



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2024 – 01:31 PM JST

PDB ID : 8IR9
Title : XFEL structure of cyanobacterial photosystem II following one flash (1F) with a 30-microsecond delay
Authors : Li, H.; Suga, M.; Shen, J.R.
Deposited on : 2023-03-17
Resolution : 2.20 Å(reported)

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

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

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)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

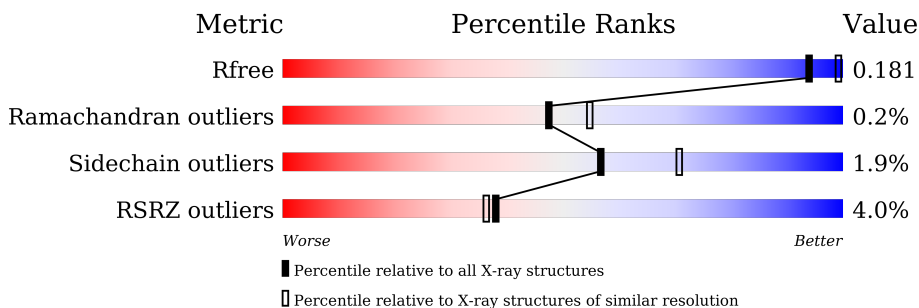
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	 2% % 99% .
2	b	505	 5% % 98% .
3	C	455	 % 98% ..
3	c	455	 2% % 99% .
4	D	342	 % 99% .

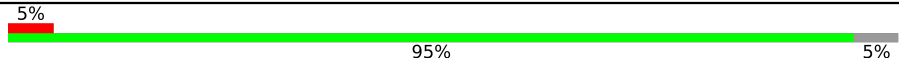
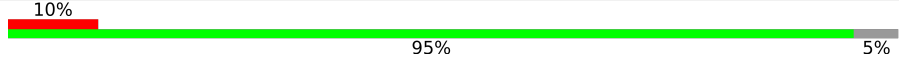
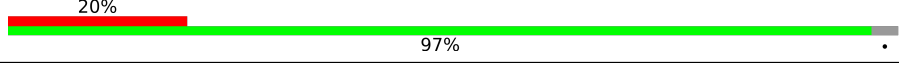
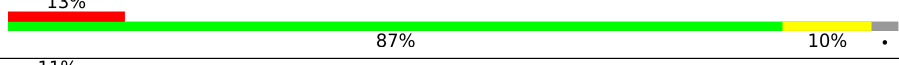
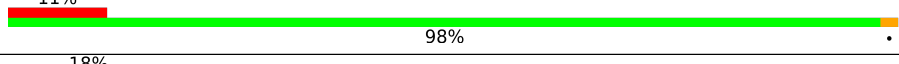
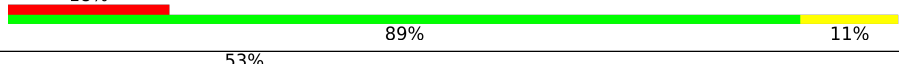
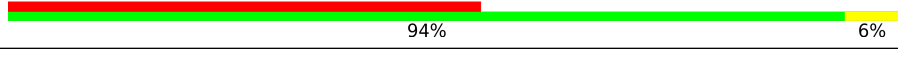
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Mol	Chain	Length	Quality of chain
4	d	342	99%
5	E	84	94%
5	e	84	92% 6%
6	F	44	77% 23%
6	f	44	70% 30%
7	H	65	94% 5%
7	h	65	95%
8	I	38	89% 11%
8	i	38	95% 5%
9	J	39	95%
9	j	39	97%
10	K	37	89% 11%
10	k	37	92% 8%
11	L	37	97%
11	l	37	97%
12	M	36	86% 6% 8%
12	m	36	89% 6% 6%
13	O	244	97%
13	o	244	98%
14	T	32	88% 6% 6%
14	t	32	91% 6%
15	U	104	90% 8%
15	u	104	92% 7%
16	V	137	99%
16	v	137	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	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	402[A]	X	-	-	-
23	CLA	D	402[B]	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	a	404[A]	X	-	-	-
23	CLA	a	404[B]	X	-	-	-
23	CLA	a	405[A]	X	-	-	-
23	CLA	a	405[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	-	-	-
23	CLA	d	402[A]	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	d	402[B]	X	-	-	-
23	CLA	d	403	X	-	-	-
27	GOL	D	412	-	X	-	-
27	GOL	a	417	-	-	-	X
33	LMT	F	101	-	-	-	X
33	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
			Total	C	N	O	S			
12	m	34	286	190	43	52	1	0	2	0

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
			Total	C	N	O	S			
13	O	243	1958	1221	335	398	4	0	10	0
13	o	243	1933	1207	330	392	4	0	8	0

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

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

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

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

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

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

- 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).

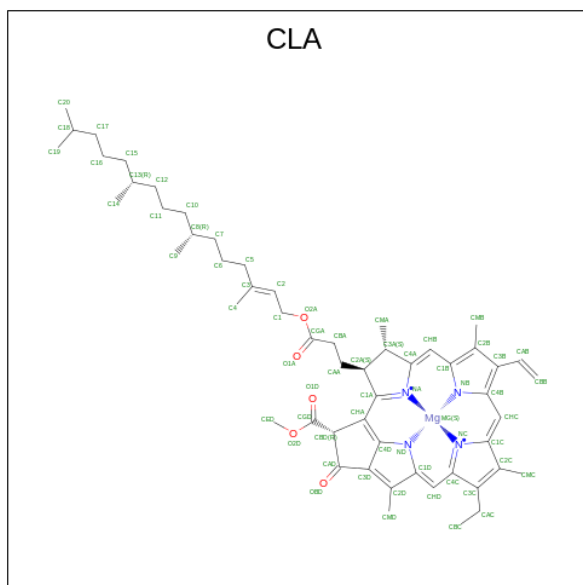
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	2
			4	4		

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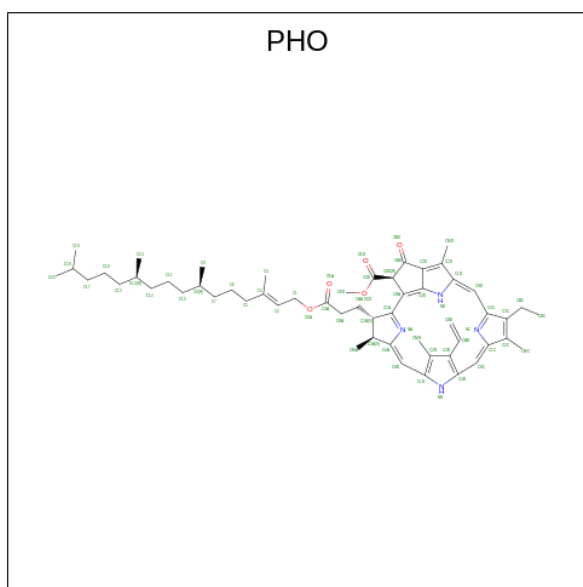
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
23	C	1	65	55	1	4	5	0	0
23	C	1	65	55	1	4	5	0	0
23	D	1	130	110	2	8	10	0	1
23	D	1	65	55	1	4	5	0	0
23	a	1	130	110	2	8	10	0	1
23	a	1	130	110	2	8	10	0	1
23	a	1	130	110	2	8	10	0	1
23	a	1	65	55	1	4	5	0	0
23	b	1	65	55	1	4	5	0	0
23	b	1	65	55	1	4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

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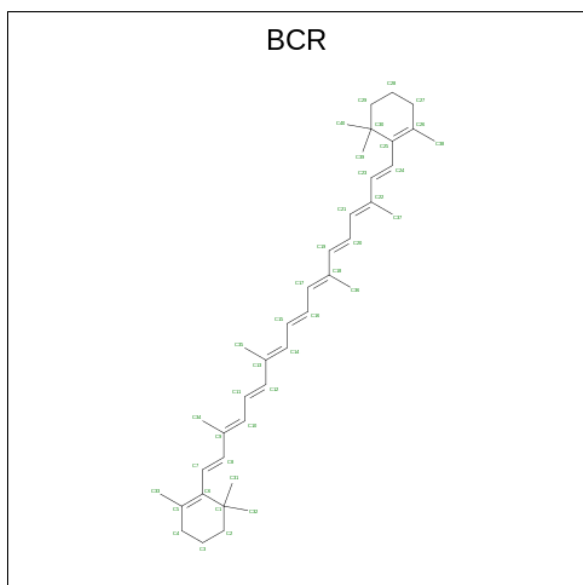
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
23	b	1	65	55	1	4	5	0	0
23	b	1	65	55	1	4	5	0	0
23	b	1	65	55	1	4	5	0	0
23	c	1	65	55	1	4	5	0	0
23	c	1	65	55	1	4	5	0	0
23	c	1	65	55	1	4	5	0	0
23	c	1	65	55	1	4	5	0	0
23	c	1	65	55	1	4	5	0	0
23	c	1	65	55	1	4	5	0	0
23	c	1	65	55	1	4	5	0	0
23	c	1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

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



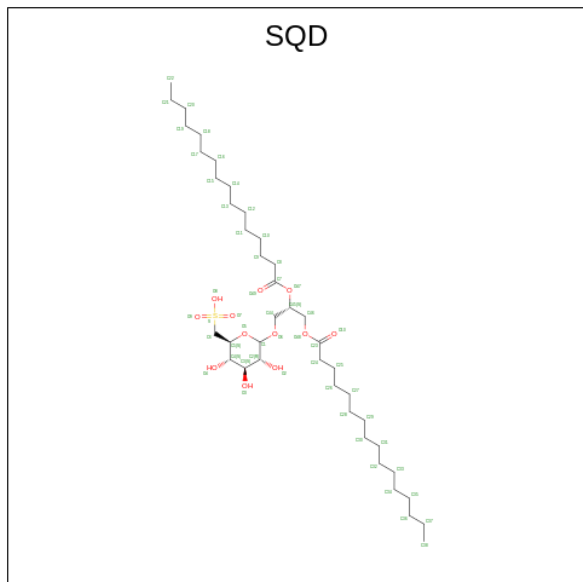
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	1
			128	110	8	10		

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



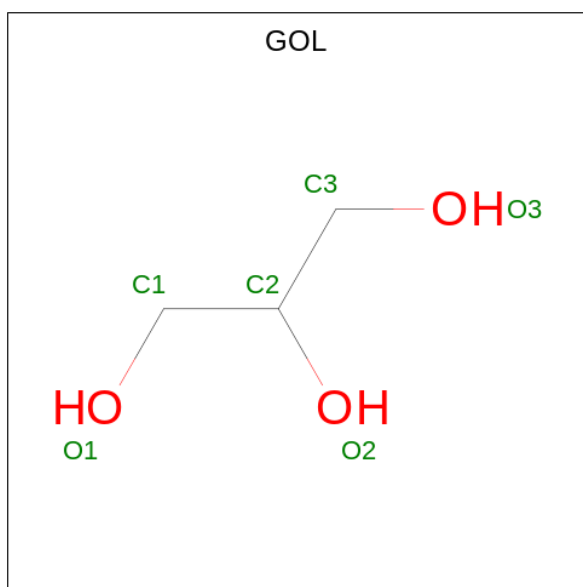
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total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

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



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

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



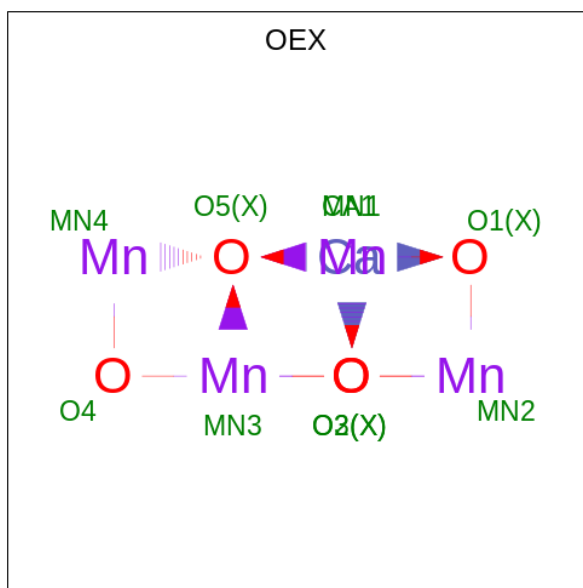
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 6 3 3	0	0
27	A	1	Total C O 6 3 3	0	0
27	B	1	Total C O 6 3 3	0	0
27	B	1	Total C O 6 3 3	0	0
27	B	1	Total C O 6 3 3	0	0
27	C	1	Total C O 12 6 6	0	1
27	D	1	Total C O 6 3 3	0	0
27	O	1	Total C O 6 3 3	0	0
27	O	1	Total C O 6 3 3	0	0
27	V	1	Total C O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

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

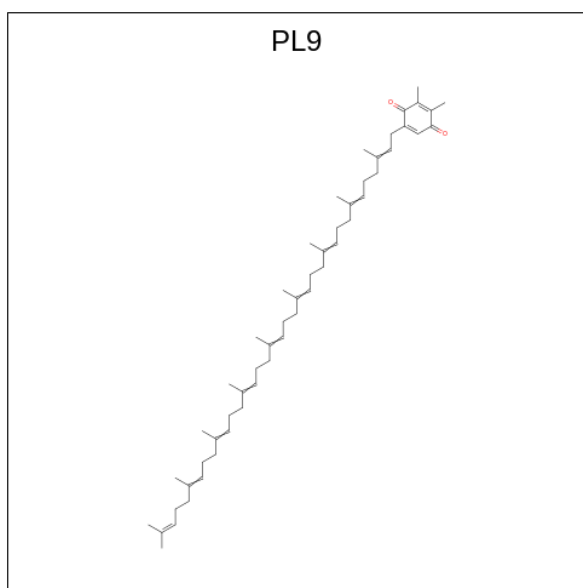
- Molecule 28 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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:).

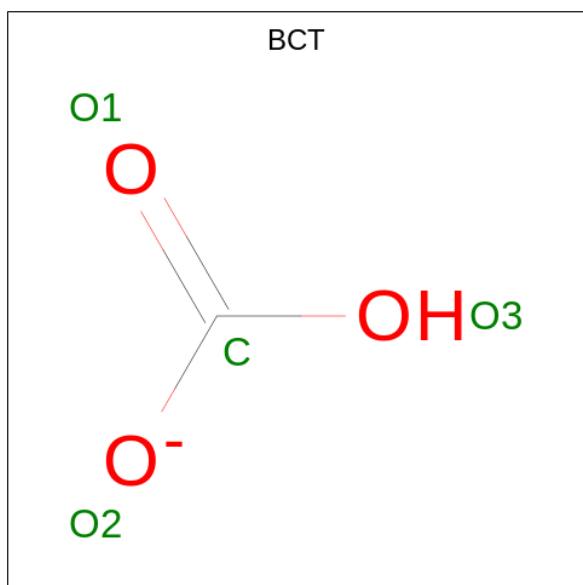
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			28	23	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	I	1	Total	C	O	0	0
			40	35	5		
30	J	1	Total	C		0	0
			10	10			
30	K	1	Total	C	O	0	1
			68	58	10		
30	X	1	Total	C	O	0	0
			18	16	2		

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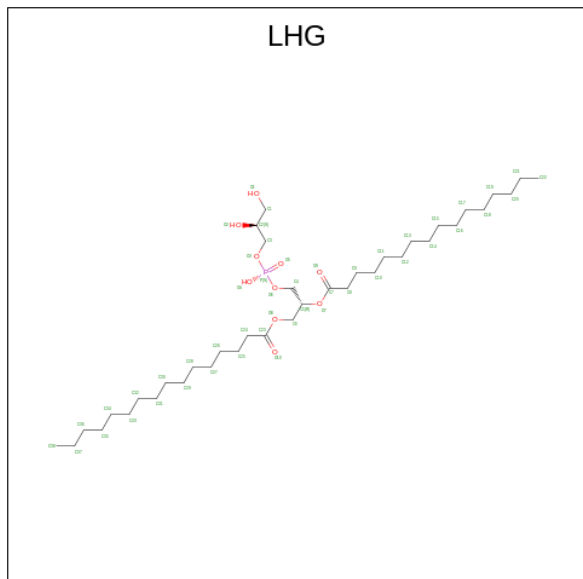
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	a	1	Total	C	O	0	0
			30	25	5		
30	b	2	Total	C	O	0	0
			69	59	10		
30	c	1	Total	C	O	0	1
			64	54	10		
30	d	1	Total	C	O	0	0
			17	16	1		
30	i	1	Total	C	O	0	0
			40	35	5		
30	j	1	Total	C		0	0
			10	10			
30	l	1	Total	C		0	0
			10	10			
30	m	1	Total	C		0	0
			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).



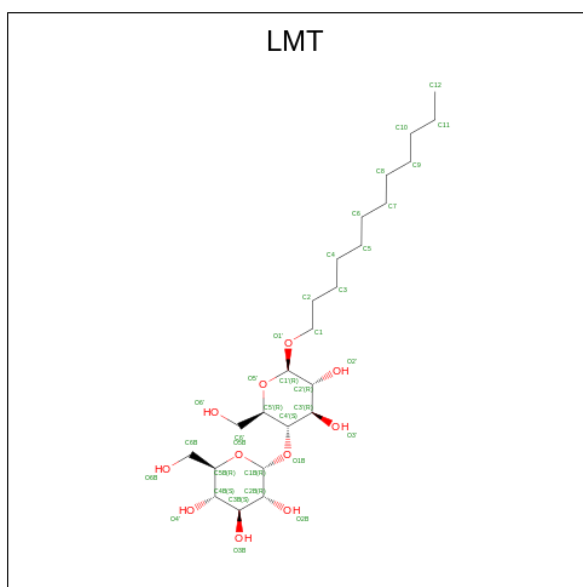
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	1
			8	2	6		
31	d	1	Total	C	O	0	1
			8	2	6		

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



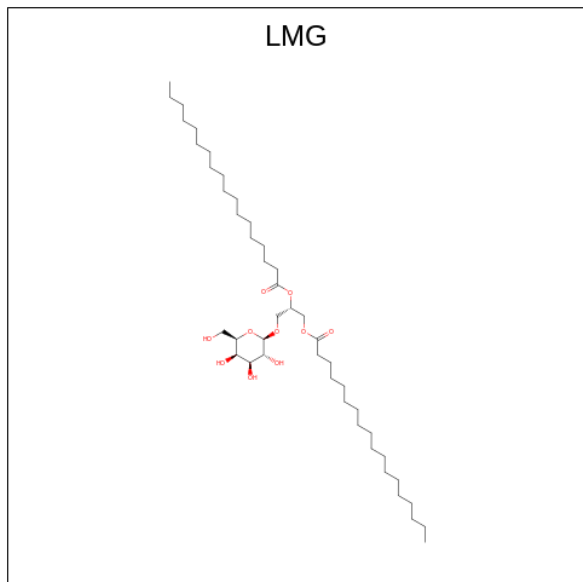
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
32	A	1	98	76	20	2	0	1
32	D	1	98	76	20	2	0	1
32	D	1	98	76	20	2	0	1
32	E	1	84	62	20	2	0	1
32	L	1	98	76	20	2	0	1
32	a	1	84	62	20	2	0	1
32	b	1	98	76	20	2	0	1
32	d	1	98	76	20	2	0	1
32	d	1	98	76	20	2	0	1
32	d	1	98	76	20	2	0	1

- Molecule 33 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



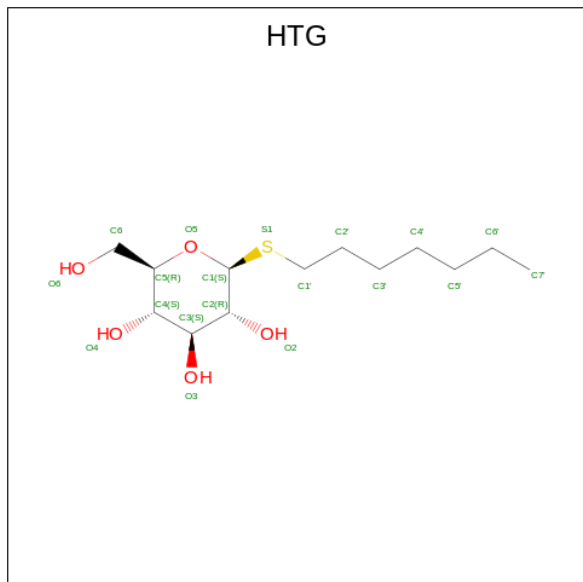
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	A	1	Total	C	O	0	0
			35	24	11		
33	B	1	Total	C	O	0	0
			35	24	11		
33	B	1	Total	C	O	0	0
			35	24	11		
33	B	1	Total	C	O	0	0
			25	19	6		
33	D	1	Total	C	O	0	0
			35	24	11		
33	F	1	Total	C	O	0	0
			35	24	11		
33	M	1	Total	C	O	0	0
			35	24	11		
33	T	1	Total	C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

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



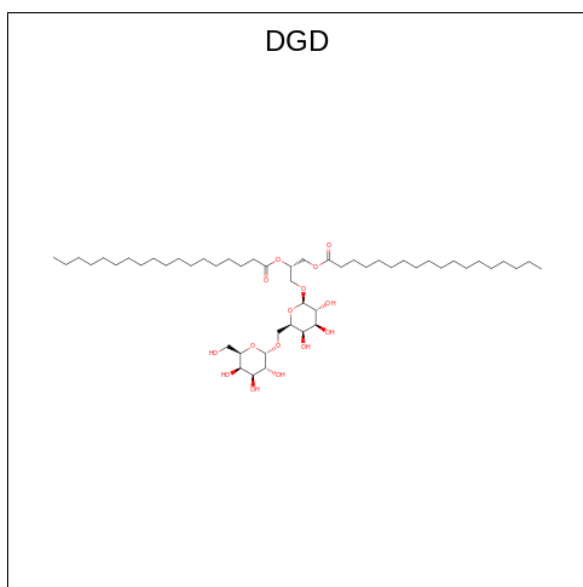
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	B	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	D	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		
34	d	1	Total	C	O	0	0
			51	41	10		
34	m	1	Total	C	O	0	0
			51	41	10		
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: $C_{13}H_{26}O_5S$).



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

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



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

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

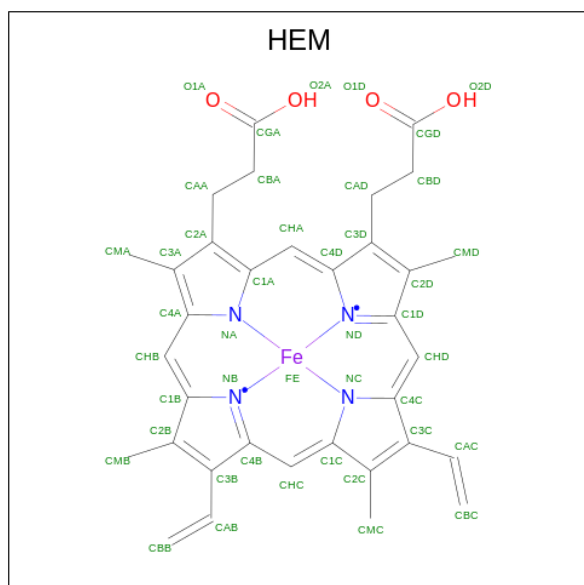
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	C	1	Total	Ca	0	0
			1	1		
37	F	1	Total	Ca	0	0
			1	1		
37	O	1	Total	Ca	0	0
			1	1		
37	c	2	Total	Ca	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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: $C_{34}H_{32}FeN_4O_4$).

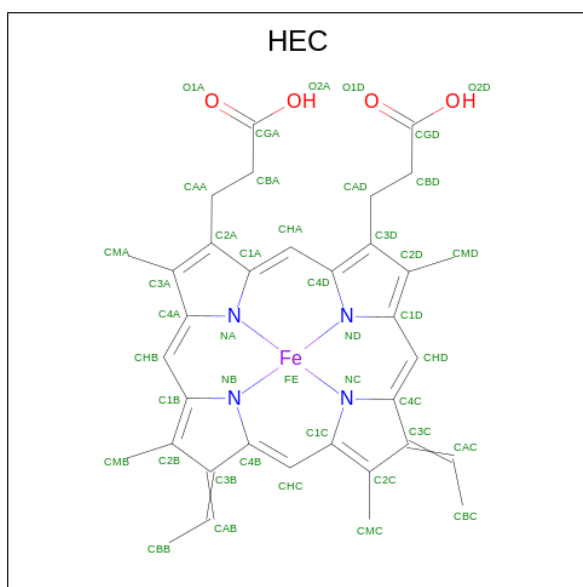


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	F	1	Total C Fe N O 43 34 1 4 4	0	0
38	f	1	Total C Fe N O 43 34 1 4 4	0	0

- 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
39	j	1	Total Mg 1 1	0	0

- Molecule 40 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	136	Total	O	0	85
			220	220		
41	B	187	Total	O	0	2
			189	189		
41	C	169	Total	O	0	38
			206	206		
41	D	122	Total	O	0	34
			156	156		
41	E	17	Total	O	0	0
			17	17		
41	F	5	Total	O	0	0
			5	5		
41	H	22	Total	O	0	0
			22	22		
41	I	5	Total	O	0	0
			5	5		
41	J	7	Total	O	0	0
			7	7		
41	K	5	Total	O	0	0
			5	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	L	9	Total O 10 10	0	1
41	M	6	Total O 6 6	0	0
41	O	104	Total O 109 109	0	5
41	T	10	Total O 13 13	0	3
41	U	46	Total O 49 49	0	3
41	V	82	Total O 83 83	0	1
41	X	8	Total O 8 8	0	0
41	a	130	Total O 211 211	0	82
41	b	200	Total O 203 203	0	3
41	c	160	Total O 193 193	0	34
41	d	115	Total O 146 146	0	31
41	e	9	Total O 9 9	0	0
41	f	3	Total O 3 3	0	0
41	h	17	Total O 17 17	0	0
41	i	2	Total O 2 2	0	0
41	j	1	Total O 1 1	0	0
41	k	3	Total O 3 3	0	0
41	l	8	Total O 10 10	0	2
41	m	12	Total O 12 12	0	0
41	o	100	Total O 104 104	0	4
41	t	7	Total O 10 10	0	3

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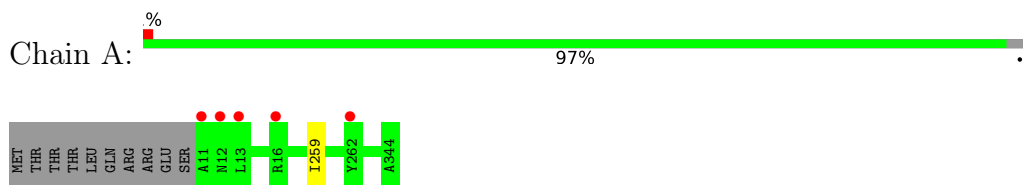
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	u	50	Total O 51 51	0	1
41	v	58	Total O 60 60	0	2
41	x	8	Total O 8 8	0	0
41	y	2	Total O 2 2	0	0

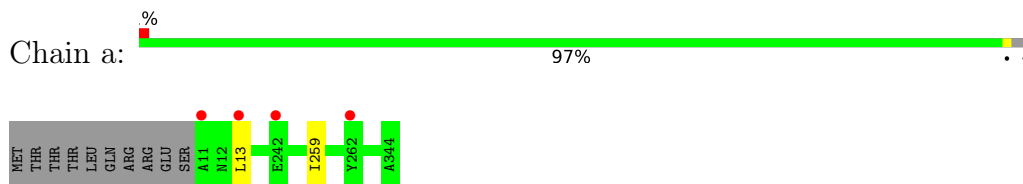
3 Residue-property plots [i](#)

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.

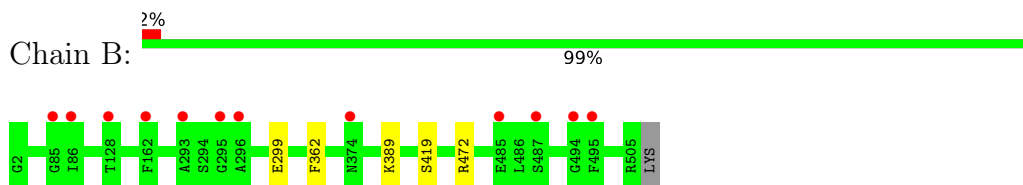
- Molecule 1: Photosystem II protein D1



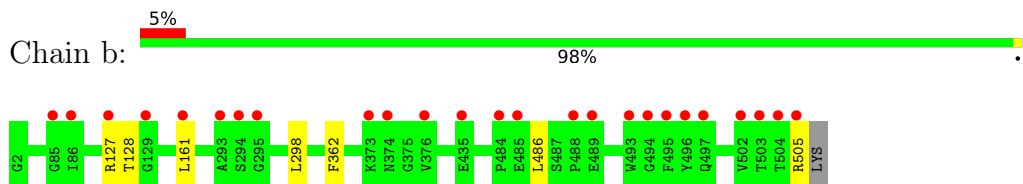
- Molecule 1: Photosystem II protein D1



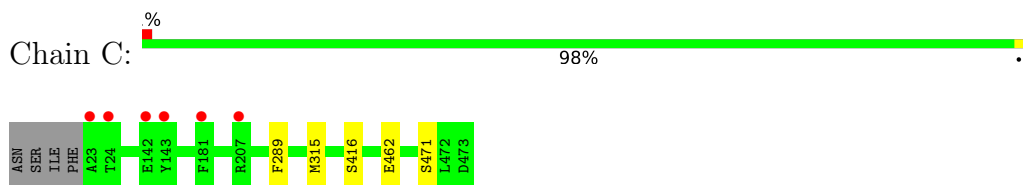
- Molecule 2: Photosystem II CP47 reaction center protein



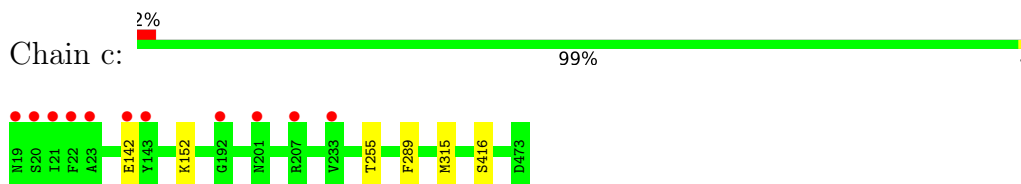
- Molecule 2: Photosystem II CP47 reaction center protein



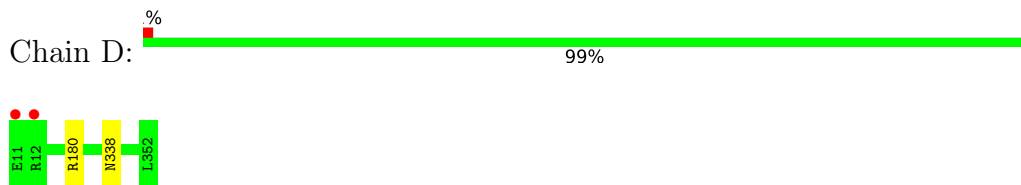
- Molecule 3: Photosystem II CP43 reaction center protein



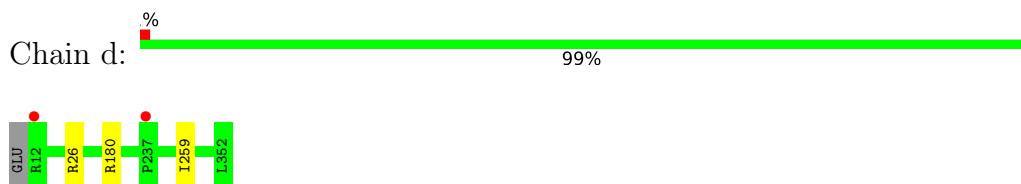
- Molecule 3: Photosystem II CP43 reaction center protein



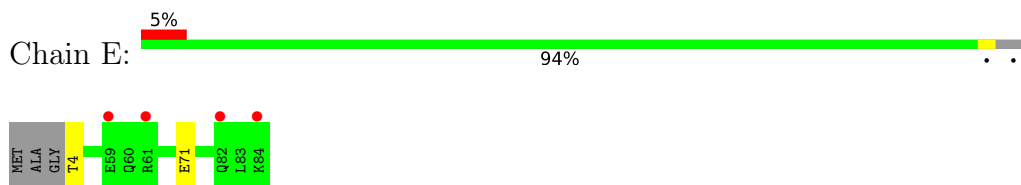
• Molecule 4: Photosystem II D2 protein



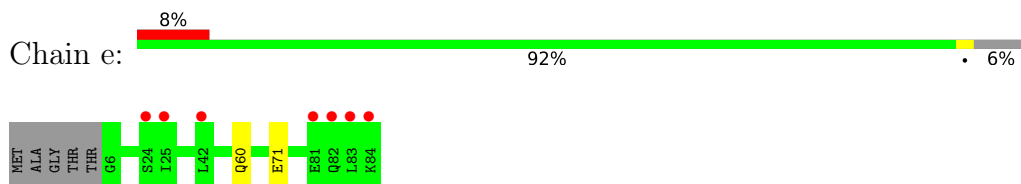
• Molecule 4: Photosystem II D2 protein



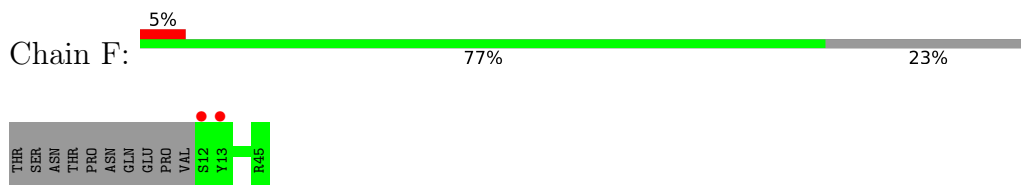
• Molecule 5: Cytochrome b559 subunit alpha



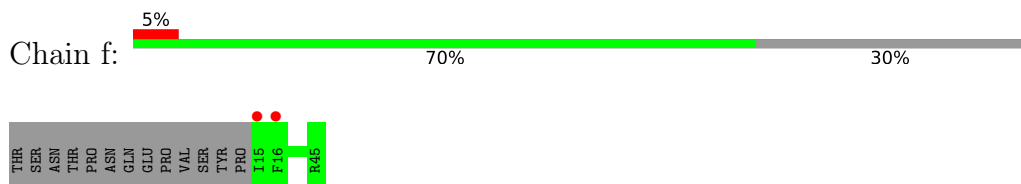
• Molecule 5: Cytochrome b559 subunit alpha



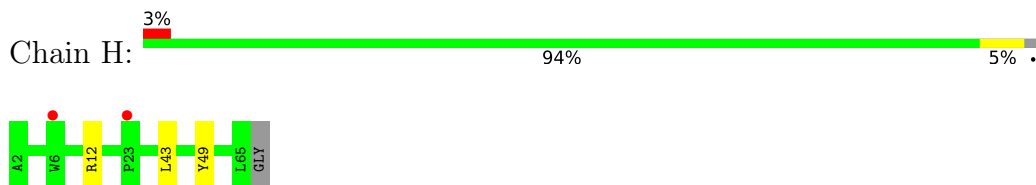
• Molecule 6: Cytochrome b559 subunit beta



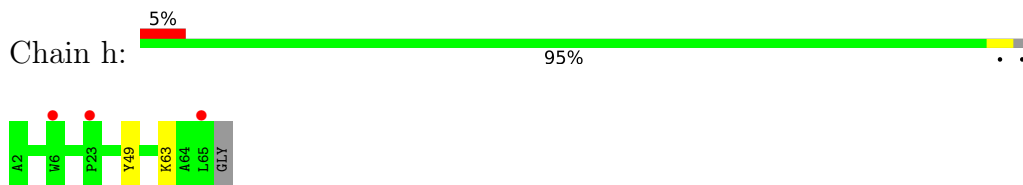
• Molecule 6: Cytochrome b559 subunit beta



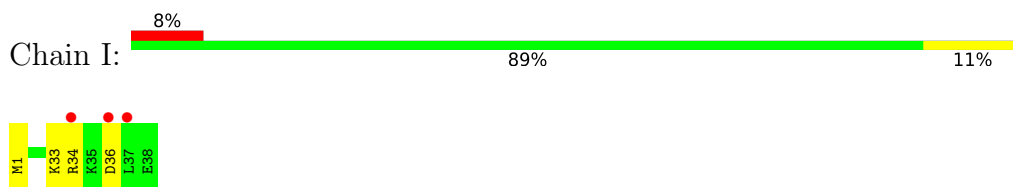
- Molecule 7: Photosystem II reaction center protein H



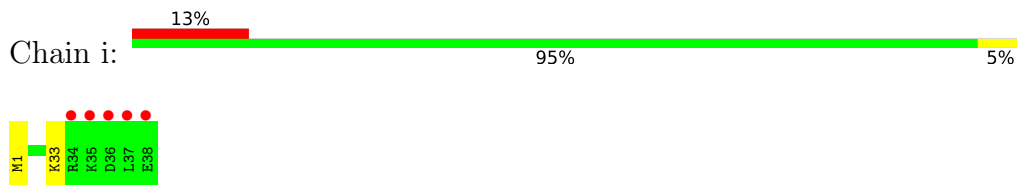
- Molecule 7: Photosystem II reaction center protein H



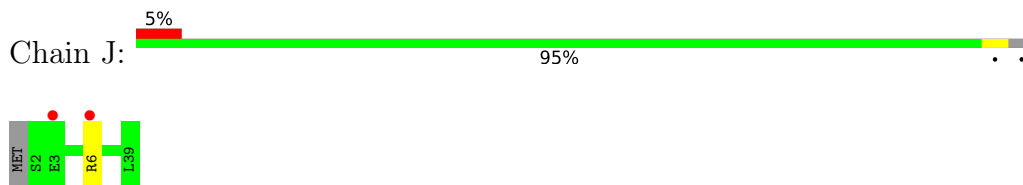
- Molecule 8: Photosystem II reaction center protein I



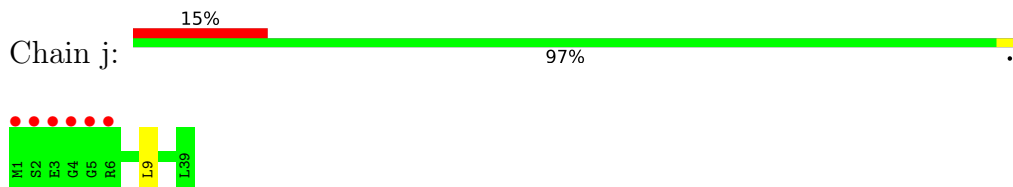
- Molecule 8: Photosystem II reaction center protein I



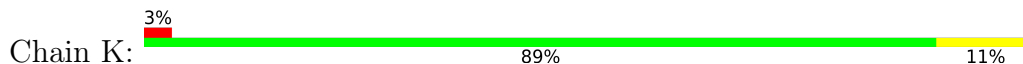
- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J

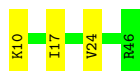


- Molecule 10: Photosystem II reaction center protein K

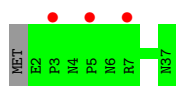




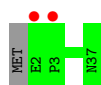
- Molecule 10: Photosystem II reaction center protein K



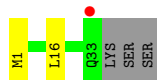
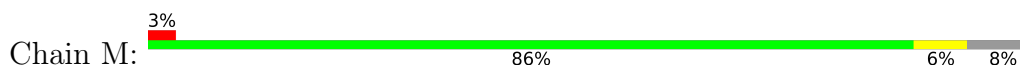
- Molecule 11: Photosystem II reaction center protein L



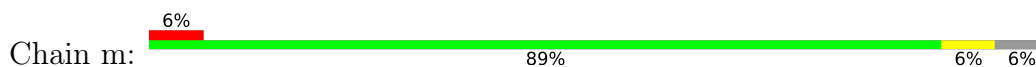
- Molecule 11: Photosystem II reaction center protein L



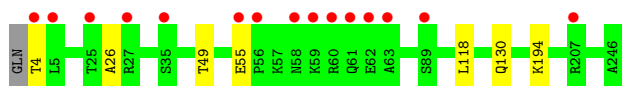
- Molecule 12: Photosystem II reaction center protein M



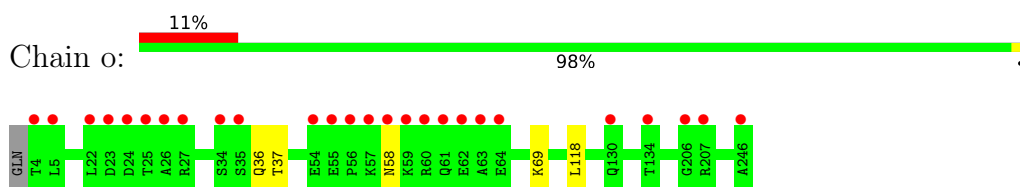
- Molecule 12: Photosystem II reaction center protein M



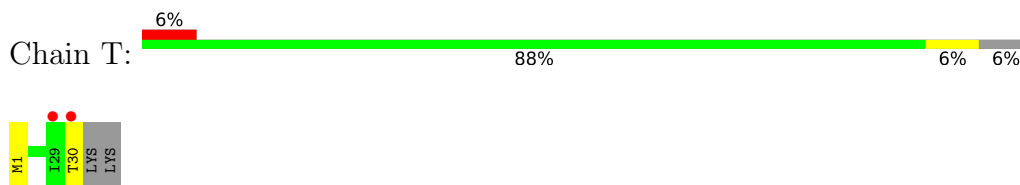
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



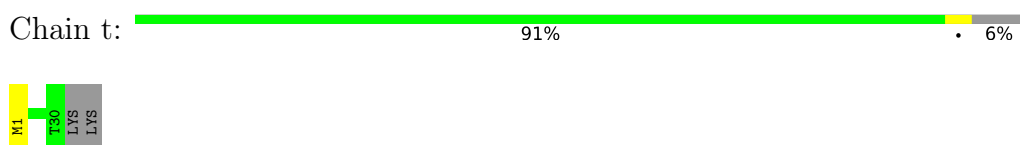
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



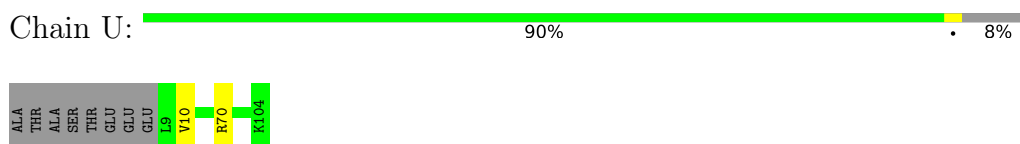
- Molecule 14: Photosystem II reaction center protein T



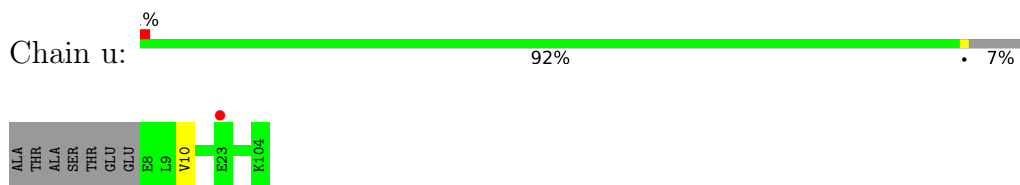
- Molecule 14: Photosystem II reaction center protein T



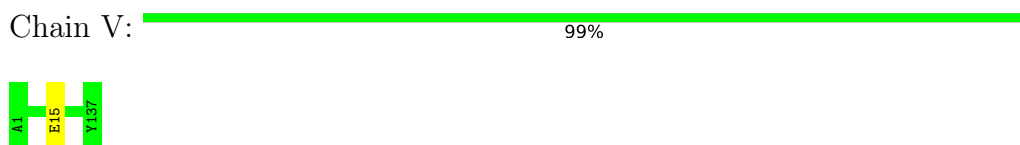
- Molecule 15: Photosystem II 12 kDa extrinsic protein



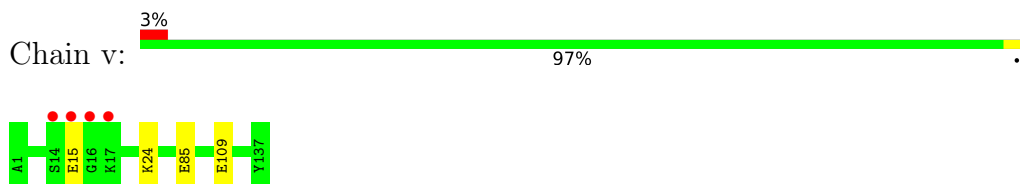
- Molecule 15: Photosystem II 12 kDa extrinsic protein



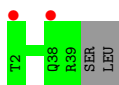
- Molecule 16: Cytochrome c-550



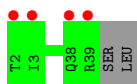
- Molecule 16: Cytochrome c-550



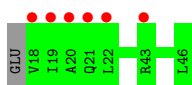
- Molecule 17: Photosystem II reaction center protein X



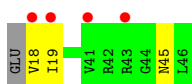
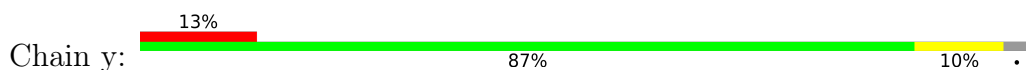
- Molecule 17: Photosystem II reaction center protein X



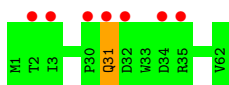
- Molecule 18: Photosystem II reaction center protein Ycf12



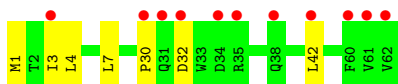
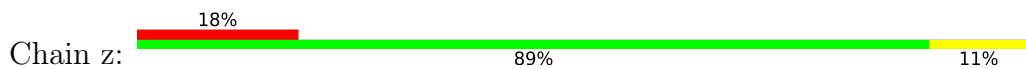
- Molecule 18: Photosystem II reaction center protein Ycf12



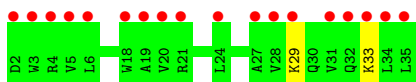
- Molecule 19: Photosystem II reaction center protein Z



- 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 – 2.20 19.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.98-2.20) 99.9 (19.98-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.19Å)	Xtrriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.140 , 0.176 0.152 , 0.181	Depositor DCC
R_{free} test set	21144 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	50.0	Xtrriage
Anisotropy	0.485	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 81.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	62674	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% 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: CL, HEC, LMT, DGD, MG, HEM, OEX, PHO, PL9, UNL, HTG, FME, SQD, FE2, BCT, LHG, GOL, LMG, CA, BCR, CLA

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	0.42	0/4478	0.58	0/6098
1	a	0.42	0/4457	0.56	0/6069
2	B	0.43	0/4314	0.58	0/5879
2	b	0.41	0/4285	0.57	0/5841
3	C	0.40	0/4416	0.55	0/6013
3	c	0.40	0/4467	0.54	0/6082
4	D	0.46	0/3746	0.59	0/5102
4	d	0.44	0/3780	0.57	0/5147
5	E	0.39	0/681	0.57	0/928
5	e	0.38	0/690	0.54	0/939
6	F	0.41	0/284	0.53	0/387
6	f	0.35	0/269	0.50	0/365
7	H	0.39	0/519	0.60	0/708
7	h	0.37	0/530	0.57	0/722
8	I	0.35	0/311	0.53	0/419
8	i	0.40	0/311	0.55	0/419
9	J	0.38	0/278	0.51	0/376
9	j	0.36	0/283	0.52	0/383
10	K	0.39	0/303	0.53	0/416
10	k	0.37	0/303	0.50	0/416
11	L	0.40	0/318	0.57	0/433
11	l	0.43	0/318	0.54	0/433
12	M	0.43	0/261	0.51	0/357
12	m	0.38	0/279	0.49	0/380
13	O	0.41	0/1991	0.64	0/2698
13	o	0.40	0/1966	0.63	0/2665
14	T	0.46	0/310	0.61	0/419
14	t	0.46	0/301	0.58	0/406
15	U	0.43	0/811	0.62	0/1095
15	u	0.44	0/826	0.61	0/1116
16	V	0.40	0/1142	0.58	0/1545

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.36	0/1139	0.55	0/1542
17	X	0.33	0/292	0.49	0/395
17	x	0.33	0/284	0.48	0/384
18	Y	0.32	0/216	0.52	0/289
18	y	0.30	0/216	0.50	0/289
19	Z	0.32	0/490	0.44	0/669
19	z	0.32	0/490	0.42	0/669
20	R	0.31	0/279	0.53	0/383
All	All	0.41	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%)	544 (98%)	7 (1%)	2 (0%)	34	37
1	a	551/344 (160%)	541 (98%)	8 (2%)	2 (0%)	34	37
2	B	524/505 (104%)	518 (99%)	6 (1%)	0	100	100
2	b	521/505 (103%)	509 (98%)	12 (2%)	0	100	100
3	C	548/455 (120%)	540 (98%)	7 (1%)	1 (0%)	47	55
3	c	554/455 (122%)	544 (98%)	9 (2%)	1 (0%)	47	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	454/342 (133%)	438 (96%)	16 (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%)	62 (100%)	0	0	100	100
7	h	63/65 (97%)	60 (95%)	2 (3%)	1 (2%)	9	7
8	I	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	5	2
8	i	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
9	J	36/39 (92%)	36 (100%)	0	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%)	8 (3%)	1 (0%)	34	37
13	o	249/244 (102%)	244 (98%)	5 (2%)	0	100	100
14	T	33/32 (103%)	33 (100%)	0	0	100	100
14	t	32/32 (100%)	32 (100%)	0	0	100	100
15	U	97/104 (93%)	92 (95%)	5 (5%)	0	100	100
15	u	99/104 (95%)	95 (96%)	4 (4%)	0	100	100
16	V	140/137 (102%)	136 (97%)	4 (3%)	0	100	100
16	v	140/137 (102%)	135 (96%)	5 (4%)	0	100	100
17	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
17	x	36/40 (90%)	36 (100%)	0	0	100	100
18	Y	27/30 (90%)	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	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	9	6
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	6180/5384 (115%)	6047 (98%)	122 (2%)	11 (0%)	47	55

All (11) 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
1	A	259[A]	ILE
1	A	259[B]	ILE
1	a	259[A]	ILE
1	a	259[B]	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	444/279 (159%)	444 (100%)	0	100	100
1	a	442/279 (158%)	441 (100%)	1 (0%)	93	97
2	B	423/403 (105%)	418 (99%)	5 (1%)	71	83
2	b	420/403 (104%)	412 (98%)	8 (2%)	57	71
3	C	431/356 (121%)	426 (99%)	5 (1%)	71	83
3	c	437/356 (123%)	431 (99%)	6 (1%)	67	80
4	D	368/277 (133%)	366 (100%)	2 (0%)	88	94
4	d	372/277 (134%)	368 (99%)	4 (1%)	73	85
5	E	72/73 (99%)	70 (97%)	2 (3%)	43	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	72/73 (99%)	70 (97%)	2 (3%)	43	56
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	26/38 (68%)	26 (100%)	0	100	100
7	H	54/54 (100%)	51 (94%)	3 (6%)	21	25
7	h	55/54 (102%)	54 (98%)	1 (2%)	59	72
8	I	34/34 (100%)	32 (94%)	2 (6%)	19	23
8	i	34/34 (100%)	33 (97%)	1 (3%)	42	54
9	J	26/27 (96%)	25 (96%)	1 (4%)	33	42
9	j	26/27 (96%)	25 (96%)	1 (4%)	33	42
10	K	30/30 (100%)	26 (87%)	4 (13%)	4	3
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	7
11	L	36/35 (103%)	36 (100%)	0	100	100
11	l	36/35 (103%)	36 (100%)	0	100	100
12	M	30/32 (94%)	28 (93%)	2 (7%)	16	18
12	m	32/32 (100%)	30 (94%)	2 (6%)	18	20
13	O	216/207 (104%)	210 (97%)	6 (3%)	43	56
13	o	213/207 (103%)	208 (98%)	5 (2%)	50	63
14	T	32/28 (114%)	30 (94%)	2 (6%)	18	20
14	t	31/28 (111%)	31 (100%)	0	100	100
15	U	86/89 (97%)	84 (98%)	2 (2%)	50	63
15	u	88/89 (99%)	86 (98%)	2 (2%)	50	63
16	V	123/117 (105%)	122 (99%)	1 (1%)	81	90
16	v	123/117 (105%)	119 (97%)	4 (3%)	38	49
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	71
19	z	52/52 (100%)	46 (88%)	6 (12%)	5	5
20	R	29/29 (100%)	27 (93%)	2 (7%)	15	16
All	All	5110/4403 (116%)	5021 (98%)	89 (2%)	57	74

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

Mol	Chain	Res	Type
2	B	299	GLU
2	B	362	PHE
2	B	389	LYS
2	B	419	SER
2	B	472	ARG
3	C	289	PHE
3	C	315[A]	MET
3	C	315[B]	MET
3	C	462	GLU
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	4	THR
13	O	49	THR
13	O	55	GLU
13	O	118	LEU
13	O	130	GLN
13	O	194	LYS
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
2	b	127	ARG
2	b	128	THR
2	b	161	LEU
2	b	298	LEU

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Mol	Chain	Res	Type
2	b	362	PHE
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	36	GLN
13	o	37	THR
13	o	58	ASN
13	o	69	LYS
13	o	118	LEU
15	u	10[A]	VAL
15	u	10[B]	VAL
16	v	15	GLU
16	v	24	LYS
16	v	85	GLU
16	v	109	GLU
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

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Mol	Chain	Res	Type
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
4	D	61	HIS
5	E	60	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	0.63	0	7,9,11	1.62	2 (28%)
14	FME	t	1	14	8,9,10	0.65	0	7,9,11	1.47	2 (28%)
8	FME	i	1	8	8,9,10	0.70	0	7,9,11	1.20	1 (14%)
12	FME	M	1	12	8,9,10	0.57	0	7,9,11	1.33	1 (14%)
8	FME	I	1	8	8,9,10	0.58	0	7,9,11	1.20	1 (14%)
12	FME	m	1	12	8,9,10	0.52	0	7,9,11	1.52	2 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	m	1	FME	CA-N-CN	-2.62	118.80	122.82
14	T	1	FME	CA-N-CN	2.49	126.66	122.82
14	t	1	FME	O-C-CA	-2.39	118.50	124.78
14	T	1	FME	CG-CB-CA	2.39	119.59	112.95
14	t	1	FME	CA-N-CN	-2.38	119.17	122.82
12	m	1	FME	O1-CN-N	-2.30	119.20	125.27
12	M	1	FME	O-C-CA	-2.25	118.89	124.78
8	I	1	FME	O-C-CA	-2.20	119.00	124.78
8	i	1	FME	O-C-CA	-2.08	119.33	124.78

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

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
24	PHO	a	407[B]	-	51,69,69	1.85	8 (15%)	47,99,99	1.81	11 (23%)
27	GOL	v	202[A]	-	5,5,5	1.27	0	5,5,5	0.72	0
23	CLA	c	503	-	65,73,73	2.02	14 (21%)	76,113,113	2.65	26 (34%)
23	CLA	B	609	-	65,73,73	1.99	16 (24%)	76,113,113	2.76	26 (34%)
40	HEC	V	201	16	32,50,50	1.95	4 (12%)	24,82,82	2.25	7 (29%)
23	CLA	C	502	-	65,73,73	1.98	16 (24%)	76,113,113	2.81	30 (39%)
23	CLA	c	509	-	65,73,73	2.15	16 (24%)	76,113,113	2.72	27 (35%)
25	BCR	c	515	-	41,41,41	0.98	1 (2%)	56,56,56	1.64	11 (19%)
28	OEX	A	413[B]	41,1,3	0,15,15	-	-	-	-	-
29	PL9	d	405[A]	-	55,55,55	0.65	1 (1%)	68,69,69	1.63	17 (25%)
32	LHG	L	102[B]	-	48,48,48	0.92	2 (4%)	51,54,54	1.08	2 (3%)
23	CLA	b	605	-	65,73,73	1.94	15 (23%)	76,113,113	2.94	27 (35%)
36	DGD	c	519	-	63,63,67	0.88	4 (6%)	77,77,81	1.02	5 (6%)
28	OEX	A	413[A]	41,1,3	0,15,15	-	-	-	-	-
24	PHO	A	407[B]	-	51,69,69	1.75	7 (13%)	47,99,99	1.82	12 (25%)
23	CLA	A	406[A]	41	65,73,73	1.96	16 (24%)	76,113,113	2.81	29 (38%)
32	LHG	b	630[A]	-	48,48,48	0.85	3 (6%)	51,54,54	1.03	4 (7%)
34	LMG	C	501	-	51,51,55	0.92	2 (3%)	59,59,63	1.44	7 (11%)
23	CLA	d	402[B]	-	65,73,73	2.02	16 (24%)	76,113,113	2.83	29 (38%)
36	DGD	C	517[B]	-	63,63,67	0.85	2 (3%)	77,77,81	1.09	7 (9%)
28	OEX	a	412[B]	41,1,3	0,15,15	-	-	-	-	-
35	HTG	d	409	-	16,16,19	1.01	1 (6%)	20,21,24	1.60	2 (10%)
25	BCR	B	618	-	41,41,41	0.97	1 (2%)	56,56,56	1.37	9 (16%)
23	CLA	C	513	-	65,73,73	2.06	15 (23%)	76,113,113	2.75	32 (42%)
27	GOL	l	102[A]	-	5,5,5	0.96	0	5,5,5	0.97	0
23	CLA	B	607	41	65,73,73	1.99	18 (27%)	76,113,113	2.83	28 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	608	-	65,73,73	1.96	14 (21%)	76,113,113	2.84	33 (43%)
23	CLA	D	402[B]	-	65,73,73	2.07	16 (24%)	76,113,113	2.85	29 (38%)
26	SQD	a	410[B]	-	53,54,54	0.97	3 (5%)	62,65,65	1.64	11 (17%)
23	CLA	b	613	-	65,73,73	1.97	14 (21%)	76,113,113	2.74	28 (36%)
27	GOL	b	624	-	5,5,5	1.12	1 (20%)	5,5,5	0.79	0
26	SQD	F	103	-	42,43,54	1.19	4 (9%)	51,54,65	2.14	14 (27%)
35	HTG	b	622	-	19,19,19	1.15	2 (10%)	23,24,24	1.94	7 (30%)
23	CLA	D	402[A]	-	65,73,73	1.99	16 (24%)	76,113,113	2.87	29 (38%)
26	SQD	b	620	-	53,54,54	1.05	3 (5%)	62,65,65	1.69	12 (19%)
31	BCT	A	416[A]	21	2,3,3	0.54	0	2,3,3	1.81	1 (50%)
32	LHG	D	407[B]	-	48,48,48	0.91	2 (4%)	51,54,54	1.00	3 (5%)
25	BCR	C	515	-	41,41,41	1.04	1 (2%)	56,56,56	1.42	8 (14%)
33	LMT	M	101	-	36,36,36	1.10	3 (8%)	47,47,47	1.17	4 (8%)
36	DGD	H	102	-	63,63,67	0.86	4 (6%)	77,77,81	1.03	6 (7%)
26	SQD	A	410[B]	-	53,54,54	0.93	3 (5%)	62,65,65	1.77	11 (17%)
32	LHG	d	407[B]	-	48,48,48	0.91	2 (4%)	51,54,54	1.03	3 (5%)
34	LMG	c	501	-	51,51,55	0.91	2 (3%)	59,59,63	1.23	6 (10%)
27	GOL	D	412	-	5,5,5	1.42	2 (40%)	5,5,5	0.89	0
33	LMT	D	401	-	36,36,36	0.93	2 (5%)	47,47,47	1.07	2 (4%)
23	CLA	C	514	-	65,73,73	2.05	15 (23%)	76,113,113	2.72	28 (36%)
27	GOL	a	418	-	5,5,5	1.31	1 (20%)	5,5,5	0.85	0
32	LHG	D	406[B]	-	48,48,48	0.85	2 (4%)	51,54,54	0.99	3 (5%)
33	LMT	B	626	-	36,36,36	1.18	4 (11%)	47,47,47	1.38	5 (10%)
27	GOL	O	303	-	5,5,5	1.00	0	5,5,5	1.07	1 (20%)
25	BCR	h	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.43	11 (19%)
32	LHG	D	406[A]	-	48,48,48	0.86	2 (4%)	51,54,54	0.99	3 (5%)
34	LMG	Z	101	-	37,37,55	1.01	2 (5%)	45,45,63	1.48	6 (13%)
25	BCR	C	516	-	41,41,41	1.03	1 (2%)	56,56,56	1.29	6 (10%)
29	PL9	a	413[B]	-	55,55,55	0.64	2 (3%)	68,69,69	1.90	22 (32%)
23	CLA	B	603	-	65,73,73	2.03	16 (24%)	76,113,113	2.87	28 (36%)
27	GOL	B	625	-	5,5,5	1.01	0	5,5,5	0.95	0
31	BCT	d	401[B]	21	2,3,3	0.60	0	2,3,3	1.27	0
23	CLA	b	602	-	65,73,73	2.05	16 (24%)	76,113,113	2.87	33 (43%)
23	CLA	B	605	-	65,73,73	1.98	16 (24%)	76,113,113	2.92	27 (35%)
23	CLA	b	611	-	65,73,73	1.96	17 (26%)	76,113,113	2.86	26 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	511	-	65,73,73	2.01	16 (24%)	76,113,113	2.81	31 (40%)
23	CLA	b	616	-	65,73,73	2.02	15 (23%)	76,113,113	2.85	27 (35%)
27	GOL	A	418	-	5,5,5	1.42	1 (20%)	5,5,5	0.96	1 (20%)
32	LHG	A	419[B]	-	48,48,48	0.86	2 (4%)	51,54,54	1.19	5 (9%)
36	DGD	c	517[A]	-	63,63,67	0.85	2 (3%)	77,77,81	1.12	6 (7%)
32	LHG	D	407[A]	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	4 (7%)
23	CLA	c	502	-	65,73,73	1.97	16 (24%)	76,113,113	2.75	27 (35%)
24	PHO	a	407[A]	-	51,69,69	1.83	8 (15%)	47,99,99	1.71	10 (21%)
32	LHG	E	101[B]	-	41,41,48	1.05	2 (4%)	44,47,54	1.10	4 (9%)
25	BCR	A	409	-	41,41,41	0.98	1 (2%)	56,56,56	1.43	9 (16%)
25	BCR	c	516	-	41,41,41	1.02	1 (2%)	56,56,56	1.40	11 (19%)
27	GOL	o	304	-	5,5,5	0.97	0	5,5,5	1.10	0
23	CLA	b	603	-	65,73,73	2.05	16 (24%)	76,113,113	2.86	33 (43%)
29	PL9	D	405[B]	-	55,55,55	0.63	2 (3%)	68,69,69	1.67	17 (25%)
32	LHG	L	102[A]	-	48,48,48	0.89	2 (4%)	51,54,54	1.15	3 (5%)
24	PHO	A	407[A]	-	51,69,69	1.78	8 (15%)	47,99,99	1.77	11 (23%)
23	CLA	c	514	-	65,73,73	2.10	17 (26%)	76,113,113	2.79	29 (38%)
23	CLA	c	507	-	65,73,73	2.04	16 (24%)	76,113,113	2.76	28 (36%)
27	GOL	B	627	-	5,5,5	0.97	0	5,5,5	1.01	0
25	BCR	k	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.50	11 (19%)
23	CLA	d	402[A]	-	65,73,73	1.94	17 (26%)	76,113,113	2.79	29 (38%)
32	LHG	a	419[B]	-	41,41,48	1.03	2 (4%)	44,47,54	0.94	2 (4%)
28	OEX	a	412[A]	41,1,3	0,15,15	-	-	-	-	-
36	DGD	C	517[A]	-	63,63,67	0.81	2 (3%)	77,77,81	1.21	8 (10%)
23	CLA	C	504	-	65,73,73	1.98	16 (24%)	76,113,113	2.81	27 (35%)
27	GOL	A	411	-	5,5,5	1.11	0	5,5,5	0.80	0
33	LMT	b	627	-	25,25,36	0.87	0	30,30,47	1.12	3 (10%)
36	DGD	C	519	-	63,63,67	0.89	3 (4%)	77,77,81	1.00	4 (5%)
23	CLA	C	511	-	65,73,73	2.03	17 (26%)	76,113,113	2.91	29 (38%)
38	HEM	f	101	6,5	41,50,50	1.30	5 (12%)	45,82,82	1.84	10 (22%)
26	SQD	a	410[A]	-	53,54,54	0.95	3 (5%)	62,65,65	1.77	13 (20%)
25	BCR	B	619	-	41,41,41	1.06	1 (2%)	56,56,56	1.32	7 (12%)
23	CLA	c	512	3	65,73,73	2.10	17 (26%)	76,113,113	2.84	29 (38%)
27	GOL	d	411	-	5,5,5	0.98	0	5,5,5	1.10	0
23	CLA	b	607	41	65,73,73	1.99	17 (26%)	76,113,113	2.72	27 (35%)
34	LMG	C	521	-	51,51,55	1.06	3 (5%)	59,59,63	1.34	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	a	406[B]	41	65,73,73	2.00	15 (23%)	76,113,113	2.84	27 (35%)
27	GOL	c	526[B]	-	5,5,5	1.02	0	5,5,5	0.91	0
27	GOL	o	303	-	5,5,5	0.97	0	5,5,5	0.97	0
35	HTG	D	410	-	16,16,19	1.04	1 (6%)	20,21,24	1.59	1 (5%)
33	LMT	a	416	-	36,36,36	1.00	1 (2%)	47,47,47	1.01	1 (2%)
23	CLA	A	404[B]	-	65,73,73	2.09	16 (24%)	76,113,113	2.81	30 (39%)
25	BCR	H	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.44	7 (12%)
26	SQD	A	410[A]	-	53,54,54	0.93	3 (5%)	62,65,65	1.81	10 (16%)
23	CLA	D	403	-	65,73,73	2.07	16 (24%)	76,113,113	2.77	29 (38%)
32	LHG	d	407[A]	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	3 (5%)
32	LHG	d	406[B]	-	48,48,48	0.90	2 (4%)	51,54,54	1.07	4 (7%)
34	LMG	D	411	39	51,51,55	0.82	3 (5%)	59,59,63	1.04	3 (5%)
23	CLA	C	506	-	65,73,73	1.96	16 (24%)	76,113,113	2.73	27 (35%)
23	CLA	C	510	-	65,73,73	2.08	17 (26%)	76,113,113	2.76	28 (36%)
33	LMT	A	420	-	36,36,36	1.03	2 (5%)	47,47,47	1.14	4 (8%)
33	LMT	T	101	-	36,36,36	1.06	3 (8%)	47,47,47	1.06	3 (6%)
36	DGD	C	518[B]	-	63,63,67	0.88	2 (3%)	77,77,81	0.97	4 (5%)
33	LMT	B	629	-	25,25,36	0.89	2 (8%)	30,30,47	1.14	3 (10%)
29	PL9	a	413[A]	-	55,55,55	0.65	2 (3%)	68,69,69	2.00	22 (32%)
34	LMG	d	410	39	51,51,55	0.87	2 (3%)	59,59,63	1.14	5 (8%)
23	CLA	a	404[B]	-	65,73,73	2.03	16 (24%)	76,113,113	2.85	32 (42%)
31	BCT	d	401[A]	21	2,3,3	0.57	0	2,3,3	1.58	1 (50%)
27	GOL	b	628	-	5,5,5	0.31	0	5,5,5	1.43	1 (20%)
27	GOL	c	527	-	5,5,5	1.13	0	5,5,5	0.92	0
36	DGD	C	518[A]	-	63,63,67	0.89	3 (4%)	77,77,81	1.02	5 (6%)
23	CLA	C	512	3	65,73,73	2.06	17 (26%)	76,113,113	2.67	26 (34%)
23	CLA	a	408	-	65,73,73	1.96	15 (23%)	76,113,113	2.91	29 (38%)
32	LHG	A	419[A]	-	48,48,48	0.84	2 (4%)	51,54,54	1.31	6 (11%)
32	LHG	E	101[A]	-	41,41,48	1.06	2 (4%)	44,47,54	1.11	3 (6%)
25	BCR	t	102	-	41,41,41	1.00	1 (2%)	56,56,56	1.67	13 (23%)
27	GOL	V	203[B]	-	5,5,5	1.01	0	5,5,5	0.94	0
23	CLA	A	405[B]	41	65,73,73	2.02	15 (23%)	76,113,113	2.73	29 (38%)
33	LMT	F	101	-	36,36,36	1.08	1 (2%)	47,47,47	1.06	3 (6%)
27	GOL	B	622	-	5,5,5	0.97	0	5,5,5	1.14	1 (20%)
23	CLA	c	513	-	65,73,73	2.07	16 (24%)	76,113,113	2.78	29 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	615	-	65,73,73	1.98	15 (23%)	76,113,113	2.86	26 (34%)
29	PL9	D	405[A]	-	55,55,55	0.62	2 (3%)	68,69,69	1.64	18 (26%)
33	LMT	m	103	-	36,36,36	1.03	2 (5%)	47,47,47	1.08	3 (6%)
23	CLA	c	504	-	65,73,73	2.05	16 (24%)	76,113,113	2.78	25 (32%)
34	LMG	C	520	-	51,51,55	0.92	2 (3%)	59,59,63	1.12	4 (6%)
35	HTG	B	623	-	19,19,19	0.99	2 (10%)	23,24,24	1.13	3 (13%)
35	HTG	B	621	-	19,19,19	0.77	1 (5%)	23,24,24	1.49	1 (4%)
38	HEM	F	102	6,5	41,50,50	1.30	5 (12%)	45,82,82	2.14	13 (28%)
23	CLA	B	604	-	65,73,73	2.01	18 (27%)	76,113,113	2.63	26 (34%)
23	CLA	B	610	41	65,73,73	2.04	17 (26%)	76,113,113	2.83	29 (38%)
23	CLA	C	509	-	65,73,73	2.11	17 (26%)	76,113,113	2.72	25 (32%)
24	PHO	A	417[B]	-	51,69,69	1.86	8 (15%)	47,99,99	1.89	12 (25%)
32	LHG	a	419[A]	-	41,41,48	1.04	2 (4%)	44,47,54	0.92	2 (4%)
25	BCR	B	617	-	41,41,41	1.08	1 (2%)	56,56,56	1.29	4 (7%)
24	PHO	a	415[B]	-	51,69,69	1.89	8 (15%)	47,99,99	1.88	11 (23%)
32	LHG	d	412[B]	-	48,48,48	0.92	2 (4%)	51,54,54	1.08	5 (9%)
24	PHO	A	417[A]	-	51,69,69	1.87	8 (15%)	47,99,99	1.93	12 (25%)
23	CLA	d	403	-	65,73,73	2.03	16 (24%)	76,113,113	2.79	28 (36%)
35	HTG	c	522	-	19,19,19	0.94	1 (5%)	23,24,24	1.64	3 (13%)
24	PHO	a	415[A]	-	51,69,69	1.86	9 (17%)	47,99,99	1.99	13 (27%)
35	HTG	V	202	-	11,11,19	0.31	0	15,15,24	1.01	1 (6%)
23	CLA	b	609	-	65,73,73	2.01	15 (23%)	76,113,113	2.76	28 (36%)
26	SQD	f	102	-	42,43,54	1.18	3 (7%)	51,54,65	1.57	11 (21%)
35	HTG	b	623	-	19,19,19	1.06	1 (5%)	23,24,24	1.88	2 (8%)
29	PL9	A	414[B]	-	55,55,55	0.65	1 (1%)	68,69,69	2.01	25 (36%)
25	BCR	D	404	-	41,41,41	1.13	2 (4%)	56,56,56	1.83	17 (30%)
34	LMG	m	101	-	51,51,55	0.87	2 (3%)	59,59,63	1.29	7 (11%)
27	GOL	v	202[B]	-	5,5,5	1.07	0	5,5,5	0.84	0
23	CLA	C	503	-	65,73,73	2.05	16 (24%)	76,113,113	2.62	25 (32%)
23	CLA	A	408	-	65,73,73	1.99	15 (23%)	76,113,113	2.91	32 (42%)
23	CLA	a	406[A]	41	65,73,73	1.94	16 (24%)	76,113,113	2.81	27 (35%)
23	CLA	b	606	-	65,73,73	1.98	15 (23%)	76,113,113	2.87	28 (36%)
27	GOL	c	526[A]	-	5,5,5	0.94	0	5,5,5	0.95	0
23	CLA	B	613	-	65,73,73	2.04	17 (26%)	76,113,113	2.69	29 (38%)
23	CLA	c	506	-	65,73,73	2.01	15 (23%)	76,113,113	2.68	24 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	A	404[A]	-	65,73,73	2.02	16 (24%)	76,113,113	2.77	32 (42%)
23	CLA	b	614	-	65,73,73	2.00	16 (24%)	76,113,113	2.88	28 (36%)
23	CLA	c	510	-	65,73,73	2.06	14 (21%)	76,113,113	2.78	28 (36%)
23	CLA	C	508	41	65,73,73	1.98	16 (24%)	76,113,113	2.81	26 (34%)
29	PL9	d	405[B]	-	55,55,55	0.66	1 (1%)	68,69,69	1.63	17 (25%)
32	LHG	d	406[A]	-	48,48,48	0.86	2 (4%)	51,54,54	1.08	4 (7%)
34	LMG	z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.05	2 (4%)
23	CLA	A	406[B]	41	65,73,73	2.02	16 (24%)	76,113,113	2.75	28 (36%)
32	LHG	b	630[B]	-	48,48,48	0.87	2 (4%)	51,54,54	1.02	3 (5%)
23	CLA	B	612	-	65,73,73	2.05	19 (29%)	76,113,113	2.84	29 (38%)
23	CLA	a	405[B]	41	65,73,73	2.08	14 (21%)	76,113,113	2.75	29 (38%)
35	HTG	C	522	-	19,19,19	0.89	1 (5%)	23,24,24	1.43	1 (4%)
23	CLA	C	505	41	65,73,73	2.00	17 (26%)	76,113,113	2.82	25 (32%)
27	GOL	a	417	-	5,5,5	1.14	0	5,5,5	1.06	1 (20%)
26	SQD	L	101	-	53,54,54	1.06	4 (7%)	62,65,65	1.75	10 (16%)
27	GOL	l	102[B]	-	5,5,5	0.91	0	5,5,5	0.96	0
35	HTG	o	301	-	19,19,19	1.06	2 (10%)	23,24,24	1.49	4 (17%)
23	CLA	a	405[A]	41	65,73,73	2.00	14 (21%)	76,113,113	2.75	26 (34%)
25	BCR	b	619	-	41,41,41	1.09	1 (2%)	56,56,56	1.35	9 (16%)
23	CLA	B	601	41	65,73,73	2.09	16 (24%)	76,113,113	2.81	28 (36%)
23	CLA	a	404[A]	-	65,73,73	1.99	15 (23%)	76,113,113	2.87	32 (42%)
23	CLA	B	606	-	65,73,73	1.99	17 (26%)	76,113,113	2.90	28 (36%)
23	CLA	b	610	41	65,73,73	2.06	16 (24%)	76,113,113	2.81	30 (39%)
26	SQD	A	412	-	53,54,54	1.02	3 (5%)	62,65,65	1.24	6 (9%)
25	BCR	b	617	-	41,41,41	1.04	1 (2%)	56,56,56	1.37	5 (8%)
33	LMT	t	101	-	26,26,36	0.90	2 (7%)	31,31,47	1.32	3 (9%)
34	LMG	B	620	-	51,51,55	0.92	2 (3%)	59,59,63	1.34	5 (8%)
23	CLA	b	604	-	65,73,73	2.05	17 (26%)	76,113,113	2.71	25 (32%)
40	HEC	v	201	16	32,50,50	2.06	3 (9%)	24,82,82	2.12	6 (25%)
23	CLA	b	612	-	65,73,73	2.02	17 (26%)	76,113,113	2.69	27 (35%)
27	GOL	V	203[A]	-	5,5,5	1.22	0	5,5,5	0.91	0
36	DGD	h	102	-	63,63,67	0.86	3 (4%)	77,77,81	1.11	7 (9%)
23	CLA	b	601	41	65,73,73	2.12	15 (23%)	76,113,113	2.73	26 (34%)
23	CLA	A	405[A]	41	65,73,73	1.90	16 (24%)	76,113,113	2.85	30 (39%)
31	BCT	A	416[B]	21	2,3,3	0.63	0	2,3,3	1.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	GOL	O	302	-	5,5,5	0.87	0	5,5,5	0.90	0
23	CLA	c	508	41	65,73,73	2.03	16 (24%)	76,113,113	2.85	27 (35%)
23	CLA	B	614	-	65,73,73	2.02	17 (26%)	76,113,113	3.00	28 (36%)
23	CLA	b	608	-	65,73,73	2.01	16 (24%)	76,113,113	2.73	30 (39%)
33	LMT	b	621	-	25,25,36	0.95	1 (4%)	30,30,47	1.17	2 (6%)
27	GOL	C	523[B]	-	5,5,5	1.31	0	5,5,5	0.75	0
33	LMT	B	628	-	36,36,36	1.02	3 (8%)	47,47,47	1.15	5 (10%)
36	DGD	c	518[B]	-	63,63,67	0.86	3 (4%)	77,77,81	0.96	5 (6%)
25	BCR	Y	101	-	41,41,41	0.99	1 (2%)	56,56,56	1.73	12 (21%)
33	LMT	e	101	-	36,36,36	1.02	2 (5%)	47,47,47	0.99	1 (2%)
34	LMG	c	520	-	51,51,55	0.90	2 (3%)	59,59,63	1.15	5 (8%)
25	BCR	K	102	-	41,41,41	1.06	1 (2%)	56,56,56	1.43	10 (17%)
27	GOL	C	523[A]	-	5,5,5	1.18	0	5,5,5	0.83	0
26	SQD	a	411	-	53,54,54	1.07	3 (5%)	62,65,65	1.19	8 (12%)
25	BCR	T	102	-	41,41,41	1.00	1 (2%)	56,56,56	1.57	12 (21%)
36	DGD	c	518[A]	-	63,63,67	0.84	2 (3%)	77,77,81	0.97	5 (6%)
35	HTG	b	625	-	19,19,19	1.10	2 (10%)	23,24,24	1.46	4 (17%)
23	CLA	b	615	-	65,73,73	1.98	16 (24%)	76,113,113	2.80	28 (36%)
23	CLA	B	611	-	65,73,73	2.67	17 (26%)	76,113,113	3.18	28 (36%)
32	LHG	d	412[A]	-	48,48,48	0.89	2 (4%)	51,54,54	1.12	4 (7%)
23	CLA	B	602	-	65,73,73	2.03	16 (24%)	76,113,113	2.80	29 (38%)
23	CLA	B	616	-	65,73,73	2.01	16 (24%)	76,113,113	2.85	26 (34%)
25	BCR	a	409	-	41,41,41	1.02	1 (2%)	56,56,56	1.35	7 (12%)
25	BCR	d	404	-	41,41,41	1.11	2 (4%)	56,56,56	1.96	18 (32%)
23	CLA	C	507	-	65,73,73	2.02	18 (27%)	76,113,113	2.74	30 (39%)
23	CLA	c	505	41	65,73,73	2.10	17 (26%)	76,113,113	2.74	27 (35%)
29	PL9	A	414[A]	-	55,55,55	0.68	2 (3%)	68,69,69	2.08	25 (36%)
34	LMG	c	521	-	51,51,55	1.00	2 (3%)	59,59,63	1.37	7 (11%)
25	BCR	y	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.68	13 (23%)
36	DGD	c	517[B]	-	63,63,67	0.86	2 (3%)	77,77,81	1.07	5 (6%)
25	BCR	b	618	-	41,41,41	0.98	1 (2%)	56,56,56	1.31	9 (16%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PHO	a	407[B]	-	-	5/37/103/103	0/5/6/6
27	GOL	v	202[A]	-	-	1/4/4/4	-
23	CLA	c	503	-	1/1/15/20	7/37/115/115	-
23	CLA	B	609	-	1/1/15/20	1/37/115/115	-
40	HEC	V	201	16	-	2/10/54/54	-
23	CLA	C	502	-	1/1/15/20	6/37/115/115	-
23	CLA	c	509	-	1/1/15/20	4/37/115/115	-
25	BCR	c	515	-	-	1/29/63/63	0/2/2/2
29	PL9	d	405[A]	-	-	6/53/73/73	0/1/1/1
32	LHG	L	102[B]	-	-	16/53/53/53	-
23	CLA	b	605	-	1/1/15/20	7/37/115/115	-
36	DGD	c	519	-	-	9/51/91/95	0/2/2/2
24	PHO	A	407[B]	-	-	2/37/103/103	0/5/6/6
23	CLA	A	406[A]	41	-	5/37/115/115	-
32	LHG	b	630[A]	-	-	20/53/53/53	-
34	LMG	C	501	-	-	11/46/66/70	0/1/1/1
23	CLA	d	402[B]	-	1/1/15/20	4/37/115/115	-
36	DGD	C	517[B]	-	-	14/51/91/95	0/2/2/2
35	HTG	d	409	-	-	1/7/27/30	0/1/1/1
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
23	CLA	C	513	-	1/1/15/20	10/37/115/115	-
27	GOL	l	102[A]	-	-	2/4/4/4	-
23	CLA	B	607	41	1/1/15/20	4/37/115/115	-
23	CLA	B	608	-	-	4/37/115/115	-
23	CLA	D	402[B]	-	1/1/15/20	0/37/115/115	-
26	SQD	a	410[B]	-	-	10/49/69/69	0/1/1/1
23	CLA	b	613	-	1/1/15/20	6/37/115/115	-
27	GOL	b	624	-	-	2/4/4/4	-
26	SQD	F	103	-	-	15/38/58/69	0/1/1/1
35	HTG	b	622	-	-	5/10/30/30	0/1/1/1
23	CLA	D	402[A]	-	1/1/15/20	0/37/115/115	-
26	SQD	b	620	-	-	17/49/69/69	0/1/1/1
33	LMT	M	101	-	-	5/21/61/61	0/2/2/2
32	LHG	D	407[B]	-	-	16/53/53/53	-
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
36	DGD	H	102	-	-	10/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	SQD	A	410[B]	-	-	10/49/69/69	0/1/1/1
32	LHG	d	407[B]	-	-	13/53/53/53	-
34	LMG	c	501	-	-	14/46/66/70	0/1/1/1
27	GOL	D	412	-	-	4/4/4/4	-
33	LMT	D	401	-	-	6/21/61/61	0/2/2/2
23	CLA	C	514	-	1/1/15/20	7/37/115/115	-
27	GOL	a	418	-	-	1/4/4/4	-
32	LHG	D	406[B]	-	-	19/53/53/53	-
33	LMT	B	626	-	-	11/21/61/61	0/2/2/2
27	GOL	O	303	-	-	2/4/4/4	-
25	BCR	h	101	-	-	2/29/63/63	0/2/2/2
32	LHG	D	406[A]	-	-	16/53/53/53	-
34	LMG	Z	101	-	-	11/31/51/70	0/1/1/1
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
29	PL9	a	413[B]	-	-	15/53/73/73	0/1/1/1
23	CLA	B	603	-	1/1/15/20	7/37/115/115	-
27	GOL	B	625	-	-	1/4/4/4	-
23	CLA	b	602	-	1/1/15/20	4/37/115/115	-
23	CLA	B	605	-	1/1/15/20	7/37/115/115	-
23	CLA	b	611	-	1/1/15/20	3/37/115/115	-
23	CLA	c	511	-	1/1/15/20	10/37/115/115	-
23	CLA	b	616	-	1/1/15/20	8/37/115/115	-
27	GOL	A	418	-	-	2/4/4/4	-
32	LHG	A	419[B]	-	-	12/53/53/53	-
36	DGD	c	517[A]	-	-	20/51/91/95	0/2/2/2
32	LHG	D	407[A]	-	-	14/53/53/53	-
23	CLA	c	502	-	1/1/15/20	2/37/115/115	-
24	PHO	a	407[A]	-	-	6/37/103/103	0/5/6/6
32	LHG	E	101[B]	-	-	21/46/46/53	-
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
25	BCR	c	516	-	-	0/29/63/63	0/2/2/2
27	GOL	o	304	-	-	2/4/4/4	-
23	CLA	b	603	-	1/1/15/20	5/37/115/115	-
29	PL9	D	405[B]	-	-	8/53/73/73	0/1/1/1
32	LHG	L	102[A]	-	-	19/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PHO	A	407[A]	-	-	4/37/103/103	0/5/6/6
23	CLA	c	514	-	1/1/15/20	10/37/115/115	-
23	CLA	c	507	-	1/1/15/20	8/37/115/115	-
27	GOL	B	627	-	-	4/4/4/4	-
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
23	CLA	d	402[A]	-	1/1/15/20	2/37/115/115	-
32	LHG	a	419[B]	-	-	16/46/46/53	-
36	DGD	C	517[A]	-	-	11/51/91/95	0/2/2/2
23	CLA	C	504	-	-	4/37/115/115	-
27	GOL	A	411	-	-	2/4/4/4	-
33	LMT	b	627	-	-	11/17/37/61	0/1/1/2
36	DGD	C	519	-	-	15/51/91/95	0/2/2/2
23	CLA	C	511	-	1/1/15/20	14/37/115/115	-
38	HEM	f	101	6,5	-	6/12/54/54	-
26	SQD	a	410[A]	-	-	10/49/69/69	0/1/1/1
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
23	CLA	c	512	3	1/1/15/20	5/37/115/115	-
27	GOL	d	411	-	-	3/4/4/4	-
23	CLA	b	607	41	1/1/15/20	2/37/115/115	-
34	LMG	C	521	-	-	13/46/66/70	0/1/1/1
23	CLA	a	406[B]	41	-	5/37/115/115	-
27	GOL	c	526[B]	-	-	0/4/4/4	-
27	GOL	o	303	-	-	1/4/4/4	-
35	HTG	D	410	-	-	3/7/27/30	0/1/1/1
33	LMT	a	416	-	-	11/21/61/61	0/2/2/2
23	CLA	A	404[B]	-	1/1/15/20	5/37/115/115	-
25	BCR	H	101	-	-	2/29/63/63	0/2/2/2
26	SQD	A	410[A]	-	-	12/49/69/69	0/1/1/1
23	CLA	D	403	-	1/1/15/20	14/37/115/115	-
32	LHG	d	407[A]	-	-	11/53/53/53	-
32	LHG	d	406[B]	-	-	15/53/53/53	-
34	LMG	D	411	39	-	10/46/66/70	0/1/1/1
23	CLA	C	506	-	1/1/15/20	7/37/115/115	-
23	CLA	C	510	-	1/1/15/20	5/37/115/115	-
33	LMT	A	420	-	-	15/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMT	T	101	-	-	7/21/61/61	0/2/2/2
36	DGD	C	518[B]	-	-	13/51/91/95	0/2/2/2
33	LMT	B	629	-	-	11/17/37/61	0/1/1/2
29	PL9	a	413[A]	-	-	14/53/73/73	0/1/1/1
34	LMG	d	410	39	-	9/46/66/70	0/1/1/1
23	CLA	a	404[B]	-	1/1/15/20	4/37/115/115	-
36	DGD	C	518[A]	-	-	15/51/91/95	0/2/2/2
27	GOL	b	628	-	-	0/4/4/4	-
27	GOL	c	527	-	-	3/4/4/4	-
23	CLA	C	512	3	1/1/15/20	2/37/115/115	-
23	CLA	a	408	-	-	9/37/115/115	-
32	LHG	A	419[A]	-	-	10/53/53/53	-
32	LHG	E	101[A]	-	-	22/46/46/53	-
25	BCR	t	102	-	-	3/29/63/63	0/2/2/2
27	GOL	V	203[B]	-	-	2/4/4/4	-
23	CLA	A	405[B]	41	1/1/15/20	4/37/115/115	-
33	LMT	F	101	-	-	8/21/61/61	0/2/2/2
27	GOL	B	622	-	-	2/4/4/4	-
23	CLA	c	513	-	1/1/15/20	13/37/115/115	-
23	CLA	B	615	-	1/1/15/20	7/37/115/115	-
29	PL9	D	405[A]	-	-	8/53/73/73	0/1/1/1
33	LMT	m	103	-	-	6/21/61/61	0/2/2/2
23	CLA	c	504	-	1/1/15/20	3/37/115/115	-
34	LMG	C	520	-	-	9/46/66/70	0/1/1/1
35	HTG	B	623	-	-	5/10/30/30	0/1/1/1
35	HTG	B	621	-	-	4/10/30/30	0/1/1/1
38	HEM	F	102	6,5	-	4/12/54/54	-
23	CLA	B	604	-	1/1/15/20	2/37/115/115	-
23	CLA	B	610	41	1/1/15/20	8/37/115/115	-
23	CLA	C	509	-	1/1/15/20	7/37/115/115	-
24	PHO	A	417[B]	-	-	1/37/103/103	0/5/6/6
32	LHG	a	419[A]	-	-	16/46/46/53	-
25	BCR	B	617	-	-	2/29/63/63	0/2/2/2
24	PHO	a	415[B]	-	-	1/37/103/103	0/5/6/6
32	LHG	d	412[B]	-	-	11/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PHO	A	417[A]	-	-	1/37/103/103	0/5/6/6
23	CLA	d	403	-	1/1/15/20	8/37/115/115	-
35	HTG	c	522	-	-	2/10/30/30	0/1/1/1
24	PHO	a	415[A]	-	-	2/37/103/103	0/5/6/6
35	HTG	V	202	-	-	0/2/19/30	0/1/1/1
23	CLA	b	609	-	1/1/15/20	3/37/115/115	-
26	SQD	f	102	-	-	11/38/58/69	0/1/1/1
35	HTG	b	623	-	-	3/10/30/30	0/1/1/1
29	PL9	A	414[B]	-	-	16/53/73/73	0/1/1/1
25	BCR	D	404	-	-	4/29/63/63	0/2/2/2
34	LMG	m	101	-	-	10/46/66/70	0/1/1/1
27	GOL	v	202[B]	-	-	2/4/4/4	-
23	CLA	C	503	-	1/1/15/20	9/37/115/115	-
23	CLA	A	408	-	1/1/15/20	9/37/115/115	-
23	CLA	a	406[A]	41	-	5/37/115/115	-
23	CLA	b	606	-	1/1/15/20	12/37/115/115	-
27	GOL	c	526[A]	-	-	0/4/4/4	-
23	CLA	B	613	-	1/1/15/20	8/37/115/115	-
23	CLA	c	506	-	1/1/15/20	7/37/115/115	-
23	CLA	A	404[A]	-	1/1/15/20	5/37/115/115	-
23	CLA	b	614	-	1/1/15/20	14/37/115/115	-
23	CLA	c	510	-	1/1/15/20	14/37/115/115	-
23	CLA	C	508	41	1/1/15/20	7/37/115/115	-
29	PL9	d	405[B]	-	-	9/53/73/73	0/1/1/1
32	LHG	d	406[A]	-	-	13/53/53/53	-
34	LMG	z	101	-	-	9/34/54/70	0/1/1/1
23	CLA	A	406[B]	41	-	5/37/115/115	-
32	LHG	b	630[B]	-	-	20/53/53/53	-
23	CLA	B	612	-	1/1/15/20	7/37/115/115	-
23	CLA	a	405[B]	41	1/1/15/20	6/37/115/115	-
35	HTG	C	522	-	-	0/10/30/30	0/1/1/1
23	CLA	C	505	41	1/1/15/20	5/37/115/115	-
27	GOL	a	417	-	-	2/4/4/4	-
26	SQD	L	101	-	-	12/49/69/69	0/1/1/1
27	GOL	l	102[B]	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HTG	o	301	-	-	3/10/30/30	0/1/1/1
23	CLA	a	405[A]	41	1/1/15/20	8/37/115/115	-
25	BCR	b	619	-	-	5/29/63/63	0/2/2/2
23	CLA	B	601	41	1/1/15/20	11/37/115/115	-
23	CLA	a	404[A]	-	1/1/15/20	3/37/115/115	-
23	CLA	B	606	-	1/1/15/20	10/37/115/115	-
23	CLA	b	610	41	1/1/15/20	5/37/115/115	-
26	SQD	A	412	-	-	12/49/69/69	0/1/1/1
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
33	LMT	t	101	-	-	9/17/38/61	0/1/1/2
34	LMG	B	620	-	-	14/46/66/70	0/1/1/1
23	CLA	b	604	-	1/1/15/20	9/37/115/115	-
40	HEC	v	201	16	-	2/10/54/54	-
23	CLA	b	612	-	1/1/15/20	4/37/115/115	-
27	GOL	V	203[A]	-	-	2/4/4/4	-
36	DGD	h	102	-	-	13/51/91/95	0/2/2/2
23	CLA	b	601	41	1/1/15/20	17/37/115/115	-
23	CLA	A	405[A]	41	-	4/37/115/115	-
27	GOL	O	302	-	-	2/4/4/4	-
23	CLA	c	508	41	1/1/15/20	7/37/115/115	-
23	CLA	B	614	-	1/1/15/20	13/37/115/115	-
23	CLA	b	608	-	-	4/37/115/115	-
33	LMT	b	621	-	-	8/17/37/61	0/1/1/2
27	GOL	C	523[B]	-	-	0/4/4/4	-
33	LMT	B	628	-	-	12/21/61/61	0/2/2/2
36	DGD	c	518[B]	-	-	17/51/91/95	0/2/2/2
25	BCR	Y	101	-	-	2/29/63/63	0/2/2/2
33	LMT	e	101	-	-	15/21/61/61	0/2/2/2
34	LMG	c	520	-	-	12/46/66/70	0/1/1/1
25	BCR	K	102	-	-	0/29/63/63	0/2/2/2
27	GOL	C	523[A]	-	-	0/4/4/4	-
26	SQD	a	411	-	-	14/49/69/69	0/1/1/1
25	BCR	T	102	-	-	3/29/63/63	0/2/2/2
36	DGD	c	518[A]	-	-	17/51/91/95	0/2/2/2
35	HTG	b	625	-	-	4/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	615	-	1/1/15/20	7/37/115/115	-
23	CLA	B	611	-	1/1/15/20	2/37/115/115	-
32	LHG	d	412[A]	-	-	13/53/53/53	-
23	CLA	B	602	-	1/1/15/20	7/37/115/115	-
23	CLA	B	616	-	1/1/15/20	5/37/115/115	-
25	BCR	a	409	-	-	0/29/63/63	0/2/2/2
25	BCR	d	404	-	-	4/29/63/63	0/2/2/2
23	CLA	C	507	-	1/1/15/20	10/37/115/115	-
23	CLA	c	505	41	1/1/15/20	8/37/115/115	-
29	PL9	A	414[A]	-	-	15/53/73/73	0/1/1/1
34	LMG	c	521	-	-	13/46/66/70	0/1/1/1
25	BCR	y	101	-	-	5/29/63/63	0/2/2/2
36	DGD	c	517[B]	-	-	19/51/91/95	0/2/2/2
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2

All (1545) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	611	CLA	C3B-C2B	11.00	1.55	1.40
23	B	611	CLA	CMB-C2B	7.09	1.66	1.51
23	B	611	CLA	C1D-ND	6.98	1.46	1.37
23	C	509	CLA	C3B-C2B	6.85	1.49	1.40
23	b	603	CLA	C3B-C2B	6.72	1.49	1.40
23	c	503	CLA	C3B-C2B	6.68	1.49	1.40
23	B	612	CLA	C3B-C2B	6.59	1.49	1.40
23	C	512	CLA	C3B-C2B	6.59	1.49	1.40
23	B	616	CLA	C3B-C2B	6.52	1.49	1.40
23	b	614	CLA	C3B-C2B	6.46	1.49	1.40
23	c	509	CLA	C3B-C2B	6.43	1.49	1.40
23	c	512	CLA	C3B-C2B	6.42	1.49	1.40
24	a	407[B]	PHO	C3B-C2B	6.41	1.49	1.40
23	c	505	CLA	C3B-C2B	6.40	1.49	1.40
23	A	404[B]	CLA	C3B-C2B	6.40	1.49	1.40
23	B	608	CLA	C3B-C2B	6.39	1.49	1.40
23	a	404[B]	CLA	C3B-C2B	6.37	1.49	1.40
24	a	407[A]	PHO	C3B-C2B	6.36	1.49	1.40
24	a	415[B]	PHO	C3B-C2B	6.33	1.49	1.40
23	B	603	CLA	C3B-C2B	6.32	1.49	1.40
23	b	604	CLA	C3B-C2B	6.32	1.49	1.40
23	d	402[B]	CLA	C3B-C2B	6.31	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	v	201	HEC	C2B-C3B	-6.27	1.34	1.40
23	a	404[A]	CLA	C3B-C2B	6.26	1.49	1.40
23	A	404[A]	CLA	C3B-C2B	6.26	1.49	1.40
23	A	408	CLA	C3B-C2B	6.21	1.49	1.40
23	b	608	CLA	C3B-C2B	6.21	1.49	1.40
24	A	417[B]	PHO	C3B-C2B	6.20	1.49	1.40
23	b	612	CLA	C3B-C2B	6.19	1.49	1.40
24	A	407[A]	PHO	C3B-C2B	6.19	1.49	1.40
23	C	510	CLA	C3B-C2B	6.18	1.48	1.40
23	D	402[B]	CLA	C3B-C2B	6.15	1.48	1.40
23	b	610	CLA	C3B-C2B	6.14	1.48	1.40
24	A	417[A]	PHO	C3B-C2B	6.12	1.48	1.40
23	D	403	CLA	C1D-ND	6.05	1.45	1.37
23	b	613	CLA	C3B-C2B	6.05	1.48	1.40
23	C	514	CLA	C3B-C2B	6.04	1.48	1.40
23	C	503	CLA	C3B-C2B	6.03	1.48	1.40
23	b	601	CLA	C3B-C2B	6.03	1.48	1.40
23	B	601	CLA	C3B-C2B	6.02	1.48	1.40
23	c	510	CLA	C3B-C2B	6.01	1.48	1.40
23	B	607	CLA	C3B-C2B	5.99	1.48	1.40
23	B	613	CLA	C3B-C2B	5.99	1.48	1.40
23	a	405[B]	CLA	C1D-ND	5.97	1.45	1.37
23	D	402[A]	CLA	C3B-C2B	5.94	1.48	1.40
23	c	511	CLA	C3B-C2B	5.94	1.48	1.40
23	c	507	CLA	C3B-C2B	5.93	1.48	1.40
23	B	611	CLA	CHC-C1C	5.91	1.50	1.35
24	a	415[A]	PHO	C3B-C2B	5.90	1.48	1.40
24	A	407[B]	PHO	C3B-C2B	5.90	1.48	1.40
23	B	602	CLA	C3B-C2B	5.88	1.48	1.40
23	C	508	CLA	C3B-C2B	5.87	1.48	1.40
23	c	514	CLA	C3B-C2B	5.86	1.48	1.40
23	C	505	CLA	C3B-C2B	5.84	1.48	1.40
23	b	611	CLA	C3B-C2B	5.81	1.48	1.40
23	B	604	CLA	C3B-C2B	5.80	1.48	1.40
23	C	511	CLA	C1D-ND	5.78	1.44	1.37
23	A	405[B]	CLA	C3B-C2B	5.78	1.48	1.40
23	C	502	CLA	C3B-C2B	5.74	1.48	1.40
23	D	403	CLA	C3C-C2C	5.70	1.48	1.36
23	B	614	CLA	C3B-C2B	5.69	1.48	1.40
23	c	509	CLA	C3C-C2C	5.68	1.48	1.36
23	c	513	CLA	C3C-C2C	5.67	1.48	1.36
24	a	407[B]	PHO	C3D-C2D	5.66	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	511	CLA	C3B-C2B	5.65	1.48	1.40
23	B	611	CLA	C3C-C2C	5.65	1.48	1.36
23	b	606	CLA	C3B-C2B	5.65	1.48	1.40
23	d	402[A]	CLA	C3B-C2B	5.65	1.48	1.40
23	C	513	CLA	C3B-C2B	5.63	1.48	1.40
23	b	616	CLA	C3B-C2B	5.62	1.48	1.40
23	c	510	CLA	C3C-C2C	5.61	1.48	1.36
23	B	606	CLA	C3B-C2B	5.59	1.48	1.40
23	b	601	CLA	C1D-ND	5.57	1.44	1.37
23	b	612	CLA	C3C-C2C	5.57	1.48	1.36
23	C	503	CLA	C1D-ND	5.56	1.44	1.37
23	b	607	CLA	C3B-C2B	5.54	1.48	1.40
23	C	513	CLA	CHC-C1C	5.53	1.49	1.35
23	b	616	CLA	C1D-ND	5.52	1.44	1.37
23	c	514	CLA	C1D-ND	5.52	1.44	1.37
23	a	405[B]	CLA	C3B-C2B	5.52	1.48	1.40
23	d	403	CLA	C3B-C2B	5.50	1.48	1.40
23	B	610	CLA	C3C-C2C	5.50	1.48	1.36
23	a	406[B]	CLA	C3C-C2C	5.49	1.48	1.36
23	C	509	CLA	C3C-C2C	5.48	1.48	1.36
23	b	602	CLA	C3C-C2C	5.48	1.48	1.36
40	V	201	HEC	C2B-C3B	-5.48	1.35	1.40
23	a	406[B]	CLA	C3B-C2B	5.48	1.48	1.40
23	a	408	CLA	C3B-C2B	5.47	1.48	1.40
23	c	505	CLA	C1D-ND	5.46	1.44	1.37
23	C	513	CLA	C3C-C2C	5.46	1.48	1.36
23	A	404[B]	CLA	C3C-C2C	5.45	1.48	1.36
23	A	404[A]	CLA	C3C-C2C	5.45	1.48	1.36
23	c	512	CLA	C1D-ND	5.44	1.44	1.37
23	c	504	CLA	CHC-C1C	5.44	1.48	1.35
23	c	504	CLA	C3C-C2C	5.43	1.48	1.36
23	b	615	CLA	C3C-C2C	5.43	1.48	1.36
23	b	609	CLA	O2D-CGD	5.43	1.46	1.33
24	a	407[A]	PHO	C3D-C2D	5.41	1.49	1.39
23	b	614	CLA	C3C-C2C	5.41	1.48	1.36
23	a	408	CLA	C3C-C2C	5.41	1.48	1.36
23	c	513	CLA	C3B-C2B	5.41	1.47	1.40
23	d	403	CLA	C3C-C2C	5.39	1.48	1.36
23	b	605	CLA	C3C-C2C	5.38	1.48	1.36
23	a	404[B]	CLA	C3C-C2C	5.38	1.48	1.36
23	b	602	CLA	CHC-C1C	5.37	1.48	1.35
23	B	605	CLA	C1D-ND	5.37	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	405[B]	CLA	C3C-C2C	5.37	1.48	1.36
24	a	415[B]	PHO	C3D-C2D	5.36	1.49	1.39
23	C	507	CLA	C3B-C2B	5.36	1.47	1.40
23	d	402[B]	CLA	C3C-C2C	5.35	1.48	1.36
23	A	408	CLA	C3C-C2C	5.35	1.48	1.36
23	B	609	CLA	C3B-C2B	5.35	1.47	1.40
23	a	405[A]	CLA	C3C-C2C	5.35	1.48	1.36
23	B	601	CLA	C3C-C2C	5.35	1.48	1.36
23	C	504	CLA	C3C-C2C	5.35	1.48	1.36
23	A	406[B]	CLA	C3C-C2C	5.35	1.48	1.36
23	b	609	CLA	C3B-C2B	5.35	1.47	1.40
23	b	607	CLA	C3C-C2C	5.35	1.48	1.36
23	c	508	CLA	C3B-C2B	5.35	1.47	1.40
23	b	606	CLA	C3C-C2C	5.34	1.48	1.36
23	c	513	CLA	CHC-C1C	5.34	1.48	1.35
23	a	406[A]	CLA	C3C-C2C	5.34	1.48	1.36
23	c	514	CLA	C3C-C2C	5.34	1.48	1.36
23	c	506	CLA	C3C-C2C	5.33	1.48	1.36
23	b	603	CLA	C3C-C2C	5.32	1.48	1.36
23	b	601	CLA	C3C-C2C	5.31	1.48	1.36
23	C	514	CLA	C3C-C2C	5.31	1.48	1.36
23	b	615	CLA	C3B-C2B	5.30	1.47	1.40
23	C	504	CLA	C3B-C2B	5.30	1.47	1.40
23	A	404[B]	CLA	C1D-ND	5.30	1.44	1.37
23	b	613	CLA	CHC-C1C	5.29	1.48	1.35
23	c	506	CLA	CHC-C1C	5.29	1.48	1.35
23	C	511	CLA	C3C-C2C	5.29	1.48	1.36
23	d	403	CLA	CHC-C1C	5.29	1.48	1.35
23	B	612	CLA	C3C-C2C	5.28	1.48	1.36
24	a	415[A]	PHO	C3D-C2D	5.28	1.48	1.39
23	B	609	CLA	CHC-C1C	5.27	1.48	1.35
23	c	509	CLA	O2D-CGD	5.26	1.46	1.33
23	B	601	CLA	CHC-C1C	5.26	1.48	1.35
24	A	417[A]	PHO	C3D-C2D	5.25	1.48	1.39
23	B	612	CLA	CHC-C1C	5.25	1.48	1.35
23	A	406[B]	CLA	C3B-C2B	5.25	1.47	1.40
23	a	405[B]	CLA	O2D-CGD	5.25	1.46	1.33
23	B	601	CLA	C1D-ND	5.24	1.44	1.37
23	c	511	CLA	O2D-CGD	5.24	1.46	1.33
23	B	616	CLA	CHC-C1C	5.24	1.48	1.35
23	B	603	CLA	C3C-C2C	5.24	1.47	1.36
23	b	610	CLA	CHC-C1C	5.24	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402[A]	CLA	C3C-C2C	5.23	1.47	1.36
23	C	510	CLA	C3C-C2C	5.23	1.47	1.36
23	B	606	CLA	CHC-C1C	5.23	1.48	1.35
23	C	502	CLA	CHC-C1C	5.23	1.48	1.35
23	b	610	CLA	C3C-C2C	5.23	1.47	1.36
23	a	406[A]	CLA	C3B-C2B	5.22	1.47	1.40
23	c	512	CLA	C3C-C2C	5.22	1.47	1.36
23	C	504	CLA	CHC-C1C	5.22	1.48	1.35
40	v	201	HEC	C3D-C2D	5.22	1.53	1.37
23	D	402[A]	CLA	C3C-C2C	5.22	1.47	1.36
23	a	408	CLA	CHC-C1C	5.22	1.48	1.35
23	B	613	CLA	CHC-C1C	5.22	1.48	1.35
23	a	404[A]	CLA	C3C-C2C	5.22	1.47	1.36
23	c	505	CLA	O2D-CGD	5.22	1.45	1.33
23	D	402[B]	CLA	C3C-C2C	5.21	1.47	1.36
23	b	602	CLA	O2D-CGD	5.21	1.45	1.33
23	B	606	CLA	C3C-C2C	5.21	1.47	1.36
23	d	403	CLA	C1D-ND	5.20	1.44	1.37
23	C	508	CLA	C3C-C2C	5.20	1.47	1.36
23	B	605	CLA	C3C-C2C	5.20	1.47	1.36
23	D	403	CLA	CHC-C1C	5.19	1.48	1.35
23	A	405[A]	CLA	C3B-C2B	5.18	1.47	1.40
23	B	604	CLA	C3C-C2C	5.18	1.47	1.36
23	a	406[B]	CLA	CHC-C1C	5.17	1.48	1.35
23	c	502	CLA	C1D-ND	5.16	1.44	1.37
23	b	616	CLA	C3C-C2C	5.16	1.47	1.36
23	a	405[A]	CLA	C1D-ND	5.16	1.44	1.37
23	C	513	CLA	C1D-ND	5.15	1.44	1.37
23	B	602	CLA	CHC-C1C	5.15	1.48	1.35
23	C	506	CLA	C3B-C2B	5.15	1.47	1.40
23	C	505	CLA	C3C-C2C	5.14	1.47	1.36
23	A	406[B]	CLA	CHC-C1C	5.14	1.48	1.35
23	c	509	CLA	CHC-C1C	5.14	1.48	1.35
23	c	509	CLA	C1D-ND	5.14	1.44	1.37
23	c	502	CLA	C3B-C2B	5.14	1.47	1.40
23	B	604	CLA	CHC-C1C	5.14	1.48	1.35
23	b	611	CLA	C3C-C2C	5.14	1.47	1.36
23	b	616	CLA	CHC-C1C	5.13	1.48	1.35
23	C	506	CLA	CHC-C1C	5.13	1.48	1.35
23	c	510	CLA	O2D-CGD	5.13	1.45	1.33
23	c	502	CLA	C3C-C2C	5.13	1.47	1.36
23	B	614	CLA	C3C-C2C	5.13	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	503	CLA	C3C-C2C	5.13	1.47	1.36
23	b	605	CLA	C1D-ND	5.13	1.44	1.37
23	A	406[A]	CLA	CHC-C1C	5.12	1.48	1.35
23	B	602	CLA	C1D-ND	5.11	1.44	1.37
23	b	615	CLA	CHC-C1C	5.11	1.48	1.35
24	A	417[B]	PHO	C3D-C2D	5.11	1.48	1.39
23	B	601	CLA	O2D-CGD	5.11	1.45	1.33
23	C	503	CLA	C3C-C2C	5.11	1.47	1.36
23	b	606	CLA	CHC-C1C	5.11	1.48	1.35
23	C	507	CLA	O2D-CGD	5.11	1.45	1.33
23	B	615	CLA	C1D-ND	5.10	1.44	1.37
23	C	511	CLA	CHC-C1C	5.10	1.48	1.35
23	C	508	CLA	CHC-C1C	5.10	1.48	1.35
23	c	511	CLA	C3C-C2C	5.10	1.47	1.36
23	A	404[B]	CLA	CHC-C1C	5.09	1.48	1.35
25	C	515	BCR	C23-C22	-5.09	1.35	1.45
23	c	514	CLA	O2D-CGD	5.08	1.45	1.33
23	c	512	CLA	CHC-C1C	5.08	1.48	1.35
23	B	614	CLA	C1D-ND	5.07	1.44	1.37
23	c	504	CLA	C1D-ND	5.07	1.44	1.37
23	c	514	CLA	CHC-C1C	5.07	1.48	1.35
23	C	510	CLA	O2D-CGD	5.06	1.45	1.33
23	c	508	CLA	CHC-C1C	5.06	1.47	1.35
23	B	609	CLA	C3C-C2C	5.06	1.47	1.36
23	A	406[A]	CLA	C3C-C2C	5.05	1.47	1.36
23	b	604	CLA	CHC-C1C	5.05	1.47	1.35
23	c	507	CLA	C3C-C2C	5.05	1.47	1.36
23	c	504	CLA	C3B-C2B	5.04	1.47	1.40
23	B	616	CLA	C3C-C2C	5.04	1.47	1.36
40	V	201	HEC	C3D-C2D	5.04	1.52	1.37
23	b	601	CLA	CHC-C1C	5.04	1.47	1.35
23	C	502	CLA	C3C-C2C	5.04	1.47	1.36
23	A	405[B]	CLA	C3C-C2C	5.03	1.47	1.36
23	b	603	CLA	O2D-CGD	5.03	1.45	1.33
23	B	615	CLA	O2D-CGD	5.03	1.45	1.33
24	a	407[A]	PHO	O2D-CGD	5.03	1.45	1.33
23	c	505	CLA	C3C-C2C	5.03	1.47	1.36
24	a	407[B]	PHO	O2D-CGD	5.02	1.45	1.33
23	D	402[B]	CLA	C1D-ND	5.02	1.44	1.37
23	A	405[B]	CLA	CHC-C1C	5.02	1.47	1.35
23	c	502	CLA	CHC-C1C	5.02	1.47	1.35
23	C	512	CLA	O2D-CGD	5.02	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	503	CLA	O2D-CGD	5.01	1.45	1.33
23	a	406[A]	CLA	CHC-C1C	5.01	1.47	1.35
23	a	405[A]	CLA	C3B-C2B	5.01	1.47	1.40
23	B	601	CLA	O2A-CGA	5.01	1.48	1.33
23	B	605	CLA	C3B-C2B	5.00	1.47	1.40
23	B	602	CLA	C3C-C2C	5.00	1.47	1.36
23	B	615	CLA	C3B-C2B	4.99	1.47	1.40
23	B	606	CLA	C1D-ND	4.99	1.43	1.37
23	b	613	CLA	C1D-ND	4.99	1.43	1.37
23	A	405[A]	CLA	CHC-C1C	4.99	1.47	1.35
24	a	415[B]	PHO	O2D-CGD	4.99	1.45	1.33
23	C	509	CLA	C1D-ND	4.99	1.43	1.37
23	b	614	CLA	CHC-C1C	4.98	1.47	1.35
23	B	609	CLA	O2D-CGD	4.98	1.45	1.33
23	B	613	CLA	O2D-CGD	4.98	1.45	1.33
23	C	507	CLA	C3C-C2C	4.98	1.47	1.36
23	c	507	CLA	CHC-C1C	4.98	1.47	1.35
23	a	405[A]	CLA	O2D-CGD	4.98	1.45	1.33
23	c	507	CLA	C1D-ND	4.97	1.43	1.37
23	A	406[B]	CLA	O2D-CGD	4.97	1.45	1.33
25	D	404	BCR	C23-C22	-4.97	1.35	1.45
25	K	102	BCR	C23-C22	-4.97	1.35	1.45
23	c	508	CLA	C1D-ND	4.96	1.43	1.37
23	c	513	CLA	C1D-ND	4.96	1.43	1.37
23	b	605	CLA	CHC-C1C	4.96	1.47	1.35
23	A	405[B]	CLA	C1D-ND	4.96	1.43	1.37
23	C	510	CLA	C1D-ND	4.96	1.43	1.37
23	b	610	CLA	O2D-CGD	4.96	1.45	1.33
23	B	605	CLA	O2D-CGD	4.96	1.45	1.33
23	b	605	CLA	C3B-C2B	4.96	1.47	1.40
23	D	402[B]	CLA	O2D-CGD	4.96	1.45	1.33
23	b	609	CLA	CHC-C1C	4.95	1.47	1.35
23	C	509	CLA	O2D-CGD	4.95	1.45	1.33
23	D	402[B]	CLA	CHC-C1C	4.95	1.47	1.35
24	a	415[A]	PHO	O2D-CGD	4.95	1.45	1.33
23	B	610	CLA	C1D-ND	4.95	1.43	1.37
23	B	607	CLA	CHC-C1C	4.95	1.47	1.35
23	A	404[B]	CLA	O2D-CGD	4.95	1.45	1.33
23	B	608	CLA	C1D-ND	4.94	1.43	1.37
23	B	605	CLA	CHC-C1C	4.94	1.47	1.35
23	b	601	CLA	O2D-CGD	4.94	1.45	1.33
25	k	101	BCR	C23-C22	-4.93	1.35	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	506	CLA	C3B-C2B	4.93	1.47	1.40
23	A	406[A]	CLA	C3B-C2B	4.93	1.47	1.40
23	C	506	CLA	C3C-C2C	4.93	1.47	1.36
23	c	512	CLA	O2D-CGD	4.92	1.45	1.33
23	a	405[B]	CLA	CHC-C1C	4.92	1.47	1.35
23	D	403	CLA	C3B-C2B	4.92	1.47	1.40
23	b	604	CLA	C1D-ND	4.92	1.43	1.37
23	b	607	CLA	CHC-C1C	4.92	1.47	1.35
23	C	509	CLA	CHC-C1C	4.92	1.47	1.35
23	b	604	CLA	C3C-C2C	4.91	1.47	1.36
23	c	511	CLA	CHC-C1C	4.91	1.47	1.35
24	A	417[A]	PHO	O2D-CGD	4.91	1.45	1.33
23	C	514	CLA	C1D-ND	4.91	1.43	1.37
23	C	512	CLA	C3C-C2C	4.91	1.47	1.36
24	A	417[B]	PHO	O2D-CGD	4.90	1.45	1.33
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	C	503	CLA	CHC-C1C	4.90	1.47	1.35
24	A	407[B]	PHO	O2D-CGD	4.90	1.45	1.33
23	b	603	CLA	C1D-ND	4.89	1.43	1.37
23	A	408	CLA	CHC-C1C	4.89	1.47	1.35
23	B	615	CLA	CHC-C1C	4.89	1.47	1.35
23	B	610	CLA	CHC-C1C	4.89	1.47	1.35
23	A	405[B]	CLA	O2D-CGD	4.89	1.45	1.33
23	a	404[B]	CLA	CHC-C1C	4.89	1.47	1.35
25	b	619	BCR	C23-C22	-4.89	1.35	1.45
23	b	611	CLA	CHC-C1C	4.88	1.47	1.35
25	d	404	BCR	C23-C22	-4.88	1.35	1.45
23	B	613	CLA	C1D-ND	4.88	1.43	1.37
24	A	407[A]	PHO	C3D-C2D	4.88	1.48	1.39
23	B	604	CLA	O2D-CGD	4.88	1.45	1.33
23	a	405[A]	CLA	CHC-C1C	4.87	1.47	1.35
23	c	503	CLA	O2D-CGD	4.87	1.45	1.33
23	A	405[A]	CLA	C3C-C2C	4.87	1.47	1.36
23	C	512	CLA	CHC-C1C	4.87	1.47	1.35
23	b	606	CLA	C1D-ND	4.86	1.43	1.37
23	c	508	CLA	C3C-C2C	4.86	1.47	1.36
23	b	605	CLA	O2D-CGD	4.86	1.45	1.33
23	C	514	CLA	O2D-CGD	4.85	1.45	1.33
23	C	510	CLA	CHC-C1C	4.85	1.47	1.35
23	c	507	CLA	O2D-CGD	4.85	1.45	1.33
23	c	513	CLA	O2D-CGD	4.85	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	508	CLA	O2D-CGD	4.84	1.45	1.33
40	V	201	HEC	C3C-C2C	-4.84	1.35	1.40
23	C	502	CLA	C1D-ND	4.84	1.43	1.37
24	a	415[A]	PHO	OBD-CAD	4.84	1.29	1.22
23	a	404[A]	CLA	CHC-C1C	4.84	1.47	1.35
23	B	607	CLA	C3C-C2C	4.84	1.47	1.36
23	b	612	CLA	CHC-C1C	4.83	1.47	1.35
23	b	608	CLA	CHC-C1C	4.83	1.47	1.35
23	B	615	CLA	C3C-C2C	4.83	1.47	1.36
26	F	103	SQD	O47-C7	4.83	1.47	1.34
23	c	510	CLA	C1D-ND	4.82	1.43	1.37
23	B	610	CLA	O2D-CGD	4.82	1.45	1.33
23	c	511	CLA	C1D-ND	4.82	1.43	1.37
23	b	609	CLA	C3C-C2C	4.82	1.47	1.36
23	C	505	CLA	CHC-C1C	4.81	1.47	1.35
40	v	201	HEC	C3C-C2C	-4.80	1.35	1.40
23	D	402[A]	CLA	O2D-CGD	4.80	1.44	1.33
23	A	404[A]	CLA	CHC-C1C	4.80	1.47	1.35
25	C	516	BCR	C23-C22	-4.80	1.35	1.45
23	C	505	CLA	O2D-CGD	4.80	1.44	1.33
25	B	617	BCR	C23-C22	-4.79	1.35	1.45
24	a	415[B]	PHO	OBD-CAD	4.78	1.29	1.22
23	B	614	CLA	CHC-C1C	4.78	1.47	1.35
23	C	514	CLA	CHC-C1C	4.78	1.47	1.35
23	a	406[B]	CLA	C1D-ND	4.77	1.43	1.37
23	C	504	CLA	C1D-ND	4.77	1.43	1.37
23	c	503	CLA	CHC-C1C	4.77	1.47	1.35
23	a	406[B]	CLA	O2D-CGD	4.76	1.44	1.33
23	b	603	CLA	CHC-C1C	4.76	1.47	1.35
23	b	601	CLA	O2A-CGA	4.76	1.47	1.33
23	B	610	CLA	C3B-C2B	4.75	1.47	1.40
23	d	402[B]	CLA	CHC-C1C	4.75	1.47	1.35
23	D	402[A]	CLA	CHC-C1C	4.75	1.47	1.35
23	b	608	CLA	C3C-C2C	4.74	1.46	1.36
23	b	613	CLA	C3C-C2C	4.74	1.46	1.36
23	b	613	CLA	O2D-CGD	4.74	1.44	1.33
25	B	619	BCR	C23-C22	-4.74	1.35	1.45
23	B	613	CLA	C3C-C2C	4.74	1.46	1.36
23	b	614	CLA	O2D-CGD	4.74	1.44	1.33
23	B	608	CLA	C3C-C2C	4.74	1.46	1.36
23	A	404[A]	CLA	O2D-CGD	4.73	1.44	1.33
23	b	615	CLA	O2D-CGD	4.73	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	408	CLA	O2D-CGD	4.73	1.44	1.33
23	c	505	CLA	CHC-C1C	4.72	1.47	1.35
23	B	603	CLA	C1D-ND	4.72	1.43	1.37
23	C	506	CLA	O2D-CGD	4.71	1.44	1.33
23	B	603	CLA	CHC-C1C	4.71	1.47	1.35
23	b	602	CLA	C3B-C2B	4.71	1.46	1.40
23	C	507	CLA	CHC-C1C	4.70	1.47	1.35
23	D	403	CLA	O2D-CGD	4.67	1.44	1.33
23	a	404[B]	CLA	O2D-CGD	4.67	1.44	1.33
23	d	402[A]	CLA	O2D-CGD	4.66	1.44	1.33
23	b	602	CLA	C1D-ND	4.66	1.43	1.37
23	B	603	CLA	O2D-CGD	4.66	1.44	1.33
23	b	611	CLA	O2D-CGD	4.66	1.44	1.33
23	b	616	CLA	O2D-CGD	4.66	1.44	1.33
23	d	402[A]	CLA	CHC-C1C	4.66	1.46	1.35
23	C	513	CLA	O2D-CGD	4.65	1.44	1.33
23	b	609	CLA	C1D-ND	4.64	1.43	1.37
34	c	521	LMG	O7-C10	4.64	1.47	1.34
25	T	102	BCR	C23-C22	-4.63	1.36	1.45
34	C	521	LMG	O7-C10	4.63	1.47	1.34
26	a	411	SQD	O48-C23	4.62	1.46	1.33
23	a	404[B]	CLA	C1D-ND	4.62	1.43	1.37
23	C	511	CLA	O2D-CGD	4.62	1.44	1.33
23	a	404[A]	CLA	C1D-ND	4.62	1.43	1.37
23	b	615	CLA	C1D-ND	4.61	1.43	1.37
25	b	617	BCR	C23-C22	-4.61	1.36	1.45
23	d	402[B]	CLA	O2D-CGD	4.61	1.44	1.33
23	b	606	CLA	O2D-CGD	4.60	1.44	1.33
24	A	417[B]	PHO	OBD-CAD	4.59	1.28	1.22
25	y	101	BCR	C23-C22	-4.59	1.36	1.45
23	d	402[B]	CLA	C1D-ND	4.58	1.43	1.37
23	B	602	CLA	O2D-CGD	4.58	1.44	1.33
23	c	506	CLA	O2D-CGD	4.58	1.44	1.33
23	A	408	CLA	O2D-CGD	4.58	1.44	1.33
23	b	602	CLA	CHD-C1D	4.57	1.47	1.38
23	c	510	CLA	CHC-C1C	4.57	1.46	1.35
25	c	516	BCR	C23-C22	-4.56	1.36	1.45
23	B	606	CLA	O2D-CGD	4.55	1.44	1.33
23	b	604	CLA	O2D-CGD	4.55	1.44	1.33
23	C	505	CLA	C1D-ND	4.55	1.43	1.37
23	a	404[A]	CLA	O2D-CGD	4.54	1.44	1.33
23	B	608	CLA	O2D-CGD	4.53	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	614	CLA	C1D-ND	4.53	1.43	1.37
23	b	604	CLA	CHD-C1D	4.53	1.47	1.38
24	A	407[B]	PHO	C3D-C2D	4.52	1.47	1.39
23	B	616	CLA	O2D-CGD	4.51	1.44	1.33
26	f	102	SQD	O47-C7	4.50	1.47	1.34
26	L	101	SQD	O47-C7	4.50	1.47	1.34
23	a	406[A]	CLA	O2D-CGD	4.50	1.44	1.33
25	c	515	BCR	C23-C22	-4.50	1.36	1.45
23	b	607	CLA	C1D-ND	4.49	1.43	1.37
23	c	514	CLA	O2A-CGA	4.49	1.46	1.33
23	B	614	CLA	O2D-CGD	4.48	1.44	1.33
23	b	608	CLA	O2D-CGD	4.48	1.44	1.33
32	E	101[A]	LHG	O8-C23	4.48	1.46	1.33
34	C	521	LMG	O8-C28	4.47	1.46	1.33
25	h	101	BCR	C23-C22	-4.47	1.36	1.45
34	z	101	LMG	O8-C28	4.46	1.46	1.33
32	E	101[B]	LHG	O8-C23	4.46	1.46	1.33
25	A	409	BCR	C23-C22	-4.46	1.36	1.45
23	B	604	CLA	C1D-ND	4.45	1.43	1.37
23	C	506	CLA	C1D-ND	4.45	1.43	1.37
23	B	610	CLA	OBD-CAD	4.45	1.30	1.22
23	b	607	CLA	O2D-CGD	4.44	1.44	1.33
25	H	101	BCR	C23-C22	-4.43	1.36	1.45
23	b	607	CLA	CHD-C1D	4.43	1.47	1.38
23	C	507	CLA	C1D-ND	4.43	1.43	1.37
23	b	609	CLA	CHD-C1D	4.43	1.47	1.38
23	c	513	CLA	O2A-CGA	4.43	1.46	1.33
23	c	509	CLA	CHD-C1D	4.42	1.47	1.38
23	b	611	CLA	O2A-CGA	4.41	1.46	1.33
25	a	409	BCR	C23-C22	-4.41	1.36	1.45
23	B	604	CLA	CHD-C1D	4.41	1.46	1.38
23	D	403	CLA	CHD-C1D	4.41	1.46	1.38
25	t	102	BCR	C23-C22	-4.41	1.36	1.45
23	b	612	CLA	O2D-CGD	4.40	1.43	1.33
23	c	506	CLA	CHD-C1D	4.40	1.46	1.38
23	a	405[B]	CLA	C3D-C2D	4.40	1.51	1.39
23	c	504	CLA	CHD-C1D	4.40	1.46	1.38
23	A	406[B]	CLA	CHD-C1D	4.39	1.46	1.38
32	a	419[A]	LHG	O8-C23	4.39	1.46	1.33
23	C	507	CLA	CHD-C1D	4.39	1.46	1.38
23	b	610	CLA	CHD-C1D	4.39	1.46	1.38
34	B	620	LMG	O8-C28	4.39	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	405[A]	CLA	C3D-C2D	4.38	1.51	1.39
23	c	506	CLA	C1D-ND	4.38	1.43	1.37
23	B	616	CLA	C1D-ND	4.38	1.43	1.37
26	A	412	SQD	O48-C23	4.37	1.46	1.33
32	a	419[B]	LHG	O8-C23	4.37	1.46	1.33
23	C	502	CLA	CHD-C1D	4.37	1.46	1.38
23	c	514	CLA	CHD-C1D	4.37	1.46	1.38
23	B	608	CLA	CHC-C1C	4.36	1.46	1.35
23	C	508	CLA	O2D-CGD	4.36	1.43	1.33
26	b	620	SQD	O47-C7	4.36	1.46	1.34
23	B	602	CLA	CHD-C1D	4.36	1.46	1.38
23	C	514	CLA	CHD-C1D	4.36	1.46	1.38
25	Y	101	BCR	C23-C22	-4.36	1.36	1.45
23	B	611	CLA	O2D-CGD	4.36	1.43	1.33
24	a	407[A]	PHO	OBD-CAD	4.36	1.28	1.22
23	d	403	CLA	CHD-C1D	4.35	1.46	1.38
23	A	405[A]	CLA	O2D-CGD	4.35	1.43	1.33
23	C	510	CLA	CHD-C1D	4.34	1.46	1.38
23	C	508	CLA	C1D-ND	4.34	1.43	1.37
23	C	509	CLA	C3D-C2D	4.33	1.51	1.39
23	C	512	CLA	C1D-ND	4.33	1.43	1.37
23	b	601	CLA	CHD-C1D	4.33	1.46	1.38
23	b	608	CLA	C1D-ND	4.32	1.43	1.37
24	A	417[A]	PHO	OBD-CAD	4.31	1.28	1.22
26	b	620	SQD	O48-C23	4.31	1.45	1.33
23	c	513	CLA	CHD-C1D	4.31	1.46	1.38
23	B	609	CLA	C1D-ND	4.31	1.43	1.37
32	d	407[A]	LHG	O8-C23	4.31	1.45	1.33
36	c	519	DGD	O1G-C1A	4.31	1.45	1.33
23	c	503	CLA	O2A-CGA	4.30	1.45	1.33
23	d	403	CLA	O2A-CGA	4.30	1.45	1.33
23	b	602	CLA	CHD-C4C	4.29	1.49	1.39
23	b	609	CLA	OBD-CAD	4.28	1.29	1.22
23	A	406[B]	CLA	C1D-ND	4.28	1.43	1.37
23	c	507	CLA	O2A-CGA	4.27	1.45	1.33
23	c	503	CLA	C1D-ND	4.27	1.43	1.37
23	D	402[A]	CLA	C1D-ND	4.27	1.43	1.37
23	C	504	CLA	O2D-CGD	4.27	1.43	1.33
23	b	612	CLA	C1D-ND	4.26	1.43	1.37
23	B	609	CLA	CHD-C1D	4.26	1.46	1.38
23	A	408	CLA	O2A-CGA	4.25	1.45	1.33
23	A	405[B]	CLA	CHD-C1D	4.24	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	408	CLA	C1D-ND	4.24	1.43	1.37
23	C	511	CLA	CHD-C4C	4.24	1.48	1.39
25	b	618	BCR	C23-C22	-4.23	1.36	1.45
23	b	601	CLA	C3D-C2D	4.23	1.50	1.39
23	A	404[A]	CLA	C1D-ND	4.22	1.43	1.37
23	D	402[A]	CLA	O2A-CGA	4.22	1.45	1.33
34	Z	101	LMG	O7-C10	4.22	1.46	1.34
23	b	610	CLA	C1D-ND	4.22	1.43	1.37
23	c	504	CLA	O2D-CGD	4.22	1.43	1.33
34	m	101	LMG	O8-C28	4.21	1.45	1.33
24	A	407[B]	PHO	OBD-CAD	4.21	1.28	1.22
23	a	408	CLA	O2A-CGA	4.21	1.45	1.33
23	c	505	CLA	CHD-C1D	4.21	1.46	1.38
23	B	613	CLA	C3D-C2D	4.20	1.50	1.39
23	c	510	CLA	CHD-C1D	4.20	1.46	1.38
23	C	514	CLA	O2A-CGA	4.20	1.45	1.33
23	c	503	CLA	CHD-C1D	4.20	1.46	1.38
34	c	521	LMG	O8-C28	4.20	1.45	1.33
23	B	615	CLA	CHD-C1D	4.20	1.46	1.38
26	f	102	SQD	O48-C23	4.19	1.45	1.33
23	d	403	CLA	O2D-CGD	4.19	1.43	1.33
23	B	611	CLA	C1C-C2C	4.19	1.52	1.44
23	c	512	CLA	O2A-CGA	4.19	1.45	1.33
32	E	101[A]	LHG	O7-C7	4.19	1.46	1.34
23	C	512	CLA	CHD-C1D	4.19	1.46	1.38
23	B	609	CLA	O2A-CGA	4.19	1.45	1.33
23	C	508	CLA	O2A-CGA	4.19	1.45	1.33
26	L	101	SQD	O48-C23	4.19	1.45	1.33
24	a	407[B]	PHO	OBD-CAD	4.19	1.28	1.22
23	C	512	CLA	O2A-CGA	4.19	1.45	1.33
23	d	402[B]	CLA	O2A-CGA	4.18	1.45	1.33
23	A	406[A]	CLA	CHD-C1D	4.18	1.46	1.38
23	D	402[B]	CLA	O2A-CGA	4.18	1.45	1.33
23	c	508	CLA	CHD-C1D	4.18	1.46	1.38
34	c	520	LMG	O7-C10	4.18	1.46	1.34
23	c	509	CLA	C3D-C2D	4.17	1.50	1.39
23	c	504	CLA	O2A-CGA	4.17	1.45	1.33
23	C	513	CLA	O2A-CGA	4.17	1.45	1.33
23	c	504	CLA	CHD-C4C	4.17	1.48	1.39
23	C	509	CLA	O2A-CGA	4.16	1.45	1.33
23	c	508	CLA	O2A-CGA	4.16	1.45	1.33
23	B	607	CLA	O2D-CGD	4.15	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	406[A]	CLA	C1D-ND	4.15	1.42	1.37
23	A	404[B]	CLA	CHD-C1D	4.15	1.46	1.38
32	E	101[B]	LHG	O7-C7	4.15	1.46	1.34
34	C	520	LMG	O8-C28	4.15	1.45	1.33
23	B	609	CLA	C3D-C2D	4.15	1.50	1.39
23	d	403	CLA	C3D-C2D	4.15	1.50	1.39
36	C	517[B]	DGD	O2G-C1B	4.15	1.46	1.34
23	B	614	CLA	CHD-C4C	4.14	1.48	1.39
23	C	514	CLA	CHD-C4C	4.14	1.48	1.39
23	c	508	CLA	OBD-CAD	4.14	1.29	1.22
32	a	419[B]	LHG	O7-C7	4.14	1.46	1.34
24	A	407[A]	PHO	OBD-CAD	4.14	1.28	1.22
23	C	502	CLA	O2A-CGA	4.14	1.45	1.33
23	c	509	CLA	O2A-CGA	4.14	1.45	1.33
23	B	608	CLA	CHD-C1D	4.14	1.46	1.38
23	c	513	CLA	CHD-C4C	4.13	1.48	1.39
32	a	419[A]	LHG	O7-C7	4.13	1.46	1.34
23	a	405[B]	CLA	O2A-CGA	4.13	1.45	1.33
23	C	503	CLA	CHD-C1D	4.13	1.46	1.38
23	a	406[A]	CLA	O2A-CGA	4.12	1.45	1.33
23	C	504	CLA	CHD-C1D	4.12	1.46	1.38
23	B	606	CLA	CHD-C1D	4.12	1.46	1.38
23	b	608	CLA	O2A-CGA	4.11	1.45	1.33
36	C	519	DGD	O1G-C1A	4.11	1.45	1.33
23	C	513	CLA	CHD-C1D	4.11	1.46	1.38
36	c	518[B]	DGD	O1G-C1A	4.11	1.45	1.33
23	a	404[B]	CLA	CHD-C4C	4.11	1.48	1.39
26	A	412	SQD	O47-C7	4.11	1.45	1.34
23	A	405[B]	CLA	C3D-C2D	4.10	1.50	1.39
23	c	512	CLA	CHD-C1D	4.10	1.46	1.38
23	c	511	CLA	C3D-C2D	4.10	1.50	1.39
23	a	406[B]	CLA	O2A-CGA	4.10	1.45	1.33
34	c	501	LMG	O7-C10	4.10	1.45	1.34
23	A	405[B]	CLA	O2A-CGA	4.10	1.45	1.33
23	C	502	CLA	O2D-CGD	4.09	1.43	1.33
36	c	517[A]	DGD	O2G-C1B	4.09	1.45	1.34
23	B	610	CLA	CHD-C1D	4.09	1.46	1.38
23	b	615	CLA	CHD-C1D	4.09	1.46	1.38
23	B	603	CLA	CHD-C1D	4.09	1.46	1.38
23	b	613	CLA	C3D-C2D	4.09	1.50	1.39
23	a	405[A]	CLA	O2A-CGA	4.08	1.45	1.33
23	C	508	CLA	CHD-C1D	4.08	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	410[B]	SQD	O47-C7	4.08	1.45	1.34
32	L	102[B]	LHG	O8-C23	4.08	1.45	1.33
26	a	410[B]	SQD	O48-C23	4.08	1.45	1.33
23	b	611	CLA	C1D-ND	4.08	1.42	1.37
26	a	410[A]	SQD	O47-C7	4.07	1.45	1.34
26	a	411	SQD	O47-C7	4.07	1.45	1.34
23	c	502	CLA	CHD-C1D	4.06	1.46	1.38
23	B	613	CLA	CHD-C1D	4.06	1.46	1.38
34	C	520	LMG	O7-C10	4.06	1.45	1.34
23	b	616	CLA	CHD-C1D	4.06	1.46	1.38
36	C	517[A]	DGD	O2G-C1B	4.06	1.45	1.34
34	z	101	LMG	O7-C10	4.05	1.45	1.34
23	a	404[B]	CLA	CHD-C1D	4.05	1.46	1.38
23	b	608	CLA	CHD-C1D	4.05	1.46	1.38
23	A	405[A]	CLA	C3D-C2D	4.05	1.50	1.39
23	d	402[A]	CLA	O2A-CGA	4.05	1.45	1.33
23	C	506	CLA	CHD-C1D	4.05	1.46	1.38
23	C	512	CLA	CHD-C4C	4.05	1.48	1.39
23	B	616	CLA	C3D-C2D	4.04	1.50	1.39
25	B	618	BCR	C23-C22	-4.04	1.37	1.45
23	c	507	CLA	CHD-C1D	4.04	1.46	1.38
23	c	505	CLA	C3D-C2D	4.04	1.50	1.39
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
34	c	501	LMG	O8-C28	4.03	1.45	1.33
23	b	601	CLA	CHD-C4C	4.03	1.48	1.39
23	b	607	CLA	C3D-C2D	4.03	1.50	1.39
23	C	503	CLA	C3D-C2D	4.03	1.50	1.39
23	C	509	CLA	CHD-C1D	4.03	1.46	1.38
36	C	518[B]	DGD	O1G-C1A	4.03	1.45	1.33
23	D	403	CLA	CHD-C4C	4.02	1.48	1.39
34	C	501	LMG	O7-C10	4.02	1.45	1.34
23	b	603	CLA	CHD-C1D	4.02	1.46	1.38
23	A	406[A]	CLA	C1D-ND	4.02	1.42	1.37
34	C	501	LMG	O8-C28	4.02	1.45	1.33
23	b	612	CLA	CHD-C1D	4.02	1.46	1.38
36	c	517[B]	DGD	O2G-C1B	4.02	1.45	1.34
23	B	615	CLA	O2A-CGA	4.02	1.45	1.33
23	A	404[B]	CLA	CHD-C4C	4.02	1.48	1.39
26	F	103	SQD	O48-C23	4.02	1.45	1.33
32	d	406[B]	LHG	O7-C7	4.01	1.45	1.34
24	A	417[B]	PHO	C3C-C2C	4.01	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	602	CLA	CHD-C4C	4.01	1.48	1.39
23	c	514	CLA	CHD-C4C	4.01	1.48	1.39
23	D	403	CLA	C3D-C2D	4.01	1.50	1.39
23	c	506	CLA	CHD-C4C	4.01	1.48	1.39
32	d	412[B]	LHG	O8-C23	4.01	1.45	1.33
23	A	406[B]	CLA	O2A-CGA	4.01	1.45	1.33
23	B	608	CLA	C3D-C2D	4.00	1.50	1.39
32	d	407[B]	LHG	O8-C23	4.00	1.45	1.33
23	B	615	CLA	CHD-C4C	4.00	1.48	1.39
23	a	404[A]	CLA	CHD-C1D	3.99	1.46	1.38
23	c	502	CLA	O2D-CGD	3.99	1.42	1.33
23	A	406[B]	CLA	C3D-C2D	3.99	1.50	1.39
34	c	520	LMG	O8-C28	3.98	1.45	1.33
23	B	601	CLA	CHD-C1D	3.98	1.46	1.38
23	c	512	CLA	CHD-C4C	3.98	1.48	1.39
32	D	407[A]	LHG	O7-C7	3.98	1.45	1.34
23	B	611	CLA	OBD-CAD	3.98	1.29	1.22
26	a	410[A]	SQD	O48-C23	3.98	1.45	1.33
23	b	615	CLA	CHD-C4C	3.98	1.48	1.39
23	b	614	CLA	CHD-C1D	3.98	1.46	1.38
23	b	615	CLA	O2A-CGA	3.98	1.45	1.33
23	C	513	CLA	C3D-C2D	3.97	1.50	1.39
23	B	603	CLA	C3D-C2D	3.97	1.50	1.39
24	a	415[A]	PHO	C3C-C2C	3.97	1.49	1.37
23	B	612	CLA	C1D-ND	3.97	1.42	1.37
32	D	407[B]	LHG	O7-C7	3.96	1.45	1.34
23	a	406[B]	CLA	C3D-C2D	3.96	1.49	1.39
23	C	505	CLA	CHD-C1D	3.96	1.46	1.38
23	c	509	CLA	OBD-CAD	3.96	1.29	1.22
23	a	404[A]	CLA	CHD-C4C	3.96	1.48	1.39
23	B	612	CLA	O2D-CGD	3.95	1.42	1.33
23	C	504	CLA	CHD-C4C	3.95	1.48	1.39
24	a	415[B]	PHO	O2A-CGA	3.95	1.44	1.33
26	A	410[B]	SQD	O48-C23	3.95	1.44	1.33
23	c	505	CLA	O2A-CGA	3.94	1.44	1.33
23	A	404[B]	CLA	C3D-C2D	3.94	1.49	1.39
23	b	606	CLA	CHD-C1D	3.94	1.46	1.38
23	C	504	CLA	O2A-CGA	3.94	1.44	1.33
23	C	514	CLA	C3D-C2D	3.94	1.49	1.39
36	h	102	DGD	O2G-C1B	3.93	1.45	1.34
23	b	616	CLA	O2A-CGA	3.93	1.44	1.33
23	B	610	CLA	C3D-C2D	3.93	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	508	CLA	C3D-C2D	3.93	1.49	1.39
23	D	402[B]	CLA	CHD-C1D	3.93	1.46	1.38
23	D	402[A]	CLA	CHD-C1D	3.92	1.46	1.38
23	C	507	CLA	O2A-CGA	3.92	1.44	1.33
32	L	102[B]	LHG	O7-C7	3.92	1.45	1.34
23	B	611	CLA	O2A-CGA	3.92	1.44	1.33
36	c	517[B]	DGD	O1G-C1A	3.92	1.44	1.33
23	b	610	CLA	OBD-CAD	3.91	1.29	1.22
23	A	406[B]	CLA	OBD-CAD	3.91	1.29	1.22
23	a	408	CLA	C1D-ND	3.91	1.42	1.37
24	a	415[B]	PHO	C3C-C2C	3.91	1.49	1.37
23	C	506	CLA	CHD-C4C	3.91	1.48	1.39
32	D	407[A]	LHG	O8-C23	3.90	1.44	1.33
23	c	507	CLA	CHD-C4C	3.90	1.48	1.39
23	c	502	CLA	O2A-CGA	3.90	1.44	1.33
23	a	406[A]	CLA	C3D-C2D	3.90	1.49	1.39
23	C	511	CLA	CHD-C1D	3.90	1.46	1.38
23	D	402[A]	CLA	CHD-C4C	3.89	1.48	1.39
23	a	405[B]	CLA	CHD-C4C	3.89	1.48	1.39
23	c	506	CLA	C3D-C2D	3.89	1.49	1.39
23	A	405[A]	CLA	C1D-ND	3.89	1.42	1.37
23	B	611	CLA	CHD-C1D	3.88	1.45	1.38
23	B	607	CLA	CHD-C1D	3.88	1.45	1.38
36	h	102	DGD	O1G-C1A	3.87	1.44	1.33
23	C	509	CLA	OBD-CAD	3.87	1.29	1.22
23	D	402[B]	CLA	CHD-C4C	3.87	1.48	1.39
23	c	510	CLA	O2A-CGA	3.87	1.44	1.33
23	B	615	CLA	OBD-CAD	3.87	1.29	1.22
23	A	405[B]	CLA	CHD-C4C	3.86	1.48	1.39
24	A	407[B]	PHO	O2A-CGA	3.86	1.44	1.33
23	c	508	CLA	CHD-C4C	3.86	1.48	1.39
34	B	620	LMG	O7-C10	3.86	1.45	1.34
23	B	602	CLA	C3D-C2D	3.86	1.49	1.39
23	C	503	CLA	O2A-CGA	3.86	1.44	1.33
23	C	510	CLA	O2A-CGA	3.86	1.44	1.33
23	b	602	CLA	OBD-CAD	3.86	1.29	1.22
23	c	510	CLA	C3D-C2D	3.86	1.49	1.39
24	A	417[A]	PHO	O2A-CGA	3.86	1.44	1.33
23	C	510	CLA	C3D-C2D	3.85	1.49	1.39
23	b	616	CLA	C3D-C2D	3.85	1.49	1.39
23	c	507	CLA	C3D-C2D	3.85	1.49	1.39
23	B	615	CLA	C3D-C2D	3.85	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	518[A]	DGD	O2G-C1B	3.85	1.45	1.34
23	b	611	CLA	CHD-C4C	3.85	1.48	1.39
26	A	410[A]	SQD	O48-C23	3.85	1.44	1.33
23	C	507	CLA	CHD-C4C	3.84	1.48	1.39
23	b	609	CLA	C3D-C2D	3.84	1.49	1.39
32	d	407[B]	LHG	O7-C7	3.84	1.45	1.34
23	b	612	CLA	C3D-C2D	3.84	1.49	1.39
23	B	606	CLA	O2A-CGA	3.84	1.44	1.33
32	L	102[A]	LHG	O8-C23	3.84	1.44	1.33
23	A	406[A]	CLA	C3D-C2D	3.84	1.49	1.39
23	b	612	CLA	OBD-CAD	3.84	1.29	1.22
36	c	518[A]	DGD	O1G-C1A	3.83	1.44	1.33
32	D	407[B]	LHG	O8-C23	3.83	1.44	1.33
23	b	603	CLA	CHD-C4C	3.83	1.48	1.39
23	A	405[A]	CLA	O2A-CGA	3.83	1.44	1.33
23	B	616	CLA	O2A-CGA	3.83	1.44	1.33
23	C	505	CLA	C3D-C2D	3.83	1.49	1.39
35	b	623	HTG	C1'-S1	-3.83	1.76	1.81
23	a	405[B]	CLA	CHD-C1D	3.83	1.45	1.38
24	a	415[A]	PHO	O2A-CGA	3.83	1.44	1.33
23	B	607	CLA	CHD-C4C	3.83	1.48	1.39
23	b	605	CLA	CHD-C4C	3.83	1.48	1.39
24	A	417[B]	PHO	O2A-CGA	3.82	1.44	1.33
23	b	610	CLA	CHD-C4C	3.82	1.48	1.39
32	L	102[A]	LHG	O7-C7	3.82	1.45	1.34
23	a	404[B]	CLA	OBD-CAD	3.81	1.29	1.22
23	A	406[B]	CLA	CHD-C4C	3.81	1.47	1.39
32	d	412[B]	LHG	O7-C7	3.81	1.45	1.34
23	d	402[A]	CLA	CHD-C1D	3.81	1.45	1.38
23	b	607	CLA	CHD-C4C	3.80	1.47	1.39
36	C	517[B]	DGD	O1G-C1A	3.80	1.44	1.33
23	c	502	CLA	CHD-C4C	3.80	1.47	1.39
23	b	602	CLA	O2A-CGA	3.80	1.44	1.33
23	A	406[A]	CLA	O2A-CGA	3.80	1.44	1.33
23	C	506	CLA	O2A-CGA	3.80	1.44	1.33
23	a	405[A]	CLA	CHD-C1D	3.80	1.45	1.38
34	d	410	LMG	O8-C28	3.79	1.44	1.33
23	C	512	CLA	C3D-C2D	3.79	1.49	1.39
23	C	502	CLA	CHD-C4C	3.79	1.47	1.39
23	c	502	CLA	C3D-C2D	3.79	1.49	1.39
24	A	417[A]	PHO	CHA-CBD	-3.79	1.47	1.52
23	a	408	CLA	CHD-C1D	3.79	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	H	102	DGD	O1G-C1A	3.79	1.44	1.33
36	C	518[B]	DGD	O2G-C1B	3.78	1.45	1.34
23	b	608	CLA	CHD-C4C	3.78	1.47	1.39
23	C	513	CLA	CHD-C4C	3.78	1.47	1.39
23	c	509	CLA	CHD-C4C	3.78	1.47	1.39
23	c	503	CLA	C3D-C2D	3.78	1.49	1.39
24	a	407[B]	PHO	C3C-C2C	3.78	1.48	1.37
23	b	603	CLA	C3D-C2D	3.78	1.49	1.39
23	a	405[A]	CLA	OBD-CAD	3.77	1.29	1.22
34	d	410	LMG	O7-C10	3.77	1.44	1.34
23	A	408	CLA	CHD-C1D	3.77	1.45	1.38
23	a	404[B]	CLA	C3D-C2D	3.77	1.49	1.39
36	c	518[B]	DGD	O2G-C1B	3.77	1.44	1.34
23	B	612	CLA	CHD-C1D	3.76	1.45	1.38
23	A	408	CLA	CHD-C4C	3.76	1.47	1.39
23	b	609	CLA	O2A-CGA	3.76	1.44	1.33
23	c	511	CLA	O2A-CGA	3.76	1.44	1.33
23	b	608	CLA	C3D-C2D	3.76	1.49	1.39
23	b	602	CLA	C3D-C2D	3.75	1.49	1.39
32	A	419[B]	LHG	O8-C23	3.75	1.44	1.33
23	B	614	CLA	O2A-CGA	3.75	1.44	1.33
32	b	630[B]	LHG	O7-C7	3.75	1.44	1.34
32	d	412[A]	LHG	O8-C23	3.75	1.44	1.33
24	A	407[B]	PHO	C3C-C2C	3.75	1.48	1.37
23	D	402[B]	CLA	C3D-C2D	3.75	1.49	1.39
23	a	406[B]	CLA	CHD-C4C	3.74	1.47	1.39
23	C	510	CLA	OBD-CAD	3.74	1.28	1.22
23	B	605	CLA	C3D-C2D	3.74	1.49	1.39
24	a	407[B]	PHO	O2A-CGA	3.74	1.44	1.33
23	c	514	CLA	C3D-C2D	3.74	1.49	1.39
23	b	604	CLA	CHD-C4C	3.74	1.47	1.39
23	A	406[A]	CLA	OBD-CAD	3.74	1.28	1.22
23	C	510	CLA	CHD-C4C	3.73	1.47	1.39
23	A	404[A]	CLA	CHD-C4C	3.73	1.47	1.39
23	B	610	CLA	CHD-C4C	3.73	1.47	1.39
23	b	608	CLA	OBD-CAD	3.73	1.28	1.22
36	C	519	DGD	O2G-C1B	3.73	1.44	1.34
23	b	605	CLA	CHD-C1D	3.73	1.45	1.38
32	D	406[B]	LHG	O7-C7	3.73	1.44	1.34
23	b	611	CLA	C3D-C2D	3.73	1.49	1.39
23	C	513	CLA	OBD-CAD	3.73	1.28	1.22
23	C	503	CLA	CHD-C4C	3.72	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402[B]	CLA	CHD-C1D	3.72	1.45	1.38
32	d	406[A]	LHG	O7-C7	3.72	1.44	1.34
23	c	510	CLA	CHD-C4C	3.72	1.47	1.39
23	D	403	CLA	O2A-CGA	3.72	1.44	1.33
23	A	405[A]	CLA	CHD-C1D	3.72	1.45	1.38
23	b	606	CLA	O2A-CGA	3.72	1.44	1.33
23	B	612	CLA	O2A-CGA	3.72	1.44	1.33
36	C	518[A]	DGD	O1G-C1A	3.71	1.44	1.33
23	B	613	CLA	OBD-CAD	3.71	1.28	1.22
23	B	605	CLA	O2A-CGA	3.71	1.44	1.33
23	C	507	CLA	C3D-C2D	3.71	1.49	1.39
23	B	607	CLA	C1D-ND	3.70	1.42	1.37
23	d	402[B]	CLA	CHD-C4C	3.70	1.47	1.39
32	b	630[B]	LHG	O8-C23	3.70	1.44	1.33
26	A	410[B]	SQD	O47-C7	3.70	1.44	1.34
23	b	614	CLA	O2A-CGA	3.70	1.44	1.33
23	b	604	CLA	C3D-C2D	3.70	1.49	1.39
23	C	506	CLA	C3D-C2D	3.69	1.49	1.39
23	C	505	CLA	O2A-CGA	3.69	1.44	1.33
23	b	603	CLA	O2A-CGA	3.69	1.44	1.33
24	A	407[A]	PHO	C3C-C2C	3.68	1.48	1.37
23	b	605	CLA	C3D-C2D	3.68	1.49	1.39
23	b	606	CLA	C3D-C2D	3.68	1.49	1.39
35	b	622	HTG	C1'-S1	-3.68	1.76	1.81
26	A	410[A]	SQD	O47-C7	3.68	1.44	1.34
23	B	605	CLA	CHD-C4C	3.68	1.47	1.39
23	a	406[A]	CLA	OBD-CAD	3.68	1.28	1.22
23	B	601	CLA	CHD-C4C	3.68	1.47	1.39
35	o	301	HTG	C1'-S1	-3.68	1.76	1.81
23	D	403	CLA	OBD-CAD	3.67	1.28	1.22
23	C	508	CLA	C3D-C2D	3.67	1.49	1.39
23	c	504	CLA	C3D-C2D	3.67	1.49	1.39
23	C	503	CLA	OBD-CAD	3.67	1.28	1.22
23	A	406[A]	CLA	CHD-C4C	3.67	1.47	1.39
23	B	608	CLA	O2A-CGA	3.67	1.44	1.33
23	B	607	CLA	OBD-CAD	3.67	1.28	1.22
23	a	406[B]	CLA	CHD-C1D	3.66	1.45	1.38
23	c	513	CLA	C3D-C2D	3.66	1.49	1.39
23	a	404[A]	CLA	C3D-C2D	3.66	1.49	1.39
23	b	601	CLA	OBD-CAD	3.66	1.28	1.22
32	d	407[A]	LHG	O7-C7	3.66	1.44	1.34
23	c	513	CLA	OBD-CAD	3.65	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	614	CLA	C3D-C2D	3.65	1.49	1.39
23	B	604	CLA	O2A-CGA	3.65	1.44	1.33
23	d	403	CLA	CHD-C4C	3.65	1.47	1.39
23	b	614	CLA	CHD-C4C	3.64	1.47	1.39
24	A	407[A]	PHO	O2A-CGA	3.64	1.44	1.33
23	b	613	CLA	CHD-C4C	3.64	1.47	1.39
23	c	512	CLA	OBD-CAD	3.64	1.28	1.22
23	B	605	CLA	CHD-C1D	3.64	1.45	1.38
23	A	404[A]	CLA	C3D-C2D	3.63	1.49	1.39
23	D	402[B]	CLA	OBD-CAD	3.63	1.28	1.22
23	b	616	CLA	CHD-C4C	3.63	1.47	1.39
23	a	408	CLA	OBD-CAD	3.63	1.28	1.22
23	b	611	CLA	CHD-C1D	3.63	1.45	1.38
23	B	602	CLA	O2A-CGA	3.62	1.43	1.33
23	B	601	CLA	C3D-C2D	3.62	1.49	1.39
24	a	407[A]	PHO	C3C-C2C	3.62	1.48	1.37
36	c	517[A]	DGD	O1G-C1A	3.62	1.43	1.33
23	a	405[A]	CLA	CHD-C4C	3.62	1.47	1.39
23	b	616	CLA	OBD-CAD	3.62	1.28	1.22
23	c	506	CLA	OBD-CAD	3.62	1.28	1.22
23	b	615	CLA	C3D-C2D	3.62	1.49	1.39
32	b	630[A]	LHG	O7-C7	3.62	1.44	1.34
23	a	404[A]	CLA	OBD-CAD	3.61	1.28	1.22
23	c	503	CLA	CHD-C4C	3.61	1.47	1.39
23	d	402[B]	CLA	C3D-C2D	3.61	1.49	1.39
23	C	505	CLA	CHD-C4C	3.61	1.47	1.39
23	a	404[B]	CLA	O2A-CGA	3.61	1.43	1.33
23	B	603	CLA	CHD-C4C	3.61	1.47	1.39
23	d	402[B]	CLA	OBD-CAD	3.60	1.28	1.22
23	c	511	CLA	CHD-C4C	3.60	1.47	1.39
23	C	511	CLA	O2A-CGA	3.60	1.43	1.33
32	d	406[B]	LHG	O8-C23	3.60	1.43	1.33
23	b	613	CLA	O2A-CGA	3.60	1.43	1.33
23	B	606	CLA	CHD-C4C	3.60	1.47	1.39
32	D	406[A]	LHG	O7-C7	3.60	1.44	1.34
23	b	605	CLA	OBD-CAD	3.60	1.28	1.22
34	m	101	LMG	O7-C10	3.60	1.44	1.34
23	b	610	CLA	C3D-C2D	3.59	1.48	1.39
23	b	606	CLA	CHD-C4C	3.59	1.47	1.39
23	c	505	CLA	CHD-C4C	3.59	1.47	1.39
23	c	505	CLA	OBD-CAD	3.59	1.28	1.22
23	B	604	CLA	CHD-C4C	3.58	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	408	CLA	C3D-C2D	3.58	1.48	1.39
23	c	507	CLA	OBD-CAD	3.58	1.28	1.22
23	a	406[A]	CLA	CHD-C4C	3.58	1.47	1.39
23	B	614	CLA	CHD-C1D	3.57	1.45	1.38
23	c	510	CLA	OBD-CAD	3.57	1.28	1.22
23	d	402[A]	CLA	CHD-C4C	3.57	1.47	1.39
23	B	614	CLA	C3D-C2D	3.57	1.48	1.39
23	A	405[A]	CLA	CHD-C4C	3.56	1.47	1.39
23	B	603	CLA	OBD-CAD	3.55	1.28	1.22
36	C	517[A]	DGD	O1G-C1A	3.55	1.43	1.33
23	d	402[A]	CLA	C3D-C2D	3.55	1.48	1.39
23	B	601	CLA	OBD-CAD	3.55	1.28	1.22
23	a	406[B]	CLA	OBD-CAD	3.54	1.28	1.22
23	a	406[A]	CLA	CHD-C1D	3.54	1.45	1.38
23	B	616	CLA	CHD-C1D	3.54	1.45	1.38
23	c	506	CLA	O2A-CGA	3.54	1.43	1.33
36	c	518[A]	DGD	O2G-C1B	3.53	1.44	1.34
32	d	406[A]	LHG	O8-C23	3.53	1.43	1.33
23	a	408	CLA	CHD-C4C	3.53	1.47	1.39
32	D	406[A]	LHG	O8-C23	3.53	1.43	1.33
23	B	606	CLA	C3D-C2D	3.53	1.48	1.39
38	f	101	HEM	C4D-ND	-3.52	1.34	1.40
32	A	419[A]	LHG	O8-C23	3.52	1.43	1.33
23	C	502	CLA	C3D-C2D	3.52	1.48	1.39
23	B	609	CLA	CHD-C4C	3.51	1.47	1.39
23	c	511	CLA	CHD-C1D	3.51	1.45	1.38
32	A	419[B]	LHG	O7-C7	3.51	1.44	1.34
32	d	412[A]	LHG	O7-C7	3.50	1.44	1.34
23	c	512	CLA	C3D-C2D	3.50	1.48	1.39
32	A	419[A]	LHG	O7-C7	3.49	1.44	1.34
32	b	630[A]	LHG	O8-C23	3.49	1.43	1.33
23	b	604	CLA	O2A-CGA	3.49	1.43	1.33
23	A	404[B]	CLA	OBD-CAD	3.49	1.28	1.22
23	b	609	CLA	CHD-C4C	3.49	1.47	1.39
23	c	503	CLA	OBD-CAD	3.49	1.28	1.22
23	C	507	CLA	OBD-CAD	3.48	1.28	1.22
23	B	612	CLA	C3D-C2D	3.48	1.48	1.39
23	a	408	CLA	C3D-C2D	3.47	1.48	1.39
23	C	514	CLA	OBD-CAD	3.47	1.28	1.22
23	B	604	CLA	OBD-CAD	3.46	1.28	1.22
34	D	411	LMG	O7-C10	3.46	1.44	1.34
32	D	406[B]	LHG	O8-C23	3.46	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	611	CLA	CHD-C4C	3.46	1.47	1.39
36	H	102	DGD	O2G-C1B	3.45	1.44	1.34
23	A	405[B]	CLA	OBD-CAD	3.43	1.28	1.22
23	D	402[A]	CLA	C3D-C2D	3.43	1.48	1.39
23	b	613	CLA	CHD-C1D	3.42	1.45	1.38
38	F	102	HEM	C1B-NB	-3.42	1.34	1.40
23	d	402[A]	CLA	OBD-CAD	3.41	1.28	1.22
23	A	408	CLA	OBD-CAD	3.41	1.28	1.22
23	A	404[B]	CLA	O2A-CGA	3.41	1.43	1.33
23	b	604	CLA	OBD-CAD	3.41	1.28	1.22
23	a	405[B]	CLA	OBD-CAD	3.40	1.28	1.22
23	B	613	CLA	O2A-CGA	3.40	1.43	1.33
23	B	610	CLA	O2A-CGA	3.40	1.43	1.33
23	C	509	CLA	CHD-C4C	3.40	1.47	1.39
24	a	407[A]	PHO	O2A-CGA	3.39	1.43	1.33
23	B	608	CLA	CHD-C4C	3.38	1.46	1.39
23	C	504	CLA	C3D-C2D	3.37	1.48	1.39
23	B	612	CLA	CHD-C4C	3.37	1.46	1.39
23	C	512	CLA	OBD-CAD	3.37	1.28	1.22
23	B	612	CLA	OBD-CAD	3.37	1.28	1.22
23	C	511	CLA	C3D-C2D	3.37	1.48	1.39
23	B	604	CLA	C3D-C2D	3.36	1.48	1.39
23	C	508	CLA	CHD-C4C	3.35	1.46	1.39
23	b	614	CLA	OBD-CAD	3.35	1.28	1.22
23	c	514	CLA	OBD-CAD	3.35	1.28	1.22
23	b	615	CLA	OBD-CAD	3.34	1.28	1.22
23	A	404[A]	CLA	OBD-CAD	3.34	1.28	1.22
23	B	603	CLA	O2A-CGA	3.34	1.43	1.33
34	D	411	LMG	O8-C28	3.33	1.43	1.33
23	b	612	CLA	O2A-CGA	3.33	1.43	1.33
36	c	519	DGD	O2G-C1B	3.32	1.43	1.34
23	b	612	CLA	CHD-C4C	3.31	1.46	1.39
23	b	606	CLA	OBD-CAD	3.31	1.28	1.22
23	B	607	CLA	O2A-CGA	3.31	1.43	1.33
23	d	403	CLA	OBD-CAD	3.30	1.28	1.22
23	b	603	CLA	OBD-CAD	3.29	1.28	1.22
23	B	611	CLA	C3D-C2D	3.29	1.48	1.39
23	B	607	CLA	C3D-C2D	3.28	1.48	1.39
23	d	402[A]	CLA	C1D-ND	3.27	1.41	1.37
23	C	506	CLA	OBD-CAD	3.27	1.28	1.22
23	D	402[A]	CLA	OBD-CAD	3.26	1.28	1.22
35	B	623	HTG	C1'-S1	-3.26	1.77	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	611	CLA	C4B-NB	-3.26	1.32	1.35
23	b	605	CLA	O2A-CGA	3.25	1.42	1.33
35	b	625	HTG	C1'-S1	-3.25	1.77	1.81
23	C	505	CLA	OBD-CAD	3.24	1.28	1.22
23	B	613	CLA	CHD-C4C	3.24	1.46	1.39
38	f	101	HEM	C1B-NB	-3.24	1.34	1.40
35	d	409	HTG	C1'-S1	-3.23	1.77	1.81
35	b	625	HTG	C1-S1	-3.23	1.75	1.80
23	B	611	CLA	C4B-CHC	3.22	1.50	1.41
38	F	102	HEM	C4D-ND	-3.21	1.34	1.40
23	c	502	CLA	OBD-CAD	3.21	1.28	1.22
23	A	404[A]	CLA	O2A-CGA	3.19	1.42	1.33
35	D	410	HTG	C1'-S1	-3.18	1.77	1.81
23	B	602	CLA	C1C-C2C	3.17	1.50	1.44
23	B	602	CLA	OBD-CAD	3.17	1.27	1.22
23	c	511	CLA	OBD-CAD	3.17	1.27	1.22
24	A	417[B]	PHO	CHA-CBD	-3.16	1.48	1.52
23	b	610	CLA	O2A-CGA	3.15	1.42	1.33
23	B	611	CLA	C1B-NB	3.15	1.38	1.35
23	C	511	CLA	OBD-CAD	3.14	1.27	1.22
35	c	522	HTG	C1'-S1	-3.13	1.77	1.81
23	B	607	CLA	C1C-C2C	3.13	1.50	1.44
23	A	405[A]	CLA	OBD-CAD	3.12	1.27	1.22
23	c	506	CLA	C4C-C3C	3.09	1.50	1.45
23	B	612	CLA	C1B-NB	-3.08	1.32	1.35
23	a	404[A]	CLA	O2A-CGA	3.07	1.42	1.33
23	b	602	CLA	C1C-C2C	3.05	1.50	1.44
23	B	616	CLA	CHD-C4C	3.04	1.46	1.39
35	C	522	HTG	C1'-S1	-3.03	1.77	1.81
23	B	614	CLA	C1B-CHB	3.03	1.49	1.41
23	C	504	CLA	OBD-CAD	3.03	1.27	1.22
23	C	513	CLA	C1C-C2C	3.02	1.50	1.44
23	C	505	CLA	C4D-CHA	3.02	1.49	1.38
23	B	606	CLA	OBD-CAD	3.01	1.27	1.22
23	C	508	CLA	OBD-CAD	3.01	1.27	1.22
23	B	614	CLA	OBD-CAD	3.01	1.27	1.22
23	c	504	CLA	OBD-CAD	3.00	1.27	1.22
23	b	607	CLA	O2A-CGA	2.99	1.42	1.33
23	B	609	CLA	OBD-CAD	2.97	1.27	1.22
23	b	607	CLA	C1B-NB	-2.97	1.32	1.35
23	b	611	CLA	OBD-CAD	2.96	1.27	1.22
23	B	606	CLA	C1C-C2C	2.96	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	404[A]	CLA	C4C-C3C	2.96	1.50	1.45
23	B	603	CLA	C1B-NB	-2.95	1.32	1.35
23	B	610	CLA	C4C-C3C	2.94	1.50	1.45
23	b	602	CLA	C4B-CHC	2.94	1.49	1.41
24	A	407[B]	PHO	CHA-CBD	-2.93	1.48	1.52
23	c	504	CLA	C1C-C2C	2.93	1.50	1.44
23	B	612	CLA	C4D-CHA	2.90	1.48	1.38
23	b	613	CLA	OBD-CAD	2.90	1.27	1.22
23	D	403	CLA	C1C-C2C	2.89	1.50	1.44
23	B	613	CLA	C1B-NB	-2.89	1.32	1.35
23	C	512	CLA	C4D-CHA	2.88	1.48	1.38
23	c	512	CLA	C1B-CHB	2.87	1.49	1.41
23	c	509	CLA	C1C-C2C	2.86	1.50	1.44
23	C	508	CLA	C1C-C2C	2.86	1.50	1.44
23	D	402[B]	CLA	C1C-C2C	2.86	1.50	1.44
23	b	609	CLA	C1B-CHB	2.86	1.48	1.41
23	B	616	CLA	C4D-CHA	2.85	1.48	1.38
23	b	607	CLA	OBD-CAD	2.84	1.27	1.22
23	c	506	CLA	C1C-C2C	2.84	1.50	1.44
23	c	505	CLA	C1C-C2C	2.83	1.50	1.44
23	B	612	CLA	C1B-CHB	2.83	1.48	1.41
24	A	407[A]	PHO	CBD-CGD	-2.83	1.48	1.52
23	c	504	CLA	C4B-CHC	2.83	1.48	1.41
23	b	612	CLA	C1C-C2C	2.82	1.50	1.44
23	B	612	CLA	C1C-C2C	2.82	1.50	1.44
23	C	508	CLA	C4D-CHA	2.82	1.48	1.38
23	B	607	CLA	C1B-NB	-2.82	1.32	1.35
23	C	511	CLA	C1B-CHB	2.81	1.48	1.41
23	c	508	CLA	C1C-C2C	2.81	1.50	1.44
23	b	604	CLA	C4B-CHC	2.80	1.48	1.41
23	C	507	CLA	C4C-C3C	2.80	1.49	1.45
23	B	601	CLA	C1C-C2C	2.79	1.50	1.44
24	a	415[B]	PHO	CHA-CBD	-2.79	1.49	1.52
23	A	408	CLA	C4D-CHA	2.79	1.48	1.38
26	a	410[B]	SQD	C6-S	-2.78	1.67	1.77
23	B	612	CLA	C4B-NB	-2.78	1.32	1.35
23	c	511	CLA	C1C-C2C	2.78	1.50	1.44
23	C	511	CLA	C4C-C3C	2.78	1.49	1.45
34	Z	101	LMG	O8-C28	2.77	1.47	1.33
23	B	604	CLA	C1B-CHB	2.76	1.48	1.41
29	A	414[A]	PL9	C6-C5	2.76	1.49	1.35
23	C	505	CLA	C1B-CHB	2.76	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	610	CLA	C1C-C2C	2.76	1.49	1.44
23	c	511	CLA	C1B-CHB	2.76	1.48	1.41
23	c	510	CLA	C4C-C3C	2.76	1.49	1.45
23	b	604	CLA	C1B-CHB	2.75	1.48	1.41
29	a	413[A]	PL9	C6-C5	2.75	1.49	1.35
23	B	605	CLA	OBD-CAD	2.75	1.27	1.22
23	d	402[A]	CLA	C1B-CHB	2.75	1.48	1.41
23	d	402[B]	CLA	C1B-CHB	2.75	1.48	1.41
23	C	505	CLA	C1C-C2C	2.75	1.49	1.44
23	b	604	CLA	C4D-CHA	2.75	1.48	1.38
23	c	508	CLA	C4D-CHA	2.75	1.48	1.38
23	C	504	CLA	C4D-CHA	2.74	1.48	1.38
36	H	102	DGD	O5D-C1E	2.74	1.44	1.40
23	B	614	CLA	C1C-C2C	2.73	1.49	1.44
26	a	410[A]	SQD	C6-S	-2.73	1.67	1.77
23	B	613	CLA	C1C-C2C	2.73	1.49	1.44
29	a	413[B]	PL9	C6-C5	2.73	1.49	1.35
23	c	506	CLA	C4D-CHA	2.73	1.48	1.38
23	C	513	CLA	C4B-CHC	2.73	1.48	1.41
26	A	410[A]	SQD	C6-S	-2.73	1.67	1.77
23	c	506	CLA	C4B-CHC	2.73	1.48	1.41
23	C	502	CLA	C4D-CHA	2.73	1.48	1.38
23	A	406[A]	CLA	C4D-CHA	2.72	1.48	1.38
23	a	406[A]	CLA	C1C-C2C	2.72	1.49	1.44
23	b	607	CLA	C4D-CHA	2.72	1.48	1.38
23	B	608	CLA	OBD-CAD	2.72	1.27	1.22
23	c	509	CLA	C4D-CHA	2.72	1.48	1.38
23	B	613	CLA	C4C-C3C	2.72	1.49	1.45
23	B	609	CLA	C1C-C2C	2.72	1.49	1.44
23	D	402[B]	CLA	C1B-CHB	2.72	1.48	1.41
23	b	616	CLA	C1C-C2C	2.72	1.49	1.44
23	b	612	CLA	C1B-CHB	2.72	1.48	1.41
23	B	601	CLA	C4B-CHC	2.72	1.48	1.41
23	c	514	CLA	C1C-C2C	2.72	1.49	1.44
23	C	511	CLA	C1C-C2C	2.72	1.49	1.44
23	D	402[A]	CLA	C4D-CHA	2.71	1.48	1.38
23	c	505	CLA	C4C-C3C	2.71	1.49	1.45
23	b	613	CLA	C4D-CHA	2.71	1.48	1.38
23	a	406[B]	CLA	C1C-C2C	2.71	1.49	1.44
26	A	410[B]	SQD	C6-S	-2.71	1.67	1.77
23	C	504	CLA	C4B-CHC	2.71	1.48	1.41
23	D	402[A]	CLA	C1B-CHB	2.70	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	C1C-C2C	2.70	1.49	1.44
23	a	408	CLA	C1C-C2C	2.70	1.49	1.44
24	a	415[B]	PHO	C3A-C2A	-2.70	1.52	1.54
23	B	608	CLA	C4D-CHA	2.70	1.48	1.38
23	C	509	CLA	C4D-CHA	2.70	1.48	1.38
23	b	610	CLA	C4D-CHA	2.69	1.48	1.38
23	D	403	CLA	C4C-C3C	2.69	1.49	1.45
23	B	616	CLA	OBD-CAD	2.69	1.27	1.22
23	B	614	CLA	C4B-NB	-2.69	1.32	1.35
23	B	614	CLA	C4D-CHA	2.69	1.48	1.38
23	d	403	CLA	C4D-CHA	2.69	1.48	1.38
23	A	405[A]	CLA	C4D-CHA	2.68	1.47	1.38
29	A	414[B]	PL9	C6-C5	2.68	1.49	1.35
23	B	605	CLA	C4B-CHC	2.68	1.48	1.41
23	C	506	CLA	C4B-CHC	2.68	1.48	1.41
23	C	502	CLA	OBD-CAD	2.68	1.27	1.22
23	c	511	CLA	C4D-CHA	2.68	1.47	1.38
23	b	609	CLA	C4D-CHA	2.67	1.47	1.38
23	B	610	CLA	C4D-CHA	2.67	1.47	1.38
23	c	513	CLA	C4B-CHC	2.67	1.48	1.41
23	A	405[B]	CLA	C4D-CHA	2.67	1.47	1.38
23	d	403	CLA	C1C-C2C	2.67	1.49	1.44
26	f	102	SQD	C6-S	-2.67	1.67	1.77
23	B	605	CLA	C1B-CHB	2.66	1.48	1.41
23	B	609	CLA	C4B-CHC	2.66	1.48	1.41
23	b	610	CLA	C1B-CHB	2.66	1.48	1.41
23	B	603	CLA	C4C-C3C	2.66	1.49	1.45
23	b	610	CLA	C3D-C4D	-2.66	1.38	1.44
23	B	613	CLA	C4D-CHA	2.65	1.47	1.38
38	F	102	HEM	FE-NB	2.65	2.10	1.96
23	C	506	CLA	C4D-CHA	2.65	1.47	1.38
23	b	611	CLA	C1B-CHB	2.65	1.48	1.41
23	B	614	CLA	C3D-C4D	-2.65	1.38	1.44
23	C	506	CLA	C1C-C2C	2.65	1.49	1.44
23	B	610	CLA	C3D-C4D	-2.65	1.38	1.44
23	C	513	CLA	C4D-CHA	2.65	1.47	1.38
23	c	504	CLA	C4D-CHA	2.64	1.47	1.38
23	c	510	CLA	C1B-CHB	2.64	1.48	1.41
26	a	411	SQD	C6-S	-2.63	1.67	1.77
23	c	504	CLA	C1B-CHB	2.63	1.48	1.41
23	C	507	CLA	C4D-CHA	2.63	1.47	1.38
23	c	510	CLA	C4D-CHA	2.63	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	512	CLA	C1C-C2C	2.63	1.49	1.44
23	c	503	CLA	C4D-CHA	2.62	1.47	1.38
38	f	101	HEM	FE-NB	2.62	2.09	1.96
23	B	616	CLA	C1C-NC	-2.62	1.33	1.37
23	A	404[B]	CLA	C4D-CHA	2.62	1.47	1.38
23	B	607	CLA	C4D-CHA	2.62	1.47	1.38
23	B	605	CLA	C1C-C2C	2.62	1.49	1.44
23	a	406[A]	CLA	C4D-CHA	2.62	1.47	1.38
23	D	403	CLA	C4B-CHC	2.61	1.48	1.41
23	C	506	CLA	C1B-CHB	2.61	1.48	1.41
23	B	607	CLA	C1B-CHB	2.61	1.48	1.41
23	B	615	CLA	C1C-C2C	2.61	1.49	1.44
23	c	502	CLA	C4C-C3C	2.61	1.49	1.45
23	C	507	CLA	C3D-C4D	-2.61	1.38	1.44
23	B	606	CLA	C4D-CHA	2.61	1.47	1.38
36	c	519	DGD	O2G-C2G	-2.60	1.40	1.46
23	A	408	CLA	C3D-C4D	-2.60	1.38	1.44
23	C	510	CLA	C1B-CHB	2.60	1.48	1.41
26	A	412	SQD	C6-S	-2.60	1.67	1.77
23	c	509	CLA	C4B-CHC	2.60	1.48	1.41
23	c	502	CLA	C4D-CHA	2.60	1.47	1.38
23	C	509	CLA	C4C-C3C	2.60	1.49	1.45
23	b	606	CLA	C1C-C2C	2.59	1.49	1.44
23	c	512	CLA	C1C-C2C	2.59	1.49	1.44
23	D	402[B]	CLA	C4C-C3C	2.59	1.49	1.45
23	C	514	CLA	C4D-CHA	2.59	1.47	1.38
23	c	513	CLA	C4D-CHA	2.59	1.47	1.38
23	b	606	CLA	C4D-CHA	2.58	1.47	1.38
33	B	626	LMT	C3'-C2'	2.58	1.58	1.52
36	C	519	DGD	O2G-C2G	-2.58	1.40	1.46
23	A	406[B]	CLA	C1C-C2C	2.58	1.49	1.44
23	d	402[B]	CLA	C4D-CHA	2.58	1.47	1.38
23	C	504	CLA	C1C-C2C	2.57	1.49	1.44
23	b	613	CLA	C4B-CHC	2.57	1.48	1.41
23	C	510	CLA	C1C-C2C	2.57	1.49	1.44
23	b	610	CLA	C4B-CHC	2.57	1.48	1.41
23	B	602	CLA	C4B-CHC	2.57	1.48	1.41
23	A	404[A]	CLA	C4D-CHA	2.57	1.47	1.38
23	b	603	CLA	C4B-CHC	2.57	1.48	1.41
23	b	610	CLA	C4C-C3C	2.57	1.49	1.45
23	B	611	CLA	C1B-CHB	2.56	1.48	1.41
23	C	510	CLA	C4C-C3C	2.56	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	601	CLA	C4D-CHA	2.56	1.47	1.38
23	B	613	CLA	C1B-CHB	2.56	1.48	1.41
23	b	615	CLA	C4D-CHA	2.56	1.47	1.38
23	d	402[A]	CLA	C4C-C3C	2.56	1.49	1.45
23	b	603	CLA	C4D-CHA	2.55	1.47	1.38
35	B	623	HTG	C1-S1	-2.55	1.76	1.80
23	C	502	CLA	C1C-C2C	2.55	1.49	1.44
38	f	101	HEM	C1D-ND	-2.55	1.33	1.38
23	c	507	CLA	C1B-CHB	2.55	1.48	1.41
23	B	607	CLA	C4B-CHC	2.55	1.48	1.41
23	C	512	CLA	C1B-CHB	2.55	1.48	1.41
27	A	418	GOL	O2-C2	-2.55	1.35	1.43
23	C	503	CLA	C4C-C3C	2.55	1.49	1.45
24	a	415[A]	PHO	C3A-C2A	-2.55	1.52	1.54
23	c	512	CLA	C4D-CHA	2.55	1.47	1.38
23	c	503	CLA	C1B-CHB	2.54	1.48	1.41
23	B	608	CLA	C4C-C3C	2.54	1.49	1.45
33	t	101	LMT	O3'-C3'	-2.54	1.37	1.43
23	b	607	CLA	C1C-C2C	2.54	1.49	1.44
23	a	405[B]	CLA	C4D-CHA	2.54	1.47	1.38
23	b	603	CLA	C1C-C2C	2.54	1.49	1.44
23	c	502	CLA	C1C-C2C	2.53	1.49	1.44
23	B	605	CLA	C4D-CHA	2.53	1.47	1.38
23	B	606	CLA	C1B-CHB	2.53	1.48	1.41
23	b	611	CLA	C4B-CHC	2.53	1.48	1.41
23	B	614	CLA	C4B-CHC	2.53	1.48	1.41
24	a	407[B]	PHO	CHA-CBD	-2.53	1.49	1.52
33	A	420	LMT	O3'-C3'	-2.53	1.37	1.43
23	A	404[B]	CLA	C4C-C3C	2.52	1.49	1.45
33	m	103	LMT	O2B-C2B	-2.52	1.37	1.43
23	c	502	CLA	C1B-CHB	2.52	1.48	1.41
23	a	404[B]	CLA	C4C-C3C	2.52	1.49	1.45
23	c	513	CLA	C1B-CHB	2.52	1.48	1.41
23	c	508	CLA	C4B-CHC	2.52	1.48	1.41
23	b	606	CLA	C1B-CHB	2.52	1.48	1.41
23	B	602	CLA	C3D-C4D	-2.52	1.38	1.44
23	B	609	CLA	C4D-CHA	2.52	1.47	1.38
24	a	407[A]	PHO	CHA-CBD	-2.51	1.49	1.52
35	b	622	HTG	O5-C1	2.51	1.46	1.42
23	C	514	CLA	C1C-C2C	2.51	1.49	1.44
23	C	503	CLA	C1C-C2C	2.51	1.49	1.44
23	b	614	CLA	C3D-C4D	-2.50	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	508	CLA	C1B-CHB	2.50	1.47	1.41
23	B	604	CLA	C4D-CHA	2.50	1.47	1.38
26	b	620	SQD	C6-S	-2.50	1.68	1.77
23	d	402[B]	CLA	C4C-C3C	2.50	1.49	1.45
23	b	616	CLA	C4D-CHA	2.50	1.47	1.38
23	b	608	CLA	C3D-C4D	-2.50	1.38	1.44
23	A	404[A]	CLA	C1C-C2C	2.49	1.49	1.44
23	a	404[A]	CLA	C4C-C3C	2.49	1.49	1.45
23	A	406[A]	CLA	C4B-CHC	2.49	1.47	1.41
23	b	612	CLA	C4B-CHC	2.49	1.47	1.41
34	C	521	LMG	O1-C1	2.49	1.44	1.40
23	C	506	CLA	C4C-C3C	2.49	1.49	1.45
33	B	626	LMT	O3'-C3'	-2.49	1.37	1.43
23	C	511	CLA	C4D-CHA	2.49	1.47	1.38
23	b	606	CLA	C3D-C4D	-2.49	1.38	1.44
23	c	508	CLA	C1B-CHB	2.49	1.47	1.41
23	B	605	CLA	C3D-C4D	-2.48	1.38	1.44
23	B	608	CLA	C1B-CHB	2.48	1.47	1.41
23	A	405[A]	CLA	C1B-CHB	2.48	1.47	1.41
23	b	614	CLA	C4B-CHC	2.48	1.47	1.41
23	a	404[A]	CLA	C4D-CHA	2.48	1.47	1.38
23	a	405[A]	CLA	C4D-CHA	2.48	1.47	1.38
23	a	406[B]	CLA	C4D-CHA	2.48	1.47	1.38
23	B	603	CLA	C4D-CHA	2.47	1.47	1.38
23	C	514	CLA	C1B-CHB	2.47	1.47	1.41
23	B	602	CLA	C1B-CHB	2.46	1.47	1.41
23	c	504	CLA	C3D-C4D	-2.46	1.38	1.44
23	C	504	CLA	C3D-C4D	-2.46	1.38	1.44
33	B	629	LMT	O3'-C3'	-2.46	1.37	1.43
23	b	607	CLA	C4C-C3C	2.46	1.49	1.45
23	a	406[A]	CLA	C1B-CHB	2.46	1.47	1.41
23	b	608	CLA	C4B-NB	-2.46	1.33	1.35
23	C	507	CLA	C1C-C2C	2.46	1.49	1.44
23	C	510	CLA	C4D-CHA	2.45	1.47	1.38
23	C	503	CLA	C1B-CHB	2.45	1.47	1.41
23	d	403	CLA	C4B-CHC	2.45	1.47	1.41
23	A	406[B]	CLA	C4D-CHA	2.45	1.47	1.38
33	e	101	LMT	O3'-C3'	-2.45	1.37	1.43
23	c	514	CLA	C4D-CHA	2.45	1.47	1.38
23	C	502	CLA	C4B-CHC	2.45	1.47	1.41
23	b	614	CLA	C4D-CHA	2.44	1.47	1.38
23	d	402[A]	CLA	C1B-NB	-2.44	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	402[B]	CLA	C4D-CHA	2.44	1.47	1.38
23	a	406[A]	CLA	C3D-C4D	-2.44	1.38	1.44
23	c	506	CLA	C1B-CHB	2.44	1.47	1.41
23	B	610	CLA	C1B-CHB	2.44	1.47	1.41
23	c	505	CLA	C4D-CHA	2.44	1.47	1.38
23	c	514	CLA	C1B-CHB	2.43	1.47	1.41
23	A	404[B]	CLA	C3D-C4D	-2.43	1.38	1.44
23	B	610	CLA	C1C-C2C	2.43	1.49	1.44
23	b	601	CLA	C1C-C2C	2.43	1.49	1.44
33	B	628	LMT	O2'-C2'	-2.43	1.37	1.43
23	b	611	CLA	C4D-CHA	2.43	1.47	1.38
23	B	604	CLA	C1C-C2C	2.43	1.49	1.44
23	A	406[B]	CLA	C4B-CHC	2.42	1.47	1.41
23	C	514	CLA	C3D-C4D	-2.42	1.38	1.44
26	L	101	SQD	C6-S	-2.42	1.68	1.77
23	C	511	CLA	C3D-C4D	-2.42	1.38	1.44
24	A	407[A]	PHO	CHA-CBD	-2.42	1.49	1.52
29	d	405[B]	PL9	C6-C5	2.42	1.47	1.35
23	C	507	CLA	C1B-CHB	2.42	1.47	1.41
23	B	602	CLA	C4D-CHA	2.41	1.47	1.38
23	c	502	CLA	C3D-C4D	-2.41	1.38	1.44
23	b	602	CLA	C3D-C4D	-2.41	1.38	1.44
23	C	510	CLA	C4B-NB	-2.41	1.33	1.35
23	b	602	CLA	C4C-C3C	2.41	1.49	1.45
23	b	612	CLA	C4D-CHA	2.41	1.47	1.38
23	c	507	CLA	C4C-C3C	2.41	1.49	1.45
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	B	601	CLA	C4D-CHA	2.41	1.47	1.38
23	a	404[A]	CLA	C1B-CHB	2.41	1.47	1.41
23	b	605	CLA	C4D-CHA	2.41	1.47	1.38
23	c	513	CLA	C1C-C2C	2.41	1.49	1.44
23	b	611	CLA	C1C-C2C	2.41	1.49	1.44
23	B	612	CLA	C4C-C3C	2.41	1.49	1.45
24	a	407[B]	PHO	C3A-C2A	-2.40	1.52	1.54
23	a	404[B]	CLA	C4D-CHA	2.40	1.46	1.38
23	b	608	CLA	C4D-CHA	2.40	1.46	1.38
35	B	621	HTG	C1'-S1	-2.40	1.78	1.81
29	D	405[B]	PL9	C6-C5	2.40	1.47	1.35
33	F	101	LMT	O3'-C3'	-2.40	1.37	1.43
33	b	621	LMT	C3'-C2'	2.40	1.58	1.52
36	h	102	DGD	O5D-C1E	2.40	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	610	CLA	C4B-CHC	2.40	1.47	1.41
23	C	502	CLA	C3D-C4D	-2.40	1.38	1.44
23	D	402[A]	CLA	C3D-C4D	-2.39	1.38	1.44
23	C	503	CLA	C4B-CHC	2.39	1.47	1.41
23	b	609	CLA	C4B-CHC	2.39	1.47	1.41
23	b	603	CLA	C1B-CHB	2.39	1.47	1.41
23	B	604	CLA	C4B-CHC	2.39	1.47	1.41
23	b	615	CLA	C3D-C4D	-2.39	1.38	1.44
23	c	509	CLA	C1B-CHB	2.39	1.47	1.41
23	a	408	CLA	C4D-CHA	2.39	1.46	1.38
40	V	201	HEC	C3C-C4C	2.39	1.47	1.43
23	B	616	CLA	C4B-CHC	2.39	1.47	1.41
23	B	616	CLA	C1B-CHB	2.38	1.47	1.41
23	d	402[B]	CLA	C3D-C4D	-2.38	1.38	1.44
23	b	604	CLA	C4C-C3C	2.38	1.49	1.45
33	M	101	LMT	O3'-C3'	-2.38	1.37	1.43
23	B	603	CLA	C1B-CHB	2.38	1.47	1.41
23	d	402[A]	CLA	C4D-CHA	2.38	1.46	1.38
23	b	603	CLA	C4C-C3C	2.38	1.49	1.45
23	B	615	CLA	C4D-CHA	2.38	1.46	1.38
23	B	615	CLA	C1B-CHB	2.38	1.47	1.41
23	a	406[B]	CLA	C4B-CHC	2.38	1.47	1.41
23	C	505	CLA	C4B-CHC	2.37	1.47	1.41
23	D	403	CLA	C1B-CHB	2.37	1.47	1.41
23	b	613	CLA	C1C-C2C	2.37	1.49	1.44
23	C	509	CLA	C1B-CHB	2.37	1.47	1.41
23	b	614	CLA	C1B-CHB	2.37	1.47	1.41
23	c	502	CLA	C4B-CHC	2.37	1.47	1.41
23	D	403	CLA	C4D-CHA	2.37	1.46	1.38
33	M	101	LMT	O2'-C2'	-2.37	1.37	1.43
23	C	508	CLA	C4B-CHC	2.36	1.47	1.41
23	B	606	CLA	C3D-C4D	-2.36	1.38	1.44
23	a	405[B]	CLA	C1B-CHB	2.36	1.47	1.41
23	a	408	CLA	C4B-CHC	2.36	1.47	1.41
23	B	602	CLA	C4C-C3C	2.36	1.49	1.45
23	C	502	CLA	C1B-CHB	2.36	1.47	1.41
23	b	607	CLA	C3D-C4D	-2.36	1.38	1.44
23	c	514	CLA	C3D-C4D	-2.36	1.38	1.44
23	B	613	CLA	C4B-CHC	2.36	1.47	1.41
23	b	616	CLA	C4B-CHC	2.35	1.47	1.41
29	d	405[A]	PL9	C6-C5	2.35	1.47	1.35
23	c	507	CLA	C4D-CHA	2.35	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	612	CLA	C1B-NB	-2.35	1.33	1.35
23	c	510	CLA	C1B-NB	-2.35	1.33	1.35
24	a	415[A]	PHO	CHA-CBD	-2.35	1.49	1.52
23	d	402[B]	CLA	C1C-C2C	2.35	1.49	1.44
23	b	608	CLA	C1B-CHB	2.35	1.47	1.41
23	C	504	CLA	C1B-CHB	2.34	1.47	1.41
33	T	101	LMT	O3'-C3'	-2.34	1.37	1.43
24	A	417[A]	PHO	C3A-C2A	-2.34	1.52	1.54
23	C	509	CLA	C4B-CHC	2.34	1.47	1.41
23	b	615	CLA	C1B-CHB	2.34	1.47	1.41
26	F	103	SQD	C6-S	-2.34	1.68	1.77
23	A	405[A]	CLA	C3D-C4D	-2.34	1.38	1.44
23	c	514	CLA	C4B-CHC	2.34	1.47	1.41
23	a	405[B]	CLA	C4B-CHC	2.34	1.47	1.41
23	b	602	CLA	C4D-CHA	2.34	1.46	1.38
29	D	405[A]	PL9	C6-C5	2.34	1.47	1.35
23	b	612	CLA	C3D-C4D	-2.34	1.38	1.44
33	M	101	LMT	O2B-C2B	-2.34	1.37	1.43
23	C	512	CLA	C4C-C3C	2.34	1.49	1.45
23	B	609	CLA	C3D-C4D	-2.34	1.38	1.44
23	A	404[B]	CLA	C1B-CHB	2.33	1.47	1.41
23	A	405[B]	CLA	C1C-C2C	2.33	1.49	1.44
24	a	407[A]	PHO	CBD-CGD	-2.33	1.49	1.52
23	b	609	CLA	C1C-C2C	2.33	1.49	1.44
23	c	505	CLA	C1C-NC	-2.33	1.34	1.37
23	b	601	CLA	C4C-C3C	2.33	1.49	1.45
23	D	402[B]	CLA	C4B-CHC	2.33	1.47	1.41
23	B	609	CLA	C1B-CHB	2.32	1.47	1.41
23	a	406[B]	CLA	C1B-CHB	2.32	1.47	1.41
23	b	611	CLA	C4C-C3C	2.32	1.49	1.45
23	a	408	CLA	C1B-CHB	2.32	1.47	1.41
23	c	509	CLA	C4C-C3C	2.32	1.49	1.45
23	A	405[B]	CLA	C4B-CHC	2.31	1.47	1.41
26	F	103	SQD	O6-C1	2.31	1.44	1.40
23	b	615	CLA	C1B-NB	-2.31	1.33	1.35
23	B	606	CLA	C4B-CHC	2.31	1.47	1.41
23	c	513	CLA	C3D-C4D	-2.31	1.39	1.44
23	b	612	CLA	C4C-C3C	2.31	1.49	1.45
23	b	604	CLA	MG-NA	2.31	2.11	2.06
23	d	403	CLA	C1B-CHB	2.31	1.47	1.41
23	D	402[B]	CLA	C3D-C4D	-2.31	1.39	1.44
23	C	509	CLA	C1C-C2C	2.31	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402[A]	CLA	C1C-C2C	2.30	1.49	1.44
23	d	402[A]	CLA	C3D-C4D	-2.30	1.39	1.44
33	a	416	LMT	O3'-C3'	-2.30	1.37	1.43
23	B	603	CLA	C4B-CHC	2.30	1.47	1.41
23	A	404[B]	CLA	C1C-C2C	2.30	1.49	1.44
23	C	512	CLA	C3D-C4D	-2.30	1.39	1.44
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	B	616	CLA	C3D-C4D	-2.30	1.39	1.44
23	C	503	CLA	C4D-CHA	2.30	1.46	1.38
23	c	511	CLA	C4B-CHC	2.29	1.47	1.41
23	A	405[B]	CLA	C3D-C4D	-2.29	1.39	1.44
23	a	404[B]	CLA	C4B-CHC	2.29	1.47	1.41
23	B	604	CLA	MG-NA	2.29	2.11	2.06
23	C	504	CLA	C4C-C3C	2.28	1.49	1.45
23	B	612	CLA	C1C-NC	-2.28	1.34	1.37
23	b	605	CLA	C1B-CHB	2.28	1.47	1.41
25	d	404	BCR	C30-C25	-2.28	1.50	1.53
23	B	607	CLA	C1C-NC	-2.28	1.34	1.37
23	b	616	CLA	C1B-CHB	2.27	1.47	1.41
23	d	402[B]	CLA	C4B-CHC	2.27	1.47	1.41
23	b	607	CLA	C1B-CHB	2.27	1.47	1.41
33	D	401	LMT	O2'-C2'	-2.27	1.37	1.43
23	c	504	CLA	C4C-C3C	2.27	1.48	1.45
23	b	601	CLA	C1B-CHB	2.27	1.47	1.41
23	B	611	CLA	C4D-CHA	2.27	1.46	1.38
24	A	417[B]	PHO	C3A-C2A	-2.26	1.52	1.54
23	B	605	CLA	C4C-C3C	2.26	1.48	1.45
23	C	511	CLA	C4B-CHC	2.26	1.47	1.41
23	b	606	CLA	C4B-CHC	2.26	1.47	1.41
27	a	418	GOL	C1-C2	2.26	1.61	1.51
23	a	404[A]	CLA	C1C-C2C	2.25	1.48	1.44
23	a	408	CLA	C4C-C3C	2.25	1.48	1.45
23	c	507	CLA	C4B-CHC	2.25	1.47	1.41
23	b	615	CLA	C4B-CHC	2.25	1.47	1.41
23	b	604	CLA	C1C-C2C	2.25	1.48	1.44
23	A	406[A]	CLA	C3D-C4D	-2.24	1.39	1.44
23	B	607	CLA	C3D-C4D	-2.24	1.39	1.44
23	D	402[A]	CLA	C1B-NB	-2.24	1.33	1.35
23	B	612	CLA	C4B-CHC	2.24	1.47	1.41
23	a	405[A]	CLA	C1B-CHB	2.24	1.47	1.41
23	C	512	CLA	C4B-CHC	2.23	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	513	CLA	C4C-C3C	2.23	1.48	1.45
23	A	405[B]	CLA	C1B-CHB	2.23	1.47	1.41
23	d	403	CLA	C3D-C4D	-2.23	1.39	1.44
23	a	405[A]	CLA	C4B-CHC	2.23	1.47	1.41
27	D	412	GOL	C3-C2	2.23	1.60	1.51
23	b	601	CLA	C4B-CHC	2.23	1.47	1.41
38	F	102	HEM	C3B-C4B	2.22	1.49	1.44
23	C	507	CLA	C4B-NB	-2.21	1.33	1.35
23	a	406[B]	CLA	C3D-C4D	-2.21	1.39	1.44
36	C	518[A]	DGD	O5D-C1E	2.21	1.44	1.40
33	A	420	LMT	O2'-C2'	-2.21	1.37	1.43
23	D	402[A]	CLA	C4C-C3C	2.21	1.48	1.45
29	D	405[B]	PL9	C2-C3	2.21	1.40	1.34
23	c	509	CLA	C3D-C4D	-2.20	1.39	1.44
23	b	616	CLA	C3D-C4D	-2.20	1.39	1.44
33	B	628	LMT	O2B-C2B	-2.20	1.37	1.43
23	B	604	CLA	C1A-CHA	2.20	1.52	1.43
23	B	608	CLA	C3D-C4D	-2.20	1.39	1.44
23	A	406[A]	CLA	C1B-CHB	2.20	1.47	1.41
38	F	102	HEM	CHB-C1B	2.20	1.40	1.35
23	B	601	CLA	C1B-CHB	2.20	1.47	1.41
29	a	413[A]	PL9	C2-C3	2.19	1.40	1.34
23	d	402[A]	CLA	C4B-CHC	2.19	1.47	1.41
33	B	628	LMT	O3'-C3'	-2.19	1.37	1.43
23	c	512	CLA	MG-NA	2.18	2.11	2.06
23	A	404[A]	CLA	C4B-NB	-2.18	1.33	1.35
23	b	615	CLA	C4C-C3C	2.18	1.48	1.45
23	A	408	CLA	C1B-CHB	2.17	1.47	1.41
33	m	103	LMT	C3'-C2'	2.17	1.57	1.52
23	A	406[A]	CLA	C1B-NB	-2.17	1.33	1.35
23	B	604	CLA	C4C-C3C	2.17	1.48	1.45
23	C	505	CLA	C3D-C4D	-2.17	1.39	1.44
23	B	610	CLA	C1B-NB	-2.17	1.33	1.35
29	a	413[B]	PL9	C2-C3	2.17	1.40	1.34
23	b	608	CLA	C1C-C2C	2.17	1.48	1.44
23	C	508	CLA	C3D-C4D	-2.17	1.39	1.44
23	b	608	CLA	C1B-NB	-2.16	1.33	1.35
23	c	507	CLA	C3D-C4D	-2.16	1.39	1.44
23	A	406[B]	CLA	C3D-C4D	-2.16	1.39	1.44
23	a	404[B]	CLA	C1C-C2C	2.16	1.48	1.44
23	d	403	CLA	C4C-C3C	2.16	1.48	1.45
23	c	511	CLA	C4C-C3C	2.16	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	404[B]	CLA	C1B-CHB	2.16	1.47	1.41
23	a	405[B]	CLA	C1C-C2C	2.16	1.48	1.44
23	A	404[B]	CLA	C4B-CHC	2.16	1.47	1.41
23	C	506	CLA	C3D-C4D	-2.15	1.39	1.44
23	C	513	CLA	C1B-CHB	2.15	1.47	1.41
23	A	405[A]	CLA	C1B-NB	-2.15	1.33	1.35
23	B	601	CLA	C3D-C4D	-2.15	1.39	1.44
23	B	615	CLA	MG-NA	2.15	2.11	2.06
23	b	613	CLA	C1B-CHB	2.15	1.47	1.41
23	C	503	CLA	C3D-C4D	-2.15	1.39	1.44
23	b	614	CLA	C4C-C3C	2.15	1.48	1.45
23	C	513	CLA	C3D-C4D	-2.14	1.39	1.44
23	a	404[A]	CLA	C4B-CHC	2.14	1.46	1.41
23	A	406[B]	CLA	C4C-C3C	2.14	1.48	1.45
38	f	101	HEM	CHB-C1B	2.14	1.40	1.35
33	T	101	LMT	O3B-C3B	-2.14	1.37	1.43
23	B	607	CLA	C4C-C3C	2.13	1.48	1.45
23	c	512	CLA	C4B-CHC	2.13	1.46	1.41
23	a	404[B]	CLA	C3D-C4D	-2.13	1.39	1.44
23	c	505	CLA	C1B-CHB	2.13	1.46	1.41
29	A	414[A]	PL9	C2-C1	-2.12	1.39	1.44
23	c	503	CLA	C3D-C4D	-2.12	1.39	1.44
23	C	508	CLA	C4C-C3C	2.12	1.48	1.45
23	D	402[A]	CLA	C4B-CHC	2.12	1.46	1.41
23	A	406[B]	CLA	C1B-CHB	2.12	1.46	1.41
23	a	405[A]	CLA	C1C-C2C	2.12	1.48	1.44
27	D	412	GOL	O2-C2	-2.12	1.37	1.43
23	c	505	CLA	C4B-CHC	2.12	1.46	1.41
23	B	614	CLA	C4C-C3C	2.12	1.48	1.45
23	C	507	CLA	C4B-CHC	2.11	1.46	1.41
36	H	102	DGD	O2G-C2G	-2.11	1.41	1.46
23	C	510	CLA	C4B-CHC	2.11	1.46	1.41
23	b	611	CLA	C3D-C4D	-2.11	1.39	1.44
23	B	613	CLA	C3D-C4D	-2.11	1.39	1.44
23	c	514	CLA	C1D-C2D	2.11	1.49	1.45
35	o	301	HTG	O5-C1	2.10	1.45	1.42
33	D	401	LMT	O3'-C3'	-2.10	1.38	1.43
23	b	609	CLA	C3D-C4D	-2.10	1.39	1.44
23	c	511	CLA	C3D-C4D	-2.10	1.39	1.44
23	B	604	CLA	C3D-C4D	-2.10	1.39	1.44
23	C	505	CLA	C4C-C3C	2.10	1.48	1.45
23	B	609	CLA	C4C-C3C	2.09	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	605	CLA	C1D-C2D	2.09	1.49	1.45
23	B	615	CLA	C4B-CHC	2.09	1.46	1.41
23	B	606	CLA	C4C-C3C	2.09	1.48	1.45
23	c	514	CLA	C4C-C3C	2.09	1.48	1.45
33	B	626	LMT	O5'-C5'	-2.09	1.39	1.44
23	c	507	CLA	C1C-C2C	2.09	1.48	1.44
23	b	602	CLA	C1B-CHB	2.09	1.46	1.41
23	b	607	CLA	C4B-CHC	2.09	1.46	1.41
23	a	406[A]	CLA	C4C-C3C	2.08	1.48	1.45
23	A	408	CLA	C4B-CHC	2.08	1.46	1.41
23	c	508	CLA	C3D-C4D	-2.08	1.39	1.44
23	b	605	CLA	C4B-CHC	2.07	1.46	1.41
23	b	611	CLA	C1D-C2D	2.07	1.49	1.45
27	b	624	GOL	C3-C2	2.07	1.60	1.51
23	A	408	CLA	C1C-NC	-2.07	1.34	1.37
23	c	503	CLA	C4B-CHC	2.07	1.46	1.41
36	c	518[B]	DGD	O3G-C1D	2.07	1.43	1.40
33	B	629	LMT	O2'-C2'	-2.07	1.38	1.43
23	C	502	CLA	C4C-C3C	2.06	1.48	1.45
23	C	507	CLA	C1D-C2D	2.06	1.49	1.45
26	L	101	SQD	O6-C1	2.06	1.43	1.40
23	b	603	CLA	C3D-C4D	-2.06	1.39	1.44
23	c	512	CLA	C4C-C3C	2.06	1.48	1.45
23	c	505	CLA	C3D-C4D	-2.06	1.39	1.44
23	C	514	CLA	C1C-NC	-2.05	1.34	1.37
23	b	605	CLA	C1C-C2C	2.05	1.48	1.44
23	a	406[A]	CLA	C4B-CHC	2.04	1.46	1.41
29	D	405[A]	PL9	C2-C3	2.04	1.40	1.34
23	C	509	CLA	C1A-CHA	2.04	1.51	1.43
23	b	614	CLA	C1C-C2C	2.04	1.48	1.44
23	B	603	CLA	C3D-C4D	-2.03	1.39	1.44
23	B	612	CLA	C3D-C4D	-2.03	1.39	1.44
33	e	101	LMT	O2B-C2B	-2.03	1.38	1.43
25	D	404	BCR	C5-C6	2.03	1.37	1.34
32	b	630[A]	LHG	O7-C5	-2.02	1.41	1.46
23	C	509	CLA	C3D-C4D	-2.02	1.39	1.44
23	b	604	CLA	C1A-CHA	2.02	1.51	1.43
23	B	606	CLA	MG-NA	2.02	2.11	2.06
23	A	404[A]	CLA	C3D-C4D	-2.02	1.39	1.44
23	C	510	CLA	C1B-NB	-2.02	1.33	1.35
33	T	101	LMT	O2'-C2'	-2.01	1.38	1.43
23	C	512	CLA	C4B-NB	-2.01	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	c	519	DGD	O5D-C1E	2.01	1.43	1.40
34	D	411	LMG	O7-C8	-2.01	1.41	1.46
23	c	508	CLA	C4C-C3C	2.01	1.48	1.45
23	C	505	CLA	C1B-NB	-2.01	1.33	1.35
23	D	403	CLA	C3D-C4D	-2.01	1.39	1.44
23	c	512	CLA	C1D-C2D	2.01	1.49	1.45
23	B	601	CLA	C4C-C3C	2.01	1.48	1.45
33	B	626	LMT	O4'-C4B	-2.01	1.38	1.43
33	t	101	LMT	O2'-C2'	-2.00	1.38	1.43
24	a	415[A]	PHO	CBD-CGD	-2.00	1.49	1.52
23	C	511	CLA	C1D-C2D	2.00	1.49	1.45

