519:**

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

**Electron density around DGD H 102:**

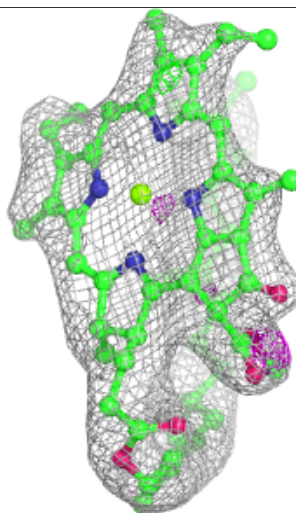
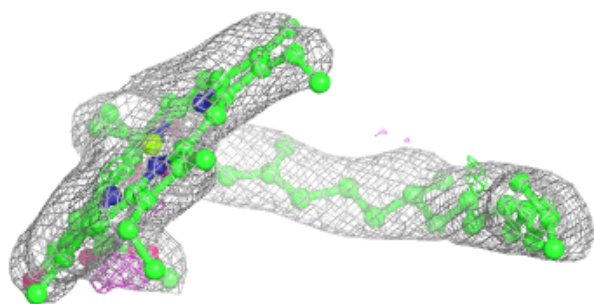
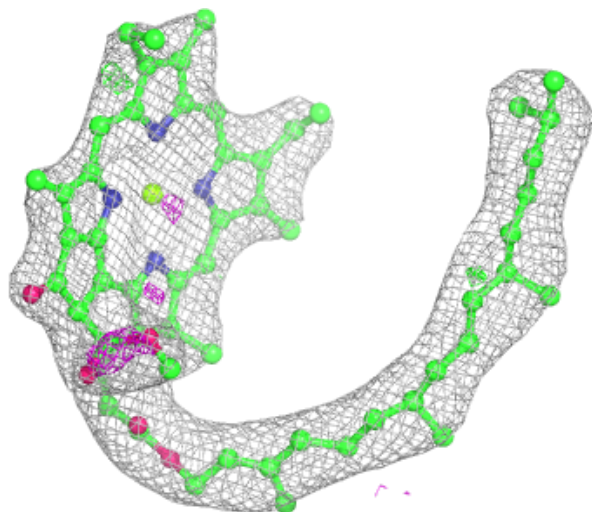
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA c 507:**

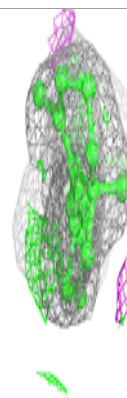
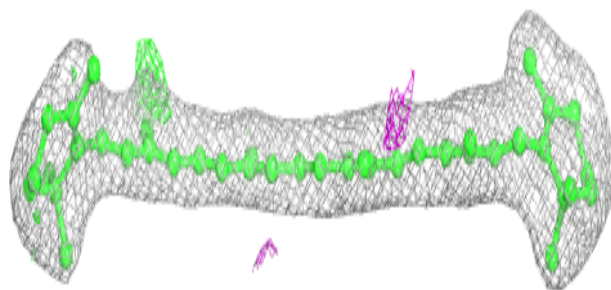
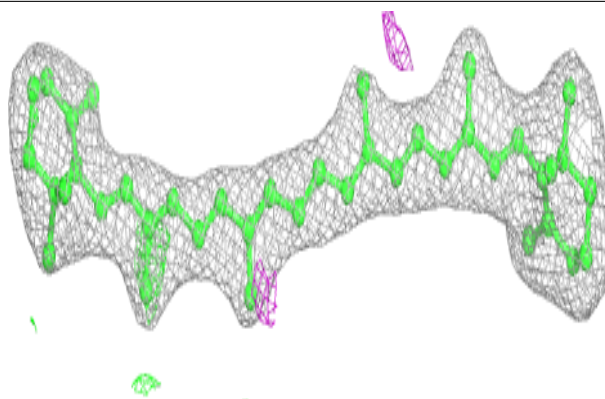
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



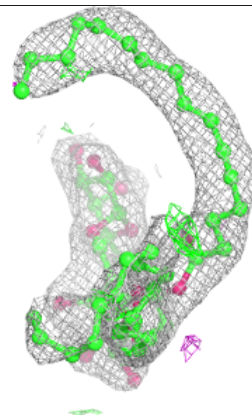
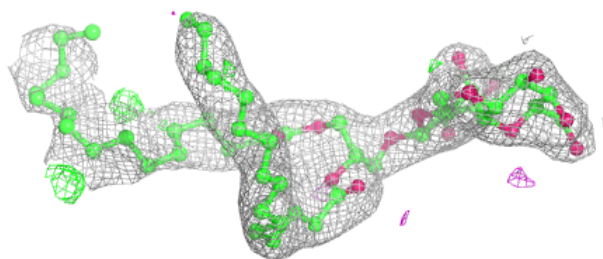
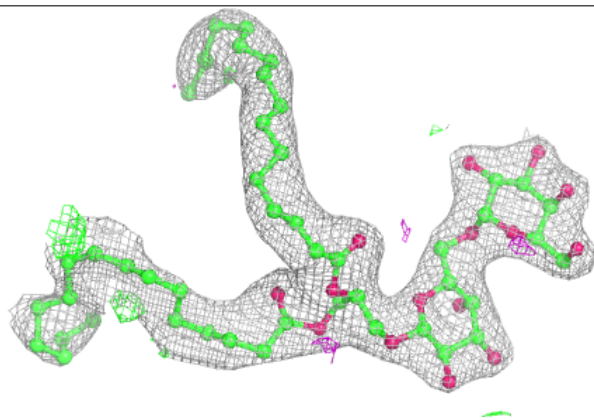


**Electron density around BCR b 618:**

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

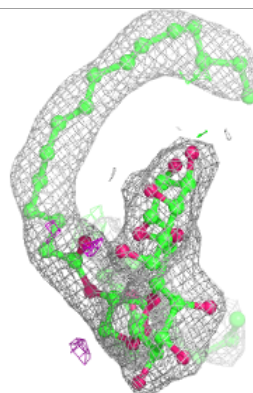
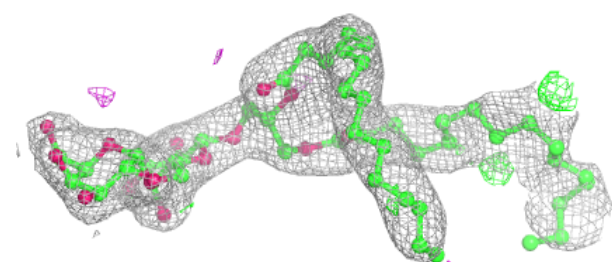
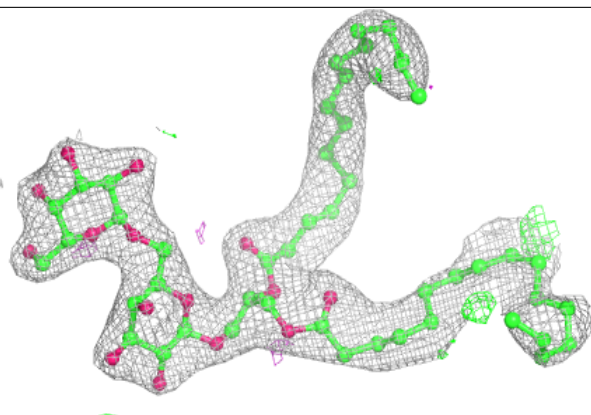
**Electron density around DGD C 518 (A):**

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

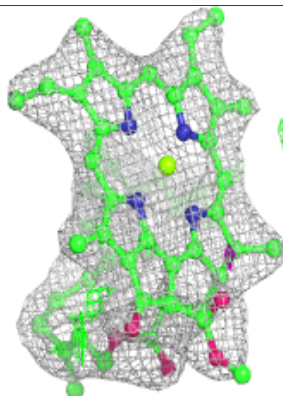
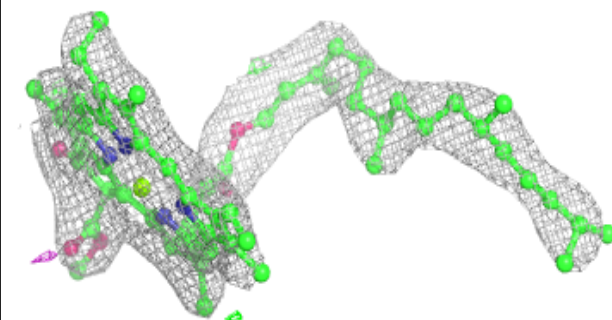
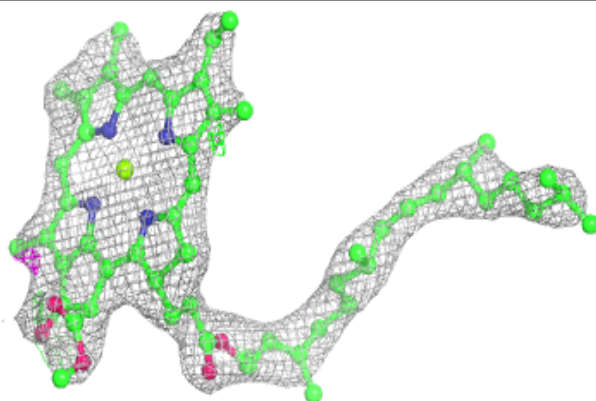


**Electron density around DGD C 518 (B):**

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

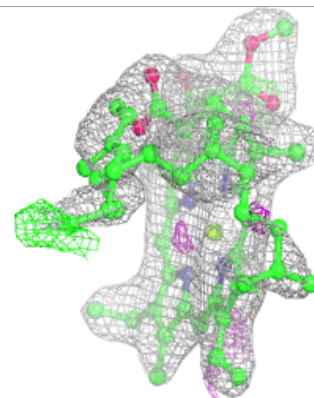
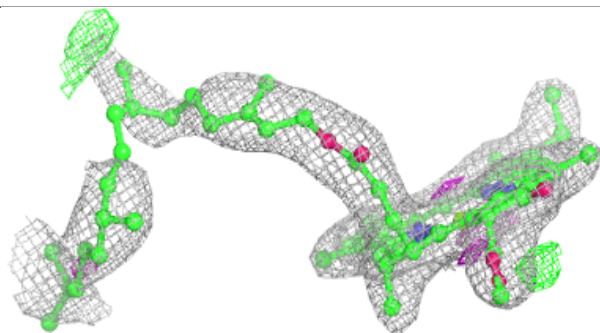
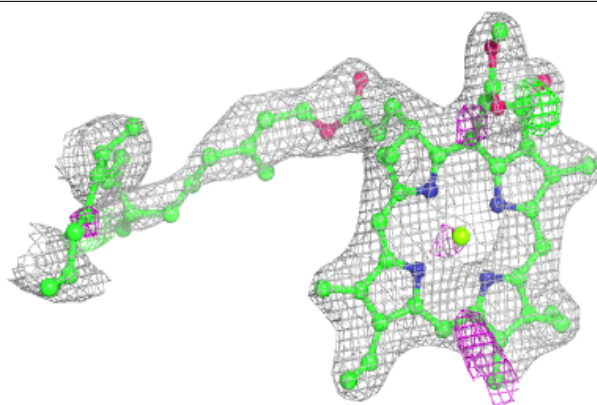
**Electron density around CLA c 511:**

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

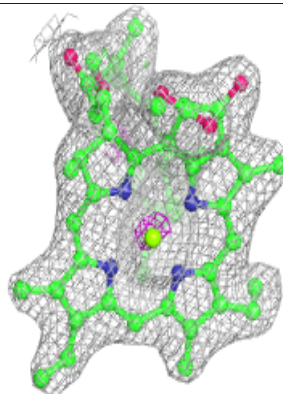
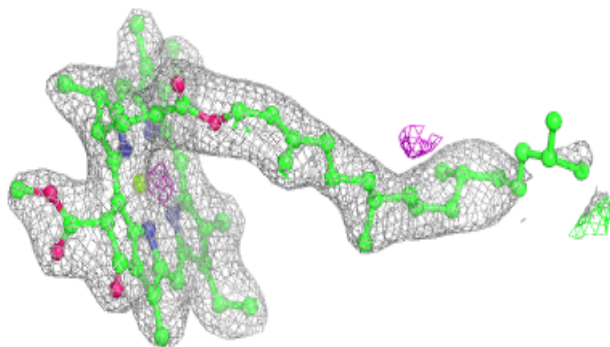
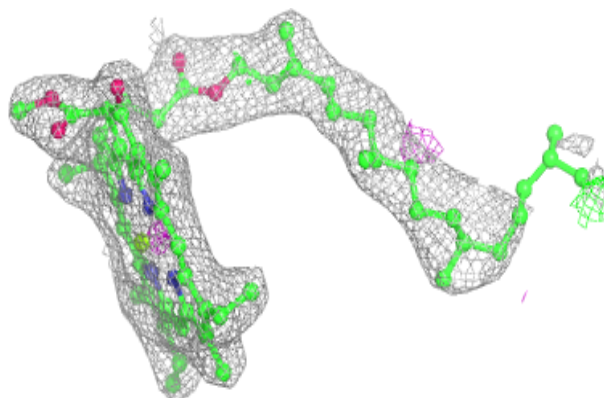


**Electron density around CLA A 408:**

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

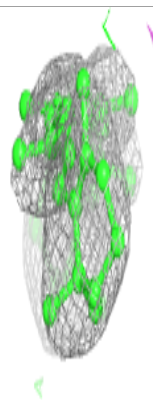
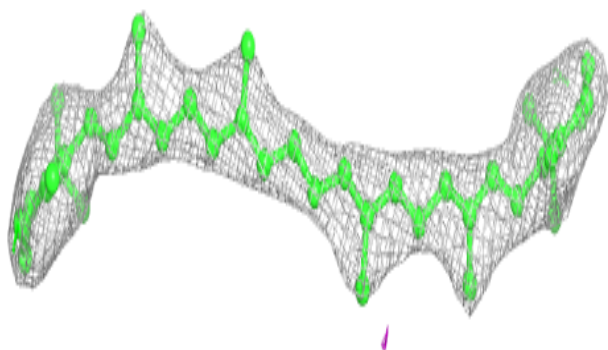
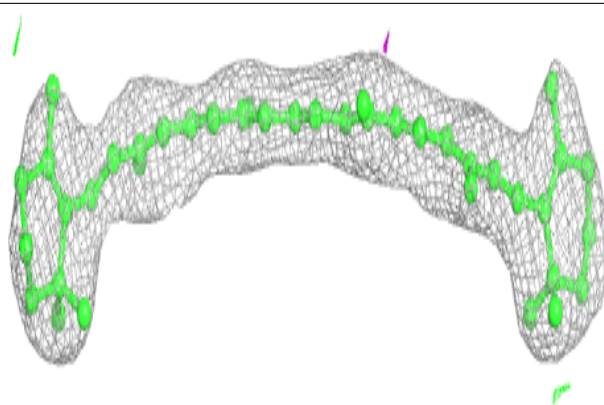
**Electron density around CLA C 509:**

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

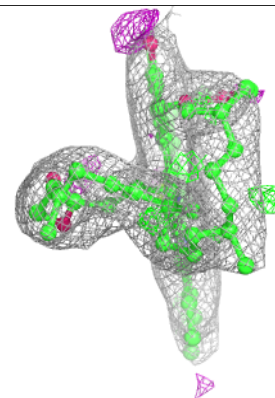
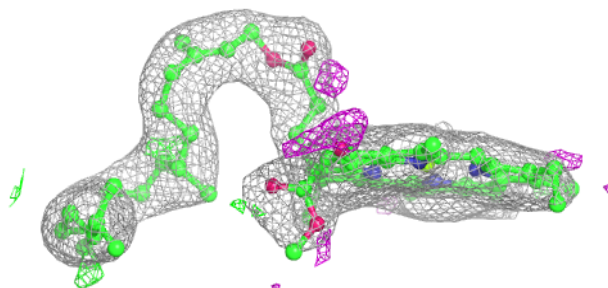
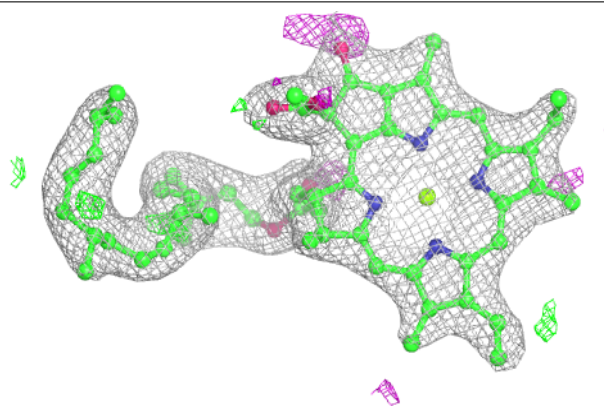


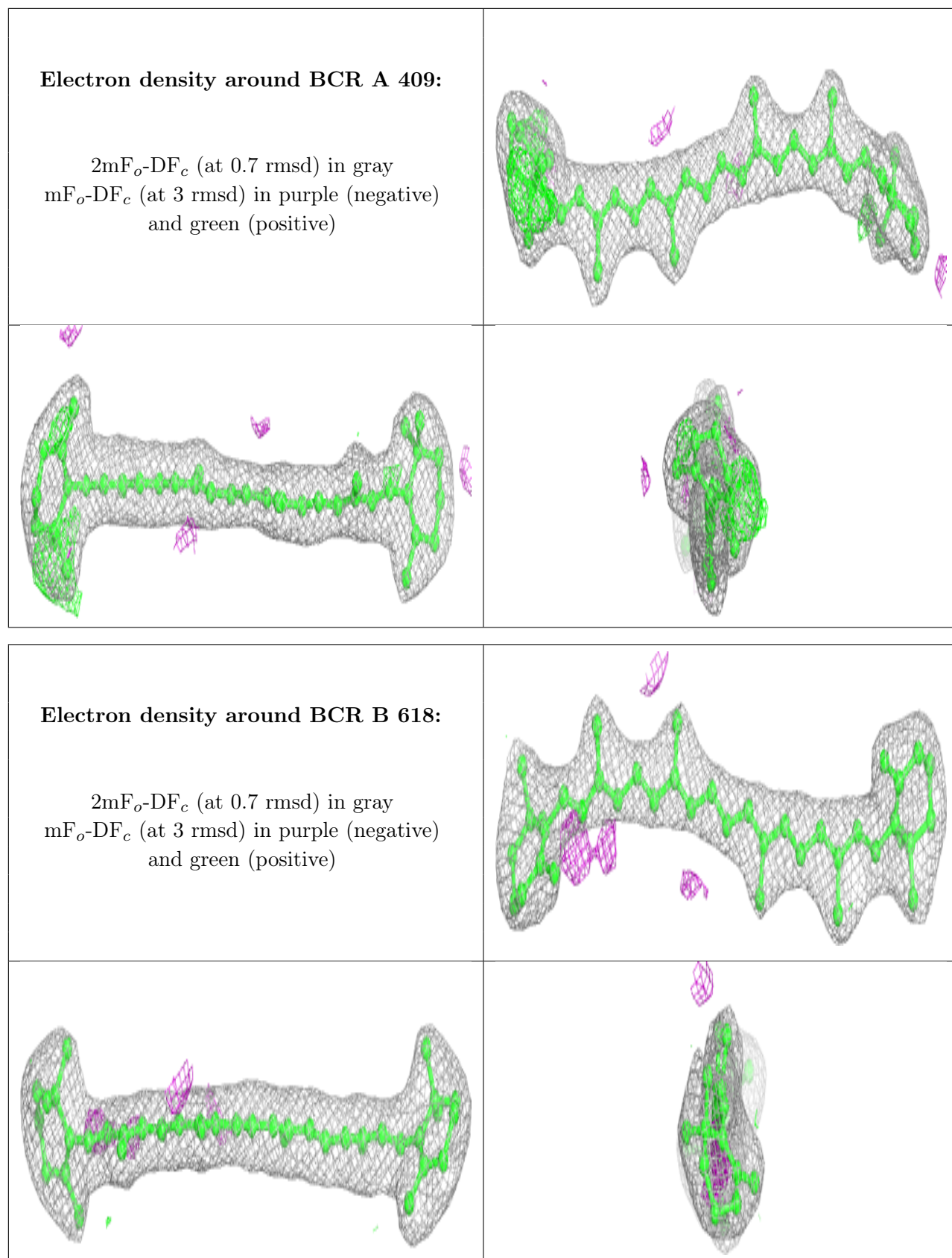
**Electron density around BCR k 101:**

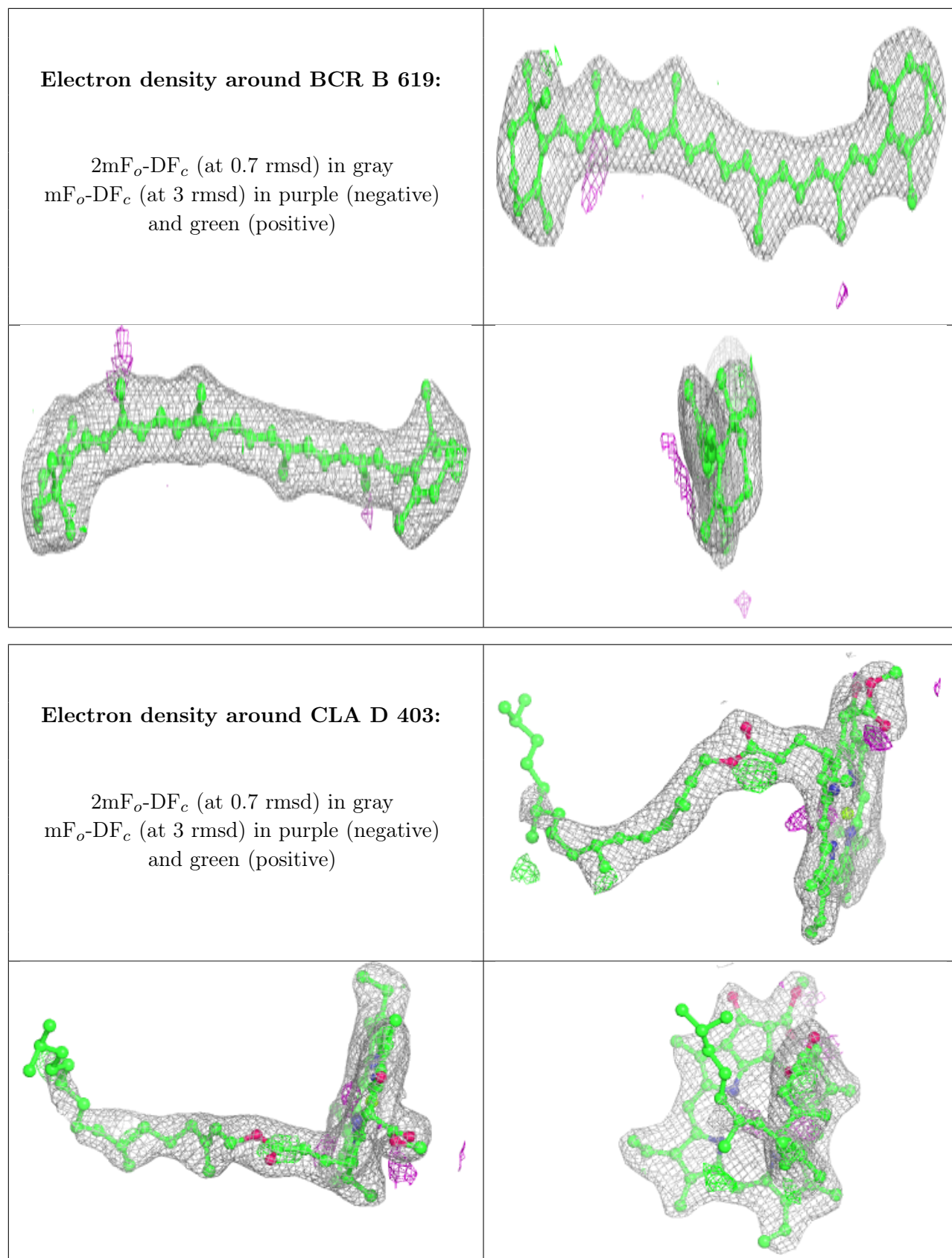
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

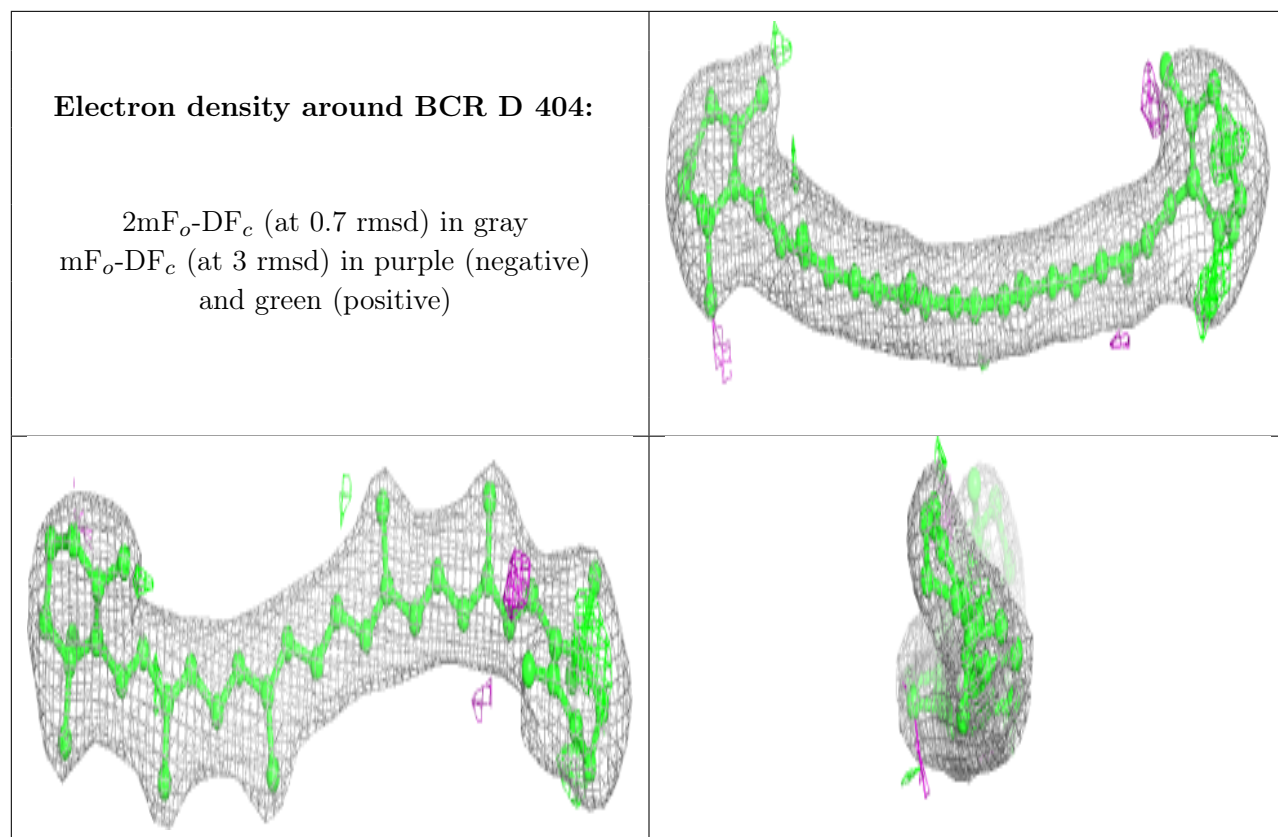
**Electron density around CLA b 612:**

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



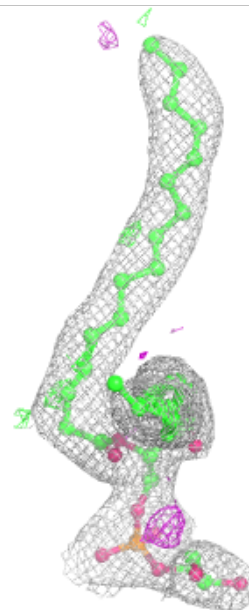
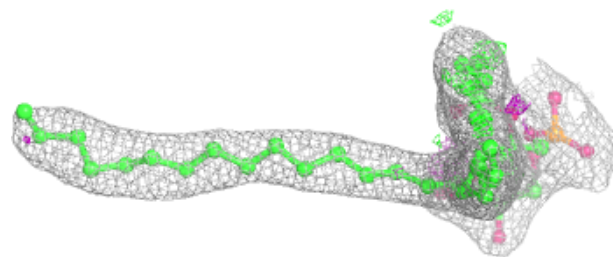
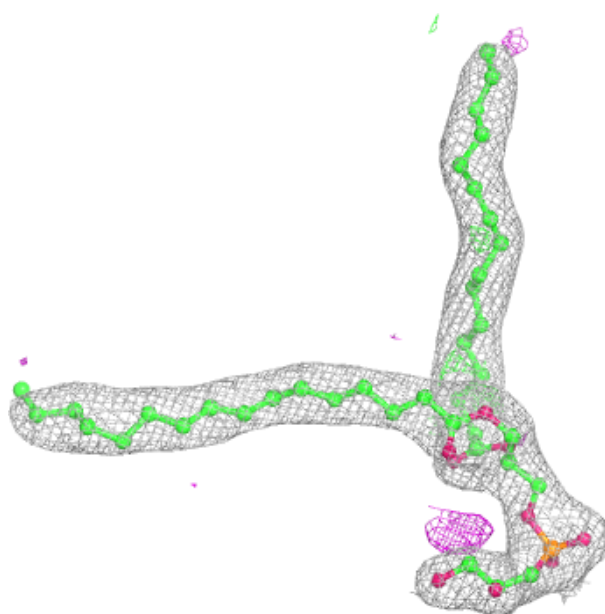






**Electron density around LHG b 629 (B):**

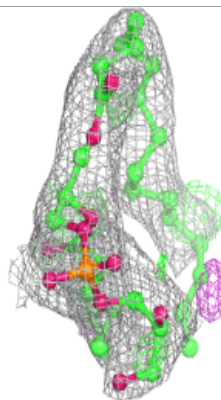
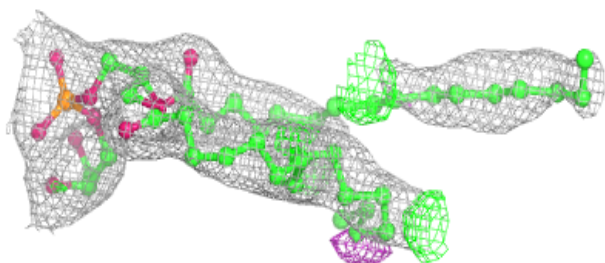
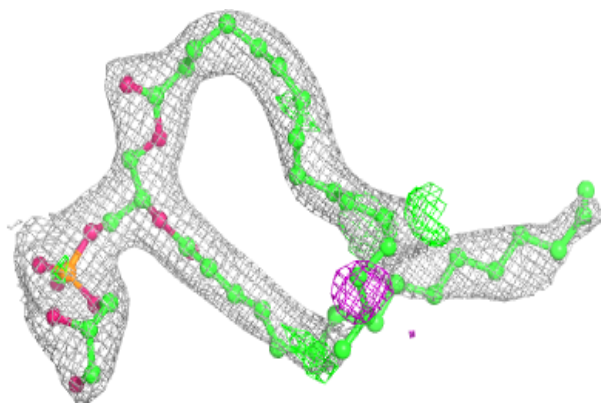
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



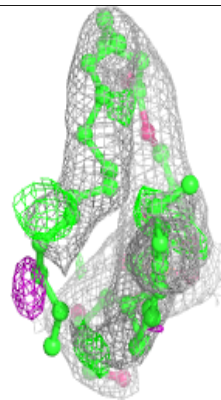
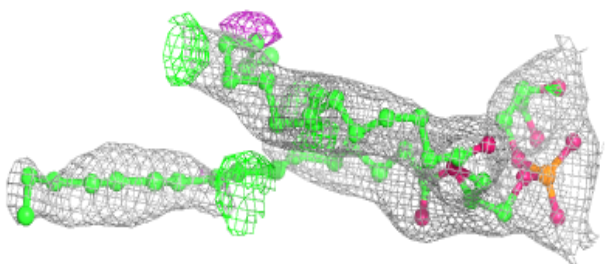
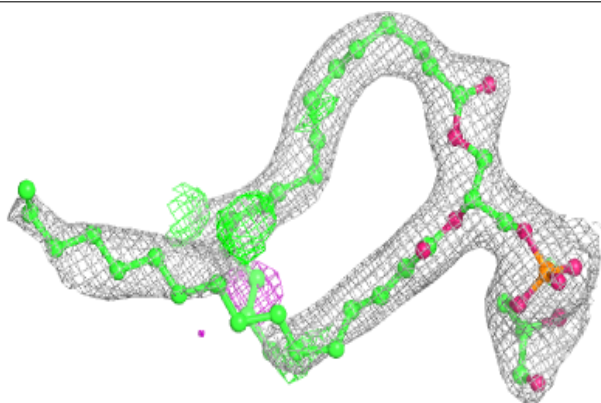


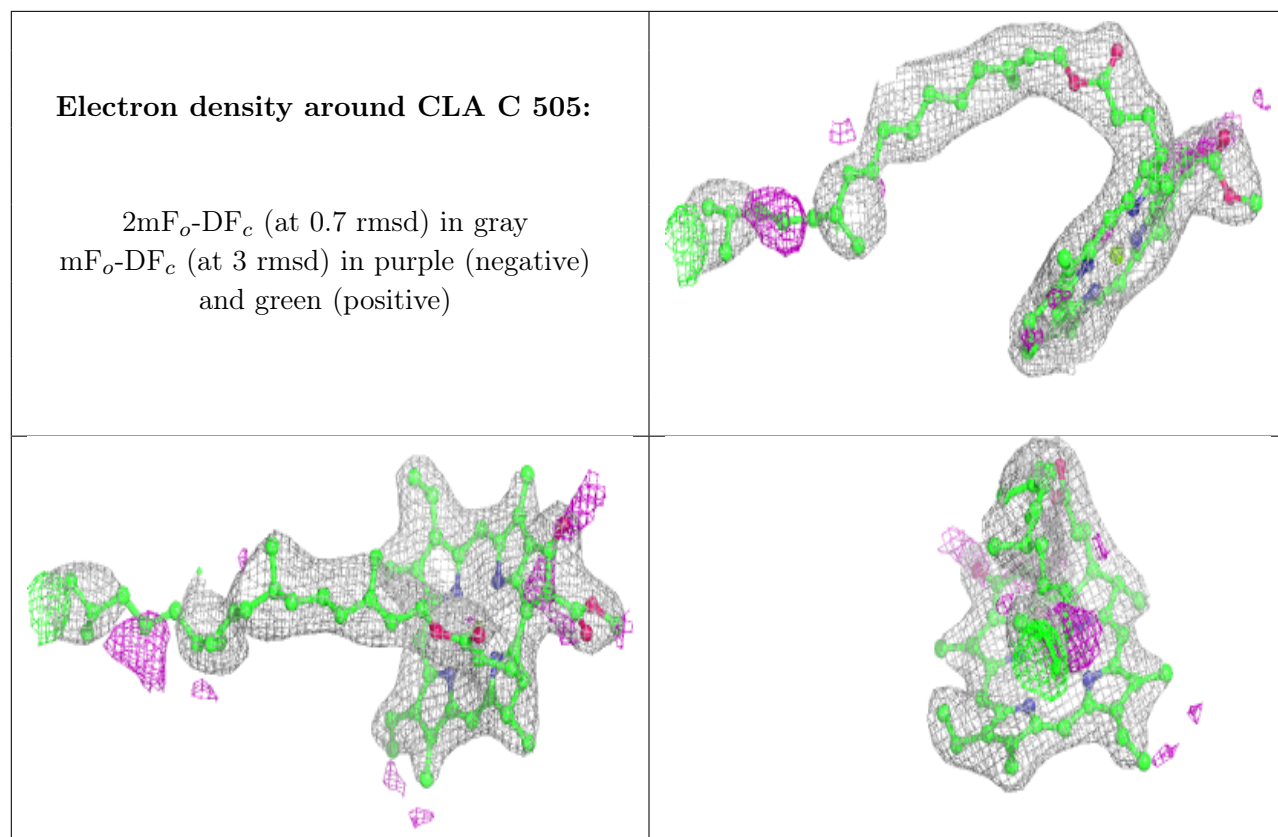
**Electron density around LHG d 408 (A):**

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

**Electron density around LHG d 408 (B):**

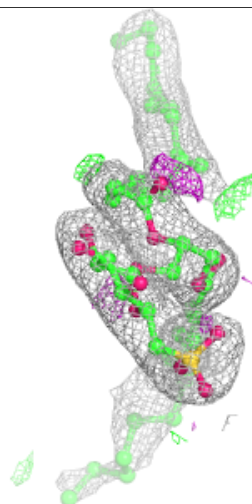
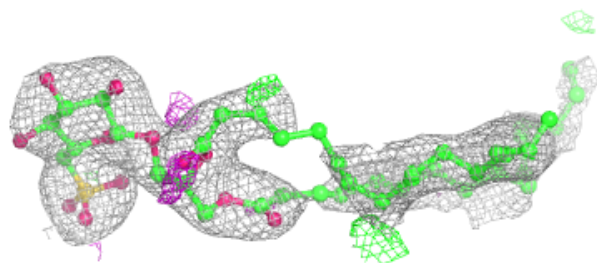
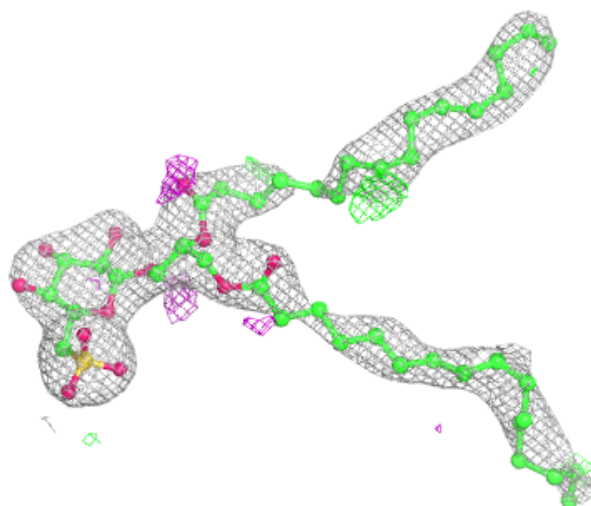
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





