



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2024 – 02:26 PM JST

PDB ID : 8IRH
Title : XFEL structure of cyanobacterial photosystem II following two flashes (2F) with a 200-microsecond delay
Authors : Li, H.; Suga, M.; Shen, J.R.
Deposited on : 2023-03-17
Resolution : 2.25 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

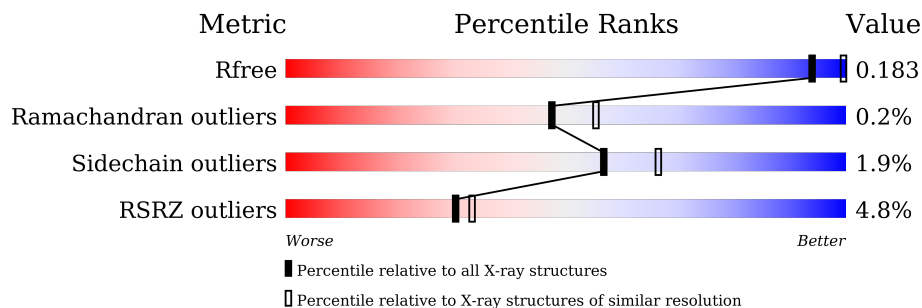
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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.



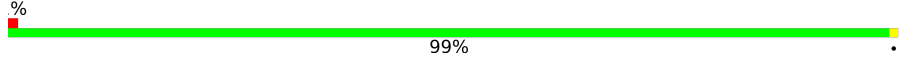
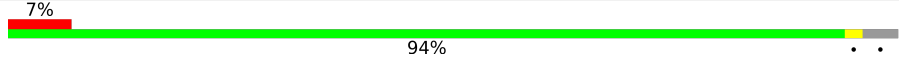
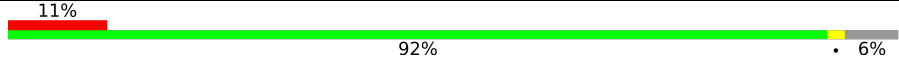

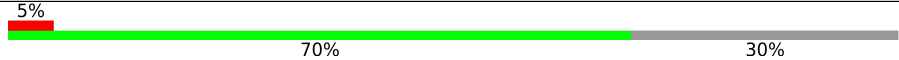
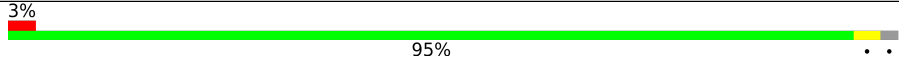
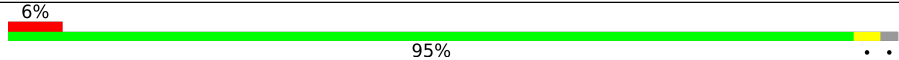
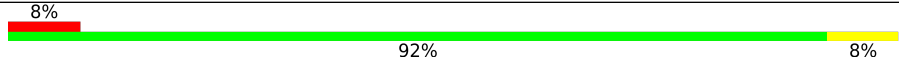
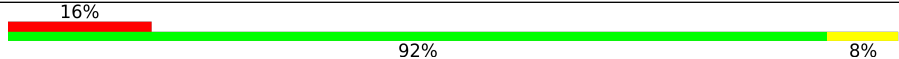
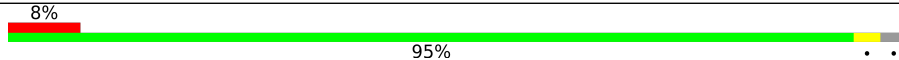
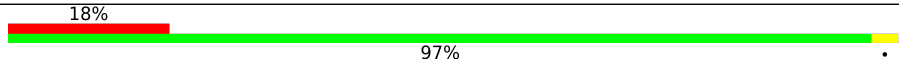
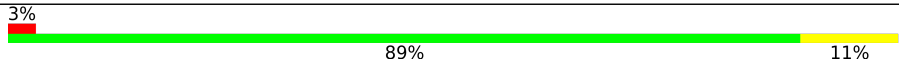
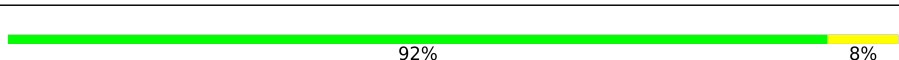
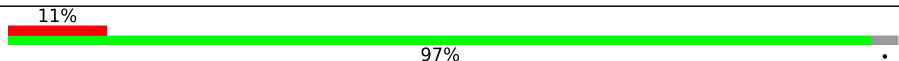
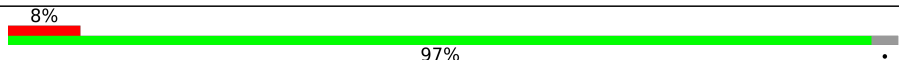
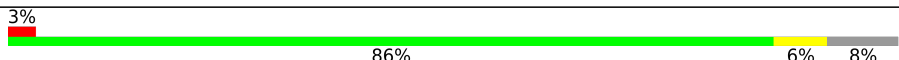
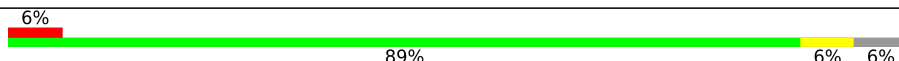
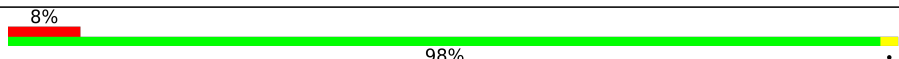
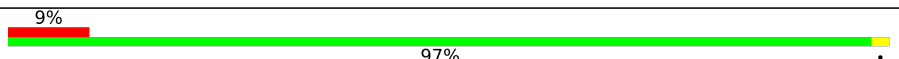

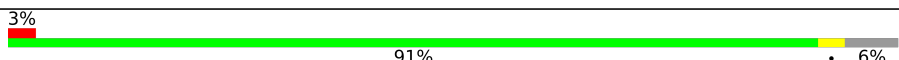
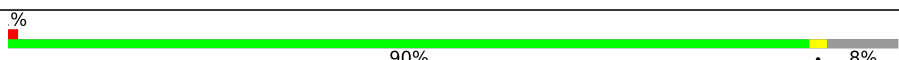
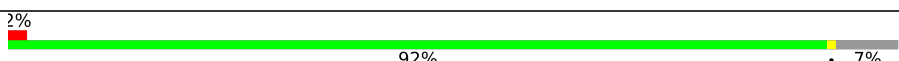
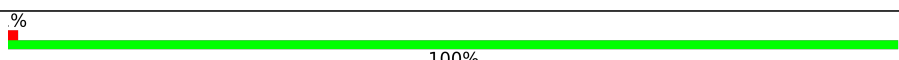
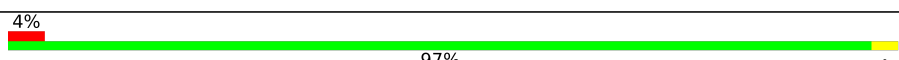
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1377 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	<p>96%</p>
1	a	344	<p>96%</p>
2	B	505	<p>99%</p>
2	b	505	<p>98%</p>
3	C	455	<p>98%</p>
3	c	455	<p>98%</p>
4	D	342	<p>99%</p>

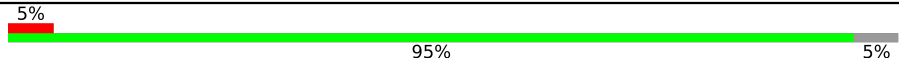
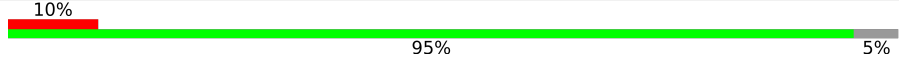
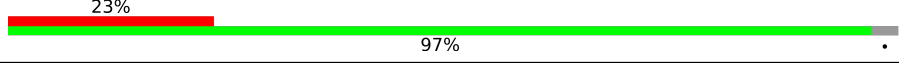
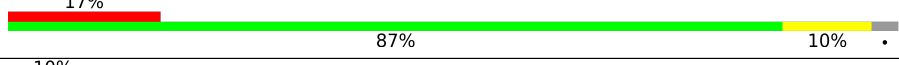
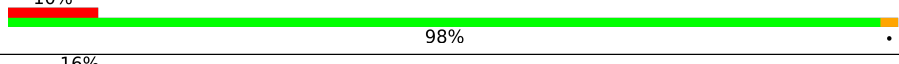
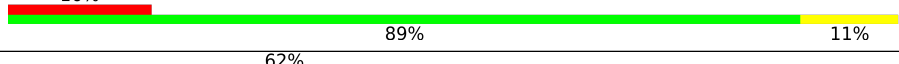
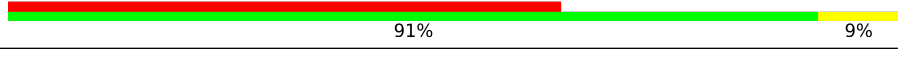
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Mol	Chain	Length	Quality of chain
4	d	342	 99%
5	E	84	 94%
5	e	84	 92% 6%
6	F	44	 77% 23%
6	f	44	 70% 30%
7	H	65	 95%
7	h	65	 95%
8	I	38	 92% 8%
8	i	38	 92% 8%
9	J	39	 95%
9	j	39	 97%
10	K	37	 89% 11%
10	k	37	 92% 8%
11	L	37	 97%
11	l	37	 97%
12	M	36	 86% 6% 8%
12	m	36	 89% 6% 6%
13	O	244	 98%
13	o	244	 97%
14	T	32	 88% 6% 6%
14	t	32	 91% 6%
15	U	104	 90% 8%
15	u	104	 92% 7%
16	V	137	 100%
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
24	CLA	A	405[A]	X	-	-	-
24	CLA	A	405[B]	X	-	-	-
24	CLA	A	406[A]	X	-	-	-
24	CLA	A	406[B]	X	-	-	-
24	CLA	A	409	X	-	-	-
24	CLA	B	601	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	C	514	X	-	-	-
24	CLA	D	402[A]	X	-	-	-
24	CLA	D	402[B]	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	a	405[A]	X	-	-	-
24	CLA	a	405[B]	X	-	-	-
24	CLA	a	406[A]	X	-	-	-
24	CLA	a	406[B]	X	-	-	-
24	CLA	a	409	X	-	-	-
24	CLA	b	601	X	-	-	-
24	CLA	b	602	X	-	-	-
24	CLA	b	603	X	-	-	-
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24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	c	502	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	c	514	X	-	-	-
24	CLA	d	403[A]	X	-	-	-
24	CLA	d	403[B]	X	-	-	-
24	CLA	d	404	X	-	-	-
28	GOL	a	418	-	-	-	X
31	UNL	c	525[A]	-	-	-	X
31	UNL	c	525[B]	-	-	-	X
32	LMT	F	101	-	-	-	X
32	LMT	c	501	-	-	-	X
32	LMT	e	102	-	-	-	X
34	HTG	b	622	-	-	-	X

2 Entry composition [i](#)

There are 42 unique types of molecules in this entry. The entry contains 62605 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	4330	2830	716	759	25	0	221	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	4146	2721	692	720	13	0	20	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	4260	2788	713	741	18	0	97	0
3	c	455	4308	2821	719	750	18	0	100	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	114	0
			3620	2387	596	622	15			
4	d	341	Total	C	N	O	S	0	116	0
			3628	2391	599	623	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	S	0	0	0
			662	432	107	123				
5	e	79	Total	C	N	O	S	0	2	0
			670	439	110	121				

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	0	0
			293	204	43	46			
10	k	37	Total	C	N	O	0	0	0
			293	204	43	46			

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	96	Total	C	N	O	0	4	0
			800	508	133	159			
15	u	97	Total	C	N	O	0	4	0
			807	513	134	160			

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

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

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

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

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

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

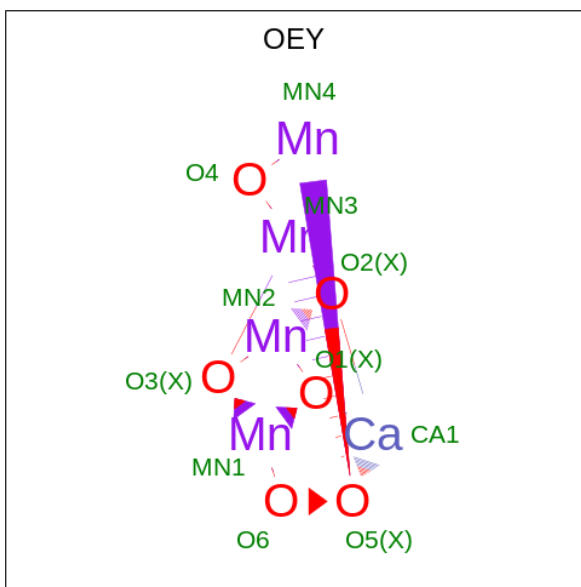
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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

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

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

- Molecule 21 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula: CaMn_4O_6).



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

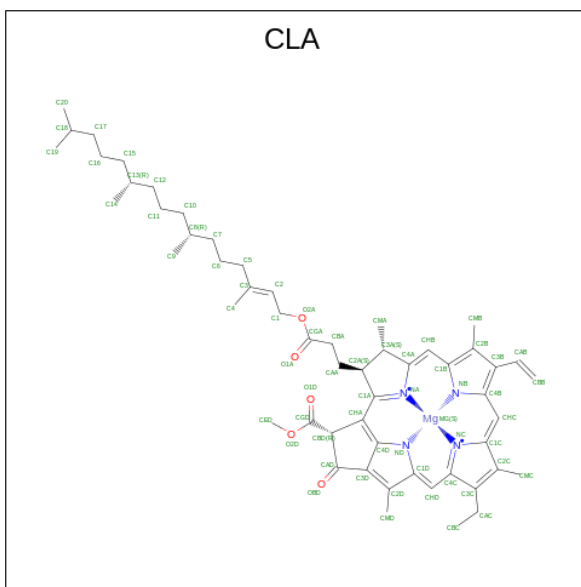
- Molecule 22 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 23 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



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

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

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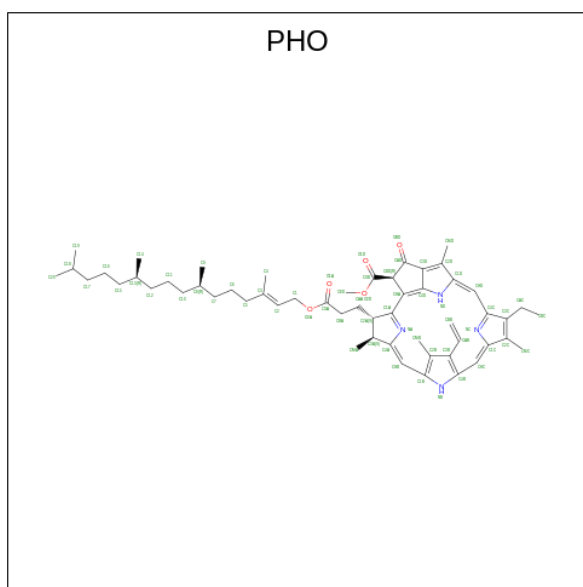
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
24	a	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
24	a	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65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

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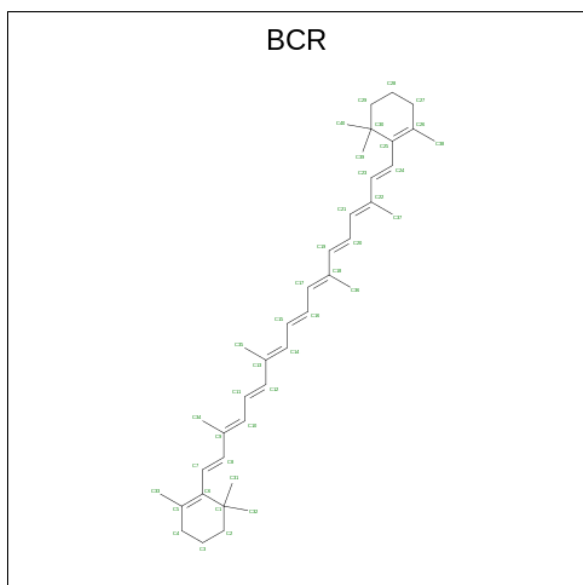
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



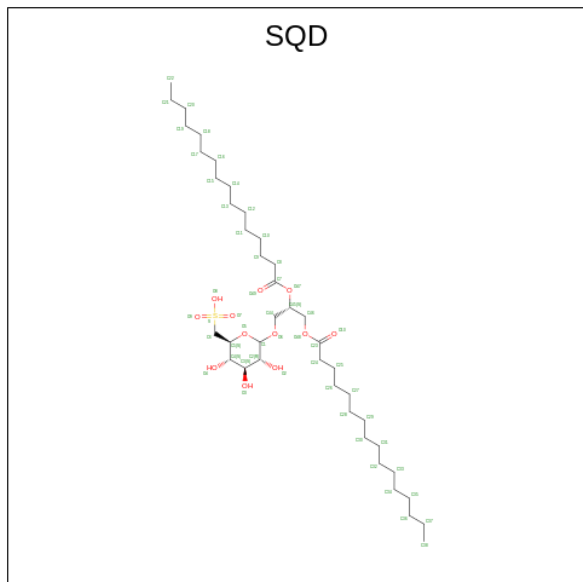
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
25	A	1	Total	C	N	O	0	1
			128	110	8	10		
25	A	1	Total	C	N	O	0	1
			128	110	8	10		
25	a	1	Total	C	N	O	0	1
			128	110	8	10		
25	d	1	Total	C	N	O	0	1
			128	110	8	10		

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



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

- Molecule 27 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		
27	A	1	Total 108	C 82	O 24	S 2	0	1
27	A	1	Total 54	C 41	O 12	S 1	0	0
27	B	1	Total 54	C 41	O 12	S 1	0	0
27	L	1	Total 54	C 41	O 12	S 1	0	0
27	X	1	Total 43	C 30	O 12	S 1	0	0
27	a	1	Total 108	C 82	O 24	S 2	0	1
27	a	1	Total 54	C 41	O 12	S 1	0	0
27	f	1	Total 43	C 30	O 12	S 1	0	0

- Molecule 28 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



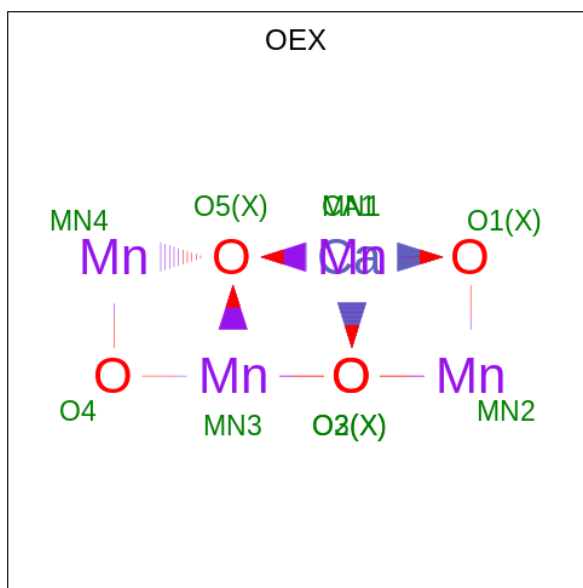
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 6 3 3	0	0
28	A	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	C	1	Total C O 12 6 6	0	1
28	D	1	Total C O 6 3 3	0	0
28	O	1	Total C O 6 3 3	0	0
28	O	1	Total C O 6 3 3	0	0
28	V	1	Total C O 12 6 6	0	1
28	a	1	Total C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

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

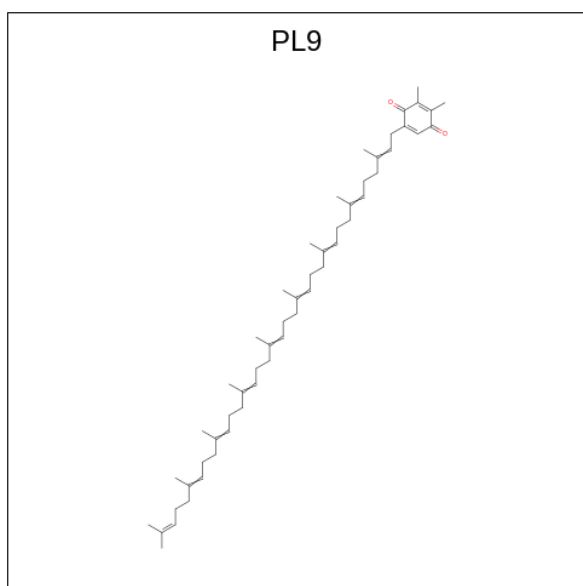
- Molecule 29 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 30 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
30	A	1	Total	C	O	0	1
			110	106	4		
30	D	1	Total	C	O	0	1
			110	106	4		
30	a	1	Total	C	O	0	1
			110	106	4		
30	d	1	Total	C	O	0	1
			110	106	4		

- Molecule 31 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

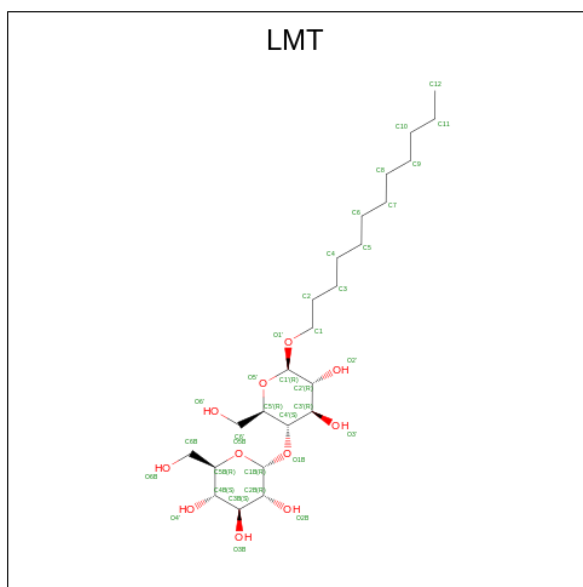
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			28	23	5		
31	B	2	Total	C	O	0	0
			73	63	10		
31	D	2	Total	C	O	0	0
			57	51	6		
31	I	1	Total	C	O	0	0
			40	35	5		
31	J	1	Total	C		0	0
			10	10			
31	K	1	Total	C	O	0	1
			68	58	10		
31	M	1	Total	C		0	0
			10	10			

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

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



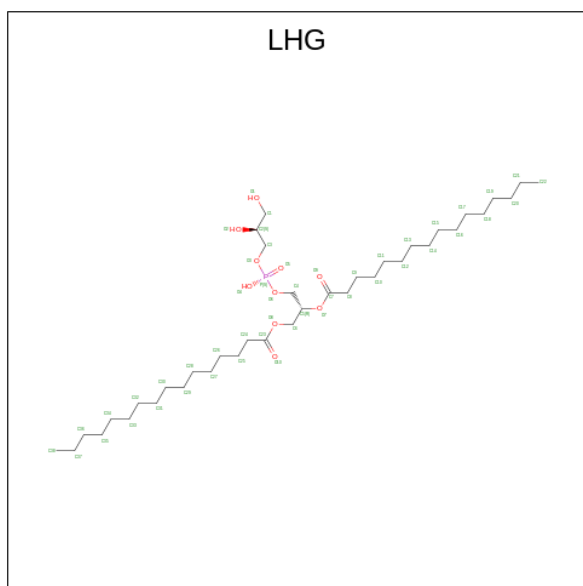
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			35	24	11		
32	A	1	Total	C	O	0	0
			35	24	11		
32	B	1	Total	C	O	0	0
			35	24	11		

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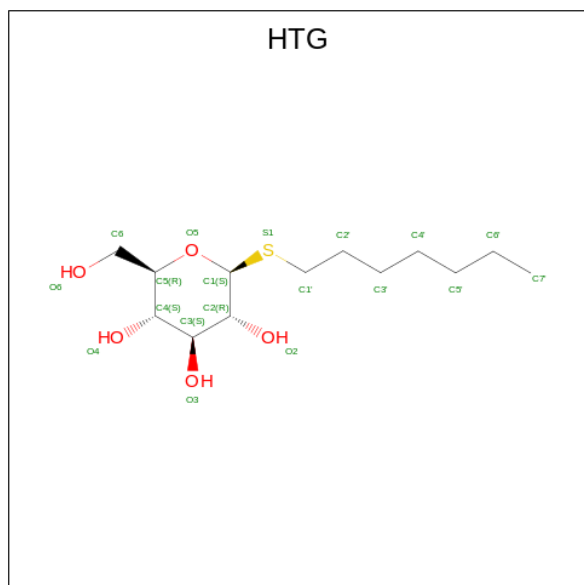
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	B	1	Total	C	O	0	0
			35	24	11		
32	B	1	Total	C	O	0	0
			25	19	6		
32	F	1	Total	C	O	0	0
			35	24	11		
32	M	1	Total	C	O	0	0
			35	24	11		
32	M	1	Total	C	O	0	0
			35	24	11		
32	b	1	Total	C	O	0	0
			25	19	6		
32	b	1	Total	C	O	0	0
			25	19	6		
32	c	1	Total	C	O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

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



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

- Molecule 34 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: C₁₃H₂₆O₅S).