All (3093) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	C1D-ND-C4D	-12.02	97.79	106.33
23	a	408	CLA	C1D-ND-C4D	-10.70	98.73	106.33
23	B	612	CLA	C1D-ND-C4D	-10.65	98.77	106.33
23	B	611	CLA	C2D-C1D-ND	10.27	117.67	110.10
23	A	408	CLA	C1D-ND-C4D	-10.19	99.10	106.33
23	b	605	CLA	C1D-ND-C4D	-10.15	99.13	106.33
23	C	511	CLA	C1D-ND-C4D	-10.11	99.15	106.33
23	a	406[B]	CLA	C1D-ND-C4D	-10.08	99.17	106.33
23	B	615	CLA	C1D-ND-C4D	-10.02	99.22	106.33
23	c	512	CLA	C1D-ND-C4D	-9.96	99.26	106.33
23	C	504	CLA	C1D-ND-C4D	-9.86	99.33	106.33
23	B	601	CLA	C1D-ND-C4D	-9.79	99.38	106.33
23	B	614	CLA	C1D-ND-C4D	-9.73	99.42	106.33
23	a	406[A]	CLA	C1D-ND-C4D	-9.69	99.45	106.33
23	d	402[B]	CLA	C1D-ND-C4D	-9.69	99.45	106.33
23	b	614	CLA	C1D-ND-C4D	-9.67	99.47	106.33
23	b	611	CLA	C1D-ND-C4D	-9.62	99.50	106.33
23	B	605	CLA	C1D-ND-C4D	-9.56	99.55	106.33
23	c	504	CLA	C1D-ND-C4D	-9.53	99.56	106.33
23	a	408	CLA	C2D-C1D-ND	9.50	117.10	110.10
23	C	502	CLA	C1D-ND-C4D	-9.49	99.59	106.33
23	c	507	CLA	C1D-ND-C4D	-9.46	99.62	106.33
23	B	615	CLA	C2D-C1D-ND	9.44	117.06	110.10
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	D	402[B]	CLA	C1D-ND-C4D	-9.37	99.68	106.33
23	a	404[B]	CLA	C1D-ND-C4D	-9.33	99.71	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	612	CLA	C2D-C1D-ND	9.33	116.98	110.10
23	C	505	CLA	C1D-ND-C4D	-9.29	99.73	106.33
23	C	506	CLA	C1D-ND-C4D	-9.29	99.74	106.33
23	A	408	CLA	C2D-C1D-ND	9.27	116.93	110.10
23	A	406[B]	CLA	C1D-ND-C4D	-9.26	99.76	106.33
23	b	615	CLA	C1D-ND-C4D	-9.26	99.76	106.33
23	B	607	CLA	C1D-ND-C4D	-9.23	99.78	106.33
23	B	606	CLA	C1D-ND-C4D	-9.22	99.78	106.33
23	d	403	CLA	C1D-ND-C4D	-9.20	99.80	106.33
23	C	505	CLA	C2D-C1D-ND	9.20	116.88	110.10
23	D	402[A]	CLA	C1D-ND-C4D	-9.14	99.84	106.33
23	b	603	CLA	C1D-ND-C4D	-9.14	99.85	106.33
23	c	502	CLA	C1D-ND-C4D	-9.12	99.86	106.33
23	b	616	CLA	C1D-ND-C4D	-9.12	99.86	106.33
23	b	613	CLA	C2D-C1D-ND	9.11	116.82	110.10
23	b	614	CLA	C2D-C1D-ND	9.10	116.81	110.10
23	b	602	CLA	C1D-ND-C4D	-9.09	99.88	106.33
23	c	506	CLA	C1D-ND-C4D	-9.08	99.88	106.33
23	b	601	CLA	C1D-ND-C4D	-9.08	99.88	106.33
23	A	405[A]	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	c	510	CLA	C1D-ND-C4D	-9.06	99.90	106.33
23	c	513	CLA	C1D-ND-C4D	-9.05	99.90	106.33
23	b	609	CLA	C1D-ND-C4D	-9.04	99.91	106.33
23	d	402[A]	CLA	C1D-ND-C4D	-9.03	99.92	106.33
23	a	406[B]	CLA	C2D-C1D-ND	9.01	116.75	110.10
23	a	404[A]	CLA	C1D-ND-C4D	-8.97	99.96	106.33
23	B	614	CLA	C2D-C1D-ND	8.95	116.70	110.10
23	b	606	CLA	C1D-ND-C4D	-8.95	99.98	106.33
23	C	514	CLA	C1D-ND-C4D	-8.92	100.00	106.33
23	b	611	CLA	C2D-C1D-ND	8.88	116.65	110.10
23	B	609	CLA	C1D-ND-C4D	-8.87	100.03	106.33
23	b	610	CLA	C1D-ND-C4D	-8.84	100.05	106.33
23	b	605	CLA	C2D-C1D-ND	8.84	116.62	110.10
23	B	602	CLA	C1D-ND-C4D	-8.83	100.06	106.33
23	D	403	CLA	C1D-ND-C4D	-8.83	100.06	106.33
23	C	510	CLA	C1D-ND-C4D	-8.82	100.07	106.33
23	a	406[A]	CLA	C2D-C1D-ND	8.81	116.60	110.10
23	C	504	CLA	C2D-C1D-ND	8.81	116.59	110.10
23	c	512	CLA	C2D-C1D-ND	8.80	116.59	110.10
23	B	606	CLA	C2D-C1D-ND	8.77	116.57	110.10
23	c	508	CLA	C1D-ND-C4D	-8.75	100.12	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	505	CLA	C1D-ND-C4D	-8.75	100.12	106.33
23	B	608	CLA	C1D-ND-C4D	-8.71	100.15	106.33
23	B	616	CLA	C2D-C1D-ND	8.70	116.52	110.10
23	b	613	CLA	C1D-ND-C4D	-8.70	100.16	106.33
23	a	405[A]	CLA	C1D-ND-C4D	-8.67	100.18	106.33
23	b	607	CLA	C1D-ND-C4D	-8.67	100.18	106.33
23	A	405[B]	CLA	C1D-ND-C4D	-8.66	100.18	106.33
23	B	608	CLA	C2D-C1D-ND	8.63	116.47	110.10
23	c	503	CLA	C1D-ND-C4D	-8.62	100.21	106.33
23	A	406[A]	CLA	C2D-C1D-ND	8.61	116.45	110.10
23	C	503	CLA	C1D-ND-C4D	-8.57	100.25	106.33
23	C	512	CLA	C1D-ND-C4D	-8.56	100.25	106.33
23	B	605	CLA	C2D-C1D-ND	8.56	116.41	110.10
23	C	508	CLA	C1D-ND-C4D	-8.56	100.25	106.33
23	A	404[B]	CLA	C1D-ND-C4D	-8.54	100.27	106.33
23	B	601	CLA	C2D-C1D-ND	8.53	116.39	110.10
23	a	405[A]	CLA	C2D-C1D-ND	8.52	116.39	110.10
23	b	608	CLA	C1D-ND-C4D	-8.52	100.28	106.33
23	a	405[B]	CLA	C1D-ND-C4D	-8.49	100.31	106.33
23	D	402[A]	CLA	C2D-C1D-ND	8.48	116.35	110.10
23	C	513	CLA	C1D-ND-C4D	-8.47	100.32	106.33
23	b	612	CLA	C1D-ND-C4D	-8.45	100.33	106.33
23	b	616	CLA	C2D-C1D-ND	8.43	116.32	110.10
23	D	402[B]	CLA	C2D-C1D-ND	8.43	116.31	110.10
23	C	507	CLA	C1D-ND-C4D	-8.40	100.37	106.33
23	C	508	CLA	C2D-C1D-ND	8.39	116.29	110.10
23	c	511	CLA	C1D-ND-C4D	-8.39	100.38	106.33
23	B	613	CLA	C2D-C1D-ND	8.35	116.26	110.10
23	B	610	CLA	C1D-ND-C4D	-8.35	100.40	106.33
23	C	509	CLA	C2D-C1D-ND	8.32	116.24	110.10
23	c	509	CLA	C2D-C1D-ND	8.32	116.24	110.10
23	B	616	CLA	C1D-ND-C4D	-8.32	100.42	106.33
23	d	403	CLA	C2D-C1D-ND	8.31	116.23	110.10
23	A	406[B]	CLA	C2D-C1D-ND	8.30	116.22	110.10
23	B	603	CLA	C1D-ND-C4D	-8.30	100.44	106.33
23	B	613	CLA	C1D-ND-C4D	-8.29	100.44	106.33
23	c	509	CLA	C1D-ND-C4D	-8.24	100.48	106.33
23	B	611	CLA	CHD-C4C-C3C	-8.24	112.73	124.84
23	c	504	CLA	C2D-C1D-ND	8.24	116.17	110.10
23	B	607	CLA	C2D-C1D-ND	8.23	116.17	110.10
23	b	606	CLA	C2D-C1D-ND	8.21	116.15	110.10
23	b	615	CLA	C2D-C1D-ND	8.20	116.15	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	507	CLA	C2D-C1D-ND	8.20	116.14	110.10
23	c	503	CLA	C2D-C1D-ND	8.19	116.14	110.10
23	c	511	CLA	C2D-C1D-ND	8.19	116.14	110.10
23	C	509	CLA	C1D-ND-C4D	-8.18	100.52	106.33
23	c	508	CLA	C2D-C1D-ND	8.18	116.14	110.10
23	C	510	CLA	C2D-C1D-ND	8.18	116.13	110.10
23	d	402[B]	CLA	C2D-C1D-ND	8.15	116.11	110.10
23	b	609	CLA	C2D-C1D-ND	8.14	116.10	110.10
23	D	403	CLA	C2D-C1D-ND	8.08	116.06	110.10
23	a	405[B]	CLA	C2D-C1D-ND	8.08	116.06	110.10
23	c	502	CLA	C2D-C1D-ND	8.07	116.05	110.10
23	C	502	CLA	C2D-C1D-ND	8.07	116.05	110.10
23	c	505	CLA	C2D-C1D-ND	8.05	116.03	110.10
23	b	601	CLA	C2D-C1D-ND	8.04	116.03	110.10
23	B	609	CLA	C2D-C1D-ND	8.04	116.03	110.10
23	b	604	CLA	C1D-ND-C4D	-8.04	100.63	106.33
23	a	404[A]	CLA	C2D-C1D-ND	8.03	116.02	110.10
23	b	603	CLA	C2D-C1D-ND	8.03	116.02	110.10
23	B	610	CLA	C2D-C1D-ND	7.94	115.95	110.10
23	d	402[A]	CLA	C2D-C1D-ND	7.92	115.94	110.10
24	a	407[B]	PHO	O2D-CGD-CBD	7.90	121.00	111.00
23	C	511	CLA	C2D-C1D-ND	7.86	115.89	110.10
23	A	405[B]	CLA	C2D-C1D-ND	7.86	115.89	110.10
23	c	513	CLA	C2D-C1D-ND	7.82	115.87	110.10
23	C	512	CLA	C2D-C1D-ND	7.82	115.87	110.10
23	b	607	CLA	C2D-C1D-ND	7.81	115.86	110.10
23	C	514	CLA	C2D-C1D-ND	7.81	115.86	110.10
23	a	404[B]	CLA	C2D-C1D-ND	7.81	115.86	110.10
23	c	514	CLA	C2D-C1D-ND	7.81	115.86	110.10
23	c	510	CLA	C2D-C1D-ND	7.79	115.85	110.10
23	B	603	CLA	C2D-C1D-ND	7.79	115.85	110.10
23	C	506	CLA	C2D-C1D-ND	7.76	115.83	110.10
23	B	604	CLA	C1D-ND-C4D	-7.76	100.82	106.33
23	b	602	CLA	C4A-NA-C1A	-7.76	103.22	106.71
23	A	404[A]	CLA	C1D-ND-C4D	-7.69	100.87	106.33
23	C	513	CLA	C2D-C1D-ND	7.67	115.76	110.10
23	C	503	CLA	C2D-C1D-ND	7.66	115.75	110.10
24	A	407[B]	PHO	O2D-CGD-CBD	7.66	120.70	111.00
23	B	602	CLA	C2D-C1D-ND	7.64	115.73	110.10
23	c	506	CLA	C2D-C1D-ND	7.59	115.70	110.10
23	b	608	CLA	C2D-C1D-ND	7.58	115.69	110.10
23	C	511	CLA	CMD-C2D-C1D	7.55	138.01	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	404[A]	CLA	C2D-C1D-ND	7.53	115.66	110.10
23	b	610	CLA	C2D-C1D-ND	7.52	115.65	110.10
23	c	504	CLA	C4A-NA-C1A	-7.50	103.33	106.71
23	b	604	CLA	C2D-C1D-ND	7.44	115.58	110.10
35	b	623	HTG	C1'-S1-C1	7.38	113.89	100.09
24	A	417[A]	PHO	O2D-CGD-CBD	7.38	120.34	111.00
23	b	615	CLA	C4A-NA-C1A	-7.34	103.41	106.71
23	b	602	CLA	C2D-C1D-ND	7.24	115.44	110.10
23	B	616	CLA	CHD-C4C-C3C	-7.24	114.20	124.84
23	b	612	CLA	C2D-C1D-ND	7.24	115.44	110.10
23	C	504	CLA	C4A-NA-C1A	-7.22	103.46	106.71
24	a	415[A]	PHO	O2D-CGD-CBD	7.21	120.13	111.00
24	a	415[B]	PHO	O2D-CGD-CBD	7.20	120.12	111.00
23	B	609	CLA	C4A-NA-C1A	-7.20	103.47	106.71
26	F	103	SQD	O6-C1-C2	7.19	119.53	108.30
23	c	508	CLA	O2D-CGD-CBD	7.19	124.04	111.27
24	a	407[A]	PHO	O2D-CGD-CBD	7.16	120.07	111.00
23	A	404[B]	CLA	C2D-C1D-ND	7.16	115.38	110.10
23	B	606	CLA	CMD-C2D-C1D	7.12	137.25	124.71
23	B	605	CLA	CHD-C4C-C3C	-7.09	114.41	124.84
23	B	614	CLA	CMD-C2D-C1D	7.07	137.18	124.71
24	A	417[B]	PHO	O2D-CGD-CBD	7.04	119.92	111.00
23	C	507	CLA	C2D-C1D-ND	7.04	115.29	110.10
23	B	616	CLA	O2D-CGD-CBD	6.98	123.68	111.27
24	A	407[A]	PHO	O2D-CGD-CBD	6.91	119.75	111.00
23	b	605	CLA	C4A-NA-C1A	-6.91	103.60	106.71
23	b	606	CLA	CHD-C4C-C3C	-6.91	114.69	124.84
23	c	508	CLA	CMD-C2D-C1D	6.89	136.86	124.71
23	B	604	CLA	C2D-C1D-ND	6.87	115.17	110.10
23	B	603	CLA	O2D-CGD-CBD	6.81	123.36	111.27
23	c	514	CLA	CMD-C2D-C1D	6.79	136.69	124.71
23	c	502	CLA	CMD-C2D-C1D	6.78	136.66	124.71
23	B	603	CLA	C4A-NA-C1A	-6.75	103.67	106.71
23	A	404[B]	CLA	C4A-NA-C1A	-6.74	103.68	106.71
23	a	406[B]	CLA	CHD-C4C-C3C	-6.74	114.93	124.84
23	B	610	CLA	O2D-CGD-CBD	6.73	123.23	111.27
23	B	606	CLA	CHD-C1D-ND	-6.71	118.28	124.45
35	D	410	HTG	C1'-S1-C1	6.69	112.61	100.09
23	C	508	CLA	O2D-CGD-CBD	6.68	123.14	111.27
23	b	605	CLA	CHD-C1D-ND	-6.66	118.33	124.45
23	C	508	CLA	CMD-C2D-C1D	6.66	136.45	124.71
23	b	616	CLA	C4A-NA-C1A	-6.65	103.72	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402[B]	CLA	C2C-C1C-NC	6.63	116.18	109.97
23	A	404[A]	CLA	CMD-C2D-C1D	6.62	136.38	124.71
23	B	611	CLA	CMD-C2D-C1D	6.62	136.38	124.71
23	b	606	CLA	CMD-C2D-C1D	6.61	136.37	124.71
23	b	604	CLA	C2C-C1C-NC	6.61	116.16	109.97
23	C	513	CLA	C4A-NA-C1A	-6.60	103.74	106.71
23	B	615	CLA	C4A-NA-C1A	-6.59	103.74	106.71
23	b	616	CLA	CHD-C4C-C3C	-6.58	115.17	124.84
23	B	601	CLA	CMD-C2D-C1D	6.58	136.31	124.71
23	A	404[B]	CLA	CMD-C2D-C1D	6.57	136.30	124.71
23	C	508	CLA	CHD-C4C-C3C	-6.56	115.20	124.84
23	B	601	CLA	CHD-C4C-C3C	-6.55	115.22	124.84
23	c	511	CLA	CHD-C4C-C3C	-6.55	115.22	124.84
23	C	509	CLA	C2C-C1C-NC	6.54	116.10	109.97
23	C	513	CLA	CHD-C4C-C3C	-6.54	115.23	124.84
23	D	402[A]	CLA	C4A-NA-C1A	-6.52	103.77	106.71
23	b	605	CLA	CHD-C4C-C3C	-6.52	115.25	124.84
23	b	606	CLA	C4A-NA-C1A	-6.52	103.78	106.71
23	d	402[A]	CLA	C2C-C1C-NC	6.51	116.07	109.97
23	A	408	CLA	CMD-C2D-C1D	6.51	136.19	124.71
23	C	504	CLA	CMD-C2D-C1D	6.50	136.17	124.71
23	c	502	CLA	CHD-C1D-ND	-6.50	118.48	124.45
23	a	406[B]	CLA	CHD-C1D-ND	-6.48	118.50	124.45
23	c	508	CLA	CHD-C1D-ND	-6.48	118.50	124.45
23	D	402[B]	CLA	CMD-C2D-C1D	6.47	136.11	124.71
23	D	402[B]	CLA	CHD-C1D-ND	-6.47	118.51	124.45
23	D	402[A]	CLA	CMD-C2D-C1D	6.46	136.10	124.71
35	c	522	HTG	C1'-S1-C1	6.46	112.17	100.09
23	b	613	CLA	CHD-C4C-C3C	-6.46	115.35	124.84
23	b	615	CLA	CMD-C2D-C1D	6.45	136.09	124.71
23	C	507	CLA	C2C-C1C-NC	6.45	116.01	109.97
23	C	505	CLA	C2C-C1C-NC	6.44	116.00	109.97
23	B	605	CLA	CMD-C2D-C1D	6.43	136.05	124.71
23	d	403	CLA	CHD-C1D-ND	-6.41	118.57	124.45
23	c	505	CLA	CHD-C1D-ND	-6.41	118.57	124.45
23	b	611	CLA	CHD-C4C-C3C	-6.38	115.46	124.84
23	c	512	CLA	CHD-C4C-C3C	-6.38	115.46	124.84
23	c	504	CLA	CHD-C4C-C3C	-6.38	115.47	124.84
23	D	403	CLA	CMD-C2D-C1D	6.38	135.95	124.71
23	C	507	CLA	CMD-C2D-C1D	6.35	135.91	124.71
23	B	615	CLA	CHD-C1D-ND	-6.35	118.62	124.45
23	c	513	CLA	CMD-C2D-C1D	6.35	135.90	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	408	CLA	CHD-C4C-C3C	-6.35	115.51	124.84
23	b	607	CLA	C2C-C1C-NC	6.34	115.91	109.97
26	F	103	SQD	O47-C7-C8	6.34	125.17	111.50
23	a	406[A]	CLA	CHD-C4C-C3C	-6.34	115.52	124.84
23	c	504	CLA	CMD-C2D-C1D	6.34	135.88	124.71
23	C	504	CLA	CHD-C4C-C3C	-6.33	115.54	124.84
23	d	402[B]	CLA	CMD-C2D-C1D	6.33	135.86	124.71
23	c	513	CLA	C4A-NA-C1A	-6.31	103.87	106.71
23	B	614	CLA	CHD-C1D-ND	-6.31	118.66	124.45
23	a	406[A]	CLA	CHD-C1D-ND	-6.31	118.66	124.45
23	B	605	CLA	C4A-NA-C1A	-6.29	103.88	106.71
23	C	502	CLA	C4A-NA-C1A	-6.28	103.88	106.71
23	B	615	CLA	CHD-C4C-C3C	-6.28	115.61	124.84
23	B	609	CLA	CHD-C4C-C3C	-6.27	115.62	124.84
23	d	403	CLA	CMD-C2D-C1D	6.26	135.75	124.71
23	b	610	CLA	CHD-C4C-C3C	-6.26	115.64	124.84
23	D	402[A]	CLA	C2C-C1C-NC	6.26	115.84	109.97
23	B	614	CLA	CHD-C4C-C3C	-6.26	115.64	124.84
23	a	404[A]	CLA	C2C-C1C-NC	6.26	115.83	109.97
23	b	616	CLA	O2D-CGD-CBD	6.24	122.36	111.27
23	c	514	CLA	CHD-C1D-ND	-6.23	118.73	124.45
23	B	608	CLA	C2C-C1C-NC	6.23	115.81	109.97
23	D	402[B]	CLA	C2C-C1C-NC	6.22	115.80	109.97
23	a	405[A]	CLA	CHD-C4C-C3C	-6.22	115.70	124.84
23	b	605	CLA	CMD-C2D-C1D	6.21	135.67	124.71
23	b	603	CLA	C4A-NA-C1A	-6.21	103.91	106.71
23	a	405[B]	CLA	CHD-C4C-C3C	-6.21	115.71	124.84
23	c	503	CLA	C2C-C1C-NC	6.20	115.78	109.97
23	a	404[B]	CLA	CHD-C1D-ND	-6.20	118.76	124.45
23	C	511	CLA	CHD-C1D-ND	-6.19	118.76	124.45
23	c	505	CLA	CMD-C2D-C1D	6.19	135.63	124.71
23	a	404[A]	CLA	C4A-NA-C1A	-6.19	103.92	106.71
23	b	601	CLA	O2D-CGD-CBD	6.18	122.26	111.27
23	B	606	CLA	CHD-C4C-C3C	-6.18	115.75	124.84
23	b	611	CLA	CMD-C2D-C1D	6.17	135.59	124.71
23	C	514	CLA	CHD-C1D-ND	-6.17	118.78	124.45
23	A	408	CLA	CHD-C1D-ND	-6.16	118.79	124.45
23	D	402[A]	CLA	CHD-C1D-ND	-6.16	118.79	124.45
23	C	505	CLA	CHD-C1D-ND	-6.16	118.79	124.45
23	a	404[B]	CLA	CMD-C2D-C1D	6.15	135.56	124.71
23	B	614	CLA	C2C-C1C-NC	6.15	115.73	109.97
23	b	614	CLA	CMD-C2D-C1D	6.15	135.55	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	610	CLA	CMD-C2D-C1D	6.14	135.54	124.71
23	B	602	CLA	CHD-C4C-C3C	-6.14	115.81	124.84
23	c	512	CLA	CMD-C2D-C1D	6.13	135.51	124.71
23	c	503	CLA	CHD-C4C-C3C	-6.13	115.83	124.84
23	C	506	CLA	CHD-C4C-C3C	-6.12	115.84	124.84
23	a	404[B]	CLA	C2C-C1C-NC	6.12	115.70	109.97
23	c	508	CLA	CHD-C4C-C3C	-6.11	115.85	124.84
23	c	507	CLA	CHD-C1D-ND	-6.10	118.84	124.45
23	b	609	CLA	CHD-C4C-C3C	-6.10	115.87	124.84
23	B	610	CLA	C2C-C1C-NC	6.09	115.68	109.97
23	b	601	CLA	C4A-NA-C1A	-6.08	103.97	106.71
23	B	612	CLA	CHD-C4C-C3C	-6.08	115.90	124.84
23	A	404[A]	CLA	C2C-C1C-NC	6.08	115.67	109.97
23	D	403	CLA	CHD-C4C-C3C	-6.08	115.90	124.84
23	A	406[B]	CLA	CHD-C1D-ND	-6.08	118.87	124.45
23	B	603	CLA	C2C-C1C-NC	6.07	115.66	109.97
23	d	403	CLA	O2D-CGD-CBD	6.06	122.04	111.27
23	b	614	CLA	O2D-CGD-CBD	6.06	122.03	111.27
23	A	408	CLA	CHD-C4C-C3C	-6.04	115.96	124.84
23	c	512	CLA	CHD-C1D-ND	-6.04	118.91	124.45
23	b	612	CLA	CHD-C4C-C3C	-6.04	115.97	124.84
26	A	410[A]	SQD	O6-C1-C2	6.03	117.72	108.30
23	d	402[A]	CLA	C4A-NA-C1A	-6.03	104.00	106.71
23	B	601	CLA	CHD-C1D-ND	-6.02	118.92	124.45
23	C	503	CLA	C2C-C1C-NC	5.99	115.59	109.97
23	b	602	CLA	CHD-C1D-ND	-5.99	118.95	124.45
23	C	502	CLA	O2D-CGD-CBD	5.99	121.91	111.27
23	c	509	CLA	CHD-C4C-C3C	-5.99	116.04	124.84
23	B	602	CLA	CMD-C2D-C1D	5.98	135.26	124.71
23	A	406[A]	CLA	CHD-C4C-C3C	-5.98	116.05	124.84
23	C	509	CLA	CHD-C4C-C3C	-5.98	116.05	124.84
23	b	611	CLA	CHD-C1D-ND	-5.98	118.96	124.45
23	b	615	CLA	CHD-C1D-ND	-5.98	118.96	124.45
23	a	404[B]	CLA	C4A-NA-C1A	-5.97	104.02	106.71
23	c	514	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
23	C	507	CLA	CHD-C1D-ND	-5.96	118.98	124.45
23	b	602	CLA	CHD-C4C-C3C	-5.95	116.09	124.84
23	C	502	CLA	CMD-C2D-C1D	5.95	135.21	124.71
23	B	604	CLA	C2C-C1C-NC	5.95	115.55	109.97
23	C	511	CLA	CHD-C4C-C3C	-5.95	116.09	124.84
23	B	616	CLA	C3C-C4C-NC	5.94	117.24	110.57
23	c	513	CLA	CHD-C1D-ND	-5.94	118.99	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	510	CLA	C2C-C1C-NC	5.94	115.53	109.97
23	b	616	CLA	CMD-C2D-C1D	5.93	135.16	124.71
23	c	507	CLA	CMD-C2D-C1D	5.93	135.16	124.71
23	b	602	CLA	CMD-C2D-C1D	5.93	135.16	124.71
23	B	607	CLA	CHD-C4C-C3C	-5.92	116.13	124.84
23	B	607	CLA	CHD-C1D-ND	-5.92	119.01	124.45
23	a	405[B]	CLA	CMD-C2D-C1D	5.92	135.15	124.71
23	c	506	CLA	CHD-C4C-C3C	-5.92	116.14	124.84
23	A	406[B]	CLA	CHD-C4C-C3C	-5.91	116.15	124.84
23	B	602	CLA	C4A-NA-C1A	-5.91	104.05	106.71
26	L	101	SQD	O6-C1-C2	5.91	117.53	108.30
23	b	610	CLA	CMD-C2D-C1D	5.91	135.13	124.71
23	B	601	CLA	O2D-CGD-CBD	5.91	121.77	111.27
23	B	615	CLA	CMD-C2D-C1D	5.91	135.12	124.71
23	b	603	CLA	CMD-C2D-C1D	5.91	135.12	124.71
23	b	602	CLA	O2D-CGD-CBD	5.91	121.76	111.27
23	C	502	CLA	CHD-C4C-C3C	-5.90	116.17	124.84
23	b	603	CLA	CHD-C4C-C3C	-5.90	116.17	124.84
23	B	606	CLA	C4A-NA-C1A	-5.90	104.06	106.71
23	A	405[A]	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
29	A	414[A]	PL9	C7-C8-C9	-5.89	116.99	126.79
23	b	606	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	d	402[B]	CLA	CHD-C1D-ND	-5.88	119.05	124.45
23	A	406[A]	CLA	CHD-C1D-ND	-5.88	119.05	124.45
23	C	504	CLA	CHD-C1D-ND	-5.87	119.06	124.45
23	d	403	CLA	CHD-C4C-C3C	-5.87	116.21	124.84
23	b	601	CLA	CHD-C4C-C3C	-5.87	116.22	124.84
23	C	508	CLA	C2C-C1C-NC	5.86	115.46	109.97
23	b	610	CLA	O2D-CGD-CBD	5.86	121.69	111.27
23	A	405[B]	CLA	C2C-C1C-NC	5.86	115.46	109.97
23	B	612	CLA	O2D-CGD-CBD	5.86	121.68	111.27
40	V	201	HEC	CBD-CAD-C3D	-5.86	102.62	112.62
23	b	601	CLA	CMD-C2D-C1D	5.86	135.03	124.71
23	C	514	CLA	CMD-C2D-C1D	5.82	134.97	124.71
23	A	404[A]	CLA	CHD-C1D-ND	-5.81	119.11	124.45
23	C	510	CLA	C2C-C1C-NC	5.81	115.41	109.97
23	B	610	CLA	CHD-C4C-C3C	-5.81	116.31	124.84
23	B	607	CLA	C2C-C1C-NC	5.80	115.41	109.97
23	c	511	CLA	CMD-C2D-C1D	5.80	134.93	124.71
23	C	510	CLA	CMD-C2D-C1D	5.79	134.92	124.71
23	C	512	CLA	CHD-C4C-C3C	-5.79	116.33	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	606	CLA	O2D-CGD-CBD	5.79	121.56	111.27
23	B	611	CLA	C3D-C2D-C1D	-5.79	97.94	105.83
23	b	614	CLA	CHD-C4C-C3C	-5.78	116.34	124.84
23	a	405[B]	CLA	C2C-C1C-NC	5.78	115.39	109.97
23	B	609	CLA	CHD-C1D-ND	-5.78	119.14	124.45
23	c	507	CLA	C2C-C1C-NC	5.78	115.38	109.97
23	b	601	CLA	CHD-C1D-ND	-5.78	119.15	124.45
23	B	602	CLA	O2D-CGD-CBD	5.77	121.53	111.27
23	A	404[B]	CLA	CHD-C1D-ND	-5.77	119.15	124.45
23	b	608	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
23	c	504	CLA	CHD-C1D-ND	-5.76	119.16	124.45
23	B	613	CLA	C2C-C1C-NC	5.75	115.36	109.97
23	a	404[A]	CLA	CMD-C2D-C1D	5.75	134.84	124.71
23	a	405[A]	CLA	C4A-NA-C1A	-5.75	104.12	106.71
23	C	512	CLA	CMD-C2D-C1D	5.74	134.84	124.71
23	D	403	CLA	C4A-NA-C1A	-5.74	104.12	106.71
23	A	405[B]	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
23	c	513	CLA	O2D-CGD-CBD	5.74	121.46	111.27
23	c	510	CLA	C1-C2-C3	-5.73	116.13	126.04
23	C	510	CLA	CHD-C4C-C3C	-5.73	116.41	124.84
23	d	402[B]	CLA	CHD-C4C-C3C	-5.73	116.41	124.84
23	c	506	CLA	C2C-C1C-NC	5.73	115.34	109.97
23	A	406[A]	CLA	C4A-NA-C1A	-5.72	104.13	106.71
23	A	404[B]	CLA	CHD-C4C-C3C	-5.72	116.43	124.84
23	c	506	CLA	O2D-CGD-CBD	5.72	121.42	111.27
23	C	503	CLA	CHD-C4C-C3C	-5.72	116.44	124.84
23	c	509	CLA	C2C-C1C-NC	5.72	115.33	109.97
23	a	405[B]	CLA	CHD-C1D-ND	-5.71	119.20	124.45
35	d	409	HTG	C1'-S1-C1	5.71	110.78	100.09
23	B	608	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
23	c	510	CLA	CMD-C2D-C1D	5.71	134.78	124.71
23	b	614	CLA	CHD-C1D-ND	-5.71	119.21	124.45
23	C	503	CLA	CMD-C2D-C1D	5.70	134.76	124.71
38	F	102	HEM	CAD-CBD-CGD	5.70	125.86	113.60
23	D	402[B]	CLA	C4A-NA-C1A	-5.69	104.15	106.71
23	C	502	CLA	CHD-C1D-ND	-5.69	119.23	124.45
23	A	404[B]	CLA	C2C-C1C-NC	5.68	115.30	109.97
23	b	608	CLA	CMD-C2D-C1D	5.68	134.73	124.71
23	c	513	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
23	c	509	CLA	C4A-NA-C1A	-5.68	104.15	106.71
23	b	603	CLA	C2C-C1C-NC	5.67	115.29	109.97
23	C	505	CLA	CMD-C2D-C1D	5.66	134.69	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	604	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
35	B	621	HTG	C1'-S1-C1	5.66	110.67	100.09
23	C	511	CLA	O2D-CGD-CBD	5.65	121.31	111.27
23	b	615	CLA	CHD-C4C-C3C	-5.65	116.53	124.84
23	b	615	CLA	C2C-C1C-NC	5.64	115.26	109.97
23	C	514	CLA	C2C-C1C-NC	5.64	115.26	109.97
23	d	402[A]	CLA	CMD-C2D-C1D	5.64	134.65	124.71
23	A	406[B]	CLA	CMD-C2D-C1D	5.63	134.64	124.71
23	B	603	CLA	CHD-C4C-C3C	-5.63	116.56	124.84
23	b	604	CLA	O2D-CGD-CBD	5.63	121.27	111.27
23	b	608	CLA	C2C-C1C-NC	5.62	115.24	109.97
23	B	603	CLA	CMD-C2D-C1D	5.62	134.62	124.71
23	B	609	CLA	CMD-C2D-C1D	5.62	134.62	124.71
23	c	507	CLA	CHD-C4C-C3C	-5.62	116.58	124.84
23	B	616	CLA	C4A-NA-C1A	-5.61	104.18	106.71
23	b	611	CLA	O2D-CGD-CBD	5.61	121.24	111.27
23	b	607	CLA	CHD-C1D-ND	-5.61	119.30	124.45
23	C	506	CLA	C2C-C1C-NC	5.61	115.23	109.97
35	C	522	HTG	C1'-S1-C1	5.61	110.58	100.09
23	a	405[A]	CLA	C2C-C1C-NC	5.61	115.22	109.97
23	A	405[B]	CLA	CHD-C1D-ND	-5.60	119.30	124.45
23	D	402[B]	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
23	B	605	CLA	CHD-C1D-ND	-5.60	119.31	124.45
23	A	408	CLA	C2C-C1C-NC	5.60	115.22	109.97
23	a	406[B]	CLA	CMD-C2D-C1D	5.60	134.58	124.71
23	c	514	CLA	C4A-NA-C1A	-5.58	104.20	106.71
26	a	410[A]	SQD	O6-C1-C2	5.58	117.02	108.30
23	A	405[A]	CLA	C2C-C1C-NC	5.58	115.19	109.97
23	b	603	CLA	CHD-C1D-ND	-5.57	119.33	124.45
23	b	612	CLA	C2C-C1C-NC	5.57	115.19	109.97
23	a	408	CLA	O2D-CGD-CBD	5.56	121.16	111.27
26	A	410[A]	SQD	C1-O5-C5	-5.56	102.77	113.69
23	b	607	CLA	CHD-C4C-C3C	-5.56	116.66	124.84
26	A	410[B]	SQD	O6-C1-C2	5.56	116.98	108.30
23	d	402[A]	CLA	CHD-C1D-ND	-5.56	119.35	124.45
23	a	406[A]	CLA	C4A-NA-C1A	-5.55	104.21	106.71
23	c	505	CLA	CHD-C4C-C3C	-5.55	116.68	124.84
23	C	513	CLA	CMD-C2D-C1D	5.55	134.50	124.71
23	C	506	CLA	O2D-CGD-CBD	5.55	121.13	111.27
23	A	406[B]	CLA	C4A-NA-C1A	-5.55	104.21	106.71
23	d	402[A]	CLA	CHD-C4C-C3C	-5.55	116.69	124.84
23	B	613	CLA	CHD-C4C-C3C	-5.54	116.69	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	510	CLA	CHD-C1D-ND	-5.54	119.37	124.45
23	C	514	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
23	b	611	CLA	C2C-C1C-NC	5.53	115.16	109.97
23	D	402[A]	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
23	A	405[A]	CLA	CHD-C1D-ND	-5.53	119.37	124.45
23	C	508	CLA	CHD-C1D-ND	-5.53	119.37	124.45
23	C	511	CLA	C2C-C1C-NC	5.53	115.15	109.97
25	Y	101	BCR	C33-C5-C6	-5.52	118.33	124.53
23	B	603	CLA	CHD-C1D-ND	-5.52	119.38	124.45
23	B	614	CLA	C4A-NA-C1A	-5.51	104.23	106.71
23	B	612	CLA	CHD-C1D-ND	-5.50	119.39	124.45
23	c	505	CLA	C2C-C1C-NC	5.49	115.12	109.97
23	c	511	CLA	C4A-NA-C1A	-5.49	104.24	106.71
23	b	613	CLA	C2C-C1C-NC	5.48	115.11	109.97
23	B	611	CLA	CHD-C1D-ND	-5.48	119.42	124.45
23	b	607	CLA	CMD-C2D-C1D	5.48	134.37	124.71
23	a	406[B]	CLA	C4A-NA-C1A	-5.47	104.25	106.71
23	b	609	CLA	CMD-C2D-C1D	5.47	134.35	124.71
23	b	613	CLA	CHD-C1D-ND	-5.47	119.43	124.45
23	b	606	CLA	O2D-CGD-CBD	5.46	120.97	111.27
23	D	403	CLA	CHD-C1D-ND	-5.46	119.43	124.45
23	b	604	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
23	b	609	CLA	CHD-C1D-ND	-5.44	119.45	124.45
23	B	606	CLA	C2C-C1C-NC	5.44	115.07	109.97
23	A	408	CLA	C3D-C2D-C1D	-5.44	98.41	105.83
23	B	614	CLA	O2D-CGD-CBD	5.44	120.94	111.27
23	a	405[A]	CLA	CHD-C1D-ND	-5.44	119.46	124.45
23	C	512	CLA	C2C-C1C-NC	5.44	115.06	109.97
23	B	607	CLA	O2D-CGD-CBD	5.43	120.92	111.27
26	b	620	SQD	O6-C1-C2	5.42	116.76	108.30
23	B	606	CLA	C3D-C2D-C1D	-5.41	98.44	105.83
23	B	608	CLA	CHD-C1D-ND	-5.41	119.48	124.45
23	B	604	CLA	CMD-C2D-C1D	5.41	134.24	124.71
23	C	505	CLA	CHD-C4C-C3C	-5.40	116.90	124.84
23	B	607	CLA	CMD-C2D-C1D	5.39	134.21	124.71
23	a	404[A]	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
23	c	508	CLA	C2C-C1C-NC	5.38	115.01	109.97
23	C	505	CLA	C3D-C2D-C1D	-5.38	98.49	105.83
23	B	611	CLA	O2D-CGD-CBD	5.37	120.81	111.27
23	B	614	CLA	C3D-C2D-C1D	-5.37	98.51	105.83
24	a	415[A]	PHO	C1-C2-C3	-5.37	116.76	126.04
23	b	610	CLA	C4A-NA-C1A	-5.36	104.30	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	604	CLA	CMD-C2D-C1D	5.35	134.15	124.71
23	A	405[A]	CLA	O2D-CGD-CBD	5.35	120.78	111.27
23	b	613	CLA	CMD-C2D-C1D	5.35	134.14	124.71
23	c	511	CLA	CHD-C1D-ND	-5.35	119.54	124.45
23	A	405[B]	CLA	CMD-C2D-C1D	5.34	134.12	124.71
23	c	502	CLA	CHD-C4C-C3C	-5.34	116.99	124.84
23	a	406[A]	CLA	CMD-C2D-C1D	5.34	134.12	124.71
29	A	414[B]	PL9	C7-C8-C9	-5.34	117.91	126.79
23	b	611	CLA	C4A-NA-C1A	-5.34	104.31	106.71
23	B	604	CLA	O2D-CGD-CBD	5.33	120.74	111.27
23	A	406[A]	CLA	C2C-C1C-NC	5.33	114.97	109.97
23	a	404[B]	CLA	CHD-C4C-C3C	-5.33	117.01	124.84
23	b	604	CLA	CHD-C1D-ND	-5.33	119.56	124.45
23	B	605	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
23	a	408	CLA	C2C-C1C-NC	5.32	114.95	109.97
23	D	403	CLA	O2D-CGD-CBD	5.31	120.71	111.27
23	B	604	CLA	C3C-C4C-NC	5.30	116.52	110.57
25	D	404	BCR	C7-C8-C9	-5.30	118.23	126.23
23	B	615	CLA	C3D-C2D-C1D	-5.29	98.61	105.83
23	c	510	CLA	CHD-C4C-C3C	-5.29	117.06	124.84
23	a	404[A]	CLA	CHD-C1D-ND	-5.29	119.59	124.45
23	B	616	CLA	C3D-C2D-C1D	-5.29	98.62	105.83
23	B	608	CLA	CMD-C2D-C1D	5.28	134.02	124.71
23	b	614	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
23	b	609	CLA	C2C-C1C-NC	5.26	114.90	109.97
23	A	405[B]	CLA	C4A-NA-C1A	-5.25	104.34	106.71
23	c	511	CLA	C2C-C1C-NC	5.25	114.89	109.97
26	A	410[A]	SQD	C1-C2-C3	-5.25	99.07	110.00
23	b	608	CLA	CHD-C1D-ND	-5.24	119.64	124.45
23	b	614	CLA	C2C-C1C-NC	5.24	114.88	109.97
23	B	613	CLA	CMD-C2D-C1D	5.24	133.94	124.71
23	A	406[B]	CLA	C2C-C1C-NC	5.23	114.87	109.97
23	C	507	CLA	CHD-C4C-C3C	-5.22	117.16	124.84
23	b	609	CLA	C4A-NA-C1A	-5.22	104.36	106.71
23	B	609	CLA	C2C-C1C-NC	5.21	114.86	109.97
26	a	410[A]	SQD	O47-C7-C8	5.21	122.73	111.50
23	C	506	CLA	C4A-NA-C1A	-5.21	104.36	106.71
23	B	605	CLA	C2C-C1C-NC	5.21	114.85	109.97
23	B	611	CLA	CMB-C2B-C1B	5.21	136.47	128.46
23	b	613	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
23	C	509	CLA	O2D-CGD-CBD	5.20	120.51	111.27
23	B	605	CLA	O2D-CGD-CBD	5.20	120.51	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	502	CLA	C2C-C1C-NC	5.20	114.84	109.97
26	L	101	SQD	O47-C7-C8	5.19	122.69	111.50
23	A	405[A]	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
23	a	405[A]	CLA	CMD-C2D-C1D	5.19	133.85	124.71
23	b	616	CLA	CHD-C1D-ND	-5.18	119.69	124.45
23	C	512	CLA	CHD-C1D-ND	-5.17	119.70	124.45
23	B	616	CLA	C2C-C1C-NC	5.17	114.81	109.97
23	C	508	CLA	C3C-C4C-NC	5.17	116.37	110.57
23	B	602	CLA	C2C-C1C-NC	5.17	114.81	109.97
23	B	611	CLA	CMC-C2C-C1C	5.16	132.90	125.04
23	C	506	CLA	C3C-C4C-NC	5.15	116.35	110.57
23	B	613	CLA	C1-C2-C3	-5.14	117.15	126.04
23	B	608	CLA	C3D-C2D-C1D	-5.14	98.82	105.83
26	b	620	SQD	O47-C7-C8	5.14	122.57	111.50
23	B	608	CLA	O2D-CGD-CBD	5.13	120.39	111.27
23	C	506	CLA	CMD-C2D-C1D	5.13	133.76	124.71
25	t	102	BCR	C33-C5-C6	-5.13	118.77	124.53
23	D	402[A]	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
23	A	406[A]	CLA	CMD-C2D-C1D	5.12	133.74	124.71
23	B	610	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
23	c	512	CLA	C2C-C1C-NC	5.12	114.77	109.97
23	C	504	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
23	c	509	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
23	b	616	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
23	C	512	CLA	O2D-CGD-CBD	5.10	120.32	111.27
23	B	602	CLA	CHD-C1D-ND	-5.09	119.78	124.45
23	b	608	CLA	C4A-NA-C1A	-5.09	104.42	106.71
23	c	503	CLA	O2D-CGD-CBD	5.08	120.29	111.27
23	b	613	CLA	C3C-C4C-NC	5.08	116.26	110.57
23	c	509	CLA	O2D-CGD-CBD	5.07	120.28	111.27
23	C	503	CLA	CHD-C1D-ND	-5.06	119.80	124.45
23	c	509	CLA	CMD-C2D-C1D	5.05	133.62	124.71
38	f	101	HEM	CHC-C4B-NB	5.05	129.92	124.43
23	b	605	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
23	b	603	CLA	O2D-CGD-CBD	5.05	120.24	111.27
23	b	606	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
23	C	505	CLA	O2D-CGD-CBD	5.04	120.23	111.27
23	a	408	CLA	CHD-C1D-ND	-5.04	119.82	124.45
23	c	506	CLA	CMD-C2D-C1D	5.04	133.59	124.71
23	c	508	CLA	C4A-NA-C1A	-5.04	104.44	106.71
26	F	103	SQD	C1-O5-C5	-5.03	103.81	113.69
23	C	508	CLA	C3D-C2D-C1D	-5.02	98.97	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	514	CLA	C2C-C1C-NC	5.02	114.68	109.97
23	B	604	CLA	C4A-NA-C1A	-5.02	104.45	106.71
23	C	513	CLA	CHD-C1D-ND	-5.02	119.84	124.45
23	B	608	CLA	C4A-NA-C1A	-5.01	104.45	106.71
23	b	605	CLA	O2D-CGD-CBD	5.01	120.17	111.27
23	C	513	CLA	O2D-CGD-CBD	5.01	120.17	111.27
23	c	502	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
23	c	510	CLA	CHD-C1D-ND	-5.00	119.86	124.45
23	b	611	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
23	B	613	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
23	c	506	CLA	C3C-C4C-NC	4.98	116.16	110.57
23	C	509	CLA	C3C-C4C-NC	4.98	116.15	110.57
23	C	509	CLA	C4A-NA-C1A	-4.98	104.47	106.71
23	D	403	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
23	C	506	CLA	CHD-C1D-ND	-4.97	119.88	124.45
23	c	512	CLA	C3D-C2D-C1D	-4.97	99.04	105.83
23	b	612	CLA	C3C-C4C-NC	4.97	116.15	110.57
23	d	403	CLA	C2C-C1C-NC	4.97	114.62	109.97
23	c	502	CLA	O2D-CGD-CBD	4.96	120.08	111.27
26	f	102	SQD	O47-C7-C8	4.95	122.17	111.50
23	B	615	CLA	C2C-C1C-NC	4.95	114.61	109.97
23	a	406[A]	CLA	C2C-C1C-NC	4.94	114.60	109.97
23	D	402[B]	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
23	b	610	CLA	C3C-C4C-NC	4.93	116.10	110.57
23	b	601	CLA	C2C-C1C-NC	4.93	114.59	109.97
40	v	201	HEC	CBD-CAD-C3D	-4.92	104.23	112.62
23	a	406[A]	CLA	C3D-C2D-C1D	-4.91	99.12	105.83
23	B	604	CLA	C1-C2-C3	-4.91	117.56	126.04
23	b	610	CLA	C2C-C1C-NC	4.91	114.57	109.97
23	B	610	CLA	CHD-C1D-ND	-4.91	119.95	124.45
23	c	506	CLA	CHD-C1D-ND	-4.90	119.95	124.45
23	a	405[A]	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
26	a	410[B]	SQD	O6-C1-C2	4.88	115.93	108.30
23	C	502	CLA	C2C-C1C-NC	4.88	114.55	109.97
23	A	405[B]	CLA	C1C-C2C-C3C	-4.87	101.84	106.96
23	c	508	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
23	b	612	CLA	C4A-NA-C1A	-4.86	104.52	106.71
23	A	405[A]	CLA	C4A-NA-C1A	-4.85	104.53	106.71
23	a	405[B]	CLA	C3D-C2D-C1D	-4.85	99.22	105.83
23	d	403	CLA	C3D-C2D-C1D	-4.85	99.22	105.83
25	d	404	BCR	C7-C8-C9	-4.84	118.92	126.23
23	c	504	CLA	C2C-C1C-NC	4.84	114.51	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	610	CLA	C1-C2-C3	-4.84	117.67	126.04
23	c	507	CLA	C4A-NA-C1A	-4.84	104.53	106.71
23	A	404[A]	CLA	CHD-C4C-C3C	-4.84	117.73	124.84
23	c	505	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
23	C	507	CLA	C4A-NA-C1A	-4.84	104.53	106.71
23	b	606	CLA	C2C-C1C-NC	4.84	114.50	109.97
23	B	601	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
23	c	510	CLA	O2D-CGD-CBD	4.83	119.85	111.27
23	B	612	CLA	C3C-C4C-NC	4.83	115.99	110.57
23	a	406[B]	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
23	c	504	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
23	c	506	CLA	C4A-NA-C1A	-4.80	104.55	106.71
23	C	508	CLA	C4A-NA-C1A	-4.80	104.55	106.71
23	b	607	CLA	C3C-C4C-NC	4.80	115.95	110.57
23	b	612	CLA	CMD-C2D-C1D	4.79	133.16	124.71
23	C	509	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
23	B	609	CLA	C3C-C4C-NC	4.79	115.94	110.57
23	B	611	CLA	C3C-C4C-NC	4.79	115.94	110.57
23	c	502	CLA	O2D-CGD-O1D	-4.79	114.47	123.84
23	c	511	CLA	C3C-C4C-NC	4.79	115.94	110.57
23	B	613	CLA	C3C-C4C-NC	4.79	115.94	110.57
23	a	405[B]	CLA	O2D-CGD-CBD	4.78	119.77	111.27
23	b	614	CLA	C4A-NA-C1A	-4.78	104.56	106.71
23	b	604	CLA	C4A-NA-C1A	-4.78	104.56	106.71
23	B	612	CLA	O2D-CGD-O1D	-4.77	114.51	123.84
23	c	514	CLA	C3D-C2D-C1D	-4.77	99.33	105.83
23	b	604	CLA	C1-C2-C3	-4.76	117.81	126.04
23	C	511	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
23	b	605	CLA	C2C-C1C-NC	4.76	114.43	109.97
23	b	611	CLA	C3C-C4C-NC	4.75	115.90	110.57
23	c	502	CLA	C4A-NA-C1A	-4.75	104.57	106.71
23	c	505	CLA	O2D-CGD-CBD	4.75	119.71	111.27
23	B	606	CLA	C3C-C4C-NC	4.75	115.90	110.57
23	C	502	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
23	A	406[A]	CLA	O2D-CGD-CBD	4.74	119.69	111.27
23	a	405[B]	CLA	C4A-NA-C1A	-4.74	104.58	106.71
23	b	605	CLA	C3D-C4D-ND	4.74	117.91	110.24
24	a	415[B]	PHO	C1-C2-C3	-4.73	117.86	126.04
23	C	514	CLA	O2D-CGD-CBD	4.73	119.67	111.27
23	c	511	CLA	O2D-CGD-CBD	4.73	119.67	111.27
23	a	408	CLA	C3D-C4D-ND	4.72	117.88	110.24
23	b	615	CLA	C3D-C2D-C1D	-4.72	99.38	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	505	CLA	C4A-NA-C1A	-4.72	104.58	106.71
23	B	612	CLA	C2C-C1C-NC	4.72	114.39	109.97
23	A	405[B]	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
26	a	410[B]	SQD	O47-C7-C8	4.72	121.66	111.50
23	C	504	CLA	C2C-C1C-NC	4.71	114.39	109.97
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	C	505	CLA	C1C-C2C-C3C	-4.71	102.01	106.96
38	F	102	HEM	CBA-CAA-C2A	-4.71	104.59	112.62
23	c	507	CLA	C3D-C2D-C1D	-4.70	99.41	105.83
23	a	406[B]	CLA	C3D-C4D-ND	4.70	117.84	110.24
23	c	503	CLA	C1C-C2C-C3C	-4.70	102.02	106.96
23	B	607	CLA	C3C-C4C-NC	4.69	115.83	110.57
23	c	504	CLA	C3C-C4C-NC	4.69	115.83	110.57
23	b	607	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
23	c	504	CLA	O2D-CGD-CBD	4.69	119.59	111.27
23	b	609	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
23	a	406[A]	CLA	C3D-C4D-ND	4.68	117.81	110.24
23	B	611	CLA	C1D-CHD-C4C	-4.68	115.96	126.06
23	B	616	CLA	CMD-C2D-C1D	4.68	132.96	124.71
23	c	512	CLA	O2D-CGD-CBD	4.68	119.58	111.27
23	C	510	CLA	O2D-CGD-CBD	4.67	119.57	111.27
23	C	505	CLA	C3C-C4C-NC	4.67	115.81	110.57
23	b	604	CLA	C3C-C4C-NC	4.67	115.81	110.57
23	b	602	CLA	C3D-C4D-ND	4.67	117.79	110.24
23	d	402[A]	CLA	C3C-C4C-NC	4.67	115.80	110.57
23	a	408	CLA	C3C-C4C-NC	4.67	115.80	110.57
34	C	501	LMG	C7-O1-C1	-4.67	104.62	113.74
23	c	512	CLA	C4A-NA-C1A	-4.66	104.61	106.71
23	B	601	CLA	C4A-NA-C1A	-4.66	104.61	106.71
23	c	511	CLA	C3D-C2D-C1D	-4.66	99.48	105.83
23	B	605	CLA	C3C-C4C-NC	4.65	115.79	110.57
35	b	622	HTG	C1-O5-C5	4.65	121.16	112.58
25	b	617	BCR	C7-C8-C9	-4.65	119.21	126.23
23	C	510	CLA	C1-C2-C3	-4.65	118.00	126.04
23	a	408	CLA	C3D-C2D-C1D	-4.64	99.49	105.83
23	A	406[B]	CLA	C3D-C4D-ND	4.64	117.75	110.24
23	C	509	CLA	CMD-C2D-C1D	4.64	132.89	124.71
25	H	101	BCR	C38-C26-C25	-4.64	119.32	124.53
23	C	511	CLA	C3D-C4D-ND	4.63	117.73	110.24
23	A	406[A]	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
23	C	503	CLA	C3D-C2D-C1D	-4.62	99.52	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	507	CLA	O2D-CGD-CBD	4.62	119.48	111.27
23	c	514	CLA	O2D-CGD-CBD	4.62	119.48	111.27
24	A	417[B]	PHO	C1-C2-C3	-4.62	118.06	126.04
38	F	102	HEM	CHC-C4B-NB	4.61	129.44	124.43
23	b	606	CLA	C3C-C4C-NC	4.61	115.74	110.57
23	c	509	CLA	CHD-C1D-ND	-4.61	120.22	124.45
29	a	413[A]	PL9	C7-C8-C9	-4.60	119.13	126.79
23	B	610	CLA	C4A-NA-C1A	-4.60	104.64	106.71
23	A	406[B]	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
23	B	609	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
23	c	503	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
23	C	510	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
23	c	509	CLA	C3C-C4C-NC	4.60	115.72	110.57
23	C	509	CLA	CHD-C1D-ND	-4.59	120.23	124.45
23	C	514	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
23	a	404[B]	CLA	C3D-C4D-ND	4.59	117.66	110.24
23	c	513	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
23	a	404[A]	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
23	a	405[B]	CLA	C1C-C2C-C3C	-4.58	102.14	106.96
23	a	406[A]	CLA	O2D-CGD-CBD	4.58	119.40	111.27
23	A	404[B]	CLA	C3D-C2D-C1D	-4.56	99.60	105.83
23	B	602	CLA	C3D-C2D-C1D	-4.56	99.60	105.83
23	D	402[B]	CLA	C3C-C4C-NC	4.56	115.69	110.57
23	c	507	CLA	C3D-C4D-ND	4.56	117.62	110.24
23	D	402[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
26	f	102	SQD	C1-O5-C5	4.55	122.62	113.69
23	C	510	CLA	C4A-NA-C1A	-4.55	104.66	106.71
23	A	405[A]	CLA	CMD-C2D-C1D	4.55	132.73	124.71
23	B	612	CLA	C3D-C4D-ND	4.55	117.59	110.24
23	d	402[B]	CLA	C4A-NA-C1A	-4.55	104.66	106.71
23	B	612	CLA	CMD-C2D-C1D	4.55	132.72	124.71
23	B	603	CLA	C3D-C2D-C1D	-4.55	99.63	105.83
23	d	402[B]	CLA	C3D-C4D-ND	4.55	117.59	110.24
23	B	613	CLA	CHD-C1D-ND	-4.54	120.28	124.45
23	B	602	CLA	C3C-C4C-NC	4.54	115.67	110.57
23	B	607	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
23	c	506	CLA	C3D-C4D-ND	4.54	117.58	110.24
23	a	408	CLA	CMD-C2D-C1D	4.54	132.71	124.71
23	C	507	CLA	C1C-C2C-C3C	-4.53	102.19	106.96
23	c	507	CLA	O2D-CGD-CBD	4.53	119.32	111.27
23	A	408	CLA	C3D-C4D-ND	4.53	117.57	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	405[B]	CLA	O2D-CGD-CBD	4.53	119.31	111.27
23	B	607	CLA	C4A-NA-C1A	-4.53	104.67	106.71
24	A	417[A]	PHO	C1-C2-C3	-4.53	118.22	126.04
26	A	410[B]	SQD	C1-O5-C5	-4.52	104.81	113.69
23	C	503	CLA	O2D-CGD-CBD	4.52	119.31	111.27
23	C	512	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
23	B	603	CLA	C3C-C4C-NC	4.52	115.64	110.57
23	d	402[B]	CLA	C3C-C4C-NC	4.52	115.64	110.57
23	B	611	CLA	CHD-C4C-NC	4.52	131.32	124.20
23	C	513	CLA	C3C-C4C-NC	4.52	115.64	110.57
23	b	608	CLA	O2D-CGD-CBD	4.51	119.28	111.27
23	C	506	CLA	C3D-C4D-ND	4.51	117.53	110.24
23	b	601	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
23	b	603	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
34	B	620	LMG	O7-C10-C11	4.50	121.19	111.50
23	b	613	CLA	C4A-NA-C1A	-4.50	104.69	106.71
23	D	403	CLA	C2C-C1C-NC	4.49	114.18	109.97
23	A	406[B]	CLA	O2D-CGD-CBD	4.49	119.25	111.27
23	C	507	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
23	B	611	CLA	C3D-C4D-ND	4.49	117.50	110.24
23	a	405[A]	CLA	C1C-C2C-C3C	-4.49	102.24	106.96
23	b	603	CLA	C3C-C4C-NC	4.49	115.60	110.57
23	b	608	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
23	b	610	CLA	CHD-C1D-ND	-4.48	120.34	124.45
23	B	610	CLA	O2A-CGA-CBA	4.48	125.96	111.91
23	a	408	CLA	C4A-NA-C1A	-4.47	104.70	106.71
23	c	513	CLA	C2C-C1C-NC	4.47	114.16	109.97
23	b	612	CLA	CHD-C1D-ND	-4.47	120.35	124.45
25	y	101	BCR	C33-C5-C6	-4.47	119.51	124.53
23	b	612	CLA	O2D-CGD-CBD	4.46	119.20	111.27
23	B	610	CLA	C1C-C2C-C3C	-4.45	102.28	106.96
25	d	404	BCR	C15-C14-C13	-4.45	120.96	127.31
23	d	402[A]	CLA	C1C-C2C-C3C	-4.45	102.28	106.96
23	d	402[B]	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
23	B	613	CLA	O2D-CGD-CBD	4.44	119.16	111.27
23	b	608	CLA	C1C-C2C-C3C	-4.44	102.29	106.96
23	d	402[A]	CLA	C3D-C4D-ND	4.44	117.42	110.24
23	d	402[B]	CLA	C1C-C2C-C3C	-4.44	102.29	106.96
23	B	609	CLA	C3D-C4D-ND	4.44	117.41	110.24
23	b	610	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
23	c	510	CLA	C4A-NA-C1A	-4.43	104.71	106.71
23	B	614	CLA	C1C-C2C-C3C	-4.43	102.30	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	513	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
33	t	101	LMT	C3'-C4'-C5'	-4.42	100.78	110.93
23	a	406[B]	CLA	C2C-C1C-NC	4.42	114.11	109.97
23	C	505	CLA	C4A-NA-C1A	-4.42	104.72	106.71
23	c	508	CLA	CMC-C2C-C1C	4.41	131.75	125.04
23	C	510	CLA	C3C-C4C-NC	4.40	115.51	110.57
23	B	608	CLA	C3C-C4C-NC	4.40	115.51	110.57
23	C	503	CLA	C3C-C4C-NC	4.40	115.51	110.57
23	b	609	CLA	C3C-C4C-NC	4.40	115.51	110.57
23	b	614	CLA	O2D-CGD-O1D	-4.40	115.24	123.84
23	b	607	CLA	C3D-C4D-ND	4.40	117.35	110.24
23	b	604	CLA	C1C-C2C-C3C	-4.39	102.34	106.96
23	a	405[A]	CLA	O2D-CGD-CBD	4.39	119.07	111.27
23	b	611	CLA	C3D-C4D-ND	4.39	117.34	110.24
23	b	602	CLA	C2C-C1C-NC	4.39	114.08	109.97
26	A	410[B]	SQD	O9-S-C6	4.39	112.15	106.94
23	b	601	CLA	C3D-C4D-ND	4.38	117.33	110.24
23	A	404[B]	CLA	C1D-CHD-C4C	-4.38	116.61	126.06
29	a	413[A]	PL9	C7-C3-C4	4.38	120.44	116.88
23	a	406[B]	CLA	O2D-CGD-CBD	4.38	119.04	111.27
23	C	513	CLA	C2C-C1C-NC	4.38	114.07	109.97
23	b	612	CLA	C1-C2-C3	-4.37	118.48	126.04
23	b	603	CLA	C3D-C4D-ND	4.37	117.31	110.24
23	B	611	CLA	CMB-C2B-C3B	4.36	132.84	124.68
23	b	616	CLA	C1D-CHD-C4C	-4.36	116.66	126.06
23	A	408	CLA	C4A-NA-C1A	-4.36	104.75	106.71
23	B	615	CLA	C3D-C4D-ND	4.36	117.28	110.24
23	B	614	CLA	C3C-C4C-NC	4.35	115.45	110.57
23	C	502	CLA	O2D-CGD-O1D	-4.35	115.34	123.84
23	B	607	CLA	C1C-C2C-C3C	-4.35	102.39	106.96
23	C	502	CLA	C3D-C4D-ND	4.34	117.26	110.24
23	C	512	CLA	C4A-NA-C1A	-4.34	104.75	106.71
23	B	616	CLA	O2D-CGD-O1D	-4.34	115.35	123.84
23	c	503	CLA	CMD-C2D-C1D	4.34	132.36	124.71
23	B	612	CLA	C3D-C2D-C1D	-4.34	99.91	105.83
38	F	102	HEM	C1B-NB-C4B	4.34	109.55	105.07
23	c	508	CLA	C3C-C4C-NC	4.33	115.43	110.57
23	c	511	CLA	C1-C2-C3	-4.33	118.56	126.04
32	E	101[A]	LHG	O7-C7-C8	4.32	120.82	111.50
34	c	521	LMG	O6-C5-C4	4.32	117.55	109.69
23	A	404[A]	CLA	C1C-C2C-C3C	-4.32	102.41	106.96
23	d	403	CLA	O2D-CGD-O1D	-4.32	115.39	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	510	CLA	C3D-C4D-ND	4.32	117.22	110.24
23	c	514	CLA	C3D-C4D-ND	4.32	117.22	110.24
23	B	601	CLA	C2C-C1C-NC	4.32	114.02	109.97
23	D	402[A]	CLA	C3C-C4C-NC	4.31	115.41	110.57
23	a	404[B]	CLA	C3D-C2D-C1D	-4.31	99.94	105.83
34	Z	101	LMG	O7-C10-C11	4.31	120.79	111.50
23	B	605	CLA	C3D-C4D-ND	4.30	117.20	110.24
23	b	609	CLA	C3D-C4D-ND	4.30	117.20	110.24
23	B	601	CLA	C3D-C4D-ND	4.30	117.20	110.24
34	c	501	LMG	O7-C10-C11	4.30	120.77	111.50
23	A	404[B]	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	C	504	CLA	C3C-C4C-NC	4.30	115.39	110.57
23	c	503	CLA	C4A-NA-C1A	-4.30	104.78	106.71
23	d	403	CLA	C3D-C4D-ND	4.29	117.18	110.24
25	d	404	BCR	C40-C30-C25	-4.29	103.34	110.30
23	b	604	CLA	C3D-C2D-C1D	-4.29	99.98	105.83
23	B	603	CLA	O2D-CGD-O1D	-4.29	115.46	123.84
23	a	404[A]	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
23	B	601	CLA	C3C-C4C-NC	4.28	115.37	110.57
23	b	610	CLA	C3D-C4D-ND	4.27	117.15	110.24
23	D	402[B]	CLA	C1C-C2C-C3C	-4.27	102.47	106.96
23	c	514	CLA	C1D-CHD-C4C	-4.26	116.86	126.06
23	C	514	CLA	C3D-C4D-ND	4.26	117.13	110.24
26	b	620	SQD	C1-O5-C5	-4.26	105.33	113.69
23	d	403	CLA	C4A-NA-C1A	-4.26	104.79	106.71
23	b	607	CLA	C3B-C4B-NB	4.26	114.71	109.21
29	D	405[B]	PL9	C42-C43-C44	-4.26	117.41	127.66
23	D	402[B]	CLA	C3D-C4D-ND	4.25	117.12	110.24
23	a	406[A]	CLA	C3C-C4C-NC	4.25	115.34	110.57
25	b	617	BCR	C33-C5-C6	-4.25	119.75	124.53
23	A	405[B]	CLA	C3D-C4D-ND	4.25	117.11	110.24
23	c	514	CLA	C3C-C4C-NC	4.25	115.33	110.57
23	c	504	CLA	C1D-CHD-C4C	-4.25	116.90	126.06
23	C	514	CLA	C4A-NA-C1A	-4.24	104.80	106.71
23	b	607	CLA	C4A-NA-C1A	-4.24	104.80	106.71
23	b	616	CLA	C3C-C4C-NC	4.24	115.33	110.57
23	c	512	CLA	C3C-C4C-NC	4.24	115.33	110.57
23	A	406[B]	CLA	C3C-C4C-NC	4.24	115.33	110.57
23	c	504	CLA	C3D-C4D-ND	4.24	117.09	110.24
23	b	607	CLA	C1C-C2C-C3C	-4.23	102.51	106.96
23	C	511	CLA	C1-C2-C3	-4.23	118.72	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	512	CLA	C3C-C4C-NC	4.23	115.32	110.57
23	C	504	CLA	O2D-CGD-CBD	4.23	118.79	111.27
23	C	507	CLA	C3D-C4D-ND	4.23	117.07	110.24
26	A	410[B]	SQD	C1-C2-C3	-4.22	101.20	110.00
23	D	403	CLA	O2D-CGD-O1D	-4.22	115.58	123.84
23	b	606	CLA	O2D-CGD-O1D	-4.22	115.59	123.84
23	a	404[A]	CLA	C3D-C4D-ND	4.22	117.06	110.24
23	C	504	CLA	C3D-C4D-ND	4.22	117.06	110.24
23	B	602	CLA	C3D-C4D-ND	4.21	117.05	110.24
23	b	602	CLA	C3D-C2D-C1D	-4.21	100.08	105.83
23	c	502	CLA	C3D-C4D-ND	4.21	117.05	110.24
23	a	404[A]	CLA	C1D-CHD-C4C	-4.21	116.98	126.06
23	B	615	CLA	C3C-C4C-NC	4.20	115.29	110.57
32	E	101[B]	LHG	O7-C7-C8	4.20	120.56	111.50
23	C	503	CLA	C3D-C4D-ND	4.20	117.03	110.24
29	A	414[B]	PL9	C32-C33-C34	-4.20	117.56	127.66
29	a	413[B]	PL9	C7-C8-C9	-4.20	119.81	126.79
23	b	603	CLA	C1D-CHD-C4C	-4.20	117.01	126.06
23	b	602	CLA	C3C-C4C-NC	4.19	115.27	110.57
26	a	410[A]	SQD	C1-C2-C3	-4.19	101.27	110.00
23	a	404[B]	CLA	C1C-C2C-C3C	-4.19	102.55	106.96
23	c	505	CLA	C3C-C4C-NC	4.19	115.27	110.57
23	b	615	CLA	C3D-C4D-ND	4.19	117.01	110.24
23	d	402[B]	CLA	O2D-CGD-CBD	4.18	118.70	111.27
23	B	613	CLA	CAC-C3C-C4C	4.18	130.24	124.81
23	B	607	CLA	C3D-C4D-ND	4.18	117.00	110.24
23	b	614	CLA	C3D-C4D-ND	4.18	117.00	110.24
23	a	404[A]	CLA	CAA-C2A-C3A	-4.18	101.34	112.78
23	C	503	CLA	C4A-NA-C1A	-4.17	104.83	106.71
23	C	514	CLA	C1C-C2C-C3C	-4.17	102.58	106.96
23	c	510	CLA	C3D-C2D-C1D	-4.17	100.15	105.83
40	v	201	HEC	CMB-C2B-C1B	-4.16	122.06	128.46
23	B	616	CLA	C1D-CHD-C4C	-4.16	117.08	126.06
23	a	406[B]	CLA	C3C-C4C-NC	4.16	115.24	110.57
23	b	616	CLA	C2C-C1C-NC	4.16	113.87	109.97
23	b	609	CLA	O2D-CGD-CBD	4.16	118.66	111.27
34	d	410	LMG	O7-C10-C11	4.16	120.46	111.50
23	A	406[A]	CLA	C1C-C2C-C3C	-4.16	102.59	106.96
40	v	201	HEC	CMC-C2C-C1C	-4.15	122.08	128.46
34	C	501	LMG	O1-C1-C2	4.14	114.77	108.30
23	B	616	CLA	C4C-C3C-C2C	-4.14	100.86	106.90
23	A	404[B]	CLA	C3C-C4C-NC	4.14	115.22	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	402[A]	CLA	C1C-C2C-C3C	-4.14	102.60	106.96
23	c	512	CLA	C3D-C4D-ND	4.14	116.94	110.24
34	C	501	LMG	O7-C10-C11	4.14	120.42	111.50
23	C	511	CLA	C1C-C2C-C3C	-4.14	102.61	106.96
23	b	612	CLA	C3D-C4D-ND	4.13	116.92	110.24
23	b	606	CLA	C1D-CHD-C4C	-4.12	117.17	126.06
23	a	405[A]	CLA	C3D-C4D-ND	4.12	116.90	110.24
23	b	607	CLA	O2D-CGD-CBD	4.12	118.58	111.27
23	D	403	CLA	C1D-CHD-C4C	-4.12	117.18	126.06
29	A	414[A]	PL9	C7-C3-C2	-4.12	117.89	123.30
23	c	503	CLA	C3D-C4D-ND	4.12	116.89	110.24
23	d	402[A]	CLA	O2D-CGD-CBD	4.11	118.58	111.27
23	d	402[A]	CLA	C3D-C2D-C1D	-4.11	100.22	105.83
23	c	508	CLA	C1C-C2C-C3C	-4.11	102.63	106.96
23	a	408	CLA	CMC-C2C-C1C	4.11	131.30	125.04
23	c	505	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	C	514	CLA	C3B-C4B-NB	4.11	114.52	109.21
23	A	404[B]	CLA	CAA-C2A-C3A	-4.11	101.54	112.78
26	L	101	SQD	C3-C4-C5	4.10	117.56	110.24
23	A	405[A]	CLA	C3D-C4D-ND	4.10	116.87	110.24
23	C	504	CLA	C1D-CHD-C4C	-4.10	117.22	126.06
23	c	513	CLA	C3D-C4D-ND	4.09	116.86	110.24
23	b	605	CLA	C3C-C4C-NC	4.08	115.15	110.57
23	c	503	CLA	C3C-C4C-NC	4.08	115.15	110.57
23	c	503	CLA	C1D-CHD-C4C	-4.08	117.25	126.06
34	c	521	LMG	O7-C10-C11	4.08	120.30	111.50
23	b	609	CLA	C1-C2-C3	-4.08	118.98	126.04
23	c	503	CLA	CHD-C1D-ND	-4.08	120.70	124.45
23	B	609	CLA	O2D-CGD-CBD	4.08	118.52	111.27
23	C	513	CLA	C1D-CHD-C4C	-4.08	117.26	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
25	A	409	BCR	C24-C23-C22	-4.08	120.08	126.23
23	D	402[B]	CLA	O2D-CGD-CBD	4.07	118.51	111.27
26	a	410[A]	SQD	C1-O5-C5	-4.07	105.69	113.69
23	D	402[A]	CLA	C3D-C4D-ND	4.07	116.82	110.24
25	d	404	BCR	C29-C30-C25	4.06	116.74	110.48
23	A	406[A]	CLA	C3C-C4C-NC	4.06	115.13	110.57
23	c	507	CLA	C3C-C4C-NC	4.06	115.13	110.57
23	A	408	CLA	C3C-C4C-NC	4.06	115.12	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	405[A]	CLA	C3C-C4C-NC	4.06	115.12	110.57
26	A	410[B]	SQD	C44-O6-C1	-4.06	105.82	113.74
23	C	505	CLA	C3D-C4D-ND	4.05	116.80	110.24
23	a	404[B]	CLA	C1D-CHD-C4C	-4.05	117.31	126.06
26	L	101	SQD	O7-S-C6	4.05	111.76	106.94
23	B	606	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
23	b	616	CLA	C3D-C4D-ND	4.05	116.79	110.24
34	C	521	LMG	O7-C10-C11	4.04	120.22	111.50
23	c	509	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
23	C	503	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
23	B	614	CLA	CMC-C2C-C1C	4.04	131.19	125.04
23	C	510	CLA	C3D-C4D-ND	4.04	116.77	110.24
26	a	410[B]	SQD	C1-O5-C5	-4.04	105.76	113.69
23	d	403	CLA	C3C-C4C-NC	4.04	115.10	110.57
23	C	511	CLA	C1D-CHD-C4C	-4.04	117.35	126.06
23	C	509	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
23	B	603	CLA	C3D-C4D-ND	4.03	116.75	110.24
23	b	608	CLA	C3D-C4D-ND	4.02	116.75	110.24
34	m	101	LMG	O7-C10-C11	4.02	120.17	111.50
23	C	502	CLA	C1D-CHD-C4C	-4.02	117.38	126.06
34	c	520	LMG	O7-C10-C11	4.02	120.16	111.50
23	c	513	CLA	C1-C2-C3	-4.02	119.09	126.04
23	c	510	CLA	C3B-C4B-NB	4.02	114.40	109.21
23	C	510	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
34	C	521	LMG	O6-C5-C4	4.01	116.98	109.69
23	c	502	CLA	C3C-C4C-NC	4.01	115.07	110.57
23	a	405[A]	CLA	C1D-CHD-C4C	-4.01	117.41	126.06
23	b	602	CLA	O2D-CGD-O1D	-4.01	116.00	123.84
23	b	601	CLA	C3C-C4C-NC	4.01	115.07	110.57
38	f	101	HEM	CAD-CBD-CGD	4.01	122.23	113.60
23	c	512	CLA	C1D-CHD-C4C	-4.01	117.42	126.06
23	C	514	CLA	C3C-C4C-NC	4.00	115.06	110.57
23	C	513	CLA	C1-C2-C3	-4.00	119.12	126.04
23	c	510	CLA	C3C-C4C-NC	4.00	115.06	110.57
23	C	508	CLA	O2D-CGD-O1D	-4.00	116.01	123.84
23	B	605	CLA	C1D-CHD-C4C	-4.00	117.44	126.06
23	C	512	CLA	C3D-C4D-ND	3.99	116.70	110.24
23	B	601	CLA	C1D-CHD-C4C	-3.99	117.45	126.06
23	C	506	CLA	C3D-C2D-C1D	-3.99	100.39	105.83
23	a	408	CLA	C1D-CHD-C4C	-3.98	117.47	126.06
34	c	521	LMG	C3-C4-C5	3.98	117.34	110.24
23	b	610	CLA	C1D-CHD-C4C	-3.98	117.47	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	510	CLA	C1D-CHD-C4C	-3.98	117.48	126.06
23	B	610	CLA	C3C-C4C-NC	3.97	115.03	110.57
33	B	626	LMT	C1'-O5'-C5'	-3.97	105.89	113.69
23	D	403	CLA	C3D-C4D-ND	3.97	116.66	110.24
23	A	405[B]	CLA	CBC-CAC-C3C	-3.97	101.49	112.43
23	c	508	CLA	C3D-C4D-ND	3.97	116.66	110.24
23	a	404[B]	CLA	CAA-C2A-C3A	-3.97	101.92	112.78
23	a	405[B]	CLA	C3D-C4D-ND	3.97	116.65	110.24
23	A	405[B]	CLA	C1D-CHD-C4C	-3.96	117.52	126.06
25	y	101	BCR	C15-C14-C13	-3.95	121.67	127.31
23	a	404[A]	CLA	C3C-C4C-NC	3.95	115.00	110.57
23	b	606	CLA	C3D-C4D-ND	3.95	116.63	110.24
23	D	403	CLA	C3C-C4C-NC	3.95	115.00	110.57
23	b	615	CLA	C1D-CHD-C4C	-3.95	117.53	126.06
23	a	404[A]	CLA	C3B-C4B-NB	3.95	114.31	109.21
23	A	404[A]	CLA	C3C-C4C-NC	3.95	115.00	110.57
23	b	614	CLA	C3C-C4C-NC	3.94	114.99	110.57
23	a	408	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
23	B	602	CLA	C1D-CHD-C4C	-3.94	117.57	126.06
29	d	405[A]	PL9	C42-C43-C44	-3.93	118.19	127.66
23	C	508	CLA	C1C-C2C-C3C	-3.93	102.82	106.96
23	c	505	CLA	C1-O2A-CGA	3.93	126.76	116.44
26	F	103	SQD	O8-S-C6	3.93	112.00	105.74
23	a	406[B]	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
23	D	402[A]	CLA	C1-C2-C3	-3.93	119.25	126.04
23	b	615	CLA	C3C-C4C-NC	3.93	114.98	110.57
23	a	406[A]	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
23	B	604	CLA	CHD-C1D-ND	-3.93	120.84	124.45
23	B	608	CLA	C3D-C4D-ND	3.93	116.59	110.24
26	A	410[B]	SQD	O47-C7-C8	3.93	119.96	111.50
23	a	405[B]	CLA	C1D-CHD-C4C	-3.92	117.59	126.06
23	b	606	CLA	C4-C3-C5	3.92	121.87	115.27
23	C	513	CLA	C3D-C4D-ND	3.92	116.58	110.24
23	b	601	CLA	C1D-CHD-C4C	-3.92	117.60	126.06
23	b	612	CLA	C3B-C4B-NB	3.92	114.28	109.21
23	B	614	CLA	C1-C2-C3	-3.92	119.26	126.04
36	c	518[B]	DGD	O2G-C1B-C2B	3.92	119.94	111.50
26	a	410[A]	SQD	C44-O6-C1	-3.91	106.09	113.74
23	C	509	CLA	C3B-C4B-NB	3.91	114.27	109.21
23	a	404[B]	CLA	C3C-C4C-NC	3.91	114.95	110.57
29	A	414[A]	PL9	C7-C3-C4	3.91	120.05	116.88
29	a	413[A]	PL9	C32-C33-C34	-3.89	118.28	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	608	CLA	CAC-C3C-C4C	3.89	129.86	124.81
34	C	520	LMG	O7-C10-C11	3.89	119.88	111.50
23	b	608	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
23	A	406[B]	CLA	C1C-C2C-C3C	-3.88	102.87	106.96
32	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	C	506	CLA	CAC-C3C-C4C	3.88	129.85	124.81
23	A	405[A]	CLA	CMC-C2C-C1C	3.88	130.95	125.04
23	b	610	CLA	O2A-CGA-CBA	3.88	124.09	111.91
23	B	614	CLA	C3D-C4D-ND	3.88	116.51	110.24
23	c	505	CLA	C3B-C4B-NB	3.88	114.22	109.21
40	V	201	HEC	CBA-CAA-C2A	-3.88	106.07	112.60
23	a	405[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
29	a	413[B]	PL9	C32-C33-C34	-3.86	118.36	127.66
23	B	603	CLA	C1C-C2C-C3C	-3.86	102.89	106.96
26	A	412	SQD	O8-S-C6	3.86	111.90	105.74
23	b	608	CLA	C3B-C4B-NB	3.86	114.20	109.21
23	C	509	CLA	C3D-C4D-ND	3.86	116.48	110.24
23	C	511	CLA	C4A-NA-C1A	-3.86	104.97	106.71
23	B	602	CLA	O2D-CGD-O1D	-3.86	116.29	123.84
23	b	608	CLA	CMB-C2B-C3B	3.86	131.90	124.68
23	C	512	CLA	C1D-CHD-C4C	-3.86	117.74	126.06
23	B	604	CLA	C3D-C2D-C1D	-3.86	100.57	105.83
23	c	509	CLA	C1-C2-C3	-3.86	119.38	126.04
23	B	610	CLA	C3D-C4D-ND	3.85	116.47	110.24
23	A	405[A]	CLA	C3C-C4C-NC	3.85	114.89	110.57
23	A	408	CLA	C3B-C4B-NB	3.85	114.19	109.21
23	B	615	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
23	c	509	CLA	C3D-C4D-ND	3.85	116.47	110.24
23	B	608	CLA	C3B-C4B-NB	3.85	114.19	109.21
23	C	505	CLA	C3B-C4B-NB	3.85	114.19	109.21
23	C	508	CLA	C1D-CHD-C4C	-3.85	117.76	126.06
23	a	408	CLA	O2D-CGD-O1D	-3.84	116.32	123.84
23	b	612	CLA	CAC-C3C-C4C	3.84	129.80	124.81
23	b	612	CLA	C3D-C2D-C1D	-3.84	100.59	105.83
36	C	517[B]	DGD	O2G-C1B-C2B	3.84	119.78	111.50
29	a	413[A]	PL9	C7-C3-C2	-3.84	118.25	123.30
23	a	405[B]	CLA	C3C-C4C-NC	3.84	114.87	110.57
23	b	616	CLA	O2A-CGA-CBA	3.83	123.94	111.91
23	a	404[B]	CLA	C3B-C4B-NB	3.83	114.16	109.21
40	V	201	HEC	C1D-C2D-C3D	-3.83	104.33	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	507	CLA	C1-C2-C3	-3.83	119.42	126.04
23	B	613	CLA	C3D-C4D-ND	3.83	116.43	110.24
23	B	615	CLA	C1D-CHD-C4C	-3.82	117.81	126.06
23	b	611	CLA	C1-C2-C3	-3.82	119.43	126.04
40	v	201	HEC	CBA-CAA-C2A	-3.82	106.16	112.60
23	B	606	CLA	C3D-C4D-ND	3.82	116.42	110.24
23	A	404[B]	CLA	C3B-C4B-NB	3.82	114.14	109.21
23	B	616	CLA	C3D-C4D-ND	3.82	116.41	110.24
23	C	502	CLA	C3C-C4C-NC	3.82	114.85	110.57
23	B	603	CLA	CMB-C2B-C3B	3.81	131.81	124.68
23	c	511	CLA	CMC-C2C-C1C	3.81	130.84	125.04
23	B	603	CLA	C1D-CHD-C4C	-3.81	117.84	126.06
29	A	414[B]	PL9	C7-C3-C2	-3.80	118.30	123.30
23	B	614	CLA	C1D-CHD-C4C	-3.80	117.85	126.06
29	a	413[B]	PL9	C7-C3-C4	3.80	119.97	116.88
23	b	615	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
32	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
23	A	404[B]	CLA	C1C-C2C-C3C	-3.80	102.97	106.96
23	b	610	CLA	C4C-C3C-C2C	-3.80	101.36	106.90
23	b	608	CLA	CMC-C2C-C1C	3.79	130.82	125.04
23	c	506	CLA	C3D-C2D-C1D	-3.79	100.66	105.83
29	A	414[B]	PL9	C37-C38-C39	-3.79	118.54	127.66
34	Z	101	LMG	C1-C2-C3	3.79	117.89	110.00
25	C	516	BCR	C7-C8-C9	-3.79	120.51	126.23
23	B	610	CLA	C1D-CHD-C4C	-3.79	117.89	126.06
23	C	509	CLA	C1-C2-C3	-3.78	119.50	126.04
23	A	408	CLA	C1D-CHD-C4C	-3.78	117.90	126.06
32	L	102[B]	LHG	O7-C7-C8	3.78	119.65	111.50
26	A	410[A]	SQD	C44-O6-C1	-3.78	106.36	113.74
23	B	612	CLA	C4C-C3C-C2C	-3.78	101.39	106.90
23	B	616	CLA	CMB-C2B-C3B	3.78	131.75	124.68
23	A	408	CLA	C1C-C2C-C3C	-3.78	102.99	106.96
38	F	102	HEM	CBD-CAD-C3D	-3.78	102.14	112.63
23	B	615	CLA	CMC-C2C-C1C	3.78	130.79	125.04
23	d	402[B]	CLA	C3B-C4B-NB	3.77	114.09	109.21
25	Y	101	BCR	C15-C14-C13	-3.77	121.92	127.31
25	Y	101	BCR	C16-C17-C18	-3.77	121.93	127.31
23	A	405[A]	CLA	CBC-CAC-C3C	-3.77	102.04	112.43
23	b	605	CLA	O2D-CGD-O1D	-3.76	116.48	123.84
32	d	412[B]	LHG	O7-C7-C8	3.76	119.61	111.50
23	b	614	CLA	C1D-CHD-C4C	-3.76	117.94	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	616	CLA	O2D-CGD-O1D	-3.76	116.49	123.84
24	a	415[A]	PHO	C4-C3-C5	3.76	121.59	115.27
23	c	513	CLA	C1D-CHD-C4C	-3.76	117.95	126.06
23	C	509	CLA	O2D-CGD-O1D	-3.76	116.49	123.84
23	a	404[B]	CLA	O2D-CGD-CBD	3.76	117.94	111.27
25	t	102	BCR	C11-C10-C9	-3.75	121.95	127.31
23	c	511	CLA	C3D-C4D-ND	3.75	116.31	110.24
23	c	503	CLA	O2D-CGD-O1D	-3.75	116.50	123.84
23	b	605	CLA	C1D-CHD-C4C	-3.75	117.97	126.06
23	c	513	CLA	C3C-C4C-NC	3.75	114.77	110.57
23	c	506	CLA	CAC-C3C-C4C	3.75	129.67	124.81
23	B	616	CLA	C3B-C4B-NB	3.74	114.05	109.21
34	B	620	LMG	O8-C28-C29	3.74	123.65	111.91
25	K	102	BCR	C7-C8-C9	-3.74	120.58	126.23
26	A	410[A]	SQD	O47-C7-C8	3.74	119.56	111.50
23	C	510	CLA	C3B-C4B-NB	3.74	114.04	109.21
23	D	402[B]	CLA	C3B-C4B-NB	3.74	114.04	109.21
23	d	403	CLA	C1C-C2C-C3C	-3.74	103.03	106.96
29	a	413[A]	PL9	C15-C14-C16	3.74	121.56	115.27
23	A	406[A]	CLA	C1D-CHD-C4C	-3.73	118.01	126.06
23	b	612	CLA	C4-C3-C5	3.73	121.55	115.27
23	C	507	CLA	C3C-C4C-NC	3.72	114.75	110.57
23	c	507	CLA	C1C-C2C-C3C	-3.72	103.04	106.96
23	C	511	CLA	C3B-C4B-NB	3.72	114.02	109.21
23	b	613	CLA	C3D-C4D-ND	3.72	116.26	110.24
26	a	411	SQD	O47-C7-C8	3.72	119.52	111.50
23	A	404[A]	CLA	C3D-C4D-ND	3.72	116.25	110.24
23	b	603	CLA	C3B-C4B-NB	3.72	114.02	109.21
23	B	608	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
23	B	607	CLA	C4-C3-C5	3.72	121.52	115.27
25	H	101	BCR	C16-C17-C18	-3.72	122.01	127.31
23	a	405[B]	CLA	CAA-C2A-C3A	-3.72	102.60	112.78
32	d	407[B]	LHG	O7-C7-C8	3.71	119.51	111.50
23	b	604	CLA	C3B-C4B-NB	3.71	114.01	109.21
23	B	616	CLA	CHD-C1D-ND	-3.71	121.04	124.45
23	C	507	CLA	C1-C2-C3	-3.71	119.63	126.04
26	A	412	SQD	O47-C7-C8	3.71	119.50	111.50
23	B	606	CLA	C1D-CHD-C4C	-3.71	118.06	126.06
23	b	604	CLA	C3D-C4D-ND	3.70	116.23	110.24
25	B	618	BCR	C29-C30-C25	3.70	116.18	110.48
23	c	505	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
23	c	506	CLA	O2D-CGD-O1D	-3.70	116.61	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	613	CLA	C1-C2-C3	-3.70	119.65	126.04
36	C	518[A]	DGD	O2G-C1B-C2B	3.69	119.46	111.50
23	b	608	CLA	C3C-C4C-NC	3.69	114.71	110.57
23	C	514	CLA	C1D-CHD-C4C	-3.69	118.09	126.06
23	b	613	CLA	C3B-C4B-NB	3.69	113.98	109.21
23	b	603	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
23	c	511	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
23	B	613	CLA	C3B-C4B-NB	3.69	113.98	109.21
23	B	604	CLA	C1C-C2C-C3C	-3.68	103.08	106.96
26	F	103	SQD	C44-O6-C1	-3.68	106.54	113.74
23	C	508	CLA	C3D-C4D-ND	3.68	116.19	110.24
32	L	102[A]	LHG	O7-C7-C8	3.68	119.43	111.50
29	A	414[A]	PL9	C37-C38-C39	-3.67	118.82	127.66
23	c	512	CLA	O2D-CGD-O1D	-3.67	116.67	123.84
36	c	517[B]	DGD	O2G-C1B-C2B	3.67	119.40	111.50
23	a	404[A]	CLA	O2A-CGA-O1A	-3.67	114.34	123.59
23	d	402[B]	CLA	C1-C2-C3	-3.66	119.71	126.04
23	c	509	CLA	C1D-CHD-C4C	-3.66	118.16	126.06
23	b	614	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
25	a	409	BCR	C38-C26-C25	-3.66	120.42	124.53
23	A	405[B]	CLA	CMC-C2C-C1C	3.66	130.61	125.04
23	C	506	CLA	C1D-CHD-C4C	-3.66	118.17	126.06
29	d	405[B]	PL9	C42-C43-C44	-3.66	118.86	127.66
38	f	101	HEM	C1B-NB-C4B	3.66	108.85	105.07
23	B	607	CLA	CMC-C2C-C1C	3.65	130.60	125.04
23	a	404[A]	CLA	CMB-C2B-C3B	3.65	131.51	124.68
23	b	613	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
23	B	605	CLA	C4-C3-C5	3.65	121.41	115.27
23	B	607	CLA	O2D-CGD-O1D	-3.65	116.71	123.84
26	a	410[B]	SQD	C44-O6-C1	-3.64	106.63	113.74
23	b	609	CLA	CBC-CAC-C3C	-3.64	102.39	112.43
23	C	507	CLA	C3B-C4B-NB	3.63	113.90	109.21
26	a	410[A]	SQD	O9-S-C6	3.63	111.25	106.94
23	D	402[A]	CLA	C3B-C4B-NB	3.62	113.89	109.21
35	b	622	HTG	C1'-S1-C1	3.62	106.86	100.09
23	C	512	CLA	C4-C3-C5	3.62	121.36	115.27
23	b	602	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
23	A	405[A]	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
23	B	610	CLA	CAA-C2A-C3A	-3.62	102.88	112.78
23	C	512	CLA	C1C-C2C-C3C	-3.62	103.16	106.96
23	B	613	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
23	B	603	CLA	CAA-C2A-C3A	-3.61	102.89	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	515	BCR	C33-C5-C6	-3.61	120.48	124.53
23	B	602	CLA	CMC-C2C-C1C	3.61	130.53	125.04
23	B	615	CLA	O2D-CGD-CBD	3.61	117.68	111.27
29	A	414[B]	PL9	C7-C3-C4	3.60	119.81	116.88
23	A	408	CLA	C1-C2-C3	-3.60	119.81	126.04
23	b	611	CLA	C3B-C4B-NB	3.60	113.87	109.21
23	A	408	CLA	O2D-CGD-CBD	3.60	117.67	111.27
23	b	607	CLA	C1D-CHD-C4C	-3.60	118.29	126.06
23	b	606	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
23	b	604	CLA	CAC-C3C-C4C	3.60	129.48	124.81
23	c	512	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
40	V	201	HEC	CMC-C2C-C1C	-3.60	122.94	128.46
23	b	603	CLA	CAA-C2A-C3A	-3.59	102.94	112.78
23	c	510	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
23	c	502	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
23	c	508	CLA	O2D-CGD-O1D	-3.59	116.82	123.84
23	B	604	CLA	C1D-CHD-C4C	-3.59	118.32	126.06
23	C	512	CLA	O2D-CGD-O1D	-3.59	116.83	123.84
23	B	608	CLA	O2D-CGD-O1D	-3.59	116.83	123.84
23	A	405[A]	CLA	O2D-CGD-O1D	-3.58	116.83	123.84
23	b	614	CLA	C1-C2-C3	-3.58	119.85	126.04
23	d	402[A]	CLA	C3B-C4B-NB	3.58	113.84	109.21
23	c	511	CLA	C1D-CHD-C4C	-3.58	118.33	126.06
25	h	101	BCR	C38-C26-C25	-3.58	120.51	124.53
23	B	604	CLA	C3D-C4D-ND	3.58	116.03	110.24
23	c	507	CLA	C3B-C4B-NB	3.58	113.83	109.21
23	c	510	CLA	CAC-C3C-C4C	3.58	129.45	124.81
24	A	407[B]	PHO	C1A-C2A-C3A	-3.57	99.44	102.84
23	b	603	CLA	O2D-CGD-O1D	-3.57	116.85	123.84
23	c	511	CLA	C3B-C4B-NB	3.57	113.83	109.21
23	a	406[B]	CLA	CHD-C4C-NC	3.57	129.83	124.20
23	b	612	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
23	b	611	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
23	B	614	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
23	d	402[A]	CLA	C1-C2-C3	-3.56	119.89	126.04
23	c	514	CLA	C3B-C4B-NB	3.56	113.81	109.21
23	B	613	CLA	O2A-CGA-O1A	-3.56	114.62	123.59
23	C	502	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
23	B	602	CLA	CAA-C2A-C3A	-3.55	103.06	112.78
23	B	611	CLA	CHB-C4A-NA	3.55	129.42	124.51
23	B	605	CLA	CHD-C4C-NC	3.55	129.79	124.20
23	C	503	CLA	C3B-C4B-NB	3.55	113.79	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	d	405[A]	PL9	C40-C39-C41	3.55	121.23	115.27
23	D	402[B]	CLA	C1-C2-C3	-3.54	119.91	126.04
29	a	413[A]	PL9	C27-C28-C29	-3.54	119.13	127.66
23	b	609	CLA	C1D-CHD-C4C	-3.54	118.42	126.06
25	k	101	BCR	C29-C30-C25	3.54	115.93	110.48
25	T	102	BCR	C11-C10-C9	-3.54	122.26	127.31
23	d	402[B]	CLA	C1D-CHD-C4C	-3.54	118.43	126.06
23	a	404[B]	CLA	CMB-C2B-C3B	3.54	131.29	124.68
23	B	607	CLA	C3B-C4B-NB	3.53	113.78	109.21
26	L	101	SQD	O9-S-C6	3.53	111.14	106.94
23	B	605	CLA	O2D-CGD-O1D	-3.53	116.93	123.84
23	A	404[A]	CLA	O2D-CGD-CBD	3.53	117.54	111.27
23	B	606	CLA	O2D-CGD-O1D	-3.53	116.93	123.84
26	F	103	SQD	C1-C2-C3	-3.53	102.64	110.00
29	d	405[B]	PL9	C7-C8-C9	-3.53	120.92	126.79
23	b	615	CLA	O2D-CGD-CBD	3.53	117.54	111.27
23	B	607	CLA	O2A-CGA-O1A	-3.53	114.69	123.59
23	b	611	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
23	B	608	CLA	C1D-CHD-C4C	-3.52	118.46	126.06
23	C	513	CLA	C4-C3-C5	3.52	121.19	115.27
29	A	414[A]	PL9	C22-C23-C24	-3.52	119.19	127.66
23	A	406[B]	CLA	C1D-CHD-C4C	-3.52	118.47	126.06
25	c	515	BCR	C11-C10-C9	-3.51	122.30	127.31
23	B	603	CLA	C3B-C4B-NB	3.51	113.75	109.21
29	A	414[A]	PL9	C15-C14-C16	3.51	121.18	115.27
23	B	610	CLA	CAA-CBA-CGA	-3.51	103.00	113.25
23	A	404[A]	CLA	C1D-CHD-C4C	-3.51	118.49	126.06
23	B	604	CLA	C3B-C4B-NB	3.51	113.75	109.21
23	C	507	CLA	C1D-CHD-C4C	-3.51	118.49	126.06
40	V	201	HEC	CMB-C2B-C1B	-3.50	123.08	128.46
23	c	503	CLA	CBC-CAC-C3C	-3.50	102.78	112.43
23	c	509	CLA	O2D-CGD-O1D	-3.50	116.99	123.84
29	D	405[A]	PL9	C53-C6-C1	3.50	122.15	114.99
23	B	609	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
36	C	518[B]	DGD	O2G-C1B-C2B	3.50	119.04	111.50
29	A	414[B]	PL9	C15-C14-C16	3.50	121.15	115.27
23	a	406[A]	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
23	b	613	CLA	O2D-CGD-CBD	3.49	117.47	111.27
23	b	602	CLA	CAA-C2A-C3A	-3.49	103.23	112.78
23	b	611	CLA	C1D-CHD-C4C	-3.49	118.54	126.06
23	B	614	CLA	C3B-C4B-NB	3.49	113.72	109.21
23	b	612	CLA	CMC-C2C-C1C	3.48	130.34	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	512	CLA	C3B-C4B-NB	3.48	113.71	109.21
29	A	414[B]	PL9	C22-C23-C24	-3.48	119.28	127.66
29	a	413[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
34	C	521	LMG	C3-C4-C5	3.48	116.45	110.24
23	b	612	CLA	C1D-CHD-C4C	-3.48	118.55	126.06
23	B	605	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
23	b	609	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
23	b	614	CLA	C3B-C4B-NB	3.48	113.70	109.21
23	c	512	CLA	C4-C3-C5	3.48	121.12	115.27
29	D	405[A]	PL9	C42-C43-C44	-3.47	119.29	127.66
23	b	616	CLA	O2A-CGA-O1A	-3.47	114.83	123.59
23	c	514	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
23	B	604	CLA	CAC-C3C-C4C	3.47	129.31	124.81
23	a	404[A]	CLA	O2D-CGD-CBD	3.47	117.43	111.27
23	C	506	CLA	C4C-C3C-C2C	-3.47	101.84	106.90
38	F	102	HEM	CHD-C1D-ND	3.47	128.20	124.43
25	d	404	BCR	C38-C26-C25	-3.46	120.64	124.53
29	a	413[B]	PL9	C15-C14-C16	3.46	121.10	115.27
23	A	406[A]	CLA	O2A-CGA-O1A	-3.46	114.85	123.59
32	A	419[B]	LHG	O8-C23-O10	-3.46	114.85	123.59
23	d	402[A]	CLA	O2A-CGA-CBA	3.46	122.77	111.91
25	D	404	BCR	C29-C30-C25	3.45	115.80	110.48
29	d	405[B]	PL9	C40-C39-C41	3.45	121.08	115.27
32	b	630[B]	LHG	O7-C7-C8	3.45	118.94	111.50
23	b	602	CLA	C1-C2-C3	-3.45	120.08	126.04
34	c	501	LMG	C7-O1-C1	-3.45	107.00	113.74
23	c	506	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
23	c	504	CLA	O2D-CGD-O1D	-3.45	117.10	123.84
35	b	625	HTG	C1-O5-C5	3.45	118.94	112.58
23	C	509	CLA	C1D-CHD-C4C	-3.45	118.62	126.06
25	c	516	BCR	C7-C8-C9	-3.45	121.03	126.23
32	A	419[B]	LHG	O7-C7-C8	3.45	118.93	111.50
23	c	511	CLA	C4-C3-C5	3.44	121.06	115.27
23	c	513	CLA	C4-C3-C5	3.44	121.06	115.27
23	b	610	CLA	CAA-C2A-C3A	-3.44	103.35	112.78
25	c	515	BCR	C15-C14-C13	-3.44	122.40	127.31
23	c	506	CLA	C4C-C3C-C2C	-3.44	101.89	106.90
23	b	610	CLA	CAC-C3C-C4C	3.44	129.27	124.81
23	C	506	CLA	C1-C2-C3	-3.43	120.10	126.04
23	B	602	CLA	C1C-C2C-C3C	-3.43	103.35	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	406[B]	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
23	c	509	CLA	C3B-C4B-NB	3.43	113.65	109.21
23	c	505	CLA	C1D-CHD-C4C	-3.43	118.65	126.06
24	a	415[B]	PHO	C4-C3-C5	3.43	121.04	115.27
34	Z	101	LMG	O6-C1-C2	3.43	117.61	110.35
23	b	612	CLA	C4C-C3C-C2C	-3.43	101.90	106.90
23	B	615	CLA	C4-C3-C5	3.43	121.04	115.27
23	C	511	CLA	CHD-C4C-NC	3.43	129.60	124.20
23	b	605	CLA	CHD-C4C-NC	3.42	129.60	124.20
25	T	102	BCR	C15-C16-C17	-3.42	116.46	123.47
23	C	512	CLA	C3B-C4B-NB	3.42	113.63	109.21
23	d	403	CLA	C1D-CHD-C4C	-3.41	118.69	126.06
29	D	405[B]	PL9	C53-C6-C1	3.41	121.97	114.99
23	a	404[A]	CLA	O2A-CGA-CBA	3.41	122.61	111.91
23	A	404[B]	CLA	CMB-C2B-C3B	3.41	131.06	124.68
29	a	413[A]	PL9	C35-C34-C36	3.41	121.01	115.27
23	b	616	CLA	C3B-C4B-NB	3.41	113.61	109.21
32	d	412[B]	LHG	O8-C23-C24	3.41	122.60	111.91
23	b	606	CLA	CHD-C4C-NC	3.41	129.57	124.20
23	C	509	CLA	C4C-C3C-C2C	-3.41	101.93	106.90
23	B	610	CLA	O2A-CGA-O1A	-3.40	115.01	123.59
23	B	614	CLA	O2A-CGA-O1A	-3.39	115.03	123.59
23	B	609	CLA	C1D-CHD-C4C	-3.39	118.74	126.06
23	A	406[A]	CLA	C3B-C4B-NB	3.39	113.59	109.21
25	t	102	BCR	C15-C16-C17	-3.39	116.53	123.47
29	D	405[A]	PL9	C25-C24-C26	3.39	120.97	115.27
23	B	613	CLA	C4A-NA-C1A	-3.39	105.18	106.71
25	D	404	BCR	C28-C27-C26	-3.38	108.03	114.08
23	b	604	CLA	CMC-C2C-C1C	3.38	130.19	125.04
23	b	612	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
25	B	619	BCR	C24-C23-C22	-3.38	121.13	126.23
23	a	405[B]	CLA	C3B-C4B-NB	3.37	113.57	109.21
23	B	609	CLA	CMC-C2C-C1C	3.37	130.18	125.04
23	c	510	CLA	CHC-C1C-C2C	-3.37	117.39	126.72
36	c	518[A]	DGD	O2G-C1B-C2B	3.37	118.77	111.50
23	a	408	CLA	C3B-C4B-NB	3.37	113.57	109.21
38	f	101	HEM	CHA-C4D-ND	3.37	128.54	124.38
23	c	506	CLA	C1D-CHD-C4C	-3.37	118.79	126.06
23	b	616	CLA	CHD-C4C-NC	3.36	129.50	124.20
25	y	101	BCR	C38-C26-C25	-3.36	120.75	124.53
23	B	611	CLA	C4C-C3C-C2C	-3.36	102.00	106.90
23	C	503	CLA	C1D-CHD-C4C	-3.35	118.82	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	o	301	HTG	C1'-S1-C1	3.35	106.36	100.09
26	a	410[B]	SQD	C1-C2-C3	-3.35	103.02	110.00
23	C	511	CLA	C4-C3-C5	3.35	120.91	115.27
29	a	413[B]	PL9	C30-C29-C31	3.35	120.91	115.27
24	A	417[A]	PHO	CMC-C2C-C3C	3.35	131.26	124.94
23	B	611	CLA	O2D-CGD-O1D	-3.35	117.30	123.84
23	C	507	CLA	CAC-C3C-C4C	3.34	129.15	124.81
23	b	603	CLA	C2A-C1A-CHA	-3.34	118.01	123.86
23	B	604	CLA	C4C-C3C-C2C	-3.34	102.03	106.90
23	c	502	CLA	C3B-C4B-NB	3.34	113.52	109.21
23	b	609	CLA	CAC-C3C-C4C	3.34	129.14	124.81
23	C	510	CLA	C1D-CHD-C4C	-3.34	118.86	126.06
25	d	404	BCR	C10-C11-C12	-3.33	112.81	123.22
23	d	402[A]	CLA	C1D-CHD-C4C	-3.33	118.87	126.06
23	A	404[B]	CLA	O2A-CGA-CBA	3.33	122.36	111.91
23	C	511	CLA	C3C-C4C-NC	3.33	114.31	110.57
25	C	515	BCR	C15-C14-C13	-3.33	122.56	127.31
23	c	507	CLA	C1D-CHD-C4C	-3.33	118.88	126.06
23	A	405[A]	CLA	C3B-C4B-NB	3.33	113.51	109.21
23	C	507	CLA	O2D-CGD-O1D	-3.33	117.34	123.84
25	k	101	BCR	C7-C8-C9	-3.32	121.21	126.23
23	c	502	CLA	CAC-C3C-C4C	3.32	129.12	124.81
29	a	413[B]	PL9	C27-C28-C29	-3.32	119.66	127.66
23	D	403	CLA	C1C-C2C-C3C	-3.32	103.47	106.96
24	A	407[A]	PHO	CMA-C3A-C4A	-3.32	107.11	114.38
23	c	504	CLA	C4C-C3C-C2C	-3.31	102.07	106.90
23	B	613	CLA	O2A-CGA-CBA	3.31	122.31	111.91
23	C	505	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
23	c	510	CLA	C4C-C3C-C2C	-3.31	102.07	106.90
29	a	413[B]	PL9	C7-C3-C2	-3.31	118.95	123.30
23	a	405[B]	CLA	CHD-C4C-NC	3.31	129.42	124.20
25	A	409	BCR	C15-C14-C13	-3.31	122.59	127.31
23	B	612	CLA	CMB-C2B-C3B	3.31	130.86	124.68
23	A	405[B]	CLA	C3C-C4C-NC	3.30	114.28	110.57
23	A	405[B]	CLA	C3B-C4B-NB	3.30	113.48	109.21
23	B	601	CLA	CHD-C4C-NC	3.30	129.41	124.20
34	c	501	LMG	C8-O7-C10	-3.30	109.66	117.79
23	b	608	CLA	C1-C2-C3	-3.30	120.34	126.04
23	C	506	CLA	C1C-C2C-C3C	-3.30	103.49	106.96
23	b	604	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
23	b	604	CLA	C1D-CHD-C4C	-3.30	118.94	126.06
23	c	507	CLA	CAC-C3C-C4C	3.30	129.09	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	d	412[A]	LHG	O8-C23-O10	-3.30	115.27	123.59
23	A	408	CLA	CAA-C2A-C3A	-3.30	103.75	112.78
23	B	612	CLA	C1D-CHD-C4C	-3.30	118.95	126.06
32	d	407[A]	LHG	O7-C7-C8	3.29	118.59	111.50
33	D	401	LMT	O5B-C5B-C4B	3.29	115.67	109.69
23	b	601	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
25	D	404	BCR	C16-C17-C18	-3.29	122.62	127.31
23	B	612	CLA	C11-C12-C13	-3.28	105.30	115.92
25	D	404	BCR	C38-C26-C25	-3.28	120.84	124.53
23	C	513	CLA	C1C-C2C-C3C	-3.28	103.50	106.96
23	b	613	CLA	C1D-CHD-C4C	-3.28	118.98	126.06
25	B	617	BCR	C33-C5-C6	-3.28	120.84	124.53
25	b	618	BCR	C15-C14-C13	-3.28	122.63	127.31
23	b	615	CLA	C4-C3-C5	3.28	120.78	115.27
23	c	503	CLA	C3B-C4B-NB	3.27	113.44	109.21
25	c	515	BCR	C16-C17-C18	-3.27	122.64	127.31
23	C	508	CLA	C4C-C3C-C2C	-3.27	102.13	106.90
23	A	405[B]	CLA	CAA-C2A-C3A	-3.27	103.82	112.78
23	B	610	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
23	c	508	CLA	C4-C3-C5	3.27	120.77	115.27
23	B	601	CLA	C4C-C3C-C2C	-3.27	102.14	106.90
23	B	608	CLA	CHC-C1C-C2C	-3.27	117.68	126.72
23	C	513	CLA	CMC-C2C-C1C	3.27	130.01	125.04
23	c	513	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
23	b	611	CLA	C4C-C3C-C2C	-3.27	102.14	106.90
35	V	202	HTG	C1-O5-C5	3.27	116.62	112.19
23	B	602	CLA	C3B-C4B-NB	3.27	113.43	109.21
34	z	101	LMG	O7-C10-C11	3.26	118.53	111.50
23	b	607	CLA	CHC-C1C-C2C	-3.26	117.70	126.72
35	b	622	HTG	O2-C2-C1	3.26	116.26	110.27
23	b	613	CLA	C4C-C3C-C2C	-3.26	102.15	106.90
23	C	510	CLA	CAC-C3C-C4C	3.26	129.04	124.81
29	A	414[B]	PL9	C20-C19-C21	3.26	120.75	115.27
23	c	508	CLA	C1D-CHD-C4C	-3.26	119.03	126.06
23	a	405[A]	CLA	C3B-C4B-NB	3.25	113.42	109.21
23	b	602	CLA	CMC-C2C-C1C	3.25	129.99	125.04
23	b	605	CLA	C1C-C2C-C3C	-3.25	103.54	106.96
23	a	408	CLA	CAA-C2A-C3A	-3.25	103.88	112.78
23	A	404[A]	CLA	CMB-C2B-C3B	3.25	130.75	124.68
23	C	502	CLA	CMC-C2C-C1C	3.25	129.99	125.04
32	d	412[A]	LHG	O7-C7-C8	3.25	118.50	111.50
25	C	515	BCR	C7-C8-C9	-3.25	121.33	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	405[B]	CLA	CHD-C4C-NC	3.25	129.32	124.20
23	b	609	CLA	CMC-C2C-C1C	3.25	129.98	125.04
25	d	404	BCR	C16-C17-C18	-3.25	122.68	127.31
34	c	521	LMG	C9-C8-C7	-3.24	104.11	111.79
23	B	606	CLA	C3B-C4B-NB	3.24	113.40	109.21
29	a	413[B]	PL9	C25-C24-C26	3.24	120.72	115.27
23	b	612	CLA	O2A-CGA-O1A	-3.24	115.42	123.59
23	b	602	CLA	C1C-C2C-C3C	-3.23	103.56	106.96
23	C	506	CLA	CMC-C2C-C1C	3.23	129.96	125.04
23	C	507	CLA	CHC-C1C-C2C	-3.23	117.78	126.72
33	B	626	LMT	C4B-C3B-C2B	3.23	116.46	110.82
23	c	513	CLA	O2A-CGA-CBA	3.23	122.04	111.91
23	B	611	CLA	C1-C2-C3	-3.23	120.46	126.04
23	C	504	CLA	C1C-C2C-C3C	-3.23	103.56	106.96
32	d	406[B]	LHG	O7-C7-C8	3.22	118.45	111.50
23	C	509	CLA	CHC-C1C-C2C	-3.22	117.81	126.72
24	a	415[A]	PHO	C4A-C3A-C2A	-3.22	99.77	102.84
23	a	404[B]	CLA	CHC-C1C-C2C	-3.22	117.82	126.72
26	a	411	SQD	O48-C23-C24	3.22	122.01	111.91
23	B	603	CLA	C4C-C3C-C2C	-3.22	102.21	106.90
32	d	412[A]	LHG	O8-C23-C24	3.22	122.00	111.91
23	B	603	CLA	CHC-C1C-C2C	-3.22	117.83	126.72
23	b	614	CLA	O2A-CGA-O1A	-3.21	115.48	123.59
23	b	607	CLA	C4-C3-C5	3.21	120.68	115.27
23	A	406[B]	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
23	B	615	CLA	C3B-C4B-NB	3.21	113.36	109.21
23	B	611	CLA	C2A-C1A-CHA	-3.21	118.25	123.86
25	T	102	BCR	C12-C13-C14	-3.20	114.02	118.94
29	d	405[B]	PL9	C7-C3-C4	3.20	119.48	116.88
35	o	301	HTG	O5-C1-C2	3.20	114.34	110.31
23	a	404[A]	CLA	CHC-C1C-C2C	-3.20	117.86	126.72
23	a	406[A]	CLA	C3B-C4B-NB	3.20	113.34	109.21
25	h	101	BCR	C7-C8-C9	-3.19	121.41	126.23
23	B	605	CLA	O2A-CGA-O1A	-3.19	115.53	123.59
38	F	102	HEM	CHB-C1B-NB	3.19	128.32	124.38
23	a	404[A]	CLA	CAA-C2A-C1A	-3.19	101.52	111.97
23	B	610	CLA	C3B-C4B-NB	3.19	113.34	109.21
26	b	620	SQD	O8-S-C6	3.19	110.82	105.74
23	b	601	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
23	C	505	CLA	C1-O2A-CGA	3.19	124.81	116.44
23	B	608	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
23	C	512	CLA	CAC-C3C-C4C	3.19	128.94	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	413[A]	PL9	C17-C18-C19	-3.19	119.99	127.66
23	b	601	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
32	D	407[B]	LHG	O7-C7-C8	3.18	118.36	111.50
23	C	511	CLA	CHC-C1C-C2C	-3.18	117.91	126.72
25	D	404	BCR	C10-C11-C12	-3.18	113.29	123.22
23	A	406[A]	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
23	b	616	CLA	C4C-C3C-C2C	-3.18	102.27	106.90
29	A	414[A]	PL9	C27-C28-C29	-3.18	120.01	127.66
23	c	512	CLA	CHD-C4C-NC	3.18	129.21	124.20
23	B	612	CLA	CAC-C3C-C4C	3.17	128.93	124.81
26	F	103	SQD	O7-S-C6	3.17	110.71	106.94
24	a	407[B]	PHO	CMA-C3A-C4A	-3.17	107.43	114.38
29	a	413[A]	PL9	C25-C24-C26	3.17	120.61	115.27
23	A	404[A]	CLA	O2A-CGA-O1A	-3.17	115.59	123.59
23	D	402[A]	CLA	C1D-CHD-C4C	-3.17	119.22	126.06
23	C	512	CLA	C1-O2A-CGA	3.17	124.76	116.44
23	b	609	CLA	C3B-C4B-NB	3.17	113.31	109.21
26	b	620	SQD	O7-S-C6	3.17	110.70	106.94
29	D	405[B]	PL9	C17-C18-C19	-3.16	120.04	127.66
23	A	406[B]	CLA	CAA-C2A-C3A	-3.16	104.11	112.78
23	B	607	CLA	CBC-CAC-C3C	-3.16	103.72	112.43
23	b	613	CLA	O2A-CGA-O1A	-3.16	115.62	123.59
25	a	409	BCR	C40-C30-C25	-3.16	105.18	110.30
23	C	506	CLA	C4-C3-C5	3.16	120.58	115.27
24	A	417[A]	PHO	C4-C3-C5	3.15	120.58	115.27
23	b	603	CLA	C4C-C3C-C2C	-3.15	102.30	106.90
23	C	514	CLA	C1-C2-C3	-3.15	120.59	126.04
23	a	405[A]	CLA	CHD-C4C-NC	3.15	129.17	124.20
38	f	101	HEM	CHD-C1D-ND	3.15	127.85	124.43
32	A	419[A]	LHG	C5-O7-C7	-3.15	110.03	117.79
23	C	513	CLA	O2A-CGA-CBA	3.15	121.79	111.91
32	A	419[A]	LHG	O8-C23-C24	3.15	121.79	111.91
29	D	405[A]	PL9	C17-C18-C19	-3.15	120.08	127.66
35	b	625	HTG	O5-C5-C4	3.15	115.41	109.69
23	B	614	CLA	O2A-CGA-CBA	3.15	121.78	111.91
38	f	101	HEM	C4D-ND-C1D	3.14	108.32	105.07
23	b	612	CLA	C2A-C1A-CHA	-3.14	118.36	123.86
40	v	201	HEC	CMB-C2B-C3B	3.14	129.51	125.82
23	c	505	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
25	c	515	BCR	C37-C22-C21	-3.14	118.52	122.92
23	B	605	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
23	A	406[B]	CLA	C3B-C4B-NB	3.14	113.27	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	504	CLA	C1C-C2C-C3C	-3.14	103.66	106.96
23	a	408	CLA	C4-C3-C5	3.14	120.55	115.27
26	f	102	SQD	O5-C1-C2	3.14	116.99	110.35
23	c	507	CLA	CHC-C1C-C2C	-3.14	118.05	126.72
23	C	503	CLA	CHC-C1C-C2C	-3.14	118.05	126.72
23	B	613	CLA	CMC-C2C-C1C	3.13	129.81	125.04
23	b	616	CLA	CBC-CAC-C3C	-3.13	103.79	112.43
23	b	602	CLA	C4C-C3C-C2C	-3.13	102.33	106.90
23	D	402[B]	CLA	CAC-C3C-C4C	3.13	128.87	124.81
23	B	616	CLA	C1-O2A-CGA	3.13	124.66	116.44
34	m	101	LMG	O8-C28-C29	3.13	121.73	111.91
23	a	406[A]	CLA	CHD-C4C-NC	3.13	129.13	124.20
23	B	613	CLA	C4-C3-C5	3.13	120.53	115.27
23	C	513	CLA	CHD-C4C-NC	3.13	129.13	124.20
23	a	406[A]	CLA	C1-C2-C3	-3.13	120.64	126.04
23	D	402[B]	CLA	CMC-C2C-C1C	3.13	129.80	125.04
23	d	402[A]	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
23	b	604	CLA	CHC-C1C-C2C	-3.13	118.08	126.72
33	b	627	LMT	C3'-C4'-C5'	-3.12	103.77	110.93
23	a	408	CLA	O2A-CGA-CBA	3.12	121.70	111.91
23	b	615	CLA	CHC-C1C-C2C	-3.12	118.09	126.72
23	A	404[B]	CLA	O2D-CGD-CBD	3.12	116.81	111.27
23	c	505	CLA	CAC-C3C-C4C	3.12	128.86	124.81
32	A	419[B]	LHG	O8-C23-C24	3.12	121.69	111.91
29	D	405[A]	PL9	C51-C49-C50	3.12	121.49	114.60
23	C	503	CLA	CAC-C3C-C4C	3.12	128.85	124.81
23	C	505	CLA	C1D-CHD-C4C	-3.11	119.34	126.06
26	f	102	SQD	C4-C3-C2	-3.11	105.39	110.82
23	c	503	CLA	CMC-C2C-C1C	3.11	129.78	125.04
24	A	417[B]	PHO	C1A-C2A-C3A	-3.11	99.88	102.84
23	B	601	CLA	C1C-C2C-C3C	-3.11	103.69	106.96
36	C	519	DGD	O1G-C1A-C2A	3.11	121.66	111.91
23	B	615	CLA	CHD-C4C-NC	3.11	129.10	124.20
23	b	603	CLA	C4-C3-C5	3.11	120.50	115.27
23	a	404[B]	CLA	O2A-CGA-CBA	3.11	121.66	111.91
29	D	405[A]	PL9	C10-C9-C11	3.11	120.50	115.27
23	D	403	CLA	CHD-C4C-NC	3.10	129.09	124.20
23	C	511	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
23	B	614	CLA	CAC-C3C-C4C	3.10	128.83	124.81
23	b	606	CLA	C3B-C4B-NB	3.10	113.22	109.21
23	C	507	CLA	CMC-C2C-C1C	3.10	129.76	125.04
23	b	601	CLA	C4-C3-C5	3.10	120.48	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	414[A]	PL9	C10-C9-C11	3.10	120.48	115.27
23	c	511	CLA	CAC-C3C-C4C	3.10	128.83	124.81
23	b	607	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
23	C	504	CLA	CHD-C4C-NC	3.09	129.08	124.20
32	b	630[A]	LHG	O7-C7-C8	3.09	118.16	111.50
23	C	510	CLA	O2A-CGA-CBA	3.09	121.61	111.91
23	b	614	CLA	CHC-C1C-C2C	-3.09	118.18	126.72
29	d	405[B]	PL9	C10-C9-C11	3.09	120.47	115.27
23	C	506	CLA	C3B-C4B-NB	3.09	113.20	109.21
25	D	404	BCR	C40-C30-C25	-3.09	105.29	110.30
23	c	507	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
23	B	613	CLA	C4C-C3C-C2C	-3.09	102.40	106.90
23	A	408	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
23	C	503	CLA	O2D-CGD-O1D	-3.09	117.81	123.84
23	B	606	CLA	O2A-CGA-O1A	-3.08	115.81	123.59
23	B	605	CLA	C1-C2-C3	-3.08	120.71	126.04
24	a	415[A]	PHO	CMB-C2B-C3B	3.08	130.44	124.68
29	A	414[B]	PL9	C27-C28-C29	-3.08	120.24	127.66
29	a	413[A]	PL9	C10-C9-C11	3.08	120.45	115.27
23	d	403	CLA	CAA-C2A-C3A	-3.08	104.34	112.78
34	C	521	LMG	O8-C28-C29	3.08	121.56	111.91
23	C	503	CLA	C1-C2-C3	-3.08	120.72	126.04
26	A	412	SQD	O48-C23-C24	3.08	121.56	111.91
23	C	510	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
23	c	510	CLA	C4-C3-C5	3.07	120.44	115.27
23	a	404[A]	CLA	C1-C2-C3	-3.07	120.73	126.04
32	a	419[B]	LHG	O7-C7-C8	3.07	118.12	111.50
23	c	502	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
23	b	615	CLA	C11-C10-C8	-3.07	106.00	115.92
23	d	402[B]	CLA	O2A-CGA-CBA	3.06	121.52	111.91
23	c	514	CLA	C4C-C3C-C2C	-3.06	102.43	106.90
33	B	628	LMT	O1'-C1'-C2'	3.06	113.08	108.30
34	C	520	LMG	O8-C28-C29	3.06	121.51	111.91
23	A	406[B]	CLA	O2A-CGA-O1A	-3.06	115.87	123.59
23	B	609	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
23	B	603	CLA	CAC-C3C-C4C	3.06	128.78	124.81
23	c	509	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
32	A	419[B]	LHG	C5-O7-C7	-3.06	110.27	117.79
23	B	613	CLA	C1D-CHD-C4C	-3.06	119.46	126.06
23	D	403	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
34	Z	101	LMG	C4-C3-C2	3.06	116.16	110.82
23	C	512	CLA	CMC-C2C-C1C	3.06	129.69	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	D	406[B]	LHG	O7-C7-C8	3.06	118.08	111.50
25	K	102	BCR	C20-C21-C22	-3.05	122.95	127.31
29	d	405[A]	PL9	C10-C9-C11	3.05	120.41	115.27
23	c	503	CLA	CHD-C4C-NC	3.05	129.01	124.20
23	a	404[A]	CLA	C4-C3-C5	3.05	120.41	115.27
23	D	402[A]	CLA	O2A-CGA-CBA	3.05	121.48	111.91
23	a	406[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	610	CLA	CAA-CBA-CGA	-3.05	104.34	113.25
23	c	511	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
23	c	509	CLA	C4-C3-C5	3.05	120.40	115.27
23	a	406[B]	CLA	C4C-C3C-C2C	-3.05	102.46	106.90
23	b	605	CLA	C4C-C3C-C2C	-3.05	102.46	106.90
23	d	402[A]	CLA	C2A-C1A-CHA	-3.05	118.53	123.86
23	D	403	CLA	C3B-C4B-NB	3.05	113.15	109.21
23	A	408	CLA	C4C-C3C-C2C	-3.05	102.46	106.90
23	A	404[B]	CLA	O2A-CGA-O1A	-3.05	115.90	123.59
23	d	402[A]	CLA	C4C-C3C-C2C	-3.04	102.46	106.90
23	a	404[B]	CLA	CAA-C2A-C1A	-3.04	102.01	111.97
23	D	402[B]	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
29	A	414[A]	PL9	C20-C19-C21	3.04	120.38	115.27
23	c	506	CLA	CMC-C2C-C1C	3.04	129.66	125.04
23	A	404[B]	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
23	c	503	CLA	CHC-C1C-C2C	-3.04	118.33	126.72
23	B	614	CLA	C2A-C1A-CHA	-3.04	118.55	123.86
23	C	502	CLA	C3B-C4B-NB	3.03	113.13	109.21
23	C	513	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
23	B	604	CLA	CMC-C2C-C1C	3.03	129.66	125.04
26	L	101	SQD	O48-C23-C24	3.03	121.42	111.91
23	C	502	CLA	CHD-C4C-NC	3.03	128.98	124.20
23	c	513	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
23	d	402[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	A	404[A]	CLA	C1-C2-C3	-3.03	120.81	126.04
23	c	502	CLA	C1-C2-C3	-3.02	120.81	126.04
23	d	402[A]	CLA	C4-C3-C5	3.02	120.36	115.27
29	d	405[A]	PL9	C37-C38-C39	-3.02	120.38	127.66
23	b	605	CLA	O2A-CGA-O1A	-3.02	115.97	123.59
23	C	502	CLA	CAC-C3C-C4C	3.02	128.73	124.81
29	A	414[B]	PL9	C17-C18-C19	-3.02	120.39	127.66
23	B	602	CLA	CAC-C3C-C4C	3.02	128.72	124.81
23	A	404[A]	CLA	CAA-C2A-C1A	-3.01	102.09	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	510	CLA	O2A-CGA-CBA	3.01	121.37	111.91
29	a	413[A]	PL9	C42-C43-C44	-3.01	120.41	127.66
23	b	605	CLA	C2A-C1A-CHA	-3.01	118.59	123.86
29	D	405[B]	PL9	C25-C24-C26	3.01	120.34	115.27
29	d	405[B]	PL9	C37-C38-C39	-3.01	120.41	127.66
23	a	408	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
32	d	406[A]	LHG	O7-C7-C8	3.01	117.99	111.50
23	D	402[A]	CLA	CAC-C3C-C4C	3.01	128.71	124.81
23	B	603	CLA	O2A-CGA-O1A	-3.01	116.00	123.59
23	c	510	CLA	O2A-C1-C2	3.01	116.54	108.64
25	b	618	BCR	C37-C22-C21	-3.01	118.71	122.92
23	D	403	CLA	CAA-C2A-C3A	-3.01	104.55	112.78
33	B	626	LMT	O1'-C1'-C2'	3.00	112.99	108.30
24	a	407[B]	PHO	C1A-C2A-C3A	-3.00	99.98	102.84
23	c	512	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
23	A	404[A]	CLA	CHC-C1C-C2C	-3.00	118.43	126.72
23	B	608	CLA	CMB-C2B-C3B	3.00	130.29	124.68
23	A	406[B]	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
23	A	405[A]	CLA	CHD-C4C-NC	3.00	128.93	124.20
26	a	410[A]	SQD	C45-O47-C7	-3.00	110.42	117.79
23	b	608	CLA	CHD-C4C-NC	2.99	128.92	124.20
23	D	402[B]	CLA	O2A-CGA-CBA	2.99	121.31	111.91
23	d	403	CLA	C4-C3-C5	2.99	120.31	115.27
23	A	408	CLA	CHD-C4C-NC	2.99	128.92	124.20
23	C	512	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
23	b	603	CLA	CAC-C3C-C4C	2.99	128.68	124.81
29	a	413[B]	PL9	C37-C38-C39	-2.98	120.47	127.66
32	D	407[A]	LHG	O8-C23-C24	2.98	121.27	111.91
23	b	608	CLA	CAC-C3C-C4C	2.98	128.68	124.81
23	c	507	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
23	d	402[B]	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
29	a	413[B]	PL9	C22-C23-C24	-2.98	120.49	127.66
23	B	616	CLA	CAC-C3C-C4C	2.98	128.67	124.81
23	B	609	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
32	d	412[B]	LHG	O8-C23-O10	-2.97	116.09	123.59
23	A	405[B]	CLA	CHC-C1C-C2C	-2.97	118.50	126.72
32	E	101[A]	LHG	O8-C23-C24	2.97	121.23	111.91
23	b	614	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
29	a	413[B]	PL9	C17-C18-C19	-2.97	120.51	127.66
32	D	407[B]	LHG	O8-C23-C24	2.97	121.23	111.91
23	c	502	CLA	C1D-CHD-C4C	-2.97	119.65	126.06
24	A	407[B]	PHO	O1D-CGD-CBD	-2.97	119.79	124.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	606	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
23	b	605	CLA	C4-C3-C5	2.97	120.27	115.27
23	B	614	CLA	CHD-C4C-NC	2.97	128.88	124.20
23	b	608	CLA	CBC-CAC-C3C	-2.97	104.25	112.43
23	B	612	CLA	C4A-NA-C1A	-2.97	105.37	106.71
23	c	502	CLA	CHC-C1C-C2C	-2.96	118.52	126.72
36	h	102	DGD	O2G-C1B-C2B	2.96	117.89	111.50
23	B	602	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
23	B	610	CLA	CHC-C1C-C2C	-2.96	118.52	126.72
23	b	609	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
23	d	402[B]	CLA	CHC-C1C-C2C	-2.96	118.53	126.72
23	c	510	CLA	C1-O2A-CGA	2.96	124.22	116.44
23	a	405[A]	CLA	CHC-C1C-C2C	-2.96	118.53	126.72
23	b	613	CLA	O2A-CGA-CBA	2.96	121.20	111.91
25	b	619	BCR	C24-C23-C22	-2.96	121.76	126.23
24	A	417[B]	PHO	C4-C3-C5	2.96	120.25	115.27
23	C	509	CLA	CMB-C2B-C3B	2.96	130.21	124.68
24	A	407[A]	PHO	O1D-CGD-CBD	-2.96	119.81	124.74
23	a	405[B]	CLA	CHC-C1C-C2C	-2.96	118.55	126.72
35	b	622	HTG	O5-C5-C4	2.95	115.06	109.69
23	c	510	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
26	A	410[B]	SQD	O48-C23-C24	2.95	121.17	111.91
23	C	510	CLA	CHC-C1C-C2C	-2.95	118.56	126.72
23	B	604	CLA	C6-C5-C3	-2.95	105.72	113.45
24	a	407[B]	PHO	O1D-CGD-CBD	-2.95	119.83	124.74
23	B	601	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
26	L	101	SQD	C1-O5-C5	-2.95	107.91	113.69
29	A	414[B]	PL9	C30-C29-C31	2.95	120.23	115.27
26	A	410[A]	SQD	O9-S-C6	2.95	110.44	106.94
23	B	611	CLA	C4A-NA-C1A	-2.94	105.38	106.71
25	B	618	BCR	C7-C8-C9	-2.94	121.79	126.23
23	c	506	CLA	CHC-C1C-C2C	-2.94	118.58	126.72
23	A	408	CLA	CBC-CAC-C3C	-2.94	104.31	112.43
23	d	403	CLA	C3B-C4B-NB	2.94	113.02	109.21
23	c	511	CLA	CHD-C4C-NC	2.94	128.84	124.20
23	B	605	CLA	CMC-C2C-C1C	2.94	129.52	125.04
29	A	414[A]	PL9	C30-C29-C31	2.94	120.22	115.27
40	v	201	HEC	C1D-C2D-C3D	-2.94	104.95	107.00
25	C	516	BCR	C33-C5-C6	-2.94	121.23	124.53
32	E	101[B]	LHG	O8-C23-C24	2.94	121.12	111.91
32	a	419[A]	LHG	O7-C7-C8	2.94	117.83	111.50
23	C	514	CLA	CBC-CAC-C3C	-2.93	104.34	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406[A]	CLA	CHD-C4C-NC	2.93	128.83	124.20
29	A	414[A]	PL9	C17-C18-C19	-2.93	120.59	127.66
23	B	612	CLA	C3B-C4B-NB	2.93	113.00	109.21
32	D	406[A]	LHG	O8-C23-O10	-2.93	116.19	123.59
23	B	607	CLA	C1D-CHD-C4C	-2.93	119.73	126.06
23	C	507	CLA	C4-C3-C5	2.93	120.20	115.27
29	d	405[A]	PL9	C22-C23-C24	-2.93	120.60	127.66
24	a	415[B]	PHO	C4A-C3A-C2A	-2.93	100.05	102.84
23	b	605	CLA	C3B-C4B-NB	2.93	113.00	109.21
23	b	613	CLA	CHC-C1C-C2C	-2.93	118.62	126.72
23	c	512	CLA	O2A-CGA-CBA	2.93	121.10	111.91
23	b	610	CLA	C4-C3-C5	2.93	120.19	115.27
29	d	405[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	606	CLA	O2A-CGA-CBA	2.93	121.09	111.91
23	D	403	CLA	O2A-CGA-O1A	-2.92	116.21	123.59
29	a	413[B]	PL9	C35-C34-C36	2.92	120.19	115.27
25	d	404	BCR	C28-C27-C26	-2.92	108.86	114.08
23	b	612	CLA	O2A-CGA-CBA	2.92	121.08	111.91
23	c	506	CLA	C3B-C4B-NB	2.92	112.99	109.21
23	a	405[A]	CLA	CBC-CAC-C3C	-2.92	104.38	112.43
23	A	406[A]	CLA	CAA-C2A-C3A	-2.92	104.78	112.78
23	b	611	CLA	CHC-C1C-C2C	-2.92	118.65	126.72
23	C	511	CLA	O2A-CGA-O1A	-2.92	116.22	123.59
23	C	514	CLA	CHC-C1C-C2C	-2.92	118.65	126.72
23	B	615	CLA	C11-C10-C8	-2.92	106.49	115.92
29	d	405[A]	PL9	C53-C6-C1	2.92	120.95	114.99
23	B	601	CLA	C3B-C4B-NB	2.92	112.98	109.21
29	a	413[A]	PL9	C22-C23-C24	-2.92	120.64	127.66
23	d	402[B]	CLA	C4-C3-C5	2.91	120.17	115.27
23	A	408	CLA	CHC-C1C-C2C	-2.91	118.66	126.72
23	b	608	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
23	D	402[B]	CLA	C1D-CHD-C4C	-2.91	119.78	126.06
26	A	410[A]	SQD	O48-C23-C24	2.91	121.04	111.91
25	B	617	BCR	C7-C8-C9	-2.91	121.84	126.23
32	D	407[A]	LHG	O8-C23-O10	-2.91	116.25	123.59
23	c	512	CLA	CMC-C2C-C1C	2.91	129.47	125.04
25	b	619	BCR	C38-C26-C25	-2.91	121.26	124.53
23	A	405[A]	CLA	C4-C3-C5	2.91	120.16	115.27
23	C	511	CLA	O2A-CGA-CBA	2.91	121.03	111.91
23	a	404[A]	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
23	a	406[A]	CLA	C4C-C3C-C2C	-2.90	102.67	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	602	CLA	CMA-C3A-C4A	-2.90	103.97	111.77
23	c	513	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
23	C	510	CLA	O2A-CGA-O1A	-2.90	116.27	123.59
23	C	504	CLA	O2A-CGA-O1A	-2.90	116.28	123.59
23	a	405[A]	CLA	CMA-C3A-C2A	-2.90	102.14	113.83
25	a	409	BCR	C24-C23-C22	-2.90	121.86	126.23
29	a	413[B]	PL9	C42-C43-C44	-2.90	120.69	127.66
23	B	608	CLA	C1-C2-C3	-2.89	121.04	126.04
23	c	508	CLA	C3B-C4B-NB	2.89	112.95	109.21
26	b	620	SQD	C3-C4-C5	2.89	115.40	110.24
23	b	615	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
23	B	616	CLA	C1C-C2C-C3C	-2.89	103.92	106.96
23	A	405[A]	CLA	CHC-C1C-C2C	-2.89	118.72	126.72
23	C	510	CLA	CMB-C2B-C3B	2.89	130.09	124.68
23	D	402[A]	CLA	CHC-C1C-C2C	-2.89	118.72	126.72
23	a	406[B]	CLA	C3B-C4B-NB	2.89	112.94	109.21
25	K	102	BCR	C24-C23-C22	-2.89	121.87	126.23
23	b	603	CLA	O2A-CGA-CBA	2.89	120.97	111.91
23	D	402[A]	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
23	C	502	CLA	C1-O2A-CGA	2.89	124.02	116.44
23	C	510	CLA	CMC-C2C-C1C	2.89	129.43	125.04
24	a	415[B]	PHO	CMB-C2B-C3B	2.89	130.08	124.68
23	C	506	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
25	D	404	BCR	C37-C22-C23	2.88	122.62	118.08
29	a	413[B]	PL9	C53-C6-C1	2.88	120.89	114.99
23	B	606	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
23	b	607	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
33	A	420	LMT	O5B-C5B-C4B	2.88	114.92	109.69
25	k	101	BCR	C24-C23-C22	-2.88	121.89	126.23
23	c	513	CLA	CHD-C4C-NC	2.88	128.74	124.20
23	c	511	CLA	CMB-C2B-C3B	2.87	130.06	124.68
23	b	606	CLA	CMC-C2C-C1C	2.87	129.41	125.04
24	a	407[A]	PHO	O2A-CGA-CBA	2.87	120.92	111.91
23	C	505	CLA	CHC-C1C-C2C	-2.87	118.78	126.72
26	a	410[B]	SQD	O9-S-C6	2.87	110.35	106.94
23	D	402[A]	CLA	O2A-CGA-O1A	-2.87	116.35	123.59
23	c	504	CLA	C3B-C4B-NB	2.87	112.92	109.21
23	a	406[B]	CLA	CAA-C2A-C3A	-2.87	104.92	112.78
29	D	405[B]	PL9	C51-C49-C50	2.87	120.94	114.60
23	B	607	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
29	A	414[B]	PL9	C10-C9-C11	2.87	120.09	115.27
23	A	404[B]	CLA	CHC-C1C-C2C	-2.87	118.79	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	610	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
23	C	503	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
23	b	601	CLA	CHD-C4C-NC	2.86	128.72	124.20
23	B	604	CLA	CHC-C1C-C2C	-2.86	118.80	126.72
29	a	413[A]	PL9	C37-C38-C39	-2.86	120.77	127.66
23	B	607	CLA	CAA-C2A-C3A	-2.86	104.94	112.78
23	B	605	CLA	C2A-C1A-CHA	-2.86	118.85	123.86
23	c	508	CLA	CHD-C4C-NC	2.86	128.71	124.20
23	c	505	CLA	CHC-C1C-C2C	-2.86	118.81	126.72
25	y	101	BCR	C24-C23-C22	-2.86	121.92	126.23
26	a	410[B]	SQD	O8-S-C6	2.86	110.29	105.74
34	D	411	LMG	O8-C28-O10	-2.85	116.39	123.59
23	d	403	CLA	CMC-C2C-C1C	2.85	129.38	125.04
23	A	404[B]	CLA	C2A-C1A-CHA	-2.85	118.87	123.86
23	C	513	CLA	CBC-CAC-C3C	-2.85	104.57	112.43
24	a	407[A]	PHO	C1A-C2A-C3A	-2.85	100.13	102.84
23	b	603	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
23	b	603	CLA	CMA-C3A-C2A	-2.85	102.33	113.83
32	b	630[A]	LHG	O8-C23-C24	2.85	120.84	111.91
25	c	515	BCR	C36-C18-C17	-2.85	118.93	122.92
23	a	408	CLA	CHD-C4C-NC	2.85	128.69	124.20
23	c	508	CLA	CAC-C3C-C4C	2.85	128.50	124.81
23	d	403	CLA	CHD-C4C-NC	2.85	128.69	124.20
23	B	608	CLA	CMC-C2C-C1C	2.85	129.37	125.04
23	B	612	CLA	C1C-C2C-C3C	-2.85	103.97	106.96
23	b	616	CLA	C1C-C2C-C3C	-2.85	103.97	106.96
24	A	407[B]	PHO	CMB-C2B-C3B	2.85	130.00	124.68
23	C	506	CLA	CHC-C1C-C2C	-2.84	118.85	126.72
23	b	601	CLA	CMB-C2B-C3B	2.84	130.00	124.68
24	a	407[A]	PHO	O1D-CGD-CBD	-2.84	120.01	124.74
23	b	610	CLA	O2A-CGA-O1A	-2.84	116.42	123.59
23	c	504	CLA	CHD-C4C-NC	2.84	128.68	124.20
25	K	102	BCR	C38-C26-C25	-2.84	121.34	124.53
23	b	610	CLA	CMC-C2C-C1C	2.84	129.36	125.04
25	c	516	BCR	C11-C10-C9	-2.84	123.26	127.31
23	b	608	CLA	CHC-C1C-C2C	-2.84	118.88	126.72
23	D	402[B]	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
23	B	609	CLA	CBC-CAC-C3C	-2.84	104.61	112.43
23	B	610	CLA	CHD-C4C-NC	2.83	128.67	124.20
23	b	614	CLA	CHD-C4C-NC	2.83	128.67	124.20
23	D	403	CLA	O2A-CGA-CBA	2.83	120.79	111.91
23	b	601	CLA	C3B-C4B-NB	2.83	112.87	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	504	CLA	C1-C2-C3	-2.83	121.15	126.04
25	D	404	BCR	C3-C4-C5	-2.83	109.03	114.08
23	c	513	CLA	CHC-C1C-C2C	-2.82	118.91	126.72
23	D	402[B]	CLA	C4-C3-C5	2.82	120.02	115.27
23	a	405[B]	CLA	CBC-CAC-C3C	-2.82	104.65	112.43
23	b	602	CLA	C2A-C1A-CHA	-2.82	118.93	123.86
23	B	606	CLA	CHC-C1C-C2C	-2.82	118.92	126.72
23	B	613	CLA	CHC-C1C-C2C	-2.82	118.92	126.72
23	D	403	CLA	C4-C3-C5	2.82	120.01	115.27
23	b	602	CLA	CHD-C4C-NC	2.82	128.64	124.20
23	b	611	CLA	CHD-C4C-NC	2.82	128.64	124.20
36	c	517[A]	DGD	O3G-C3G-C2G	-2.82	104.11	110.90
23	B	609	CLA	C3B-C4B-NB	2.81	112.85	109.21
23	a	406[B]	CLA	C1-C2-C3	-2.81	121.18	126.04
23	B	606	CLA	CMC-C2C-C1C	2.81	129.32	125.04
34	z	101	LMG	O8-C28-C29	2.81	120.72	111.91
38	f	101	HEM	CHB-C1B-NB	2.81	127.85	124.38
24	a	415[A]	PHO	CMC-C2C-C3C	2.81	130.23	124.94
23	c	514	CLA	O2A-CGA-CBA	2.80	120.71	111.91
24	A	407[B]	PHO	CMC-C2C-C3C	2.80	130.23	124.94
23	d	402[A]	CLA	CHC-C1C-C2C	-2.80	118.97	126.72
23	c	514	CLA	CAC-C3C-C4C	2.80	128.45	124.81
23	B	604	CLA	C6-C7-C8	-2.80	106.86	115.92
23	B	611	CLA	C3B-C4B-NB	2.80	112.83	109.21
34	c	520	LMG	O8-C28-C29	2.80	120.70	111.91
34	c	520	LMG	O1-C7-C8	-2.80	104.14	110.90
23	d	403	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
25	d	404	BCR	C21-C20-C19	-2.80	114.48	123.22
23	A	408	CLA	CMB-C2B-C3B	2.80	129.92	124.68
23	b	609	CLA	CHD-C4C-NC	2.80	128.61	124.20
23	b	613	CLA	CMB-C2B-C3B	2.80	129.91	124.68
23	A	406[A]	CLA	CHC-C1C-C2C	-2.80	118.99	126.72
36	C	517[A]	DGD	O3G-C3G-C2G	-2.79	104.16	110.90
25	c	516	BCR	C32-C1-C6	-2.79	105.77	110.30
24	A	407[A]	PHO	CMC-C2C-C3C	2.79	130.21	124.94
23	C	504	CLA	C4-C3-C5	2.79	119.96	115.27
36	c	519	DGD	O3G-C3G-C2G	-2.79	104.17	110.90
35	B	623	HTG	C1'-S1-C1	2.79	105.31	100.09
23	b	609	CLA	CHC-C1C-C2C	-2.79	119.02	126.72
32	D	407[A]	LHG	O7-C7-C8	2.79	117.50	111.50
23	C	510	CLA	C4-C3-C5	2.78	119.95	115.27
26	a	410[A]	SQD	O47-C7-O49	-2.78	116.98	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	D	411	LMG	O7-C10-C11	2.78	117.50	111.50
25	t	102	BCR	C35-C13-C12	2.78	122.46	118.08
23	c	506	CLA	O2A-CGA-O1A	-2.78	116.58	123.59
24	A	417[B]	PHO	O2D-CGD-O1D	-2.78	118.41	123.84
23	A	404[A]	CLA	CAA-CBA-CGA	-2.78	105.14	113.25
23	B	612	CLA	C2A-C1A-CHA	-2.78	119.00	123.86
23	b	601	CLA	CHC-C1C-C2C	-2.78	119.04	126.72
23	c	514	CLA	CHD-C4C-NC	2.77	128.57	124.20
26	b	620	SQD	O9-S-C6	2.77	110.23	106.94
29	a	413[B]	PL9	C10-C9-C11	2.77	119.93	115.27
25	t	102	BCR	C28-C27-C26	-2.77	109.13	114.08
23	B	610	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
26	L	101	SQD	C4-C3-C2	2.77	115.66	110.82
23	c	503	CLA	O2A-CGA-CBA	2.77	120.59	111.91
33	B	626	LMT	C2'-C3'-C4'	2.77	116.00	109.68
35	b	622	HTG	O2-C2-C3	-2.76	103.96	110.35
23	D	402[B]	CLA	CHC-C1C-C2C	-2.76	119.08	126.72
23	B	616	CLA	CHD-C4C-NC	2.76	128.56	124.20
23	A	405[B]	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
23	c	514	CLA	CMC-C2C-C1C	2.76	129.25	125.04
32	b	630[B]	LHG	O8-C23-C24	2.76	120.58	111.91
29	a	413[A]	PL9	C53-C6-C1	2.76	120.64	114.99
24	a	407[B]	PHO	O2A-CGA-CBA	2.76	120.57	111.91
29	D	405[B]	PL9	C27-C28-C29	-2.76	121.02	127.66
23	b	604	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
23	C	514	CLA	C2A-C1A-CHA	-2.75	119.05	123.86
23	a	404[B]	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
23	C	502	CLA	CBC-CAC-C3C	-2.75	104.85	112.43
29	A	414[A]	PL9	C40-C39-C41	2.75	119.90	115.27
23	c	509	CLA	CHC-C1C-C2C	-2.75	119.12	126.72
23	a	408	CLA	CAC-C3C-C4C	2.75	128.38	124.81
23	B	616	CLA	O2A-CGA-CBA	2.75	120.53	111.91
23	b	613	CLA	CMA-C3A-C4A	-2.75	104.39	111.77
23	d	402[B]	CLA	C2A-C1A-CHA	-2.75	119.06	123.86
24	A	417[B]	PHO	CED-O2D-CGD	2.75	122.15	115.94
23	A	406[B]	CLA	CHD-C4C-NC	2.75	128.53	124.20
32	D	406[B]	LHG	O8-C23-O10	-2.74	116.67	123.59
23	B	611	CLA	O2A-CGA-O1A	-2.74	116.67	123.59
23	B	608	CLA	CMA-C3A-C4A	-2.74	104.40	111.77
29	A	414[B]	PL9	C53-C6-C1	2.74	120.59	114.99
25	k	101	BCR	C11-C10-C9	-2.74	123.40	127.31
23	c	508	CLA	O2A-CGA-CBA	2.74	120.50	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	602	CLA	CHD-C4C-NC	2.74	128.52	124.20
23	D	402[B]	CLA	CAA-C2A-C3A	-2.74	105.28	112.78
33	M	101	LMT	C3'-C4'-C5'	-2.74	104.65	110.93
29	A	414[A]	PL9	C10-C9-C8	-2.74	116.66	123.68
36	H	102	DGD	O1G-C1A-C2A	2.73	120.49	111.91
23	a	405[B]	CLA	O2A-CGA-O1A	-2.73	116.69	123.59
23	A	404[A]	CLA	CAC-C3C-C4C	2.73	128.36	124.81
23	B	601	CLA	CBC-CAC-C3C	-2.73	104.90	112.43
23	D	403	CLA	CHC-C1C-C2C	-2.73	119.17	126.72
23	A	406[A]	CLA	CBC-CAC-C3C	-2.73	104.90	112.43
23	C	509	CLA	CAC-C3C-C4C	2.73	128.35	124.81
23	B	614	CLA	CHC-C1C-C2C	-2.73	119.17	126.72
23	C	505	CLA	CMC-C2C-C1C	2.73	129.20	125.04
23	C	514	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
29	D	405[B]	PL9	C10-C9-C11	2.73	119.86	115.27
23	C	507	CLA	CAA-C2A-C3A	-2.73	105.31	112.78
36	C	517[A]	DGD	C2G-O2G-C1B	-2.73	111.07	117.79
23	c	514	CLA	C2A-C1A-CHA	-2.73	119.09	123.86
25	y	101	BCR	C11-C10-C9	-2.73	123.42	127.31
23	A	406[B]	CLA	CHC-C1C-C2C	-2.73	119.18	126.72
23	b	610	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
32	d	407[A]	LHG	O8-C23-C24	2.73	120.46	111.91
32	D	407[B]	LHG	O8-C23-O10	-2.72	116.72	123.59
23	B	613	CLA	CMB-C2B-C3B	2.72	129.78	124.68
23	c	509	CLA	CAA-C2A-C3A	-2.72	105.32	112.78
23	b	606	CLA	CHC-C1C-C2C	-2.72	119.19	126.72
25	A	409	BCR	C16-C17-C18	-2.72	123.42	127.31
23	a	405[A]	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
26	a	410[B]	SQD	C45-O47-C7	-2.72	111.09	117.79
23	c	502	CLA	CMB-C2B-C1B	2.72	132.65	128.46
23	b	609	CLA	O2A-CGA-O1A	-2.72	116.72	123.59
29	D	405[A]	PL9	C42-C41-C39	-2.72	104.03	112.98
23	D	402[A]	CLA	CAA-C2A-C3A	-2.72	105.33	112.78
23	b	615	CLA	CHD-C4C-NC	2.72	128.49	124.20
25	T	102	BCR	C21-C20-C19	-2.72	114.73	123.22
23	C	502	CLA	CHC-C1C-C2C	-2.72	119.20	126.72
26	f	102	SQD	O8-S-C6	2.72	110.07	105.74
23	C	512	CLA	CMB-C2B-C3B	2.72	129.76	124.68
25	k	101	BCR	C20-C21-C22	-2.72	123.43	127.31
32	A	419[A]	LHG	O7-C7-O9	-2.72	117.13	123.70
26	A	412	SQD	C4-C3-C2	-2.72	106.08	110.82
25	h	101	BCR	C24-C23-C22	-2.72	122.13	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	505	CLA	CMB-C2B-C3B	2.72	129.76	124.68
23	b	612	CLA	CHC-C1C-C2C	-2.71	119.21	126.72
25	c	515	BCR	C36-C18-C19	2.71	122.35	118.08
29	d	405[A]	PL9	C36-C34-C33	-2.71	115.63	121.12
23	A	404[B]	CLA	C1-C2-C3	-2.71	121.35	126.04
23	a	406[B]	CLA	C4-C3-C5	2.71	119.83	115.27
23	B	602	CLA	C11-C12-C13	-2.71	107.16	115.92
25	H	101	BCR	C24-C23-C22	-2.71	122.14	126.23
23	C	512	CLA	CHC-C1C-C2C	-2.71	119.23	126.72
23	a	406[A]	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
23	b	616	CLA	CHC-C1C-C2C	-2.71	119.23	126.72
24	a	407[A]	PHO	CMA-C3A-C4A	-2.71	108.45	114.38
23	b	605	CLA	CHC-C1C-C2C	-2.71	119.24	126.72
23	D	402[B]	CLA	C2A-C1A-CHA	-2.71	119.13	123.86
23	c	504	CLA	CMC-C2C-C1C	2.71	129.16	125.04
23	A	406[A]	CLA	C2A-C1A-CHA	-2.71	119.13	123.86
23	c	514	CLA	CAA-C2A-C3A	-2.70	105.37	112.78
23	A	404[A]	CLA	C2A-C1A-CHA	-2.70	119.13	123.86
34	m	101	LMG	C8-O7-C10	-2.70	111.14	117.79
32	d	406[B]	LHG	O8-C23-O10	-2.70	116.77	123.59
36	h	102	DGD	O1G-C1A-C2A	2.70	120.39	111.91
23	c	506	CLA	O2A-CGA-CBA	2.70	120.39	111.91
23	A	406[B]	CLA	O2A-CGA-CBA	2.70	120.38	111.91
34	c	521	LMG	O8-C28-C29	2.70	120.38	111.91
23	B	601	CLA	C1-O2A-CGA	2.70	123.52	116.44
36	C	518[A]	DGD	O1G-C1A-O1A	-2.70	116.78	123.59
23	D	402[A]	CLA	CMC-C2C-C1C	2.70	129.15	125.04
27	b	628	GOL	C3-C2-C1	-2.70	101.22	111.70
23	a	404[B]	CLA	C4-C3-C5	2.70	119.81	115.27
38	F	102	HEM	CHA-C4D-ND	2.69	127.71	124.38
23	B	613	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
23	C	514	CLA	C4C-C3C-C2C	-2.69	102.97	106.90
36	c	519	DGD	O1G-C1A-C2A	2.69	120.36	111.91
26	a	411	SQD	O7-S-C6	2.69	110.14	106.94
23	B	608	CLA	C11-C12-C13	-2.69	107.23	115.92
23	B	603	CLA	O2A-CGA-CBA	2.69	120.34	111.91
23	a	404[A]	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
23	a	406[A]	CLA	CHC-C1C-C2C	-2.69	119.29	126.72
25	h	101	BCR	C16-C17-C18	-2.69	123.48	127.31
23	D	403	CLA	CMA-C3A-C4A	-2.68	104.56	111.77
25	T	102	BCR	C3-C4-C5	-2.68	109.28	114.08
25	t	102	BCR	C36-C18-C19	2.68	122.31	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	h	102	DGD	O1G-C1A-O1A	-2.68	116.82	123.59
35	b	622	HTG	O5-C1-C2	2.68	113.69	110.31
33	a	416	LMT	C3'-C4'-C5'	-2.68	104.78	110.93
36	h	102	DGD	O3G-C1D-C2D	2.68	112.49	108.30
23	A	406[A]	CLA	CMC-C2C-C1C	2.68	129.12	125.04
34	C	501	LMG	C6-C5-C4	2.68	119.28	113.00
23	A	405[A]	CLA	CAC-C3C-C4C	2.68	128.29	124.81
25	T	102	BCR	C35-C13-C12	2.68	122.30	118.08
23	a	405[B]	CLA	O2A-CGA-CBA	2.68	120.32	111.91
23	a	404[B]	CLA	C2A-C1A-CHA	-2.68	119.17	123.86
23	B	609	CLA	CHD-C4C-NC	2.68	128.43	124.20
23	C	508	CLA	CHD-C4C-NC	2.68	128.43	124.20
26	f	102	SQD	O5-C5-C4	2.68	114.56	109.69
23	C	503	CLA	C2A-C1A-CHA	-2.68	119.18	123.86
32	a	419[A]	LHG	O8-C23-C24	2.68	120.30	111.91
24	a	415[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	405[A]	PL9	C37-C38-C39	-2.67	121.22	127.66
24	a	415[B]	PHO	O2D-CGD-O1D	-2.67	118.61	123.84
23	A	406[A]	CLA	C1-C2-C3	-2.67	121.42	126.04
23	b	607	CLA	CAA-C2A-C3A	-2.67	105.46	112.78
23	B	606	CLA	CBC-CAC-C3C	-2.67	105.06	112.43
25	Y	101	BCR	C15-C16-C17	-2.67	118.00	123.47
23	A	408	CLA	O2A-CGA-CBA	2.67	120.29	111.91
23	a	404[B]	CLA	O2A-CGA-O1A	-2.67	116.86	123.59
23	b	614	CLA	O2A-CGA-CBA	2.67	120.28	111.91
29	a	413[B]	PL9	C20-C19-C21	2.67	119.76	115.27
24	A	417[B]	PHO	CMC-C2C-C3C	2.67	129.97	124.94
23	C	510	CLA	C16-C15-C13	-2.67	107.30	115.92
23	b	610	CLA	C3B-C4B-NB	2.67	112.66	109.21
25	c	515	BCR	C28-C27-C26	-2.67	109.32	114.08
23	B	601	CLA	O2A-CGA-CBA	2.67	120.27	111.91
23	a	404[B]	CLA	C1-C2-C3	-2.66	121.44	126.04
25	Y	101	BCR	C10-C11-C12	-2.66	114.91	123.22
23	c	513	CLA	C3B-C4B-NB	2.66	112.65	109.21
23	a	405[B]	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
23	b	603	CLA	CMB-C2B-C3B	2.66	129.66	124.68
23	c	511	CLA	CHC-C1C-C2C	-2.66	119.37	126.72
23	a	406[A]	CLA	CAA-C2A-C3A	-2.66	105.50	112.78
23	C	502	CLA	C4C-C3C-C2C	-2.66	103.03	106.90
23	C	511	CLA	CMC-C2C-C1C	2.65	129.08	125.04
26	A	410[A]	SQD	O48-C23-O10	-2.65	116.89	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	613	CLA	CHD-C4C-NC	2.65	128.38	124.20
23	a	404[A]	CLA	CAC-C3C-C4C	2.65	128.25	124.81
23	A	404[B]	CLA	CMA-C3A-C2A	-2.65	103.13	113.83
23	b	611	CLA	C2A-C1A-CHA	-2.65	119.22	123.86
25	C	515	BCR	C16-C17-C18	-2.65	123.53	127.31
23	B	608	CLA	CHB-C4A-NA	2.65	128.18	124.51
25	H	101	BCR	C7-C8-C9	-2.65	122.23	126.23
29	D	405[B]	PL9	C20-C19-C21	2.65	119.73	115.27
23	c	512	CLA	CHC-C1C-C2C	-2.65	119.39	126.72
23	C	505	CLA	C4C-C3C-C2C	-2.65	103.04	106.90
29	D	405[A]	PL9	C40-C39-C41	2.65	119.72	115.27
23	B	610	CLA	CMC-C2C-C1C	2.65	129.07	125.04
23	d	403	CLA	CHC-C1C-C2C	-2.65	119.40	126.72
38	F	102	HEM	O2A-CGA-CBA	2.64	122.53	114.03
24	A	417[B]	PHO	CMB-C2B-C3B	2.64	129.62	124.68
26	a	411	SQD	C3-C4-C5	2.64	114.95	110.24
25	b	617	BCR	C29-C30-C25	2.64	114.55	110.48
23	B	615	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
26	F	103	SQD	O5-C1-O6	2.64	116.22	109.97
23	b	613	CLA	CED-O2D-CGD	2.64	121.91	115.94
23	a	408	CLA	O2A-CGA-O1A	-2.64	116.94	123.59
23	A	406[A]	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
23	D	402[B]	CLA	O2A-CGA-O1A	-2.63	116.94	123.59
23	A	406[A]	CLA	C4-C3-C5	2.63	119.70	115.27
23	C	512	CLA	CHD-C4C-NC	2.63	128.35	124.20
36	c	519	DGD	O2G-C1B-C2B	2.63	117.18	111.50
24	A	417[A]	PHO	O2D-CGD-O1D	-2.63	118.69	123.84
23	B	609	CLA	O2A-CGA-CBA	2.63	120.17	111.91
23	B	616	CLA	CHC-C1C-C2C	-2.63	119.44	126.72
23	B	608	CLA	C11-C10-C8	-2.63	107.42	115.92
25	b	619	BCR	C11-C10-C9	-2.63	123.56	127.31
23	A	404[B]	CLA	CHD-C4C-NC	2.63	128.35	124.20
23	B	606	CLA	CHD-C4C-NC	2.63	128.35	124.20
35	b	625	HTG	C1'-S1-C1	2.63	105.01	100.09
23	B	609	CLA	CAC-C3C-C4C	2.63	128.22	124.81
25	a	409	BCR	C7-C8-C9	-2.63	122.27	126.23
23	c	508	CLA	O1D-CGD-CBD	-2.62	119.12	124.48
29	a	413[B]	PL9	C40-C39-C41	2.62	119.68	115.27
32	a	419[B]	LHG	O8-C23-C24	2.62	120.13	111.91
23	D	402[A]	CLA	CMB-C2B-C3B	2.62	129.58	124.68
23	d	402[A]	CLA	CAA-C2A-C3A	-2.62	105.61	112.78
34	D	411	LMG	O8-C28-C29	2.62	120.13	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	405[B]	PL9	C42-C41-C39	-2.62	104.37	112.98
29	A	414[B]	PL9	C40-C39-C41	2.62	119.67	115.27
23	b	609	CLA	C16-C15-C13	-2.62	107.46	115.92
32	d	406[B]	LHG	O8-C23-C24	2.62	120.12	111.91
25	c	515	BCR	C20-C21-C22	-2.61	123.58	127.31
26	f	102	SQD	O48-C23-C24	2.61	120.11	111.91
29	D	405[B]	PL9	C37-C38-C39	-2.61	121.37	127.66
23	C	511	CLA	CAC-C3C-C4C	2.61	128.20	124.81
29	A	414[A]	PL9	C53-C6-C1	2.61	120.33	114.99
23	B	609	CLA	CHC-C1C-C2C	-2.61	119.50	126.72
23	C	508	CLA	C4-C3-C5	2.61	119.66	115.27
29	d	405[B]	PL9	C36-C37-C38	-2.61	103.30	111.88
33	b	621	LMT	C1'-O5'-C5'	-2.61	108.57	113.69
23	c	508	CLA	C4C-C3C-C2C	-2.61	103.09	106.90
32	D	406[A]	LHG	O8-C23-C24	2.61	120.09	111.91
23	b	614	CLA	CBC-CAC-C3C	-2.61	105.24	112.43
32	D	406[A]	LHG	O7-C7-C8	2.61	117.12	111.50
23	B	615	CLA	C6-C7-C8	-2.61	107.50	115.92
23	b	602	CLA	C1B-CHB-C4A	-2.61	124.96	130.12
24	A	407[B]	PHO	CMA-C3A-C4A	-2.61	108.67	114.38
25	B	619	BCR	C21-C20-C19	-2.60	115.10	123.22
23	C	505	CLA	CBC-CAC-C3C	-2.60	105.26	112.43
23	C	511	CLA	CMB-C2B-C3B	2.60	129.54	124.68
23	c	509	CLA	O2A-CGA-CBA	2.60	120.07	111.91
32	L	102[A]	LHG	O8-C23-C24	2.60	120.06	111.91
23	B	614	CLA	CMB-C2B-C3B	2.60	129.54	124.68
23	b	605	CLA	C1-C2-C3	-2.60	121.55	126.04
25	H	101	BCR	C16-C15-C14	-2.60	118.16	123.47
25	B	618	BCR	C37-C22-C21	-2.60	119.29	122.92
23	C	514	CLA	O2A-CGA-CBA	2.60	120.05	111.91
23	d	402[B]	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
23	c	504	CLA	C4-C3-C5	2.59	119.64	115.27
23	a	406[B]	CLA	CBC-CAC-C3C	-2.59	105.28	112.43
23	a	405[A]	CLA	O2A-CGA-CBA	2.59	120.05	111.91
23	A	405[A]	CLA	OBD-CAD-C3D	-2.59	122.28	128.52
23	c	507	CLA	CHD-C4C-NC	2.59	128.29	124.20
23	B	607	CLA	C2A-C1A-CHA	-2.59	119.33	123.86
23	b	609	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
32	D	406[B]	LHG	O8-C23-C24	2.59	120.03	111.91
23	C	504	CLA	CMC-C2C-C1C	2.59	128.98	125.04
23	b	612	CLA	CMB-C2B-C3B	2.59	129.52	124.68
23	a	404[A]	CLA	C2A-C1A-CHA	-2.59	119.34	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	618	BCR	C2-C1-C6	2.59	114.46	110.48
23	b	602	CLA	C11-C12-C13	-2.59	107.56	115.92
40	V	201	HEC	CAD-CBD-CGD	-2.59	106.51	113.76
23	a	406[B]	CLA	CHC-C1C-C2C	-2.59	119.57	126.72
23	B	614	CLA	C4C-C3C-C2C	-2.59	103.13	106.90
23	C	504	CLA	CHC-C1C-C2C	-2.58	119.57	126.72
23	a	404[B]	CLA	CMA-C3A-C4A	-2.58	104.83	111.77
23	B	605	CLA	CHC-C1C-C2C	-2.58	119.58	126.72
38	f	101	HEM	CBD-CAD-C3D	-2.58	105.45	112.63
23	b	601	CLA	C1-O2A-CGA	2.58	123.22	116.44
29	d	405[A]	PL9	C36-C37-C38	-2.58	103.40	111.88
23	b	610	CLA	CHD-C4C-NC	2.58	128.27	124.20
40	V	201	HEC	CMB-C2B-C3B	2.58	128.85	125.82
25	T	102	BCR	C15-C14-C13	2.58	130.99	127.31
25	Y	101	BCR	C34-C9-C8	2.58	122.14	118.08
23	B	604	CLA	O2A-CGA-O1A	-2.58	117.09	123.59
23	b	606	CLA	CAA-C2A-C3A	-2.57	105.73	112.78
25	B	618	BCR	C37-C22-C23	2.57	122.13	118.08
25	d	404	BCR	C39-C30-C25	-2.57	106.13	110.30
25	h	101	BCR	C36-C18-C17	-2.57	119.32	122.92
23	B	603	CLA	C4-C3-C5	2.57	119.60	115.27
23	B	603	CLA	C2A-C1A-CHA	-2.57	119.36	123.86
23	C	507	CLA	CBC-CAC-C3C	-2.57	105.34	112.43
23	d	403	CLA	CBC-CAC-C3C	-2.57	105.34	112.43
23	C	508	CLA	CHC-C1C-C2C	-2.57	119.61	126.72
23	a	404[A]	CLA	CMA-C3A-C4A	-2.57	104.87	111.77
23	A	404[B]	CLA	CAA-C2A-C1A	-2.57	103.56	111.97
23	B	612	CLA	CMC-C2C-C1C	2.57	128.95	125.04
23	C	504	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
23	C	502	CLA	C4-C3-C5	2.56	119.58	115.27
33	T	101	LMT	C3'-C4'-C5'	-2.56	105.05	110.93
23	D	402[A]	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
23	D	402[A]	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
23	B	608	CLA	CMA-C3A-C2A	-2.56	103.50	113.83
23	b	615	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
36	c	517[A]	DGD	O1G-C1A-O1A	-2.56	117.13	123.59
23	C	513	CLA	C3B-C4B-NB	2.56	112.52	109.21
34	c	501	LMG	O6-C5-C4	2.56	114.34	109.69
25	B	618	BCR	C38-C26-C25	-2.56	121.66	124.53
23	C	514	CLA	CHD-C4C-NC	2.56	128.23	124.20
23	A	408	CLA	C4-C3-C5	2.56	119.57	115.27
23	c	509	CLA	CHD-C4C-NC	2.56	128.23	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	F	103	SQD	O48-C23-C24	2.56	119.93	111.91
29	D	405[B]	PL9	C7-C8-C9	-2.56	122.54	126.79
23	B	604	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
25	t	102	BCR	C37-C22-C23	2.56	122.10	118.08
23	c	507	CLA	C2A-C1A-CHA	-2.56	119.39	123.86
23	c	514	CLA	CHC-C1C-C2C	-2.55	119.66	126.72
23	b	614	CLA	CAC-C3C-C4C	2.55	128.12	124.81
23	B	607	CLA	CED-O2D-CGD	2.55	121.71	115.94
35	c	522	HTG	O5-C1-C2	2.55	113.52	110.31
25	T	102	BCR	C2-C1-C6	2.55	114.41	110.48
23	b	603	CLA	CHD-C4C-NC	2.55	128.22	124.20
25	y	101	BCR	C10-C11-C12	-2.55	115.26	123.22
23	b	616	CLA	CAC-C3C-C4C	2.55	128.12	124.81
23	b	610	CLA	CHC-C1C-C2C	-2.55	119.67	126.72
23	C	508	CLA	C3B-C4B-NB	2.55	112.50	109.21
25	A	409	BCR	C38-C26-C25	-2.55	121.67	124.53
26	F	103	SQD	O47-C7-O49	-2.54	117.56	123.70
23	A	405[A]	CLA	CMA-C3A-C2A	-2.54	103.58	113.83
23	C	505	CLA	C4-C3-C5	2.54	119.54	115.27
24	a	415[A]	PHO	O1D-CGD-CBD	-2.54	120.51	124.74
23	A	404[B]	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
23	B	601	CLA	CMC-C2C-C1C	2.54	128.90	125.04
23	b	603	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
23	B	609	CLA	C1-C2-C3	-2.54	121.66	126.04
23	C	507	CLA	O2A-CGA-CBA	2.54	119.86	111.91
23	b	607	CLA	CBC-CAC-C3C	-2.54	105.44	112.43
23	b	607	CLA	O2A-CGA-O1A	-2.54	117.19	123.59
25	y	101	BCR	C21-C20-C19	-2.53	115.31	123.22
23	B	612	CLA	C1-C2-C3	-2.53	121.66	126.04
36	H	102	DGD	O1G-C1A-O1A	-2.53	117.20	123.59
23	b	607	CLA	CMB-C2B-C3B	2.53	129.41	124.68
29	A	414[A]	PL9	C35-C34-C36	2.53	119.53	115.27
23	b	604	CLA	O2A-CGA-CBA	2.53	119.85	111.91
23	A	405[A]	CLA	C2A-C1A-CHA	-2.53	119.44	123.86
23	b	609	CLA	CMA-C3A-C4A	-2.53	104.97	111.77
23	C	512	CLA	C1-C2-C3	-2.53	121.67	126.04
34	B	620	LMG	O8-C28-O10	-2.53	117.22	123.59
23	B	610	CLA	O1D-CGD-CBD	-2.53	119.32	124.48
23	B	605	CLA	C3B-C4B-NB	2.52	112.47	109.21
36	C	519	DGD	O3G-C3G-C2G	-2.52	104.81	110.90
23	B	609	CLA	C2A-C1A-CHA	-2.52	119.45	123.86
23	B	615	CLA	CMB-C2B-C1B	2.52	132.34	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	e	101	LMT	O1'-C1'-C2'	2.52	112.24	108.30
23	a	406[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
24	A	417[B]	PHO	C4A-C3A-C2A	-2.52	100.44	102.84
23	b	611	CLA	O2A-CGA-O1A	-2.52	117.23	123.59
23	C	508	CLA	C1-C2-C3	-2.52	121.69	126.04
26	a	411	SQD	O8-S-C6	2.52	109.75	105.74
25	b	618	BCR	C29-C30-C25	2.52	114.36	110.48
26	a	410[B]	SQD	O48-C23-C24	2.52	119.81	111.91
32	d	407[B]	LHG	O8-C23-C24	2.52	119.81	111.91
23	d	402[A]	CLA	CMB-C2B-C3B	2.52	129.39	124.68
23	D	403	CLA	CMA-C3A-C2A	-2.52	103.68	113.83
23	A	405[B]	CLA	O2A-CGA-O1A	-2.52	117.24	123.59
23	B	608	CLA	O2A-CGA-O1A	-2.52	117.24	123.59
23	c	514	CLA	CMB-C2B-C3B	2.52	129.38	124.68
23	c	512	CLA	CBC-CAC-C3C	-2.52	105.50	112.43
23	b	616	CLA	CMC-C2C-C1C	2.51	128.87	125.04
23	B	609	CLA	C16-C15-C13	-2.51	107.79	115.92
24	A	407[B]	PHO	C1-C2-C3	-2.51	121.69	126.04
23	A	405[B]	CLA	C2A-C1A-CHA	-2.51	119.46	123.86
34	C	501	LMG	C8-O7-C10	-2.51	111.60	117.79
29	a	413[A]	PL9	C47-C48-C49	-2.51	119.16	127.75
23	c	511	CLA	O2A-CGA-CBA	2.51	119.79	111.91
29	A	414[B]	PL9	C35-C34-C36	2.51	119.50	115.27
23	a	405[A]	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
24	A	407[A]	PHO	O2A-CGA-CBA	2.51	119.78	111.91
24	A	407[A]	PHO	CMB-C2B-C3B	2.51	129.37	124.68
23	A	405[B]	CLA	C4-C3-C5	2.51	119.49	115.27
23	b	602	CLA	C4-C3-C5	2.51	119.49	115.27
23	C	511	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
23	a	406[A]	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
23	b	614	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
25	Y	101	BCR	C36-C18-C17	-2.51	119.41	122.92
26	f	102	SQD	O47-C7-O49	-2.50	117.65	123.70
33	A	420	LMT	O5'-C5'-C6'	2.50	112.66	106.44
25	c	516	BCR	C33-C5-C6	-2.50	121.72	124.53
26	a	411	SQD	C1-O5-C5	2.50	118.60	113.69
33	B	629	LMT	C3'-C4'-C5'	-2.50	105.19	110.93
23	c	507	CLA	O2A-CGA-O1A	-2.50	117.28	123.59
25	Y	101	BCR	C37-C22-C23	2.50	122.02	118.08
23	d	402[B]	CLA	O2A-CGA-O1A	-2.50	117.28	123.59
26	b	620	SQD	C1-C2-C3	-2.50	104.79	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	507	CLA	C4-C3-C5	2.50	119.47	115.27
23	a	404[A]	CLA	CMC-C2C-C1C	2.50	128.84	125.04
23	b	607	CLA	CAC-C3C-C4C	2.50	128.05	124.81
23	d	402[B]	CLA	CMB-C2B-C3B	2.50	129.35	124.68
23	a	404[B]	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
23	B	614	CLA	OBD-CAD-C3D	-2.49	122.52	128.52
23	C	503	CLA	C4-C3-C5	2.49	119.46	115.27
23	c	502	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
23	d	403	CLA	O2A-CGA-CBA	2.49	119.72	111.91
33	B	629	LMT	O1'-C1'-C2'	2.49	112.19	108.30
23	d	402[B]	CLA	CAA-C2A-C3A	-2.49	105.96	112.78
25	T	102	BCR	C16-C17-C18	-2.49	123.76	127.31
23	a	406[A]	CLA	O2A-CGA-CBA	2.49	119.72	111.91
36	C	518[B]	DGD	O1G-C1A-C2A	2.49	119.71	111.91
25	k	101	BCR	C2-C1-C6	2.49	114.31	110.48
24	a	407[A]	PHO	CMB-C2B-C3B	2.48	129.33	124.68
23	C	508	CLA	CMC-C2C-C1C	2.48	128.82	125.04
23	b	603	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
35	b	623	HTG	O5-C1-C2	2.48	113.43	110.31
23	B	612	CLA	O2A-CGA-CBA	2.48	119.69	111.91
36	c	517[B]	DGD	O3G-C3G-C2G	-2.48	104.91	110.90
29	A	414[B]	PL9	C12-C13-C14	-2.48	121.69	127.66
36	C	517[A]	DGD	O5D-C6D-C5D	-2.48	104.46	109.05
29	d	405[A]	PL9	C17-C18-C19	-2.48	121.69	127.66
23	b	606	CLA	CBC-CAC-C3C	-2.48	105.60	112.43
23	C	510	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
23	b	616	CLA	C4-C3-C5	2.48	119.44	115.27
23	c	514	CLA	C1-C2-C3	-2.48	121.76	126.04
23	B	615	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
25	D	404	BCR	C24-C23-C22	-2.48	122.49	126.23
36	C	517[B]	DGD	O5D-C6D-C5D	-2.48	104.47	109.05
24	A	407[A]	PHO	O2A-CGA-O1A	-2.48	117.34	123.59
33	F	101	LMT	C1'-O5'-C5'	-2.47	108.83	113.69
23	A	404[A]	CLA	CMA-C3A-C2A	-2.47	103.85	113.83
23	b	606	CLA	C1-C2-C3	-2.47	121.77	126.04
25	h	101	BCR	C11-C10-C9	-2.47	123.78	127.31
36	c	518[B]	DGD	O1G-C1A-C2A	2.47	119.67	111.91
23	C	514	CLA	CMC-C2C-C1C	2.47	128.80	125.04
25	A	409	BCR	C31-C1-C6	-2.47	106.29	110.30
23	B	612	CLA	CHD-C4C-NC	2.47	128.09	124.20
25	t	102	BCR	C21-C20-C19	-2.47	115.52	123.22
29	a	413[B]	PL9	C47-C48-C49	-2.47	119.32	127.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	516	BCR	C37-C22-C21	-2.47	119.47	122.92
23	C	507	CLA	CHD-C4C-NC	2.47	128.09	124.20
23	B	602	CLA	C2A-C1A-CHA	-2.47	119.55	123.86
23	c	510	CLA	C2A-C1A-CHA	-2.47	119.55	123.86
23	b	601	CLA	C2A-C1A-CHA	-2.46	119.55	123.86
23	a	405[B]	CLA	CMC-C2C-C1C	2.46	128.79	125.04
32	d	406[A]	LHG	O8-C23-O10	-2.46	117.38	123.59
23	a	405[B]	CLA	C4C-C3C-C2C	-2.46	103.31	106.90
23	B	602	CLA	CHC-C1C-C2C	-2.46	119.92	126.72
26	a	410[A]	SQD	O7-S-C6	2.46	109.86	106.94
23	C	513	CLA	O2A-CGA-O1A	-2.46	117.39	123.59
23	C	510	CLA	CHD-C4C-NC	2.46	128.07	124.20
33	B	628	LMT	O5'-C5'-C6'	2.45	112.54	106.44
23	B	611	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
33	m	103	LMT	C3'-C4'-C5'	-2.45	105.30	110.93
25	t	102	BCR	C12-C13-C14	-2.45	115.18	118.94
23	a	405[A]	CLA	C4C-C3C-C2C	-2.45	103.32	106.90
23	a	406[B]	CLA	O2A-CGA-CBA	2.45	119.60	111.91
24	A	407[B]	PHO	O2A-CGA-CBA	2.45	119.60	111.91
23	C	513	CLA	CMA-C3A-C4A	-2.45	105.18	111.77
25	c	515	BCR	C7-C8-C9	-2.45	122.53	126.23
23	B	605	CLA	OBD-CAD-C3D	-2.45	122.62	128.52
23	A	405[A]	CLA	CMA-C3A-C4A	-2.45	105.19	111.77
32	b	630[B]	LHG	O8-C23-O10	-2.45	117.41	123.59
23	C	507	CLA	C2A-C1A-CHA	-2.45	119.58	123.86
23	B	601	CLA	CHC-C1C-C2C	-2.45	119.95	126.72
23	C	507	CLA	C4C-C3C-C2C	-2.45	103.33	106.90
29	a	413[A]	PL9	C40-C39-C41	2.45	119.39	115.27
23	B	610	CLA	CBC-CAC-C3C	-2.45	105.69	112.43
25	c	516	BCR	C29-C30-C25	2.45	114.25	110.48
23	C	513	CLA	CHB-C4A-NA	2.45	127.89	124.51
23	B	606	CLA	C4-C3-C5	2.45	119.39	115.27
23	D	402[B]	CLA	CMB-C2B-C3B	2.45	129.25	124.68
24	a	407[B]	PHO	C1-C2-C3	-2.45	121.81	126.04
23	a	405[B]	CLA	CAA-CBA-CGA	2.45	120.40	113.25
23	c	509	CLA	O2A-CGA-O1A	-2.45	117.42	123.59
29	D	405[A]	PL9	C27-C28-C29	-2.44	121.77	127.66
23	c	505	CLA	CHD-C4C-NC	2.44	128.06	124.20
29	a	413[A]	PL9	C20-C19-C21	2.44	119.38	115.27
23	C	503	CLA	CHD-C4C-NC	2.44	128.06	124.20
23	A	405[B]	CLA	CAA-CBA-CGA	2.44	120.39	113.25
23	b	604	CLA	C4-C3-C5	2.44	119.38	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	607	CLA	C1-O2A-CGA	2.44	122.85	116.44
23	b	602	CLA	CAC-C3C-C4C	2.44	127.98	124.81
26	L	101	SQD	O48-C23-O10	-2.44	117.43	123.59
24	a	415[B]	PHO	C1A-C2A-C3A	-2.44	100.52	102.84
23	A	405[A]	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
23	A	406[B]	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
23	a	404[A]	CLA	CHD-C4C-NC	2.44	128.05	124.20
29	d	405[B]	PL9	C47-C48-C49	-2.44	119.42	127.75
26	A	410[B]	SQD	O48-C23-O10	-2.44	117.44	123.59
23	c	503	CLA	C4C-C3C-C2C	-2.44	103.34	106.90
23	a	404[B]	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
23	B	612	CLA	CHC-C1C-C2C	-2.44	119.98	126.72
23	c	505	CLA	C1-C2-C3	-2.44	121.83	126.04
23	C	507	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
25	B	619	BCR	C38-C26-C25	-2.43	121.79	124.53
23	B	608	CLA	CHD-C4C-NC	2.43	128.04	124.20
34	c	520	LMG	C8-O7-C10	-2.43	111.80	117.79
25	D	404	BCR	C21-C20-C19	-2.43	115.62	123.22
23	a	404[B]	CLA	CHD-C4C-NC	2.43	128.04	124.20
23	B	608	CLA	CAA-C2A-C3A	-2.43	106.12	112.78
29	D	405[B]	PL9	C45-C44-C46	2.43	119.36	115.27
29	D	405[B]	PL9	C12-C13-C14	-2.43	121.81	127.66
23	C	503	CLA	CMC-C2C-C1C	2.43	128.74	125.04
23	B	607	CLA	CHD-C4C-NC	2.43	128.03	124.20
23	A	406[B]	CLA	C1-C2-C3	-2.43	121.84	126.04
24	a	407[A]	PHO	O2A-CGA-O1A	-2.43	117.46	123.59
26	A	410[B]	SQD	O8-S-C6	2.43	109.61	105.74
23	c	505	CLA	CMC-C2C-C1C	2.43	128.74	125.04
25	T	102	BCR	C33-C5-C6	-2.43	121.80	124.53
23	c	508	CLA	O2A-CGA-O1A	-2.43	117.47	123.59
23	B	615	CLA	CHC-C1C-C2C	-2.43	120.01	126.72
23	a	408	CLA	C2A-C1A-CHA	-2.43	119.62	123.86
23	A	408	CLA	C2A-C1A-CHA	-2.43	119.62	123.86
29	d	405[A]	PL9	C47-C48-C49	-2.42	119.47	127.75
23	C	511	CLA	C4C-C3C-C2C	-2.42	103.36	106.90
23	c	508	CLA	CHC-C1C-C2C	-2.42	120.02	126.72
23	B	601	CLA	CHB-C4A-NA	2.42	127.85	124.51
29	A	414[B]	PL9	C42-C43-C44	-2.42	121.84	127.66
23	d	402[B]	CLA	CBC-CAC-C3C	-2.42	105.77	112.43
26	a	410[A]	SQD	O8-S-C6	2.41	109.59	105.74
24	a	407[B]	PHO	O2A-CGA-O1A	-2.41	117.50	123.59
29	A	414[A]	PL9	C35-C34-C33	-2.41	117.49	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	M	101	LMT	C1'-O5'-C5'	-2.41	108.95	113.69
38	F	102	HEM	O2D-CGD-CBD	2.41	121.78	114.03
25	b	619	BCR	C39-C30-C25	-2.41	106.39	110.30
23	a	406[B]	CLA	CMC-C2C-C1C	2.41	128.71	125.04
23	c	512	CLA	C1-O2A-CGA	2.41	122.77	116.44
23	C	508	CLA	O2A-CGA-CBA	2.41	119.47	111.91
23	A	404[A]	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
29	A	414[A]	PL9	C42-C43-C44	-2.41	121.87	127.66
23	B	612	CLA	C4-C3-C5	2.40	119.32	115.27
23	C	511	CLA	CBC-CAC-C3C	-2.40	105.80	112.43
23	C	504	CLA	CBC-CAC-C3C	-2.40	105.80	112.43
33	B	628	LMT	O5'-C5'-C4'	2.40	114.82	109.75
36	c	518[B]	DGD	C2G-O2G-C1B	-2.40	111.88	117.79
23	b	601	CLA	CAC-C3C-C4C	2.40	127.92	124.81
33	A	420	LMT	O1'-C1'-C2'	2.40	112.05	108.30
23	b	609	CLA	O2A-CGA-CBA	2.40	119.44	111.91
23	C	504	CLA	O2A-CGA-CBA	2.40	119.43	111.91
25	K	102	BCR	C3-C4-C5	-2.40	109.80	114.08
23	b	605	CLA	CMC-C2C-C1C	2.40	128.69	125.04
25	k	101	BCR	C10-C11-C12	-2.40	115.74	123.22
23	C	506	CLA	O2A-CGA-CBA	2.40	119.43	111.91
35	b	625	HTG	C1-C2-C3	-2.40	105.86	110.59
23	c	505	CLA	CBC-CAC-C3C	-2.40	105.83	112.43
23	A	408	CLA	CHB-C4A-NA	2.40	127.82	124.51
23	B	613	CLA	CHB-C4A-NA	2.40	127.82	124.51
38	F	102	HEM	C4D-ND-C1D	2.39	107.55	105.07
23	B	612	CLA	O2A-CGA-O1A	-2.39	117.55	123.59
23	a	405[B]	CLA	C2A-C1A-CHA	-2.39	119.67	123.86
33	B	626	LMT	C1B-C2B-C3B	2.39	114.98	110.00
25	k	101	BCR	C15-C14-C13	-2.39	123.89	127.31
23	c	504	CLA	O2A-CGA-CBA	2.39	119.42	111.91
23	B	602	CLA	CMB-C2B-C3B	2.39	129.15	124.68
29	D	405[B]	PL9	C40-C39-C41	2.39	119.29	115.27
23	d	403	CLA	CHB-C4A-NA	2.39	127.82	124.51
24	a	407[B]	PHO	O2D-CGD-O1D	-2.39	119.16	123.84
23	C	502	CLA	C2A-C1A-CHA	-2.39	119.68	123.86
29	A	414[B]	PL9	C47-C48-C49	-2.39	119.59	127.75
23	C	503	CLA	O2A-CGA-CBA	2.39	119.40	111.91
32	A	419[B]	LHG	O7-C7-O9	-2.39	117.94	123.70
25	H	101	BCR	C10-C11-C12	-2.38	115.78	123.22
23	c	504	CLA	C2A-C1A-CHA	-2.38	119.69	123.86
23	B	610	CLA	CMA-C3A-C4A	-2.38	105.37	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	504	CLA	C1-C2-C3	-2.38	121.92	126.04
23	c	502	CLA	C4-C3-C5	2.38	119.28	115.27
29	A	414[B]	PL9	C45-C44-C46	2.38	119.28	115.27
26	A	412	SQD	O48-C23-O10	-2.38	117.58	123.59
32	L	102[A]	LHG	O8-C23-O10	-2.38	117.59	123.59
25	d	404	BCR	C36-C18-C17	-2.38	119.59	122.92
23	a	404[B]	CLA	CAC-C3C-C4C	2.38	127.90	124.81
23	B	607	CLA	C11-C10-C8	-2.38	108.23	115.92
23	A	406[B]	CLA	CBC-CAC-C3C	-2.38	105.88	112.43
29	a	413[A]	PL9	C10-C9-C8	-2.38	117.58	123.68
23	d	402[B]	CLA	CHD-C4C-NC	2.38	127.95	124.20
23	c	507	CLA	CMB-C2B-C3B	2.38	129.12	124.68
29	d	405[A]	PL9	C7-C8-C9	-2.38	122.84	126.79
33	B	629	LMT	O5'-C5'-C4'	2.38	114.76	109.75
29	D	405[A]	PL9	C45-C44-C46	2.38	119.27	115.27
23	c	512	CLA	CAC-C3C-C4C	2.38	127.89	124.81
25	A	409	BCR	C37-C22-C21	-2.38	119.60	122.92
23	c	512	CLA	CMA-C3A-C4A	2.37	118.15	111.77
23	C	509	CLA	C4-C3-C5	2.37	119.26	115.27
23	A	404[B]	CLA	C4-C3-C5	2.37	119.26	115.27
23	b	608	CLA	CMA-C3A-C4A	-2.37	105.40	111.77
36	C	517[B]	DGD	C2G-O2G-C1B	-2.37	111.95	117.79
34	C	521	LMG	C9-C8-C7	-2.37	106.18	111.79
23	C	514	CLA	C4-C3-C5	2.37	119.26	115.27
23	C	507	CLA	CGD-CBD-CAD	-2.37	103.06	110.73
23	A	404[B]	CLA	CAA-CBA-CGA	-2.37	106.33	113.25
23	c	502	CLA	CHD-C4C-NC	2.37	127.93	124.20
23	c	505	CLA	O2A-CGA-CBA	2.37	119.34	111.91
23	b	611	CLA	CMB-C2B-C3B	2.37	129.11	124.68
32	d	406[B]	LHG	C6-C5-C4	-2.37	106.19	111.79
36	h	102	DGD	C6D-C5D-C4D	2.37	117.03	112.09
25	B	619	BCR	C7-C8-C9	-2.37	122.66	126.23
23	C	510	CLA	C11-C12-C13	-2.37	108.27	115.92
23	c	512	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
29	d	405[B]	PL9	C17-C18-C19	-2.36	121.97	127.66
23	C	503	CLA	O2A-CGA-O1A	-2.36	117.62	123.59
23	A	408	CLA	CMC-C2C-C1C	2.36	128.64	125.04
23	C	514	CLA	CMB-C2B-C3B	2.36	129.10	124.68
34	m	101	LMG	C7-O1-C1	-2.36	109.12	113.74
23	a	408	CLA	CHC-C1C-C2C	-2.36	120.18	126.72
23	a	406[B]	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
23	b	606	CLA	O2A-CGA-O1A	-2.36	117.63	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	509	CLA	CMC-C2C-C1C	2.36	128.63	125.04
23	B	615	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
29	D	405[A]	PL9	C22-C23-C24	-2.36	121.98	127.66
25	a	409	BCR	C33-C5-C6	-2.36	121.88	124.53
25	b	617	BCR	C24-C23-C22	-2.36	122.67	126.23
34	C	520	LMG	O8-C28-O10	-2.36	117.64	123.59
23	c	513	CLA	CAC-C3C-C4C	2.36	127.87	124.81
23	a	405[B]	CLA	C4-C3-C5	2.36	119.23	115.27
25	A	409	BCR	C33-C5-C6	-2.36	121.88	124.53
23	A	404[B]	CLA	CAC-C3C-C4C	2.36	127.87	124.81
23	b	608	CLA	C11-C10-C8	-2.36	108.31	115.92
23	C	505	CLA	C2A-C1A-CHA	-2.36	119.74	123.86
23	c	503	CLA	CAC-C3C-C4C	2.35	127.86	124.81
24	A	417[A]	PHO	CMA-C3A-C4A	-2.35	109.23	114.38
23	b	615	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
23	A	404[B]	CLA	CMC-C2C-C1C	2.35	128.62	125.04
29	A	414[A]	PL9	C45-C44-C46	2.35	119.22	115.27
36	C	518[A]	DGD	O6E-C5E-C6E	2.35	112.28	106.44
29	a	413[A]	PL9	C45-C44-C46	2.35	119.22	115.27
23	a	405[A]	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
23	B	601	CLA	CAC-C3C-C4C	2.35	127.85	124.81
23	b	604	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
25	K	102	BCR	C29-C30-C25	2.35	114.09	110.48
23	C	508	CLA	CBC-CAC-C3C	-2.35	105.97	112.43
23	A	406[B]	CLA	CMC-C2C-C1C	2.34	128.61	125.04
23	C	509	CLA	O2A-CGA-CBA	2.34	119.26	111.91
36	C	518[B]	DGD	O1G-C1A-O1A	-2.34	117.68	123.59
25	h	101	BCR	C36-C18-C19	2.34	121.77	118.08
25	Y	101	BCR	C38-C26-C25	-2.34	121.90	124.53
23	C	505	CLA	CAC-C3C-C4C	2.34	127.85	124.81
23	c	513	CLA	CBA-CAA-C2A	-2.34	106.95	113.86
23	C	513	CLA	CHC-C1C-C2C	-2.34	120.25	126.72
26	A	410[B]	SQD	O9-S-O7	-2.34	105.85	113.95
23	b	606	CLA	C1-O2A-CGA	2.34	122.58	116.44
29	d	405[B]	PL9	C53-C6-C1	2.34	119.77	114.99
36	H	102	DGD	C3B-C2B-C1B	-2.34	105.12	113.62
23	d	402[B]	CLA	CAC-C3C-C4C	2.34	127.84	124.81
24	a	407[A]	PHO	CMC-C2C-C3C	2.34	129.35	124.94
23	c	505	CLA	C2A-C1A-CHA	-2.34	119.77	123.86
25	H	101	BCR	C31-C1-C6	-2.34	106.51	110.30
23	c	504	CLA	CAC-C3C-C4C	2.34	127.84	124.81
23	b	612	CLA	CHD-C4C-NC	2.34	127.88	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	510	CLA	CHD-C4C-NC	2.33	127.88	124.20
23	b	608	CLA	O2A-CGA-CBA	2.33	119.23	111.91
33	A	420	LMT	O5'-C5'-C4'	2.33	114.67	109.75
23	D	402[A]	CLA	CHD-C4C-NC	2.33	127.88	124.20
38	f	101	HEM	CMD-C2D-C1D	2.33	128.59	125.04
23	a	405[A]	CLA	C1-O2A-CGA	2.33	122.56	116.44
29	A	414[B]	PL9	C37-C36-C34	-2.33	105.32	112.98
23	B	608	CLA	CBC-CAC-C3C	-2.33	106.01	112.43
29	a	413[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
35	o	301	HTG	C2'-C1'-S1	-2.33	104.88	112.40
23	B	607	CLA	O2A-CGA-CBA	2.33	119.21	111.91
36	c	518[A]	DGD	O1G-C1A-C2A	2.33	119.21	111.91
23	C	507	CLA	CMB-C2B-C3B	2.33	129.03	124.68
23	B	610	CLA	CMA-C3A-C2A	-2.33	104.45	113.83
32	d	406[A]	LHG	O8-C23-C24	2.33	119.21	111.91
23	b	603	CLA	CMC-C2C-C1C	2.33	128.58	125.04
26	a	410[B]	SQD	O47-C7-O49	-2.32	118.09	123.70
36	c	517[A]	DGD	C2G-O2G-C1B	-2.32	112.07	117.79
23	a	406[A]	CLA	C4-C3-C5	2.32	119.17	115.27
23	b	613	CLA	C4-C3-C5	2.32	119.17	115.27
23	B	607	CLA	CHC-C1C-C2C	-2.32	120.31	126.72
23	A	405[B]	CLA	CED-O2D-CGD	2.32	121.18	115.94
23	b	607	CLA	C2A-C1A-CHA	-2.32	119.81	123.86
23	A	404[A]	CLA	CMA-C3A-C4A	-2.32	105.54	111.77
26	a	410[A]	SQD	O48-C23-C24	2.32	119.17	111.91
25	B	619	BCR	C2-C1-C6	2.32	114.05	110.48
23	C	504	CLA	CMB-C2B-C3B	2.31	129.01	124.68
23	c	511	CLA	C4-C3-C2	-2.31	117.74	123.68
23	c	511	CLA	O2A-CGA-O1A	-2.31	117.75	123.59
23	C	514	CLA	CAA-C2A-C3A	-2.31	106.44	112.78
23	C	505	CLA	O2A-CGA-O1A	-2.31	117.75	123.59
25	B	618	BCR	C28-C27-C26	-2.31	109.95	114.08
34	m	101	LMG	O8-C28-O10	-2.31	117.76	123.59
23	B	601	CLA	CMB-C2B-C3B	2.31	129.00	124.68
29	A	414[A]	PL9	C37-C36-C34	-2.31	105.38	112.98
34	d	410	LMG	O7-C10-O9	-2.31	118.12	123.70
23	c	510	CLA	CMB-C2B-C3B	2.31	129.00	124.68
23	b	603	CLA	C7-C6-C5	-2.31	107.09	113.36
25	D	404	BCR	C15-C14-C13	-2.31	124.02	127.31
23	c	505	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
23	a	404[A]	CLA	C1B-CHB-C4A	-2.31	125.55	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	511	CLA	C2A-C1A-CHA	-2.30	119.83	123.86
26	b	620	SQD	O48-C23-C24	2.30	119.14	111.91
23	d	402[A]	CLA	CMC-C2C-C1C	2.30	128.55	125.04
23	b	615	CLA	C6-C7-C8	-2.30	108.47	115.92
23	A	406[B]	CLA	C4-C3-C5	2.30	119.14	115.27
36	C	517[B]	DGD	O3G-C3G-C2G	-2.30	105.34	110.90
26	a	411	SQD	O48-C23-O10	-2.30	117.78	123.59
33	T	101	LMT	C1'-O5'-C5'	-2.30	109.17	113.69
23	c	505	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
29	A	414[A]	PL9	C2-C3-C4	2.30	121.97	118.80
23	D	403	CLA	CAC-C3C-C4C	2.30	127.80	124.81
23	C	514	CLA	CAC-C3C-C4C	2.30	127.80	124.81
34	c	521	LMG	O8-C28-O10	-2.30	117.79	123.59
25	B	619	BCR	C3-C4-C5	-2.30	109.97	114.08
23	A	404[A]	CLA	CMC-C2C-C1C	2.30	128.54	125.04
23	C	504	CLA	C3B-C4B-NB	2.30	112.18	109.21
29	D	405[B]	PL9	C30-C29-C31	2.30	119.14	115.27
25	b	618	BCR	C8-C7-C6	-2.30	120.75	127.20
23	C	508	CLA	C6-C7-C8	-2.29	108.50	115.92
29	A	414[B]	PL9	C51-C49-C50	2.29	119.67	114.60
25	C	516	BCR	C32-C1-C6	-2.29	106.58	110.30
23	c	507	CLA	CMC-C2C-C1C	2.29	128.53	125.04
24	A	407[B]	PHO	C4A-C3A-C2A	-2.29	100.66	102.84
23	C	513	CLA	CAC-C3C-C4C	2.29	127.78	124.81
29	A	414[A]	PL9	C47-C48-C49	-2.29	119.92	127.75
24	a	415[A]	PHO	O2D-CGD-O1D	-2.29	119.36	123.84
23	a	404[B]	CLA	C7-C6-C5	-2.29	107.14	113.36
32	d	407[A]	LHG	O8-C23-O10	-2.29	117.82	123.59
25	d	404	BCR	C40-C30-C39	2.29	115.55	108.53
23	a	406[A]	CLA	CBC-CAC-C3C	-2.29	106.12	112.43
23	B	612	CLA	CMA-C3A-C2A	-2.29	104.60	113.83
23	C	506	CLA	CHD-C4C-NC	2.29	127.81	124.20
23	C	510	CLA	C2A-C1A-CHA	-2.29	119.86	123.86
23	b	601	CLA	O2A-CGA-CBA	2.29	119.08	111.91
23	b	608	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
23	b	608	CLA	C4C-C3C-C2C	-2.28	103.57	106.90
23	b	611	CLA	O2A-CGA-CBA	2.28	119.07	111.91
25	b	618	BCR	C37-C22-C23	2.28	121.67	118.08
23	C	509	CLA	CHD-C4C-NC	2.28	127.80	124.20
23	b	606	CLA	CMB-C2B-C3B	2.28	128.95	124.68
23	c	513	CLA	CHB-C4A-NA	2.28	127.67	124.51
23	a	405[B]	CLA	CMA-C3A-C2A	-2.28	104.63	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	602	CLA	CMA-C3A-C4A	-2.28	105.65	111.77
25	d	404	BCR	C11-C10-C9	-2.28	124.06	127.31
23	b	614	CLA	CMB-C2B-C3B	2.28	128.94	124.68
23	B	603	CLA	CHD-C4C-NC	2.28	127.79	124.20
33	m	103	LMT	C1'-O5'-C5'	-2.27	109.22	113.69
23	b	608	CLA	C11-C12-C13	-2.27	108.57	115.92
23	a	404[A]	CLA	CMA-C3A-C2A	-2.27	104.66	113.83
29	d	405[A]	PL9	C31-C32-C33	-2.27	104.42	111.88
23	C	513	CLA	CMB-C2B-C3B	2.27	128.93	124.68
25	c	516	BCR	C21-C20-C19	-2.27	116.13	123.22
29	a	413[B]	PL9	C45-C44-C46	2.27	119.09	115.27
25	C	516	BCR	C29-C30-C25	2.27	113.97	110.48
23	B	605	CLA	CED-O2D-CGD	2.27	121.07	115.94
24	A	417[A]	PHO	O1D-CGD-CBD	-2.27	120.96	124.74
23	A	408	CLA	OBD-CAD-C3D	-2.27	123.07	128.52
23	c	508	CLA	CBC-CAC-C3C	-2.27	106.18	112.43
23	a	406[B]	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
25	c	515	BCR	C38-C26-C25	-2.27	121.98	124.53
23	c	513	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
34	d	410	LMG	C7-O1-C1	-2.26	109.32	113.74
23	B	605	CLA	CBC-CAC-C3C	-2.26	106.19	112.43
25	t	102	BCR	C20-C21-C22	-2.26	124.08	127.31
36	c	517[B]	DGD	C3G-C2G-C1G	-2.26	106.44	111.79
35	b	622	HTG	C6-C5-C4	-2.26	107.71	113.00
32	d	412[A]	LHG	O7-C7-O9	-2.26	118.24	123.70
35	B	623	HTG	O5-C5-C4	2.26	113.80	109.69
25	b	617	BCR	C11-C10-C9	-2.26	124.08	127.31
23	c	503	CLA	C1-O2A-CGA	2.26	122.37	116.44
25	b	618	BCR	C33-C5-C6	-2.26	121.99	124.53
23	D	402[A]	CLA	C4-C3-C5	2.26	119.07	115.27
23	C	511	CLA	C4-C3-C2	-2.26	117.88	123.68
29	d	405[B]	PL9	C51-C49-C50	2.26	119.59	114.60
32	d	406[A]	LHG	C6-C5-C4	-2.26	106.44	111.79
25	B	617	BCR	C31-C1-C6	-2.26	106.63	110.30
23	A	408	CLA	CMA-C3A-C2A	-2.26	104.72	113.83
35	o	301	HTG	O2-C2-C3	-2.26	105.13	110.35
23	b	602	CLA	C11-C10-C8	-2.26	108.62	115.92
23	c	512	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
23	a	408	CLA	CMB-C2B-C3B	2.26	128.90	124.68
32	b	630[A]	LHG	O8-C23-O10	-2.26	117.90	123.59
23	c	507	CLA	O2A-CGA-CBA	2.26	118.99	111.91
24	a	415[A]	PHO	C4-C3-C2	-2.26	117.89	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	603	CLA	CMC-C2C-C1C	2.25	128.47	125.04
23	B	603	CLA	CMA-C3A-C2A	-2.25	104.73	113.83
23	b	615	CLA	CBC-CAC-C3C	-2.25	106.22	112.43
26	f	102	SQD	O7-S-C6	2.25	109.61	106.94
23	c	502	CLA	CMC-C2C-C1C	2.25	128.47	125.04
29	D	405[A]	PL9	C20-C19-C21	2.25	119.05	115.27
32	d	412[B]	LHG	O7-C7-O9	-2.25	118.27	123.70
24	A	417[A]	PHO	CMB-C2B-C3B	2.25	128.88	124.68
34	C	520	LMG	C8-O7-C10	-2.25	112.26	117.79
25	B	617	BCR	C15-C14-C13	-2.25	124.10	127.31
23	a	408	CLA	CMA-C3A-C2A	-2.25	104.76	113.83
23	C	513	CLA	C4-C3-C2	-2.25	117.91	123.68
23	A	405[B]	CLA	CAC-C3C-C4C	2.25	127.72	124.81
23	D	403	CLA	C2A-C1A-CHA	-2.25	119.93	123.86
23	b	602	CLA	CHC-C1C-C2C	-2.24	120.51	126.72
35	B	623	HTG	C3-C4-C5	2.24	114.24	110.24
23	a	406[B]	CLA	C2A-C1A-CHA	-2.24	119.94	123.86
23	c	503	CLA	C1-C2-C3	-2.24	122.17	126.04
24	a	415[A]	PHO	CED-O2D-CGD	2.24	121.00	115.94
23	d	403	CLA	CAC-C3C-C4C	2.24	127.72	124.81
23	c	514	CLA	C4-C3-C5	2.24	119.04	115.27
23	C	506	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
25	y	101	BCR	C35-C13-C14	-2.24	119.79	122.92
23	c	504	CLA	CHC-C1C-C2C	-2.24	120.53	126.72
23	d	403	CLA	C2A-C1A-CHA	-2.24	119.95	123.86
23	A	405[B]	CLA	CMA-C3A-C2A	-2.24	104.81	113.83
34	m	101	LMG	O7-C10-O9	-2.24	118.30	123.70
23	c	514	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
25	c	516	BCR	C15-C14-C13	-2.23	124.12	127.31
26	F	103	SQD	O48-C23-O10	-2.23	117.95	123.59
29	D	405[A]	PL9	C36-C37-C38	-2.23	104.54	111.88
23	b	615	CLA	CHA-C1A-NA	-2.23	121.29	126.40
23	a	405[B]	CLA	C1-C2-C3	-2.23	122.18	126.04
29	A	414[B]	PL9	C25-C24-C26	2.23	119.02	115.27
25	t	102	BCR	C1-C6-C7	2.23	122.08	115.78
23	c	510	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
34	d	410	LMG	O8-C28-O10	-2.23	117.97	123.59
36	C	517[B]	DGD	O6D-C1D-O3G	-2.23	104.70	109.97
23	a	408	CLA	CBC-CAC-C3C	-2.23	106.30	112.43
23	b	615	CLA	O2A-CGA-CBA	2.23	118.89	111.91
36	c	518[B]	DGD	O2G-C1B-O1B	-2.22	118.33	123.70
23	B	602	CLA	O2A-CGA-CBA	2.22	118.89	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	d	405[B]	PL9	C12-C13-C14	-2.22	122.31	127.66
26	F	103	SQD	C46-C45-C44	-2.22	106.53	111.79
23	a	404[A]	CLA	C7-C6-C5	-2.22	107.32	113.36
23	b	605	CLA	O2A-C1-C2	-2.22	102.79	108.64
23	D	402[B]	CLA	CHD-C4C-NC	2.22	127.71	124.20
23	d	402[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
23	d	403	CLA	C1-O2A-CGA	2.22	122.27	116.44
23	c	506	CLA	CHD-C4C-NC	2.22	127.70	124.20
25	Y	101	BCR	C1-C6-C7	2.22	122.06	115.78
23	A	408	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
29	A	414[B]	PL9	C2-C3-C4	2.22	121.86	118.80
23	B	601	CLA	C2A-C1A-CHA	-2.22	119.98	123.86
23	b	602	CLA	C1-O2A-CGA	2.22	122.27	116.44
36	h	102	DGD	O4D-C4D-C3D	-2.22	105.22	110.35
26	a	410[B]	SQD	C3-C4-C5	2.22	114.20	110.24
23	A	405[A]	CLA	CHB-C4A-NA	2.22	127.58	124.51
23	c	507	CLA	CAA-C2A-C3A	-2.22	106.70	112.78
24	A	407[B]	PHO	O2D-CGD-O1D	-2.22	119.50	123.84
23	C	502	CLA	C1-C2-C3	-2.22	122.21	126.04
23	c	512	CLA	C1-C2-C3	-2.22	122.21	126.04
36	C	517[A]	DGD	C3G-C2G-C1G	-2.22	106.55	111.79
34	d	410	LMG	O8-C28-C29	2.22	118.86	111.91
36	c	518[A]	DGD	O4E-C4E-C3E	-2.22	105.23	110.35
25	Y	101	BCR	C36-C18-C19	2.22	121.57	118.08
25	T	102	BCR	C1-C6-C7	2.21	122.04	115.78
26	F	103	SQD	O5-C1-C2	-2.21	105.66	110.35
25	C	516	BCR	C11-C10-C9	-2.21	124.15	127.31
23	b	614	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
29	d	405[B]	PL9	C20-C19-C21	2.21	118.99	115.27
23	b	602	CLA	CHB-C4A-NA	2.21	127.57	124.51
23	B	611	CLA	OBD-CAD-C3D	-2.21	123.20	128.52
36	H	102	DGD	O6E-C5E-C6E	2.21	111.94	106.44
23	B	606	CLA	C7-C6-C5	-2.21	107.35	113.36
23	C	513	CLA	CBA-CAA-C2A	-2.21	107.34	113.86
23	A	405[B]	CLA	CMB-C2B-C3B	2.21	128.81	124.68
23	C	513	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
23	C	506	CLA	CHA-C1A-NA	-2.21	121.34	126.40
23	B	611	CLA	O2A-CGA-CBA	2.21	118.84	111.91
23	B	616	CLA	C2A-C1A-CHA	-2.21	120.00	123.86
25	c	515	BCR	C33-C5-C6	-2.21	122.05	124.53
23	c	502	CLA	O2A-CGA-CBA	2.21	118.84	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	504	CLA	CAC-C3C-C4C	2.21	127.67	124.81
23	b	615	CLA	C11-C12-C13	-2.21	108.78	115.92
23	b	608	CLA	CAA-C2A-C3A	-2.21	106.73	112.78
32	L	102[B]	LHG	O8-C23-C24	2.21	118.83	111.91
23	a	406[B]	CLA	CMB-C2B-C3B	2.21	128.80	124.68
23	B	613	CLA	CBC-CAC-C3C	-2.20	106.36	112.43
23	d	402[B]	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
23	c	502	CLA	C2A-C1A-CHA	-2.20	120.01	123.86
34	c	521	LMG	C1-C2-C3	-2.20	105.41	110.00
24	A	417[B]	PHO	C6-C5-C3	-2.20	107.68	113.45
23	B	608	CLA	O2A-CGA-CBA	2.20	118.81	111.91
24	A	407[A]	PHO	C1-C2-C3	-2.20	122.24	126.04
23	a	406[A]	CLA	CAC-C3C-C4C	2.20	127.67	124.81
25	d	404	BCR	C37-C22-C23	2.20	121.54	118.08
25	C	515	BCR	C40-C30-C25	-2.20	106.73	110.30
29	A	414[A]	PL9	C51-C49-C50	2.20	119.46	114.60
23	C	512	CLA	CBC-CAC-C3C	-2.20	106.38	112.43
25	K	102	BCR	C36-C18-C19	2.20	121.54	118.08
23	c	511	CLA	C11-C10-C8	-2.20	108.82	115.92
24	A	417[A]	PHO	O2A-CGA-CBA	2.20	118.80	111.91
25	b	618	BCR	C7-C8-C9	-2.20	122.92	126.23
23	B	608	CLA	C2A-C1A-CHA	-2.19	120.02	123.86
23	a	404[B]	CLA	CMA-C3A-C2A	-2.19	104.97	113.83
25	b	619	BCR	C16-C15-C14	-2.19	118.98	123.47
25	K	102	BCR	C32-C1-C6	-2.19	106.74	110.30
23	b	605	CLA	C1-O2A-CGA	2.19	122.19	116.44
23	B	604	CLA	C11-C12-C13	-2.19	108.84	115.92
23	b	614	CLA	CMC-C2C-C1C	2.19	128.37	125.04
23	c	503	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
24	A	407[B]	PHO	CBA-CAA-C2A	-2.19	107.42	113.81
36	H	102	DGD	O2G-C1B-C2B	2.19	116.21	111.50
23	C	502	CLA	O2A-CGA-CBA	2.19	118.77	111.91
24	a	415[B]	PHO	CBA-CAA-C2A	-2.19	107.42	113.81
29	d	405[B]	PL9	C7-C3-C2	-2.19	120.42	123.30
25	B	618	BCR	C15-C14-C13	-2.19	124.19	127.31
23	D	402[A]	CLA	CED-O2D-CGD	2.19	120.88	115.94
38	f	101	HEM	C3C-C4C-NC	-2.18	106.82	110.94
25	C	515	BCR	C24-C23-C22	-2.18	122.94	126.23
26	a	410[A]	SQD	O9-S-O7	-2.18	106.39	113.95
23	b	602	CLA	CMB-C2B-C3B	2.18	128.76	124.68
23	b	615	CLA	C1-C2-C3	-2.18	122.27	126.04
24	a	407[B]	PHO	CMB-C2B-C3B	2.18	128.76	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	610	CLA	CAC-C3C-C4C	2.18	127.64	124.81
23	b	604	CLA	C6-C5-C3	-2.18	107.74	113.45
29	A	414[B]	PL9	C10-C9-C8	-2.18	118.09	123.68
26	L	101	SQD	C44-O6-C1	-2.18	109.48	113.74
29	d	405[A]	PL9	C51-C49-C50	2.18	119.42	114.60
38	F	102	HEM	C4B-C3B-C2B	-2.18	105.39	107.11
32	d	407[B]	LHG	O8-C23-O10	-2.18	118.09	123.59
35	c	522	HTG	C1-O5-C5	2.18	116.60	112.58
23	d	402[A]	CLA	CAC-C3C-C4C	2.18	127.64	124.81
36	c	518[A]	DGD	C2G-O2G-C1B	-2.18	112.43	117.79
23	b	616	CLA	C1-C2-C3	-2.18	122.28	126.04
33	t	101	LMT	C1-O1'-C1'	2.17	117.45	113.84
34	Z	101	LMG	C1-O6-C5	2.17	117.95	113.69
25	D	404	BCR	C15-C16-C17	-2.17	119.03	123.47
23	B	604	CLA	O2A-CGA-CBA	2.17	118.72	111.91
23	b	611	CLA	CMC-C2C-C1C	2.17	128.34	125.04
34	C	501	LMG	O6-C1-O1	-2.17	104.83	109.97
23	b	602	CLA	CAA-CBA-CGA	-2.17	106.92	113.25
24	a	407[A]	PHO	CBA-CAA-C2A	-2.17	107.47	113.81
32	A	419[A]	LHG	O4-P-O5	2.17	122.95	112.24
23	C	502	CLA	C11-C12-C13	-2.17	108.92	115.92
23	c	511	CLA	C7-C6-C5	-2.17	107.48	113.36
23	D	402[B]	CLA	CBC-CAC-C3C	-2.17	106.46	112.43
23	B	609	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
25	y	101	BCR	C40-C30-C25	-2.16	106.79	110.30
29	d	405[B]	PL9	C15-C14-C16	2.16	118.91	115.27
27	B	622	GOL	C3-C2-C1	-2.16	103.29	111.70
23	A	408	CLA	CAC-C3C-C4C	2.16	127.62	124.81
23	A	405[A]	CLA	C4C-C3C-C2C	-2.16	103.75	106.90
26	b	620	SQD	C44-O6-C1	-2.16	109.52	113.74
25	b	618	BCR	C38-C26-C25	-2.16	122.10	124.53
29	d	405[B]	PL9	C45-C44-C46	2.16	118.90	115.27
26	A	410[A]	SQD	O9-S-O7	-2.16	106.48	113.95
23	C	509	CLA	CAA-C2A-C3A	-2.16	106.87	112.78
23	C	511	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
25	h	101	BCR	C16-C15-C14	-2.16	119.06	123.47
23	d	402[B]	CLA	CMC-C2C-C1C	2.16	128.32	125.04
23	b	603	CLA	CBC-CAC-C3C	-2.15	106.49	112.43
34	C	521	LMG	O1-C1-C2	2.15	111.67	108.30
23	A	406[B]	CLA	CAC-C3C-C4C	2.15	127.60	124.81
23	b	610	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
23	B	605	CLA	O2A-CGA-CBA	2.15	118.66	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	t	102	BCR	C29-C28-C27	-2.15	106.57	111.38
23	c	513	CLA	CMB-C2B-C3B	2.15	128.70	124.68
25	C	515	BCR	C38-C26-C25	-2.15	122.11	124.53
36	C	518[A]	DGD	C2G-O2G-C1B	-2.15	112.50	117.79
23	b	610	CLA	C4-C3-C2	-2.15	118.16	123.68
23	B	615	CLA	CED-O2D-CGD	2.15	120.80	115.94
25	b	619	BCR	C29-C30-C25	2.15	113.79	110.48
26	A	410[B]	SQD	O6-C44-C45	-2.15	105.71	110.90
23	c	514	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
36	c	517[A]	DGD	O6D-C1D-O3G	-2.15	104.89	109.97
29	d	405[A]	PL9	C35-C34-C36	2.15	118.88	115.27
25	C	516	BCR	C37-C22-C23	2.15	121.46	118.08
36	c	517[B]	DGD	C2G-O2G-C1B	-2.14	112.51	117.79
25	d	404	BCR	C38-C26-C27	2.14	117.73	113.62
26	A	412	SQD	O6-C44-C45	-2.14	105.73	110.90
36	c	519	DGD	O3G-C1D-C2D	-2.14	104.96	108.30
29	A	414[A]	PL9	C25-C24-C26	2.14	118.87	115.27
23	B	606	CLA	C2A-C1A-CHA	-2.14	120.12	123.86
23	b	605	CLA	C6-C7-C8	-2.14	109.00	115.92
23	C	509	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
23	B	606	CLA	CAC-C3C-C4C	2.14	127.58	124.81
23	b	613	CLA	CAC-C3C-C4C	2.14	127.58	124.81
25	y	101	BCR	C35-C13-C12	2.14	121.44	118.08
24	A	407[A]	PHO	CBA-CAA-C2A	-2.14	107.57	113.81
34	c	520	LMG	O8-C28-O10	-2.13	118.20	123.59
23	b	606	CLA	C2A-C1A-CHA	-2.13	120.13	123.86
29	a	413[B]	PL9	C51-C49-C50	2.13	119.32	114.60
23	c	509	CLA	CAC-C3C-C4C	2.13	127.58	124.81
25	h	101	BCR	C10-C11-C12	-2.13	116.57	123.22
25	b	618	BCR	C35-C13-C14	-2.13	119.94	122.92
24	A	417[B]	PHO	O2A-CGA-CBA	2.13	118.59	111.91
23	c	510	CLA	C4-C3-C2	-2.13	118.22	123.68
33	m	103	LMT	C3B-C4B-C5B	-2.13	106.44	110.24
25	a	409	BCR	C8-C7-C6	-2.13	121.22	127.20
23	C	506	CLA	CMB-C2B-C1B	2.13	131.73	128.46
36	C	517[A]	DGD	O1G-C1A-O1A	-2.13	118.22	123.59
24	a	415[B]	PHO	O2A-CGA-CBA	2.13	118.58	111.91
36	c	518[A]	DGD	O1G-C1A-O1A	-2.13	118.23	123.59
23	B	602	CLA	CHB-C4A-NA	2.13	127.45	124.51
23	a	405[B]	CLA	CHB-C4A-NA	2.13	127.45	124.51
32	E	101[B]	LHG	O7-C7-O9	-2.13	118.57	123.70
23	b	603	CLA	CGD-CBD-CAD	-2.12	103.85	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	404	BCR	C33-C5-C6	-2.12	122.14	124.53
26	b	620	SQD	O5-C1-C2	-2.12	105.85	110.35
24	a	415[A]	PHO	C1A-C2A-C3A	-2.12	100.82	102.84
33	b	621	LMT	C2'-C3'-C4'	2.12	114.53	109.68
33	M	101	LMT	O5B-C5B-C6B	2.12	111.72	106.44
23	C	502	CLA	OBD-CAD-C3D	-2.12	123.41	128.52
23	B	611	CLA	C11-C12-C13	-2.12	109.06	115.92
36	C	517[A]	DGD	O6D-C1D-O3G	-2.12	104.95	109.97
23	A	405[A]	CLA	O2A-CGA-CBA	2.12	118.56	111.91
29	D	405[B]	PL9	C36-C37-C38	-2.12	104.92	111.88
25	d	404	BCR	C29-C28-C27	-2.12	106.64	111.38
25	A	409	BCR	C8-C7-C6	-2.12	121.25	127.20
36	C	517[B]	DGD	C3G-C2G-C1G	-2.12	106.78	111.79
29	A	414[A]	PL9	C12-C13-C14	-2.12	122.56	127.66
23	D	403	CLA	OBD-CAD-C3D	-2.12	123.43	128.52
33	t	101	LMT	O5'-C1'-O1'	-2.12	104.96	109.97
25	c	516	BCR	C2-C1-C6	2.12	113.74	110.48
23	B	601	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
38	F	102	HEM	C3C-C4C-NC	-2.11	106.95	110.94
23	D	403	CLA	CMC-C2C-C1C	2.11	128.25	125.04
36	C	517[B]	DGD	O1G-C1A-O1A	-2.11	118.27	123.59
23	b	604	CLA	C2A-C1A-CHA	-2.11	120.17	123.86
25	B	618	BCR	C40-C30-C25	-2.11	106.88	110.30
23	B	616	CLA	OBD-CAD-C3D	-2.11	123.45	128.52
23	c	502	CLA	CBC-CAC-C3C	-2.11	106.63	112.43
23	B	610	CLA	C1-C2-C3	-2.11	122.40	126.04
23	C	502	CLA	CAA-C2A-C3A	-2.11	107.01	112.78
24	A	417[A]	PHO	C6-C5-C3	-2.11	107.94	113.45
23	B	606	CLA	C11-C10-C8	-2.10	109.11	115.92
23	b	605	CLA	CMB-C2B-C3B	2.10	128.61	124.68
36	h	102	DGD	C3B-C2B-C1B	-2.10	105.97	113.62
23	c	514	CLA	CBC-CAC-C3C	-2.10	106.64	112.43
29	d	405[A]	PL9	C12-C13-C14	-2.10	122.60	127.66
23	b	611	CLA	CAC-C3C-C4C	2.10	127.54	124.81
25	C	515	BCR	C37-C22-C23	2.10	121.39	118.08
23	B	606	CLA	OBD-CAD-C3D	-2.10	123.47	128.52
32	b	630[A]	LHG	O7-C7-O9	-2.10	118.63	123.70
36	H	102	DGD	O3G-C3G-C2G	-2.10	105.83	110.90
23	d	403	CLA	C6-C7-C8	-2.10	109.13	115.92
25	B	619	BCR	C16-C15-C14	-2.10	119.18	123.47
33	F	101	LMT	C2'-C3'-C4'	2.10	114.47	109.68
26	b	620	SQD	O47-C7-O49	-2.10	118.64	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	610	CLA	CMA-C3A-C4A	-2.10	106.14	111.77
23	C	504	CLA	CHA-C1A-NA	-2.10	121.60	126.40
25	y	101	BCR	C16-C15-C14	-2.09	119.18	123.47
32	E	101[A]	LHG	O7-C7-O9	-2.09	118.64	123.70
25	b	619	BCR	C7-C6-C5	2.09	126.53	121.46
23	c	512	CLA	C11-C10-C8	-2.09	109.16	115.92
23	b	607	CLA	C1-C2-C3	-2.09	122.43	126.04
25	k	101	BCR	C36-C18-C19	2.09	121.37	118.08
24	a	415[B]	PHO	CMC-C2C-C3C	2.09	128.88	124.94
23	A	404[A]	CLA	C7-C6-C5	-2.09	107.69	113.36
33	F	101	LMT	C3B-C4B-C5B	-2.09	106.52	110.24
33	M	101	LMT	C3B-C4B-C5B	-2.09	106.52	110.24
29	a	413[B]	PL9	C10-C9-C8	-2.09	118.33	123.68
23	B	611	CLA	C2C-C1C-NC	2.08	111.92	109.97
23	c	504	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
23	d	402[A]	CLA	CHD-C4C-NC	2.08	127.49	124.20
24	a	415[B]	PHO	O1D-CGD-CBD	-2.08	121.27	124.74
26	f	102	SQD	O48-C23-O10	-2.08	118.33	123.59
23	b	608	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
33	D	401	LMT	C4B-C3B-C2B	-2.08	107.19	110.82
23	A	408	CLA	C11-C12-C13	-2.08	109.19	115.92
23	a	404[B]	CLA	CHB-C4A-NA	2.08	127.39	124.51
23	B	602	CLA	C1-O2A-CGA	2.08	121.90	116.44
25	D	404	BCR	C29-C28-C27	-2.08	106.73	111.38
29	A	414[B]	PL9	C35-C34-C33	-2.08	118.34	123.68
34	B	620	LMG	C8-O7-C10	-2.08	112.67	117.79
23	c	507	CLA	CAA-CBA-CGA	2.08	119.33	113.25
25	K	102	BCR	C37-C22-C21	-2.08	120.01	122.92
36	C	519	DGD	O1G-C1A-O1A	-2.08	118.34	123.59
23	b	610	CLA	C11-C12-C13	-2.08	109.20	115.92
23	b	614	CLA	C4-C3-C5	2.08	118.77	115.27
23	B	616	CLA	C4-C3-C2	-2.08	118.35	123.68
25	K	102	BCR	C2-C1-C6	2.08	113.68	110.48
23	B	616	CLA	CMC-C2C-C1C	2.08	128.20	125.04
23	D	402[B]	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
23	b	603	CLA	C1-O2A-CGA	2.08	121.89	116.44
33	B	628	LMT	O5B-C5B-C6B	2.07	111.59	106.44
23	c	506	CLA	C1-C2-C3	-2.07	122.46	126.04
23	B	607	CLA	CMA-C3A-C2A	-2.07	105.47	113.83
23	A	404[A]	CLA	C4-C3-C5	2.07	118.75	115.27
29	D	405[A]	PL9	C12-C13-C14	-2.07	122.68	127.66
33	b	627	LMT	O1'-C1'-C2'	2.07	111.53	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	614	CLA	CBC-CAC-C3C	-2.07	106.73	112.43
29	D	405[B]	PL9	C22-C23-C24	-2.07	122.68	127.66
23	C	512	CLA	O2A-CGA-CBA	2.07	118.39	111.91
23	B	613	CLA	C2A-C1A-CHA	-2.07	120.25	123.86
34	Z	101	LMG	C9-C8-C7	-2.07	106.90	111.79
29	D	405[A]	PL9	C30-C29-C31	2.07	118.75	115.27
29	a	413[A]	PL9	C51-C49-C50	2.07	119.17	114.60
25	c	516	BCR	C37-C22-C23	2.07	121.33	118.08
25	A	409	BCR	C11-C10-C9	-2.07	124.36	127.31
23	B	601	CLA	C4-C3-C5	2.06	118.74	115.27
29	D	405[A]	PL9	C25-C24-C23	-2.06	118.38	123.68
23	c	508	CLA	CMB-C2B-C1B	2.06	131.63	128.46
25	k	101	BCR	C34-C9-C8	2.06	121.33	118.08
32	E	101[B]	LHG	C5-O7-C7	-2.06	112.72	117.79
23	B	611	CLA	CAC-C3C-C4C	2.06	127.48	124.81
25	d	404	BCR	C24-C23-C22	-2.06	123.12	126.23
25	D	404	BCR	C30-C25-C24	2.06	121.60	115.78
25	b	619	BCR	C15-C14-C13	-2.06	124.37	127.31
23	c	514	CLA	C1-O2A-CGA	2.06	121.84	116.44
23	b	611	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
24	a	407[B]	PHO	CBA-CAA-C2A	-2.06	107.80	113.81
35	d	409	HTG	C4-C3-C2	-2.06	107.23	110.82
36	c	517[B]	DGD	O6D-C1D-O3G	-2.05	105.11	109.97
23	B	612	CLA	C7-C6-C5	-2.05	107.78	113.36
36	C	517[A]	DGD	C3E-C4E-C5E	2.05	113.90	110.24
23	C	508	CLA	CHA-C1A-NA	-2.05	121.70	126.40
23	C	505	CLA	OBD-CAD-C3D	-2.05	123.58	128.52
34	B	620	LMG	C4-C3-C2	-2.05	107.24	110.82
25	h	101	BCR	C20-C21-C22	-2.05	124.38	127.31
23	b	609	CLA	CAA-C2A-C3A	-2.05	107.16	112.78
23	A	406[A]	CLA	CMA-C3A-C4A	-2.05	106.26	111.77
23	c	509	CLA	C2A-C1A-CHA	-2.05	120.28	123.86
32	d	412[B]	LHG	C5-O7-C7	-2.05	112.75	117.79
23	A	404[A]	CLA	CHB-C4A-NA	2.05	127.34	124.51
34	C	501	LMG	C9-C8-C7	-2.05	106.94	111.79
36	C	518[B]	DGD	C6D-C5D-C4D	2.05	116.37	112.09
23	c	509	CLA	CHA-C1A-NA	-2.05	121.71	126.40
25	h	101	BCR	C34-C9-C8	2.05	121.30	118.08
26	F	103	SQD	O8-S-O7	-2.05	106.28	111.27
23	C	514	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
29	a	413[B]	PL9	C35-C34-C33	-2.04	118.44	123.68
32	D	407[A]	LHG	O4-P-O5	2.04	122.34	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	503	CLA	C2A-C1A-CHA	-2.04	120.29	123.86
25	D	404	BCR	C37-C22-C21	-2.04	120.06	122.92
33	b	627	LMT	C1'-O5'-C5'	-2.04	109.68	113.69
24	A	407[A]	PHO	C4-C3-C5	2.04	118.70	115.27
27	O	303	GOL	C3-C2-C1	-2.04	103.77	111.70
23	b	612	CLA	C4D-CHA-C1A	-2.04	118.77	121.25
23	C	513	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
25	T	102	BCR	C39-C30-C25	-2.04	106.99	110.30
29	d	405[B]	PL9	C32-C33-C34	-2.04	122.75	127.66
23	c	511	CLA	CBC-CAC-C3C	-2.04	106.81	112.43
23	B	613	CLA	CMA-C3A-C4A	-2.04	106.30	111.77
24	A	407[B]	PHO	O2A-CGA-O1A	-2.04	118.45	123.59
26	a	411	SQD	O5-C5-C4	2.04	113.39	109.69
33	B	628	LMT	C3B-C4B-C5B	-2.04	106.61	110.24
23	b	602	CLA	CMA-C3A-C2A	-2.04	105.62	113.83
26	f	102	SQD	C44-O6-C1	-2.04	109.76	113.74
23	C	502	CLA	O2A-CGA-O1A	-2.04	118.46	123.59
23	C	513	CLA	C2A-C1A-CHA	-2.03	120.30	123.86
34	c	501	LMG	O8-C28-C29	2.03	118.29	111.91
25	t	102	BCR	C37-C22-C21	-2.03	120.07	122.92
33	T	101	LMT	O5B-C5B-C6B	2.03	111.49	106.44
23	C	508	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
36	C	519	DGD	O2G-C1B-C2B	2.03	115.88	111.50
25	y	101	BCR	C1-C6-C7	2.03	121.53	115.78
23	a	408	CLA	CHB-C4A-NA	2.03	127.32	124.51
23	b	601	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
23	B	604	CLA	C4-C3-C5	2.03	118.69	115.27
23	a	405[A]	CLA	CAC-C3C-C2C	2.03	131.00	127.53
24	a	407[B]	PHO	CMC-C2C-C3C	2.03	128.77	124.94
26	a	410[A]	SQD	O48-C23-O10	-2.03	118.47	123.59
25	a	409	BCR	C2-C3-C4	-2.03	106.85	111.38
23	c	511	CLA	CED-O2D-CGD	2.03	120.52	115.94
25	D	404	BCR	C38-C26-C27	2.03	117.51	113.62
29	d	405[A]	PL9	C45-C44-C46	2.03	118.68	115.27
23	b	615	CLA	C2A-C1A-CHA	-2.03	120.32	123.86
23	c	508	CLA	C1-C2-C3	-2.02	122.54	126.04
23	B	603	CLA	C2A-C3A-C4A	-2.02	98.60	101.87
23	b	613	CLA	O2D-CGD-O1D	-2.02	119.88	123.84
23	c	511	CLA	O1D-CGD-CBD	-2.02	120.34	124.48
23	b	603	CLA	C5-C3-C2	-2.02	117.02	121.12
34	c	501	LMG	O7-C10-O9	-2.02	118.82	123.70
24	a	415[A]	PHO	O2A-CGA-CBA	2.02	118.25	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	101	BCR	C3-C4-C5	-2.02	110.47	114.08
23	B	614	CLA	CMA-C3A-C2A	-2.02	105.68	113.83
23	c	513	CLA	CMC-C2C-C1C	2.02	128.12	125.04
23	b	609	CLA	CHA-C1A-NA	-2.02	121.77	126.40
23	A	406[A]	CLA	CHB-C4A-NA	2.02	127.30	124.51
23	c	513	CLA	C2A-C1A-CHA	-2.02	120.33	123.86
25	k	101	BCR	C39-C30-C25	-2.02	107.03	110.30
23	B	602	CLA	C4-C3-C5	2.02	118.67	115.27
23	c	506	CLA	C4-C3-C5	2.02	118.66	115.27
23	b	607	CLA	CHD-C4C-NC	2.02	127.38	124.20
24	A	417[A]	PHO	CED-O2D-CGD	2.01	120.49	115.94
23	d	402[A]	CLA	CBC-CAC-C3C	-2.01	106.88	112.43
23	A	405[B]	CLA	O2A-CGA-CBA	2.01	118.23	111.91
24	a	407[A]	PHO	O2D-CGD-O1D	-2.01	119.90	123.84
25	y	101	BCR	C37-C22-C23	2.01	121.25	118.08
23	A	406[B]	CLA	CHB-C4A-NA	2.01	127.30	124.51
23	b	613	CLA	CHB-C4A-NA	2.01	127.30	124.51
23	C	506	CLA	C11-C10-C8	-2.01	109.42	115.92
24	A	417[B]	PHO	CBA-CAA-C2A	-2.01	107.93	113.81
31	A	416[A]	BCT	O2-C-O1	2.01	124.76	119.55
27	A	418	GOL	C3-C2-C1	-2.01	103.89	111.70
23	D	402[A]	CLA	CBC-CAC-C3C	-2.01	106.89	112.43
31	d	401[A]	BCT	O2-C-O1	2.01	124.76	119.55
23	D	403	CLA	CHB-C4A-NA	2.01	127.29	124.51
23	B	608	CLA	OBD-CAD-C3D	-2.01	123.68	128.52
23	b	613	CLA	CHA-C1A-NA	-2.01	121.80	126.40
36	c	519	DGD	O2G-C1B-O1B	-2.01	118.85	123.70
23	B	613	CLA	CHD-C4C-NC	2.01	127.37	124.20
29	D	405[A]	PL9	O2-C1-C6	-2.01	117.11	120.59
23	b	602	CLA	O2A-CGA-CBA	2.01	118.21	111.91
23	C	507	CLA	CHB-C4A-NA	2.01	127.29	124.51
23	b	606	CLA	OBD-CAD-C3D	-2.01	123.69	128.52
25	b	619	BCR	C31-C1-C6	-2.01	107.05	110.30
23	b	616	CLA	OBD-CAD-C3D	-2.01	123.69	128.52
23	b	601	CLA	CAA-C2A-C3A	-2.01	107.29	112.78
27	a	417	GOL	C3-C2-C1	-2.01	103.91	111.70
23	c	513	CLA	OBD-CAD-C3D	-2.00	123.70	128.52
23	b	616	CLA	C2A-C1A-CHA	-2.00	120.36	123.86
36	c	518[B]	DGD	O1G-C1A-O1A	-2.00	118.54	123.59
25	c	516	BCR	C16-C17-C18	-2.00	124.45	127.31
34	m	101	LMG	C3-C4-C5	2.00	113.81	110.24
23	B	615	CLA	O2A-CGA-O1A	-2.00	118.54	123.59