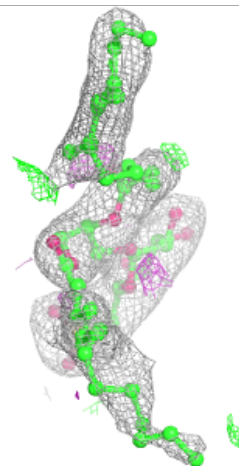
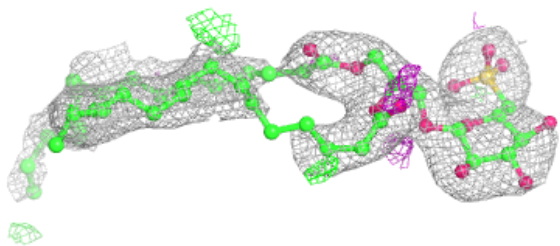
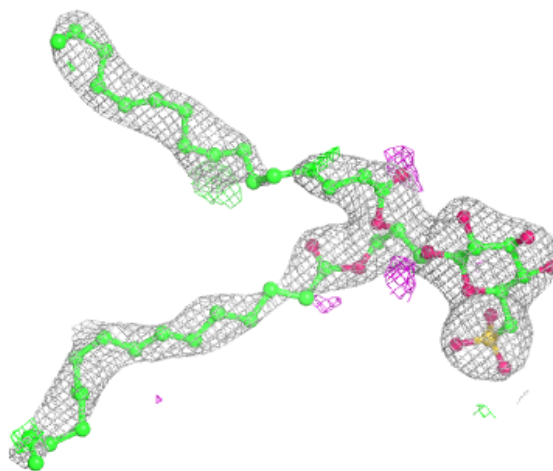
**Electron density around SQD a 409 (A):**

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



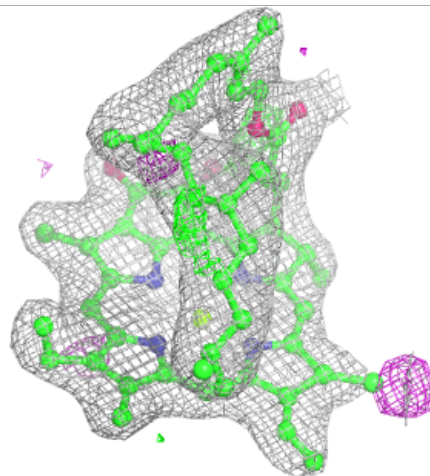
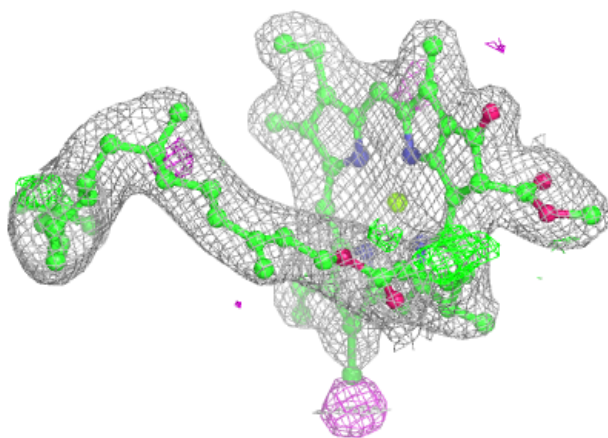
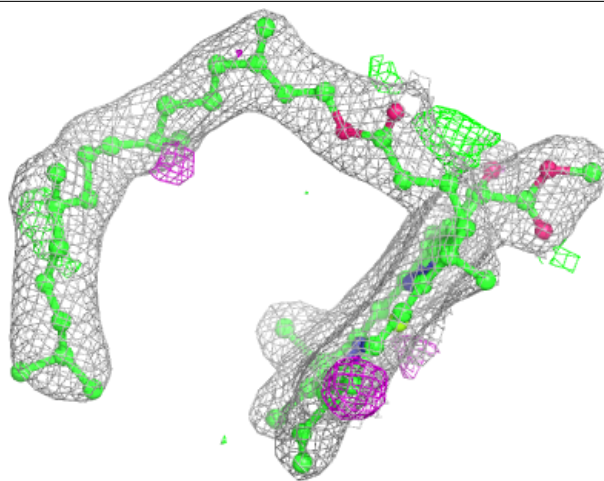
**Electron density around SQD a 409 (B):**

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



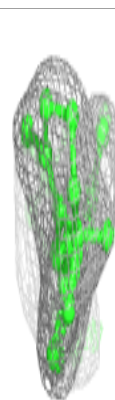
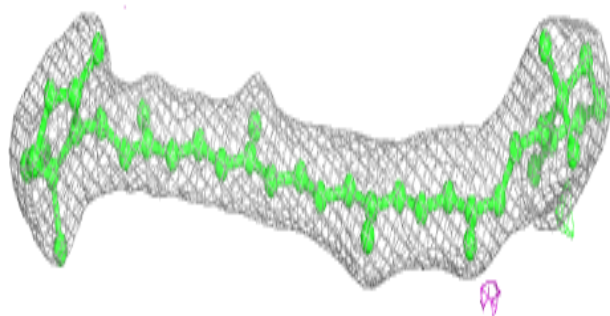
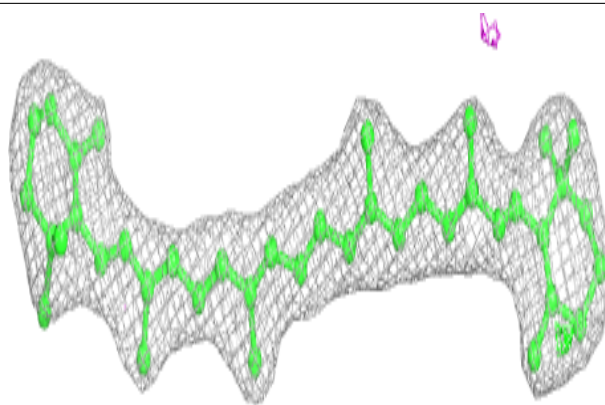
**Electron density around CLA B 611:**

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

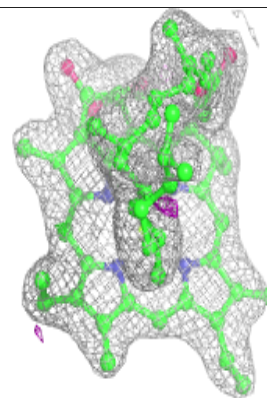
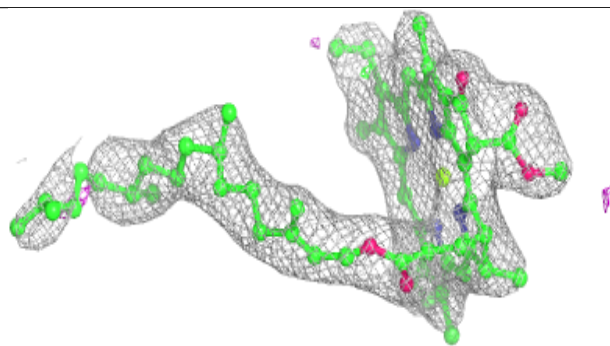
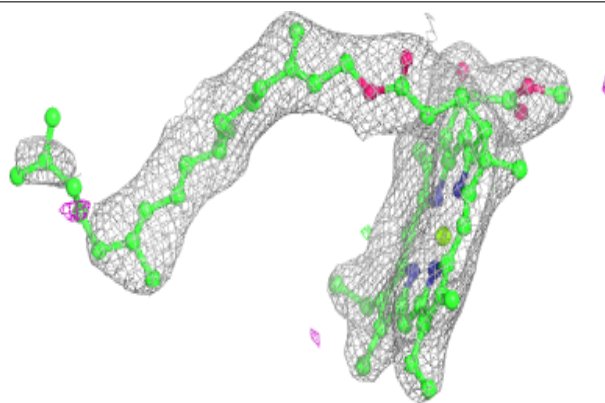


**Electron density around BCR b 619:**

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

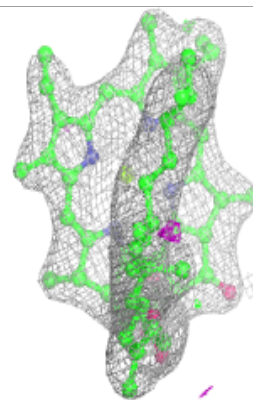
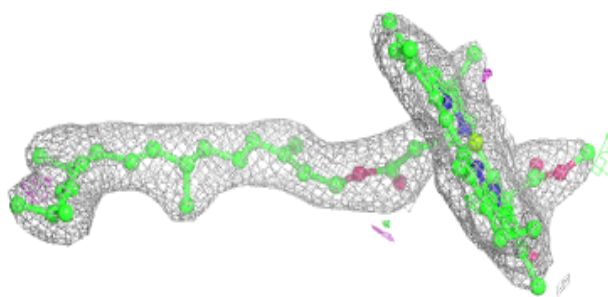
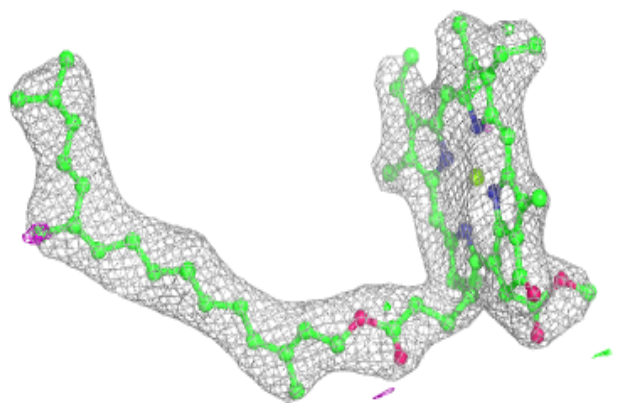
**Electron density around CLA c 508:**

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

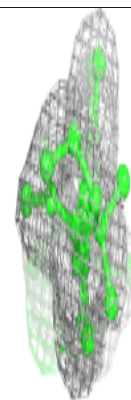
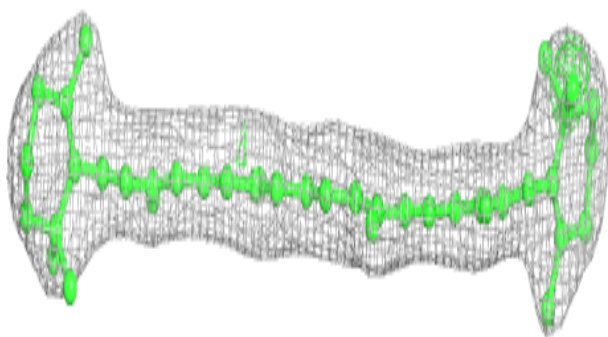
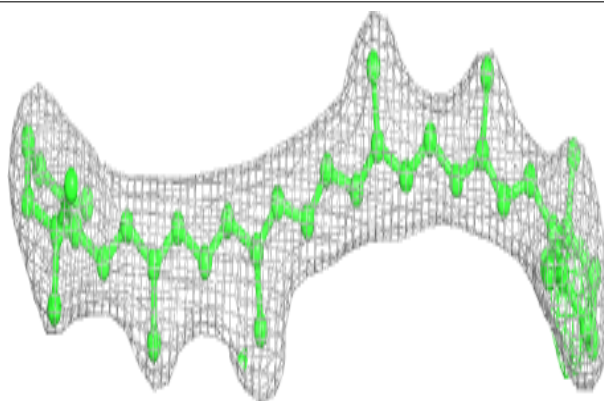


**Electron density around CLA b 609:**

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

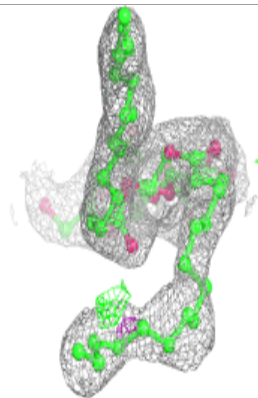
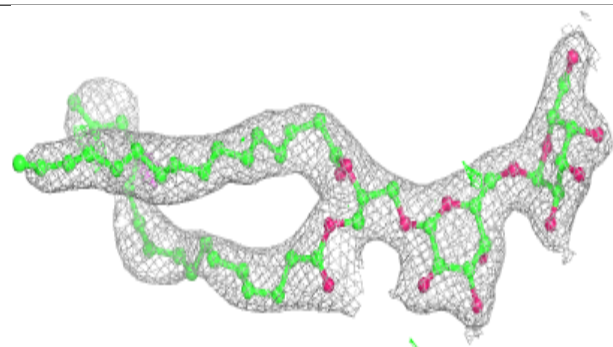
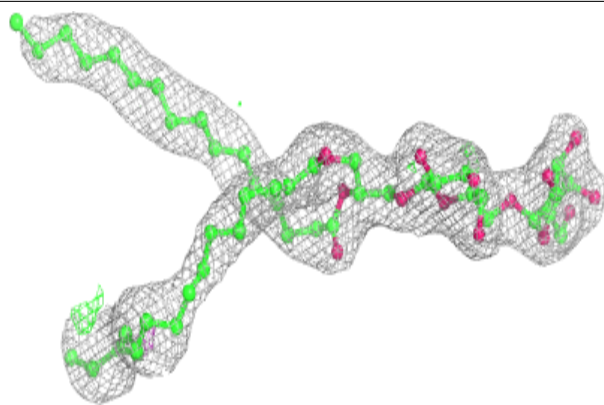
**Electron density around BCR C 516:**

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

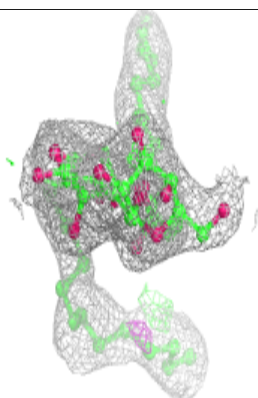
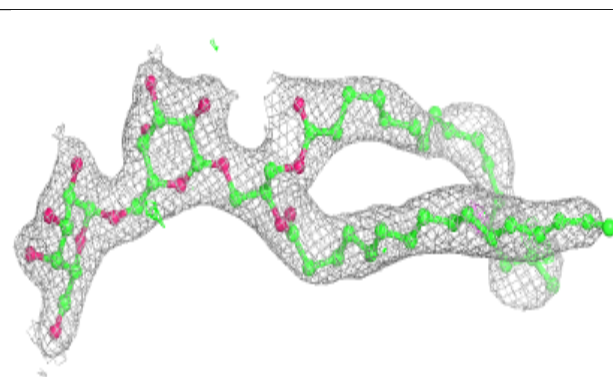
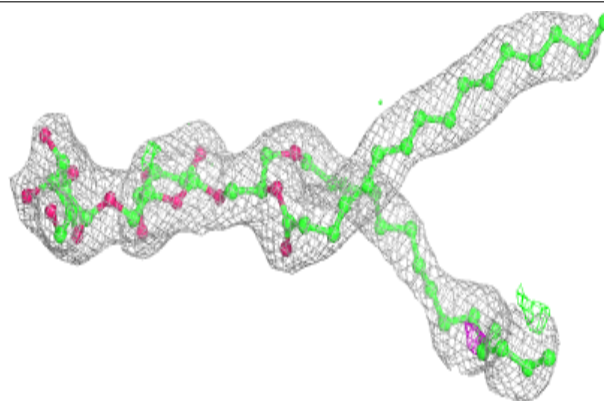


**Electron density around DGD c 516 (A):**

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

**Electron density around DGD c 516 (B):**

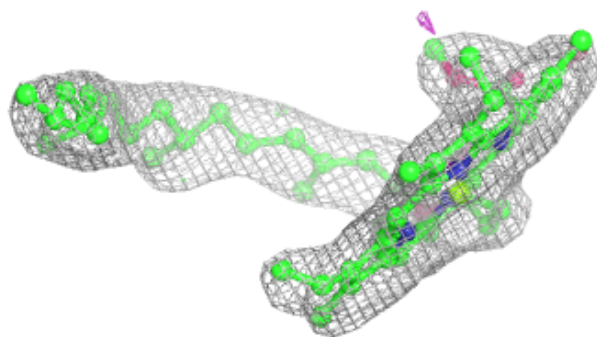
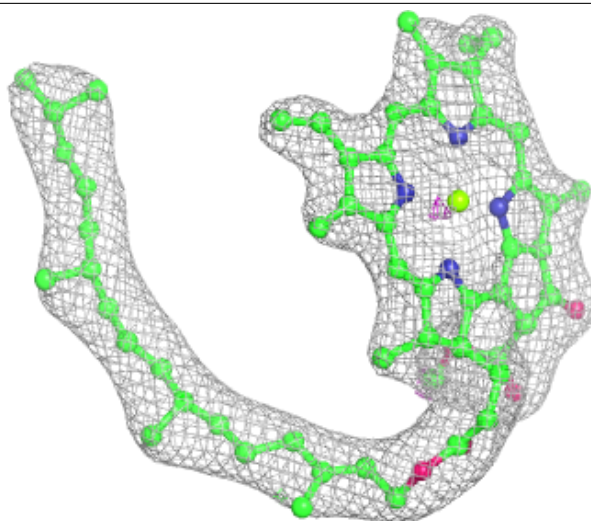
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





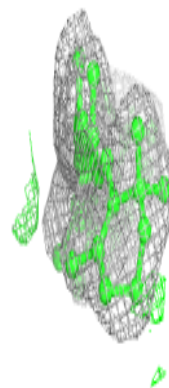
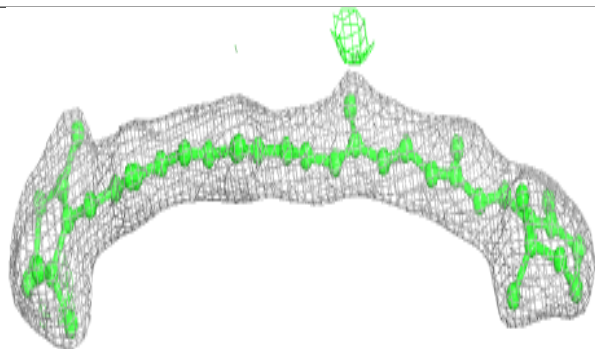
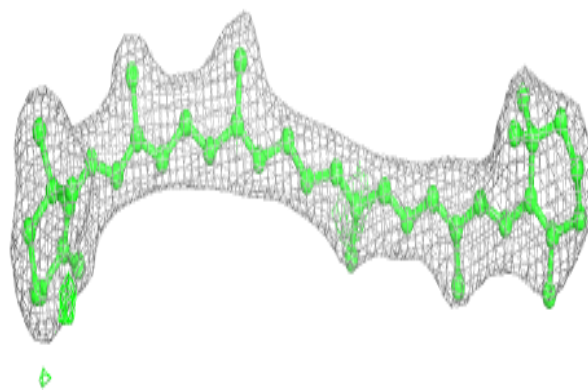
**Electron density around CLA C 508:**

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



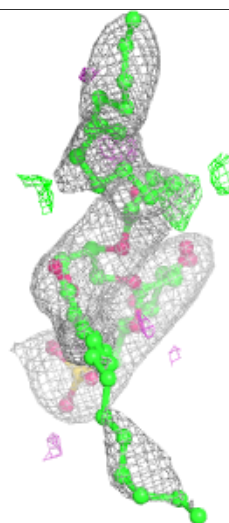
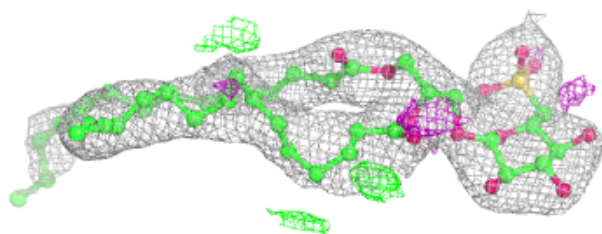
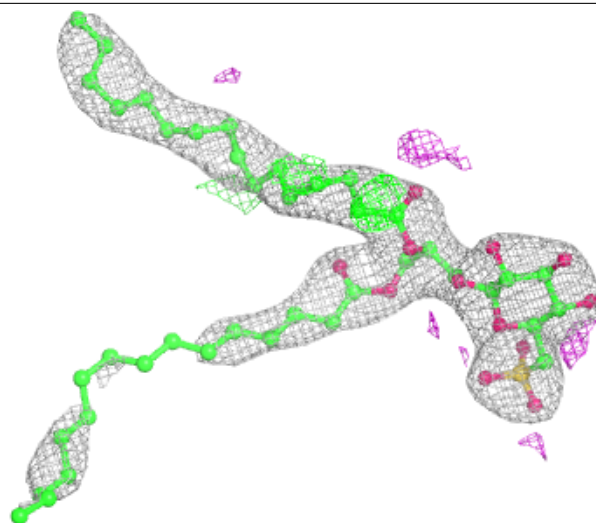
**Electron density around BCR t 102:**

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



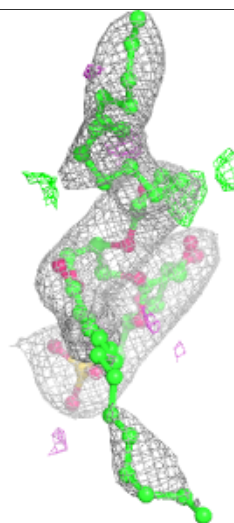
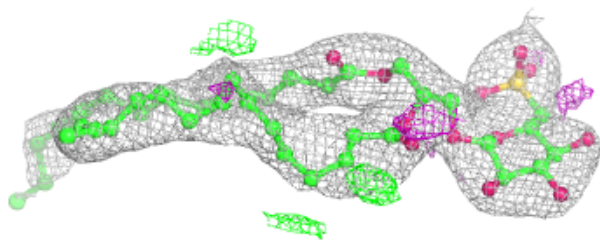
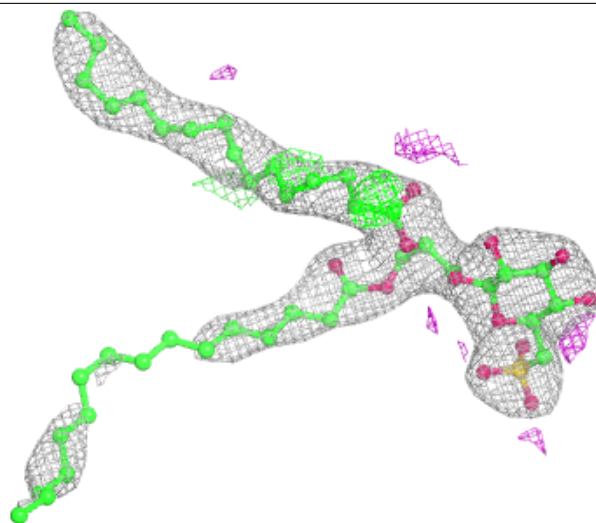
**Electron density around SQD A 410 (A):**

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



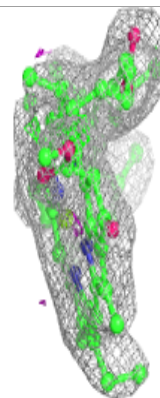
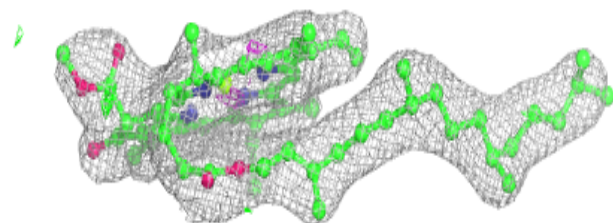
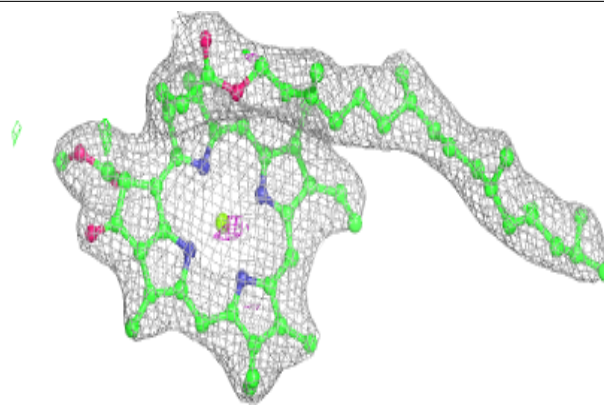
**Electron density around SQD A 410 (B):**

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

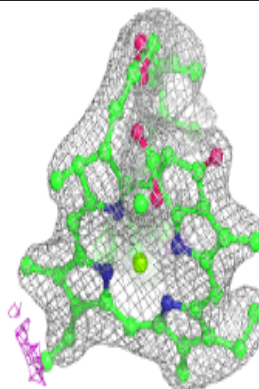
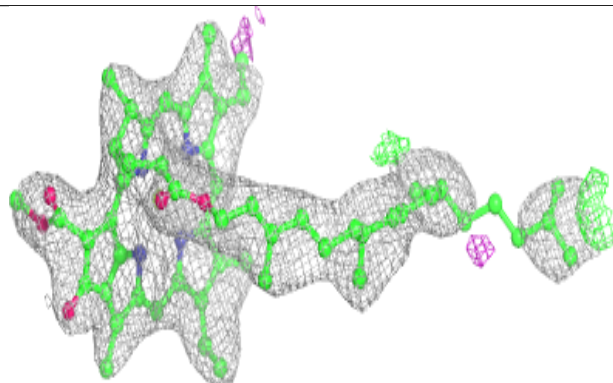
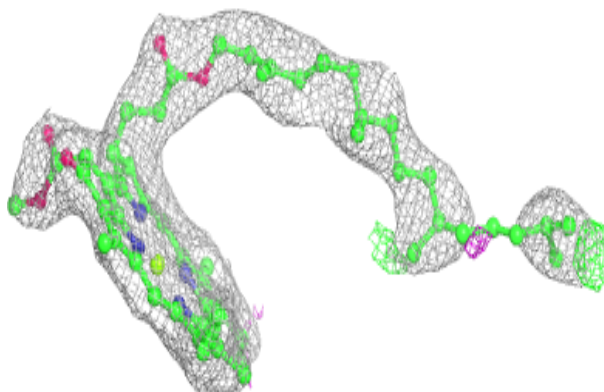


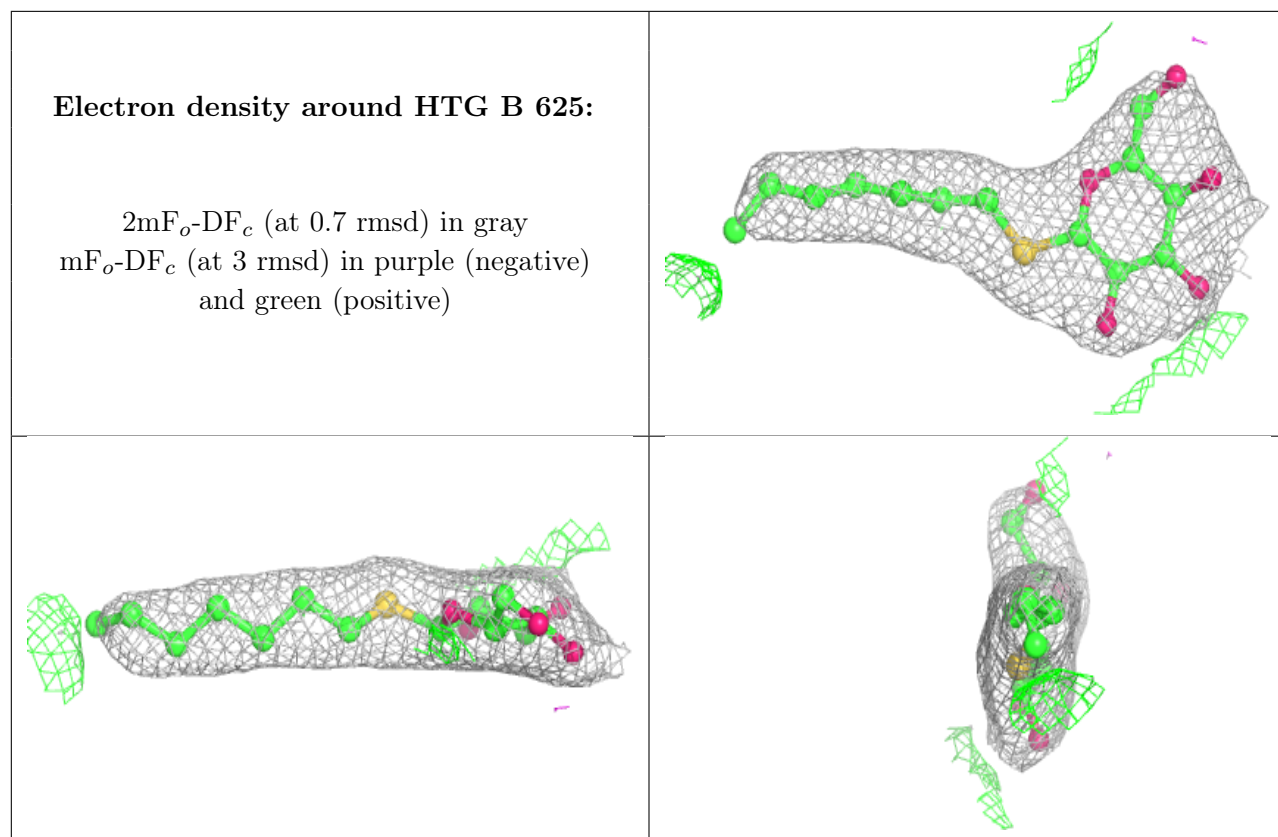
**Electron density around CLA C 502:**

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

**Electron density around CLA c 504:**

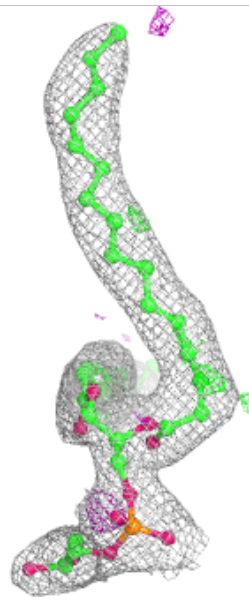
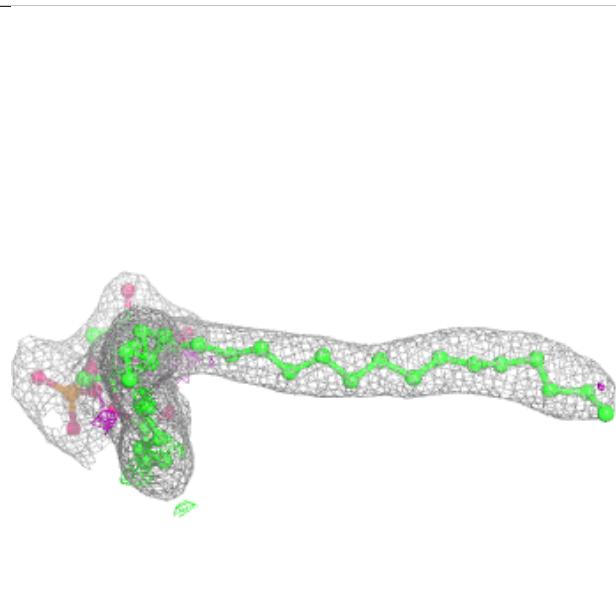
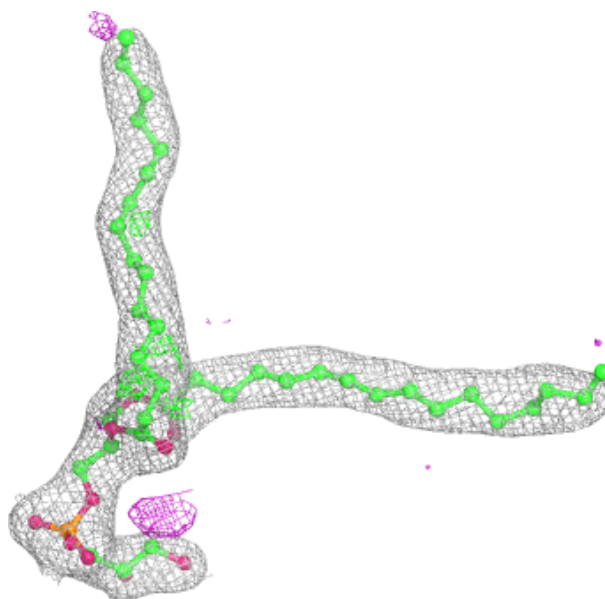
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





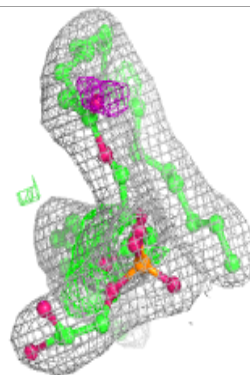
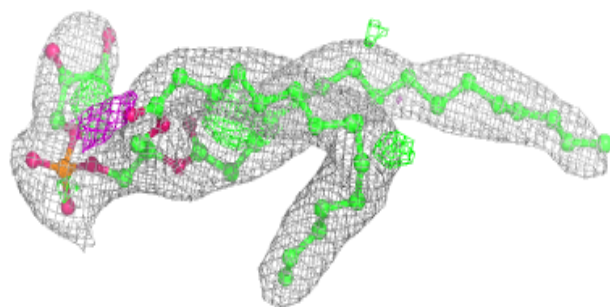
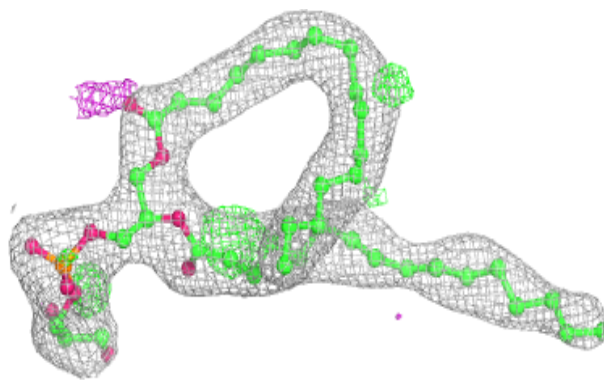
**Electron density around LHG b 629 (A):**

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

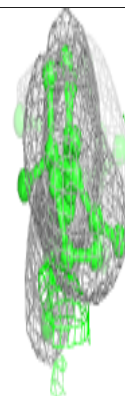
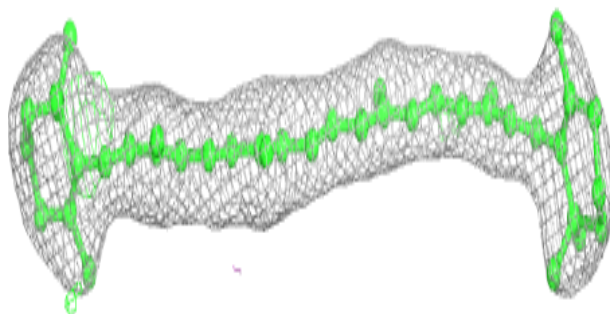
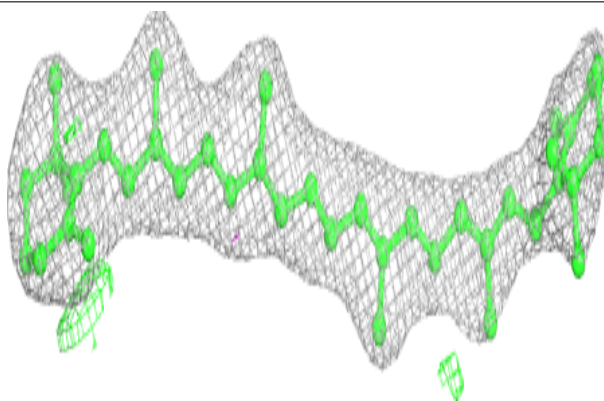


**Electron density around LHG d 414 (B):**

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

**Electron density around BCR c 515:**

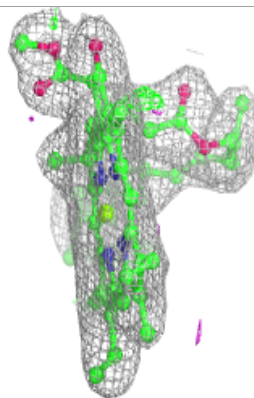
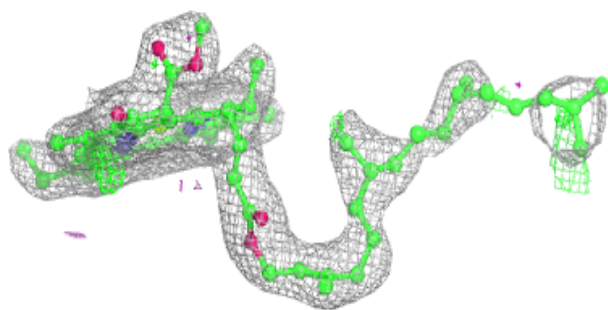
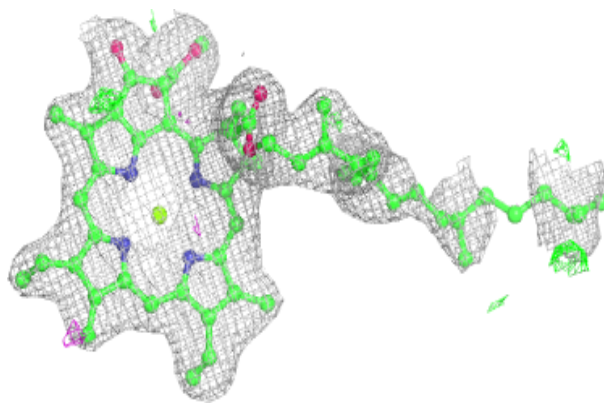
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



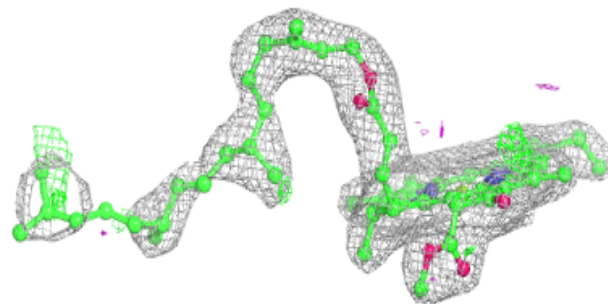
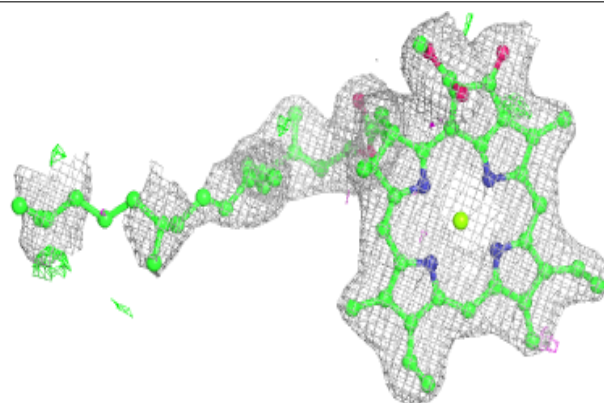