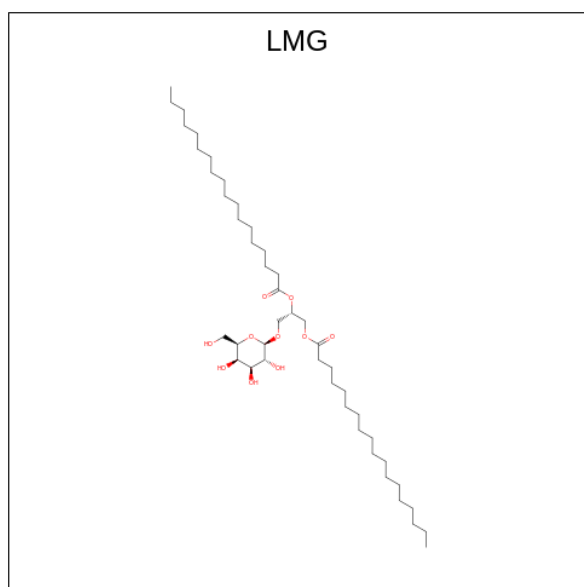
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	O	S	0	0
			19	13	5	1		

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

- Molecule 35 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



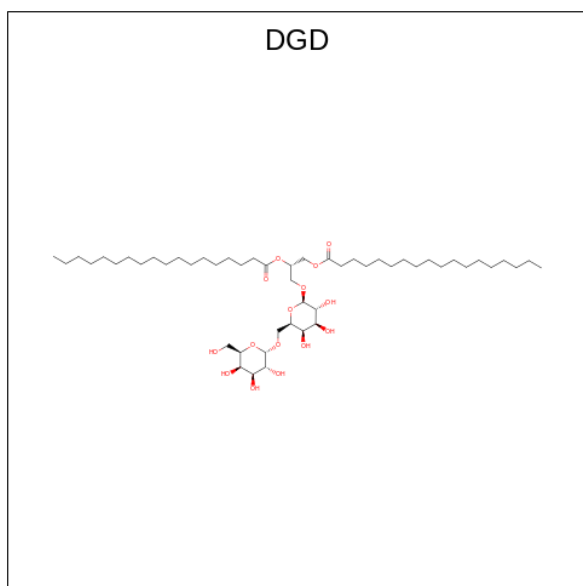
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
35	C	1	Total 51	C 41	O 10	0	0

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

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

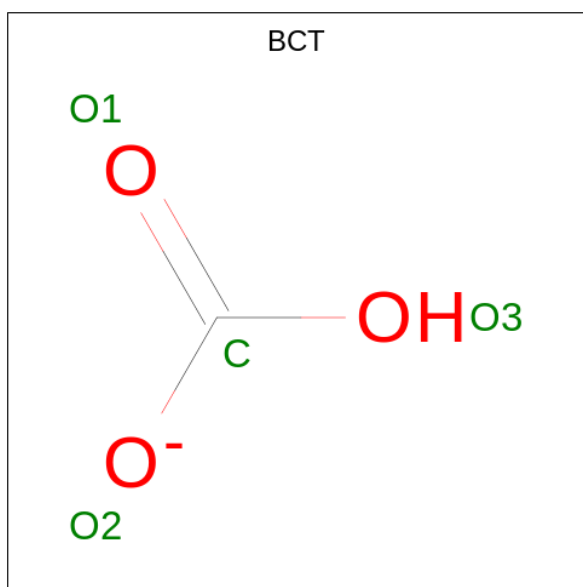


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	C	1	Total C O 124 94 30	0	1
36	C	1	Total C O 124 94 30	0	1
36	C	1	Total C O 62 47 15	0	0
36	H	1	Total C O 62 47 15	0	0
36	c	1	Total C O 124 94 30	0	1
36	c	1	Total C O 124 94 30	0	1
36	c	1	Total C O 62 47 15	0	0
36	h	1	Total C O 62 47 15	0	0

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

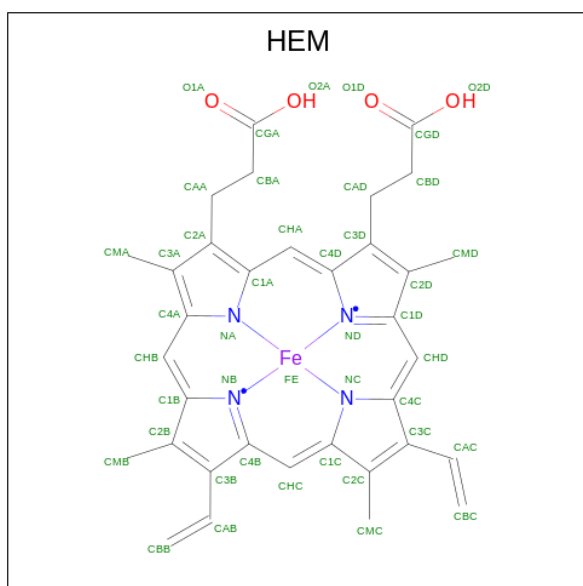
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	C	1	Total Ca 1 1	0	0
37	F	1	Total Ca 1 1	0	0
37	O	1	Total Ca 1 1	0	0
37	c	2	Total Ca 2 2	0	0
37	f	1	Total Ca 1 1	0	0
37	o	1	Total Ca 1 1	0	0

- Molecule 38 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 39 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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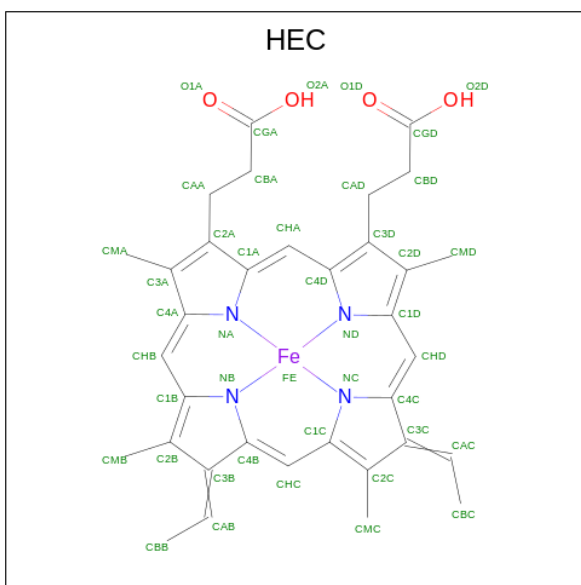
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
39	e	1	43	34	1	4	4	0	0

- Molecule 40 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 41 is HEME C (three-letter code: HEC) (formula: C₃₄H₃₄FeN₄O₄).



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

- Molecule 42 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
42	A	137	218	218	0	84
42	B	183	186	186	0	3

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
42	C	166	Total O 203 203	0	37
42	D	123	Total O 158 158	0	35
42	E	16	Total O 16 16	0	0
42	F	5	Total O 5 5	0	0
42	H	24	Total O 24 24	0	0
42	I	7	Total O 7 7	0	0
42	J	7	Total O 7 7	0	0
42	K	5	Total O 5 5	0	0
42	L	9	Total O 10 10	0	1
42	M	10	Total O 10 10	0	0
42	O	101	Total O 105 105	0	4
42	T	10	Total O 13 13	0	3
42	U	46	Total O 49 49	0	3
42	V	82	Total O 84 84	0	2
42	X	8	Total O 8 8	0	0
42	a	130	Total O 208 208	0	80
42	b	203	Total O 206 206	0	3
42	c	158	Total O 191 191	0	33
42	d	118	Total O 151 151	0	33
42	e	8	Total O 8 8	0	0
42	f	3	Total O 3 3	0	0

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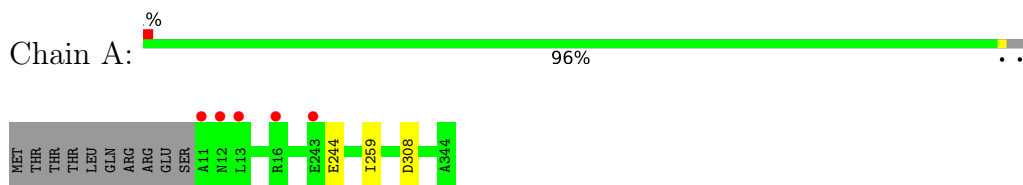
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
42	h	18	Total O 18 18	0	0
42	i	3	Total O 3 3	0	0
42	j	2	Total O 2 2	0	0
42	k	3	Total O 3 3	0	0
42	l	8	Total O 9 9	0	1
42	m	9	Total O 9 9	0	0
42	o	97	Total O 102 102	0	5
42	t	8	Total O 11 11	0	3
42	u	50	Total O 51 51	0	1
42	v	59	Total O 62 62	0	3
42	x	8	Total O 8 8	0	0
42	y	2	Total O 2 2	0	0

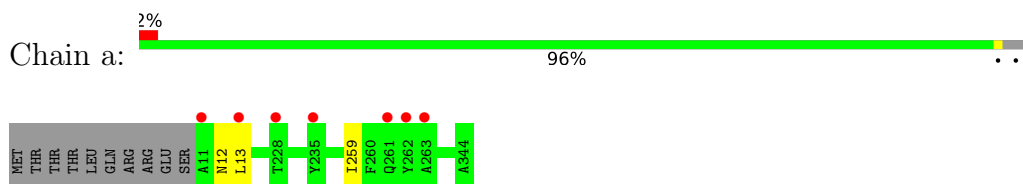
3 Residue-property plots [i](#)

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.

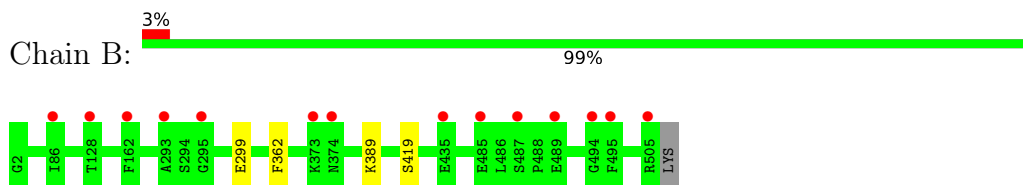
- Molecule 1: Photosystem II protein D1



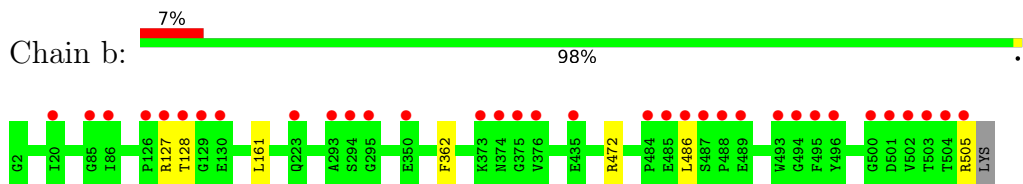
- Molecule 1: Photosystem II protein D1



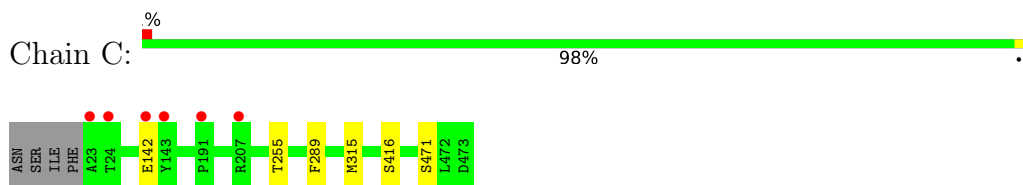
- Molecule 2: Photosystem II CP47 reaction center protein



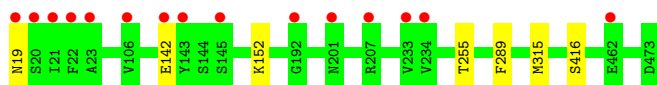
- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein



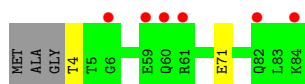
- Molecule 4: Photosystem II D2 protein



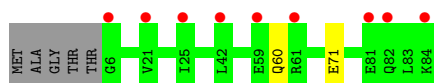
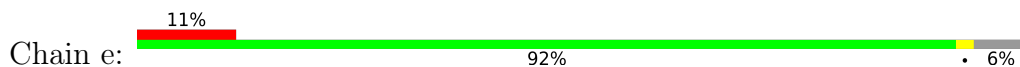
- Molecule 4: Photosystem II D2 protein



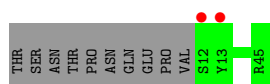
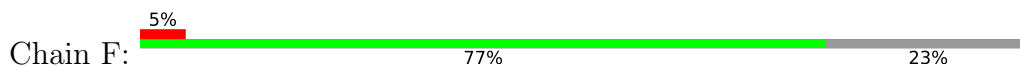
- Molecule 5: Cytochrome b559 subunit alpha



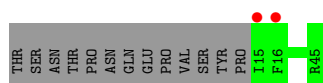
- Molecule 5: Cytochrome b559 subunit alpha



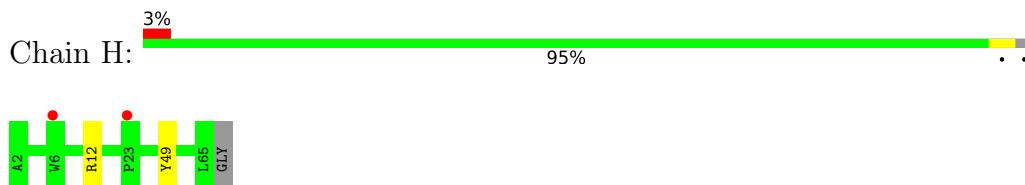
- Molecule 6: Cytochrome b559 subunit beta



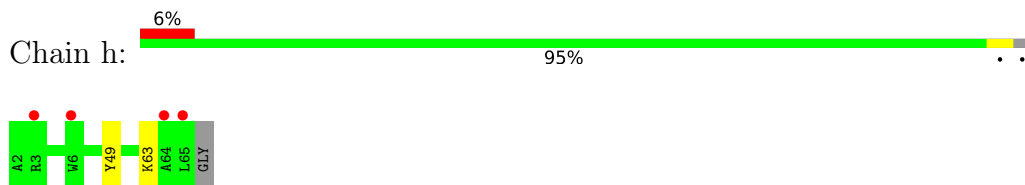
- Molecule 6: Cytochrome b559 subunit beta



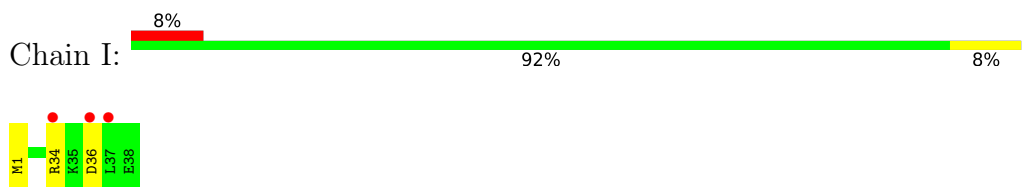
- Molecule 7: Photosystem II reaction center protein H



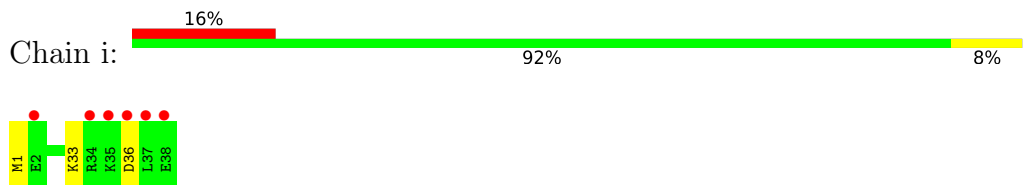
- Molecule 7: Photosystem II reaction center protein H



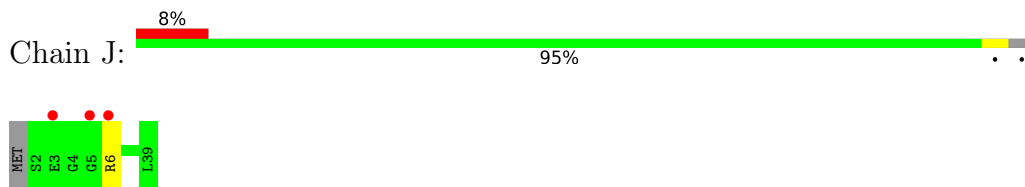
- Molecule 8: Photosystem II reaction center protein I



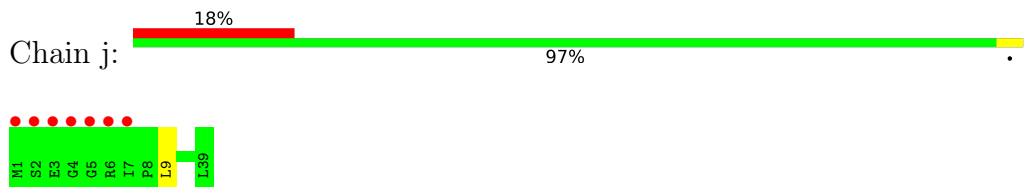
- Molecule 8: Photosystem II reaction center protein I



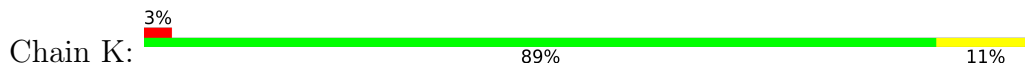
- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K

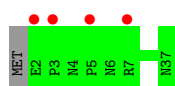




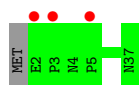
- Molecule 10: Photosystem II reaction center protein K



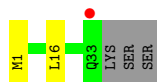
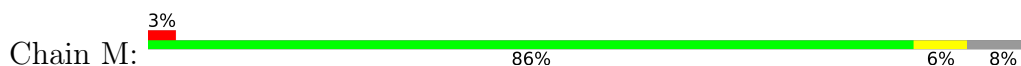
- Molecule 11: Photosystem II reaction center protein L



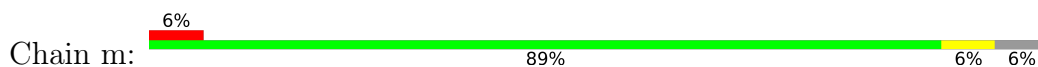
- Molecule 11: Photosystem II reaction center protein L



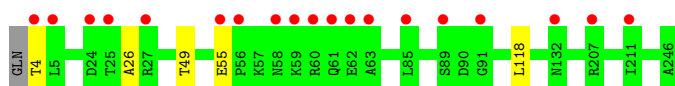
- Molecule 12: Photosystem II reaction center protein M



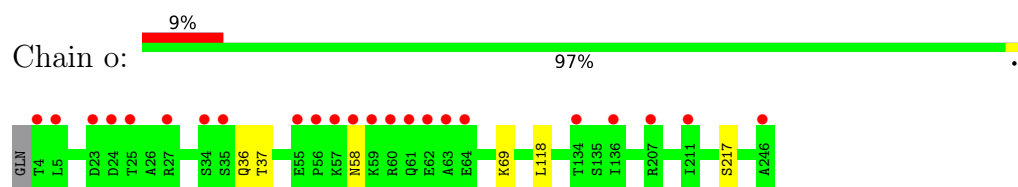
- Molecule 12: Photosystem II reaction center protein M



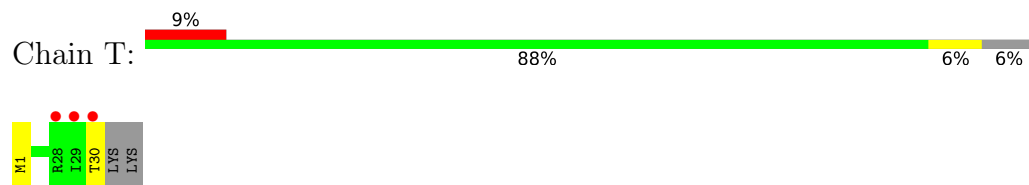
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



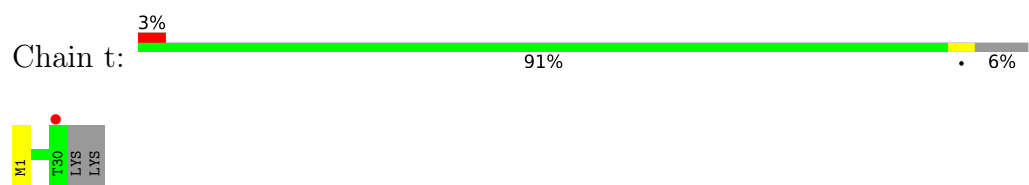
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



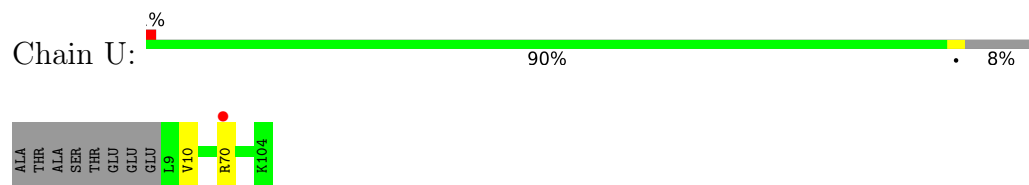
- Molecule 14: Photosystem II reaction center protein T



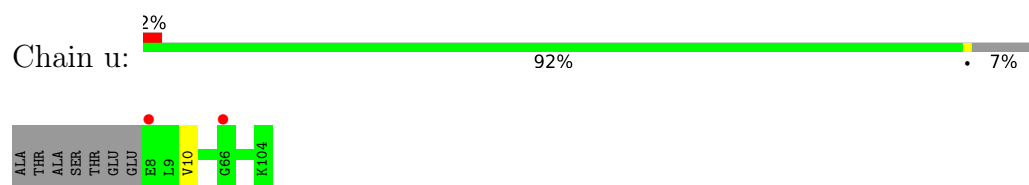
- Molecule 14: Photosystem II reaction center protein T



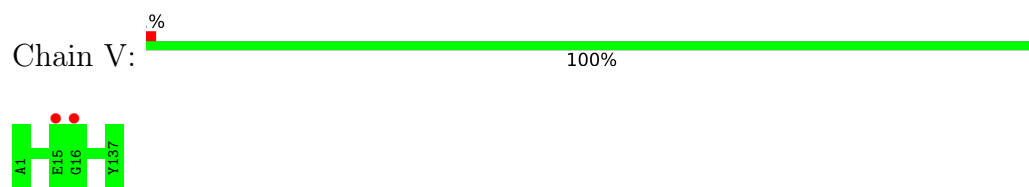
- Molecule 15: Photosystem II 12 kDa extrinsic protein



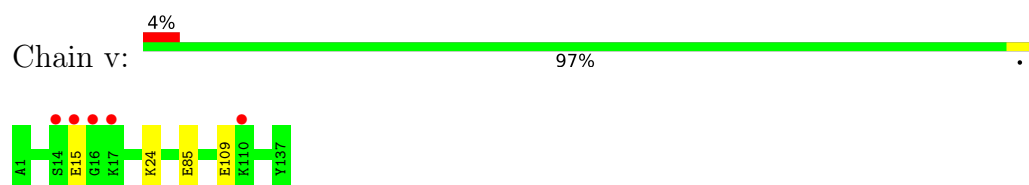
- Molecule 15: Photosystem II 12 kDa extrinsic protein



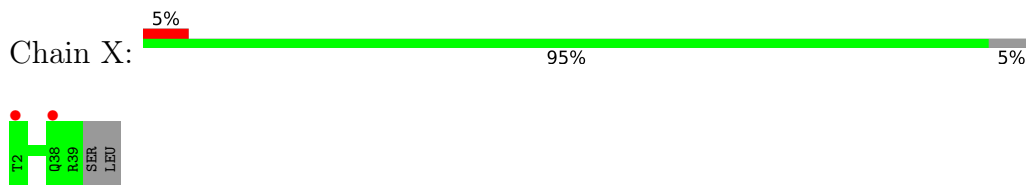
- Molecule 16: Cytochrome c-550



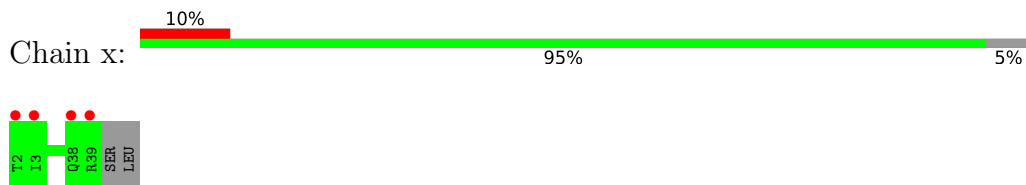
- Molecule 16: Cytochrome c-550



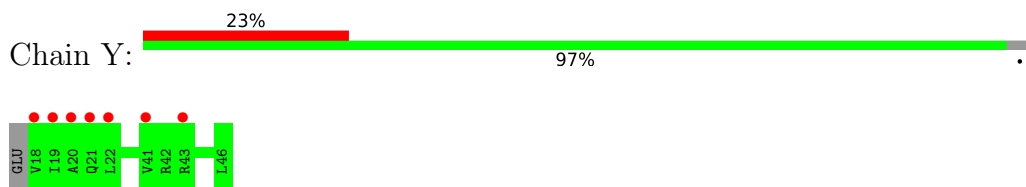
- Molecule 17: Photosystem II reaction center protein X