All (69) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404[A]	CLA	ND
23	A	404[B]	CLA	ND
23	A	405[B]	CLA	ND
23	A	408	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND
23	B	604	CLA	ND
23	B	605	CLA	ND
23	B	606	CLA	ND
23	B	607	CLA	ND
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	505	CLA	ND
23	C	506	CLA	ND
23	C	507	CLA	ND
23	C	508	CLA	ND
23	C	509	CLA	ND
23	C	510	CLA	ND
23	C	511	CLA	ND
23	C	512	CLA	ND
23	C	513	CLA	ND
23	C	514	CLA	ND
23	D	402[A]	CLA	ND
23	D	402[B]	CLA	ND
23	D	403	CLA	ND
23	a	404[A]	CLA	ND
23	a	404[B]	CLA	ND
23	a	405[A]	CLA	ND
23	a	405[B]	CLA	ND
23	b	601	CLA	ND
23	b	602	CLA	ND
23	b	603	CLA	ND
23	b	604	CLA	ND

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Mol	Chain	Res	Type	Atom
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	402[A]	CLA	ND
23	d	402[B]	CLA	ND
23	d	403	CLA	ND

All (1625) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	408	CLA	C4-C3-C5-C6
23	B	606	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	C	509	CLA	CHA-CBD-CGD-O1D
23	C	509	CLA	CHA-CBD-CGD-O2D
23	b	605	CLA	C4-C3-C5-C6
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	C2-C3-C5-C6
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	403	CLA	C4-C3-C5-C6
25	y	101	BCR	C1-C6-C7-C8
25	y	101	BCR	C5-C6-C7-C8
26	A	410[A]	SQD	O49-C7-O47-C45
26	A	410[B]	SQD	C8-C7-O47-C45
26	A	412	SQD	O6-C44-C45-O47
26	F	103	SQD	C2-C1-O6-C44
26	F	103	SQD	O49-C7-O47-C45
26	F	103	SQD	C8-C7-O47-C45
26	L	101	SQD	O5-C1-O6-C44
26	L	101	SQD	O49-C7-O47-C45
26	a	411	SQD	O6-C44-C45-O47
26	a	411	SQD	C5-C6-S-O7
26	a	411	SQD	C5-C6-S-O8
26	a	411	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	B	622	GOL	C1-C2-C3-O3
27	B	622	GOL	O2-C2-C3-O3
27	B	627	GOL	O1-C1-C2-C3
27	D	412	GOL	C1-C2-C3-O3
27	V	203[A]	GOL	C1-C2-C3-O3
27	V	203[B]	GOL	C1-C2-C3-O3
27	V	203[B]	GOL	O2-C2-C3-O3
27	b	624	GOL	C1-C2-C3-O3
27	c	527	GOL	C1-C2-C3-O3
27	c	527	GOL	O2-C2-C3-O3
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

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Mol	Chain	Res	Type	Atoms
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	413[A]	PL9	C9-C11-C12-C13
29	a	413[A]	PL9	C14-C16-C17-C18
29	a	413[A]	PL9	C25-C24-C26-C27
29	a	413[B]	PL9	C9-C11-C12-C13
29	a	413[B]	PL9	C14-C16-C17-C18
29	a	413[B]	PL9	C23-C24-C26-C27
29	a	413[B]	PL9	C25-C24-C26-C27
32	D	406[A]	LHG	O2-C2-C3-O3
32	D	406[A]	LHG	C3-O3-P-O4
32	D	406[A]	LHG	C3-O3-P-O5
32	D	406[A]	LHG	C3-O3-P-O6
32	D	406[A]	LHG	C4-O6-P-O4
32	D	406[B]	LHG	O2-C2-C3-O3
32	D	406[B]	LHG	C3-O3-P-O4
32	D	406[B]	LHG	C4-O6-P-O4
32	D	406[B]	LHG	C4-O6-P-O5
32	D	407[B]	LHG	C4-O6-P-O4
32	E	101[A]	LHG	C3-O3-P-O4
32	E	101[A]	LHG	C3-O3-P-O5
32	E	101[A]	LHG	O10-C23-O8-C6
32	E	101[A]	LHG	C24-C23-O8-C6
32	E	101[B]	LHG	C3-O3-P-O4
32	E	101[B]	LHG	C3-O3-P-O5
32	E	101[B]	LHG	O10-C23-O8-C6
32	E	101[B]	LHG	C24-C23-O8-C6
32	L	102[A]	LHG	C4-O6-P-O4
32	L	102[A]	LHG	C4-O6-P-O5
32	L	102[B]	LHG	C4-O6-P-O4
32	a	419[A]	LHG	C3-O3-P-O4
32	a	419[A]	LHG	C4-O6-P-O5
32	a	419[A]	LHG	O10-C23-O8-C6
32	a	419[A]	LHG	C24-C23-O8-C6
32	a	419[B]	LHG	C3-O3-P-O4
32	a	419[B]	LHG	C4-O6-P-O5
32	a	419[B]	LHG	O10-C23-O8-C6
32	a	419[B]	LHG	C24-C23-O8-C6
32	b	630[A]	LHG	C4-O6-P-O3
32	b	630[A]	LHG	C4-O6-P-O4
32	b	630[A]	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
32	b	630[B]	LHG	C4-O6-P-O4
32	b	630[B]	LHG	C4-O6-P-O5
32	d	406[A]	LHG	C3-O3-P-O5
32	d	406[A]	LHG	C4-O6-P-O4
32	d	406[B]	LHG	C3-O3-P-O4
32	d	406[B]	LHG	C3-O3-P-O5
32	d	406[B]	LHG	C3-O3-P-O6
32	d	406[B]	LHG	C4-O6-P-O4
32	d	412[A]	LHG	C3-O3-P-O5
33	A	420	LMT	O5'-C1'-O1'-C1
33	B	628	LMT	C2'-C1'-O1'-C1
33	B	629	LMT	O5'-C1'-O1'-C1
33	B	629	LMT	C2-C1-O1'-C1'
33	D	401	LMT	C2'-C1'-O1'-C1
33	D	401	LMT	O5'-C1'-O1'-C1
33	F	101	LMT	C2'-C1'-O1'-C1
33	F	101	LMT	O5'-C1'-O1'-C1
33	T	101	LMT	C2-C1-O1'-C1'
33	b	627	LMT	C2'-C1'-O1'-C1
33	b	627	LMT	O5'-C1'-O1'-C1
33	t	101	LMT	O5'-C1'-O1'-C1
33	t	101	LMT	C2-C1-O1'-C1'
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	c	522	HTG	C2'-C1'-S1-C1
35	o	301	HTG	C2'-C1'-S1-C1
33	B	628	LMT	C4'-C5'-C6'-O6'
33	A	420	LMT	O5B-C1B-O1B-C4'
26	A	410[B]	SQD	O49-C7-O47-C45
26	b	620	SQD	O49-C7-O47-C45
34	z	101	LMG	O9-C10-O7-C8
23	b	616	CLA	C3-C5-C6-C7
23	c	513	CLA	C3-C5-C6-C7
23	d	403	CLA	C3-C5-C6-C7
33	a	416	LMT	O5B-C5B-C6B-O6B
26	A	410[A]	SQD	C8-C7-O47-C45
26	L	101	SQD	C8-C7-O47-C45
34	c	521	LMG	C11-C10-O7-C8
34	z	101	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
33	T	101	LMT	O5'-C5'-C6'-O6'
23	C	505	CLA	C4-C3-C5-C6
23	a	408	CLA	C4-C3-C5-C6
23	c	514	CLA	C4-C3-C5-C6
33	B	626	LMT	C4'-C5'-C6'-O6'
33	T	101	LMT	C4B-C5B-C6B-O6B
23	A	408	CLA	C2-C3-C5-C6
23	C	505	CLA	C2-C3-C5-C6
23	b	605	CLA	C2-C3-C5-C6
23	d	403	CLA	C2-C3-C5-C6
29	A	414[A]	PL9	C18-C19-C21-C22
29	A	414[B]	PL9	C18-C19-C21-C22
23	B	614	CLA	C3-C5-C6-C7
23	D	403	CLA	C3-C5-C6-C7
33	B	626	LMT	O5'-C5'-C6'-O6'
33	F	101	LMT	O5'-C5'-C6'-O6'
35	D	410	HTG	O5-C5-C6-O6
33	m	103	LMT	C4B-C5B-C6B-O6B
33	B	626	LMT	C6-C7-C8-C9
35	D	410	HTG	S1-C1'-C2'-C3'
35	b	625	HTG	S1-C1'-C2'-C3'
33	m	103	LMT	O5B-C5B-C6B-O6B
34	C	521	LMG	O9-C10-O7-C8
33	B	628	LMT	O5B-C5B-C6B-O6B
33	b	621	LMT	O5'-C5'-C6'-O6'
23	C	514	CLA	CBD-CGD-O2D-CED
32	E	101[A]	LHG	O2-C2-C3-O3
32	d	406[A]	LHG	O2-C2-C3-O3
32	d	406[B]	LHG	O2-C2-C3-O3
23	B	616	CLA	C3-C5-C6-C7
34	c	521	LMG	C4-C5-C6-O5
23	C	504	CLA	CBD-CGD-O2D-CED
23	c	514	CLA	CBD-CGD-O2D-CED
34	C	521	LMG	O6-C5-C6-O5
35	b	625	HTG	O5-C5-C6-O6
33	a	416	LMT	C4B-C5B-C6B-O6B
35	D	410	HTG	C4-C5-C6-O6
33	A	420	LMT	O5B-C5B-C6B-O6B
33	A	420	LMT	O5'-C5'-C6'-O6'
33	B	629	LMT	O5'-C5'-C6'-O6'
33	b	627	LMT	O5'-C5'-C6'-O6'
33	T	101	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
33	e	101	LMT	C4'-C5'-C6'-O6'
23	B	605	CLA	C4-C3-C5-C6
23	C	508	CLA	C4-C3-C5-C6
23	b	603	CLA	C4-C3-C5-C6
23	b	614	CLA	C4-C3-C5-C6
29	A	414[A]	PL9	C20-C19-C21-C22
29	A	414[B]	PL9	C20-C19-C21-C22
29	a	413[A]	PL9	C15-C14-C16-C17
29	a	413[A]	PL9	C30-C29-C31-C32
29	a	413[B]	PL9	C15-C14-C16-C17
29	a	413[B]	PL9	C30-C29-C31-C32
33	F	101	LMT	C4'-C5'-C6'-O6'
23	B	605	CLA	C2-C3-C5-C6
23	C	508	CLA	C2-C3-C5-C6
23	b	603	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	413[A]	PL9	C13-C14-C16-C17
29	a	413[A]	PL9	C28-C29-C31-C32
29	a	413[B]	PL9	C13-C14-C16-C17
29	a	413[B]	PL9	C28-C29-C31-C32
23	b	606	CLA	C2A-CAA-CBA-CGA
36	h	102	DGD	C6B-C7B-C8B-C9B
33	B	626	LMT	O5B-C5B-C6B-O6B
33	B	628	LMT	O5'-C5'-C6'-O6'
33	T	101	LMT	O5B-C5B-C6B-O6B
33	e	101	LMT	O5'-C1'-O1'-C1
29	A	414[B]	PL9	C44-C46-C47-C48
29	D	405[A]	PL9	C39-C41-C42-C43
36	C	519	DGD	C6B-C7B-C8B-C9B
23	B	605	CLA	CBD-CGD-O2D-CED
33	t	101	LMT	O5'-C5'-C6'-O6'
33	B	628	LMT	C4B-C5B-C6B-O6B
33	A	420	LMT	C4B-C5B-C6B-O6B
34	B	620	LMG	C39-C40-C41-C42
34	B	620	LMG	C15-C16-C17-C18
32	d	406[A]	LHG	C1-C2-C3-O3
23	A	408	CLA	C3-C5-C6-C7
23	a	408	CLA	CBA-CGA-O2A-C1
23	C	509	CLA	CBD-CGD-O2D-CED
35	b	623	HTG	C1'-C2'-C3'-C4'

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Mol	Chain	Res	Type	Atoms
32	D	407[A]	LHG	C33-C34-C35-C36
33	B	629	LMT	C4'-C5'-C6'-O6'
23	B	601	CLA	C5-C6-C7-C8
23	b	601	CLA	C10-C11-C12-C13
23	b	604	CLA	C8-C10-C11-C12
32	E	101[B]	LHG	O2-C2-C3-O3
33	A	420	LMT	C2'-C1'-O1'-C1
33	B	629	LMT	C2'-C1'-O1'-C1
33	t	101	LMT	C2'-C1'-O1'-C1
34	c	521	LMG	O6-C5-C6-O5
33	b	621	LMT	C4'-C5'-C6'-O6'
23	a	408	CLA	C2-C3-C5-C6
29	a	413[A]	PL9	C23-C24-C26-C27
23	B	602	CLA	C6-C7-C8-C9
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	514	CLA	C6-C7-C8-C9
26	L	101	SQD	C30-C31-C32-C33
23	B	606	CLA	C2A-CAA-CBA-CGA
33	b	627	LMT	C4'-C5'-C6'-O6'
23	B	601	CLA	C10-C11-C12-C13
23	B	606	CLA	C10-C11-C12-C13
23	b	611	CLA	C15-C16-C17-C18
23	c	513	CLA	C15-C16-C17-C18
35	B	623	HTG	O5-C5-C6-O6
36	c	518[B]	DGD	C1B-C2B-C3B-C4B
33	B	626	LMT	C4B-C5B-C6B-O6B
33	A	420	LMT	C5'-C4'-O1B-C1B
33	B	626	LMT	C5'-C4'-O1B-C1B
33	e	101	LMT	O5'-C5'-C6'-O6'
23	A	408	CLA	C5-C6-C7-C8
23	B	602	CLA	C13-C15-C16-C17
23	C	508	CLA	C5-C6-C7-C8
23	b	611	CLA	C8-C10-C11-C12
23	b	614	CLA	C8-C10-C11-C12
26	b	620	SQD	C18-C19-C20-C21
27	B	627	GOL	O1-C1-C2-O2
27	O	302	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
27	V	203[A]	GOL	O2-C2-C3-O3
26	A	410[B]	SQD	C7-C8-C9-C10
26	F	103	SQD	C23-C24-C25-C26
26	L	101	SQD	C7-C8-C9-C10
23	B	603	CLA	C13-C15-C16-C17
23	c	510	CLA	CBA-CGA-O2A-C1
35	b	622	HTG	S1-C1'-C2'-C3'
35	d	409	HTG	S1-C1'-C2'-C3'
23	B	616	CLA	C2-C1-O2A-CGA
33	A	420	LMT	O1'-C1-C2-C3
32	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
23	C	502	CLA	CBD-CGD-O2D-CED
23	c	513	CLA	CBD-CGD-O2D-CED
23	A	408	CLA	C12-C13-C15-C16
23	C	511	CLA	C11-C12-C13-C15
23	D	403	CLA	C11-C10-C8-C7
23	b	606	CLA	C12-C13-C15-C16
23	c	510	CLA	C3-C5-C6-C7
23	a	408	CLA	O1A-CGA-O2A-C1
23	c	510	CLA	O1A-CGA-O2A-C1
33	a	416	LMT	O1'-C1-C2-C3
23	B	614	CLA	C8-C10-C11-C12
23	C	511	CLA	C10-C11-C12-C13
33	A	420	LMT	C4'-C5'-C6'-O6'
26	F	103	SQD	O5-C1-O6-C44
33	B	628	LMT	O5'-C1'-O1'-C1
33	b	621	LMT	O5'-C1'-O1'-C1
29	A	414[A]	PL9	C44-C46-C47-C48
29	D	405[B]	PL9	C39-C41-C42-C43
29	d	405[A]	PL9	C39-C41-C42-C43
29	d	405[B]	PL9	C39-C41-C42-C43
32	E	101[B]	LHG	C23-C24-C25-C26
35	B	623	HTG	S1-C1'-C2'-C3'
36	c	517[B]	DGD	O6D-C5D-C6D-O5D
32	D	407[B]	LHG	C33-C34-C35-C36
33	e	101	LMT	O5B-C5B-C6B-O6B
23	C	512	CLA	C3-C5-C6-C7
23	c	514	CLA	C10-C11-C12-C13
36	C	519	DGD	CAB-CBB-CCB-CDB
23	a	404[B]	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	b	606	CLA	C10-C11-C12-C13
23	c	507	CLA	C15-C16-C17-C18
23	B	614	CLA	C10-C11-C12-C13
23	C	509	CLA	C10-C11-C12-C13
23	a	404[A]	CLA	C15-C16-C17-C18
23	b	606	CLA	C13-C15-C16-C17
32	D	406[B]	LHG	C3-O3-P-O6
32	D	406[B]	LHG	C4-O6-P-O3
32	E	101[A]	LHG	C3-O3-P-O6
32	E	101[A]	LHG	C4-O6-P-O3
32	E	101[B]	LHG	C3-O3-P-O6
32	E	101[B]	LHG	C4-O6-P-O3
32	L	102[A]	LHG	C4-O6-P-O3
32	L	102[B]	LHG	C4-O6-P-O3
32	a	419[A]	LHG	C3-O3-P-O6
32	a	419[A]	LHG	C4-O6-P-O3
32	a	419[B]	LHG	C3-O3-P-O6
32	a	419[B]	LHG	C4-O6-P-O3
32	b	630[B]	LHG	C4-O6-P-O3
32	d	406[A]	LHG	C3-O3-P-O6
35	o	301	HTG	C1'-C2'-C3'-C4'
26	A	410[A]	SQD	C7-C8-C9-C10
32	D	406[A]	LHG	C1-C2-C3-O3
32	D	406[B]	LHG	C1-C2-C3-O3
32	d	406[B]	LHG	C1-C2-C3-O3
34	Z	101	LMG	O6-C5-C6-O5
34	B	620	LMG	O9-C10-O7-C8
23	b	604	CLA	C5-C6-C7-C8
23	b	610	CLA	C2A-CAA-CBA-CGA
36	C	519	DGD	C2B-C3B-C4B-C5B
25	T	102	BCR	C13-C14-C15-C16
26	A	410[A]	SQD	C15-C16-C17-C18
32	L	102[A]	LHG	C12-C13-C14-C15
32	L	102[B]	LHG	C12-C13-C14-C15
23	D	403	CLA	CBD-CGD-O2D-CED
34	B	620	LMG	C11-C10-O7-C8
26	F	103	SQD	C30-C31-C32-C33
26	f	102	SQD	C32-C33-C34-C35
32	D	406[B]	LHG	C16-C17-C18-C19
32	L	102[A]	LHG	C17-C18-C19-C20
32	d	412[A]	LHG	C16-C17-C18-C19
33	b	627	LMT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
34	B	620	LMG	C34-C35-C36-C37
36	C	517[B]	DGD	C5B-C6B-C7B-C8B
36	c	517[B]	DGD	C2B-C3B-C4B-C5B
36	c	518[A]	DGD	CAA-CBA-CCA-CDA
36	c	518[B]	DGD	C9A-CAA-CBA-CCA
36	h	102	DGD	C7B-C8B-C9B-CAB
23	a	408	CLA	C16-C17-C18-C19
23	c	510	CLA	C16-C17-C18-C20
32	L	102[B]	LHG	C13-C14-C15-C16
33	A	420	LMT	C3-C4-C5-C6
34	D	411	LMG	C35-C36-C37-C38
35	b	622	HTG	C2'-C3'-C4'-C5'
36	c	518[A]	DGD	C9A-CAA-CBA-CCA
36	c	518[B]	DGD	CAA-CBA-CCA-CDA
36	c	518[B]	DGD	CBA-CCA-CDA-CEA
26	A	410[B]	SQD	C15-C16-C17-C18
32	L	102[B]	LHG	C17-C18-C19-C20
34	C	521	LMG	C18-C19-C20-C21
36	C	518[A]	DGD	CCB-CDB-CEB-CFB
33	M	101	LMT	O5'-C5'-C6'-O6'
34	D	411	LMG	C30-C31-C32-C33
35	B	621	HTG	C3'-C4'-C5'-C6'
36	c	517[A]	DGD	C2B-C3B-C4B-C5B
36	c	517[B]	DGD	C9A-CAA-CBA-CCA
23	D	403	CLA	C10-C11-C12-C13
23	b	605	CLA	C8-C10-C11-C12
26	F	103	SQD	C24-C25-C26-C27
32	L	102[B]	LHG	C25-C26-C27-C28
33	D	401	LMT	O1'-C1-C2-C3
36	C	517[A]	DGD	C4B-C5B-C6B-C7B
26	A	412	SQD	C2-C1-O6-C44
33	b	621	LMT	C2'-C1'-O1'-C1
33	e	101	LMT	C2'-C1'-O1'-C1
36	C	518[A]	DGD	C2E-C1E-O5D-C6D
32	D	407[B]	LHG	C32-C33-C34-C35
34	C	501	LMG	C17-C18-C19-C20
34	D	411	LMG	C19-C20-C21-C22
36	C	517[A]	DGD	C5B-C6B-C7B-C8B
36	c	517[A]	DGD	C9A-CAA-CBA-CCA
23	b	614	CLA	C16-C17-C18-C20
23	c	509	CLA	C16-C17-C18-C19
29	A	414[A]	PL9	C45-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
32	A	419[B]	LHG	C34-C35-C36-C37
32	D	406[A]	LHG	C16-C17-C18-C19
32	a	419[A]	LHG	C26-C27-C28-C29
32	b	630[A]	LHG	C14-C15-C16-C17
32	b	630[B]	LHG	C14-C15-C16-C17
32	d	412[B]	LHG	C16-C17-C18-C19
33	e	101	LMT	C4-C5-C6-C7
33	t	101	LMT	C4-C5-C6-C7
34	C	501	LMG	C12-C13-C14-C15
36	H	102	DGD	C5B-C6B-C7B-C8B
29	d	405[A]	PL9	C13-C14-C16-C17
23	B	603	CLA	C11-C12-C13-C14
23	a	406[A]	CLA	C11-C12-C13-C14
23	a	406[B]	CLA	C11-C12-C13-C14
23	c	505	CLA	C14-C13-C15-C16
32	D	407[A]	LHG	C32-C33-C34-C35
32	L	102[A]	LHG	C15-C16-C17-C18
34	C	521	LMG	C17-C18-C19-C20
34	c	520	LMG	C34-C35-C36-C37
36	c	519	DGD	CBB-CCB-CDB-CEB
23	B	610	CLA	C2A-CAA-CBA-CGA
23	c	508	CLA	C2A-CAA-CBA-CGA
36	c	517[B]	DGD	C4D-C5D-C6D-O5D
25	b	619	BCR	C7-C8-C9-C34
32	a	419[B]	LHG	C26-C27-C28-C29
32	d	412[A]	LHG	C32-C33-C34-C35
33	B	628	LMT	C2-C3-C4-C5
33	e	101	LMT	C5-C6-C7-C8
36	C	518[B]	DGD	CCB-CDB-CEB-CFB
36	c	518[A]	DGD	CBA-CCA-CDA-CEA
27	A	411	GOL	O1-C1-C2-C3
27	B	627	GOL	C1-C2-C3-O3
27	D	412	GOL	O1-C1-C2-C3
27	O	302	GOL	O1-C1-C2-C3
27	O	303	GOL	O1-C1-C2-C3
27	a	417	GOL	O1-C1-C2-C3
27	d	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	b	619	BCR	C7-C8-C9-C10
23	C	510	CLA	C3-C5-C6-C7
36	c	517[B]	DGD	O6E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
32	A	419[B]	LHG	C12-C13-C14-C15
32	L	102[A]	LHG	C25-C26-C27-C28
33	t	101	LMT	C4'-C5'-C6'-O6'
34	c	520	LMG	C10-C11-C12-C13
26	A	412	SQD	C17-C18-C19-C20
32	A	419[A]	LHG	C34-C35-C36-C37
32	d	406[A]	LHG	C11-C10-C9-C8
33	B	628	LMT	C5-C6-C7-C8
34	c	501	LMG	C30-C31-C32-C33
34	c	501	LMG	C34-C35-C36-C37
34	m	101	LMG	C39-C40-C41-C42
36	C	517[B]	DGD	C4B-C5B-C6B-C7B
36	H	102	DGD	CCB-CDB-CEB-CFB
23	B	603	CLA	C16-C17-C18-C20
23	B	615	CLA	C16-C17-C18-C19
23	B	615	CLA	C16-C17-C18-C20
23	a	408	CLA	C16-C17-C18-C20
23	b	615	CLA	C16-C17-C18-C19
23	d	403	CLA	C16-C17-C18-C19
23	d	403	CLA	C16-C17-C18-C20
26	A	412	SQD	O5-C1-O6-C44
23	b	606	CLA	C15-C16-C17-C18
26	A	410[A]	SQD	C12-C13-C14-C15
32	d	407[B]	LHG	C27-C28-C29-C30
33	B	626	LMT	C5-C6-C7-C8
32	L	102[A]	LHG	C13-C14-C15-C16
32	d	406[A]	LHG	C34-C35-C36-C37
34	m	101	LMG	C35-C36-C37-C38
36	H	102	DGD	C7A-C8A-C9A-CAA
26	a	411	SQD	C25-C26-C27-C28
32	d	407[A]	LHG	C27-C28-C29-C30
33	B	629	LMT	C3-C4-C5-C6
33	B	629	LMT	C4-C5-C6-C7
34	d	410	LMG	C29-C30-C31-C32
33	A	420	LMT	C1-C2-C3-C4
23	C	513	CLA	CBA-CGA-O2A-C1
36	C	517[B]	DGD	O6D-C5D-C6D-O5D
32	E	101[B]	LHG	C24-C25-C26-C27
34	C	501	LMG	C19-C20-C21-C22
34	C	520	LMG	C16-C17-C18-C19
34	C	520	LMG	C17-C18-C19-C20
23	C	507	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
33	a	416	LMT	C1-C2-C3-C4
33	A	420	LMT	C2-C1-O1'-C1'
33	F	101	LMT	C2-C1-O1'-C1'
33	b	627	LMT	C2-C1-O1'-C1'
34	c	520	LMG	C33-C34-C35-C36
23	C	514	CLA	O1D-CGD-O2D-CED
23	B	603	CLA	C16-C17-C18-C19
23	b	602	CLA	C16-C17-C18-C19
23	b	602	CLA	C16-C17-C18-C20
26	a	411	SQD	C31-C32-C33-C34
32	A	419[A]	LHG	C12-C13-C14-C15
32	b	630[A]	LHG	C16-C17-C18-C19
33	M	101	LMT	C3-C4-C5-C6
33	T	101	LMT	C7-C8-C9-C10
32	E	101[A]	LHG	C24-C25-C26-C27
32	d	406[B]	LHG	C34-C35-C36-C37
33	m	103	LMT	C7-C8-C9-C10
34	B	620	LMG	C17-C18-C19-C20
36	h	102	DGD	C9A-CAA-CBA-CCA
36	h	102	DGD	CAA-CBA-CCA-CDA
36	c	517[A]	DGD	O6D-C5D-C6D-O5D
34	C	501	LMG	C10-C11-C12-C13
26	F	103	SQD	C29-C30-C31-C32
29	D	405[B]	PL9	C15-C14-C16-C17
29	d	405[A]	PL9	C15-C14-C16-C17
36	c	517[A]	DGD	C2A-C1A-O1G-C1G
24	a	407[B]	PHO	C2-C3-C5-C6
29	A	414[A]	PL9	C12-C11-C9-C8
29	A	414[A]	PL9	C43-C44-C46-C47
29	D	405[A]	PL9	C13-C14-C16-C17
29	d	405[B]	PL9	C13-C14-C16-C17
36	c	519	DGD	C2B-C3B-C4B-C5B
27	D	412	GOL	O1-C1-C2-O2
27	b	624	GOL	O2-C2-C3-O3
27	v	202[B]	GOL	O1-C1-C2-O2
32	d	412[B]	LHG	C32-C33-C34-C35
34	m	101	LMG	C38-C39-C40-C41
36	c	518[A]	DGD	CBB-CCB-CDB-CEB
23	b	615	CLA	C16-C17-C18-C20
23	c	510	CLA	C16-C17-C18-C19
23	A	406[B]	CLA	C13-C15-C16-C17
32	D	407[A]	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
34	C	521	LMG	C19-C20-C21-C22
36	H	102	DGD	C9B-CAB-CBB-CCB
36	c	517[A]	DGD	C5A-C6A-C7A-C8A
36	c	517[A]	DGD	CAA-CBA-CCA-CDA
23	C	510	CLA	C2-C1-O2A-CGA
23	b	601	CLA	C2-C1-O2A-CGA
26	b	620	SQD	C13-C14-C15-C16
32	d	412[A]	LHG	C29-C30-C31-C32
34	D	411	LMG	C36-C37-C38-C39
23	A	404[B]	CLA	C13-C15-C16-C17
23	C	513	CLA	C10-C11-C12-C13
33	B	629	LMT	O1'-C1-C2-C3
33	B	629	LMT	C11-C10-C9-C8
36	c	517[A]	DGD	C7A-C8A-C9A-CAA
34	c	501	LMG	C10-C11-C12-C13
33	b	621	LMT	C3'-C4'-O1B-C1B
25	D	404	BCR	C23-C24-C25-C30
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	b	617	BCR	C5-C6-C7-C8
25	b	619	BCR	C5-C6-C7-C8
36	c	518[B]	DGD	CBB-CCB-CDB-CEB
36	h	102	DGD	C2B-C3B-C4B-C5B
23	C	503	CLA	C15-C16-C17-C18
34	m	101	LMG	C11-C10-O7-C8
36	c	518[A]	DGD	C6A-C7A-C8A-C9A
23	C	513	CLA	O1A-CGA-O2A-C1
35	b	622	HTG	C3'-C4'-C5'-C6'
36	c	519	DGD	CBA-CCA-CDA-CEA
23	B	608	CLA	C13-C15-C16-C17
23	b	614	CLA	C10-C11-C12-C13
33	B	626	LMT	C3'-C4'-O1B-C1B
34	C	501	LMG	C36-C37-C38-C39
23	D	403	CLA	C4-C3-C5-C6
24	a	407[B]	PHO	C4-C3-C5-C6
29	A	414[A]	PL9	C30-C29-C31-C32
29	D	405[A]	PL9	C15-C14-C16-C17
23	B	603	CLA	C11-C12-C13-C15
23	B	614	CLA	C11-C10-C8-C7
23	a	406[A]	CLA	C11-C12-C13-C15
23	a	406[B]	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
23	c	505	CLA	C12-C13-C15-C16
29	A	414[B]	PL9	C12-C11-C9-C8
29	D	405[B]	PL9	C13-C14-C16-C17
33	A	420	LMT	C3'-C4'-O1B-C1B
34	c	520	LMG	C31-C32-C33-C34
26	A	412	SQD	C26-C27-C28-C29
26	L	101	SQD	C11-C10-C9-C8
32	D	407[A]	LHG	C29-C30-C31-C32
32	D	407[B]	LHG	C15-C16-C17-C18
33	e	101	LMT	C1-C2-C3-C4
23	C	512	CLA	C8-C10-C11-C12
26	b	620	SQD	C27-C28-C29-C30
32	D	406[A]	LHG	C13-C14-C15-C16
32	b	630[B]	LHG	C12-C13-C14-C15
33	B	628	LMT	C6-C7-C8-C9
33	b	627	LMT	C5-C6-C7-C8
32	b	630[B]	LHG	C27-C28-C29-C30
32	d	407[B]	LHG	C25-C26-C27-C28
32	d	412[B]	LHG	C24-C25-C26-C27
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-C19
36	C	518[A]	DGD	O6E-C1E-O5D-C6D
36	c	517[B]	DGD	O6E-C1E-O5D-C6D
36	c	518[B]	DGD	O6E-C1E-O5D-C6D
23	b	604	CLA	C15-C16-C17-C18
26	a	410[A]	SQD	C9-C10-C11-C12
26	a	410[B]	SQD	C9-C10-C11-C12
26	a	410[B]	SQD	C12-C13-C14-C15
32	b	630[B]	LHG	C16-C17-C18-C19
33	b	621	LMT	C11-C10-C9-C8
34	C	521	LMG	C13-C14-C15-C16
36	C	517[B]	DGD	C8A-C9A-CAA-CBA
26	L	101	SQD	C34-C35-C36-C37
32	d	407[B]	LHG	C29-C30-C31-C32
33	b	627	LMT	C3-C4-C5-C6
26	f	102	SQD	C25-C26-C27-C28
36	c	517[B]	DGD	CAA-CBA-CCA-CDA
34	m	101	LMG	O9-C10-O7-C8
36	C	517[B]	DGD	C4D-C5D-C6D-O5D
26	A	412	SQD	C27-C28-C29-C30
32	L	102[B]	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
36	c	518[B]	DGD	C2B-C3B-C4B-C5B
23	C	504	CLA	O1D-CGD-O2D-CED
36	c	517[B]	DGD	C2E-C1E-O5D-C6D
36	c	518[B]	DGD	C2E-C1E-O5D-C6D
26	A	410[A]	SQD	O6-C44-C45-O47
26	A	410[B]	SQD	O6-C44-C45-O47
34	C	520	LMG	C31-C32-C33-C34
36	C	517[B]	DGD	C9A-CAA-CBA-CCA
23	B	610	CLA	C16-C17-C18-C20
26	b	620	SQD	C14-C15-C16-C17
36	C	517[A]	DGD	C9A-CAA-CBA-CCA
36	c	518[A]	DGD	C2B-C3B-C4B-C5B
29	A	414[B]	PL9	C45-C44-C46-C47
23	D	403	CLA	C2-C3-C5-C6
23	b	609	CLA	C2-C3-C5-C6
23	c	514	CLA	C2-C3-C5-C6
23	D	403	CLA	C11-C10-C8-C9
23	b	606	CLA	C11-C10-C8-C9
36	C	517[A]	DGD	O6E-C5E-C6E-O5E
26	b	620	SQD	C26-C27-C28-C29
32	b	630[A]	LHG	C13-C14-C15-C16
36	c	518[B]	DGD	C6A-C7A-C8A-C9A
23	b	607	CLA	C3-C5-C6-C7
23	B	601	CLA	C2A-CAA-CBA-CGA
33	B	626	LMT	C1-C2-C3-C4
32	d	412[B]	LHG	C25-C26-C27-C28
34	c	501	LMG	C35-C36-C37-C38
23	A	405[A]	CLA	C1A-C2A-CAA-CBA
23	b	614	CLA	C16-C17-C18-C19
23	c	509	CLA	C16-C17-C18-C20
32	D	407[A]	LHG	C17-C18-C19-C20
35	o	301	HTG	C2'-C3'-C4'-C5'
23	A	406[A]	CLA	C13-C15-C16-C17
33	t	101	LMT	O1'-C1-C2-C3
34	m	101	LMG	C37-C38-C39-C40
23	c	514	CLA	O1D-CGD-O2D-CED
34	c	520	LMG	C4-C5-C6-O5
32	d	406[B]	LHG	C24-C23-O8-C6
36	c	517[B]	DGD	C2A-C1A-O1G-C1G
36	h	102	DGD	CAB-CBB-CCB-CDB
36	C	517[B]	DGD	O6E-C5E-C6E-O5E
23	A	404[A]	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
23	C	511	CLA	C13-C15-C16-C17
23	d	402[A]	CLA	C16-C17-C18-C20
32	d	407[A]	LHG	C25-C26-C27-C28
32	d	412[B]	LHG	C29-C30-C31-C32
36	c	517[B]	DGD	C5A-C6A-C7A-C8A
23	B	605	CLA	O1D-CGD-O2D-CED
23	c	513	CLA	CBA-CGA-O2A-C1
23	d	403	CLA	CBA-CGA-O2A-C1
26	b	620	SQD	C31-C32-C33-C34
34	c	501	LMG	C29-C30-C31-C32
34	C	520	LMG	C36-C37-C38-C39
36	c	518[A]	DGD	C4A-C5A-C6A-C7A
36	c	518[B]	DGD	C4A-C5A-C6A-C7A
26	A	410[A]	SQD	O6-C44-C45-C46
26	A	412	SQD	O6-C44-C45-C46
26	L	101	SQD	C44-C45-C46-O48
26	a	410[A]	SQD	O6-C44-C45-C46
26	a	410[B]	SQD	O6-C44-C45-C46
26	f	102	SQD	O6-C44-C45-C46
26	f	102	SQD	C44-C45-C46-O48
32	D	407[B]	LHG	C29-C30-C31-C32
32	E	101[B]	LHG	C4-C5-C6-O8
34	c	501	LMG	C7-C8-C9-O8
23	B	614	CLA	C5-C6-C7-C8
23	b	601	CLA	C8-C10-C11-C12
32	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[B]	DGD	C2G-C3G-O3G-C1D
36	C	518[B]	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
34	D	411	LMG	C12-C13-C14-C15
35	c	522	HTG	C4'-C5'-C6'-C7'
36	C	518[A]	DGD	CDA-CEA-CFA-CGA
23	C	503	CLA	C13-C15-C16-C17
32	L	102[B]	LHG	C27-C28-C29-C30
33	a	416	LMT	C2-C3-C4-C5
36	C	518[B]	DGD	CDA-CEA-CFA-CGA
36	c	517[A]	DGD	C4D-C5D-C6D-O5D
34	D	411	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
35	b	623	HTG	O5-C5-C6-O6
23	d	403	CLA	O1A-CGA-O2A-C1
36	C	517[A]	DGD	C3B-C4B-C5B-C6B
23	B	615	CLA	C10-C11-C12-C13
29	a	413[B]	PL9	C24-C26-C27-C28
27	A	411	GOL	O1-C1-C2-O2
27	B	627	GOL	O2-C2-C3-O3
27	D	412	GOL	O2-C2-C3-O3
27	o	304	GOL	O2-C2-C3-O3
23	b	610	CLA	C15-C16-C17-C18
33	a	416	LMT	O5'-C5'-C6'-O6'
32	d	412[B]	LHG	C33-C34-C35-C36
23	A	405[A]	CLA	C15-C16-C17-C18
23	B	615	CLA	C5-C6-C7-C8
34	d	410	LMG	O6-C5-C6-O5
36	c	517[A]	DGD	O6E-C5E-C6E-O5E
23	C	511	CLA	C4-C3-C5-C6
23	b	609	CLA	C4-C3-C5-C6
23	c	506	CLA	C4-C3-C5-C6
29	a	413[A]	PL9	C12-C11-C9-C10
29	a	413[B]	PL9	C12-C11-C9-C10
32	d	407[B]	LHG	C28-C29-C30-C31
36	h	102	DGD	CDB-CEB-CFB-CGB
34	c	520	LMG	C28-C29-C30-C31
33	A	420	LMT	C4-C5-C6-C7
34	C	521	LMG	C35-C36-C37-C38
23	B	602	CLA	C15-C16-C17-C18
23	a	405[A]	CLA	C2C-C3C-CAC-CBC
32	d	412[A]	LHG	C33-C34-C35-C36
26	b	620	SQD	C46-C45-O47-C7
33	m	103	LMT	O5'-C5'-C6'-O6'
23	b	608	CLA	C2-C1-O2A-CGA
23	b	614	CLA	C2-C1-O2A-CGA
26	b	620	SQD	C11-C10-C9-C8
32	d	407[A]	LHG	C34-C35-C36-C37
34	z	101	LMG	C14-C15-C16-C17
26	a	410[A]	SQD	C12-C13-C14-C15
32	D	406[A]	LHG	C12-C13-C14-C15
33	a	416	LMT	C9-C10-C11-C12
33	e	101	LMT	C3-C4-C5-C6
26	b	620	SQD	C24-C23-O48-C46
34	c	521	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
36	c	519	DGD	C2A-C1A-O1G-C1G
23	d	402[B]	CLA	C16-C17-C18-C20
36	H	102	DGD	CAB-CBB-CCB-CDB
32	d	406[B]	LHG	O10-C23-O8-C6
23	a	405[B]	CLA	C2C-C3C-CAC-CBC
34	C	501	LMG	C13-C14-C15-C16
35	b	622	HTG	C1'-C2'-C3'-C4'
23	B	601	CLA	C13-C15-C16-C17
23	B	601	CLA	C15-C16-C17-C18
36	C	518[B]	DGD	C2E-C1E-O5D-C6D
34	B	620	LMG	O8-C28-C29-C30
26	a	410[B]	SQD	O6-C44-C45-O47
32	D	406[B]	LHG	C13-C14-C15-C16
36	C	517[A]	DGD	O6D-C5D-C6D-O5D
36	c	517[B]	DGD	O1A-C1A-O1G-C1G
23	d	402[A]	CLA	C16-C17-C18-C19
32	D	407[B]	LHG	C13-C14-C15-C16
32	D	407[B]	LHG	C17-C18-C19-C20
32	d	407[A]	LHG	C29-C30-C31-C32
34	C	520	LMG	C30-C31-C32-C33
32	d	407[B]	LHG	C34-C35-C36-C37
23	A	406[A]	CLA	C12-C13-C15-C16
23	A	406[B]	CLA	C12-C13-C15-C16
23	B	602	CLA	C11-C12-C13-C15
23	B	606	CLA	C11-C10-C8-C7
23	C	503	CLA	C12-C13-C15-C16
23	C	505	CLA	C12-C13-C15-C16
23	C	511	CLA	C2-C3-C5-C6
23	D	403	CLA	C12-C13-C15-C16
23	a	408	CLA	C11-C10-C8-C7
23	b	601	CLA	C11-C10-C8-C7
23	b	606	CLA	C11-C10-C8-C7
23	c	505	CLA	C11-C12-C13-C15
23	c	506	CLA	C2-C3-C5-C6
23	c	507	CLA	C11-C10-C8-C7
23	B	602	CLA	C11-C12-C13-C14
23	B	606	CLA	C11-C10-C8-C9
23	C	505	CLA	C14-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C14
23	C	514	CLA	C11-C10-C8-C9
23	D	403	CLA	C14-C13-C15-C16
23	b	601	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	c	506	CLA	C11-C12-C13-C14
32	d	407[A]	LHG	C28-C29-C30-C31
33	b	621	LMT	C7-C8-C9-C10
34	C	501	LMG	C39-C40-C41-C42
32	D	407[B]	LHG	C24-C23-O8-C6
32	A	419[B]	LHG	C18-C19-C20-C21
23	b	606	CLA	C16-C17-C18-C20
36	c	517[B]	DGD	C7A-C8A-C9A-CAA
27	B	625	GOL	C1-C2-C3-O3
32	b	630[A]	LHG	C27-C28-C29-C30
33	A	420	LMT	C5-C6-C7-C8
23	b	601	CLA	CBA-CGA-O2A-C1
26	a	411	SQD	C16-C17-C18-C19
35	B	623	HTG	C4'-C5'-C6'-C7'
36	C	518[A]	DGD	C5B-C6B-C7B-C8B
23	B	613	CLA	C13-C15-C16-C17
32	E	101[A]	LHG	O6-C4-C5-C6
32	b	630[A]	LHG	O6-C4-C5-C6
23	C	509	CLA	O1D-CGD-O2D-CED
32	D	406[A]	LHG	C10-C11-C12-C13
32	D	407[A]	LHG	C13-C14-C15-C16
32	d	407[A]	LHG	C9-C10-C11-C12
23	B	610	CLA	C13-C15-C16-C17
23	c	513	CLA	C10-C11-C12-C13
33	b	621	LMT	C3-C4-C5-C6
29	d	405[A]	PL9	C45-C44-C46-C47
32	A	419[A]	LHG	C26-C27-C28-C29
32	d	406[A]	LHG	C13-C14-C15-C16
32	d	406[B]	LHG	C11-C10-C9-C8
23	B	608	CLA	C16-C17-C18-C20
33	a	416	LMT	C3-C4-C5-C6
33	e	101	LMT	C9-C10-C11-C12
23	c	512	CLA	CBA-CGA-O2A-C1
34	C	520	LMG	C37-C38-C39-C40
36	C	517[A]	DGD	C7A-C8A-C9A-CAA
36	C	517[B]	DGD	C3B-C4B-C5B-C6B
23	c	513	CLA	O1D-CGD-O2D-CED
32	D	406[B]	LHG	C12-C13-C14-C15
33	B	626	LMT	C2-C1-O1'-C1'
33	e	101	LMT	C2-C1-O1'-C1'
32	d	407[B]	LHG	C9-C10-C11-C12
36	h	102	DGD	C9B-CAB-CBB-CCB

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Mol	Chain	Res	Type	Atoms
32	E	101[B]	LHG	C25-C26-C27-C28
34	Z	101	LMG	C19-C20-C21-C22
36	c	518[A]	DGD	CDA-CEA-CFA-CGA
23	c	510	CLA	C15-C16-C17-C18
26	A	410[B]	SQD	O6-C44-C45-C46
26	a	411	SQD	O6-C44-C45-C46
26	b	620	SQD	C44-C45-C46-O48
32	a	419[A]	LHG	C4-C5-C6-O8
32	a	419[B]	LHG	C4-C5-C6-O8
32	L	102[A]	LHG	C24-C25-C26-C27
32	a	419[A]	LHG	C10-C11-C12-C13
33	t	101	LMT	C7-C8-C9-C10
34	C	520	LMG	C34-C35-C36-C37
36	C	517[B]	DGD	C7A-C8A-C9A-CAA
32	b	630[A]	LHG	C12-C13-C14-C15
24	a	407[A]	PHO	O2A-C1-C2-C3
32	D	407[B]	LHG	C10-C11-C12-C13
23	C	502	CLA	O1D-CGD-O2D-CED
36	c	518[A]	DGD	C5A-C6A-C7A-C8A
36	h	102	DGD	CBA-CCA-CDA-CEA
36	c	519	DGD	O1A-C1A-O1G-C1G
24	a	407[A]	PHO	C4-C3-C5-C6
29	A	414[B]	PL9	C30-C29-C31-C32
29	D	405[A]	PL9	C43-C44-C46-C47
26	F	103	SQD	C34-C35-C36-C37
32	L	102[A]	LHG	C11-C12-C13-C14
32	b	630[B]	LHG	C17-C18-C19-C20
32	d	406[B]	LHG	C4-O6-P-O3
32	a	419[A]	LHG	C7-C8-C9-C10
32	D	407[B]	LHG	O10-C23-O8-C6
35	b	622	HTG	O5-C5-C6-O6
27	a	417	GOL	O1-C1-C2-O2
27	c	527	GOL	O1-C1-C2-O2
27	o	303	GOL	O2-C2-C3-O3
32	E	101[B]	LHG	C17-C18-C19-C20
34	m	101	LMG	C11-C12-C13-C14
32	E	101[A]	LHG	O6-C4-C5-O7
26	A	410[B]	SQD	C12-C13-C14-C15
32	D	406[B]	LHG	C10-C11-C12-C13
33	a	416	LMT	C4'-C5'-C6'-O6'
23	c	513	CLA	O1A-CGA-O2A-C1
26	b	620	SQD	O10-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
34	c	521	LMG	O10-C28-O8-C9
23	A	406[A]	CLA	C16-C17-C18-C20
23	b	606	CLA	C16-C17-C18-C19
23	d	402[B]	CLA	C16-C17-C18-C19
32	b	630[A]	LHG	C31-C32-C33-C34
23	c	512	CLA	O1A-CGA-O2A-C1
26	a	410[A]	SQD	C34-C35-C36-C37
26	a	410[A]	SQD	O6-C44-C45-O47
26	b	620	SQD	O47-C45-C46-O48
26	f	102	SQD	O47-C45-C46-O48
34	c	501	LMG	O7-C8-C9-O8
32	d	407[B]	LHG	C24-C23-O8-C6
23	B	615	CLA	C13-C15-C16-C17
32	b	630[B]	LHG	C13-C14-C15-C16
36	C	518[A]	DGD	C8B-C9B-CAB-CBB
23	C	502	CLA	C16-C17-C18-C20
32	E	101[A]	LHG	C17-C18-C19-C20
29	a	413[A]	PL9	C24-C26-C27-C28
26	b	620	SQD	C28-C29-C30-C31
32	D	407[A]	LHG	C10-C11-C12-C13
32	a	419[B]	LHG	C10-C11-C12-C13
32	b	630[B]	LHG	C25-C26-C27-C28
32	b	630[B]	LHG	C34-C35-C36-C37
36	C	519	DGD	CDB-CEB-CFB-CGB
23	B	610	CLA	C14-C13-C15-C16
23	B	613	CLA	C11-C12-C13-C14
23	a	406[B]	CLA	C6-C7-C8-C9
23	c	511	CLA	C11-C10-C8-C9
23	d	403	CLA	C11-C12-C13-C14
23	C	511	CLA	CBA-CGA-O2A-C1
33	M	101	LMT	C2-C3-C4-C5
33	F	101	LMT	C2-C3-C4-C5
36	C	518[B]	DGD	C5B-C6B-C7B-C8B
32	D	407[B]	LHG	C2-C3-O3-P
32	d	407[B]	LHG	C2-C3-O3-P
34	B	620	LMG	C36-C37-C38-C39
34	C	501	LMG	C11-C12-C13-C14
36	C	518[A]	DGD	C8A-C9A-CAA-CBA
23	C	503	CLA	C16-C17-C18-C19
25	B	617	BCR	C5-C6-C7-C8
25	D	404	BCR	C23-C24-C25-C26
25	H	101	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
25	b	619	BCR	C1-C6-C7-C8
32	d	412[A]	LHG	C25-C26-C27-C28
34	Z	101	LMG	C11-C12-C13-C14
25	D	404	BCR	C21-C22-C23-C24
25	d	404	BCR	C21-C22-C23-C24
23	B	612	CLA	C10-C11-C12-C13
23	b	602	CLA	C10-C11-C12-C13
32	D	406[B]	LHG	C26-C27-C28-C29
34	C	501	LMG	C18-C19-C20-C21
23	B	605	CLA	C5-C6-C7-C8
32	D	406[B]	LHG	O6-C4-C5-C6
32	b	630[B]	LHG	O6-C4-C5-C6
26	F	103	SQD	C32-C33-C34-C35
23	B	610	CLA	C12-C13-C15-C16
23	B	614	CLA	C12-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C15
23	C	507	CLA	C6-C7-C8-C10
23	C	511	CLA	C12-C13-C15-C16
23	C	514	CLA	C11-C10-C8-C7
23	b	601	CLA	C6-C7-C8-C10
23	b	616	CLA	C6-C7-C8-C10
23	c	506	CLA	C11-C12-C13-C15
23	c	510	CLA	C6-C7-C8-C10
23	c	510	CLA	C11-C10-C8-C7
23	c	511	CLA	C11-C10-C8-C7
24	a	407[A]	PHO	C2-C3-C5-C6
29	A	414[B]	PL9	C43-C44-C46-C47
32	E	101[B]	LHG	C13-C14-C15-C16
23	c	510	CLA	C8-C10-C11-C12
23	c	512	CLA	C8-C10-C11-C12
25	t	102	BCR	C13-C14-C15-C16
32	L	102[A]	LHG	C11-C10-C9-C8
32	d	412[A]	LHG	C24-C25-C26-C27
34	d	410	LMG	C10-C11-C12-C13
32	b	630[A]	LHG	C34-C35-C36-C37
36	C	519	DGD	C8A-C9A-CAA-CBA
36	c	518[B]	DGD	C5A-C6A-C7A-C8A
23	C	508	CLA	C13-C15-C16-C17
23	b	601	CLA	C13-C15-C16-C17
36	C	517[A]	DGD	CCA-CDA-CEA-CFA
32	b	630[A]	LHG	C9-C10-C11-C12
32	D	407[B]	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
32	d	406[B]	LHG	C13-C14-C15-C16
34	B	620	LMG	C20-C21-C22-C23
23	c	513	CLA	C13-C15-C16-C17
26	a	410[B]	SQD	C34-C35-C36-C37
36	C	519	DGD	CAA-CBA-CCA-CDA
23	B	610	CLA	CAD-CBD-CGD-O2D
23	B	616	CLA	CAD-CBD-CGD-O2D
23	b	612	CLA	CAD-CBD-CGD-O2D
23	c	513	CLA	CAD-CBD-CGD-O2D
24	A	407[A]	PHO	CAD-CBD-CGD-O2D
24	a	407[A]	PHO	CAD-CBD-CGD-O2D
24	a	407[B]	PHO	CAD-CBD-CGD-O2D
26	L	101	SQD	C46-C45-O47-C7
38	f	101	HEM	C2B-C3B-CAB-CBB
32	E	101[A]	LHG	C13-C14-C15-C16
35	b	625	HTG	C4-C5-C6-O6
26	a	410[A]	SQD	C27-C28-C29-C30
34	C	501	LMG	C20-C21-C22-C23
34	z	101	LMG	C19-C20-C21-C22
23	B	608	CLA	C16-C17-C18-C19
32	D	406[A]	LHG	C34-C35-C36-C37
36	C	518[B]	DGD	O6E-C1E-O5D-C6D
32	E	101[A]	LHG	C4-C5-C6-O8
32	b	630[A]	LHG	O6-C4-C5-O7
32	b	630[B]	LHG	O6-C4-C5-O7
36	C	518[A]	DGD	C7A-C8A-C9A-CAA
23	A	406[B]	CLA	C16-C17-C18-C20
32	A	419[B]	LHG	C1-C2-C3-O3
23	B	601	CLA	CHA-CBD-CGD-O1D
23	B	601	CLA	CHA-CBD-CGD-O2D
23	C	503	CLA	CHA-CBD-CGD-O1D
23	C	503	CLA	CHA-CBD-CGD-O2D
23	c	503	CLA	CHA-CBD-CGD-O1D
23	c	503	CLA	CHA-CBD-CGD-O2D
23	C	511	CLA	O1A-CGA-O2A-C1
23	b	601	CLA	O1A-CGA-O2A-C1
26	F	103	SQD	O47-C45-C46-O48
32	a	419[A]	LHG	O7-C5-C6-O8
23	c	511	CLA	C4-C3-C5-C6
29	D	405[A]	PL9	C45-C44-C46-C47
29	d	405[B]	PL9	C45-C44-C46-C47
32	d	407[B]	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
36	c	518[A]	DGD	C1A-C2A-C3A-C4A
29	a	413[B]	PL9	C4-C3-C7-C8
23	B	614	CLA	C14-C13-C15-C16
36	C	517[A]	DGD	C4D-C5D-C6D-O5D
23	B	601	CLA	O1A-CGA-O2A-C1
23	b	604	CLA	C13-C15-C16-C17
23	B	601	CLA	CAA-CBA-CGA-O2A
23	b	601	CLA	CAA-CBA-CGA-O2A
25	d	404	BCR	C37-C22-C23-C24
23	b	613	CLA	CBD-CGD-O2D-CED
23	a	404[A]	CLA	C2C-C3C-CAC-CBC
34	c	501	LMG	C4-C5-C6-O5
23	B	604	CLA	C1A-C2A-CAA-CBA
23	a	405[A]	CLA	C1A-C2A-CAA-CBA
23	c	512	CLA	C1A-C2A-CAA-CBA
36	C	518[B]	DGD	C1A-C2A-C3A-C4A
23	B	601	CLA	CBA-CGA-O2A-C1
26	F	103	SQD	C24-C23-O48-C46
32	d	407[A]	LHG	C24-C23-O8-C6
32	A	419[A]	LHG	C32-C33-C34-C35
32	D	406[A]	LHG	C4-O6-P-O3
32	D	407[B]	LHG	C4-O6-P-O3
32	d	412[A]	LHG	C3-O3-P-O6
32	a	419[A]	LHG	C23-C24-C25-C26
26	a	410[A]	SQD	C35-C36-C37-C38
34	c	501	LMG	C21-C22-C23-C24
29	D	405[B]	PL9	C45-C44-C46-C47
36	H	102	DGD	O2G-C1B-C2B-C3B
32	D	407[A]	LHG	C2-C3-O3-P
32	d	407[A]	LHG	C2-C3-O3-P
32	D	406[A]	LHG	C4-O6-P-O5
32	E	101[A]	LHG	C4-O6-P-O5
32	E	101[B]	LHG	C4-O6-P-O5
32	L	102[B]	LHG	C4-O6-P-O5
32	a	419[A]	LHG	C4-O6-P-O4
32	a	419[B]	LHG	C4-O6-P-O4
32	d	406[A]	LHG	C3-O3-P-O4
32	d	406[B]	LHG	C4-O6-P-O5
23	c	503	CLA	C16-C17-C18-C19
26	F	103	SQD	C7-C8-C9-C10
34	z	101	LMG	C10-C11-C12-C13
32	L	102[B]	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
36	C	517[B]	DGD	CCA-CDA-CEA-CFA
36	c	517[A]	DGD	O6E-C1E-O5D-C6D
32	L	102[A]	LHG	O6-C4-C5-C6
26	A	410[A]	SQD	C18-C19-C20-C21
36	C	518[B]	DGD	C8B-C9B-CAB-CBB
26	A	412	SQD	C30-C31-C32-C33
33	F	101	LMT	C4-C5-C6-C7
34	C	520	LMG	C11-C12-C13-C14
32	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	605	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	503	CLA	CAD-CBD-CGD-O1D
23	c	505	CLA	CAD-CBD-CGD-O1D
23	c	507	CLA	CAD-CBD-CGD-O1D
33	B	628	LMT	C1-C2-C3-C4
23	c	508	CLA	C5-C6-C7-C8
34	Z	101	LMG	C29-C28-O8-C9
32	a	419[B]	LHG	C23-C24-C25-C26
32	D	407[A]	LHG	C24-C23-O8-C6
33	b	627	LMT	C1-C2-C3-C4
23	D	403	CLA	O1D-CGD-O2D-CED
32	E	101[A]	LHG	C1-C2-C3-O3
23	B	616	CLA	C12-C13-C15-C16
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	511	CLA	C12-C13-C15-C16
23	c	513	CLA	C12-C13-C15-C16
23	d	402[B]	CLA	C11-C12-C13-C15
29	d	405[B]	PL9	C28-C29-C31-C32
23	A	405[B]	CLA	C15-C16-C17-C18
32	d	407[A]	LHG	O10-C23-O8-C6
34	c	501	LMG	C33-C34-C35-C36
33	b	627	LMT	O1'-C1-C2-C3
36	C	518[A]	DGD	C1A-C2A-C3A-C4A
36	C	519	DGD	CBA-CCA-CDA-CEA
32	D	407[A]	LHG	O10-C23-O8-C6
36	c	517[A]	DGD	C8B-C9B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	C	503	CLA	C16-C17-C18-C20
26	A	410[A]	SQD	C34-C35-C36-C37
33	B	628	LMT	C3-C4-C5-C6
26	L	101	SQD	O47-C45-C46-O48
32	E	101[A]	LHG	O7-C5-C6-O8
32	a	419[B]	LHG	O7-C5-C6-O8
34	C	501	LMG	C29-C30-C31-C32
34	C	521	LMG	C38-C39-C40-C41
34	c	520	LMG	C29-C30-C31-C32
26	a	410[A]	SQD	C11-C12-C13-C14
36	c	518[B]	DGD	C2G-C3G-O3G-C1D
33	M	101	LMT	O1'-C1-C2-C3
32	D	406[B]	LHG	C11-C10-C9-C8
23	b	616	CLA	C5-C6-C7-C8
29	d	405[B]	PL9	C15-C14-C16-C17
23	c	507	CLA	C13-C15-C16-C17
23	A	406[A]	CLA	C14-C13-C15-C16
23	B	610	CLA	C11-C12-C13-C14
23	C	507	CLA	C6-C7-C8-C9
23	C	511	CLA	C11-C12-C13-C14
23	C	511	CLA	C14-C13-C15-C16
23	a	408	CLA	C11-C10-C8-C9
23	b	610	CLA	C11-C12-C13-C14
23	c	510	CLA	C6-C7-C8-C9
23	c	513	CLA	C6-C7-C8-C9
23	B	607	CLA	C3-C5-C6-C7
34	B	620	LMG	C37-C38-C39-C40
24	a	407[A]	PHO	C8-C10-C11-C12
23	B	611	CLA	C8-C10-C11-C12
26	F	103	SQD	O10-C23-O48-C46
23	C	513	CLA	C3-C5-C6-C7
26	a	410[B]	SQD	C35-C36-C37-C38
32	d	406[B]	LHG	C16-C17-C18-C19
34	C	521	LMG	C12-C13-C14-C15
23	c	511	CLA	C2-C3-C5-C6
29	a	413[A]	PL9	C12-C11-C9-C8
29	a	413[B]	PL9	C43-C44-C46-C47
32	d	412[A]	LHG	C34-C35-C36-C37
23	B	613	CLA	C15-C16-C17-C18
32	d	407[A]	LHG	C32-C33-C34-C35
34	m	101	LMG	C14-C15-C16-C17
32	a	419[B]	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
23	C	502	CLA	C2A-CAA-CBA-CGA
23	A	408	CLA	C2-C1-O2A-CGA
23	B	613	CLA	C2-C1-O2A-CGA
23	C	507	CLA	C2-C1-O2A-CGA
23	C	514	CLA	C2-C1-O2A-CGA
23	a	404[B]	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
33	b	627	LMT	C6-C7-C8-C9
34	z	101	LMG	C13-C14-C15-C16
36	c	518[B]	DGD	C7B-C8B-C9B-CAB
32	d	406[A]	LHG	O10-C23-O8-C6
32	D	406[B]	LHG	O6-C4-C5-O7
32	L	102[A]	LHG	O6-C4-C5-O7
34	d	410	LMG	C16-C17-C18-C19
25	B	617	BCR	C1-C6-C7-C8
25	H	101	BCR	C23-C24-C25-C26
25	d	404	BCR	C23-C24-C25-C30
29	A	414[A]	PL9	C28-C29-C31-C32
29	a	413[B]	PL9	C12-C11-C9-C8
33	D	401	LMT	O5B-C5B-C6B-O6B
32	d	406[A]	LHG	C24-C23-O8-C6
23	a	405[A]	CLA	C4C-C3C-CAC-CBC
33	B	629	LMT	C1-C2-C3-C4
36	H	102	DGD	CCA-CDA-CEA-CFA
36	c	518[A]	DGD	O6E-C1E-O5D-C6D
34	m	101	LMG	C32-C33-C34-C35
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
32	L	102[A]	LHG	C26-C27-C28-C29
36	c	519	DGD	CDA-CEA-CFA-CGA
32	E	101[B]	LHG	O7-C5-C6-O8
23	C	507	CLA	C15-C16-C17-C18
32	D	406[B]	LHG	C34-C35-C36-C37
32	d	412[B]	LHG	C3-O3-P-O6
32	d	407[B]	LHG	C33-C34-C35-C36
32	L	102[A]	LHG	C27-C28-C29-C30
32	D	406[B]	LHG	C28-C29-C30-C31
23	C	514	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
23	b	614	CLA	C12-C13-C15-C16
23	c	503	CLA	C11-C12-C13-C15
33	T	101	LMT	C9-C10-C11-C12
34	c	501	LMG	C31-C32-C33-C34
23	A	406[B]	CLA	C14-C13-C15-C16
23	B	614	CLA	C11-C10-C8-C9
23	b	615	CLA	C14-C13-C15-C16
23	c	507	CLA	C11-C10-C8-C9
34	d	410	LMG	C35-C36-C37-C38
36	c	519	DGD	O6D-C5D-C6D-O5D
26	A	410[B]	SQD	C11-C10-C9-C8
33	B	629	LMT	C6-C7-C8-C9
23	b	615	CLA	C10-C11-C12-C13
23	c	507	CLA	C10-C11-C12-C13
23	a	404[A]	CLA	C4C-C3C-CAC-CBC
26	A	410[B]	SQD	C16-C17-C18-C19
32	L	102[B]	LHG	C26-C27-C28-C29
32	a	419[B]	LHG	C24-C25-C26-C27
36	C	518[B]	DGD	C7A-C8A-C9A-CAA
26	a	410[B]	SQD	C11-C12-C13-C14
32	D	407[A]	LHG	C27-C28-C29-C30
36	C	518[B]	DGD	C3B-C4B-C5B-C6B
25	D	404	BCR	C37-C22-C23-C24
25	T	102	BCR	C11-C12-C13-C35
23	c	503	CLA	C16-C17-C18-C20
36	h	102	DGD	C3B-C4B-C5B-C6B
23	b	612	CLA	C10-C11-C12-C13
33	B	626	LMT	C9-C10-C11-C12
36	c	517[A]	DGD	C4B-C5B-C6B-C7B
32	A	419[B]	LHG	C17-C18-C19-C20
32	d	412[A]	LHG	C1-C2-C3-O3
27	l	102[B]	GOL	O1-C1-C2-O2
23	b	616	CLA	CBA-CGA-O2A-C1
32	d	407[A]	LHG	C33-C34-C35-C36
23	b	616	CLA	O1A-CGA-O2A-C1
23	B	606	CLA	C16-C17-C18-C19
36	C	517[B]	DGD	O6E-C1E-O5D-C6D
36	c	517[B]	DGD	CCB-CDB-CEB-CFB
23	c	510	CLA	C10-C11-C12-C13
34	d	410	LMG	C11-C12-C13-C14
26	L	101	SQD	C29-C30-C31-C32
23	b	601	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	A	414[B]	PL9	C25-C24-C26-C27
33	e	101	LMT	C2-C3-C4-C5
36	C	519	DGD	CDA-CEA-CFA-CGA
23	C	506	CLA	C2-C3-C5-C6
26	A	410[A]	SQD	C11-C10-C9-C8
23	C	509	CLA	C5-C6-C7-C8
23	b	612	CLA	C8-C10-C11-C12
32	b	630[A]	LHG	C25-C26-C27-C28
34	c	501	LMG	O8-C28-C29-C30
23	C	502	CLA	C16-C17-C18-C19
32	D	406[A]	LHG	C11-C10-C9-C8
33	F	101	LMT	C6-C7-C8-C9
32	A	419[B]	LHG	C26-C27-C28-C29
23	C	508	CLA	C2A-CAA-CBA-CGA
26	a	410[B]	SQD	C27-C28-C29-C30
32	a	419[A]	LHG	C24-C25-C26-C27
23	c	507	CLA	C3A-C2A-CAA-CBA
38	F	102	HEM	CAD-CBD-CGD-O1D
23	C	507	CLA	C16-C17-C18-C20
34	C	520	LMG	C29-C30-C31-C32
23	a	405[B]	CLA	C4C-C3C-CAC-CBC
29	A	414[B]	PL9	C4-C3-C7-C8
29	a	413[A]	PL9	C4-C3-C7-C8
23	B	611	CLA	C11-C12-C13-C14
23	B	615	CLA	C14-C13-C15-C16
23	a	406[A]	CLA	C6-C7-C8-C9
23	d	402[B]	CLA	C11-C12-C13-C14
34	d	410	LMG	C18-C19-C20-C21
36	C	517[B]	DGD	CDB-CEB-CFB-CGB
36	c	518[A]	DGD	C7B-C8B-C9B-CAB
23	b	608	CLA	C13-C15-C16-C17
36	H	102	DGD	O1G-C1G-C2G-C3G
32	L	102[A]	LHG	C23-C24-C25-C26
32	d	412[B]	LHG	C34-C35-C36-C37
24	A	407[B]	PHO	O2A-C1-C2-C3
34	C	521	LMG	C4-C5-C6-O5
33	a	416	LMT	O5'-C1'-O1'-C1
36	h	102	DGD	C6A-C7A-C8A-C9A
32	d	407[B]	LHG	C32-C33-C34-C35
23	a	405[A]	CLA	C15-C16-C17-C18
26	a	410[B]	SQD	C10-C11-C12-C13
26	A	410[A]	SQD	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
23	b	616	CLA	C4-C3-C5-C6
29	a	413[B]	PL9	C45-C44-C46-C47
23	C	502	CLA	C1A-C2A-CAA-CBA
23	B	615	CLA	C12-C13-C15-C16
23	C	506	CLA	C12-C13-C15-C16
23	C	507	CLA	C12-C13-C15-C16
23	a	406[B]	CLA	C6-C7-C8-C10
23	b	608	CLA	C12-C13-C15-C16
23	c	514	CLA	C12-C13-C15-C16
23	A	404[A]	CLA	C2C-C3C-CAC-CBC
35	b	625	HTG	C1'-C2'-C3'-C4'
32	A	419[A]	LHG	C18-C19-C20-C21
32	b	630[A]	LHG	C17-C18-C19-C20
32	L	102[B]	LHG	C11-C10-C9-C8
26	a	411	SQD	C26-C27-C28-C29
23	b	605	CLA	C3-C5-C6-C7
23	a	405[B]	CLA	C15-C16-C17-C18
36	C	519	DGD	C2A-C1A-O1G-C1G
32	D	406[A]	LHG	C26-C27-C28-C29
38	F	102	HEM	CAD-CBD-CGD-O2D
40	V	201	HEC	CAD-CBD-CGD-O1D
40	V	201	HEC	CAD-CBD-CGD-O2D
26	A	412	SQD	C31-C32-C33-C34
32	d	406[A]	LHG	C16-C17-C18-C19
34	D	411	LMG	C34-C35-C36-C37
23	b	601	CLA	C2-C3-C5-C6
29	d	405[A]	PL9	C43-C44-C46-C47
34	d	410	LMG	C19-C20-C21-C22
36	C	519	DGD	O1A-C1A-O1G-C1G
23	c	512	CLA	C3-C5-C6-C7
32	L	102[B]	LHG	C11-C12-C13-C14
36	H	102	DGD	O1G-C1G-C2G-O2G
36	C	518[B]	DGD	C8A-C9A-CAA-CBA
23	A	406[A]	CLA	C16-C17-C18-C19
36	c	517[B]	DGD	C8B-C9B-CAB-CBB
23	C	511	CLA	C15-C16-C17-C18
34	D	411	LMG	C18-C19-C20-C21
23	D	403	CLA	O1A-CGA-O2A-C1
23	b	613	CLA	O1D-CGD-O2D-CED
29	A	414[A]	PL9	C39-C41-C42-C43
29	A	414[B]	PL9	C39-C41-C42-C43
29	D	405[B]	PL9	C35-C34-C36-C37

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Mol	Chain	Res	Type	Atoms
29	a	413[A]	PL9	C45-C44-C46-C47
32	d	412[B]	LHG	C17-C18-C19-C20
23	A	404[B]	CLA	C2-C1-O2A-CGA
23	D	403	CLA	C8-C10-C11-C12
23	C	513	CLA	C6-C7-C8-C9
23	a	406[B]	CLA	C14-C13-C15-C16
23	c	503	CLA	C11-C12-C13-C14
34	d	410	LMG	C38-C39-C40-C41
36	C	519	DGD	C7A-C8A-C9A-CAA
23	b	601	CLA	C3-C5-C6-C7
36	h	102	DGD	O2G-C1B-C2B-C3B
32	A	419[A]	LHG	C29-C30-C31-C32
36	c	517[A]	DGD	CAB-CBB-CCB-CDB
23	B	612	CLA	O1A-CGA-O2A-C1
25	c	515	BCR	C23-C24-C25-C30
25	d	404	BCR	C23-C24-C25-C26
25	h	101	BCR	C23-C24-C25-C30
25	y	101	BCR	C23-C24-C25-C30
23	a	408	CLA	C15-C16-C17-C18
23	b	615	CLA	C5-C6-C7-C8
36	C	517[B]	DGD	C6A-C7A-C8A-C9A
27	l	102[A]	GOL	O1-C1-C2-C3
27	v	202[A]	GOL	O1-C1-C2-C3
32	d	412[B]	LHG	C13-C14-C15-C16
29	D	405[A]	PL9	C35-C34-C36-C37
36	c	519	DGD	O6E-C5E-C6E-O5E
23	c	504	CLA	C8-C10-C11-C12
29	D	405[B]	PL9	C43-C44-C46-C47
29	a	413[A]	PL9	C43-C44-C46-C47
29	d	405[B]	PL9	C43-C44-C46-C47
34	B	620	LMG	O10-C28-C29-C30
32	D	406[B]	LHG	C32-C33-C34-C35
33	e	101	LMT	C2B-C1B-O1B-C4'
36	c	517[B]	DGD	C5D-C6D-O5D-C1E
36	c	518[B]	DGD	CDA-CEA-CFA-CGA
26	a	410[B]	SQD	C18-C19-C20-C21
23	C	511	CLA	C8-C10-C11-C12
34	z	101	LMG	O7-C10-C11-C12
23	A	404[A]	CLA	C16-C17-C18-C19
32	E	101[B]	LHG	O6-C4-C5-O7
26	f	102	SQD	C23-C24-C25-C26
32	A	419[A]	LHG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
23	C	510	CLA	CBD-CGD-O2D-CED
23	A	408	CLA	C16-C17-C18-C19
32	b	630[A]	LHG	C10-C11-C12-C13
23	C	506	CLA	C4-C3-C5-C6
23	c	505	CLA	C4-C3-C5-C6
23	B	613	CLA	C11-C12-C13-C15
23	a	406[A]	CLA	C6-C7-C8-C10
23	b	615	CLA	C11-C12-C13-C15
23	b	616	CLA	C2-C3-C5-C6
32	L	102[A]	LHG	C16-C17-C18-C19
32	b	630[B]	LHG	C28-C29-C30-C31
33	B	628	LMT	C7-C8-C9-C10
35	b	623	HTG	S1-C1'-C2'-C3'
34	m	101	LMG	C2-C1-O1-C7
36	C	517[B]	DGD	C2E-C1E-O5D-C6D
23	a	404[B]	CLA	C2C-C3C-CAC-CBC
32	E	101[B]	LHG	C1-C2-C3-O3
34	c	521	LMG	O1-C7-C8-O7
34	C	521	LMG	C20-C21-C22-C23
33	t	101	LMT	C2-C3-C4-C5
36	c	517[B]	DGD	CBA-CCA-CDA-CEA
36	c	517[B]	DGD	CAB-CBB-CCB-CDB
23	b	604	CLA	C10-C11-C12-C13
23	D	403	CLA	C15-C16-C17-C18
23	B	606	CLA	C16-C17-C18-C20
23	C	513	CLA	CAA-CBA-CGA-O2A
32	A	419[A]	LHG	O8-C23-C24-C25
23	c	508	CLA	C8-C10-C11-C12
34	z	101	LMG	C20-C21-C22-C23
29	D	405[B]	PL9	C18-C19-C21-C22
35	B	621	HTG	C4'-C5'-C6'-C7'
36	c	518[A]	DGD	C9B-CAB-CBB-CCB
32	A	419[B]	LHG	C11-C12-C13-C14
23	A	408	CLA	C11-C12-C13-C14
23	A	408	CLA	C14-C13-C15-C16
23	B	616	CLA	C14-C13-C15-C16
23	C	514	CLA	C6-C7-C8-C9
23	a	406[A]	CLA	C14-C13-C15-C16
23	c	506	CLA	C14-C13-C15-C16
23	c	507	CLA	C6-C7-C8-C9
34	c	521	LMG	C28-C29-C30-C31
34	c	521	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
36	c	519	DGD	C7B-C8B-C9B-CAB
34	c	521	LMG	C31-C32-C33-C34
23	B	603	CLA	CAD-CBD-CGD-O2D
23	B	604	CLA	CAD-CBD-CGD-O2D
23	B	612	CLA	CAD-CBD-CGD-O2D
23	C	513	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
23	c	511	CLA	CAD-CBD-CGD-O2D
24	A	407[B]	PHO	CAD-CBD-CGD-O2D
24	a	415[A]	PHO	CAD-CBD-CGD-O2D
32	D	407[A]	LHG	C28-C29-C30-C31
23	c	502	CLA	C2A-CAA-CBA-CGA
32	b	630[A]	LHG	C30-C31-C32-C33
23	B	612	CLA	C8-C10-C11-C12
23	B	608	CLA	C2-C1-O2A-CGA
23	a	404[B]	CLA	C4C-C3C-CAC-CBC
32	L	102[A]	LHG	O7-C7-C8-C9
32	a	419[A]	LHG	O8-C23-C24-C25
34	c	520	LMG	O7-C10-C11-C12
23	b	605	CLA	C13-C15-C16-C17
23	C	507	CLA	C4-C3-C5-C6
29	A	414[A]	PL9	C25-C24-C26-C27
32	b	630[B]	LHG	C31-C32-C33-C34
25	T	102	BCR	C11-C12-C13-C14
25	b	619	BCR	C21-C22-C23-C24
25	y	101	BCR	C21-C22-C23-C24
32	A	419[B]	LHG	C32-C33-C34-C35
34	c	520	LMG	C30-C31-C32-C33
34	C	521	LMG	C10-C11-C12-C13
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
24	a	407[A]	PHO	C2C-C3C-CAC-CBC
24	a	415[A]	PHO	C2C-C3C-CAC-CBC
24	a	415[B]	PHO	C2C-C3C-CAC-CBC
26	F	103	SQD	C44-C45-C46-O48
34	B	620	LMG	O1-C7-C8-C9
32	b	630[A]	LHG	O7-C7-C8-C9
32	b	630[B]	LHG	O7-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
34	Z	101	LMG	O7-C10-C11-C12
35	B	623	HTG	C4-C5-C6-O6
36	c	517[B]	DGD	C7B-C8B-C9B-CAB
36	c	518[B]	DGD	C1A-C2A-C3A-C4A
23	A	404[A]	CLA	C15-C16-C17-C18
23	B	606	CLA	C8-C10-C11-C12
23	B	602	CLA	O2A-C1-C2-C3
24	A	407[A]	PHO	O2A-C1-C2-C3
24	a	407[B]	PHO	O2A-C1-C2-C3
23	A	404[A]	CLA	C4C-C3C-CAC-CBC
36	C	519	DGD	C6A-C7A-C8A-C9A
38	f	101	HEM	C4B-C3B-CAB-CBB
23	B	612	CLA	CBA-CGA-O2A-C1
23	A	404[B]	CLA	C2A-CAA-CBA-CGA
40	v	201	HEC	CAD-CBD-CGD-O2D
23	A	404[B]	CLA	C16-C17-C18-C19
32	L	102[B]	LHG	C23-C24-C25-C26
32	A	419[B]	LHG	O2-C2-C3-O3
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-O2D
23	B	607	CLA	CHA-CBD-CGD-O1D
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	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-O2D
23	b	612	CLA	CHA-CBD-CGD-O2D
23	c	504	CLA	CHA-CBD-CGD-O2D
23	c	505	CLA	CHA-CBD-CGD-O1D
23	c	508	CLA	CHA-CBD-CGD-O1D
23	c	508	CLA	CHA-CBD-CGD-O2D
23	c	510	CLA	CHA-CBD-CGD-O1D
38	f	101	HEM	CAD-CBD-CGD-O1D
40	v	201	HEC	CAD-CBD-CGD-O1D
32	L	102[B]	LHG	O7-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
26	f	102	SQD	C26-C27-C28-C29
23	c	513	CLA	CAA-CBA-CGA-O2A
32	E	101[B]	LHG	O7-C7-C8-C9
32	A	419[A]	LHG	C17-C18-C19-C20
32	d	412[A]	LHG	C13-C14-C15-C16
32	d	406[B]	LHG	O7-C5-C6-O8
36	C	518[A]	DGD	CAB-CBB-CCB-CDB
23	C	504	CLA	C8-C10-C11-C12
24	A	407[A]	PHO	CHA-CBD-CGD-O1D
27	O	303	GOL	O1-C1-C2-O2
27	d	411	GOL	O1-C1-C2-O2
26	A	410[B]	SQD	C34-C35-C36-C37
34	c	501	LMG	C13-C14-C15-C16
33	D	401	LMT	C2B-C1B-O1B-C4'
26	b	620	SQD	C10-C11-C12-C13
23	C	511	CLA	CAA-CBA-CGA-O2A
38	f	101	HEM	CAD-CBD-CGD-O2D
35	B	623	HTG	C2'-C3'-C4'-C5'
36	h	102	DGD	CDA-CEA-CFA-CGA
23	a	405[A]	CLA	C11-C12-C13-C15
29	A	414[A]	PL9	C4-C3-C7-C8
23	b	613	CLA	CAA-CBA-CGA-O2A
23	c	511	CLA	CAA-CBA-CGA-O2A
23	C	506	CLA	C14-C13-C15-C16
23	C	513	CLA	C11-C10-C8-C9
23	b	606	CLA	C14-C13-C15-C16
23	b	614	CLA	C11-C12-C13-C14
23	c	514	CLA	C14-C13-C15-C16
26	A	412	SQD	C24-C23-O48-C46
23	B	613	CLA	CAA-CBA-CGA-O2A
34	D	411	LMG	O7-C10-C11-C12
32	d	412[A]	LHG	C18-C19-C20-C21
23	B	614	CLA	C2A-CAA-CBA-CGA
29	D	405[B]	PL9	C11-C12-C13-C14
29	d	405[B]	PL9	C11-C12-C13-C14
32	b	630[A]	LHG	C24-C25-C26-C27
23	B	612	CLA	CAA-CBA-CGA-O2A
32	a	419[B]	LHG	O8-C23-C24-C25
26	L	101	SQD	C24-C25-C26-C27
23	b	604	CLA	C4-C3-C5-C6
34	c	521	LMG	C39-C40-C41-C42
27	A	418	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
27	A	418	GOL	C1-C2-C3-O3
27	a	418	GOL	C1-C2-C3-O3
27	d	411	GOL	C1-C2-C3-O3
27	l	102[A]	GOL	C1-C2-C3-O3
27	l	102[B]	GOL	C1-C2-C3-O3
35	B	621	HTG	C1'-C2'-C3'-C4'
23	c	511	CLA	O1A-CGA-O2A-C1
29	D	405[A]	PL9	C28-C29-C31-C32
33	D	401	LMT	C1-C2-C3-C4
23	C	513	CLA	CAA-CBA-CGA-O1A
23	D	403	CLA	CBA-CGA-O2A-C1
23	B	606	CLA	C15-C16-C17-C18
32	D	407[B]	LHG	C28-C29-C30-C31
32	A	419[A]	LHG	O10-C23-C24-C25
33	e	101	LMT	C4B-C5B-C6B-O6B
34	Z	101	LMG	O10-C28-O8-C9
32	a	419[A]	LHG	O10-C23-C24-C25
32	b	630[A]	LHG	O9-C7-C8-C9
36	c	517[A]	DGD	O2G-C1B-C2B-C3B
23	b	602	CLA	C2A-CAA-CBA-CGA
23	b	603	CLA	C2A-CAA-CBA-CGA
24	a	407[B]	PHO	C8-C10-C11-C12
32	A	419[B]	LHG	C30-C31-C32-C33
36	H	102	DGD	C6A-C7A-C8A-C9A
32	E	101[A]	LHG	O7-C7-C8-C9
34	c	501	LMG	O9-C10-O7-C8
23	c	513	CLA	CAA-CBA-CGA-O1A
34	c	520	LMG	O9-C10-C11-C12
29	A	414[B]	PL9	C23-C24-C26-C27
26	a	411	SQD	O10-C23-O48-C46
33	a	416	LMT	C2'-C1'-O1'-C1
23	b	603	CLA	C5-C6-C7-C8
23	b	611	CLA	C13-C15-C16-C17
33	e	101	LMT	O1'-C1-C2-C3
32	D	406[B]	LHG	C3-O3-P-O5
32	D	407[B]	LHG	C4-O6-P-O5
32	d	406[A]	LHG	C4-O6-P-O5
32	d	412[B]	LHG	C3-O3-P-O5
33	m	103	LMT	C9-C10-C11-C12
23	B	613	CLA	CAA-CBA-CGA-O1A
32	E	101[B]	LHG	O9-C7-C8-C9
32	a	419[B]	LHG	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
36	c	517[B]	DGD	O2G-C1B-C2B-C3B
34	B	620	LMG	O6-C1-O1-C7
38	f	101	HEM	CAA-CBA-CGA-O2A
23	c	514	CLA	C3-C5-C6-C7
25	h	101	BCR	C23-C24-C25-C26
25	t	102	BCR	C1-C6-C7-C8
25	t	102	BCR	C5-C6-C7-C8
25	y	101	BCR	C23-C24-C25-C26
32	L	102[A]	LHG	O9-C7-C8-C9
32	L	102[B]	LHG	O9-C7-C8-C9
32	b	630[B]	LHG	O9-C7-C8-C9
34	Z	101	LMG	O9-C10-C11-C12
36	c	517[A]	DGD	C1A-C2A-C3A-C4A
38	F	102	HEM	CAA-CBA-CGA-O2A
36	C	518[B]	DGD	O2G-C1B-C2B-C3B
23	A	404[B]	CLA	C15-C16-C17-C18
34	c	520	LMG	C14-C15-C16-C17
23	b	613	CLA	CAA-CBA-CGA-O1A
23	c	511	CLA	CAA-CBA-CGA-O1A
29	d	405[B]	PL9	C35-C34-C36-C37
29	d	405[A]	PL9	C11-C12-C13-C14
23	B	607	CLA	CAD-CBD-CGD-O1D
23	C	507	CLA	CAD-CBD-CGD-O1D
23	a	405[B]	CLA	CAD-CBD-CGD-O1D
23	b	601	CLA	CAD-CBD-CGD-O1D
23	b	605	CLA	CAD-CBD-CGD-O1D
23	b	607	CLA	CAD-CBD-CGD-O1D
23	b	609	CLA	CAD-CBD-CGD-O1D
26	f	102	SQD	O5-C5-C6-S
26	a	410[A]	SQD	C10-C11-C12-C13
32	b	630[B]	LHG	C10-C11-C12-C13
34	c	520	LMG	C32-C33-C34-C35
23	B	607	CLA	C14-C13-C15-C16
23	a	405[A]	CLA	C11-C12-C13-C14
23	b	601	CLA	C11-C12-C13-C14
23	b	603	CLA	C11-C10-C8-C9
23	b	608	CLA	C14-C13-C15-C16
23	c	511	CLA	CBD-CGD-O2D-CED
23	b	613	CLA	C5-C6-C7-C8
26	A	412	SQD	O10-C23-O48-C46
23	C	506	CLA	CAA-CBA-CGA-O2A
26	a	411	SQD	O48-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
32	A	419[B]	LHG	O8-C23-C24-C25
32	D	407[A]	LHG	O8-C23-C24-C25
23	c	505	CLA	O1A-CGA-O2A-C1
32	b	630[B]	LHG	C9-C10-C11-C12
23	B	603	CLA	C2A-CAA-CBA-CGA
32	D	407[B]	LHG	O8-C23-C24-C25
36	C	519	DGD	O1G-C1A-C2A-C3A
23	C	509	CLA	C13-C15-C16-C17
36	c	518[B]	DGD	C9B-CAB-CBB-CCB
26	a	410[A]	SQD	C19-C20-C21-C22
32	A	419[B]	LHG	C25-C26-C27-C28
29	A	414[B]	PL9	C12-C11-C9-C10
29	D	405[A]	PL9	C40-C39-C41-C42
29	a	413[B]	PL9	C35-C34-C36-C37
29	d	405[B]	PL9	C30-C29-C31-C32
23	A	405[B]	CLA	C13-C15-C16-C17
36	c	517[A]	DGD	CBA-CCA-CDA-CEA
23	A	406[B]	CLA	C11-C10-C8-C7
23	B	602	CLA	C6-C7-C8-C10
23	B	613	CLA	C12-C13-C15-C16
23	C	513	CLA	C11-C10-C8-C7
23	b	601	CLA	C11-C12-C13-C15
23	b	614	CLA	C11-C10-C8-C7
38	f	101	HEM	CAA-CBA-CGA-O1A
36	C	519	DGD	C8B-C9B-CAB-CBB
32	E	101[A]	LHG	O8-C23-C24-C25
32	E	101[B]	LHG	O8-C23-C24-C25
32	d	407[B]	LHG	O8-C23-C24-C25
34	c	521	LMG	O7-C10-C11-C12
36	C	518[A]	DGD	O2G-C1B-C2B-C3B
26	a	411	SQD	C15-C16-C17-C18
32	D	406[A]	LHG	C28-C29-C30-C31
35	B	621	HTG	C2'-C3'-C4'-C5'
32	D	407[A]	LHG	O10-C23-C24-C25
32	d	407[B]	LHG	O10-C23-C24-C25
36	c	517[A]	DGD	O1B-C1B-C2B-C3B
38	F	102	HEM	CAA-CBA-CGA-O1A
36	C	518[A]	DGD	C3A-C4A-C5A-C6A
33	m	103	LMT	C2-C1-O1'-C1'
34	B	620	LMG	O7-C10-C11-C12
33	M	101	LMT	O5'-C1'-O1'-C1
34	D	411	LMG	O9-C10-C11-C12

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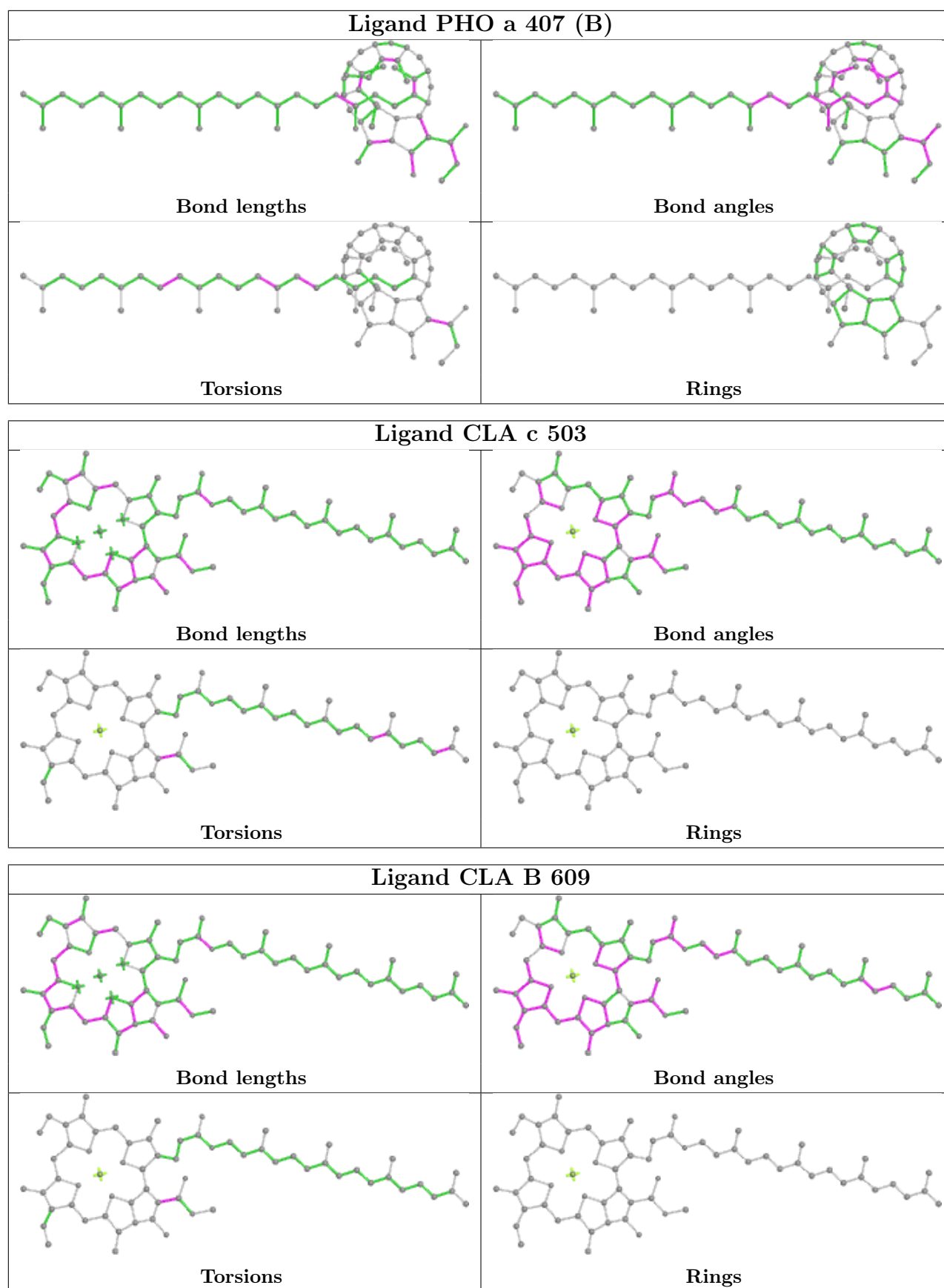
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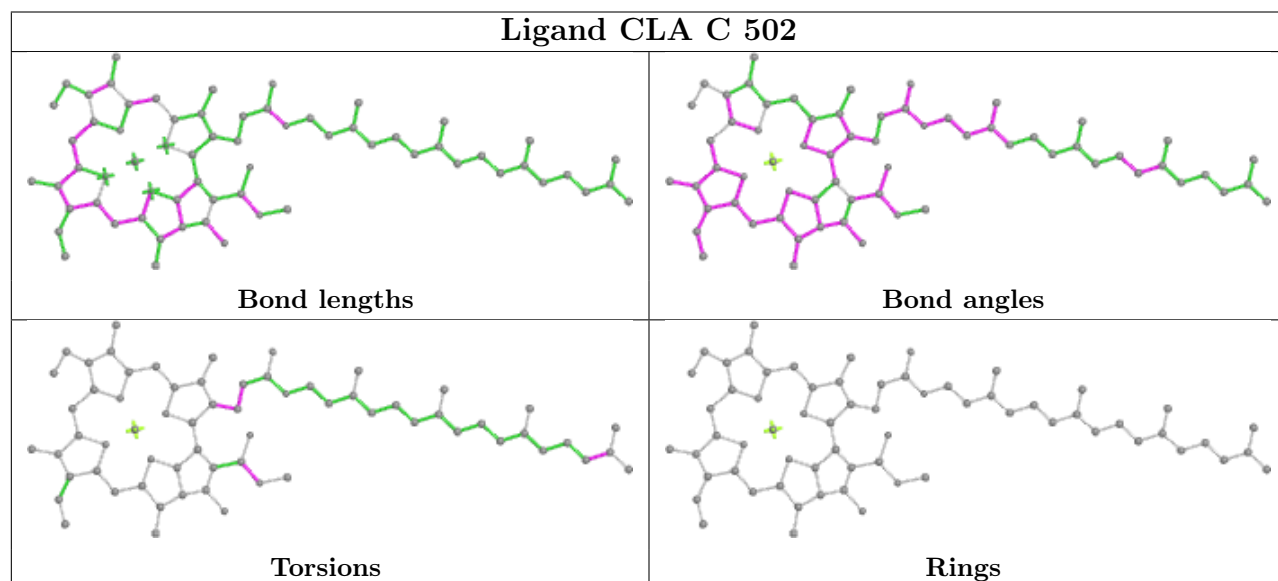
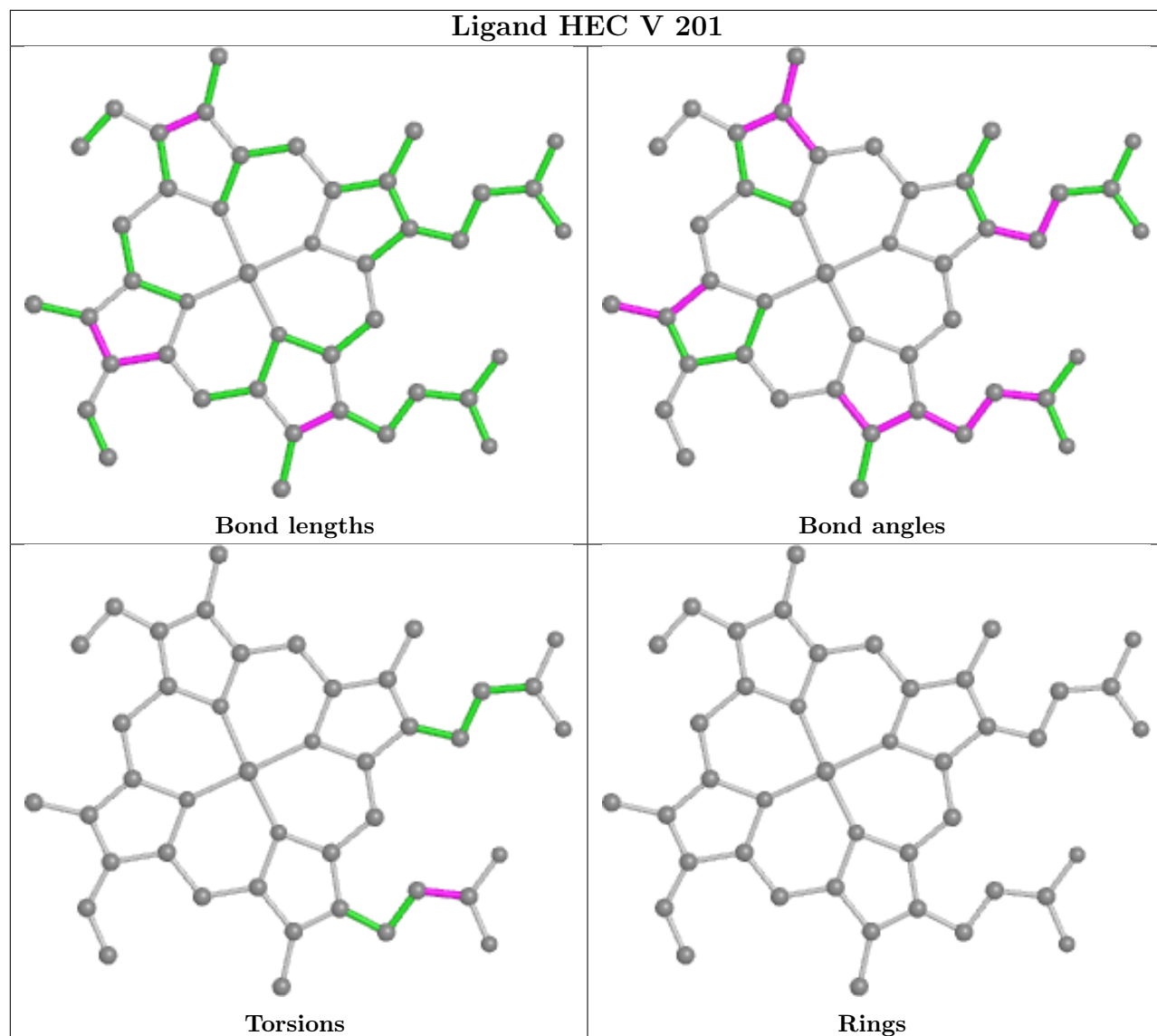
Mol	Chain	Res	Type	Atoms
26	a	411	SQD	C24-C23-O48-C46
23	b	610	CLA	C5-C6-C7-C8
23	B	612	CLA	CAA-CBA-CGA-O1A
23	C	511	CLA	CAA-CBA-CGA-O1A
32	E	101[A]	LHG	O9-C7-C8-C9
32	E	101[A]	LHG	O10-C23-C24-C25
34	c	521	LMG	O9-C10-C11-C12
23	C	504	CLA	C2A-CAA-CBA-CGA
23	c	504	CLA	C2A-CAA-CBA-CGA
23	B	605	CLA	C8-C10-C11-C12
23	b	605	CLA	C5-C6-C7-C8
26	a	411	SQD	O10-C23-C24-C25
32	E	101[B]	LHG	O10-C23-C24-C25
36	C	518[A]	DGD	O1B-C1B-C2B-C3B
26	b	620	SQD	C16-C17-C18-C19
32	b	630[B]	LHG	C11-C12-C13-C14
36	C	519	DGD	C9A-CAA-CBA-CCA
26	A	412	SQD	O48-C23-C24-C25

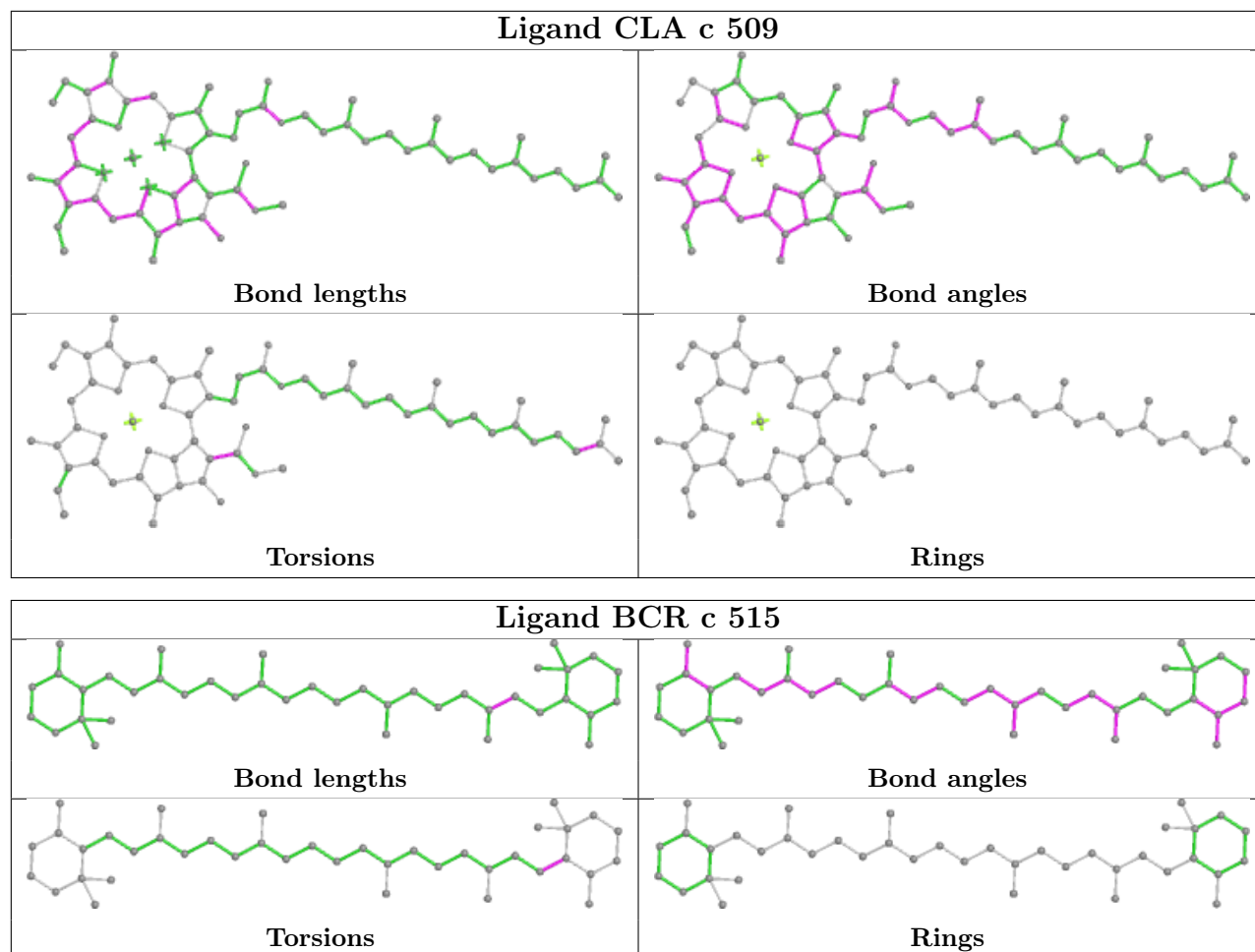
There are no ring outliers.