**Electron density around CLA a 405 (A):**

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

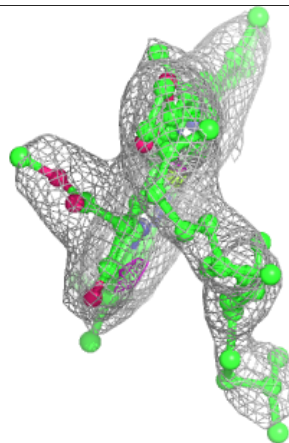
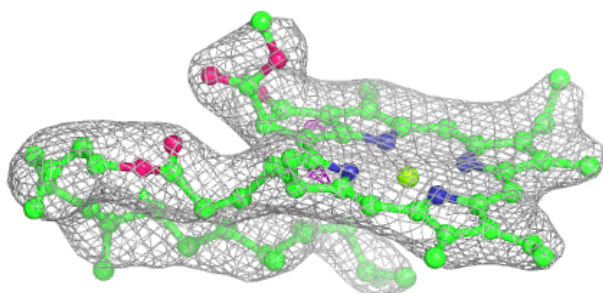
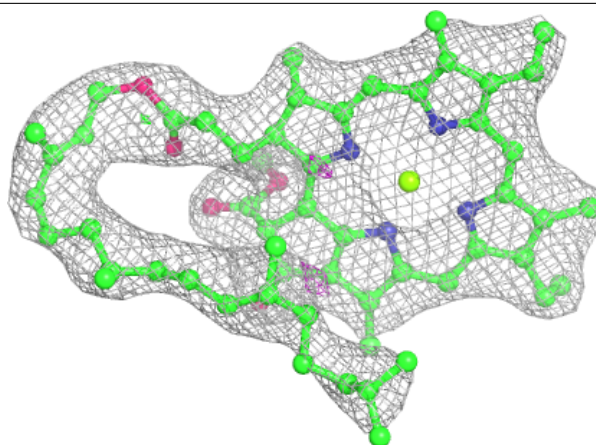
**Electron density around CLA a 405 (B):**

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

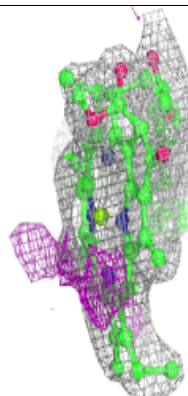
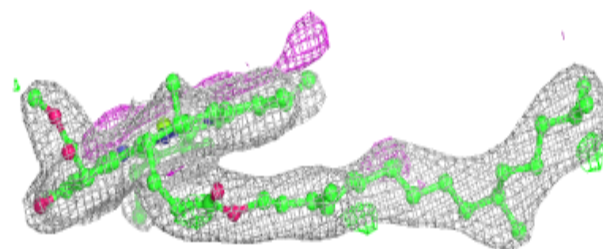
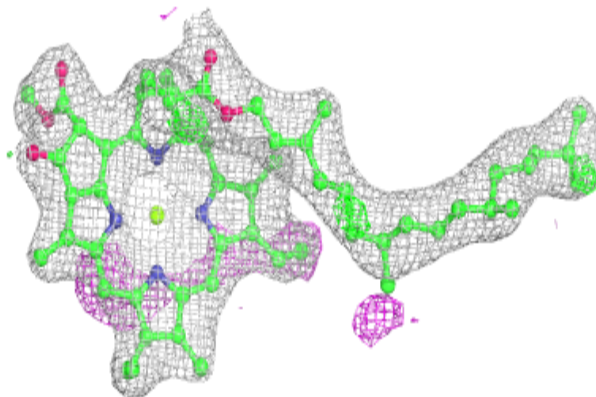


**Electron density around CLA c 509:**

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

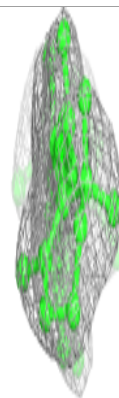
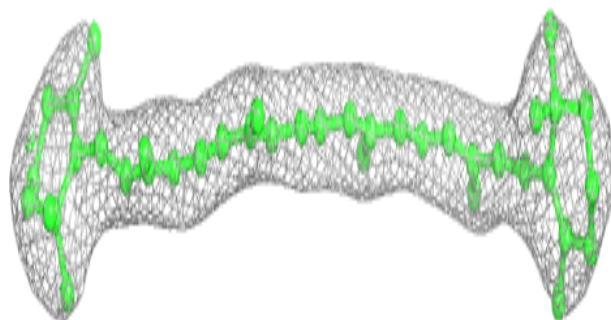
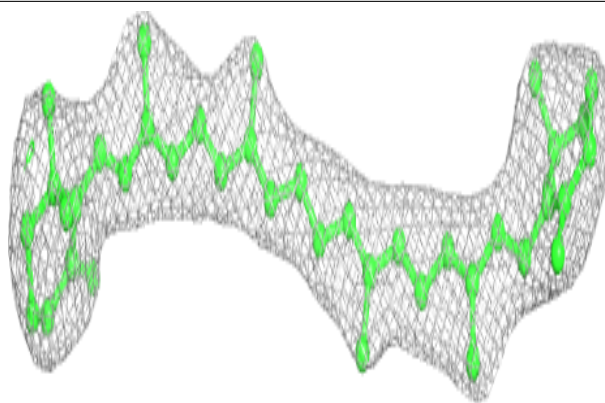
**Electron density around CLA B 603:**

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

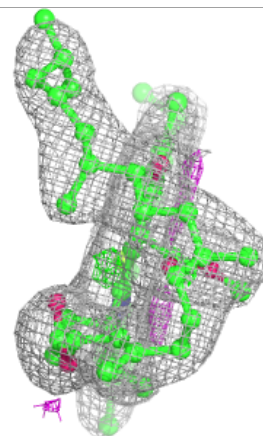
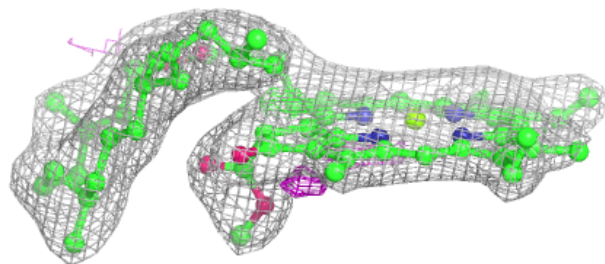
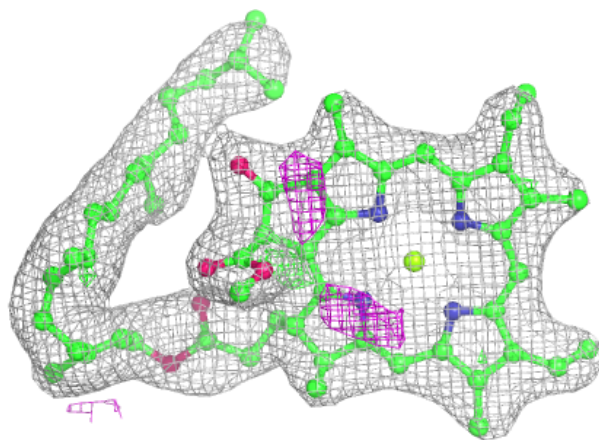


**Electron density around BCR y 101:**

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

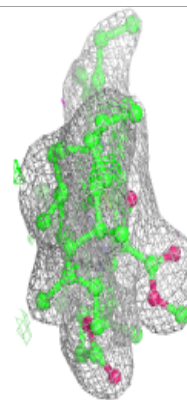
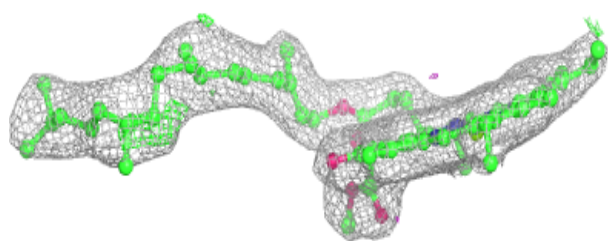
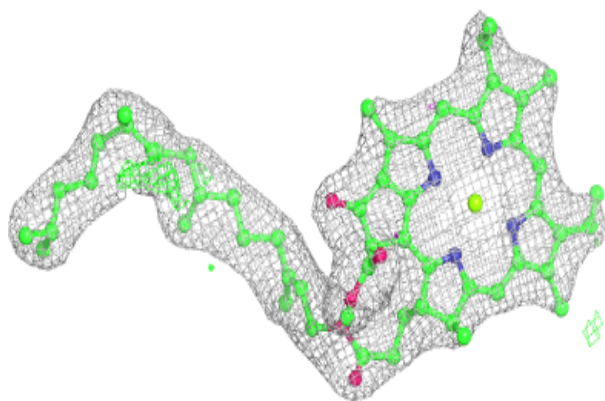
**Electron density around CLA B 610:**

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

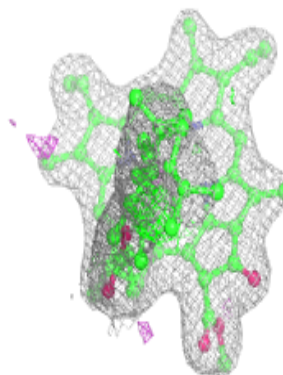
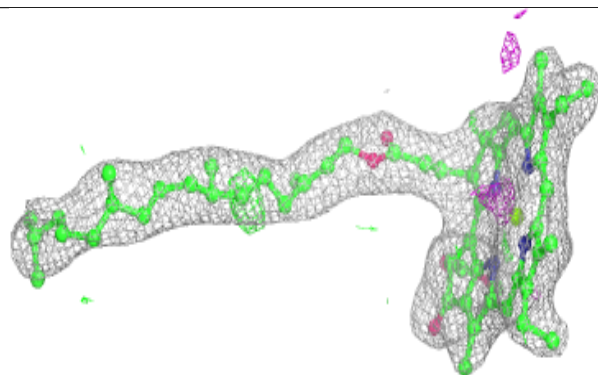
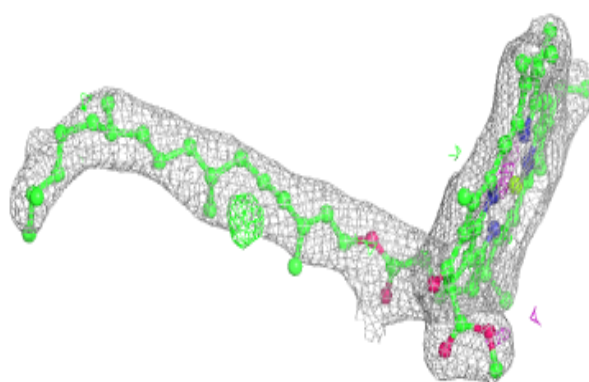


**Electron density around CLA b 602:**

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

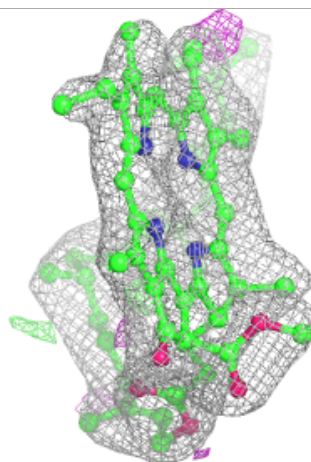
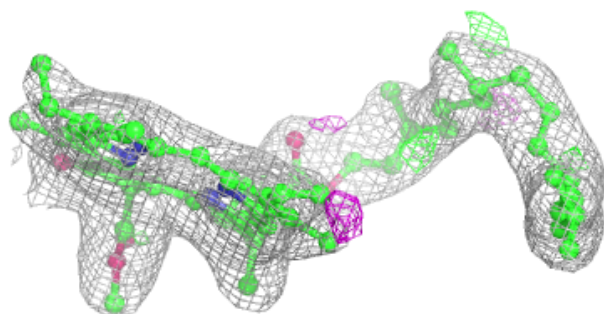
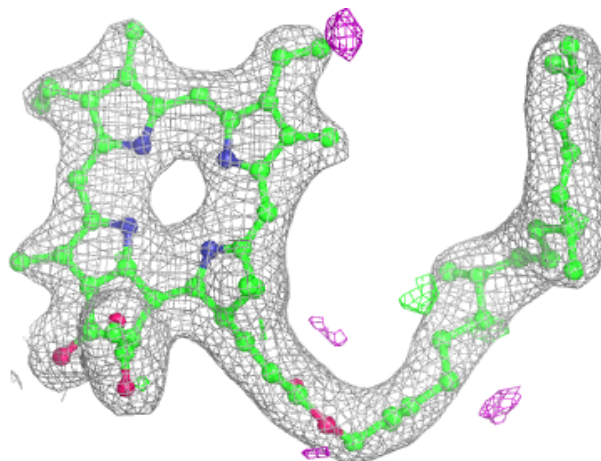
**Electron density around CLA b 604:**

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



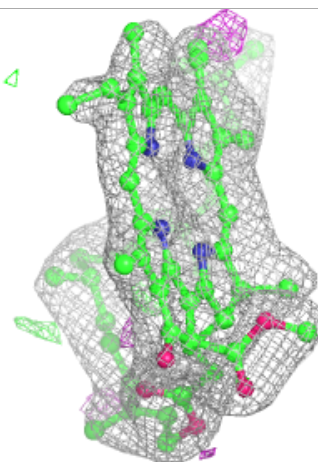
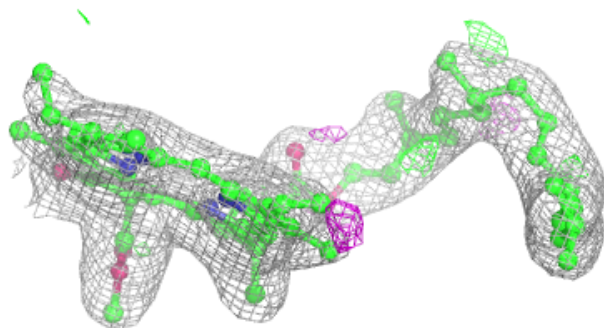
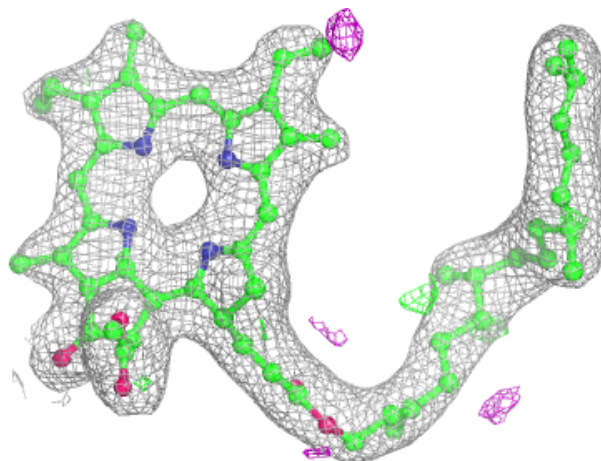
**Electron density around PHO a 414 (A):**

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



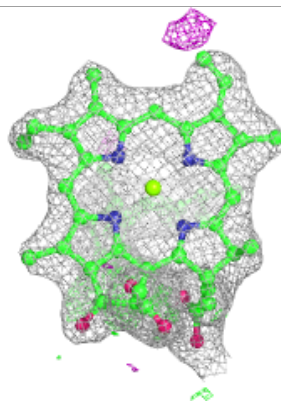
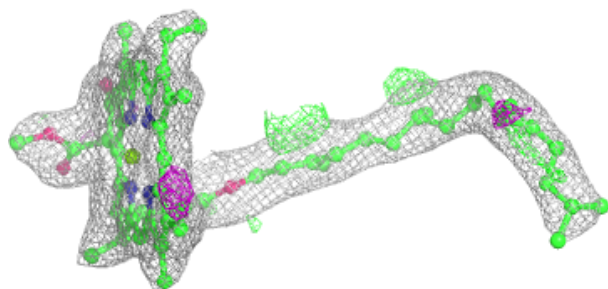
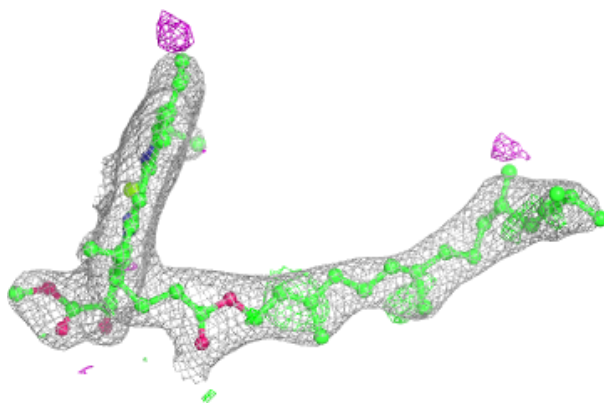
**Electron density around PHO a 414 (B):**

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

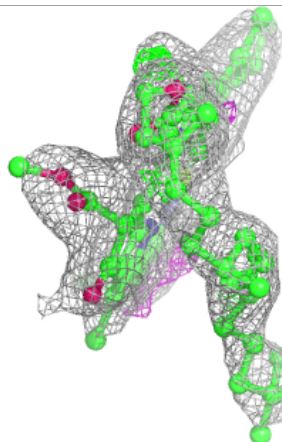
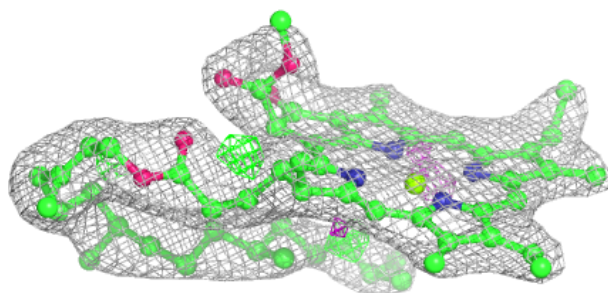
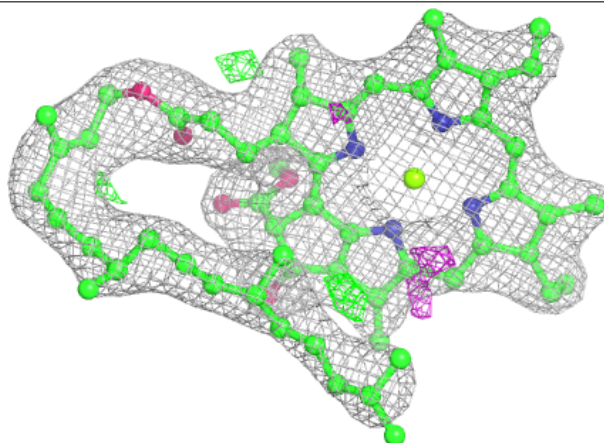


**Electron density around CLA b 605:**

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

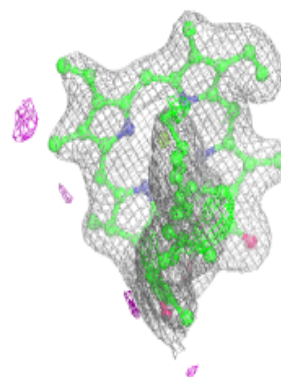
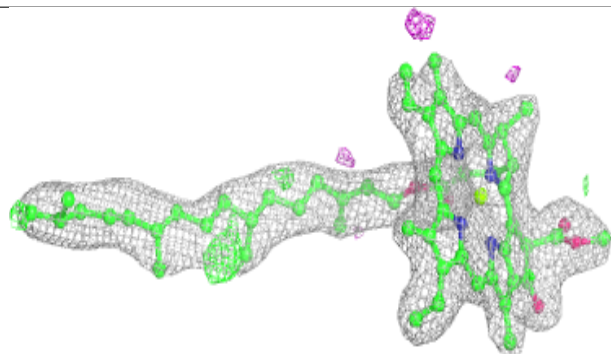
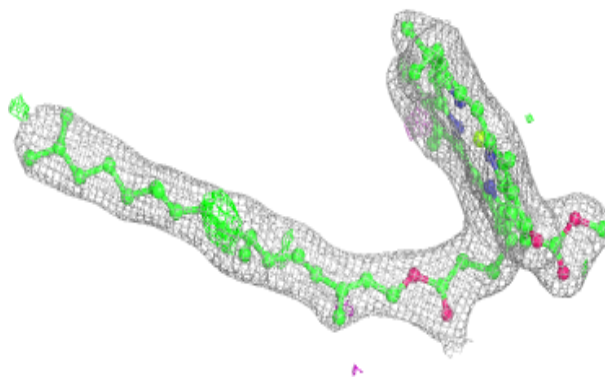
**Electron density around CLA C 510:**

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

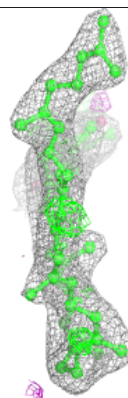
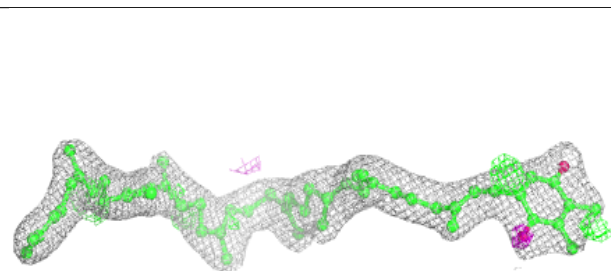
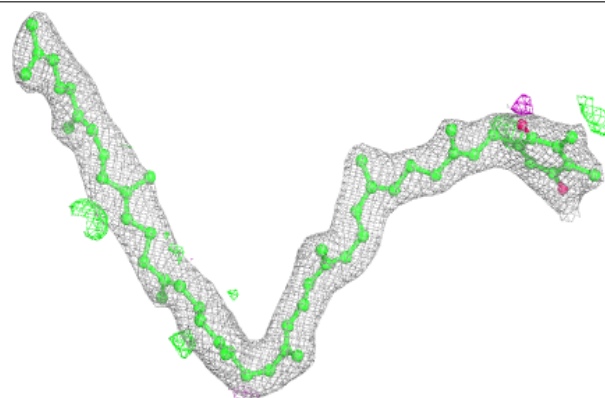


**Electron density around CLA b 607:**

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

**Electron density around PL9 D 405 (A):**

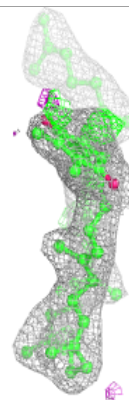
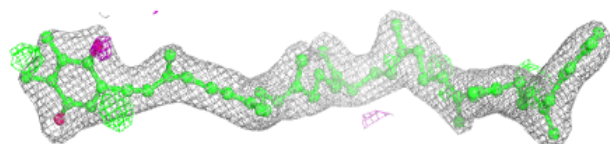
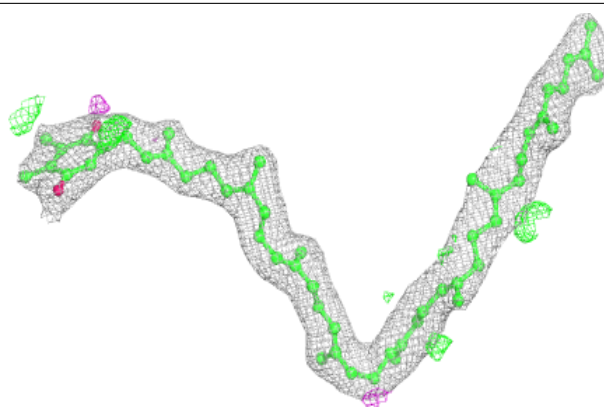
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





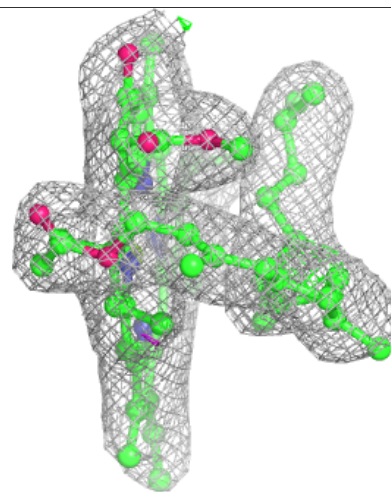
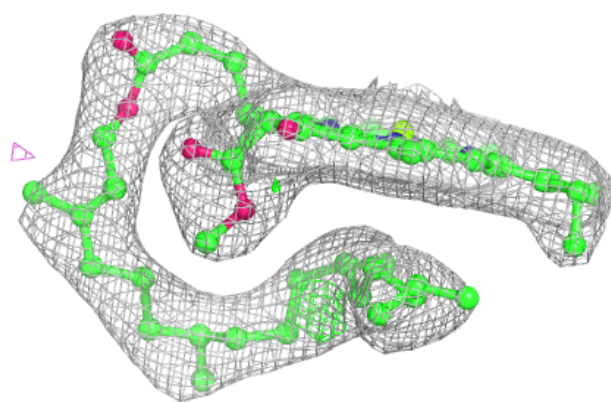
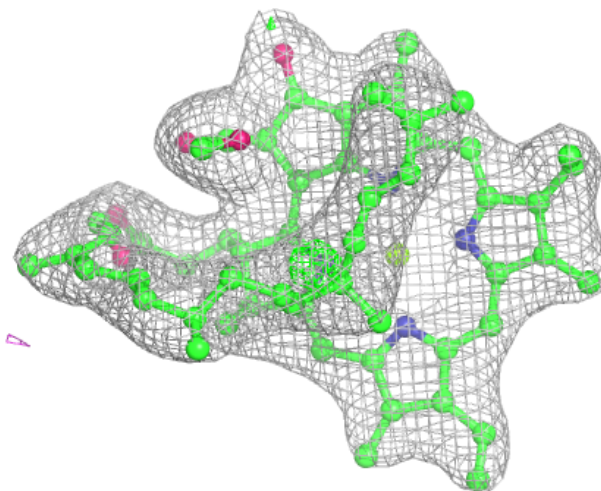
**Electron density around PL9 D 405 (B):**

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



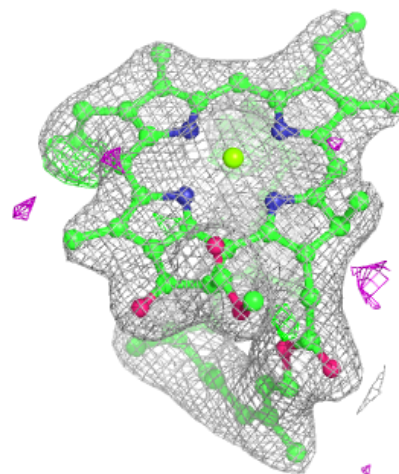
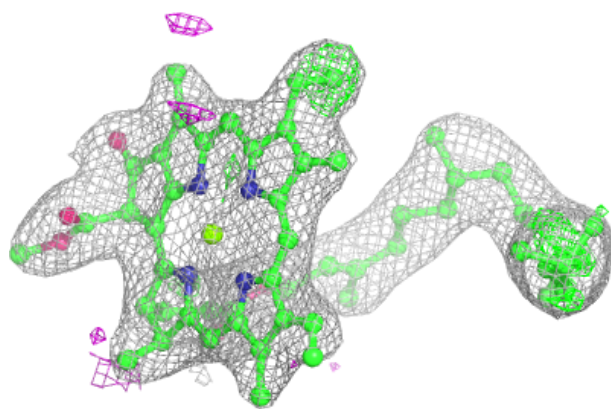
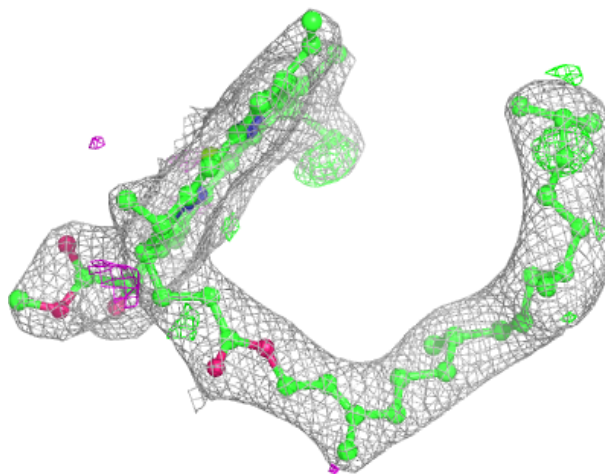
**Electron density around CLA C 511:**

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



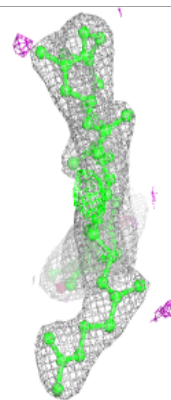
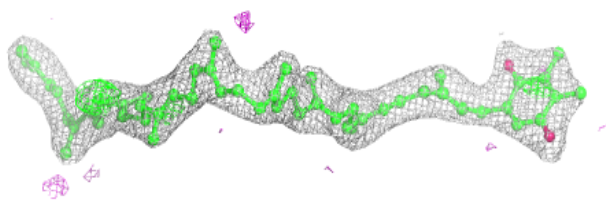
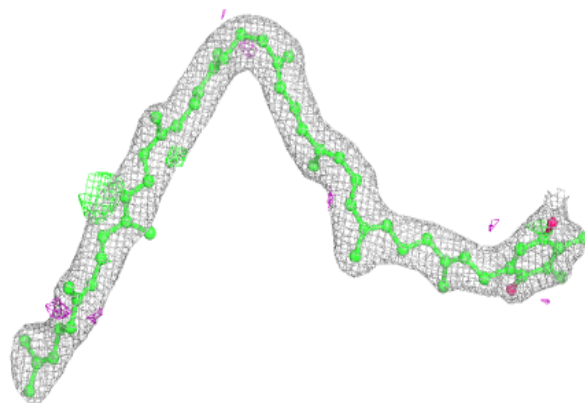
**Electron density around CLA b 611:**

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

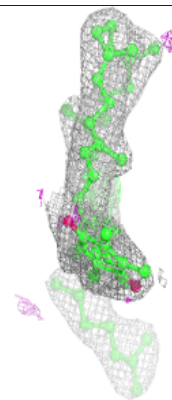
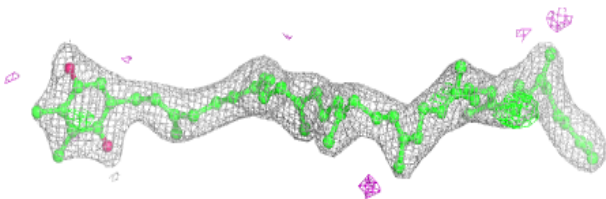
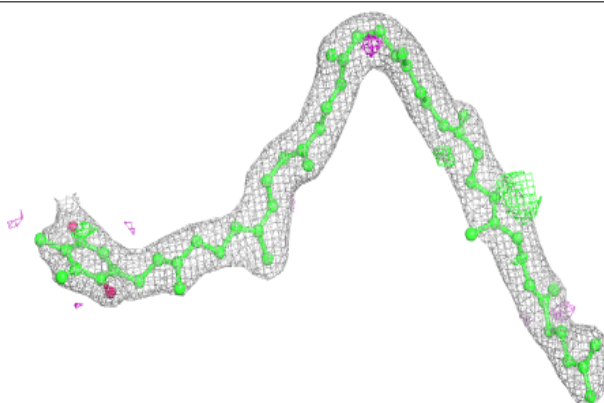


**Electron density around PL9 d 406 (A):**

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

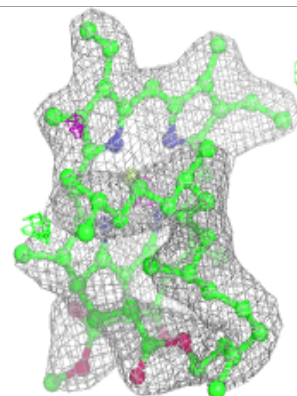
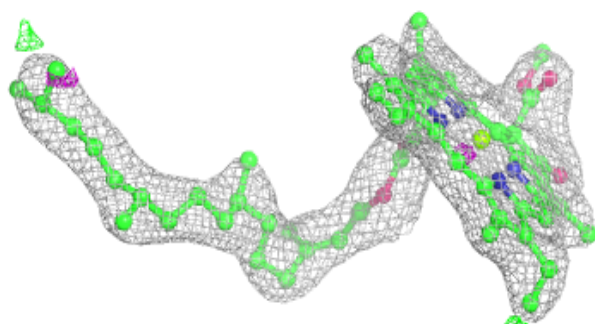
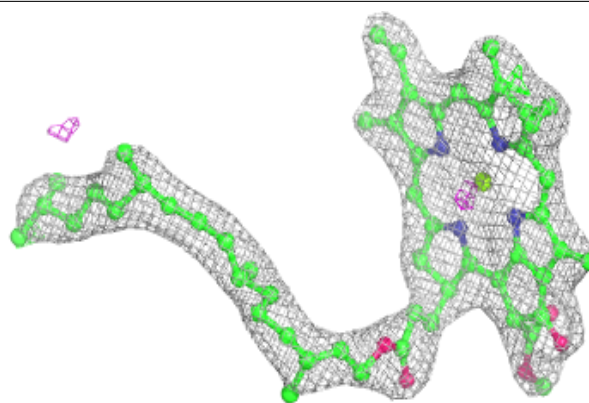
**Electron density around PL9 d 406 (B):**

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

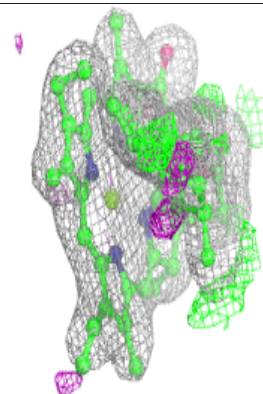
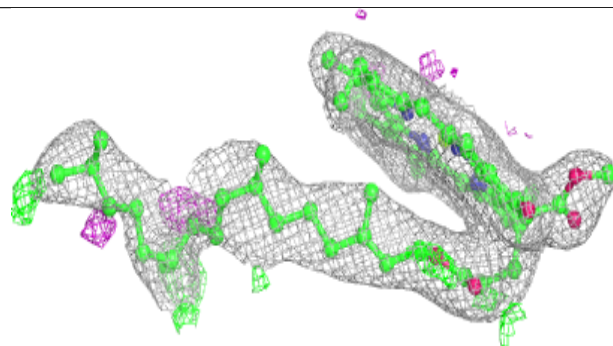
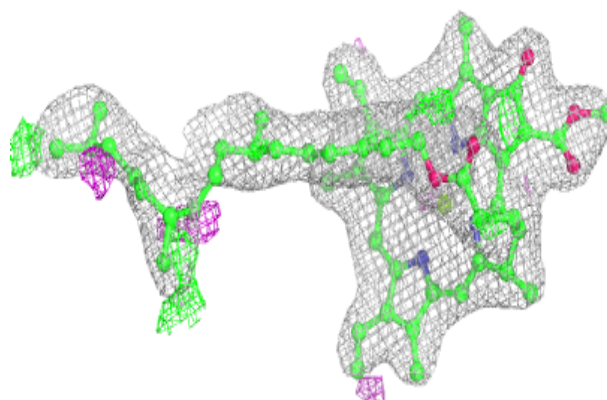


**Electron density around CLA C 512:**

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

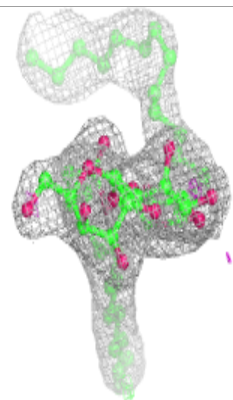
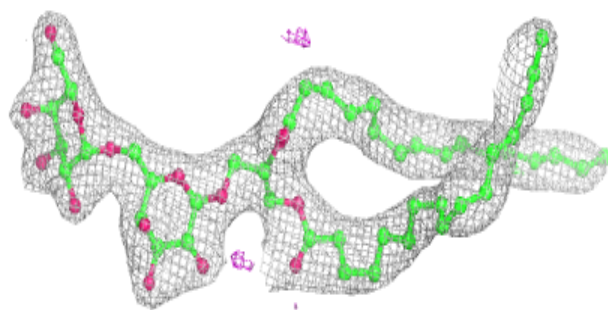
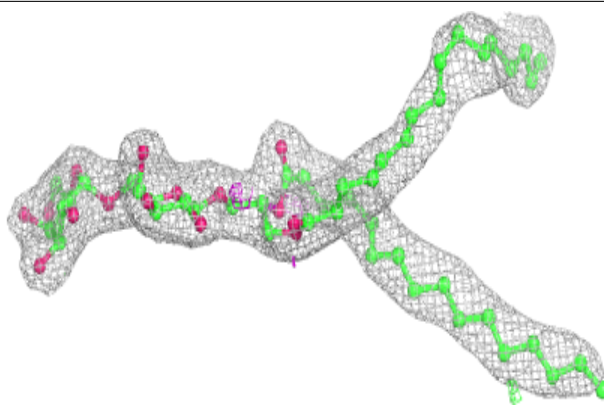
**Electron density around CLA b 614:**

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

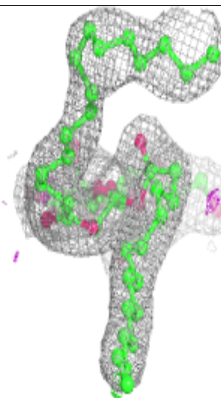
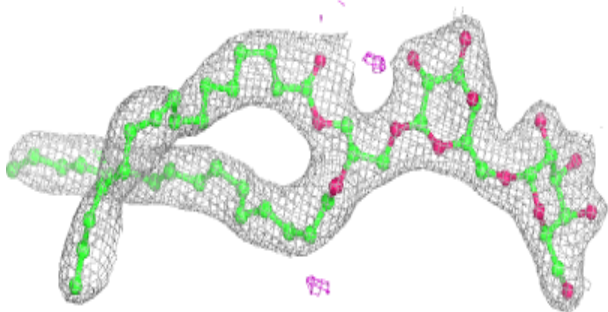
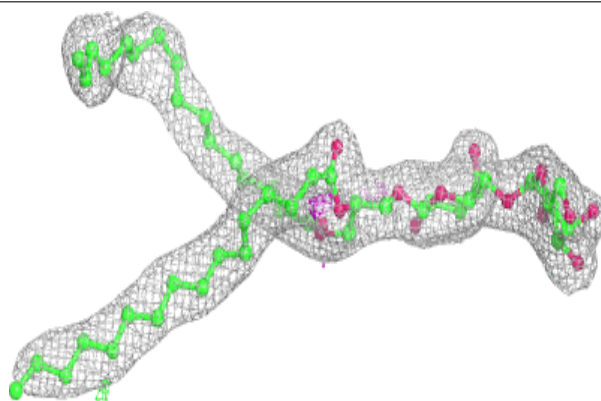


