



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2024 – 01:10 PM JST

PDB ID : 8IRB
Title : XFEL structure of cyanobacterial photosystem II following one flash (1F) with a 5-millisecond delay
Authors : Li, H.; Suga, M.; Shen, J.R.
Deposited on : 2023-03-17
Resolution : 2.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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)
Xtrriage (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

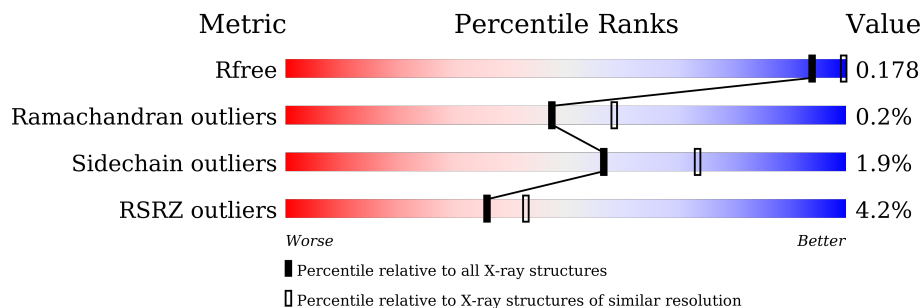
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	344	97% .
1	a	344	97% ..
2	B	505	99% .
2	b	505	98% .
3	C	455	97% ..
3	c	455	99% .
4	D	342	99% .

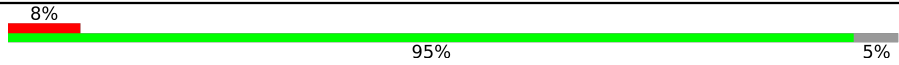
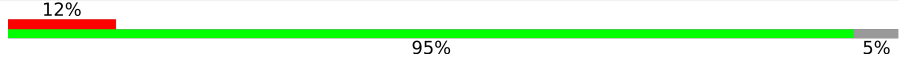
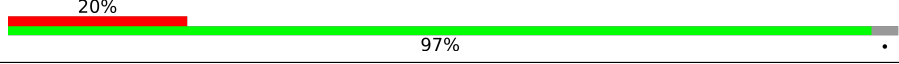
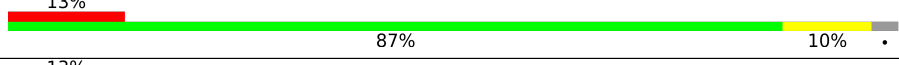
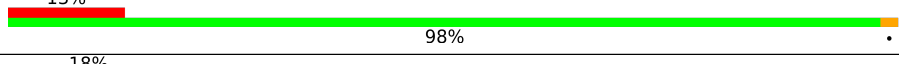
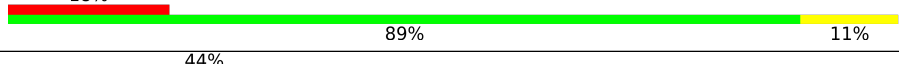
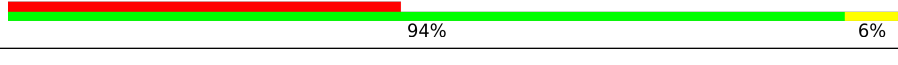
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Mol	Chain	Length	Quality of chain
4	d	342	99%
5	E	84	4% 94%
5	e	84	7% 92% 6%
6	F	44	5% 77% 23%
6	f	44	5% 70% 30%
7	H	65	3% 94% 5%
7	h	65	5% 95%
8	I	38	5% 89% 11%
8	i	38	13% 97%
9	J	39	5% 95%
9	j	39	15% 97%
10	K	37	3% 89% 11%
10	k	37	92% 8%
11	L	37	8% 97%
11	l	37	5% 97%
12	M	36	3% 86% 6% 8%
12	m	36	6% 89% 6% 6%
13	O	244	7% 98%
13	o	244	11% 97%
14	T	32	3% 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	3% 97%

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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	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	C	514	X	-	-	-
23	CLA	D	702[A]	X	-	-	-
23	CLA	D	702[B]	X	-	-	-
23	CLA	D	703	X	-	-	-
23	CLA	a	405[A]	X	-	-	-
23	CLA	a	405[B]	X	-	-	-
23	CLA	a	406[A]	X	-	-	-
23	CLA	a	406[B]	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	503	X	-	-	-
23	CLA	c	504	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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	d	401[A]	X	-	-	-
23	CLA	d	401[B]	X	-	-	-
23	CLA	d	402	X	-	-	-
27	GOL	D	712	-	X	-	-
27	GOL	a	418	-	-	-	X
27	GOL	l	102[A]	-	-	-	X
27	GOL	l	102[B]	-	-	-	X
32	LMT	F	101	-	-	-	X
32	LMT	e	101	-	-	-	X
35	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).

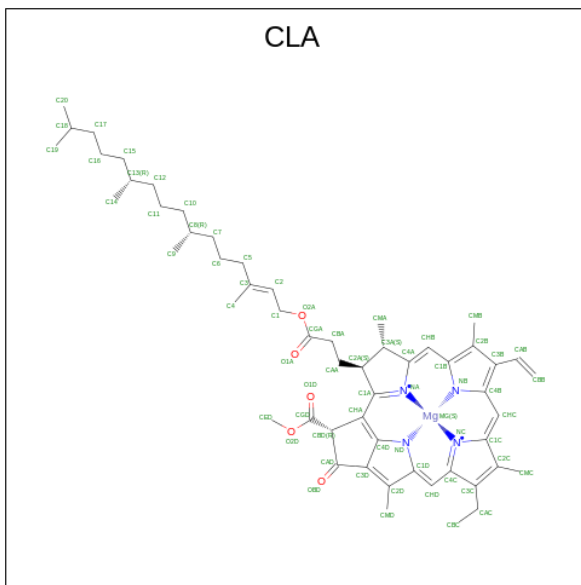
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	2
			4	4		

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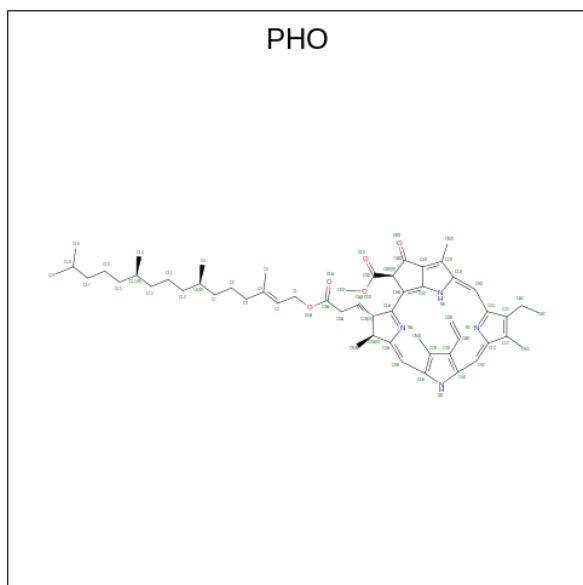
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	D	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	a	1	Total	C	Mg	N	O	0	1
			130	110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

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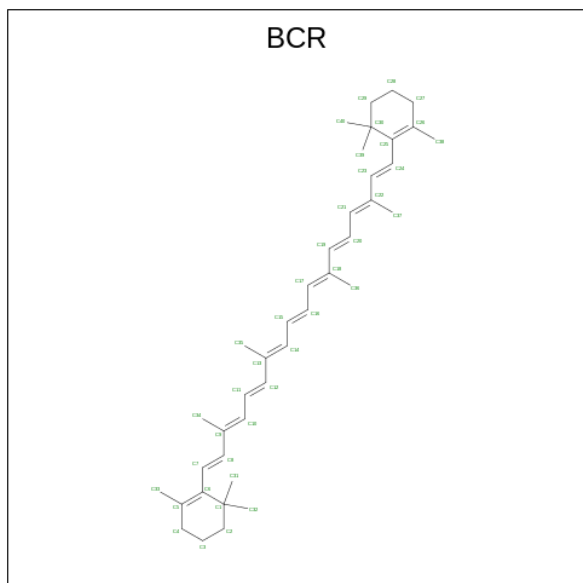
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



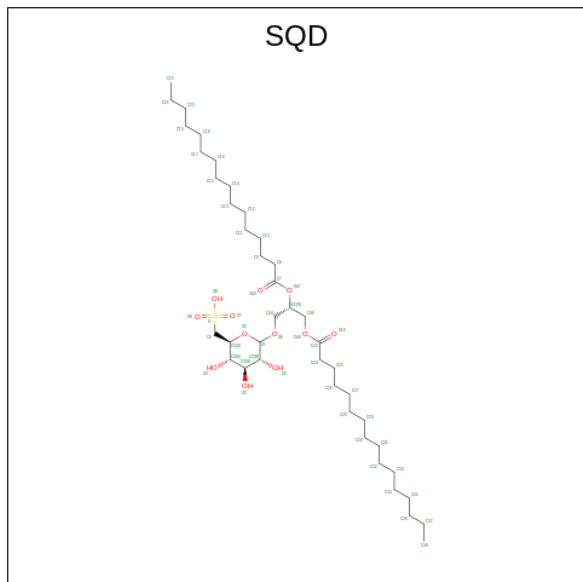
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
24	A	1	Total 128	C 110	N 8	O 10	0	1
24	A	1	Total 128	C 110	N 8	O 10	0	1
24	a	1	Total 128	C 110	N 8	O 10	0	1
24	a	1	Total 128	C 110	N 8	O 10	0	1

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



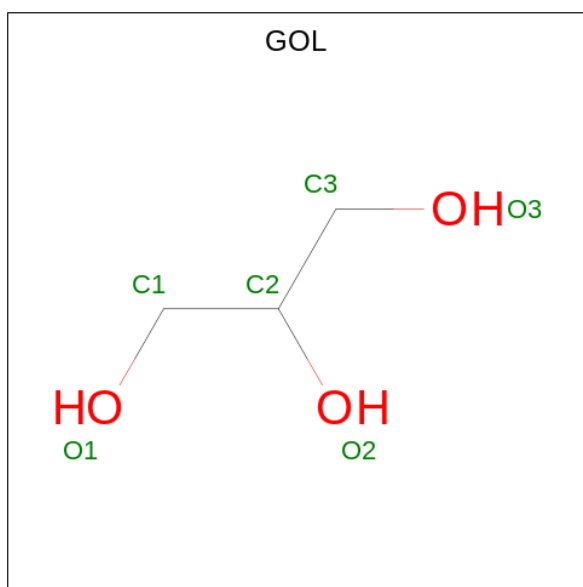
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total 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	X	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: $C_3H_8O_3$).



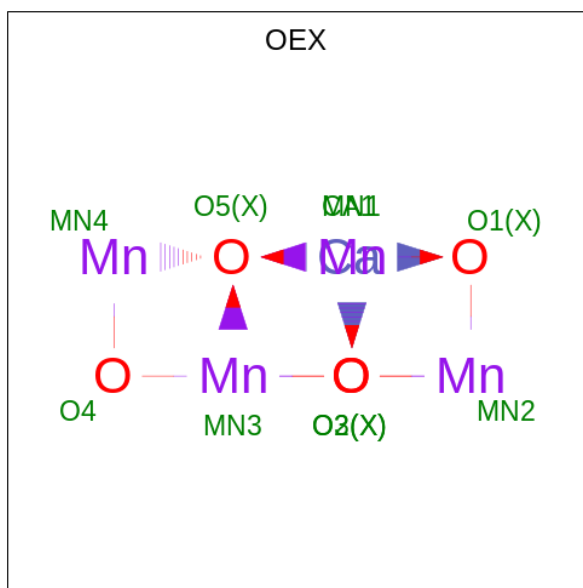
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 6 3 3	0	0
27	B	1	Total C O 6 3 3	0	0
27	B	1	Total C O 6 3 3	0	0
27	B	1	Total C O 6 3 3	0	0
27	C	1	Total C O 12 6 6	0	1
27	D	1	Total C O 6 3 3	0	0
27	D	1	Total C O 6 3 3	0	0
27	O	1	Total C O 6 3 3	0	0
27	O	1	Total C O 6 3 3	0	0
27	V	1	Total C O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

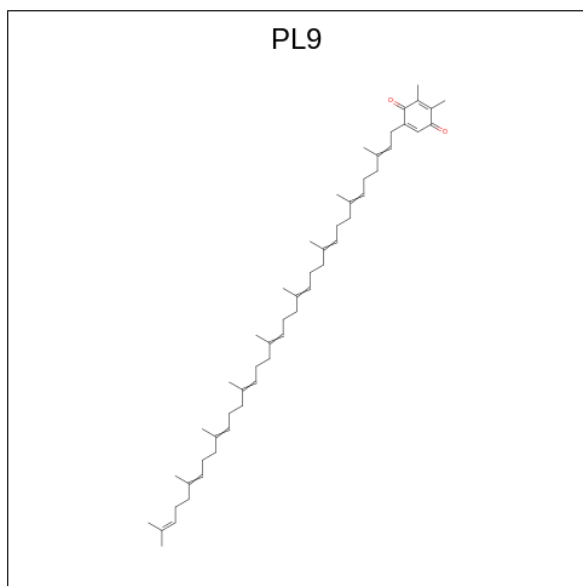
- Molecule 28 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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:

C₅₃H₈₀O₂) (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:).

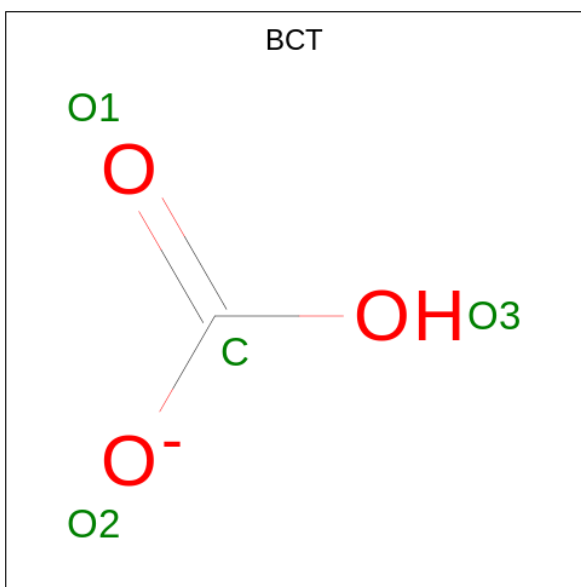
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			28	23	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	I	1	Total	C	O	0	0
			40	35	5		
30	J	1	Total	C		0	0
			10	10			
30	K	1	Total	C	O	0	1
			68	58	10		
30	X	1	Total	C	O	0	0
			18	16	2		

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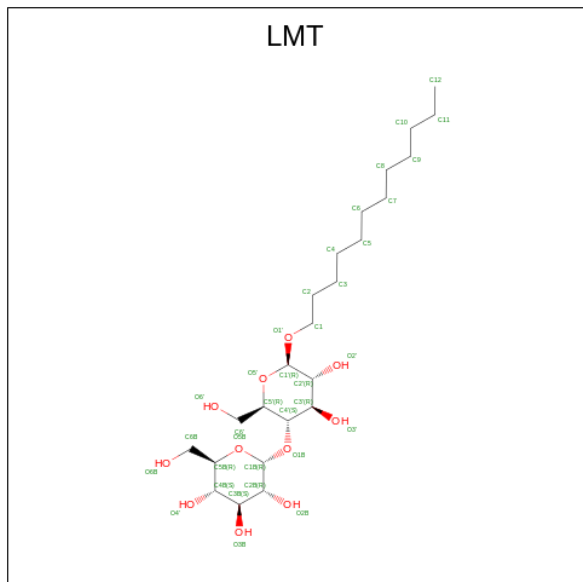
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	a	1	Total	C	O	0	0
			30	25	5		
30	b	1	Total	C	O	0	0
			33	28	5		
30	c	1	Total	C	O	0	1
			64	54	10		
30	d	2	Total	C	O	0	0
			53	47	6		
30	i	1	Total	C	O	0	0
			40	35	5		
30	j	1	Total	C		0	0
			10	10			
30	l	1	Total	C		0	0
			10	10			
30	m	1	Total	C		0	0
		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

- Molecule 31 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	1
			8	2	6		
31	a	1	Total	C	O	0	1
			8	2	6		

- Molecule 32 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



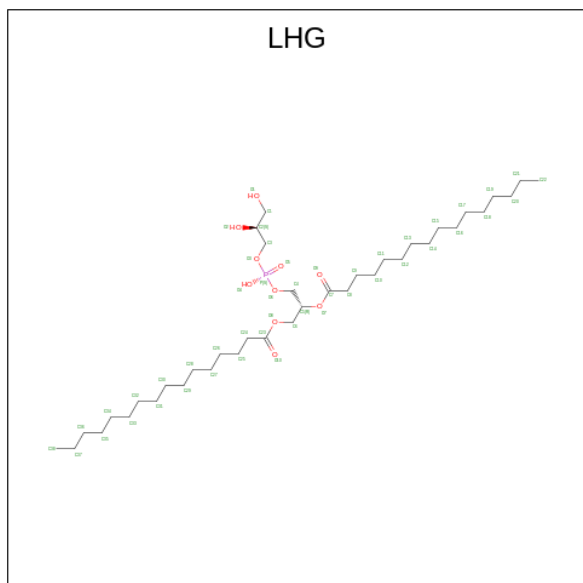
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total C O 35 24 11	0	0
32	A	1	Total C O 35 24 11	0	0
32	B	1	Total C O 35 24 11	0	0
32	B	1	Total C O 35 24 11	0	0
32	B	1	Total C O 25 19 6	0	0
32	F	1	Total C O 35 24 11	0	0
32	M	1	Total C O 35 24 11	0	0
32	T	1	Total C O 35 24 11	0	0
32	a	1	Total C O 35 24 11	0	0
32	b	1	Total C O 25 19 6	0	0
32	b	1	Total C O 25 19 6	0	0
32	e	1	Total C O 35 24 11	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	m	1	Total	C	O	0	0
			35	24	11		
32	t	1	Total	C	O	0	0
			26	19	7		

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{76}O_{10}P$).



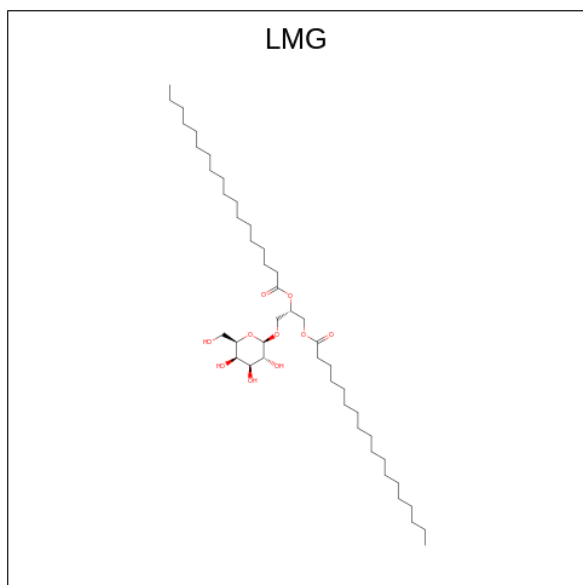
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	A	1	Total	C	O	P	0	1
			98	76	20	2		
33	D	1	Total	C	O	P	0	1
			98	76	20	2		
33	D	1	Total	C	O	P	0	1
			98	76	20	2		
33	E	1	Total	C	O	P	0	1
			84	62	20	2		
33	L	1	Total	C	O	P	0	1
			98	76	20	2		
33	a	1	Total	C	O	P	0	1
			84	62	20	2		
33	b	1	Total	C	O	P	0	1
			98	76	20	2		
33	d	1	Total	C	O	P	0	1
			98	76	20	2		
33	d	1	Total	C	O	P	0	1
			98	76	20	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
33	d	1	98	76	20	2	0	1

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



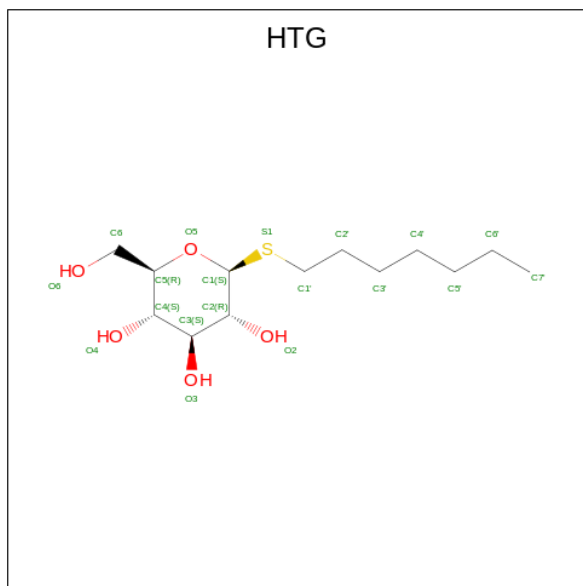
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
34	B	1	51	41	10	0	0
34	C	1	51	41	10	0	0
34	C	1	51	41	10	0	0
34	C	1	51	41	10	0	0
34	D	1	51	41	10	0	0
34	c	1	51	41	10	0	0
34	c	1	51	41	10	0	0
34	c	1	51	41	10	0	0
34	d	1	51	41	10	0	0
34	m	1	51	41	10	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	Z	1	Total	C	O	0	0
			37	27	10		
34	z	1	Total	C	O	0	0
			39	29	10		

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: C₁₃H₂₆O₅S).



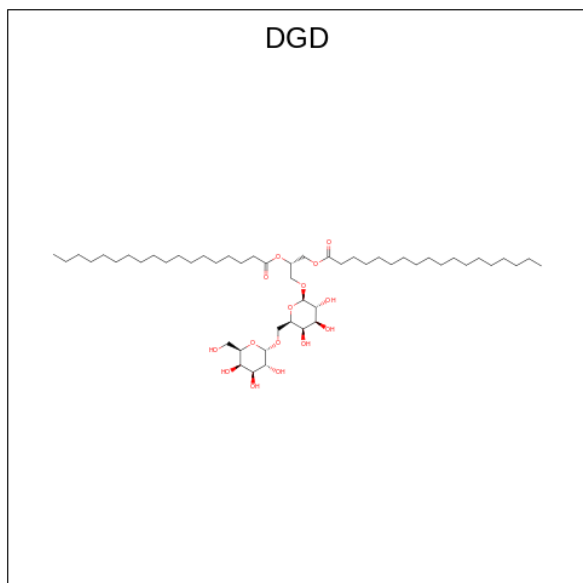
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	D	1	Total	C	O	S	0	0
			16	10	5	1		
35	V	1	Total	C	O		0	0
			11	6	5			
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
35	d	1	16	10	5	1	0	0
35	o	1	19	13	5	1	0	0

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).

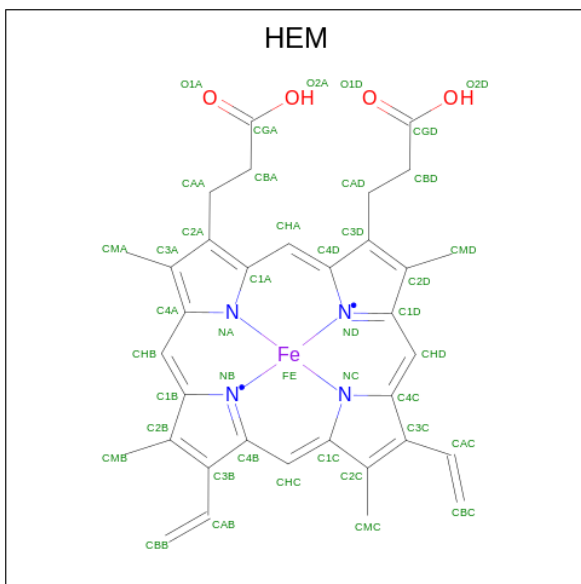


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
36	C	1	124	94	30	0	1
36	C	1	124	94	30	0	1
36	C	1	62	47	15	0	0
36	H	1	62	47	15	0	0
36	c	1	124	94	30	0	1
36	c	1	124	94	30	0	1
36	c	1	62	47	15	0	0
36	h	1	62	47	15	0	0

- Molecule 37 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- 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	F	1	Total C Fe N O 43 34 1 4 4	0	0
38	f	1	Total C Fe N O 43 34 1 4 4	0	0

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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	H	21	Total O 21 21	0	0
41	I	5	Total O 5 5	0	0
41	J	7	Total O 7 7	0	0
41	K	5	Total O 5 5	0	0
41	L	8	Total O 9 9	0	1
41	M	6	Total O 6 6	0	0
41	O	105	Total O 109 109	0	4
41	T	11	Total O 14 14	0	3
41	U	46	Total O 48 48	0	2
41	V	79	Total O 80 80	0	1
41	X	9	Total O 9 9	0	0
41	a	134	Total O 215 215	0	82
41	b	199	Total O 202 202	0	3
41	c	160	Total O 193 193	0	34
41	d	116	Total O 147 147	0	31
41	e	9	Total O 9 9	0	0
41	f	3	Total O 3 3	0	0
41	h	18	Total O 18 18	0	0
41	i	2	Total O 2 2	0	0
41	j	2	Total O 2 2	0	0
41	k	3	Total O 3 3	0	0

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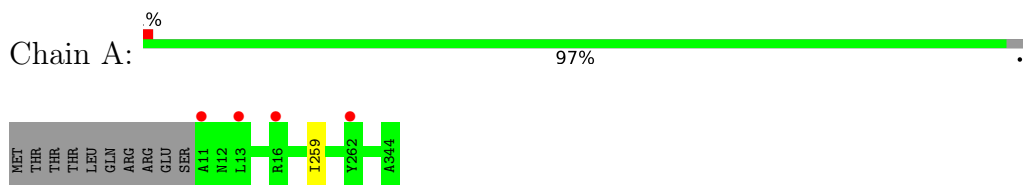
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	l	8	Total O 10 10	0	2
41	m	13	Total O 13 13	0	0
41	o	99	Total O 103 103	0	4
41	t	6	Total O 9 9	0	3
41	u	50	Total O 51 51	0	1
41	v	57	Total O 59 59	0	2
41	x	6	Total O 6 6	0	0
41	y	2	Total O 2 2	0	0

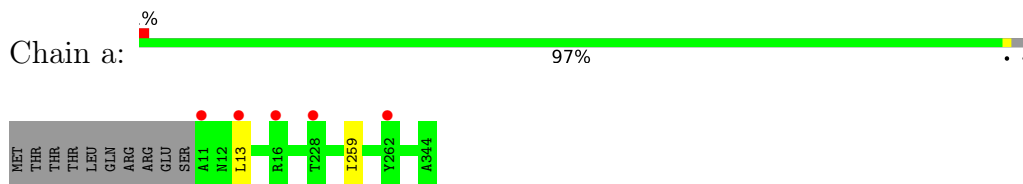
3 Residue-property plots [i](#)

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.

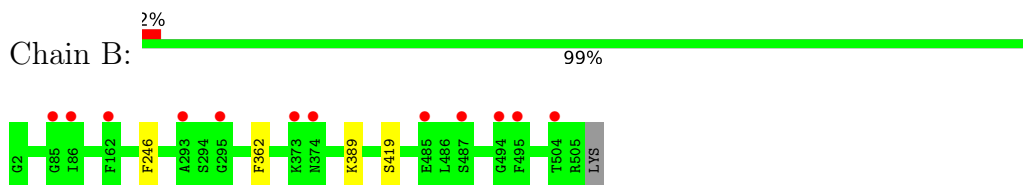
- Molecule 1: Photosystem II protein D1



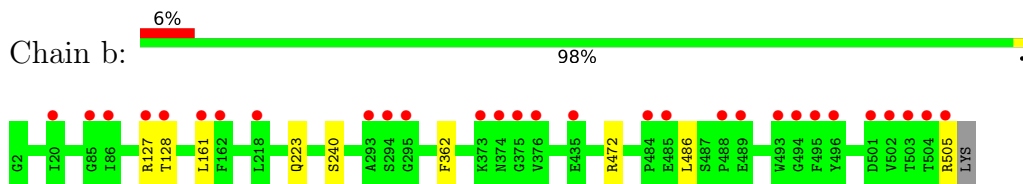
- Molecule 1: Photosystem II protein D1



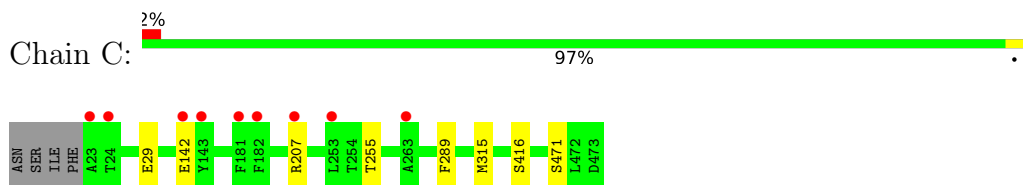
- Molecule 2: Photosystem II CP47 reaction center protein



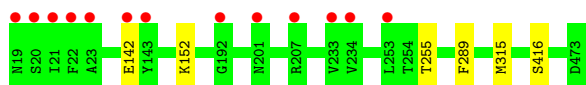
- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein



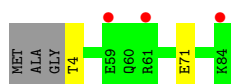
- Molecule 4: Photosystem II D2 protein



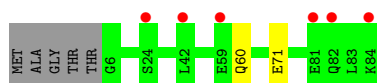
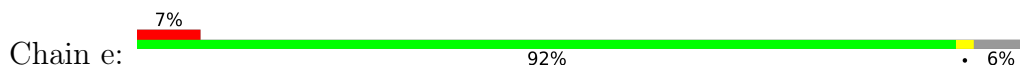
- Molecule 4: Photosystem II D2 protein



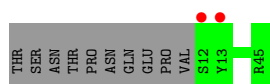
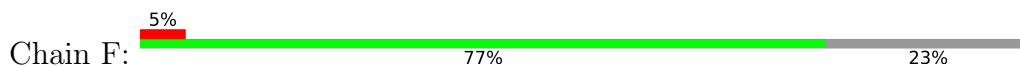
- Molecule 5: Cytochrome b559 subunit alpha



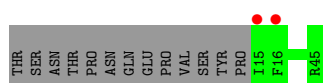
- Molecule 5: Cytochrome b559 subunit alpha



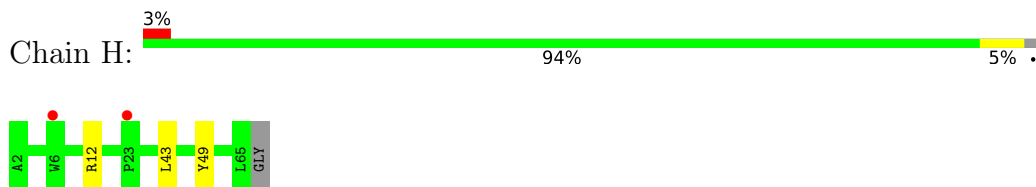
- Molecule 6: Cytochrome b559 subunit beta



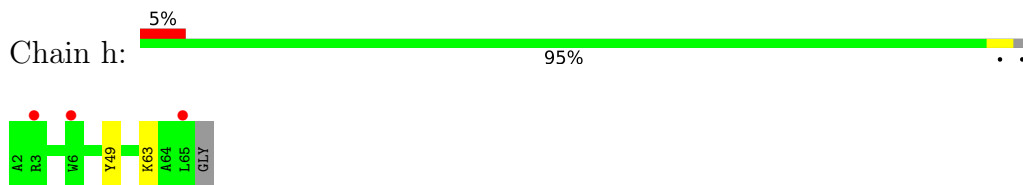
- Molecule 6: Cytochrome b559 subunit beta



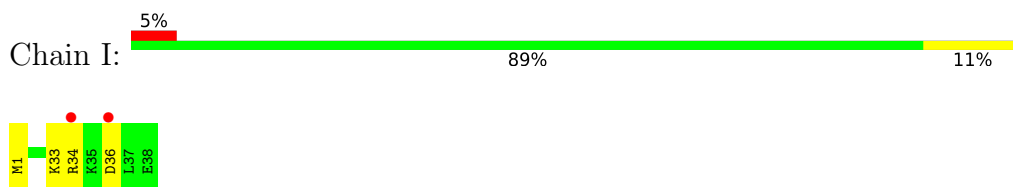
- Molecule 7: Photosystem II reaction center protein H



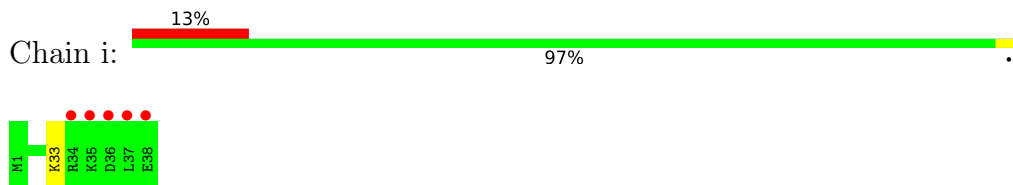
- Molecule 7: Photosystem II reaction center protein H



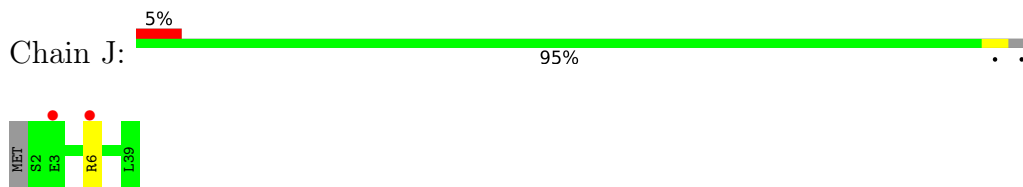
- Molecule 8: Photosystem II reaction center protein I



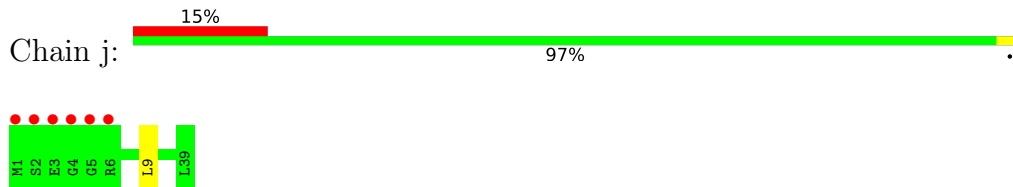
- Molecule 8: Photosystem II reaction center protein I



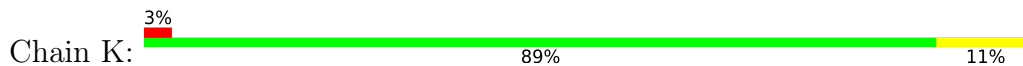
- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K

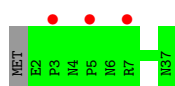




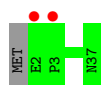
- Molecule 10: Photosystem II reaction center protein K



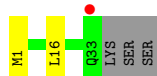
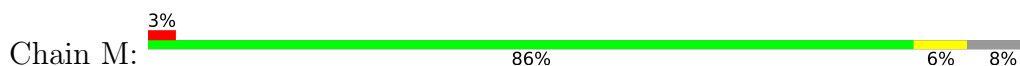
- Molecule 11: Photosystem II reaction center protein L



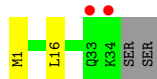
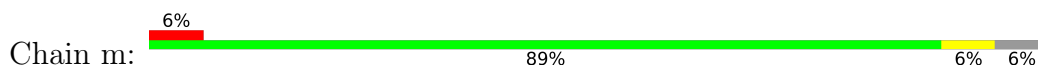
- Molecule 11: Photosystem II reaction center protein L



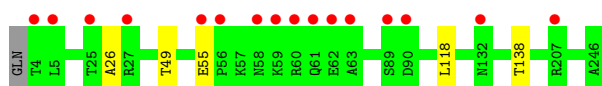
- Molecule 12: Photosystem II reaction center protein M



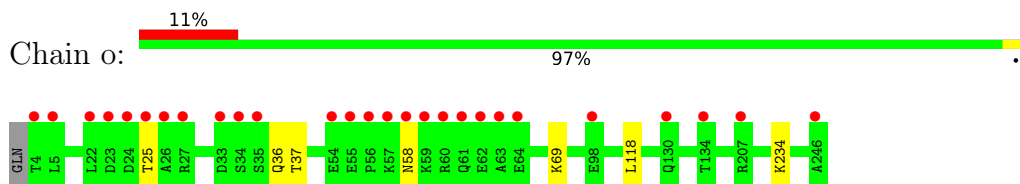
- Molecule 12: Photosystem II reaction center protein M



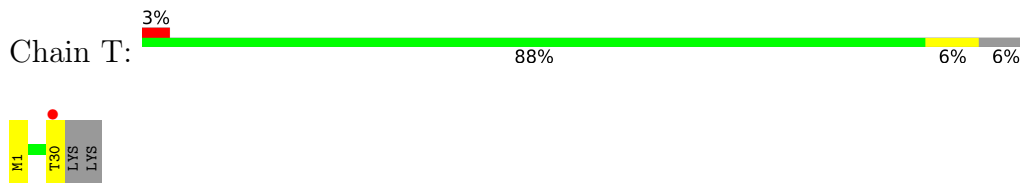
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



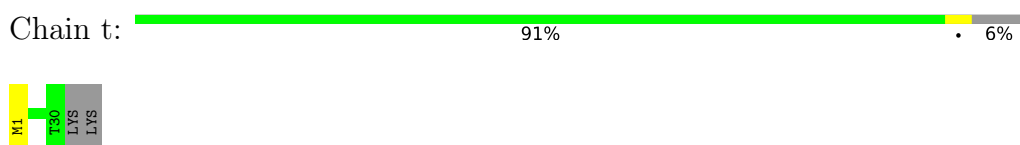
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



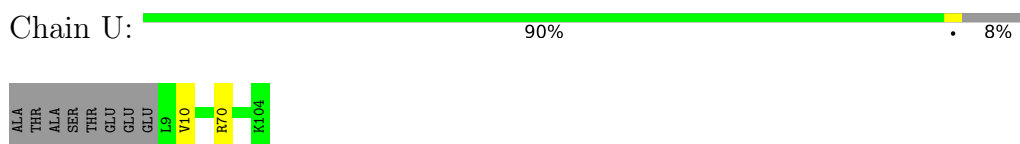
- Molecule 14: Photosystem II reaction center protein T



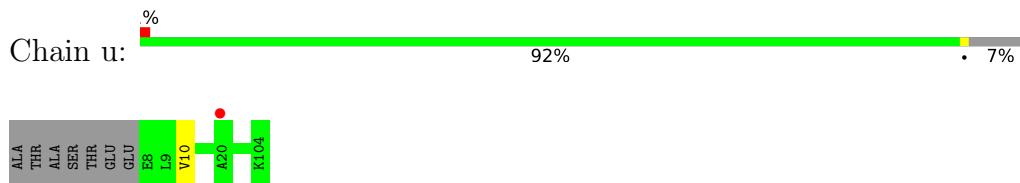
- Molecule 14: Photosystem II reaction center protein T



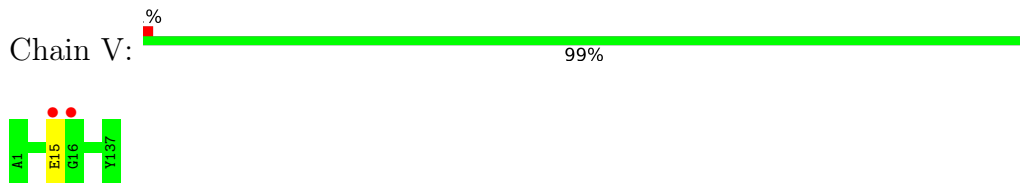
- Molecule 15: Photosystem II 12 kDa extrinsic protein



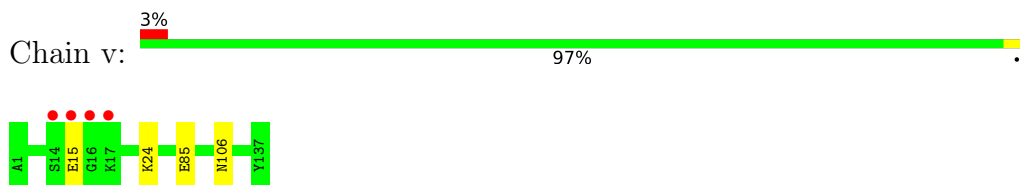
- Molecule 15: Photosystem II 12 kDa extrinsic protein



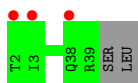
- Molecule 16: Cytochrome c-550



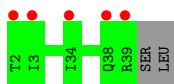
- Molecule 16: Cytochrome c-550



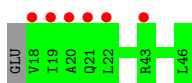
- Molecule 17: Photosystem II reaction center protein X



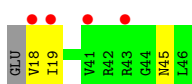
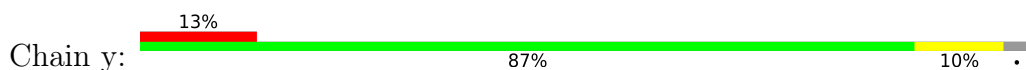
- Molecule 17: Photosystem II reaction center protein X



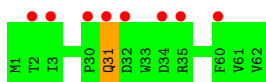
- Molecule 18: Photosystem II reaction center protein Ycf12



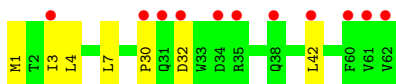
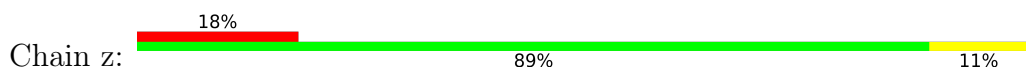
- Molecule 18: Photosystem II reaction center protein Ycf12



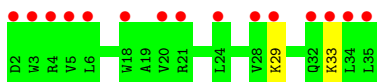
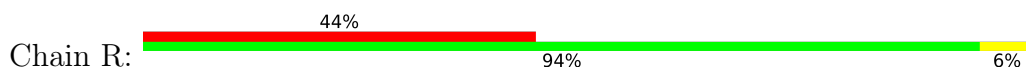
- Molecule 19: Photosystem II reaction center protein Z



- 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, α , β , γ	125.75Å 231.60Å 288.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.30 19.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.98-2.30) 99.9 (19.98-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.30Å)	Xtrriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.139 , 0.180 0.144 , 0.178	Depositor DCC
R_{free} test set	18620 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	50.8	Xtrriage
Anisotropy	0.541	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 84.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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 ²)	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FME, HEM, CLA, GOL, HEC, BCR, LMG, OEX, UNL, CA, LMT, FE2, LHG, SQD, PL9, PHO, MG, HTG, CL, BCT, 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	0/6098
1	a	0.42	0/4457	0.57	0/6069
2	B	0.44	0/4314	0.58	0/5879
2	b	0.42	0/4285	0.57	0/5841
3	C	0.40	0/4416	0.55	0/6013
3	c	0.40	0/4467	0.54	0/6082
4	D	0.46	0/3746	0.60	0/5102
4	d	0.45	0/3780	0.58	0/5147
5	E	0.42	0/681	0.57	0/928
5	e	0.39	0/690	0.54	0/939
6	F	0.41	0/284	0.56	0/387
6	f	0.37	0/269	0.53	0/365
7	H	0.39	0/519	0.58	0/708
7	h	0.38	0/530	0.59	0/722
8	I	0.38	0/311	0.52	0/419
8	i	0.42	0/311	0.55	0/419
9	J	0.41	0/278	0.54	0/376
9	j	0.35	0/283	0.54	0/383
10	K	0.39	0/303	0.52	0/416
10	k	0.40	0/303	0.49	0/416
11	L	0.43	0/318	0.57	0/433
11	l	0.44	0/318	0.54	0/433
12	M	0.43	0/261	0.51	0/357
12	m	0.38	0/279	0.51	0/380
13	O	0.42	0/1991	0.64	0/2698
13	o	0.40	0/1966	0.63	0/2665
14	T	0.43	0/310	0.61	0/419
14	t	0.45	0/301	0.58	0/406
15	U	0.44	0/811	0.62	0/1095
15	u	0.44	0/826	0.63	0/1116
16	V	0.41	0/1142	0.58	0/1545

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.38	0/1139	0.56	0/1542
17	X	0.33	0/292	0.49	0/395
17	x	0.32	0/284	0.48	0/384
18	Y	0.32	0/216	0.52	0/289
18	y	0.31	0/216	0.51	0/289
19	Z	0.34	0/490	0.45	0/669
19	z	0.32	0/490	0.42	0/669
20	R	0.34	0/279	0.53	0/383
All	All	0.42	0/50634	0.57	0/68876

There are no bond length outliers.

There are no bond angle outliers.

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%)	546 (99%)	5 (1%)	2 (0%)	34	42
1	a	551/344 (160%)	544 (99%)	5 (1%)	2 (0%)	34	42
2	B	524/505 (104%)	514 (98%)	10 (2%)	0	100	100
2	b	521/505 (103%)	510 (98%)	11 (2%)	0	100	100
3	C	548/455 (120%)	539 (98%)	8 (2%)	1 (0%)	47	58
3	c	554/455 (122%)	542 (98%)	11 (2%)	1 (0%)	47	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	454/342 (133%)	437 (96%)	17 (4%)	0	100	100
4	d	457/342 (134%)	445 (97%)	12 (3%)	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%)	61 (98%)	1 (2%)	0	100	100
7	h	63/65 (97%)	58 (92%)	4 (6%)	1 (2%)	9	9
8	I	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	5	3
8	i	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
9	J	36/39 (92%)	33 (92%)	3 (8%)	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%)	34 (100%)	0	0	100	100
13	O	251/244 (103%)	242 (96%)	7 (3%)	2 (1%)	19	23
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%)	92 (95%)	5 (5%)	0	100	100
15	u	99/104 (95%)	96 (97%)	3 (3%)	0	100	100
16	V	140/137 (102%)	137 (98%)	3 (2%)	0	100	100
16	v	140/137 (102%)	134 (96%)	6 (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%)	25 (93%)	2 (7%)	0	100	100
18	y	27/30 (90%)	27 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	9	8
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	6180/5384 (115%)	6040 (98%)	128 (2%)	12 (0%)	47	58

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
8	I	36	ASP
13	O	26	ALA
3	c	416	SER
19	Z	31	GLN
19	z	30	PRO
7	h	63	LYS
13	O	138	THR
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%)	419 (99%)	4 (1%)	78	89
2	b	420/403 (104%)	410 (98%)	10 (2%)	49	66
3	C	431/356 (121%)	423 (98%)	8 (2%)	57	73
3	c	437/356 (123%)	431 (99%)	6 (1%)	67	81
4	D	368/277 (133%)	366 (100%)	2 (0%)	88	95
4	d	372/277 (134%)	368 (99%)	4 (1%)	73	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	72/73 (99%)	70 (97%)	2 (3%)	43	60
5	e	72/73 (99%)	70 (97%)	2 (3%)	43	60
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	29
7	h	55/54 (102%)	54 (98%)	1 (2%)	59	75
8	I	34/34 (100%)	32 (94%)	2 (6%)	19	27
8	i	34/34 (100%)	33 (97%)	1 (3%)	42	58
9	J	26/27 (96%)	25 (96%)	1 (4%)	33	47
9	j	26/27 (96%)	25 (96%)	1 (4%)	33	47
10	K	30/30 (100%)	26 (87%)	4 (13%)	4	4
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	9
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	21
12	m	32/32 (100%)	30 (94%)	2 (6%)	18	24
13	O	216/207 (104%)	213 (99%)	3 (1%)	67	81
13	o	213/207 (103%)	206 (97%)	7 (3%)	38	53
14	T	32/28 (114%)	30 (94%)	2 (6%)	18	24
14	t	31/28 (111%)	31 (100%)	0	100	100
15	U	86/89 (97%)	84 (98%)	2 (2%)	50	67
15	u	88/89 (99%)	86 (98%)	2 (2%)	50	67
16	V	123/117 (105%)	122 (99%)	1 (1%)	81	91
16	v	123/117 (105%)	119 (97%)	4 (3%)	38	53
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%)	19 (86%)	3 (14%)	3	3
19	Z	52/52 (100%)	51 (98%)	1 (2%)	57	73
19	z	52/52 (100%)	46 (88%)	6 (12%)	5	6
20	R	29/29 (100%)	27 (93%)	2 (7%)	15	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5110/4403 (116%)	5018 (98%)	92 (2%)	57 75

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	246	PHE
2	B	362	PHE
2	B	389	LYS
2	B	419	SER
3	C	29	GLU
3	C	142	GLU
3	C	207	ARG
3	C	255	THR
3	C	289	PHE
3	C	315[A]	MET
3	C	315[B]	MET
3	C	471	SER
4	D	180	ARG
4	D	338	ASN
5	E	4	THR
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	118	LEU
14	T	30[A]	THR
14	T	30[B]	THR
15	U	10	VAL
15	U	70	ARG
16	V	15	GLU
1	a	13	LEU

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Mol	Chain	Res	Type
2	b	127	ARG
2	b	128	THR
2	b	161	LEU
2	b	223	GLN
2	b	240	SER
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	152	LYS
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	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	58	ASN
13	o	69	LYS
13	o	118	LEU
13	o	234	LYS
15	u	10[A]	VAL
15	u	10[B]	VAL
16	v	15	GLU
16	v	24	LYS
16	v	85	GLU

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Mol	Chain	Res	Type
16	v	106	ASN
18	y	18	VAL
18	y	19	ILE
18	y	45	ASN
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
11	l	8	GLN
13	o	58	ASN

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	$\# Z > 2$
14	FME	t	1	14	8,9,10	0.74	0	7,9,11	1.65	2 (28%)
12	FME	m	1	12	8,9,10	0.49	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
12	FME	M	1	12	8,9,10	0.62	0	7,9,11	1.32	1 (14%)
8	FME	I	1	8	8,9,10	0.51	0	7,9,11	1.21	1 (14%)
14	FME	T	1	14	8,9,10	0.65	0	7,9,11	1.78	3 (42%)
8	FME	i	1	8	8,9,10	0.68	0	7,9,11	1.33	0

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

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

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	CA-N-CN	2.47	126.62	122.82
12	m	1	FME	CA-N-CN	-2.45	119.06	122.82
14	t	1	FME	O-C-CA	-2.42	118.43	124.78
14	t	1	FME	CA-N-CN	-2.41	119.12	122.82
12	m	1	FME	O1-CN-N	-2.41	118.93	125.27
14	T	1	FME	CG-CB-CA	2.34	119.44	112.95
12	M	1	FME	O-C-CA	-2.23	118.93	124.78
14	T	1	FME	C-CA-N	2.18	113.67	109.73
8	I	1	FME	O-C-CA	-2.14	119.17	124.78

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	O1-CN-N-CA
12	M	1	FME	O-C-CA-CB
8	i	1	FME	O-C-CA-CB
14	t	1	FME	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
14	T	1	FME	N-CA-CB-CG
14	T	1	FME	C-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
27	GOL	a	419	-	5,5,5	1.28	1 (20%)	5,5,5	0.93	0
32	LMT	F	101	-	36,36,36	1.06	1 (2%)	47,47,47	1.04	3 (6%)
23	CLA	b	616	-	65,73,73	2.02	15 (23%)	76,113,113	2.91	27 (35%)
24	PHO	a	408[A]	-	51,69,69	1.83	8 (15%)	47,99,99	1.71	10 (21%)
33	LHG	b	629[B]	-	48,48,48	0.89	2 (4%)	51,54,54	1.05	5 (9%)
28	OEX	A	413[A]	3,41,1	0,15,15	-	-	-	-	-
32	LMT	B	627	-	36,36,36	1.15	3 (8%)	47,47,47	1.41	6 (12%)
25	BCR	T	102	-	41,41,41	1.02	1 (2%)	56,56,56	1.76	13 (23%)
33	LHG	L	101[B]	-	48,48,48	0.95	2 (4%)	51,54,54	1.09	2 (3%)
32	LMT	b	621	-	25,25,36	0.98	2 (8%)	30,30,47	1.19	2 (6%)
36	DGD	c	518[B]	-	63,63,67	0.87	2 (3%)	77,77,81	0.92	2 (2%)
23	CLA	C	507	-	65,73,73	2.04	17 (26%)	76,113,113	2.79	29 (38%)
31	BCT	A	416[A]	21	2,3,3	0.54	0	2,3,3	1.81	1 (50%)
25	BCR	C	515	-	41,41,41	1.04	1 (2%)	56,56,56	1.49	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	A	408	-	65,73,73	2.02	16 (24%)	76,113,113	2.91	33 (43%)
27	GOL	B	628	-	5,5,5	0.88	0	5,5,5	1.13	0
29	PL9	d	404[B]	-	55,55,55	0.64	1 (1%)	68,69,69	1.65	16 (23%)
31	BCT	a	404[B]	21	2,3,3	0.64	0	2,3,3	1.26	0
25	BCR	B	617	-	41,41,41	1.04	1 (2%)	56,56,56	1.28	6 (10%)
23	CLA	B	616	-	65,73,73	2.01	16 (24%)	76,113,113	2.92	26 (34%)
27	GOL	D	701	-	5,5,5	1.57	2 (40%)	5,5,5	1.06	1 (20%)
36	DGD	H	102	-	63,63,67	0.85	3 (4%)	77,77,81	1.09	7 (9%)
23	CLA	C	511	-	65,73,73	2.05	17 (26%)	76,113,113	2.90	30 (39%)
23	CLA	B	615	-	65,73,73	2.03	16 (24%)	76,113,113	2.83	29 (38%)
32	LMT	m	103	-	36,36,36	1.07	2 (5%)	47,47,47	1.16	4 (8%)
34	LMG	d	410	39	51,51,55	0.89	2 (3%)	59,59,63	1.17	5 (8%)
23	CLA	a	406[A]	41	65,73,73	2.00	14 (21%)	76,113,113	2.75	26 (34%)
24	PHO	A	407[A]	-	51,69,69	1.78	8 (15%)	47,99,99	1.77	11 (23%)
27	GOL	C	523[A]	-	5,5,5	1.18	0	5,5,5	0.83	0
27	GOL	l	102[B]	-	5,5,5	0.90	0	5,5,5	1.02	0
26	SQD	B	620	-	53,54,54	1.08	4 (7%)	62,65,65	1.73	11 (17%)
34	LMG	C	501	-	51,51,55	0.93	2 (3%)	59,59,63	1.53	7 (11%)
34	LMG	C	520	-	51,51,55	0.95	2 (3%)	59,59,63	1.11	6 (10%)
34	LMG	c	520	-	51,51,55	0.91	2 (3%)	59,59,63	1.17	5 (8%)
33	LHG	D	707[A]	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	4 (7%)
23	CLA	b	612	-	65,73,73	2.05	16 (24%)	76,113,113	2.69	26 (34%)
23	CLA	d	402	-	65,73,73	2.05	15 (23%)	76,113,113	2.84	29 (38%)
27	GOL	a	418	-	5,5,5	1.21	0	5,5,5	1.01	0
32	LMT	B	629	-	36,36,36	1.01	3 (8%)	47,47,47	1.20	5 (10%)
33	LHG	d	405[A]	-	48,48,48	0.86	2 (4%)	51,54,54	1.08	4 (7%)
33	LHG	d	412[A]	-	48,48,48	0.89	2 (4%)	51,54,54	1.12	4 (7%)
36	DGD	C	518[B]	-	63,63,67	0.88	3 (4%)	77,77,81	1.03	6 (7%)
27	GOL	c	526[B]	-	5,5,5	0.86	0	5,5,5	0.98	0
29	PL9	D	705[B]	-	55,55,55	0.63	2 (3%)	68,69,69	1.68	18 (26%)
23	CLA	B	604	-	65,73,73	2.01	18 (27%)	76,113,113	2.69	27 (35%)
25	BCR	c	516	-	41,41,41	1.03	1 (2%)	56,56,56	1.34	8 (14%)
25	BCR	C	516	-	41,41,41	1.07	1 (2%)	56,56,56	1.34	7 (12%)
23	CLA	b	610	41	65,73,73	2.07	16 (24%)	76,113,113	2.88	28 (36%)
27	GOL	O	302	-	5,5,5	0.82	0	5,5,5	0.94	0
35	HTG	B	624	-	19,19,19	1.01	2 (10%)	23,24,24	1.29	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	DGD	c	517[A]	-	63,63,67	0.85	2 (3%)	77,77,81	1.12	6 (7%)
23	CLA	B	602	-	65,73,73	2.04	16 (24%)	76,113,113	2.84	29 (38%)
36	DGD	c	519	-	63,63,67	0.87	4 (6%)	77,77,81	1.07	6 (7%)
23	CLA	c	511	-	65,73,73	2.02	16 (24%)	76,113,113	2.80	31 (40%)
32	LMT	t	101	-	26,26,36	0.91	2 (7%)	31,31,47	1.29	1 (3%)
23	CLA	B	606	-	65,73,73	1.96	16 (24%)	76,113,113	2.96	29 (38%)
32	LMT	a	417	-	36,36,36	1.00	2 (5%)	47,47,47	1.04	2 (4%)
34	LMG	c	501	-	51,51,55	0.92	2 (3%)	59,59,63	1.25	6 (10%)
38	HEM	f	101	5,6	41,50,50	1.31	5 (12%)	45,82,82	1.82	11 (24%)
23	CLA	c	509	-	65,73,73	2.12	16 (24%)	76,113,113	2.67	25 (32%)
34	LMG	D	711	39	51,51,55	0.79	2 (3%)	59,59,63	1.09	3 (5%)
34	LMG	B	621	-	51,51,55	0.93	2 (3%)	59,59,63	1.27	4 (6%)
24	PHO	a	408[B]	-	51,69,69	1.86	7 (13%)	47,99,99	1.82	9 (19%)
28	OEX	A	413[B]	3,41,1	0,15,15	-	-	-	-	-
23	CLA	c	502	-	65,73,73	2.00	16 (24%)	76,113,113	2.79	27 (35%)
26	SQD	A	410[A]	-	53,54,54	0.93	3 (5%)	62,65,65	1.81	10 (16%)
26	SQD	f	102	-	42,43,54	1.19	3 (7%)	51,54,65	1.55	12 (23%)
23	CLA	C	504	-	65,73,73	1.98	16 (24%)	76,113,113	2.87	27 (35%)
23	CLA	b	615	-	65,73,73	1.98	16 (24%)	76,113,113	2.78	30 (39%)
27	GOL	V	203[A]	-	5,5,5	1.22	0	5,5,5	0.91	0
31	BCT	A	416[B]	21	2,3,3	0.59	0	2,3,3	1.20	0
26	SQD	A	412	-	53,54,54	1.06	3 (5%)	62,65,65	1.23	6 (9%)
35	HTG	b	623	-	19,19,19	1.09	1 (5%)	23,24,24	1.91	2 (8%)
23	CLA	a	405[A]	-	65,73,73	1.99	15 (23%)	76,113,113	2.87	32 (42%)
23	CLA	c	513	-	65,73,73	2.07	16 (24%)	76,113,113	2.72	28 (36%)
23	CLA	B	608	-	65,73,73	1.98	17 (26%)	76,113,113	2.90	34 (44%)
23	CLA	D	702[A]	-	65,73,73	1.99	16 (24%)	76,113,113	2.87	29 (38%)
25	BCR	k	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.43	11 (19%)
27	GOL	d	411	-	5,5,5	1.12	0	5,5,5	0.90	0
23	CLA	a	406[B]	41	65,73,73	2.08	16 (24%)	76,113,113	2.77	30 (39%)
23	CLA	A	406[B]	41	65,73,73	2.03	17 (26%)	76,113,113	2.84	29 (38%)
25	BCR	d	403	-	41,41,41	1.15	2 (4%)	56,56,56	1.98	14 (25%)
24	PHO	A	407[B]	-	51,69,69	1.79	7 (13%)	47,99,99	1.82	11 (23%)
25	BCR	b	617	-	41,41,41	1.08	1 (2%)	56,56,56	1.26	5 (8%)
27	GOL	C	523[B]	-	5,5,5	1.19	0	5,5,5	0.79	0
23	CLA	A	405[A]	41	65,73,73	1.90	16 (24%)	76,113,113	2.85	30 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	601	41	65,73,73	2.08	16 (24%)	76,113,113	2.77	26 (34%)
33	LHG	D	707[B]	-	48,48,48	0.90	2 (4%)	51,54,54	1.02	3 (5%)
28	OEX	a	413[A]	3,41,1	0,15,15	-	-	-	-	-
33	LHG	d	405[B]	-	48,48,48	0.89	2 (4%)	51,54,54	1.04	4 (7%)
33	LHG	d	412[B]	-	48,48,48	0.92	2 (4%)	51,54,54	1.07	3 (5%)
23	CLA	A	406[A]	41	65,73,73	1.96	16 (24%)	76,113,113	2.81	29 (38%)
32	LMT	M	101	-	36,36,36	1.14	4 (11%)	47,47,47	1.20	3 (6%)
33	LHG	D	706[A]	-	48,48,48	0.86	2 (4%)	51,54,54	0.99	3 (5%)
23	CLA	c	506	-	65,73,73	2.01	16 (24%)	76,113,113	2.78	25 (32%)
23	CLA	a	407[B]	41	65,73,73	2.02	16 (24%)	76,113,113	2.74	28 (36%)
36	DGD	c	517[B]	-	63,63,67	0.85	2 (3%)	77,77,81	1.11	6 (7%)
27	GOL	b	628	-	5,5,5	0.49	0	5,5,5	1.34	1 (20%)
23	CLA	b	607	41	65,73,73	1.99	18 (27%)	76,113,113	2.83	27 (35%)
23	CLA	a	407[A]	41	65,73,73	1.94	16 (24%)	76,113,113	2.81	27 (35%)
34	LMG	c	521	-	51,51,55	1.02	2 (3%)	59,59,63	1.38	7 (11%)
23	CLA	c	514	-	65,73,73	2.13	17 (26%)	76,113,113	2.82	28 (36%)
23	CLA	c	508	41	65,73,73	1.99	16 (24%)	76,113,113	2.82	26 (34%)
25	BCR	h	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.49	12 (21%)
36	DGD	C	517[A]	-	63,63,67	0.81	2 (3%)	77,77,81	1.21	8 (10%)
27	GOL	v	202[A]	-	5,5,5	1.27	0	5,5,5	0.72	0
25	BCR	K	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.42	11 (19%)
25	BCR	b	618	-	41,41,41	0.96	1 (2%)	56,56,56	1.34	11 (19%)
27	GOL	B	623	-	5,5,5	0.75	0	5,5,5	1.11	1 (20%)
23	CLA	b	601	41	65,73,73	2.13	15 (23%)	76,113,113	2.74	28 (36%)
29	PL9	a	414[A]	-	55,55,55	0.65	2 (3%)	68,69,69	2.00	22 (32%)
26	SQD	a	411[A]	-	53,54,54	0.95	3 (5%)	62,65,65	1.77	13 (20%)
26	SQD	A	410[B]	-	53,54,54	0.92	3 (5%)	62,65,65	1.75	12 (19%)
26	SQD	a	412	-	53,54,54	1.09	3 (5%)	62,65,65	1.17	8 (12%)
26	SQD	X	101	-	42,43,54	1.21	4 (9%)	51,54,65	2.24	15 (29%)
27	GOL	V	203[B]	-	5,5,5	1.11	0	5,5,5	0.89	0
35	HTG	D	710	-	16,16,19	0.99	1 (6%)	20,21,24	1.54	1 (5%)
23	CLA	c	510	-	65,73,73	2.10	16 (24%)	76,113,113	2.76	27 (35%)
27	GOL	B	626	-	5,5,5	1.09	0	5,5,5	0.92	0
24	PHO	A	417[A]	-	51,69,69	1.87	8 (15%)	47,99,99	1.93	12 (25%)
27	GOL	c	527	-	5,5,5	1.19	0	5,5,5	0.91	0
23	CLA	a	405[B]	-	65,73,73	2.02	14 (21%)	76,113,113	2.88	32 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	614	-	65,73,73	2.06	15 (23%)	76,113,113	2.92	29 (38%)
23	CLA	C	502	-	65,73,73	1.99	17 (26%)	76,113,113	2.81	27 (35%)
23	CLA	D	702[B]	-	65,73,73	2.05	16 (24%)	76,113,113	2.86	28 (36%)
33	LHG	A	419[A]	-	48,48,48	0.84	2 (4%)	51,54,54	1.31	6 (11%)
23	CLA	C	505	41	65,73,73	2.03	15 (23%)	76,113,113	2.73	26 (34%)
25	BCR	B	619	-	41,41,41	1.10	2 (4%)	56,56,56	1.31	5 (8%)
33	LHG	d	406[A]	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	3 (5%)
32	LMT	A	420	-	36,36,36	1.04	2 (5%)	47,47,47	1.14	4 (8%)
38	HEM	F	102	5,6	41,50,50	1.31	4 (9%)	45,82,82	2.08	15 (33%)
23	CLA	B	611	-	65,73,73	2.60	17 (26%)	76,113,113	3.17	27 (35%)
23	CLA	b	611	-	65,73,73	2.00	15 (23%)	76,113,113	2.82	27 (35%)
25	BCR	a	410	-	41,41,41	1.02	1 (2%)	56,56,56	1.33	8 (14%)
25	BCR	c	515	-	41,41,41	1.01	1 (2%)	56,56,56	1.64	11 (19%)
35	HTG	V	202	-	11,11,19	0.33	0	15,15,24	1.26	2 (13%)
23	CLA	A	405[B]	41	65,73,73	2.02	15 (23%)	76,113,113	2.78	29 (38%)
23	CLA	B	610	41	65,73,73	2.07	18 (27%)	76,113,113	2.89	28 (36%)
28	OEX	a	413[B]	3,41,1	0,15,15	-	-	-	-	-
25	BCR	t	102	-	41,41,41	1.02	1 (2%)	56,56,56	1.69	14 (25%)
35	HTG	b	622	-	19,19,19	1.28	2 (10%)	23,24,24	1.94	8 (34%)
23	CLA	B	614	-	65,73,73	2.02	17 (26%)	76,113,113	2.99	29 (38%)
33	LHG	D	706[B]	-	48,48,48	0.87	2 (4%)	51,54,54	0.98	3 (5%)
27	GOL	O	303	-	5,5,5	1.02	0	5,5,5	1.02	0
23	CLA	B	607	41	65,73,73	1.95	18 (27%)	76,113,113	2.81	29 (38%)
23	CLA	C	508	41	65,73,73	1.99	16 (24%)	76,113,113	2.72	25 (32%)
32	LMT	A	418	-	36,36,36	0.93	3 (8%)	47,47,47	1.05	2 (4%)
23	CLA	A	404[A]	-	65,73,73	2.02	16 (24%)	76,113,113	2.77	32 (42%)
23	CLA	B	605	-	65,73,73	1.98	16 (24%)	76,113,113	2.87	27 (35%)
32	LMT	b	627	-	25,25,36	0.89	1 (4%)	30,30,47	1.12	2 (6%)
35	HTG	B	622	-	19,19,19	0.80	1 (5%)	23,24,24	1.41	2 (8%)
36	DGD	h	102	-	63,63,67	0.85	3 (4%)	77,77,81	1.16	8 (10%)
23	CLA	B	612	-	65,73,73	2.05	18 (27%)	76,113,113	2.82	27 (35%)
23	CLA	D	703	-	65,73,73	2.08	16 (24%)	76,113,113	2.73	29 (38%)
29	PL9	A	414[A]	-	55,55,55	0.68	2 (3%)	68,69,69	2.08	25 (36%)
32	LMT	T	101	-	36,36,36	1.10	3 (8%)	47,47,47	1.08	2 (4%)
23	CLA	C	506	-	65,73,73	2.02	16 (24%)	76,113,113	2.67	27 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	DGD	C	517[B]	-	63,63,67	0.83	2 (3%)	77,77,81	1.14	8 (10%)
23	CLA	B	603	-	65,73,73	2.06	18 (27%)	76,113,113	2.90	31 (40%)
33	LHG	a	420[A]	-	41,41,48	1.04	2 (4%)	44,47,54	0.92	2 (4%)
27	GOL	v	202[B]	-	5,5,5	1.06	0	5,5,5	0.84	0
27	GOL	A	411	-	5,5,5	1.21	0	5,5,5	0.66	0
23	CLA	C	509	-	65,73,73	2.13	16 (24%)	76,113,113	2.69	28 (36%)
26	SQD	b	620	-	53,54,54	1.06	3 (5%)	62,65,65	1.69	12 (19%)
26	SQD	a	411[B]	-	53,54,54	0.97	3 (5%)	62,65,65	1.58	12 (19%)
29	PL9	a	414[B]	-	55,55,55	0.62	2 (3%)	68,69,69	1.95	22 (32%)
23	CLA	b	608	-	65,73,73	2.01	16 (24%)	76,113,113	2.72	30 (39%)
27	GOL	b	624	-	5,5,5	1.18	1 (20%)	5,5,5	0.78	0
25	BCR	H	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.44	8 (14%)
34	LMG	m	101	-	51,51,55	0.87	2 (3%)	59,59,63	1.28	7 (11%)
32	LMT	B	630	-	25,25,36	0.89	2 (8%)	30,30,47	1.18	3 (10%)
35	HTG	C	522	-	19,19,19	0.88	1 (5%)	23,24,24	1.34	2 (8%)
25	BCR	Y	101	-	41,41,41	0.92	1 (2%)	56,56,56	1.69	15 (26%)
23	CLA	b	604	-	65,73,73	2.00	17 (26%)	76,113,113	2.70	26 (34%)
23	CLA	C	503	-	65,73,73	2.05	16 (24%)	76,113,113	2.59	25 (32%)
24	PHO	A	417[B]	-	51,69,69	1.91	8 (15%)	47,99,99	1.88	10 (21%)
25	BCR	b	619	-	41,41,41	1.08	1 (2%)	56,56,56	1.40	11 (19%)
27	GOL	D	712	-	5,5,5	1.56	2 (40%)	5,5,5	0.88	0
23	CLA	B	609	-	65,73,73	2.00	15 (23%)	76,113,113	2.78	27 (35%)
33	LHG	E	101[A]	-	41,41,48	1.06	2 (4%)	44,47,54	1.11	3 (6%)
23	CLA	b	602	-	65,73,73	2.05	14 (21%)	76,113,113	2.95	31 (40%)
23	CLA	d	401[B]	-	65,73,73	2.02	16 (24%)	76,113,113	2.75	29 (38%)
25	BCR	y	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.62	12 (21%)
34	LMG	z	101	-	39,39,55	1.10	2 (5%)	47,47,63	1.04	2 (4%)
33	LHG	A	419[B]	-	48,48,48	0.86	2 (4%)	51,54,54	1.18	5 (9%)
23	CLA	c	504	-	65,73,73	2.02	15 (23%)	76,113,113	2.84	24 (31%)
33	LHG	d	406[B]	-	48,48,48	0.93	2 (4%)	51,54,54	0.96	2 (3%)
23	CLA	b	609	-	65,73,73	2.00	16 (24%)	76,113,113	2.77	29 (38%)
25	BCR	D	704	-	41,41,41	1.10	1 (2%)	56,56,56	1.96	20 (35%)
32	LMT	e	101	-	36,36,36	1.03	3 (8%)	47,47,47	0.97	1 (2%)
33	LHG	b	629[A]	-	48,48,48	0.85	3 (6%)	51,54,54	1.03	4 (7%)
40	HEC	V	201	16	32,50,50	2.07	4 (12%)	24,82,82	2.06	6 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	d	401[A]	-	65,73,73	1.94	17 (26%)	76,113,113	2.79	29 (38%)
36	DGD	C	519	-	63,63,67	0.85	3 (4%)	77,77,81	1.01	3 (3%)
36	DGD	c	518[A]	-	63,63,67	0.84	2 (3%)	77,77,81	0.97	5 (6%)
33	LHG	L	101[A]	-	48,48,48	0.89	2 (4%)	51,54,54	1.15	3 (5%)
40	HEC	v	201	16	32,50,50	1.97	4 (12%)	24,82,82	1.95	6 (25%)
35	HTG	c	522	-	19,19,19	0.91	1 (5%)	23,24,24	1.45	2 (8%)
23	CLA	b	606	-	65,73,73	1.99	16 (24%)	76,113,113	2.89	29 (38%)
25	BCR	B	618	-	41,41,41	0.97	1 (2%)	56,56,56	1.42	8 (14%)
23	CLA	c	503	-	65,73,73	2.07	16 (24%)	76,113,113	2.64	25 (32%)
24	PHO	a	416[B]	-	51,69,69	1.91	8 (15%)	47,99,99	1.89	9 (19%)
29	PL9	d	404[A]	-	55,55,55	0.65	1 (1%)	68,69,69	1.63	17 (25%)
31	BCT	a	404[A]	21	2,3,3	0.57	0	2,3,3	1.58	1 (50%)
23	CLA	b	605	-	65,73,73	1.95	13 (20%)	76,113,113	2.95	29 (38%)
23	CLA	B	613	-	65,73,73	1.98	17 (26%)	76,113,113	2.77	31 (40%)
23	CLA	b	613	-	65,73,73	1.99	15 (23%)	76,113,113	2.85	29 (38%)
23	CLA	A	404[B]	-	65,73,73	2.10	16 (24%)	76,113,113	2.81	30 (39%)
23	CLA	C	510	-	65,73,73	2.11	17 (26%)	76,113,113	2.80	28 (36%)
23	CLA	b	603	-	65,73,73	2.03	16 (24%)	76,113,113	2.94	29 (38%)
34	LMG	Z	101	-	37,37,55	1.01	2 (5%)	45,45,63	1.42	6 (13%)
24	PHO	a	416[A]	-	51,69,69	1.86	9 (17%)	47,99,99	1.99	13 (27%)
27	GOL	l	102[A]	-	5,5,5	0.96	0	5,5,5	0.97	0
23	CLA	c	507	-	65,73,73	2.06	16 (24%)	76,113,113	2.75	30 (39%)
29	PL9	A	414[B]	-	55,55,55	0.65	2 (3%)	68,69,69	1.99	24 (35%)
35	HTG	d	409	-	16,16,19	0.97	1 (6%)	20,21,24	1.49	1 (5%)
36	DGD	C	518[A]	-	63,63,67	0.89	3 (4%)	77,77,81	1.02	5 (6%)
25	BCR	A	409	-	41,41,41	0.99	1 (2%)	56,56,56	1.34	8 (14%)
23	CLA	C	513	-	65,73,73	2.04	15 (23%)	76,113,113	2.80	29 (38%)
27	GOL	c	526[A]	-	5,5,5	0.94	0	5,5,5	0.95	0
29	PL9	D	705[A]	-	55,55,55	0.62	2 (3%)	68,69,69	1.64	18 (26%)
33	LHG	a	420[B]	-	41,41,48	1.04	2 (4%)	44,47,54	0.93	2 (4%)
34	LMG	C	521	-	51,51,55	1.08	3 (5%)	59,59,63	1.35	6 (10%)
23	CLA	c	505	41	65,73,73	2.14	16 (24%)	76,113,113	2.78	29 (38%)
23	CLA	c	512	3	65,73,73	2.13	15 (23%)	76,113,113	2.76	29 (38%)
27	GOL	o	303	-	5,5,5	1.12	0	5,5,5	0.87	0
23	CLA	C	514	-	65,73,73	2.07	17 (26%)	76,113,113	2.79	28 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	GOL	o	304	-	5,5,5	1.08	1 (20%)	5,5,5	1.06	0
35	HTG	o	301	-	19,19,19	1.15	2 (10%)	23,24,24	1.67	5 (21%)
23	CLA	C	512	3	65,73,73	2.09	19 (29%)	76,113,113	2.69	26 (34%)
23	CLA	a	409	-	65,73,73	1.99	14 (21%)	76,113,113	2.92	29 (38%)
33	LHG	E	101[B]	-	41,41,48	1.06	2 (4%)	44,47,54	1.11	3 (6%)
35	HTG	b	625	-	19,19,19	1.11	2 (10%)	23,24,24	1.53	4 (17%)

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
27	GOL	a	419	-	-	1/4/4/4	-
32	LMT	F	101	-	-	8/21/61/61	0/2/2/2
23	CLA	b	616	-	1/1/15/20	9/37/115/115	-
24	PHO	a	408[A]	-	-	6/37/103/103	0/5/6/6
33	LHG	b	629[B]	-	-	16/53/53/53	-
32	LMT	B	627	-	-	12/21/61/61	0/2/2/2
25	BCR	T	102	-	-	1/29/63/63	0/2/2/2
33	LHG	L	101[B]	-	-	17/53/53/53	-
32	LMT	b	621	-	-	8/17/37/61	0/1/1/2
36	DGD	c	518[B]	-	-	16/51/91/95	0/2/2/2
23	CLA	C	507	-	1/1/15/20	12/37/115/115	-
25	BCR	C	515	-	-	1/29/63/63	0/2/2/2
23	CLA	A	408	-	1/1/15/20	9/37/115/115	-
27	GOL	B	628	-	-	4/4/4/4	-
29	PL9	d	404[B]	-	-	10/53/73/73	0/1/1/1
25	BCR	B	617	-	-	2/29/63/63	0/2/2/2
23	CLA	B	616	-	1/1/15/20	5/37/115/115	-
27	GOL	D	701	-	-	2/4/4/4	-
36	DGD	H	102	-	-	7/51/91/95	0/2/2/2
23	CLA	C	511	-	1/1/15/20	11/37/115/115	-
23	CLA	B	615	-	1/1/15/20	7/37/115/115	-
32	LMT	m	103	-	-	5/21/61/61	0/2/2/2
34	LMG	d	410	39	-	11/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	a	406[A]	41	1/1/15/20	8/37/115/115	-
24	PHO	A	407[A]	-	-	4/37/103/103	0/5/6/6
27	GOL	C	523[A]	-	-	0/4/4/4	-
27	GOL	l	102[B]	-	-	2/4/4/4	-
26	SQD	B	620	-	-	13/49/69/69	0/1/1/1
34	LMG	C	501	-	-	13/46/66/70	0/1/1/1
34	LMG	C	520	-	-	11/46/66/70	0/1/1/1
34	LMG	c	520	-	-	13/46/66/70	0/1/1/1
33	LHG	D	707[A]	-	-	14/53/53/53	-
23	CLA	b	612	-	1/1/15/20	4/37/115/115	-
23	CLA	d	402	-	1/1/15/20	8/37/115/115	-
27	GOL	a	418	-	-	2/4/4/4	-
32	LMT	B	629	-	-	11/21/61/61	0/2/2/2
33	LHG	d	405[A]	-	-	13/53/53/53	-
33	LHG	d	412[A]	-	-	13/53/53/53	-
36	DGD	C	518[B]	-	-	14/51/91/95	0/2/2/2
27	GOL	c	526[B]	-	-	0/4/4/4	-
29	PL9	D	705[B]	-	-	6/53/73/73	0/1/1/1
23	CLA	B	604	-	1/1/15/20	2/37/115/115	-
25	BCR	c	516	-	-	0/29/63/63	0/2/2/2
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
23	CLA	b	610	41	1/1/15/20	7/37/115/115	-
27	GOL	O	302	-	-	2/4/4/4	-
35	HTG	B	624	-	-	3/10/30/30	0/1/1/1
36	DGD	c	517[A]	-	-	20/51/91/95	0/2/2/2
23	CLA	B	602	-	1/1/15/20	8/37/115/115	-
36	DGD	c	519	-	-	8/51/91/95	0/2/2/2
23	CLA	c	511	-	1/1/15/20	12/37/115/115	-
32	LMT	t	101	-	-	10/17/38/61	0/1/1/2
23	CLA	B	606	-	1/1/15/20	9/37/115/115	-
32	LMT	a	417	-	-	12/21/61/61	0/2/2/2
34	LMG	c	501	-	-	11/46/66/70	0/1/1/1
38	HEM	f	101	5,6	-	6/12/54/54	-
23	CLA	c	509	-	1/1/15/20	4/37/115/115	-
34	LMG	D	711	39	-	9/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMG	B	621	-	-	20/46/66/70	0/1/1/1
24	PHO	a	408[B]	-	-	5/37/103/103	0/5/6/6
23	CLA	c	502	-	1/1/15/20	5/37/115/115	-
26	SQD	A	410[A]	-	-	12/49/69/69	0/1/1/1
26	SQD	f	102	-	-	9/38/58/69	0/1/1/1
23	CLA	C	504	-	1/1/15/20	4/37/115/115	-
23	CLA	b	615	-	1/1/15/20	8/37/115/115	-
27	GOL	V	203[A]	-	-	2/4/4/4	-
35	HTG	b	623	-	-	5/10/30/30	0/1/1/1
26	SQD	A	412	-	-	13/49/69/69	0/1/1/1
23	CLA	a	405[A]	-	1/1/15/20	3/37/115/115	-
23	CLA	c	513	-	1/1/15/20	12/37/115/115	-
23	CLA	B	608	-	-	4/37/115/115	-
23	CLA	D	702[A]	-	1/1/15/20	0/37/115/115	-
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
27	GOL	d	411	-	-	4/4/4/4	-
23	CLA	a	406[B]	41	1/1/15/20	6/37/115/115	-
23	CLA	A	406[B]	41	-	4/37/115/115	-
25	BCR	d	403	-	-	5/29/63/63	0/2/2/2
24	PHO	A	407[B]	-	-	3/37/103/103	0/5/6/6
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
27	GOL	C	523[B]	-	-	0/4/4/4	-
23	CLA	A	405[A]	41	-	4/37/115/115	-
23	CLA	B	601	41	1/1/15/20	11/37/115/115	-
33	LHG	D	707[B]	-	-	16/53/53/53	-
33	LHG	d	412[B]	-	-	13/53/53/53	-
33	LHG	d	405[B]	-	-	14/53/53/53	-
23	CLA	A	406[A]	41	-	5/37/115/115	-
32	LMT	M	101	-	-	5/21/61/61	0/2/2/2
33	LHG	D	706[A]	-	-	16/53/53/53	-
23	CLA	c	506	-	1/1/15/20	7/37/115/115	-
23	CLA	a	407[B]	41	-	6/37/115/115	-
36	DGD	c	517[B]	-	-	19/51/91/95	0/2/2/2
27	GOL	b	628	-	-	0/4/4/4	-
23	CLA	b	607	41	1/1/15/20	3/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	a	407[A]	41	-	5/37/115/115	-
34	LMG	c	521	-	-	13/46/66/70	0/1/1/1
23	CLA	c	514	-	1/1/15/20	10/37/115/115	-
23	CLA	c	508	41	1/1/15/20	7/37/115/115	-
25	BCR	h	101	-	-	2/29/63/63	0/2/2/2
36	DGD	C	517[A]	-	-	11/51/91/95	0/2/2/2
27	GOL	v	202[A]	-	-	1/4/4/4	-
25	BCR	K	102	-	-	2/29/63/63	0/2/2/2
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
27	GOL	B	623	-	-	4/4/4/4	-
23	CLA	b	601	41	1/1/15/20	19/37/115/115	-
29	PL9	a	414[A]	-	-	14/53/73/73	0/1/1/1
26	SQD	a	411[A]	-	-	10/49/69/69	0/1/1/1
26	SQD	A	410[B]	-	-	11/49/69/69	0/1/1/1
26	SQD	a	412	-	-	13/49/69/69	0/1/1/1
26	SQD	X	101	-	-	16/38/58/69	0/1/1/1
27	GOL	V	203[B]	-	-	2/4/4/4	-
35	HTG	D	710	-	-	3/7/27/30	0/1/1/1
23	CLA	c	510	-	1/1/15/20	16/37/115/115	-
27	GOL	B	626	-	-	1/4/4/4	-
24	PHO	A	417[A]	-	-	1/37/103/103	0/5/6/6
27	GOL	c	527	-	-	2/4/4/4	-
23	CLA	a	405[B]	-	1/1/15/20	4/37/115/115	-
23	CLA	b	614	-	1/1/15/20	14/37/115/115	-
23	CLA	C	502	-	1/1/15/20	5/37/115/115	-
23	CLA	D	702[B]	-	1/1/15/20	0/37/115/115	-
33	LHG	A	419[A]	-	-	10/53/53/53	-
23	CLA	C	505	41	1/1/15/20	8/37/115/115	-
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
33	LHG	d	406[A]	-	-	11/53/53/53	-
32	LMT	A	420	-	-	15/21/61/61	0/2/2/2
38	HEM	F	102	5,6	-	4/12/54/54	-
23	CLA	B	611	-	1/1/15/20	2/37/115/115	-
23	CLA	b	611	-	1/1/15/20	3/37/115/115	-
25	BCR	a	410	-	-	1/29/63/63	0/2/2/2
25	BCR	c	515	-	-	1/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HTG	V	202	-	-	0/2/19/30	0/1/1/1
23	CLA	A	405[B]	41	1/1/15/20	4/37/115/115	-
23	CLA	B	610	41	1/1/15/20	8/37/115/115	-
25	BCR	t	102	-	-	5/29/63/63	0/2/2/2
35	HTG	b	622	-	-	4/10/30/30	0/1/1/1
23	CLA	B	614	-	1/1/15/20	15/37/115/115	-
33	LHG	D	706[B]	-	-	17/53/53/53	-
27	GOL	O	303	-	-	2/4/4/4	-
23	CLA	B	607	41	1/1/15/20	6/37/115/115	-
23	CLA	C	508	41	1/1/15/20	7/37/115/115	-
32	LMT	A	418	-	-	6/21/61/61	0/2/2/2
23	CLA	A	404[A]	-	1/1/15/20	5/37/115/115	-
23	CLA	B	605	-	1/1/15/20	4/37/115/115	-
32	LMT	b	627	-	-	11/17/37/61	0/1/1/2
35	HTG	B	622	-	-	1/10/30/30	0/1/1/1
36	DGD	h	102	-	-	15/51/91/95	0/2/2/2
23	CLA	B	612	-	1/1/15/20	5/37/115/115	-
23	CLA	D	703	-	1/1/15/20	13/37/115/115	-
29	PL9	A	414[A]	-	-	15/53/73/73	0/1/1/1
32	LMT	T	101	-	-	9/21/61/61	0/2/2/2
23	CLA	C	506	-	1/1/15/20	7/37/115/115	-
36	DGD	C	517[B]	-	-	12/51/91/95	0/2/2/2
23	CLA	B	603	-	1/1/15/20	9/37/115/115	-
33	LHG	a	420[A]	-	-	16/46/46/53	-
27	GOL	v	202[B]	-	-	2/4/4/4	-
27	GOL	A	411	-	-	2/4/4/4	-
23	CLA	C	509	-	1/1/15/20	6/37/115/115	-
26	SQD	b	620	-	-	18/49/69/69	0/1/1/1
26	SQD	a	411[B]	-	-	10/49/69/69	0/1/1/1
29	PL9	a	414[B]	-	-	14/53/73/73	0/1/1/1
23	CLA	b	608	-	-	4/37/115/115	-
27	GOL	b	624	-	-	2/4/4/4	-
25	BCR	H	101	-	-	2/29/63/63	0/2/2/2
34	LMG	m	101	-	-	9/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LMT	B	630	-	-	10/17/37/61	0/1/1/2
35	HTG	C	522	-	-	0/10/30/30	0/1/1/1
25	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
23	CLA	b	604	-	1/1/15/20	9/37/115/115	-
23	CLA	C	503	-	1/1/15/20	10/37/115/115	-
24	PHO	A	417[B]	-	-	1/37/103/103	0/5/6/6
25	BCR	b	619	-	-	4/29/63/63	0/2/2/2
27	GOL	D	712	-	-	4/4/4/4	-
23	CLA	B	609	-	1/1/15/20	3/37/115/115	-
33	LHG	E	101[A]	-	-	22/46/46/53	-
23	CLA	b	602	-	1/1/15/20	5/37/115/115	-
23	CLA	d	401[B]	-	1/1/15/20	4/37/115/115	-
25	BCR	y	101	-	-	5/29/63/63	0/2/2/2
34	LMG	z	101	-	-	9/34/54/70	0/1/1/1
33	LHG	A	419[B]	-	-	13/53/53/53	-
23	CLA	c	504	-	1/1/15/20	3/37/115/115	-
33	LHG	d	406[B]	-	-	13/53/53/53	-
23	CLA	b	609	-	1/1/15/20	1/37/115/115	-
25	BCR	D	704	-	-	4/29/63/63	0/2/2/2
32	LMT	e	101	-	-	15/21/61/61	0/2/2/2
33	LHG	b	629[A]	-	-	20/53/53/53	-
40	HEC	V	201	16	-	2/10/54/54	-
23	CLA	d	401[A]	-	1/1/15/20	2/37/115/115	-
36	DGD	C	519	-	-	19/51/91/95	0/2/2/2
36	DGD	c	518[A]	-	-	17/51/91/95	0/2/2/2
33	LHG	L	101[A]	-	-	19/53/53/53	-
40	HEC	v	201	16	-	2/10/54/54	-
35	HTG	c	522	-	-	2/10/30/30	0/1/1/1
23	CLA	b	606	-	1/1/15/20	12/37/115/115	-
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
23	CLA	c	503	-	1/1/15/20	4/37/115/115	-
24	PHO	a	416[B]	-	-	0/37/103/103	0/5/6/6
29	PL9	d	404[A]	-	-	6/53/73/73	0/1/1/1
23	CLA	b	605	-	1/1/15/20	6/37/115/115	-
23	CLA	B	613	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	613	-	1/1/15/20	4/37/115/115	-
23	CLA	A	404[B]	-	1/1/15/20	4/37/115/115	-
23	CLA	C	510	-	1/1/15/20	8/37/115/115	-
23	CLA	b	603	-	1/1/15/20	5/37/115/115	-
34	LMG	Z	101	-	-	12/31/51/70	0/1/1/1
24	PHO	a	416[A]	-	-	2/37/103/103	0/5/6/6
27	GOL	l	102[A]	-	-	2/4/4/4	-
23	CLA	c	507	-	1/1/15/20	6/37/115/115	-
29	PL9	A	414[B]	-	-	16/53/73/73	0/1/1/1
35	HTG	d	409	-	-	1/7/27/30	0/1/1/1
36	DGD	C	518[A]	-	-	15/51/91/95	0/2/2/2
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
23	CLA	C	513	-	1/1/15/20	8/37/115/115	-
27	GOL	c	526[A]	-	-	0/4/4/4	-
29	PL9	D	705[A]	-	-	8/53/73/73	0/1/1/1
33	LHG	a	420[B]	-	-	16/46/46/53	-
34	LMG	C	521	-	-	14/46/66/70	0/1/1/1
23	CLA	c	505	41	1/1/15/20	6/37/115/115	-
23	CLA	c	512	3	1/1/15/20	6/37/115/115	-
27	GOL	o	303	-	-	2/4/4/4	-
23	CLA	C	514	-	1/1/15/20	6/37/115/115	-
27	GOL	o	304	-	-	4/4/4/4	-
35	HTG	o	301	-	-	4/10/30/30	0/1/1/1
23	CLA	C	512	3	1/1/15/20	3/37/115/115	-
23	CLA	a	409	-	-	10/37/115/115	-
33	LHG	E	101[B]	-	-	23/46/46/53	-
35	HTG	b	625	-	-	5/10/30/30	0/1/1/1

All (1553) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	611	CLA	C3B-C2B	10.56	1.55	1.40
23	C	510	CLA	C3B-C2B	6.89	1.49	1.40
23	C	512	CLA	C3B-C2B	6.78	1.49	1.40
23	C	509	CLA	C3B-C2B	6.78	1.49	1.40
23	B	616	CLA	C3B-C2B	6.70	1.49	1.40
23	b	603	CLA	C3B-C2B	6.67	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	505	CLA	C3B-C2B	6.65	1.49	1.40
23	A	408	CLA	C3B-C2B	6.64	1.49	1.40
23	A	404[B]	CLA	C3B-C2B	6.63	1.49	1.40
23	c	503	CLA	C3B-C2B	6.58	1.49	1.40
23	B	608	CLA	C3B-C2B	6.57	1.49	1.40
23	B	611	CLA	C1D-ND	6.56	1.45	1.37
23	C	503	CLA	C3B-C2B	6.52	1.49	1.40
23	B	603	CLA	C3B-C2B	6.50	1.49	1.40
23	C	514	CLA	C3B-C2B	6.48	1.49	1.40
24	a	408[B]	PHO	C3B-C2B	6.42	1.49	1.40
23	b	613	CLA	C3B-C2B	6.39	1.49	1.40
24	a	416[B]	PHO	C3B-C2B	6.38	1.49	1.40
23	c	512	CLA	C3B-C2B	6.38	1.49	1.40
24	a	408[A]	PHO	C3B-C2B	6.36	1.49	1.40
23	a	405[B]	CLA	C3B-C2B	6.35	1.49	1.40
23	b	601	CLA	C3B-C2B	6.34	1.49	1.40
23	c	514	CLA	C3B-C2B	6.31	1.49	1.40
23	B	611	CLA	CMB-C2B	6.30	1.64	1.51
23	D	702[B]	CLA	C3B-C2B	6.29	1.49	1.40
23	B	612	CLA	C3B-C2B	6.26	1.49	1.40
23	a	405[A]	CLA	C3B-C2B	6.26	1.49	1.40
23	A	404[A]	CLA	C3B-C2B	6.26	1.49	1.40
23	c	510	CLA	C3B-C2B	6.25	1.49	1.40
24	A	417[B]	PHO	C3B-C2B	6.25	1.49	1.40
24	A	407[B]	PHO	C3B-C2B	6.25	1.49	1.40
23	b	604	CLA	C3B-C2B	6.22	1.49	1.40
23	d	401[B]	CLA	C3B-C2B	6.21	1.49	1.40
23	b	614	CLA	C3B-C2B	6.21	1.49	1.40
24	A	407[A]	PHO	C3B-C2B	6.19	1.49	1.40
23	c	509	CLA	C3B-C2B	6.16	1.48	1.40
23	b	612	CLA	C3B-C2B	6.13	1.48	1.40
23	C	505	CLA	C3B-C2B	6.12	1.48	1.40
24	A	417[A]	PHO	C3B-C2B	6.12	1.48	1.40
23	B	604	CLA	C3B-C2B	6.09	1.48	1.40
23	B	602	CLA	C3B-C2B	6.08	1.48	1.40
23	b	611	CLA	C3B-C2B	6.08	1.48	1.40
23	c	511	CLA	C3B-C2B	6.03	1.48	1.40
23	c	507	CLA	C3B-C2B	6.03	1.48	1.40
23	a	409	CLA	C3B-C2B	6.02	1.48	1.40
40	V	201	HEC	C2B-C3B	-6.00	1.34	1.40
23	b	607	CLA	C3B-C2B	5.98	1.48	1.40
23	B	601	CLA	C3B-C2B	5.98	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	608	CLA	C3B-C2B	5.98	1.48	1.40
23	b	610	CLA	C3B-C2B	5.94	1.48	1.40
23	D	702[A]	CLA	C3B-C2B	5.94	1.48	1.40
23	A	405[B]	CLA	C3B-C2B	5.93	1.48	1.40
23	B	613	CLA	C3B-C2B	5.92	1.48	1.40
24	a	416[A]	PHO	C3B-C2B	5.90	1.48	1.40
23	C	507	CLA	C3B-C2B	5.84	1.48	1.40
23	B	610	CLA	C3C-C2C	5.83	1.49	1.36
23	C	511	CLA	C1D-ND	5.81	1.44	1.37
23	B	607	CLA	C3B-C2B	5.79	1.48	1.40
23	C	511	CLA	C3B-C2B	5.77	1.48	1.40
23	C	513	CLA	C3B-C2B	5.76	1.48	1.40
23	b	616	CLA	C3B-C2B	5.75	1.48	1.40
23	B	611	CLA	CHC-C1C	5.73	1.49	1.35
23	B	606	CLA	C3B-C2B	5.72	1.48	1.40
40	v	201	HEC	C2B-C3B	-5.71	1.34	1.40
23	a	406[B]	CLA	C3B-C2B	5.69	1.48	1.40
23	a	407[B]	CLA	C3B-C2B	5.69	1.48	1.40
23	c	513	CLA	C3C-C2C	5.68	1.48	1.36
23	b	606	CLA	C3B-C2B	5.66	1.48	1.40
23	b	612	CLA	C3C-C2C	5.66	1.48	1.36
23	B	611	CLA	C3C-C2C	5.65	1.48	1.36
23	D	703	CLA	C1D-ND	5.65	1.44	1.37
23	c	512	CLA	C1D-ND	5.65	1.44	1.37
23	d	401[A]	CLA	C3B-C2B	5.65	1.48	1.40
23	c	509	CLA	C3C-C2C	5.63	1.48	1.36
23	D	703	CLA	C3C-C2C	5.61	1.48	1.36
23	b	607	CLA	C3C-C2C	5.60	1.48	1.36
23	C	513	CLA	CHC-C1C	5.60	1.49	1.35
23	b	605	CLA	C3B-C2B	5.60	1.48	1.40
23	d	402	CLA	C3B-C2B	5.59	1.48	1.40
23	C	513	CLA	C3C-C2C	5.57	1.48	1.36
23	a	406[B]	CLA	C1D-ND	5.57	1.44	1.37
23	d	402	CLA	C3C-C2C	5.57	1.48	1.36
24	a	408[B]	PHO	C3D-C2D	5.56	1.49	1.39
40	V	201	HEC	C3C-C2C	-5.56	1.34	1.40
23	c	505	CLA	C1D-ND	5.56	1.44	1.37
23	A	404[B]	CLA	C3C-C2C	5.56	1.48	1.36
23	b	602	CLA	CHC-C1C	5.55	1.49	1.35
23	c	506	CLA	C3B-C2B	5.53	1.48	1.40
23	b	614	CLA	C3C-C2C	5.52	1.48	1.36
23	b	606	CLA	C3C-C2C	5.52	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	605	CLA	C1D-ND	5.52	1.44	1.37
23	C	508	CLA	C3B-C2B	5.51	1.48	1.40
23	b	609	CLA	C3B-C2B	5.51	1.48	1.40
23	b	601	CLA	C1D-ND	5.49	1.44	1.37
23	b	610	CLA	C3C-C2C	5.46	1.48	1.36
23	C	509	CLA	C3C-C2C	5.46	1.48	1.36
23	B	616	CLA	C3C-C2C	5.45	1.48	1.36
23	A	404[A]	CLA	C3C-C2C	5.45	1.48	1.36
23	c	514	CLA	C1D-ND	5.44	1.44	1.37
23	d	402	CLA	CHC-C1C	5.44	1.48	1.35
23	a	405[B]	CLA	C3C-C2C	5.43	1.48	1.36
23	a	409	CLA	C3C-C2C	5.42	1.48	1.36
23	B	601	CLA	C3C-C2C	5.42	1.48	1.36
23	c	502	CLA	C1D-ND	5.42	1.44	1.37
24	a	408[A]	PHO	C3D-C2D	5.41	1.49	1.39
23	c	506	CLA	C3C-C2C	5.41	1.48	1.36
23	c	510	CLA	C3C-C2C	5.41	1.48	1.36
23	c	505	CLA	O2D-CGD	5.40	1.46	1.33
23	b	611	CLA	C3C-C2C	5.39	1.48	1.36
23	a	406[B]	CLA	C3C-C2C	5.39	1.48	1.36
23	c	509	CLA	O2D-CGD	5.38	1.46	1.33
23	B	606	CLA	CHC-C1C	5.37	1.48	1.35
23	A	404[B]	CLA	C1D-ND	5.37	1.44	1.37
23	b	605	CLA	C3C-C2C	5.37	1.48	1.36
23	C	509	CLA	C1D-ND	5.37	1.44	1.37
23	c	504	CLA	C3C-C2C	5.37	1.48	1.36
23	C	506	CLA	CHC-C1C	5.36	1.48	1.35
23	c	513	CLA	CHC-C1C	5.36	1.48	1.35
23	A	405[B]	CLA	C3C-C2C	5.36	1.48	1.36
23	d	402	CLA	C1D-ND	5.36	1.44	1.37
24	a	416[B]	PHO	C3D-C2D	5.36	1.49	1.39
23	C	508	CLA	C3C-C2C	5.35	1.48	1.36
23	A	406[B]	CLA	C3B-C2B	5.35	1.47	1.40
23	a	406[A]	CLA	C3C-C2C	5.35	1.48	1.36
23	b	613	CLA	C1D-ND	5.35	1.44	1.37
23	B	616	CLA	CHC-C1C	5.35	1.48	1.35
23	b	610	CLA	CHC-C1C	5.35	1.48	1.35
23	A	406[B]	CLA	C3C-C2C	5.34	1.48	1.36
23	B	614	CLA	C3B-C2B	5.34	1.47	1.40
24	A	417[B]	PHO	C3D-C2D	5.34	1.49	1.39
23	a	407[A]	CLA	C3C-C2C	5.34	1.48	1.36
23	c	504	CLA	CHC-C1C	5.33	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	506	CLA	CHC-C1C	5.33	1.48	1.35
23	b	603	CLA	C3C-C2C	5.33	1.48	1.36
23	D	702[B]	CLA	C3C-C2C	5.32	1.48	1.36
23	C	504	CLA	C3C-C2C	5.32	1.48	1.36
23	a	407[B]	CLA	C3C-C2C	5.31	1.48	1.36
23	d	401[B]	CLA	C3C-C2C	5.31	1.48	1.36
23	c	508	CLA	C3B-C2B	5.31	1.47	1.40
23	c	510	CLA	O2D-CGD	5.31	1.46	1.33
23	b	615	CLA	C3C-C2C	5.30	1.48	1.36
23	b	614	CLA	O2D-CGD	5.30	1.46	1.33
23	c	511	CLA	C3C-C2C	5.30	1.48	1.36
23	C	505	CLA	C3C-C2C	5.29	1.48	1.36
23	C	502	CLA	C3B-C2B	5.29	1.47	1.40
23	b	614	CLA	CHC-C1C	5.29	1.48	1.35
23	b	601	CLA	C3C-C2C	5.28	1.48	1.36
24	a	416[A]	PHO	C3D-C2D	5.28	1.48	1.39
23	B	613	CLA	CHC-C1C	5.28	1.48	1.35
40	v	201	HEC	C3D-C2D	5.28	1.53	1.37
23	C	508	CLA	CHC-C1C	5.28	1.48	1.35
23	B	615	CLA	C1D-ND	5.28	1.44	1.37
23	c	511	CLA	O2D-CGD	5.27	1.46	1.33
23	C	504	CLA	CHC-C1C	5.27	1.48	1.35
23	B	609	CLA	CHC-C1C	5.27	1.48	1.35
23	c	512	CLA	C3C-C2C	5.27	1.47	1.36
23	c	514	CLA	CHC-C1C	5.26	1.48	1.35
24	A	417[A]	PHO	C3D-C2D	5.25	1.48	1.39
23	b	613	CLA	CHC-C1C	5.24	1.48	1.35
23	B	610	CLA	C1D-ND	5.24	1.44	1.37
23	B	602	CLA	C3C-C2C	5.23	1.47	1.36
23	d	401[A]	CLA	C3C-C2C	5.23	1.47	1.36
23	c	505	CLA	C3C-C2C	5.23	1.47	1.36
23	a	407[A]	CLA	C3B-C2B	5.22	1.47	1.40
23	b	602	CLA	C3C-C2C	5.22	1.47	1.36
23	D	702[A]	CLA	C3C-C2C	5.22	1.47	1.36
23	A	404[B]	CLA	CHC-C1C	5.22	1.48	1.35
23	a	405[A]	CLA	C3C-C2C	5.22	1.47	1.36
23	b	615	CLA	CHC-C1C	5.22	1.48	1.35
23	B	614	CLA	C1D-ND	5.21	1.44	1.37
23	a	409	CLA	CHC-C1C	5.21	1.48	1.35
23	c	514	CLA	C3C-C2C	5.21	1.47	1.36
23	b	616	CLA	CHC-C1C	5.21	1.48	1.35
23	a	406[B]	CLA	O2D-CGD	5.21	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	613	CLA	O2D-CGD	5.20	1.45	1.33
23	a	407[B]	CLA	CHC-C1C	5.19	1.48	1.35
23	C	511	CLA	C3C-C2C	5.19	1.47	1.36
23	C	511	CLA	CHC-C1C	5.19	1.48	1.35
23	c	507	CLA	C3C-C2C	5.19	1.47	1.36
23	C	510	CLA	C3C-C2C	5.19	1.47	1.36
23	A	405[A]	CLA	C3B-C2B	5.18	1.47	1.40
23	c	503	CLA	C3C-C2C	5.18	1.47	1.36
23	B	614	CLA	C3C-C2C	5.18	1.47	1.36
23	C	505	CLA	CHC-C1C	5.18	1.48	1.35
23	C	502	CLA	C1D-ND	5.17	1.44	1.37
23	B	605	CLA	C3C-C2C	5.17	1.47	1.36
23	D	703	CLA	CHC-C1C	5.17	1.48	1.35
23	B	612	CLA	CHC-C1C	5.16	1.48	1.35
23	c	508	CLA	CHC-C1C	5.16	1.48	1.35
23	a	406[A]	CLA	C1D-ND	5.16	1.44	1.37
23	B	603	CLA	C1D-ND	5.16	1.44	1.37
23	B	601	CLA	CHC-C1C	5.16	1.48	1.35
24	A	417[B]	PHO	O2D-CGD	5.16	1.45	1.33
23	b	603	CLA	O2D-CGD	5.15	1.45	1.33
23	b	606	CLA	CHC-C1C	5.15	1.48	1.35
23	B	601	CLA	O2A-CGA	5.15	1.48	1.33
23	C	502	CLA	CHC-C1C	5.15	1.48	1.35
23	C	503	CLA	C3C-C2C	5.15	1.47	1.36
23	C	514	CLA	C3C-C2C	5.15	1.47	1.36
23	c	511	CLA	C1D-ND	5.15	1.44	1.37
25	C	516	BCR	C23-C22	-5.14	1.34	1.45
23	c	504	CLA	C1D-ND	5.14	1.44	1.37
23	b	609	CLA	CHC-C1C	5.14	1.48	1.35
25	C	515	BCR	C23-C22	-5.14	1.34	1.45
23	B	609	CLA	O2D-CGD	5.14	1.45	1.33
24	a	416[B]	PHO	OBD-CAD	5.13	1.29	1.22
23	b	609	CLA	O2D-CGD	5.13	1.45	1.33
23	b	615	CLA	C3B-C2B	5.13	1.47	1.40
23	B	610	CLA	C3B-C2B	5.13	1.47	1.40
23	B	604	CLA	C3C-C2C	5.13	1.47	1.36
23	b	602	CLA	O2D-CGD	5.13	1.45	1.33
23	B	609	CLA	C3B-C2B	5.13	1.47	1.40
23	C	506	CLA	C3B-C2B	5.13	1.47	1.40
23	C	504	CLA	C3B-C2B	5.13	1.47	1.40
23	B	608	CLA	C3C-C2C	5.12	1.47	1.36
23	A	406[A]	CLA	CHC-C1C	5.12	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	504	CLA	C3B-C2B	5.12	1.47	1.40
23	A	406[B]	CLA	CHC-C1C	5.12	1.48	1.35
23	c	513	CLA	C1D-ND	5.11	1.44	1.37
23	c	509	CLA	CHC-C1C	5.11	1.48	1.35
23	C	503	CLA	O2D-CGD	5.11	1.45	1.33
23	A	408	CLA	C3C-C2C	5.10	1.47	1.36
23	b	616	CLA	C1D-ND	5.10	1.44	1.37
23	C	502	CLA	C3C-C2C	5.09	1.47	1.36
23	c	514	CLA	O2D-CGD	5.09	1.45	1.33
24	a	408[B]	PHO	O2D-CGD	5.08	1.45	1.33
23	B	615	CLA	C3C-C2C	5.08	1.47	1.36
25	d	403	BCR	C23-C22	-5.08	1.35	1.45
23	b	616	CLA	C3C-C2C	5.07	1.47	1.36
23	b	603	CLA	CHC-C1C	5.07	1.48	1.35
23	B	605	CLA	CHC-C1C	5.07	1.48	1.35
23	c	502	CLA	CHC-C1C	5.06	1.47	1.35
23	c	502	CLA	C3B-C2B	5.06	1.47	1.40
23	C	506	CLA	C3C-C2C	5.06	1.47	1.36
23	B	601	CLA	C1D-ND	5.06	1.44	1.37
23	c	513	CLA	C3B-C2B	5.06	1.47	1.40
23	A	406[A]	CLA	C3C-C2C	5.05	1.47	1.36
23	c	509	CLA	C1D-ND	5.05	1.44	1.37
23	B	609	CLA	C3C-C2C	5.05	1.47	1.36
23	C	507	CLA	O2D-CGD	5.04	1.45	1.33
23	C	509	CLA	O2D-CGD	5.03	1.45	1.33
23	B	606	CLA	C3C-C2C	5.03	1.47	1.36
24	a	408[A]	PHO	O2D-CGD	5.03	1.45	1.33
23	c	503	CLA	O2D-CGD	5.03	1.45	1.33
23	B	601	CLA	O2D-CGD	5.03	1.45	1.33
23	D	703	CLA	C3B-C2B	5.02	1.47	1.40
23	b	615	CLA	C1D-ND	5.02	1.44	1.37
23	c	503	CLA	C1D-ND	5.02	1.44	1.37
23	a	407[A]	CLA	CHC-C1C	5.01	1.47	1.35
23	c	510	CLA	C1D-ND	5.01	1.43	1.37
23	a	406[A]	CLA	C3B-C2B	5.01	1.47	1.40
23	b	607	CLA	CHC-C1C	5.01	1.47	1.35
23	B	612	CLA	C3C-C2C	5.01	1.47	1.36
23	A	405[B]	CLA	CHC-C1C	5.00	1.47	1.35
23	C	514	CLA	C1D-ND	5.00	1.43	1.37
23	b	605	CLA	O2D-CGD	5.00	1.45	1.33
23	a	405[B]	CLA	C1D-ND	5.00	1.43	1.37
23	B	603	CLA	C3C-C2C	4.99	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	512	CLA	CHC-C1C	4.99	1.47	1.35
40	V	201	HEC	C3D-C2D	4.99	1.52	1.37
25	k	101	BCR	C23-C22	-4.99	1.35	1.45
23	c	507	CLA	O2D-CGD	4.99	1.45	1.33
23	A	405[A]	CLA	CHC-C1C	4.99	1.47	1.35
23	b	604	CLA	C3C-C2C	4.98	1.47	1.36
23	c	507	CLA	C1D-ND	4.98	1.43	1.37
23	a	406[A]	CLA	O2D-CGD	4.98	1.45	1.33
24	a	416[B]	PHO	O2D-CGD	4.98	1.45	1.33
23	C	512	CLA	CHC-C1C	4.97	1.47	1.35
23	C	503	CLA	C1D-ND	4.97	1.43	1.37
23	B	602	CLA	CHC-C1C	4.96	1.47	1.35
23	C	511	CLA	O2D-CGD	4.96	1.45	1.33
23	C	512	CLA	O2D-CGD	4.96	1.45	1.33
23	b	616	CLA	O2D-CGD	4.95	1.45	1.33
24	a	416[A]	PHO	O2D-CGD	4.95	1.45	1.33
26	X	101	SQD	O47-C7	4.95	1.48	1.34
23	b	610	CLA	O2D-CGD	4.95	1.45	1.33
23	c	505	CLA	CHC-C1C	4.95	1.47	1.35
23	C	506	CLA	C1D-ND	4.95	1.43	1.37
23	B	610	CLA	CHC-C1C	4.94	1.47	1.35
23	b	613	CLA	C3C-C2C	4.94	1.47	1.36
23	B	603	CLA	O2D-CGD	4.94	1.45	1.33
23	b	601	CLA	CHC-C1C	4.94	1.47	1.35
24	A	407[B]	PHO	O2D-CGD	4.94	1.45	1.33
23	D	702[B]	CLA	CHC-C1C	4.93	1.47	1.35
23	B	615	CLA	CHC-C1C	4.93	1.47	1.35
23	a	407[B]	CLA	O2D-CGD	4.93	1.45	1.33
23	A	406[A]	CLA	C3B-C2B	4.93	1.47	1.40
24	A	417[B]	PHO	OBD-CAD	4.92	1.29	1.22
23	D	702[B]	CLA	O2D-CGD	4.92	1.45	1.33
23	b	612	CLA	CHC-C1C	4.92	1.47	1.35
23	C	510	CLA	O2D-CGD	4.92	1.45	1.33
24	A	407[B]	PHO	C3D-C2D	4.91	1.48	1.39
24	A	417[A]	PHO	O2D-CGD	4.91	1.45	1.33
23	B	602	CLA	C1D-ND	4.91	1.43	1.37
23	c	502	CLA	C3C-C2C	4.90	1.47	1.36
23	C	512	CLA	C3C-C2C	4.90	1.47	1.36
24	A	407[A]	PHO	O2D-CGD	4.90	1.45	1.33
23	A	406[A]	CLA	O2D-CGD	4.90	1.45	1.33
23	b	611	CLA	C1D-ND	4.90	1.43	1.37
23	c	512	CLA	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[B]	CLA	O2D-CGD	4.89	1.45	1.33
23	B	606	CLA	C1D-ND	4.89	1.43	1.37
24	A	407[A]	PHO	C3D-C2D	4.88	1.48	1.39
23	a	406[B]	CLA	CHC-C1C	4.88	1.47	1.35
23	a	406[A]	CLA	CHC-C1C	4.87	1.47	1.35
23	A	405[B]	CLA	C1D-ND	4.87	1.43	1.37
23	b	611	CLA	CHC-C1C	4.87	1.47	1.35
23	B	607	CLA	C3C-C2C	4.87	1.47	1.36
23	A	405[A]	CLA	C3C-C2C	4.87	1.47	1.36
23	d	401[B]	CLA	CHC-C1C	4.86	1.47	1.35
23	B	615	CLA	O2D-CGD	4.86	1.45	1.33
25	B	619	BCR	C23-C22	-4.86	1.35	1.45
23	C	505	CLA	O2D-CGD	4.86	1.45	1.33
23	C	513	CLA	C1D-ND	4.86	1.43	1.37
23	B	615	CLA	C3B-C2B	4.86	1.47	1.40
25	T	102	BCR	C23-C22	-4.86	1.35	1.45
23	c	507	CLA	CHC-C1C	4.85	1.47	1.35
23	b	601	CLA	O2D-CGD	4.85	1.45	1.33
23	a	407[B]	CLA	C1D-ND	4.84	1.43	1.37
24	a	416[A]	PHO	OBD-CAD	4.84	1.29	1.22
23	B	614	CLA	CHC-C1C	4.84	1.47	1.35
23	a	405[A]	CLA	CHC-C1C	4.84	1.47	1.35
23	B	604	CLA	CHC-C1C	4.84	1.47	1.35
23	A	408	CLA	CHC-C1C	4.82	1.47	1.35
23	B	605	CLA	O2D-CGD	4.82	1.45	1.33
23	C	503	CLA	CHC-C1C	4.81	1.47	1.35
23	D	703	CLA	O2D-CGD	4.81	1.44	1.33
23	b	608	CLA	C3C-C2C	4.81	1.47	1.36
25	D	704	BCR	C23-C22	-4.81	1.35	1.45
23	C	507	CLA	C3C-C2C	4.81	1.46	1.36
23	C	514	CLA	CHC-C1C	4.80	1.47	1.35
23	c	511	CLA	CHC-C1C	4.80	1.47	1.35
23	D	702[A]	CLA	O2D-CGD	4.80	1.44	1.33
23	A	404[A]	CLA	CHC-C1C	4.80	1.47	1.35
23	b	609	CLA	C1D-ND	4.80	1.43	1.37
23	b	614	CLA	C1D-ND	4.79	1.43	1.37
23	b	609	CLA	C3C-C2C	4.79	1.46	1.36
23	d	401[B]	CLA	O2D-CGD	4.79	1.44	1.33
25	K	102	BCR	C23-C22	-4.78	1.35	1.45
23	C	510	CLA	C1D-ND	4.78	1.43	1.37
23	c	508	CLA	O2D-CGD	4.77	1.44	1.33
23	b	613	CLA	O2D-CGD	4.77	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	601	CLA	O2A-CGA	4.77	1.47	1.33
23	B	613	CLA	C3C-C2C	4.77	1.46	1.36
23	a	405[B]	CLA	CHC-C1C	4.76	1.47	1.35
23	A	405[B]	CLA	O2D-CGD	4.76	1.44	1.33
23	c	506	CLA	O2D-CGD	4.76	1.44	1.33
34	c	521	LMG	O7-C10	4.75	1.47	1.34
23	D	702[A]	CLA	CHC-C1C	4.75	1.47	1.35
23	C	514	CLA	O2D-CGD	4.75	1.44	1.33
23	b	604	CLA	CHC-C1C	4.75	1.47	1.35
23	B	603	CLA	CHC-C1C	4.75	1.47	1.35
23	b	602	CLA	C1D-ND	4.74	1.43	1.37
23	d	402	CLA	O2D-CGD	4.74	1.44	1.33
23	A	404[A]	CLA	O2D-CGD	4.73	1.44	1.33
25	b	617	BCR	C23-C22	-4.73	1.35	1.45
23	A	408	CLA	O2D-CGD	4.72	1.44	1.33
23	B	613	CLA	C1D-ND	4.72	1.43	1.37
34	C	521	LMG	O7-C10	4.72	1.47	1.34
25	y	101	BCR	C23-C22	-4.72	1.35	1.45
25	c	515	BCR	C23-C22	-4.72	1.35	1.45
23	a	409	CLA	O2D-CGD	4.72	1.44	1.33
23	C	510	CLA	CHC-C1C	4.71	1.47	1.35
23	b	608	CLA	CHC-C1C	4.71	1.47	1.35
23	c	510	CLA	CHC-C1C	4.71	1.47	1.35
23	D	702[B]	CLA	C1D-ND	4.70	1.43	1.37
23	B	610	CLA	O2D-CGD	4.70	1.44	1.33
23	c	508	CLA	C3C-C2C	4.70	1.46	1.36
23	b	606	CLA	C1D-ND	4.69	1.43	1.37
23	b	602	CLA	C3B-C2B	4.69	1.46	1.40
26	a	412	SQD	O48-C23	4.68	1.47	1.33
23	b	615	CLA	O2D-CGD	4.68	1.44	1.33
23	C	508	CLA	O2D-CGD	4.68	1.44	1.33
23	B	611	CLA	O2D-CGD	4.67	1.44	1.33
23	A	404[B]	CLA	O2D-CGD	4.67	1.44	1.33
23	b	605	CLA	CHC-C1C	4.67	1.46	1.35
25	c	516	BCR	C23-C22	-4.67	1.35	1.45
23	C	504	CLA	C1D-ND	4.67	1.43	1.37
23	d	401[A]	CLA	O2D-CGD	4.66	1.44	1.33
23	B	607	CLA	CHC-C1C	4.66	1.46	1.35
23	d	401[A]	CLA	CHC-C1C	4.66	1.46	1.35
23	B	608	CLA	CHC-C1C	4.66	1.46	1.35
23	C	507	CLA	CHC-C1C	4.65	1.46	1.35
25	B	617	BCR	C23-C22	-4.65	1.35	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	619	BCR	C23-C22	-4.65	1.36	1.45
23	C	509	CLA	CHC-C1C	4.64	1.46	1.35
23	c	503	CLA	CHC-C1C	4.64	1.46	1.35
23	B	604	CLA	O2D-CGD	4.64	1.44	1.33
23	a	405[B]	CLA	O2D-CGD	4.63	1.44	1.33
23	b	608	CLA	O2D-CGD	4.63	1.44	1.33
23	C	506	CLA	CHD-C1D	4.62	1.47	1.38
23	C	507	CLA	C1D-ND	4.62	1.43	1.37
23	a	405[A]	CLA	C1D-ND	4.62	1.43	1.37
23	c	508	CLA	C1D-ND	4.60	1.43	1.37
23	B	609	CLA	C1D-ND	4.60	1.43	1.37
23	B	614	CLA	O2D-CGD	4.59	1.44	1.33
23	d	401[B]	CLA	C1D-ND	4.59	1.43	1.37
23	c	513	CLA	O2D-CGD	4.59	1.44	1.33
25	A	409	BCR	C23-C22	-4.59	1.36	1.45
23	b	605	CLA	C1D-ND	4.59	1.43	1.37
23	b	612	CLA	O2D-CGD	4.58	1.44	1.33
26	B	620	SQD	O47-C7	4.58	1.47	1.34
23	b	606	CLA	O2D-CGD	4.57	1.44	1.33
25	h	101	BCR	C23-C22	-4.57	1.36	1.45
23	B	604	CLA	CHD-C1D	4.56	1.47	1.38
26	A	412	SQD	O48-C23	4.56	1.46	1.33
25	t	102	BCR	C23-C22	-4.56	1.36	1.45
23	C	507	CLA	CHD-C1D	4.55	1.47	1.38
23	b	611	CLA	O2D-CGD	4.55	1.44	1.33
23	a	405[A]	CLA	O2D-CGD	4.54	1.44	1.33
40	v	201	HEC	C3C-C2C	-4.53	1.36	1.40
23	C	510	CLA	CHD-C1D	4.52	1.47	1.38
34	C	521	LMG	O8-C28	4.52	1.46	1.33
23	b	604	CLA	C1D-ND	4.51	1.43	1.37
23	A	406[B]	CLA	CHD-C1D	4.51	1.47	1.38
24	a	408[B]	PHO	OBD-CAD	4.51	1.28	1.22
26	f	102	SQD	O47-C7	4.51	1.47	1.34
23	A	408	CLA	O2A-CGA	4.50	1.46	1.33
23	a	407[A]	CLA	O2D-CGD	4.50	1.44	1.33
23	B	602	CLA	O2D-CGD	4.49	1.44	1.33
34	z	101	LMG	O8-C28	4.49	1.46	1.33
23	C	502	CLA	CHD-C1D	4.49	1.47	1.38
33	E	101[A]	LHG	O8-C23	4.48	1.46	1.33
23	b	602	CLA	CHD-C1D	4.47	1.47	1.38
23	B	612	CLA	O2D-CGD	4.47	1.44	1.33
23	b	607	CLA	O2D-CGD	4.47	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	514	CLA	O2A-CGA	4.47	1.46	1.33
23	c	504	CLA	O2A-CGA	4.46	1.46	1.33
23	B	605	CLA	C3B-C2B	4.46	1.46	1.40
23	C	506	CLA	O2D-CGD	4.45	1.44	1.33
23	c	513	CLA	CHD-C1D	4.45	1.47	1.38
33	E	101[B]	LHG	O8-C23	4.44	1.46	1.33
23	C	513	CLA	O2D-CGD	4.44	1.44	1.33
23	b	610	CLA	C1D-ND	4.44	1.43	1.37
23	B	608	CLA	C1D-ND	4.44	1.43	1.37
23	a	409	CLA	O2A-CGA	4.43	1.46	1.33
34	B	621	LMG	O8-C28	4.42	1.46	1.33
23	c	504	CLA	CHD-C1D	4.41	1.47	1.38
23	B	610	CLA	OBD-CAD	4.41	1.30	1.22
25	H	101	BCR	C23-C22	-4.41	1.36	1.45
23	B	609	CLA	CHD-C1D	4.41	1.46	1.38
36	c	519	DGD	O1G-C1A	4.40	1.46	1.33
33	a	420[B]	LHG	O8-C23	4.40	1.46	1.33
33	a	420[A]	LHG	O8-C23	4.39	1.46	1.33
24	A	407[B]	PHO	OBD-CAD	4.39	1.28	1.22
23	d	402	CLA	O2A-CGA	4.39	1.46	1.33
23	B	606	CLA	O2D-CGD	4.39	1.43	1.33
23	A	405[B]	CLA	O2A-CGA	4.39	1.46	1.33
23	B	615	CLA	CHD-C1D	4.39	1.46	1.38
23	A	408	CLA	C1D-ND	4.38	1.43	1.37
23	c	502	CLA	CHD-C1D	4.38	1.46	1.38
23	a	406[A]	CLA	C3D-C2D	4.38	1.51	1.39
26	b	620	SQD	O47-C7	4.38	1.46	1.34
33	d	406[B]	LHG	O8-C23	4.38	1.46	1.33
23	c	514	CLA	CHD-C1D	4.38	1.46	1.38
23	B	614	CLA	CHD-C4C	4.38	1.49	1.39
23	b	601	CLA	CHD-C1D	4.37	1.46	1.38
23	b	604	CLA	O2D-CGD	4.36	1.43	1.33
24	a	408[A]	PHO	OBD-CAD	4.36	1.28	1.22
23	c	513	CLA	O2A-CGA	4.35	1.46	1.33
23	C	505	CLA	C1D-ND	4.35	1.43	1.37
23	C	504	CLA	O2D-CGD	4.35	1.43	1.33
23	A	405[A]	CLA	O2D-CGD	4.35	1.43	1.33
23	b	612	CLA	C1D-ND	4.34	1.43	1.37
23	a	406[B]	CLA	O2A-CGA	4.33	1.46	1.33
26	f	102	SQD	O48-C23	4.33	1.46	1.33
23	D	703	CLA	CHD-C1D	4.33	1.46	1.38
23	B	602	CLA	CHD-C1D	4.32	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	C	520	LMG	O8-C28	4.32	1.46	1.33
24	A	417[A]	PHO	OBD-CAD	4.31	1.28	1.22
23	b	613	CLA	C3D-C2D	4.31	1.50	1.39
23	c	503	CLA	C3D-C2D	4.31	1.50	1.39
33	d	406[A]	LHG	O8-C23	4.31	1.45	1.33
25	a	410	BCR	C23-C22	-4.29	1.36	1.45
23	c	506	CLA	C1D-ND	4.29	1.43	1.37
23	B	609	CLA	O2A-CGA	4.29	1.45	1.33
23	A	406[B]	CLA	C1D-ND	4.29	1.43	1.37
23	b	609	CLA	CHD-C1D	4.28	1.46	1.38
23	c	508	CLA	CHD-C1D	4.28	1.46	1.38
23	B	616	CLA	O2D-CGD	4.28	1.43	1.33
23	c	512	CLA	CHD-C1D	4.28	1.46	1.38
26	b	620	SQD	O48-C23	4.28	1.45	1.33
23	C	512	CLA	C1D-ND	4.28	1.43	1.37
23	C	514	CLA	O2A-CGA	4.27	1.45	1.33
23	a	409	CLA	C1D-ND	4.27	1.43	1.37
23	D	702[A]	CLA	C1D-ND	4.27	1.43	1.37
34	c	521	LMG	O8-C28	4.27	1.45	1.33
23	b	603	CLA	C1D-ND	4.26	1.43	1.37
33	L	101[B]	LHG	O8-C23	4.26	1.45	1.33
23	B	608	CLA	O2D-CGD	4.23	1.43	1.33
23	C	512	CLA	CHD-C1D	4.23	1.46	1.38
23	c	507	CLA	CHD-C1D	4.22	1.46	1.38
35	b	622	HTG	C1'-S1	-4.22	1.76	1.81
23	A	404[A]	CLA	C1D-ND	4.22	1.43	1.37
23	b	607	CLA	CHD-C1D	4.22	1.46	1.38
25	b	618	BCR	C23-C22	-4.22	1.36	1.45
23	D	702[A]	CLA	O2A-CGA	4.22	1.45	1.33
23	c	512	CLA	O2A-CGA	4.22	1.45	1.33
26	B	620	SQD	O48-C23	4.21	1.45	1.33
23	B	615	CLA	OBD-CAD	4.21	1.29	1.22
23	C	503	CLA	CHD-C1D	4.21	1.46	1.38
34	m	101	LMG	O8-C28	4.21	1.45	1.33
23	C	504	CLA	CHD-C4C	4.21	1.48	1.39
23	C	513	CLA	O2A-CGA	4.21	1.45	1.33
23	D	702[B]	CLA	O2A-CGA	4.20	1.45	1.33
23	a	407[B]	CLA	C3D-C2D	4.20	1.50	1.39
36	C	517[B]	DGD	O2G-C1B	4.20	1.46	1.34
23	C	514	CLA	CHD-C1D	4.20	1.46	1.38
23	A	406[B]	CLA	O2A-CGA	4.19	1.45	1.33
33	E	101[B]	LHG	O7-C7	4.19	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	610	CLA	CHD-C1D	4.19	1.46	1.38
23	B	613	CLA	C3D-C2D	4.19	1.50	1.39
36	c	518[B]	DGD	O1G-C1A	4.19	1.45	1.33
33	E	101[A]	LHG	O7-C7	4.19	1.46	1.34
23	c	502	CLA	O2D-CGD	4.19	1.43	1.33
23	A	406[A]	CLA	CHD-C1D	4.18	1.46	1.38
23	c	509	CLA	C3D-C2D	4.18	1.50	1.39
33	a	420[B]	LHG	O7-C7	4.18	1.46	1.34
34	Z	101	LMG	O7-C10	4.17	1.46	1.34
23	C	512	CLA	O2A-CGA	4.17	1.45	1.33
23	c	505	CLA	C3D-C2D	4.16	1.50	1.39
23	C	512	CLA	CHD-C4C	4.16	1.48	1.39
36	C	519	DGD	O1G-C1A	4.16	1.45	1.33
23	A	404[B]	CLA	CHD-C1D	4.16	1.46	1.38
23	b	608	CLA	C1D-ND	4.16	1.42	1.37
23	C	509	CLA	C3D-C2D	4.15	1.50	1.39
23	a	407[A]	CLA	C1D-ND	4.15	1.42	1.37
23	C	508	CLA	O2A-CGA	4.15	1.45	1.33
23	c	508	CLA	O2A-CGA	4.15	1.45	1.33
26	A	412	SQD	O47-C7	4.15	1.46	1.34
23	b	608	CLA	OBD-CAD	4.15	1.29	1.22
23	b	601	CLA	C3D-C2D	4.15	1.50	1.39
23	b	608	CLA	O2A-CGA	4.15	1.45	1.33
23	a	406[B]	CLA	CHD-C1D	4.14	1.46	1.38
23	b	610	CLA	CHD-C4C	4.14	1.48	1.39
23	b	604	CLA	CHD-C1D	4.14	1.46	1.38
24	A	407[A]	PHO	OBD-CAD	4.14	1.28	1.22
34	c	501	LMG	O7-C10	4.14	1.46	1.34
23	b	602	CLA	CHD-C4C	4.14	1.48	1.39
33	a	420[A]	LHG	O7-C7	4.13	1.46	1.34
23	B	610	CLA	CHD-C1D	4.13	1.46	1.38
23	c	503	CLA	CHD-C4C	4.13	1.48	1.39
23	C	508	CLA	C1D-ND	4.13	1.42	1.37
23	c	509	CLA	O2A-CGA	4.13	1.45	1.33
34	z	101	LMG	O7-C10	4.13	1.45	1.34
23	b	611	CLA	CHD-C1D	4.12	1.46	1.38
34	c	520	LMG	O8-C28	4.12	1.45	1.33
23	B	603	CLA	C3D-C2D	4.12	1.50	1.39
23	a	407[A]	CLA	O2A-CGA	4.12	1.45	1.33
23	B	611	CLA	OBD-CAD	4.12	1.29	1.22
23	c	502	CLA	O2A-CGA	4.12	1.45	1.33
23	b	612	CLA	CHD-C1D	4.12	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	510	CLA	CHD-C1D	4.11	1.46	1.38
23	c	507	CLA	CHD-C4C	4.11	1.48	1.39
23	C	511	CLA	CHD-C4C	4.11	1.48	1.39
23	c	509	CLA	OBD-CAD	4.11	1.29	1.22
23	C	509	CLA	CHD-C1D	4.11	1.46	1.38
23	c	507	CLA	O2A-CGA	4.10	1.45	1.33
26	a	412	SQD	O47-C7	4.10	1.45	1.34
23	B	612	CLA	C1D-ND	4.09	1.42	1.37
23	c	503	CLA	CHD-C1D	4.09	1.46	1.38
23	A	404[B]	CLA	CHD-C4C	4.09	1.48	1.39
26	a	411[B]	SQD	O47-C7	4.09	1.45	1.34
23	C	506	CLA	CHD-C4C	4.09	1.48	1.39
36	c	517[A]	DGD	O2G-C1B	4.09	1.45	1.34
23	a	406[B]	CLA	C3D-C2D	4.09	1.50	1.39
34	c	520	LMG	O7-C10	4.09	1.45	1.34
23	B	608	CLA	CHD-C1D	4.08	1.46	1.38
23	B	614	CLA	O2A-CGA	4.08	1.45	1.33
23	b	616	CLA	CHD-C1D	4.08	1.46	1.38
23	a	406[A]	CLA	O2A-CGA	4.08	1.45	1.33
23	c	506	CLA	CHD-C1D	4.08	1.46	1.38
23	d	402	CLA	CHD-C1D	4.08	1.46	1.38
23	c	504	CLA	CHD-C4C	4.08	1.48	1.39
23	b	611	CLA	O2A-CGA	4.08	1.45	1.33
23	c	503	CLA	O2A-CGA	4.08	1.45	1.33
23	c	510	CLA	O2A-CGA	4.08	1.45	1.33
23	C	503	CLA	C3D-C2D	4.07	1.50	1.39
23	c	512	CLA	OBD-CAD	4.07	1.29	1.22
23	C	509	CLA	O2A-CGA	4.07	1.45	1.33
23	A	405[B]	CLA	C3D-C2D	4.07	1.50	1.39
26	a	411[A]	SQD	O47-C7	4.07	1.45	1.34
23	B	601	CLA	CHD-C1D	4.07	1.46	1.38
34	C	501	LMG	O8-C28	4.07	1.45	1.33
23	b	614	CLA	CHD-C1D	4.06	1.46	1.38
36	C	517[A]	DGD	O2G-C1B	4.06	1.45	1.34
26	a	411[B]	SQD	O48-C23	4.06	1.45	1.33
23	c	514	CLA	CHD-C4C	4.05	1.48	1.39
23	A	405[A]	CLA	C3D-C2D	4.05	1.50	1.39
23	d	401[A]	CLA	O2A-CGA	4.05	1.45	1.33
23	b	601	CLA	CHD-C4C	4.05	1.48	1.39
34	c	501	LMG	O8-C28	4.05	1.45	1.33
23	b	605	CLA	CHD-C1D	4.05	1.46	1.38
23	C	514	CLA	C3D-C2D	4.04	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	c	517[B]	DGD	O2G-C1B	4.04	1.45	1.34
26	X	101	SQD	O48-C23	4.04	1.45	1.33
24	A	417[A]	PHO	C3C-C2C	4.04	1.49	1.37
23	A	404[A]	CLA	CHD-C1D	4.03	1.46	1.38
25	Y	101	BCR	C23-C22	-4.03	1.37	1.45
23	C	504	CLA	CHD-C1D	4.02	1.46	1.38
23	b	608	CLA	CHD-C1D	4.02	1.46	1.38
23	A	406[A]	CLA	C1D-ND	4.02	1.42	1.37
23	d	401[B]	CLA	O2A-CGA	4.02	1.45	1.33
36	C	518[B]	DGD	O1G-C1A	4.02	1.45	1.33
35	b	623	HTG	C1'-S1	-4.01	1.76	1.81
23	B	606	CLA	O2A-CGA	4.01	1.45	1.33
23	a	406[B]	CLA	CHD-C4C	4.01	1.48	1.39
23	a	407[B]	CLA	O2A-CGA	4.01	1.45	1.33
23	C	508	CLA	C3D-C2D	4.01	1.50	1.39
23	A	408	CLA	CHD-C1D	4.00	1.46	1.38
34	d	410	LMG	O8-C28	4.00	1.45	1.33
23	b	606	CLA	CHD-C1D	4.00	1.46	1.38
23	c	512	CLA	CHD-C4C	4.00	1.48	1.39
23	c	505	CLA	CHD-C1D	4.00	1.46	1.38
34	C	520	LMG	O7-C10	3.99	1.45	1.34
23	a	405[B]	CLA	CHD-C4C	3.99	1.48	1.39
23	b	614	CLA	C3D-C2D	3.99	1.50	1.39
36	h	102	DGD	O2G-C1B	3.99	1.45	1.34
23	C	505	CLA	C3D-C2D	3.99	1.50	1.39
23	a	405[A]	CLA	CHD-C1D	3.99	1.46	1.38
23	B	609	CLA	C3D-C2D	3.99	1.50	1.39
33	d	412[B]	LHG	O8-C23	3.99	1.45	1.33
23	c	513	CLA	CHD-C4C	3.98	1.48	1.39
23	A	406[B]	CLA	CHD-C4C	3.98	1.48	1.39
23	c	502	CLA	CHD-C4C	3.98	1.48	1.39
33	L	101[B]	LHG	O7-C7	3.98	1.45	1.34
33	D	707[A]	LHG	O7-C7	3.98	1.45	1.34
23	A	405[B]	CLA	CHD-C1D	3.98	1.46	1.38
23	C	513	CLA	C3D-C2D	3.98	1.50	1.39
26	a	411[A]	SQD	O48-C23	3.98	1.45	1.33
23	b	616	CLA	O2A-CGA	3.98	1.45	1.33
34	B	621	LMG	O7-C10	3.98	1.45	1.34
23	B	615	CLA	C3D-C2D	3.98	1.50	1.39
23	B	616	CLA	O2A-CGA	3.97	1.45	1.33
24	a	416[A]	PHO	C3C-C2C	3.97	1.49	1.37
23	c	504	CLA	O2D-CGD	3.97	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	d	405[B]	LHG	O7-C7	3.97	1.45	1.34
23	C	507	CLA	O2A-CGA	3.96	1.44	1.33
24	A	417[B]	PHO	O2A-CGA	3.96	1.44	1.33
23	C	510	CLA	O2A-CGA	3.96	1.44	1.33
23	b	615	CLA	O2A-CGA	3.96	1.44	1.33
23	c	509	CLA	CHD-C1D	3.96	1.46	1.38
23	c	513	CLA	C3D-C2D	3.96	1.49	1.39
23	c	507	CLA	C3D-C2D	3.96	1.49	1.39
23	a	405[A]	CLA	CHD-C4C	3.96	1.48	1.39
23	B	616	CLA	C1D-ND	3.95	1.42	1.37
23	D	703	CLA	C3D-C2D	3.95	1.49	1.39
23	C	513	CLA	CHD-C1D	3.95	1.46	1.38
23	B	604	CLA	OBD-CAD	3.95	1.29	1.22
23	B	615	CLA	O2A-CGA	3.95	1.44	1.33
23	D	702[B]	CLA	CHD-C1D	3.95	1.46	1.38
23	c	508	CLA	OBD-CAD	3.95	1.29	1.22
23	b	615	CLA	CHD-C1D	3.95	1.46	1.38
23	C	505	CLA	CHD-C1D	3.94	1.46	1.38
33	D	707[B]	LHG	O8-C23	3.94	1.44	1.33
23	B	607	CLA	O2D-CGD	3.94	1.42	1.33
23	b	607	CLA	C1D-ND	3.94	1.42	1.37
23	B	616	CLA	C3D-C2D	3.94	1.49	1.39
23	C	502	CLA	O2D-CGD	3.94	1.42	1.33
23	D	703	CLA	CHD-C4C	3.93	1.48	1.39
23	c	505	CLA	O2A-CGA	3.93	1.44	1.33
23	d	402	CLA	C3D-C2D	3.93	1.49	1.39
23	C	503	CLA	CHD-C4C	3.93	1.48	1.39
23	B	610	CLA	C3D-C2D	3.93	1.49	1.39
23	B	612	CLA	CHD-C1D	3.93	1.46	1.38
23	C	509	CLA	OBD-CAD	3.92	1.29	1.22
23	D	702[A]	CLA	CHD-C1D	3.92	1.46	1.38
23	b	612	CLA	C3D-C2D	3.92	1.49	1.39
23	d	401[B]	CLA	CHD-C1D	3.92	1.46	1.38
36	c	518[B]	DGD	O2G-C1B	3.91	1.45	1.34
23	c	510	CLA	CHD-C4C	3.91	1.48	1.39
23	B	611	CLA	CHD-C1D	3.91	1.46	1.38
23	C	510	CLA	C3D-C2D	3.91	1.49	1.39
24	a	416[B]	PHO	C3C-C2C	3.91	1.49	1.37
23	B	611	CLA	C1C-C2C	3.91	1.52	1.44
33	D	707[A]	LHG	O8-C23	3.90	1.44	1.33
23	C	505	CLA	O2A-CGA	3.90	1.44	1.33
23	C	512	CLA	C3D-C2D	3.90	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	C	501	LMG	O7-C10	3.90	1.45	1.34
23	B	616	CLA	CHD-C1D	3.90	1.46	1.38
23	a	407[A]	CLA	C3D-C2D	3.90	1.49	1.39
23	D	702[A]	CLA	CHD-C4C	3.89	1.48	1.39
23	A	405[A]	CLA	C1D-ND	3.89	1.42	1.37
33	b	629[B]	LHG	O8-C23	3.88	1.44	1.33
23	B	605	CLA	CHD-C1D	3.88	1.45	1.38
23	C	508	CLA	CHD-C1D	3.88	1.45	1.38
24	a	416[B]	PHO	O2A-CGA	3.88	1.44	1.33
36	c	517[B]	DGD	O1G-C1A	3.88	1.44	1.33
23	b	606	CLA	OBD-CAD	3.88	1.29	1.22
23	C	507	CLA	CHD-C4C	3.87	1.48	1.39
23	c	508	CLA	CHD-C4C	3.87	1.48	1.39
36	C	517[B]	DGD	O1G-C1A	3.86	1.44	1.33
23	b	609	CLA	OBD-CAD	3.86	1.29	1.22
23	B	611	CLA	O2A-CGA	3.86	1.44	1.33
23	b	608	CLA	C3D-C2D	3.86	1.49	1.39
24	A	417[A]	PHO	O2A-CGA	3.86	1.44	1.33
23	B	614	CLA	CHD-C1D	3.86	1.45	1.38
23	c	510	CLA	C3D-C2D	3.86	1.49	1.39
23	b	605	CLA	CHD-C4C	3.85	1.48	1.39
23	b	615	CLA	C3D-C2D	3.85	1.49	1.39
36	C	518[A]	DGD	O2G-C1B	3.85	1.45	1.34
23	D	702[B]	CLA	CHD-C4C	3.85	1.48	1.39
26	A	410[A]	SQD	O48-C23	3.85	1.44	1.33
23	c	512	CLA	C3D-C2D	3.84	1.49	1.39
33	b	629[B]	LHG	O7-C7	3.84	1.45	1.34
23	C	503	CLA	O2A-CGA	3.84	1.44	1.33
33	L	101[A]	LHG	O8-C23	3.84	1.44	1.33
23	A	406[B]	CLA	C3D-C2D	3.84	1.49	1.39
23	A	406[A]	CLA	C3D-C2D	3.84	1.49	1.39
36	c	518[A]	DGD	O1G-C1A	3.83	1.44	1.33
23	d	401[B]	CLA	CHD-C4C	3.83	1.48	1.39
23	B	610	CLA	CHD-C4C	3.83	1.48	1.39
23	A	405[A]	CLA	O2A-CGA	3.83	1.44	1.33
23	c	514	CLA	C3D-C2D	3.83	1.49	1.39
25	B	618	BCR	C23-C22	-3.83	1.37	1.45
34	d	410	LMG	O7-C10	3.83	1.45	1.34
23	c	506	CLA	CHD-C4C	3.83	1.48	1.39
24	a	416[A]	PHO	O2A-CGA	3.83	1.44	1.33
36	C	518[B]	DGD	O2G-C1B	3.83	1.45	1.34
33	d	412[B]	LHG	O7-C7	3.83	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	417[B]	PHO	C3C-C2C	3.83	1.49	1.37
23	B	603	CLA	CHD-C1D	3.82	1.45	1.38
23	a	405[B]	CLA	CHD-C1D	3.82	1.45	1.38
26	A	410[B]	SQD	O48-C23	3.82	1.44	1.33
33	L	101[A]	LHG	O7-C7	3.82	1.45	1.34
23	a	409	CLA	CHD-C1D	3.82	1.45	1.38
23	B	602	CLA	C3D-C2D	3.82	1.49	1.39
23	B	604	CLA	C1D-ND	3.81	1.42	1.37
23	b	612	CLA	O2A-CGA	3.81	1.44	1.33
23	B	602	CLA	CHD-C4C	3.81	1.47	1.39
23	C	502	CLA	CHD-C4C	3.81	1.47	1.39
23	b	602	CLA	OBD-CAD	3.81	1.29	1.22
23	d	401[A]	CLA	CHD-C1D	3.81	1.45	1.38
33	A	419[B]	LHG	O8-C23	3.80	1.44	1.33
24	A	407[B]	PHO	O2A-CGA	3.80	1.44	1.33
23	c	513	CLA	OBD-CAD	3.80	1.29	1.22
23	c	509	CLA	CHD-C4C	3.80	1.47	1.39
23	A	406[A]	CLA	O2A-CGA	3.80	1.44	1.33
23	b	601	CLA	OBD-CAD	3.80	1.29	1.22
23	a	406[A]	CLA	CHD-C1D	3.80	1.45	1.38
23	b	605	CLA	OBD-CAD	3.80	1.29	1.22
23	C	514	CLA	CHD-C4C	3.79	1.47	1.39
24	A	417[A]	PHO	CHA-CBD	-3.79	1.47	1.52
23	b	609	CLA	O2A-CGA	3.79	1.44	1.33
23	C	511	CLA	O2A-CGA	3.79	1.44	1.33
33	D	706[B]	LHG	O7-C7	3.79	1.45	1.34
23	C	510	CLA	OBD-CAD	3.79	1.29	1.22
35	o	301	HTG	C1'-S1	-3.78	1.76	1.81
23	c	511	CLA	CHD-C1D	3.78	1.45	1.38
23	A	408	CLA	C3D-C2D	3.78	1.49	1.39
23	c	502	CLA	C3D-C2D	3.78	1.49	1.39
23	B	603	CLA	O2A-CGA	3.78	1.44	1.33
23	B	611	CLA	C4B-NB	-3.78	1.31	1.35
23	A	405[B]	CLA	CHD-C4C	3.77	1.47	1.39
23	b	609	CLA	C3D-C2D	3.77	1.49	1.39
33	d	406[B]	LHG	O7-C7	3.77	1.44	1.34
23	b	616	CLA	CHD-C4C	3.77	1.47	1.39
23	a	406[A]	CLA	OBD-CAD	3.77	1.29	1.22
23	b	602	CLA	O2A-CGA	3.77	1.44	1.33
23	c	503	CLA	OBD-CAD	3.77	1.29	1.22
23	B	607	CLA	CHD-C4C	3.77	1.47	1.39
23	b	603	CLA	CHD-C1D	3.77	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	601	CLA	CHD-C4C	3.77	1.47	1.39
23	b	605	CLA	C3D-C2D	3.77	1.49	1.39
23	C	507	CLA	C3D-C2D	3.77	1.49	1.39
24	A	407[B]	PHO	C3C-C2C	3.76	1.48	1.37
23	b	612	CLA	OBD-CAD	3.76	1.29	1.22
23	B	607	CLA	CHD-C1D	3.76	1.45	1.38
23	C	511	CLA	CHD-C1D	3.76	1.45	1.38
23	c	506	CLA	C3D-C2D	3.75	1.49	1.39
23	A	408	CLA	CHD-C4C	3.75	1.47	1.39
23	B	615	CLA	CHD-C4C	3.75	1.47	1.39
33	d	412[A]	LHG	O8-C23	3.75	1.44	1.33
23	b	610	CLA	C3D-C2D	3.75	1.49	1.39
23	B	606	CLA	CHD-C1D	3.74	1.45	1.38
23	A	406[B]	CLA	OBD-CAD	3.74	1.28	1.22
33	D	707[B]	LHG	O7-C7	3.74	1.44	1.34
23	B	605	CLA	C3D-C2D	3.74	1.49	1.39
23	C	506	CLA	O2A-CGA	3.74	1.44	1.33
23	c	505	CLA	CHD-C4C	3.74	1.47	1.39
24	a	408[B]	PHO	C3C-C2C	3.74	1.48	1.37
23	c	507	CLA	OBD-CAD	3.74	1.28	1.22
23	A	406[A]	CLA	OBD-CAD	3.74	1.28	1.22
23	b	611	CLA	CHD-C4C	3.74	1.47	1.39
23	a	406[B]	CLA	OBD-CAD	3.74	1.28	1.22
23	c	511	CLA	C3D-C2D	3.73	1.49	1.39
23	c	511	CLA	O2A-CGA	3.73	1.44	1.33
23	A	404[A]	CLA	CHD-C4C	3.73	1.47	1.39
23	a	407[B]	CLA	CHD-C1D	3.73	1.45	1.38
23	C	502	CLA	O2A-CGA	3.73	1.44	1.33
23	b	604	CLA	CHD-C4C	3.73	1.47	1.39
23	c	511	CLA	CHD-C4C	3.73	1.47	1.39
23	c	506	CLA	OBD-CAD	3.72	1.28	1.22
23	B	602	CLA	O2A-CGA	3.72	1.44	1.33
33	d	405[A]	LHG	O7-C7	3.72	1.44	1.34
23	A	405[A]	CLA	CHD-C1D	3.72	1.45	1.38
23	b	616	CLA	C3D-C2D	3.72	1.49	1.39
23	B	601	CLA	C3D-C2D	3.71	1.49	1.39
36	C	518[A]	DGD	O1G-C1A	3.71	1.44	1.33
23	C	509	CLA	CHD-C4C	3.71	1.47	1.39
23	D	703	CLA	OBD-CAD	3.71	1.28	1.22
23	b	603	CLA	OBD-CAD	3.71	1.28	1.22
23	b	606	CLA	C3D-C2D	3.70	1.49	1.39
23	C	502	CLA	C3D-C2D	3.70	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	504	CLA	O2A-CGA	3.70	1.44	1.33
23	C	510	CLA	CHD-C4C	3.70	1.47	1.39
23	B	603	CLA	CHD-C4C	3.70	1.47	1.39
23	D	702[B]	CLA	C3D-C2D	3.70	1.49	1.39
33	d	405[B]	LHG	O8-C23	3.70	1.44	1.33
36	H	102	DGD	O1G-C1A	3.70	1.44	1.33
23	b	610	CLA	OBD-CAD	3.70	1.28	1.22
23	b	613	CLA	O2A-CGA	3.70	1.44	1.33
23	C	505	CLA	CHD-C4C	3.69	1.47	1.39
23	a	405[B]	CLA	OBD-CAD	3.69	1.28	1.22
23	B	608	CLA	C3D-C2D	3.69	1.49	1.39
23	B	607	CLA	OBD-CAD	3.69	1.28	1.22
24	A	407[A]	PHO	C3C-C2C	3.68	1.48	1.37
23	b	602	CLA	C3D-C2D	3.68	1.49	1.39
26	A	410[A]	SQD	O47-C7	3.68	1.44	1.34
23	a	407[A]	CLA	OBD-CAD	3.68	1.28	1.22
23	a	407[B]	CLA	OBD-CAD	3.68	1.28	1.22
23	b	604	CLA	C3D-C2D	3.68	1.49	1.39
23	B	605	CLA	O2A-CGA	3.67	1.44	1.33
23	A	406[A]	CLA	CHD-C4C	3.67	1.47	1.39
23	B	607	CLA	O2A-CGA	3.66	1.44	1.33
23	A	404[B]	CLA	C3D-C2D	3.66	1.49	1.39
23	b	606	CLA	O2A-CGA	3.66	1.44	1.33
23	B	609	CLA	CHD-C4C	3.66	1.47	1.39
26	A	410[B]	SQD	O47-C7	3.66	1.44	1.34
23	a	405[A]	CLA	C3D-C2D	3.66	1.49	1.39
23	b	603	CLA	CHD-C4C	3.66	1.47	1.39
33	d	406[A]	LHG	O7-C7	3.66	1.44	1.34
23	a	407[B]	CLA	CHD-C4C	3.66	1.47	1.39
23	c	508	CLA	C3D-C2D	3.65	1.49	1.39
24	A	407[A]	PHO	O2A-CGA	3.64	1.44	1.33
23	C	504	CLA	OBD-CAD	3.64	1.28	1.22
23	d	401[B]	CLA	C3D-C2D	3.63	1.49	1.39
23	A	404[A]	CLA	C3D-C2D	3.63	1.49	1.39
23	b	616	CLA	OBD-CAD	3.63	1.28	1.22
24	a	408[A]	PHO	C3C-C2C	3.62	1.48	1.37
33	D	706[B]	LHG	O8-C23	3.62	1.43	1.33
36	c	517[A]	DGD	O1G-C1A	3.62	1.43	1.33
23	B	612	CLA	CHD-C4C	3.62	1.47	1.39
23	a	406[A]	CLA	CHD-C4C	3.62	1.47	1.39
33	b	629[A]	LHG	O7-C7	3.62	1.44	1.34
23	C	513	CLA	CHD-C4C	3.62	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	405[A]	CLA	OBD-CAD	3.61	1.28	1.22
23	B	607	CLA	C1D-ND	3.61	1.42	1.37
33	D	706[A]	LHG	O7-C7	3.60	1.44	1.34
23	a	405[B]	CLA	C3D-C2D	3.60	1.48	1.39
23	b	611	CLA	C3D-C2D	3.60	1.48	1.39
23	a	405[B]	CLA	O2A-CGA	3.59	1.43	1.33
23	C	514	CLA	OBD-CAD	3.59	1.28	1.22
23	B	604	CLA	CHD-C4C	3.59	1.47	1.39
23	b	614	CLA	CHD-C4C	3.59	1.47	1.39
23	C	511	CLA	C3D-C2D	3.58	1.48	1.39
23	a	407[A]	CLA	CHD-C4C	3.58	1.47	1.39
23	B	605	CLA	CHD-C4C	3.58	1.47	1.39
23	B	606	CLA	C3D-C2D	3.58	1.48	1.39
23	d	402	CLA	CHD-C4C	3.58	1.47	1.39
23	C	513	CLA	OBD-CAD	3.58	1.28	1.22
23	d	401[A]	CLA	CHD-C4C	3.57	1.47	1.39
23	B	610	CLA	O2A-CGA	3.57	1.43	1.33
23	b	603	CLA	C3D-C2D	3.57	1.48	1.39
36	h	102	DGD	O1G-C1A	3.57	1.43	1.33
34	m	101	LMG	O7-C10	3.56	1.44	1.34
23	B	608	CLA	CHD-C4C	3.56	1.47	1.39
23	A	405[A]	CLA	CHD-C4C	3.56	1.47	1.39
23	b	615	CLA	CHD-C4C	3.56	1.47	1.39
36	C	517[A]	DGD	O1G-C1A	3.55	1.43	1.33
23	d	401[A]	CLA	C3D-C2D	3.55	1.48	1.39
23	C	507	CLA	OBD-CAD	3.55	1.28	1.22
23	B	613	CLA	CHD-C1D	3.54	1.45	1.38
23	a	407[A]	CLA	CHD-C1D	3.54	1.45	1.38
23	B	607	CLA	C3D-C2D	3.54	1.48	1.39
23	b	604	CLA	OBD-CAD	3.53	1.28	1.22
36	c	518[A]	DGD	O2G-C1B	3.53	1.44	1.34
23	B	603	CLA	OBD-CAD	3.53	1.28	1.22
38	f	101	HEM	C1B-NB	-3.53	1.34	1.40
33	d	405[A]	LHG	O8-C23	3.53	1.43	1.33
23	b	604	CLA	O2A-CGA	3.53	1.43	1.33
23	B	604	CLA	O2A-CGA	3.53	1.43	1.33
23	b	614	CLA	O2A-CGA	3.53	1.43	1.33
33	D	706[A]	LHG	O8-C23	3.53	1.43	1.33
23	c	506	CLA	O2A-CGA	3.52	1.43	1.33
33	A	419[A]	LHG	O8-C23	3.52	1.43	1.33
24	a	408[B]	PHO	O2A-CGA	3.51	1.43	1.33
33	A	419[B]	LHG	O7-C7	3.51	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	608	CLA	O2A-CGA	3.51	1.43	1.33
23	C	506	CLA	C3D-C2D	3.51	1.48	1.39
23	b	615	CLA	OBD-CAD	3.50	1.28	1.22
33	d	412[A]	LHG	O7-C7	3.50	1.44	1.34
36	C	519	DGD	O2G-C1B	3.50	1.44	1.34
23	D	703	CLA	O2A-CGA	3.50	1.43	1.33
23	C	506	CLA	OBD-CAD	3.50	1.28	1.22
23	b	607	CLA	C3D-C2D	3.49	1.48	1.39
33	A	419[A]	LHG	O7-C7	3.49	1.44	1.34
33	b	629[A]	LHG	O8-C23	3.49	1.43	1.33
23	B	611	CLA	C3D-C2D	3.49	1.48	1.39
23	c	510	CLA	OBD-CAD	3.49	1.28	1.22
23	b	606	CLA	CHD-C4C	3.49	1.47	1.39
23	b	605	CLA	O2A-CGA	3.48	1.43	1.33
23	c	514	CLA	OBD-CAD	3.47	1.28	1.22
23	b	608	CLA	CHD-C4C	3.46	1.47	1.39
23	b	612	CLA	CHD-C4C	3.46	1.47	1.39
36	H	102	DGD	O2G-C1B	3.45	1.44	1.34
23	b	613	CLA	CHD-C1D	3.45	1.45	1.38
23	C	508	CLA	CHD-C4C	3.44	1.47	1.39
23	C	505	CLA	OBD-CAD	3.44	1.28	1.22
23	B	612	CLA	O2A-CGA	3.44	1.43	1.33
23	b	611	CLA	OBD-CAD	3.44	1.28	1.22
23	D	702[A]	CLA	C3D-C2D	3.43	1.48	1.39
38	f	101	HEM	C4D-ND	-3.43	1.34	1.40
23	C	504	CLA	C3D-C2D	3.43	1.48	1.39
23	B	613	CLA	O2A-CGA	3.43	1.43	1.33
23	B	601	CLA	OBD-CAD	3.42	1.28	1.22
38	F	102	HEM	C1B-NB	-3.42	1.34	1.40
23	B	612	CLA	OBD-CAD	3.42	1.28	1.22
23	c	504	CLA	C3D-C2D	3.42	1.48	1.39
23	b	609	CLA	CHD-C4C	3.41	1.47	1.39
23	d	401[A]	CLA	OBD-CAD	3.41	1.28	1.22
35	b	625	HTG	C1-S1	-3.41	1.75	1.80
23	b	602	CLA	C1C-C2C	3.40	1.51	1.44
35	B	624	HTG	C1'-S1	-3.40	1.77	1.81
23	b	610	CLA	O2A-CGA	3.39	1.43	1.33
23	D	702[B]	CLA	OBD-CAD	3.39	1.28	1.22
24	a	408[A]	PHO	O2A-CGA	3.39	1.43	1.33
23	B	611	CLA	CHD-C4C	3.39	1.47	1.39
23	B	606	CLA	CHD-C4C	3.38	1.47	1.39
23	B	616	CLA	CHD-C4C	3.38	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	c	519	DGD	O2G-C1B	3.37	1.43	1.34
23	A	404[B]	CLA	OBD-CAD	3.37	1.28	1.22
23	c	511	CLA	OBD-CAD	3.36	1.28	1.22
23	C	512	CLA	OBD-CAD	3.35	1.28	1.22
23	b	607	CLA	CHD-C4C	3.35	1.46	1.39
34	D	711	LMG	O7-C10	3.35	1.43	1.34
23	c	505	CLA	OBD-CAD	3.35	1.28	1.22
23	A	404[A]	CLA	OBD-CAD	3.34	1.28	1.22
23	B	612	CLA	C3D-C2D	3.33	1.48	1.39
23	b	607	CLA	O2A-CGA	3.33	1.43	1.33
23	A	404[B]	CLA	O2A-CGA	3.32	1.43	1.33
23	b	603	CLA	O2A-CGA	3.32	1.43	1.33
23	B	614	CLA	C3D-C2D	3.31	1.48	1.39
23	C	503	CLA	OBD-CAD	3.30	1.28	1.22
23	b	613	CLA	CHD-C4C	3.30	1.46	1.39
23	a	409	CLA	C3D-C2D	3.29	1.48	1.39
23	d	401[B]	CLA	OBD-CAD	3.29	1.28	1.22
23	b	614	CLA	OBD-CAD	3.29	1.28	1.22
23	a	409	CLA	CHD-C4C	3.28	1.46	1.39
23	B	613	CLA	CHD-C4C	3.28	1.46	1.39
23	d	401[A]	CLA	C1D-ND	3.27	1.41	1.37
23	B	602	CLA	OBD-CAD	3.27	1.28	1.22
23	D	702[A]	CLA	OBD-CAD	3.26	1.28	1.22
23	B	602	CLA	C1C-C2C	3.25	1.50	1.44
38	F	102	HEM	C4D-ND	-3.25	1.34	1.40
24	A	417[B]	PHO	CHA-CBD	-3.24	1.48	1.52
23	C	511	CLA	OBD-CAD	3.24	1.28	1.22
23	B	604	CLA	C3D-C2D	3.23	1.48	1.39
23	B	613	CLA	OBD-CAD	3.22	1.28	1.22
34	D	711	LMG	O8-C28	3.22	1.42	1.33
23	B	612	CLA	C1C-C2C	3.21	1.50	1.44
23	B	612	CLA	C1B-CHB	3.21	1.49	1.41
23	A	405[B]	CLA	OBD-CAD	3.20	1.28	1.22
23	A	404[A]	CLA	O2A-CGA	3.19	1.42	1.33
23	B	609	CLA	OBD-CAD	3.18	1.28	1.22
35	d	409	HTG	C1'-S1	-3.18	1.77	1.81
23	B	611	CLA	C4B-CHC	3.17	1.49	1.41
23	C	502	CLA	OBD-CAD	3.15	1.27	1.22
23	C	507	CLA	C4C-C3C	3.15	1.50	1.45
23	A	405[A]	CLA	OBD-CAD	3.12	1.27	1.22
35	b	625	HTG	C1'-S1	-3.11	1.77	1.81
23	B	614	CLA	OBD-CAD	3.11	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	502	CLA	OBD-CAD	3.11	1.27	1.22
23	C	508	CLA	OBD-CAD	3.08	1.27	1.22
23	a	405[A]	CLA	O2A-CGA	3.07	1.42	1.33
23	a	409	CLA	OBD-CAD	3.06	1.27	1.22
23	C	513	CLA	C1C-C2C	3.03	1.50	1.44
23	B	615	CLA	C1C-C2C	3.02	1.50	1.44
23	d	402	CLA	OBD-CAD	3.02	1.27	1.22
35	D	710	HTG	C1'-S1	-3.01	1.77	1.81
23	D	703	CLA	C1C-C2C	3.00	1.50	1.44
23	b	604	CLA	C4D-CHA	2.98	1.49	1.38
24	a	408[B]	PHO	CHA-CBD	-2.96	1.48	1.52
23	B	608	CLA	OBD-CAD	2.96	1.27	1.22
23	B	605	CLA	C4B-CHC	2.96	1.49	1.41
35	c	522	HTG	C1'-S1	-2.96	1.77	1.81
23	A	404[A]	CLA	C4C-C3C	2.96	1.50	1.45
23	B	612	CLA	C1B-NB	-2.95	1.32	1.35
23	b	612	CLA	C1C-C2C	2.94	1.50	1.44
23	B	611	CLA	C1B-NB	2.93	1.37	1.35
23	C	512	CLA	C4D-CHA	2.93	1.48	1.38
23	B	606	CLA	OBD-CAD	2.91	1.27	1.22
35	C	522	HTG	C1'-S1	-2.91	1.77	1.81
23	a	409	CLA	C1C-C2C	2.91	1.50	1.44
23	b	602	CLA	C4B-CHC	2.90	1.49	1.41
23	A	408	CLA	OBD-CAD	2.88	1.27	1.22
23	c	504	CLA	OBD-CAD	2.88	1.27	1.22
23	B	607	CLA	C1B-NB	-2.88	1.32	1.35
23	B	616	CLA	OBD-CAD	2.87	1.27	1.22
24	a	416[B]	PHO	C3A-C2A	-2.87	1.52	1.54
23	C	502	CLA	C1C-C2C	2.85	1.50	1.44
23	b	612	CLA	C1B-CHB	2.85	1.48	1.41
23	b	616	CLA	C1C-C2C	2.85	1.50	1.44
23	c	505	CLA	C1C-C2C	2.84	1.50	1.44
23	C	508	CLA	C4D-CHA	2.83	1.48	1.38
23	c	510	CLA	C1B-NB	-2.83	1.32	1.35
24	A	407[A]	PHO	CBD-CGD	-2.83	1.48	1.52
23	B	614	CLA	C1B-CHB	2.82	1.48	1.41
23	b	609	CLA	C1B-CHB	2.81	1.48	1.41
23	c	511	CLA	C1C-C2C	2.81	1.50	1.44
23	B	606	CLA	C1C-C2C	2.80	1.50	1.44
23	c	510	CLA	C4C-C3C	2.80	1.49	1.45
23	c	504	CLA	C1C-C2C	2.80	1.50	1.44
23	a	407[B]	CLA	C1C-C2C	2.80	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	411[B]	SQD	C6-S	-2.79	1.67	1.77
34	Z	101	LMG	O8-C28	2.78	1.47	1.33
23	B	612	CLA	C4D-CHA	2.78	1.48	1.38
23	b	610	CLA	C1C-C2C	2.77	1.49	1.44
23	c	513	CLA	C4B-CHC	2.77	1.48	1.41
29	A	414[A]	PL9	C6-C5	2.76	1.49	1.35
23	A	404[B]	CLA	C1C-C2C	2.76	1.49	1.44
23	c	514	CLA	C1C-C2C	2.76	1.49	1.44
23	b	607	CLA	C1B-NB	-2.76	1.32	1.35
29	a	414[A]	PL9	C6-C5	2.75	1.49	1.35
23	B	605	CLA	OBD-CAD	2.75	1.27	1.22
23	d	401[A]	CLA	C1B-CHB	2.75	1.48	1.41
23	c	504	CLA	C4B-CHC	2.75	1.48	1.41
23	d	401[B]	CLA	C4C-C3C	2.75	1.49	1.45
23	B	604	CLA	C4D-CHA	2.75	1.48	1.38
23	B	614	CLA	C4D-CHA	2.74	1.48	1.38
23	B	605	CLA	C1B-CHB	2.74	1.48	1.41
23	B	605	CLA	C1C-C2C	2.74	1.49	1.44
23	C	506	CLA	C4D-CHA	2.74	1.48	1.38
23	c	512	CLA	C1B-CHB	2.74	1.48	1.41
26	a	411[A]	SQD	C6-S	-2.73	1.67	1.77
23	c	512	CLA	C4D-CHA	2.73	1.48	1.38
26	A	410[A]	SQD	C6-S	-2.73	1.67	1.77
23	A	408	CLA	C4D-CHA	2.73	1.48	1.38
23	D	703	CLA	C4B-CHC	2.73	1.48	1.41
23	c	509	CLA	C4D-CHA	2.73	1.48	1.38
29	A	414[B]	PL9	C6-C5	2.72	1.49	1.35
23	C	502	CLA	C4D-CHA	2.72	1.48	1.38
23	A	406[A]	CLA	C4D-CHA	2.72	1.48	1.38
23	a	407[A]	CLA	C1C-C2C	2.72	1.49	1.44
23	B	614	CLA	C4B-NB	-2.72	1.32	1.35
23	B	605	CLA	C3D-C4D	-2.72	1.38	1.44
29	a	414[B]	PL9	C6-C5	2.72	1.49	1.35
24	A	417[B]	PHO	C3A-C2A	-2.71	1.52	1.54
23	B	607	CLA	C4D-CHA	2.71	1.48	1.38
23	c	502	CLA	C1B-CHB	2.71	1.48	1.41
23	D	702[A]	CLA	C4D-CHA	2.71	1.48	1.38
23	c	513	CLA	C4D-CHA	2.71	1.48	1.38
23	B	604	CLA	C1B-CHB	2.70	1.48	1.41
23	D	702[A]	CLA	C1B-CHB	2.70	1.48	1.41
23	C	509	CLA	C4C-C3C	2.70	1.49	1.45
23	C	505	CLA	C4D-CHA	2.70	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	512	CLA	C1B-CHB	2.70	1.48	1.41
23	B	616	CLA	C4D-CHA	2.69	1.48	1.38
23	C	505	CLA	C1C-C2C	2.69	1.49	1.44
26	A	410[B]	SQD	C6-S	-2.69	1.67	1.77
23	C	508	CLA	C1C-C2C	2.69	1.49	1.44
23	B	614	CLA	C4B-CHC	2.69	1.48	1.41
23	b	603	CLA	C1C-C2C	2.69	1.49	1.44
23	A	405[A]	CLA	C4D-CHA	2.68	1.47	1.38
23	A	404[B]	CLA	C4C-C3C	2.68	1.49	1.45
23	C	511	CLA	C1C-C2C	2.68	1.49	1.44
23	c	502	CLA	C4D-CHA	2.68	1.47	1.38
23	C	510	CLA	C1C-C2C	2.68	1.49	1.44
23	b	610	CLA	C4C-C3C	2.68	1.49	1.45
23	C	509	CLA	C1B-CHB	2.68	1.48	1.41
23	C	506	CLA	C1B-CHB	2.68	1.48	1.41
23	B	610	CLA	C4D-CHA	2.67	1.47	1.38
23	B	606	CLA	C3D-C4D	-2.66	1.38	1.44
23	C	513	CLA	C4B-CHC	2.66	1.48	1.41
23	B	603	CLA	C1B-CHB	2.66	1.48	1.41
23	c	508	CLA	C1C-C2C	2.65	1.49	1.44
23	B	609	CLA	C4B-CHC	2.65	1.48	1.41
23	c	510	CLA	C1B-CHB	2.65	1.48	1.41
23	c	510	CLA	C4D-CHA	2.65	1.47	1.38
35	o	301	HTG	O5-C1	2.64	1.46	1.42
23	B	608	CLA	C4D-CHA	2.64	1.47	1.38
23	d	401[B]	CLA	C4D-CHA	2.64	1.47	1.38
26	A	412	SQD	C6-S	-2.64	1.67	1.77
23	c	509	CLA	C4C-C3C	2.64	1.49	1.45
38	f	101	HEM	FE-NB	2.64	2.09	1.96
23	c	508	CLA	C4D-CHA	2.63	1.47	1.38
23	c	506	CLA	C1C-C2C	2.63	1.49	1.44
23	b	607	CLA	C1C-C2C	2.63	1.49	1.44
23	c	506	CLA	C4B-CHC	2.63	1.48	1.41
23	D	702[B]	CLA	C1C-C2C	2.63	1.49	1.44
26	f	102	SQD	C6-S	-2.63	1.67	1.77
23	B	601	CLA	C4B-CHC	2.63	1.48	1.41
23	B	606	CLA	C1B-CHB	2.63	1.48	1.41
23	c	506	CLA	C4D-CHA	2.63	1.47	1.38
23	C	512	CLA	C1C-C2C	2.63	1.49	1.44
23	d	402	CLA	C4D-CHA	2.62	1.47	1.38
23	C	510	CLA	C4D-CHA	2.62	1.47	1.38
23	b	612	CLA	C4B-CHC	2.62	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	607	CLA	C1C-C2C	2.62	1.49	1.44
23	c	502	CLA	C1C-C2C	2.62	1.49	1.44
23	a	407[A]	CLA	C4D-CHA	2.62	1.47	1.38
23	b	616	CLA	C3D-C4D	-2.62	1.38	1.44
38	F	102	HEM	FE-NB	2.61	2.09	1.96
23	C	507	CLA	C1C-C2C	2.61	1.49	1.44
23	B	613	CLA	C4D-CHA	2.61	1.47	1.38
23	C	504	CLA	C4B-CHC	2.61	1.48	1.41
23	C	507	CLA	C4D-CHA	2.61	1.47	1.38
23	C	502	CLA	C4B-CHC	2.61	1.48	1.41
32	t	101	LMT	O3'-C3'	-2.61	1.36	1.43
23	C	506	CLA	C1C-C2C	2.61	1.49	1.44
23	B	603	CLA	C4D-CHA	2.60	1.47	1.38
24	A	407[B]	PHO	CHA-CBD	-2.60	1.49	1.52
23	C	506	CLA	C4B-CHC	2.60	1.48	1.41
23	B	611	CLA	C1B-CHB	2.60	1.48	1.41
23	b	613	CLA	C4D-CHA	2.60	1.47	1.38
23	c	511	CLA	C4D-CHA	2.60	1.47	1.38
26	b	620	SQD	C6-S	-2.60	1.67	1.77
23	C	514	CLA	C1C-C2C	2.60	1.49	1.44
24	a	416[B]	PHO	CHA-CBD	-2.60	1.49	1.52
23	B	613	CLA	C1B-CHB	2.59	1.48	1.41
23	b	612	CLA	C4D-CHA	2.59	1.47	1.38
35	b	622	HTG	O5-C1	2.59	1.46	1.42
23	b	609	CLA	C1C-C2C	2.59	1.49	1.44
23	C	509	CLA	C4D-CHA	2.59	1.47	1.38
23	b	611	CLA	C4C-C3C	2.59	1.49	1.45
23	b	608	CLA	C1B-CHB	2.59	1.48	1.41
23	a	407[B]	CLA	C4D-CHA	2.59	1.47	1.38
23	C	513	CLA	C4D-CHA	2.59	1.47	1.38
23	c	504	CLA	C3D-C4D	-2.58	1.38	1.44
23	c	507	CLA	C1B-CHB	2.58	1.48	1.41
23	B	610	CLA	C1B-CHB	2.58	1.48	1.41
23	c	502	CLA	C4C-C3C	2.58	1.49	1.45
23	b	609	CLA	C4D-CHA	2.58	1.47	1.38
23	C	511	CLA	C4C-C3C	2.58	1.49	1.45
23	B	615	CLA	C1B-CHB	2.58	1.48	1.41
26	a	412	SQD	C6-S	-2.58	1.67	1.77
23	b	601	CLA	C4D-CHA	2.57	1.47	1.38
23	B	602	CLA	C4D-CHA	2.57	1.47	1.38
23	B	612	CLA	C4B-CHC	2.57	1.48	1.41
23	b	615	CLA	C4D-CHA	2.57	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	606	CLA	C1C-C2C	2.57	1.49	1.44
23	d	401[B]	CLA	C1B-CHB	2.57	1.48	1.41
23	b	615	CLA	C3D-C4D	-2.57	1.38	1.44
23	A	404[A]	CLA	C4D-CHA	2.57	1.47	1.38
23	A	405[B]	CLA	C4D-CHA	2.57	1.47	1.38
23	c	505	CLA	C4D-CHA	2.57	1.47	1.38
23	b	614	CLA	C4D-CHA	2.56	1.47	1.38
23	b	610	CLA	C1B-CHB	2.56	1.48	1.41
23	c	504	CLA	C4D-CHA	2.56	1.47	1.38
23	d	401[A]	CLA	C4C-C3C	2.56	1.49	1.45
23	b	610	CLA	C4B-CHC	2.55	1.48	1.41
23	C	514	CLA	C4D-CHA	2.55	1.47	1.38
23	b	610	CLA	C4D-CHA	2.55	1.47	1.38
23	B	615	CLA	C4D-CHA	2.55	1.47	1.38
23	b	604	CLA	C4B-CHC	2.55	1.48	1.41
24	a	416[A]	PHO	C3A-C2A	-2.55	1.52	1.54
32	A	420	LMT	O3'-C3'	-2.54	1.37	1.43
23	C	510	CLA	C4C-C3C	2.54	1.49	1.45
23	b	614	CLA	C4B-CHC	2.54	1.48	1.41
23	c	513	CLA	C1B-CHB	2.54	1.48	1.41
23	b	607	CLA	C4D-CHA	2.54	1.47	1.38
23	C	504	CLA	C3D-C4D	-2.54	1.38	1.44
23	B	608	CLA	C1B-CHB	2.54	1.48	1.41
23	B	612	CLA	C4C-C3C	2.54	1.49	1.45
23	b	608	CLA	C4D-CHA	2.54	1.47	1.38
23	a	406[B]	CLA	C4D-CHA	2.54	1.47	1.38
23	D	703	CLA	C4C-C3C	2.53	1.49	1.45
23	D	702[B]	CLA	C4C-C3C	2.53	1.49	1.45
32	B	627	LMT	C3'-C2'	2.53	1.58	1.52
23	C	505	CLA	C4B-CHC	2.53	1.48	1.41
23	C	505	CLA	C1B-CHB	2.53	1.48	1.41
23	B	609	CLA	C1C-C2C	2.53	1.49	1.44
35	B	624	HTG	C1-S1	-2.52	1.76	1.80
23	c	512	CLA	C1C-C2C	2.52	1.49	1.44
23	C	514	CLA	C1B-CHB	2.52	1.48	1.41
23	D	703	CLA	C1B-CHB	2.52	1.48	1.41
23	b	614	CLA	C1C-C2C	2.52	1.49	1.44
29	D	705[B]	PL9	C6-C5	2.51	1.48	1.35
24	a	408[A]	PHO	CHA-CBD	-2.51	1.49	1.52
23	c	509	CLA	C1B-CHB	2.51	1.48	1.41
23	B	601	CLA	C4D-CHA	2.51	1.47	1.38
23	d	402	CLA	C1C-C2C	2.51	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	m	103	LMT	C3'-C2'	2.51	1.58	1.52
23	C	504	CLA	C4D-CHA	2.51	1.47	1.38
23	A	406[B]	CLA	C4B-CHC	2.51	1.48	1.41
23	A	404[B]	CLA	C4D-CHA	2.50	1.47	1.38
23	b	616	CLA	C4B-CHC	2.50	1.47	1.41
23	C	502	CLA	C4C-C3C	2.50	1.49	1.45
34	C	521	LMG	O1-C1	2.50	1.44	1.40
23	b	602	CLA	C4D-CHA	2.50	1.47	1.38
23	b	608	CLA	C1C-C2C	2.50	1.49	1.44
23	c	508	CLA	C4B-CHC	2.50	1.47	1.41
35	B	622	HTG	C1'-S1	-2.50	1.78	1.81
23	a	409	CLA	C1B-CHB	2.50	1.47	1.41
23	c	502	CLA	C4B-CHC	2.50	1.47	1.41
23	C	506	CLA	C4C-C3C	2.50	1.49	1.45
23	A	404[A]	CLA	C1C-C2C	2.49	1.49	1.44
23	a	405[A]	CLA	C4C-C3C	2.49	1.49	1.45
23	A	406[A]	CLA	C4B-CHC	2.49	1.47	1.41
23	B	606	CLA	C4D-CHA	2.49	1.47	1.38
36	c	519	DGD	O2G-C2G	-2.49	1.40	1.46
23	d	402	CLA	C4B-CHC	2.49	1.47	1.41
23	c	507	CLA	C4C-C3C	2.49	1.49	1.45
23	c	506	CLA	C4C-C3C	2.49	1.49	1.45
23	B	610	CLA	C1C-C2C	2.49	1.49	1.44
23	B	603	CLA	C1B-NB	-2.49	1.33	1.35
23	D	702[B]	CLA	C1B-CHB	2.49	1.47	1.41
23	B	616	CLA	C1C-C2C	2.49	1.49	1.44
23	a	409	CLA	C4B-CHC	2.48	1.47	1.41
32	T	101	LMT	O3'-C3'	-2.48	1.37	1.43
23	A	405[A]	CLA	C1B-CHB	2.48	1.47	1.41
23	d	402	CLA	C1B-CHB	2.48	1.47	1.41
23	b	613	CLA	OBD-CAD	2.48	1.26	1.22
23	B	607	CLA	C3D-C4D	-2.48	1.38	1.44
23	C	511	CLA	C1B-CHB	2.48	1.47	1.41
23	A	405[B]	CLA	C3D-C4D	-2.48	1.38	1.44
23	a	405[A]	CLA	C4D-CHA	2.48	1.47	1.38
23	a	406[A]	CLA	C4D-CHA	2.48	1.47	1.38
23	A	406[B]	CLA	C1C-C2C	2.47	1.49	1.44
23	B	606	CLA	C4B-CHC	2.47	1.47	1.41
23	B	602	CLA	C1B-CHB	2.47	1.47	1.41
23	b	603	CLA	C4B-CHC	2.47	1.47	1.41
23	C	503	CLA	C1B-CHB	2.46	1.47	1.41
23	b	607	CLA	OBD-CAD	2.46	1.26	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	503	CLA	C4D-CHA	2.46	1.47	1.38
23	a	407[A]	CLA	C1B-CHB	2.46	1.47	1.41
23	b	616	CLA	C4D-CHA	2.46	1.47	1.38
23	C	508	CLA	C4B-CHC	2.46	1.47	1.41
23	c	503	CLA	C1B-CHB	2.46	1.47	1.41
23	b	613	CLA	C1C-C2C	2.45	1.49	1.44
23	B	601	CLA	C1C-C2C	2.45	1.49	1.44
23	c	507	CLA	C4D-CHA	2.45	1.47	1.38
23	B	609	CLA	C4D-CHA	2.45	1.47	1.38
23	B	602	CLA	C4B-CHC	2.45	1.47	1.41
23	C	505	CLA	C3D-C4D	-2.45	1.38	1.44
23	B	602	CLA	C4C-C3C	2.45	1.49	1.45
23	b	613	CLA	C1B-CHB	2.45	1.47	1.41
23	C	504	CLA	C1C-C2C	2.45	1.49	1.44
23	B	608	CLA	C3D-C4D	-2.44	1.38	1.44
23	d	401[A]	CLA	C1B-NB	-2.44	1.33	1.35
32	b	621	LMT	C3'-C2'	2.44	1.58	1.52
23	a	407[A]	CLA	C3D-C4D	-2.44	1.38	1.44
23	b	606	CLA	C4D-CHA	2.44	1.47	1.38
23	A	406[B]	CLA	C3D-C4D	-2.44	1.38	1.44
23	D	702[B]	CLA	C3D-C4D	-2.44	1.38	1.44
23	b	615	CLA	C1B-CHB	2.44	1.47	1.41
23	C	507	CLA	C3D-C4D	-2.44	1.38	1.44
23	b	608	CLA	C1B-NB	-2.44	1.33	1.35
23	C	510	CLA	C4B-NB	-2.43	1.33	1.35
23	a	405[B]	CLA	C4C-C3C	2.43	1.49	1.45
23	c	504	CLA	C1B-CHB	2.43	1.47	1.41
36	C	519	DGD	O2G-C2G	-2.43	1.40	1.46
23	C	510	CLA	C1B-CHB	2.43	1.47	1.41
23	D	702[B]	CLA	C4B-CHC	2.42	1.47	1.41
23	C	504	CLA	C1B-CHB	2.42	1.47	1.41
23	c	514	CLA	C1B-CHB	2.42	1.47	1.41
23	c	505	CLA	C4C-C3C	2.42	1.49	1.45
23	B	610	CLA	C4C-C3C	2.42	1.49	1.45
23	c	511	CLA	C1B-CHB	2.42	1.47	1.41
23	b	605	CLA	C4D-CHA	2.42	1.47	1.38
23	b	601	CLA	C1C-C2C	2.42	1.49	1.44
32	M	101	LMT	O2'-C2'	-2.42	1.37	1.43
27	D	701	GOL	O2-C2	-2.42	1.36	1.43
24	A	407[A]	PHO	CHA-CBD	-2.42	1.49	1.52
23	c	514	CLA	C4D-CHA	2.41	1.47	1.38
23	C	503	CLA	C3D-C4D	-2.41	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	405[A]	CLA	C1C-C2C	2.41	1.49	1.44
23	A	406[A]	CLA	C1C-C2C	2.41	1.49	1.44
23	a	405[A]	CLA	C1B-CHB	2.41	1.47	1.41
23	c	511	CLA	C4B-CHC	2.41	1.47	1.41
27	D	701	GOL	C3-C2	2.41	1.61	1.51
23	b	604	CLA	C1B-CHB	2.41	1.47	1.41
23	a	405[B]	CLA	C1B-CHB	2.41	1.47	1.41
23	B	608	CLA	C4C-C3C	2.41	1.49	1.45
23	C	508	CLA	C1B-CHB	2.40	1.47	1.41
36	H	102	DGD	O5D-C1E	2.40	1.44	1.40
25	d	403	BCR	C30-C25	-2.40	1.50	1.53
23	A	406[B]	CLA	C4D-CHA	2.40	1.46	1.38
23	B	607	CLA	C4C-C3C	2.40	1.49	1.45
23	c	509	CLA	C1C-C2C	2.39	1.49	1.44
23	b	602	CLA	C3D-C4D	-2.39	1.38	1.44
23	D	702[A]	CLA	C3D-C4D	-2.39	1.38	1.44
23	a	405[B]	CLA	C4D-CHA	2.39	1.46	1.38
23	b	611	CLA	C4D-CHA	2.39	1.46	1.38
23	B	614	CLA	C3D-C4D	-2.39	1.38	1.44
23	C	511	CLA	C4D-CHA	2.39	1.46	1.38
32	e	101	LMT	O3'-C3'	-2.39	1.37	1.43
26	B	620	SQD	C6-S	-2.39	1.68	1.77
23	a	409	CLA	C4D-CHA	2.38	1.46	1.38
32	F	101	LMT	O3'-C3'	-2.38	1.37	1.43
23	B	605	CLA	C4D-CHA	2.38	1.46	1.38
23	B	612	CLA	C4B-NB	-2.38	1.33	1.35
23	d	401[A]	CLA	C4D-CHA	2.38	1.46	1.38
23	c	513	CLA	C1C-C2C	2.38	1.49	1.44
23	b	611	CLA	C1B-CHB	2.37	1.47	1.41
23	b	614	CLA	C1B-CHB	2.37	1.47	1.41
23	b	610	CLA	C3D-C4D	-2.37	1.38	1.44
23	B	604	CLA	C3D-C4D	-2.37	1.38	1.44
23	b	608	CLA	C3D-C4D	-2.37	1.38	1.44
23	b	611	CLA	C3D-C4D	-2.37	1.38	1.44
23	C	507	CLA	C1B-CHB	2.37	1.47	1.41
32	A	420	LMT	O2'-C2'	-2.37	1.37	1.43
23	B	613	CLA	C1C-C2C	2.36	1.49	1.44
23	B	607	CLA	C4B-CHC	2.36	1.47	1.41
23	D	703	CLA	C4D-CHA	2.36	1.46	1.38
23	c	505	CLA	C4B-CHC	2.36	1.47	1.41
23	C	502	CLA	C3D-C4D	-2.36	1.38	1.44
23	c	511	CLA	C3D-C4D	-2.35	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	d	404[A]	PL9	C6-C5	2.35	1.47	1.35
32	B	627	LMT	O3'-C3'	-2.35	1.37	1.43
24	a	416[A]	PHO	CHA-CBD	-2.35	1.49	1.52
26	X	101	SQD	C6-S	-2.35	1.68	1.77
27	a	419	GOL	C1-C2	2.35	1.61	1.51
23	B	604	CLA	C4B-CHC	2.35	1.47	1.41
23	B	607	CLA	C1B-CHB	2.35	1.47	1.41
23	B	602	CLA	C3D-C4D	-2.35	1.38	1.44
32	T	101	LMT	O2'-C2'	-2.35	1.37	1.43
23	C	509	CLA	C1C-C2C	2.35	1.49	1.44
29	d	404[B]	PL9	C6-C5	2.35	1.47	1.35
23	B	615	CLA	C4C-C3C	2.35	1.49	1.45
24	A	417[A]	PHO	C3A-C2A	-2.34	1.52	1.54
23	A	405[A]	CLA	C3D-C4D	-2.34	1.38	1.44
23	B	605	CLA	C4C-C3C	2.34	1.49	1.45
23	b	613	CLA	C4B-CHC	2.34	1.47	1.41
32	B	630	LMT	O3'-C3'	-2.34	1.37	1.43
23	b	607	CLA	C1B-CHB	2.34	1.47	1.41
23	C	511	CLA	C1B-NB	-2.34	1.33	1.35
23	b	603	CLA	C1B-CHB	2.34	1.47	1.41
29	D	705[A]	PL9	C6-C5	2.34	1.47	1.35
23	d	401[B]	CLA	C3D-C4D	-2.34	1.38	1.44
23	C	512	CLA	C4B-NB	-2.34	1.33	1.35
23	c	512	CLA	C4C-C3C	2.33	1.49	1.45
23	C	511	CLA	C3D-C4D	-2.33	1.38	1.44
23	A	405[B]	CLA	C1C-C2C	2.33	1.49	1.44
23	B	616	CLA	C1B-CHB	2.33	1.47	1.41
23	c	509	CLA	C4B-CHC	2.33	1.47	1.41
24	a	408[A]	PHO	CBD-CGD	-2.33	1.49	1.52
23	A	404[B]	CLA	C3D-C4D	-2.33	1.38	1.44
38	f	101	HEM	C1D-ND	-2.32	1.34	1.38
23	d	401[B]	CLA	C1C-C2C	2.32	1.49	1.44
23	C	503	CLA	C4C-C3C	2.32	1.49	1.45
23	C	503	CLA	C1C-C2C	2.32	1.49	1.44
23	A	405[B]	CLA	C4B-CHC	2.31	1.47	1.41
23	B	612	CLA	C3D-C4D	-2.31	1.39	1.44
23	A	408	CLA	C1C-NC	-2.31	1.34	1.37
23	D	702[B]	CLA	C4D-CHA	2.31	1.46	1.38
32	M	101	LMT	O1'-C1'	-2.31	1.36	1.40
23	a	407[B]	CLA	C1B-CHB	2.31	1.47	1.41
23	b	609	CLA	C3D-C4D	-2.31	1.39	1.44
23	d	401[A]	CLA	C1C-C2C	2.30	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	401[A]	CLA	C3D-C4D	-2.30	1.39	1.44
23	A	408	CLA	C3D-C4D	-2.30	1.39	1.44
32	M	101	LMT	O3'-C3'	-2.30	1.37	1.43
23	C	512	CLA	C4C-C3C	2.30	1.49	1.45
32	B	629	LMT	O2'-C2'	-2.30	1.37	1.43
23	A	405[A]	CLA	C4B-CHC	2.30	1.47	1.41
23	A	404[A]	CLA	C1B-CHB	2.30	1.47	1.41
23	A	404[B]	CLA	C1B-CHB	2.30	1.47	1.41
32	M	101	LMT	O2B-C2B	-2.30	1.37	1.43
23	C	512	CLA	C1C-NC	-2.30	1.34	1.37
23	C	503	CLA	C4D-CHA	2.29	1.46	1.38
23	B	608	CLA	C1C-NC	-2.29	1.34	1.37
23	b	606	CLA	C3D-C4D	-2.29	1.39	1.44
23	b	612	CLA	C3D-C4D	-2.29	1.39	1.44
23	B	608	CLA	C1C-C2C	2.29	1.49	1.44
23	c	506	CLA	C1B-CHB	2.29	1.47	1.41
23	a	407[B]	CLA	C3D-C4D	-2.29	1.39	1.44
26	X	101	SQD	O6-C1	2.29	1.44	1.40
23	A	405[B]	CLA	C1B-CHB	2.29	1.47	1.41
23	b	604	CLA	C1C-C2C	2.29	1.49	1.44
23	B	616	CLA	C4B-CHC	2.28	1.47	1.41
23	c	513	CLA	C4C-C3C	2.28	1.49	1.45
23	c	514	CLA	C4B-CHC	2.28	1.47	1.41
23	a	406[B]	CLA	C3D-C4D	-2.27	1.39	1.44
36	h	102	DGD	O5D-C1E	2.27	1.44	1.40
25	B	619	BCR	C30-C25	-2.27	1.50	1.53
23	B	610	CLA	C4B-CHC	2.27	1.47	1.41
23	c	503	CLA	C4C-C3C	2.26	1.48	1.45
23	b	607	CLA	C4B-CHC	2.26	1.47	1.41
23	b	601	CLA	C1B-CHB	2.26	1.47	1.41
23	b	614	CLA	C3D-C4D	-2.26	1.39	1.44
23	C	502	CLA	C1B-CHB	2.26	1.47	1.41
23	a	406[B]	CLA	C4B-CHC	2.26	1.47	1.41
23	c	514	CLA	C3D-C4D	-2.26	1.39	1.44
23	c	513	CLA	C3D-C4D	-2.26	1.39	1.44
23	B	616	CLA	C3D-C4D	-2.26	1.39	1.44
23	b	603	CLA	C3D-C4D	-2.26	1.39	1.44
23	d	402	CLA	C3D-C4D	-2.25	1.39	1.44
23	a	407[B]	CLA	C4C-C3C	2.25	1.48	1.45
23	B	611	CLA	C4D-CHA	2.25	1.46	1.38
23	a	405[A]	CLA	C1C-C2C	2.25	1.48	1.44
23	b	607	CLA	C3D-C4D	-2.25	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	406[B]	CLA	C1B-NB	-2.25	1.33	1.35
23	B	601	CLA	C1B-CHB	2.25	1.47	1.41
32	a	417	LMT	O3'-C3'	-2.25	1.37	1.43
32	T	101	LMT	O3B-C3B	-2.24	1.37	1.43
23	A	406[A]	CLA	C3D-C4D	-2.24	1.39	1.44
23	b	601	CLA	C4C-C3C	2.24	1.48	1.45
23	b	603	CLA	C4C-C3C	2.24	1.48	1.45
40	V	201	HEC	C3C-C4C	2.24	1.47	1.43
23	D	702[A]	CLA	C1B-NB	-2.24	1.33	1.35
23	B	603	CLA	C1C-C2C	2.24	1.48	1.44
23	b	606	CLA	C4B-CHC	2.24	1.47	1.41
23	a	406[A]	CLA	C1B-CHB	2.24	1.47	1.41
23	C	512	CLA	C3D-C4D	-2.24	1.39	1.44
27	o	304	GOL	C1-C2	2.24	1.60	1.51
23	B	609	CLA	C3D-C4D	-2.23	1.39	1.44
23	b	609	CLA	C4B-CHC	2.23	1.47	1.41
23	B	614	CLA	C1C-C2C	2.23	1.48	1.44
23	b	603	CLA	C4D-CHA	2.23	1.46	1.38
27	D	712	GOL	C3-C2	2.23	1.60	1.51
23	B	609	CLA	C1B-CHB	2.23	1.47	1.41
23	a	406[A]	CLA	C4B-CHC	2.23	1.47	1.41
23	c	514	CLA	C4C-C3C	2.23	1.48	1.45
23	A	404[B]	CLA	C4B-CHC	2.23	1.47	1.41
23	c	508	CLA	C1B-CHB	2.22	1.47	1.41
23	C	512	CLA	C4B-CHC	2.22	1.47	1.41
32	B	629	LMT	O2B-C2B	-2.21	1.37	1.43
36	C	518[A]	DGD	O5D-C1E	2.21	1.44	1.40
23	D	702[A]	CLA	C4C-C3C	2.21	1.48	1.45
23	C	508	CLA	C3D-C4D	-2.20	1.39	1.44
23	c	505	CLA	C3D-C4D	-2.20	1.39	1.44
23	a	405[B]	CLA	C4B-CHC	2.20	1.47	1.41
23	b	615	CLA	C4B-CHC	2.20	1.47	1.41
23	A	406[A]	CLA	C1B-CHB	2.20	1.47	1.41
23	B	603	CLA	C4B-CHC	2.20	1.47	1.41
23	c	507	CLA	C4B-CHC	2.20	1.47	1.41
23	B	603	CLA	C4C-C3C	2.19	1.48	1.45
23	b	604	CLA	C4C-C3C	2.19	1.48	1.45
27	b	624	GOL	C3-C2	2.19	1.60	1.51
23	C	506	CLA	C3D-C4D	-2.19	1.39	1.44
29	a	414[A]	PL9	C2-C3	2.19	1.40	1.34
23	d	401[A]	CLA	C4B-CHC	2.19	1.47	1.41
23	d	401[B]	CLA	C4B-CHC	2.19	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	620	SQD	O6-C1	2.19	1.43	1.40
23	c	505	CLA	C1B-CHB	2.19	1.47	1.41
23	A	408	CLA	C1C-C2C	2.18	1.48	1.44
32	t	101	LMT	O2'-C2'	-2.18	1.37	1.43
23	A	404[A]	CLA	C4B-NB	-2.18	1.33	1.35
23	b	601	CLA	C4B-CHC	2.18	1.47	1.41
23	c	512	CLA	C4B-CHC	2.18	1.47	1.41
23	b	605	CLA	C3D-C4D	-2.17	1.39	1.44
23	c	506	CLA	C3D-C4D	-2.17	1.39	1.44
27	D	712	GOL	O2-C2	-2.17	1.36	1.43
23	a	407[B]	CLA	C4B-CHC	2.17	1.47	1.41
32	B	629	LMT	O3'-C3'	-2.17	1.37	1.43
23	A	406[A]	CLA	C1B-NB	-2.17	1.33	1.35
32	e	101	LMT	O2B-C2B	-2.17	1.37	1.43
23	B	603	CLA	C3D-C4D	-2.17	1.39	1.44
29	D	705[B]	PL9	C2-C3	2.17	1.40	1.34
23	c	502	CLA	C3D-C4D	-2.16	1.39	1.44
23	B	616	CLA	C1C-NC	-2.16	1.34	1.37
23	B	610	CLA	C3D-C4D	-2.16	1.39	1.44
23	D	703	CLA	C3D-C4D	-2.16	1.39	1.44
23	c	507	CLA	C3D-C4D	-2.16	1.39	1.44
23	a	406[B]	CLA	C1B-CHB	2.16	1.47	1.41
23	C	514	CLA	C3D-C4D	-2.15	1.39	1.44
38	F	102	HEM	C3B-C4B	2.15	1.49	1.44
23	A	405[A]	CLA	C1B-NB	-2.15	1.33	1.35
32	b	627	LMT	O3'-C3'	-2.15	1.37	1.43
23	B	607	CLA	C1C-NC	-2.15	1.34	1.37
23	C	508	CLA	C4C-C3C	2.15	1.48	1.45
23	a	405[A]	CLA	C4B-CHC	2.14	1.46	1.41
23	B	603	CLA	C1C-NC	-2.14	1.34	1.37
23	B	604	CLA	C4C-C3C	2.14	1.48	1.45
23	B	604	CLA	C1A-CHA	2.14	1.52	1.43
23	c	503	CLA	C3D-C4D	-2.13	1.39	1.44
23	A	406[B]	CLA	C4C-C3C	2.13	1.48	1.45
23	c	509	CLA	C3D-C4D	-2.13	1.39	1.44
23	b	608	CLA	C4B-CHC	2.13	1.46	1.41
32	b	621	LMT	O3'-C3'	-2.13	1.38	1.43
23	C	509	CLA	C4B-CHC	2.13	1.46	1.41
29	A	414[A]	PL9	C2-C1	-2.12	1.39	1.44
23	C	503	CLA	C4B-CHC	2.12	1.46	1.41
23	b	606	CLA	C1B-NB	-2.12	1.33	1.35
23	D	702[A]	CLA	C4B-CHC	2.12	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	606	CLA	C1B-CHB	2.12	1.46	1.41
23	a	406[B]	CLA	C1B-NB	-2.12	1.33	1.35
23	C	510	CLA	C4B-CHC	2.12	1.46	1.41
23	a	406[A]	CLA	C1C-C2C	2.12	1.48	1.44
23	B	610	CLA	C1B-NB	-2.11	1.33	1.35
23	b	607	CLA	C1C-NC	-2.11	1.34	1.37
23	C	502	CLA	C1B-NB	-2.11	1.33	1.35
23	C	513	CLA	C3D-C4D	-2.11	1.39	1.44
23	c	510	CLA	C4B-NB	-2.11	1.33	1.35
23	c	511	CLA	C4C-C3C	2.11	1.48	1.45
32	a	417	LMT	O2'-C2'	-2.11	1.38	1.43
23	B	604	CLA	MG-NA	2.10	2.11	2.06
23	b	604	CLA	C3D-C4D	-2.10	1.39	1.44
23	B	613	CLA	C4C-C3C	2.10	1.48	1.45
23	B	604	CLA	C1C-C2C	2.09	1.48	1.44
23	c	514	CLA	C1D-C2D	2.09	1.49	1.45
32	B	627	LMT	O5'-C5'	-2.09	1.39	1.44
23	C	504	CLA	C4C-C3C	2.09	1.48	1.45
23	c	510	CLA	C1C-NC	-2.09	1.34	1.37
40	v	201	HEC	C3C-C4C	2.08	1.46	1.43
23	a	407[A]	CLA	C4C-C3C	2.08	1.48	1.45
36	C	518[B]	DGD	O5D-C1E	2.08	1.43	1.40
23	c	508	CLA	C3D-C4D	-2.08	1.39	1.44
23	B	613	CLA	C4B-CHC	2.08	1.46	1.41
23	b	615	CLA	C1C-C2C	2.08	1.48	1.44
23	C	507	CLA	C1D-C2D	2.08	1.49	1.45
23	c	508	CLA	C4C-C3C	2.08	1.48	1.45
23	B	608	CLA	C4B-CHC	2.07	1.46	1.41
23	C	513	CLA	C1B-CHB	2.07	1.46	1.41
23	B	601	CLA	C3D-C4D	-2.07	1.39	1.44
23	C	514	CLA	C4C-C3C	2.07	1.48	1.45
23	b	604	CLA	MG-NA	2.06	2.11	2.06
23	A	406[B]	CLA	C1B-CHB	2.06	1.46	1.41
32	B	630	LMT	O2'-C2'	-2.06	1.38	1.43
23	b	605	CLA	C1B-CHB	2.05	1.46	1.41
32	e	101	LMT	O3B-C3B	-2.05	1.38	1.43
32	A	418	LMT	O2'-C2'	-2.05	1.38	1.43
23	C	509	CLA	C3D-C4D	-2.05	1.39	1.44
23	C	514	CLA	C4B-CHC	2.05	1.46	1.41
23	C	514	CLA	C1B-NB	-2.05	1.33	1.35
36	c	519	DGD	O5D-C1E	2.05	1.43	1.40
23	B	610	CLA	C1C-NC	-2.05	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	414[B]	PL9	C2-C1	-2.05	1.39	1.44
23	c	507	CLA	C1C-C2C	2.04	1.48	1.44
23	B	614	CLA	C4C-C3C	2.04	1.48	1.45
23	a	407[A]	CLA	C4B-CHC	2.04	1.46	1.41
23	B	601	CLA	C4C-C3C	2.04	1.48	1.45
29	D	705[A]	PL9	C2-C3	2.04	1.40	1.34
23	b	607	CLA	C4C-C3C	2.04	1.48	1.45
23	A	408	CLA	C4B-CHC	2.03	1.46	1.41
23	C	507	CLA	C4B-CHC	2.03	1.46	1.41
23	b	612	CLA	C4C-C3C	2.03	1.48	1.45
23	C	511	CLA	C4B-CHC	2.03	1.46	1.41
23	b	616	CLA	C1B-CHB	2.03	1.46	1.41
29	a	414[B]	PL9	C2-C3	2.03	1.40	1.34
32	A	418	LMT	O3'-C3'	-2.03	1.38	1.43
23	B	615	CLA	C3D-C4D	-2.03	1.39	1.44
23	c	503	CLA	C4B-CHC	2.03	1.46	1.41
23	a	406[B]	CLA	C1C-C2C	2.03	1.48	1.44
23	B	606	CLA	MG-NA	2.03	2.11	2.06
23	b	615	CLA	C4C-C3C	2.03	1.48	1.45
33	b	629[A]	LHG	O7-C5	-2.02	1.41	1.46
23	C	510	CLA	C1C-NC	-2.02	1.34	1.37
23	B	613	CLA	C1B-NB	-2.02	1.33	1.35
23	b	609	CLA	C4C-C3C	2.02	1.48	1.45
23	A	404[A]	CLA	C3D-C4D	-2.02	1.39	1.44
23	B	615	CLA	MG-NA	2.02	2.11	2.06
23	C	512	CLA	C1A-CHA	2.01	1.51	1.43
38	f	101	HEM	CHB-C1B	2.01	1.40	1.35
23	B	613	CLA	C3D-C4D	-2.01	1.39	1.44
23	b	613	CLA	C4C-C3C	2.01	1.48	1.45
32	m	103	LMT	O3'-C3'	-2.01	1.38	1.43
32	A	418	LMT	O2B-C2B	-2.01	1.38	1.43
23	A	408	CLA	C4C-C3C	2.00	1.48	1.45
23	c	503	CLA	C1C-C2C	2.00	1.48	1.44
23	b	611	CLA	C4B-CHC	2.00	1.46	1.41
24	a	416[A]	PHO	CBD-CGD	-2.00	1.49	1.52