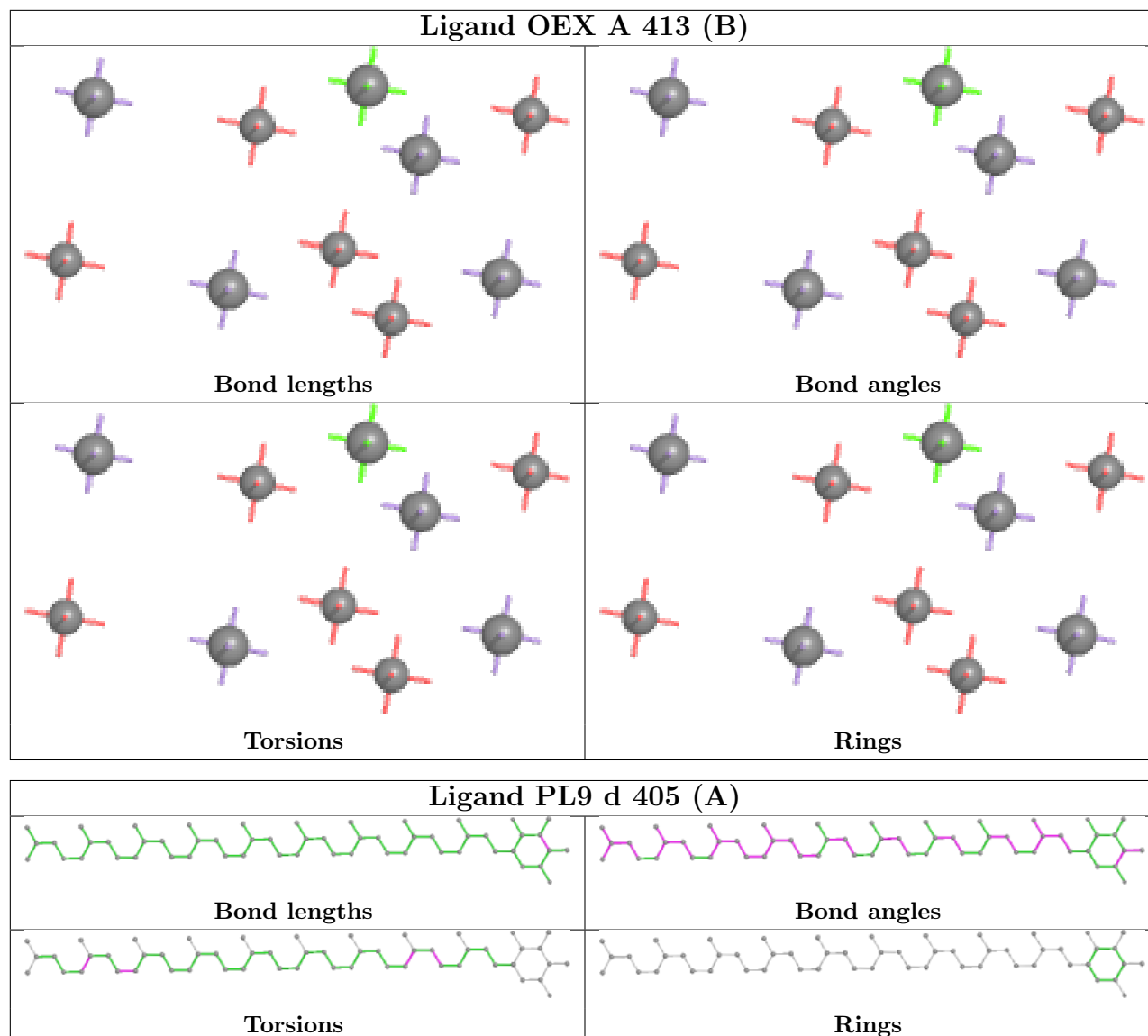
No monomer is involved in short contacts.

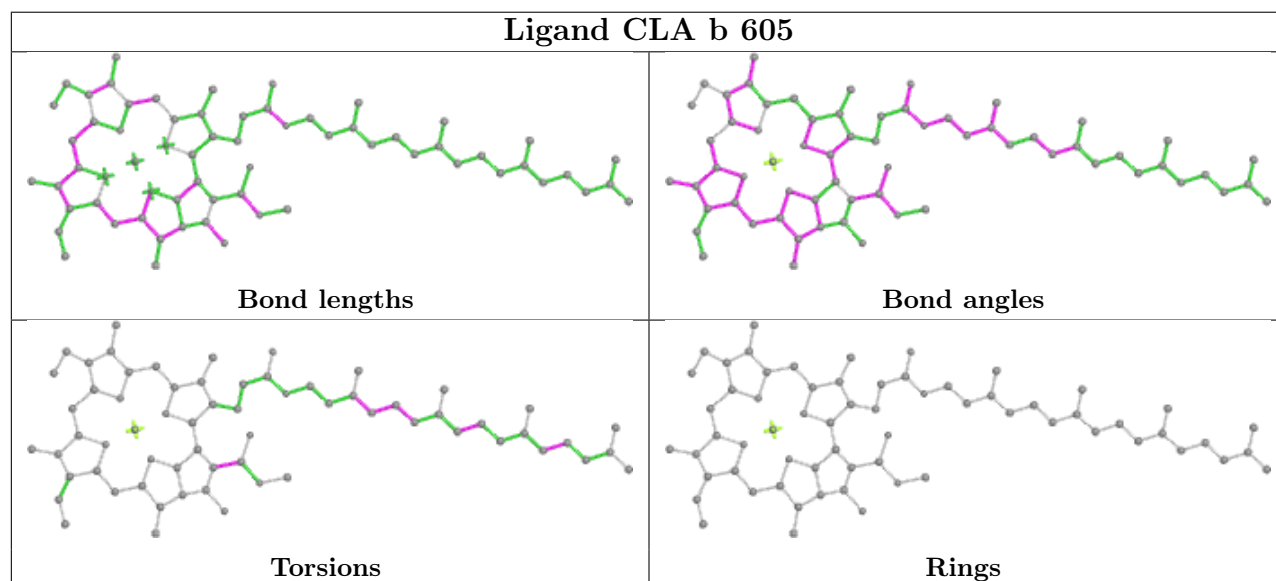
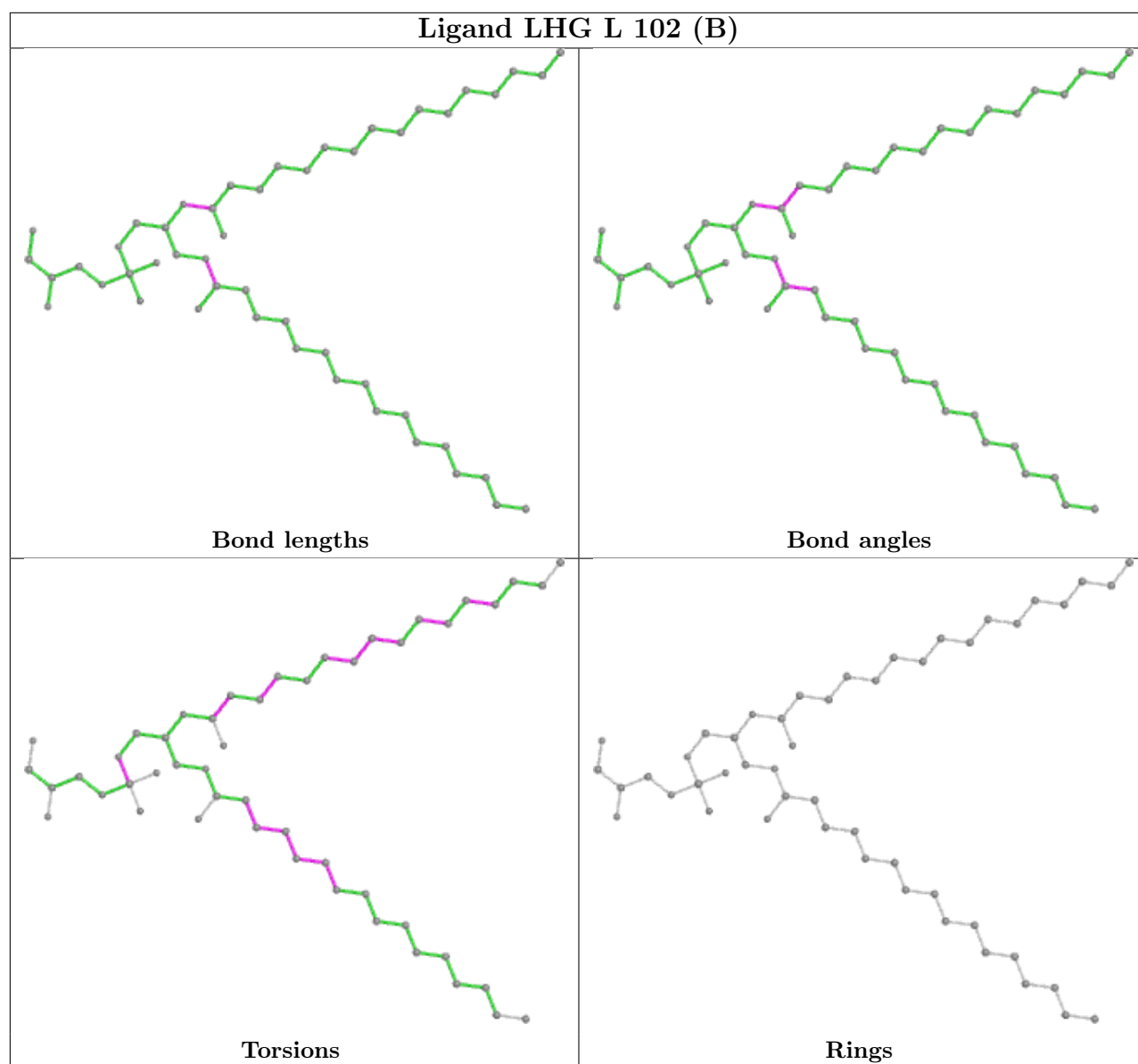
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

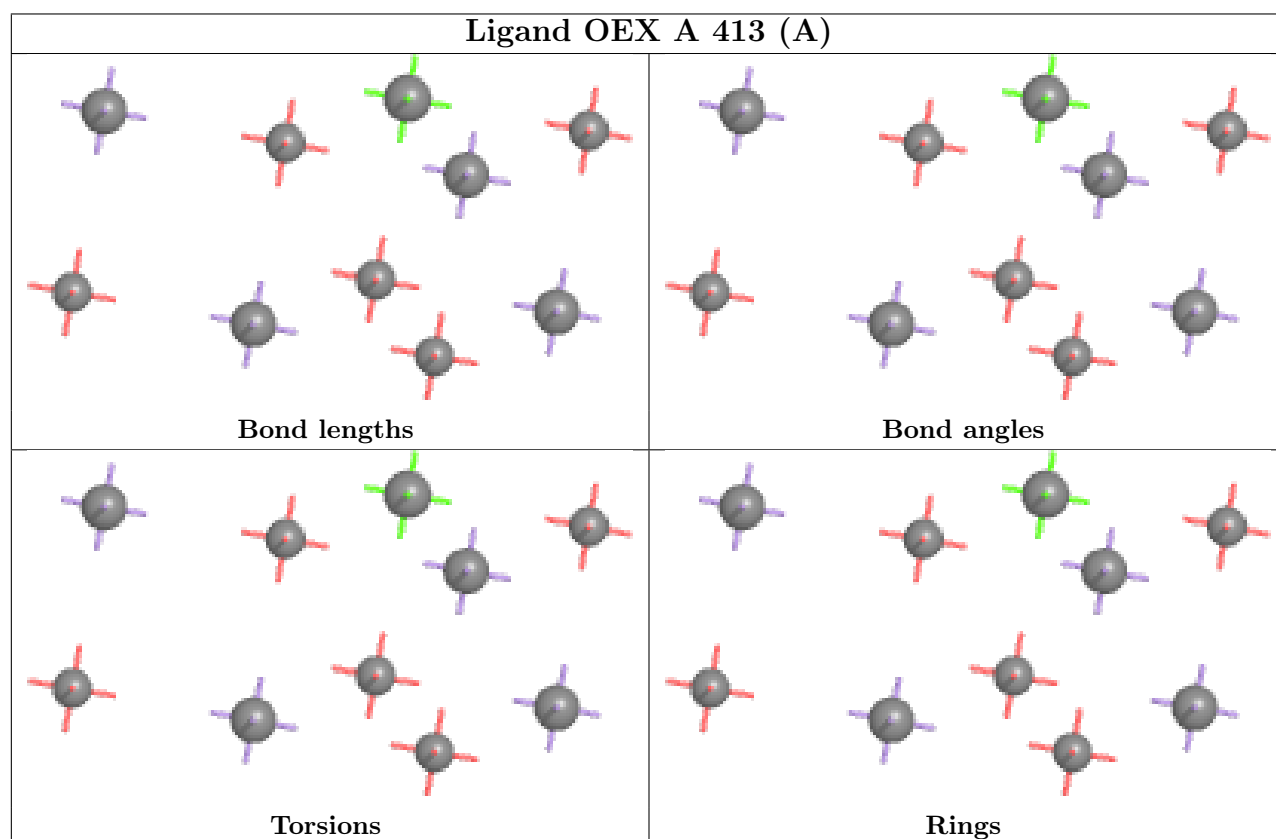
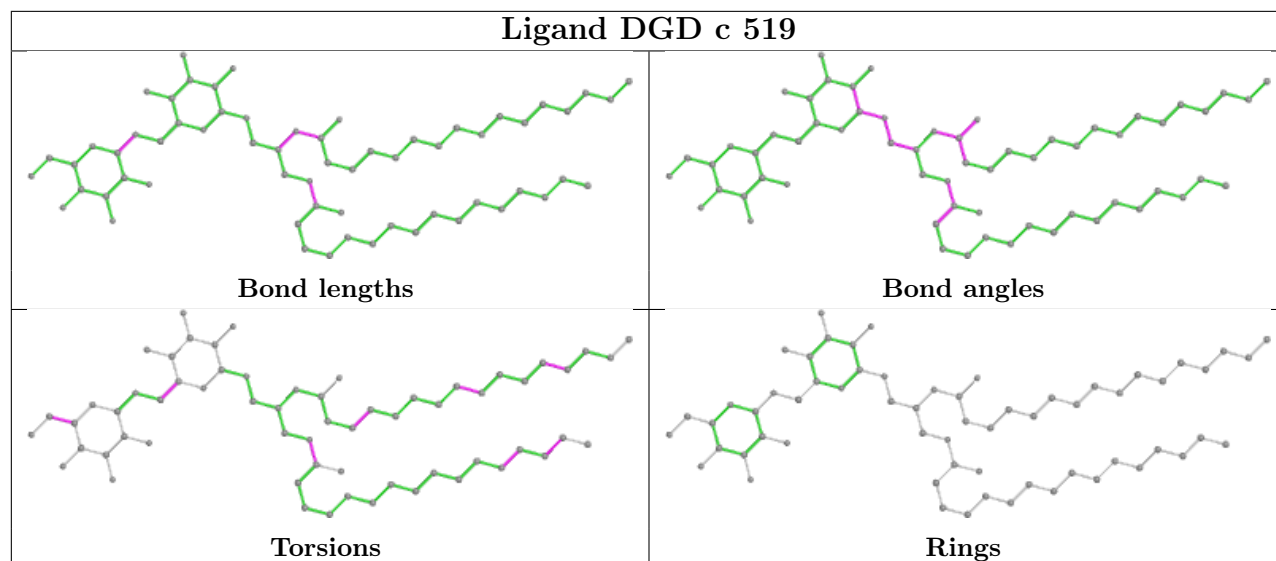


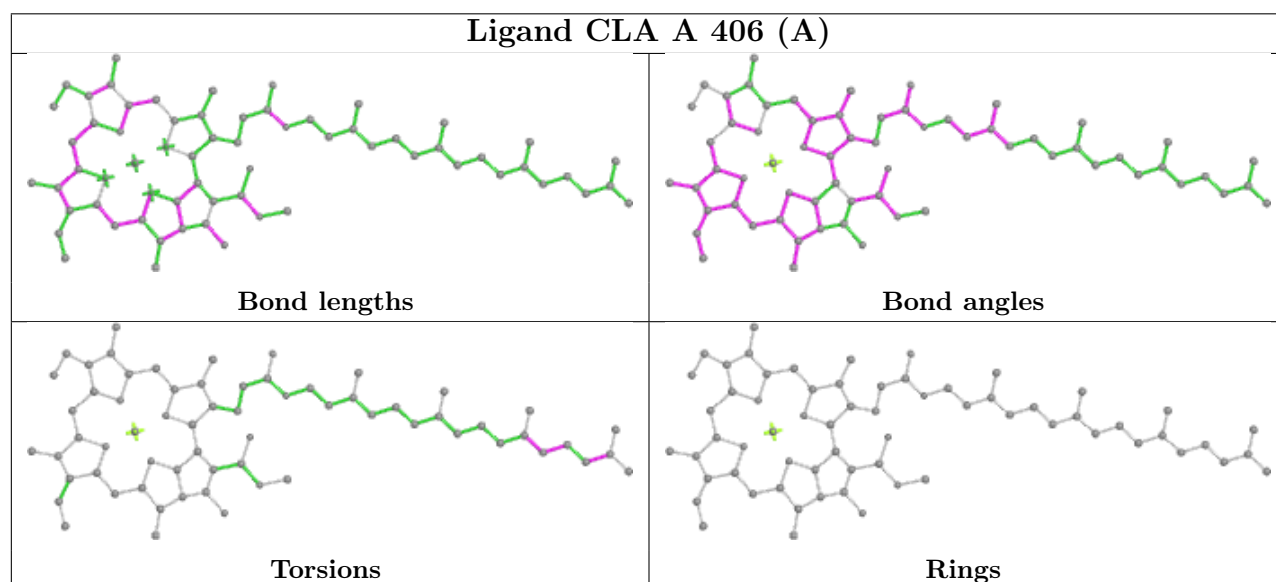
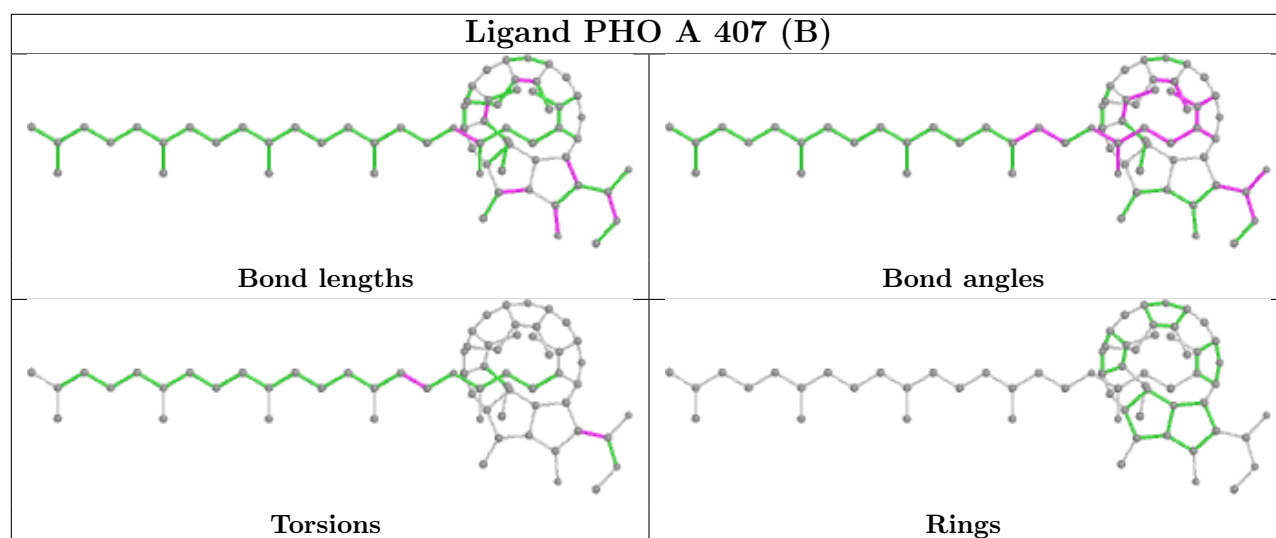


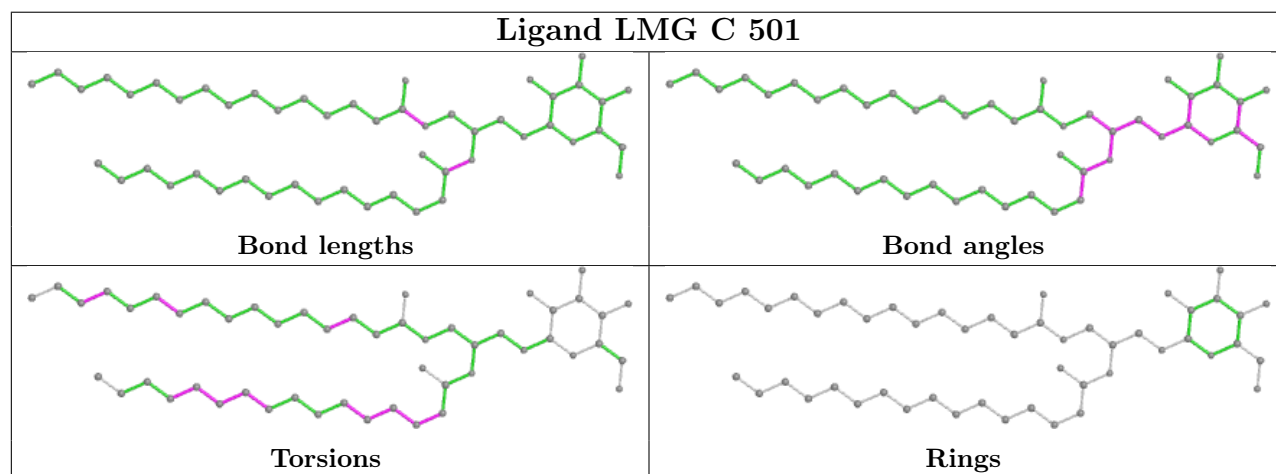
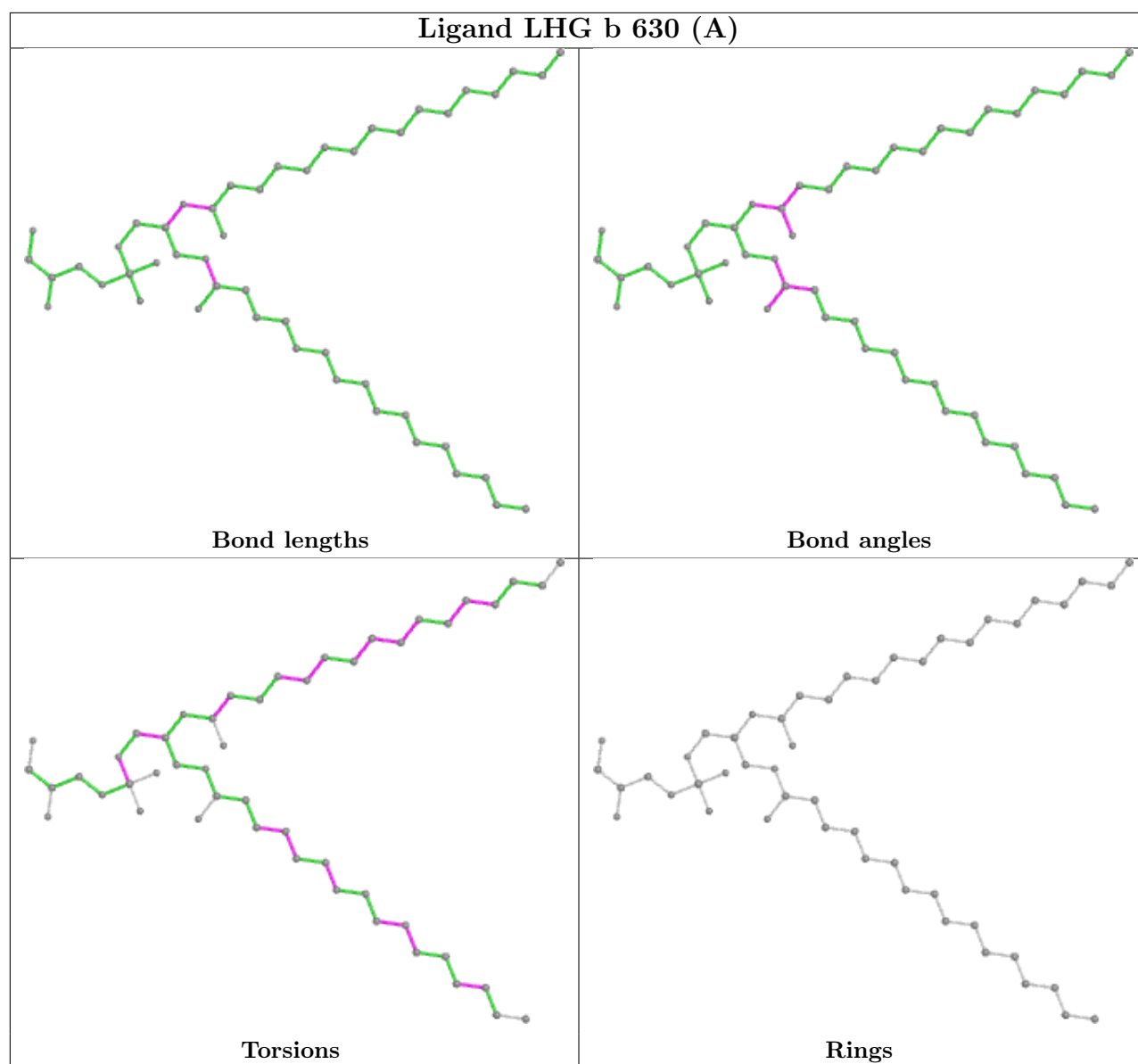


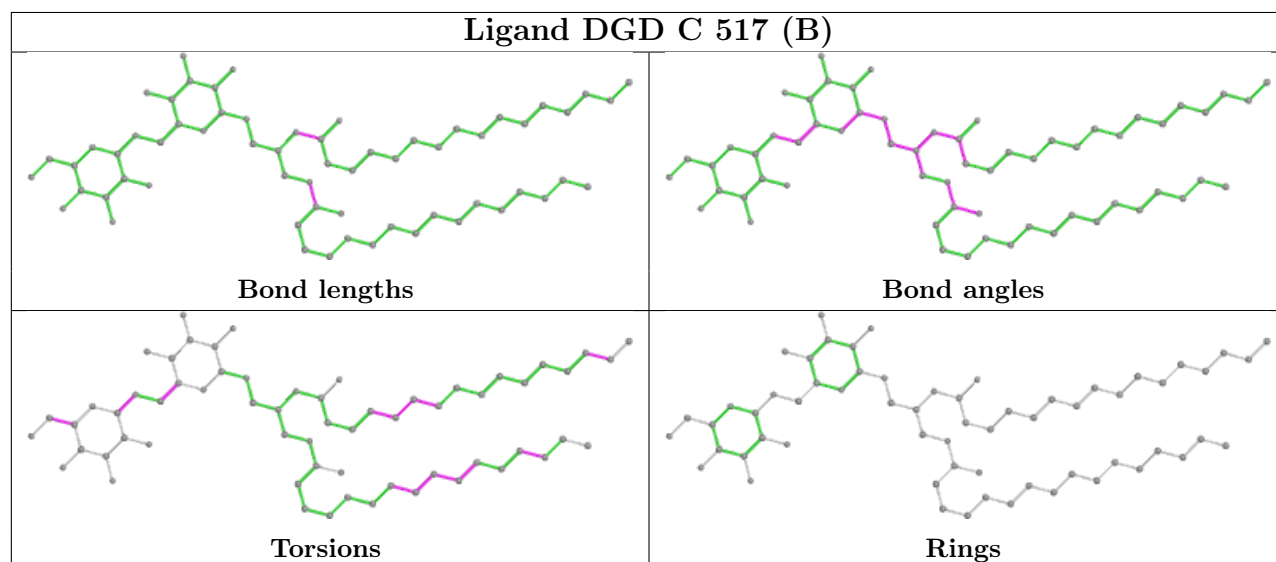
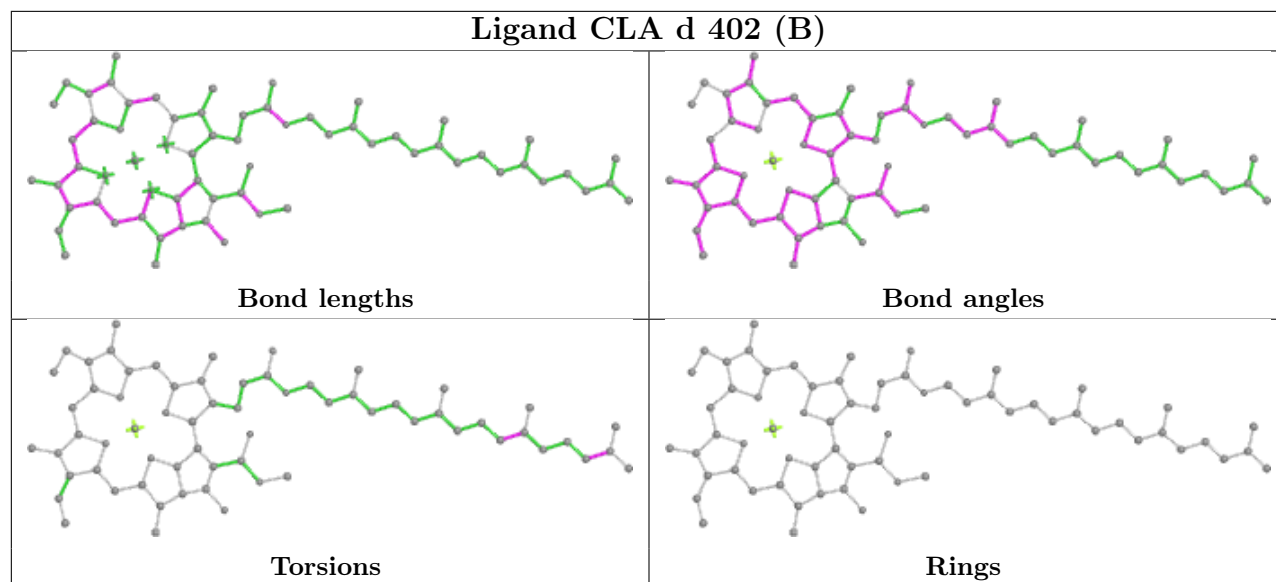


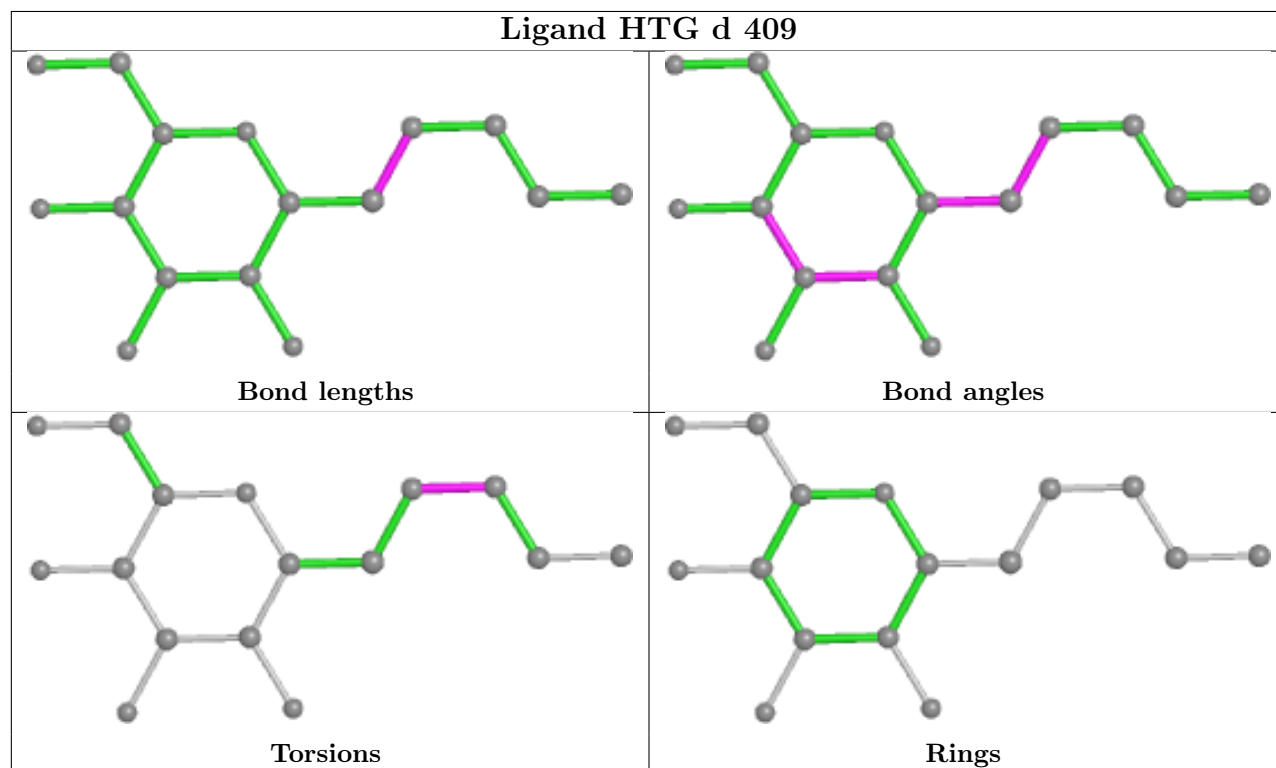
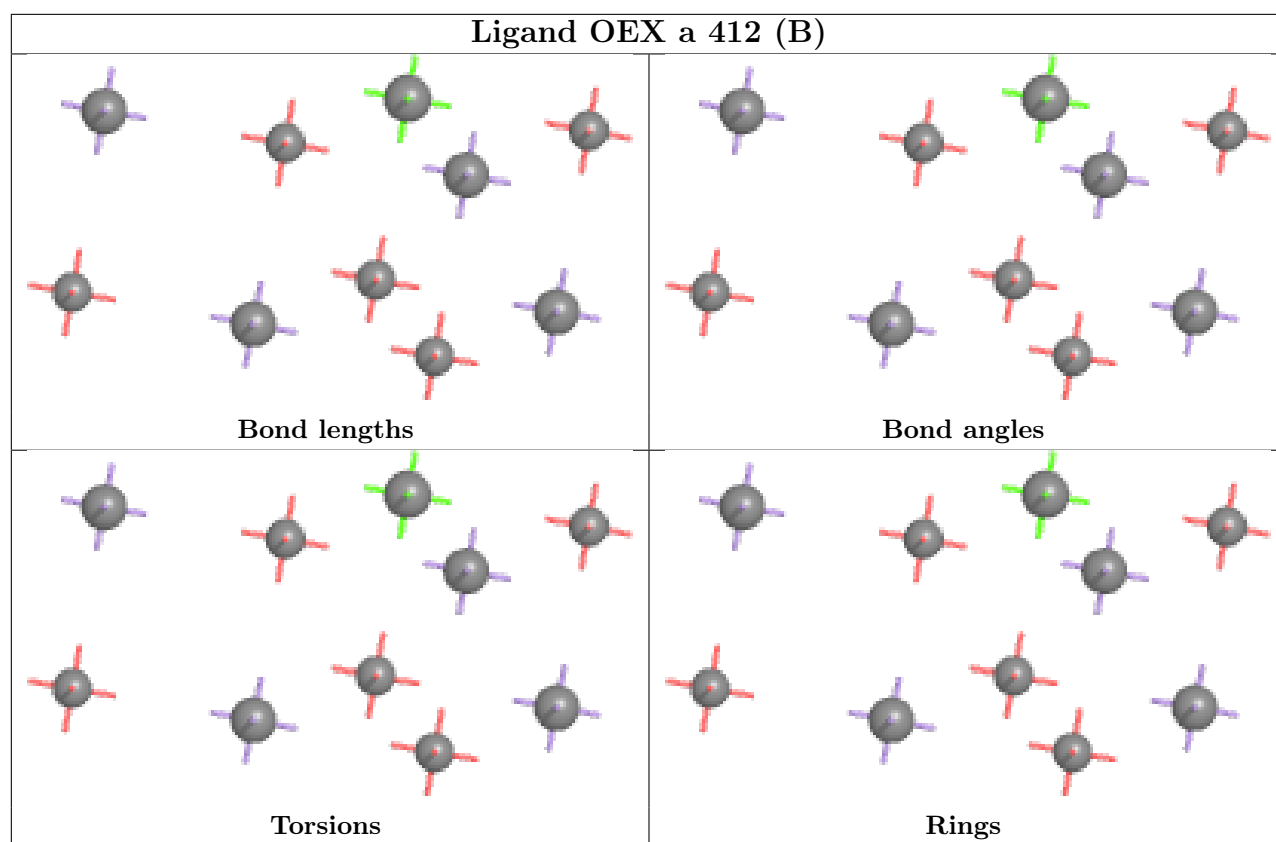


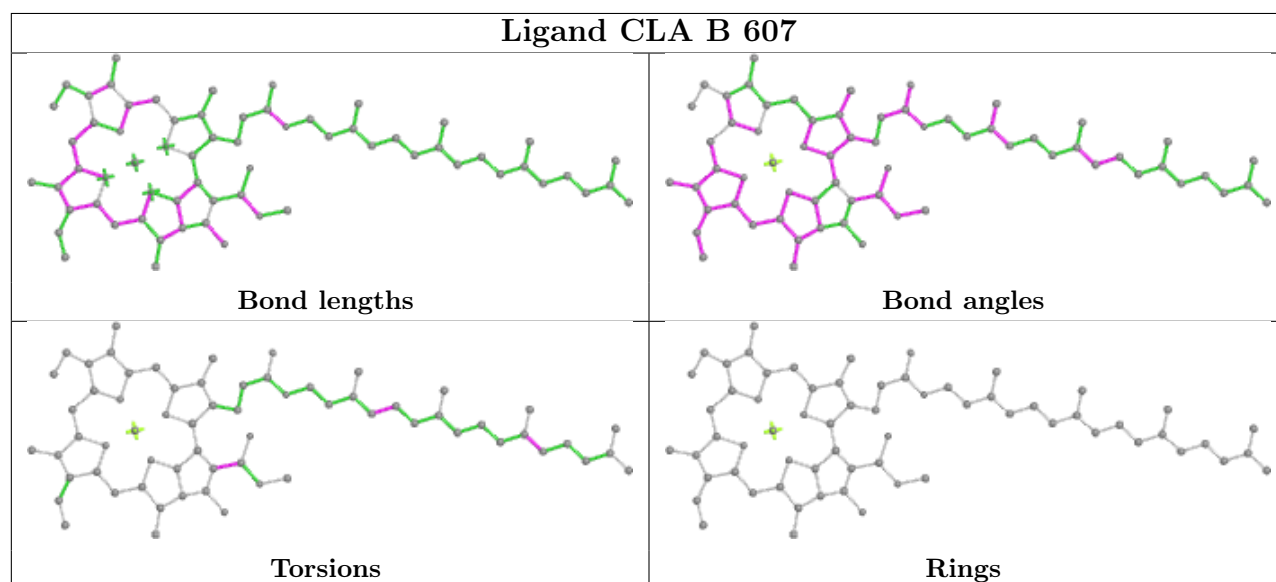
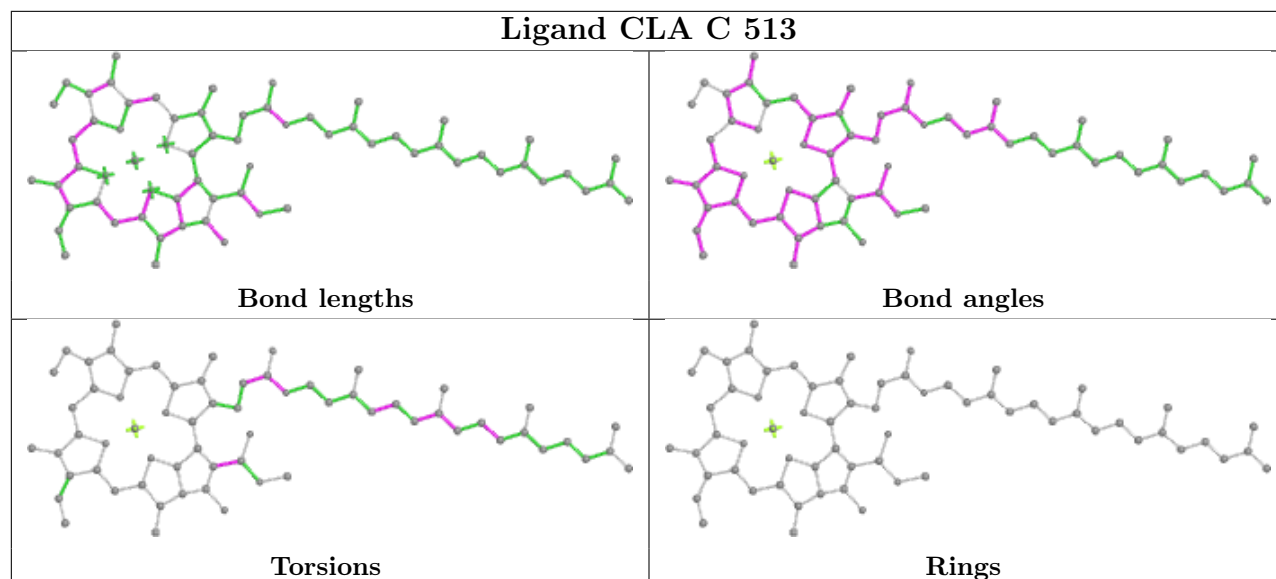
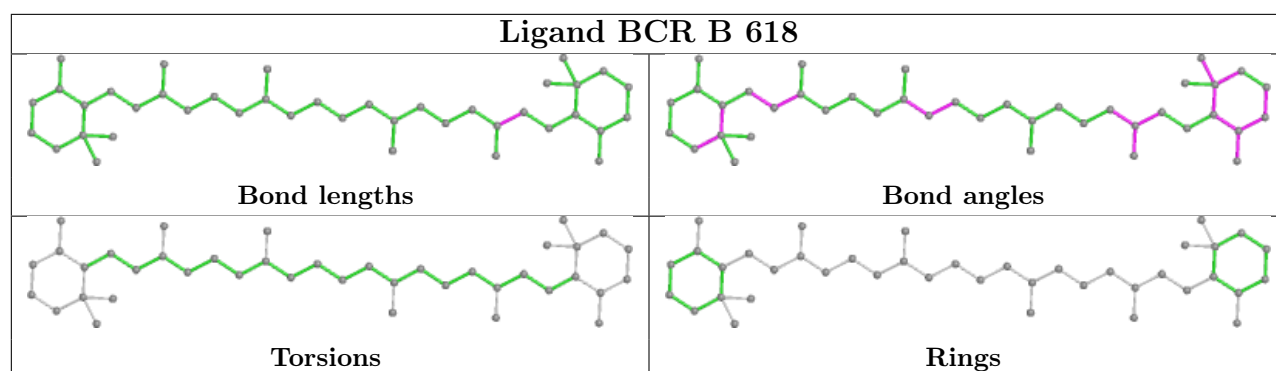


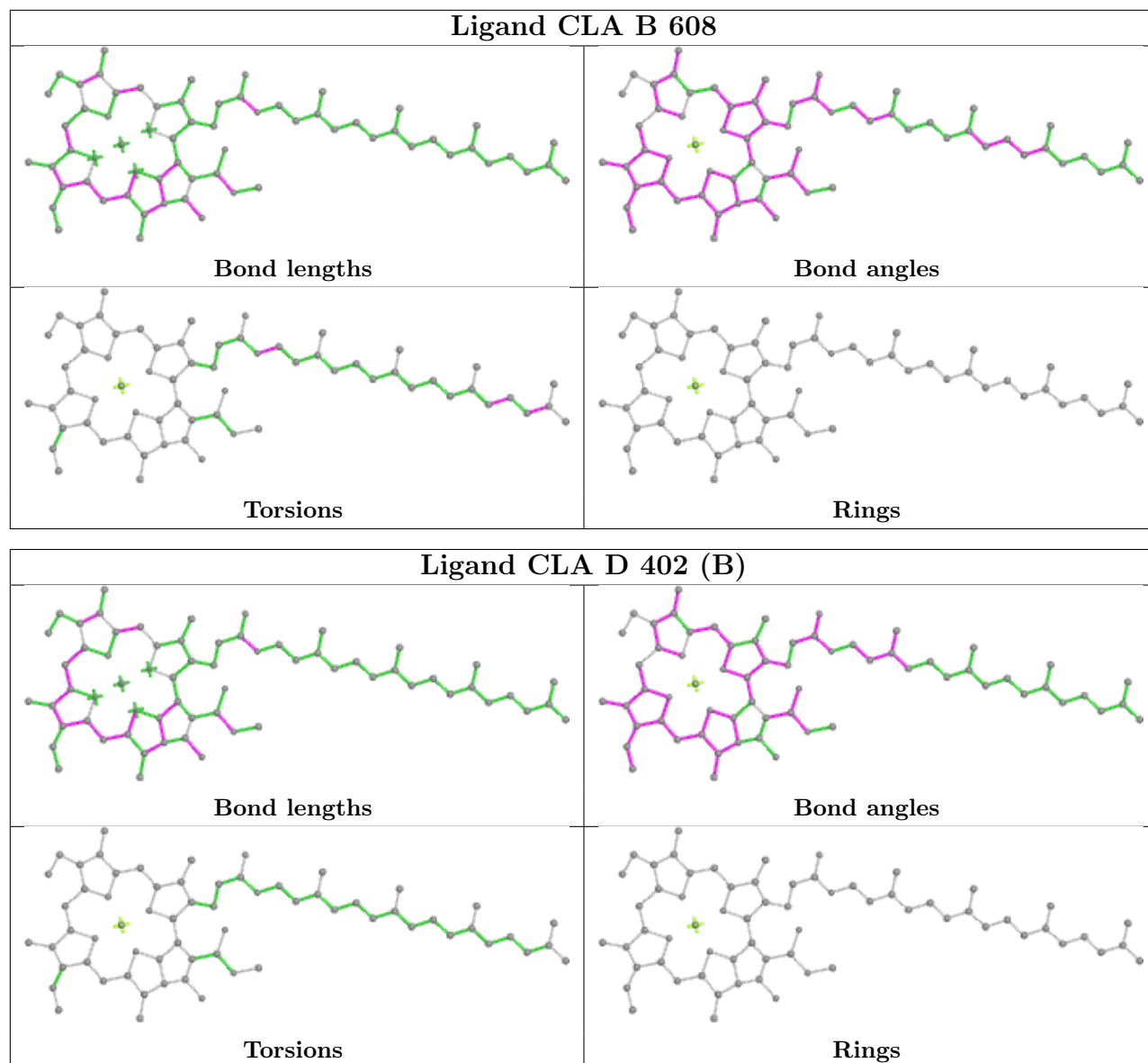


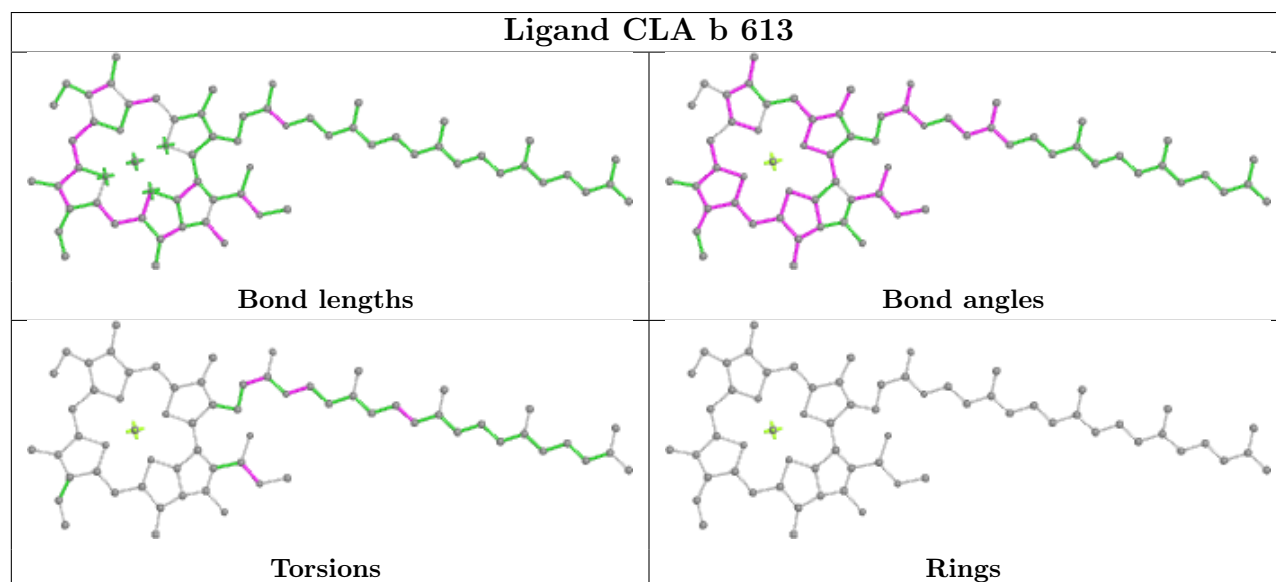
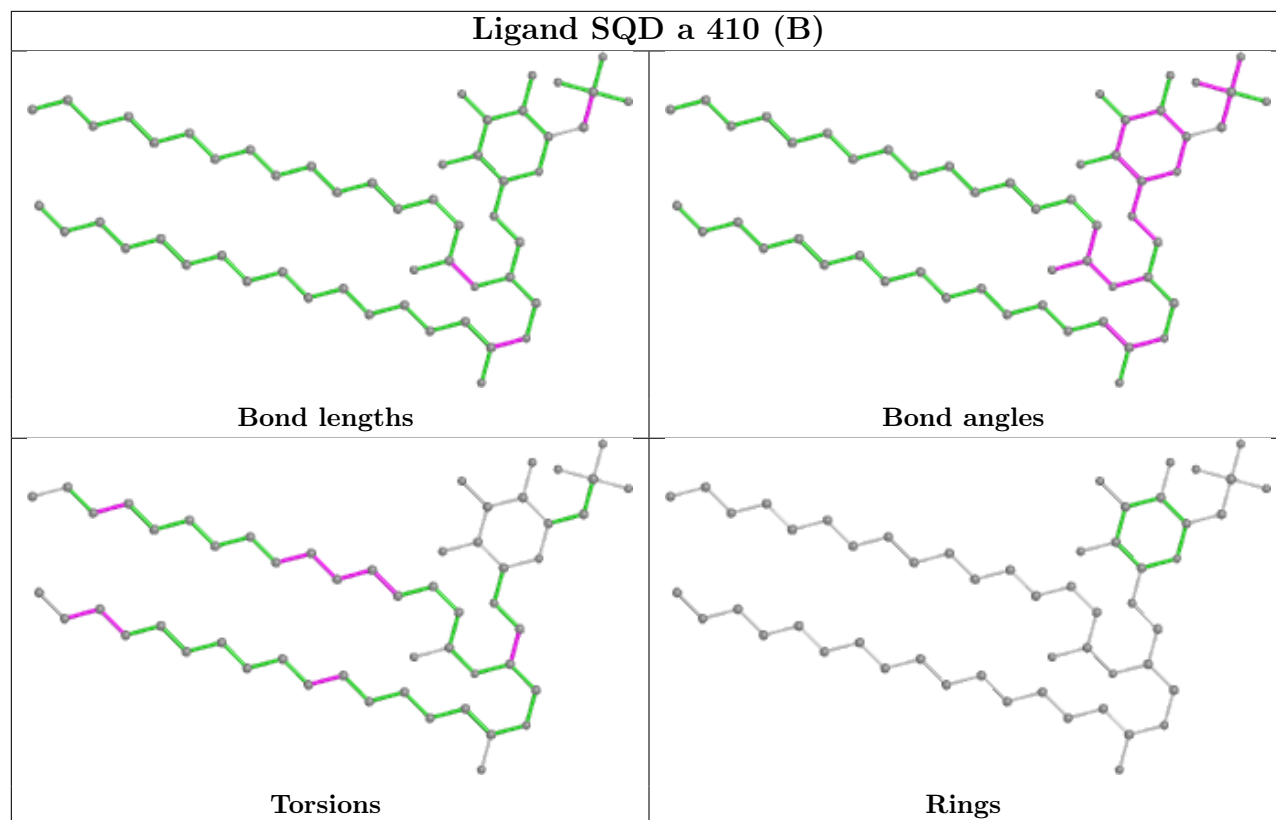


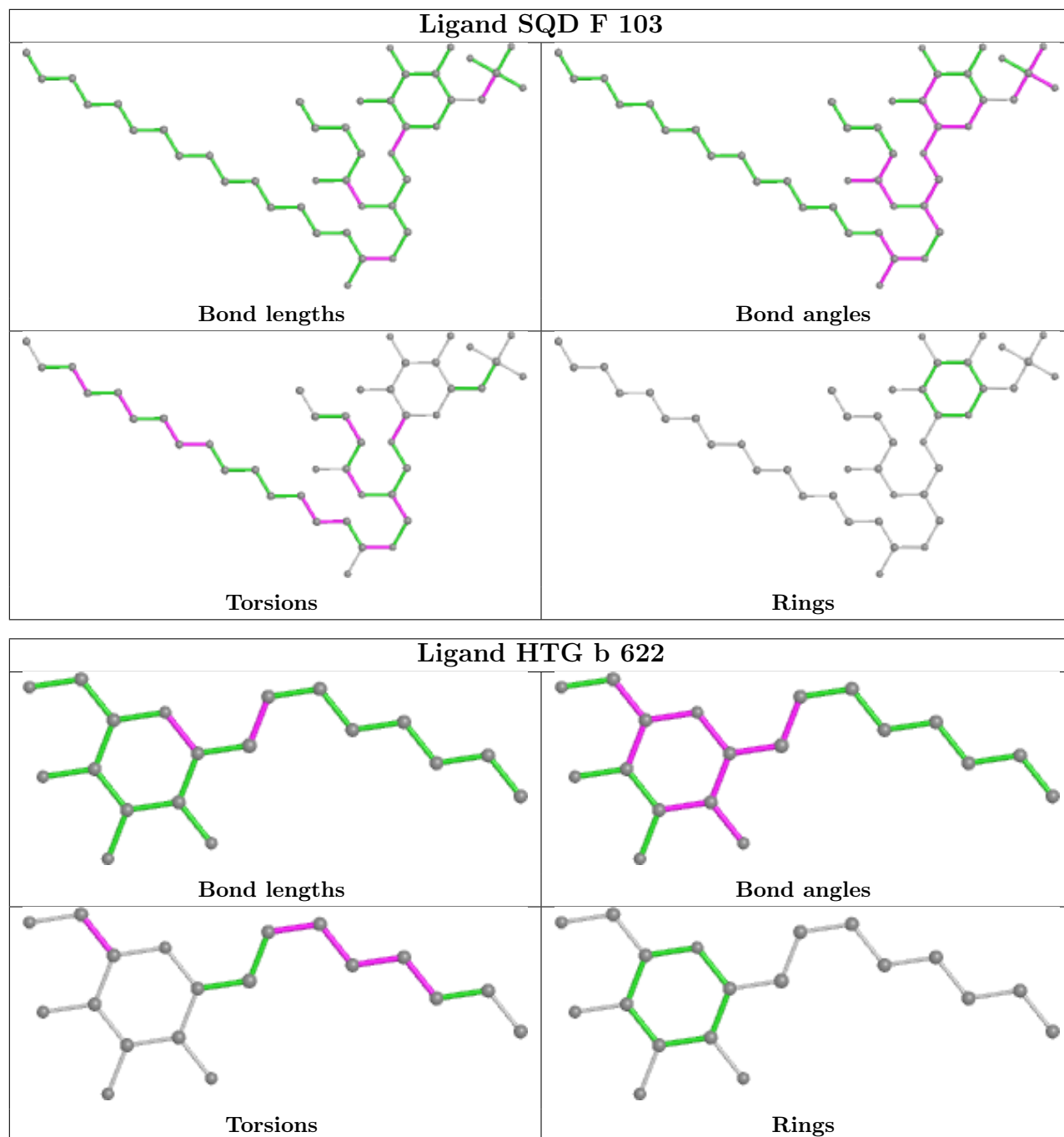


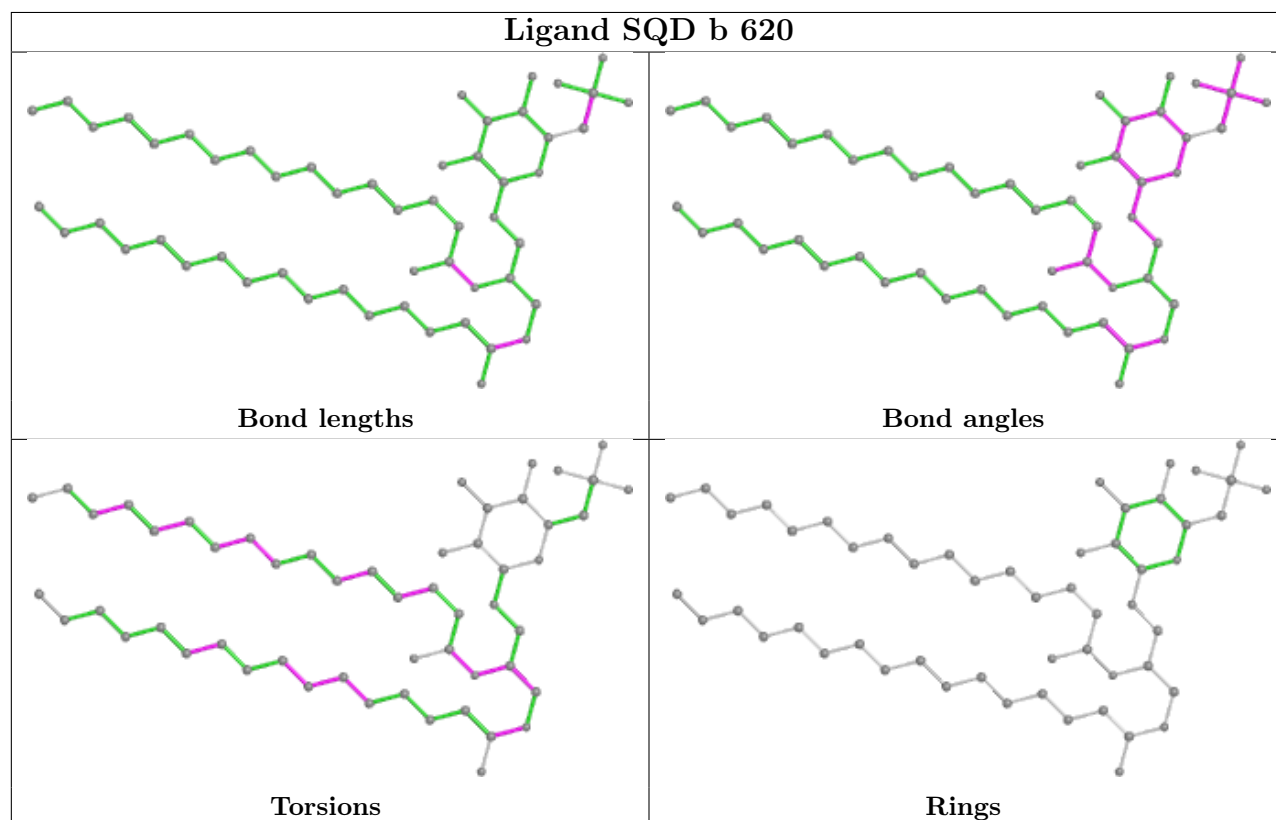
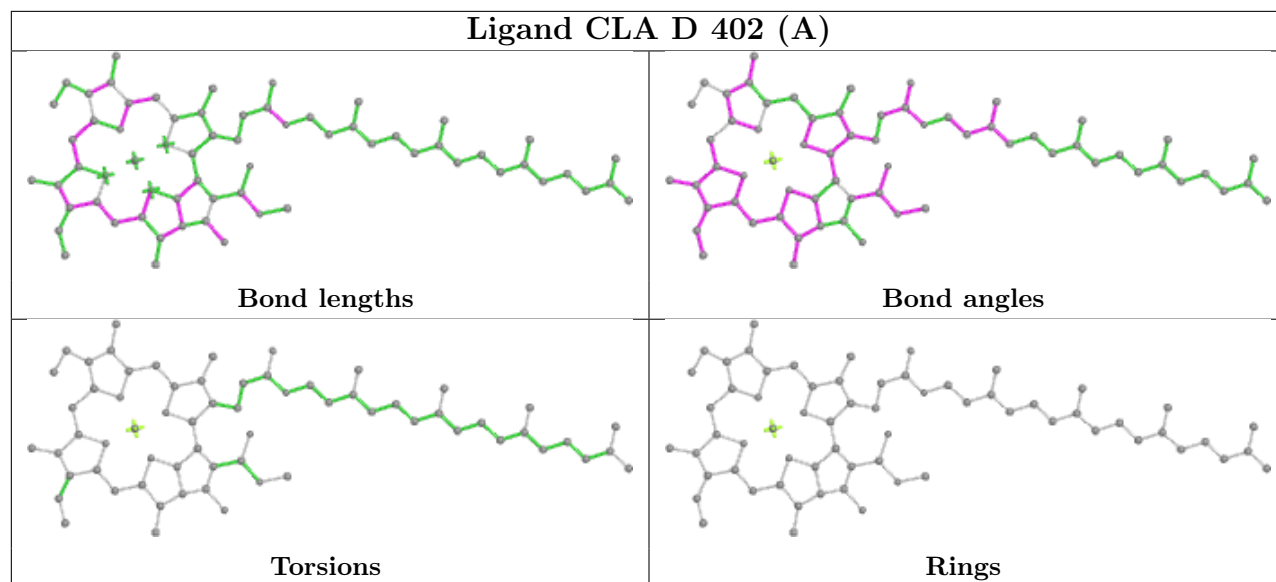


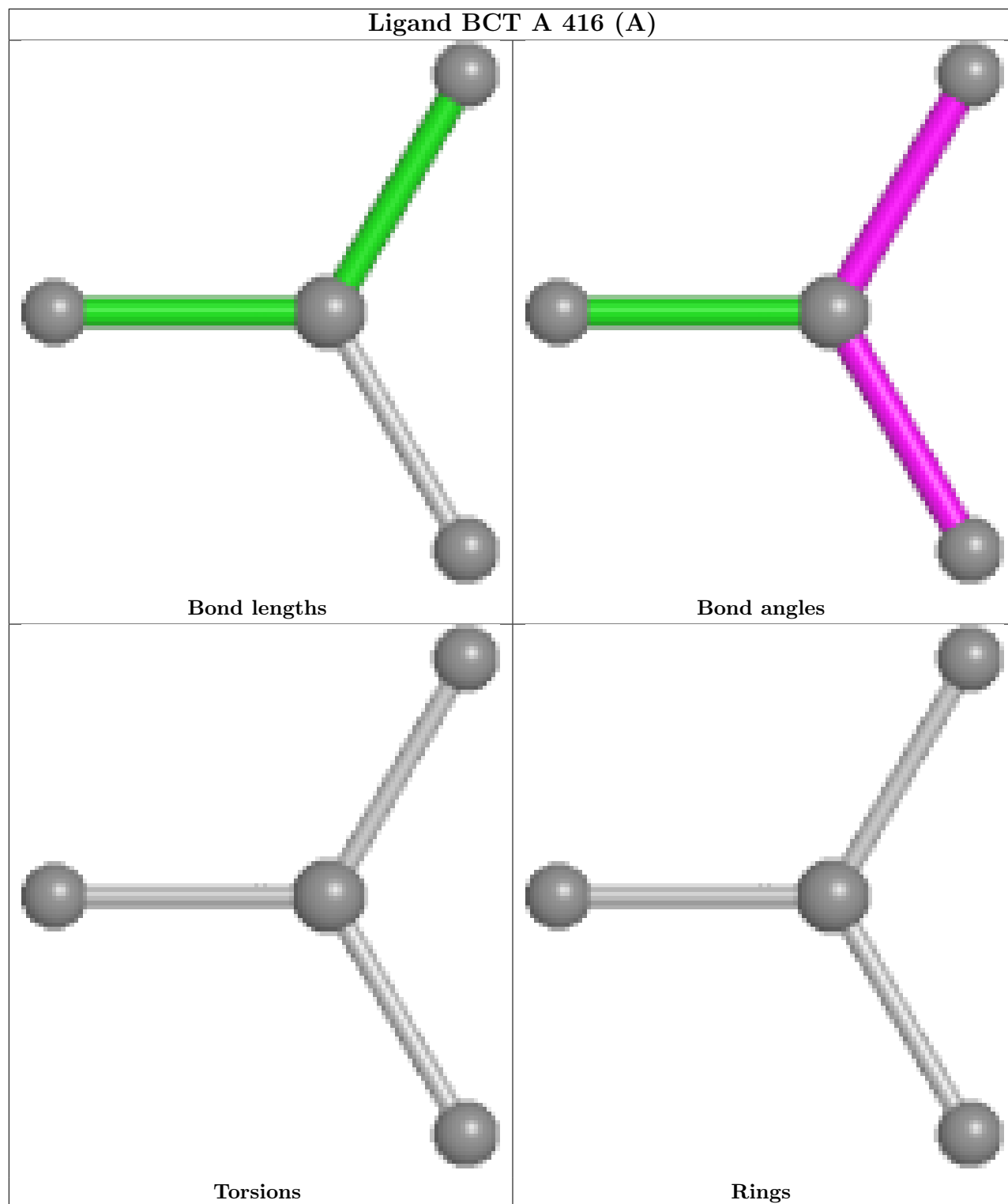


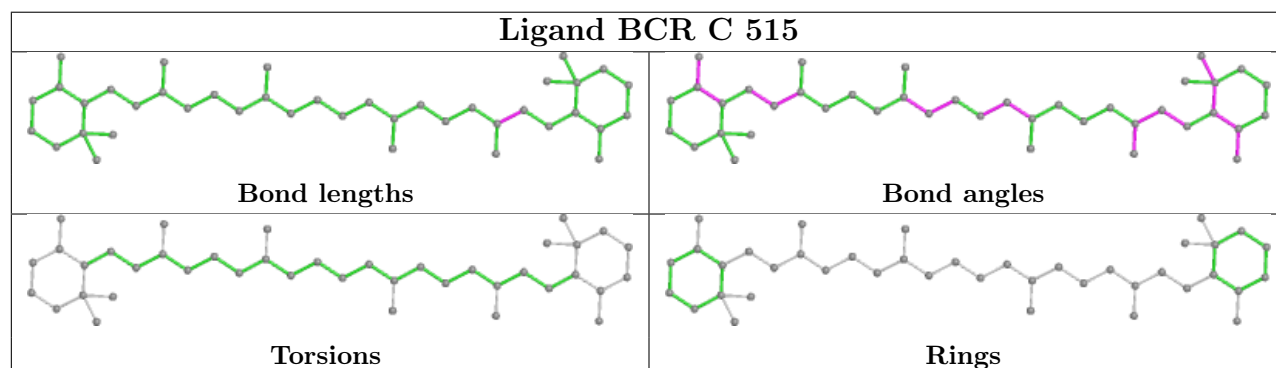
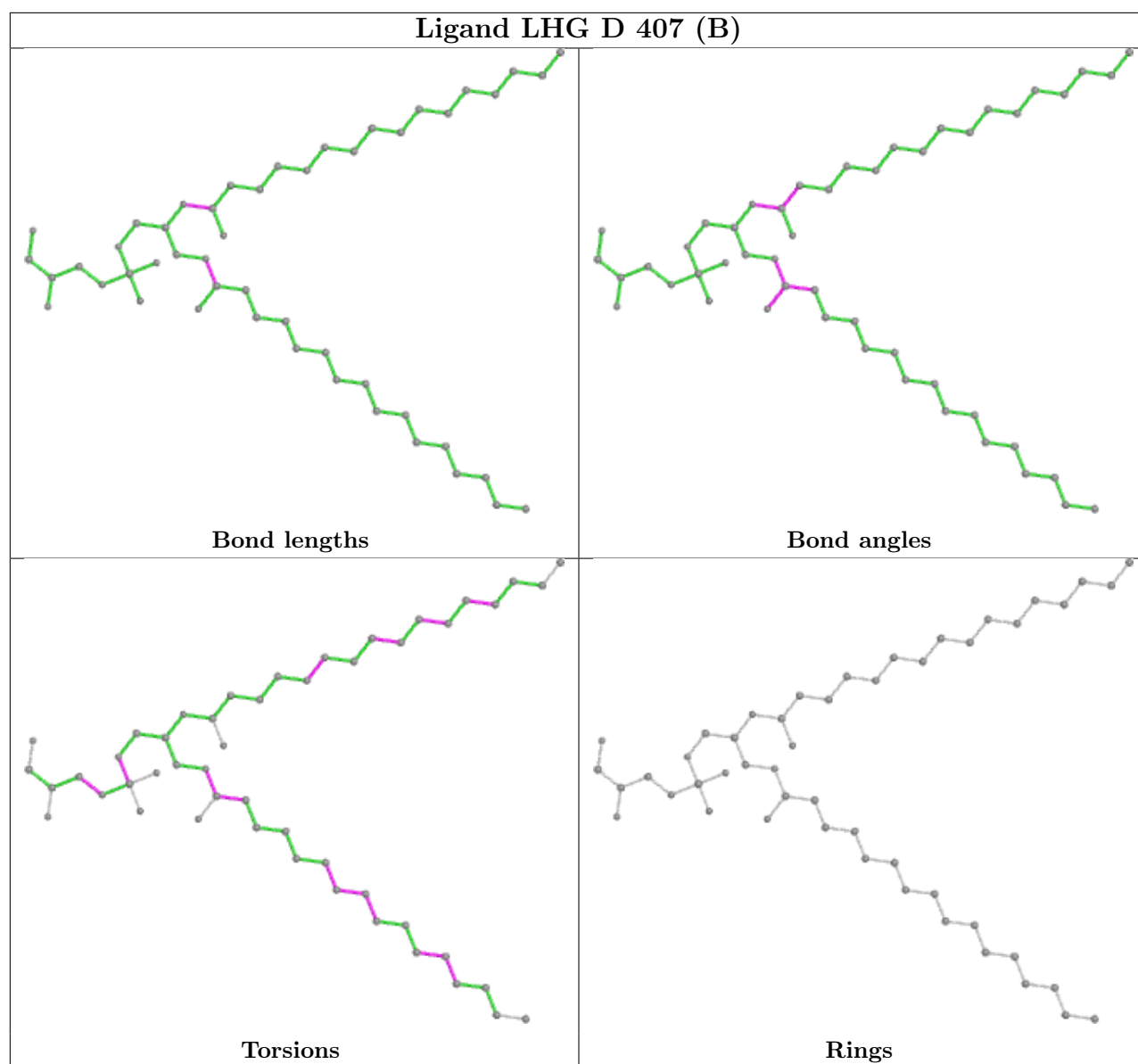


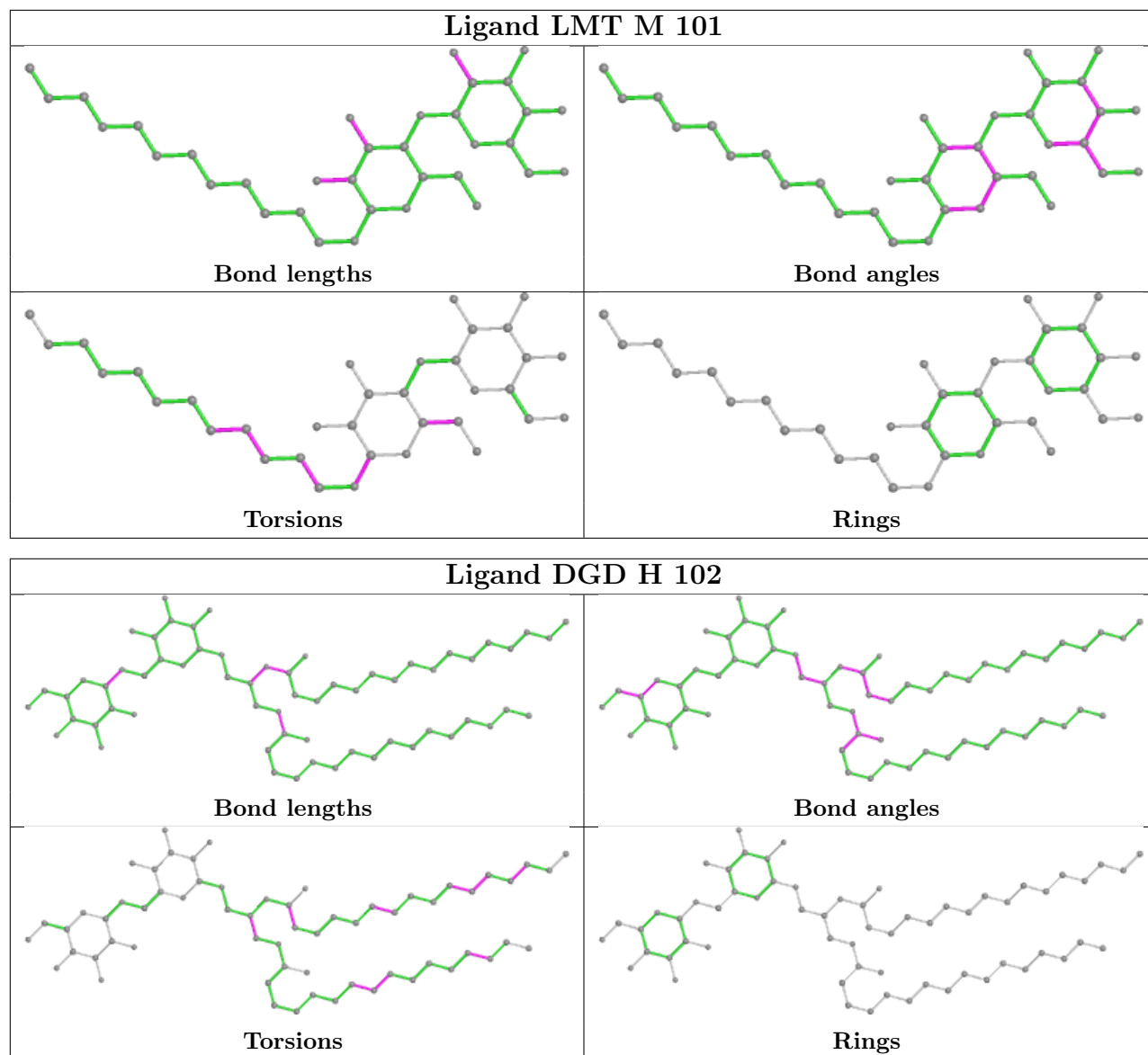


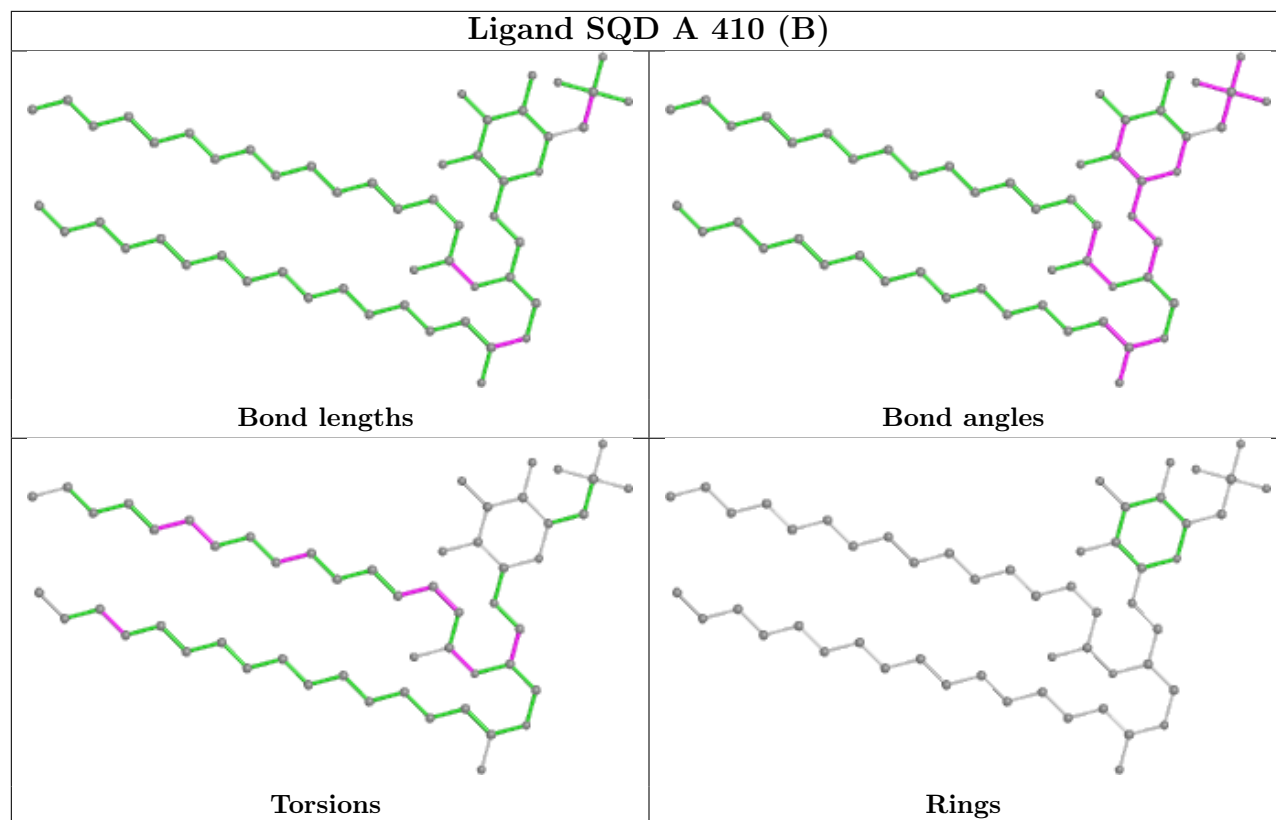


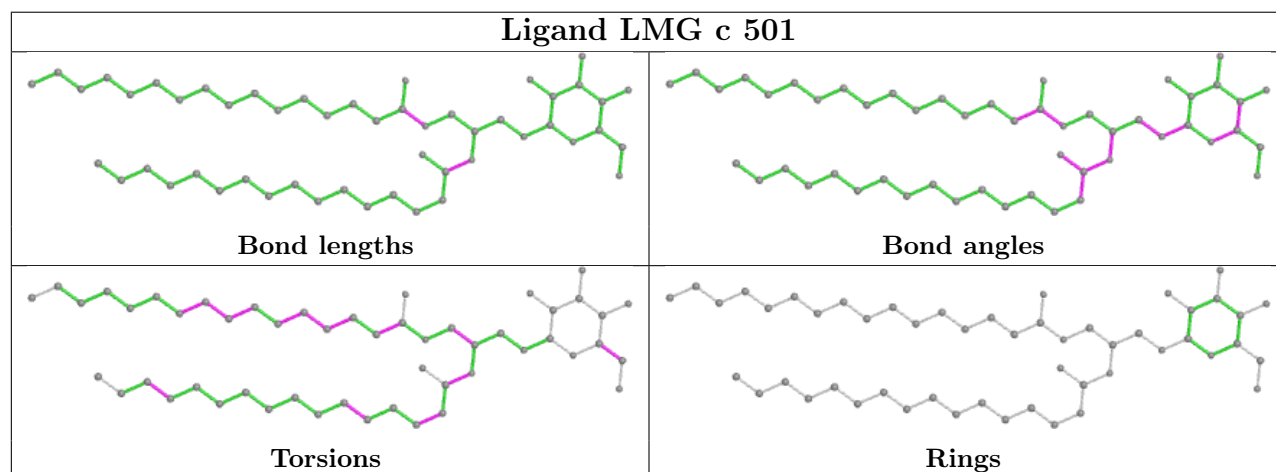
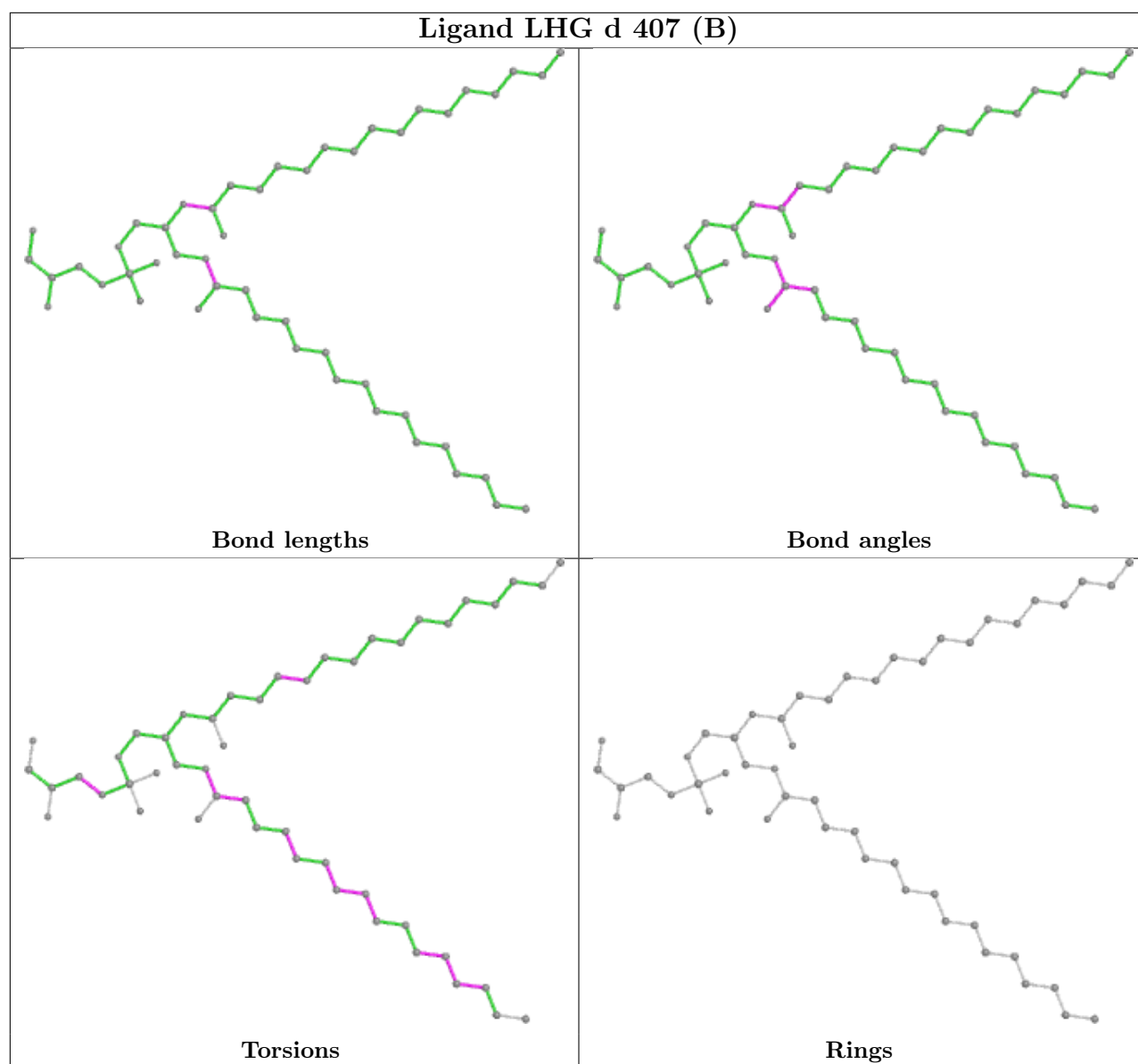


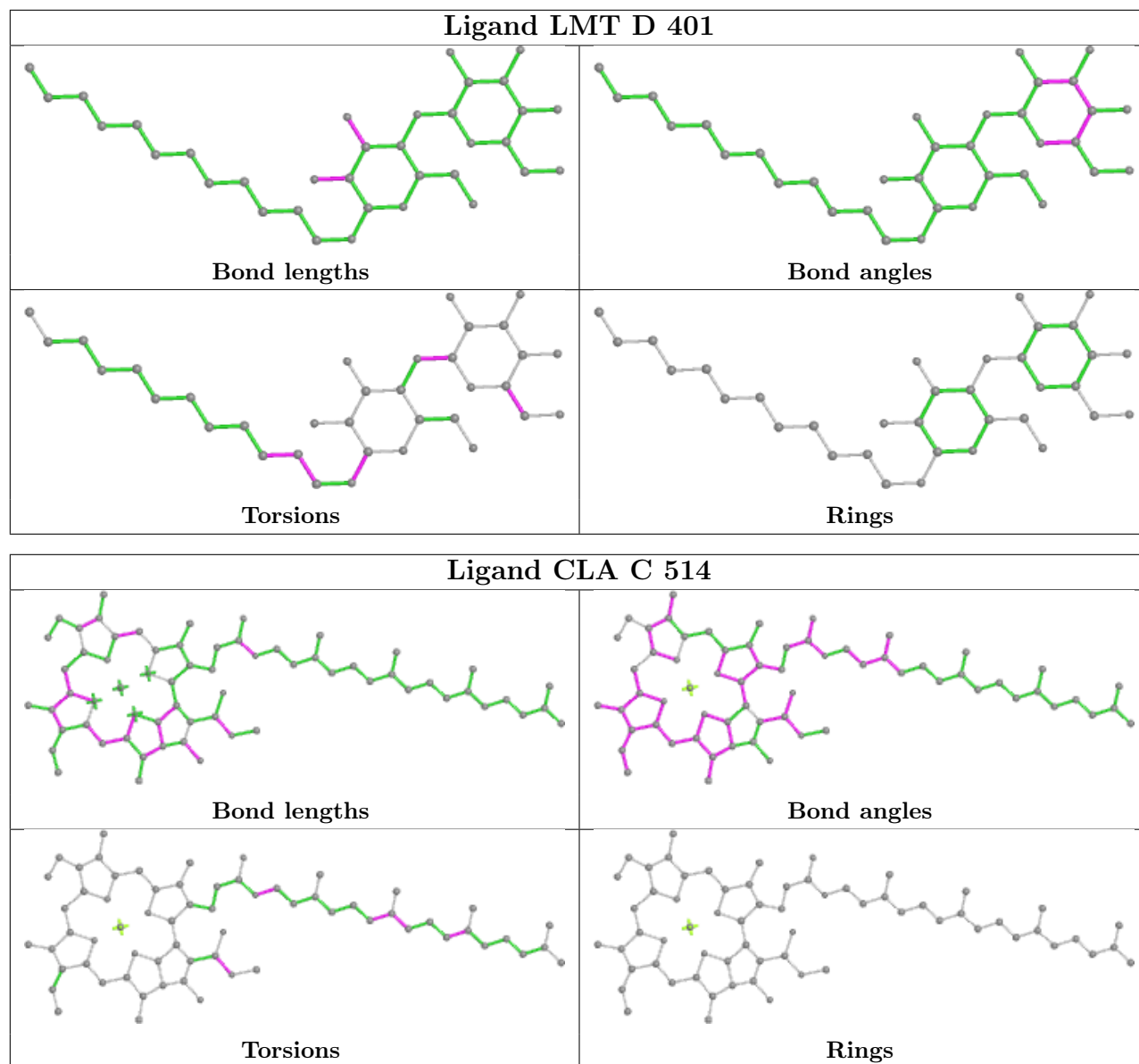


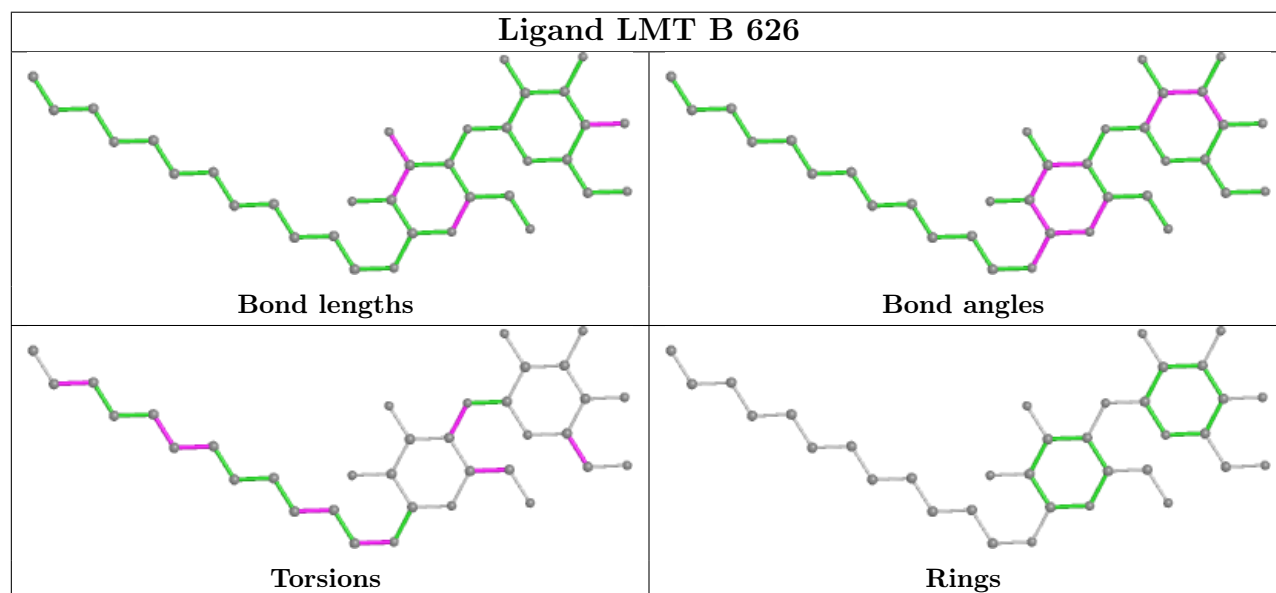
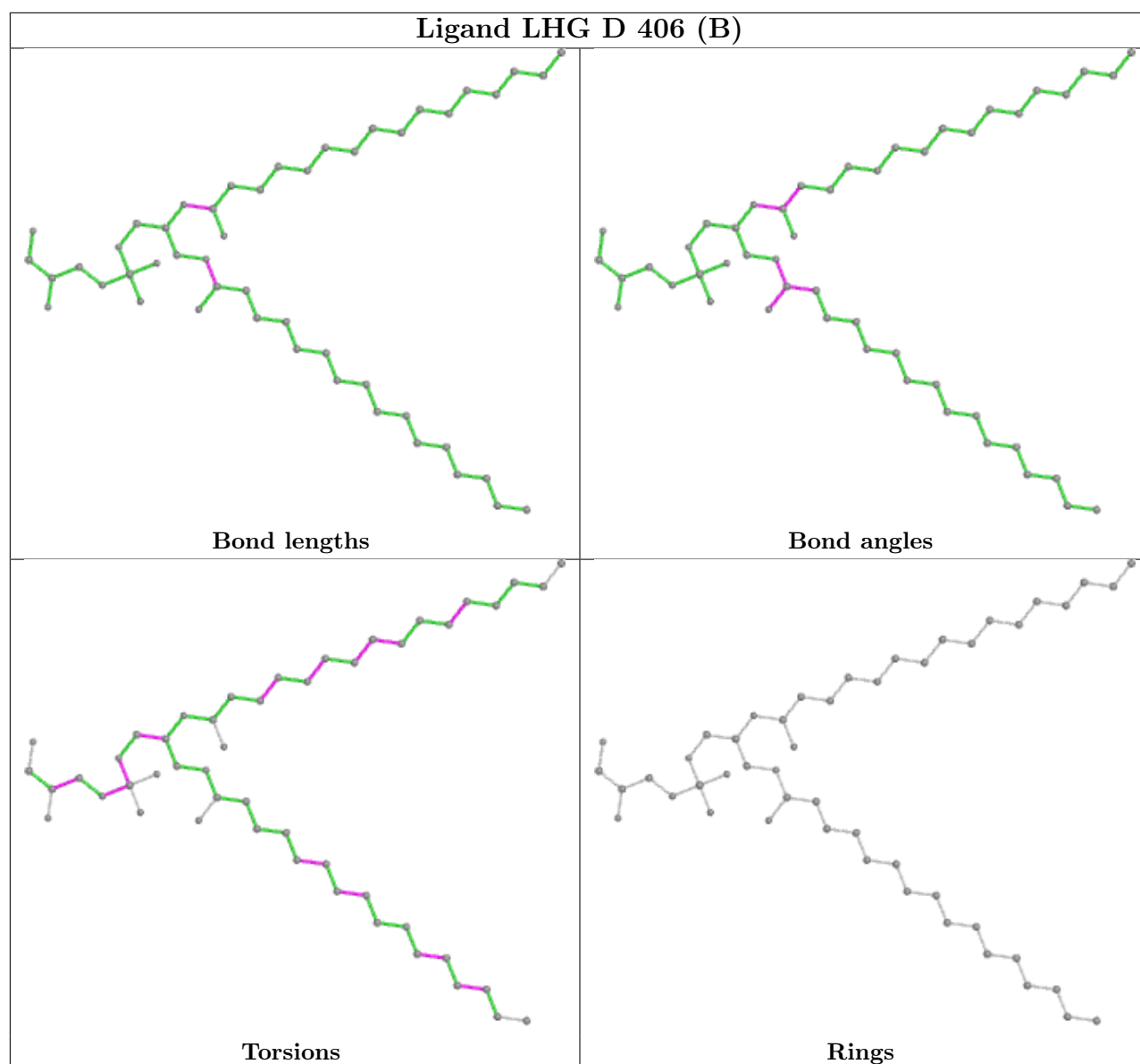


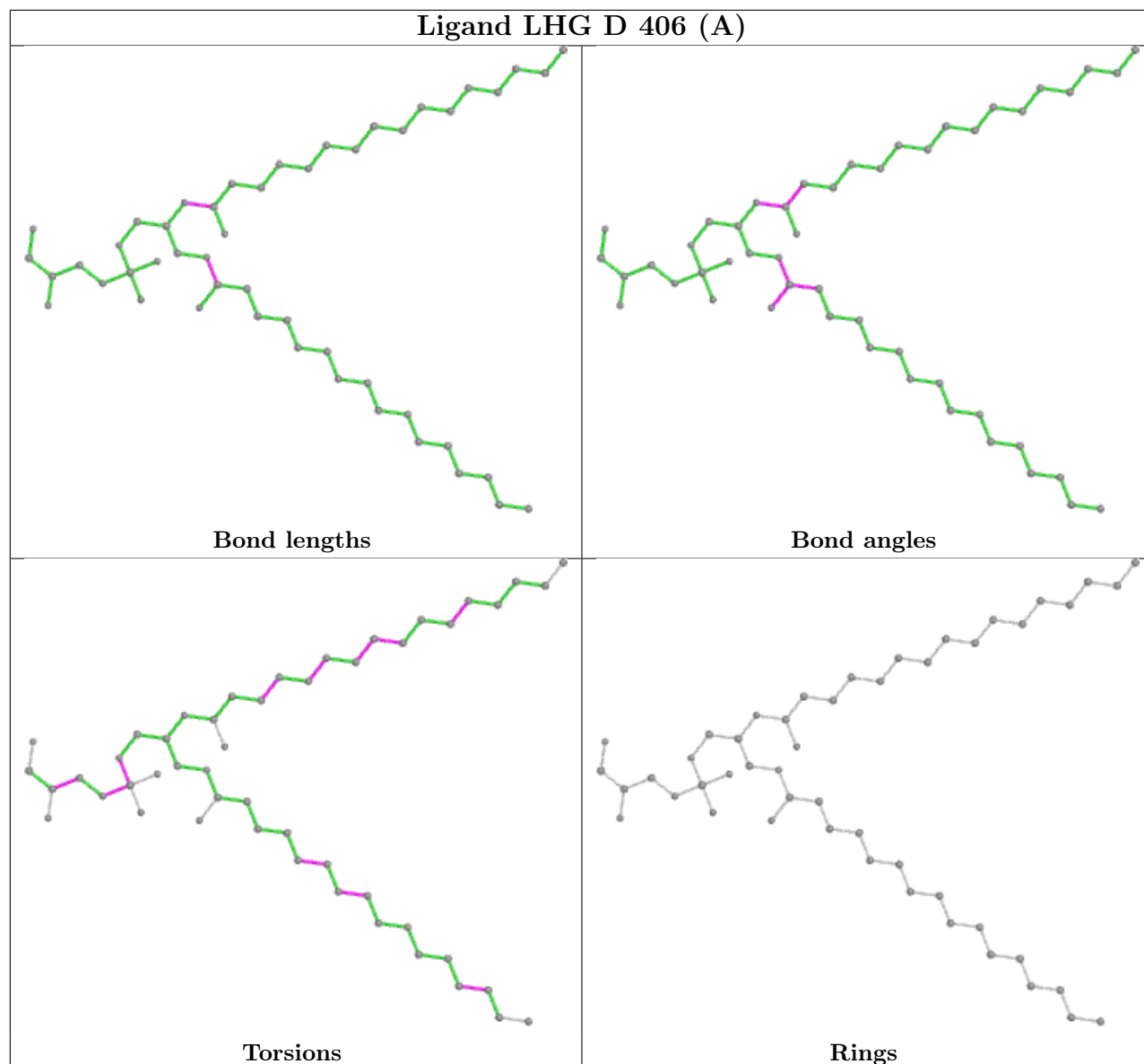
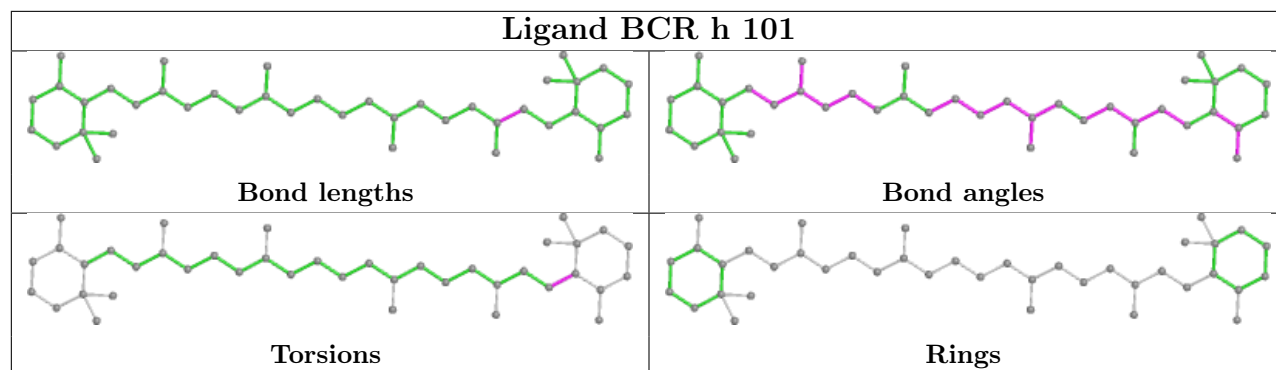


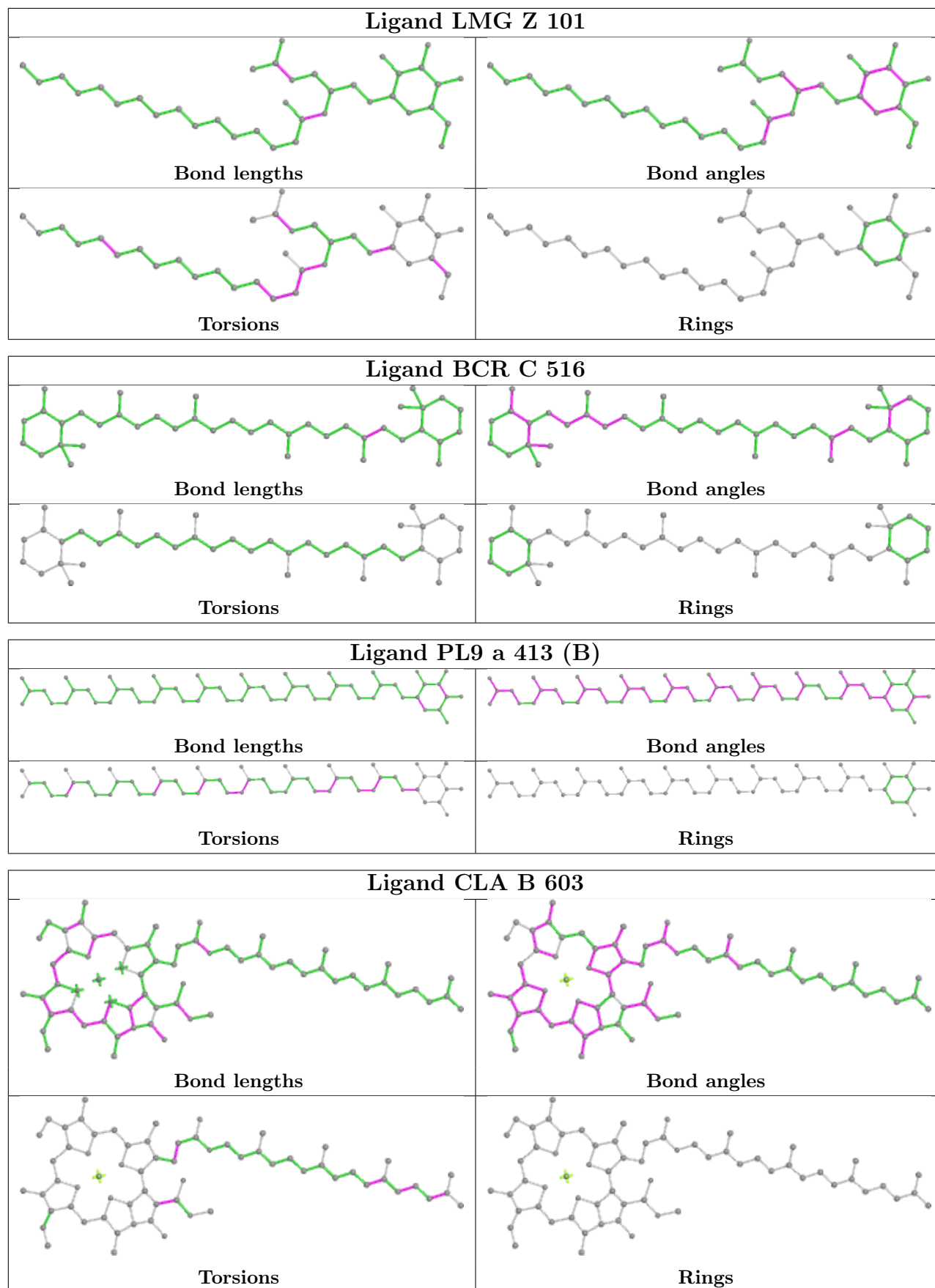


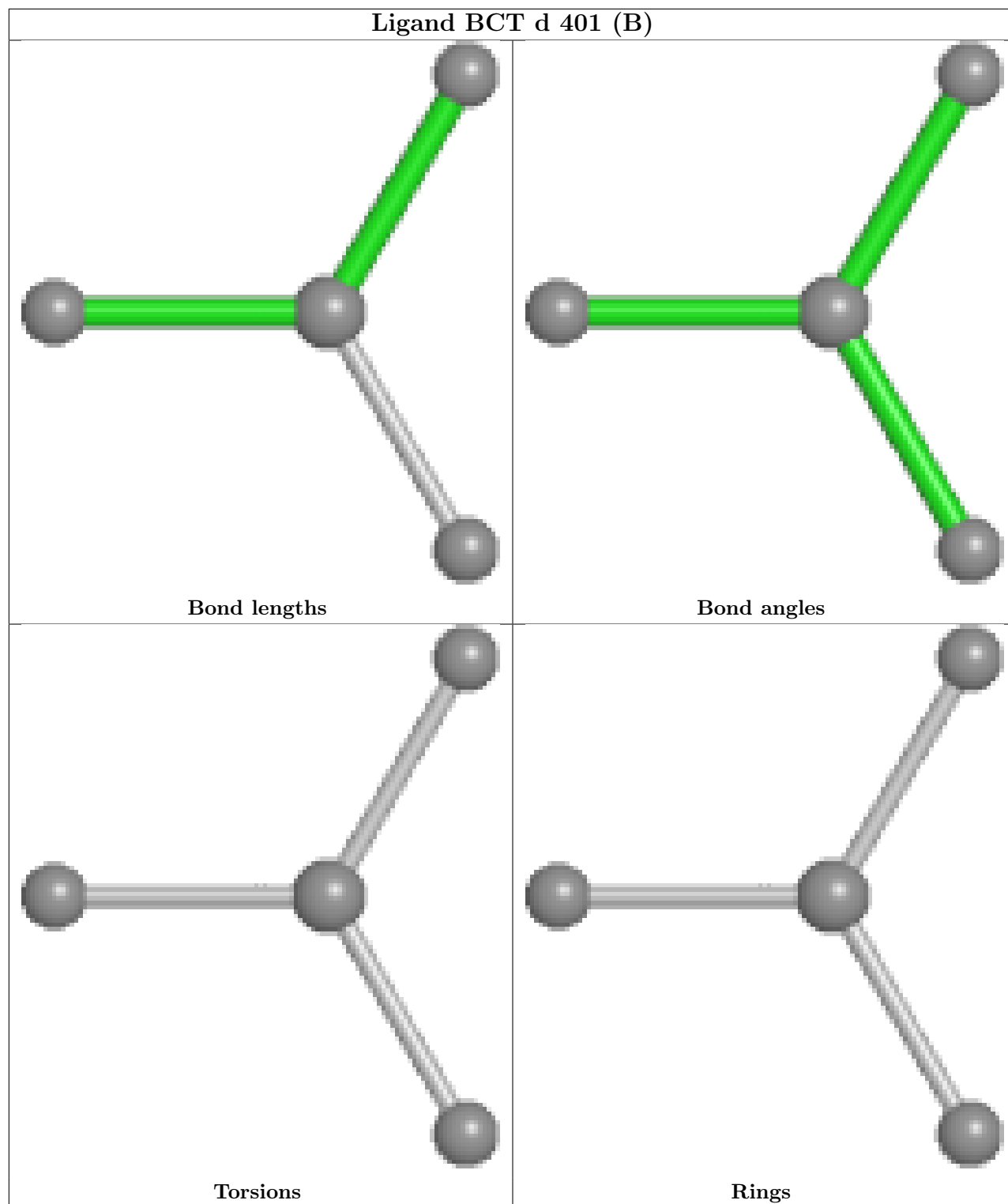


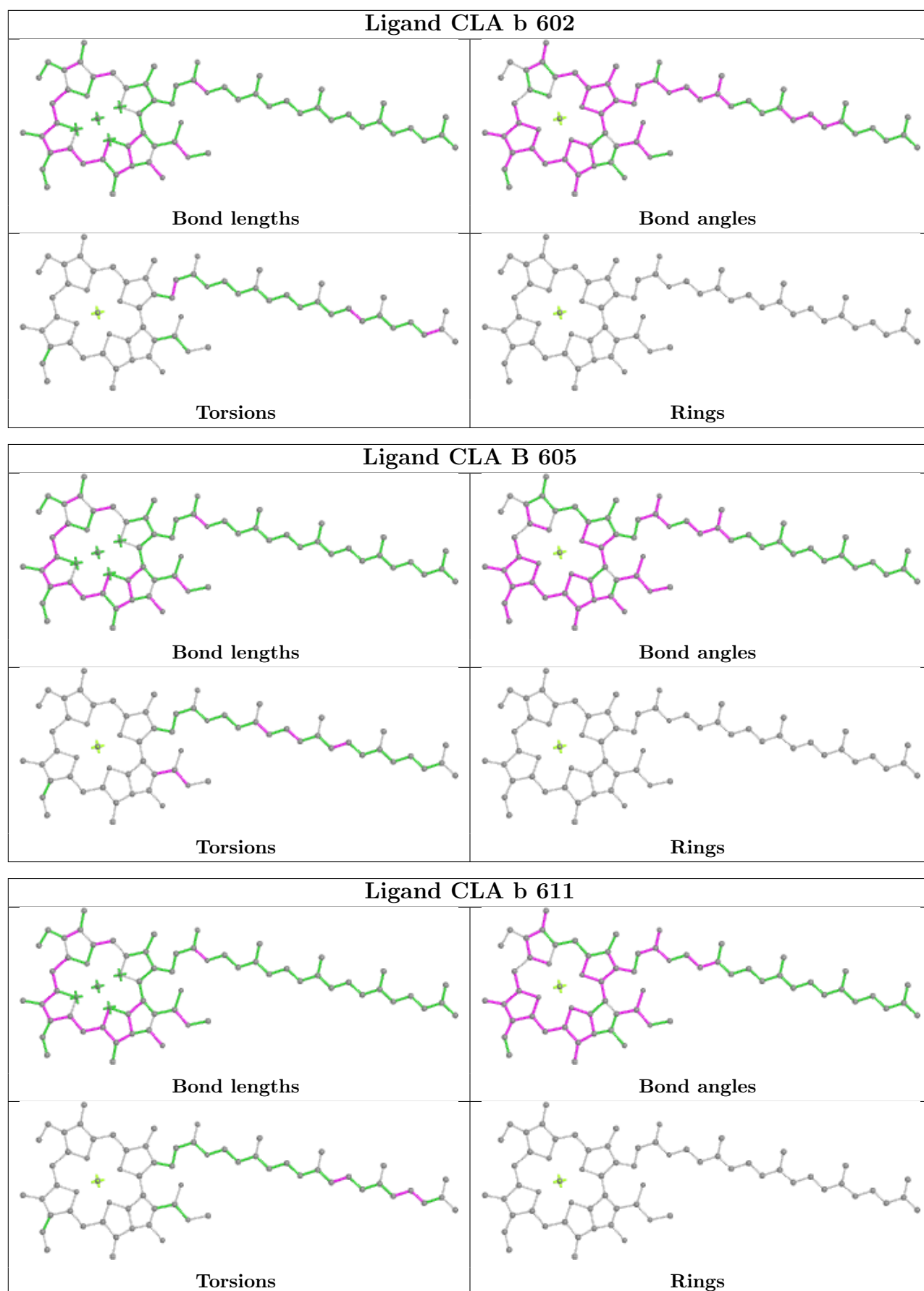


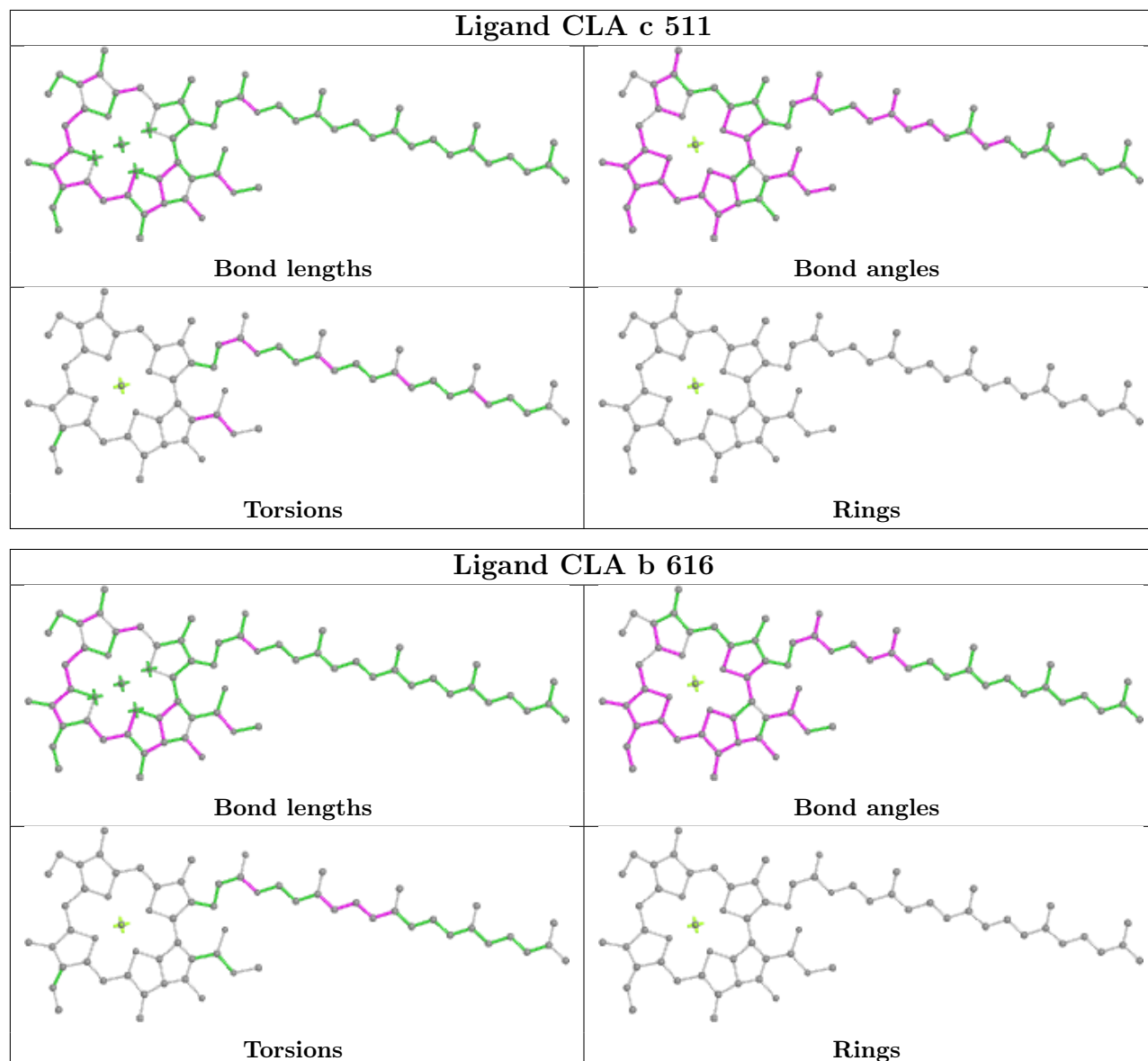


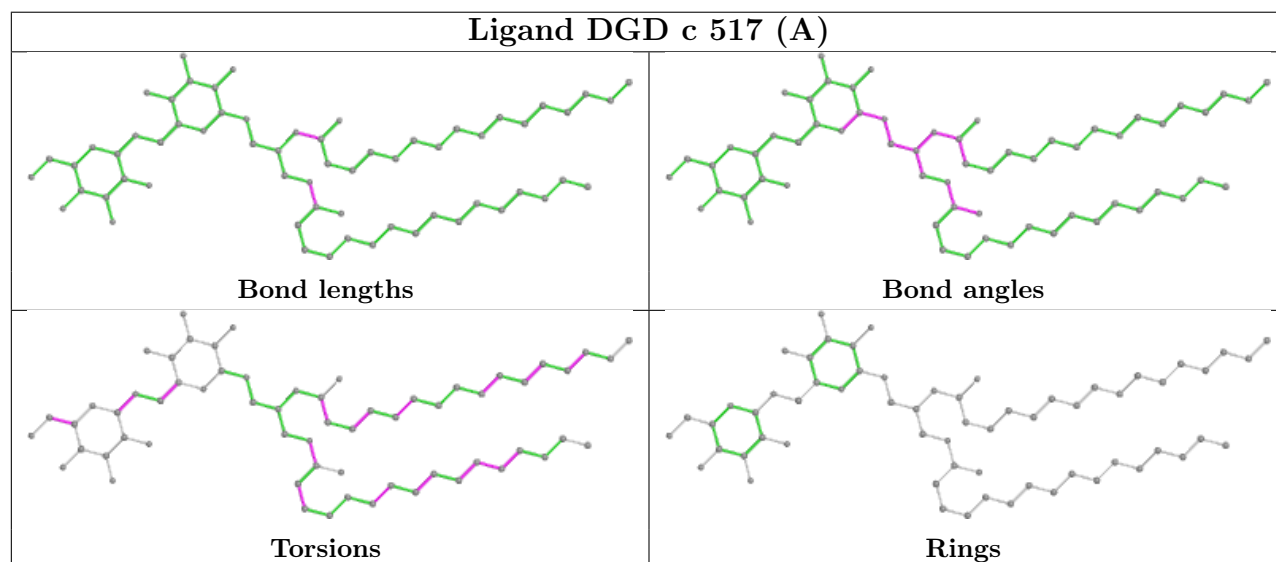
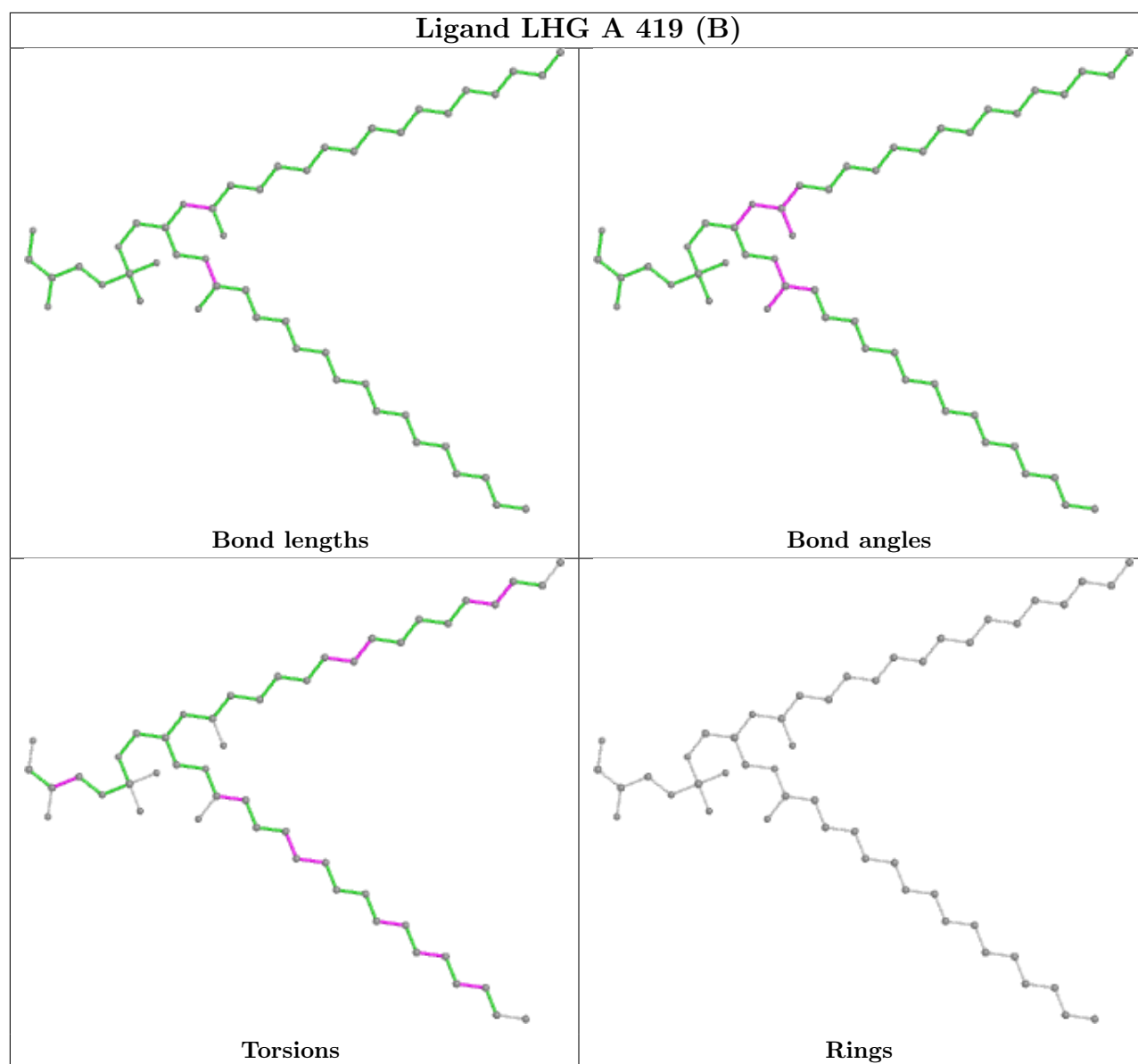


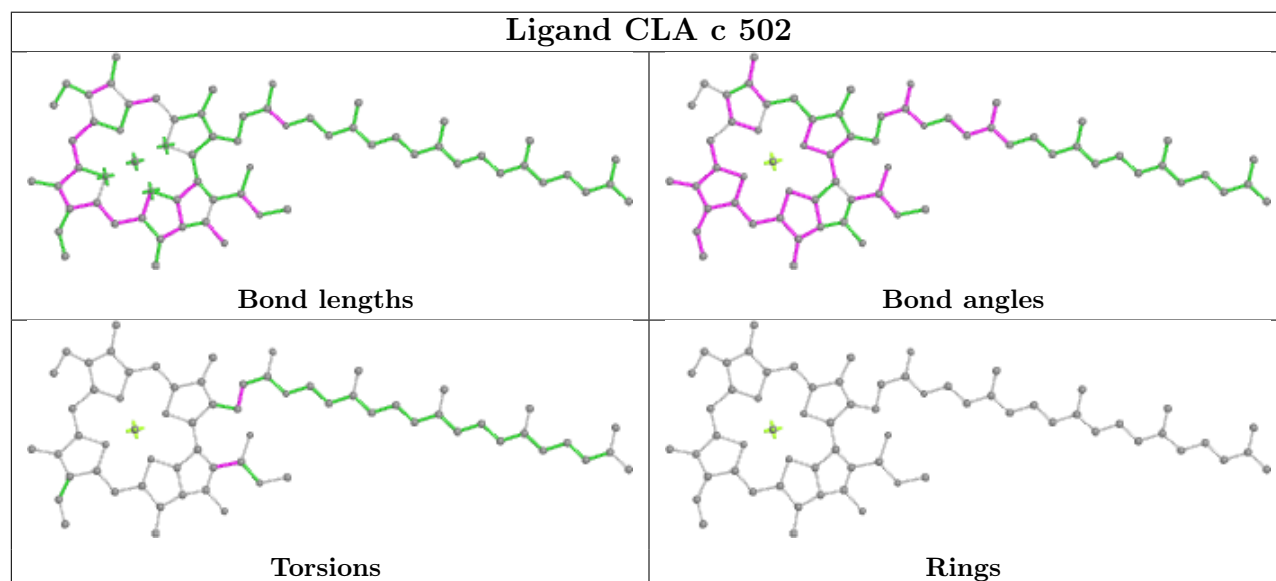
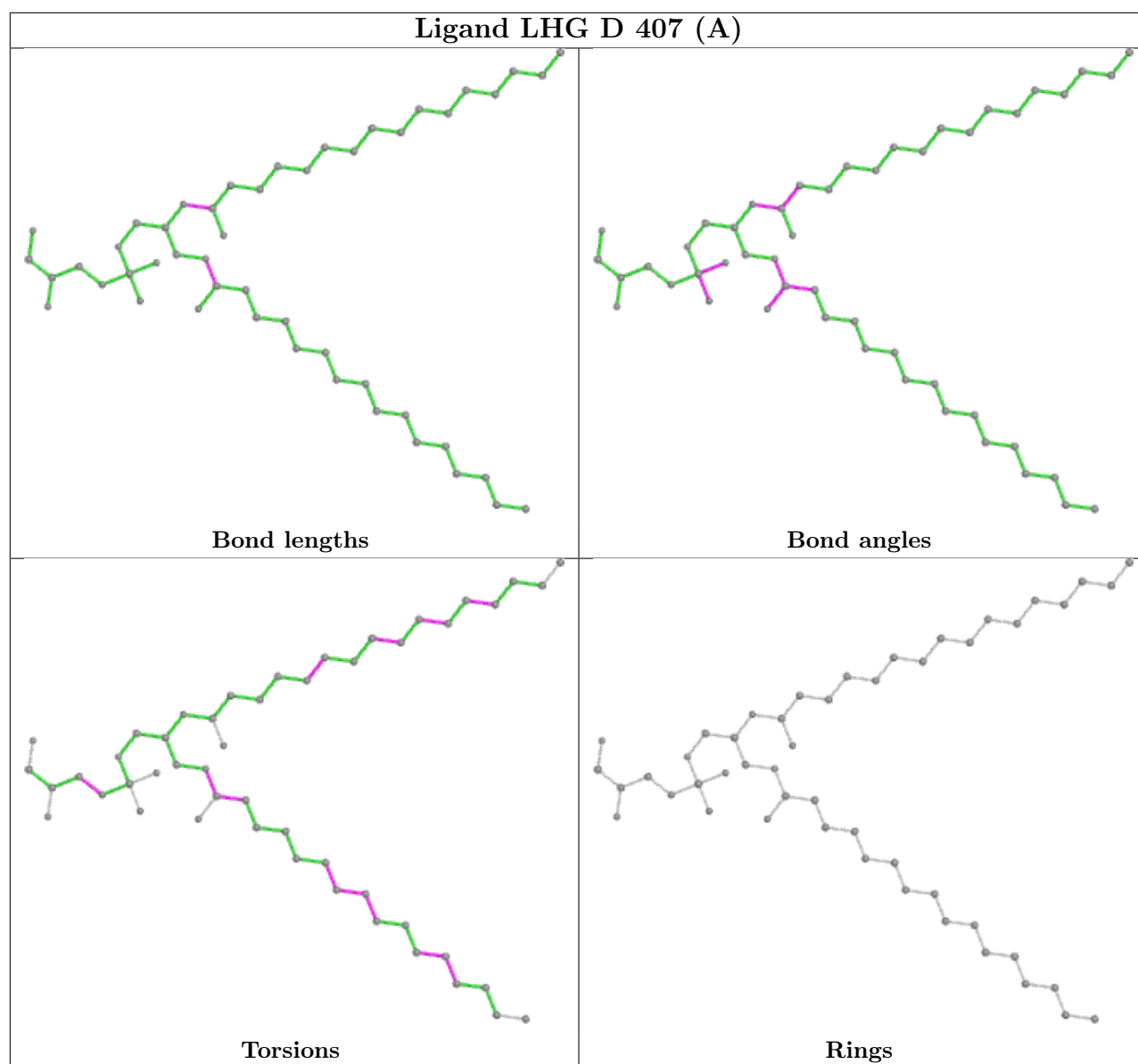


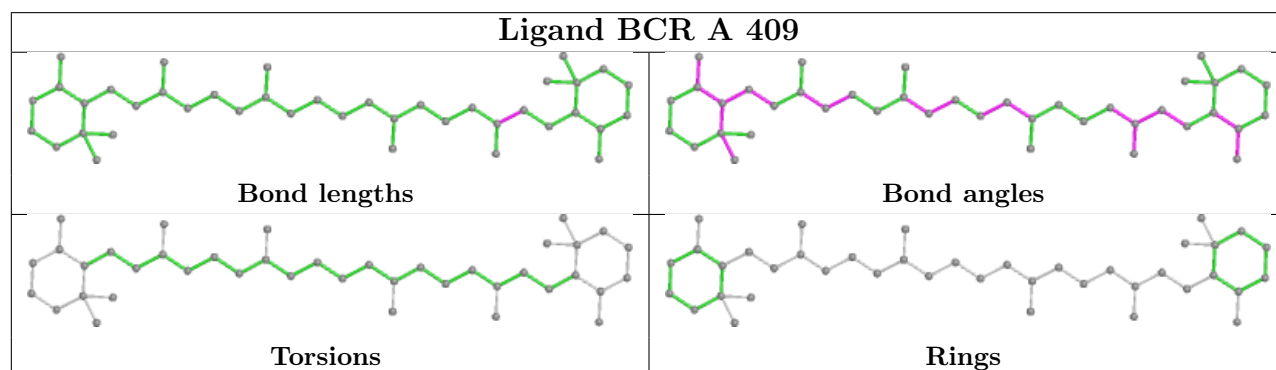
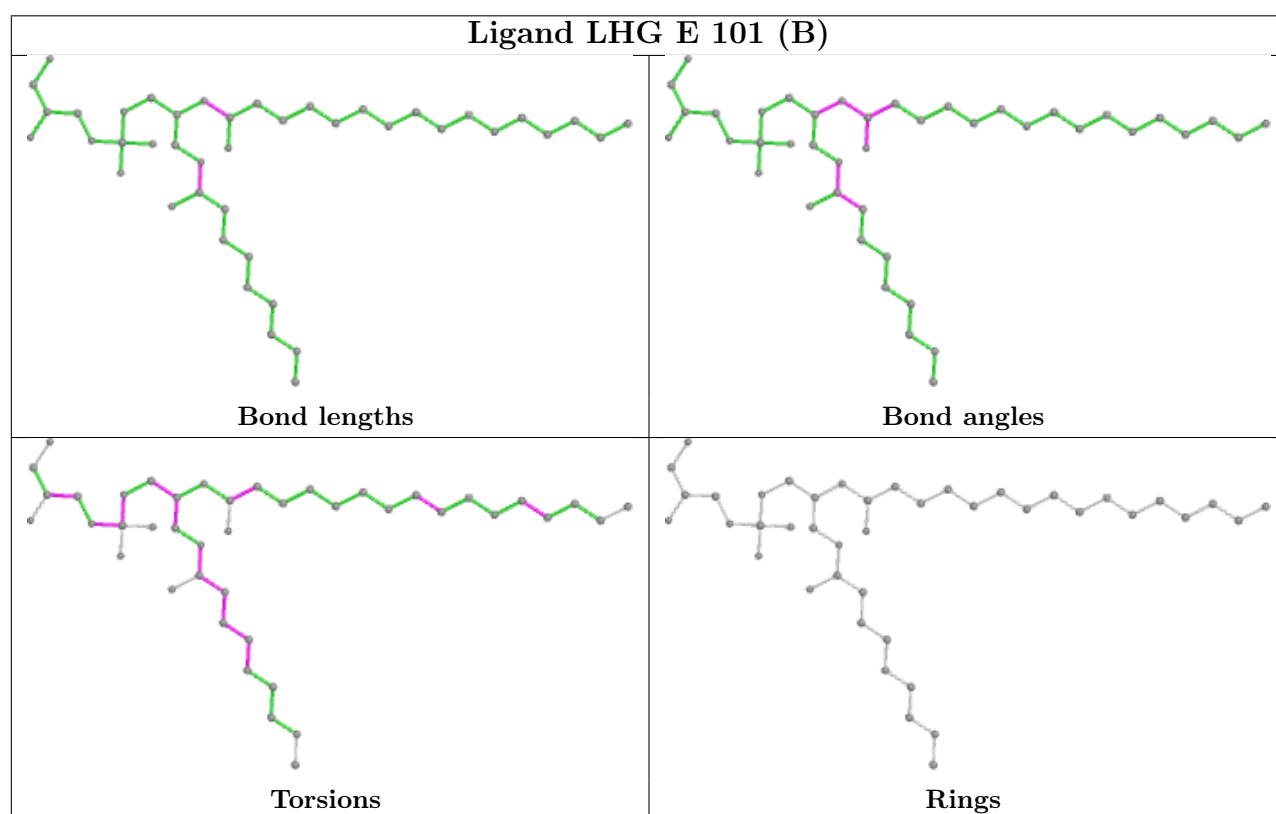
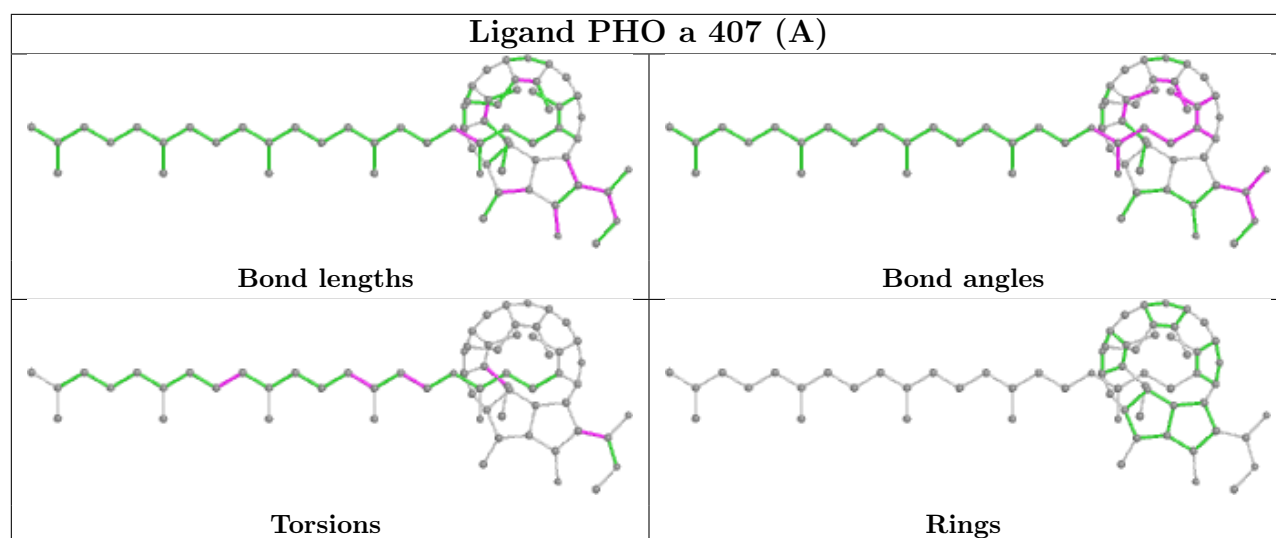


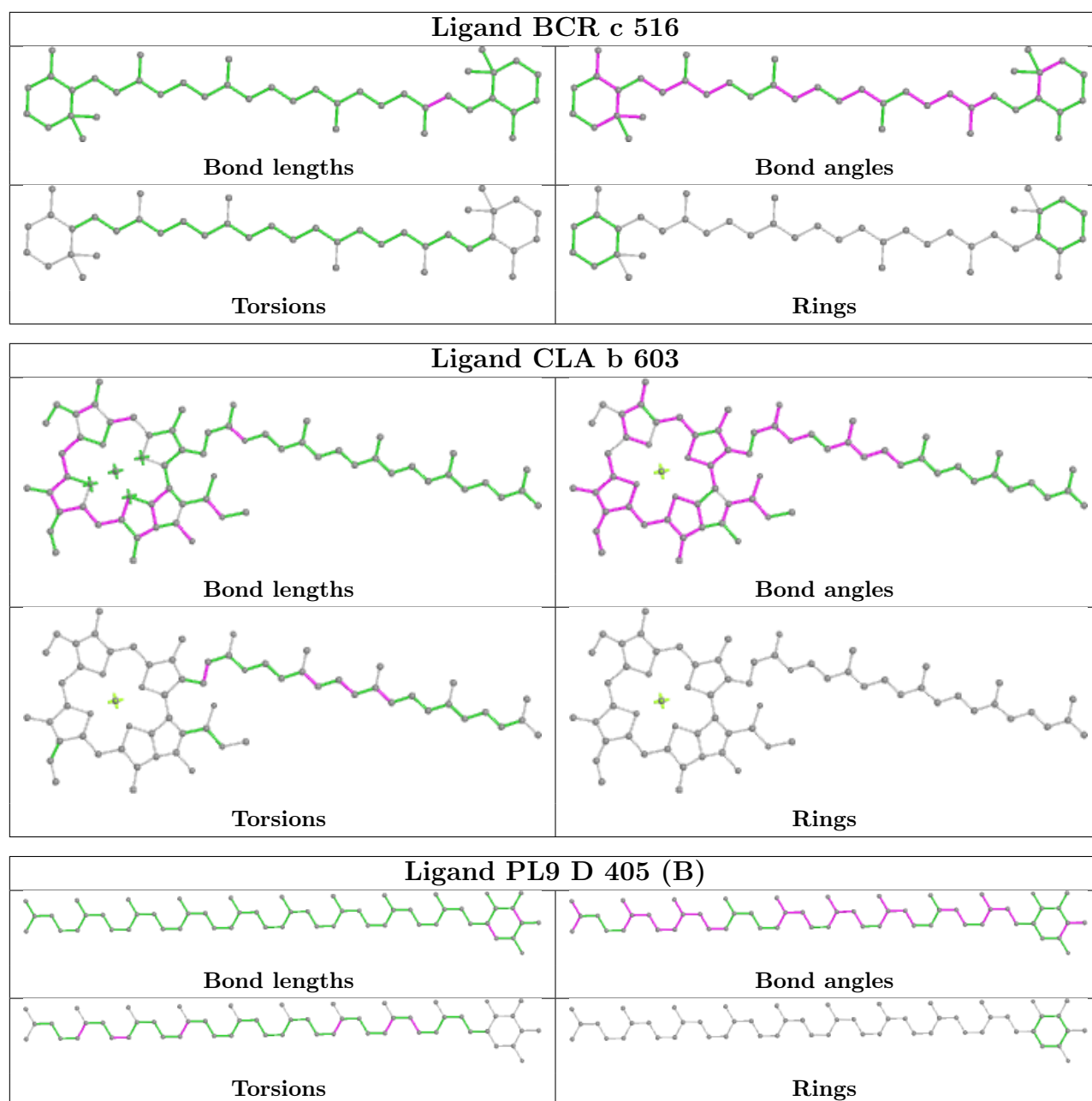


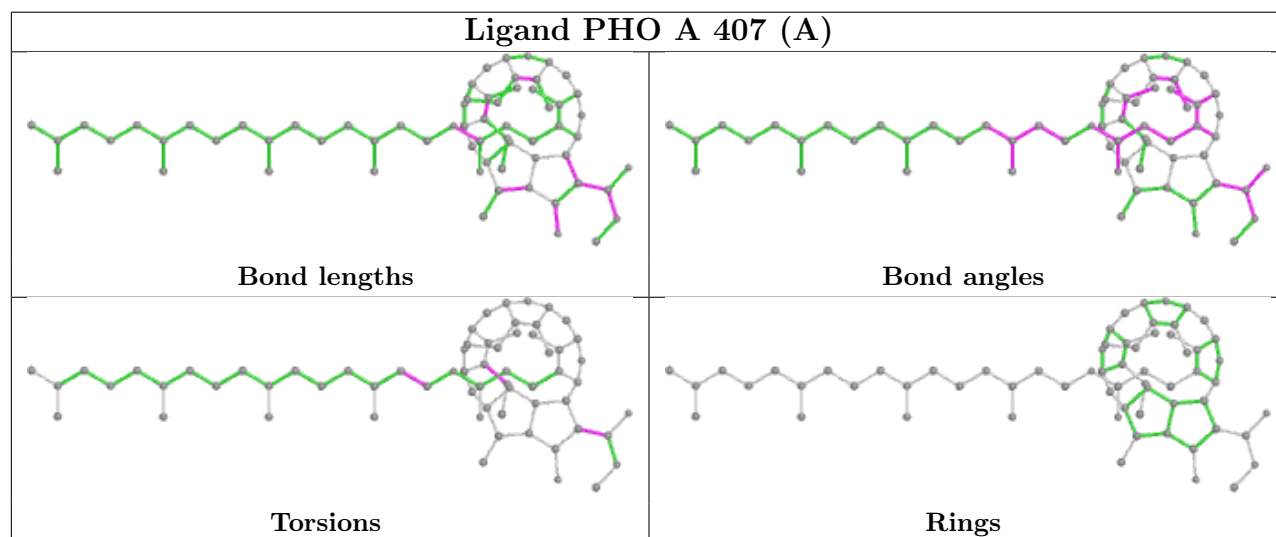
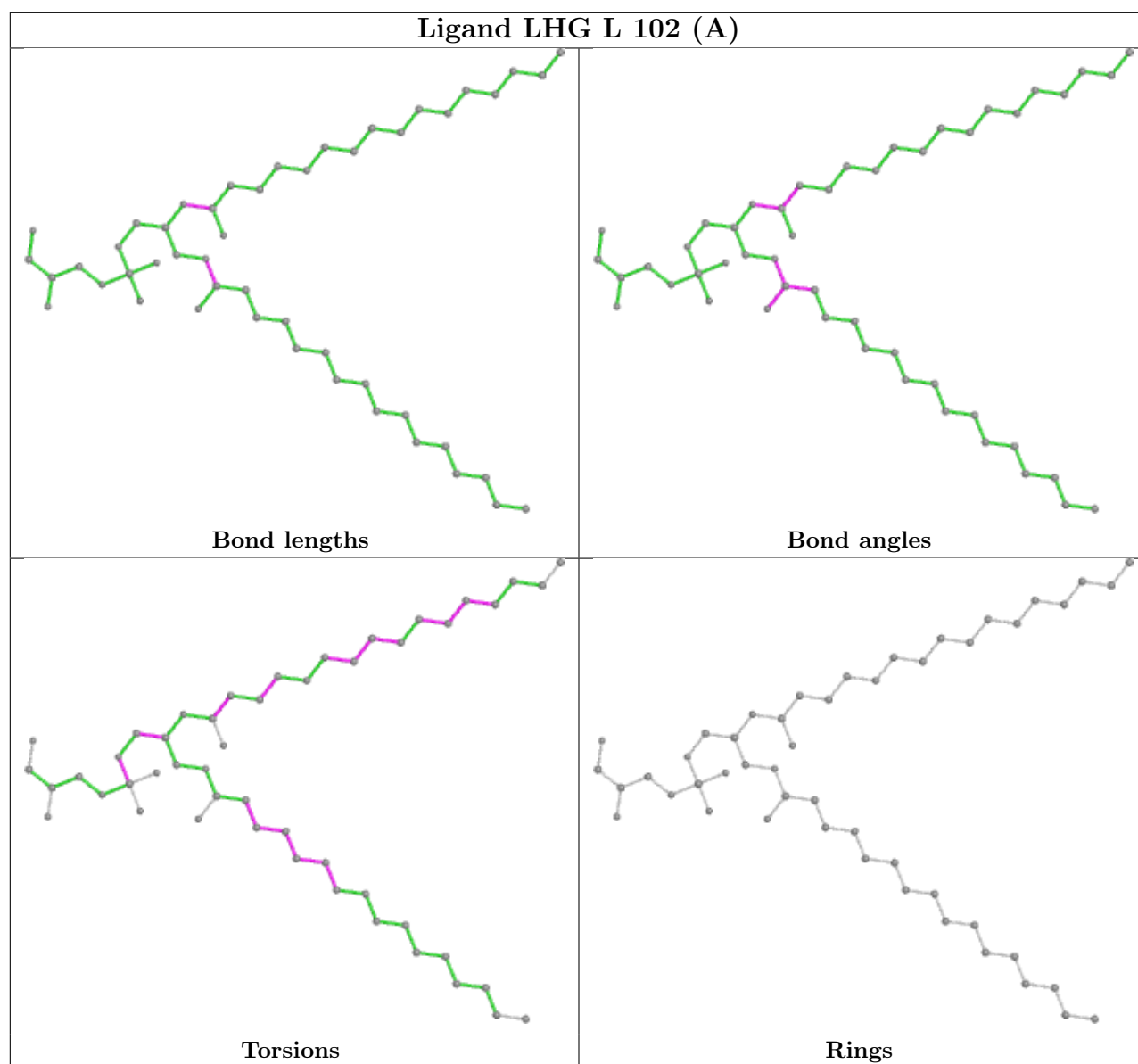


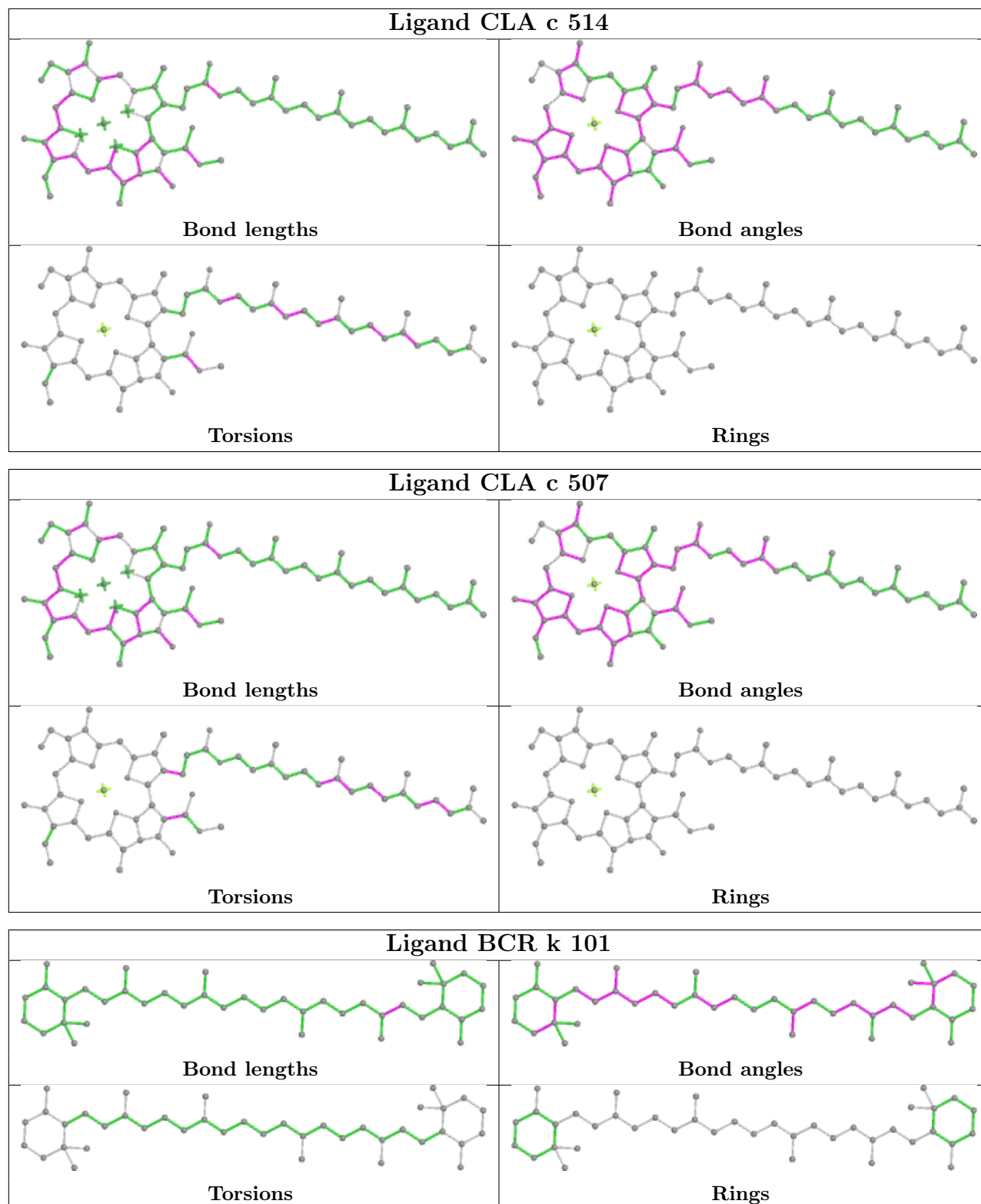


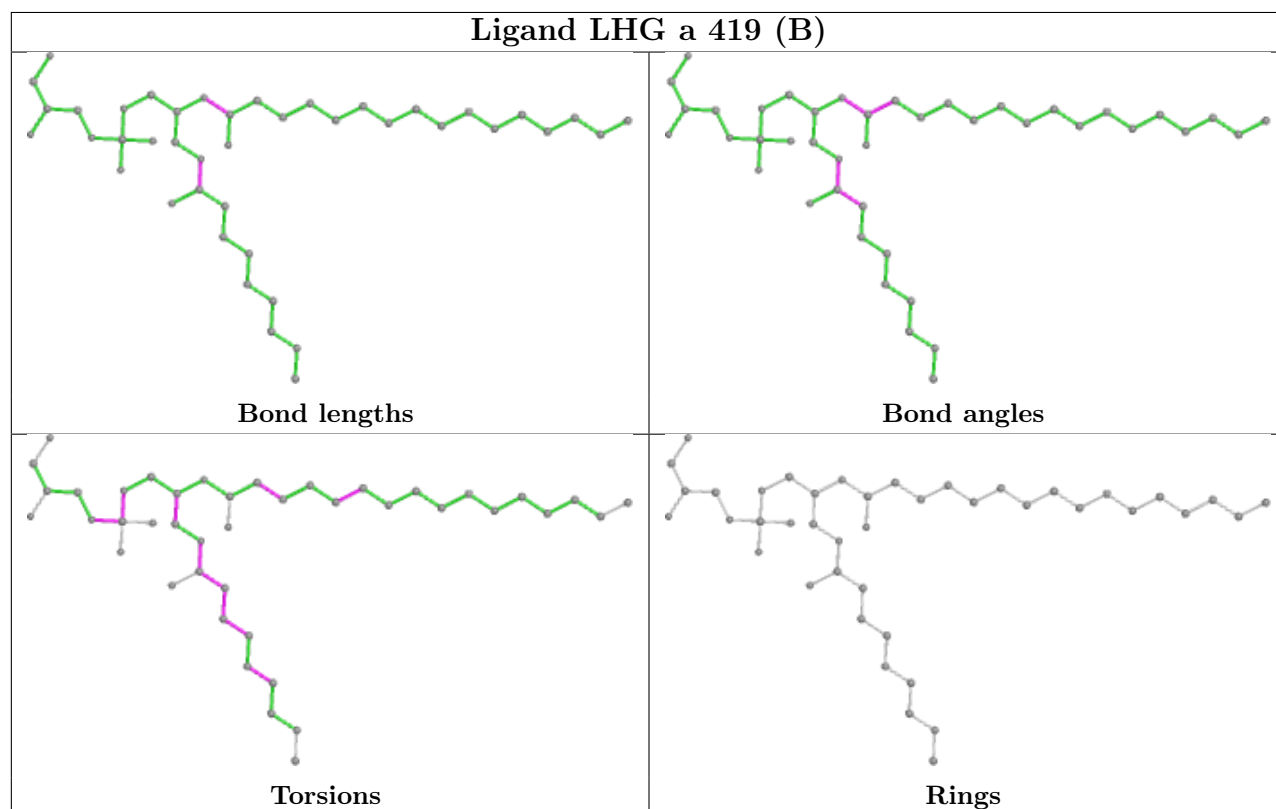
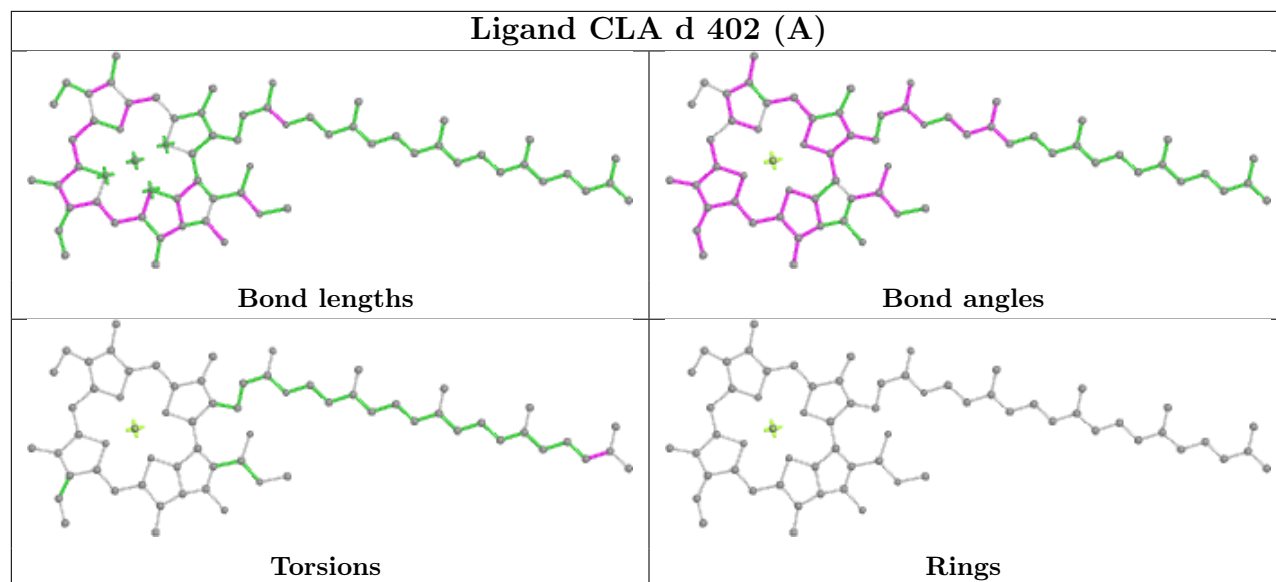


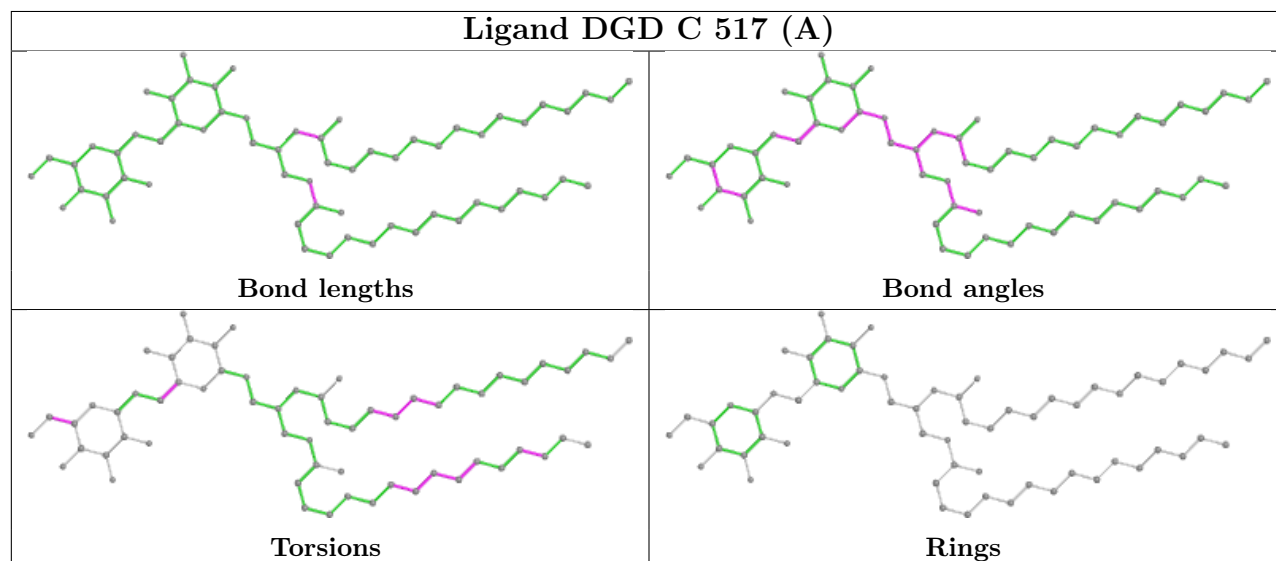
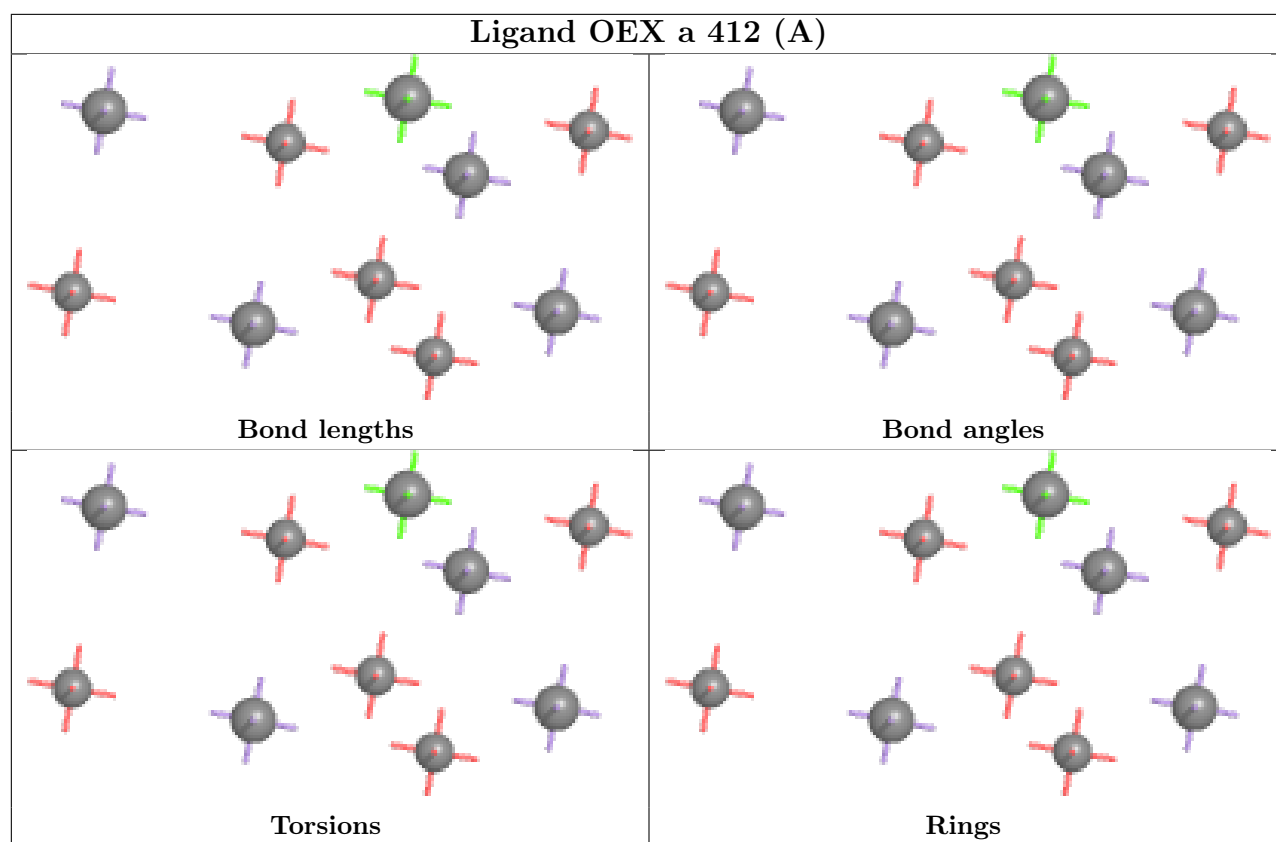