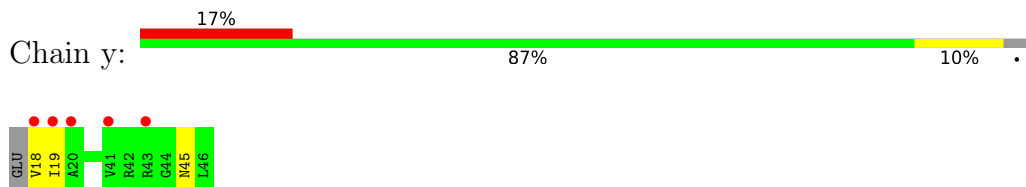
- Molecule 17: Photosystem II reaction center protein X



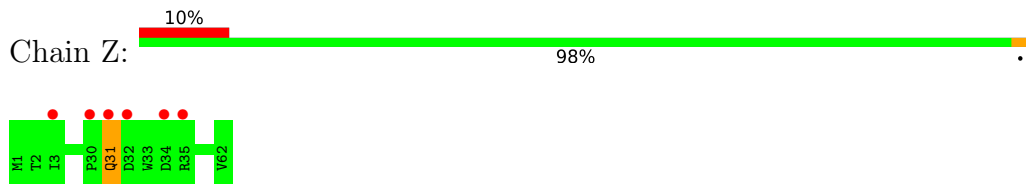
- Molecule 18: Photosystem II reaction center protein Ycf12



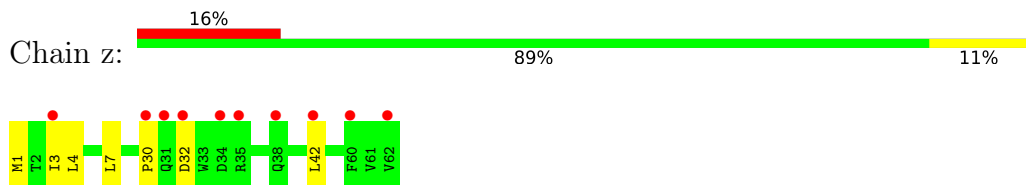
- Molecule 18: Photosystem II reaction center protein Ycf12



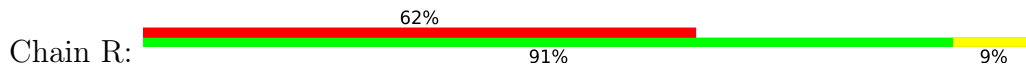
- Molecule 19: Photosystem II reaction center protein Z

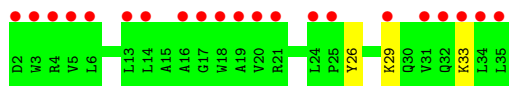


- Molecule 19: Photosystem II reaction center protein Z



- 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	125.77Å 231.76Å 288.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.25 19.99 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.25) 100.0 (19.99-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.26Å)	Xtrriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.143 , 0.183 0.143 , 0.183	Depositor DCC
R_{free} test set	19877 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	51.6	Xtrriage
Anisotropy	0.461	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 87.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	62605	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% 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: BCT, LMT, PL9, HTG, MG, DGD, FE2, CL, GOL, UNL, CLA, HEM, HEC, BCR, OEY, CA, FME, PHO, OEX, LMG, SQD, LHG

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	0.44	0/4478	0.58	1/6098 (0.0%)
1	a	0.42	0/4470	0.56	0/6087
2	B	0.46	0/4293	0.59	0/5851
2	b	0.43	0/4285	0.59	0/5841
3	C	0.41	0/4404	0.56	0/5997
3	c	0.40	0/4459	0.55	0/6071
4	D	0.48	0/3741	0.60	0/5095
4	d	0.46	0/3749	0.58	0/5106
5	E	0.41	0/681	0.58	0/928
5	e	0.39	0/690	0.54	0/939
6	F	0.39	0/284	0.54	0/387
6	f	0.36	0/269	0.51	0/365
7	H	0.40	0/519	0.62	0/708
7	h	0.37	0/530	0.59	0/722
8	I	0.39	0/311	0.54	0/419
8	i	0.41	0/311	0.53	0/419
9	J	0.40	0/278	0.54	0/376
9	j	0.37	0/283	0.55	0/383
10	K	0.39	0/303	0.53	0/416
10	k	0.40	0/303	0.52	0/416
11	L	0.47	0/318	0.60	0/433
11	l	0.46	0/318	0.56	0/433
12	M	0.47	0/261	0.54	0/357
12	m	0.41	0/279	0.54	0/380
13	O	0.42	0/1991	0.65	0/2698
13	o	0.40	0/1966	0.66	0/2665
14	T	0.50	0/310	0.61	0/419
14	t	0.44	0/301	0.59	0/406
15	U	0.45	0/811	0.61	0/1095
15	u	0.45	0/818	0.62	0/1105
16	V	0.42	0/1142	0.58	0/1545

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.36	0/1139	0.58	0/1542
17	X	0.33	0/292	0.50	0/395
17	x	0.33	0/284	0.50	0/384
18	Y	0.32	0/216	0.53	0/289
18	y	0.29	0/216	0.52	0/289
19	Z	0.32	0/490	0.45	0/669
19	z	0.32	0/490	0.43	0/669
20	R	0.30	0/279	0.51	0/383
All	All	0.42	0/50562	0.58	1/68780 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	308	ASP	CB-CG-OD1	6.13	123.82	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	553/344 (161%)	542 (98%)	9 (2%)	2 (0%)	34	37
1	a	552/344 (160%)	544 (99%)	6 (1%)	2 (0%)	34	37
2	B	522/505 (103%)	516 (99%)	6 (1%)	0	100	100
2	b	521/505 (103%)	510 (98%)	11 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	546/455 (120%)	535 (98%)	10 (2%)	1 (0%)	47	55
3	c	553/455 (122%)	544 (98%)	8 (1%)	1 (0%)	47	55
4	D	453/342 (132%)	438 (97%)	15 (3%)	0	100	100
4	d	454/342 (133%)	444 (98%)	10 (2%)	0	100	100
5	E	79/84 (94%)	78 (99%)	1 (1%)	0	100	100
5	e	79/84 (94%)	79 (100%)	0	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
7	h	63/65 (97%)	58 (92%)	4 (6%)	1 (2%)	9	5
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%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	37 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	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%)	243 (97%)	7 (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	98/104 (94%)	94 (96%)	4 (4%)	0	100	100
16	V	140/137 (102%)	136 (97%)	4 (3%)	0	100	100
16	v	140/137 (102%)	134 (96%)	6 (4%)	0	100	100
17	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
17	x	36/40 (90%)	36 (100%)	0	0	100	100
18	Y	27/30 (90%)	25 (93%)	2 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	y	27/30 (90%)	27 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9	4
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	9	4
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	6171/5384 (115%)	6037 (98%)	123 (2%)	11 (0%)	47	55

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
8	I	36	ASP
19	Z	31	GLN
3	c	416	SER
19	z	30	PRO
13	O	26	ALA
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%)	442 (100%)	2 (0%)	88	92
1	a	443/279 (159%)	441 (100%)	2 (0%)	88	92
2	B	421/403 (104%)	417 (99%)	4 (1%)	76	84
2	b	420/403 (104%)	412 (98%)	8 (2%)	57	66
3	C	430/356 (121%)	424 (99%)	6 (1%)	67	76
3	c	436/356 (122%)	429 (98%)	7 (2%)	62	73
4	D	368/277 (133%)	366 (100%)	2 (0%)	88	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	d	369/277 (133%)	364 (99%)	5 (1%)	67	76
5	E	72/73 (99%)	70 (97%)	2 (3%)	43	52
5	e	72/73 (99%)	70 (97%)	2 (3%)	43	52
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%)	52 (96%)	2 (4%)	34	40
7	h	55/54 (102%)	54 (98%)	1 (2%)	59	68
8	I	34/34 (100%)	33 (97%)	1 (3%)	42	51
8	i	34/34 (100%)	32 (94%)	2 (6%)	19	19
9	J	26/27 (96%)	25 (96%)	1 (4%)	33	39
9	j	26/27 (96%)	25 (96%)	1 (4%)	33	39
10	K	30/30 (100%)	26 (87%)	4 (13%)	4	2
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	5
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	15
12	m	32/32 (100%)	30 (94%)	2 (6%)	18	17
13	O	216/207 (104%)	212 (98%)	4 (2%)	57	66
13	o	213/207 (103%)	207 (97%)	6 (3%)	43	52
14	T	32/28 (114%)	30 (94%)	2 (6%)	18	17
14	t	31/28 (111%)	31 (100%)	0	100	100
15	U	86/89 (97%)	84 (98%)	2 (2%)	50	59
15	u	87/89 (98%)	85 (98%)	2 (2%)	50	59
16	V	123/117 (105%)	123 (100%)	0	100	100
16	v	123/117 (105%)	119 (97%)	4 (3%)	38	46
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	2
19	Z	52/52 (100%)	51 (98%)	1 (2%)	57	66
19	z	52/52 (100%)	46 (88%)	6 (12%)	5	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	R	29/29 (100%)	26 (90%)	3 (10%)	7	5
All	All	5103/4403 (116%)	5011 (98%)	92 (2%)	57	68

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

Mol	Chain	Res	Type
1	A	244[A]	GLU
1	A	244[B]	GLU
2	B	299	GLU
2	B	362	PHE
2	B	389	LYS
2	B	419	SER
3	C	142	GLU
3	C	255	THR
3	C	289	PHE
3	C	315[A]	MET
3	C	315[B]	MET
3	C	471	SER
4	D	180	ARG
4	D	338	ASN
5	E	4	THR
5	E	71	GLU
7	H	12	ARG
7	H	49	TYR
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
14	T	30[A]	THR
14	T	30[B]	THR
15	U	10	VAL
15	U	70	ARG
1	a	12	ASN
1	a	13	LEU

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Mol	Chain	Res	Type
2	b	127	ARG
2	b	128	THR
2	b	161	LEU
2	b	362	PHE
2	b	472	ARG
2	b	486[A]	LEU
2	b	486[B]	LEU
2	b	505	ARG
3	c	19	ASN
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	171	PRO
4	d	180	ARG
4	d	230[A]	SER
4	d	230[B]	SER
5	e	60	GLN
5	e	71	GLU
7	h	49	TYR
8	i	33	LYS
8	i	36	ASP
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
13	o	217	SER
15	u	10[A]	VAL
15	u	10[B]	VAL
16	v	15	GLU
16	v	24	LYS
16	v	85	GLU

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Mol	Chain	Res	Type
16	v	109	GLU
18	y	18	VAL
18	y	19	ILE
18	y	45	ASN
19	Z	31	GLN
20	R	26	TYR
20	R	29	LYS
20	R	33	LYS
19	z	1	MET
19	z	3	ILE
19	z	4	LEU
19	z	7	LEU
19	z	32	ASP
19	z	42	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	61	HIS
5	E	60	GLN
3	c	28	GLN
11	l	8	GLN
13	o	58	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	FME	t	1	14	8,9,10	0.65	0	7,9,11	1.39	1 (14%)
14	FME	T	1	14	8,9,10	0.60	0	7,9,11	1.71	3 (42%)
8	FME	I	1	8	8,9,10	0.62	0	7,9,11	1.18	1 (14%)
8	FME	i	1	8	8,9,10	0.62	0	7,9,11	1.05	1 (14%)
12	FME	m	1	12	8,9,10	0.52	0	7,9,11	1.47	2 (28%)
12	FME	M	1	12	8,9,10	0.60	0	7,9,11	1.35	1 (14%)

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	-	3/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
8	FME	i	1	8	-	2/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
12	FME	M	1	12	-	0/7/9/11	-

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	CA-N-CN	2.40	126.52	122.82
12	m	1	FME	O1-CN-N	-2.39	118.98	125.27
12	M	1	FME	O-C-CA	-2.34	118.66	124.78
14	t	1	FME	O-C-CA	-2.26	118.85	124.78
14	T	1	FME	C-CA-N	2.22	113.75	109.73
8	I	1	FME	O-C-CA	-2.20	119.02	124.78
14	T	1	FME	CG-CB-CA	2.12	118.85	112.95
8	i	1	FME	O-C-CA	-2.02	119.49	124.78
12	m	1	FME	O-C-CA	-2.02	119.49	124.78