**Electron density around DGD C 517 (A):**

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

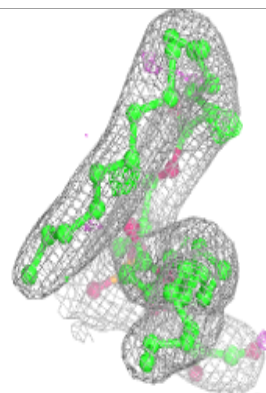
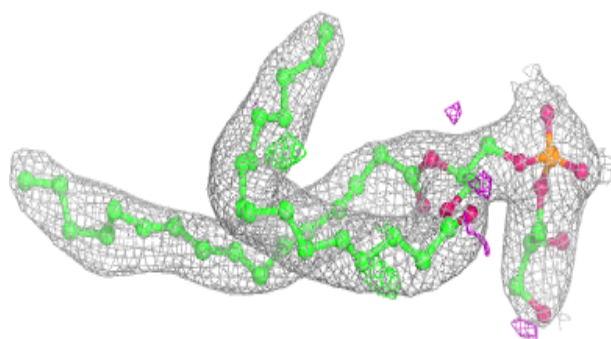
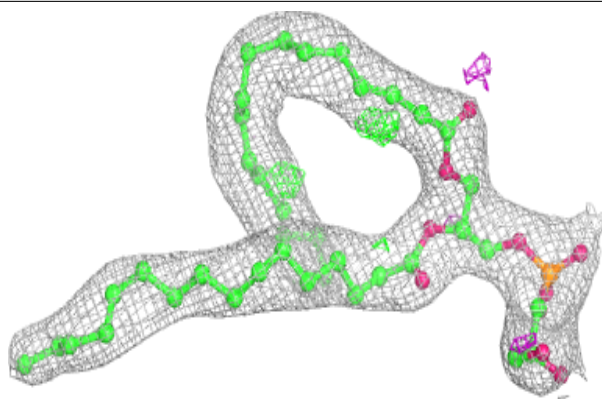
**Electron density around DGD C 517 (B):**

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

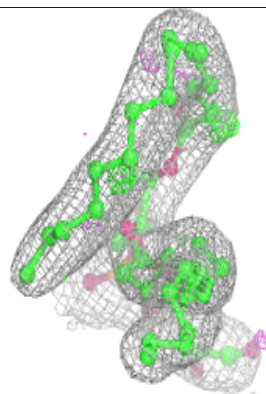
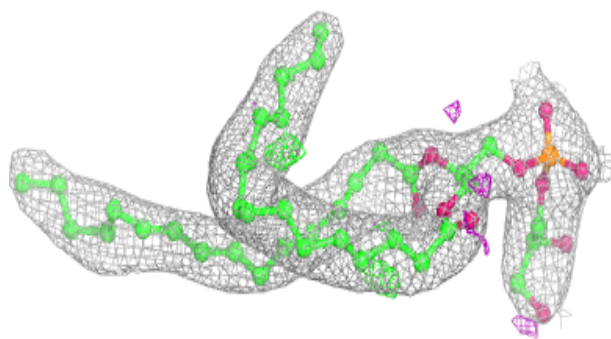
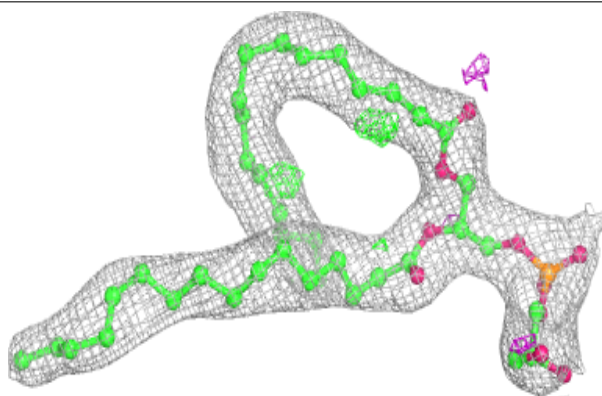


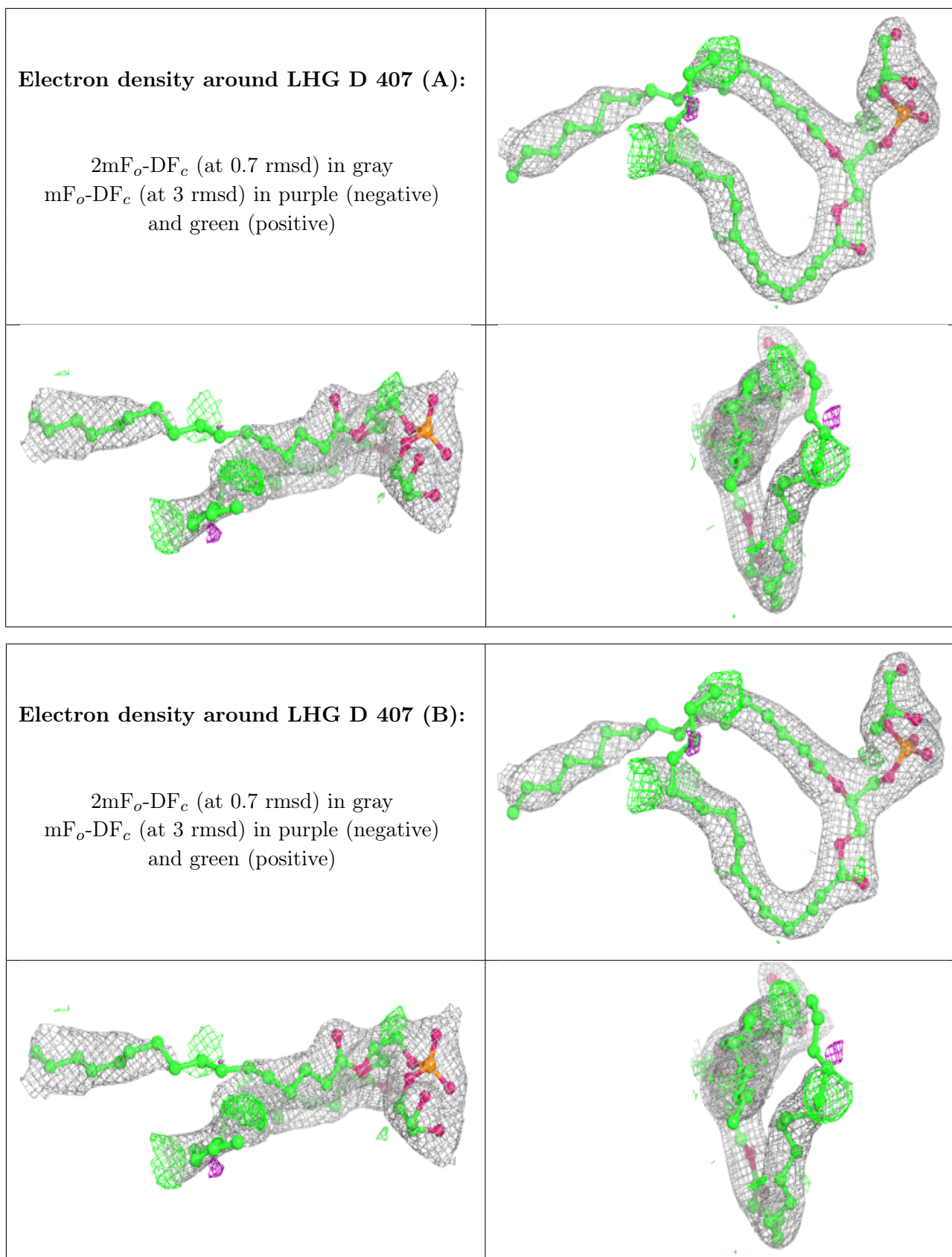
**Electron density around LHG A 419 (A):**

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

**Electron density around LHG A 419 (B):**

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

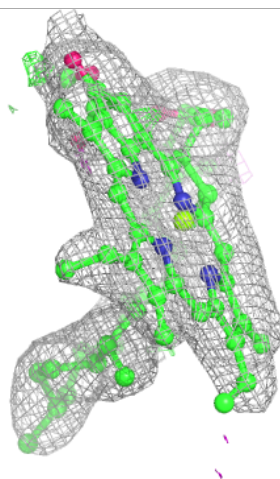
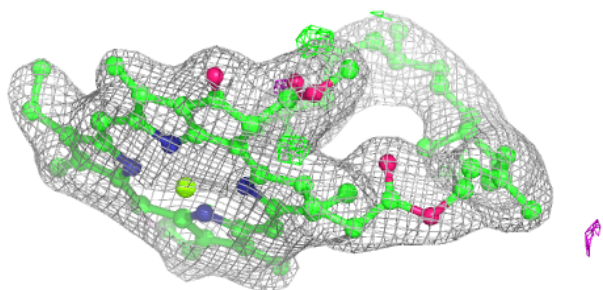
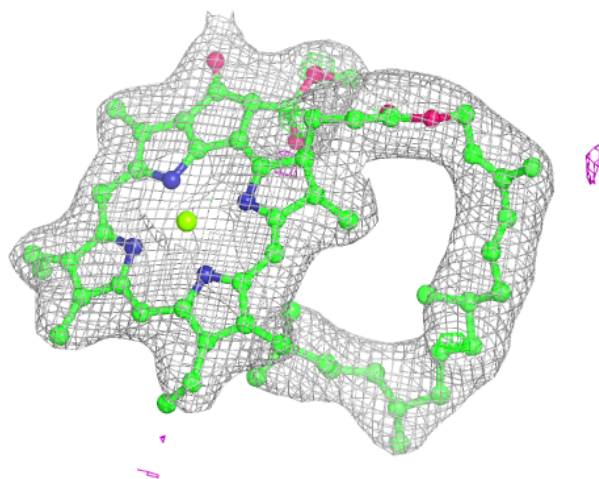


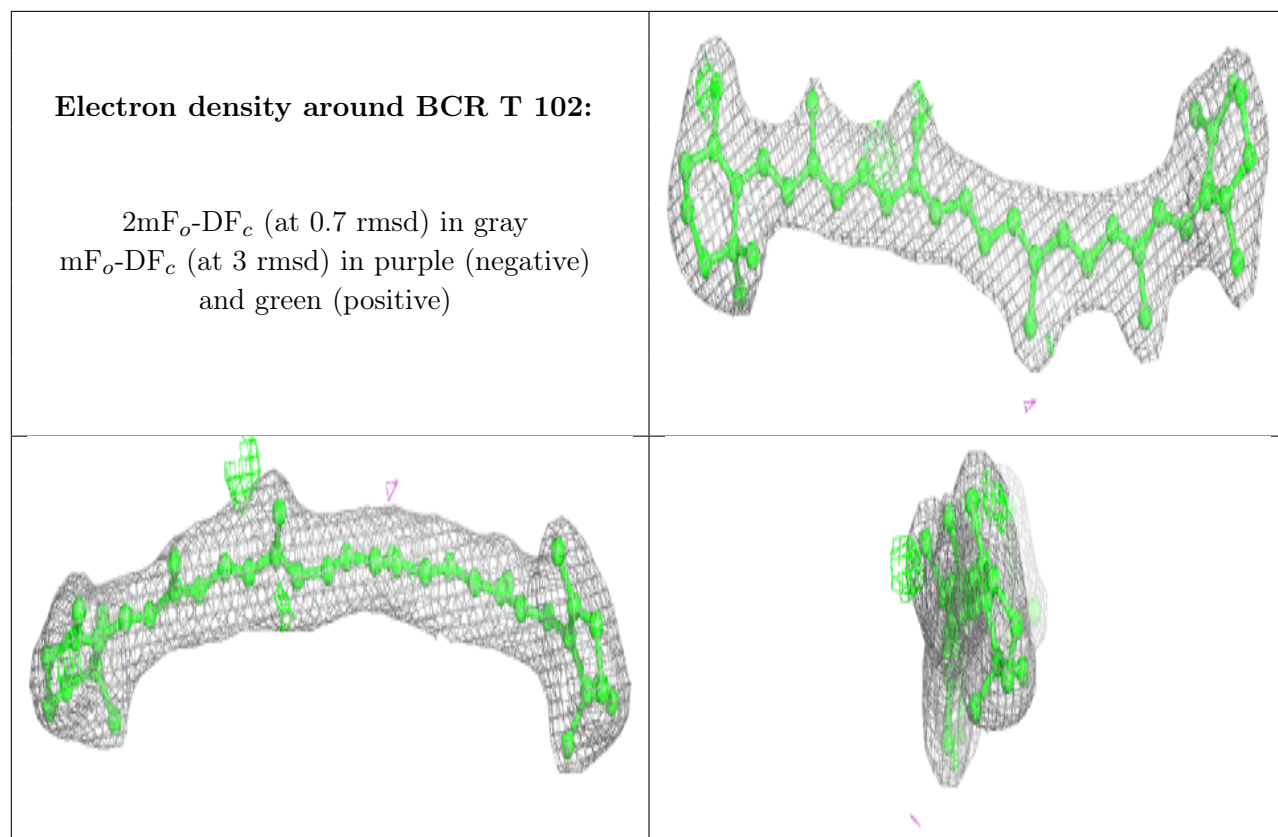




**Electron density around CLA b 615:**

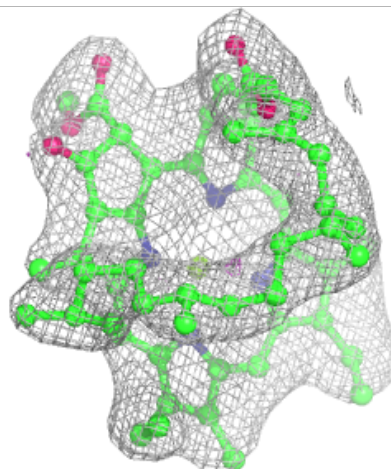
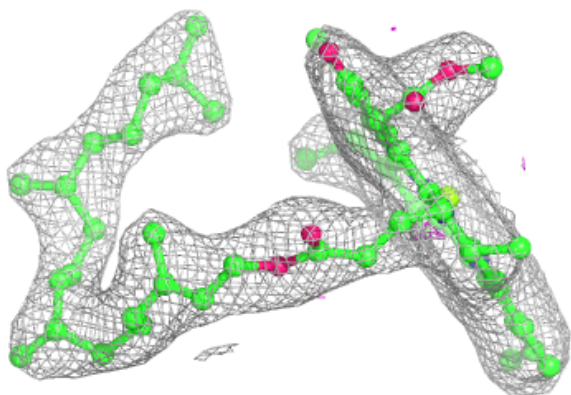
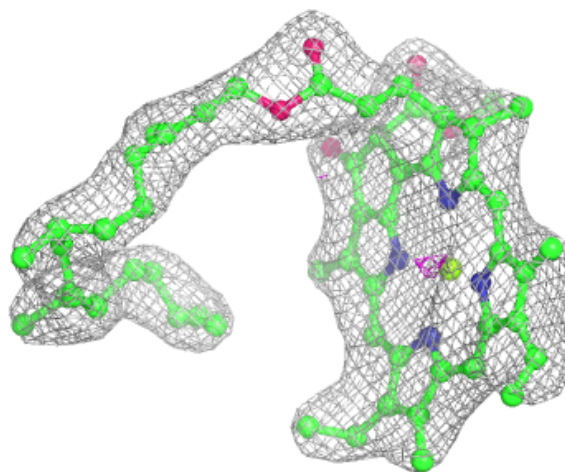
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





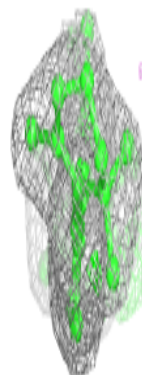
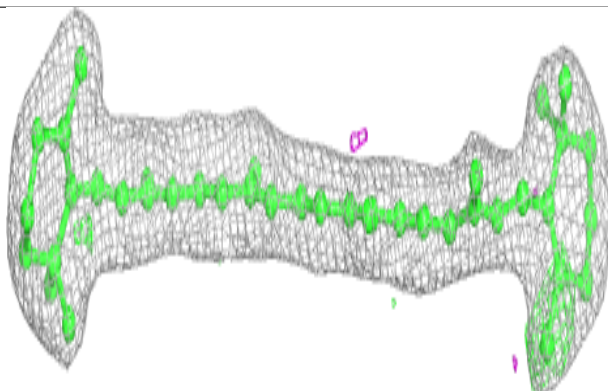
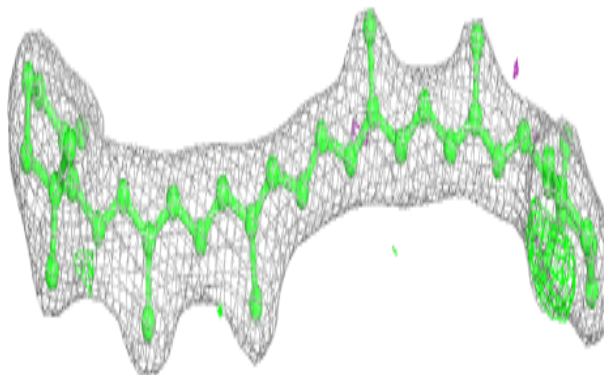
**Electron density around CLA C 504:**

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

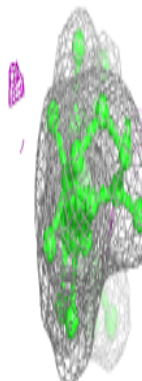
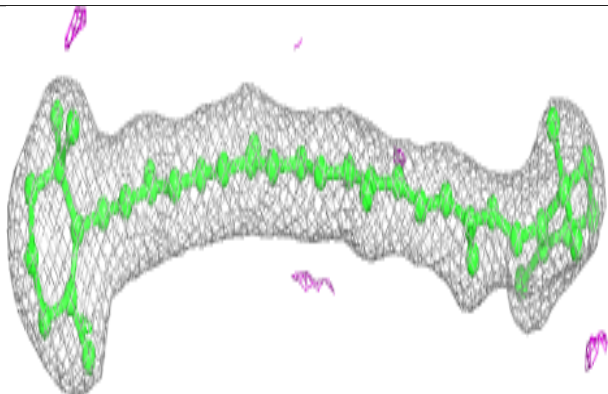
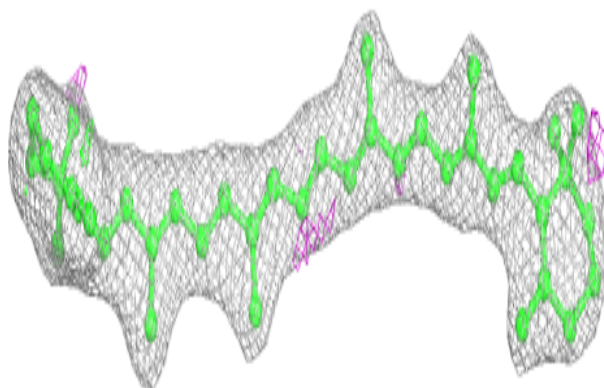


**Electron density around BCR a 408:**

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

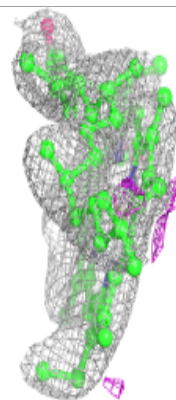
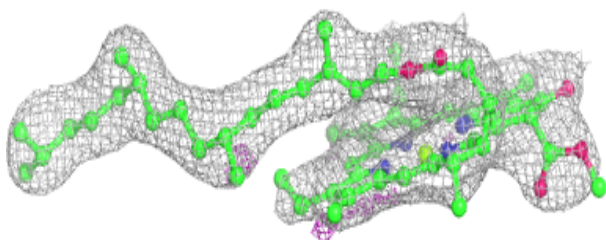
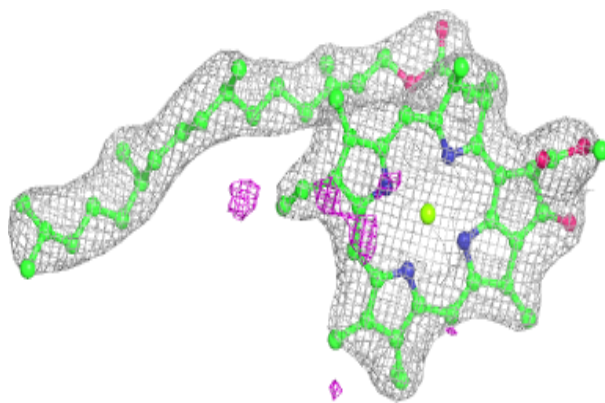
**Electron density around BCR b 617:**

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

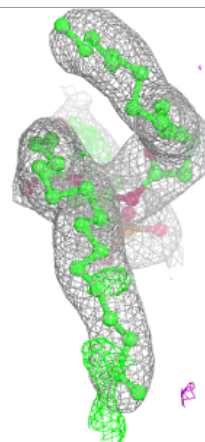
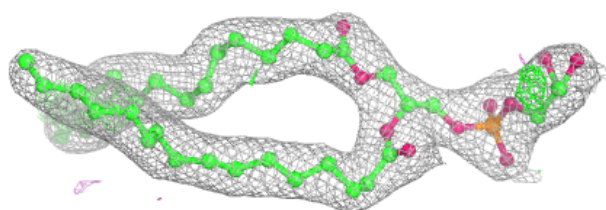
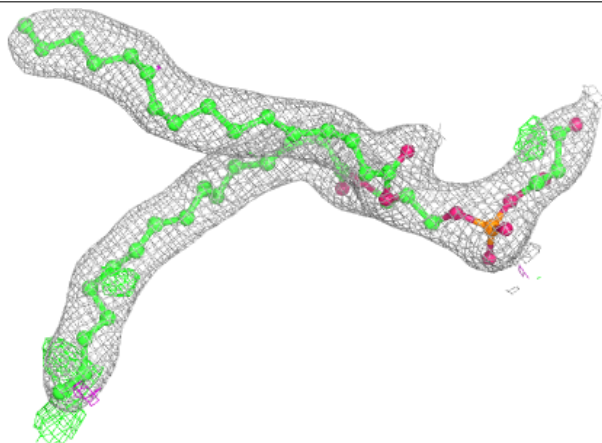


**Electron density around CLA c 501:**

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

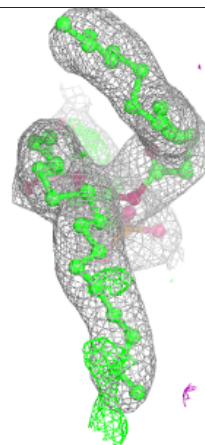
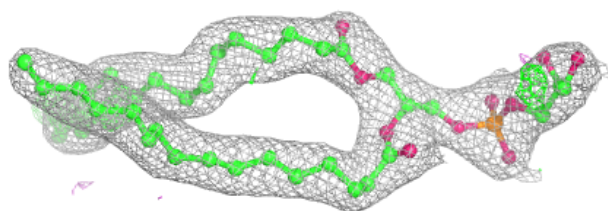
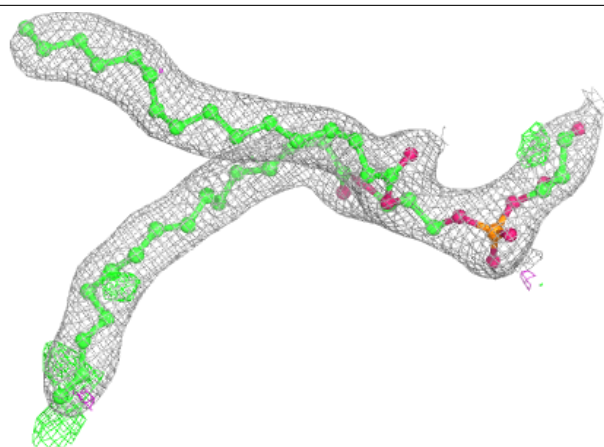
**Electron density around LHG d 407 (A):**

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

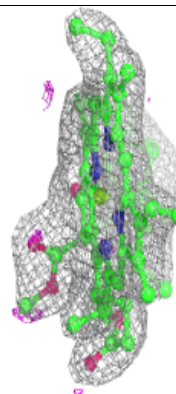
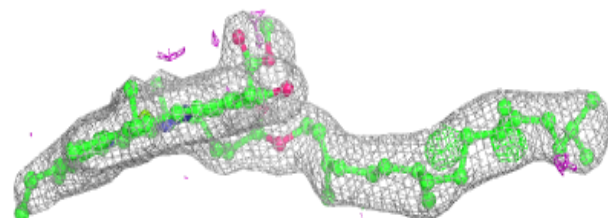
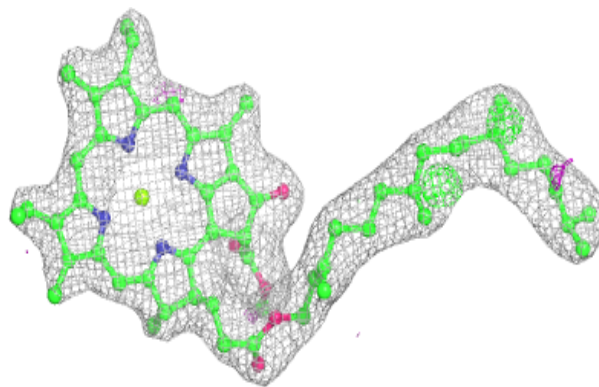


**Electron density around LHG d 407 (B):**

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

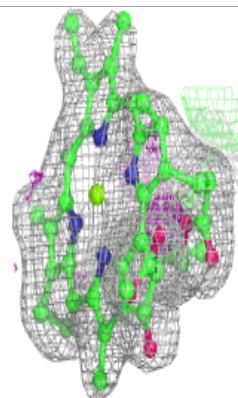
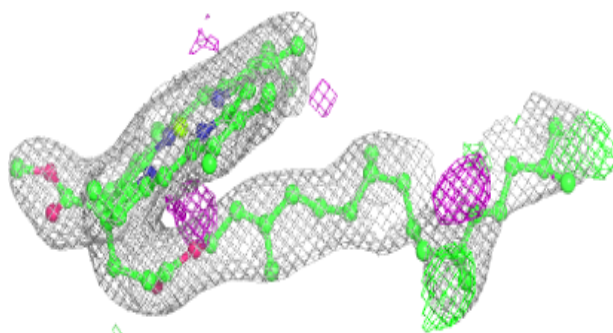
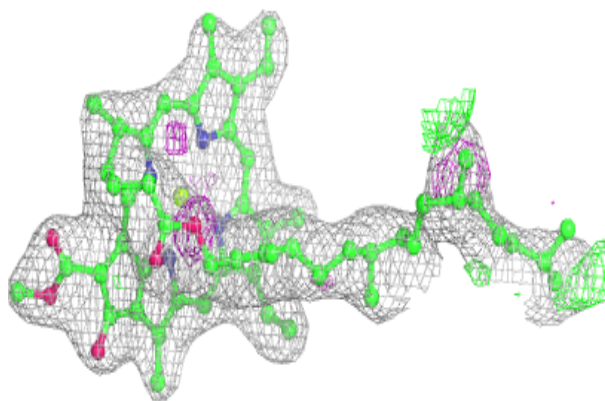
**Electron density around CLA B 602:**

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

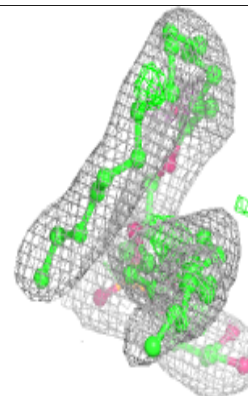
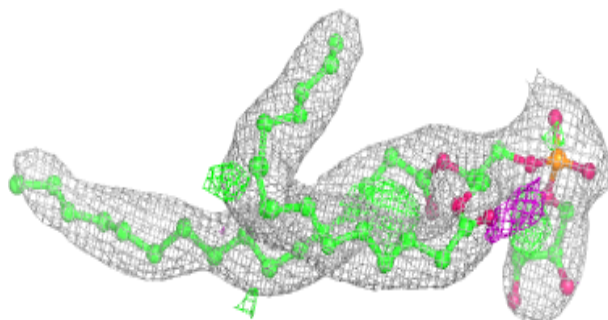
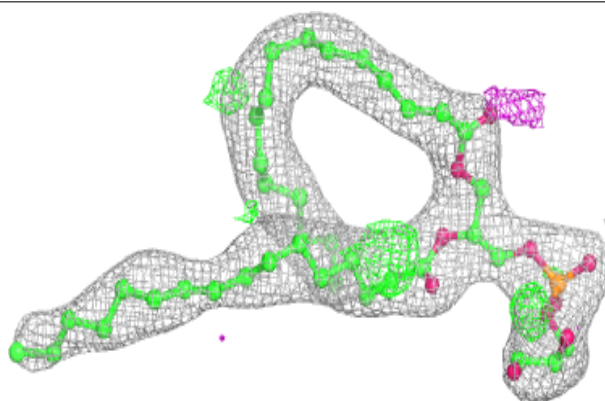


**Electron density around CLA B 614:**

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

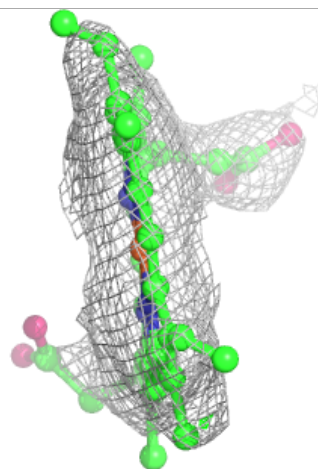
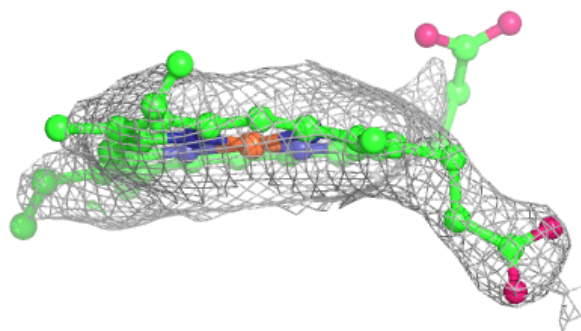
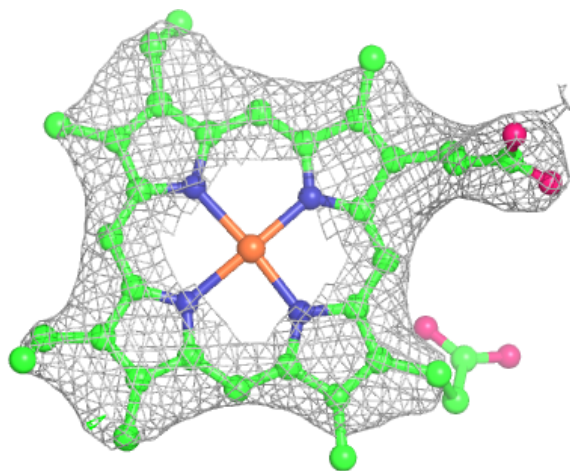
**Electron density around LHG d 414 (A):**

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



**Electron density around HEM f 101:**

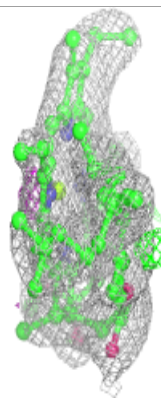
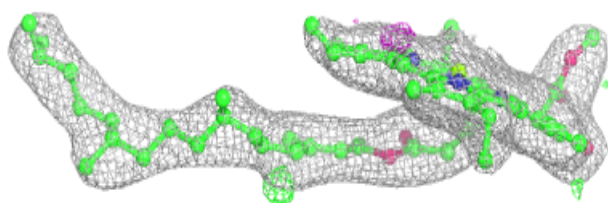
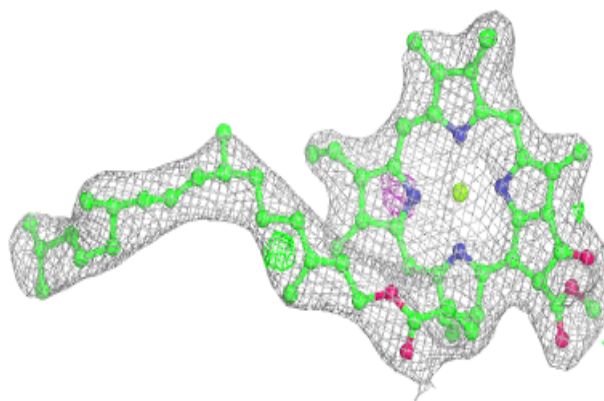
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



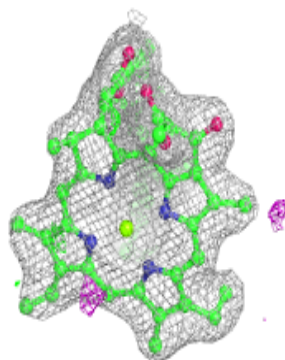
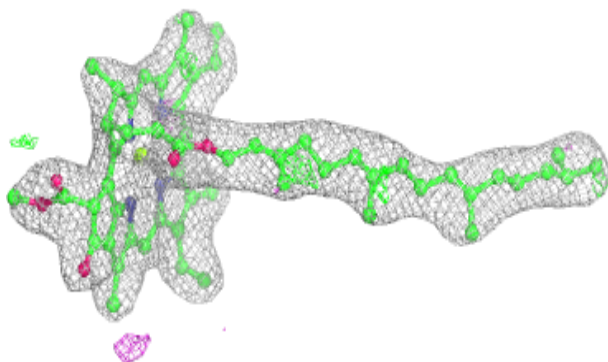
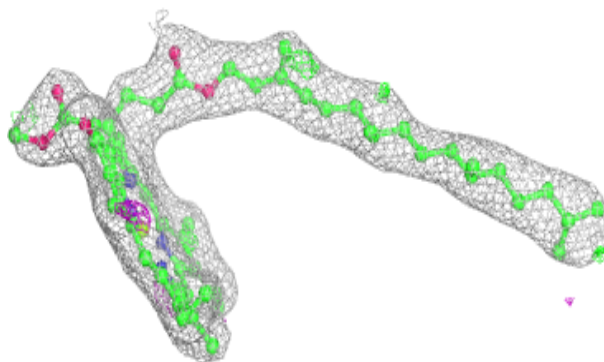


**Electron density around CLA b 603:**

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

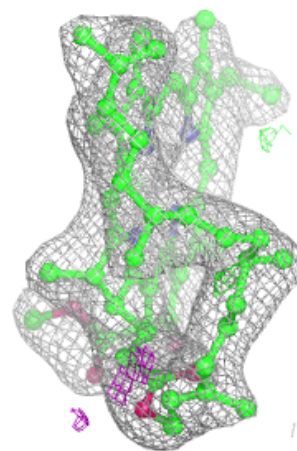
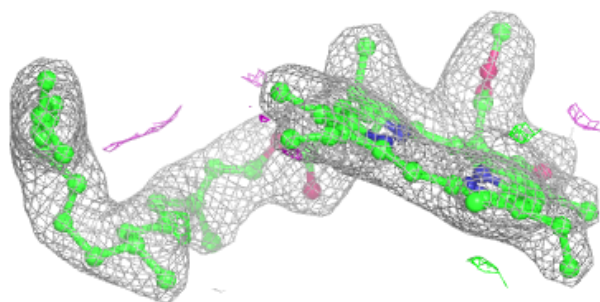
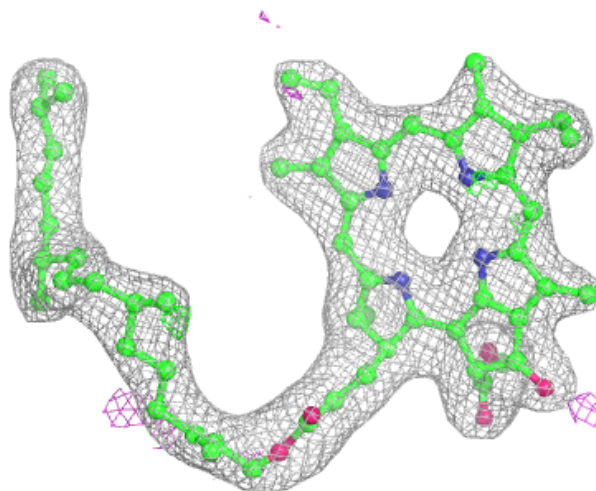
**Electron density around CLA B 607:**

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



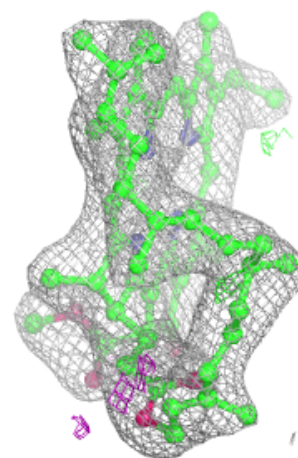
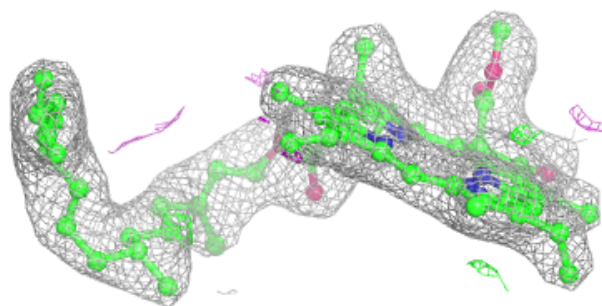
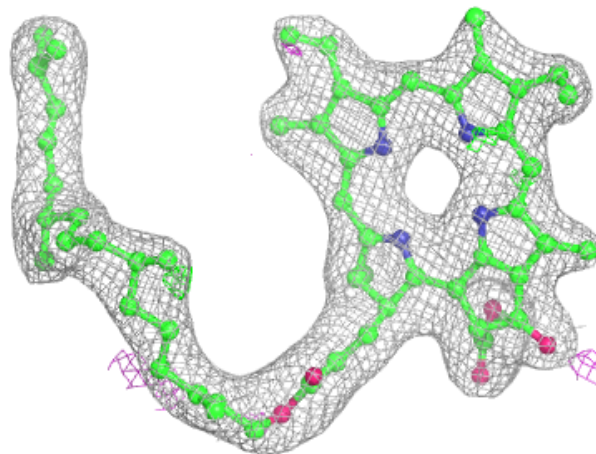
**Electron density around PHO A 416 (A):**