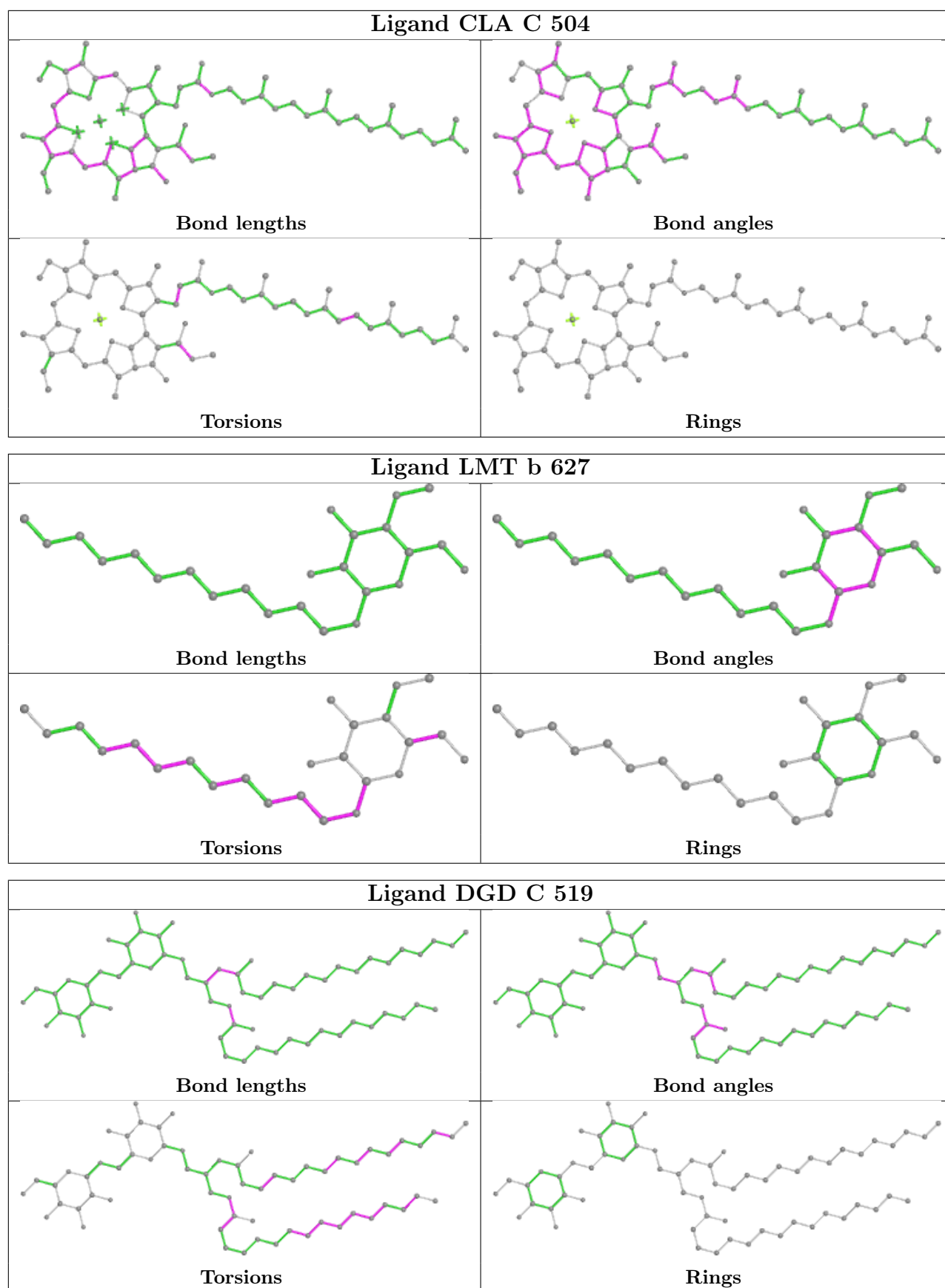


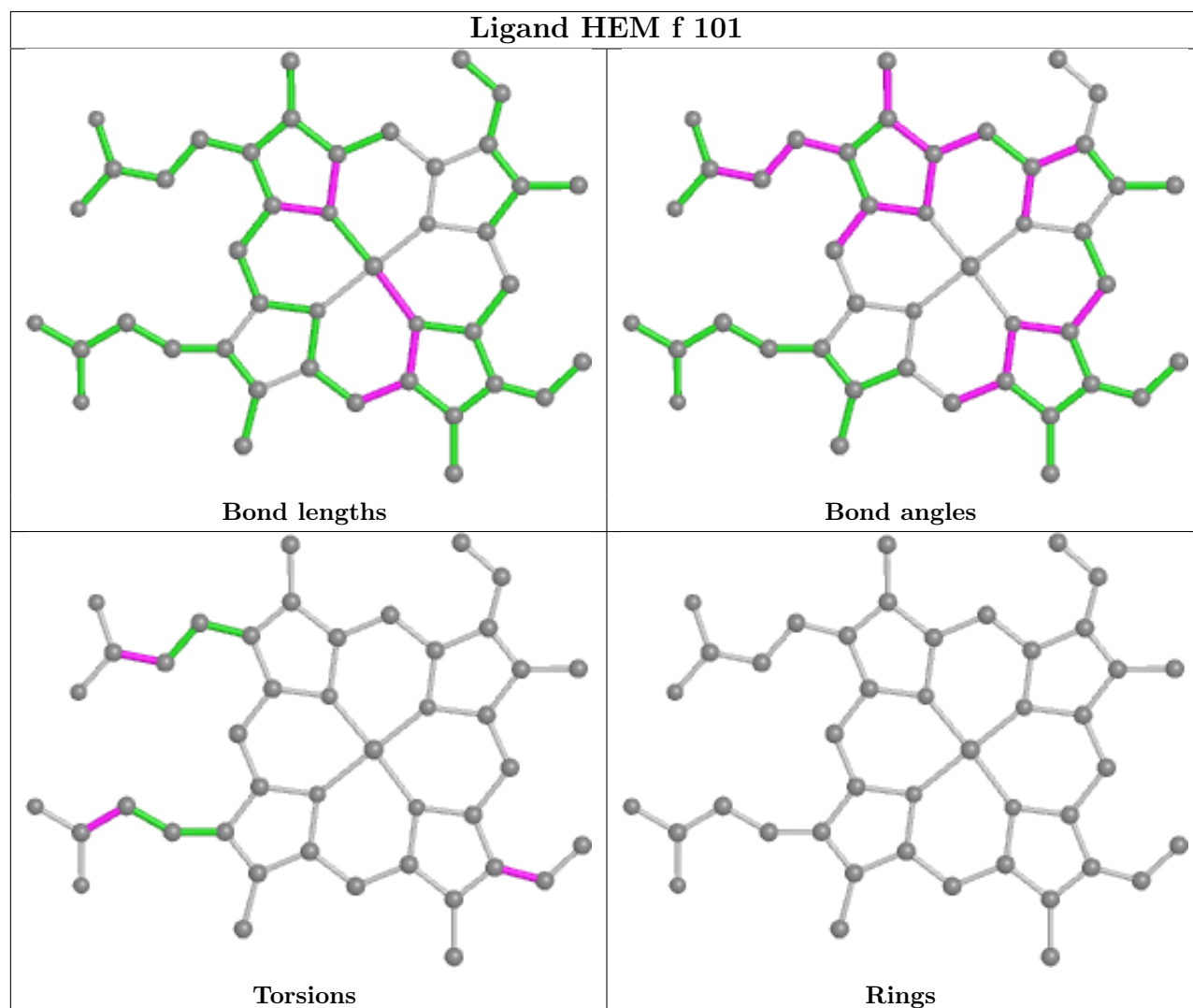
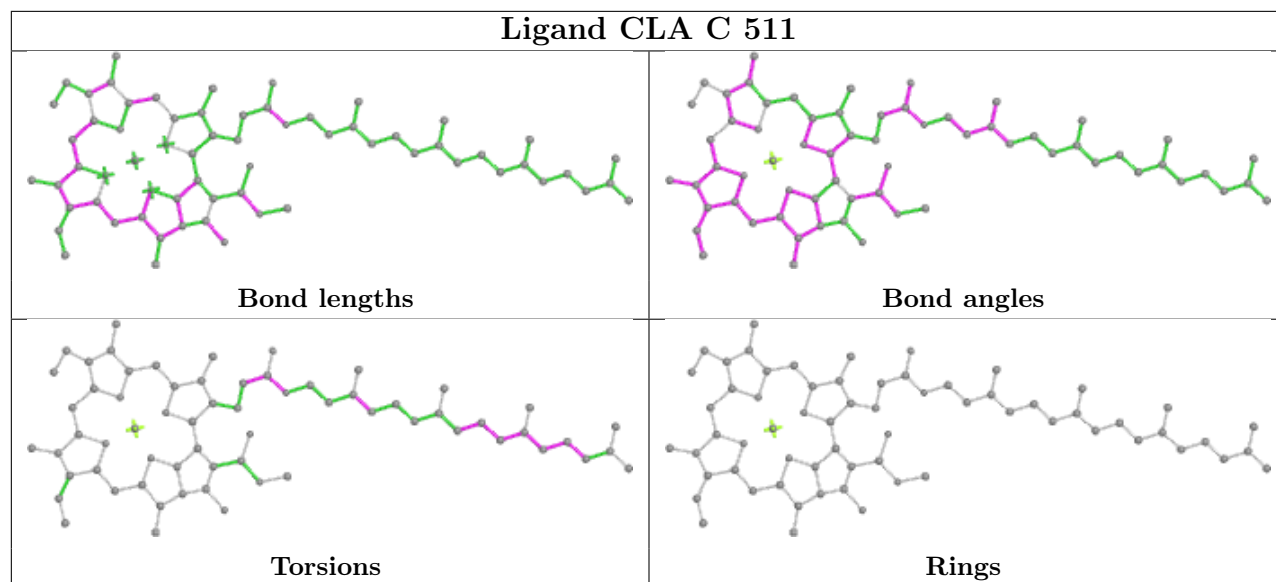


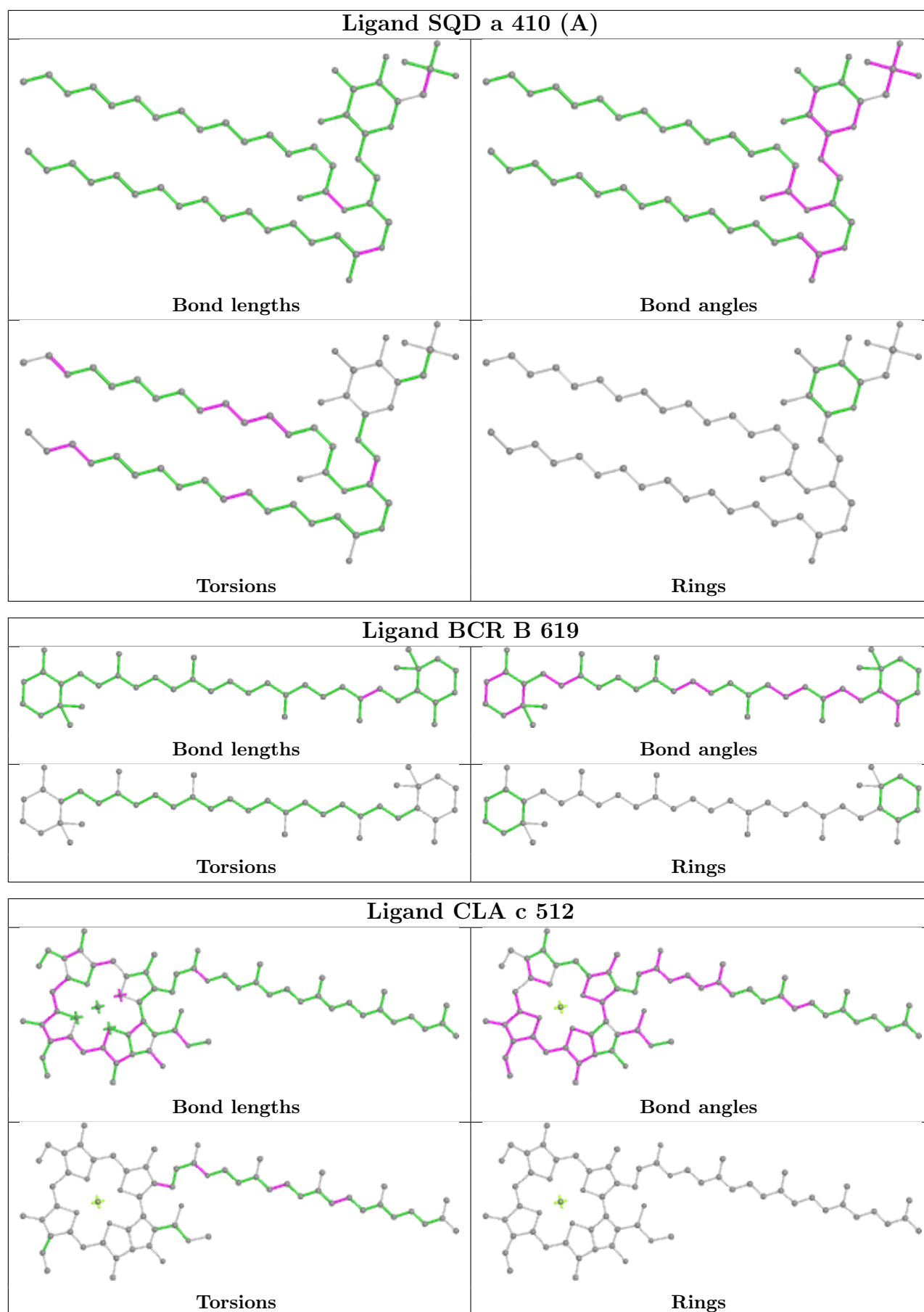


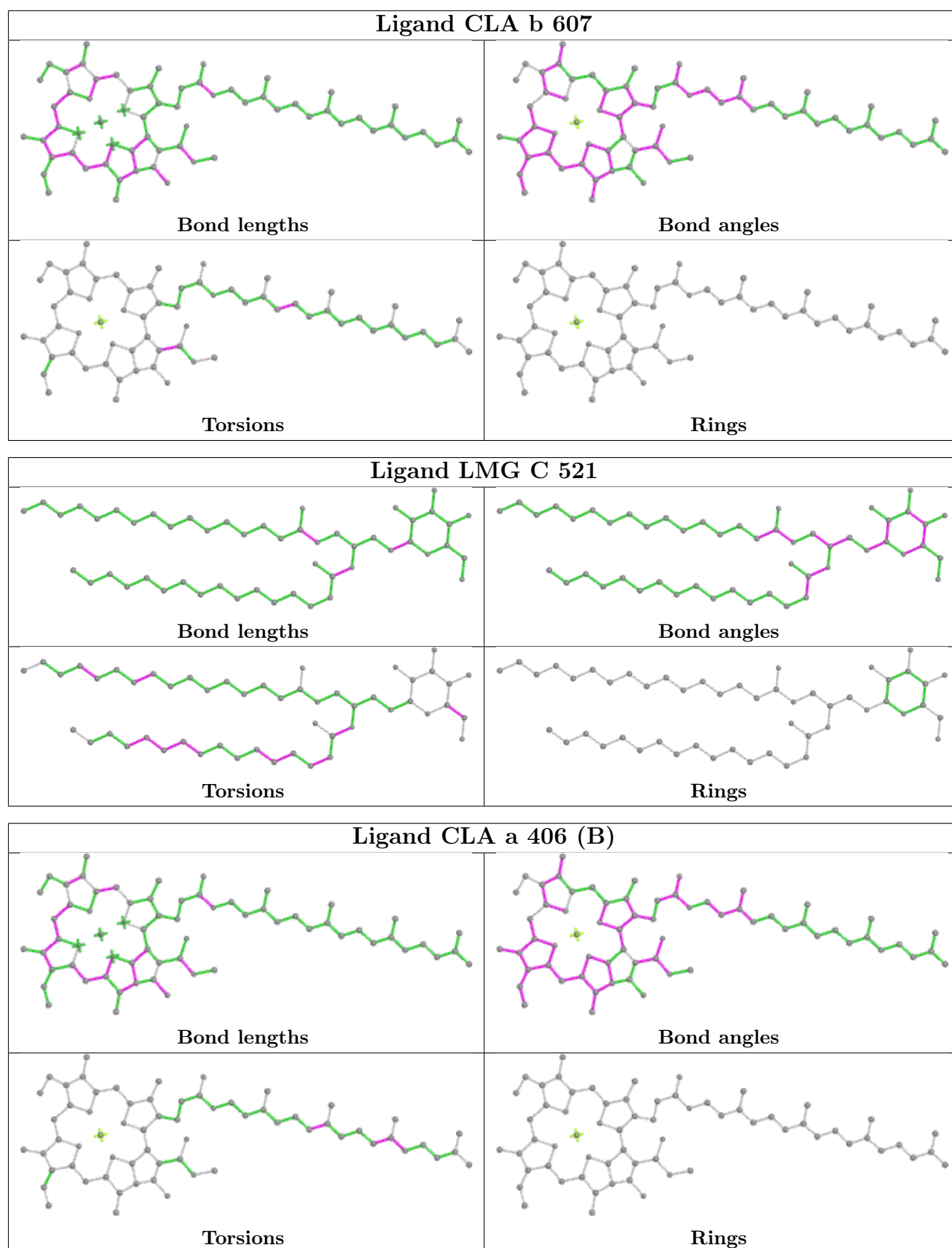


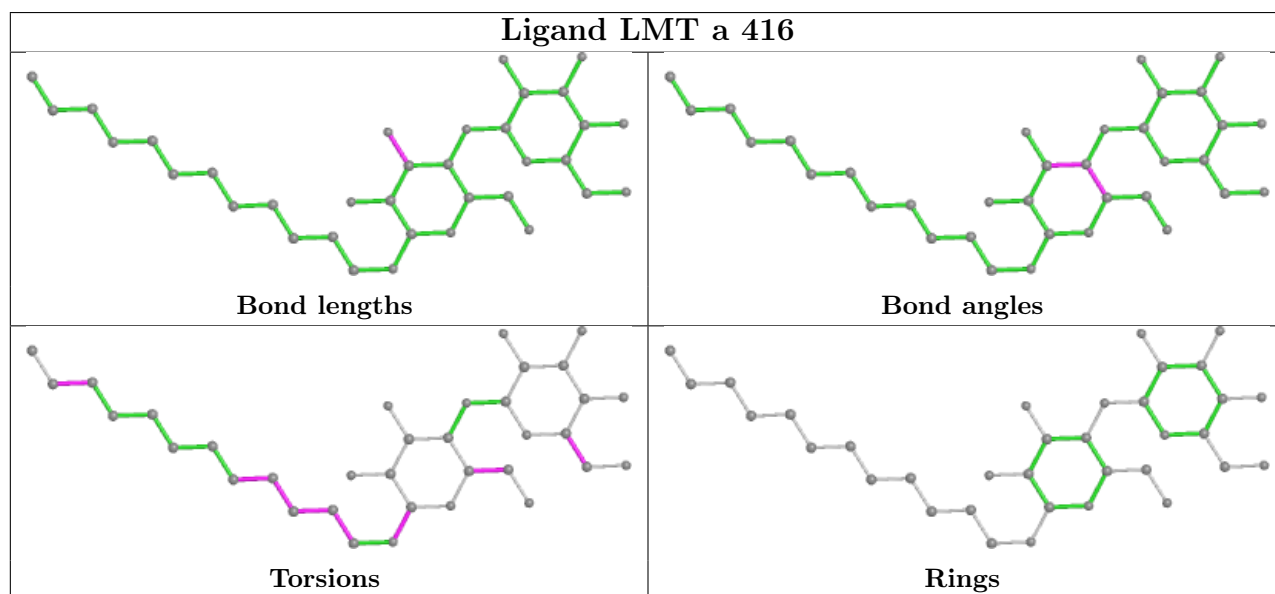
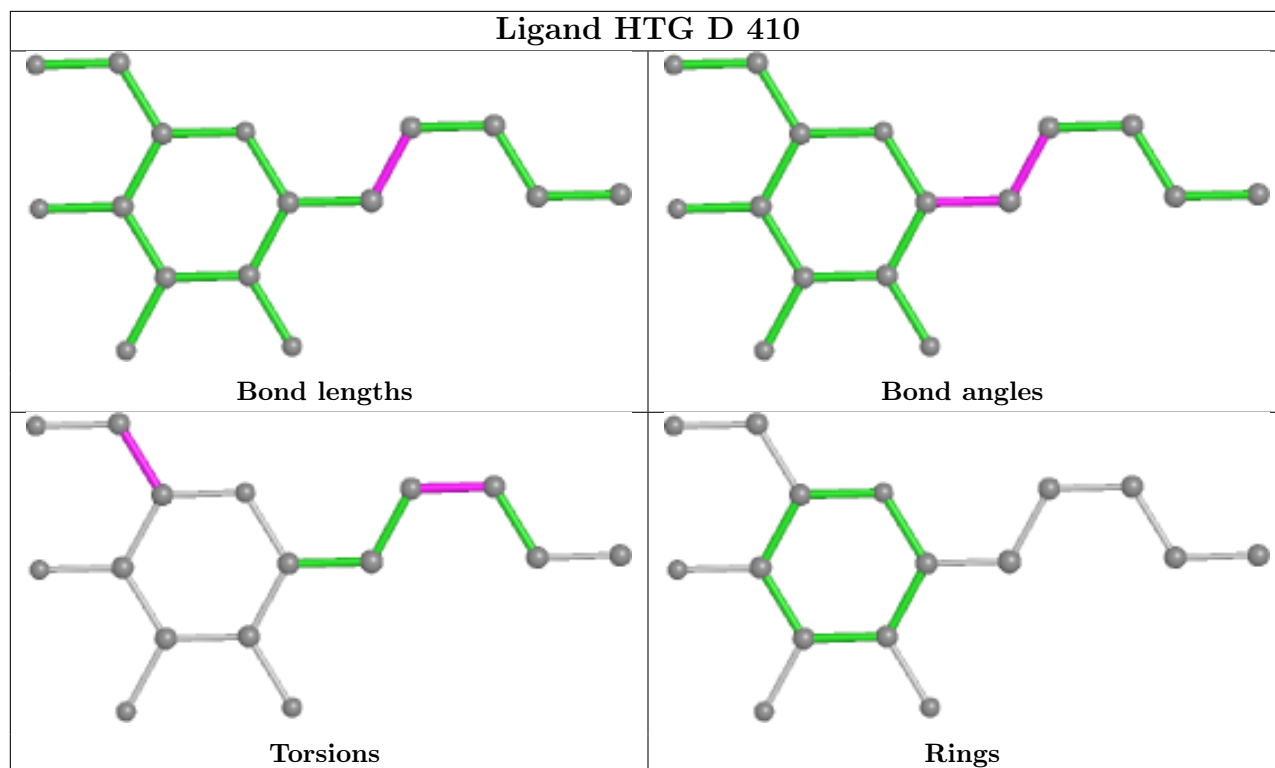


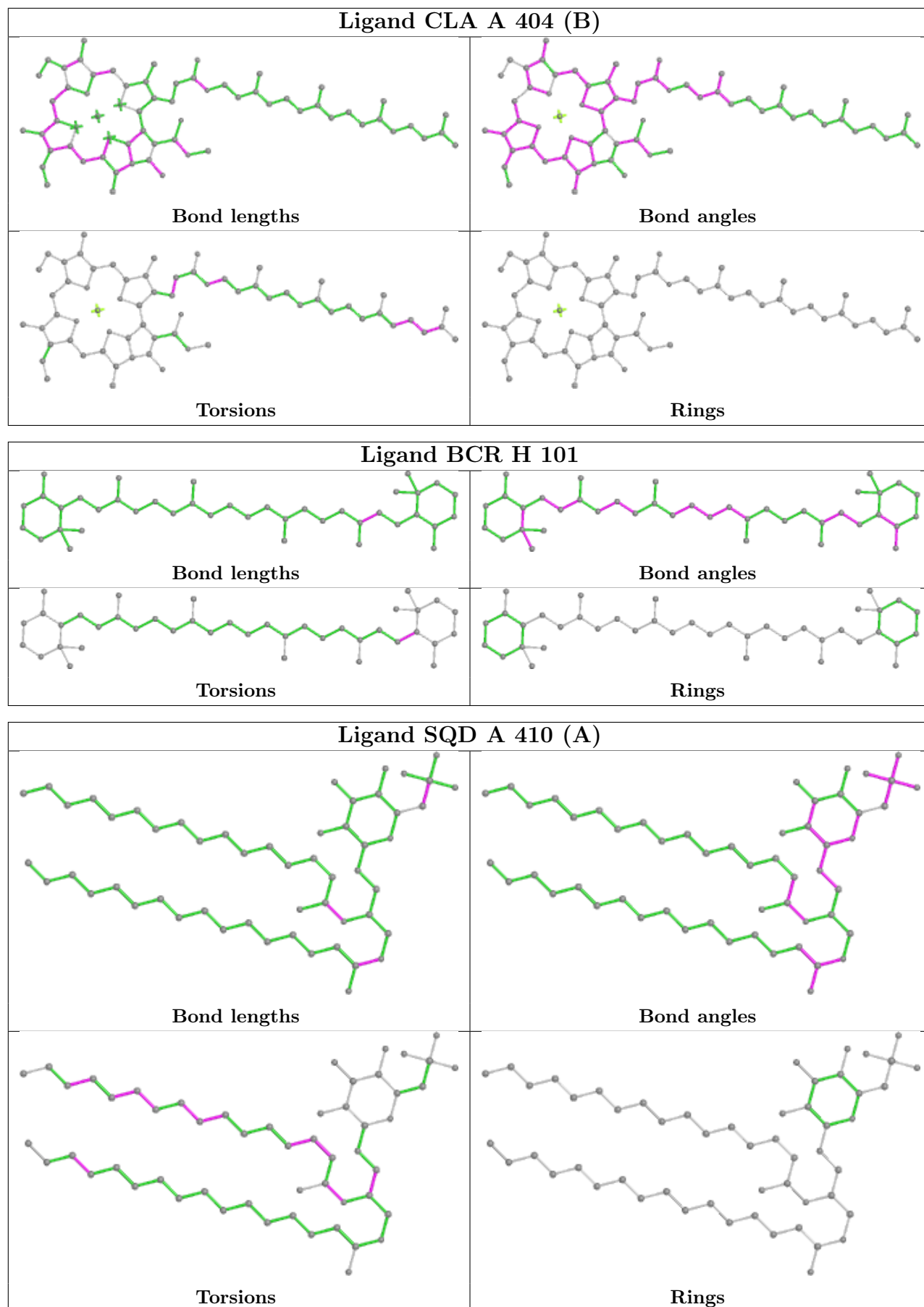


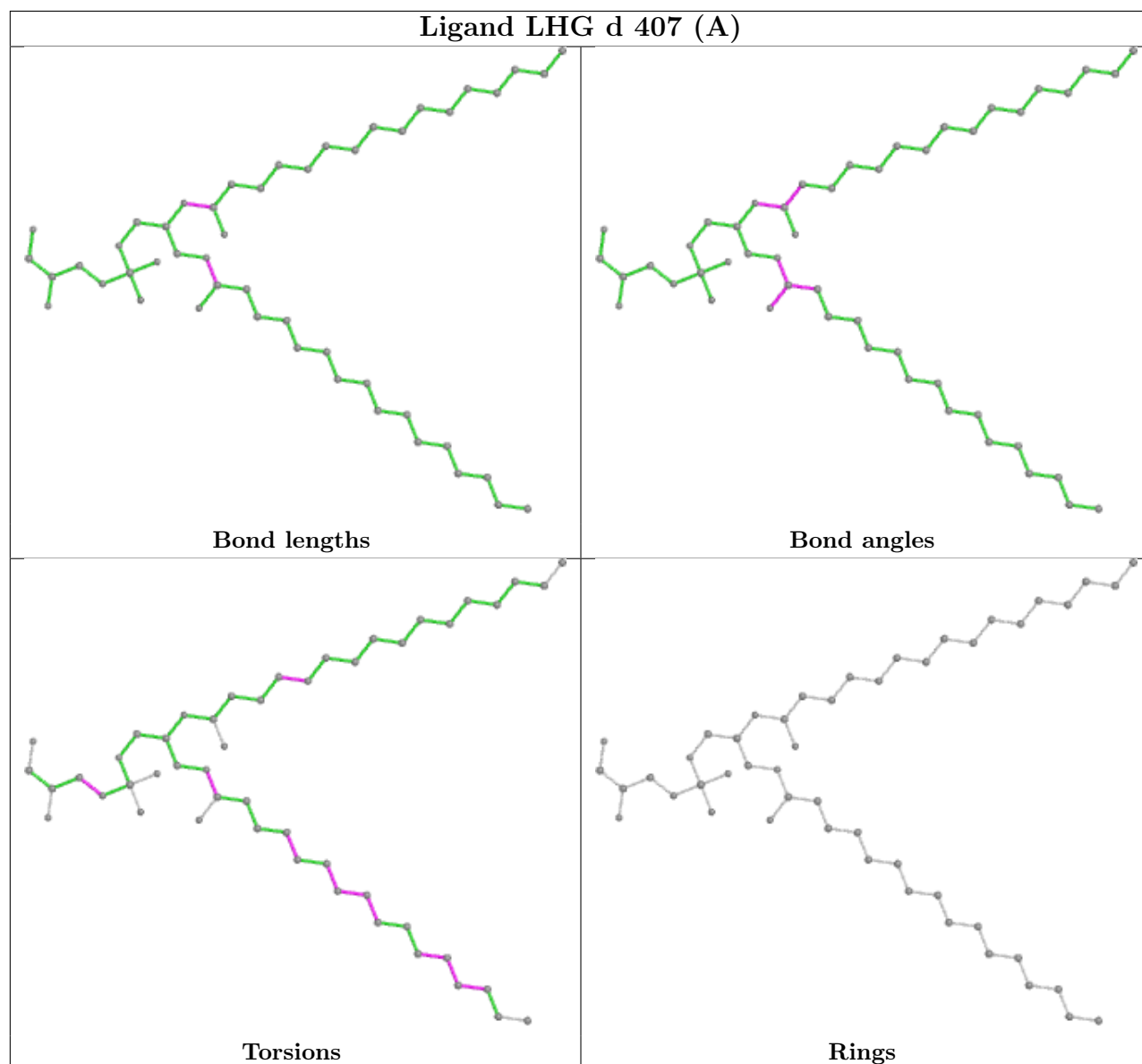
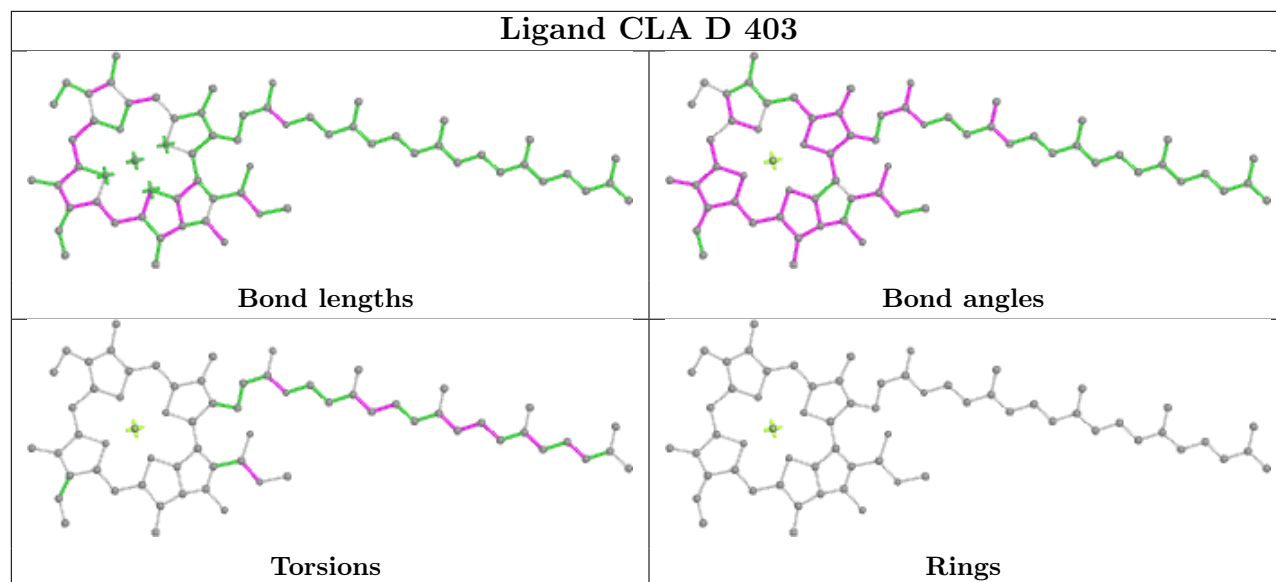


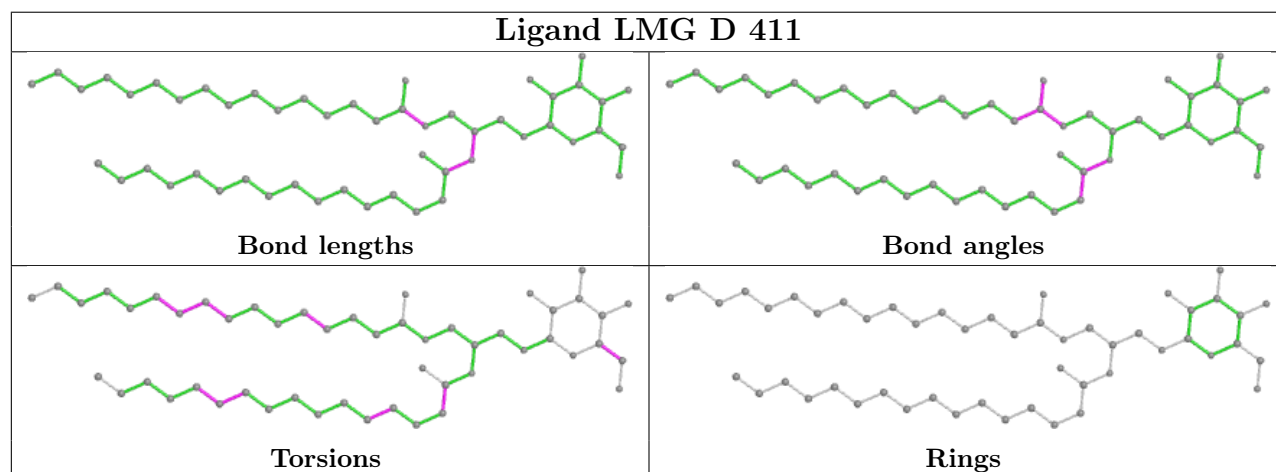
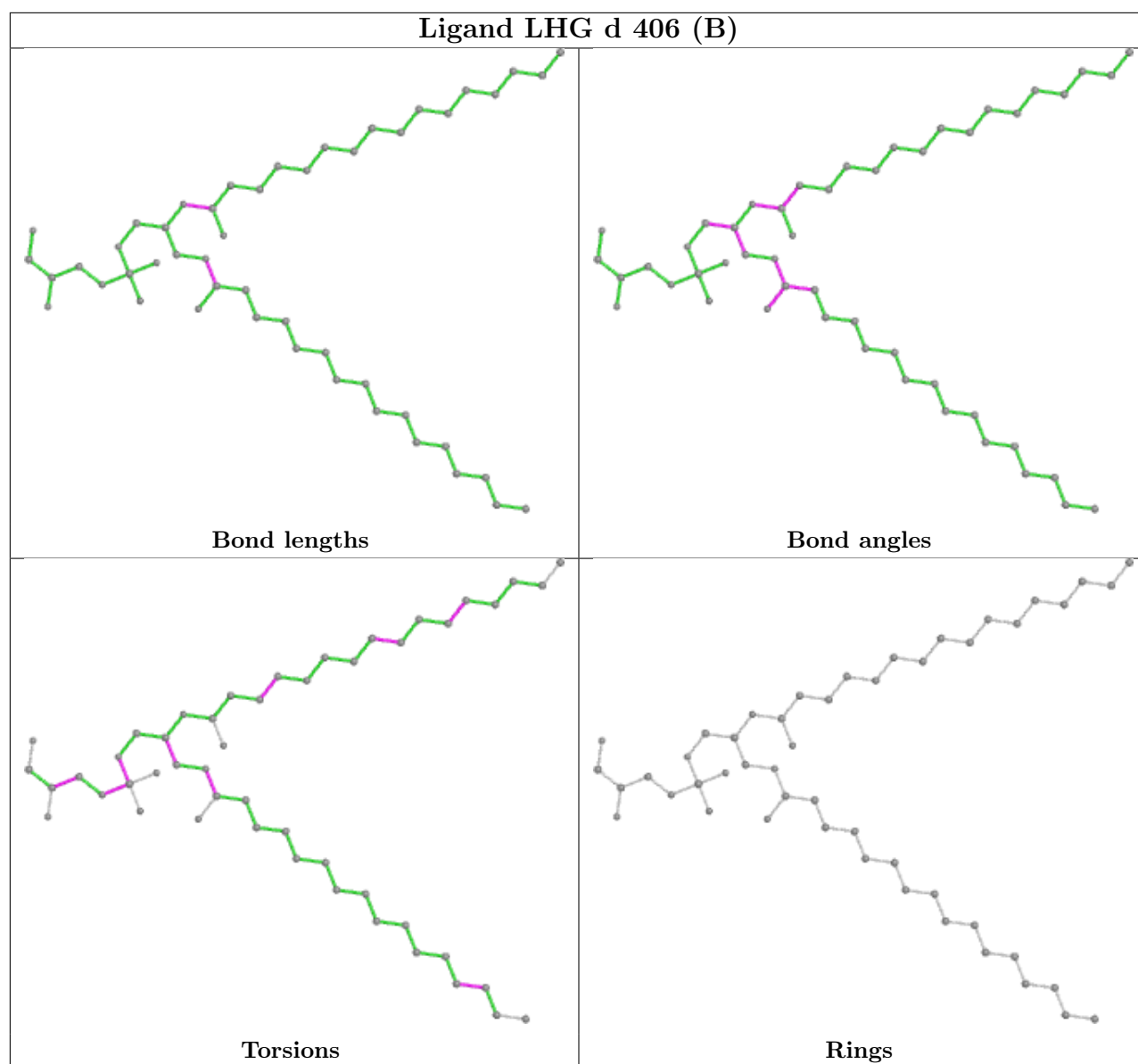


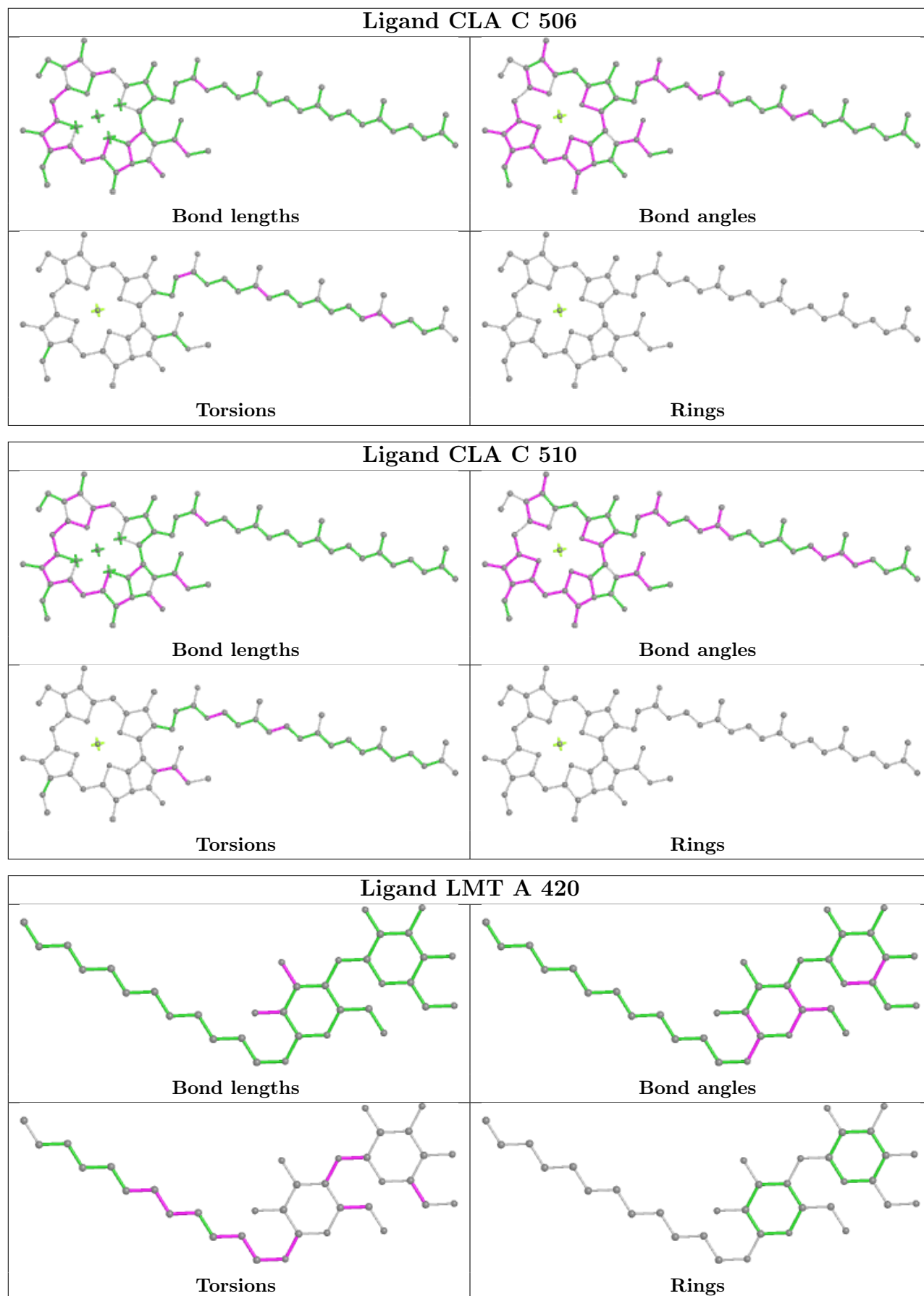


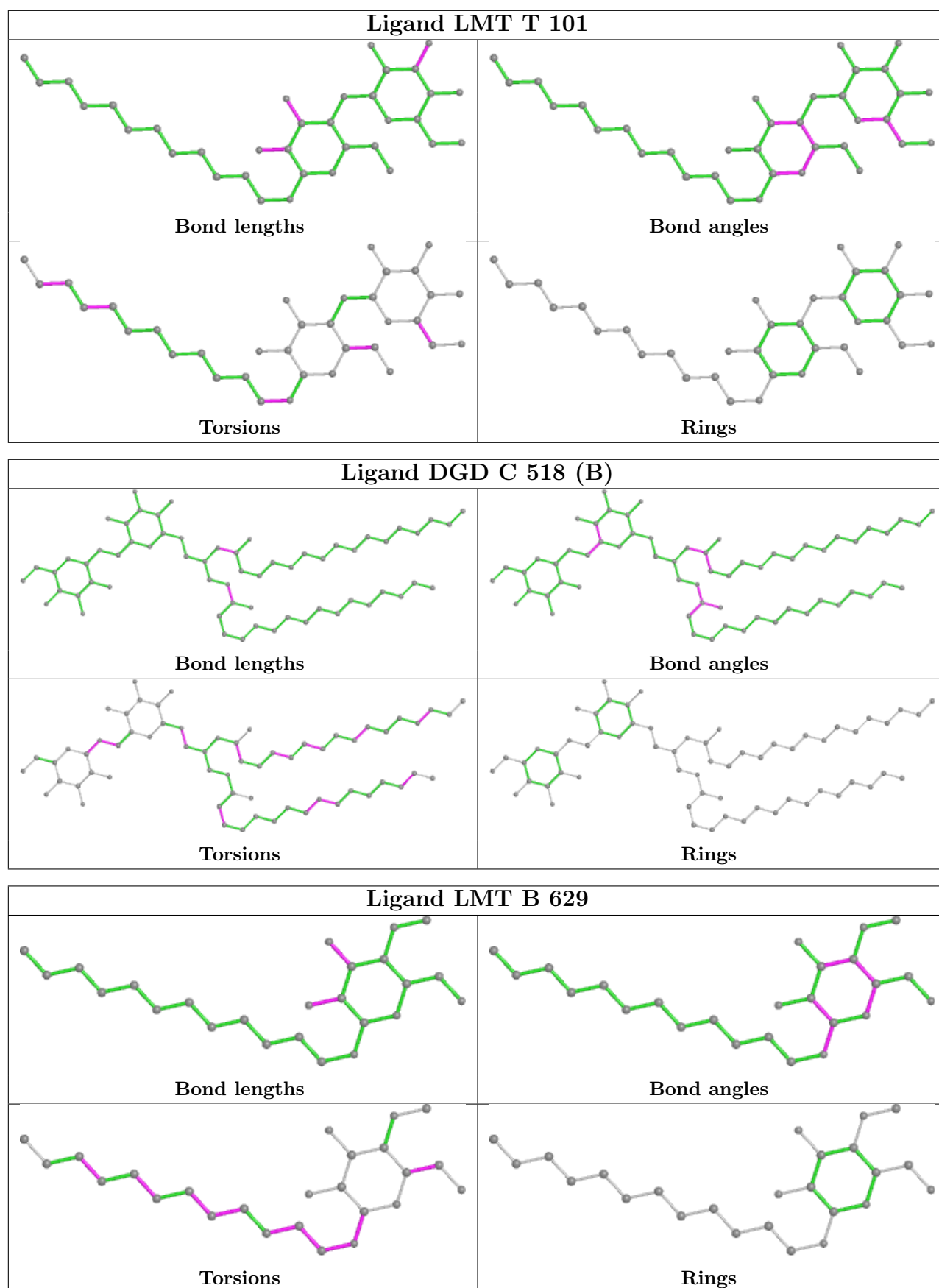


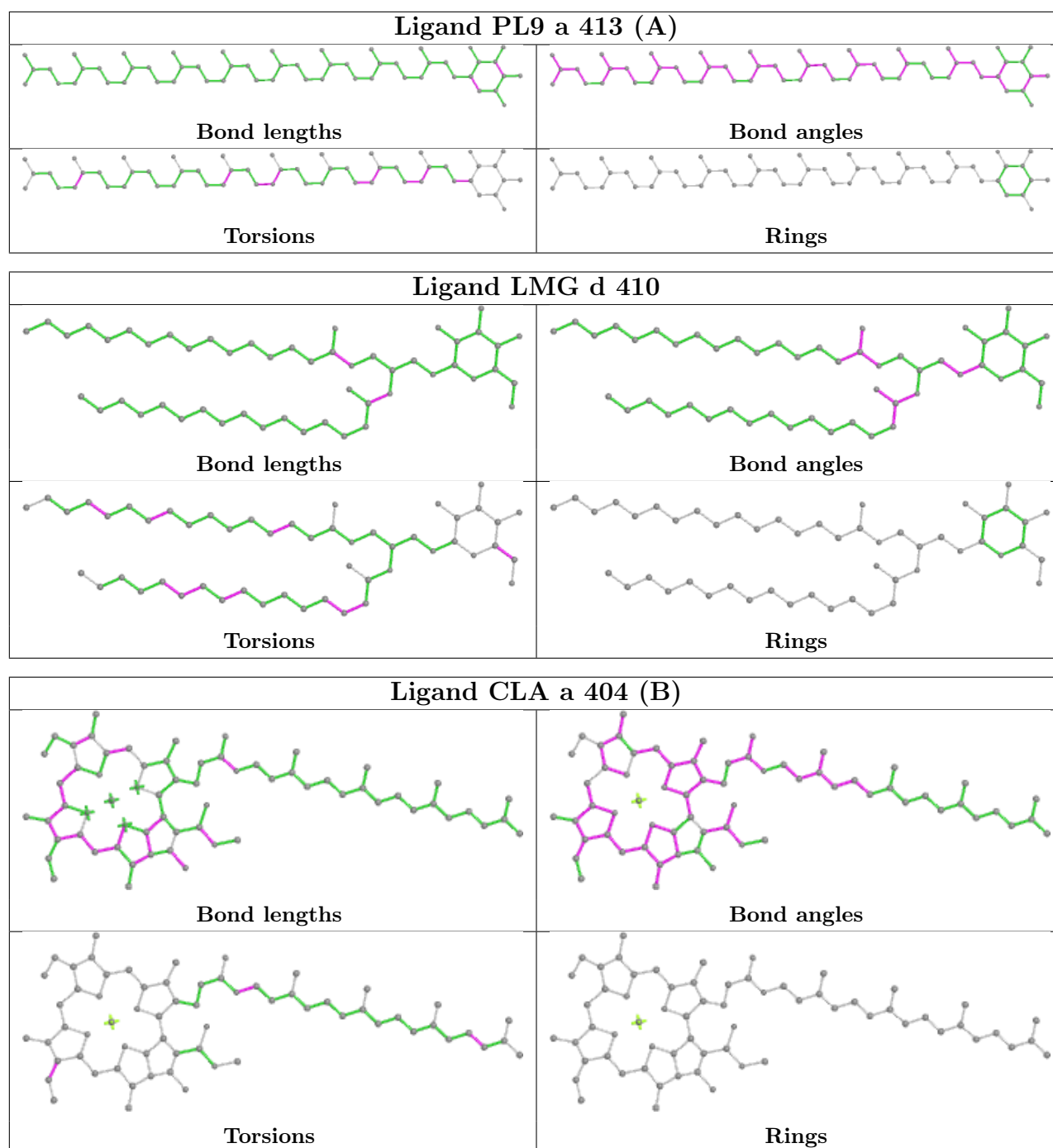


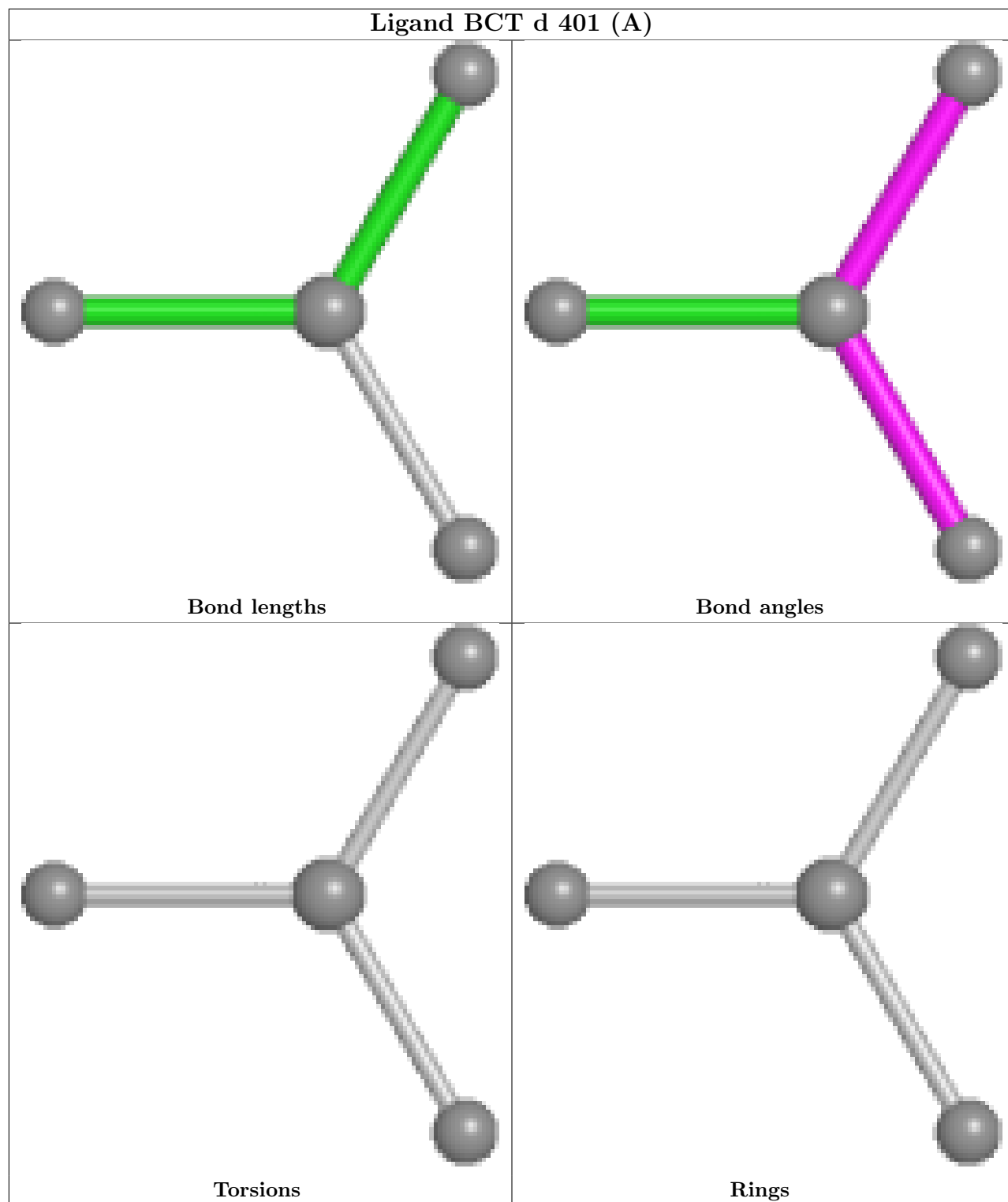


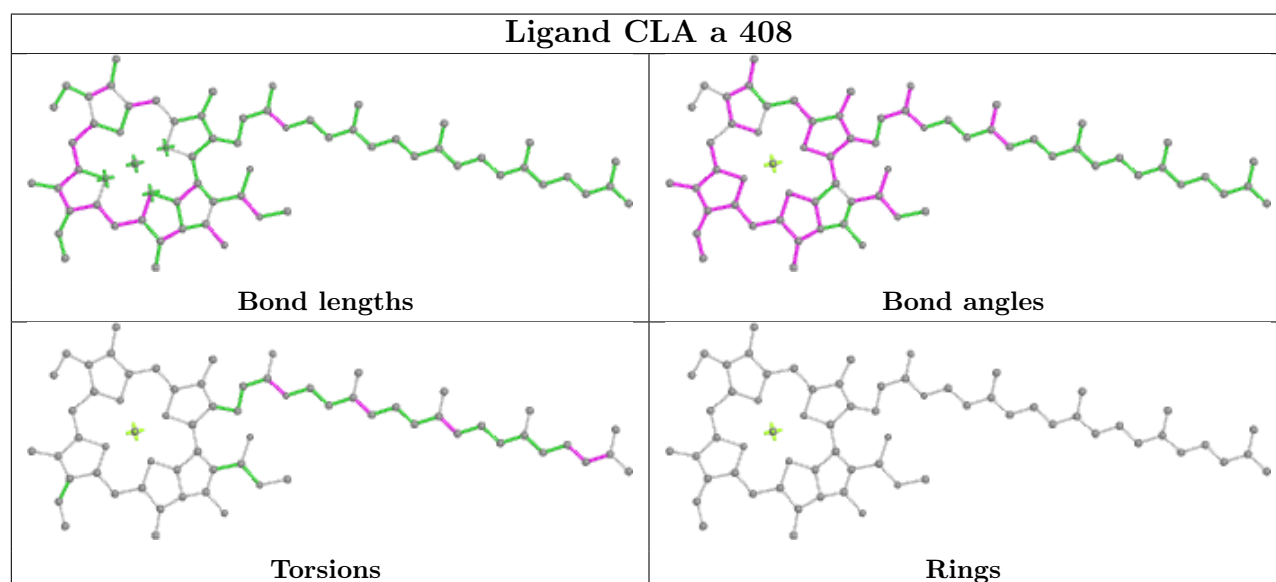
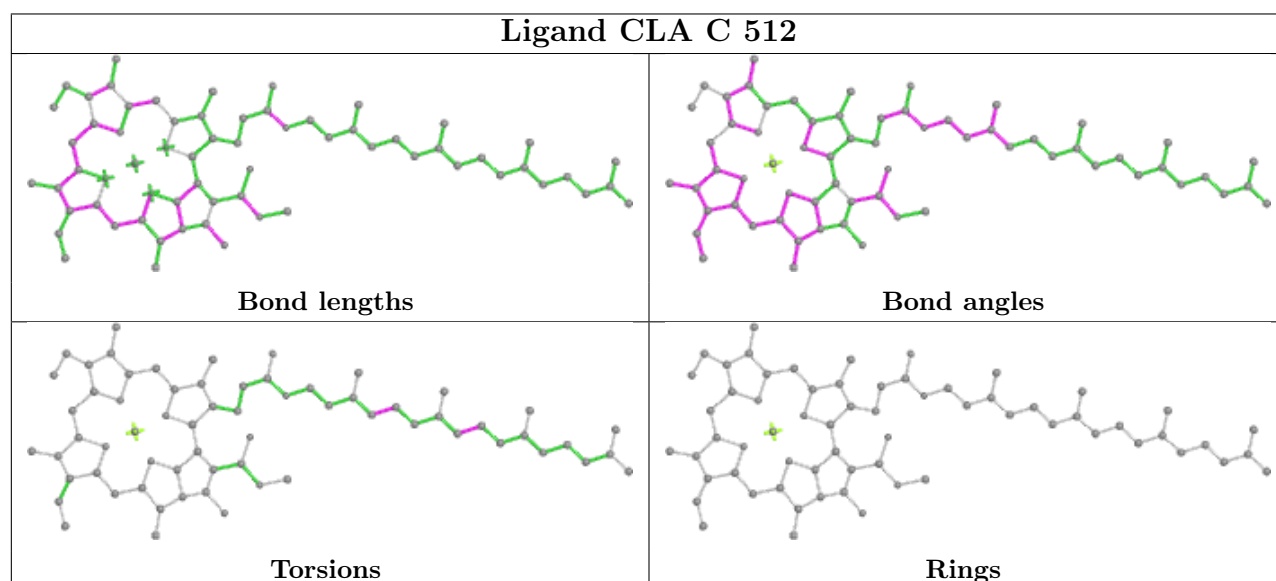
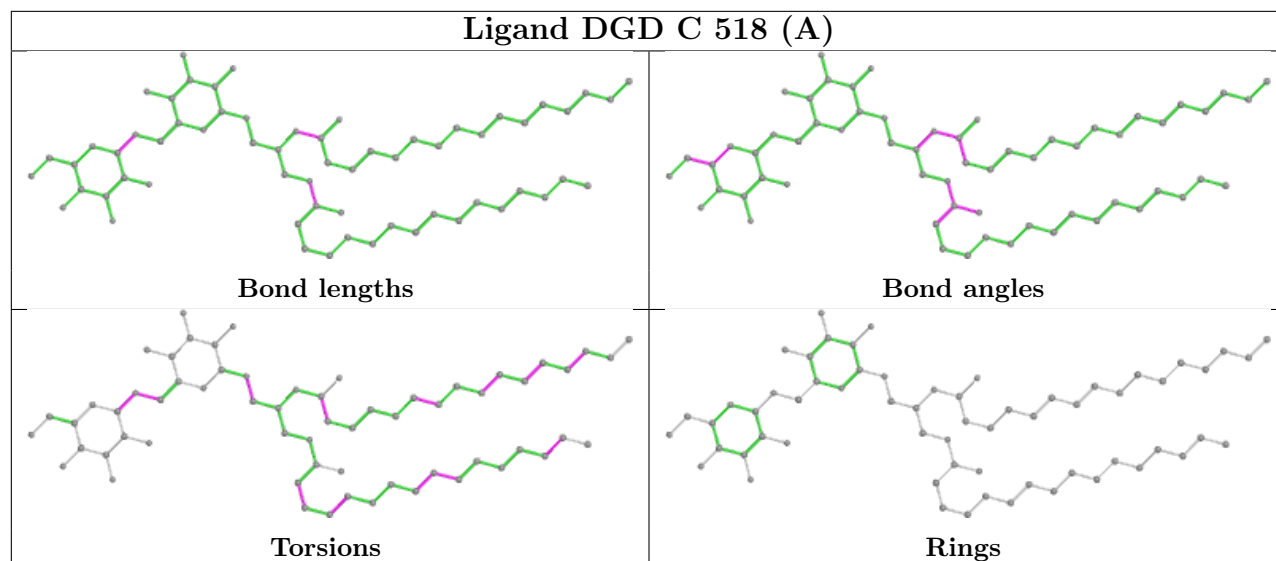


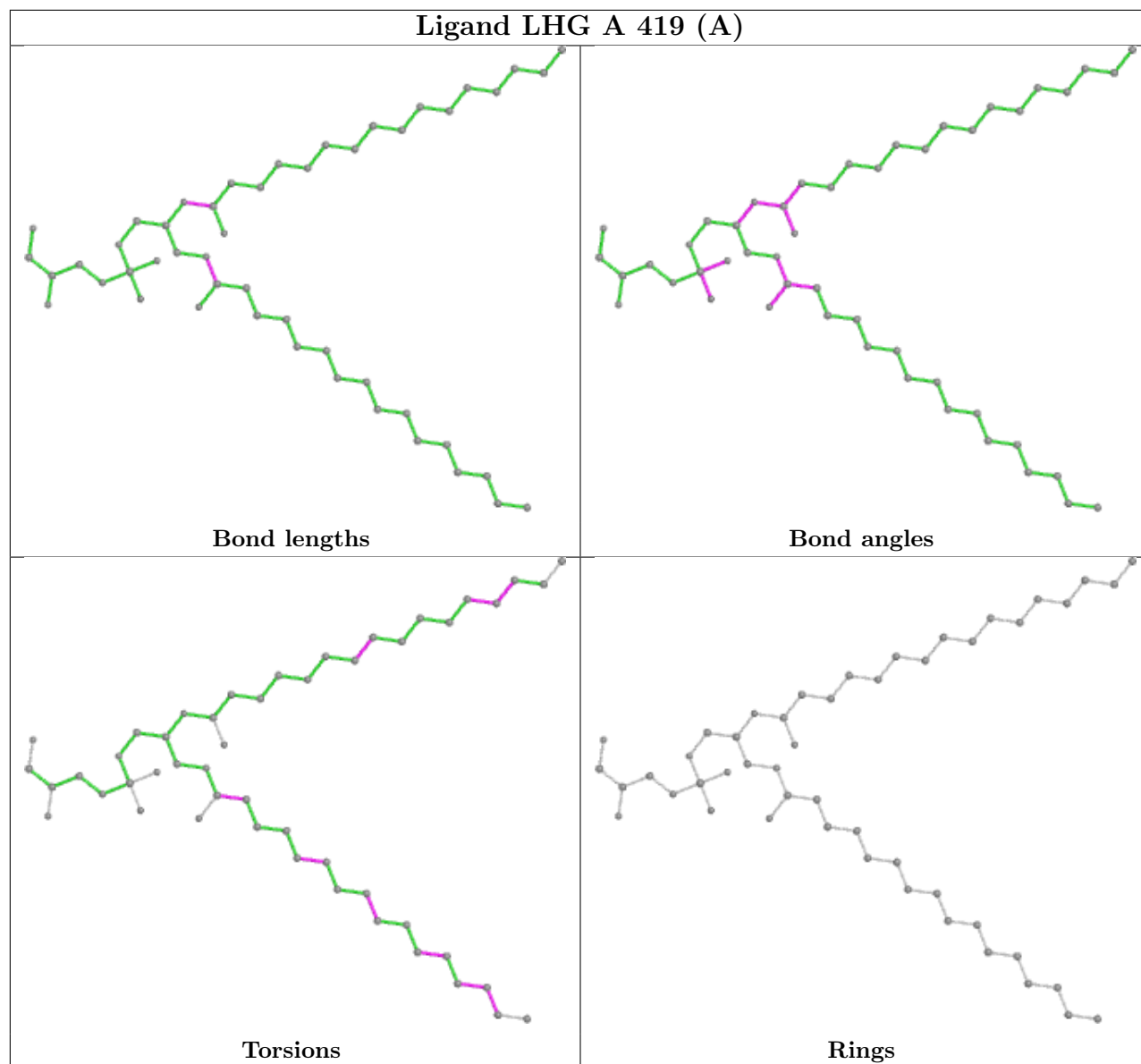


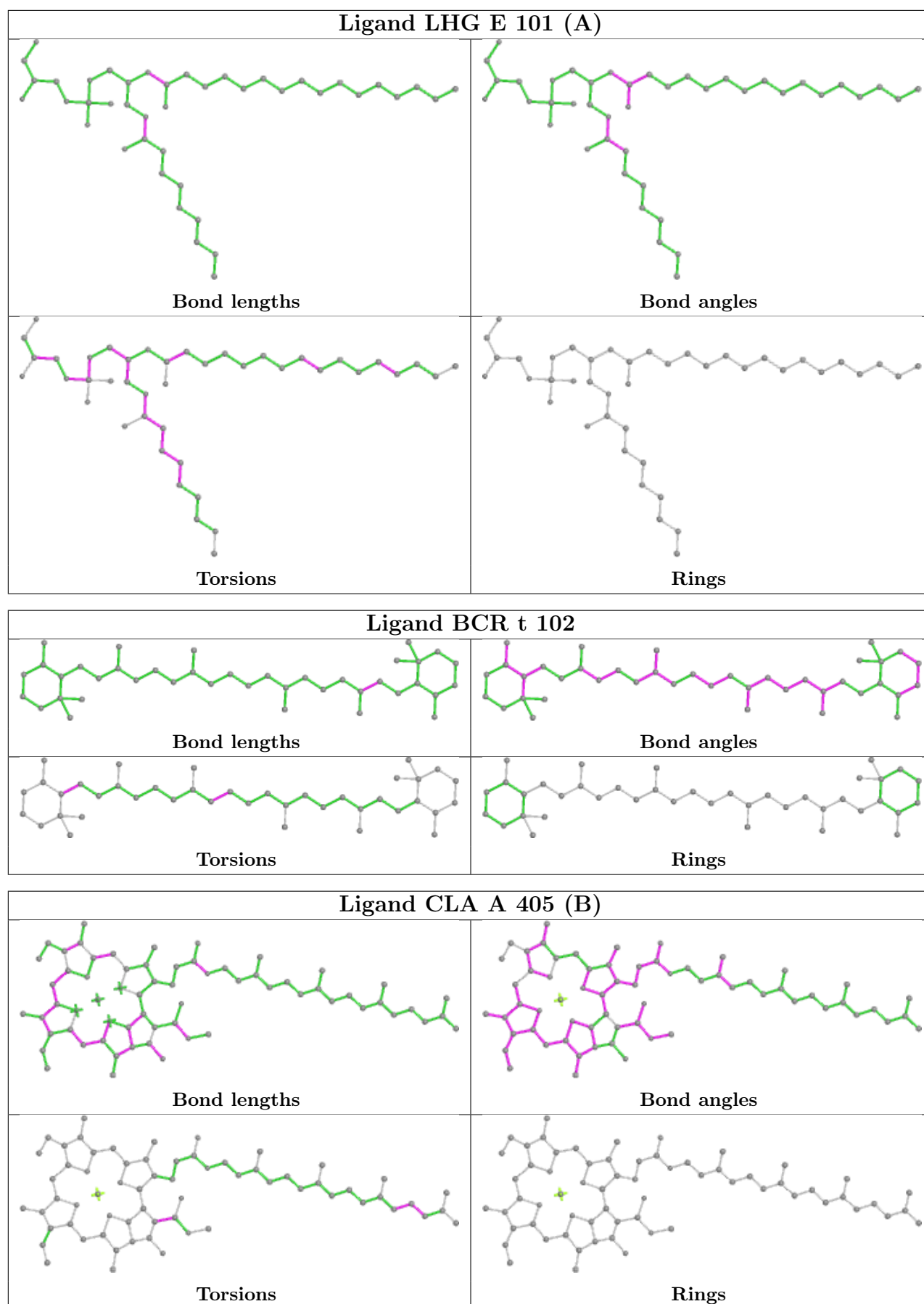


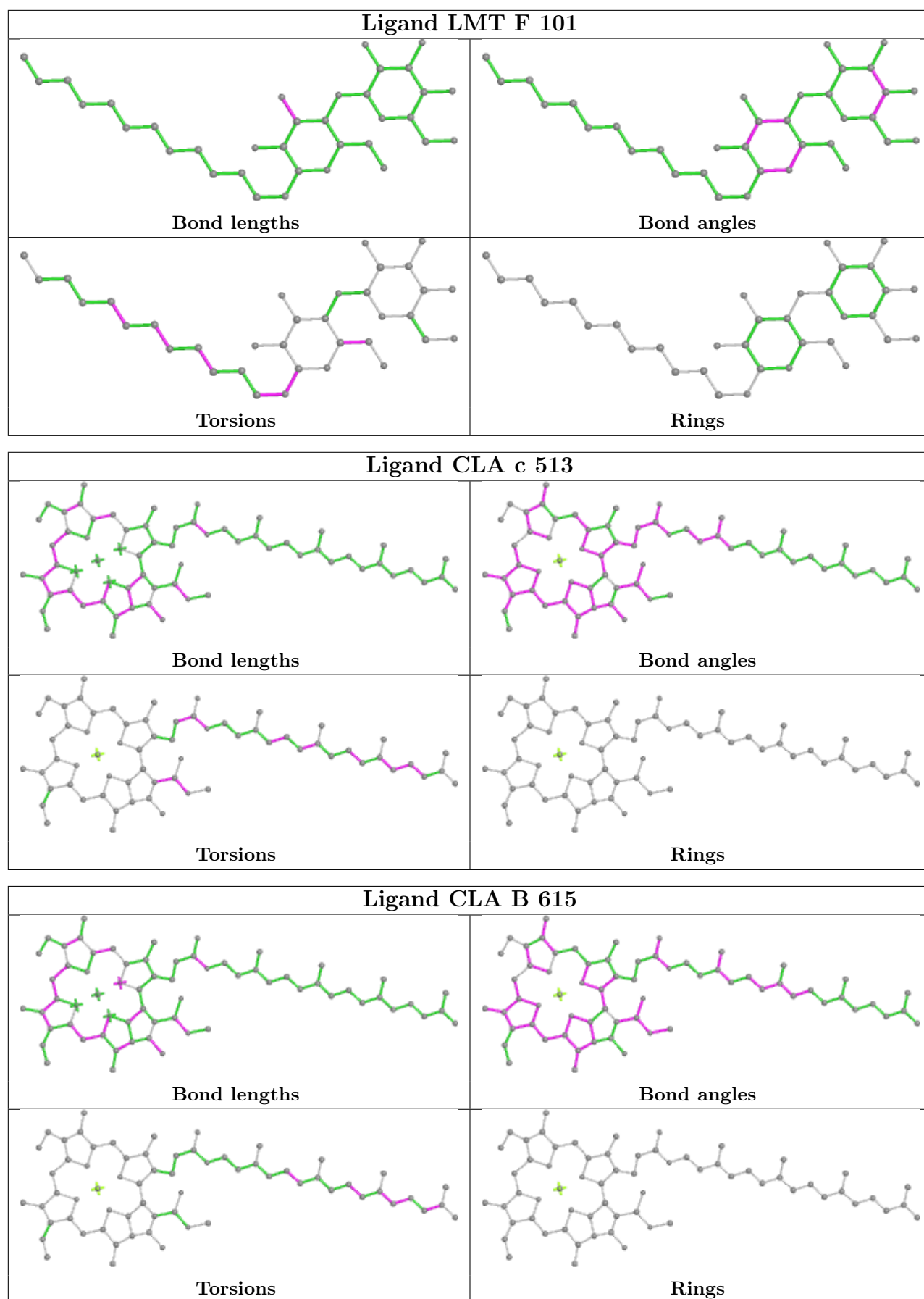


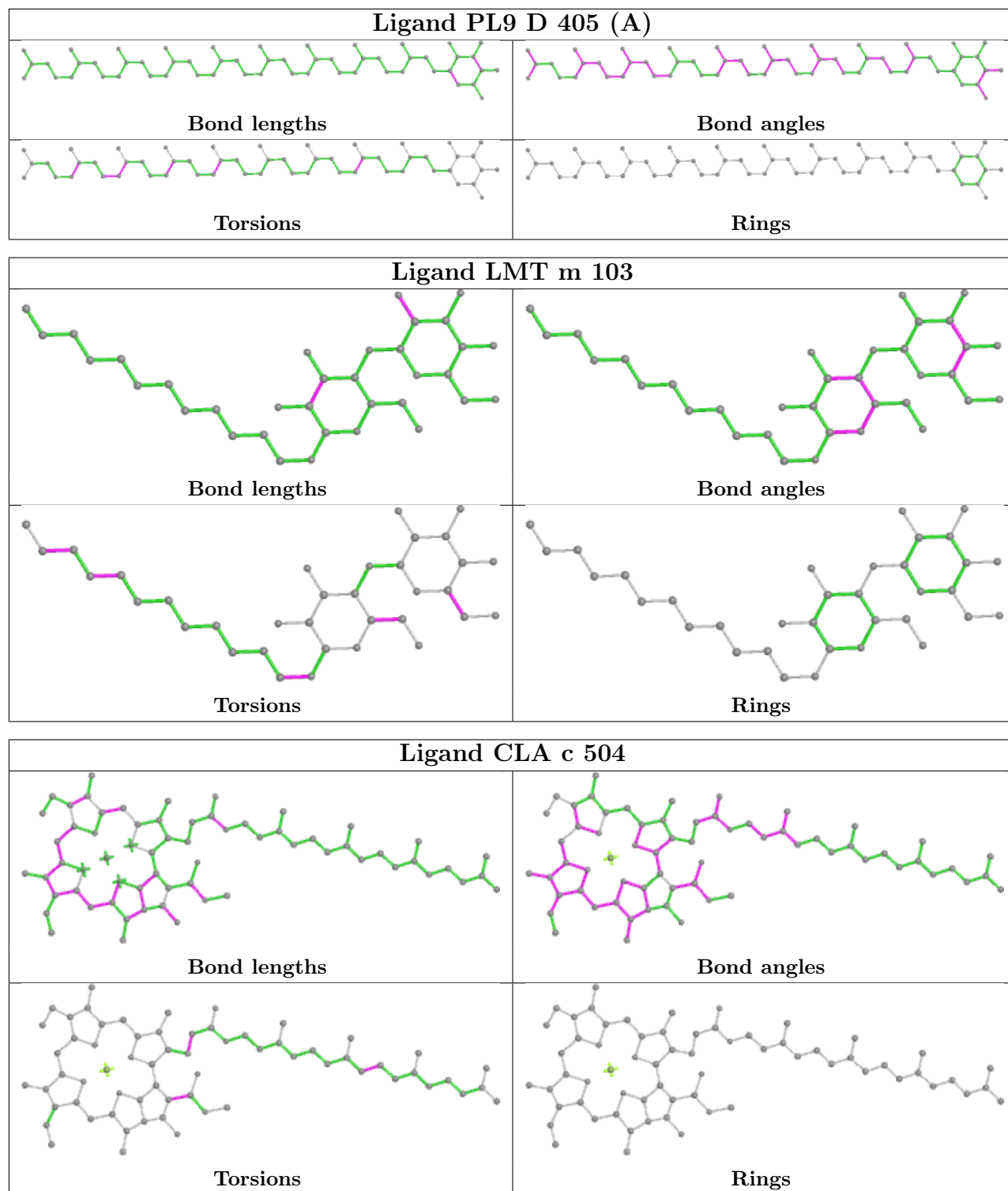


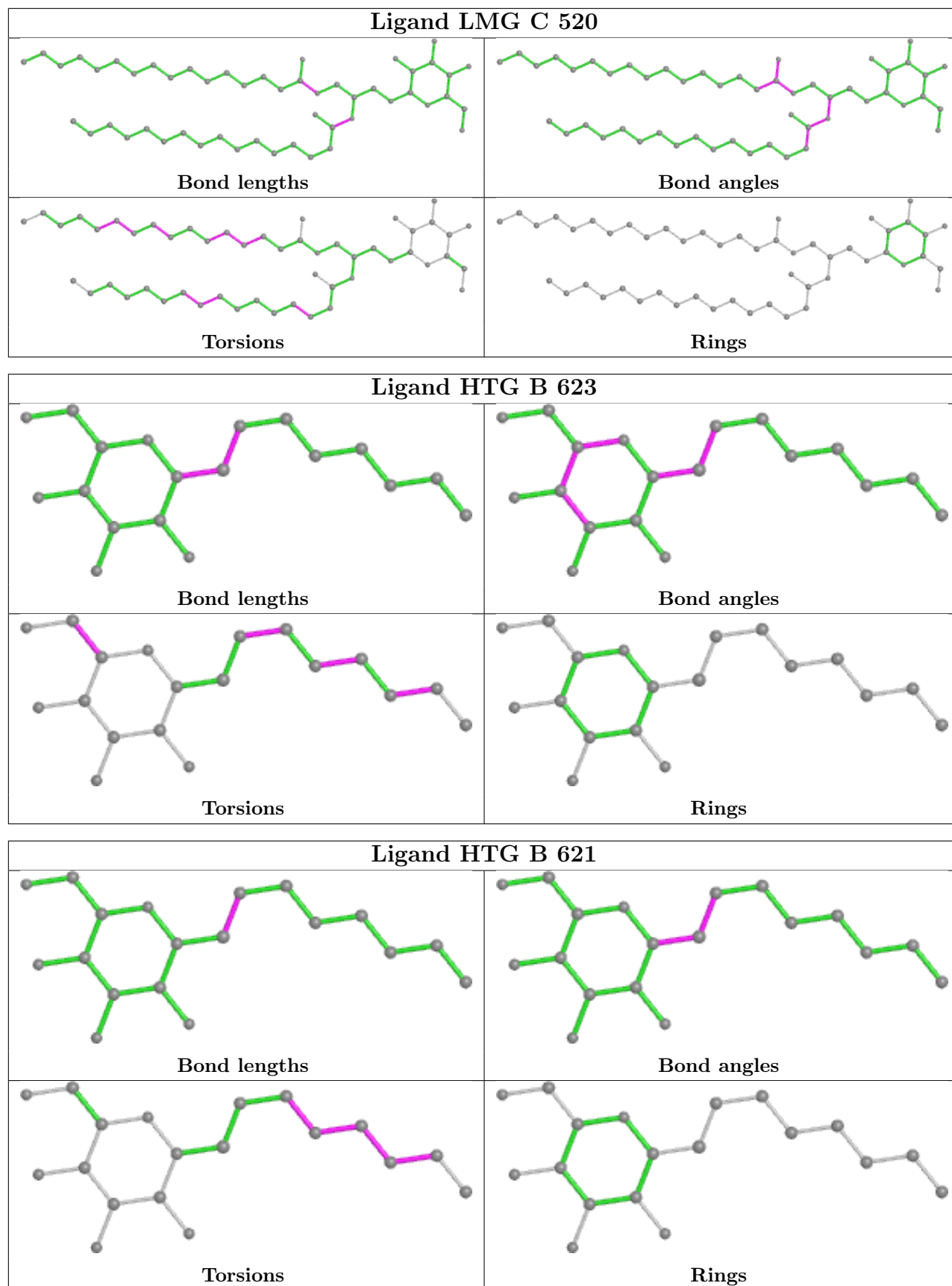


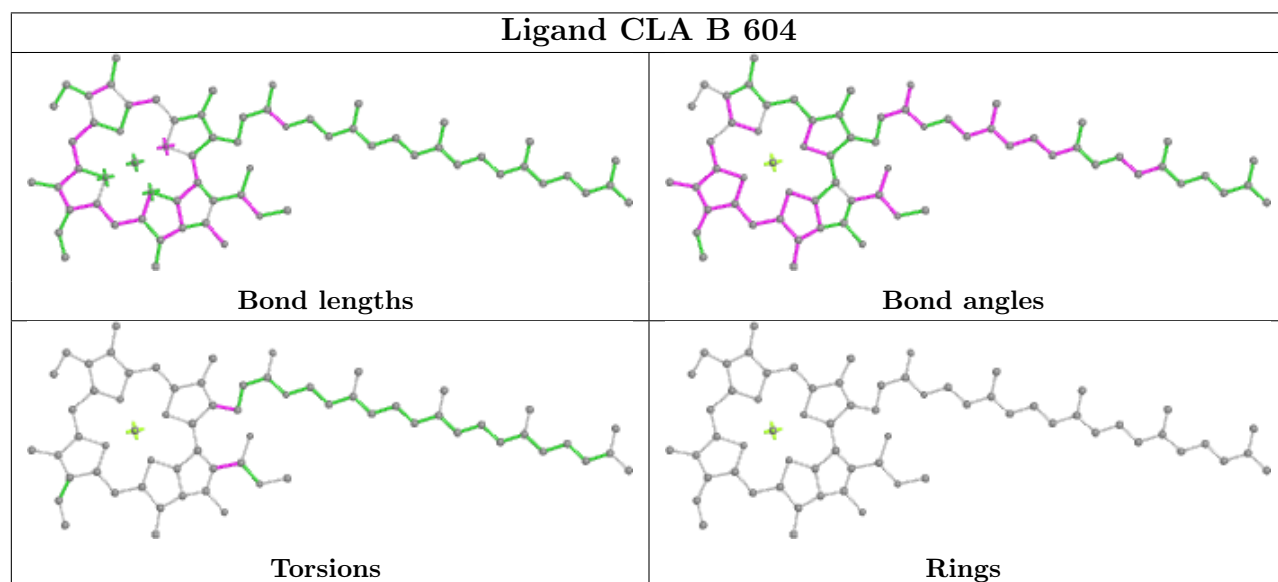
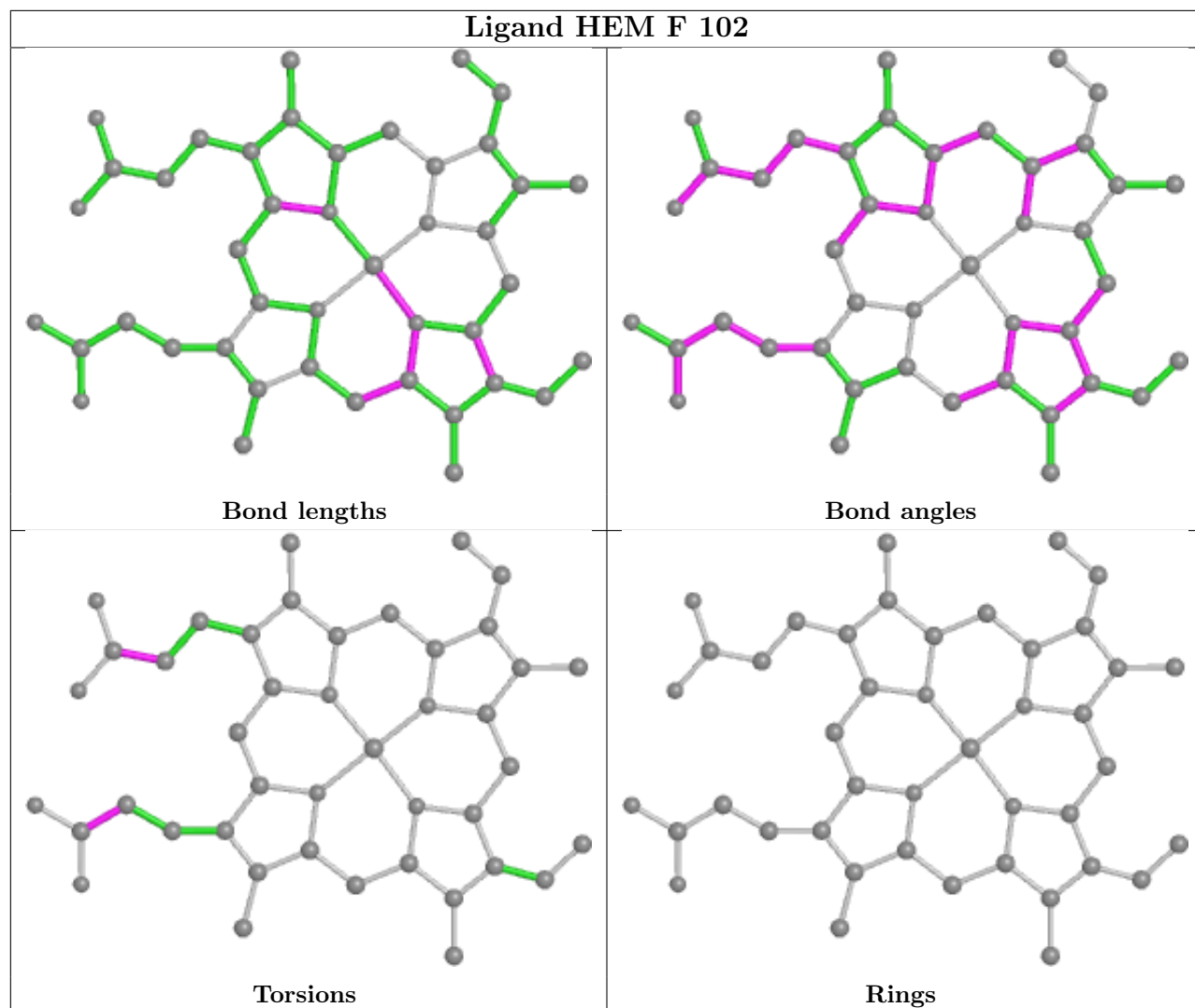


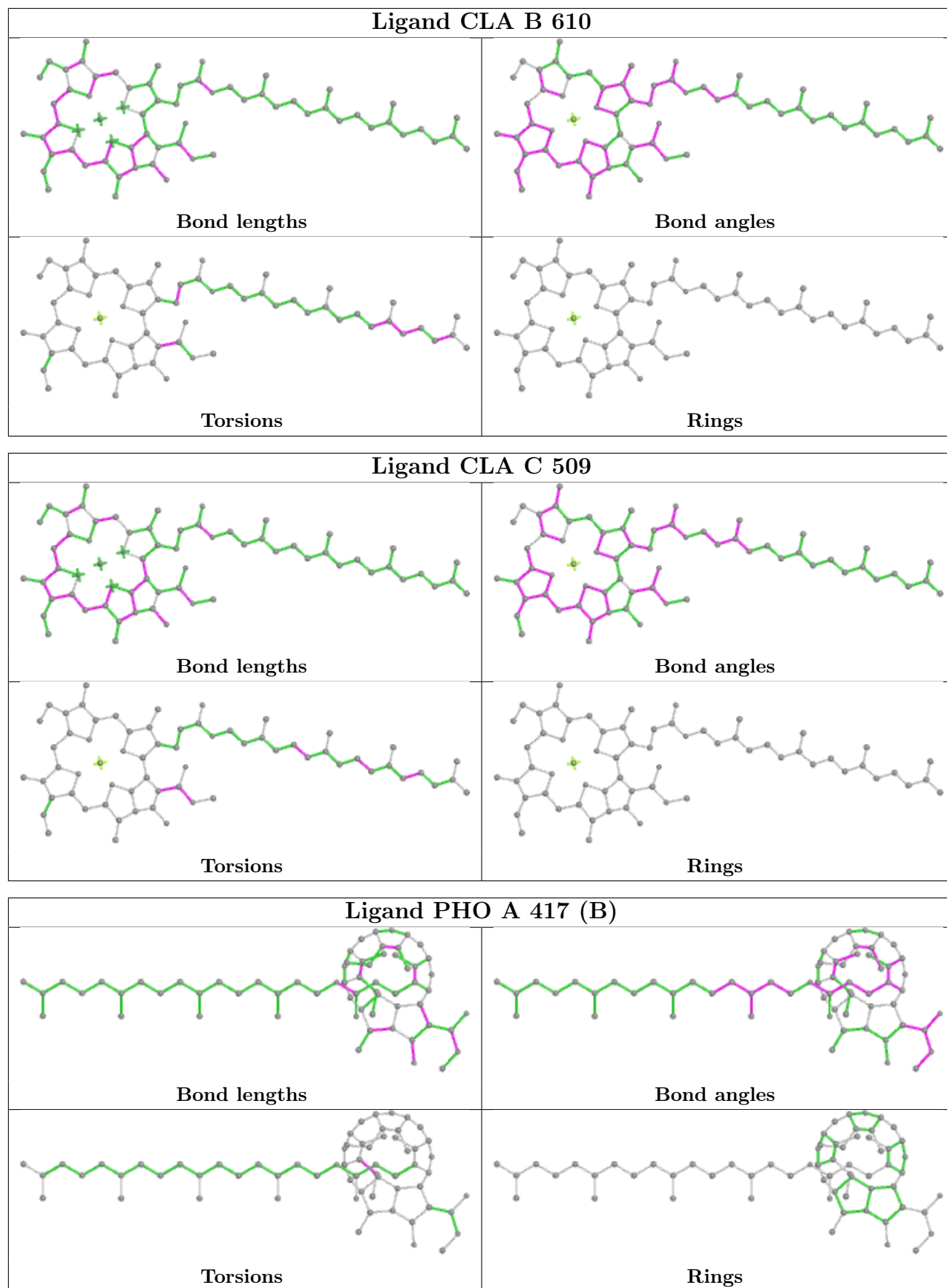


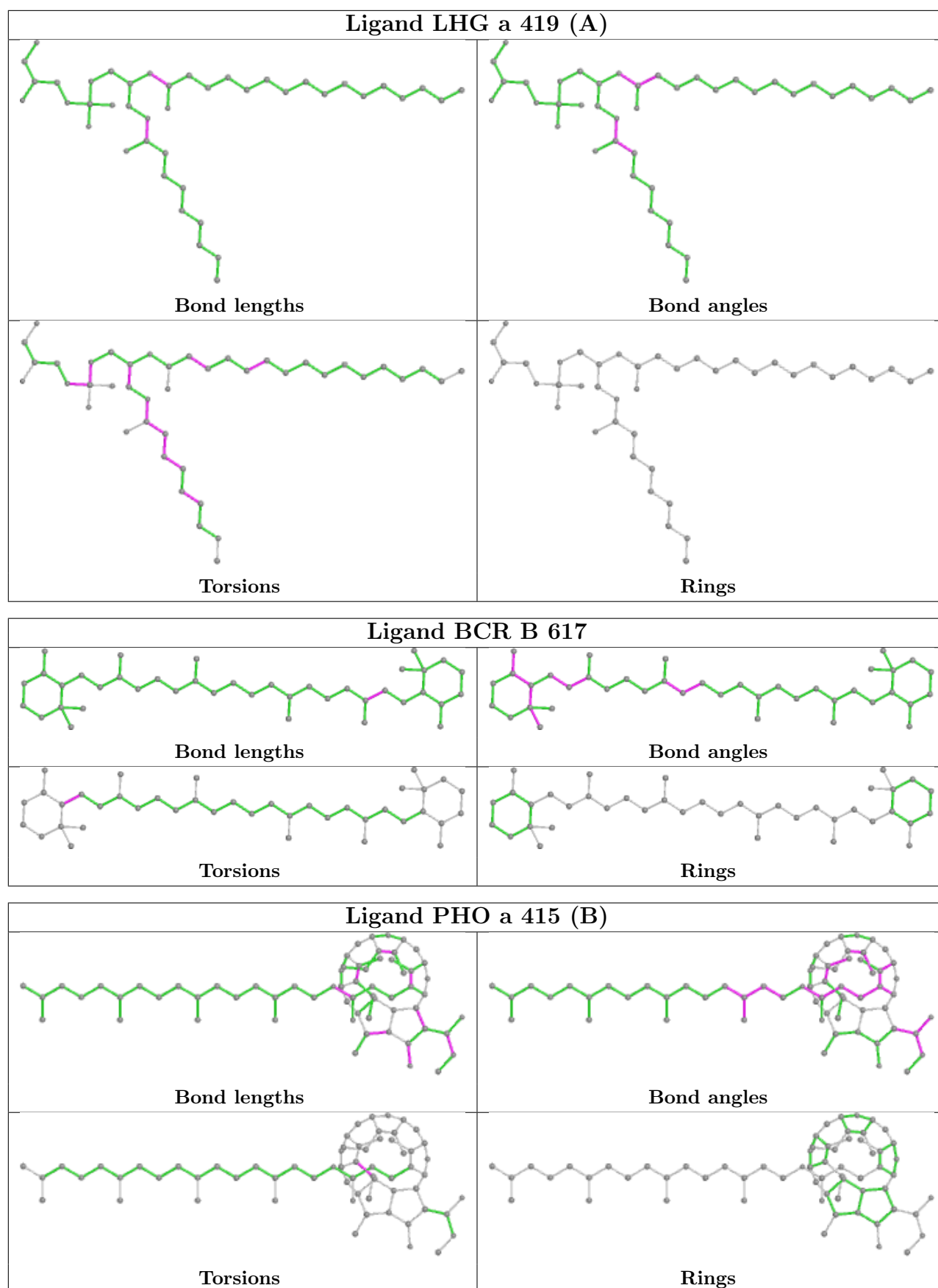


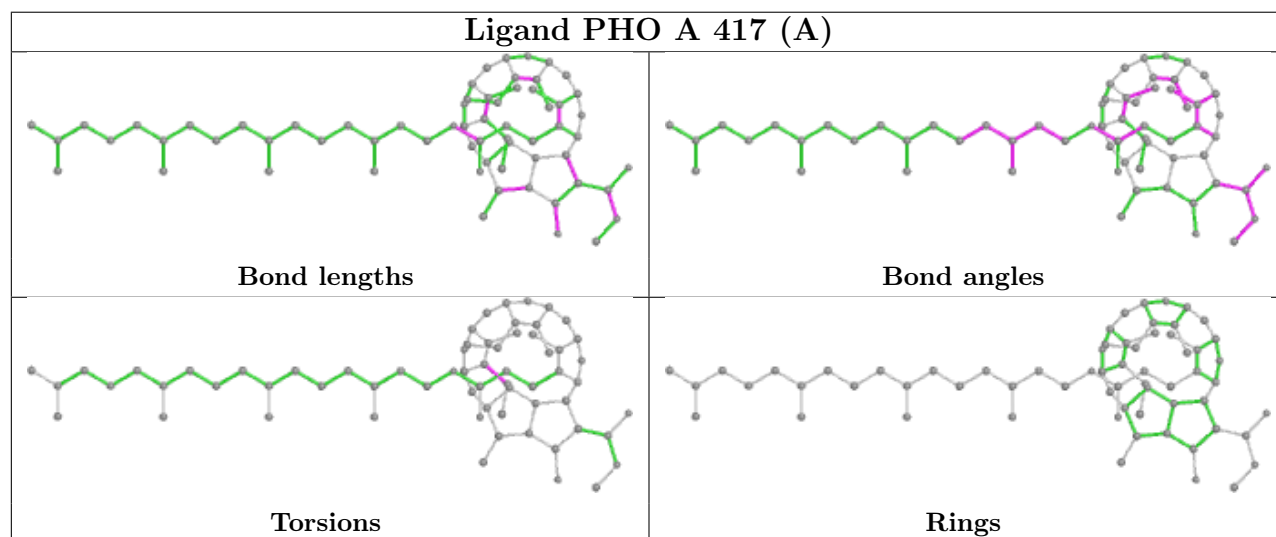
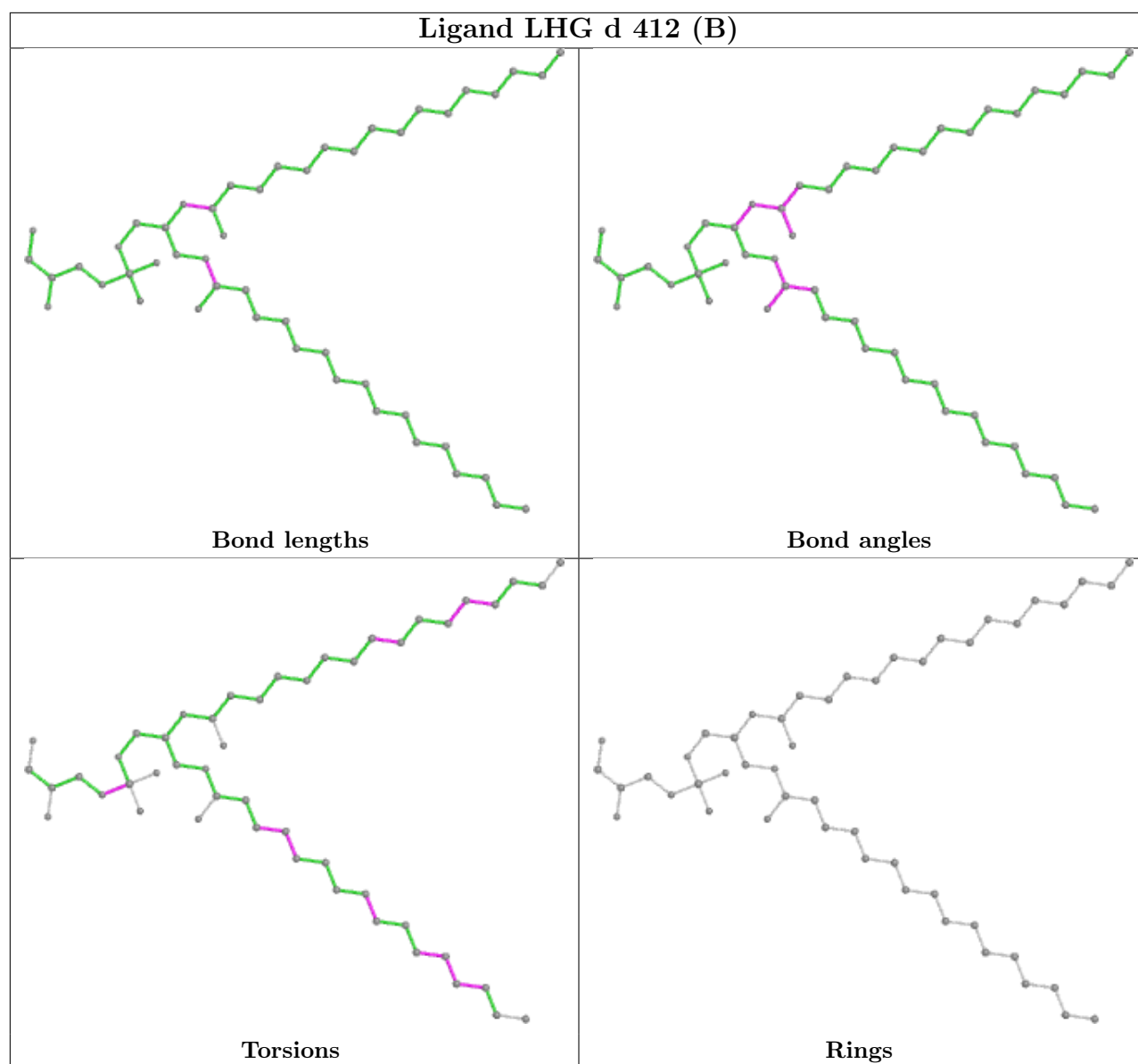


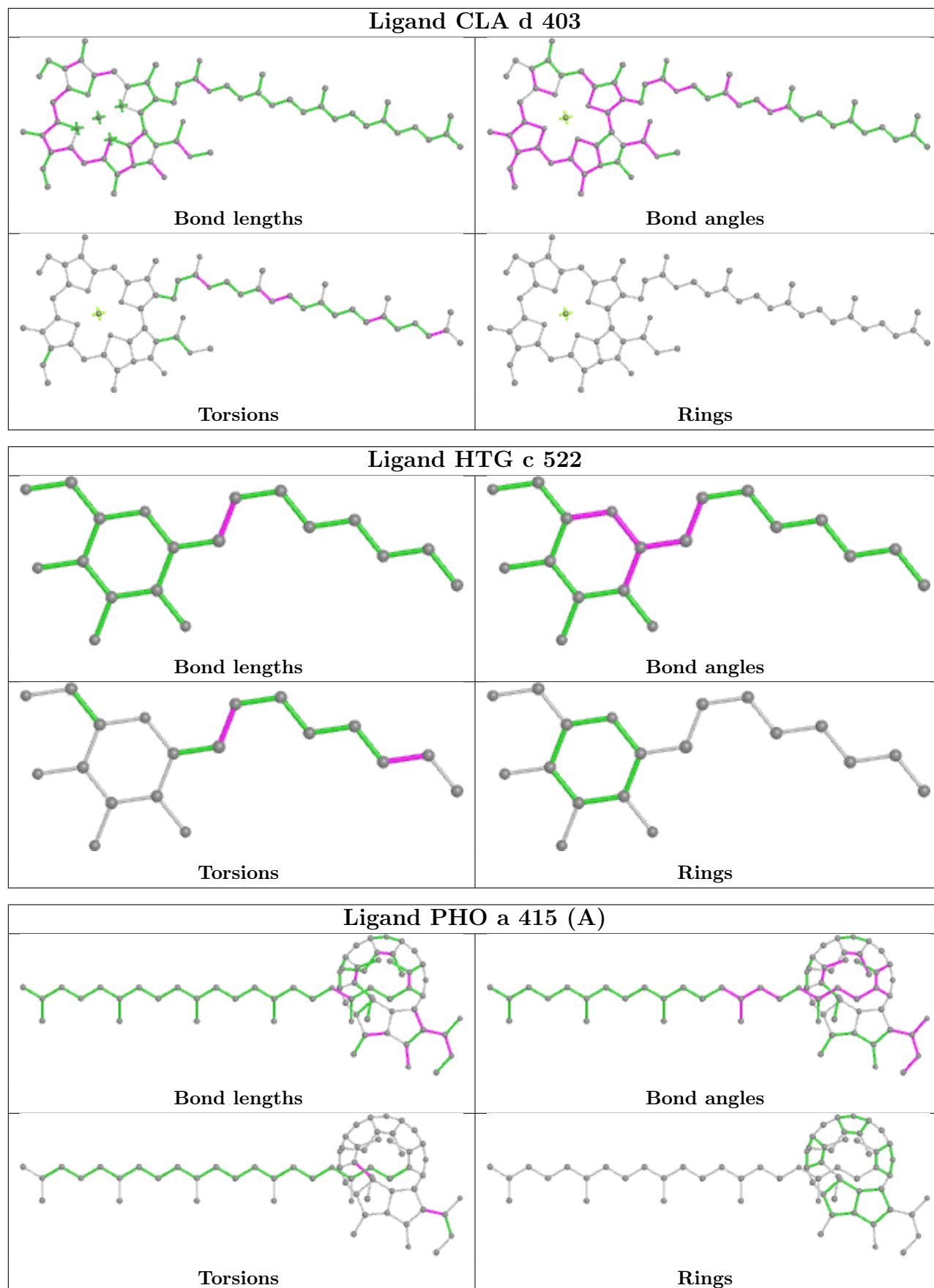


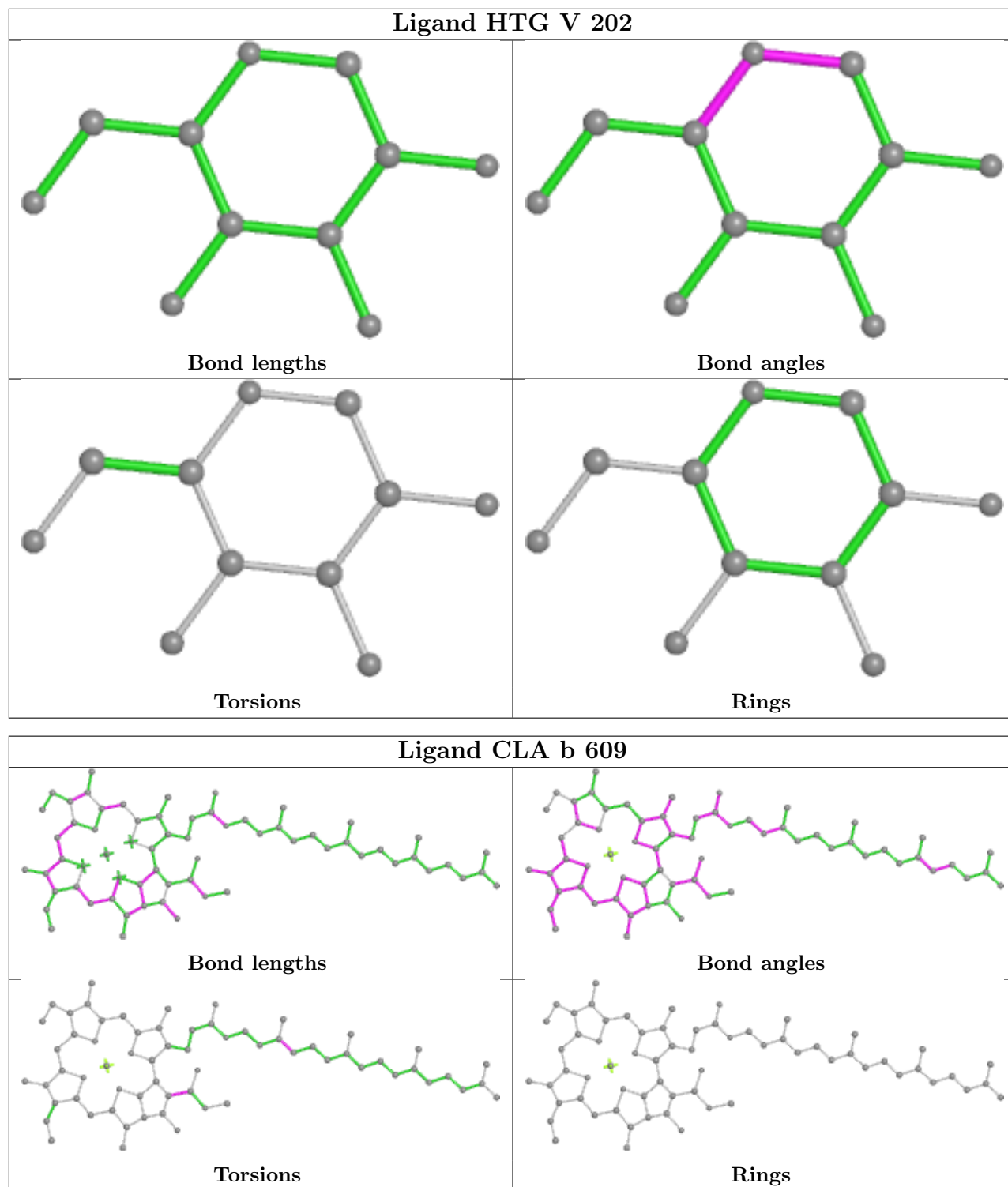


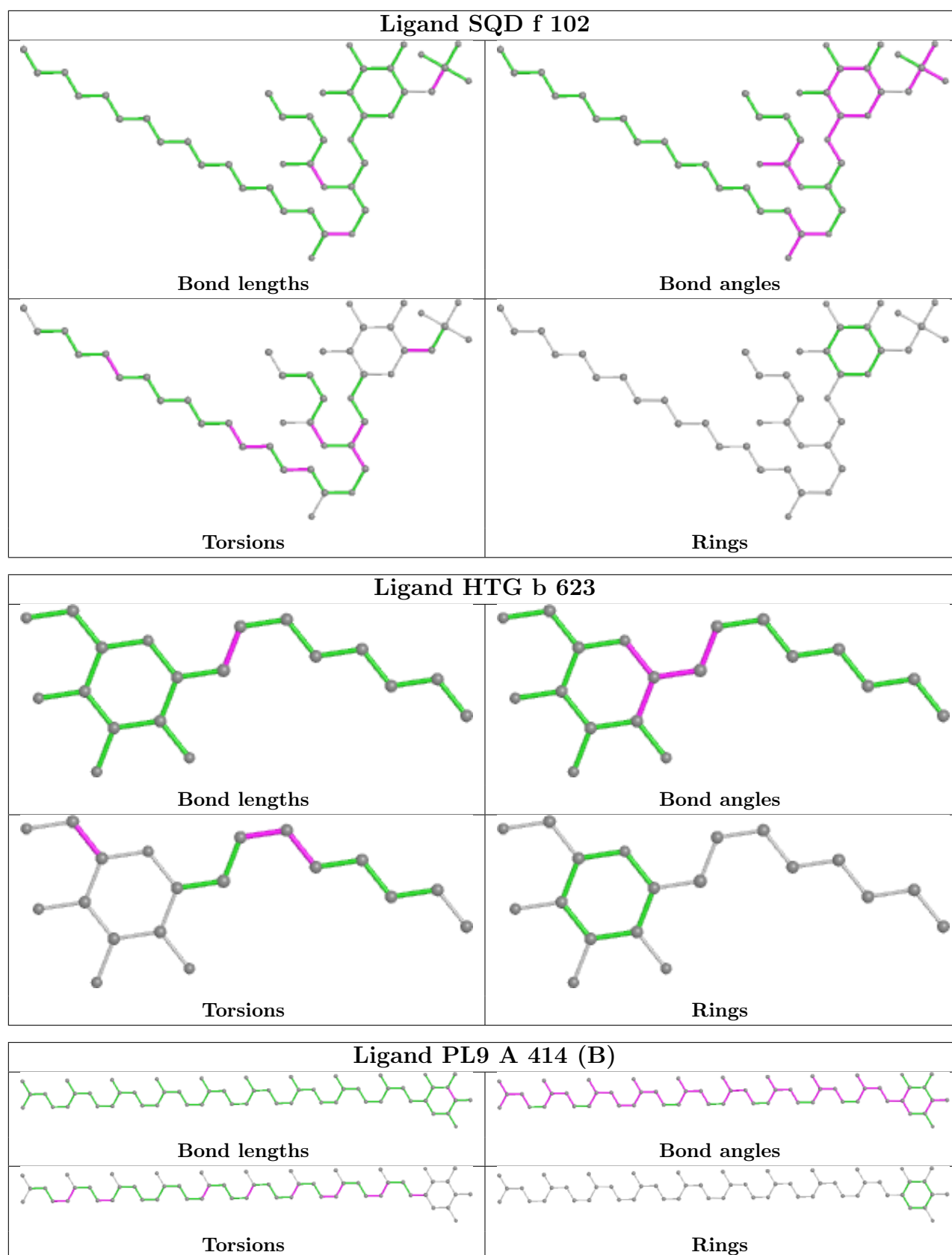


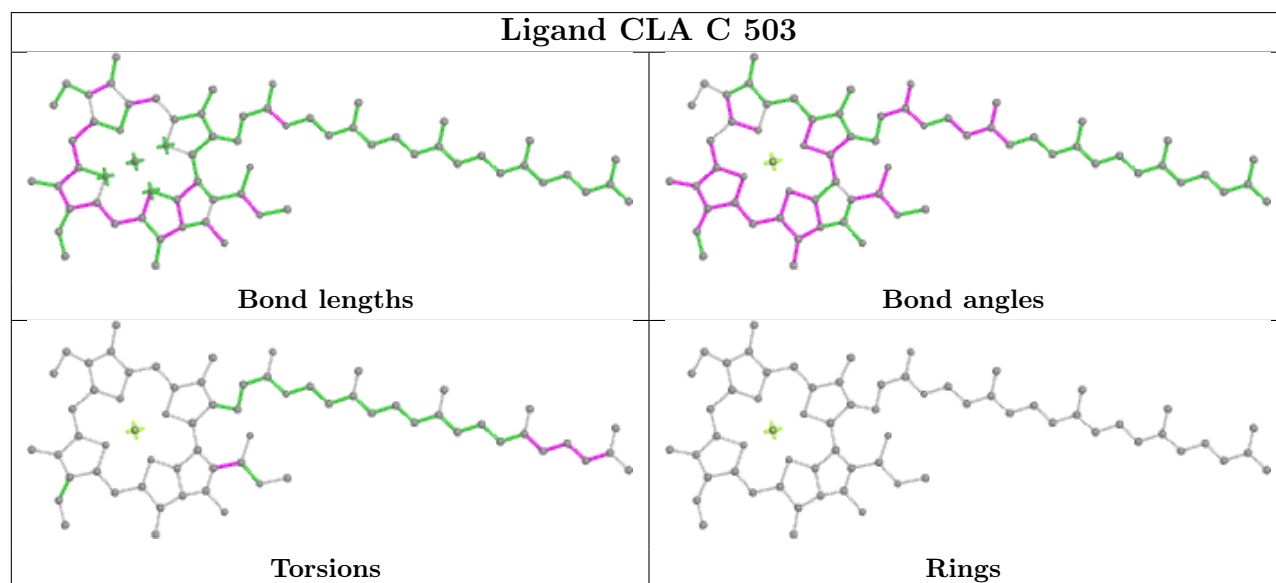
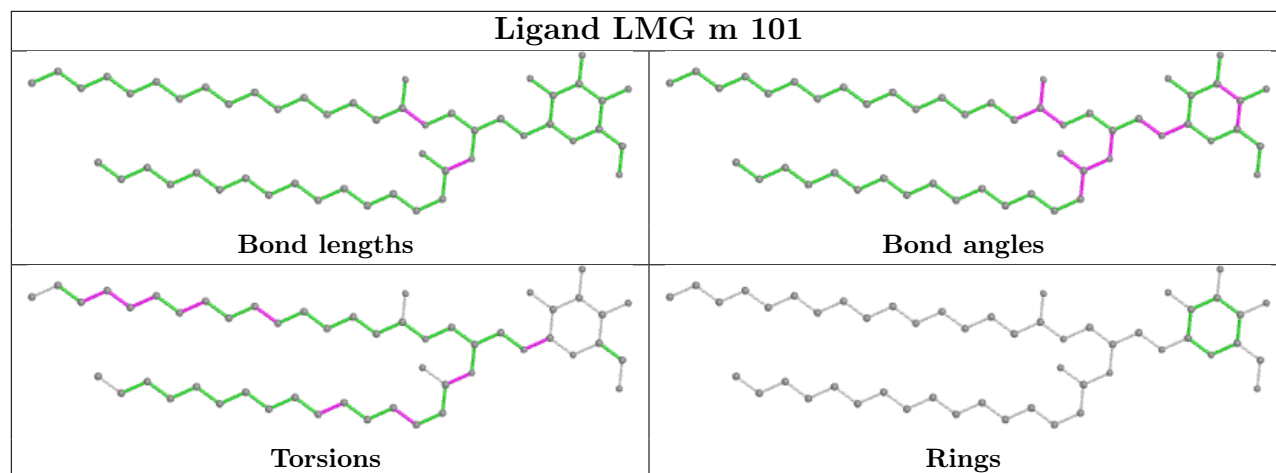
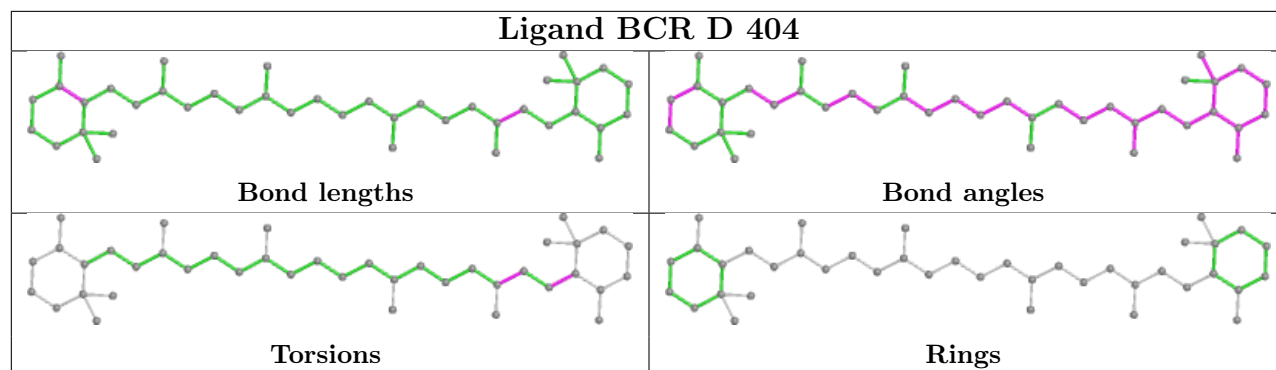


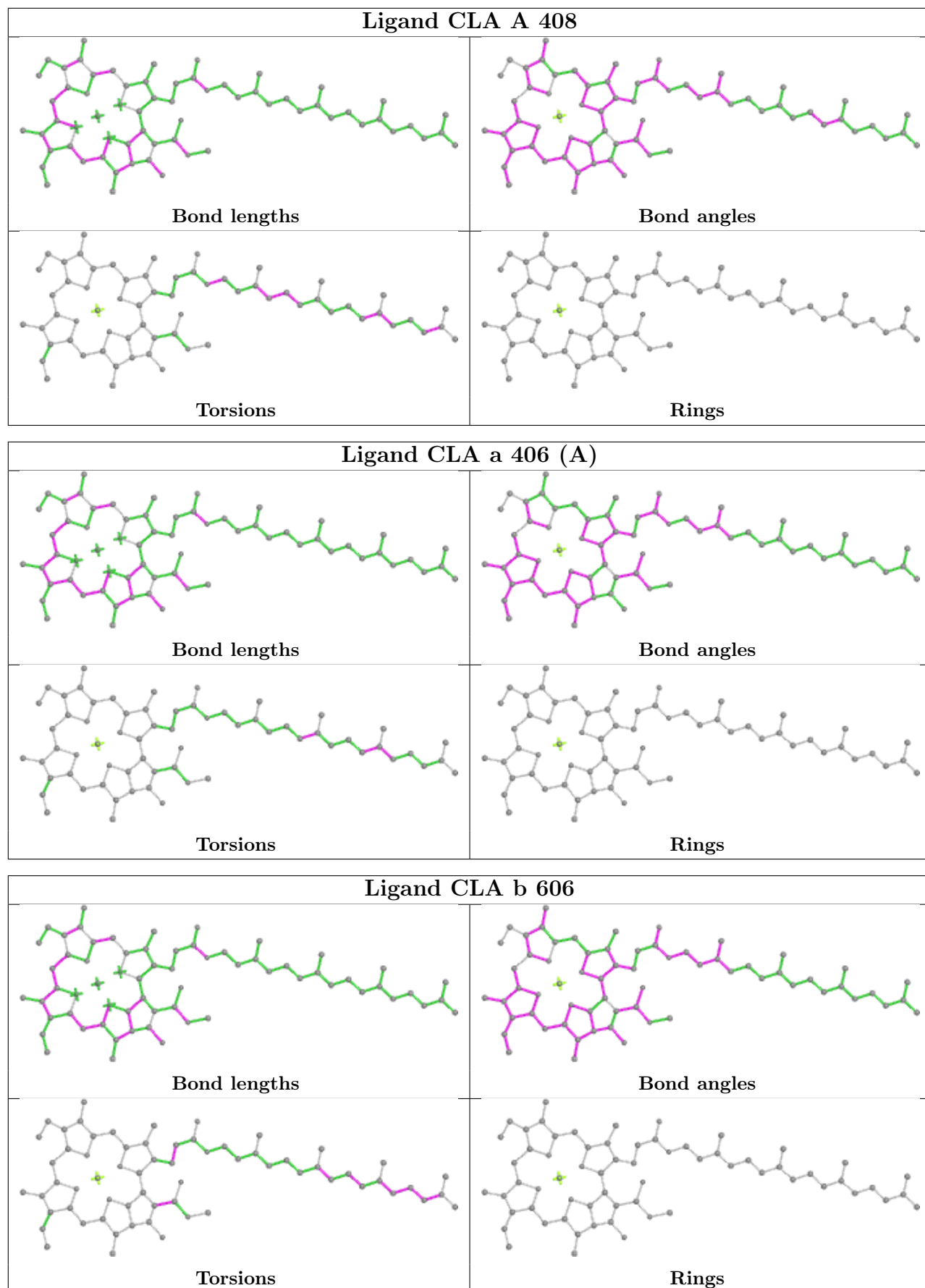


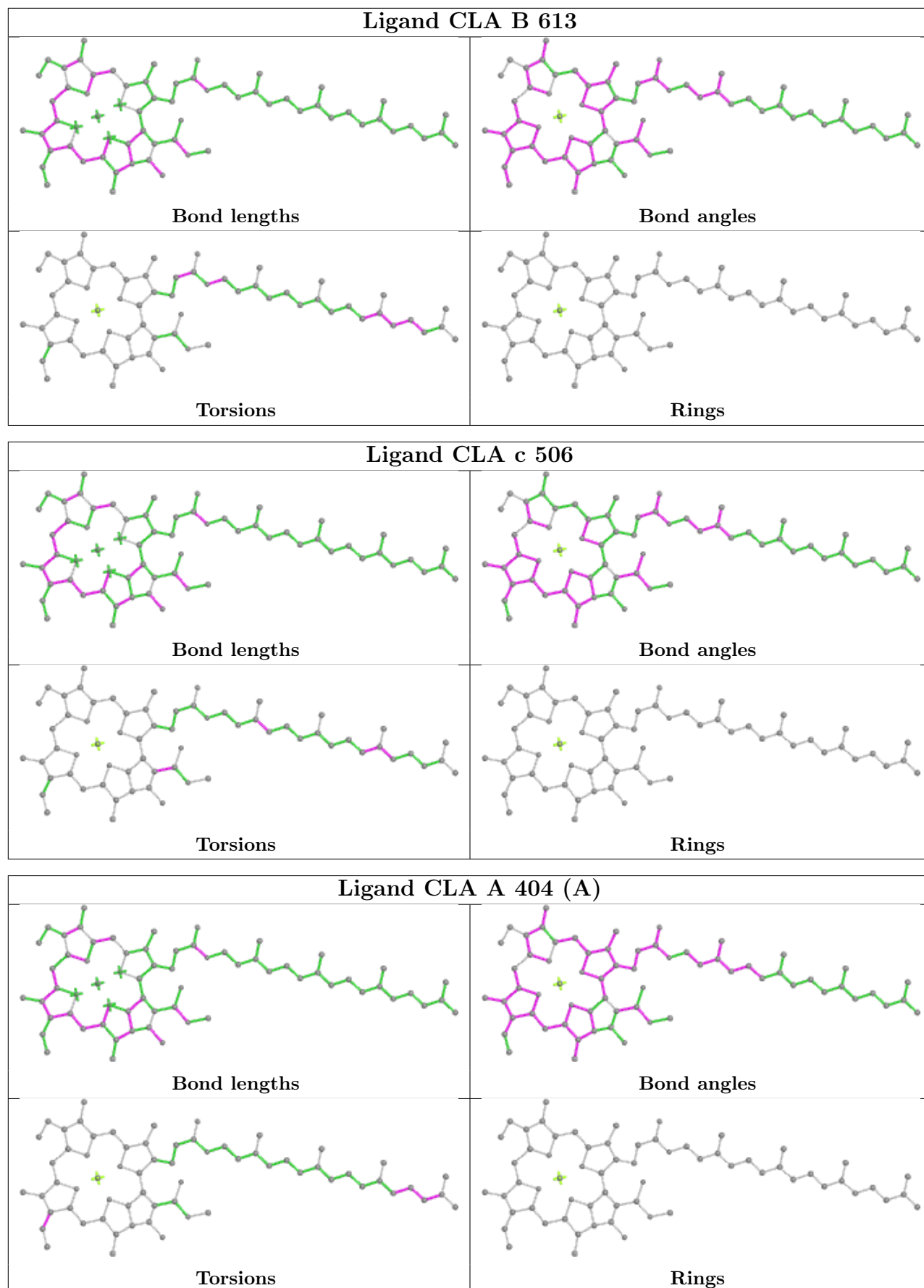


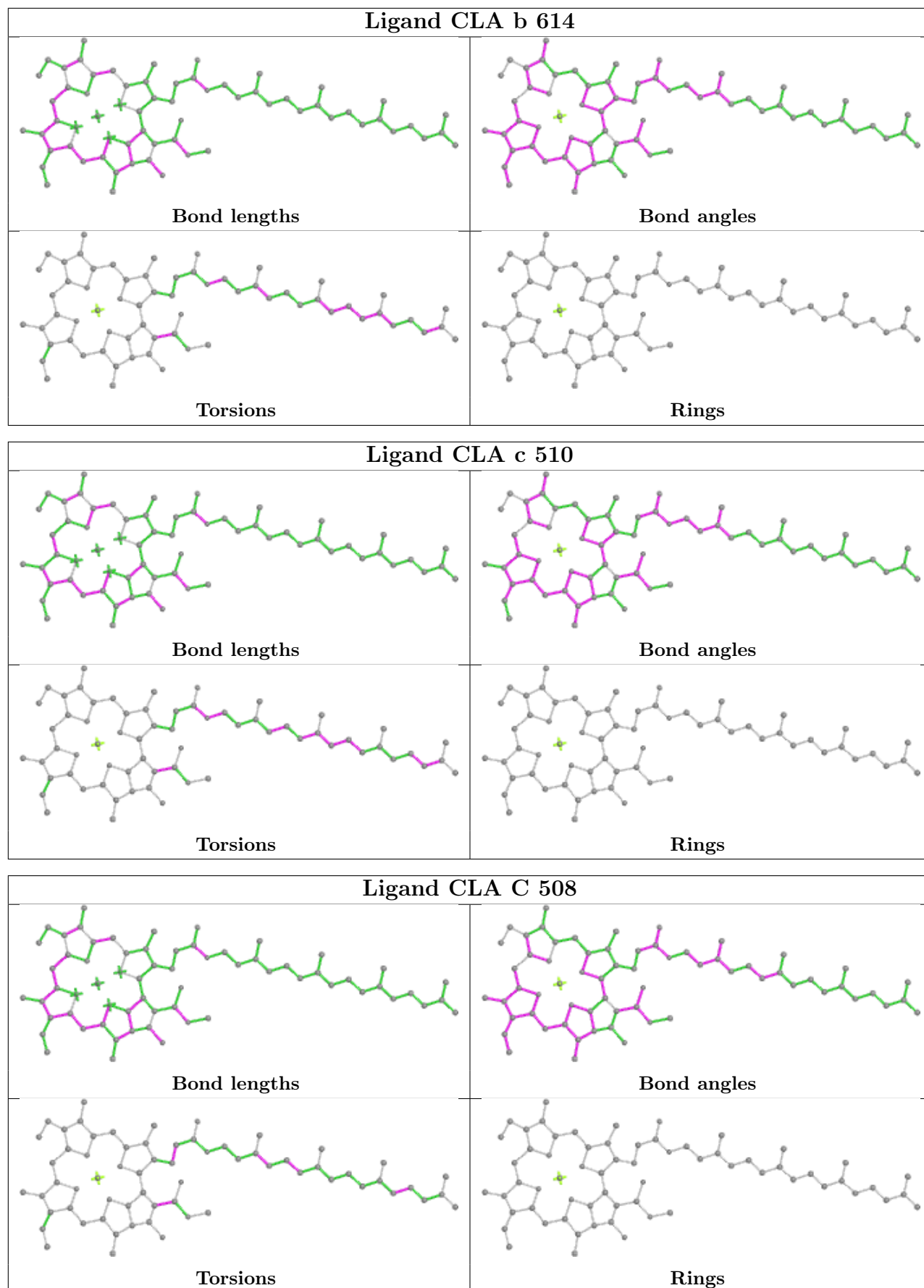


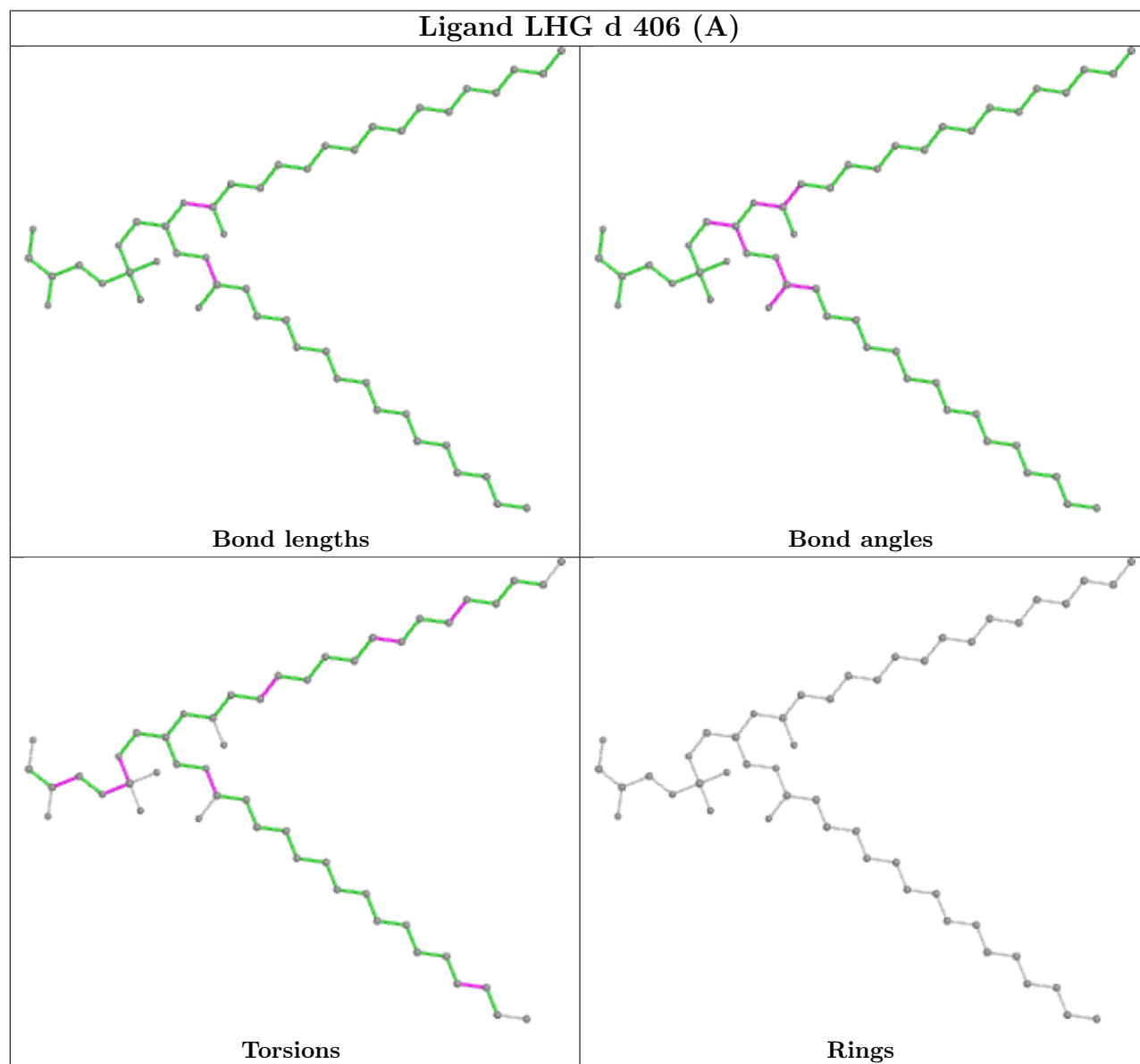
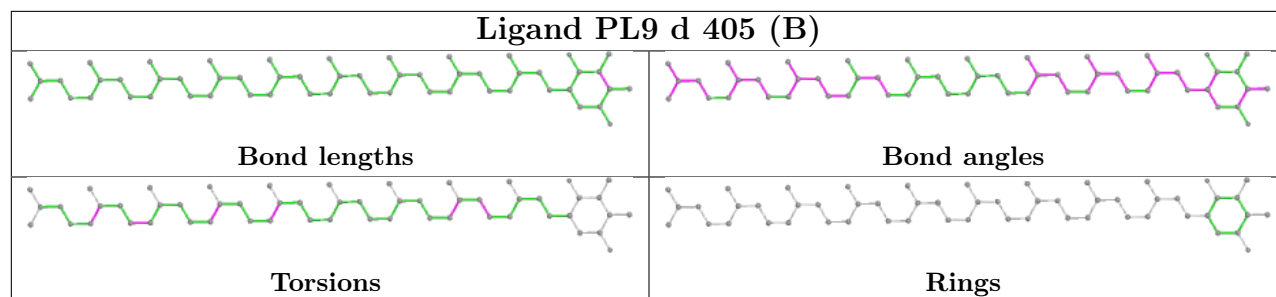


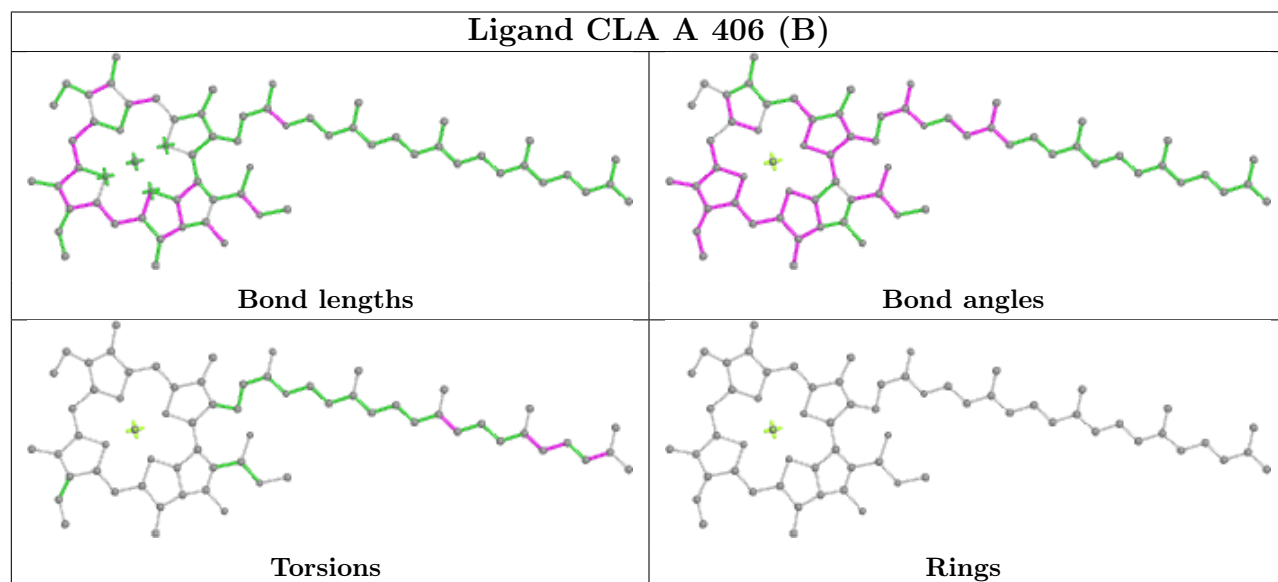
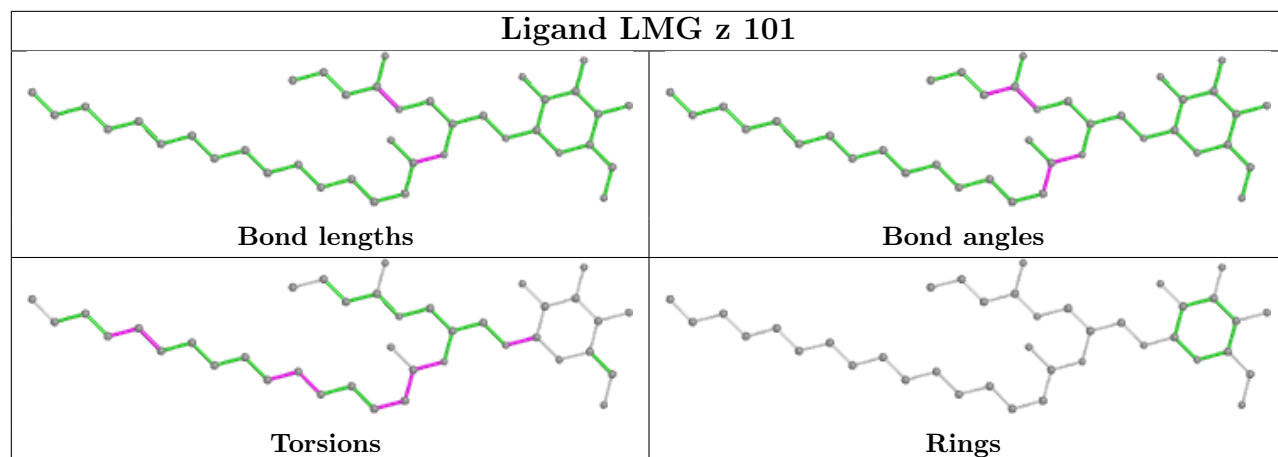


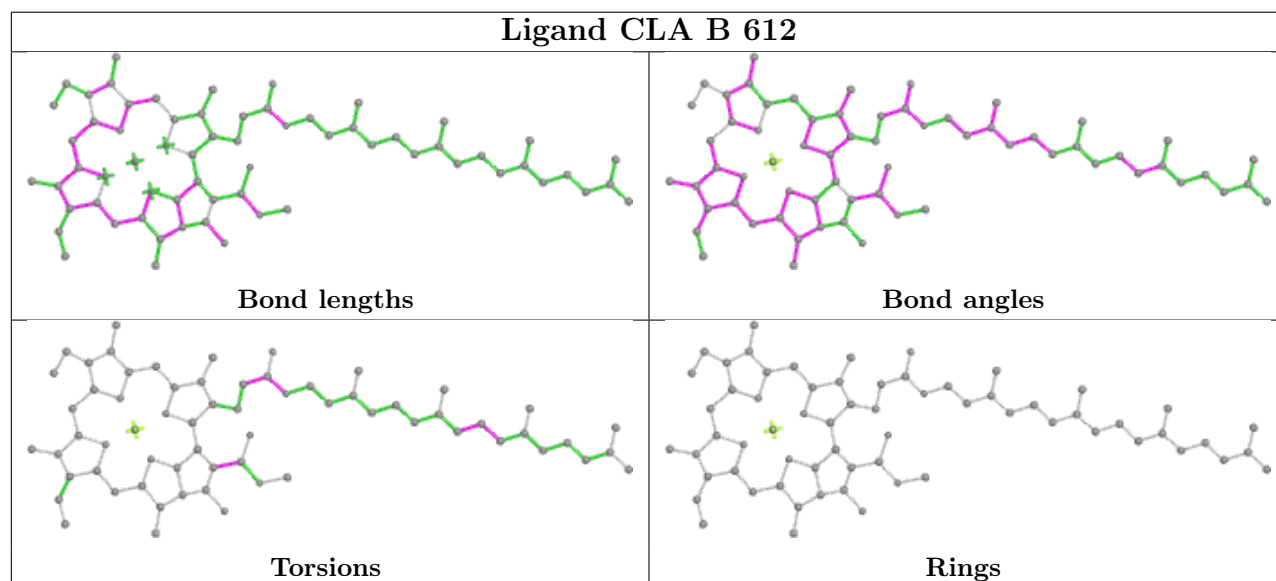
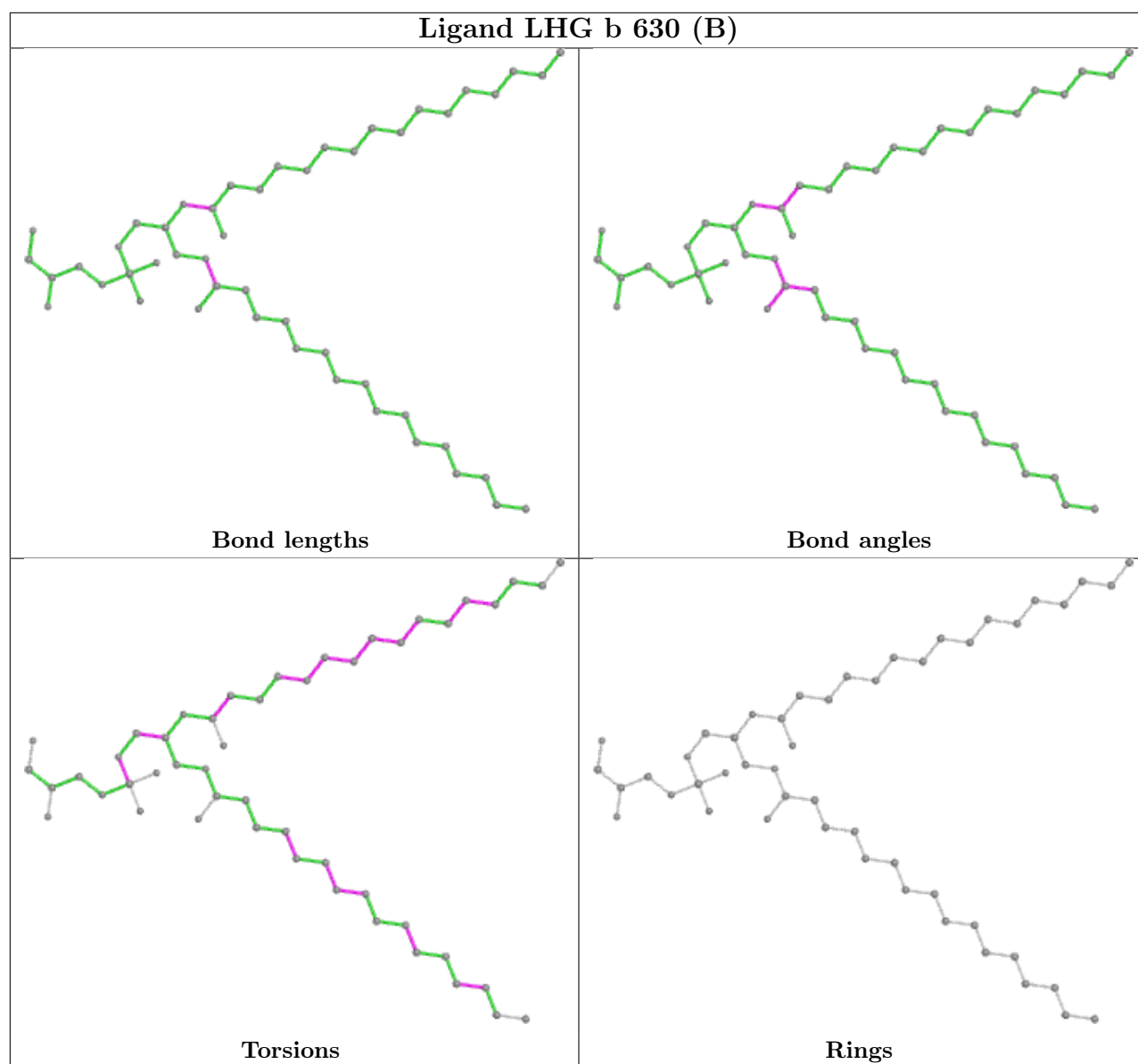


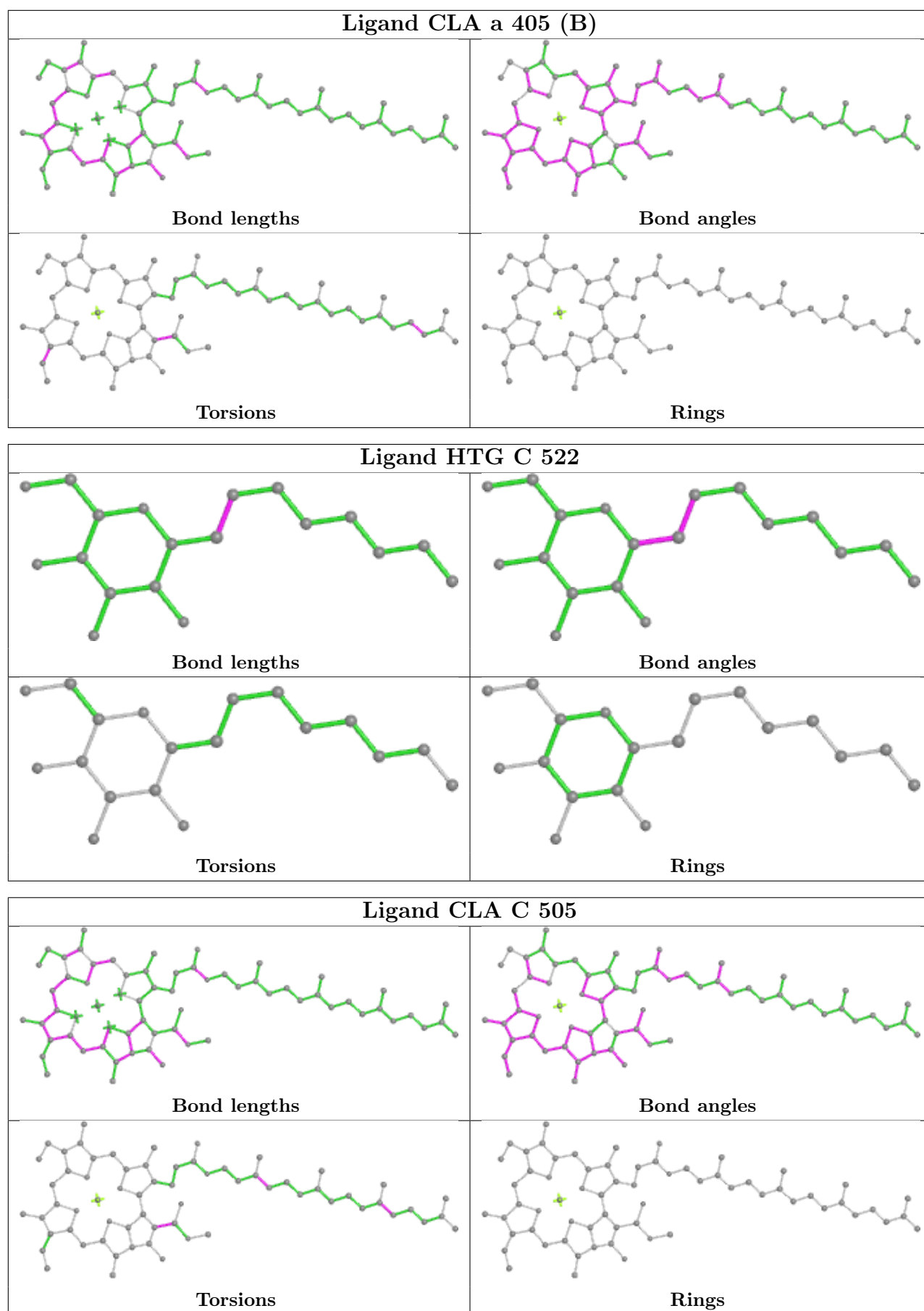


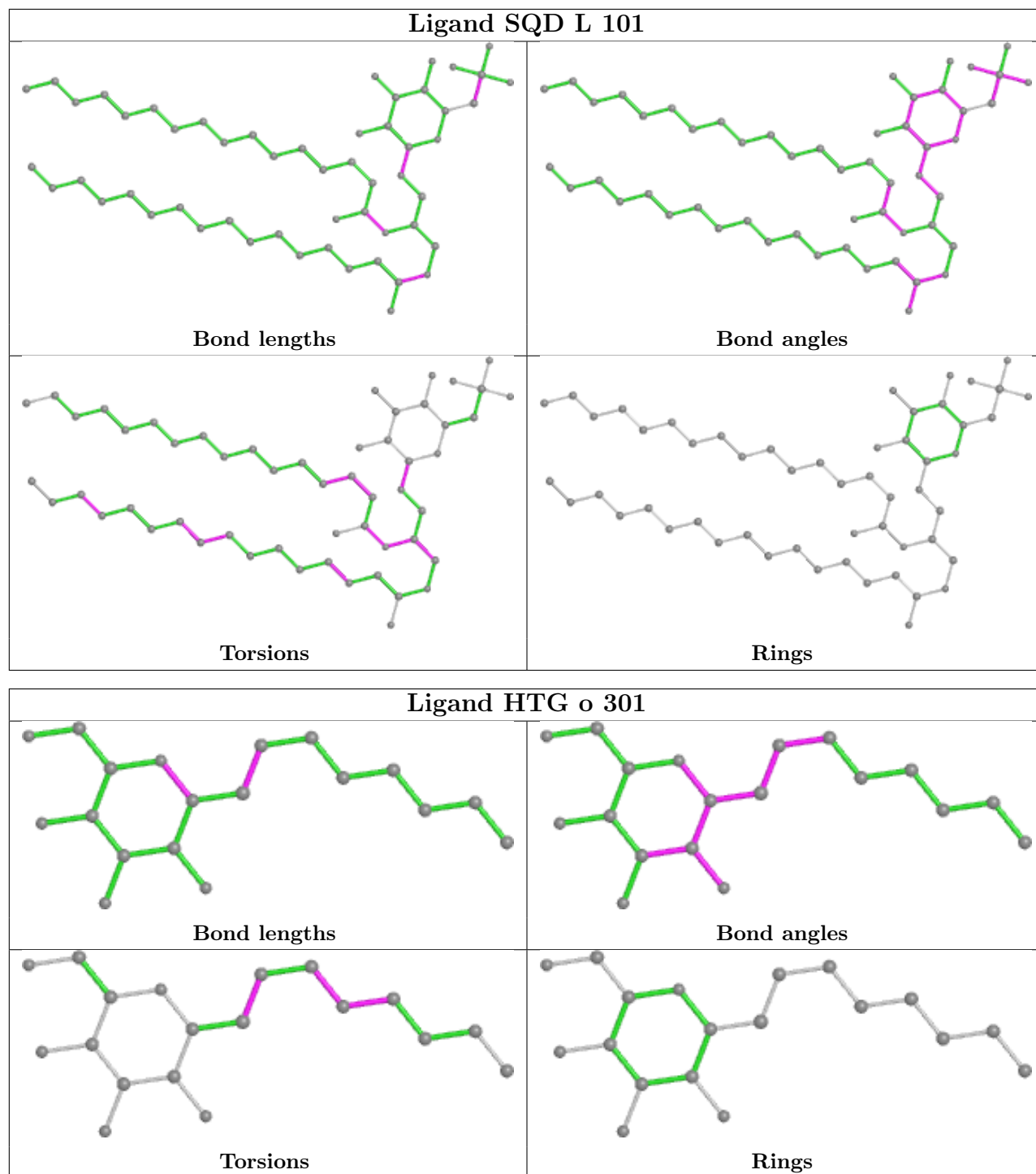


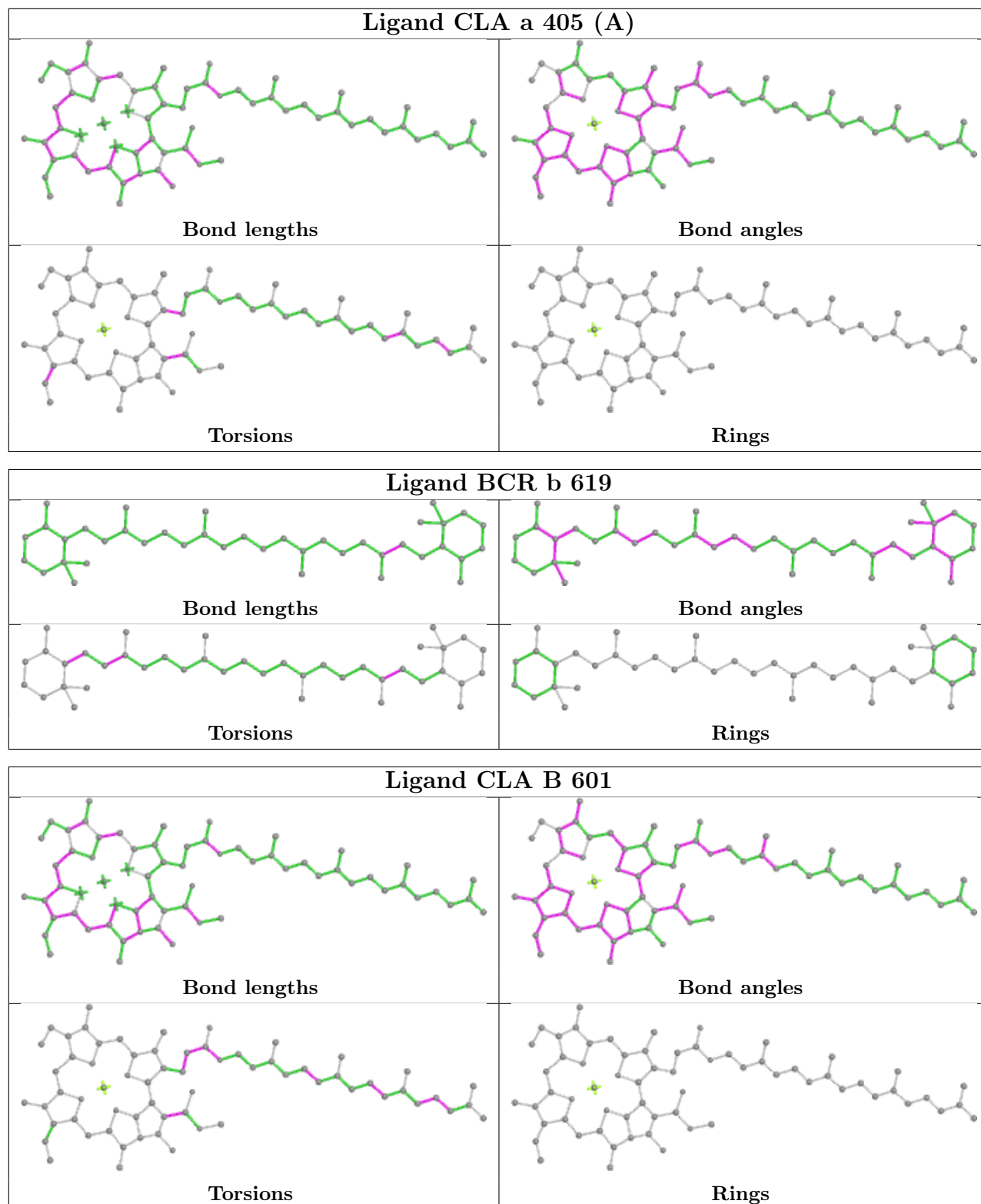


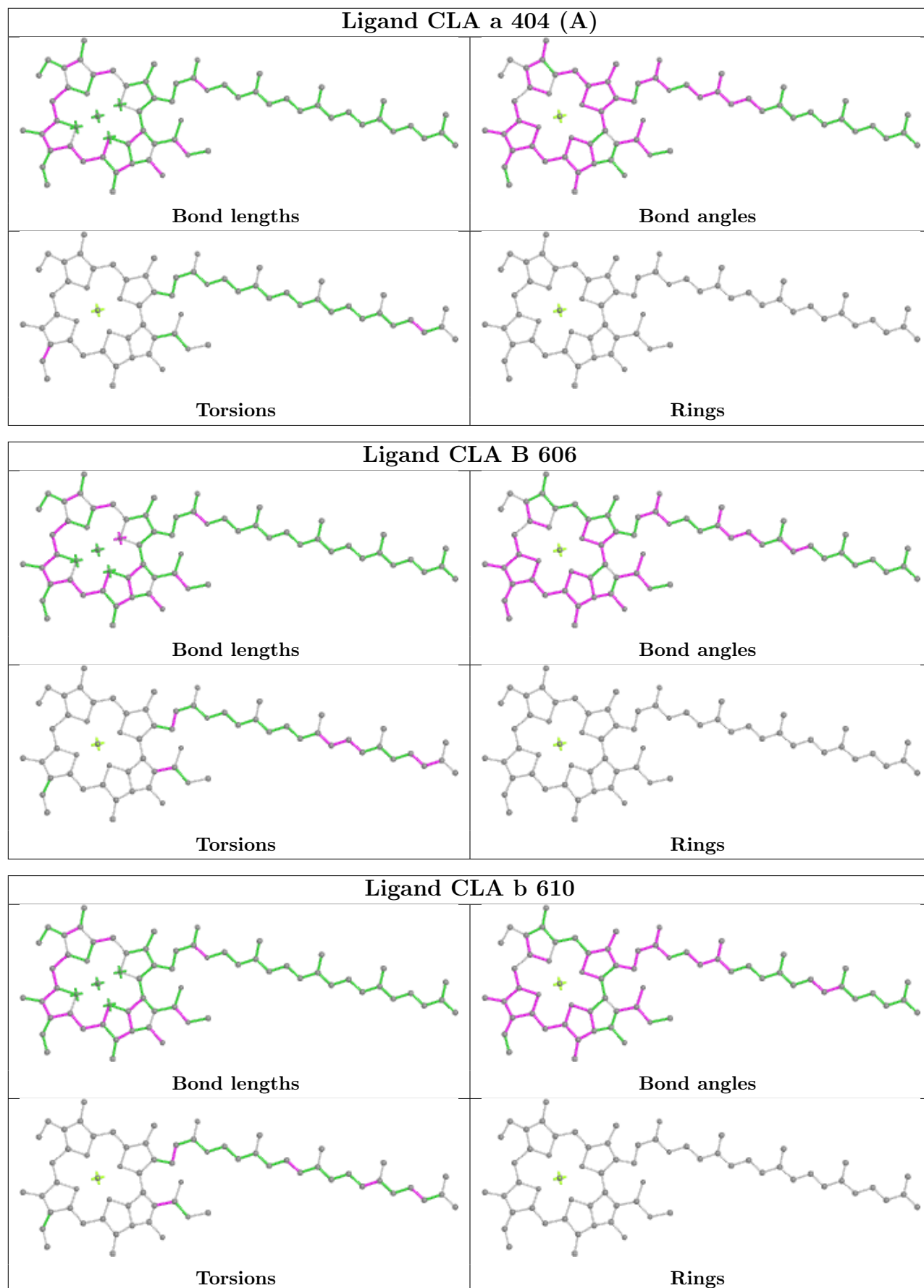


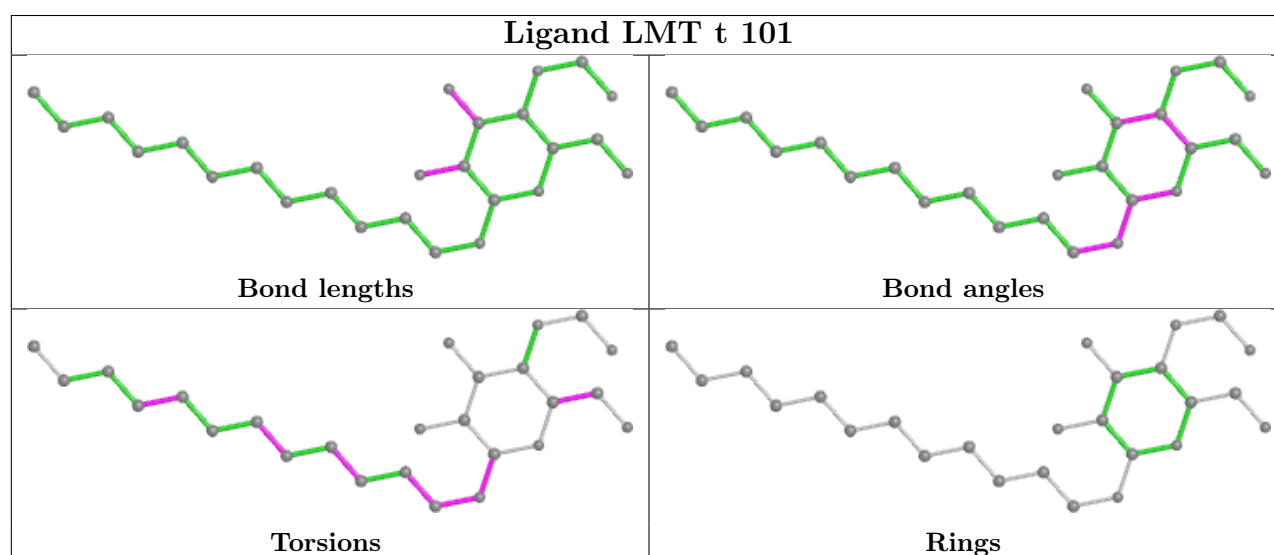
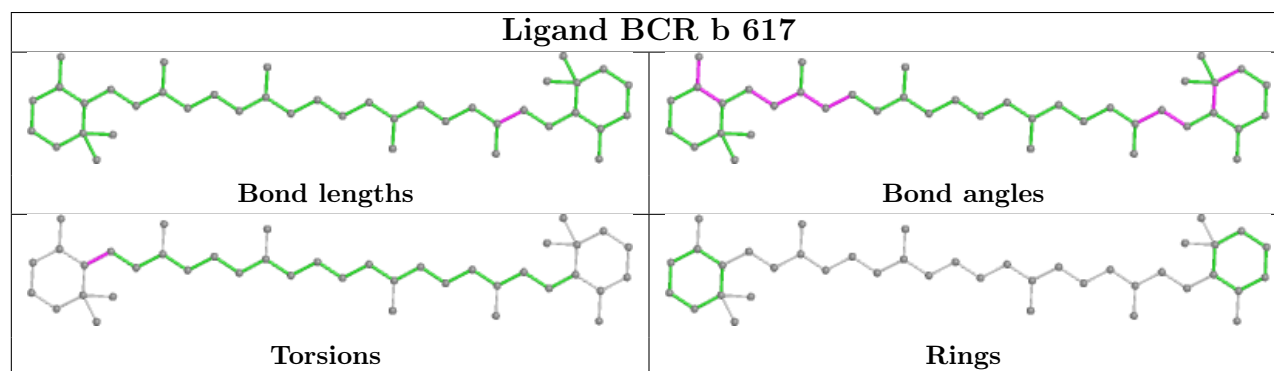
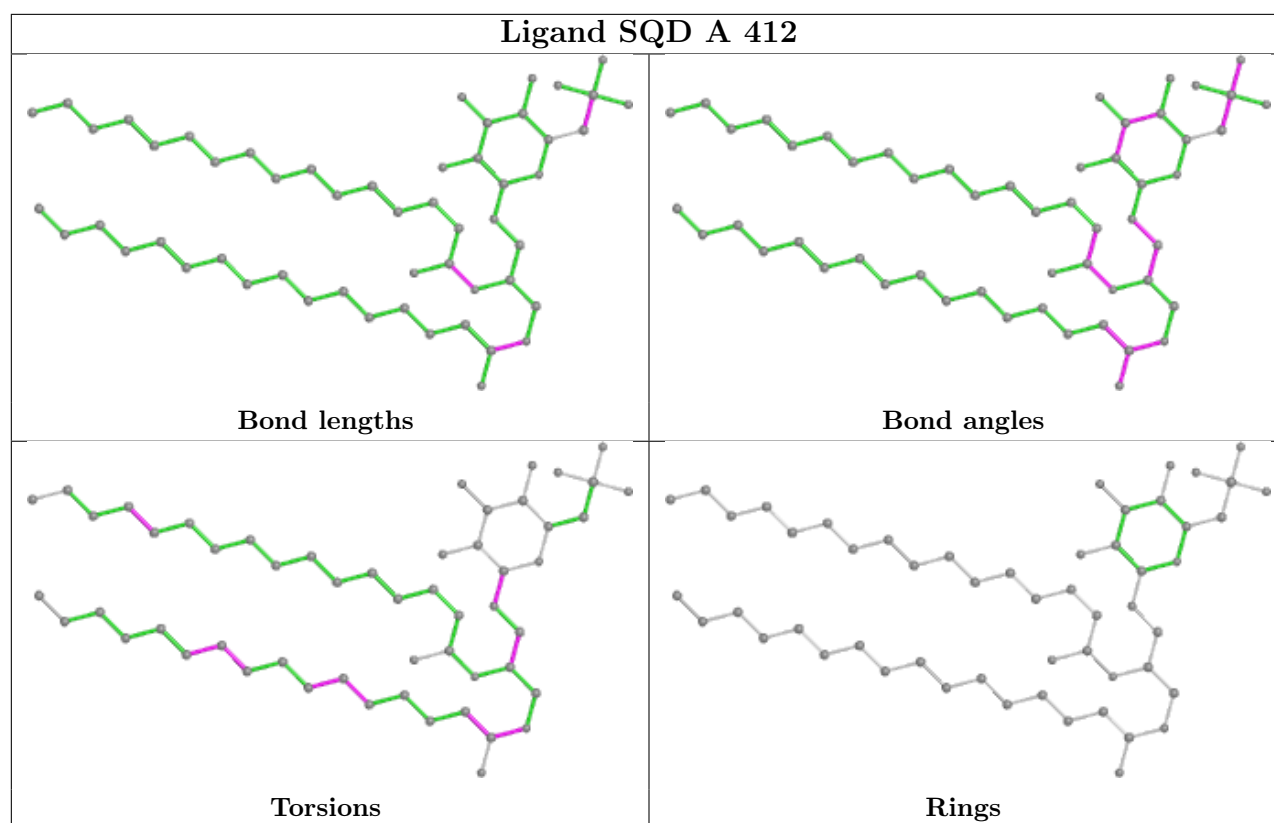


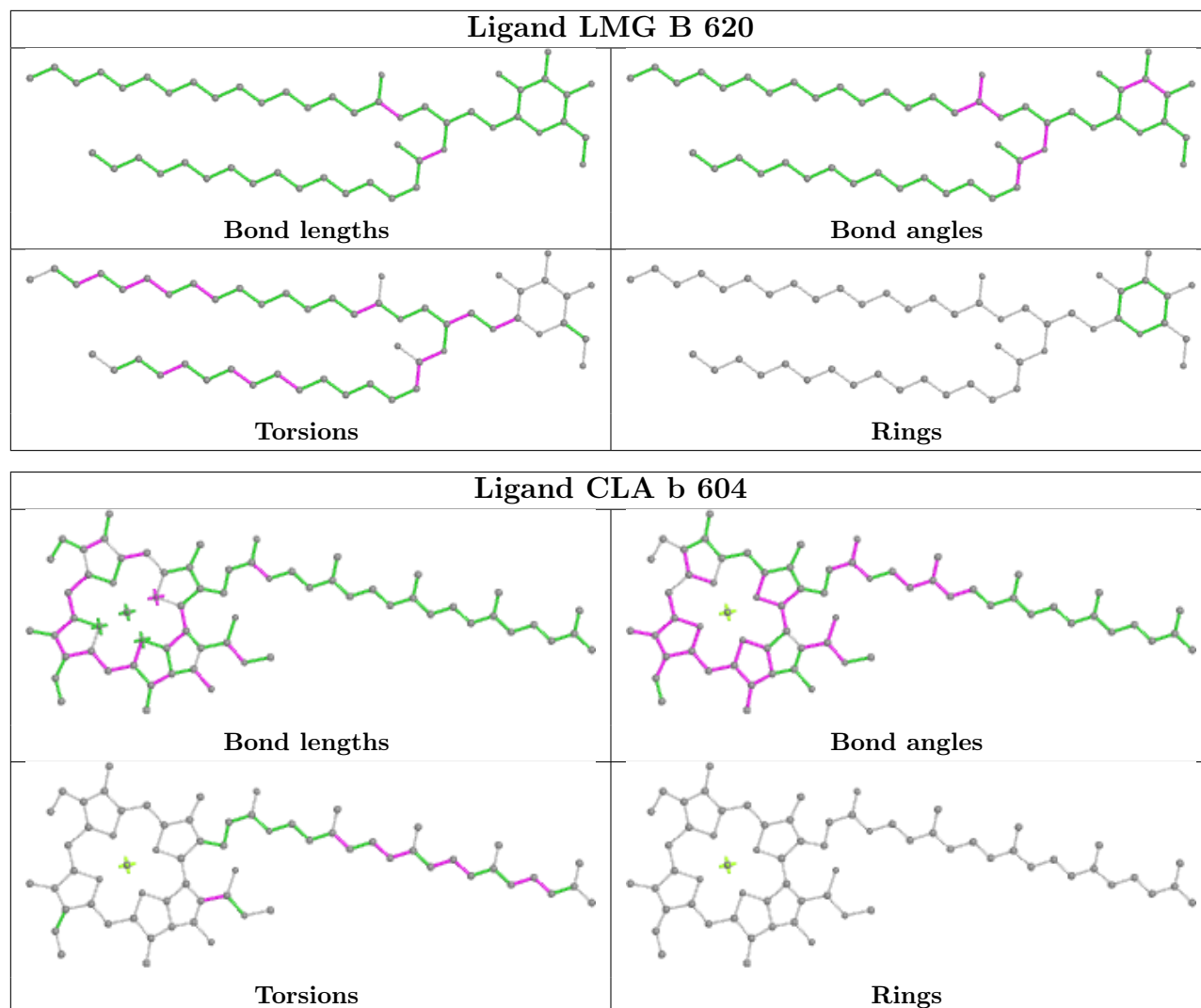


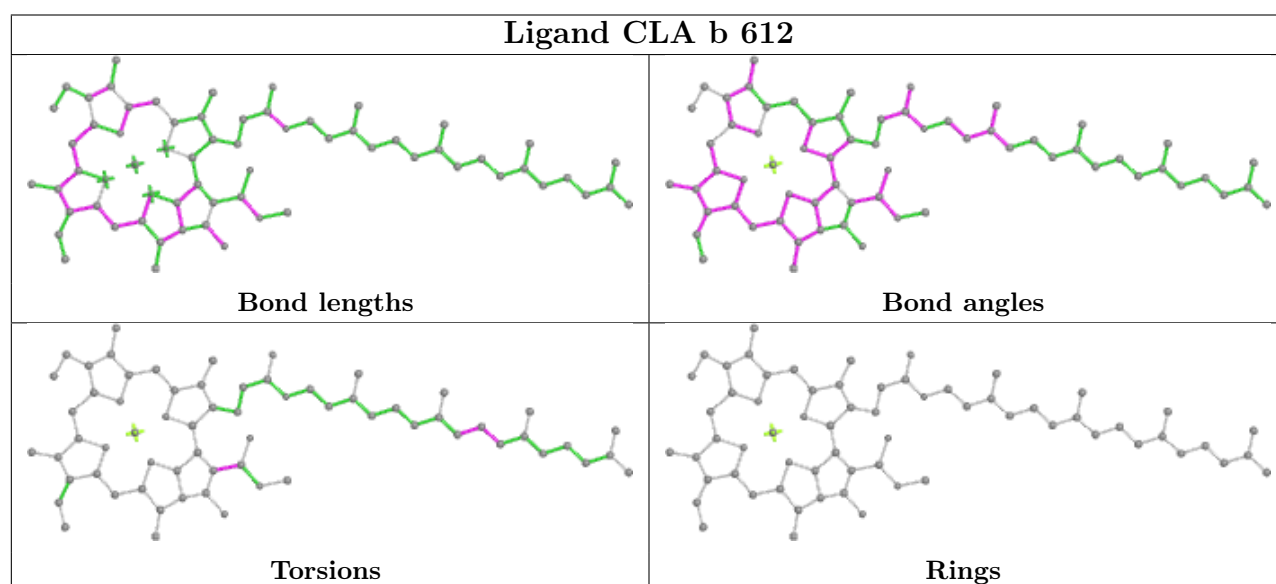
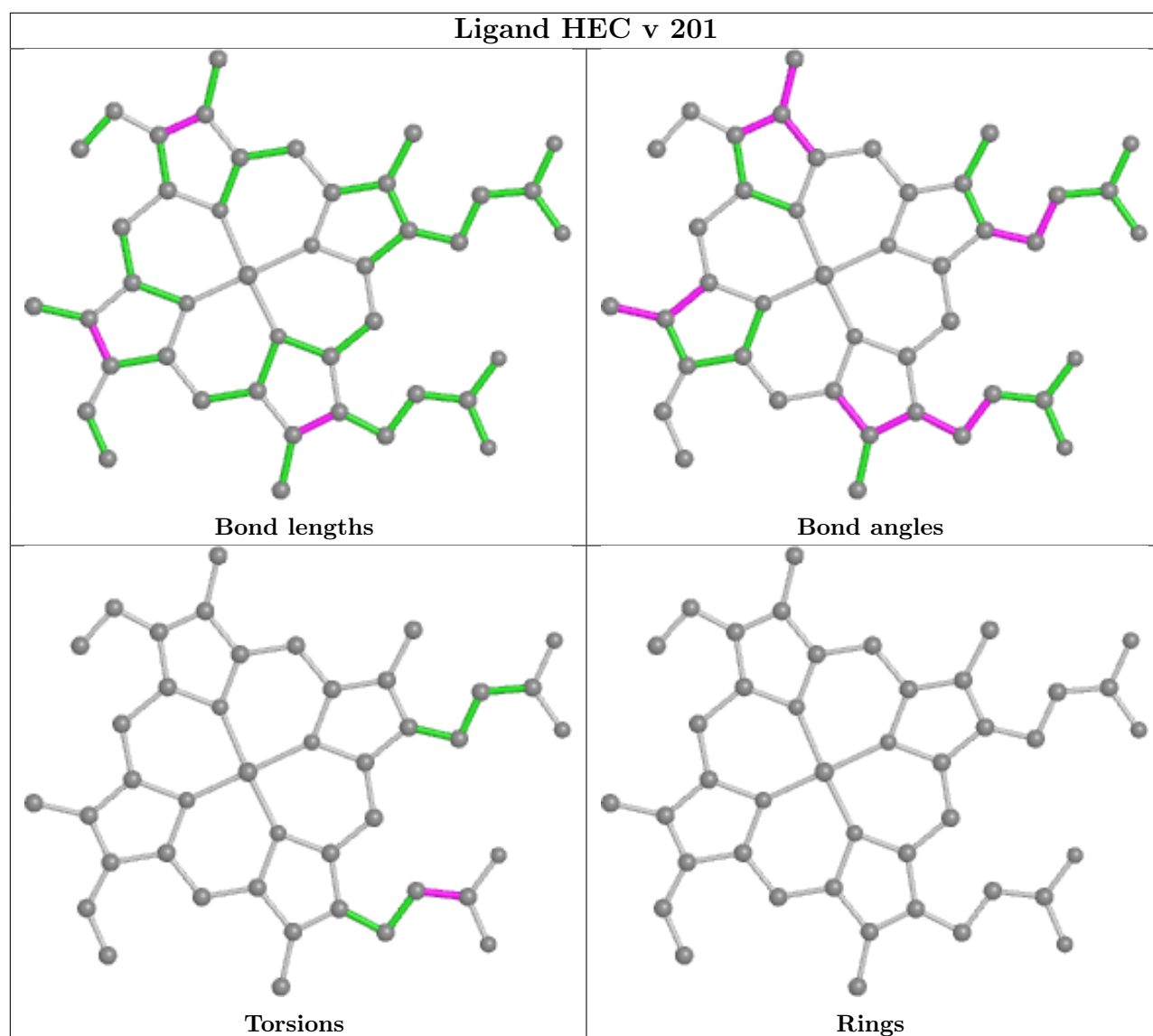