All (3111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	C1D-ND-C4D	-11.83	97.93	106.33
23	a	409	CLA	C1D-ND-C4D	-10.60	98.80	106.33
23	B	614	CLA	C1D-ND-C4D	-10.32	99.00	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	612	CLA	C1D-ND-C4D	-10.31	99.01	106.33
23	C	504	CLA	C1D-ND-C4D	-10.29	99.02	106.33
23	B	611	CLA	C2D-C1D-ND	10.29	117.68	110.10
23	b	605	CLA	C1D-ND-C4D	-10.12	99.15	106.33
23	b	603	CLA	C1D-ND-C4D	-10.04	99.20	106.33
23	B	615	CLA	C1D-ND-C4D	-9.76	99.40	106.33
23	c	504	CLA	C1D-ND-C4D	-9.74	99.41	106.33
23	b	613	CLA	C2D-C1D-ND	9.73	117.27	110.10
23	c	502	CLA	C1D-ND-C4D	-9.72	99.43	106.33
23	d	402	CLA	C1D-ND-C4D	-9.71	99.44	106.33
23	a	407[A]	CLA	C1D-ND-C4D	-9.69	99.45	106.33
23	b	614	CLA	C1D-ND-C4D	-9.68	99.46	106.33
23	A	406[B]	CLA	C1D-ND-C4D	-9.65	99.48	106.33
23	a	405[B]	CLA	C1D-ND-C4D	-9.64	99.49	106.33
23	A	408	CLA	C1D-ND-C4D	-9.62	99.50	106.33
23	B	601	CLA	C1D-ND-C4D	-9.56	99.54	106.33
23	c	514	CLA	C1D-ND-C4D	-9.56	99.54	106.33
23	b	610	CLA	C1D-ND-C4D	-9.56	99.55	106.33
23	a	407[B]	CLA	C1D-ND-C4D	-9.52	99.57	106.33
23	a	409	CLA	C2D-C1D-ND	9.52	117.12	110.10
23	C	511	CLA	C1D-ND-C4D	-9.51	99.58	106.33
23	b	602	CLA	C1D-ND-C4D	-9.50	99.58	106.33
23	c	512	CLA	C1D-ND-C4D	-9.49	99.59	106.33
23	b	611	CLA	C1D-ND-C4D	-9.47	99.61	106.33
23	B	606	CLA	C1D-ND-C4D	-9.47	99.61	106.33
23	A	408	CLA	C2D-C1D-ND	9.44	117.06	110.10
23	b	607	CLA	C1D-ND-C4D	-9.44	99.63	106.33
23	A	406[A]	CLA	C1D-ND-C4D	-9.41	99.65	106.33
23	C	514	CLA	C1D-ND-C4D	-9.40	99.66	106.33
23	C	510	CLA	C1D-ND-C4D	-9.36	99.69	106.33
23	B	610	CLA	C1D-ND-C4D	-9.35	99.69	106.33
23	b	606	CLA	C1D-ND-C4D	-9.34	99.70	106.33
23	b	614	CLA	C2D-C1D-ND	9.32	116.97	110.10
23	B	608	CLA	C1D-ND-C4D	-9.29	99.73	106.33
23	c	506	CLA	C1D-ND-C4D	-9.29	99.74	106.33
23	C	502	CLA	C1D-ND-C4D	-9.25	99.76	106.33
23	B	613	CLA	C2D-C1D-ND	9.22	116.90	110.10
23	B	605	CLA	C1D-ND-C4D	-9.21	99.79	106.33
23	B	614	CLA	C2D-C1D-ND	9.18	116.87	110.10
23	D	702[A]	CLA	C1D-ND-C4D	-9.14	99.84	106.33
23	D	702[B]	CLA	C1D-ND-C4D	-9.12	99.85	106.33
23	A	405[A]	CLA	C2D-C1D-ND	9.08	116.79	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	606	CLA	C2D-C1D-ND	9.08	116.79	110.10
23	A	405[A]	CLA	C1D-ND-C4D	-9.06	99.90	106.33
23	B	609	CLA	C1D-ND-C4D	-9.04	99.91	106.33
23	A	405[B]	CLA	C1D-ND-C4D	-9.04	99.91	106.33
23	b	615	CLA	C1D-ND-C4D	-9.04	99.91	106.33
23	b	608	CLA	C1D-ND-C4D	-9.03	99.92	106.33
23	d	401[A]	CLA	C1D-ND-C4D	-9.03	99.92	106.33
23	B	602	CLA	C1D-ND-C4D	-9.02	99.93	106.33
23	b	607	CLA	C2D-C1D-ND	9.01	116.74	110.10
23	b	609	CLA	C1D-ND-C4D	-8.99	99.95	106.33
23	a	405[A]	CLA	C1D-ND-C4D	-8.97	99.96	106.33
23	D	703	CLA	C1D-ND-C4D	-8.95	99.98	106.33
23	B	613	CLA	C1D-ND-C4D	-8.92	100.00	106.33
23	a	406[B]	CLA	C1D-ND-C4D	-8.90	100.02	106.33
23	c	507	CLA	C1D-ND-C4D	-8.90	100.02	106.33
23	B	616	CLA	C2D-C1D-ND	8.88	116.65	110.10
23	B	615	CLA	C2D-C1D-ND	8.88	116.65	110.10
23	C	513	CLA	C1D-ND-C4D	-8.86	100.04	106.33
23	d	402	CLA	C2D-C1D-ND	8.83	116.61	110.10
23	a	407[A]	CLA	C2D-C1D-ND	8.81	116.60	110.10
23	C	505	CLA	C1D-ND-C4D	-8.81	100.08	106.33
23	b	605	CLA	C2D-C1D-ND	8.81	116.59	110.10
23	B	607	CLA	C1D-ND-C4D	-8.80	100.08	106.33
23	c	508	CLA	C1D-ND-C4D	-8.79	100.09	106.33
23	B	616	CLA	C1D-ND-C4D	-8.76	100.11	106.33
23	c	505	CLA	C1D-ND-C4D	-8.74	100.13	106.33
23	C	504	CLA	C2D-C1D-ND	8.73	116.54	110.10
23	b	601	CLA	C1D-ND-C4D	-8.72	100.14	106.33
23	C	505	CLA	C2D-C1D-ND	8.71	116.53	110.10
23	c	513	CLA	C1D-ND-C4D	-8.71	100.15	106.33
23	c	510	CLA	C1D-ND-C4D	-8.70	100.15	106.33
23	c	511	CLA	C1D-ND-C4D	-8.69	100.16	106.33
23	b	616	CLA	C1D-ND-C4D	-8.69	100.16	106.33
23	B	603	CLA	C1D-ND-C4D	-8.69	100.16	106.33
23	A	404[B]	CLA	C1D-ND-C4D	-8.68	100.17	106.33
23	C	506	CLA	C1D-ND-C4D	-8.68	100.17	106.33
23	a	406[A]	CLA	C1D-ND-C4D	-8.67	100.18	106.33
23	d	401[B]	CLA	C1D-ND-C4D	-8.64	100.19	106.33
23	b	603	CLA	C2D-C1D-ND	8.62	116.46	110.10
23	A	406[A]	CLA	C2D-C1D-ND	8.61	116.45	110.10
23	B	608	CLA	C2D-C1D-ND	8.61	116.45	110.10
23	b	613	CLA	C1D-ND-C4D	-8.59	100.23	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	612	CLA	C1D-ND-C4D	-8.59	100.23	106.33
23	B	610	CLA	C2D-C1D-ND	8.56	116.41	110.10
23	a	406[A]	CLA	C2D-C1D-ND	8.52	116.39	110.10
23	C	512	CLA	C1D-ND-C4D	-8.52	100.28	106.33
23	b	606	CLA	C2D-C1D-ND	8.50	116.37	110.10
23	a	407[B]	CLA	C2D-C1D-ND	8.49	116.36	110.10
23	c	502	CLA	C2D-C1D-ND	8.49	116.36	110.10
23	D	702[A]	CLA	C2D-C1D-ND	8.48	116.35	110.10
23	C	514	CLA	C2D-C1D-ND	8.43	116.31	110.10
23	B	607	CLA	C2D-C1D-ND	8.42	116.31	110.10
23	c	512	CLA	C2D-C1D-ND	8.41	116.30	110.10
23	b	611	CLA	C2D-C1D-ND	8.40	116.29	110.10
23	c	509	CLA	C2D-C1D-ND	8.38	116.28	110.10
23	b	610	CLA	C2D-C1D-ND	8.38	116.28	110.10
23	C	507	CLA	C1D-ND-C4D	-8.38	100.38	106.33
23	C	513	CLA	C2D-C1D-ND	8.37	116.28	110.10
23	c	503	CLA	C1D-ND-C4D	-8.36	100.40	106.33
23	B	612	CLA	C2D-C1D-ND	8.35	116.26	110.10
23	C	508	CLA	C1D-ND-C4D	-8.34	100.41	106.33
23	B	603	CLA	C2D-C1D-ND	8.34	116.25	110.10
23	A	406[B]	CLA	C2D-C1D-ND	8.33	116.25	110.10
23	a	405[B]	CLA	C2D-C1D-ND	8.33	116.24	110.10
23	B	601	CLA	C2D-C1D-ND	8.32	116.24	110.10
23	C	510	CLA	C2D-C1D-ND	8.29	116.21	110.10
23	c	504	CLA	C2D-C1D-ND	8.29	116.21	110.10
23	B	602	CLA	C2D-C1D-ND	8.24	116.18	110.10
23	b	616	CLA	C2D-C1D-ND	8.20	116.15	110.10
23	c	509	CLA	C1D-ND-C4D	-8.19	100.52	106.33
23	C	511	CLA	C2D-C1D-ND	8.18	116.13	110.10
23	A	405[B]	CLA	C2D-C1D-ND	8.17	116.12	110.10
23	B	605	CLA	C2D-C1D-ND	8.15	116.11	110.10
23	c	505	CLA	C2D-C1D-ND	8.15	116.11	110.10
23	B	609	CLA	C2D-C1D-ND	8.14	116.11	110.10
23	C	503	CLA	C1D-ND-C4D	-8.14	100.56	106.33
23	C	508	CLA	C2D-C1D-ND	8.10	116.07	110.10
23	C	512	CLA	C2D-C1D-ND	8.08	116.06	110.10
23	b	602	CLA	C4A-NA-C1A	-8.05	103.09	106.71
23	b	615	CLA	C2D-C1D-ND	8.03	116.02	110.10
23	a	405[A]	CLA	C2D-C1D-ND	8.03	116.02	110.10
23	C	509	CLA	C1D-ND-C4D	-8.00	100.65	106.33
23	b	609	CLA	C2D-C1D-ND	7.98	115.98	110.10
23	c	514	CLA	C2D-C1D-ND	7.95	115.96	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	504	CLA	C4A-NA-C1A	-7.93	103.14	106.71
23	d	401[A]	CLA	C2D-C1D-ND	7.92	115.94	110.10
23	c	506	CLA	C2D-C1D-ND	7.92	115.94	110.10
23	a	406[B]	CLA	C2D-C1D-ND	7.92	115.94	110.10
23	B	611	CLA	CHD-C4C-C3C	-7.89	113.24	124.84
23	c	508	CLA	C2D-C1D-ND	7.88	115.91	110.10
23	B	604	CLA	C1D-ND-C4D	-7.88	100.74	106.33
35	b	623	HTG	C1'-S1-C1	7.84	114.76	100.09
23	B	616	CLA	O2D-CGD-CBD	7.84	125.20	111.27
24	a	408[B]	PHO	O2D-CGD-CBD	7.84	120.93	111.00
23	D	702[B]	CLA	C2D-C1D-ND	7.83	115.87	110.10
23	b	601	CLA	C2D-C1D-ND	7.81	115.86	110.10
23	c	507	CLA	C2D-C1D-ND	7.78	115.83	110.10
23	C	511	CLA	CMD-C2D-C1D	7.76	138.38	124.71
23	C	509	CLA	C2D-C1D-ND	7.74	115.81	110.10
26	X	101	SQD	O6-C1-C2	7.73	120.37	108.30
23	C	502	CLA	C2D-C1D-ND	7.72	115.79	110.10
23	A	404[A]	CLA	C1D-ND-C4D	-7.69	100.87	106.33
23	c	510	CLA	C2D-C1D-ND	7.65	115.74	110.10
24	A	407[B]	PHO	O2D-CGD-CBD	7.65	120.69	111.00
23	c	503	CLA	C2D-C1D-ND	7.61	115.72	110.10
24	A	417[B]	PHO	O2D-CGD-CBD	7.60	120.62	111.00
23	c	513	CLA	C2D-C1D-ND	7.58	115.69	110.10
23	b	602	CLA	C2D-C1D-ND	7.55	115.67	110.10
23	A	404[A]	CLA	C2D-C1D-ND	7.53	115.66	110.10
23	b	608	CLA	C2D-C1D-ND	7.53	115.65	110.10
23	c	511	CLA	C2D-C1D-ND	7.52	115.64	110.10
23	d	401[B]	CLA	C2D-C1D-ND	7.51	115.64	110.10
23	b	604	CLA	C1D-ND-C4D	-7.50	101.01	106.33
23	b	612	CLA	C2D-C1D-ND	7.48	115.62	110.10
23	C	504	CLA	C4A-NA-C1A	-7.44	103.36	106.71
24	A	417[A]	PHO	O2D-CGD-CBD	7.38	120.34	111.00
23	B	606	CLA	CMD-C2D-C1D	7.31	137.60	124.71
23	C	507	CLA	C2D-C1D-ND	7.25	115.44	110.10
24	a	416[A]	PHO	O2D-CGD-CBD	7.21	120.13	111.00
23	D	703	CLA	C2D-C1D-ND	7.20	115.41	110.10
23	b	616	CLA	O2D-CGD-CBD	7.20	124.06	111.27
23	A	404[B]	CLA	C2D-C1D-ND	7.17	115.39	110.10
24	a	408[A]	PHO	O2D-CGD-CBD	7.16	120.07	111.00
23	C	503	CLA	C2D-C1D-ND	7.15	115.37	110.10
23	b	604	CLA	C2D-C1D-ND	7.14	115.37	110.10
23	B	614	CLA	CMD-C2D-C1D	7.13	137.28	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	605	CLA	CHD-C4C-C3C	-7.11	114.39	124.84
23	B	604	CLA	C2D-C1D-ND	7.09	115.33	110.10
23	c	503	CLA	C2C-C1C-NC	7.01	116.54	109.97
24	a	416[B]	PHO	O2D-CGD-CBD	7.01	119.88	111.00
23	C	506	CLA	C2D-C1D-ND	6.94	115.22	110.10
23	b	616	CLA	CHD-C4C-C3C	-6.93	114.66	124.84
23	B	603	CLA	O2D-CGD-CBD	6.92	123.56	111.27
23	c	502	CLA	CMD-C2D-C1D	6.92	136.90	124.71
24	A	407[A]	PHO	O2D-CGD-CBD	6.91	119.75	111.00
23	c	504	CLA	CMD-C2D-C1D	6.90	136.88	124.71
23	c	508	CLA	O2D-CGD-CBD	6.88	123.50	111.27
23	b	615	CLA	C4A-NA-C1A	-6.88	103.61	106.71
23	B	609	CLA	C4A-NA-C1A	-6.87	103.62	106.71
23	C	513	CLA	CHD-C4C-C3C	-6.85	114.78	124.84
23	b	606	CLA	CHD-C4C-C3C	-6.85	114.78	124.84
23	B	616	CLA	CHD-C4C-C3C	-6.85	114.78	124.84
23	d	401[B]	CLA	C2C-C1C-NC	6.81	116.36	109.97
23	A	406[B]	CLA	CHD-C1D-ND	-6.80	118.21	124.45
23	c	514	CLA	CMD-C2D-C1D	6.77	136.65	124.71
23	b	605	CLA	CHD-C1D-ND	-6.75	118.25	124.45
23	C	507	CLA	C2C-C1C-NC	6.75	116.29	109.97
23	B	606	CLA	CHD-C4C-C3C	-6.74	114.94	124.84
23	D	703	CLA	C4A-NA-C1A	-6.72	103.68	106.71
23	D	702[B]	CLA	C4A-NA-C1A	-6.72	103.69	106.71
23	B	606	CLA	CHD-C1D-ND	-6.71	118.28	124.45
23	b	613	CLA	CHD-C4C-C3C	-6.71	114.97	124.84
23	b	607	CLA	CHD-C1D-ND	-6.71	118.29	124.45
23	c	502	CLA	CHD-C1D-ND	-6.70	118.30	124.45
23	b	604	CLA	C2C-C1C-NC	6.70	116.25	109.97
23	c	508	CLA	CHD-C1D-ND	-6.69	118.30	124.45
23	C	509	CLA	C2C-C1C-NC	6.69	116.24	109.97
23	d	402	CLA	CMD-C2D-C1D	6.68	136.49	124.71
23	a	409	CLA	CHD-C4C-C3C	-6.68	115.02	124.84
23	b	616	CLA	C4A-NA-C1A	-6.68	103.70	106.71
23	b	612	CLA	CHD-C4C-C3C	-6.67	115.03	124.84
23	B	610	CLA	O2D-CGD-CBD	6.66	123.10	111.27
23	C	504	CLA	CMD-C2D-C1D	6.65	136.43	124.71
23	d	402	CLA	CHD-C1D-ND	-6.63	118.36	124.45
23	c	508	CLA	CMD-C2D-C1D	6.63	136.40	124.71
23	A	404[A]	CLA	CMD-C2D-C1D	6.62	136.38	124.71
23	A	404[B]	CLA	CMD-C2D-C1D	6.62	136.38	124.71
23	b	605	CLA	CMD-C2D-C1D	6.62	136.38	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	605	CLA	CHD-C4C-C3C	-6.61	115.12	124.84
23	B	614	CLA	CHD-C1D-ND	-6.60	118.39	124.45
23	b	614	CLA	CHD-C4C-C3C	-6.59	115.16	124.84
23	a	405[B]	CLA	C2C-C1C-NC	6.58	116.13	109.97
23	B	611	CLA	CMD-C2D-C1D	6.57	136.30	124.71
23	c	514	CLA	CHD-C1D-ND	-6.56	118.43	124.45
23	b	607	CLA	CMD-C2D-C1D	6.55	136.26	124.71
23	c	507	CLA	CMD-C2D-C1D	6.54	136.25	124.71
23	C	502	CLA	C4A-NA-C1A	-6.53	103.77	106.71
23	B	604	CLA	C2C-C1C-NC	6.53	116.09	109.97
23	D	702[A]	CLA	C4A-NA-C1A	-6.52	103.77	106.71
23	C	513	CLA	C4A-NA-C1A	-6.51	103.78	106.71
23	d	401[A]	CLA	C2C-C1C-NC	6.51	116.07	109.97
26	X	101	SQD	O47-C7-C8	6.51	125.53	111.50
23	B	605	CLA	CMD-C2D-C1D	6.51	136.19	124.71
23	b	606	CLA	C4A-NA-C1A	-6.51	103.78	106.71
23	C	507	CLA	CMD-C2D-C1D	6.51	136.18	124.71
23	b	610	CLA	CHD-C4C-C3C	-6.49	115.30	124.84
23	b	616	CLA	CMD-C2D-C1D	6.48	136.14	124.71
23	D	702[A]	CLA	CMD-C2D-C1D	6.46	136.10	124.71
23	b	601	CLA	O2D-CGD-CBD	6.45	122.74	111.27
23	b	606	CLA	CMD-C2D-C1D	6.45	136.08	124.71
23	b	602	CLA	CMD-C2D-C1D	6.45	136.08	124.71
23	C	502	CLA	O2D-CGD-CBD	6.44	122.72	111.27
23	b	606	CLA	CHD-C1D-ND	-6.42	118.56	124.45
23	b	602	CLA	CHD-C1D-ND	-6.41	118.56	124.45
23	b	615	CLA	CMD-C2D-C1D	6.40	135.99	124.71
26	B	620	SQD	O6-C1-C2	6.40	118.29	108.30
23	C	504	CLA	CHD-C1D-ND	-6.39	118.58	124.45
23	d	401[B]	CLA	CMD-C2D-C1D	6.38	135.97	124.71
23	b	602	CLA	CHD-C4C-C3C	-6.38	115.47	124.84
23	C	511	CLA	CHD-C1D-ND	-6.37	118.60	124.45
23	B	607	CLA	C2C-C1C-NC	6.36	115.93	109.97
23	B	616	CLA	C4A-NA-C1A	-6.36	103.85	106.71
23	c	507	CLA	CHD-C1D-ND	-6.34	118.63	124.45
23	a	407[A]	CLA	CHD-C4C-C3C	-6.34	115.52	124.84
23	a	406[B]	CLA	CHD-C4C-C3C	-6.33	115.53	124.84
23	b	609	CLA	C4A-NA-C1A	-6.31	103.87	106.71
23	a	407[A]	CLA	CHD-C1D-ND	-6.31	118.66	124.45
23	A	405[B]	CLA	CHD-C1D-ND	-6.30	118.66	124.45
23	d	402	CLA	CHD-C4C-C3C	-6.30	115.58	124.84
35	D	710	HTG	C1'-S1-C1	6.29	111.85	100.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	511	CLA	CMD-C2D-C1D	6.29	135.79	124.71
23	b	610	CLA	CMD-C2D-C1D	6.28	135.79	124.71
23	C	508	CLA	CHD-C4C-C3C	-6.28	115.61	124.84
23	A	408	CLA	CHD-C4C-C3C	-6.27	115.62	124.84
23	a	405[B]	CLA	CMD-C2D-C1D	6.27	135.76	124.71
23	c	506	CLA	CHD-C4C-C3C	-6.26	115.63	124.84
23	c	513	CLA	C4A-NA-C1A	-6.26	103.89	106.71
23	D	702[A]	CLA	C2C-C1C-NC	6.26	115.84	109.97
23	B	601	CLA	CMD-C2D-C1D	6.26	135.75	124.71
23	b	609	CLA	CHD-C4C-C3C	-6.26	115.64	124.84
23	c	505	CLA	CMD-C2D-C1D	6.26	135.74	124.71
23	a	405[A]	CLA	C2C-C1C-NC	6.26	115.83	109.97
23	B	606	CLA	C4A-NA-C1A	-6.25	103.89	106.71
23	C	504	CLA	CHD-C4C-C3C	-6.25	115.65	124.84
23	C	506	CLA	CMD-C2D-C1D	6.25	135.73	124.71
23	b	603	CLA	CHD-C4C-C3C	-6.25	115.66	124.84
23	D	702[B]	CLA	C2C-C1C-NC	6.24	115.82	109.97
23	B	610	CLA	CMD-C2D-C1D	6.24	135.71	124.71
23	c	512	CLA	CHD-C4C-C3C	-6.24	115.67	124.84
23	b	613	CLA	C2C-C1C-NC	6.24	115.81	109.97
23	D	702[B]	CLA	CMD-C2D-C1D	6.23	135.70	124.71
23	a	406[A]	CLA	CHD-C4C-C3C	-6.22	115.70	124.84
23	B	609	CLA	CHD-C4C-C3C	-6.21	115.72	124.84
23	B	612	CLA	CHD-C4C-C3C	-6.20	115.72	124.84
23	C	507	CLA	CHD-C1D-ND	-6.20	118.76	124.45
23	c	504	CLA	CHD-C4C-C3C	-6.19	115.73	124.84
23	a	405[A]	CLA	C4A-NA-C1A	-6.19	103.92	106.71
23	C	508	CLA	O2D-CGD-CBD	6.18	122.25	111.27
23	b	611	CLA	CMD-C2D-C1D	6.16	135.58	124.71
23	D	702[A]	CLA	CHD-C1D-ND	-6.16	118.79	124.45
23	c	511	CLA	CHD-C4C-C3C	-6.16	115.78	124.84
23	B	615	CLA	CHD-C4C-C3C	-6.16	115.79	124.84
23	A	406[B]	CLA	CMD-C2D-C1D	6.16	135.56	124.71
23	A	404[B]	CLA	C4A-NA-C1A	-6.14	103.94	106.71
23	A	406[B]	CLA	C4A-NA-C1A	-6.14	103.94	106.71
23	c	510	CLA	C2C-C1C-NC	6.14	115.72	109.97
23	a	406[B]	CLA	CMD-C2D-C1D	6.13	135.52	124.71
23	B	601	CLA	CHD-C4C-C3C	-6.13	115.83	124.84
23	B	602	CLA	CHD-C4C-C3C	-6.13	115.83	124.84
23	A	408	CLA	CHD-C1D-ND	-6.11	118.84	124.45
23	B	608	CLA	CHD-C1D-ND	-6.11	118.84	124.45
23	c	504	CLA	CHD-C1D-ND	-6.09	118.86	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	514	CLA	C4A-NA-C1A	-6.09	103.97	106.71
23	c	509	CLA	C2C-C1C-NC	6.09	115.67	109.97
23	C	506	CLA	CHD-C4C-C3C	-6.09	115.89	124.84
23	C	502	CLA	CMD-C2D-C1D	6.09	135.44	124.71
23	A	404[A]	CLA	C2C-C1C-NC	6.08	115.67	109.97
23	C	503	CLA	C2C-C1C-NC	6.07	115.66	109.97
23	D	702[B]	CLA	CHD-C1D-ND	-6.07	118.88	124.45
23	D	703	CLA	CMD-C2D-C1D	6.06	135.39	124.71
23	C	511	CLA	CHD-C4C-C3C	-6.05	115.95	124.84
23	c	506	CLA	C4A-NA-C1A	-6.05	103.99	106.71
23	b	601	CLA	C4A-NA-C1A	-6.04	103.99	106.71
23	c	505	CLA	CHD-C1D-ND	-6.04	118.91	124.45
26	A	410[A]	SQD	O6-C1-C2	6.03	117.72	108.30
23	C	503	CLA	CMD-C2D-C1D	6.03	135.35	124.71
23	b	601	CLA	CMD-C2D-C1D	6.03	135.35	124.71
23	d	401[A]	CLA	C4A-NA-C1A	-6.03	104.00	106.71
23	B	603	CLA	CHD-C4C-C3C	-6.03	115.98	124.84
25	D	704	BCR	C7-C8-C9	-6.03	117.13	126.23
23	C	505	CLA	CHD-C1D-ND	-6.02	118.92	124.45
23	A	405[B]	CLA	CHD-C4C-C3C	-6.01	116.00	124.84
23	b	614	CLA	O2D-CGD-CBD	6.01	121.95	111.27
23	A	405[B]	CLA	CMD-C2D-C1D	6.01	135.31	124.71
23	C	512	CLA	CHD-C4C-C3C	-6.01	116.01	124.84
23	c	506	CLA	O2D-CGD-CBD	6.00	121.92	111.27
23	B	601	CLA	CHD-C1D-ND	-5.99	118.94	124.45
23	b	615	CLA	CHD-C4C-C3C	-5.99	116.03	124.84
23	c	510	CLA	CMD-C2D-C1D	5.99	135.27	124.71
23	C	514	CLA	CHD-C1D-ND	-5.99	118.95	124.45
23	B	614	CLA	CHD-C4C-C3C	-5.99	116.04	124.84
23	A	406[A]	CLA	CHD-C4C-C3C	-5.98	116.05	124.84
23	B	608	CLA	CHD-C4C-C3C	-5.98	116.06	124.84
23	B	610	CLA	CHD-C1D-ND	-5.96	118.97	124.45
38	F	102	HEM	CAD-CBD-CGD	5.96	126.43	113.60
23	a	407[B]	CLA	CHD-C1D-ND	-5.96	118.98	124.45
23	c	507	CLA	C2C-C1C-NC	5.95	115.55	109.97
35	c	522	HTG	C1'-S1-C1	5.93	111.19	100.09
23	B	608	CLA	CMD-C2D-C1D	5.93	135.16	124.71
23	C	514	CLA	CHD-C4C-C3C	-5.93	116.12	124.84
23	b	603	CLA	CMD-C2D-C1D	5.92	135.15	124.71
23	B	615	CLA	CHD-C1D-ND	-5.92	119.02	124.45
23	B	615	CLA	CMD-C2D-C1D	5.91	135.13	124.71
23	a	407[B]	CLA	CHD-C4C-C3C	-5.90	116.17	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	603	CLA	C4A-NA-C1A	-5.89	104.06	106.71
23	A	405[A]	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
23	b	607	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	b	601	CLA	CHD-C1D-ND	-5.89	119.04	124.45
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	b	602	CLA	O2D-CGD-CBD	5.88	121.71	111.27
23	c	513	CLA	CMD-C2D-C1D	5.87	135.07	124.71
23	C	510	CLA	C2C-C1C-NC	5.87	115.47	109.97
23	B	609	CLA	CMD-C2D-C1D	5.87	135.06	124.71
23	B	602	CLA	O2D-CGD-CBD	5.87	121.70	111.27
23	c	508	CLA	C4A-NA-C1A	-5.87	104.07	106.71
26	A	410[B]	SQD	O6-C1-C2	5.87	117.46	108.30
23	c	512	CLA	CMD-C2D-C1D	5.86	135.03	124.71
23	A	404[B]	CLA	C2C-C1C-NC	5.85	115.46	109.97
24	a	416[B]	PHO	C1-C2-C3	-5.85	115.93	126.04
23	A	404[B]	CLA	CHD-C1D-ND	-5.85	119.08	124.45
23	c	505	CLA	CHD-C4C-C3C	-5.84	116.25	124.84
23	B	604	CLA	CMD-C2D-C1D	5.84	135.01	124.71
23	a	405[B]	CLA	CHD-C1D-ND	-5.84	119.09	124.45
23	B	613	CLA	CHD-C4C-C3C	-5.83	116.27	124.84
23	b	601	CLA	CHD-C4C-C3C	-5.82	116.28	124.84
23	B	611	CLA	C3D-C2D-C1D	-5.82	97.89	105.83
23	B	601	CLA	O2D-CGD-CBD	5.82	121.61	111.27
23	b	611	CLA	CHD-C1D-ND	-5.81	119.11	124.45
23	A	404[A]	CLA	CHD-C1D-ND	-5.81	119.11	124.45
23	b	608	CLA	CHD-C4C-C3C	-5.81	116.30	124.84
23	B	615	CLA	C4A-NA-C1A	-5.81	104.10	106.71
23	C	505	CLA	C2C-C1C-NC	5.80	115.40	109.97
23	B	611	CLA	O2D-CGD-CBD	5.79	121.55	111.27
23	C	508	CLA	CMD-C2D-C1D	5.79	134.91	124.71
23	B	609	CLA	CHD-C1D-ND	-5.78	119.15	124.45
23	b	604	CLA	O2D-CGD-CBD	5.77	121.53	111.27
23	c	511	CLA	C4A-NA-C1A	-5.77	104.11	106.71
23	C	502	CLA	CHD-C4C-C3C	-5.76	116.37	124.84
23	a	405[A]	CLA	CMD-C2D-C1D	5.75	134.84	124.71
23	a	406[A]	CLA	C4A-NA-C1A	-5.75	104.12	106.71
23	A	404[B]	CLA	CHD-C4C-C3C	-5.75	116.39	124.84
23	B	602	CLA	CMD-C2D-C1D	5.75	134.84	124.71
23	c	513	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
23	c	511	CLA	CHD-C1D-ND	-5.74	119.18	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	703	CLA	CHD-C1D-ND	-5.73	119.19	124.45
23	c	514	CLA	CHD-C4C-C3C	-5.72	116.43	124.84
23	A	406[A]	CLA	C4A-NA-C1A	-5.72	104.13	106.71
23	a	406[B]	CLA	C2C-C1C-NC	5.71	115.33	109.97
23	d	402	CLA	O2D-CGD-CBD	5.70	121.40	111.27
23	B	611	CLA	CHD-C1D-ND	-5.69	119.22	124.45
23	b	605	CLA	O2D-CGD-CBD	5.69	121.39	111.27
23	b	611	CLA	O2D-CGD-CBD	5.69	121.38	111.27
23	c	508	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
23	B	602	CLA	C2C-C1C-NC	5.69	115.30	109.97
23	B	607	CLA	C4A-NA-C1A	-5.69	104.15	106.71
23	A	408	CLA	C2C-C1C-NC	5.68	115.29	109.97
23	b	612	CLA	C2C-C1C-NC	5.67	115.28	109.97
23	C	510	CLA	CHD-C1D-ND	-5.66	119.25	124.45
23	b	613	CLA	C3D-C2D-C1D	-5.66	98.10	105.83
23	D	703	CLA	CHD-C4C-C3C	-5.65	116.53	124.84
23	D	702[B]	CLA	CHD-C4C-C3C	-5.65	116.54	124.84
23	B	603	CLA	CHD-C1D-ND	-5.65	119.27	124.45
23	C	512	CLA	C2C-C1C-NC	5.64	115.26	109.97
23	b	604	CLA	CMD-C2D-C1D	5.64	134.66	124.71
40	V	201	HEC	CBD-CAD-C3D	-5.64	103.00	112.62
23	b	609	CLA	CMD-C2D-C1D	5.64	134.65	124.71
23	C	509	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
23	d	401[A]	CLA	CMD-C2D-C1D	5.64	134.65	124.71
23	A	405[B]	CLA	C2C-C1C-NC	5.64	115.25	109.97
25	Y	101	BCR	C33-C5-C6	-5.64	118.20	124.53
23	b	611	CLA	CHD-C4C-C3C	-5.64	116.56	124.84
23	b	614	CLA	CHD-C1D-ND	-5.63	119.28	124.45
23	C	510	CLA	CMD-C2D-C1D	5.63	134.63	124.71
23	A	408	CLA	CMD-C2D-C1D	5.62	134.62	124.71
23	c	506	CLA	CMD-C2D-C1D	5.61	134.60	124.71
23	B	606	CLA	O2D-CGD-CBD	5.61	121.23	111.27
23	B	610	CLA	CHD-C4C-C3C	-5.61	116.60	124.84
23	a	406[A]	CLA	C2C-C1C-NC	5.61	115.22	109.97
23	c	509	CLA	CHD-C4C-C3C	-5.61	116.60	124.84
23	B	607	CLA	CMD-C2D-C1D	5.60	134.59	124.71
23	C	510	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
23	C	514	CLA	C2C-C1C-NC	5.59	115.21	109.97
23	B	612	CLA	O2D-CGD-CBD	5.59	121.20	111.27
26	b	620	SQD	O6-C1-C2	5.59	117.03	108.30
23	C	503	CLA	CHD-C1D-ND	-5.59	119.32	124.45
26	a	411[A]	SQD	O6-C1-C2	5.58	117.02	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	503	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
23	A	405[A]	CLA	C2C-C1C-NC	5.58	115.19	109.97
23	b	615	CLA	C2C-C1C-NC	5.58	115.19	109.97
23	B	602	CLA	C4A-NA-C1A	-5.57	104.20	106.71
23	C	505	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
23	c	502	CLA	CHD-C4C-C3C	-5.57	116.66	124.84
23	b	603	CLA	C2C-C1C-NC	5.57	115.19	109.97
26	A	410[A]	SQD	C1-O5-C5	-5.56	102.77	113.69
23	B	614	CLA	C2C-C1C-NC	5.56	115.18	109.97
23	b	611	CLA	C4A-NA-C1A	-5.56	104.21	106.71
23	d	401[A]	CLA	CHD-C1D-ND	-5.56	119.35	124.45
23	b	611	CLA	C2C-C1C-NC	5.55	115.18	109.97
23	a	407[A]	CLA	C4A-NA-C1A	-5.55	104.21	106.71
23	B	606	CLA	C3D-C2D-C1D	-5.55	98.25	105.83
23	d	401[A]	CLA	CHD-C4C-C3C	-5.55	116.69	124.84
23	B	616	CLA	C3C-C4C-NC	5.55	116.79	110.57
23	B	607	CLA	CHD-C1D-ND	-5.54	119.36	124.45
23	c	503	CLA	O2D-CGD-CBD	5.54	121.11	111.27
23	D	702[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	C2C-C1C-NC	5.53	115.15	109.97
23	c	510	CLA	C1-C2-C3	-5.53	116.48	126.04
23	A	408	CLA	C3D-C2D-C1D	-5.53	98.29	105.83
23	C	502	CLA	CHD-C1D-ND	-5.52	119.38	124.45
23	B	614	CLA	O2D-CGD-CBD	5.52	121.07	111.27
35	d	409	HTG	C1'-S1-C1	5.51	110.41	100.09
23	C	508	CLA	C4A-NA-C1A	-5.51	104.23	106.71
23	B	603	CLA	CMD-C2D-C1D	5.51	134.42	124.71
23	a	407[B]	CLA	C4A-NA-C1A	-5.51	104.23	106.71
23	c	512	CLA	C2C-C1C-NC	5.50	115.12	109.97
23	c	513	CLA	CHD-C1D-ND	-5.49	119.41	124.45
23	b	603	CLA	CHD-C1D-ND	-5.49	119.41	124.45
23	B	603	CLA	C4A-NA-C1A	-5.49	104.24	106.71
23	B	608	CLA	C2C-C1C-NC	5.48	115.10	109.97
23	C	513	CLA	CMD-C2D-C1D	5.48	134.37	124.71
23	B	605	CLA	C4A-NA-C1A	-5.48	104.24	106.71
23	B	602	CLA	CHD-C1D-ND	-5.47	119.42	124.45
23	b	610	CLA	CHD-C1D-ND	-5.47	119.43	124.45
23	a	406[B]	CLA	CHD-C1D-ND	-5.46	119.43	124.45
34	C	501	LMG	C7-O1-C1	-5.46	103.07	113.74
23	C	512	CLA	O2D-CGD-CBD	5.46	120.97	111.27
23	B	603	CLA	C2C-C1C-NC	5.45	115.08	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	620	SQD	O47-C7-C8	5.45	123.25	111.50
23	c	503	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
23	a	406[A]	CLA	CHD-C1D-ND	-5.44	119.46	124.45
23	A	406[B]	CLA	CHD-C4C-C3C	-5.44	116.85	124.84
23	C	508	CLA	CHD-C1D-ND	-5.43	119.47	124.45
23	b	603	CLA	O2D-CGD-CBD	5.42	120.91	111.27
23	B	604	CLA	CHD-C4C-C3C	-5.42	116.87	124.84
23	b	607	CLA	C3D-C2D-C1D	-5.42	98.43	105.83
23	C	511	CLA	C2C-C1C-NC	5.42	115.05	109.97
23	c	506	CLA	CHD-C1D-ND	-5.42	119.48	124.45
23	C	506	CLA	C2C-C1C-NC	5.41	115.04	109.97
23	c	506	CLA	C2C-C1C-NC	5.40	115.03	109.97
23	B	614	CLA	C3D-C2D-C1D	-5.40	98.47	105.83
23	a	405[A]	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
23	a	405[B]	CLA	CHD-C4C-C3C	-5.38	116.93	124.84
23	c	503	CLA	C1C-C2C-C3C	-5.38	101.30	106.96
23	B	604	CLA	C3C-C4C-NC	5.38	116.60	110.57
23	b	614	CLA	C2C-C1C-NC	5.37	115.01	109.97
24	a	416[A]	PHO	C1-C2-C3	-5.37	116.76	126.04
23	d	401[B]	CLA	CHD-C4C-C3C	-5.37	116.95	124.84
23	C	505	CLA	CMD-C2D-C1D	5.36	134.17	124.71
23	C	514	CLA	CMD-C2D-C1D	5.36	134.16	124.71
23	b	607	CLA	C2C-C1C-NC	5.36	114.99	109.97
23	d	401[B]	CLA	CHD-C1D-ND	-5.36	119.53	124.45
23	A	405[A]	CLA	O2D-CGD-CBD	5.35	120.78	111.27
23	B	612	CLA	CMD-C2D-C1D	5.35	134.15	124.71
23	b	614	CLA	CMD-C2D-C1D	5.35	134.14	124.71
23	b	610	CLA	O2D-CGD-CBD	5.34	120.76	111.27
23	a	407[A]	CLA	CMD-C2D-C1D	5.34	134.12	124.71
23	A	406[A]	CLA	C2C-C1C-NC	5.33	114.97	109.97
23	c	508	CLA	C2C-C1C-NC	5.33	114.96	109.97
23	D	703	CLA	O2D-CGD-CBD	5.32	120.72	111.27
23	B	605	CLA	C2C-C1C-NC	5.32	114.95	109.97
23	c	505	CLA	O2D-CGD-CBD	5.31	120.70	111.27
23	b	609	CLA	CHD-C1D-ND	-5.30	119.59	124.45
23	C	512	CLA	CMD-C2D-C1D	5.29	134.04	124.71
23	b	604	CLA	CHD-C4C-C3C	-5.29	117.06	124.84
23	a	405[A]	CLA	CHD-C1D-ND	-5.29	119.59	124.45
23	C	509	CLA	CMD-C2D-C1D	5.29	134.03	124.71
25	d	403	BCR	C7-C8-C9	-5.29	118.25	126.23
23	b	610	CLA	C1-C2-C3	-5.28	116.92	126.04
23	b	612	CLA	C3C-C4C-NC	5.27	116.48	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	511	CLA	O2D-CGD-CBD	5.27	120.63	111.27
23	C	513	CLA	CHD-C1D-ND	-5.27	119.61	124.45
23	B	609	CLA	C2C-C1C-NC	5.27	114.91	109.97
23	b	608	CLA	C2C-C1C-NC	5.26	114.90	109.97
23	B	608	CLA	O2D-CGD-CBD	5.26	120.61	111.27
23	c	512	CLA	CHD-C1D-ND	-5.26	119.62	124.45
23	C	513	CLA	O2D-CGD-CBD	5.25	120.60	111.27
23	c	507	CLA	CHD-C4C-C3C	-5.25	117.12	124.84
26	A	410[A]	SQD	C1-C2-C3	-5.25	99.07	110.00
23	B	604	CLA	O2D-CGD-CBD	5.25	120.59	111.27
23	b	613	CLA	CMD-C2D-C1D	5.25	133.96	124.71
23	C	507	CLA	C4A-NA-C1A	-5.24	104.35	106.71
23	c	509	CLA	CMD-C2D-C1D	5.24	133.95	124.71
23	c	513	CLA	O2D-CGD-CBD	5.24	120.57	111.27
23	b	614	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
23	B	607	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
23	C	505	CLA	O2D-CGD-CBD	5.23	120.57	111.27
23	B	605	CLA	C3D-C2D-C1D	-5.23	98.69	105.83
23	B	612	CLA	CHD-C1D-ND	-5.23	119.65	124.45
23	B	613	CLA	C3D-C2D-C1D	-5.23	98.70	105.83
23	c	510	CLA	CHD-C4C-C3C	-5.23	117.16	124.84
23	b	616	CLA	C3D-C2D-C1D	-5.22	98.70	105.83
35	B	622	HTG	C1'-S1-C1	5.22	109.85	100.09
23	b	605	CLA	C4A-NA-C1A	-5.21	104.36	106.71
26	a	411[A]	SQD	O47-C7-C8	5.21	122.73	111.50
23	a	409	CLA	O2D-CGD-CBD	5.21	120.53	111.27
23	C	506	CLA	O2D-CGD-CBD	5.20	120.51	111.27
23	C	508	CLA	C2C-C1C-NC	5.20	114.85	109.97
23	B	605	CLA	O2D-CGD-CBD	5.20	120.51	111.27
23	b	610	CLA	C2C-C1C-NC	5.20	114.84	109.97
23	A	405[A]	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
23	a	406[A]	CLA	CMD-C2D-C1D	5.19	133.85	124.71
23	b	601	CLA	C2C-C1C-NC	5.18	114.83	109.97
23	c	505	CLA	C4A-NA-C1A	-5.17	104.38	106.71
23	b	615	CLA	CHD-C1D-ND	-5.17	119.70	124.45
23	B	616	CLA	C3D-C2D-C1D	-5.17	98.78	105.83
23	c	511	CLA	C2C-C1C-NC	5.16	114.81	109.97
23	c	510	CLA	CHD-C1D-ND	-5.15	119.72	124.45
23	b	606	CLA	O2D-CGD-CBD	5.14	120.40	111.27
23	C	511	CLA	C3D-C2D-C1D	-5.14	98.82	105.83
23	B	608	CLA	C4A-NA-C1A	-5.13	104.40	106.71
23	D	702[A]	CLA	C3D-C2D-C1D	-5.12	98.84	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	604	CLA	C1-C2-C3	-5.12	117.19	126.04
23	A	406[A]	CLA	CMD-C2D-C1D	5.12	133.74	124.71
34	B	621	LMG	O7-C10-C11	5.12	122.53	111.50
23	B	611	CLA	CMB-C2B-C1B	5.12	136.33	128.46
23	B	612	CLA	C3C-C4C-NC	5.11	116.31	110.57
23	A	406[B]	CLA	C2C-C1C-NC	5.11	114.76	109.97
23	d	402	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
23	B	613	CLA	C2C-C1C-NC	5.11	114.76	109.97
23	B	613	CLA	CHD-C1D-ND	-5.10	119.77	124.45
23	C	505	CLA	C3D-C2D-C1D	-5.09	98.88	105.83
23	c	505	CLA	C3D-C2D-C1D	-5.09	98.88	105.83
23	b	605	CLA	C2C-C1C-NC	5.09	114.74	109.97
23	b	613	CLA	C3C-C4C-NC	5.08	116.27	110.57
23	c	509	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
23	B	604	CLA	C4A-NA-C1A	-5.08	104.42	106.71
23	C	512	CLA	CHD-C1D-ND	-5.07	119.80	124.45
23	c	502	CLA	C2C-C1C-NC	5.06	114.72	109.97
23	B	613	CLA	CMD-C2D-C1D	5.06	133.63	124.71
23	B	608	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
23	b	608	CLA	CHD-C1D-ND	-5.05	119.81	124.45
25	H	101	BCR	C38-C26-C25	-5.05	118.86	124.53
23	d	402	CLA	C4A-NA-C1A	-5.04	104.44	106.71
23	a	407[B]	CLA	CMD-C2D-C1D	5.04	133.60	124.71
23	B	610	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
23	a	409	CLA	C2C-C1C-NC	5.04	114.69	109.97
23	c	506	CLA	C3C-C4C-NC	5.03	116.21	110.57
23	B	616	CLA	CMD-C2D-C1D	5.02	133.55	124.71
23	C	508	CLA	C3C-C4C-NC	5.00	116.18	110.57
23	B	610	CLA	C2C-C1C-NC	5.00	114.66	109.97
23	c	504	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
23	b	611	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
26	B	620	SQD	O47-C7-C8	5.00	122.27	111.50
23	b	604	CLA	CHD-C1D-ND	-4.99	119.86	124.45
23	B	605	CLA	C3C-C4C-NC	4.99	116.17	110.57
23	C	502	CLA	C2C-C1C-NC	4.99	114.65	109.97
23	B	601	CLA	C4A-NA-C1A	-4.99	104.46	106.71
23	a	409	CLA	CMD-C2D-C1D	4.99	133.50	124.71
23	B	604	CLA	C1-C2-C3	-4.98	117.42	126.04
23	B	605	CLA	CHD-C1D-ND	-4.98	119.88	124.45
23	B	610	CLA	C4A-NA-C1A	-4.98	104.47	106.71
23	B	615	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
23	C	514	CLA	O2D-CGD-CBD	4.98	120.11	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	507	CLA	C4A-NA-C1A	-4.97	104.47	106.71
23	b	612	CLA	O2D-CGD-CBD	4.97	120.11	111.27
23	a	409	CLA	CHD-C1D-ND	-4.97	119.89	124.45
23	C	507	CLA	CHD-C4C-C3C	-4.97	117.54	124.84
23	a	406[B]	CLA	O2D-CGD-CBD	4.96	120.09	111.27
23	c	512	CLA	O2D-CGD-CBD	4.96	120.08	111.27
23	A	405[B]	CLA	C3D-C2D-C1D	-4.96	99.07	105.83
23	c	502	CLA	C3D-C2D-C1D	-4.96	99.07	105.83
23	a	409	CLA	C3C-C4C-NC	4.96	116.13	110.57
23	B	616	CLA	CHD-C1D-ND	-4.95	119.91	124.45
23	c	504	CLA	C2C-C1C-NC	4.95	114.61	109.97
23	c	510	CLA	O2D-CGD-CBD	4.94	120.05	111.27
23	C	506	CLA	C4A-NA-C1A	-4.94	104.48	106.71
23	B	616	CLA	O2D-CGD-O1D	-4.94	114.18	123.84
23	B	603	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
23	C	504	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
23	a	407[A]	CLA	C2C-C1C-NC	4.94	114.60	109.97
23	a	409	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
23	b	608	CLA	C4A-NA-C1A	-4.94	104.49	106.71
23	b	608	CLA	CMD-C2D-C1D	4.93	133.41	124.71
23	c	502	CLA	O2D-CGD-CBD	4.93	120.02	111.27
23	c	505	CLA	C2C-C1C-NC	4.93	114.59	109.97
23	B	607	CLA	O2D-CGD-CBD	4.92	120.02	111.27
23	c	514	CLA	C2C-C1C-NC	4.91	114.58	109.97
23	a	407[A]	CLA	C3D-C2D-C1D	-4.91	99.12	105.83
23	a	406[B]	CLA	C3D-C2D-C1D	-4.91	99.14	105.83
23	b	607	CLA	C3C-C4C-NC	4.90	116.07	110.57
23	c	509	CLA	C4A-NA-C1A	-4.90	104.50	106.71
23	C	513	CLA	C3C-C4C-NC	4.89	116.06	110.57
23	a	406[A]	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
26	f	102	SQD	O47-C7-C8	4.89	122.03	111.50
23	c	509	CLA	CHD-C1D-ND	-4.89	119.96	124.45
23	b	616	CLA	CHD-C1D-ND	-4.88	119.97	124.45
23	C	506	CLA	C3C-C4C-NC	4.88	116.04	110.57
35	C	522	HTG	C1'-S1-C1	4.88	109.21	100.09
23	c	509	CLA	O2D-CGD-CBD	4.87	119.93	111.27
23	B	611	CLA	C3C-C4C-NC	4.87	116.03	110.57
23	D	702[B]	CLA	C1-C2-C3	-4.87	117.62	126.04
23	b	609	CLA	C2C-C1C-NC	4.86	114.53	109.97
23	b	613	CLA	C1-C2-C3	-4.86	117.64	126.04
26	A	410[B]	SQD	C1-O5-C5	-4.85	104.17	113.69
23	A	405[A]	CLA	C4A-NA-C1A	-4.85	104.53	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	404[A]	CLA	CHD-C4C-C3C	-4.84	117.73	124.84
23	B	613	CLA	C1-C2-C3	-4.84	117.67	126.04
23	B	607	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
23	b	605	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
26	a	411[B]	SQD	O6-C1-C2	4.84	115.85	108.30
23	b	606	CLA	C2C-C1C-NC	4.83	114.50	109.97
23	b	606	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
25	t	102	BCR	C33-C5-C6	-4.82	119.12	124.53
23	B	613	CLA	C3C-C4C-NC	4.82	115.98	110.57
23	C	507	CLA	O2D-CGD-CBD	4.82	119.83	111.27
23	C	505	CLA	C4A-NA-C1A	-4.81	104.54	106.71
23	B	616	CLA	C2C-C1C-NC	4.81	114.48	109.97
23	B	602	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
23	b	615	CLA	C3D-C2D-C1D	-4.80	99.27	105.83
23	A	405[B]	CLA	C1C-C2C-C3C	-4.80	101.91	106.96
23	C	511	CLA	C1-C2-C3	-4.80	117.74	126.04
23	b	608	CLA	O2D-CGD-CBD	4.79	119.78	111.27
23	a	407[B]	CLA	C2C-C1C-NC	4.78	114.45	109.97
23	C	513	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
23	C	503	CLA	C4A-NA-C1A	-4.77	104.56	106.71
26	X	101	SQD	C1-O5-C5	-4.77	104.33	113.69
23	B	607	CLA	C1C-C2C-C3C	-4.77	101.94	106.96
23	a	409	CLA	C4A-NA-C1A	-4.76	104.56	106.71
23	C	506	CLA	CHD-C1D-ND	-4.76	120.08	124.45
23	A	405[B]	CLA	C4A-NA-C1A	-4.76	104.57	106.71
25	y	101	BCR	C33-C5-C6	-4.76	119.19	124.53
23	A	406[B]	CLA	O2D-CGD-CBD	4.76	119.72	111.27
23	c	512	CLA	C3D-C2D-C1D	-4.75	99.34	105.83
23	a	405[B]	CLA	C4A-NA-C1A	-4.75	104.57	106.71
23	b	609	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
23	A	406[B]	CLA	C3D-C4D-ND	4.75	117.92	110.24
23	A	406[A]	CLA	O2D-CGD-CBD	4.74	119.69	111.27
23	b	604	CLA	C1C-C2C-C3C	-4.74	101.98	106.96
23	B	611	CLA	CMC-C2C-C1C	4.74	132.25	125.04
23	B	612	CLA	C2C-C1C-NC	4.74	114.41	109.97
23	b	606	CLA	C3C-C4C-NC	4.73	115.88	110.57
23	C	510	CLA	C4A-NA-C1A	-4.73	104.58	106.71
23	D	703	CLA	C2C-C1C-NC	4.73	114.41	109.97
23	a	407[B]	CLA	O2D-CGD-CBD	4.73	119.67	111.27
23	B	609	CLA	C3C-C4C-NC	4.73	115.87	110.57
23	C	509	CLA	C3C-C4C-NC	4.73	115.87	110.57
23	d	401[B]	CLA	C1C-C2C-C3C	-4.73	101.99	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	605	CLA	C3D-C4D-ND	4.72	117.88	110.24
23	b	602	CLA	C3D-C4D-ND	4.72	117.87	110.24
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	b	603	CLA	C3D-C4D-ND	4.71	117.85	110.24
23	b	613	CLA	CHD-C1D-ND	-4.71	120.13	124.45
23	B	606	CLA	C2C-C1C-NC	4.70	114.38	109.97
23	b	610	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
23	C	514	CLA	C4A-NA-C1A	-4.70	104.59	106.71
23	a	405[B]	CLA	C1C-C2C-C3C	-4.69	102.02	106.96
23	b	610	CLA	C3C-C4C-NC	4.69	115.83	110.57
25	d	403	BCR	C15-C14-C13	-4.69	120.62	127.31
23	C	508	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
23	a	407[A]	CLA	C3D-C4D-ND	4.68	117.81	110.24
23	b	613	CLA	C1C-C2C-C3C	-4.68	102.03	106.96
23	b	603	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
23	b	614	CLA	C3C-C4C-NC	4.68	115.82	110.57
23	d	401[B]	CLA	C4A-NA-C1A	-4.68	104.60	106.71
23	C	509	CLA	C1-C2-C3	-4.67	117.96	126.04
23	a	407[B]	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
23	C	509	CLA	O2D-CGD-CBD	4.67	119.57	111.27
24	A	417[B]	PHO	C1-C2-C3	-4.67	117.97	126.04
23	C	507	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
23	d	401[A]	CLA	C3C-C4C-NC	4.67	115.80	110.57
23	b	607	CLA	C4A-NA-C1A	-4.66	104.61	106.71
23	B	609	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
23	c	514	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
23	C	512	CLA	C4A-NA-C1A	-4.65	104.62	106.71
23	c	514	CLA	O2D-CGD-CBD	4.65	119.53	111.27
23	B	611	CLA	C3D-C4D-ND	4.65	117.76	110.24
23	a	407[B]	CLA	C3D-C4D-ND	4.64	117.75	110.24
23	C	514	CLA	C3D-C2D-C1D	-4.64	99.49	105.83
23	D	702[B]	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
23	B	601	CLA	C2C-C1C-NC	4.64	114.32	109.97
23	d	401[B]	CLA	O2D-CGD-CBD	4.64	119.51	111.27
23	A	406[B]	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
23	C	507	CLA	C1C-C2C-C3C	-4.63	102.08	106.96
23	C	509	CLA	C3D-C2D-C1D	-4.63	99.52	105.83
23	A	406[A]	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
23	B	601	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
38	F	102	HEM	CHC-C4B-NB	4.62	129.45	124.43
26	X	101	SQD	O8-S-C6	4.62	113.09	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	507	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
23	b	610	CLA	C4A-NA-C1A	-4.61	104.63	106.71
23	a	405[B]	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
29	a	414[A]	PL9	C7-C8-C9	-4.60	119.13	126.79
23	C	505	CLA	C1C-C2C-C3C	-4.60	102.12	106.96
23	B	612	CLA	C3D-C4D-ND	4.59	117.67	110.24
23	c	504	CLA	C3C-C4C-NC	4.59	115.72	110.57
23	C	505	CLA	C3C-C4C-NC	4.58	115.71	110.57
23	a	405[A]	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
23	a	407[A]	CLA	O2D-CGD-CBD	4.58	119.40	111.27
23	b	601	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
23	C	504	CLA	C3D-C4D-ND	4.57	117.63	110.24
23	A	408	CLA	C3C-C4C-NC	4.57	115.69	110.57
23	c	508	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
23	b	603	CLA	C3C-C4C-NC	4.57	115.69	110.57
23	D	702[A]	CLA	O2D-CGD-CBD	4.55	119.36	111.27
23	A	406[A]	CLA	C3D-C4D-ND	4.55	117.61	110.24
23	b	616	CLA	C3C-C4C-NC	4.55	115.68	110.57
23	b	608	CLA	C3D-C4D-ND	4.55	117.59	110.24
23	A	405[A]	CLA	CMD-C2D-C1D	4.55	132.73	124.71
23	B	608	CLA	C3C-C4C-NC	4.54	115.67	110.57
26	a	411[B]	SQD	O47-C7-C8	4.54	121.28	111.50
23	b	609	CLA	C3C-C4C-NC	4.53	115.66	110.57
24	A	417[A]	PHO	C1-C2-C3	-4.53	118.22	126.04
23	c	513	CLA	C3D-C2D-C1D	-4.53	99.66	105.83
23	C	510	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
23	b	606	CLA	C4-C3-C5	4.52	122.88	115.27
23	c	506	CLA	C3D-C4D-ND	4.52	117.55	110.24
23	B	602	CLA	C3C-C4C-NC	4.52	115.64	110.57
23	C	512	CLA	C3D-C2D-C1D	-4.52	99.67	105.83
23	c	504	CLA	O2D-CGD-CBD	4.52	119.30	111.27
29	a	414[B]	PL9	C7-C8-C9	-4.51	119.28	126.79
23	b	609	CLA	O2D-CGD-CBD	4.51	119.28	111.27
23	B	603	CLA	C3C-C4C-NC	4.50	115.62	110.57
23	a	409	CLA	C3D-C4D-ND	4.49	117.51	110.24
23	c	505	CLA	C1-O2A-CGA	4.49	128.22	116.44
23	a	406[A]	CLA	C1C-C2C-C3C	-4.49	102.24	106.96
23	b	610	CLA	C3D-C4D-ND	4.49	117.49	110.24
26	A	410[B]	SQD	C1-C2-C3	-4.48	100.67	110.00
23	C	502	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
23	c	511	CLA	C1-C2-C3	-4.47	118.31	126.04
23	C	514	CLA	C3C-C4C-NC	4.47	115.58	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	f	101	HEM	CHC-C4B-NB	4.47	129.28	124.43
23	D	702[B]	CLA	C3C-C4C-NC	4.46	115.58	110.57
23	c	510	CLA	C4A-NA-C1A	-4.46	104.70	106.71
23	C	510	CLA	C3D-C4D-ND	4.46	117.44	110.24
23	C	513	CLA	C2C-C1C-NC	4.45	114.14	109.97
23	d	401[A]	CLA	C1C-C2C-C3C	-4.45	102.28	106.96
23	A	404[B]	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
23	c	511	CLA	O2D-CGD-CBD	4.44	119.15	111.27
23	d	401[A]	CLA	C3D-C4D-ND	4.44	117.42	110.24
23	b	612	CLA	CMD-C2D-C1D	4.44	132.53	124.71
23	a	405[B]	CLA	C3D-C4D-ND	4.44	117.41	110.24
38	F	102	HEM	CBA-CAA-C2A	-4.44	105.05	112.62
23	c	513	CLA	C2C-C1C-NC	4.43	114.12	109.97
32	t	101	LMT	C3'-C4'-C5'	-4.43	100.78	110.93
23	C	512	CLA	C3C-C4C-NC	4.43	115.53	110.57
23	b	616	CLA	C1D-CHD-C4C	-4.42	116.51	126.06
29	A	414[B]	PL9	C7-C8-C9	-4.42	119.43	126.79
23	c	514	CLA	C3D-C4D-ND	4.42	117.38	110.24
23	b	614	CLA	C4A-NA-C1A	-4.41	104.72	106.71
34	c	521	LMG	O6-C5-C4	4.40	117.69	109.69
23	c	511	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
23	B	610	CLA	O2A-CGA-CBA	4.40	125.70	111.91
23	c	507	CLA	C3D-C4D-ND	4.40	117.35	110.24
34	d	410	LMG	O7-C10-C11	4.39	120.97	111.50
23	b	605	CLA	O2D-CGD-O1D	-4.39	115.25	123.84
23	B	606	CLA	C3C-C4C-NC	4.39	115.50	110.57
23	a	406[A]	CLA	O2D-CGD-CBD	4.39	119.07	111.27
23	B	609	CLA	C3D-C4D-ND	4.39	117.34	110.24
23	A	408	CLA	C4A-NA-C1A	-4.39	104.73	106.71
29	a	414[A]	PL9	C7-C3-C4	4.38	120.44	116.88
23	D	703	CLA	C3D-C4D-ND	4.38	117.32	110.24
23	d	401[B]	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
23	B	615	CLA	C3C-C4C-NC	4.38	115.48	110.57
23	C	514	CLA	C3D-C4D-ND	4.38	117.32	110.24
23	D	702[B]	CLA	C3D-C4D-ND	4.38	117.32	110.24
23	C	511	CLA	C4A-NA-C1A	-4.38	104.74	106.71
23	b	604	CLA	C4A-NA-C1A	-4.37	104.74	106.71
23	C	510	CLA	O2D-CGD-CBD	4.37	119.03	111.27
23	c	502	CLA	C3D-C4D-ND	4.36	117.30	110.24
23	B	615	CLA	C3D-C4D-ND	4.36	117.30	110.24
23	C	502	CLA	O2D-CGD-O1D	-4.36	115.31	123.84
23	C	504	CLA	O2D-CGD-CBD	4.36	119.02	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	603	CLA	C1D-CHD-C4C	-4.36	116.65	126.06
23	A	404[B]	CLA	C1D-CHD-C4C	-4.36	116.66	126.06
33	E	101[B]	LHG	O7-C7-C8	4.35	120.88	111.50
23	c	510	CLA	C3D-C2D-C1D	-4.34	99.90	105.83
23	c	512	CLA	C1D-CHD-C4C	-4.34	116.69	126.06
23	A	405[B]	CLA	C3D-C4D-ND	4.34	117.26	110.24
23	C	509	CLA	CHD-C1D-ND	-4.34	120.47	124.45
23	C	510	CLA	C1-C2-C3	-4.34	118.54	126.04
23	c	510	CLA	C3B-C4B-NB	4.34	114.82	109.21
23	B	601	CLA	C3D-C4D-ND	4.34	117.25	110.24
34	C	501	LMG	O7-C10-C11	4.33	120.84	111.50
33	E	101[A]	LHG	O7-C7-C8	4.32	120.82	111.50
23	B	610	CLA	CAA-C2A-C3A	-4.32	100.94	112.78
23	A	404[A]	CLA	C1C-C2C-C3C	-4.32	102.41	106.96
23	c	508	CLA	CMC-C2C-C1C	4.32	131.62	125.04
23	D	702[A]	CLA	C3C-C4C-NC	4.31	115.41	110.57
23	b	615	CLA	C3C-C4C-NC	4.31	115.41	110.57
23	d	402	CLA	C2C-C1C-NC	4.31	114.01	109.97
23	C	503	CLA	O2D-CGD-CBD	4.31	118.93	111.27
23	C	502	CLA	C3D-C4D-ND	4.30	117.20	110.24
23	B	607	CLA	C3C-C4C-NC	4.30	115.40	110.57
23	c	503	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
23	C	504	CLA	C2C-C1C-NC	4.30	114.00	109.97
23	C	503	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
23	c	503	CLA	C3D-C4D-ND	4.30	117.19	110.24
38	F	102	HEM	C1B-NB-C4B	4.30	109.51	105.07
23	B	610	CLA	C3D-C4D-ND	4.30	117.19	110.24
29	A	414[A]	PL9	C32-C33-C34	-4.30	117.31	127.66
23	b	607	CLA	C3D-C4D-ND	4.30	117.19	110.24
23	b	614	CLA	C3D-C4D-ND	4.30	117.19	110.24
23	d	402	CLA	C3D-C4D-ND	4.30	117.19	110.24
23	a	406[B]	CLA	C4A-NA-C1A	-4.30	104.78	106.71
23	b	611	CLA	C3D-C4D-ND	4.29	117.18	110.24
23	a	406[B]	CLA	C1C-C2C-C3C	-4.29	102.44	106.96
23	b	612	CLA	C4A-NA-C1A	-4.29	104.78	106.71
29	D	705[B]	PL9	C42-C43-C44	-4.29	117.34	127.66
23	a	405[A]	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
23	b	609	CLA	C3D-C4D-ND	4.28	117.16	110.24
23	b	616	CLA	O2D-CGD-O1D	-4.28	115.47	123.84
23	D	702[B]	CLA	C1C-C2C-C3C	-4.28	102.46	106.96
23	c	508	CLA	C1C-C2C-C3C	-4.28	102.46	106.96
23	D	702[B]	CLA	O2D-CGD-CBD	4.28	118.87	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	504	CLA	C3D-C4D-ND	4.28	117.15	110.24
29	A	414[B]	PL9	C32-C33-C34	-4.27	117.37	127.66
23	c	502	CLA	C4A-NA-C1A	-4.27	104.78	106.71
23	C	509	CLA	C3B-C4B-NB	4.27	114.73	109.21
34	C	501	LMG	O1-C1-C2	4.27	114.97	108.30
23	B	611	CLA	C1D-CHD-C4C	-4.27	116.85	126.06
23	B	605	CLA	C1D-CHD-C4C	-4.27	116.86	126.06
23	b	604	CLA	C3B-C4B-NB	4.26	114.72	109.21
23	a	406[B]	CLA	C1D-CHD-C4C	-4.26	116.87	126.06
23	c	509	CLA	C3C-C4C-NC	4.26	115.35	110.57
23	A	404[B]	CLA	CAA-C2A-C3A	-4.25	101.13	112.78
23	a	407[A]	CLA	C3C-C4C-NC	4.25	115.34	110.57
23	b	602	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
23	b	613	CLA	O2D-CGD-CBD	4.24	118.81	111.27
26	f	102	SQD	C1-O5-C5	4.24	122.01	113.69
34	c	501	LMG	O7-C10-C11	4.24	120.64	111.50
23	B	613	CLA	C4A-NA-C1A	-4.24	104.80	106.71
23	b	605	CLA	C3C-C4C-NC	4.24	115.32	110.57
23	b	604	CLA	C3D-C2D-C1D	-4.24	100.05	105.83
23	b	604	CLA	C3C-C4C-NC	4.23	115.32	110.57
23	D	703	CLA	C3D-C2D-C1D	-4.23	100.06	105.83
34	C	521	LMG	O6-C5-C4	4.23	117.37	109.69
23	b	615	CLA	C1D-CHD-C4C	-4.22	116.95	126.06
40	v	201	HEC	CBD-CAD-C3D	-4.22	105.42	112.62
23	C	507	CLA	C3D-C4D-ND	4.22	117.06	110.24
23	a	405[A]	CLA	C3D-C4D-ND	4.22	117.06	110.24
23	a	406[B]	CLA	C3D-C4D-ND	4.22	117.06	110.24
23	c	507	CLA	O2D-CGD-CBD	4.21	118.75	111.27
25	b	617	BCR	C7-C8-C9	-4.21	119.88	126.23
23	a	405[A]	CLA	C1D-CHD-C4C	-4.21	116.98	126.06
23	b	601	CLA	C3D-C4D-ND	4.20	117.04	110.24
23	c	504	CLA	C1D-CHD-C4C	-4.20	116.99	126.06
23	c	509	CLA	C1C-C2C-C3C	-4.20	102.54	106.96
23	A	406[B]	CLA	C1C-C2C-C3C	-4.20	102.54	106.96
23	A	404[B]	CLA	C3C-C4C-NC	4.20	115.28	110.57
23	B	614	CLA	C3D-C4D-ND	4.20	117.03	110.24
23	C	510	CLA	C3C-C4C-NC	4.19	115.27	110.57
26	a	411[A]	SQD	C1-C2-C3	-4.19	101.27	110.00
23	A	408	CLA	C3D-C4D-ND	4.19	117.01	110.24
23	b	606	CLA	C3D-C4D-ND	4.18	117.00	110.24
23	c	502	CLA	O2D-CGD-O1D	-4.18	115.66	123.84
23	c	503	CLA	CHD-C1D-ND	-4.18	120.61	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	506	CLA	C3D-C2D-C1D	-4.18	100.13	105.83
23	C	511	CLA	C3D-C4D-ND	4.18	117.00	110.24
25	T	102	BCR	C15-C16-C17	-4.18	114.92	123.47
23	a	405[A]	CLA	CAA-C2A-C3A	-4.18	101.34	112.78
23	c	503	CLA	CMD-C2D-C1D	4.17	132.07	124.71
23	b	608	CLA	C1C-C2C-C3C	-4.17	102.57	106.96
23	B	608	CLA	C3D-C4D-ND	4.17	116.98	110.24
35	b	622	HTG	C1-O5-C5	4.17	120.26	112.58
23	c	513	CLA	C3D-C4D-ND	4.16	116.97	110.24
23	A	404[B]	CLA	C3D-C4D-ND	4.16	116.96	110.24
23	A	406[A]	CLA	C1C-C2C-C3C	-4.16	102.59	106.96
23	D	703	CLA	C3C-C4C-NC	4.16	115.23	110.57
23	b	608	CLA	CMC-C2C-C1C	4.16	131.37	125.04
23	B	611	CLA	CMB-C2B-C3B	4.15	132.45	124.68
23	c	511	CLA	C1C-C2C-C3C	-4.15	102.60	106.96
23	B	602	CLA	C3D-C4D-ND	4.14	116.94	110.24
23	D	702[A]	CLA	C1C-C2C-C3C	-4.14	102.60	106.96
23	C	503	CLA	C3C-C4C-NC	4.14	115.21	110.57
23	c	512	CLA	C3D-C4D-ND	4.14	116.93	110.24
23	b	615	CLA	C3D-C4D-ND	4.14	116.93	110.24
23	B	611	CLA	CHD-C4C-NC	4.13	130.72	124.20
23	b	609	CLA	C1-C2-C3	-4.13	118.90	126.04
25	d	403	BCR	C29-C30-C25	4.13	116.84	110.48
23	B	601	CLA	C3C-C4C-NC	4.13	115.20	110.57
23	d	402	CLA	C3C-C4C-NC	4.13	115.20	110.57
26	b	620	SQD	C1-O5-C5	-4.13	105.59	113.69
23	C	506	CLA	C3D-C4D-ND	4.12	116.91	110.24
23	b	602	CLA	C3C-C4C-NC	4.12	115.19	110.57
23	A	408	CLA	O2D-CGD-CBD	4.12	118.59	111.27
23	a	406[A]	CLA	C3D-C4D-ND	4.12	116.90	110.24
23	d	401[B]	CLA	C3D-C4D-ND	4.12	116.90	110.24
23	B	609	CLA	O2D-CGD-CBD	4.12	118.59	111.27
24	A	407[B]	PHO	C1A-C2A-C3A	-4.12	98.92	102.84
29	A	414[A]	PL9	C7-C3-C2	-4.12	117.89	123.30
23	d	401[A]	CLA	O2D-CGD-CBD	4.11	118.58	111.27
23	d	401[A]	CLA	C3D-C2D-C1D	-4.11	100.22	105.83
34	c	521	LMG	O7-C10-C11	4.11	120.36	111.50
23	B	614	CLA	C4A-NA-C1A	-4.11	104.86	106.71
23	B	608	CLA	O2D-CGD-O1D	-4.11	115.80	123.84
23	c	510	CLA	C3D-C4D-ND	4.11	116.88	110.24
23	A	404[A]	CLA	C3B-C4B-NB	4.11	114.52	109.21
23	B	607	CLA	O2D-CGD-O1D	-4.11	115.81	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	409	CLA	C1D-CHD-C4C	-4.10	117.20	126.06
23	B	604	CLA	C3D-C2D-C1D	-4.10	100.23	105.83
23	C	509	CLA	C1C-C2C-C3C	-4.10	102.64	106.96
23	C	503	CLA	C3D-C4D-ND	4.10	116.87	110.24
23	c	503	CLA	C1D-CHD-C4C	-4.10	117.22	126.06
23	A	405[A]	CLA	C3D-C4D-ND	4.10	116.87	110.24
23	B	602	CLA	C1C-C2C-C3C	-4.10	102.65	106.96
34	Z	101	LMG	O7-C10-C11	4.09	120.33	111.50
23	b	612	CLA	C3D-C4D-ND	4.09	116.86	110.24
23	b	612	CLA	CHD-C1D-ND	-4.09	120.69	124.45
23	B	607	CLA	C3D-C4D-ND	4.09	116.85	110.24
23	B	602	CLA	CMC-C2C-C1C	4.09	131.26	125.04
23	B	605	CLA	C3D-C4D-ND	4.09	116.85	110.24
23	d	401[B]	CLA	C3C-C4C-NC	4.08	115.15	110.57
23	c	514	CLA	C1D-CHD-C4C	-4.08	117.25	126.06
23	b	616	CLA	C2C-C1C-NC	4.08	113.80	109.97
23	a	405[B]	CLA	C1D-CHD-C4C	-4.08	117.25	126.06
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
36	C	517[A]	DGD	O2G-C1B-C2B	4.08	120.29	111.50
23	B	606	CLA	C1D-CHD-C4C	-4.08	117.26	126.06
23	c	505	CLA	C3D-C4D-ND	4.08	116.83	110.24
23	b	610	CLA	O2A-CGA-CBA	4.08	124.70	111.91
23	C	513	CLA	C1D-CHD-C4C	-4.07	117.27	126.06
26	a	411[A]	SQD	C1-O5-C5	-4.07	105.69	113.69
23	a	405[B]	CLA	CAA-C2A-C3A	-4.07	101.62	112.78
23	b	608	CLA	C3D-C2D-C1D	-4.07	100.27	105.83
23	C	502	CLA	C1D-CHD-C4C	-4.07	117.27	126.06
34	C	521	LMG	O7-C10-C11	4.07	120.28	111.50
23	b	607	CLA	O2D-CGD-CBD	4.07	118.50	111.27
35	B	624	HTG	C1'-S1-C1	4.07	107.70	100.09
23	D	702[A]	CLA	C3D-C4D-ND	4.07	116.82	110.24
23	c	514	CLA	C3C-C4C-NC	4.07	115.13	110.57
29	a	414[B]	PL9	C32-C33-C34	-4.07	117.87	127.66
23	c	503	CLA	O2D-CGD-O1D	-4.06	115.89	123.84
26	A	410[B]	SQD	C44-O6-C1	-4.06	105.80	113.74
23	b	616	CLA	O2A-CGA-CBA	4.06	124.66	111.91
23	A	406[A]	CLA	C3C-C4C-NC	4.06	115.13	110.57
23	C	510	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
23	a	406[A]	CLA	C3C-C4C-NC	4.06	115.12	110.57
34	C	520	LMG	O7-C10-C11	4.05	120.24	111.50
23	b	611	CLA	C3C-C4C-NC	4.05	115.11	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	404[B]	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
23	B	615	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
23	B	613	CLA	O2D-CGD-CBD	4.05	118.46	111.27
23	a	406[B]	CLA	CAA-C2A-C3A	-4.04	101.71	112.78
23	c	505	CLA	C3C-C4C-NC	4.04	115.10	110.57
23	a	405[B]	CLA	C3B-C4B-NB	4.04	114.43	109.21
35	b	625	HTG	C1-O5-C5	4.03	120.01	112.58
34	m	101	LMG	O7-C10-C11	4.03	120.19	111.50
25	c	515	BCR	C11-C10-C9	-4.03	121.56	127.31
23	C	513	CLA	C3D-C4D-ND	4.03	116.75	110.24
23	b	603	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
23	B	616	CLA	C3D-C4D-ND	4.02	116.74	110.24
23	A	408	CLA	C1-C2-C3	-4.02	119.09	126.04
23	C	503	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
23	c	507	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
23	b	611	CLA	C3B-C4B-NB	4.02	114.40	109.21
23	b	603	CLA	CAA-C2A-C3A	-4.01	101.79	112.78
23	B	613	CLA	C3B-C4B-NB	4.01	114.40	109.21
23	a	406[A]	CLA	C1D-CHD-C4C	-4.01	117.41	126.06
23	A	405[B]	CLA	O2D-CGD-CBD	4.00	118.38	111.27
23	B	603	CLA	C3D-C4D-ND	4.00	116.71	110.24
40	v	201	HEC	CMC-C2C-C1C	-4.00	122.31	128.46
23	B	612	CLA	C3D-C2D-C1D	-4.00	100.37	105.83
23	b	609	CLA	C1D-CHD-C4C	-4.00	117.44	126.06
23	a	405[B]	CLA	O2D-CGD-CBD	3.99	118.36	111.27
23	b	612	CLA	C1D-CHD-C4C	-3.99	117.44	126.06
23	b	603	CLA	O2D-CGD-O1D	-3.99	116.04	123.84
23	C	505	CLA	C3D-C4D-ND	3.99	116.69	110.24
23	C	512	CLA	C1D-CHD-C4C	-3.99	117.45	126.06
23	b	601	CLA	C1D-CHD-C4C	-3.99	117.45	126.06
23	C	504	CLA	C3C-C4C-NC	3.98	115.03	110.57
23	C	512	CLA	C3D-C4D-ND	3.98	116.67	110.24
23	B	616	CLA	CMB-C2B-C3B	3.98	132.12	124.68
23	B	615	CLA	C1D-CHD-C4C	-3.98	117.48	126.06
23	c	508	CLA	C3C-C4C-NC	3.97	115.02	110.57
23	c	508	CLA	C3D-C4D-ND	3.97	116.66	110.24
23	c	503	CLA	C4A-NA-C1A	-3.96	104.92	106.71
23	C	506	CLA	C1D-CHD-C4C	-3.96	117.51	126.06
23	B	610	CLA	C3C-C4C-NC	3.96	115.01	110.57
23	c	511	CLA	C3D-C4D-ND	3.96	116.64	110.24
23	B	603	CLA	C1D-CHD-C4C	-3.95	117.53	126.06
23	a	405[A]	CLA	C3C-C4C-NC	3.95	115.00	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	405[A]	CLA	C3B-C4B-NB	3.95	114.31	109.21
26	X	101	SQD	C44-O6-C1	-3.95	106.03	113.74
23	A	404[A]	CLA	C3C-C4C-NC	3.95	115.00	110.57
23	B	614	CLA	C1D-CHD-C4C	-3.95	117.55	126.06
23	C	502	CLA	C3C-C4C-NC	3.94	115.00	110.57
23	B	616	CLA	C4C-C3C-C2C	-3.94	101.15	106.90
23	B	612	CLA	CAC-C3C-C4C	3.94	129.93	124.81
23	C	508	CLA	O2D-CGD-O1D	-3.94	116.13	123.84
23	C	511	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
23	c	511	CLA	C3C-C4C-NC	3.94	114.99	110.57
23	b	614	CLA	O2D-CGD-O1D	-3.94	116.14	123.84
29	d	404[A]	PL9	C42-C43-C44	-3.93	118.19	127.66
25	C	515	BCR	C7-C8-C9	-3.93	120.30	126.23
23	D	702[A]	CLA	C1-C2-C3	-3.93	119.25	126.04
34	c	520	LMG	O7-C10-C11	3.93	119.97	111.50
23	a	407[A]	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
23	b	606	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
23	C	504	CLA	C1D-CHD-C4C	-3.92	117.60	126.06
23	c	512	CLA	C3C-C4C-NC	3.92	114.97	110.57
23	b	608	CLA	C3B-C4B-NB	3.92	114.27	109.21
23	C	508	CLA	C1D-CHD-C4C	-3.92	117.61	126.06
38	f	101	HEM	CAD-CBD-CGD	3.92	122.03	113.60
23	C	514	CLA	C3B-C4B-NB	3.92	114.27	109.21
23	D	703	CLA	O2D-CGD-O1D	-3.92	116.18	123.84
26	a	411[A]	SQD	C44-O6-C1	-3.91	106.09	113.74
23	b	614	CLA	C1-C2-C3	-3.91	119.28	126.04
25	B	618	BCR	C29-C30-C25	3.91	116.50	110.48
29	A	414[A]	PL9	C7-C3-C4	3.91	120.05	116.88
25	t	102	BCR	C11-C10-C9	-3.91	121.73	127.31
23	B	605	CLA	C4-C3-C5	3.91	121.84	115.27
23	b	612	CLA	C1-C2-C3	-3.91	119.29	126.04
23	b	602	CLA	CMC-C2C-C1C	3.91	130.99	125.04
26	B	620	SQD	O7-S-C6	3.90	111.58	106.94
23	C	510	CLA	C3B-C4B-NB	3.90	114.26	109.21
23	B	603	CLA	O2D-CGD-O1D	-3.90	116.21	123.84
23	c	512	CLA	C3B-C4B-NB	3.90	114.25	109.21
23	B	614	CLA	C1C-C2C-C3C	-3.90	102.86	106.96
29	a	414[A]	PL9	C32-C33-C34	-3.89	118.28	127.66
23	B	601	CLA	C1D-CHD-C4C	-3.89	117.66	126.06
23	a	407[B]	CLA	C1C-C2C-C3C	-3.89	102.86	106.96
23	C	506	CLA	C3D-C2D-C1D	-3.89	100.52	105.83
23	a	407[B]	CLA	C3C-C4C-NC	3.89	114.93	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	507	CLA	CAC-C3C-C4C	3.89	129.85	124.81
23	b	606	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
33	A	419[A]	LHG	O8-C23-O10	-3.88	113.79	123.59
36	c	517[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
25	T	102	BCR	C11-C10-C9	-3.88	121.77	127.31
25	c	515	BCR	C15-C14-C13	-3.88	121.78	127.31
23	B	614	CLA	C1-C2-C3	-3.88	119.34	126.04
29	A	414[B]	PL9	C7-C3-C4	3.87	120.02	116.88
23	a	406[A]	CLA	CAA-C2A-C3A	-3.87	102.19	112.78
24	A	407[A]	PHO	C1A-C2A-C3A	-3.87	99.16	102.84
23	c	510	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
23	B	606	CLA	C3D-C4D-ND	3.86	116.48	110.24
23	b	604	CLA	CMC-C2C-C1C	3.86	130.91	125.04
23	b	608	CLA	C1D-CHD-C4C	-3.85	117.74	126.06
23	A	405[A]	CLA	C3C-C4C-NC	3.85	114.89	110.57
23	B	613	CLA	C3D-C4D-ND	3.85	116.47	110.24
23	a	409	CLA	O2D-CGD-O1D	-3.85	116.32	123.84
23	B	604	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
23	b	614	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
32	B	627	LMT	C1'-O5'-C5'	-3.84	106.15	113.69
23	c	510	CLA	C1D-CHD-C4C	-3.84	117.78	126.06
23	b	615	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
29	a	414[A]	PL9	C7-C3-C2	-3.84	118.25	123.30
23	A	405[B]	CLA	C1D-CHD-C4C	-3.84	117.78	126.06
23	B	604	CLA	C1D-CHD-C4C	-3.83	117.79	126.06
23	A	404[B]	CLA	CMB-C2B-C3B	3.83	131.85	124.68
23	b	612	CLA	C3D-C2D-C1D	-3.83	100.60	105.83
23	C	514	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
23	C	512	CLA	O2D-CGD-O1D	-3.83	116.35	123.84
23	c	507	CLA	C3B-C4B-NB	3.83	114.16	109.21
23	c	502	CLA	C3C-C4C-NC	3.83	114.86	110.57
34	Z	101	LMG	C1-C2-C3	3.83	117.97	110.00
23	b	610	CLA	C1D-CHD-C4C	-3.83	117.80	126.06
23	D	703	CLA	C1D-CHD-C4C	-3.83	117.81	126.06
23	c	513	CLA	C1D-CHD-C4C	-3.82	117.81	126.06
23	a	406[B]	CLA	C3C-C4C-NC	3.82	114.86	110.57
23	C	507	CLA	C1-C2-C3	-3.82	119.44	126.04
23	C	509	CLA	C4A-NA-C1A	-3.81	104.99	106.71
23	b	612	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
23	c	512	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
23	B	614	CLA	C3B-C4B-NB	3.81	114.14	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	C	518[B]	DGD	O2G-C1B-C2B	3.81	119.72	111.50
23	C	508	CLA	C3D-C4D-ND	3.81	116.41	110.24
23	B	603	CLA	C3B-C4B-NB	3.81	114.14	109.21
36	C	517[B]	DGD	O2G-C1B-C2B	3.81	119.71	111.50
25	D	704	BCR	C10-C11-C12	-3.81	111.33	123.22
23	C	507	CLA	C3C-C4C-NC	3.81	114.84	110.57
23	b	614	CLA	C1D-CHD-C4C	-3.80	117.85	126.06
23	C	513	CLA	C1-C2-C3	-3.80	119.47	126.04
33	A	419[A]	LHG	O7-C7-C8	3.80	119.69	111.50
24	A	417[A]	PHO	C1A-C2A-C3A	-3.80	99.22	102.84
35	V	202	HTG	C1-O5-C5	3.80	117.34	112.19
23	b	611	CLA	O2D-CGD-O1D	-3.80	116.41	123.84
23	b	616	CLA	C3D-C4D-ND	3.80	116.38	110.24
23	C	511	CLA	C4-C3-C5	3.80	121.66	115.27
23	C	511	CLA	C1D-CHD-C4C	-3.79	117.88	126.06
23	B	612	CLA	O2D-CGD-O1D	-3.79	116.42	123.84
23	d	401[B]	CLA	C3B-C4B-NB	3.79	114.11	109.21
23	c	513	CLA	C1-C2-C3	-3.79	119.49	126.04
23	b	602	CLA	C2C-C1C-NC	3.79	113.52	109.97
23	A	408	CLA	C1D-CHD-C4C	-3.79	117.89	126.06
29	A	414[B]	PL9	C37-C38-C39	-3.79	118.54	127.66
23	C	511	CLA	C3B-C4B-NB	3.78	114.10	109.21
26	X	101	SQD	C1-C2-C3	-3.78	102.12	110.00
26	A	410[A]	SQD	C44-O6-C1	-3.78	106.36	113.74
34	c	521	LMG	C3-C4-C5	3.78	116.97	110.24
23	C	509	CLA	C3D-C4D-ND	3.78	116.35	110.24
23	c	503	CLA	C3B-C4B-NB	3.77	114.09	109.21
23	B	606	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
23	A	405[A]	CLA	CBC-CAC-C3C	-3.77	102.04	112.43
23	C	510	CLA	CAC-C3C-C4C	3.77	129.70	124.81
23	B	609	CLA	C1C-C2C-C3C	-3.77	103.00	106.96
23	b	602	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
23	A	405[B]	CLA	CBC-CAC-C3C	-3.77	102.05	112.43
23	c	512	CLA	C4A-NA-C1A	-3.76	105.01	106.71
23	B	603	CLA	CMB-C2B-C3B	3.76	131.72	124.68
23	c	509	CLA	C3D-C4D-ND	3.76	116.33	110.24
23	b	605	CLA	C1D-CHD-C4C	-3.76	117.94	126.06
23	b	601	CLA	C3C-C4C-NC	3.76	114.79	110.57
23	b	608	CLA	C3C-C4C-NC	3.76	114.79	110.57
23	B	603	CLA	CAA-C2A-C3A	-3.76	102.48	112.78
23	C	504	CLA	C4-C3-C5	3.76	121.59	115.27
24	a	416[A]	PHO	C4-C3-C5	3.76	121.59	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	409	CLA	CMC-C2C-C1C	3.76	130.76	125.04
25	D	704	BCR	C16-C17-C18	-3.75	121.95	127.31
33	L	101[B]	LHG	O7-C7-C8	3.75	119.58	111.50
25	D	704	BCR	C38-C26-C25	-3.75	120.32	124.53
23	d	401[B]	CLA	C1D-CHD-C4C	-3.75	117.97	126.06
26	A	410[A]	SQD	O47-C7-C8	3.74	119.56	111.50
23	A	408	CLA	C1C-C2C-C3C	-3.74	103.03	106.96
29	a	414[A]	PL9	C15-C14-C16	3.74	121.56	115.27
23	b	612	CLA	C4-C3-C5	3.74	121.56	115.27
26	A	412	SQD	O47-C7-C8	3.74	119.55	111.50
25	b	617	BCR	C33-C5-C6	-3.74	120.33	124.53
23	A	406[A]	CLA	C1D-CHD-C4C	-3.73	118.01	126.06
23	C	505	CLA	O2D-CGD-O1D	-3.73	116.55	123.84
23	A	408	CLA	C3B-C4B-NB	3.73	114.03	109.21
23	B	610	CLA	C3B-C4B-NB	3.72	114.02	109.21
23	A	404[A]	CLA	C3D-C4D-ND	3.72	116.25	110.24
23	A	404[B]	CLA	C3B-C4B-NB	3.72	114.02	109.21
23	C	511	CLA	C3C-C4C-NC	3.72	114.74	110.57
23	B	602	CLA	O2D-CGD-O1D	-3.71	116.58	123.84
35	o	301	HTG	O5-C1-C2	3.71	114.98	110.31
23	B	607	CLA	C3B-C4B-NB	3.71	114.01	109.21
38	f	101	HEM	C1B-NB-C4B	3.70	108.90	105.07
33	b	629[B]	LHG	O7-C7-C8	3.70	119.48	111.50
29	a	414[B]	PL9	C15-C14-C16	3.70	121.49	115.27
23	b	604	CLA	O2D-CGD-O1D	-3.70	116.61	123.84
23	b	612	CLA	C3B-C4B-NB	3.69	113.99	109.21
36	C	518[A]	DGD	O2G-C1B-C2B	3.69	119.46	111.50
23	B	611	CLA	O2D-CGD-O1D	-3.69	116.62	123.84
23	a	409	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
23	c	510	CLA	C3C-C4C-NC	3.69	114.70	110.57
23	A	404[B]	CLA	O2D-CGD-CBD	3.68	117.81	111.27
26	B	620	SQD	C3-C4-C5	3.68	116.81	110.24
33	L	101[A]	LHG	O7-C7-C8	3.68	119.43	111.50
23	C	509	CLA	O2D-CGD-O1D	-3.68	116.65	123.84
23	B	604	CLA	C3B-C4B-NB	3.67	113.96	109.21
25	C	515	BCR	C33-C5-C6	-3.67	120.40	124.53
23	B	604	CLA	C3D-C4D-ND	3.67	116.18	110.24
36	c	517[B]	DGD	O2G-C1B-C2B	3.67	119.41	111.50
29	A	414[A]	PL9	C37-C38-C39	-3.67	118.82	127.66
26	A	412	SQD	O8-S-C6	3.67	111.59	105.74
23	B	616	CLA	C1D-CHD-C4C	-3.67	118.14	126.06
25	k	101	BCR	C29-C30-C25	3.67	116.13	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	405[A]	CLA	O2A-CGA-O1A	-3.67	114.34	123.59
23	B	610	CLA	CAA-CBA-CGA	-3.67	102.54	113.25
23	b	607	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
25	d	403	BCR	C38-C26-C25	-3.66	120.42	124.53
23	c	507	CLA	C1-C2-C3	-3.66	119.72	126.04
29	D	705[B]	PL9	C10-C9-C11	3.66	121.42	115.27
26	A	410[B]	SQD	O47-C7-C8	3.65	119.38	111.50
25	d	403	BCR	C40-C30-C25	-3.65	104.37	110.30
32	B	627	LMT	C4B-C3B-C2B	3.65	117.20	110.82
23	b	612	CLA	O2D-CGD-O1D	-3.65	116.70	123.84
23	a	405[A]	CLA	CMB-C2B-C3B	3.65	131.51	124.68
23	B	602	CLA	C1D-CHD-C4C	-3.65	118.19	126.06
23	b	609	CLA	CAC-C3C-C4C	3.65	129.54	124.81
25	T	102	BCR	C12-C13-C14	-3.65	113.34	118.94
23	B	616	CLA	C3B-C4B-NB	3.65	113.92	109.21
29	A	414[B]	PL9	C22-C23-C24	-3.64	118.88	127.66
40	V	201	HEC	CMC-C2C-C1C	-3.64	122.86	128.46
25	B	617	BCR	C33-C5-C6	-3.64	120.44	124.53
23	c	513	CLA	C3C-C4C-NC	3.64	114.65	110.57
23	B	611	CLA	CHB-C4A-NA	3.64	129.54	124.51
23	A	406[B]	CLA	O2D-CGD-O1D	-3.64	116.72	123.84
23	B	614	CLA	C3C-C4C-NC	3.64	114.65	110.57
23	C	503	CLA	C1D-CHD-C4C	-3.64	118.21	126.06
23	c	508	CLA	O2D-CGD-O1D	-3.64	116.72	123.84
23	B	608	CLA	CAC-C3C-C4C	3.64	129.53	124.81
23	C	509	CLA	C1D-CHD-C4C	-3.64	118.21	126.06
23	b	602	CLA	O2D-CGD-O1D	-3.63	116.73	123.84
23	c	509	CLA	C1-C2-C3	-3.63	119.76	126.04
23	c	505	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
26	a	411[A]	SQD	O9-S-C6	3.63	111.25	106.94
25	B	619	BCR	C24-C23-C22	-3.63	120.75	126.23
35	b	622	HTG	O2-C2-C1	3.63	116.93	110.27
25	C	516	BCR	C7-C8-C9	-3.63	120.75	126.23
23	B	613	CLA	CAC-C3C-C4C	3.62	129.51	124.81
40	v	201	HEC	CMB-C2B-C1B	-3.62	122.90	128.46
23	c	512	CLA	O2D-CGD-O1D	-3.62	116.76	123.84
23	D	702[A]	CLA	C3B-C4B-NB	3.62	113.89	109.21
23	A	405[A]	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
23	B	610	CLA	C1C-C2C-C3C	-3.62	103.16	106.96
29	a	414[B]	PL9	C7-C3-C4	3.61	119.81	116.88
23	b	613	CLA	C1D-CHD-C4C	-3.61	118.26	126.06
23	b	601	CLA	C1C-C2C-C3C	-3.61	103.16	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	612	CLA	C4A-NA-C1A	-3.60	105.09	106.71
23	C	512	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
23	b	615	CLA	O2D-CGD-CBD	3.60	117.67	111.27
23	B	614	CLA	CMC-C2C-C1C	3.60	130.52	125.04
23	A	406[B]	CLA	C3C-C4C-NC	3.60	114.60	110.57
23	B	612	CLA	C4C-C3C-C2C	-3.59	101.66	106.90
23	c	507	CLA	C3C-C4C-NC	3.59	114.60	110.57
23	c	505	CLA	C1D-CHD-C4C	-3.59	118.31	126.06
25	K	102	BCR	C7-C8-C9	-3.59	120.81	126.23
25	h	101	BCR	C38-C26-C25	-3.59	120.50	124.53
23	B	609	CLA	CBC-CAC-C3C	-3.58	102.55	112.43
23	A	405[A]	CLA	O2D-CGD-O1D	-3.58	116.83	123.84
23	a	405[B]	CLA	C3C-C4C-NC	3.58	114.59	110.57
23	d	401[A]	CLA	C3B-C4B-NB	3.58	113.84	109.21
23	C	512	CLA	C4-C3-C5	3.58	121.29	115.27
23	c	511	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
23	c	502	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
23	c	510	CLA	CAC-C3C-C4C	3.57	129.44	124.81
29	d	404[B]	PL9	C7-C8-C9	-3.57	120.86	126.79
23	B	615	CLA	CMC-C2C-C1C	3.56	130.46	125.04
23	d	401[A]	CLA	C1-C2-C3	-3.56	119.89	126.04
23	c	506	CLA	C4C-C3C-C2C	-3.56	101.72	106.90
23	B	606	CLA	O2D-CGD-O1D	-3.55	116.89	123.84
23	B	610	CLA	O2D-CGD-O1D	-3.55	116.89	123.84
23	C	507	CLA	C3B-C4B-NB	3.55	113.80	109.21
29	A	414[B]	PL9	C15-C14-C16	3.55	121.24	115.27
29	A	414[B]	PL9	C7-C3-C2	-3.55	118.64	123.30
29	d	404[A]	PL9	C40-C39-C41	3.55	121.23	115.27
29	a	414[A]	PL9	C27-C28-C29	-3.54	119.13	127.66
23	C	503	CLA	C3B-C4B-NB	3.54	113.79	109.21
23	c	511	CLA	CMC-C2C-C1C	3.54	130.43	125.04
23	b	608	CLA	CAC-C3C-C4C	3.54	129.40	124.81
23	B	608	CLA	C1C-C2C-C3C	-3.54	103.24	106.96
23	b	604	CLA	C1D-CHD-C4C	-3.53	118.43	126.06
33	A	419[B]	LHG	O7-C7-C8	3.53	119.12	111.50
23	A	404[A]	CLA	O2D-CGD-CBD	3.53	117.54	111.27
23	c	505	CLA	CMB-C2B-C3B	3.52	131.27	124.68
33	d	412[B]	LHG	O8-C23-C24	3.52	122.95	111.91
23	C	514	CLA	C1D-CHD-C4C	-3.52	118.47	126.06
23	C	512	CLA	C3B-C4B-NB	3.52	113.76	109.21
23	C	502	CLA	CAC-C3C-C4C	3.52	129.37	124.81
29	A	414[A]	PL9	C22-C23-C24	-3.52	119.19	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	506	CLA	C4C-C3C-C2C	-3.51	101.78	106.90
25	c	516	BCR	C7-C8-C9	-3.51	120.92	126.23
23	C	508	CLA	C4C-C3C-C2C	-3.51	101.78	106.90
24	a	408[B]	PHO	C1A-C2A-C3A	-3.51	99.50	102.84
29	A	414[A]	PL9	C15-C14-C16	3.51	121.18	115.27
23	c	503	CLA	C3C-C4C-NC	3.51	114.51	110.57
23	A	404[A]	CLA	C1D-CHD-C4C	-3.51	118.49	126.06
23	B	612	CLA	C1D-CHD-C4C	-3.51	118.49	126.06
23	a	406[B]	CLA	C3B-C4B-NB	3.51	113.74	109.21
23	A	406[B]	CLA	CBC-CAC-C3C	-3.50	102.77	112.43
23	b	616	CLA	O2A-CGA-O1A	-3.50	114.75	123.59
23	B	608	CLA	C3B-C4B-NB	3.50	113.74	109.21
23	B	611	CLA	C4C-C3C-C2C	-3.50	101.80	106.90
29	D	705[A]	PL9	C53-C6-C1	3.50	122.15	114.99
23	C	510	CLA	CMC-C2C-C1C	3.50	130.37	125.04
40	v	201	HEC	CBA-CAA-C2A	-3.49	106.71	112.60
23	c	514	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
23	a	407[A]	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
23	a	407[B]	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
23	C	506	CLA	CAC-C3C-C4C	3.49	129.33	124.81
29	a	414[A]	PL9	C30-C29-C31	3.48	121.13	115.27
23	B	615	CLA	C3B-C4B-NB	3.48	113.71	109.21
23	A	404[A]	CLA	O2A-CGA-CBA	3.48	122.83	111.91
23	b	613	CLA	C3D-C4D-ND	3.48	115.86	110.24
40	V	201	HEC	CBA-CAA-C2A	-3.48	106.75	112.60
29	D	705[A]	PL9	C42-C43-C44	-3.47	119.29	127.66
23	c	509	CLA	C1D-CHD-C4C	-3.47	118.57	126.06
26	a	412	SQD	O47-C7-C8	3.47	118.98	111.50
25	d	403	BCR	C16-C17-C18	-3.47	122.35	127.31
23	b	610	CLA	O2A-CGA-O1A	-3.47	114.83	123.59
23	B	603	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
23	c	510	CLA	CHC-C1C-C2C	-3.47	117.12	126.72
35	o	301	HTG	C1'-S1-C1	3.47	106.58	100.09
23	B	609	CLA	CMC-C2C-C1C	3.47	130.32	125.04
23	A	405[B]	CLA	CHD-C4C-NC	3.47	129.67	124.20
23	B	605	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
23	a	405[A]	CLA	O2D-CGD-CBD	3.47	117.43	111.27
23	b	607	CLA	C4C-C3C-C2C	-3.47	101.84	106.90
23	b	610	CLA	C4C-C3C-C2C	-3.47	101.84	106.90
29	a	414[B]	PL9	C7-C3-C2	-3.47	118.74	123.30
34	c	501	LMG	C7-O1-C1	-3.47	106.97	113.74
23	b	616	CLA	CHD-C4C-NC	3.47	129.66	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	613	CLA	O2A-CGA-O1A	-3.46	114.85	123.59
23	b	605	CLA	C1C-C2C-C3C	-3.46	103.31	106.96
23	A	406[A]	CLA	O2A-CGA-O1A	-3.46	114.85	123.59
23	d	401[A]	CLA	O2A-CGA-CBA	3.46	122.77	111.91
23	C	506	CLA	C1-C2-C3	-3.46	120.06	126.04
23	C	507	CLA	O2D-CGD-O1D	-3.46	117.07	123.84
23	B	612	CLA	CMB-C2B-C3B	3.46	131.15	124.68
23	b	603	CLA	C3B-C4B-NB	3.46	113.68	109.21
23	d	402	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
23	A	404[B]	CLA	O2A-CGA-CBA	3.45	122.75	111.91
34	C	521	LMG	C3-C4-C5	3.45	116.40	110.24
23	B	604	CLA	C4C-C3C-C2C	-3.45	101.87	106.90
25	H	101	BCR	C16-C17-C18	-3.45	122.39	127.31
23	B	613	CLA	C4-C3-C5	3.45	121.07	115.27
23	b	613	CLA	C3B-C4B-NB	3.44	113.66	109.21
29	a	414[B]	PL9	C27-C28-C29	-3.44	119.38	127.66
23	C	502	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
23	A	405[B]	CLA	CAA-C2A-C3A	-3.43	103.38	112.78
23	B	608	CLA	C4C-C3C-C2C	-3.43	101.90	106.90
23	a	406[B]	CLA	CHD-C4C-NC	3.43	129.61	124.20
23	b	611	CLA	C1D-CHD-C4C	-3.43	118.67	126.06
23	b	616	CLA	C4C-C3C-C2C	-3.42	101.91	106.90
23	B	610	CLA	C1D-CHD-C4C	-3.42	118.68	126.06
23	C	508	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
23	B	605	CLA	C4C-C3C-C2C	-3.42	101.92	106.90
36	h	102	DGD	O2G-C1B-C2B	3.42	118.86	111.50
23	b	614	CLA	C3B-C4B-NB	3.41	113.62	109.21
23	a	405[A]	CLA	O2A-CGA-CBA	3.41	122.61	111.91
23	B	607	CLA	O2A-CGA-O1A	-3.41	114.98	123.59
29	a	414[A]	PL9	C35-C34-C36	3.41	121.01	115.27
23	d	402	CLA	C1D-CHD-C4C	-3.41	118.70	126.06
25	D	704	BCR	C28-C27-C26	-3.40	108.00	114.08
26	a	411[B]	SQD	C1-O5-C5	-3.40	107.01	113.69
23	D	703	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
23	C	510	CLA	C1D-CHD-C4C	-3.40	118.72	126.06
23	B	609	CLA	C1D-CHD-C4C	-3.40	118.72	126.06
32	A	418	LMT	O5B-C5B-C4B	3.40	115.87	109.69
23	B	614	CLA	CAC-C3C-C4C	3.40	129.22	124.81
23	B	606	CLA	CHD-C4C-NC	3.40	129.56	124.20
23	b	610	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
23	c	514	CLA	C3B-C4B-NB	3.40	113.60	109.21
23	c	502	CLA	CAC-C3C-C4C	3.40	129.22	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	507	CLA	C1D-CHD-C4C	-3.39	118.74	126.06
23	c	503	CLA	CHC-C1C-C2C	-3.39	117.34	126.72
23	b	609	CLA	CMC-C2C-C1C	3.39	130.20	125.04
23	b	605	CLA	CHD-C4C-NC	3.39	129.54	124.20
23	A	406[A]	CLA	C3B-C4B-NB	3.39	113.59	109.21
29	D	705[A]	PL9	C25-C24-C26	3.39	120.97	115.27
23	c	506	CLA	C1D-CHD-C4C	-3.39	118.75	126.06
23	b	604	CLA	CAC-C3C-C4C	3.39	129.20	124.81
23	b	607	CLA	C3B-C4B-NB	3.38	113.59	109.21
23	b	611	CLA	C1C-C2C-C3C	-3.38	103.40	106.96
23	b	606	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
23	b	612	CLA	C4C-C3C-C2C	-3.38	101.97	106.90
33	A	419[B]	LHG	C5-O7-C7	-3.38	109.47	117.79
33	d	412[B]	LHG	O7-C7-C8	3.38	118.78	111.50
23	b	603	CLA	C2A-C1A-CHA	-3.38	117.95	123.86
23	c	508	CLA	C4-C3-C5	3.38	120.95	115.27
23	B	607	CLA	C4-C3-C5	3.38	120.95	115.27
23	B	614	CLA	O2A-CGA-O1A	-3.37	115.08	123.59
36	c	518[A]	DGD	O2G-C1B-C2B	3.37	118.77	111.50
25	D	704	BCR	C29-C30-C25	3.37	115.67	110.48
23	b	601	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
23	b	602	CLA	C1-C2-C3	-3.37	120.22	126.04
29	a	414[B]	PL9	C25-C24-C26	3.36	120.93	115.27
23	b	604	CLA	C3D-C4D-ND	3.36	115.68	110.24
38	f	101	HEM	CHA-C4D-ND	3.36	128.53	124.38
23	B	611	CLA	C1-C2-C3	-3.36	120.23	126.04
23	B	604	CLA	CHD-C1D-ND	-3.36	121.37	124.45
23	c	506	CLA	C1-C2-C3	-3.36	120.23	126.04
23	c	511	CLA	C3B-C4B-NB	3.36	113.55	109.21
29	a	414[B]	PL9	C37-C38-C39	-3.35	119.58	127.66
34	c	521	LMG	C9-C8-C7	-3.35	103.86	111.79
38	F	102	HEM	CBD-CAD-C3D	-3.35	103.31	112.63
25	B	618	BCR	C37-C22-C21	-3.35	118.23	122.92
23	A	405[B]	CLA	C3C-C4C-NC	3.35	114.33	110.57
24	A	417[A]	PHO	CMC-C2C-C3C	3.35	131.26	124.94
23	a	409	CLA	C3B-C4B-NB	3.35	113.54	109.21
23	b	614	CLA	O2A-CGA-O1A	-3.35	115.14	123.59
23	b	613	CLA	C4A-NA-C1A	-3.35	105.20	106.71
36	c	518[B]	DGD	O2G-C1B-C2B	3.34	118.71	111.50
23	b	615	CLA	C3B-C4B-NB	3.34	113.53	109.21
23	B	612	CLA	CMC-C2C-C1C	3.34	130.13	125.04
23	b	602	CLA	CAA-C2A-C3A	-3.34	103.62	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	b	622	HTG	C1'-S1-C1	3.34	106.34	100.09
23	B	613	CLA	C4C-C3C-C2C	-3.34	102.03	106.90
23	C	505	CLA	C3B-C4B-NB	3.34	113.53	109.21
23	B	615	CLA	O2D-CGD-CBD	3.34	117.20	111.27
24	a	408[B]	PHO	CMA-C3A-C4A	-3.34	107.07	114.38
26	b	620	SQD	O8-S-C6	3.33	111.05	105.74
23	B	613	CLA	C1D-CHD-C4C	-3.33	118.87	126.06
23	C	504	CLA	C1-C2-C3	-3.33	120.28	126.04
23	d	401[A]	CLA	C1D-CHD-C4C	-3.33	118.87	126.06
23	A	406[B]	CLA	C3B-C4B-NB	3.33	113.51	109.21
23	C	513	CLA	C4C-C3C-C2C	-3.33	102.05	106.90
23	c	513	CLA	C4-C3-C5	3.33	120.86	115.27
23	A	405[A]	CLA	C3B-C4B-NB	3.33	113.51	109.21
23	C	506	CLA	C3B-C4B-NB	3.32	113.51	109.21
33	D	707[B]	LHG	O7-C7-C8	3.32	118.66	111.50
25	K	102	BCR	C38-C26-C25	-3.32	120.80	124.53
34	c	520	LMG	O1-C7-C8	-3.32	102.88	110.90
34	Z	101	LMG	O6-C1-C2	3.32	117.38	110.35
23	c	514	CLA	CAC-C3C-C4C	3.32	129.12	124.81
23	B	605	CLA	CHD-C4C-NC	3.32	129.44	124.20
23	B	613	CLA	O2A-CGA-CBA	3.32	122.32	111.91
34	B	621	LMG	O8-C28-C29	3.32	122.31	111.91
24	A	407[A]	PHO	CMA-C3A-C4A	-3.32	107.11	114.38
23	c	506	CLA	C1C-C2C-C3C	-3.32	103.47	106.96
23	D	702[B]	CLA	CAA-C2A-C3A	-3.31	103.70	112.78
23	B	611	CLA	C2A-C1A-CHA	-3.31	118.07	123.86
23	C	507	CLA	CMC-C2C-C1C	3.31	130.08	125.04
23	c	511	CLA	C4-C3-C5	3.31	120.84	115.27
25	t	102	BCR	C28-C27-C26	-3.31	108.17	114.08
34	z	101	LMG	O7-C10-C11	3.31	118.62	111.50
23	B	603	CLA	C4C-C3C-C2C	-3.30	102.08	106.90
25	A	409	BCR	C11-C10-C9	-3.30	122.59	127.31
25	T	102	BCR	C16-C17-C18	-3.30	122.60	127.31
33	d	412[A]	LHG	O8-C23-O10	-3.30	115.27	123.59
23	A	406[B]	CLA	CAA-C2A-C3A	-3.30	103.75	112.78
23	B	601	CLA	C1C-C2C-C3C	-3.29	103.49	106.96
29	d	404[B]	PL9	C42-C43-C44	-3.29	119.73	127.66
29	a	414[B]	PL9	C30-C29-C31	3.29	120.81	115.27
23	B	604	CLA	O2A-CGA-O1A	-3.29	115.28	123.59
33	d	406[A]	LHG	O7-C7-C8	3.29	118.59	111.50
29	D	705[B]	PL9	C25-C24-C26	3.29	120.80	115.27
23	c	507	CLA	CHC-C1C-C2C	-3.29	117.63	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	506	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
23	c	502	CLA	C1D-CHD-C4C	-3.29	118.97	126.06
23	B	602	CLA	CAA-C2A-C3A	-3.28	103.78	112.78
23	B	605	CLA	O2A-CGA-O1A	-3.28	115.31	123.59
23	C	514	CLA	CMC-C2C-C1C	3.28	130.04	125.04
23	c	514	CLA	CMC-C2C-C1C	3.28	130.04	125.04
23	c	504	CLA	C1C-C2C-C3C	-3.28	103.51	106.96
23	C	507	CLA	CHC-C1C-C2C	-3.28	117.66	126.72
33	A	419[B]	LHG	O8-C23-O10	-3.28	115.32	123.59
23	A	405[B]	CLA	C3B-C4B-NB	3.28	113.44	109.21
23	B	615	CLA	CED-O2D-CGD	3.27	123.34	115.94
23	A	406[B]	CLA	C1D-CHD-C4C	-3.27	119.00	126.06
23	b	615	CLA	C4-C3-C5	3.27	120.77	115.27
23	b	606	CLA	C3B-C4B-NB	3.27	113.44	109.21
23	B	603	CLA	CAC-C3C-C4C	3.27	129.05	124.81
23	c	512	CLA	CHD-C4C-NC	3.27	129.35	124.20
29	d	404[B]	PL9	C10-C9-C11	3.27	120.77	115.27
23	A	408	CLA	C4C-C3C-C2C	-3.26	102.14	106.90
23	c	513	CLA	C1C-C2C-C3C	-3.26	103.53	106.96
23	b	613	CLA	O2A-CGA-O1A	-3.26	115.36	123.59
23	b	606	CLA	CHD-C4C-NC	3.26	129.34	124.20
23	c	509	CLA	C3B-C4B-NB	3.26	113.42	109.21
23	b	602	CLA	CHD-C4C-NC	3.26	129.34	124.20
23	a	405[B]	CLA	CAA-C2A-C1A	-3.26	101.30	111.97
23	b	611	CLA	C4C-C3C-C2C	-3.26	102.15	106.90
23	a	406[A]	CLA	C3B-C4B-NB	3.25	113.42	109.21
23	B	606	CLA	CMC-C2C-C1C	3.25	130.00	125.04
38	f	101	HEM	CHD-C1D-ND	3.25	127.97	124.43
25	Y	101	BCR	C15-C14-C13	-3.25	122.67	127.31
23	A	408	CLA	CAA-C2A-C3A	-3.25	103.88	112.78
26	a	412	SQD	O48-C23-C24	3.25	122.10	111.91
23	a	405[B]	CLA	CHC-C1C-C2C	-3.25	117.73	126.72
23	A	404[A]	CLA	CMB-C2B-C3B	3.25	130.75	124.68
33	d	412[A]	LHG	O7-C7-C8	3.25	118.50	111.50
23	C	504	CLA	CHD-C4C-NC	3.25	129.32	124.20
23	a	409	CLA	C4-C3-C5	3.24	120.73	115.27
29	A	414[B]	PL9	C27-C28-C29	-3.24	119.85	127.66
23	C	513	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
32	b	627	LMT	C3'-C4'-C5'	-3.24	103.49	110.93
23	B	604	CLA	CAC-C3C-C4C	3.24	129.01	124.81
23	C	510	CLA	CMB-C2B-C3B	3.24	130.74	124.68
23	C	509	CLA	C4C-C3C-C2C	-3.24	102.18	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	507	CLA	CBC-CAC-C3C	-3.24	103.51	112.43
25	Y	101	BCR	C16-C17-C18	-3.24	122.69	127.31
23	C	511	CLA	CHD-C4C-NC	3.23	129.30	124.20
25	T	102	BCR	C33-C5-C6	-3.23	120.90	124.53
25	b	618	BCR	C37-C22-C21	-3.23	118.40	122.92
23	B	608	CLA	C1D-CHD-C4C	-3.23	119.09	126.06
23	B	614	CLA	CHD-C4C-NC	3.23	129.28	124.20
23	c	507	CLA	O2D-CGD-O1D	-3.22	117.53	123.84
23	c	510	CLA	O2A-CGA-CBA	3.22	122.02	111.91
23	b	611	CLA	C1-C2-C3	-3.22	120.47	126.04
24	a	416[A]	PHO	C4A-C3A-C2A	-3.22	99.77	102.84
23	B	612	CLA	C1-C2-C3	-3.22	120.47	126.04
23	A	408	CLA	CMB-C2B-C3B	3.22	130.70	124.68
23	B	605	CLA	C1-C2-C3	-3.22	120.48	126.04
23	d	401[B]	CLA	C1-C2-C3	-3.22	120.48	126.04
23	B	610	CLA	C4C-C3C-C2C	-3.22	102.21	106.90
33	d	412[A]	LHG	O8-C23-C24	3.22	122.00	111.91
23	B	613	CLA	C1C-C2C-C3C	-3.22	103.58	106.96
23	b	609	CLA	CBC-CAC-C3C	-3.22	103.57	112.43
23	c	502	CLA	C3B-C4B-NB	3.21	113.36	109.21
23	d	401[B]	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
38	f	101	HEM	CHB-C1B-NB	3.21	128.34	124.38
23	b	616	CLA	CBC-CAC-C3C	-3.20	103.60	112.43
23	a	405[A]	CLA	CHC-C1C-C2C	-3.20	117.86	126.72
23	D	702[B]	CLA	C1D-CHD-C4C	-3.20	119.15	126.06
23	a	407[A]	CLA	C3B-C4B-NB	3.20	113.34	109.21
25	c	515	BCR	C16-C17-C18	-3.20	122.75	127.31
23	c	513	CLA	O2A-CGA-CBA	3.20	121.94	111.91
23	b	603	CLA	C4-C3-C5	3.20	120.65	115.27
23	B	605	CLA	C1C-C2C-C3C	-3.19	103.60	106.96
24	A	417[B]	PHO	C4-C3-C5	3.19	120.64	115.27
23	a	405[A]	CLA	CAA-C2A-C1A	-3.19	101.52	111.97
23	b	605	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
29	d	404[B]	PL9	C40-C39-C41	3.19	120.64	115.27
23	b	614	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
23	c	511	CLA	CHD-C4C-NC	3.19	129.23	124.20
23	a	405[B]	CLA	O2A-CGA-CBA	3.19	121.91	111.91
23	C	505	CLA	C1D-CHD-C4C	-3.19	119.18	126.06
29	a	414[A]	PL9	C17-C18-C19	-3.19	119.99	127.66
24	a	416[B]	PHO	C4-C3-C5	3.19	120.63	115.27
23	b	602	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
23	c	504	CLA	O2D-CGD-O1D	-3.18	117.61	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	611	CLA	CHC-C1C-C2C	-3.18	117.92	126.72
23	B	609	CLA	O2A-CGA-CBA	3.18	121.89	111.91
23	A	408	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
23	d	402	CLA	CHD-C4C-NC	3.18	129.22	124.20
23	C	507	CLA	C4-C3-C5	3.18	120.62	115.27
23	A	406[A]	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
23	c	504	CLA	C4C-C3C-C2C	-3.18	102.27	106.90
29	A	414[A]	PL9	C27-C28-C29	-3.18	120.01	127.66
26	a	411[B]	SQD	C1-C2-C3	-3.18	103.38	110.00
23	D	702[B]	CLA	C3B-C4B-NB	3.17	113.31	109.21
23	B	601	CLA	C4C-C3C-C2C	-3.17	102.27	106.90
29	a	414[A]	PL9	C25-C24-C26	3.17	120.61	115.27
23	B	605	CLA	CMC-C2C-C1C	3.17	129.87	125.04
23	A	404[A]	CLA	O2A-CGA-O1A	-3.17	115.59	123.59
23	D	702[A]	CLA	C1D-CHD-C4C	-3.17	119.22	126.06
23	B	602	CLA	C3B-C4B-NB	3.17	113.30	109.21
23	b	609	CLA	C1C-C2C-C3C	-3.16	103.63	106.96
23	C	507	CLA	C1D-CHD-C4C	-3.16	119.24	126.06
23	C	512	CLA	C4C-C3C-C2C	-3.16	102.29	106.90
29	A	414[B]	PL9	C17-C18-C19	-3.16	120.06	127.66
33	d	412[B]	LHG	O8-C23-O10	-3.16	115.62	123.59
23	c	506	CLA	C3B-C4B-NB	3.16	113.29	109.21
23	b	609	CLA	C4C-C3C-C2C	-3.16	102.30	106.90
23	B	614	CLA	O2A-CGA-CBA	3.16	121.81	111.91
23	C	503	CLA	CHC-C1C-C2C	-3.15	118.00	126.72
24	A	417[A]	PHO	C4-C3-C5	3.15	120.58	115.27
25	T	102	BCR	C15-C14-C13	3.15	131.81	127.31
23	d	401[B]	CLA	O2A-CGA-CBA	3.15	121.80	111.91
23	a	406[A]	CLA	CHD-C4C-NC	3.15	129.17	124.20
40	V	201	HEC	CMB-C2B-C1B	-3.15	123.62	128.46
33	A	419[A]	LHG	C5-O7-C7	-3.15	110.03	117.79
23	b	608	CLA	CBC-CAC-C3C	-3.15	103.75	112.43
23	C	510	CLA	C16-C15-C13	-3.15	105.74	115.92
23	C	513	CLA	CHD-C4C-NC	3.15	129.16	124.20
33	A	419[A]	LHG	O8-C23-C24	3.15	121.79	111.91
29	D	705[A]	PL9	C17-C18-C19	-3.15	120.08	127.66
23	d	402	CLA	CAA-C2A-C3A	-3.15	104.16	112.78
23	C	514	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
23	C	502	CLA	CMC-C2C-C1C	3.15	129.83	125.04
35	b	625	HTG	O5-C5-C4	3.15	115.41	109.69
32	m	103	LMT	C1'-O5'-C5'	-3.14	107.52	113.69
23	b	601	CLA	CMB-C2B-C3B	3.14	130.56	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	609	CLA	C3B-C4B-NB	3.14	113.27	109.21
23	a	409	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
23	D	702[B]	CLA	O2A-CGA-CBA	3.14	121.76	111.91
23	b	601	CLA	C3B-C4B-NB	3.14	113.27	109.21
25	A	409	BCR	C24-C23-C22	-3.14	121.50	126.23
23	c	505	CLA	C3B-C4B-NB	3.13	113.26	109.21
25	T	102	BCR	C7-C8-C9	-3.13	121.50	126.23
23	B	602	CLA	CAC-C3C-C4C	3.13	128.88	124.81
34	C	521	LMG	O8-C28-C29	3.13	121.74	111.91
25	a	410	BCR	C38-C26-C25	-3.13	121.01	124.53
23	a	407[B]	CLA	CMC-C2C-C1C	3.13	129.81	125.04
34	m	101	LMG	O8-C28-C29	3.13	121.74	111.91
23	a	407[A]	CLA	CHD-C4C-NC	3.13	129.13	124.20
23	A	404[B]	CLA	O2A-CGA-O1A	-3.13	115.70	123.59
23	a	407[A]	CLA	C1-C2-C3	-3.13	120.64	126.04
23	d	401[B]	CLA	C4-C3-C5	3.13	120.53	115.27
23	C	506	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
23	d	401[A]	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
23	C	502	CLA	C3B-C4B-NB	3.13	113.25	109.21
25	C	516	BCR	C24-C23-C22	-3.13	121.51	126.23
23	C	509	CLA	CHC-C1C-C2C	-3.12	118.08	126.72
23	C	510	CLA	O2A-CGA-CBA	3.12	121.71	111.91
26	a	411[B]	SQD	C44-O6-C1	-3.12	107.64	113.74
33	d	406[B]	LHG	O7-C7-C8	3.12	118.23	111.50
23	b	616	CLA	CMC-C2C-C1C	3.12	129.79	125.04
34	D	711	LMG	O8-C28-O10	-3.12	115.72	123.59
29	D	705[A]	PL9	C51-C49-C50	3.12	121.49	114.60
34	C	520	LMG	O8-C28-C29	3.11	121.68	111.91
25	k	101	BCR	C7-C8-C9	-3.11	121.53	126.23
23	B	612	CLA	O2A-CGA-CBA	3.11	121.67	111.91
29	A	414[B]	PL9	C20-C19-C21	3.11	120.50	115.27
23	b	615	CLA	C11-C10-C8	-3.11	105.87	115.92
23	b	613	CLA	CHC-C1C-C2C	-3.11	118.12	126.72
25	h	101	BCR	C16-C17-C18	-3.11	122.87	127.31
23	C	506	CLA	C1C-C2C-C3C	-3.11	103.69	106.96
23	B	603	CLA	CHC-C1C-C2C	-3.11	118.13	126.72
29	D	705[A]	PL9	C10-C9-C11	3.11	120.50	115.27
25	b	619	BCR	C15-C14-C13	-3.10	122.88	127.31
29	A	414[A]	PL9	C10-C9-C11	3.10	120.48	115.27
23	B	606	CLA	O2A-CGA-CBA	3.09	121.61	111.91
33	b	629[A]	LHG	O7-C7-C8	3.09	118.16	111.50
23	C	503	CLA	C4-C3-C5	3.09	120.47	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	t	102	BCR	C15-C16-C17	-3.09	117.14	123.47
23	B	609	CLA	C3B-C4B-NB	3.08	113.20	109.21
23	c	508	CLA	C1D-CHD-C4C	-3.08	119.41	126.06
25	d	403	BCR	C39-C30-C25	-3.08	105.30	110.30
24	a	416[A]	PHO	CMB-C2B-C3B	3.08	130.44	124.68
23	B	616	CLA	C1-O2A-CGA	3.08	124.53	116.44
25	D	704	BCR	C37-C22-C23	3.08	122.93	118.08
29	a	414[A]	PL9	C10-C9-C11	3.08	120.45	115.27
23	b	601	CLA	C4-C3-C5	3.08	120.45	115.27
26	b	620	SQD	C3-C4-C5	3.08	115.73	110.24
23	b	612	CLA	CMC-C2C-C1C	3.08	129.72	125.04
23	a	405[A]	CLA	C1-C2-C3	-3.07	120.73	126.04
23	d	401[B]	CLA	CHC-C1C-C2C	-3.07	118.23	126.72
23	c	514	CLA	O2A-CGA-CBA	3.07	121.54	111.91
23	b	611	CLA	O2A-CGA-O1A	-3.06	115.86	123.59
23	B	607	CLA	C1D-CHD-C4C	-3.06	119.45	126.06
38	F	102	HEM	CHB-C1B-NB	3.06	128.16	124.38
23	A	405[B]	CLA	CHC-C1C-C2C	-3.06	118.25	126.72
23	B	603	CLA	O2A-CGA-O1A	-3.06	115.87	123.59
23	b	614	CLA	CHD-C4C-NC	3.06	129.02	124.20
29	d	404[A]	PL9	C10-C9-C11	3.05	120.41	115.27
23	b	605	CLA	CHC-C1C-C2C	-3.05	118.27	126.72
29	a	414[B]	PL9	C35-C34-C36	3.05	120.41	115.27
23	a	405[A]	CLA	C4-C3-C5	3.05	120.41	115.27
23	D	702[A]	CLA	O2A-CGA-CBA	3.05	121.48	111.91
23	a	407[A]	CLA	CMC-C2C-C1C	3.05	129.68	125.04
23	C	504	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
23	B	601	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
23	b	603	CLA	CMA-C3A-C2A	-3.05	101.54	113.83
23	d	401[A]	CLA	C2A-C1A-CHA	-3.05	118.53	123.86
23	B	607	CLA	CAA-C2A-C3A	-3.05	104.44	112.78
23	c	510	CLA	C4C-C3C-C2C	-3.05	102.46	106.90
29	a	414[B]	PL9	C42-C43-C44	-3.04	120.33	127.66
23	D	703	CLA	C4C-C3C-C2C	-3.04	102.46	106.90
23	d	401[A]	CLA	C4C-C3C-C2C	-3.04	102.46	106.90
23	C	514	CLA	C1-C2-C3	-3.04	120.78	126.04
23	b	609	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
29	A	414[A]	PL9	C20-C19-C21	3.04	120.38	115.27
23	c	503	CLA	CBC-CAC-C3C	-3.04	104.06	112.43
25	K	102	BCR	C24-C23-C22	-3.03	121.65	126.23
25	C	515	BCR	C15-C14-C13	-3.03	122.98	127.31
23	b	607	CLA	C1D-CHD-C4C	-3.03	119.52	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	401[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	b	612	CLA	O2A-CGA-O1A	-3.03	115.95	123.59
23	A	404[A]	CLA	C1-C2-C3	-3.03	120.81	126.04
23	d	401[A]	CLA	C4-C3-C5	3.02	120.36	115.27
23	C	511	CLA	CHC-C1C-C2C	-3.02	118.36	126.72
23	B	601	CLA	CHD-C4C-NC	3.02	128.97	124.20
29	d	404[A]	PL9	C37-C38-C39	-3.02	120.38	127.66
23	c	503	CLA	C1-C2-C3	-3.02	120.82	126.04
33	D	706[B]	LHG	O8-C23-O10	-3.02	115.97	123.59
34	c	501	LMG	C8-O7-C10	-3.02	110.36	117.79
23	C	512	CLA	CAC-C3C-C4C	3.02	128.72	124.81
23	A	404[A]	CLA	CAA-C2A-C1A	-3.01	102.09	111.97
33	a	420[B]	LHG	O7-C7-C8	3.01	118.00	111.50
23	b	611	CLA	O2A-CGA-CBA	3.01	121.36	111.91
29	a	414[A]	PL9	C42-C43-C44	-3.01	120.41	127.66
25	d	403	BCR	C21-C20-C19	-3.01	113.82	123.22
23	b	613	CLA	O2A-CGA-CBA	3.01	121.36	111.91
25	D	704	BCR	C15-C14-C13	-3.01	123.01	127.31
23	d	402	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
23	b	604	CLA	CHC-C1C-C2C	-3.01	118.39	126.72
32	A	420	LMT	O5B-C5B-C4B	3.01	115.16	109.69
23	c	505	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
33	d	405[A]	LHG	O7-C7-C8	3.01	117.99	111.50
23	b	603	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
23	c	513	CLA	CHD-C4C-NC	3.01	128.94	124.20
23	a	407[B]	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
23	D	702[A]	CLA	CAC-C3C-C4C	3.01	128.71	124.81
23	a	406[B]	CLA	CHC-C1C-C2C	-3.01	118.40	126.72
29	D	705[B]	PL9	C17-C18-C19	-3.01	120.42	127.66
34	D	711	LMG	O7-C10-C11	3.01	117.98	111.50
33	d	405[B]	LHG	O7-C7-C8	3.00	117.97	111.50
23	c	509	CLA	C4C-C3C-C2C	-3.00	102.52	106.90
35	b	622	HTG	O5-C5-C4	3.00	115.15	109.69
23	A	404[A]	CLA	CHC-C1C-C2C	-3.00	118.43	126.72
38	F	102	HEM	CHD-C1D-ND	3.00	127.69	124.43
23	A	405[B]	CLA	CMC-C2C-C1C	3.00	129.60	125.04
23	A	405[A]	CLA	CHD-C4C-NC	3.00	128.93	124.20
26	a	411[A]	SQD	C45-O47-C7	-3.00	110.42	117.79
23	B	612	CLA	C1C-C2C-C3C	-3.00	103.81	106.96
23	A	406[B]	CLA	O2A-CGA-CBA	2.99	121.30	111.91
23	b	601	CLA	CHD-C4C-NC	2.99	128.92	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	505	CLA	CMC-C2C-C1C	2.99	129.60	125.04
23	B	608	CLA	CHC-C1C-C2C	-2.99	118.45	126.72
23	b	608	CLA	CHD-C4C-NC	2.99	128.91	124.20
23	C	513	CLA	O2A-CGA-CBA	2.99	121.28	111.91
23	C	514	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
23	c	514	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
23	a	409	CLA	O2A-CGA-CBA	2.98	121.27	111.91
33	D	707[A]	LHG	O8-C23-C24	2.98	121.27	111.91
36	h	102	DGD	O1G-C1A-O1A	-2.98	116.07	123.59
25	T	102	BCR	C2-C1-C6	2.98	115.07	110.48
23	c	507	CLA	CAC-C3C-C4C	2.98	128.68	124.81
29	a	414[B]	PL9	C17-C18-C19	-2.98	120.48	127.66
23	C	504	CLA	O2A-CGA-O1A	-2.98	116.08	123.59
23	B	612	CLA	C11-C12-C13	-2.98	106.29	115.92
23	a	407[B]	CLA	CHD-C4C-NC	2.98	128.90	124.20
23	D	703	CLA	O2A-CGA-O1A	-2.98	116.08	123.59
23	B	615	CLA	C4-C3-C5	2.98	120.28	115.27
23	c	514	CLA	CAA-C2A-C3A	-2.97	104.63	112.78
23	B	612	CLA	O2A-CGA-O1A	-2.97	116.09	123.59
23	C	504	CLA	C1C-C2C-C3C	-2.97	103.83	106.96
33	E	101[A]	LHG	O8-C23-C24	2.97	121.23	111.91
23	b	605	CLA	C1-C2-C3	-2.97	120.90	126.04
23	A	404[B]	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
23	B	608	CLA	CMA-C3A-C4A	-2.97	103.79	111.77
23	B	616	CLA	C1C-C2C-C3C	-2.97	103.84	106.96
23	b	611	CLA	C2A-C1A-CHA	-2.97	118.67	123.86
23	c	509	CLA	CHC-C1C-C2C	-2.97	118.52	126.72
23	b	616	CLA	CAC-C3C-C4C	2.96	128.66	124.81
23	b	614	CLA	CBC-CAC-C3C	-2.96	104.26	112.43
23	D	703	CLA	CAC-C3C-C4C	2.96	128.65	124.81
23	a	406[A]	CLA	CHC-C1C-C2C	-2.96	118.53	126.72
23	b	602	CLA	C2A-C1A-CHA	-2.96	118.68	123.86
23	c	511	CLA	CMB-C2B-C3B	2.96	130.22	124.68
23	c	510	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
36	h	102	DGD	O1G-C1A-C2A	2.96	121.19	111.91
23	b	610	CLA	CHD-C4C-NC	2.96	128.86	124.20
24	A	407[A]	PHO	O1D-CGD-CBD	-2.96	119.81	124.74
23	b	608	CLA	CMB-C2B-C3B	2.96	130.21	124.68
23	b	615	CLA	CHC-C1C-C2C	-2.96	118.55	126.72
23	b	612	CLA	O2A-CGA-CBA	2.95	121.17	111.91
26	B	620	SQD	O9-S-C6	2.95	110.45	106.94
23	c	512	CLA	C4-C3-C5	2.95	120.23	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	412	SQD	O7-S-C6	2.95	110.44	106.94
23	B	614	CLA	CHC-C1C-C2C	-2.95	118.57	126.72
23	c	513	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
26	A	410[A]	SQD	O9-S-C6	2.95	110.44	106.94
33	D	706[B]	LHG	O7-C7-C8	2.94	117.85	111.50
23	a	409	CLA	CHD-C4C-NC	2.94	128.84	124.20
23	b	613	CLA	C4-C3-C5	2.94	120.22	115.27
23	b	608	CLA	C1-C2-C3	-2.94	120.95	126.04
23	c	504	CLA	C1-C2-C3	-2.94	120.95	126.04
29	D	705[B]	PL9	C20-C19-C21	2.94	120.22	115.27
36	C	519	DGD	O1G-C1A-C2A	2.94	121.14	111.91
23	B	611	CLA	C3B-C4B-NB	2.94	113.01	109.21
38	f	101	HEM	CBD-CAD-C3D	-2.94	104.45	112.63
29	A	414[A]	PL9	C30-C29-C31	2.94	120.22	115.27
23	d	402	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
23	b	605	CLA	C2A-C1A-CHA	-2.94	118.72	123.86
23	C	505	CLA	C1-O2A-CGA	2.94	124.16	116.44
23	a	405[B]	CLA	CMB-C2B-C3B	2.94	130.18	124.68
23	b	607	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
23	C	510	CLA	C4C-C3C-C2C	-2.94	102.62	106.90
32	B	629	LMT	O1'-C1'-C2'	2.94	112.89	108.30
33	a	420[A]	LHG	O7-C7-C8	2.94	117.83	111.50
23	C	510	CLA	O2A-CGA-O1A	-2.94	116.18	123.59
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
33	D	706[A]	LHG	O8-C23-O10	-2.93	116.19	123.59
29	d	404[A]	PL9	C22-C23-C24	-2.93	120.60	127.66
23	C	502	CLA	C1-C2-C3	-2.93	120.97	126.04
23	B	608	CLA	C1-C2-C3	-2.93	120.98	126.04
23	c	512	CLA	CHC-C1C-C2C	-2.93	118.63	126.72
29	d	404[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	B	615	CLA	CMB-C2B-C1B	2.92	132.96	128.46
23	b	610	CLA	CAA-C2A-C3A	-2.92	104.77	112.78
23	C	512	CLA	CHC-C1C-C2C	-2.92	118.64	126.72
33	A	419[B]	LHG	O8-C23-C24	2.92	121.08	111.91
23	a	406[A]	CLA	CBC-CAC-C3C	-2.92	104.38	112.43
23	b	613	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
38	f	101	HEM	C4D-ND-C1D	2.92	108.09	105.07
23	A	406[A]	CLA	CAA-C2A-C3A	-2.92	104.78	112.78
23	B	601	CLA	C3B-C4B-NB	2.92	112.98	109.21
23	C	513	CLA	CMC-C2C-C1C	2.92	129.48	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	613	CLA	CMC-C2C-C1C	2.92	129.48	125.04
29	d	404[A]	PL9	C53-C6-C1	2.92	120.95	114.99
26	B	620	SQD	O48-C23-C24	2.92	121.06	111.91
23	a	405[B]	CLA	CMA-C3A-C4A	-2.92	103.94	111.77
24	A	417[B]	PHO	C1A-C2A-C3A	-2.92	100.06	102.84
29	a	414[A]	PL9	C22-C23-C24	-2.92	120.64	127.66
23	b	606	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
23	B	613	CLA	CMB-C2B-C3B	2.91	130.13	124.68
33	D	707[B]	LHG	O8-C23-C24	2.91	121.05	111.91
23	b	607	CLA	CAA-C2A-C3A	-2.91	104.81	112.78
26	A	410[A]	SQD	O48-C23-C24	2.91	121.04	111.91
33	D	707[A]	LHG	O8-C23-O10	-2.91	116.25	123.59
23	a	407[B]	CLA	C3B-C4B-NB	2.91	112.97	109.21
23	A	405[A]	CLA	C4-C3-C5	2.91	120.16	115.27
23	b	605	CLA	C3B-C4B-NB	2.91	112.97	109.21
24	a	408[B]	PHO	O2A-CGA-CBA	2.90	121.02	111.91
34	z	101	LMG	O8-C28-C29	2.90	121.02	111.91
23	a	405[A]	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
23	b	603	CLA	O2A-CGA-O1A	-2.90	116.27	123.59
23	B	604	CLA	CHC-C1C-C2C	-2.90	118.69	126.72
26	a	411[B]	SQD	O9-S-C6	2.90	110.39	106.94
23	a	407[A]	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
23	B	609	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
23	a	406[A]	CLA	CMA-C3A-C2A	-2.90	102.14	113.83
23	c	502	CLA	CMC-C2C-C1C	2.89	129.45	125.04
34	C	501	LMG	O6-C1-O1	-2.89	103.12	109.97
23	b	607	CLA	C4-C3-C5	2.89	120.14	115.27
23	A	405[A]	CLA	CHC-C1C-C2C	-2.89	118.72	126.72
23	D	702[A]	CLA	CHC-C1C-C2C	-2.89	118.72	126.72
26	A	412	SQD	O48-C23-C24	2.89	120.98	111.91
32	T	101	LMT	C1'-O5'-C5'	-2.89	108.01	113.69
23	c	511	CLA	O2A-CGA-CBA	2.89	120.98	111.91
23	C	509	CLA	C4-C3-C5	2.89	120.13	115.27
23	A	406[B]	CLA	O2A-CGA-O1A	-2.89	116.30	123.59
23	D	702[A]	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
23	B	606	CLA	O2A-CGA-O1A	-2.89	116.31	123.59
23	C	514	CLA	CAC-C3C-C4C	2.88	128.55	124.81
23	b	613	CLA	CHD-C4C-NC	2.88	128.75	124.20
23	c	504	CLA	C3B-C4B-NB	2.88	112.94	109.21
23	c	511	CLA	O2A-CGA-O1A	-2.88	116.32	123.59
23	c	502	CLA	CHC-C1C-C2C	-2.88	118.75	126.72
25	y	101	BCR	C38-C26-C25	-2.88	121.29	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	609	CLA	O2A-CGA-O1A	-2.88	116.32	123.59
23	C	505	CLA	CMC-C2C-C1C	2.88	129.43	125.04
29	a	414[B]	PL9	C22-C23-C24	-2.88	120.73	127.66
29	A	414[B]	PL9	C30-C29-C31	2.88	120.11	115.27
23	C	513	CLA	C4-C3-C5	2.88	120.11	115.27
23	b	614	CLA	CHC-C1C-C2C	-2.88	118.76	126.72
23	b	601	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
23	b	614	CLA	O2A-CGA-CBA	2.87	120.93	111.91
23	a	405[B]	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
26	X	101	SQD	O7-S-C6	2.87	110.36	106.94
23	C	506	CLA	C4-C3-C5	2.87	120.10	115.27
23	b	608	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
23	b	615	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
24	a	408[A]	PHO	O2A-CGA-CBA	2.87	120.92	111.91
25	D	704	BCR	C40-C30-C25	-2.87	105.64	110.30
23	D	702[A]	CLA	O2A-CGA-O1A	-2.87	116.35	123.59
34	C	501	LMG	C6-C5-C4	2.87	119.72	113.00
23	B	610	CLA	CHC-C1C-C2C	-2.87	118.79	126.72
23	c	513	CLA	CHC-C1C-C2C	-2.87	118.79	126.72
23	b	601	CLA	CHC-C1C-C2C	-2.87	118.80	126.72
25	c	516	BCR	C37-C22-C23	2.86	122.59	118.08
29	a	414[A]	PL9	C37-C38-C39	-2.86	120.77	127.66
26	b	620	SQD	O7-S-C6	2.86	110.34	106.94
24	A	407[B]	PHO	CMB-C2B-C3B	2.86	130.03	124.68
23	B	613	CLA	CMC-C2C-C1C	2.86	129.40	125.04
23	D	702[B]	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
23	B	611	CLA	C4A-NA-C1A	-2.86	105.42	106.71
23	b	616	CLA	C3B-C4B-NB	2.86	112.91	109.21
23	B	615	CLA	CHD-C4C-NC	2.86	128.71	124.20
26	A	410[B]	SQD	O48-C23-C24	2.85	120.86	111.91
34	c	520	LMG	O8-C28-C29	2.85	120.86	111.91
23	D	702[B]	CLA	CHC-C1C-C2C	-2.85	118.83	126.72
23	C	514	CLA	C2A-C1A-CHA	-2.85	118.87	123.86
23	A	408	CLA	CBC-CAC-C3C	-2.85	104.57	112.43
24	a	408[A]	PHO	C1A-C2A-C3A	-2.85	100.13	102.84
25	h	101	BCR	C7-C8-C9	-2.85	121.93	126.23
33	b	629[A]	LHG	O8-C23-C24	2.85	120.84	111.91
40	V	201	HEC	C1D-C2D-C3D	-2.85	105.02	107.00
23	C	510	CLA	CHC-C1C-C2C	-2.85	118.85	126.72
23	b	602	CLA	C11-C12-C13	-2.85	106.72	115.92
23	B	608	CLA	CMC-C2C-C1C	2.84	129.37	125.04
23	A	406[B]	CLA	CHC-C1C-C2C	-2.84	118.85	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	511	CLA	CHC-C1C-C2C	-2.84	118.85	126.72
23	A	408	CLA	CHD-C4C-NC	2.84	128.69	124.20
23	B	607	CLA	CMC-C2C-C1C	2.84	129.37	125.04
23	c	505	CLA	CAC-C3C-C4C	2.84	128.50	124.81
25	h	101	BCR	C33-C5-C6	-2.84	121.34	124.53
24	a	408[A]	PHO	O1D-CGD-CBD	-2.84	120.01	124.74
25	T	102	BCR	C35-C13-C12	2.84	122.55	118.08
23	c	513	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
23	b	609	CLA	CHD-C4C-NC	2.84	128.68	124.20
23	b	602	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
23	c	502	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
25	d	403	BCR	C10-C11-C12	-2.84	114.36	123.22
23	c	514	CLA	CMB-C2B-C3B	2.83	129.98	124.68
23	B	614	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
23	C	502	CLA	O2A-CGA-O1A	-2.83	116.44	123.59
24	a	416[B]	PHO	CMB-C2B-C3B	2.83	129.98	124.68
25	d	403	BCR	C33-C5-C6	-2.83	121.35	124.53
34	D	711	LMG	O8-C28-C29	2.83	120.79	111.91
23	a	409	CLA	CAA-C2A-C3A	-2.83	105.03	112.78
23	c	503	CLA	CHD-C4C-NC	2.83	128.66	124.20
29	d	404[B]	PL9	C37-C38-C39	-2.83	120.85	127.66
32	B	627	LMT	C2'-C3'-C4'	2.83	116.14	109.68
23	C	506	CLA	CHC-C1C-C2C	-2.83	118.90	126.72
26	a	411[B]	SQD	O8-S-C6	2.83	110.25	105.74
23	b	603	CLA	CHD-C4C-NC	2.82	128.65	124.20
23	c	505	CLA	CHD-C4C-NC	2.82	128.64	124.20
23	b	605	CLA	C4-C3-C5	2.82	120.01	115.27
34	Z	101	LMG	C4-C3-C2	2.82	115.74	110.82
36	c	517[A]	DGD	O3G-C3G-C2G	-2.82	104.11	110.90
23	C	502	CLA	CHD-C4C-NC	2.81	128.64	124.20
25	h	101	BCR	C36-C18-C17	-2.81	118.98	122.92
25	y	101	BCR	C15-C14-C13	-2.81	123.30	127.31
23	a	409	CLA	C2A-C1A-CHA	-2.81	118.95	123.86
24	a	416[A]	PHO	CMC-C2C-C3C	2.81	130.23	124.94
25	C	516	BCR	C33-C5-C6	-2.81	121.38	124.53
40	v	201	HEC	C1D-C2D-C3D	-2.81	105.04	107.00
23	A	408	CLA	CHC-C1C-C2C	-2.80	118.96	126.72
23	d	401[A]	CLA	CHC-C1C-C2C	-2.80	118.97	126.72
23	C	514	CLA	CMB-C2B-C3B	2.80	129.92	124.68
23	B	604	CLA	O2A-CGA-CBA	2.80	120.70	111.91
23	d	401[B]	CLA	CMB-C2B-C3B	2.80	129.92	124.68
26	f	102	SQD	C4-C3-C2	-2.80	105.94	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	E	101[B]	LHG	O8-C23-C24	2.80	120.69	111.91
25	h	101	BCR	C16-C15-C14	-2.80	117.74	123.47
23	A	406[A]	CLA	CHC-C1C-C2C	-2.80	118.99	126.72
26	A	412	SQD	C4-C3-C2	-2.80	105.94	110.82
26	f	102	SQD	O5-C1-C2	2.79	116.26	110.35
36	C	517[A]	DGD	O3G-C3G-C2G	-2.79	104.16	110.90
23	a	405[B]	CLA	O2A-CGA-O1A	-2.79	116.54	123.59
23	c	512	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
23	b	602	CLA	C4-C3-C5	2.79	119.97	115.27
24	A	407[A]	PHO	CMC-C2C-C3C	2.79	130.21	124.94
23	D	702[B]	CLA	C2A-C1A-CHA	-2.79	118.98	123.86
23	C	502	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
33	b	629[B]	LHG	O8-C23-C24	2.79	120.66	111.91
23	B	608	CLA	CAA-C2A-C3A	-2.79	105.14	112.78
23	c	506	CLA	CHC-C1C-C2C	-2.79	119.01	126.72
23	a	406[B]	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
23	C	502	CLA	CHC-C1C-C2C	-2.79	119.01	126.72
23	C	503	CLA	C4C-C3C-C2C	-2.79	102.84	106.90
33	D	707[A]	LHG	O7-C7-C8	2.79	117.50	111.50
23	a	407[B]	CLA	CBC-CAC-C3C	-2.79	104.75	112.43
26	B	620	SQD	C4-C3-C2	2.78	115.68	110.82
23	C	505	CLA	CHC-C1C-C2C	-2.78	119.02	126.72
23	B	610	CLA	O2A-CGA-O1A	-2.78	116.57	123.59
26	a	411[A]	SQD	O47-C7-O49	-2.78	116.98	123.70
29	D	705[B]	PL9	C45-C44-C46	2.78	119.95	115.27
23	B	602	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
23	B	615	CLA	C4C-C3C-C2C	-2.78	102.85	106.90
23	B	608	CLA	O2A-CGA-O1A	-2.78	116.58	123.59
23	b	608	CLA	CHC-C1C-C2C	-2.78	119.04	126.72
23	A	404[A]	CLA	CAA-CBA-CGA	-2.78	105.14	113.25
23	C	509	CLA	CAC-C3C-C4C	2.78	128.41	124.81
23	c	508	CLA	CAC-C3C-C4C	2.78	128.41	124.81
23	b	613	CLA	C4C-C3C-C2C	-2.77	102.85	106.90
29	d	404[B]	PL9	C17-C18-C19	-2.77	120.98	127.66
24	A	407[B]	PHO	C1-C2-C3	-2.77	121.25	126.04
23	B	612	CLA	C3B-C4B-NB	2.77	112.79	109.21
25	A	409	BCR	C33-C5-C6	-2.77	121.42	124.53
24	a	408[B]	PHO	O1D-CGD-CBD	-2.77	120.12	124.74
23	C	514	CLA	CBC-CAC-C3C	-2.77	104.79	112.43
23	C	511	CLA	O2A-CGA-O1A	-2.77	116.60	123.59
24	a	408[B]	PHO	O2A-CGA-O1A	-2.77	116.60	123.59
32	b	621	LMT	C1'-O5'-C5'	-2.77	108.25	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	M	101	LMT	C1'-O5'-C5'	-2.77	108.25	113.69
35	b	622	HTG	O2-C2-C3	-2.77	103.95	110.35
23	b	615	CLA	CHD-C4C-NC	2.77	128.56	124.20
23	B	601	CLA	C1-O2A-CGA	2.77	123.70	116.44
23	D	703	CLA	C4-C3-C5	2.77	119.92	115.27
23	b	613	CLA	CMB-C2B-C3B	2.77	129.85	124.68
26	f	102	SQD	O48-C23-C24	2.76	120.58	111.91
23	b	615	CLA	O2A-CGA-O1A	-2.76	116.62	123.59
29	A	414[B]	PL9	C40-C39-C41	2.76	119.92	115.27
23	B	603	CLA	CBC-CAC-C3C	-2.76	104.81	112.43
29	a	414[A]	PL9	C53-C6-C1	2.76	120.64	114.99
23	C	511	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
23	B	606	CLA	C3B-C4B-NB	2.76	112.78	109.21
23	C	506	CLA	CMC-C2C-C1C	2.76	129.24	125.04
23	A	406[B]	CLA	CHD-C4C-NC	2.76	128.55	124.20
23	B	608	CLA	CMA-C3A-C2A	-2.76	102.71	113.83
23	B	608	CLA	O2A-CGA-CBA	2.76	120.56	111.91
23	B	615	CLA	C11-C10-C8	-2.75	107.02	115.92
23	D	702[B]	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
23	d	402	CLA	C3B-C4B-NB	2.75	112.77	109.21
23	A	404[B]	CLA	CHC-C1C-C2C	-2.75	119.11	126.72
23	b	603	CLA	O2A-CGA-CBA	2.75	120.55	111.91
23	c	508	CLA	O2A-CGA-CBA	2.75	120.54	111.91
23	c	504	CLA	CHD-C4C-NC	2.75	128.54	124.20
23	b	610	CLA	C3B-C4B-NB	2.75	112.77	109.21
23	b	610	CLA	C4-C3-C5	2.75	119.90	115.27
23	a	407[B]	CLA	C4-C3-C5	2.75	119.90	115.27
29	A	414[A]	PL9	C40-C39-C41	2.75	119.90	115.27
23	B	614	CLA	CBC-CAC-C3C	-2.75	104.86	112.43
25	b	618	BCR	C15-C14-C13	-2.75	123.39	127.31
23	c	511	CLA	CAC-C3C-C4C	2.75	128.37	124.81
26	X	101	SQD	O48-C23-C24	2.75	120.52	111.91
23	B	602	CLA	CHD-C4C-NC	2.75	128.53	124.20
29	D	705[B]	PL9	C27-C28-C29	-2.74	121.05	127.66
25	k	101	BCR	C24-C23-C22	-2.74	122.09	126.23
23	c	510	CLA	C1-O2A-CGA	2.74	123.64	116.44
25	B	617	BCR	C7-C8-C9	-2.74	122.09	126.23
23	C	504	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
23	b	606	CLA	CAA-C2A-C3A	-2.74	105.28	112.78
35	o	301	HTG	O2-C2-C3	-2.74	104.02	110.35
25	y	101	BCR	C34-C9-C8	2.74	122.39	118.08
29	A	414[A]	PL9	C10-C9-C8	-2.74	116.66	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	606	CLA	CHC-C1C-C2C	-2.74	119.16	126.72
23	A	404[A]	CLA	CAC-C3C-C4C	2.73	128.36	124.81
23	c	505	CLA	CBC-CAC-C3C	-2.73	104.89	112.43
23	c	504	CLA	CMC-C2C-C1C	2.73	129.20	125.04
23	a	407[B]	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
23	A	406[A]	CLA	CBC-CAC-C3C	-2.73	104.90	112.43
25	B	618	BCR	C37-C22-C23	2.73	122.38	118.08
23	B	606	CLA	CBC-CAC-C3C	-2.73	104.91	112.43
36	C	517[A]	DGD	C2G-O2G-C1B	-2.73	111.07	117.79
25	c	516	BCR	C21-C20-C19	-2.73	114.70	123.22
33	d	405[B]	LHG	O8-C23-O10	-2.73	116.71	123.59
23	c	508	CLA	CHD-C4C-NC	2.73	128.50	124.20
23	B	603	CLA	O2A-CGA-CBA	2.73	120.46	111.91
33	d	406[A]	LHG	O8-C23-C24	2.73	120.46	111.91
24	A	417[B]	PHO	O2D-CGD-O1D	-2.73	118.51	123.84
36	C	519	DGD	O3G-C3G-C2G	-2.72	104.32	110.90
23	C	512	CLA	C1-O2A-CGA	2.72	123.59	116.44
23	a	406[A]	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
29	D	705[A]	PL9	C42-C41-C39	-2.72	104.03	112.98
23	D	702[A]	CLA	CAA-C2A-C3A	-2.72	105.33	112.78
29	d	404[B]	PL9	C51-C49-C50	2.72	120.61	114.60
33	A	419[A]	LHG	O7-C7-O9	-2.72	117.13	123.70
23	D	703	CLA	C3B-C4B-NB	2.72	112.72	109.21
25	c	516	BCR	C32-C1-C6	-2.72	105.89	110.30
23	c	514	CLA	C2A-C1A-CHA	-2.72	119.11	123.86
23	c	502	CLA	CHD-C4C-NC	2.71	128.48	124.20
29	A	414[B]	PL9	C12-C13-C14	-2.71	121.13	127.66
29	d	404[A]	PL9	C36-C34-C33	-2.71	115.63	121.12
23	b	610	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
23	b	615	CLA	O2A-CGA-CBA	2.71	120.41	111.91
23	c	507	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
29	a	414[B]	PL9	C53-C6-C1	2.71	120.53	114.99
23	B	615	CLA	CHC-C1C-C2C	-2.71	119.23	126.72
23	d	402	CLA	C2A-C1A-CHA	-2.71	119.12	123.86
23	a	407[A]	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
23	b	612	CLA	CHD-C4C-NC	2.71	128.47	124.20
24	a	408[A]	PHO	CMA-C3A-C4A	-2.71	108.45	114.38
23	a	405[B]	CLA	CHD-C4C-NC	2.71	128.47	124.20
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
33	D	707[B]	LHG	O8-C23-O10	-2.70	116.77	123.59
23	C	504	CLA	CMC-C2C-C1C	2.70	129.16	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	412	SQD	C3-C4-C5	2.70	115.06	110.24
25	A	409	BCR	C8-C7-C6	-2.70	119.61	127.20
23	C	512	CLA	C1-C2-C3	-2.70	121.37	126.04
23	D	703	CLA	CMC-C2C-C1C	2.70	129.15	125.04
23	A	406[B]	CLA	C2A-C1A-CHA	-2.70	119.14	123.86
25	c	515	BCR	C34-C9-C10	-2.70	119.14	122.92
23	c	506	CLA	CAC-C3C-C4C	2.70	128.31	124.81
23	B	608	CLA	CHB-C4A-NA	2.70	128.25	124.51
25	a	410	BCR	C29-C30-C25	2.70	114.63	110.48
36	C	518[A]	DGD	O1G-C1A-O1A	-2.70	116.78	123.59
23	D	702[A]	CLA	CMC-C2C-C1C	2.70	129.15	125.04
23	C	512	CLA	CHD-C4C-NC	2.70	128.45	124.20
23	C	512	CLA	CMB-C2B-C3B	2.69	129.72	124.68
23	B	607	CLA	CHC-C1C-C2C	-2.69	119.27	126.72
29	d	404[B]	PL9	C36-C37-C38	-2.69	103.03	111.88
34	c	521	LMG	O8-C28-C29	2.69	120.36	111.91
24	a	416[B]	PHO	O2D-CGD-O1D	-2.69	118.58	123.84
25	b	619	BCR	C24-C23-C22	-2.69	122.17	126.23
26	a	411[B]	SQD	C45-O47-C7	-2.69	111.17	117.79
23	A	404[B]	CLA	CMC-C2C-C1C	2.69	129.13	125.04
23	B	603	CLA	C4-C3-C5	2.69	119.79	115.27
23	a	405[A]	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
34	C	501	LMG	C8-O7-C10	-2.69	111.18	117.79
25	b	618	BCR	C29-C30-C25	2.69	114.62	110.48
23	D	703	CLA	O2A-CGA-CBA	2.69	120.34	111.91
23	a	407[A]	CLA	CHC-C1C-C2C	-2.69	119.29	126.72
23	b	609	CLA	CHC-C1C-C2C	-2.68	119.30	126.72
23	c	514	CLA	CHD-C4C-NC	2.68	128.43	124.20
23	d	402	CLA	O2A-CGA-CBA	2.68	120.33	111.91
23	D	702[B]	CLA	C4-C3-C5	2.68	119.79	115.27
23	B	608	CLA	CMB-C2B-C3B	2.68	129.70	124.68
23	b	608	CLA	C11-C12-C13	-2.68	107.25	115.92
23	A	406[A]	CLA	CMC-C2C-C1C	2.68	129.12	125.04
23	A	405[A]	CLA	CAC-C3C-C4C	2.68	128.29	124.81
36	c	517[B]	DGD	O3G-C3G-C2G	-2.68	104.44	110.90
23	B	616	CLA	CHD-C4C-NC	2.68	128.42	124.20
23	b	603	CLA	CHC-C1C-C2C	-2.68	119.32	126.72
33	a	420[A]	LHG	O8-C23-C24	2.68	120.30	111.91
24	a	416[A]	PHO	CBA-CAA-C2A	-2.68	105.99	113.81
36	c	517[A]	DGD	C3G-C2G-C1G	-2.68	105.46	111.79
29	D	705[A]	PL9	C37-C38-C39	-2.67	121.22	127.66
24	A	407[B]	PHO	O2D-CGD-O1D	-2.67	118.61	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	609	CLA	CHC-C1C-C2C	-2.67	119.33	126.72
23	A	406[A]	CLA	C1-C2-C3	-2.67	121.42	126.04
23	c	512	CLA	CMC-C2C-C1C	2.67	129.11	125.04
23	B	601	CLA	CHC-C1C-C2C	-2.67	119.33	126.72
23	D	702[B]	CLA	O2A-CGA-O1A	-2.67	116.85	123.59
23	D	703	CLA	C2A-C1A-CHA	-2.67	119.19	123.86
25	y	101	BCR	C21-C20-C19	-2.67	114.88	123.22
23	c	502	CLA	CBC-CAC-C3C	-2.67	105.07	112.43
23	A	408	CLA	CMC-C2C-C1C	2.67	129.10	125.04
23	b	614	CLA	CMC-C2C-C1C	2.67	129.10	125.04
25	B	619	BCR	C38-C26-C25	-2.67	121.53	124.53
25	k	101	BCR	C15-C14-C13	-2.67	123.50	127.31
23	B	609	CLA	CHD-C4C-NC	2.67	128.41	124.20
36	c	517[B]	DGD	C2G-O2G-C1B	-2.66	111.23	117.79
23	c	509	CLA	O2A-CGA-CBA	2.66	120.27	111.91
23	C	508	CLA	C1-C2-C3	-2.66	121.44	126.04
25	B	617	BCR	C31-C1-C6	-2.66	105.98	110.30
23	B	603	CLA	CHD-C4C-NC	2.66	128.40	124.20
25	b	617	BCR	C24-C23-C22	-2.66	122.21	126.23
25	Y	101	BCR	C10-C11-C12	-2.66	114.91	123.22
25	t	102	BCR	C21-C20-C19	-2.66	114.91	123.22
23	C	503	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
25	H	101	BCR	C31-C1-C6	-2.66	105.98	110.30
23	c	512	CLA	O2A-CGA-CBA	2.66	120.26	111.91
23	C	510	CLA	C11-C12-C13	-2.66	107.32	115.92
23	b	616	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
23	a	407[A]	CLA	CAA-C2A-C3A	-2.66	105.50	112.78
23	B	610	CLA	CHD-C4C-NC	2.66	128.39	124.20
23	B	604	CLA	C6-C7-C8	-2.66	107.33	115.92
26	A	410[A]	SQD	O48-C23-O10	-2.65	116.89	123.59
23	b	612	CLA	CHC-C1C-C2C	-2.65	119.38	126.72
23	a	405[A]	CLA	CAC-C3C-C4C	2.65	128.25	124.81
23	a	407[B]	CLA	C1-C2-C3	-2.65	121.46	126.04
36	H	102	DGD	O1G-C1A-O1A	-2.65	116.90	123.59
25	C	516	BCR	C11-C10-C9	-2.65	123.53	127.31
23	B	607	CLA	C4C-C3C-C2C	-2.65	103.03	106.90
23	C	514	CLA	CHC-C1C-C2C	-2.65	119.39	126.72
25	t	102	BCR	C35-C13-C12	2.65	122.25	118.08
23	B	606	CLA	C4C-C3C-C2C	-2.65	103.04	106.90
29	D	705[A]	PL9	C40-C39-C41	2.65	119.72	115.27
25	t	102	BCR	C12-C13-C14	-2.65	114.88	118.94
36	H	102	DGD	O1G-C1A-C2A	2.65	120.21	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	505	CLA	C4C-C3C-C2C	-2.65	103.04	106.90
23	B	616	CLA	CHC-C1C-C2C	-2.64	119.41	126.72
23	c	506	CLA	O2A-CGA-CBA	2.64	120.20	111.91
23	c	509	CLA	CAA-C2A-C3A	-2.64	105.54	112.78
23	a	409	CLA	CMA-C3A-C2A	-2.64	103.17	113.83
23	C	506	CLA	CMB-C2B-C1B	2.64	132.52	128.46
23	a	406[B]	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
25	D	704	BCR	C3-C4-C5	-2.64	109.36	114.08
33	d	406[B]	LHG	O8-C23-C24	2.64	120.19	111.91
23	A	406[A]	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
29	D	705[B]	PL9	C37-C38-C39	-2.64	121.31	127.66
23	b	616	CLA	OBD-CAD-C3D	-2.64	122.18	128.52
25	b	619	BCR	C38-C26-C25	-2.64	121.57	124.53
23	A	406[A]	CLA	C4-C3-C5	2.63	119.70	115.27
23	B	603	CLA	C7-C6-C5	-2.63	106.20	113.36
23	b	604	CLA	C4-C3-C5	2.63	119.70	115.27
23	B	607	CLA	CBC-CAC-C3C	-2.63	105.17	112.43
24	A	417[A]	PHO	O2D-CGD-O1D	-2.63	118.69	123.84
25	c	515	BCR	C36-C18-C17	-2.63	119.24	122.92
23	d	401[B]	CLA	C4C-C3C-C2C	-2.63	103.06	106.90
23	c	502	CLA	C1-C2-C3	-2.63	121.49	126.04
32	B	627	LMT	C1B-C2B-C3B	2.63	115.47	110.00
23	B	604	CLA	CMC-C2C-C1C	2.63	129.04	125.04
23	B	606	CLA	CHC-C1C-C2C	-2.63	119.45	126.72
23	c	505	CLA	CHC-C1C-C2C	-2.63	119.45	126.72
29	a	414[B]	PL9	C40-C39-C41	2.62	119.69	115.27
23	b	607	CLA	CHC-C1C-C2C	-2.62	119.47	126.72
23	b	614	CLA	C4-C3-C5	2.62	119.68	115.27
36	H	102	DGD	C3E-C4E-C5E	-2.62	105.56	110.24
23	A	408	CLA	O2A-CGA-CBA	2.62	120.14	111.91
33	a	420[B]	LHG	O8-C23-C24	2.62	120.14	111.91
23	b	610	CLA	CHC-C1C-C2C	-2.62	119.47	126.72
32	a	417	LMT	C3'-C4'-C5'	-2.62	104.92	110.93
23	D	702[A]	CLA	CMB-C2B-C3B	2.62	129.58	124.68
23	b	611	CLA	CHD-C4C-NC	2.62	128.33	124.20
32	A	420	LMT	O5'-C5'-C6'	2.62	112.95	106.44
23	d	401[A]	CLA	CAA-C2A-C3A	-2.62	105.61	112.78
23	d	402	CLA	CBC-CAC-C3C	-2.62	105.21	112.43
25	k	101	BCR	C39-C30-C25	-2.62	106.05	110.30
23	B	604	CLA	C4-C3-C5	2.62	119.67	115.27
23	a	406[B]	CLA	CBC-CAC-C3C	-2.62	105.22	112.43
35	o	301	HTG	C2'-C1'-S1	-2.62	103.95	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	407[B]	CLA	CHC-C1C-C2C	-2.62	119.49	126.72
23	A	404[B]	CLA	CHD-C4C-NC	2.61	128.32	124.20
25	B	618	BCR	C2-C1-C6	2.61	114.51	110.48
23	b	612	CLA	CAC-C3C-C4C	2.61	128.20	124.81
23	C	509	CLA	CMB-C2B-C3B	2.61	129.57	124.68
29	A	414[A]	PL9	C53-C6-C1	2.61	120.33	114.99
32	m	103	LMT	C3'-C4'-C5'	-2.61	104.94	110.93
25	B	619	BCR	C21-C20-C19	-2.61	115.06	123.22
23	a	409	CLA	O2A-CGA-O1A	-2.61	117.00	123.59
23	b	602	CLA	CMA-C3A-C4A	-2.61	104.75	111.77
23	c	510	CLA	C4-C3-C5	2.61	119.66	115.27
33	D	706[A]	LHG	O8-C23-C24	2.61	120.09	111.91
23	B	602	CLA	CMA-C3A-C4A	-2.61	104.76	111.77
23	D	703	CLA	CAA-C2A-C3A	-2.61	105.64	112.78
26	b	620	SQD	C44-O6-C1	-2.61	108.64	113.74
23	c	506	CLA	C4-C3-C5	2.61	119.66	115.27
33	D	706[A]	LHG	O7-C7-C8	2.61	117.12	111.50
23	a	407[B]	CLA	CAA-C2A-C3A	-2.61	105.64	112.78
32	B	630	LMT	O5'-C5'-C4'	2.60	115.24	109.75
23	b	603	CLA	CBC-CAC-C3C	-2.60	105.25	112.43
24	A	407[B]	PHO	O2A-CGA-CBA	2.60	120.08	111.91
23	b	605	CLA	O2A-CGA-O1A	-2.60	117.03	123.59
23	c	513	CLA	C3B-C4B-NB	2.60	112.57	109.21
23	C	508	CLA	O2A-CGA-CBA	2.60	120.07	111.91
25	Y	101	BCR	C37-C22-C23	2.60	122.17	118.08
33	L	101[A]	LHG	O8-C23-C24	2.60	120.06	111.91
32	B	627	LMT	O1'-C1'-C2'	2.60	112.36	108.30
23	A	408	CLA	C4-C3-C5	2.60	119.64	115.27
23	a	406[A]	CLA	O2A-CGA-CBA	2.59	120.05	111.91
23	C	504	CLA	CHC-C1C-C2C	-2.59	119.55	126.72
23	A	405[A]	CLA	OBD-CAD-C3D	-2.59	122.28	128.52
29	d	404[B]	PL9	C53-C6-C1	2.59	120.29	114.99
23	C	514	CLA	CHD-C4C-NC	2.59	128.29	124.20
23	a	407[B]	CLA	CAC-C3C-C4C	2.59	128.17	124.81
23	A	406[B]	CLA	CMC-C2C-C1C	2.59	128.99	125.04
23	c	503	CLA	CMC-C2C-C1C	2.59	128.99	125.04
23	a	407[B]	CLA	O2A-CGA-O1A	-2.59	117.05	123.59
23	a	405[B]	CLA	C2A-C1A-CHA	-2.59	119.33	123.86
25	h	101	BCR	C24-C23-C22	-2.59	122.32	126.23
36	H	102	DGD	C3G-C2G-C1G	-2.59	105.66	111.79
23	C	507	CLA	C2A-C1A-CHA	-2.59	119.33	123.86
23	a	405[A]	CLA	C2A-C1A-CHA	-2.59	119.34	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	508	CLA	CBC-CAC-C3C	-2.59	105.30	112.43
23	C	503	CLA	CAC-C3C-C4C	2.59	128.16	124.81
23	B	608	CLA	CHD-C4C-NC	2.59	128.28	124.20
23	c	507	CLA	CHD-C4C-NC	2.58	128.28	124.20
25	d	403	BCR	C37-C22-C23	2.58	122.15	118.08
23	d	402	CLA	CHC-C1C-C2C	-2.58	119.58	126.72
23	d	401[B]	CLA	CBC-CAC-C3C	-2.58	105.31	112.43
23	B	616	CLA	CAC-C3C-C4C	2.58	128.16	124.81
23	B	601	CLA	O2A-CGA-CBA	2.58	120.01	111.91
23	b	602	CLA	O2A-CGA-O1A	-2.58	117.08	123.59
29	d	404[A]	PL9	C36-C37-C38	-2.58	103.40	111.88
23	C	514	CLA	O2A-CGA-CBA	2.58	120.00	111.91
23	C	505	CLA	CAC-C3C-C4C	2.58	128.16	124.81
29	A	414[B]	PL9	C42-C43-C44	-2.58	121.45	127.66
32	M	101	LMT	C3'-C4'-C5'	-2.58	105.02	110.93
23	b	615	CLA	C1-C2-C3	-2.58	121.58	126.04
23	C	502	CLA	CBC-CAC-C3C	-2.58	105.33	112.43
23	B	604	CLA	C11-C12-C13	-2.58	107.59	115.92
26	X	101	SQD	O5-C1-O6	2.58	116.08	109.97
23	C	503	CLA	C2A-C1A-CHA	-2.58	119.35	123.86
26	X	101	SQD	O47-C7-O49	-2.57	117.48	123.70
23	b	607	CLA	CBC-CAC-C3C	-2.57	105.33	112.43
36	C	517[B]	DGD	O6D-C1D-O3G	-2.57	103.88	109.97
23	B	613	CLA	CHC-C1C-C2C	-2.57	119.61	126.72
23	C	502	CLA	O2A-CGA-CBA	2.57	119.98	111.91
36	c	519	DGD	O1G-C1A-C2A	2.57	119.98	111.91
23	B	615	CLA	C6-C7-C8	-2.57	107.61	115.92
23	b	614	CLA	C2A-C1A-CHA	-2.57	119.36	123.86
23	a	407[B]	CLA	C2A-C1A-CHA	-2.57	119.36	123.86
23	a	405[A]	CLA	CMA-C3A-C4A	-2.57	104.87	111.77
23	b	607	CLA	C2A-C1A-CHA	-2.57	119.37	123.86
29	A	414[B]	PL9	C53-C6-C1	2.57	120.24	114.99
23	d	401[B]	CLA	CAA-C2A-C3A	-2.57	105.75	112.78
25	a	410	BCR	C33-C5-C6	-2.57	121.64	124.53
33	D	706[B]	LHG	O8-C23-C24	2.57	119.97	111.91
23	C	511	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
23	B	606	CLA	C1-C2-C3	-2.57	121.61	126.04
23	b	616	CLA	C4-C3-C5	2.57	119.59	115.27
26	f	102	SQD	O8-S-C6	2.56	109.83	105.74
23	a	405[B]	CLA	C4-C3-C5	2.56	119.58	115.27
23	b	601	CLA	C1-O2A-CGA	2.56	123.17	116.44
23	C	506	CLA	O2A-CGA-CBA	2.56	119.95	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	d	405[B]	LHG	O8-C23-C24	2.56	119.95	111.91
29	a	414[B]	PL9	C20-C19-C21	2.56	119.58	115.27
23	C	508	CLA	CHC-C1C-C2C	-2.56	119.63	126.72
23	D	702[A]	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
23	D	702[A]	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
25	H	101	BCR	C7-C8-C9	-2.56	122.36	126.23
23	c	512	CLA	CMB-C2B-C3B	2.56	129.47	124.68
23	b	612	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
36	c	517[A]	DGD	O1G-C1A-O1A	-2.56	117.13	123.59
23	D	703	CLA	CHD-C4C-NC	2.56	128.24	124.20
23	c	506	CLA	O2A-CGA-O1A	-2.56	117.13	123.59
23	B	605	CLA	C2A-C1A-CHA	-2.56	119.39	123.86
23	D	703	CLA	CHC-C1C-C2C	-2.56	119.65	126.72
23	C	509	CLA	O2A-CGA-O1A	-2.55	117.14	123.59
29	d	404[B]	PL9	C27-C28-C29	-2.55	121.51	127.66
34	C	520	LMG	O8-C28-O10	-2.55	117.15	123.59
36	C	517[B]	DGD	C2G-O2G-C1B	-2.55	111.51	117.79
26	A	410[B]	SQD	O9-S-C6	2.55	109.97	106.94
33	A	419[B]	LHG	O7-C7-O9	-2.55	117.54	123.70
23	B	601	CLA	CAC-C3C-C4C	2.55	128.12	124.81
25	H	101	BCR	C10-C11-C12	-2.55	115.26	123.22
23	c	512	CLA	CBC-CAC-C3C	-2.55	105.40	112.43
23	b	604	CLA	O2A-CGA-CBA	2.55	119.91	111.91
23	C	505	CLA	C4-C3-C5	2.55	119.56	115.27
36	c	517[B]	DGD	O6D-C1D-O3G	-2.55	103.94	109.97
29	A	414[B]	PL9	C47-C48-C49	-2.55	119.04	127.75
23	A	404[B]	CLA	C1-C2-C3	-2.55	121.63	126.04
23	C	508	CLA	C3B-C4B-NB	2.55	112.50	109.21
26	B	620	SQD	C44-O6-C1	-2.55	108.76	113.74
26	B	620	SQD	C1-O5-C5	-2.55	108.69	113.69
26	A	410[B]	SQD	O48-C23-O10	-2.54	117.17	123.59
23	c	513	CLA	O2A-CGA-O1A	-2.54	117.17	123.59
35	b	622	HTG	O5-C1-C2	2.54	113.51	110.31
23	C	508	CLA	CHD-C4C-NC	2.54	128.21	124.20
23	C	505	CLA	CBC-CAC-C3C	-2.54	105.42	112.43
23	b	607	CLA	CMB-C2B-C3B	2.54	129.43	124.68
23	A	405[A]	CLA	CMA-C3A-C2A	-2.54	103.58	113.83
24	a	416[B]	PHO	CBA-CAA-C2A	-2.54	106.39	113.81
23	b	611	CLA	CMB-C2B-C3B	2.54	129.43	124.68
24	a	416[A]	PHO	O1D-CGD-CBD	-2.54	120.51	124.74
25	C	515	BCR	C20-C21-C22	-2.54	123.69	127.31
32	B	630	LMT	O1'-C1'-C2'	2.54	112.27	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B	629	LMT	O5B-C5B-C4B	2.54	114.30	109.69
23	B	614	CLA	CMB-C2B-C3B	2.53	129.42	124.68
29	D	705[B]	PL9	C42-C41-C39	-2.53	104.64	112.98
26	a	412	SQD	C1-O5-C5	2.53	118.66	113.69
36	C	518[B]	DGD	C2G-O2G-C1B	-2.53	111.55	117.79
25	a	410	BCR	C24-C23-C22	-2.53	122.41	126.23
29	a	414[B]	PL9	C10-C9-C11	2.53	119.53	115.27
29	A	414[A]	PL9	C35-C34-C36	2.53	119.53	115.27
23	C	507	CLA	O2A-CGA-CBA	2.53	119.85	111.91
23	A	405[A]	CLA	C2A-C1A-CHA	-2.53	119.44	123.86
25	b	618	BCR	C28-C27-C26	-2.53	109.56	114.08
23	c	503	CLA	O2A-CGA-CBA	2.53	119.84	111.91
23	B	613	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
23	B	608	CLA	C11-C12-C13	-2.53	107.75	115.92
25	B	618	BCR	C28-C27-C26	-2.53	109.56	114.08
23	C	511	CLA	CAC-C3C-C4C	2.53	128.09	124.81
23	c	508	CLA	C3B-C4B-NB	2.53	112.48	109.21
23	D	702[B]	CLA	CMC-C2C-C1C	2.52	128.88	125.04
23	a	406[B]	CLA	O2A-CGA-CBA	2.52	119.82	111.91
23	a	407[A]	CLA	C2A-C1A-CHA	-2.52	119.45	123.86
23	A	406[A]	CLA	CMA-C3A-C2A	-2.52	103.66	113.83
23	c	513	CLA	CAC-C3C-C4C	2.52	128.08	124.81
23	d	401[B]	CLA	O2A-CGA-O1A	-2.52	117.23	123.59
23	c	504	CLA	C4-C3-C5	2.52	119.50	115.27
23	c	509	CLA	C4-C3-C5	2.52	119.50	115.27
23	d	401[A]	CLA	CMB-C2B-C3B	2.52	129.39	124.68
23	C	504	CLA	CBC-CAC-C3C	-2.52	105.50	112.43
23	c	511	CLA	C2A-C1A-CHA	-2.52	119.46	123.86
23	B	605	CLA	CED-O2D-CGD	2.52	121.63	115.94
29	D	705[B]	PL9	C7-C8-C9	-2.51	122.61	126.79
23	c	514	CLA	O2A-CGA-O1A	-2.51	117.25	123.59
23	B	607	CLA	C2A-C1A-CHA	-2.51	119.46	123.86
23	c	511	CLA	C11-C10-C8	-2.51	107.79	115.92
25	h	101	BCR	C37-C22-C21	-2.51	119.40	122.92
29	a	414[A]	PL9	C47-C48-C49	-2.51	119.16	127.75
23	B	614	CLA	C4C-C3C-C2C	-2.51	103.23	106.90
23	a	406[B]	CLA	C1-C2-C3	-2.51	121.70	126.04
36	c	519	DGD	O2G-C1B-C2B	2.51	116.91	111.50
23	a	406[A]	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
29	A	414[B]	PL9	C10-C9-C11	2.51	119.50	115.27
23	A	408	CLA	CAC-C3C-C4C	2.51	128.07	124.81
24	A	407[A]	PHO	O2A-CGA-CBA	2.51	119.78	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	407[A]	PHO	CMB-C2B-C3B	2.51	129.37	124.68
24	a	408[B]	PHO	O2D-CGD-O1D	-2.51	118.93	123.84
25	t	102	BCR	C37-C22-C23	2.51	122.03	118.08
23	a	407[A]	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
23	A	406[B]	CLA	C4C-C3C-C2C	-2.51	103.24	106.90
29	A	414[B]	PL9	C35-C34-C36	2.51	119.49	115.27
23	c	506	CLA	CHD-C4C-NC	2.51	128.15	124.20
23	C	514	CLA	C4-C3-C5	2.50	119.48	115.27
23	B	602	CLA	CHC-C1C-C2C	-2.50	119.79	126.72
23	C	503	CLA	CHD-C4C-NC	2.50	128.15	124.20
36	C	517[B]	DGD	O5D-C6D-C5D	-2.50	104.42	109.05
23	C	507	CLA	CAA-C2A-C3A	-2.50	105.93	112.78
25	c	515	BCR	C37-C22-C21	-2.50	119.42	122.92
23	B	601	CLA	CMB-C2B-C3B	2.50	129.35	124.68
23	C	502	CLA	C4-C3-C5	2.50	119.48	115.27
23	A	408	CLA	CMA-C3A-C2A	-2.50	103.75	113.83
32	F	101	LMT	C1'-O5'-C5'	-2.50	108.78	113.69
23	c	510	CLA	CHD-C4C-NC	2.50	128.14	124.20
23	B	615	CLA	CAC-C3C-C4C	2.50	128.05	124.81
23	a	405[A]	CLA	CMC-C2C-C1C	2.50	128.84	125.04
23	B	609	CLA	CAC-C3C-C4C	2.50	128.05	124.81
23	B	610	CLA	CAC-C3C-C4C	2.50	128.05	124.81
25	Y	101	BCR	C15-C16-C17	-2.49	118.36	123.47
23	B	606	CLA	C1-O2A-CGA	2.49	122.98	116.44
24	A	407[B]	PHO	CMC-C2C-C3C	2.49	129.64	124.94
26	f	102	SQD	O7-S-C6	2.49	109.90	106.94
23	A	405[B]	CLA	C4-C3-C5	2.49	119.46	115.27
23	C	508	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
32	T	101	LMT	C3'-C4'-C5'	-2.49	105.22	110.93
23	a	407[A]	CLA	O2A-CGA-CBA	2.49	119.72	111.91
34	c	520	LMG	C8-O7-C10	-2.49	111.67	117.79
25	b	619	BCR	C16-C17-C18	-2.49	123.76	127.31
23	C	507	CLA	O2A-CGA-O1A	-2.49	117.32	123.59
23	C	510	CLA	CHD-C4C-NC	2.48	128.12	124.20
24	a	408[A]	PHO	CMB-C2B-C3B	2.48	129.33	124.68
25	K	102	BCR	C29-C30-C25	2.48	114.30	110.48
23	c	514	CLA	CHC-C1C-C2C	-2.48	119.86	126.72
36	C	517[A]	DGD	O5D-C6D-C5D	-2.48	104.46	109.05
23	c	507	CLA	CAA-C2A-C3A	-2.48	105.99	112.78
29	d	404[A]	PL9	C17-C18-C19	-2.48	121.69	127.66
23	C	511	CLA	O2A-CGA-CBA	2.48	119.69	111.91
23	c	508	CLA	CHC-C1C-C2C	-2.48	119.87	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	o	301	HTG	C1-O5-C5	2.48	117.15	112.58
25	y	101	BCR	C16-C17-C18	-2.48	123.78	127.31
23	A	404[B]	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
24	A	407[A]	PHO	O2A-CGA-O1A	-2.48	117.34	123.59
25	b	618	BCR	C20-C21-C22	-2.47	123.78	127.31
32	B	630	LMT	C3'-C4'-C5'	-2.47	105.25	110.93
23	A	404[A]	CLA	CMA-C3A-C2A	-2.47	103.85	113.83
23	B	612	CLA	C4-C3-C5	2.47	119.43	115.27
27	b	628	GOL	C3-C2-C1	-2.47	102.09	111.70
23	b	616	CLA	CHC-C1C-C2C	-2.47	119.88	126.72
23	B	614	CLA	C2A-C1A-CHA	-2.47	119.54	123.86
23	B	602	CLA	CMB-C2B-C3B	2.47	129.30	124.68
23	b	601	CLA	CMC-C2C-C1C	2.47	128.80	125.04
29	D	705[B]	PL9	C51-C49-C50	2.47	120.05	114.60
25	c	516	BCR	C37-C22-C21	-2.47	119.47	122.92
26	f	102	SQD	O5-C5-C4	2.47	114.17	109.69
23	C	513	CLA	CHB-C4A-NA	2.47	127.92	124.51
25	c	515	BCR	C20-C21-C22	-2.46	123.79	127.31
23	b	607	CLA	O2A-CGA-O1A	-2.46	117.37	123.59
23	b	602	CLA	CAA-CBA-CGA	-2.46	106.06	113.25
23	c	513	CLA	CMA-C3A-C4A	-2.46	105.16	111.77
33	d	405[A]	LHG	O8-C23-O10	-2.46	117.38	123.59
25	b	619	BCR	C11-C10-C9	-2.46	123.80	127.31
23	c	507	CLA	O2A-CGA-O1A	-2.46	117.38	123.59
23	A	404[B]	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
23	C	513	CLA	C3B-C4B-NB	2.46	112.39	109.21
26	a	411[A]	SQD	O7-S-C6	2.46	109.86	106.94
23	C	511	CLA	CMC-C2C-C1C	2.46	128.78	125.04
23	A	405[B]	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
23	B	612	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
23	c	509	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
23	B	616	CLA	O2A-CGA-CBA	2.46	119.62	111.91
23	c	504	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
23	b	615	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
23	c	505	CLA	CED-O2D-CGD	2.46	121.49	115.94
23	c	507	CLA	C4-C3-C5	2.46	119.40	115.27
23	a	406[B]	CLA	CMA-C3A-C2A	-2.46	103.92	113.83
23	C	512	CLA	CMC-C2C-C1C	2.45	128.78	125.04
23	a	405[B]	CLA	C4C-C3C-C2C	-2.45	103.32	106.90
23	c	507	CLA	CMB-C2B-C3B	2.45	129.27	124.68
23	a	406[A]	CLA	C4C-C3C-C2C	-2.45	103.32	106.90
23	c	511	CLA	C4C-C3C-C2C	-2.45	103.32	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	403	BCR	C40-C30-C39	2.45	116.06	108.53
23	C	513	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
23	A	404[B]	CLA	C4-C3-C5	2.45	119.39	115.27
23	A	405[A]	CLA	CMA-C3A-C4A	-2.45	105.19	111.77
35	b	625	HTG	C1-C2-C3	-2.45	105.75	110.59
38	f	101	HEM	CMD-C2D-C1D	2.45	128.77	125.04
23	a	407[B]	CLA	O2A-CGA-CBA	2.45	119.59	111.91
38	F	102	HEM	O2D-CGD-CBD	2.45	121.89	114.03
29	a	414[A]	PL9	C40-C39-C41	2.45	119.39	115.27
23	C	506	CLA	CHD-C4C-NC	2.45	128.06	124.20
25	T	102	BCR	C21-C20-C19	-2.45	115.58	123.22
29	D	705[A]	PL9	C27-C28-C29	-2.44	121.77	127.66
23	d	402	CLA	CMC-C2C-C1C	2.44	128.76	125.04
29	a	414[A]	PL9	C20-C19-C21	2.44	119.38	115.27
26	f	102	SQD	O47-C7-O49	-2.44	117.80	123.70
23	c	512	CLA	C1-O2A-CGA	2.44	122.85	116.44
23	c	509	CLA	CHD-C4C-NC	2.44	128.05	124.20
38	F	102	HEM	CMD-C2D-C1D	2.44	128.75	125.04
23	A	405[A]	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
23	a	405[A]	CLA	CHD-C4C-NC	2.44	128.05	124.20
23	c	511	CLA	CBC-CAC-C3C	-2.44	105.71	112.43
23	C	514	CLA	CAA-C2A-C3A	-2.44	106.10	112.78
23	b	613	CLA	CMA-C3A-C4A	-2.44	105.23	111.77
23	C	503	CLA	O2A-CGA-O1A	-2.44	117.45	123.59
23	B	616	CLA	CBC-CAC-C3C	-2.44	105.72	112.43
24	A	407[B]	PHO	CMA-C3A-C4A	-2.43	109.05	114.38
32	B	629	LMT	O5'-C5'-C6'	2.43	112.48	106.44
23	b	601	CLA	CBC-CAC-C3C	-2.43	105.73	112.43
24	a	408[A]	PHO	O2A-CGA-O1A	-2.43	117.46	123.59
23	c	509	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
26	B	620	SQD	O48-C23-O10	-2.43	117.46	123.59
23	c	505	CLA	C2A-C1A-CHA	-2.43	119.61	123.86
24	A	407[B]	PHO	O1D-CGD-CBD	-2.43	120.70	124.74
25	c	515	BCR	C28-C27-C26	-2.43	109.74	114.08
23	C	506	CLA	O2A-CGA-O1A	-2.43	117.47	123.59
29	D	705[B]	PL9	C40-C39-C41	2.43	119.35	115.27
23	c	510	CLA	O2A-C1-C2	2.43	115.01	108.64
26	X	101	SQD	O8-S-O7	-2.42	105.35	111.27
29	d	404[A]	PL9	C47-C48-C49	-2.42	119.47	127.75
23	C	507	CLA	C4C-C3C-C2C	-2.42	103.36	106.90
23	C	511	CLA	C2A-C1A-CHA	-2.42	119.62	123.86
23	C	509	CLA	O2A-CGA-CBA	2.42	119.50	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	510	CLA	CMB-C2B-C3B	2.42	129.21	124.68
23	a	409	CLA	CAC-C3C-C4C	2.42	127.95	124.81
24	A	417[B]	PHO	CMB-C2B-C3B	2.42	129.20	124.68
23	a	405[B]	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
23	B	602	CLA	C2A-C1A-CHA	-2.42	119.63	123.86
23	B	611	CLA	C2C-C1C-NC	2.42	112.24	109.97
26	X	101	SQD	C46-C45-C44	-2.42	106.08	111.79
26	a	411[A]	SQD	O8-S-C6	2.41	109.59	105.74
23	B	605	CLA	CHC-C1C-C2C	-2.41	120.04	126.72
29	A	414[A]	PL9	C35-C34-C33	-2.41	117.49	123.68
23	B	614	CLA	CED-O2D-CGD	2.41	121.39	115.94
23	c	507	CLA	C2A-C1A-CHA	-2.41	119.64	123.86
23	B	612	CLA	CHC-C1C-C2C	-2.41	120.05	126.72
25	c	516	BCR	C15-C14-C13	-2.41	123.87	127.31
23	c	505	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
26	b	620	SQD	C1-C2-C3	-2.41	104.98	110.00
23	a	405[B]	CLA	C1-C2-C3	-2.41	121.88	126.04
29	d	404[B]	PL9	C36-C34-C33	-2.41	116.24	121.12
23	d	401[B]	CLA	C2A-C1A-CHA	-2.41	119.65	123.86
23	A	404[A]	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
25	C	515	BCR	C38-C26-C25	-2.41	121.83	124.53
23	b	604	CLA	O2A-CGA-O1A	-2.41	117.52	123.59
23	c	505	CLA	O2A-CGA-CBA	2.41	119.46	111.91
29	A	414[A]	PL9	C42-C43-C44	-2.41	121.87	127.66
36	c	517[B]	DGD	C3G-C2G-C1G	-2.40	106.10	111.79
23	b	608	CLA	C11-C10-C8	-2.40	108.15	115.92
23	C	503	CLA	O2A-CGA-CBA	2.40	119.45	111.91
24	a	408[B]	PHO	CMB-C2B-C3B	2.40	129.17	124.68
23	C	504	CLA	C3B-C4B-NB	2.40	112.31	109.21
29	D	705[B]	PL9	C53-C6-C1	2.40	119.90	114.99
23	D	702[B]	CLA	CAC-C3C-C4C	2.40	127.92	124.81
26	a	411[B]	SQD	O48-C23-C24	2.40	119.43	111.91
29	D	705[B]	PL9	C12-C13-C14	-2.39	121.89	127.66
23	b	606	CLA	CAC-C3C-C2C	2.39	131.62	127.53
29	A	414[B]	PL9	C45-C44-C46	2.39	119.29	115.27
34	d	410	LMG	O8-C28-C29	2.39	119.41	111.91
23	c	506	CLA	CMC-C2C-C1C	2.39	128.68	125.04
23	D	702[B]	CLA	CBC-CAC-C3C	-2.39	105.84	112.43
24	A	407[B]	PHO	C4-C3-C5	2.39	119.29	115.27
26	f	102	SQD	C44-O6-C1	-2.39	109.07	113.74
23	B	613	CLA	CHB-C4A-NA	2.39	127.81	124.51
25	t	102	BCR	C7-C8-C9	-2.39	122.63	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	612	CLA	CHD-C4C-NC	2.39	127.97	124.20
23	a	406[B]	CLA	C1-O2A-CGA	2.39	122.71	116.44
26	a	412	SQD	O8-S-C6	2.39	109.54	105.74
25	c	515	BCR	C36-C18-C19	2.39	121.83	118.08
23	c	513	CLA	CHB-C4A-NA	2.38	127.81	124.51
26	A	410[B]	SQD	O7-S-C6	2.38	109.77	106.94
23	B	601	CLA	CBC-CAC-C3C	-2.38	105.86	112.43
23	b	605	CLA	CMC-C2C-C1C	2.38	128.66	125.04
23	c	502	CLA	O2A-CGA-CBA	2.38	119.38	111.91
33	L	101[A]	LHG	O8-C23-O10	-2.38	117.59	123.59
23	d	402	CLA	C6-C7-C8	-2.38	108.23	115.92
23	C	507	CLA	CGD-CBD-CAD	-2.38	103.03	110.73
29	a	414[A]	PL9	C10-C9-C8	-2.38	117.58	123.68
23	B	608	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
29	d	404[A]	PL9	C7-C8-C9	-2.38	122.84	126.79
29	D	705[A]	PL9	C45-C44-C46	2.38	119.27	115.27
23	B	609	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
23	b	608	CLA	O2A-CGA-CBA	2.38	119.36	111.91
25	y	101	BCR	C16-C15-C14	-2.37	118.61	123.47
36	c	519	DGD	O3G-C3G-C2G	-2.37	105.17	110.90
23	c	514	CLA	C1-C2-C3	-2.37	121.94	126.04
23	B	611	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
24	A	417[B]	PHO	CMC-C2C-C3C	2.37	129.42	124.94
23	b	603	CLA	CMC-C2C-C1C	2.37	128.65	125.04
23	A	406[B]	CLA	CAC-C3C-C4C	2.37	127.89	124.81
23	B	604	CLA	C6-C5-C3	-2.37	107.25	113.45
23	b	604	CLA	C4C-C3C-C2C	-2.37	103.45	106.90
26	b	620	SQD	O47-C7-O49	-2.37	117.98	123.70
29	a	414[B]	PL9	C45-C44-C46	2.36	119.25	115.27
23	A	408	CLA	C1-O2A-CGA	2.36	122.64	116.44
25	y	101	BCR	C24-C23-C22	-2.36	122.66	126.23
23	A	408	CLA	CHB-C4A-NA	2.36	127.78	124.51
23	c	502	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
23	c	505	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
23	d	402	CLA	C4-C3-C5	2.36	119.24	115.27
23	b	606	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
24	a	416[B]	PHO	C4-C3-C2	-2.36	117.63	123.68
29	D	705[A]	PL9	C22-C23-C24	-2.36	121.98	127.66
23	b	608	CLA	C4C-C3C-C2C	-2.36	103.46	106.90
26	X	101	SQD	O48-C23-O10	-2.36	117.64	123.59
29	a	414[B]	PL9	C47-C48-C49	-2.36	119.69	127.75
23	c	504	CLA	CAC-C3C-C4C	2.36	127.87	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	409	BCR	C37-C22-C23	2.36	121.79	118.08
23	c	503	CLA	O2A-CGA-O1A	-2.35	117.65	123.59
24	A	417[A]	PHO	CMA-C3A-C4A	-2.35	109.23	114.38
23	b	604	CLA	C6-C5-C3	-2.35	107.29	113.45
23	c	507	CLA	O2A-CGA-CBA	2.35	119.29	111.91
36	c	518[B]	DGD	O1G-C1A-C2A	2.35	119.29	111.91
29	A	414[A]	PL9	C45-C44-C46	2.35	119.22	115.27
23	B	611	CLA	C1C-C2C-C3C	-2.35	104.49	106.96
36	C	518[A]	DGD	O6E-C5E-C6E	2.35	112.28	106.44
32	A	420	LMT	O1'-C1'-C2'	2.35	111.97	108.30
29	a	414[A]	PL9	C45-C44-C46	2.35	119.22	115.27
23	C	504	CLA	O2A-CGA-CBA	2.35	119.28	111.91
23	B	605	CLA	C3B-C4B-NB	2.35	112.25	109.21
23	C	502	CLA	C2A-C1A-CHA	-2.35	119.75	123.86
23	b	603	CLA	C7-C6-C5	-2.35	106.98	113.36
23	a	406[A]	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
23	C	508	CLA	C4-C3-C5	2.35	119.22	115.27
23	C	505	CLA	C2A-C1A-CHA	-2.35	119.76	123.86
29	d	404[B]	PL9	C22-C23-C24	-2.35	122.01	127.66
23	B	605	CLA	CAC-C3C-C4C	2.34	127.85	124.81
23	d	401[B]	CLA	CHD-C4C-NC	2.34	127.89	124.20
34	C	521	LMG	C9-C8-C7	-2.34	106.25	111.79
32	e	101	LMT	O1'-C1'-C2'	2.34	111.96	108.30
25	k	101	BCR	C38-C26-C25	-2.34	121.90	124.53
24	a	408[A]	PHO	CMC-C2C-C3C	2.34	129.35	124.94
23	B	606	CLA	C4-C3-C5	2.34	119.20	115.27
23	b	606	CLA	C1-O2A-CGA	2.34	122.58	116.44
23	C	511	CLA	CBC-CAC-C3C	-2.34	105.99	112.43
23	b	610	CLA	CAA-CBA-CGA	-2.34	106.42	113.25
23	b	609	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
26	A	410[B]	SQD	O8-S-C6	2.34	109.46	105.74
23	a	407[B]	CLA	CMB-C2B-C3B	2.34	129.05	124.68
23	D	702[B]	CLA	CHD-C4C-NC	2.33	127.88	124.20
23	b	614	CLA	CAC-C3C-C4C	2.33	127.84	124.81
25	H	101	BCR	C36-C18-C17	-2.33	119.65	122.92
33	L	101[B]	LHG	O8-C23-C24	2.33	119.23	111.91
25	y	101	BCR	C11-C10-C9	-2.33	123.98	127.31
25	D	704	BCR	C15-C16-C17	-2.33	118.70	123.47
23	D	702[A]	CLA	CHD-C4C-NC	2.33	127.88	124.20
24	a	416[B]	PHO	C1A-C2A-C3A	-2.33	100.62	102.84
23	a	406[A]	CLA	C1-O2A-CGA	2.33	122.56	116.44
34	m	101	LMG	C8-O7-C10	-2.33	112.06	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	619	BCR	C34-C9-C8	2.33	121.75	118.08
23	C	504	CLA	CAC-C3C-C4C	2.33	127.83	124.81
36	C	517[B]	DGD	O3G-C3G-C2G	-2.33	105.28	110.90
29	d	404[B]	PL9	C20-C19-C21	2.33	119.19	115.27
29	a	414[A]	PL9	C35-C34-C33	-2.33	117.70	123.68
36	C	518[A]	DGD	O1G-C1A-C2A	2.33	119.21	111.91
36	c	518[A]	DGD	O1G-C1A-C2A	2.33	119.21	111.91
23	b	615	CLA	C6-C7-C8	-2.33	108.40	115.92
26	f	102	SQD	O6-C1-C2	2.33	111.93	108.30
33	d	405[A]	LHG	O8-C23-C24	2.33	119.21	111.91
23	c	513	CLA	CBA-CAA-C2A	-2.32	107.00	113.86
24	A	417[B]	PHO	O1D-CGD-CBD	-2.32	120.87	124.74
25	K	102	BCR	C36-C18-C19	2.32	121.74	118.08
36	c	517[A]	DGD	C2G-O2G-C1B	-2.32	112.07	117.79
25	D	704	BCR	C21-C20-C19	-2.32	115.97	123.22
25	B	618	BCR	C3-C4-C5	-2.32	109.93	114.08
23	c	513	CLA	CMC-C2C-C1C	2.32	128.57	125.04
23	b	609	CLA	O2A-CGA-CBA	2.32	119.19	111.91
23	A	408	CLA	C2A-C1A-CHA	-2.32	119.80	123.86
23	c	508	CLA	O1D-CGD-CBD	-2.32	119.74	124.48
38	F	102	HEM	O2A-CGA-CBA	2.32	121.48	114.03
23	a	407[A]	CLA	C4-C3-C5	2.32	119.17	115.27
25	c	515	BCR	C38-C26-C25	-2.32	121.92	124.53
25	K	102	BCR	C2-C1-C6	2.32	114.05	110.48
23	b	608	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
23	A	404[A]	CLA	CMA-C3A-C4A	-2.32	105.54	111.77
25	C	515	BCR	C40-C30-C25	-2.32	106.54	110.30
23	a	405[B]	CLA	CHB-C4A-NA	2.32	127.71	124.51
26	a	411[A]	SQD	O48-C23-C24	2.32	119.17	111.91
23	C	513	CLA	CHC-C1C-C2C	-2.32	120.32	126.72
36	h	102	DGD	C6D-C5D-C4D	2.32	116.93	112.09
23	B	609	CLA	C2A-C1A-CHA	-2.31	119.81	123.86
25	B	618	BCR	C7-C8-C9	-2.31	122.74	126.23
23	b	606	CLA	C1-C2-C3	-2.31	122.04	126.04
23	b	602	CLA	O2A-CGA-CBA	2.31	119.17	111.91
23	b	602	CLA	CMB-C2B-C3B	2.31	129.01	124.68
23	c	511	CLA	CED-O2D-CGD	2.31	121.17	115.94
26	a	412	SQD	O48-C23-O10	-2.31	117.76	123.59
29	A	414[B]	PL9	C51-C49-C50	2.31	119.71	114.60
34	B	621	LMG	C12-C11-C10	-2.31	105.22	113.62
29	A	414[A]	PL9	C37-C36-C34	-2.31	105.38	112.98
25	K	102	BCR	C39-C30-C25	-2.31	106.55	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	507	CLA	CMB-C2B-C3B	2.31	129.00	124.68
38	F	102	HEM	C3C-C4C-NC	-2.31	106.58	110.94
23	A	405[B]	CLA	CMA-C3A-C4A	-2.31	105.57	111.77
23	b	601	CLA	CAC-C3C-C4C	2.31	127.80	124.81
23	a	405[A]	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
23	c	502	CLA	CMB-C2B-C1B	2.31	132.01	128.46
25	T	102	BCR	C7-C6-C5	-2.30	115.88	121.46
23	d	401[A]	CLA	CMC-C2C-C1C	2.30	128.55	125.04
23	c	508	CLA	CBC-CAC-C3C	-2.30	106.08	112.43
23	B	616	CLA	C2A-C1A-CHA	-2.30	119.83	123.86
23	A	404[B]	CLA	CAA-CBA-CGA	-2.30	106.53	113.25
29	A	414[A]	PL9	C2-C3-C4	2.30	121.97	118.80
23	a	409	CLA	CMB-C2B-C3B	2.30	128.98	124.68
23	A	404[A]	CLA	CMC-C2C-C1C	2.30	128.54	125.04
25	T	102	BCR	C1-C6-C7	2.30	122.28	115.78
23	B	604	CLA	O1D-CGD-CBD	-2.30	119.78	124.48
23	A	404[B]	CLA	CAC-C3C-C4C	2.30	127.79	124.81
36	H	102	DGD	O6E-C5E-C6E	2.30	112.15	106.44
25	k	101	BCR	C2-C1-C6	2.30	114.02	110.48
23	C	504	CLA	C2A-C1A-CHA	-2.30	119.84	123.86
23	b	605	CLA	CAC-C3C-C4C	2.29	127.79	124.81
32	B	629	LMT	O5'-C5'-C4'	2.29	114.59	109.75
23	C	511	CLA	CMB-C2B-C3B	2.29	128.97	124.68
29	A	414[A]	PL9	C47-C48-C49	-2.29	119.92	127.75
24	a	416[A]	PHO	O2D-CGD-O1D	-2.29	119.36	123.84
33	d	406[A]	LHG	O8-C23-O10	-2.29	117.82	123.59
23	a	407[A]	CLA	CBC-CAC-C3C	-2.29	106.12	112.43
25	h	101	BCR	C36-C18-C19	2.29	121.68	118.08
23	c	507	CLA	CBC-CAC-C3C	-2.29	106.13	112.43
34	m	101	LMG	C7-O1-C1	-2.28	109.28	113.74
29	D	705[B]	PL9	C30-C29-C31	2.28	119.11	115.27
23	a	406[B]	CLA	C4-C3-C5	2.28	119.11	115.27
23	C	505	CLA	CMB-C2B-C3B	2.28	128.95	124.68
23	C	510	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
23	A	404[B]	CLA	CAA-C2A-C1A	-2.28	104.50	111.97
23	b	608	CLA	CAA-C2A-C3A	-2.28	106.54	112.78
23	b	602	CLA	C11-C10-C8	-2.28	108.55	115.92
23	B	607	CLA	O2A-CGA-CBA	2.28	119.06	111.91
23	B	601	CLA	C2A-C1A-CHA	-2.28	119.88	123.86
23	B	601	CLA	CHB-C4A-NA	2.28	127.66	124.51
23	C	513	CLA	CMB-C2B-C3B	2.28	128.94	124.68
23	b	605	CLA	CHB-C4A-NA	2.27	127.66	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	410	BCR	C40-C30-C25	-2.27	106.61	110.30
23	a	406[B]	CLA	CHB-C4A-NA	2.27	127.66	124.51
23	c	512	CLA	CAC-C3C-C4C	2.27	127.76	124.81
23	a	405[A]	CLA	CMA-C3A-C2A	-2.27	104.66	113.83
23	c	514	CLA	CBC-CAC-C3C	-2.27	106.17	112.43
25	k	101	BCR	C3-C4-C5	-2.27	110.02	114.08
29	d	404[A]	PL9	C31-C32-C33	-2.27	104.42	111.88
23	a	406[B]	CLA	C2A-C1A-CHA	-2.27	119.89	123.86
26	f	102	SQD	O48-C23-O10	-2.27	117.87	123.59
24	A	417[A]	PHO	O1D-CGD-CBD	-2.27	120.96	124.74
34	c	501	LMG	O8-C28-C29	2.27	119.02	111.91
23	b	606	CLA	CMC-C2C-C1C	2.26	128.49	125.04
23	B	608	CLA	CBC-CAC-C3C	-2.26	106.19	112.43
23	c	508	CLA	C1-C2-C3	-2.26	122.13	126.04
23	B	603	CLA	CMA-C3A-C2A	-2.26	104.71	113.83
33	d	412[A]	LHG	O7-C7-O9	-2.26	118.24	123.70
23	D	702[A]	CLA	C4-C3-C5	2.26	119.07	115.27
33	d	405[A]	LHG	C6-C5-C4	-2.26	106.44	111.79
25	t	102	BCR	C36-C18-C19	2.26	121.64	118.08
25	Y	101	BCR	C28-C27-C26	-2.26	110.04	114.08
23	b	602	CLA	CAC-C3C-C4C	2.26	127.74	124.81
25	C	515	BCR	C16-C17-C18	-2.26	124.09	127.31
23	b	606	CLA	CMB-C2B-C3B	2.26	128.90	124.68
25	Y	101	BCR	C36-C18-C17	-2.26	119.76	122.92
23	B	606	CLA	CMB-C2B-C3B	2.26	128.90	124.68
33	b	629[B]	LHG	O8-C23-O10	-2.26	117.89	123.59
23	c	508	CLA	C4C-C3C-C2C	-2.26	103.61	106.90
33	b	629[A]	LHG	O8-C23-O10	-2.26	117.90	123.59
34	d	410	LMG	C7-O1-C1	-2.26	109.33	113.74
23	c	502	CLA	C4-C3-C5	2.26	119.07	115.27
24	a	416[A]	PHO	C4-C3-C2	-2.26	117.89	123.68
23	C	512	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
23	c	504	CLA	CHC-C1C-C2C	-2.26	120.48	126.72
25	c	515	BCR	C35-C13-C14	-2.25	119.77	122.92
25	D	704	BCR	C34-C9-C10	-2.25	119.77	122.92
23	C	513	CLA	CBA-CAA-C2A	-2.25	107.22	113.86
23	d	401[B]	CLA	CAC-C3C-C4C	2.25	127.73	124.81
23	D	702[B]	CLA	CMB-C2B-C3B	2.25	128.89	124.68
23	B	606	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
23	B	603	CLA	CMC-C2C-C1C	2.25	128.47	125.04
23	b	607	CLA	CHD-C4C-NC	2.25	127.75	124.20
29	D	705[A]	PL9	C20-C19-C21	2.25	119.05	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	613	CLA	CHD-C4C-NC	2.25	127.75	124.20
23	a	409	CLA	OBD-CAD-C3D	-2.25	123.11	128.52
24	A	417[A]	PHO	CMB-C2B-C3B	2.25	128.88	124.68
23	C	503	CLA	CBC-CAC-C3C	-2.25	106.24	112.43
25	h	101	BCR	C34-C9-C8	2.24	121.61	118.08
23	b	608	CLA	C2A-C1A-CHA	-2.24	119.93	123.86
24	A	407[B]	PHO	O2A-CGA-O1A	-2.24	117.93	123.59
29	A	414[B]	PL9	C25-C24-C26	2.24	119.04	115.27
24	a	416[A]	PHO	CED-O2D-CGD	2.24	121.00	115.94
26	A	412	SQD	C1-C2-C3	-2.24	105.33	110.00
34	d	410	LMG	O8-C28-O10	-2.24	117.94	123.59
25	b	618	BCR	C37-C22-C23	2.24	121.60	118.08
38	f	101	HEM	C3C-C4C-NC	-2.24	106.72	110.94
23	b	608	CLA	CMA-C3A-C4A	-2.24	105.76	111.77
26	B	620	SQD	O5-C1-C2	-2.24	105.62	110.35
34	c	501	LMG	O6-C5-C4	2.23	113.75	109.69
25	y	101	BCR	C10-C11-C12	-2.23	116.25	123.22
23	b	615	CLA	CHA-C1A-NA	-2.23	121.28	126.40
29	D	705[A]	PL9	C36-C37-C38	-2.23	104.54	111.88
23	A	408	CLA	C11-C12-C13	-2.23	108.70	115.92
25	b	619	BCR	C37-C22-C23	2.23	121.59	118.08
26	a	412	SQD	O5-C5-C4	2.23	113.75	109.69
23	b	610	CLA	CAC-C3C-C2C	2.23	131.34	127.53
23	b	601	CLA	O2A-CGA-CBA	2.23	118.90	111.91
23	C	511	CLA	C4-C3-C2	-2.23	117.96	123.68
25	t	102	BCR	C1-C6-C7	2.23	122.08	115.78
33	E	101[B]	LHG	O7-C7-O9	-2.23	118.32	123.70
25	B	617	BCR	C34-C9-C8	2.22	121.58	118.08
23	a	405[A]	CLA	C7-C6-C5	-2.22	107.32	113.36
32	m	103	LMT	C3B-C4B-C5B	-2.22	106.27	110.24
35	b	625	HTG	C1'-S1-C1	2.22	104.25	100.09
33	b	629[B]	LHG	C5-O7-C7	-2.22	112.32	117.79
36	c	519	DGD	O2E-C2E-C3E	-2.22	105.21	110.35
23	b	607	CLA	CAC-C3C-C4C	2.22	127.69	124.81
23	d	401[A]	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
26	A	410[A]	SQD	O8-S-C6	2.22	109.28	105.74
29	A	414[B]	PL9	C37-C36-C34	-2.22	105.67	112.98
36	C	518[B]	DGD	O1G-C1A-C2A	2.22	118.88	111.91
23	A	405[B]	CLA	CMA-C3A-C2A	-2.22	104.88	113.83
23	A	405[A]	CLA	CHB-C4A-NA	2.22	127.58	124.51
23	c	508	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
23	B	615	CLA	O2D-CGD-O1D	-2.22	119.50	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	C	517[A]	DGD	C3G-C2G-C1G	-2.22	106.55	111.79
36	c	518[A]	DGD	O4E-C4E-C3E	-2.22	105.23	110.35
23	b	613	CLA	CED-O2D-CGD	2.21	120.95	115.94
26	a	411[B]	SQD	O47-C7-O49	-2.21	118.35	123.70
23	a	409	CLA	CHC-C1C-C2C	-2.21	120.60	126.72
26	X	101	SQD	O6-C44-C45	2.21	116.23	110.90
23	B	611	CLA	OBD-CAD-C3D	-2.21	123.20	128.52
29	d	404[B]	PL9	C15-C14-C16	2.21	118.99	115.27
36	C	519	DGD	O2G-C1B-C2B	2.21	116.27	111.50
29	D	705[B]	PL9	C22-C23-C24	-2.21	122.34	127.66
34	c	521	LMG	O8-C28-O10	-2.21	118.02	123.59
25	b	619	BCR	C39-C30-C25	-2.21	106.72	110.30
34	c	520	LMG	O8-C28-O10	-2.21	118.02	123.59
25	D	704	BCR	C29-C28-C27	-2.21	106.45	111.38
23	b	605	CLA	C1-O2A-CGA	2.21	122.23	116.44
23	A	406[B]	CLA	CHB-C4A-NA	2.21	127.56	124.51
38	F	102	HEM	CAD-C3D-C4D	2.21	128.51	124.66
34	Z	101	LMG	C1-O6-C5	2.20	118.02	113.69
23	B	605	CLA	O2A-CGA-CBA	2.20	118.83	111.91
23	C	513	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
25	C	515	BCR	C29-C30-C25	2.20	113.87	110.48
23	b	606	CLA	C4-C3-C2	-2.20	118.03	123.68
23	c	504	CLA	O2A-CGA-CBA	2.20	118.82	111.91
34	C	520	LMG	C8-O7-C10	-2.20	112.37	117.79
23	C	508	CLA	CMB-C2B-C1B	2.20	131.85	128.46
24	A	407[A]	PHO	C1-C2-C3	-2.20	122.24	126.04
23	a	407[A]	CLA	CAC-C3C-C4C	2.20	127.67	124.81
23	c	507	CLA	CGD-CBD-CAD	-2.20	103.61	110.73
23	B	615	CLA	C2A-C1A-CHA	-2.20	120.01	123.86
23	a	406[B]	CLA	OBD-CAD-C3D	-2.20	123.23	128.52
23	c	511	CLA	C4-C3-C2	-2.20	118.04	123.68
23	A	405[B]	CLA	CED-O2D-CGD	2.20	120.91	115.94
23	C	506	CLA	CHA-C1A-NA	-2.20	121.36	126.40
25	D	704	BCR	C11-C10-C9	-2.20	124.17	127.31
29	A	414[A]	PL9	C51-C49-C50	2.20	119.46	114.60
23	b	615	CLA	CBC-CAC-C3C	-2.20	106.37	112.43
23	c	514	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
23	B	609	CLA	CMB-C2B-C1B	2.20	131.84	128.46
24	A	417[A]	PHO	O2A-CGA-CBA	2.20	118.80	111.91
23	b	611	CLA	OBD-CAD-C3D	-2.20	123.24	128.52
29	d	404[B]	PL9	C12-C13-C14	-2.19	122.38	127.66
26	X	101	SQD	O5-C1-C2	-2.19	105.70	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	510	CLA	C2A-C1A-CHA	-2.19	120.02	123.86
36	C	517[B]	DGD	O1G-C1A-C2A	2.19	118.79	111.91
23	B	602	CLA	CHB-C4A-NA	2.19	127.55	124.51
25	b	618	BCR	C33-C5-C6	-2.19	122.06	124.53
26	A	412	SQD	O48-C23-O10	-2.19	118.06	123.59
27	D	701	GOL	C3-C2-C1	-2.19	103.18	111.70
25	K	102	BCR	C15-C14-C13	-2.19	124.18	127.31
23	B	605	CLA	OBD-CAD-C3D	-2.19	123.25	128.52
25	y	101	BCR	C1-C6-C7	2.19	121.97	115.78
23	A	405[B]	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
23	B	606	CLA	OBD-CAD-C3D	-2.19	123.25	128.52
23	B	610	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
26	a	411[B]	SQD	C3-C4-C5	2.19	114.14	110.24
23	b	601	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
23	B	602	CLA	C11-C10-C8	-2.19	108.85	115.92
35	b	622	HTG	C3-C4-C5	2.19	114.14	110.24
23	D	702[A]	CLA	CED-O2D-CGD	2.19	120.88	115.94
23	a	405[B]	CLA	CMA-C3A-C2A	-2.19	105.01	113.83
23	c	514	CLA	C4-C3-C5	2.18	118.95	115.27
23	C	505	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
26	a	411[A]	SQD	O9-S-O7	-2.18	106.39	113.95
25	b	618	BCR	C3-C4-C5	-2.18	110.18	114.08
23	b	610	CLA	C11-C12-C13	-2.18	108.86	115.92
23	B	601	CLA	CMC-C2C-C1C	2.18	128.36	125.04
23	B	611	CLA	CBC-CAC-C3C	-2.18	106.42	112.43
23	b	609	CLA	C7-C6-C5	-2.18	107.44	113.36
23	b	606	CLA	O2A-CGA-CBA	2.18	118.75	111.91
29	d	404[A]	PL9	C51-C49-C50	2.18	119.42	114.60
23	B	610	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
32	B	629	LMT	O5B-C5B-C6B	2.18	111.85	106.44
23	d	401[A]	CLA	CAC-C3C-C4C	2.18	127.64	124.81
23	b	606	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
25	K	102	BCR	C35-C13-C14	-2.18	119.87	122.92
23	B	606	CLA	C7-C6-C5	-2.18	107.45	113.36
36	c	518[A]	DGD	C2G-O2G-C1B	-2.18	112.43	117.79
25	d	403	BCR	C28-C27-C26	-2.18	110.19	114.08
26	A	410[B]	SQD	O9-S-O7	-2.18	106.42	113.95
35	C	522	HTG	C1-O5-C5	2.17	116.59	112.58
25	Y	101	BCR	C40-C30-C25	-2.17	106.77	110.30
23	C	505	CLA	CHD-C4C-NC	2.17	127.63	124.20
23	B	604	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
26	b	620	SQD	O9-S-C6	2.17	109.52	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	409	BCR	C40-C30-C25	-2.17	106.78	110.30
23	B	607	CLA	OBD-CAD-C3D	-2.17	123.30	128.52
24	a	408[A]	PHO	CBA-CAA-C2A	-2.17	107.47	113.81
34	C	501	LMG	O8-C28-C29	2.17	118.71	111.91
23	b	610	CLA	CMC-C2C-C1C	2.17	128.34	125.04
23	b	604	CLA	CHD-C4C-NC	2.17	127.62	124.20
33	A	419[A]	LHG	O4-P-O5	2.17	122.95	112.24
23	b	607	CLA	C1-O2A-CGA	2.16	122.12	116.44
34	C	521	LMG	O1-C1-C2	2.16	111.68	108.30
23	C	507	CLA	CHD-C4C-NC	2.16	127.61	124.20
32	b	621	LMT	C2'-C3'-C4'	2.16	114.62	109.68
38	F	102	HEM	CHA-C4D-ND	2.16	127.05	124.38
32	A	420	LMT	O5'-C5'-C4'	2.16	114.31	109.75
36	H	102	DGD	O3G-C3G-C2G	-2.16	105.68	110.90
23	A	405[A]	CLA	C4C-C3C-C2C	-2.16	103.75	106.90
36	H	102	DGD	O2G-C1B-C2B	2.16	116.16	111.50
23	C	502	CLA	C1-O2A-CGA	2.16	122.11	116.44
25	a	410	BCR	C2-C1-C6	2.16	113.81	110.48
34	m	101	LMG	C3-C4-C5	2.16	114.09	110.24
23	b	602	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
29	a	414[B]	PL9	C51-C49-C50	2.16	119.37	114.60
36	c	519	DGD	O3G-C1D-C2D	-2.16	104.93	108.30
26	A	410[A]	SQD	O9-S-O7	-2.16	106.48	113.95
23	B	610	CLA	CHB-C4A-NA	2.16	127.50	124.51
23	b	602	CLA	CMA-C3A-C2A	-2.16	105.13	113.83
36	h	102	DGD	O4D-C4D-C3D	-2.16	105.36	110.35
25	B	619	BCR	C31-C1-C6	-2.16	106.80	110.30
23	B	608	CLA	C11-C10-C8	-2.16	108.95	115.92
25	d	403	BCR	C3-C4-C5	-2.16	110.23	114.08
23	b	613	CLA	CAC-C3C-C4C	2.15	127.61	124.81
23	B	615	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
23	c	502	CLA	C2A-C1A-CHA	-2.15	120.09	123.86
23	B	610	CLA	C4-C3-C5	2.15	118.89	115.27
25	b	619	BCR	C7-C6-C5	2.15	126.68	121.46
23	b	614	CLA	CMB-C2B-C3B	2.15	128.71	124.68
23	c	503	CLA	CMB-C2B-C3B	2.15	128.71	124.68
23	d	402	CLA	CMA-C3A-C2A	-2.15	105.15	113.83
36	c	517[B]	DGD	C4E-C3E-C2E	-2.15	107.07	110.82
36	C	518[B]	DGD	O1G-C1A-O1A	-2.15	118.17	123.59
36	C	518[A]	DGD	C2G-O2G-C1B	-2.15	112.50	117.79
23	A	405[B]	CLA	O2A-CGA-CBA	2.15	118.65	111.91
24	A	417[B]	PHO	CED-O2D-CGD	2.15	120.80	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	512	CLA	O2A-CGA-CBA	2.15	118.65	111.91
23	C	510	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
36	c	517[A]	DGD	O6D-C1D-O3G	-2.15	104.89	109.97
23	c	506	CLA	CHA-C1A-NA	-2.15	121.48	126.40
23	c	512	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
29	d	404[A]	PL9	C35-C34-C36	2.15	118.88	115.27
23	A	406[B]	CLA	C1-C2-C3	-2.15	122.33	126.04
25	Y	101	BCR	C29-C30-C25	2.15	113.78	110.48
25	C	515	BCR	C11-C10-C9	-2.15	124.25	127.31
34	d	410	LMG	O7-C10-O9	-2.14	118.52	123.70
36	C	518[B]	DGD	O2G-C1B-O1B	-2.14	118.52	123.70
24	A	417[B]	PHO	O2A-CGA-CBA	2.14	118.63	111.91
23	b	604	CLA	C11-C12-C13	-2.14	109.00	115.92
29	A	414[A]	PL9	C25-C24-C26	2.14	118.87	115.27
23	C	509	CLA	CHD-C4C-NC	2.14	127.58	124.20
23	d	401[B]	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
24	A	407[A]	PHO	CBA-CAA-C2A	-2.14	107.57	113.81
23	D	703	CLA	C1-C2-C3	-2.14	122.35	126.04
25	Y	101	BCR	C38-C26-C25	-2.13	122.13	124.53
23	D	703	CLA	CMA-C3A-C4A	-2.13	106.04	111.77
23	C	504	CLA	CMB-C2B-C3B	2.13	128.67	124.68
23	C	510	CLA	C4-C3-C5	2.13	118.86	115.27
24	a	408[B]	PHO	C1-C2-C3	-2.13	122.36	126.04
32	B	627	LMT	O1B-C4'-C5'	-2.13	103.61	109.45
23	B	613	CLA	CMA-C3A-C4A	-2.13	106.05	111.77
25	C	516	BCR	C3-C4-C5	-2.13	110.28	114.08
36	C	517[A]	DGD	O1G-C1A-O1A	-2.13	118.22	123.59
25	D	704	BCR	C37-C22-C21	-2.13	119.94	122.92
36	c	518[A]	DGD	O1G-C1A-O1A	-2.13	118.23	123.59
25	A	409	BCR	C37-C22-C21	-2.13	119.94	122.92
32	b	627	LMT	O1'-C1'-C2'	2.13	111.62	108.30
26	b	620	SQD	O5-C1-C2	-2.12	105.85	110.35
29	a	414[B]	PL9	C35-C34-C33	-2.12	118.23	123.68
34	C	520	LMG	O7-C10-O9	-2.12	118.57	123.70
24	a	416[A]	PHO	C1A-C2A-C3A	-2.12	100.82	102.84
33	b	629[B]	LHG	O7-C7-O9	-2.12	118.57	123.70
36	C	517[A]	DGD	O6D-C1D-O3G	-2.12	104.95	109.97
35	B	622	HTG	C1-C2-C3	2.12	114.78	110.59
23	B	616	CLA	C4-C3-C2	-2.12	118.24	123.68
23	b	609	CLA	CHA-C1A-NA	-2.12	121.54	126.40
23	A	405[A]	CLA	O2A-CGA-CBA	2.12	118.56	111.91
25	A	409	BCR	C15-C14-C13	-2.12	124.29	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	414[A]	PL9	C12-C13-C14	-2.12	122.56	127.66
25	k	101	BCR	C36-C18-C19	2.12	121.41	118.08
23	d	401[B]	CLA	CMC-C2C-C1C	2.12	128.26	125.04
23	b	614	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
35	b	622	HTG	C6-C5-C4	-2.12	108.05	113.00
36	C	517[B]	DGD	C3G-C2G-C1G	-2.12	106.78	111.79
23	b	613	CLA	CBC-CAC-C3C	-2.12	106.60	112.43
23	B	615	CLA	O2A-CGA-CBA	2.12	118.55	111.91
23	C	514	CLA	O2A-CGA-O1A	-2.11	118.25	123.59
23	b	611	CLA	C4-C3-C5	2.11	118.83	115.27
23	B	607	CLA	CAC-C3C-C4C	2.11	127.55	124.81
25	a	410	BCR	C8-C7-C6	-2.11	121.27	127.20
23	B	610	CLA	CMA-C3A-C2A	-2.11	105.31	113.83
23	C	509	CLA	C7-C6-C5	-2.11	107.62	113.36
23	C	503	CLA	CMC-C2C-C1C	2.11	128.25	125.04
23	c	505	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
23	B	613	CLA	C2A-C1A-CHA	-2.11	120.17	123.86
25	K	102	BCR	C20-C21-C22	-2.11	124.30	127.31
23	C	509	CLA	C2A-C1A-CHA	-2.11	120.17	123.86
29	A	414[B]	PL9	C10-C9-C8	-2.11	118.27	123.68
23	C	509	CLA	CMC-C2C-C1C	2.11	128.25	125.04
40	v	201	HEC	CMB-C2B-C3B	2.11	128.30	125.82
24	a	416[B]	PHO	C4A-C3A-C2A	-2.11	100.83	102.84
23	b	616	CLA	C11-C12-C13	-2.11	109.11	115.92
36	h	102	DGD	O3G-C1D-C2D	2.11	111.59	108.30
24	A	417[A]	PHO	C6-C5-C3	-2.11	107.94	113.45
23	B	603	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
23	B	602	CLA	C1B-CHB-C4A	-2.10	125.95	130.12
25	c	516	BCR	C33-C5-C6	-2.10	122.17	124.53
25	k	101	BCR	C34-C9-C8	2.10	121.39	118.08
25	b	617	BCR	C29-C30-C25	2.10	113.72	110.48
23	b	605	CLA	C6-C7-C8	-2.10	109.13	115.92
29	d	404[A]	PL9	C12-C13-C14	-2.10	122.60	127.66
23	C	513	CLA	C2A-C1A-CHA	-2.10	120.19	123.86
23	B	608	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
25	D	704	BCR	C39-C30-C25	-2.10	106.89	110.30
33	b	629[A]	LHG	O7-C7-O9	-2.10	118.63	123.70
36	h	102	DGD	C3E-C4E-C5E	-2.10	106.49	110.24
34	c	521	LMG	C1-C2-C3	-2.10	105.62	110.00
23	b	603	CLA	CMB-C2B-C3B	2.10	128.60	124.68
23	d	402	CLA	CHB-C4A-NA	2.10	127.41	124.51
25	b	617	BCR	C21-C20-C19	-2.10	116.67	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	101	BCR	C3-C4-C5	-2.10	110.33	114.08
23	A	406[B]	CLA	CMA-C3A-C2A	-2.10	105.37	113.83
23	B	613	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
25	B	618	BCR	C15-C14-C13	-2.10	124.32	127.31
23	b	609	CLA	CAA-C2A-C3A	-2.09	107.04	112.78
23	C	511	CLA	CMD-C2D-C3D	-2.09	122.80	127.61
33	E	101[A]	LHG	O7-C7-O9	-2.09	118.64	123.70
23	A	406[B]	CLA	C4-C3-C5	2.09	118.79	115.27
25	b	618	BCR	C2-C1-C6	2.09	113.70	110.48
25	C	516	BCR	C21-C20-C19	-2.09	116.69	123.22
29	d	404[B]	PL9	C45-C44-C46	2.09	118.79	115.27
25	k	101	BCR	C20-C21-C22	-2.09	124.33	127.31
23	b	601	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
25	Y	101	BCR	C1-C6-C7	2.09	121.69	115.78
23	B	602	CLA	C11-C12-C13	-2.09	109.17	115.92
25	y	101	BCR	C37-C22-C23	2.09	121.37	118.08
23	B	613	CLA	C4-C3-C2	-2.09	118.32	123.68
23	B	616	CLA	OBD-CAD-C3D	-2.09	123.50	128.52
23	A	404[A]	CLA	C7-C6-C5	-2.09	107.69	113.36
32	a	417	LMT	O5B-C5B-C4B	2.09	113.48	109.69
23	b	605	CLA	CMB-C2B-C3B	2.09	128.58	124.68
32	F	101	LMT	C3B-C4B-C5B	-2.09	106.52	110.24
23	B	607	CLA	CAA-CBA-CGA	2.09	119.35	113.25
23	d	401[A]	CLA	CHD-C4C-NC	2.08	127.49	124.20
34	m	101	LMG	C12-C11-C10	-2.08	106.04	113.62
35	B	624	HTG	O5-C5-C4	2.08	113.48	109.69
40	V	201	HEC	CAD-CBD-CGD	-2.08	107.92	113.76
25	D	704	BCR	C38-C26-C27	2.08	117.62	113.62
27	B	623	GOL	C3-C2-C1	-2.08	103.61	111.70
23	A	405[B]	CLA	CHB-C4A-NA	2.08	127.39	124.51
23	d	402	CLA	CMB-C2B-C3B	2.08	128.57	124.68
23	D	703	CLA	CMB-C2B-C1B	2.08	131.66	128.46
23	b	610	CLA	C4-C3-C2	-2.08	118.34	123.68
23	c	503	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
23	c	505	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
23	A	408	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
23	d	402	CLA	OBD-CAD-C3D	-2.08	123.52	128.52
23	A	405[B]	CLA	C4C-C3C-C2C	-2.08	103.87	106.90
25	t	102	BCR	C7-C6-C5	-2.08	116.43	121.46
23	a	405[B]	CLA	C7-C6-C5	-2.08	107.72	113.36
23	b	615	CLA	C6-C5-C3	-2.07	108.01	113.45
38	F	102	HEM	C4B-C3B-C2B	-2.07	105.47	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	512	CLA	C2A-C1A-CHA	-2.07	120.23	123.86
25	b	618	BCR	C7-C8-C9	-2.07	123.10	126.23
36	c	519	DGD	O2G-C1B-O1B	-2.07	118.70	123.70
32	A	418	LMT	O1'-C1'-C2'	2.07	111.53	108.30
23	A	404[A]	CLA	C4-C3-C5	2.07	118.75	115.27
29	D	705[A]	PL9	C12-C13-C14	-2.07	122.68	127.66
23	c	507	CLA	CMC-C2C-C1C	2.07	128.19	125.04
35	B	624	HTG	C3-C4-C5	2.07	113.93	110.24
36	C	518[B]	DGD	O3G-C1D-C2D	2.07	111.53	108.30
34	m	101	LMG	O8-C28-O10	-2.07	118.37	123.59
25	H	101	BCR	C24-C23-C22	-2.07	123.11	126.23
23	b	611	CLA	CBC-CAC-C3C	-2.07	106.73	112.43
25	c	516	BCR	C15-C16-C17	-2.07	119.24	123.47
29	D	705[A]	PL9	C30-C29-C31	2.07	118.75	115.27
29	a	414[A]	PL9	C51-C49-C50	2.07	119.17	114.60
23	B	607	CLA	CHD-C4C-NC	2.07	127.46	124.20
25	a	410	BCR	C11-C10-C9	-2.07	124.36	127.31
23	b	612	CLA	CMB-C2B-C3B	2.06	128.54	124.68
29	D	705[A]	PL9	C25-C24-C23	-2.06	118.38	123.68
34	c	501	LMG	C30-C29-C28	-2.06	106.12	113.62
23	B	614	CLA	CMA-C3A-C2A	-2.06	105.51	113.83
23	b	615	CLA	C2A-C1A-CHA	-2.06	120.25	123.86
25	C	516	BCR	C32-C1-C6	-2.06	106.95	110.30
38	F	102	HEM	O2D-CGD-O1D	-2.06	118.16	123.30
23	B	608	CLA	OBD-CAD-C3D	-2.06	123.56	128.52
23	b	616	CLA	CHA-C1A-NA	-2.06	121.68	126.40
36	h	102	DGD	C4D-C3D-C2D	-2.06	107.23	110.82
29	D	705[B]	PL9	C36-C37-C38	-2.06	105.11	111.88
23	b	613	CLA	C16-C15-C13	-2.06	109.27	115.92
23	c	507	CLA	C1-O2A-CGA	2.06	121.84	116.44
23	b	607	CLA	CAA-CBA-CGA	2.06	119.27	113.25
23	a	406[B]	CLA	CMC-C2C-C1C	2.06	128.17	125.04
23	c	509	CLA	CAC-C3C-C4C	2.06	127.48	124.81
23	a	406[B]	CLA	CAC-C3C-C2C	2.05	131.04	127.53
23	b	609	CLA	C4-C3-C5	2.05	118.73	115.27
25	h	101	BCR	C2-C1-C6	2.05	113.64	110.48
26	a	411[B]	SQD	O7-S-C6	2.05	109.38	106.94
23	b	611	CLA	CAC-C3C-C4C	2.05	127.47	124.81
23	C	509	CLA	CHB-C4A-NA	2.05	127.35	124.51
32	m	103	LMT	O1'-C1'-C2'	2.05	111.51	108.30
36	C	517[A]	DGD	C3E-C4E-C5E	2.05	113.90	110.24
23	C	511	CLA	OBD-CAD-C3D	-2.05	123.58	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	615	CLA	CHA-C1A-NA	-2.05	121.70	126.40
23	B	611	CLA	CAC-C3C-C4C	2.05	127.47	124.81
23	C	513	CLA	CAC-C3C-C4C	2.05	127.47	124.81
23	a	409	CLA	C1B-CHB-C4A	-2.05	126.05	130.12
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	c	511	CLA	CHB-C4A-NA	2.05	127.34	124.51
25	T	102	BCR	C29-C30-C25	2.05	113.63	110.48
36	C	517[B]	DGD	O1G-C1A-O1A	-2.05	118.43	123.59
35	b	623	HTG	O5-C1-C2	2.05	112.89	110.31
25	D	704	BCR	C30-C25-C24	2.04	121.56	115.78
23	B	602	CLA	CAA-CBA-CGA	-2.04	107.28	113.25
23	B	603	CLA	C2A-C3A-C4A	-2.04	98.57	101.87
33	D	707[A]	LHG	O4-P-O5	2.04	122.34	112.24
25	B	617	BCR	C34-C9-C10	-2.04	120.06	122.92
25	b	619	BCR	C7-C8-C9	-2.04	123.15	126.23
24	A	407[A]	PHO	C4-C3-C5	2.04	118.70	115.27
23	b	601	CLA	C2A-C1A-CHA	-2.04	120.29	123.86
25	C	515	BCR	C37-C22-C23	2.04	121.29	118.08
23	c	512	CLA	CMA-C3A-C4A	2.04	117.26	111.77
34	C	520	LMG	O1-C7-C8	-2.04	105.98	110.90
29	A	414[B]	PL9	C35-C34-C33	-2.04	118.45	123.68
23	a	405[B]	CLA	CAA-CBA-CGA	-2.04	107.30	113.25
35	V	202	HTG	C6-C5-C4	-2.04	108.23	113.00
25	K	102	BCR	C3-C4-C5	-2.04	110.44	114.08
23	b	615	CLA	CMC-C2C-C1C	2.03	128.14	125.04
25	H	101	BCR	C33-C5-C6	-2.03	122.24	124.53
25	b	619	BCR	C21-C20-C19	-2.03	116.87	123.22
25	h	101	BCR	C32-C1-C6	-2.03	107.00	110.30
23	c	510	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
23	b	605	CLA	CED-O2D-CGD	2.03	120.53	115.94
25	t	102	BCR	C29-C28-C27	-2.03	106.84	111.38
25	Y	101	BCR	C7-C6-C5	-2.03	116.55	121.46
23	a	406[A]	CLA	CAC-C3C-C2C	2.03	131.00	127.53
23	c	511	CLA	C7-C6-C5	-2.03	107.85	113.36
26	a	411[A]	SQD	O48-C23-O10	-2.03	118.47	123.59
23	A	405[B]	CLA	CAA-CBA-CGA	2.03	119.18	113.25
34	Z	101	LMG	C9-C8-C7	-2.03	107.00	111.79
29	d	404[A]	PL9	C45-C44-C46	2.03	118.68	115.27
25	B	617	BCR	C16-C17-C18	-2.03	124.42	127.31
23	C	508	CLA	CAC-C3C-C2C	2.03	130.99	127.53
23	c	512	CLA	OBD-CAD-C3D	-2.02	123.65	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	603	CLA	C2A-C1A-CHA	-2.02	120.32	123.86
23	B	613	CLA	CBC-CAC-C3C	-2.02	106.85	112.43
23	B	609	CLA	CHA-C1A-NA	-2.02	121.77	126.40
23	B	607	CLA	C6-C7-C8	-2.02	109.38	115.92
23	A	408	CLA	OBD-CAD-C3D	-2.02	123.66	128.52
24	a	416[A]	PHO	O2A-CGA-CBA	2.02	118.25	111.91
23	C	513	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
23	A	406[A]	CLA	CHB-C4A-NA	2.02	127.30	124.51
26	A	410[B]	SQD	O4-C4-C3	-2.02	105.68	110.35
25	t	102	BCR	C10-C11-C12	-2.02	116.92	123.22
25	b	618	BCR	C38-C26-C25	-2.02	122.26	124.53
23	C	506	CLA	CBC-CAC-C3C	-2.02	106.87	112.43
25	b	619	BCR	C35-C13-C14	-2.02	120.10	122.92
25	D	704	BCR	C24-C23-C22	-2.02	123.19	126.23
23	A	404[B]	CLA	CED-O2D-CGD	2.02	120.50	115.94
26	b	620	SQD	C4-C3-C2	2.02	114.34	110.82
24	A	417[A]	PHO	CED-O2D-CGD	2.01	120.49	115.94
23	c	513	CLA	CHA-C1A-NA	-2.01	121.78	126.40
38	f	101	HEM	CHA-C4D-C3D	-2.01	121.55	125.33
35	c	522	HTG	O5-C1-C2	2.01	112.85	110.31
23	d	401[A]	CLA	CBC-CAC-C3C	-2.01	106.88	112.43
24	a	408[A]	PHO	O2D-CGD-O1D	-2.01	119.90	123.84
23	D	703	CLA	CMA-C3A-C2A	-2.01	105.71	113.83
33	d	405[B]	LHG	C5-O7-C7	-2.01	112.84	117.79
23	c	509	CLA	CMB-C2B-C3B	2.01	128.44	124.68
34	B	621	LMG	O8-C28-O10	-2.01	118.52	123.59
31	A	416[A]	BCT	O2-C-O1	2.01	124.76	119.55
23	D	702[A]	CLA	CBC-CAC-C3C	-2.01	106.89	112.43
31	a	404[A]	BCT	O2-C-O1	2.01	124.76	119.55
29	a	414[B]	PL9	C10-C9-C8	-2.01	118.52	123.68
23	b	615	CLA	C11-C12-C13	-2.01	109.42	115.92
29	D	705[A]	PL9	O2-C1-C6	-2.01	117.11	120.59
25	Y	101	BCR	C36-C18-C19	2.01	121.24	118.08
23	B	614	CLA	CAA-C2A-C3A	-2.01	107.28	112.78
23	b	614	CLA	CHB-C4A-NA	2.00	127.28	124.51
29	D	705[B]	PL9	C45-C44-C43	-2.00	118.54	123.68
23	b	603	CLA	C5-C3-C2	-2.00	117.06	121.12
32	M	101	LMT	O1B-C1B-C2B	2.00	113.29	108.10
23	B	609	CLA	C16-C15-C13	-2.00	109.44	115.92
23	c	503	CLA	C4C-C3C-C2C	-2.00	103.98	106.90
32	F	101	LMT	O1'-C1'-C2'	2.00	111.43	108.30
23	b	609	CLA	C16-C15-C13	-2.00	109.45	115.92