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
14	T	1	FME	O1-CN-N-CA
8	i	1	FME	CA-CB-CG-SD
14	T	1	FME	N-CA-CB-CG
14	T	1	FME	C-CA-CB-CG
8	i	1	FME	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 274 ligands modelled in this entry, 21 are monoatomic and 20 are unknown - leaving 233 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
21	OEY	A	401[B]	42,1,3	0,16,16	-	-	-		
24	CLA	a	407[B]	42	65,73,73	2.04	16 (24%)	76,113,113	2.84	31 (40%)
24	CLA	c	514	-	65,73,73	2.10	16 (24%)	76,113,113	2.80	28 (36%)
24	CLA	A	407[B]	42	65,73,73	2.06	16 (24%)	76,113,113	2.78	29 (38%)
24	CLA	B	603	-	65,73,73	2.04	17 (26%)	76,113,113	2.87	29 (38%)
34	HTG	c	522	-	19,19,19	0.93	1 (5%)	23,24,24	1.59	3 (13%)
25	PHO	d	402[B]	-	51,69,69	1.87	8 (15%)	47,99,99	1.92	12 (25%)
27	SQD	A	411[B]	-	53,54,54	0.93	3 (5%)	62,65,65	1.70	9 (14%)
24	CLA	d	404	-	65,73,73	2.09	16 (24%)	76,113,113	2.75	27 (35%)
24	CLA	B	601	42	65,73,73	2.08	17 (26%)	76,113,113	2.77	27 (35%)
24	CLA	C	514	-	65,73,73	2.08	16 (24%)	76,113,113	2.77	28 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LHG	d	407[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.04	4 (7%)
35	LMG	z	101	-	39,39,55	1.11	2 (5%)	47,47,63	1.11	5 (10%)
24	CLA	c	507	-	65,73,73	2.02	16 (24%)	76,113,113	2.80	28 (36%)
28	GOL	A	419	-	5,5,5	1.40	1 (20%)	5,5,5	0.82	0
24	CLA	b	611	-	65,73,73	2.00	17 (26%)	76,113,113	2.90	28 (36%)
26	BCR	d	405	-	41,41,41	1.14	1 (2%)	56,56,56	1.93	13 (23%)
28	GOL	B	626	-	5,5,5	1.02	0	5,5,5	0.96	0
36	DGD	c	517[B]	-	63,63,67	0.86	2 (3%)	77,77,81	1.09	5 (6%)
36	DGD	c	519	-	63,63,67	0.88	3 (4%)	77,77,81	1.09	5 (6%)
28	GOL	c	526[B]	-	5,5,5	1.04	0	5,5,5	0.92	0
24	CLA	b	610	42	65,73,73	2.05	16 (24%)	76,113,113	2.77	28 (36%)
26	BCR	c	516	-	41,41,41	1.03	1 (2%)	56,56,56	1.46	12 (21%)
30	PL9	a	415[B]	-	55,55,55	0.63	2 (3%)	68,69,69	1.87	21 (30%)
29	OEX	A	414[A]	42,1,3	0,15,15	-	-	-	-	-
26	BCR	B	617	-	41,41,41	1.05	1 (2%)	56,56,56	1.38	9 (16%)
28	GOL	b	623	-	5,5,5	1.20	1 (20%)	5,5,5	0.84	0
24	CLA	c	506	-	65,73,73	2.00	15 (23%)	76,113,113	2.65	25 (32%)
27	SQD	A	413	-	53,54,54	1.03	3 (5%)	62,65,65	1.35	8 (12%)
33	LHG	E	101[A]	-	41,41,48	1.08	2 (4%)	44,47,54	1.10	3 (6%)
33	LHG	d	408[A]	-	48,48,48	0.92	2 (4%)	51,54,54	1.01	3 (5%)
33	LHG	D	406[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.01	3 (5%)
24	CLA	b	614	-	65,73,73	2.02	15 (23%)	76,113,113	2.87	27 (35%)
24	CLA	b	615	-	65,73,73	2.02	16 (24%)	76,113,113	2.76	28 (36%)
33	LHG	D	407[A]	-	48,48,48	0.93	2 (4%)	51,54,54	1.02	3 (5%)
26	BCR	t	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.65	11 (19%)
28	GOL	v	202[B]	-	5,5,5	1.10	0	5,5,5	0.85	0
30	PL9	D	405[B]	-	55,55,55	0.61	1 (1%)	68,69,69	1.62	16 (23%)
36	DGD	C	518[A]	-	63,63,67	0.90	3 (4%)	77,77,81	1.03	5 (6%)
24	CLA	C	513	-	65,73,73	2.05	16 (24%)	76,113,113	2.80	31 (40%)
27	SQD	B	620	-	53,54,54	1.08	4 (7%)	62,65,65	1.78	12 (19%)
24	CLA	c	510	-	65,73,73	2.06	17 (26%)	76,113,113	2.86	31 (40%)
26	BCR	A	410	-	41,41,41	1.07	1 (2%)	56,56,56	1.40	6 (10%)
28	GOL	v	202[A]	-	5,5,5	1.20	0	5,5,5	0.82	0
24	CLA	b	606	-	65,73,73	2.00	16 (24%)	76,113,113	2.81	28 (36%)
32	LMT	m	102	-	36,36,36	1.02	3 (8%)	47,47,47	1.10	3 (6%)
33	LHG	b	628[A]	-	48,48,48	0.83	2 (4%)	51,54,54	1.04	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMT	A	418	-	36,36,36	0.93	0	47,47,47	1.11	2 (4%)
24	CLA	D	402[A]	-	65,73,73	2.04	16 (24%)	76,113,113	2.87	31 (40%)
34	HTG	B	624	-	19,19,19	1.17	2 (10%)	23,24,24	1.14	2 (8%)
32	LMT	B	627	-	36,36,36	1.15	4 (11%)	47,47,47	1.30	5 (10%)
24	CLA	c	511	-	65,73,73	2.02	16 (24%)	76,113,113	2.77	29 (38%)
26	BCR	D	404	-	41,41,41	1.11	1 (2%)	56,56,56	1.80	12 (21%)
28	GOL	o	303	-	5,5,5	1.36	1 (20%)	5,5,5	1.00	0
26	BCR	c	515	-	41,41,41	1.00	1 (2%)	56,56,56	1.58	14 (25%)
24	CLA	a	406[A]	42	65,73,73	2.02	15 (23%)	76,113,113	2.80	29 (38%)
25	PHO	A	408[A]	-	51,69,69	1.77	8 (15%)	47,99,99	1.69	10 (21%)
28	GOL	a	412	-	5,5,5	0.96	0	5,5,5	0.96	0
24	CLA	b	605	-	65,73,73	1.94	18 (27%)	76,113,113	2.98	30 (39%)
30	PL9	d	406[A]	-	55,55,55	0.70	1 (1%)	68,69,69	1.63	18 (26%)
35	LMG	b	629	-	51,51,55	0.85	2 (3%)	59,59,63	1.37	8 (13%)
33	LHG	a	420[A]	-	41,41,48	1.06	2 (4%)	44,47,54	0.92	2 (4%)
24	CLA	c	513	-	65,73,73	2.06	16 (24%)	76,113,113	2.77	31 (40%)
33	LHG	A	420[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.27	6 (11%)
38	BCT	d	401[B]	22	2,3,3	0.63	0	2,3,3	0.87	0
24	CLA	B	604	-	65,73,73	2.01	18 (27%)	76,113,113	2.57	28 (36%)
26	BCR	B	618	-	41,41,41	0.97	1 (2%)	56,56,56	1.45	11 (19%)
32	LMT	F	101	-	36,36,36	1.04	1 (2%)	47,47,47	1.02	2 (4%)
35	LMG	Z	101	-	37,37,55	1.01	2 (5%)	45,45,63	1.44	6 (13%)
34	HTG	D	410	-	16,16,19	1.00	1 (6%)	20,21,24	1.56	1 (5%)
28	GOL	B	623	-	5,5,5	0.92	0	5,5,5	1.11	1 (20%)
33	LHG	d	414[A]	-	48,48,48	0.89	2 (4%)	51,54,54	1.11	4 (7%)
25	PHO	A	417[A]	-	51,69,69	1.92	8 (15%)	47,99,99	1.85	9 (19%)
32	LMT	M	102	-	36,36,36	1.17	3 (8%)	47,47,47	1.17	3 (6%)
27	SQD	a	411[B]	-	53,54,54	0.98	3 (5%)	62,65,65	1.57	13 (20%)
36	DGD	C	519	-	63,63,67	0.86	3 (4%)	77,77,81	1.07	5 (6%)
26	BCR	b	618	-	41,41,41	1.00	1 (2%)	56,56,56	1.31	9 (16%)
36	DGD	C	517[B]	-	63,63,67	0.83	2 (3%)	77,77,81	1.07	5 (6%)
24	CLA	D	402[B]	-	65,73,73	2.06	15 (23%)	76,113,113	2.81	25 (32%)
26	BCR	C	515	-	41,41,41	1.03	1 (2%)	56,56,56	1.34	7 (12%)
26	BCR	Y	101	-	41,41,41	0.96	1 (2%)	56,56,56	1.74	14 (25%)
24	CLA	A	405[A]	-	65,73,73	2.02	16 (24%)	76,113,113	2.85	30 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	GOL	V	203[A]	-	5,5,5	1.34	0	5,5,5	0.80	0
24	CLA	a	406[B]	42	65,73,73	2.03	14 (21%)	76,113,113	2.73	27 (35%)
24	CLA	B	606	-	65,73,73	1.99	17 (26%)	76,113,113	2.98	29 (38%)
24	CLA	B	612	-	65,73,73	2.07	18 (27%)	76,113,113	2.85	28 (36%)
24	CLA	b	601	42	65,73,73	2.10	15 (23%)	76,113,113	2.80	27 (35%)
24	CLA	C	507	-	65,73,73	1.98	16 (24%)	76,113,113	2.85	29 (38%)
32	LMT	A	421	-	36,36,36	1.05	2 (5%)	47,47,47	1.16	4 (8%)
28	GOL	C	523[A]	-	5,5,5	1.11	0	5,5,5	0.88	0
32	LMT	e	102	-	36,36,36	1.03	3 (8%)	47,47,47	0.94	1 (2%)
24	CLA	C	511	-	65,73,73	2.02	16 (24%)	76,113,113	2.91	32 (42%)
33	LHG	a	420[B]	-	41,41,48	1.04	2 (4%)	44,47,54	0.92	2 (4%)
34	HTG	d	411	-	16,16,19	0.97	1 (6%)	20,21,24	1.59	2 (10%)
24	CLA	B	611	-	65,73,73	2.69	20 (30%)	76,113,113	3.15	28 (36%)
26	BCR	b	617	-	41,41,41	1.05	1 (2%)	56,56,56	1.36	5 (8%)
24	CLA	B	605	-	65,73,73	1.97	16 (24%)	76,113,113	2.94	30 (39%)
30	PL9	A	415[B]	-	55,55,55	0.63	1 (1%)	68,69,69	1.95	22 (32%)
35	LMG	C	520	-	51,51,55	1.00	2 (3%)	59,59,63	1.11	4 (6%)
28	GOL	a	419	-	5,5,5	1.16	1 (20%)	5,5,5	0.94	0
24	CLA	C	510	-	65,73,73	2.03	16 (24%)	76,113,113	2.80	28 (36%)
28	GOL	b	627	-	5,5,5	0.65	0	5,5,5	1.28	1 (20%)
27	SQD	a	413	-	53,54,54	1.05	4 (7%)	62,65,65	1.23	8 (12%)
26	BCR	C	516	-	41,41,41	0.99	1 (2%)	56,56,56	1.35	7 (12%)
32	LMT	b	626	-	25,25,36	0.88	1 (4%)	30,30,47	1.15	3 (10%)
28	GOL	O	303	-	5,5,5	1.02	0	5,5,5	1.00	0
26	BCR	b	619	-	41,41,41	1.04	1 (2%)	56,56,56	1.32	7 (12%)
33	LHG	d	407[B]	-	48,48,48	0.88	2 (4%)	51,54,54	1.03	4 (7%)
21	OEY	a	401[B]	42,1,3	0,16,16	-	-	-	-	-
24	CLA	A	405[B]	-	65,73,73	2.15	16 (24%)	76,113,113	2.78	32 (42%)
28	GOL	V	203[B]	-	5,5,5	1.10	0	5,5,5	0.86	0
24	CLA	C	509	-	65,73,73	2.12	16 (24%)	76,113,113	2.66	26 (34%)
28	GOL	D	412	-	5,5,5	1.43	1 (20%)	5,5,5	0.74	0
24	CLA	c	505	42	65,73,73	2.13	18 (27%)	76,113,113	2.78	28 (36%)
33	LHG	E	101[B]	-	41,41,48	1.05	2 (4%)	44,47,54	1.11	3 (6%)
33	LHG	d	408[B]	-	48,48,48	0.91	2 (4%)	51,54,54	0.99	3 (5%)
26	BCR	a	410	-	41,41,41	1.08	2 (4%)	56,56,56	1.29	6 (10%)
41	HEC	V	201	16	32,50,50	1.95	4 (12%)	24,82,82	2.16	6 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LHG	D	406[B]	-	48,48,48	0.89	2 (4%)	51,54,54	0.99	3 (5%)
27	SQD	L	102	-	53,54,54	1.05	3 (5%)	62,65,65	1.72	10 (16%)
29	OEX	a	414[A]	42,1,3	0,15,15	-	-	-	-	-
30	PL9	A	415[A]	-	55,55,55	0.69	2 (3%)	68,69,69	2.01	24 (35%)
33	LHG	D	407[B]	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	3 (5%)
28	GOL	a	418	-	5,5,5	1.09	0	5,5,5	0.96	0
34	HTG	C	522	-	19,19,19	0.87	1 (5%)	23,24,24	1.39	2 (8%)
36	DGD	C	518[B]	-	63,63,67	0.86	2 (3%)	77,77,81	1.04	6 (7%)
26	BCR	k	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.45	9 (16%)
25	PHO	a	408[A]	-	51,69,69	1.83	8 (15%)	47,99,99	1.87	9 (19%)
33	LHG	b	628[B]	-	48,48,48	0.89	2 (4%)	51,54,54	1.09	4 (7%)
28	GOL	d	413	-	5,5,5	1.06	0	5,5,5	1.08	0
28	GOL	l	801[A]	-	5,5,5	0.93	0	5,5,5	0.98	0
24	CLA	c	509	-	65,73,73	2.13	16 (24%)	76,113,113	2.79	28 (36%)
24	CLA	A	406[A]	42	65,73,73	1.99	15 (23%)	76,113,113	2.79	30 (39%)
24	CLA	b	603	-	65,73,73	2.01	16 (24%)	76,113,113	2.78	29 (38%)
24	CLA	b	602	-	65,73,73	2.06	16 (24%)	76,113,113	2.78	33 (43%)
24	CLA	a	407[A]	42	65,73,73	1.98	16 (24%)	76,113,113	2.77	27 (35%)
25	PHO	A	408[B]	-	51,69,69	1.80	8 (15%)	47,99,99	1.77	10 (21%)
30	PL9	d	406[B]	-	55,55,55	0.64	2 (3%)	68,69,69	1.65	18 (26%)
25	PHO	d	402[A]	-	51,69,69	1.88	8 (15%)	47,99,99	1.99	12 (25%)
24	CLA	B	607	42	65,73,73	2.00	17 (26%)	76,113,113	2.89	28 (36%)
35	LMG	d	412	40	51,51,55	0.89	2 (3%)	59,59,63	1.08	5 (8%)
27	SQD	A	411[A]	-	53,54,54	0.93	3 (5%)	62,65,65	1.88	10 (16%)
32	LMT	B	628	-	36,36,36	1.00	3 (8%)	47,47,47	1.20	4 (8%)
35	LMG	c	521	-	51,51,55	1.01	2 (3%)	59,59,63	1.33	6 (10%)
24	CLA	C	502	-	65,73,73	2.01	16 (24%)	76,113,113	2.84	31 (40%)
38	BCT	D	401[A]	22	2,3,3	0.64	0	2,3,3	1.30	0
24	CLA	C	504	-	65,73,73	1.93	15 (23%)	76,113,113	2.81	24 (31%)
26	BCR	h	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.46	10 (17%)
24	CLA	B	610	42	65,73,73	2.00	17 (26%)	76,113,113	2.85	28 (36%)
24	CLA	c	508	42	65,73,73	1.99	16 (24%)	76,113,113	2.80	28 (36%)
33	LHG	A	420[B]	-	48,48,48	0.88	2 (4%)	51,54,54	1.17	6 (11%)
34	HTG	b	624	-	19,19,19	1.02	2 (10%)	23,24,24	1.56	3 (13%)
24	CLA	B	608	-	65,73,73	1.96	14 (21%)	76,113,113	2.79	33 (43%)
35	LMG	a	417	-	51,51,55	0.92	2 (3%)	59,59,63	1.23	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	B	609	-	65,73,73	2.02	17 (26%)	76,113,113	2.67	27 (35%)
36	DGD	c	517[A]	-	63,63,67	0.85	2 (3%)	77,77,81	1.10	7 (9%)
24	CLA	D	403	-	65,73,73	2.06	16 (24%)	76,113,113	2.73	28 (36%)
24	CLA	A	409	-	65,73,73	2.01	15 (23%)	76,113,113	2.89	30 (39%)
26	BCR	H	101	-	41,41,41	0.99	1 (2%)	56,56,56	1.52	9 (16%)
33	LHG	L	101[A]	-	48,48,48	0.88	2 (4%)	51,54,54	1.15	4 (7%)
35	LMG	D	411	40	51,51,55	0.86	2 (3%)	59,59,63	0.99	4 (6%)
30	PL9	a	415[A]	-	55,55,55	0.65	2 (3%)	68,69,69	2.01	22 (32%)
33	LHG	d	414[B]	-	48,48,48	0.91	2 (4%)	51,54,54	1.01	3 (5%)
26	BCR	y	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.60	13 (23%)
24	CLA	a	405[A]	-	65,73,73	2.01	16 (24%)	76,113,113	2.86	32 (42%)
25	PHO	A	417[B]	-	51,69,69	1.90	8 (15%)	47,99,99	1.82	11 (23%)
24	CLA	c	503	-	65,73,73	1.99	14 (21%)	76,113,113	2.67	25 (32%)
34	HTG	b	621	-	19,19,19	1.26	2 (10%)	23,24,24	2.09	7 (30%)
24	CLA	C	512	3	65,73,73	2.05	18 (27%)	76,113,113	2.67	27 (35%)
24	CLA	c	504	-	65,73,73	2.01	16 (24%)	76,113,113	2.77	27 (35%)
24	CLA	b	608	-	65,73,73	2.01	18 (27%)	76,113,113	2.75	32 (42%)
28	GOL	c	527	-	5,5,5	1.13	0	5,5,5	0.90	0
34	HTG	B	621	-	19,19,19	1.03	2 (10%)	23,24,24	1.55	5 (21%)
34	HTG	B	622	-	19,19,19	0.82	1 (5%)	23,24,24	1.55	2 (8%)
32	LMT	B	630	-	25,25,36	0.89	2 (8%)	30,30,47	1.13	3 (10%)
36	DGD	c	518[A]	-	63,63,67	0.85	3 (4%)	77,77,81	0.97	3 (3%)
41	HEC	v	201	16	32,50,50	2.08	4 (12%)	24,82,82	1.96	6 (25%)
28	GOL	C	523[B]	-	5,5,5	1.18	0	5,5,5	0.85	0
36	DGD	h	102	-	63,63,67	0.87	3 (4%)	77,77,81	1.21	7 (9%)
24	CLA	b	616	-	65,73,73	2.02	15 (23%)	76,113,113	2.83	27 (35%)
38	BCT	D	401[B]	22	2,3,3	0.64	0	2,3,3	0.97	0
24	CLA	B	602	-	65,73,73	2.06	16 (24%)	76,113,113	2.79	31 (40%)
24	CLA	b	613	-	65,73,73	1.98	15 (23%)	76,113,113	2.78	30 (39%)
39	HEM	e	101	6,5	41,50,50	1.29	5 (12%)	45,82,82	1.84	12 (26%)
39	HEM	F	102	6,5	41,50,50	1.29	5 (12%)	45,82,82	2.15	14 (31%)
32	LMT	c	501	-	36,36,36	1.01	1 (2%)	47,47,47	1.05	3 (6%)
24	CLA	C	505	42	65,73,73	1.99	14 (21%)	76,113,113	2.76	25 (32%)
24	CLA	b	604	-	65,73,73	2.01	18 (27%)	76,113,113	2.69	24 (31%)
24	CLA	B	613	-	65,73,73	2.00	16 (24%)	76,113,113	2.73	27 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	c	512	3	65,73,73	2.12	17 (26%)	76,113,113	2.74	28 (36%)
35	LMG	C	501	-	51,51,55	0.93	2 (3%)	59,59,63	1.57	9 (15%)
33	LHG	L	101[B]	-	48,48,48	0.93	2 (4%)	51,54,54	1.14	5 (9%)
24	CLA	b	609	-	65,73,73	2.02	16 (24%)	76,113,113	2.71	30 (39%)
34	HTG	b	622	-	19,19,19	0.99	1 (5%)	23,24,24	1.78	3 (13%)
24	CLA	C	506	-	65,73,73	1.99	16 (24%)	76,113,113	2.79	28 (36%)
38	BCT	d	401[A]	22	2,3,3	0.59	0	2,3,3	1.49	0
24	CLA	a	405[B]	-	65,73,73	2.06	15 (23%)	76,113,113	2.84	30 (39%)
24	CLA	C	503	-	65,73,73	2.06	16 (24%)	76,113,113	2.66	27 (35%)
24	CLA	d	403[A]	-	65,73,73	1.96	16 (24%)	76,113,113	2.74	29 (38%)
28	GOL	A	412	-	5,5,5	1.25	0	5,5,5	0.62	0
27	SQD	f	101	-	42,43,54	1.19	3 (7%)	51,54,65	1.41	9 (17%)
28	GOL	o	302	-	5,5,5	0.99	0	5,5,5	0.93	0
24	CLA	A	407[A]	42	65,73,73	1.98	17 (26%)	76,113,113	2.76	30 (39%)
24	CLA	B	615	-	65,73,73	2.01	15 (23%)	76,113,113	2.88	26 (34%)
26	BCR	B	619	-	41,41,41	1.10	2 (4%)	56,56,56	1.23	6 (10%)
35	LMG	c	520	-	51,51,55	0.91	2 (3%)	59,59,63	1.11	6 (10%)
24	CLA	c	502	-	65,73,73	2.00	16 (24%)	76,113,113	2.75	27 (35%)
24	CLA	C	508	42	65,73,73	1.98	16 (24%)	76,113,113	2.72	27 (35%)
28	GOL	O	302	-	5,5,5	0.88	0	5,5,5	0.95	0
36	DGD	c	518[B]	-	63,63,67	0.86	2 (3%)	77,77,81	1.04	7 (9%)
27	SQD	a	411[A]	-	53,54,54	0.96	3 (5%)	62,65,65	1.83	13 (20%)
35	LMG	M	101	-	51,51,55	0.91	2 (3%)	59,59,63	1.26	3 (5%)
36	DGD	C	517[A]	-	63,63,67	0.83	2 (3%)	77,77,81	1.20	8 (10%)
26	BCR	K	102	-	41,41,41	1.07	1 (2%)	56,56,56	1.50	12 (21%)
24	CLA	B	614	-	65,73,73	2.00	17 (26%)	76,113,113	2.93	30 (39%)
35	LMG	C	521	-	51,51,55	1.09	3 (5%)	59,59,63	1.34	6 (10%)
36	DGD	H	102	-	63,63,67	0.83	3 (4%)	77,77,81	1.13	8 (10%)
24	CLA	b	607	42	65,73,73	1.96	17 (26%)	76,113,113	2.80	28 (36%)
24	CLA	b	612	-	65,73,73	2.05	16 (24%)	76,113,113	2.76	26 (34%)
28	GOL	c	526[A]	-	5,5,5	1.00	0	5,5,5	0.98	0
32	LMT	b	620	-	25,25,36	0.98	1 (4%)	30,30,47	1.15	2 (6%)
32	LMT	t	101	-	26,26,36	0.90	2 (7%)	31,31,47	1.28	2 (6%)
26	BCR	T	101	-	41,41,41	1.10	1 (2%)	56,56,56	1.51	15 (26%)
24	CLA	a	409	-	65,73,73	2.01	15 (23%)	76,113,113	2.95	29 (38%)
32	LMT	M	104	-	36,36,36	1.06	3 (8%)	47,47,47	1.08	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PHO	a	408[B]	-	51,69,69	1.84	8 (15%)	47,99,99	1.82	11 (23%)
34	HTG	V	202	-	11,11,19	0.32	0	15,15,24	1.10	1 (6%)
27	SQD	X	101	-	42,43,54	1.21	4 (9%)	51,54,65	2.08	14 (27%)
24	CLA	d	403[B]	-	65,73,73	2.04	16 (24%)	76,113,113	2.86	30 (39%)
30	PL9	D	405[A]	-	55,55,55	0.63	1 (1%)	68,69,69	1.61	17 (25%)
28	GOL	l	801[B]	-	5,5,5	0.88	0	5,5,5	0.96	0
24	CLA	A	406[B]	42	65,73,73	2.00	15 (23%)	76,113,113	2.81	29 (38%)
24	CLA	B	616	-	65,73,73	2.05	17 (26%)	76,113,113	2.84	26 (34%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	a	407[B]	42	-	6/37/115/115	-
24	CLA	c	514	-	1/1/15/20	10/37/115/115	-
24	CLA	A	407[B]	42	-	6/37/115/115	-
24	CLA	B	603	-	1/1/15/20	8/37/115/115	-
34	HTG	c	522	-	-	2/10/30/30	0/1/1/1
25	PHO	d	402[B]	-	-	1/37/103/103	0/5/6/6
27	SQD	A	411[B]	-	-	11/49/69/69	0/1/1/1
24	CLA	d	404	-	1/1/15/20	8/37/115/115	-
24	CLA	B	601	42	1/1/15/20	11/37/115/115	-
24	CLA	C	514	-	1/1/15/20	6/37/115/115	-
33	LHG	d	407[A]	-	-	13/53/53/53	-
35	LMG	z	101	-	-	8/34/54/70	0/1/1/1
24	CLA	c	507	-	1/1/15/20	9/37/115/115	-
28	GOL	A	419	-	-	0/4/4/4	-
24	CLA	b	611	-	1/1/15/20	2/37/115/115	-
26	BCR	d	405	-	-	5/29/63/63	0/2/2/2
28	GOL	B	626	-	-	2/4/4/4	-
36	DGD	c	517[B]	-	-	16/51/91/95	0/2/2/2
36	DGD	c	519	-	-	9/51/91/95	0/2/2/2
28	GOL	c	526[B]	-	-	0/4/4/4	-
24	CLA	b	610	42	1/1/15/20	7/37/115/115	-
26	BCR	c	516	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	PL9	a	415[B]	-	-	14/53/73/73	0/1/1/1
26	BCR	B	617	-	-	2/29/63/63	0/2/2/2
28	GOL	b	623	-	-	2/4/4/4	-
24	CLA	c	506	-	1/1/15/20	6/37/115/115	-
27	SQD	A	413	-	-	12/49/69/69	0/1/1/1
33	LHG	E	101[A]	-	-	22/46/46/53	-
33	LHG	d	408[A]	-	-	13/53/53/53	-
33	LHG	D	406[A]	-	-	17/53/53/53	-
24	CLA	b	614	-	1/1/15/20	14/37/115/115	-
24	CLA	b	615	-	1/1/15/20	8/37/115/115	-
33	LHG	D	407[A]	-	-	14/53/53/53	-
26	BCR	t	102	-	-	0/29/63/63	0/2/2/2
28	GOL	v	202[B]	-	-	2/4/4/4	-
30	PL9	D	405[B]	-	-	7/53/73/73	0/1/1/1
36	DGD	C	518[A]	-	-	13/51/91/95	0/2/2/2
24	CLA	C	513	-	1/1/15/20	9/37/115/115	-
27	SQD	B	620	-	-	14/49/69/69	0/1/1/1
24	CLA	c	510	-	1/1/15/20	15/37/115/115	-
26	BCR	A	410	-	-	0/29/63/63	0/2/2/2
28	GOL	v	202[A]	-	-	2/4/4/4	-
24	CLA	b	606	-	1/1/15/20	12/37/115/115	-
32	LMT	m	102	-	-	6/21/61/61	0/2/2/2
33	LHG	b	628[A]	-	-	14/53/53/53	-
32	LMT	A	418	-	-	7/21/61/61	0/2/2/2
24	CLA	D	402[A]	-	1/1/15/20	0/37/115/115	-
34	HTG	B	624	-	-	4/10/30/30	0/1/1/1
32	LMT	B	627	-	-	10/21/61/61	0/2/2/2
24	CLA	c	511	-	1/1/15/20	11/37/115/115	-
26	BCR	D	404	-	-	4/29/63/63	0/2/2/2
28	GOL	o	303	-	-	2/4/4/4	-
26	BCR	c	515	-	-	1/29/63/63	0/2/2/2
24	CLA	a	406[A]	42	1/1/15/20	8/37/115/115	-
25	PHO	A	408[A]	-	-	3/37/103/103	0/5/6/6
28	GOL	a	412	-	-	4/4/4/4	-
24	CLA	b	605	-	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	PL9	d	406[A]	-	-	7/53/73/73	0/1/1/1
35	LMG	b	629	-	-	10/46/66/70	0/1/1/1
33	LHG	a	420[A]	-	-	16/46/46/53	-
24	CLA	c	513	-	1/1/15/20	13/37/115/115	-
33	LHG	A	420[A]	-	-	14/53/53/53	-
24	CLA	B	604	-	1/1/15/20	4/37/115/115	-
26	BCR	B	618	-	-	0/29/63/63	0/2/2/2
32	LMT	F	101	-	-	8/21/61/61	0/2/2/2
35	LMG	Z	101	-	-	10/31/51/70	0/1/1/1
34	HTG	D	410	-	-	3/7/27/30	0/1/1/1
28	GOL	B	623	-	-	4/4/4/4	-
33	LHG	d	414[A]	-	-	17/53/53/53	-
25	PHO	A	417[A]	-	-	1/37/103/103	0/5/6/6
32	LMT	M	102	-	-	4/21/61/61	0/2/2/2
27	SQD	a	411[B]	-	-	11/49/69/69	0/1/1/1
36	DGD	C	519	-	-	17/51/91/95	0/2/2/2
26	BCR	b	618	-	-	0/29/63/63	0/2/2/2
36	DGD	C	517[B]	-	-	17/51/91/95	0/2/2/2
24	CLA	D	402[B]	-	1/1/15/20	0/37/115/115	-
26	BCR	C	515	-	-	0/29/63/63	0/2/2/2
26	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
24	CLA	A	405[A]	-	1/1/15/20	3/37/115/115	-
28	GOL	V	203[A]	-	-	2/4/4/4	-
24	CLA	a	406[B]	42	1/1/15/20	6/37/115/115	-
24	CLA	B	606	-	1/1/15/20	6/37/115/115	-
24	CLA	B	612	-	1/1/15/20	3/37/115/115	-
24	CLA	b	601	42	1/1/15/20	19/37/115/115	-
24	CLA	C	507	-	1/1/15/20	11/37/115/115	-
32	LMT	A	421	-	-	16/21/61/61	0/2/2/2
28	GOL	C	523[A]	-	-	0/4/4/4	-
32	LMT	e	102	-	-	14/21/61/61	0/2/2/2
24	CLA	C	511	-	1/1/15/20	14/37/115/115	-
33	LHG	a	420[B]	-	-	16/46/46/53	-
34	HTG	d	411	-	-	1/7/27/30	0/1/1/1
24	CLA	B	611	-	1/1/15/20	4/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	b	617	-	-	2/29/63/63	0/2/2/2
24	CLA	B	605	-	1/1/15/20	7/37/115/115	-
30	PL9	A	415[B]	-	-	14/53/73/73	0/1/1/1
35	LMG	C	520	-	-	10/46/66/70	0/1/1/1
28	GOL	a	419	-	-	2/4/4/4	-
24	CLA	C	510	-	1/1/15/20	7/37/115/115	-
28	GOL	b	627	-	-	0/4/4/4	-
27	SQD	a	413	-	-	14/49/69/69	0/1/1/1
26	BCR	C	516	-	-	0/29/63/63	0/2/2/2
32	LMT	b	626	-	-	11/17/37/61	0/1/1/2
28	GOL	O	303	-	-	1/4/4/4	-
26	BCR	b	619	-	-	5/29/63/63	0/2/2/2
33	LHG	d	407[B]	-	-	17/53/53/53	-
24	CLA	A	405[B]	-	1/1/15/20	3/37/115/115	-
28	GOL	V	203[B]	-	-	4/4/4/4	-
24	CLA	C	509	-	1/1/15/20	5/37/115/115	-
28	GOL	D	412	-	-	4/4/4/4	-
24	CLA	c	505	42	1/1/15/20	6/37/115/115	-
33	LHG	E	101[B]	-	-	19/46/46/53	-
33	LHG	d	408[B]	-	-	12/53/53/53	-
26	BCR	a	410	-	-	3/29/63/63	0/2/2/2
41	HEC	V	201	16	-	2/10/54/54	-
33	LHG	D	406[B]	-	-	15/53/53/53	-
27	SQD	L	102	-	-	19/49/69/69	0/1/1/1
33	LHG	D	407[B]	-	-	14/53/53/53	-
30	PL9	A	415[A]	-	-	15/53/73/73	0/1/1/1
36	DGD	C	518[B]	-	-	14/51/91/95	0/2/2/2
28	GOL	a	418	-	-	2/4/4/4	-
34	HTG	C	522	-	-	0/10/30/30	0/1/1/1
26	BCR	k	101	-	-	1/29/63/63	0/2/2/2
25	PHO	a	408[A]	-	-	6/37/103/103	0/5/6/6
33	LHG	b	628[B]	-	-	18/53/53/53	-
28	GOL	d	413	-	-	2/4/4/4	-
28	GOL	l	801[A]	-	-	1/4/4/4	-
24	CLA	c	509	-	1/1/15/20	6/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	406[A]	42	1/1/15/20	3/37/115/115	-
24	CLA	b	603	-	1/1/15/20	9/37/115/115	-
24	CLA	b	602	-	1/1/15/20	4/37/115/115	-
24	CLA	a	407[A]	42	-	6/37/115/115	-
25	PHO	A	408[B]	-	-	6/37/103/103	0/5/6/6
30	PL9	d	406[B]	-	-	8/53/73/73	0/1/1/1
25	PHO	d	402[A]	-	-	1/37/103/103	0/5/6/6
24	CLA	B	607	42	1/1/15/20	3/37/115/115	-
35	LMG	d	412	40	-	12/46/66/70	0/1/1/1
27	SQD	A	411[A]	-	-	12/49/69/69	0/1/1/1
32	LMT	B	628	-	-	13/21/61/61	0/2/2/2
35	LMG	c	521	-	-	11/46/66/70	0/1/1/1
24	CLA	C	502	-	1/1/15/20	6/37/115/115	-
24	CLA	C	504	-	-	2/37/115/115	-
26	BCR	h	101	-	-	2/29/63/63	0/2/2/2
24	CLA	B	610	42	1/1/15/20	9/37/115/115	-
24	CLA	c	508	42	1/1/15/20	6/37/115/115	-
33	LHG	A	420[B]	-	-	12/53/53/53	-
34	HTG	b	624	-	-	4/10/30/30	0/1/1/1
24	CLA	B	608	-	-	4/37/115/115	-
35	LMG	a	417	-	-	14/46/66/70	0/1/1/1
24	CLA	B	609	-	1/1/15/20	1/37/115/115	-
36	DGD	c	517[A]	-	-	18/51/91/95	0/2/2/2
24	CLA	D	403	-	1/1/15/20	14/37/115/115	-
24	CLA	A	409	-	1/1/15/20	8/37/115/115	-
26	BCR	H	101	-	-	2/29/63/63	0/2/2/2
33	LHG	L	101[A]	-	-	20/53/53/53	-
35	LMG	D	411	40	-	10/46/66/70	0/1/1/1
30	PL9	a	415[A]	-	-	14/53/73/73	0/1/1/1
33	LHG	d	414[B]	-	-	10/53/53/53	-
26	BCR	y	101	-	-	3/29/63/63	0/2/2/2
24	CLA	a	405[A]	-	1/1/15/20	4/37/115/115	-
25	PHO	A	417[B]	-	-	5/37/103/103	0/5/6/6
24	CLA	c	503	-	1/1/15/20	6/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	HTG	b	621	-	-	3/10/30/30	0/1/1/1
24	CLA	C	512	3	1/1/15/20	3/37/115/115	-
24	CLA	c	504	-	1/1/15/20	3/37/115/115	-
24	CLA	b	608	-	-	7/37/115/115	-
28	GOL	c	527	-	-	3/4/4/4	-
34	HTG	B	621	-	-	4/10/30/30	0/1/1/1
34	HTG	B	622	-	-	3/10/30/30	0/1/1/1
32	LMT	B	630	-	-	11/17/37/61	0/1/1/2
36	DGD	c	518[A]	-	-	16/51/91/95	0/2/2/2
41	HEC	v	201	16	-	2/10/54/54	-
28	GOL	C	523[B]	-	-	0/4/4/4	-
36	DGD	h	102	-	-	16/51/91/95	0/2/2/2
24	CLA	b	616	-	1/1/15/20	9/37/115/115	-
24	CLA	B	602	-	1/1/15/20	7/37/115/115	-
24	CLA	b	613	-	1/1/15/20	5/37/115/115	-
39	HEM	e	101	6,5	-	6/12/54/54	-
39	HEM	F	102	6,5	-	2/12/54/54	-
32	LMT	c	501	-	-	11/21/61/61	0/2/2/2
24	CLA	C	505	42	1/1/15/20	7/37/115/115	-
24	CLA	b	604	-	1/1/15/20	9/37/115/115	-
24	CLA	B	613	-	1/1/15/20	7/37/115/115	-
24	CLA	c	512	3	1/1/15/20	6/37/115/115	-
35	LMG	C	501	-	-	17/46/66/70	0/1/1/1
33	LHG	L	101[B]	-	-	16/53/53/53	-
24	CLA	b	609	-	1/1/15/20	2/37/115/115	-
34	HTG	b	622	-	-	3/10/30/30	0/1/1/1
24	CLA	C	506	-	1/1/15/20	8/37/115/115	-
24	CLA	a	405[B]	-	1/1/15/20	3/37/115/115	-
24	CLA	C	503	-	1/1/15/20	7/37/115/115	-
24	CLA	d	403[A]	-	1/1/15/20	4/37/115/115	-
28	GOL	A	412	-	-	2/4/4/4	-
27	SQD	f	101	-	-	11/38/58/69	0/1/1/1
28	GOL	o	302	-	-	4/4/4/4	-
24	CLA	A	407[A]	42	-	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	615	-	1/1/15/20	6/37/115/115	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
35	LMG	c	520	-	-	12/46/66/70	0/1/1/1
24	CLA	c	502	-	1/1/15/20	2/37/115/115	-
24	CLA	C	508	42	1/1/15/20	4/37/115/115	-
28	GOL	O	302	-	-	2/4/4/4	-
36	DGD	c	518[B]	-	-	15/51/91/95	0/2/2/2
27	SQD	a	411[A]	-	-	9/49/69/69	0/1/1/1
35	LMG	M	101	-	-	18/46/66/70	0/1/1/1
36	DGD	C	517[A]	-	-	14/51/91/95	0/2/2/2
26	BCR	K	102	-	-	2/29/63/63	0/2/2/2
24	CLA	B	614	-	1/1/15/20	14/37/115/115	-
35	LMG	C	521	-	-	11/46/66/70	0/1/1/1
36	DGD	H	102	-	-	10/51/91/95	0/2/2/2
24	CLA	b	607	42	1/1/15/20	3/37/115/115	-
24	CLA	b	612	-	1/1/15/20	5/37/115/115	-
28	GOL	c	526[A]	-	-	0/4/4/4	-
32	LMT	b	620	-	-	8/17/37/61	0/1/1/2
32	LMT	t	101	-	-	9/17/38/61	0/1/1/2
26	BCR	T	101	-	-	1/29/63/63	0/2/2/2
24	CLA	a	409	-	1/1/15/20	11/37/115/115	-
32	LMT	M	104	-	-	6/21/61/61	0/2/2/2
25	PHO	a	408[B]	-	-	4/37/103/103	0/5/6/6
34	HTG	V	202	-	-	0/2/19/30	0/1/1/1
27	SQD	X	101	-	-	15/38/58/69	0/1/1/1
24	CLA	d	403[B]	-	1/1/15/20	4/37/115/115	-
30	PL9	D	405[A]	-	-	6/53/73/73	0/1/1/1
28	GOL	l	801[B]	-	-	1/4/4/4	-
24	CLA	A	406[B]	42	1/1/15/20	4/37/115/115	-
24	CLA	B	616	-	1/1/15/20	5/37/115/115	-