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



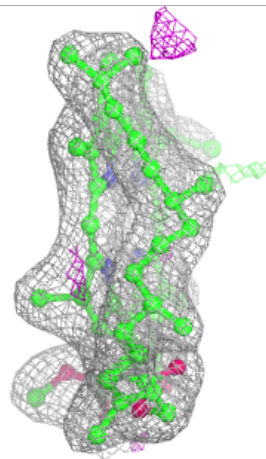
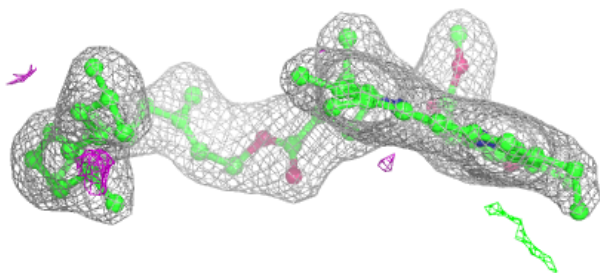
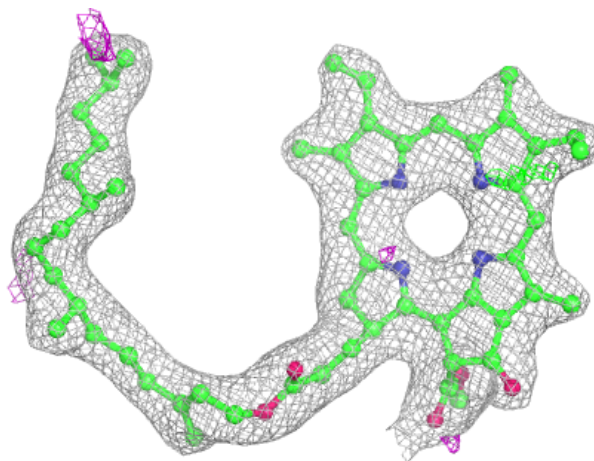
**Electron density around PHO A 416 (B):**

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



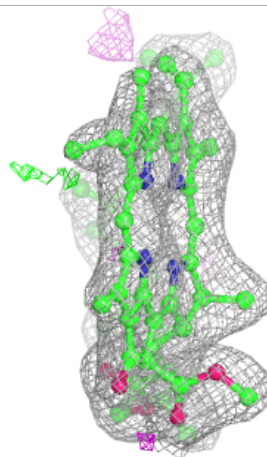
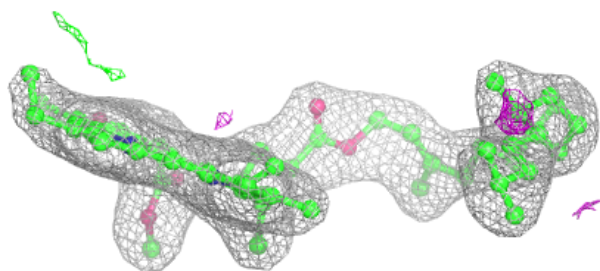
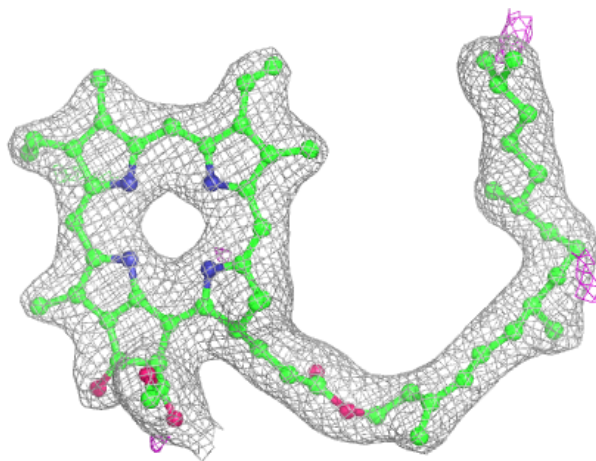
**Electron density around PHO a 406 (A):**

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



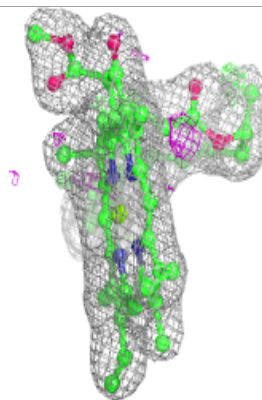
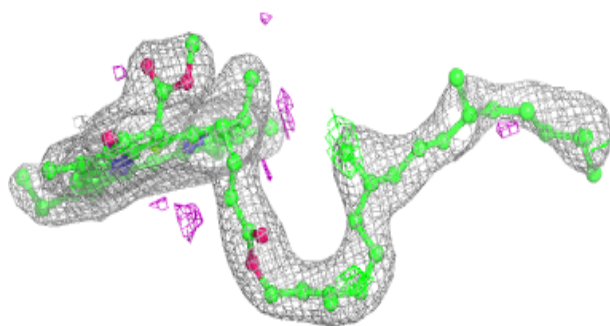
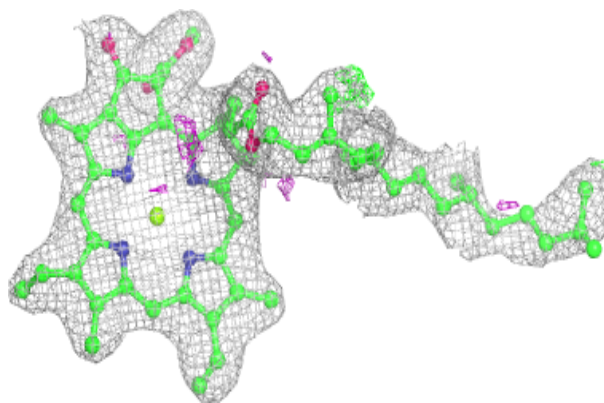
**Electron density around PHO a 406 (B):**

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



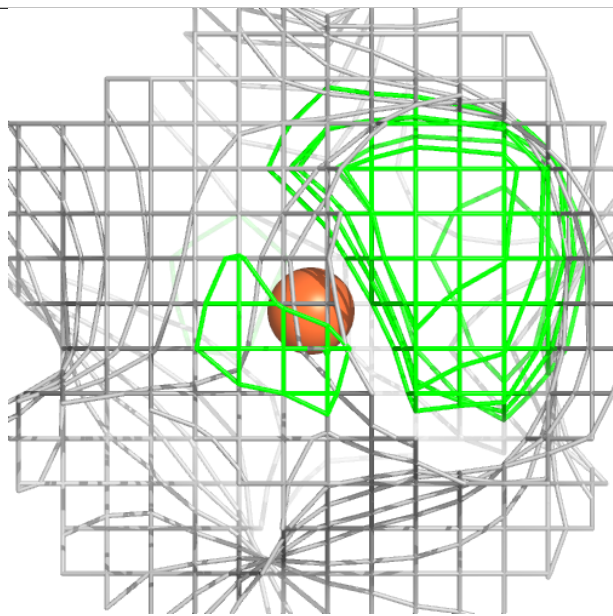
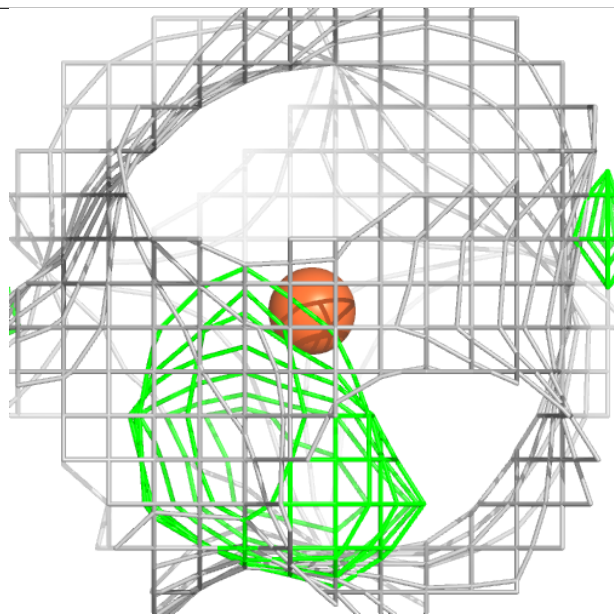
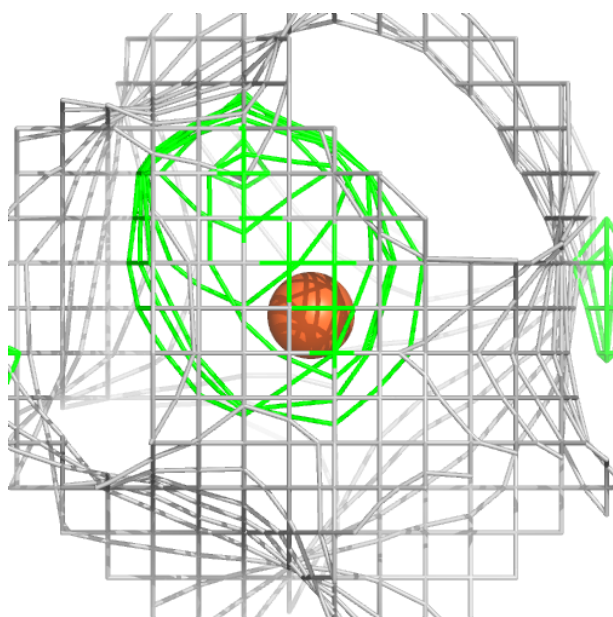
**Electron density around CLA A 406 (B):**

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



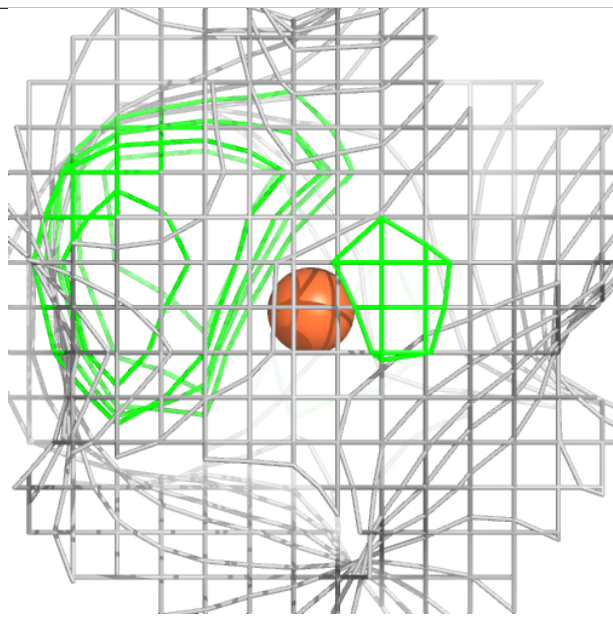
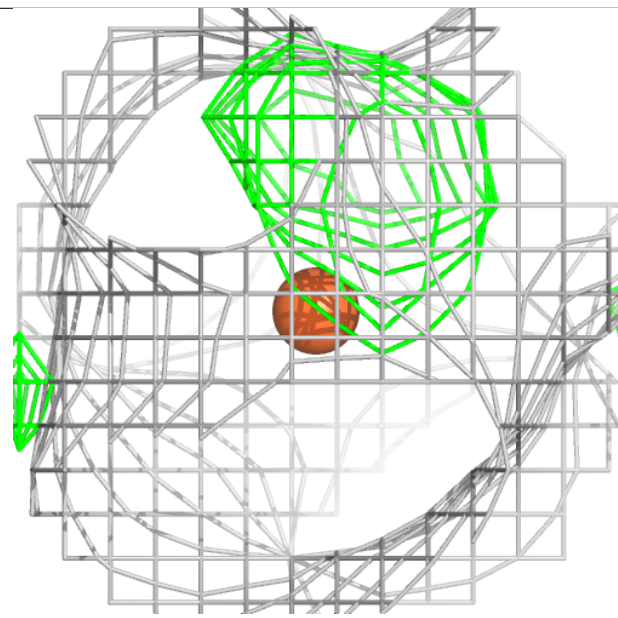
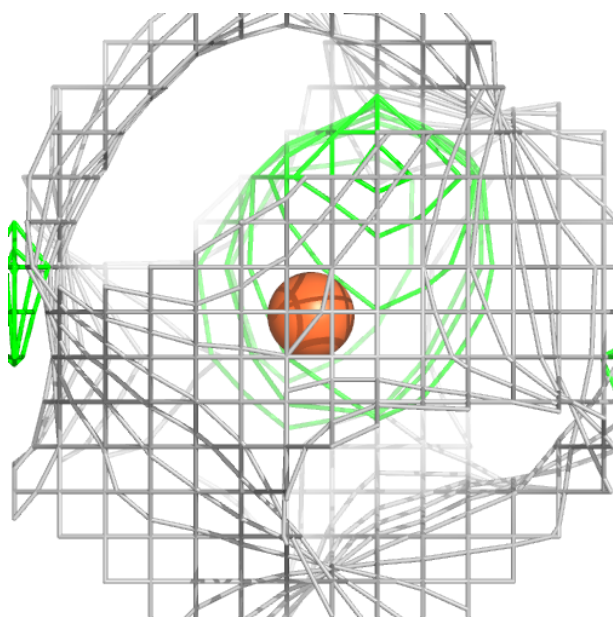
**Electron density around FE2 a 401 (A):**

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

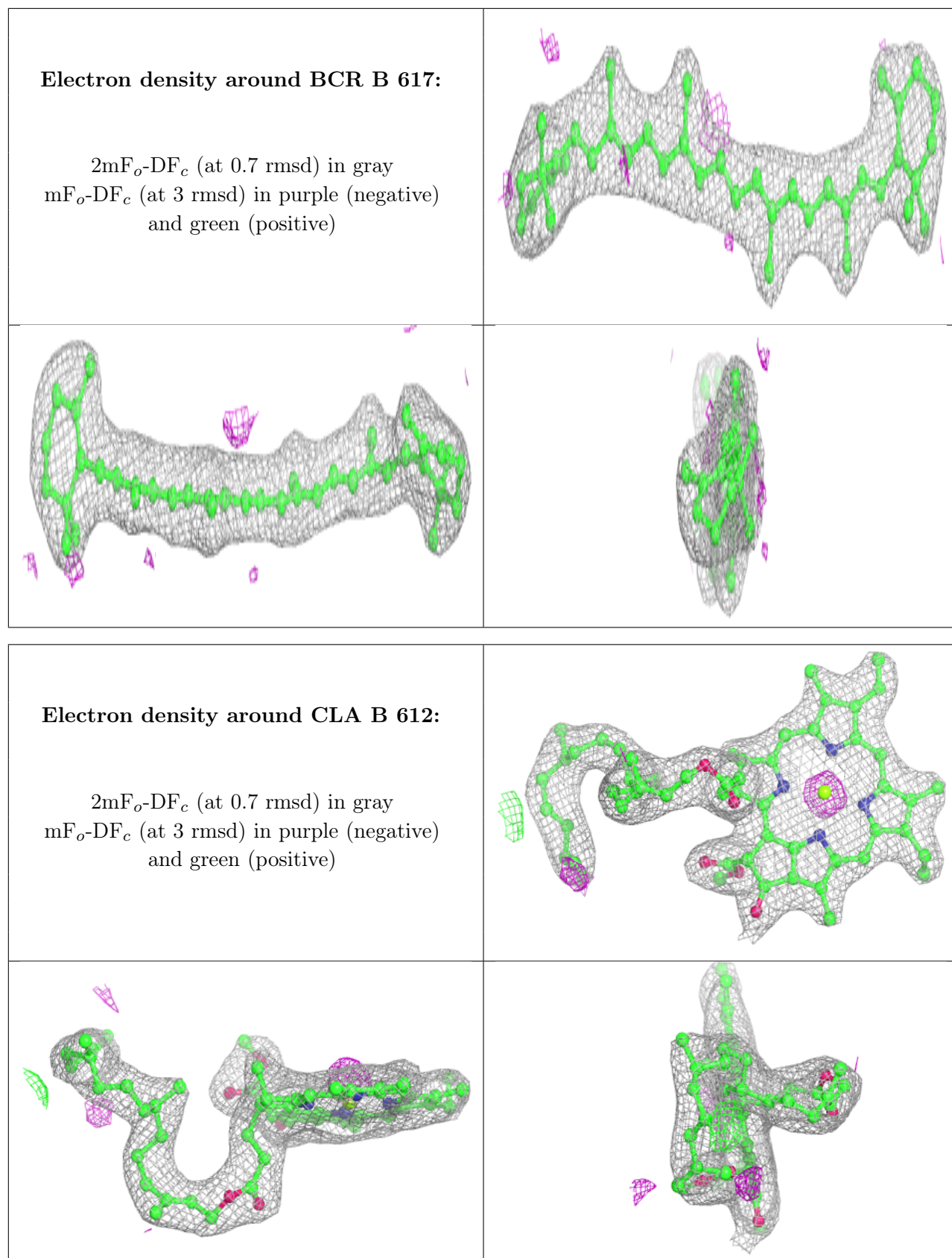


**Electron density around FE2 a 401 (B):**

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

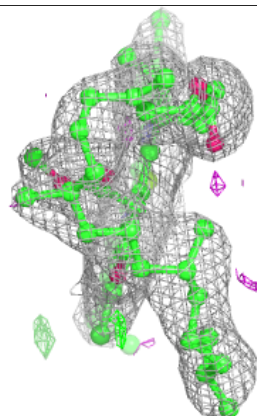
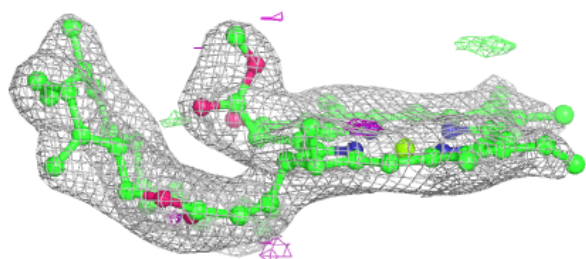
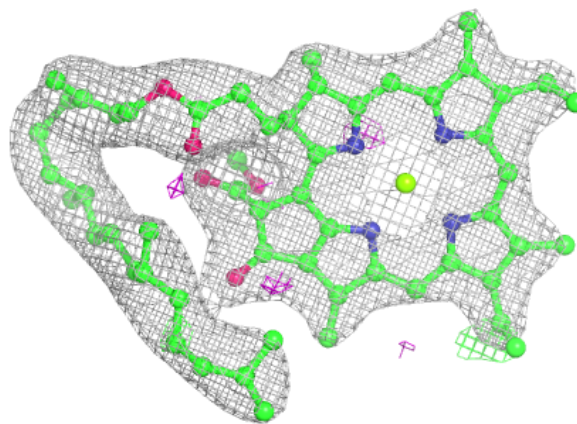






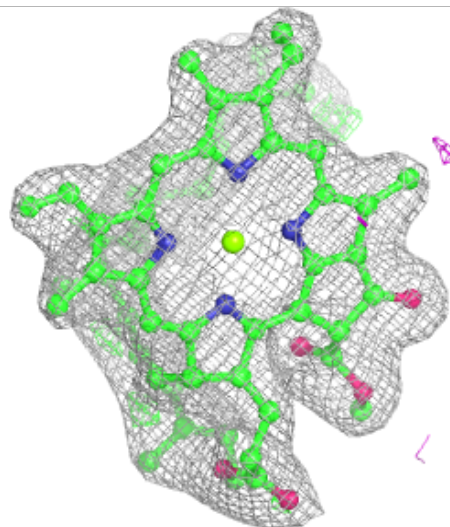
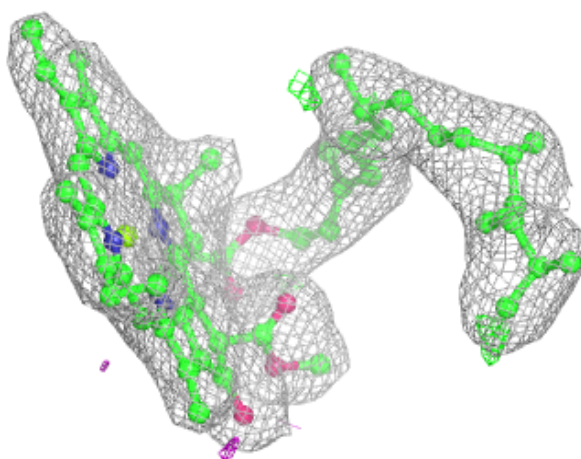
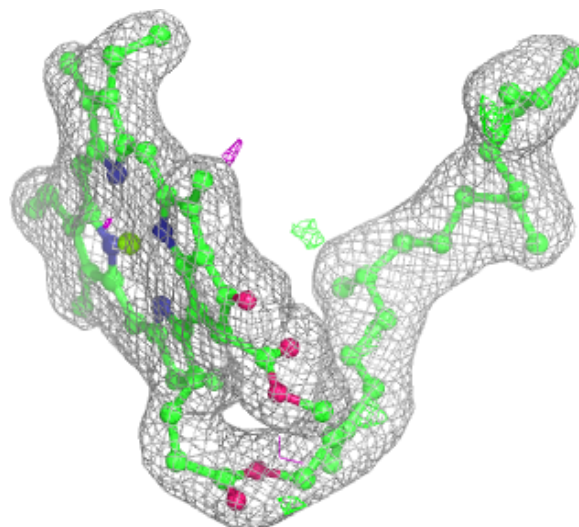
**Electron density around CLA b 610:**

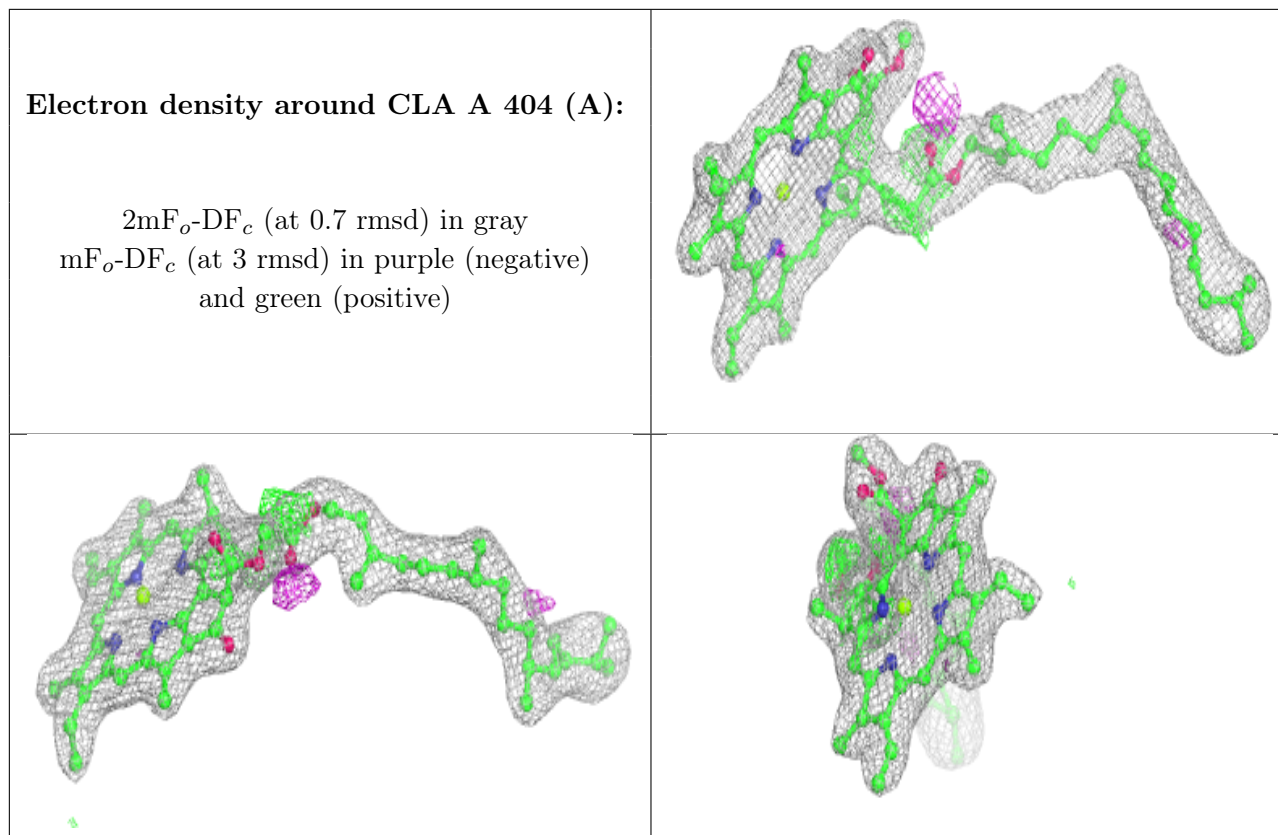
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

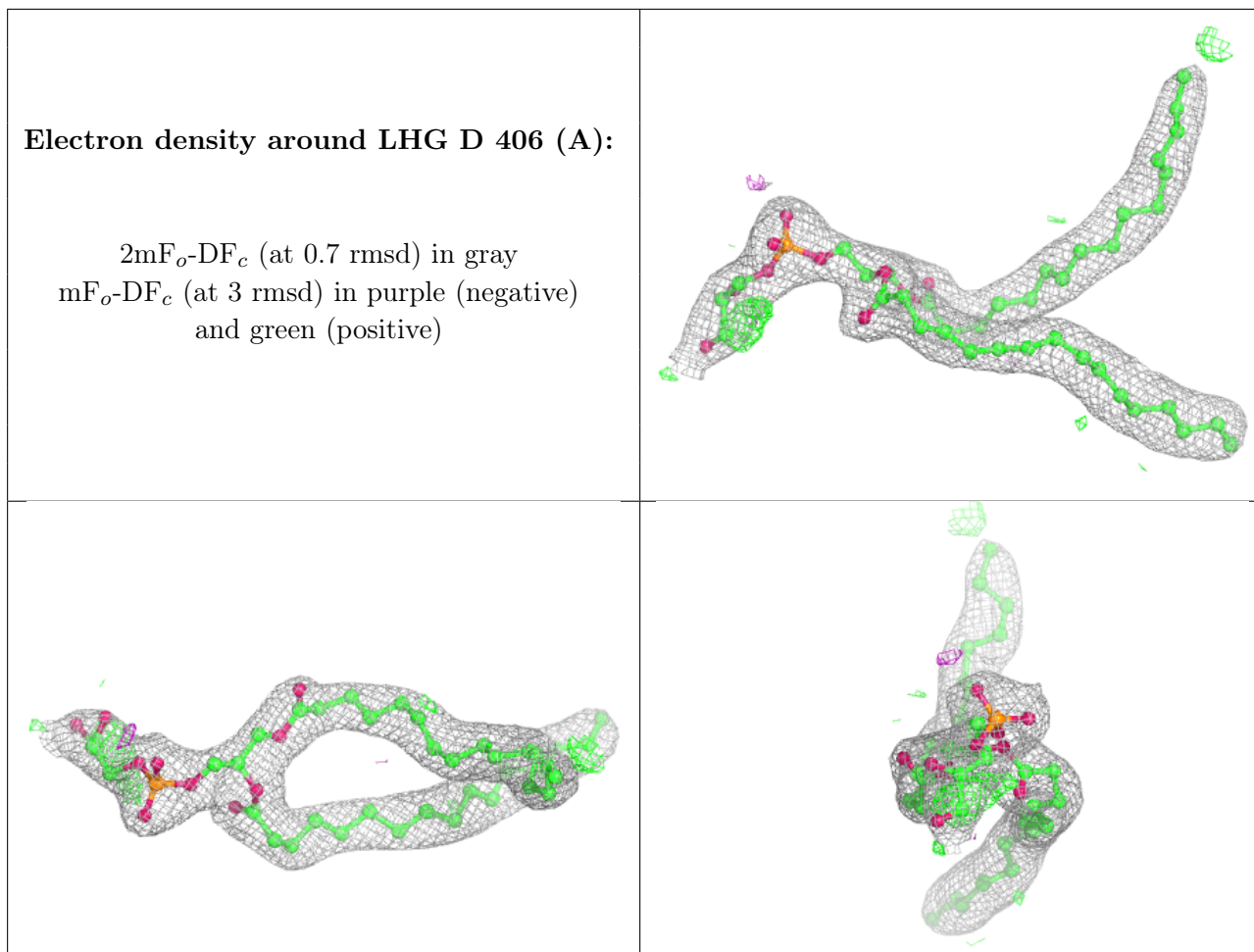


**Electron density around CLA B 613:**

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

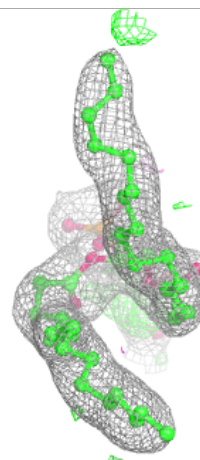
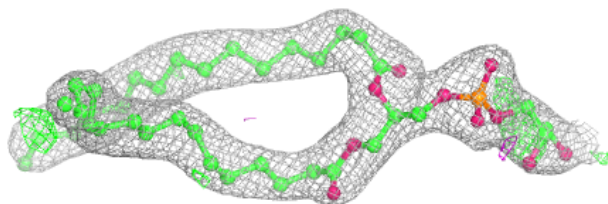
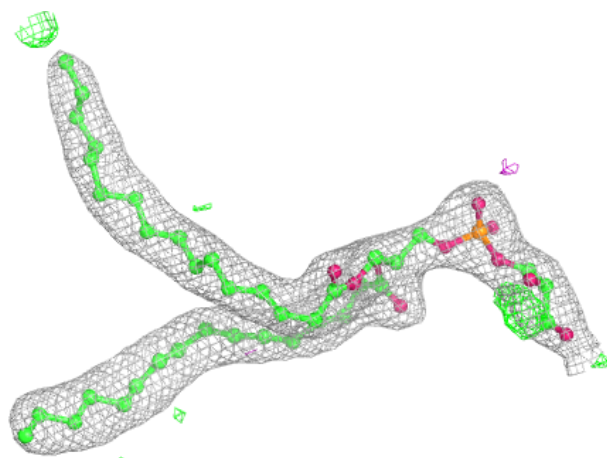






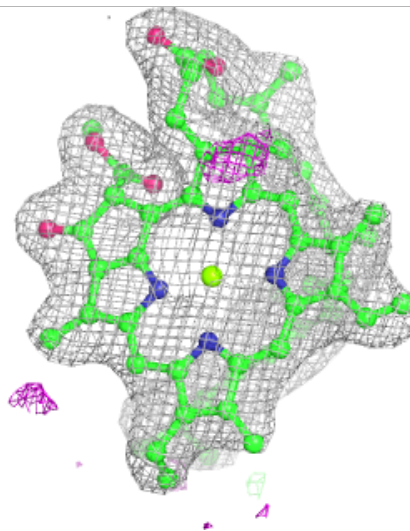
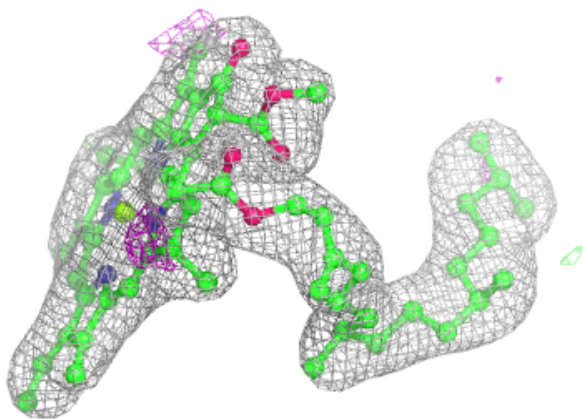
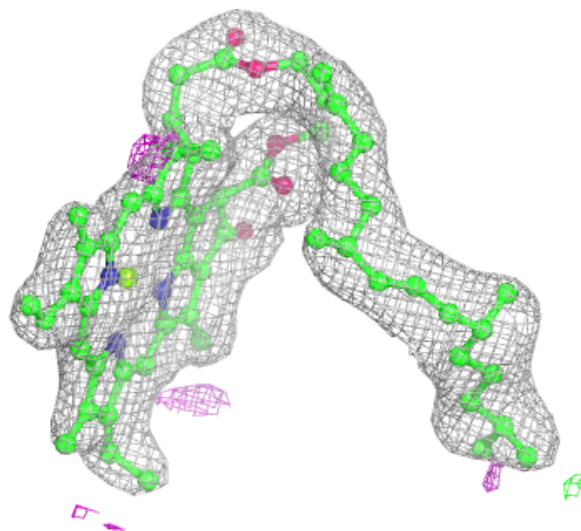
**Electron density around LHG D 406 (B):**

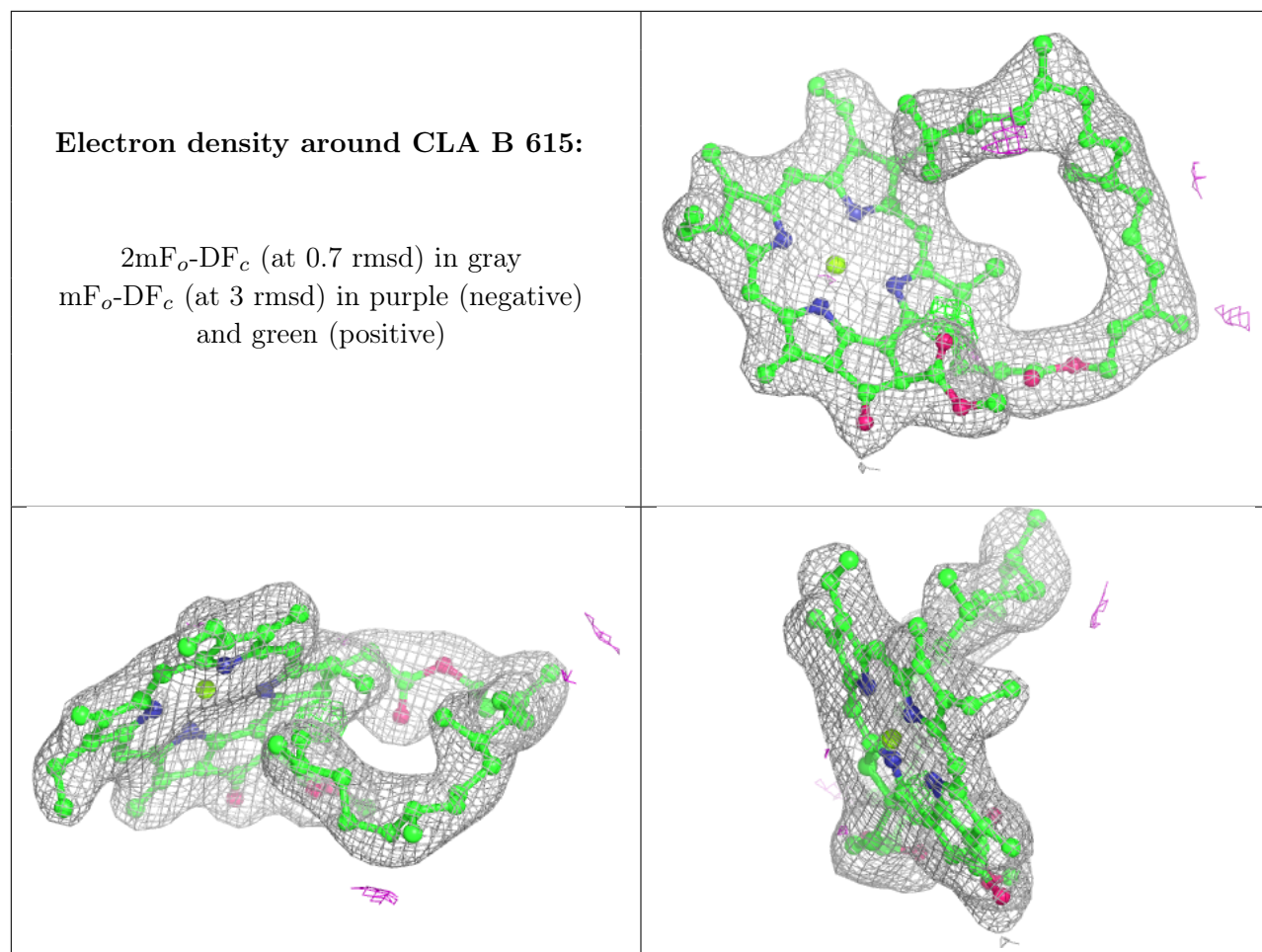
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA b 613:**

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

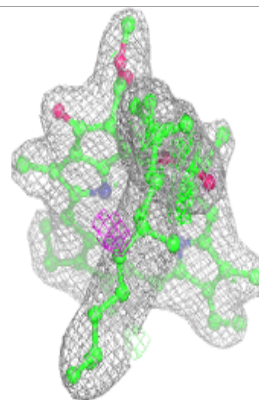
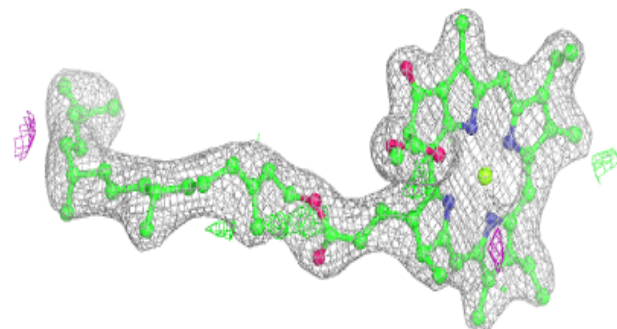
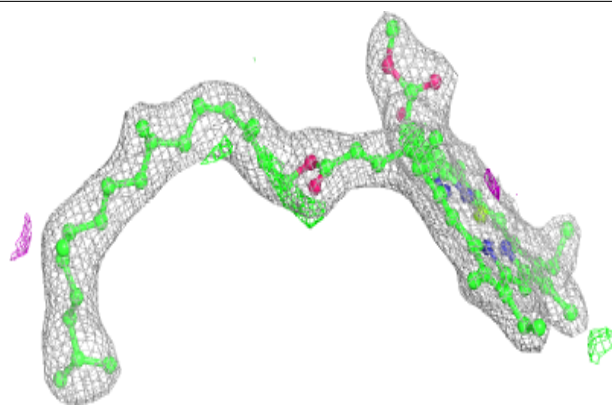