All (70) 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
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	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	C	514	CLA	ND
23	D	702[A]	CLA	ND
23	D	702[B]	CLA	ND
23	D	703	CLA	ND
23	a	405[A]	CLA	ND
23	a	405[B]	CLA	ND
23	a	406[A]	CLA	ND
23	a	406[B]	CLA	ND
23	b	601	CLA	ND
23	b	602	CLA	ND
23	b	603	CLA	ND

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Mol	Chain	Res	Type	Atom
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	502	CLA	ND
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	c	514	CLA	ND
23	d	401[A]	CLA	ND
23	d	401[B]	CLA	ND
23	d	402	CLA	ND

All (1652) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	408	CLA	C2-C3-C5-C6
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	508	CLA	C4-C3-C5-C6
23	C	509	CLA	CHA-CBD-CGD-O1D
23	C	509	CLA	CHA-CBD-CGD-O2D
23	b	606	CLA	CHA-CBD-CGD-O1D
23	b	614	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
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	508	CLA	C4-C3-C5-C6
23	c	509	CLA	CHA-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O2D
23	c	510	CLA	C2-C1-O2A-CGA
23	c	510	CLA	C11-C10-C8-C9
23	d	402	CLA	C2-C3-C5-C6
23	d	402	CLA	C4-C3-C5-C6
25	D	704	BCR	C23-C24-C25-C30
25	T	102	BCR	C13-C14-C15-C16
25	Y	101	BCR	C1-C6-C7-C8
25	Y	101	BCR	C5-C6-C7-C8
25	b	617	BCR	C1-C6-C7-C8
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	412	SQD	O6-C44-C45-O47
26	B	620	SQD	O5-C1-O6-C44
26	B	620	SQD	O49-C7-O47-C45
26	B	620	SQD	C8-C7-O47-C45
26	X	101	SQD	C2-C1-O6-C44
26	X	101	SQD	O49-C7-O47-C45
26	X	101	SQD	C8-C7-O47-C45
26	a	412	SQD	O6-C44-C45-O47
26	a	412	SQD	C5-C6-S-O7
26	a	412	SQD	C5-C6-S-O8
26	a	412	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-C3
27	B	623	GOL	C1-C2-C3-O3
27	B	628	GOL	O1-C1-C2-C3
27	D	712	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	527	GOL	C1-C2-C3-O3
27	o	303	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
27	o	304	GOL	O1-C1-C2-C3
27	o	304	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	414[A]	PL9	C9-C11-C12-C13
29	a	414[A]	PL9	C14-C16-C17-C18
29	a	414[A]	PL9	C25-C24-C26-C27
29	a	414[B]	PL9	C9-C11-C12-C13
29	a	414[B]	PL9	C14-C16-C17-C18
29	a	414[B]	PL9	C23-C24-C26-C27
29	a	414[B]	PL9	C25-C24-C26-C27
32	A	418	LMT	C2'-C1'-O1'-C1
32	A	418	LMT	O5'-C1'-O1'-C1
32	A	420	LMT	C2'-C1'-O1'-C1
32	A	420	LMT	O5'-C1'-O1'-C1
32	B	629	LMT	C2'-C1'-O1'-C1
32	B	630	LMT	O5'-C1'-O1'-C1
32	B	630	LMT	C2-C1-O1'-C1'
32	F	101	LMT	C2'-C1'-O1'-C1
32	F	101	LMT	O5'-C1'-O1'-C1
32	T	101	LMT	C2-C1-O1'-C1'
32	b	627	LMT	C2'-C1'-O1'-C1
32	b	627	LMT	O5'-C1'-O1'-C1
32	t	101	LMT	O5'-C1'-O1'-C1
32	t	101	LMT	C2-C1-O1'-C1'
33	A	419[B]	LHG	C4-O6-P-O5
33	D	706[A]	LHG	O2-C2-C3-O3
33	D	706[A]	LHG	C3-O3-P-O4
33	D	706[A]	LHG	C3-O3-P-O5
33	D	706[A]	LHG	C3-O3-P-O6
33	D	706[A]	LHG	C4-O6-P-O4
33	D	706[B]	LHG	O2-C2-C3-O3
33	D	706[B]	LHG	C3-O3-P-O4
33	D	706[B]	LHG	C4-O6-P-O4
33	E	101[A]	LHG	C3-O3-P-O4
33	E	101[A]	LHG	C3-O3-P-O5
33	E	101[A]	LHG	O10-C23-O8-C6
33	E	101[A]	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
33	E	101[B]	LHG	C3-O3-P-O4
33	E	101[B]	LHG	C3-O3-P-O5
33	E	101[B]	LHG	C3-O3-P-O6
33	E	101[B]	LHG	O10-C23-O8-C6
33	E	101[B]	LHG	C24-C23-O8-C6
33	L	101[A]	LHG	C4-O6-P-O4
33	L	101[A]	LHG	C4-O6-P-O5
33	L	101[B]	LHG	C4-O6-P-O4
33	a	420[A]	LHG	C3-O3-P-O4
33	a	420[A]	LHG	C4-O6-P-O5
33	a	420[A]	LHG	O10-C23-O8-C6
33	a	420[A]	LHG	C24-C23-O8-C6
33	a	420[B]	LHG	C3-O3-P-O4
33	a	420[B]	LHG	C4-O6-P-O5
33	a	420[B]	LHG	O10-C23-O8-C6
33	a	420[B]	LHG	C24-C23-O8-C6
33	b	629[A]	LHG	C4-O6-P-O3
33	b	629[A]	LHG	C4-O6-P-O4
33	b	629[A]	LHG	C4-O6-P-O5
33	b	629[B]	LHG	C4-O6-P-O3
33	b	629[B]	LHG	C4-O6-P-O4
33	b	629[B]	LHG	C4-O6-P-O5
33	d	405[A]	LHG	C3-O3-P-O5
33	d	405[A]	LHG	C4-O6-P-O4
33	d	405[B]	LHG	C3-O3-P-O4
33	d	405[B]	LHG	C4-O6-P-O4
33	d	412[A]	LHG	C3-O3-P-O5
34	C	521	LMG	C11-C10-O7-C8
34	c	521	LMG	O9-C10-O7-C8
34	Z	101	LMG	O9-C10-O7-C8
34	Z	101	LMG	C11-C10-O7-C8
34	z	101	LMG	O6-C1-O1-C7
35	b	623	HTG	O5-C1-S1-C1'
35	o	301	HTG	C2'-C1'-S1-C1
32	A	420	LMT	O5B-C1B-O1B-C4'
32	B	629	LMT	C4'-C5'-C6'-O6'
32	m	103	LMT	C4B-C5B-C6B-O6B
26	A	410[B]	SQD	O49-C7-O47-C45
26	b	620	SQD	O49-C7-O47-C45
32	T	101	LMT	C4B-C5B-C6B-O6B
23	D	703	CLA	C3-C5-C6-C7
23	b	616	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
23	c	513	CLA	C3-C5-C6-C7
23	d	402	CLA	C3-C5-C6-C7
32	T	101	LMT	O5'-C5'-C6'-O6'
32	a	417	LMT	O5B-C5B-C6B-O6B
26	A	410[A]	SQD	C8-C7-O47-C45
26	A	410[B]	SQD	C8-C7-O47-C45
34	c	521	LMG	C11-C10-O7-C8
32	B	629	LMT	O5B-C5B-C6B-O6B
32	m	103	LMT	O5B-C5B-C6B-O6B
35	D	710	HTG	O5-C5-C6-O6
23	C	505	CLA	C4-C3-C5-C6
23	a	409	CLA	C4-C3-C5-C6
29	A	414[B]	PL9	C30-C29-C31-C32
32	B	627	LMT	C4'-C5'-C6'-O6'
23	C	508	CLA	C2-C3-C5-C6
23	c	508	CLA	C2-C3-C5-C6
29	A	414[A]	PL9	C18-C19-C21-C22
29	A	414[B]	PL9	C18-C19-C21-C22
23	D	703	CLA	CBD-CGD-O2D-CED
23	c	512	CLA	CBD-CGD-O2D-CED
23	B	606	CLA	C2A-CAA-CBA-CGA
23	b	606	CLA	C2A-CAA-CBA-CGA
23	B	614	CLA	C3-C5-C6-C7
32	F	101	LMT	O5'-C5'-C6'-O6'
35	b	625	HTG	S1-C1'-C2'-C3'
34	C	521	LMG	O9-C10-O7-C8
32	B	627	LMT	O5'-C5'-C6'-O6'
23	c	514	CLA	CBD-CGD-O2D-CED
33	E	101[A]	LHG	O2-C2-C3-O3
33	d	405[A]	LHG	O2-C2-C3-O3
33	d	405[B]	LHG	O2-C2-C3-O3
23	A	408	CLA	C3-C5-C6-C7
23	B	616	CLA	C3-C5-C6-C7
32	B	627	LMT	O5B-C5B-C6B-O6B
34	z	101	LMG	C11-C10-O7-C8
23	C	510	CLA	CBD-CGD-O2D-CED
32	T	101	LMT	C4'-C5'-C6'-O6'
34	c	521	LMG	C4-C5-C6-O5
34	C	521	LMG	O6-C5-C6-O5
35	b	625	HTG	O5-C5-C6-O6
32	a	417	LMT	C4B-C5B-C6B-O6B
35	D	710	HTG	S1-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
35	b	622	HTG	S1-C1'-C2'-C3'
32	T	101	LMT	O5B-C5B-C6B-O6B
32	B	629	LMT	C4B-C5B-C6B-O6B
32	e	101	LMT	C4'-C5'-C6'-O6'
32	A	420	LMT	O5B-C5B-C6B-O6B
32	B	629	LMT	O5'-C5'-C6'-O6'
32	B	630	LMT	O5'-C5'-C6'-O6'
23	B	605	CLA	C4-C3-C5-C6
23	b	603	CLA	C4-C3-C5-C6
23	b	605	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	414[A]	PL9	C15-C14-C16-C17
29	a	414[A]	PL9	C30-C29-C31-C32
29	a	414[B]	PL9	C15-C14-C16-C17
29	a	414[B]	PL9	C30-C29-C31-C32
32	F	101	LMT	C4'-C5'-C6'-O6'
23	B	605	CLA	C2-C3-C5-C6
23	C	505	CLA	C2-C3-C5-C6
23	b	603	CLA	C2-C3-C5-C6
23	b	605	CLA	C2-C3-C5-C6
23	b	614	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[A]	PL9	C13-C14-C16-C17
29	a	414[A]	PL9	C28-C29-C31-C32
29	a	414[B]	PL9	C13-C14-C16-C17
29	a	414[B]	PL9	C28-C29-C31-C32
32	A	420	LMT	O5'-C5'-C6'-O6'
32	b	621	LMT	O5'-C5'-C6'-O6'
32	B	629	LMT	O5'-C1'-O1'-C1
32	b	621	LMT	O5'-C1'-O1'-C1
29	A	414[B]	PL9	C44-C46-C47-C48
29	D	705[A]	PL9	C39-C41-C42-C43
29	d	404[B]	PL9	C39-C41-C42-C43
34	B	621	LMG	C39-C40-C41-C42
32	b	627	LMT	O5'-C5'-C6'-O6'
34	c	521	LMG	O6-C5-C6-O5
35	D	710	HTG	C4-C5-C6-O6
33	D	706[B]	LHG	C1-C2-C3-O3
33	d	405[A]	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
34	z	101	LMG	O9-C10-O7-C8
32	B	627	LMT	C6-C7-C8-C9
23	a	409	CLA	CBA-CGA-O2A-C1
23	c	510	CLA	CBA-CGA-O2A-C1
32	A	420	LMT	C4B-C5B-C6B-O6B
23	b	606	CLA	C10-C11-C12-C13
32	t	101	LMT	O5'-C5'-C6'-O6'
33	D	707[A]	LHG	C33-C34-C35-C36
32	B	630	LMT	C4'-C5'-C6'-O6'
32	b	627	LMT	C4'-C5'-C6'-O6'
23	B	601	CLA	C10-C11-C12-C13
23	C	509	CLA	C10-C11-C12-C13
33	E	101[B]	LHG	O2-C2-C3-O3
32	B	630	LMT	C2'-C1'-O1'-C1
32	b	621	LMT	C2'-C1'-O1'-C1
32	t	101	LMT	C2'-C1'-O1'-C1
23	a	409	CLA	C2-C3-C5-C6
29	a	414[A]	PL9	C23-C24-C26-C27
23	B	602	CLA	C6-C7-C8-C9
23	B	613	CLA	C11-C12-C13-C14
23	C	503	CLA	C14-C13-C15-C16
23	C	507	CLA	C14-C13-C15-C16
23	b	601	CLA	C11-C10-C8-C9
23	b	604	CLA	C6-C7-C8-C9
23	b	616	CLA	C6-C7-C8-C9
23	c	505	CLA	C11-C12-C13-C14
23	C	502	CLA	CBD-CGD-O2D-CED
23	C	514	CLA	CBD-CGD-O2D-CED
23	B	602	CLA	C13-C15-C16-C17
23	b	610	CLA	C2A-CAA-CBA-CGA
25	D	704	BCR	C37-C22-C23-C24
25	d	403	BCR	C7-C8-C9-C34
32	e	101	LMT	O5B-C5B-C6B-O6B
34	c	520	LMG	C4-C5-C6-O5
23	b	601	CLA	C10-C11-C12-C13
23	b	606	CLA	C13-C15-C16-C17
23	c	513	CLA	C15-C16-C17-C18
23	B	601	CLA	C5-C6-C7-C8
23	B	603	CLA	C13-C15-C16-C17
23	B	606	CLA	C10-C11-C12-C13
23	b	604	CLA	C5-C6-C7-C8
23	b	604	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
23	b	611	CLA	C15-C16-C17-C18
23	b	614	CLA	C8-C10-C11-C12
27	A	411	GOL	O1-C1-C2-O2
27	B	628	GOL	O1-C1-C2-O2
27	V	203[A]	GOL	O2-C2-C3-O3
27	V	203[B]	GOL	O2-C2-C3-O3
27	v	202[B]	GOL	O1-C1-C2-O2
26	X	101	SQD	C23-C24-C25-C26
36	c	518[B]	DGD	C1B-C2B-C3B-C4B
32	e	101	LMT	O5'-C5'-C6'-O6'
33	D	707[B]	LHG	C33-C34-C35-C36
23	A	408	CLA	C5-C6-C7-C8
23	B	614	CLA	C8-C10-C11-C12
23	C	512	CLA	C3-C5-C6-C7
32	A	420	LMT	C5'-C4'-O1B-C1B
32	A	418	LMT	O5B-C5B-C6B-O6B
32	a	417	LMT	O1'-C1-C2-C3
33	E	101[A]	LHG	C23-C24-C25-C26
34	Z	101	LMG	C10-C11-C12-C13
36	c	518[A]	DGD	C1B-C2B-C3B-C4B
32	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	703	CLA	C11-C10-C8-C7
23	b	606	CLA	C12-C13-C15-C16
23	c	510	CLA	C3-C5-C6-C7
36	h	102	DGD	C6B-C7B-C8B-C9B
23	D	703	CLA	C10-C11-C12-C13
32	e	101	LMT	O5'-C1'-O1'-C1
23	c	514	CLA	C10-C11-C12-C13
29	A	414[A]	PL9	C44-C46-C47-C48
29	D	705[B]	PL9	C39-C41-C42-C43
29	d	404[A]	PL9	C39-C41-C42-C43
33	E	101[B]	LHG	C23-C24-C25-C26
23	C	508	CLA	C5-C6-C7-C8
34	Z	101	LMG	C11-C12-C13-C14
23	a	409	CLA	O1A-CGA-O2A-C1
23	c	510	CLA	O1A-CGA-O2A-C1
32	A	420	LMT	C4'-C5'-C6'-O6'
32	B	627	LMT	C4B-C5B-C6B-O6B
32	A	418	LMT	O1'-C1-C2-C3
36	h	102	DGD	C3B-C4B-C5B-C6B

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Mol	Chain	Res	Type	Atoms
23	C	503	CLA	C13-C15-C16-C17
23	a	405[A]	CLA	C15-C16-C17-C18
23	b	605	CLA	C8-C10-C11-C12
23	b	606	CLA	C15-C16-C17-C18
33	D	706[B]	LHG	C3-O3-P-O6
33	D	706[B]	LHG	C4-O6-P-O3
33	E	101[A]	LHG	C3-O3-P-O6
33	E	101[A]	LHG	C4-O6-P-O3
33	E	101[B]	LHG	C4-O6-P-O3
33	L	101[A]	LHG	C4-O6-P-O3
33	L	101[B]	LHG	C4-O6-P-O3
33	a	420[A]	LHG	C3-O3-P-O6
33	a	420[A]	LHG	C4-O6-P-O3
33	a	420[B]	LHG	C3-O3-P-O6
33	a	420[B]	LHG	C4-O6-P-O3
33	d	405[A]	LHG	C3-O3-P-O6
33	d	405[B]	LHG	C3-O3-P-O6
34	B	621	LMG	O6-C5-C6-O5
35	b	623	HTG	C1'-C2'-C3'-C4'
32	B	627	LMT	C5'-C4'-O1B-C1B
35	B	624	HTG	S1-C1'-C2'-C3'
26	A	410[A]	SQD	C7-C8-C9-C10
34	d	410	LMG	C10-C11-C12-C13
33	D	706[A]	LHG	C1-C2-C3-O3
33	d	405[B]	LHG	C1-C2-C3-O3
35	B	624	HTG	O5-C5-C6-O6
23	D	703	CLA	C4-C3-C5-C6
26	b	620	SQD	C18-C19-C20-C21
23	B	614	CLA	C10-C11-C12-C13
23	a	405[B]	CLA	C15-C16-C17-C18
23	B	608	CLA	C16-C17-C18-C20
23	c	509	CLA	C16-C17-C18-C19
36	c	517[B]	DGD	O6D-C5D-C6D-O5D
32	M	101	LMT	O5'-C5'-C6'-O6'
26	A	410[A]	SQD	C15-C16-C17-C18
26	A	410[B]	SQD	C15-C16-C17-C18
26	A	412	SQD	C17-C18-C19-C20
32	A	420	LMT	C3-C4-C5-C6
33	L	101[A]	LHG	C12-C13-C14-C15
34	c	501	LMG	C34-C35-C36-C37
23	c	513	CLA	CBD-CGD-O2D-CED
34	B	621	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
35	o	301	HTG	C1'-C2'-C3'-C4'
26	X	101	SQD	C30-C31-C32-C33
33	L	101[A]	LHG	C17-C18-C19-C20
33	d	405[B]	LHG	C34-C35-C36-C37
33	d	412[A]	LHG	C16-C17-C18-C19
34	C	501	LMG	C17-C18-C19-C20
35	b	622	HTG	C2'-C3'-C4'-C5'
36	C	517[B]	DGD	C5B-C6B-C7B-C8B
36	c	518[A]	DGD	CAA-CBA-CCA-CDA
36	c	518[B]	DGD	C9A-CAA-CBA-CCA
23	B	603	CLA	C16-C17-C18-C20
23	a	409	CLA	C16-C17-C18-C19
23	b	614	CLA	C16-C17-C18-C20
23	c	510	CLA	C16-C17-C18-C20
32	B	627	LMT	C5-C6-C7-C8
33	b	629[B]	LHG	C14-C15-C16-C17
34	B	621	LMG	C17-C18-C19-C20
34	C	521	LMG	C18-C19-C20-C21
34	D	711	LMG	C19-C20-C21-C22
34	m	101	LMG	C35-C36-C37-C38
35	B	622	HTG	C3'-C4'-C5'-C6'
36	c	518[A]	DGD	C9A-CAA-CBA-CCA
36	c	518[B]	DGD	CAA-CBA-CCA-CDA
34	B	621	LMG	O9-C10-O7-C8
33	d	412[B]	LHG	C16-C17-C18-C19
36	C	518[A]	DGD	CCB-CDB-CEB-CFB
36	c	518[B]	DGD	CBA-CCA-CDA-CEA
36	h	102	DGD	C7B-C8B-C9B-CAB
32	e	101	LMT	C4-C5-C6-C7
34	c	520	LMG	C33-C34-C35-C36
36	c	517[A]	DGD	C2B-C3B-C4B-C5B
32	b	621	LMT	C4'-C5'-C6'-O6'
23	B	605	CLA	C5-C6-C7-C8
32	B	630	LMT	C3-C4-C5-C6
33	D	707[B]	LHG	C32-C33-C34-C35
33	L	101[B]	LHG	C25-C26-C27-C28
36	C	517[A]	DGD	C4B-C5B-C6B-C7B
34	c	501	LMG	C10-C11-C12-C13
23	c	512	CLA	O1D-CGD-O2D-CED
26	A	412	SQD	C2-C1-O6-C44
32	e	101	LMT	C2'-C1'-O1'-C1
34	B	621	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
36	C	518[A]	DGD	C2E-C1E-O5D-C6D
36	C	518[B]	DGD	C2E-C1E-O5D-C6D
32	b	627	LMT	C7-C8-C9-C10
33	d	405[B]	LHG	C11-C10-C9-C8
36	C	517[A]	DGD	C5B-C6B-C7B-C8B
36	c	517[A]	DGD	C9A-CAA-CBA-CCA
23	B	615	CLA	C5-C6-C7-C8
23	C	513	CLA	C10-C11-C12-C13
23	b	614	CLA	C10-C11-C12-C13
23	c	507	CLA	C15-C16-C17-C18
23	B	603	CLA	C16-C17-C18-C19
23	B	615	CLA	C16-C17-C18-C19
23	b	615	CLA	C16-C17-C18-C19
29	A	414[A]	PL9	C45-C44-C46-C47
29	d	404[B]	PL9	C15-C14-C16-C17
33	D	706[A]	LHG	C16-C17-C18-C19
33	L	101[B]	LHG	C12-C13-C14-C15
33	a	420[A]	LHG	C26-C27-C28-C29
33	b	629[A]	LHG	C14-C15-C16-C17
34	C	501	LMG	C12-C13-C14-C15
34	C	521	LMG	C17-C18-C19-C20
34	c	520	LMG	C34-C35-C36-C37
36	C	518[B]	DGD	CCB-CDB-CEB-CFB
29	d	404[A]	PL9	C13-C14-C16-C17
23	a	407[A]	CLA	C11-C12-C13-C14
23	a	407[B]	CLA	C11-C12-C13-C14
23	b	610	CLA	C11-C12-C13-C14
23	c	505	CLA	C14-C13-C15-C16
33	D	707[A]	LHG	C32-C33-C34-C35
33	L	101[A]	LHG	C15-C16-C17-C18
33	a	420[B]	LHG	C26-C27-C28-C29
34	C	521	LMG	C19-C20-C21-C22
34	D	711	LMG	C35-C36-C37-C38
34	c	501	LMG	C30-C31-C32-C33
36	c	517[B]	DGD	C9A-CAA-CBA-CCA
34	Z	101	LMG	O6-C5-C6-O5
36	c	517[B]	DGD	C4D-C5D-C6D-O5D
25	b	619	BCR	C7-C8-C9-C34
32	e	101	LMT	C5-C6-C7-C8
33	D	706[B]	LHG	C16-C17-C18-C19
33	L	101[B]	LHG	C15-C16-C17-C18
33	d	412[A]	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
36	c	517[B]	DGD	C2B-C3B-C4B-C5B
36	c	518[A]	DGD	CBA-CCA-CDA-CEA
27	B	623	GOL	O1-C1-C2-C3
27	B	628	GOL	C1-C2-C3-O3
27	D	712	GOL	O1-C1-C2-C3
27	O	302	GOL	O1-C1-C2-C3
27	a	418	GOL	O1-C1-C2-C3
27	d	411	GOL	O1-C1-C2-C3
27	l	102[B]	GOL	O1-C1-C2-C3
27	v	202[B]	GOL	O1-C1-C2-C3
25	D	704	BCR	C21-C22-C23-C24
25	b	619	BCR	C7-C8-C9-C10
23	B	602	CLA	C3-C5-C6-C7
33	A	419[B]	LHG	C34-C35-C36-C37
33	L	101[A]	LHG	C25-C26-C27-C28
26	a	412	SQD	C31-C32-C33-C34
32	t	101	LMT	C4-C5-C6-C7
33	A	419[A]	LHG	C34-C35-C36-C37
33	L	101[B]	LHG	C13-C14-C15-C16
33	d	405[A]	LHG	C11-C10-C9-C8
23	B	610	CLA	C16-C17-C18-C19
23	a	409	CLA	C16-C17-C18-C20
23	b	602	CLA	C16-C17-C18-C19
23	b	602	CLA	C16-C17-C18-C20
23	c	510	CLA	C16-C17-C18-C19
23	d	402	CLA	C16-C17-C18-C20
26	X	101	SQD	O5-C1-O6-C44
36	C	518[B]	DGD	O6E-C1E-O5D-C6D
23	B	614	CLA	C5-C6-C7-C8
23	C	503	CLA	C15-C16-C17-C18
23	b	611	CLA	C8-C10-C11-C12
26	A	410[A]	SQD	C12-C13-C14-C15
32	B	629	LMT	C2-C3-C4-C5
32	B	629	LMT	C5-C6-C7-C8
32	b	627	LMT	C3-C4-C5-C6
33	L	101[B]	LHG	C17-C18-C19-C20
34	d	410	LMG	C29-C30-C31-C32
36	H	102	DGD	C5B-C6B-C7B-C8B
26	f	102	SQD	C32-C33-C34-C35
33	L	101[A]	LHG	C13-C14-C15-C16
33	d	405[A]	LHG	C34-C35-C36-C37
36	C	517[B]	DGD	C8A-C9A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
33	d	406[A]	LHG	C27-C28-C29-C30
34	m	101	LMG	C39-C40-C41-C42
32	A	420	LMT	C1-C2-C3-C4
26	X	101	SQD	C24-C25-C26-C27
23	D	703	CLA	O1D-CGD-O2D-CED
32	A	420	LMT	C2-C1-O1'-C1'
32	b	627	LMT	C2-C1-O1'-C1'
36	h	102	DGD	CAA-CBA-CCA-CDA
23	b	615	CLA	C16-C17-C18-C20
32	B	630	LMT	C4-C5-C6-C7
33	A	419[A]	LHG	C12-C13-C14-C15
33	b	629[A]	LHG	C16-C17-C18-C19
33	d	412[B]	LHG	C24-C25-C26-C27
34	C	501	LMG	C19-C20-C21-C22
32	T	101	LMT	C7-C8-C9-C10
32	t	101	LMT	O1'-C1-C2-C3
33	E	101[A]	LHG	C24-C25-C26-C27
34	D	711	LMG	C30-C31-C32-C33
36	C	517[B]	DGD	C4B-C5B-C6B-C7B
36	c	517[A]	DGD	O6D-C5D-C6D-O5D
26	B	620	SQD	C7-C8-C9-C10
32	a	417	LMT	C1-C2-C3-C4
26	X	101	SQD	C29-C30-C31-C32
23	C	511	CLA	C4-C3-C5-C6
29	A	414[B]	PL9	C45-C44-C46-C47
29	d	404[A]	PL9	C15-C14-C16-C17
36	c	517[A]	DGD	C2A-C1A-O1G-C1G
23	C	511	CLA	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	D	705[A]	PL9	C13-C14-C16-C17
29	D	705[B]	PL9	C13-C14-C16-C17
34	m	101	LMG	C11-C10-O7-C8
36	H	102	DGD	C9B-CAB-CBB-CCB
36	H	102	DGD	CCB-CDB-CEB-CFB
27	B	623	GOL	O2-C2-C3-O3
27	D	712	GOL	O1-C1-C2-O2
27	O	302	GOL	O1-C1-C2-O2
27	b	624	GOL	O2-C2-C3-O3
27	c	527	GOL	O2-C2-C3-O3
27	o	303	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
32	b	627	LMT	C5-C6-C7-C8
36	c	518[A]	DGD	CBB-CCB-CDB-CEB
34	C	520	LMG	C16-C17-C18-C19
32	b	621	LMT	C3'-C4'-O1B-C1B
33	D	707[A]	LHG	C15-C16-C17-C18
36	c	517[A]	DGD	C5A-C6A-C7A-C8A
36	c	519	DGD	CBA-CCA-CDA-CEA
32	e	101	LMT	C1-C2-C3-C4
26	b	620	SQD	C27-C28-C29-C30
26	f	102	SQD	C25-C26-C27-C28
34	D	711	LMG	C12-C13-C14-C15
35	d	409	HTG	S1-C1'-C2'-C3'
26	b	620	SQD	C26-C27-C28-C29
32	t	101	LMT	C7-C8-C9-C10
34	c	501	LMG	C21-C22-C23-C24
36	C	517[B]	DGD	C9A-CAA-CBA-CCA
36	c	517[A]	DGD	CAA-CBA-CCA-CDA
23	B	616	CLA	C2-C1-O2A-CGA
33	D	707[B]	LHG	C29-C30-C31-C32
33	d	412[A]	LHG	C29-C30-C31-C32
33	d	412[B]	LHG	C32-C33-C34-C35
33	E	101[B]	LHG	C24-C25-C26-C27
36	c	517[A]	DGD	C7A-C8A-C9A-CAA
34	C	501	LMG	C10-C11-C12-C13
25	D	704	BCR	C23-C24-C25-C26
25	b	617	BCR	C5-C6-C7-C8
25	b	619	BCR	C1-C6-C7-C8
25	b	619	BCR	C5-C6-C7-C8
33	b	629[B]	LHG	C16-C17-C18-C19
23	c	514	CLA	O1D-CGD-O2D-CED
36	c	518[A]	DGD	C6A-C7A-C8A-C9A
36	h	102	DGD	C9B-CAB-CBB-CCB
26	A	410[B]	SQD	C7-C8-C9-C10
26	B	620	SQD	C30-C31-C32-C33
32	B	630	LMT	C11-C10-C9-C8
23	b	604	CLA	C15-C16-C17-C18
23	b	605	CLA	C5-C6-C7-C8
26	B	620	SQD	C11-C10-C9-C8
33	D	707[B]	LHG	C17-C18-C19-C20
34	C	521	LMG	C13-C14-C15-C16
23	C	506	CLA	C4-C3-C5-C6
23	c	506	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	A	414[A]	PL9	C30-C29-C31-C32
29	D	705[A]	PL9	C15-C14-C16-C17
29	D	705[B]	PL9	C15-C14-C16-C17
23	B	603	CLA	C11-C12-C13-C15
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	506	CLA	C2-C3-C5-C6
23	a	407[A]	CLA	C11-C12-C13-C15
23	a	407[B]	CLA	C11-C12-C13-C15
23	b	606	CLA	C11-C10-C8-C7
23	c	505	CLA	C12-C13-C15-C16
23	c	506	CLA	C2-C3-C5-C6
24	a	408[B]	PHO	C2-C3-C5-C6
26	A	412	SQD	C27-C28-C29-C30
23	B	601	CLA	C13-C15-C16-C17
23	b	601	CLA	C13-C15-C16-C17
23	B	615	CLA	C16-C17-C18-C20
23	d	402	CLA	C16-C17-C18-C19
34	m	101	LMG	O9-C10-O7-C8
23	d	402	CLA	CBA-CGA-O2A-C1
26	b	620	SQD	C24-C23-O48-C46
33	D	707[A]	LHG	C29-C30-C31-C32
34	B	621	LMG	C34-C35-C36-C37
36	C	519	DGD	C6B-C7B-C8B-C9B
23	B	610	CLA	C2A-CAA-CBA-CGA
23	B	615	CLA	C10-C11-C12-C13
33	D	706[A]	LHG	C13-C14-C15-C16
34	C	501	LMG	C36-C37-C38-C39
26	a	412	SQD	C25-C26-C27-C28
36	c	517[B]	DGD	C5A-C6A-C7A-C8A
33	A	419[B]	LHG	C12-C13-C14-C15
33	d	406[B]	LHG	C29-C30-C31-C32
34	C	520	LMG	C34-C35-C36-C37
36	c	519	DGD	CBB-CCB-CDB-CEB
33	D	707[B]	LHG	C15-C16-C17-C18
36	C	517[A]	DGD	C8A-C9A-CAA-CBA
36	c	517[A]	DGD	O1A-C1A-O1G-C1G
23	B	610	CLA	C16-C17-C18-C20
26	A	412	SQD	O5-C1-O6-C44
34	B	621	LMG	O6-C1-O1-C7
36	C	518[A]	DGD	O6E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
36	c	517[B]	DGD	O6E-C1E-O5D-C6D
26	a	411[A]	SQD	C9-C10-C11-C12
26	A	412	SQD	C26-C27-C28-C29
33	D	706[B]	LHG	C26-C27-C28-C29
36	h	102	DGD	C9A-CAA-CBA-CCA
32	b	627	LMT	C1-C2-C3-C4
23	A	406[B]	CLA	C13-C15-C16-C17
23	B	601	CLA	C15-C16-C17-C18
23	c	502	CLA	CBD-CGD-O2D-CED
32	A	420	LMT	C3'-C4'-O1B-C1B
33	d	406[B]	LHG	C27-C28-C29-C30
36	H	102	DGD	C7A-C8A-C9A-CAA
26	B	620	SQD	C34-C35-C36-C37
36	h	102	DGD	C2B-C3B-C4B-C5B
26	A	410[A]	SQD	O6-C44-C45-O47
26	A	410[B]	SQD	O6-C44-C45-O47
36	c	517[B]	DGD	O6E-C5E-C6E-O5E
23	C	513	CLA	CBA-CGA-O2A-C1
36	C	517[B]	DGD	O6D-C5D-C6D-O5D
36	C	517[A]	DGD	C9A-CAA-CBA-CCA
36	c	518[A]	DGD	C2B-C3B-C4B-C5B
35	b	623	HTG	O5-C5-C6-O6
23	A	404[B]	CLA	C13-C15-C16-C17
24	a	408[B]	PHO	C4-C3-C5-C6
29	a	414[B]	PL9	C12-C11-C9-C10
34	c	520	LMG	C10-C11-C12-C13
23	D	703	CLA	C2-C3-C5-C6
29	A	414[B]	PL9	C43-C44-C46-C47
29	d	404[B]	PL9	C28-C29-C31-C32
23	B	602	CLA	C11-C12-C13-C14
23	B	606	CLA	C11-C10-C8-C9
23	D	703	CLA	C11-C10-C8-C9
23	b	606	CLA	C11-C10-C8-C9
36	C	517[A]	DGD	O6E-C5E-C6E-O5E
33	b	629[A]	LHG	C13-C14-C15-C16
34	d	410	LMG	C11-C12-C13-C14
23	b	607	CLA	C3-C5-C6-C7
36	C	517[B]	DGD	O6E-C5E-C6E-O5E
25	K	102	BCR	C7-C8-C9-C34
32	a	417	LMT	C2-C3-C4-C5
36	c	517[B]	DGD	CAA-CBA-CCA-CDA
23	d	402	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	A	405[A]	CLA	C1A-C2A-CAA-CBA
23	a	406[B]	CLA	C1A-C2A-CAA-CBA
23	c	514	CLA	C1A-C2A-CAA-CBA
23	B	608	CLA	C16-C17-C18-C19
23	c	509	CLA	C16-C17-C18-C20
23	d	401[B]	CLA	C16-C17-C18-C20
26	a	411[B]	SQD	C9-C10-C11-C12
32	M	101	LMT	C3-C4-C5-C6
33	D	706[B]	LHG	C13-C14-C15-C16
33	D	707[A]	LHG	C17-C18-C19-C20
33	d	406[B]	LHG	C28-C29-C30-C31
36	h	102	DGD	CBA-CCA-CDA-CEA
23	A	406[A]	CLA	C13-C15-C16-C17
23	B	602	CLA	C15-C16-C17-C18
23	c	513	CLA	C10-C11-C12-C13
33	A	419[B]	LHG	C4-O6-P-O3
33	d	405[B]	LHG	C4-O6-P-O3
33	d	412[B]	LHG	C25-C26-C27-C28
36	h	102	DGD	CAB-CBB-CCB-CDB
34	c	520	LMG	C28-C29-C30-C31
32	B	629	LMT	C6-C7-C8-C9
23	c	513	CLA	C13-C15-C16-C17
23	B	601	CLA	CBA-CGA-O2A-C1
34	d	410	LMG	O6-C5-C6-O5
32	B	630	LMT	O1'-C1-C2-C3
33	L	101[B]	LHG	C23-C24-C25-C26
23	C	510	CLA	O1D-CGD-O2D-CED
34	m	101	LMG	C38-C39-C40-C41
23	A	404[A]	CLA	C13-C15-C16-C17
23	B	613	CLA	C13-C15-C16-C17
23	d	401[A]	CLA	C16-C17-C18-C20
33	d	406[A]	LHG	C25-C26-C27-C28
34	d	410	LMG	C35-C36-C37-C38
32	t	101	LMT	C4'-C5'-C6'-O6'
35	b	623	HTG	S1-C1'-C2'-C3'
26	A	410[B]	SQD	C12-C13-C14-C15
32	b	621	LMT	C11-C10-C9-C8
33	d	406[B]	LHG	C9-C10-C11-C12
23	c	513	CLA	CBA-CGA-O2A-C1
23	C	507	CLA	C4-C3-C5-C6
26	A	410[B]	SQD	C11-C10-C9-C8
34	c	520	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
26	b	620	SQD	O10-C23-O48-C46
36	C	518[B]	DGD	CDA-CEA-CFA-CGA
36	c	518[A]	DGD	C4A-C5A-C6A-C7A
23	b	614	CLA	C16-C17-C18-C19
23	C	513	CLA	C3-C5-C6-C7
26	A	410[A]	SQD	O6-C44-C45-C46
26	A	412	SQD	O6-C44-C45-C46
26	a	411[A]	SQD	O6-C44-C45-C46
26	f	102	SQD	O6-C44-C45-C46
26	f	102	SQD	C44-C45-C46-O48
34	C	501	LMG	C11-C12-C13-C14
36	C	517[B]	DGD	CCA-CDA-CEA-CFA
36	c	518[B]	DGD	C6A-C7A-C8A-C9A
36	c	518[B]	DGD	CBB-CCB-CDB-CEB
32	m	103	LMT	O5'-C5'-C6'-O6'
32	a	417	LMT	C9-C10-C11-C12
33	E	101[A]	LHG	C25-C26-C27-C28
36	C	518[A]	DGD	C2G-C3G-O3G-C1D
36	C	518[A]	DGD	C5D-C6D-O5D-C1E
36	c	518[A]	DGD	C2G-C3G-O3G-C1D
36	c	518[A]	DGD	C5D-C6D-O5D-C1E
36	c	518[B]	DGD	C5D-C6D-O5D-C1E
26	b	620	SQD	C11-C10-C9-C8
34	D	711	LMG	C36-C37-C38-C39
36	C	518[A]	DGD	CDA-CEA-CFA-CGA
36	c	518[B]	DGD	C2B-C3B-C4B-C5B
32	A	420	LMT	C4-C5-C6-C7
34	C	520	LMG	C17-C18-C19-C20
36	c	517[A]	DGD	C4D-C5D-C6D-O5D
36	C	517[A]	DGD	C3B-C4B-C5B-C6B
27	B	628	GOL	O2-C2-C3-O3
27	D	712	GOL	O2-C2-C3-O3
27	o	304	GOL	O2-C2-C3-O3
32	B	627	LMT	C3'-C4'-O1B-C1B
23	B	601	CLA	O1A-CGA-O2A-C1
23	C	513	CLA	O1A-CGA-O2A-C1
35	B	624	HTG	C4'-C5'-C6'-C7'
23	A	405[A]	CLA	C15-C16-C17-C18
34	D	711	LMG	O6-C5-C6-O5
36	c	517[A]	DGD	O6E-C5E-C6E-O5E
35	b	622	HTG	C1'-C2'-C3'-C4'
29	a	414[A]	PL9	C12-C11-C9-C10

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Mol	Chain	Res	Type	Atoms
32	e	101	LMT	C4B-C5B-C6B-O6B
34	z	101	LMG	C10-C11-C12-C13
36	c	517[B]	DGD	C2A-C1A-O1G-C1G
32	e	101	LMT	C3-C4-C5-C6
23	C	507	CLA	C5-C6-C7-C8
23	a	406[A]	CLA	C2C-C3C-CAC-CBC
33	b	629[B]	LHG	C12-C13-C14-C15
33	d	412[A]	LHG	C33-C34-C35-C36
36	H	102	DGD	CCA-CDA-CEA-CFA
26	B	620	SQD	C46-C45-O47-C7
26	b	620	SQD	C46-C45-O47-C7
23	b	601	CLA	C2-C1-O2A-CGA
33	b	629[B]	LHG	C13-C14-C15-C16
33	d	406[A]	LHG	C34-C35-C36-C37
23	c	511	CLA	CBD-CGD-O2D-CED
26	a	411[A]	SQD	C12-C13-C14-C15
33	D	706[A]	LHG	C12-C13-C14-C15
23	C	511	CLA	C10-C11-C12-C13
34	B	621	LMG	C37-C38-C39-C40
34	C	501	LMG	C13-C14-C15-C16
34	C	520	LMG	C31-C32-C33-C34
23	d	401[B]	CLA	C16-C17-C18-C19
36	C	519	DGD	CAB-CBB-CCB-CDB
36	c	517[B]	DGD	C2E-C1E-O5D-C6D
34	c	520	LMG	O6-C5-C6-O5
26	a	412	SQD	C16-C17-C18-C19
26	b	620	SQD	C14-C15-C16-C17
36	C	517[A]	DGD	O6D-C5D-C6D-O5D
23	d	401[A]	CLA	C16-C17-C18-C19
33	d	406[A]	LHG	C29-C30-C31-C32
36	c	518[B]	DGD	C4A-C5A-C6A-C7A
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	C	505	CLA	C12-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C15
23	C	514	CLA	C11-C10-C8-C7
23	C	514	CLA	C11-C12-C13-C15
23	a	409	CLA	C11-C10-C8-C7
23	b	601	CLA	C11-C12-C13-C15
23	c	505	CLA	C11-C12-C13-C15
23	c	506	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
23	c	511	CLA	C11-C10-C8-C7
23	c	513	CLA	C12-C13-C15-C16
29	d	404[B]	PL9	C13-C14-C16-C17
23	B	603	CLA	C11-C12-C13-C14
23	C	505	CLA	C14-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C14
23	C	513	CLA	C6-C7-C8-C9
23	C	514	CLA	C11-C10-C8-C9
23	D	703	CLA	C14-C13-C15-C16
23	b	601	CLA	C6-C7-C8-C9
23	b	606	CLA	C14-C13-C15-C16
23	c	506	CLA	C11-C12-C13-C14
23	c	511	CLA	C11-C10-C8-C9
33	d	406[A]	LHG	C28-C29-C30-C31
34	c	501	LMG	C35-C36-C37-C38
36	h	102	DGD	CDB-CEB-CFB-CGB
23	b	602	CLA	C10-C11-C12-C13
23	b	606	CLA	C16-C17-C18-C20
27	O	303	GOL	O1-C1-C2-C3
32	e	101	LMT	C9-C10-C11-C12
33	D	707[B]	LHG	C13-C14-C15-C16
33	E	101[B]	LHG	C25-C26-C27-C28
26	b	620	SQD	C31-C32-C33-C34
33	b	629[A]	LHG	C27-C28-C29-C30
23	b	601	CLA	CBA-CGA-O2A-C1
36	c	519	DGD	C2A-C1A-O1G-C1G
23	C	514	CLA	O1D-CGD-O2D-CED
32	t	101	LMT	C11-C10-C9-C8
35	o	301	HTG	C2'-C3'-C4'-C5'
23	C	507	CLA	C15-C16-C17-C18
34	C	520	LMG	C37-C38-C39-C40
34	z	101	LMG	C14-C15-C16-C17
34	c	520	LMG	C29-C30-C31-C32
36	C	518[A]	DGD	C5B-C6B-C7B-C8B
33	E	101[A]	LHG	O6-C4-C5-C6
33	b	629[A]	LHG	O6-C4-C5-C6
33	b	629[B]	LHG	O6-C4-C5-C6
32	A	420	LMT	C5-C6-C7-C8
33	D	706[A]	LHG	C10-C11-C12-C13
33	D	707[A]	LHG	C13-C14-C15-C16
33	d	406[A]	LHG	C9-C10-C11-C12
29	d	404[A]	PL9	C45-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
33	A	419[A]	LHG	C26-C27-C28-C29
33	L	101[B]	LHG	C11-C12-C13-C14
33	d	405[A]	LHG	C13-C14-C15-C16
34	c	501	LMG	C29-C30-C31-C32
35	c	522	HTG	C4'-C5'-C6'-C7'
33	b	629[B]	LHG	C27-C28-C29-C30
23	C	511	CLA	CBA-CGA-O2A-C1
36	C	517[A]	DGD	C7A-C8A-C9A-CAA
23	C	502	CLA	O1D-CGD-O2D-CED
36	c	517[B]	DGD	O1A-C1A-O1G-C1G
33	L	101[B]	LHG	C24-C25-C26-C27
36	c	517[B]	DGD	C4B-C5B-C6B-C7B
32	B	627	LMT	C2-C1-O1'-C1'
32	F	101	LMT	C2-C1-O1'-C1'
32	e	101	LMT	C2-C1-O1'-C1'
32	m	103	LMT	C2-C1-O1'-C1'
26	X	101	SQD	C32-C33-C34-C35
33	E	101[B]	LHG	C17-C18-C19-C20
36	C	517[B]	DGD	C7A-C8A-C9A-CAA
36	C	519	DGD	CDB-CEB-CFB-CGB
23	c	510	CLA	C8-C10-C11-C12
26	X	101	SQD	C34-C35-C36-C37
32	F	101	LMT	C4-C5-C6-C7
33	D	707[B]	LHG	C24-C23-O8-C6
33	D	706[B]	LHG	C12-C13-C14-C15
36	c	518[A]	DGD	CDA-CEA-CFA-CGA
23	B	610	CLA	C13-C15-C16-C17
26	A	410[B]	SQD	O6-C44-C45-C46
26	B	620	SQD	C44-C45-C46-O48
26	b	620	SQD	C44-C45-C46-O48
33	a	420[A]	LHG	C4-C5-C6-O8
33	a	420[B]	LHG	C4-C5-C6-O8
34	c	501	LMG	C7-C8-C9-O8
33	L	101[A]	LHG	C24-C25-C26-C27
33	a	420[A]	LHG	C10-C11-C12-C13
36	c	517[B]	DGD	C7A-C8A-C9A-CAA
36	c	518[B]	DGD	C5A-C6A-C7A-C8A
33	b	629[A]	LHG	C12-C13-C14-C15
33	d	406[B]	LHG	C34-C35-C36-C37
34	m	101	LMG	C37-C38-C39-C40
24	a	408[A]	PHO	O2A-C1-C2-C3
32	M	101	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
32	b	621	LMT	C3-C4-C5-C6
32	a	417	LMT	C3-C4-C5-C6
36	c	518[A]	DGD	C5A-C6A-C7A-C8A
23	B	603	CLA	C4-C3-C5-C6
24	a	408[A]	PHO	C4-C3-C5-C6
23	b	606	CLA	C16-C17-C18-C19
29	D	705[A]	PL9	C43-C44-C46-C47
33	L	101[A]	LHG	C11-C12-C13-C14
36	H	102	DGD	CAB-CBB-CCB-CDB
35	b	622	HTG	C3'-C4'-C5'-C6'
33	A	419[B]	LHG	C3-O3-P-O6
33	a	420[A]	LHG	C7-C8-C9-C10
33	b	629[B]	LHG	C25-C26-C27-C28
23	c	513	CLA	O1D-CGD-O2D-CED
23	C	503	CLA	C3-C5-C6-C7
35	b	625	HTG	C4-C5-C6-O6
34	C	520	LMG	C30-C31-C32-C33
33	E	101[A]	LHG	O6-C4-C5-O7
36	C	517[B]	DGD	C4D-C5D-C6D-O5D
34	c	521	LMG	C29-C28-O8-C9
23	c	513	CLA	O1A-CGA-O2A-C1
23	A	406[A]	CLA	C16-C17-C18-C20
33	b	629[A]	LHG	C31-C32-C33-C34
32	B	627	LMT	C1-C2-C3-C4
23	b	610	CLA	C15-C16-C17-C18
34	C	521	LMG	C35-C36-C37-C38
26	a	411[A]	SQD	C34-C35-C36-C37
26	B	620	SQD	O47-C45-C46-O48
26	a	411[A]	SQD	O6-C44-C45-O47
23	c	512	CLA	CBA-CGA-O2A-C1
33	A	419[B]	LHG	C18-C19-C20-C21
34	C	520	LMG	C36-C37-C38-C39
36	C	518[A]	DGD	C8B-C9B-CAB-CBB
33	E	101[A]	LHG	C17-C18-C19-C20
33	a	420[B]	LHG	C10-C11-C12-C13
29	a	414[A]	PL9	C24-C26-C27-C28
29	a	414[B]	PL9	C24-C26-C27-C28
33	D	707[A]	LHG	C10-C11-C12-C13
23	b	608	CLA	C2-C1-O2A-CGA
23	b	613	CLA	C2-C1-O2A-CGA
23	b	614	CLA	C2-C1-O2A-CGA
23	B	612	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	c	510	CLA	C13-C15-C16-C17
23	B	614	CLA	C14-C13-C15-C16
23	C	507	CLA	C6-C7-C8-C9
23	c	513	CLA	C6-C7-C8-C9
23	c	514	CLA	C6-C7-C8-C9
33	d	406[B]	LHG	C25-C26-C27-C28
32	b	621	LMT	C7-C8-C9-C10
23	b	612	CLA	C10-C11-C12-C13
23	c	507	CLA	C13-C15-C16-C17
23	b	601	CLA	O1A-CGA-O2A-C1
26	a	411[B]	SQD	C35-C36-C37-C38
32	m	103	LMT	C7-C8-C9-C10
36	C	518[A]	DGD	C8A-C9A-CAA-CBA
25	B	617	BCR	C5-C6-C7-C8
25	H	101	BCR	C23-C24-C25-C26
25	H	101	BCR	C23-C24-C25-C30
23	C	512	CLA	C8-C10-C11-C12
33	d	412[A]	LHG	C25-C26-C27-C28
25	K	102	BCR	C7-C8-C9-C10
25	d	403	BCR	C7-C8-C9-C10
23	b	616	CLA	C5-C6-C7-C8
23	A	406[B]	CLA	C16-C17-C18-C20
33	D	706[B]	LHG	C11-C10-C9-C8
34	B	621	LMG	C32-C33-C34-C35
36	C	519	DGD	C6A-C7A-C8A-C9A
23	B	606	CLA	C15-C16-C17-C18
33	D	706[B]	LHG	C34-C35-C36-C37
23	B	610	CLA	C12-C13-C15-C16
23	B	614	CLA	C12-C13-C15-C16
23	C	503	CLA	C12-C13-C15-C16
23	C	507	CLA	C6-C7-C8-C10
23	C	511	CLA	C12-C13-C15-C16
23	D	703	CLA	C12-C13-C15-C16
23	b	601	CLA	C6-C7-C8-C10
23	b	601	CLA	C11-C10-C8-C7
23	b	604	CLA	C6-C7-C8-C10
23	b	615	CLA	C12-C13-C15-C16
23	c	506	CLA	C12-C13-C15-C16
23	c	507	CLA	C11-C10-C8-C7
23	c	510	CLA	C6-C7-C8-C10
23	c	510	CLA	C11-C10-C8-C7
23	d	401[B]	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
24	a	408[A]	PHO	C2-C3-C5-C6
29	a	414[B]	PL9	C12-C11-C9-C8
34	B	621	LMG	C18-C19-C20-C21
25	t	102	BCR	C13-C14-C15-C16
23	C	503	CLA	C16-C17-C18-C19
33	L	101[A]	LHG	C11-C10-C9-C8
33	d	412[A]	LHG	C24-C25-C26-C27
33	b	629[A]	LHG	C34-C35-C36-C37
36	C	517[A]	DGD	CCA-CDA-CEA-CFA
32	B	629	LMT	C3-C4-C5-C6
33	b	629[A]	LHG	C9-C10-C11-C12
33	d	412[B]	LHG	C33-C34-C35-C36
35	c	522	HTG	C2'-C1'-S1-C1
26	b	620	SQD	C13-C14-C15-C16
33	D	707[B]	LHG	C10-C11-C12-C13
33	E	101[B]	LHG	C13-C14-C15-C16
34	m	101	LMG	C32-C33-C34-C35
23	B	616	CLA	CAD-CBD-CGD-O2D
23	C	513	CLA	CAD-CBD-CGD-O2D
23	b	612	CLA	CAD-CBD-CGD-O2D
23	b	616	CLA	CAD-CBD-CGD-O2D
23	c	504	CLA	CAD-CBD-CGD-O2D
23	c	511	CLA	CAD-CBD-CGD-O2D
24	A	407[A]	PHO	CAD-CBD-CGD-O2D
24	a	408[A]	PHO	CAD-CBD-CGD-O2D
24	a	408[B]	PHO	CAD-CBD-CGD-O2D
38	f	101	HEM	C2B-C3B-CAB-CBB
33	E	101[A]	LHG	C13-C14-C15-C16
33	L	101[B]	LHG	C11-C10-C9-C8
26	a	411[A]	SQD	C27-C28-C29-C30
23	c	514	CLA	C4-C3-C5-C6
23	C	503	CLA	C16-C17-C18-C20
33	D	706[A]	LHG	C34-C35-C36-C37
36	c	518[B]	DGD	O6E-C1E-O5D-C6D
23	a	406[B]	CLA	C2C-C3C-CAC-CBC
26	a	412	SQD	O6-C44-C45-C46
33	D	707[B]	LHG	C2-C3-O3-P
33	E	101[A]	LHG	C4-C5-C6-O8
33	E	101[B]	LHG	C4-C5-C6-O8
33	E	101[B]	LHG	O6-C4-C5-O7
33	b	629[A]	LHG	O6-C4-C5-O7
33	b	629[B]	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
23	b	601	CLA	C8-C10-C11-C12
36	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	B	607	CLA	CHA-CBD-CGD-O1D
23	C	503	CLA	CHA-CBD-CGD-O1D
23	C	503	CLA	CHA-CBD-CGD-O2D
23	b	601	CLA	CHA-CBD-CGD-O1D
23	b	606	CLA	CHA-CBD-CGD-O2D
23	c	503	CLA	CHA-CBD-CGD-O1D
23	C	511	CLA	O1A-CGA-O2A-C1
23	c	512	CLA	O1A-CGA-O2A-C1
33	D	707[B]	LHG	O10-C23-O8-C6
36	c	519	DGD	O1A-C1A-O1G-C1G
26	a	411[B]	SQD	C12-C13-C14-C15
32	b	627	LMT	C6-C7-C8-C9
36	C	519	DGD	CBA-CCA-CDA-CEA
26	b	620	SQD	O47-C45-C46-O48
26	f	102	SQD	O47-C45-C46-O48
33	a	420[A]	LHG	O7-C5-C6-O8
33	a	420[B]	LHG	O7-C5-C6-O8
34	B	621	LMG	O1-C7-C8-O7
23	D	703	CLA	O1A-CGA-O2A-C1
34	c	521	LMG	O10-C28-O8-C9
32	M	101	LMT	C2-C3-C4-C5
34	C	501	LMG	C20-C21-C22-C23
34	C	501	LMG	C29-C30-C31-C32
34	d	410	LMG	C16-C17-C18-C19
36	c	517[B]	DGD	C8B-C9B-CAB-CBB
23	b	601	CLA	C4-C3-C5-C6
29	D	705[A]	PL9	C45-C44-C46-C47
36	c	518[A]	DGD	C1A-C2A-C3A-C4A
23	C	511	CLA	C14-C13-C15-C16
36	C	517[A]	DGD	C4D-C5D-C6D-O5D
23	B	615	CLA	C13-C15-C16-C17
23	B	601	CLA	C2A-CAA-CBA-CGA
26	A	412	SQD	C24-C23-O48-C46
26	X	101	SQD	C7-C8-C9-C10
33	d	412[B]	LHG	C7-C8-C9-C10
27	d	411	GOL	C1-C2-C3-O3
23	a	405[A]	CLA	C2C-C3C-CAC-CBC
36	C	518[B]	DGD	C3B-C4B-C5B-C6B

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Mol	Chain	Res	Type	Atoms
34	C	521	LMG	C38-C39-C40-C41
23	B	611	CLA	C1A-C2A-CAA-CBA
23	C	512	CLA	C1A-C2A-CAA-CBA
23	a	406[A]	CLA	C1A-C2A-CAA-CBA
34	C	521	LMG	C20-C21-C22-C23
23	C	510	CLA	C2-C1-O2A-CGA
33	d	405[B]	LHG	C24-C23-O8-C6
33	d	406[A]	LHG	C24-C23-O8-C6
33	A	419[A]	LHG	C32-C33-C34-C35
33	D	706[A]	LHG	C4-O6-P-O3
33	d	412[A]	LHG	C3-O3-P-O6
36	C	519	DGD	CAA-CBA-CCA-CDA
33	a	420[A]	LHG	C23-C24-C25-C26
26	a	411[A]	SQD	C35-C36-C37-C38
32	B	627	LMT	C7-C8-C9-C10
33	D	706[B]	LHG	C28-C29-C30-C31
36	C	519	DGD	C7B-C8B-C9B-CAB
36	h	102	DGD	CDA-CEA-CFA-CGA
33	D	707[A]	LHG	C2-C3-O3-P
33	d	406[A]	LHG	C2-C3-O3-P
33	d	406[B]	LHG	C2-C3-O3-P
34	m	101	LMG	C14-C15-C16-C17
33	d	405[B]	LHG	O10-C23-O8-C6
33	A	419[B]	LHG	C4-O6-P-O4
33	D	706[A]	LHG	C4-O6-P-O5
33	D	706[B]	LHG	C4-O6-P-O5
33	D	707[B]	LHG	C4-O6-P-O4
33	E	101[A]	LHG	C4-O6-P-O5
33	E	101[B]	LHG	C4-O6-P-O5
33	L	101[B]	LHG	C4-O6-P-O5
33	a	420[A]	LHG	C4-O6-P-O4
33	a	420[B]	LHG	C4-O6-P-O4
33	d	405[A]	LHG	C3-O3-P-O4
33	d	405[B]	LHG	C4-O6-P-O5
36	c	517[A]	DGD	O6E-C1E-O5D-C6D
23	D	703	CLA	CBA-CGA-O2A-C1
33	d	406[B]	LHG	C24-C23-O8-C6
33	E	101[B]	LHG	O6-C4-C5-C6
33	L	101[A]	LHG	O6-C4-C5-C6
26	A	410[A]	SQD	C18-C19-C20-C21
33	d	406[B]	LHG	O10-C23-O8-C6
34	C	501	LMG	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
32	T	101	LMT	C1-C2-C3-C4
26	B	620	SQD	C33-C34-C35-C36
33	d	412[A]	LHG	C27-C28-C29-C30
36	c	517[A]	DGD	CCB-CDB-CEB-CFB
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	607	CLA	CAD-CBD-CGD-O1D
23	B	609	CLA	CAD-CBD-CGD-O1D
23	C	503	CLA	CAD-CBD-CGD-O1D
23	C	505	CLA	CAD-CBD-CGD-O1D
23	C	507	CLA	CAD-CBD-CGD-O1D
23	b	601	CLA	CAD-CBD-CGD-O1D
23	c	503	CLA	CAD-CBD-CGD-O1D
23	b	604	CLA	C10-C11-C12-C13
32	B	630	LMT	C6-C7-C8-C9
23	b	601	CLA	C3-C5-C6-C7
33	a	420[B]	LHG	C23-C24-C25-C26
26	A	412	SQD	C30-C31-C32-C33
33	D	707[A]	LHG	C24-C23-O8-C6
33	E	101[A]	LHG	C1-C2-C3-O3
23	B	602	CLA	C6-C7-C8-C10
23	B	607	CLA	C12-C13-C15-C16
23	B	616	CLA	C12-C13-C15-C16
23	C	506	CLA	C12-C13-C15-C16
23	C	507	CLA	C12-C13-C15-C16
23	b	616	CLA	C6-C7-C8-C10
33	b	629[B]	LHG	C9-C10-C11-C12
34	C	520	LMG	C12-C13-C14-C15
36	h	102	DGD	CCB-CDB-CEB-CFB
26	A	412	SQD	O10-C23-O48-C46
33	d	406[A]	LHG	O10-C23-O8-C6
23	c	504	CLA	C8-C10-C11-C12
36	C	518[A]	DGD	C1A-C2A-C3A-C4A
33	D	707[A]	LHG	O10-C23-O8-C6
36	c	517[A]	DGD	C8B-C9B-CAB-CBB
26	A	410[A]	SQD	C34-C35-C36-C37
23	b	601	CLA	CAA-CBA-CGA-O2A
34	C	501	LMG	C18-C19-C20-C21
33	E	101[A]	LHG	O7-C5-C6-O8
34	c	501	LMG	O7-C8-C9-O8
33	b	629[B]	LHG	C34-C35-C36-C37
36	C	517[B]	DGD	C6A-C7A-C8A-C9A
26	B	620	SQD	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
26	a	411[A]	SQD	C11-C12-C13-C14
32	F	101	LMT	C2-C3-C4-C5
34	d	410	LMG	C18-C19-C20-C21
34	z	101	LMG	C20-C21-C22-C23
36	C	518[B]	DGD	C5D-C6D-O5D-C1E
34	z	101	LMG	C19-C20-C21-C22
33	a	420[B]	LHG	C7-C8-C9-C10
36	C	519	DGD	O1A-C1A-O1G-C1G
23	b	612	CLA	C8-C10-C11-C12
23	A	406[A]	CLA	C14-C13-C15-C16
23	B	607	CLA	C14-C13-C15-C16
23	B	610	CLA	C14-C13-C15-C16
23	a	409	CLA	C11-C10-C8-C9
23	b	615	CLA	C14-C13-C15-C16
23	c	506	CLA	C14-C13-C15-C16
23	c	510	CLA	C6-C7-C8-C9
23	d	401[B]	CLA	C11-C12-C13-C14
23	d	402	CLA	C11-C12-C13-C14
33	d	406[B]	LHG	C33-C34-C35-C36
23	D	703	CLA	C8-C10-C11-C12
23	c	512	CLA	C8-C10-C11-C12
36	H	102	DGD	O2G-C1B-C2B-C3B
27	D	701	GOL	O1-C1-C2-O2
27	o	304	GOL	O1-C1-C2-O2
23	c	510	CLA	C15-C16-C17-C18
24	a	408[A]	PHO	C8-C10-C11-C12
34	B	621	LMG	C14-C15-C16-C17
25	t	102	BCR	C7-C8-C9-C34
23	C	510	CLA	C3-C5-C6-C7
23	A	405[B]	CLA	C15-C16-C17-C18
32	A	418	LMT	C7-C8-C9-C10
33	D	707[B]	LHG	C27-C28-C29-C30
23	B	601	CLA	CAA-CBA-CGA-O2A
34	m	101	LMG	C11-C12-C13-C14
34	Z	101	LMG	C29-C28-O8-C9
32	F	101	LMT	C6-C7-C8-C9
23	c	511	CLA	C4-C3-C5-C6
34	c	501	LMG	O8-C28-C29-C30
33	D	706[B]	LHG	C10-C11-C12-C13
36	c	518[B]	DGD	C9B-CAB-CBB-CCB
23	B	603	CLA	C2-C3-C5-C6
29	a	414[A]	PL9	C12-C11-C9-C8

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Mol	Chain	Res	Type	Atoms
33	d	412[A]	LHG	C34-C35-C36-C37
36	c	517[B]	DGD	CCB-CDB-CEB-CFB
33	d	406[A]	LHG	C32-C33-C34-C35
34	B	621	LMG	O8-C28-C29-C30
23	b	608	CLA	C13-C15-C16-C17
33	E	101[B]	LHG	C1-C2-C3-O3
23	A	408	CLA	C2-C1-O2A-CGA
23	B	613	CLA	C2-C1-O2A-CGA
23	c	514	CLA	C2-C1-O2A-CGA
26	A	410[A]	SQD	C16-C17-C18-C19
26	A	410[B]	SQD	C16-C17-C18-C19
36	C	518[B]	DGD	C7A-C8A-C9A-CAA
23	b	616	CLA	O1A-CGA-O2A-C1
26	b	620	SQD	C10-C11-C12-C13
32	B	629	LMT	C7-C8-C9-C10
36	C	518[B]	DGD	C5B-C6B-C7B-C8B
33	A	419[B]	LHG	C26-C27-C28-C29
23	b	614	CLA	CBD-CGD-O2D-CED
36	C	518[B]	DGD	C8A-C9A-CAA-CBA
33	d	405[A]	LHG	O10-C23-O8-C6
33	L	101[A]	LHG	O6-C4-C5-O7
33	b	629[B]	LHG	C17-C18-C19-C20
29	D	705[B]	PL9	C45-C44-C46-C47
26	f	102	SQD	C26-C27-C28-C29
23	c	502	CLA	O1D-CGD-O2D-CED
25	B	617	BCR	C1-C6-C7-C8
23	b	601	CLA	C2-C3-C5-C6
29	A	414[A]	PL9	C28-C29-C31-C32
29	A	414[B]	PL9	C28-C29-C31-C32
29	a	414[B]	PL9	C43-C44-C46-C47
26	a	411[B]	SQD	C34-C35-C36-C37
33	d	405[A]	LHG	C24-C23-O8-C6
36	C	519	DGD	C2A-C1A-O1G-C1G
23	a	406[A]	CLA	C4C-C3C-CAC-CBC
33	L	101[B]	LHG	C27-C28-C29-C30
36	c	518[A]	DGD	O6E-C1E-O5D-C6D
35	o	301	HTG	C4'-C5'-C6'-C7'
36	C	517[A]	DGD	C6A-C7A-C8A-C9A
34	Z	101	LMG	C2-C1-O1-C7
36	c	517[A]	DGD	C2E-C1E-O5D-C6D
36	c	518[A]	DGD	C2E-C1E-O5D-C6D
36	c	518[B]	DGD	C2E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
33	L	101[A]	LHG	C26-C27-C28-C29
33	E	101[B]	LHG	O7-C5-C6-O8
33	d	412[B]	LHG	C3-O3-P-O6
34	d	410	LMG	C19-C20-C21-C22
33	L	101[A]	LHG	C27-C28-C29-C30
34	B	621	LMG	O1-C7-C8-C9
26	a	411[B]	SQD	C11-C12-C13-C14
23	B	613	CLA	C11-C10-C8-C7
23	C	507	CLA	C2-C3-C5-C6
23	B	607	CLA	C3-C5-C6-C7
34	D	711	LMG	C18-C19-C20-C21
36	c	519	DGD	C2B-C3B-C4B-C5B
23	A	406[B]	CLA	C14-C13-C15-C16
23	B	614	CLA	C11-C10-C8-C9
23	C	511	CLA	C11-C12-C13-C14
23	C	514	CLA	C6-C7-C8-C9
23	b	601	CLA	C11-C12-C13-C14
23	a	406[B]	CLA	C15-C16-C17-C18
23	a	405[A]	CLA	C4C-C3C-CAC-CBC
32	T	101	LMT	C3-C4-C5-C6
35	b	623	HTG	C4'-C5'-C6'-C7'
36	C	517[B]	DGD	CDB-CEB-CFB-CGB
33	D	707[A]	LHG	C27-C28-C29-C30
36	C	518[B]	DGD	C8B-C9B-CAB-CBB
23	c	511	CLA	O1A-CGA-O2A-C1
23	b	616	CLA	CBA-CGA-O2A-C1
23	A	404[B]	CLA	C2C-C3C-CAC-CBC
25	Y	101	BCR	C21-C22-C23-C24
25	d	403	BCR	C21-C22-C23-C24
33	d	405[B]	LHG	C25-C26-C27-C28
36	c	517[A]	DGD	C4B-C5B-C6B-C7B
33	d	412[A]	LHG	C1-C2-C3-O3
36	c	518[B]	DGD	C1A-C2A-C3A-C4A
26	a	412	SQD	C24-C23-O48-C46
33	d	406[A]	LHG	C33-C34-C35-C36
26	a	412	SQD	O10-C23-O48-C46
23	c	511	CLA	CBA-CGA-O2A-C1
34	d	410	LMG	C28-C29-C30-C31
38	F	102	HEM	CAD-CBD-CGD-O1D
23	b	605	CLA	C3-C5-C6-C7
29	A	414[B]	PL9	C39-C41-C42-C43
23	B	608	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
23	C	504	CLA	CBD-CGD-O2D-CED
33	a	420[B]	LHG	C24-C25-C26-C27
23	B	609	CLA	C2-C3-C5-C6
26	A	410[A]	SQD	C11-C10-C9-C8
23	B	606	CLA	C8-C10-C11-C12
32	a	417	LMT	C4-C5-C6-C7
33	b	629[A]	LHG	C25-C26-C27-C28
34	z	101	LMG	O7-C10-C11-C12
23	C	507	CLA	C2-C1-O2A-CGA
33	D	706[A]	LHG	C11-C10-C9-C8
36	C	519	DGD	CDA-CEA-CFA-CGA
23	A	404[B]	CLA	C2A-CAA-CBA-CGA
23	C	502	CLA	C2A-CAA-CBA-CGA
26	X	101	SQD	O47-C45-C46-O48
33	a	420[A]	LHG	C24-C25-C26-C27
38	f	101	HEM	CAD-CBD-CGD-O1D
34	d	410	LMG	C40-C41-C42-C43
34	d	410	LMG	C36-C37-C38-C39
23	B	609	CLA	C4-C3-C5-C6
29	A	414[B]	PL9	C12-C11-C9-C10
29	a	414[B]	PL9	C45-C44-C46-C47
29	d	404[B]	PL9	C45-C44-C46-C47
29	A	414[B]	PL9	C4-C3-C7-C8
29	a	414[A]	PL9	C4-C3-C7-C8
29	a	414[B]	PL9	C4-C3-C7-C8
36	C	519	DGD	C7A-C8A-C9A-CAA
36	h	102	DGD	O2G-C1B-C2B-C3B
23	B	614	CLA	C6-C7-C8-C9
23	B	616	CLA	C14-C13-C15-C16
23	C	506	CLA	C14-C13-C15-C16
23	C	510	CLA	C6-C7-C8-C9
23	a	407[A]	CLA	C6-C7-C8-C9
33	d	412[B]	LHG	C17-C18-C19-C20
36	c	518[A]	DGD	C7B-C8B-C9B-CAB
26	a	411[B]	SQD	O6-C44-C45-C46
33	L	101[A]	LHG	C23-C24-C25-C26
24	a	408[B]	PHO	O2A-C1-C2-C3
32	a	417	LMT	O5'-C1'-O1'-C1
38	f	101	HEM	CAD-CBD-CGD-O2D
36	c	519	DGD	C9B-CAB-CBB-CCB
23	a	406[A]	CLA	C15-C16-C17-C18
26	A	410[A]	SQD	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
36	C	519	DGD	C9A-CAA-CBA-CCA
29	d	404[B]	PL9	C30-C29-C31-C32
23	B	604	CLA	C1A-C2A-CAA-CBA
23	C	502	CLA	C1A-C2A-CAA-CBA
23	a	407[B]	CLA	C1A-C2A-CAA-CBA
23	B	615	CLA	C12-C13-C15-C16
23	C	504	CLA	C6-C7-C8-C10
23	b	603	CLA	C11-C10-C8-C7
23	b	608	CLA	C12-C13-C15-C16
23	b	614	CLA	C12-C13-C15-C16
23	A	404[A]	CLA	C2C-C3C-CAC-CBC
32	B	627	LMT	C9-C10-C11-C12
40	V	201	HEC	CAD-CBD-CGD-O1D
25	a	410	BCR	C19-C20-C21-C22
23	a	405[B]	CLA	C2C-C3C-CAC-CBC
33	A	419[A]	LHG	C18-C19-C20-C21
33	b	629[A]	LHG	C17-C18-C19-C20
33	d	406[B]	LHG	C32-C33-C34-C35
23	B	614	CLA	C2A-CAA-CBA-CGA
23	a	405[B]	CLA	C2A-CAA-CBA-CGA
23	b	602	CLA	C2A-CAA-CBA-CGA
23	B	613	CLA	C15-C16-C17-C18
34	z	101	LMG	C13-C14-C15-C16
33	D	706[A]	LHG	C26-C27-C28-C29
36	C	519	DGD	C4A-C5A-C6A-C7A
36	c	517[B]	DGD	CAB-CBB-CCB-CDB
32	e	101	LMT	O1'-C1-C2-C3
33	d	412[B]	LHG	C13-C14-C15-C16
36	C	517[B]	DGD	C3B-C4B-C5B-C6B
23	C	507	CLA	C16-C17-C18-C20
33	d	405[A]	LHG	C16-C17-C18-C19
29	D	705[B]	PL9	C35-C34-C36-C37
29	d	404[A]	PL9	C43-C44-C46-C47
23	c	510	CLA	C10-C11-C12-C13
23	a	409	CLA	C15-C16-C17-C18
38	F	102	HEM	CAD-CBD-CGD-O2D
26	a	412	SQD	C26-C27-C28-C29
26	a	411[B]	SQD	O6-C44-C45-O47
36	c	519	DGD	C1A-C2A-C3A-C4A
26	b	620	SQD	C28-C29-C30-C31
23	A	406[A]	CLA	C16-C17-C18-C19
29	A	414[A]	PL9	C39-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
34	Z	101	LMG	C21-C22-C23-C24
29	a	414[A]	PL9	C45-C44-C46-C47
32	e	101	LMT	C2-C3-C4-C5
23	c	511	CLA	C2-C3-C5-C6
23	A	404[B]	CLA	C4C-C3C-CAC-CBC
33	A	419[B]	LHG	C11-C12-C13-C14
40	V	201	HEC	CAD-CBD-CGD-O2D
23	B	610	CLA	C11-C12-C13-C14
23	a	407[B]	CLA	C6-C7-C8-C9
34	C	521	LMG	C12-C13-C14-C15
32	a	417	LMT	O5'-C5'-C6'-O6'
33	A	419[A]	LHG	C29-C30-C31-C32
36	c	517[A]	DGD	CAB-CBB-CCB-CDB
26	A	412	SQD	C15-C16-C17-C18
25	C	515	BCR	C1-C6-C7-C8
25	c	515	BCR	C23-C24-C25-C30
25	d	403	BCR	C23-C24-C25-C30
25	h	101	BCR	C23-C24-C25-C30
25	y	101	BCR	C23-C24-C25-C30
23	C	504	CLA	O1D-CGD-O2D-CED
27	D	701	GOL	O1-C1-C2-C3
27	l	102[A]	GOL	O1-C1-C2-C3
27	v	202[A]	GOL	O1-C1-C2-C3
35	b	625	HTG	C1'-C2'-C3'-C4'
26	a	411[B]	SQD	C18-C19-C20-C21
23	A	405[B]	CLA	C2C-C3C-CAC-CBC
23	b	616	CLA	C4-C3-C5-C6
23	c	505	CLA	C4-C3-C5-C6
29	D	705[A]	PL9	C35-C34-C36-C37
23	c	508	CLA	C5-C6-C7-C8
29	a	414[A]	PL9	C43-C44-C46-C47
36	c	519	DGD	O6D-C5D-C6D-O5D
36	C	518[B]	DGD	C2G-C3G-O3G-C1D
36	c	517[B]	DGD	C5D-C6D-O5D-C1E
36	c	518[B]	DGD	C2G-C3G-O3G-C1D
23	A	404[A]	CLA	C16-C17-C18-C19
26	a	411[B]	SQD	C27-C28-C29-C30
33	A	419[A]	LHG	C35-C36-C37-C38
34	B	621	LMG	C29-C30-C31-C32
36	C	518[B]	DGD	C1A-C2A-C3A-C4A
33	b	629[A]	LHG	C10-C11-C12-C13
23	B	606	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
36	h	102	DGD	C6A-C7A-C8A-C9A
23	B	613	CLA	C12-C13-C15-C16
23	a	407[A]	CLA	C6-C7-C8-C10
23	a	407[B]	CLA	C6-C7-C8-C10
23	b	613	CLA	C11-C10-C8-C7
23	b	615	CLA	C11-C12-C13-C15
23	c	514	CLA	C12-C13-C15-C16
29	D	705[B]	PL9	C43-C44-C46-C47
29	d	404[B]	PL9	C18-C19-C21-C22
29	d	404[B]	PL9	C43-C44-C46-C47
38	f	101	HEM	CAA-CBA-CGA-O2A
33	L	101[A]	LHG	C16-C17-C18-C19
34	B	621	LMG	C20-C21-C22-C23
34	c	521	LMG	C31-C32-C33-C34
27	a	418	GOL	O1-C1-C2-O2
27	d	411	GOL	O2-C2-C3-O3
27	l	102[B]	GOL	O1-C1-C2-O2
23	b	615	CLA	C10-C11-C12-C13
34	c	521	LMG	O1-C7-C8-O7
33	E	101[B]	LHG	C11-C10-C9-C8
33	d	406[B]	LHG	C11-C10-C9-C8
26	b	620	SQD	C30-C31-C32-C33
36	h	102	DGD	CCA-CDA-CEA-CFA
32	M	101	LMT	C9-C10-C11-C12
36	C	519	DGD	C2B-C3B-C4B-C5B
33	A	419[A]	LHG	O8-C23-C24-C25
33	b	629[B]	LHG	O7-C7-C8-C9
23	B	614	CLA	C4-C3-C5-C6
23	C	509	CLA	C13-C15-C16-C17
23	c	514	CLA	C2-C3-C5-C6
36	c	518[A]	DGD	C9B-CAB-CBB-CCB
23	B	612	CLA	CBA-CGA-O2A-C1
23	C	513	CLA	CAA-CBA-CGA-O2A
33	A	419[B]	LHG	O8-C23-C24-C25
33	E	101[B]	LHG	O7-C7-C8-C9
23	A	408	CLA	C11-C12-C13-C14
23	B	615	CLA	C14-C13-C15-C16
23	C	505	CLA	C11-C12-C13-C14
23	a	407[A]	CLA	C14-C13-C15-C16
23	a	407[B]	CLA	C14-C13-C15-C16
23	b	603	CLA	C11-C10-C8-C9
23	b	608	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	b	614	CLA	C11-C12-C13-C14
23	c	507	CLA	C11-C10-C8-C9
23	c	510	CLA	C11-C12-C13-C14
23	c	512	CLA	C3-C5-C6-C7
34	c	521	LMG	C32-C33-C34-C35
23	C	507	CLA	C3A-C2A-CAA-CBA
23	c	507	CLA	C3A-C2A-CAA-CBA
34	Z	101	LMG	O7-C10-C11-C12
23	B	604	CLA	CAD-CBD-CGD-O2D
23	B	610	CLA	CAD-CBD-CGD-O2D
23	B	612	CLA	CAD-CBD-CGD-O2D
23	C	506	CLA	CAD-CBD-CGD-O2D
23	b	603	CLA	CAD-CBD-CGD-O2D
23	b	604	CLA	CAD-CBD-CGD-O2D
23	b	610	CLA	CAD-CBD-CGD-O2D
23	c	502	CLA	CAD-CBD-CGD-O2D
23	c	506	CLA	CAD-CBD-CGD-O2D
24	A	407[B]	PHO	CAD-CBD-CGD-O2D
24	a	416[A]	PHO	CAD-CBD-CGD-O2D
33	D	707[A]	LHG	C28-C29-C30-C31
23	C	505	CLA	C3-C5-C6-C7
33	b	629[A]	LHG	C30-C31-C32-C33
36	c	518[B]	DGD	CDA-CEA-CFA-CGA
23	B	613	CLA	CAA-CBA-CGA-O2A
23	C	511	CLA	CAA-CBA-CGA-O2A
33	L	101[A]	LHG	O7-C7-C8-C9
33	a	420[A]	LHG	O8-C23-C24-C25
33	a	420[B]	LHG	O8-C23-C24-C25
33	d	412[B]	LHG	C29-C30-C31-C32
23	a	406[B]	CLA	C4C-C3C-CAC-CBC
36	C	519	DGD	C8A-C9A-CAA-CBA
29	A	414[A]	PL9	C25-C24-C26-C27
40	v	201	HEC	CAD-CBD-CGD-O2D
33	L	101[B]	LHG	O7-C7-C8-C9
34	c	520	LMG	C14-C15-C16-C17
36	C	518[B]	DGD	C7B-C8B-C9B-CAB
36	c	517[B]	DGD	CBA-CCA-CDA-CEA
25	t	102	BCR	C7-C8-C9-C10
25	y	101	BCR	C21-C22-C23-C24
24	A	407[A]	PHO	C2C-C3C-CAC-CBC
24	A	417[A]	PHO	C2C-C3C-CAC-CBC
24	A	417[B]	PHO	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
24	a	408[A]	PHO	C2C-C3C-CAC-CBC
24	a	408[B]	PHO	C2C-C3C-CAC-CBC
24	a	416[A]	PHO	C2C-C3C-CAC-CBC
38	f	101	HEM	CAA-CBA-CGA-O1A
26	B	620	SQD	C24-C25-C26-C27
26	b	620	SQD	C16-C17-C18-C19
23	b	604	CLA	C13-C15-C16-C17
33	b	629[A]	LHG	O7-C7-C8-C9
35	b	625	HTG	C3'-C4'-C5'-C6'
23	A	404[A]	CLA	C15-C16-C17-C18
23	B	602	CLA	O2A-C1-C2-C3
23	C	510	CLA	O2A-C1-C2-C3
23	b	613	CLA	O2A-C1-C2-C3
24	A	407[A]	PHO	O2A-C1-C2-C3
24	A	407[B]	PHO	O2A-C1-C2-C3
23	A	404[A]	CLA	C4C-C3C-CAC-CBC
34	C	501	LMG	C31-C32-C33-C34
38	f	101	HEM	C4B-C3B-CAB-CBB
23	c	513	CLA	CAA-CBA-CGA-O2A
34	B	621	LMG	C15-C16-C17-C18
23	C	502	CLA	C16-C17-C18-C20
33	d	405[B]	LHG	C12-C13-C14-C15
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	B	606	CLA	CHA-CBD-CGD-O1D
23	B	606	CLA	CHA-CBD-CGD-O2D
23	B	607	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CHA-CBD-CGD-O2D
23	C	508	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O2D
23	C	510	CLA	CHA-CBD-CGD-O1D
23	C	510	CLA	CHA-CBD-CGD-O2D
23	a	406[A]	CLA	CHA-CBD-CGD-O1D
23	a	406[A]	CLA	CHA-CBD-CGD-O2D
23	a	406[B]	CLA	CHA-CBD-CGD-O1D
23	a	406[B]	CLA	CHA-CBD-CGD-O2D
23	b	601	CLA	CHA-CBD-CGD-O2D
23	c	503	CLA	CHA-CBD-CGD-O2D
23	c	508	CLA	CHA-CBD-CGD-O1D
23	c	508	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	c	510	CLA	CHA-CBD-CGD-O2D
40	v	201	HEC	CAD-CBD-CGD-O1D
26	A	412	SQD	C19-C20-C21-C22
23	b	616	CLA	C2-C3-C5-C6
34	D	711	LMG	O7-C10-C11-C12
33	A	419[A]	LHG	C17-C18-C19-C20
33	d	412[A]	LHG	C13-C14-C15-C16
36	C	518[A]	DGD	CAB-CBB-CCB-CDB
23	c	508	CLA	C2A-CAA-CBA-CGA
24	A	407[A]	PHO	CHA-CBD-CGD-O1D
27	B	623	GOL	O1-C1-C2-O2
27	O	303	GOL	O1-C1-C2-O2
27	d	411	GOL	O1-C1-C2-O2
26	X	101	SQD	C24-C23-O48-C46
36	C	519	DGD	O1G-C1A-C2A-C3A
23	a	406[A]	CLA	C11-C12-C13-C15
29	A	414[A]	PL9	C4-C3-C7-C8
23	c	511	CLA	CAA-CBA-CGA-O2A
33	D	707[B]	LHG	O8-C23-C24-C25
34	c	520	LMG	O7-C10-C11-C12
23	A	408	CLA	C14-C13-C15-C16
23	b	607	CLA	C14-C13-C15-C16
23	a	405[B]	CLA	C4C-C3C-CAC-CBC
26	X	101	SQD	C33-C34-C35-C36
23	b	615	CLA	C5-C6-C7-C8
33	d	412[A]	LHG	C18-C19-C20-C21
33	b	629[B]	LHG	O9-C7-C8-C9
33	b	629[A]	LHG	C24-C25-C26-C27
32	T	101	LMT	O1'-C1-C2-C3
32	b	627	LMT	O1'-C1-C2-C3
34	c	501	LMG	C18-C19-C20-C21
25	Y	101	BCR	C37-C22-C23-C24
34	c	521	LMG	C28-C29-C30-C31
34	Z	101	LMG	O9-C10-C11-C12
33	d	405[B]	LHG	C13-C14-C15-C16
29	A	414[B]	PL9	C25-C24-C26-C27
26	A	410[B]	SQD	C13-C14-C15-C16
27	a	419	GOL	C1-C2-C3-O3
27	l	102[A]	GOL	C1-C2-C3-O3
29	D	705[A]	PL9	C28-C29-C31-C32
23	B	612	CLA	O1A-CGA-O2A-C1
23	c	511	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
33	d	412[B]	LHG	C1-C2-C3-O3
33	D	706[B]	LHG	C23-C24-C25-C26
36	C	519	DGD	C3B-C4B-C5B-C6B
23	C	513	CLA	CAA-CBA-CGA-O1A
33	A	419[A]	LHG	O10-C23-C24-C25
29	d	404[B]	PL9	C11-C12-C13-C14
23	B	608	CLA	C2-C1-O2A-CGA
32	a	417	LMT	C7-C8-C9-C10
33	A	419[B]	LHG	O10-C23-C24-C25
33	a	420[A]	LHG	O10-C23-C24-C25
33	b	629[A]	LHG	O9-C7-C8-C9
33	A	419[B]	LHG	C17-C18-C19-C20
26	X	101	SQD	C44-C45-C46-O48
34	C	501	LMG	C7-C8-C9-O8
36	c	517[A]	DGD	O2G-C1B-C2B-C3B
34	c	501	LMG	C13-C14-C15-C16
23	B	603	CLA	C2A-CAA-CBA-CGA
23	A	408	CLA	C16-C17-C18-C19
33	a	420[B]	LHG	O10-C23-C24-C25
38	F	102	HEM	CAA-CBA-CGA-O2A
33	E	101[A]	LHG	O7-C7-C8-C9
23	b	610	CLA	C13-C15-C16-C17
34	B	621	LMG	C4-C5-C6-O5
23	c	513	CLA	CAA-CBA-CGA-O1A
33	L	101[B]	LHG	O9-C7-C8-C9
34	c	521	LMG	C39-C40-C41-C42
32	a	417	LMT	C2'-C1'-O1'-C1
23	C	509	CLA	C5-C6-C7-C8
23	b	611	CLA	C13-C15-C16-C17
23	c	508	CLA	C8-C10-C11-C12
33	A	419[B]	LHG	C3-O3-P-O5
33	D	707[B]	LHG	C4-O6-P-O5
33	d	405[A]	LHG	C4-O6-P-O5
33	d	412[B]	LHG	C3-O3-P-O5
23	B	613	CLA	CAA-CBA-CGA-O1A
23	C	511	CLA	CAA-CBA-CGA-O1A
36	C	519	DGD	O1A-C1A-C2A-C3A
33	L	101[B]	LHG	O6-C4-C5-C6
25	d	403	BCR	C23-C24-C25-C26
25	h	101	BCR	C23-C24-C25-C26
25	t	102	BCR	C1-C6-C7-C8
25	t	102	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	y	101	BCR	C23-C24-C25-C26
23	b	615	CLA	C13-C15-C16-C17
33	L	101[B]	LHG	C7-C8-C9-C10
33	L	101[A]	LHG	O9-C7-C8-C9
26	X	101	SQD	O10-C23-O48-C46
34	c	520	LMG	O10-C28-O8-C9
33	d	412[B]	LHG	O8-C23-C24-C25
34	c	521	LMG	O7-C10-C11-C12
34	Z	101	LMG	C19-C20-C21-C22
34	C	520	LMG	C10-C11-C12-C13
36	c	517[A]	DGD	C1A-C2A-C3A-C4A
23	C	508	CLA	C2A-CAA-CBA-CGA
32	A	418	LMT	C9-C10-C11-C12
34	C	521	LMG	C4-C5-C6-O5
32	e	101	LMT	C2B-C1B-O1B-C4'
29	d	404[A]	PL9	C11-C12-C13-C14
23	b	610	CLA	C16-C17-C18-C19
38	F	102	HEM	CAA-CBA-CGA-O1A
23	B	603	CLA	CAD-CBD-CGD-O1D
23	B	605	CLA	CAD-CBD-CGD-O1D
23	b	605	CLA	CAD-CBD-CGD-O1D
23	b	609	CLA	CAD-CBD-CGD-O1D
23	c	505	CLA	CAD-CBD-CGD-O1D
23	c	507	CLA	CAD-CBD-CGD-O1D
26	a	411[B]	SQD	C7-C8-C9-C10
33	E	101[B]	LHG	O9-C7-C8-C9
34	D	711	LMG	O9-C10-C11-C12
26	a	411[A]	SQD	C10-C11-C12-C13
23	a	406[A]	CLA	C11-C12-C13-C14
23	c	514	CLA	C14-C13-C15-C16
27	B	626	GOL	O1-C1-C2-O2
23	c	504	CLA	C5-C6-C7-C8
34	c	520	LMG	O9-C10-C11-C12
26	A	412	SQD	O48-C23-C24-C25
33	D	707[A]	LHG	O8-C23-C24-C25
26	A	410[B]	SQD	C18-C19-C20-C21
23	C	504	CLA	C5-C6-C7-C8
23	a	409	CLA	C8-C10-C11-C12
32	t	101	LMT	C2-C3-C4-C5
34	B	621	LMG	C36-C37-C38-C39
34	c	520	LMG	C40-C41-C42-C43
23	c	502	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
26	a	412	SQD	O48-C23-C24-C25
33	E	101[B]	LHG	O8-C23-C24-C25
33	d	406[B]	LHG	O8-C23-C24-C25
23	B	611	CLA	C8-C10-C11-C12
33	D	706[B]	LHG	C32-C33-C34-C35
36	C	519	DGD	C2A-C3A-C4A-C5A
26	a	411[A]	SQD	C19-C20-C21-C22
34	C	521	LMG	C11-C12-C13-C14
23	c	503	CLA	C16-C17-C18-C19
34	Z	101	LMG	O10-C28-O8-C9
29	D	705[A]	PL9	C40-C39-C41-C42
34	C	520	LMG	C29-C30-C31-C32
36	c	517[A]	DGD	CBA-CCA-CDA-CEA
23	C	505	CLA	C6-C7-C8-C10
23	C	509	CLA	C12-C13-C15-C16
23	b	604	CLA	C11-C12-C13-C15
23	b	607	CLA	C12-C13-C15-C16
23	c	511	CLA	C12-C13-C15-C16
24	A	407[B]	PHO	C6-C7-C8-C10
33	D	707[B]	LHG	O10-C23-C24-C25
23	b	612	CLA	CAA-CBA-CGA-O2A
33	E	101[A]	LHG	O8-C23-C24-C25
36	C	518[A]	DGD	O2G-C1B-C2B-C3B
33	D	706[A]	LHG	C28-C29-C30-C31
23	c	502	CLA	CAA-CBA-CGA-O1A
23	c	511	CLA	CAA-CBA-CGA-O1A
26	a	412	SQD	O10-C23-C24-C25
33	D	707[A]	LHG	O10-C23-C24-C25
36	c	517[A]	DGD	O1B-C1B-C2B-C3B
34	C	521	LMG	C33-C34-C35-C36
36	C	518[A]	DGD	C3A-C4A-C5A-C6A
23	b	610	CLA	C16-C17-C18-C20
23	b	613	CLA	CAA-CBA-CGA-O2A
36	c	517[B]	DGD	O2G-C1B-C2B-C3B
23	C	508	CLA	C13-C15-C16-C17
33	E	101[B]	LHG	O10-C23-C24-C25
29	d	404[B]	PL9	C34-C36-C37-C38
23	B	612	CLA	C8-C10-C11-C12
36	C	518[B]	DGD	O2G-C1B-C2B-C3B
33	E	101[A]	LHG	O9-C7-C8-C9
33	E	101[A]	LHG	O10-C23-C24-C25
33	D	707[B]	LHG	C28-C29-C30-C31

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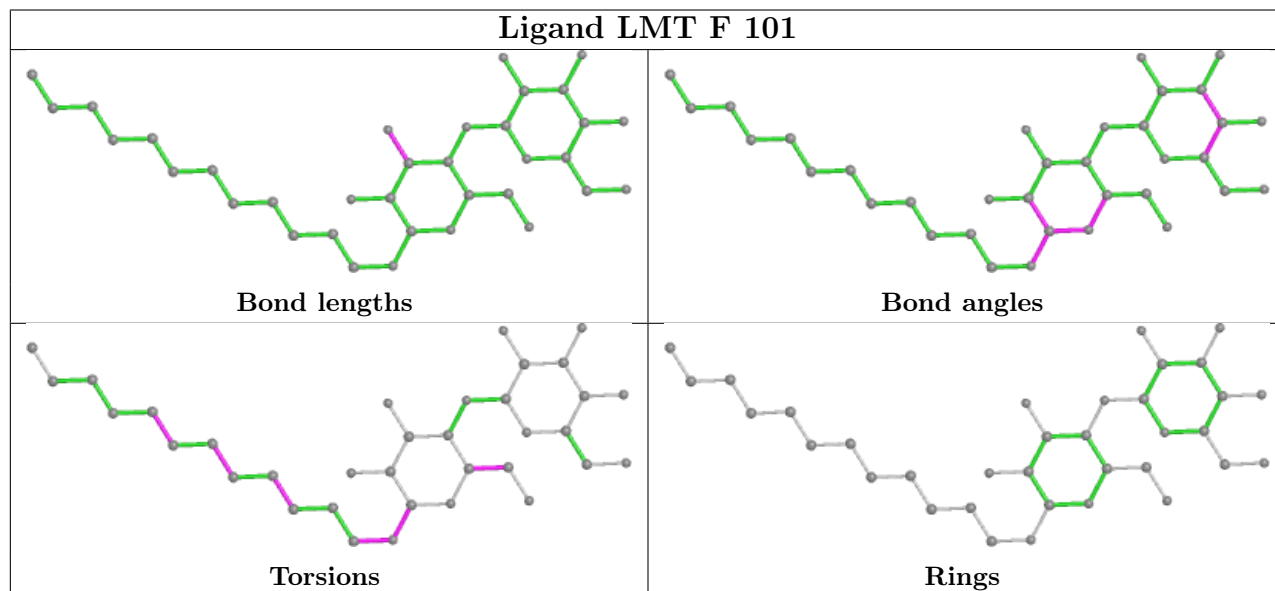
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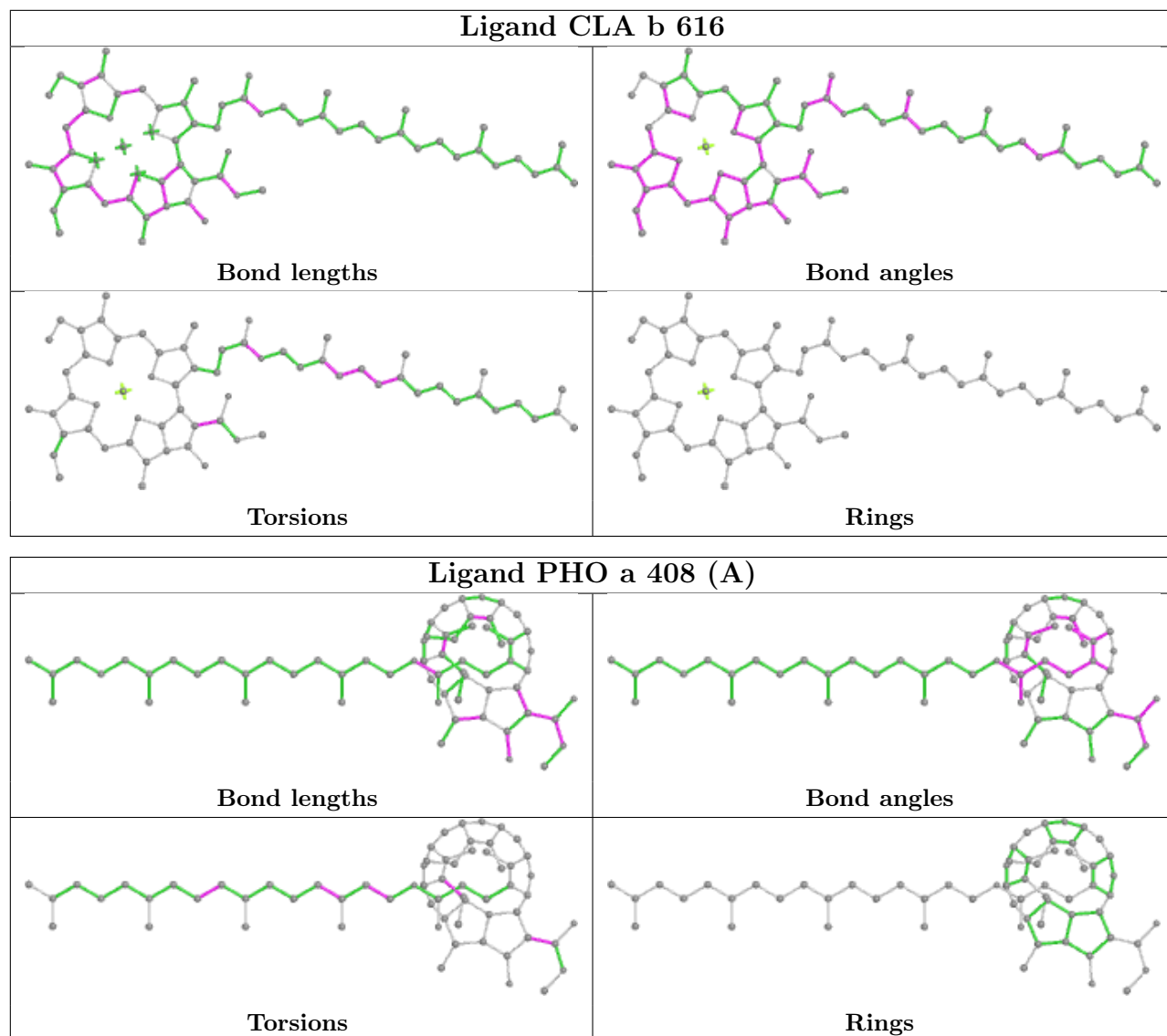
Mol	Chain	Res	Type	Atoms
34	c	521	LMG	O9-C10-C11-C12
36	C	518[A]	DGD	O1B-C1B-C2B-C3B
34	C	520	LMG	C11-C12-C13-C14
23	b	602	CLA	CAA-CBA-CGA-O2A

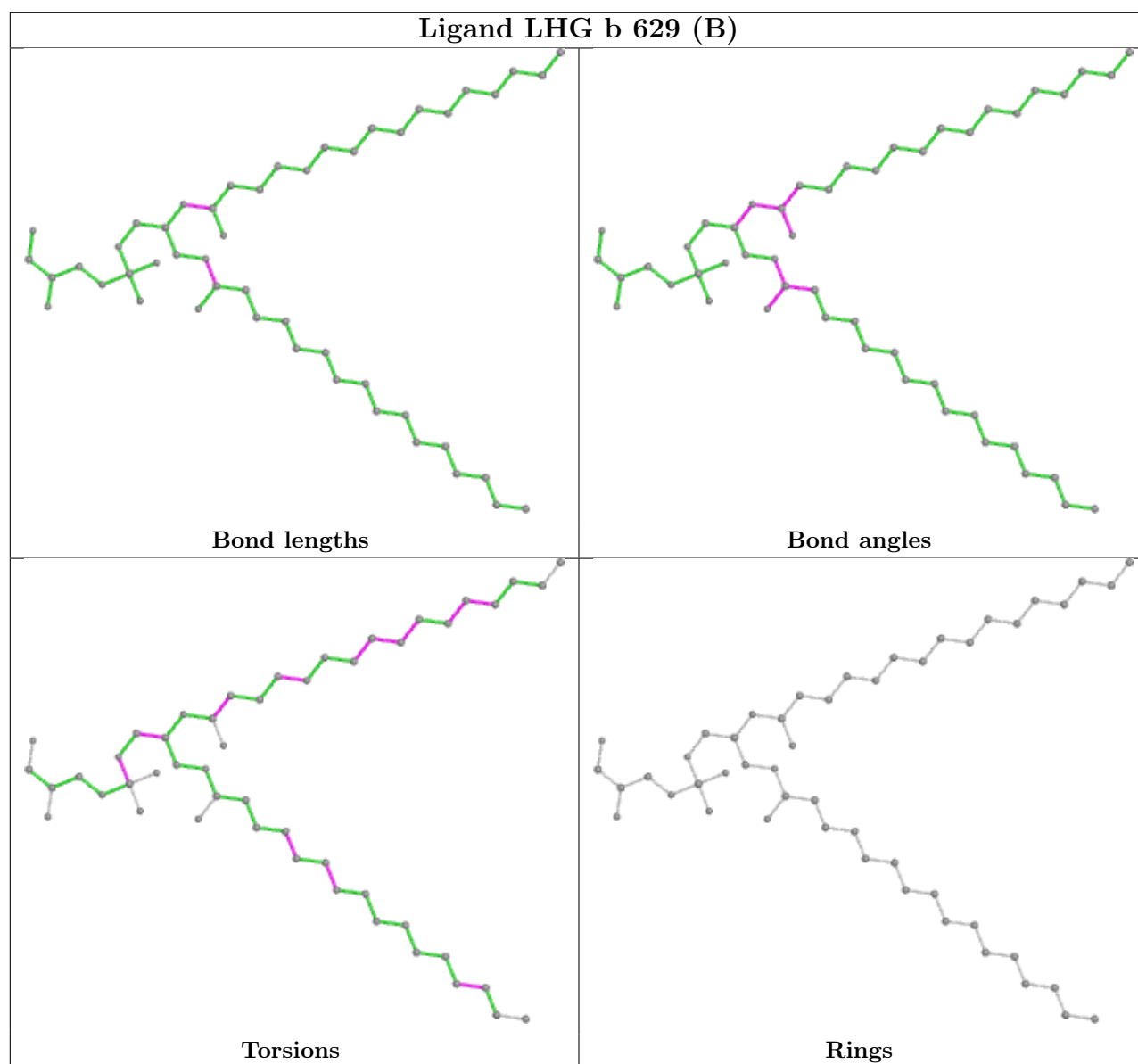
There are no ring outliers.