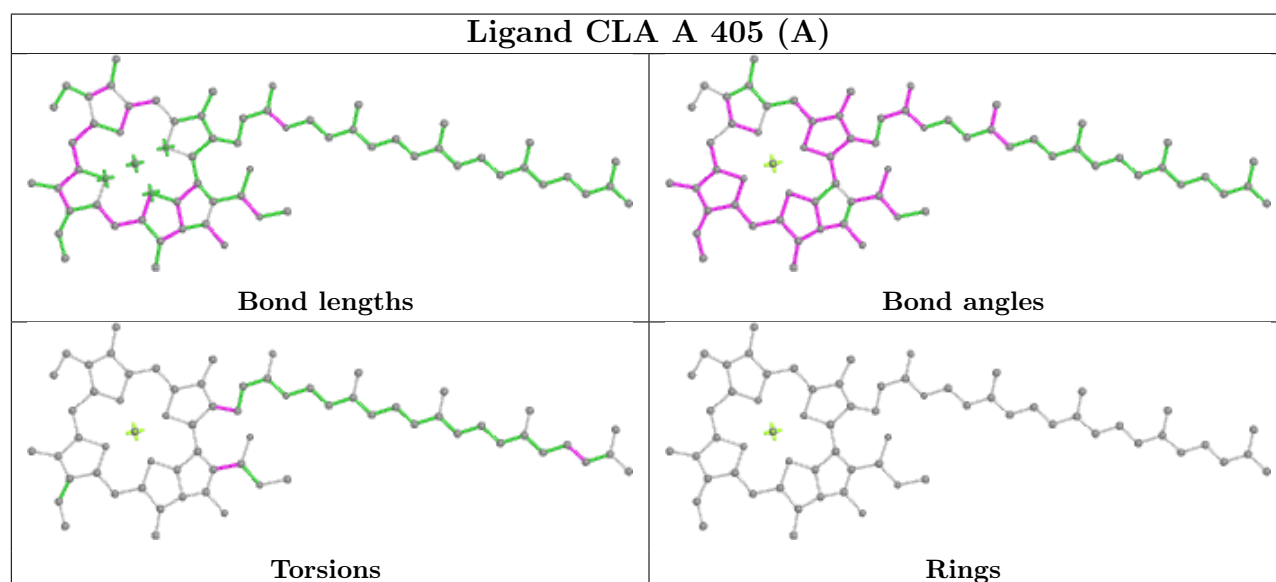
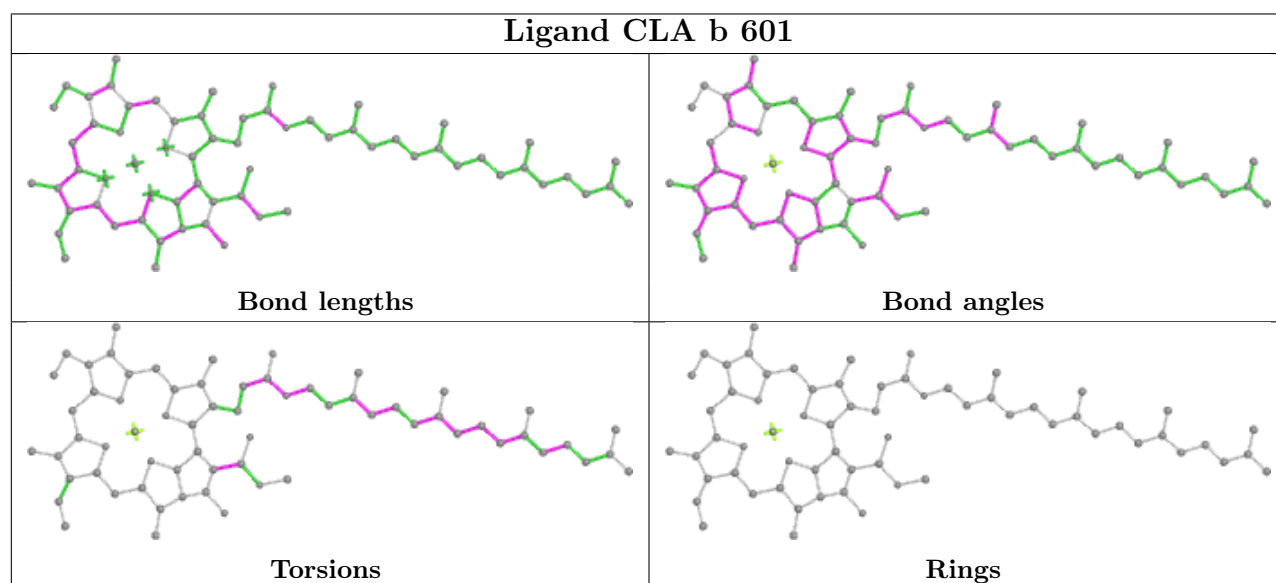
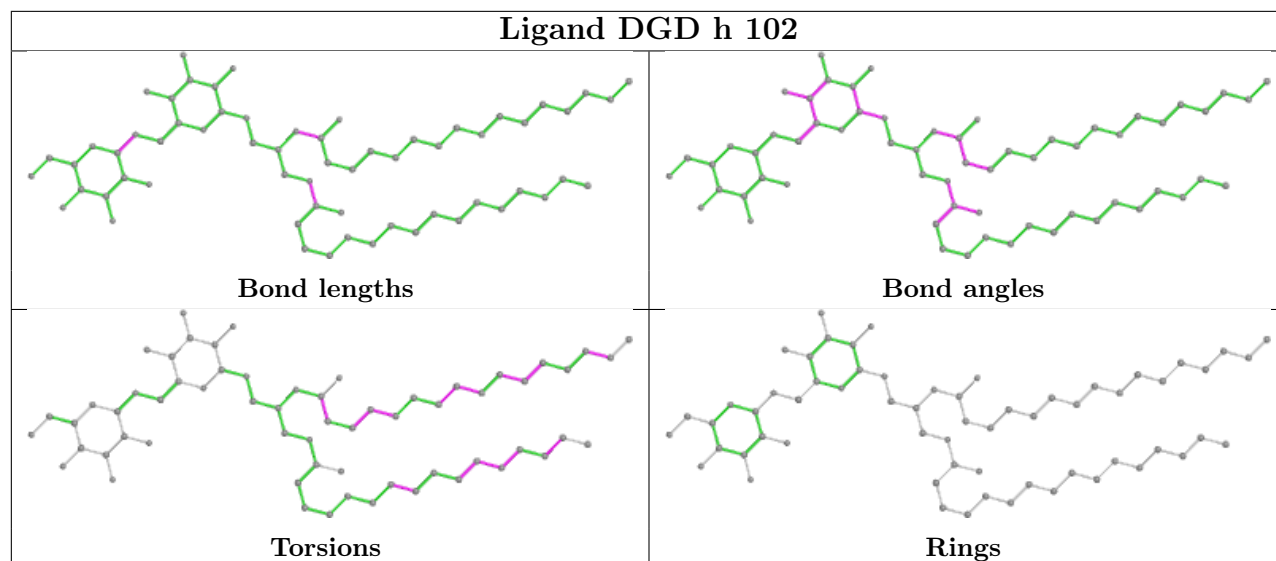


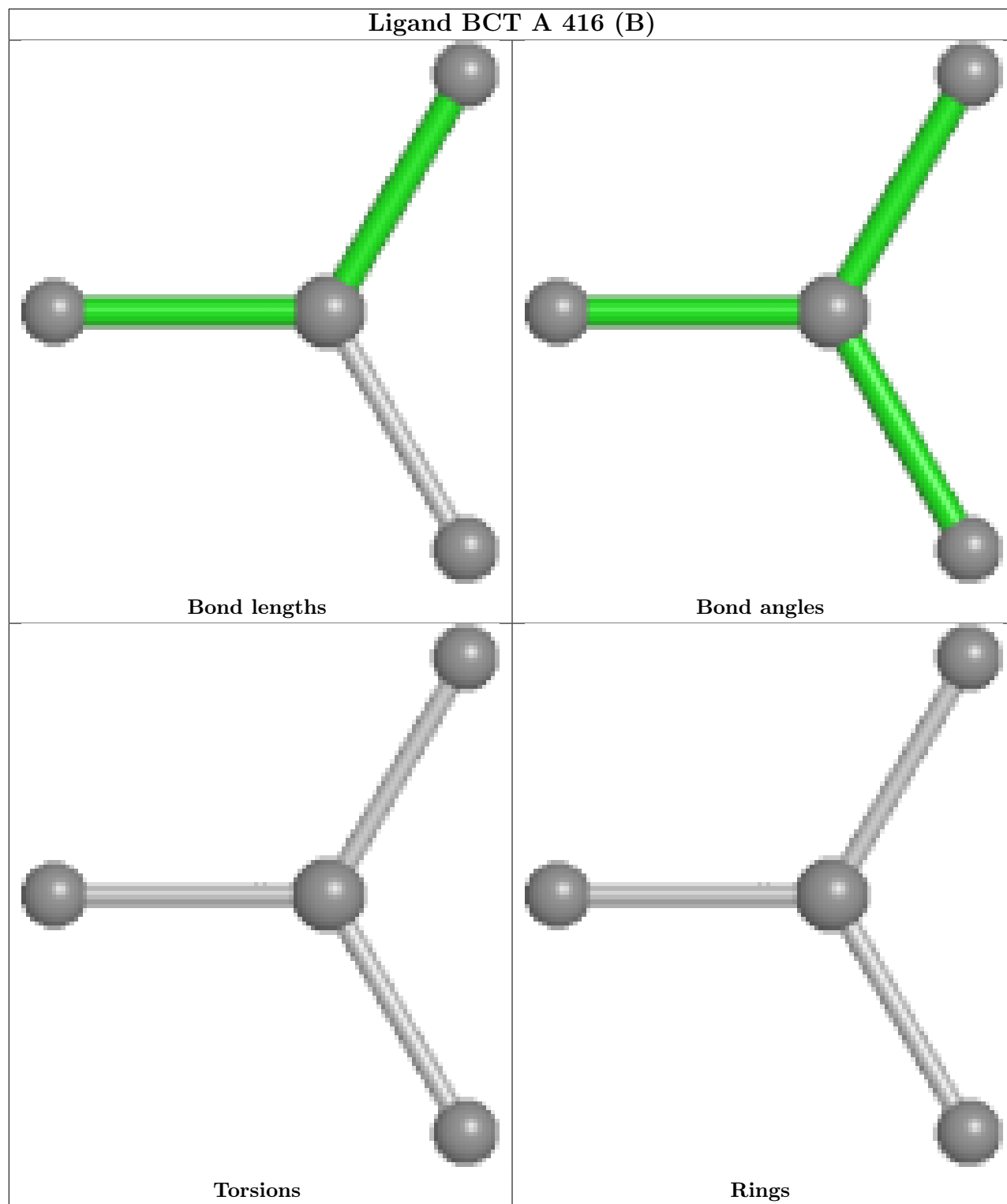


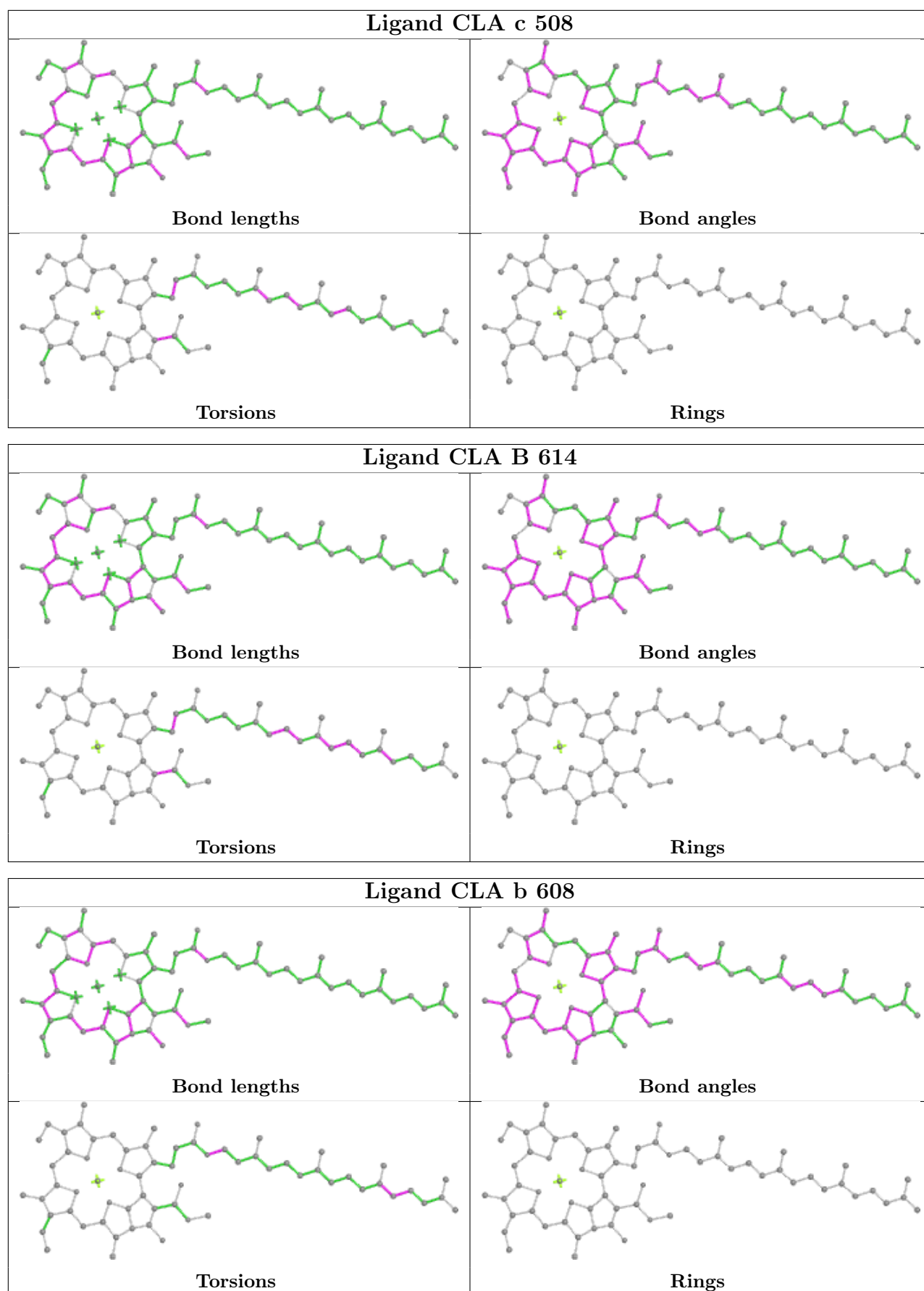


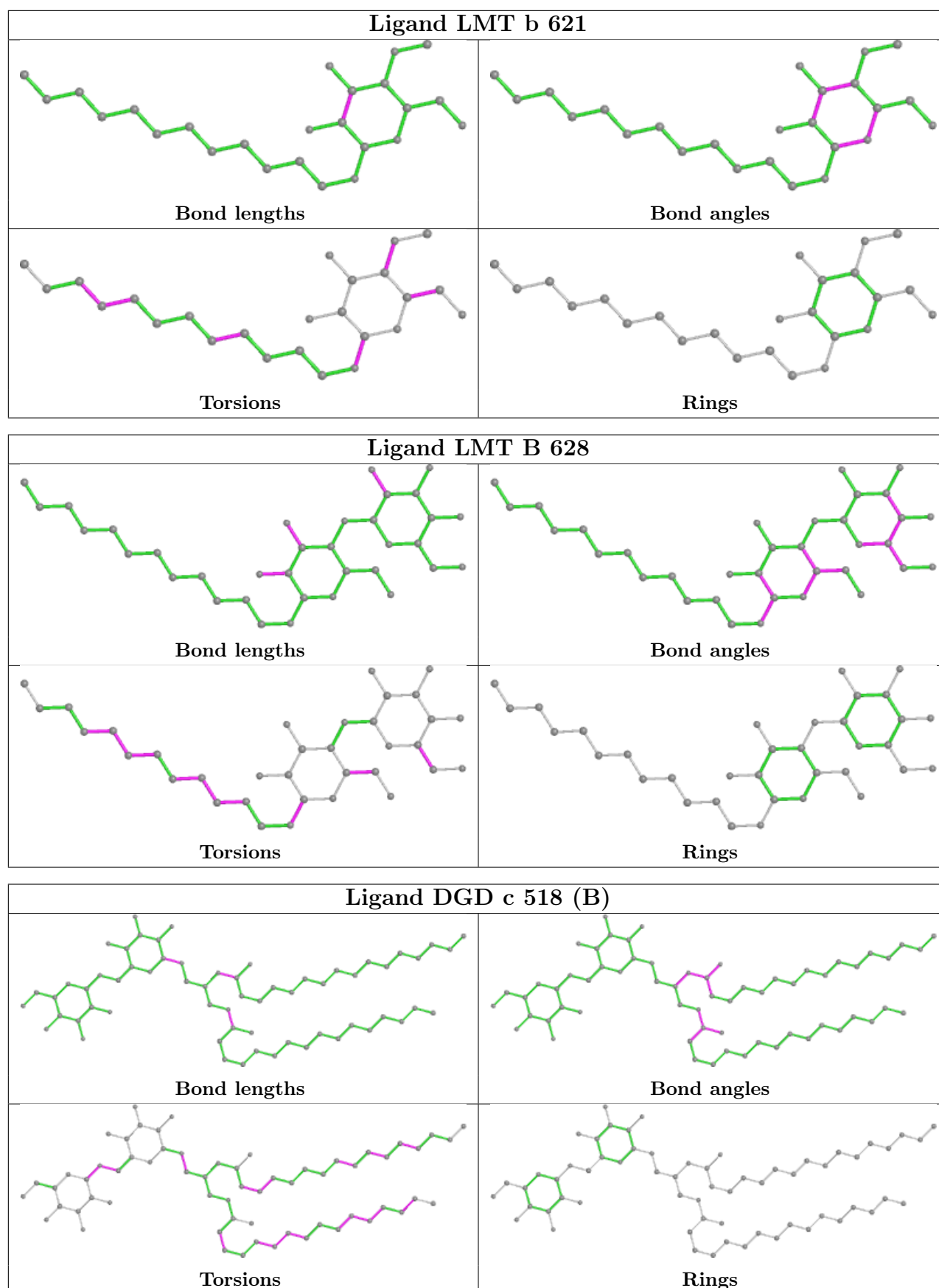


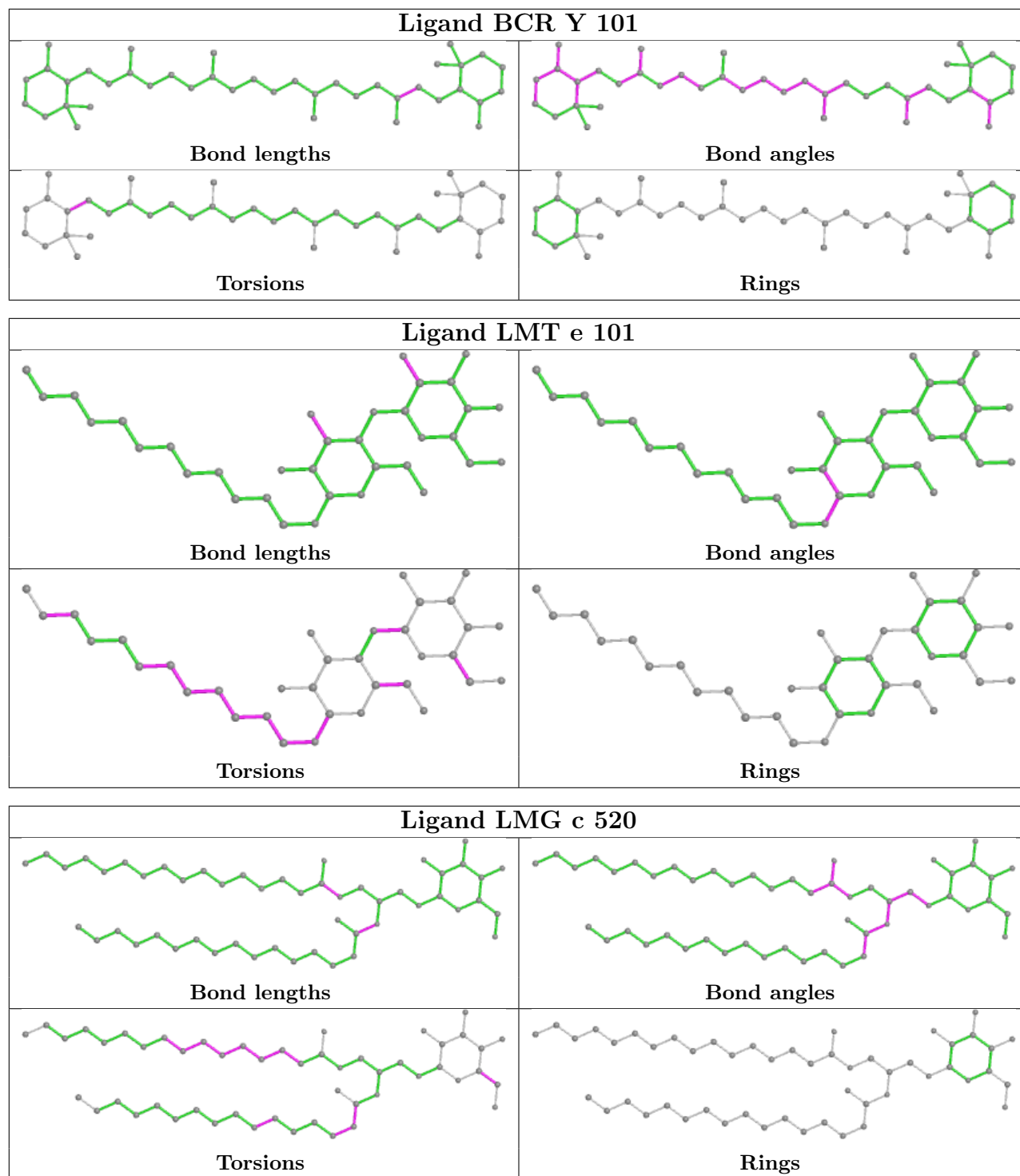


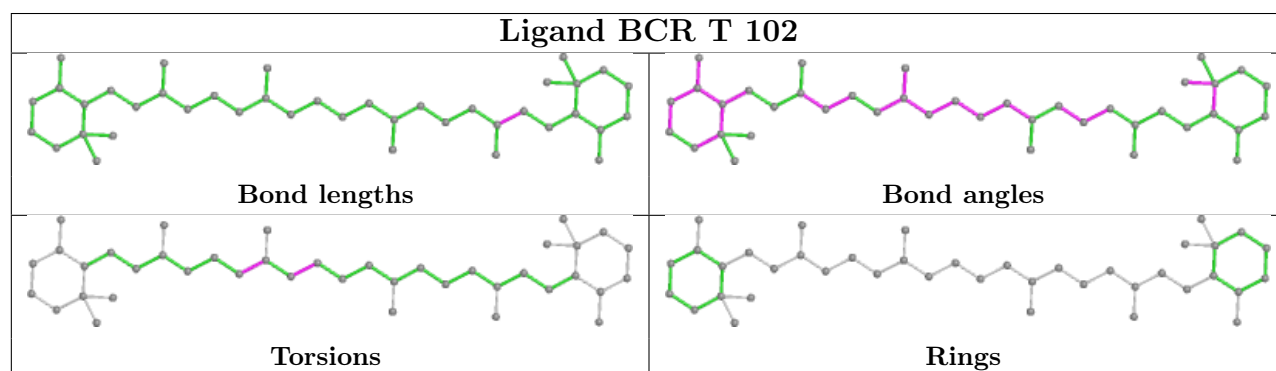
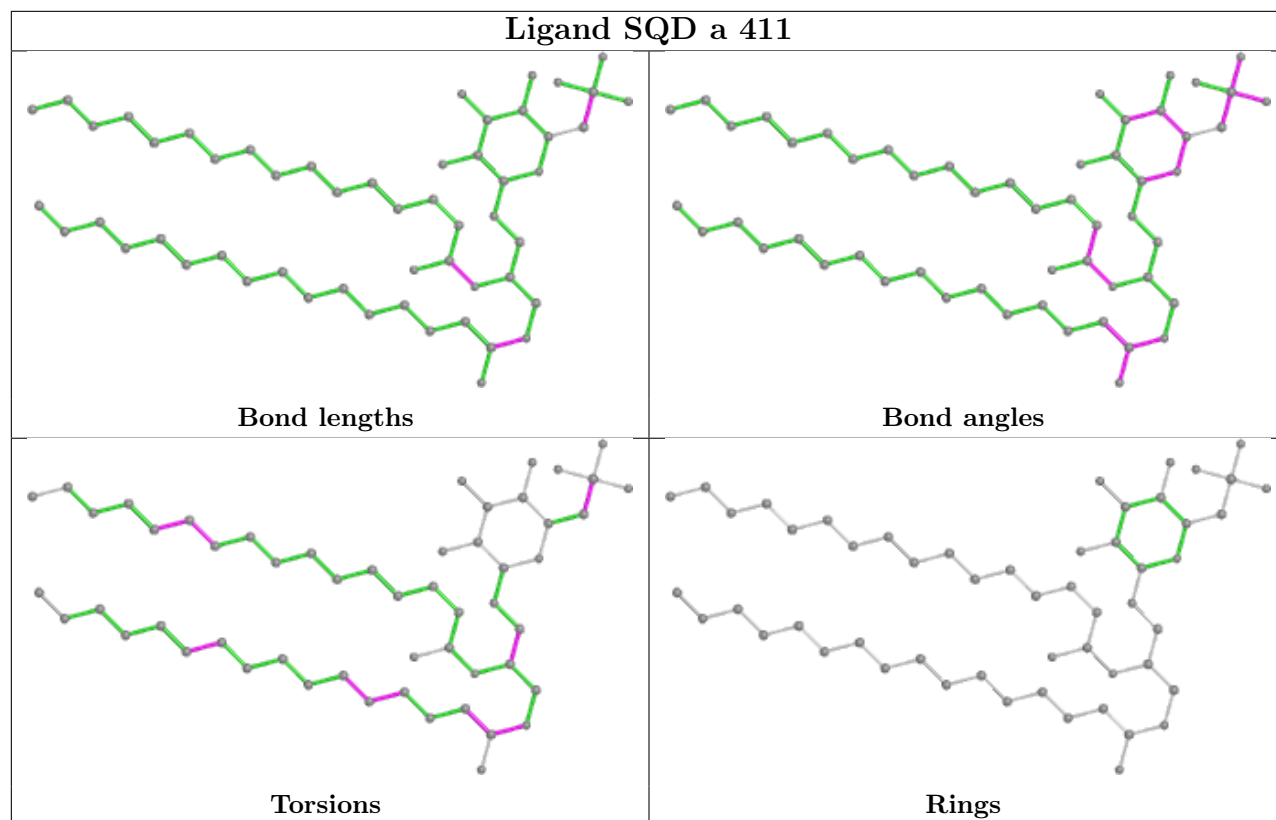
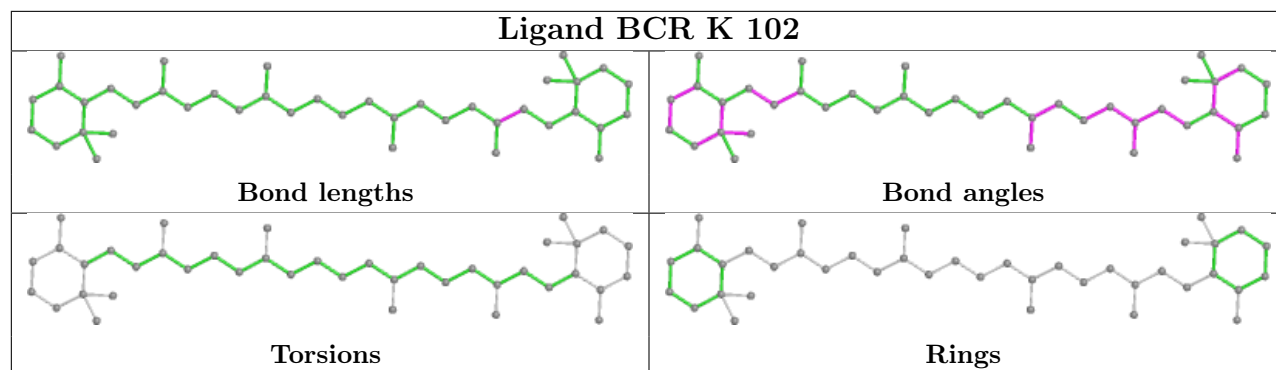


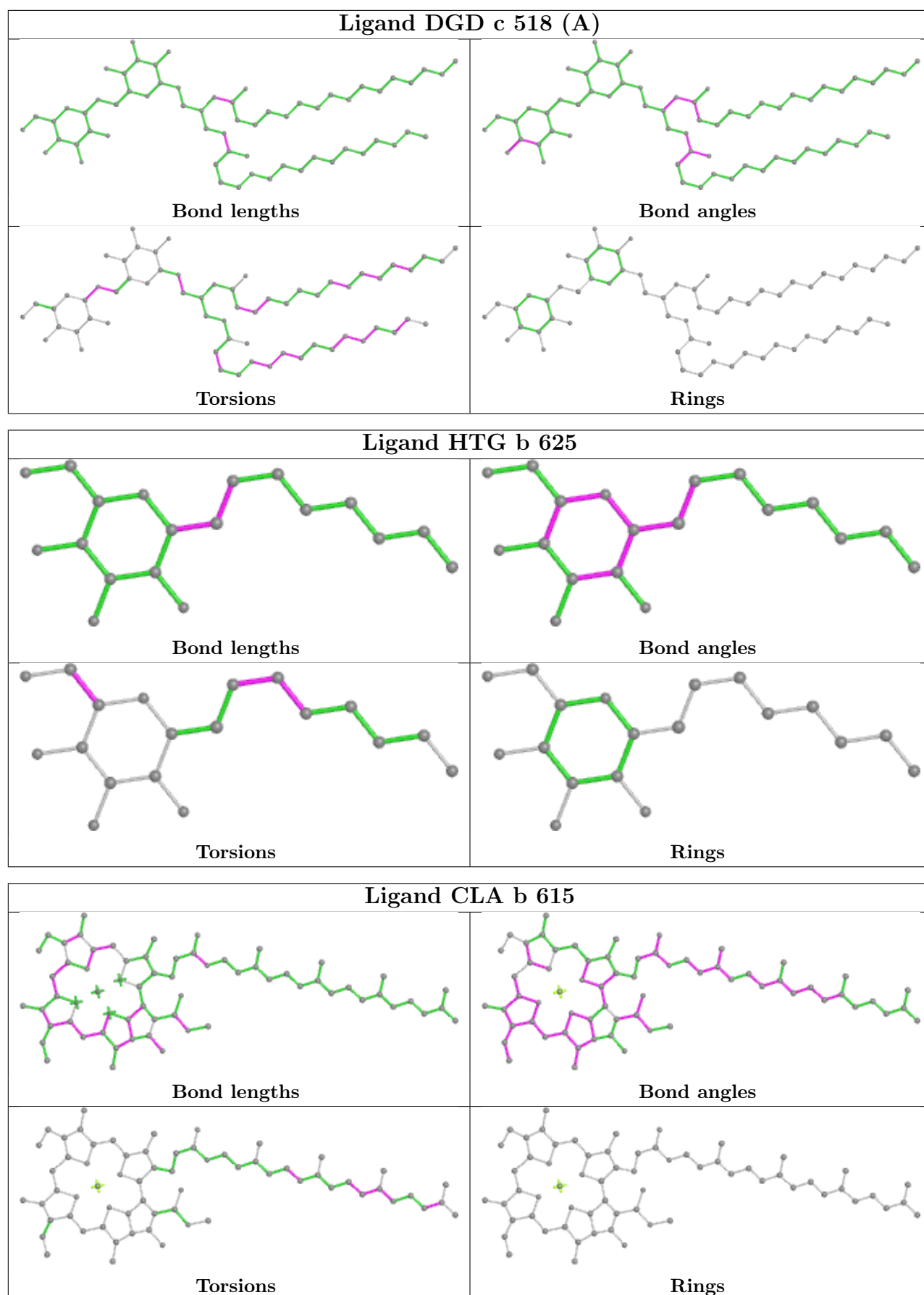


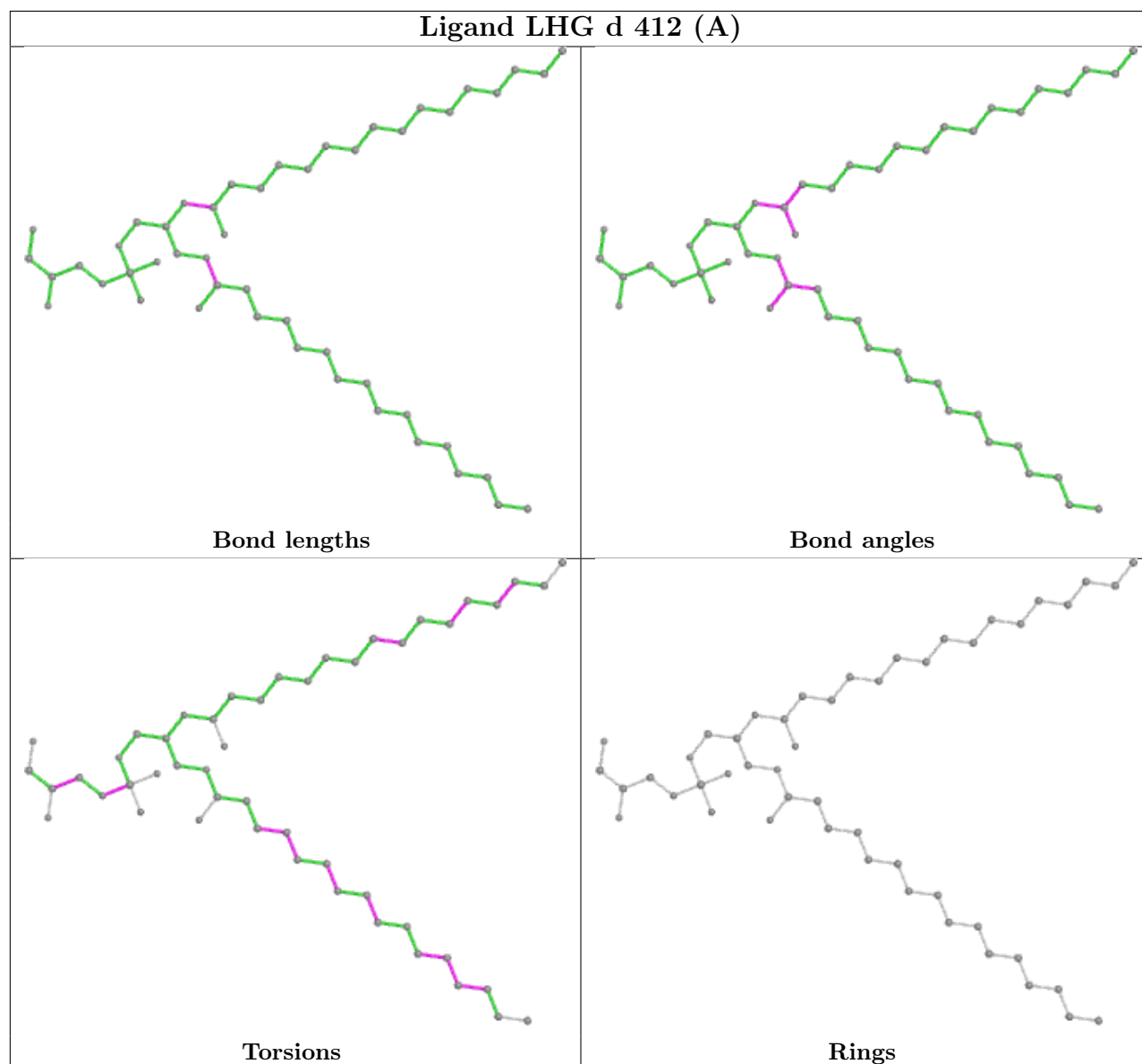
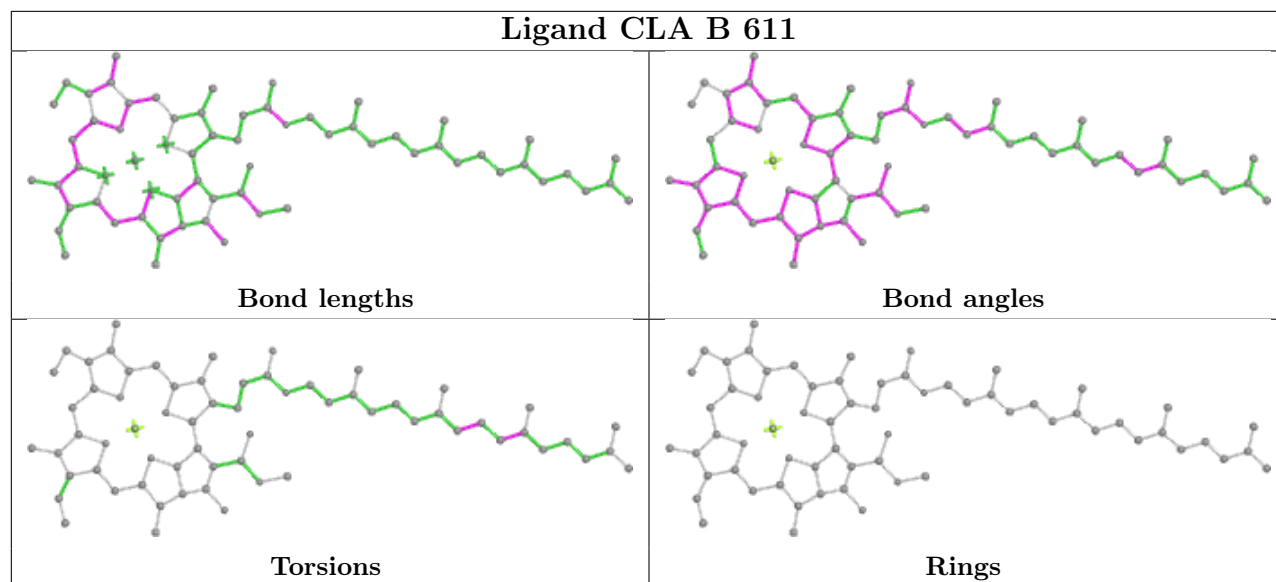


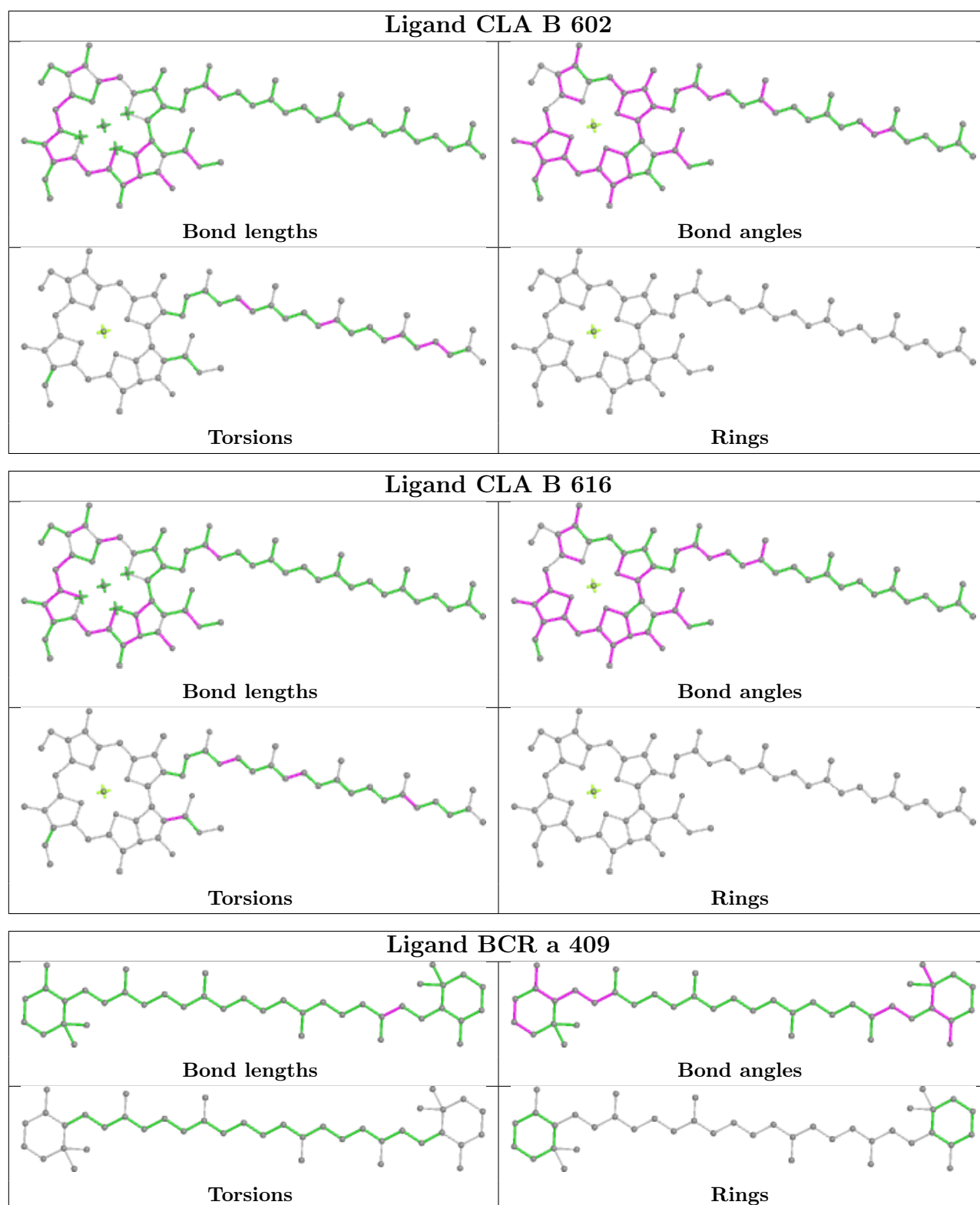


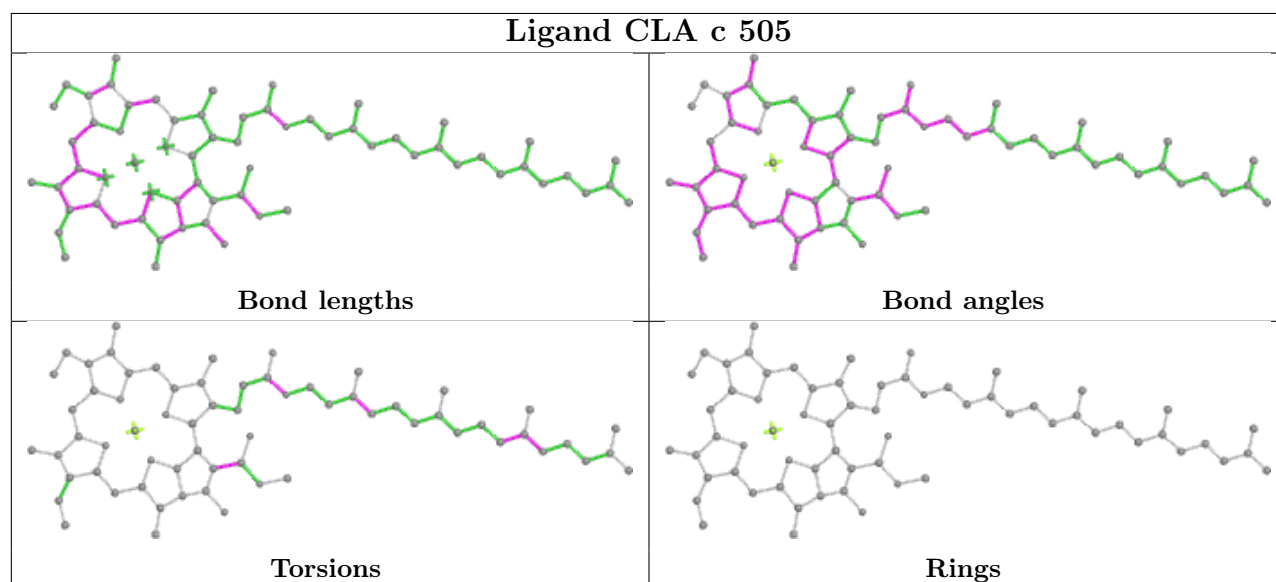
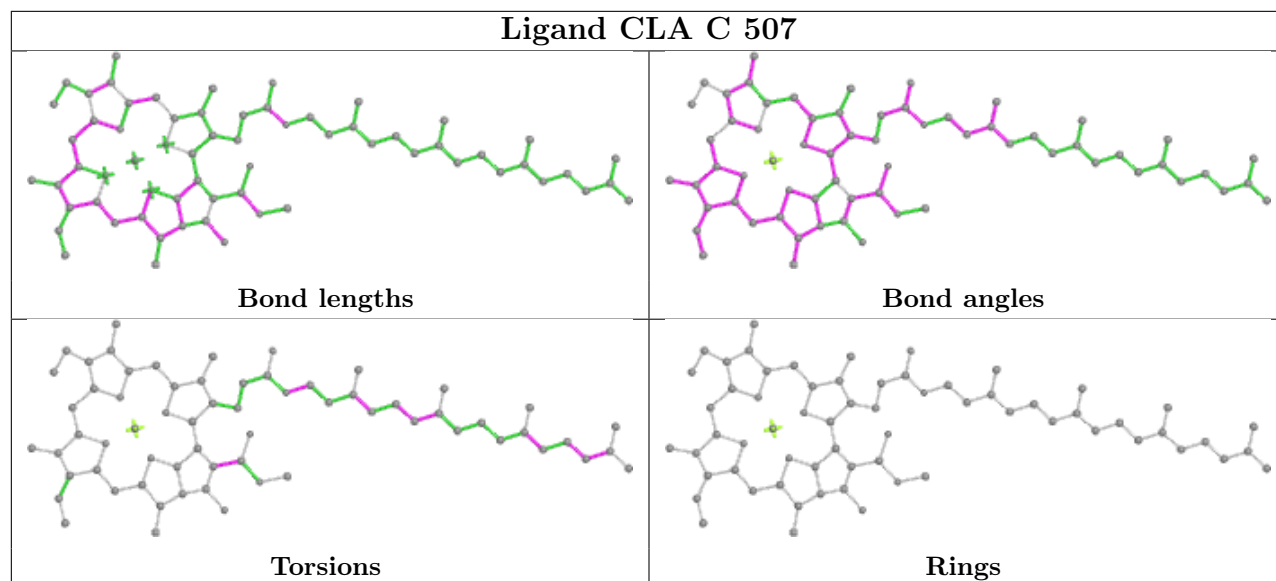
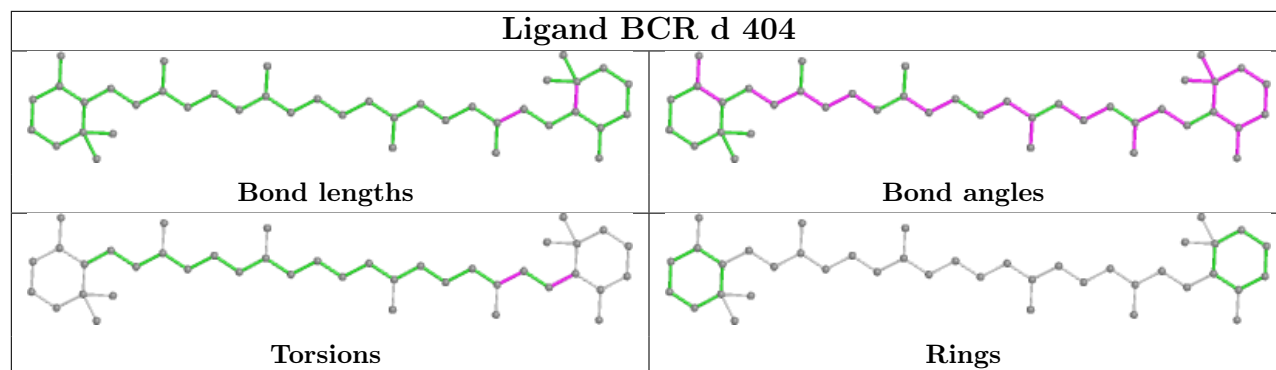


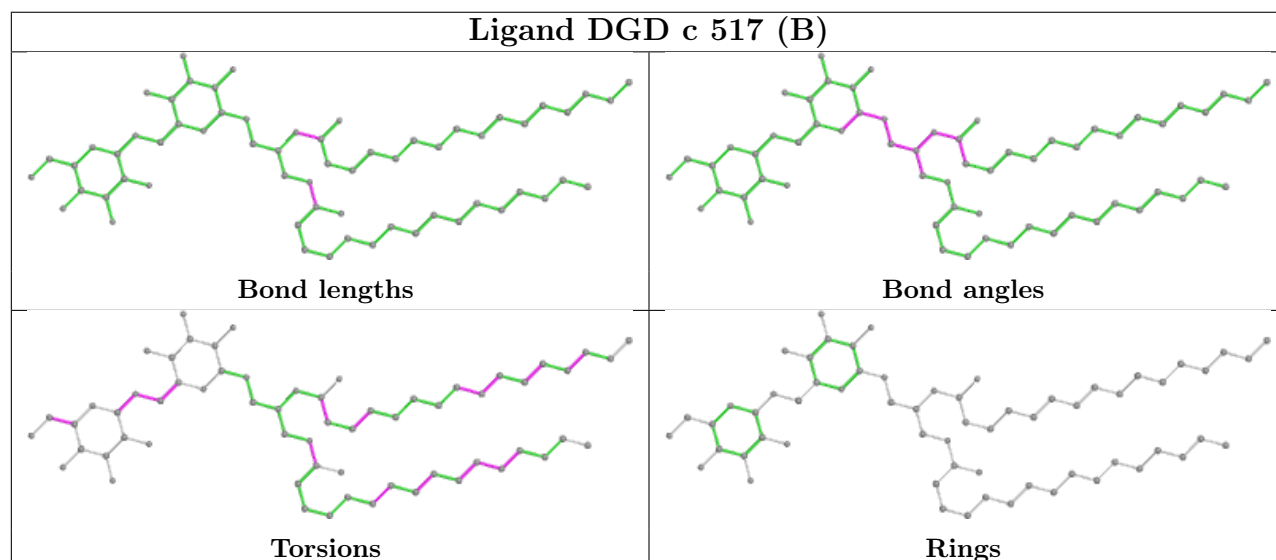
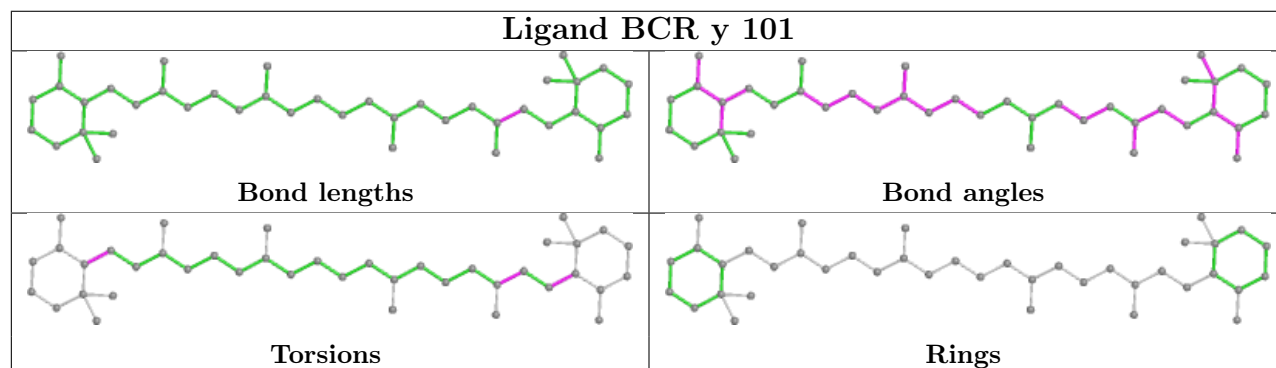
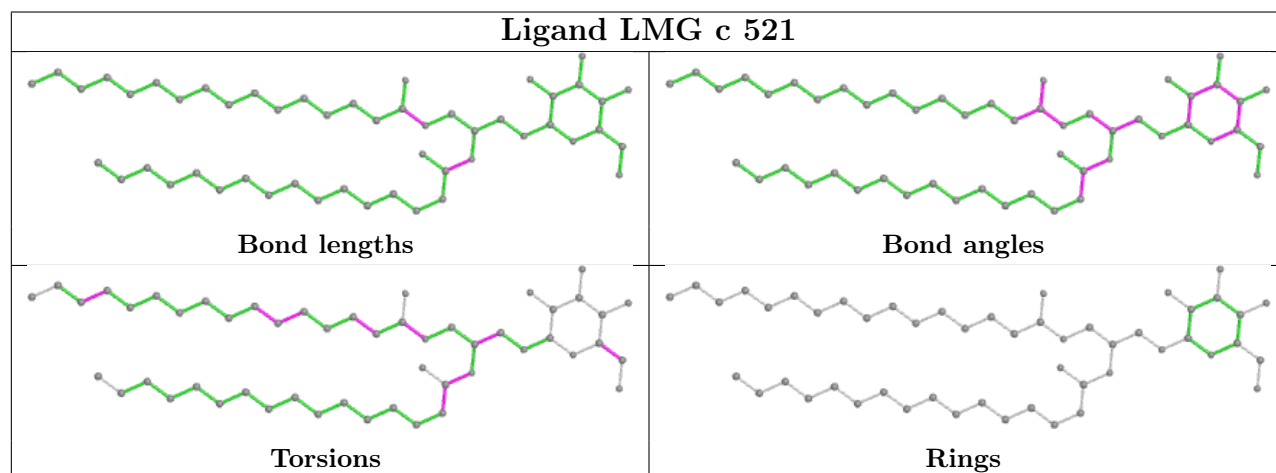
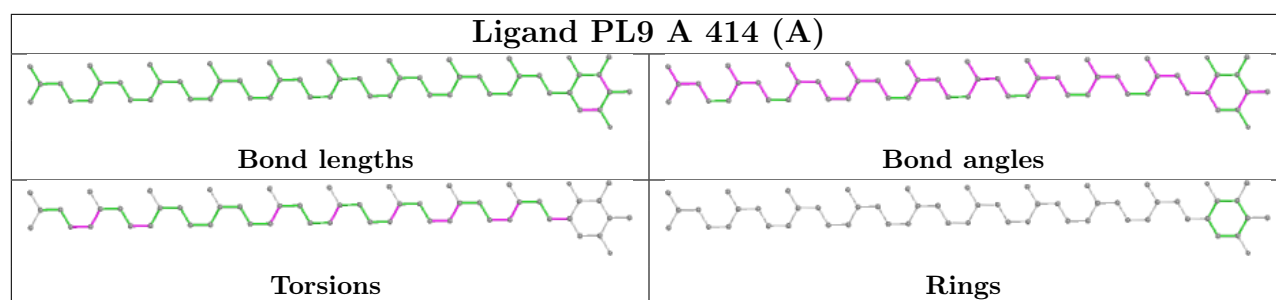


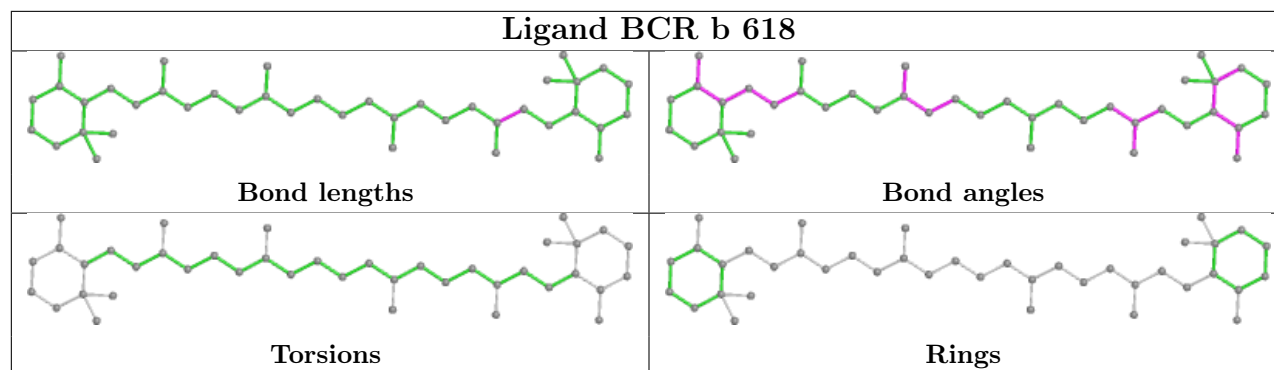












5.7 Other polymers [i](#)

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%)	-0.78	5 (1%) 73 72	41, 48, 69, 128	0
1	a	334/344 (97%)	-0.66	4 (1%) 79 77	44, 52, 81, 141	0
2	B	504/505 (99%)	-0.51	12 (2%) 59 56	43, 55, 82, 119	0
2	b	504/505 (99%)	-0.34	25 (4%) 28 27	46, 58, 99, 162	1 (0%)
3	C	451/455 (99%)	-0.58	6 (1%) 77 75	45, 60, 81, 162	0
3	c	455/455 (100%)	-0.46	11 (2%) 59 56	49, 66, 87, 126	2 (0%)
4	D	342/342 (100%)	-0.69	2 (0%) 89 88	41, 50, 68, 137	0
4	d	341/342 (99%)	-0.68	2 (0%) 89 88	43, 54, 77, 132	0
5	E	81/84 (96%)	-0.08	4 (4%) 29 28	52, 69, 101, 170	0
5	e	79/84 (94%)	0.21	7 (8%) 9 8	63, 77, 117, 152	0
6	F	34/44 (77%)	-0.47	2 (5%) 22 21	55, 61, 86, 108	0
6	f	31/44 (70%)	-0.34	2 (6%) 18 17	59, 68, 97, 148	0
7	H	64/65 (98%)	-0.29	2 (3%) 49 47	52, 63, 84, 109	0
7	h	64/65 (98%)	-0.29	3 (4%) 31 30	57, 71, 93, 108	0
8	I	37/38 (97%)	-0.12	3 (8%) 12 10	57, 63, 124, 165	0
8	i	37/38 (97%)	-0.03	5 (13%) 3 2	55, 64, 121, 139	0
9	J	38/39 (97%)	-0.28	2 (5%) 26 25	51, 70, 118, 182	0
9	j	39/39 (100%)	0.15	6 (15%) 2 1	60, 76, 127, 174	0
10	K	37/37 (100%)	-0.50	1 (2%) 54 52	59, 68, 86, 108	0
10	k	37/37 (100%)	-0.43	0 100 100	67, 74, 95, 113	0
11	L	36/37 (97%)	-0.37	3 (8%) 11 10	41, 48, 104, 147	0
11	l	36/37 (97%)	-0.42	2 (5%) 24 23	44, 49, 104, 121	0
12	M	32/36 (88%)	-0.63	1 (3%) 49 47	45, 50, 79, 143	0
12	m	33/36 (91%)	-0.41	2 (6%) 21 20	46, 50, 74, 151	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.10	15 (6%) 20 19	43, 65, 121, 186	0
13	o	243/244 (99%)	0.02	26 (10%) 6 5	45, 66, 125, 171	0
14	T	29/32 (90%)	-0.64	2 (6%) 16 15	44, 49, 75, 117	0
14	t	29/32 (90%)	-0.71	0 100 100	46, 51, 78, 133	0
15	U	96/104 (92%)	-0.46	0 100 100	48, 60, 93, 101	0
15	u	97/104 (93%)	-0.40	1 (1%) 82 81	52, 63, 84, 139	0
16	V	137/137 (100%)	-0.56	0 100 100	48, 58, 83, 107	0
16	v	137/137 (100%)	-0.21	4 (2%) 51 49	55, 71, 102, 136	0
17	X	38/40 (95%)	-0.26	2 (5%) 26 25	60, 71, 93, 113	0
17	x	38/40 (95%)	0.15	4 (10%) 6 5	63, 77, 123, 169	0
18	Y	29/30 (96%)	1.04	6 (20%) 1 1	68, 86, 120, 126	0
18	y	29/30 (96%)	0.31	4 (13%) 2 2	73, 90, 111, 118	0
19	Z	62/62 (100%)	0.10	7 (11%) 5 4	66, 81, 133, 169	0
19	z	62/62 (100%)	0.34	11 (17%) 1 1	79, 95, 146, 202	0
20	R	34/34 (100%)	2.01	18 (52%) 0 0	75, 100, 130, 139	0
All	All	5283/5384 (98%)	-0.40	212 (4%) 38 36	41, 60, 100, 202	3 (0%)

All (212) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	c	20	SER	7.9
5	E	84	LYS	7.4
2	b	495	PHE	7.3
13	O	60	ARG	6.7
1	a	11	ALA	6.5
3	C	23	ALA	6.5
13	o	4	THR	6.3
2	b	494	GLY	6.3
18	Y	19	ILE	6.1
19	Z	32	ASP	5.7
18	Y	18	VAL	5.5
13	o	56	PRO	5.3
5	e	84	LYS	5.3
17	x	2	THR	5.2
1	A	11	ALA	5.2
13	O	62	GLU	5.1
13	O	56	PRO	5.0

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Mol	Chain	Res	Type	RSRZ
20	R	32	GLN	5.0
13	O	4	THR	5.0
19	Z	31	GLN	5.0
12	m	34	LYS	4.9
3	c	19	ASN	4.9
19	z	31	GLN	4.8
13	o	60	ARG	4.8
13	o	62	GLU	4.6
3	c	21	ILE	4.6
12	M	33	GLN	4.6
13	o	63	ALA	4.6
13	O	59	LYS	4.6
20	R	35	LEU	4.5
13	O	63	ALA	4.5
13	o	59	LYS	4.5
13	o	57	LYS	4.5
17	x	38	GLN	4.4
19	z	32	ASP	4.4
19	z	60	PHE	4.4
19	z	3	ILE	4.4
3	C	143	TYR	4.4
9	j	3	GLU	4.4
6	F	12	SER	4.4
11	L	3	PRO	4.3
13	o	58	ASN	4.3
20	R	20	VAL	4.3
8	I	36	ASP	4.3
4	D	11	GLU	4.2
2	b	504	THR	4.2
19	Z	3	ILE	4.2
13	O	5	LEU	4.2
13	o	24	ASP	4.2
18	y	18	VAL	4.2
7	h	6	TRP	4.1
2	b	293	ALA	4.1
6	f	15	ILE	4.1
3	C	207	ARG	4.1
13	o	207	ARG	4.1
2	b	502	VAL	4.0
20	R	33	LYS	4.0
3	c	143	TYR	4.0
19	Z	30	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
20	R	3	TRP	3.9
14	T	30[A]	THR	3.9
19	z	38	GLN	3.9
2	b	493[A]	TRP	3.8
11	l	3	PRO	3.8
2	b	127	ARG	3.8
13	o	25	THR	3.8
19	z	42	LEU	3.8
2	b	489	GLU	3.7
5	e	81	GLU	3.7
6	f	16[A]	PHE	3.7
20	R	21	ARG	3.7
1	a	262[A]	TYR	3.6
2	b	503	THR	3.6
18	Y	20	ALA	3.6
13	o	35	SER	3.5
18	Y	21	GLN	3.5
12	m	33	GLN	3.5
4	D	12	ARG	3.5
8	I	34	ARG	3.4
2	B	494	GLY	3.4
11	l	2	GLU	3.3
1	A	13	LEU	3.3
9	j	1	MET	3.3
2	b	505	ARG	3.3
9	j	5	GLY	3.3
18	y	43	ARG	3.2
19	Z	35	ARG	3.2
19	z	35	ARG	3.2
18	Y	43	ARG	3.2
16	v	15	GLU	3.2
13	O	61	GLN	3.2
13	o	27	ARG	3.2
8	i	34	ARG	3.2
18	y	19	ILE	3.1
2	b	485	GLU	3.1
7	H	6	TRP	3.1
20	R	24	LEU	3.1
17	X	2	THR	3.1
16	v	17	LYS	3.1
3	c	23	ALA	3.1
2	B	295	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
8	i	38	GLU	3.0
18	y	41	VAL	3.0
1	a	13	LEU	3.0
9	j	6	ARG	3.0
17	X	38	GLN	3.0
11	L	7	ARG	3.0
19	Z	34	ASP	3.0
3	C	24	THR	3.0
3	c	207	ARG	2.9
20	R	31	VAL	2.9
20	R	18	TRP	2.9
20	R	4	ARG	2.9
20	R	28	VAL	2.9
9	j	4	GLY	2.9
2	b	294	SER	2.9
19	z	62	VAL	2.9
13	o	61	GLN	2.8
20	R	29	LYS	2.8
19	z	30	PRO	2.8
13	O	25	THR	2.8
5	E	59	GLU	2.8
9	J	3	GLU	2.8
13	o	134	THR	2.8
3	c	192	GLY	2.8
13	o	246	ALA	2.7
18	Y	22	LEU	2.7
2	b	86	ILE	2.7
3	c	22	PHE	2.7
13	o	23	ASP	2.7
19	Z	2	THR	2.7
19	z	34	ASP	2.7
13	o	64	GLU	2.7
13	o	206	GLY	2.7
2	b	373	LYS	2.7
8	i	36	ASP	2.6
4	d	12	ARG	2.6
2	B	86	ILE	2.6
4	d	237[A]	PRO	2.6
2	B	162	PHE	2.6
2	b	85	GLY	2.5
9	j	2	SER	2.5
20	R	34	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	85	GLY	2.5
5	e	83	LEU	2.5
17	x	39	ARG	2.5
3	C	181	PHE	2.5
2	b	374	ASN	2.5
6	F	13	TYR	2.5
5	E	61	ARG	2.5
9	J	6	ARG	2.4
11	L	5	PRO	2.4
16	v	16	GLY	2.4
8	i	35	LYS	2.4
3	c	233	VAL	2.4
2	b	484[A]	PRO	2.4
2	B	485	GLU	2.4
2	B	487	SER	2.4
13	O	35	SER	2.4
2	B	293	ALA	2.4
2	B	495	PHE	2.4
13	o	5	LEU	2.4
2	b	161	LEU	2.4
20	R	6	LEU	2.4
20	R	27	ALA	2.4
16	v	14	SER	2.4
17	x	3	ILE	2.3
5	E	82	GLN	2.3
13	o	55	GLU	2.3
2	b	488	PRO	2.3
13	o	130	GLN	2.3
2	b	295	GLY	2.3
20	R	5	VAL	2.3
1	A	16	ARG	2.3
1	A	262[A]	TYR	2.3
13	O	27	ARG	2.3
10	K	10	LYS	2.3
13	o	26	ALA	2.3
7	h	65	LEU	2.2
1	A	12	ASN	2.2
7	H	23	PRO	2.2
13	O	207	ARG	2.2
20	R	2	ASP	2.2
1	a	242[A]	GLU	2.2
5	e	82	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
2	b	376	VAL	2.2
7	h	23	PRO	2.2
15	u	23	GLU	2.2
3	c	201	ASN	2.2
20	R	19	ALA	2.2
2	b	435	GLU	2.2
8	i	37	LEU	2.1
2	B	296	ALA	2.1
19	z	61	VAL	2.1
13	O	55	GLU	2.1
13	O	89	SER	2.1
13	o	22	LEU	2.1
3	C	142	GLU	2.1
13	O	58	ASN	2.1
5	e	25	ILE	2.1
5	e	42	LEU	2.1
2	b	497	GLN	2.1
2	b	496	TYR	2.1
8	I	37	LEU	2.1
14	T	29[A]	ILE	2.1
13	o	54	GLU	2.1
2	B	374	ASN	2.1
2	B	128	THR	2.0
2	b	129	GLY	2.0
13	o	34	SER	2.0
3	c	142	GLU	2.0
5	e	24	SER	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	0.14	57,69,76,89	0
14	FME	T	1	10/11	0.94	0.11	46,60,72,76	0
12	FME	M	1	10/11	0.96	0.12	49,63,97,109	0
14	FME	t	1	10/11	0.96	0.10	43,51,58,76	0
12	FME	m	1	10/11	0.97	0.12	55,64,93,112	0
8	FME	I	1	10/11	0.97	0.07	60,70,80,86	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	624	33/-	0.46	0.39	57,106,145,153	0
30	UNL	I	101	40/-	0.48	0.35	80,106,158,169	0
30	UNL	b	626	33/-	0.50	0.36	67,100,154,165	0
33	LMT	T	101	35/35	0.52	0.31	75,127,183,186	0
30	UNL	j	101	10/-	0.54	0.28	78,94,106,108	0
33	LMT	b	621	25/35	0.55	0.29	83,115,157,170	0
30	UNL	i	101	40/-	0.56	0.31	78,110,152,169	0
34	LMG	C	521	51/55	0.57	0.31	58,118,157,172	0
27	GOL	a	417	6/6	0.61	0.48	81,102,107,110	0
33	LMT	B	628	35/35	0.62	0.37	64,119,146,159	0
30	UNL	A	415	28/-	0.62	0.37	91,115,134,158	0
30	UNL	K	101[A]	34/-	0.64	0.34	90,113,127,128	34
30	UNL	K	101[B]	34/-	0.64	0.34	89,113,127,128	34
33	LMT	F	101	35/35	0.64	0.52	106,136,178,183	0
30	UNL	c	525[B]	32/-	0.65	0.38	102,115,127,139	32
30	UNL	c	525[A]	32/-	0.65	0.38	102,115,127,138	32
33	LMT	M	101	35/35	0.66	0.25	61,101,124,129	0
33	LMT	B	629	25/35	0.66	0.26	65,91,149,165	0
35	HTG	D	410	16/19	0.66	0.29	90,106,132,143	0
34	LMG	c	521	51/55	0.68	0.28	75,136,166,190	0
35	HTG	b	623	19/19	0.68	0.49	80,130,155,167	0
33	LMT	D	401	35/35	0.69	0.33	67,118,139,144	0
33	LMT	A	420	35/35	0.70	0.36	97,135,158,172	0
30	UNL	b	629	36/-	0.70	0.20	71,98,130,143	0
30	UNL	x	101	18/-	0.70	0.23	72,83,135,137	0
34	LMG	Z	101	37/55	0.71	0.27	70,119,155,173	0
33	LMT	m	103	35/35	0.73	0.25	60,91,109,119	0
32	LHG	a	419[A]	42/49	0.73	0.35	95,143,157,167	42
32	LHG	a	419[B]	42/49	0.73	0.35	95,143,157,168	42
27	GOL	o	303	6/6	0.74	0.32	80,102,112,119	0
33	LMT	b	627	25/35	0.74	0.25	57,100,147,164	0
34	LMG	z	101	39/55	0.74	0.26	75,129,151,168	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
30	UNL	m	102	10/-	0.74	0.37	74,79,100,101	0
33	LMT	B	626	35/35	0.74	0.26	70,98,140,150	0
33	LMT	e	101	35/35	0.75	0.49	113,151,189,195	0
33	LMT	a	416	35/35	0.75	0.39	108,138,156,164	0
27	GOL	A	411	6/6	0.77	0.20	69,78,88,94	0
37	CA	F	104	1/1	0.77	0.20	131,131,131,131	0
27	GOL	b	624	6/6	0.78	0.19	91,98,104,106	0
30	UNL	X	101	18/-	0.78	0.21	61,78,111,113	0
27	GOL	B	625	6/6	0.79	0.24	69,87,98,117	0
26	SQD	f	102	43/54	0.80	0.31	96,131,177,190	0
35	HTG	d	409	16/19	0.80	0.29	96,124,142,151	0
30	UNL	a	414	30/-	0.80	0.33	95,123,145,159	0
40	HEC	V	201	43/43	0.80	0.17	38,52,72,137	0
27	GOL	o	304	6/6	0.81	0.17	82,93,102,108	0
27	GOL	l	102[A]	6/6	0.81	0.94	67,100,107,110	6
27	GOL	l	102[B]	6/6	0.81	0.94	66,101,108,110	6
27	GOL	O	302	6/6	0.81	0.22	79,86,105,110	0
29	PL9	A	414[B]	55/55	0.82	0.23	73,100,112,120	55
27	GOL	A	418	6/6	0.82	0.48	54,76,86,91	0
32	LHG	E	101[A]	42/49	0.82	0.24	79,104,116,124	42
32	LHG	E	101[B]	42/49	0.82	0.24	79,104,117,125	42
27	GOL	c	527	6/6	0.82	0.23	104,117,125,127	0
29	PL9	A	414[A]	55/55	0.82	0.23	73,100,112,119	55
30	UNL	J	101	10/-	0.82	0.18	72,83,90,96	0
30	UNL	l	101	10/-	0.83	0.25	68,79,90,99	0
26	SQD	b	620	54/54	0.83	0.17	66,97,127,132	0
27	GOL	a	418	6/6	0.83	0.44	58,83,85,95	0
29	PL9	a	413[A]	55/55	0.83	0.23	90,109,123,132	55
29	PL9	a	413[B]	55/55	0.83	0.23	90,109,123,133	55
26	SQD	A	412	54/54	0.83	0.18	70,92,134,155	0
33	LMT	t	101	26/35	0.83	0.19	75,106,147,156	0
27	GOL	O	303	6/6	0.83	0.26	84,101,109,113	0
34	LMG	c	501	51/55	0.84	0.17	67,96,114,125	0
27	GOL	V	203[B]	6/6	0.84	0.19	60,72,77,80	6
35	HTG	c	522	19/19	0.84	0.26	111,128,145,148	0
30	UNL	D	409	40/-	0.84	0.18	67,96,135,148	0
27	GOL	V	203[A]	6/6	0.84	0.19	60,72,77,80	6
37	CA	f	103	1/1	0.84	0.06	125,125,125,125	0
35	HTG	C	522	19/19	0.84	0.31	110,129,143,150	0
35	HTG	o	301	19/19	0.85	0.16	61,88,118,123	0
26	SQD	a	411	54/54	0.85	0.19	69,97,137,153	0
35	HTG	b	622	19/19	0.86	0.18	59,87,116,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
35	HTG	B	621	19/19	0.86	0.27	65,93,115,117	0
34	LMG	C	501	51/55	0.86	0.16	72,92,119,131	0
27	GOL	D	412	6/6	0.86	0.25	47,69,75,95	0
25	BCR	K	102	40/40	0.87	0.19	57,65,80,81	0
37	CA	o	302	1/1	0.87	0.06	105,105,105,105	0
26	SQD	L	101	54/54	0.87	0.14	66,95,137,148	0
23	CLA	b	616	65/65	0.88	0.17	50,64,127,139	0
27	GOL	d	411	6/6	0.88	0.24	53,74,81,90	0
23	CLA	c	514	65/65	0.88	0.18	70,90,125,145	0
34	LMG	D	411	51/55	0.88	0.18	49,70,124,136	0
25	BCR	C	515	40/40	0.88	0.13	53,75,88,91	0
23	CLA	C	514	65/65	0.88	0.15	58,87,113,121	0
34	LMG	d	410	51/55	0.88	0.17	54,71,117,148	0
34	LMG	C	520	51/55	0.89	0.19	53,86,115,129	0
27	GOL	v	202[B]	6/6	0.89	0.15	66,81,85,86	6
23	CLA	c	513	65/65	0.89	0.17	62,81,130,136	0
27	GOL	v	202[A]	6/6	0.89	0.15	66,81,84,86	6
23	CLA	B	601	65/65	0.90	0.14	56,77,109,160	0
34	LMG	c	520	51/55	0.90	0.18	60,94,129,159	0
25	BCR	h	101	40/40	0.90	0.14	53,69,93,101	0
23	CLA	b	601	65/65	0.90	0.16	59,90,127,159	0
23	CLA	d	403	65/65	0.90	0.14	46,66,124,153	0
23	CLA	B	616	65/65	0.90	0.18	48,60,131,143	0
36	DGD	c	518[B]	62/66	0.91	0.13	56,69,117,131	62
25	BCR	d	404	40/40	0.91	0.12	53,68,104,112	0
26	SQD	F	103	43/54	0.91	0.18	68,103,125,140	0
35	HTG	b	625	19/19	0.91	0.11	66,81,97,116	0
36	DGD	c	518[A]	62/66	0.91	0.13	56,69,117,131	62
30	UNL	d	408	17/-	0.92	0.12	68,83,114,123	0
23	CLA	B	606	65/65	0.92	0.14	39,56,110,130	0
36	DGD	h	102	62/66	0.92	0.12	53,66,79,85	0
23	CLA	C	513	65/65	0.92	0.14	56,73,115,137	0
23	CLA	b	606	65/65	0.92	0.14	44,60,114,128	0
34	LMG	B	620	51/55	0.92	0.12	58,73,95,116	0
25	BCR	Y	101	40/40	0.92	0.13	52,67,83,91	0
25	BCR	c	515	40/40	0.93	0.11	68,84,93,98	0
27	GOL	B	627	6/6	0.93	0.29	78,80,94,94	0
36	DGD	C	518[A]	62/66	0.93	0.12	51,64,111,116	62
36	DGD	C	518[B]	62/66	0.93	0.12	51,64,111,117	62
36	DGD	C	519	62/66	0.93	0.12	45,63,102,116	0
36	DGD	H	102	62/66	0.93	0.12	47,63,75,84	0
25	BCR	D	404	40/40	0.93	0.10	49,59,106,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
30	UNL	D	408	17/-	0.93	0.12	60,77,101,120	0
36	DGD	c	519	62/66	0.93	0.12	51,68,108,132	0
23	CLA	C	507	65/65	0.93	0.13	51,70,120,142	0
37	CA	C	524	1/1	0.93	0.05	74,74,74,74	0
25	BCR	k	101	40/40	0.93	0.14	57,73,84,88	0
23	CLA	c	507	65/65	0.93	0.13	50,70,121,138	0
25	BCR	b	618	40/40	0.93	0.10	46,58,82,94	0
34	LMG	m	101	51/55	0.93	0.13	61,77,101,115	0
23	CLA	B	609	65/65	0.94	0.16	46,60,71,85	0
23	CLA	D	403	65/65	0.94	0.12	48,58,126,139	0
35	HTG	V	202	11/19	0.94	0.38	82,114,126,133	0
23	CLA	a	408	65/65	0.94	0.16	43,56,141,159	0
23	CLA	C	509	65/65	0.94	0.10	45,57,119,142	0
23	CLA	A	408	65/65	0.94	0.12	45,53,130,148	0
23	CLA	b	609	65/65	0.94	0.14	46,65,79,89	0
23	CLA	b	612	65/65	0.94	0.11	43,53,65,73	0
37	CA	c	523	1/1	0.94	0.09	74,74,74,74	0
26	SQD	A	410[A]	54/54	0.94	0.13	56,80,114,116	54
26	SQD	A	410[B]	54/54	0.94	0.13	56,81,114,117	54
25	BCR	H	101	40/40	0.94	0.10	51,67,85,88	0
32	LHG	d	407[A]	49/49	0.95	0.15	53,64,111,128	49
32	LHG	d	407[B]	49/49	0.95	0.15	53,65,111,129	49
25	BCR	t	102	40/40	0.95	0.09	45,60,80,86	0
35	HTG	B	623	19/19	0.95	0.10	70,82,99,105	0
25	BCR	y	101	40/40	0.95	0.09	59,71,88,101	0
23	CLA	C	502	65/65	0.95	0.09	50,62,74,80	0
25	BCR	A	409	40/40	0.95	0.10	42,52,68,69	0
25	BCR	B	618	40/40	0.95	0.08	44,57,73,84	0
25	BCR	B	619	40/40	0.95	0.09	48,60,96,97	0
23	CLA	a	406[A]	65/65	0.95	0.11	42,54,123,132	65
26	SQD	a	410[A]	54/54	0.95	0.14	62,83,118,122	54
26	SQD	a	410[B]	54/54	0.95	0.14	62,83,118,123	54
25	BCR	C	516	40/40	0.95	0.12	51,64,76,88	0
23	CLA	a	406[B]	65/65	0.95	0.11	41,54,123,132	65
23	CLA	c	502	65/65	0.95	0.11	55,68,80,95	0
23	CLA	c	505	65/65	0.95	0.10	52,66,110,134	0
23	CLA	C	512	65/65	0.95	0.13	50,64,79,88	0
23	CLA	c	508	65/65	0.95	0.11	50,68,85,90	0
25	BCR	b	619	40/40	0.95	0.09	46,62,87,92	0
32	LHG	D	407[A]	49/49	0.95	0.15	50,61,110,111	49
32	LHG	D	407[B]	49/49	0.95	0.15	50,61,110,112	49
23	CLA	c	509	65/65	0.95	0.12	43,63,126,150	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	c	512	65/65	0.95	0.11	55,68,86,100	0
23	CLA	C	505	65/65	0.95	0.10	40,58,106,138	0
23	CLA	B	611	65/65	0.95	0.10	37,48,68,78	0
32	LHG	b	630[A]	49/49	0.95	0.14	54,61,73,98	49
38	HEM	f	101	43/43	0.95	0.15	56,82,118,130	0
32	LHG	b	630[B]	49/49	0.95	0.14	53,61,73,98	49
23	CLA	c	506	65/65	0.96	0.10	50,65,98,100	0
23	CLA	b	604	65/65	0.96	0.11	39,51,100,123	0
32	LHG	d	412[A]	49/49	0.96	0.14	55,69,84,93	49
32	LHG	d	412[B]	49/49	0.96	0.14	55,69,84,94	49
23	CLA	b	605	65/65	0.96	0.11	39,52,73,84	0
25	BCR	T	102	40/40	0.96	0.08	46,58,74,84	0
23	CLA	C	510	65/65	0.96	0.11	48,58,85,100	0
25	BCR	a	409	40/40	0.96	0.07	45,55,69,71	0
25	BCR	b	617	40/40	0.96	0.09	44,55,65,72	0
23	CLA	c	510	65/65	0.96	0.10	46,63,92,102	0
23	CLA	b	607	65/65	0.96	0.09	39,50,84,97	0
23	CLA	C	511	65/65	0.96	0.09	48,59,82,90	0
25	BCR	c	516	40/40	0.96	0.10	56,66,83,85	0
23	CLA	b	611	65/65	0.96	0.09	40,51,73,84	0
29	PL9	D	405[A]	55/55	0.96	0.11	38,50,61,70	55
29	PL9	D	405[B]	55/55	0.96	0.11	38,50,61,70	55
32	LHG	A	419[A]	49/49	0.96	0.13	52,66,87,90	49
36	DGD	c	517[A]	62/66	0.96	0.11	48,65,100,106	62
36	DGD	c	517[B]	62/66	0.96	0.11	47,65,100,106	62
32	LHG	A	419[B]	49/49	0.96	0.13	52,66,87,90	49
27	GOL	C	523[A]	6/6	0.96	0.10	59,64,68,70	6
27	GOL	C	523[B]	6/6	0.96	0.10	63,64,69,70	6
23	CLA	C	504	65/65	0.96	0.09	48,61,73,83	0
23	CLA	b	614	65/65	0.96	0.09	42,53,103,117	0
23	CLA	b	615	65/65	0.96	0.11	47,62,87,96	0
37	CA	O	301	1/1	0.96	0.08	105,105,105,105	0
23	CLA	C	508	65/65	0.96	0.11	48,63,87,92	0
23	CLA	B	614	65/65	0.96	0.10	39,50,105,124	0
23	CLA	b	602	65/65	0.96	0.12	48,60,82,91	0
32	LHG	d	406[A]	49/49	0.96	0.16	49,59,74,80	49
32	LHG	d	406[B]	49/49	0.96	0.16	48,59,74,80	49
40	HEC	v	201	43/43	0.96	0.12	47,61,69,71	0
23	CLA	B	602	65/65	0.97	0.11	46,56,71,88	0
23	CLA	B	603	65/65	0.97	0.10	40,54,72,91	0
23	CLA	c	503	65/65	0.97	0.09	46,59,95,113	0
23	CLA	c	504	65/65	0.97	0.09	50,69,80,97	0

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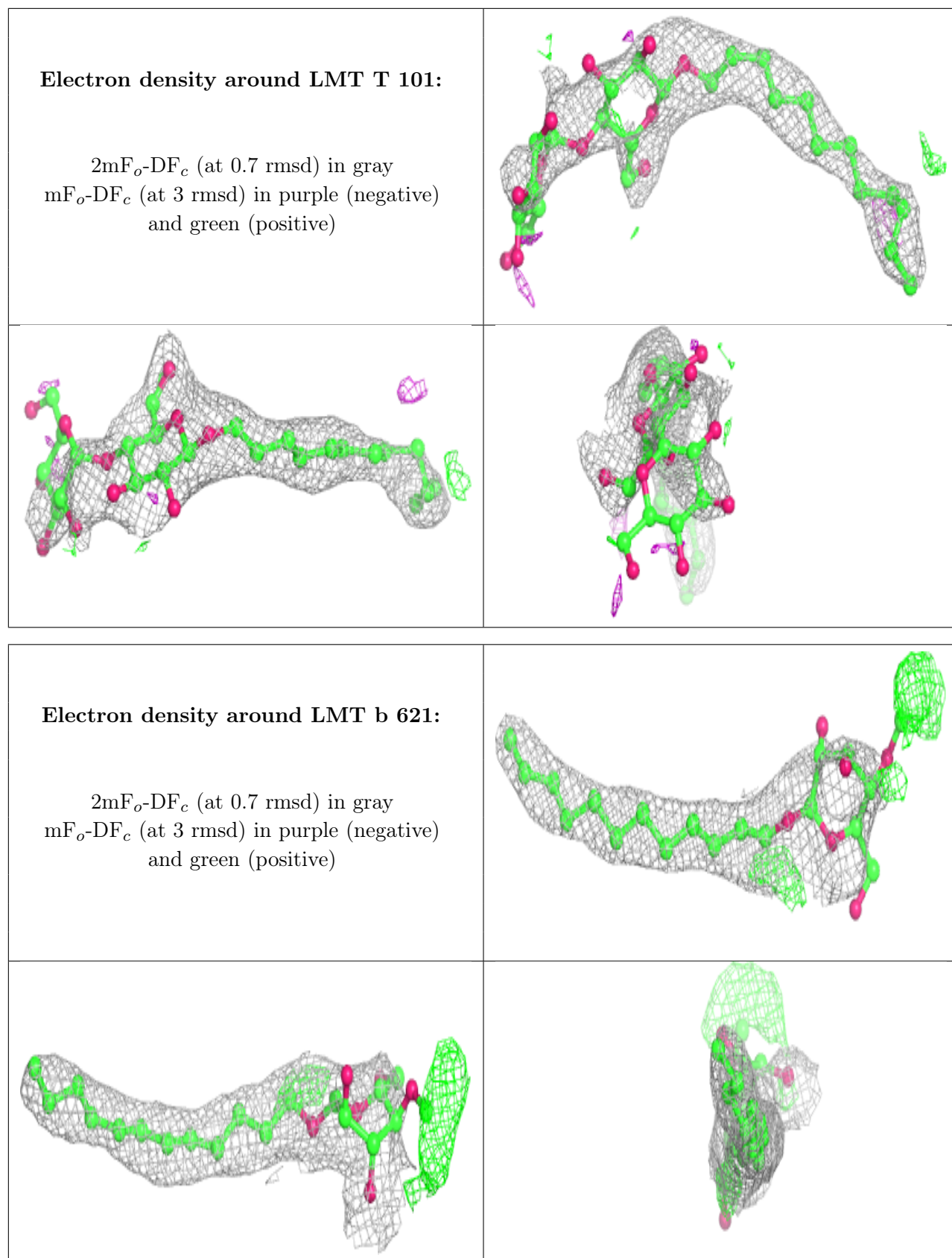
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	B	605	65/65	0.97	0.11	41,49,68,84	0
23	CLA	A	406[A]	65/65	0.97	0.09	41,49,115,126	65
23	CLA	C	506	65/65	0.97	0.09	48,61,96,107	0
27	GOL	b	628	6/6	0.97	0.20	83,90,91,96	0
27	GOL	c	526[A]	6/6	0.97	0.18	67,71,76,79	6
27	GOL	c	526[B]	6/6	0.97	0.18	67,73,77,80	6
32	LHG	D	406[A]	49/49	0.97	0.14	49,56,70,78	49
32	LHG	D	406[B]	49/49	0.97	0.14	49,56,70,79	49
23	CLA	B	607	65/65	0.97	0.09	38,48,81,86	0
23	CLA	b	603	65/65	0.97	0.08	46,57,82,94	0
23	CLA	A	406[B]	65/65	0.97	0.09	41,49,115,126	65
23	CLA	c	511	65/65	0.97	0.10	49,64,81,98	0
32	LHG	L	102[A]	49/49	0.97	0.12	50,59,69,95	49
32	LHG	L	102[B]	49/49	0.97	0.12	50,59,68,95	49
23	CLA	B	610	65/65	0.97	0.12	43,55,67,89	0
23	CLA	A	404[A]	65/65	0.97	0.12	37,44,64,71	65
23	CLA	B	612	65/65	0.97	0.08	37,50,64,68	0
23	CLA	d	402[A]	65/65	0.97	0.11	40,46,81,95	65
23	CLA	d	402[B]	65/65	0.97	0.11	40,46,81,96	65
36	DGD	C	517[A]	62/66	0.97	0.10	47,58,101,106	62
36	DGD	C	517[B]	62/66	0.97	0.10	46,59,101,106	62
23	CLA	B	613	65/65	0.97	0.08	40,48,94,111	0
24	PHO	A	407[A]	64/64	0.97	0.09	39,47,55,58	64
24	PHO	A	407[B]	64/64	0.97	0.09	38,47,55,58	64
24	PHO	A	417[A]	64/64	0.97	0.10	40,51,58,65	64
24	PHO	A	417[B]	64/64	0.97	0.10	39,51,58,65	64
29	PL9	d	405[A]	55/55	0.97	0.10	41,52,63,72	55
29	PL9	d	405[B]	55/55	0.97	0.10	41,53,63,72	55
24	PHO	a	407[A]	64/64	0.97	0.09	44,50,56,61	64
24	PHO	a	407[B]	64/64	0.97	0.09	44,50,56,61	64
24	PHO	a	415[A]	64/64	0.97	0.12	44,56,62,69	64
24	PHO	a	415[B]	64/64	0.97	0.12	44,56,62,69	64
23	CLA	b	610	65/65	0.97	0.09	46,57,68,77	0
25	BCR	B	617	40/40	0.97	0.08	42,54,65,65	0
27	GOL	B	622	6/6	0.97	0.17	72,82,89,91	0
23	CLA	A	404[B]	65/65	0.97	0.12	37,44,66,71	65
23	CLA	B	615	65/65	0.97	0.09	44,54,82,92	0
38	HEM	F	102	43/43	0.97	0.11	52,68,80,88	0
23	CLA	b	613	65/65	0.97	0.08	41,50,86,107	0
23	CLA	D	402[A]	65/65	0.97	0.11	33,44,69,79	65
23	CLA	D	402[B]	65/65	0.97	0.11	33,44,69,81	65
31	BCT	d	401[B]	4/4	0.98	0.10	58,60,70,80	4

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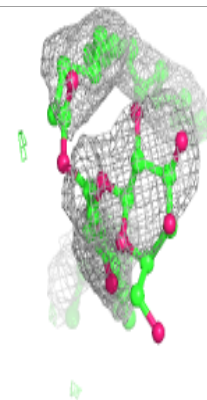
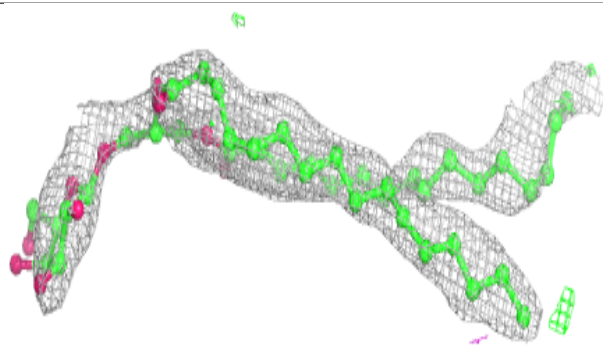
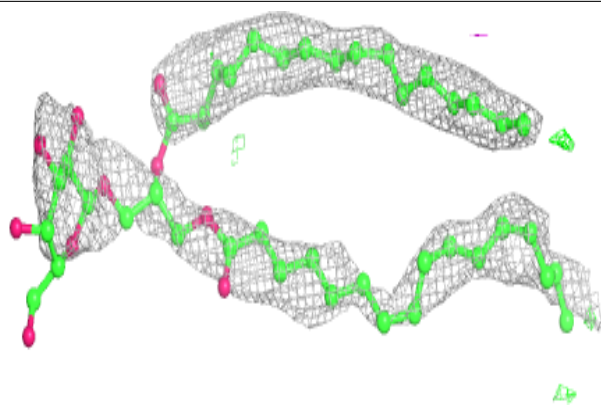
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	FE2	a	401[A]	1/1	0.98	0.06	54,54,54,54	1
21	FE2	a	401[B]	1/1	0.98	0.06	55,55,55,55	1
23	CLA	B	604	65/65	0.98	0.09	39,48,115,134	0
23	CLA	A	405[A]	65/65	0.98	0.09	37,44,58,69	65
23	CLA	A	405[B]	65/65	0.98	0.09	37,44,58,70	65
22	CL	a	402[A]	1/1	0.98	0.05	49,49,49,49	1
23	CLA	C	503	65/65	0.98	0.08	46,54,84,94	0
23	CLA	B	608	65/65	0.98	0.08	42,52,72,79	0
22	CL	a	402[B]	1/1	0.98	0.05	49,49,49,49	1
23	CLA	b	608	65/65	0.98	0.08	43,58,85,97	0
22	CL	a	403[A]	1/1	0.98	0.04	52,52,52,52	1
23	CLA	a	404[A]	65/65	0.98	0.13	41,47,67,78	65
23	CLA	a	404[B]	65/65	0.98	0.13	41,47,68,78	65
37	CA	c	524	1/1	0.98	0.05	77,77,77,77	0
23	CLA	a	405[A]	65/65	0.98	0.08	40,46,68,74	65
23	CLA	a	405[B]	65/65	0.98	0.08	40,46,68,74	65
22	CL	a	403[B]	1/1	0.98	0.04	52,52,52,52	1
31	BCT	A	416[A]	4/4	0.98	0.13	55,57,61,66	4
39	MG	J	102	1/1	0.98	0.03	60,60,60,60	0
39	MG	j	102	1/1	0.98	0.09	64,64,64,64	0
31	BCT	A	416[B]	4/4	0.98	0.13	54,56,62,72	4
31	BCT	d	401[A]	4/4	0.98	0.10	58,59,70,78	4
22	CL	A	402[A]	1/1	0.99	0.02	44,44,44,44	1
22	CL	A	402[B]	1/1	0.99	0.02	44,44,44,44	1
28	OEX	A	413[A]	10/10	0.99	0.05	40,45,49,49	10
28	OEX	A	413[B]	10/10	0.99	0.05	39,44,49,50	10
28	OEX	a	412[A]	10/10	0.99	0.06	46,49,51,55	10
28	OEX	a	412[B]	10/10	0.99	0.06	45,50,51,55	10
22	CL	A	403[A]	1/1	0.99	0.05	47,47,47,47	1
22	CL	A	403[B]	1/1	0.99	0.05	47,47,47,47	1
21	FE2	A	401[A]	1/1	0.99	0.05	51,51,51,51	1
21	FE2	A	401[B]	1/1	0.99	0.05	52,52,52,52	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.

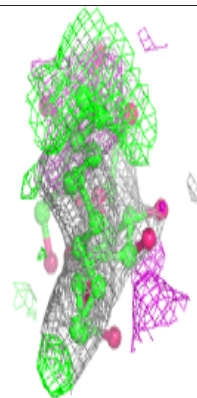
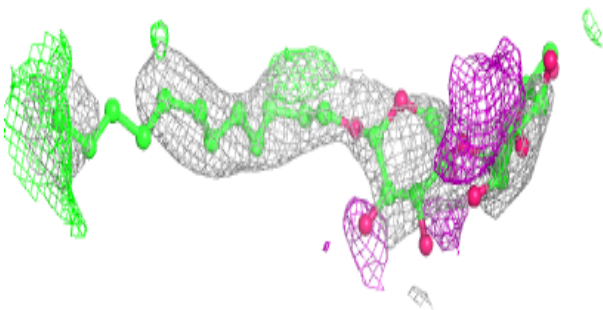
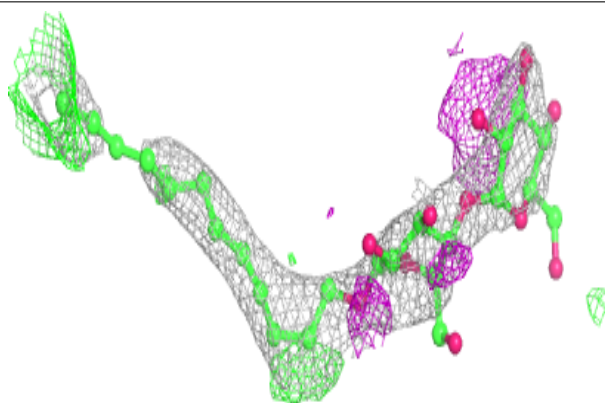


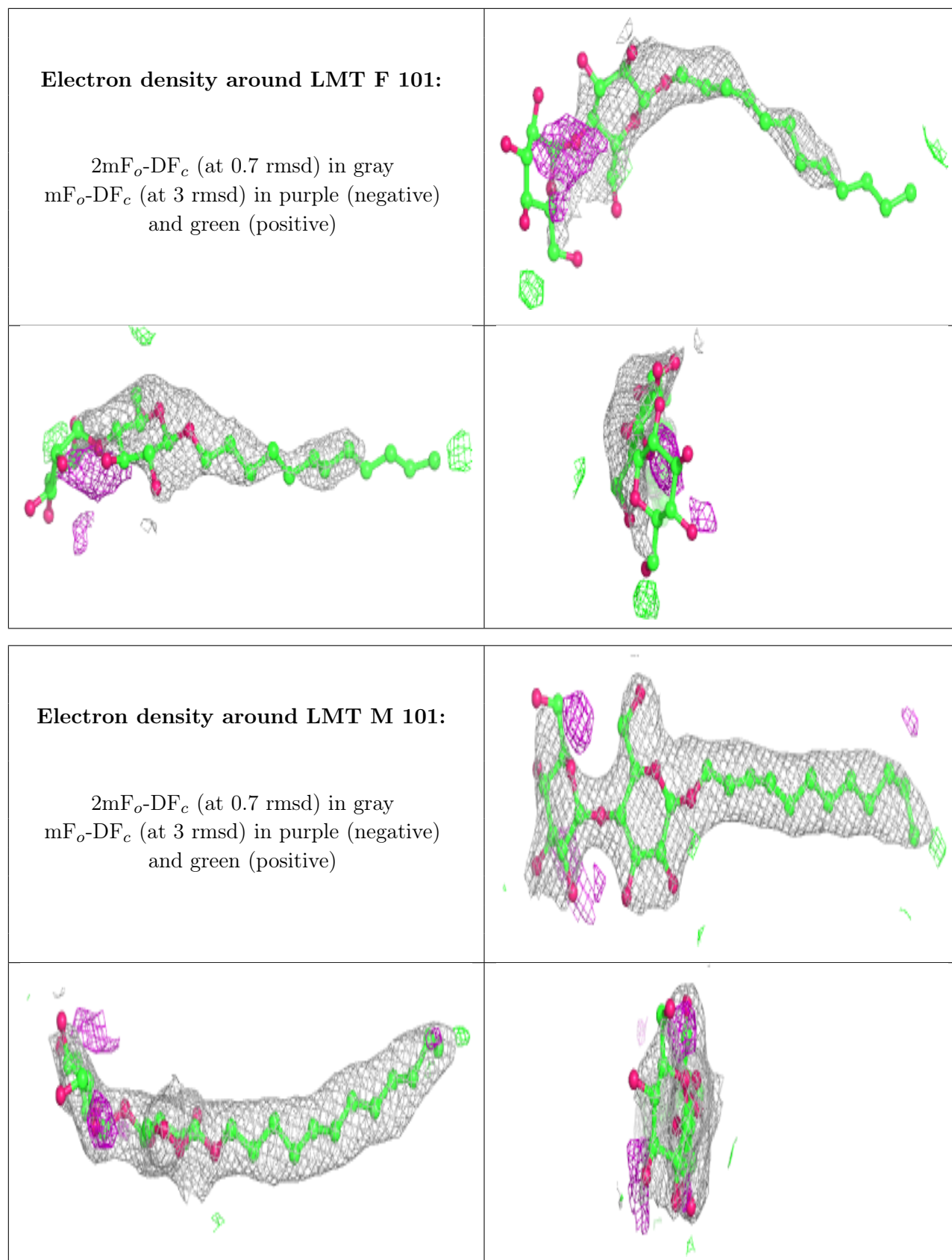
Electron density around LMG C 521:

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

**Electron density around LMT B 628:**

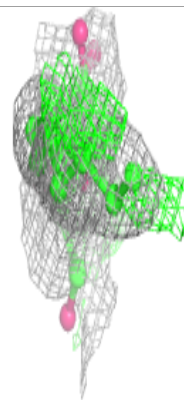
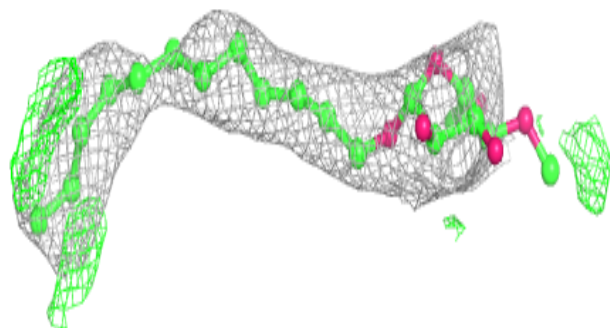
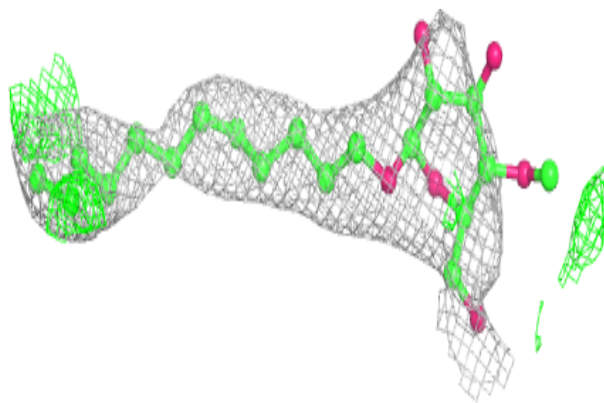
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



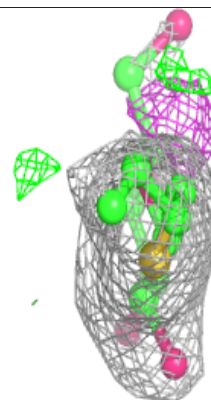
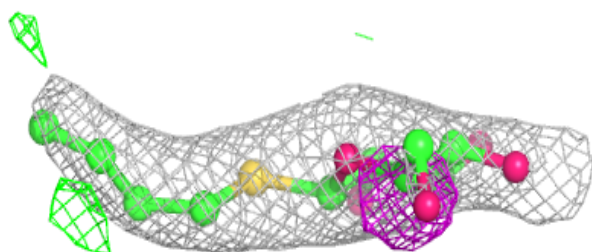
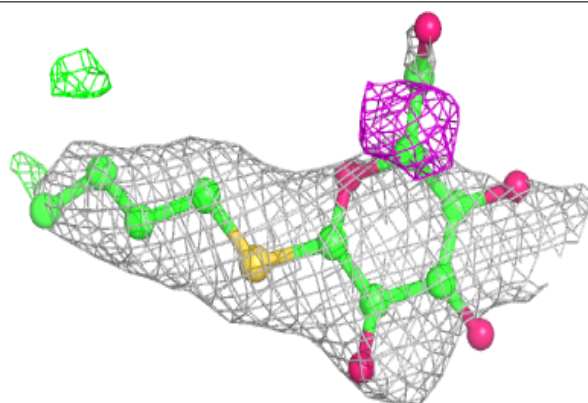


Electron density around LMT B 629:

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

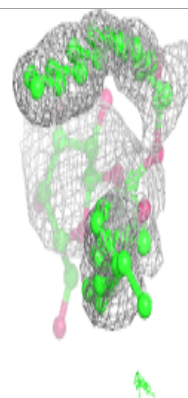
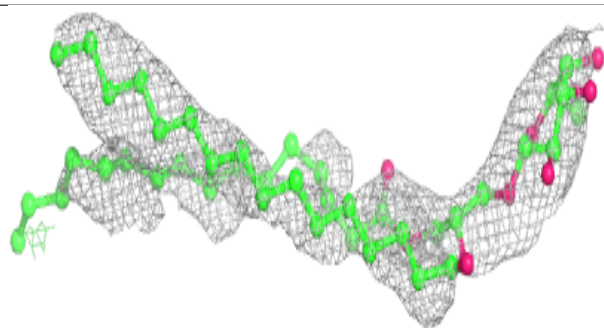
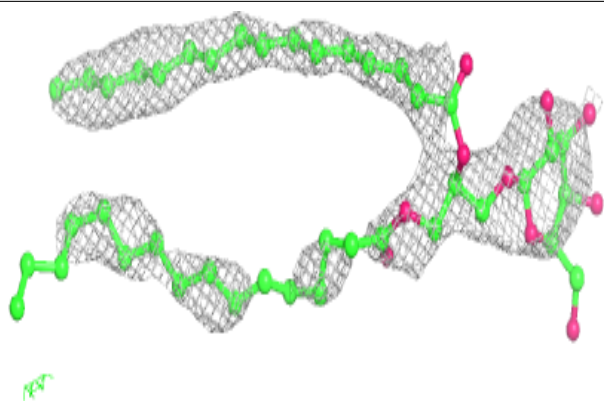
**Electron density around HTG D 410:**

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

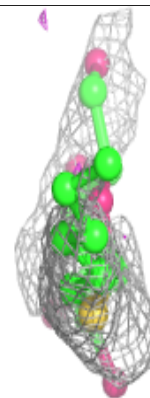
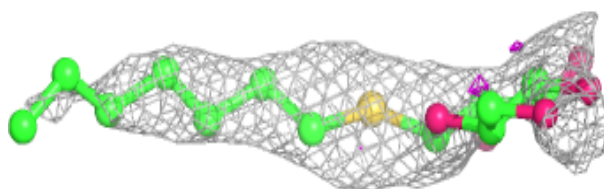
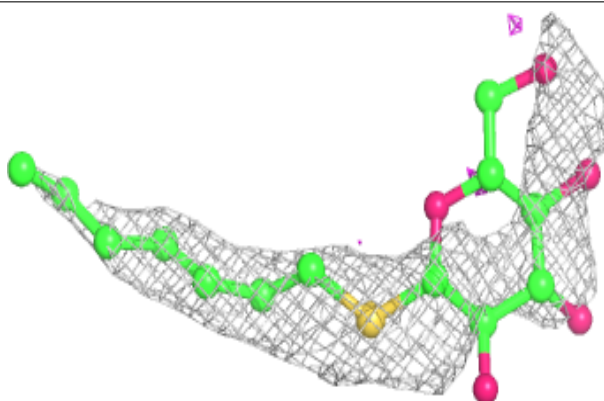


Electron density around LMG c 521:

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

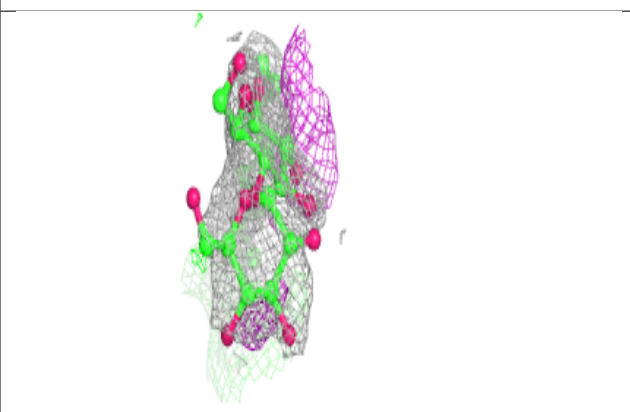
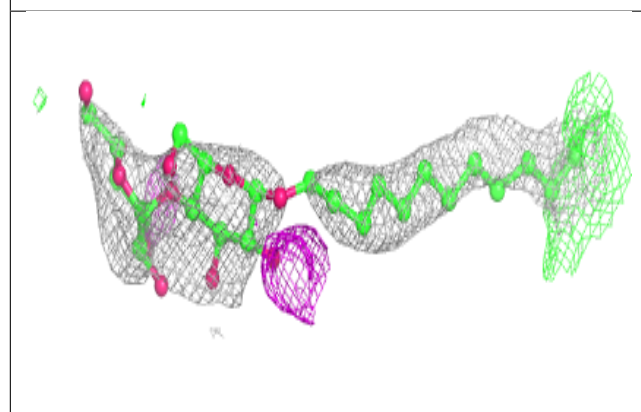
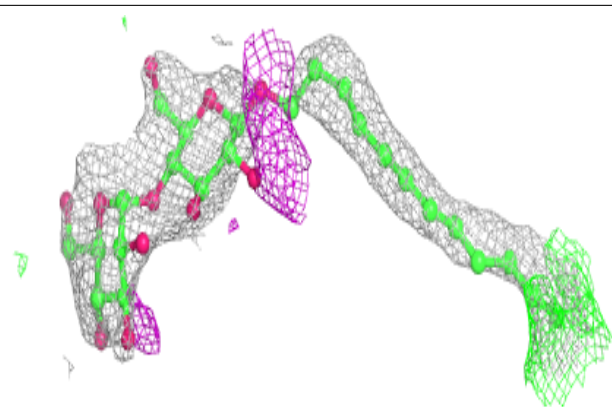
**Electron density around HTG b 623:**

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

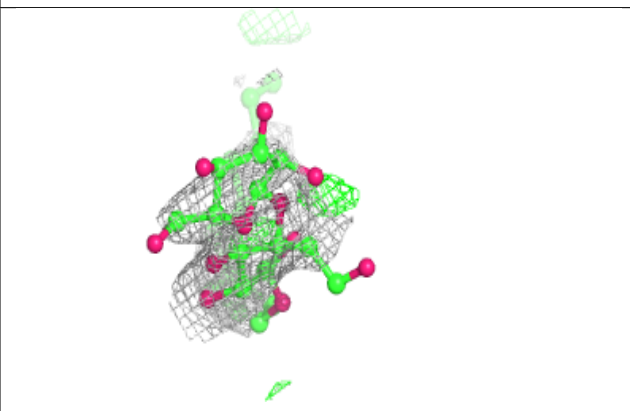
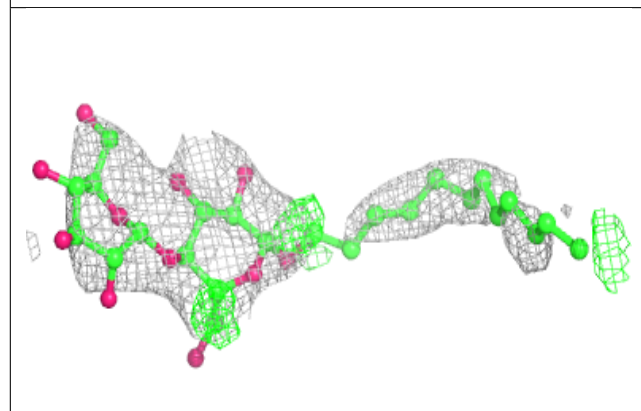
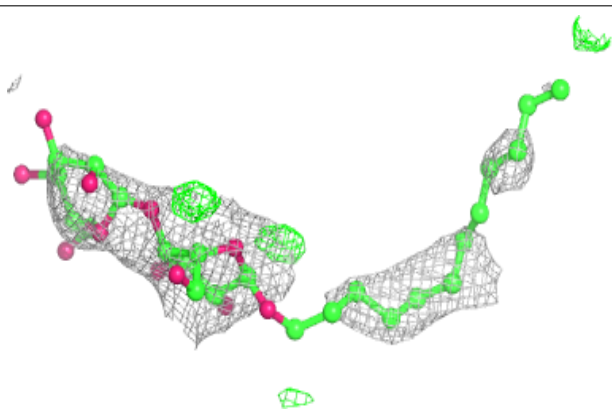


Electron density around LMT D 401:

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

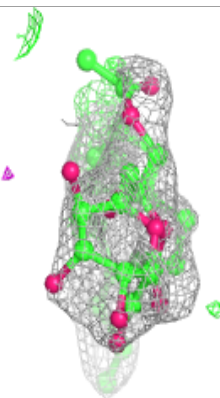
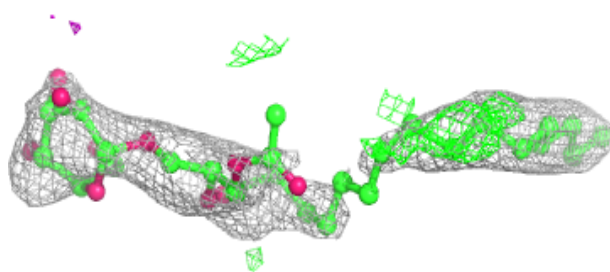
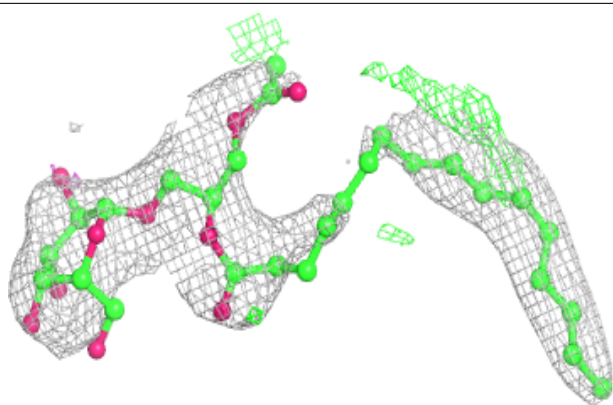
**Electron density around LMT A 420:**

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

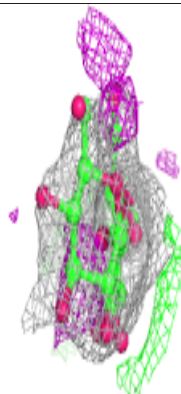
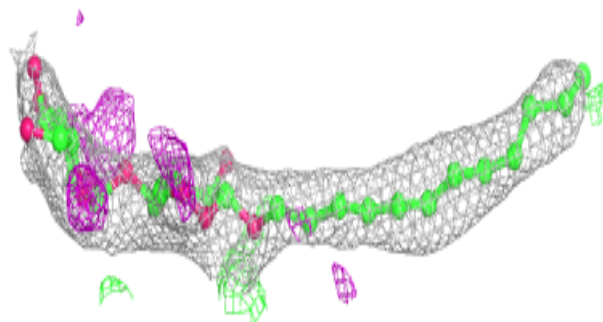
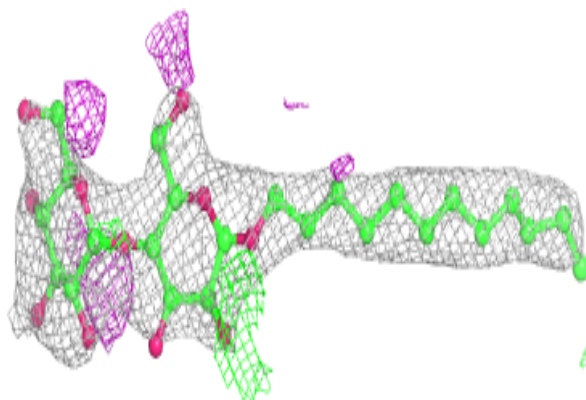


Electron density around LMG Z 101:

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

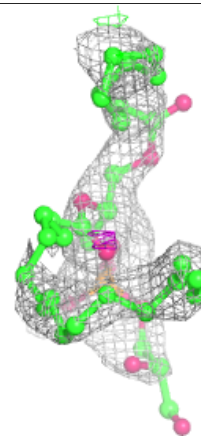
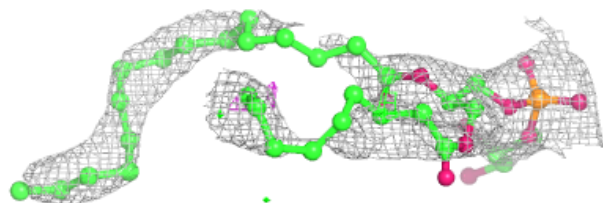
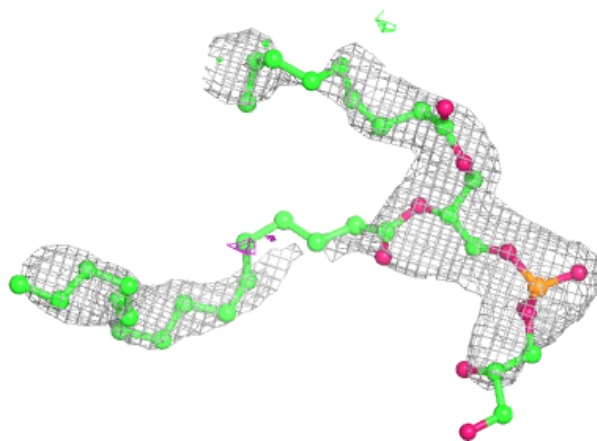
**Electron density around LMT m 103:**

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



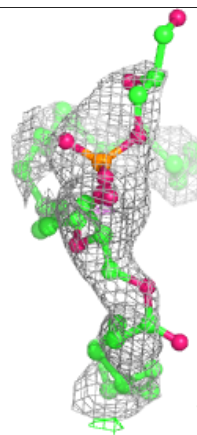
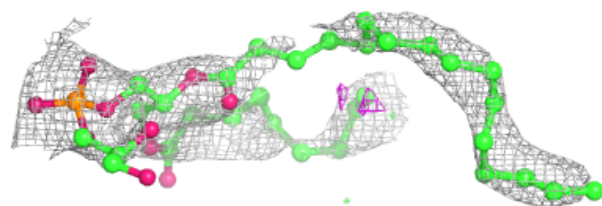
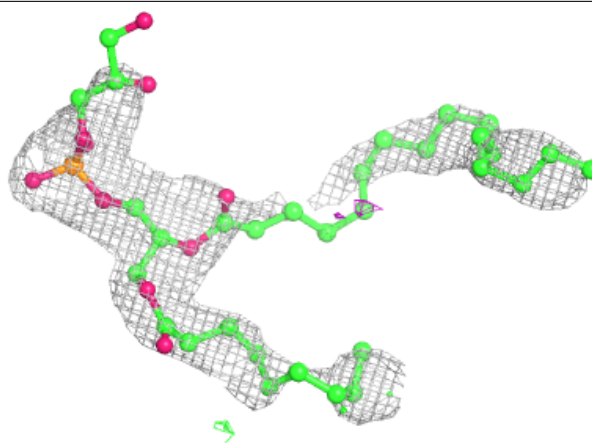
Electron density around LHG a 419 (A):

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

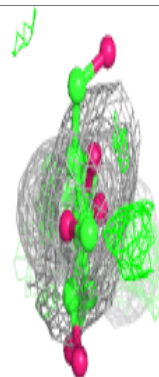
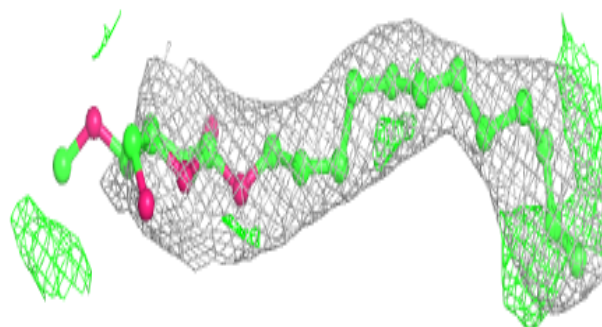
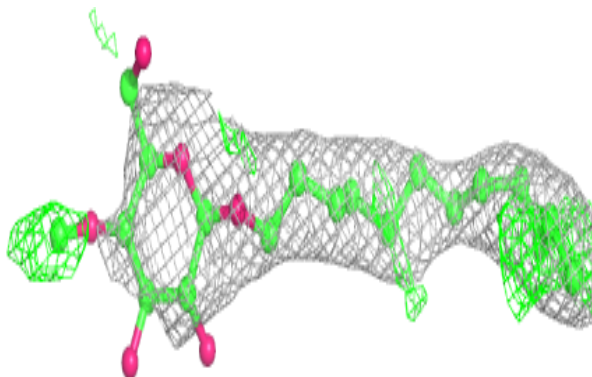


Electron density around LHG a 419 (B):

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

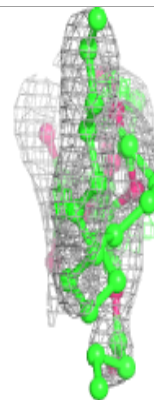
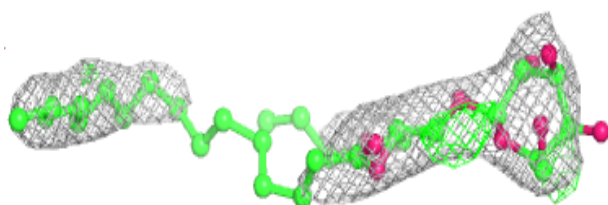
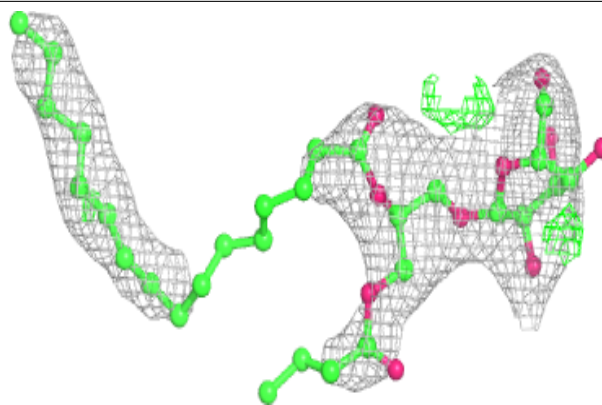
**Electron density around LMT b 627:**

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

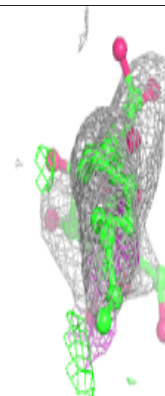
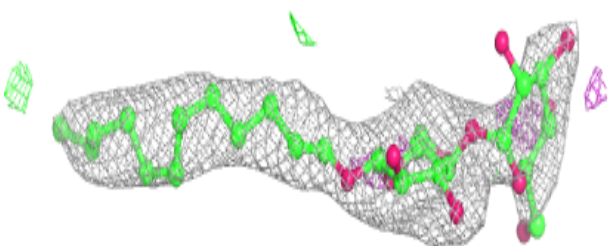
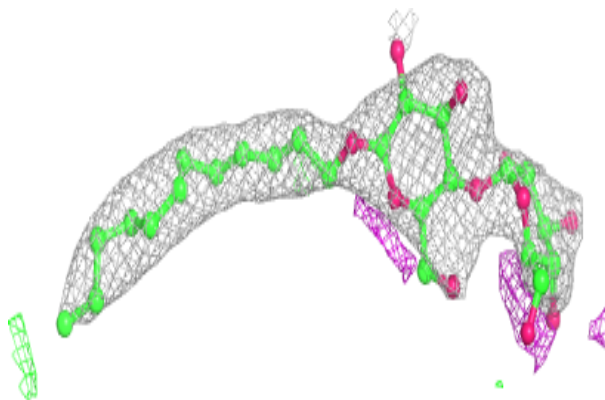


Electron density around LMG z 101:

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

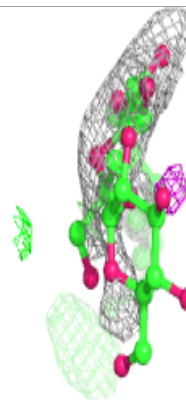
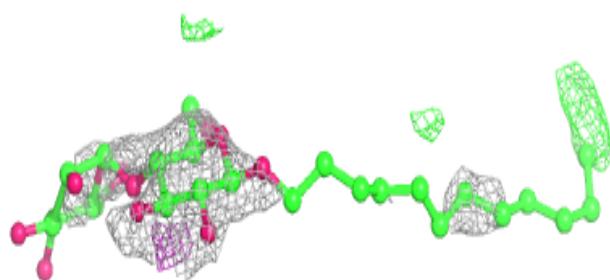
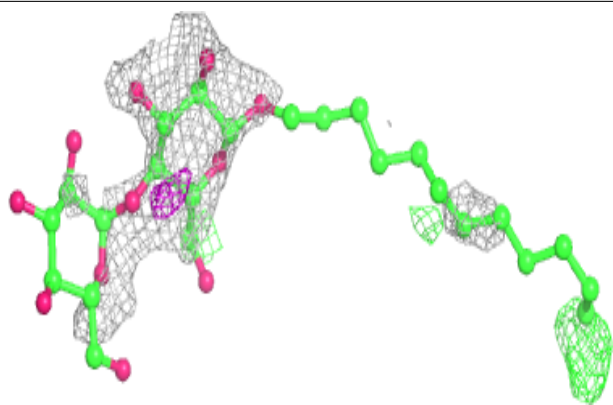
**Electron density around LMT B 626:**

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

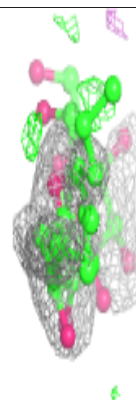
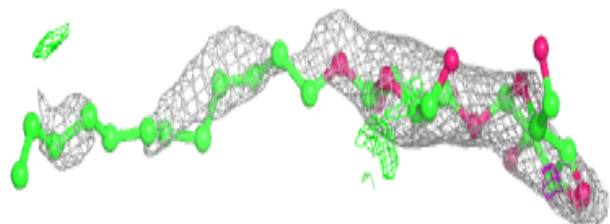
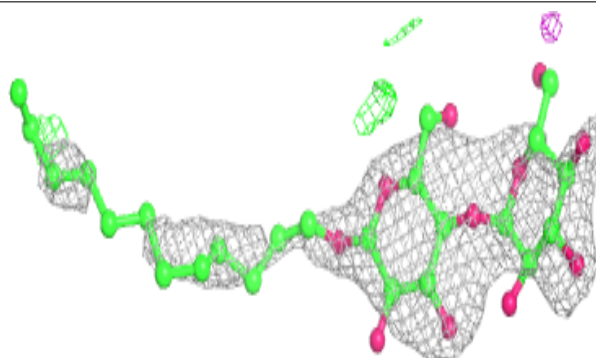


Electron density around LMT e 101:

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

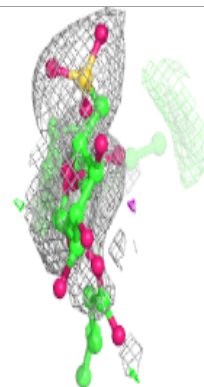
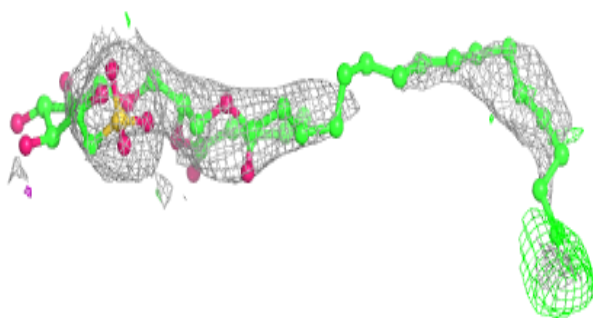
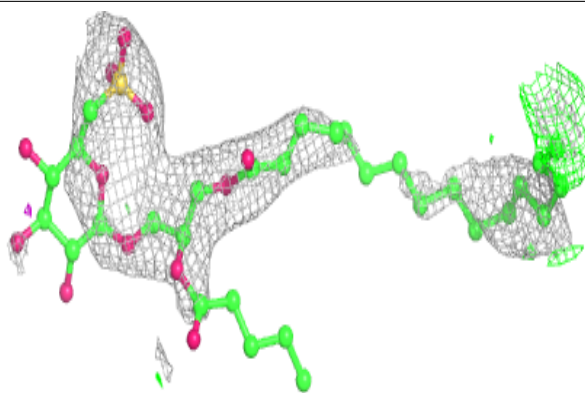
**Electron density around LMT a 416:**

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

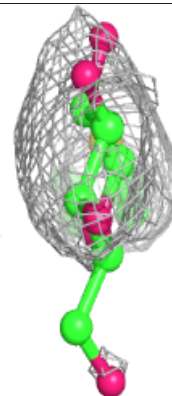
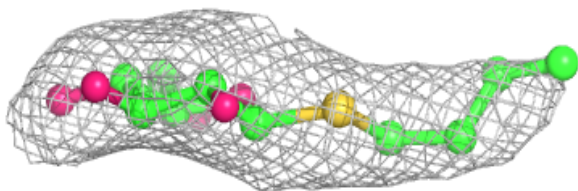
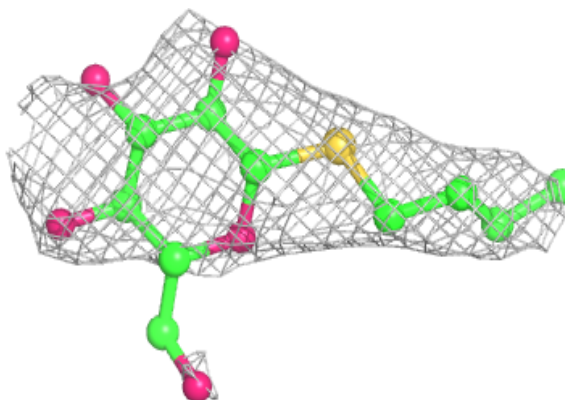


Electron density around SQD f 102:

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

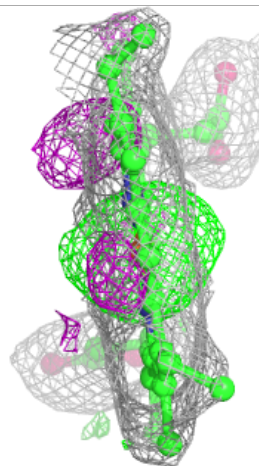
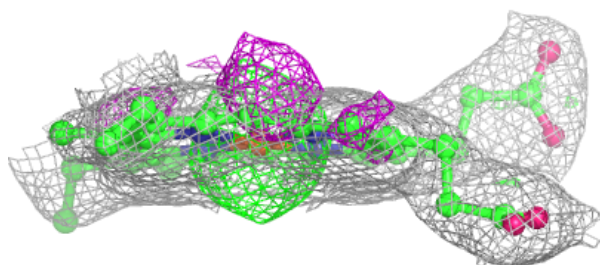
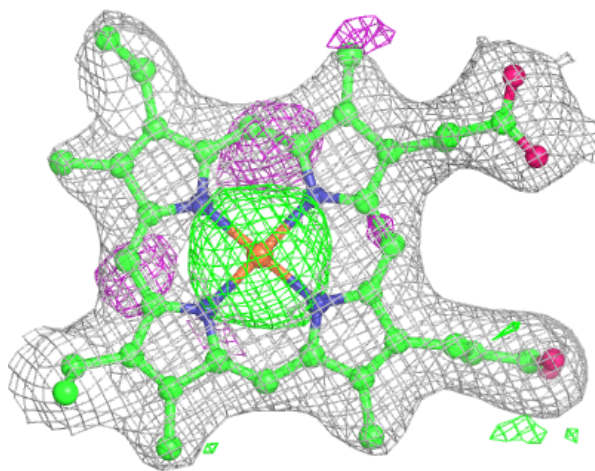
**Electron density around HTG d 409:**

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



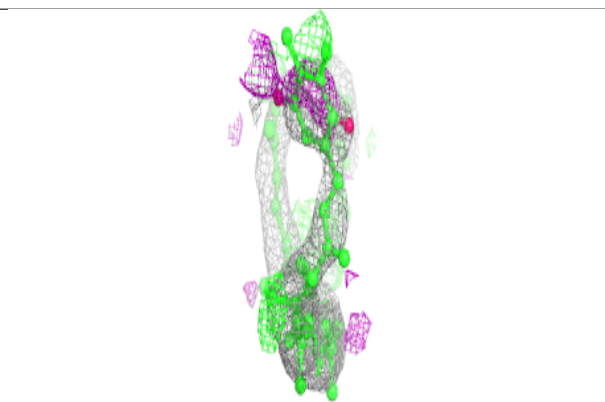
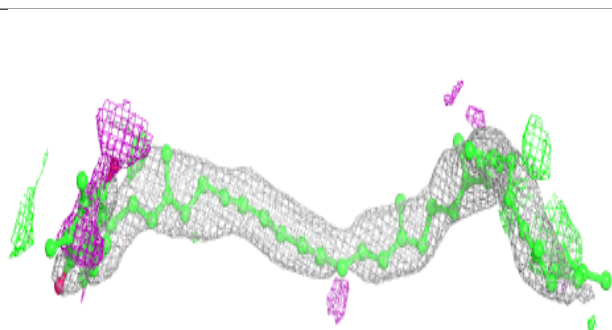
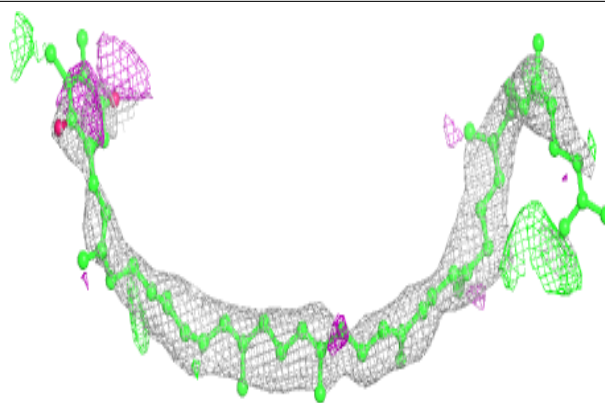
Electron density around HEC V 201:

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

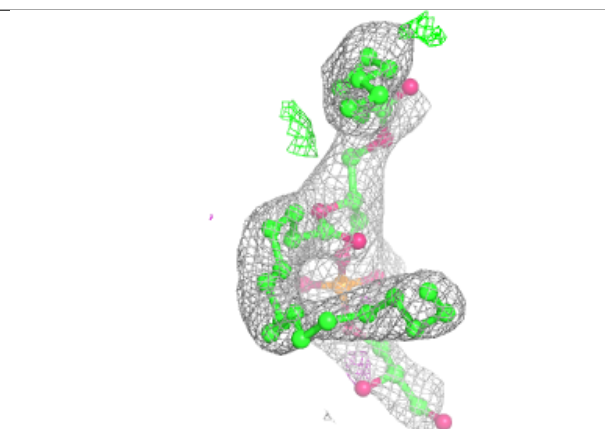
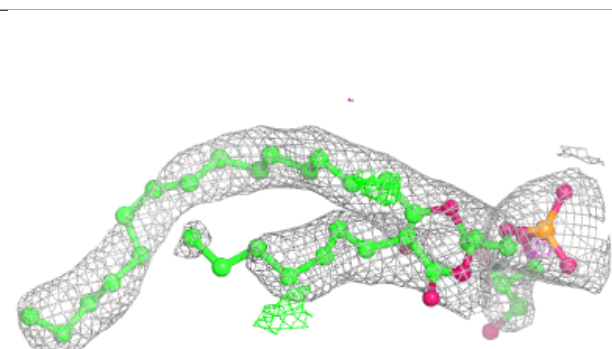
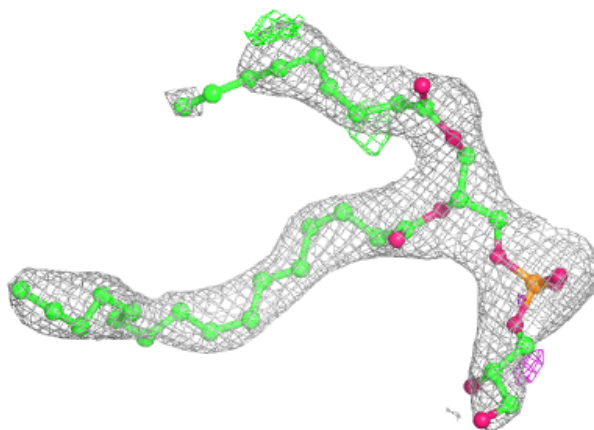


Electron density around PL9 A 414 (B):

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

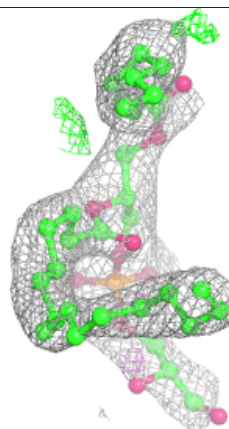
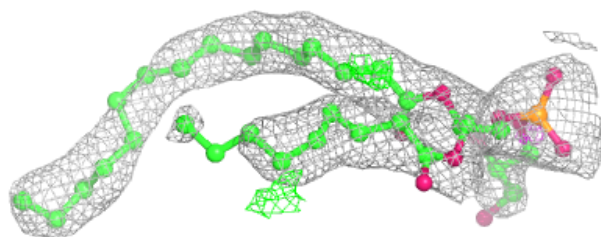
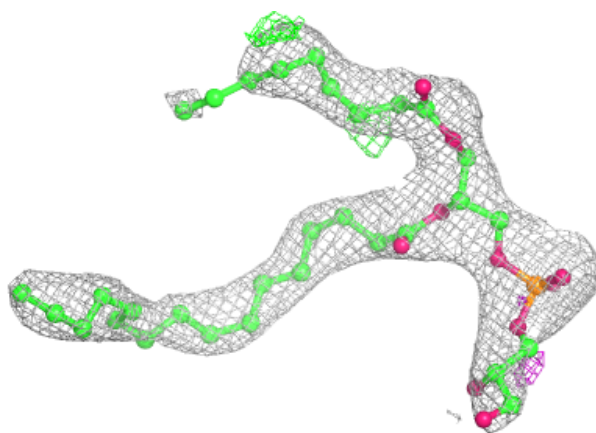
**Electron density around LHG E 101 (A):**

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

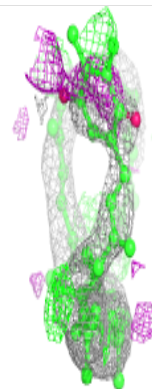
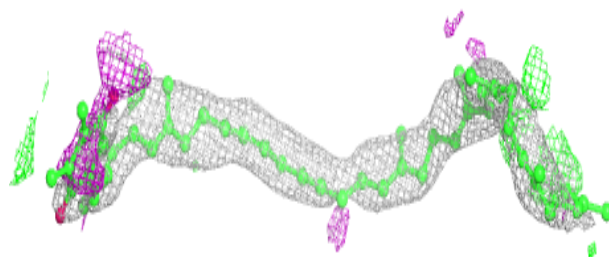
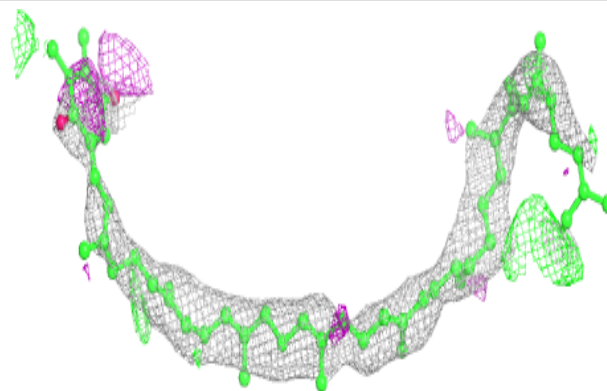


Electron density around LHG E 101 (B):

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

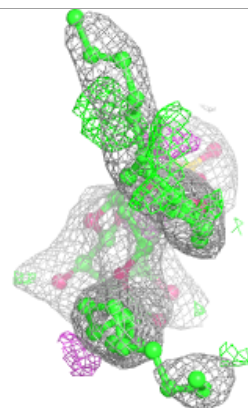
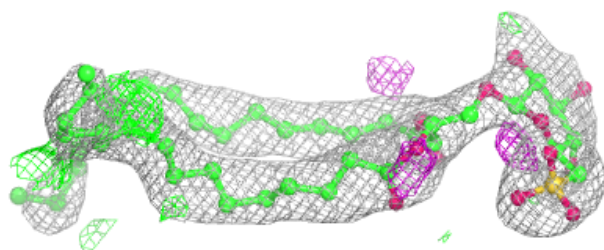
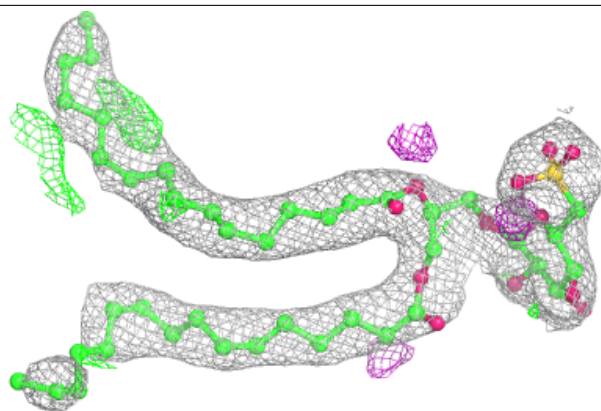
**Electron density around PL9 A 414 (A):**

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

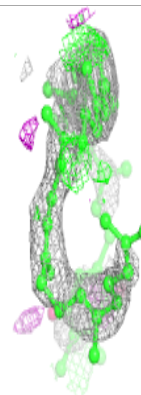
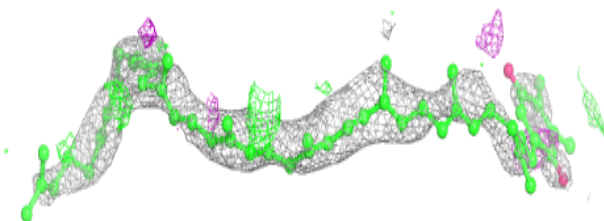
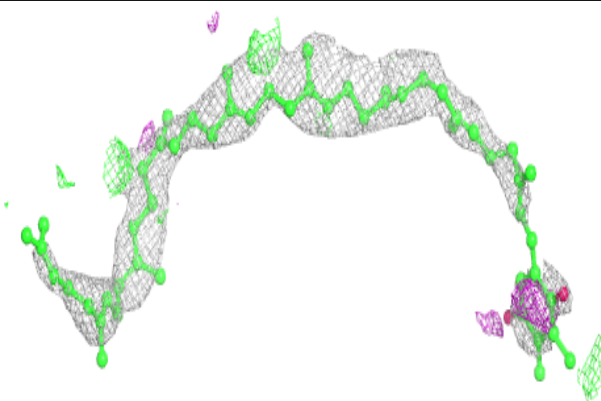


Electron density around SQD b 620:

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

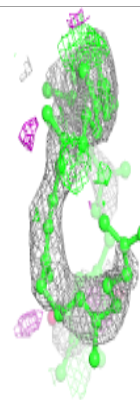
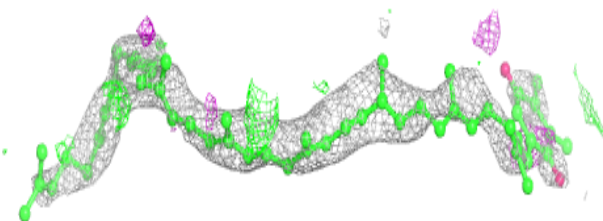
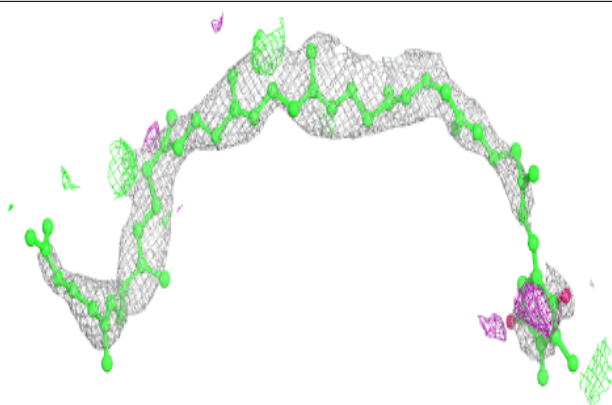
**Electron density around PL9 a 413 (A):**

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

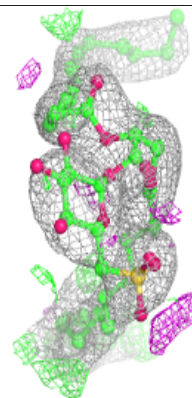
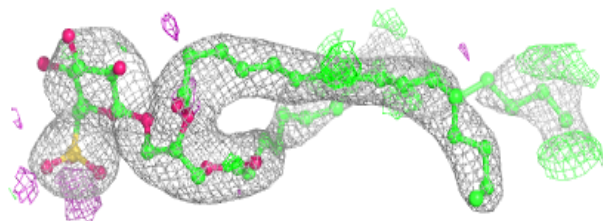
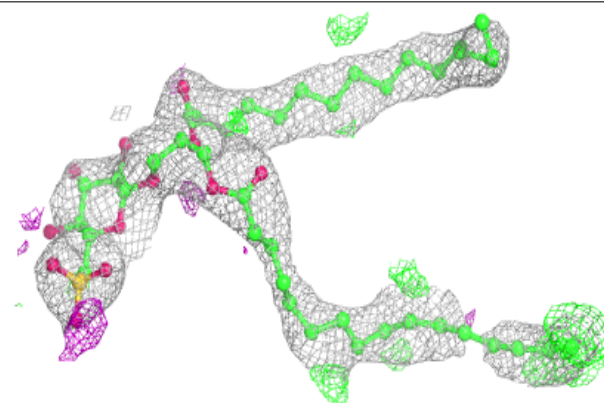


Electron density around PL9 a 413 (B):

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

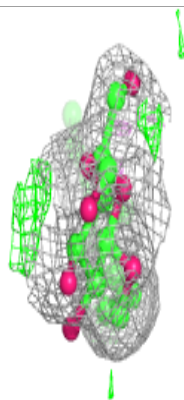
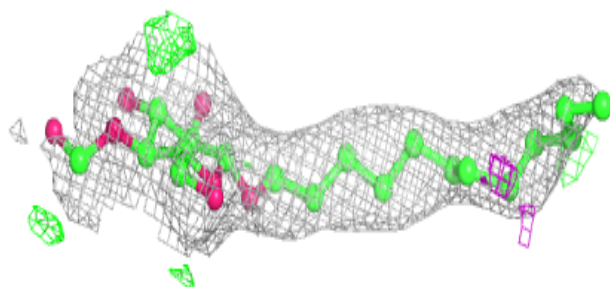
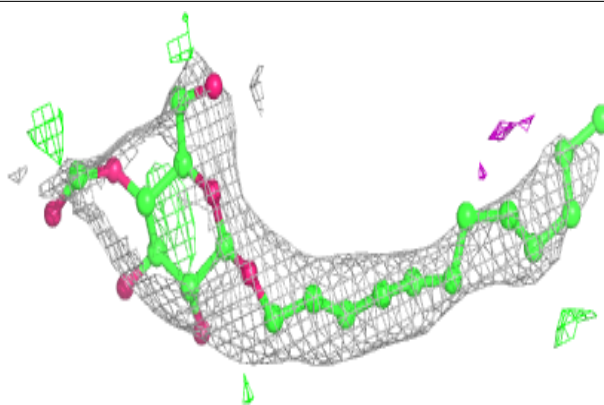
**Electron density around SQD A 412:**

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

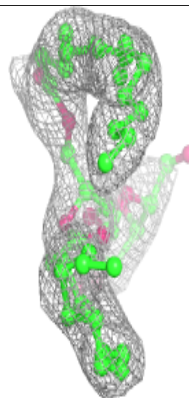
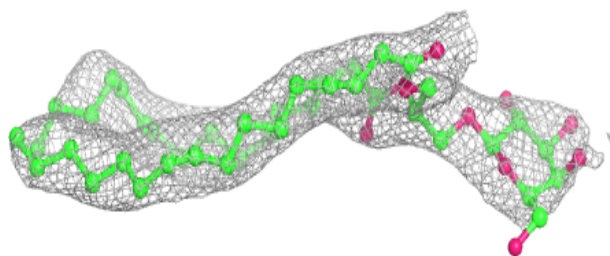
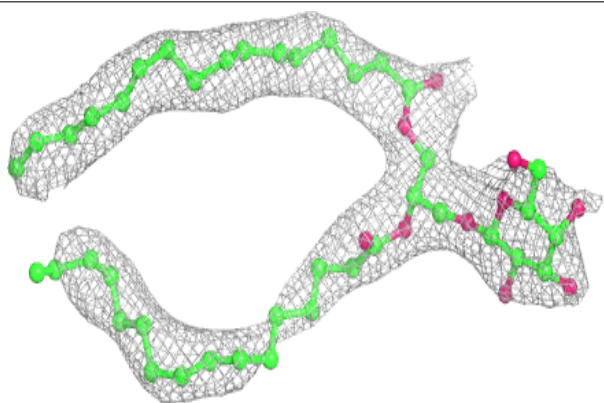


Electron density around LMT t 101:

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

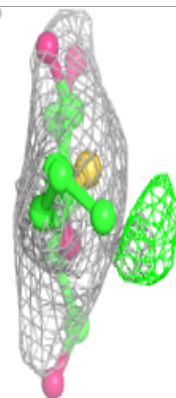
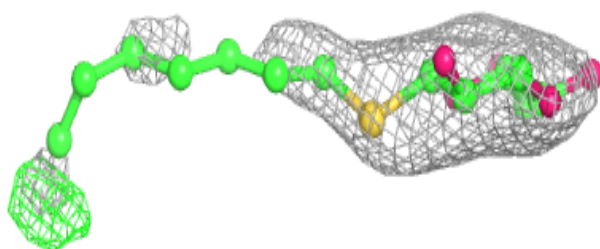
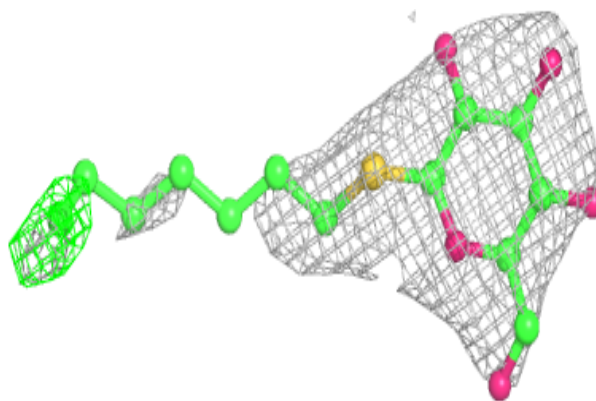
**Electron density around LMG c 501:**

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

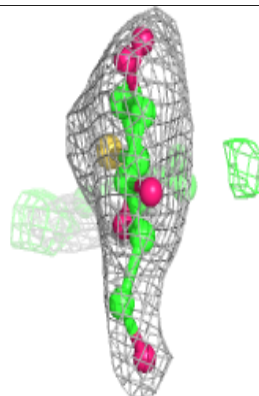
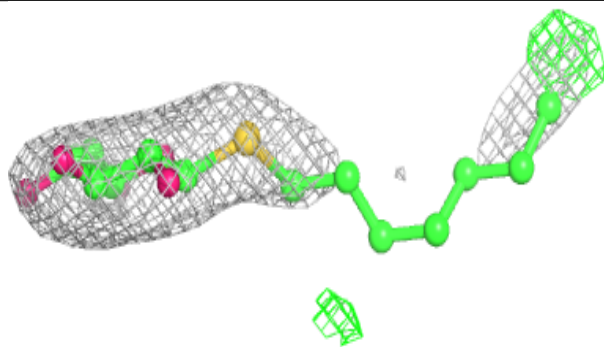
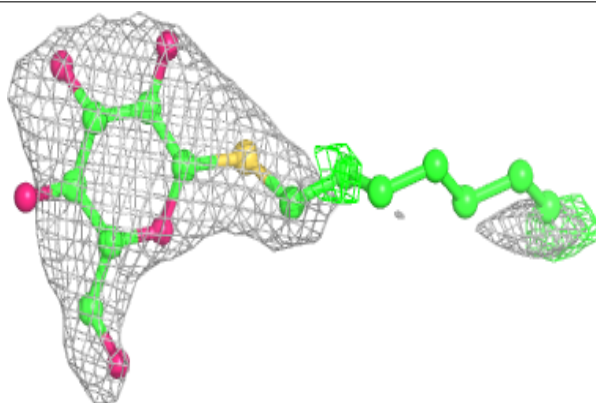


Electron density around HTG c 522:

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

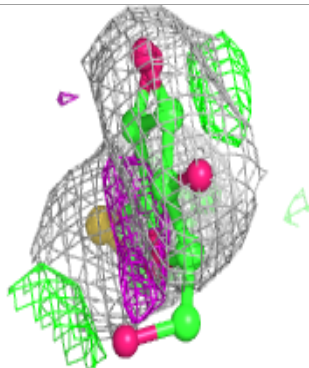
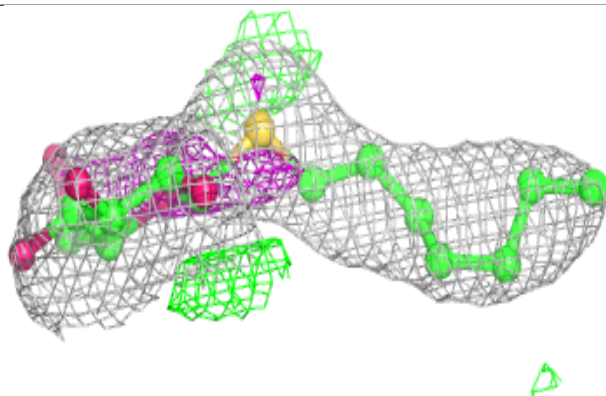
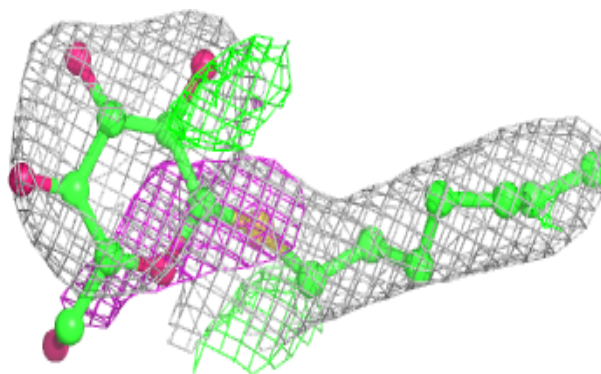
**Electron density around HTG C 522:**

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

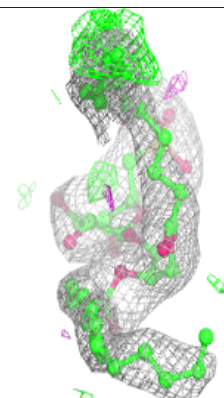
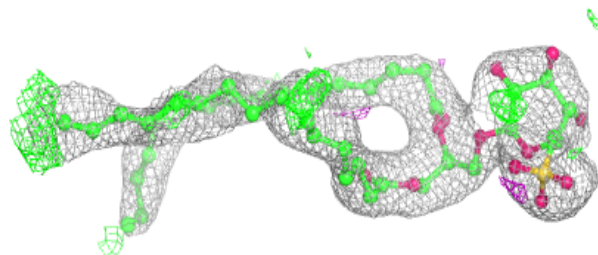
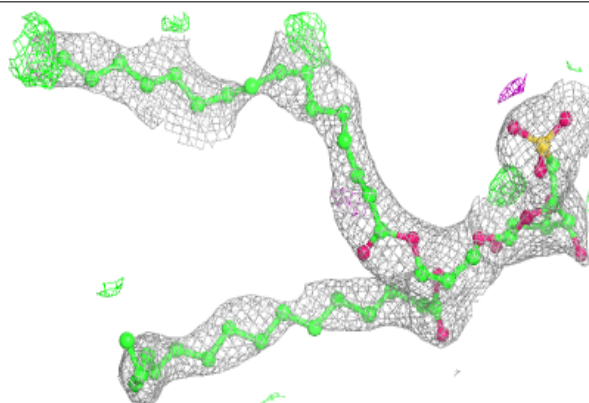


Electron density around HTG o 301:

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

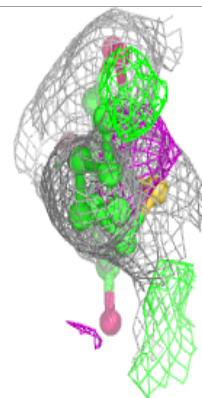
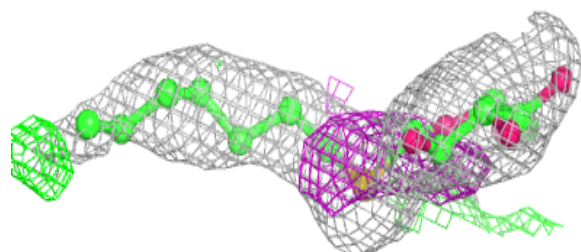
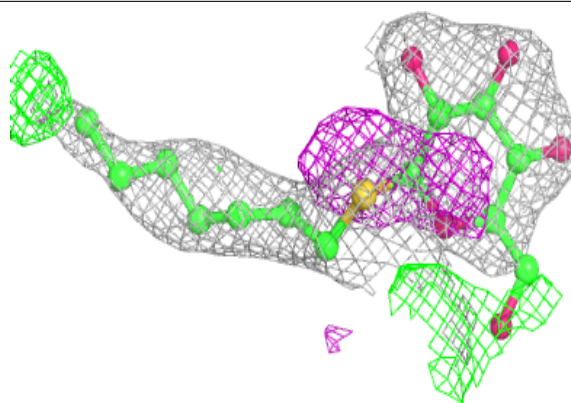
**Electron density around SQD a 411:**

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

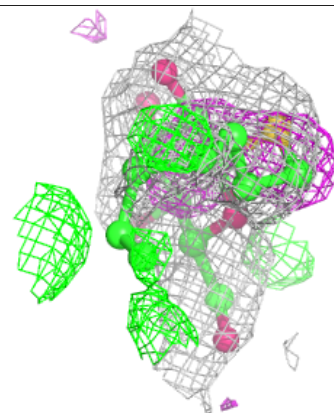
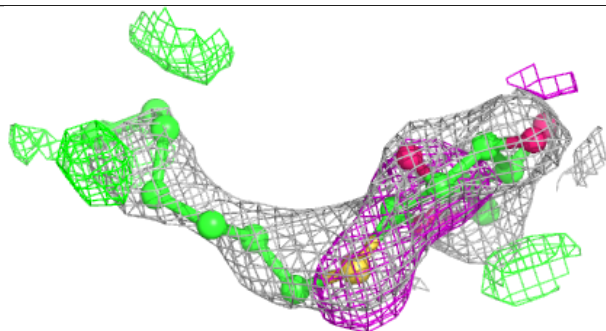
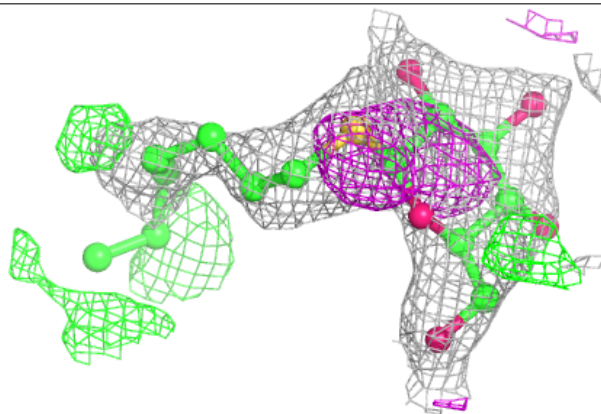


Electron density around HTG b 622:

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

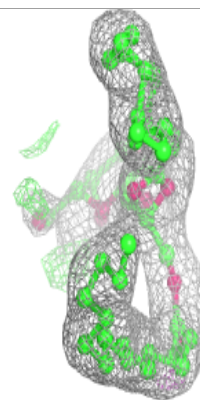
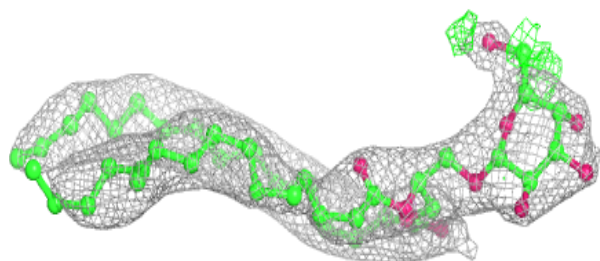
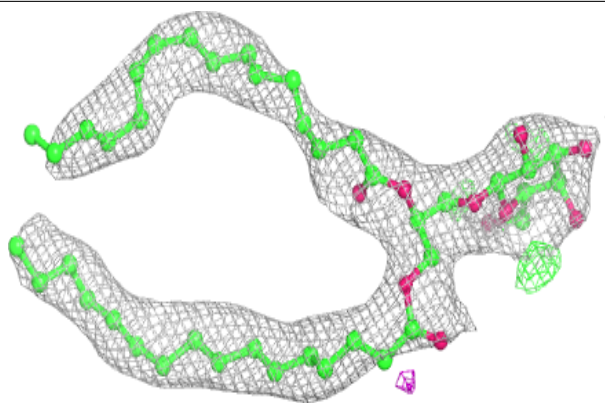
**Electron density around HTG B 621:**

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

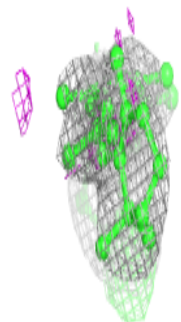
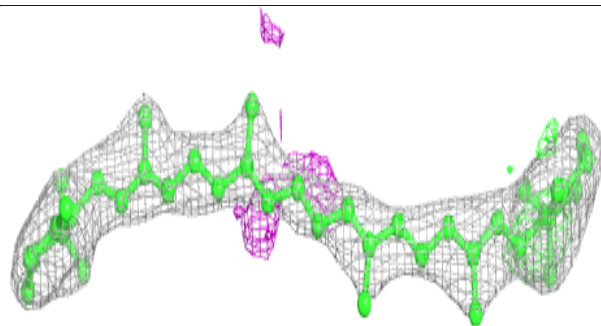
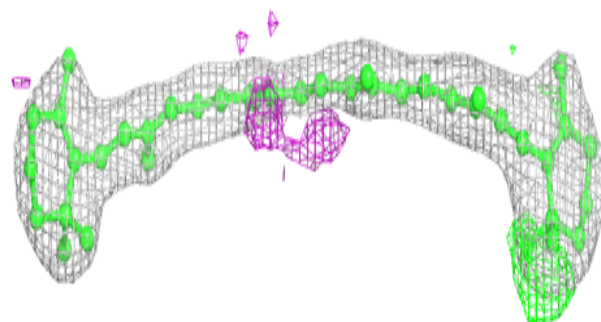


Electron density around LMG C 501:

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

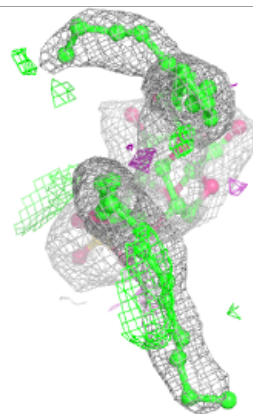
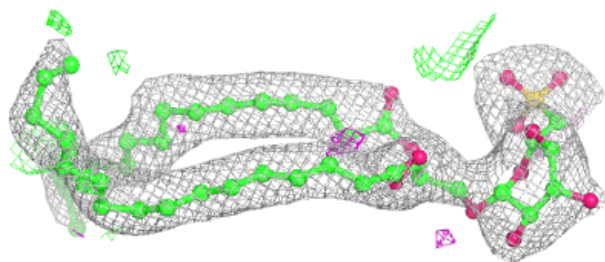
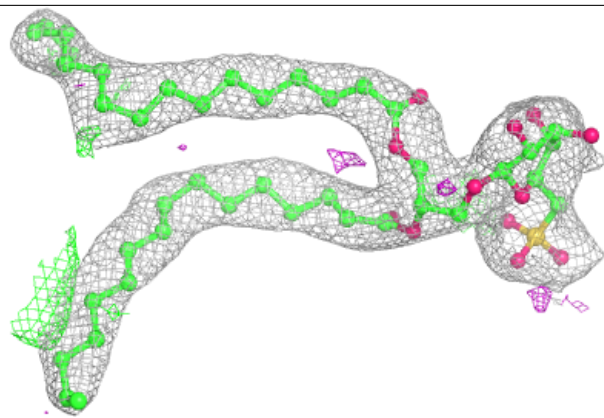
**Electron density around BCR K 102:**

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



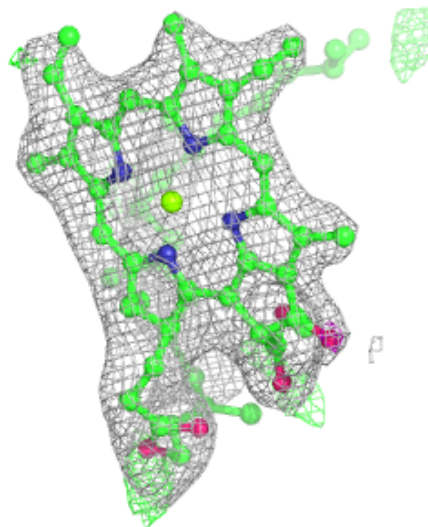
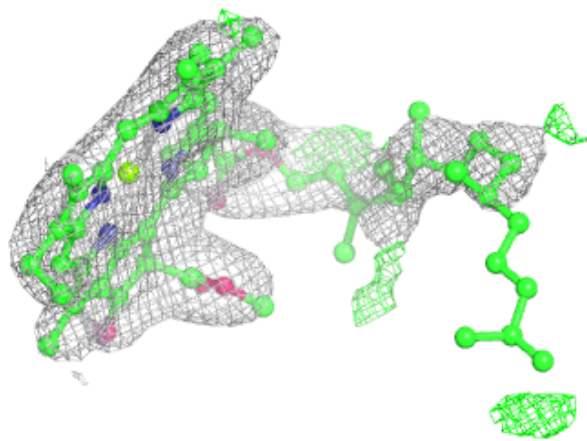
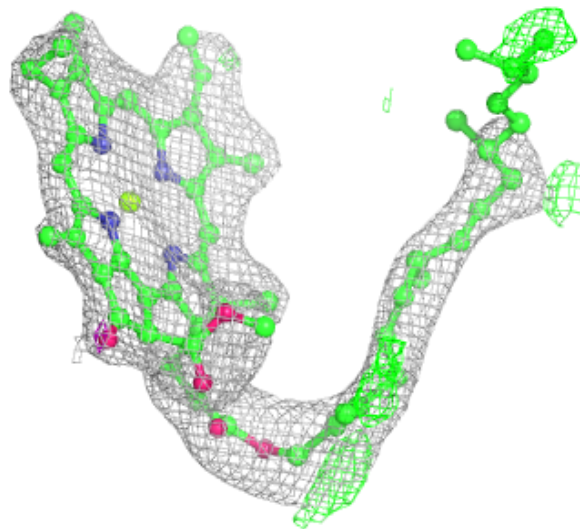
Electron density around SQD L 101:

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



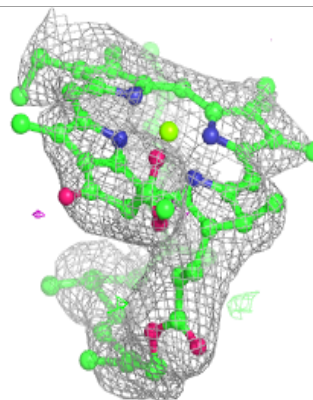
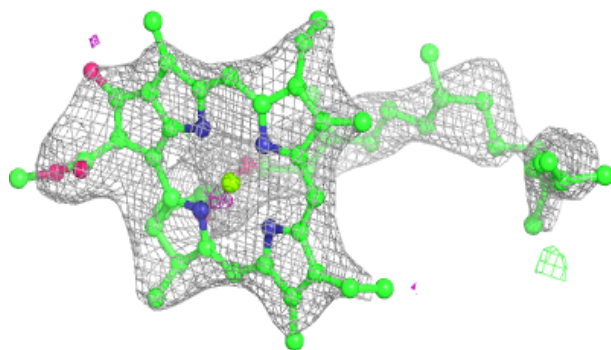
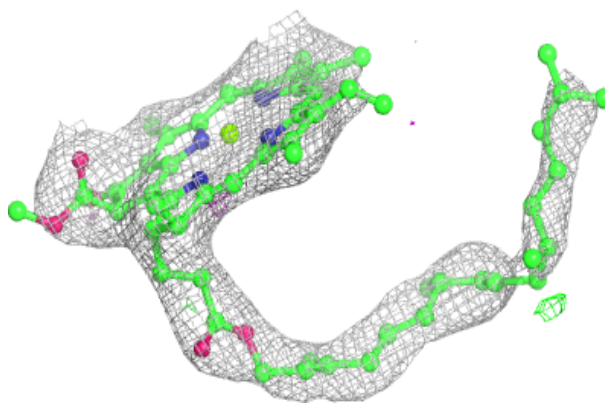
Electron density around CLA b 616:

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

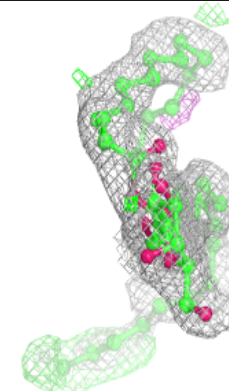
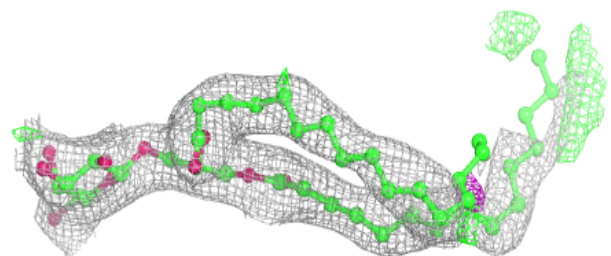
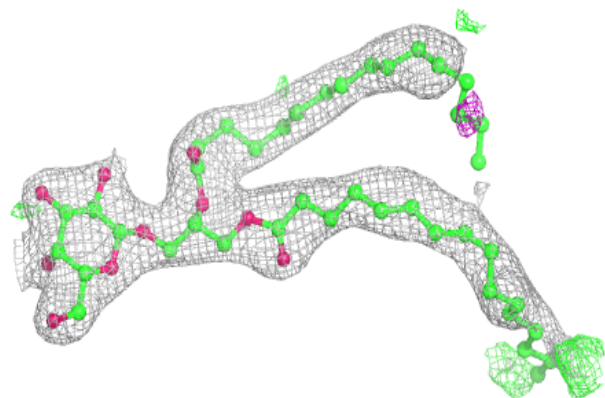


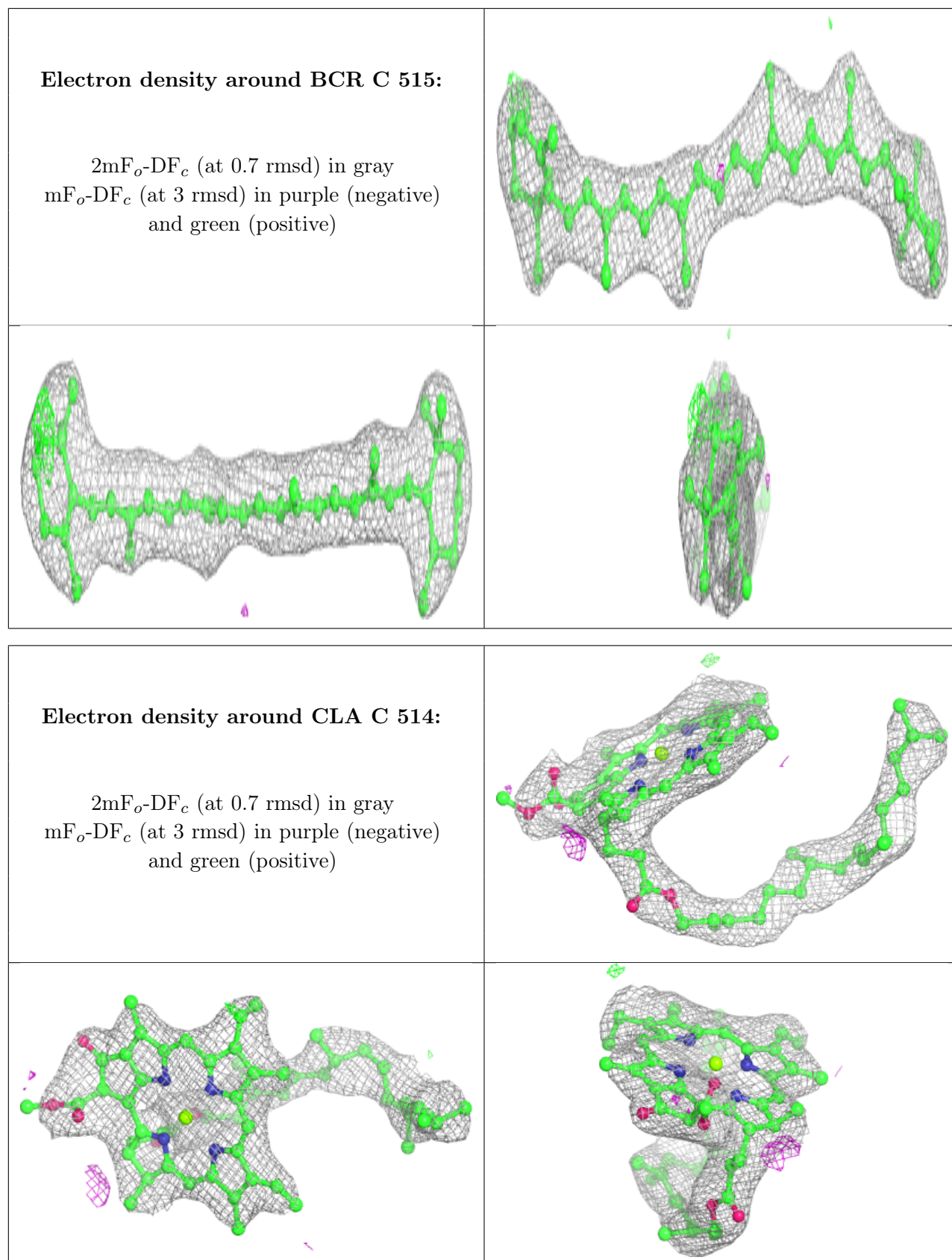
Electron density around CLA c 514:

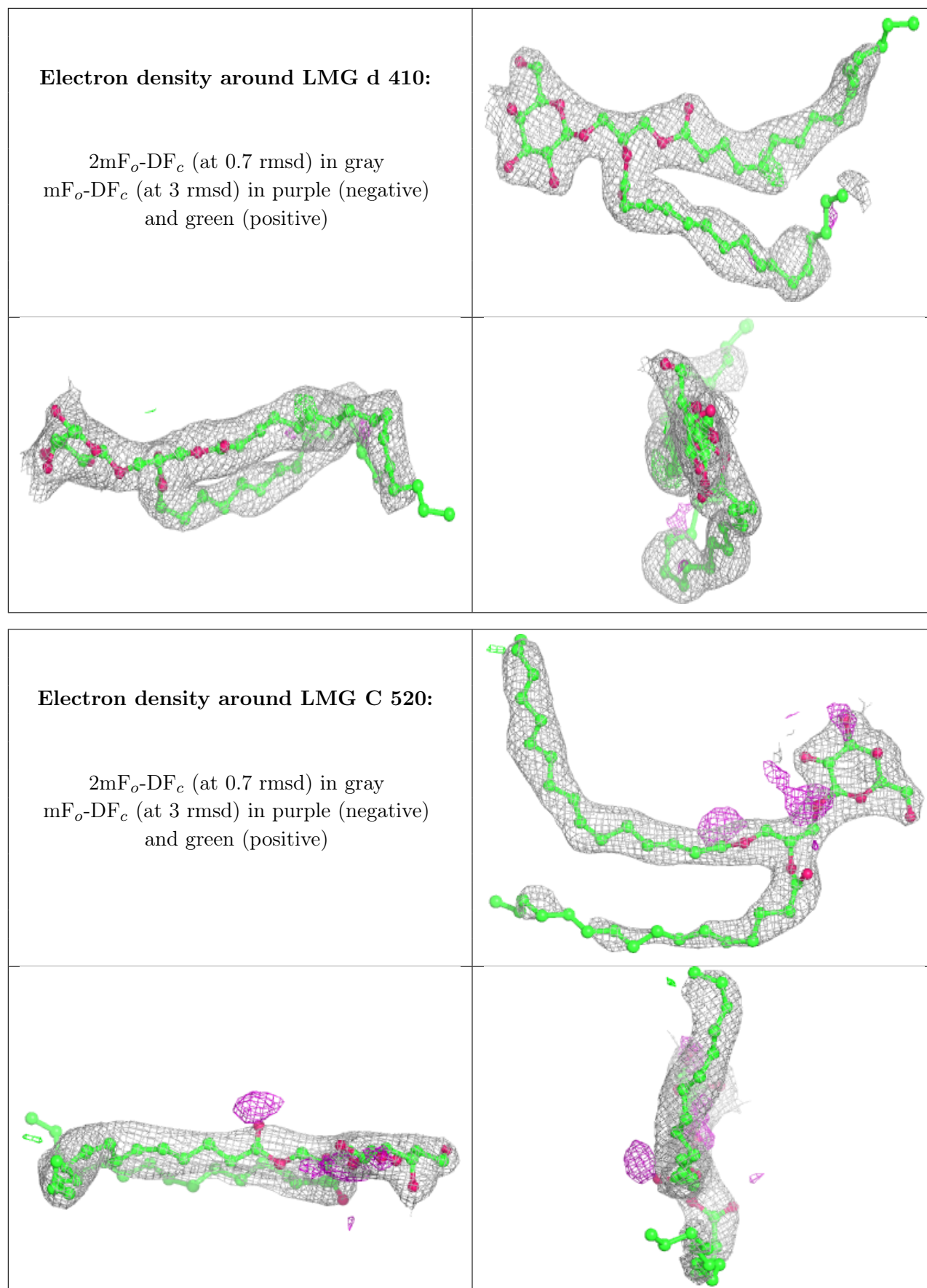
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around LMG D 411:**