All (1551) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	611	CLA	C3B-C2B	11.19	1.55	1.40
24	B	616	CLA	C3B-C2B	7.31	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	611	CLA	CMB-C2B	6.90	1.66	1.51
24	C	509	CLA	C3B-C2B	6.79	1.49	1.40
24	B	612	CLA	C3B-C2B	6.76	1.49	1.40
24	b	603	CLA	C3B-C2B	6.76	1.49	1.40
24	b	612	CLA	C3B-C2B	6.74	1.49	1.40
24	B	603	CLA	C3B-C2B	6.67	1.49	1.40
24	C	514	CLA	C3B-C2B	6.54	1.49	1.40
24	A	409	CLA	C3B-C2B	6.49	1.49	1.40
24	c	512	CLA	C3B-C2B	6.48	1.49	1.40
25	a	408[B]	PHO	C3B-C2B	6.44	1.49	1.40
24	C	512	CLA	C3B-C2B	6.41	1.49	1.40
24	D	402[A]	CLA	C3B-C2B	6.40	1.49	1.40
24	c	509	CLA	C3B-C2B	6.40	1.49	1.40
24	B	611	CLA	C1D-ND	6.39	1.45	1.37
25	a	408[A]	PHO	C3B-C2B	6.39	1.49	1.40
24	c	510	CLA	C3B-C2B	6.37	1.49	1.40
24	d	403[B]	CLA	C3B-C2B	6.31	1.49	1.40
24	C	505	CLA	C3B-C2B	6.28	1.49	1.40
24	C	503	CLA	C3B-C2B	6.23	1.49	1.40
25	A	417[B]	PHO	C3B-C2B	6.21	1.49	1.40
25	A	408[B]	PHO	C3B-C2B	6.19	1.49	1.40
24	B	611	CLA	C3C-C2C	6.17	1.49	1.36
24	a	405[B]	CLA	C3B-C2B	6.15	1.48	1.40
25	A	408[A]	PHO	C3B-C2B	6.13	1.48	1.40
25	d	402[B]	PHO	C3B-C2B	6.13	1.48	1.40
24	b	614	CLA	C3B-C2B	6.10	1.48	1.40
24	c	505	CLA	C3B-C2B	6.06	1.48	1.40
24	A	405[B]	CLA	C3B-C2B	6.06	1.48	1.40
24	B	608	CLA	C3B-C2B	6.03	1.48	1.40
24	B	610	CLA	C3C-C2C	6.02	1.49	1.36
24	C	510	CLA	C3B-C2B	6.01	1.48	1.40
24	b	611	CLA	C3B-C2B	5.98	1.48	1.40
24	B	606	CLA	C3B-C2B	5.98	1.48	1.40
24	c	507	CLA	C3B-C2B	5.98	1.48	1.40
24	b	613	CLA	C3B-C2B	5.97	1.48	1.40
24	A	405[A]	CLA	C3B-C2B	5.96	1.48	1.40
25	A	417[A]	PHO	C3B-C2B	5.94	1.48	1.40
24	b	608	CLA	C3B-C2B	5.92	1.48	1.40
24	d	404	CLA	C3B-C2B	5.91	1.48	1.40
24	B	601	CLA	C3B-C2B	5.91	1.48	1.40
24	C	511	CLA	C3B-C2B	5.91	1.48	1.40
24	c	514	CLA	C3B-C2B	5.89	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	602	CLA	C3B-C2B	5.89	1.48	1.40
24	c	511	CLA	C3B-C2B	5.88	1.48	1.40
25	d	402[A]	PHO	C3B-C2B	5.88	1.48	1.40
24	b	610	CLA	C3B-C2B	5.87	1.48	1.40
24	a	405[A]	CLA	C3B-C2B	5.86	1.48	1.40
24	b	601	CLA	C3B-C2B	5.81	1.48	1.40
24	A	407[B]	CLA	C3B-C2B	5.81	1.48	1.40
24	c	503	CLA	C3B-C2B	5.80	1.48	1.40
41	v	201	HEC	C2B-C3B	-5.78	1.34	1.40
24	B	611	CLA	CHC-C1C	5.77	1.49	1.35
24	D	402[B]	CLA	C3B-C2B	5.77	1.48	1.40
24	C	504	CLA	C3C-C2C	5.75	1.49	1.36
24	b	607	CLA	C3B-C2B	5.75	1.48	1.40
24	C	507	CLA	C3B-C2B	5.75	1.48	1.40
24	C	513	CLA	C3B-C2B	5.74	1.48	1.40
24	b	604	CLA	C3B-C2B	5.73	1.48	1.40
24	c	505	CLA	C1D-ND	5.69	1.44	1.37
24	d	403[A]	CLA	C3B-C2B	5.68	1.48	1.40
24	C	504	CLA	C3B-C2B	5.65	1.48	1.40
24	B	604	CLA	C3B-C2B	5.63	1.48	1.40
24	a	407[B]	CLA	C3C-C2C	5.62	1.48	1.36
24	C	502	CLA	C3B-C2B	5.62	1.48	1.40
24	C	513	CLA	C3C-C2C	5.61	1.48	1.36
24	A	405[B]	CLA	C3C-C2C	5.61	1.48	1.36
24	D	402[B]	CLA	C3C-C2C	5.60	1.48	1.36
25	A	417[B]	PHO	C3D-C2D	5.60	1.49	1.39
24	b	616	CLA	C3B-C2B	5.58	1.48	1.40
24	a	406[A]	CLA	C3C-C2C	5.58	1.48	1.36
24	d	404	CLA	C1D-ND	5.57	1.44	1.37
24	b	606	CLA	C3B-C2B	5.57	1.48	1.40
24	c	506	CLA	C3C-C2C	5.54	1.48	1.36
24	D	403	CLA	C1D-ND	5.53	1.44	1.37
24	A	405[B]	CLA	C1D-ND	5.52	1.44	1.37
24	c	513	CLA	C3C-C2C	5.50	1.48	1.36
24	B	607	CLA	C3B-C2B	5.49	1.48	1.40
24	c	506	CLA	CHC-C1C	5.47	1.49	1.35
41	v	201	HEC	C3C-C2C	-5.47	1.35	1.40
25	d	402[A]	PHO	C3D-C2D	5.46	1.49	1.39
24	c	512	CLA	C1D-ND	5.46	1.44	1.37
25	a	408[A]	PHO	C3D-C2D	5.46	1.49	1.39
24	b	612	CLA	C3C-C2C	5.45	1.48	1.36
24	B	613	CLA	C3B-C2B	5.45	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	511	CLA	C1D-ND	5.45	1.44	1.37
24	a	406[B]	CLA	C3C-C2C	5.45	1.48	1.36
24	a	406[B]	CLA	C1D-ND	5.45	1.44	1.37
24	A	406[B]	CLA	C3B-C2B	5.44	1.47	1.40
24	a	409	CLA	C3B-C2B	5.44	1.47	1.40
24	C	509	CLA	C3C-C2C	5.44	1.48	1.36
24	c	509	CLA	C3C-C2C	5.44	1.48	1.36
24	b	601	CLA	C1D-ND	5.44	1.44	1.37
24	A	405[A]	CLA	C3C-C2C	5.43	1.48	1.36
24	B	614	CLA	C3B-C2B	5.43	1.47	1.40
24	c	509	CLA	O2D-CGD	5.43	1.46	1.33
24	C	508	CLA	C3B-C2B	5.43	1.47	1.40
24	C	502	CLA	C1D-ND	5.42	1.44	1.37
24	a	406[A]	CLA	C1D-ND	5.42	1.44	1.37
24	a	407[A]	CLA	C3B-C2B	5.42	1.47	1.40
24	b	609	CLA	O2D-CGD	5.42	1.46	1.33
24	C	513	CLA	CHC-C1C	5.41	1.48	1.35
24	C	511	CLA	C3C-C2C	5.39	1.48	1.36
24	c	504	CLA	C3C-C2C	5.39	1.48	1.36
41	v	201	HEC	C3D-C2D	5.38	1.53	1.37
24	A	407[B]	CLA	C3C-C2C	5.38	1.48	1.36
24	B	604	CLA	C3C-C2C	5.38	1.48	1.36
24	C	508	CLA	C3C-C2C	5.38	1.48	1.36
24	c	513	CLA	C3B-C2B	5.37	1.47	1.40
24	a	406[B]	CLA	C3B-C2B	5.37	1.47	1.40
24	B	605	CLA	C3C-C2C	5.36	1.48	1.36
24	b	601	CLA	C3C-C2C	5.36	1.48	1.36
24	a	409	CLA	CHC-C1C	5.36	1.48	1.35
24	A	409	CLA	C3C-C2C	5.35	1.48	1.36
24	A	405[B]	CLA	CHC-C1C	5.33	1.48	1.35
24	a	407[B]	CLA	CHC-C1C	5.33	1.48	1.35
25	A	417[A]	PHO	C3D-C2D	5.33	1.49	1.39
24	c	509	CLA	C1D-ND	5.33	1.44	1.37
24	b	616	CLA	C3C-C2C	5.32	1.48	1.36
24	B	616	CLA	C3C-C2C	5.31	1.48	1.36
24	c	514	CLA	C3C-C2C	5.31	1.48	1.36
24	c	502	CLA	C3B-C2B	5.31	1.47	1.40
24	c	510	CLA	O2D-CGD	5.31	1.46	1.33
24	a	407[A]	CLA	C3C-C2C	5.31	1.48	1.36
24	c	511	CLA	O2D-CGD	5.31	1.46	1.33
24	c	504	CLA	CHC-C1C	5.30	1.48	1.35
24	D	402[A]	CLA	C3C-C2C	5.30	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407[A]	CLA	CHC-C1C	5.30	1.48	1.35
25	d	402[B]	PHO	C3D-C2D	5.30	1.48	1.39
25	d	402[A]	PHO	OBD-CAD	5.30	1.29	1.22
24	c	505	CLA	O2D-CGD	5.30	1.46	1.33
24	B	612	CLA	C3C-C2C	5.30	1.48	1.36
24	c	514	CLA	C1D-ND	5.30	1.44	1.37
24	b	605	CLA	C3B-C2B	5.30	1.47	1.40
24	D	403	CLA	C3C-C2C	5.30	1.48	1.36
24	a	405[B]	CLA	C3C-C2C	5.29	1.48	1.36
24	b	615	CLA	CHC-C1C	5.29	1.48	1.35
24	C	506	CLA	CHC-C1C	5.29	1.48	1.35
25	A	417[A]	PHO	OBD-CAD	5.28	1.29	1.22
24	B	613	CLA	CHC-C1C	5.28	1.48	1.35
24	d	404	CLA	C3C-C2C	5.28	1.47	1.36
24	b	607	CLA	C3C-C2C	5.28	1.47	1.36
24	B	609	CLA	CHC-C1C	5.28	1.48	1.35
24	b	614	CLA	C1D-ND	5.28	1.44	1.37
24	B	603	CLA	C3C-C2C	5.27	1.47	1.36
24	d	403[B]	CLA	C3C-C2C	5.27	1.47	1.36
24	C	503	CLA	C1D-ND	5.27	1.44	1.37
24	b	615	CLA	C3C-C2C	5.26	1.47	1.36
24	A	407[B]	CLA	CHC-C1C	5.26	1.48	1.35
24	c	510	CLA	C3C-C2C	5.26	1.47	1.36
24	d	404	CLA	CHC-C1C	5.25	1.48	1.35
24	b	610	CLA	CHC-C1C	5.24	1.48	1.35
24	b	603	CLA	O2D-CGD	5.24	1.46	1.33
25	a	408[A]	PHO	O2D-CGD	5.24	1.46	1.33
24	c	505	CLA	C3C-C2C	5.24	1.47	1.36
24	b	602	CLA	C3C-C2C	5.24	1.47	1.36
24	B	601	CLA	C3C-C2C	5.23	1.47	1.36
24	c	512	CLA	C3C-C2C	5.23	1.47	1.36
24	C	510	CLA	C3C-C2C	5.22	1.47	1.36
24	B	606	CLA	CHC-C1C	5.22	1.48	1.35
24	b	616	CLA	C1D-ND	5.22	1.44	1.37
25	a	408[B]	PHO	C3D-C2D	5.22	1.48	1.39
24	A	407[B]	CLA	O2D-CGD	5.22	1.45	1.33
24	b	602	CLA	CHC-C1C	5.21	1.48	1.35
24	c	513	CLA	CHC-C1C	5.21	1.48	1.35
24	b	602	CLA	C3B-C2B	5.21	1.47	1.40
24	C	502	CLA	CHC-C1C	5.21	1.48	1.35
24	B	607	CLA	CHC-C1C	5.19	1.48	1.35
24	b	606	CLA	C3C-C2C	5.19	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	514	CLA	CHC-C1C	5.19	1.48	1.35
25	A	417[B]	PHO	O2D-CGD	5.19	1.45	1.33
24	C	503	CLA	C3C-C2C	5.19	1.47	1.36
24	C	506	CLA	C3C-C2C	5.19	1.47	1.36
24	C	508	CLA	CHC-C1C	5.18	1.48	1.35
24	a	409	CLA	C3C-C2C	5.18	1.47	1.36
24	c	513	CLA	C1D-ND	5.17	1.44	1.37
24	b	605	CLA	C3C-C2C	5.17	1.47	1.36
24	B	615	CLA	C3B-C2B	5.17	1.47	1.40
24	C	506	CLA	C3B-C2B	5.17	1.47	1.40
24	b	615	CLA	C3B-C2B	5.16	1.47	1.40
24	b	614	CLA	CHC-C1C	5.15	1.48	1.35
26	T	101	BCR	C23-C22	-5.15	1.34	1.45
24	B	612	CLA	CHC-C1C	5.15	1.48	1.35
24	B	615	CLA	C1D-ND	5.14	1.44	1.37
24	a	405[B]	CLA	CHC-C1C	5.14	1.48	1.35
24	b	616	CLA	CHC-C1C	5.14	1.48	1.35
24	c	509	CLA	CHC-C1C	5.14	1.48	1.35
24	A	406[A]	CLA	O2D-CGD	5.14	1.45	1.33
24	B	613	CLA	O2D-CGD	5.14	1.45	1.33
24	b	606	CLA	C1D-ND	5.14	1.44	1.37
24	B	614	CLA	C3C-C2C	5.14	1.47	1.36
24	c	503	CLA	C3C-C2C	5.14	1.47	1.36
24	A	407[A]	CLA	C3C-C2C	5.13	1.47	1.36
24	a	405[A]	CLA	C1D-ND	5.13	1.44	1.37
24	A	405[A]	CLA	C1D-ND	5.13	1.44	1.37
24	B	605	CLA	C1D-ND	5.12	1.44	1.37
24	a	405[B]	CLA	C1D-ND	5.12	1.44	1.37
24	b	606	CLA	CHC-C1C	5.12	1.48	1.35
24	b	613	CLA	CHC-C1C	5.12	1.48	1.35
24	b	613	CLA	C1D-ND	5.11	1.44	1.37
24	A	406[B]	CLA	CHC-C1C	5.10	1.48	1.35
24	D	402[B]	CLA	CHC-C1C	5.10	1.48	1.35
24	B	609	CLA	C3B-C2B	5.10	1.47	1.40
24	B	601	CLA	O2A-CGA	5.09	1.48	1.33
24	a	407[B]	CLA	C3B-C2B	5.09	1.47	1.40
24	a	409	CLA	O2D-CGD	5.09	1.45	1.33
26	k	101	BCR	C23-C22	-5.09	1.35	1.45
24	d	403[A]	CLA	C3C-C2C	5.09	1.47	1.36
24	B	601	CLA	CHC-C1C	5.09	1.48	1.35
24	c	504	CLA	C3B-C2B	5.09	1.47	1.40
24	A	405[B]	CLA	O2D-CGD	5.09	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	408[B]	PHO	O2D-CGD	5.09	1.45	1.33
24	c	502	CLA	CHC-C1C	5.08	1.48	1.35
24	b	610	CLA	C3C-C2C	5.08	1.47	1.36
24	c	504	CLA	C1D-ND	5.07	1.44	1.37
24	b	609	CLA	C3B-C2B	5.07	1.47	1.40
24	A	406[B]	CLA	C3C-C2C	5.07	1.47	1.36
24	B	604	CLA	O2D-CGD	5.07	1.45	1.33
24	b	603	CLA	C3C-C2C	5.06	1.47	1.36
24	a	405[A]	CLA	CHC-C1C	5.06	1.47	1.35
24	C	505	CLA	O2D-CGD	5.06	1.45	1.33
24	b	609	CLA	CHC-C1C	5.05	1.47	1.35
24	D	403	CLA	CHC-C1C	5.05	1.47	1.35
24	b	614	CLA	C3C-C2C	5.05	1.47	1.36
24	C	514	CLA	CHC-C1C	5.05	1.47	1.35
24	C	510	CLA	C1D-ND	5.04	1.44	1.37
41	V	201	HEC	C3C-C2C	-5.04	1.35	1.40
24	b	613	CLA	O2D-CGD	5.04	1.45	1.33
24	B	602	CLA	C1D-ND	5.04	1.44	1.37
24	A	406[A]	CLA	CHC-C1C	5.04	1.47	1.35
24	B	602	CLA	CHC-C1C	5.04	1.47	1.35
24	a	407[A]	CLA	CHC-C1C	5.04	1.47	1.35
24	B	606	CLA	C3C-C2C	5.03	1.47	1.36
25	A	408[B]	PHO	C3D-C2D	5.03	1.48	1.39
24	b	602	CLA	O2D-CGD	5.03	1.45	1.33
24	B	601	CLA	C1D-ND	5.03	1.44	1.37
41	V	201	HEC	C3D-C2D	5.03	1.52	1.37
26	d	405	BCR	C23-C22	-5.03	1.35	1.45
24	a	405[A]	CLA	C3C-C2C	5.02	1.47	1.36
24	c	508	CLA	CHC-C1C	5.02	1.47	1.35
25	d	402[B]	PHO	O2D-CGD	5.02	1.45	1.33
24	C	502	CLA	C3C-C2C	5.01	1.47	1.36
24	C	514	CLA	C3C-C2C	5.00	1.47	1.36
24	C	512	CLA	O2D-CGD	5.00	1.45	1.33
24	c	504	CLA	CHD-C1D	5.00	1.48	1.38
24	C	512	CLA	C3C-C2C	4.99	1.47	1.36
24	C	506	CLA	O2D-CGD	4.99	1.45	1.33
24	D	402[A]	CLA	CHC-C1C	4.98	1.47	1.35
24	c	505	CLA	CHC-C1C	4.98	1.47	1.35
24	b	603	CLA	CHC-C1C	4.98	1.47	1.35
24	B	610	CLA	CHC-C1C	4.97	1.47	1.35
24	B	602	CLA	C3C-C2C	4.97	1.47	1.36
24	c	512	CLA	CHC-C1C	4.97	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	605	CLA	CHC-C1C	4.97	1.47	1.35
24	C	505	CLA	C3C-C2C	4.96	1.47	1.36
24	C	513	CLA	C1D-ND	4.96	1.43	1.37
24	A	406[A]	CLA	C3C-C2C	4.96	1.47	1.36
24	b	604	CLA	C3C-C2C	4.95	1.47	1.36
24	a	406[A]	CLA	O2D-CGD	4.95	1.45	1.33
24	B	606	CLA	C1D-ND	4.95	1.43	1.37
25	A	417[A]	PHO	O2D-CGD	4.95	1.45	1.33
24	A	407[B]	CLA	C1D-ND	4.95	1.43	1.37
24	C	512	CLA	CHC-C1C	4.95	1.47	1.35
25	a	408[B]	PHO	O2D-CGD	4.95	1.45	1.33
24	B	601	CLA	O2D-CGD	4.95	1.45	1.33
24	c	514	CLA	O2D-CGD	4.94	1.45	1.33
24	c	507	CLA	C3C-C2C	4.94	1.47	1.36
24	b	601	CLA	O2D-CGD	4.94	1.45	1.33
24	B	604	CLA	CHC-C1C	4.94	1.47	1.35
24	B	615	CLA	C3C-C2C	4.94	1.47	1.36
24	B	608	CLA	C1D-ND	4.94	1.43	1.37
24	b	613	CLA	C3C-C2C	4.94	1.47	1.36
24	a	406[B]	CLA	CHC-C1C	4.93	1.47	1.35
24	A	405[A]	CLA	CHC-C1C	4.93	1.47	1.35
24	C	509	CLA	O2D-CGD	4.93	1.45	1.33
24	A	406[A]	CLA	C3B-C2B	4.92	1.47	1.40
24	b	607	CLA	CHC-C1C	4.92	1.47	1.35
24	C	514	CLA	O2D-CGD	4.92	1.45	1.33
24	b	611	CLA	CHC-C1C	4.91	1.47	1.35
24	B	614	CLA	CHC-C1C	4.91	1.47	1.35
24	C	514	CLA	C1D-ND	4.91	1.43	1.37
24	b	605	CLA	C1D-ND	4.91	1.43	1.37
41	V	201	HEC	C2B-C3B	-4.91	1.35	1.40
25	A	408[A]	PHO	O2D-CGD	4.91	1.45	1.33
24	a	406[A]	CLA	CHC-C1C	4.90	1.47	1.35
24	B	608	CLA	C3C-C2C	4.90	1.47	1.36
25	A	417[B]	PHO	OBD-CAD	4.90	1.29	1.22
24	A	406[B]	CLA	O2D-CGD	4.90	1.45	1.33
24	B	609	CLA	C3C-C2C	4.90	1.47	1.36
24	c	502	CLA	C1D-ND	4.90	1.43	1.37
24	d	403[B]	CLA	CHC-C1C	4.90	1.47	1.35
24	D	402[B]	CLA	O2D-CGD	4.89	1.45	1.33
24	B	613	CLA	C3C-C2C	4.88	1.47	1.36
24	b	601	CLA	CHC-C1C	4.88	1.47	1.35
24	b	609	CLA	C3C-C2C	4.88	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	402[B]	PHO	OBD-CAD	4.88	1.29	1.22
24	D	402[A]	CLA	O2D-CGD	4.88	1.45	1.33
24	a	406[B]	CLA	O2D-CGD	4.88	1.45	1.33
24	b	612	CLA	CHC-C1C	4.88	1.47	1.35
24	B	615	CLA	CHC-C1C	4.87	1.47	1.35
24	C	505	CLA	CHC-C1C	4.87	1.47	1.35
24	c	511	CLA	C1D-ND	4.87	1.43	1.37
24	B	607	CLA	C3C-C2C	4.87	1.47	1.36
24	B	611	CLA	O2D-CGD	4.86	1.45	1.33
24	C	511	CLA	O2D-CGD	4.86	1.45	1.33
24	C	504	CLA	CHC-C1C	4.86	1.47	1.35
24	C	509	CLA	C1D-ND	4.86	1.43	1.37
24	B	610	CLA	O2D-CGD	4.86	1.45	1.33
24	b	615	CLA	O2D-CGD	4.86	1.45	1.33
26	C	515	BCR	C23-C22	-4.85	1.35	1.45
24	c	507	CLA	C1D-ND	4.85	1.43	1.37
24	B	615	CLA	O2D-CGD	4.85	1.45	1.33
24	B	609	CLA	O2D-CGD	4.85	1.45	1.33
24	b	616	CLA	O2D-CGD	4.85	1.45	1.33
25	d	402[A]	PHO	O2D-CGD	4.84	1.45	1.33
24	B	616	CLA	CHC-C1C	4.84	1.47	1.35
24	C	511	CLA	CHC-C1C	4.83	1.47	1.35
24	c	511	CLA	C3C-C2C	4.83	1.47	1.36
24	a	407[B]	CLA	O2D-CGD	4.83	1.45	1.33
24	c	508	CLA	C3C-C2C	4.83	1.47	1.36
24	a	405[B]	CLA	O2D-CGD	4.82	1.45	1.33
24	b	604	CLA	CHC-C1C	4.82	1.47	1.35
24	c	502	CLA	C3C-C2C	4.82	1.47	1.36
24	c	507	CLA	CHC-C1C	4.81	1.47	1.35
24	C	503	CLA	CHC-C1C	4.81	1.47	1.35
24	B	603	CLA	C1D-ND	4.81	1.43	1.37
24	C	507	CLA	CHC-C1C	4.81	1.47	1.35
24	C	507	CLA	O2D-CGD	4.81	1.44	1.33
24	b	611	CLA	C3C-C2C	4.80	1.46	1.36
26	K	102	BCR	C23-C22	-4.80	1.35	1.45
24	C	510	CLA	O2D-CGD	4.80	1.44	1.33
24	c	507	CLA	O2D-CGD	4.80	1.44	1.33