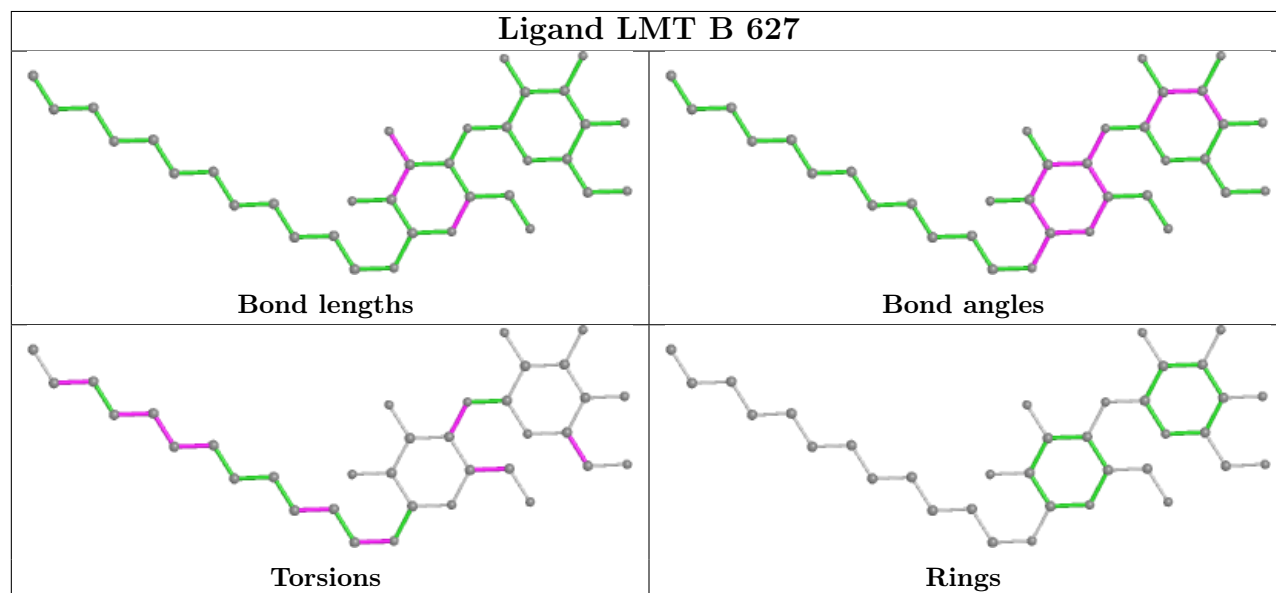
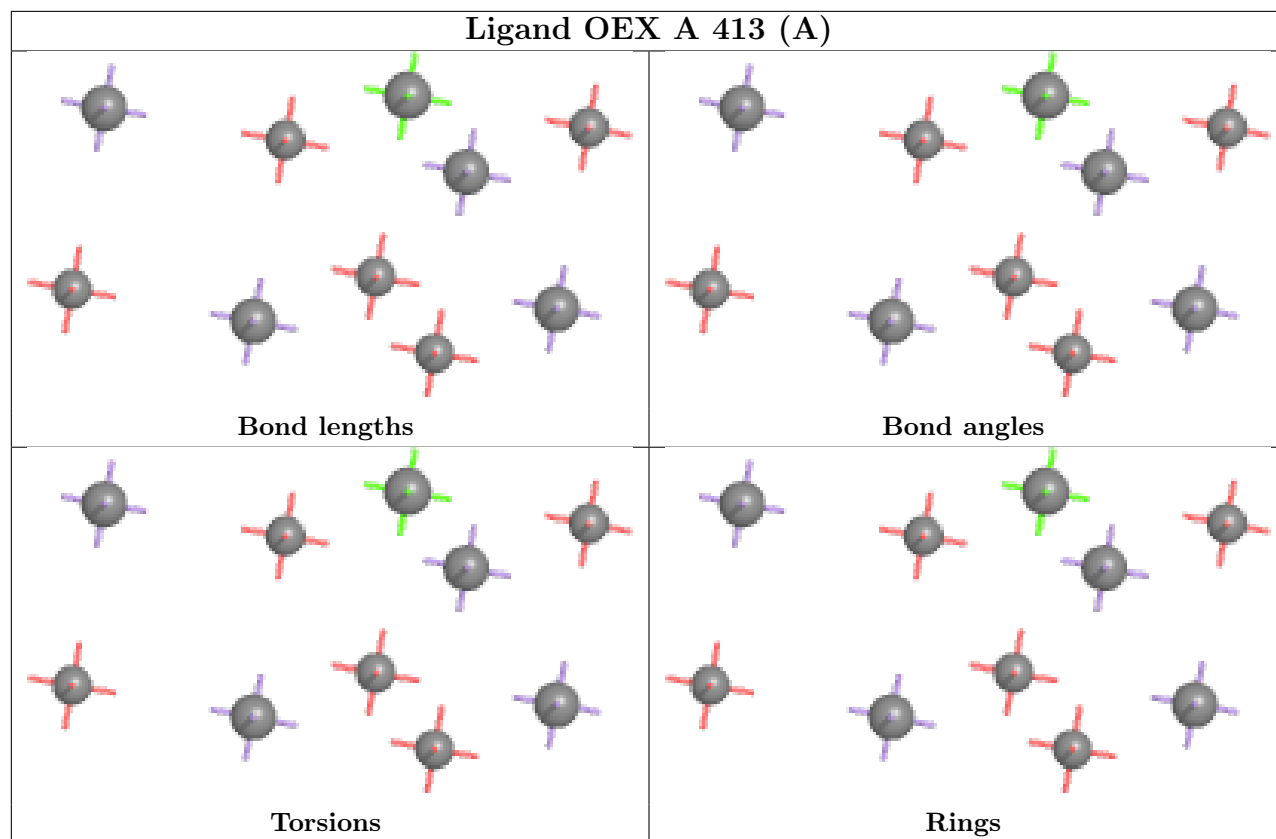
No monomer is involved in short contacts.

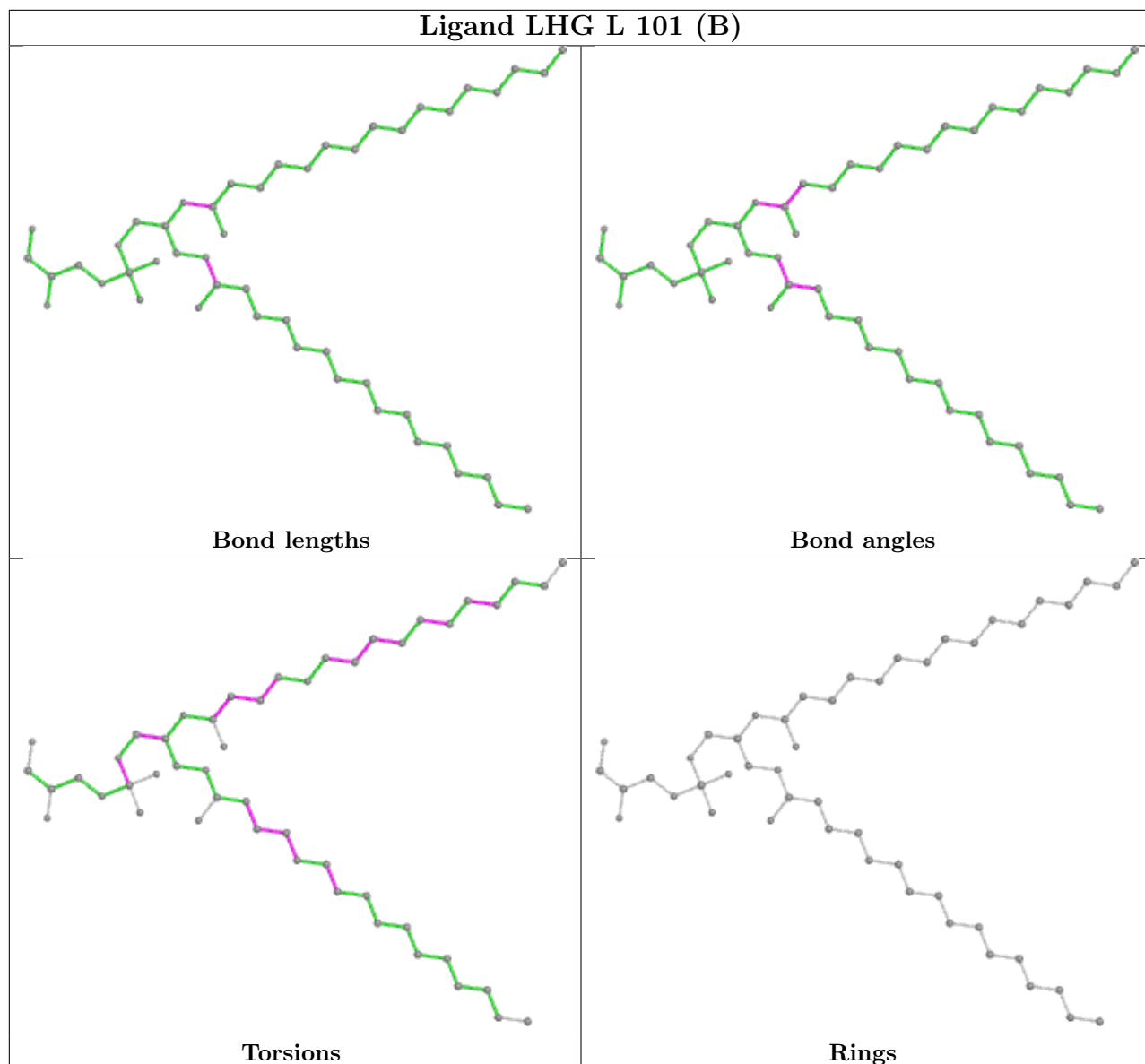
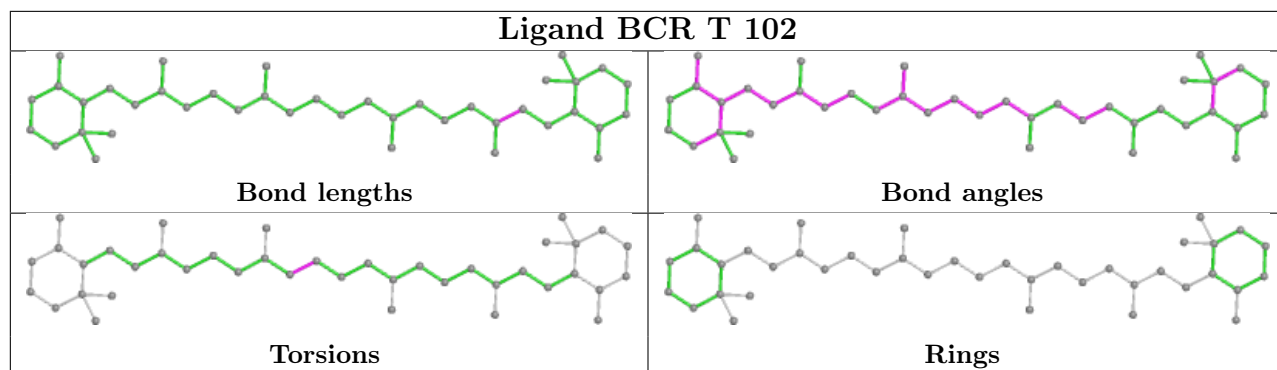
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

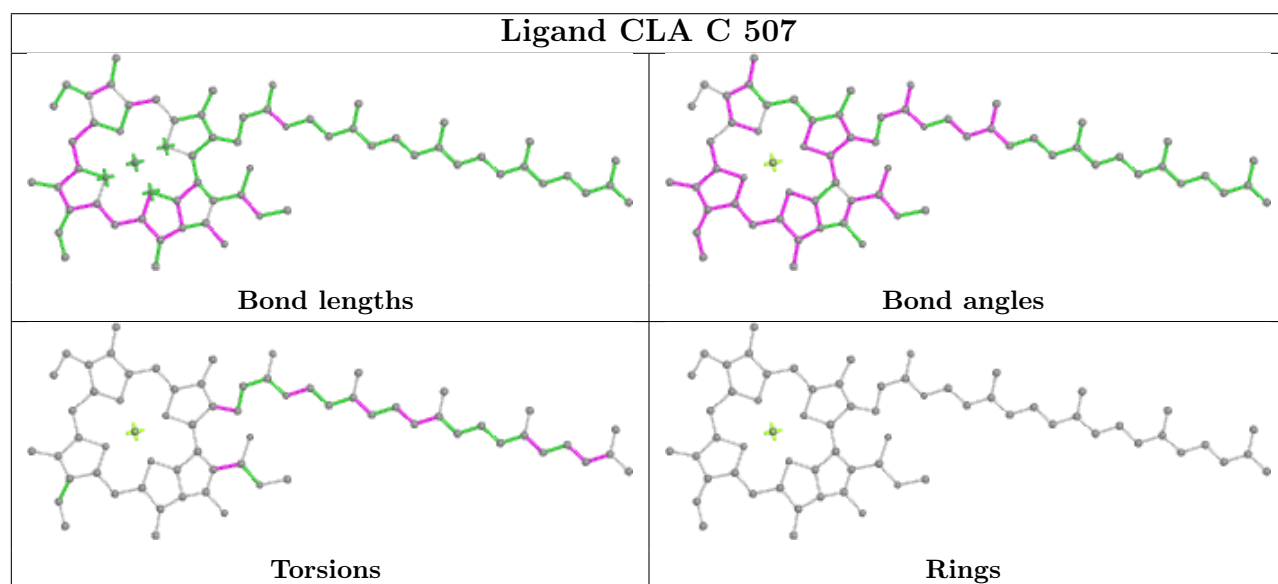
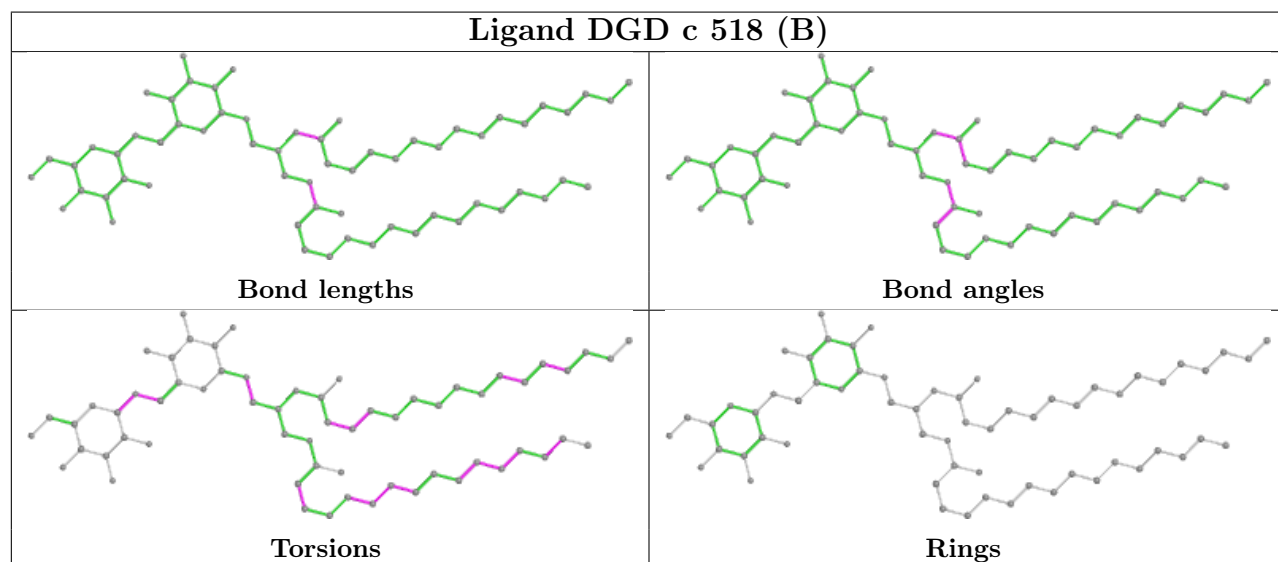
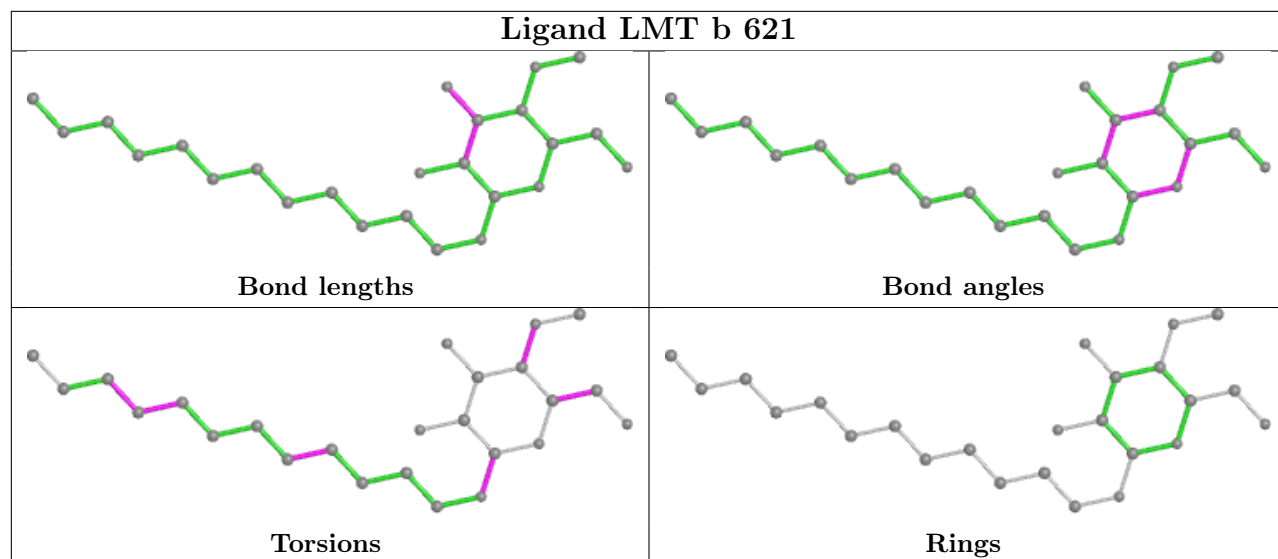


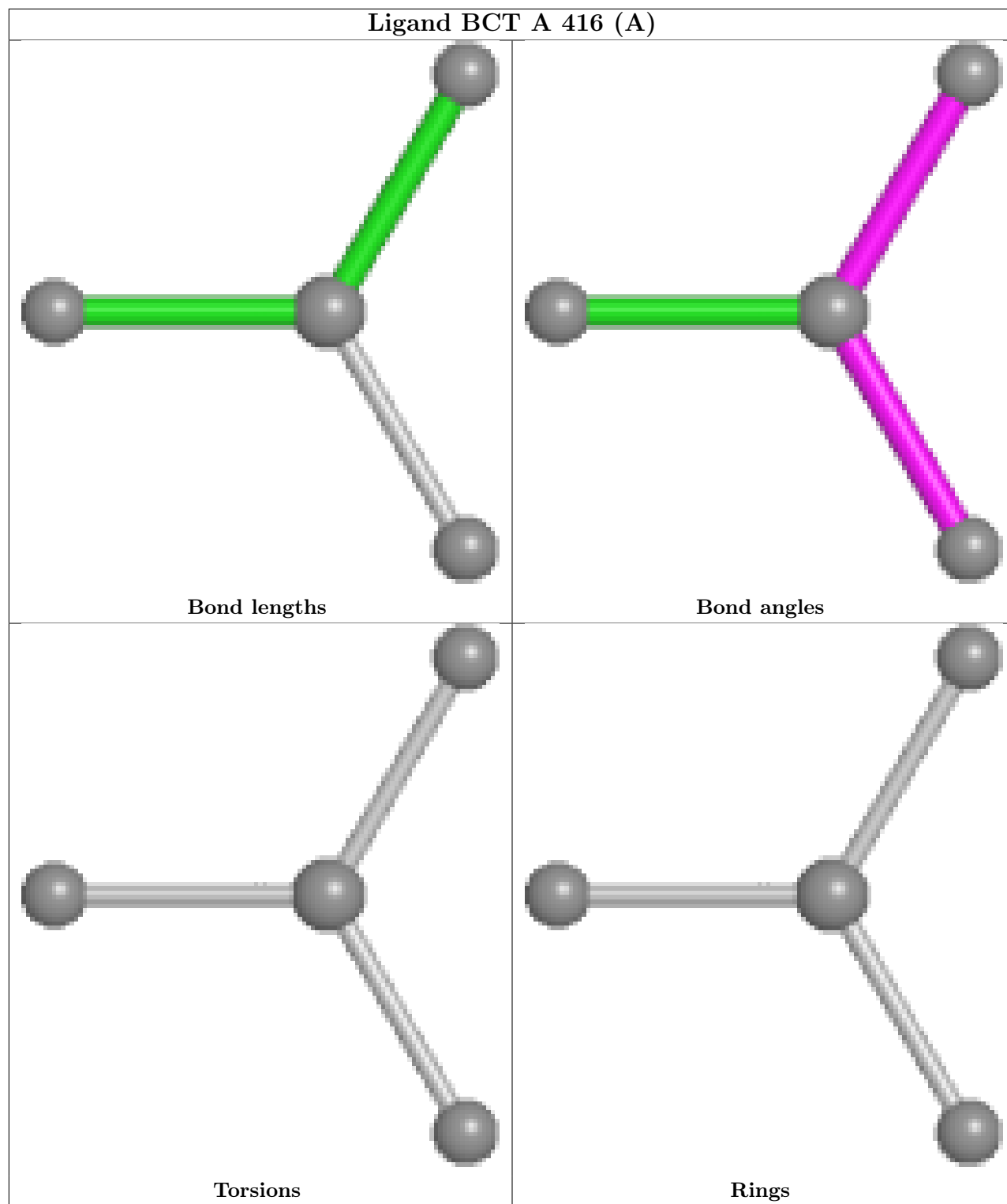


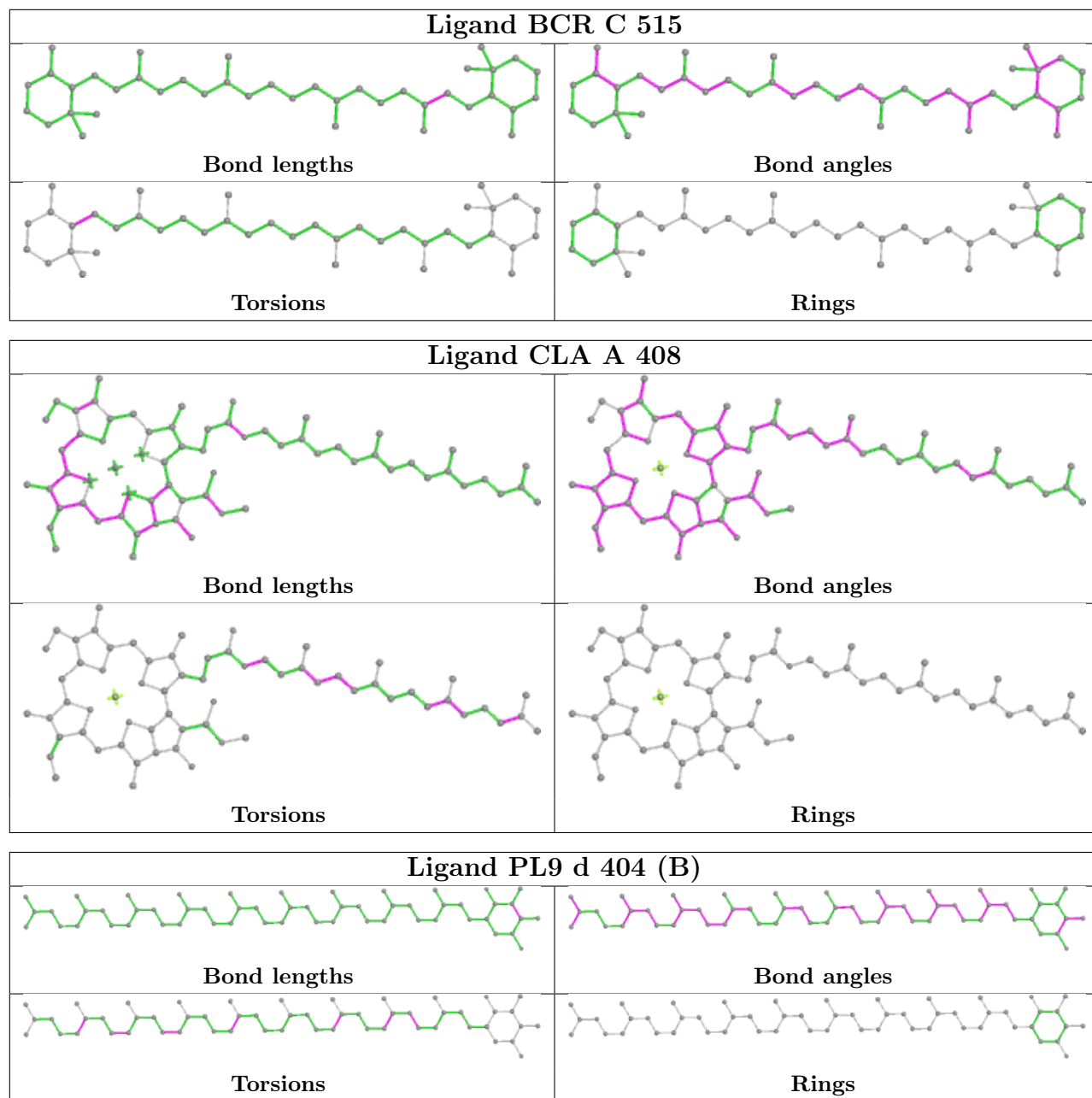


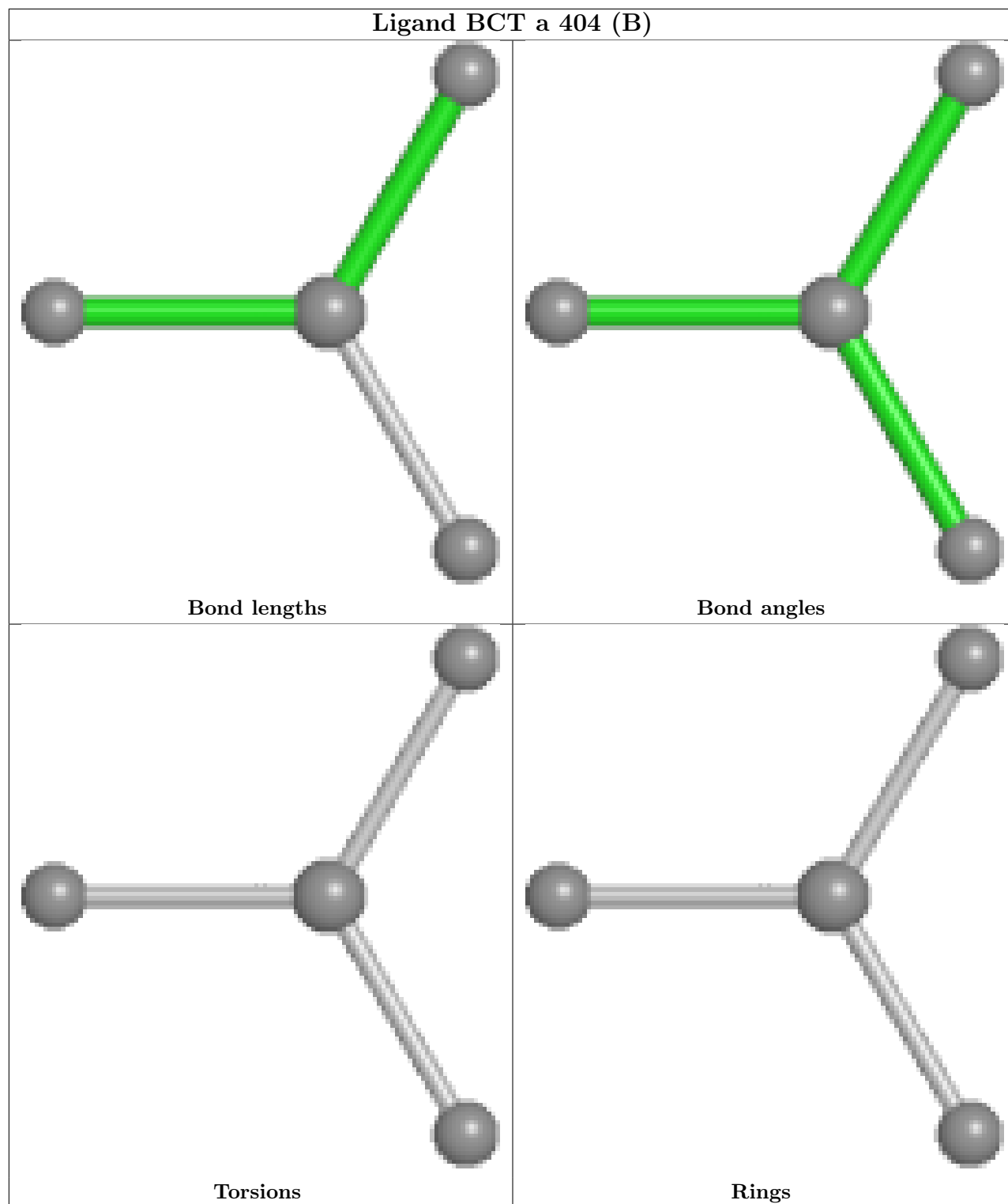


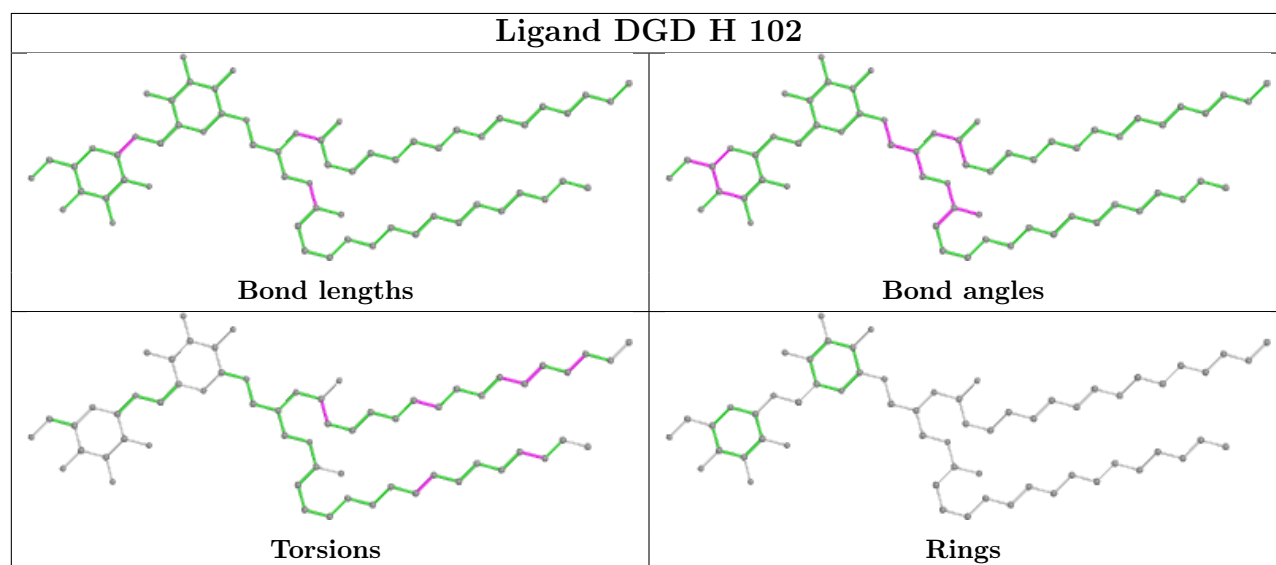
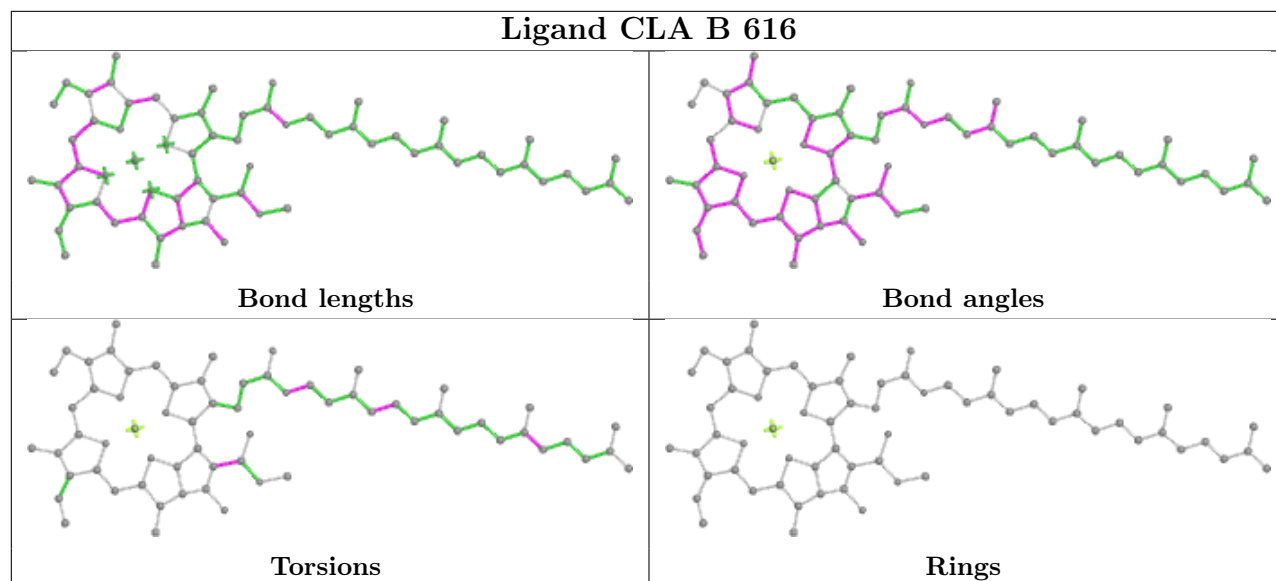
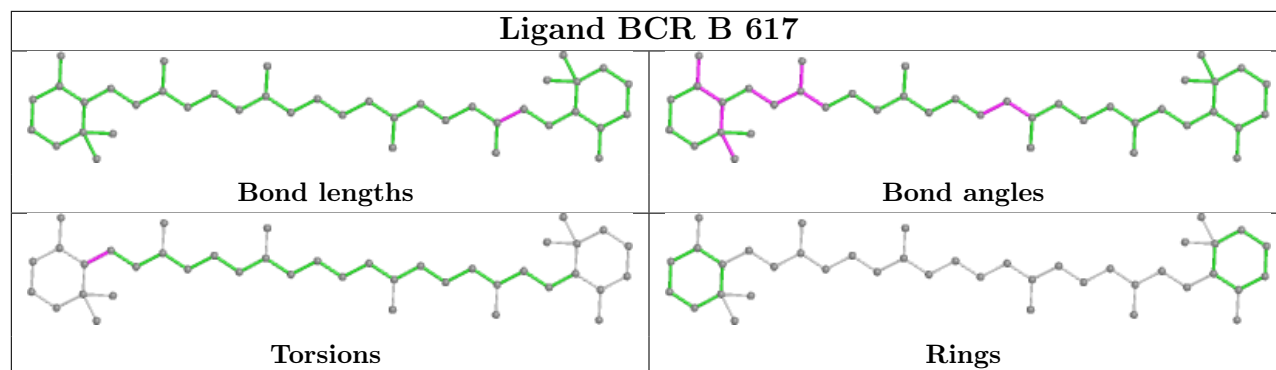


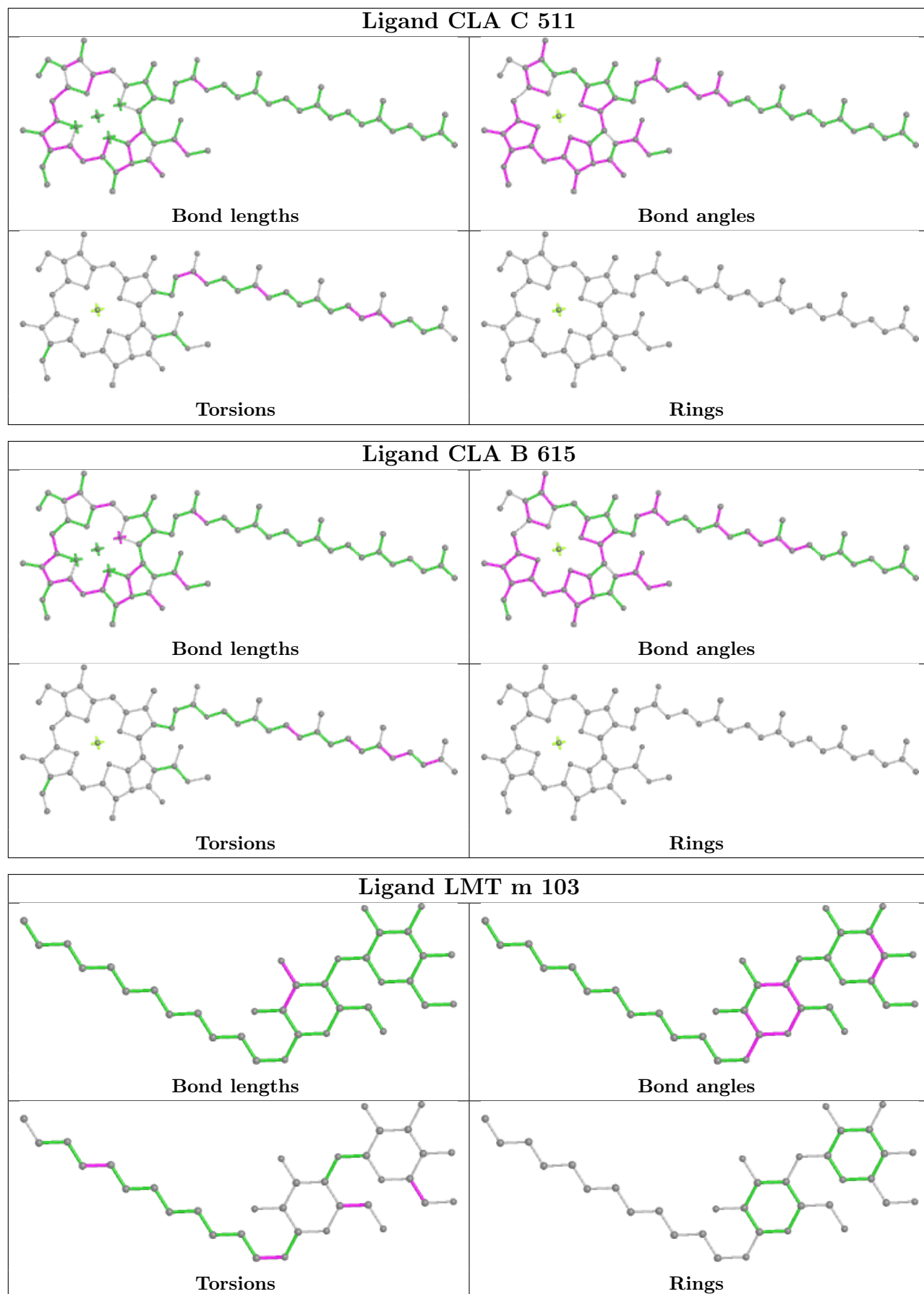


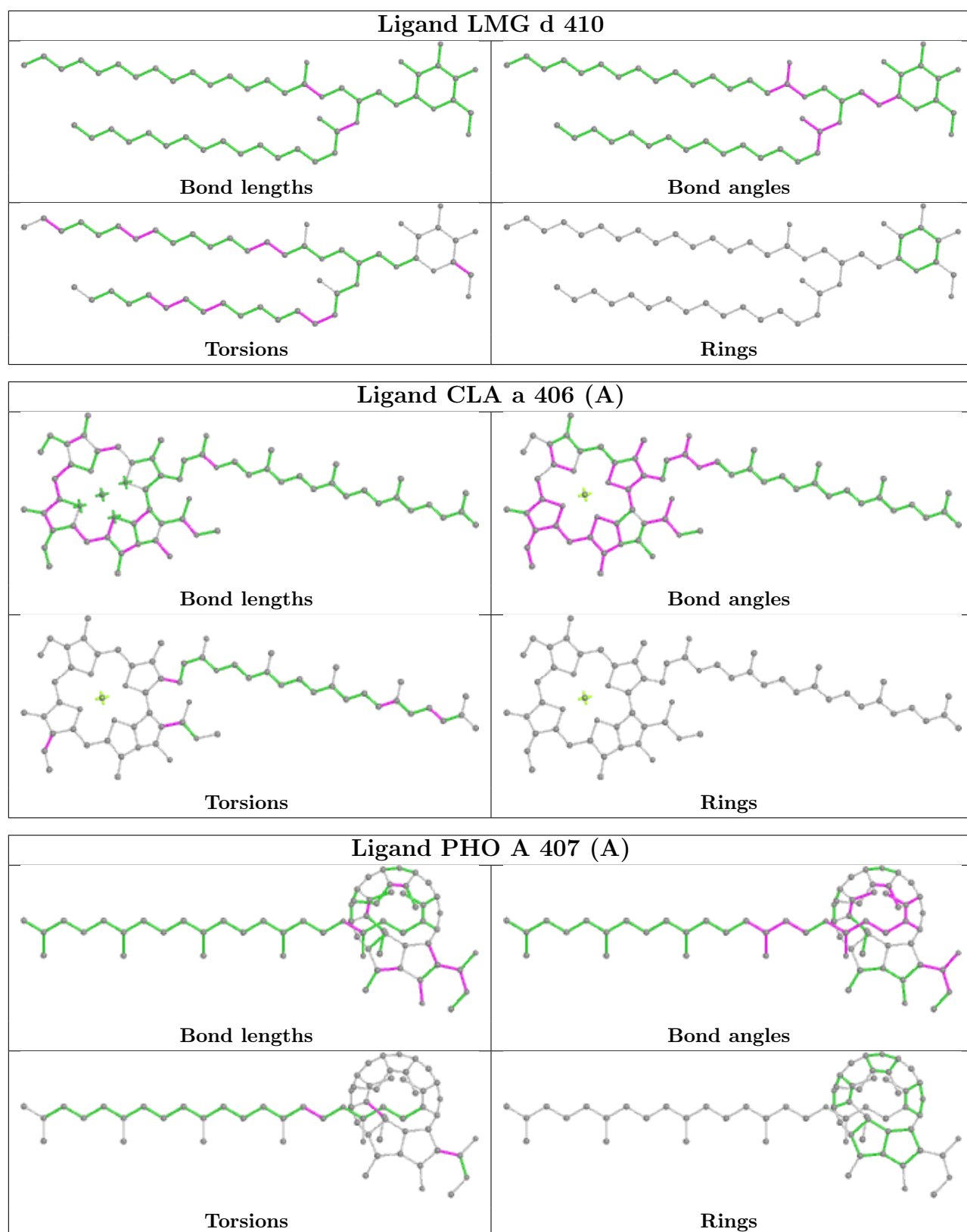


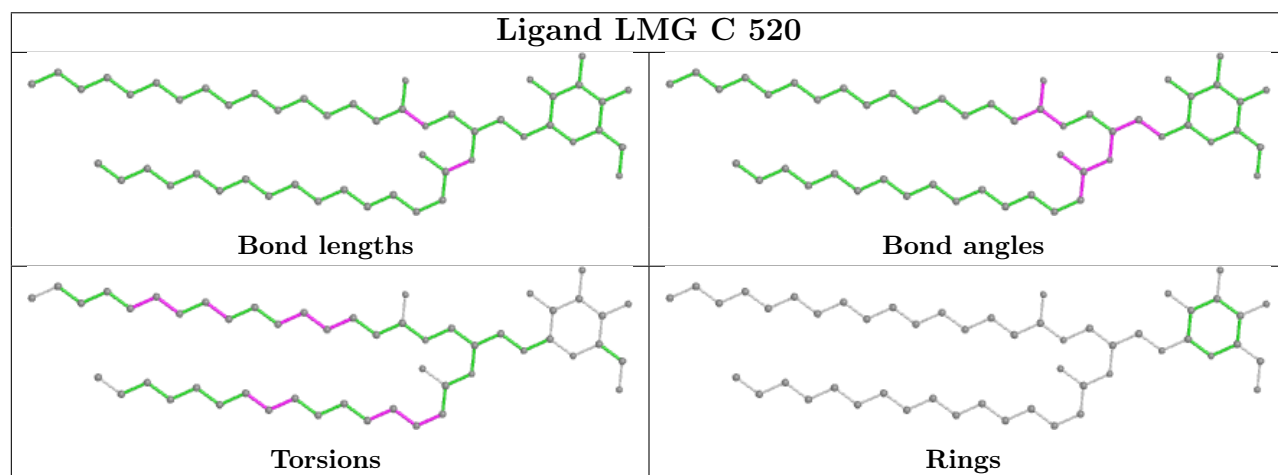
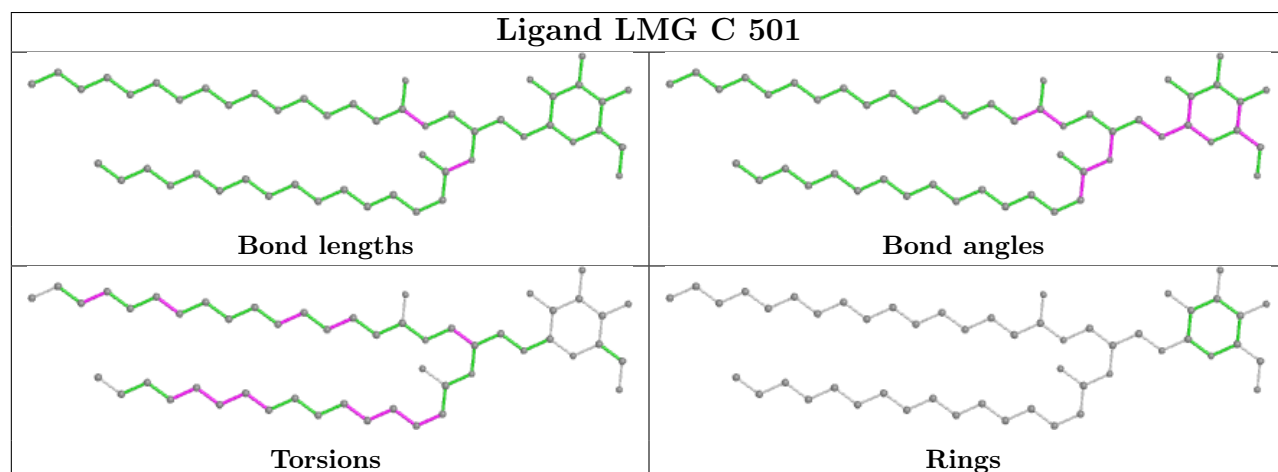
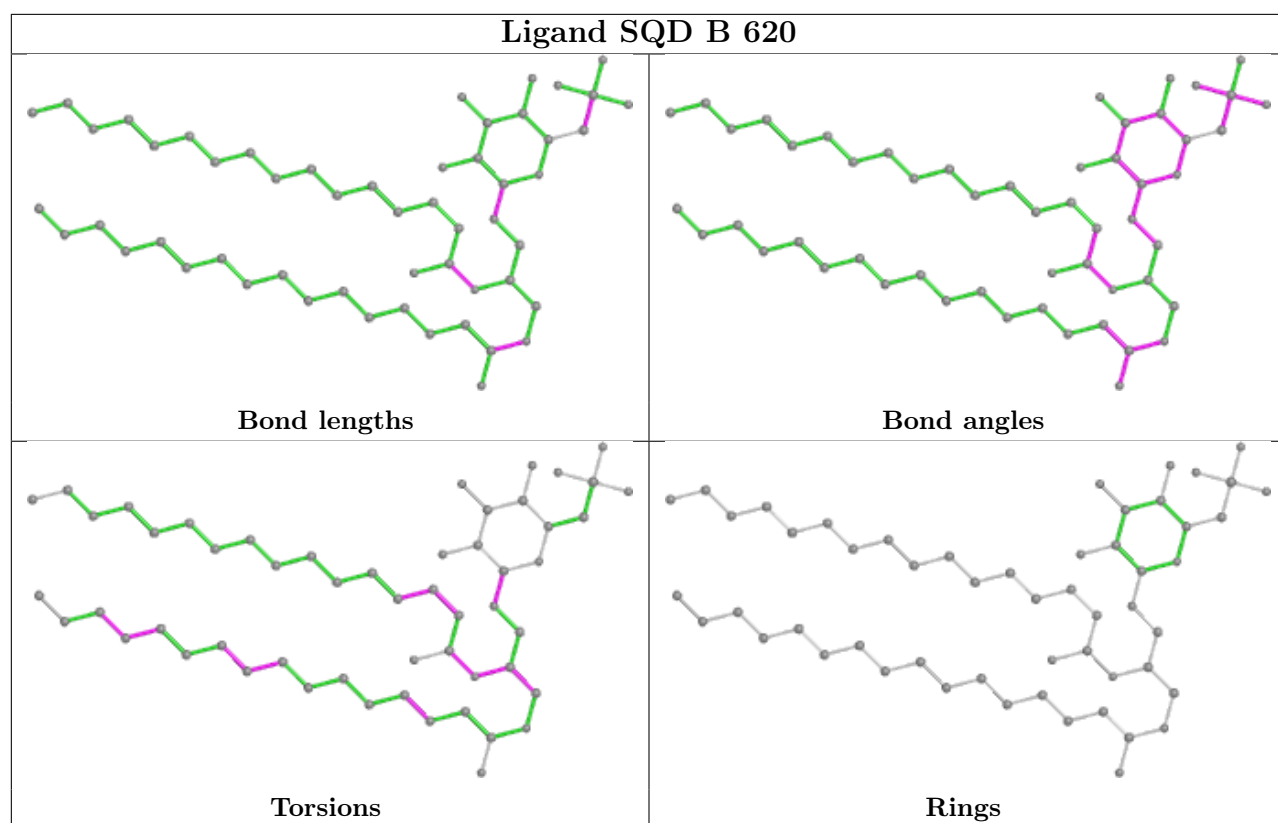


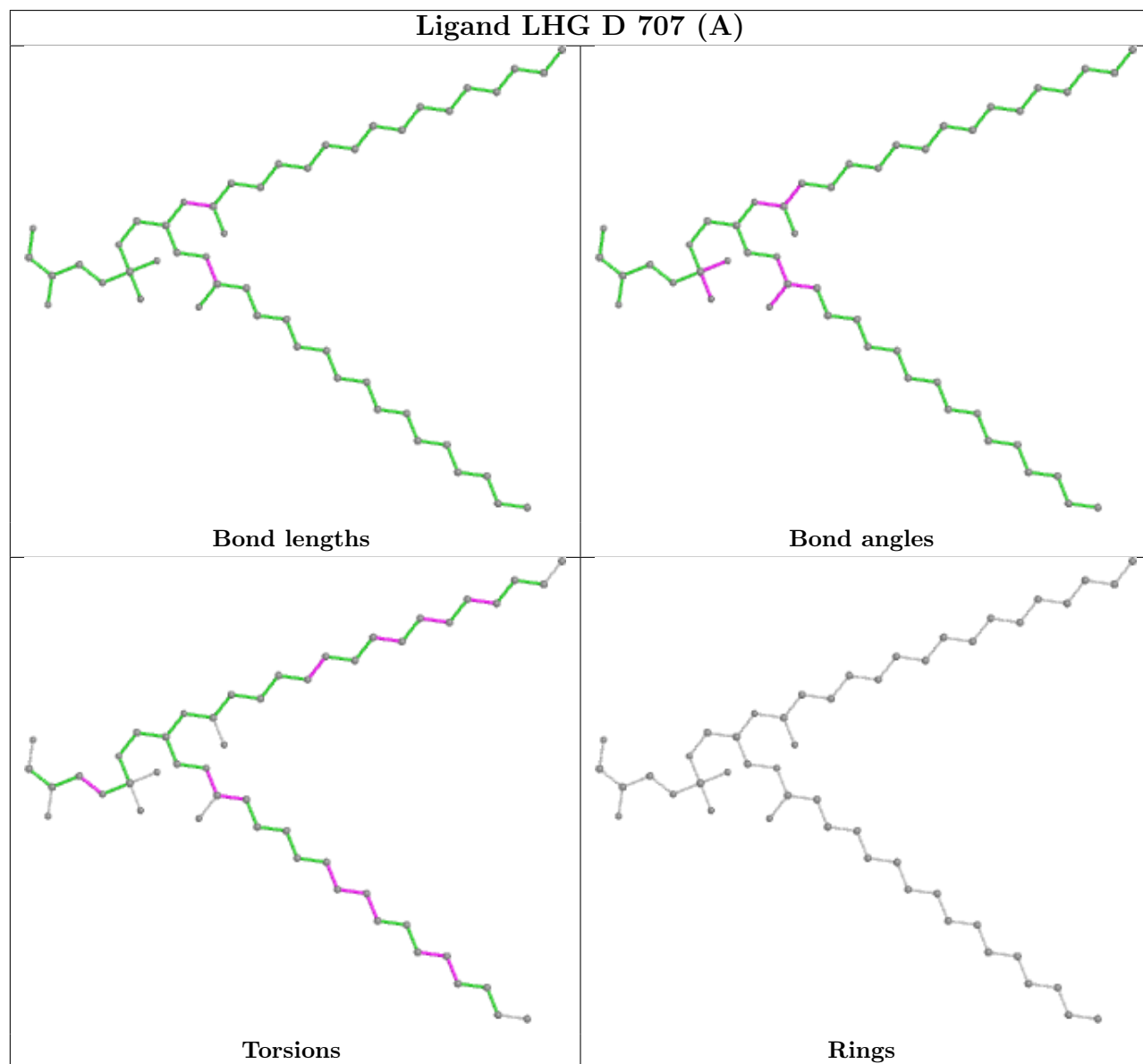
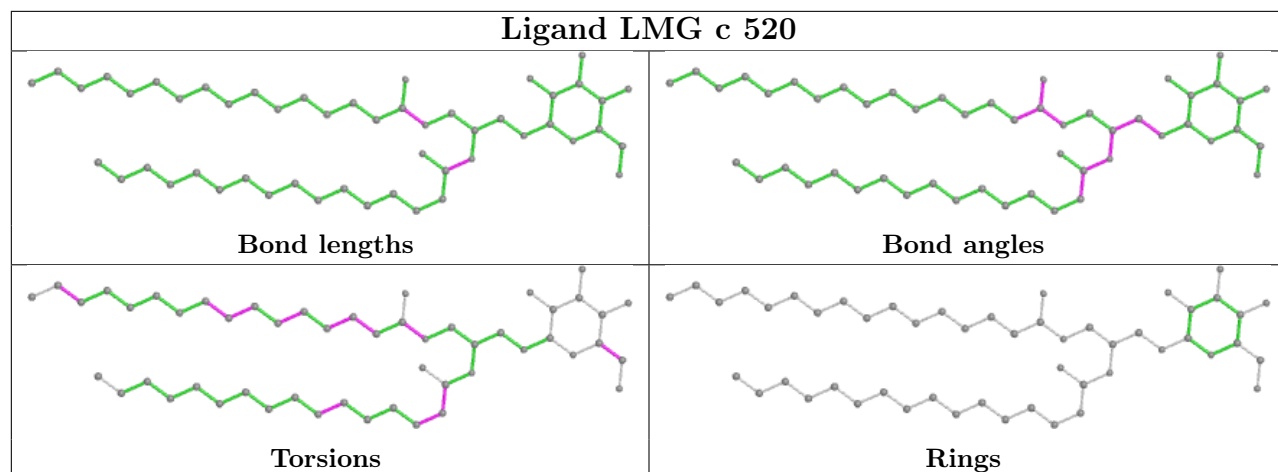


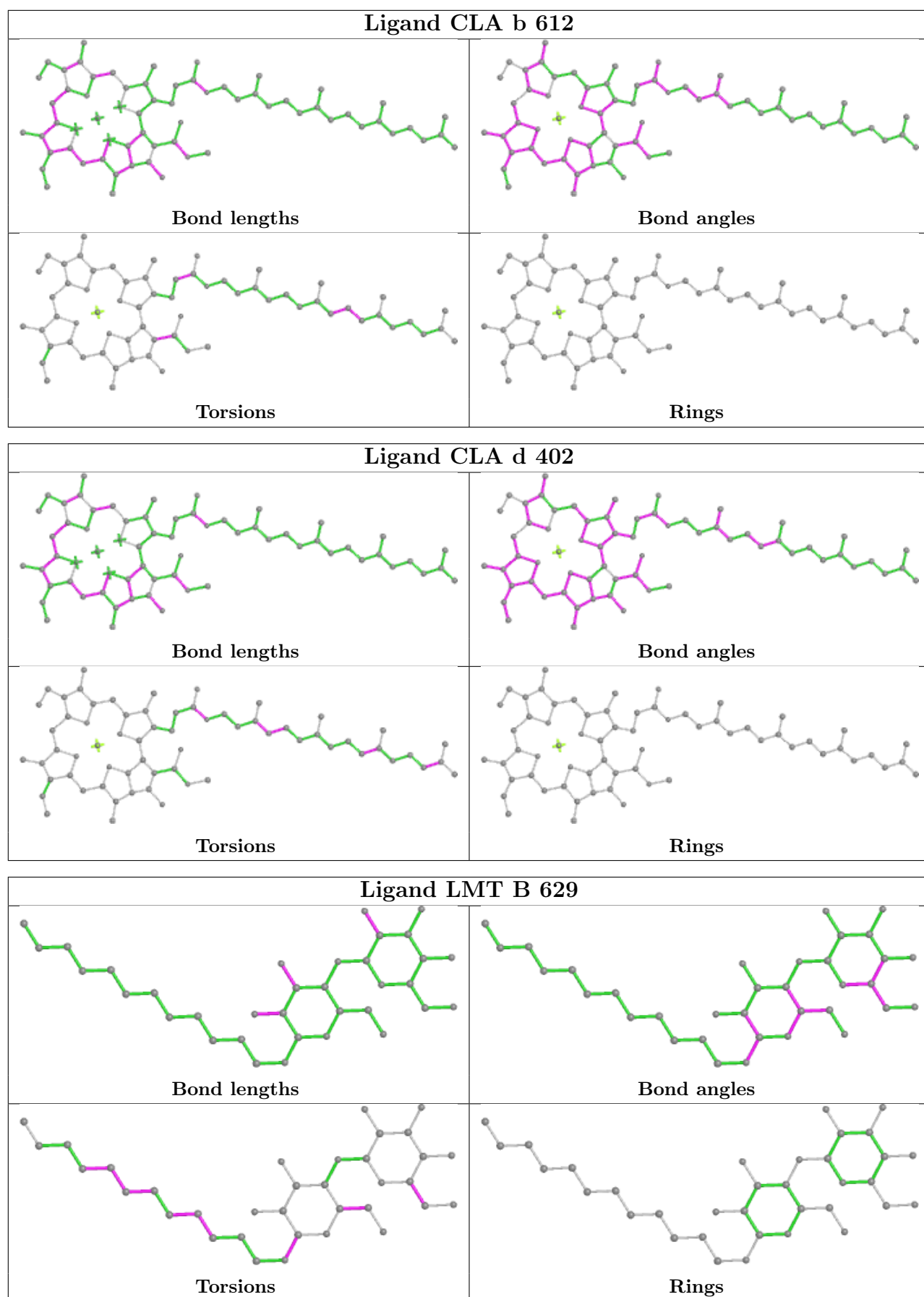


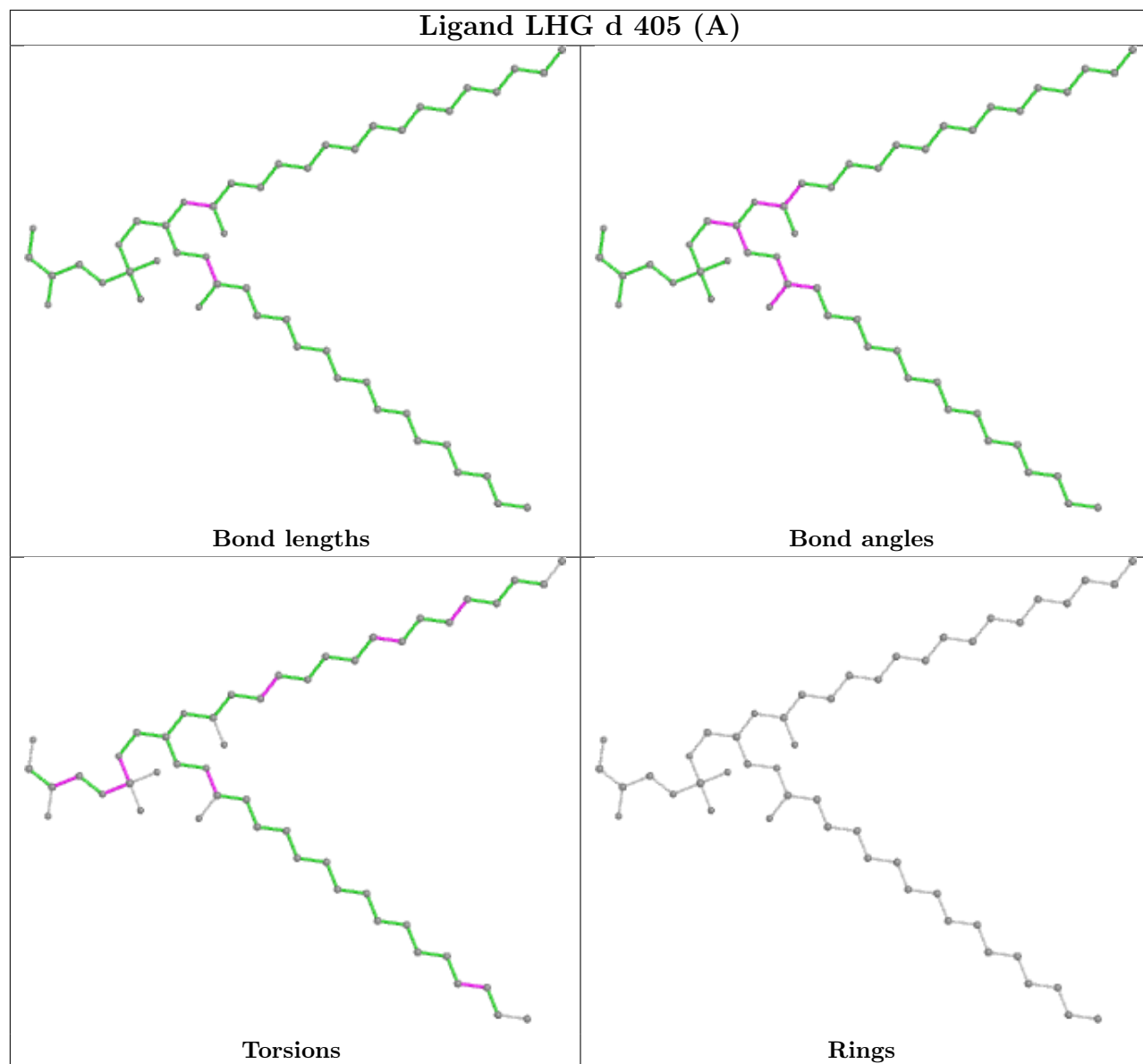


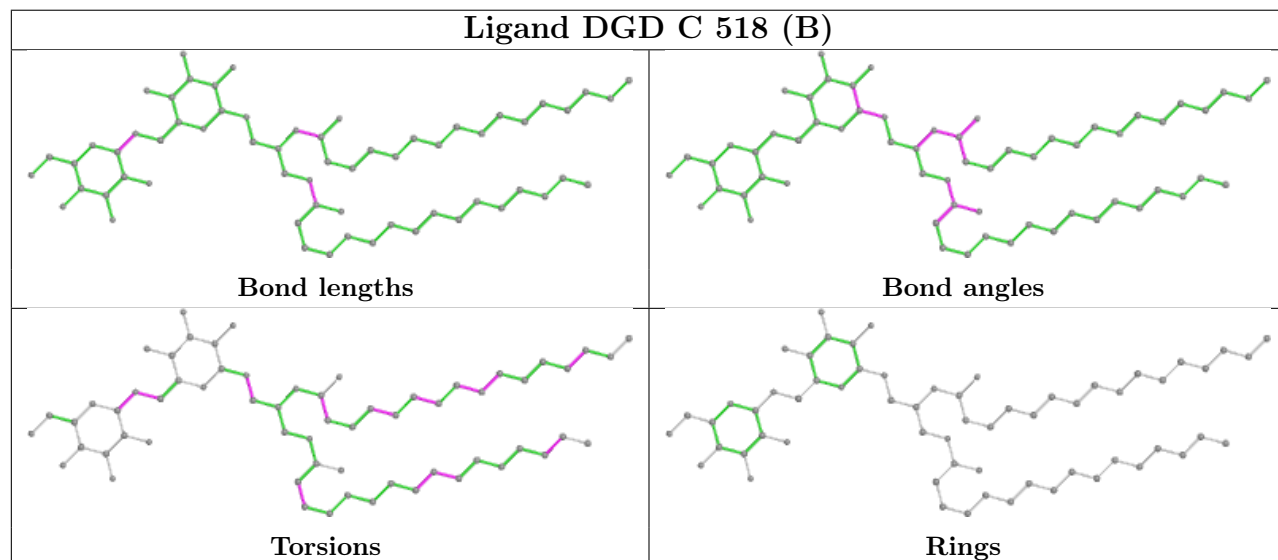
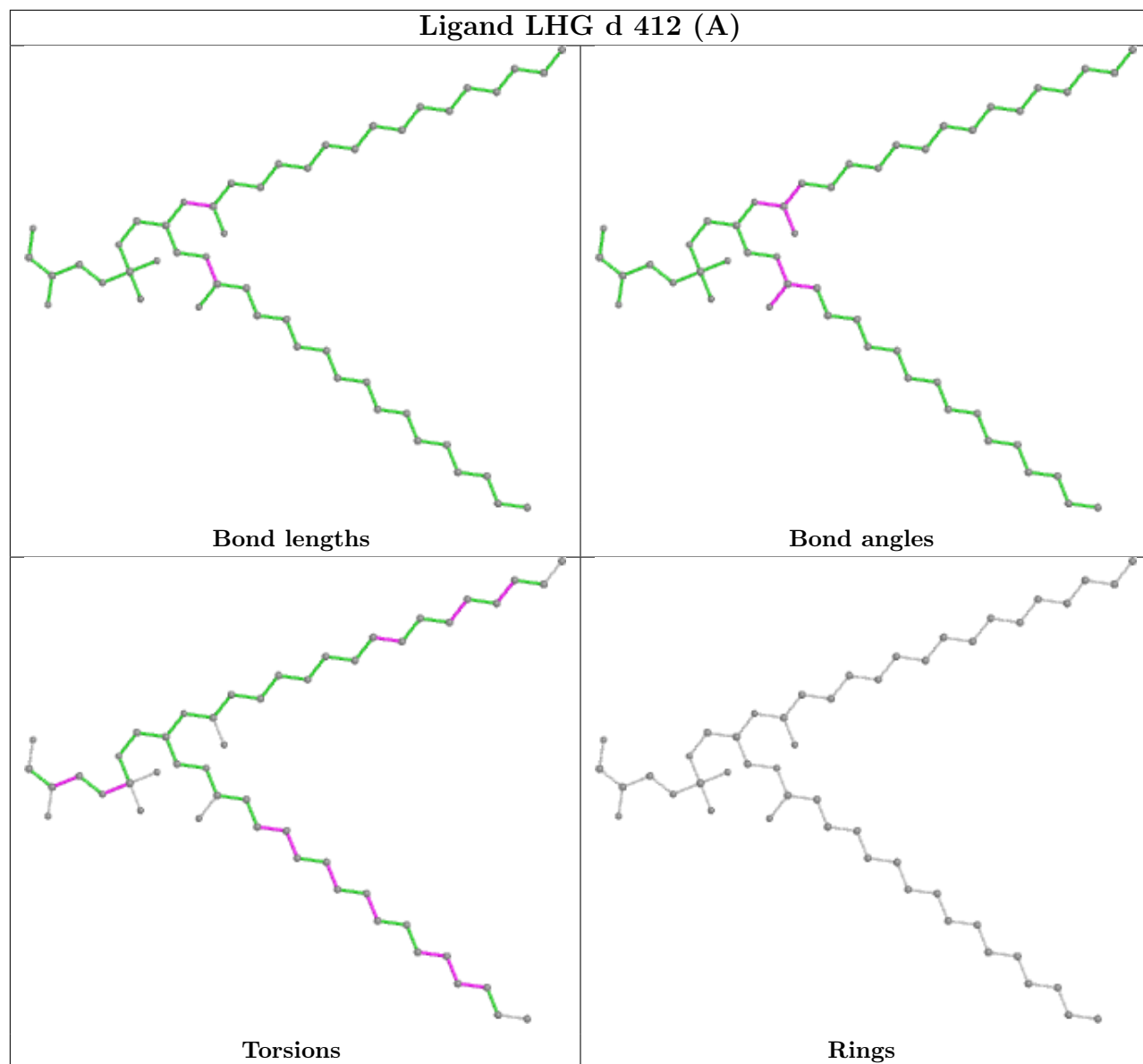


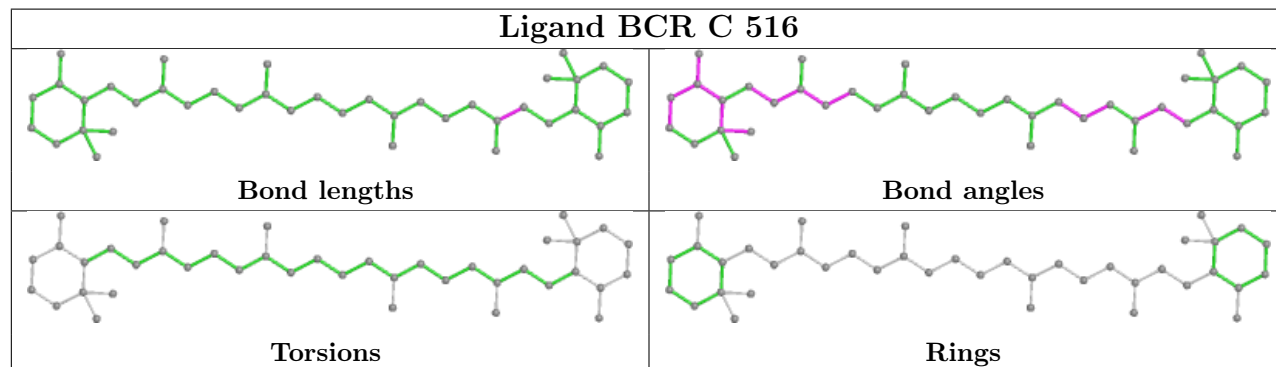
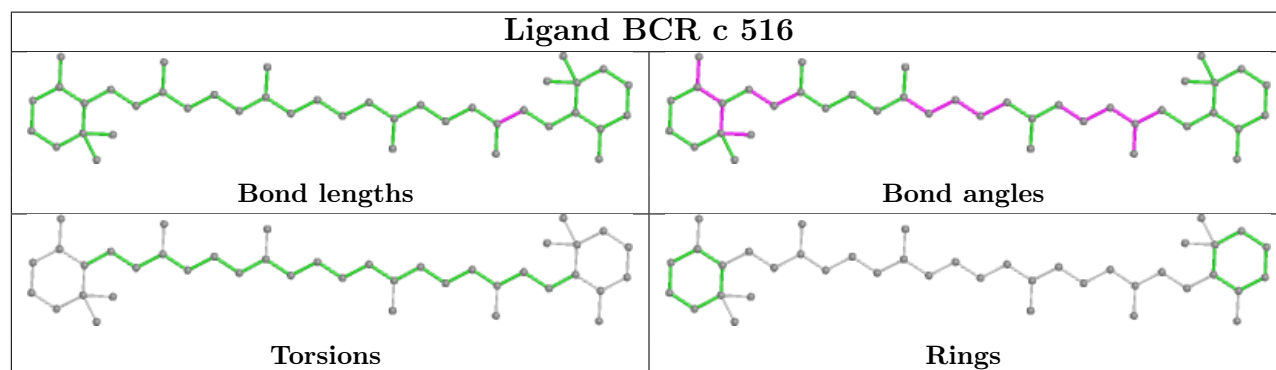
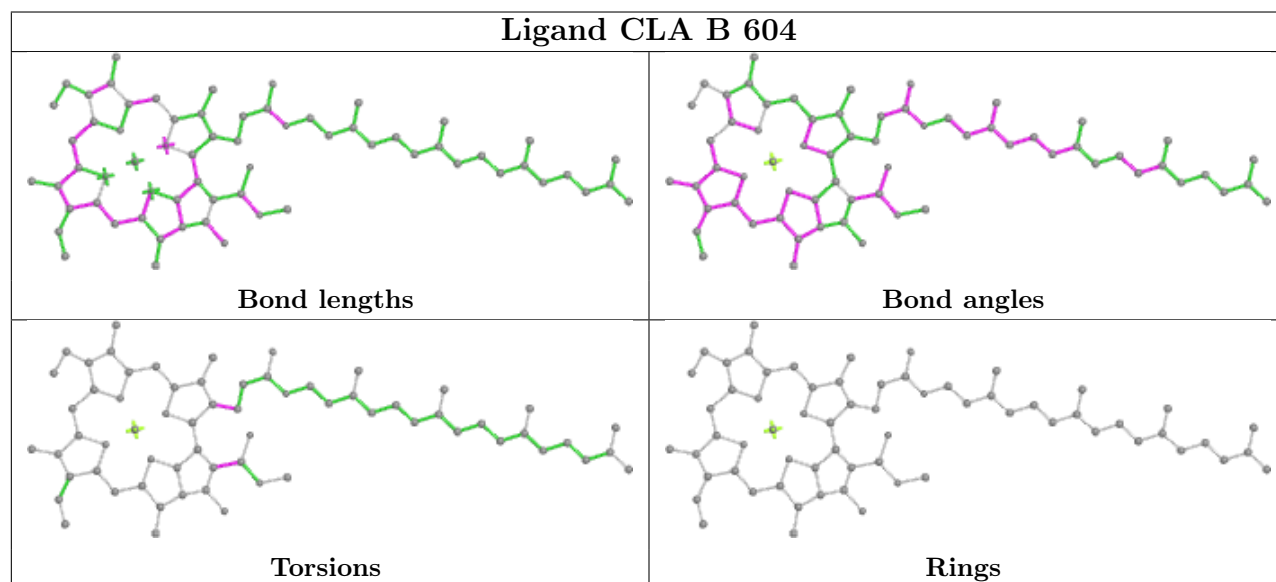
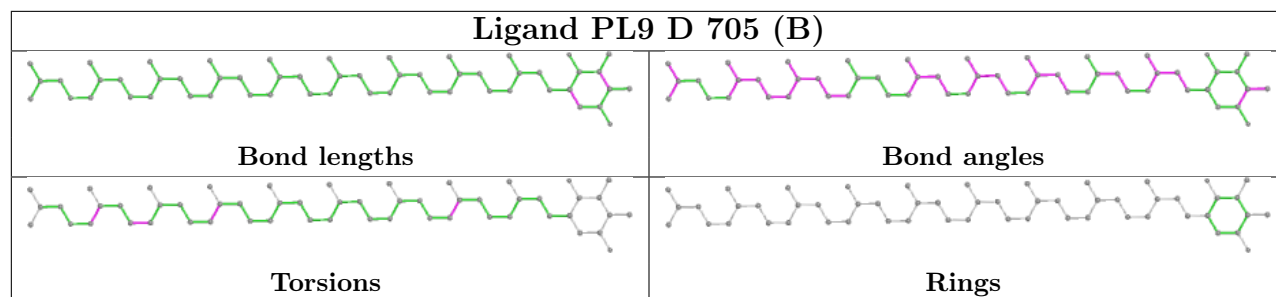


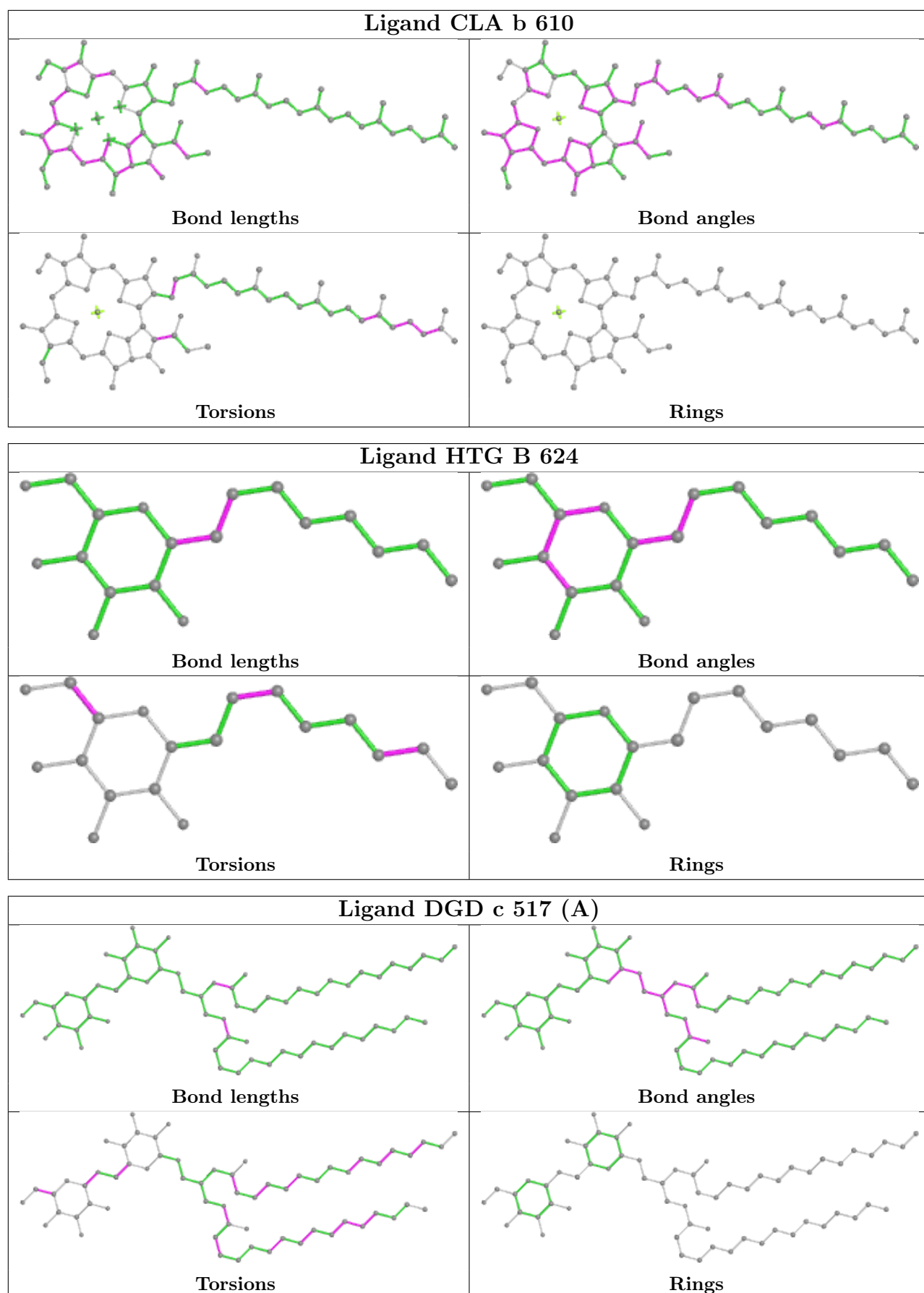


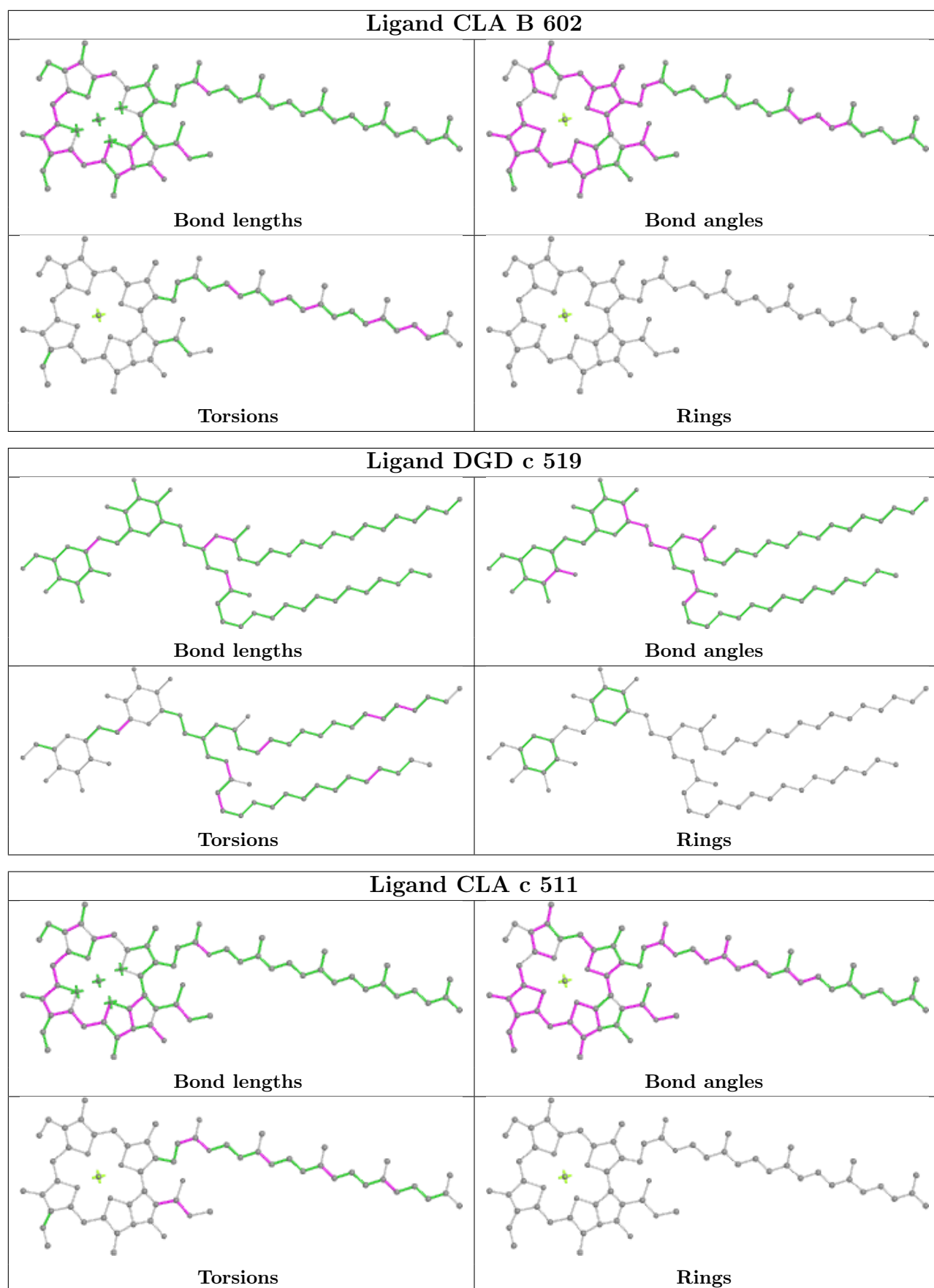


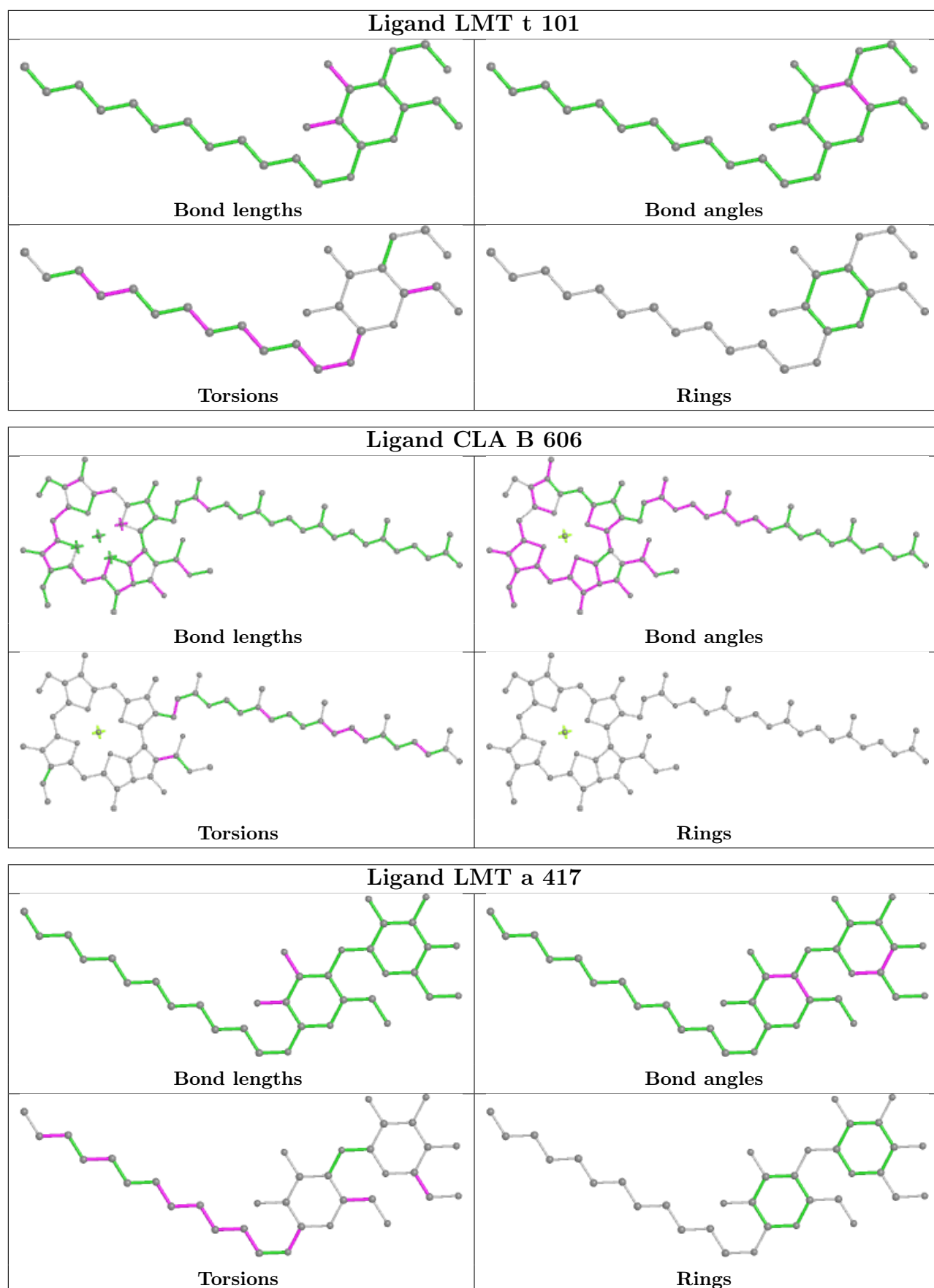


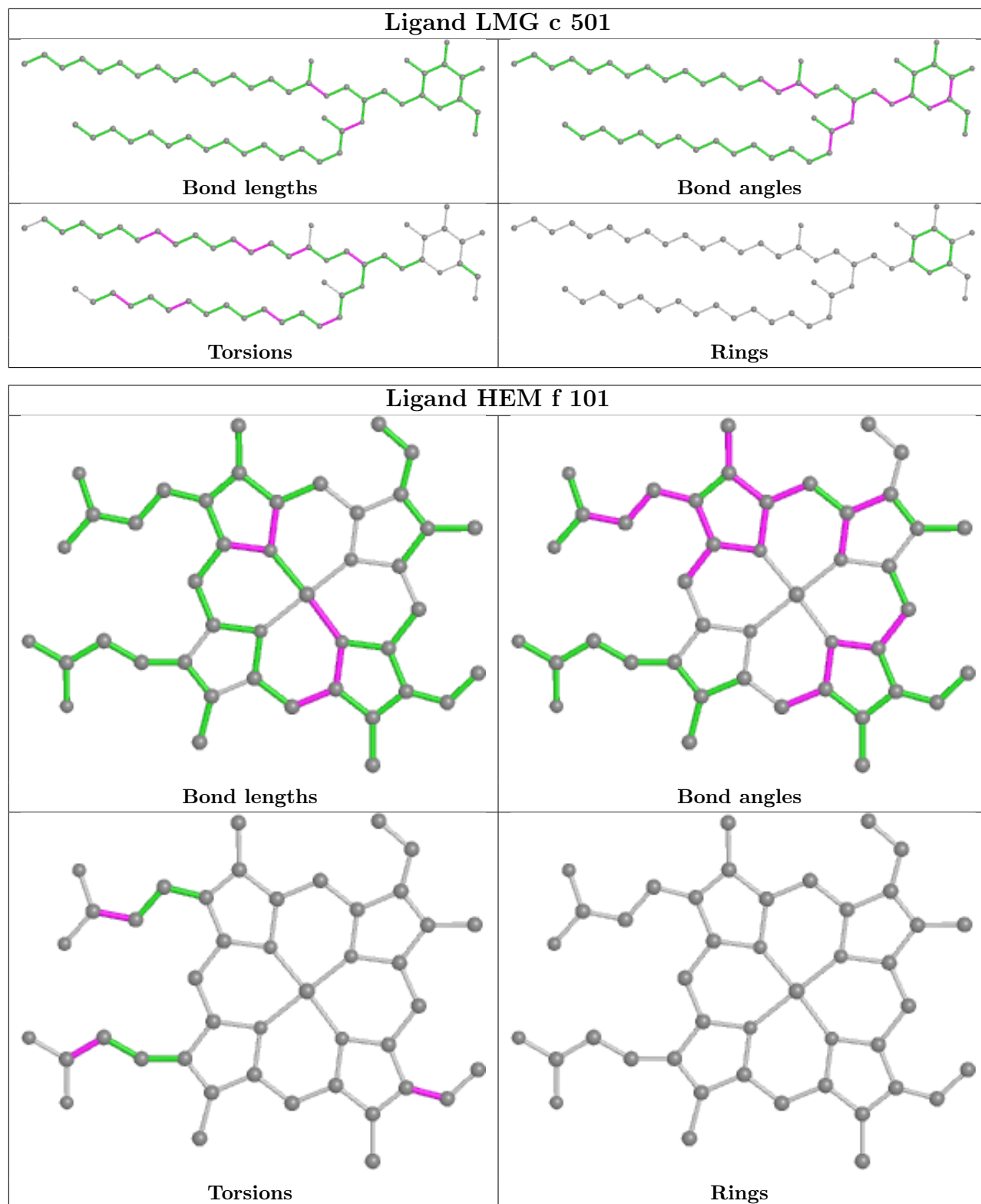


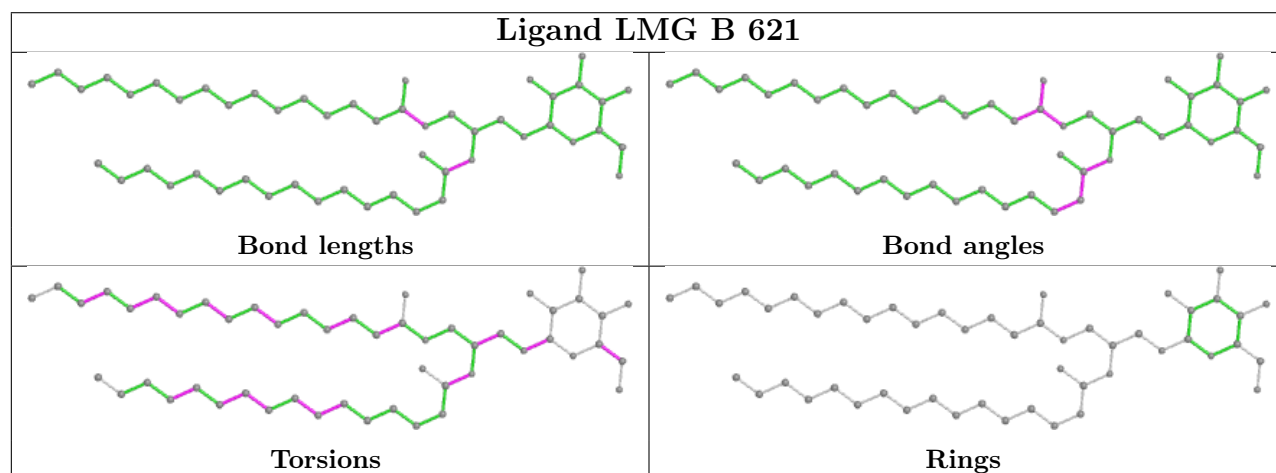
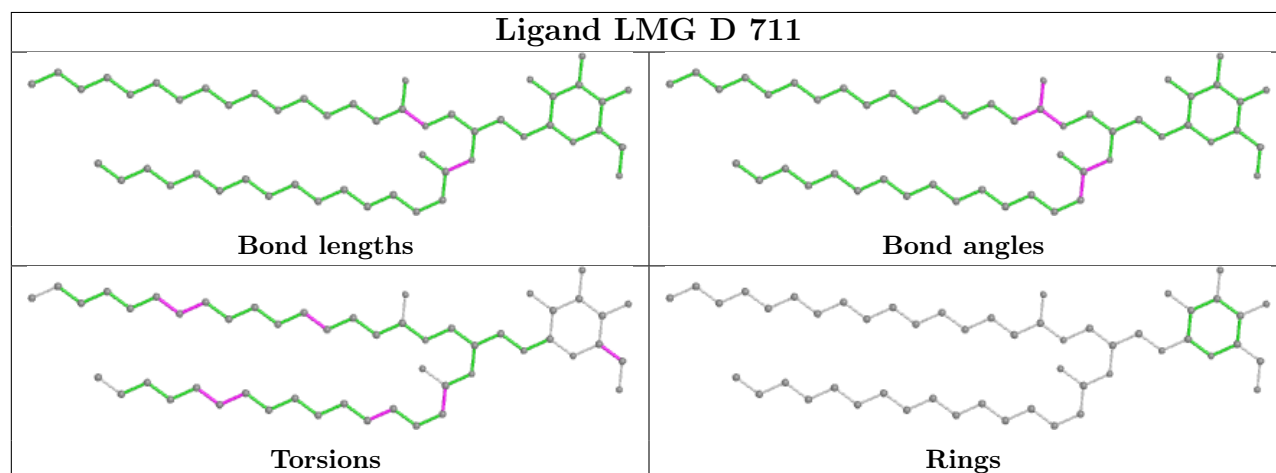
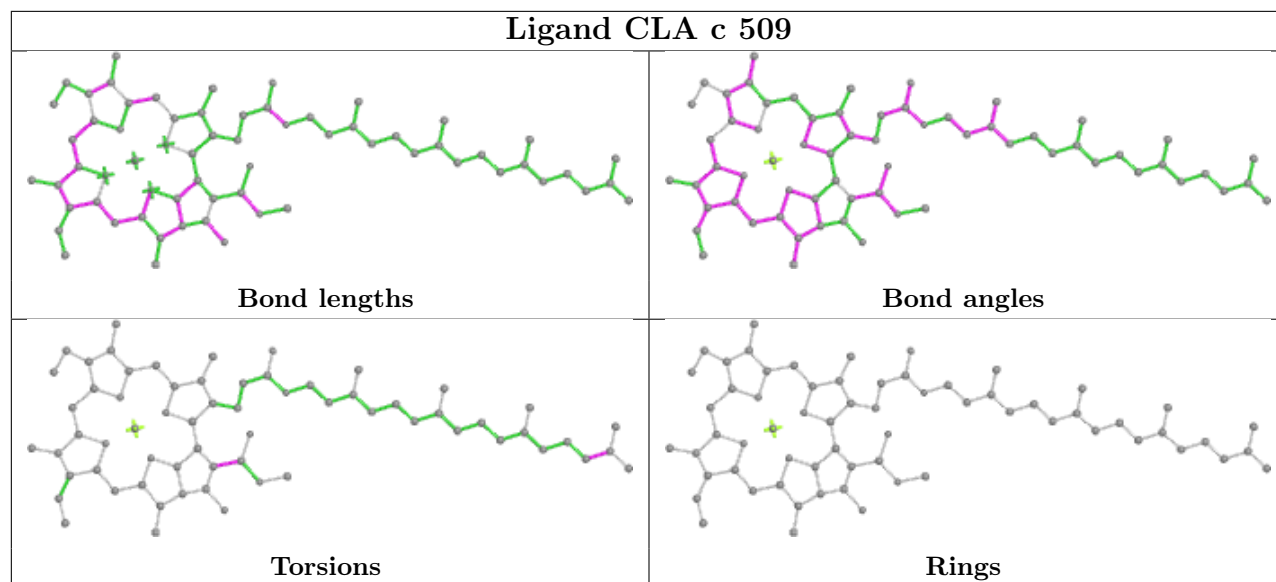


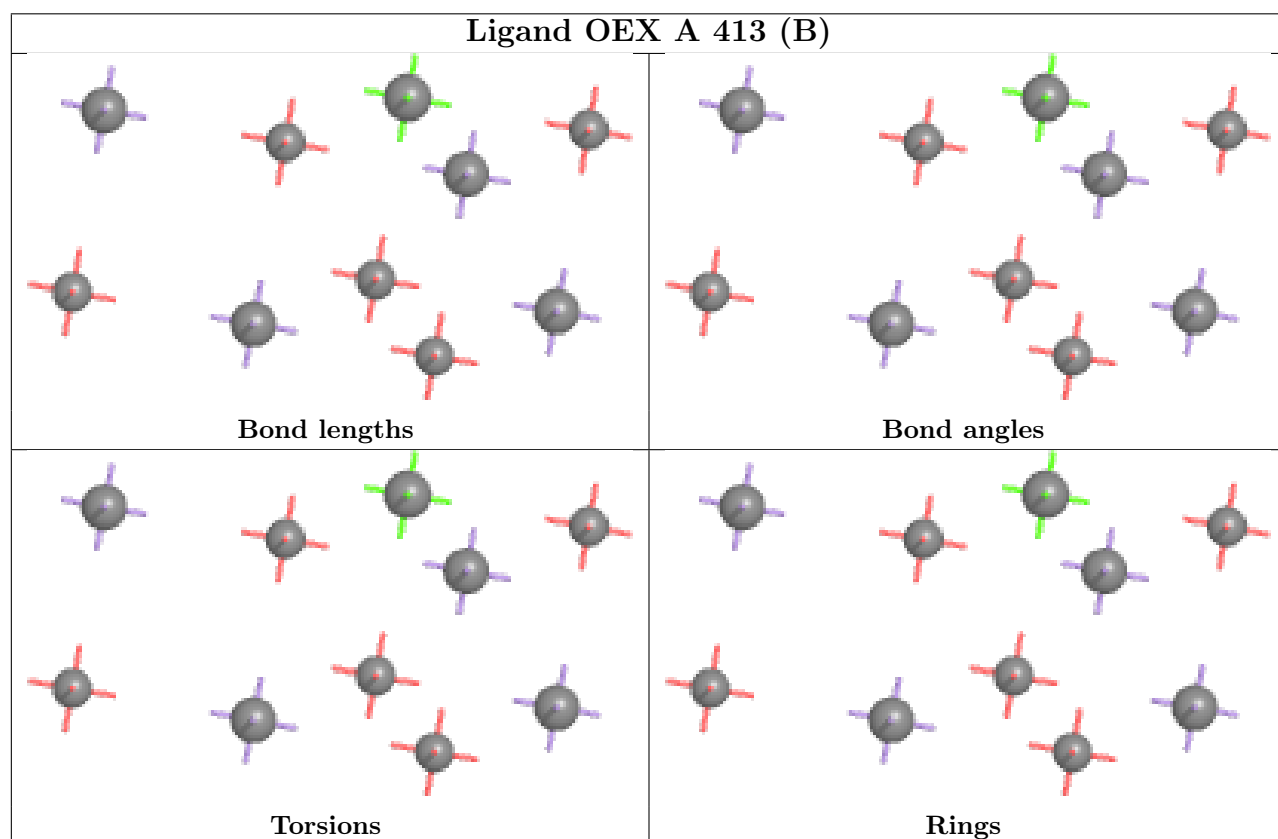
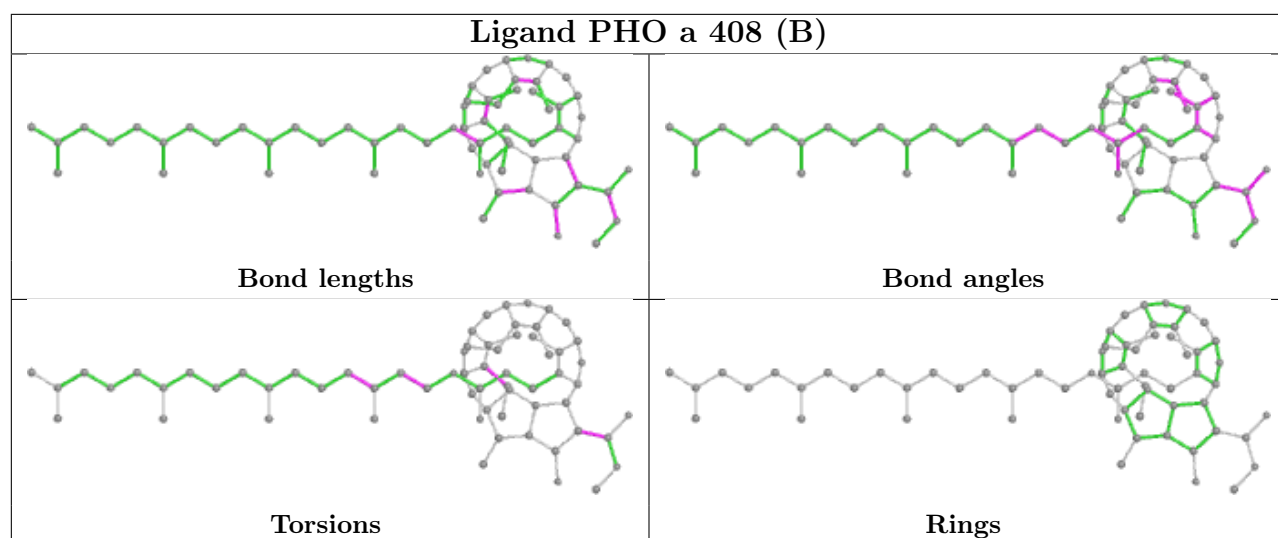


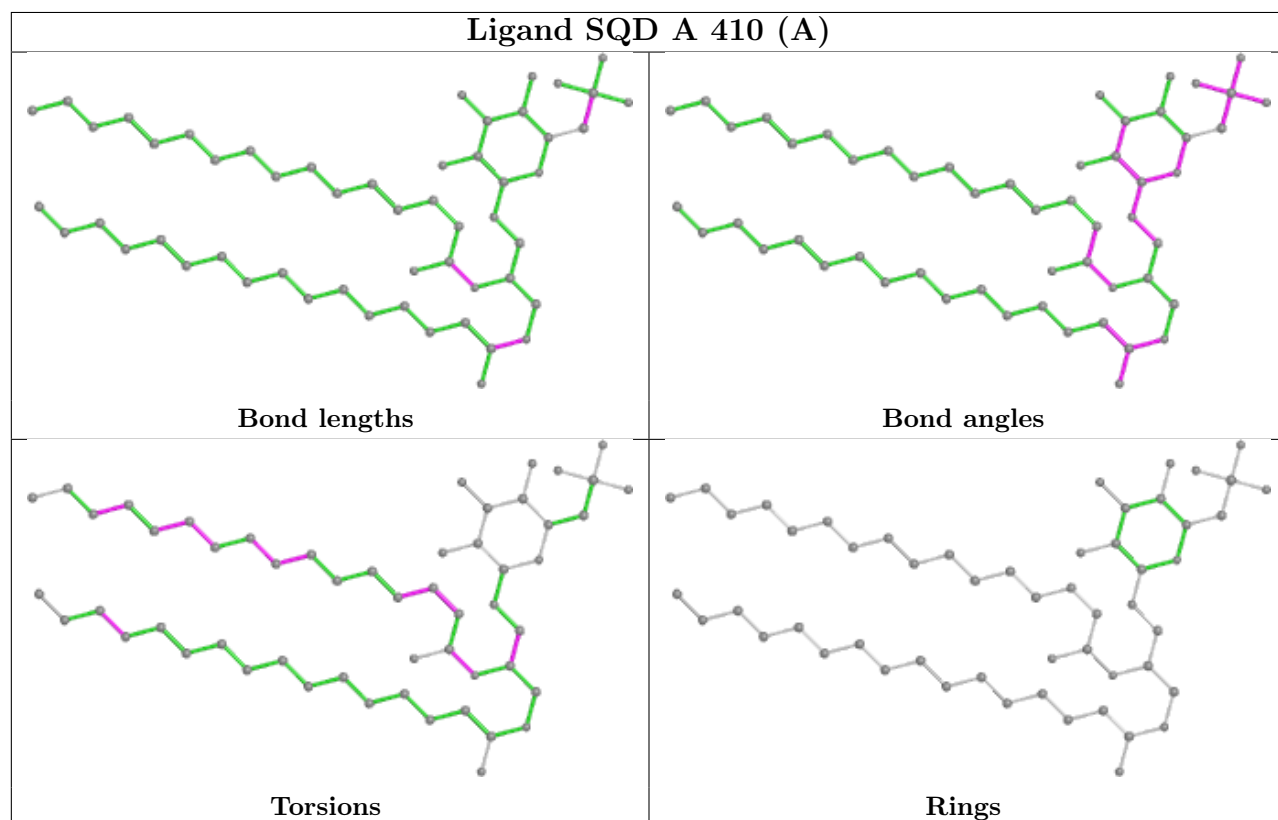
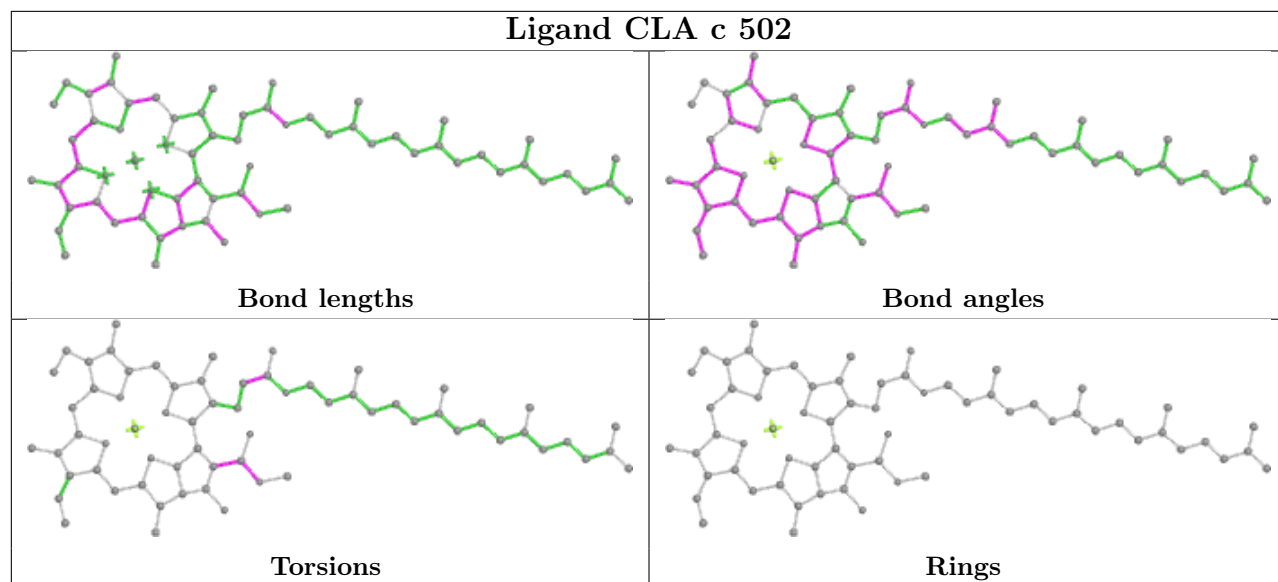


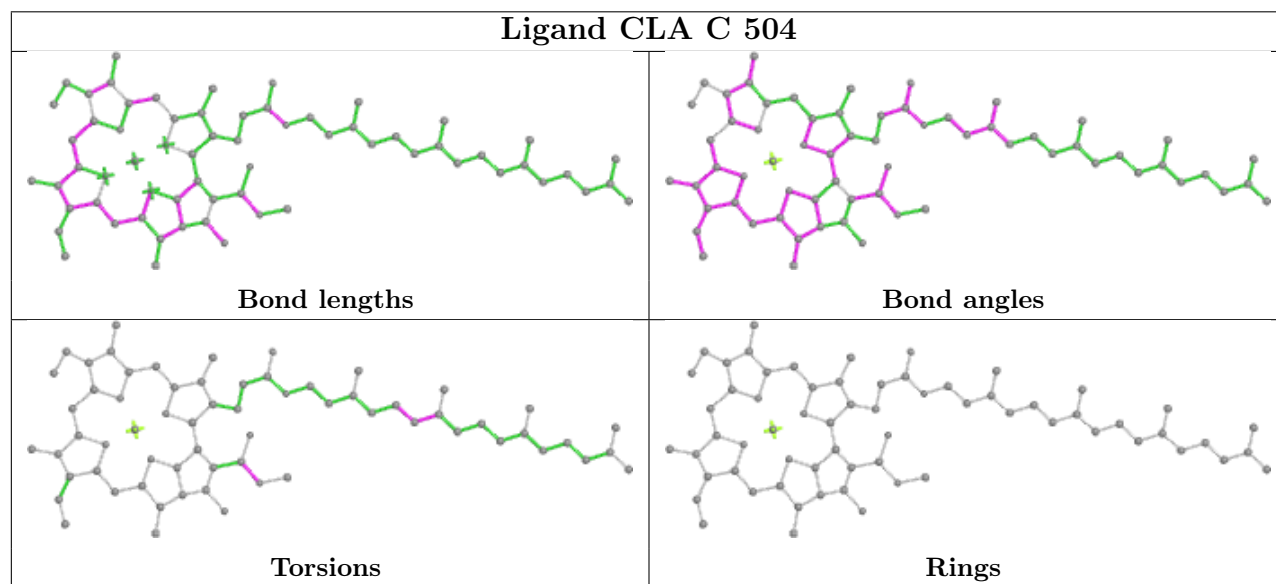
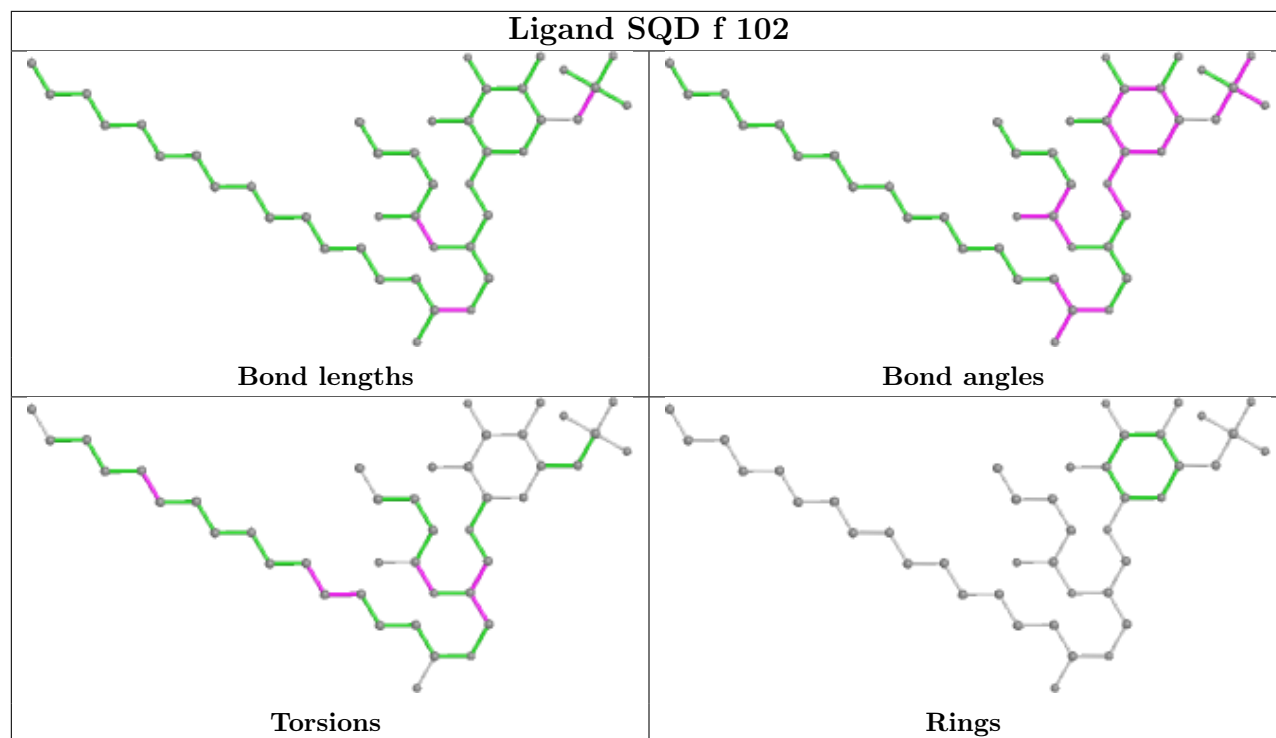


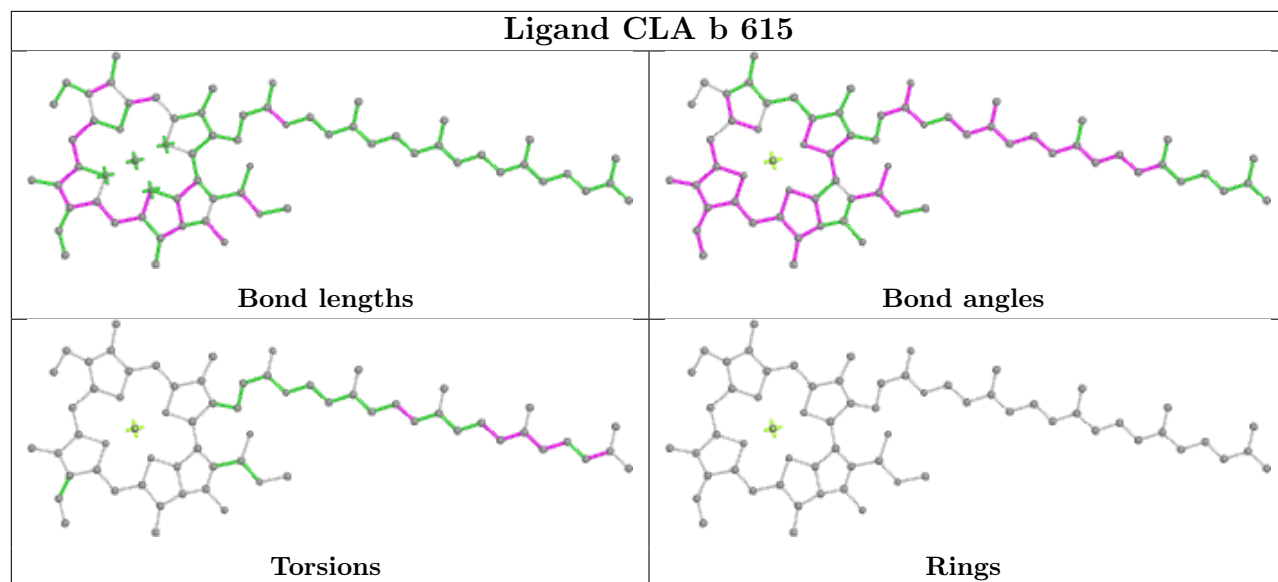


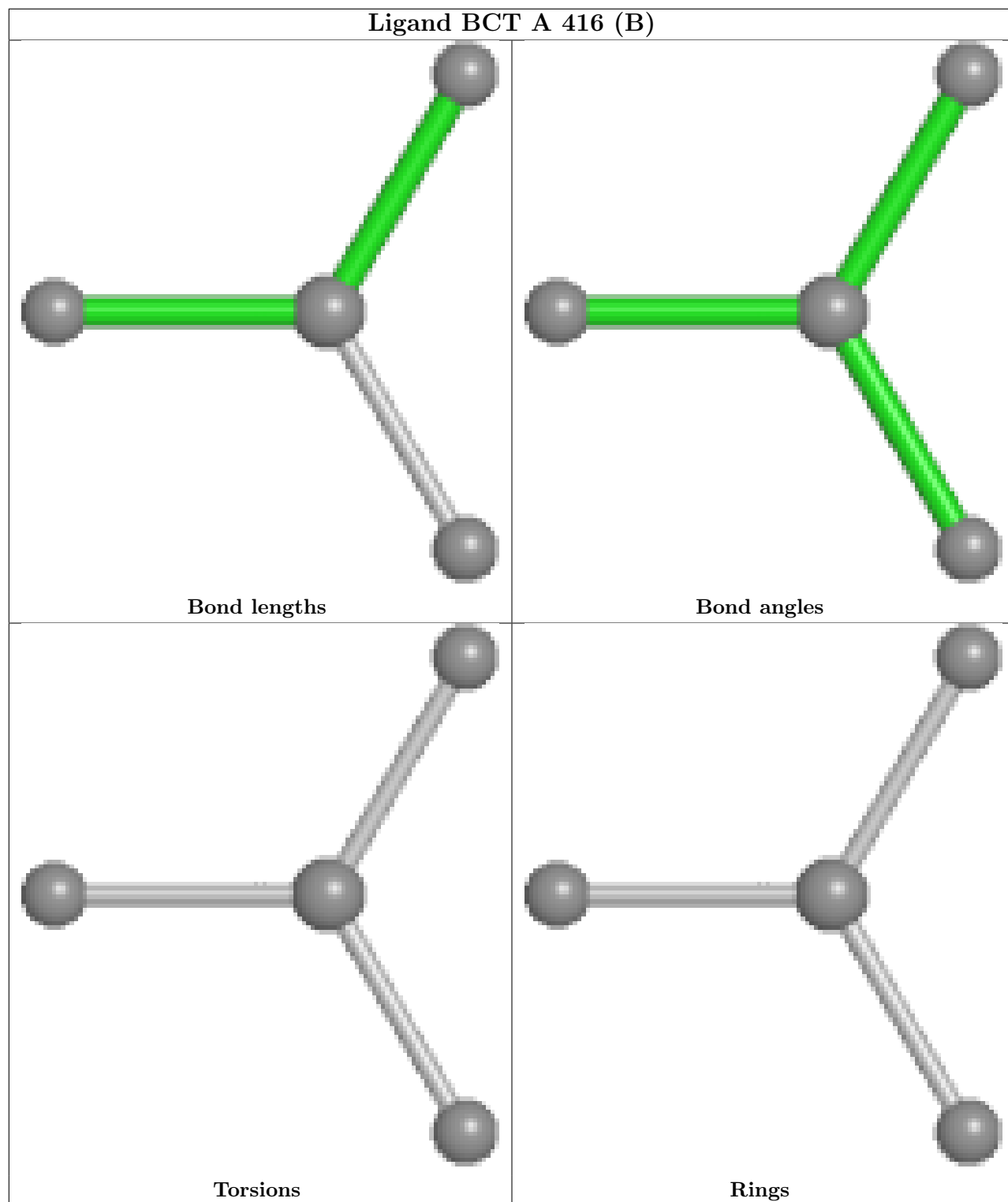


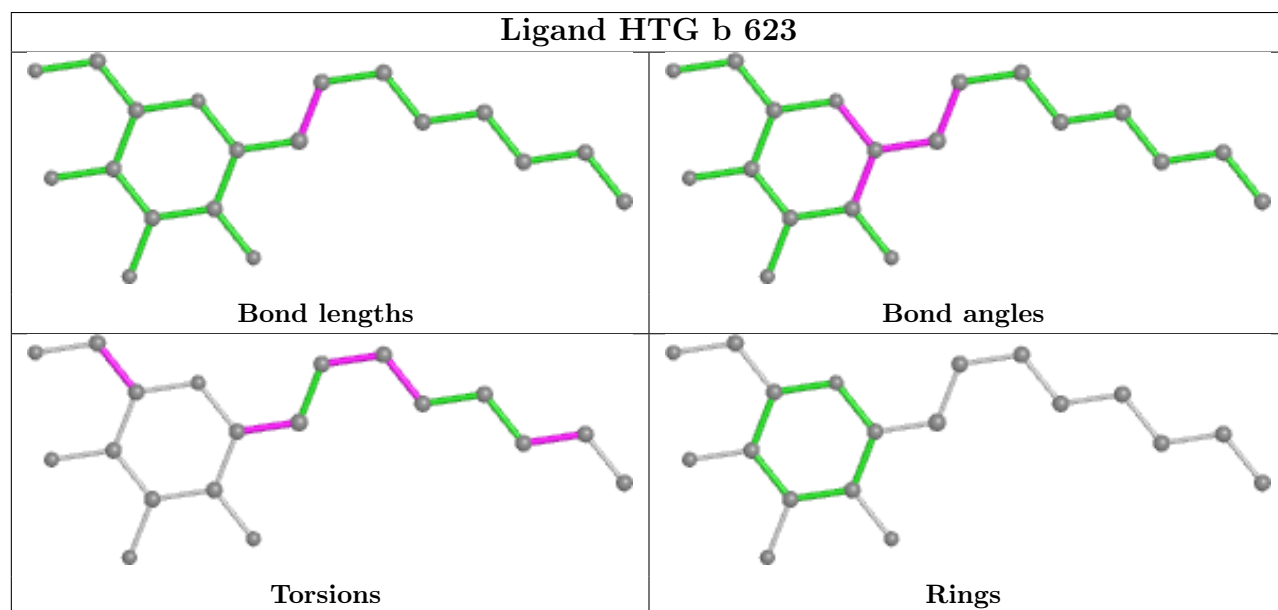
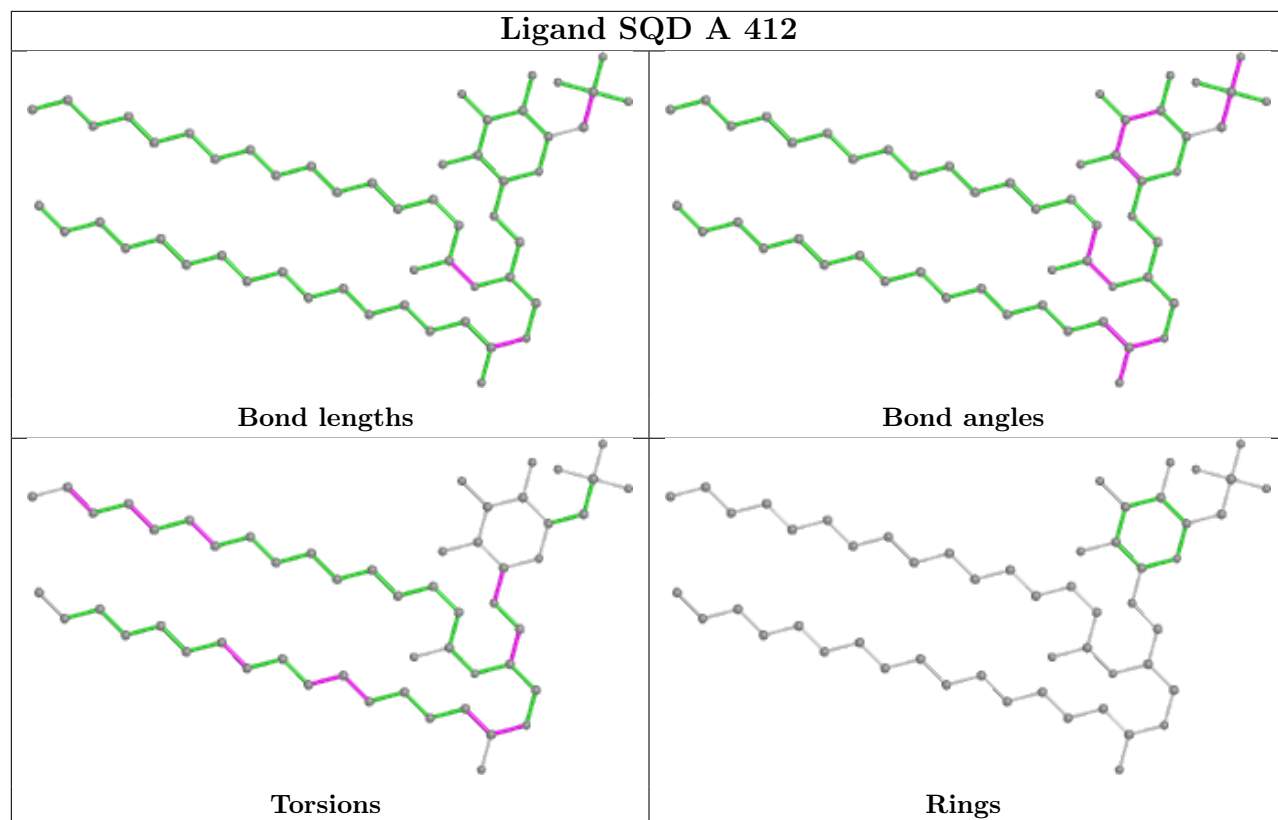


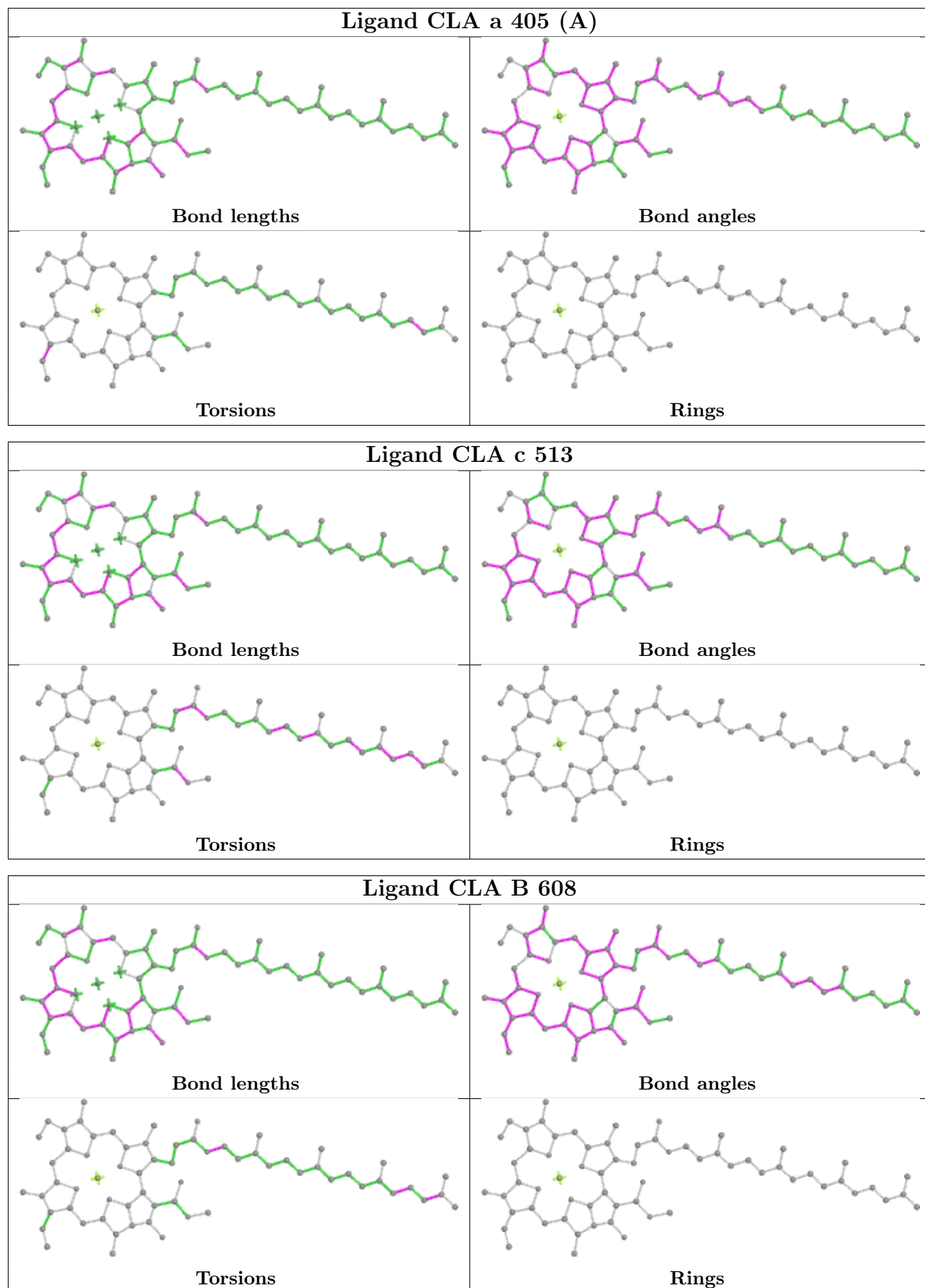


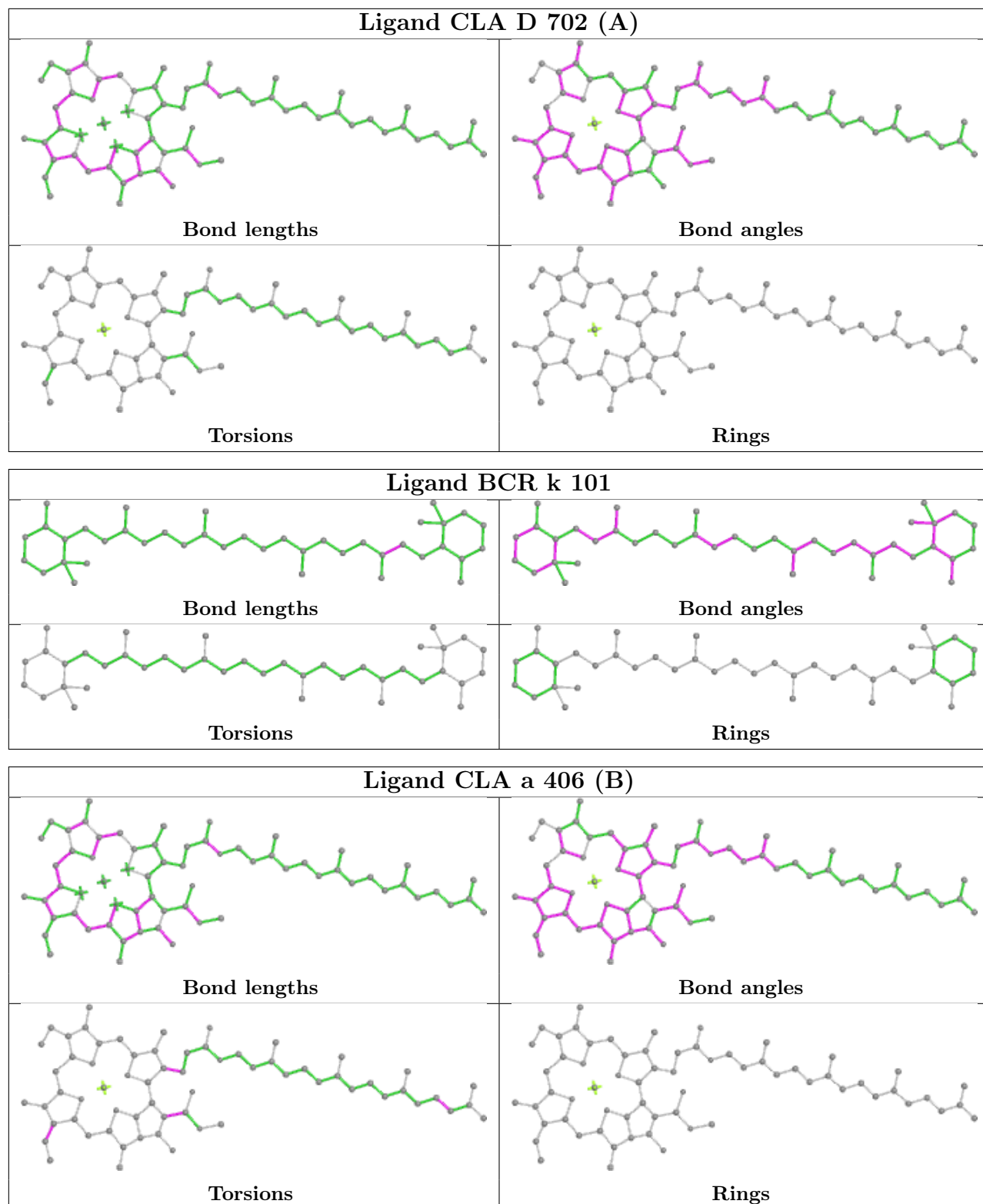


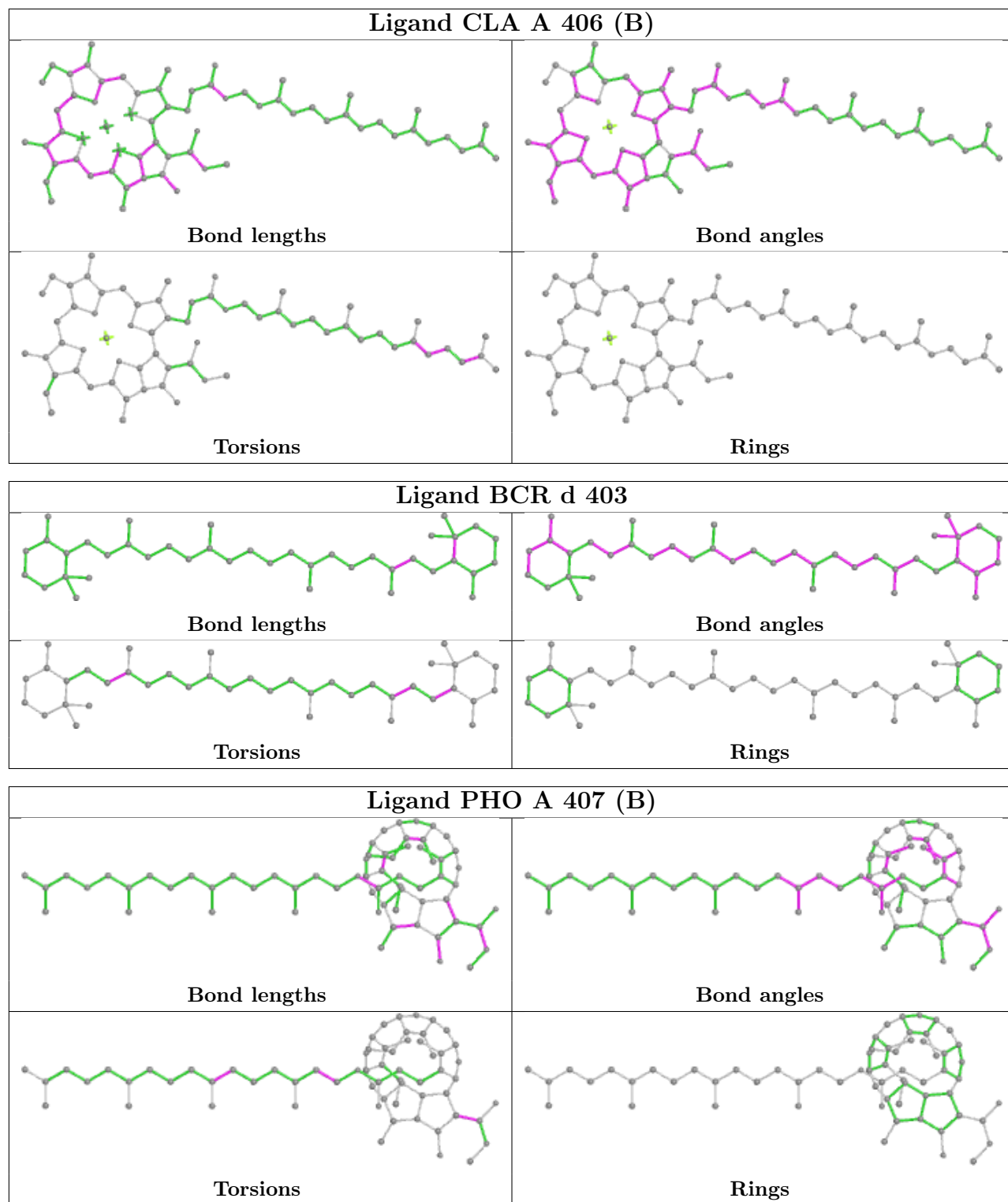


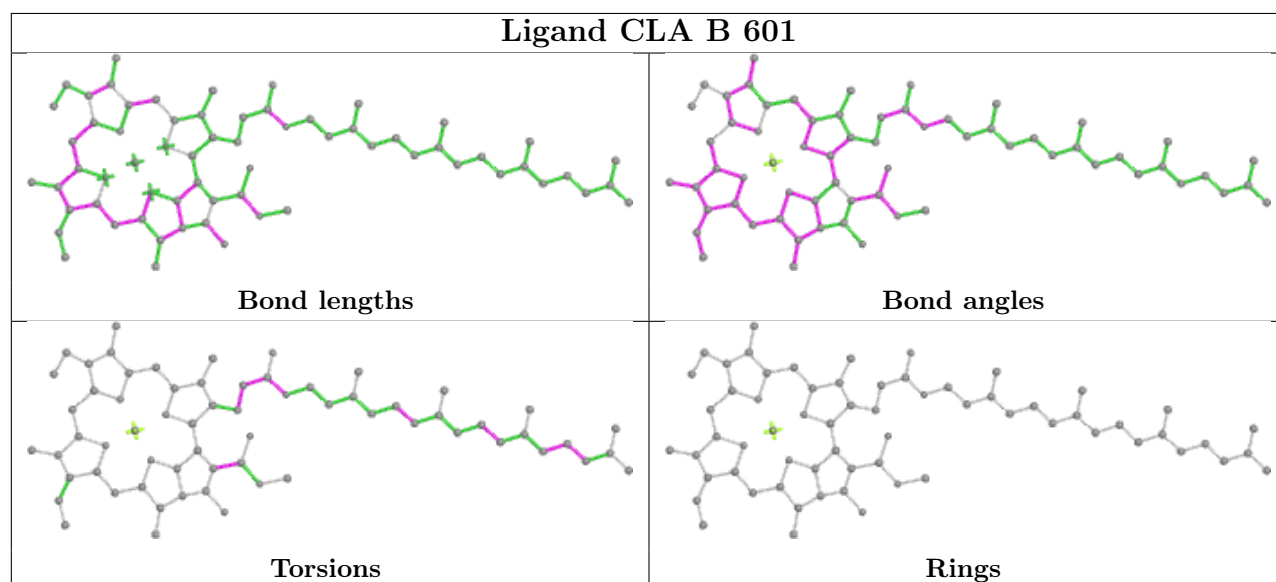
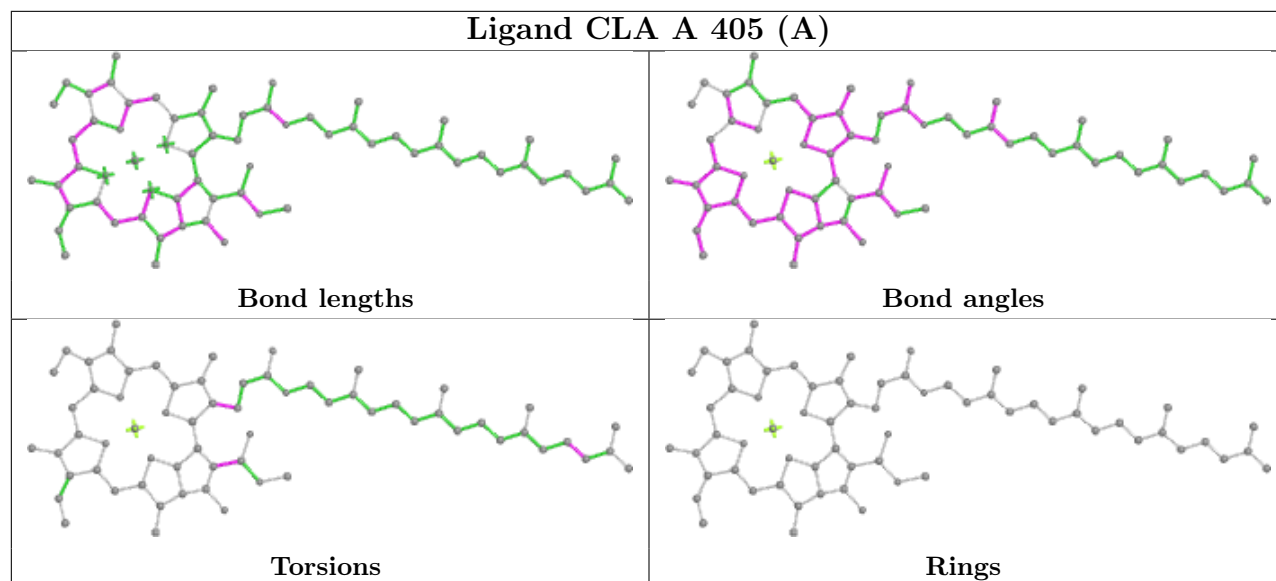
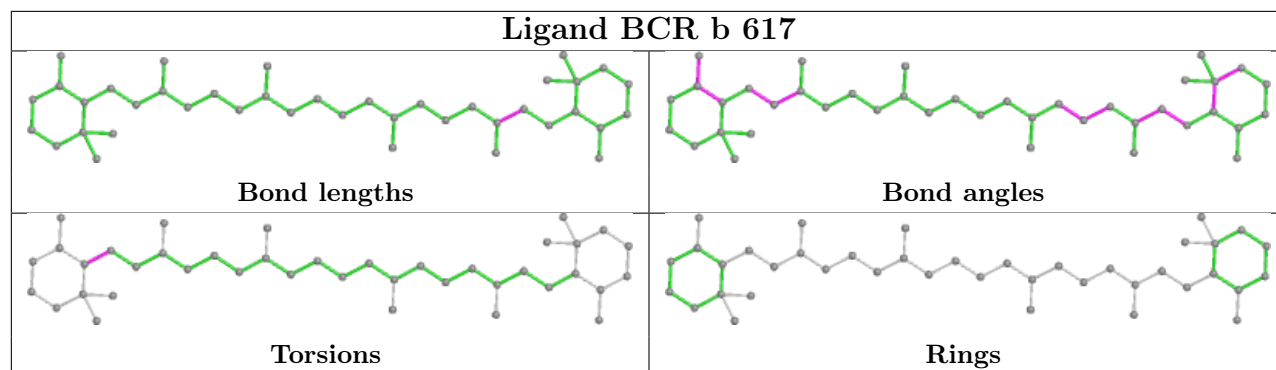


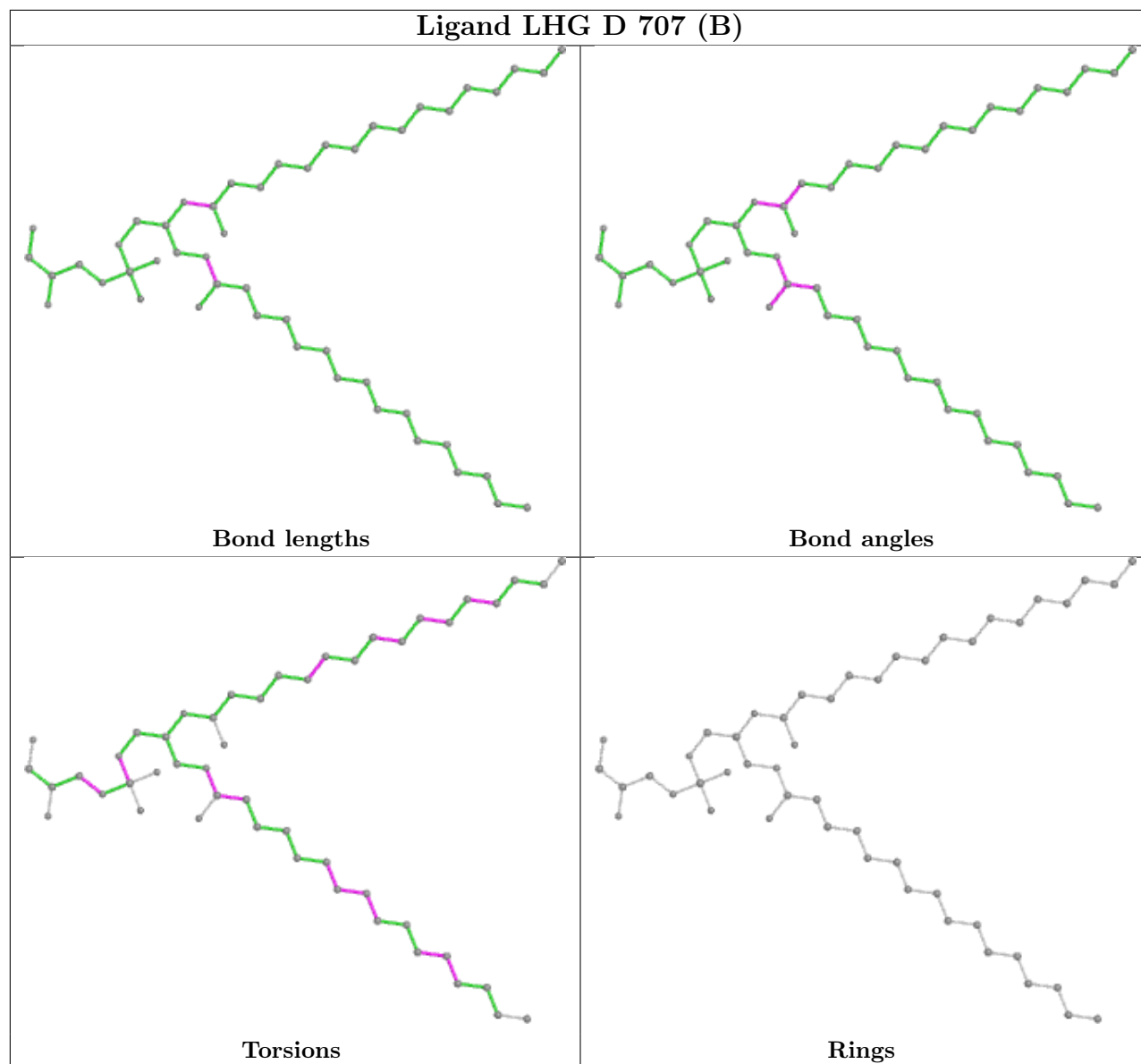


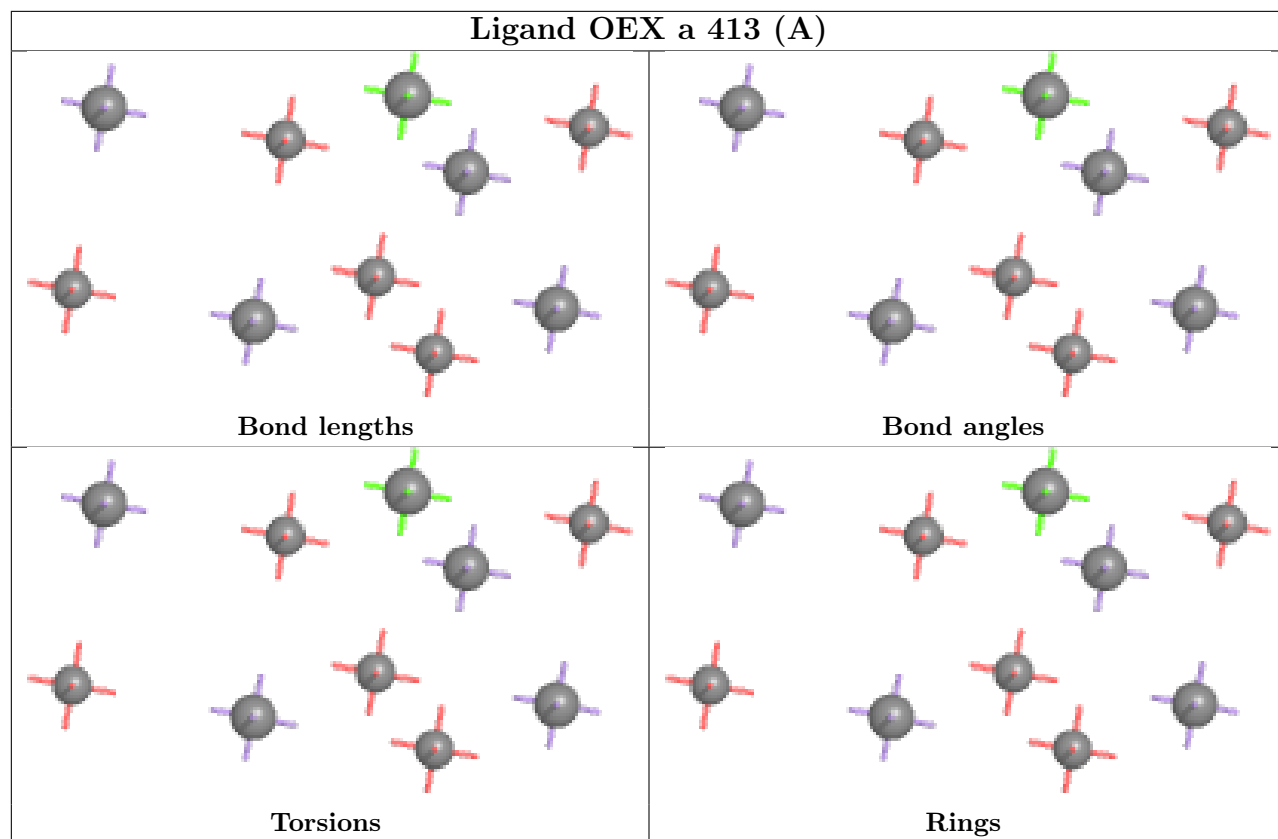


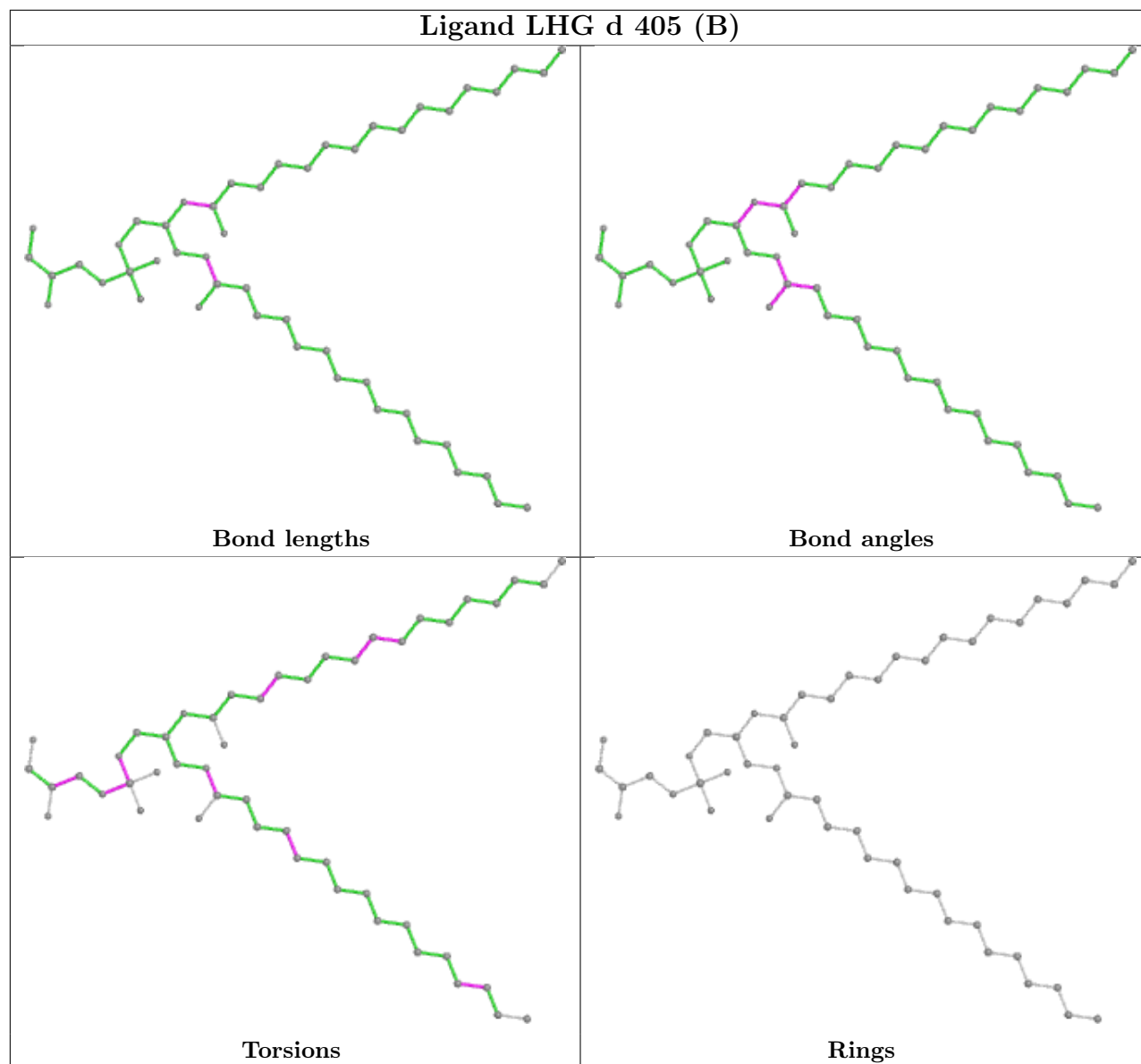


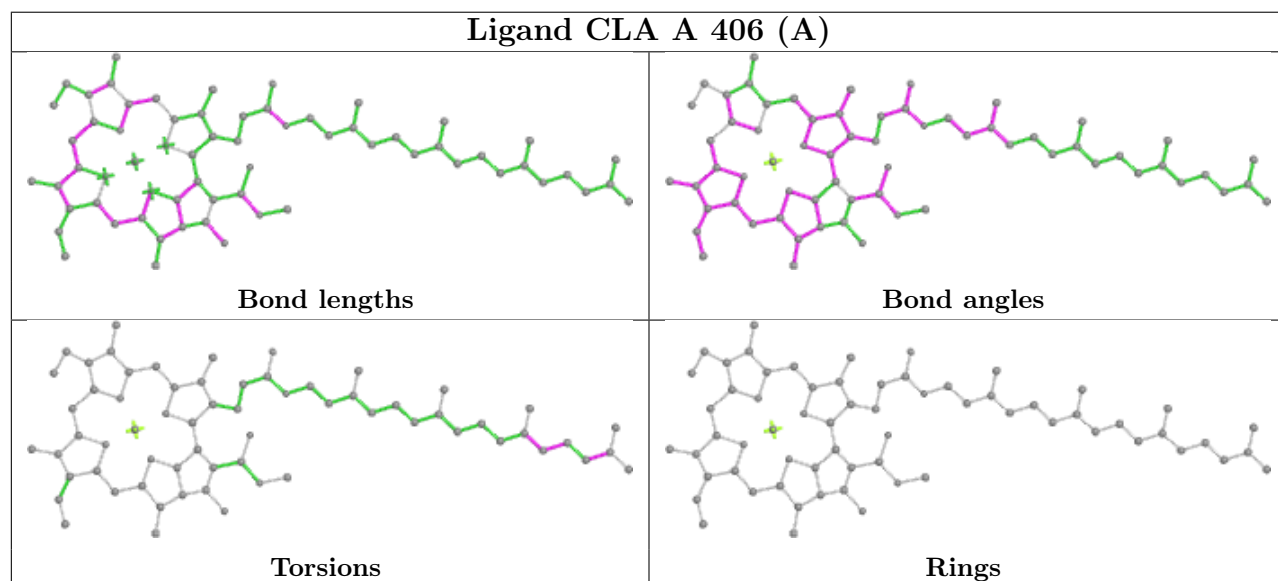
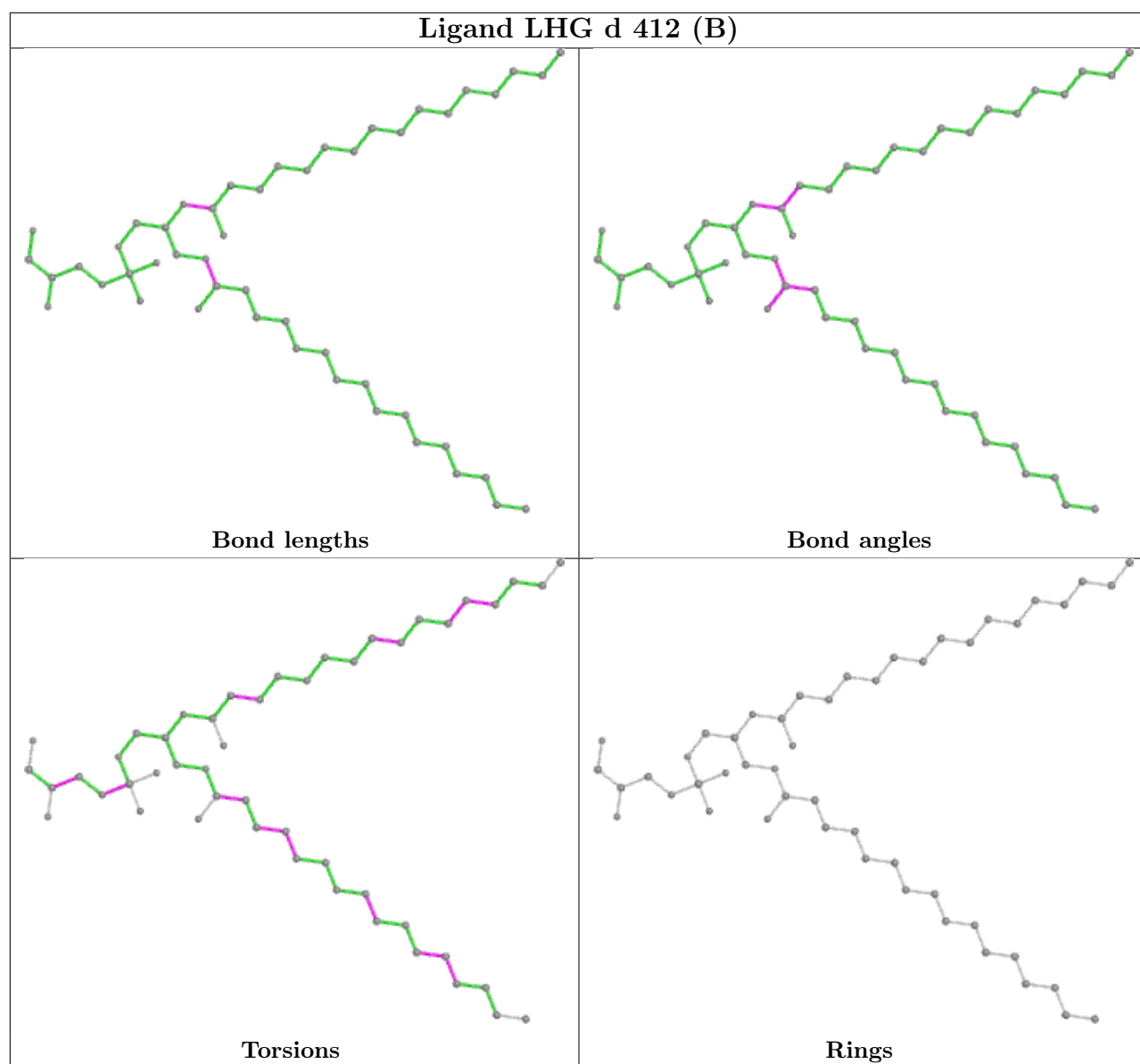


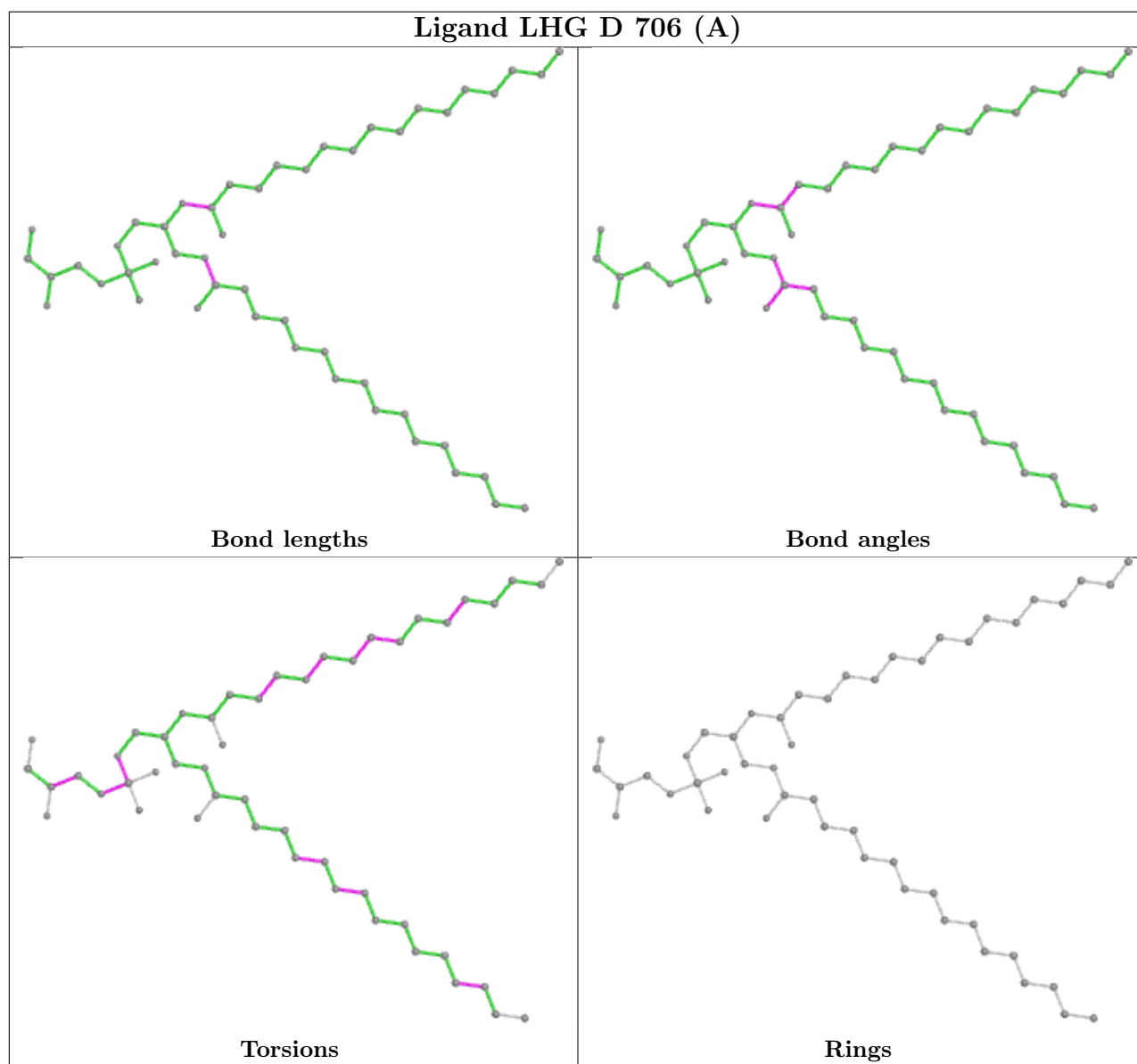
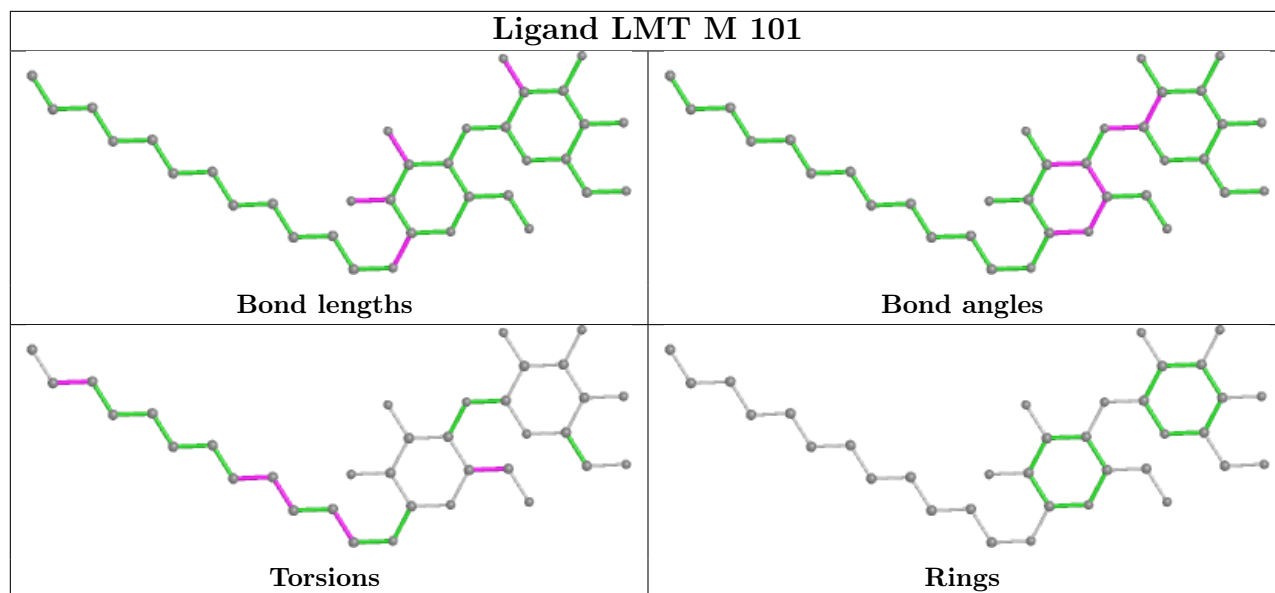


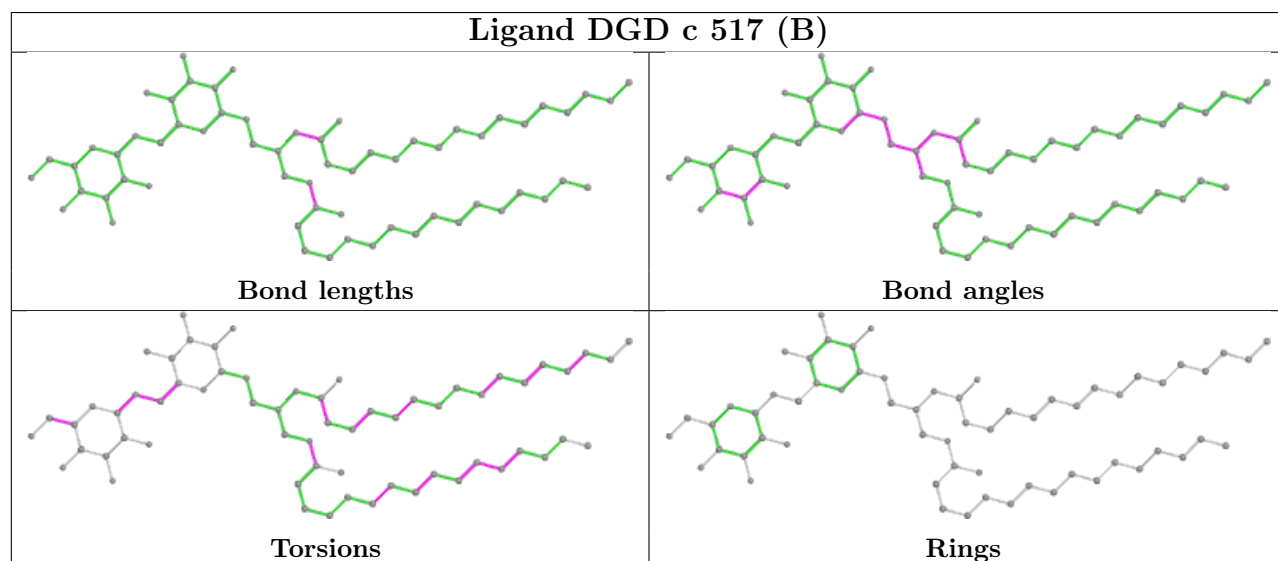
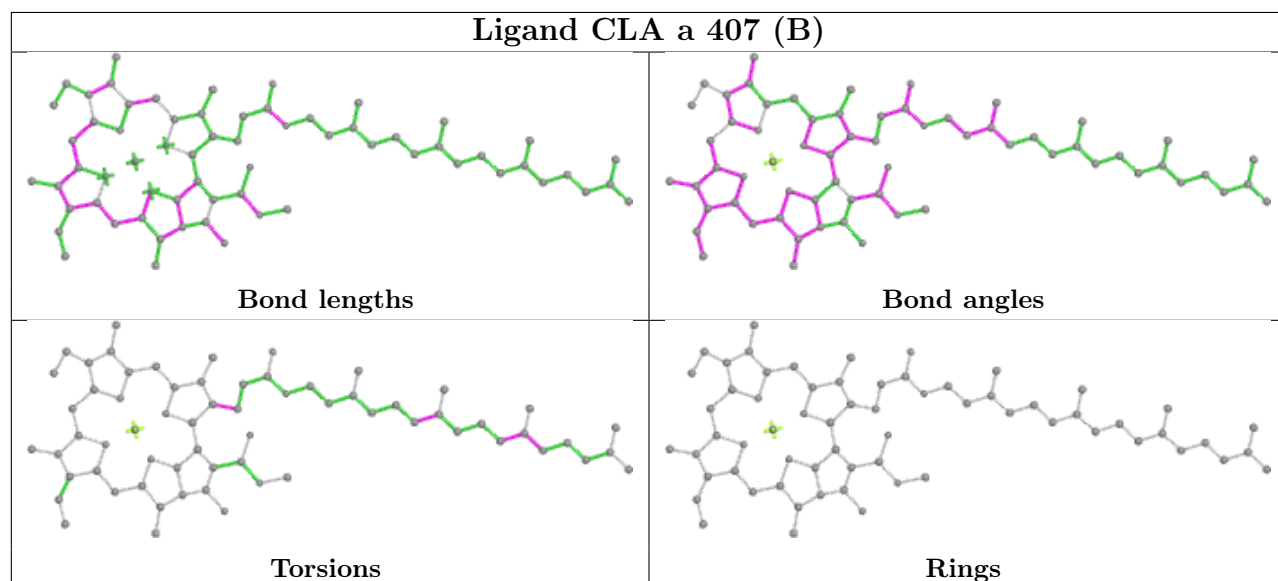
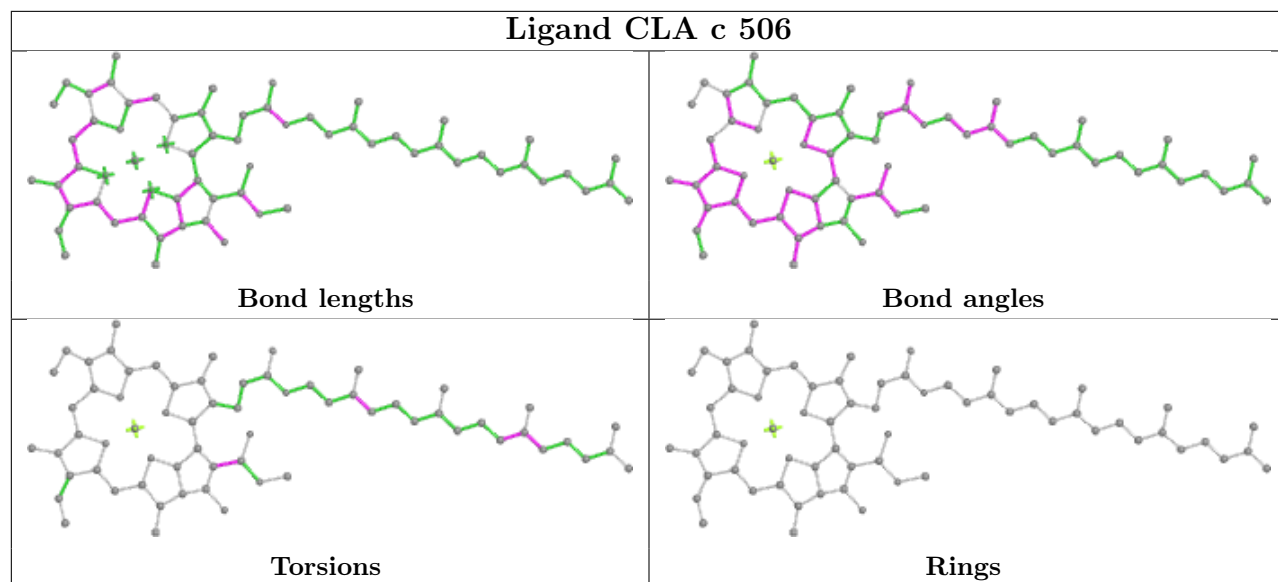