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

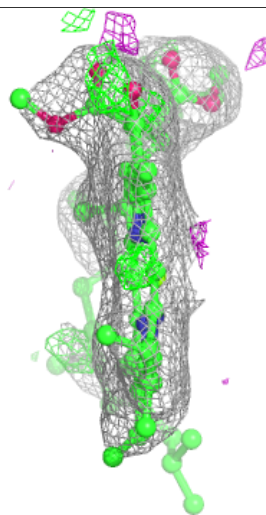
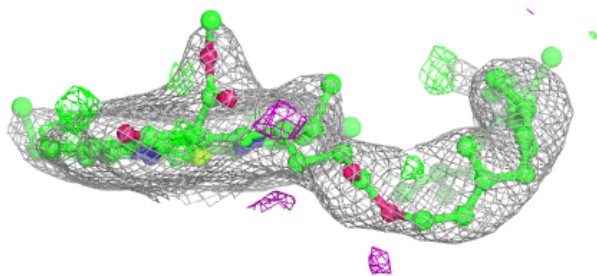
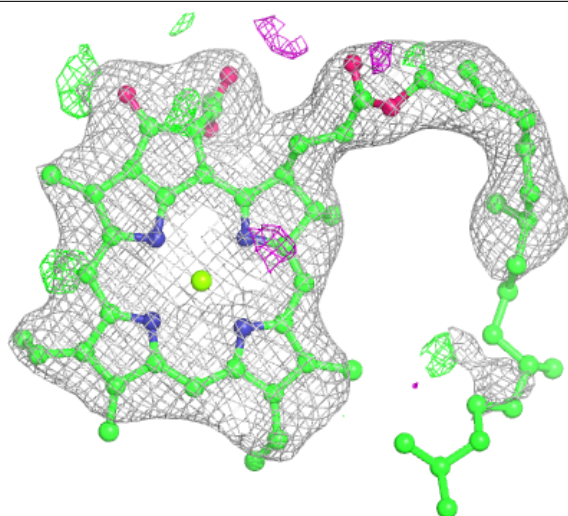






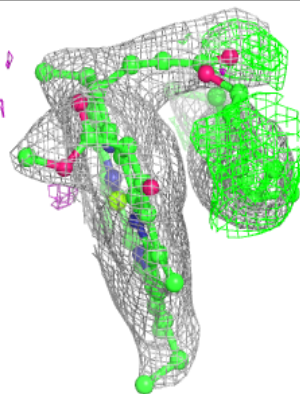
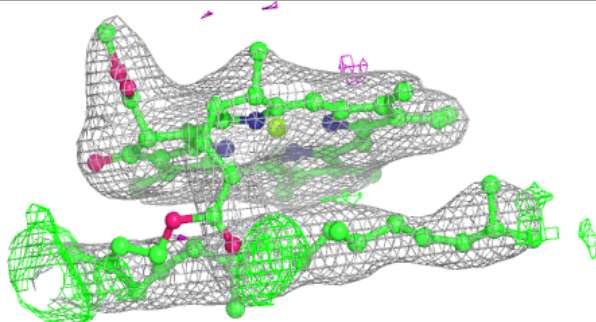
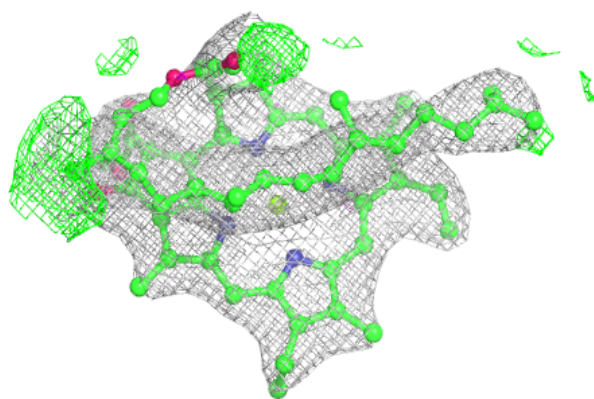
Electron density around CLA c 513:

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

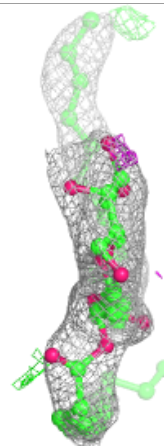
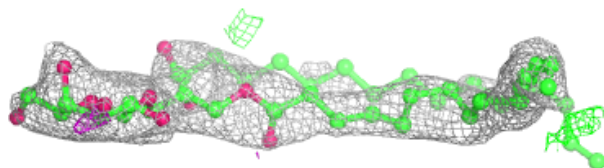
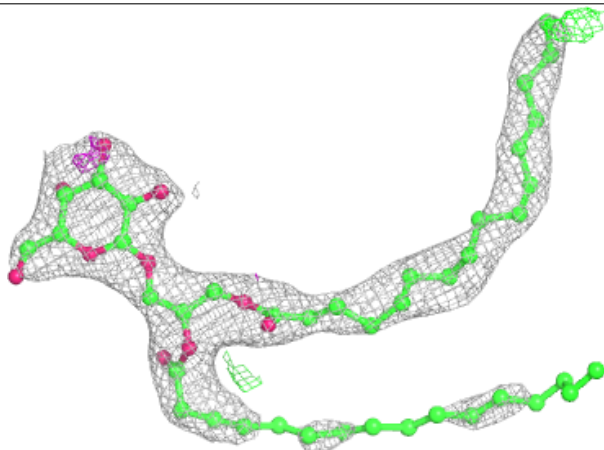


Electron density around CLA B 601:

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

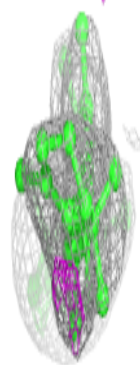
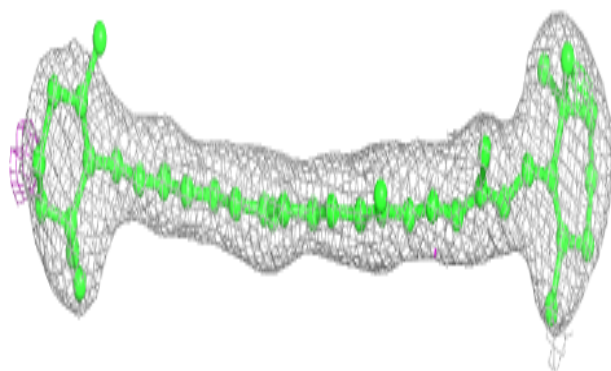
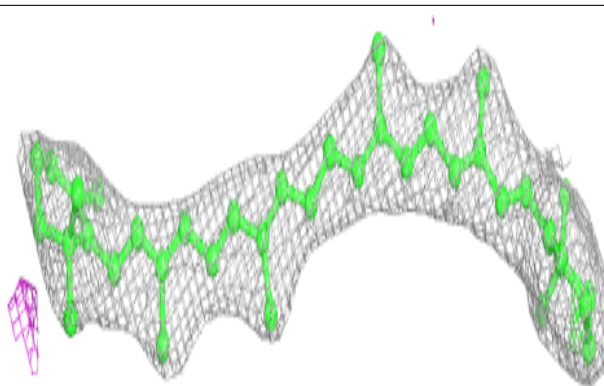
**Electron density around LMG c 520:**

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

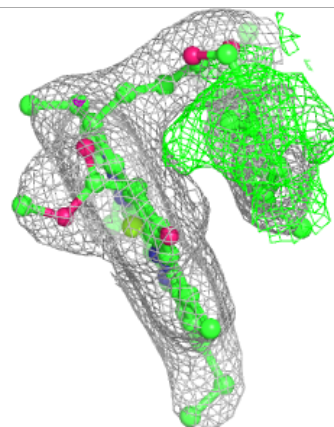
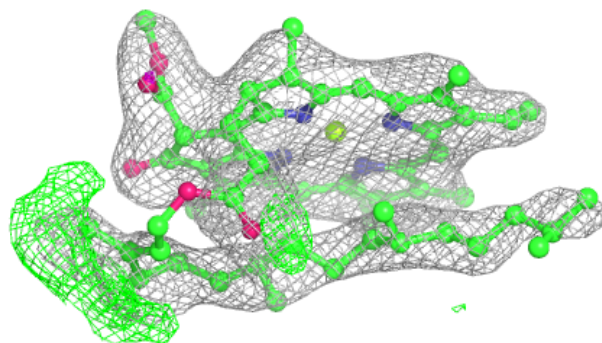
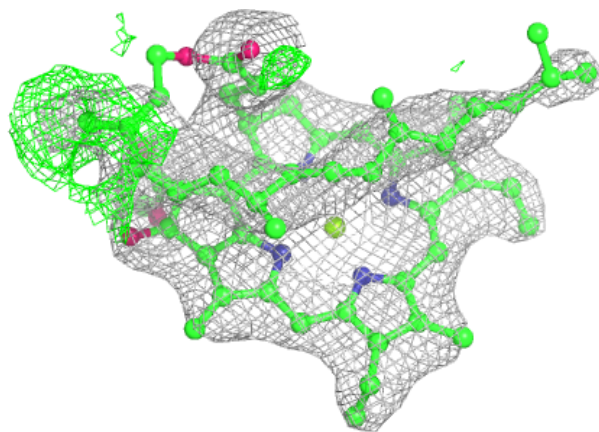


Electron density around BCR h 101:

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

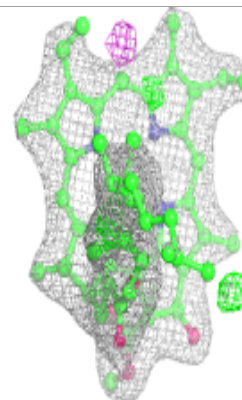
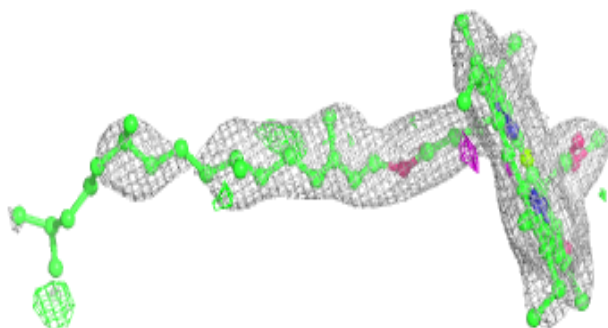
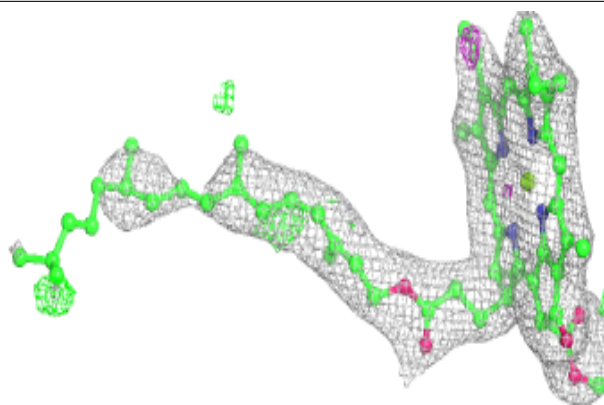
**Electron density around CLA b 601:**

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



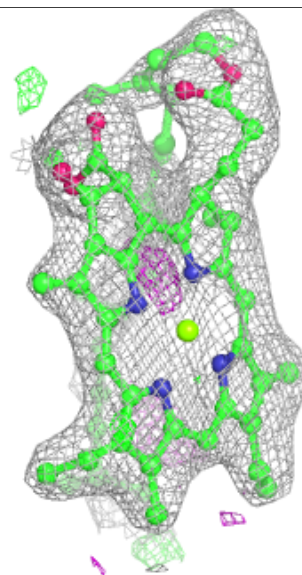
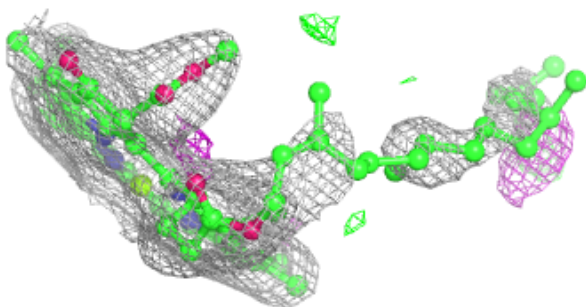
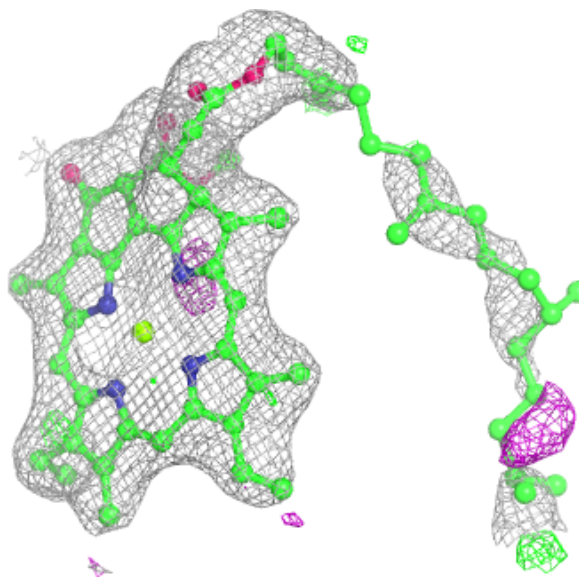
Electron density around CLA d 403:

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



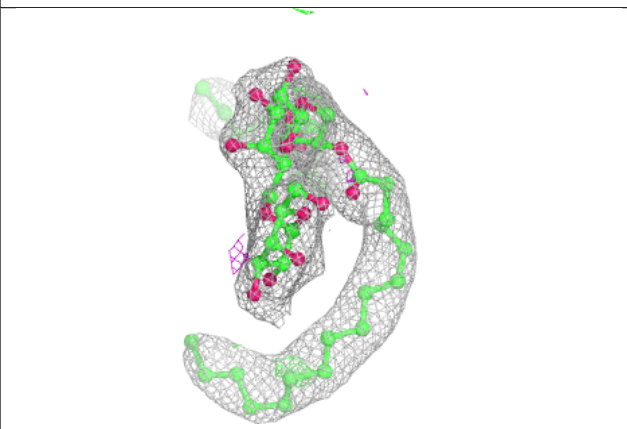
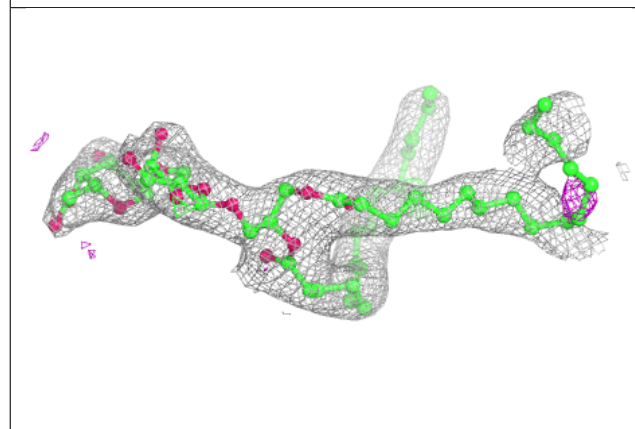
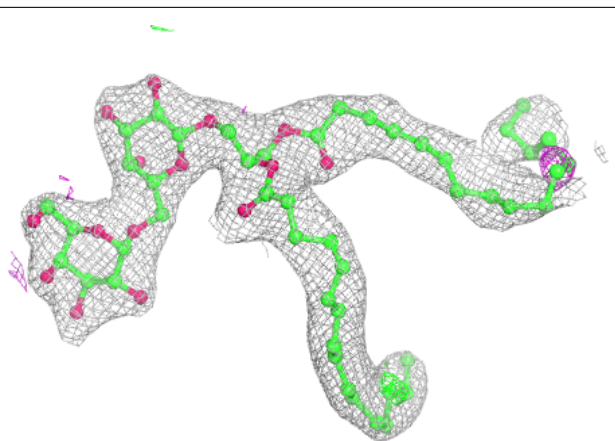
Electron density around CLA B 616:

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

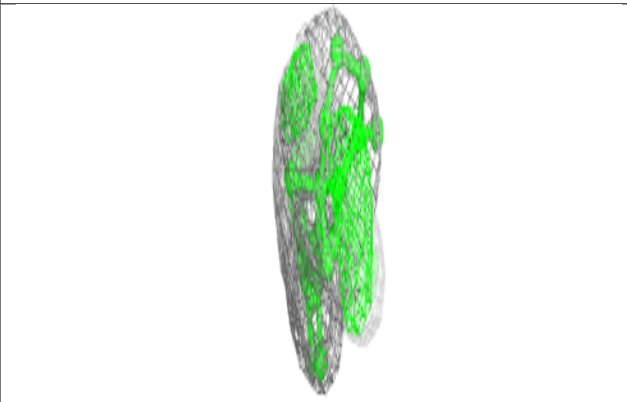
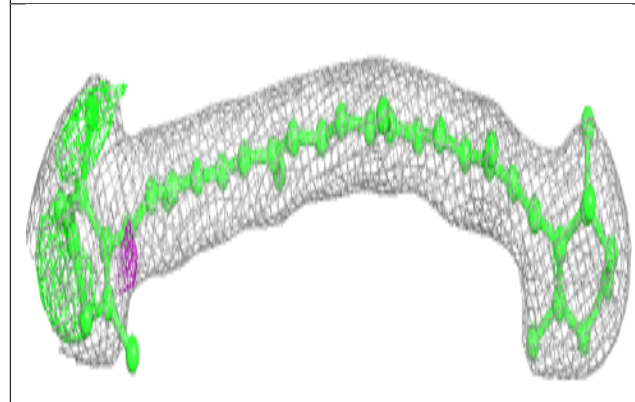
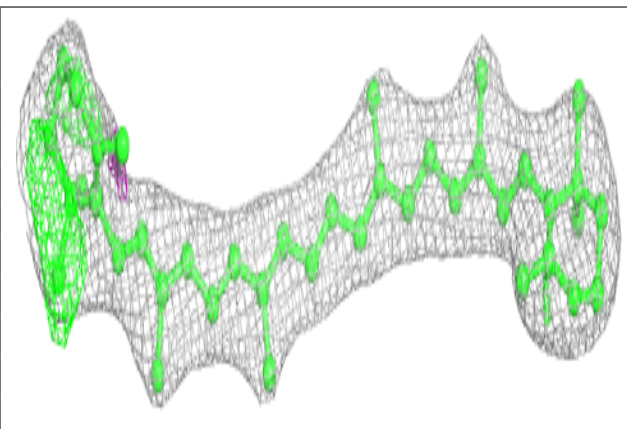


Electron density around DGD c 518 (B):

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

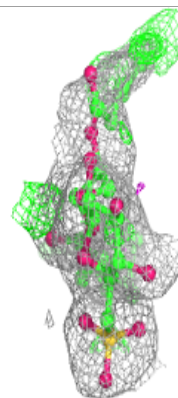
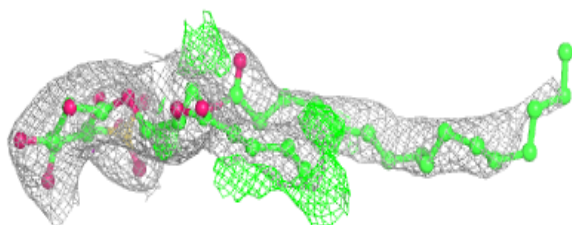
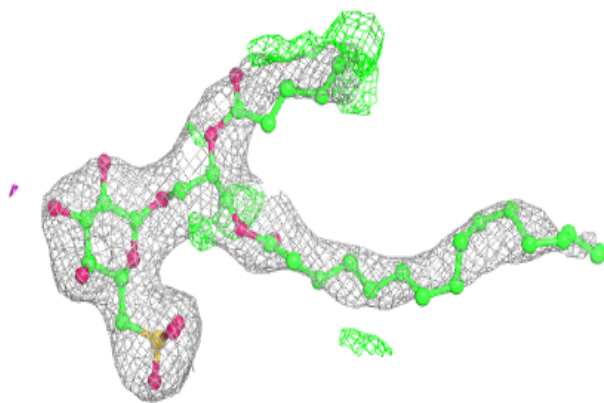
**Electron density around BCR d 404:**

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

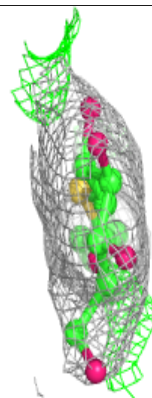
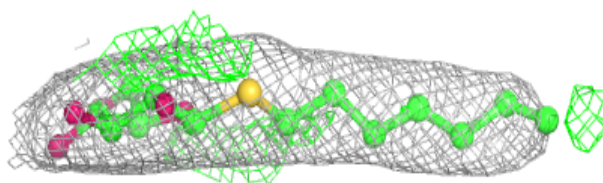
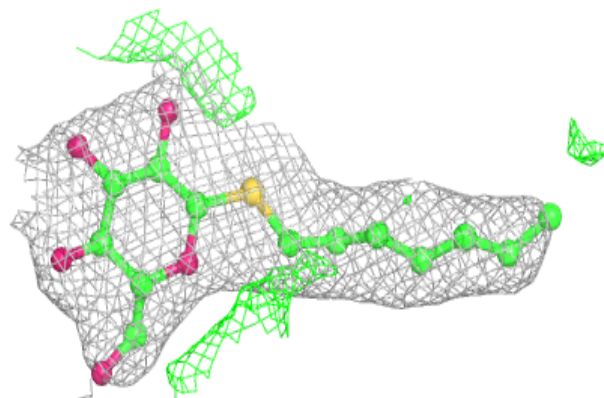


Electron density around SQD F 103:

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

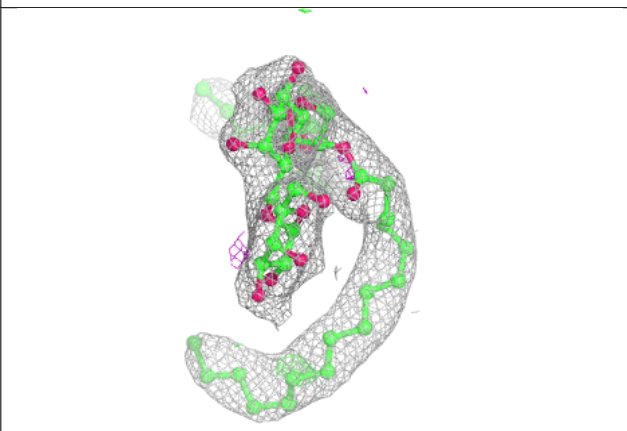
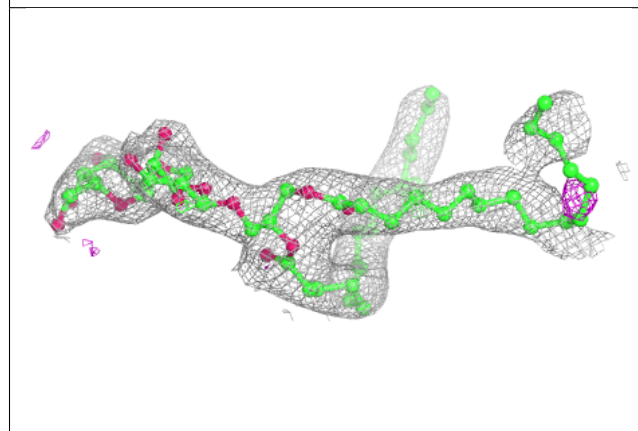
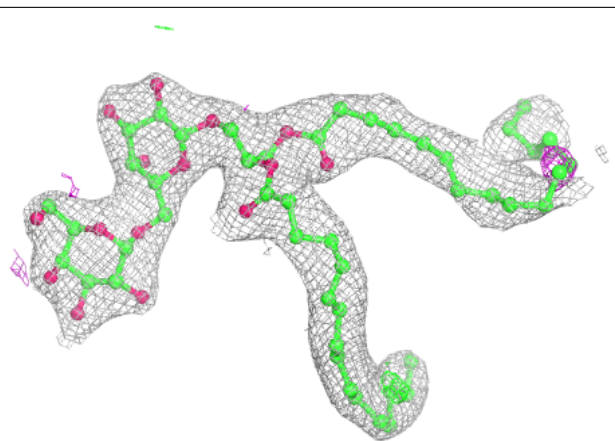
**Electron density around HTG b 625:**

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

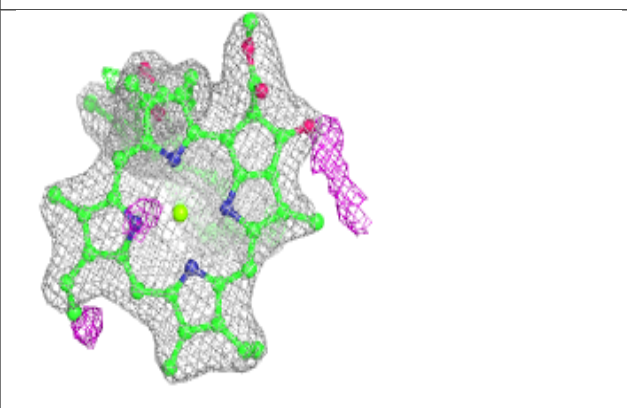
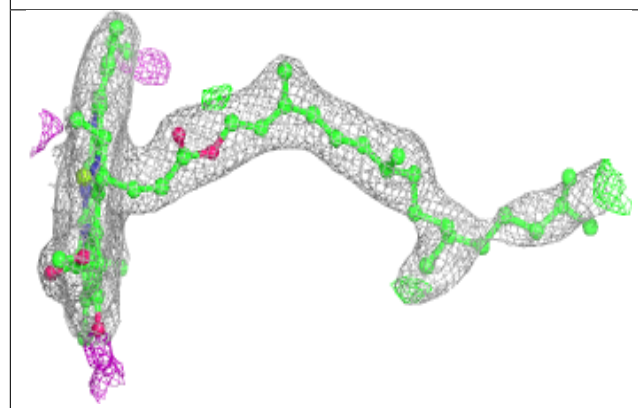
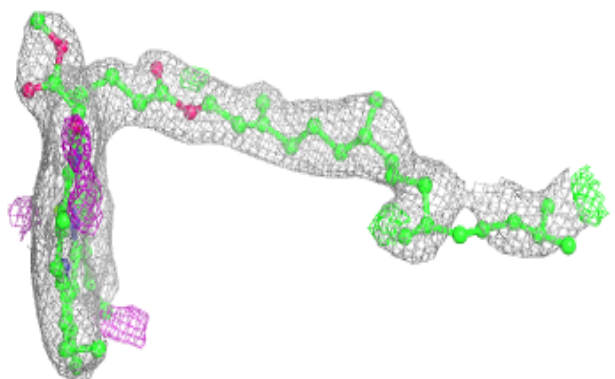


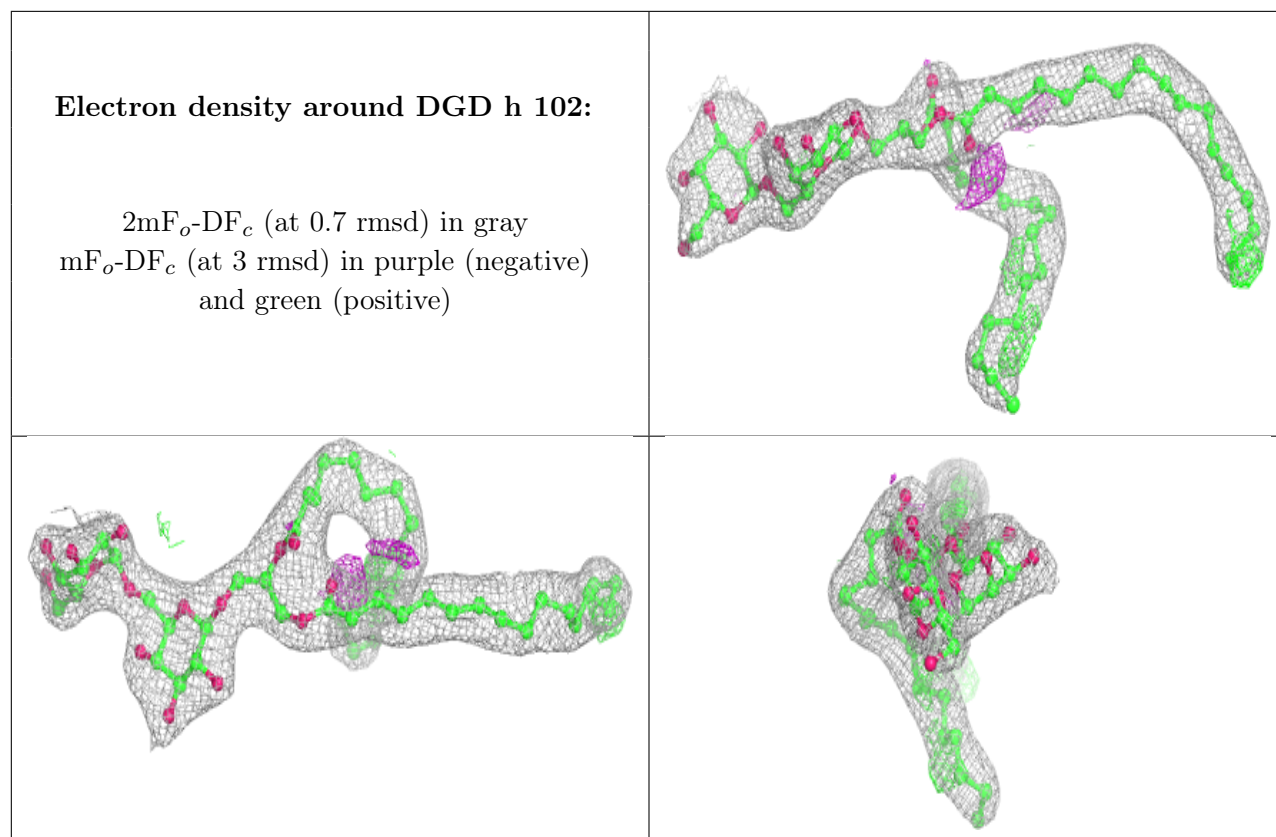
Electron density around DGD c 518 (A):

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

**Electron density around CLA B 606:**

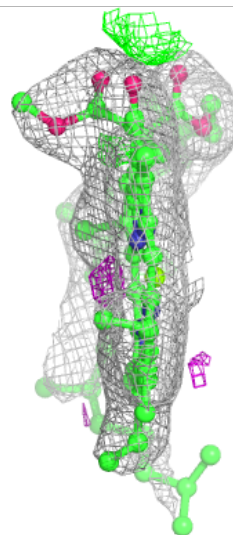
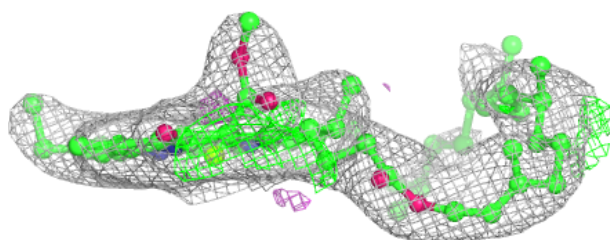
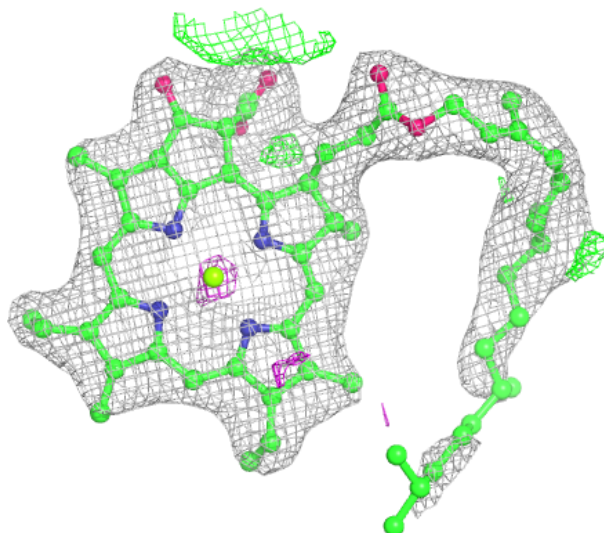
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





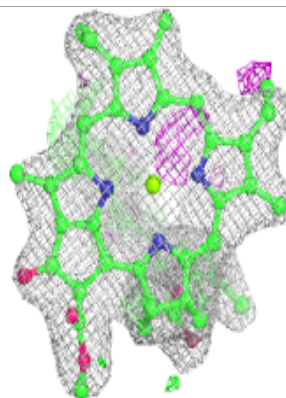
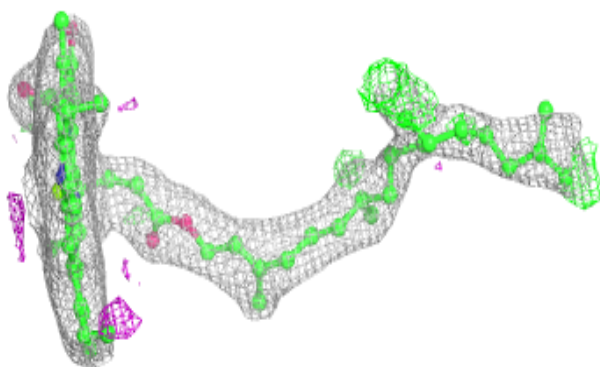
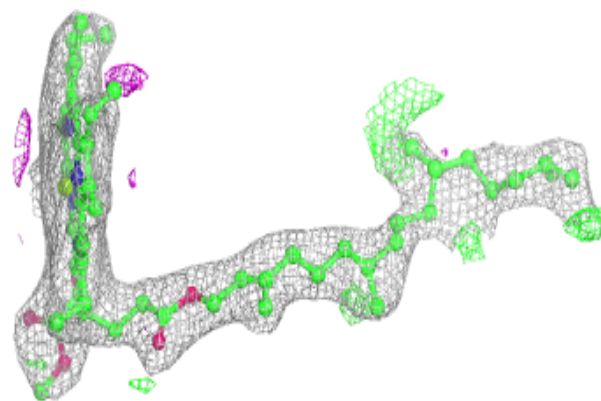
Electron density around CLA C 513:

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

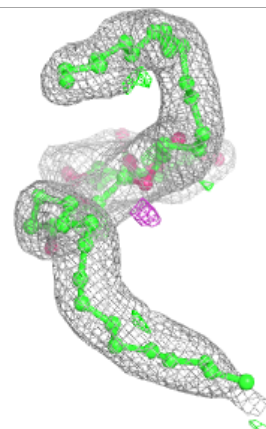
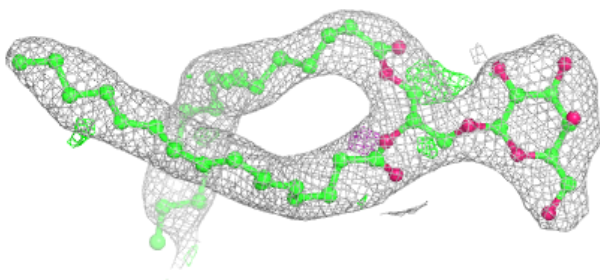
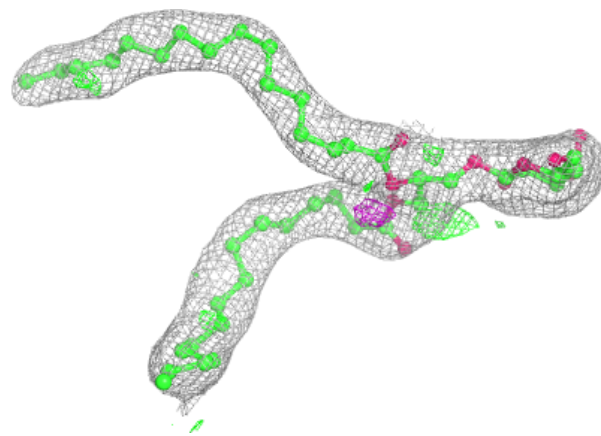


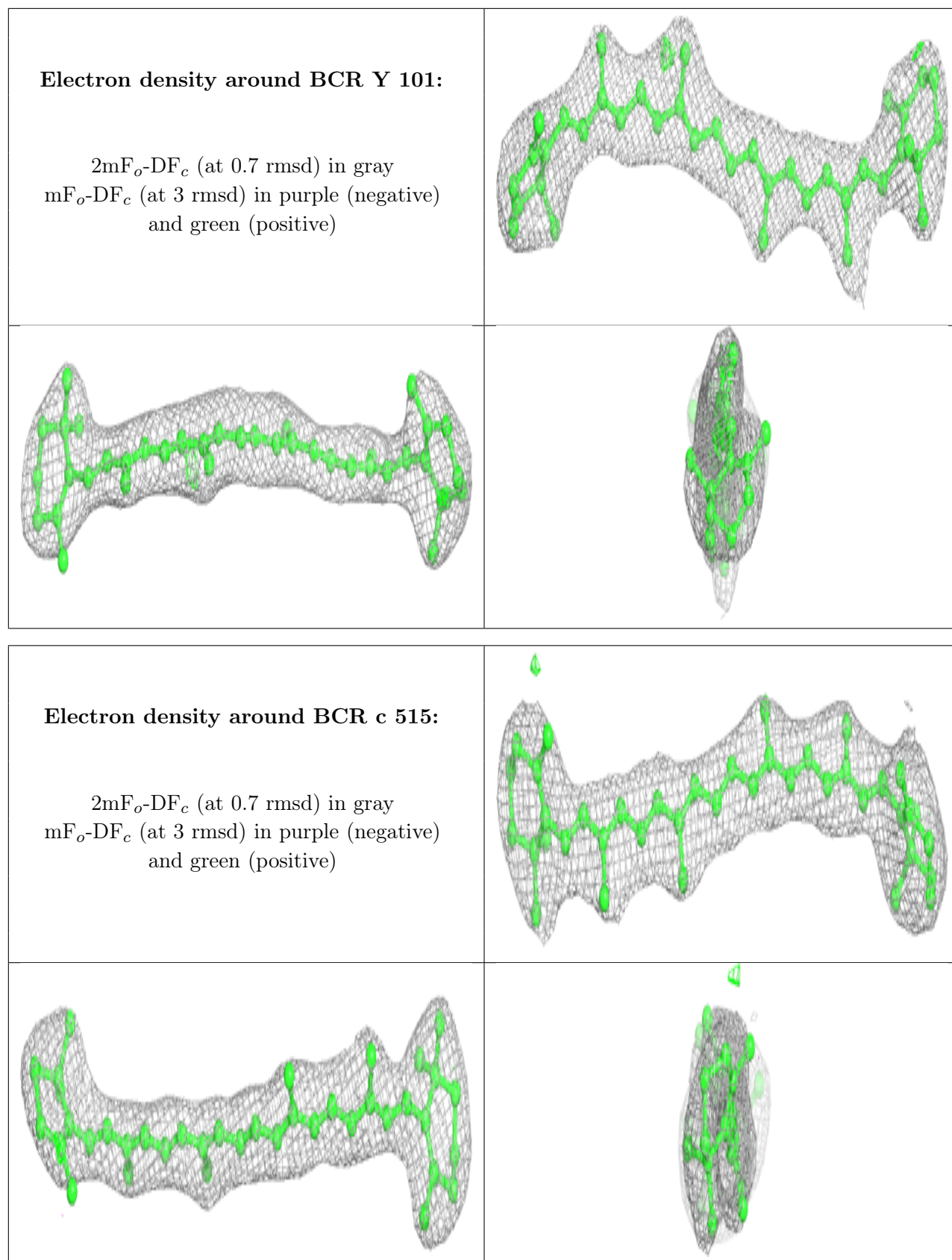
Electron density around CLA b 606:

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

**Electron density around LMG B 620:**

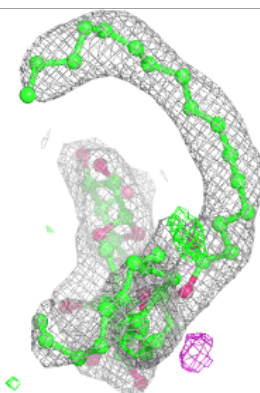
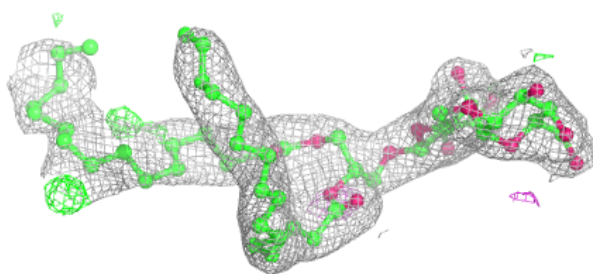
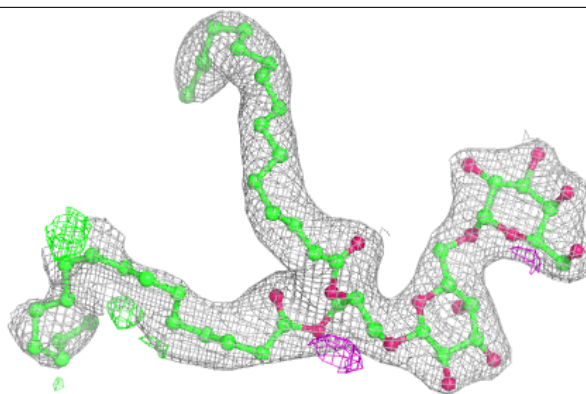
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



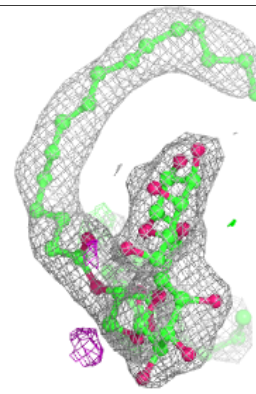
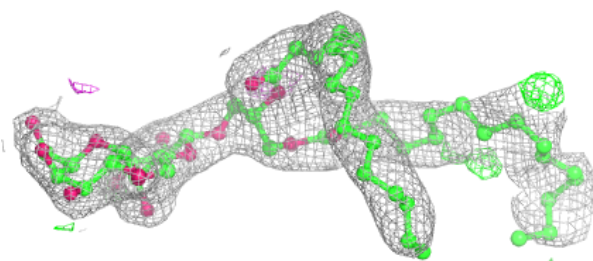
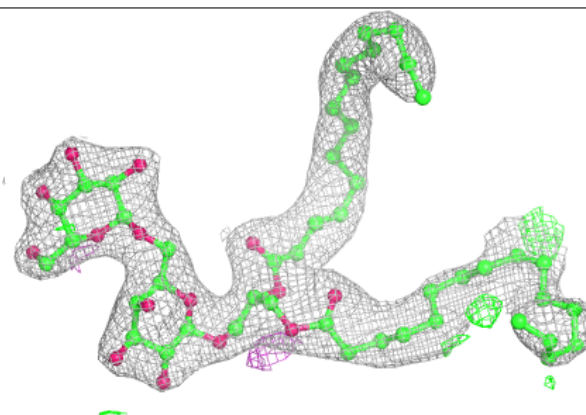


Electron density around DGD C 518 (A):

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

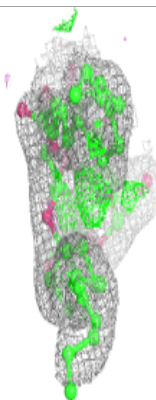
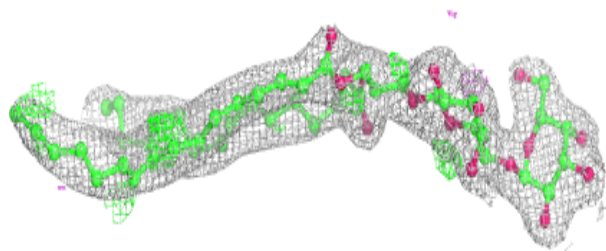
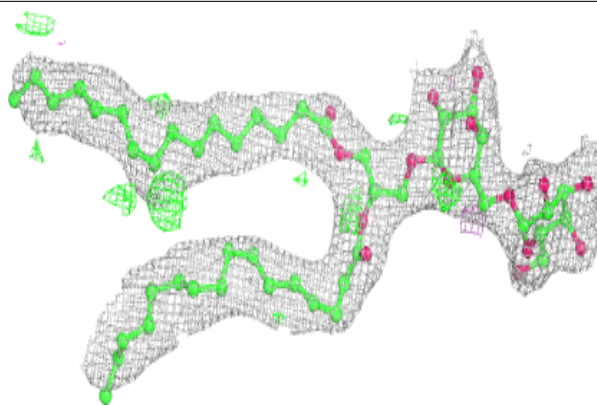
**Electron density around DGD C 518 (B):**

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

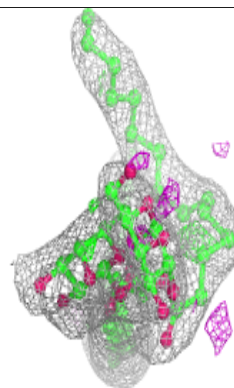
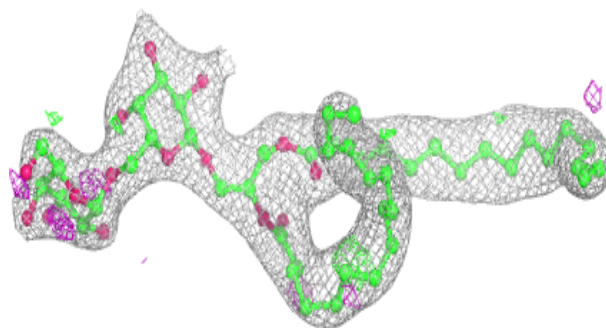
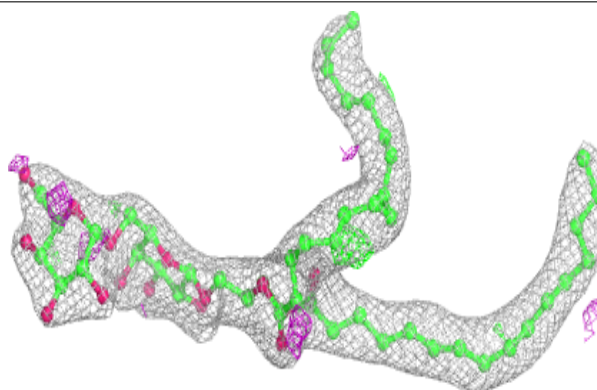


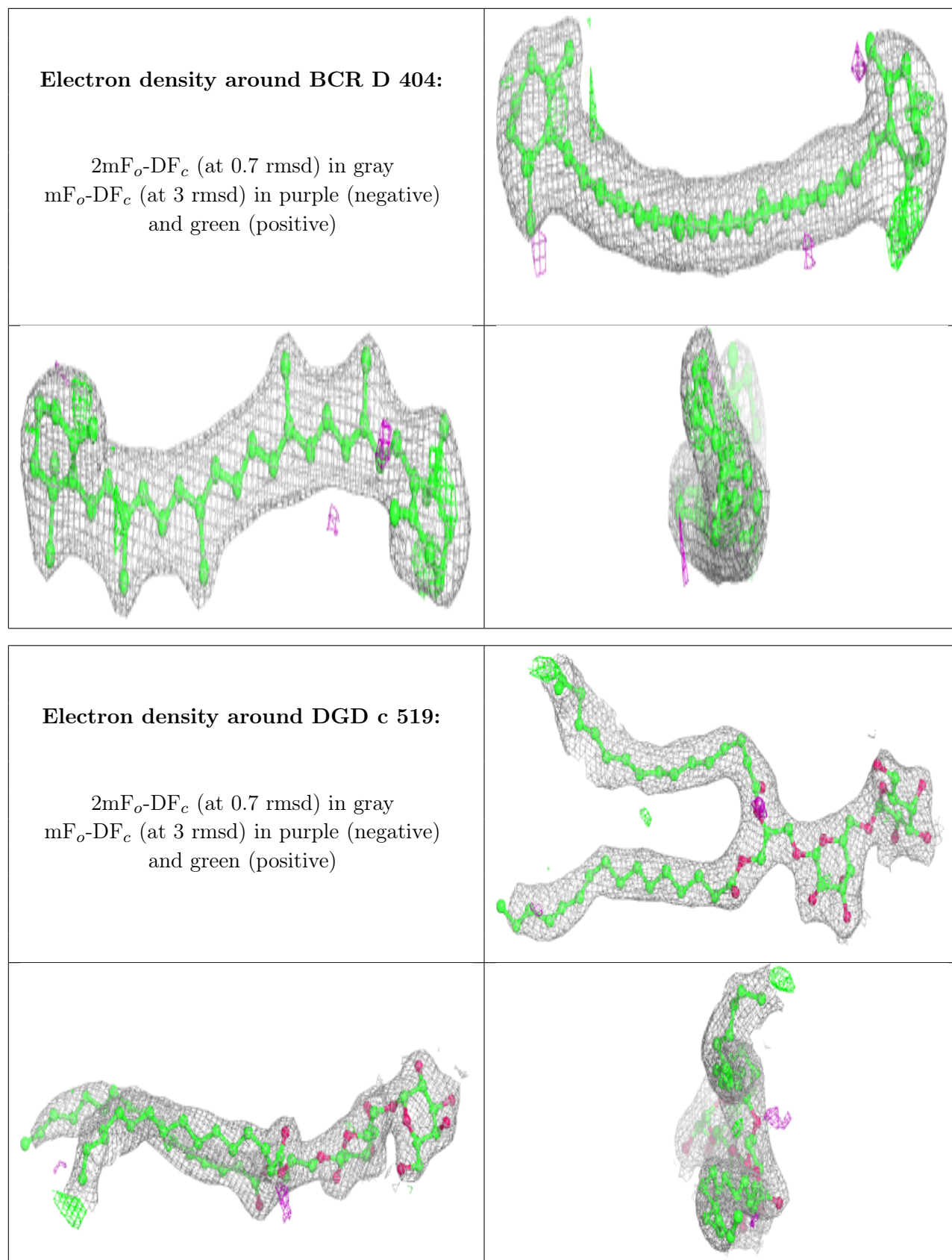
Electron density around DGD C 519:

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

**Electron density around DGD H 102:**

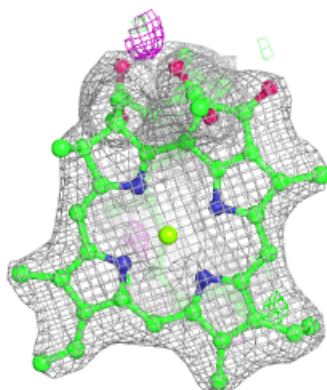
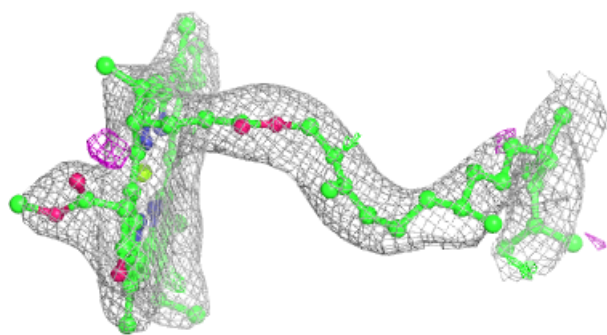
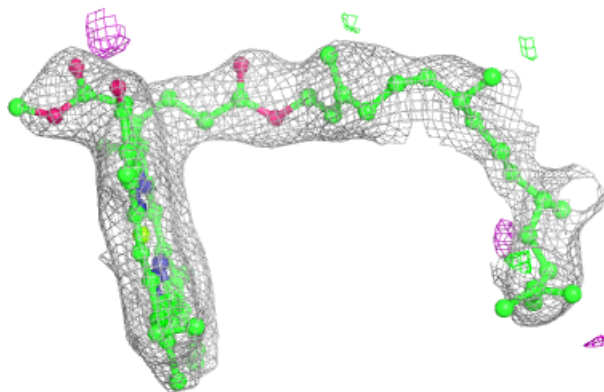
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



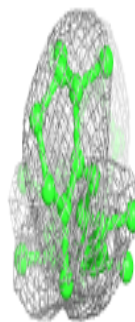
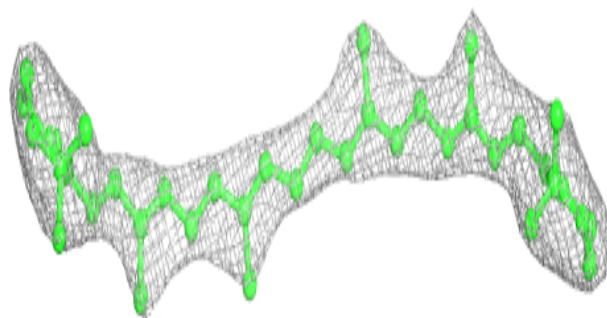
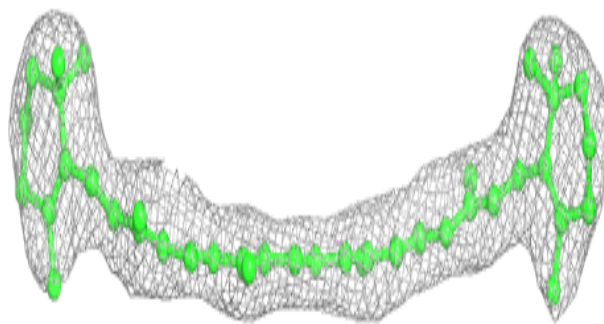


Electron density around CLA C 507:

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

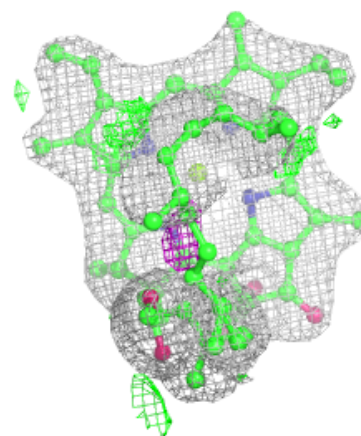
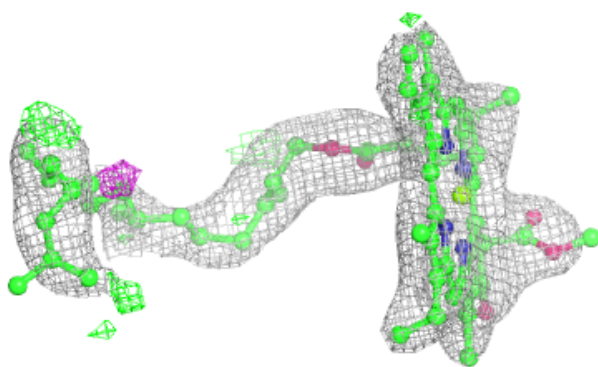
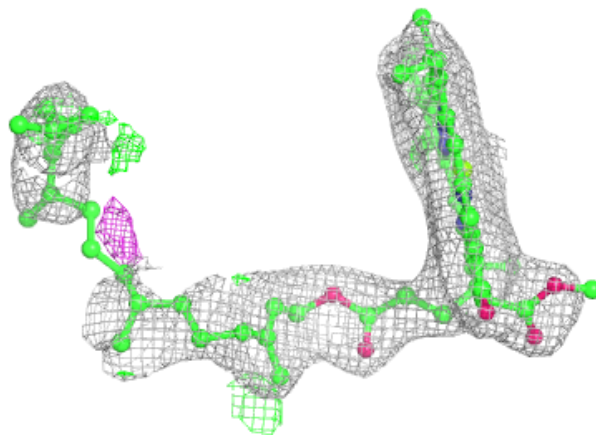
**Electron density around BCR k 101:**

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



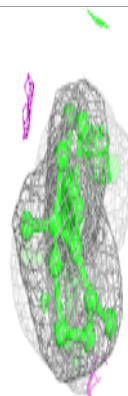
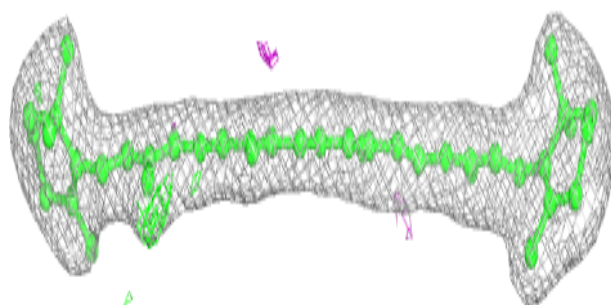
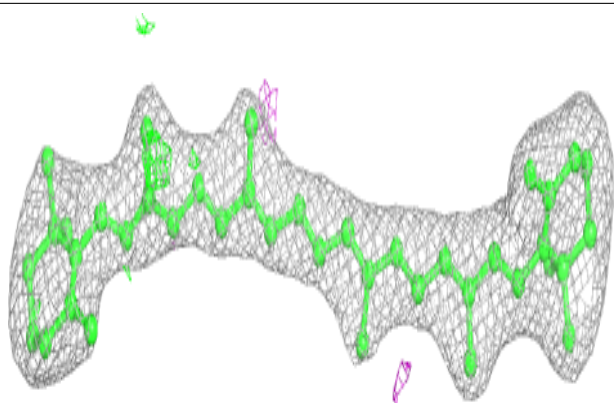
Electron density around CLA c 507:

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

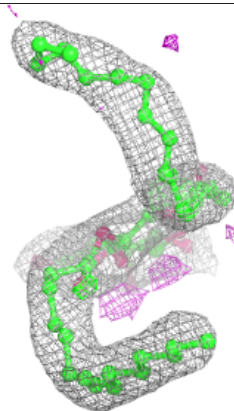
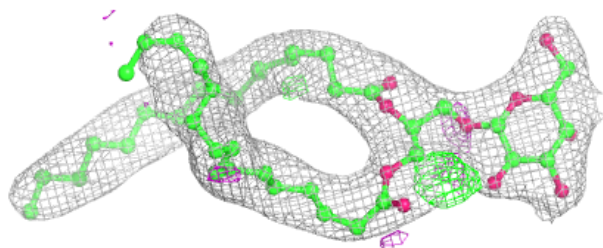
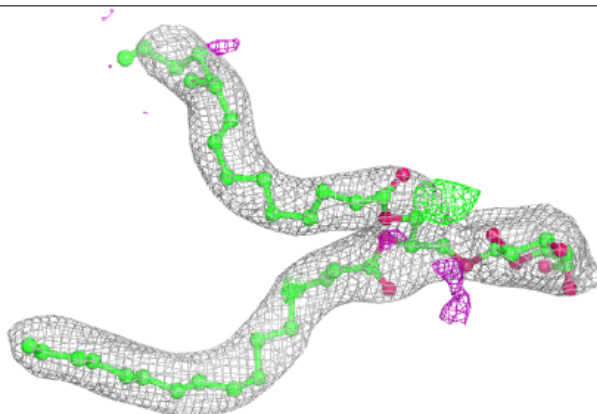


Electron density around BCR b 618:

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

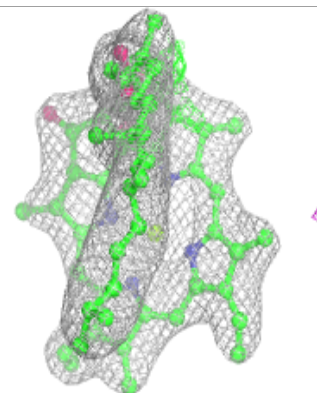
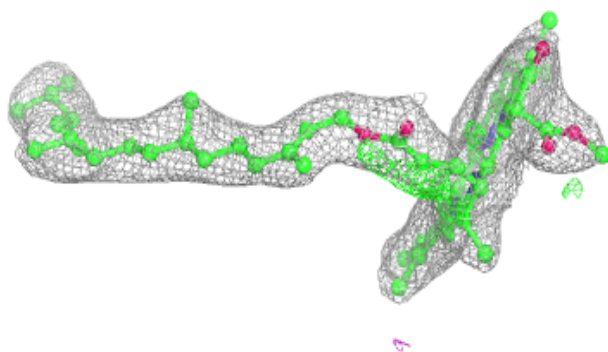
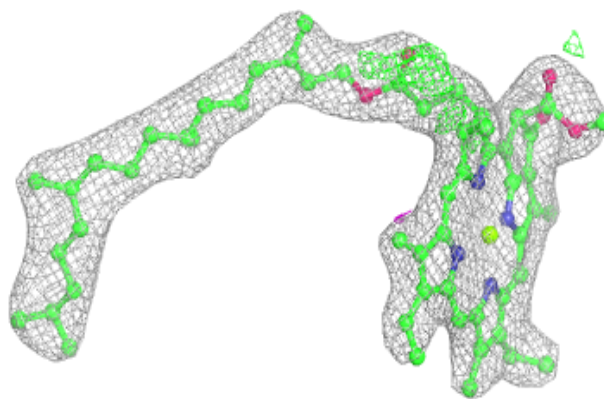
**Electron density around LMG m 101:**

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

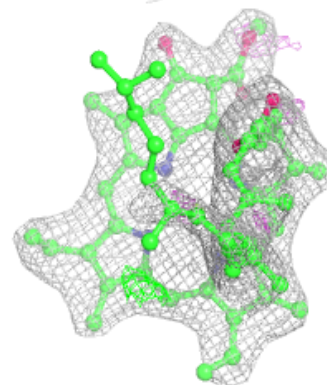
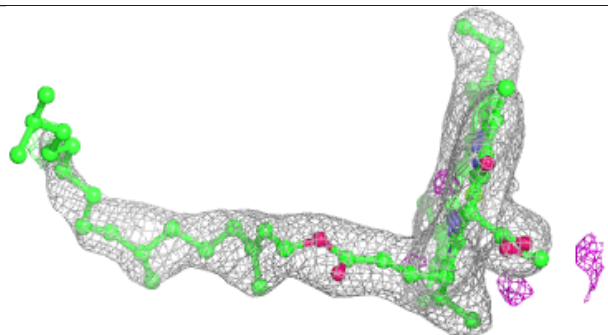
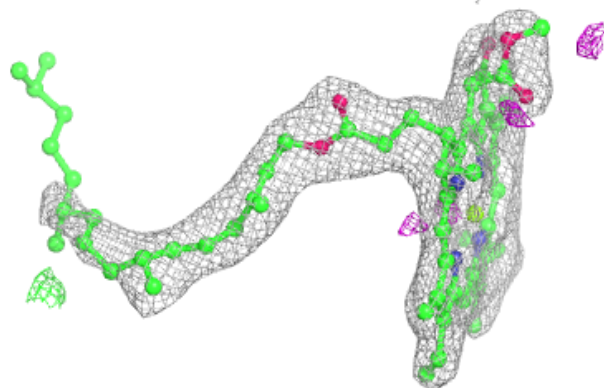


Electron density around CLA B 609:

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

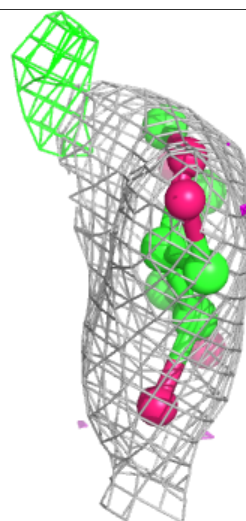
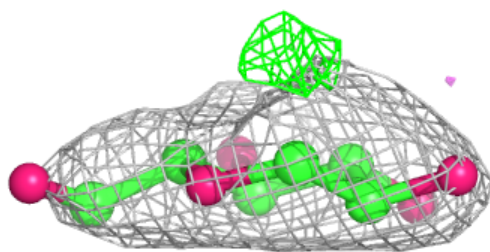
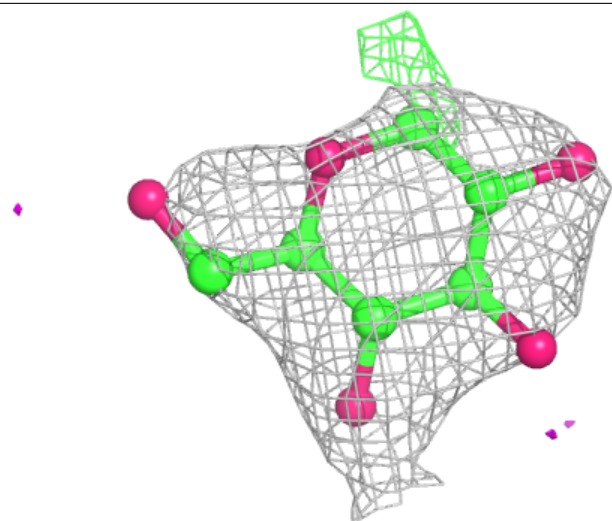
**Electron density around CLA D 403:**

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



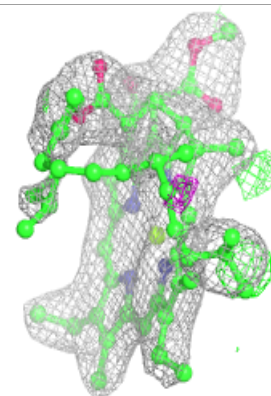
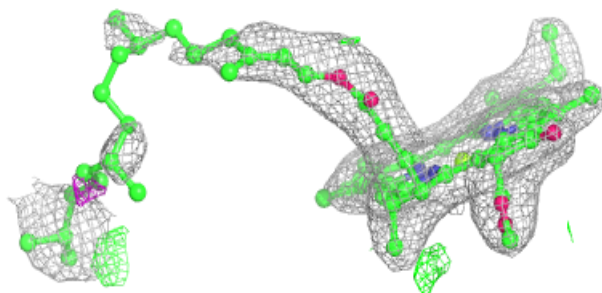
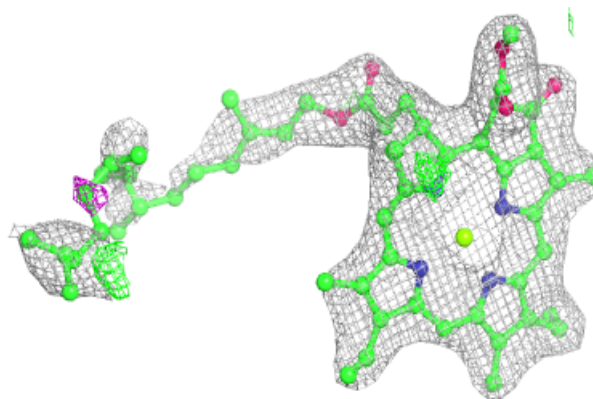
Electron density around HTG V 202:

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

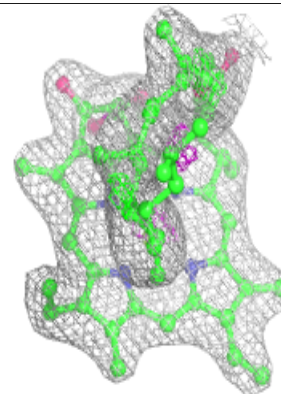
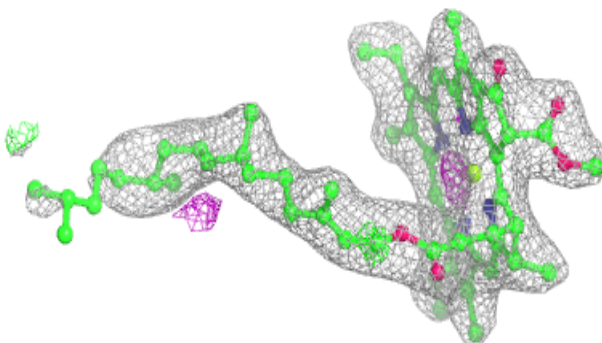
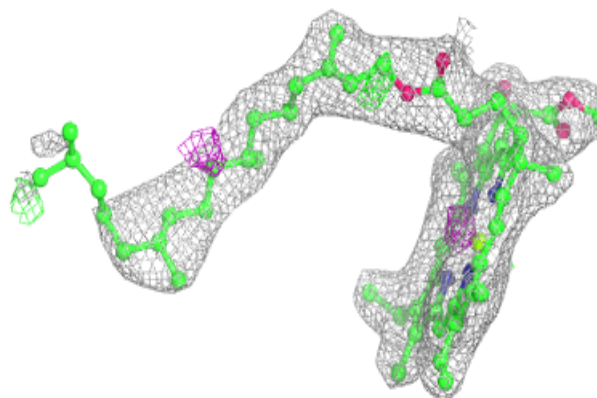


Electron density around CLA a 408:

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

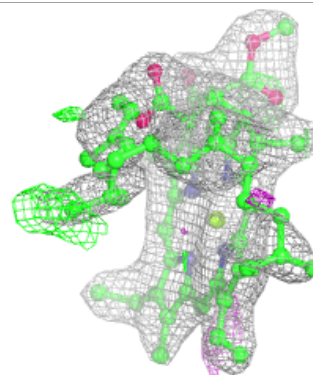
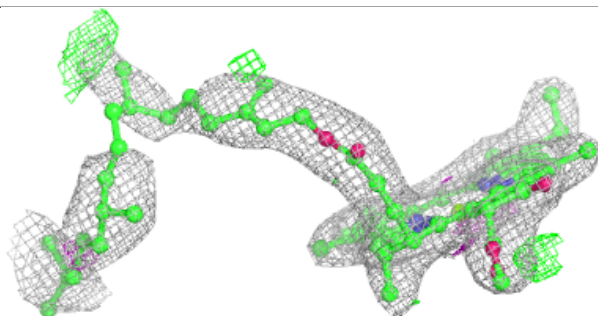
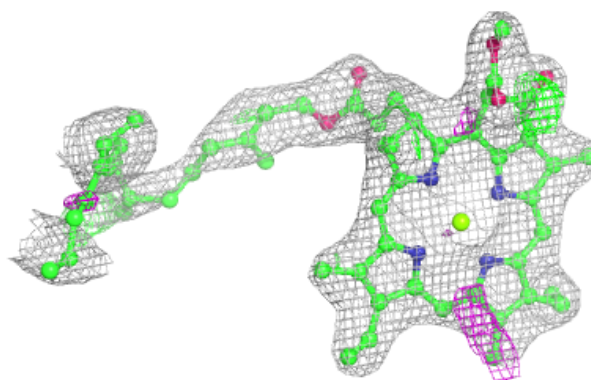
**Electron density around CLA C 509:**

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

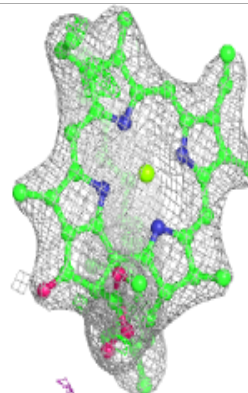
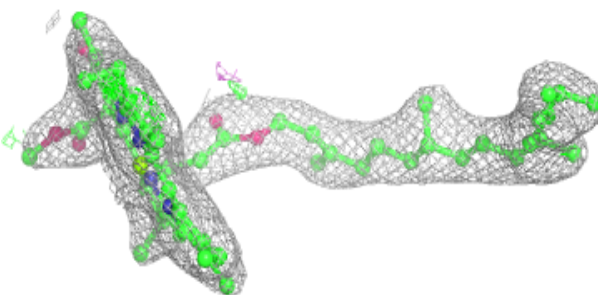
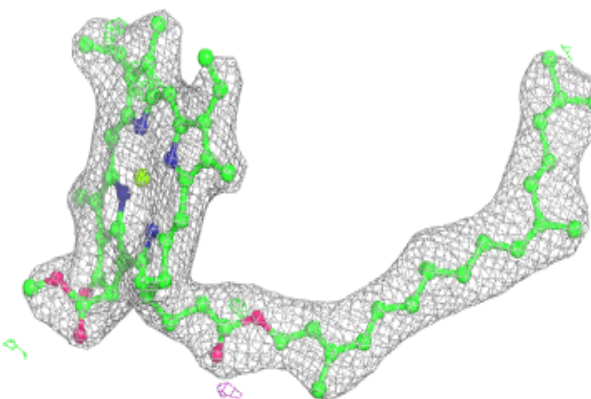


Electron density around CLA A 408:

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

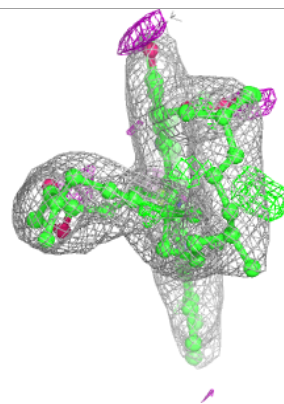
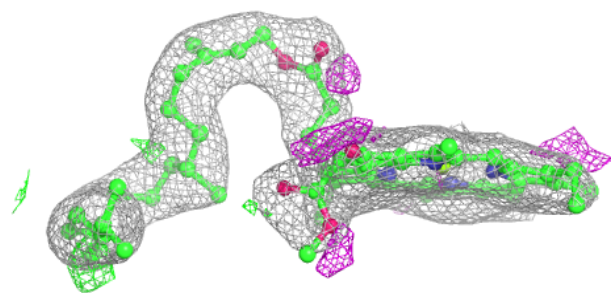
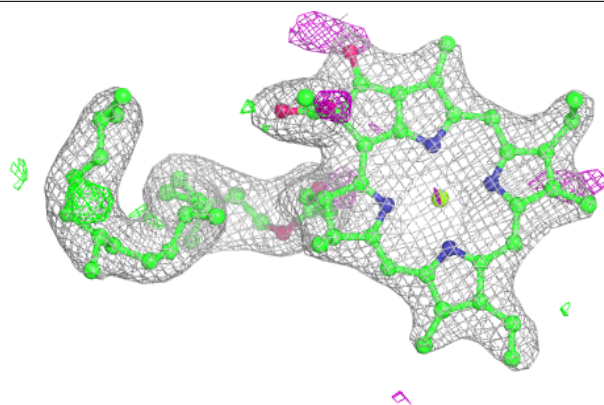
**Electron density around CLA b 609:**

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



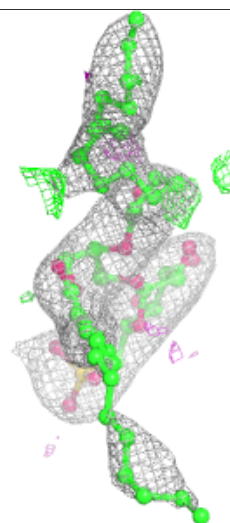
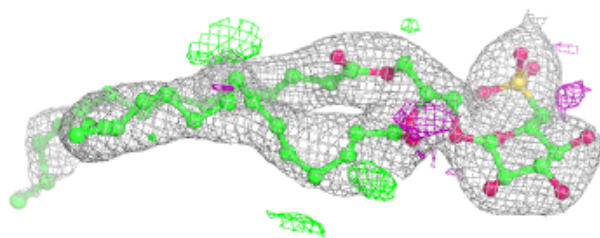
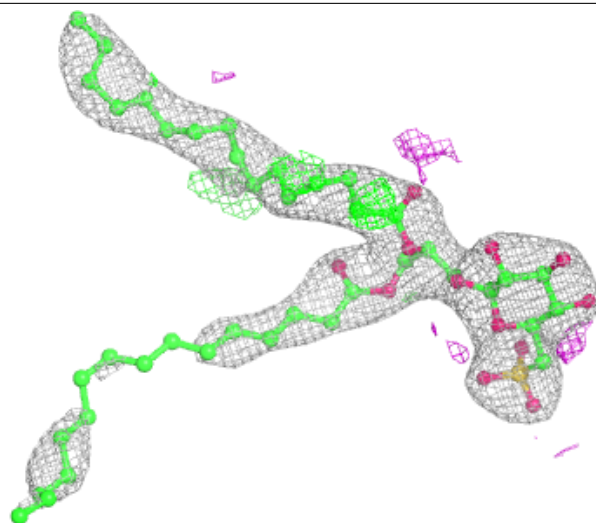
Electron density around CLA b 612:

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



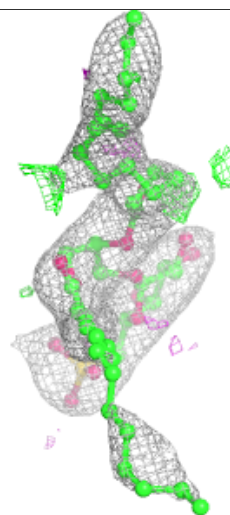
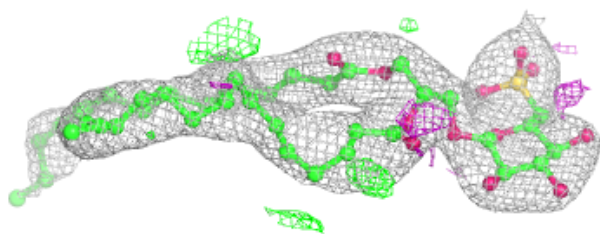
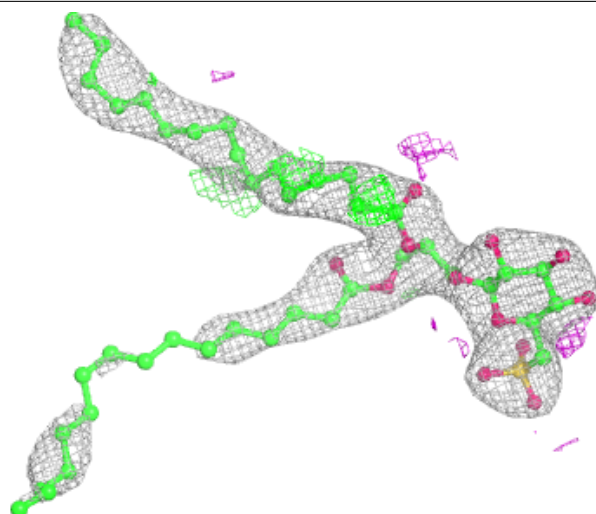
Electron density around SQD A 410 (A):

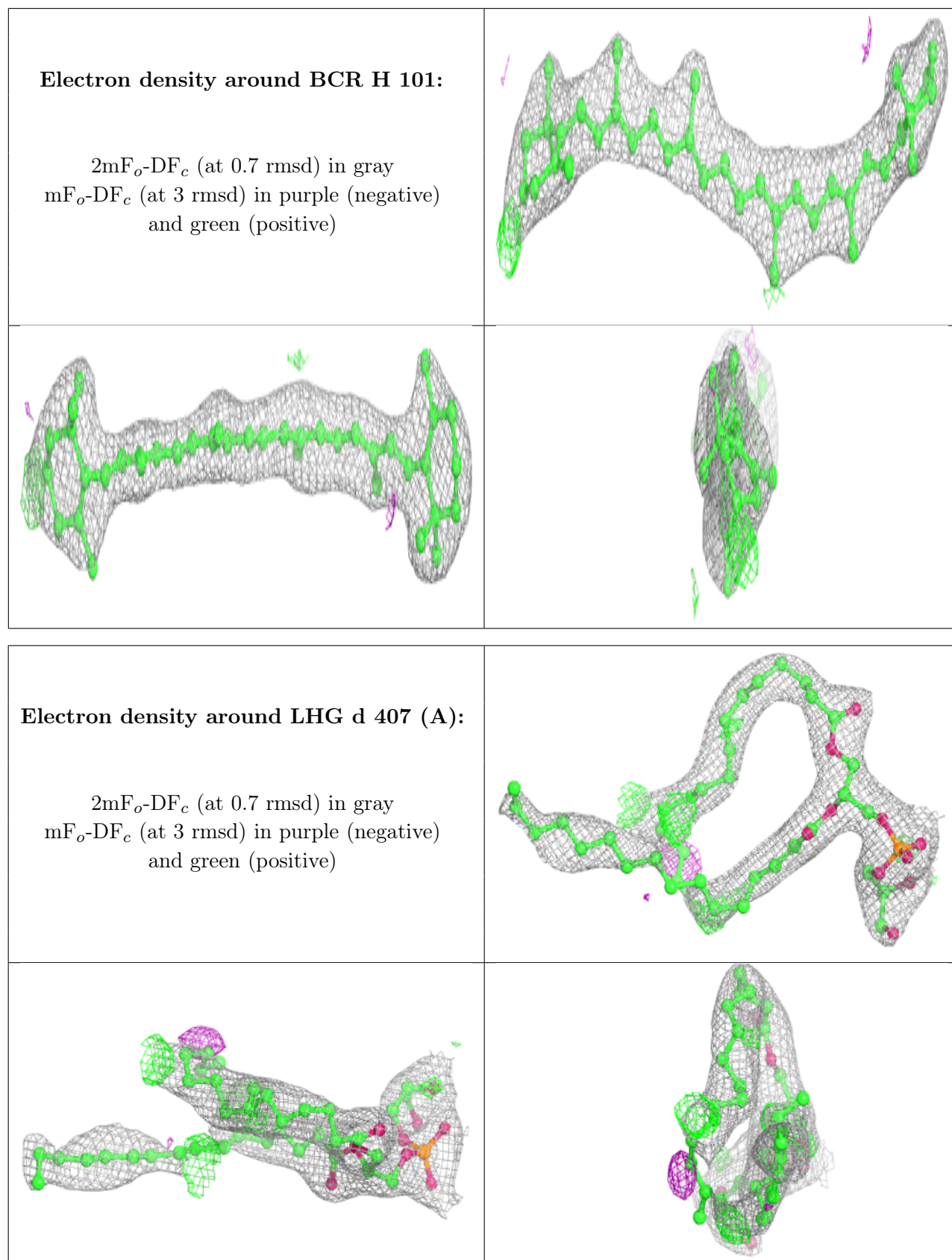
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SQD A 410 (B):

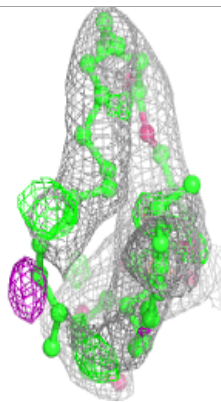
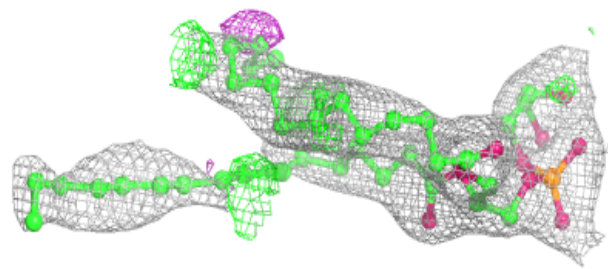
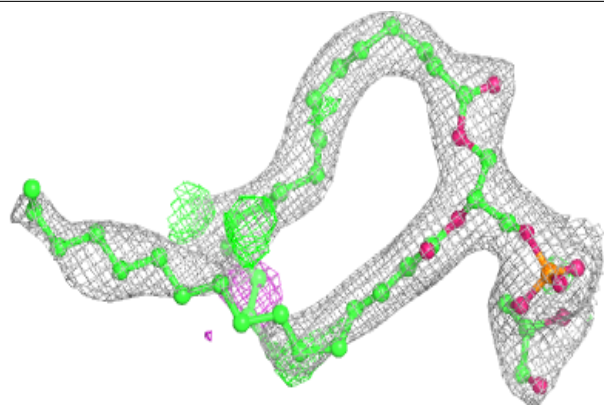
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



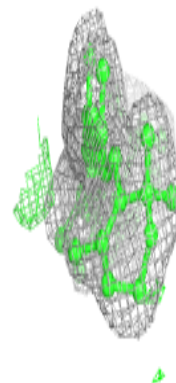
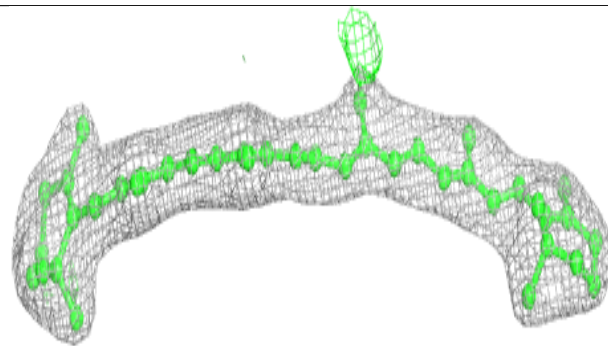
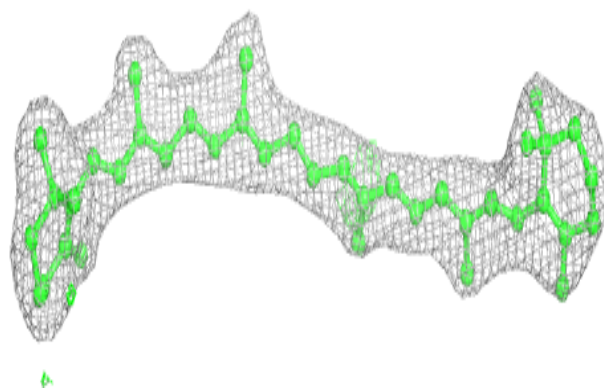


Electron density around LHG d 407 (B):

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

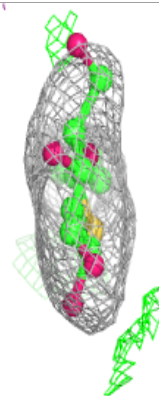
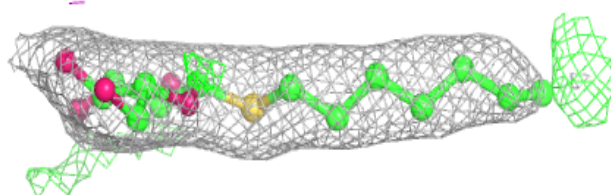
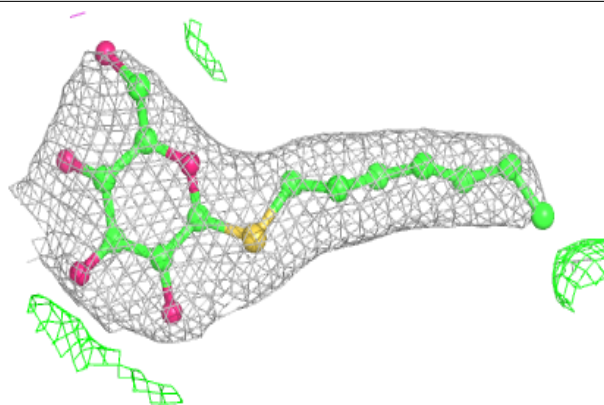
**Electron density around BCR t 102:**

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

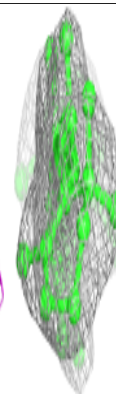
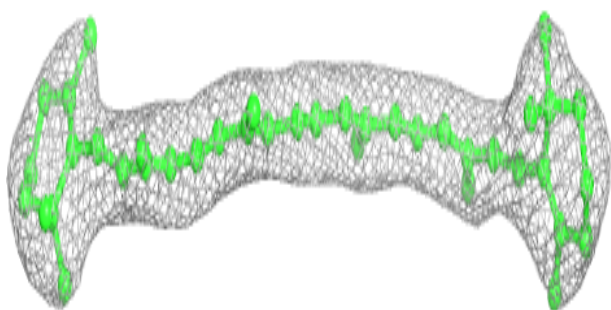
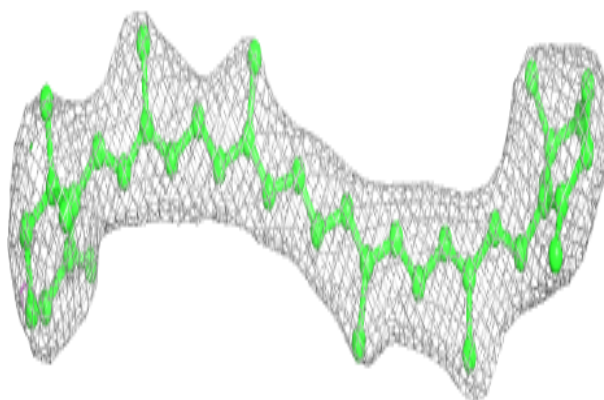


Electron density around HTG B 623:

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

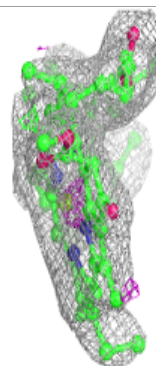
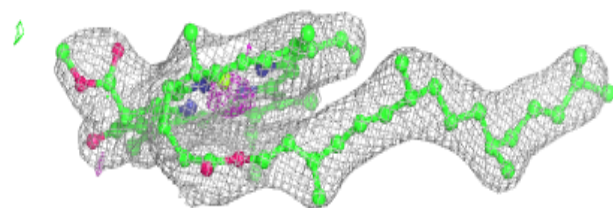
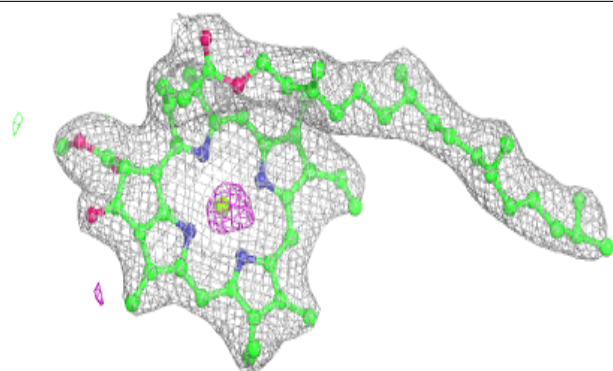
**Electron density around BCR y 101:**

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

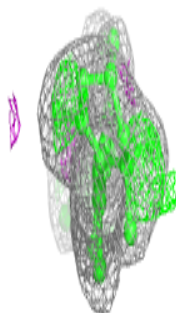
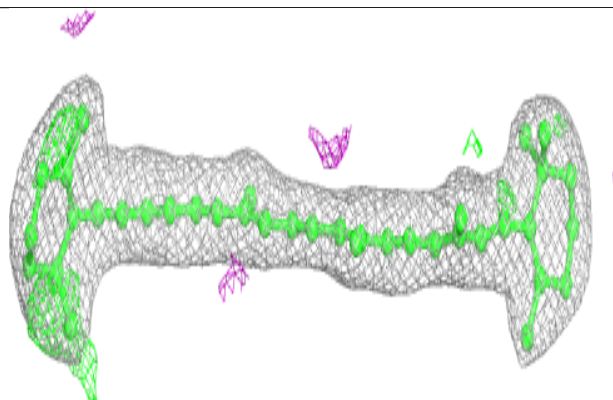
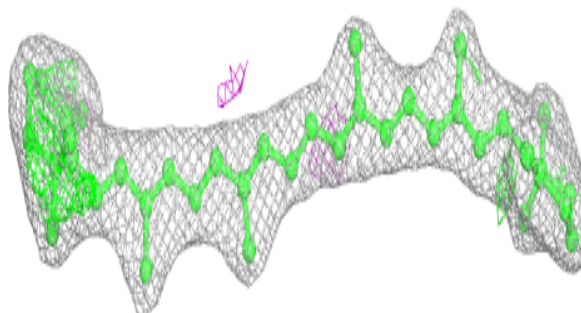


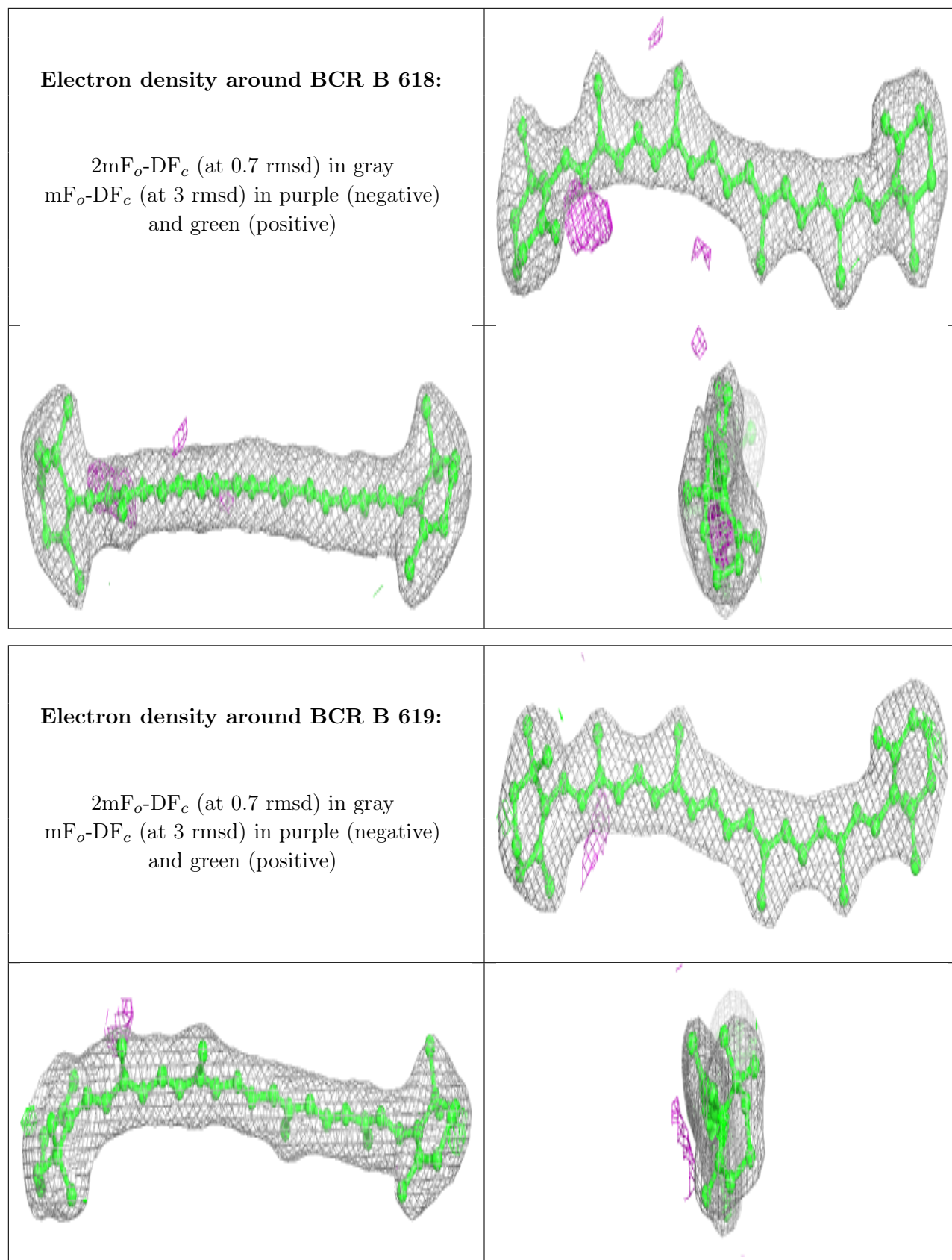
Electron density around CLA C 502:

$2mF_o-DF_c$ (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:**

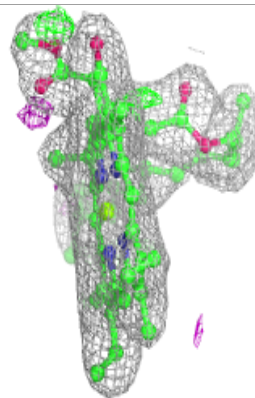
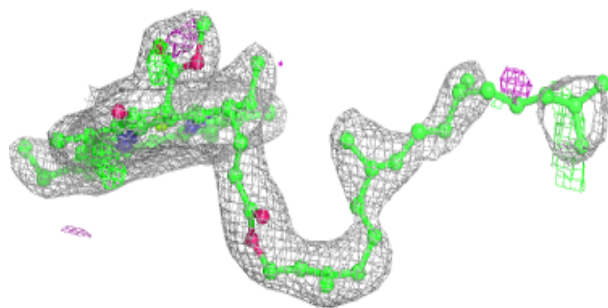
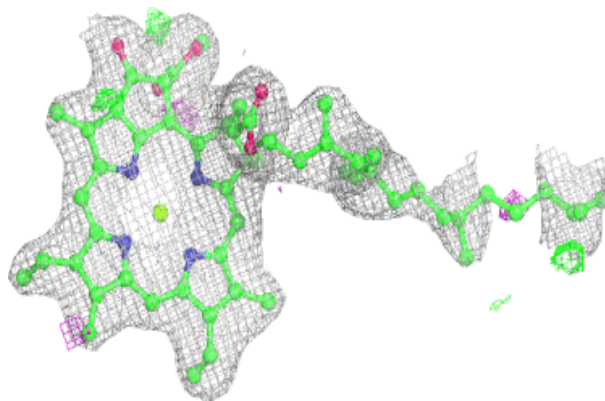
$2mF_o-DF_c$ (at 0.7 rnsd) in gray
 mF_o-DF_c (at 3 rnsd) in purple (negative)
and green (positive)





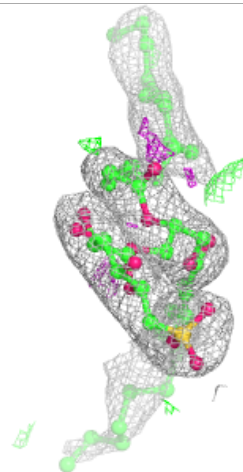
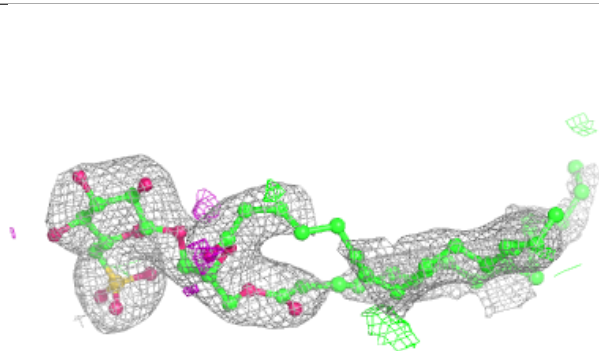
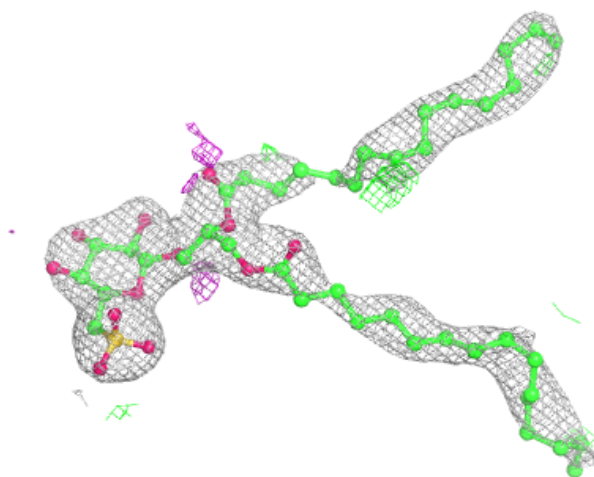
Electron density around CLA a 406 (A):

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



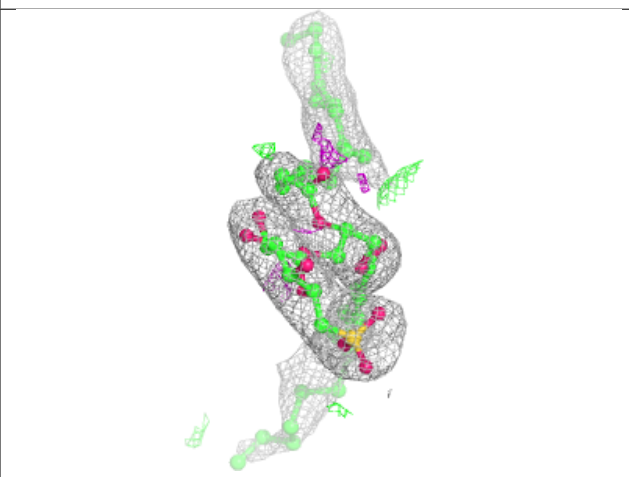
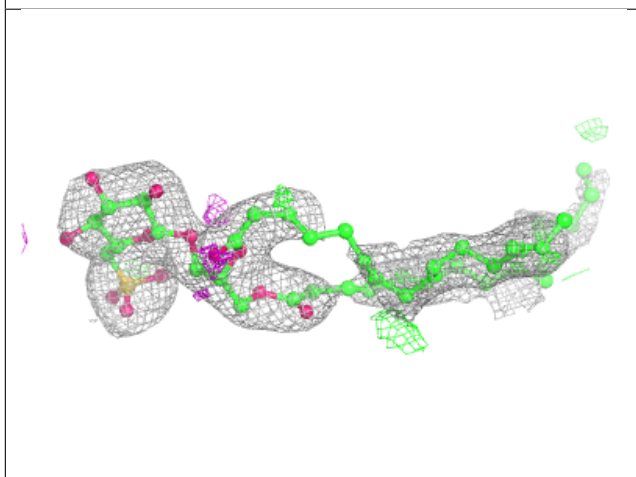
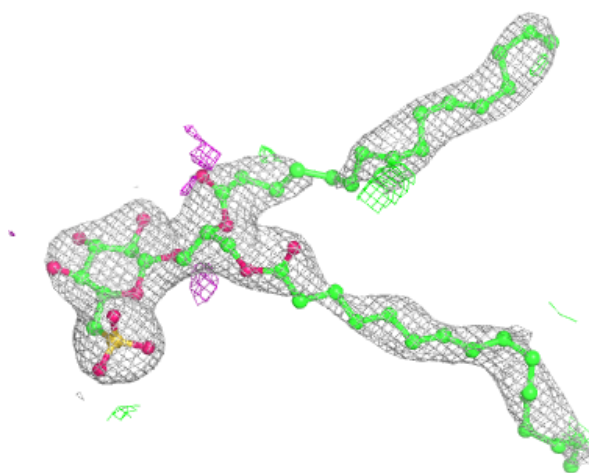
Electron density around SQD a 410 (A):

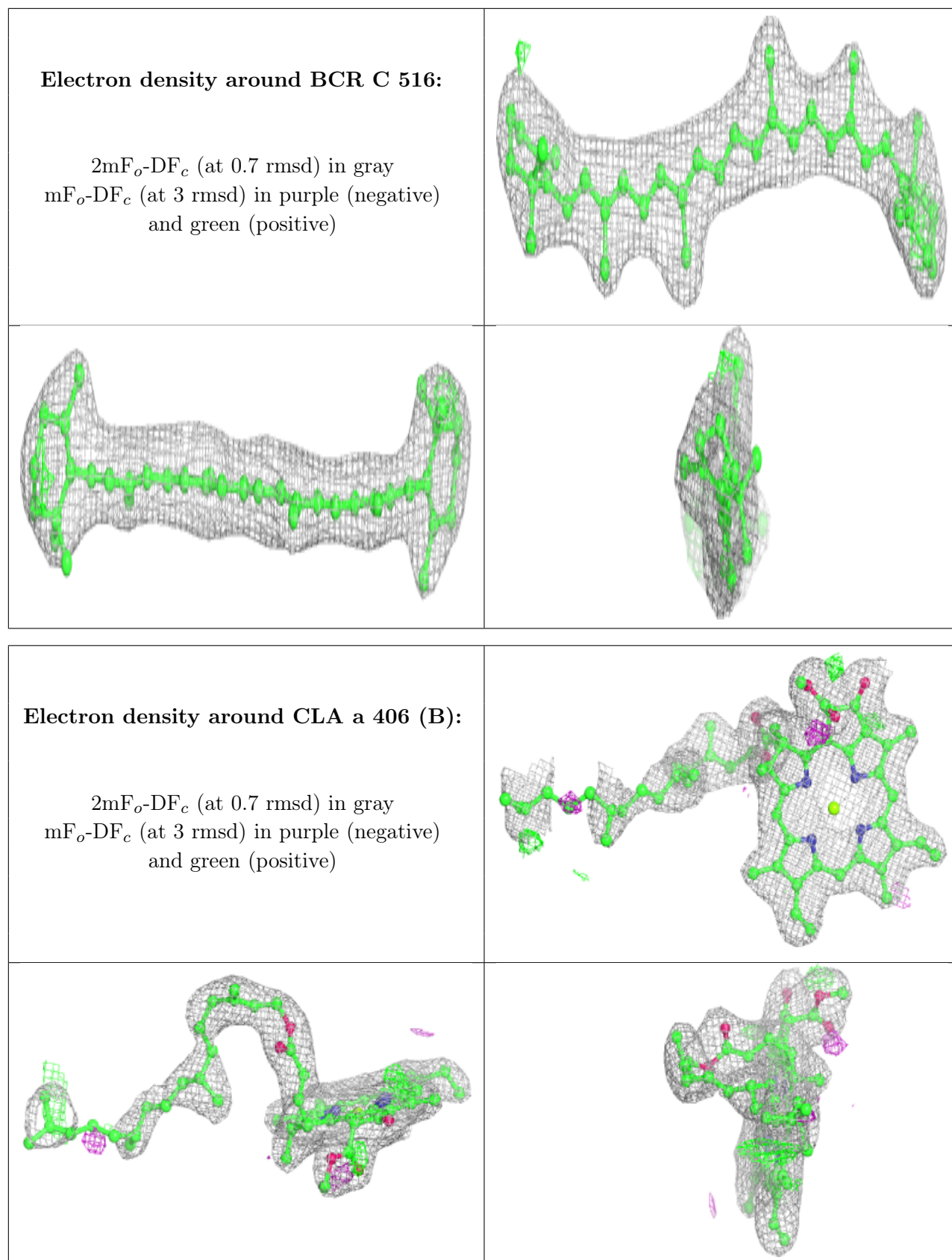
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SQD a 410 (B):

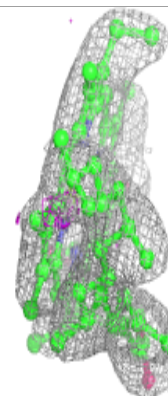
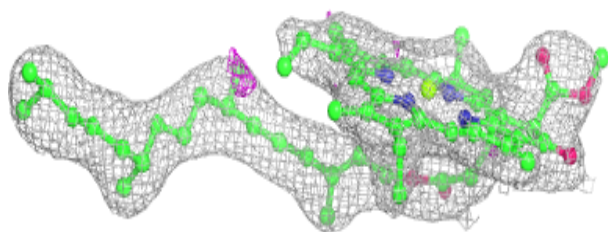
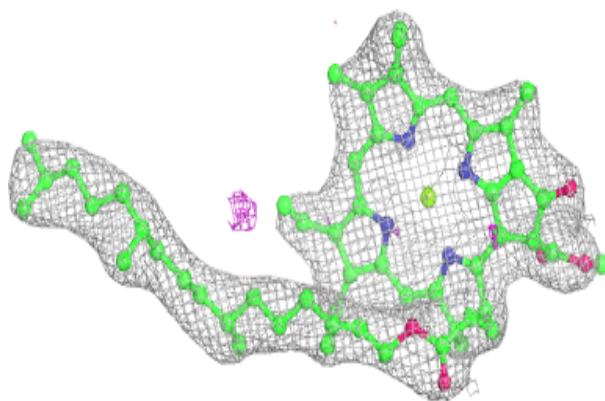
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



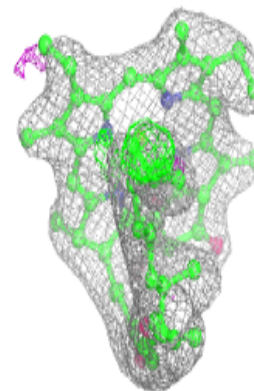
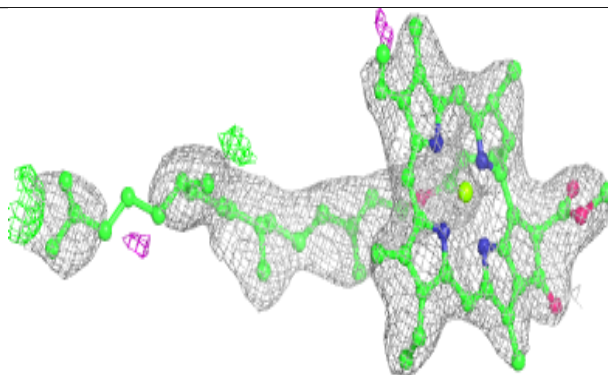
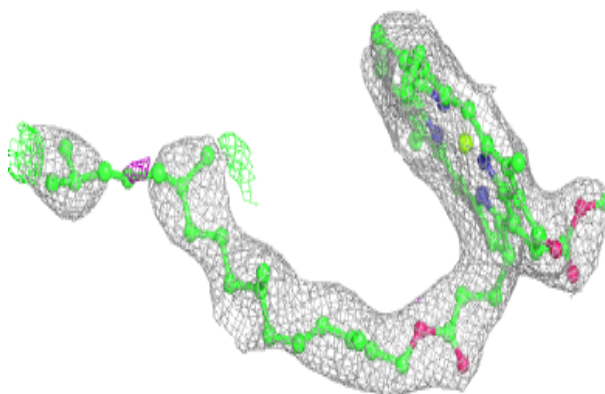


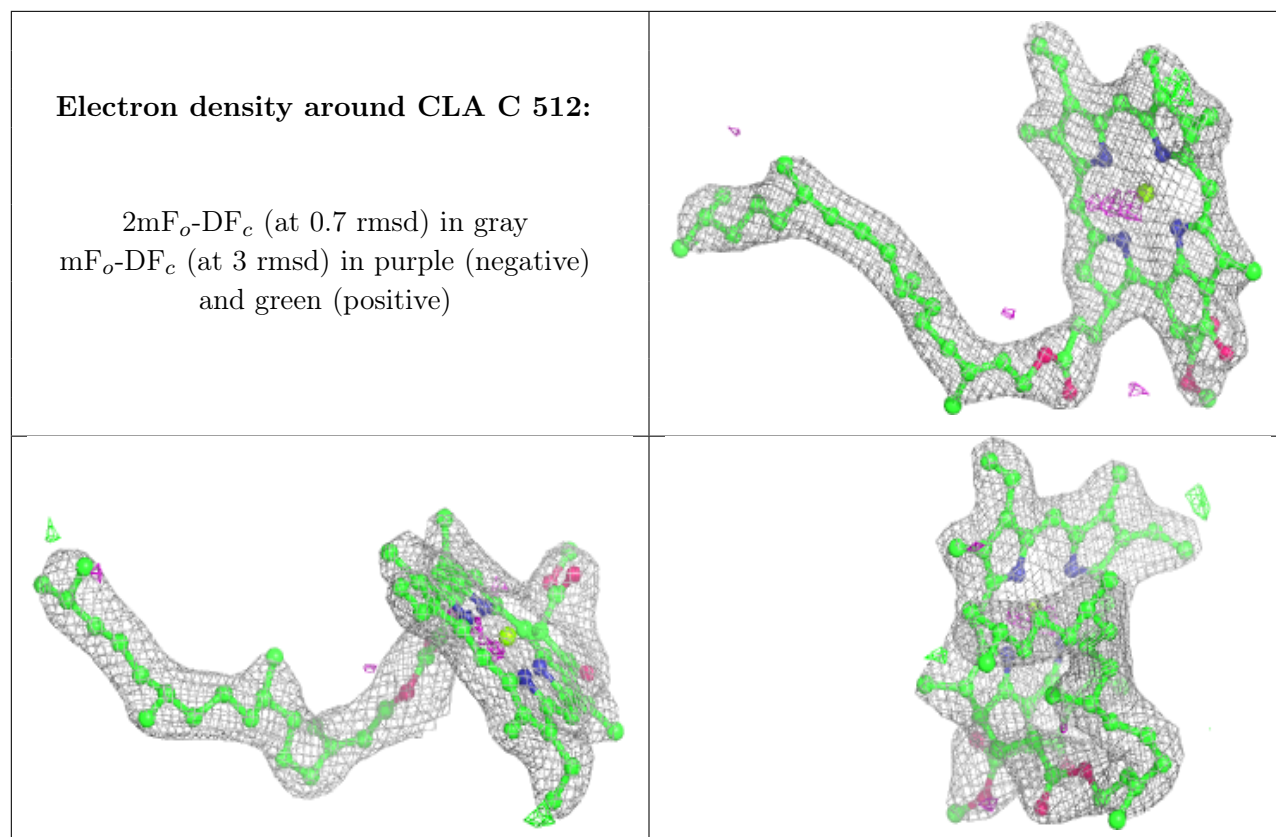
Electron density around CLA c 502:

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

**Electron density around CLA c 505:**

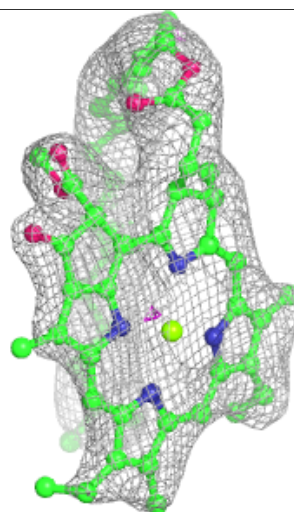
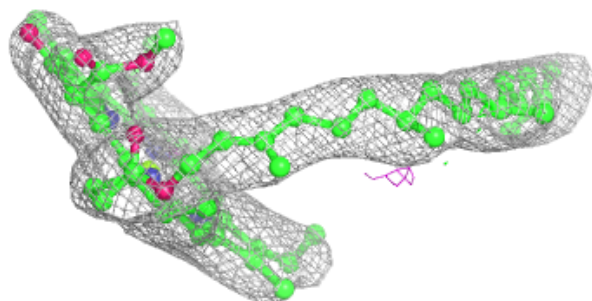
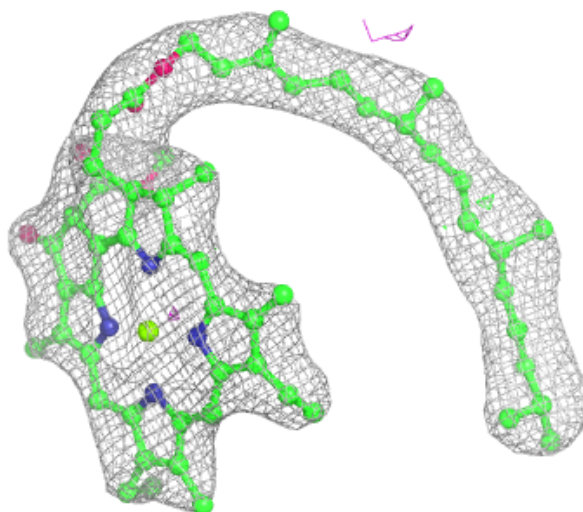
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





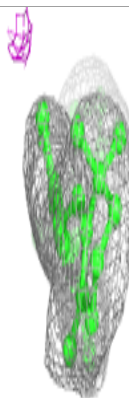
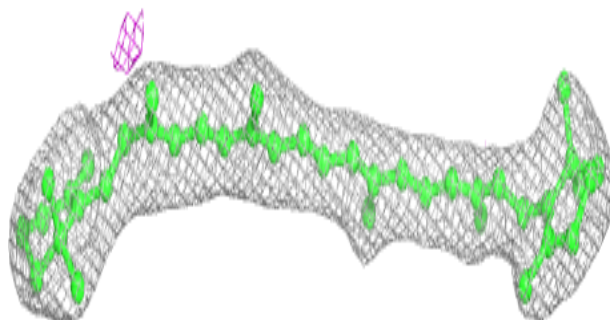
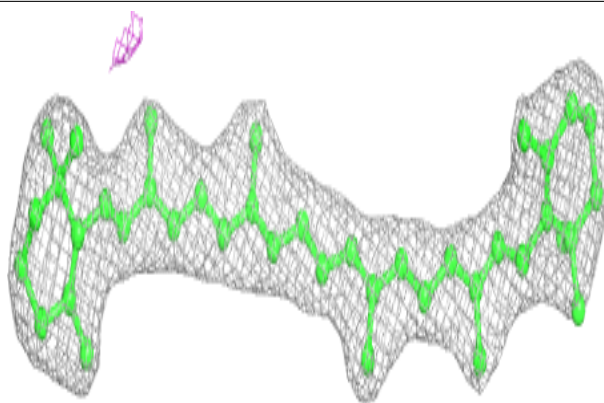
Electron density around CLA c 508:

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

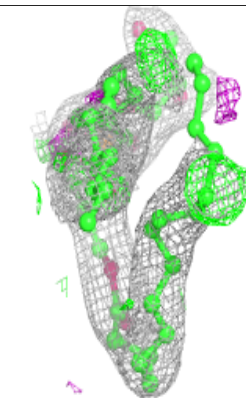
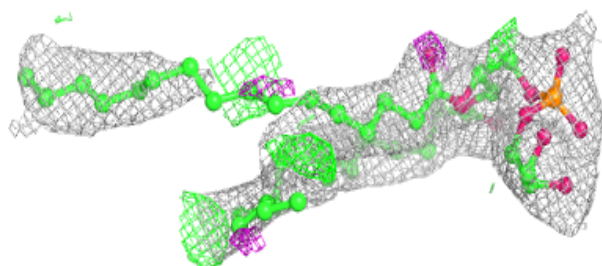
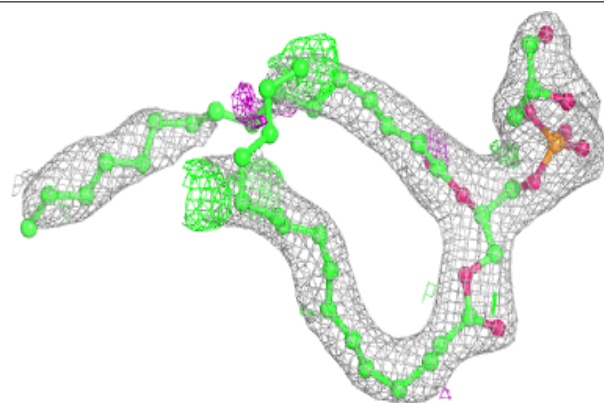


Electron density around BCR b 619:

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

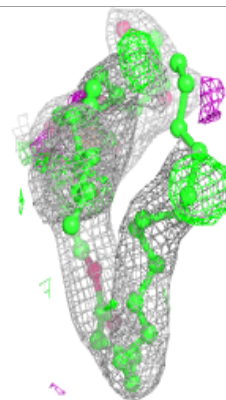
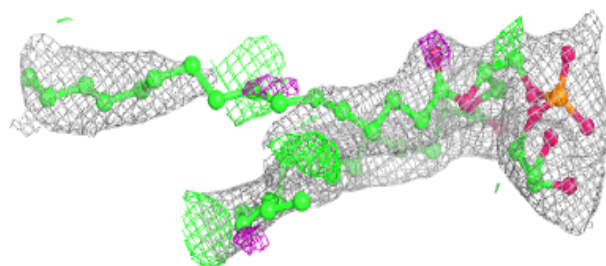
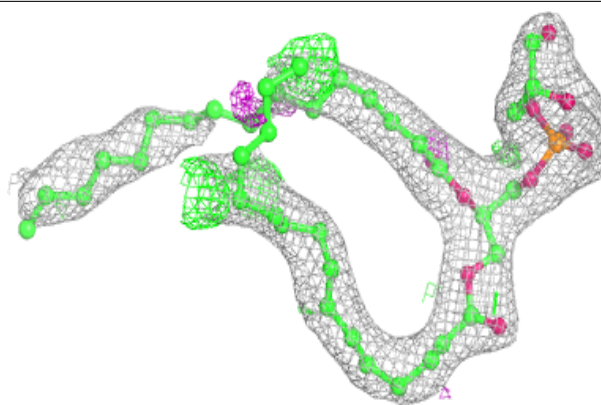
**Electron density around LHG D 407 (A):**

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

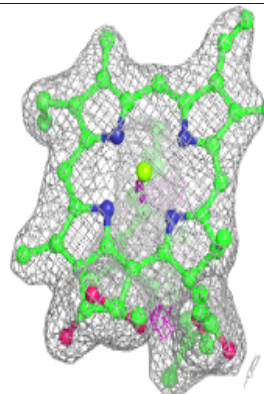
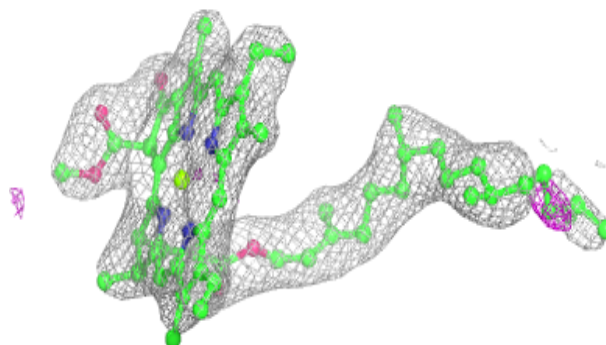
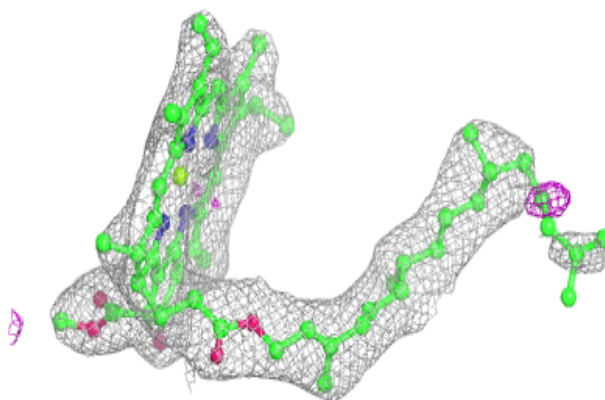


Electron density around LHG D 407 (B):

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

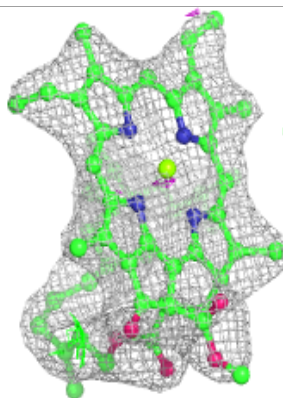
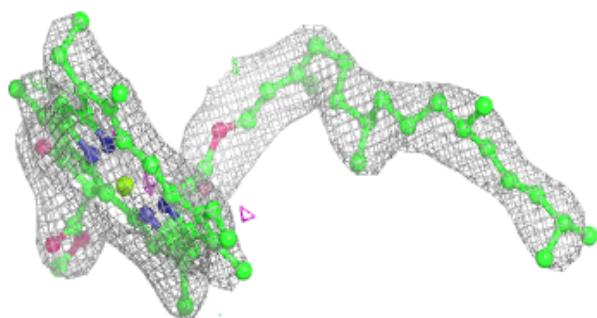
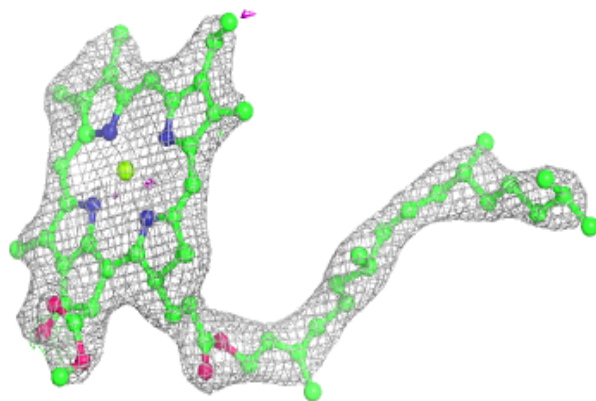
**Electron density around CLA c 509:**

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

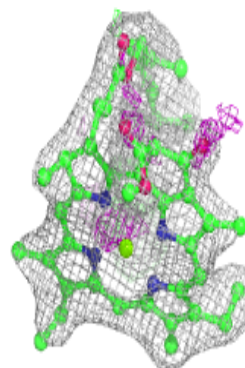
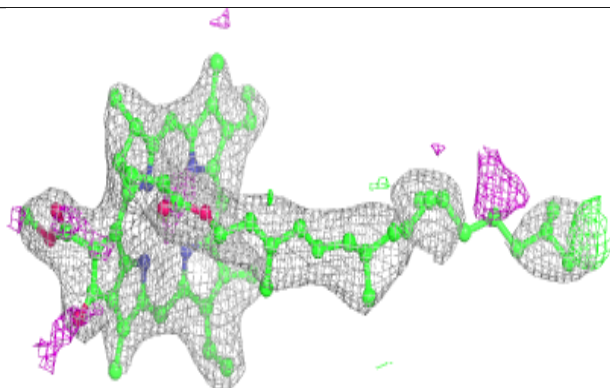
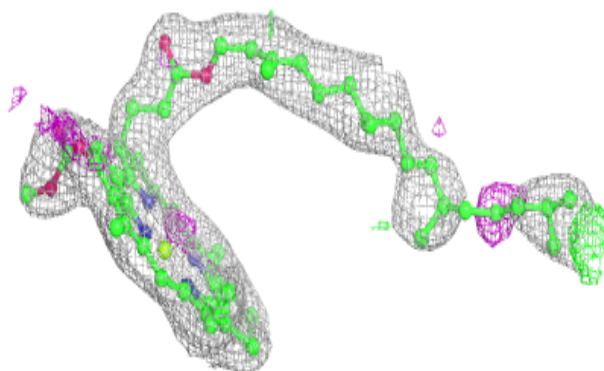


Electron density around CLA c 512:

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

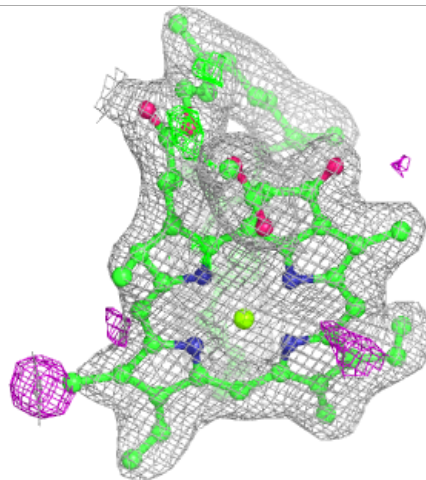
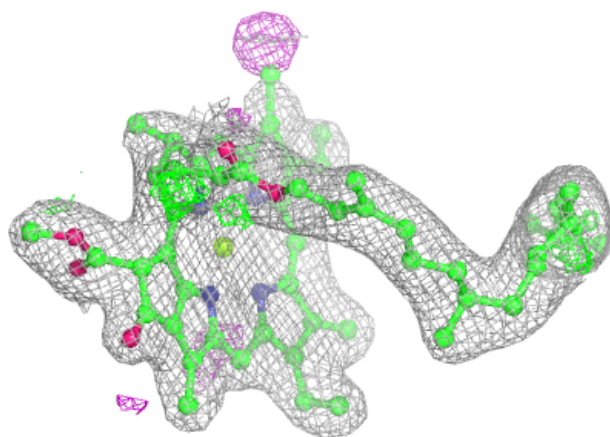
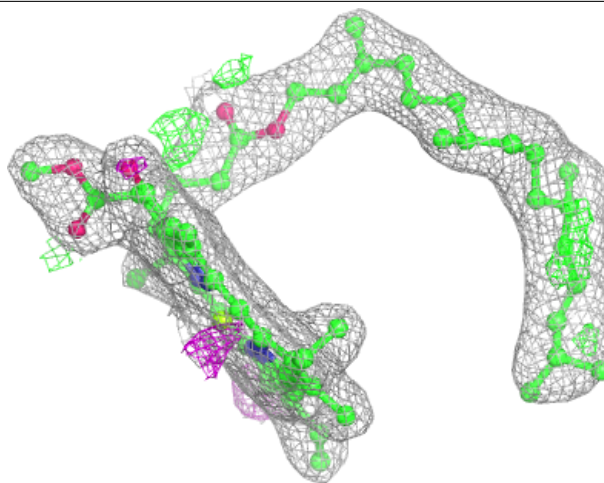
**Electron density around CLA C 505:**

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



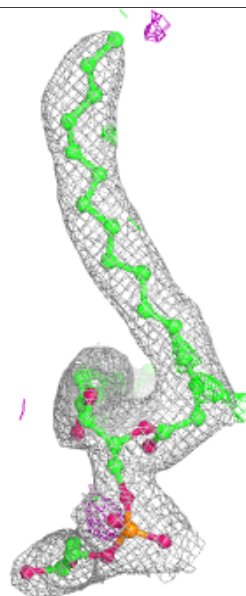
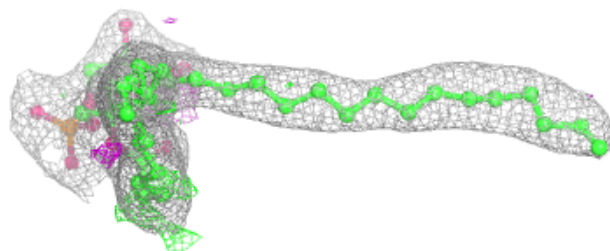
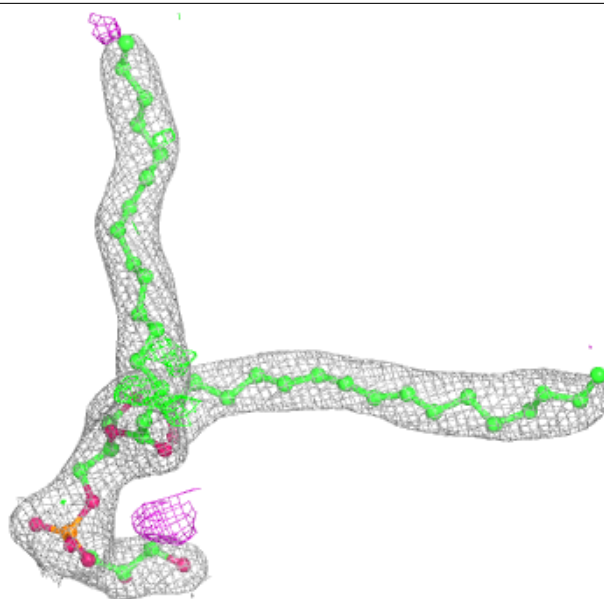
Electron density around CLA B 611:

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



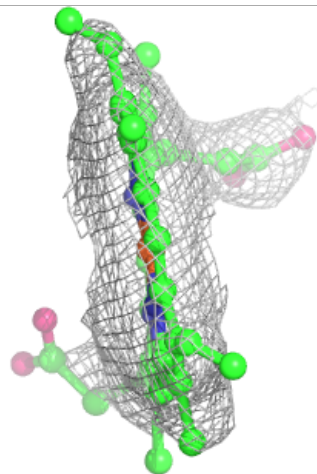
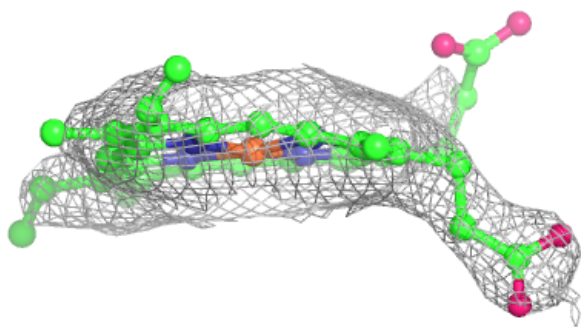
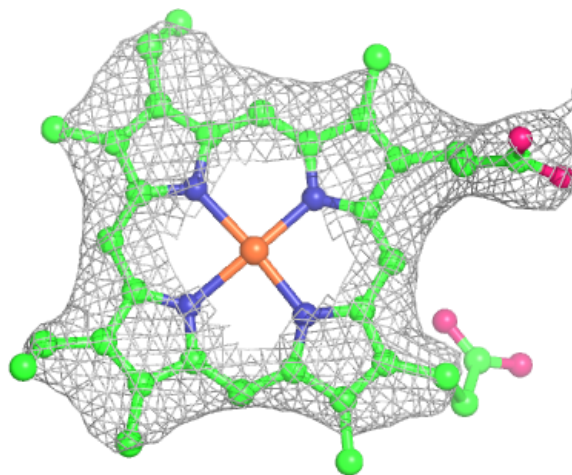
Electron density around LHG b 630 (A):

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



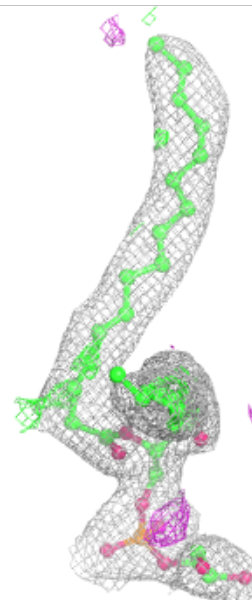
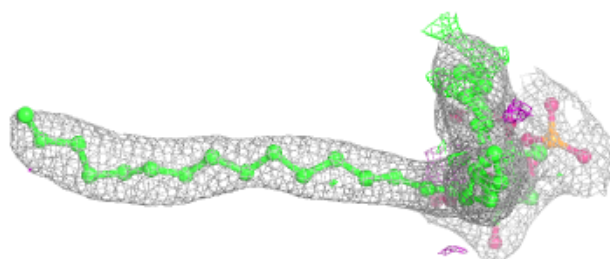
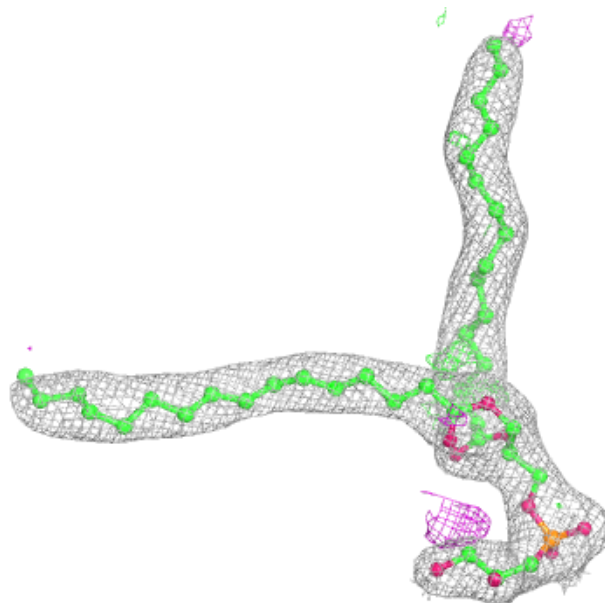
Electron density around HEM f 101:

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



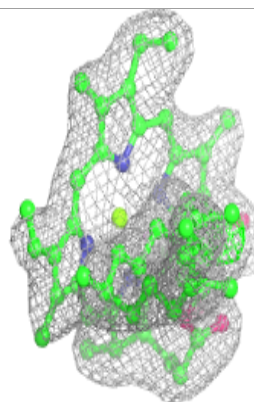
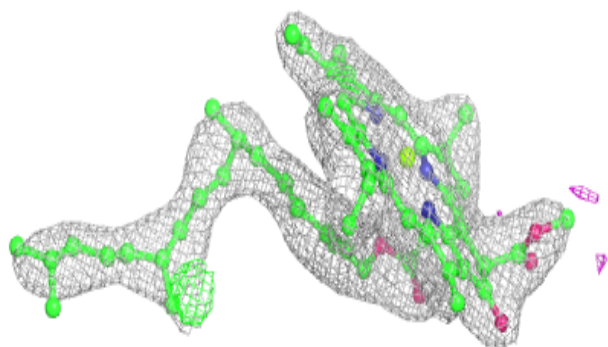
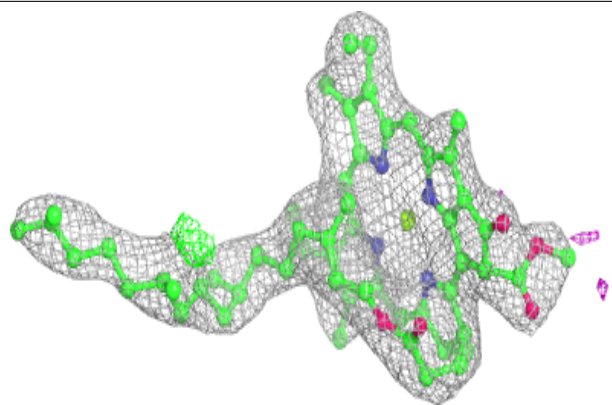
Electron density around LHG b 630 (B):

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

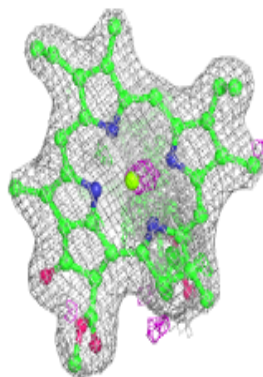
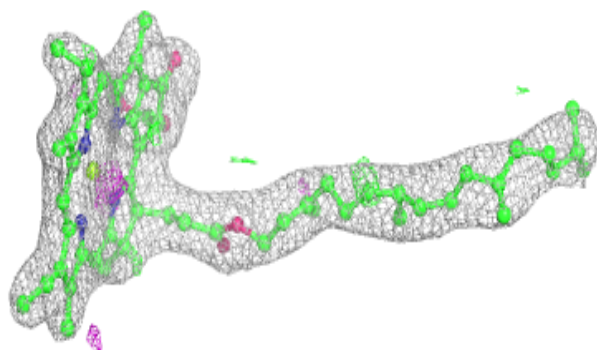
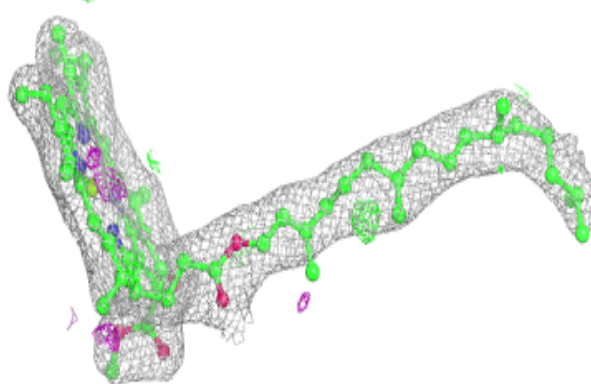


Electron density around CLA c 506:

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

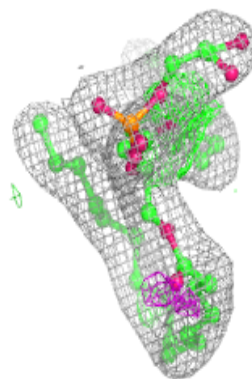
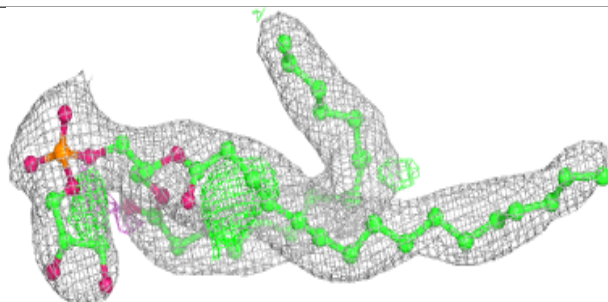
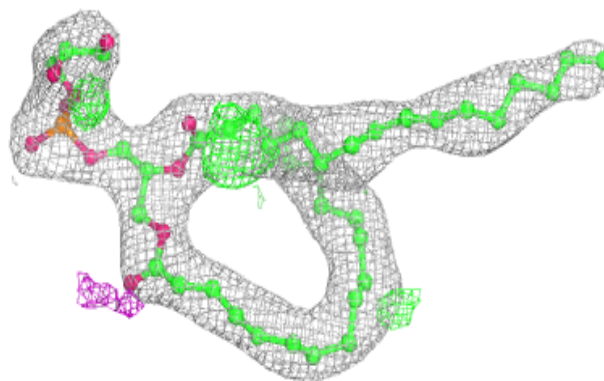
**Electron density around CLA b 604:**

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

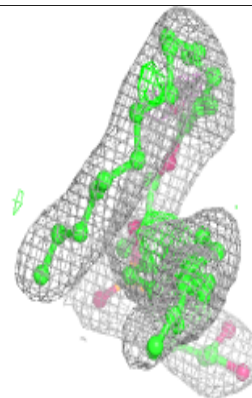
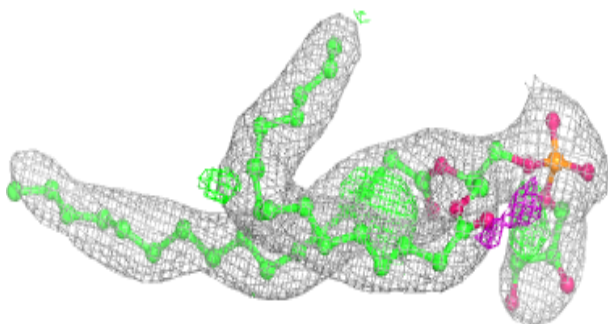
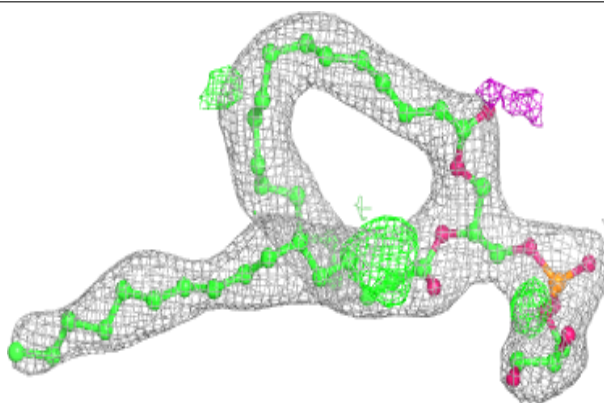


Electron density around LHG d 412 (A):

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

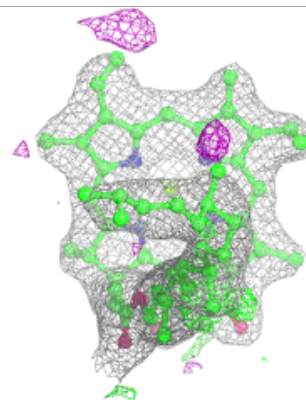
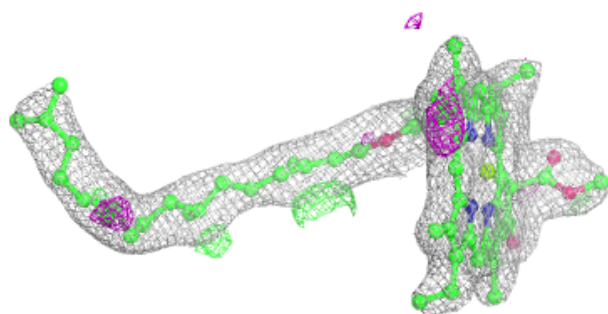
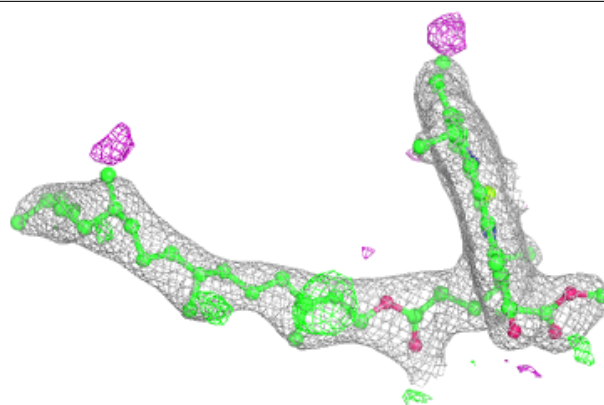
**Electron density around LHG d 412 (B):**

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

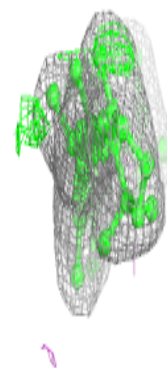
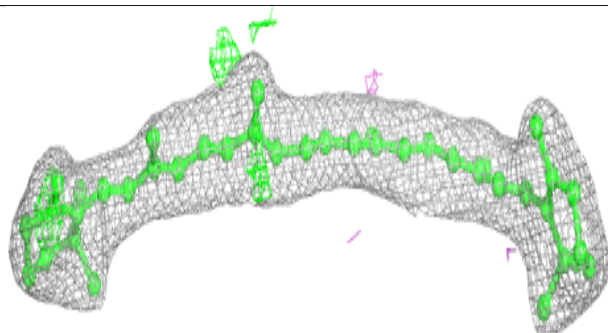
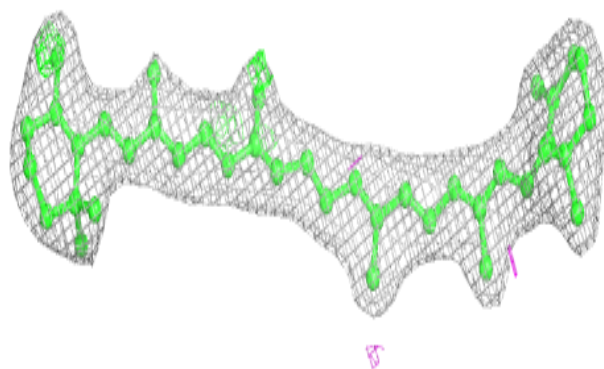


Electron density around CLA b 605:

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

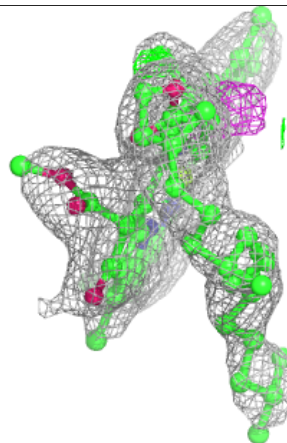
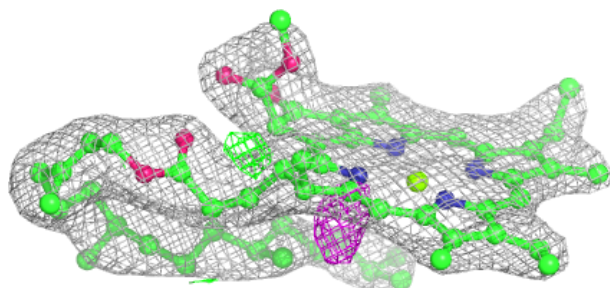
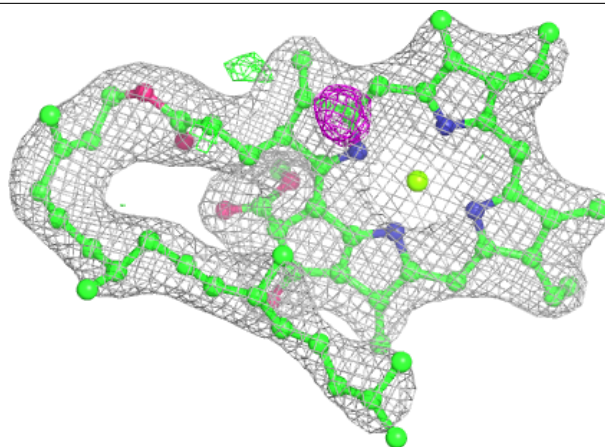
**Electron density around BCR T 102:**

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

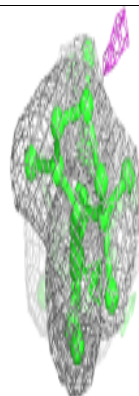
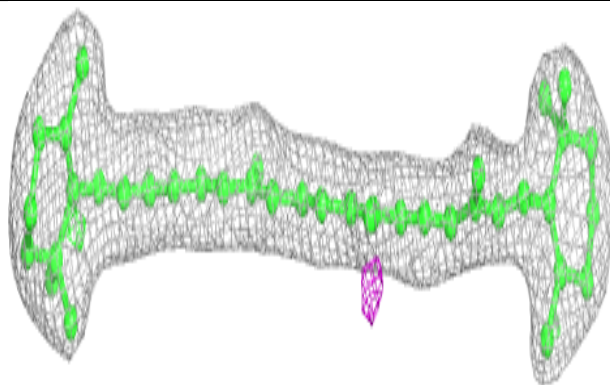
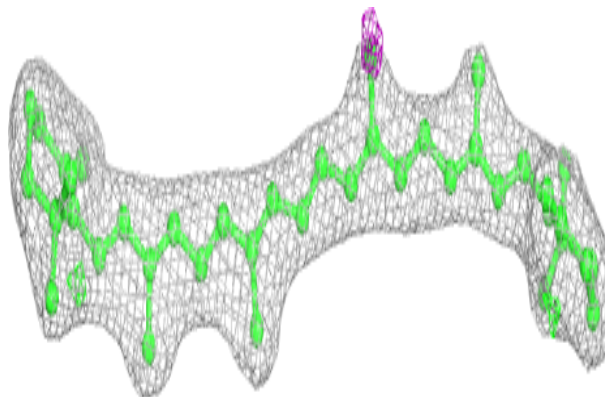


Electron density around CLA C 510:

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

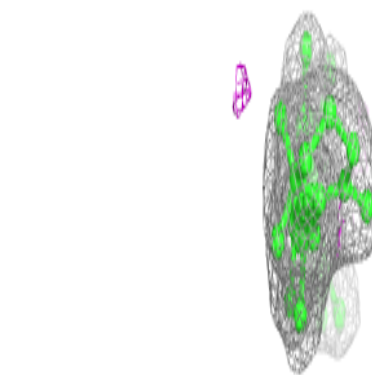
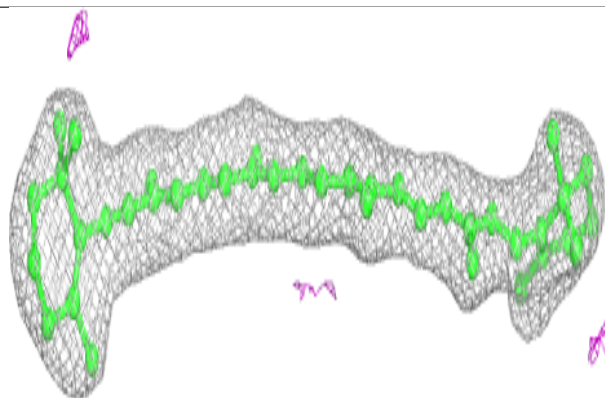
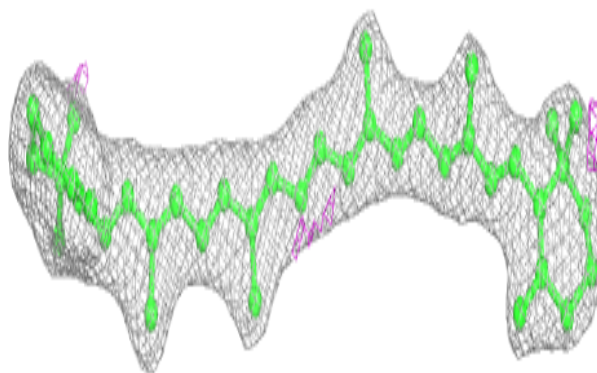
**Electron density around BCR a 409:**

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

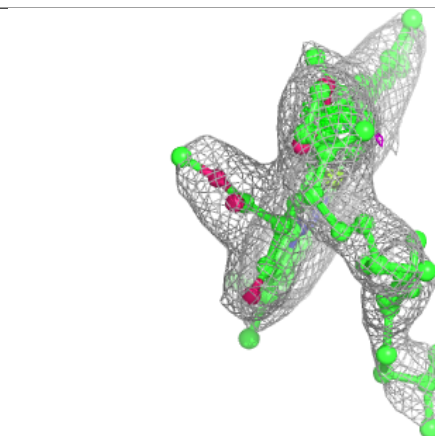
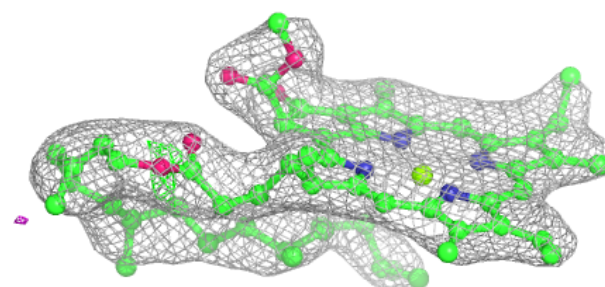
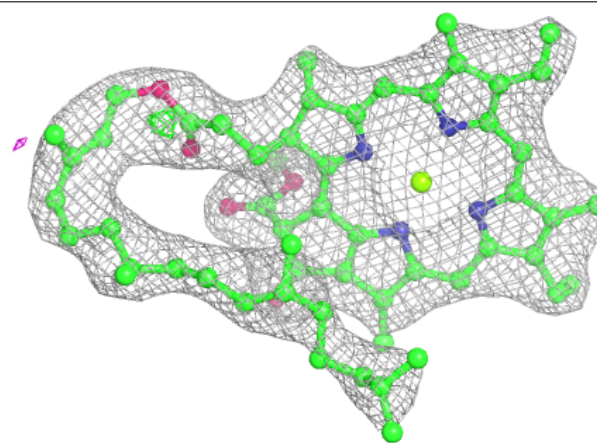


Electron density around BCR b 617:

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

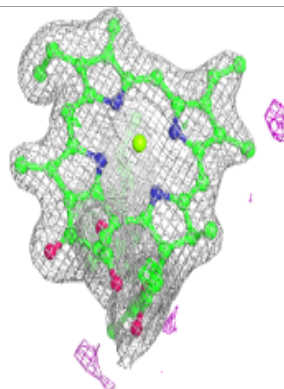
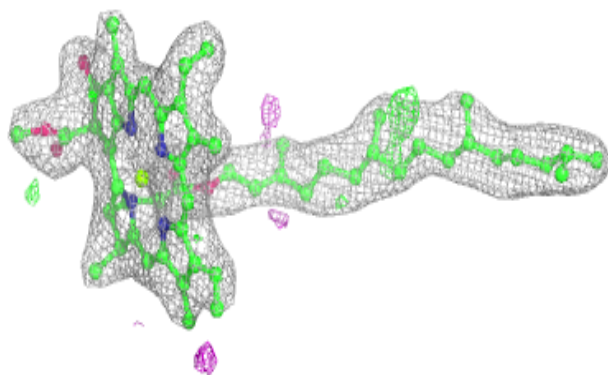
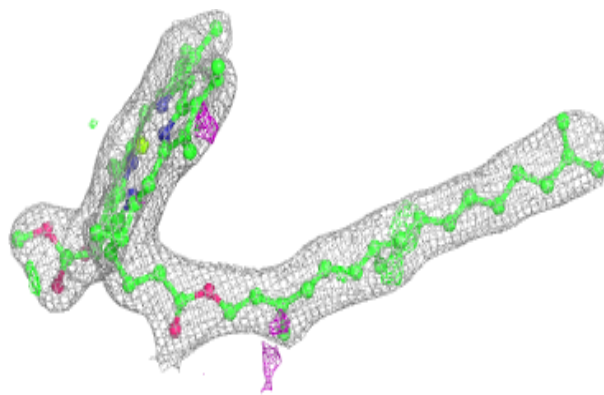
**Electron density around CLA c 510:**

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



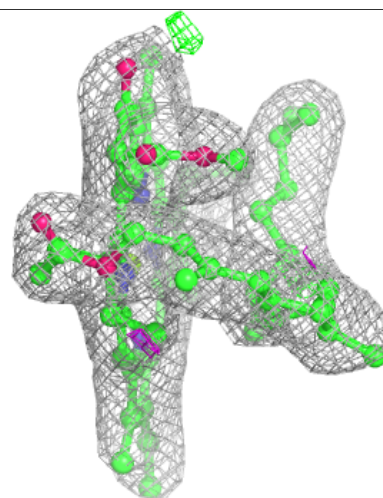
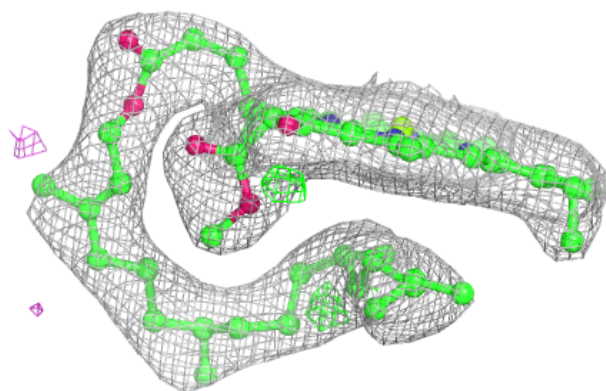
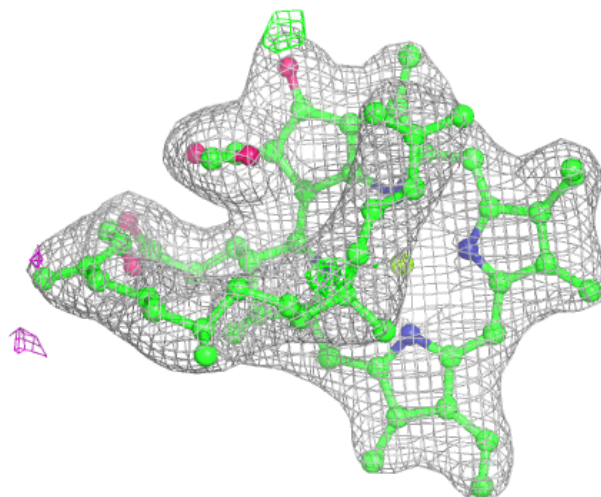
Electron density around CLA b 607:

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



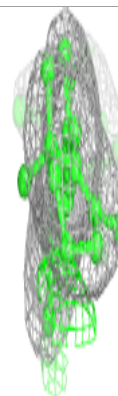
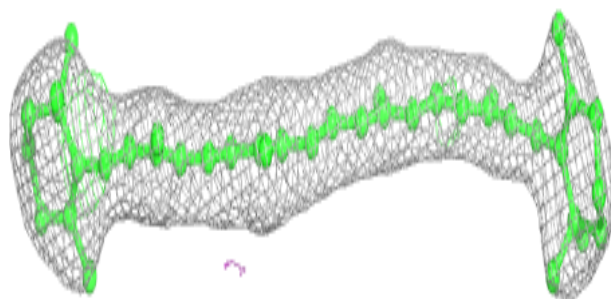
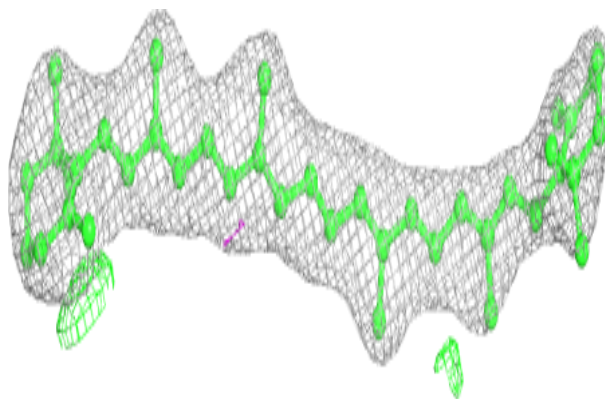
Electron density around CLA C 511:

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



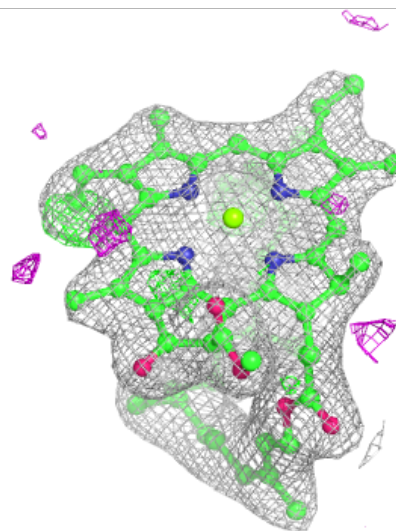
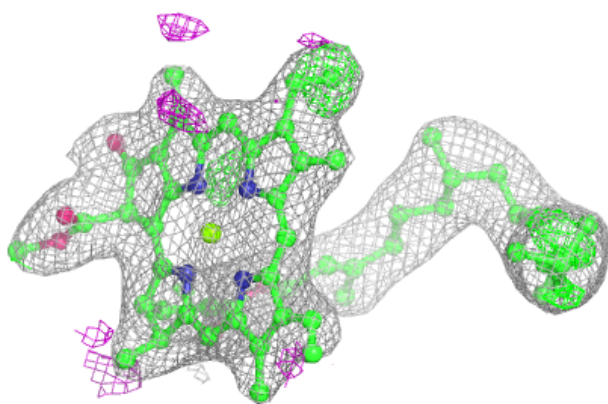
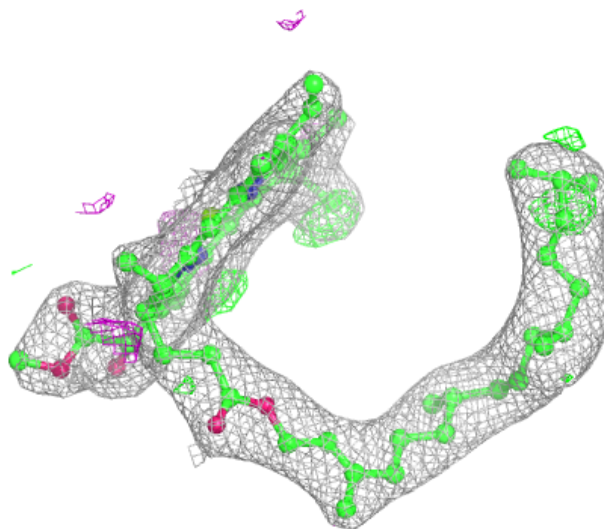
Electron density around BCR c 516:

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



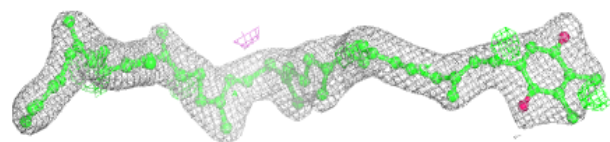
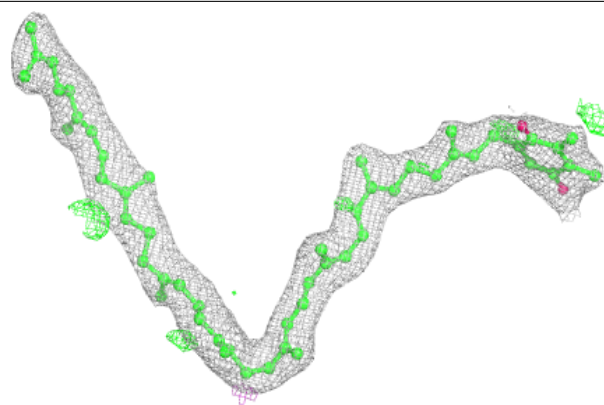
Electron density around CLA b 611:

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

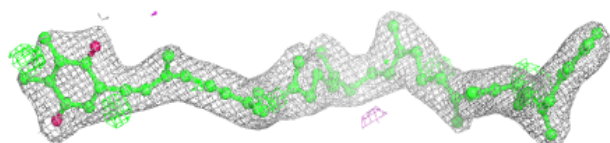
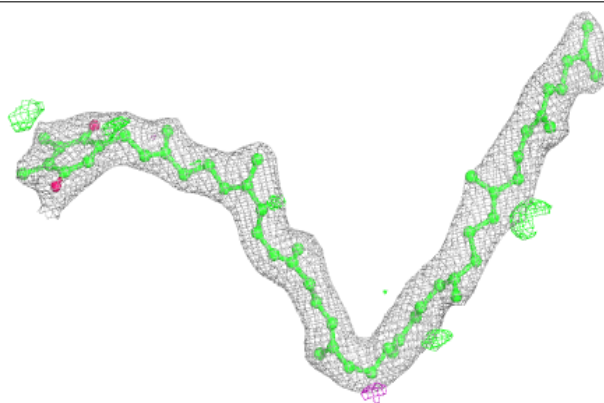


Electron density around PL9 D 405 (A):

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

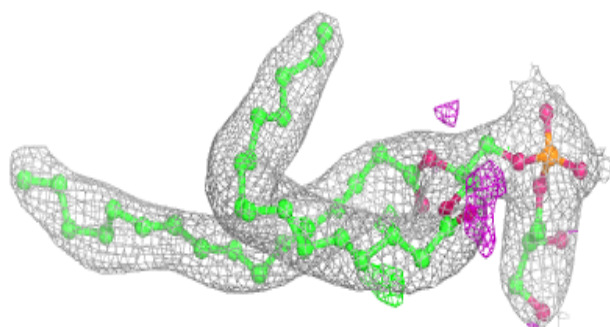
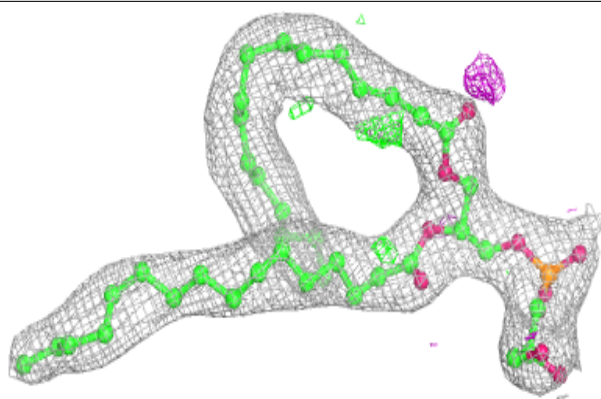
**Electron density around PL9 D 405 (B):**

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

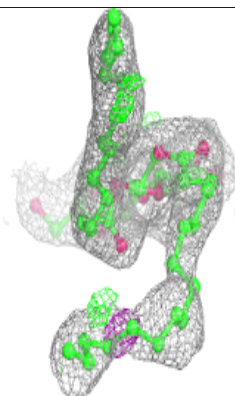
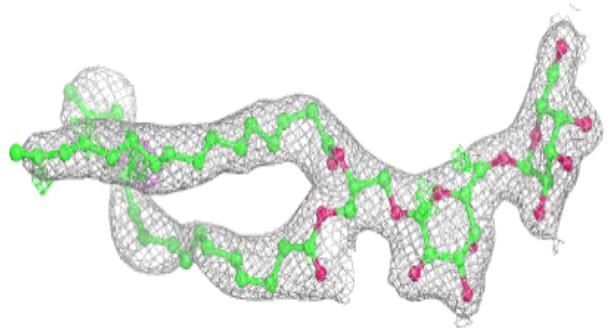
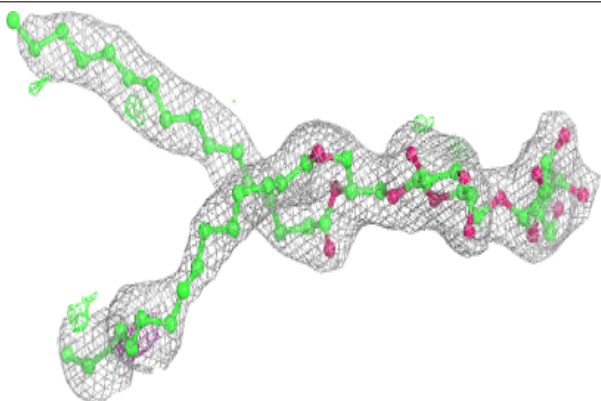


Electron density around LHG A 419 (A):

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

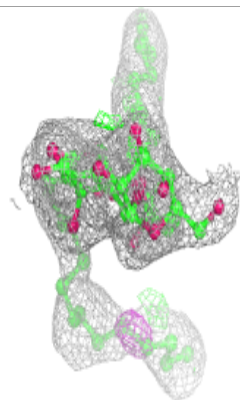
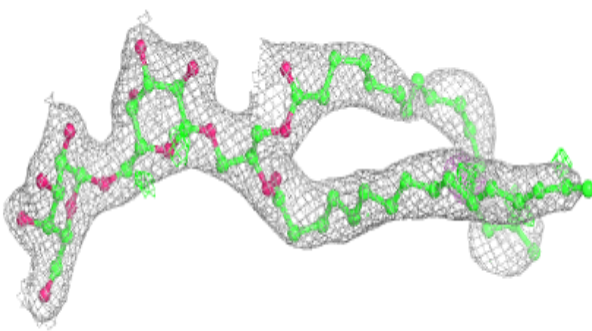
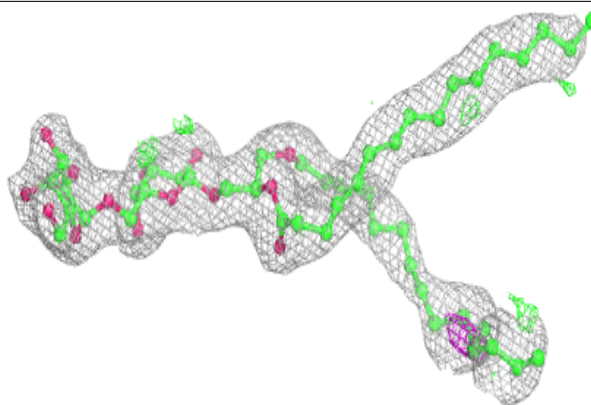
**Electron density around DGD c 517 (A):**

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

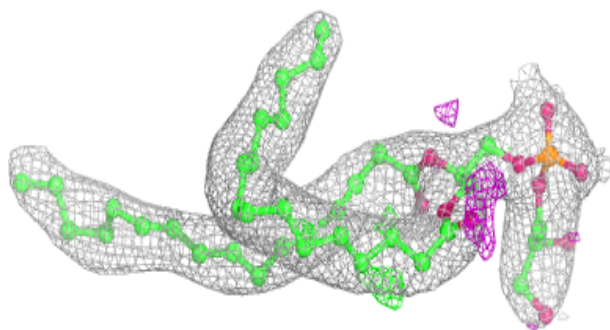
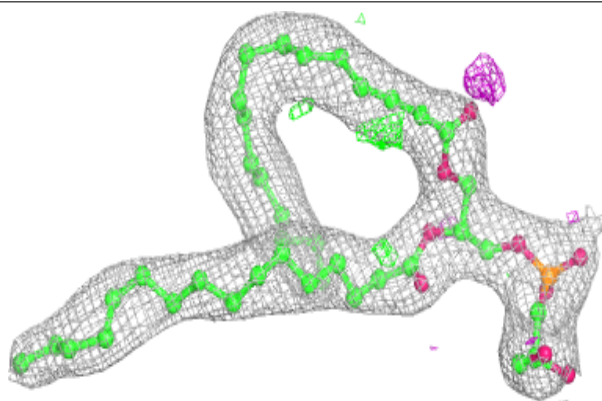


Electron density around DGD c 517 (B):

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

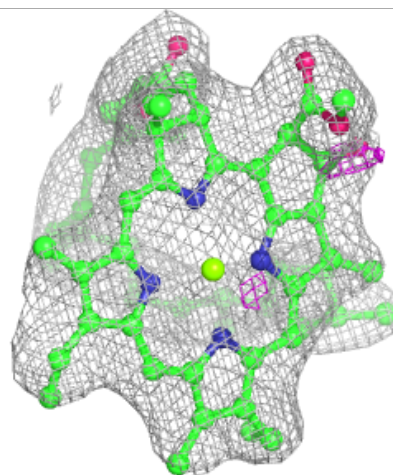
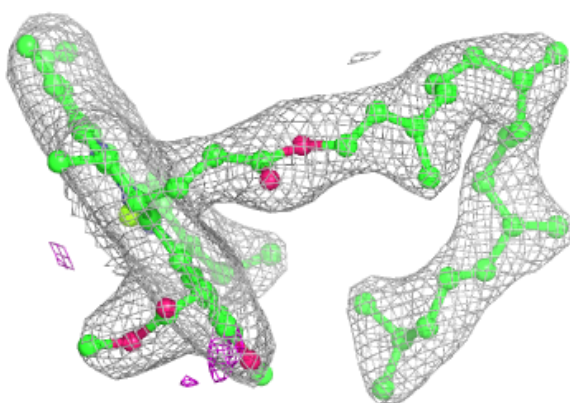
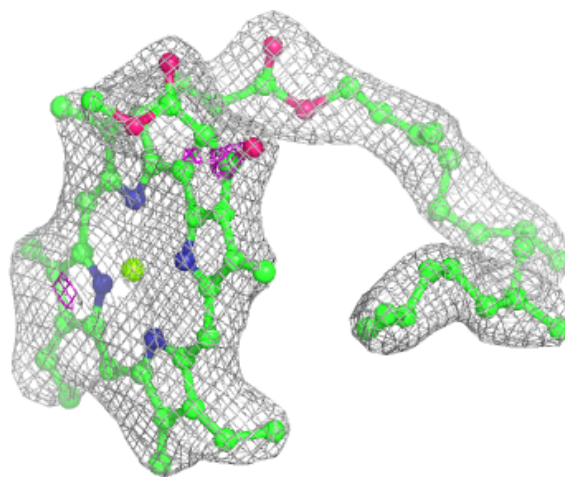
**Electron density around LHG A 419 (B):**

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



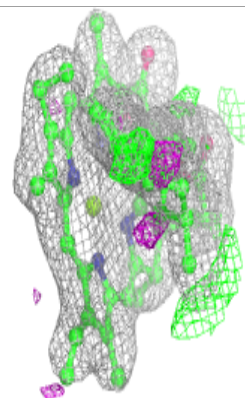
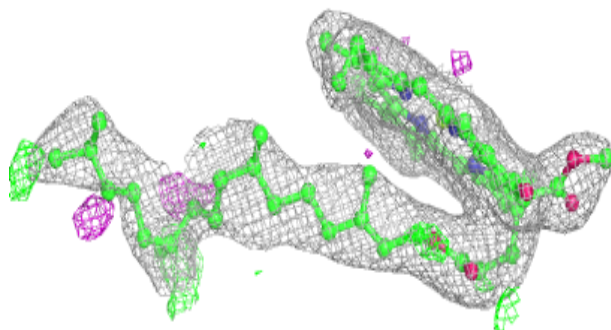
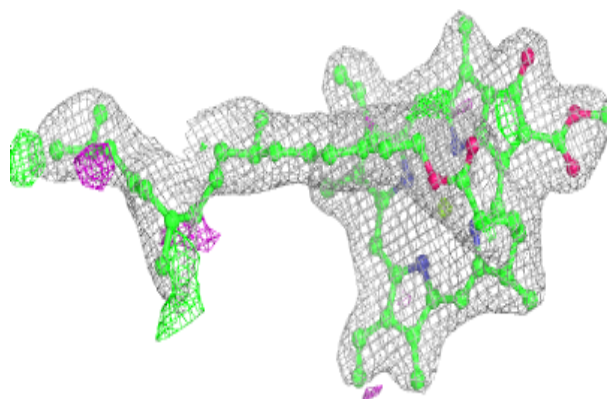
Electron density around CLA C 504:

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



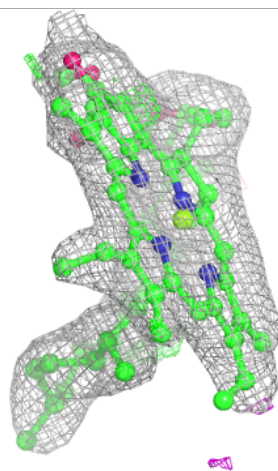
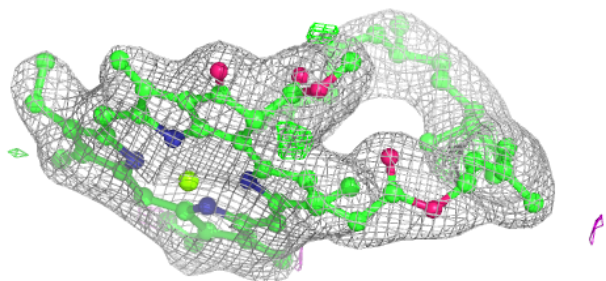
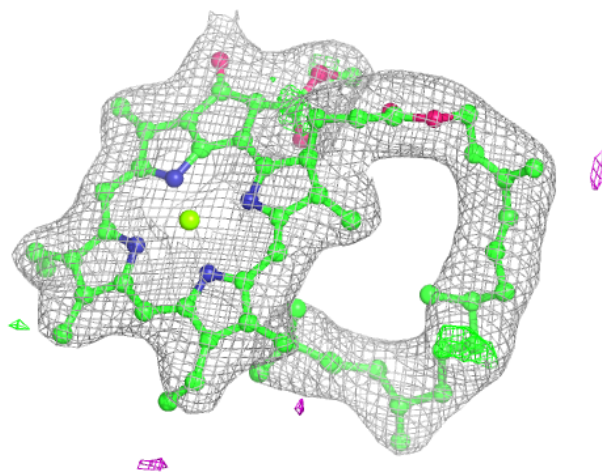
Electron density around CLA b 614:

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



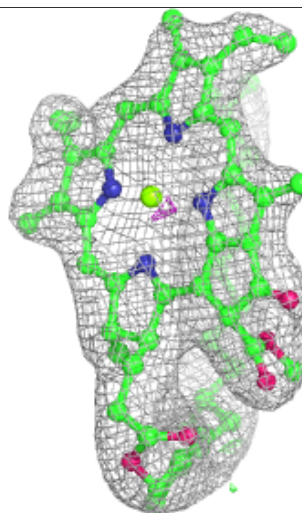
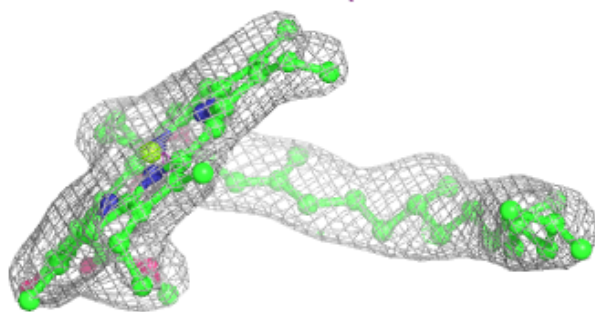
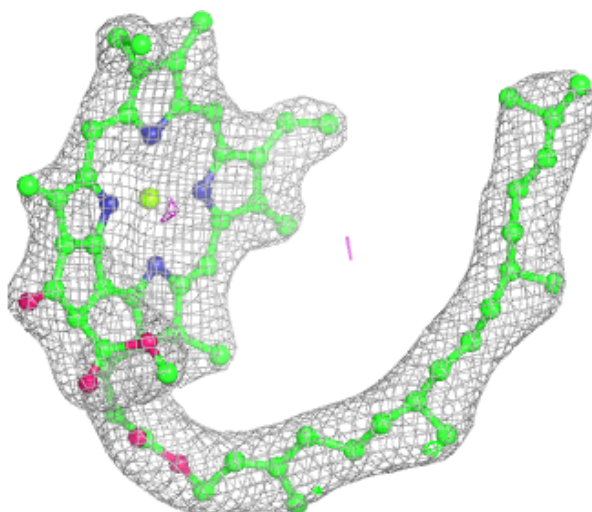
Electron density around CLA b 615:

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



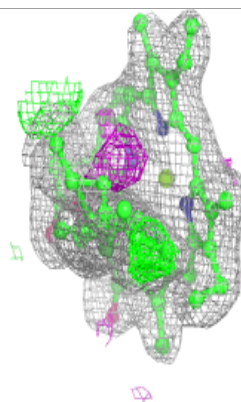
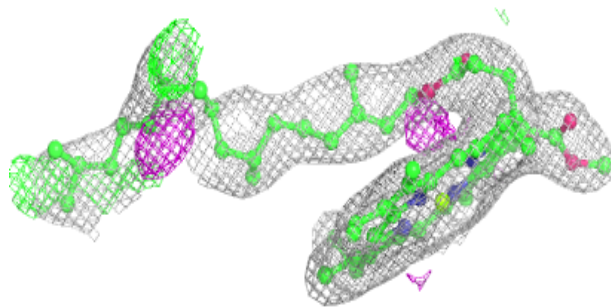
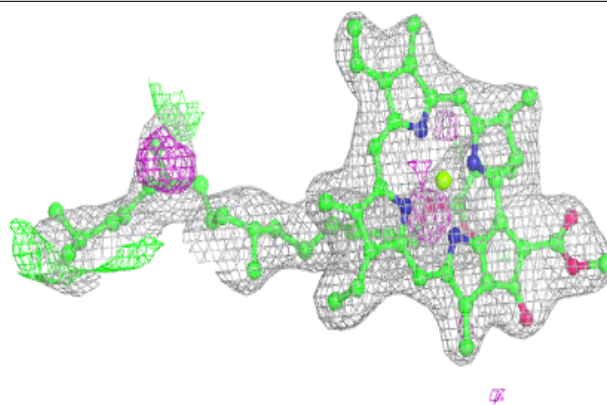
Electron density around CLA C 508:

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

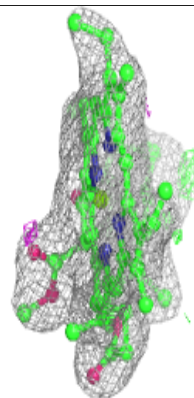
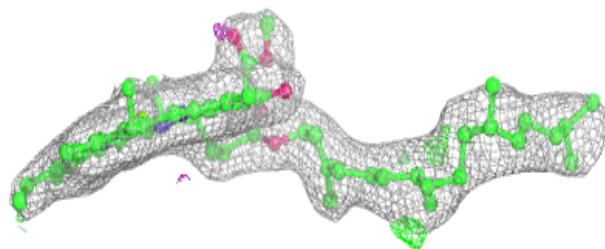
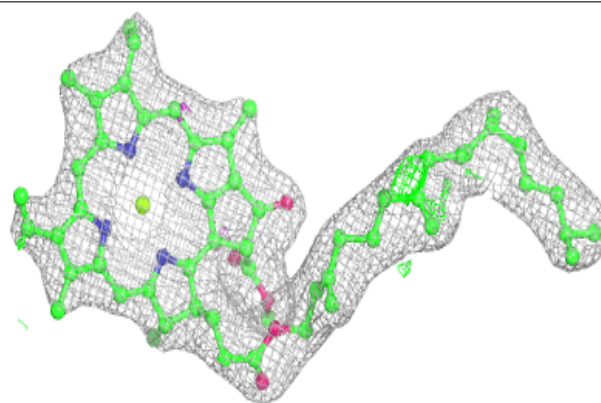


Electron density around CLA B 614:

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

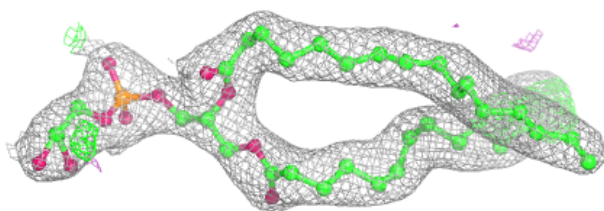
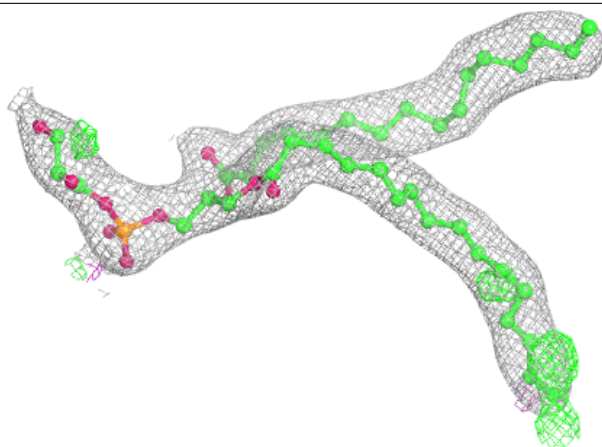
**Electron density around CLA b 602:**

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



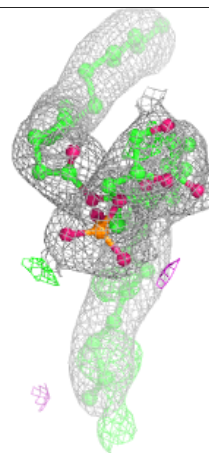
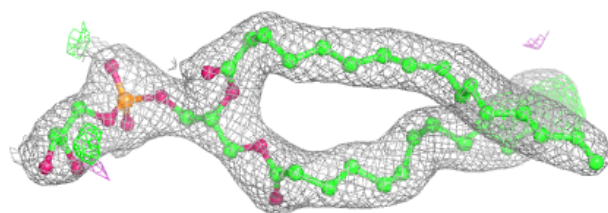
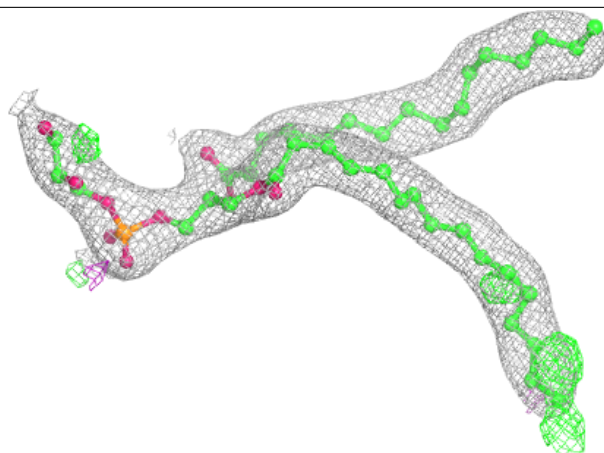
Electron density around LHG d 406 (A):

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



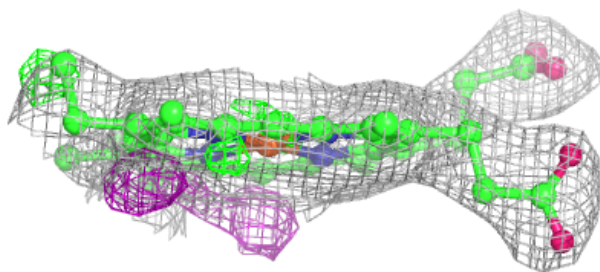
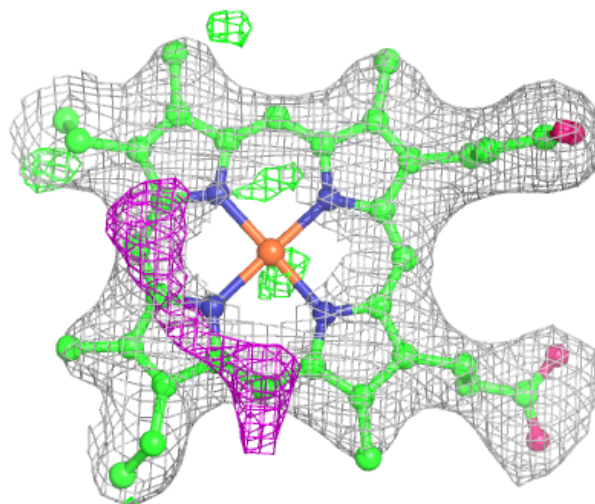
Electron density around LHG d 406 (B):

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



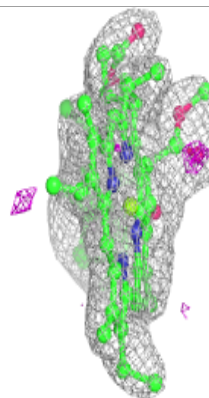
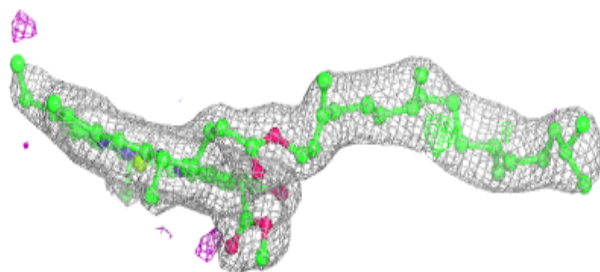
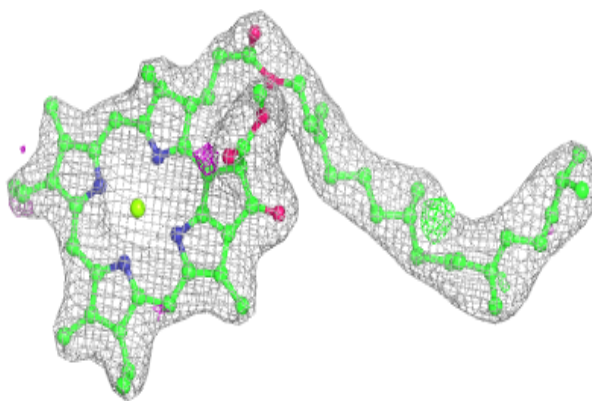
Electron density around HEC v 201:

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

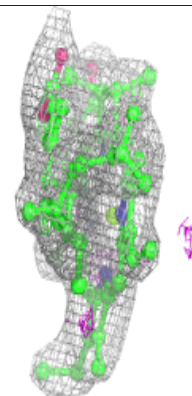
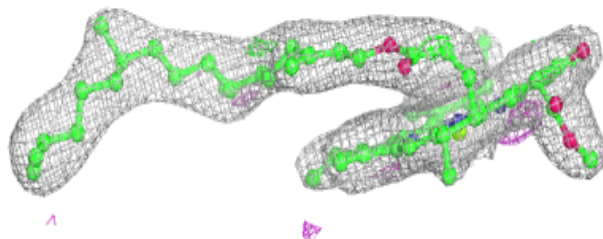
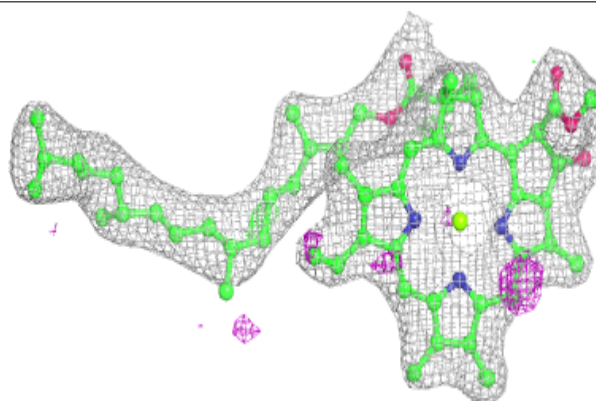


Electron density around CLA B 602:

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

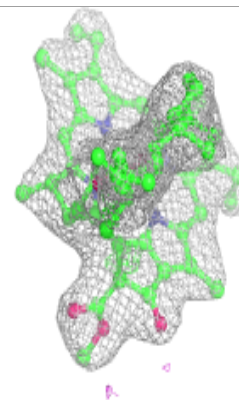
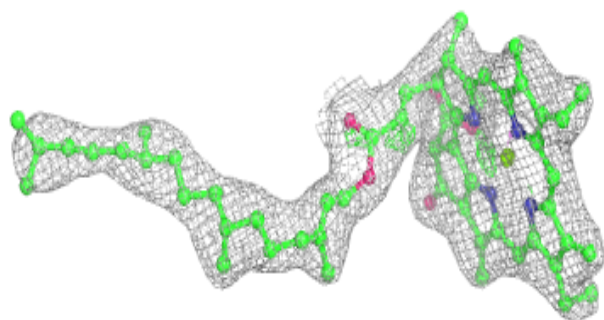
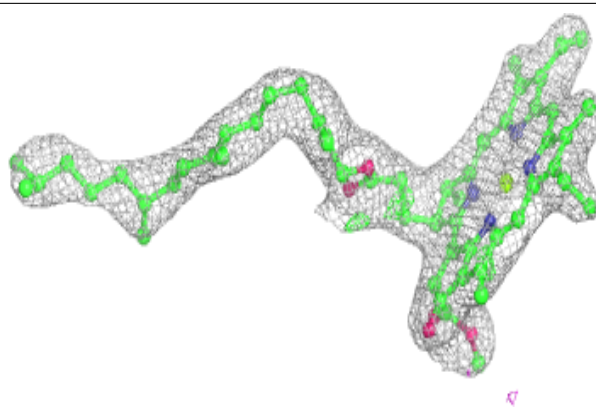
**Electron density around CLA B 603:**

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



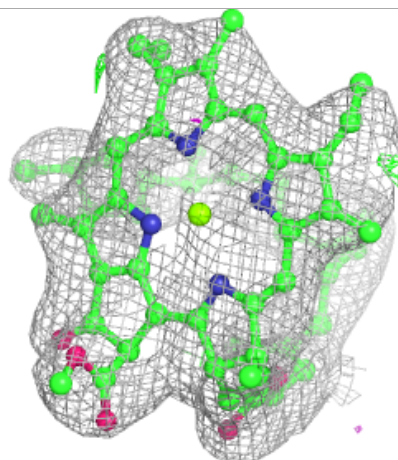
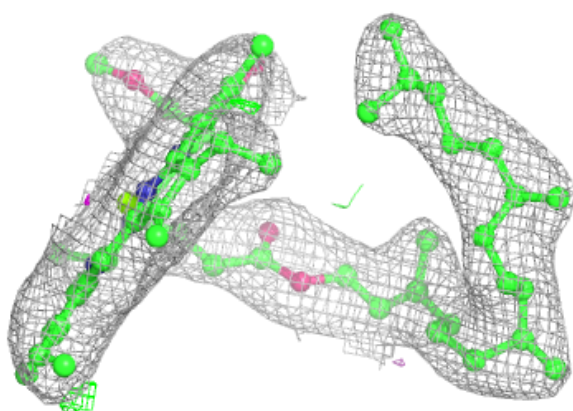
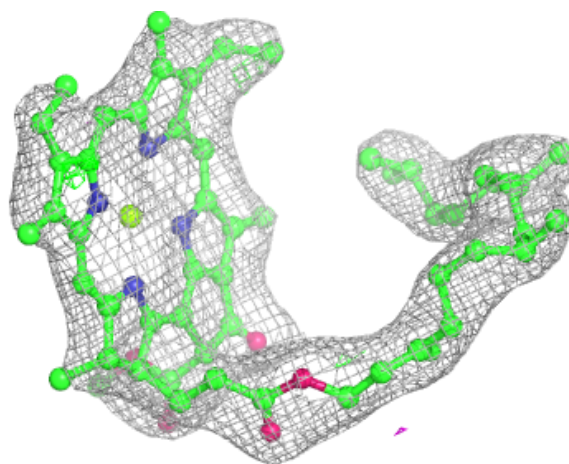
Electron density around CLA c 503:

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



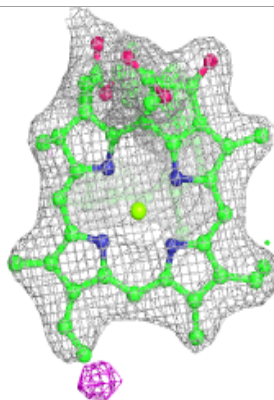
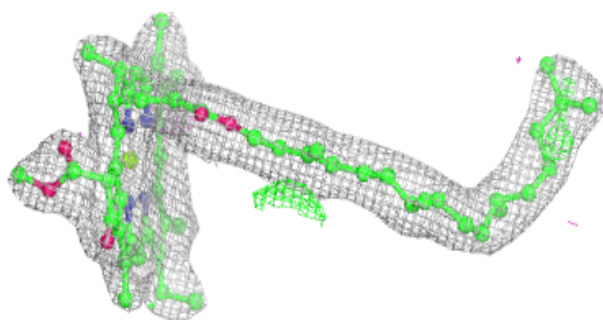
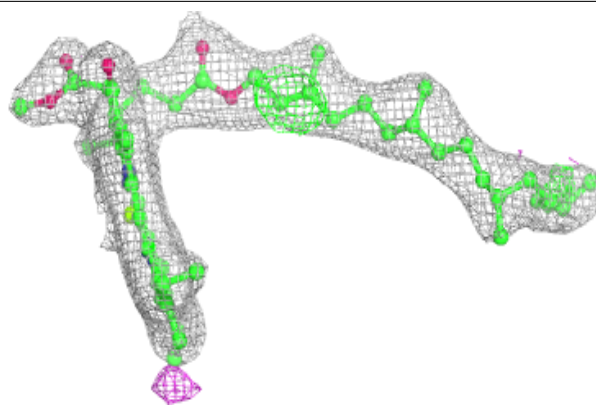
Electron density around CLA c 504:

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

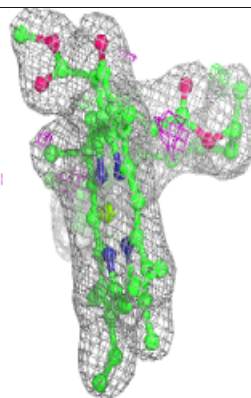
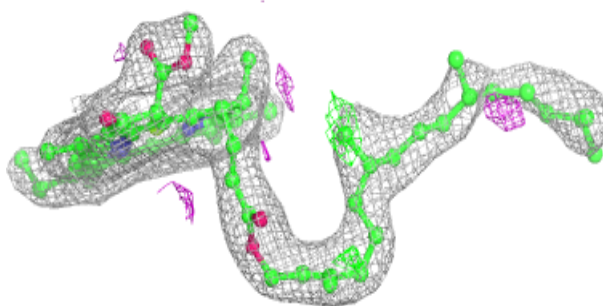
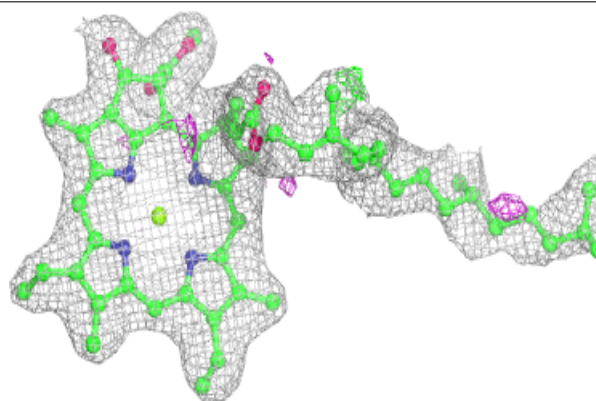


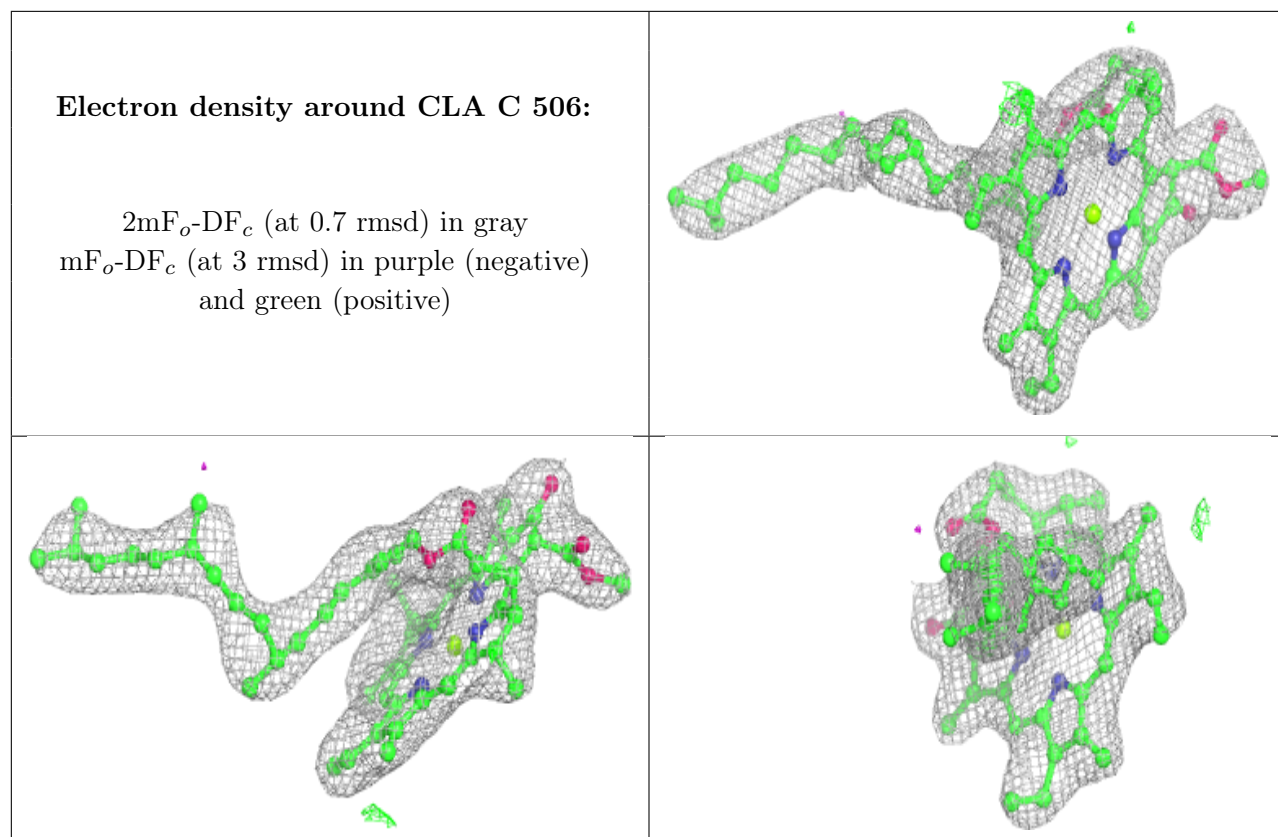
Electron density around CLA B 605:

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

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

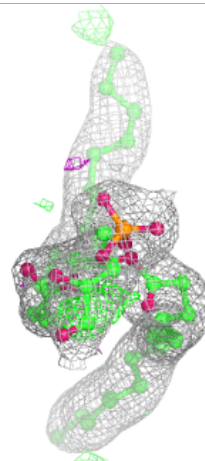
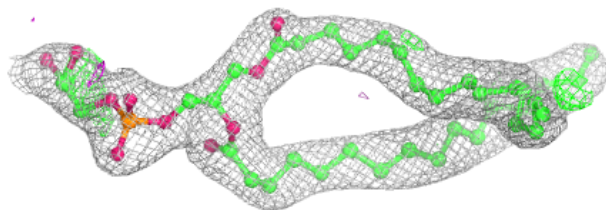
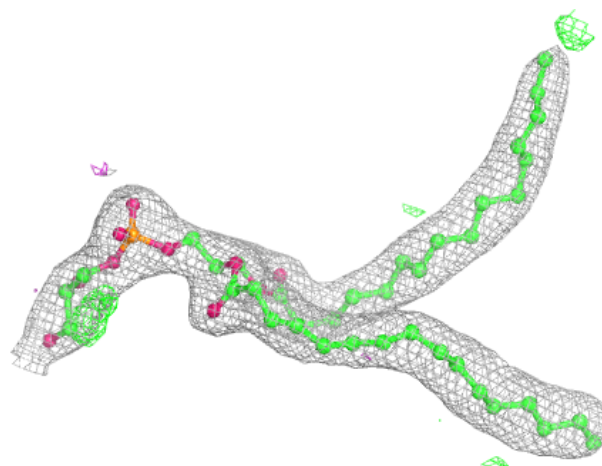
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





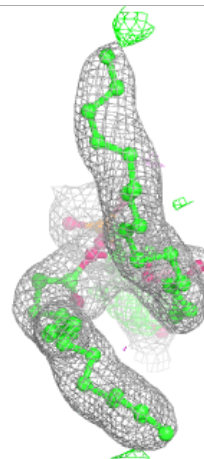
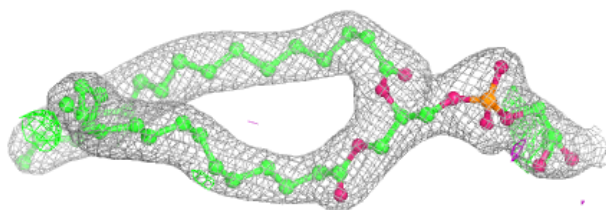
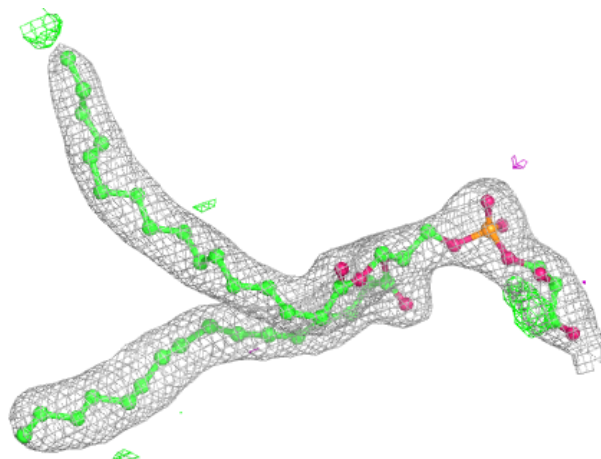
Electron density around LHG D 406 (A):

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



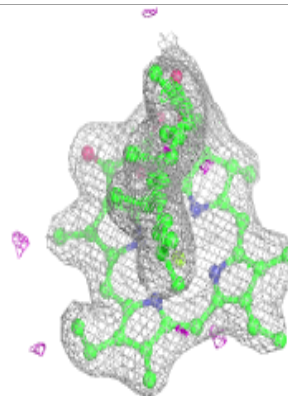
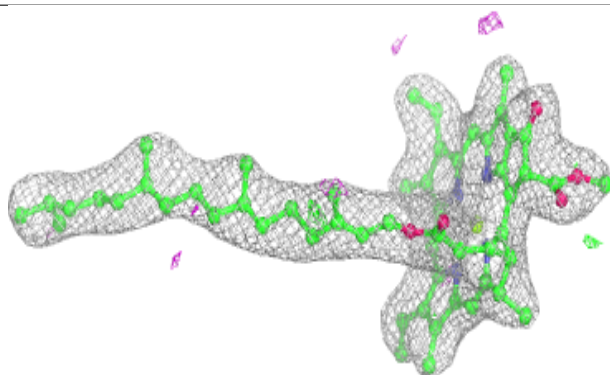
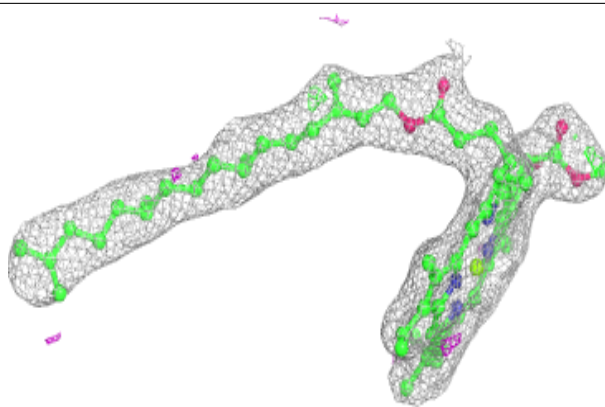
Electron density around LHG D 406 (B):

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

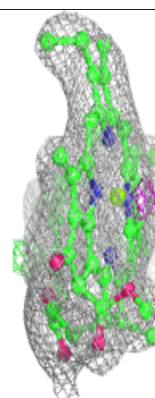
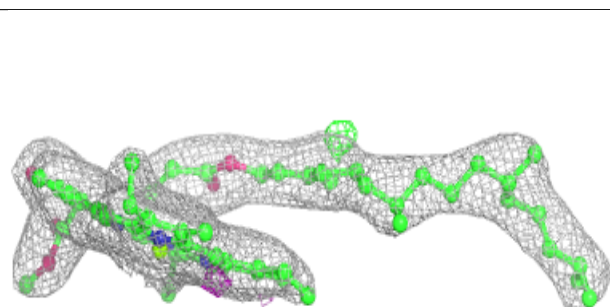
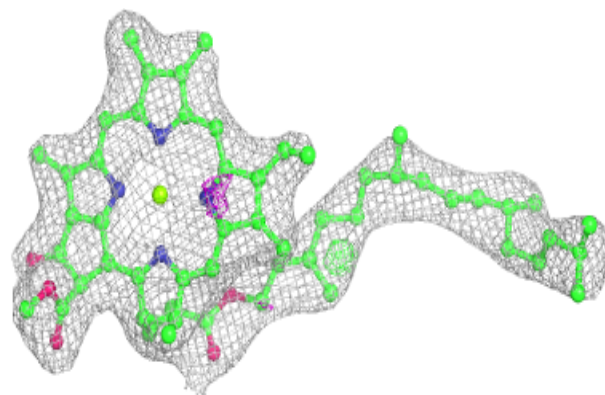


Electron density around CLA B 607:

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

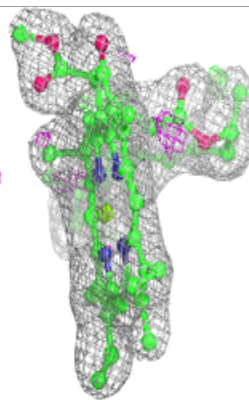
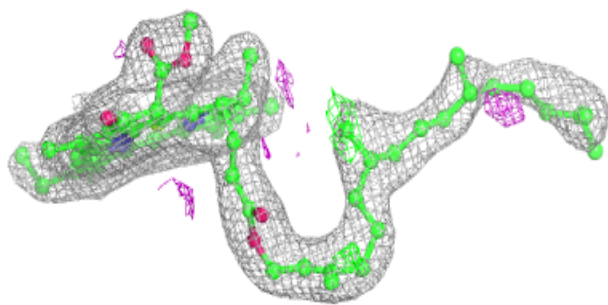
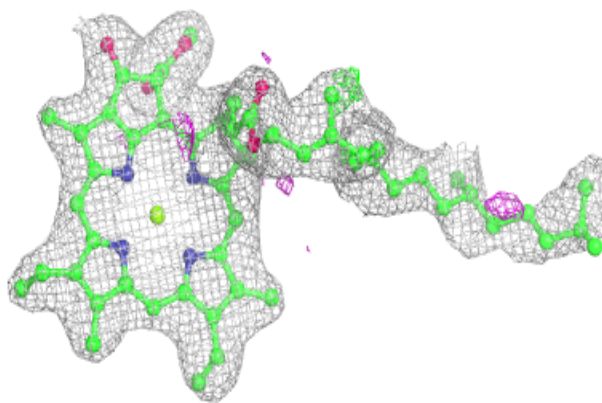
**Electron density around CLA b 603:**

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



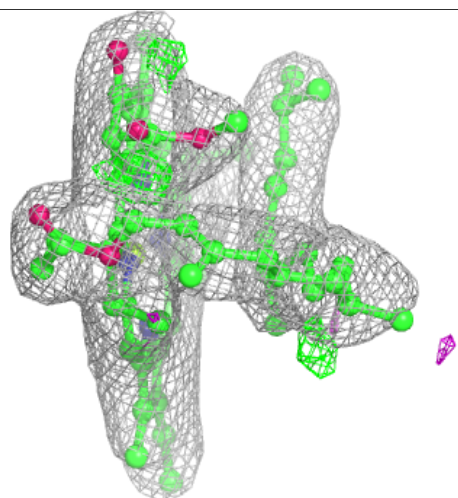
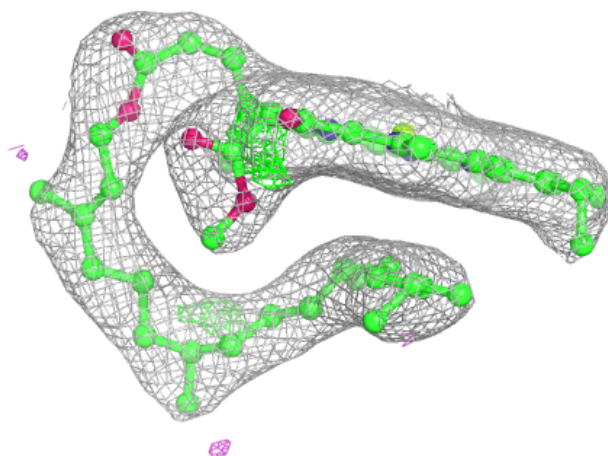
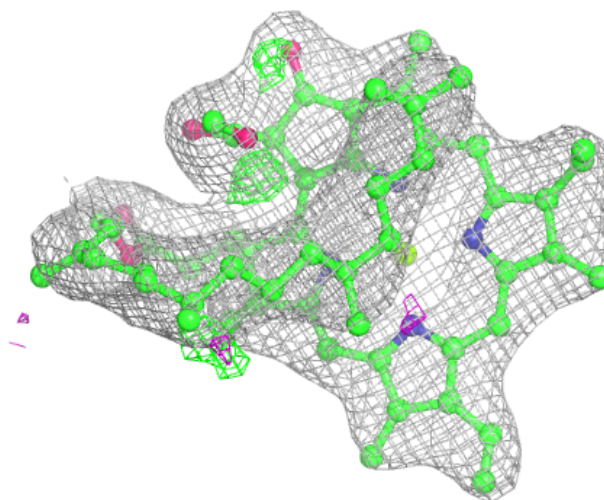
Electron density around CLA A 406 (B):

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



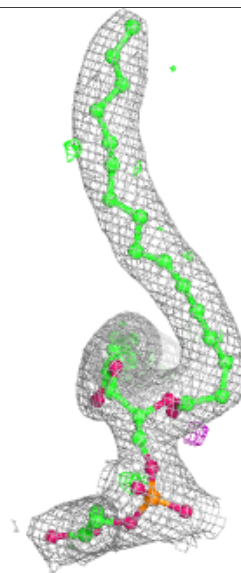
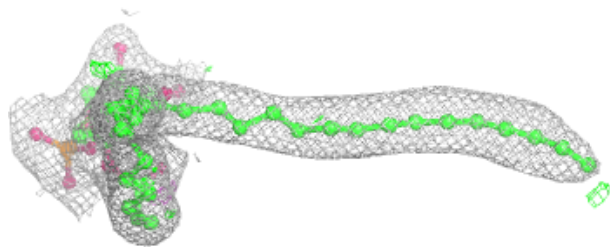
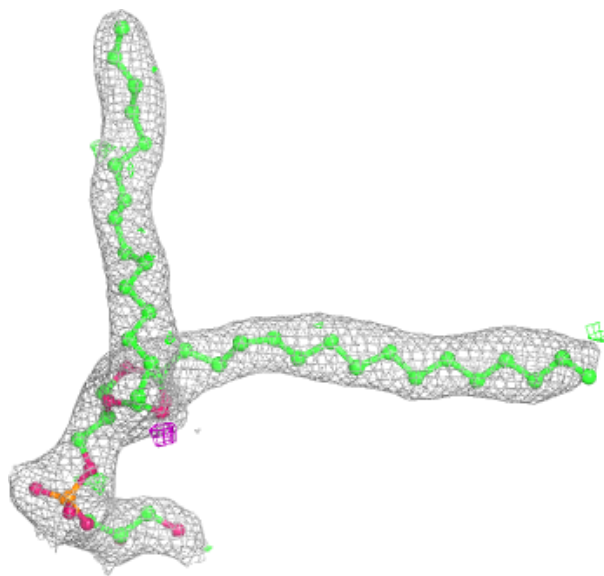
Electron density around CLA c 511:

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



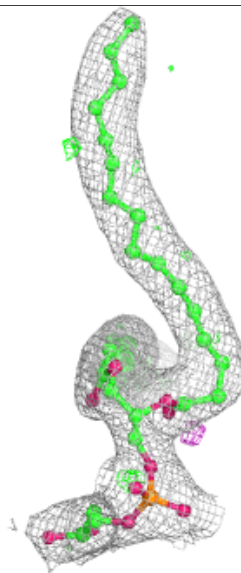
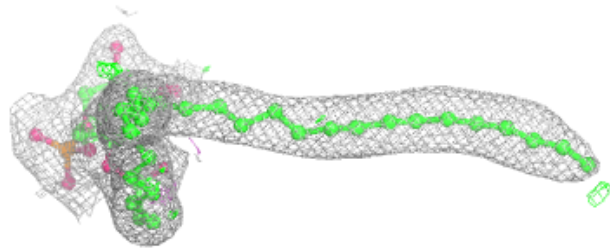
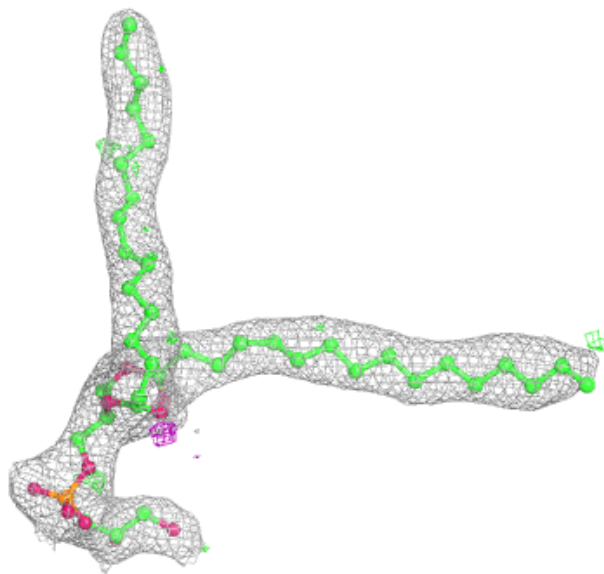
Electron density around LHG L 102 (A):

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



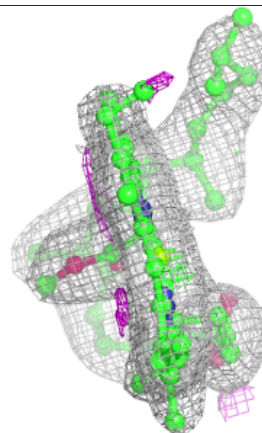
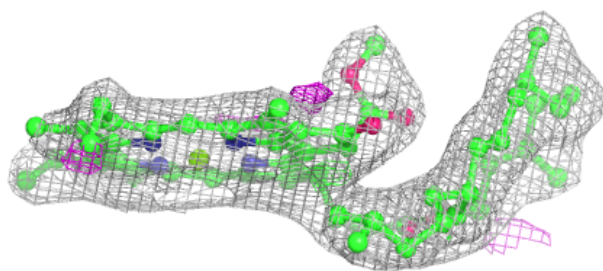
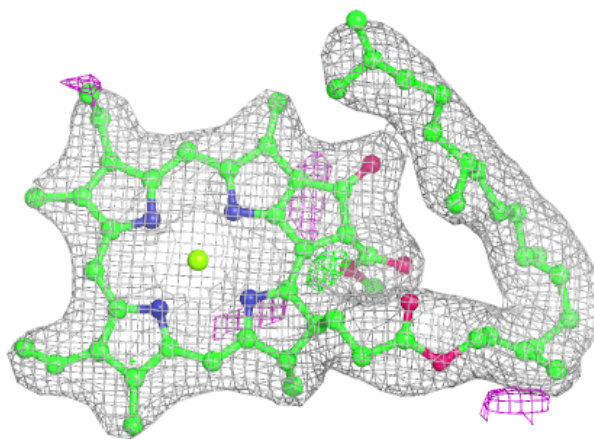
Electron density around LHG L 102 (B):

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

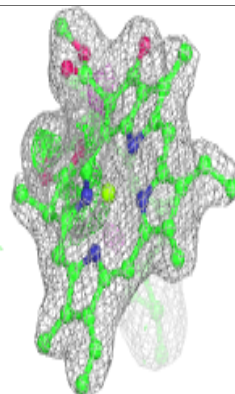
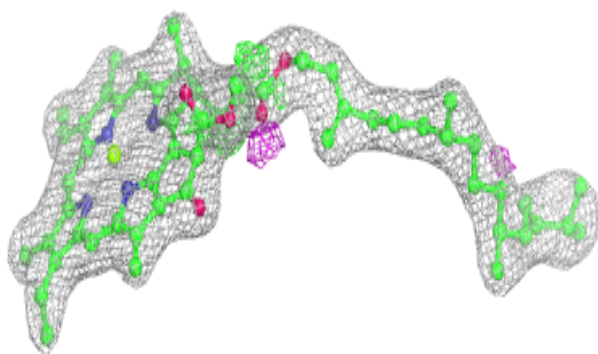
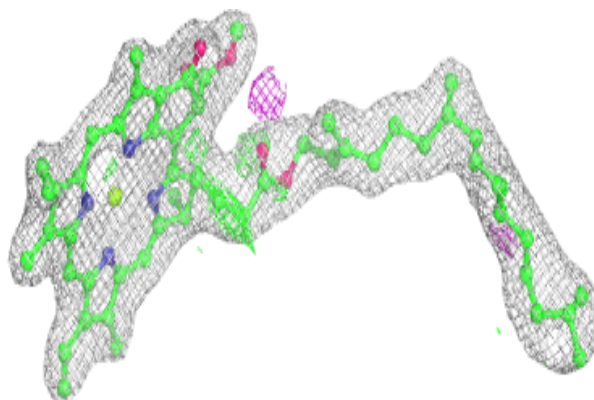


Electron density around CLA B 610:

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

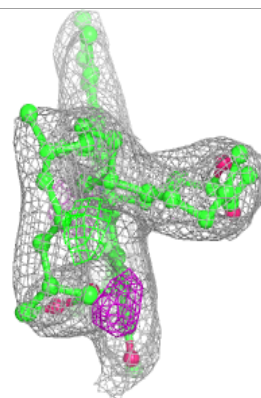
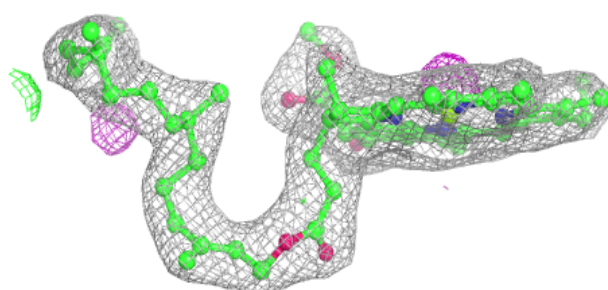
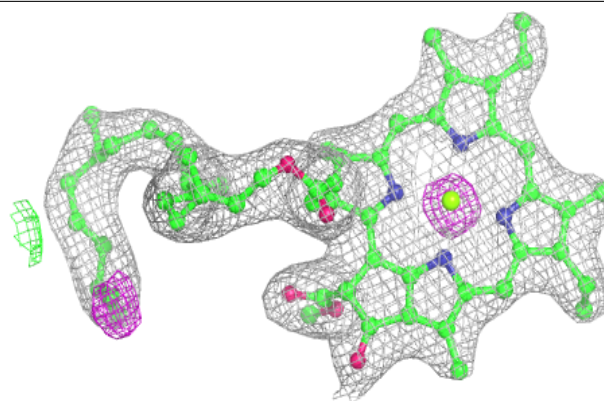
**Electron density around CLA A 404 (A):**

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

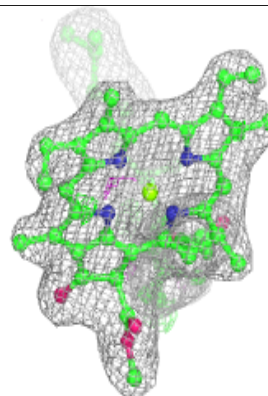
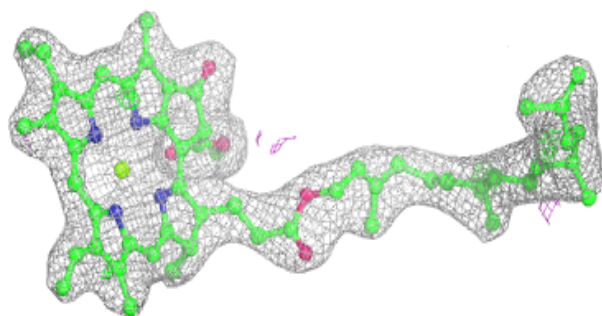
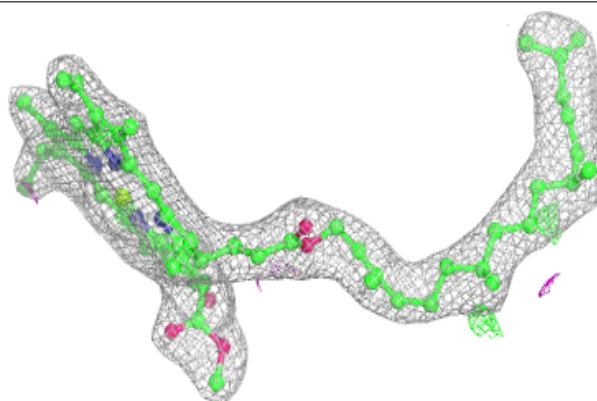


Electron density around CLA B 612:

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

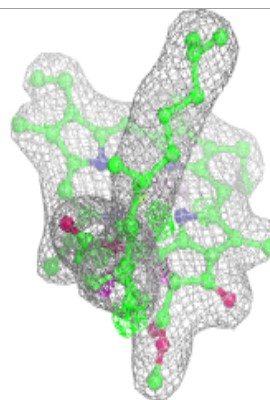
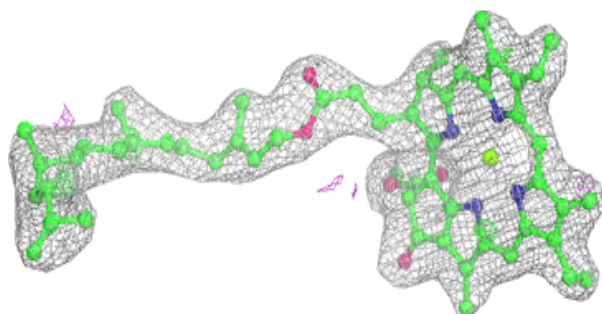
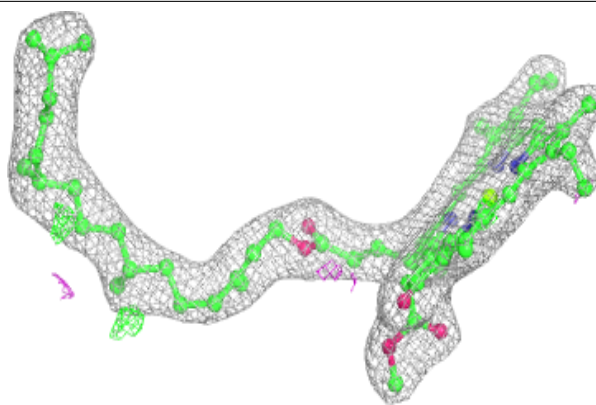
**Electron density around CLA d 402 (A):**

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

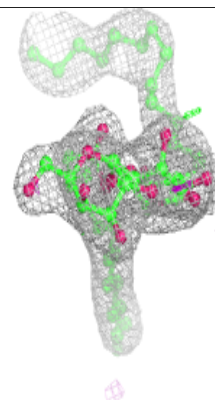
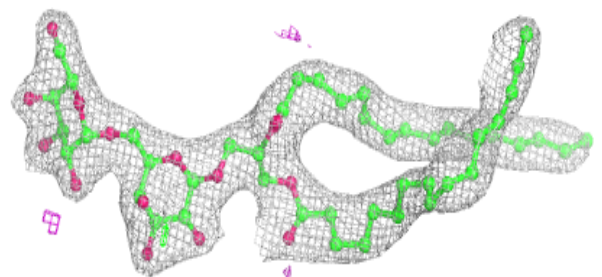
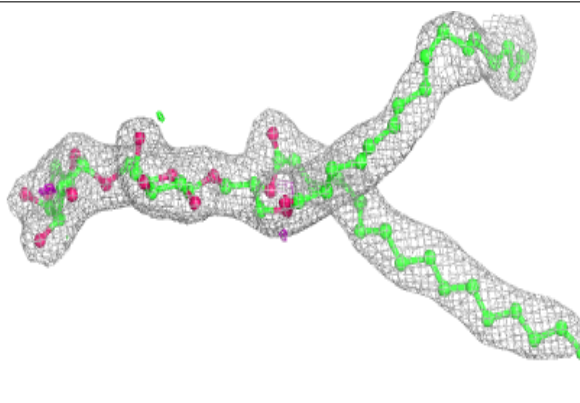


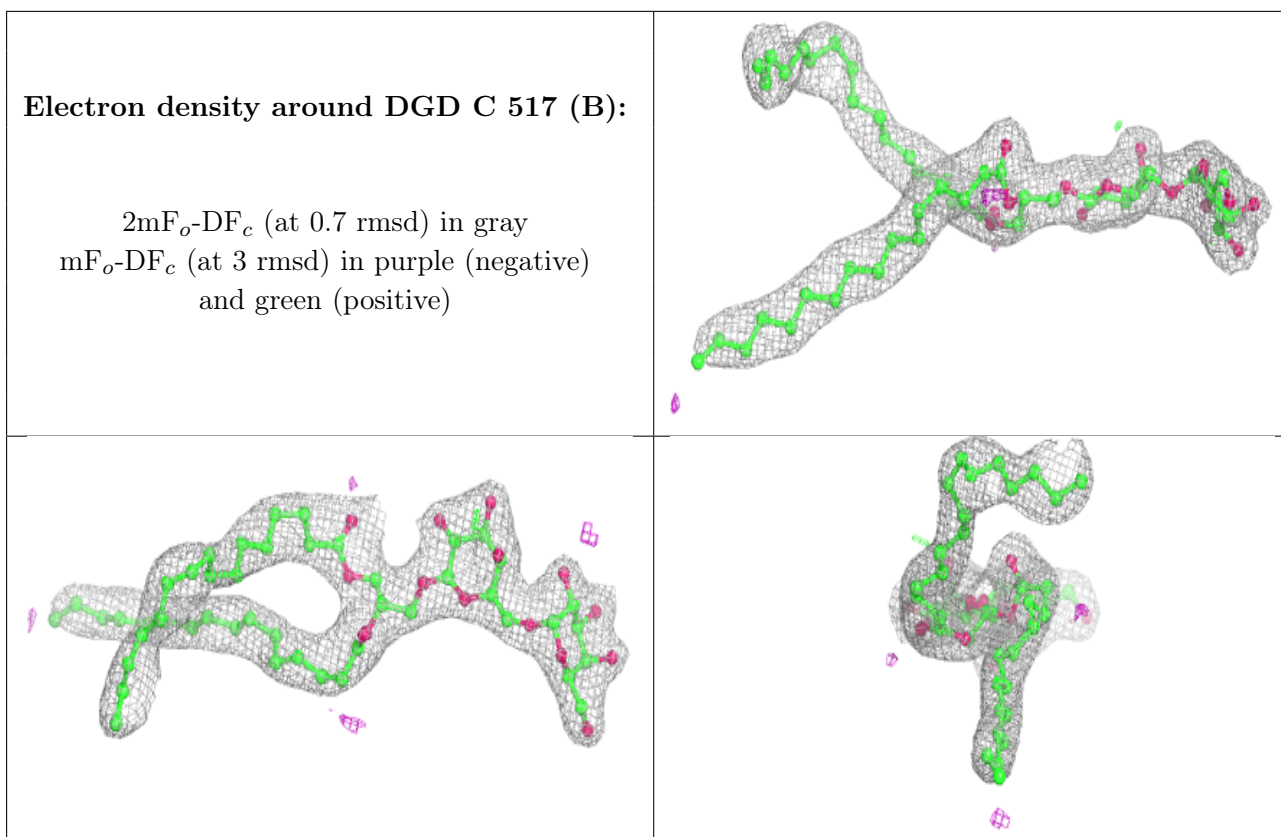
Electron density around CLA d 402 (B):

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

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

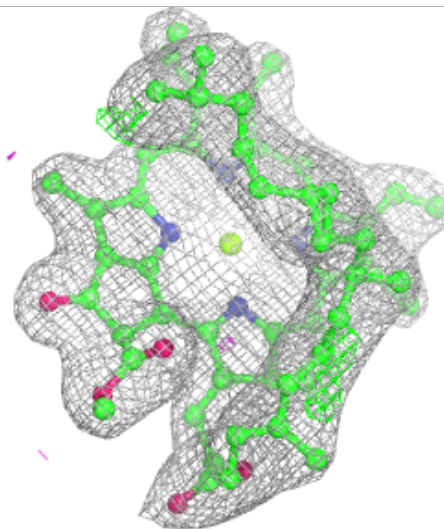
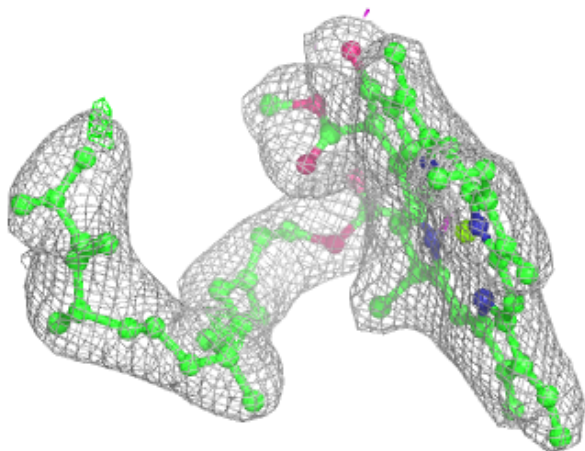
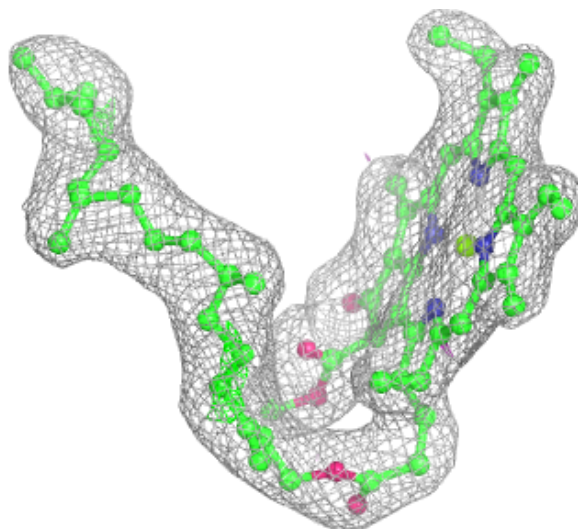
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





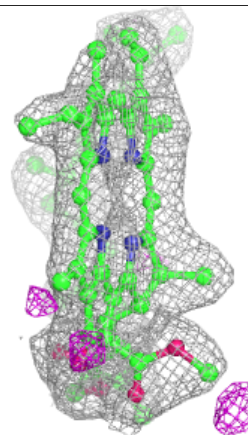
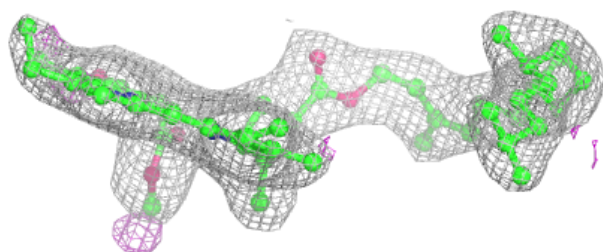
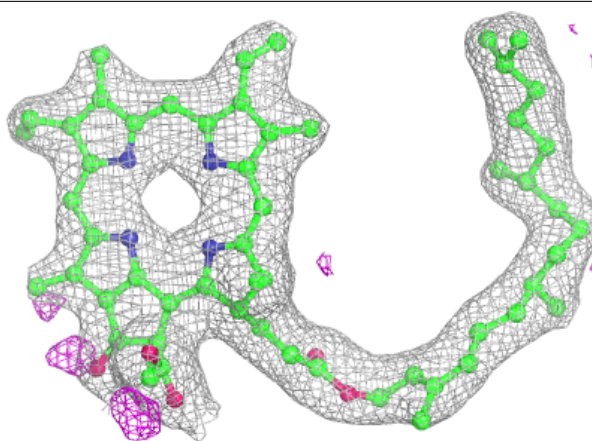
Electron density around CLA B 613:

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



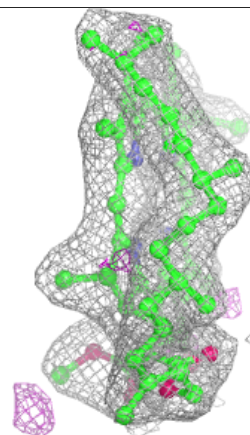
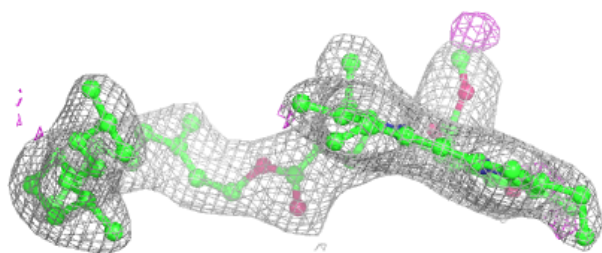
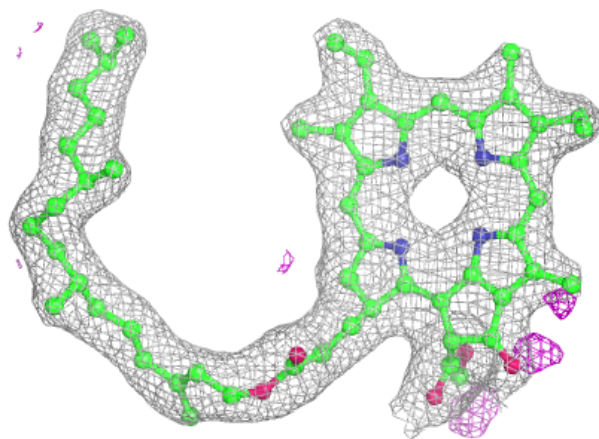
Electron density around PHO A 407 (A):

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



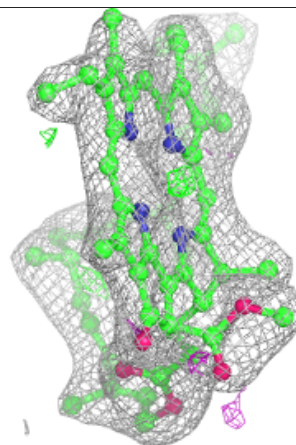
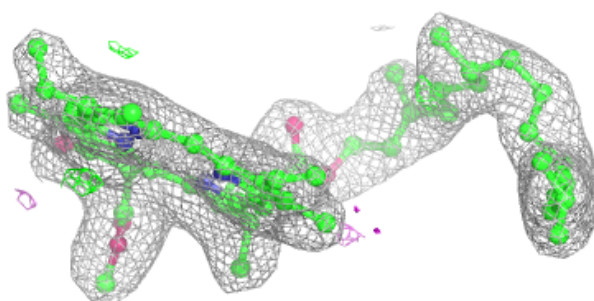
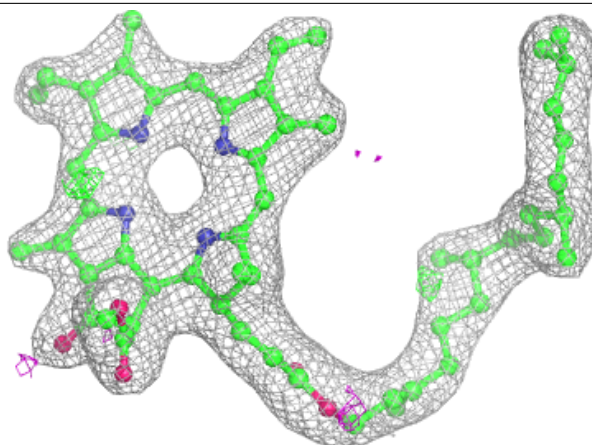
Electron density around PHO A 407 (B):

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



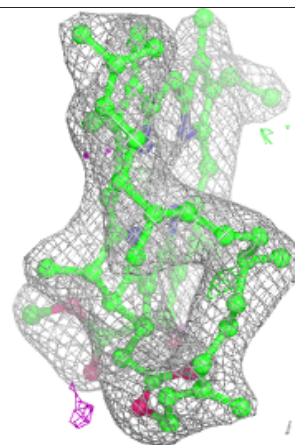
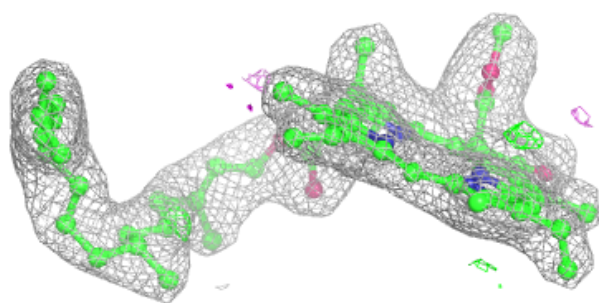
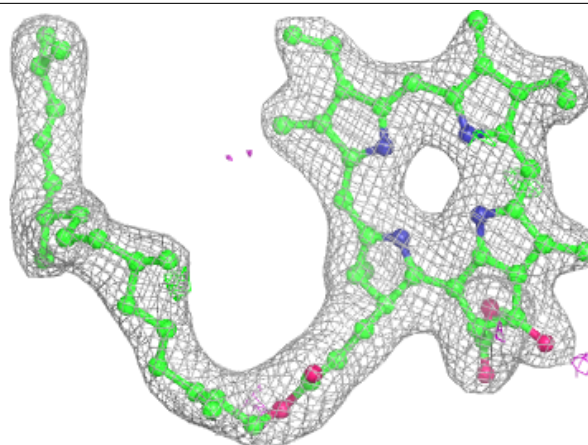
Electron density around PHO A 417 (A):

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

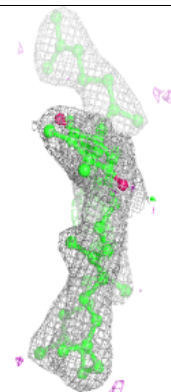
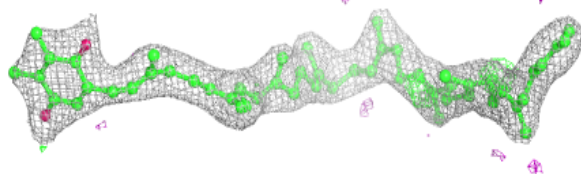
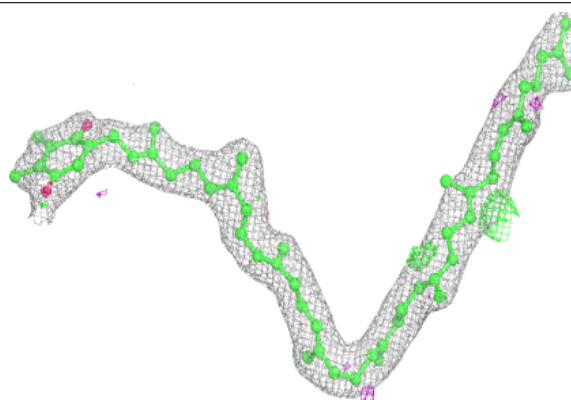


Electron density around PHO A 417 (B):

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

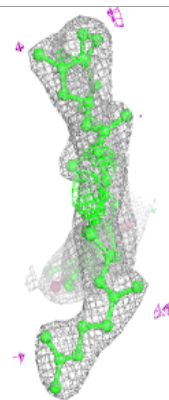
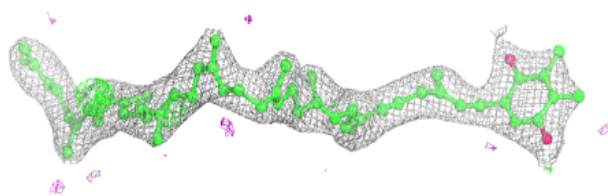
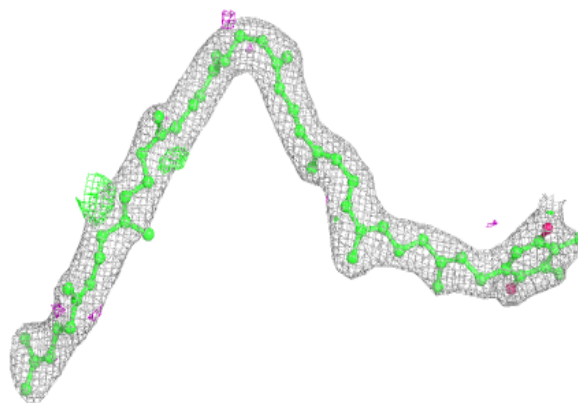
**Electron density around PL9 d 405 (A):**

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



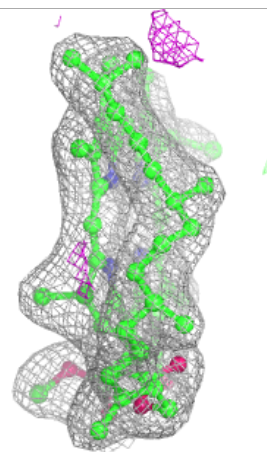
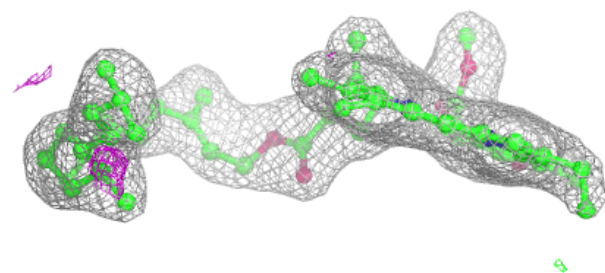
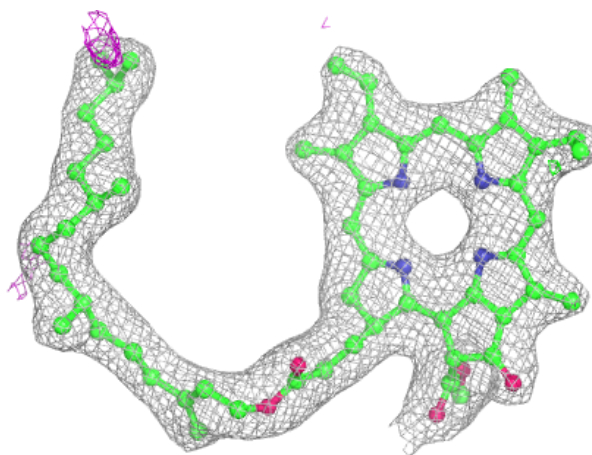
Electron density around PL9 d 405 (B):

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



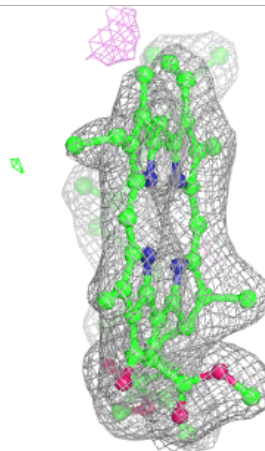
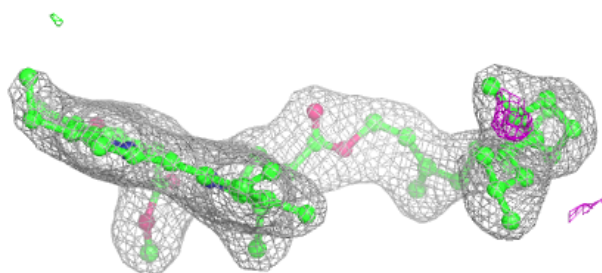
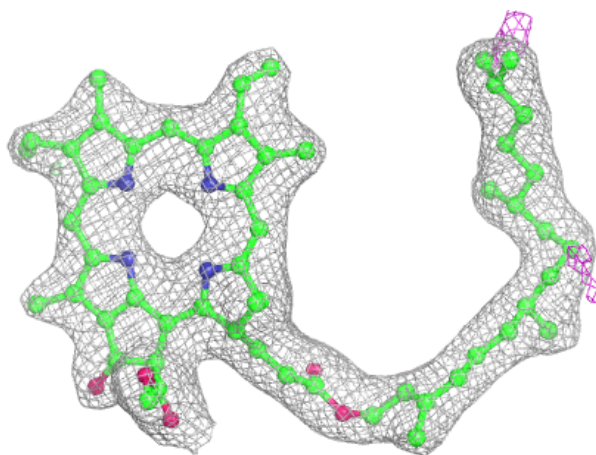
Electron density around PHO a 407 (A):

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



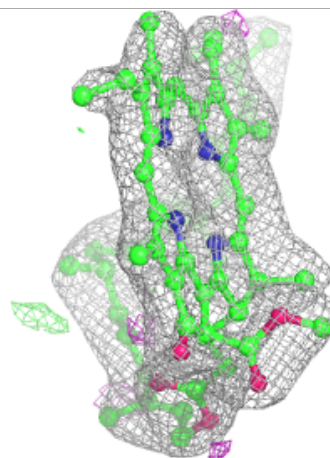
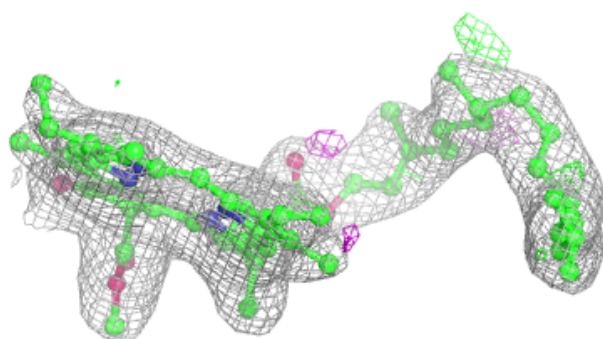
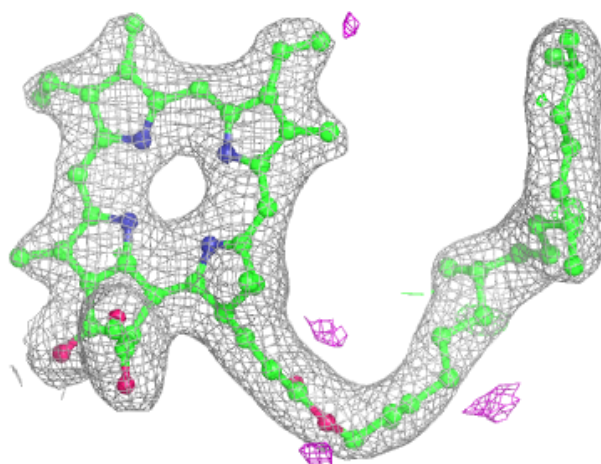
Electron density around PHO a 407 (B):

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



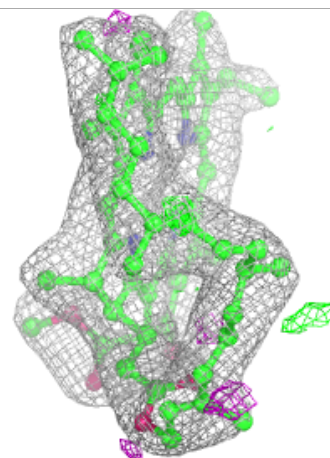
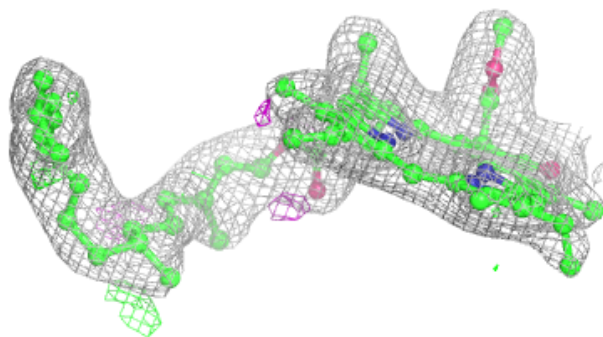
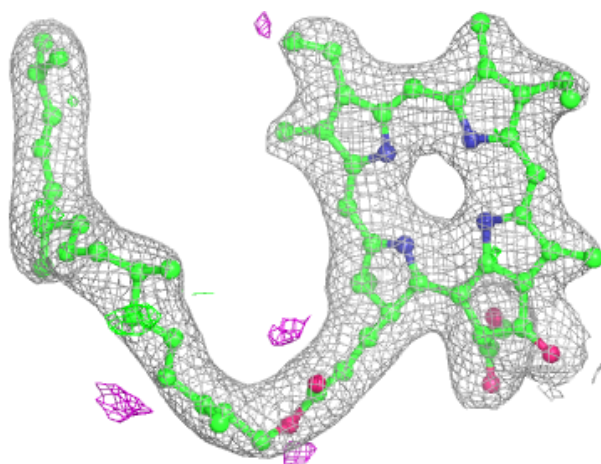
Electron density around PHO a 415 (A):

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



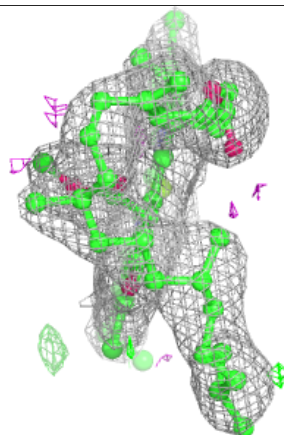
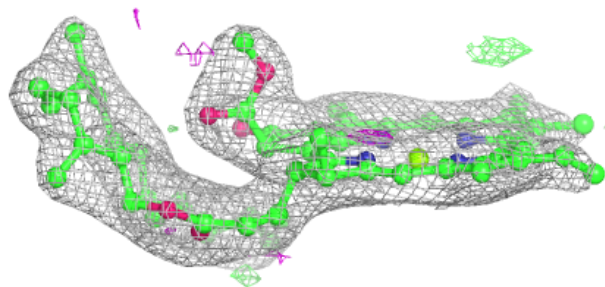
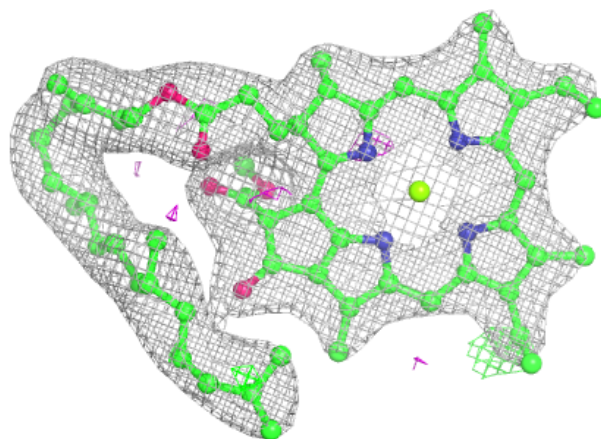
Electron density around PHO a 415 (B):

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

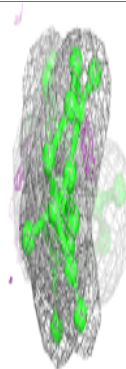
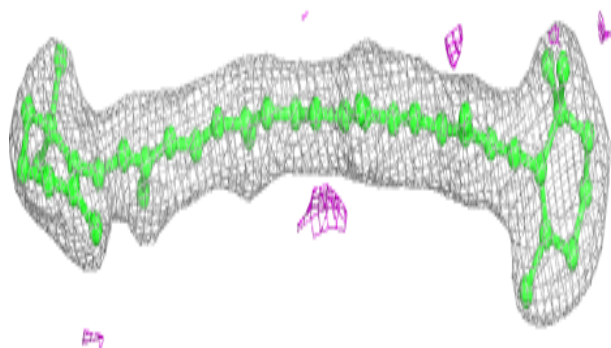
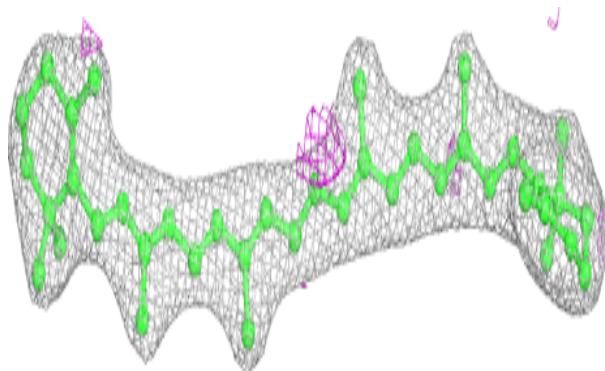


Electron density around CLA b 610:

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

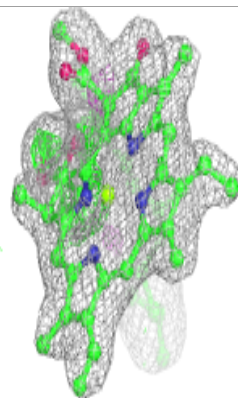
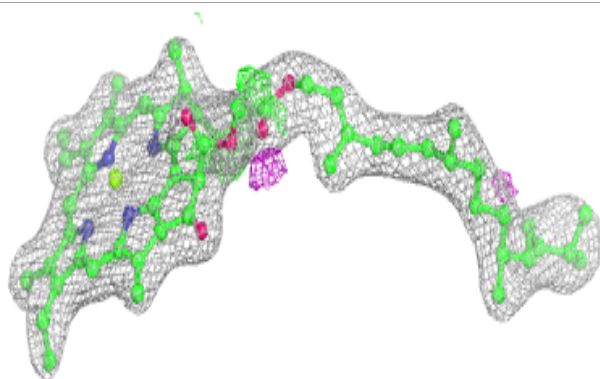
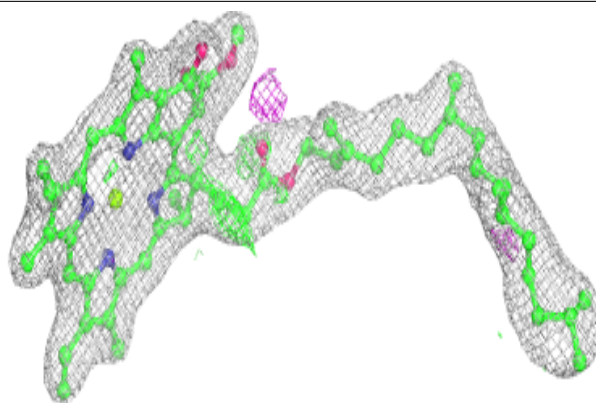
**Electron density around BCR B 617:**

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

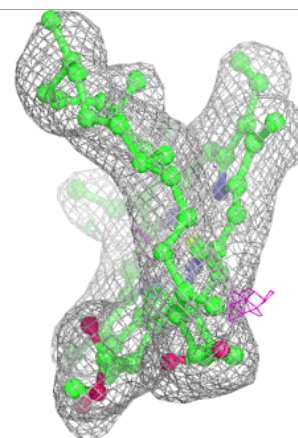
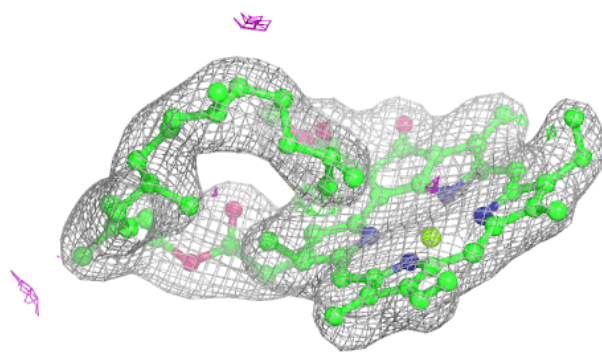
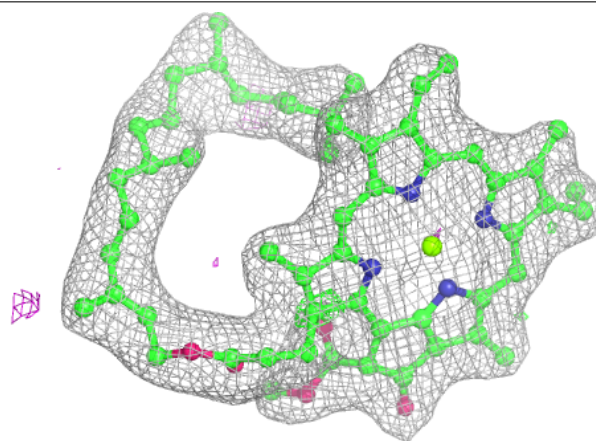


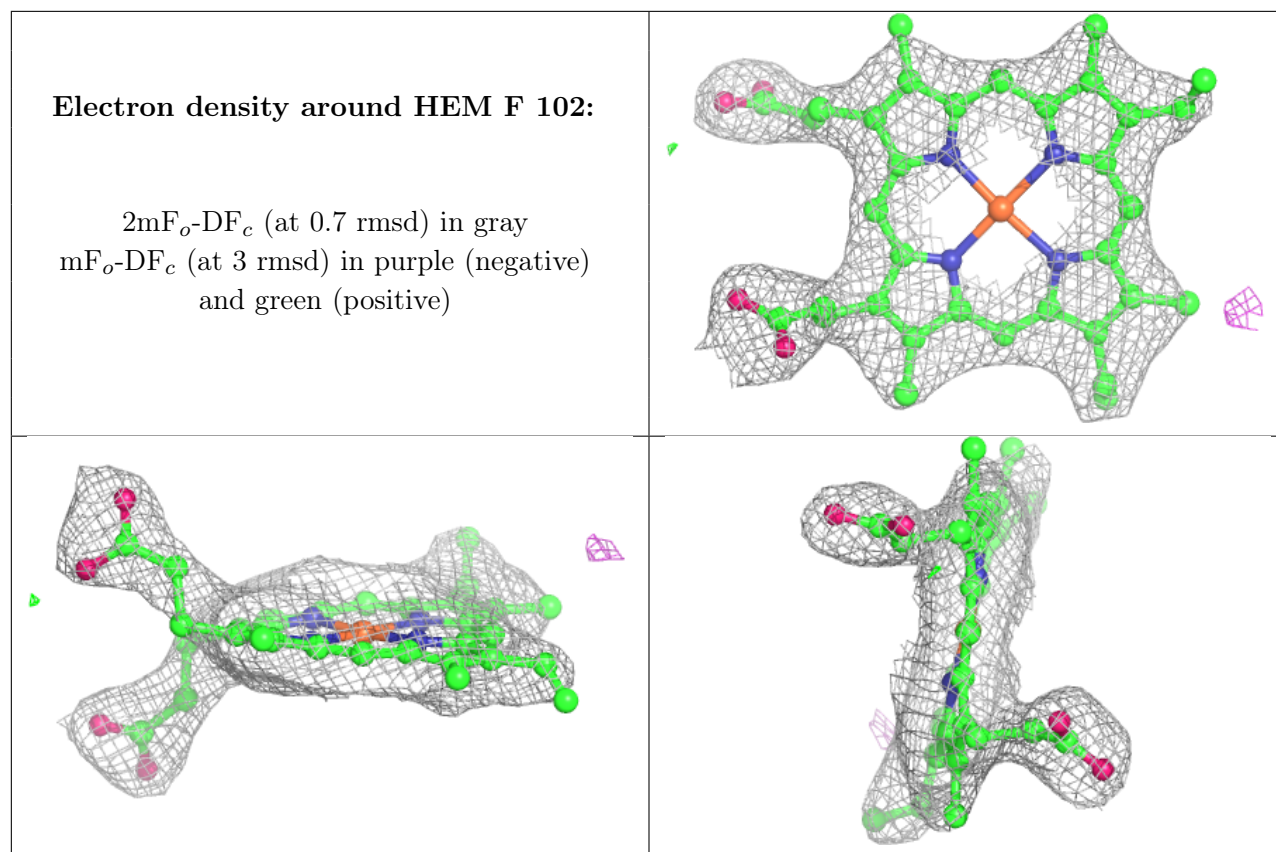
Electron density around CLA A 404 (B):

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

**Electron density around CLA B 615:**

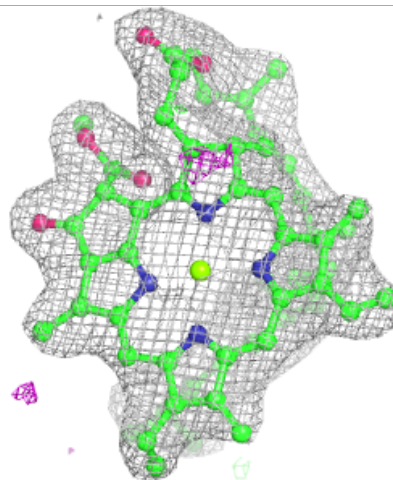
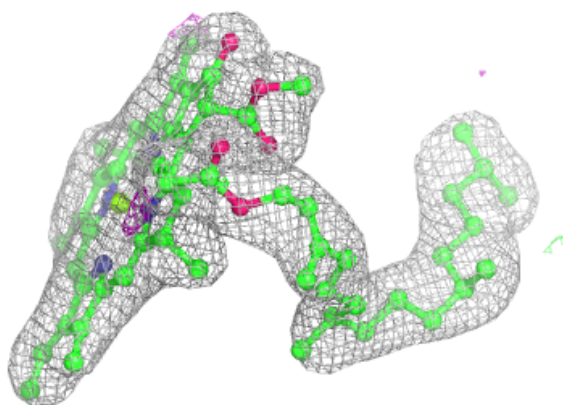
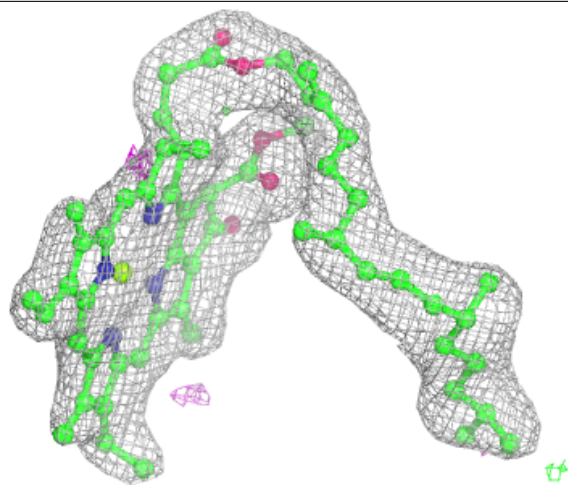
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





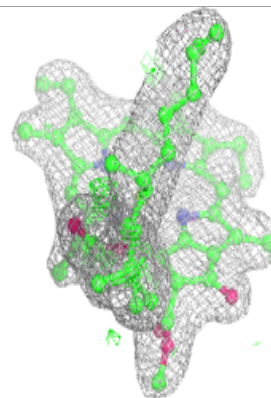
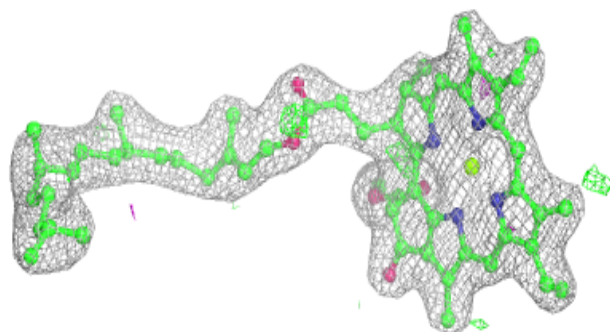
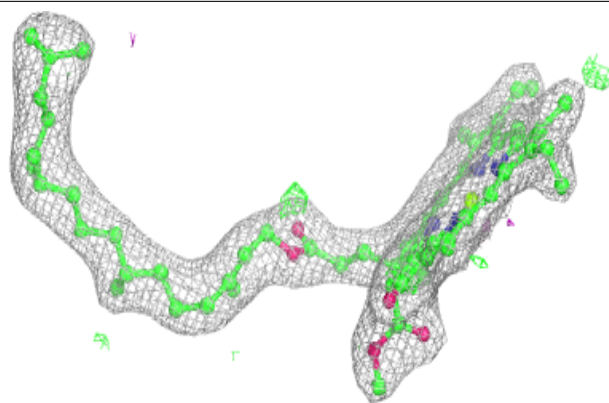
Electron density around CLA b 613:

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

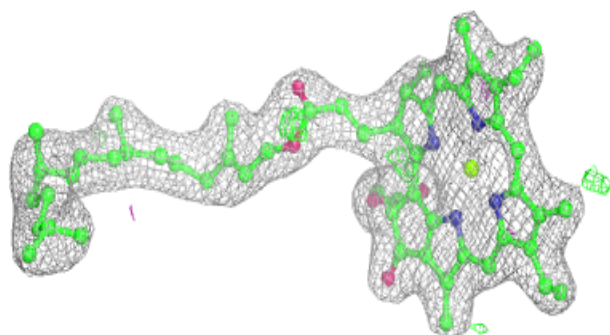
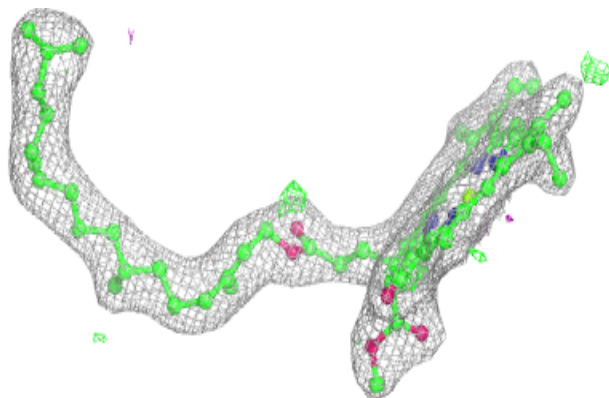


Electron density around CLA D 402 (A):

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

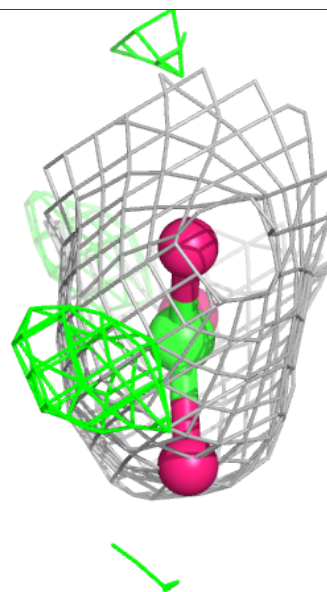
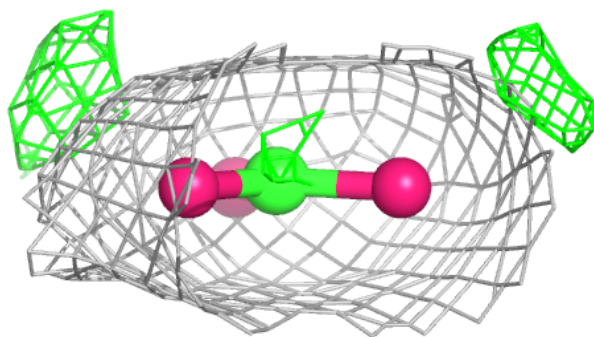
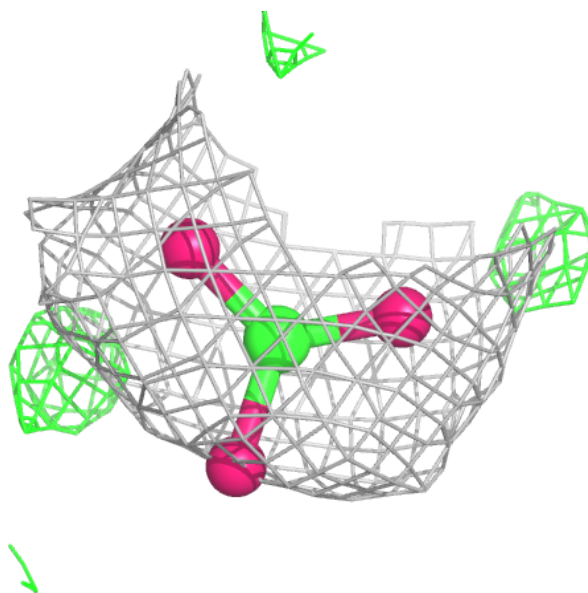
**Electron density around CLA D 402 (B):**

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



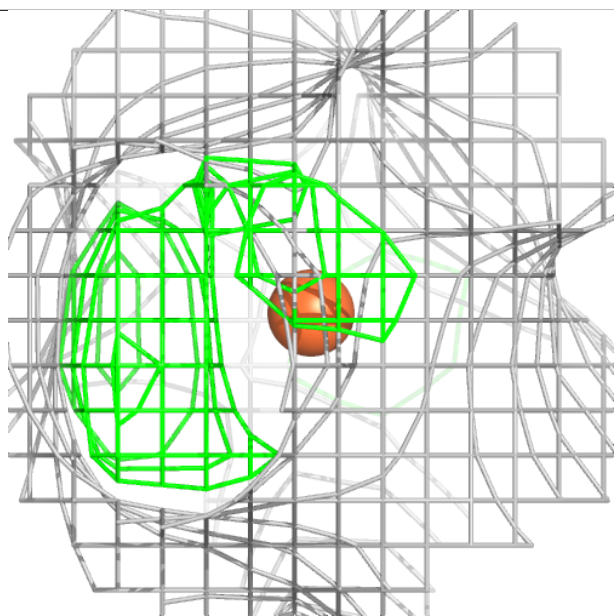
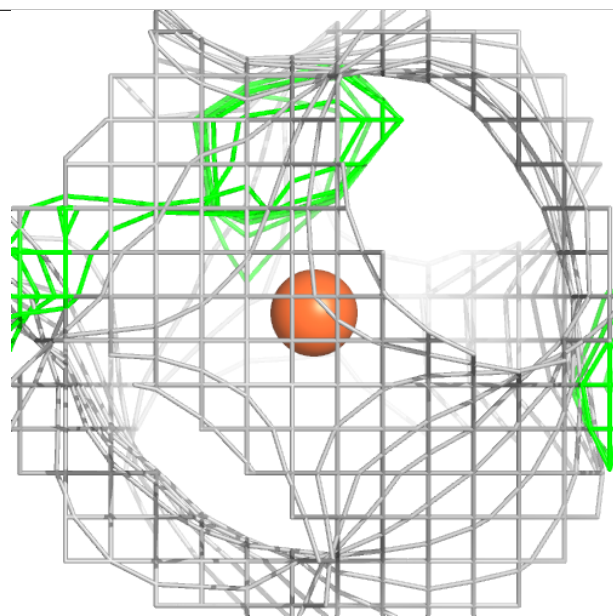
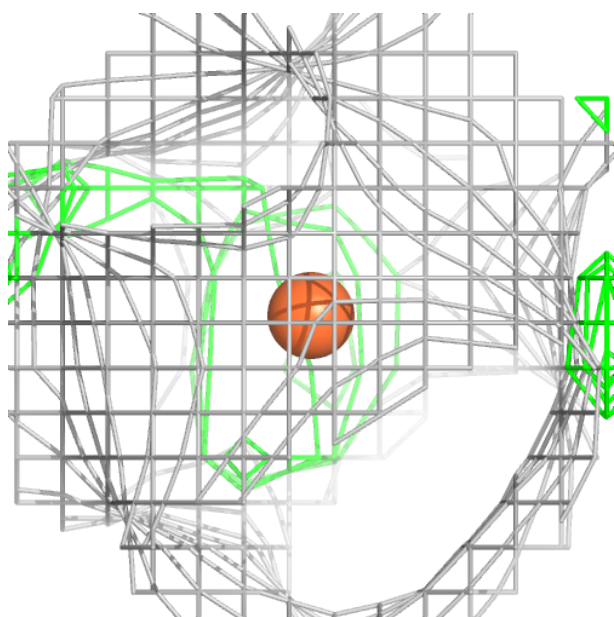
Electron density around BCT d 401 (B):

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



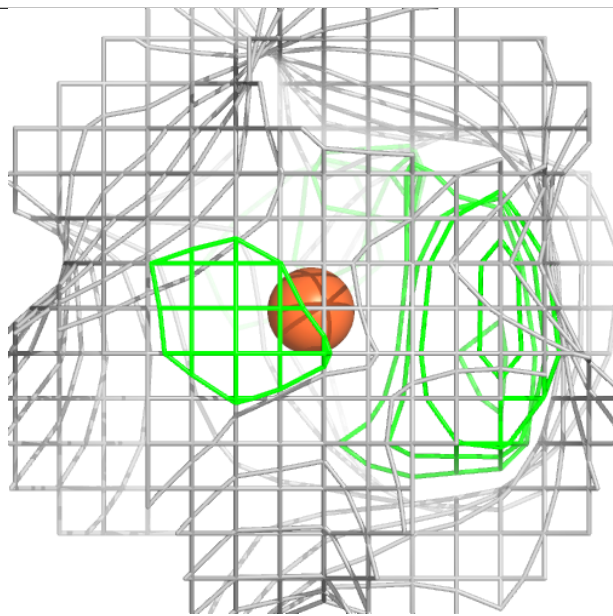
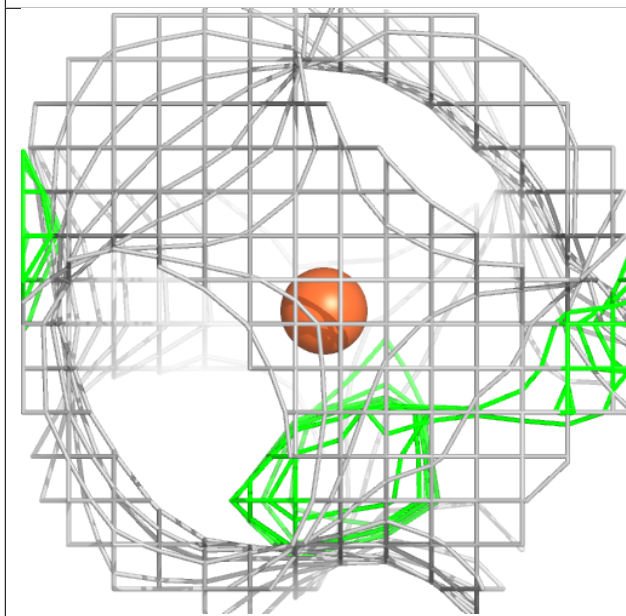
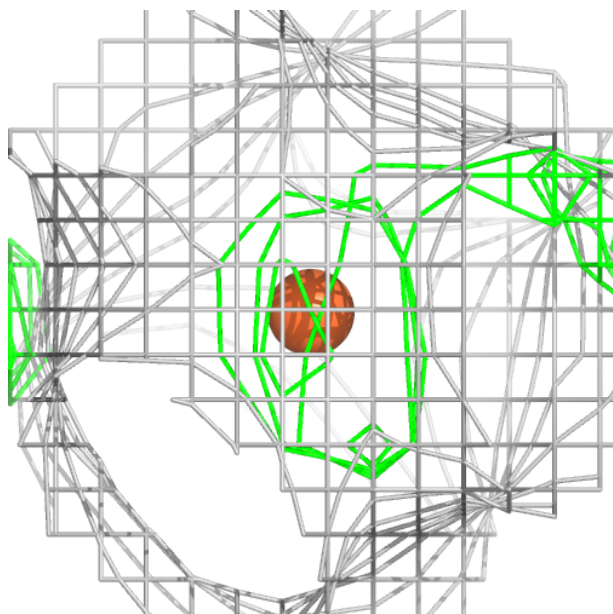
Electron density around FE2 a 401 (A):

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



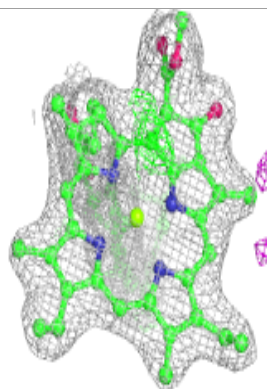
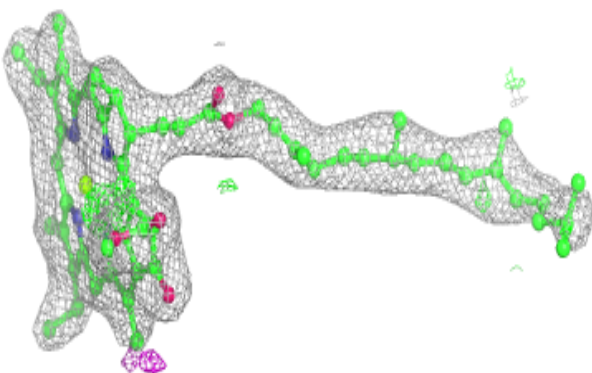
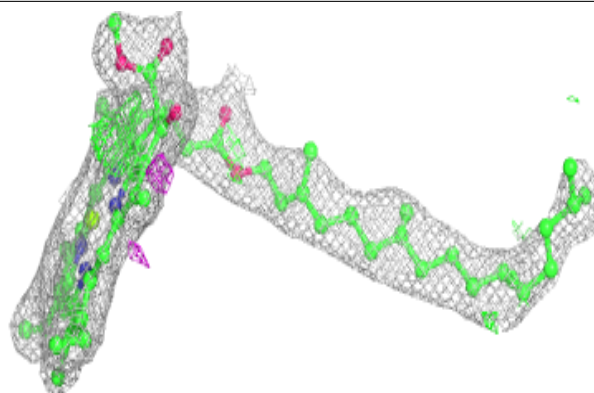
Electron density around FE2 a 401 (B):

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

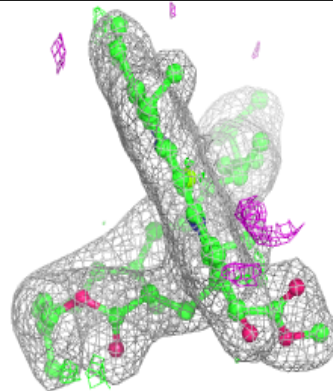
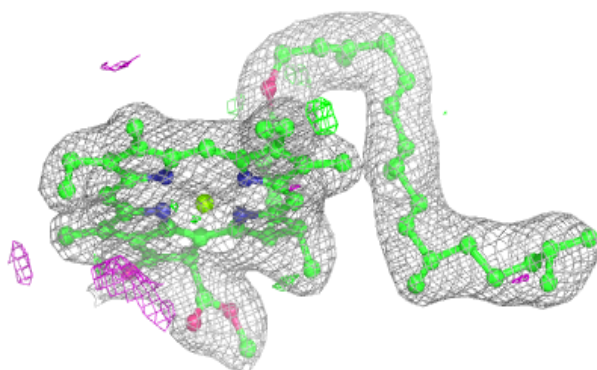
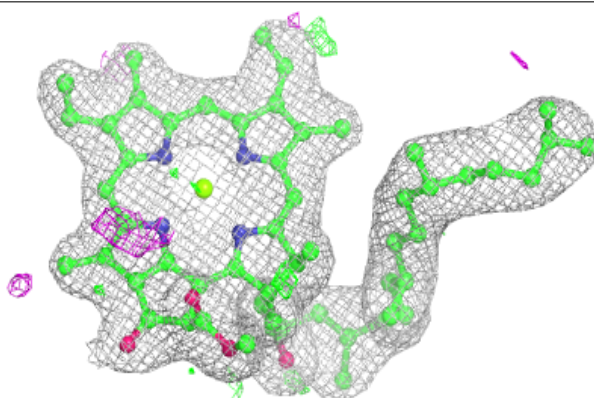


Electron density around CLA B 604:

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

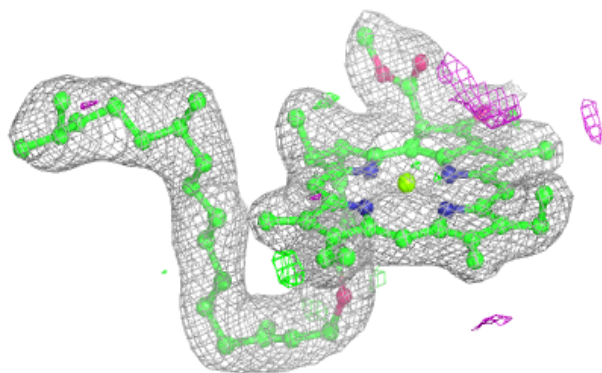
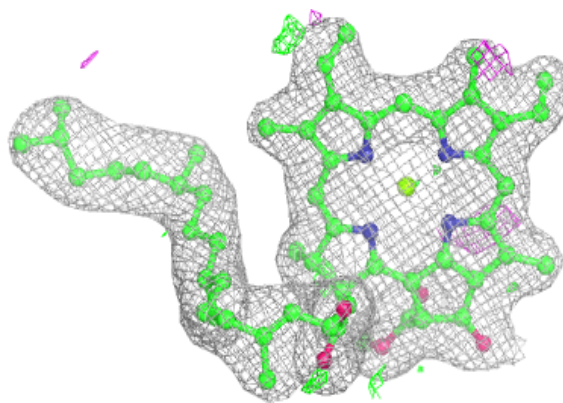
**Electron density around CLA A 405 (A):**

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



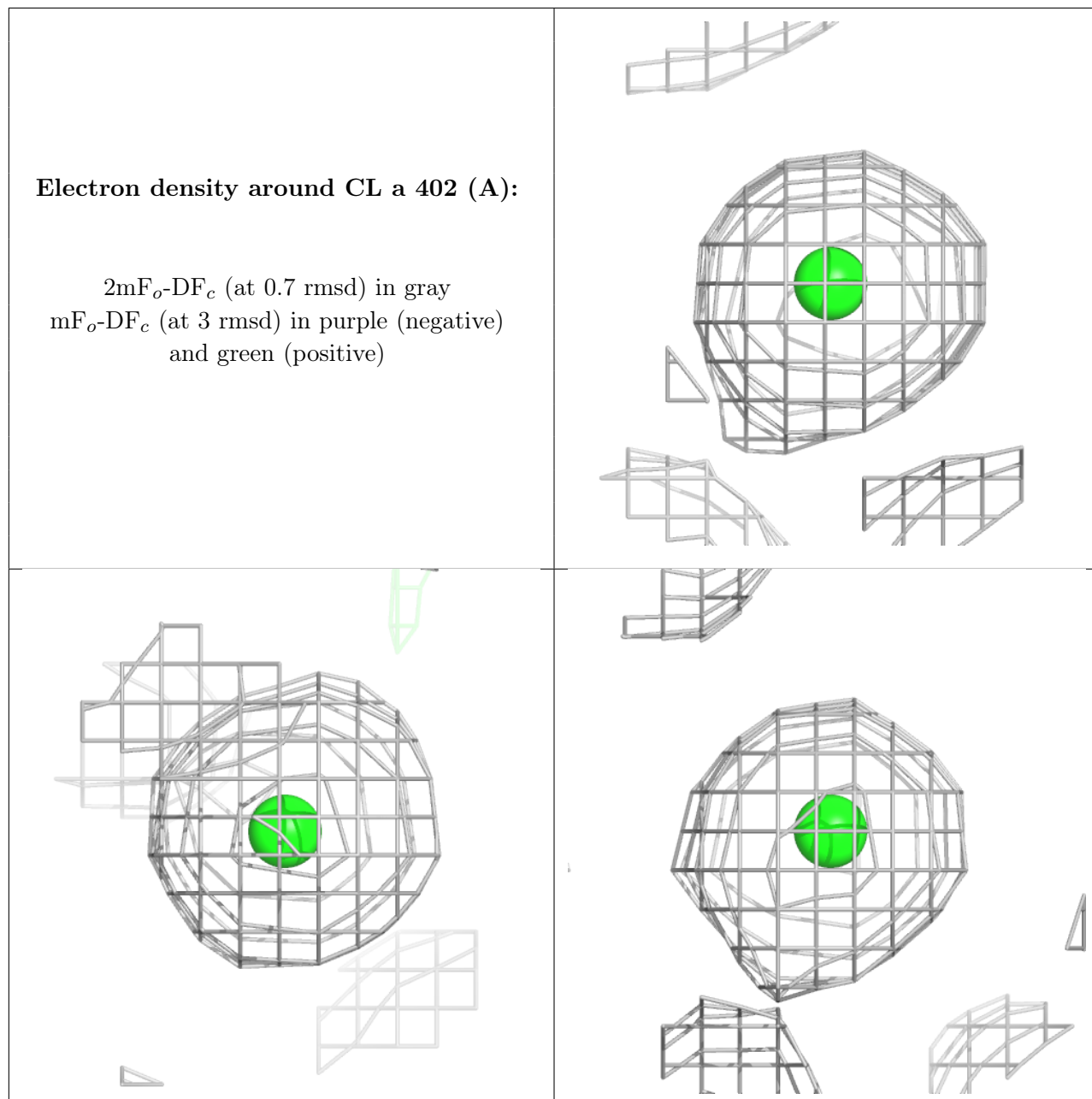
Electron density around CLA A 405 (B):

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



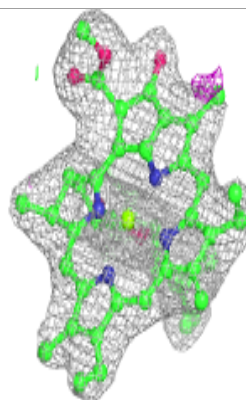
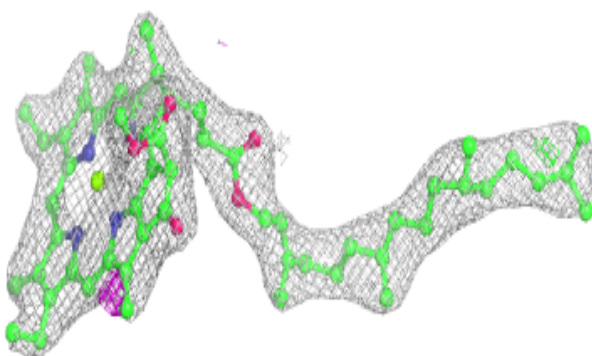
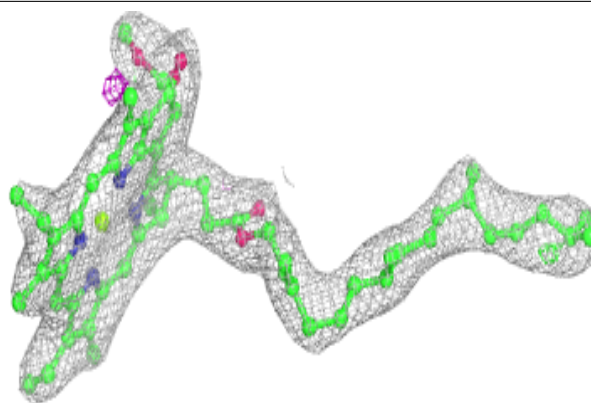
Electron density around CL a 402 (A):

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

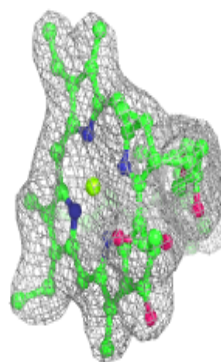
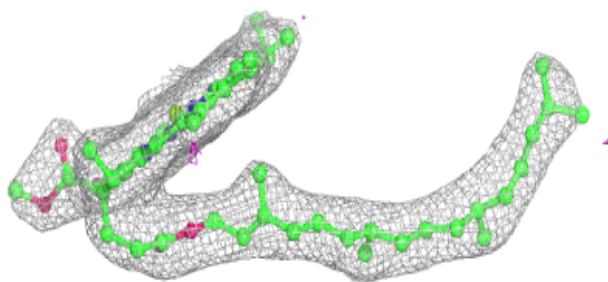
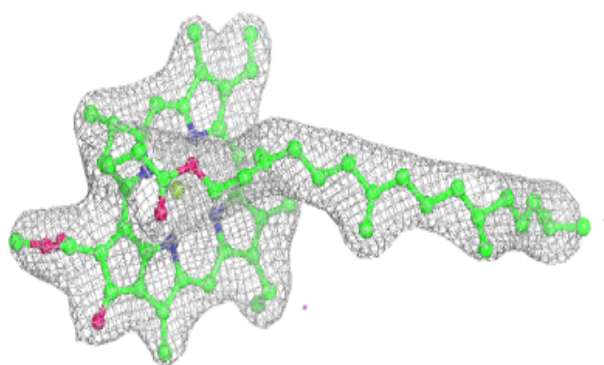


Electron density around CLA C 503:

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

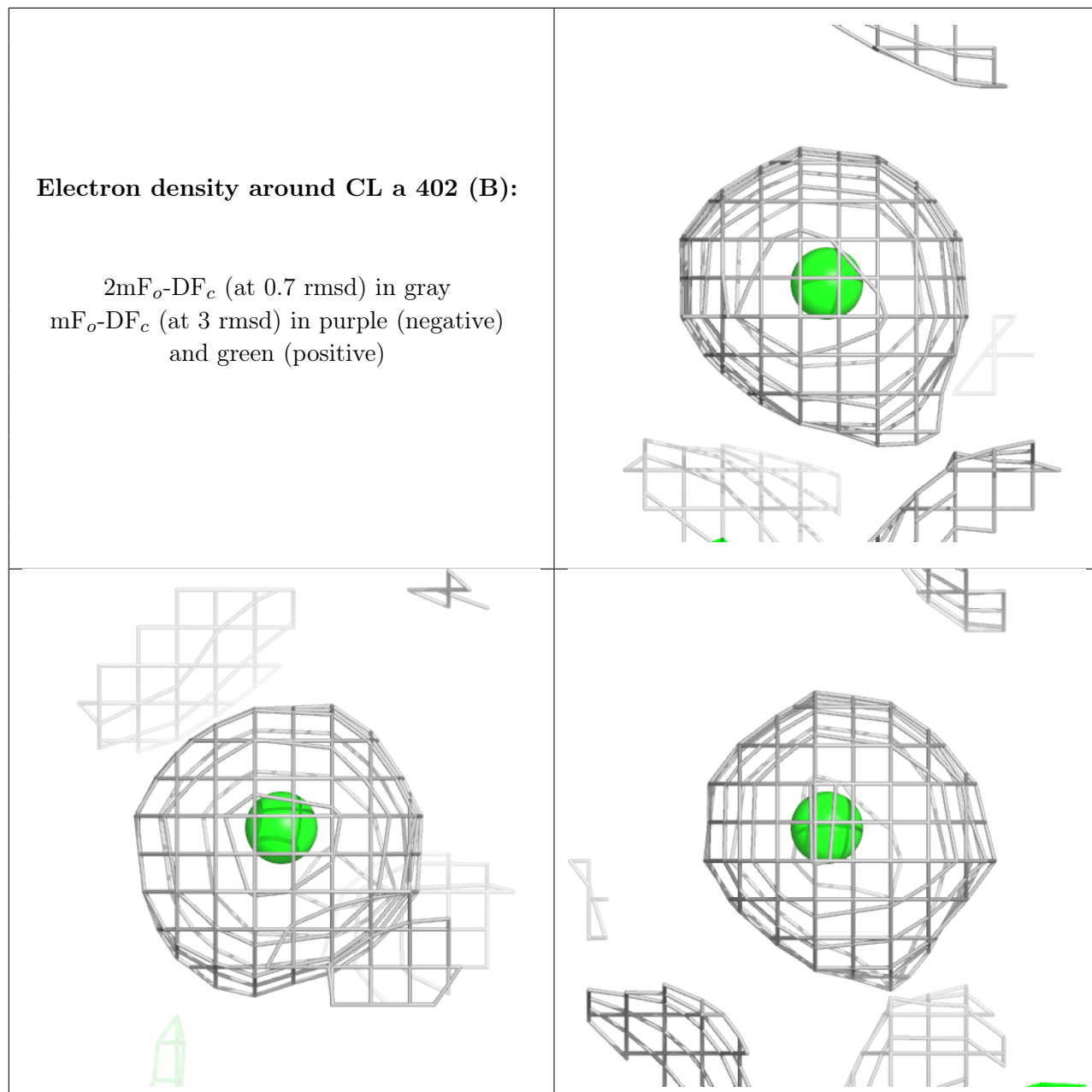
**Electron density around CLA B 608:**

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



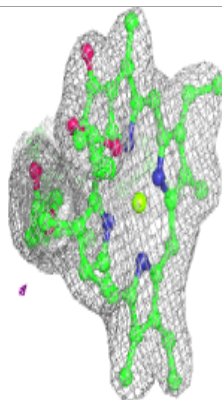
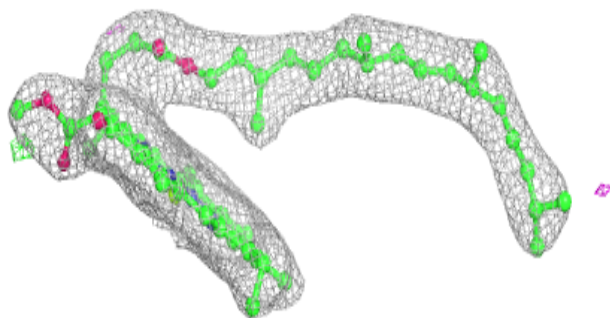
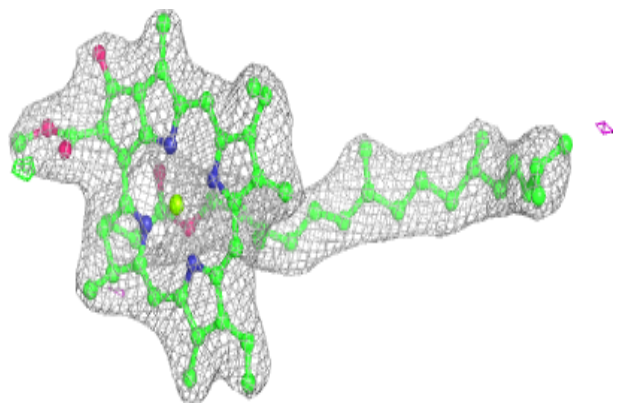
Electron density around CL a 402 (B):

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



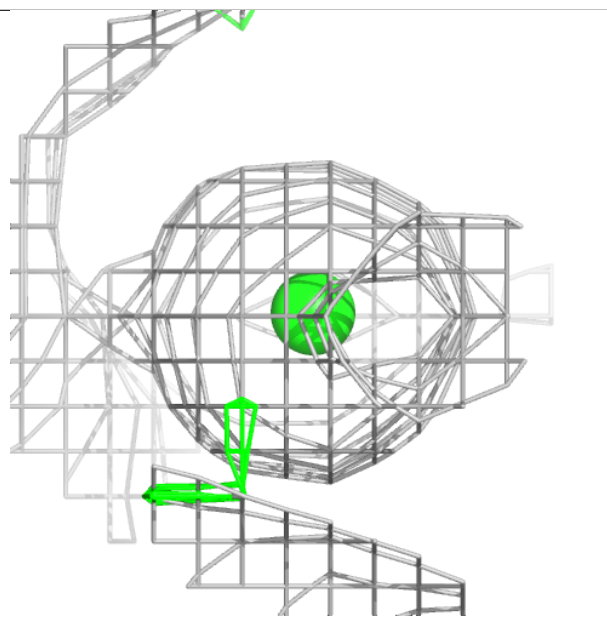
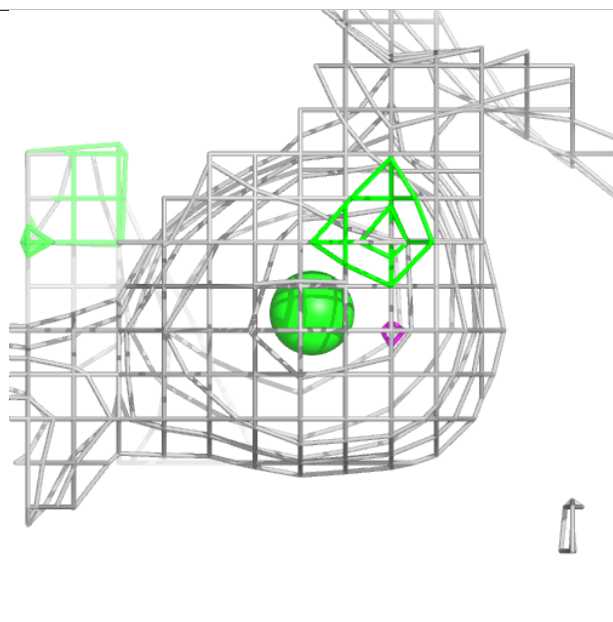
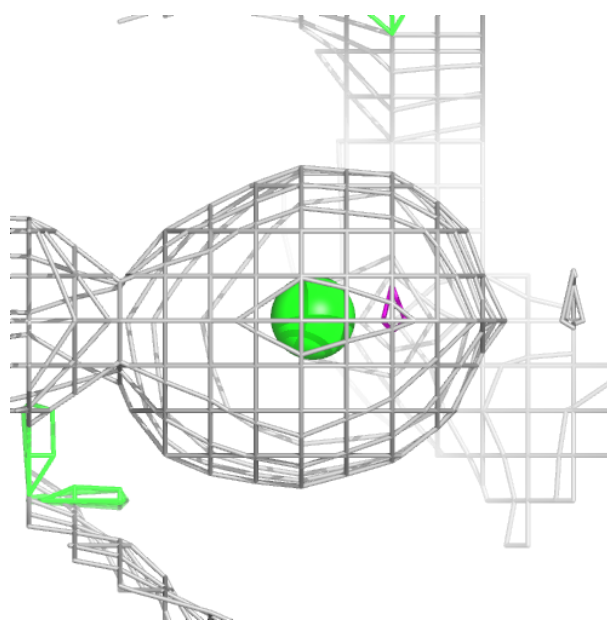
Electron density around CLA b 608:

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



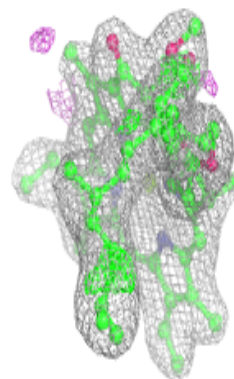
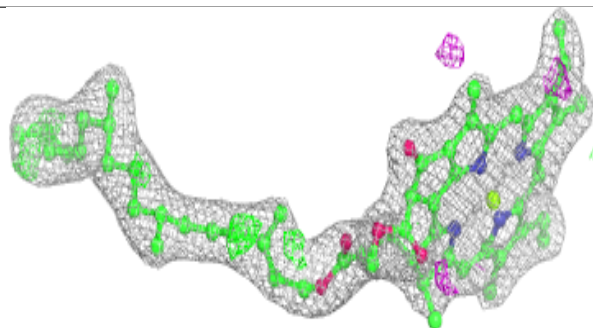
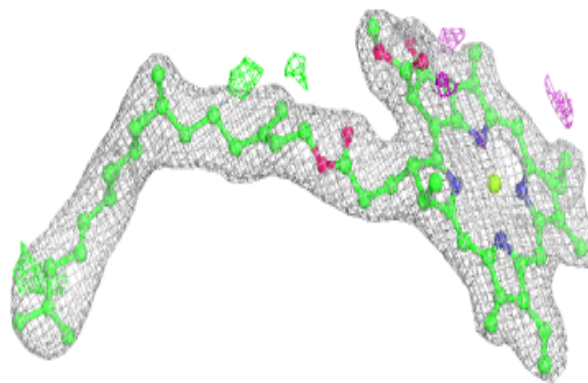
Electron density around CL a 403 (A):

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

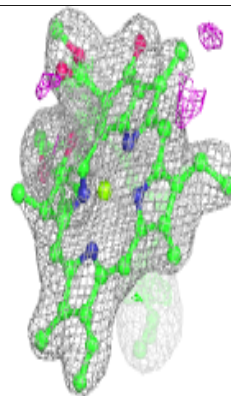
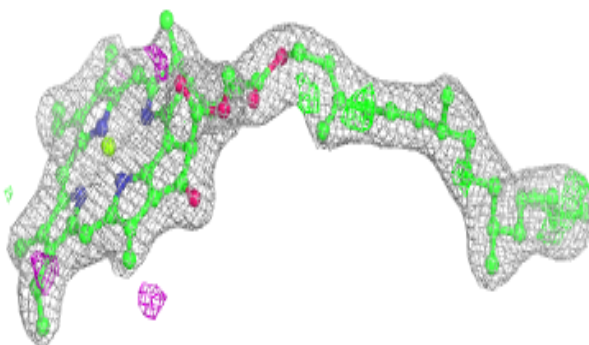
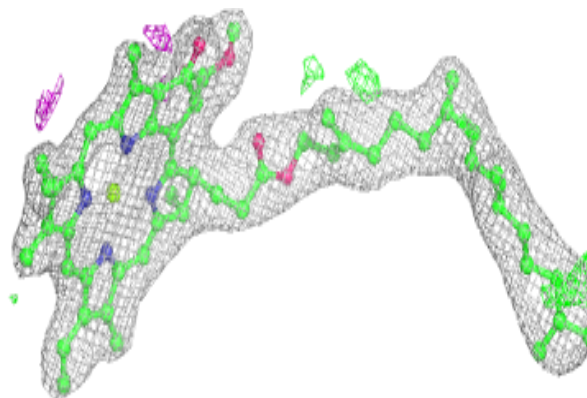


Electron density around CLA a 404 (A):

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

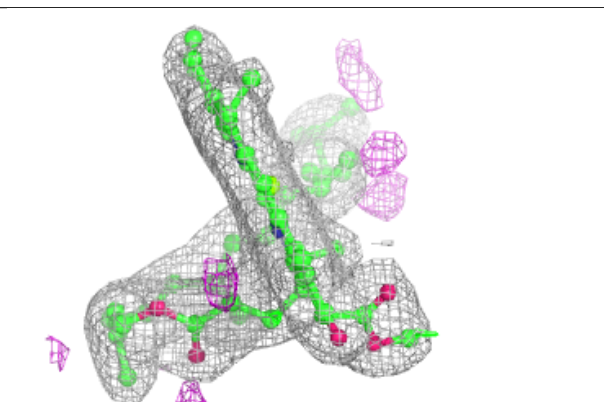
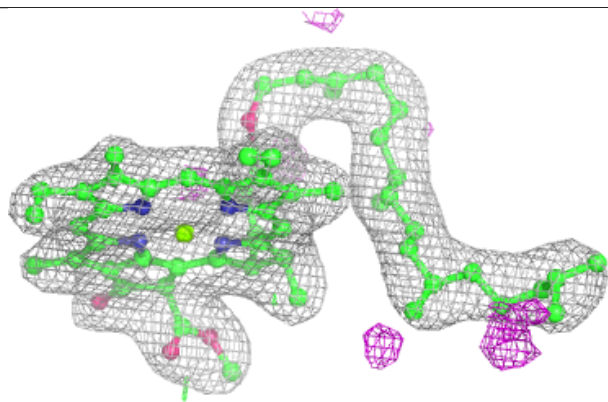
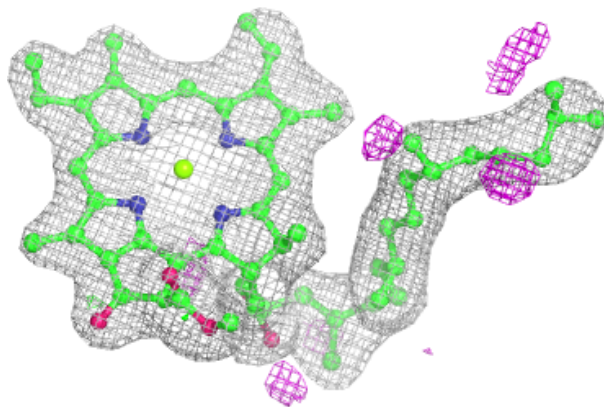
**Electron density around CLA a 404 (B):**

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

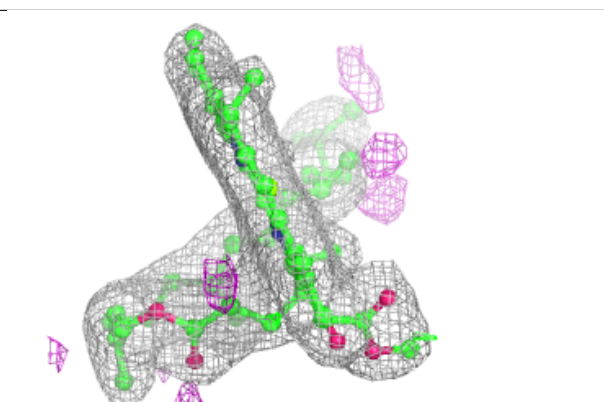
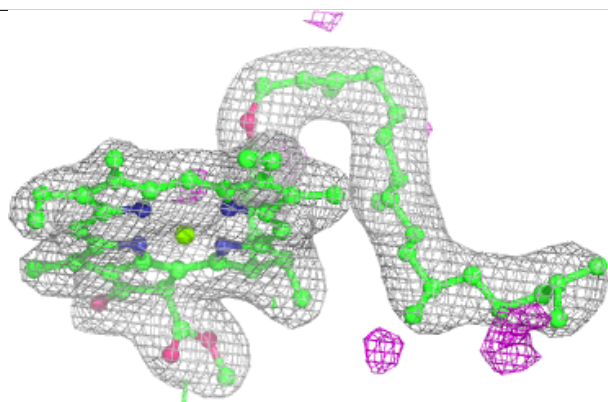
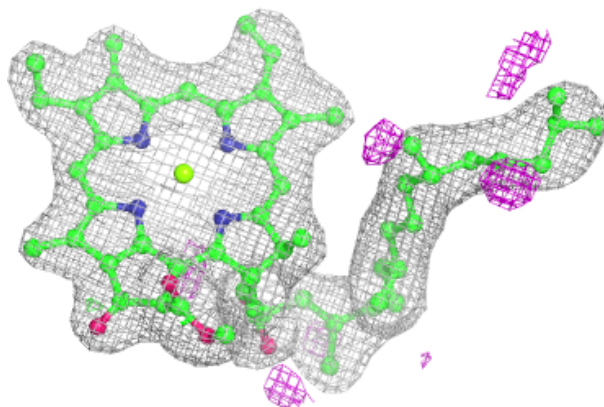


Electron density around CLA a 405 (A):

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

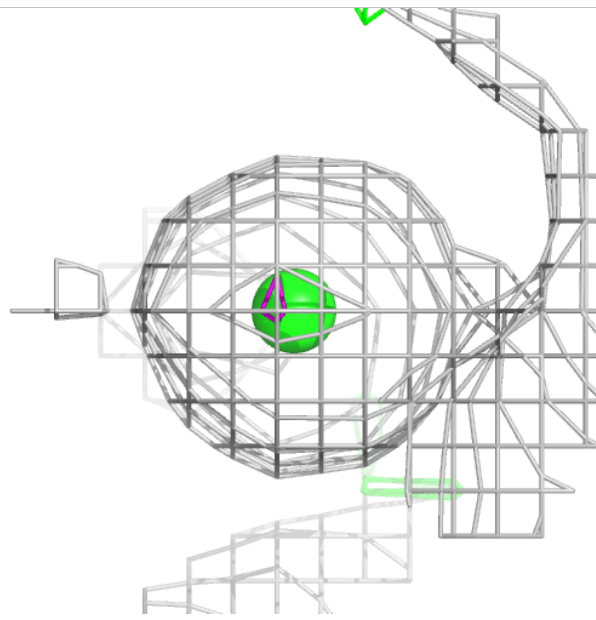
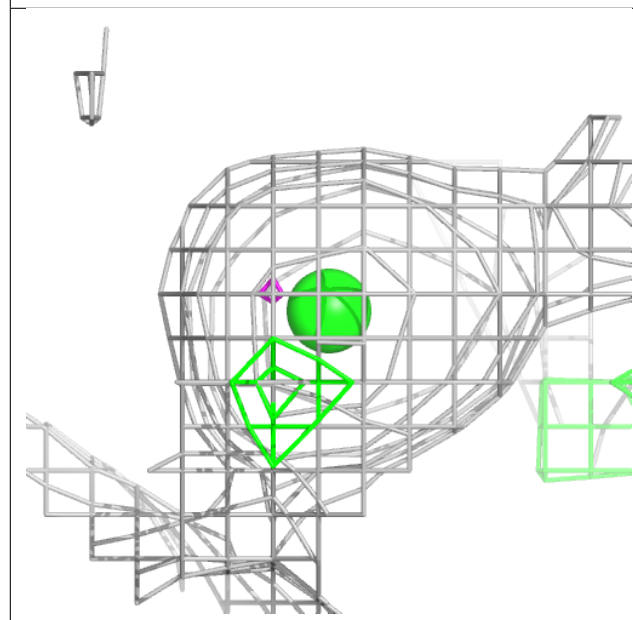
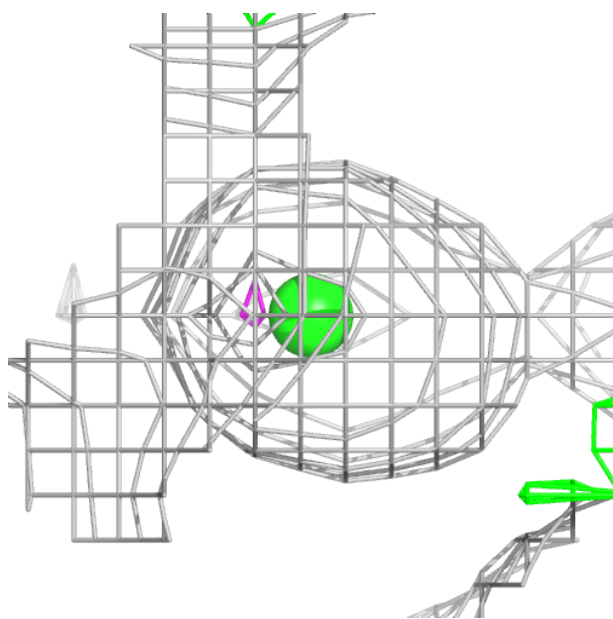
**Electron density around CLA a 405 (B):**

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



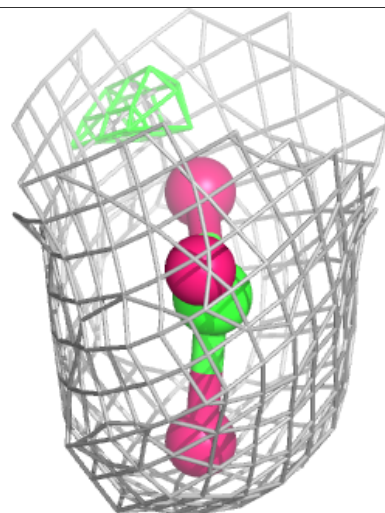
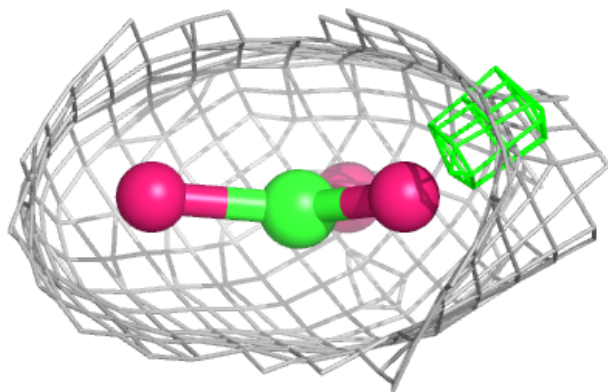
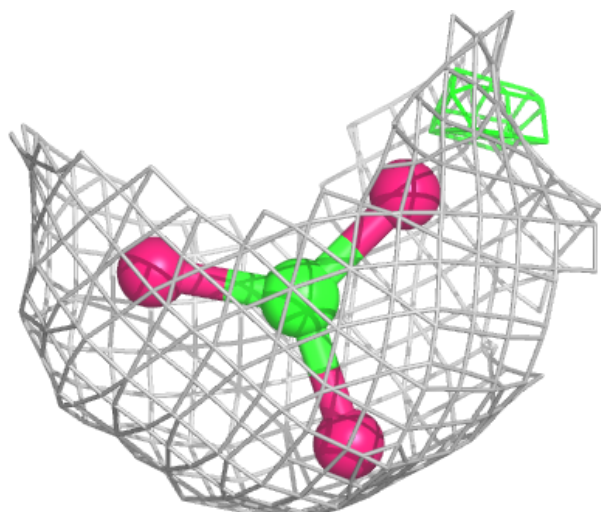
Electron density around CL a 403 (B):

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



Electron density around BCT A 416 (A):

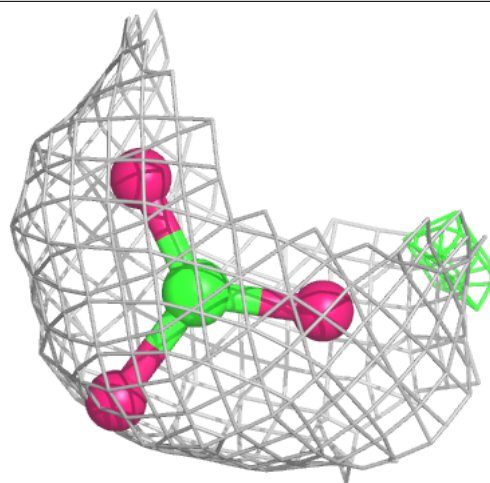
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



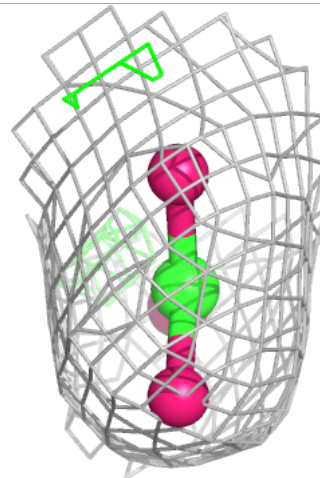
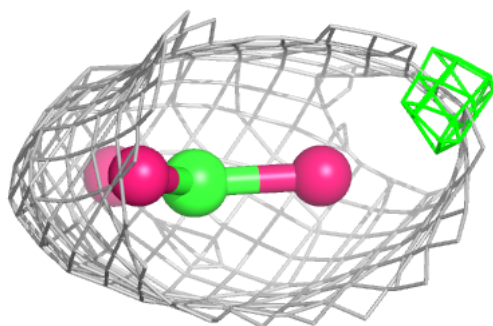
Electron density around BCT A 416 (B):

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

A

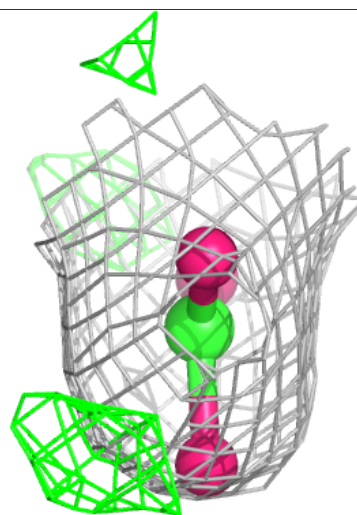
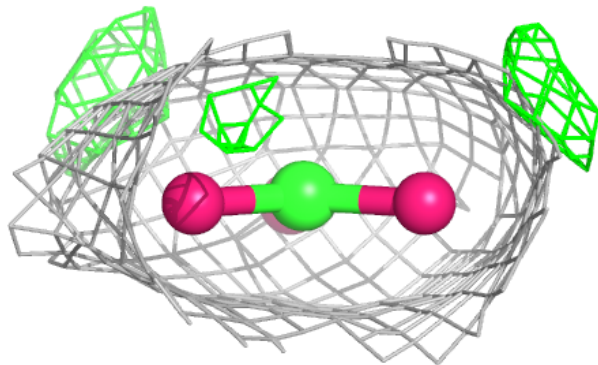
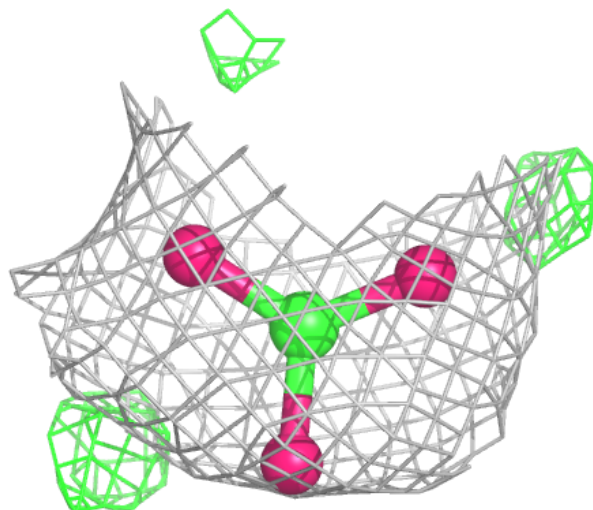


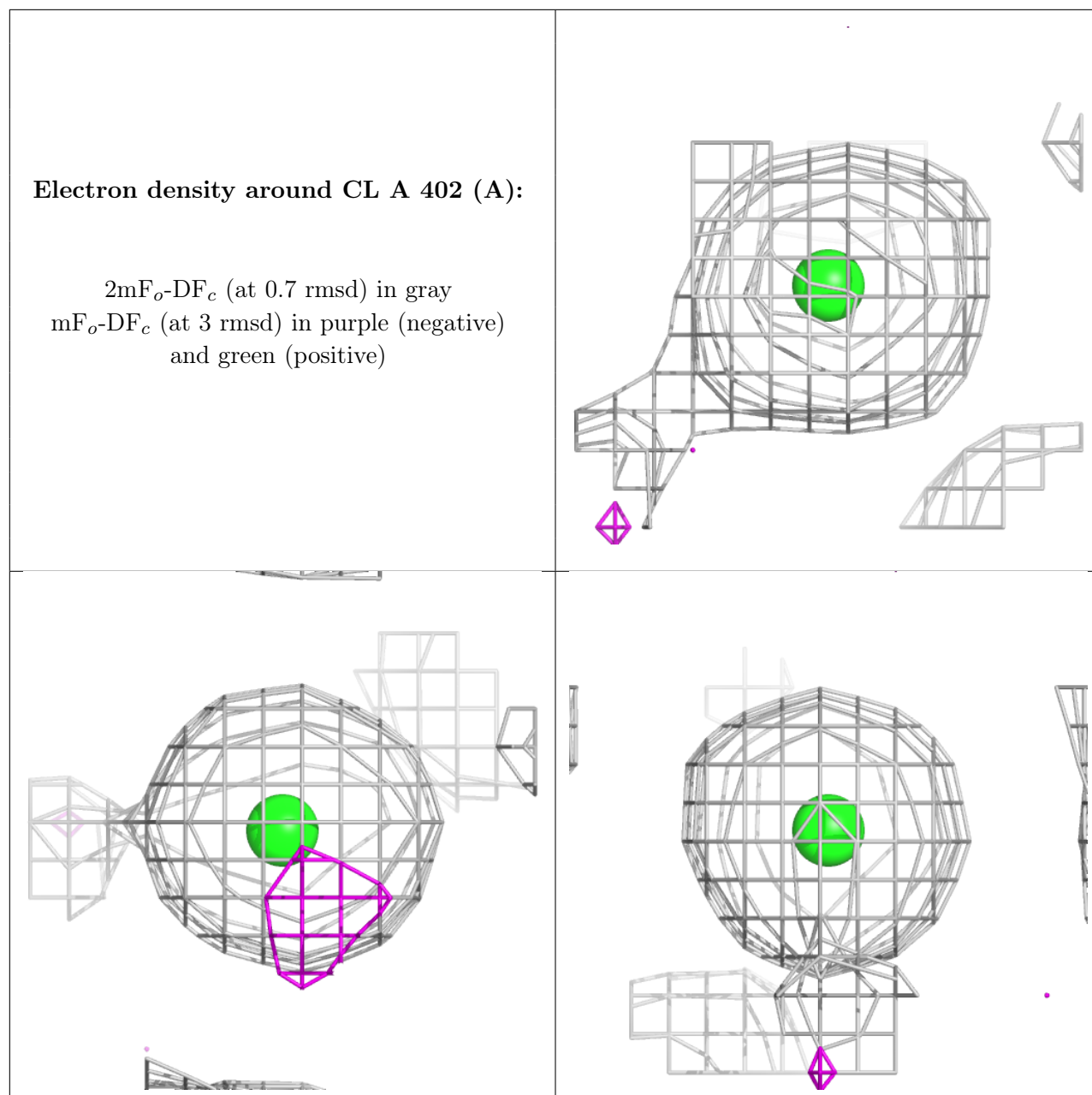
A

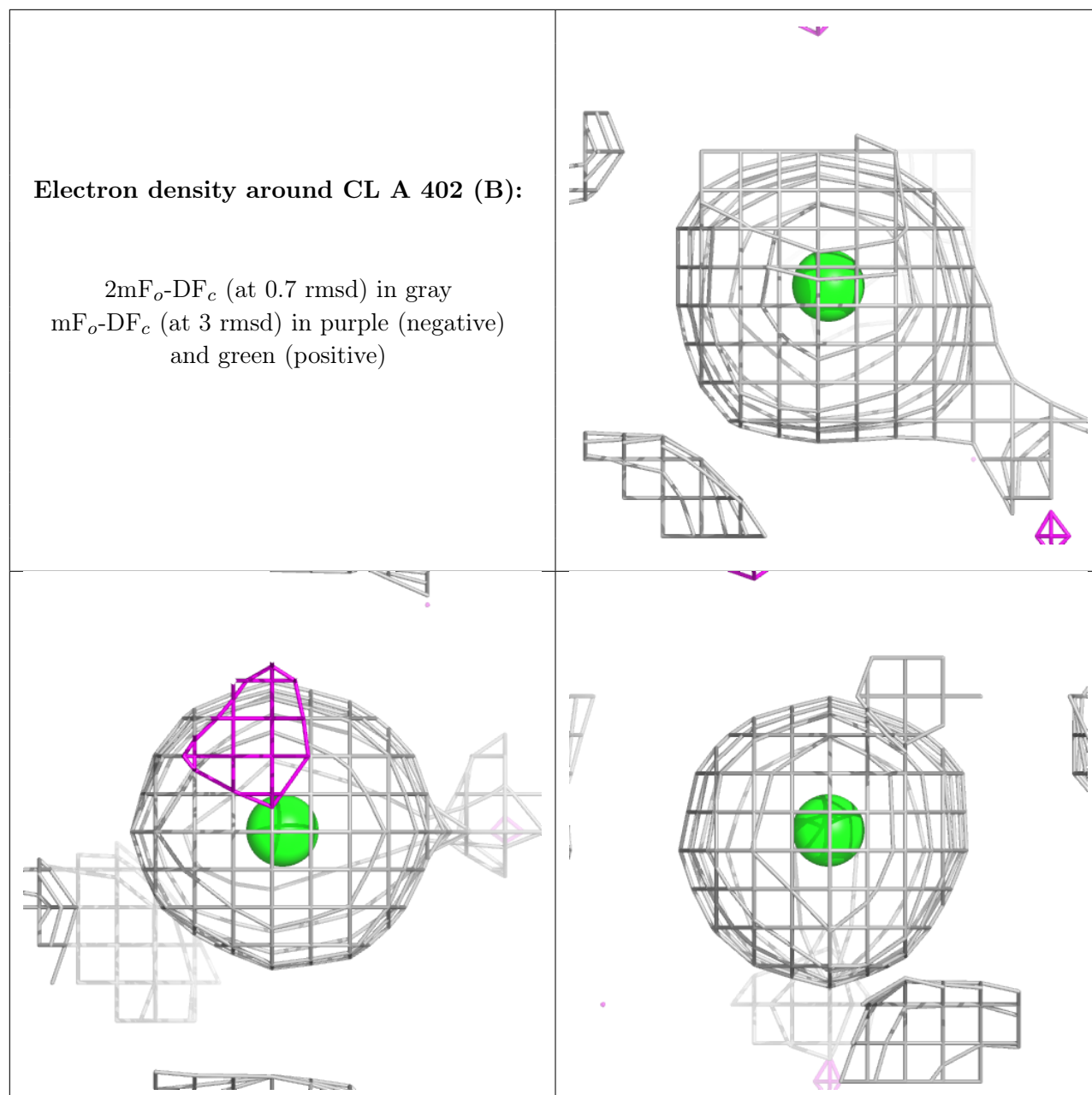


Electron density around BCT d 401 (A):

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

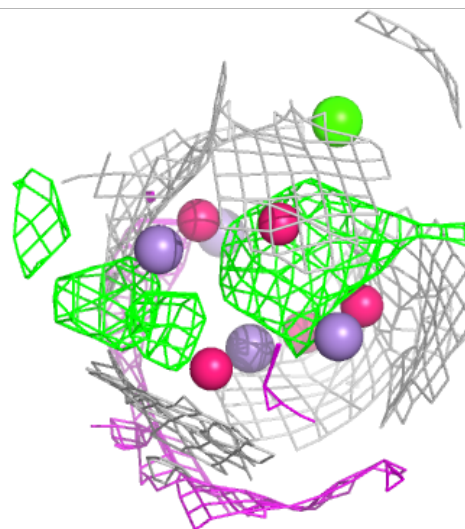
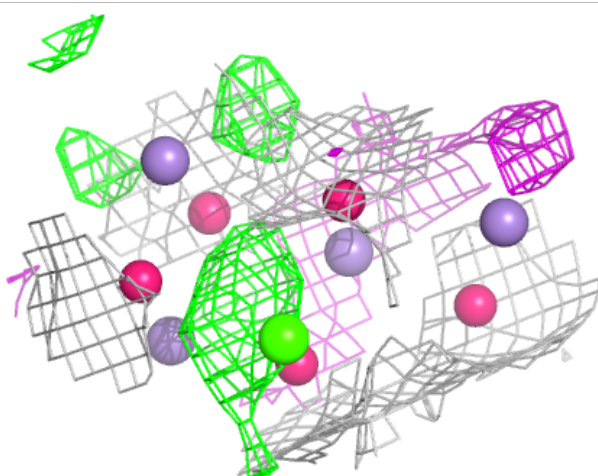
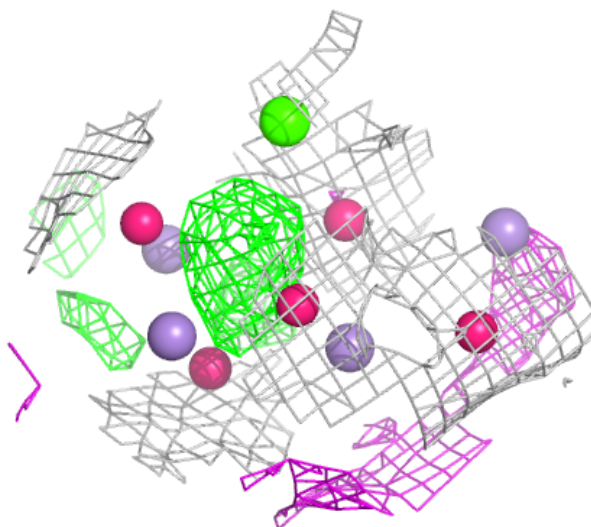






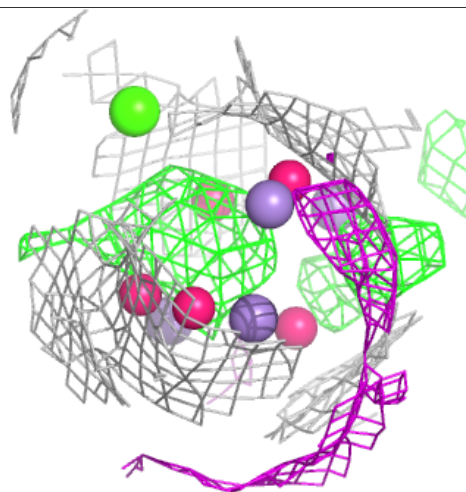
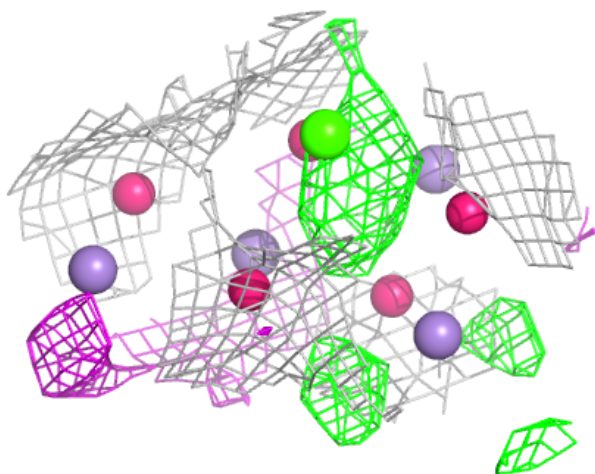
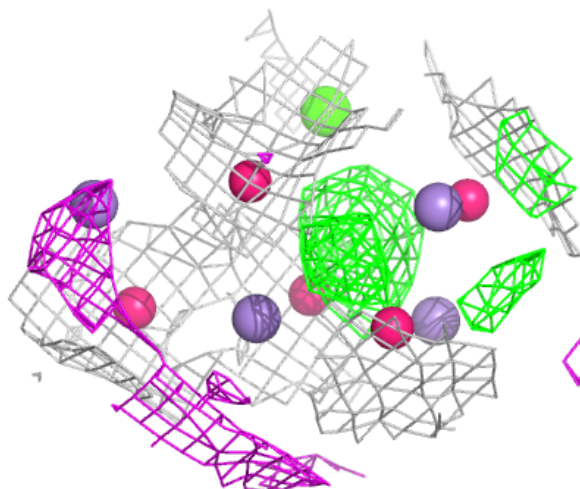
Electron density around OEX A 413 (A):

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



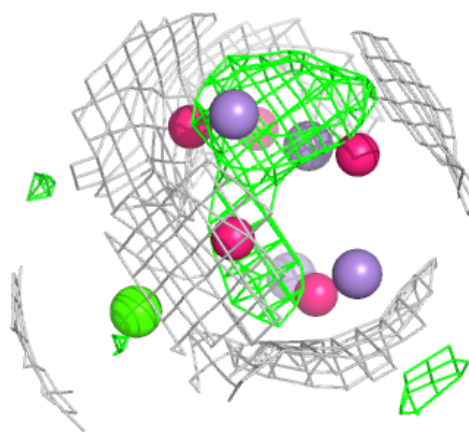
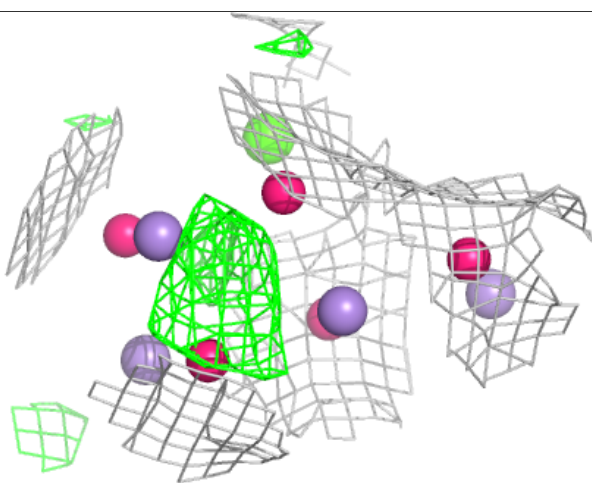
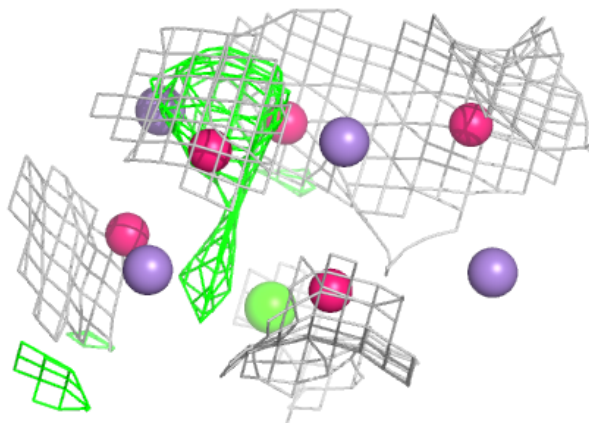
Electron density around OEX A 413 (B):

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



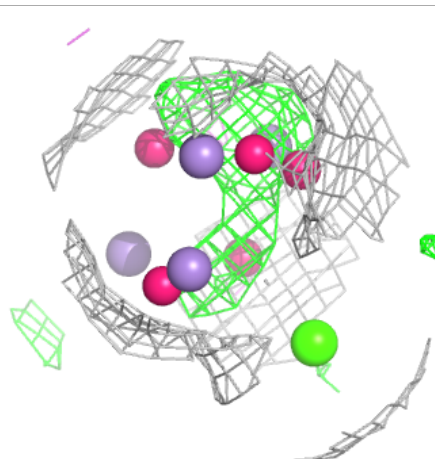
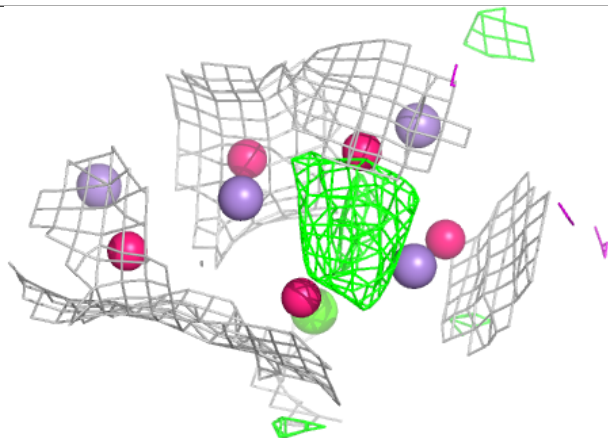
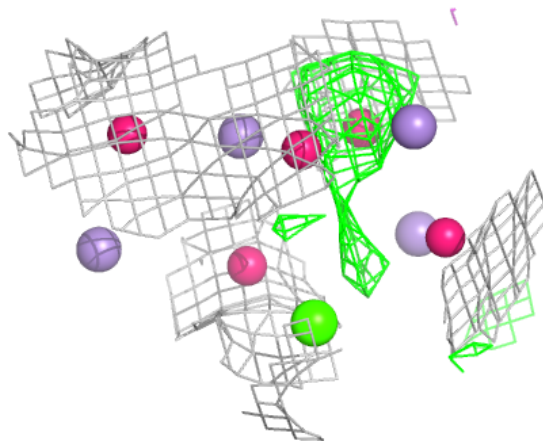
Electron density around OEX a 412 (A):

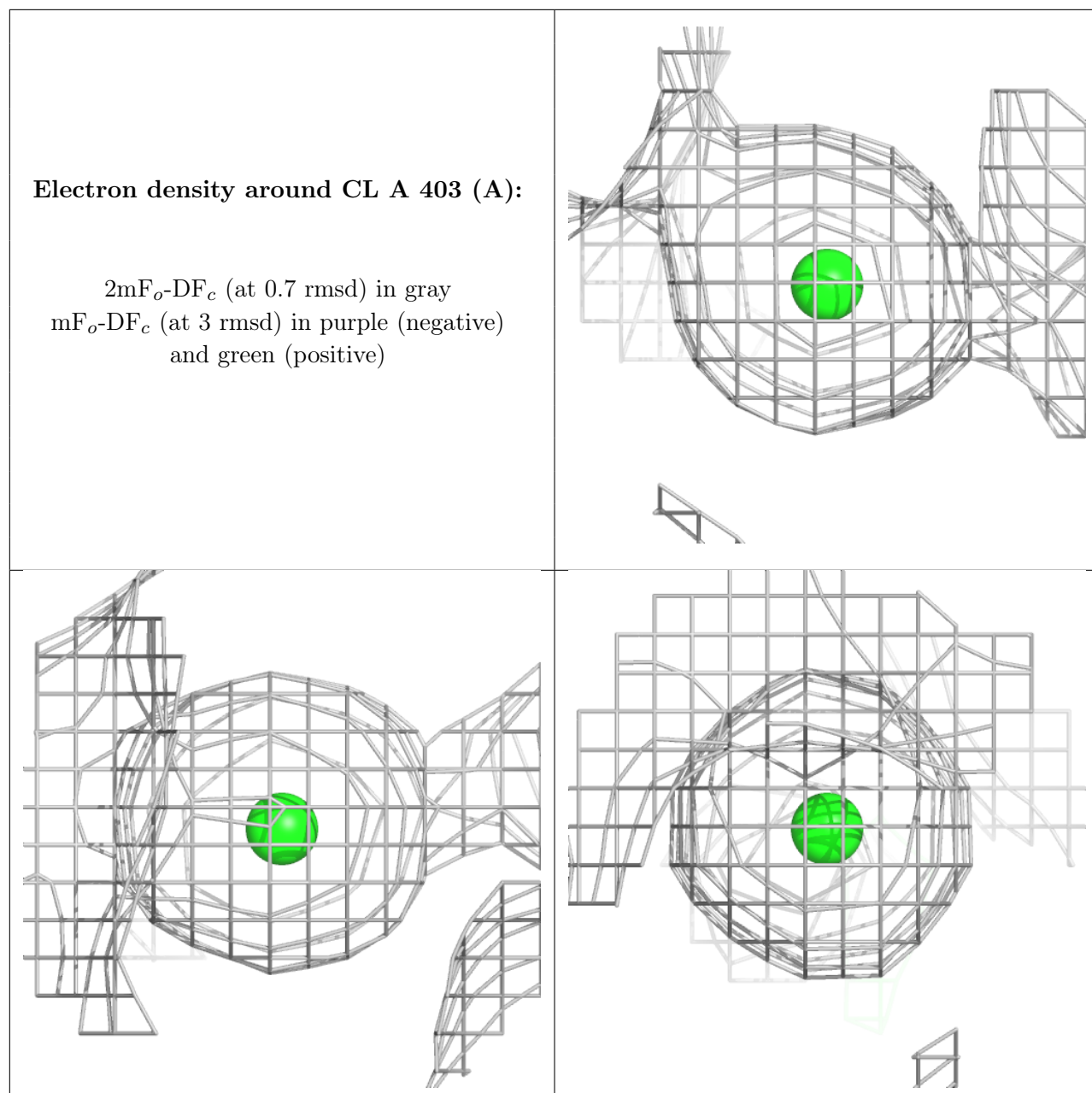
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

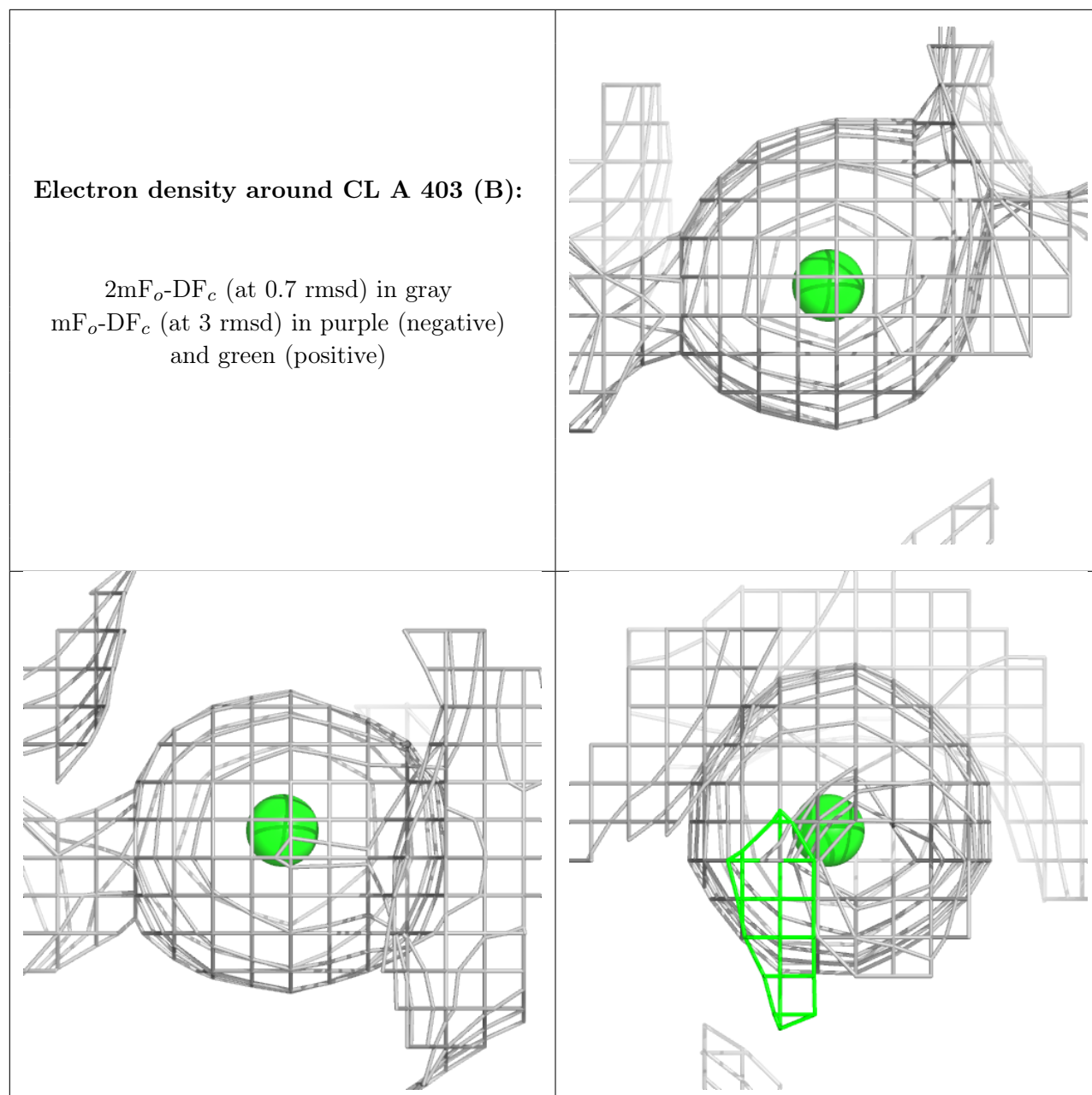


Electron density around OEX a 412 (B):

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

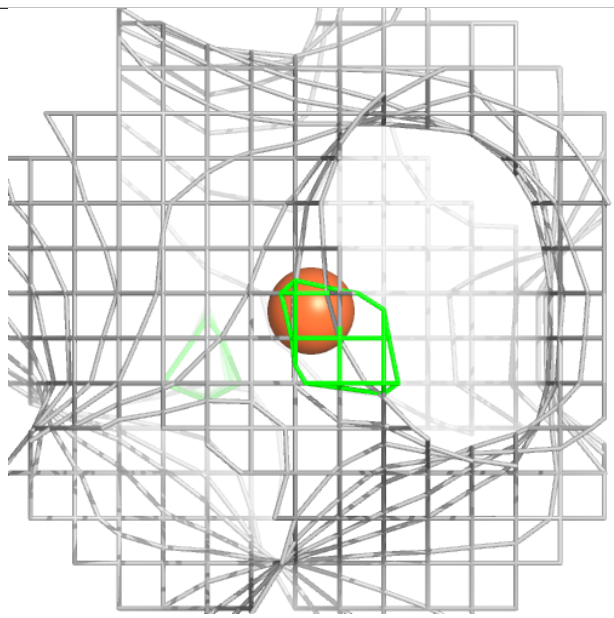
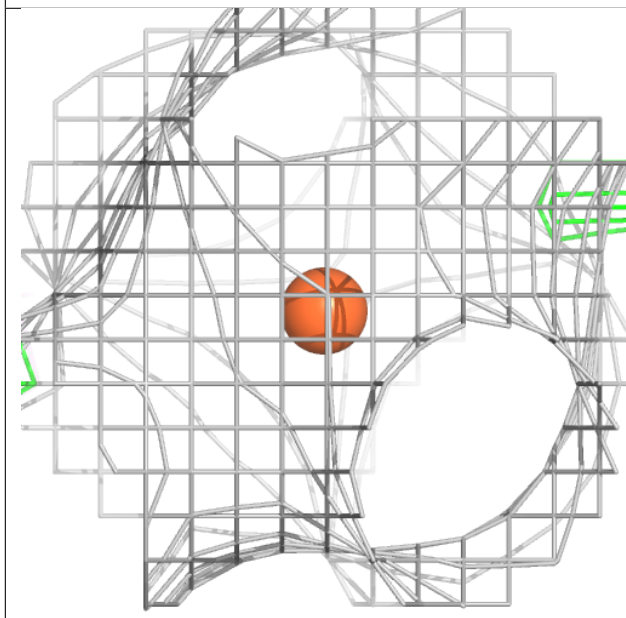
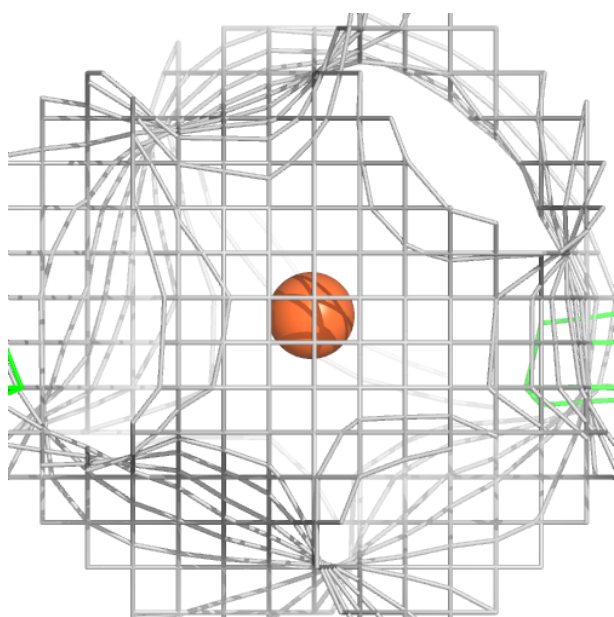


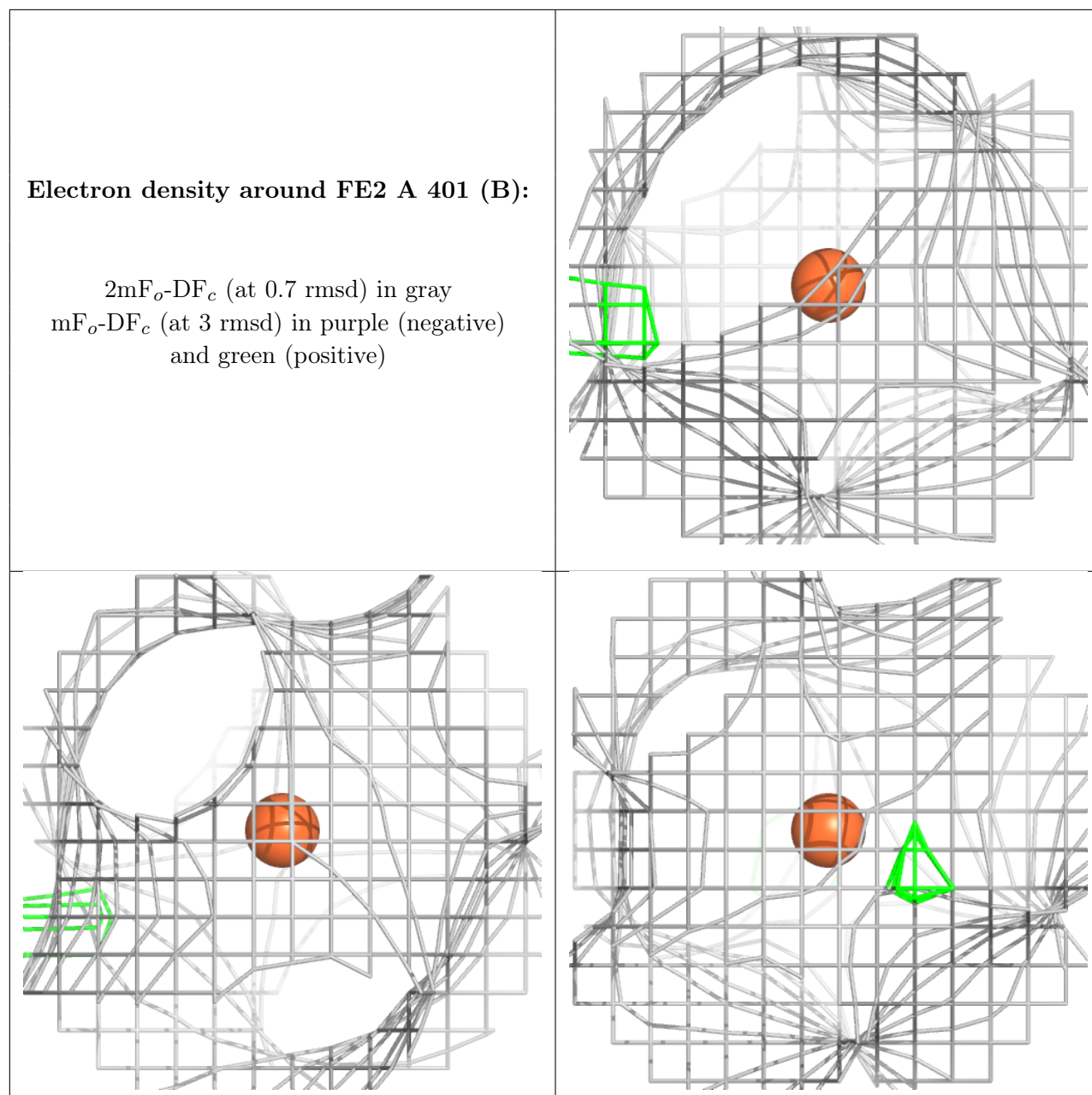




Electron density around FE2 A 401 (A):

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





6.5 Other polymers [i](#)

There are no such residues in this entry.