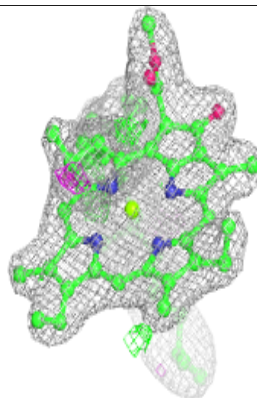
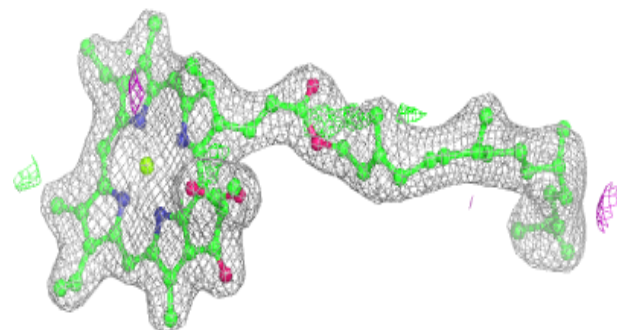
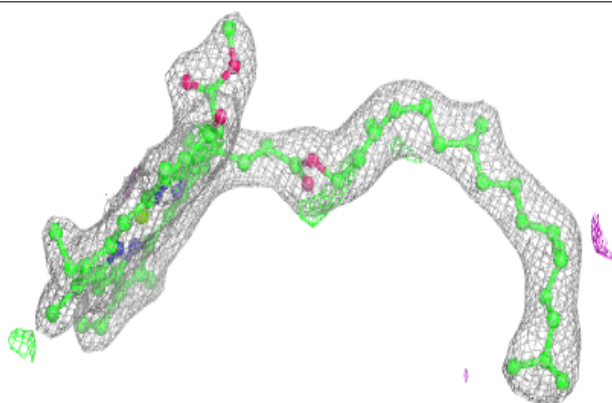


**Electron density around CLA D 402 (A):**

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

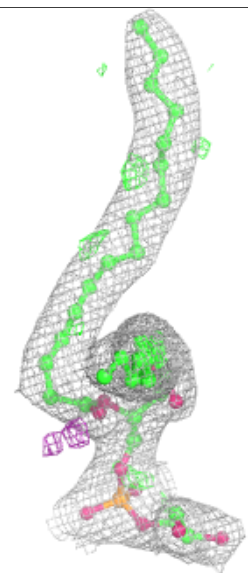
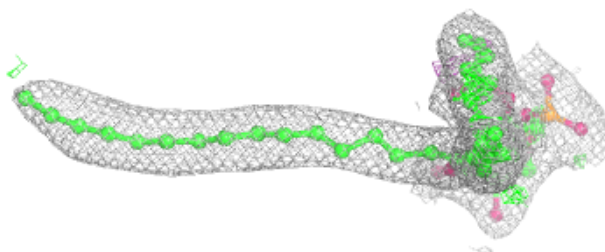
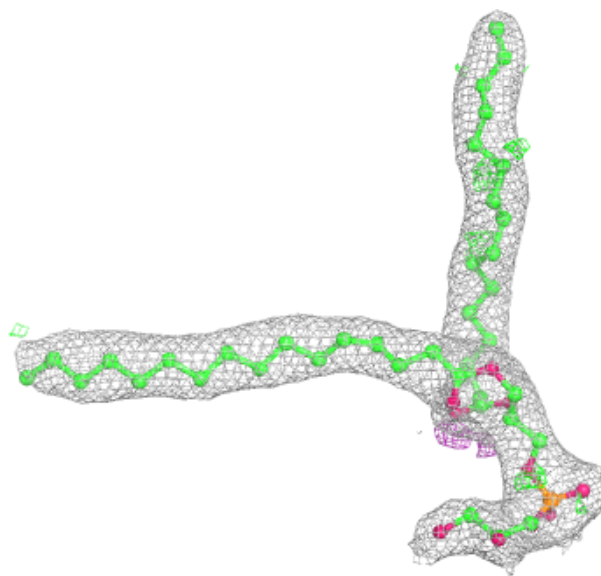
**Electron density around CLA D 402 (B):**

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



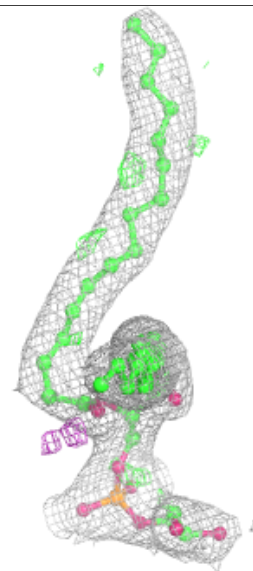
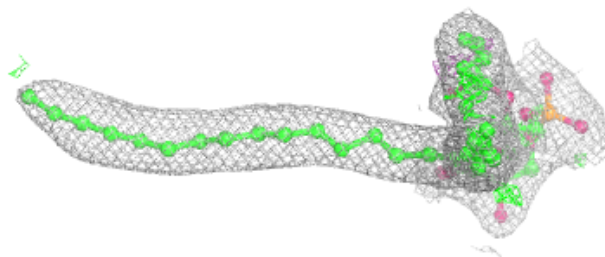
**Electron density around LHG L 101 (A):**

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



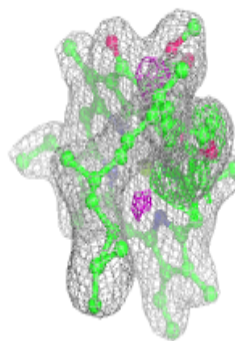
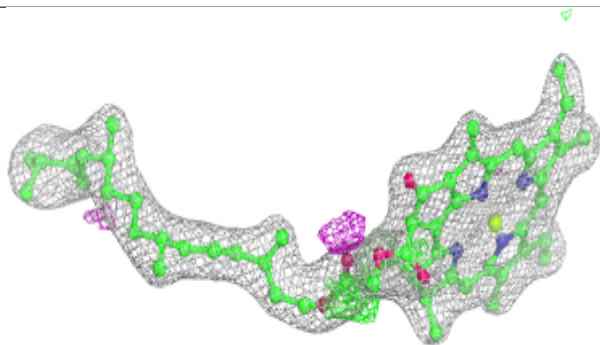
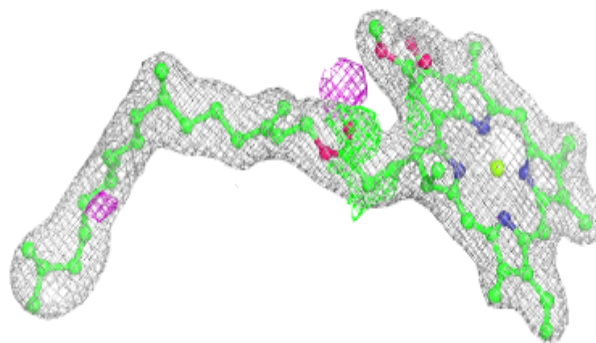
**Electron density around LHG L 101 (B):**

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

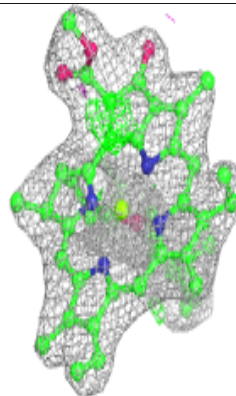
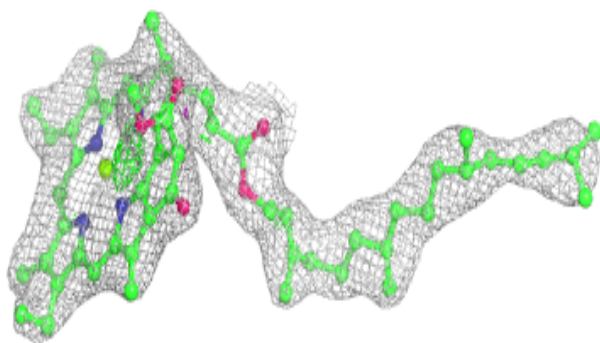
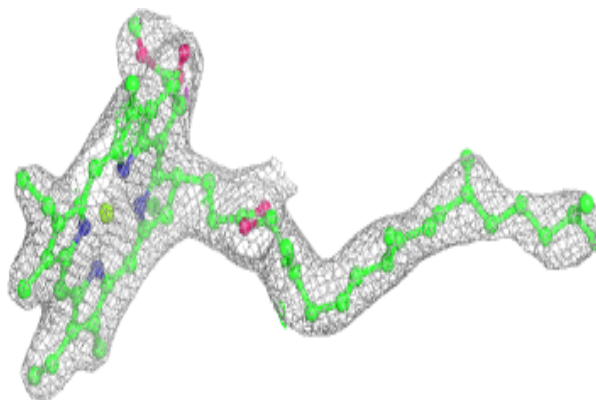


**Electron density around CLA A 404 (B):**

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

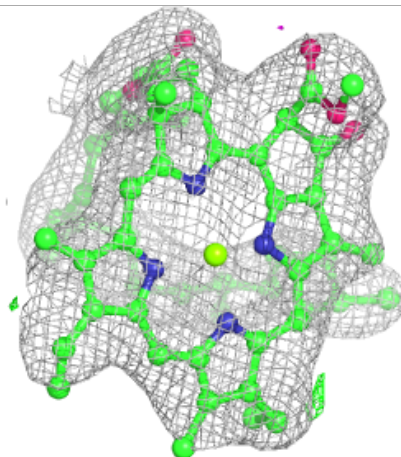
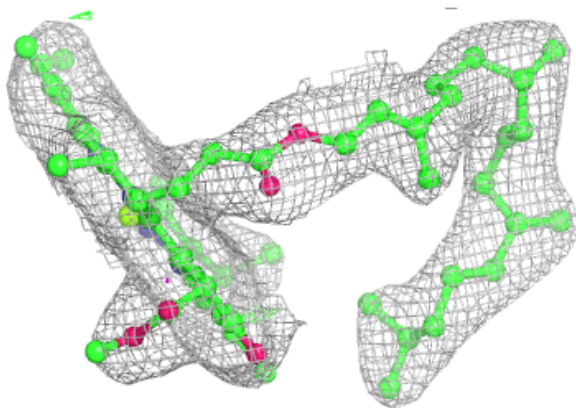
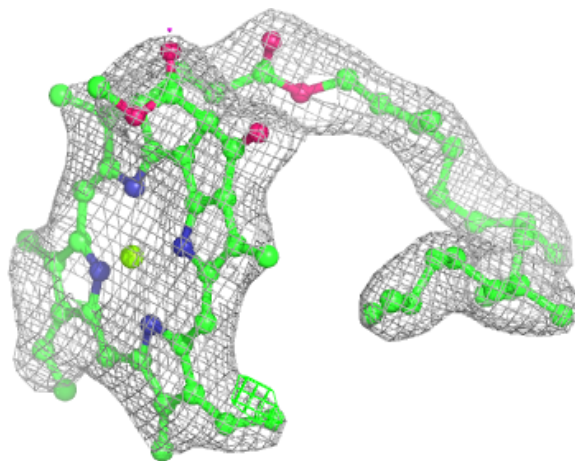
**Electron density around CLA c 502:**

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



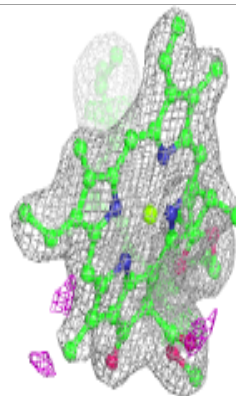
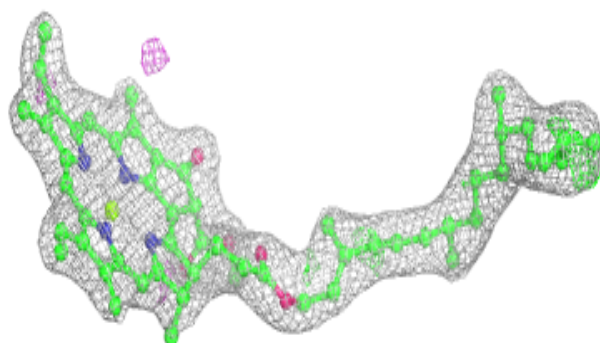
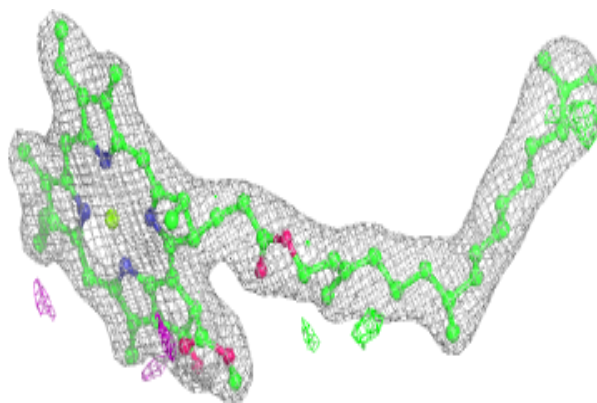
**Electron density around CLA c 503:**

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

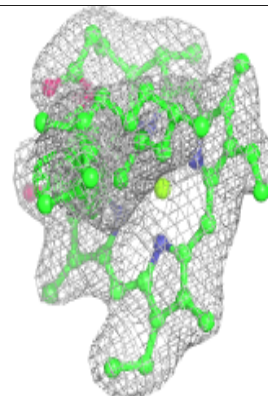
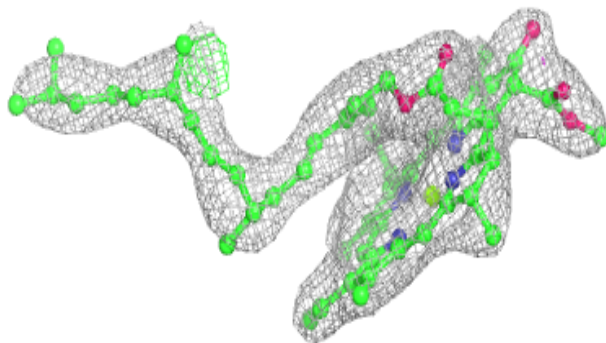
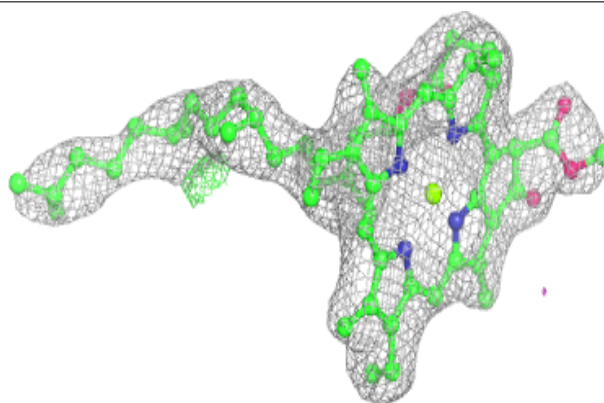


**Electron density around CLA a 404 (A):**

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

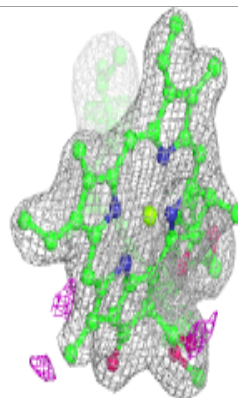
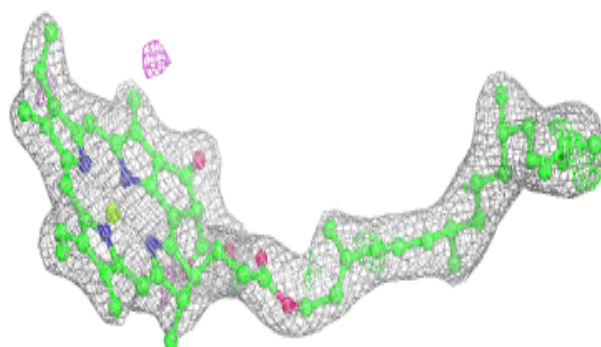
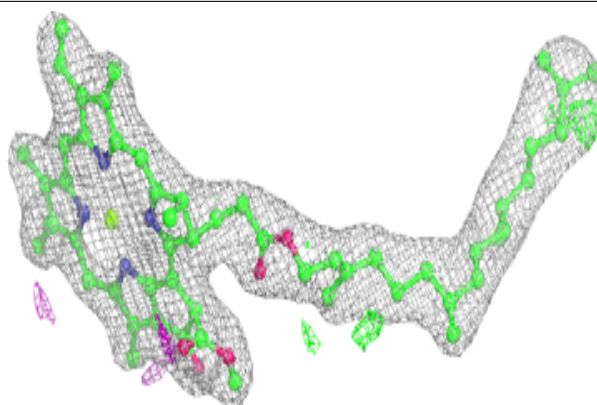
**Electron density around CLA c 505:**

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

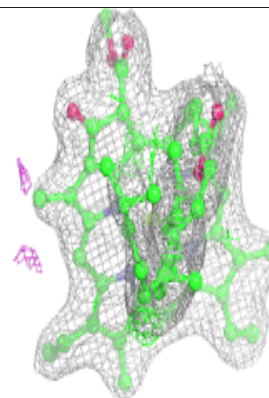
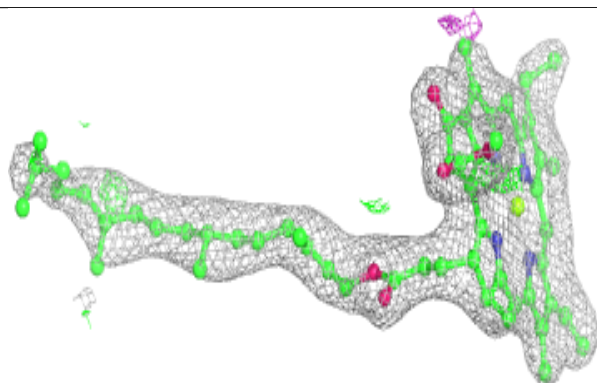
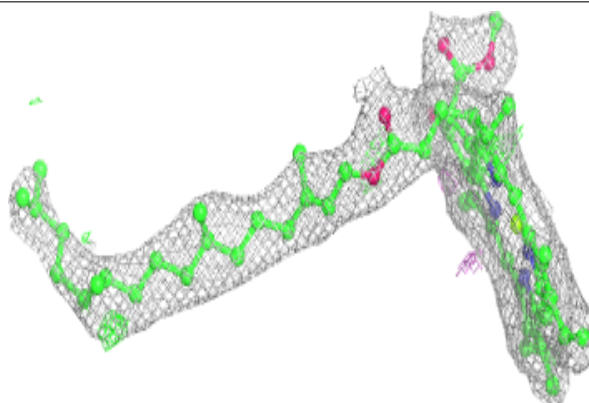


**Electron density around CLA a 404 (B):**

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

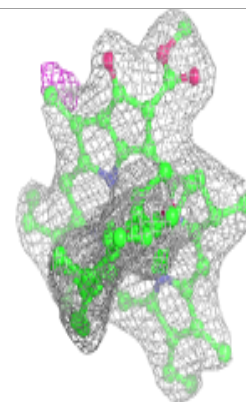
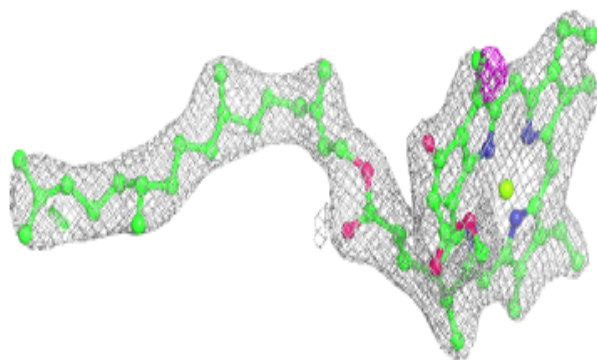
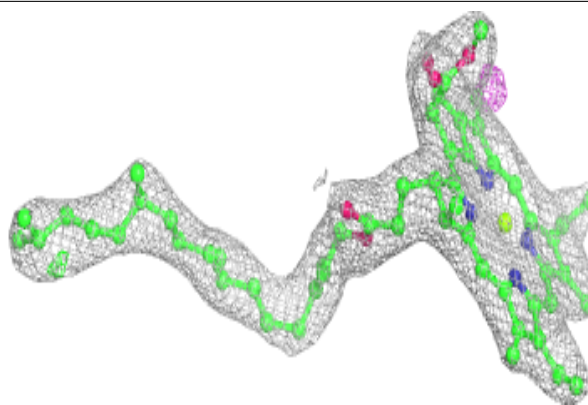
**Electron density around CLA B 604:**

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

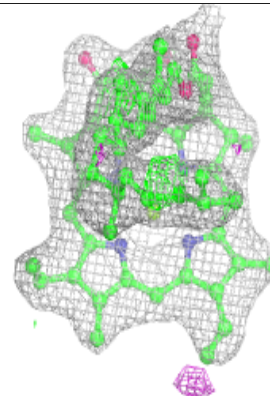
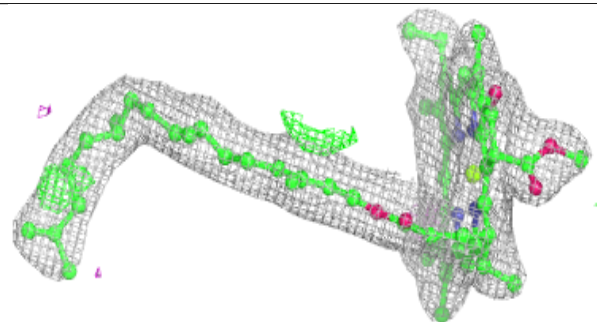
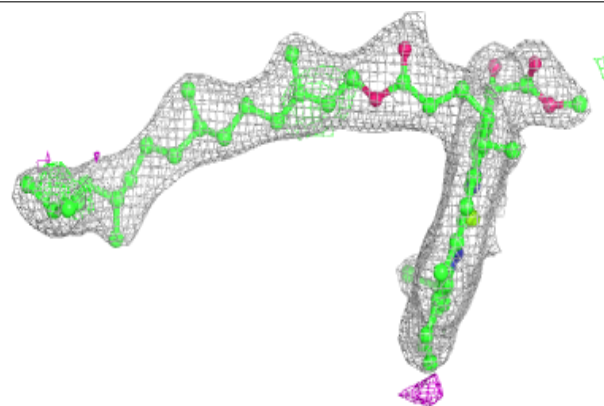


**Electron density around CLA C 503:**

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

**Electron density around CLA B 605:**

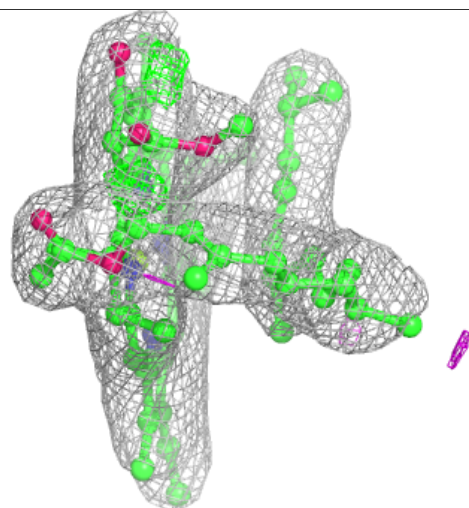
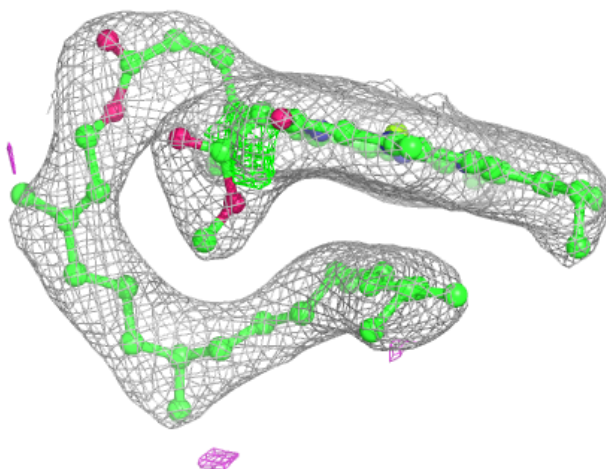
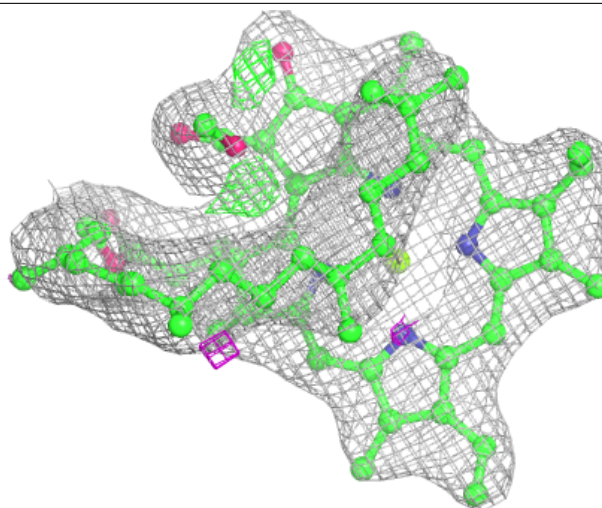
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





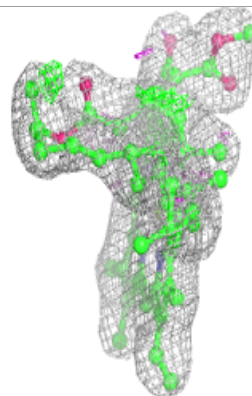
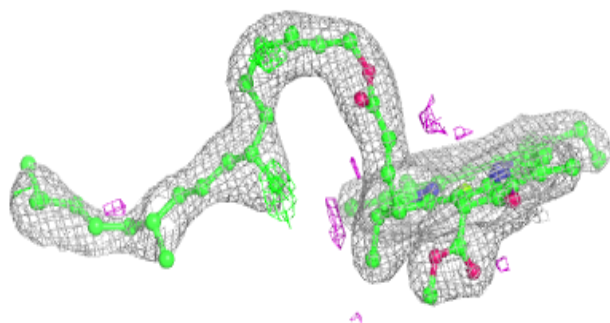
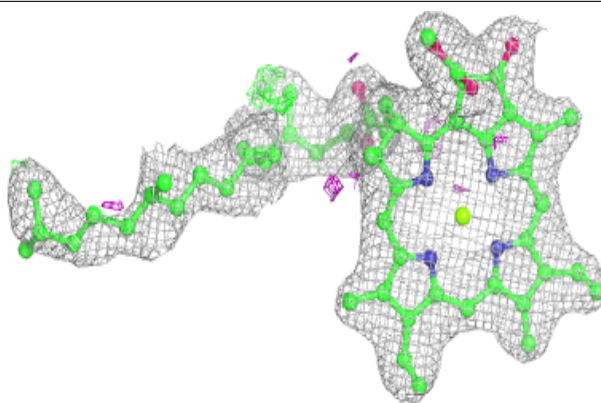
**Electron density around CLA c 510:**

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

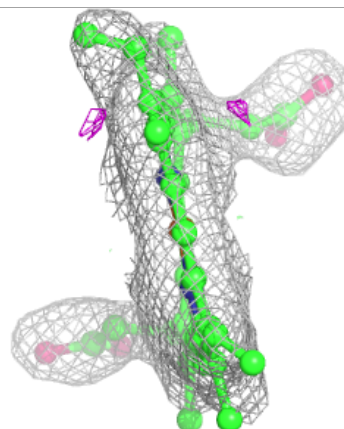
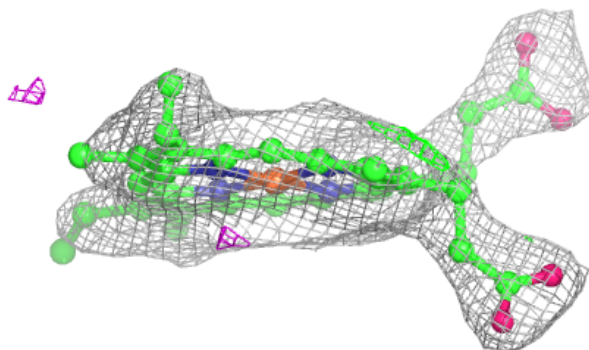
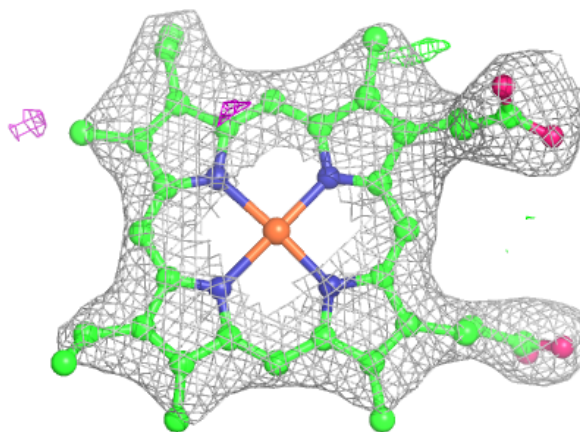


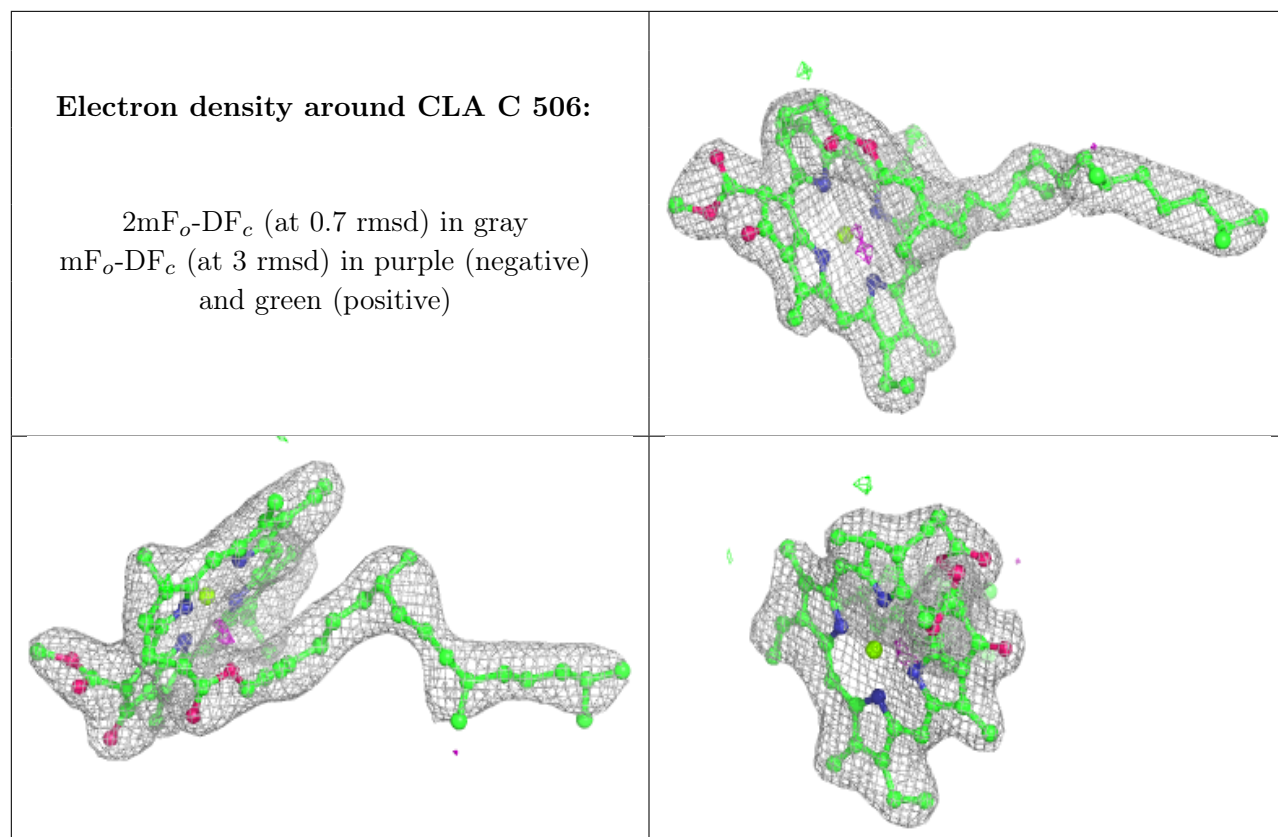
**Electron density around CLA A 406 (A):**

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

**Electron density around HEM E 102:**

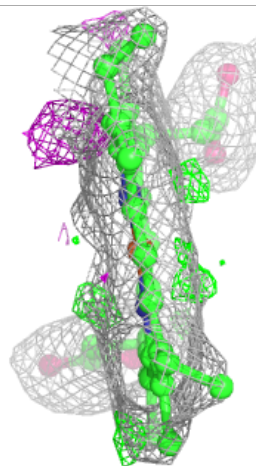
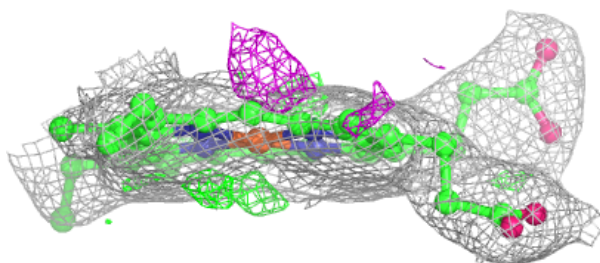
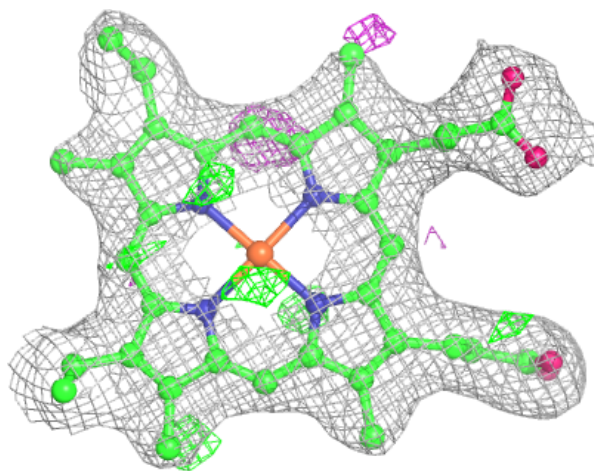
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





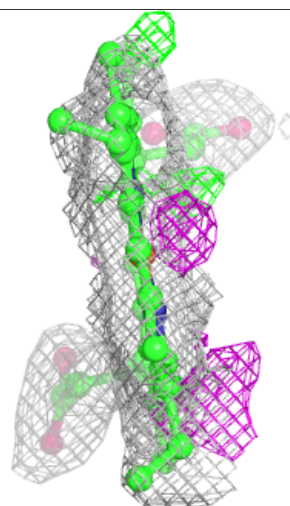
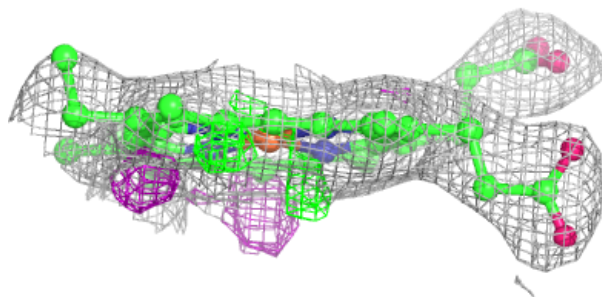
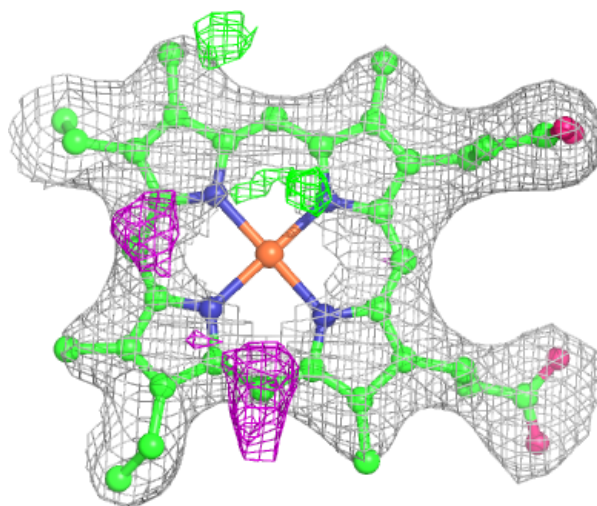
**Electron density around HEC V 201:**