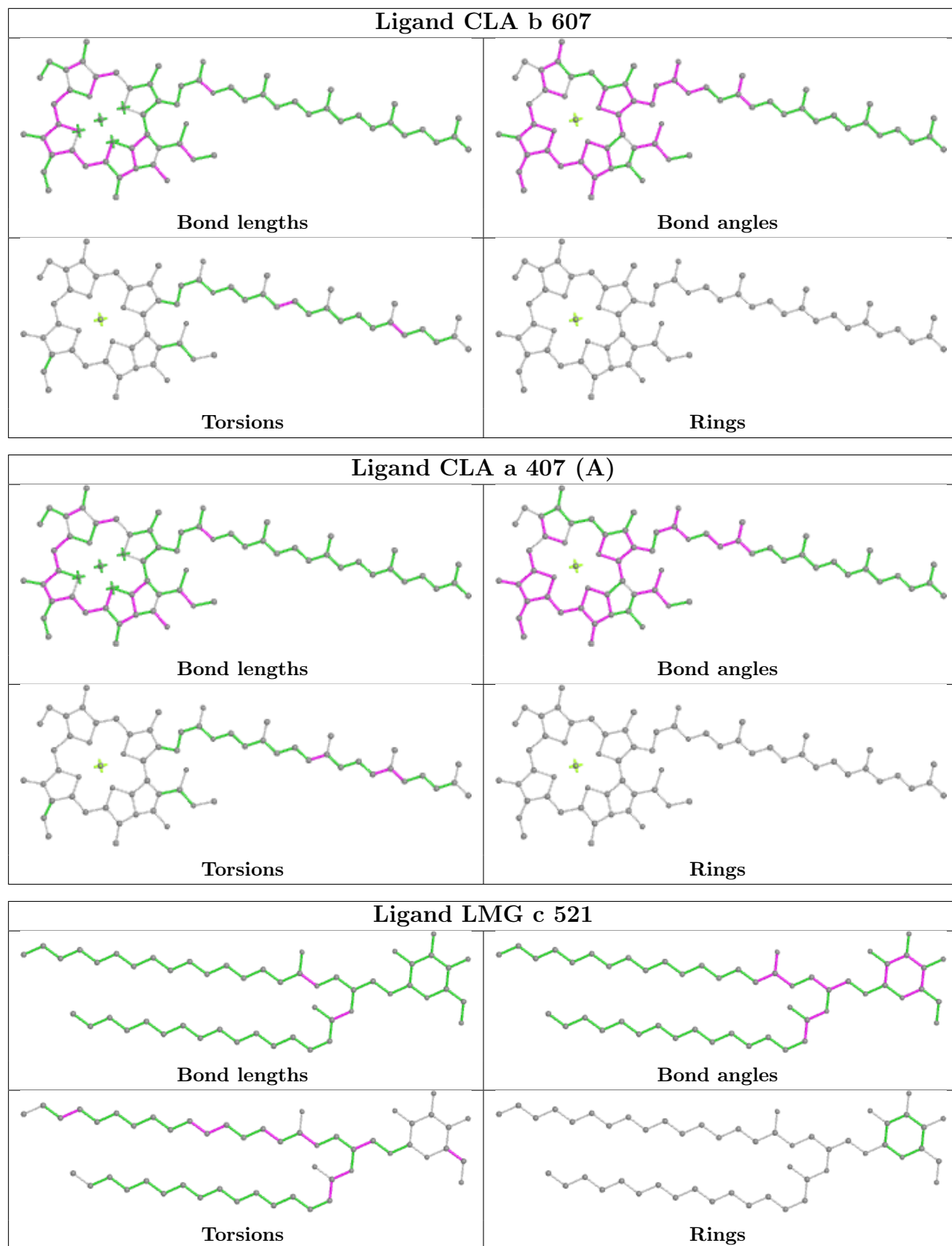


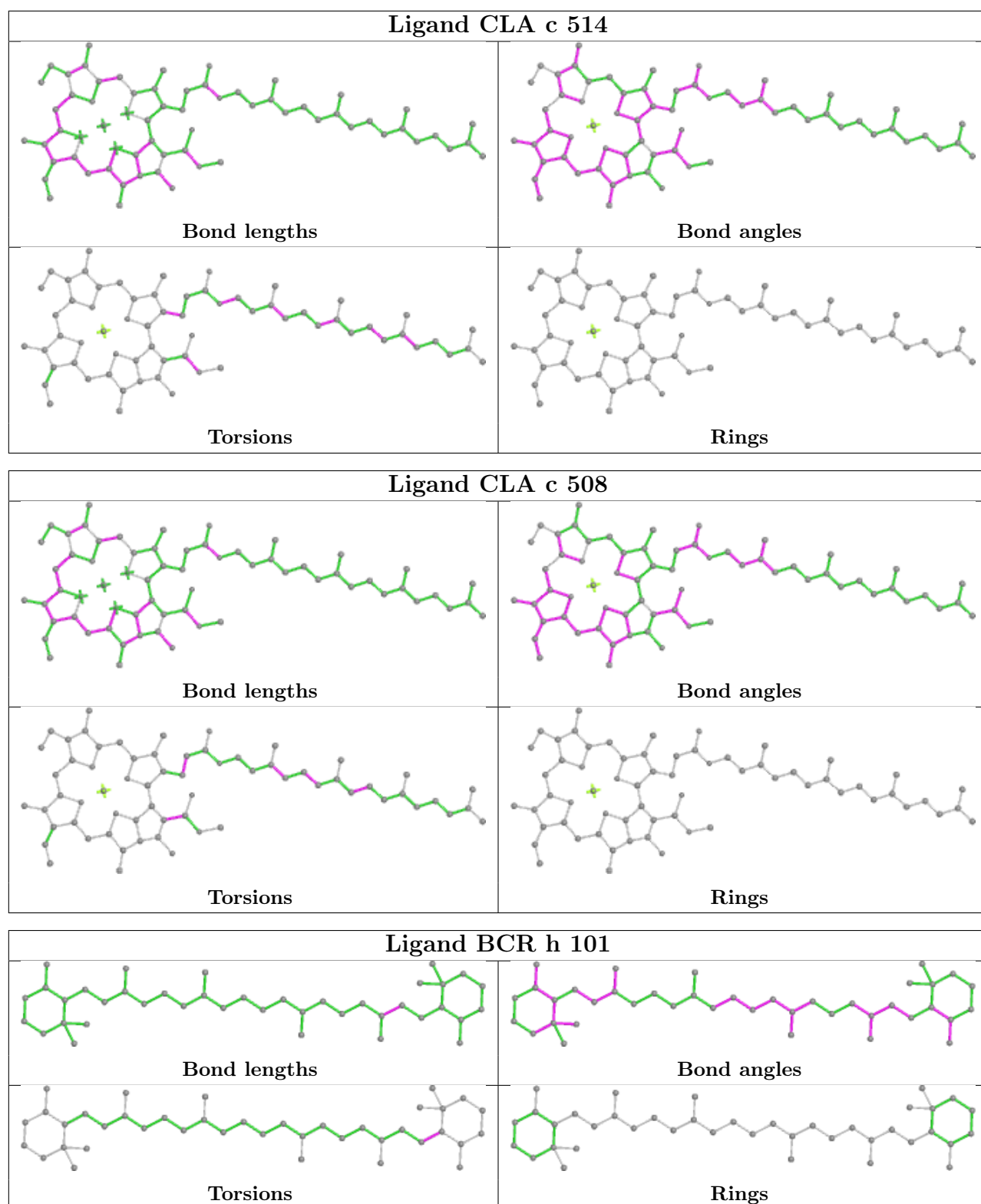


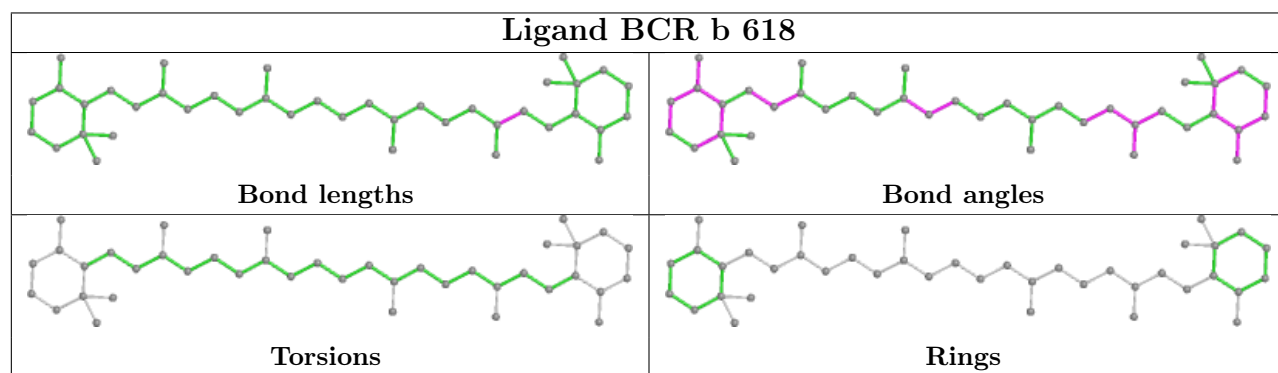
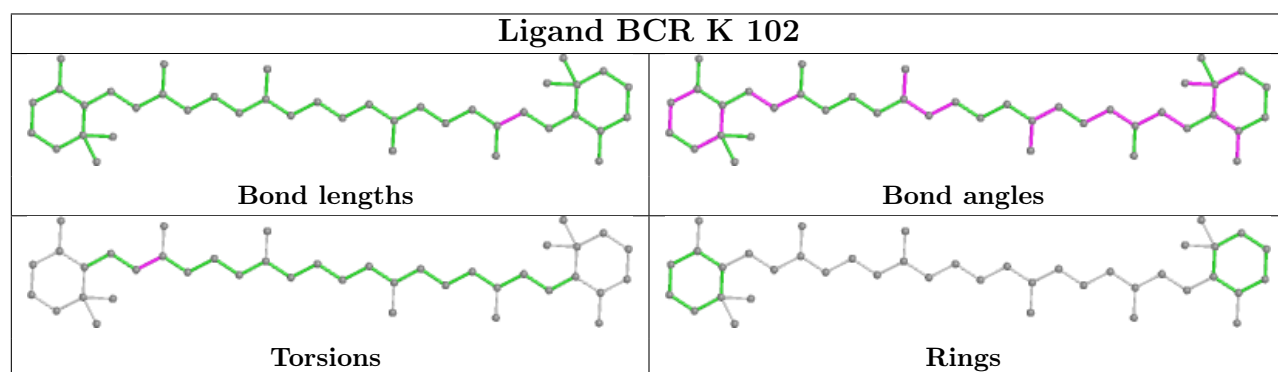
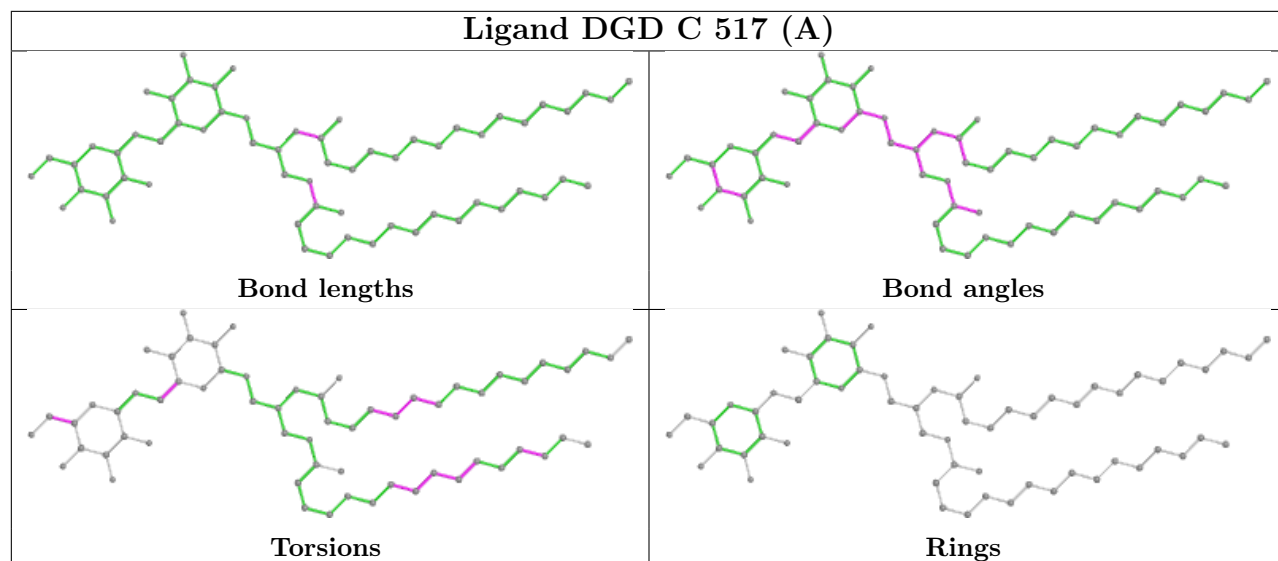


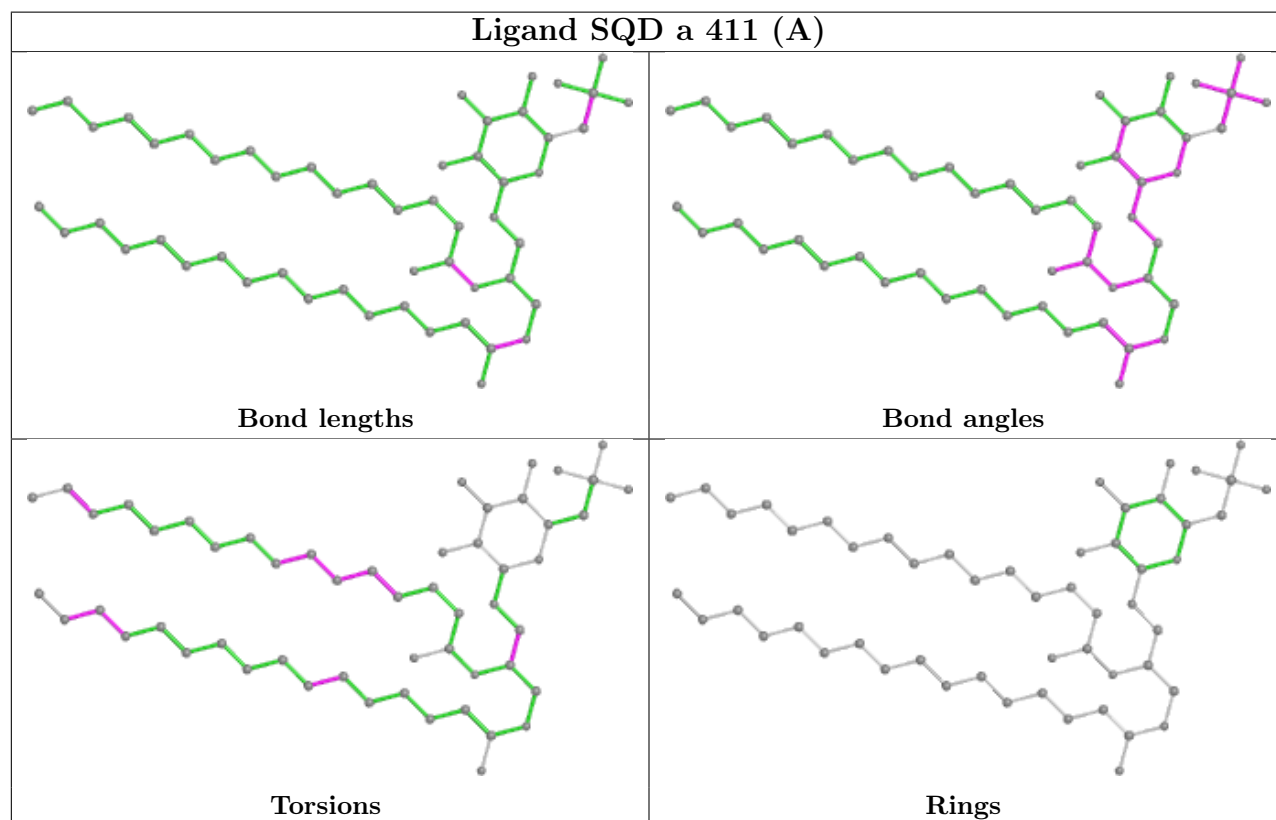
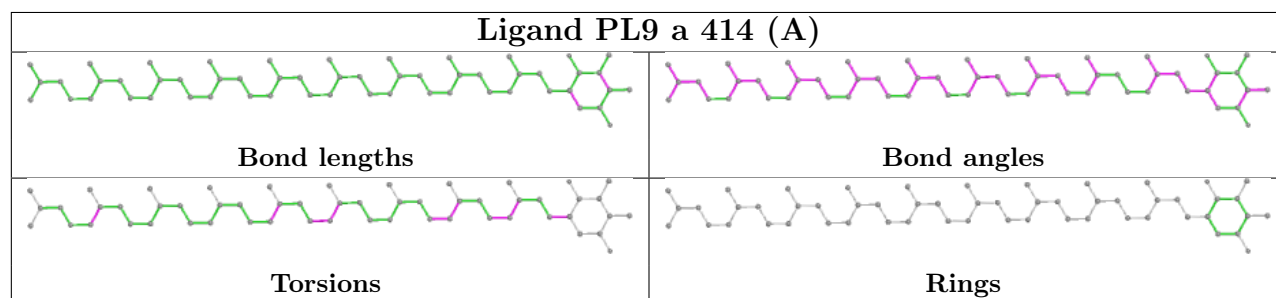
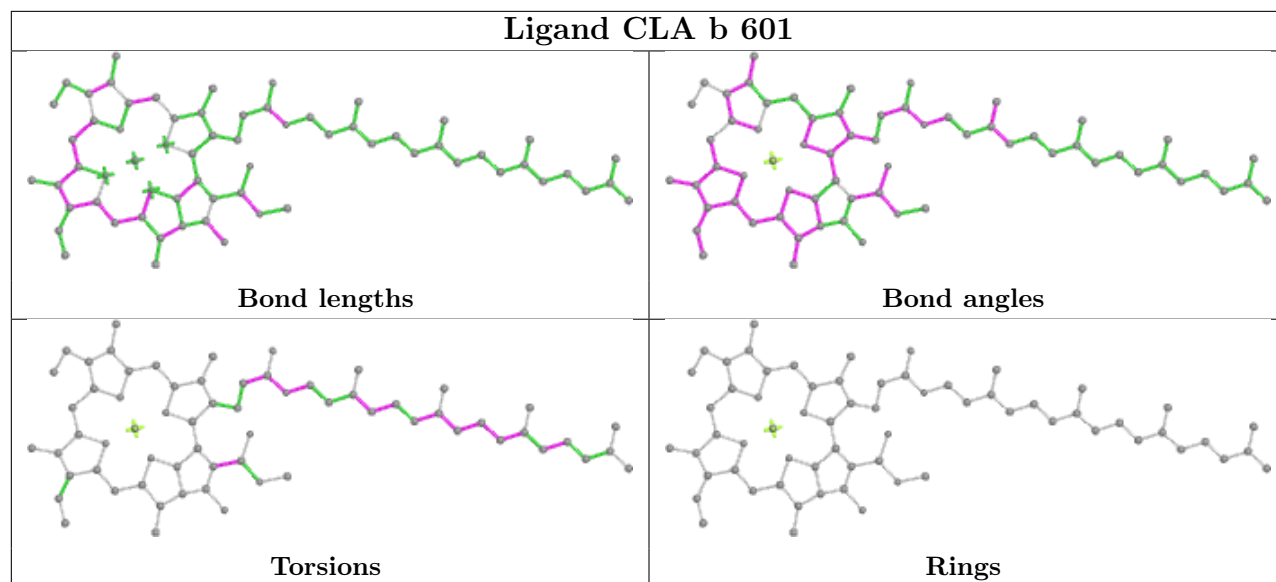


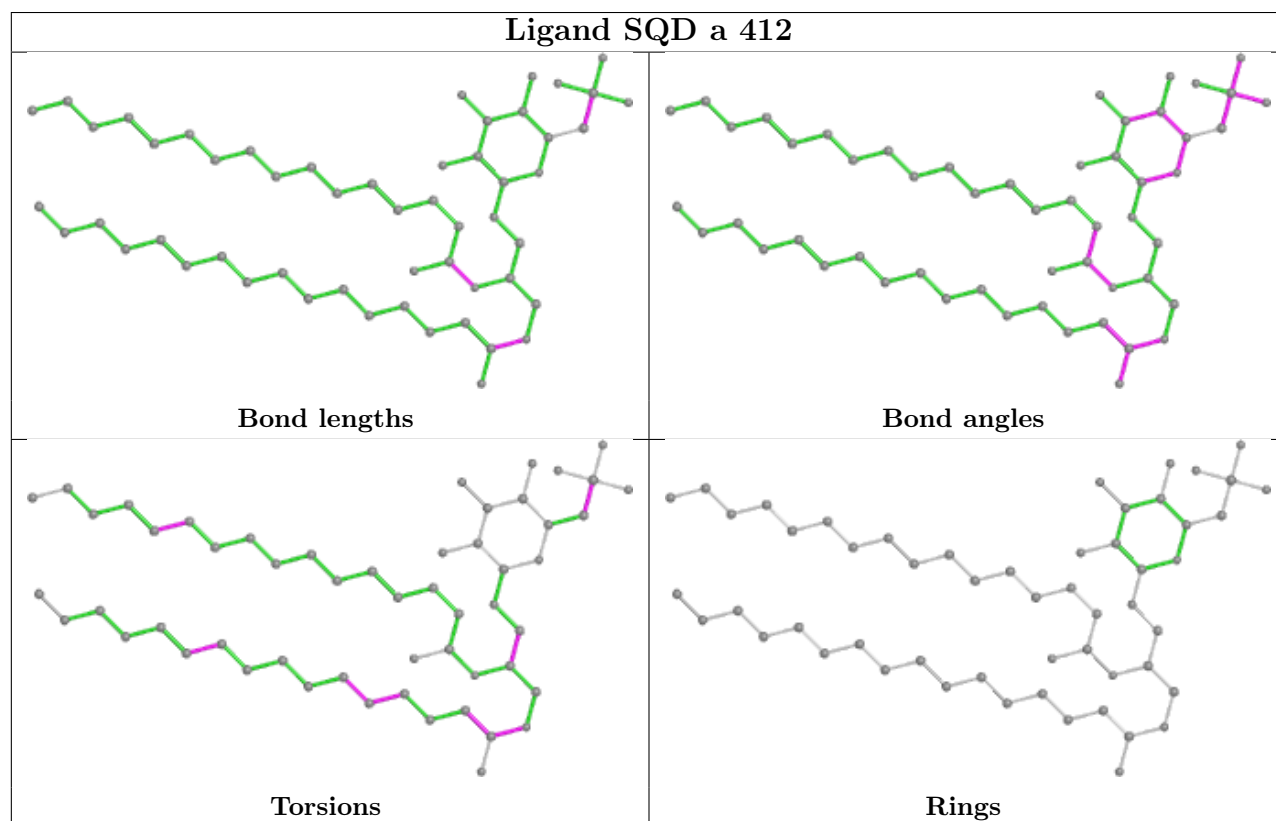
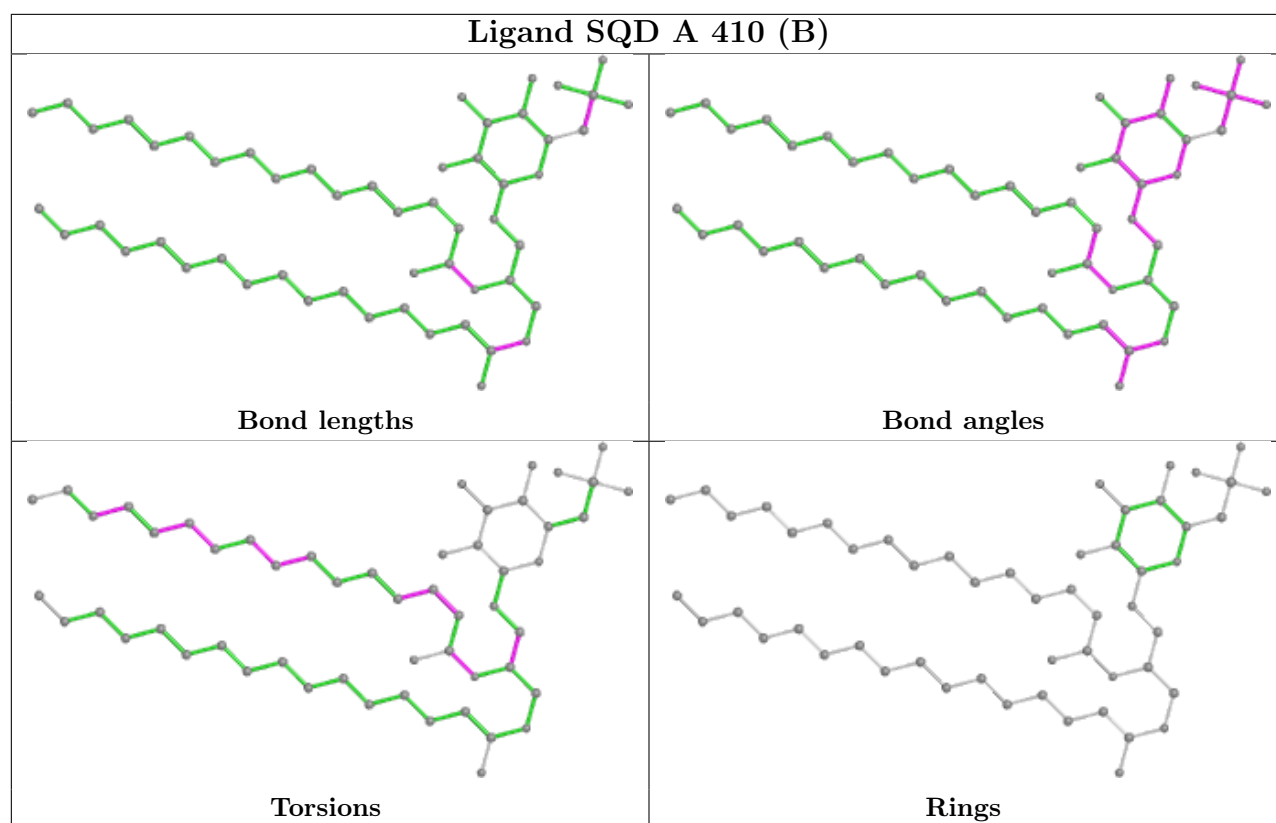


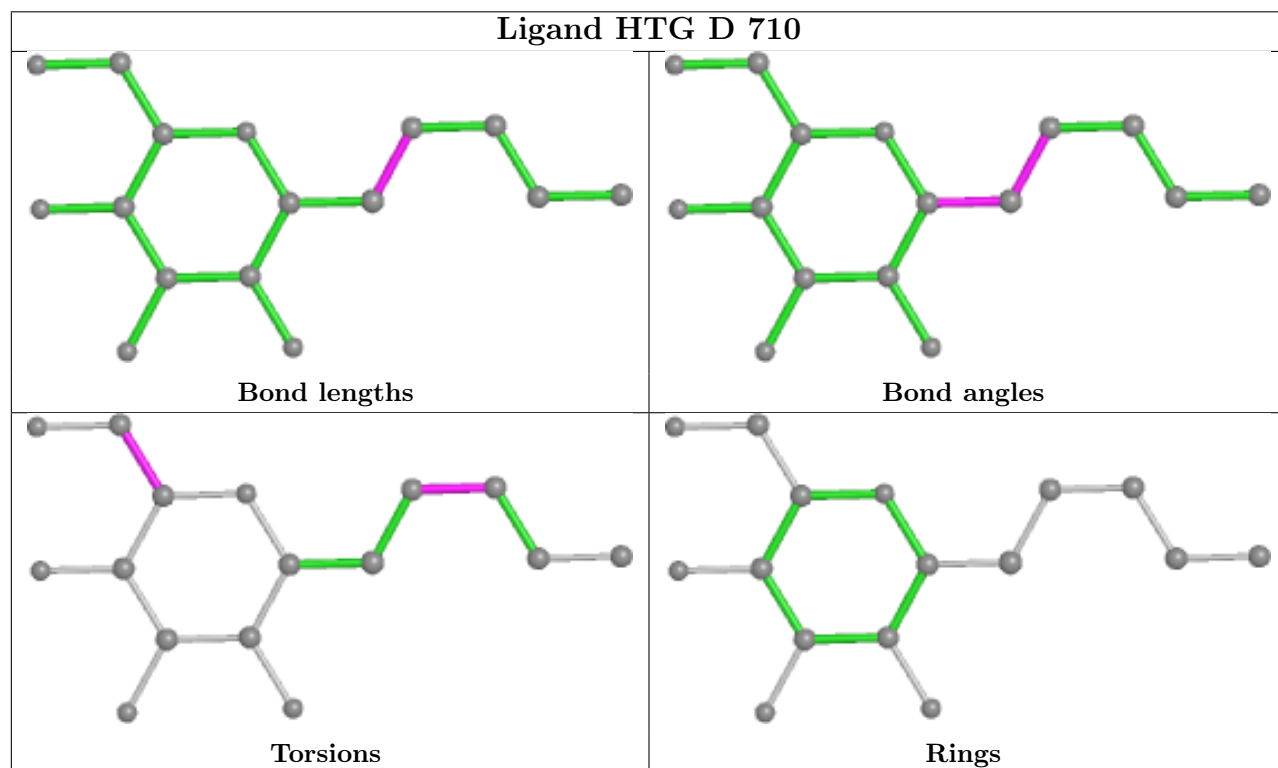
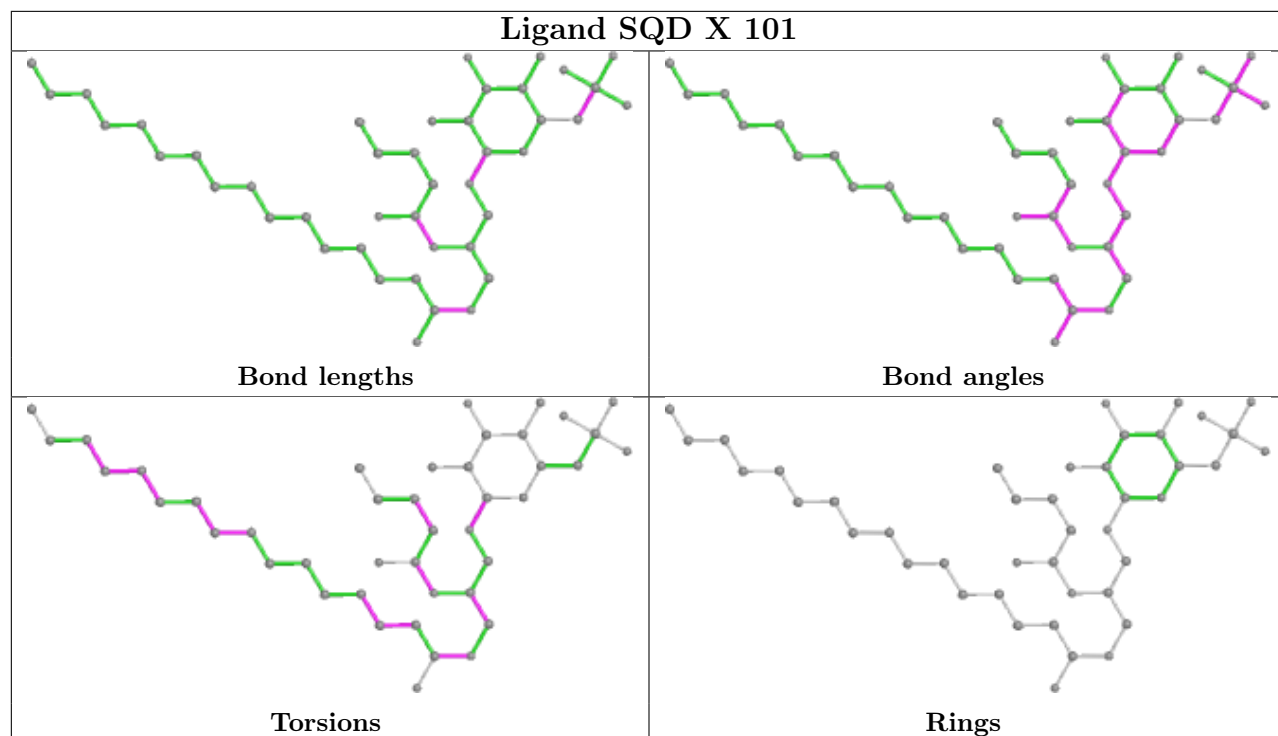


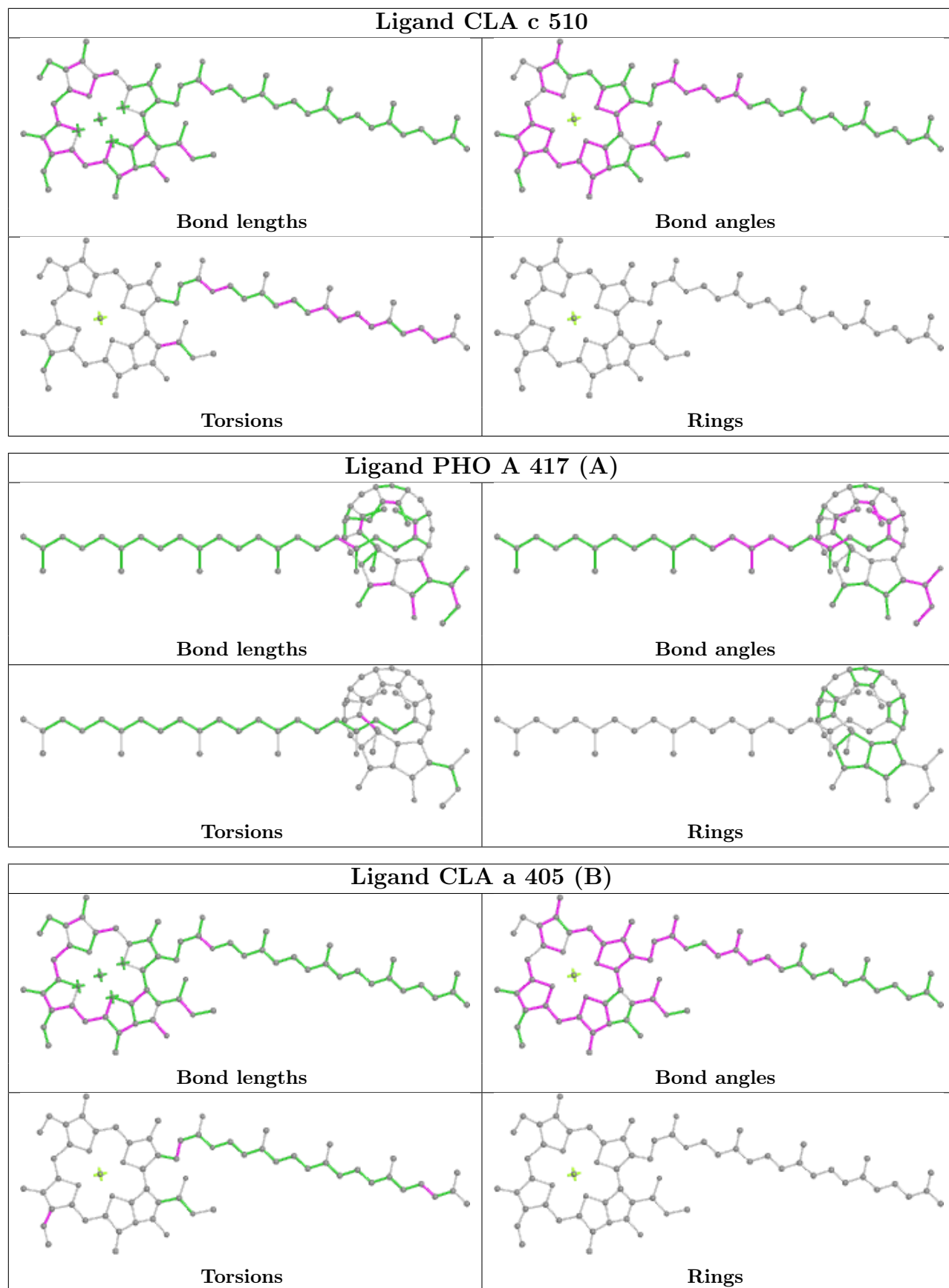


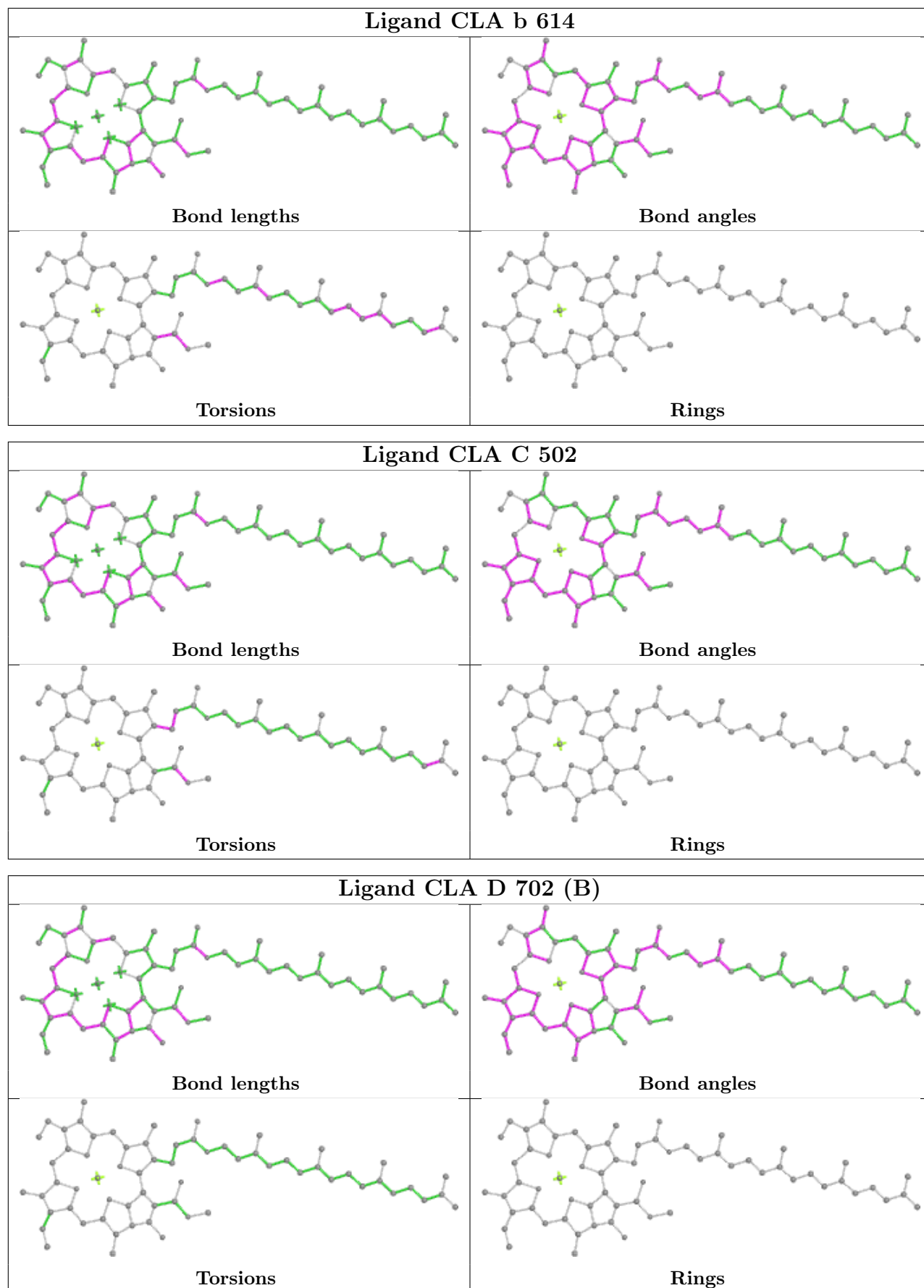


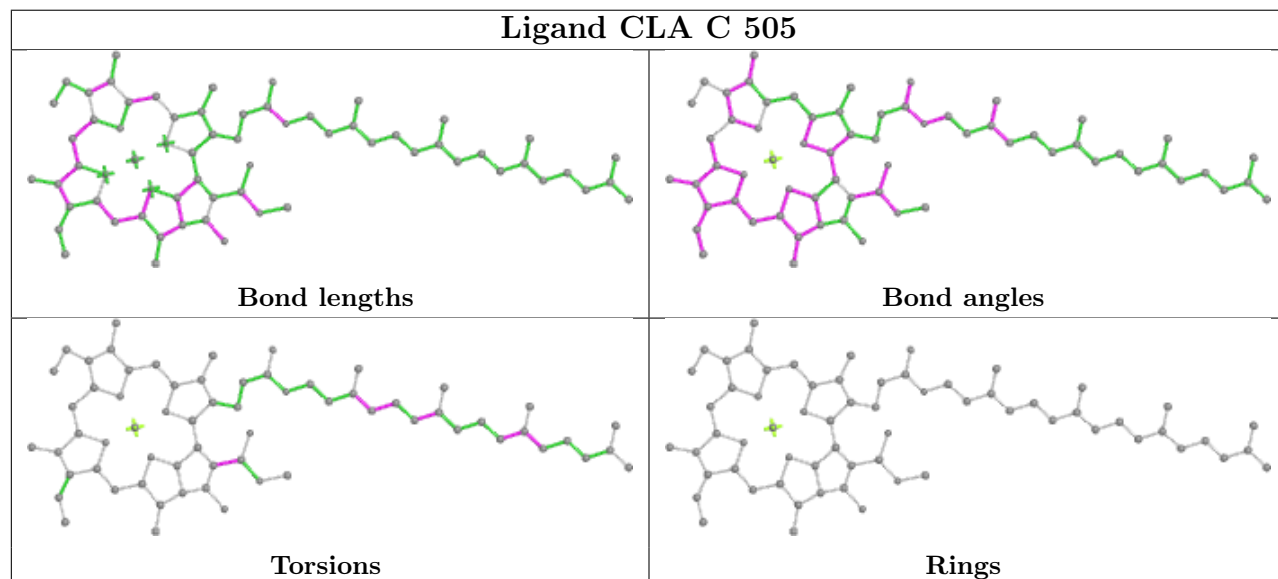
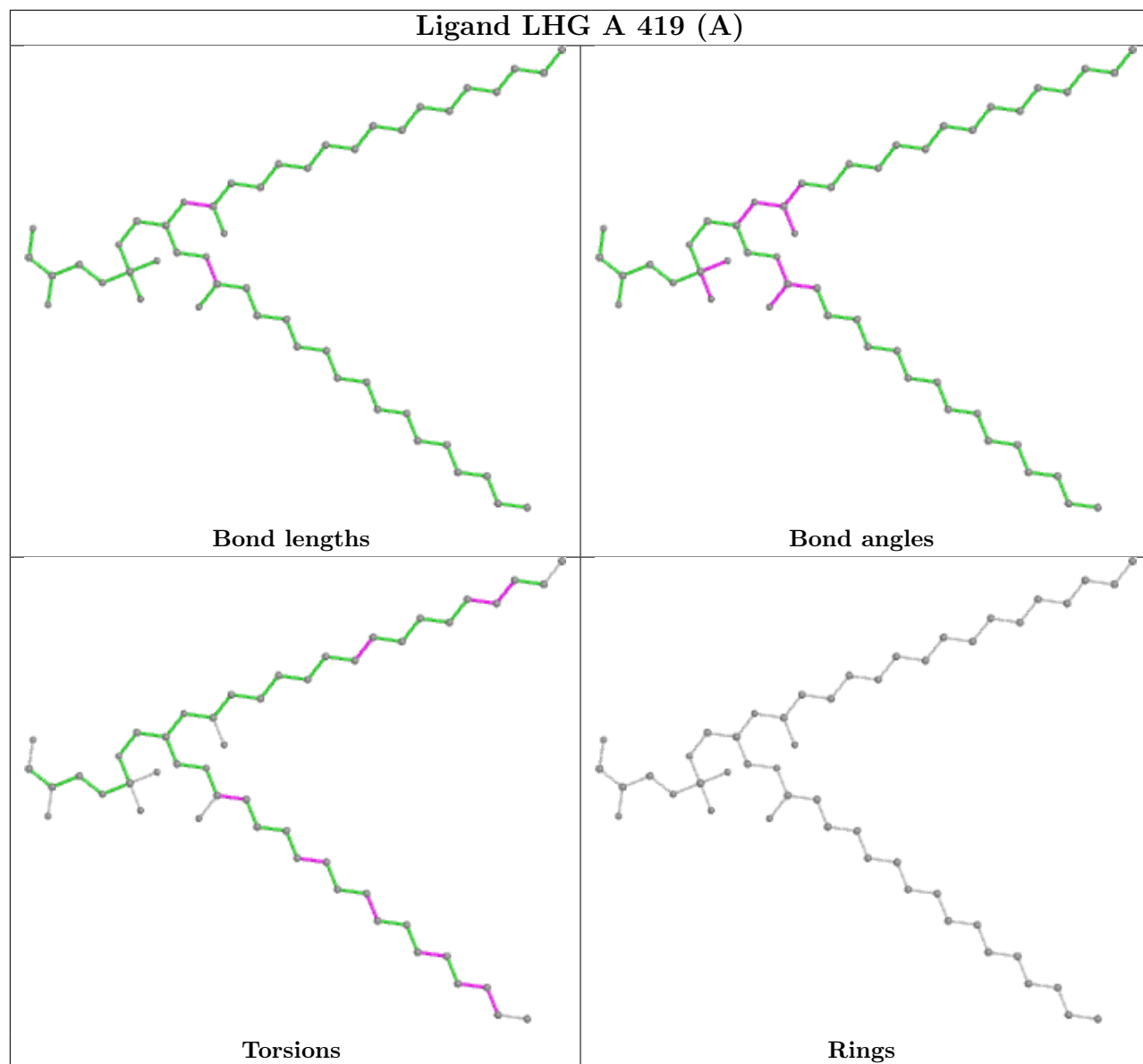


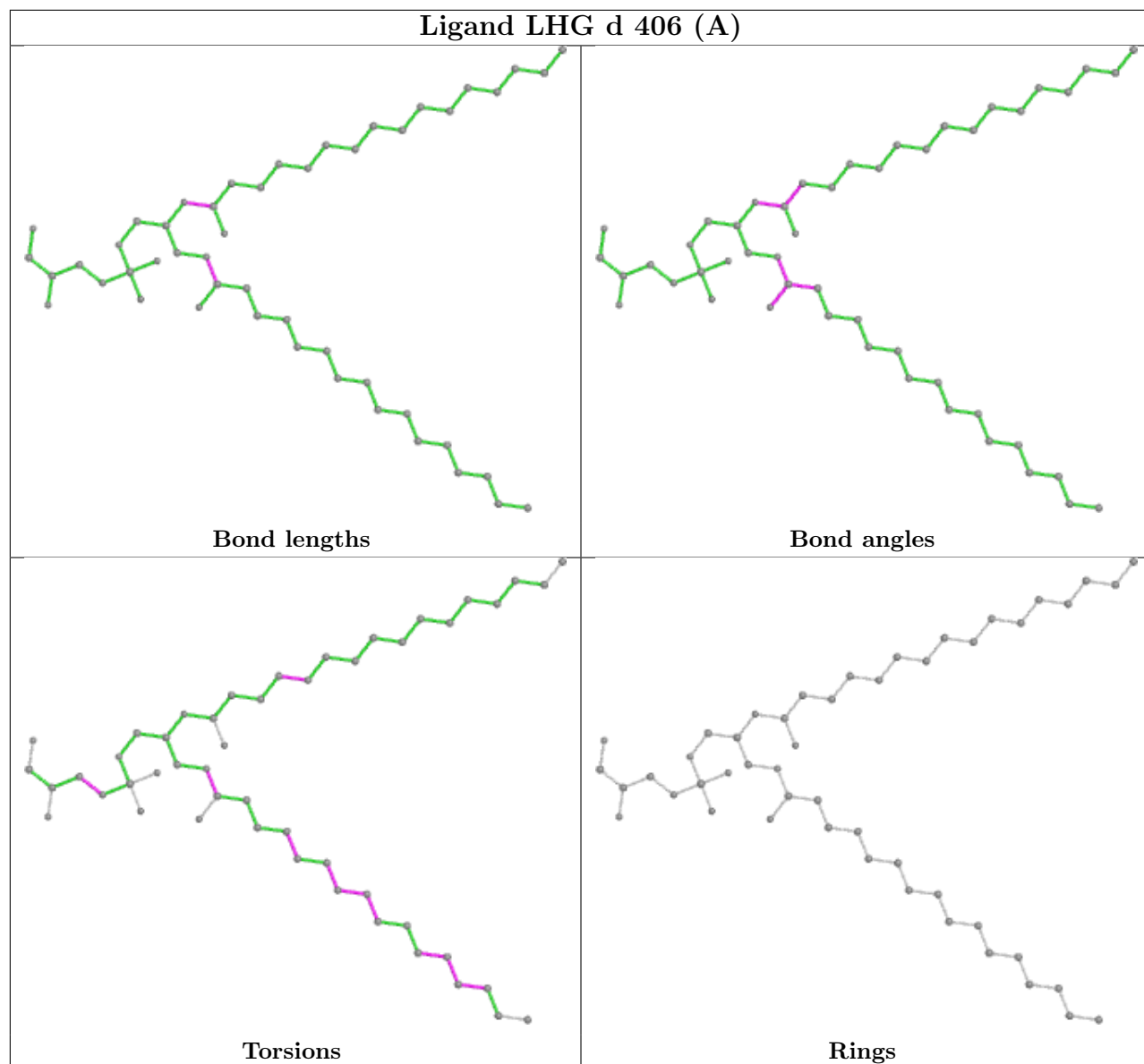
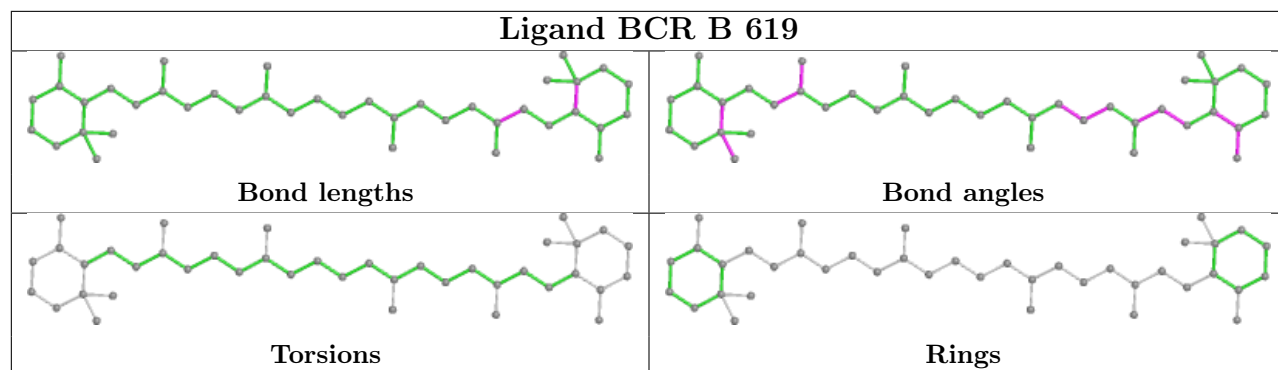


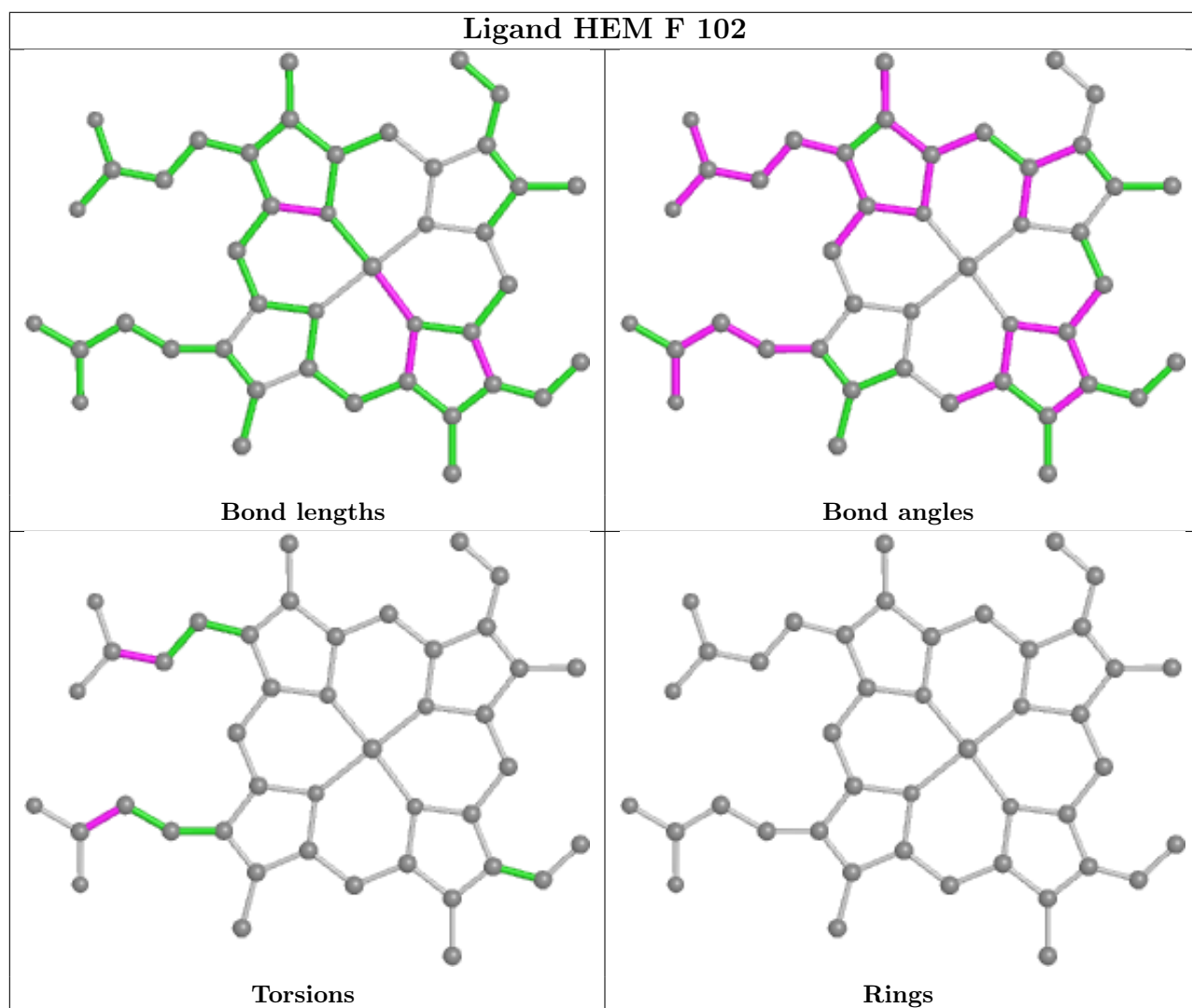
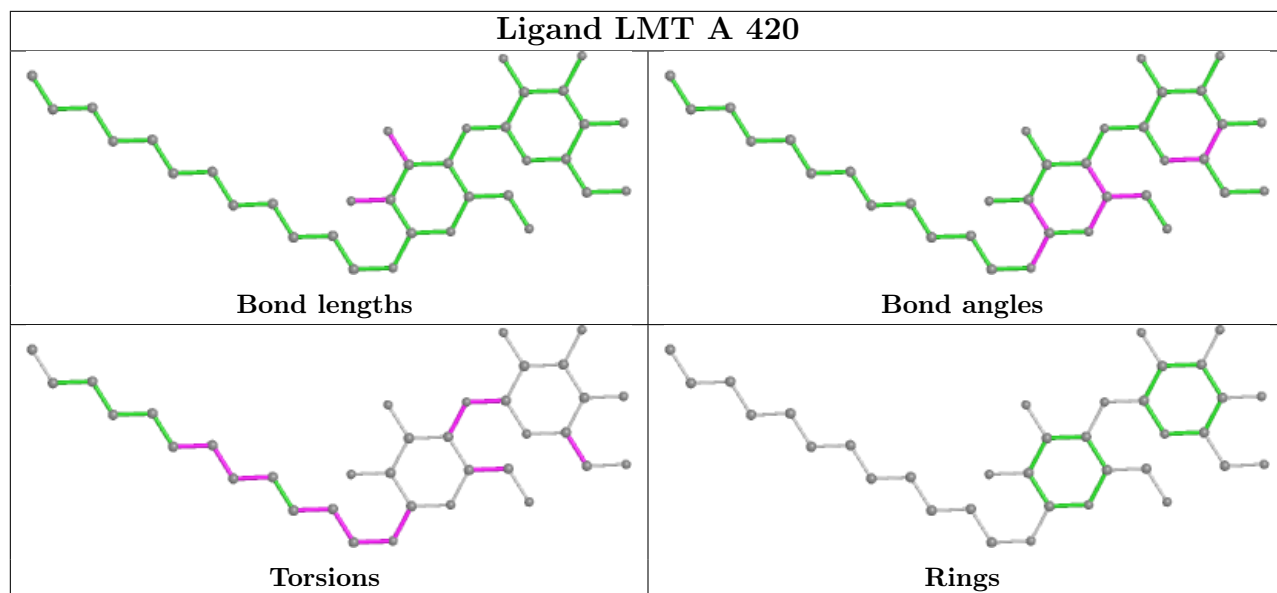


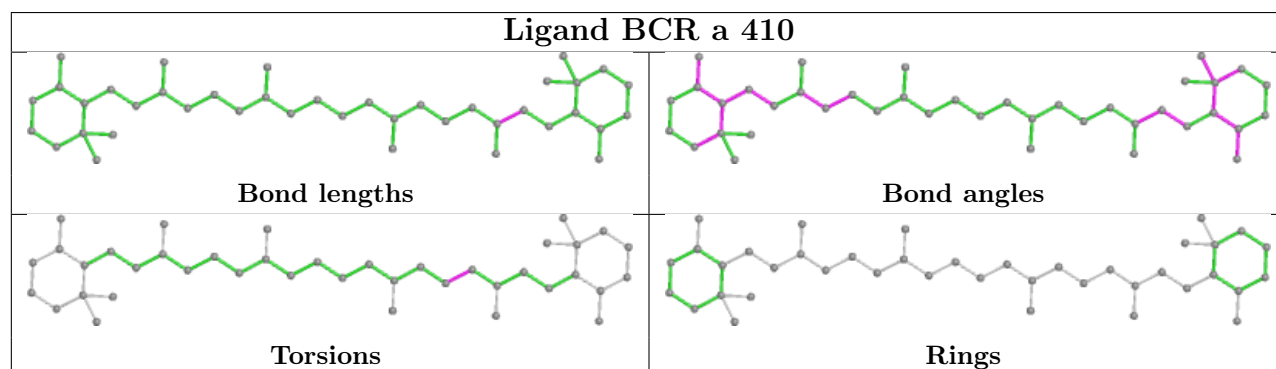
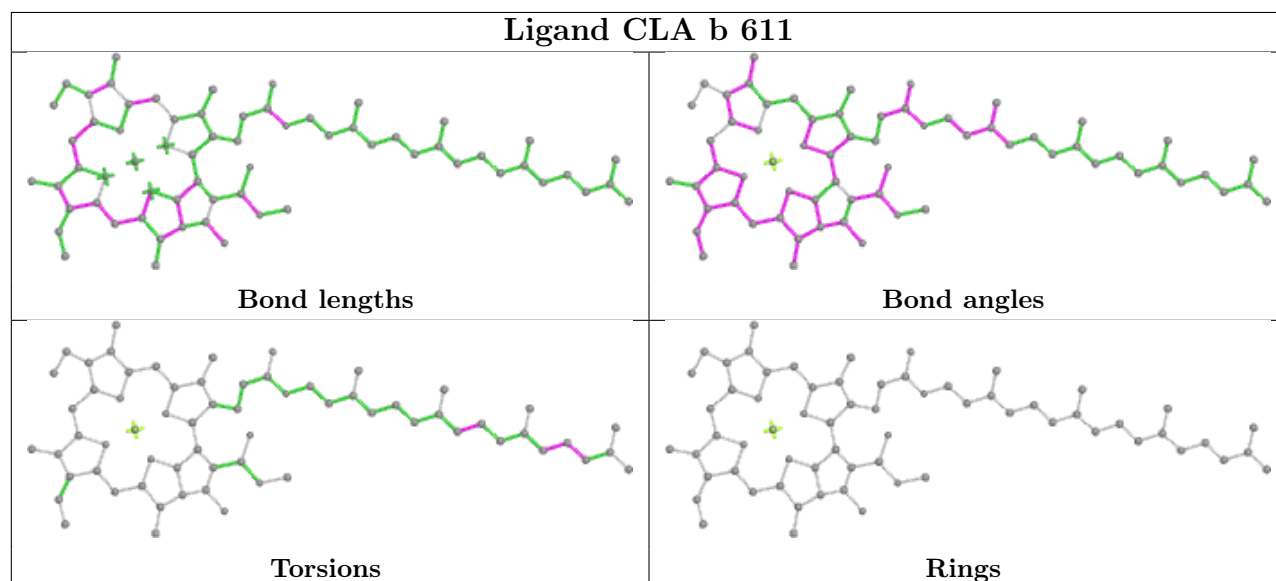
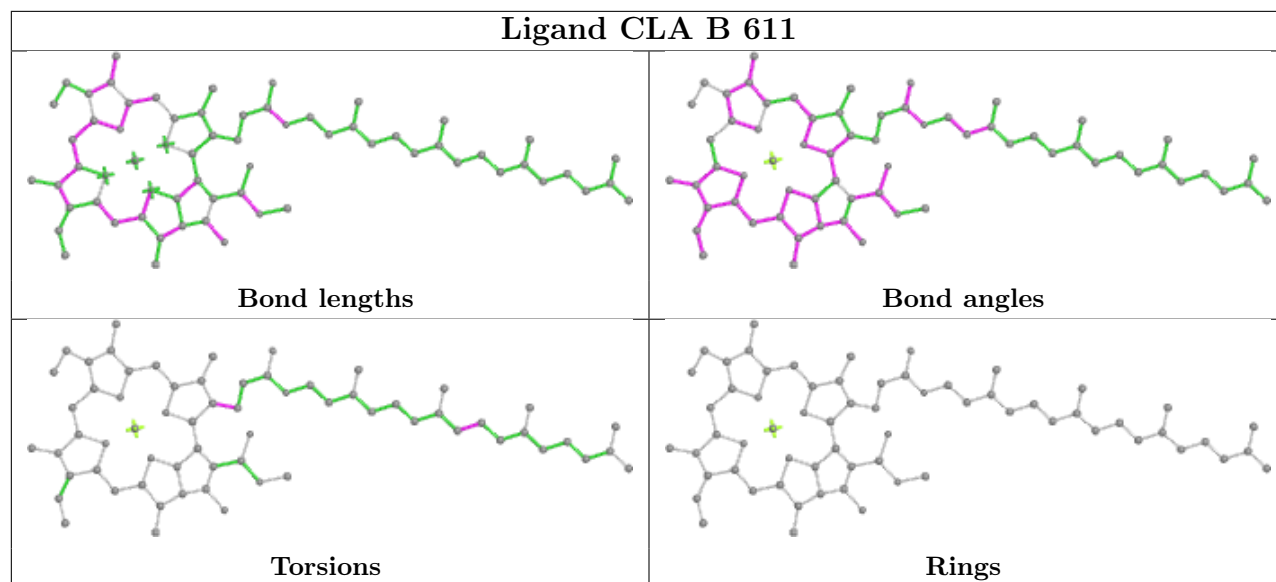


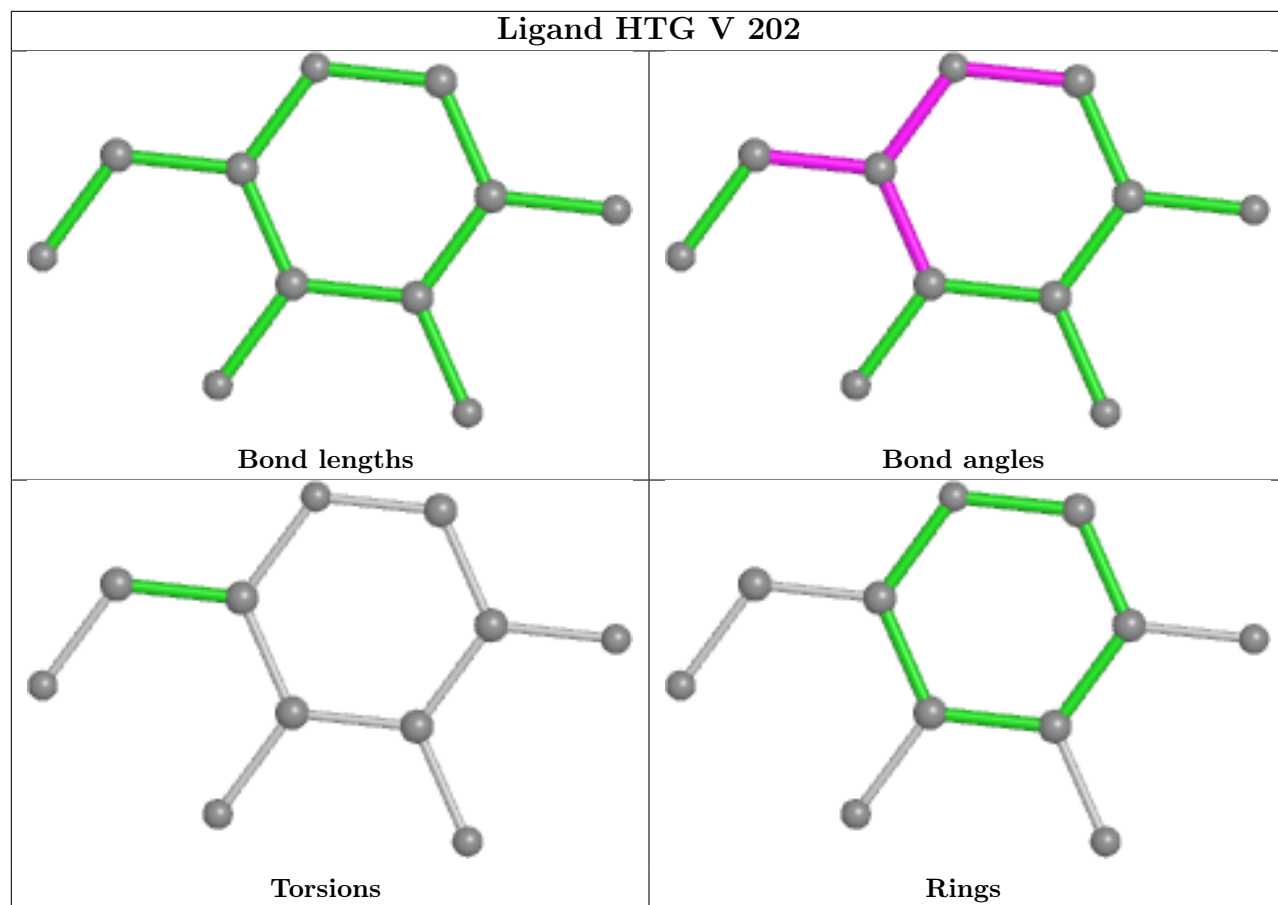
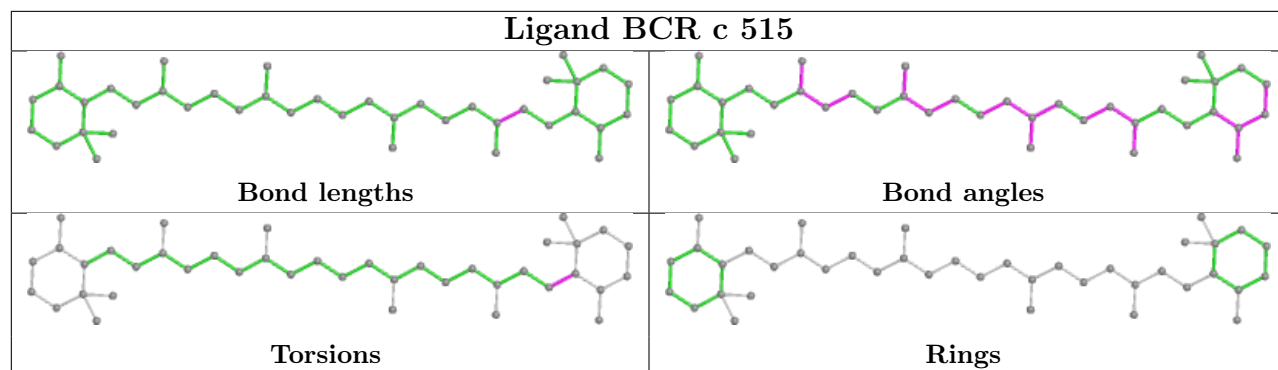


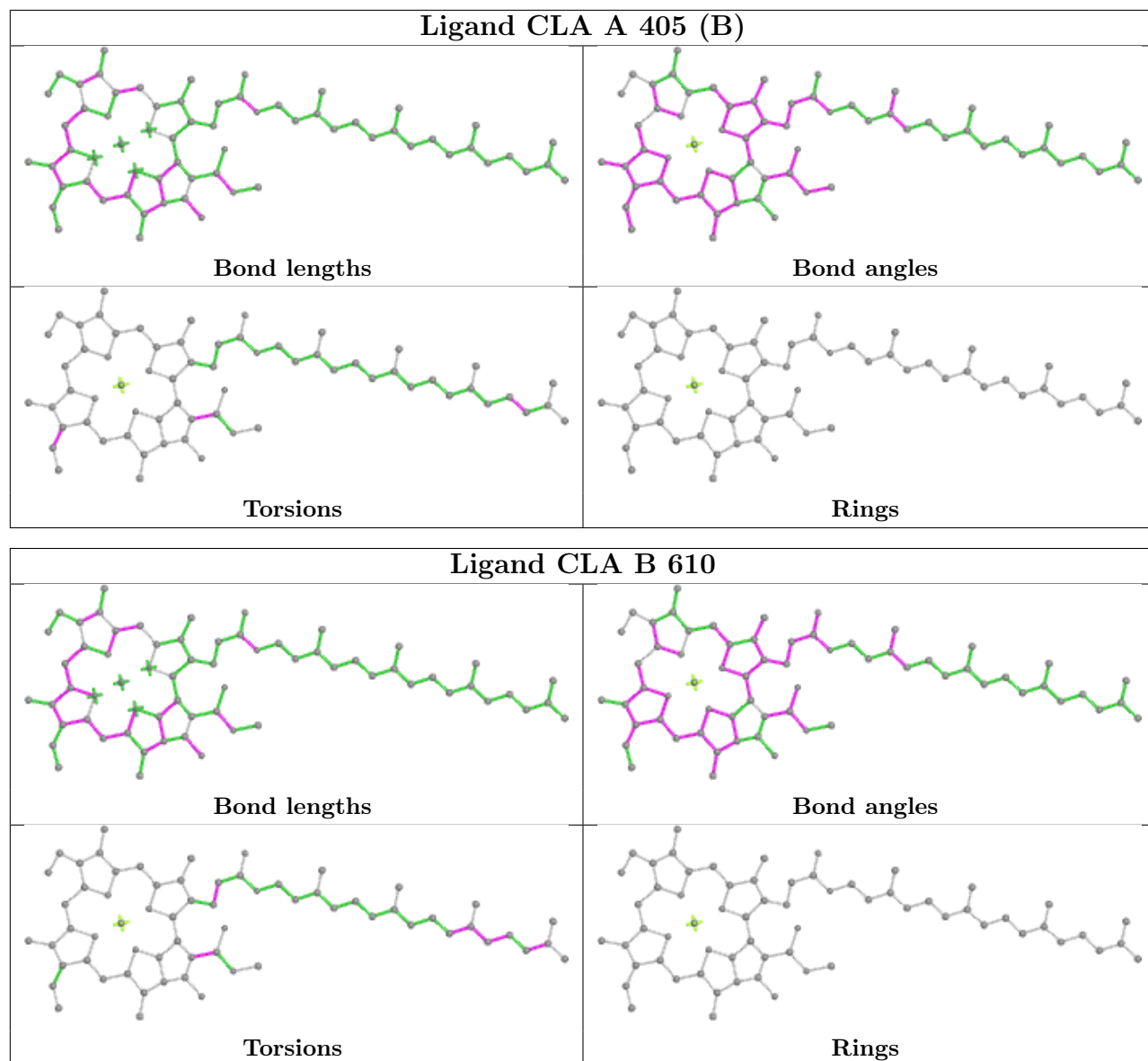


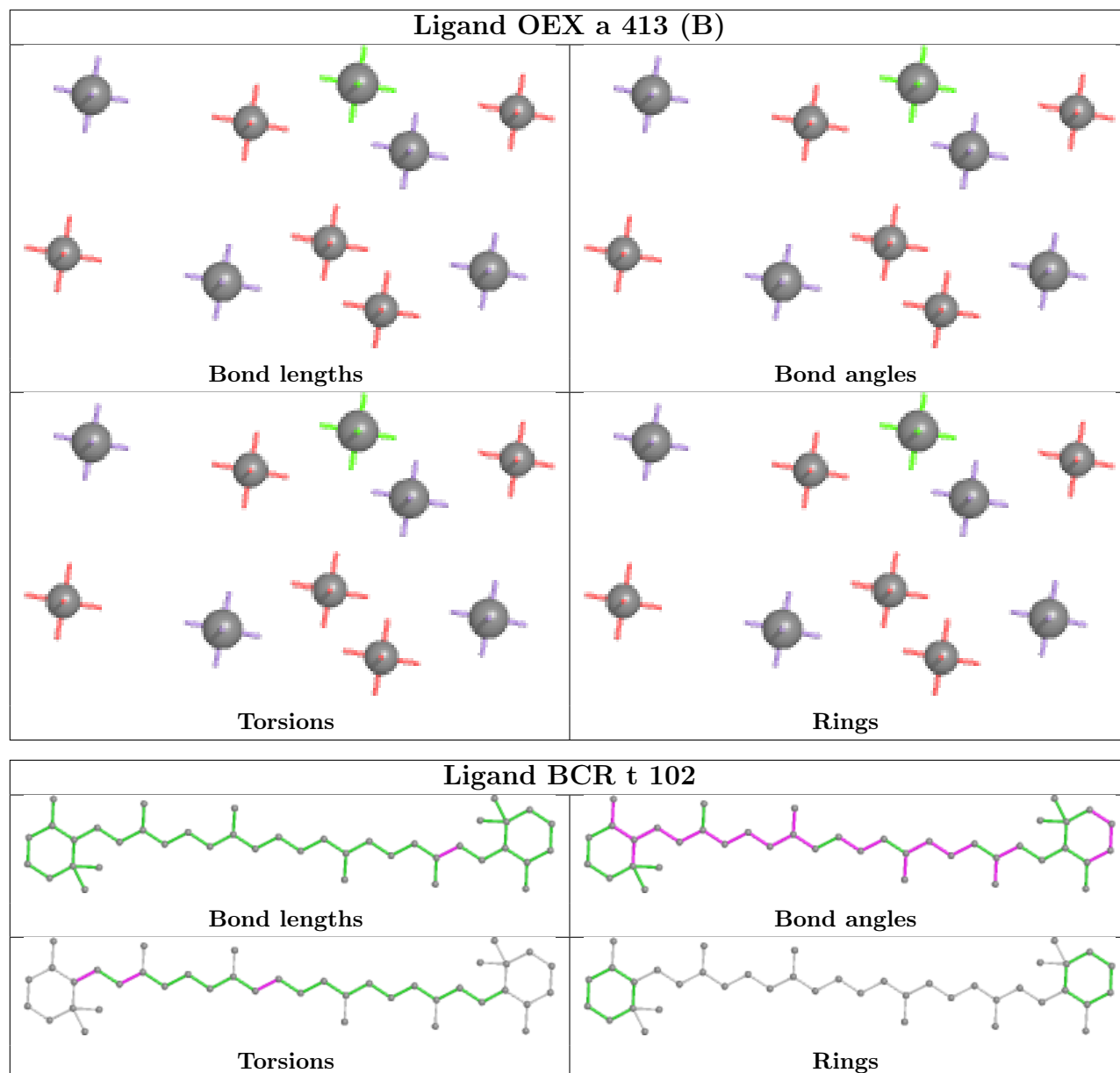


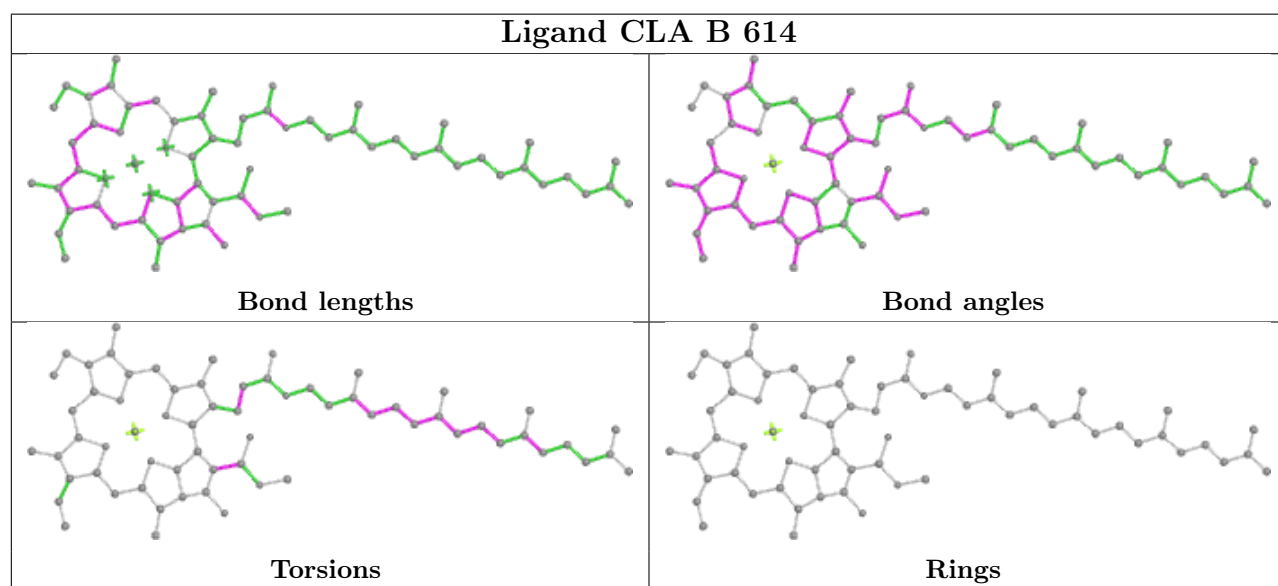
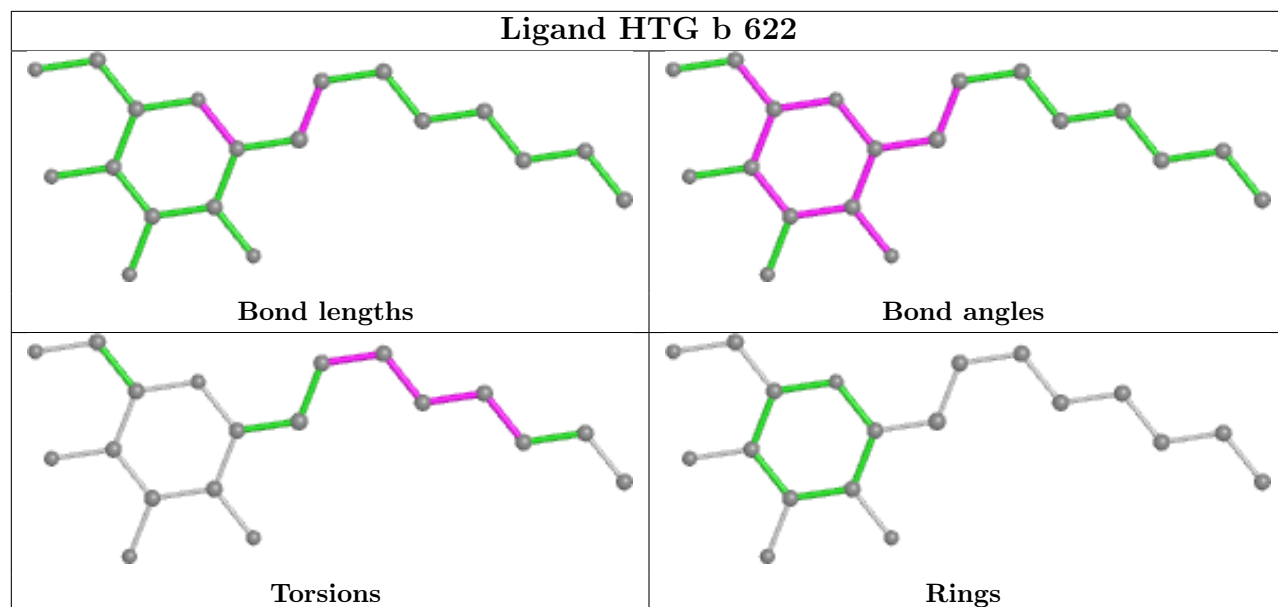


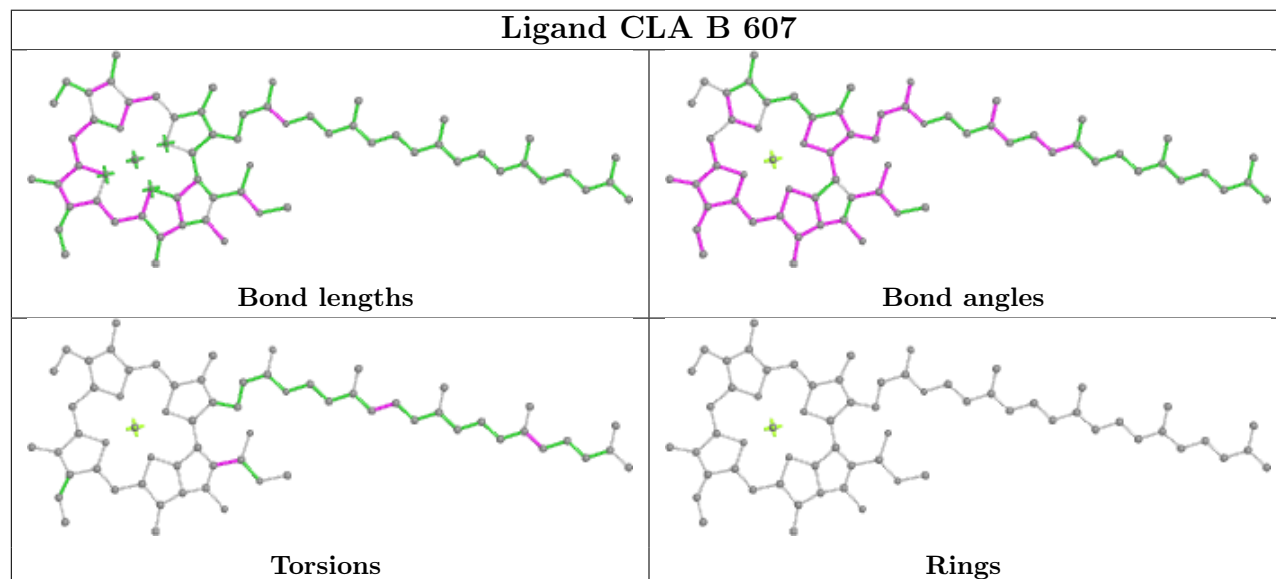
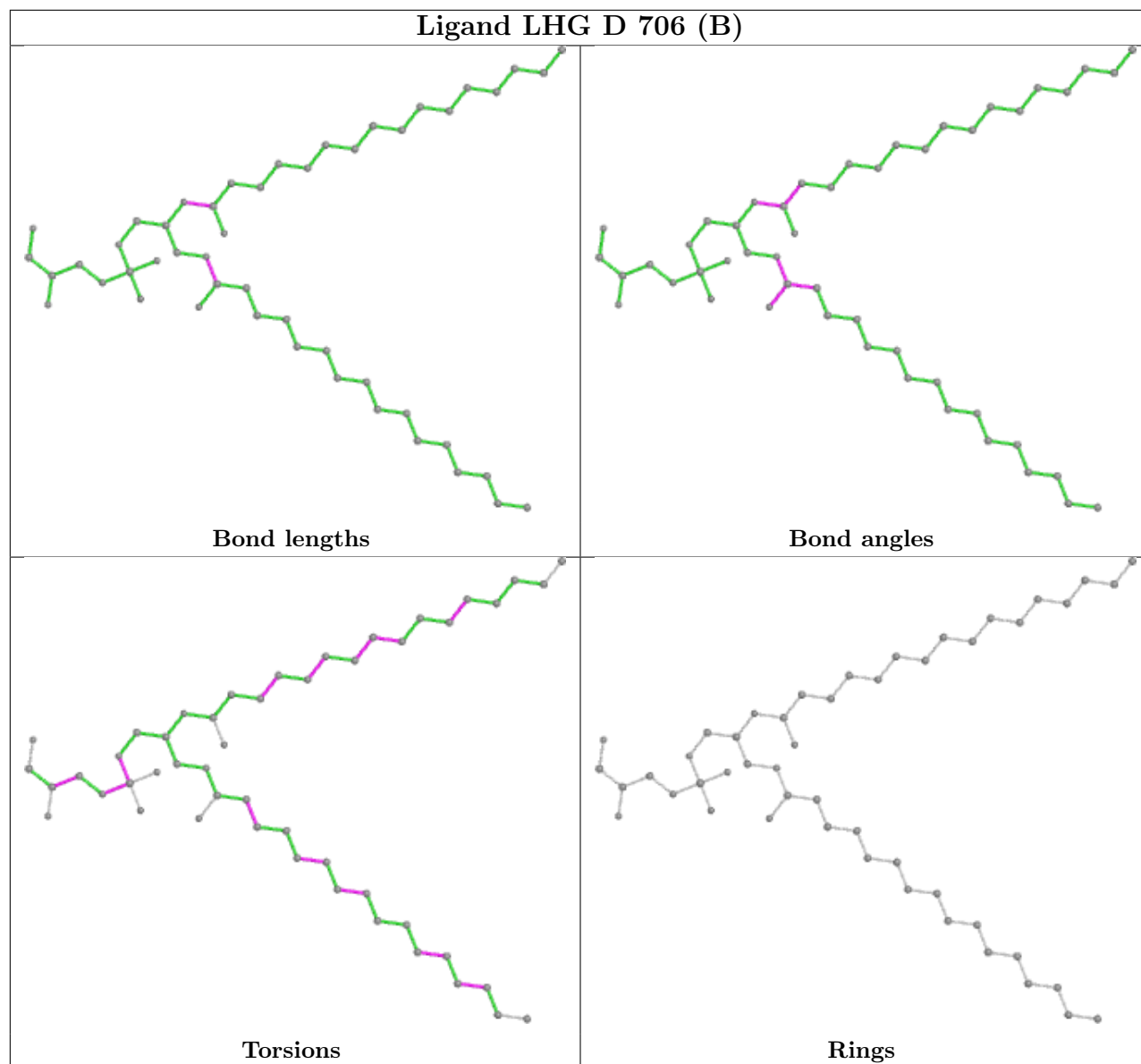


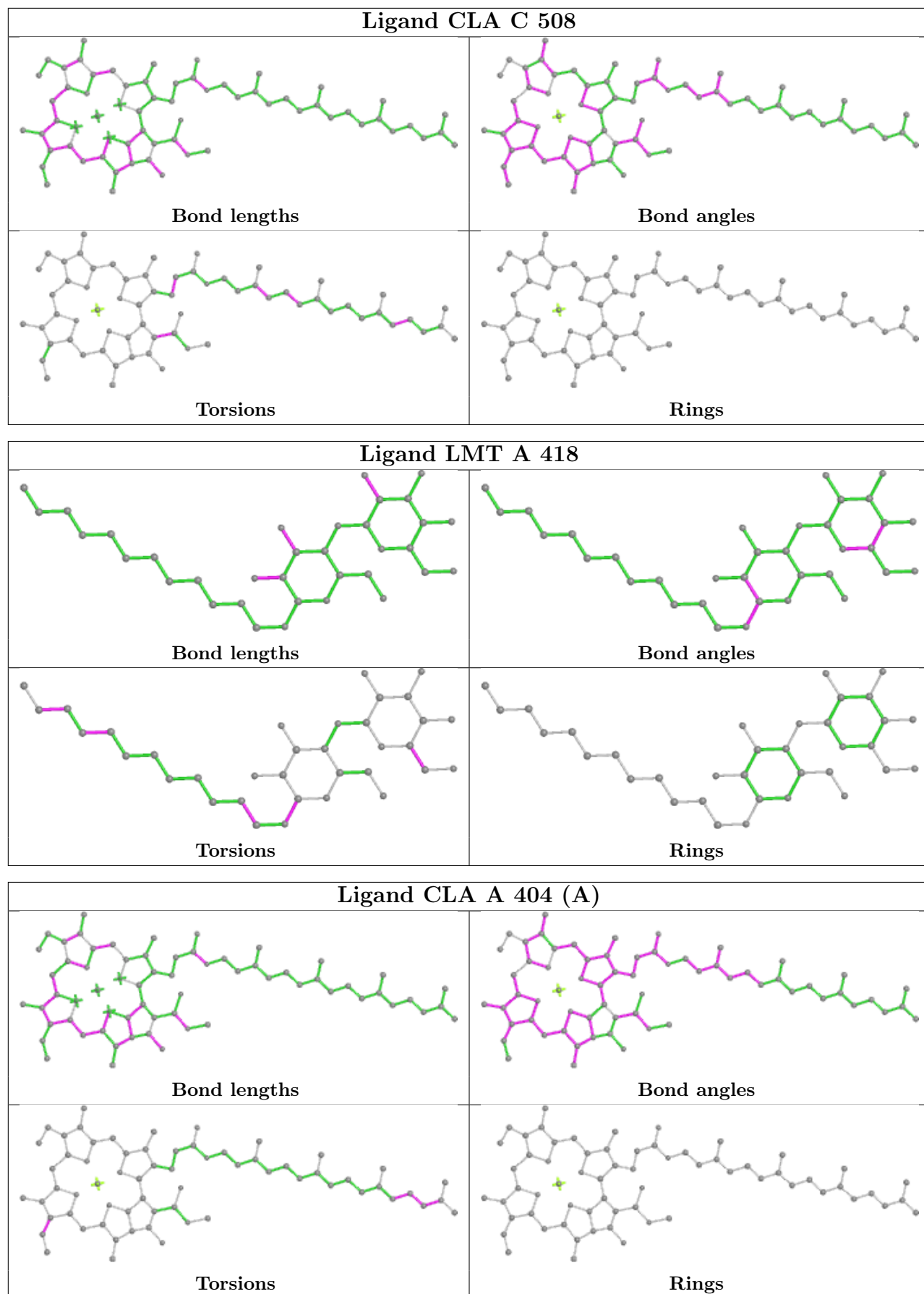


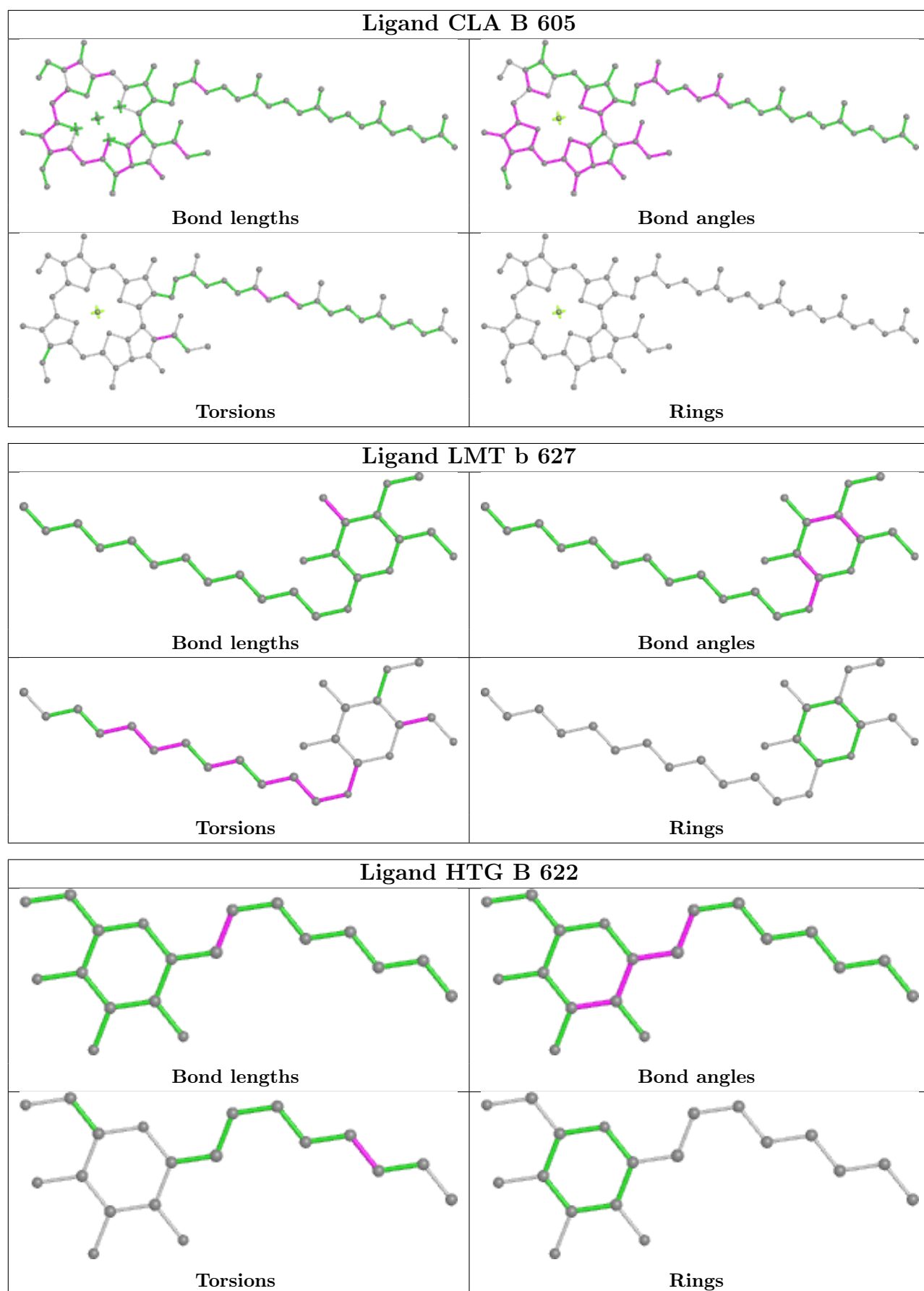


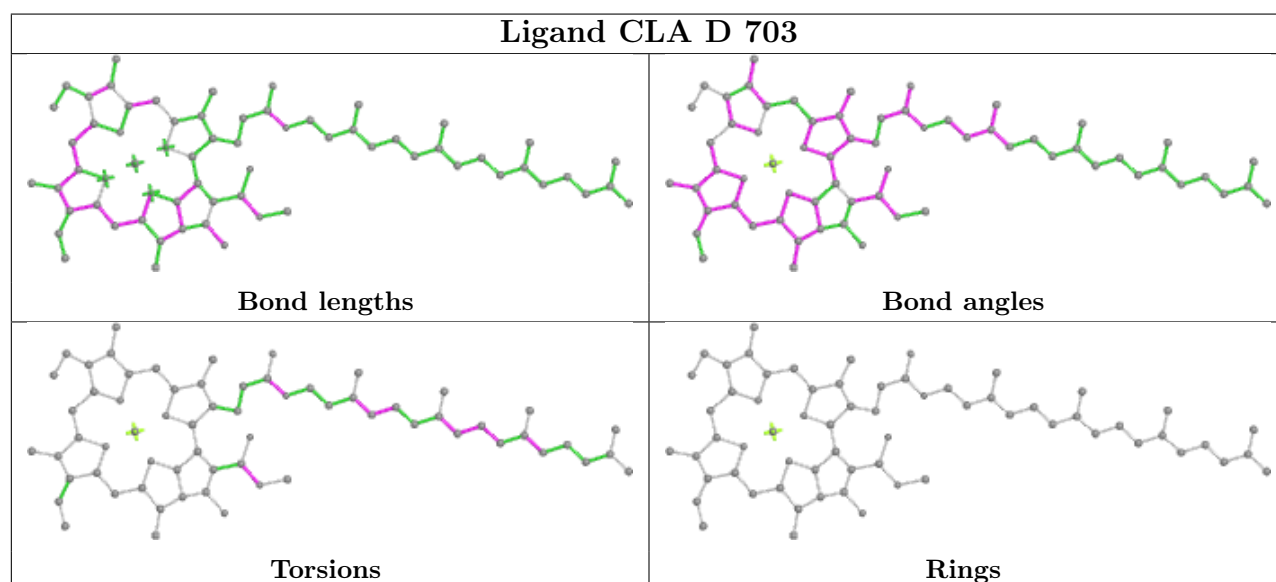
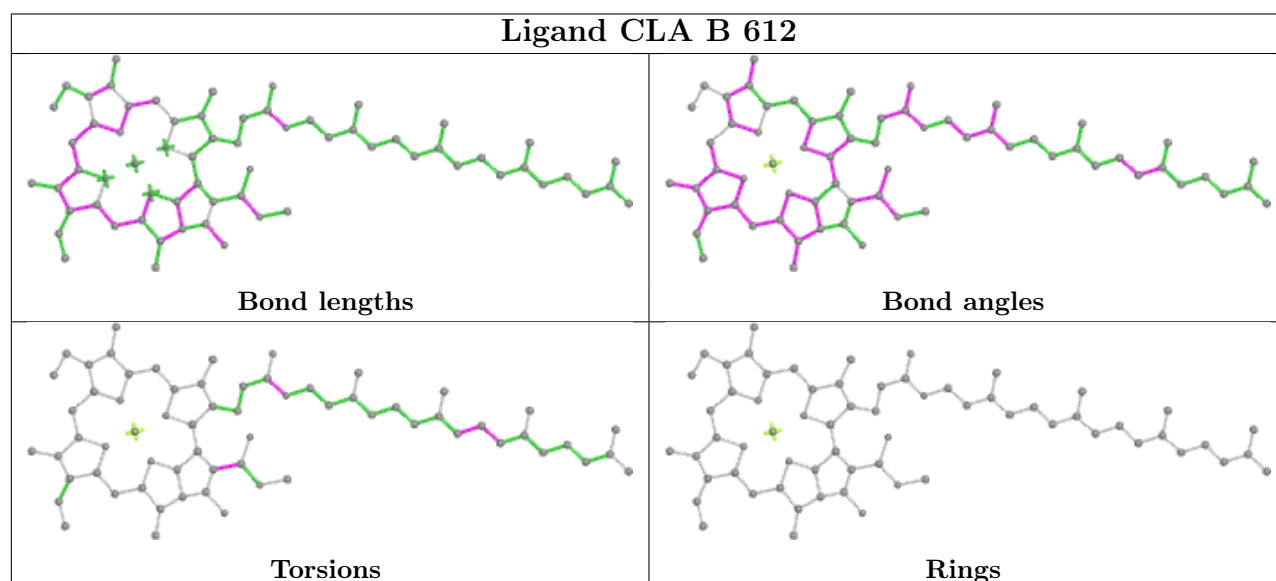
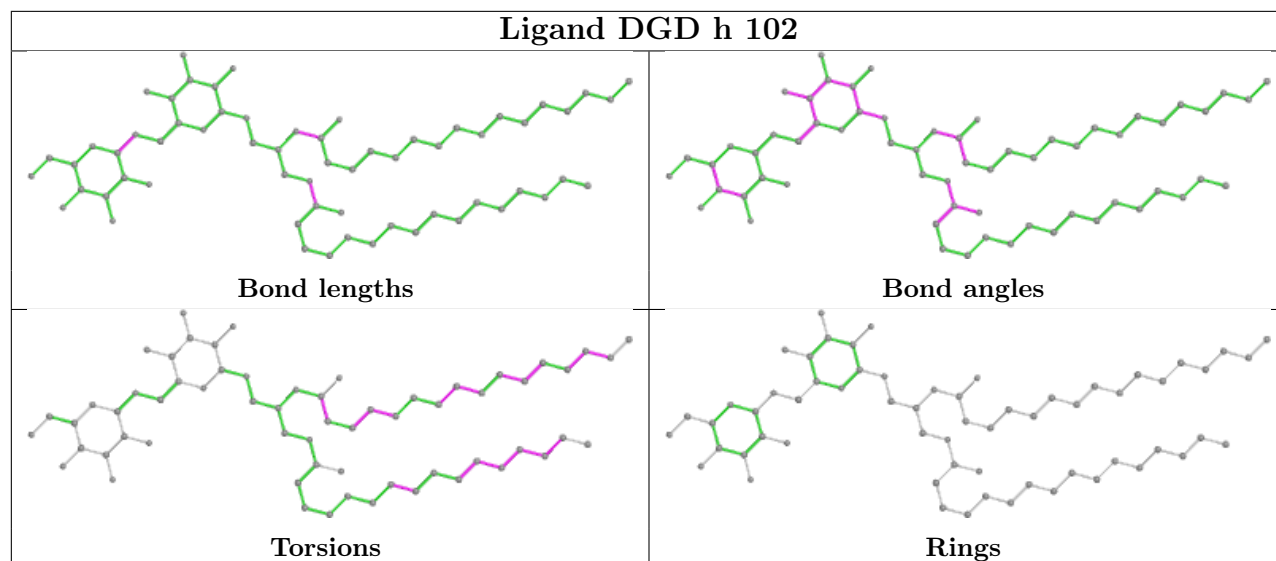


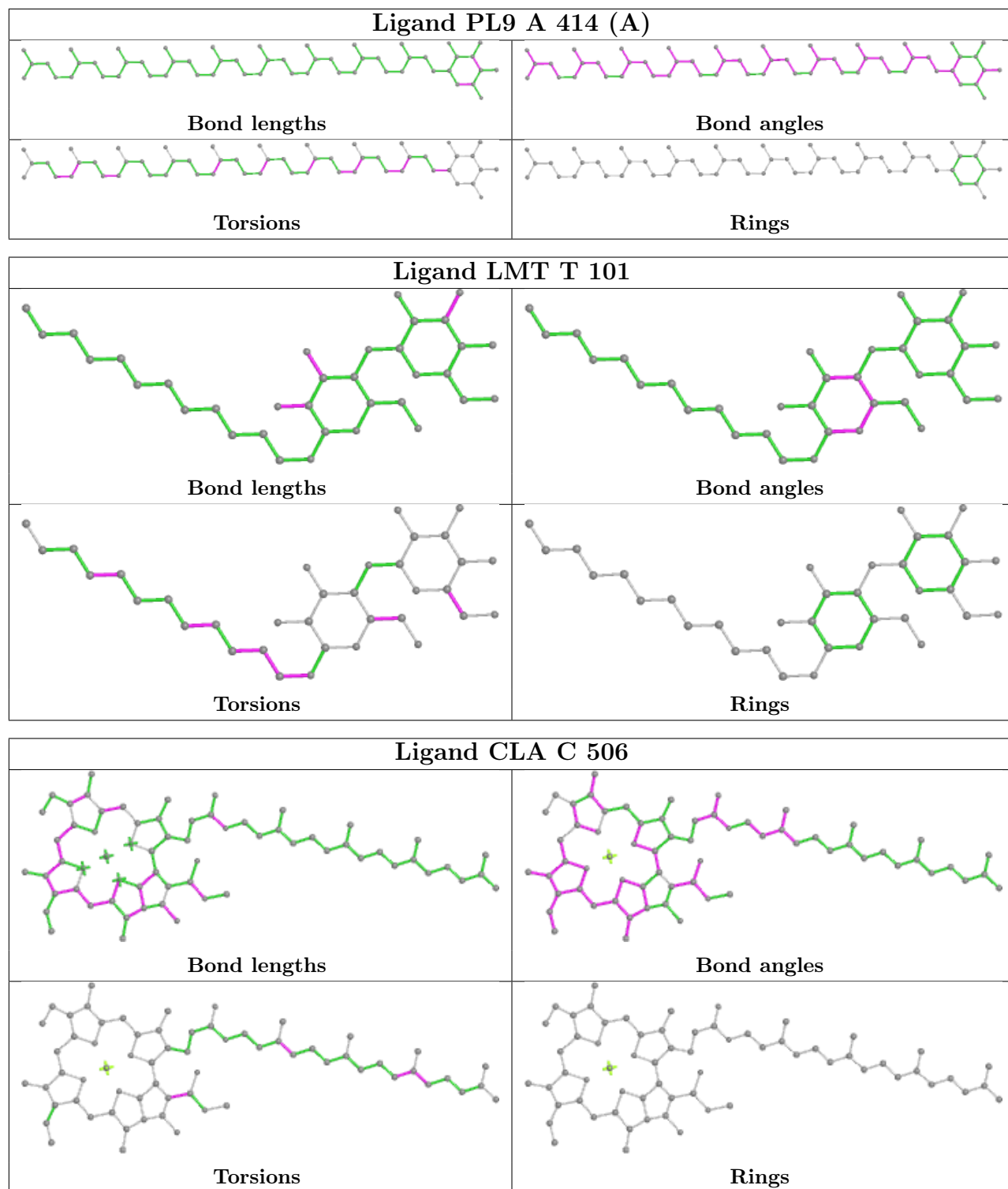


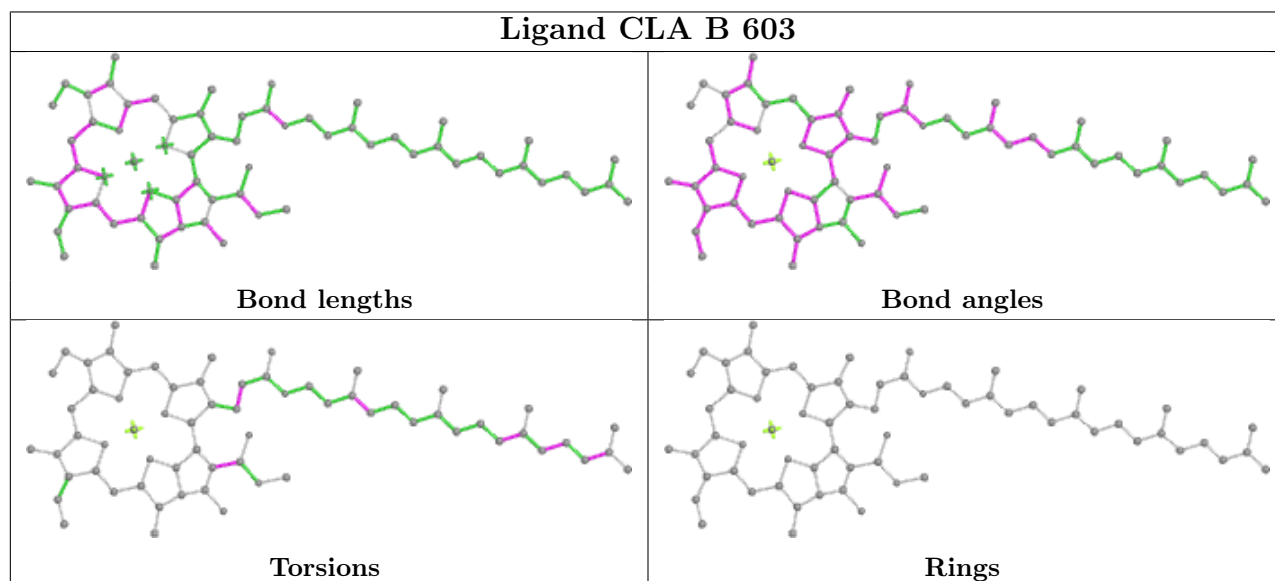
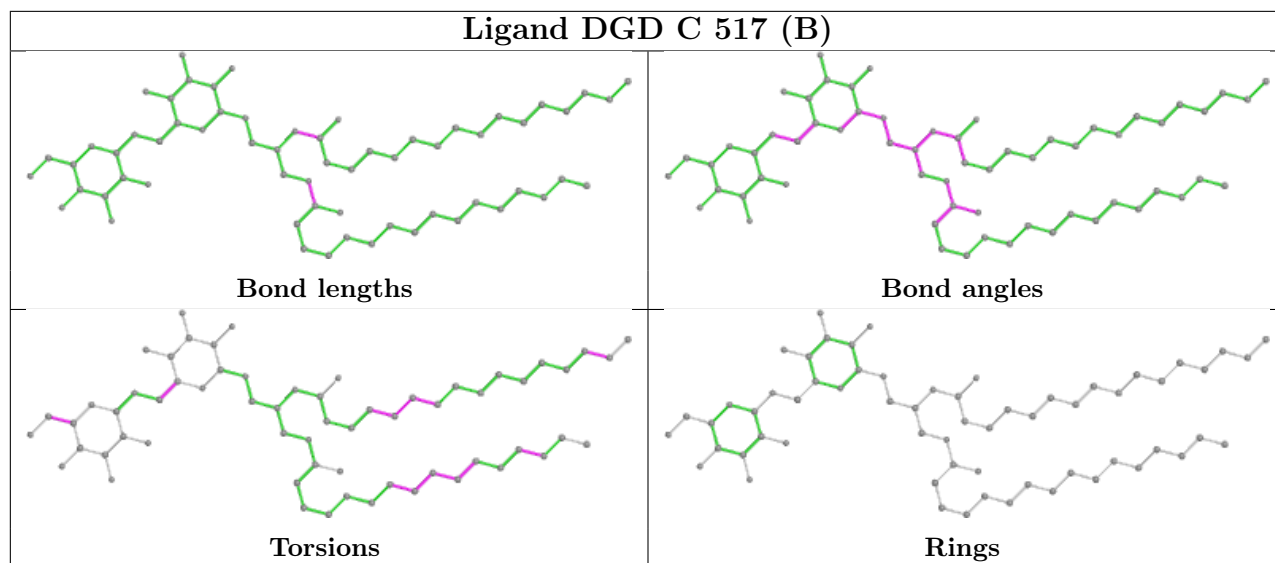


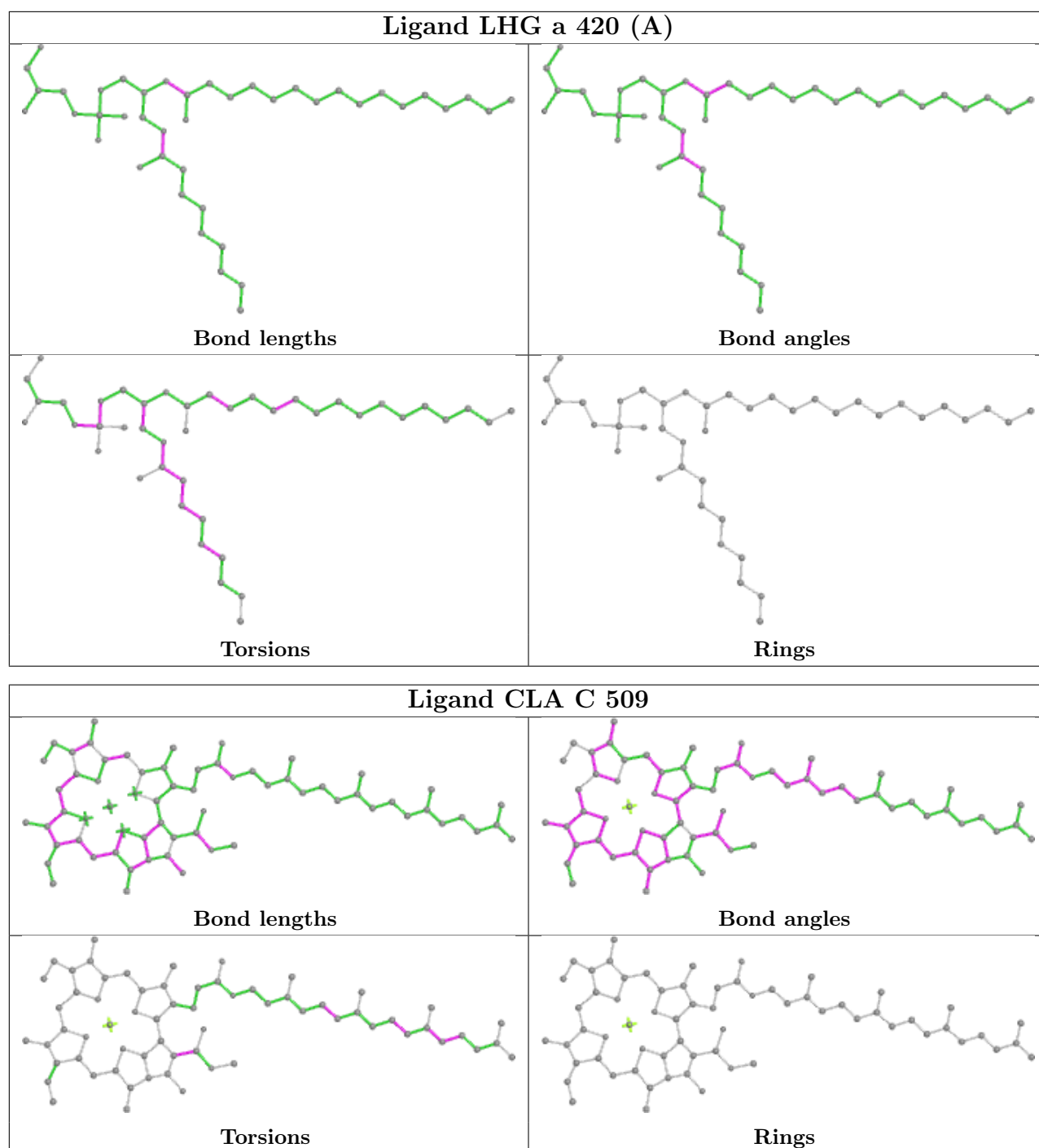


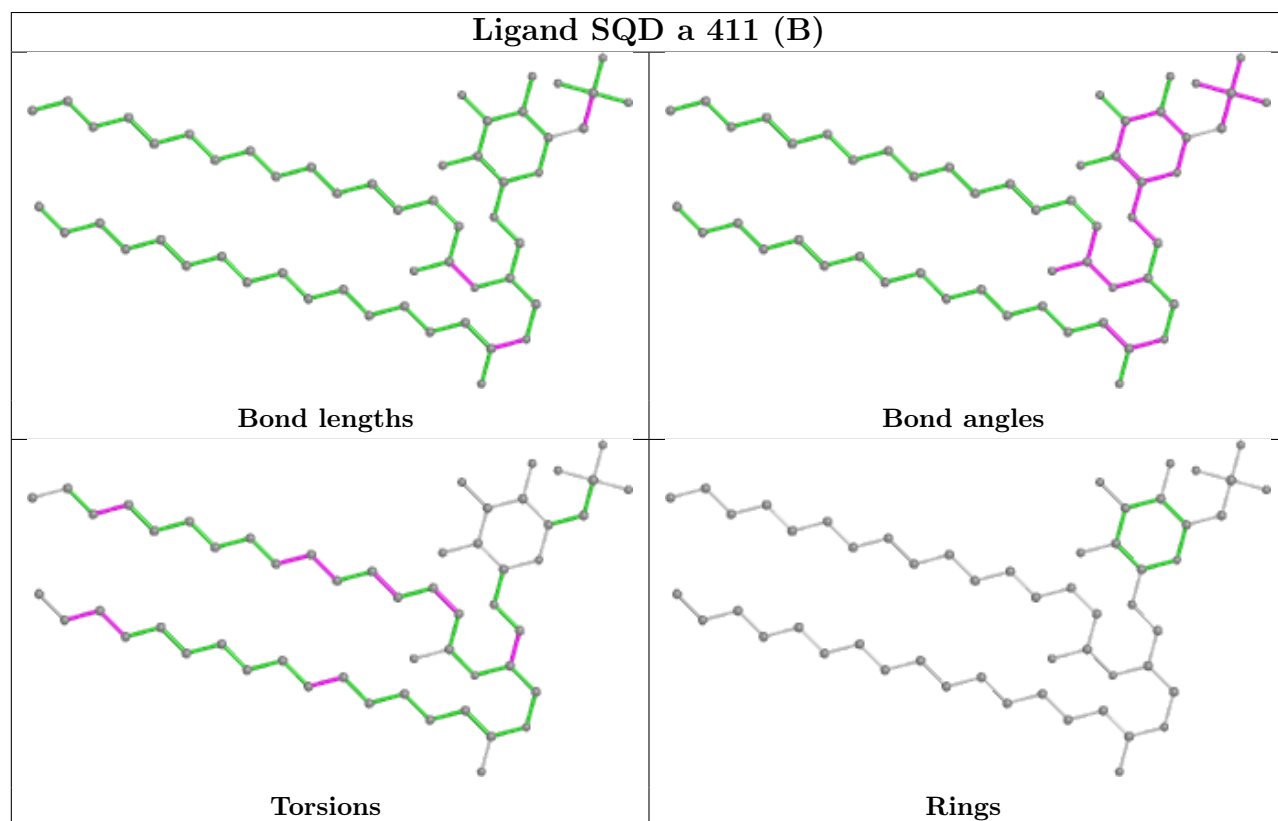
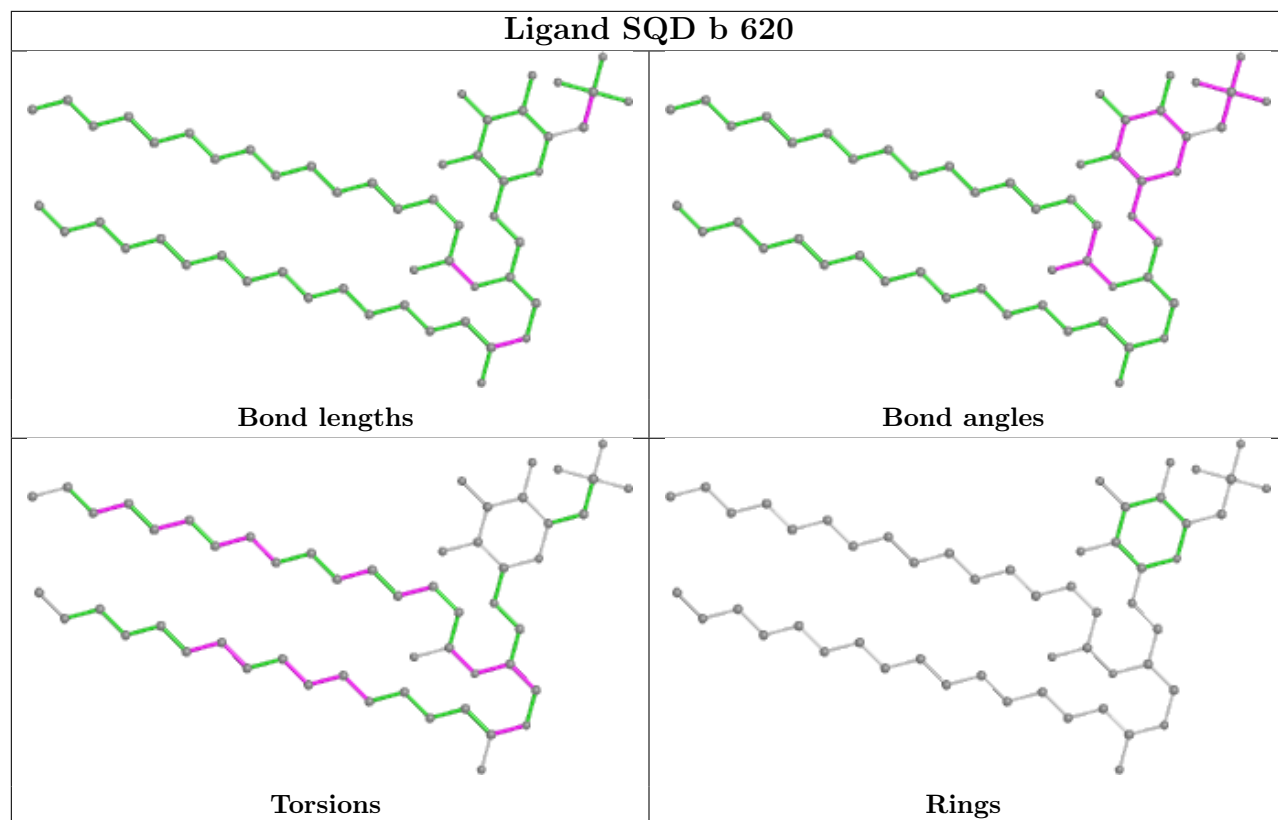


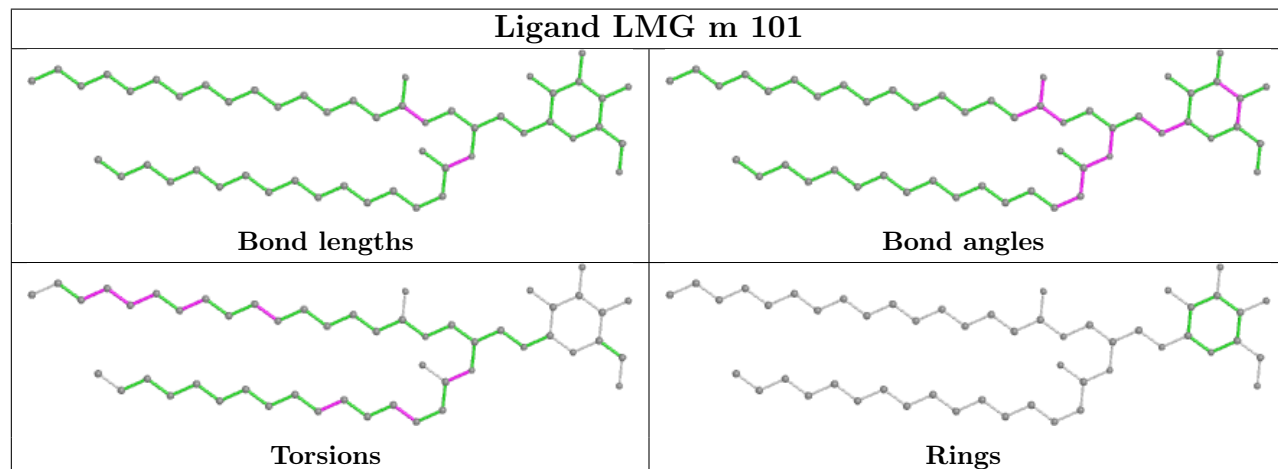
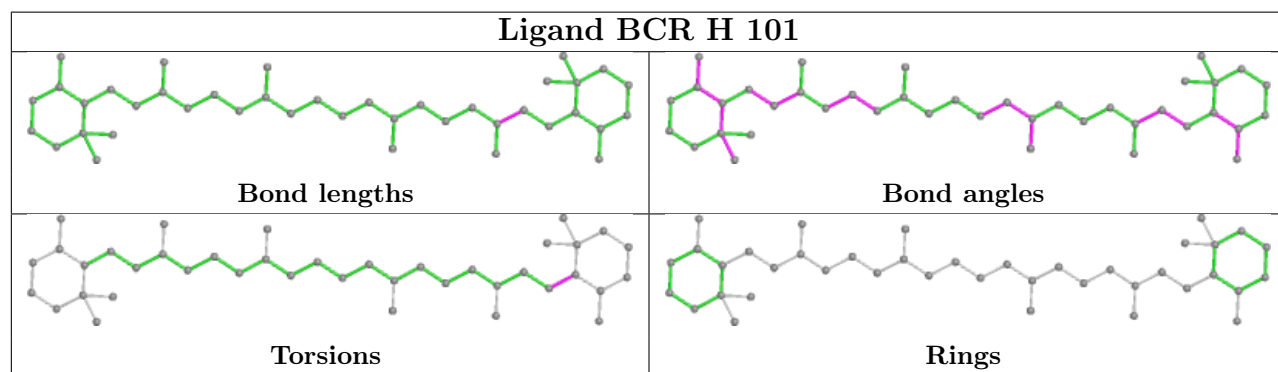
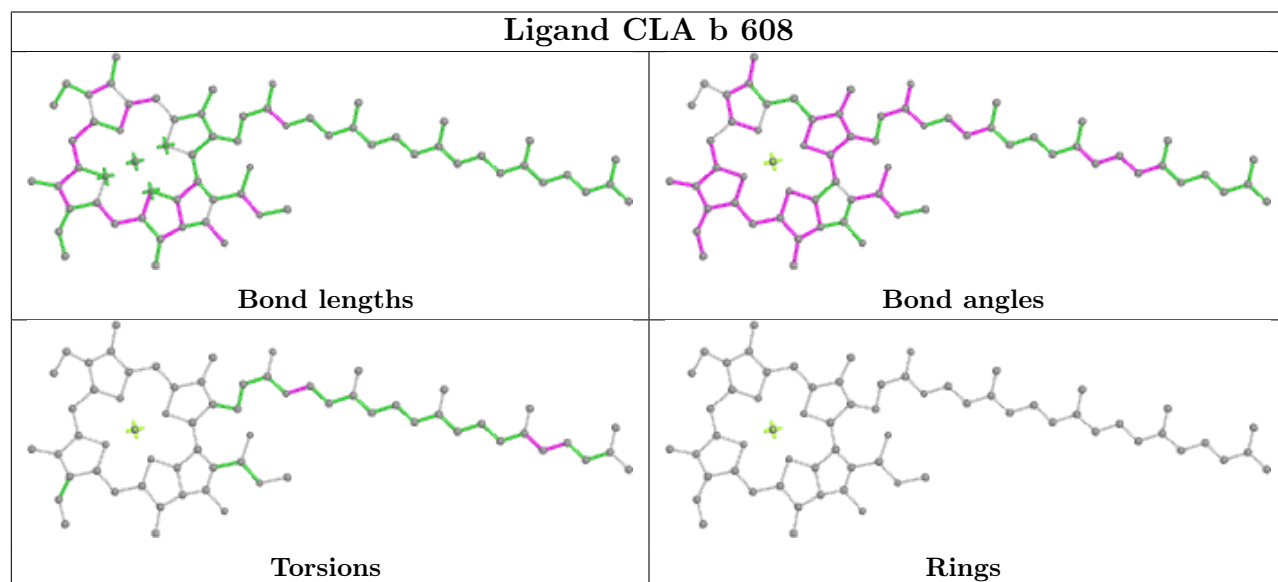
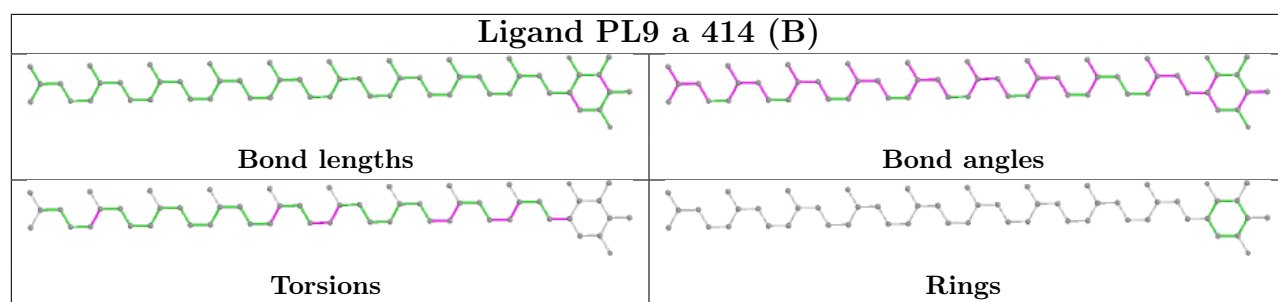


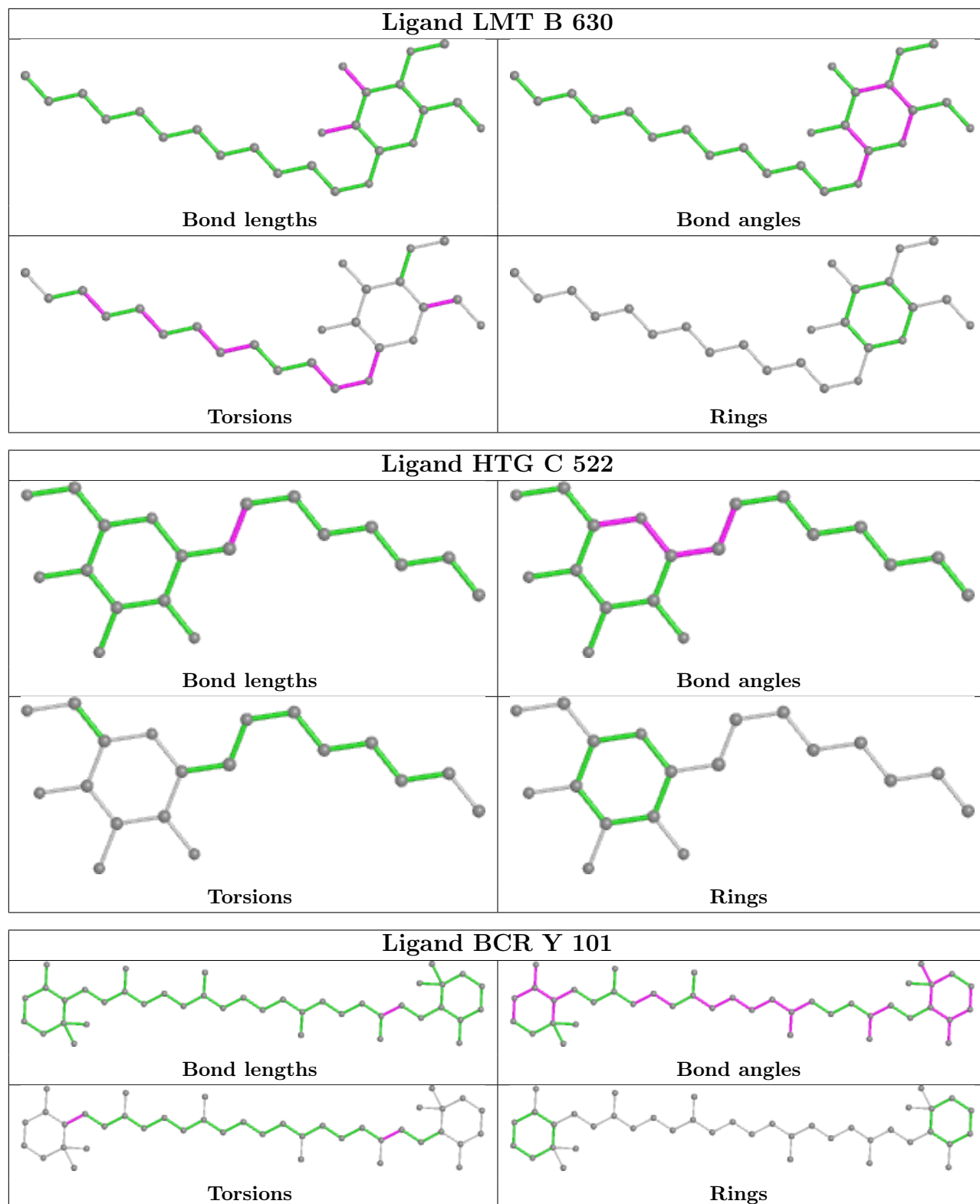


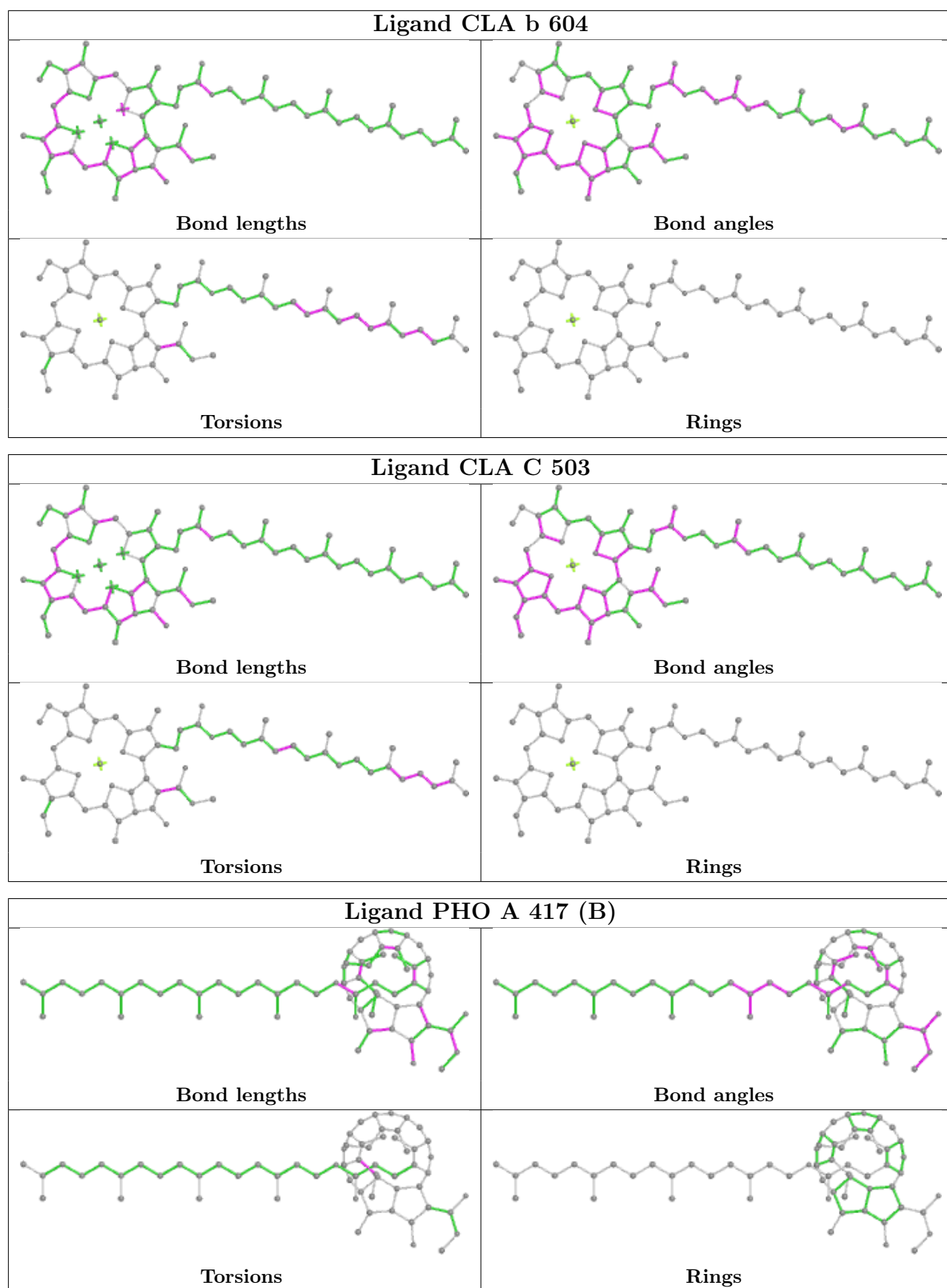


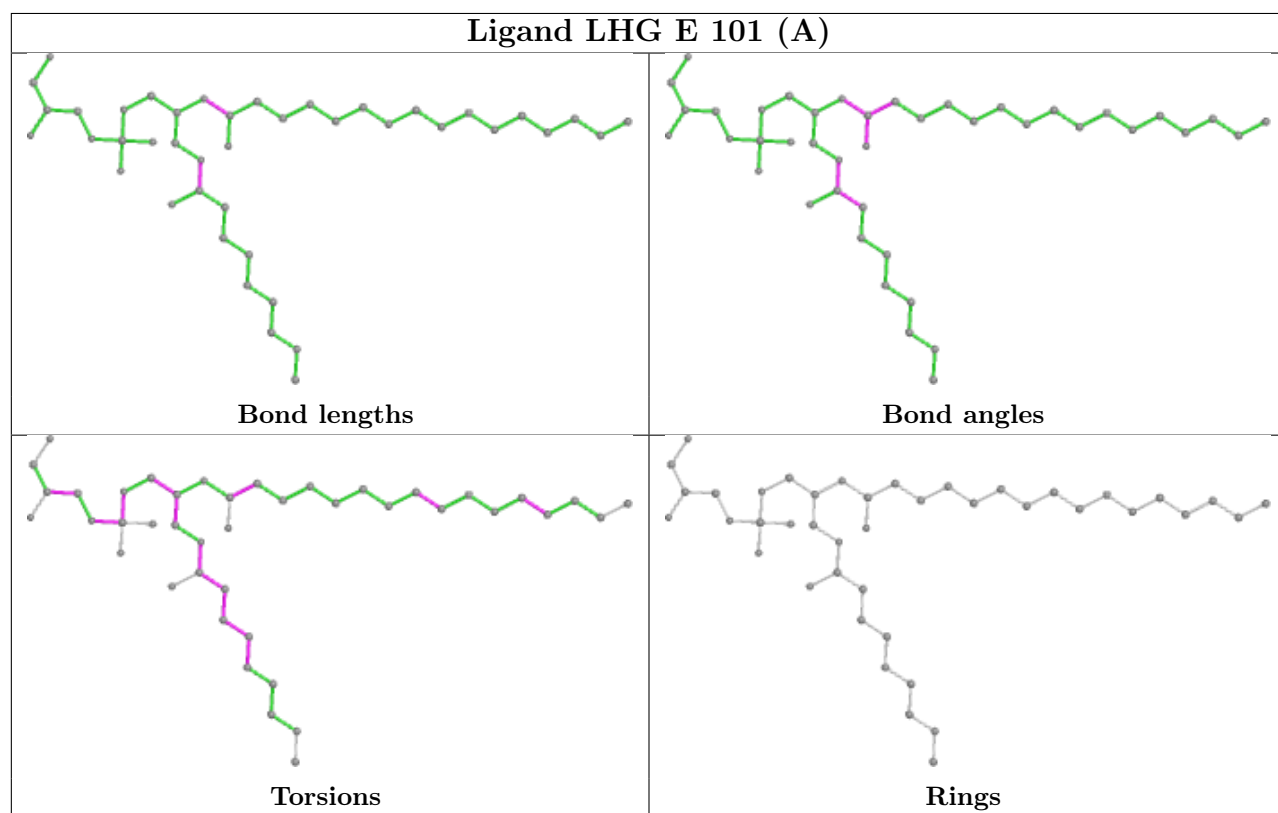
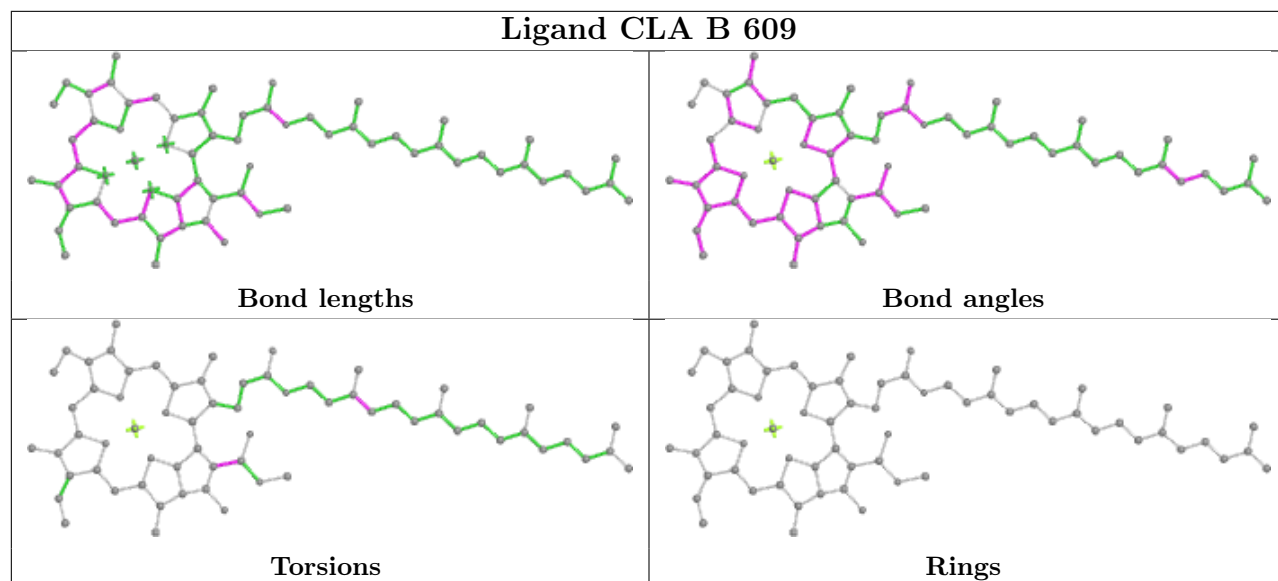
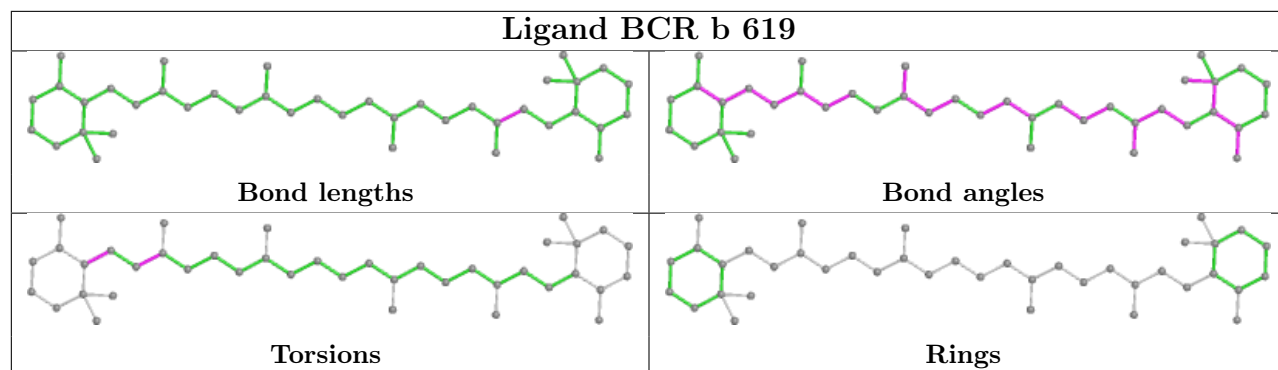


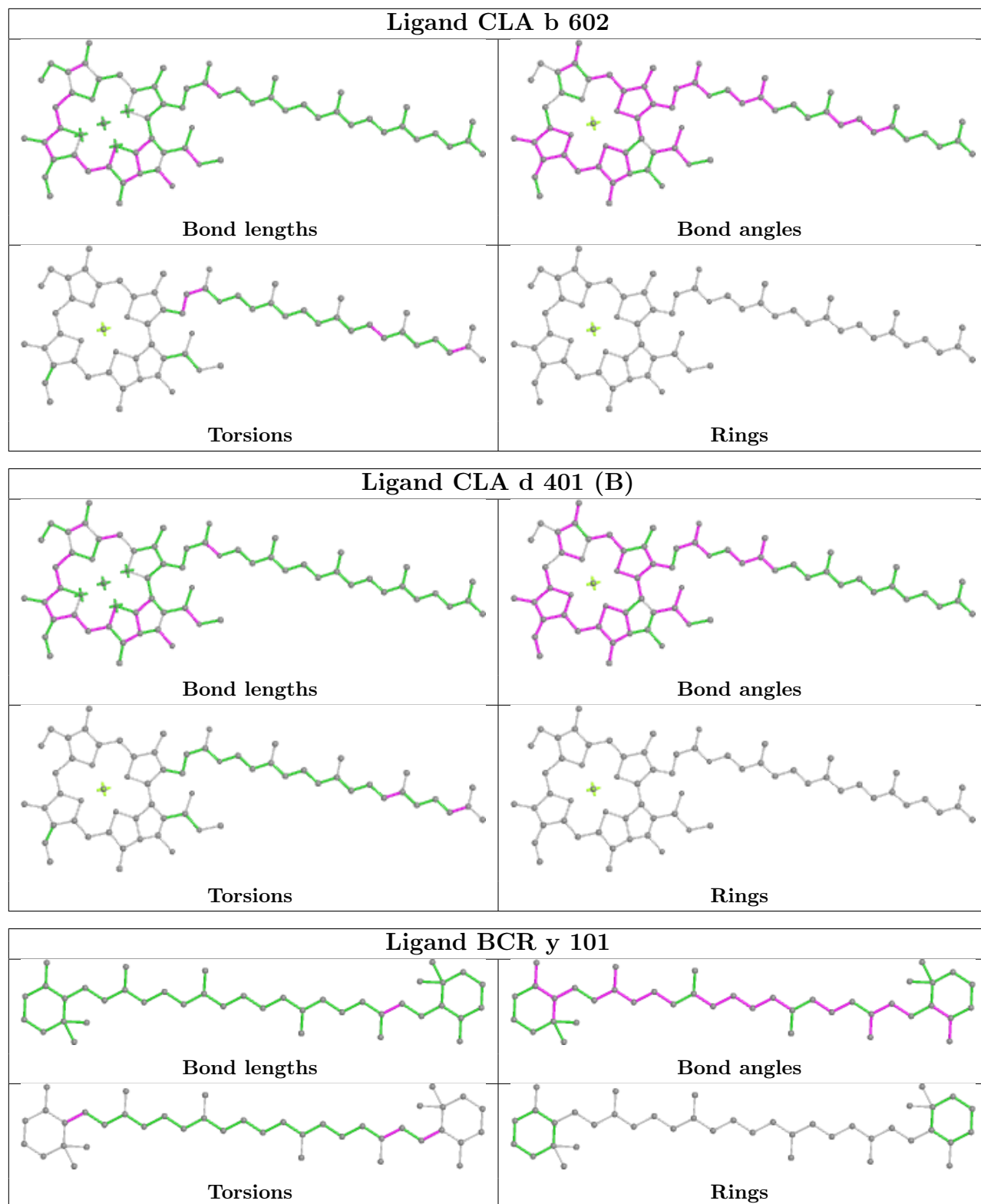


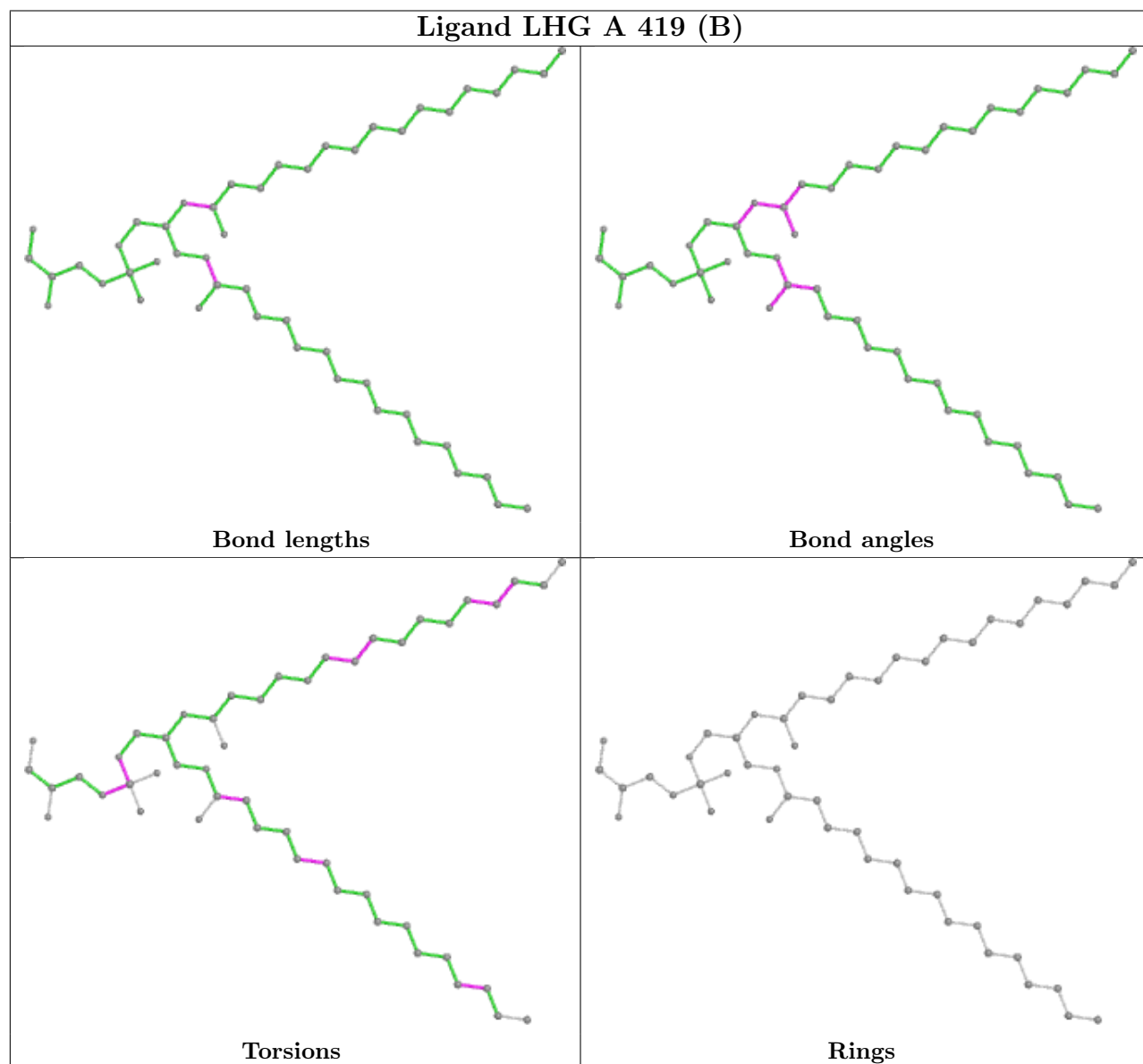
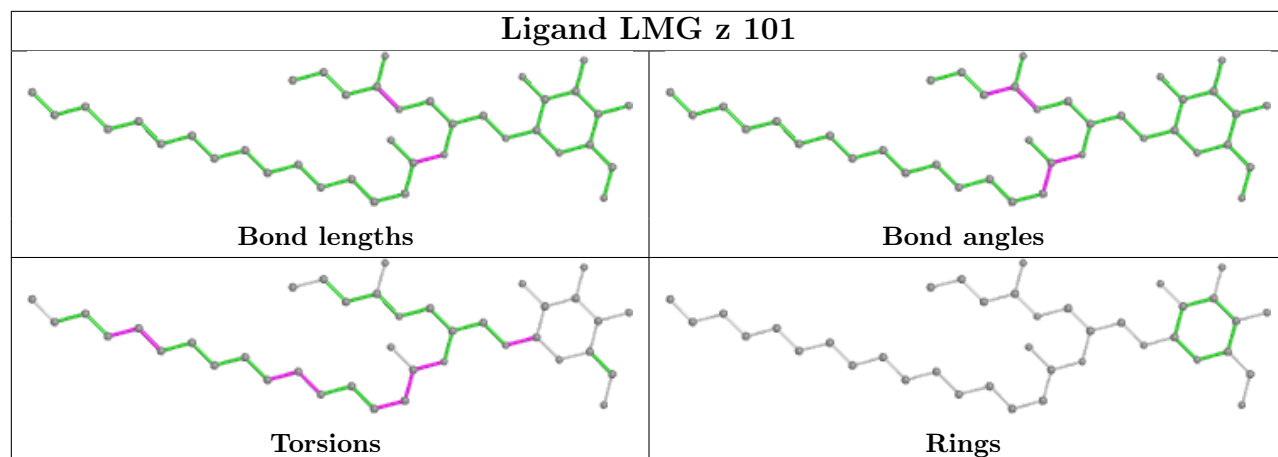


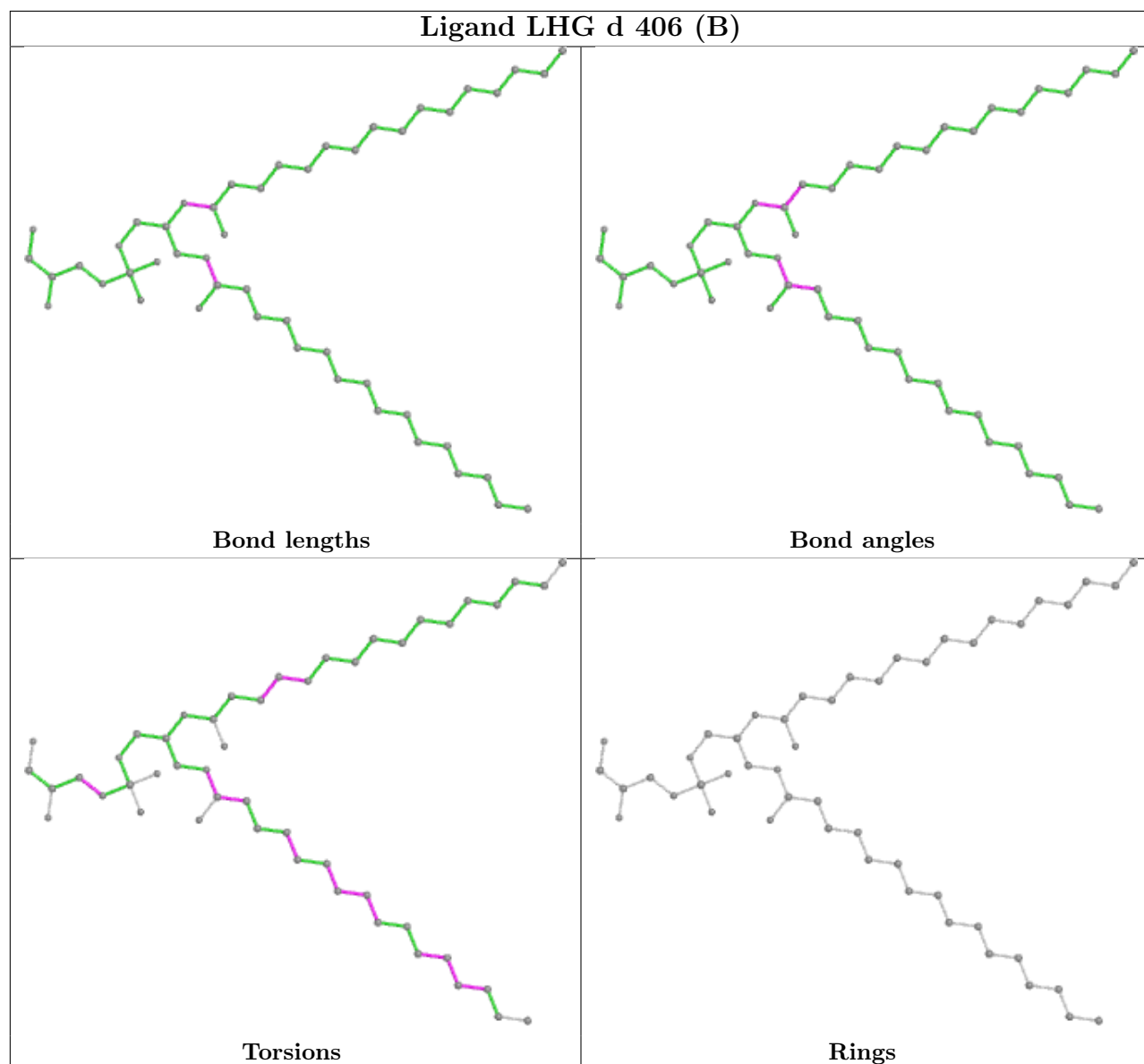
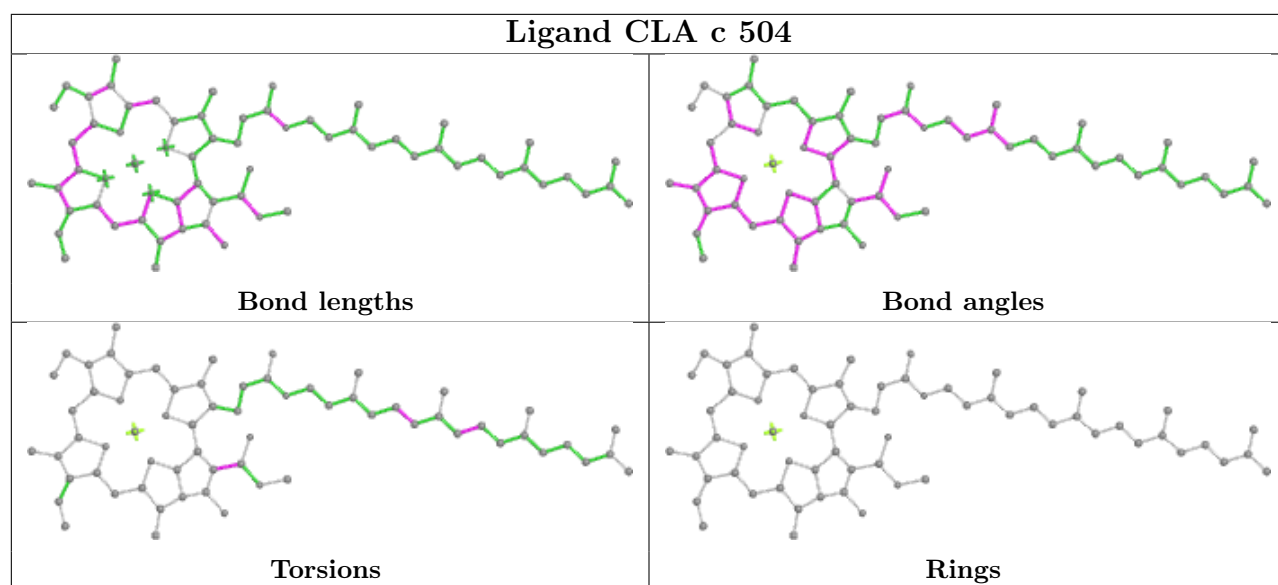


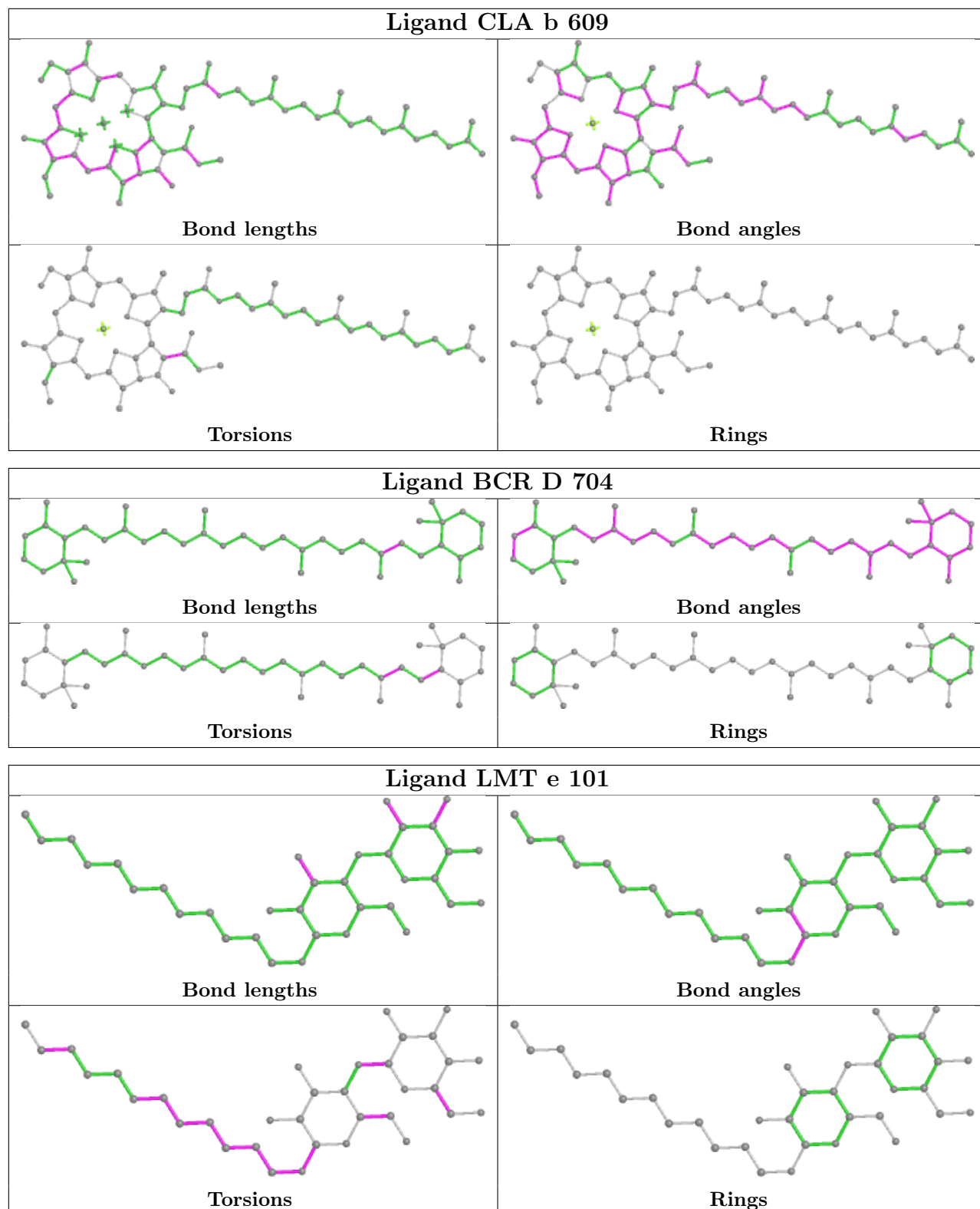


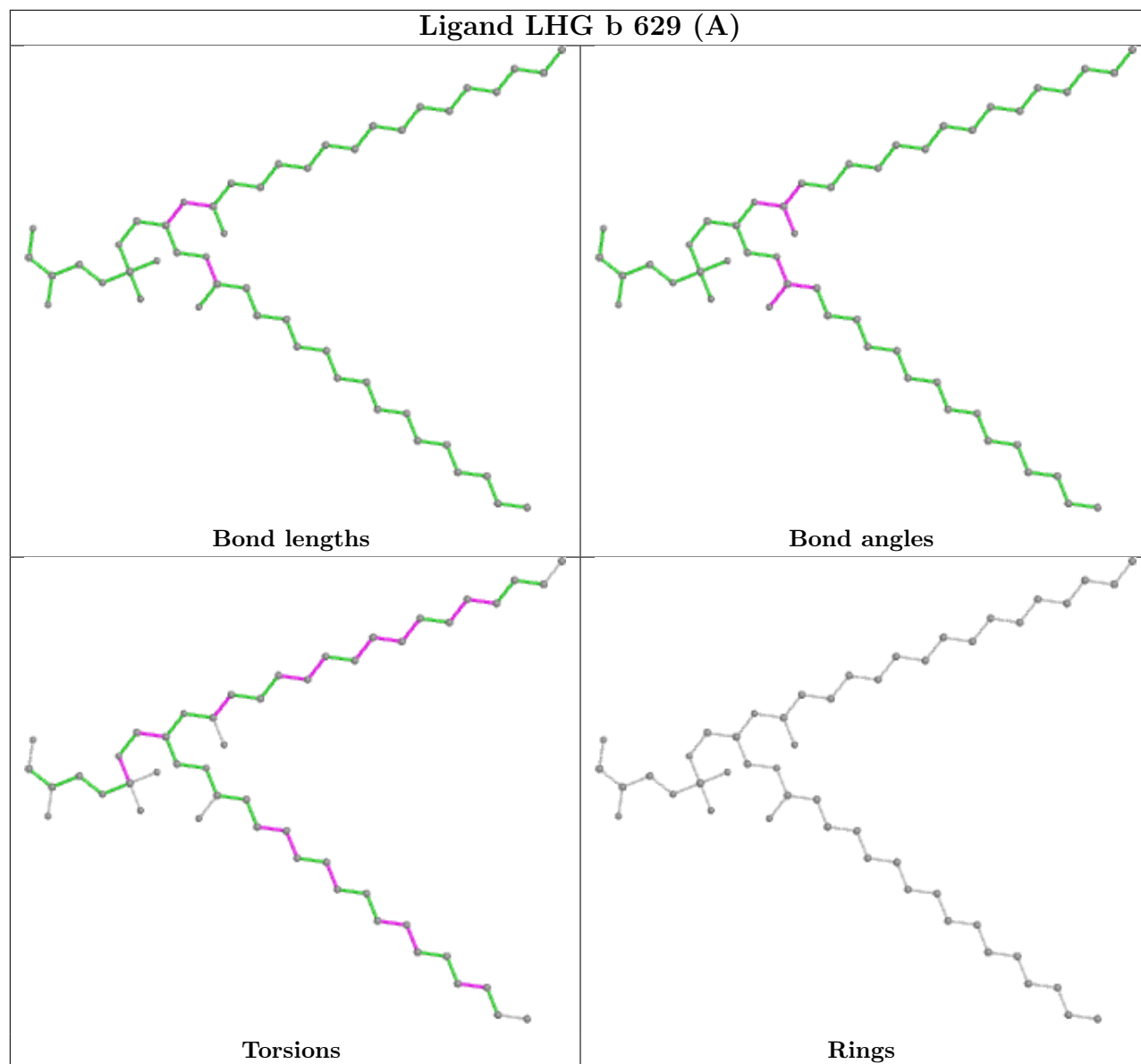


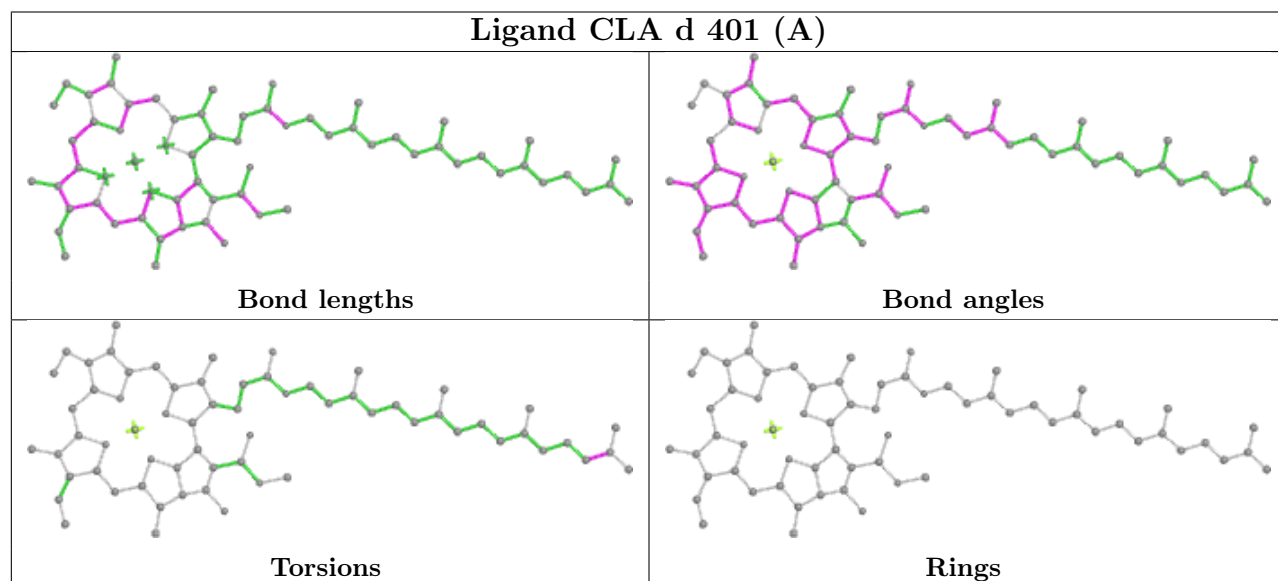
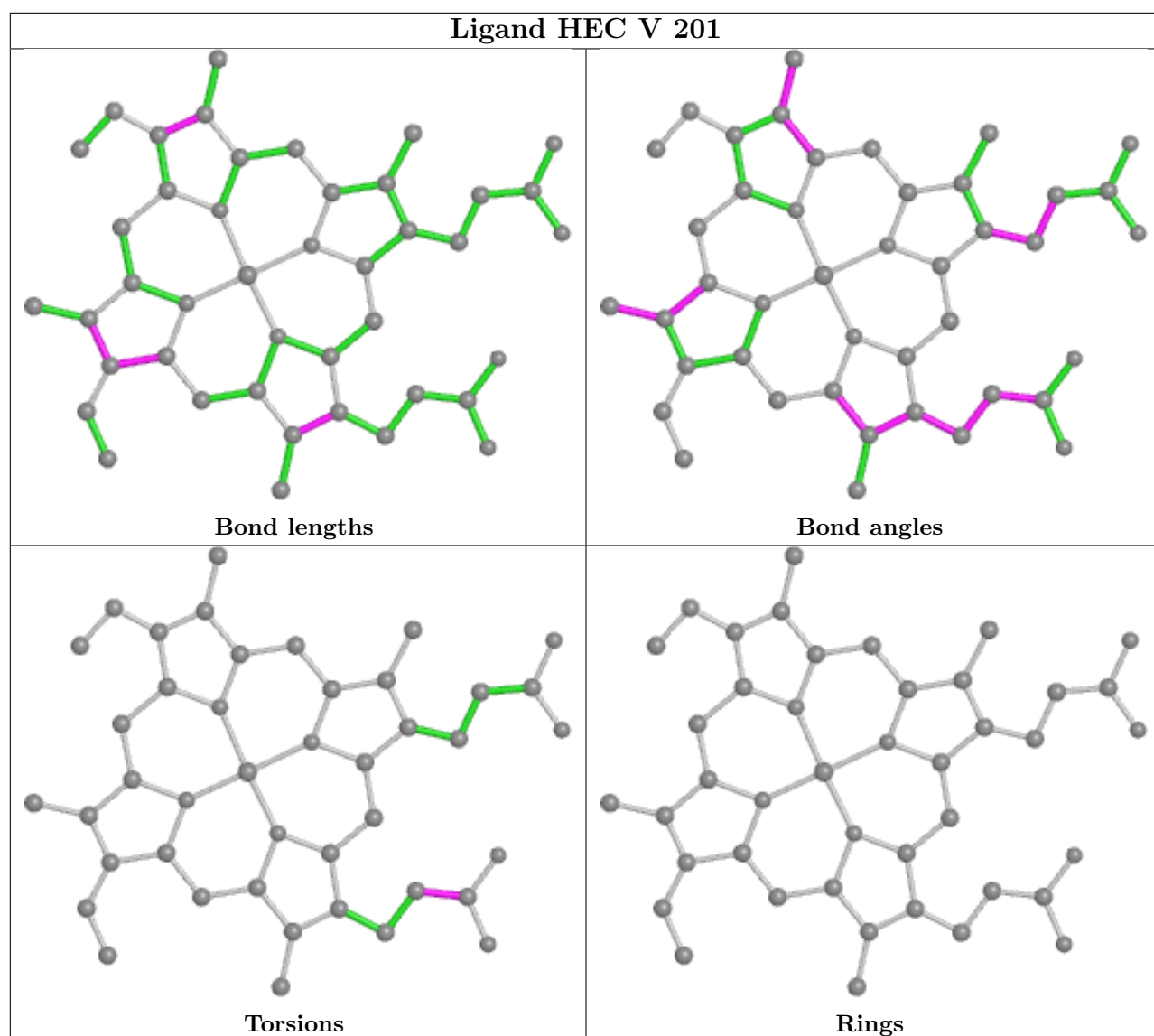


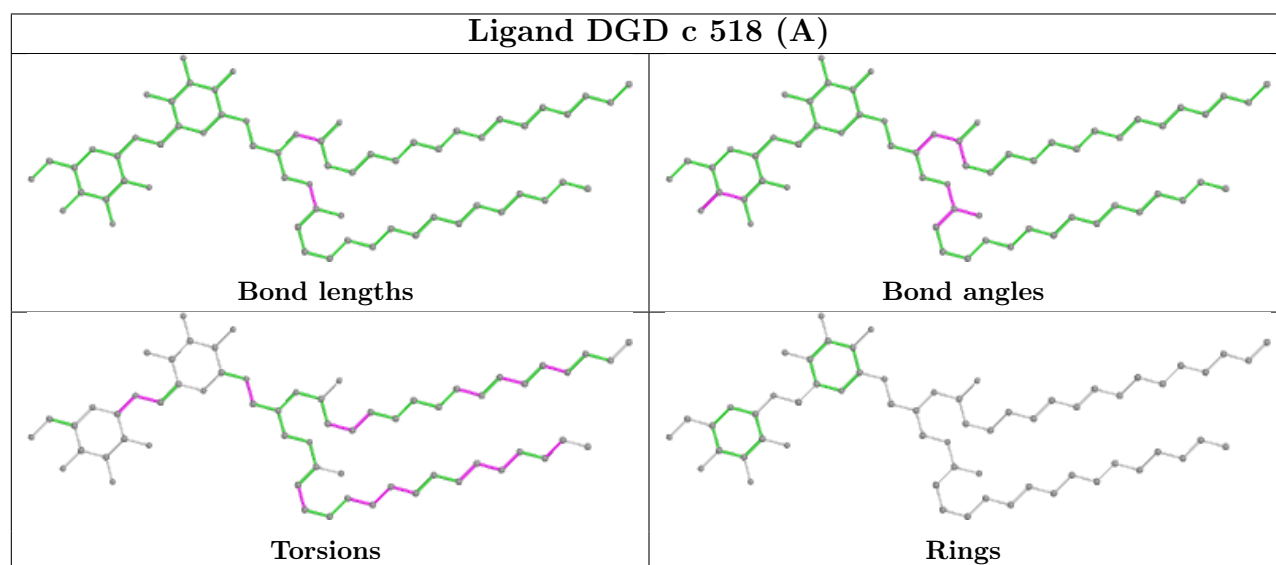
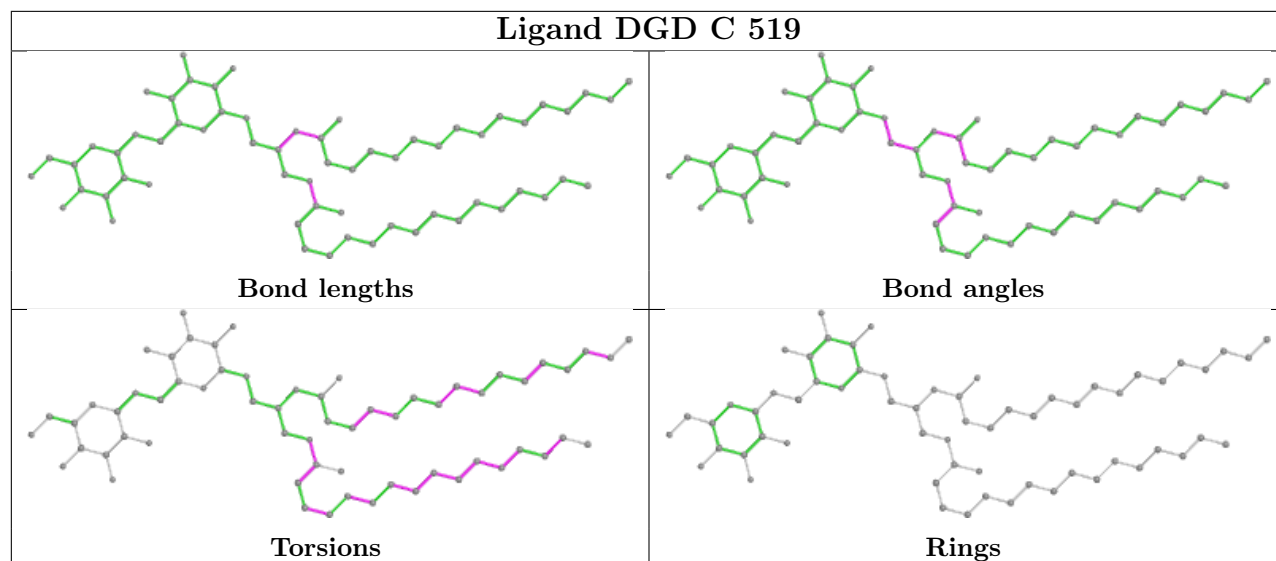