24	b	602	CLA	CHD-C1D	4.80	1.47	1.38
24	c	503	CLA	CHC-C1C	4.79	1.47	1.35
25	A	408[A]	PHO	C3D-C2D	4.79	1.48	1.39
24	c	503	CLA	C1D-ND	4.79	1.43	1.37
24	b	601	CLA	O2A-CGA	4.79	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	406[B]	CLA	C1D-ND	4.79	1.43	1.37
24	B	607	CLA	O2D-CGD	4.78	1.44	1.33
24	D	402[B]	CLA	C1D-ND	4.78	1.43	1.37
24	B	610	CLA	C3B-C2B	4.78	1.47	1.40
24	B	605	CLA	O2D-CGD	4.78	1.44	1.33
24	A	405[A]	CLA	O2D-CGD	4.77	1.44	1.33
24	b	611	CLA	C1D-ND	4.77	1.43	1.37
24	c	510	CLA	C1D-ND	4.77	1.43	1.37
24	c	508	CLA	C3B-C2B	4.77	1.47	1.40
26	t	102	BCR	C23-C22	-4.77	1.35	1.45
24	b	605	CLA	CHC-C1C	4.77	1.47	1.35
27	X	101	SQD	O47-C7	4.75	1.47	1.34
24	c	511	CLA	CHC-C1C	4.75	1.47	1.35
24	C	509	CLA	CHC-C1C	4.75	1.47	1.35
24	c	506	CLA	C3B-C2B	4.75	1.47	1.40
24	a	409	CLA	C1D-ND	4.74	1.43	1.37
26	B	619	BCR	C23-C22	-4.73	1.35	1.45
24	A	407[A]	CLA	O2D-CGD	4.73	1.44	1.33
24	d	403[B]	CLA	O2D-CGD	4.72	1.44	1.33
24	d	403[A]	CLA	CHC-C1C	4.72	1.47	1.35
24	A	409	CLA	CHC-C1C	4.71	1.47	1.35
24	B	603	CLA	CHC-C1C	4.71	1.47	1.35
24	B	609	CLA	CHD-C1D	4.69	1.47	1.38
26	D	404	BCR	C23-C22	-4.68	1.35	1.45
24	B	603	CLA	O2D-CGD	4.68	1.44	1.33
24	b	609	CLA	CHD-C1D	4.68	1.47	1.38
24	D	403	CLA	O2D-CGD	4.67	1.44	1.33
24	B	614	CLA	C1D-ND	4.67	1.43	1.37
24	C	507	CLA	C3C-C2C	4.67	1.46	1.36
24	b	610	CLA	O2D-CGD	4.67	1.44	1.33
24	B	602	CLA	O2D-CGD	4.66	1.44	1.33
24	b	614	CLA	O2D-CGD	4.66	1.44	1.33
35	c	521	LMG	O7-C10	4.66	1.47	1.34
24	B	606	CLA	O2D-CGD	4.66	1.44	1.33
24	D	403	CLA	CHD-C1D	4.65	1.47	1.38
24	a	407[A]	CLA	O2D-CGD	4.65	1.44	1.33
24	c	508	CLA	O2D-CGD	4.64	1.44	1.33
24	c	503	CLA	O2D-CGD	4.64	1.44	1.33
27	B	620	SQD	O47-C7	4.64	1.47	1.34
24	c	513	CLA	O2D-CGD	4.64	1.44	1.33
35	C	521	LMG	O7-C10	4.63	1.47	1.34
24	b	608	CLA	C3C-C2C	4.63	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	503	CLA	CHD-C1D	4.62	1.47	1.38
35	C	521	LMG	O8-C28	4.62	1.46	1.33
35	C	520	LMG	O8-C28	4.61	1.46	1.33
24	A	405[B]	CLA	CHD-C1D	4.61	1.47	1.38
24	C	503	CLA	O2D-CGD	4.61	1.44	1.33
24	C	513	CLA	O2D-CGD	4.60	1.44	1.33
27	f	101	SQD	O47-C7	4.60	1.47	1.34
24	B	605	CLA	C3B-C2B	4.60	1.46	1.40
24	B	616	CLA	O2D-CGD	4.59	1.44	1.33
24	c	512	CLA	O2D-CGD	4.59	1.44	1.33
24	d	403[A]	CLA	O2D-CGD	4.59	1.44	1.33
24	a	406[A]	CLA	C3B-C2B	4.58	1.46	1.40
26	y	101	BCR	C23-C22	-4.58	1.36	1.45
24	b	608	CLA	CHC-C1C	4.58	1.46	1.35
26	C	516	BCR	C23-C22	-4.57	1.36	1.45
33	E	101[A]	LHG	O8-C23	4.57	1.46	1.33
24	C	502	CLA	CHD-C1D	4.56	1.47	1.38
24	a	407[B]	CLA	C1D-ND	4.56	1.43	1.37
24	b	609	CLA	C1D-ND	4.55	1.43	1.37
24	b	612	CLA	O2D-CGD	4.55	1.44	1.33
24	A	409	CLA	O2D-CGD	4.55	1.44	1.33
24	A	406[A]	CLA	C1D-ND	4.55	1.43	1.37
24	b	604	CLA	CHD-C1D	4.54	1.47	1.38
24	C	506	CLA	C1D-ND	4.54	1.43	1.37
24	b	604	CLA	C1D-ND	4.54	1.43	1.37
24	c	514	CLA	O2A-CGA	4.54	1.46	1.33
24	b	602	CLA	C1D-ND	4.54	1.43	1.37
24	d	404	CLA	CHD-C1D	4.53	1.47	1.38
24	B	614	CLA	O2D-CGD	4.53	1.44	1.33
24	B	604	CLA	OBD-CAD	4.53	1.30	1.22
35	z	101	LMG	O8-C28	4.52	1.46	1.33
24	c	513	CLA	CHD-C1D	4.52	1.47	1.38
26	c	515	BCR	C23-C22	-4.52	1.36	1.45
26	c	516	BCR	C23-C22	-4.50	1.36	1.45
33	a	420[A]	LHG	O8-C23	4.50	1.46	1.33
25	a	408[B]	PHO	OBD-CAD	4.49	1.28	1.22
24	b	608	CLA	O2D-CGD	4.49	1.44	1.33
24	A	407[A]	CLA	C3B-C2B	4.48	1.46	1.40
24	a	407[A]	CLA	C1D-ND	4.48	1.43	1.37
24	D	402[B]	CLA	O2A-CGA	4.48	1.46	1.33
24	b	616	CLA	CHD-C1D	4.47	1.47	1.38
24	c	510	CLA	CHC-C1C	4.47	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	508	CLA	C1D-ND	4.46	1.43	1.37
24	D	403	CLA	C3B-C2B	4.45	1.46	1.40
27	a	413	SQD	O48-C23	4.45	1.46	1.33
27	A	413	SQD	O48-C23	4.45	1.46	1.33
24	d	403[B]	CLA	C1D-ND	4.44	1.43	1.37
24	b	615	CLA	C1D-ND	4.43	1.43	1.37
26	A	410	BCR	C23-C22	-4.43	1.36	1.45
24	C	510	CLA	CHC-C1C	4.42	1.46	1.35
24	b	605	CLA	O2D-CGD	4.42	1.44	1.33
24	B	602	CLA	CHD-C1D	4.42	1.47	1.38
24	c	513	CLA	O2A-CGA	4.41	1.46	1.33
33	E	101[B]	LHG	O8-C23	4.41	1.46	1.33
24	c	514	CLA	CHD-C1D	4.40	1.46	1.38
24	d	404	CLA	O2A-CGA	4.40	1.46	1.33
24	b	612	CLA	C1D-ND	4.40	1.43	1.37
26	H	101	BCR	C23-C22	-4.40	1.36	1.45
24	a	407[B]	CLA	O2A-CGA	4.40	1.46	1.33
26	b	619	BCR	C23-C22	-4.40	1.36	1.45
24	b	614	CLA	CHD-C1D	4.39	1.46	1.38
24	c	512	CLA	CHD-C1D	4.39	1.46	1.38
26	a	410	BCR	C23-C22	-4.39	1.36	1.45
24	b	607	CLA	O2D-CGD	4.38	1.43	1.33
24	B	609	CLA	C1D-ND	4.38	1.43	1.37
24	A	405[B]	CLA	CHD-C4C	4.38	1.49	1.39
24	a	405[A]	CLA	O2D-CGD	4.38	1.43	1.33
24	B	610	CLA	C1D-ND	4.38	1.43	1.37
26	b	618	BCR	C23-C22	-4.38	1.36	1.45
33	a	420[B]	LHG	O8-C23	4.38	1.46	1.33
24	b	606	CLA	O2D-CGD	4.38	1.43	1.33
24	C	513	CLA	CHD-C1D	4.37	1.46	1.38
24	c	502	CLA	O2D-CGD	4.37	1.43	1.33
27	L	102	SQD	O48-C23	4.36	1.46	1.33
24	C	512	CLA	CHD-C1D	4.36	1.46	1.38
24	c	506	CLA	C1D-ND	4.36	1.43	1.37
24	C	508	CLA	O2A-CGA	4.36	1.46	1.33
24	A	409	CLA	C1D-ND	4.35	1.43	1.37
24	C	507	CLA	C1D-ND	4.35	1.43	1.37
24	C	505	CLA	C1D-ND	4.35	1.43	1.37
24	b	610	CLA	C1D-ND	4.35	1.43	1.37
24	B	612	CLA	C1B-NB	-4.35	1.31	1.35
24	c	508	CLA	O2A-CGA	4.34	1.46	1.33
24	c	506	CLA	CHD-C1D	4.34	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	617	BCR	C23-C22	-4.34	1.36	1.45
24	b	608	CLA	CHD-C1D	4.33	1.46	1.38
25	A	408[B]	PHO	OBD-CAD	4.33	1.28	1.22
24	C	507	CLA	CHD-C1D	4.33	1.46	1.38
24	a	406[B]	CLA	O2A-CGA	4.33	1.46	1.33
25	A	417[A]	PHO	CHA-CBD	-4.32	1.47	1.52
26	B	617	BCR	C23-C22	-4.32	1.36	1.45
26	h	101	BCR	C23-C22	-4.31	1.36	1.45
24	a	406[A]	CLA	C3D-C2D	4.30	1.50	1.39
24	c	506	CLA	O2D-CGD	4.30	1.43	1.33
24	a	409	CLA	O2A-CGA	4.29	1.45	1.33
24	C	504	CLA	O2D-CGD	4.29	1.43	1.33
33	a	420[A]	LHG	O7-C7	4.28	1.46	1.34
24	A	406[B]	CLA	CHD-C1D	4.27	1.46	1.38
27	L	102	SQD	O47-C7	4.27	1.46	1.34
24	B	604	CLA	CHD-C1D	4.26	1.46	1.38
24	D	402[B]	CLA	CHD-C1D	4.26	1.46	1.38
24	B	616	CLA	C1D-ND	4.26	1.43	1.37
27	B	620	SQD	O48-C23	4.26	1.45	1.33
24	B	616	CLA	O2A-CGA	4.25	1.45	1.33
24	b	607	CLA	CHD-C1D	4.25	1.46	1.38
24	B	608	CLA	CHC-C1C	4.25	1.45	1.35
24	b	601	CLA	CHD-C1D	4.25	1.46	1.38
24	b	611	CLA	O2D-CGD	4.25	1.43	1.33
24	D	402[A]	CLA	C1D-ND	4.25	1.43	1.37
24	b	608	CLA	O2A-CGA	4.25	1.45	1.33
24	c	508	CLA	CHD-C1D	4.25	1.46	1.38
24	b	611	CLA	O2A-CGA	4.25	1.45	1.33
35	c	521	LMG	O8-C28	4.24	1.45	1.33
24	B	609	CLA	C3D-C2D	4.24	1.50	1.39
24	C	508	CLA	O2D-CGD	4.24	1.43	1.33
24	c	503	CLA	CHD-C1D	4.24	1.46	1.38
24	C	509	CLA	CHD-C1D	4.23	1.46	1.38
27	f	101	SQD	O48-C23	4.23	1.45	1.33
24	b	615	CLA	O2A-CGA	4.23	1.45	1.33
24	C	514	CLA	CHD-C1D	4.22	1.46	1.38
24	C	514	CLA	O2A-CGA	4.22	1.45	1.33
24	D	402[B]	CLA	CHD-C4C	4.22	1.48	1.39
24	c	513	CLA	CHD-C4C	4.22	1.48	1.39
35	M	101	LMG	O8-C28	4.22	1.45	1.33
24	B	612	CLA	O2D-CGD	4.22	1.43	1.33
33	E	101[A]	LHG	O7-C7	4.22	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	509	CLA	O2A-CGA	4.21	1.45	1.33
36	c	517[B]	DGD	O2G-C1B	4.21	1.46	1.34
24	a	406[B]	CLA	C3D-C2D	4.21	1.50	1.39
35	C	520	LMG	O7-C10	4.20	1.46	1.34
24	b	602	CLA	CHD-C4C	4.20	1.48	1.39
24	B	608	CLA	O2D-CGD	4.20	1.43	1.33
24	C	503	CLA	C3D-C2D	4.20	1.50	1.39
24	C	504	CLA	C1D-ND	4.20	1.42	1.37
33	d	408[A]	LHG	O8-C23	4.19	1.45	1.33
24	a	405[B]	CLA	CHD-C1D	4.19	1.46	1.38
27	X	101	SQD	O48-C23	4.19	1.45	1.33
24	D	402[A]	CLA	CHD-C1D	4.19	1.46	1.38
24	C	509	CLA	C3D-C2D	4.19	1.50	1.39
24	a	407[B]	CLA	CHD-C1D	4.19	1.46	1.38
24	D	402[A]	CLA	O2A-CGA	4.18	1.45	1.33
24	b	604	CLA	O2D-CGD	4.18	1.43	1.33
24	A	409	CLA	O2A-CGA	4.17	1.45	1.33
24	C	512	CLA	O2A-CGA	4.17	1.45	1.33
24	d	403[B]	CLA	CHD-C1D	4.17	1.46	1.38
24	C	513	CLA	O2A-CGA	4.17	1.45	1.33
24	C	504	CLA	CHD-C1D	4.16	1.46	1.38
24	B	615	CLA	CHD-C1D	4.16	1.46	1.38
24	b	608	CLA	OBD-CAD	4.16	1.29	1.22
35	Z	101	LMG	O7-C10	4.16	1.46	1.34
24	c	505	CLA	C3D-C2D	4.16	1.50	1.39
24	a	405[B]	CLA	CHD-C4C	4.16	1.48	1.39
33	d	408[B]	LHG	O8-C23	4.15	1.45	1.33
33	E	101[B]	LHG	O7-C7	4.15	1.46	1.34
24	c	512	CLA	O2A-CGA	4.15	1.45	1.33
33	a	420[B]	LHG	O7-C7	4.15	1.46	1.34
24	b	602	CLA	C3D-C2D	4.15	1.50	1.39
24	b	606	CLA	CHD-C1D	4.14	1.46	1.38
35	z	101	LMG	O7-C10	4.14	1.46	1.34
24	d	404	CLA	C3D-C2D	4.14	1.50	1.39
24	b	615	CLA	CHD-C1D	4.14	1.46	1.38
24	A	406[B]	CLA	O2A-CGA	4.14	1.45	1.33
24	b	601	CLA	C3D-C2D	4.13	1.50	1.39
36	C	517[A]	DGD	O2G-C1B	4.13	1.46	1.34
25	A	408[A]	PHO	OBD-CAD	4.13	1.28	1.22
34	b	621	HTG	C1'-S1	-4.13	1.76	1.81
24	c	506	CLA	CHD-C4C	4.13	1.48	1.39
24	c	503	CLA	CHD-C4C	4.13	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	612	CLA	C3D-C2D	4.12	1.50	1.39
24	a	406[A]	CLA	O2A-CGA	4.12	1.45	1.33
24	b	607	CLA	C1D-ND	4.12	1.42	1.37
24	A	407[B]	CLA	CHD-C1D	4.12	1.46	1.38
24	C	510	CLA	CHD-C1D	4.12	1.46	1.38
26	Y	101	BCR	C23-C22	-4.12	1.37	1.45
27	a	411[B]	SQD	O47-C7	4.11	1.45	1.34
24	c	507	CLA	O2A-CGA	4.11	1.45	1.33
36	c	518[B]	DGD	O1G-C1A	4.11	1.45	1.33
24	B	613	CLA	CHD-C1D	4.11	1.46	1.38
24	a	405[A]	CLA	CHD-C1D	4.11	1.46	1.38
24	B	609	CLA	O2A-CGA	4.11	1.45	1.33
24	A	407[A]	CLA	CHD-C1D	4.10	1.46	1.38
24	A	406[A]	CLA	C3D-C2D	4.10	1.50	1.39
24	B	608	CLA	CHD-C1D	4.10	1.46	1.38
24	c	505	CLA	O2A-CGA	4.10	1.45	1.33
33	L	101[B]	LHG	O8-C23	4.10	1.45	1.33
24	a	405[A]	CLA	CHD-C4C	4.10	1.48	1.39
24	B	613	CLA	C1D-ND	4.10	1.42	1.37
24	c	507	CLA	CHD-C1D	4.09	1.46	1.38
24	C	506	CLA	CHD-C1D	4.09	1.46	1.38
24	A	407[A]	CLA	C1D-ND	4.09	1.42	1.37
24	c	503	CLA	C3D-C2D	4.08	1.50	1.39
33	D	407[B]	LHG	O7-C7	4.08	1.45	1.34
24	a	407[B]	CLA	C3D-C2D	4.07	1.50	1.39
24	b	610	CLA	CHD-C1D	4.07	1.46	1.38
24	A	406[A]	CLA	O2A-CGA	4.07	1.45	1.33
24	C	507	CLA	O2A-CGA	4.07	1.45	1.33
24	B	601	CLA	CHD-C1D	4.07	1.46	1.38
24	A	409	CLA	CHD-C1D	4.07	1.46	1.38
24	B	610	CLA	C3D-C2D	4.07	1.50	1.39
35	C	501	LMG	O7-C10	4.07	1.45	1.34
24	c	514	CLA	CHD-C4C	4.06	1.48	1.39
24	C	503	CLA	O2A-CGA	4.06	1.45	1.33
24	B	615	CLA	C3D-C2D	4.06	1.50	1.39
35	c	520	LMG	O8-C28	4.06	1.45	1.33
24	c	505	CLA	CHD-C1D	4.06	1.46	1.38
24	A	407[B]	CLA	C3D-C2D	4.06	1.50	1.39
24	b	601	CLA	CHD-C4C	4.06	1.48	1.39
24	C	508	CLA	CHD-C1D	4.06	1.46	1.38
27	a	411[B]	SQD	O48-C23	4.06	1.45	1.33
24	d	403[B]	CLA	O2A-CGA	4.05	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	L	101[B]	LHG	O7-C7	4.05	1.45	1.34
35	b	629	LMG	O8-C28	4.05	1.45	1.33
35	c	520	LMG	O7-C10	4.05	1.45	1.34
27	a	411[A]	SQD	O47-C7	4.05	1.45	1.34
24	B	614	CLA	O2A-CGA	4.05	1.45	1.33
24	B	604	CLA	C1D-ND	4.04	1.42	1.37
24	b	608	CLA	C1D-ND	4.04	1.42	1.37
25	d	402[B]	PHO	O2A-CGA	4.04	1.45	1.33
24	c	509	CLA	C3D-C2D	4.04	1.50	1.39
35	a	417	LMG	O8-C28	4.04	1.45	1.33
33	D	406[B]	LHG	O7-C7	4.04	1.45	1.34
24	b	603	CLA	CHD-C1D	4.03	1.46	1.38
36	c	519	DGD	O1G-C1A	4.03	1.45	1.33
24	c	502	CLA	CHD-C1D	4.03	1.46	1.38
25	d	402[B]	PHO	C3C-C2C	4.03	1.49	1.37
36	c	517[B]	DGD	O1G-C1A	4.03	1.45	1.33
24	c	505	CLA	CHD-C4C	4.02	1.48	1.39
24	B	607	CLA	OBD-CAD	4.02	1.29	1.22
24	C	511	CLA	CHD-C1D	4.02	1.46	1.38
24	B	611	CLA	OBD-CAD	4.02	1.29	1.22
25	A	417[A]	PHO	O2A-CGA	4.02	1.45	1.33
24	B	611	CLA	CHD-C1D	4.02	1.46	1.38
24	B	607	CLA	CHD-C1D	4.01	1.46	1.38
35	M	101	LMG	O7-C10	4.01	1.45	1.34
24	b	615	CLA	C3D-C2D	4.01	1.50	1.39
24	C	510	CLA	O2A-CGA	4.01	1.45	1.33
24	C	513	CLA	CHD-C4C	4.01	1.48	1.39
24	B	605	CLA	CHD-C1D	4.01	1.46	1.38
36	c	518[A]	DGD	O1G-C1A	4.00	1.45	1.33
24	C	502	CLA	O2D-CGD	4.00	1.43	1.33
24	c	504	CLA	CHD-C4C	4.00	1.48	1.39
24	d	403[B]	CLA	CHD-C4C	4.00	1.48	1.39
24	C	509	CLA	O2A-CGA	4.00	1.45	1.33
24	b	611	CLA	CHD-C4C	3.99	1.48	1.39
36	C	517[B]	DGD	O2G-C1B	3.99	1.45	1.34
35	a	417	LMG	O7-C10	3.99	1.45	1.34
24	b	611	CLA	CHD-C1D	3.99	1.46	1.38
24	B	603	CLA	C3D-C2D	3.99	1.50	1.39
24	B	606	CLA	CHD-C1D	3.98	1.46	1.38
24	B	602	CLA	CHD-C4C	3.98	1.48	1.39
35	C	501	LMG	O8-C28	3.98	1.45	1.33
24	C	506	CLA	CHD-C4C	3.98	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	607	CLA	C1D-ND	3.98	1.42	1.37
24	B	615	CLA	O2A-CGA	3.97	1.45	1.33
24	c	503	CLA	O2A-CGA	3.97	1.45	1.33
24	d	404	CLA	O2D-CGD	3.97	1.42	1.33
24	B	616	CLA	C3D-C2D	3.97	1.50	1.39
24	A	406[A]	CLA	CHD-C1D	3.97	1.46	1.38
24	C	510	CLA	C3D-C2D	3.97	1.50	1.39
27	a	411[A]	SQD	O48-C23	3.97	1.44	1.33
24	D	403	CLA	C3D-C2D	3.97	1.50	1.39
33	b	628[B]	LHG	O8-C23	3.96	1.44	1.33
36	C	519	DGD	O1G-C1A	3.96	1.44	1.33
24	c	510	CLA	C3D-C2D	3.96	1.49	1.39
27	A	413	SQD	O47-C7	3.96	1.45	1.34
24	a	407[A]	CLA	O2A-CGA	3.96	1.44	1.33
24	a	407[A]	CLA	C3D-C2D	3.96	1.49	1.39
24	d	403[A]	CLA	O2A-CGA	3.96	1.44	1.33
24	c	512	CLA	CHD-C4C	3.95	1.48	1.39
24	A	407[A]	CLA	OBD-CAD	3.95	1.29	1.22
24	c	502	CLA	OBD-CAD	3.95	1.29	1.22
27	A	411[B]	SQD	O48-C23	3.95	1.44	1.33
24	A	407[A]	CLA	C3D-C2D	3.95	1.49	1.39
24	B	611	CLA	CHD-C4C	3.95	1.48	1.39
24	B	605	CLA	O2A-CGA	3.94	1.44	1.33
24	C	512	CLA	C1D-ND	3.94	1.42	1.37
24	C	508	CLA	C3D-C2D	3.94	1.49	1.39
24	C	511	CLA	CHD-C4C	3.94	1.48	1.39
24	A	406[B]	CLA	CHD-C4C	3.94	1.48	1.39
24	B	612	CLA	CHD-C1D	3.93	1.46	1.38
24	b	616	CLA	O2A-CGA	3.93	1.44	1.33
24	a	407[B]	CLA	CHD-C4C	3.93	1.48	1.39
24	A	407[B]	CLA	CHD-C4C	3.93	1.48	1.39
36	C	518[B]	DGD	O1G-C1A	3.93	1.44	1.33
24	d	403[A]	CLA	CHD-C1D	3.93	1.46	1.38
27	a	413	SQD	O47-C7	3.92	1.45	1.34
33	D	407[B]	LHG	O8-C23	3.92	1.44	1.33
24	b	609	CLA	OBD-CAD	3.92	1.29	1.22
24	C	509	CLA	OBD-CAD	3.92	1.29	1.22