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



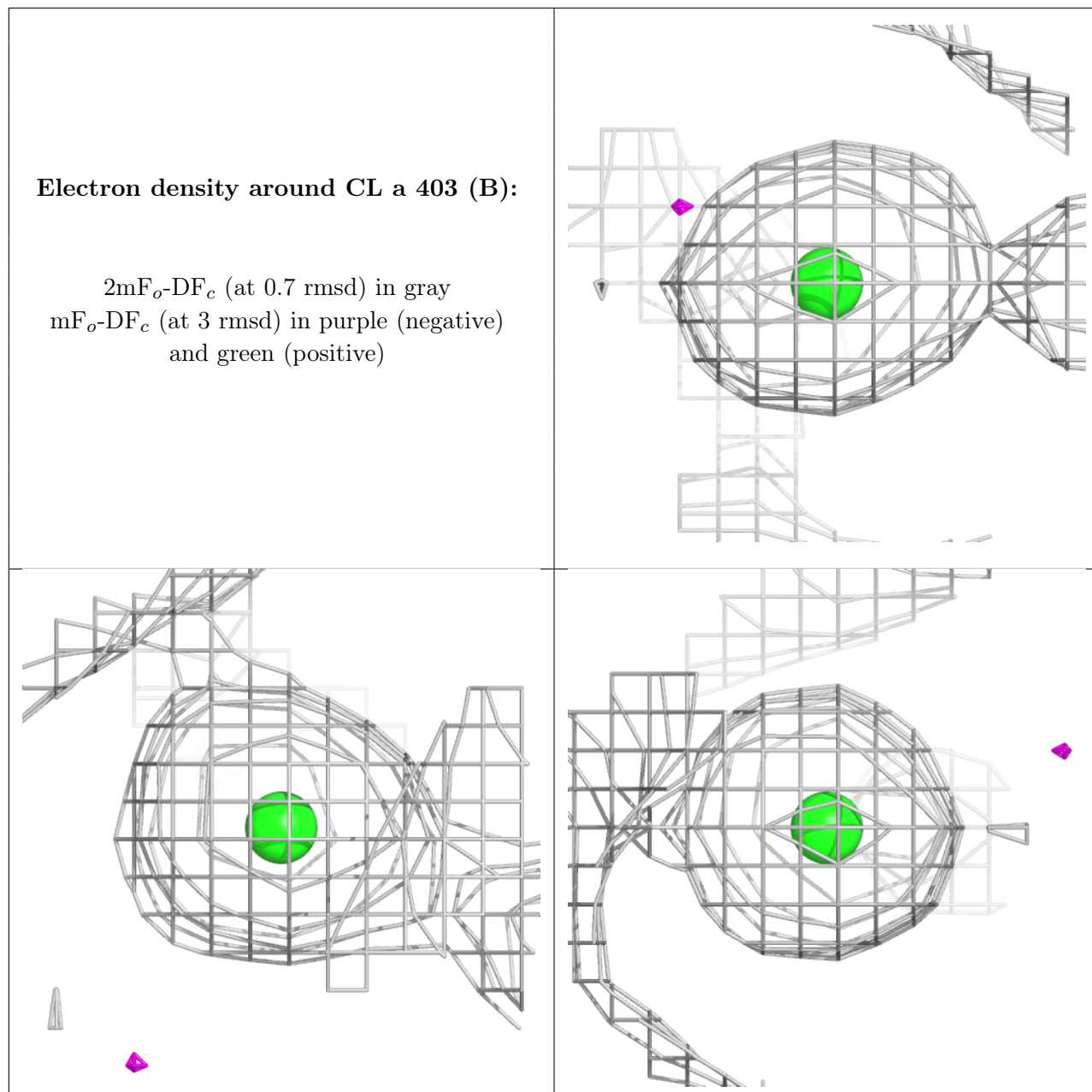
**Electron density around HEC v 201:**

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



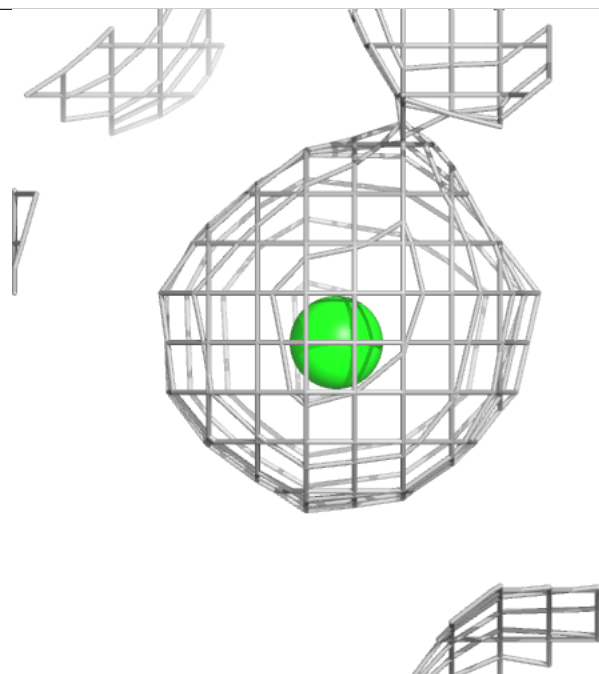
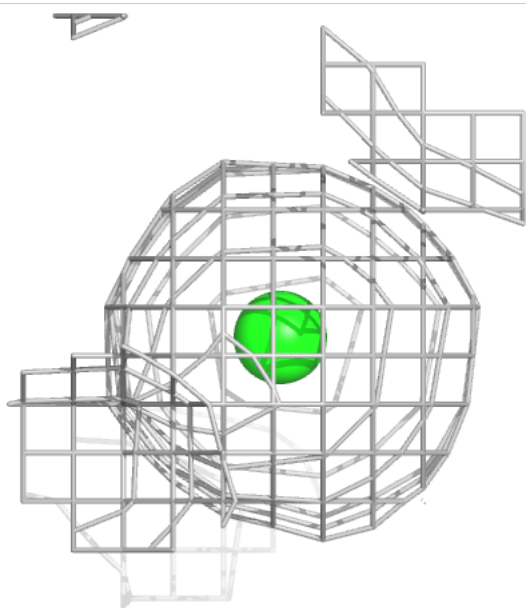
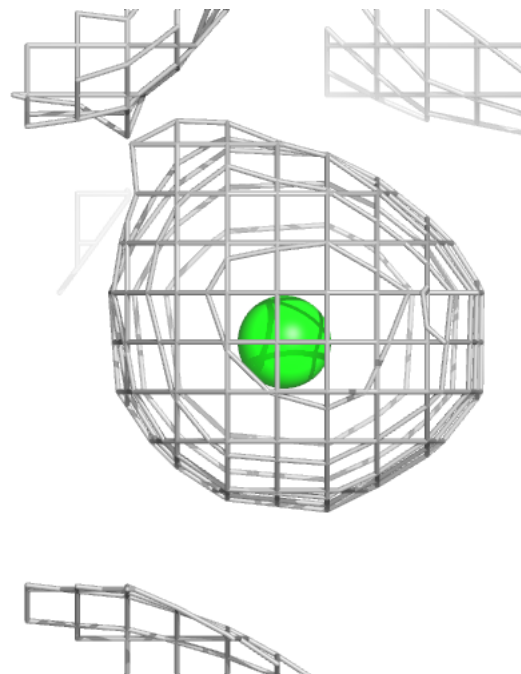
**Electron density around CL a 403 (B):**

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



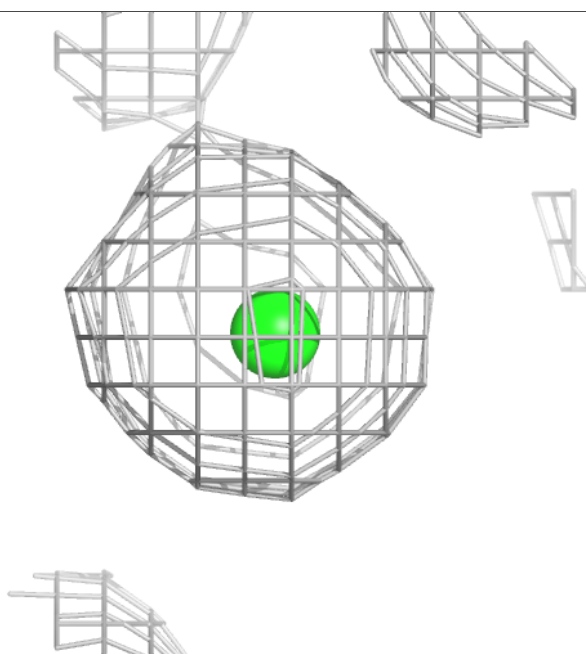
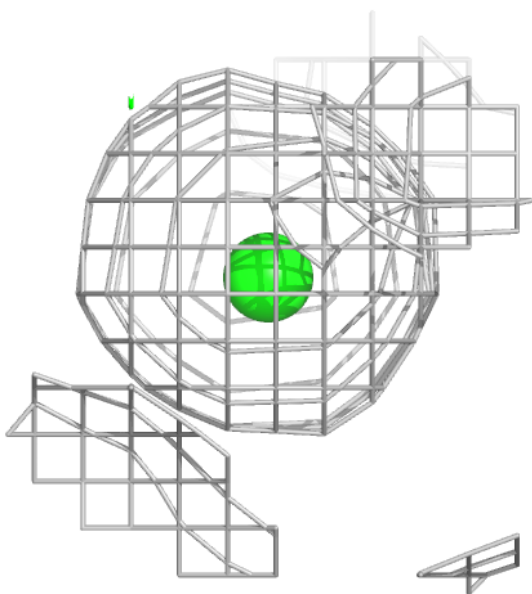
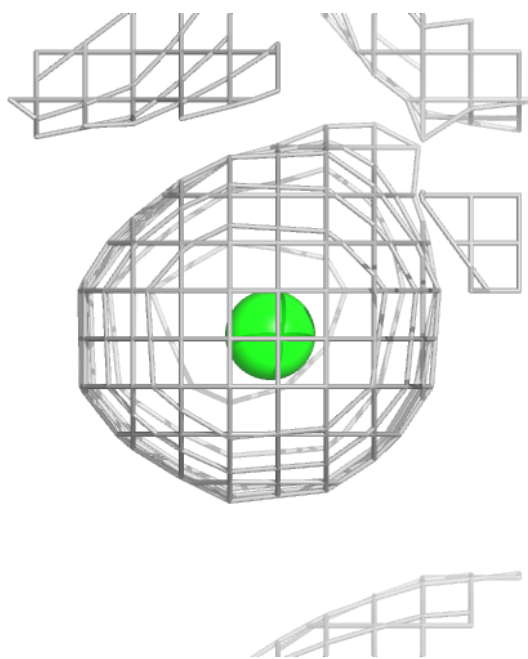
**Electron density around CL a 402 (A):**

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



**Electron density around CL a 402 (B):**

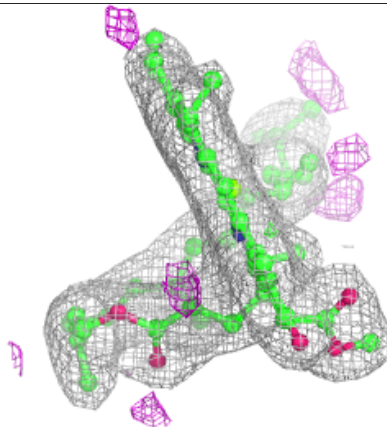
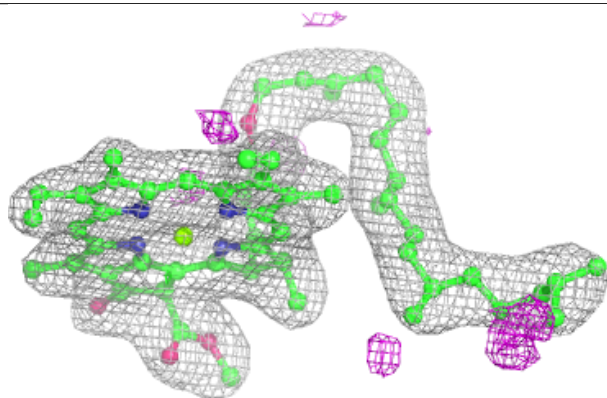
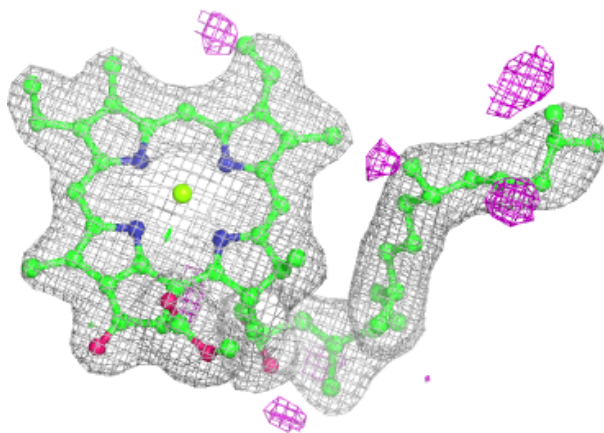
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





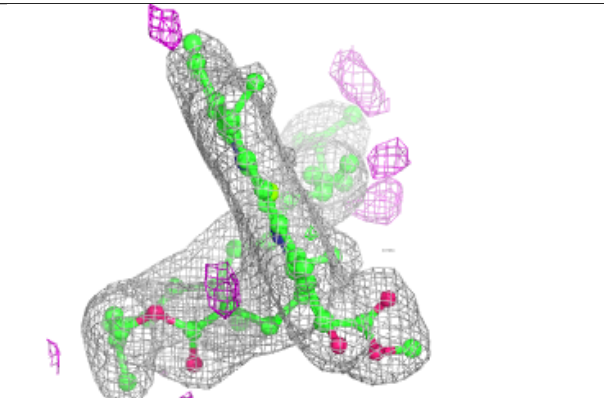
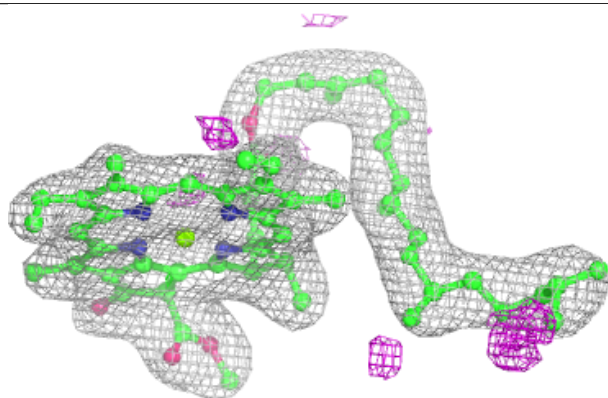
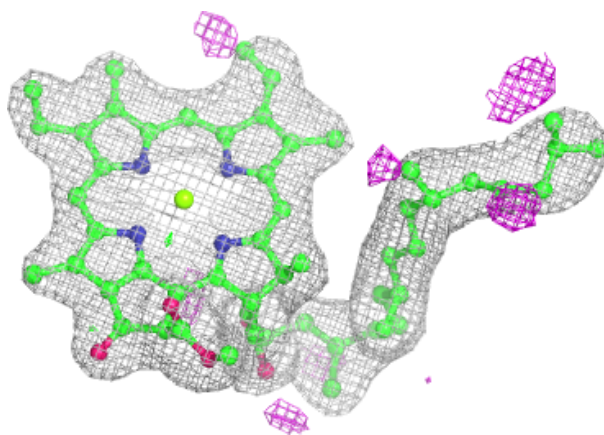
**Electron density around CLA d 402 (A):**

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

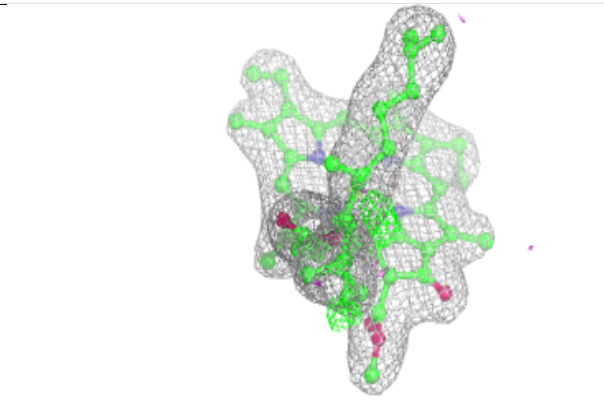
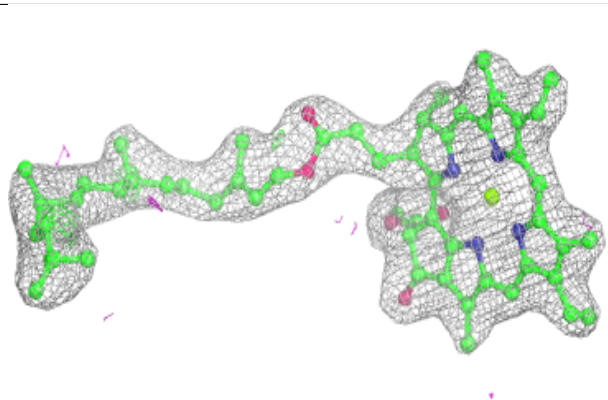
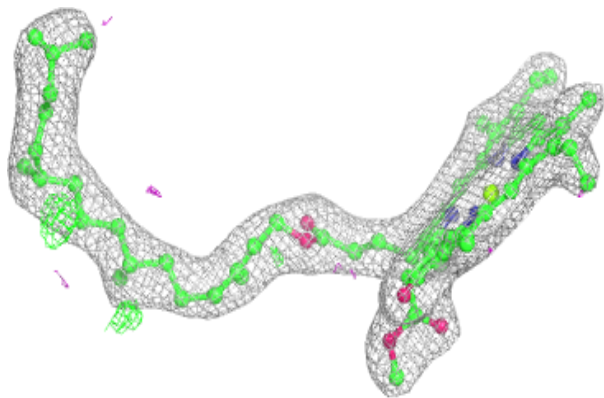


**Electron density around CLA d 402 (B):**

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

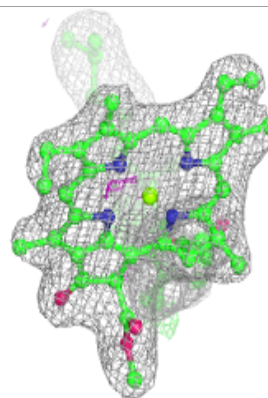
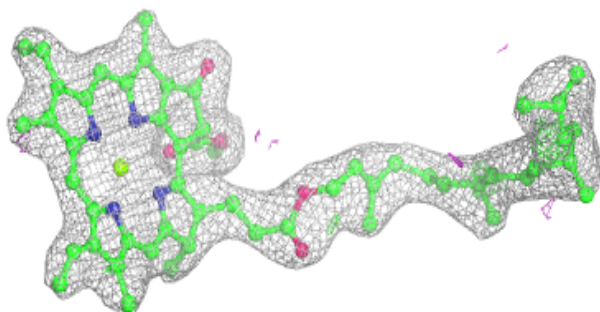
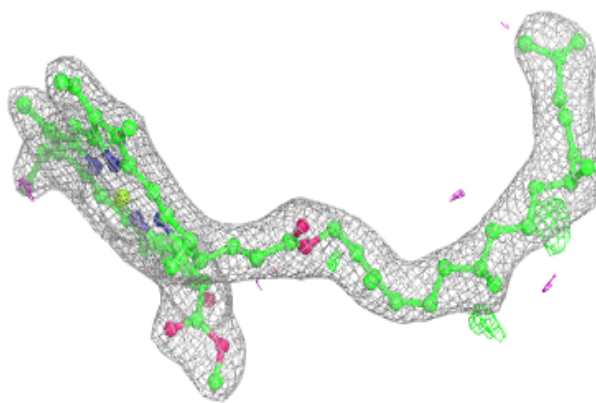
**Electron density around CLA d 403 (A):**

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

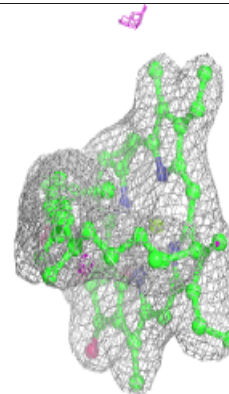
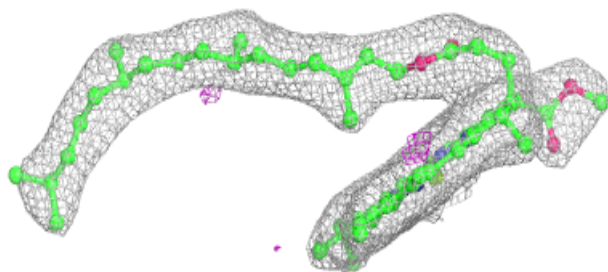
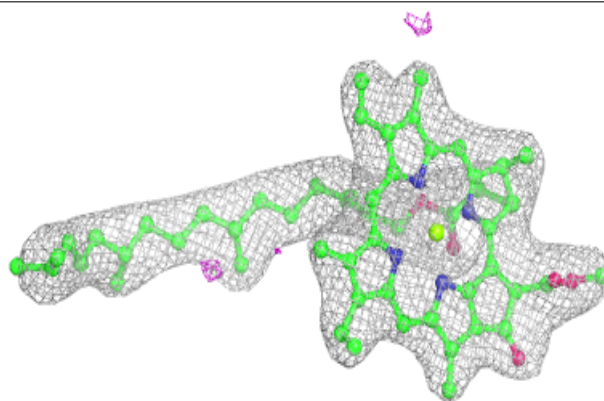


**Electron density around CLA d 403 (B):**

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

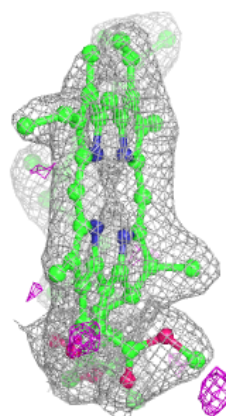
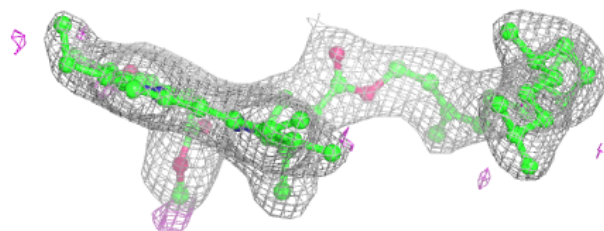
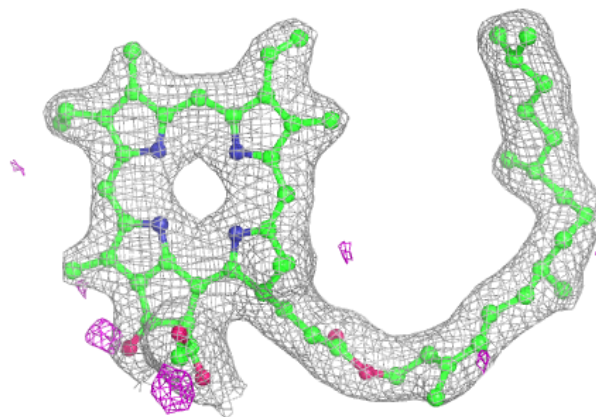
**Electron density around CLA B 608:**

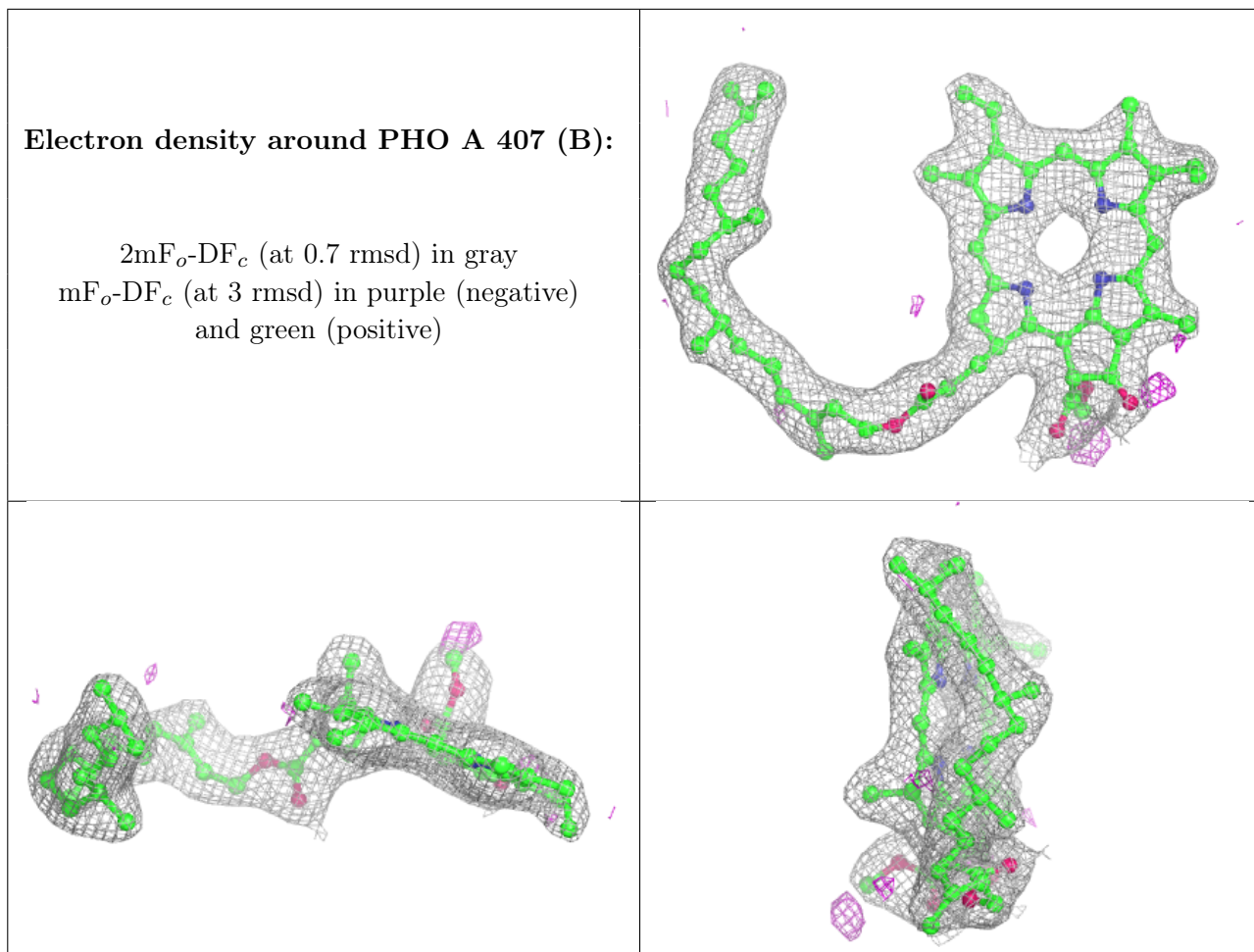
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PHO A 407 (A):**

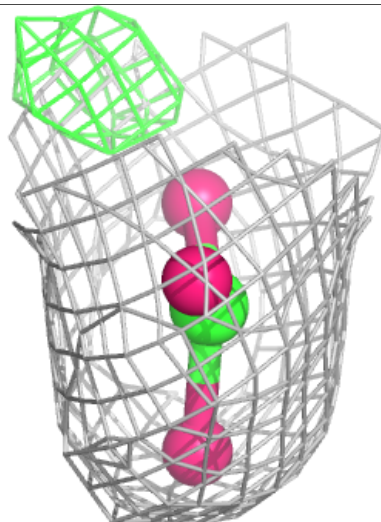
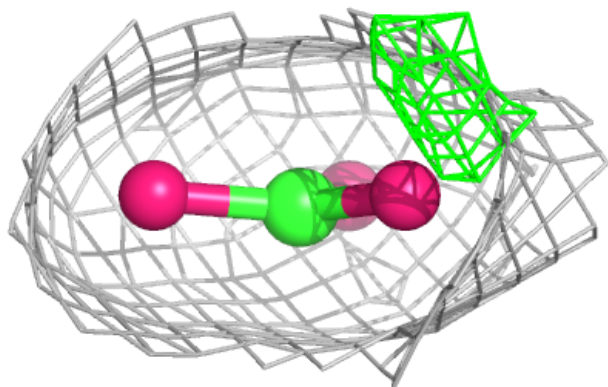
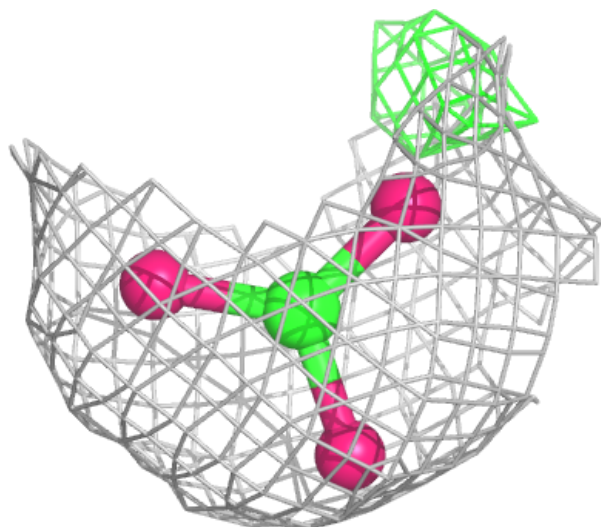
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





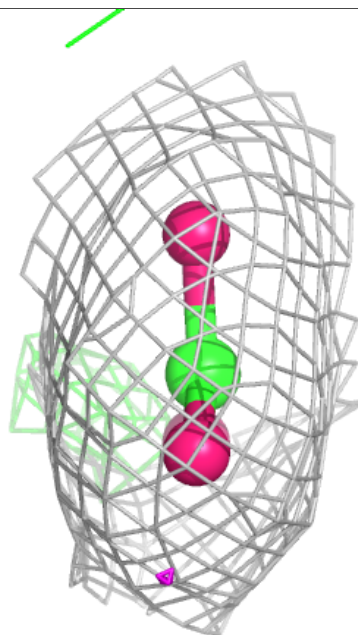
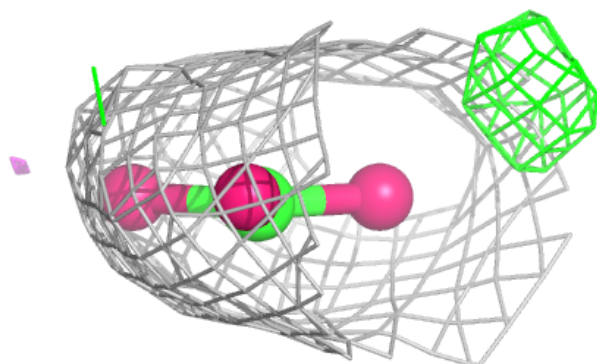
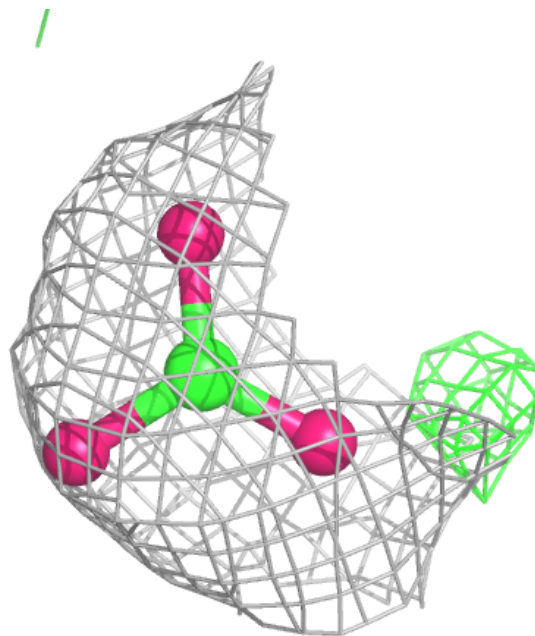
**Electron density around BCT D 401 (A):**

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



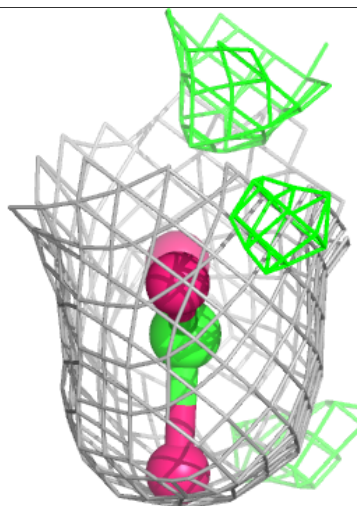
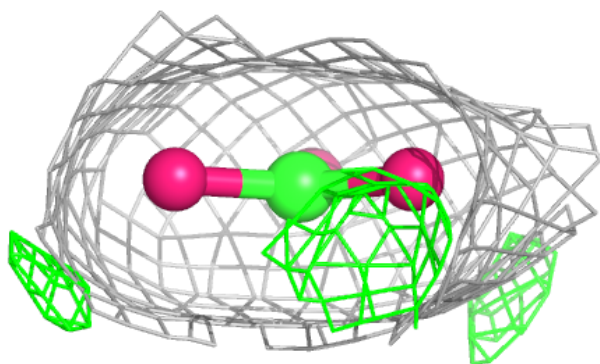
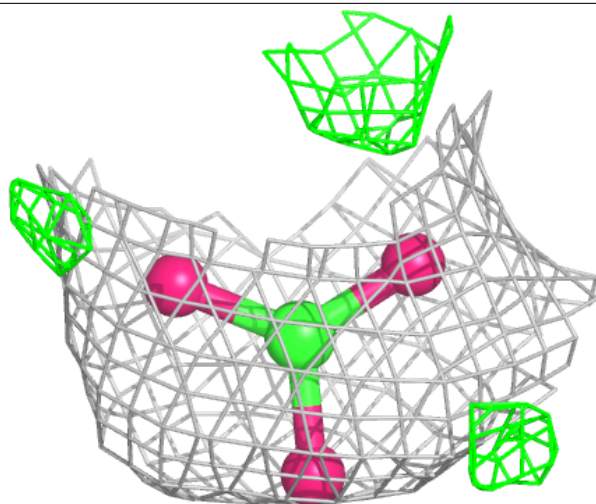
**Electron density around BCT D 401 (B):**

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



**Electron density around BCT d 401 (A):**

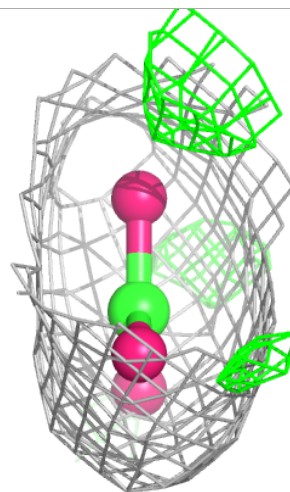
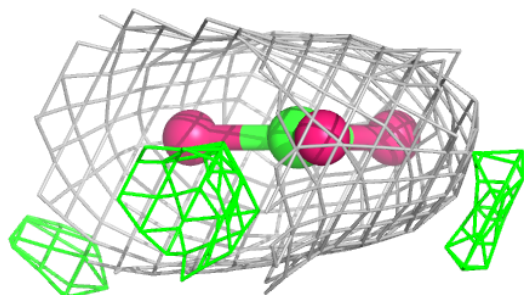
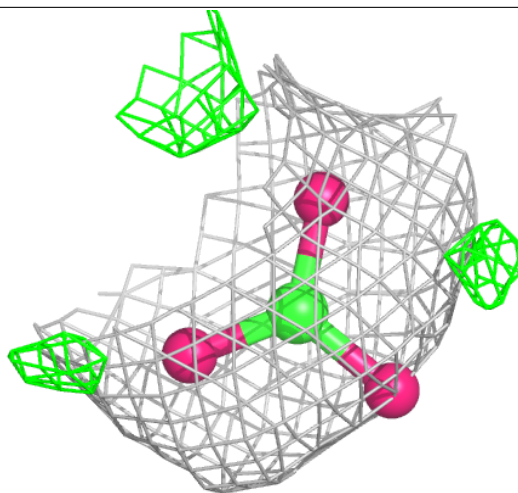
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





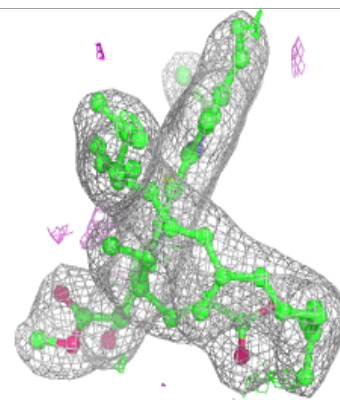
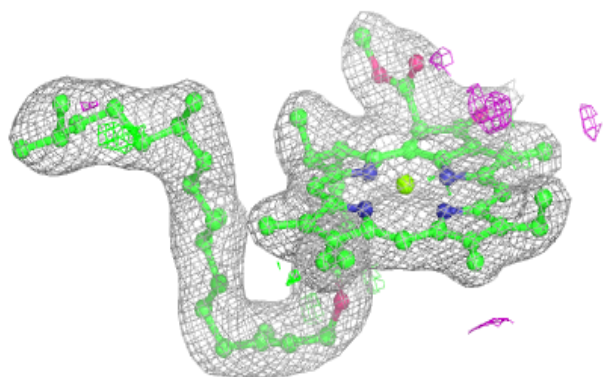
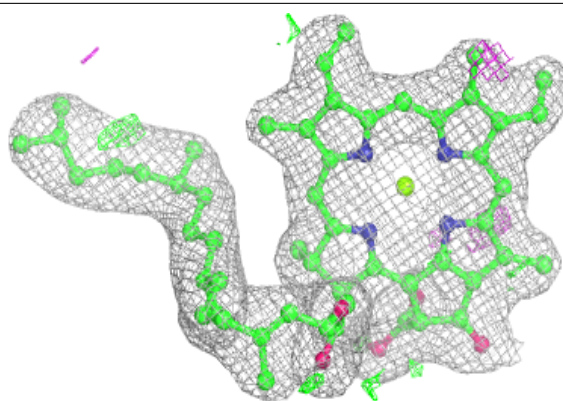
**Electron density around BCT d 401 (B):**

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

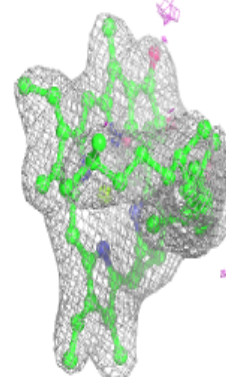
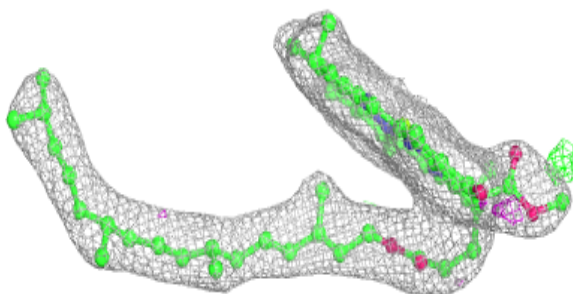
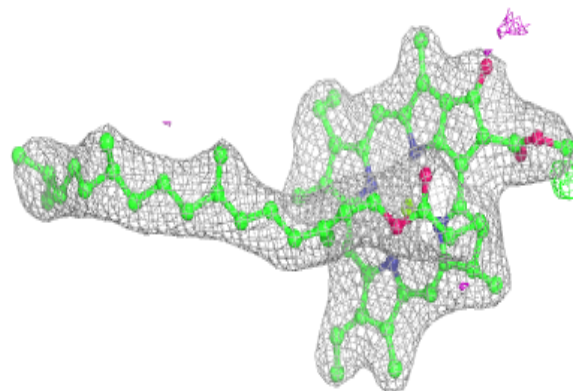