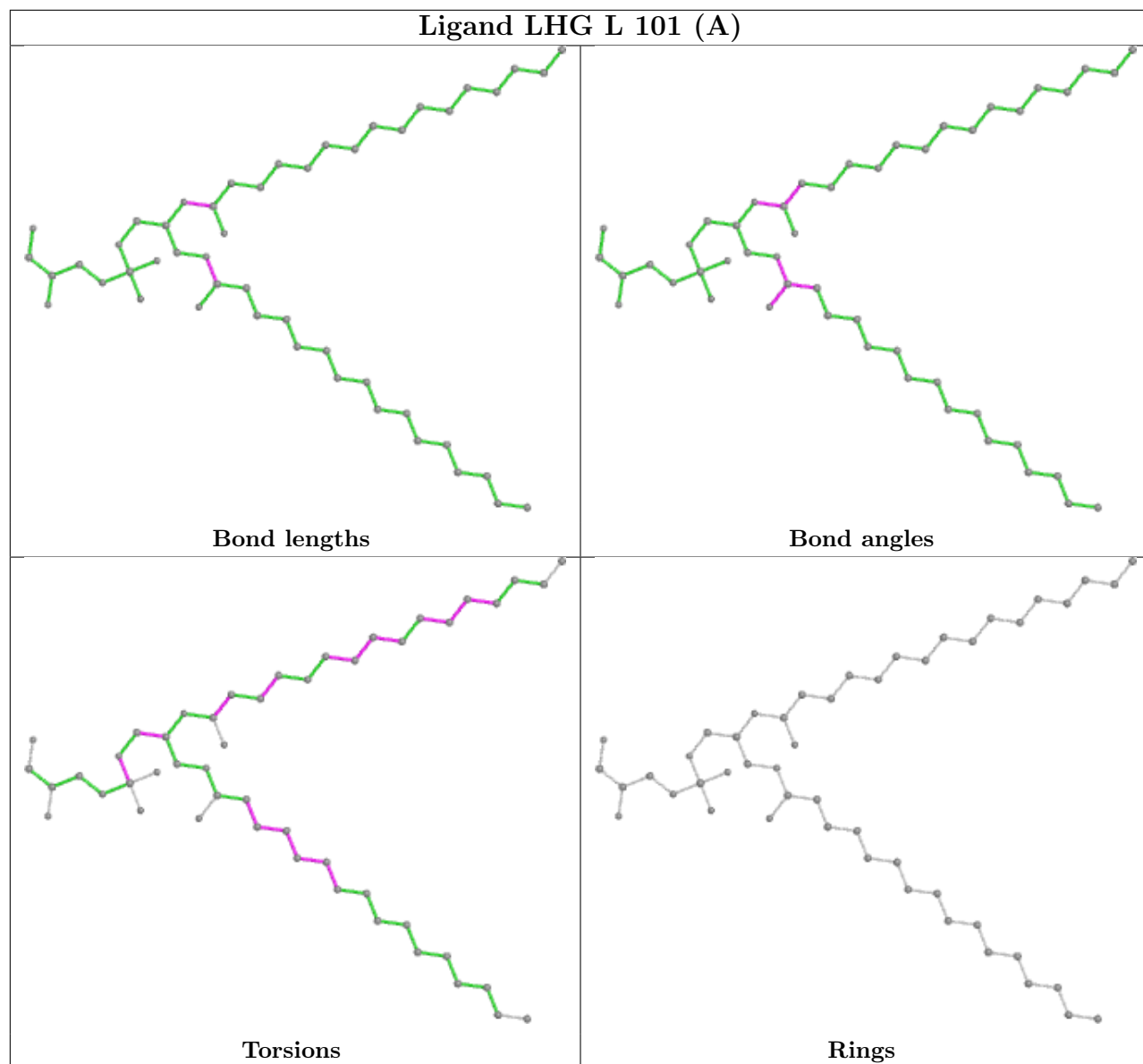


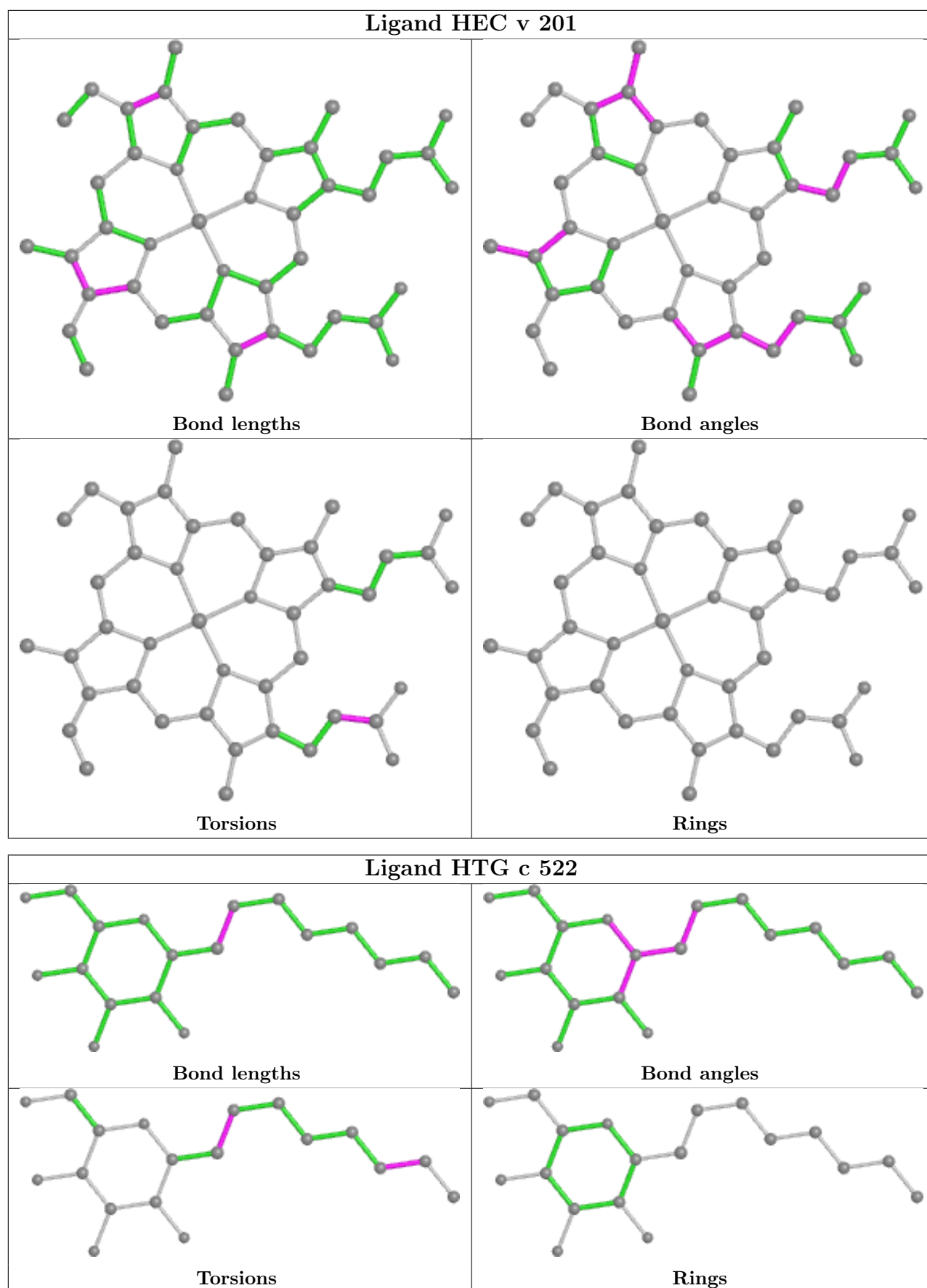


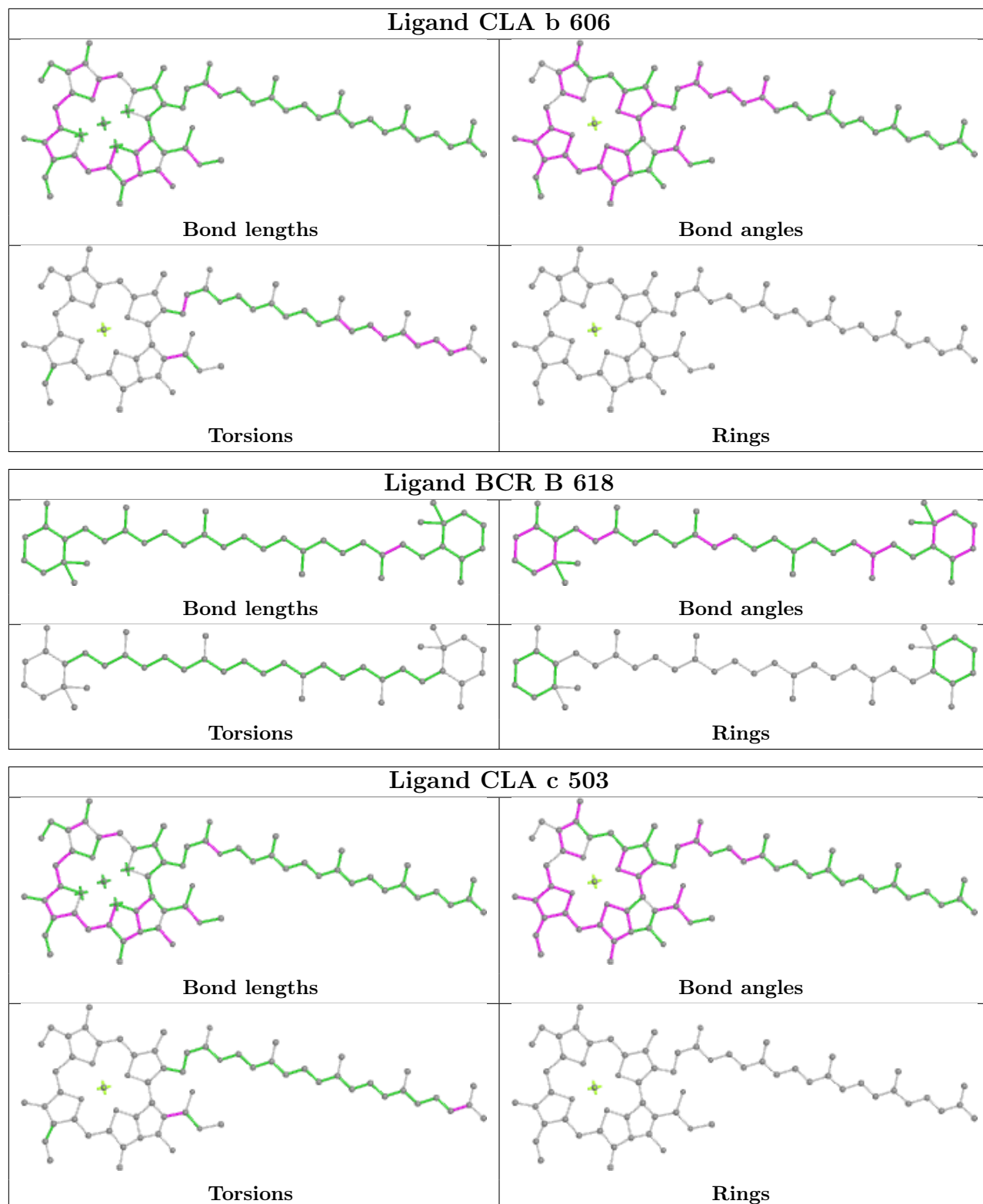


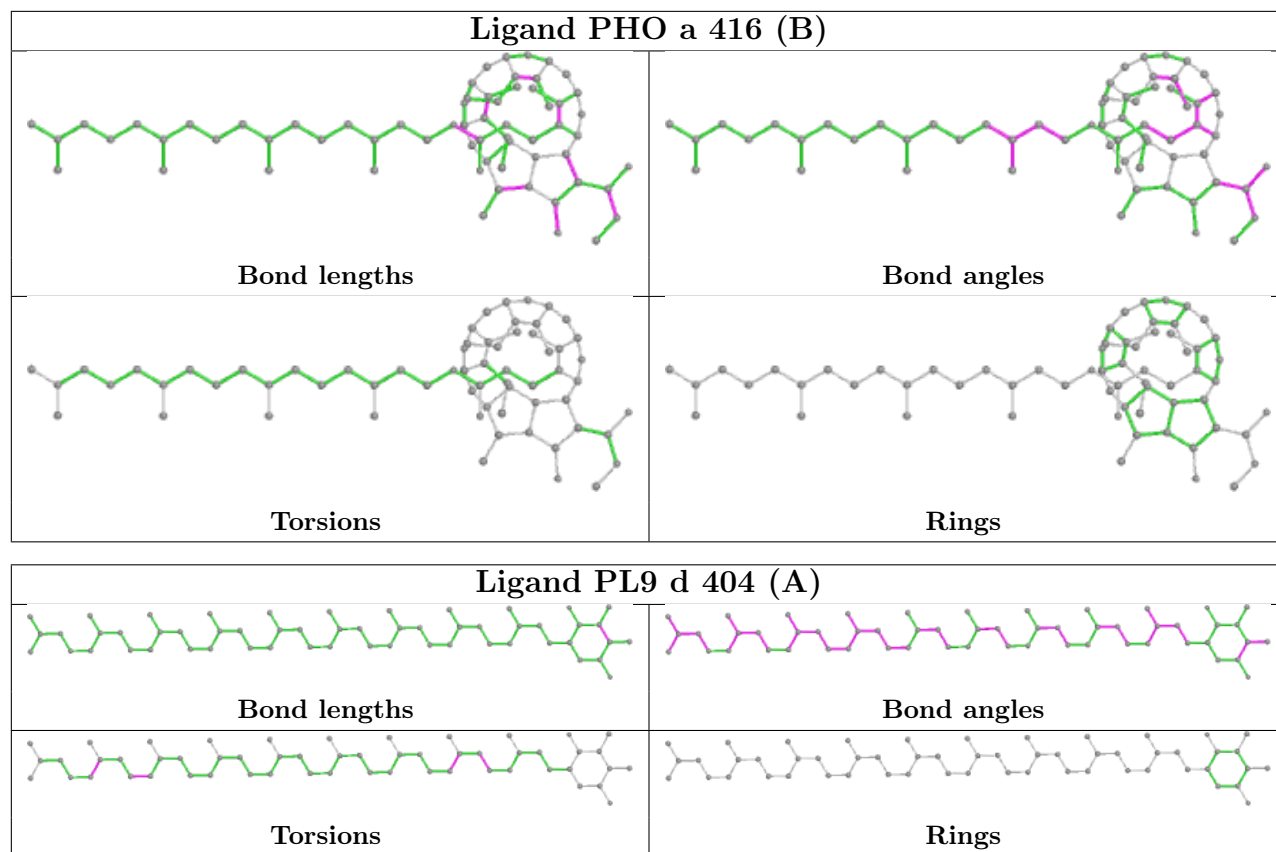


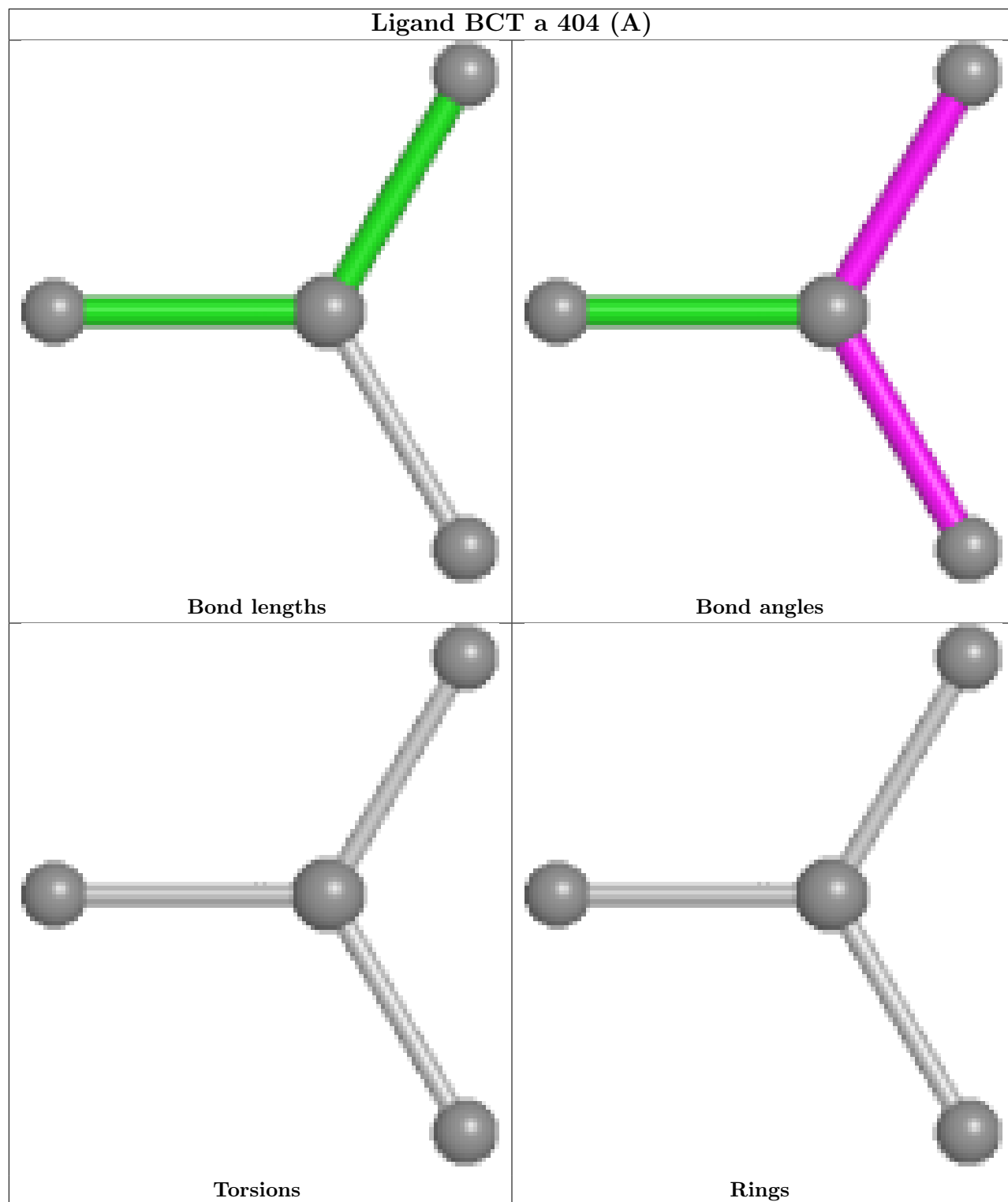


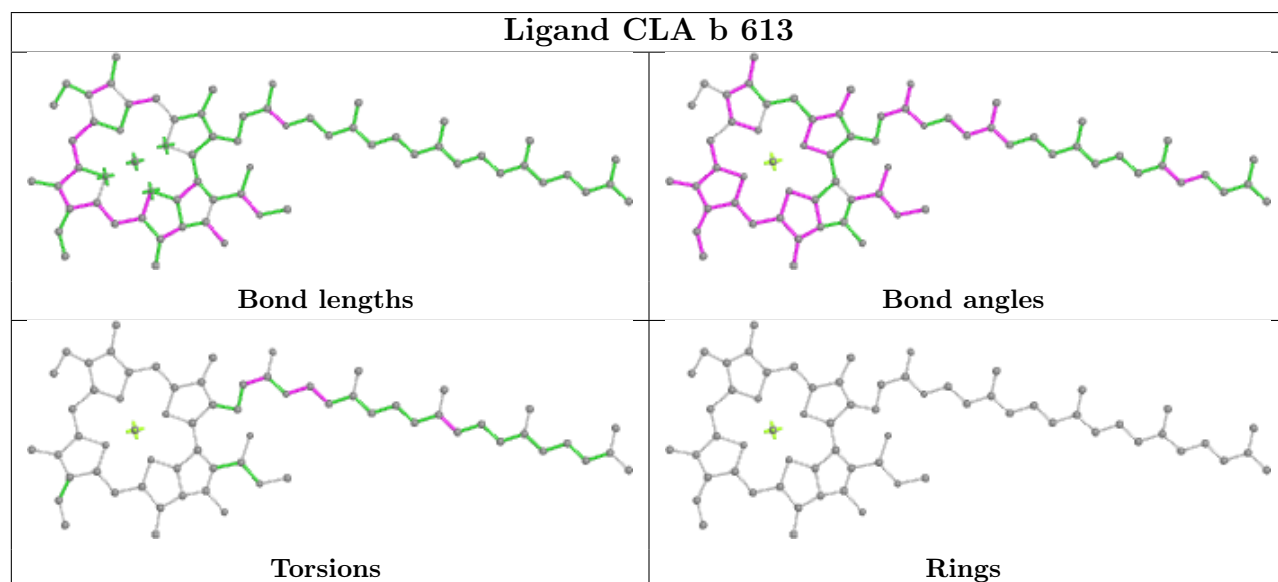
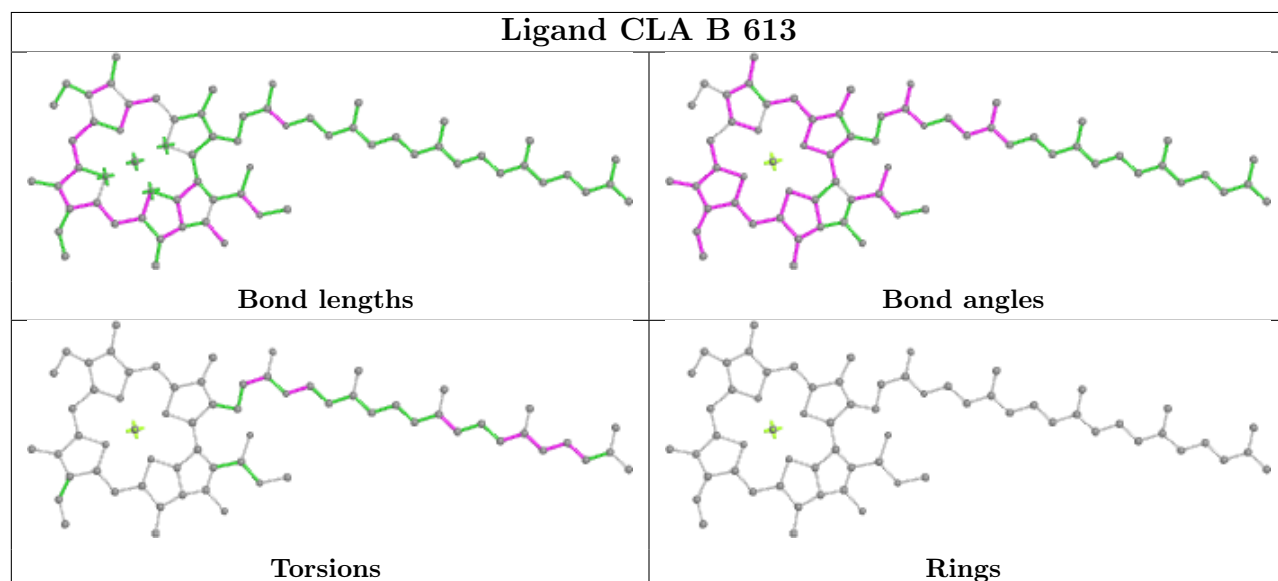
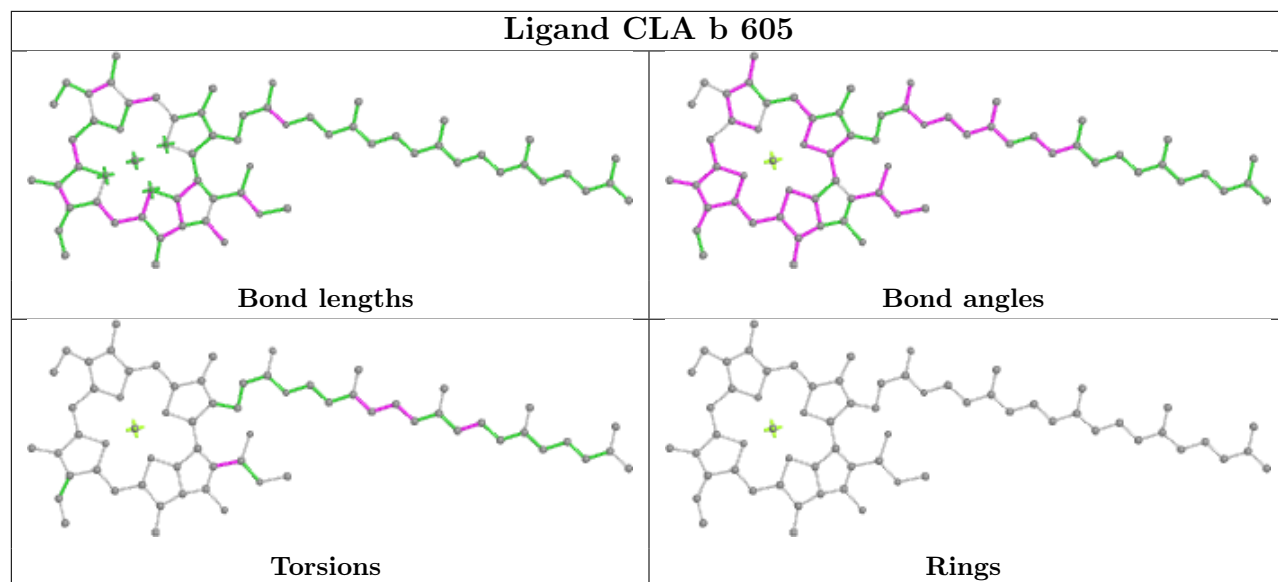


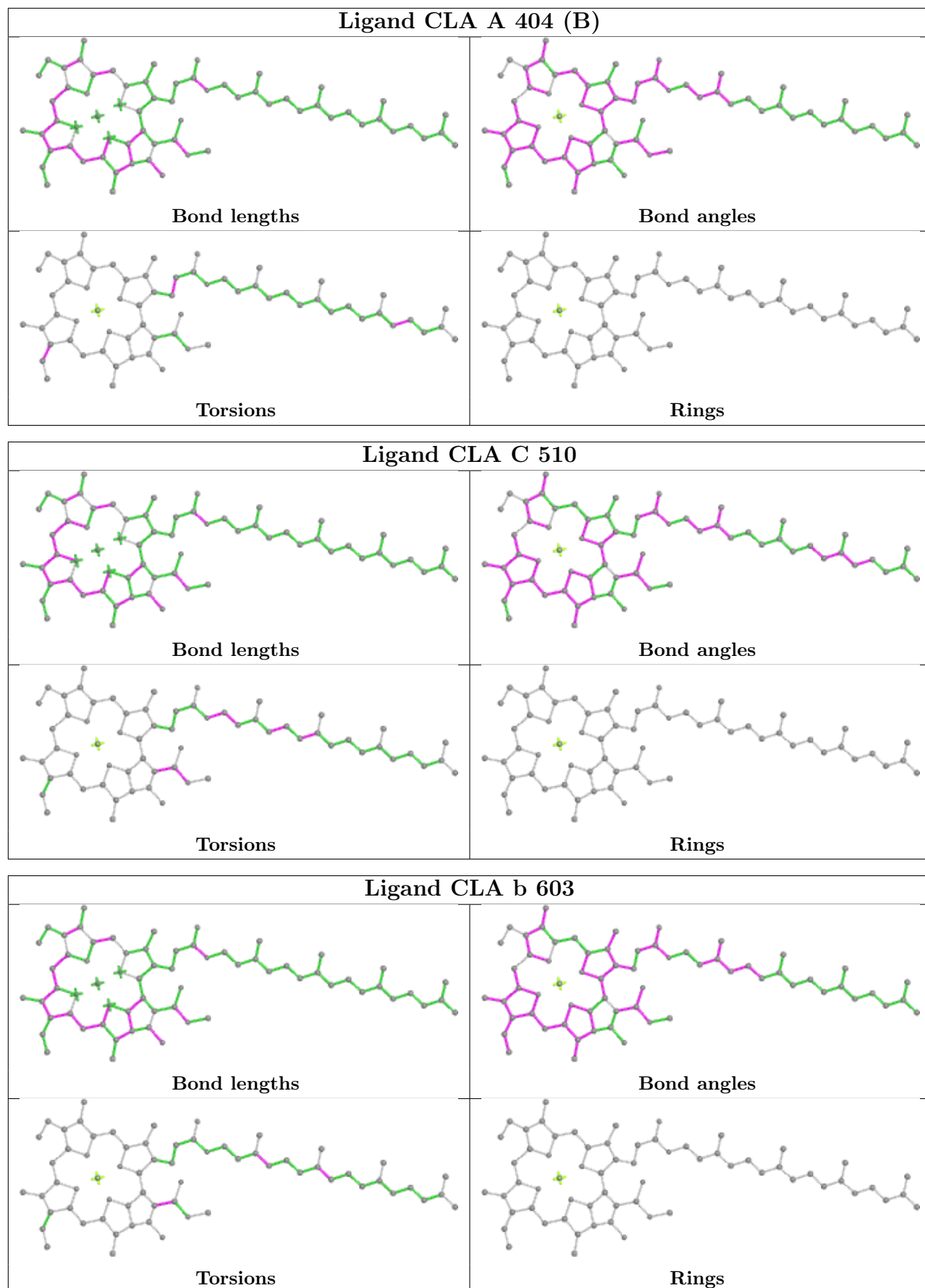


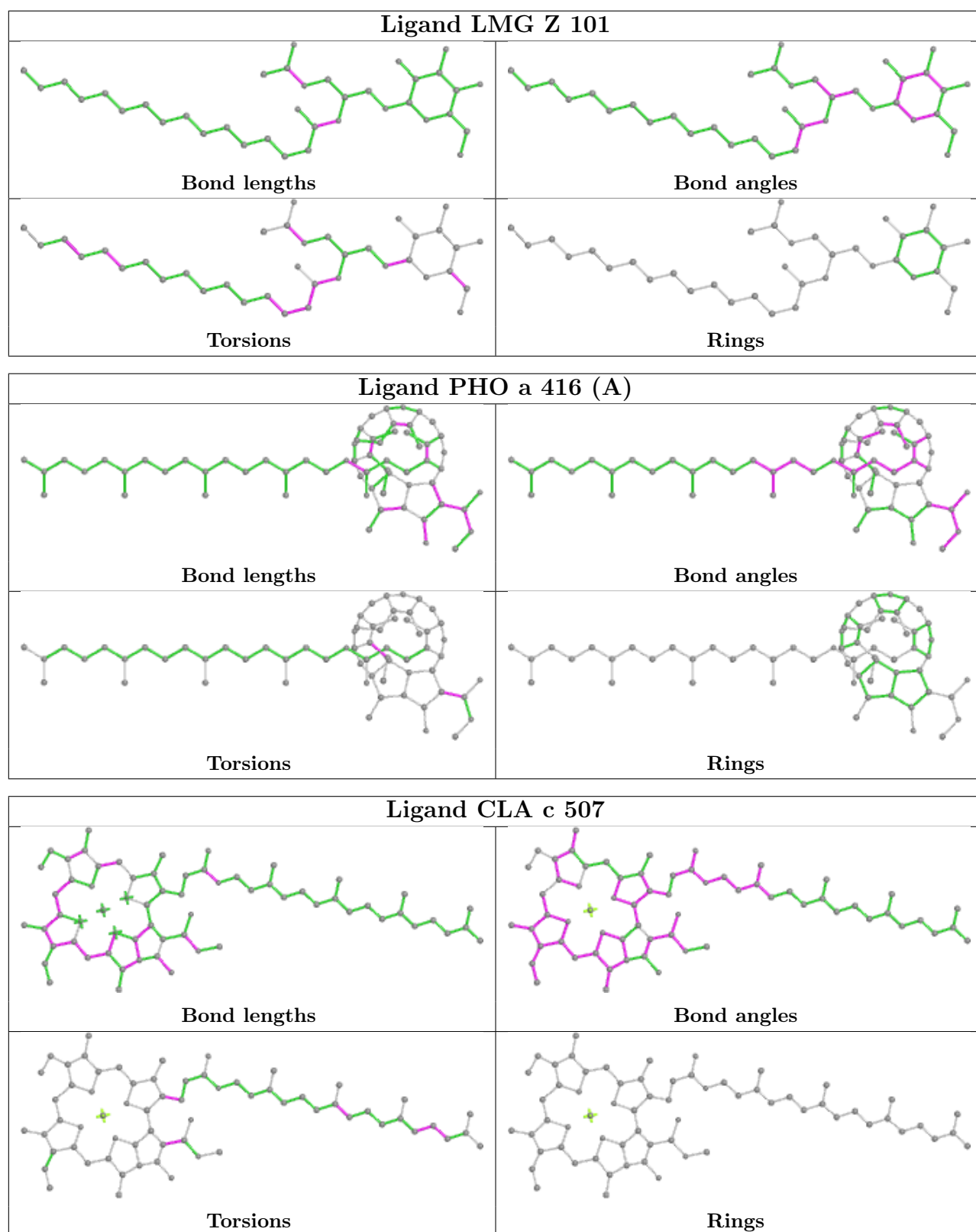


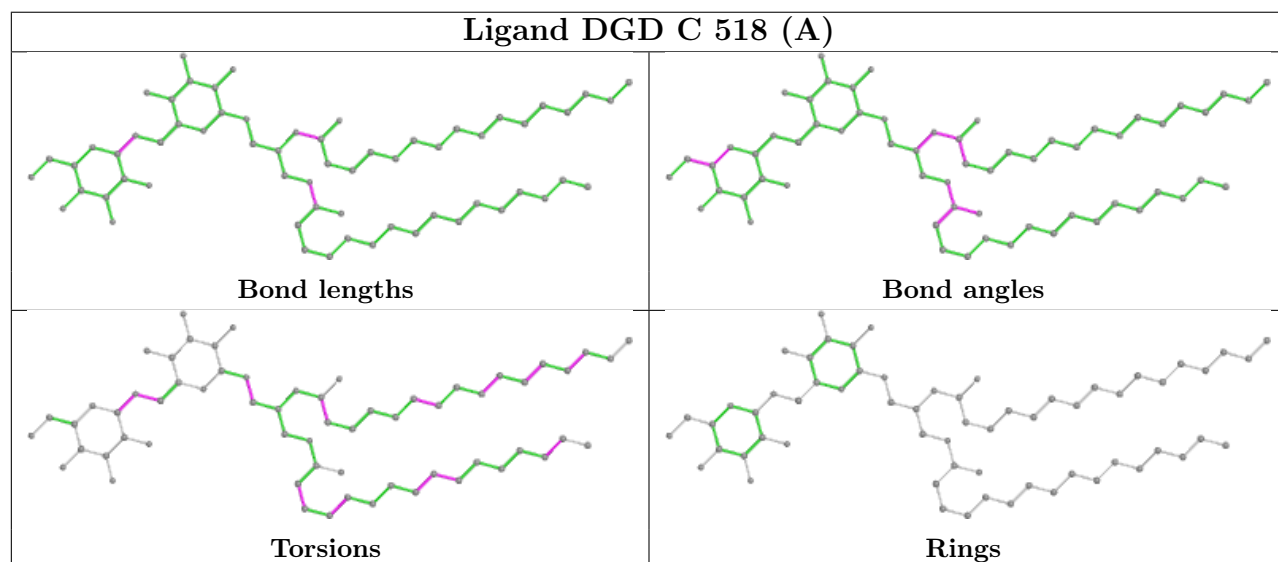
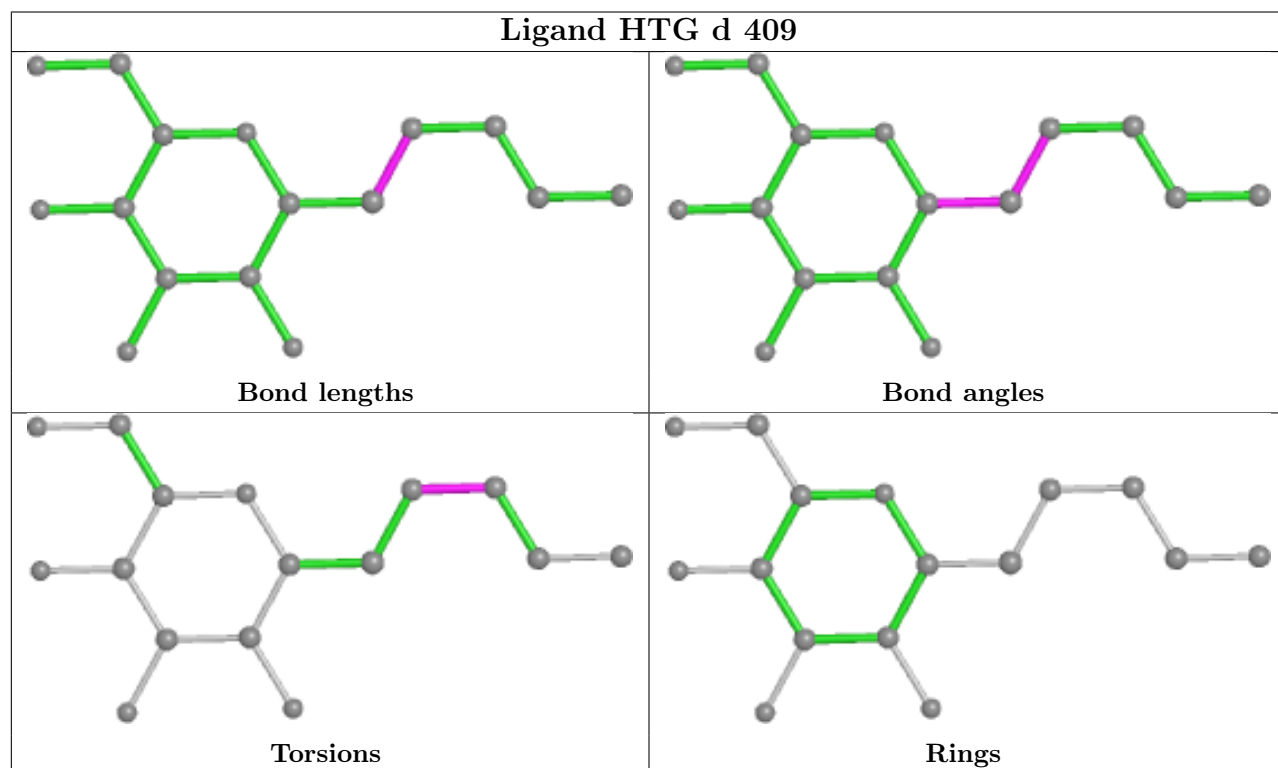
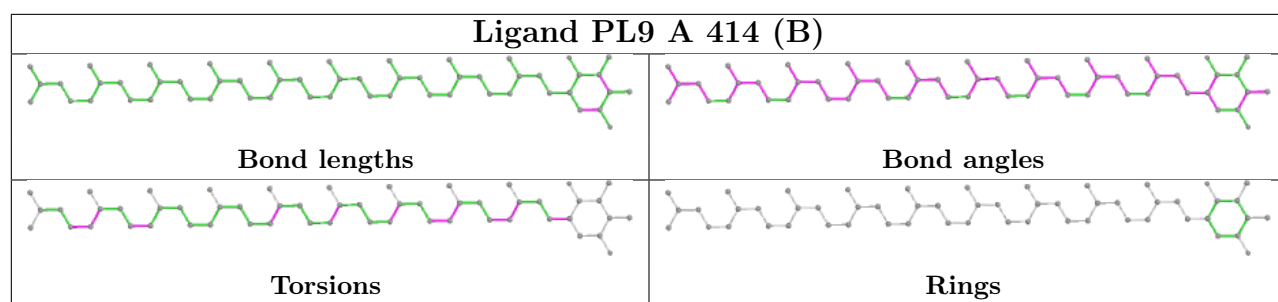


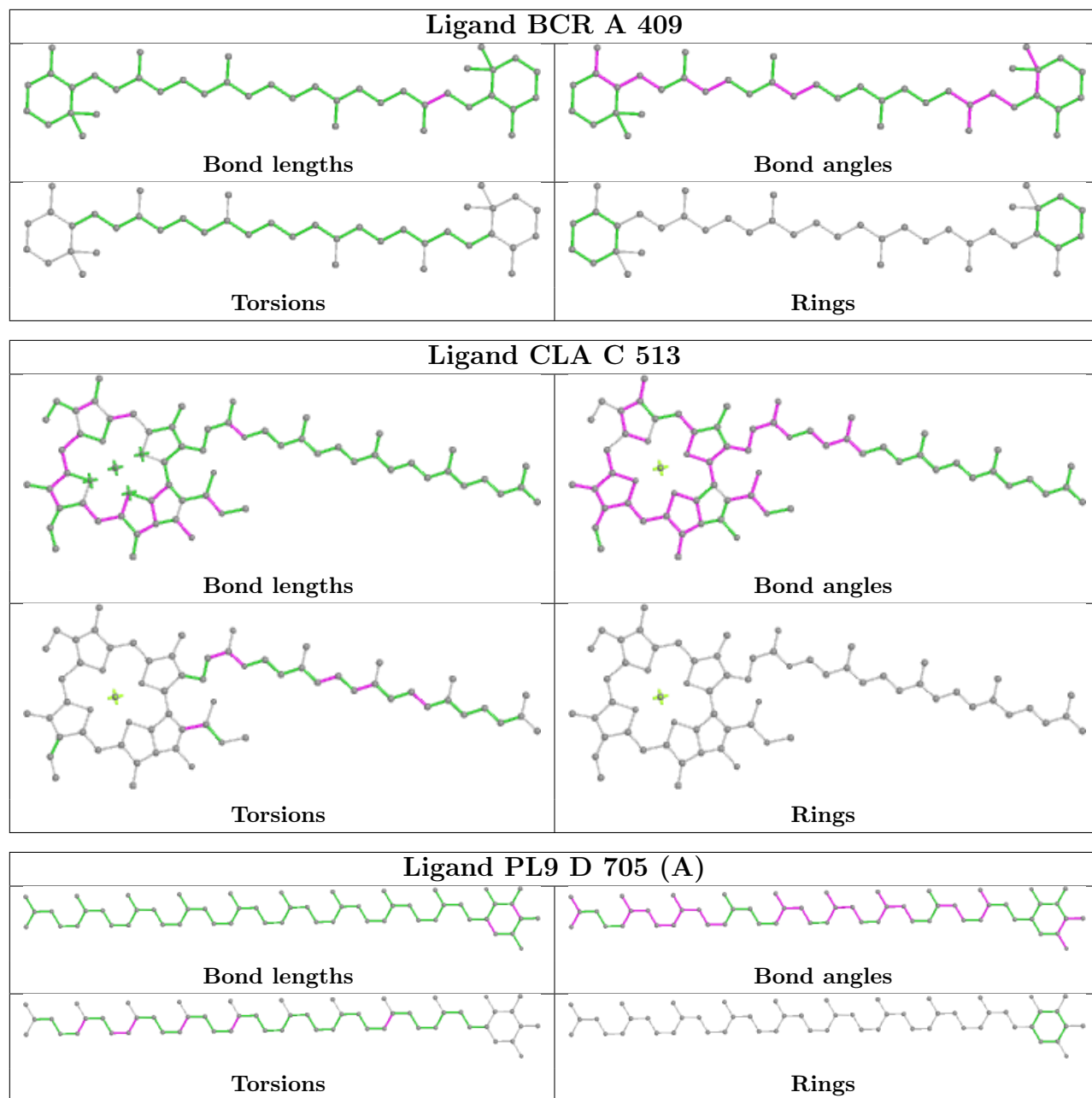


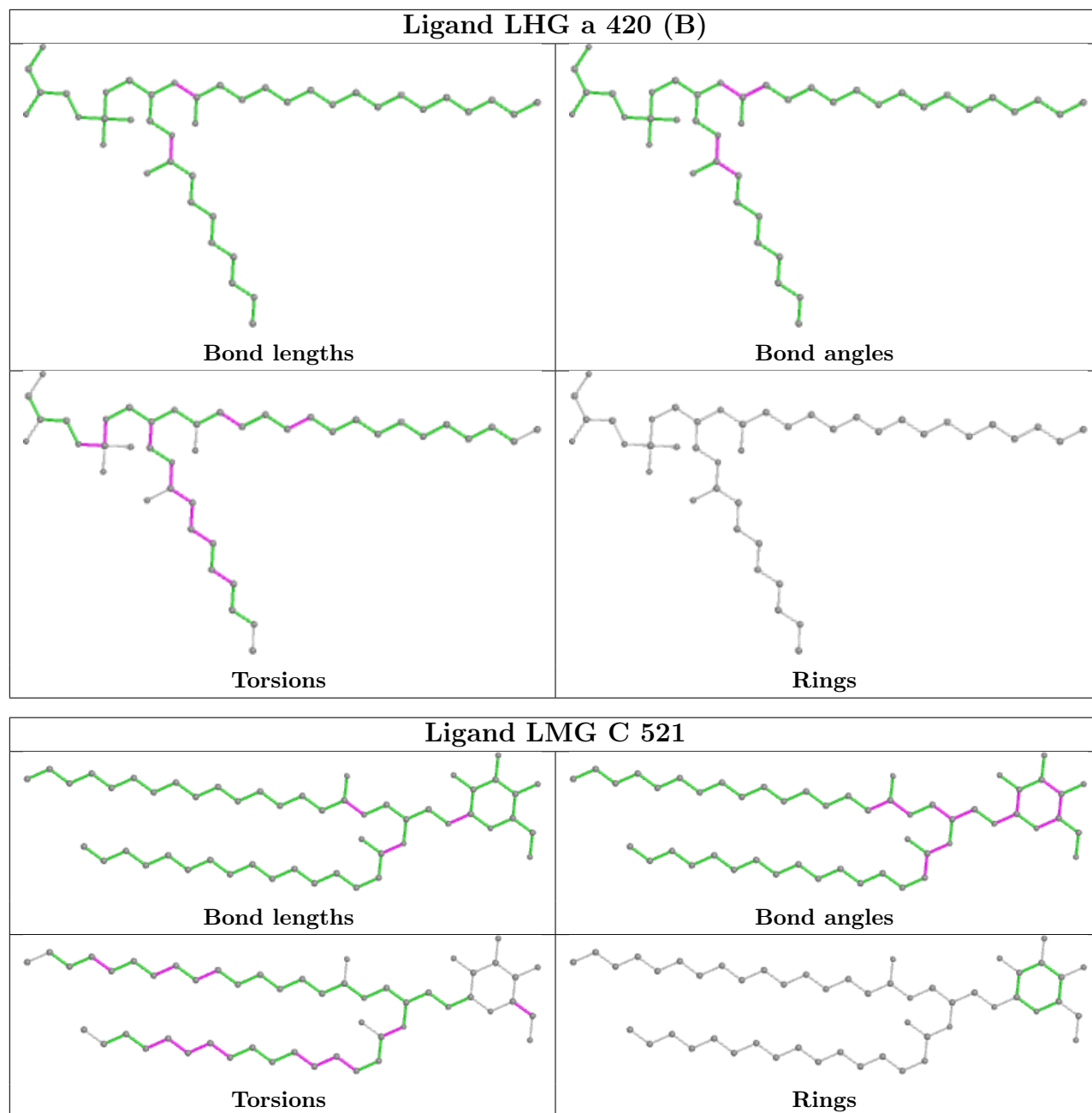


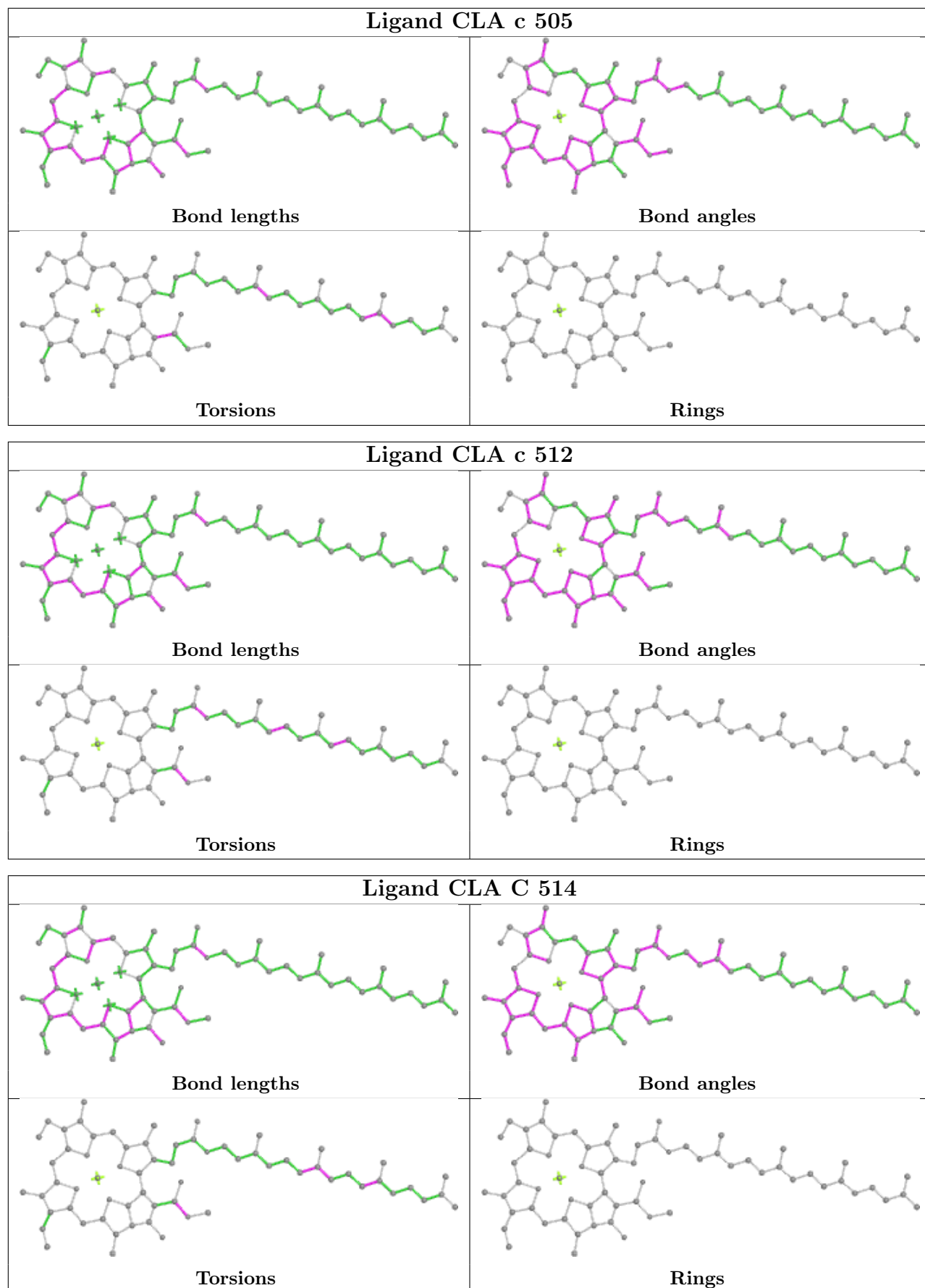


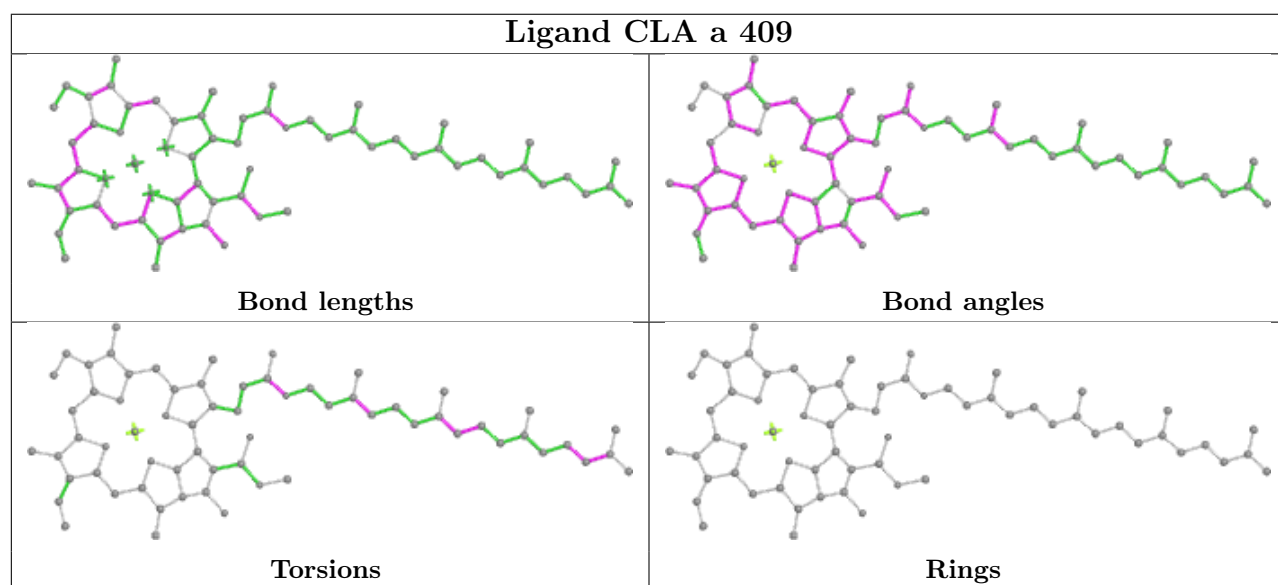
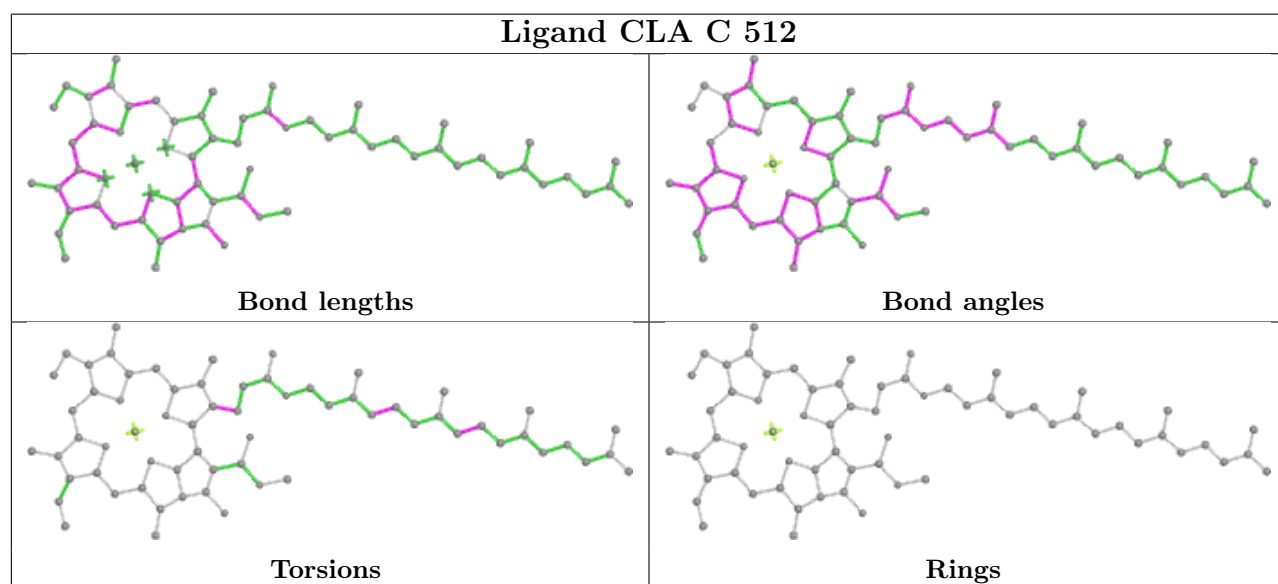
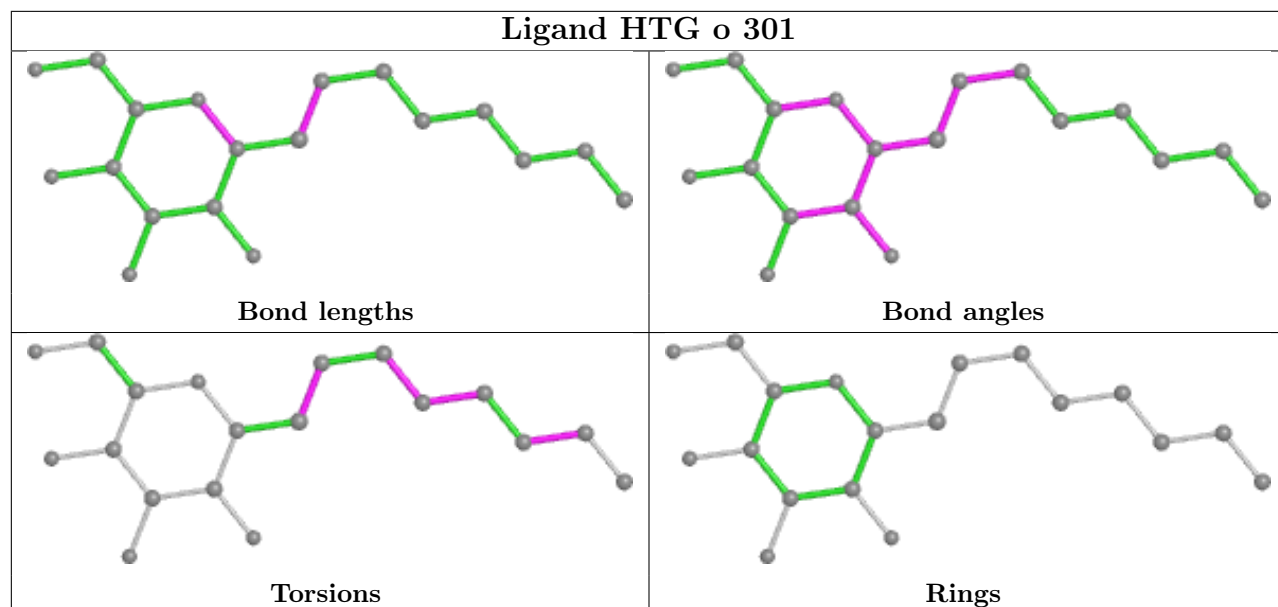


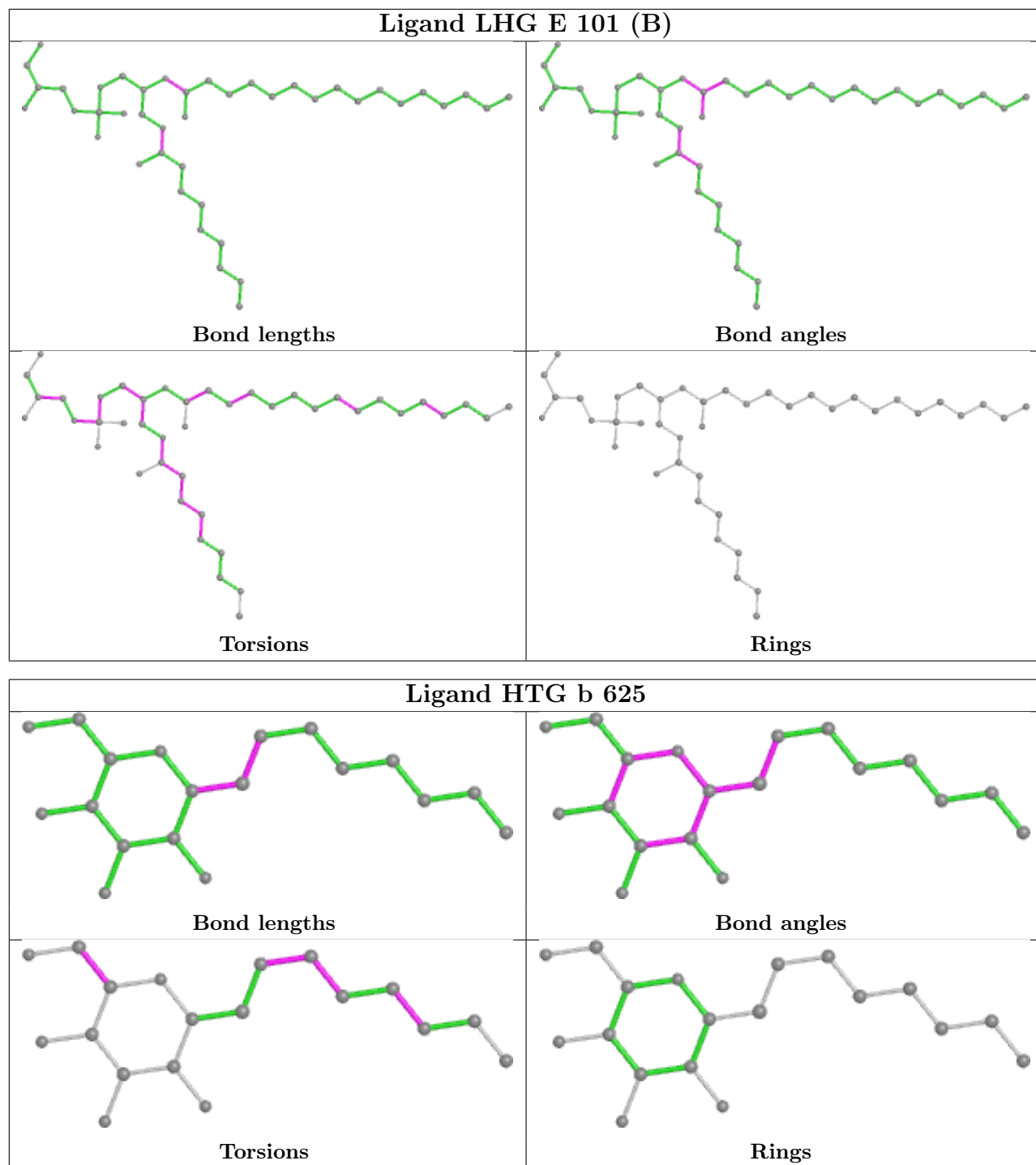












5.7 Other polymers [\(i\)](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.70	4 (1%) 79 83	41, 49, 70, 128	0
1	a	334/344 (97%)	-0.61	5 (1%) 73 79	43, 53, 82, 124	0
2	B	504/505 (99%)	-0.46	12 (2%) 59 66	43, 55, 82, 119	0
2	b	504/505 (99%)	-0.30	29 (5%) 23 29	45, 59, 97, 169	1 (0%)
3	C	451/455 (99%)	-0.53	9 (1%) 65 71	45, 60, 81, 160	0
3	c	455/455 (100%)	-0.38	13 (2%) 51 58	50, 66, 86, 130	2 (0%)
4	D	342/342 (100%)	-0.64	3 (0%) 84 88	40, 50, 69, 136	0
4	d	341/342 (99%)	-0.62	1 (0%) 94 96	44, 55, 78, 133	0
5	E	81/84 (96%)	-0.09	3 (3%) 41 48	53, 70, 99, 165	0
5	e	79/84 (94%)	0.24	6 (7%) 13 18	61, 77, 114, 152	0
6	F	34/44 (77%)	-0.44	2 (5%) 22 28	54, 62, 86, 117	0
6	f	31/44 (70%)	-0.19	2 (6%) 18 24	59, 68, 97, 155	0
7	H	64/65 (98%)	-0.24	2 (3%) 49 56	53, 64, 85, 106	0
7	h	64/65 (98%)	-0.28	3 (4%) 31 38	56, 70, 95, 115	0
8	I	37/38 (97%)	-0.14	2 (5%) 25 32	54, 63, 127, 162	0
8	i	37/38 (97%)	-0.03	5 (13%) 3 4	55, 65, 122, 143	0
9	J	38/39 (97%)	-0.17	2 (5%) 26 33	51, 70, 124, 180	0
9	j	39/39 (100%)	0.25	6 (15%) 2 3	60, 76, 128, 171	0
10	K	37/37 (100%)	-0.48	1 (2%) 54 62	59, 68, 89, 113	0
10	k	37/37 (100%)	-0.41	0 100 100	68, 75, 98, 112	0
11	L	36/37 (97%)	-0.30	3 (8%) 11 15	41, 48, 100, 142	0
11	l	36/37 (97%)	-0.38	2 (5%) 24 30	43, 50, 104, 136	0
12	M	32/36 (88%)	-0.61	1 (3%) 49 56	45, 50, 76, 147	0
12	m	33/36 (91%)	-0.38	2 (6%) 21 27	46, 51, 73, 154	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.03	16 (6%) 18 23	43, 65, 116, 187	0
13	o	243/244 (99%)	0.05	27 (11%) 5 7	45, 67, 129, 174	0
14	T	29/32 (90%)	-0.67	1 (3%) 45 52	44, 50, 78, 119	0
14	t	29/32 (90%)	-0.66	0 100 100	46, 51, 81, 133	0
15	U	96/104 (92%)	-0.40	0 100 100	49, 59, 91, 102	0
15	u	97/104 (93%)	-0.34	1 (1%) 82 86	53, 62, 84, 138	0
16	V	137/137 (100%)	-0.48	2 (1%) 73 79	47, 58, 83, 107	0
16	v	137/137 (100%)	-0.15	4 (2%) 51 58	53, 71, 104, 139	0
17	X	38/40 (95%)	-0.26	3 (7%) 12 17	62, 72, 94, 113	0
17	x	38/40 (95%)	0.05	5 (13%) 3 4	64, 79, 124, 162	0
18	Y	29/30 (96%)	1.13	6 (20%) 1 1	69, 87, 124, 125	0
18	y	29/30 (96%)	0.38	4 (13%) 2 4	76, 92, 113, 116	0
19	Z	62/62 (100%)	0.05	8 (12%) 3 5	65, 80, 134, 159	0
19	z	62/62 (100%)	0.39	11 (17%) 1 1	81, 95, 146, 205	0
20	R	34/34 (100%)	1.84	15 (44%) 0 0	82, 103, 134, 144	0
All	All	5283/5384 (98%)	-0.35	221 (4%) 36 43	40, 60, 100, 205	3 (0%)

All (221) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	23	ALA	7.9
3	c	20	SER	7.3
2	b	495	PHE	7.3
5	E	84	LYS	7.2
18	Y	18	VAL	6.9
18	Y	19	ILE	6.5
13	o	4	THR	6.3
1	a	11	ALA	6.1
13	O	60	ARG	6.0
13	o	56	PRO	6.0
2	b	494	GLY	5.8
13	O	56	PRO	5.7
19	Z	31	GLN	5.5
12	m	34	LYS	5.3
17	x	2	THR	5.3
19	z	31	GLN	5.2
3	C	143	TYR	5.2

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Mol	Chain	Res	Type	RSRZ
17	x	38	GLN	5.1
19	Z	32	ASP	5.1
13	O	62	GLU	5.1
5	e	84	LYS	5.0
13	O	4	THR	4.9
3	c	143	TYR	4.9
2	b	127	ARG	4.8
19	z	32	ASP	4.8
2	b	504	THR	4.8
13	o	60	ARG	4.8
9	j	3	GLU	4.8
19	z	38	GLN	4.8
18	y	18	VAL	4.8
20	R	35	LEU	4.8
13	o	62	GLU	4.7
1	A	11	ALA	4.7
13	o	57	LYS	4.7
20	R	32	GLN	4.7
13	o	59	LYS	4.7
6	F	12	SER	4.6
19	z	3	ILE	4.5
19	Z	3	ILE	4.5
12	M	33	GLN	4.5
13	O	5	LEU	4.5
13	o	207	ARG	4.4
13	o	63	ALA	4.4
19	z	60	PHE	4.3
6	f	15	ILE	4.3
13	O	59	LYS	4.3
3	c	19	ASN	4.2
11	L	3	PRO	4.2
14	T	30[A]	THR	4.2
20	R	3	TRP	4.1
13	o	58	ASN	4.1
2	b	293	ALA	4.1
1	A	13	LEU	4.0
13	O	63	ALA	4.0
9	j	4	GLY	4.0
2	B	494	GLY	4.0
13	o	24	ASP	4.0
11	l	3	PRO	3.9
2	b	489	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
3	C	207	ARG	3.9
4	D	11	GLU	3.9
3	c	21	ILE	3.9
2	b	503	THR	3.9
20	R	21	ARG	3.8
8	I	36	ASP	3.8
4	D	12	ARG	3.8
8	i	38	GLU	3.8
9	j	1	MET	3.7
13	O	25	THR	3.7
6	f	16[A]	PHE	3.7
18	Y	20	ALA	3.7
7	h	6	TRP	3.7
9	j	6	ARG	3.6
19	Z	30	PRO	3.5
16	v	15	GLU	3.5
3	c	23	ALA	3.4
18	y	43	ARG	3.4
2	b	505	ARG	3.4
17	X	38	GLN	3.4
19	z	42	LEU	3.4
13	o	246	ALA	3.4
20	R	4	ARG	3.4
9	j	2	SER	3.4
18	Y	21	GLN	3.4
20	R	24	LEU	3.4
7	H	6	TRP	3.3
20	R	33	LYS	3.3
13	o	35	SER	3.3
2	B	495	PHE	3.3
18	y	19	ILE	3.3
17	X	2	THR	3.3
1	a	262[A]	TYR	3.3
2	b	502	VAL	3.3
19	Z	35	ARG	3.3
2	b	484[A]	PRO	3.2
13	o	55	GLU	3.2
20	R	20	VAL	3.2
8	I	34	ARG	3.2
19	z	35	ARG	3.2
18	y	41	VAL	3.1
16	v	17	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
19	z	62	VAL	3.1
2	b	86	ILE	3.1
18	Y	22	LEU	3.1
12	m	33	GLN	3.1
19	z	34	ASP	3.1
13	O	61	GLN	3.1
2	B	162	PHE	3.1
3	c	207	ARG	3.0
13	o	22	LEU	3.0
11	L	7	ARG	3.0
18	Y	43	ARG	3.0
3	c	22	PHE	3.0
13	o	64	GLU	3.0
17	x	39	ARG	3.0
5	e	81	GLU	2.9
6	F	13	TYR	2.9
19	Z	34	ASP	2.9
2	b	85	GLY	2.9
13	o	61	GLN	2.9
13	o	23	ASP	2.9
9	J	3	GLU	2.9
1	a	16	ARG	2.9
20	R	34	LEU	2.9
3	c	192	GLY	2.8
13	o	5	LEU	2.8
2	b	488	PRO	2.8
2	B	295	GLY	2.8
2	b	373	LYS	2.8
2	b	294	SER	2.8
5	e	24	SER	2.8
4	d	12	ARG	2.8
8	i	34	ARG	2.8
17	x	3	ILE	2.8
19	z	30	PRO	2.8
2	b	161	LEU	2.8
2	b	496	TYR	2.8
20	R	28	VAL	2.7
13	o	26	ALA	2.7
13	o	25	THR	2.7
5	E	59	GLU	2.7
11	l	2	GLU	2.7
5	e	82	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
9	J	6	ARG	2.7
8	i	37	LEU	2.6
9	j	5	GLY	2.6
13	o	27	ARG	2.6
2	b	493[A]	TRP	2.6
1	a	13	LEU	2.6
20	R	29	LYS	2.6
8	i	36	ASP	2.6
8	i	35	LYS	2.6
16	v	16	GLY	2.6
13	O	132	ASN	2.6
3	c	234	VAL	2.5
3	c	142	GLU	2.5
3	c	253	LEU	2.5
2	b	435	GLU	2.5
2	b	485	GLU	2.5
2	b	374	ASN	2.5
20	R	6	LEU	2.5
2	B	485	GLU	2.5
2	b	162	PHE	2.5
1	A	262[A]	TYR	2.5
2	b	295	GLY	2.5
2	B	86	ILE	2.4
13	O	207	ARG	2.4
13	o	54	GLU	2.4
19	z	61	VAL	2.4
3	C	142	GLU	2.4
20	R	18	TRP	2.4
13	O	55	GLU	2.4
13	o	134	THR	2.4
2	b	375	GLY	2.3
3	C	24	THR	2.3
7	h	3[A]	ARG	2.3
13	O	90	ASP	2.3
2	b	376	VAL	2.3
13	O	89	SER	2.3
16	v	14	SER	2.3
19	Z	60	PHE	2.3
13	O	27	ARG	2.3
3	c	201	ASN	2.3
19	Z	2	THR	2.3
11	L	5	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	374	ASN	2.2
13	o	130	GLN	2.2
3	C	182	PHE	2.2
15	u	20	ALA	2.2
1	A	16	ARG	2.2
2	B	373	LYS	2.2
3	C	181	PHE	2.2
5	e	59	GLU	2.2
2	B	85	GLY	2.2
13	o	33	ASP	2.2
20	R	5	VAL	2.1
2	b	501	ASP	2.1
13	O	58	ASN	2.1
16	V	15	GLU	2.1
2	B	293	ALA	2.1
4	D	238[A]	THR	2.1
3	c	233	VAL	2.1
5	E	61	ARG	2.1
7	H	23	PRO	2.1
10	K	13	GLU	2.1
1	a	228	THR	2.1
2	b	128	THR	2.1
17	x	34	ILE	2.1
2	B	487	SER	2.1
13	o	34	SER	2.1
2	b	20	ILE	2.0
3	C	253	LEU	2.0
17	X	3	ILE	2.0
20	R	2	ASP	2.0
2	b	218	LEU	2.0
7	h	65	LEU	2.0
13	o	98	GLU	2.0
3	C	263	ALA	2.0
5	e	42	LEU	2.0
16	V	16	GLY	2.0
2	B	504	THR	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, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	FME	i	1	10/11	0.92	0.16	50,68,83,87	0
14	FME	T	1	10/11	0.96	0.09	47,58,69,72	0
14	FME	t	1	10/11	0.96	0.09	43,50,69,76	0
12	FME	M	1	10/11	0.97	0.13	49,61,93,102	0
12	FME	m	1	10/11	0.98	0.12	50,64,91,120	0
8	FME	I	1	10/11	0.98	0.10	60,68,82,83	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
30	UNL	b	626	33/-	0.41	0.36	69,96,158,173	0
30	UNL	I	101	40/-	0.48	0.35	75,109,159,173	0
30	UNL	B	625	33/-	0.50	0.36	58,109,143,152	0
32	LMT	T	101	35/35	0.56	0.32	76,131,174,184	0
30	UNL	i	101	40/-	0.59	0.31	74,107,162,167	0
34	LMG	C	521	51/55	0.62	0.34	59,121,157,175	0
32	LMT	b	621	25/35	0.63	0.29	86,120,162,172	0
27	GOL	a	418	6/6	0.64	0.58	80,108,110,120	0
30	UNL	K	101[A]	34/-	0.66	0.35	90,113,127,130	34
30	UNL	K	101[B]	34/-	0.66	0.35	90,113,127,130	34
32	LMT	M	101	35/35	0.66	0.26	64,95,120,130	0
30	UNL	A	415	28/-	0.67	0.39	89,115,132,142	0
32	LMT	B	629	35/35	0.67	0.40	65,117,147,151	0
32	LMT	F	101	35/35	0.68	0.50	104,135,179,184	0
32	LMT	B	630	25/35	0.69	0.25	57,92,148,164	0
30	UNL	c	525[A]	32/-	0.69	0.40	98,115,128,135	32
33	LHG	a	420[A]	42/49	0.69	0.36	99,148,163,168	42
33	LHG	a	420[B]	42/49	0.69	0.36	99,148,163,168	42
30	UNL	c	525[B]	32/-	0.69	0.40	98,115,128,135	32
35	HTG	b	623	19/19	0.69	0.47	83,133,157,164	0
34	LMG	c	521	51/55	0.70	0.28	72,137,167,189	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
32	LMT	A	418	35/35	0.70	0.33	72,119,140,144	0
30	UNL	m	102	10/-	0.73	0.38	75,77,102,106	0
30	UNL	d	408	36/-	0.73	0.20	68,97,136,143	0
32	LMT	m	103	35/35	0.73	0.26	55,95,109,123	0
30	UNL	j	101	10/-	0.73	0.32	83,96,103,107	0
35	HTG	D	710	16/19	0.75	0.26	86,105,131,151	0
34	LMG	z	101	39/55	0.75	0.28	75,130,153,169	0
30	UNL	x	101	18/-	0.76	0.23	73,81,134,142	0
34	LMG	Z	101	37/55	0.76	0.27	66,119,147,176	0
27	GOL	b	624	6/6	0.76	0.20	93,103,110,118	0
32	LMT	b	627	25/35	0.76	0.23	53,101,149,156	0
32	LMT	e	101	35/35	0.76	0.52	107,142,187,194	0
32	LMT	A	420	35/35	0.77	0.37	96,138,157,172	0
32	LMT	B	627	35/35	0.78	0.27	61,108,138,152	0
27	GOL	l	102[B]	6/6	0.78	0.80	70,107,107,108	6
27	GOL	l	102[A]	6/6	0.78	0.80	71,105,107,108	6
27	GOL	o	304	6/6	0.79	0.22	89,93,102,106	0
30	UNL	l	101	10/-	0.79	0.34	71,79,95,97	0
26	SQD	f	102	43/54	0.80	0.32	97,131,176,184	0
26	SQD	b	620	54/54	0.80	0.18	68,98,127,133	0
35	HTG	d	409	16/19	0.80	0.32	79,122,141,161	0
29	PL9	A	414[B]	55/55	0.81	0.24	66,96,111,117	55
27	GOL	B	626	6/6	0.81	0.22	68,87,96,119	0
35	HTG	B	622	19/19	0.81	0.26	66,99,118,134	0
29	PL9	A	414[A]	55/55	0.81	0.24	66,96,110,116	55
30	UNL	X	102	18/-	0.81	0.21	62,75,114,115	0
30	UNL	a	415	30/-	0.81	0.34	92,122,144,155	0
30	UNL	J	101	10/-	0.82	0.19	69,81,97,105	0
35	HTG	C	522	19/19	0.82	0.31	111,128,143,152	0
32	LMT	t	101	26/35	0.82	0.18	75,114,149,159	0
27	GOL	o	303	6/6	0.82	0.27	85,106,121,123	0
32	LMT	a	417	35/35	0.82	0.39	112,138,151,161	0
37	CA	F	103	1/1	0.82	0.16	128,128,128,128	0
27	GOL	A	411	6/6	0.83	0.18	63,80,85,90	0
26	SQD	a	412	54/54	0.83	0.19	67,97,137,156	0
27	GOL	c	527	6/6	0.83	0.26	103,117,127,128	0
27	GOL	O	302	6/6	0.83	0.22	67,88,100,104	0
37	CA	o	302	1/1	0.83	0.06	111,111,111,111	0
27	GOL	a	419	6/6	0.84	0.52	60,80,88,94	0
34	LMG	c	501	51/55	0.84	0.18	67,90,114,134	0
29	PL9	a	414[A]	55/55	0.84	0.24	87,109,123,130	55
29	PL9	a	414[B]	55/55	0.84	0.24	87,109,124,130	55

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	UNL	D	709	40/-	0.85	0.18	67,98,145,157	0
26	SQD	A	412	54/54	0.85	0.17	66,89,136,163	0
33	LHG	E	101[A]	42/49	0.85	0.23	70,107,122,131	42
35	HTG	c	522	19/19	0.85	0.26	104,126,145,148	0
33	LHG	E	101[B]	42/49	0.85	0.23	70,107,123,131	42
27	GOL	d	411	6/6	0.85	0.29	52,68,77,89	0
27	GOL	D	701	6/6	0.85	0.43	56,77,86,93	0
35	HTG	o	301	19/19	0.87	0.17	58,86,117,132	0
27	GOL	v	202[B]	6/6	0.87	0.17	68,79,85,88	6
27	GOL	v	202[A]	6/6	0.87	0.17	68,79,85,87	6
34	LMG	C	501	51/55	0.88	0.15	61,90,118,132	0
23	CLA	b	616	65/65	0.88	0.17	49,63,130,145	0
34	LMG	D	711	51/55	0.88	0.18	50,68,126,141	0
37	CA	O	301	1/1	0.88	0.05	113,113,113,113	0
37	CA	f	103	1/1	0.88	0.09	123,123,123,123	0
26	SQD	B	620	54/54	0.88	0.15	64,98,139,146	0
23	CLA	d	402	65/65	0.89	0.15	51,67,133,149	0
34	LMG	d	410	51/55	0.89	0.17	52,69,126,154	0
25	BCR	K	102	40/40	0.89	0.19	55,67,79,82	0
23	CLA	B	616	65/65	0.89	0.19	50,63,135,143	0
27	GOL	V	203[A]	6/6	0.89	0.17	59,73,76,83	6
27	GOL	V	203[B]	6/6	0.89	0.17	58,73,76,83	6
23	CLA	c	514	65/65	0.89	0.18	68,93,130,148	0
35	HTG	b	622	19/19	0.89	0.16	58,83,125,127	0
25	BCR	h	101	40/40	0.90	0.15	55,65,91,97	0
23	CLA	b	601	65/65	0.90	0.15	60,88,131,160	0
23	CLA	C	514	65/65	0.90	0.14	57,84,113,118	0
25	BCR	C	515	40/40	0.90	0.14	57,75,89,93	0
34	LMG	C	520	51/55	0.90	0.18	57,87,123,129	0
23	CLA	c	513	65/65	0.90	0.18	63,81,130,137	0
23	CLA	B	601	65/65	0.91	0.14	55,78,119,156	0
35	HTG	V	202	11/19	0.91	0.39	81,115,121,129	0
34	LMG	c	520	51/55	0.91	0.18	63,91,137,157	0
27	GOL	D	712	6/6	0.91	0.22	51,66,78,101	0
35	HTG	b	625	19/19	0.91	0.11	64,78,100,111	0
25	BCR	d	403	40/40	0.91	0.12	53,65,102,114	0
25	BCR	Y	101	40/40	0.92	0.13	51,64,84,89	0
30	UNL	D	708	17/-	0.92	0.15	65,78,110,128	0
30	UNL	d	407	17/-	0.92	0.12	67,84,111,112	0
36	DGD	c	518[A]	62/66	0.92	0.13	57,70,121,139	62
36	DGD	c	518[B]	62/66	0.92	0.13	57,70,121,139	62
36	DGD	h	102	62/66	0.92	0.12	50,66,80,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	LMG	B	621	51/55	0.92	0.13	56,72,94,121	0
27	GOL	O	303	6/6	0.92	0.17	88,102,106,117	0
26	SQD	X	101	43/54	0.92	0.17	73,104,134,142	0
23	CLA	B	606	65/65	0.92	0.14	44,58,110,134	0
36	DGD	C	519	62/66	0.93	0.12	44,61,99,122	0
23	CLA	b	606	65/65	0.93	0.13	40,59,109,127	0
34	LMG	m	101	51/55	0.93	0.12	60,76,98,112	0
23	CLA	C	507	65/65	0.93	0.13	56,72,124,142	0
23	CLA	c	507	65/65	0.93	0.13	53,69,127,138	0
23	CLA	a	409	65/65	0.93	0.17	43,56,143,159	0
27	GOL	B	628	6/6	0.93	0.26	73,79,89,102	0
23	CLA	C	513	65/65	0.93	0.14	54,74,115,133	0
36	DGD	C	518[A]	62/66	0.94	0.12	51,67,115,122	62
36	DGD	C	518[B]	62/66	0.94	0.12	51,67,116,122	62
23	CLA	D	703	65/65	0.94	0.13	47,59,126,136	0
36	DGD	H	102	62/66	0.94	0.12	48,63,76,88	0
25	BCR	k	101	40/40	0.94	0.14	56,74,83,91	0
23	CLA	A	408	65/65	0.94	0.13	42,54,132,155	0
36	DGD	c	519	62/66	0.94	0.12	50,68,104,134	0
25	BCR	c	515	40/40	0.94	0.10	71,83,93,95	0
25	BCR	D	704	40/40	0.94	0.10	47,60,103,111	0
33	LHG	d	406[A]	49/49	0.94	0.17	54,66,114,132	49
37	CA	c	523	1/1	0.94	0.09	76,76,76,76	0
37	CA	c	524	1/1	0.94	0.06	81,81,81,81	0
35	HTG	B	624	19/19	0.94	0.10	66,78,100,107	0
33	LHG	d	406[B]	49/49	0.94	0.17	54,66,114,132	49
33	LHG	D	707[B]	49/49	0.95	0.16	51,61,108,113	49
23	CLA	B	609	65/65	0.95	0.16	45,60,74,78	0
23	CLA	B	611	65/65	0.95	0.10	38,48,65,76	0
23	CLA	b	609	65/65	0.95	0.15	47,64,75,91	0
25	BCR	A	409	40/40	0.95	0.10	41,53,67,69	0
33	LHG	b	629[A]	49/49	0.95	0.15	53,61,68,92	49
33	LHG	b	629[B]	49/49	0.95	0.15	52,61,68,93	49
25	BCR	t	102	40/40	0.95	0.10	43,63,83,98	0
26	SQD	A	410[A]	54/54	0.95	0.13	58,79,110,117	54
26	SQD	A	410[B]	54/54	0.95	0.13	58,79,110,118	54
25	BCR	B	618	40/40	0.95	0.09	43,57,73,83	0
23	CLA	C	508	65/65	0.95	0.12	50,63,87,96	0
23	CLA	C	509	65/65	0.95	0.10	47,56,121,146	0
27	GOL	b	628	6/6	0.95	0.21	84,86,95,96	0
26	SQD	a	411[A]	54/54	0.95	0.15	59,82,124,129	54
26	SQD	a	411[B]	54/54	0.95	0.15	59,82,124,129	54

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
25	BCR	H	101	40/40	0.95	0.09	47,64,80,89	0
23	CLA	c	509	65/65	0.95	0.12	43,66,128,150	0
25	BCR	T	102	40/40	0.95	0.09	44,61,75,80	0
23	CLA	c	512	65/65	0.95	0.12	57,71,87,114	0
27	GOL	B	623	6/6	0.95	0.19	71,85,90,90	0
25	BCR	b	618	40/40	0.95	0.10	47,61,78,83	0
33	LHG	D	707[A]	49/49	0.95	0.16	51,61,108,113	49
39	MG	J	102	1/1	0.95	0.04	60,60,60,60	0
25	BCR	C	516	40/40	0.96	0.11	51,63,77,84	0
23	CLA	b	612	65/65	0.96	0.10	40,54,65,72	0
23	CLA	b	614	65/65	0.96	0.10	42,51,105,124	0
21	FE2	a	401[A]	1/1	0.96	0.05	54,54,54,54	1
23	CLA	c	505	65/65	0.96	0.11	50,63,111,139	0
29	PL9	D	705[A]	55/55	0.96	0.12	38,51,61,68	55
29	PL9	D	705[B]	55/55	0.96	0.12	37,51,61,69	55
23	CLA	c	506	65/65	0.96	0.10	48,65,88,99	0
25	BCR	a	410	40/40	0.96	0.08	44,56,67,73	0
29	PL9	d	404[A]	55/55	0.96	0.11	41,52,62,69	55
29	PL9	d	404[B]	55/55	0.96	0.11	41,52,63,70	55
25	BCR	b	617	40/40	0.96	0.10	46,57,65,70	0
27	GOL	C	523[A]	6/6	0.96	0.09	59,64,68,73	6
27	GOL	C	523[B]	6/6	0.96	0.09	59,64,69,73	6
21	FE2	a	401[B]	1/1	0.96	0.05	54,54,54,54	1
25	BCR	b	619	40/40	0.96	0.09	48,62,86,89	0
33	LHG	A	419[A]	49/49	0.96	0.13	51,65,85,93	49
33	LHG	A	419[B]	49/49	0.96	0.13	51,66,85,93	49
23	CLA	c	508	65/65	0.96	0.11	52,70,82,92	0
25	BCR	c	516	40/40	0.96	0.12	53,67,80,90	0
23	CLA	a	407[A]	65/65	0.96	0.11	43,56,128,136	65
23	CLA	a	407[B]	65/65	0.96	0.11	43,56,128,136	65
23	CLA	C	502	65/65	0.96	0.08	49,60,74,85	0
23	CLA	C	510	65/65	0.96	0.11	46,59,84,88	0
36	DGD	c	517[A]	62/66	0.96	0.11	49,64,104,113	62
36	DGD	c	517[B]	62/66	0.96	0.11	48,64,104,113	62
25	BCR	y	101	40/40	0.96	0.09	56,72,86,96	0
23	CLA	b	602	65/65	0.96	0.13	48,61,84,94	0
33	LHG	d	405[A]	49/49	0.96	0.16	50,59,71,78	49
33	LHG	d	405[B]	49/49	0.96	0.16	50,59,71,79	49
23	CLA	b	604	65/65	0.96	0.12	43,53,103,127	0
25	BCR	B	617	40/40	0.96	0.10	41,55,63,71	0
33	LHG	d	412[A]	49/49	0.96	0.14	52,68,81,90	49
33	LHG	d	412[B]	49/49	0.96	0.14	52,68,82,90	49

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	C	512	65/65	0.96	0.13	52,64,81,91	0
25	BCR	B	619	40/40	0.96	0.09	47,60,90,98	0
38	HEM	f	101	43/43	0.96	0.14	58,86,113,139	0
23	CLA	C	505	65/65	0.96	0.10	40,57,96,128	0
27	GOL	c	526[A]	6/6	0.97	0.25	72,74,80,83	6
27	GOL	c	526[B]	6/6	0.97	0.25	72,75,81,83	6
23	CLA	c	504	65/65	0.97	0.10	49,71,86,103	0
23	CLA	B	612	65/65	0.97	0.08	36,50,64,75	0
23	CLA	B	614	65/65	0.97	0.10	39,51,111,124	0
23	CLA	B	615	65/65	0.97	0.10	44,55,83,97	0
23	CLA	a	405[A]	65/65	0.97	0.12	41,48,64,76	65
23	CLA	a	405[B]	65/65	0.97	0.12	40,47,64,77	65
23	CLA	c	510	65/65	0.97	0.10	50,63,92,98	0
23	CLA	c	511	65/65	0.97	0.10	50,64,77,90	0
23	CLA	A	404[B]	65/65	0.97	0.12	37,44,63,71	65
23	CLA	B	602	65/65	0.97	0.11	46,56,71,86	0
23	CLA	C	504	65/65	0.97	0.09	47,62,72,85	0
23	CLA	B	603	65/65	0.97	0.10	42,54,74,83	0
24	PHO	A	407[A]	64/64	0.97	0.09	40,46,53,59	64
24	PHO	A	407[B]	64/64	0.97	0.09	40,46,53,60	64
24	PHO	a	408[A]	64/64	0.97	0.09	42,49,54,57	64
24	PHO	a	408[B]	64/64	0.97	0.09	41,49,55,57	64
24	PHO	a	416[A]	64/64	0.97	0.12	44,56,63,67	64
33	LHG	D	706[A]	49/49	0.97	0.14	48,55,68,77	49
33	LHG	D	706[B]	49/49	0.97	0.14	47,55,68,78	49
36	DGD	C	517[A]	62/66	0.97	0.11	47,59,99,108	62
36	DGD	C	517[B]	62/66	0.97	0.11	47,59,99,108	62
24	PHO	a	416[B]	64/64	0.97	0.12	43,56,63,67	64
23	CLA	C	506	65/65	0.97	0.09	45,61,91,102	0
23	CLA	b	603	65/65	0.97	0.08	45,57,83,95	0
23	CLA	A	406[A]	65/65	0.97	0.09	40,49,114,130	65
33	LHG	L	101[A]	49/49	0.97	0.12	51,59,70,92	49
33	LHG	L	101[B]	49/49	0.97	0.12	50,59,70,92	49
23	CLA	b	605	65/65	0.97	0.11	39,52,78,83	0
23	CLA	B	607	65/65	0.97	0.09	36,48,74,86	0
23	CLA	b	607	65/65	0.97	0.09	38,50,81,91	0
23	CLA	A	406[B]	65/65	0.97	0.09	40,49,114,130	65
37	CA	C	524	1/1	0.97	0.10	71,71,71,71	0
23	CLA	b	610	65/65	0.97	0.09	49,58,71,83	0
23	CLA	b	611	65/65	0.97	0.09	38,51,72,80	0
23	CLA	B	610	65/65	0.97	0.12	43,55,68,89	0
23	CLA	b	613	65/65	0.97	0.08	42,52,88,102	0

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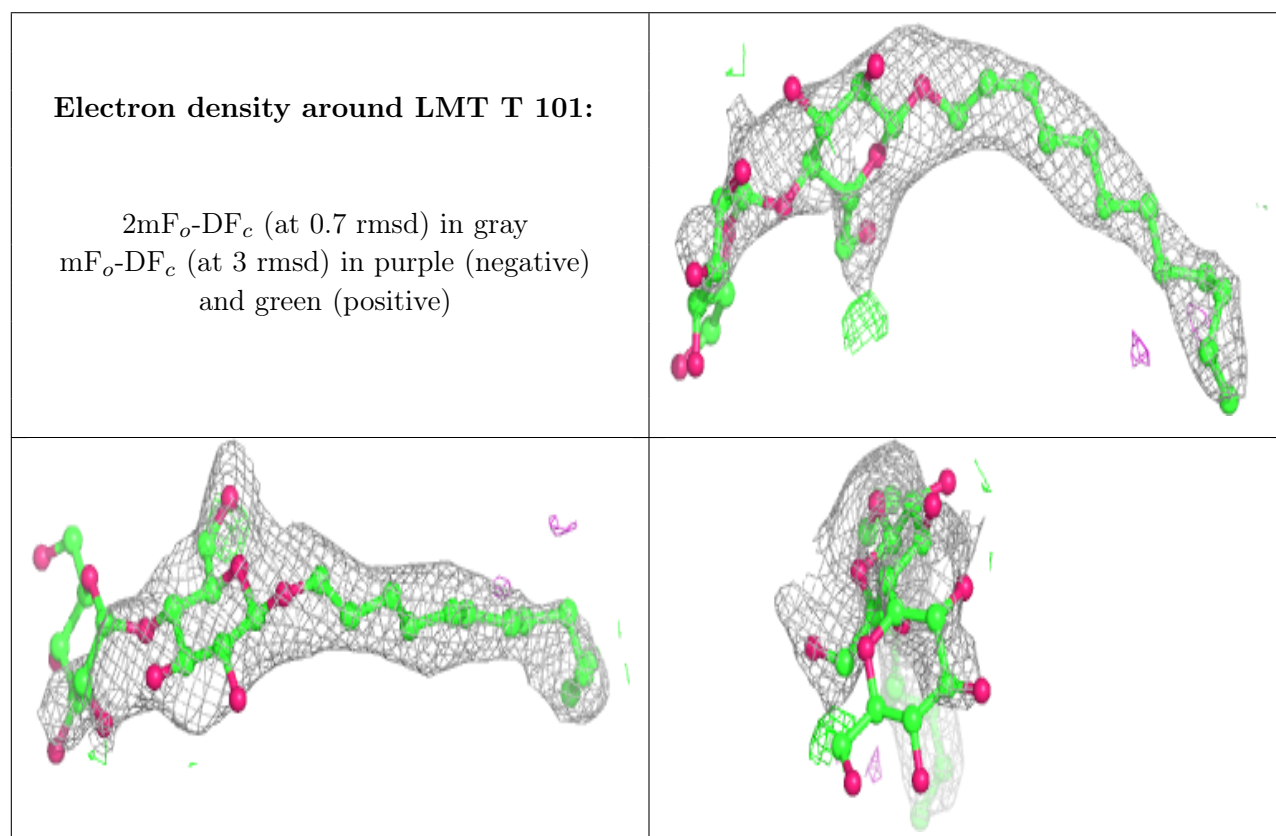
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	C	511	65/65	0.97	0.08	48,59,79,85	0
23	CLA	b	615	65/65	0.97	0.10	49,61,84,94	0
38	HEM	F	102	43/43	0.97	0.11	54,69,84,91	0
23	CLA	A	404[A]	65/65	0.97	0.12	38,44,62,71	65
23	CLA	c	502	65/65	0.97	0.10	54,67,80,89	0
39	MG	j	102	1/1	0.97	0.04	67,67,67,67	0
40	HEC	V	201	43/43	0.97	0.13	41,52,59,62	0
40	HEC	v	201	43/43	0.97	0.11	51,62,70,78	0
23	CLA	a	406[B]	65/65	0.98	0.09	39,47,67,71	65
23	CLA	A	405[B]	65/65	0.98	0.09	35,46,58,71	65
23	CLA	B	608	65/65	0.98	0.09	41,52,71,79	0
21	FE2	A	401[A]	1/1	0.98	0.06	52,52,52,52	1
23	CLA	d	401[A]	65/65	0.98	0.11	41,47,71,91	65
23	CLA	d	401[B]	65/65	0.98	0.11	41,47,72,91	65
31	BCT	A	416[A]	4/4	0.98	0.13	54,56,61,64	4
31	BCT	A	416[B]	4/4	0.98	0.13	54,54,63,63	4
31	BCT	a	404[A]	4/4	0.98	0.11	60,61,69,82	4
31	BCT	a	404[B]	4/4	0.98	0.11	61,61,71,85	4
23	CLA	C	503	65/65	0.98	0.08	43,55,81,92	0
21	FE2	A	401[B]	1/1	0.98	0.06	52,52,52,52	1
23	CLA	B	604	65/65	0.98	0.09	38,48,118,132	0
24	PHO	A	417[A]	64/64	0.98	0.10	37,50,58,62	64
24	PHO	A	417[B]	64/64	0.98	0.10	37,50,58,62	64
23	CLA	c	503	65/65	0.98	0.09	44,60,91,109	0
23	CLA	D	702[A]	65/65	0.98	0.12	36,45,68,81	65
23	CLA	D	702[B]	65/65	0.98	0.12	36,45,68,83	65
23	CLA	B	605	65/65	0.98	0.11	40,50,68,85	0
23	CLA	B	613	65/65	0.98	0.09	40,48,97,105	0
23	CLA	b	608	65/65	0.98	0.07	42,58,79,96	0
23	CLA	A	405[A]	65/65	0.98	0.09	36,46,58,71	65
23	CLA	a	406[A]	65/65	0.98	0.09	39,46,67,71	65
22	CL	a	403[A]	1/1	0.99	0.03	53,53,53,53	1
22	CL	a	403[B]	1/1	0.99	0.03	53,53,53,53	1
28	OEX	A	413[A]	10/10	0.99	0.05	43,46,49,51	10
28	OEX	A	413[B]	10/10	0.99	0.05	42,46,50,50	10
28	OEX	a	413[A]	10/10	0.99	0.06	47,50,54,56	10
28	OEX	a	413[B]	10/10	0.99	0.06	46,50,54,54	10
22	CL	A	402[A]	1/1	0.99	0.02	43,43,43,43	1
22	CL	A	402[B]	1/1	0.99	0.02	44,44,44,44	1
22	CL	A	403[A]	1/1	0.99	0.04	47,47,47,47	1
22	CL	A	403[B]	1/1	0.99	0.04	47,47,47,47	1
22	CL	a	402[A]	1/1	0.99	0.06	49,49,49,49	1

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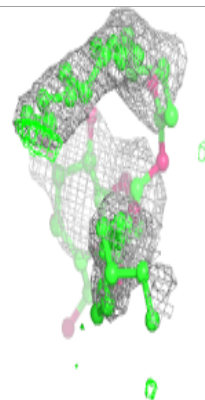
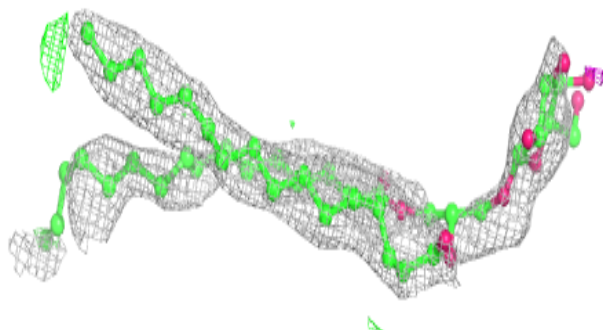
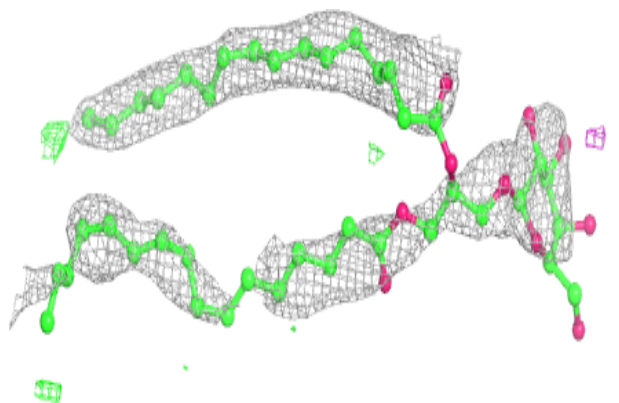
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CL	a	402[B]	1/1	0.99	0.06	50,50,50,50	1

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.

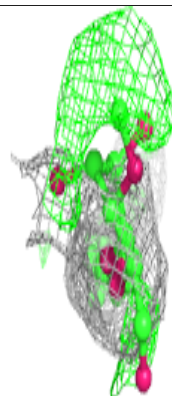
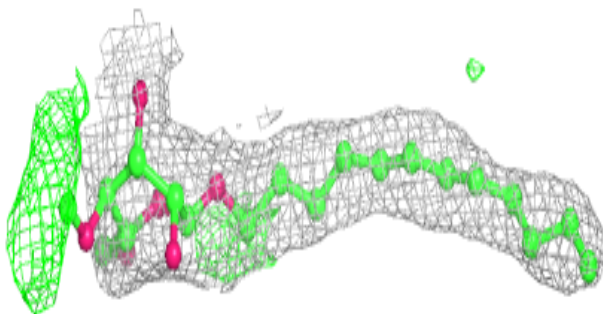
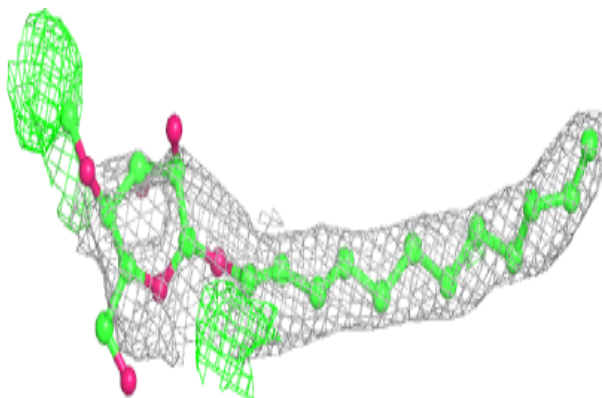


Electron density around LMG C 521:

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

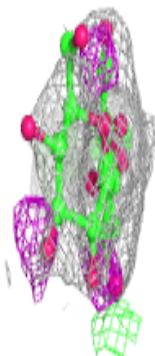
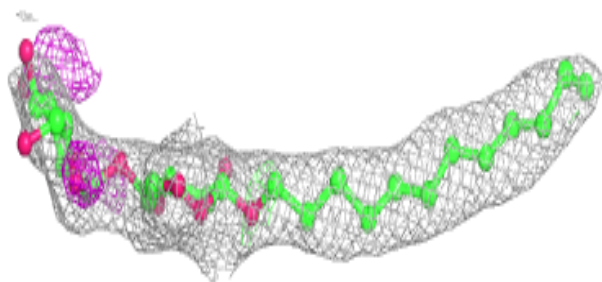
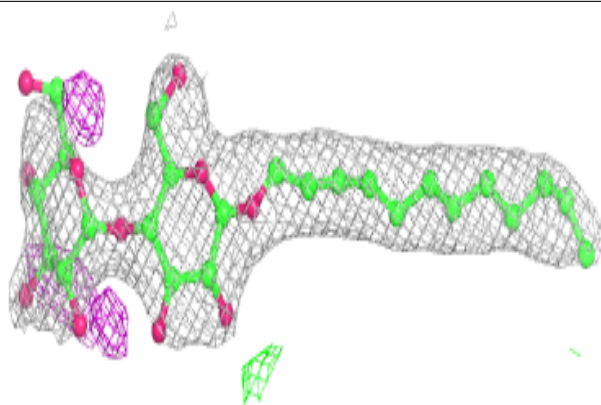
**Electron density around LMT b 621:**

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

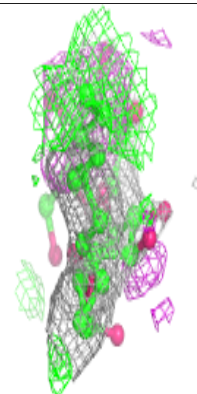
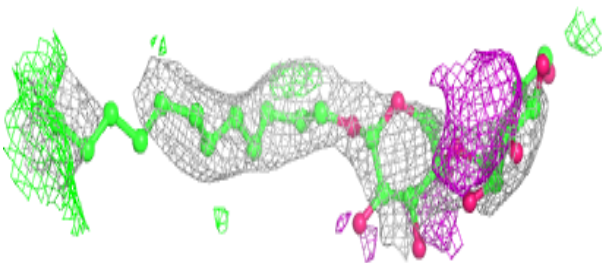
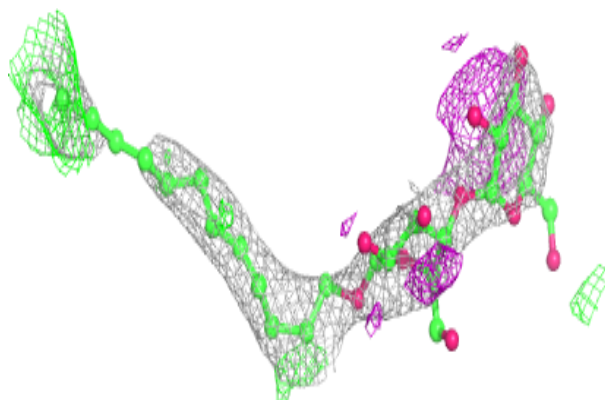


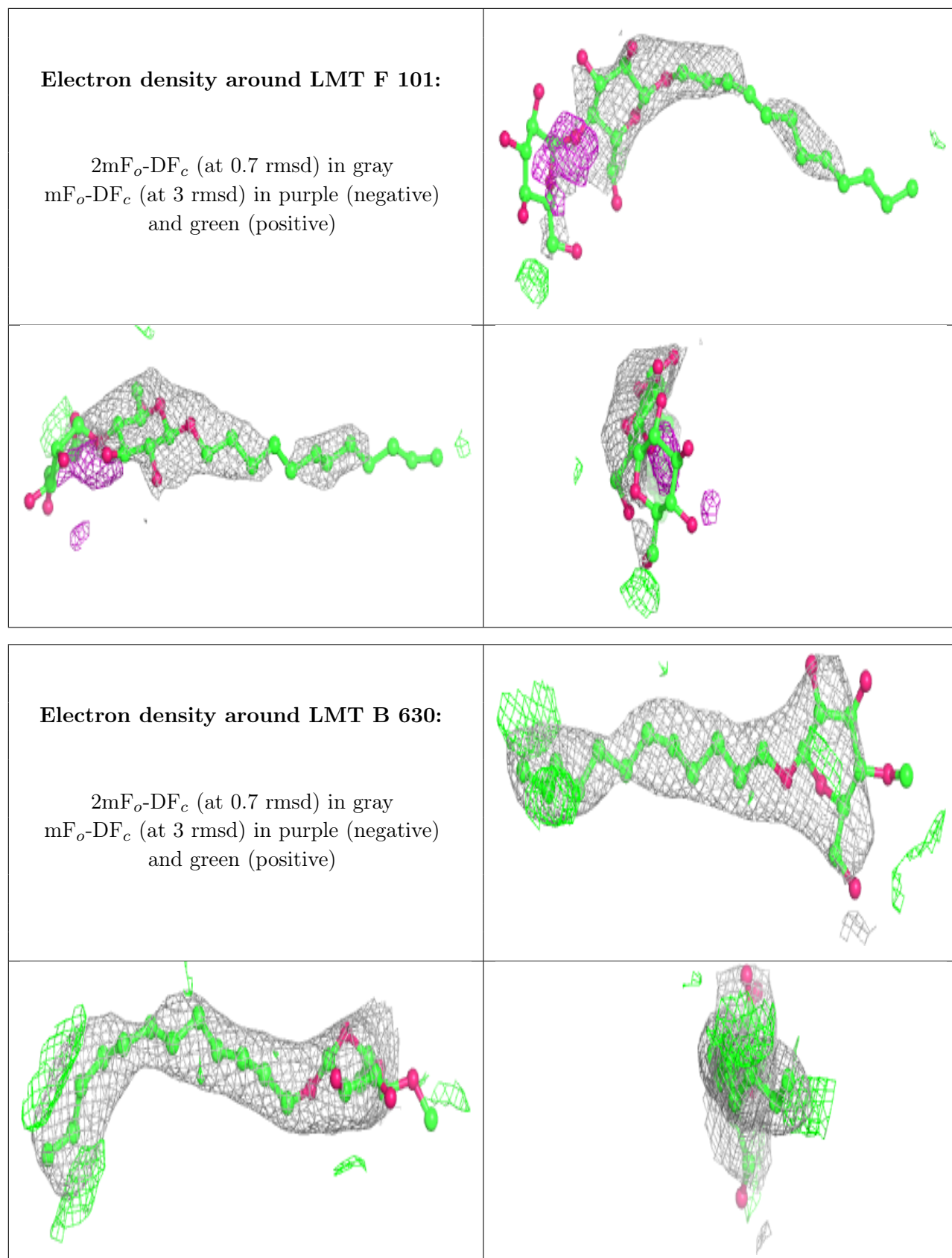
Electron density around LMT M 101:

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

**Electron density around LMT B 629:**

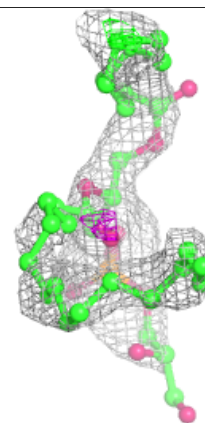
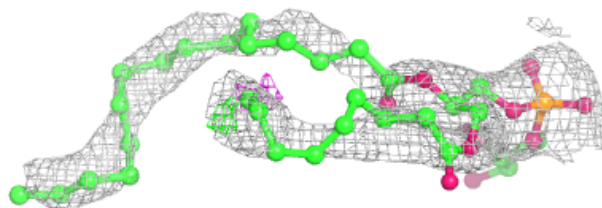
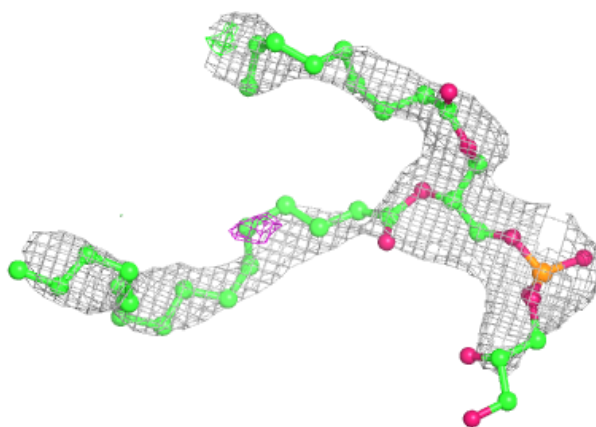
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



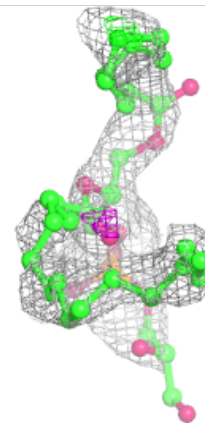
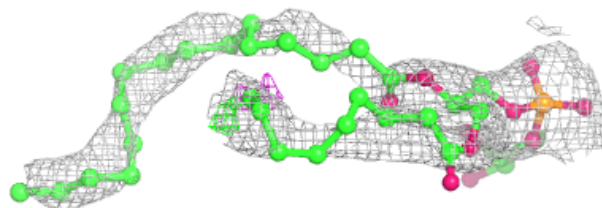
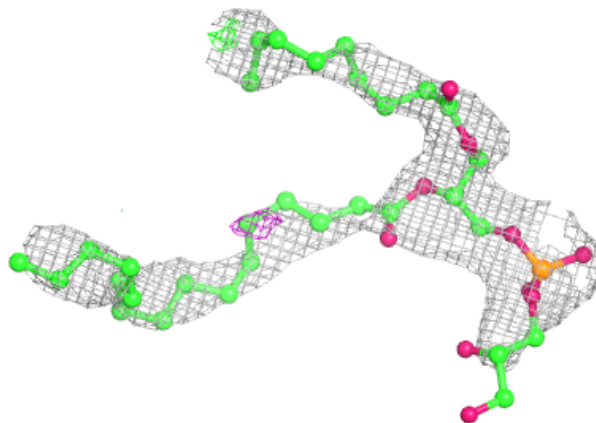


Electron density around LHG a 420 (A):

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

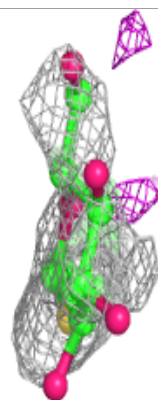
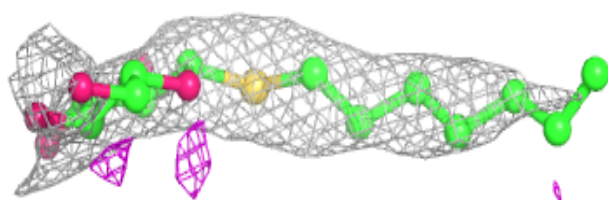
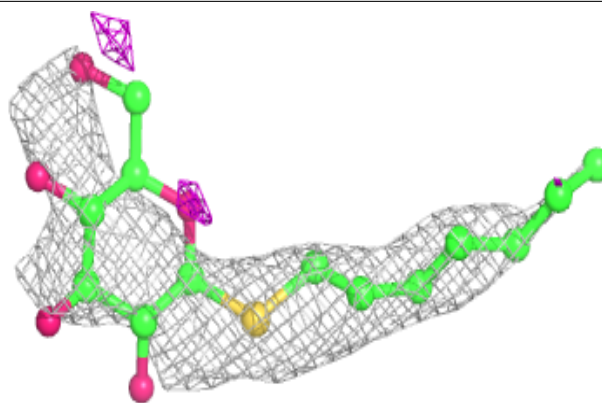
**Electron density around LHG a 420 (B):**

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

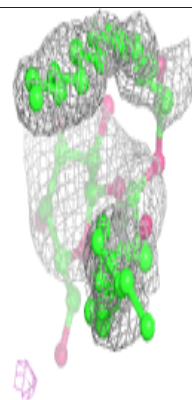
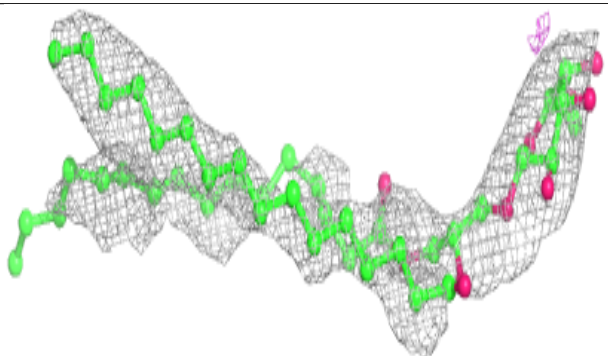
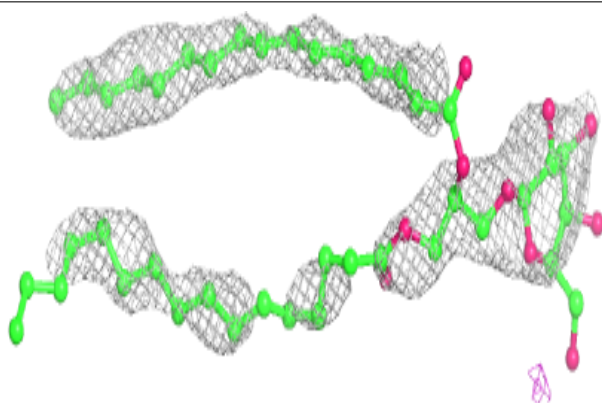


Electron density around HTG b 623:

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

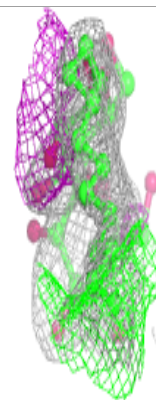
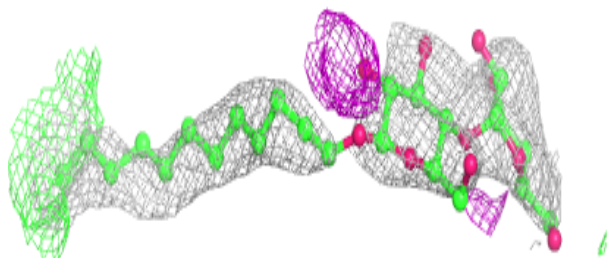
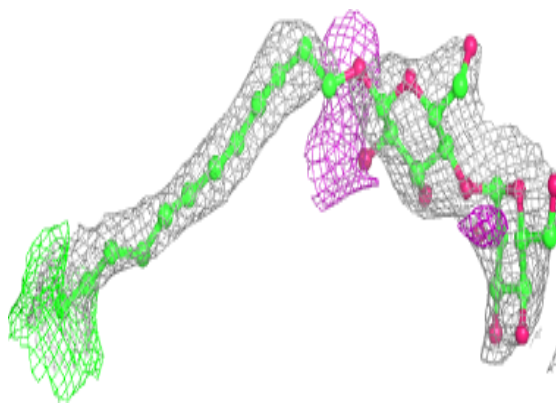
**Electron density around LMG c 521:**

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

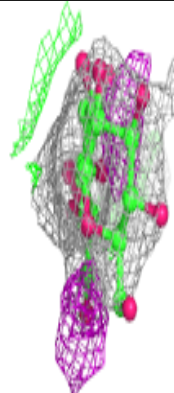
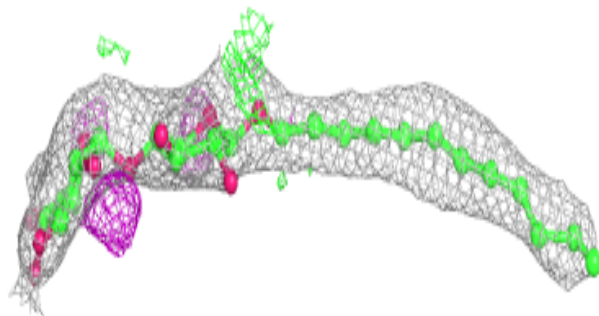
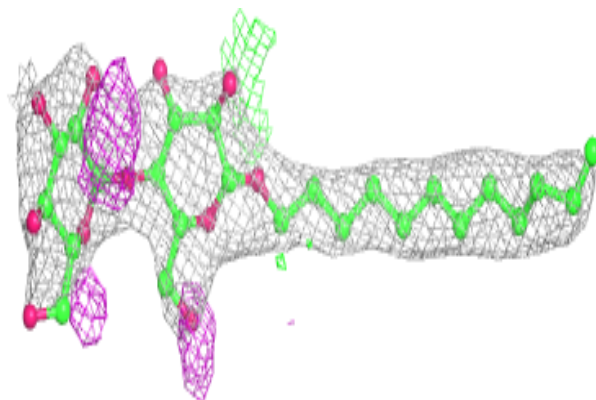


Electron density around LMT A 418:

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

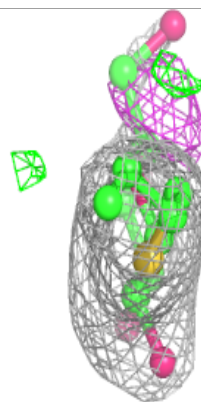
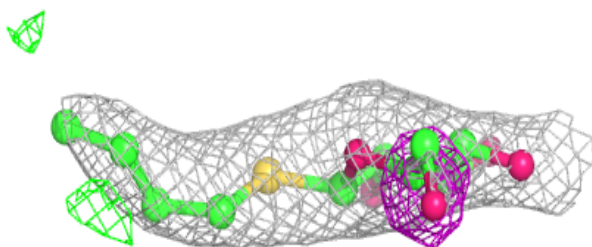
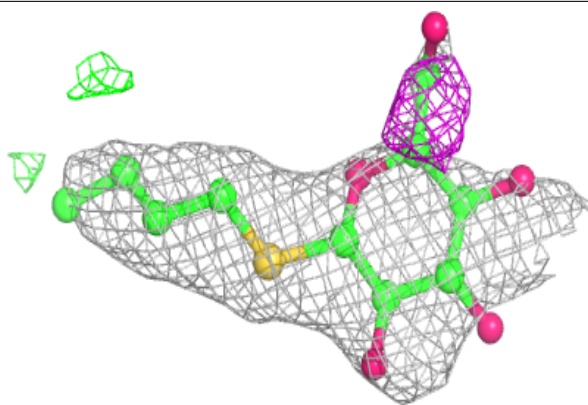
**Electron density around LMT m 103:**

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

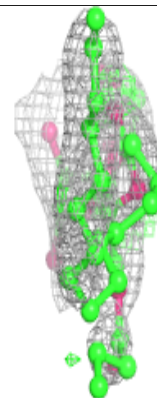
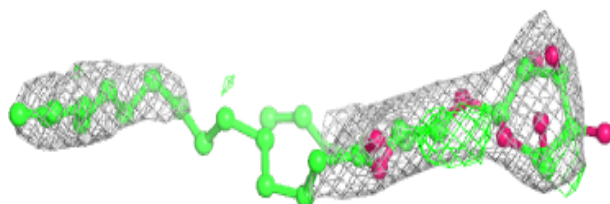
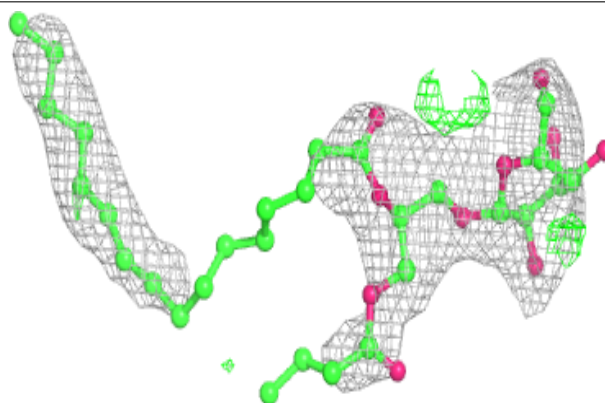


Electron density around HTG D 710:

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

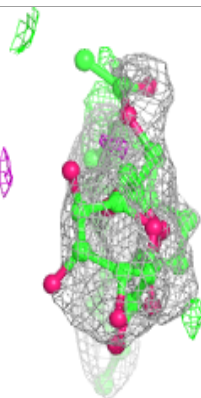
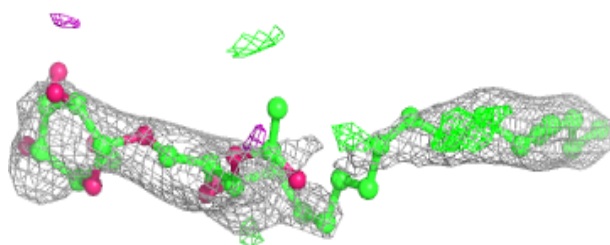
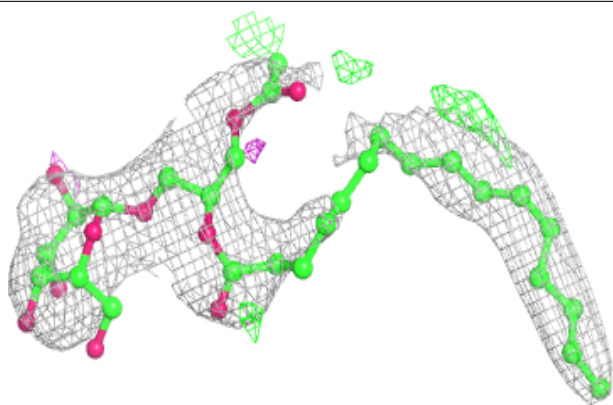
**Electron density around LMG z 101:**

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

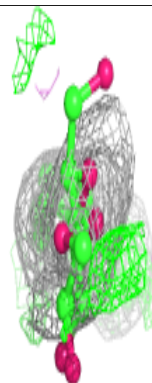
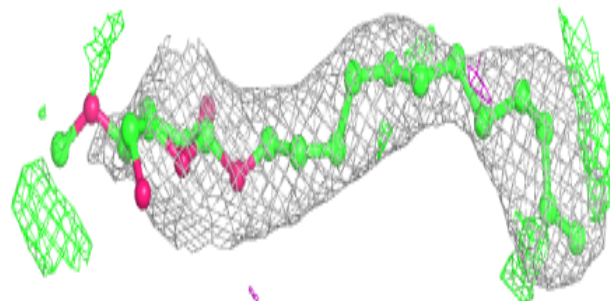
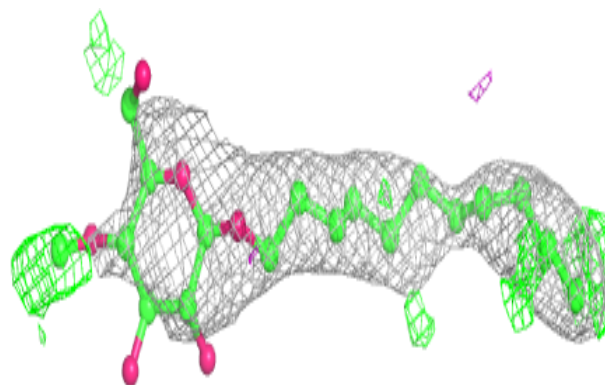


Electron density around LMG Z 101:

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

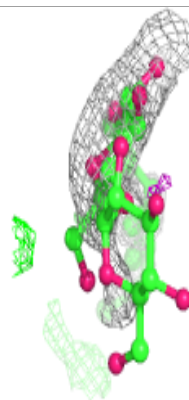
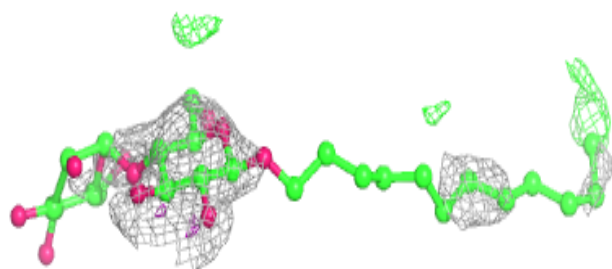
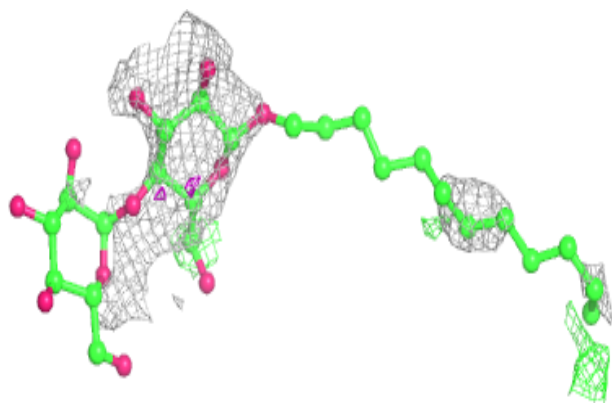
**Electron density around LMT b 627:**

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

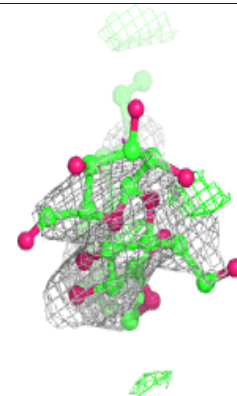
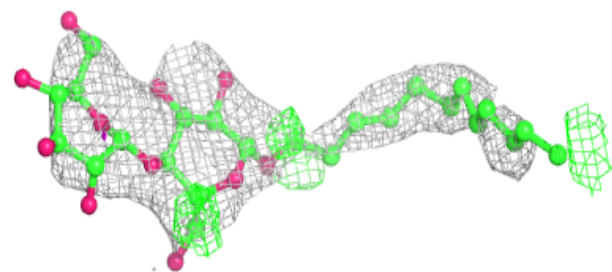
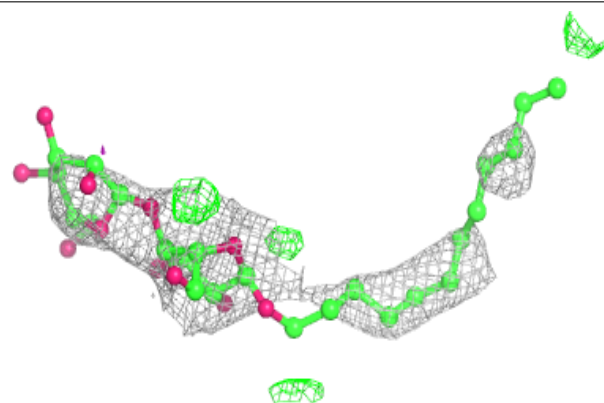


Electron density around LMT e 101:

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

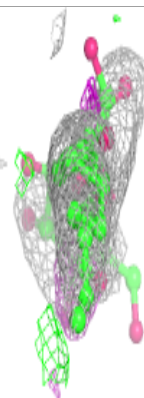
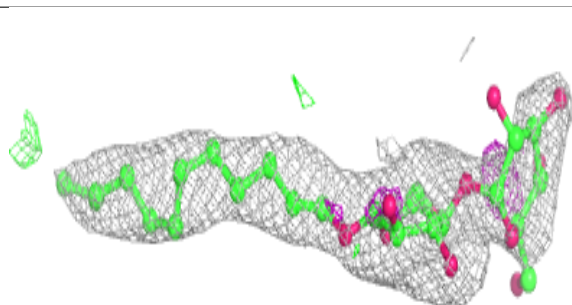
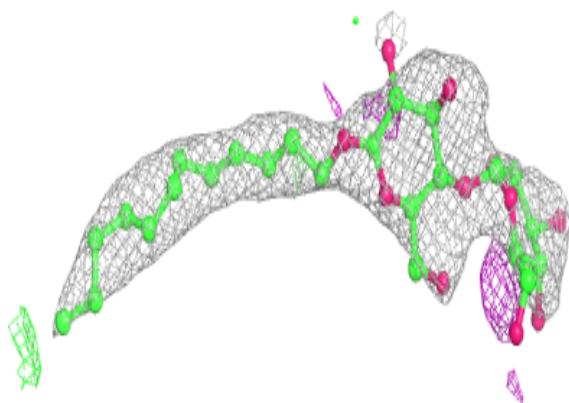
**Electron density around LMT A 420:**

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

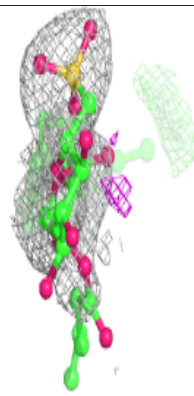
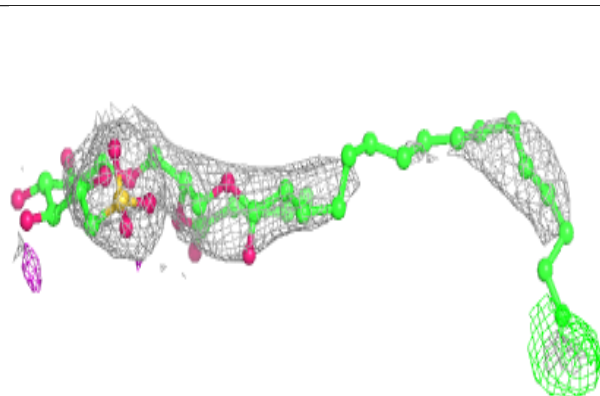
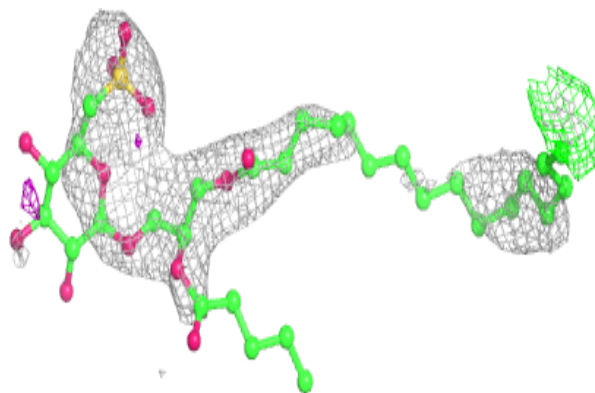


Electron density around LMT B 627:

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

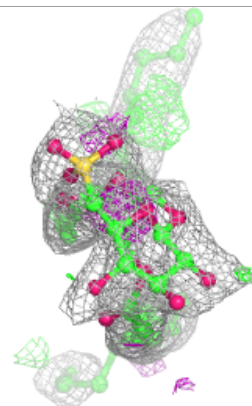
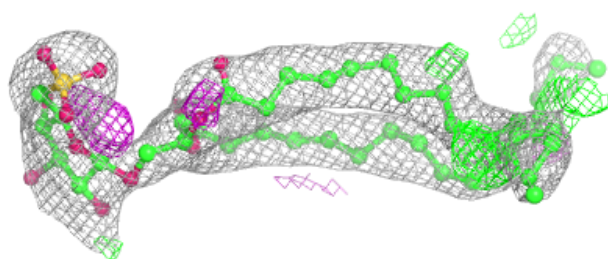
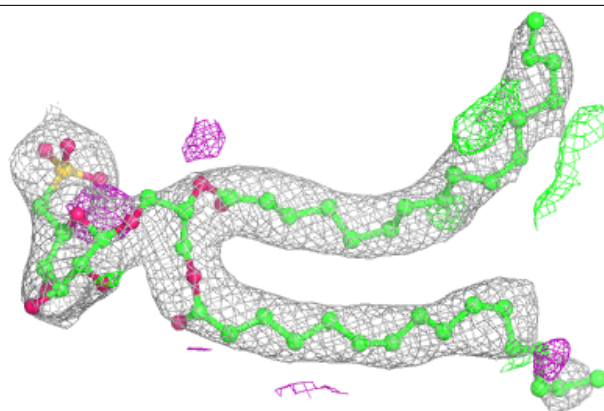
**Electron density around SQD f 102:**

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

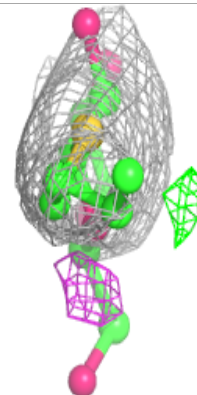
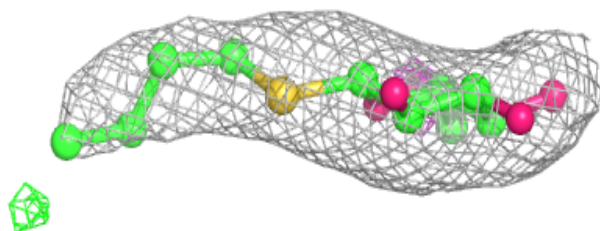
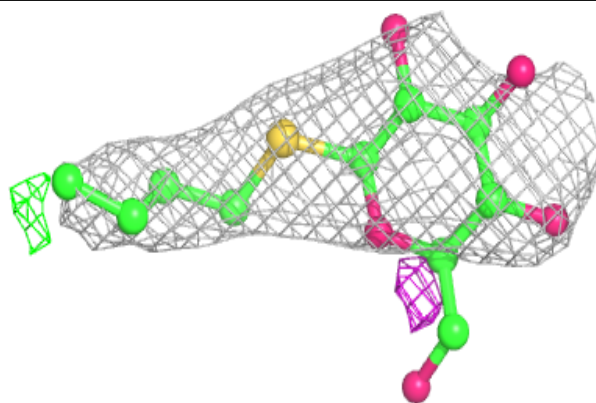


Electron density around SQD b 620:

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

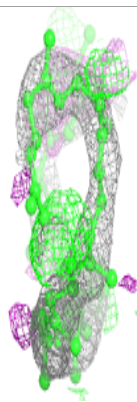
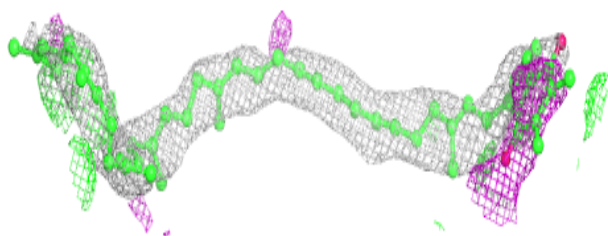
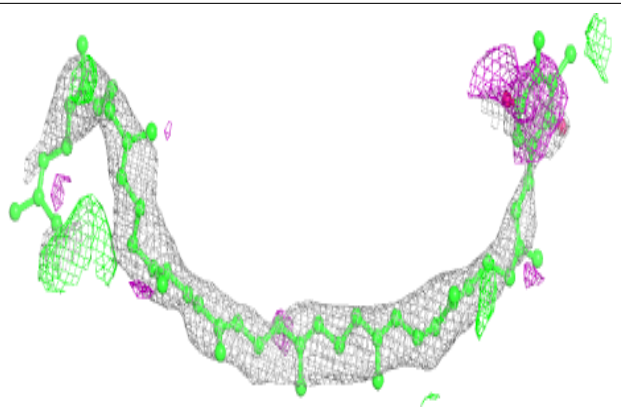
**Electron density around HTG d 409:**

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

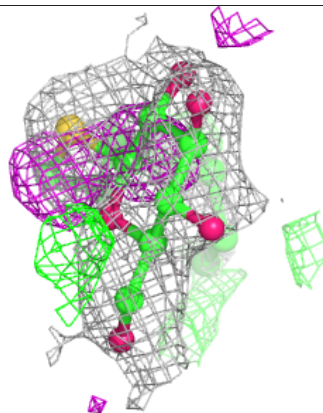
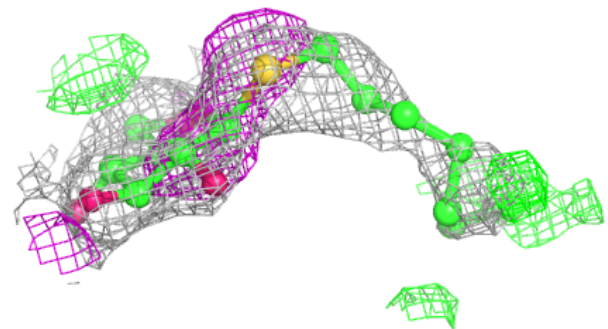
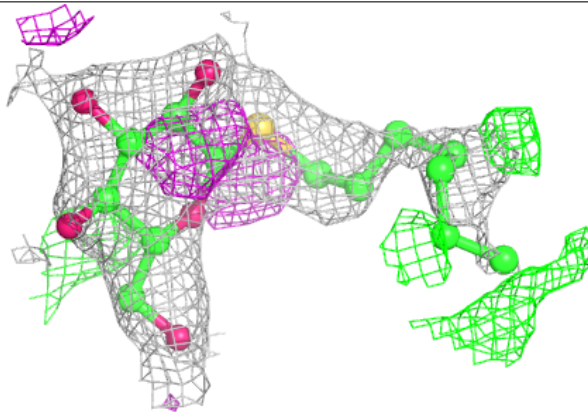


Electron density around PL9 A 414 (B):

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

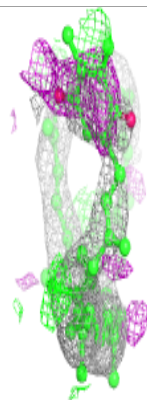
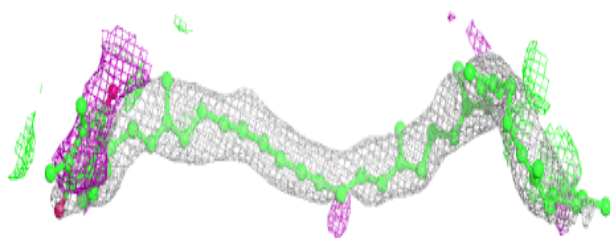
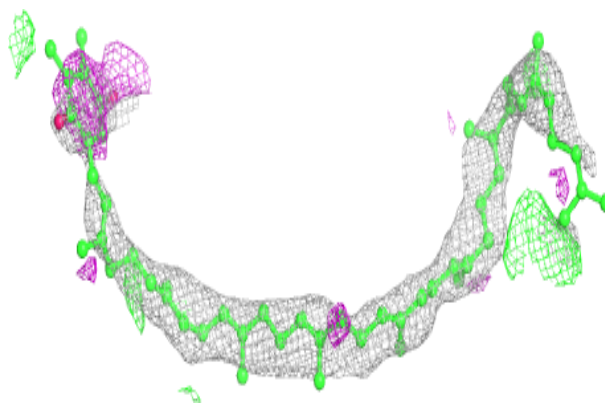
**Electron density around HTG B 622:**

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

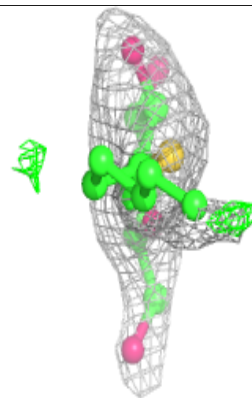
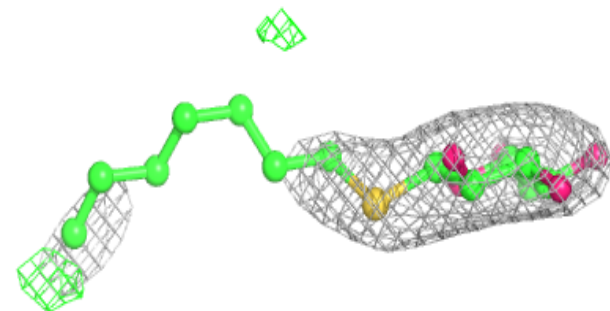
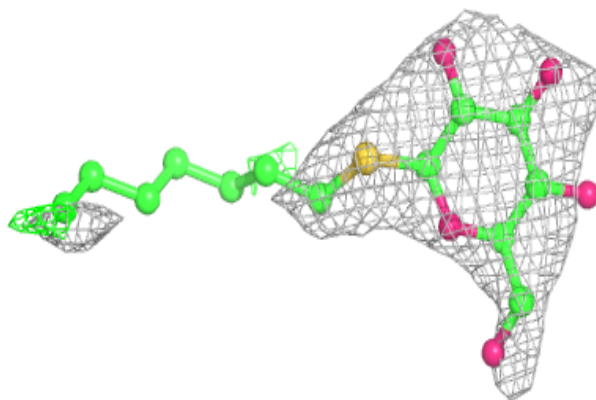


Electron density around PL9 A 414 (A):

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

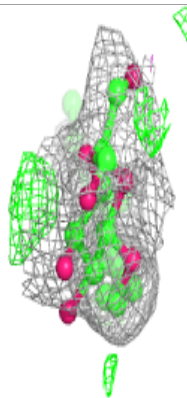
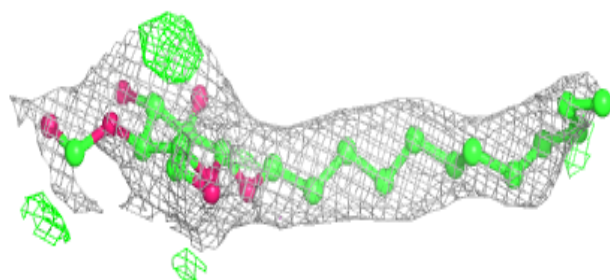
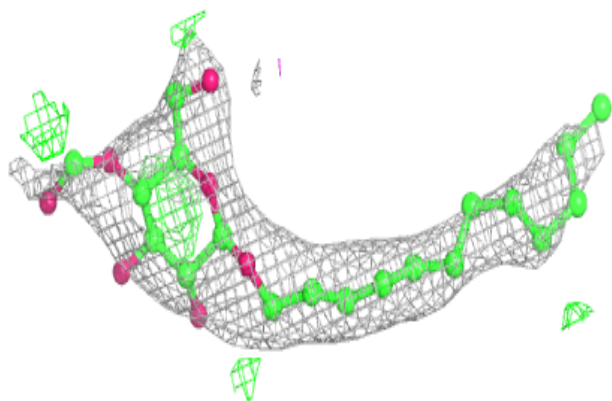
**Electron density around HTG C 522:**

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

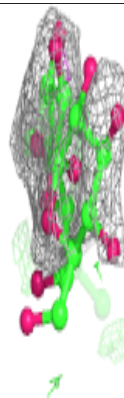
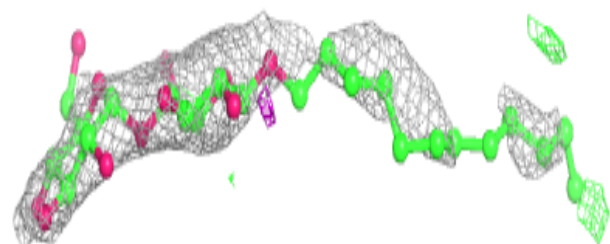
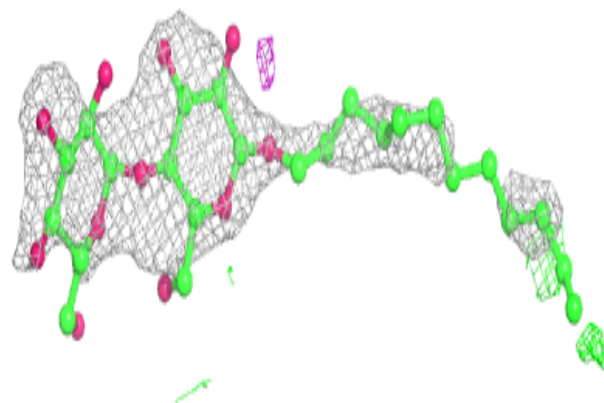


Electron density around LMT t 101:

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

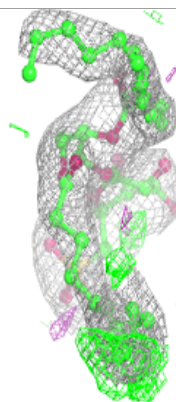
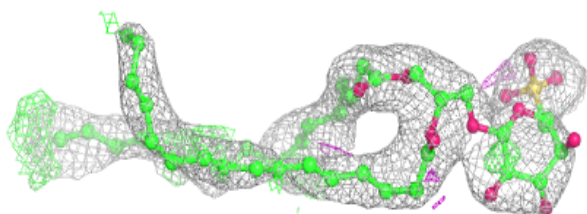
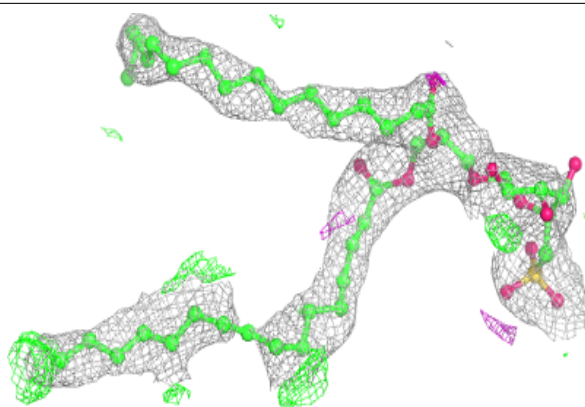
**Electron density around LMT a 417:**

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

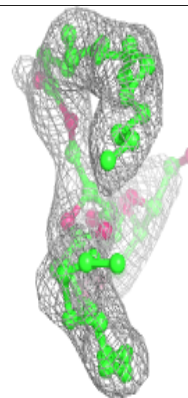
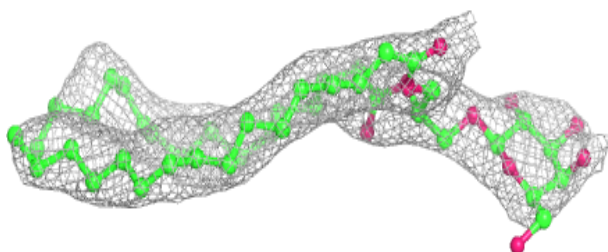
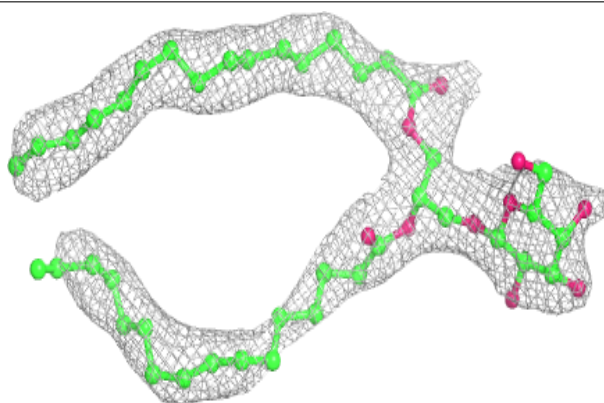


Electron density around SQD a 412:

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

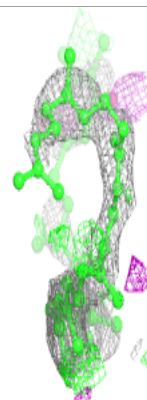
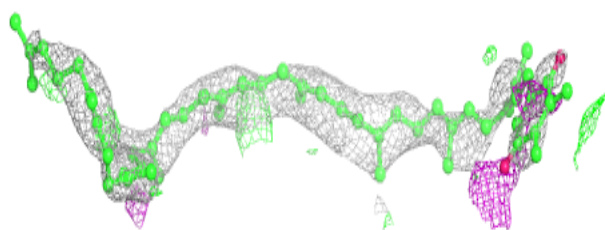
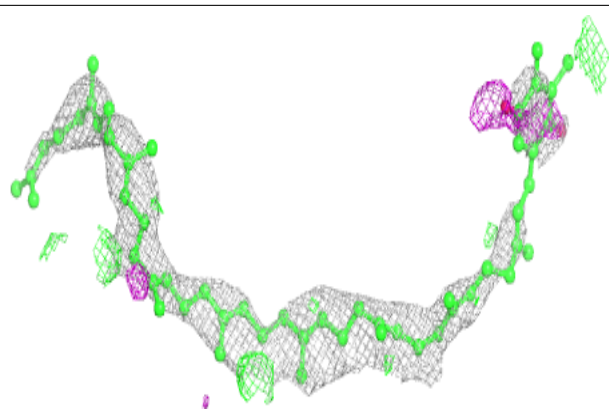
**Electron density around LMG c 501:**

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

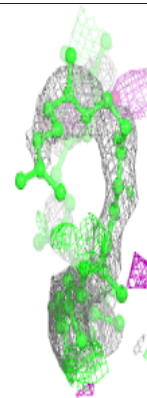
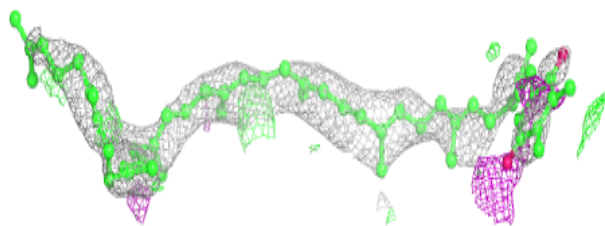
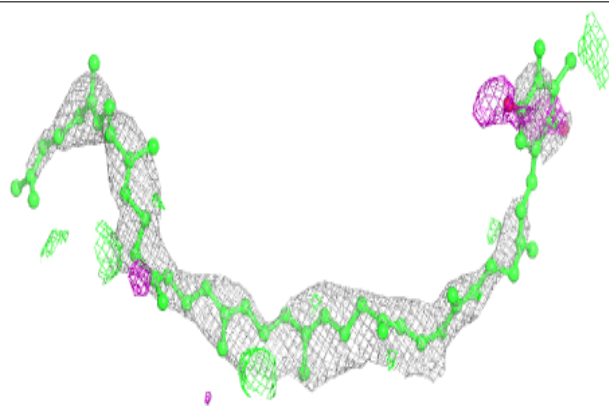


Electron density around PL9 a 414 (A):

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

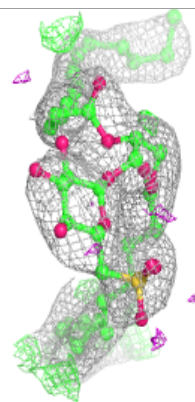
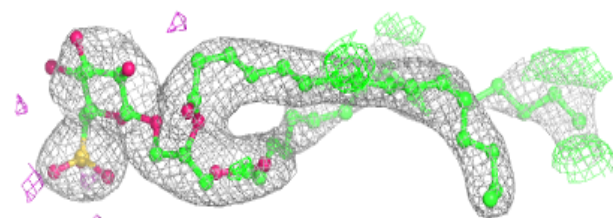
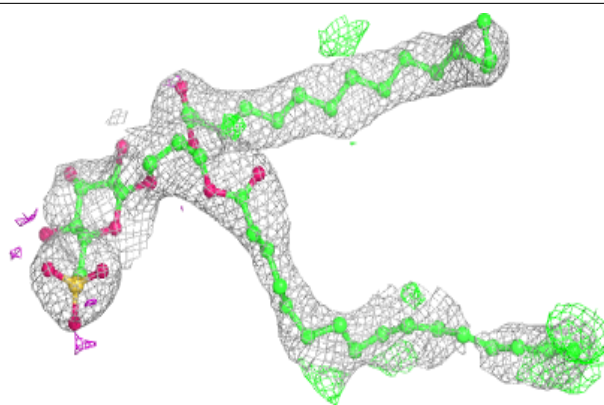
**Electron density around PL9 a 414 (B):**

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

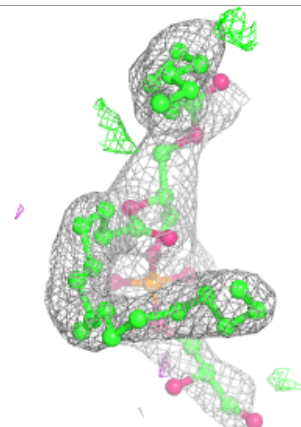
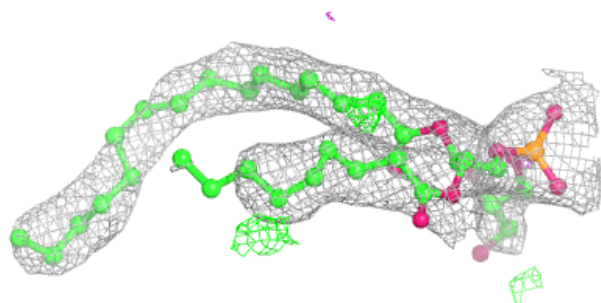
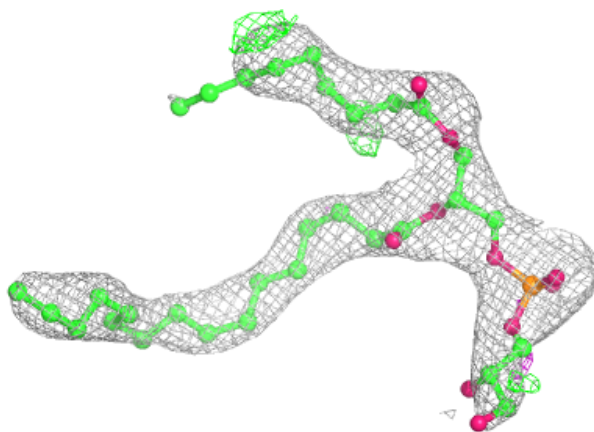


Electron density around SQD A 412:

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

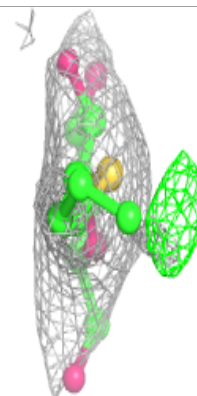
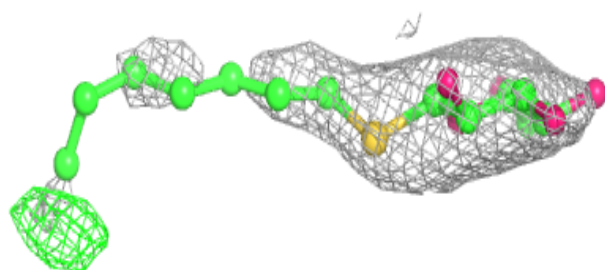
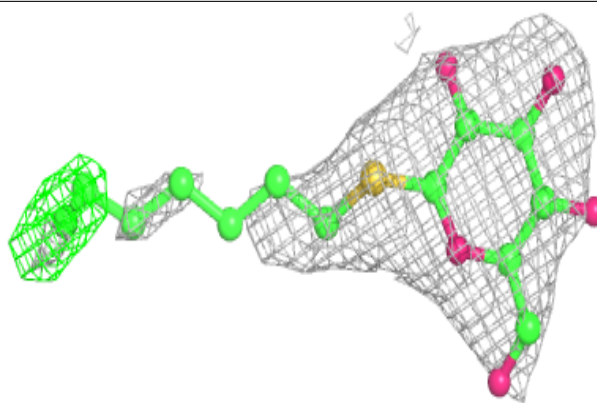
**Electron density around LHG E 101 (A):**

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

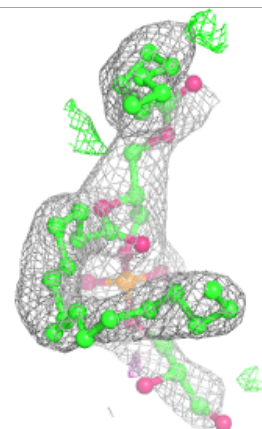
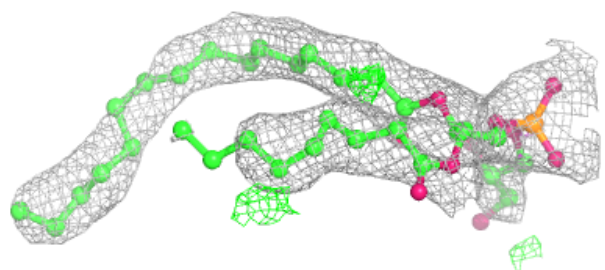
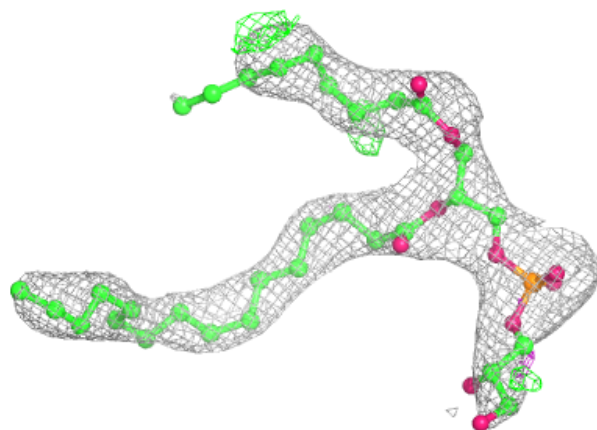


Electron density around HTG c 522:

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

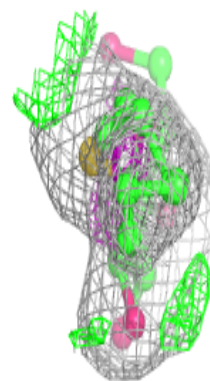
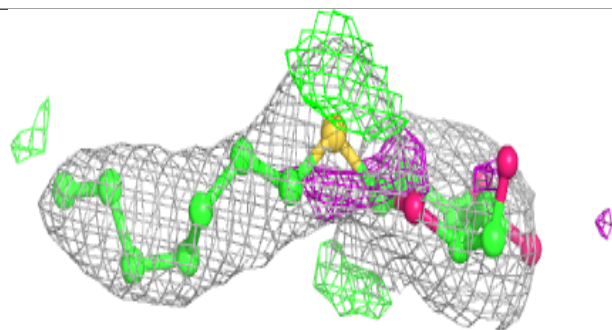
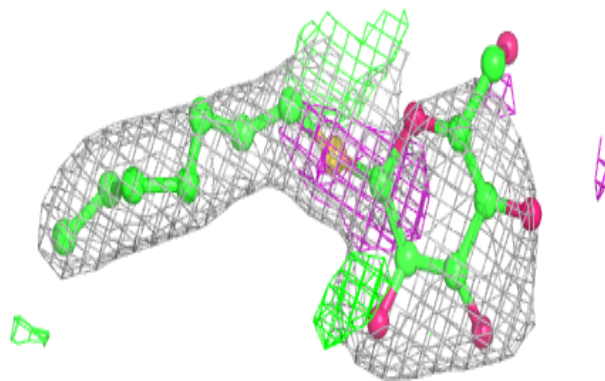
**Electron density around LHG E 101 (B):**

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

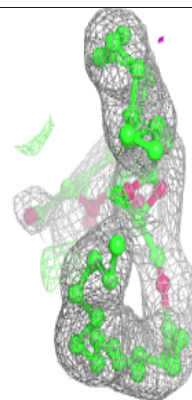
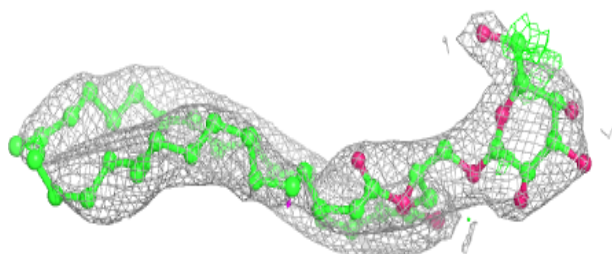
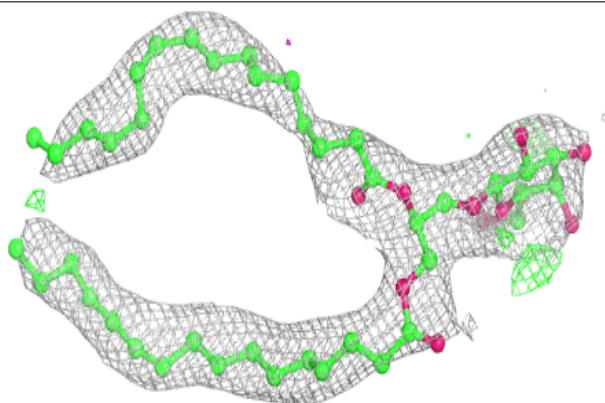


Electron density around HTG O 301:

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

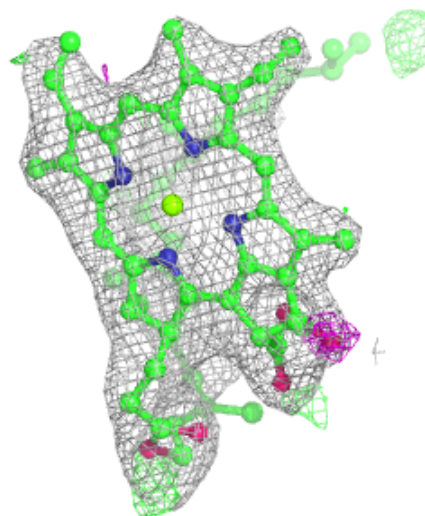
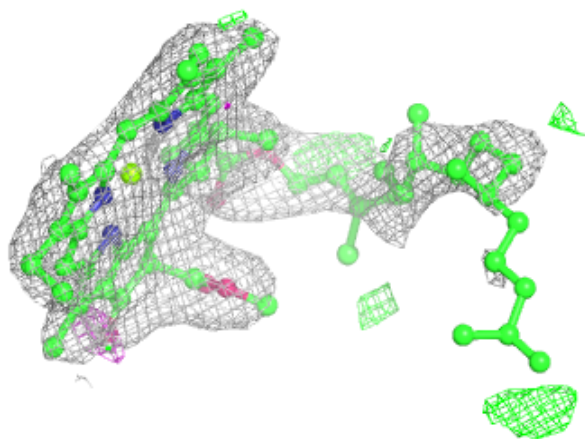
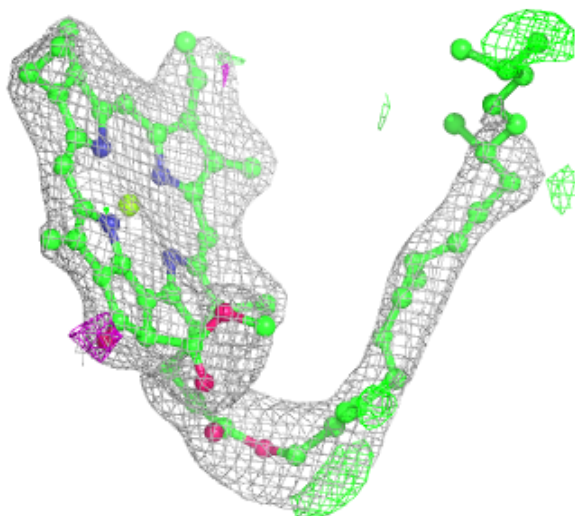
**Electron density around LMG C 501:**

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



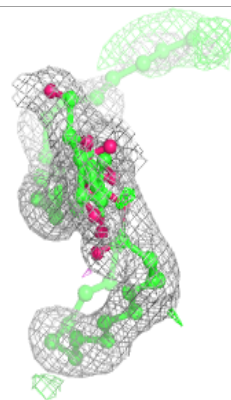
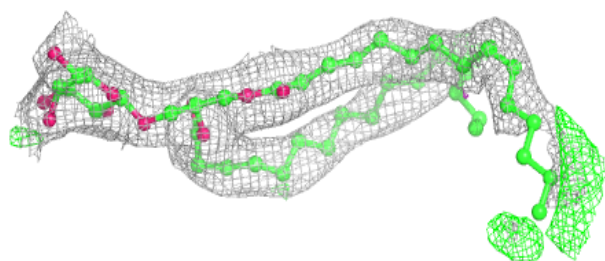
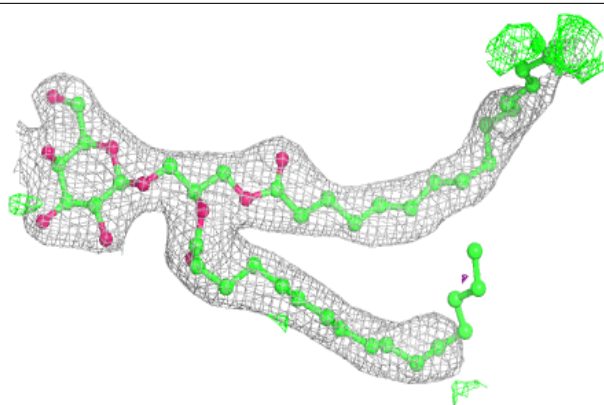
Electron density around CLA b 616:

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

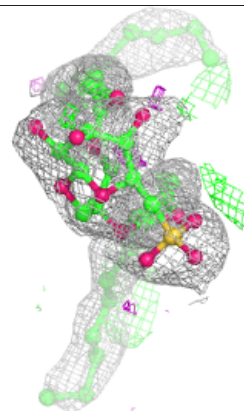
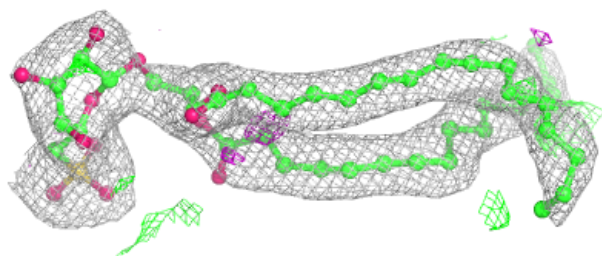
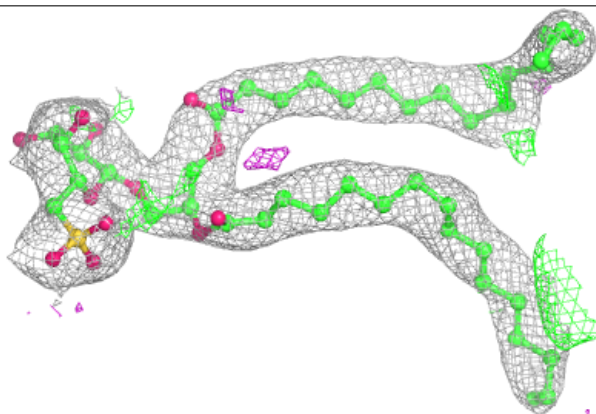


Electron density around LMG D 711:

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

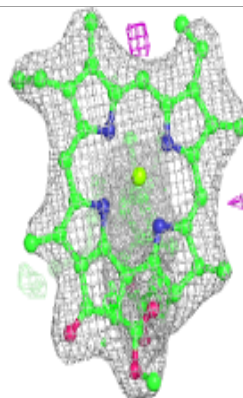
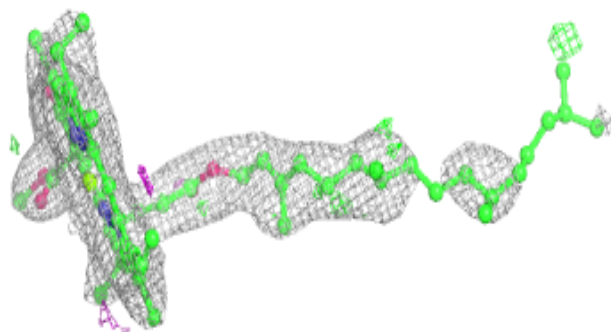
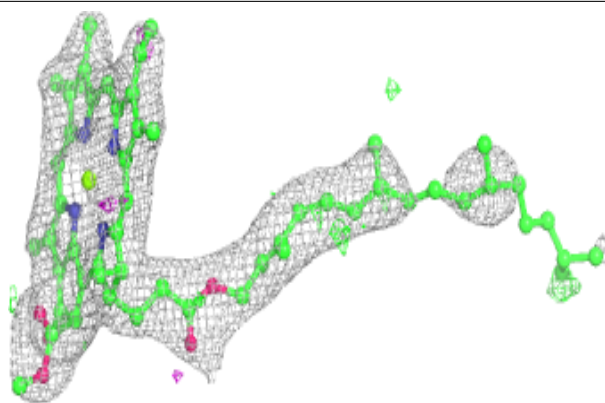
**Electron density around SQD B 620:**

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

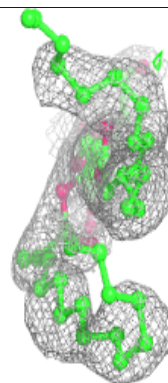
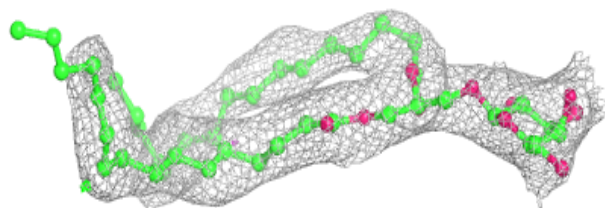
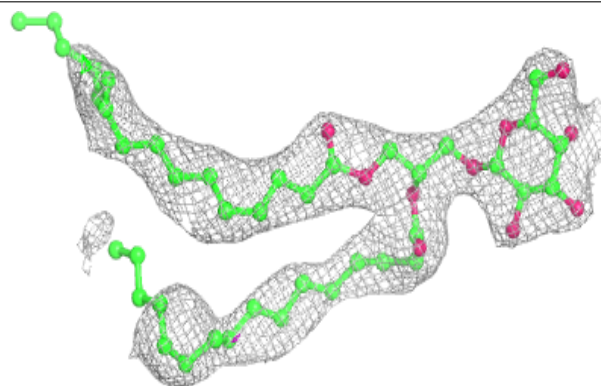


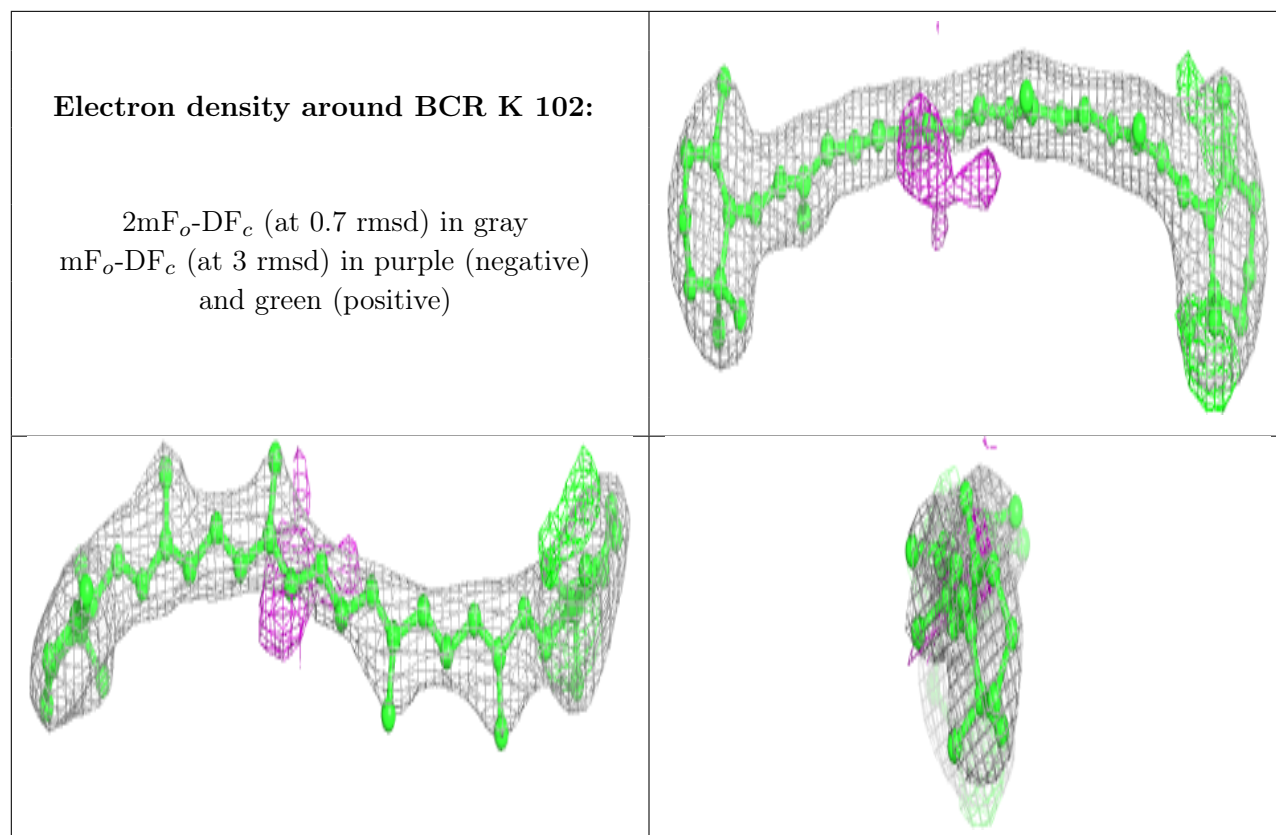
Electron density around CLA d 402:

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

**Electron density around LMG d 410:**

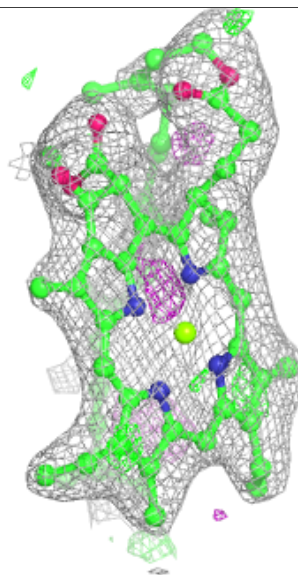
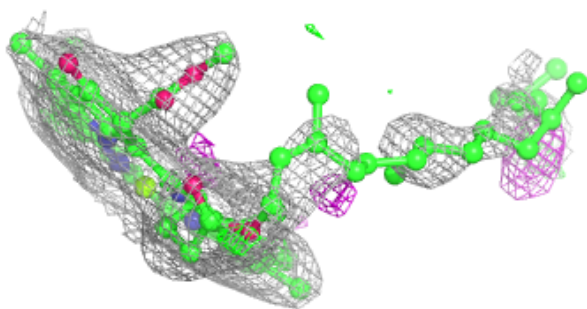
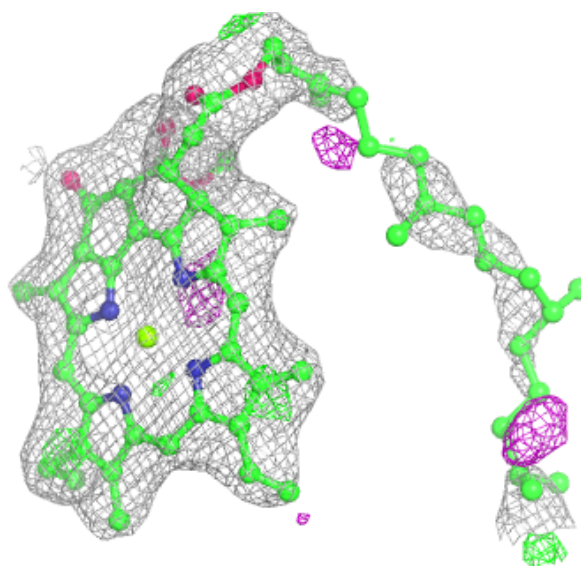
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





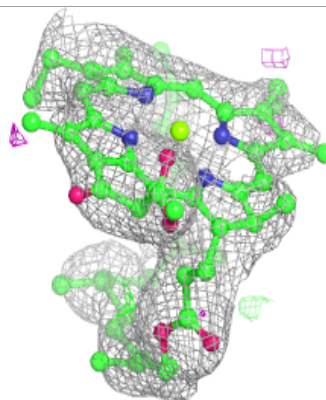
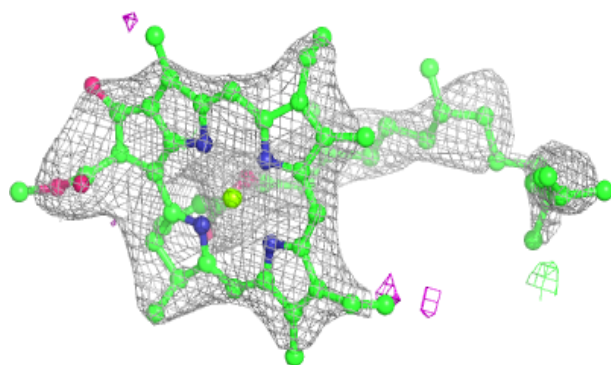
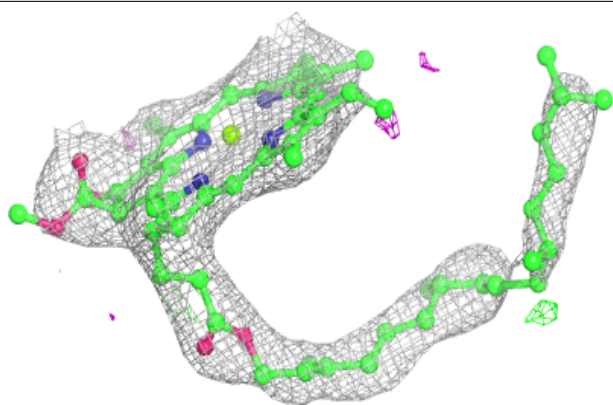
Electron density around CLA B 616:

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

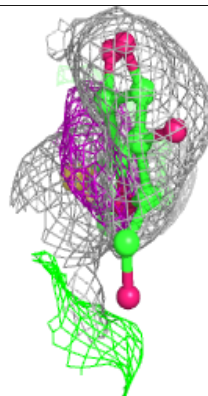
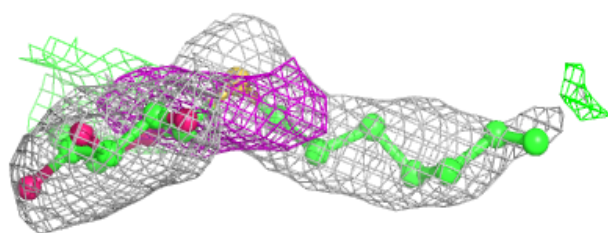
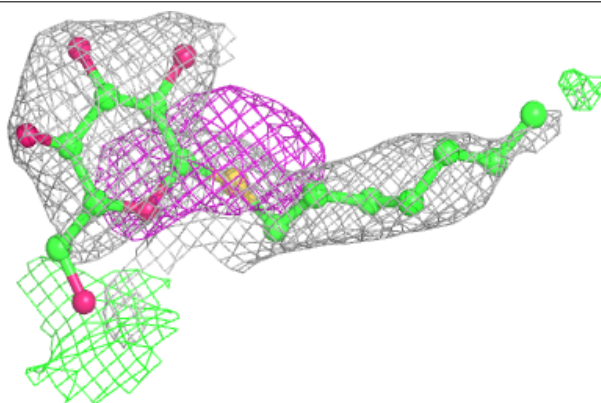


Electron density around CLA c 514:

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

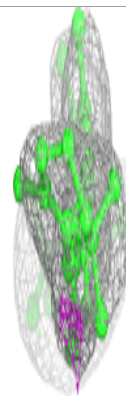
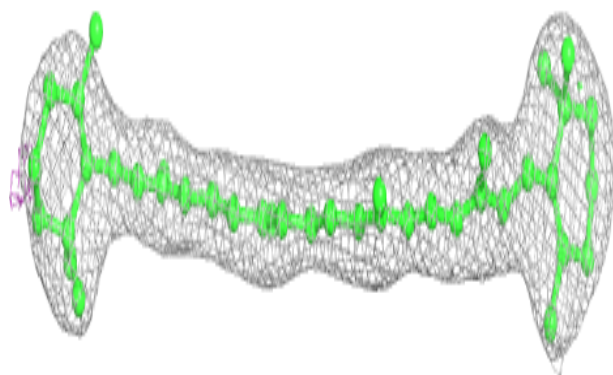
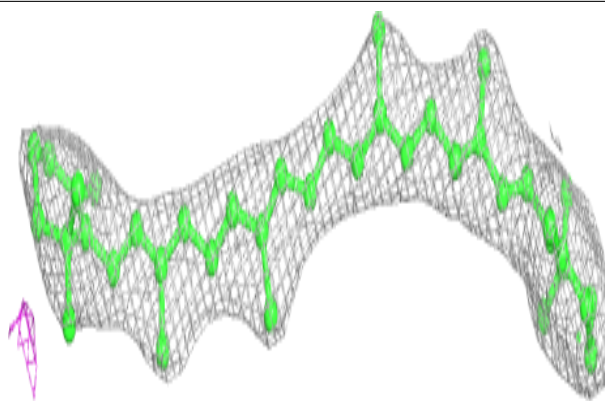
**Electron density around HTG b 622:**

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

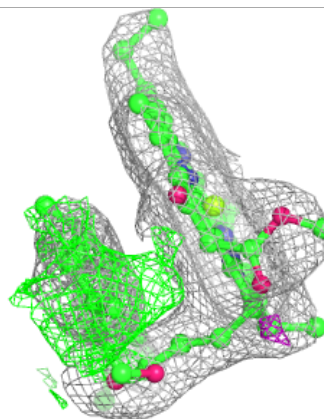
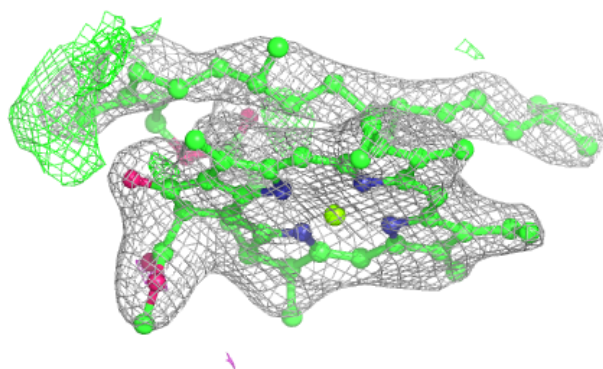
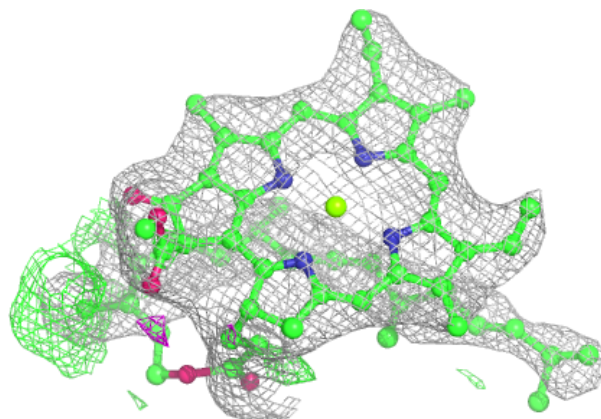


Electron density around BCR h 101:

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

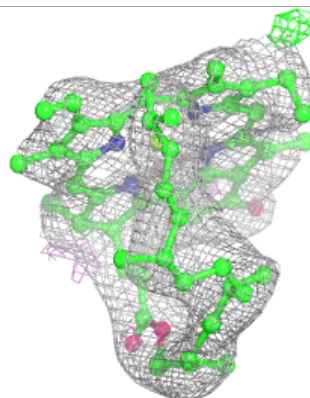
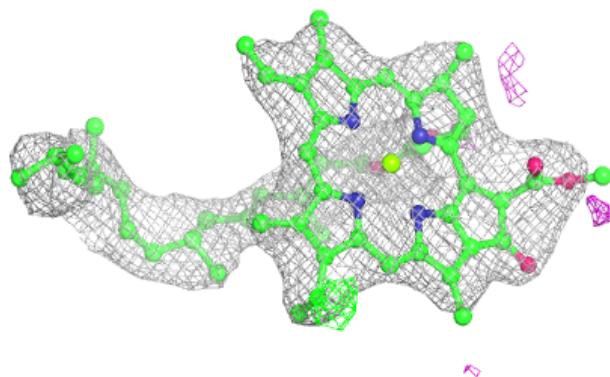
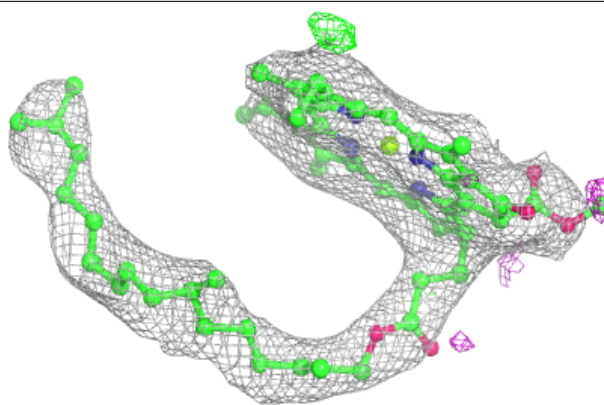
**Electron density around CLA b 601:**

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

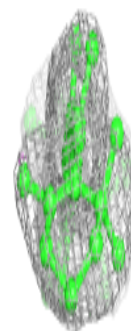
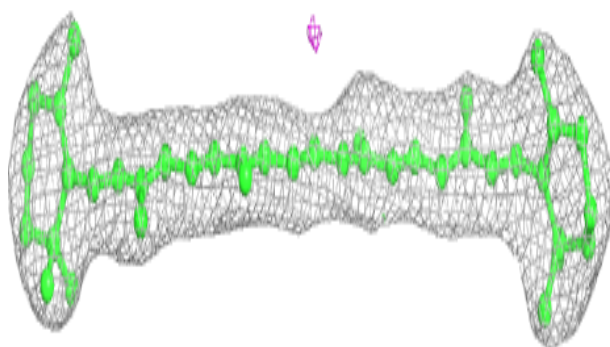
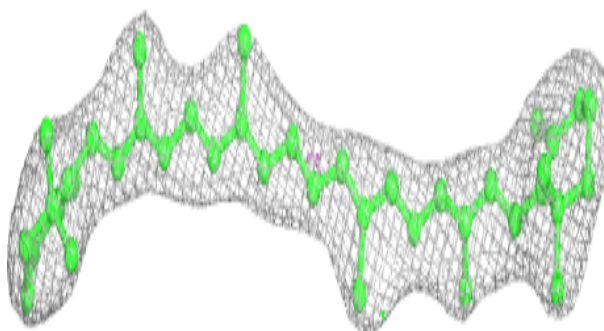


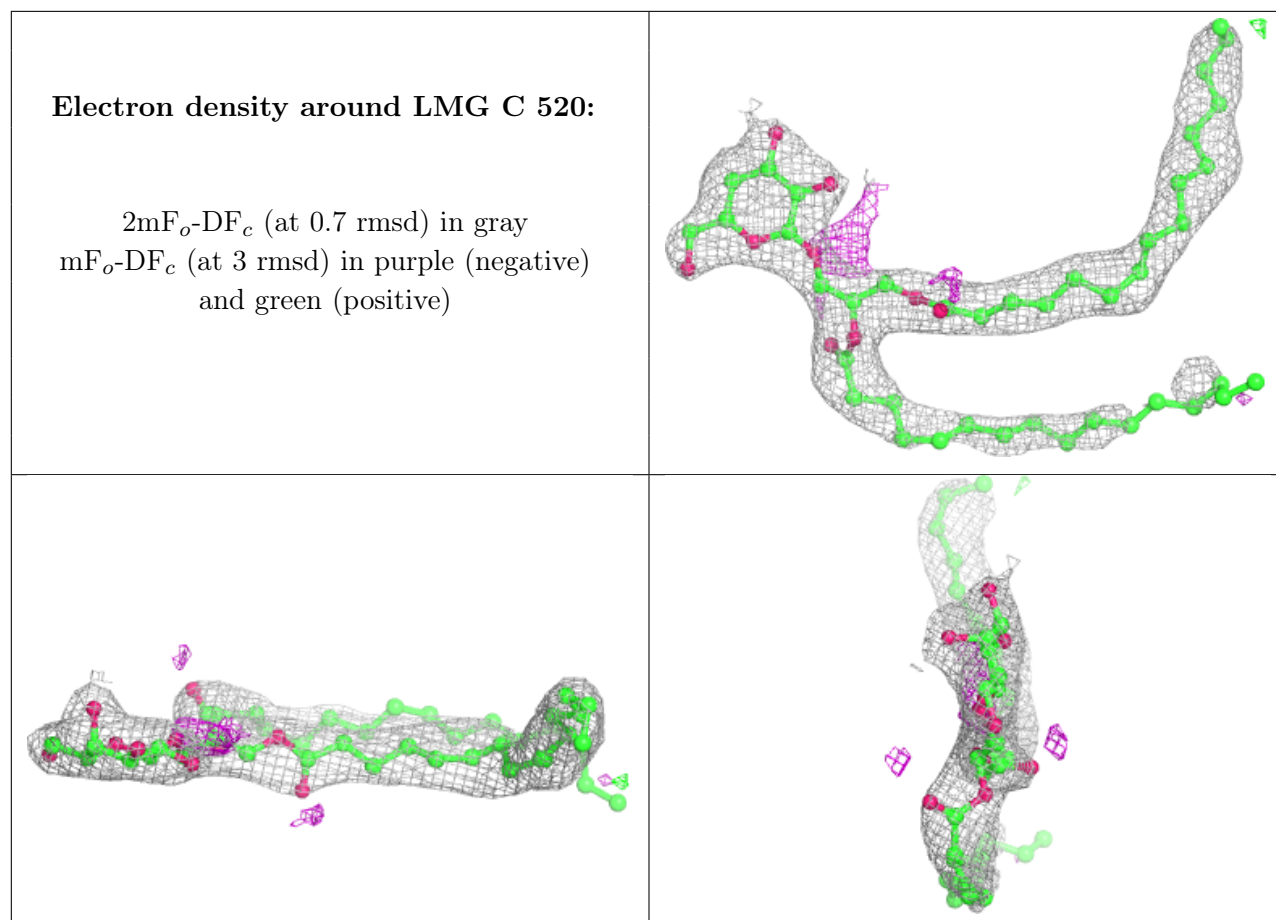
Electron density around CLA C 514:

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

**Electron density around BCR C 515:**

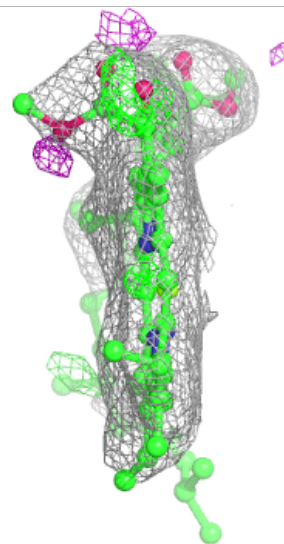
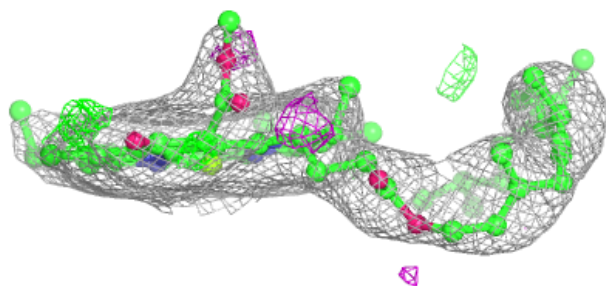
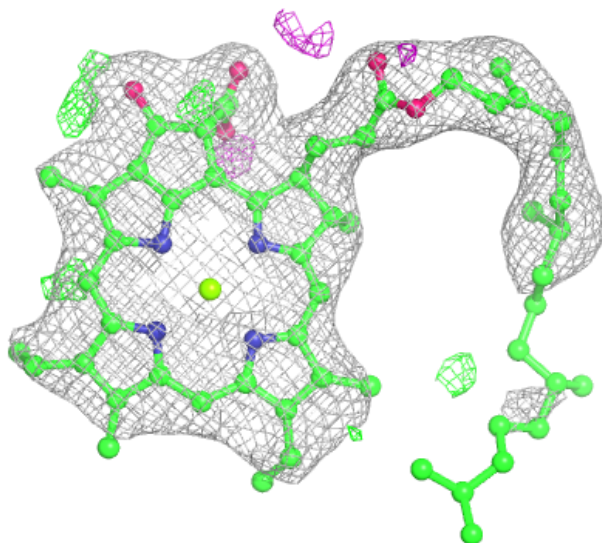
$2mF_o-DF_c$ (at 0.7 rnsd) in gray
 mF_o-DF_c (at 3 rnsd) in purple (negative)
and green (positive)

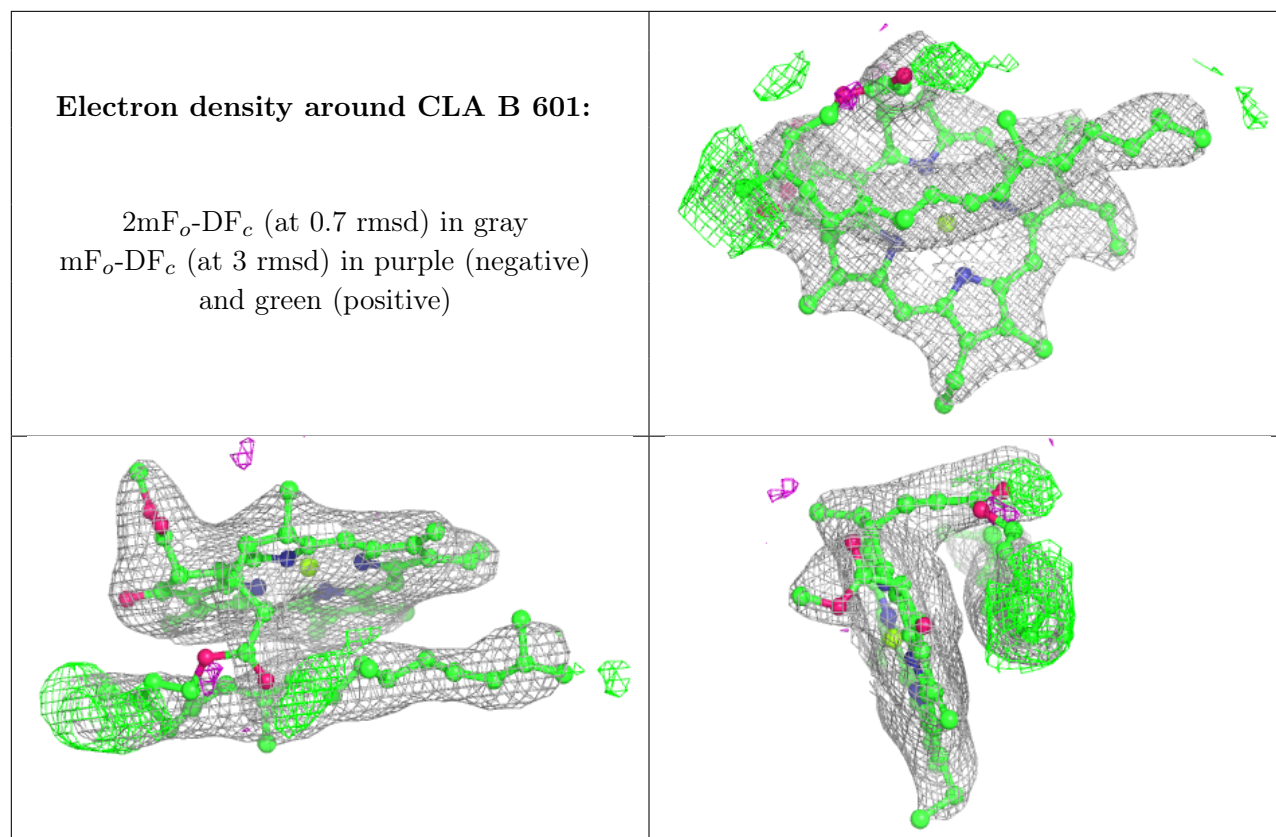




Electron density around CLA c 513:

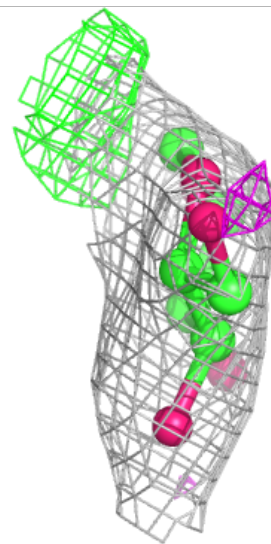
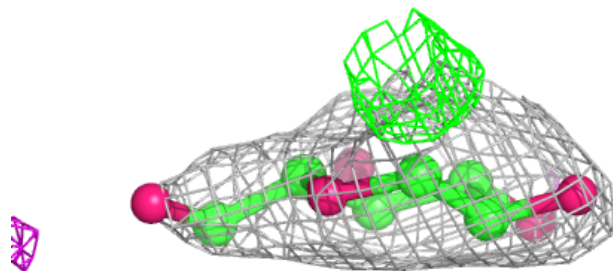
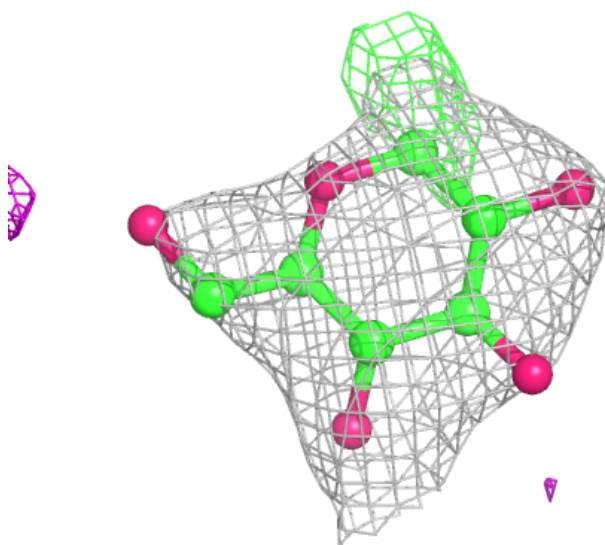
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





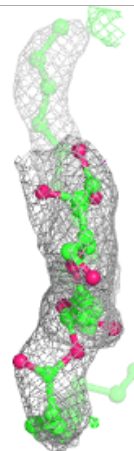
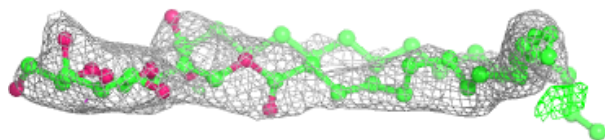
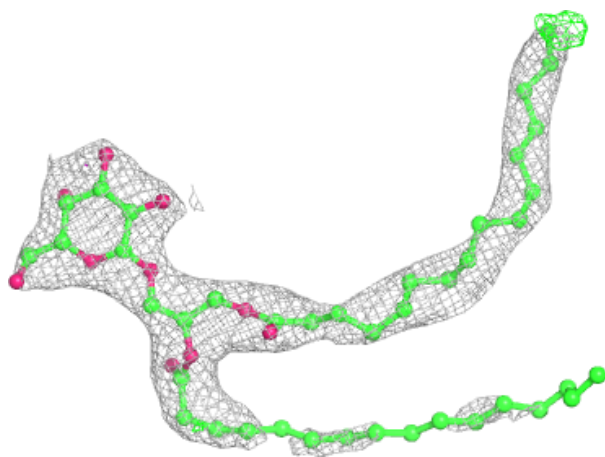
Electron density around HTG V 202:

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



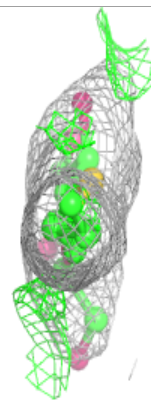
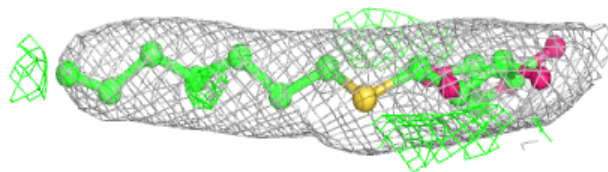
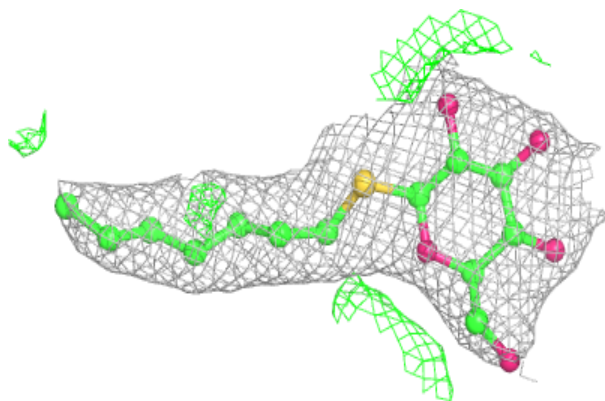
Electron density around LMG c 520:

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

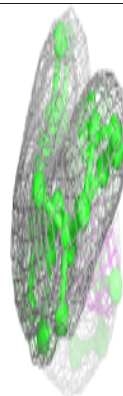
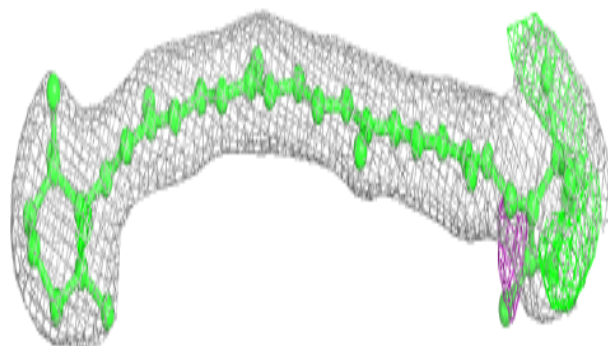
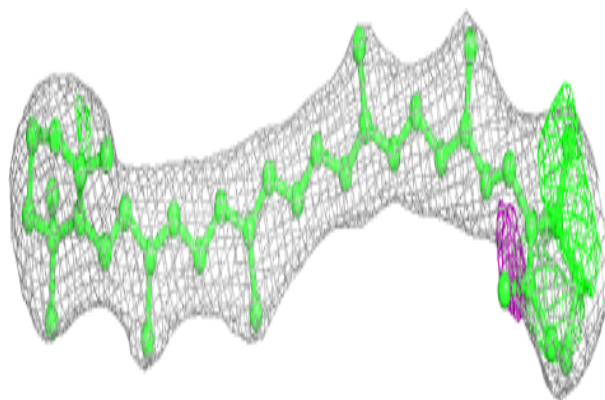


Electron density around HTG b 625:

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

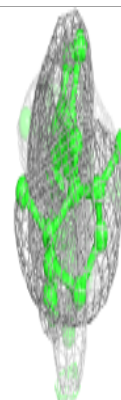
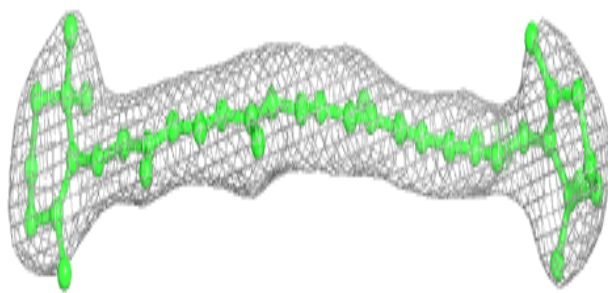
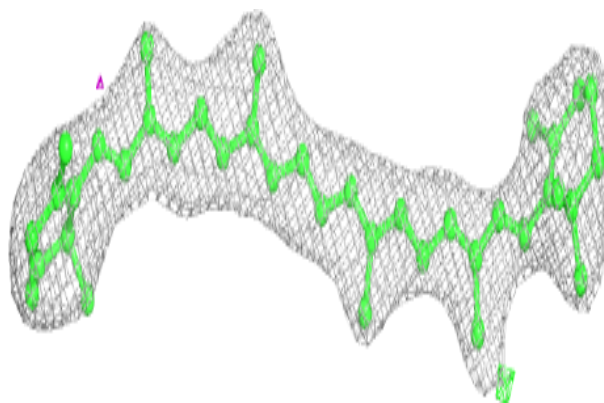
**Electron density around BCR d 403:**

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

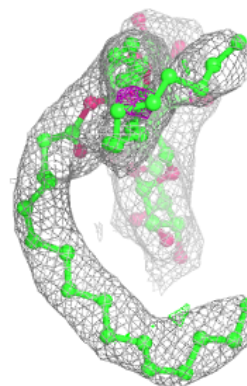
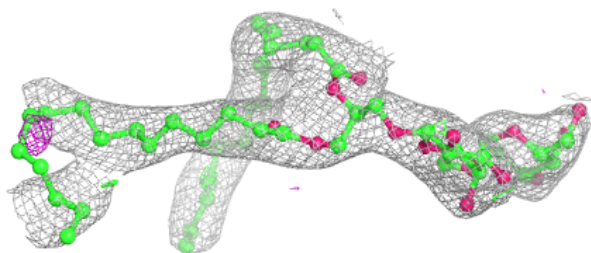
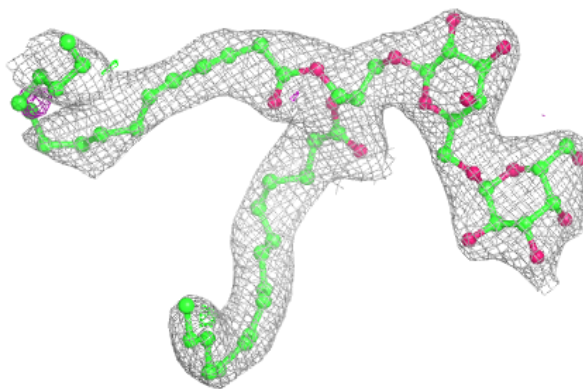


Electron density around BCR Y 101:

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

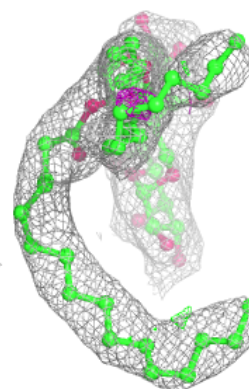
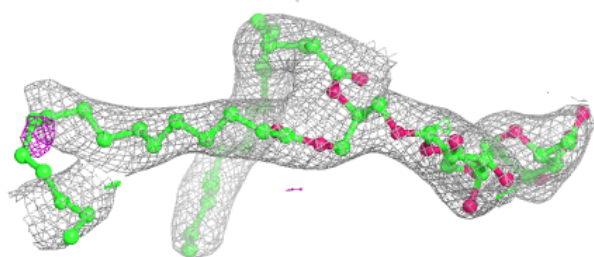
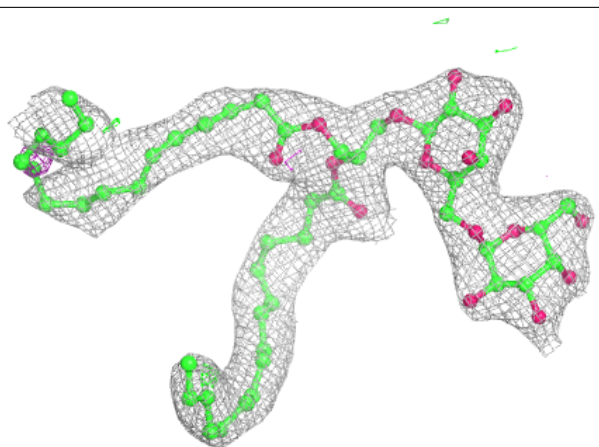
**Electron density around DGD c 518 (A):**

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

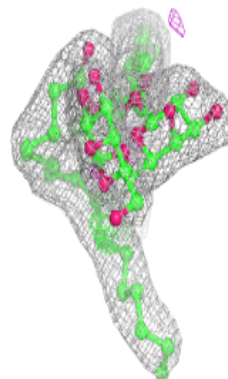
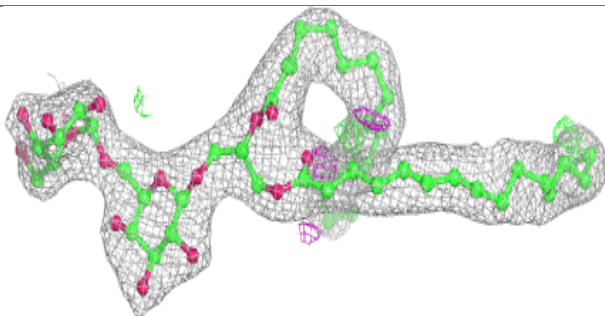
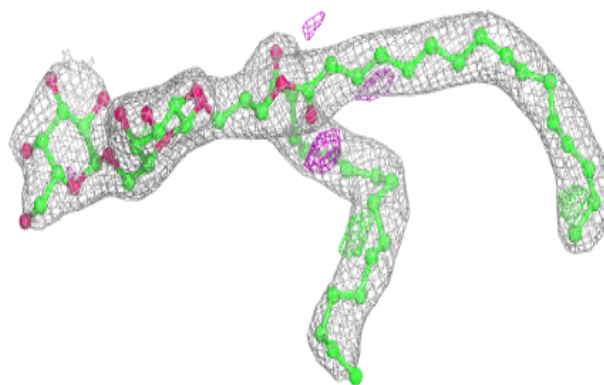


Electron density around DGD c 518 (B):

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

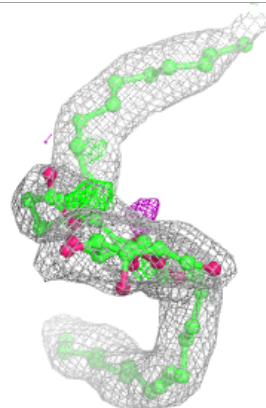
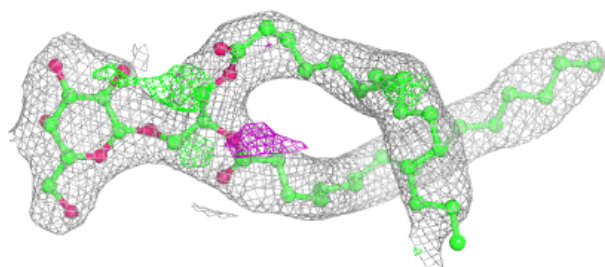
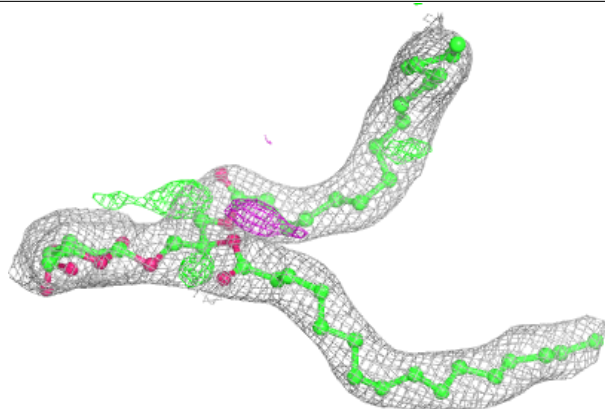
**Electron density around DGD h 102:**

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

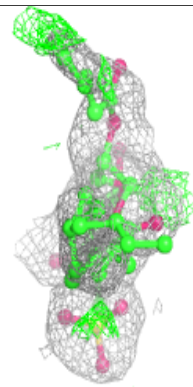
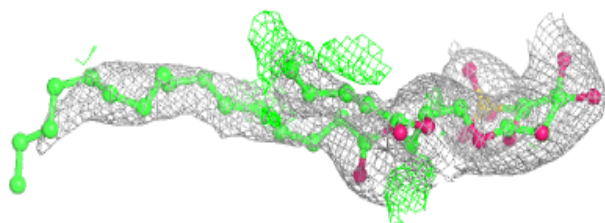
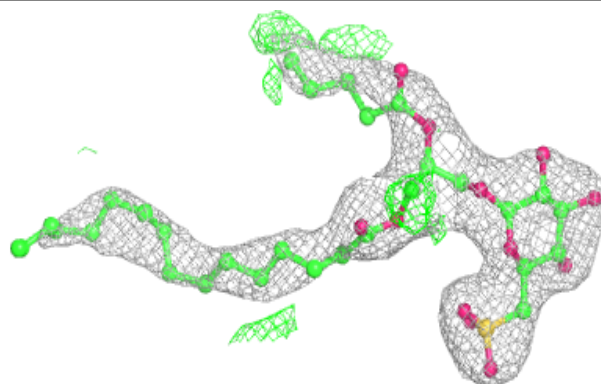


Electron density around LMG B 621:

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

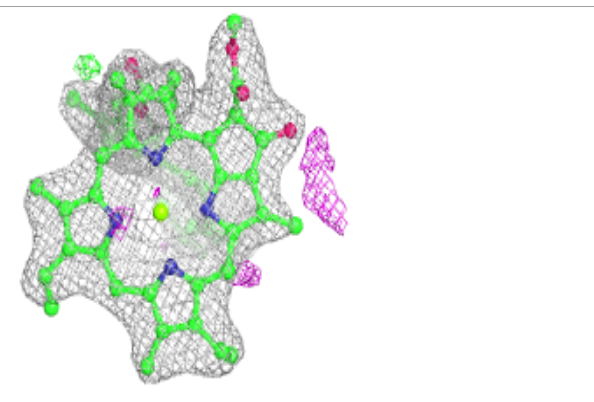
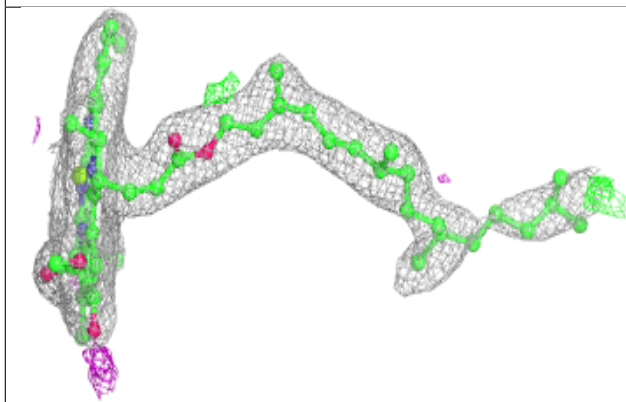
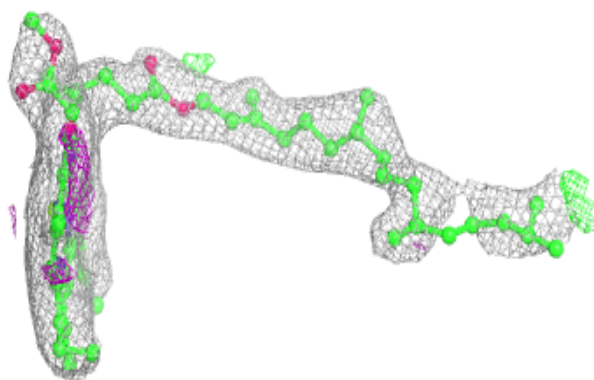
**Electron density around SQD X 101:**

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

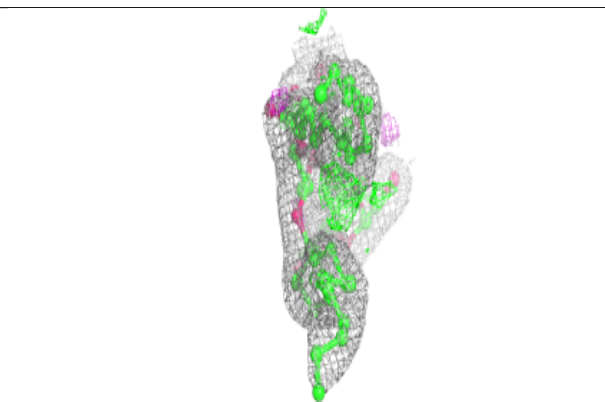
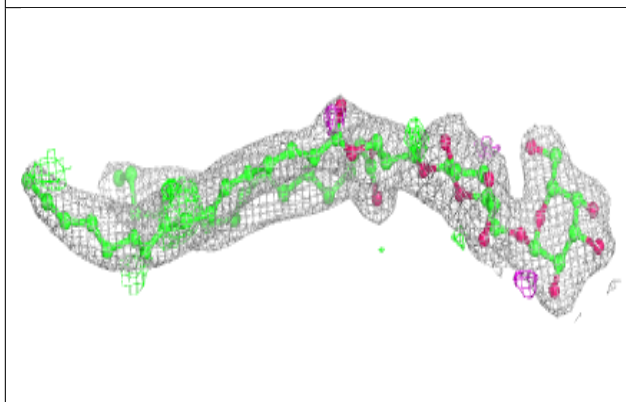
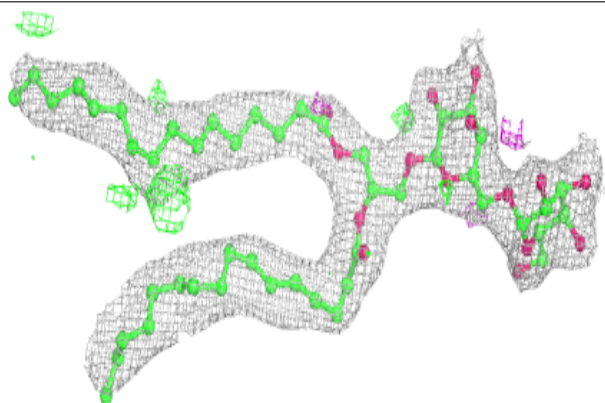


Electron density around CLA B 606:

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

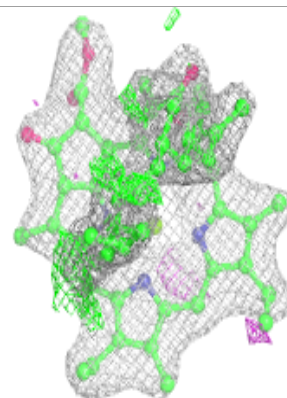
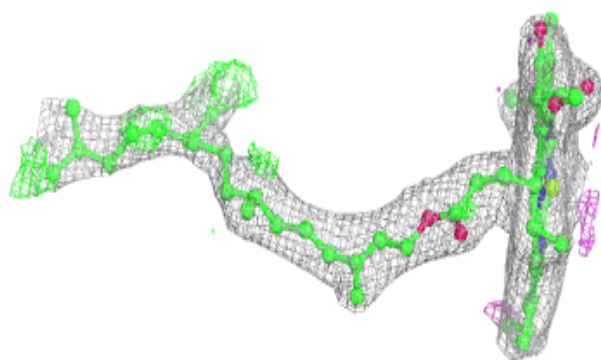
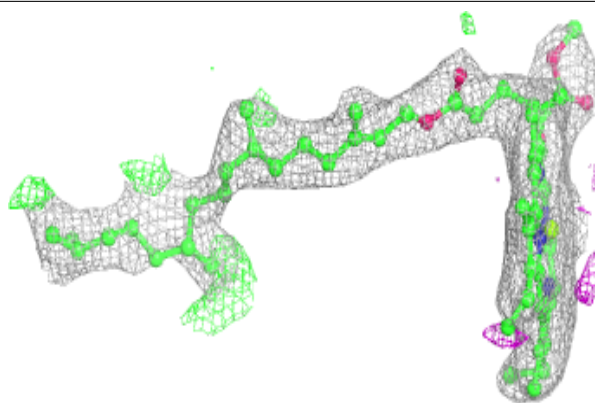
**Electron density around DGD C 519:**

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

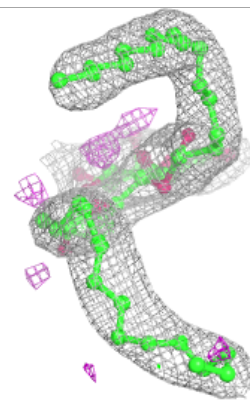
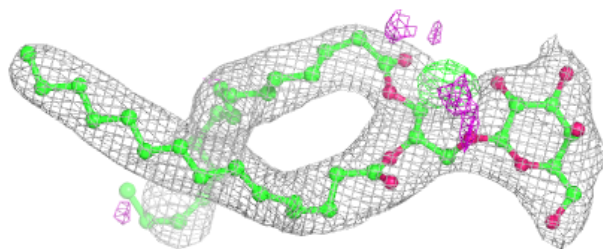
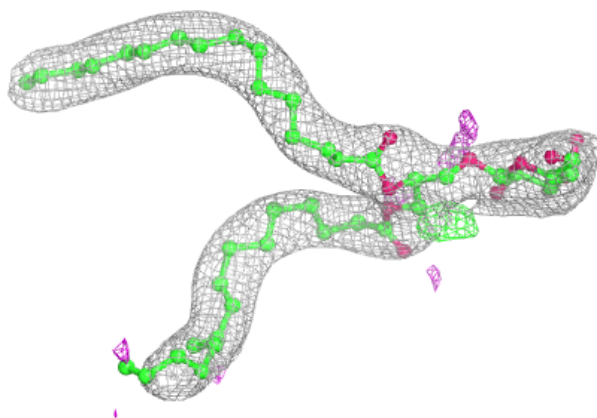


Electron density around CLA b 606:

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

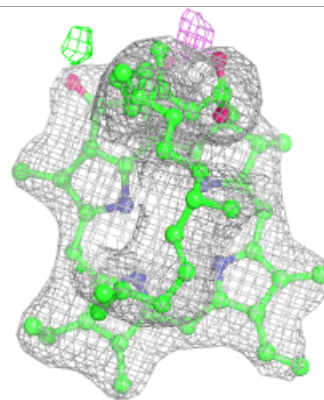
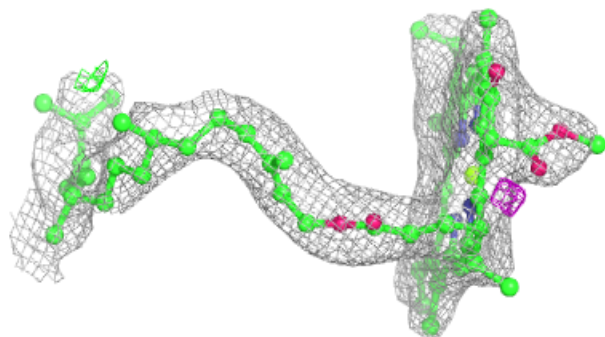
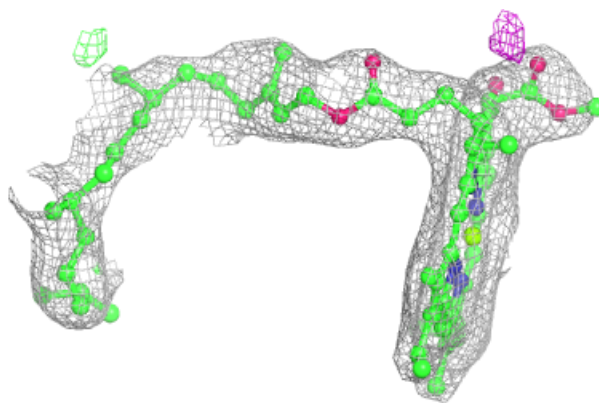
**Electron density around LMG m 101:**

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



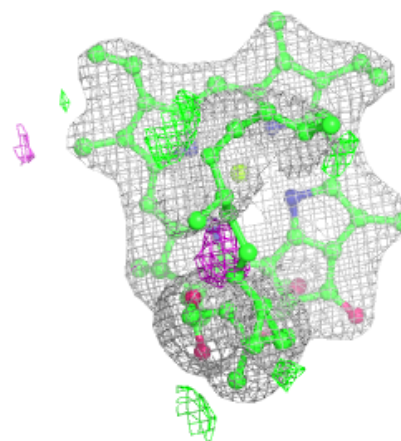
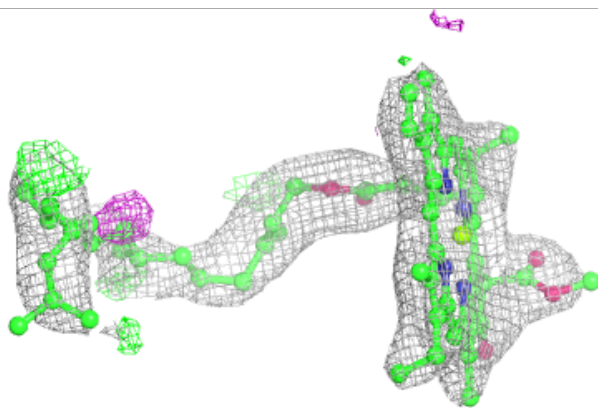
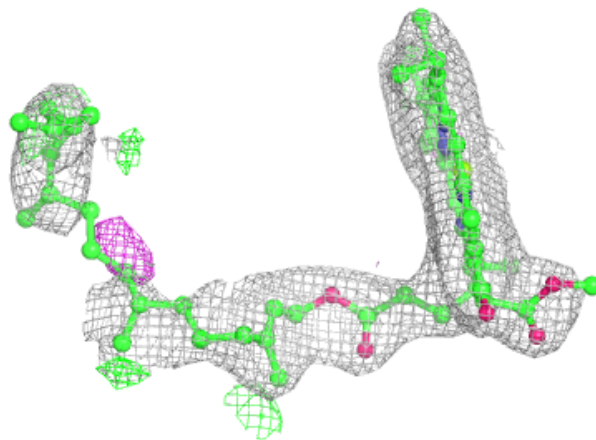
Electron density around CLA C 507:

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



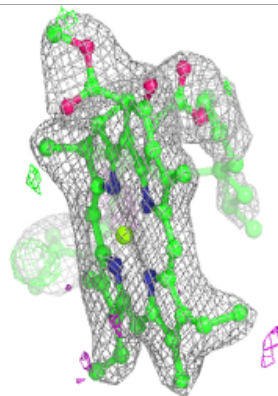
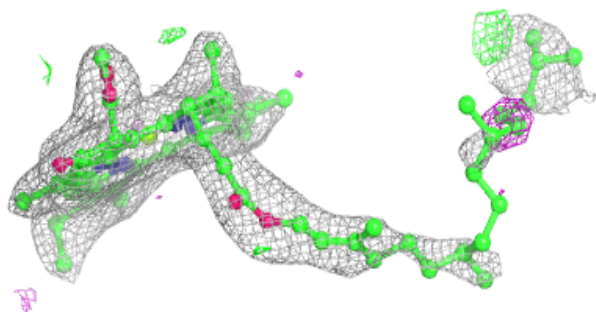
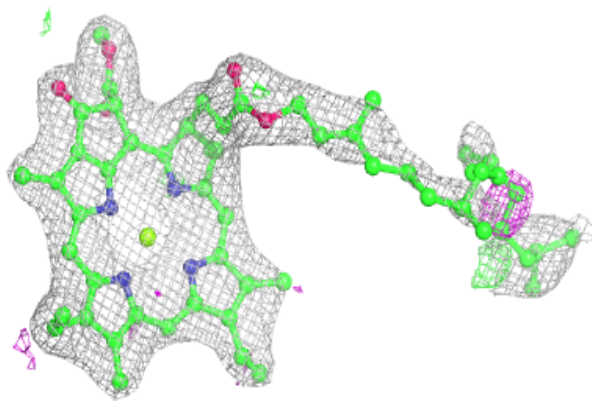
Electron density around CLA c 507:

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



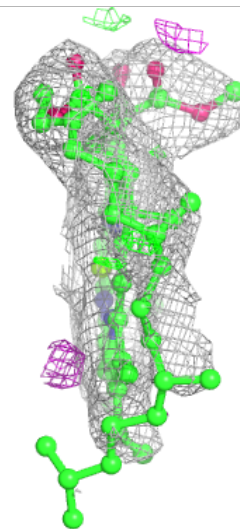
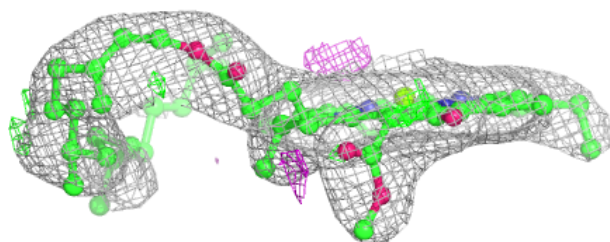
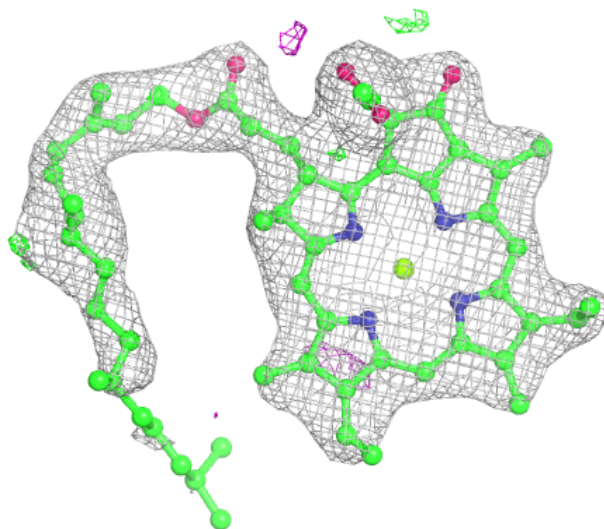
Electron density around CLA a 409:

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



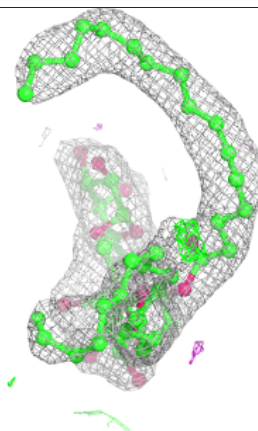
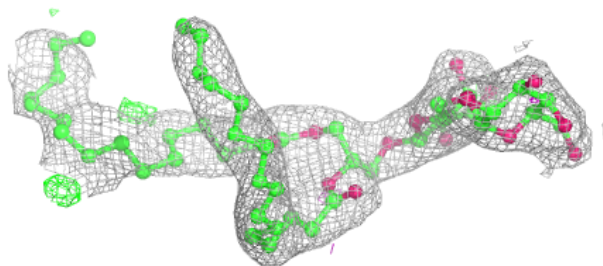
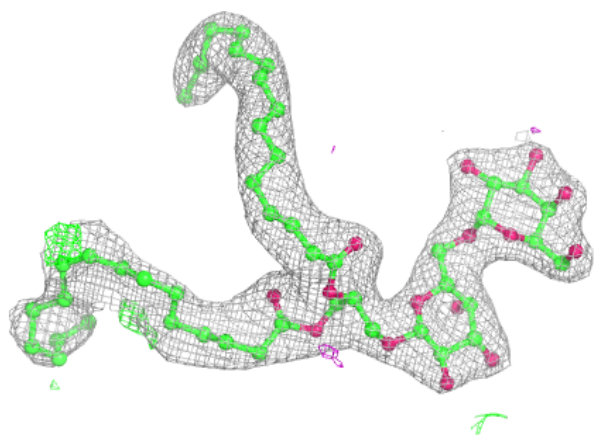
Electron density around CLA C 513:

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



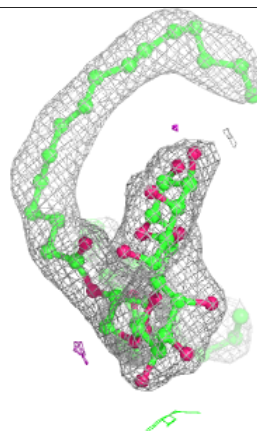
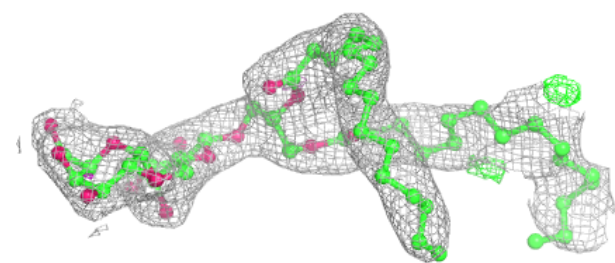
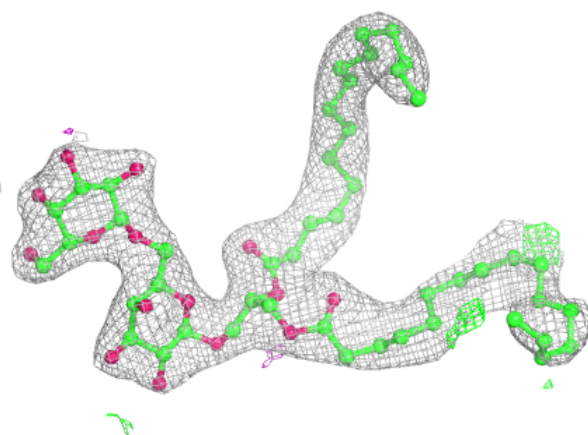
Electron density around DGD C 518 (A):

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

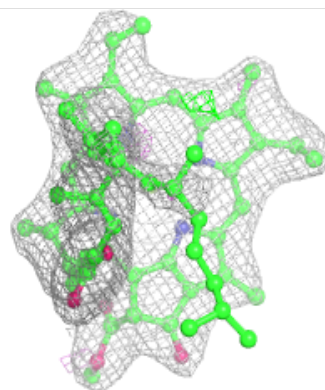
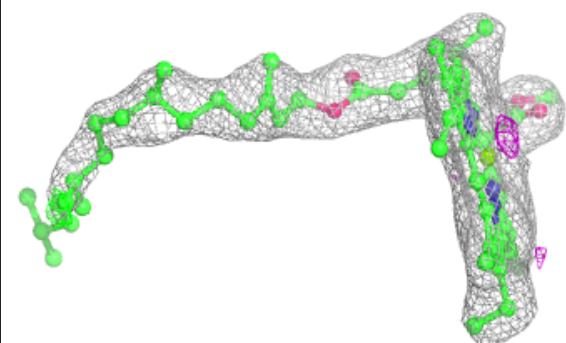
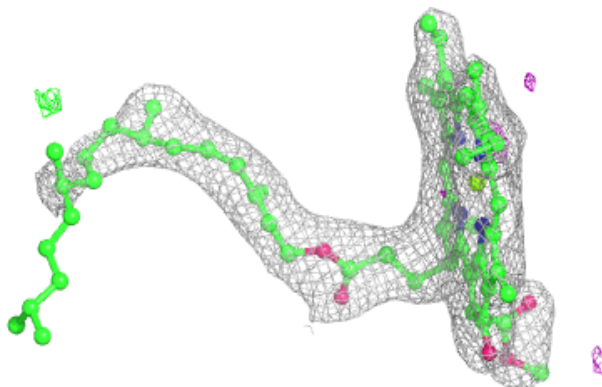


Electron density around DGD C 518 (B):

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

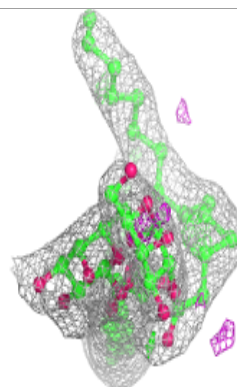
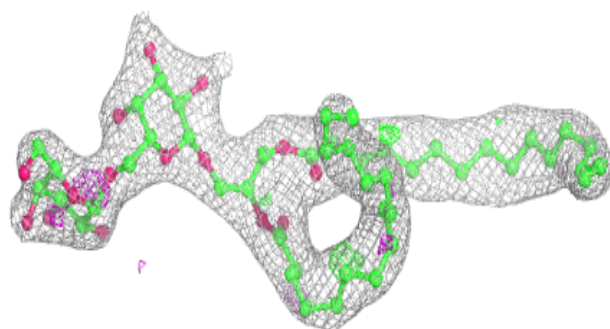
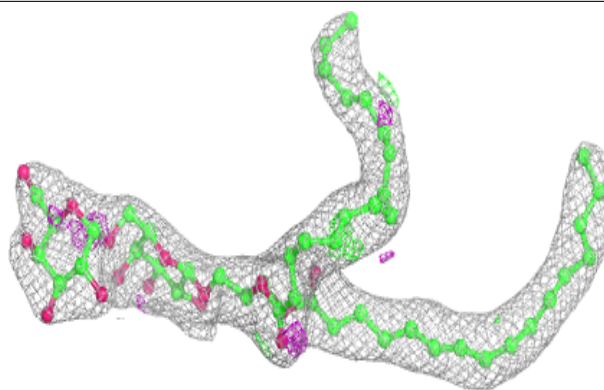
**Electron density around CLA D 703:**

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

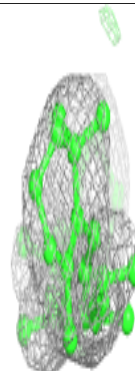
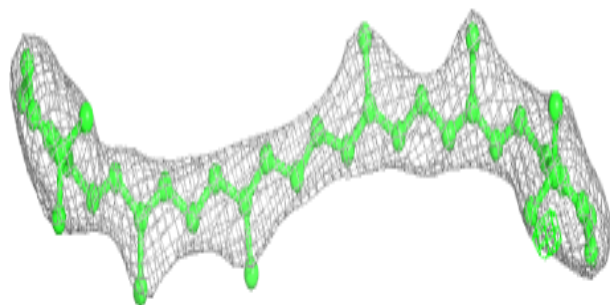
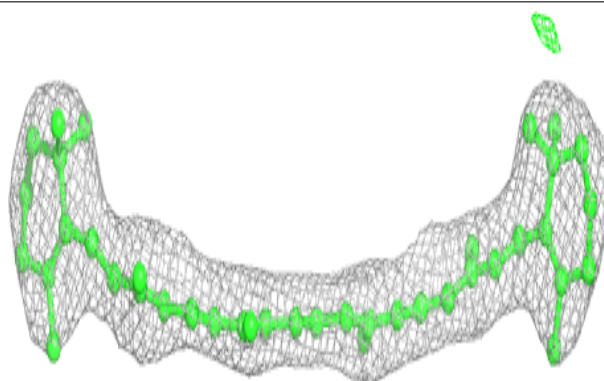


Electron density around DGD H 102:

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

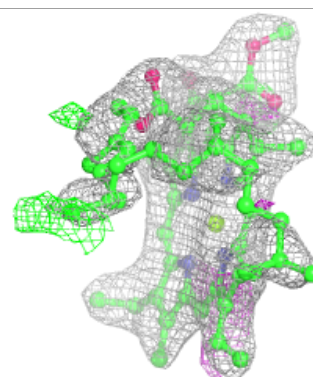
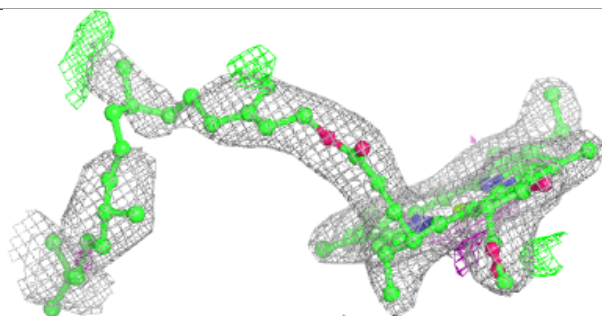
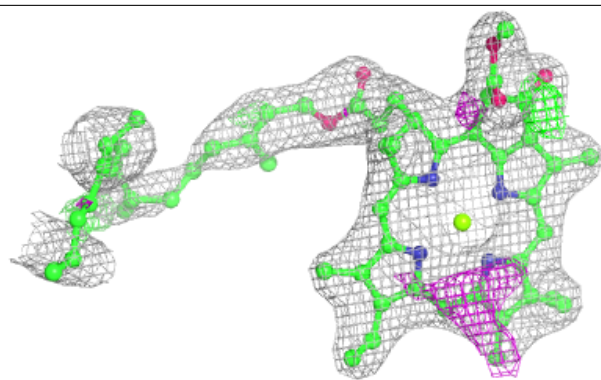
**Electron density around BCR k 101:**

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

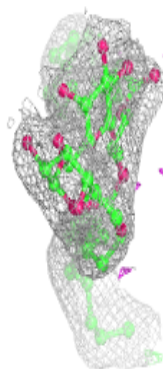
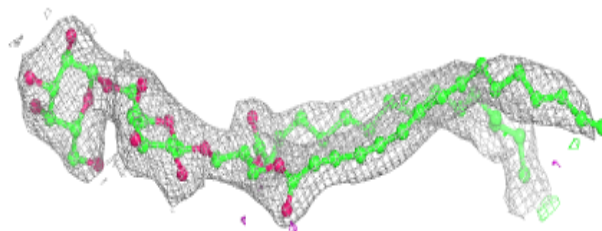
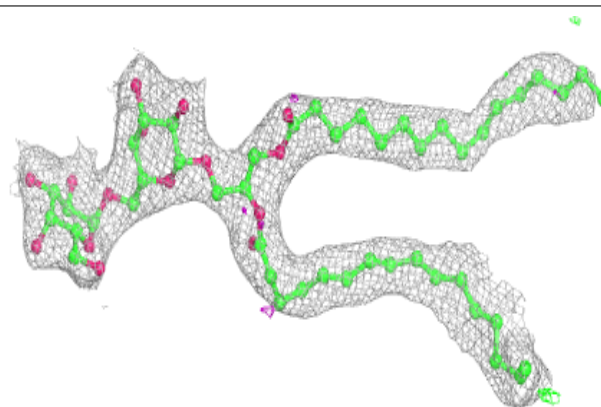


Electron density around CLA A 408:

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

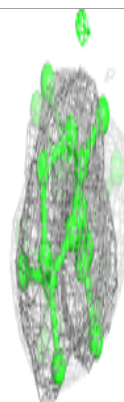
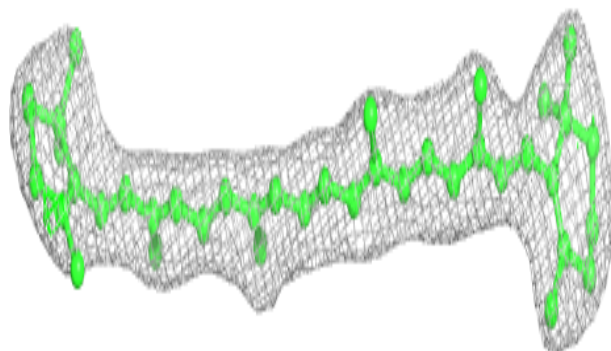
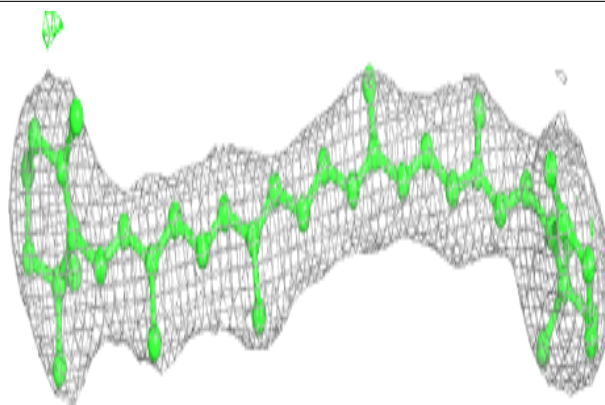
**Electron density around DGD c 519:**

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

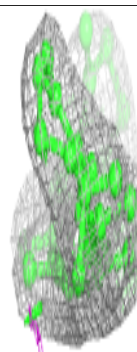
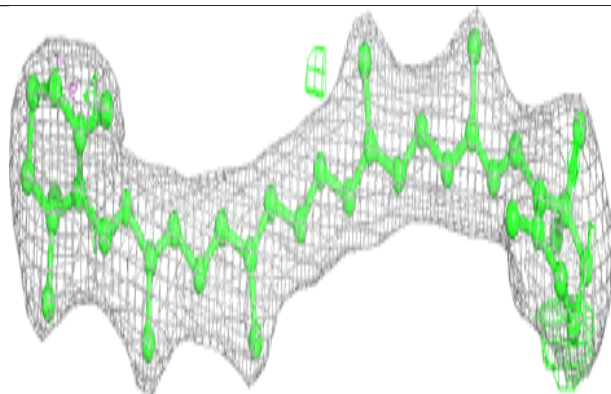
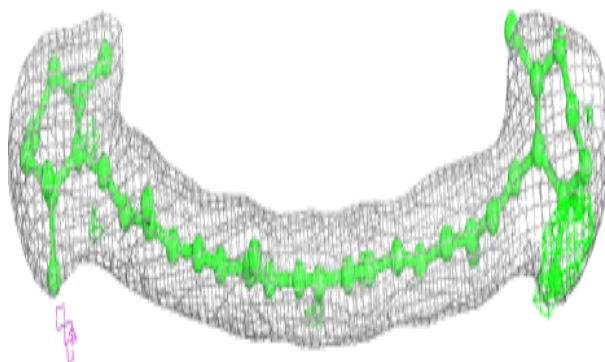


Electron density around BCR c 515:

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

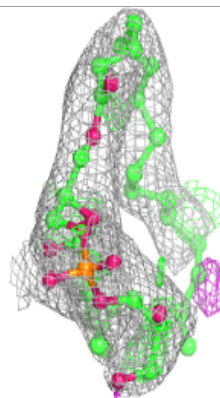
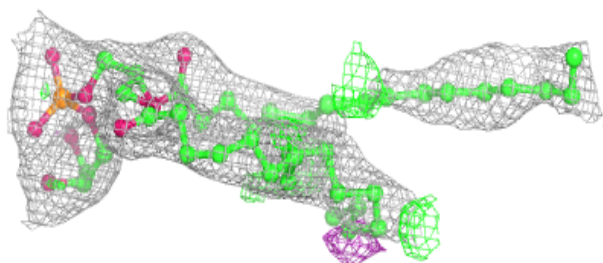
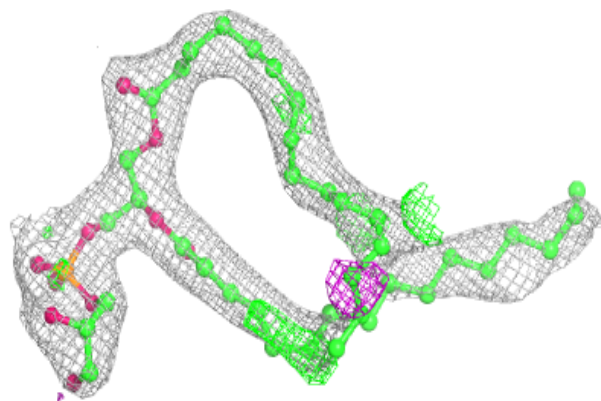
**Electron density around BCR D 704:**

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

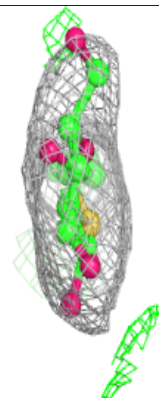
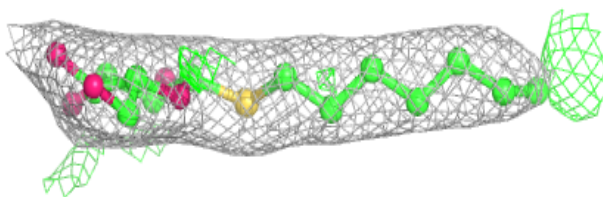
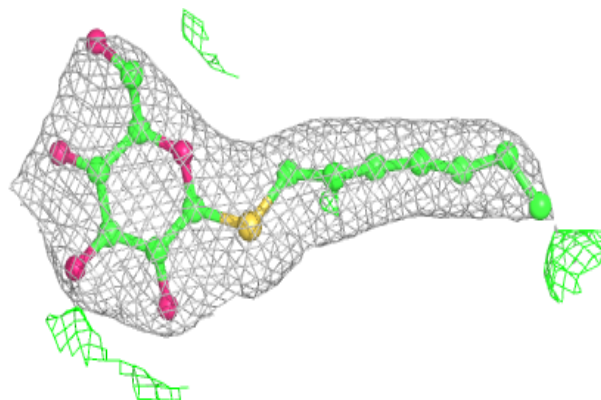


Electron density around LHG d 406 (A):

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

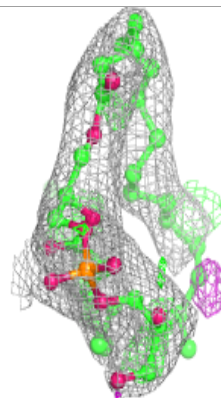
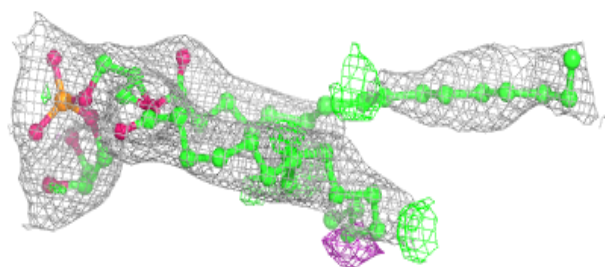
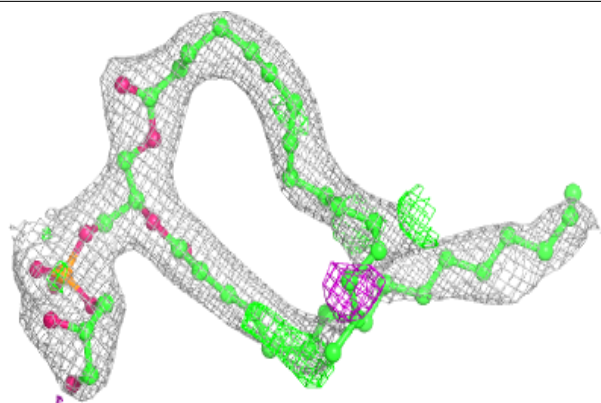
**Electron density around HTG B 624:**

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

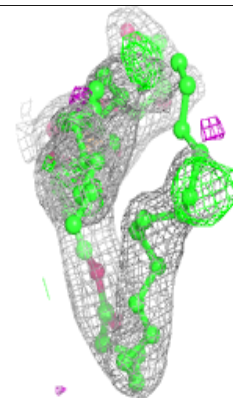
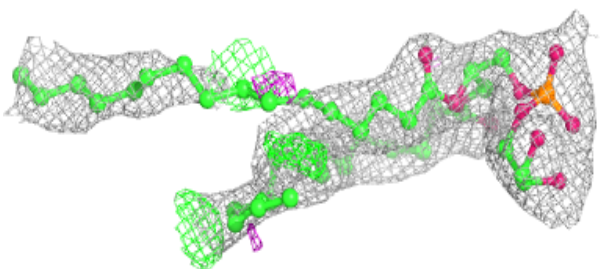
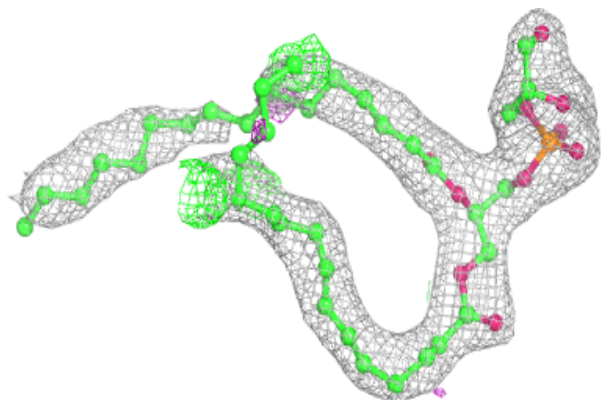


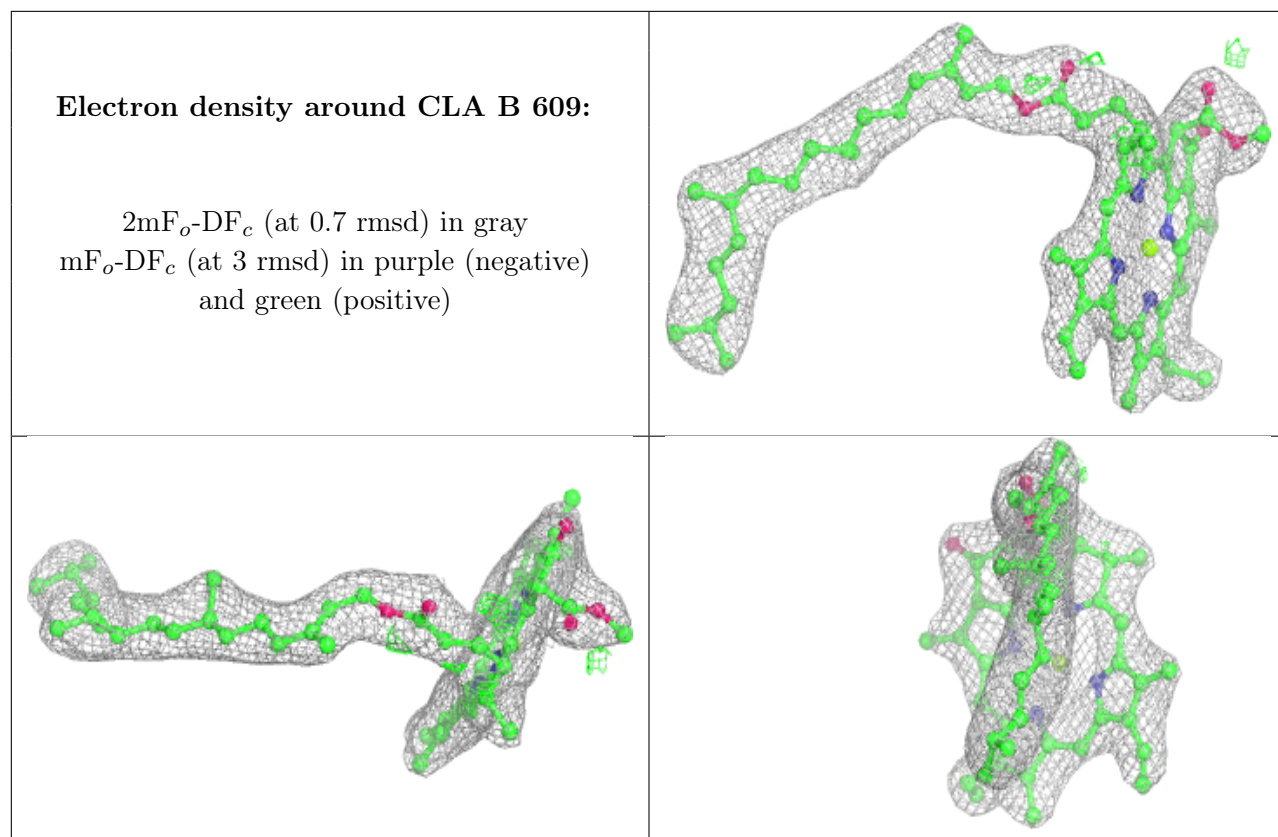
Electron density around LHG d 406 (B):

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

**Electron density around LHG D 707 (B):**

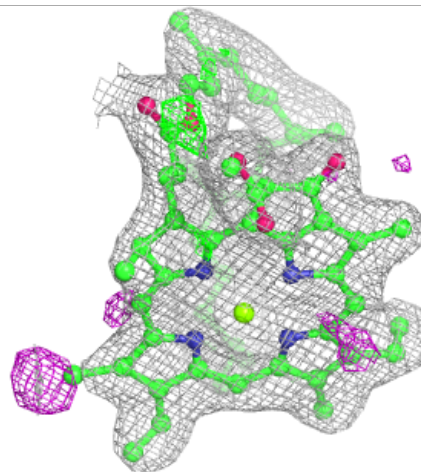
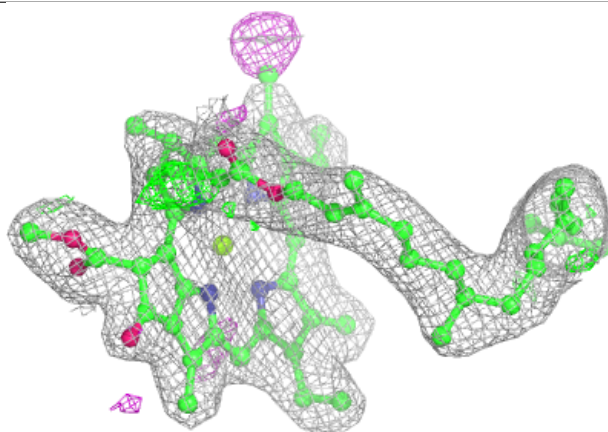
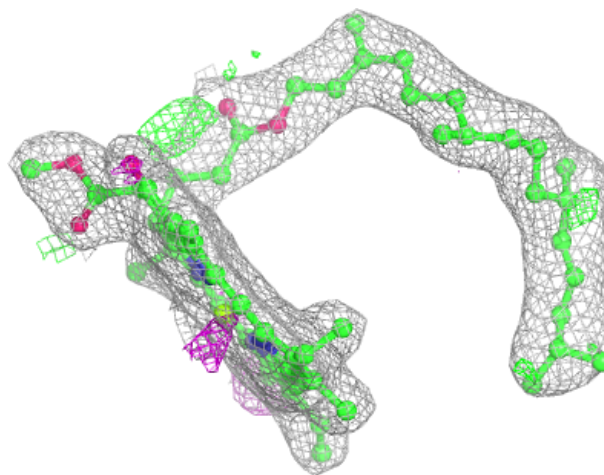
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





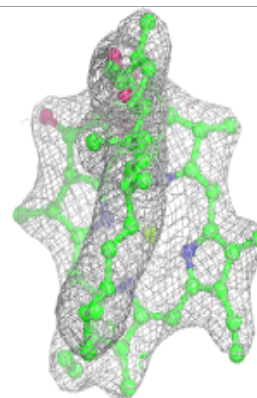
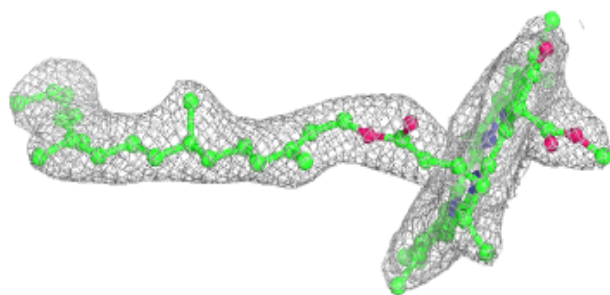
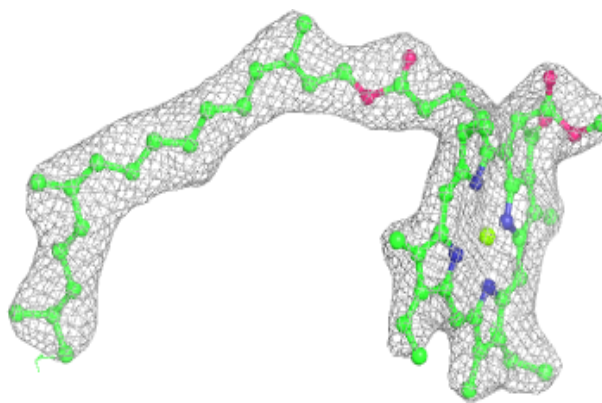
Electron density around CLA B 611:

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

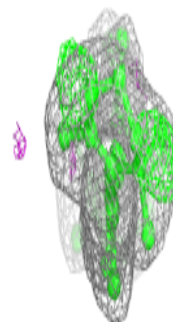
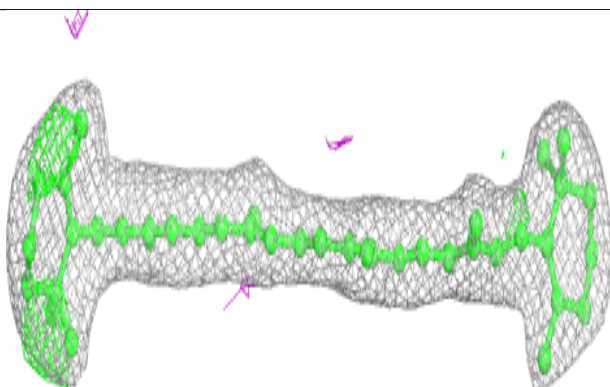
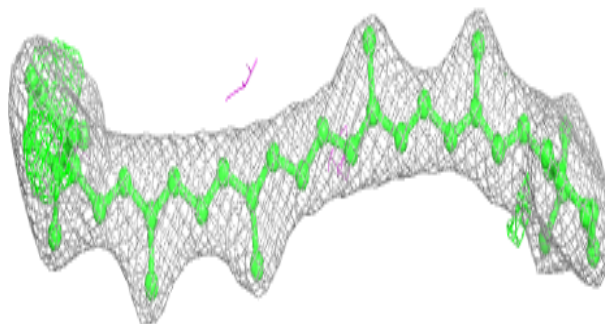


Electron density around CLA b 609:

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

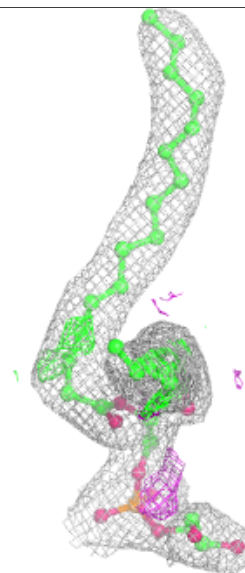
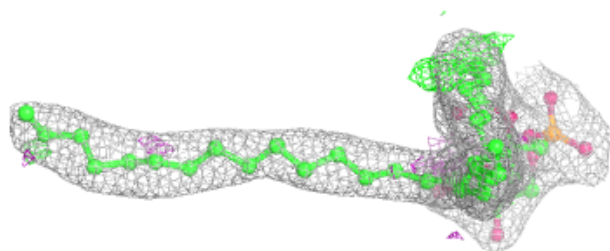
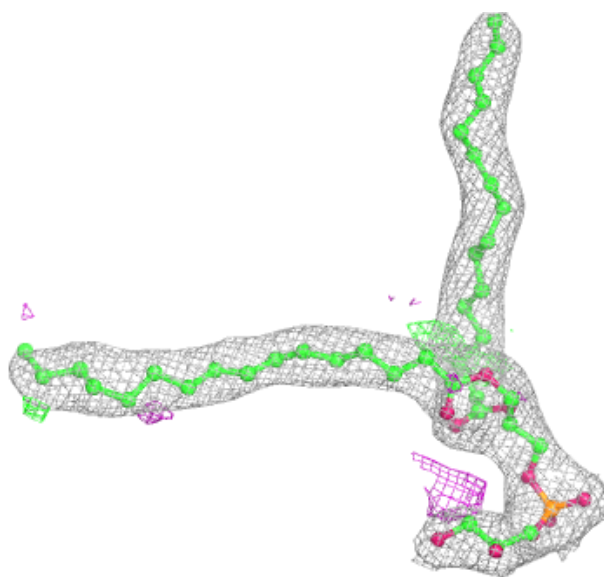
**Electron density around BCR A 409:**

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



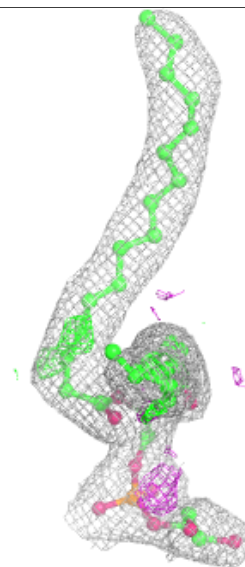
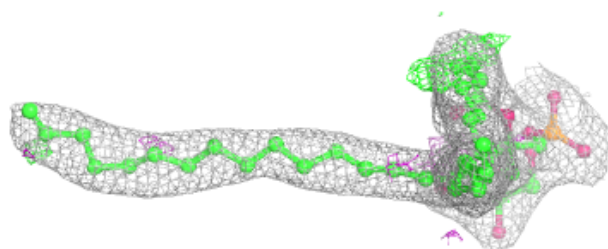
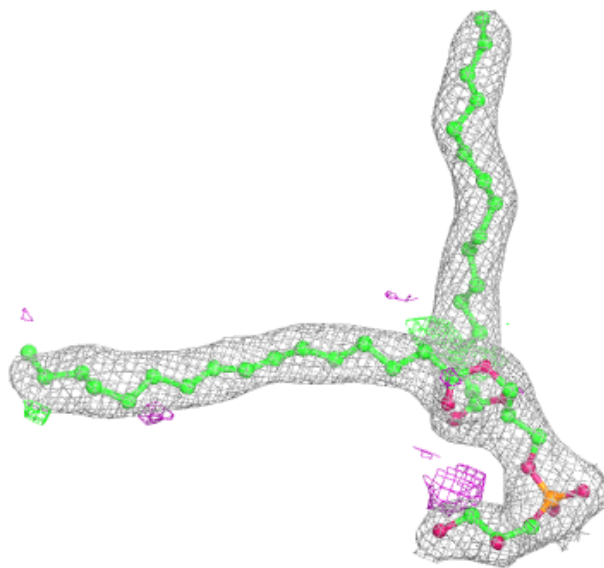
Electron density around LHG b 629 (A):

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



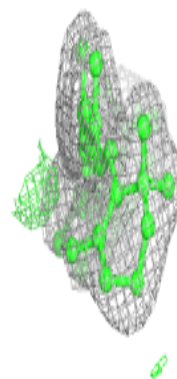
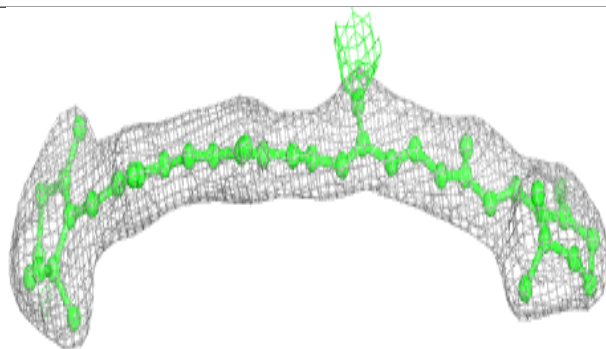
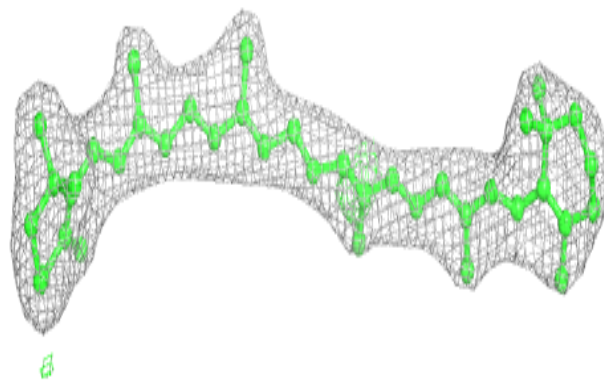
Electron density around LHG b 629 (B):

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



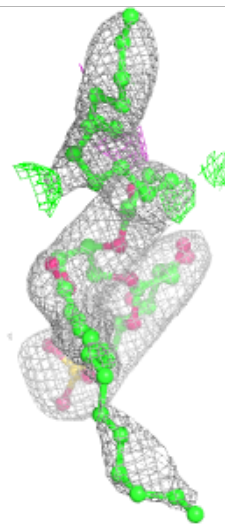
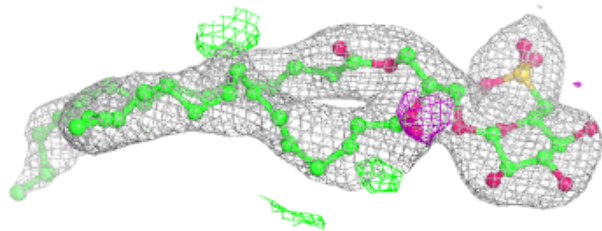
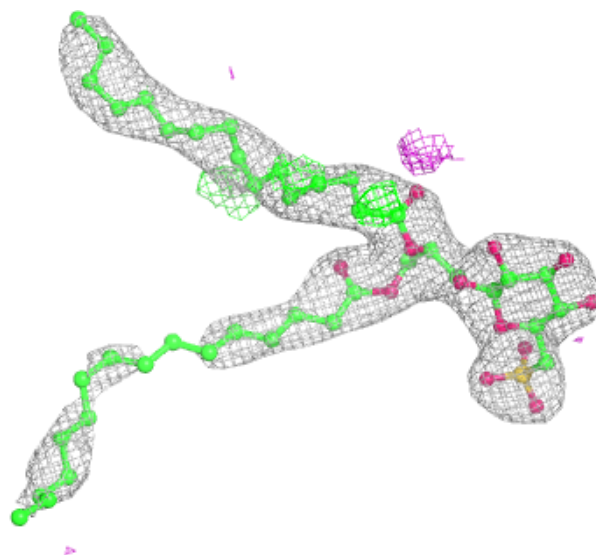
Electron density around BCR t 102:

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



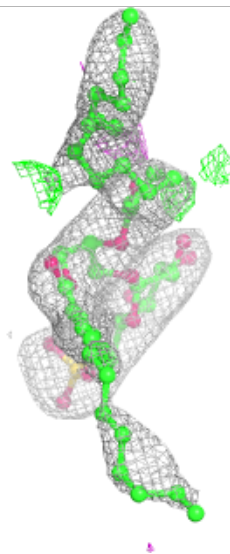
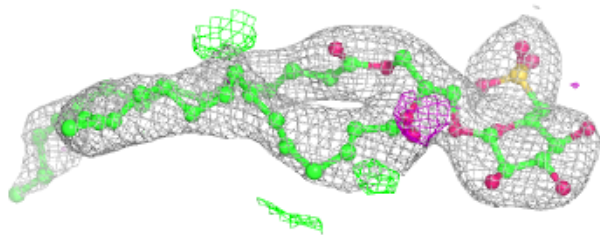
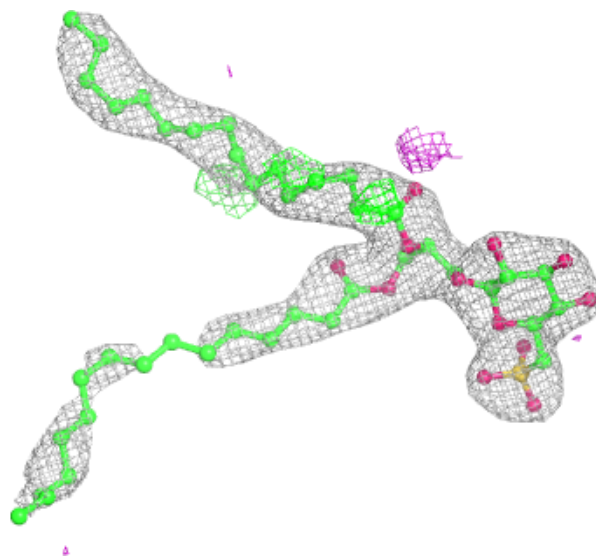
Electron density around SQD A 410 (A):

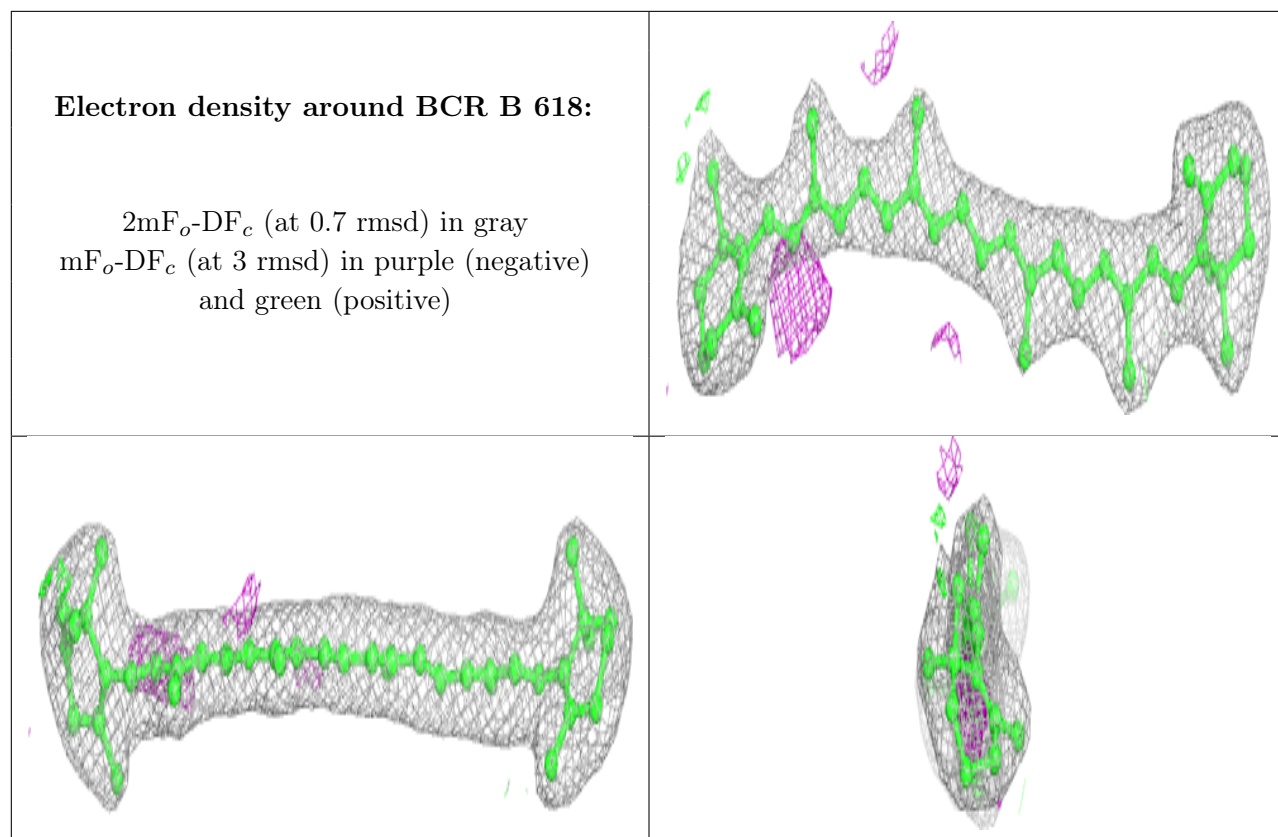
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SQD A 410 (B):

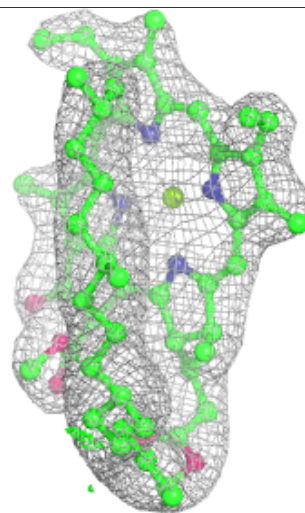
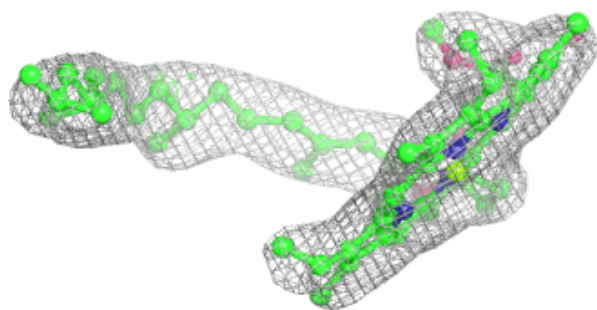
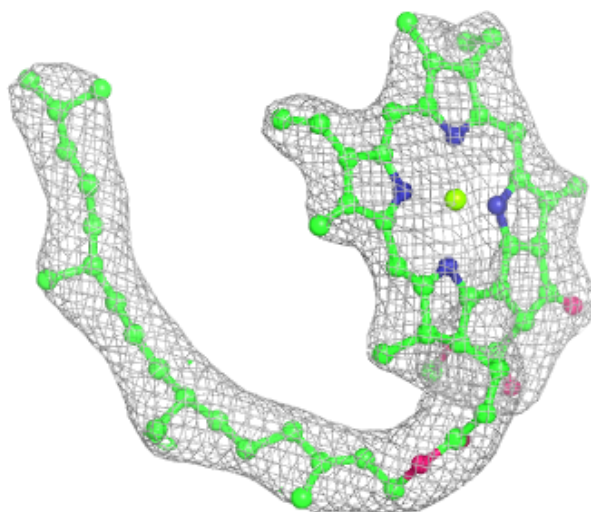
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

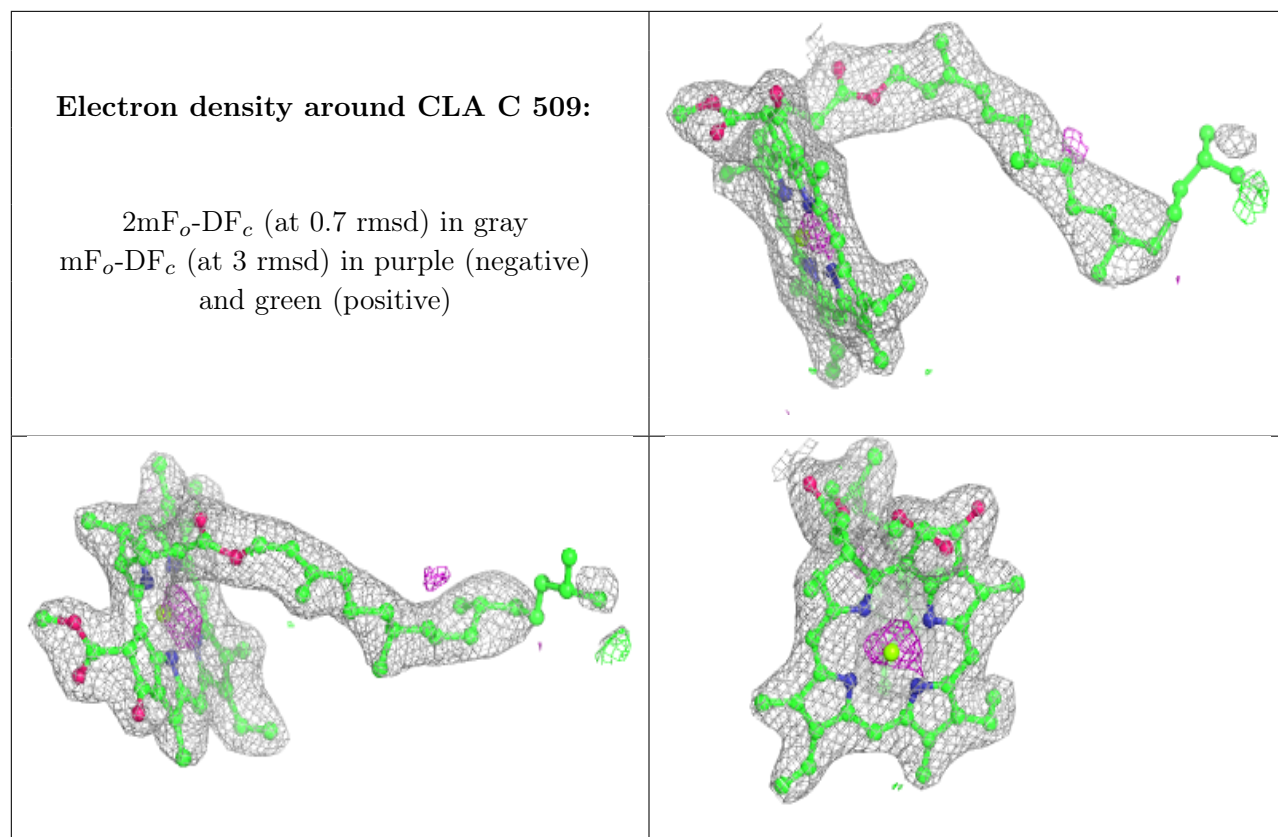




Electron density around CLA C 508:

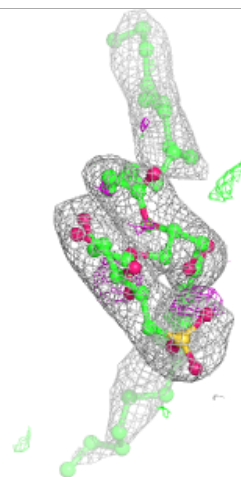
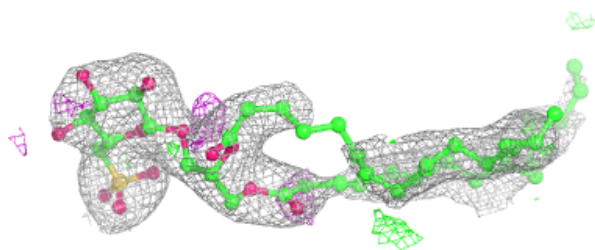
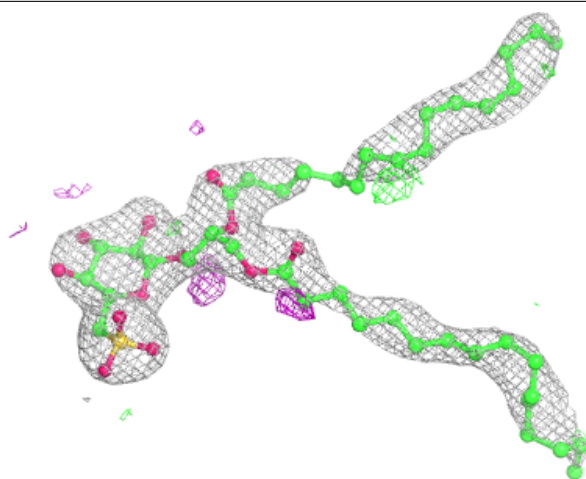
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





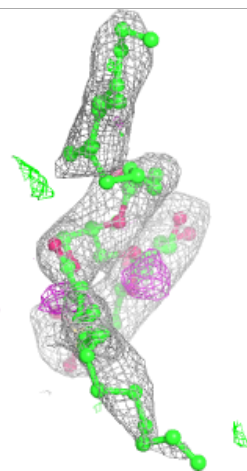
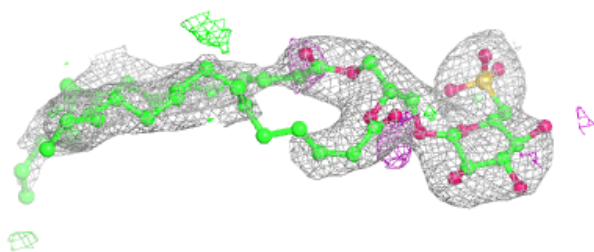
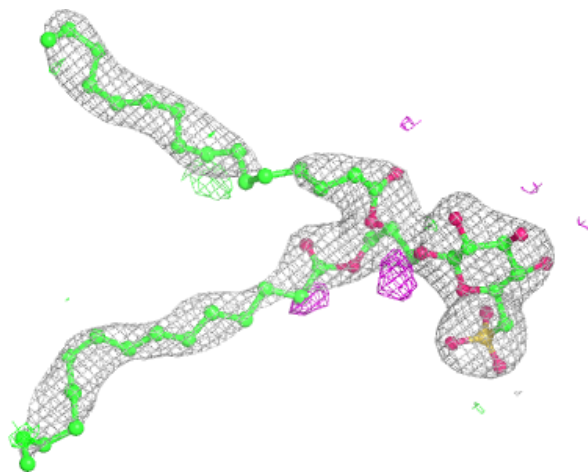
Electron density around SQD a 411 (A):

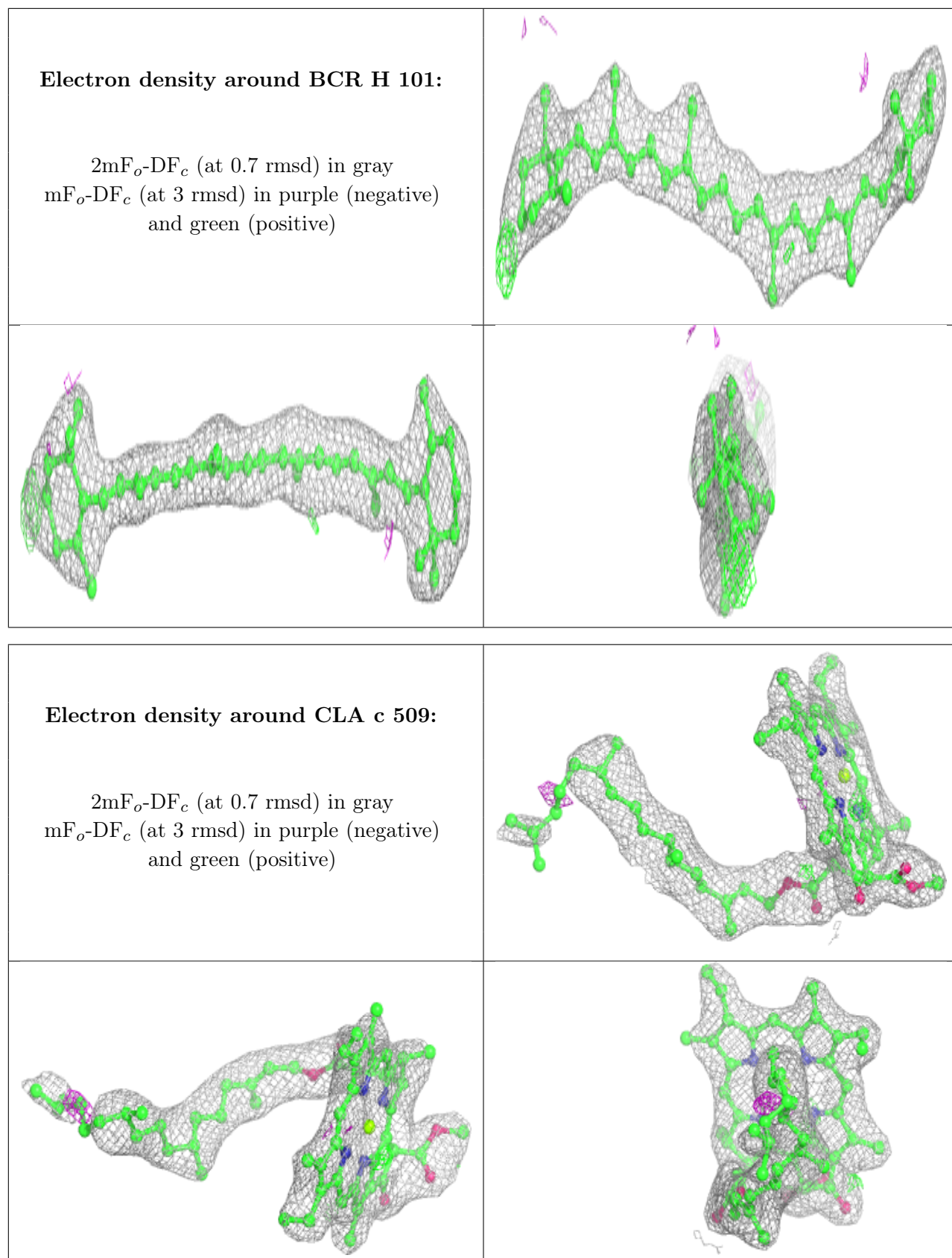
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

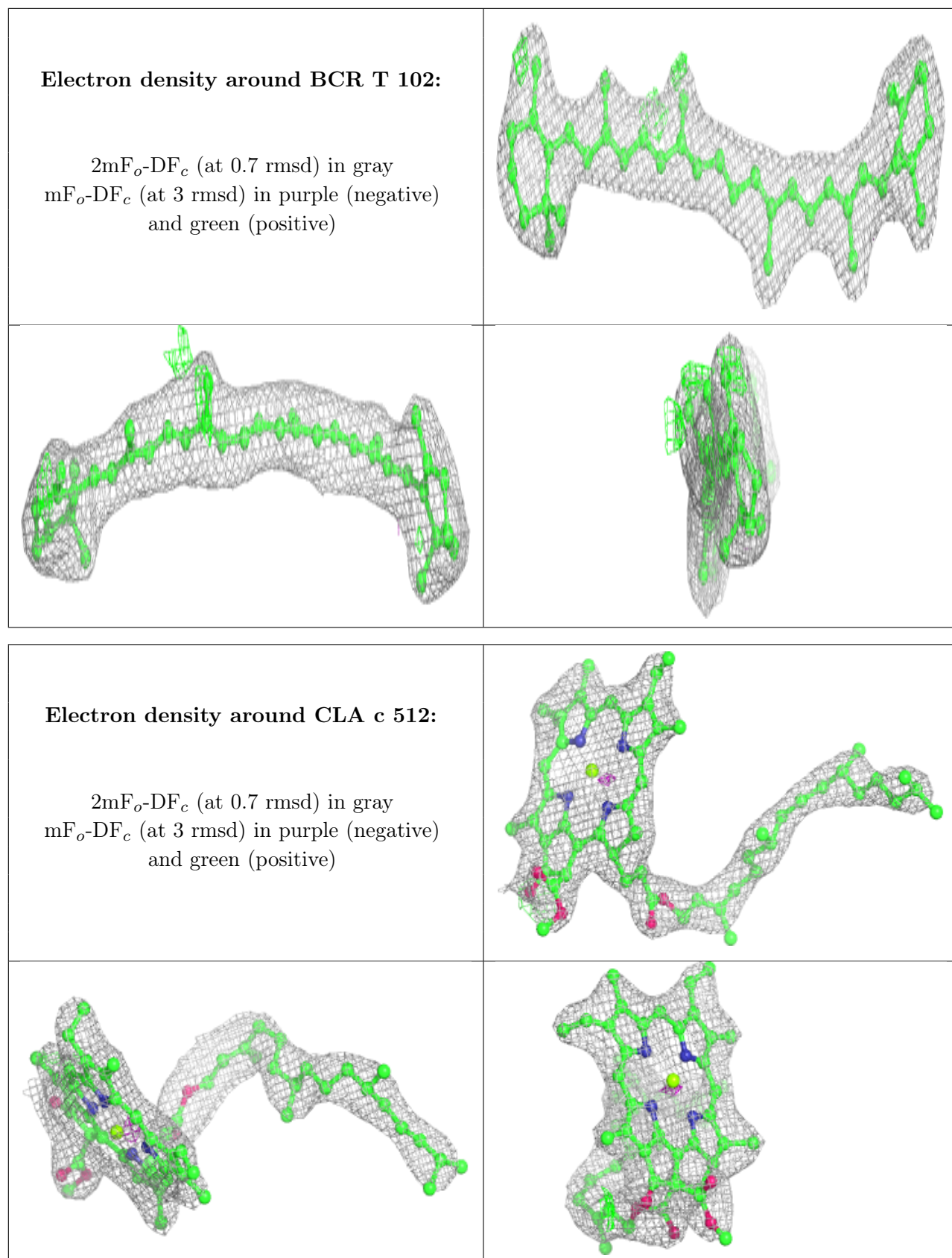


Electron density around SQD a 411 (B):

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

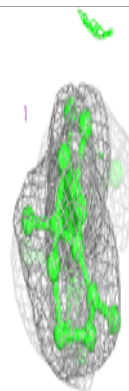
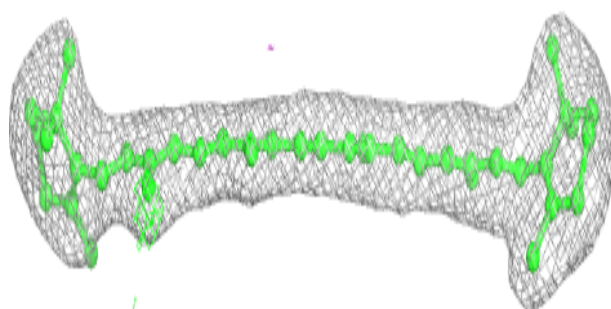
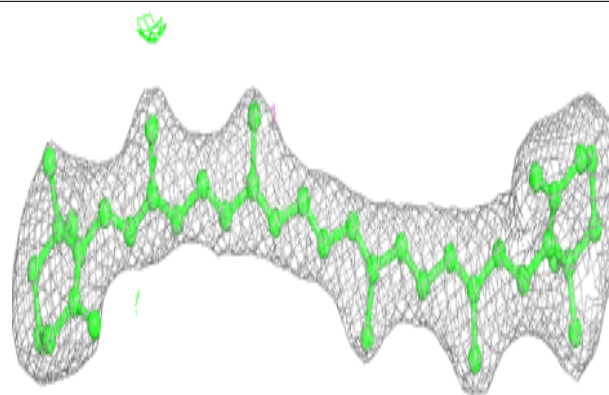




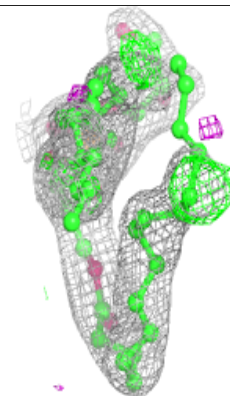
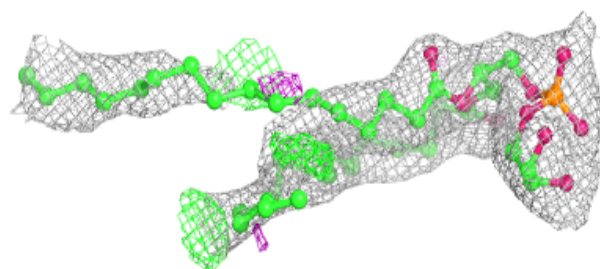
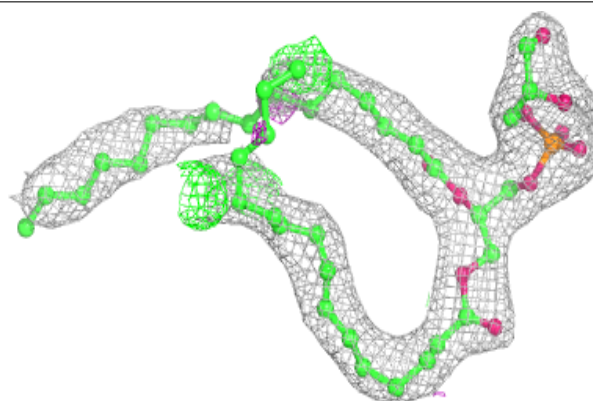


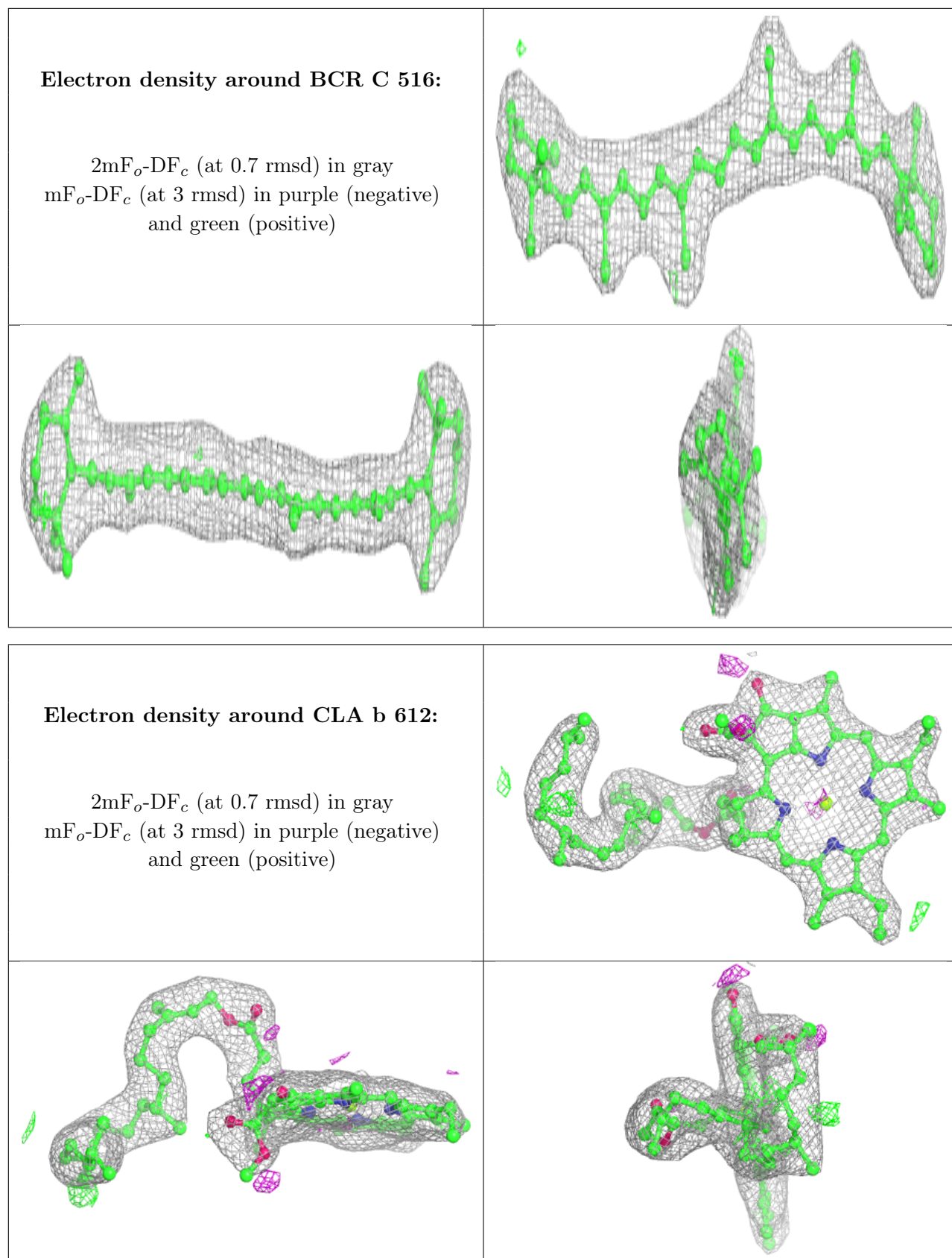
Electron density around BCR b 618:

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

**Electron density around LHG D 707 (A):**

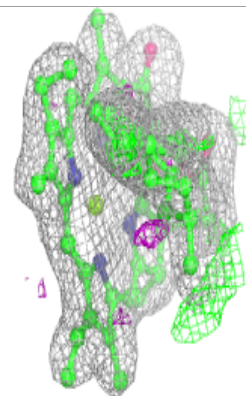
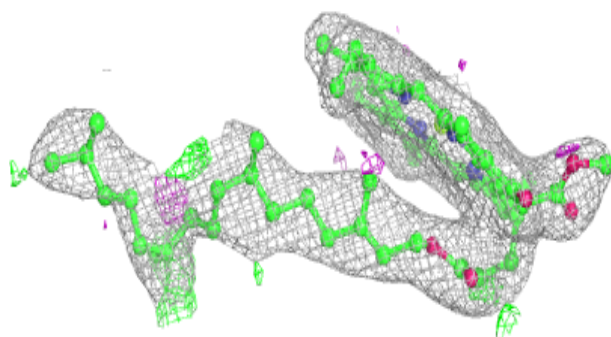
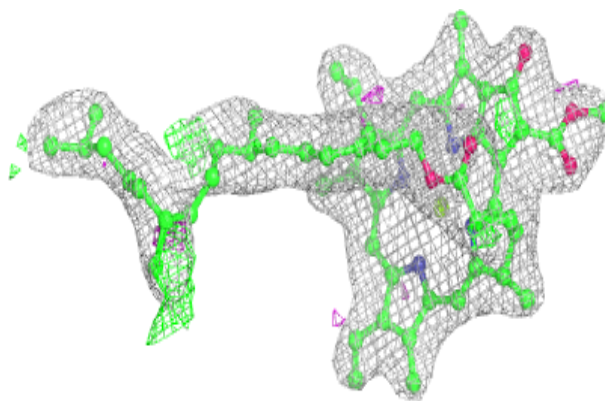
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





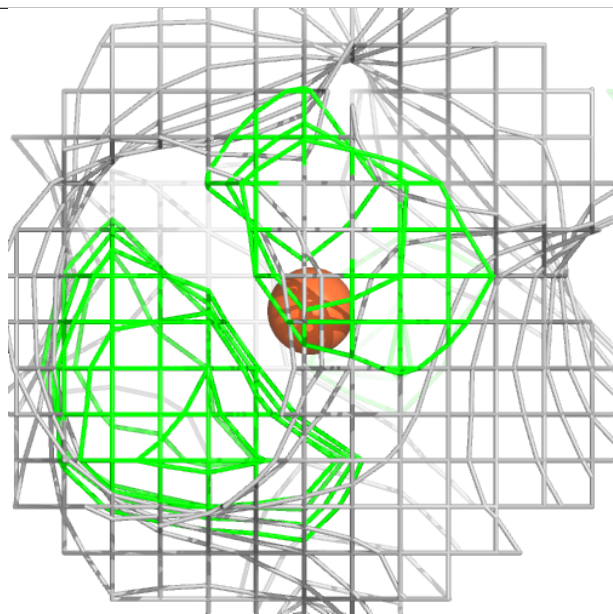
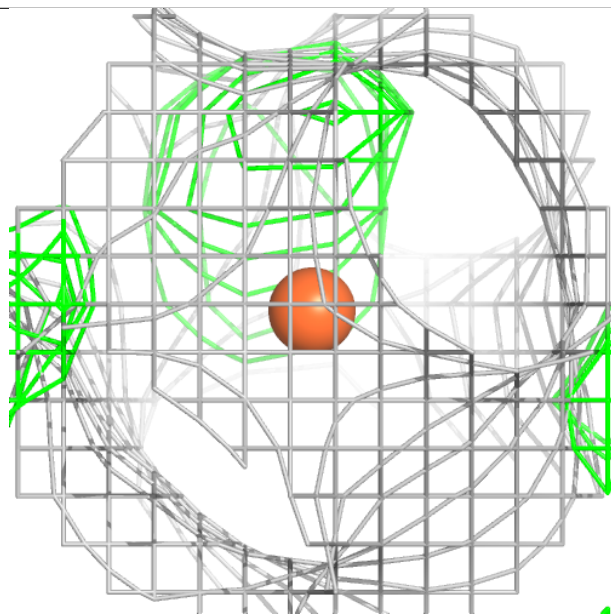
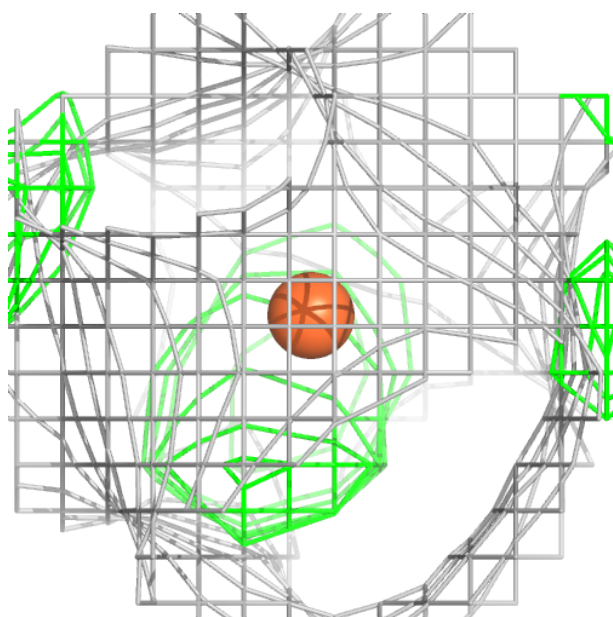
Electron density around CLA b 614:

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



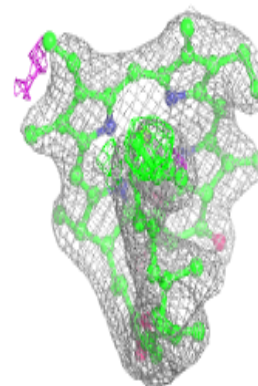
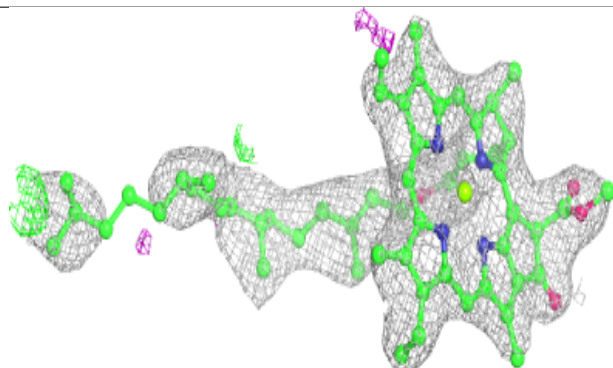
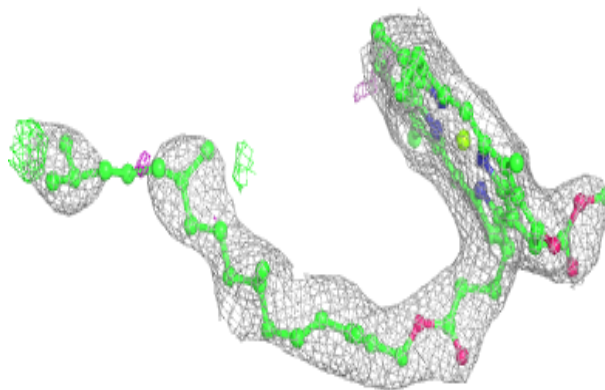
Electron density around FE2 a 401 (A):

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

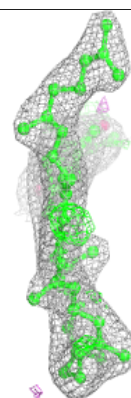
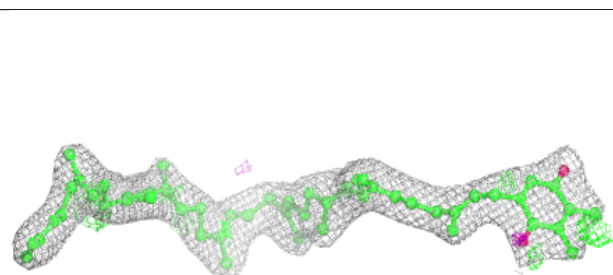
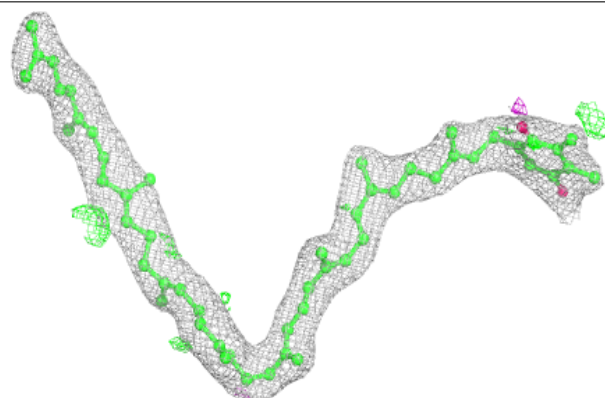


Electron density around CLA c 505:

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

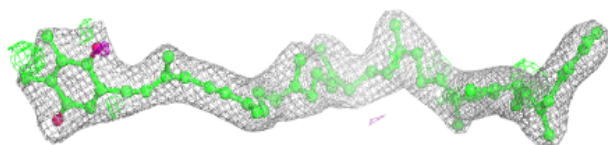
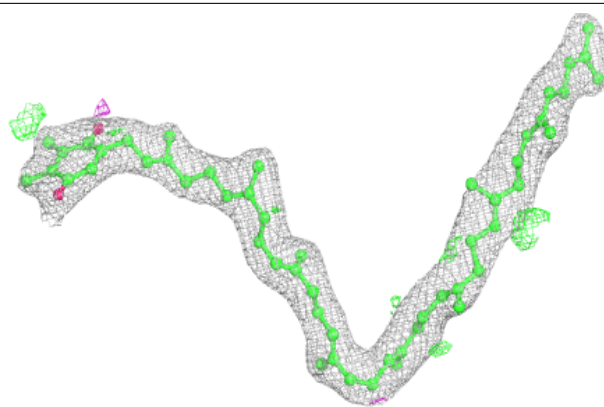
**Electron density around PL9 D 705 (A):**

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

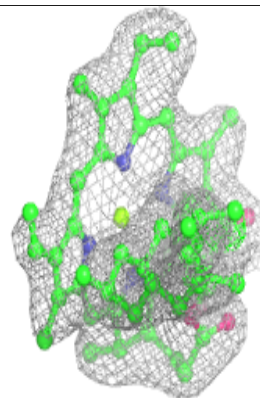
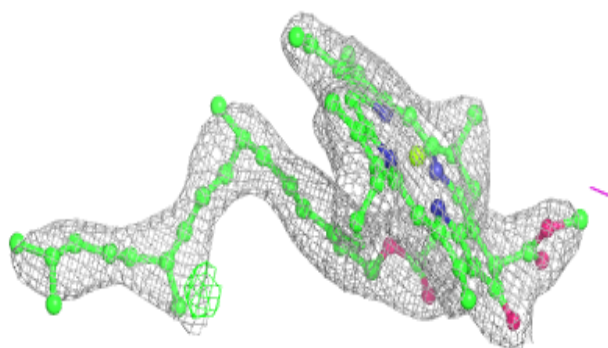
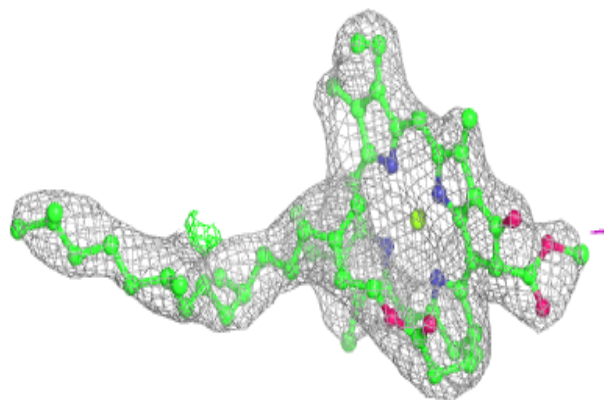


Electron density around PL9 D 705 (B):

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

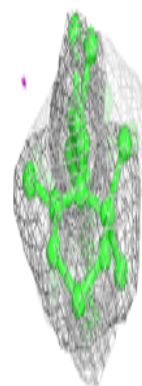
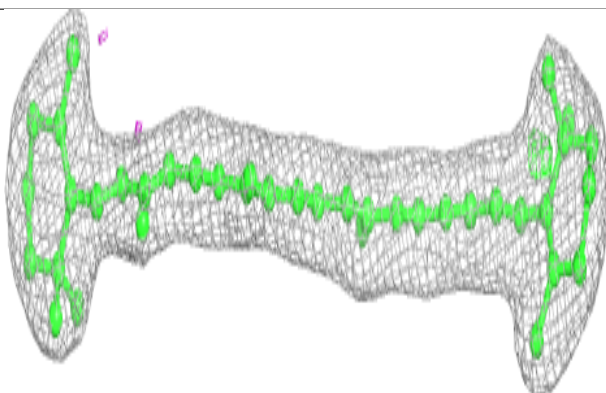
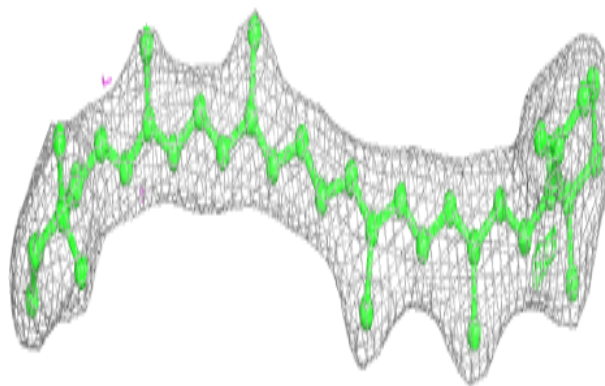
**Electron density around CLA c 506:**

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

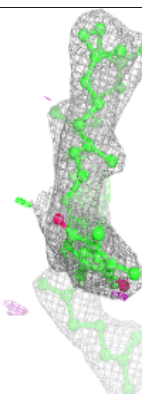
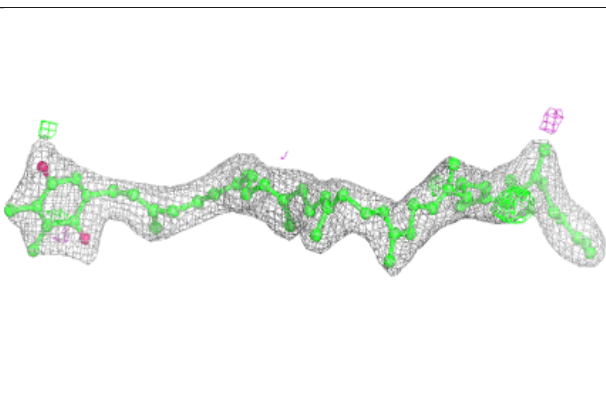
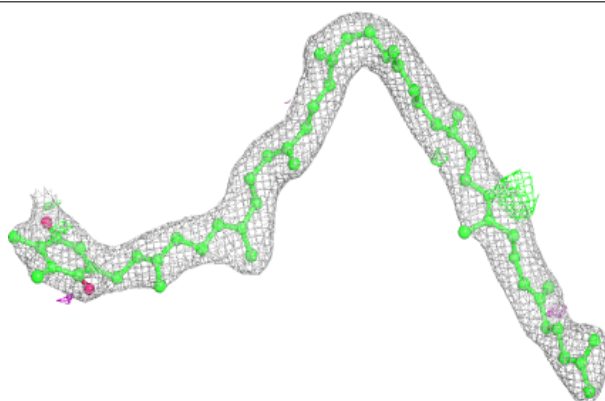


Electron density around BCR a 410:

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

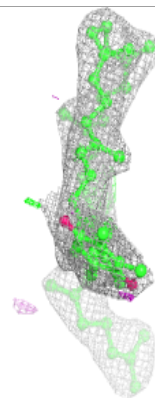
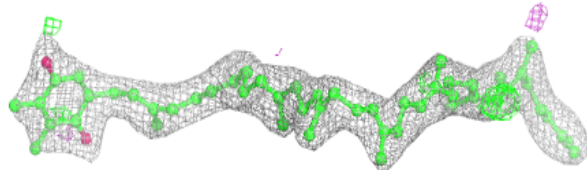
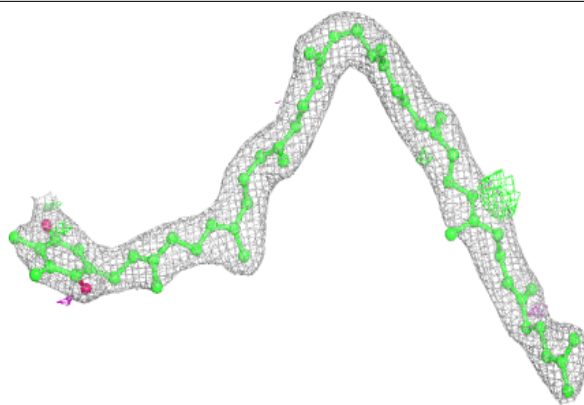
**Electron density around PL9 d 404 (A):**

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

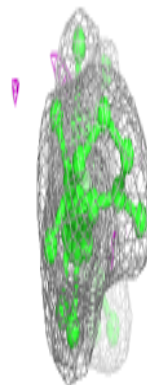
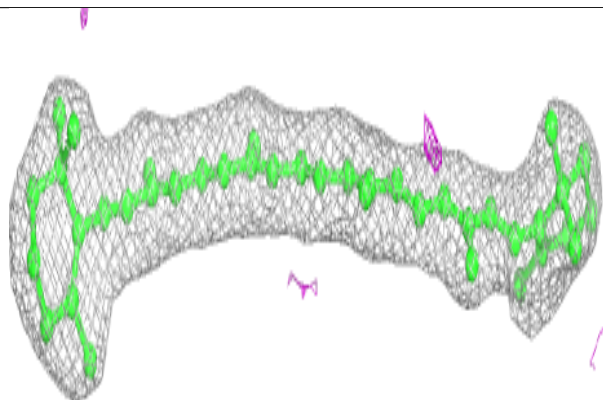
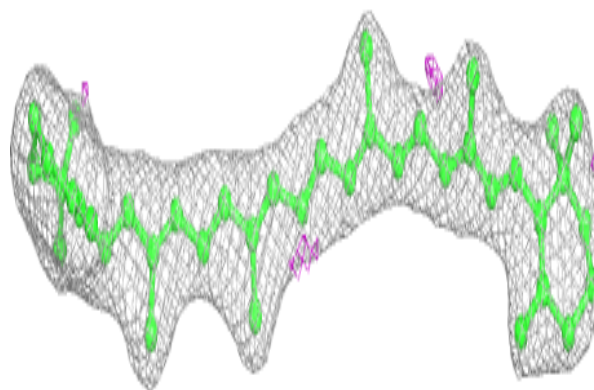


Electron density around PL9 d 404 (B):

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

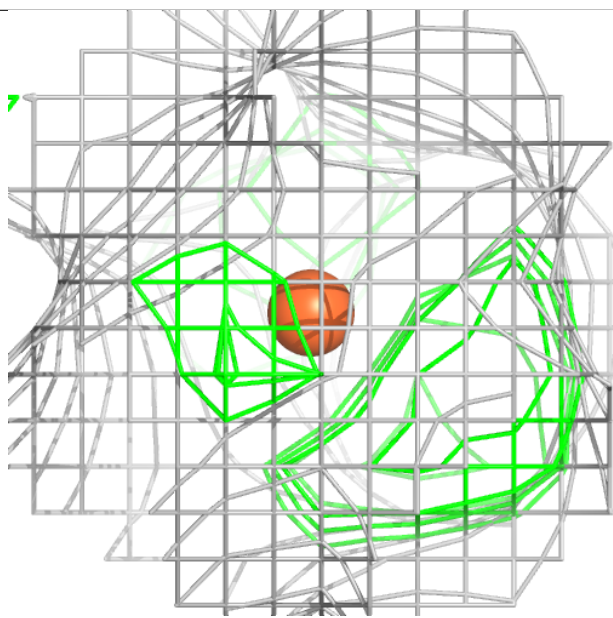
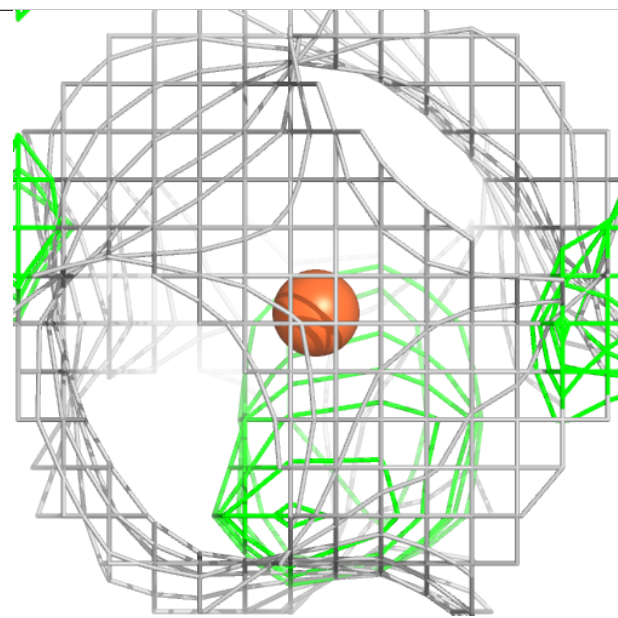
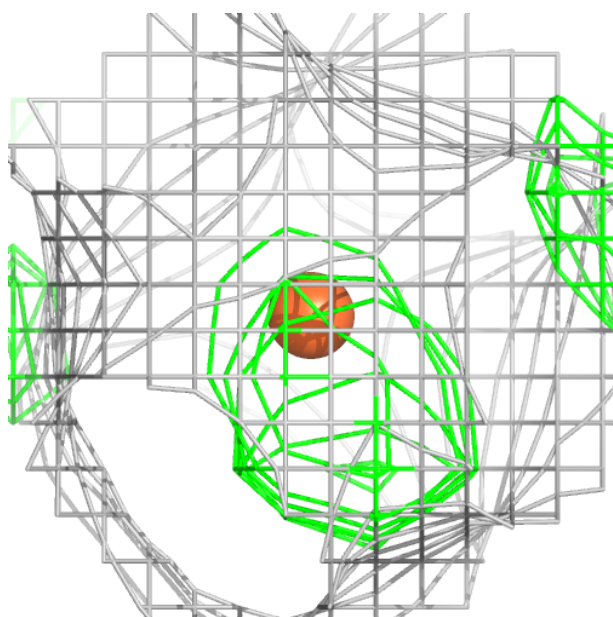
**Electron density around BCR b 617:**

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



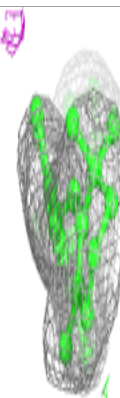
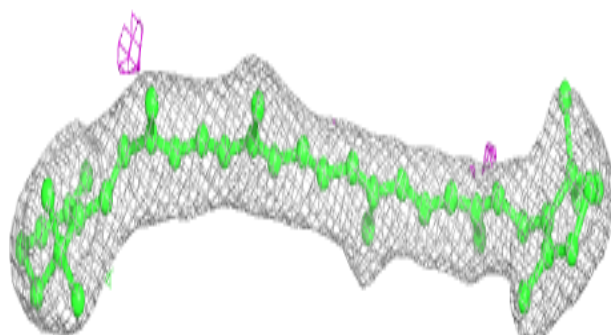
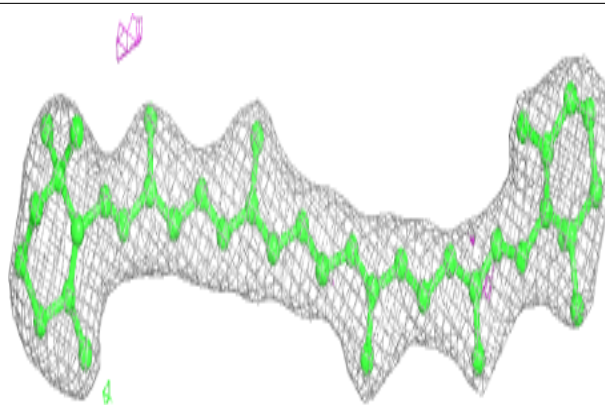
Electron density around FE2 a 401 (B):

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

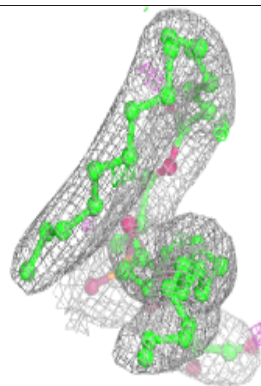
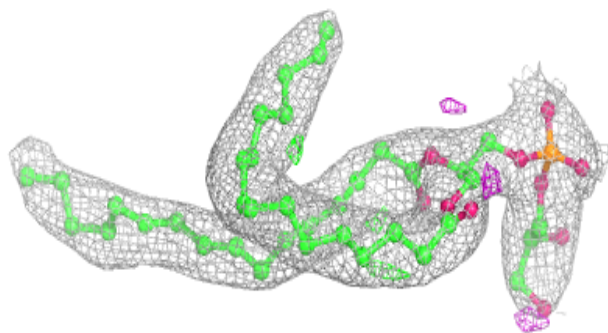
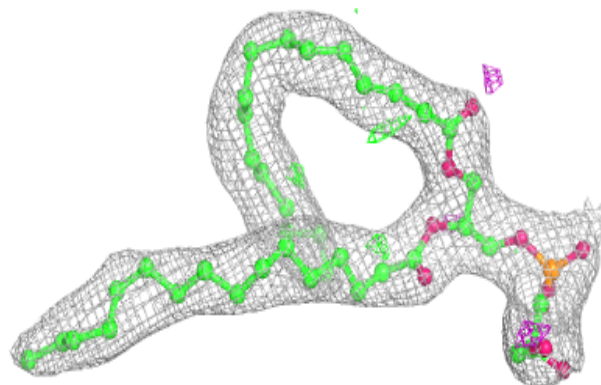


Electron density around BCR b 619:

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

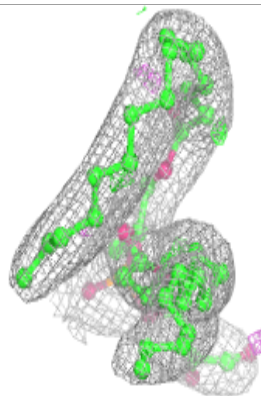
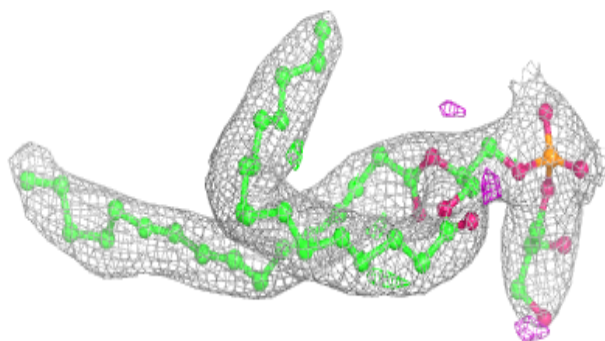
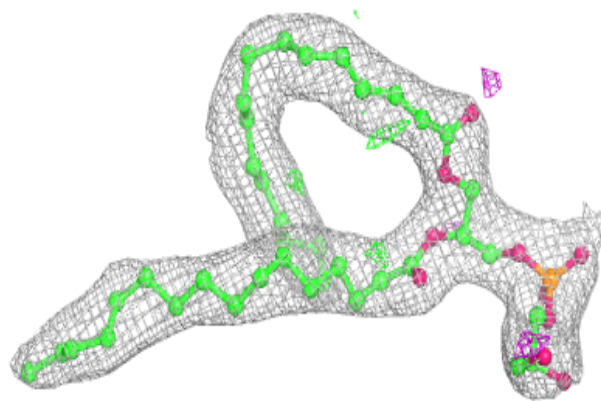
**Electron density around LHG A 419 (A):**

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



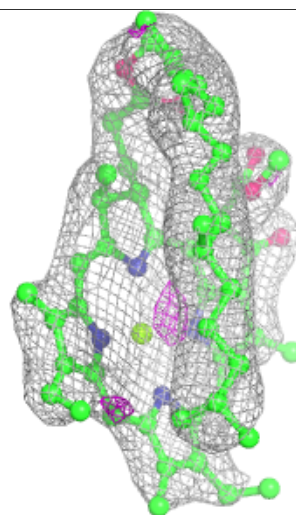
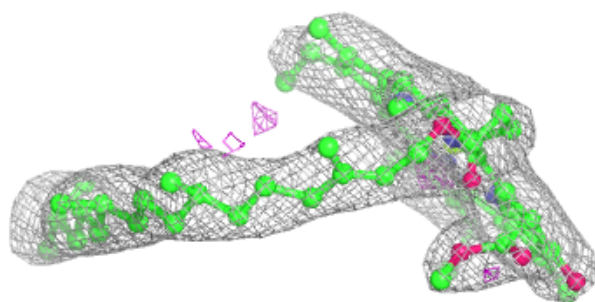
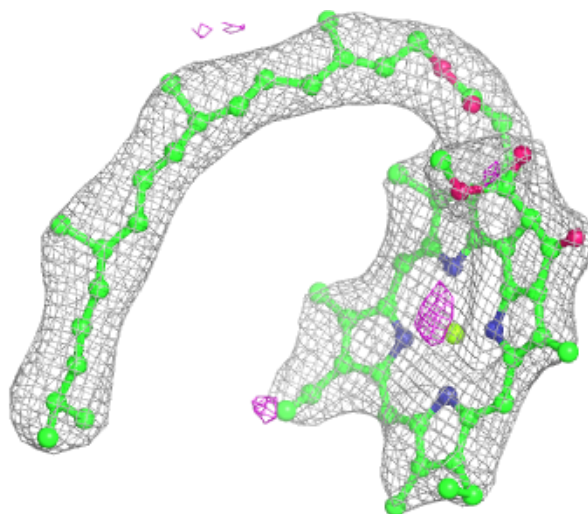
Electron density around LHG A 419 (B):

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



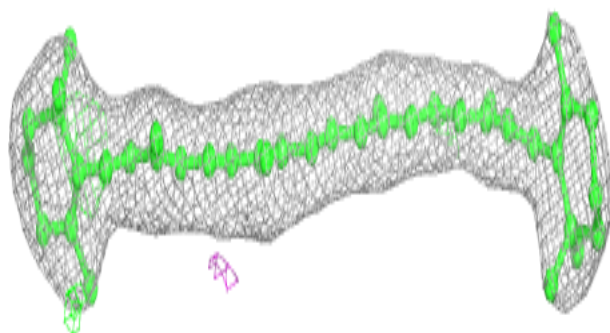
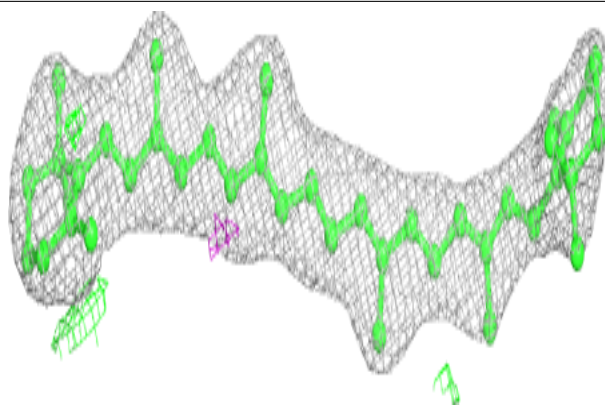
Electron density around CLA c 508:

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

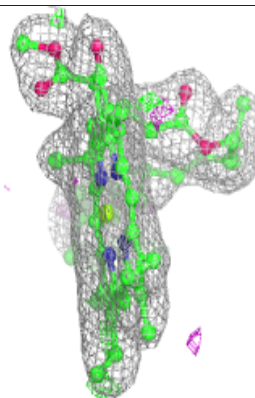
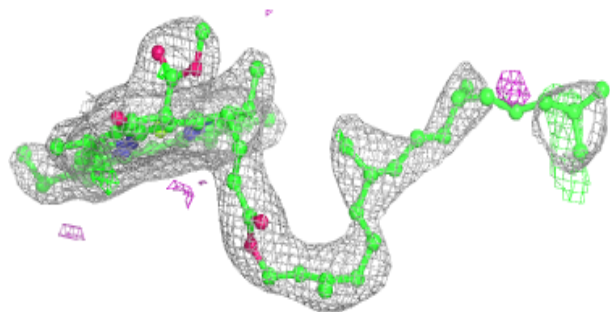
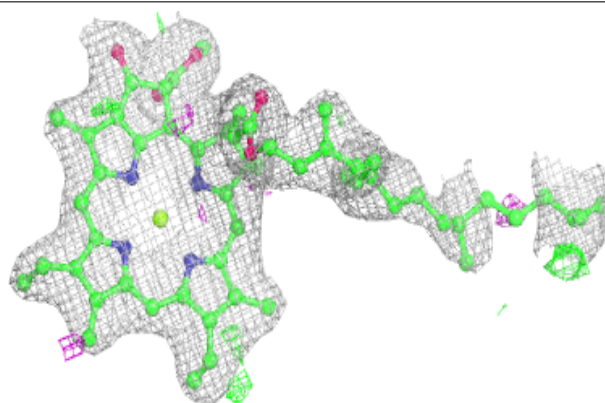


Electron density around BCR c 516:

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

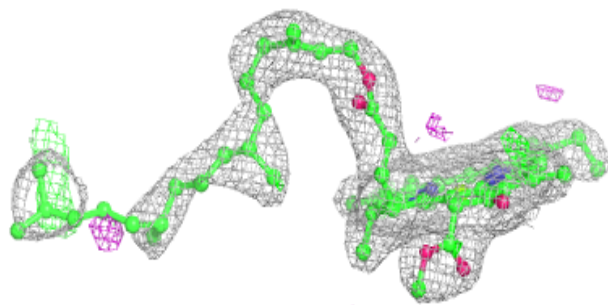
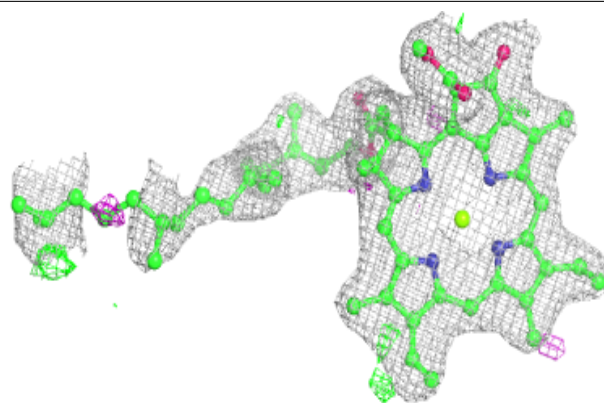
**Electron density around CLA a 407 (A):**

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

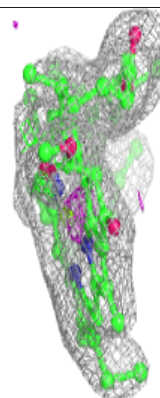
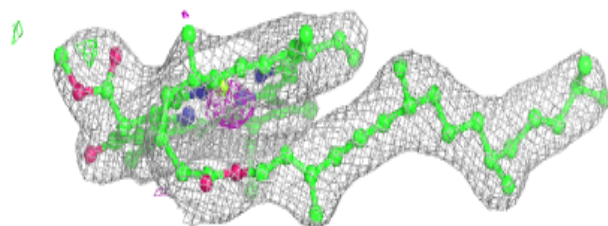
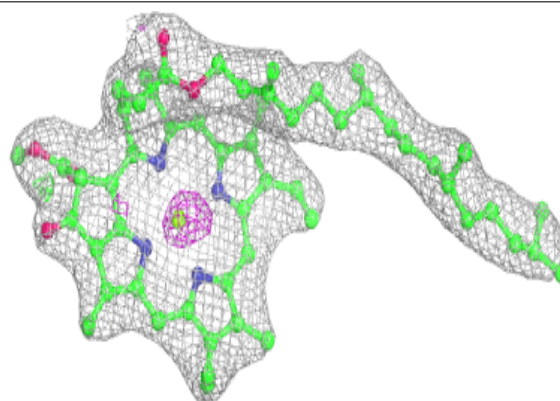


Electron density around CLA a 407 (B):

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

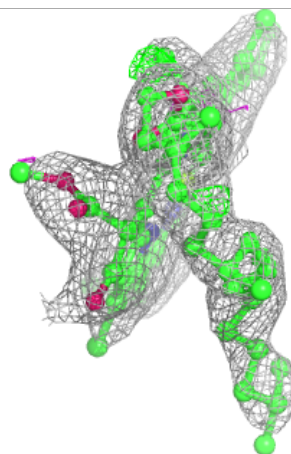
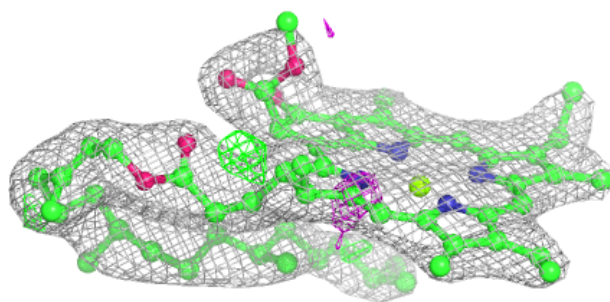
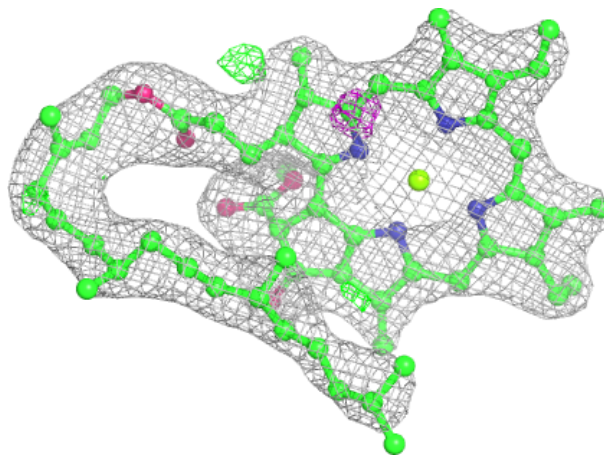
**Electron density around CLA C 502:**

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



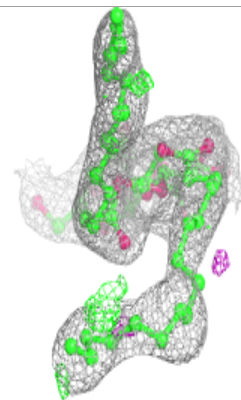
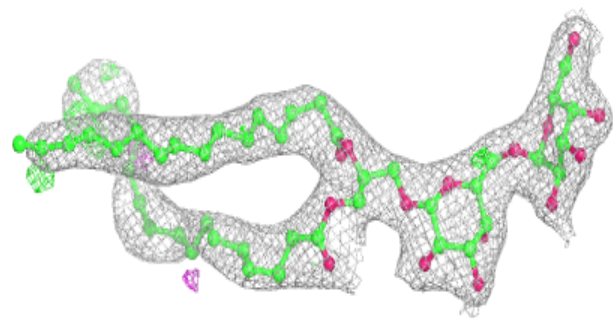
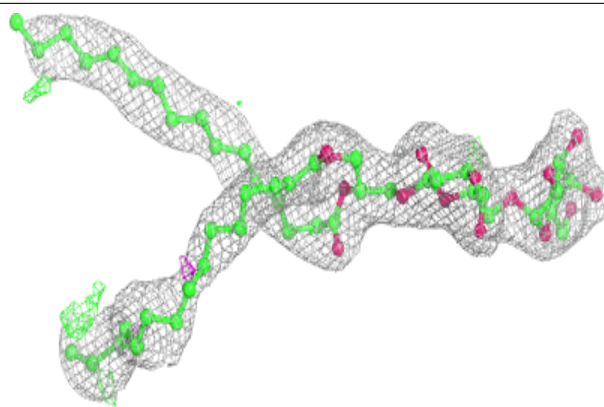
Electron density around CLA C 510:

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

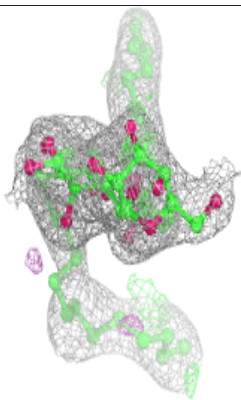
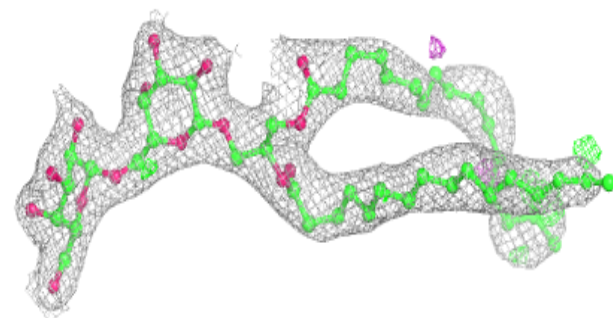
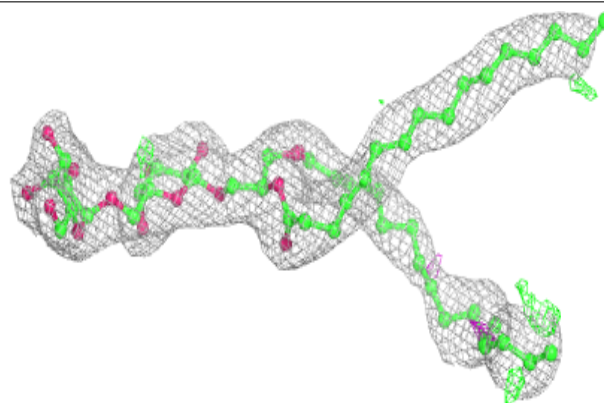


Electron density around DGD c 517 (A):

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

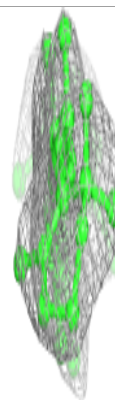
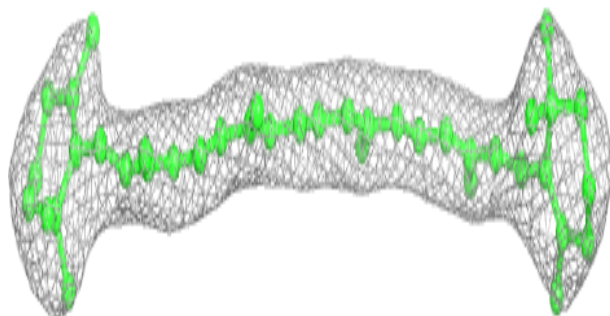
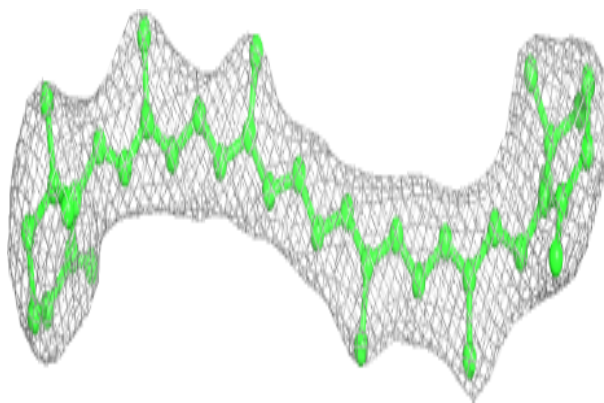
**Electron density around DGD c 517 (B):**

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

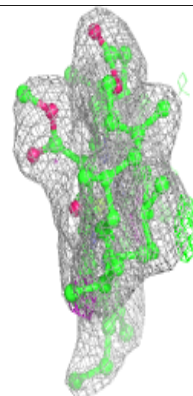
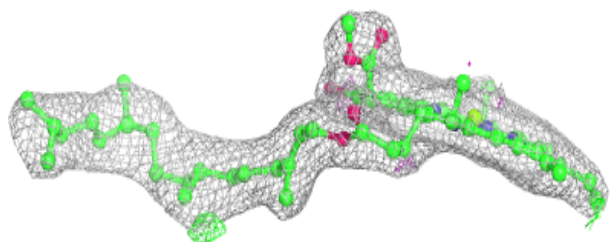
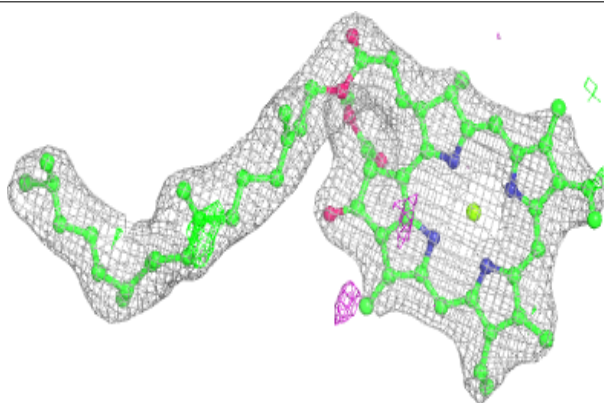


Electron density around BCR y 101:

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

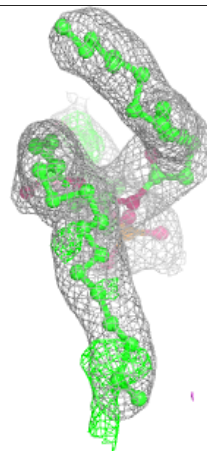
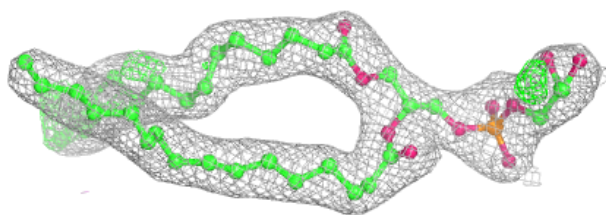
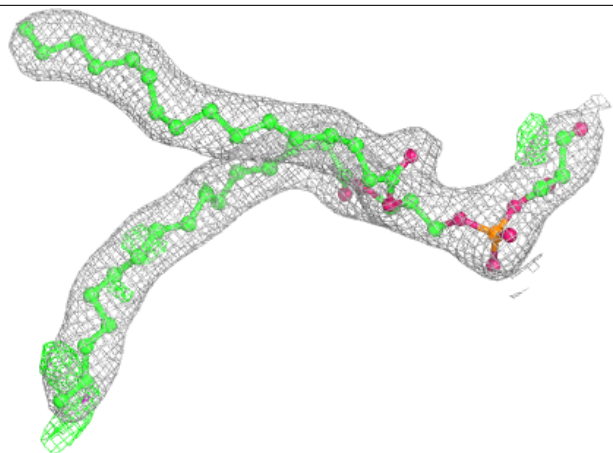
**Electron density around CLA b 602:**

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



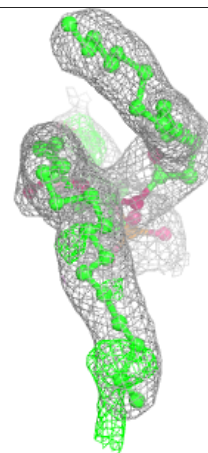
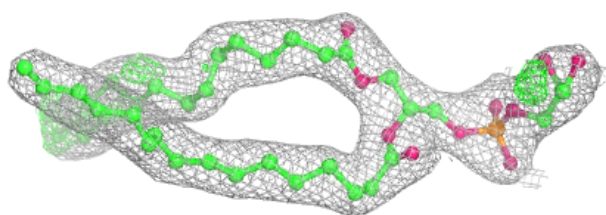
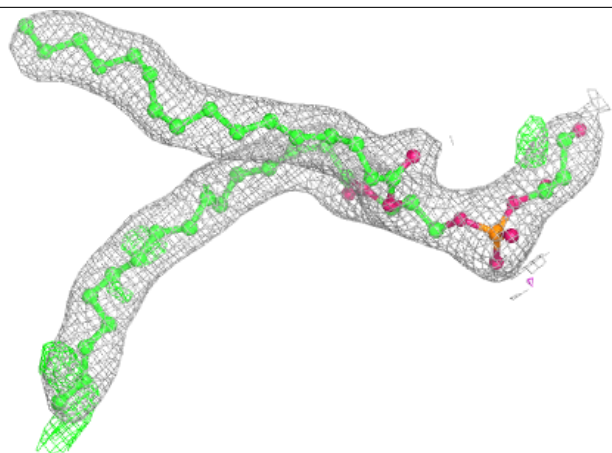
Electron density around LHG d 405 (A):

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

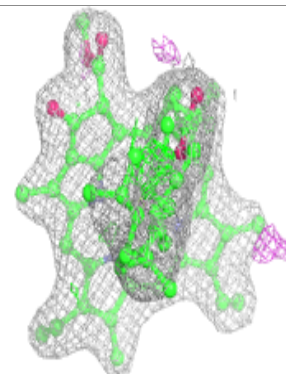
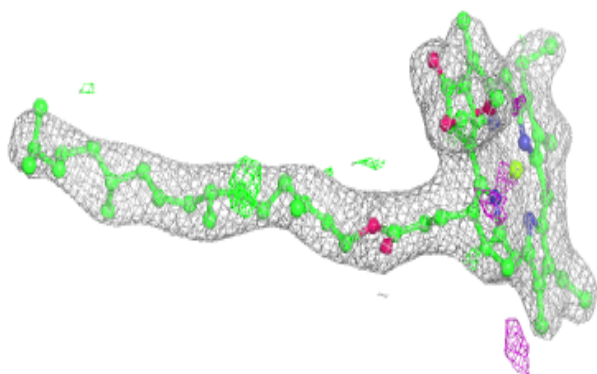
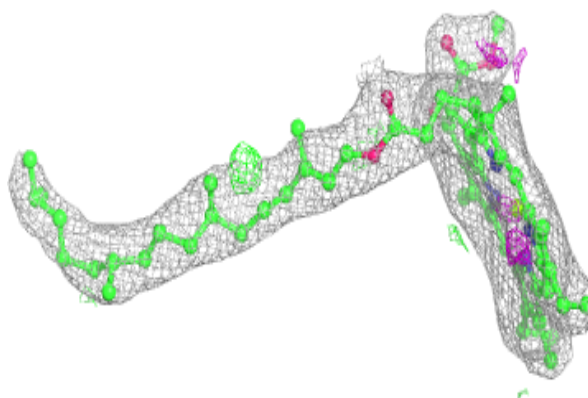


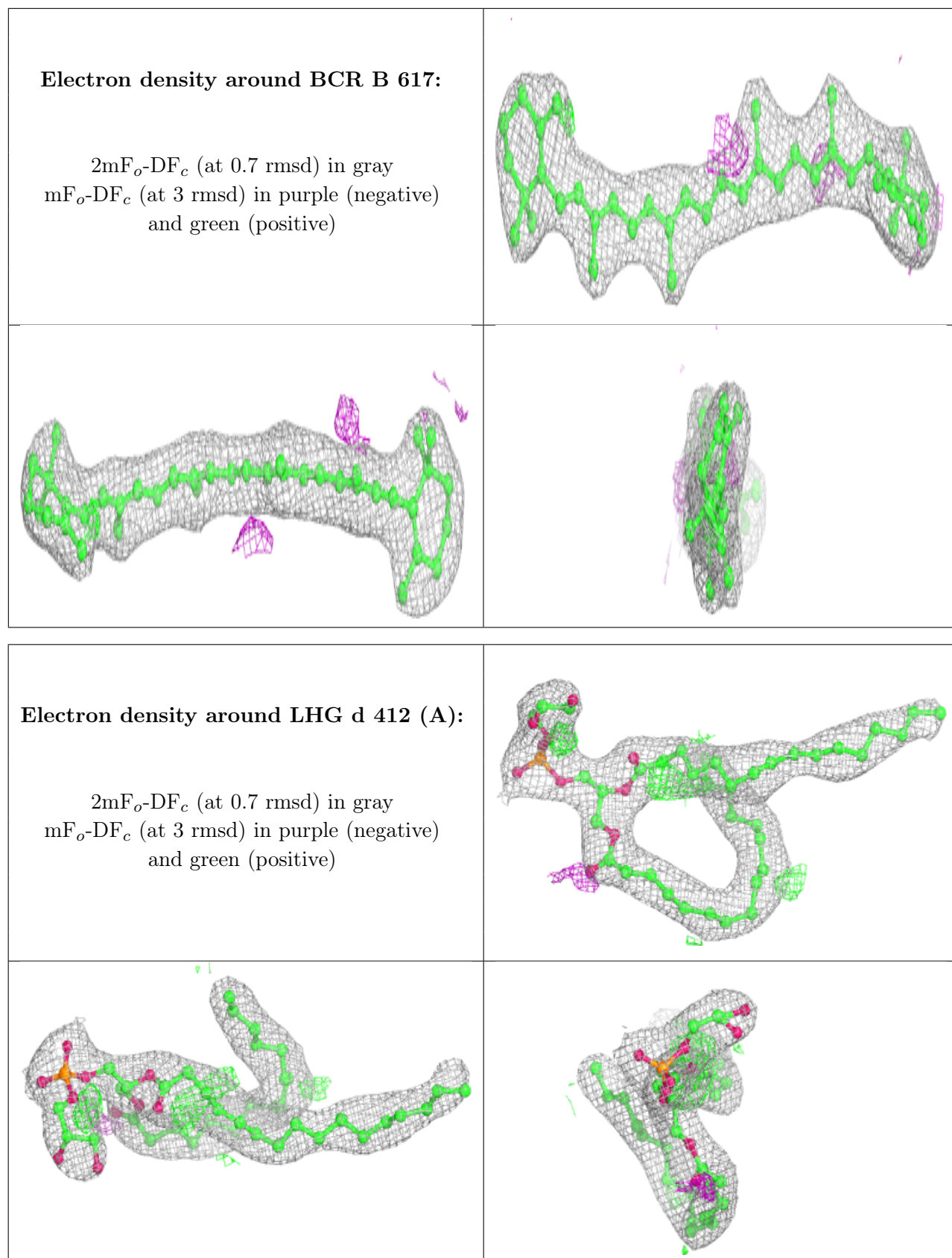
Electron density around LHG d 405 (B):

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

**Electron density around CLA b 604:**

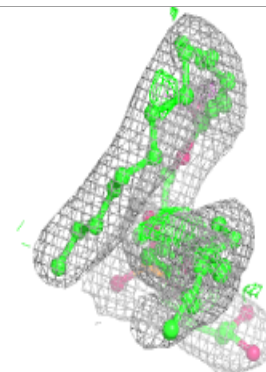
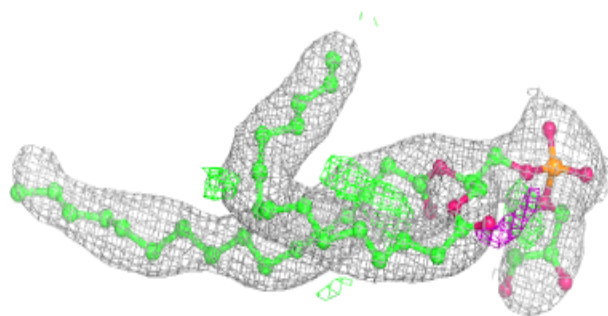
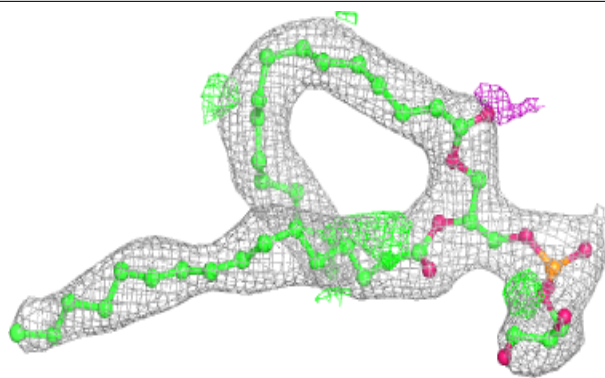
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



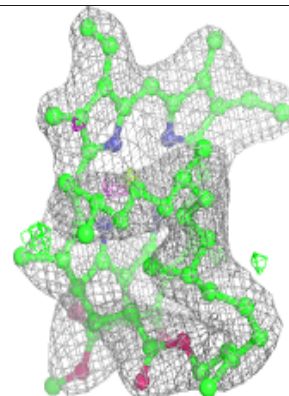
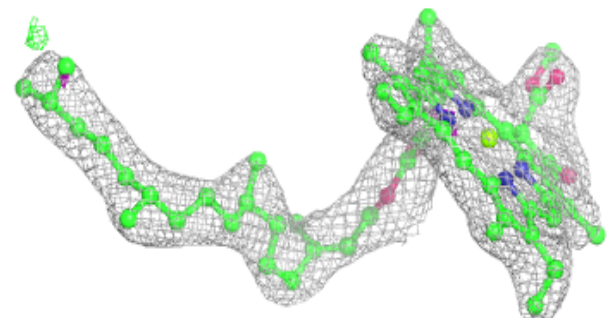
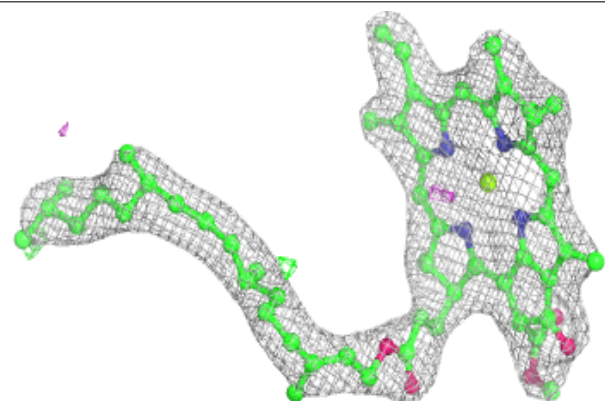


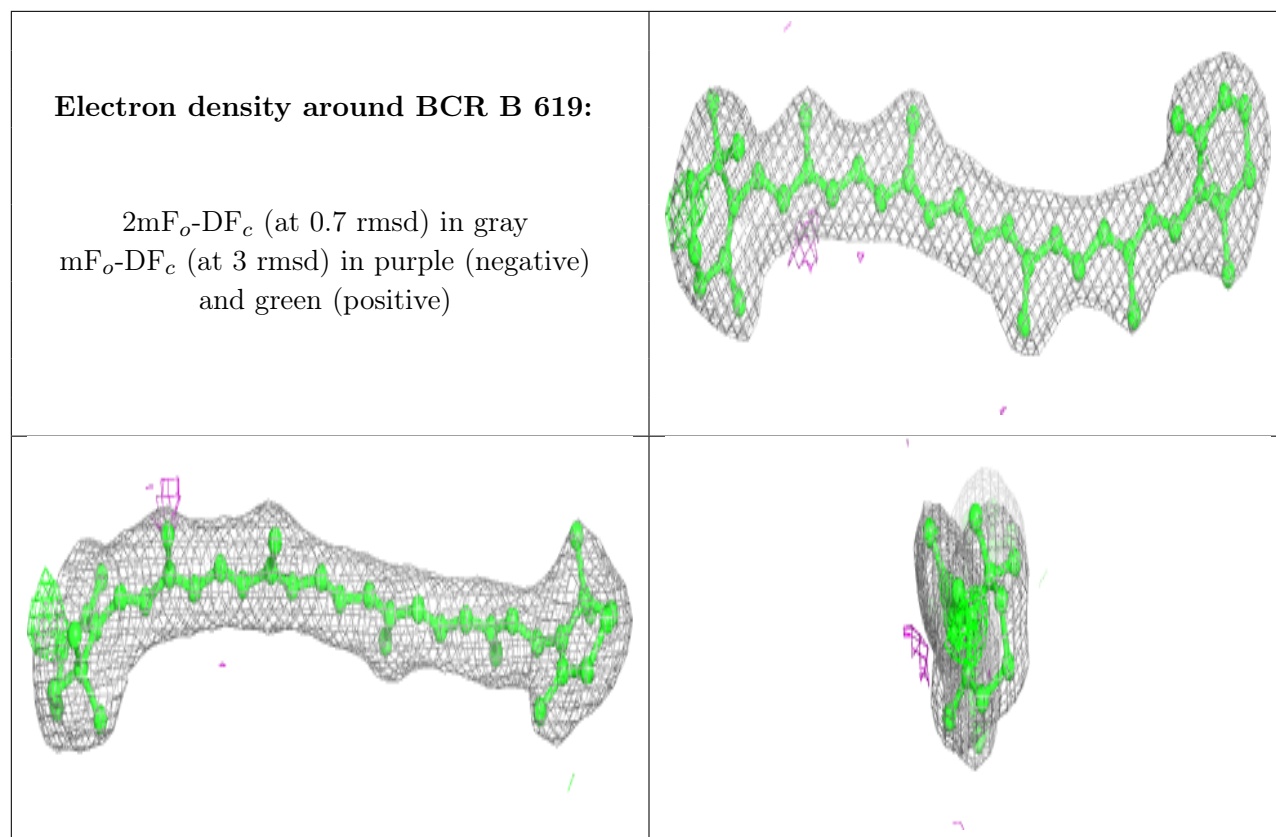
Electron density around LHG d 412 (B):

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

**Electron density around CLA C 512:**

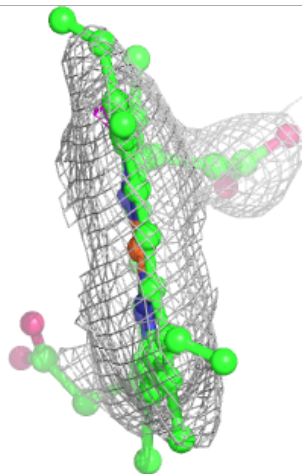
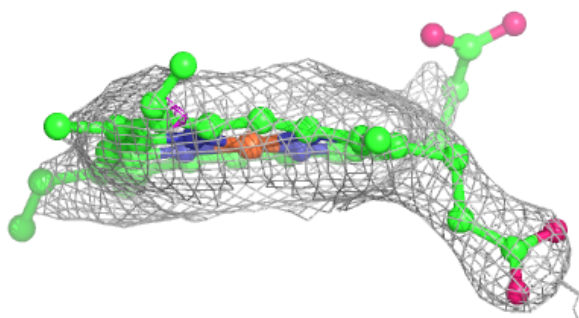
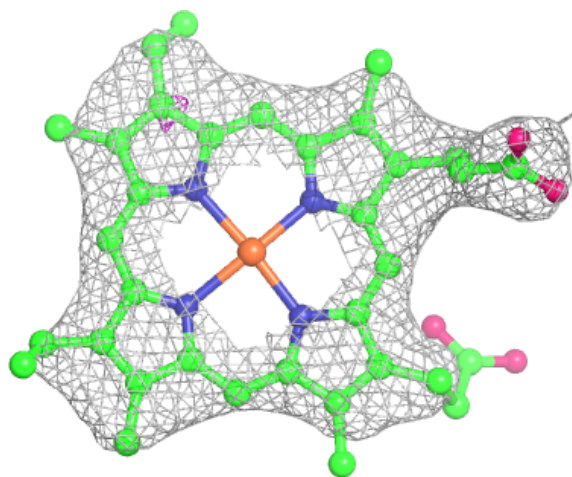
$2mF_o-DF_c$ (at 0.7 rnsd) in gray
 mF_o-DF_c (at 3 rnsd) in purple (negative)
and green (positive)





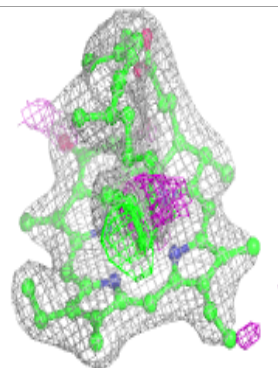
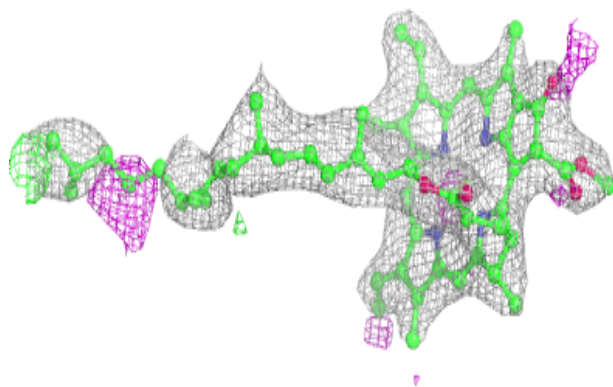
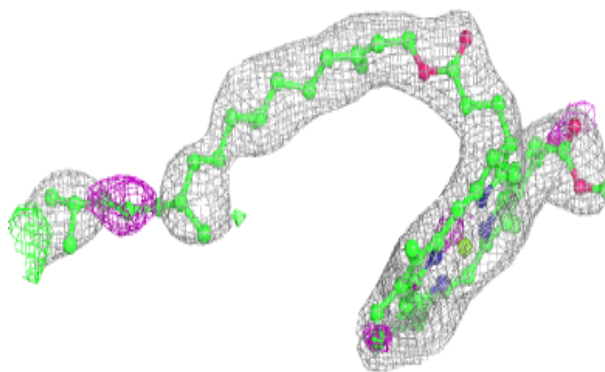
Electron density around HEM f 101:

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



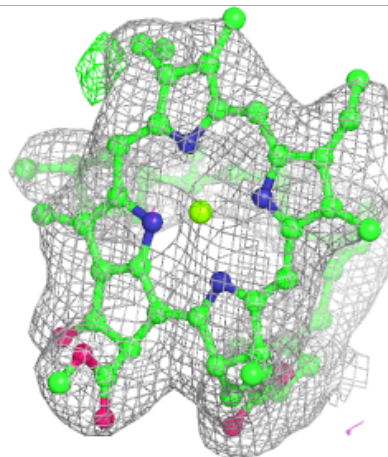
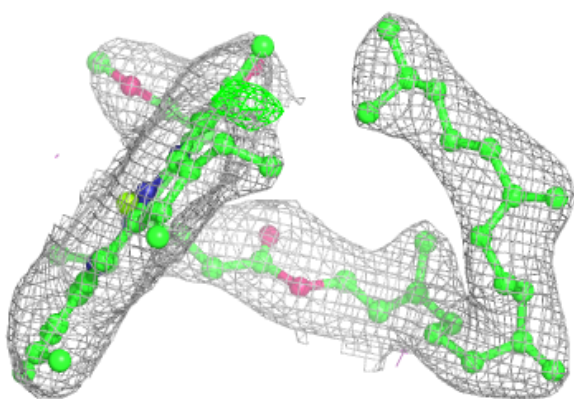
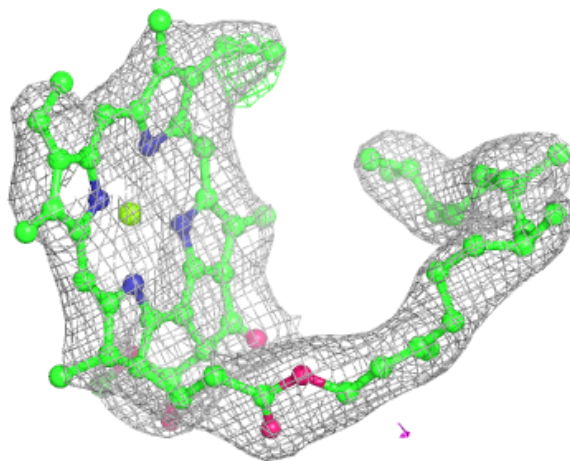
Electron density around CLA C 505:

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



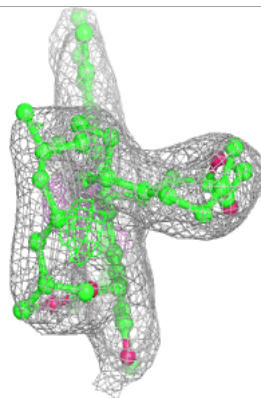
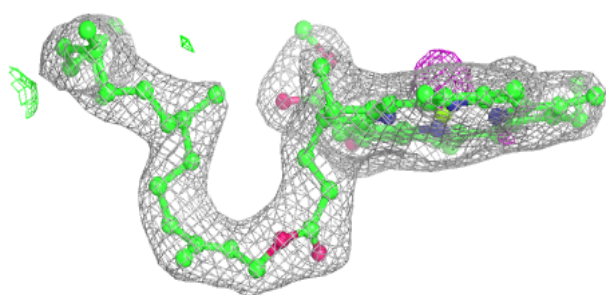
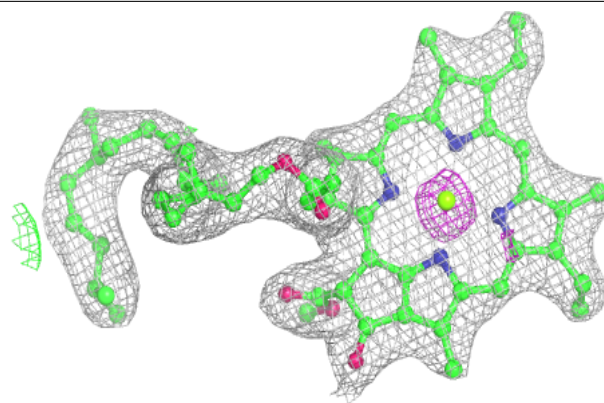
Electron density around CLA c 504:

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

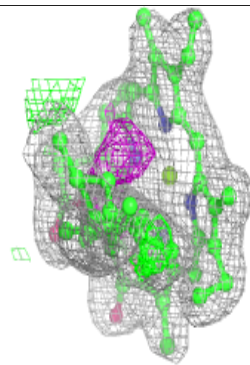
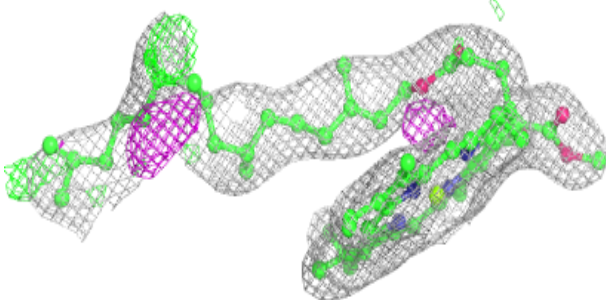
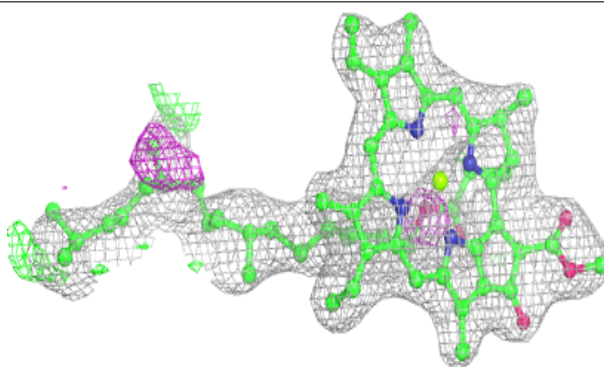


Electron density around CLA B 612:

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

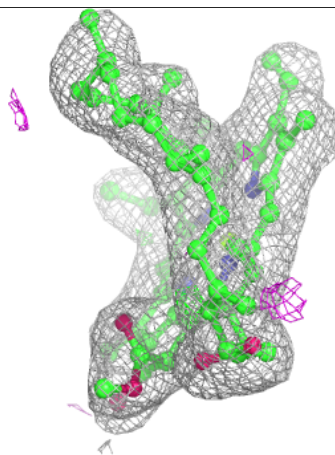
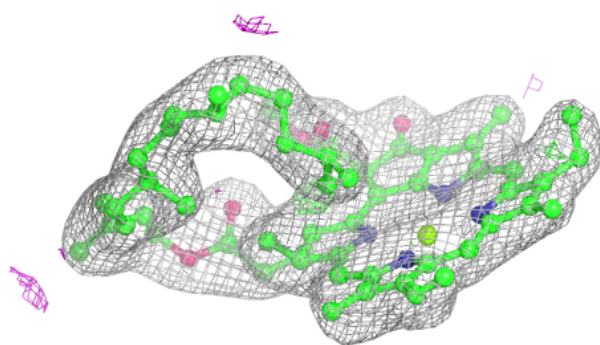
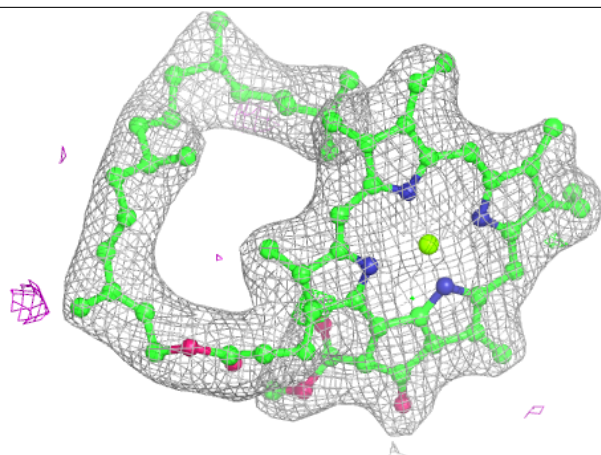
**Electron density around CLA B 614:**

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

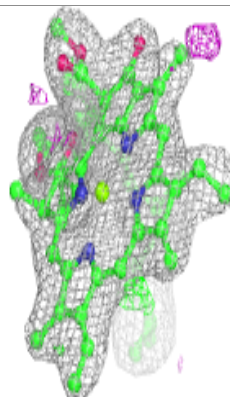
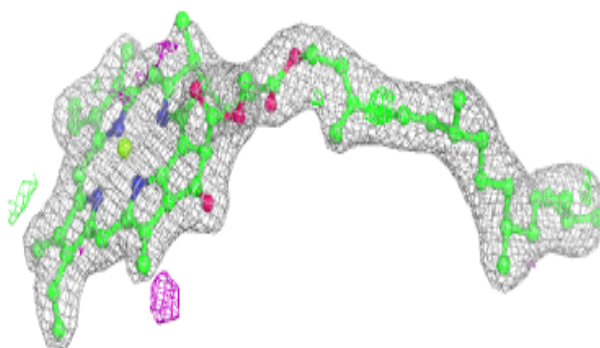
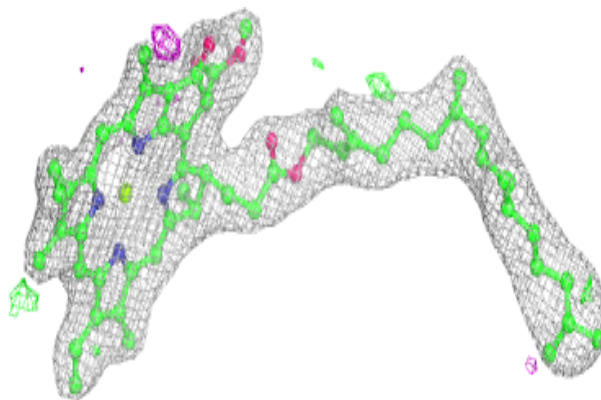


Electron density around CLA B 615:

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

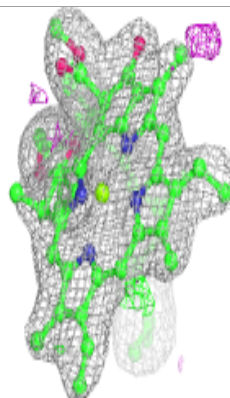
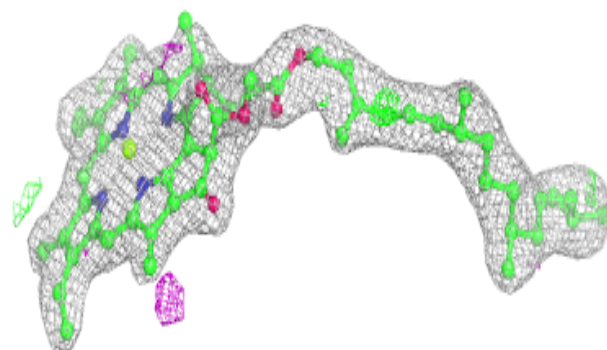
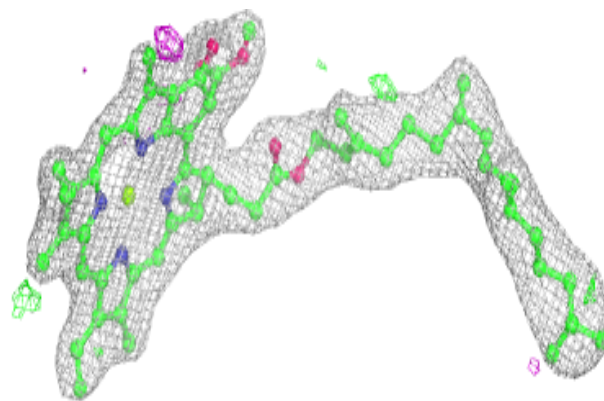
**Electron density around CLA a 405 (A):**

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



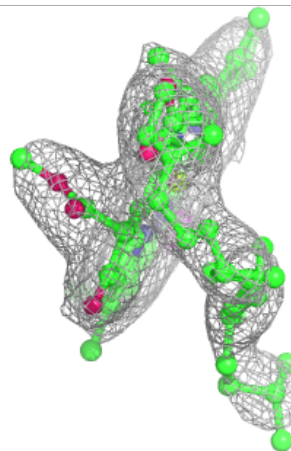
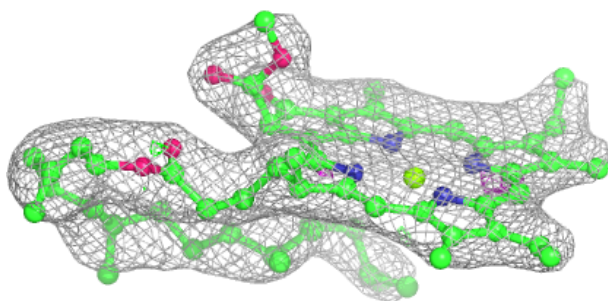
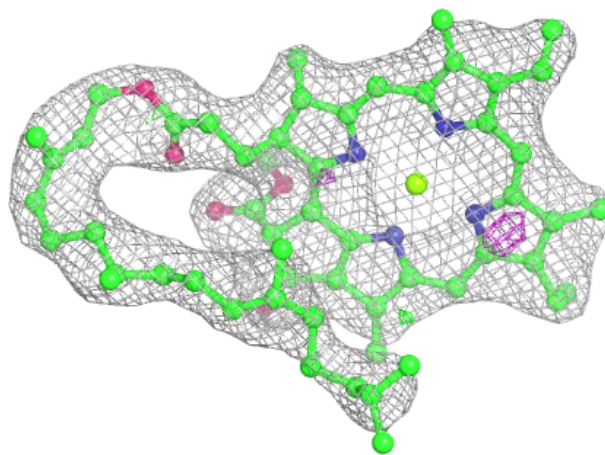
Electron density around CLA a 405 (B):

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



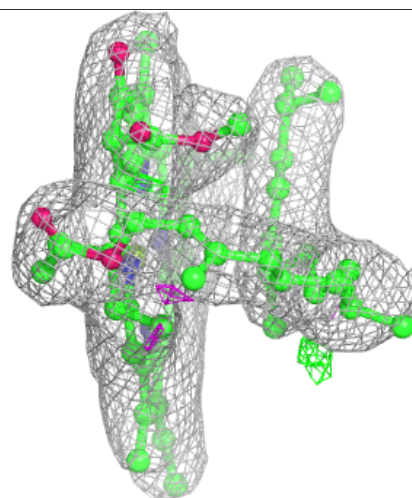
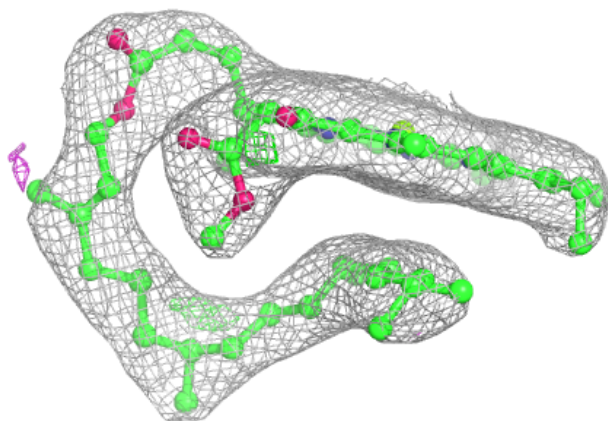
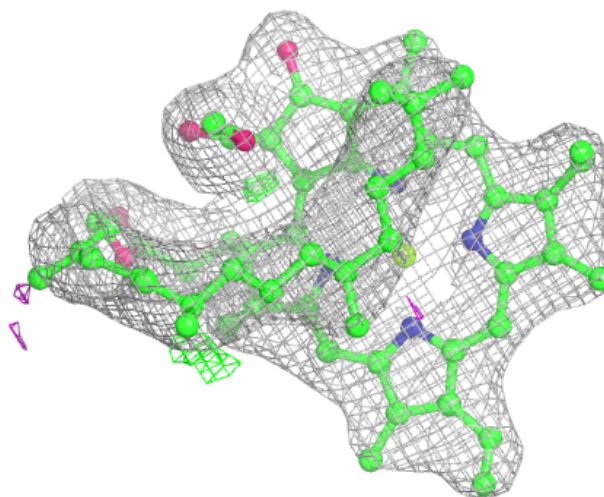
Electron density around CLA c 510:

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



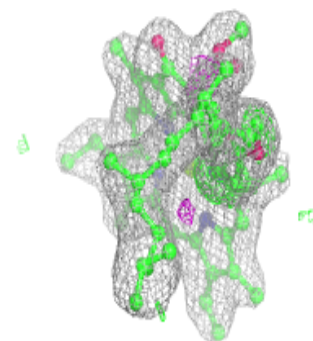
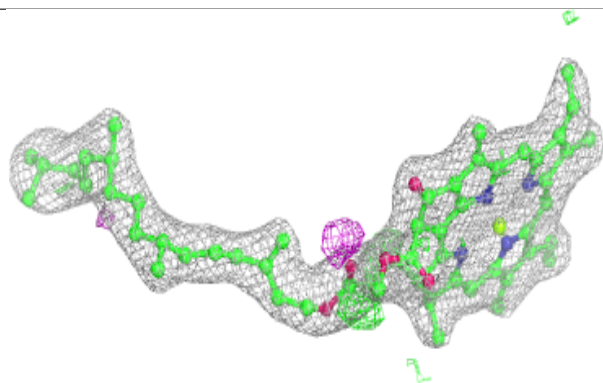
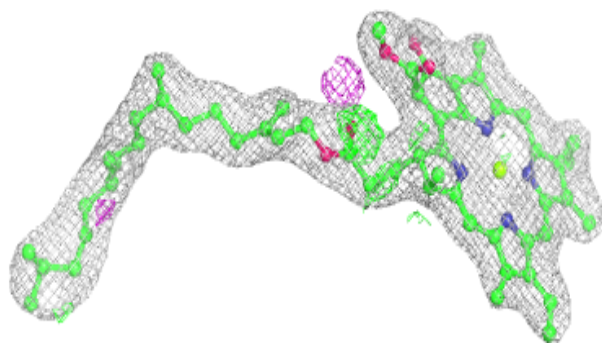
Electron density around CLA c 511:

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

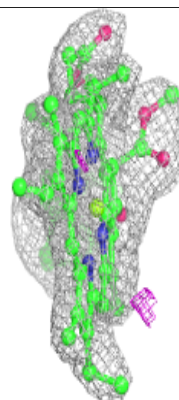
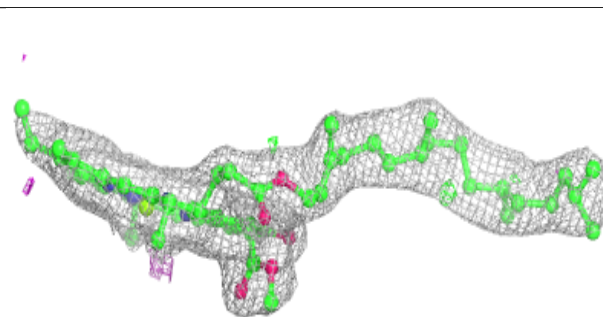
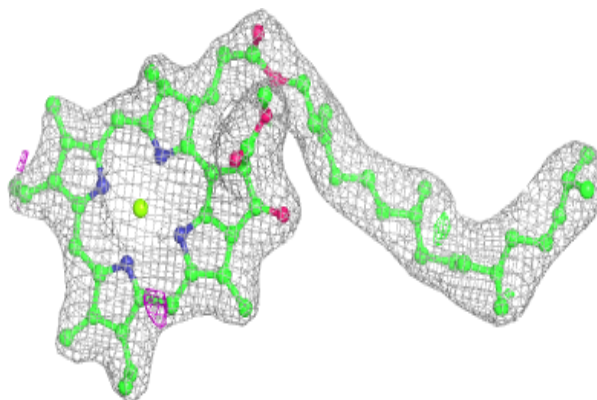


Electron density around CLA A 404 (B):

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

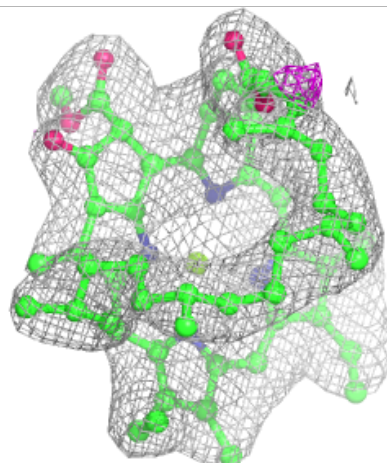
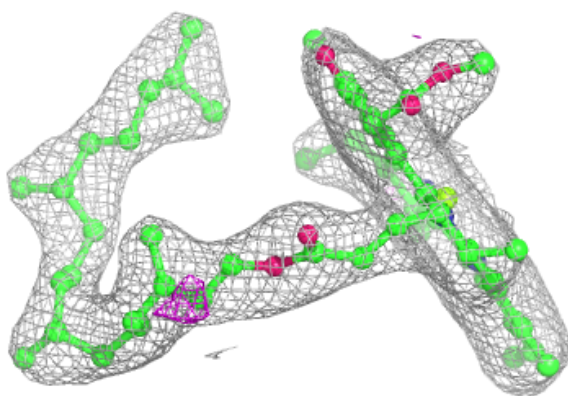
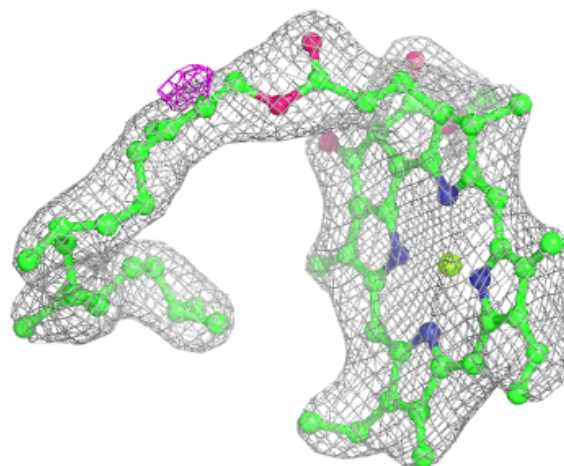
**Electron density around CLA B 602:**

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



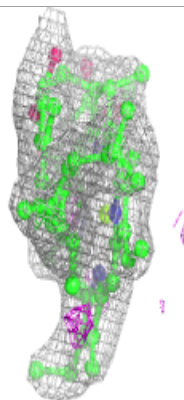
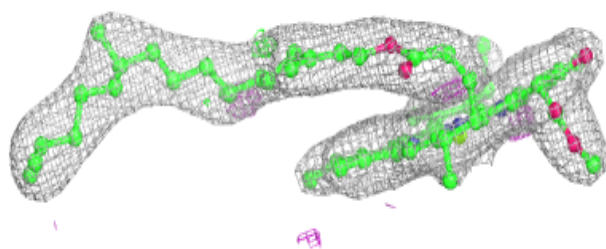
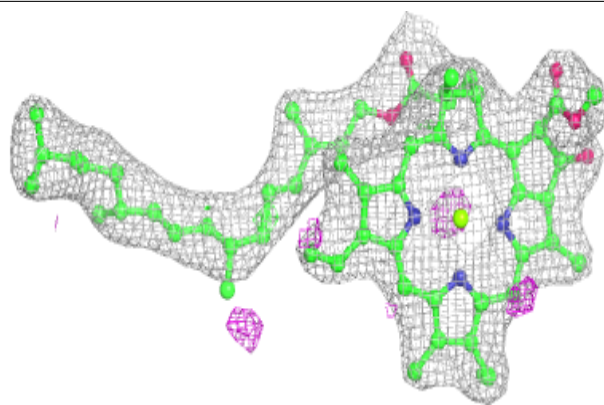
Electron density around CLA C 504:

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

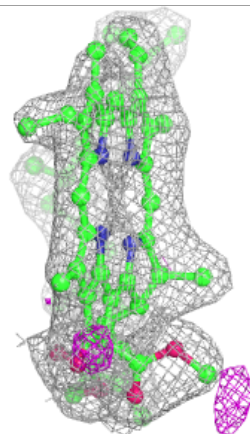
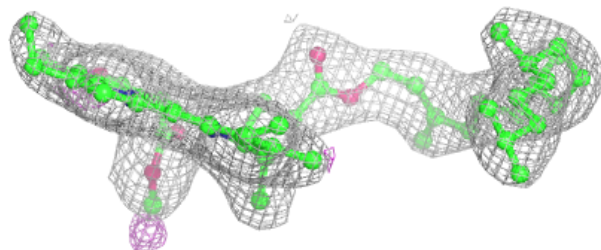
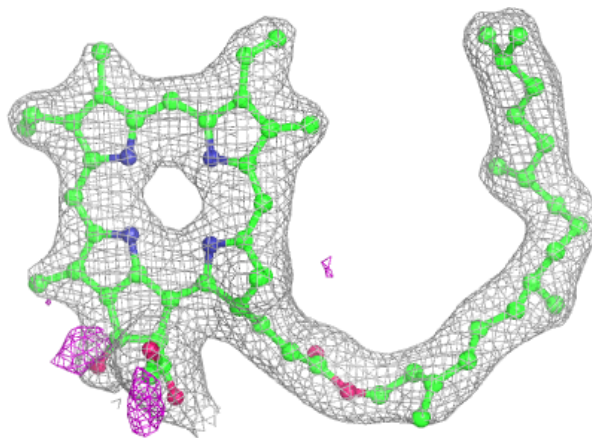


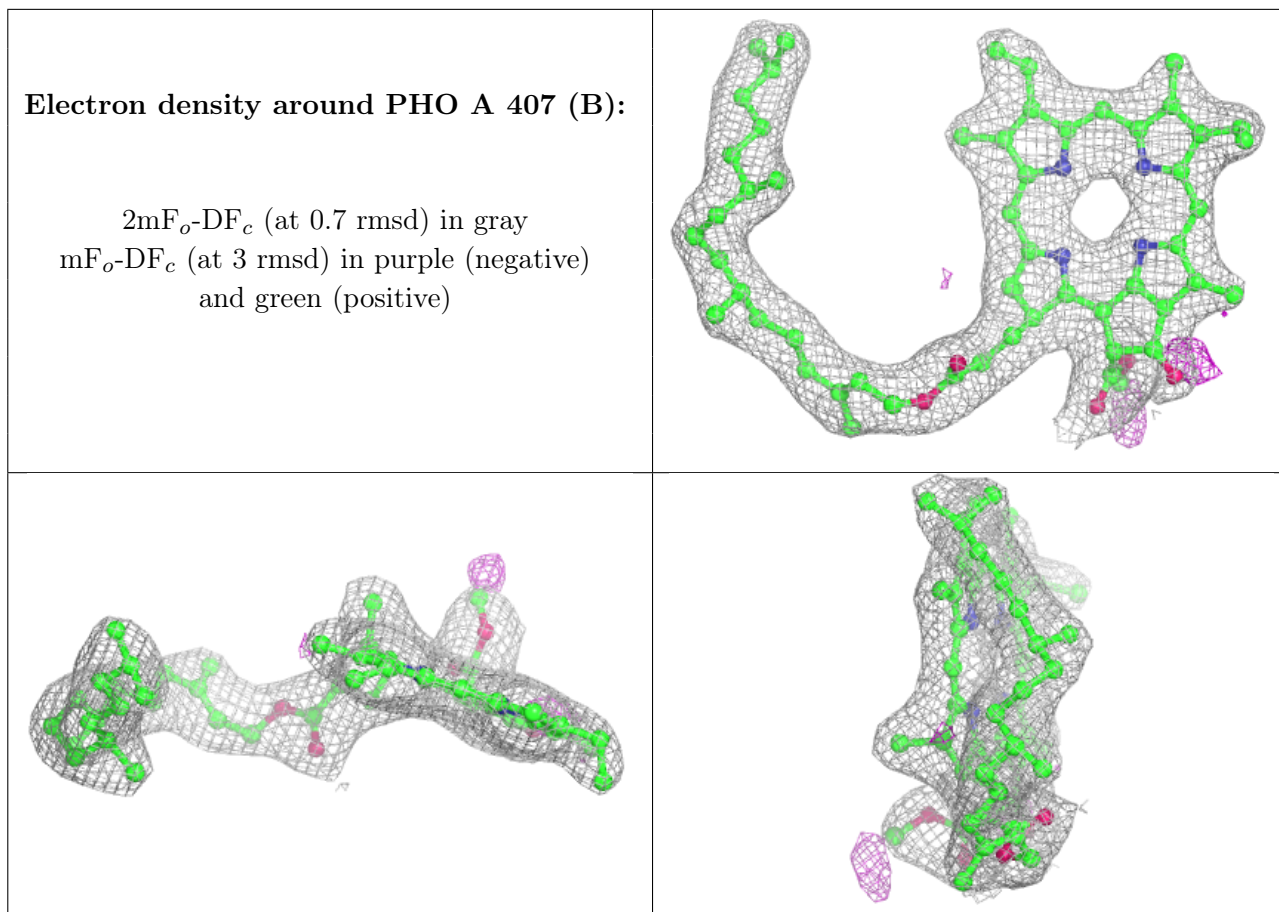
Electron density around CLA B 603:

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

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

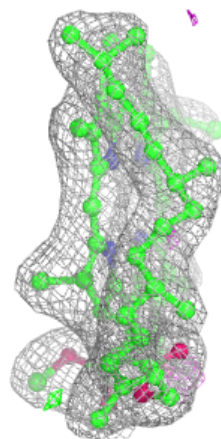
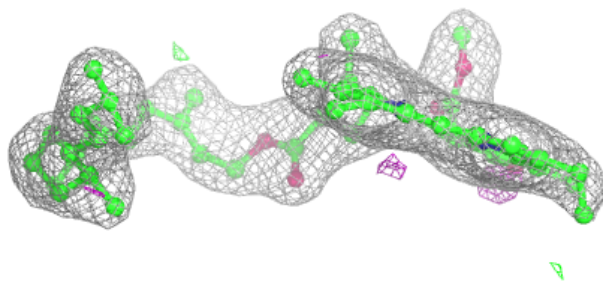
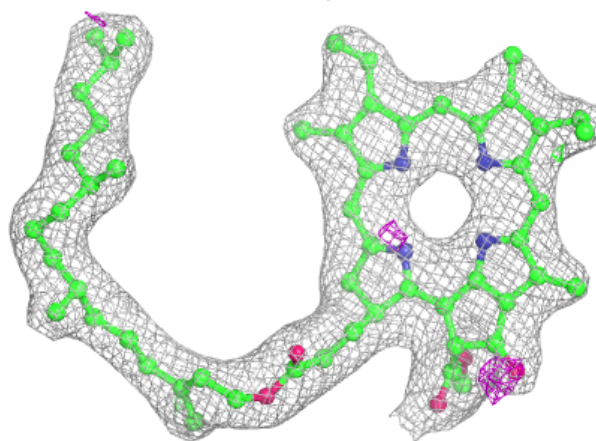
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





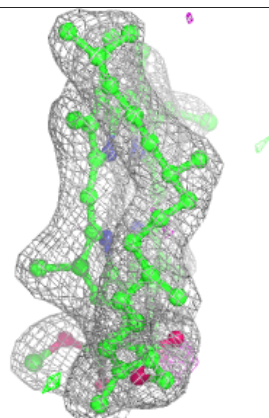
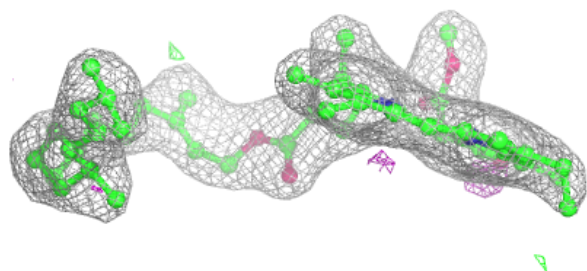
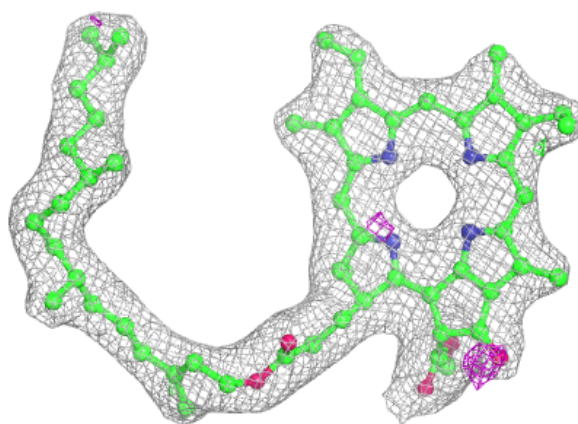
Electron density around PHO a 408 (A):

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



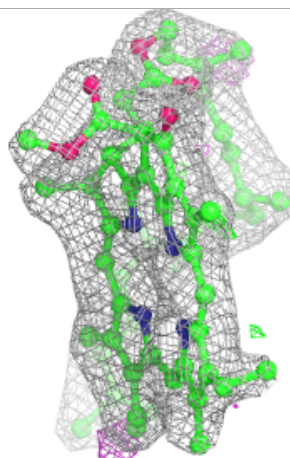
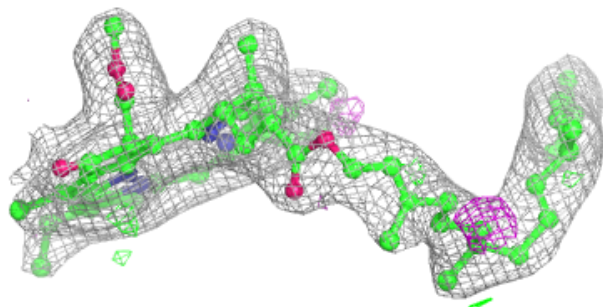
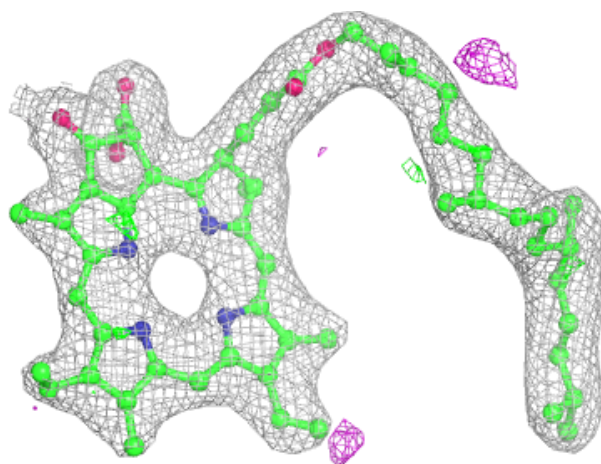
Electron density around PHO a 408 (B):

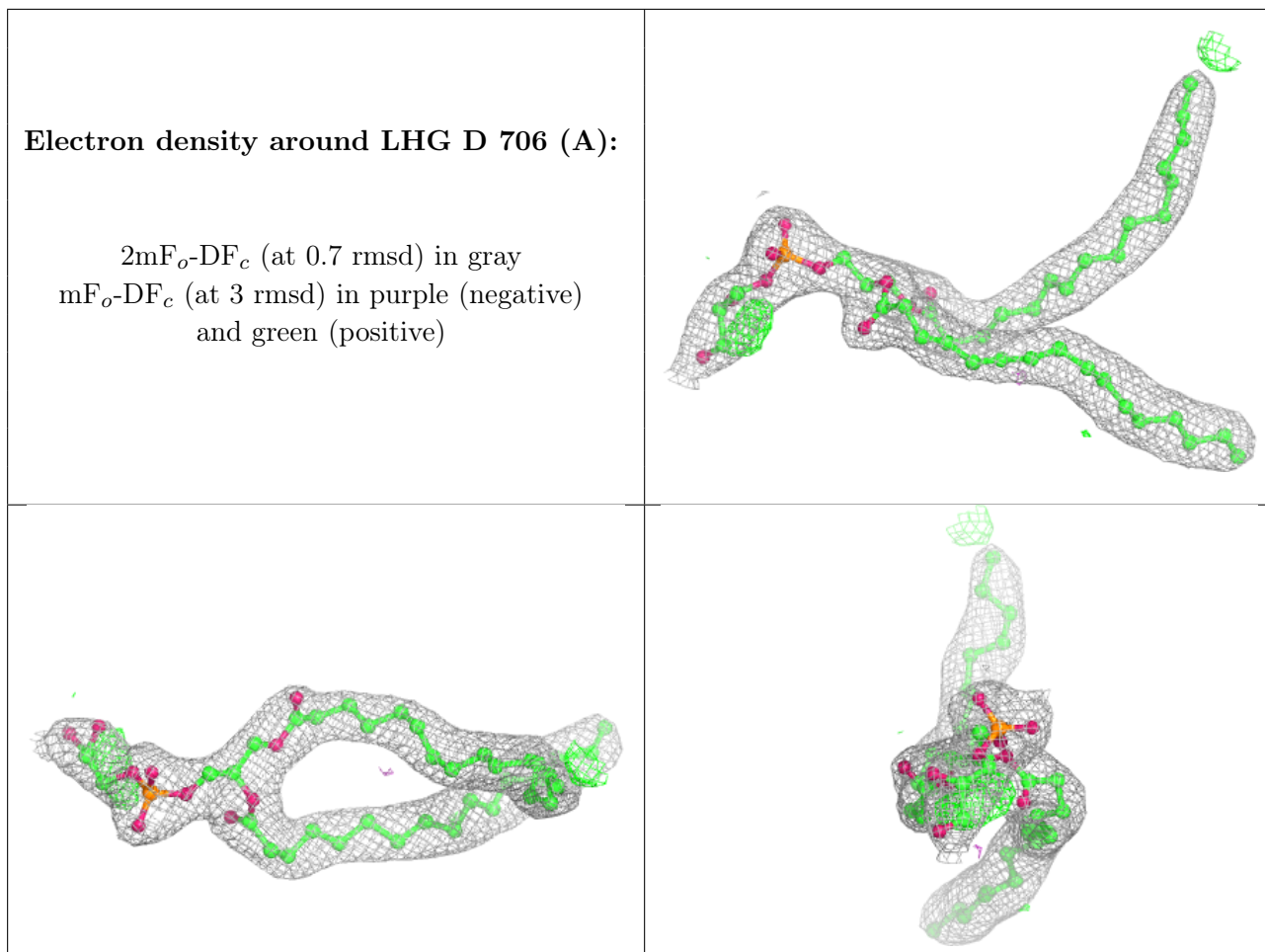
$2mF_o-DF_c$ (at 0.7 rnsd) in gray
 mF_o-DF_c (at 3 rnsd) in purple (negative)
and green (positive)

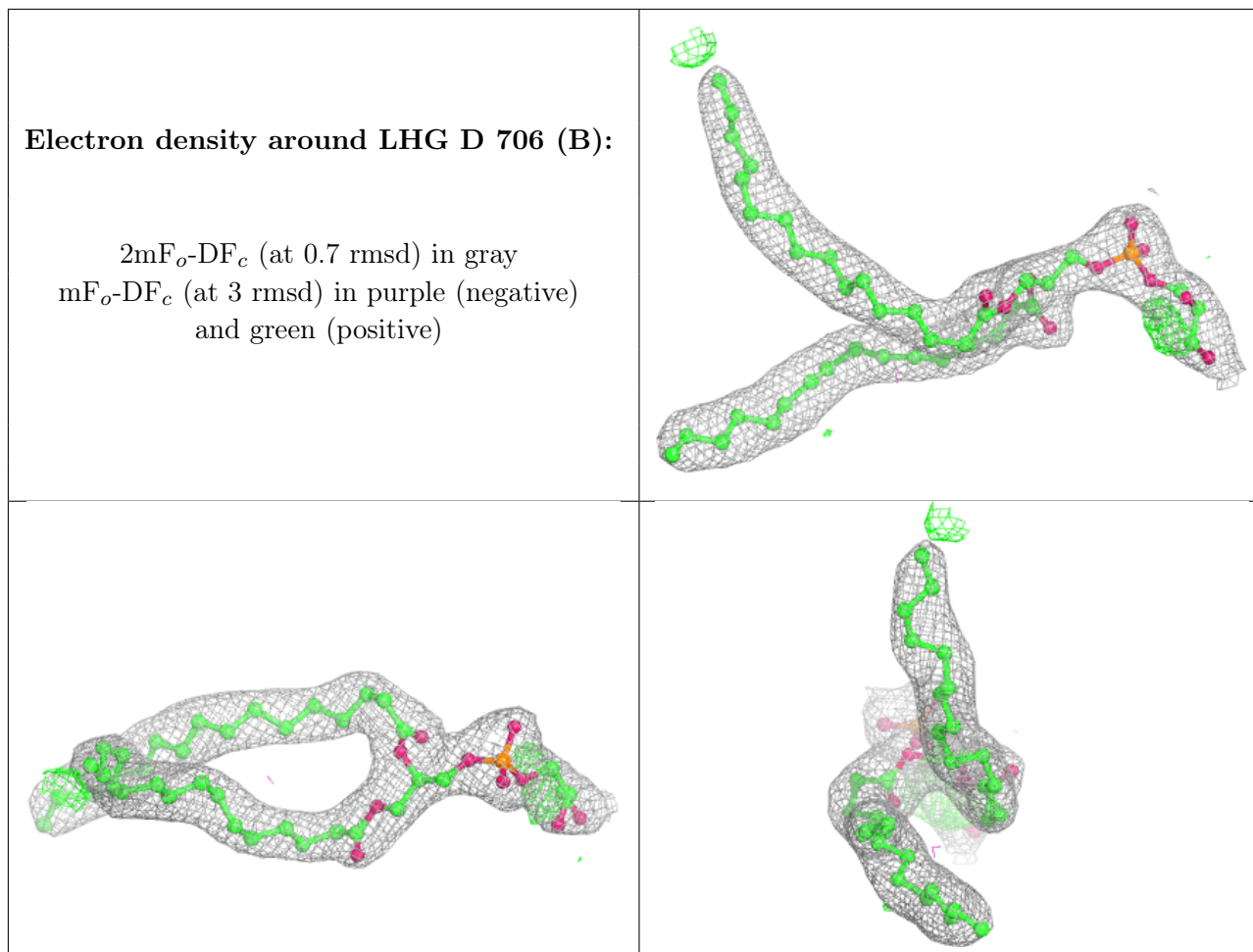


Electron density around PHO a 416 (A):

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

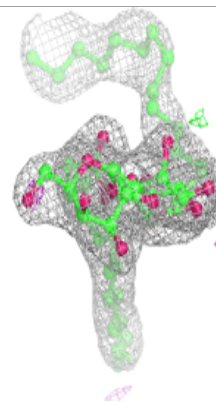
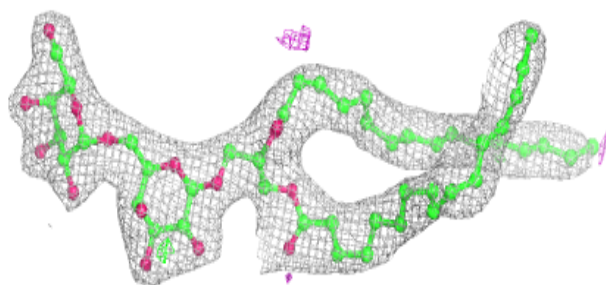
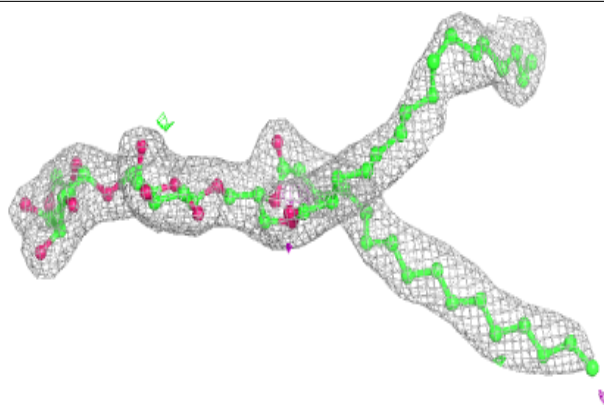




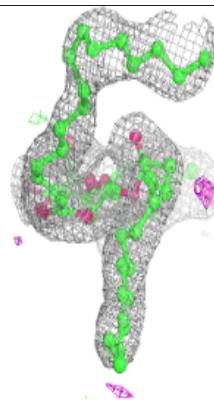
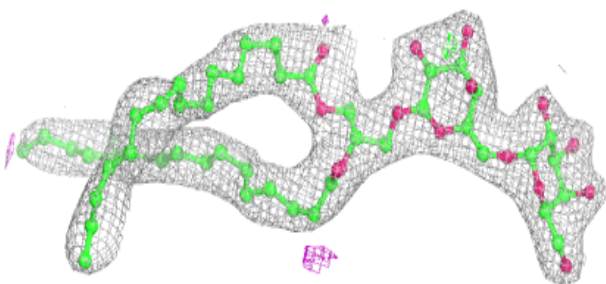
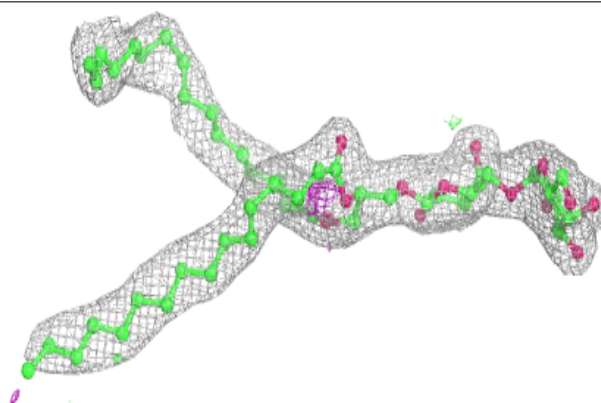


Electron density around DGD C 517 (A):

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

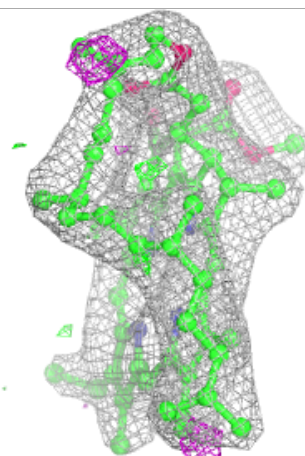
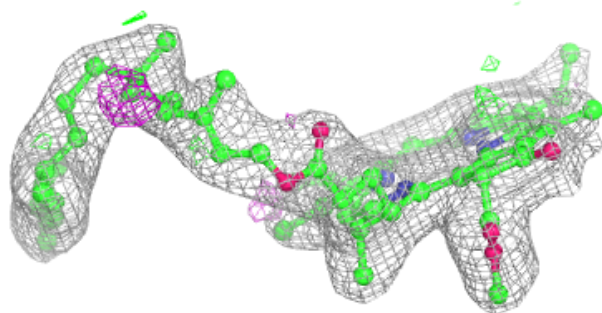
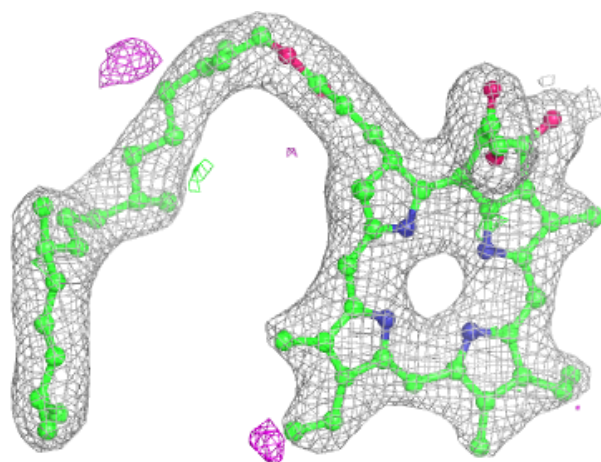
**Electron density around DGD C 517 (B):**

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



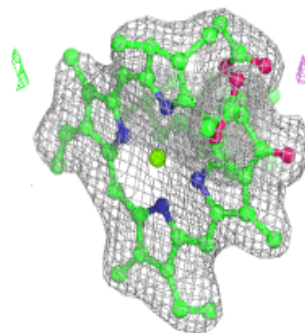
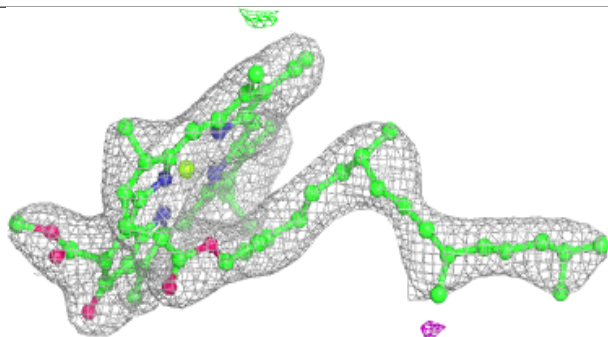
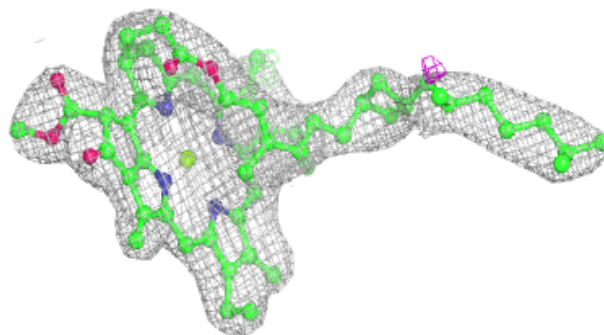
Electron density around PHO a 416 (B):

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

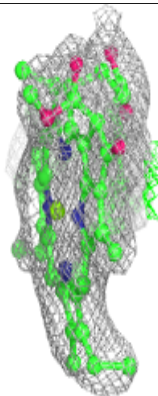
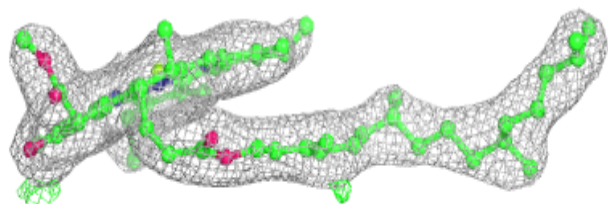
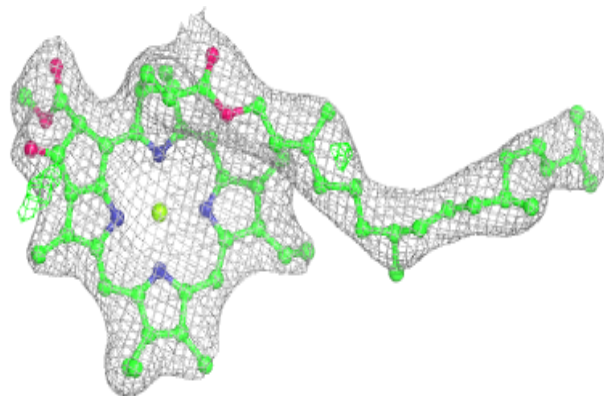


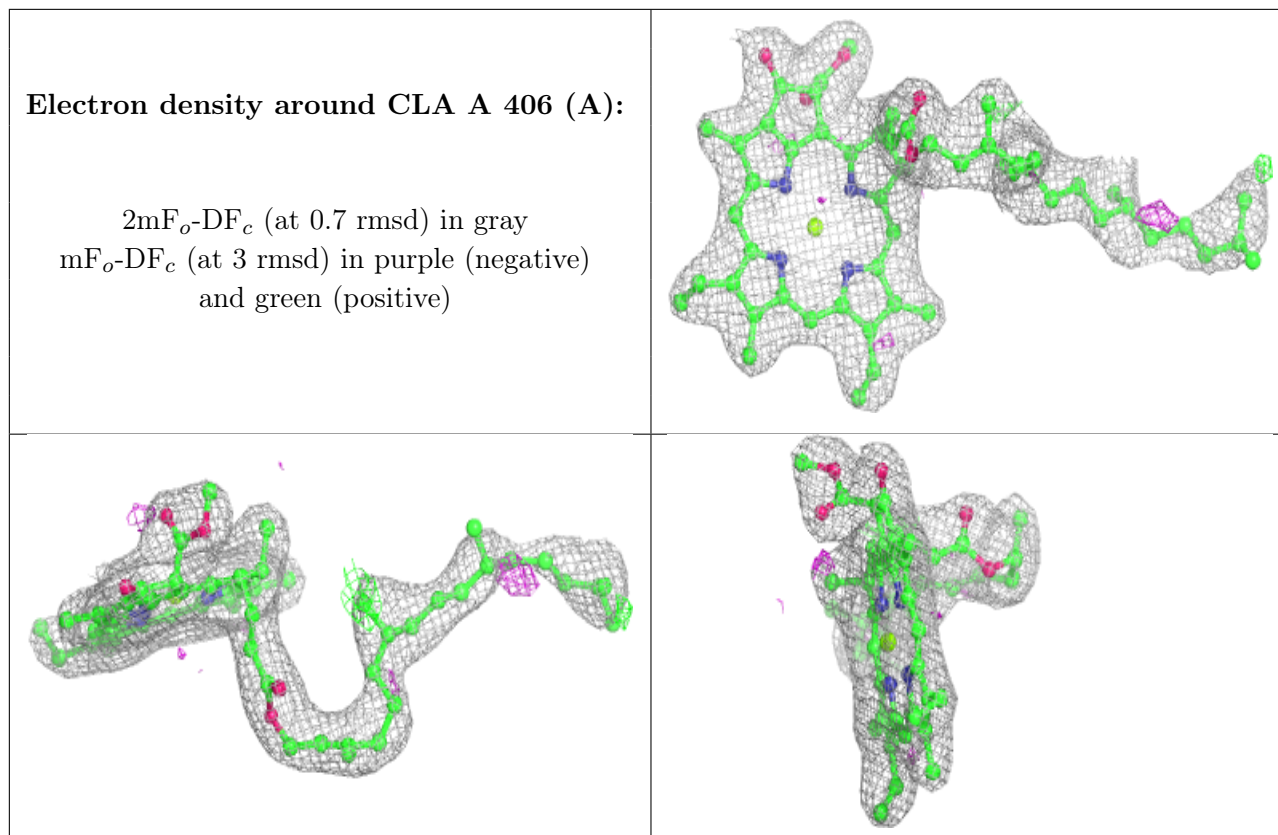
Electron density around CLA C 506:

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

**Electron density around CLA b 603:**

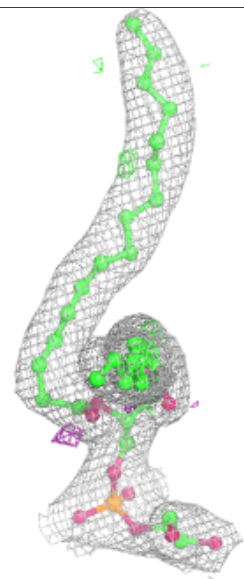
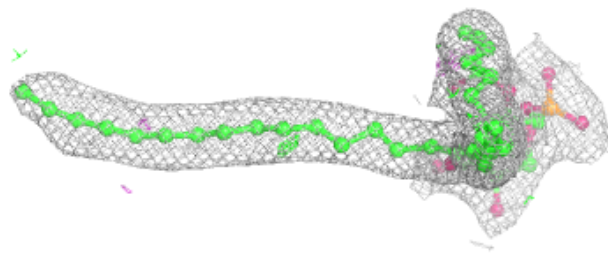
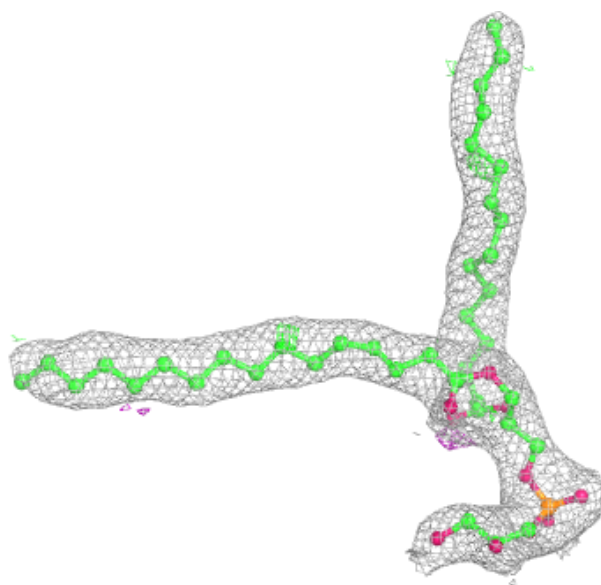
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





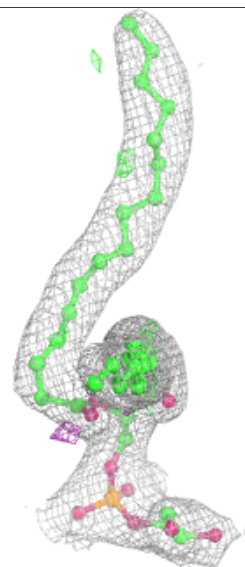
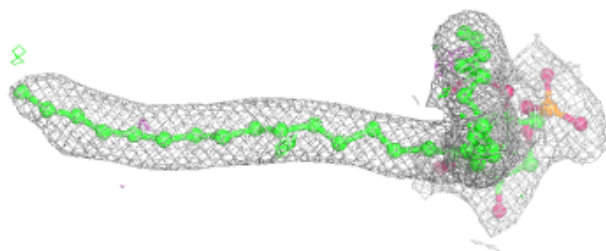
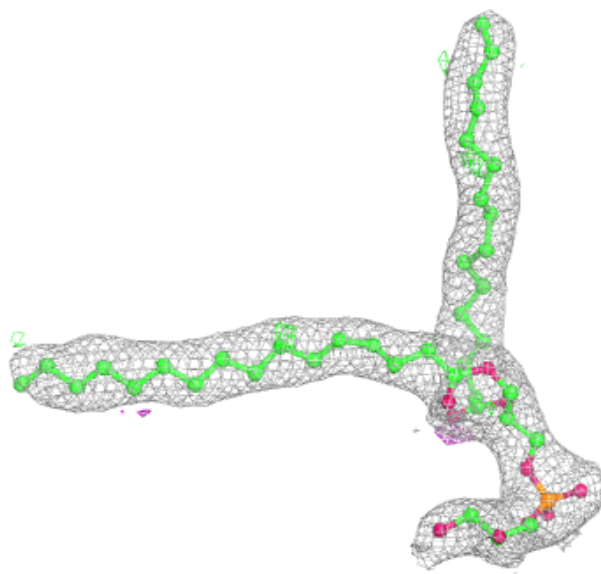
Electron density around LHG L 101 (A):

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



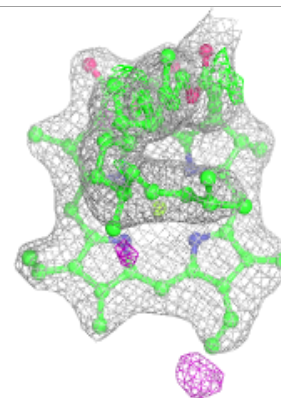
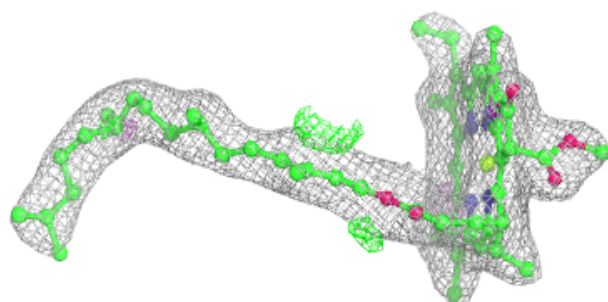
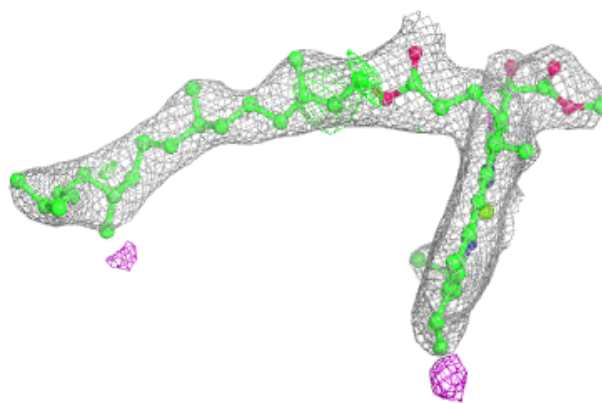
Electron density around LHG L 101 (B):

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

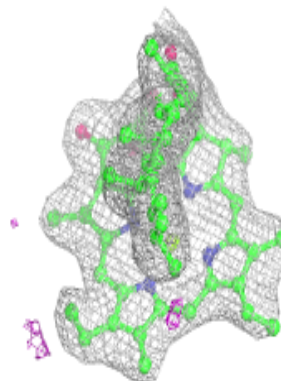
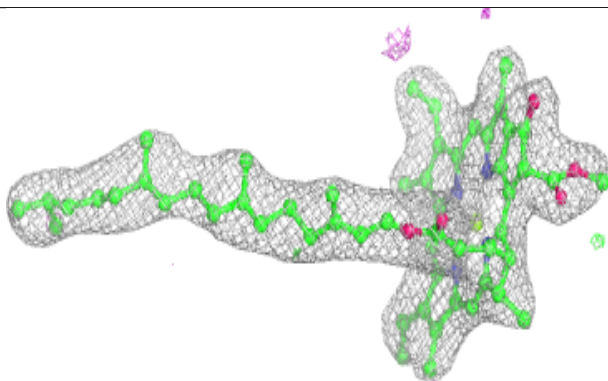
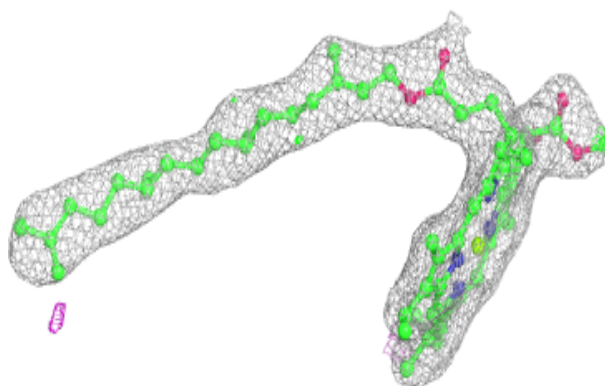


Electron density around CLA b 605:

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

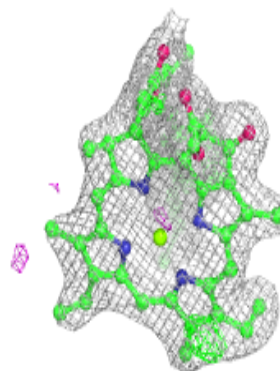
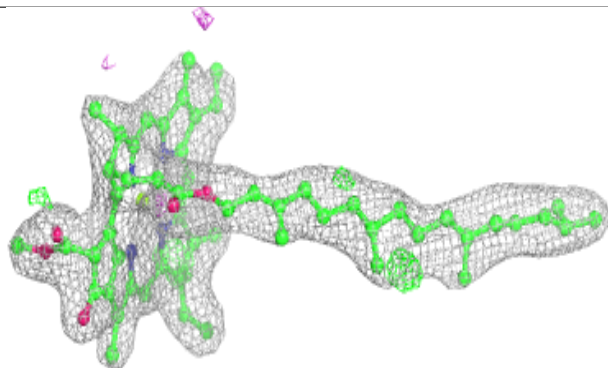
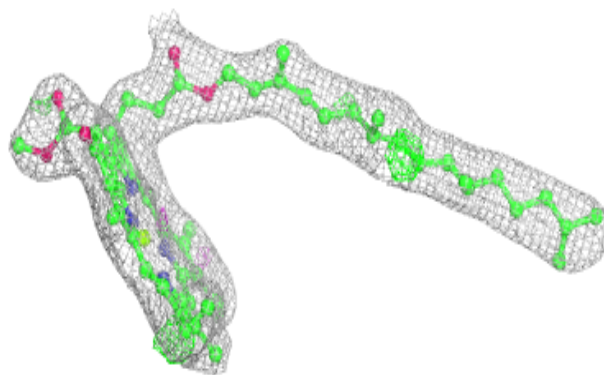
**Electron density around CLA B 607:**

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

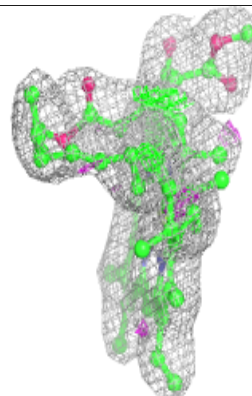
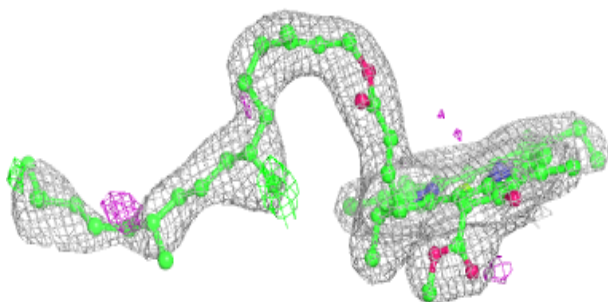
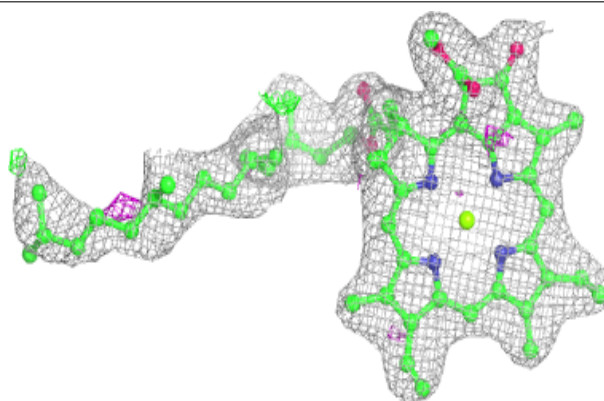


Electron density around CLA b 607:

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

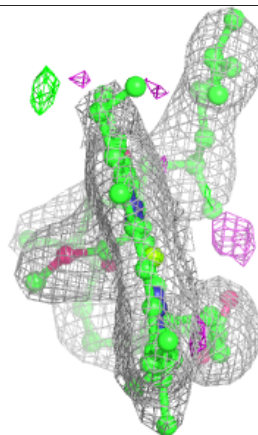
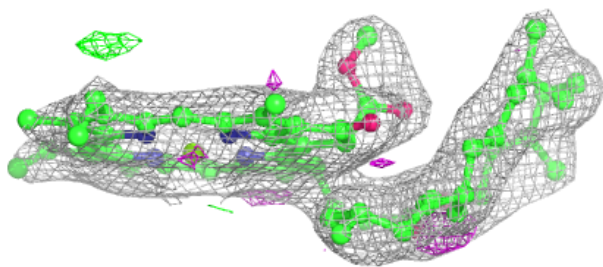
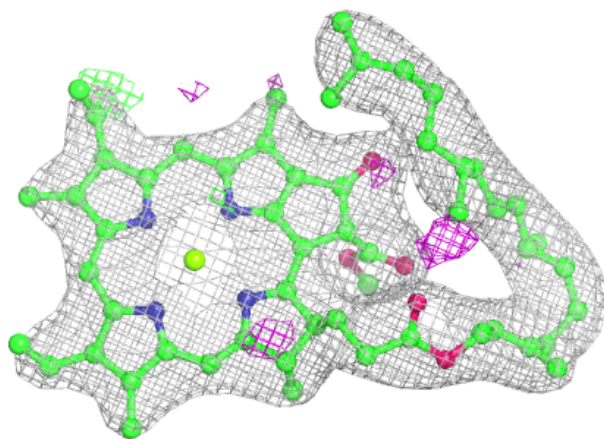
**Electron density around CLA A 406 (B):**

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



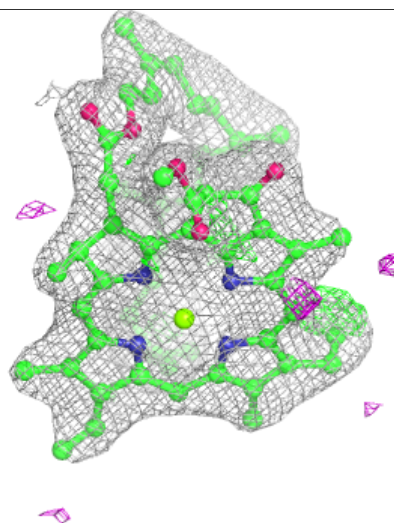
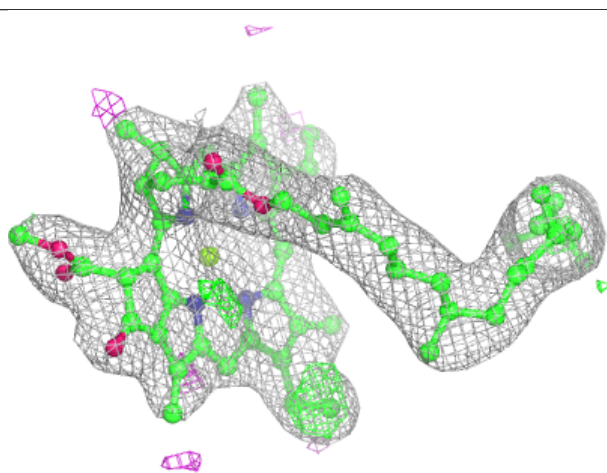
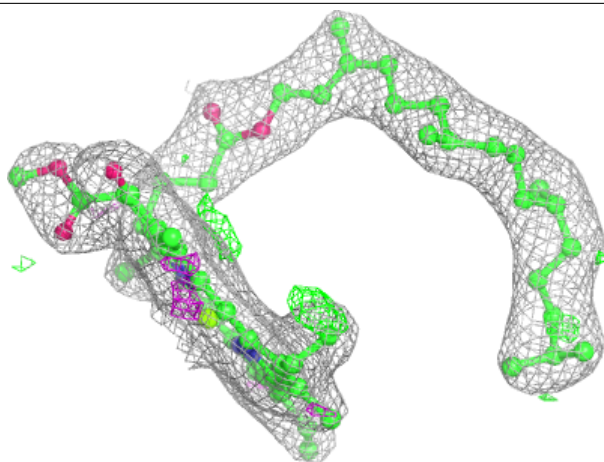
Electron density around CLA b 610:

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



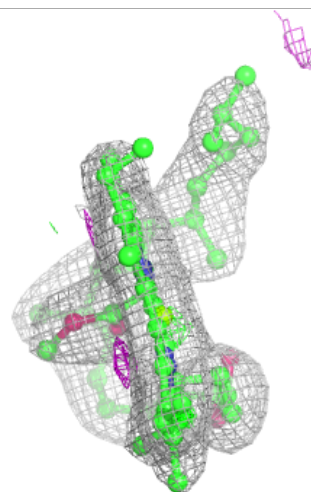
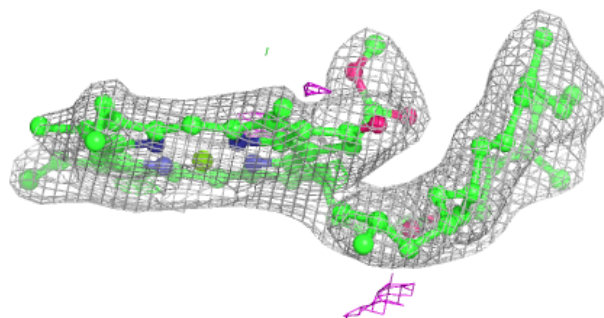
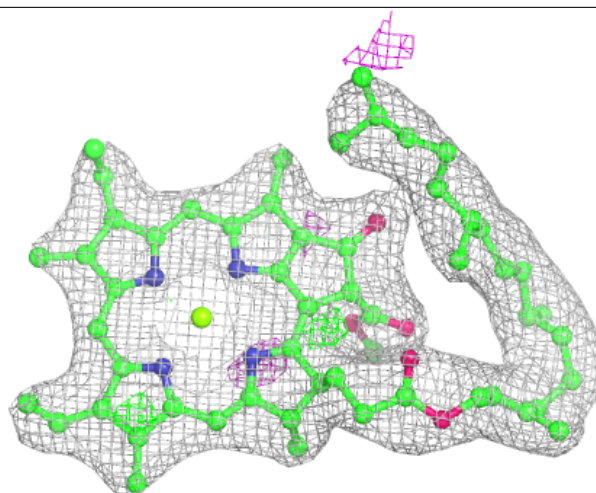
Electron density around CLA b 611:

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



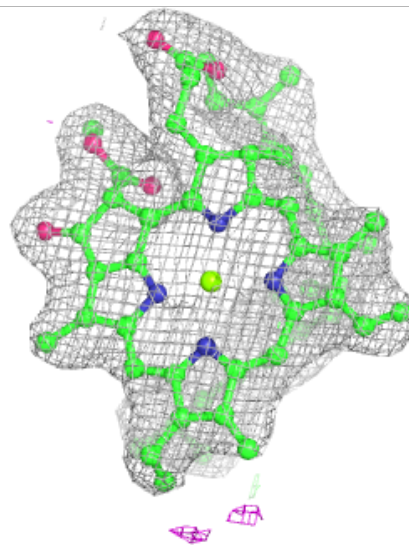
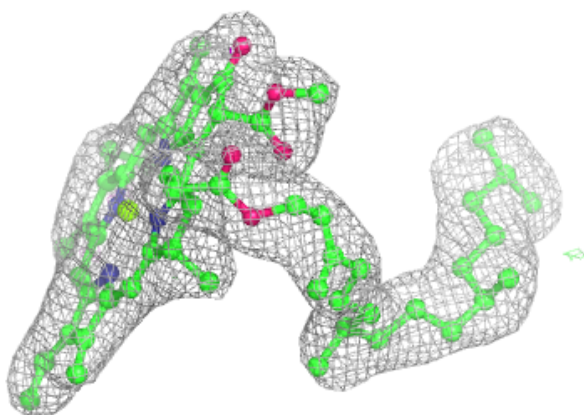
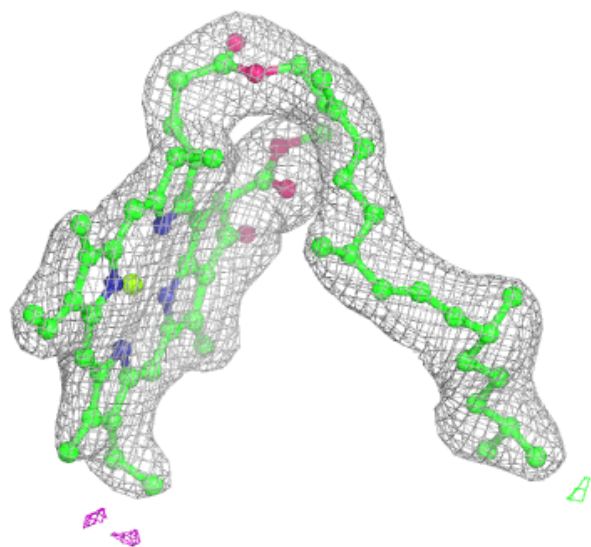
Electron density around CLA B 610:

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



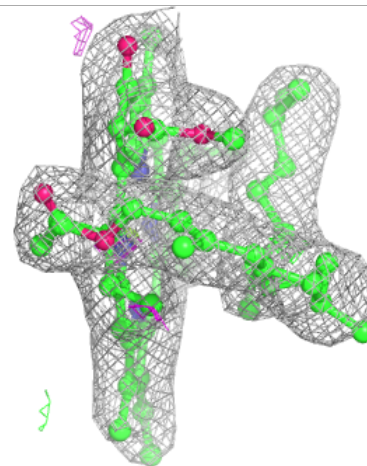
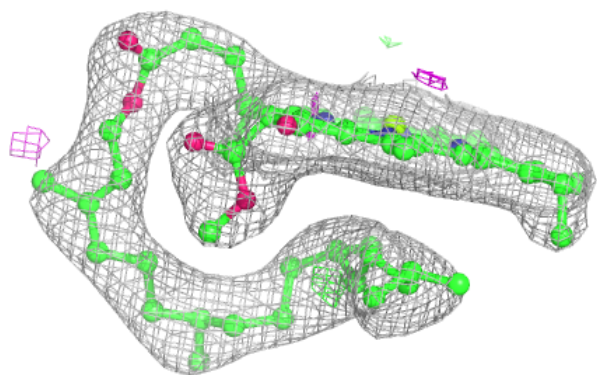
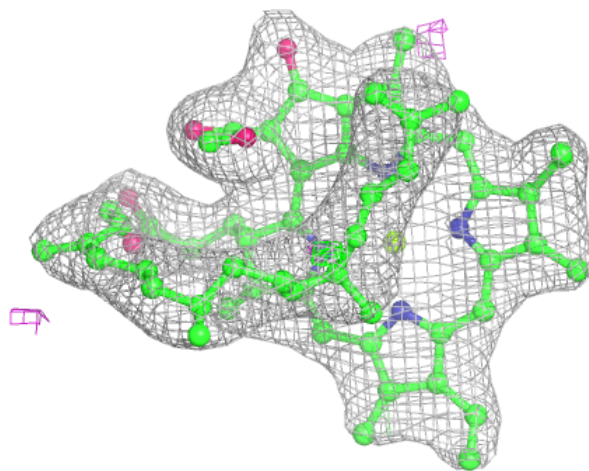
Electron density around CLA b 613:

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



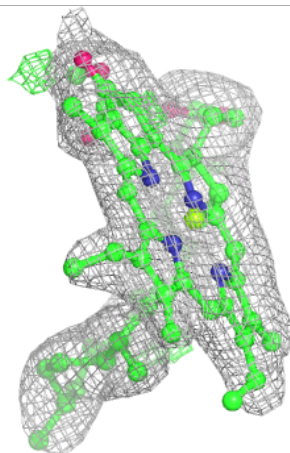
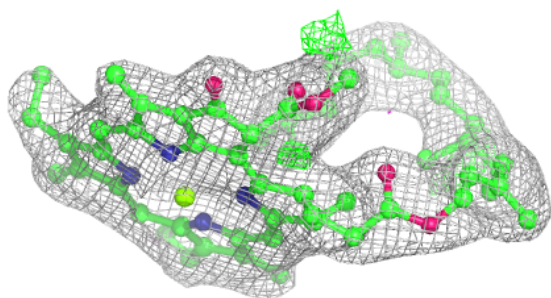
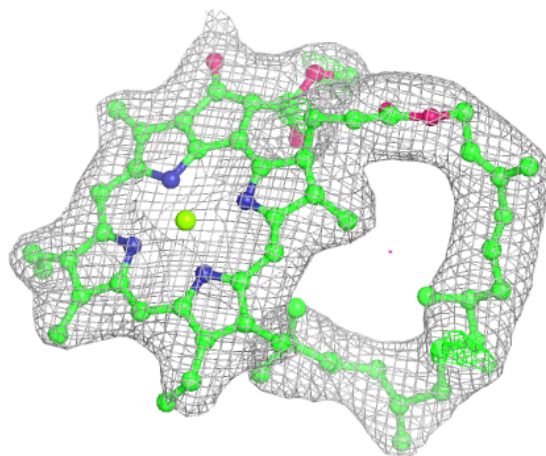
Electron density around CLA C 511:

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



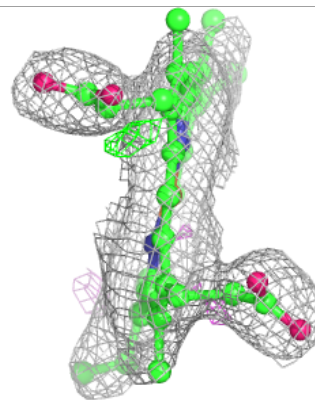
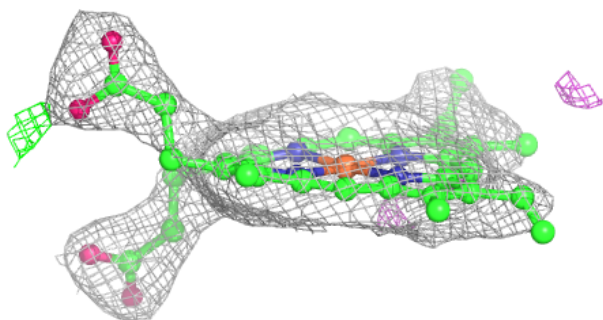
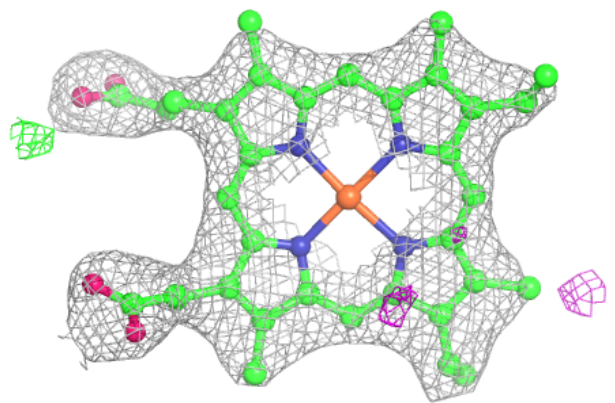
Electron density around CLA b 615:

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

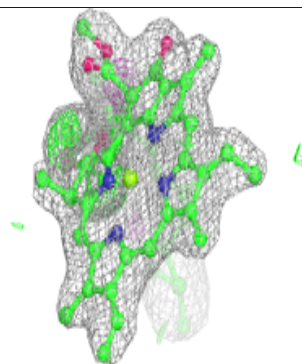
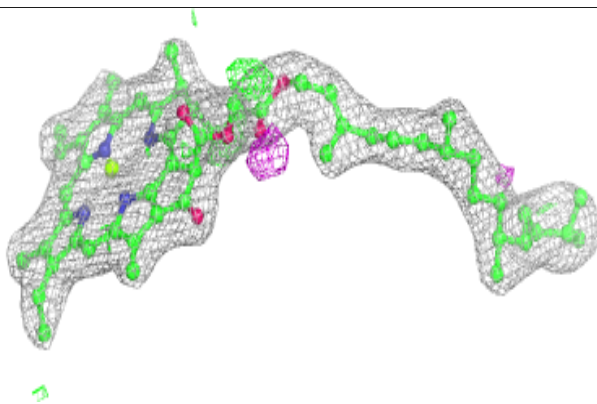
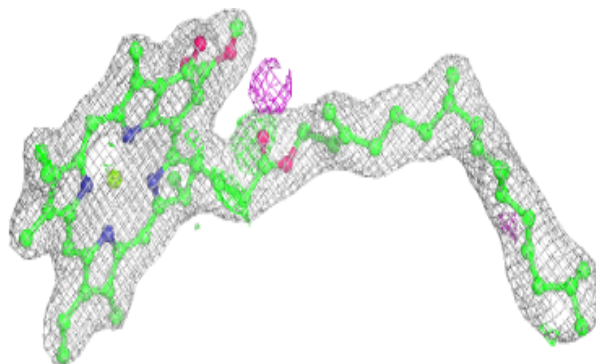


Electron density around HEM F 102:

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

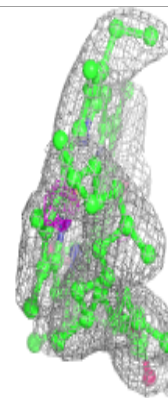
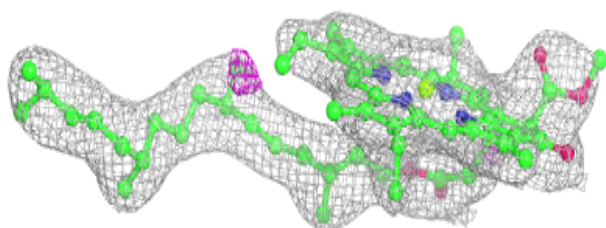
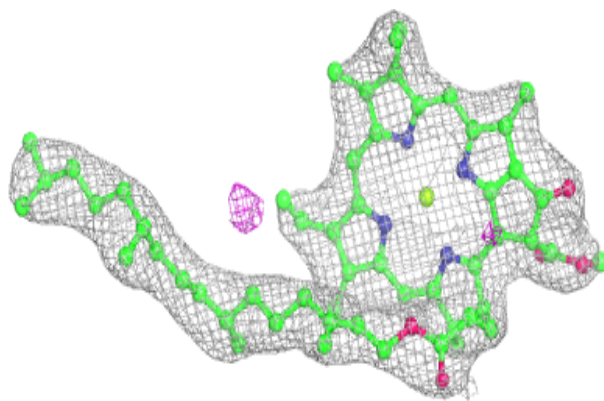
**Electron density around CLA A 404 (A):**

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



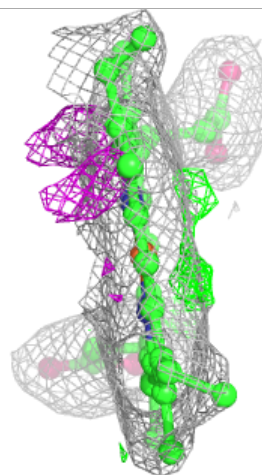
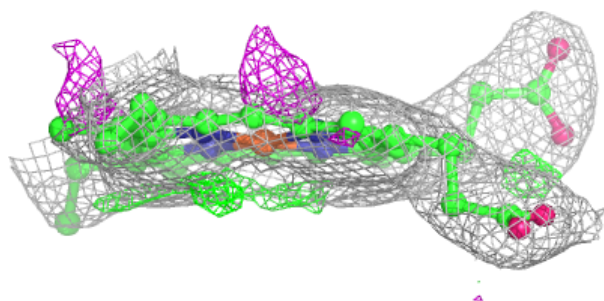
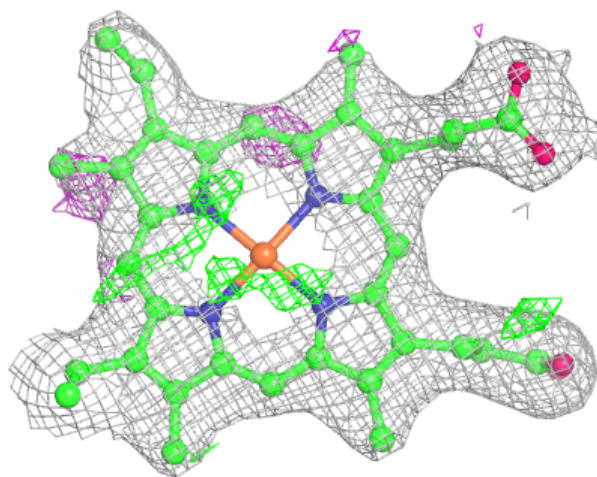
Electron density around CLA c 502:

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



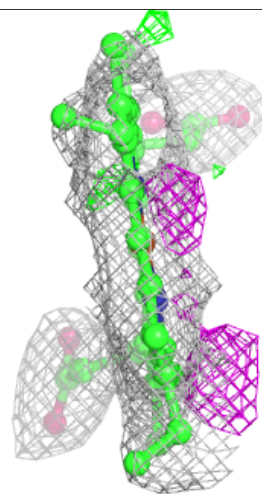
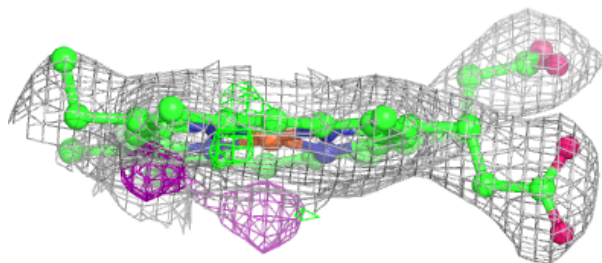
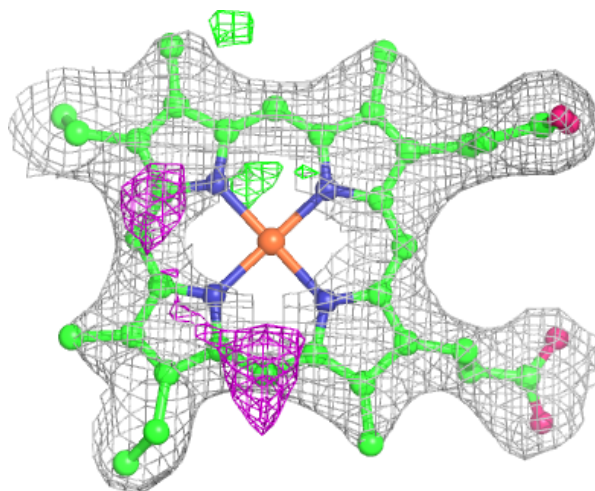
Electron density around HEC V 201:

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



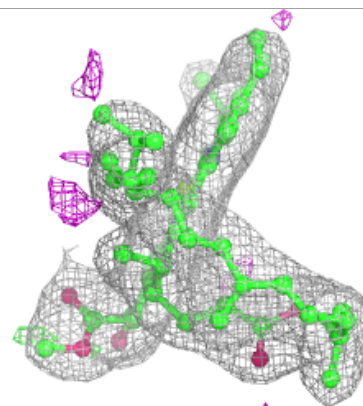
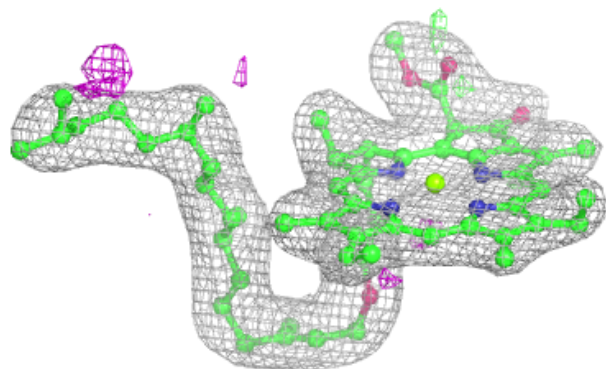
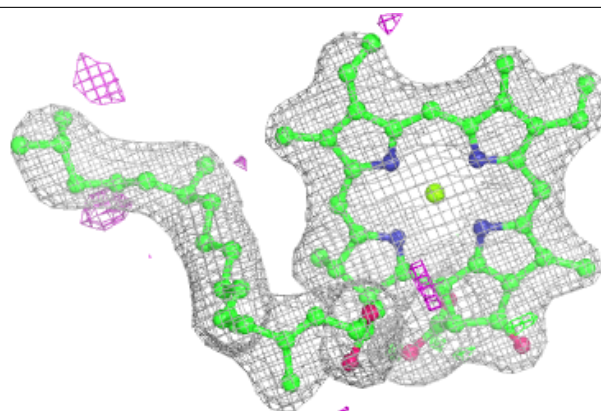
Electron density around HEC v 201:

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

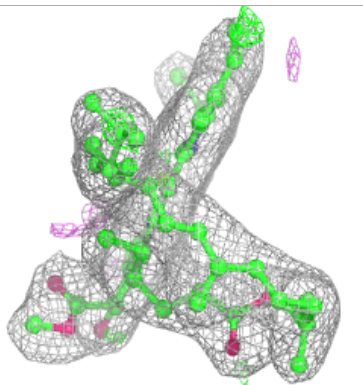
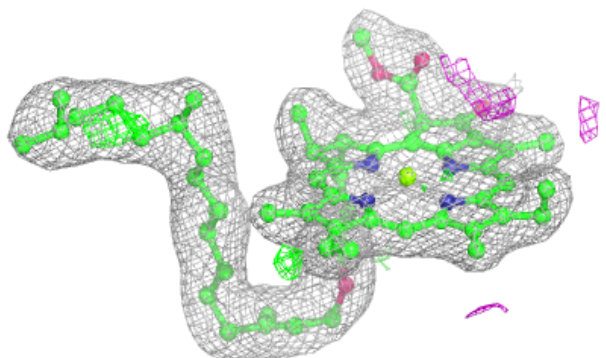
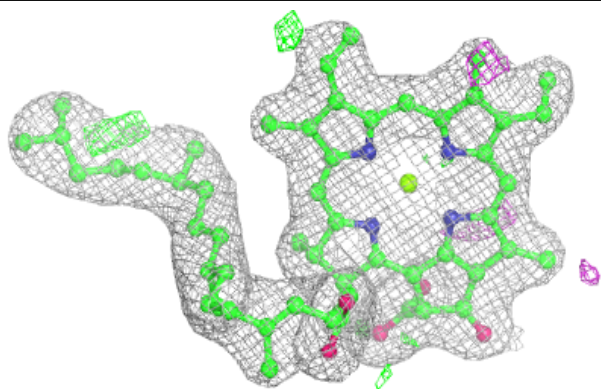


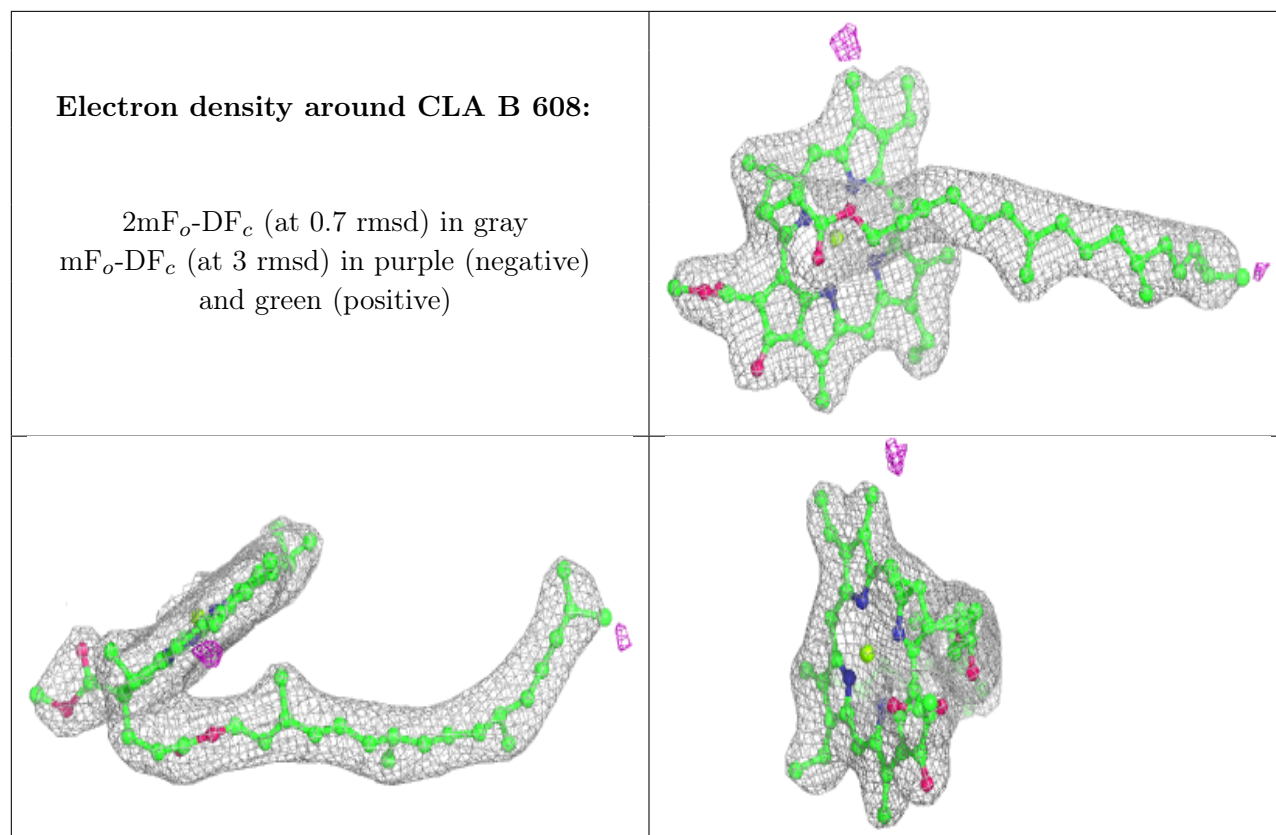
Electron density around CLA a 406 (B):

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

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

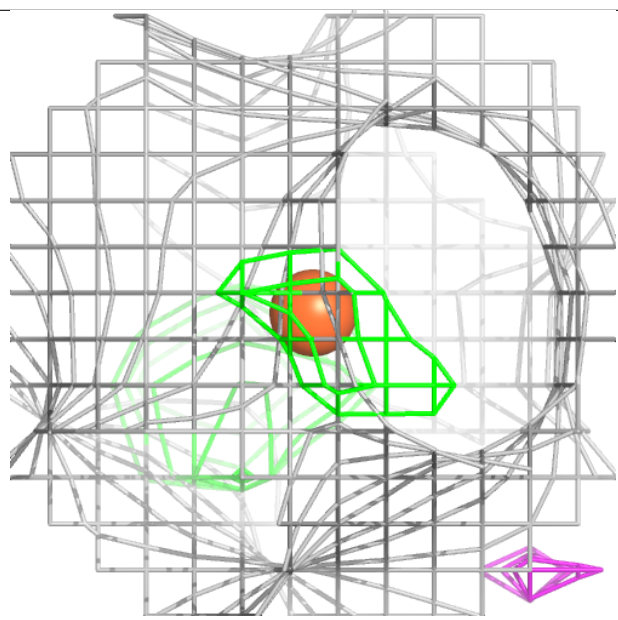
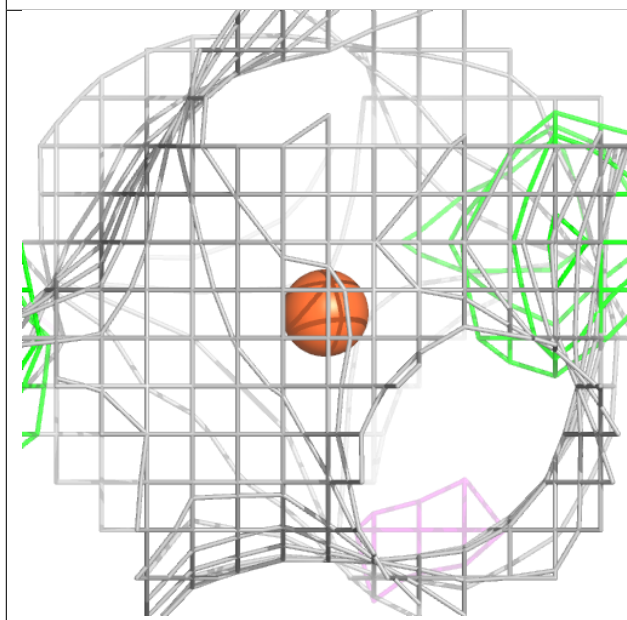
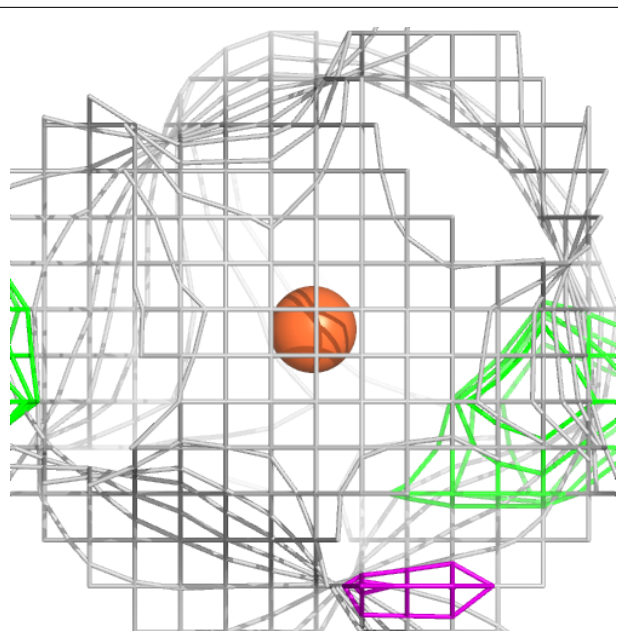
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





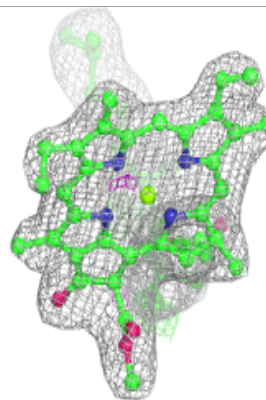
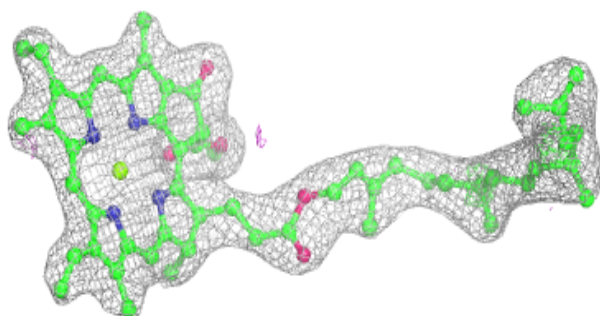
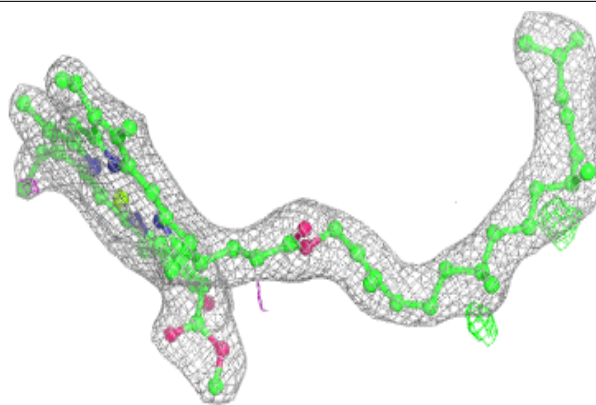
Electron density around FE2 A 401 (A):

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

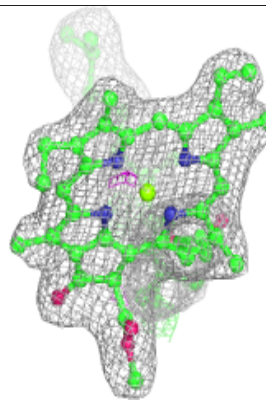
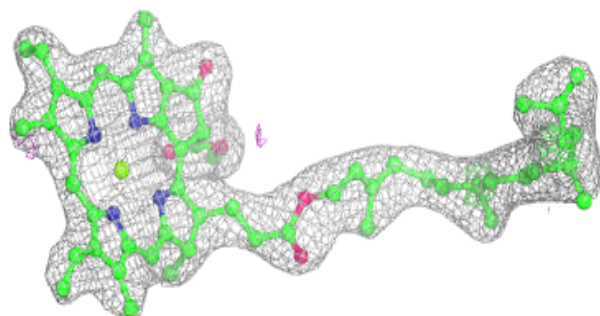
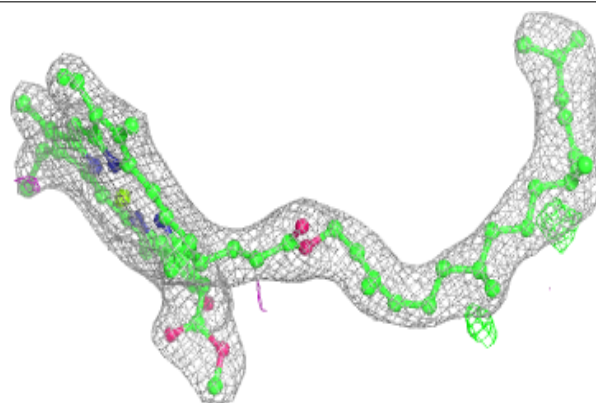


Electron density around CLA d 401 (A):

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

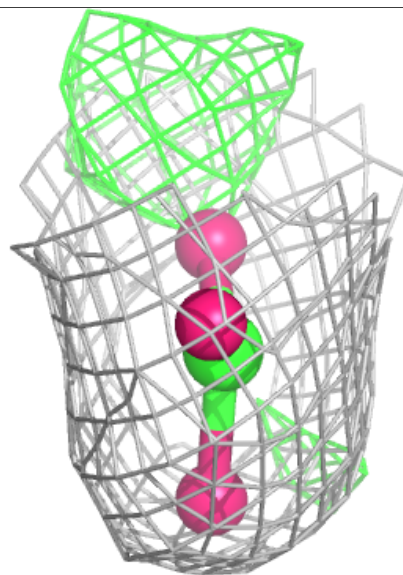
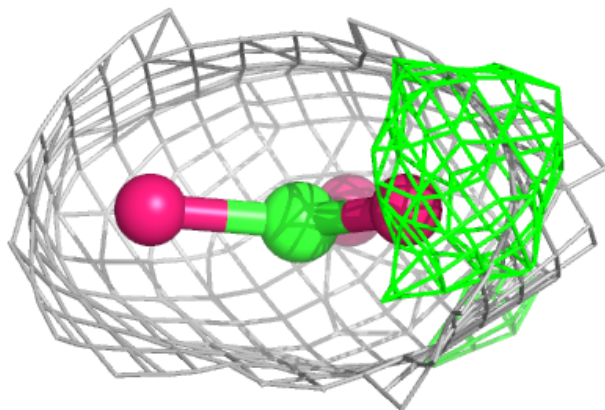
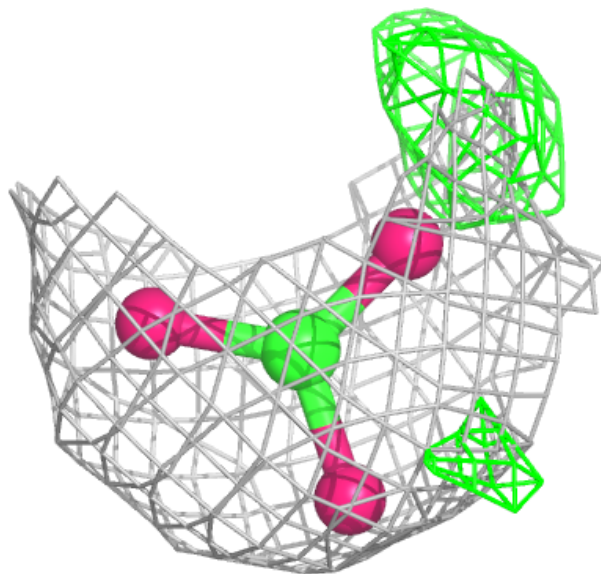
**Electron density around CLA d 401 (B):**

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



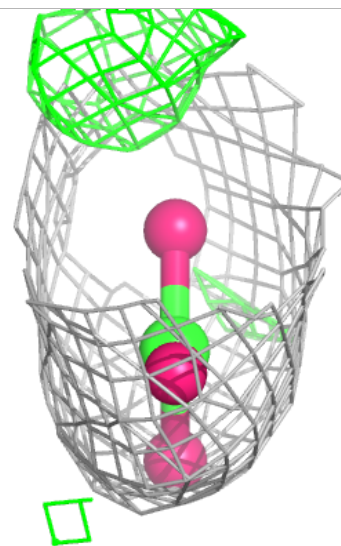
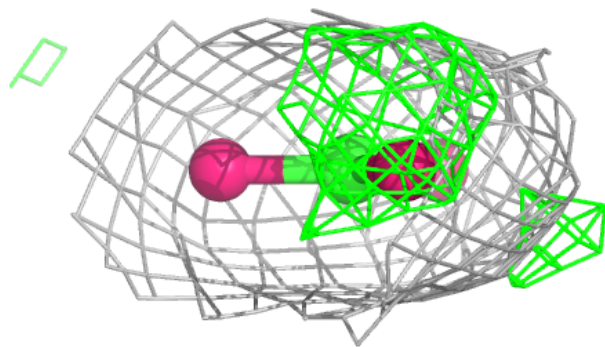
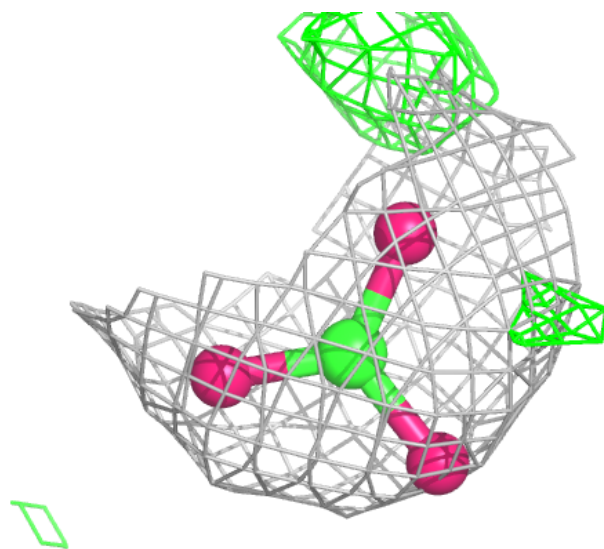
Electron density around BCT A 416 (A):

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



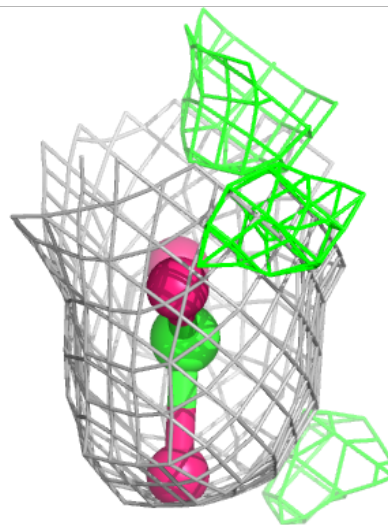
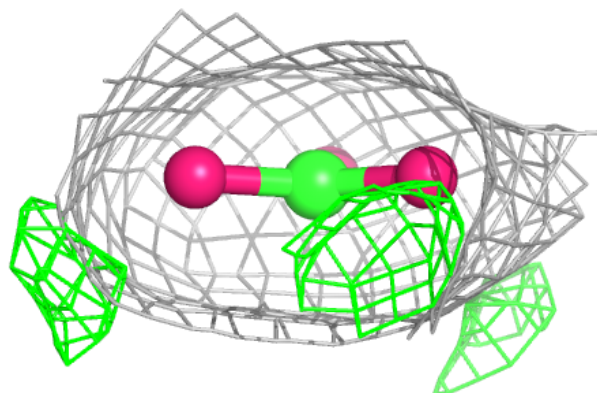
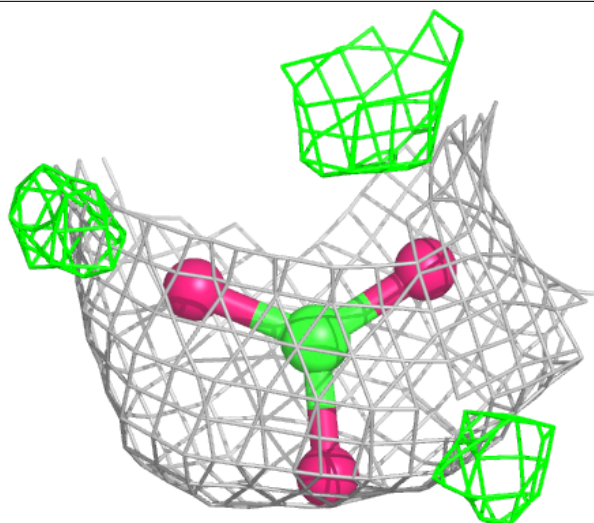
Electron density around BCT A 416 (B):

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



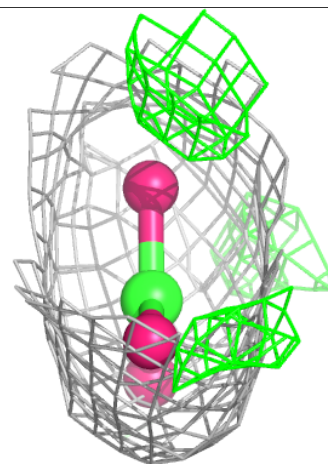
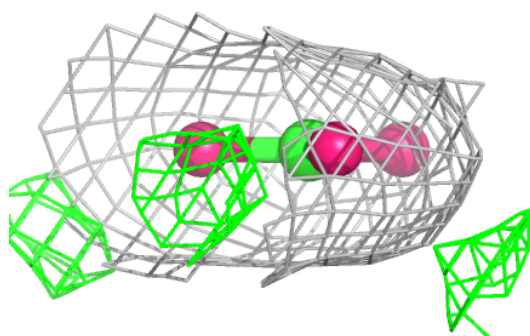
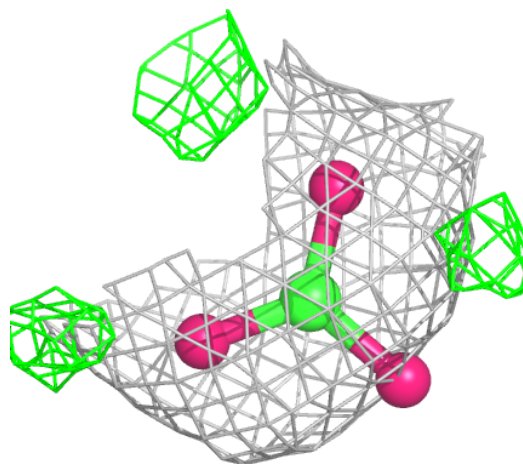
Electron density around BCT a 404 (A):

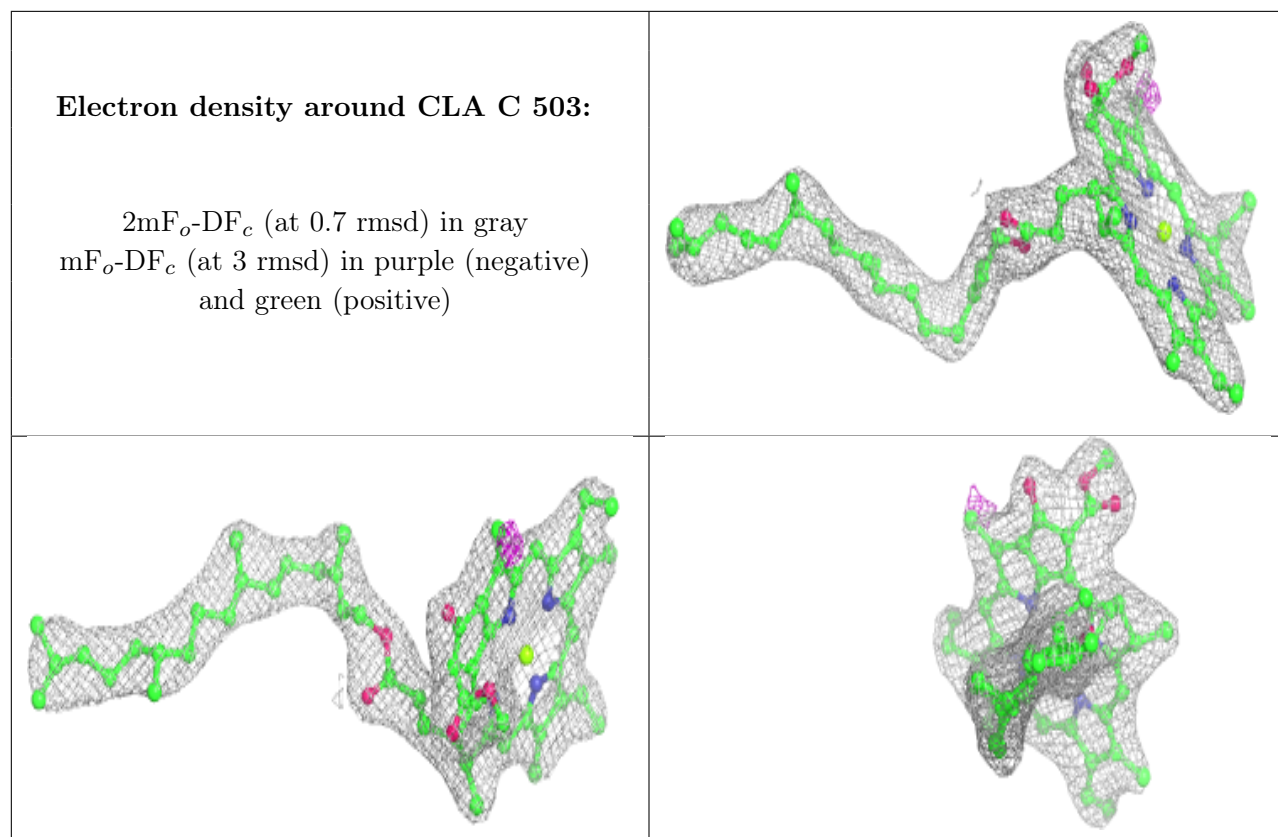
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BCT a 404 (B):

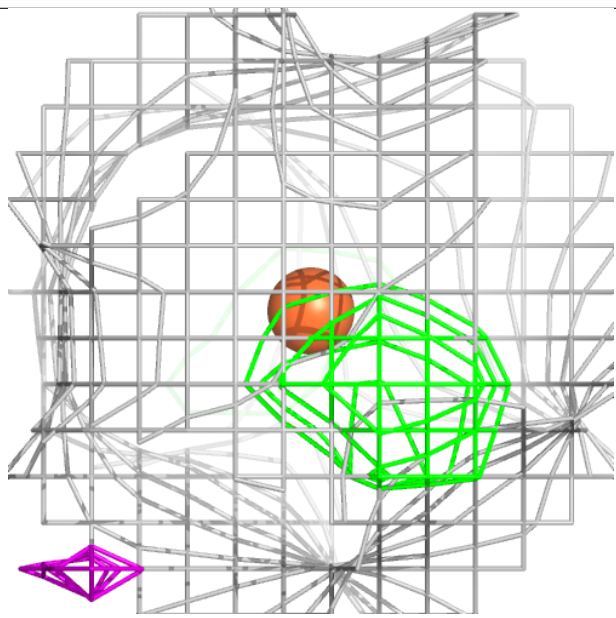
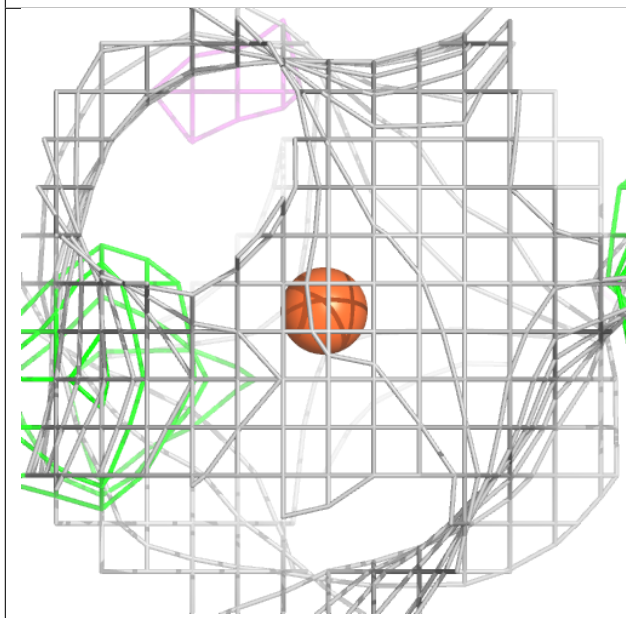
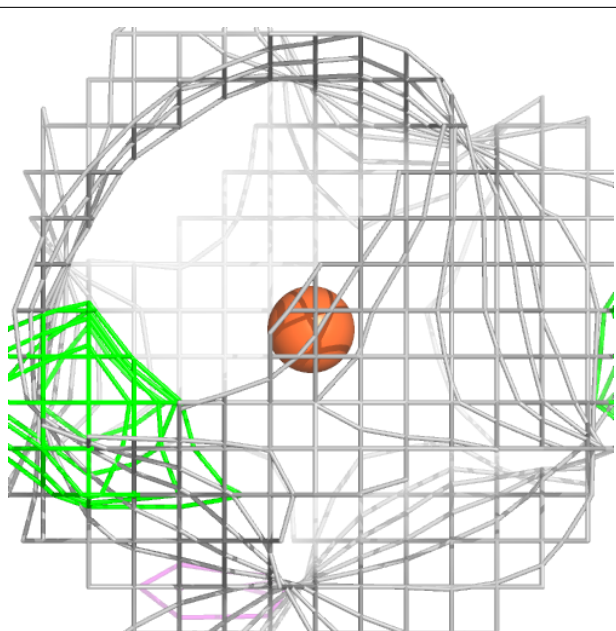
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





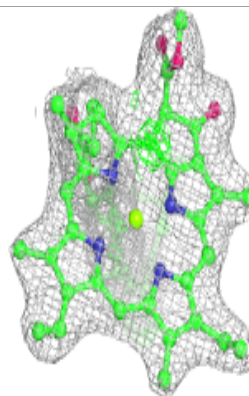
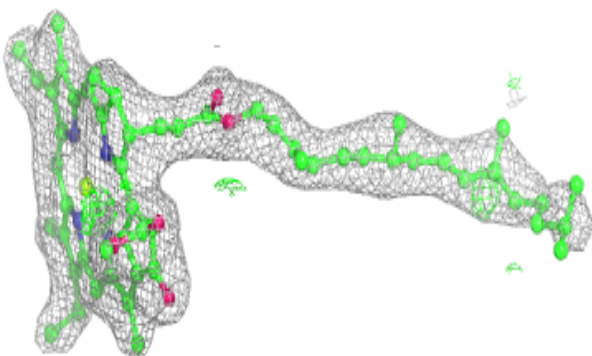
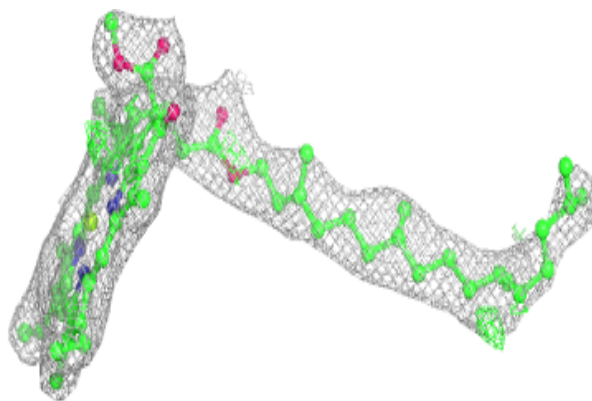
Electron density around FE2 A 401 (B):

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

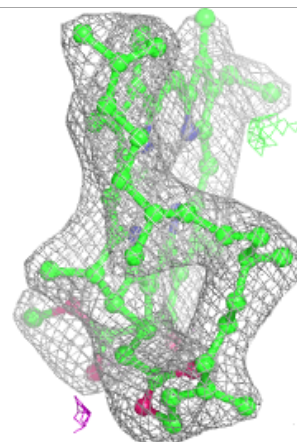
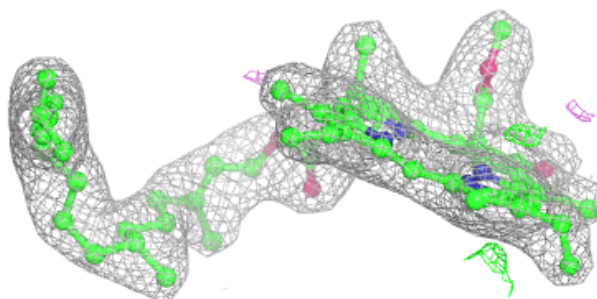
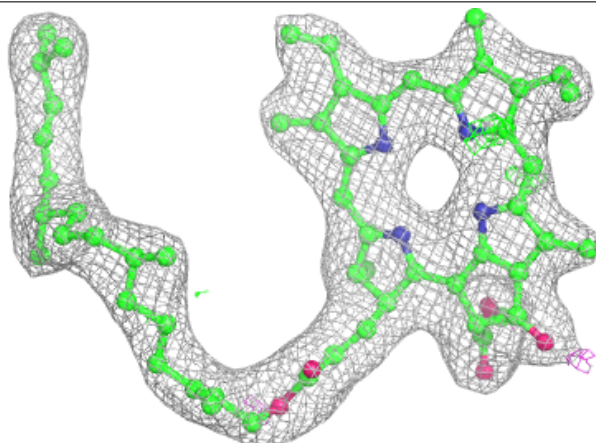


Electron density around CLA B 604:

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

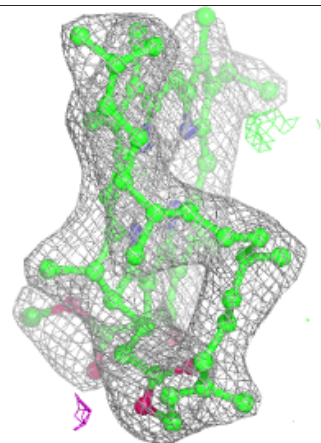
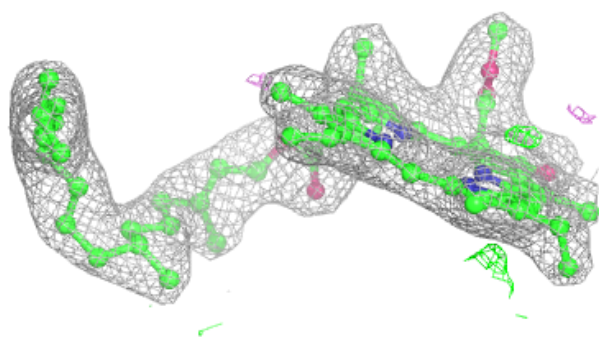
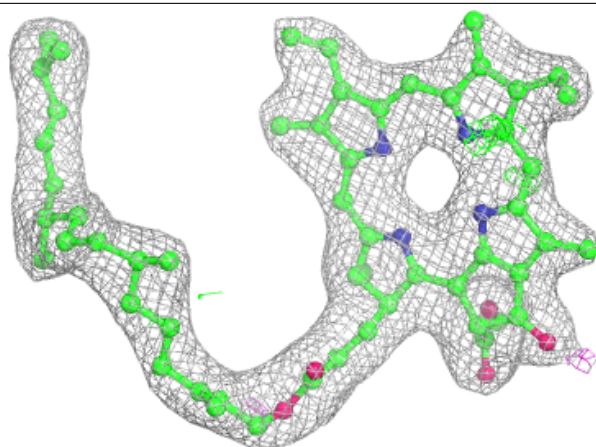
**Electron density around PHO A 417 (A):**

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

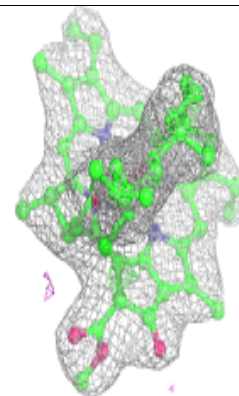
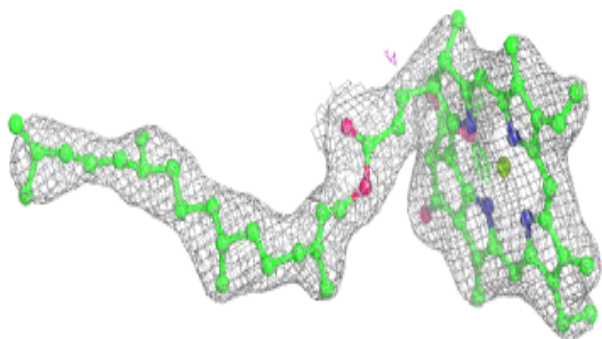
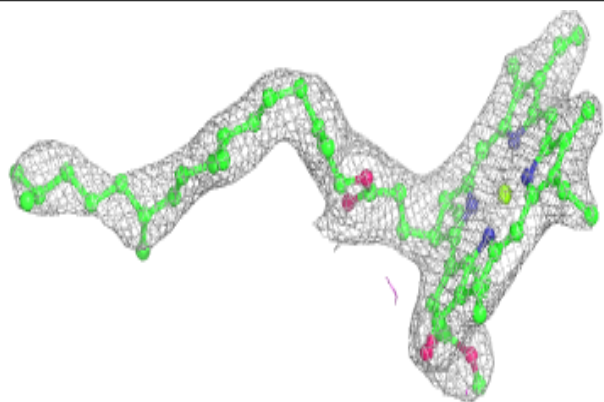


Electron density around PHO A 417 (B):

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

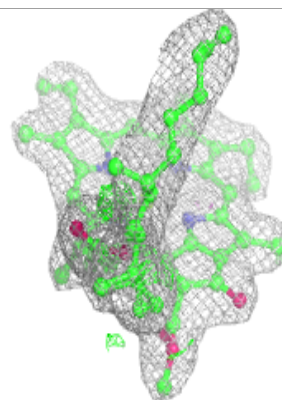
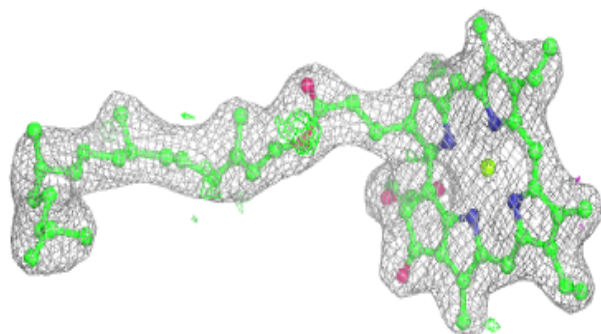
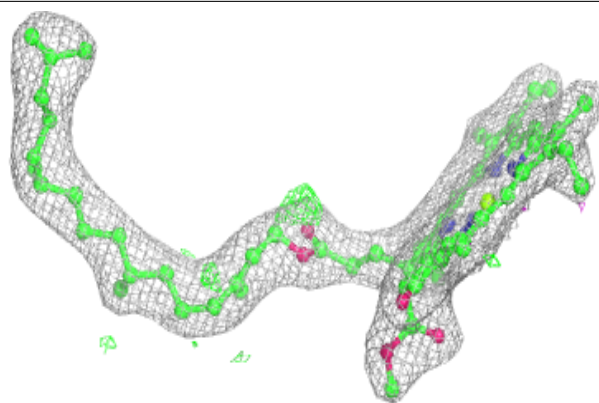
**Electron density around CLA c 503:**

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

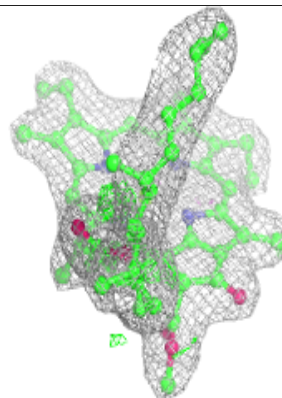
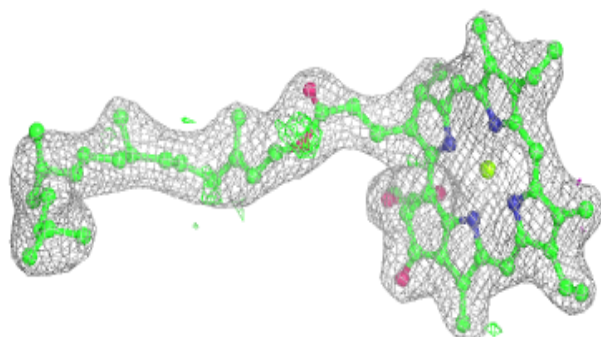
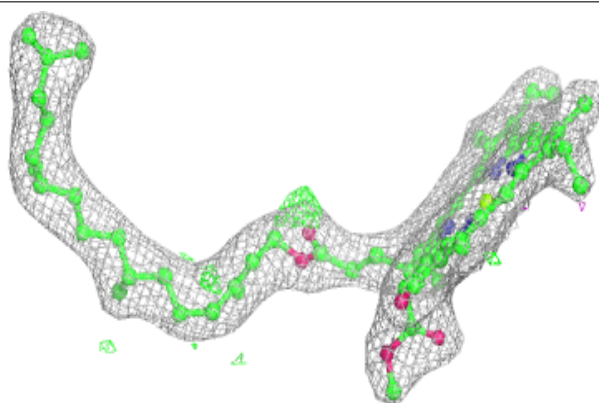


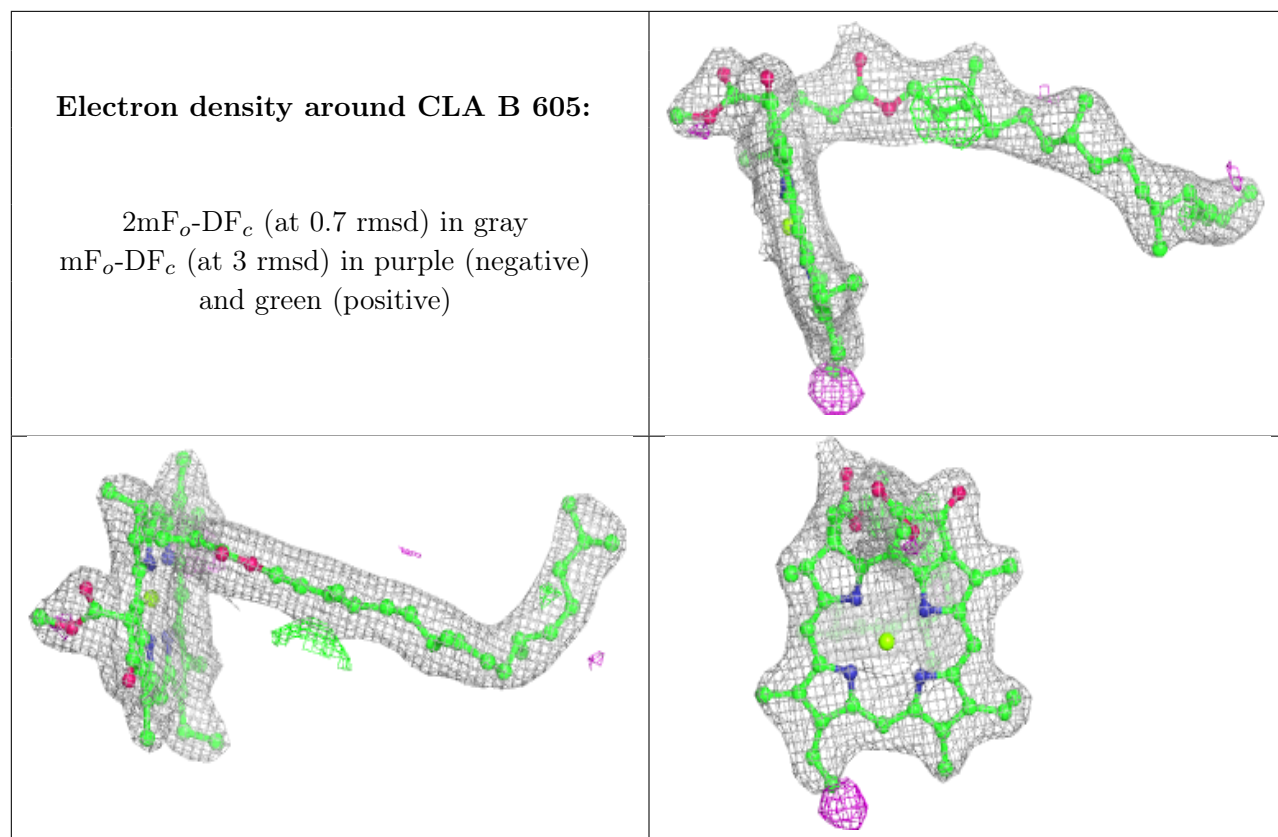
Electron density around CLA D 702 (A):

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

**Electron density around CLA D 702 (B):**

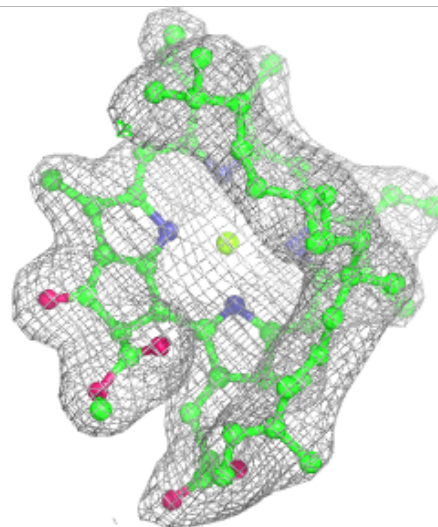
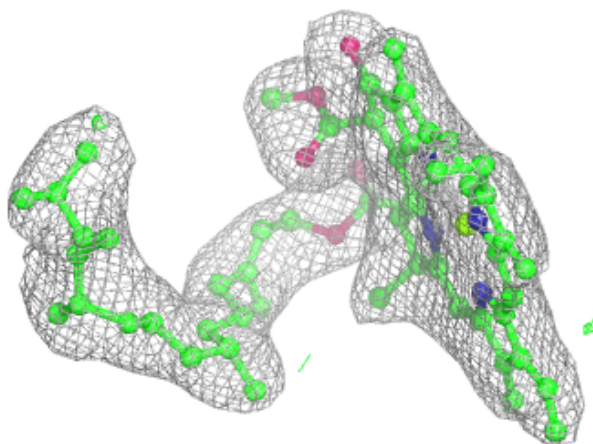
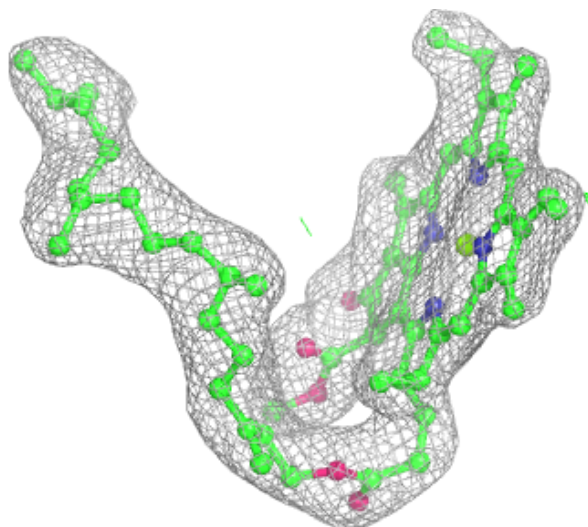
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





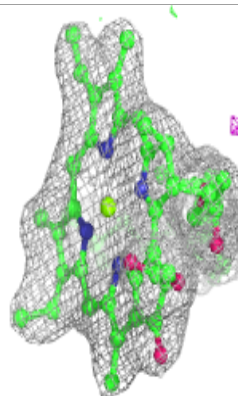
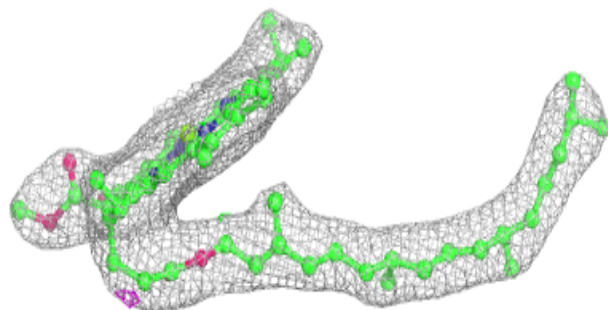
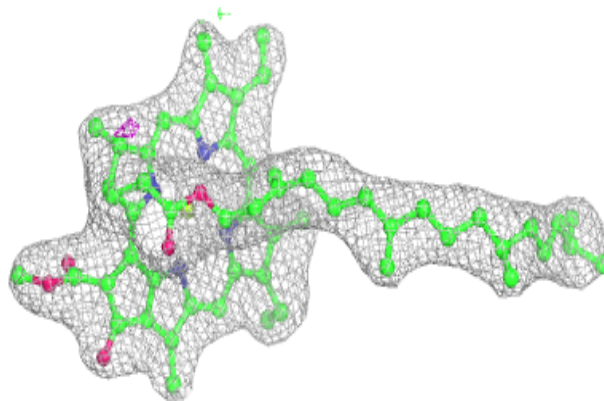
Electron density around CLA B 613:

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

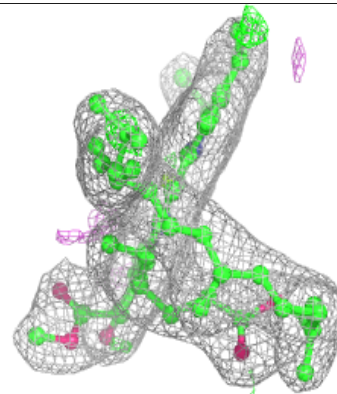
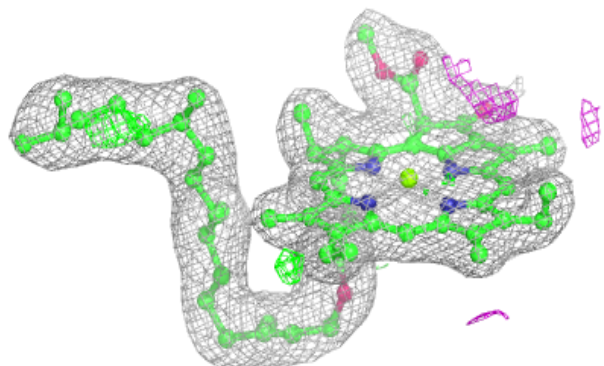
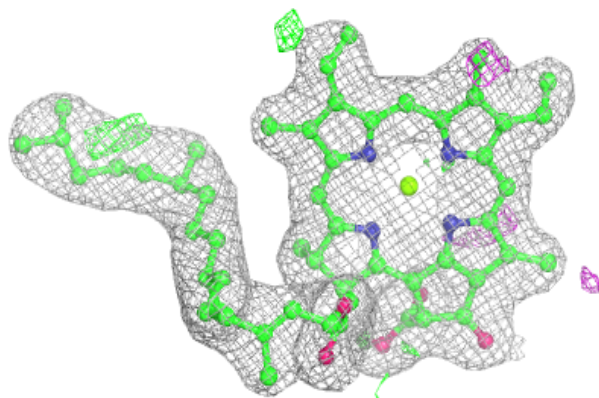


Electron density around CLA b 608:

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

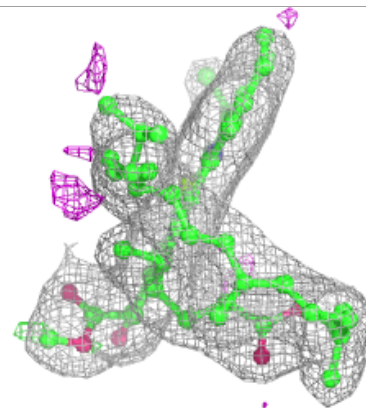
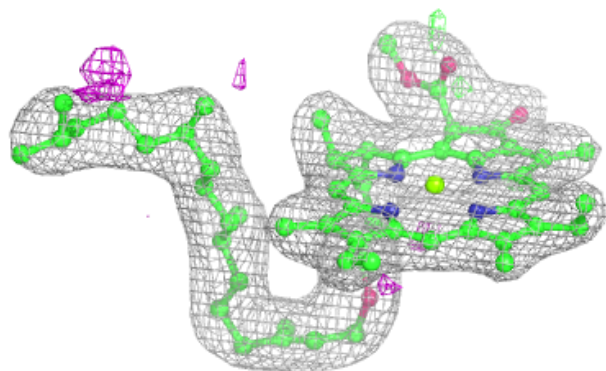
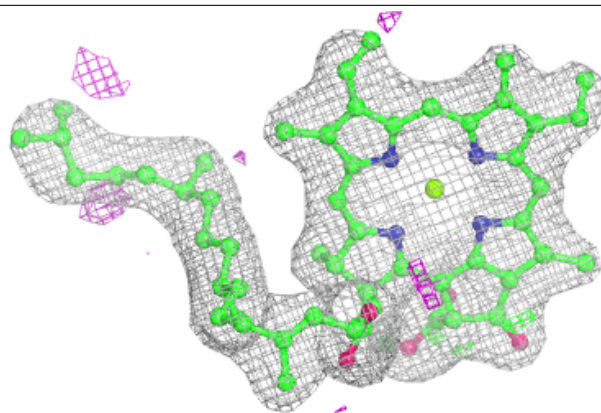
**Electron density around CLA A 405 (A):**

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



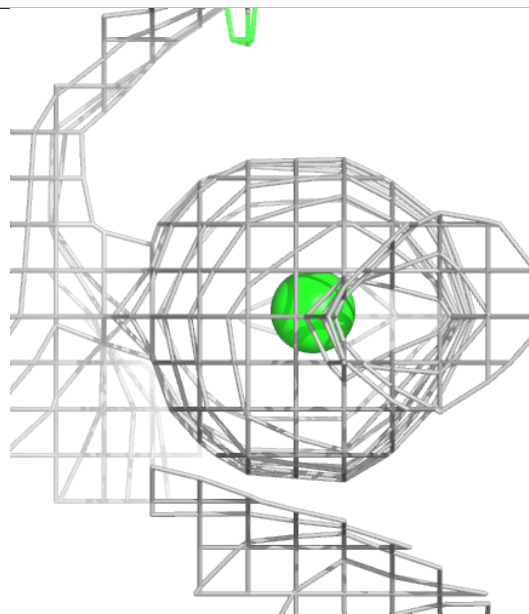
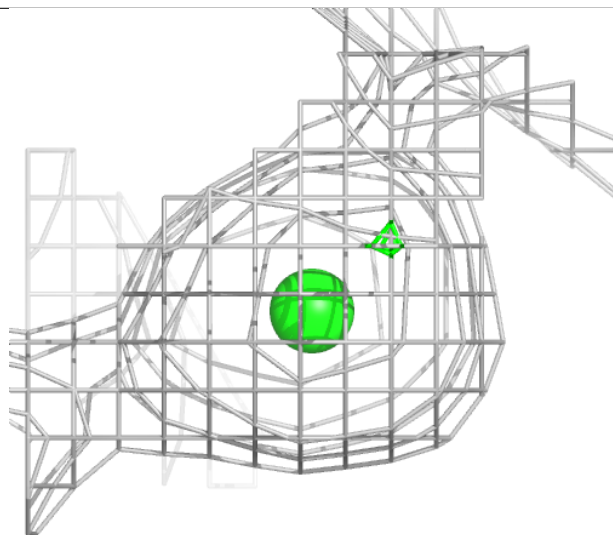
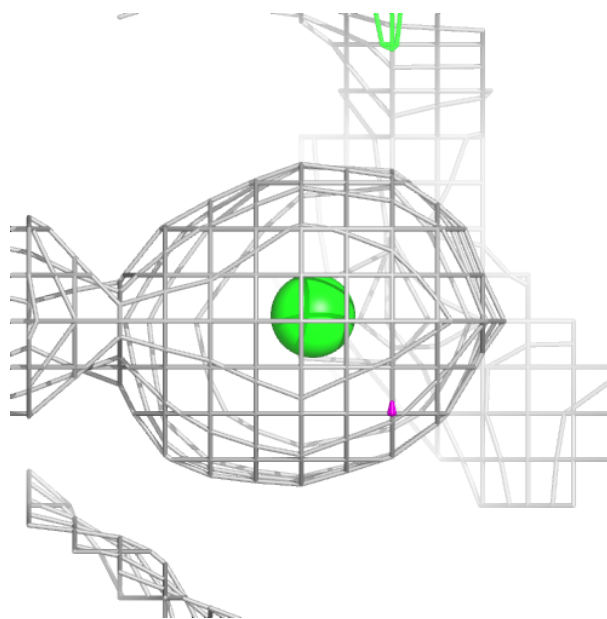
Electron density around CLA a 406 (A):

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



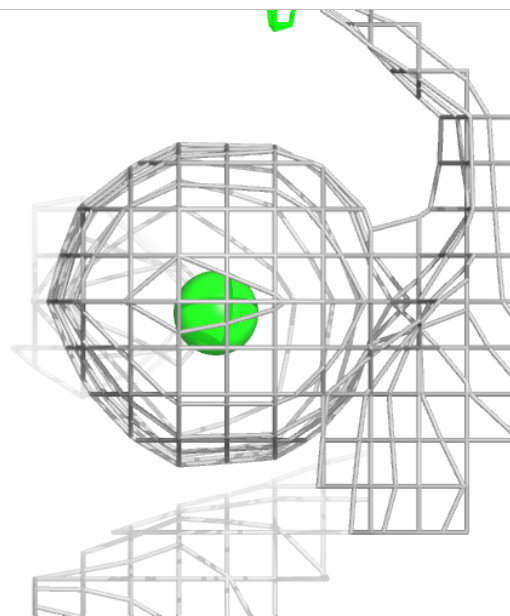
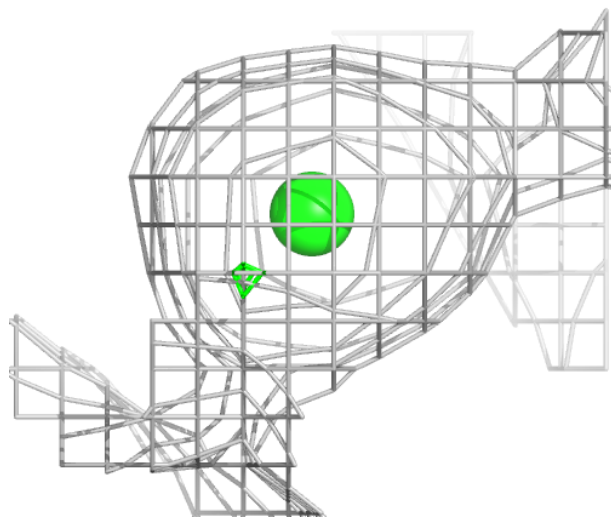
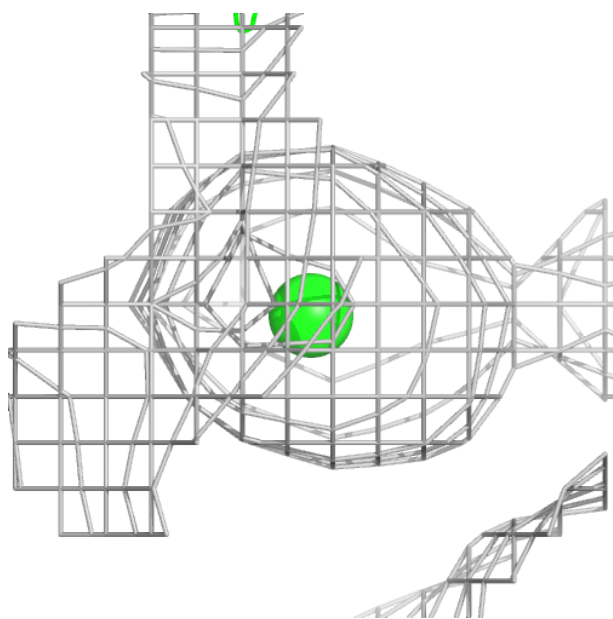
Electron density around CL a 403 (A):

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



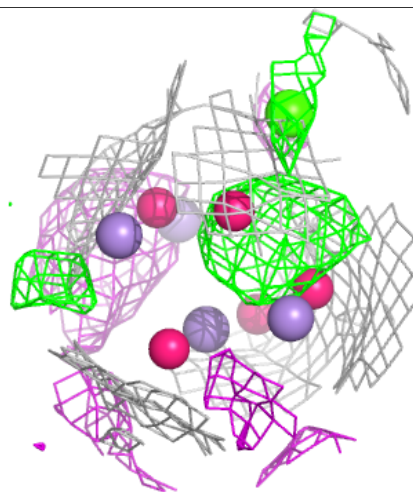
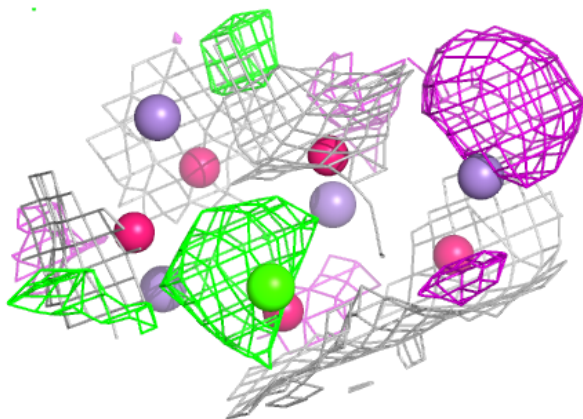
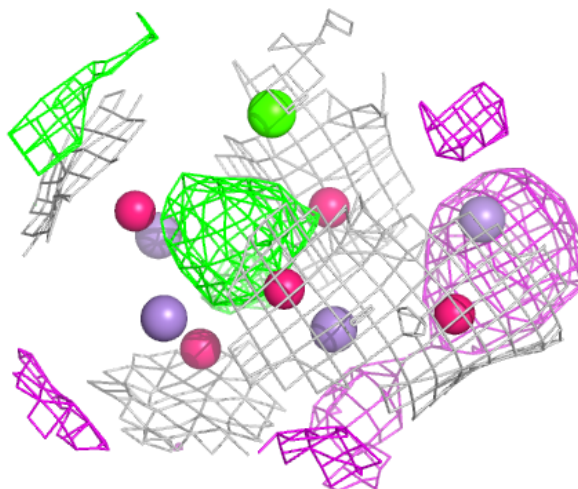
Electron density around CL a 403 (B):

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



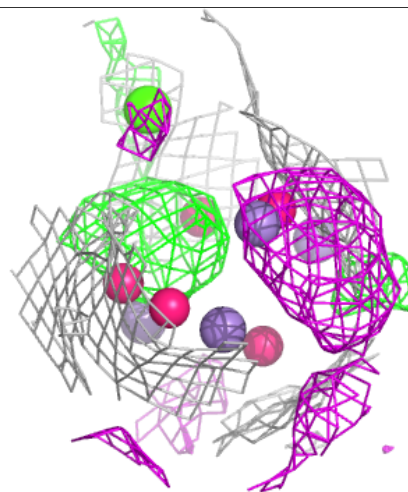
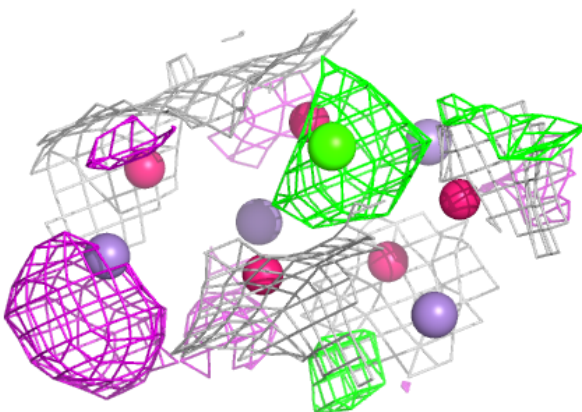
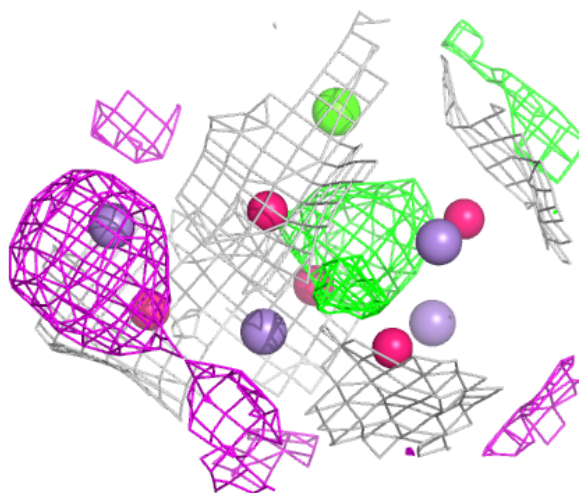
Electron density around OEX A 413 (A):

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



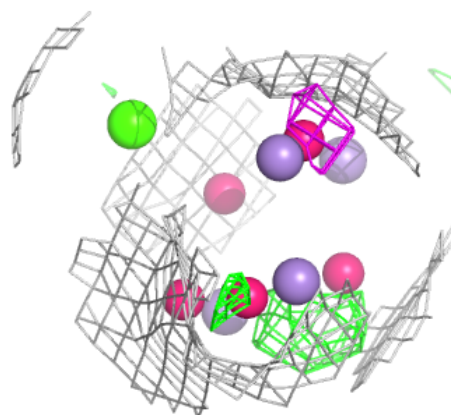
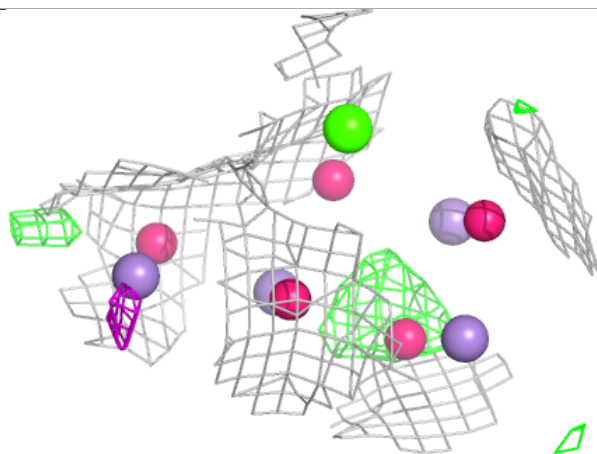
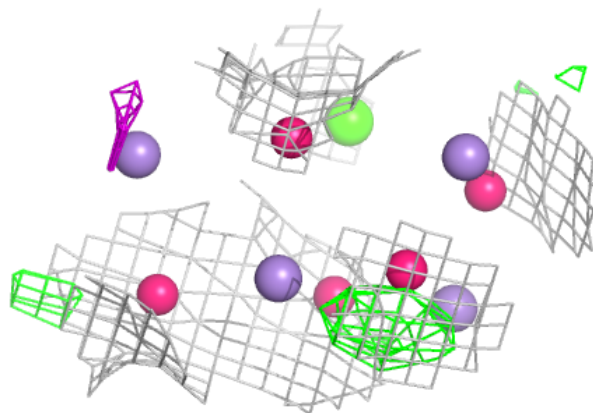
Electron density around OEX A 413 (B):

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



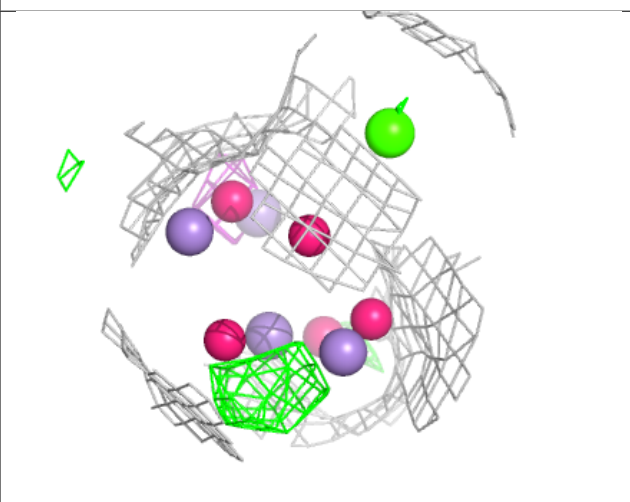
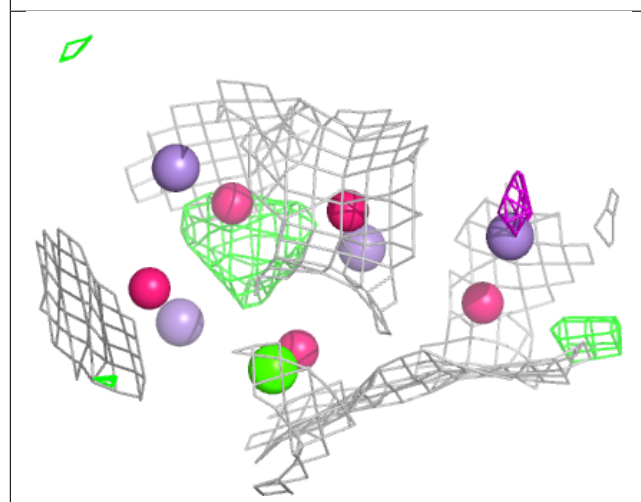
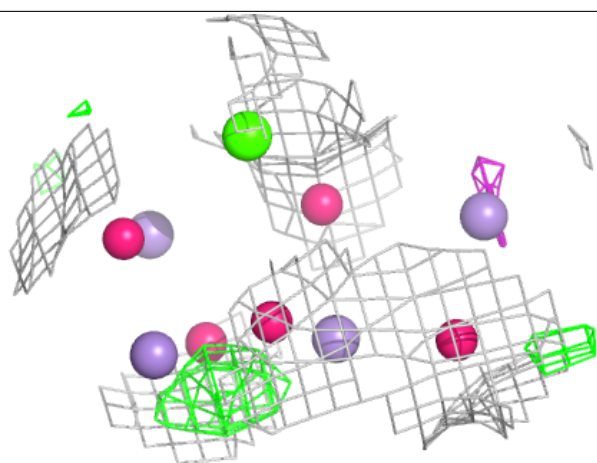
Electron density around OEX a 413 (A):

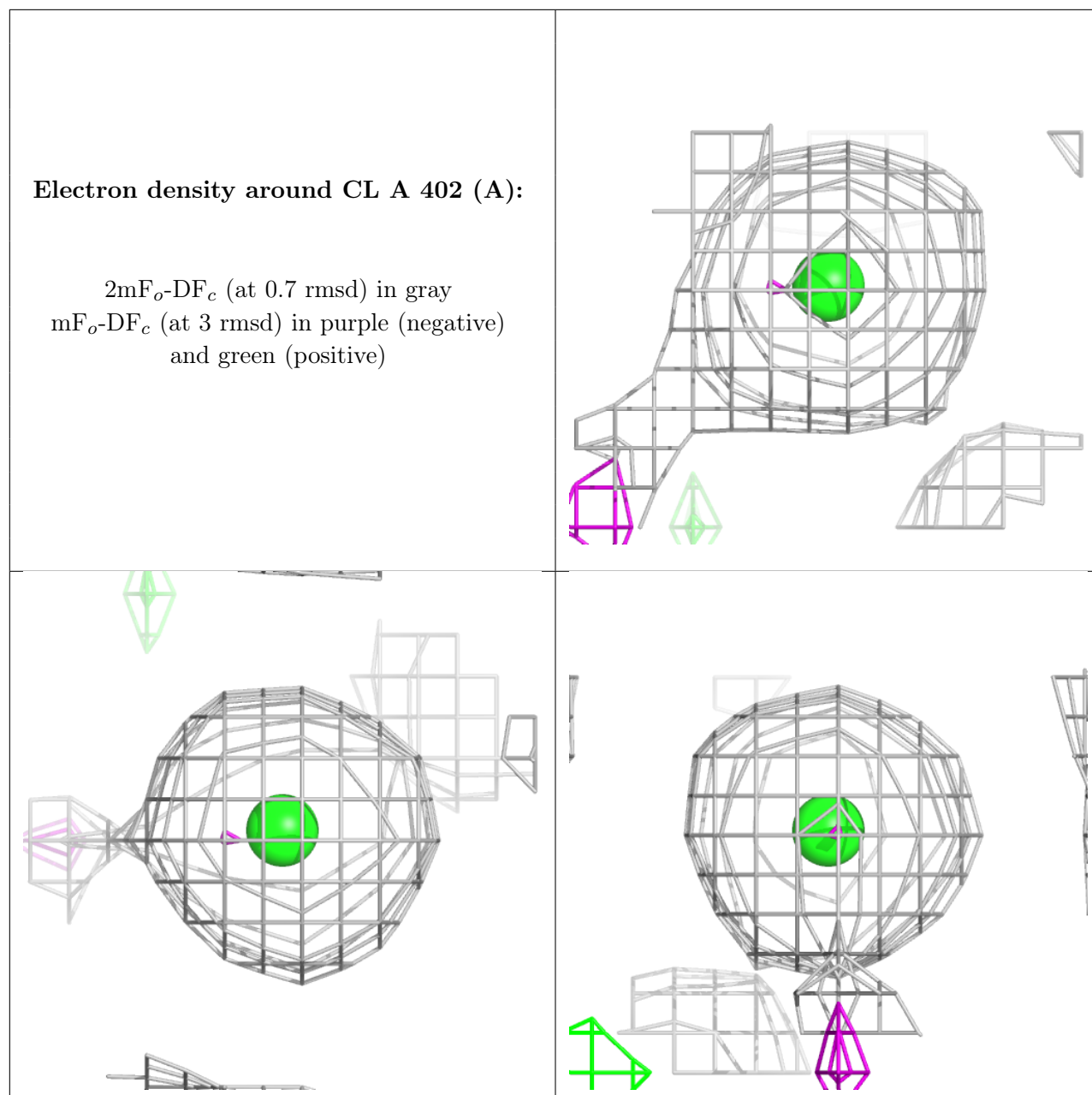
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

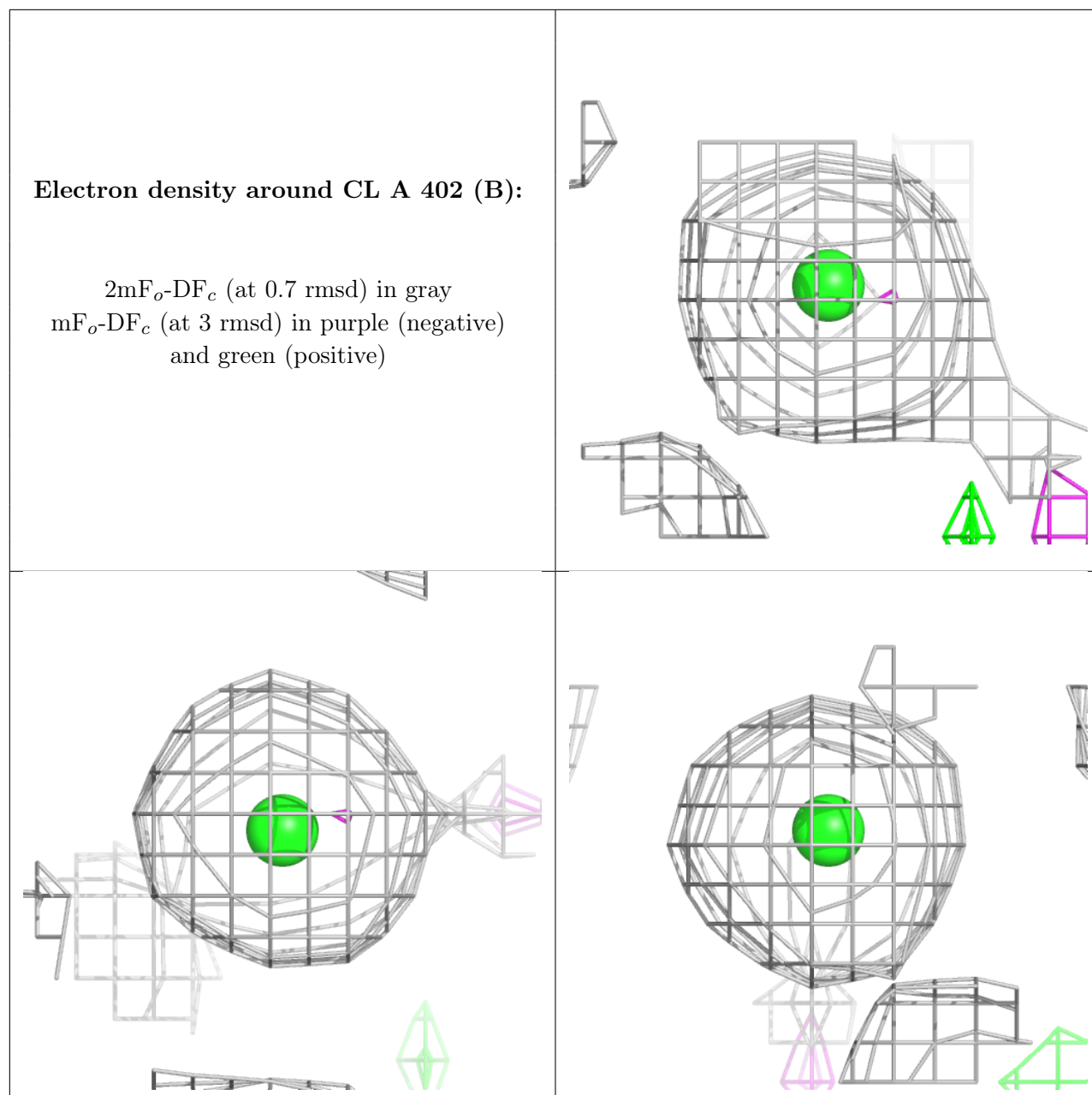


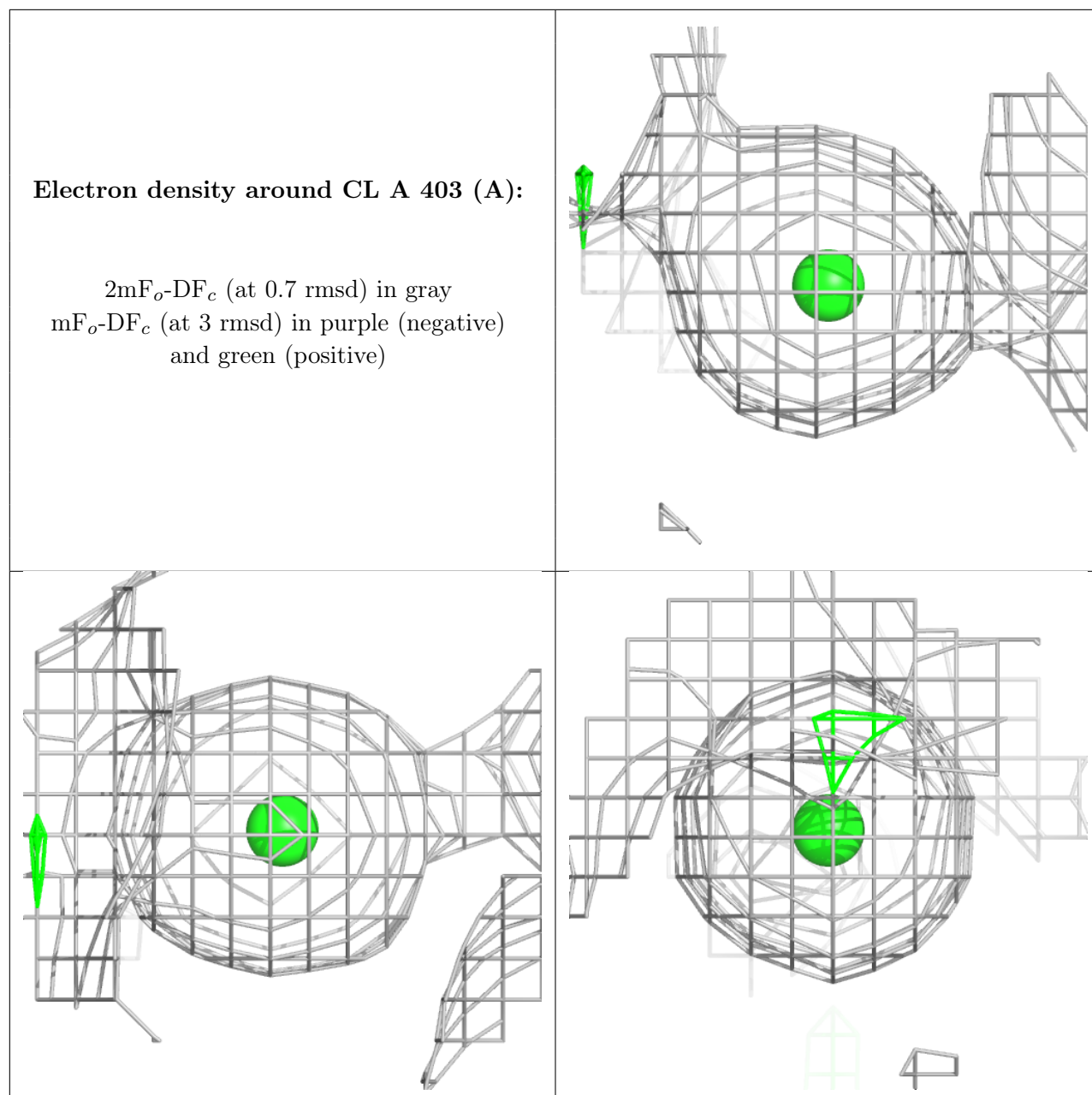
Electron density around OEX a 413 (B):

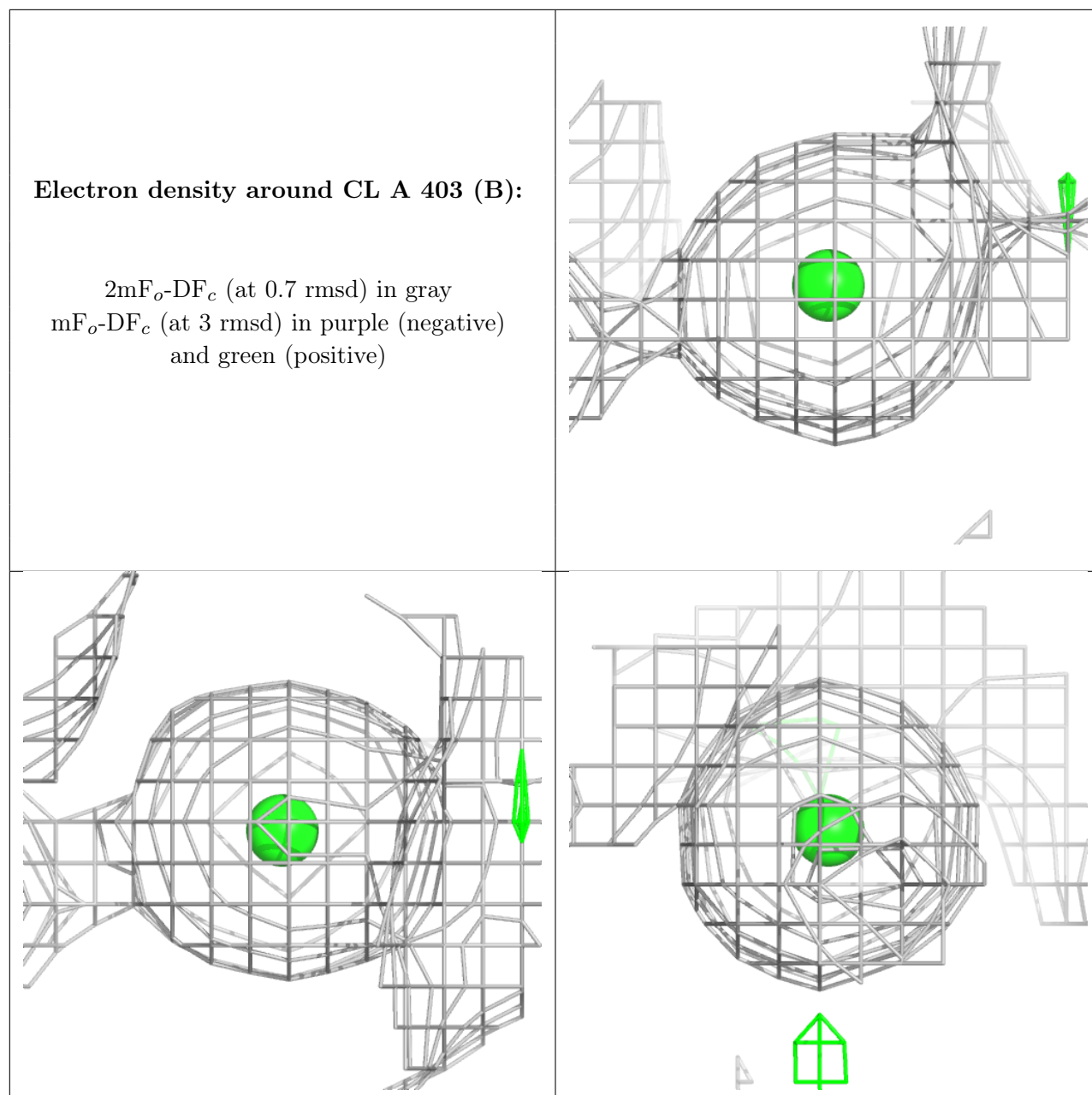
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





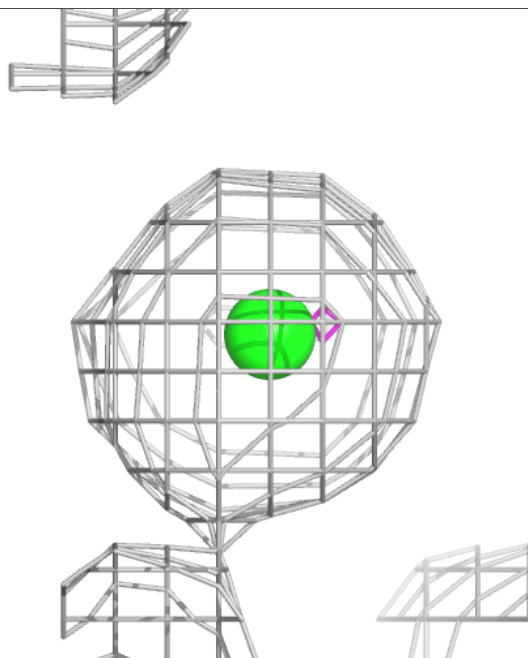
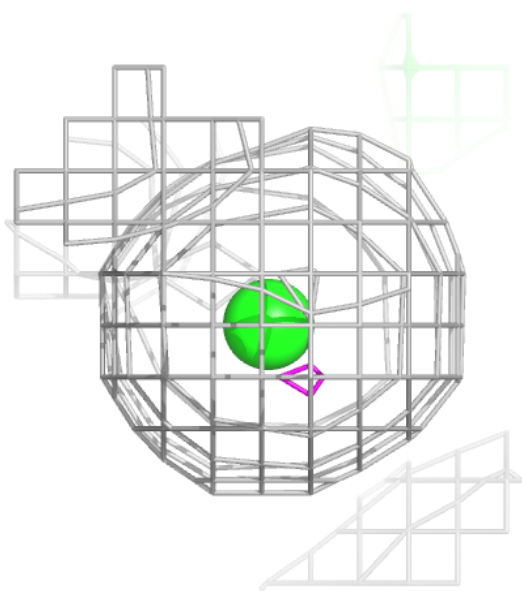
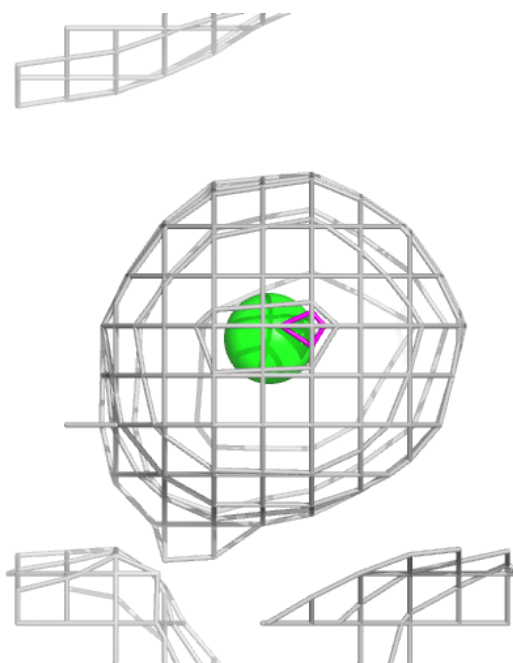


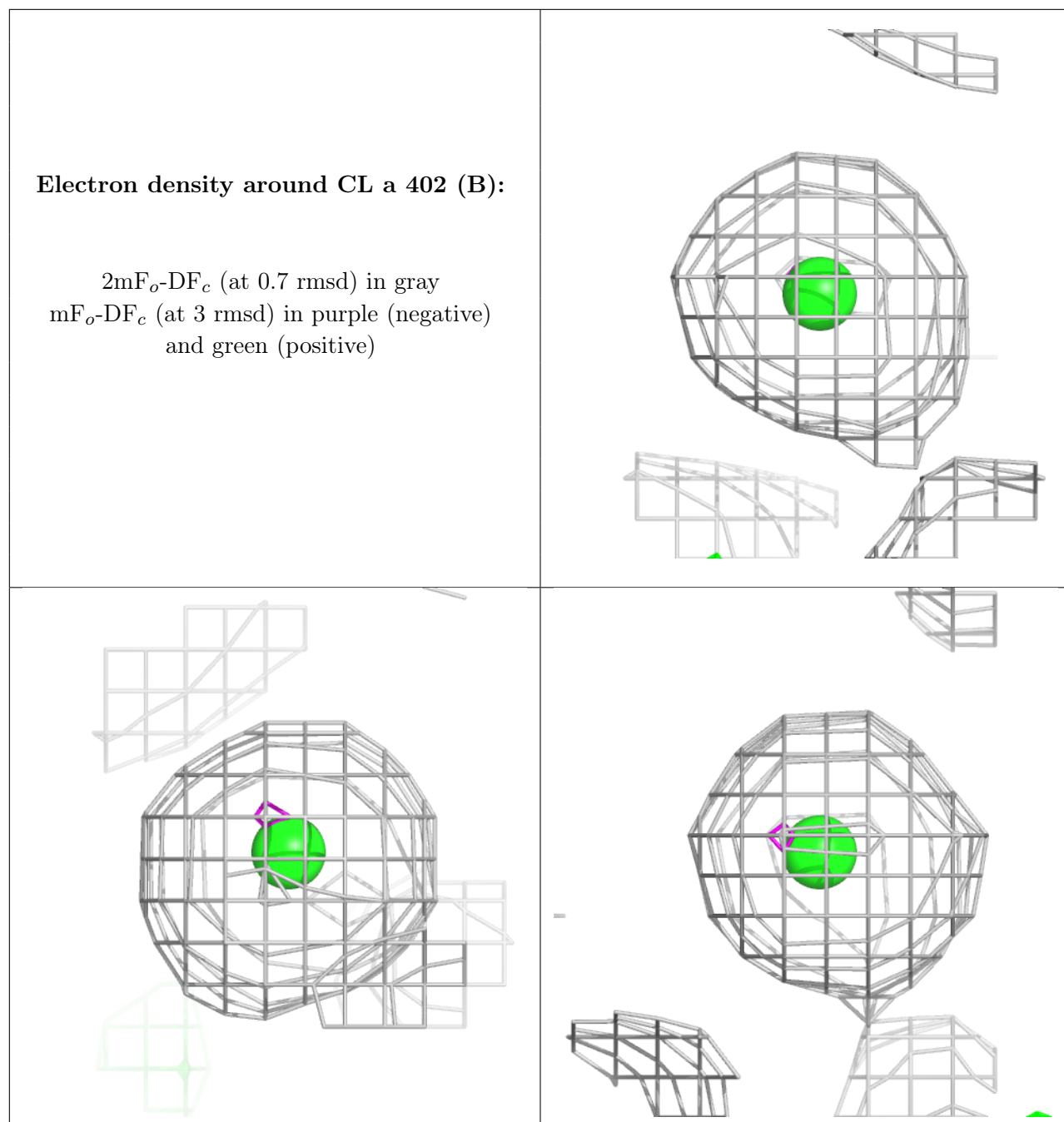




Electron density around CL a 402 (A):

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





6.5 Other polymers [i](#)

There are no such residues in this entry.