24	c	502	CLA	C3D-C2D	3.92	1.49	1.39
33	L	101[A]	LHG	O8-C23	3.92	1.44	1.33
24	b	608	CLA	C3D-C2D	3.92	1.49	1.39
24	a	409	CLA	CHD-C1D	3.91	1.46	1.38
24	c	513	CLA	C3D-C2D	3.91	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	611	CLA	O2A-CGA	3.91	1.44	1.33
33	D	407[A]	LHG	O8-C23	3.91	1.44	1.33
24	c	509	CLA	CHD-C1D	3.91	1.46	1.38
33	d	407[B]	LHG	O7-C7	3.90	1.45	1.34
33	d	407[A]	LHG	O7-C7	3.90	1.45	1.34
24	B	608	CLA	C3D-C2D	3.90	1.49	1.39
24	a	406[B]	CLA	OBD-CAD	3.89	1.29	1.22
33	D	407[A]	LHG	O7-C7	3.89	1.45	1.34
24	b	615	CLA	OBD-CAD	3.89	1.29	1.22
36	h	102	DGD	O1G-C1A	3.89	1.44	1.33
25	d	402[A]	PHO	C3C-C2C	3.89	1.49	1.37
24	C	505	CLA	CHD-C1D	3.89	1.45	1.38
24	c	502	CLA	CHD-C4C	3.88	1.48	1.39
24	c	506	CLA	C3D-C2D	3.88	1.49	1.39
24	b	610	CLA	OBD-CAD	3.88	1.29	1.22
24	c	511	CLA	CHD-C4C	3.88	1.48	1.39
24	C	508	CLA	C1D-ND	3.88	1.42	1.37
25	A	417[B]	PHO	O2A-CGA	3.88	1.44	1.33
24	B	610	CLA	CHD-C1D	3.88	1.45	1.38
24	c	507	CLA	CHD-C4C	3.87	1.48	1.39
25	a	408[A]	PHO	OBD-CAD	3.87	1.27	1.22
24	b	611	CLA	C3D-C2D	3.87	1.49	1.39
25	A	417[B]	PHO	C3C-C2C	3.87	1.49	1.37
24	a	405[B]	CLA	OBD-CAD	3.87	1.29	1.22
35	d	412	LMG	O7-C10	3.87	1.45	1.34
24	b	610	CLA	C3D-C2D	3.87	1.49	1.39
24	b	606	CLA	O2A-CGA	3.87	1.44	1.33
24	B	602	CLA	C3D-C2D	3.86	1.49	1.39
24	D	403	CLA	CHD-C4C	3.86	1.48	1.39
24	C	514	CLA	CHD-C4C	3.86	1.48	1.39
24	A	406[B]	CLA	C3D-C2D	3.85	1.49	1.39
24	c	502	CLA	O2A-CGA	3.85	1.44	1.33
24	c	514	CLA	C3D-C2D	3.85	1.49	1.39
24	b	616	CLA	CHD-C4C	3.85	1.48	1.39
33	b	628[B]	LHG	O7-C7	3.85	1.45	1.34
25	d	402[A]	PHO	O2A-CGA	3.84	1.44	1.33
33	d	408[B]	LHG	O7-C7	3.84	1.45	1.34
25	A	408[B]	PHO	O2A-CGA	3.84	1.44	1.33
36	C	518[A]	DGD	O2G-C1B	3.84	1.45	1.34
24	c	511	CLA	C3D-C2D	3.84	1.49	1.39
24	a	406[A]	CLA	OBD-CAD	3.84	1.29	1.22
24	C	502	CLA	CHD-C4C	3.84	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	c	518[B]	DGD	O2G-C1B	3.84	1.45	1.34
24	C	502	CLA	O2A-CGA	3.84	1.44	1.33
24	c	512	CLA	OBD-CAD	3.83	1.29	1.22
24	C	514	CLA	C3D-C2D	3.83	1.49	1.39
24	D	403	CLA	OBD-CAD	3.83	1.29	1.22
24	c	504	CLA	O2D-CGD	3.83	1.42	1.33
24	c	509	CLA	CHD-C4C	3.82	1.48	1.39
24	c	508	CLA	C3D-C2D	3.82	1.49	1.39
24	c	508	CLA	OBD-CAD	3.82	1.29	1.22
24	b	614	CLA	C3D-C2D	3.82	1.49	1.39
24	B	607	CLA	CHD-C4C	3.82	1.47	1.39
36	h	102	DGD	O2G-C1B	3.82	1.45	1.34
24	d	404	CLA	CHD-C4C	3.82	1.47	1.39
24	c	510	CLA	O2A-CGA	3.81	1.44	1.33
25	a	408[B]	PHO	O2A-CGA	3.81	1.44	1.33
24	C	512	CLA	C3D-C2D	3.81	1.49	1.39
24	C	513	CLA	C3D-C2D	3.81	1.49	1.39
36	c	517[A]	DGD	O2G-C1B	3.81	1.45	1.34
34	B	624	HTG	C1'-S1	-3.81	1.76	1.81
24	b	606	CLA	OBD-CAD	3.81	1.29	1.22
24	A	405[A]	CLA	C3D-C2D	3.81	1.49	1.39
33	d	414[B]	LHG	O8-C23	3.80	1.44	1.33
36	C	518[B]	DGD	O2G-C1B	3.80	1.45	1.34
24	B	603	CLA	O2A-CGA	3.80	1.44	1.33
24	A	409	CLA	C3D-C2D	3.80	1.49	1.39
24	a	406[B]	CLA	CHD-C4C	3.80	1.47	1.39
24	B	609	CLA	CHD-C4C	3.80	1.47	1.39
24	A	409	CLA	CHD-C4C	3.79	1.47	1.39
24	b	605	CLA	CHD-C4C	3.79	1.47	1.39
36	C	518[A]	DGD	O1G-C1A	3.79	1.44	1.33
24	b	616	CLA	C3D-C2D	3.79	1.49	1.39
24	A	406[A]	CLA	CHD-C4C	3.79	1.47	1.39
24	b	607	CLA	C3D-C2D	3.79	1.49	1.39
35	d	412	LMG	O8-C28	3.79	1.44	1.33
24	a	407[A]	CLA	CHD-C4C	3.79	1.47	1.39
25	A	417[A]	PHO	C3C-C2C	3.78	1.48	1.37
24	b	613	CLA	C3D-C2D	3.78	1.49	1.39
25	A	408[A]	PHO	C3C-C2C	3.78	1.48	1.37
36	c	517[A]	DGD	O1G-C1A	3.78	1.44	1.33
26	B	618	BCR	C23-C22	-3.78	1.37	1.45
24	b	604	CLA	C3D-C2D	3.78	1.49	1.39
24	c	504	CLA	O2A-CGA	3.77	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	603	CLA	CHD-C1D	3.77	1.45	1.38
25	A	408[A]	PHO	O2A-CGA	3.77	1.44	1.33
24	B	608	CLA	O2A-CGA	3.77	1.44	1.33
24	a	406[B]	CLA	CHD-C1D	3.76	1.45	1.38
24	b	613	CLA	O2A-CGA	3.76	1.44	1.33
24	B	615	CLA	CHD-C4C	3.76	1.47	1.39
24	B	610	CLA	OBD-CAD	3.76	1.29	1.22
36	C	517[B]	DGD	O1G-C1A	3.76	1.44	1.33
27	A	411[A]	SQD	O48-C23	3.76	1.44	1.33
24	A	405[B]	CLA	C3D-C2D	3.76	1.49	1.39
24	d	404	CLA	OBD-CAD	3.76	1.29	1.22
24	b	605	CLA	CHD-C1D	3.76	1.45	1.38
24	B	614	CLA	CHD-C4C	3.75	1.47	1.39
33	A	420[B]	LHG	O8-C23	3.75	1.44	1.33
24	a	407[B]	CLA	OBD-CAD	3.75	1.28	1.22
36	H	102	DGD	O1G-C1A	3.75	1.44	1.33
24	c	507	CLA	C3D-C2D	3.74	1.49	1.39
24	B	605	CLA	CHD-C4C	3.74	1.47	1.39
24	b	606	CLA	CHD-C4C	3.74	1.47	1.39
24	A	405[B]	CLA	O2A-CGA	3.74	1.44	1.33
24	a	405[A]	CLA	OBD-CAD	3.74	1.28	1.22
33	d	414[B]	LHG	O7-C7	3.74	1.44	1.34
24	b	612	CLA	CHD-C1D	3.73	1.45	1.38
24	A	407[A]	CLA	O2A-CGA	3.73	1.44	1.33
24	C	512	CLA	CHD-C4C	3.73	1.47	1.39
24	b	609	CLA	O2A-CGA	3.73	1.44	1.33
24	A	407[B]	CLA	OBD-CAD	3.73	1.28	1.22
24	B	614	CLA	CHD-C1D	3.73	1.45	1.38
24	b	603	CLA	C1D-ND	3.73	1.42	1.37
24	b	608	CLA	CHD-C4C	3.73	1.47	1.39
24	C	510	CLA	CHD-C4C	3.72	1.47	1.39
24	b	610	CLA	CHD-C4C	3.72	1.47	1.39
24	b	605	CLA	C3D-C2D	3.72	1.49	1.39
24	c	508	CLA	CHD-C4C	3.72	1.47	1.39
33	d	407[B]	LHG	O8-C23	3.71	1.44	1.33
24	B	601	CLA	CHD-C4C	3.71	1.47	1.39
24	b	613	CLA	CHD-C1D	3.71	1.45	1.38
24	b	614	CLA	CHD-C4C	3.71	1.47	1.39
24	B	607	CLA	O2A-CGA	3.71	1.44	1.33
24	C	507	CLA	CHD-C4C	3.71	1.47	1.39
24	a	405[B]	CLA	O2A-CGA	3.71	1.44	1.33
24	C	514	CLA	OBD-CAD	3.71	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407[A]	CLA	CHD-C4C	3.70	1.47	1.39
24	B	616	CLA	CHD-C1D	3.70	1.45	1.38
24	b	604	CLA	O2A-CGA	3.70	1.44	1.33
36	c	519	DGD	O2G-C1B	3.70	1.44	1.34
24	A	405[A]	CLA	CHD-C1D	3.70	1.45	1.38
24	c	510	CLA	CHD-C1D	3.69	1.45	1.38
24	B	613	CLA	C3D-C2D	3.69	1.49	1.39
24	c	511	CLA	CHD-C1D	3.69	1.45	1.38
24	C	511	CLA	O2A-CGA	3.69	1.44	1.33
24	b	602	CLA	O2A-CGA	3.68	1.44	1.33
33	L	101[A]	LHG	O7-C7	3.68	1.44	1.34
27	A	411[A]	SQD	O47-C7	3.68	1.44	1.34
33	d	408[A]	LHG	O7-C7	3.68	1.44	1.34
24	c	510	CLA	CHD-C4C	3.68	1.47	1.39
24	B	605	CLA	C3D-C2D	3.67	1.49	1.39
27	A	411[B]	SQD	O47-C7	3.67	1.44	1.34
24	c	511	CLA	O2A-CGA	3.67	1.44	1.33
24	a	405[A]	CLA	C3D-C2D	3.67	1.49	1.39
24	C	505	CLA	C3D-C2D	3.67	1.49	1.39
24	A	407[B]	CLA	O2A-CGA	3.67	1.44	1.33
24	A	405[A]	CLA	CHD-C4C	3.67	1.47	1.39
33	D	406[A]	LHG	O7-C7	3.66	1.44	1.34
24	d	403[B]	CLA	OBD-CAD	3.66	1.28	1.22
35	D	411	LMG	O8-C28	3.66	1.44	1.33
24	C	504	CLA	CHD-C4C	3.66	1.47	1.39
24	b	612	CLA	O2A-CGA	3.65	1.44	1.33
36	C	517[A]	DGD	O1G-C1A	3.65	1.44	1.33
24	a	406[A]	CLA	CHD-C1D	3.65	1.45	1.38
25	a	408[B]	PHO	C3C-C2C	3.65	1.48	1.37
24	b	615	CLA	CHD-C4C	3.64	1.47	1.39
33	d	414[A]	LHG	O8-C23	3.64	1.44	1.33
24	D	402[A]	CLA	CHD-C4C	3.64	1.47	1.39
24	A	405[B]	CLA	OBD-CAD	3.64	1.28	1.22
24	B	601	CLA	C3D-C2D	3.64	1.49	1.39
24	b	609	CLA	C3D-C2D	3.64	1.49	1.39
24	b	603	CLA	O2A-CGA	3.63	1.44	1.33
24	B	606	CLA	O2A-CGA	3.63	1.43	1.33
24	b	606	CLA	C3D-C2D	3.63	1.49	1.39
24	b	605	CLA	OBD-CAD	3.63	1.28	1.22
36	C	519	DGD	O2G-C1B	3.62	1.44	1.34
24	C	503	CLA	CHD-C4C	3.62	1.47	1.39
24	B	604	CLA	CHD-C4C	3.62	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	602	CLA	O2A-CGA	3.62	1.43	1.33
24	C	505	CLA	O2A-CGA	3.62	1.43	1.33
24	d	403[A]	CLA	C1D-ND	3.61	1.42	1.37
33	A	420[B]	LHG	O7-C7	3.61	1.44	1.34
24	a	407[A]	CLA	CHD-C1D	3.61	1.45	1.38
24	B	606	CLA	C3D-C2D	3.61	1.49	1.39
24	d	403[A]	CLA	OBD-CAD	3.61	1.28	1.22
24	a	405[B]	CLA	C3D-C2D	3.61	1.49	1.39
24	B	615	CLA	OBD-CAD	3.61	1.28	1.22
33	b	628[A]	LHG	O7-C7	3.60	1.44	1.34
33	D	406[A]	LHG	O8-C23	3.60	1.43	1.33
24	B	612	CLA	C1D-ND	3.60	1.42	1.37
24	d	403[A]	CLA	CHD-C4C	3.60	1.47	1.39
24	b	614	CLA	O2A-CGA	3.60	1.43	1.33
24	B	611	CLA	C4B-NB	-3.60	1.32	1.35
33	A	420[A]	LHG	O7-C7	3.60	1.44	1.34
24	C	507	CLA	OBD-CAD	3.58	1.28	1.22
24	C	502	CLA	C3D-C2D	3.58	1.48	1.39
24	C	509	CLA	CHD-C4C	3.58	1.47	1.39
33	d	407[A]	LHG	O8-C23	3.58	1.43	1.33
25	A	408[B]	PHO	C3C-C2C	3.57	1.48	1.37
24	C	505	CLA	CHD-C4C	3.57	1.47	1.39
24	C	506	CLA	O2A-CGA	3.57	1.43	1.33
24	c	512	CLA	C3D-C2D	3.57	1.48	1.39
33	D	406[B]	LHG	O8-C23	3.57	1.43	1.33
24	c	509	CLA	OBD-CAD	3.56	1.28	1.22
24	c	506	CLA	OBD-CAD	3.56	1.28	1.22
24	a	409	CLA	CHD-C4C	3.56	1.47	1.39
24	B	613	CLA	OBD-CAD	3.56	1.28	1.22
24	b	603	CLA	C3D-C2D	3.56	1.48	1.39
24	B	603	CLA	CHD-C4C	3.55	1.47	1.39
24	D	402[A]	CLA	C3D-C2D	3.55	1.48	1.39
24	B	609	CLA	OBD-CAD	3.55	1.28	1.22
24	c	513	CLA	OBD-CAD	3.55	1.28	1.22
24	b	609	CLA	CHD-C4C	3.54	1.47	1.39
36	c	518[A]	DGD	O2G-C1B	3.54	1.44	1.34
24	D	403	CLA	O2A-CGA	3.53	1.43	1.33
24	d	403[A]	CLA	C3D-C2D	3.53	1.48	1.39
25	a	408[A]	PHO	C3C-C2C	3.52	1.48	1.37
24	a	406[A]	CLA	CHD-C4C	3.52	1.47	1.39
24	D	402[B]	CLA	C3D-C2D	3.52	1.48	1.39
24	b	604	CLA	CHD-C4C	3.52	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	504	CLA	C3D-C2D	3.51	1.48	1.39
24	C	507	CLA	C3D-C2D	3.51	1.48	1.39
24	C	506	CLA	C3D-C2D	3.51	1.48	1.39
33	d	414[A]	LHG	O7-C7	3.50	1.44	1.34
24	a	407[A]	CLA	OBD-CAD	3.50	1.28	1.22
33	A	420[A]	LHG	O8-C23	3.49	1.43	1.33
24	a	409	CLA	C3D-C2D	3.49	1.48	1.39
24	B	613	CLA	CHD-C4C	3.49	1.47	1.39
24	B	612	CLA	C1C-C2C	3.48	1.51	1.44
24	C	511	CLA	C3D-C2D	3.48	1.48	1.39
35	D	411	LMG	O7-C10	3.48	1.44	1.34
24	B	608	CLA	CHD-C4C	3.45	1.47	1.39
24	b	602	CLA	OBD-CAD	3.45	1.28	1.22
24	B	611	CLA	C1C-C2C	3.44	1.51	1.44
35	b	629	LMG	O7-C10	3.44	1.44	1.34
24	C	506	CLA	OBD-CAD	3.44	1.28	1.22
24	b	613	CLA	CHD-C4C	3.43	1.47	1.39
24	c	514	CLA	OBD-CAD	3.42	1.28	1.22
24	c	507	CLA	OBD-CAD	3.42	1.28	1.22
24	b	604	CLA	OBD-CAD	3.41	1.28	1.22
24	B	608	CLA	OBD-CAD	3.41	1.28	1.22
24	b	612	CLA	OBD-CAD	3.40	1.28	1.22
24	c	506	CLA	O2A-CGA	3.40	1.43	1.33
24	b	601	CLA	OBD-CAD	3.40	1.28	1.22
24	b	605	CLA	O2A-CGA	3.40	1.43	1.33
24	B	612	CLA	O2A-CGA	3.40	1.43	1.33
24	C	504	CLA	O2A-CGA	3.40	1.43	1.33
24	B	606	CLA	CHD-C4C	3.39	1.47	1.39
33	b	628[A]	LHG	O8-C23	3.39	1.43	1.33
24	D	402[B]	CLA	OBD-CAD	3.39	1.28	1.22
24	b	603	CLA	CHD-C4C	3.39	1.47	1.39
24	B	611	CLA	C3D-C2D	3.39	1.48	1.39
24	d	403[B]	CLA	C3D-C2D	3.38	1.48	1.39
24	C	504	CLA	C3D-C2D	3.38	1.48	1.39
34	b	622	HTG	C1'-S1	-3.38	1.77	1.81
24	C	503	CLA	OBD-CAD	3.38	1.28	1.22
24	B	602	CLA	OBD-CAD	3.38	1.28	1.22
24	B	607	CLA	C3D-C2D	3.36	1.48	1.39
24	B	610	CLA	O2A-CGA	3.36	1.43	1.33
24	A	406[A]	CLA	OBD-CAD	3.36	1.28	1.22
24	A	406[B]	CLA	OBD-CAD	3.36	1.28	1.22
25	a	408[A]	PHO	O2A-CGA	3.35	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	610	CLA	CHD-C4C	3.35	1.46	1.39
24	b	603	CLA	OBD-CAD	3.35	1.28	1.22
24	a	409	CLA	OBD-CAD	3.35	1.28	1.22
24	C	505	CLA	OBD-CAD	3.35	1.28	1.22
24	C	513	CLA	OBD-CAD	3.34	1.28	1.22
24	C	502	CLA	OBD-CAD	3.34	1.28	1.22
24	B	612	CLA	CHD-C4C	3.34	1.46	1.39
24	B	614	CLA	C4B-NB	-3.34	1.32	1.35
24	B	601	CLA	OBD-CAD	3.34	1.28	1.22
24	B	612	CLA	C3D-C2D	3.34	1.48	1.39
24	B	603	CLA	OBD-CAD	3.33	1.28	1.22
39	e	101	HEM	C1B-NB	-3.33	1.34	1.40
24	A	405[A]	CLA	OBD-CAD	3.33	1.28	1.22
24	B	614	CLA	C3D-C2D	3.33	1.48	1.39
36	H	102	DGD	O2G-C1B	3.32	1.43	1.34
39	e	101	HEM	C4D-ND	-3.32	1.34	1.40
24	C	510	CLA	OBD-CAD	3.31	1.28	1.22
25	A	417[B]	PHO	CHA-CBD	-3.30	1.48	1.52
24	c	510	CLA	OBD-CAD	3.29	1.28	1.22
24	c	503	CLA	OBD-CAD	3.28	1.28	1.22
24	A	405[A]	CLA	O2A-CGA	3.28	1.42	1.33
24	C	511	CLA	OBD-CAD	3.28	1.28	1.22
39	F	102	HEM	C1B-NB	-3.28	1.34	1.40
24	c	505	CLA	OBD-CAD	3.26	1.28	1.22
24	D	402[A]	CLA	OBD-CAD	3.24	1.28	1.22
34	B	621	HTG	C1'-S1	-3.24	1.77	1.81
24	C	508	CLA	CHD-C4C	3.23	1.46	1.39
24	C	508	CLA	OBD-CAD	3.22	1.28	1.22
24	B	604	CLA	O2A-CGA	3.22	1.42	1.33
24	B	612	CLA	OBD-CAD	3.22	1.28	1.22
24	b	607	CLA	CHD-C4C	3.21	1.46	1.39
24	B	613	CLA	O2A-CGA	3.19	1.42	1.33
24	a	405[A]	CLA	O2A-CGA	3.19	1.42	1.33
24	b	612	CLA	CHD-C4C	3.17	1.46	1.39
34	B	624	HTG	C1-S1	-3.17	1.75	1.80
34	b	624	HTG	C1'-S1	-3.16	1.77	1.81
24	B	604	CLA	C3D-C2D	3.15	1.47	1.39
24	b	610	CLA	O2A-CGA	3.14	1.42	1.33
24	b	602	CLA	C1C-C2C	3.14	1.50	1.44
24	C	504	CLA	OBD-CAD	3.13	1.27	1.22
34	d	411	HTG	C1'-S1	-3.13	1.77	1.81
24	C	512	CLA	OBD-CAD	3.12	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	610	CLA	C1B-NB	-3.11	1.32	1.35
24	b	614	CLA	OBD-CAD	3.10	1.27	1.22
24	D	403	CLA	C1C-C2C	3.10	1.50	1.44
24	B	606	CLA	OBD-CAD	3.10	1.27	1.22
24	c	511	CLA	C1C-C2C	3.09	1.50	1.44
24	A	407[A]	CLA	C1B-NB	-3.09	1.32	1.35
24	B	602	CLA	C1C-C2C	3.08	1.50	1.44
24	B	616	CLA	CHD-C4C	3.05	1.46	1.39
24	B	612	CLA	C1B-CHB	3.04	1.49	1.41
24	b	616	CLA	OBD-CAD	3.04	1.27	1.22
24	b	602	CLA	C4B-CHC	3.03	1.49	1.41
24	c	511	CLA	OBD-CAD	2.99	1.27	1.22
34	D	410	HTG	C1'-S1	-2.99	1.77	1.81
24	B	613	CLA	C4D-CHA	2.98	1.49	1.38
24	a	409	CLA	C1C-C2C	2.97	1.50	1.44
24	b	611	CLA	OBD-CAD	2.97	1.27	1.22
24	B	611	CLA	C4B-CHC	2.97	1.49	1.41
24	B	613	CLA	C1B-NB	-2.96	1.32	1.35
24	b	609	CLA	C4D-CHA	2.95	1.48	1.38
39	F	102	HEM	C4D-ND	-2.95	1.35	1.40
24	b	604	CLA	C1C-C2C	2.94	1.50	1.44
24	b	610	CLA	C1C-C2C	2.94	1.50	1.44
24	b	604	CLA	C4D-CHA	2.94	1.48	1.38
24	c	506	CLA	C4C-C3C	2.94	1.50	1.45
34	c	522	HTG	C1'-S1	-2.94	1.77	1.81
24	b	607	CLA	OBD-CAD	2.91	1.27	1.22
24	a	407[A]	CLA	C1C-C2C	2.91	1.50	1.44
24	c	509	CLA	C1C-C2C	2.90	1.50	1.44
24	B	615	CLA	C1C-C2C	2.90	1.50	1.44
24	b	610	CLA	C4C-C3C	2.90	1.50	1.45
24	c	511	CLA	C1B-CHB	2.89	1.49	1.41
24	C	505	CLA	C4D-CHA	2.89	1.48	1.38
24	B	604	CLA	C1B-CHB	2.88	1.49	1.41
24	B	616	CLA	C1C-C2C	2.88	1.50	1.44
24	C	508	CLA	C4D-CHA	2.88	1.48	1.38
24	B	613	CLA	C4C-C3C	2.87	1.50	1.45