**Electron density around CLA A 405 (A):**

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

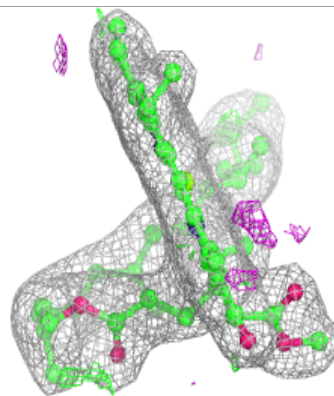
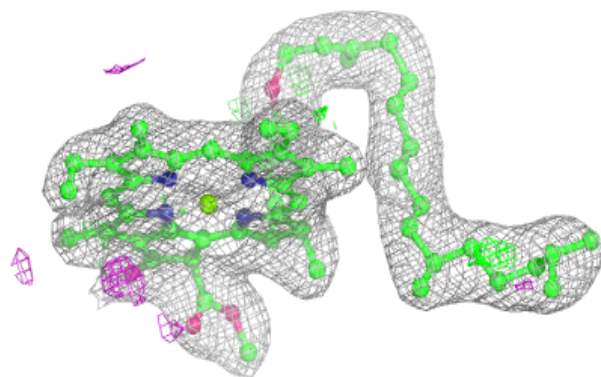
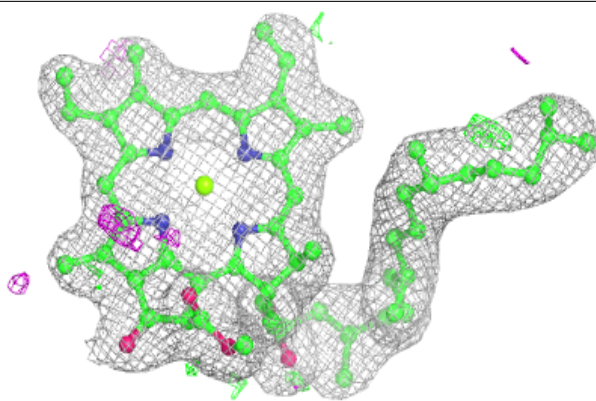
**Electron density around CLA b 608:**

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



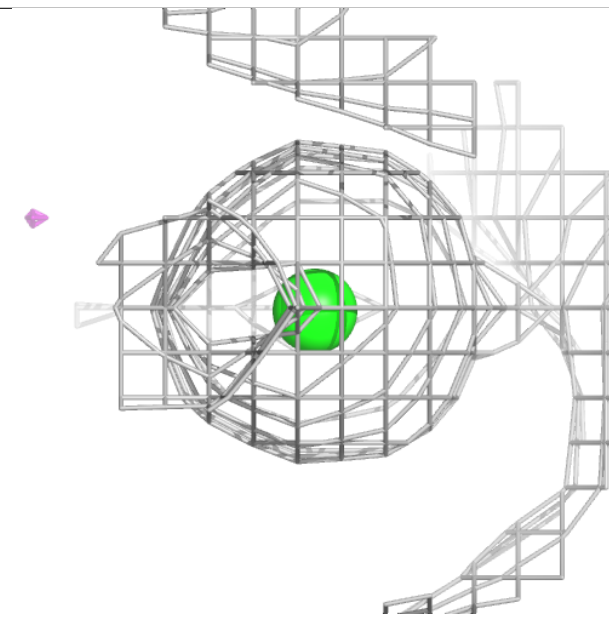
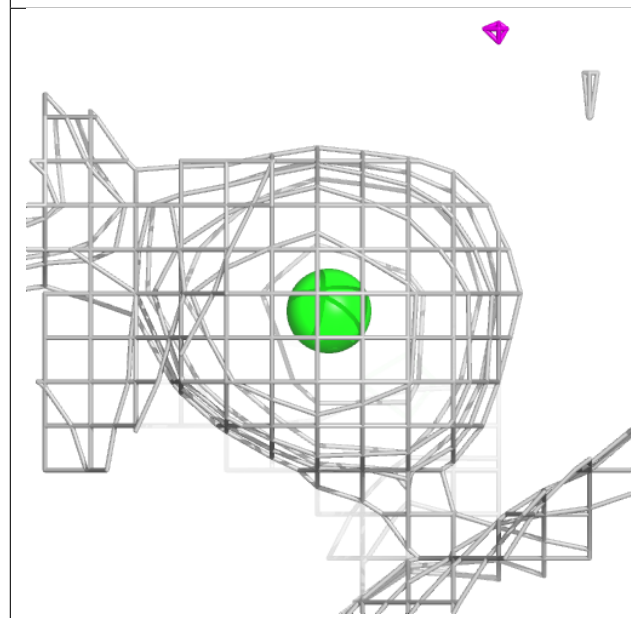
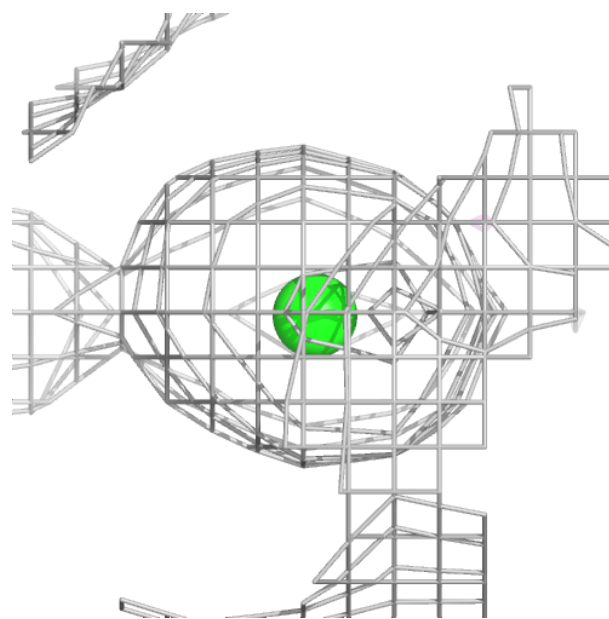
**Electron density around CLA A 405 (B):**

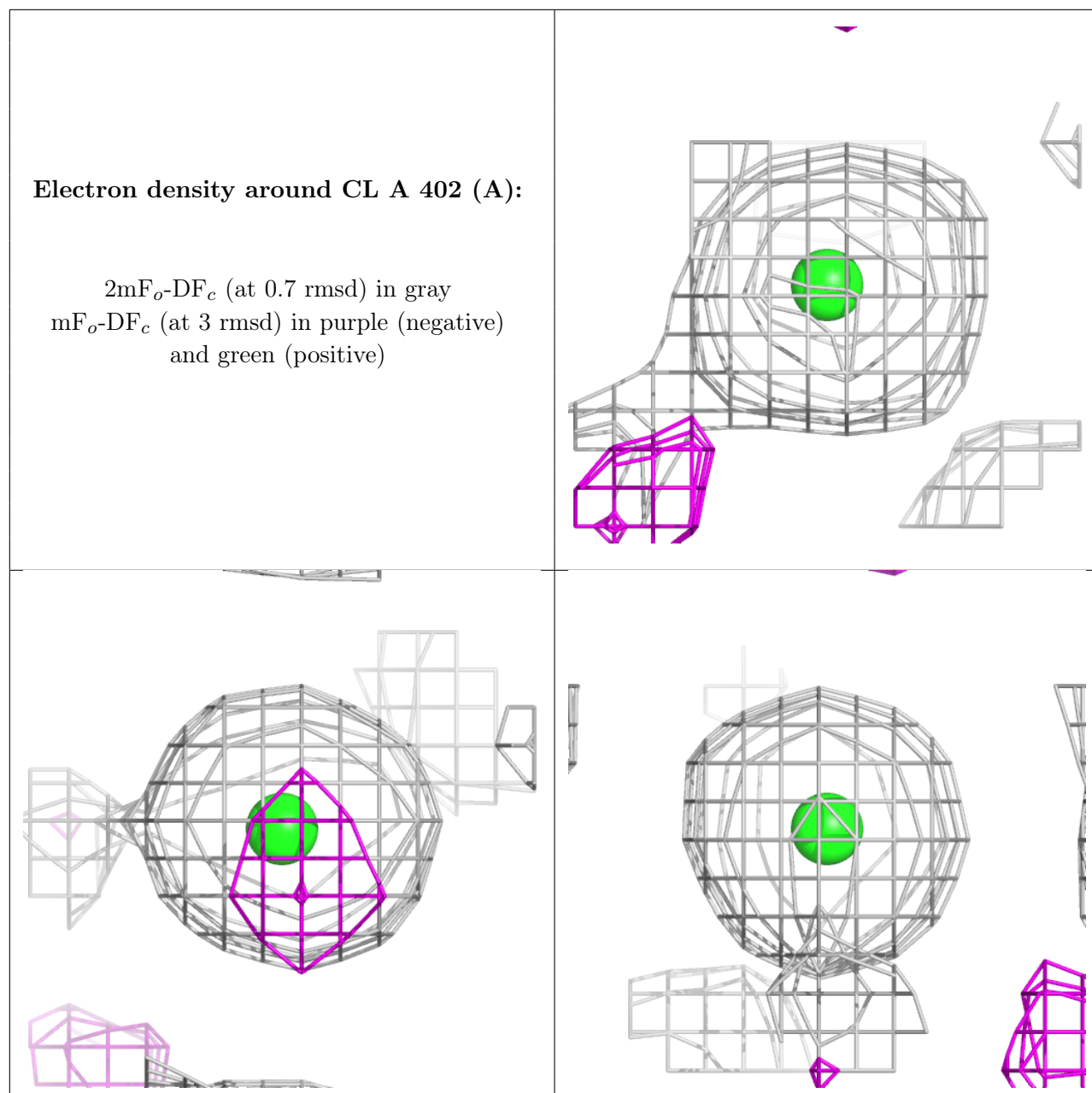
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

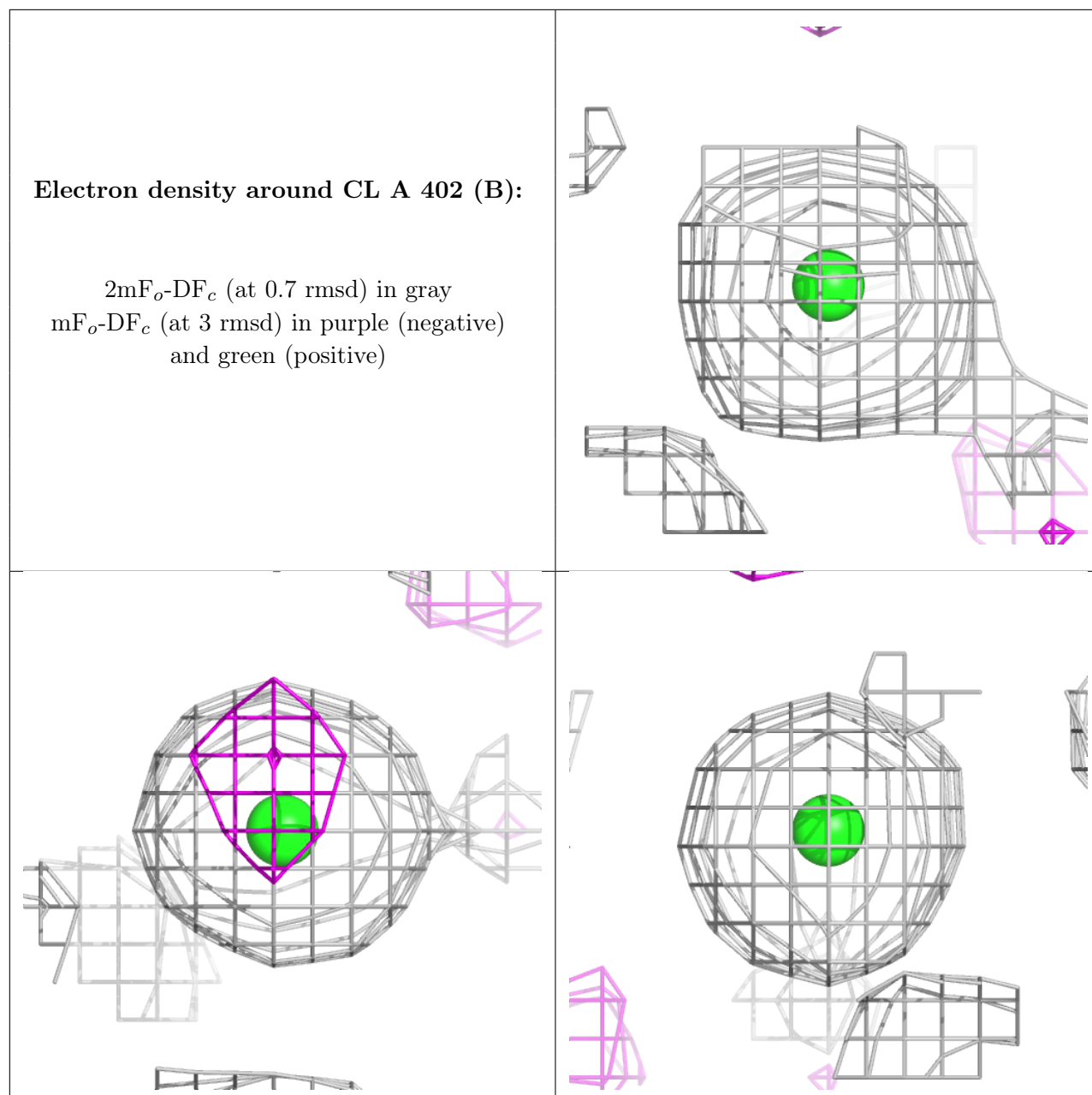


**Electron density around CL a 403 (A):**

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

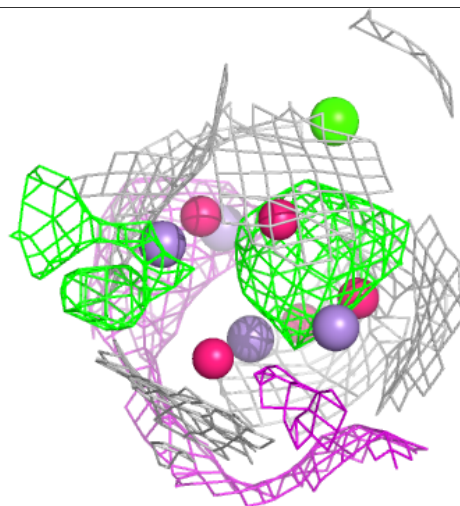
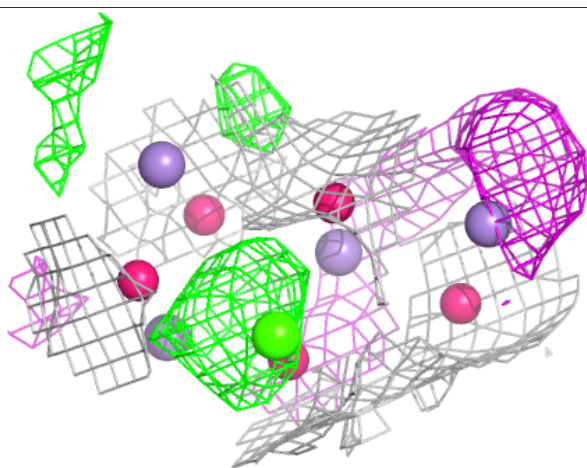
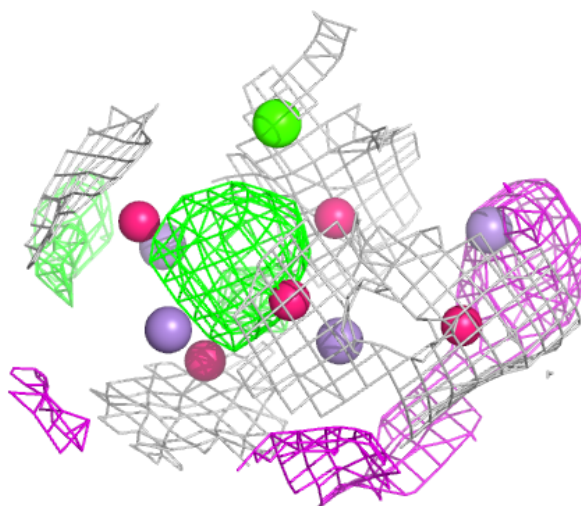






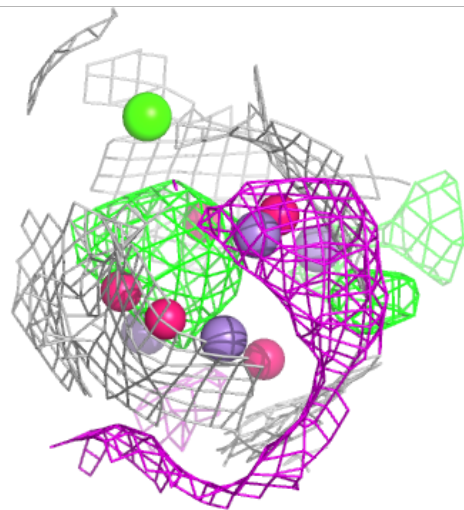
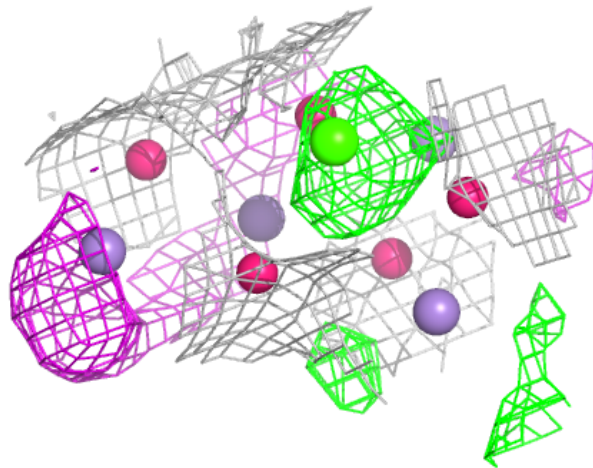
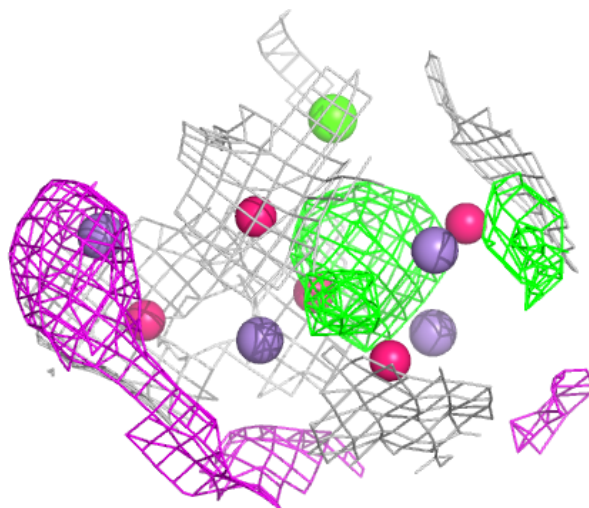
**Electron density around OEX A 413 (A):**

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



**Electron density around OEX A 413 (B):**

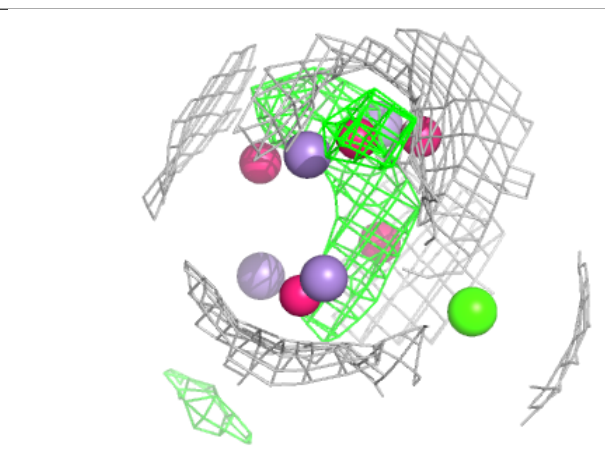
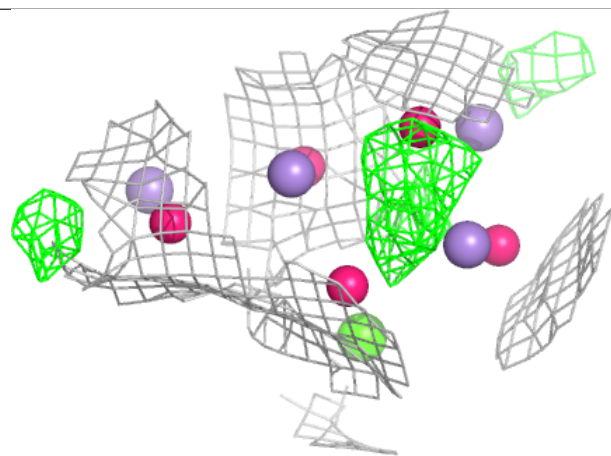
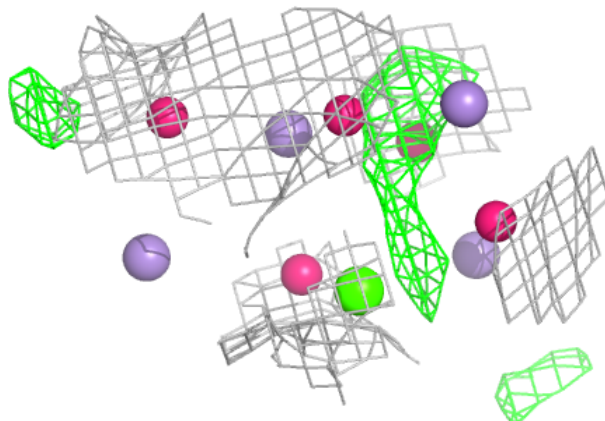
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





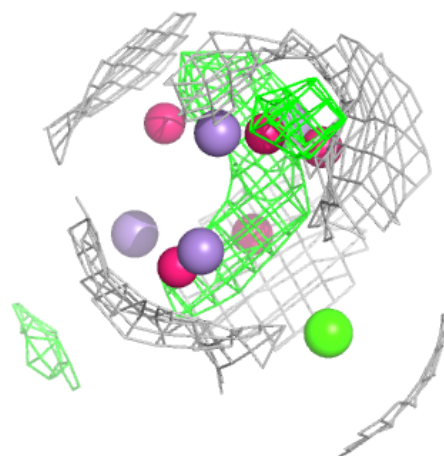
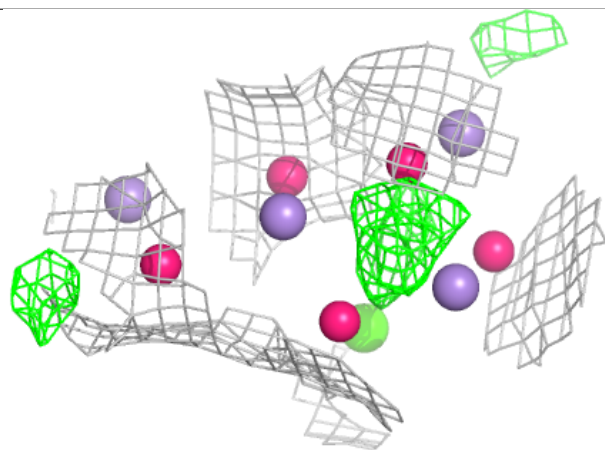
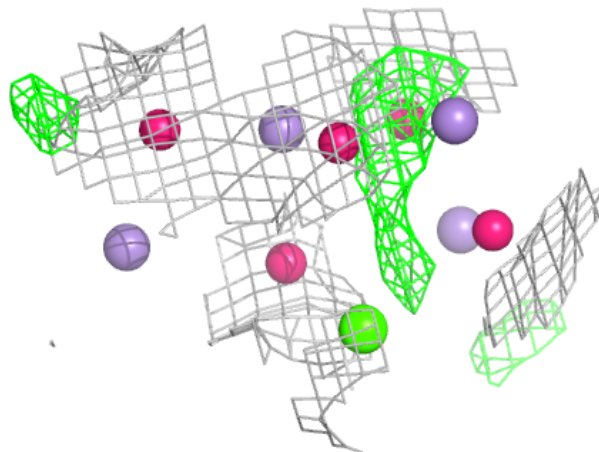
**Electron density around OEX a 411 (A):**

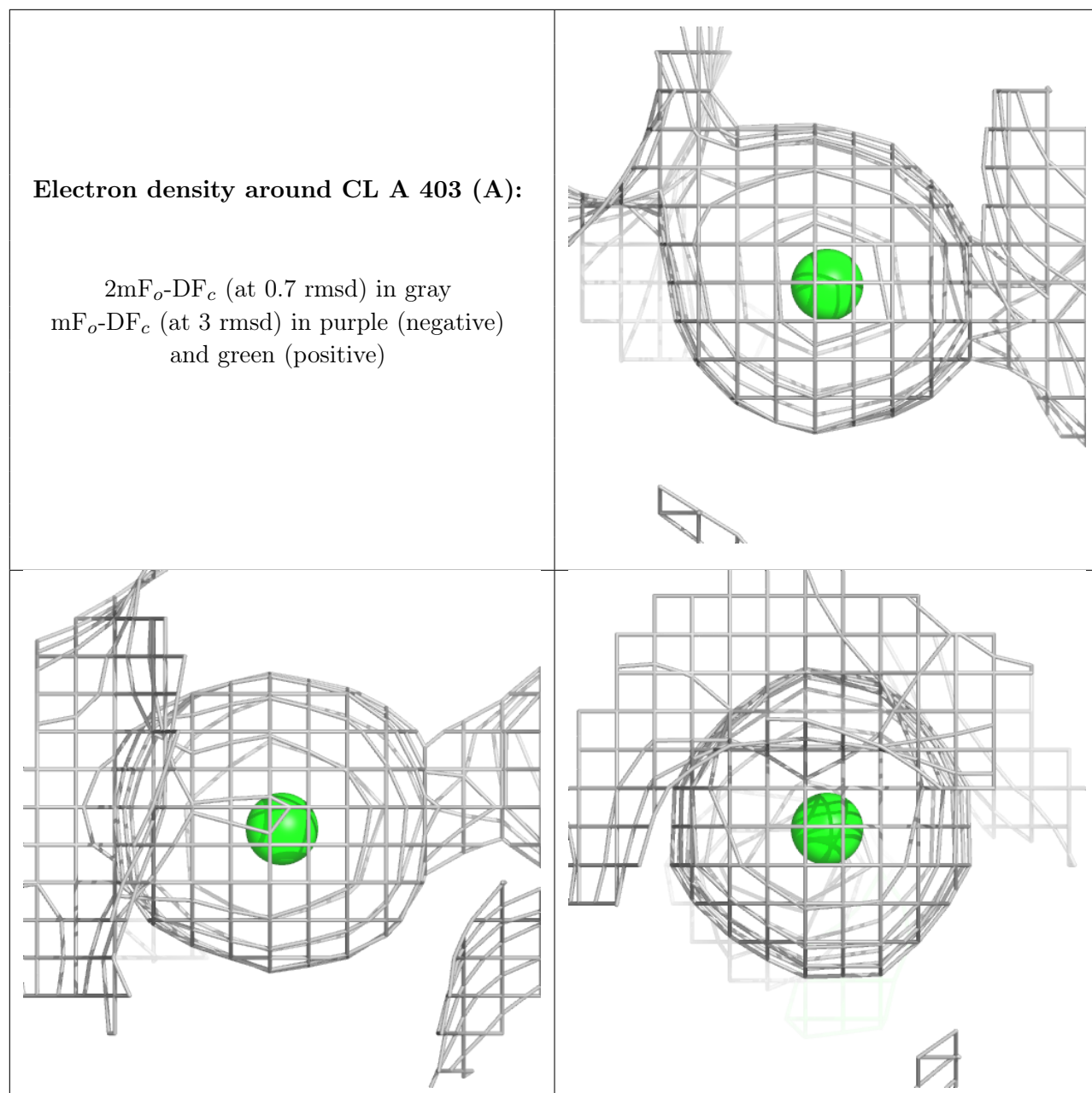
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

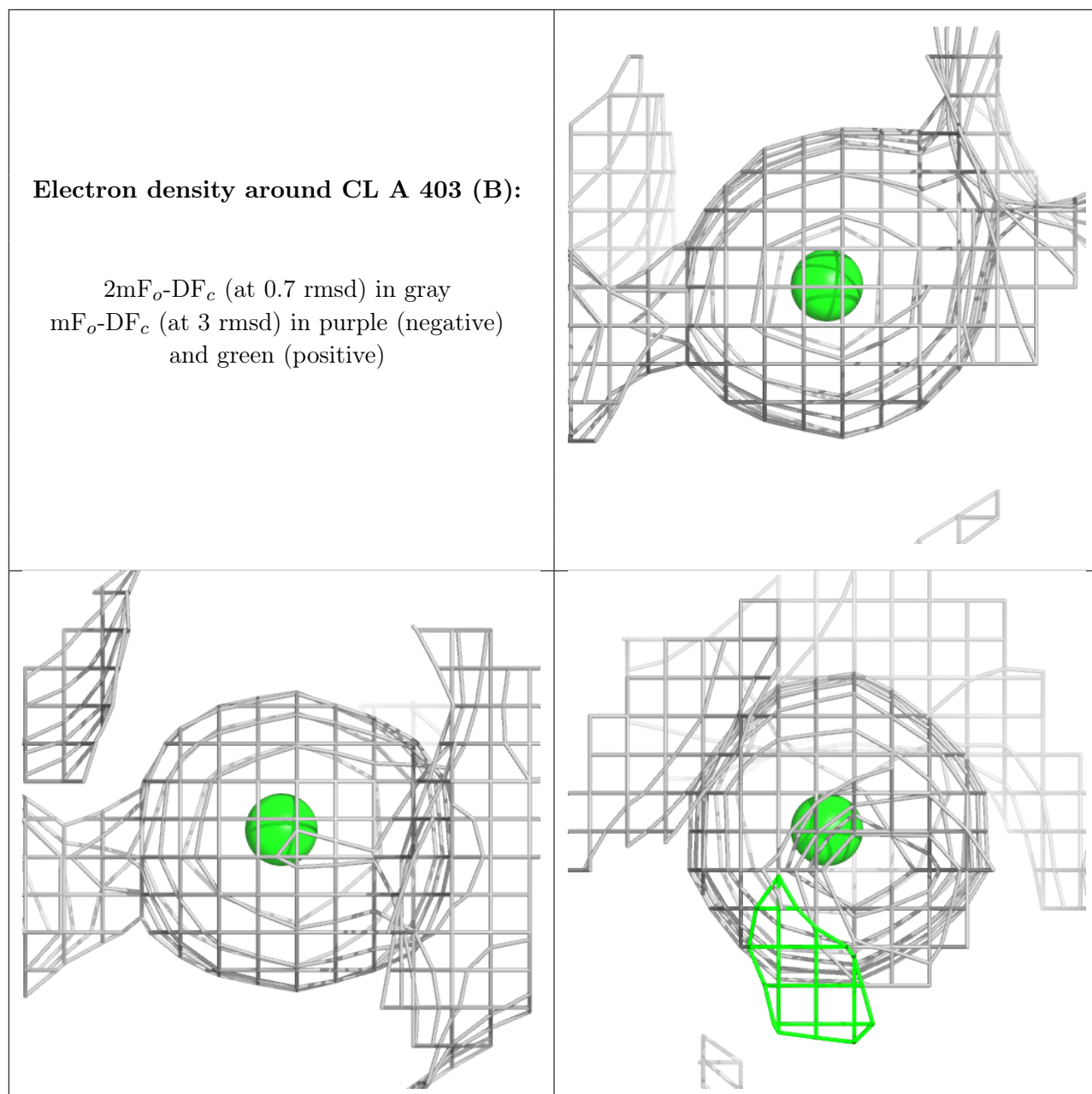


**Electron density around OEX a 411 (B):**

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

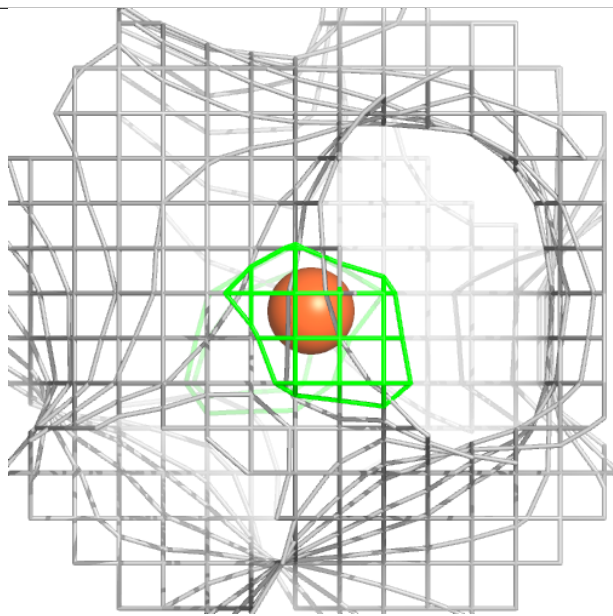
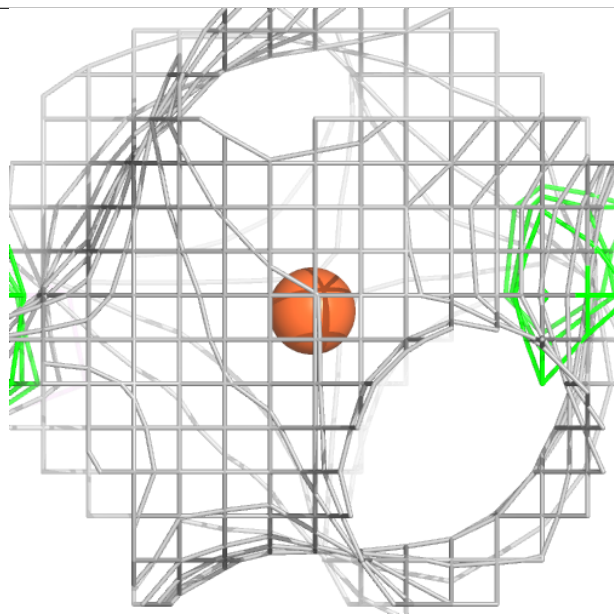
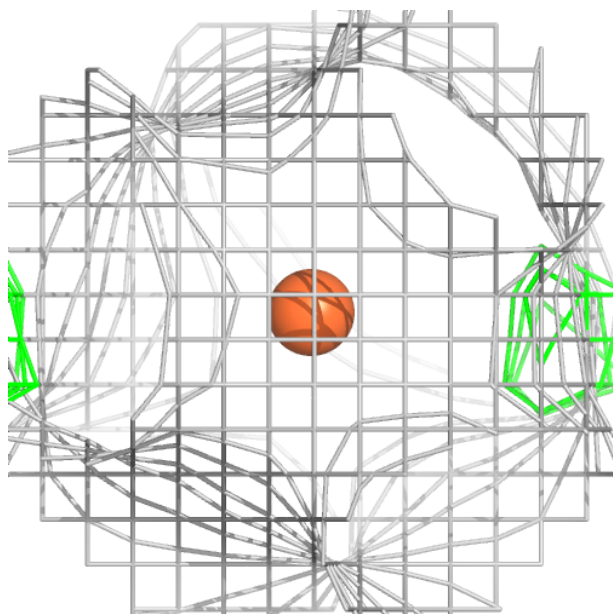


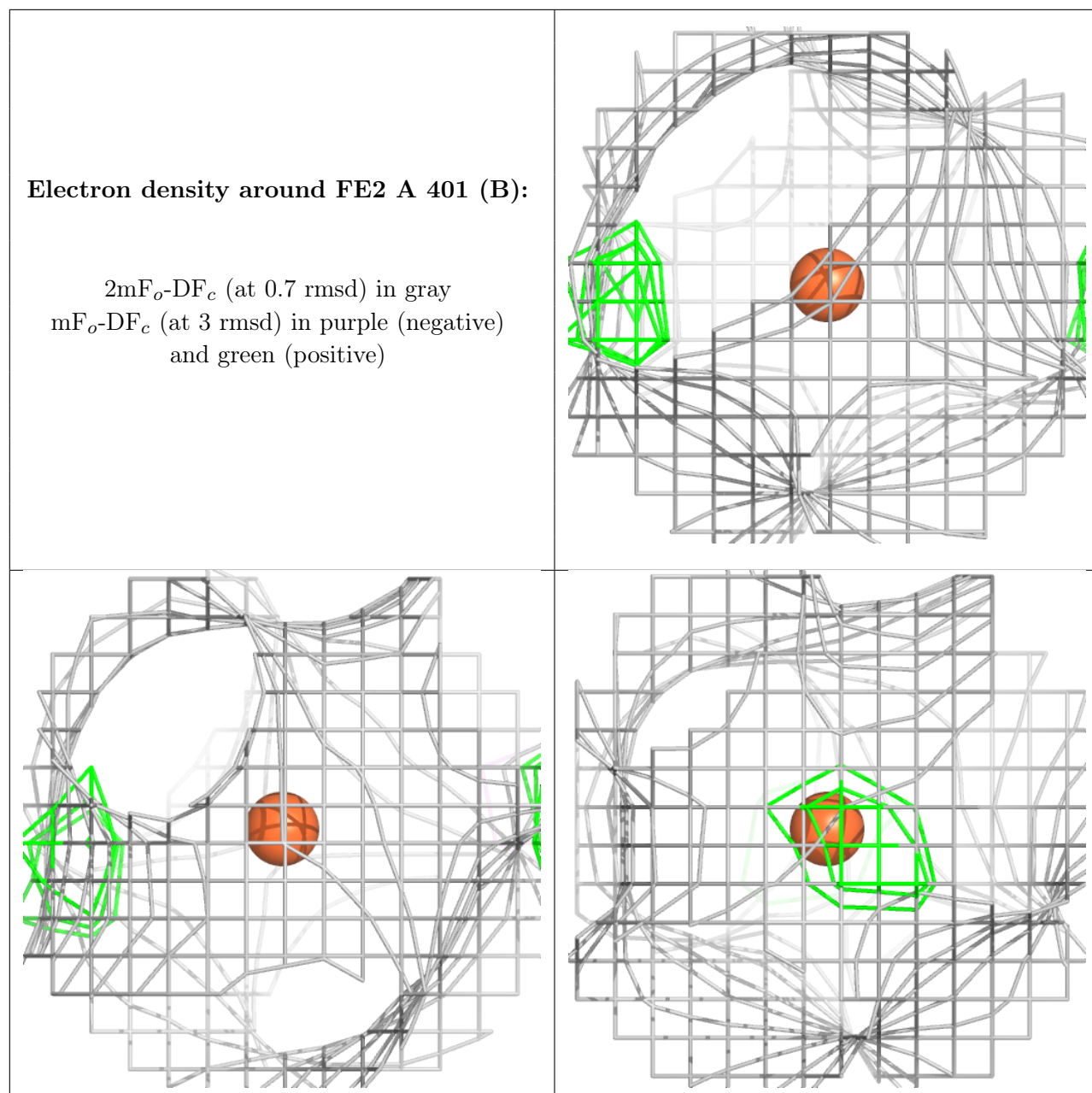




**Electron density around FE2 A 401 (A):**

$2mF_o-DF_c$  (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.