24	B	614	CLA	OBD-CAD	2.86	1.27	1.22
24	b	610	CLA	C4B-CHC	2.84	1.48	1.41
34	C	522	HTG	C1'-S1	-2.84	1.77	1.81
24	A	405[A]	CLA	C4C-C3C	2.84	1.49	1.45
27	a	411[B]	SQD	C6-S	-2.84	1.66	1.77
24	D	403	CLA	C4C-C3C	2.83	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	510	CLA	C1B-CHB	2.83	1.48	1.41
24	c	506	CLA	C4B-CHC	2.83	1.48	1.41
24	B	611	CLA	C1B-NB	2.82	1.37	1.35
24	C	514	CLA	C1C-C2C	2.82	1.50	1.44
24	B	606	CLA	C1C-C2C	2.82	1.50	1.44
34	b	624	HTG	C1-S1	-2.81	1.76	1.80
24	c	512	CLA	C1B-CHB	2.81	1.48	1.41
24	B	602	CLA	C4C-C3C	2.81	1.49	1.45
30	A	415[A]	PL9	C6-C5	2.81	1.49	1.35
24	C	502	CLA	C1C-C2C	2.81	1.50	1.44
24	B	614	CLA	C4D-CHA	2.80	1.48	1.38
24	b	602	CLA	C3D-C4D	-2.80	1.37	1.44
24	b	611	CLA	C1C-C2C	2.80	1.50	1.44
24	B	610	CLA	C3D-C4D	-2.80	1.37	1.44
24	B	613	CLA	C1C-C2C	2.80	1.50	1.44
24	c	511	CLA	C4D-CHA	2.80	1.48	1.38
25	a	408[B]	PHO	CHA-CBD	-2.79	1.49	1.52
24	d	403[A]	CLA	C4C-C3C	2.79	1.49	1.45
24	A	409	CLA	C4D-CHA	2.79	1.48	1.38
24	c	514	CLA	C1C-C2C	2.79	1.50	1.44
27	A	411[B]	SQD	C6-S	-2.79	1.67	1.77
24	B	605	CLA	C1C-C2C	2.79	1.50	1.44
24	c	506	CLA	C1C-C2C	2.78	1.50	1.44
36	h	102	DGD	O5D-C1E	2.78	1.44	1.40
24	B	615	CLA	C1B-CHB	2.78	1.48	1.41
24	A	406[B]	CLA	C4D-CHA	2.78	1.48	1.38
24	c	509	CLA	C4D-CHA	2.77	1.48	1.38
24	a	406[A]	CLA	C1B-NB	-2.77	1.32	1.35
25	A	408[A]	PHO	CBD-CGD	-2.76	1.48	1.52
24	C	512	CLA	C1C-C2C	2.76	1.49	1.44
24	B	608	CLA	C4D-CHA	2.76	1.48	1.38
24	C	510	CLA	C1C-C2C	2.76	1.49	1.44
27	A	411[A]	SQD	C6-S	-2.76	1.67	1.77
24	c	506	CLA	C1B-CHB	2.75	1.48	1.41
24	b	611	CLA	C4C-C3C	2.75	1.49	1.45
24	c	512	CLA	C4D-CHA	2.75	1.48	1.38
24	b	610	CLA	C1B-CHB	2.74	1.48	1.41
24	c	504	CLA	OBD-CAD	2.74	1.27	1.22
24	b	607	CLA	O2A-CGA	2.74	1.41	1.33
30	a	415[A]	PL9	C6-C5	2.74	1.49	1.35
24	c	504	CLA	C3D-C4D	-2.74	1.38	1.44
24	C	509	CLA	C4D-CHA	2.74	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	411[A]	SQD	C6-S	-2.73	1.67	1.77
30	a	415[B]	PL9	C6-C5	2.73	1.49	1.35
24	D	403	CLA	C1B-CHB	2.73	1.48	1.41
24	A	406[A]	CLA	C1C-C2C	2.73	1.49	1.44
24	B	605	CLA	C3D-C4D	-2.73	1.38	1.44
24	B	616	CLA	C4D-CHA	2.72	1.48	1.38
24	B	603	CLA	C1B-NB	-2.72	1.32	1.35
24	c	508	CLA	C4D-CHA	2.72	1.48	1.38
28	o	303	GOL	C1-C2	2.71	1.62	1.51
24	B	606	CLA	C1B-CHB	2.71	1.48	1.41
24	C	508	CLA	C1C-C2C	2.70	1.49	1.44
24	B	614	CLA	C3D-C4D	-2.70	1.38	1.44
24	C	511	CLA	C1C-C2C	2.70	1.49	1.44
24	c	502	CLA	C1C-C2C	2.70	1.49	1.44
24	C	507	CLA	C1C-C2C	2.70	1.49	1.44
24	c	513	CLA	C4D-CHA	2.70	1.48	1.38
24	c	504	CLA	C1C-C2C	2.70	1.49	1.44
24	B	605	CLA	C1B-CHB	2.70	1.48	1.41
24	b	611	CLA	C1B-CHB	2.70	1.48	1.41
24	c	509	CLA	C4B-CHC	2.69	1.48	1.41
24	c	510	CLA	C1C-C2C	2.69	1.49	1.44
24	B	607	CLA	C1B-CHB	2.69	1.48	1.41
24	B	601	CLA	C1C-C2C	2.69	1.49	1.44
24	A	406[A]	CLA	C4D-CHA	2.69	1.48	1.38
24	C	512	CLA	C1B-CHB	2.69	1.48	1.41
35	Z	101	LMG	O8-C28	2.69	1.46	1.33
24	C	502	CLA	C4D-CHA	2.69	1.47	1.38
24	B	616	CLA	OBD-CAD	2.68	1.27	1.22
24	C	509	CLA	C1B-CHB	2.68	1.48	1.41
24	b	610	CLA	C3D-C4D	-2.68	1.38	1.44
24	D	402[A]	CLA	C1B-CHB	2.68	1.48	1.41
24	b	604	CLA	C4B-CHC	2.68	1.48	1.41
24	c	506	CLA	C4D-CHA	2.67	1.47	1.38
24	a	407[A]	CLA	C4D-CHA	2.67	1.47	1.38
24	B	605	CLA	OBD-CAD	2.67	1.27	1.22
24	C	512	CLA	C4D-CHA	2.67	1.47	1.38
24	a	405[A]	CLA	C1B-CHB	2.67	1.48	1.41
30	A	415[B]	PL9	C6-C5	2.67	1.49	1.35
24	c	510	CLA	C4D-CHA	2.67	1.47	1.38
24	b	609	CLA	C1B-CHB	2.67	1.48	1.41
24	A	405[B]	CLA	C4C-C3C	2.67	1.49	1.45
24	C	506	CLA	C4C-C3C	2.66	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	f	101	SQD	C6-S	-2.66	1.67	1.77
34	b	621	HTG	O5-C1	2.66	1.46	1.42
24	b	614	CLA	C4B-CHC	2.66	1.48	1.41
39	e	101	HEM	FE-NB	2.66	2.10	1.96
24	c	507	CLA	C1B-CHB	2.66	1.48	1.41
24	B	607	CLA	C4D-CHA	2.65	1.47	1.38
24	b	603	CLA	C4D-CHA	2.65	1.47	1.38
27	A	413	SQD	C6-S	-2.65	1.67	1.77
28	A	419	GOL	O2-C2	-2.65	1.35	1.43
24	d	403[A]	CLA	C1B-CHB	2.65	1.48	1.41
24	c	504	CLA	C4D-CHA	2.65	1.47	1.38
24	b	613	CLA	C1C-C2C	2.64	1.49	1.44
24	B	604	CLA	C1C-C2C	2.64	1.49	1.44
24	b	614	CLA	C1B-CHB	2.64	1.48	1.41
24	d	403[B]	CLA	C1B-CHB	2.64	1.48	1.41
24	b	616	CLA	C1C-C2C	2.64	1.49	1.44
24	A	409	CLA	OBD-CAD	2.63	1.27	1.22
24	b	615	CLA	C4D-CHA	2.63	1.47	1.38
24	c	510	CLA	C4C-C3C	2.63	1.49	1.45
24	B	609	CLA	C4D-CHA	2.63	1.47	1.38
24	C	513	CLA	C1C-C2C	2.63	1.49	1.44
24	C	504	CLA	C3D-C4D	-2.62	1.38	1.44
24	c	503	CLA	C4D-CHA	2.62	1.47	1.38
24	c	505	CLA	C4D-CHA	2.62	1.47	1.38
25	d	402[B]	PHO	C3A-C2A	-2.62	1.52	1.54
24	b	601	CLA	C4D-CHA	2.62	1.47	1.38
32	M	102	LMT	O2'-C2'	-2.62	1.36	1.43
24	C	506	CLA	C1B-CHB	2.62	1.48	1.41
24	C	507	CLA	C4C-C3C	2.62	1.49	1.45
24	B	612	CLA	C4D-CHA	2.62	1.47	1.38
24	B	607	CLA	C1C-C2C	2.62	1.49	1.44
24	c	502	CLA	C3D-C4D	-2.62	1.38	1.44
24	C	507	CLA	C4D-CHA	2.62	1.47	1.38
24	b	607	CLA	C4D-CHA	2.62	1.47	1.38
24	B	601	CLA	C4B-CHC	2.61	1.48	1.41
24	c	504	CLA	C4B-CHC	2.61	1.48	1.41
24	D	402[A]	CLA	C4D-CHA	2.61	1.47	1.38
24	B	607	CLA	C1B-NB	-2.61	1.32	1.35
24	C	513	CLA	C4D-CHA	2.61	1.47	1.38
24	C	505	CLA	C1C-C2C	2.61	1.49	1.44
34	B	622	HTG	C1'-S1	-2.61	1.78	1.81
24	b	612	CLA	C1C-C2C	2.61	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	409	CLA	C4B-CHC	2.61	1.48	1.41
24	d	404	CLA	C1C-C2C	2.60	1.49	1.44
24	a	409	CLA	C4D-CHA	2.60	1.47	1.38
24	b	607	CLA	C1B-CHB	2.60	1.48	1.41
24	b	605	CLA	C4D-CHA	2.60	1.47	1.38
24	d	403[A]	CLA	C4D-CHA	2.60	1.47	1.38
24	D	402[B]	CLA	C4D-CHA	2.60	1.47	1.38
24	b	613	CLA	C4D-CHA	2.60	1.47	1.38
24	b	601	CLA	C1C-C2C	2.60	1.49	1.44
24	C	503	CLA	C4B-CHC	2.59	1.48	1.41
27	a	413	SQD	C6-S	-2.59	1.67	1.77
24	A	407[B]	CLA	C4D-CHA	2.59	1.47	1.38
25	a	408[A]	PHO	CHA-CBD	-2.59	1.49	1.52
24	c	511	CLA	C4B-CHC	2.59	1.48	1.41
24	C	505	CLA	C1B-CHB	2.58	1.48	1.41
24	b	612	CLA	C1B-CHB	2.58	1.48	1.41
24	b	616	CLA	C3D-C4D	-2.58	1.38	1.44
24	B	610	CLA	C4D-CHA	2.58	1.47	1.38
24	c	505	CLA	C4C-C3C	2.58	1.49	1.45
24	A	407[A]	CLA	C4D-CHA	2.58	1.47	1.38
25	a	408[A]	PHO	CBD-CGD	-2.58	1.49	1.52
35	C	521	LMG	O1-C1	2.57	1.44	1.40
24	c	513	CLA	C4B-CHC	2.57	1.48	1.41
24	A	409	CLA	C1C-NC	-2.57	1.34	1.37
24	a	407[B]	CLA	C1C-C2C	2.57	1.49	1.44
24	B	602	CLA	C4B-CHC	2.57	1.48	1.41
24	C	509	CLA	C4C-C3C	2.57	1.49	1.45
24	D	403	CLA	C4B-CHC	2.57	1.48	1.41
24	d	403[B]	CLA	C1C-C2C	2.56	1.49	1.44
24	C	511	CLA	C4D-CHA	2.56	1.47	1.38
25	d	402[A]	PHO	CHA-CBD	-2.56	1.49	1.52
24	B	610	CLA	C1B-CHB	2.56	1.48	1.41
24	B	604	CLA	C4D-CHA	2.56	1.47	1.38
24	B	603	CLA	C1C-C2C	2.55	1.49	1.44
24	a	405[A]	CLA	C4D-CHA	2.55	1.47	1.38
24	c	509	CLA	C4C-C3C	2.55	1.49	1.45
24	B	615	CLA	C4D-CHA	2.55	1.47	1.38
24	d	403[A]	CLA	C1C-C2C	2.55	1.49	1.44
24	d	403[B]	CLA	C4D-CHA	2.55	1.47	1.38
24	A	406[B]	CLA	C4B-CHC	2.55	1.48	1.41
24	B	614	CLA	C1B-CHB	2.55	1.48	1.41
24	B	602	CLA	C3D-C4D	-2.55	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	507	CLA	C1B-CHB	2.54	1.48	1.41
24	b	616	CLA	C4D-CHA	2.54	1.47	1.38
24	A	405[A]	CLA	C4D-CHA	2.54	1.47	1.38
24	C	514	CLA	C4D-CHA	2.54	1.47	1.38
39	F	102	HEM	FE-NB	2.54	2.09	1.96
24	d	404	CLA	C4C-C3C	2.54	1.49	1.45
24	B	605	CLA	C4B-CHC	2.54	1.48	1.41
24	c	512	CLA	C1C-C2C	2.54	1.49	1.44
24	D	403	CLA	C4D-CHA	2.54	1.47	1.38
24	D	402[B]	CLA	C1B-CHB	2.53	1.48	1.41
24	b	606	CLA	C4D-CHA	2.53	1.47	1.38
24	a	405[B]	CLA	C4C-C3C	2.53	1.49	1.45
24	B	606	CLA	C4C-C3C	2.53	1.49	1.45
24	C	509	CLA	C1C-C2C	2.53	1.49	1.44
24	b	616	CLA	C4B-CHC	2.53	1.48	1.41
24	C	510	CLA	C4D-CHA	2.52	1.47	1.38
24	a	406[A]	CLA	C4D-CHA	2.52	1.47	1.38
24	c	502	CLA	C1B-CHB	2.52	1.48	1.41
24	b	603	CLA	C4B-CHC	2.52	1.48	1.41
24	B	612	CLA	C4B-CHC	2.52	1.48	1.41
24	b	608	CLA	C1C-C2C	2.52	1.49	1.44
24	c	505	CLA	C1C-NC	-2.52	1.34	1.37
25	d	402[A]	PHO	C3A-C2A	-2.52	1.52	1.54
32	b	620	LMT	C3'-C2'	2.52	1.58	1.52
24	c	514	CLA	C1B-CHB	2.51	1.48	1.41
24	b	614	CLA	C4D-CHA	2.51	1.47	1.38
24	B	606	CLA	C3D-C4D	-2.51	1.38	1.44
32	t	101	LMT	O3'-C3'	-2.51	1.37	1.43
24	B	614	CLA	C4C-C3C	2.51	1.49	1.45
32	M	102	LMT	O3'-C3'	-2.51	1.37	1.43
41	V	201	HEC	C3C-C4C	2.51	1.47	1.43
24	B	602	CLA	C4D-CHA	2.51	1.47	1.38
24	C	502	CLA	C4B-CHC	2.50	1.48	1.41
24	C	503	CLA	C4D-CHA	2.50	1.47	1.38
24	b	607	CLA	C1B-NB	-2.50	1.33	1.35
24	B	603	CLA	C1B-CHB	2.50	1.47	1.41
24	C	506	CLA	C4D-CHA	2.50	1.47	1.38
24	b	603	CLA	C1C-C2C	2.50	1.49	1.44
32	A	421	LMT	O3'-C3'	-2.50	1.37	1.43
24	A	407[B]	CLA	C4B-CHC	2.50	1.47	1.41
24	c	502	CLA	C4D-CHA	2.50	1.47	1.38
24	c	503	CLA	C4C-C3C	2.50	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	607	CLA	C1C-C2C	2.50	1.49	1.44
24	C	506	CLA	C1C-C2C	2.50	1.49	1.44
30	D	405[A]	PL9	C6-C5	2.50	1.48	1.35
24	B	609	CLA	C3D-C4D	-2.50	1.38	1.44
24	A	405[A]	CLA	C1B-CHB	2.49	1.47	1.41
24	C	506	CLA	C4B-CHC	2.49	1.47	1.41
24	a	406[B]	CLA	C4D-CHA	2.49	1.47	1.38
24	c	511	CLA	C4C-C3C	2.49	1.49	1.45
27	L	102	SQD	C6-S	-2.49	1.68	1.77
30	d	406[B]	PL9	C6-C5	2.49	1.48	1.35
24	A	405[B]	CLA	C4D-CHA	2.48	1.47	1.38
24	d	404	CLA	C4D-CHA	2.48	1.47	1.38
36	c	519	DGD	O2G-C2G	-2.48	1.40	1.46
24	c	514	CLA	C4C-C3C	2.48	1.49	1.45
24	C	512	CLA	C3D-C4D	-2.48	1.38	1.44
24	c	508	CLA	C4B-CHC	2.48	1.47	1.41
24	B	611	CLA	C1B-CHB	2.48	1.47	1.41
24	c	508	CLA	C1B-CHB	2.48	1.47	1.41
24	B	611	CLA	C4D-CHA	2.48	1.47	1.38
24	B	603	CLA	C4D-CHA	2.48	1.47	1.38
24	C	505	CLA	C3D-C4D	-2.47	1.38	1.44
24	a	405[B]	CLA	C4D-CHA	2.47	1.47	1.38
24	a	405[A]	CLA	C1C-C2C	2.47	1.49	1.44
24	c	510	CLA	C4B-NB	-2.47	1.33	1.35
24	B	605	CLA	C4D-CHA	2.47	1.47	1.38
24	b	610	CLA	C4D-CHA	2.47	1.47	1.38
24	A	406[A]	CLA	C4B-CHC	2.47	1.47	1.41
24	b	612	CLA	C4B-NB	-2.47	1.33	1.35
24	D	402[A]	CLA	C1C-C2C	2.46	1.49	1.44
24	B	601	CLA	C4D-CHA	2.46	1.47	1.38
24	a	407[B]	CLA	C4B-CHC	2.46	1.47	1.41
24	c	507	CLA	C4D-CHA	2.46	1.47	1.38
24	b	609	CLA	C4B-CHC	2.46	1.47	1.41
30	D	405[B]	PL9	C6-C5	2.46	1.48	1.35
24	A	405[B]	CLA	C4B-CHC	2.46	1.47	1.41
24	c	508	CLA	C1C-C2C	2.46	1.49	1.44
24	C	508	CLA	C4B-CHC	2.46	1.47	1.41
24	B	616	CLA	C4B-CHC	2.45	1.47	1.41
24	C	510	CLA	C1B-CHB	2.45	1.47	1.41
24	b	608	CLA	C4D-CHA	2.45	1.47	1.38
24	b	604	CLA	C1B-CHB	2.45	1.47	1.41
24	d	403[A]	CLA	C3D-C4D	-2.45	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	403	CLA	C1B-NB	-2.45	1.33	1.35
24	B	607	CLA	C3D-C4D	-2.45	1.38	1.44
24	c	513	CLA	C1B-CHB	2.44	1.47	1.41
24	C	511	CLA	C1B-CHB	2.44	1.47	1.41
24	b	612	CLA	C4D-CHA	2.44	1.47	1.38
24	B	604	CLA	C3D-C4D	-2.44	1.38	1.44
24	B	610	CLA	C4C-C3C	2.44	1.49	1.45
24	C	504	CLA	C4D-CHA	2.44	1.47	1.38
24	b	606	CLA	C3D-C4D	-2.43	1.38	1.44
24	D	402[A]	CLA	C3D-C4D	-2.43	1.38	1.44
28	D	412	GOL	O2-C2	-2.43	1.36	1.43
24	b	615	CLA	C4B-CHC	2.43	1.47	1.41
24	D	402[B]	CLA	C4B-CHC	2.42	1.47	1.41
24	b	613	CLA	C1B-CHB	2.42	1.47	1.41
24	b	605	CLA	C4B-CHC	2.42	1.47	1.41
27	X	101	SQD	O6-C1	2.42	1.44	1.40
24	B	602	CLA	C1B-CHB	2.42	1.47	1.41
24	C	503	CLA	C1C-C2C	2.42	1.49	1.44
24	b	613	CLA	C4B-CHC	2.42	1.47	1.41
24	A	405[A]	CLA	C1C-C2C	2.42	1.49	1.44
24	c	509	CLA	C1B-CHB	2.42	1.47	1.41
24	B	610	CLA	C4B-CHC	2.42	1.47	1.41
24	A	406[B]	CLA	C3D-C4D	-2.42	1.38	1.44
24	A	407[B]	CLA	C1C-C2C	2.41	1.49	1.44
24	a	407[B]	CLA	C4D-CHA	2.41	1.47	1.38
24	B	608	CLA	C4C-C3C	2.41	1.49	1.45
24	B	604	CLA	C1A-CHA	2.41	1.53	1.43
24	b	612	CLA	C4B-CHC	2.41	1.47	1.41
24	d	403[B]	CLA	C4C-C3C	2.41	1.49	1.45
24	c	514	CLA	C4D-CHA	2.41	1.47	1.38
24	B	606	CLA	C4D-CHA	2.41	1.47	1.38
24	B	609	CLA	C1B-CHB	2.40	1.47	1.41
24	b	605	CLA	C1C-C2C	2.40	1.49	1.44
24	b	601	CLA	C4B-CHC	2.40	1.47	1.41
24	D	402[B]	CLA	C3D-C4D	-2.40	1.38	1.44
24	C	513	CLA	C4B-CHC	2.40	1.47	1.41
24	b	602	CLA	C4D-CHA	2.40	1.46	1.38
24	c	510	CLA	C1B-NB	-2.40	1.33	1.35
25	d	402[B]	PHO	CHA-CBD	-2.40	1.49	1.52
28	b	623	GOL	C3-C2	2.39	1.61	1.51
24	C	513	CLA	C3D-C4D	-2.39	1.38	1.44
24	b	607	CLA	C4C-C3C	2.39	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	519	DGD	O2G-C2G	-2.39	1.40	1.46
24	c	503	CLA	C1B-CHB	2.39	1.47	1.41
24	c	502	CLA	C4B-CHC	2.39	1.47	1.41
24	A	407[A]	CLA	C1C-C2C	2.39	1.49	1.44
24	b	602	CLA	C4C-C3C	2.39	1.49	1.45
24	b	615	CLA	C1C-C2C	2.38	1.49	1.44
32	M	104	LMT	O3'-C3'	-2.38	1.37	1.43
24	D	402[B]	CLA	C1C-C2C	2.38	1.49	1.44
24	a	409	CLA	C1B-CHB	2.38	1.47	1.41
24	c	507	CLA	C3D-C4D	-2.38	1.38	1.44
24	A	405[B]	CLA	C1B-CHB	2.38	1.47	1.41
24	A	409	CLA	C3D-C4D	-2.38	1.38	1.44
24	A	406[A]	CLA	C1B-CHB	2.37	1.47	1.41
27	B	620	SQD	C6-S	-2.37	1.68	1.77
24	B	601	CLA	C1B-CHB	2.37	1.47	1.41
24	b	603	CLA	C1B-CHB	2.37	1.47	1.41
24	b	612	CLA	C3D-C4D	-2.37	1.38	1.44
24	b	615	CLA	C1B-CHB	2.37	1.47	1.41
24	b	611	CLA	C3D-C4D	-2.37	1.38	1.44
24	A	407[A]	CLA	C4B-CHC	2.37	1.47	1.41
24	C	511	CLA	C3D-C4D	-2.37	1.38	1.44
34	B	621	HTG	O5-C1	2.37	1.46	1.42
24	a	407[A]	CLA	C3D-C4D	-2.36	1.38	1.44
25	A	417[A]	PHO	C3A-C2A	-2.36	1.52	1.54
24	b	608	CLA	C4C-C3C	2.36	1.49	1.45
24	C	507	CLA	C3D-C4D	-2.36	1.38	1.44
24	c	504	CLA	C1B-CHB	2.36	1.47	1.41
24	C	504	CLA	C1B-CHB	2.36	1.47	1.41
24	B	609	CLA	C4B-CHC	2.36	1.47	1.41
24	a	405[A]	CLA	C4C-C3C	2.36	1.49	1.45
24	B	614	CLA	C4B-CHC	2.36	1.47	1.41
24	B	613	CLA	C1B-CHB	2.36	1.47	1.41
32	B	627	LMT	C3'-C2'	2.36	1.58	1.52
24	c	512	CLA	C4C-C3C	2.35	1.49	1.45
24	b	606	CLA	C4B-CHC	2.35	1.47	1.41
24	d	404	CLA	C4B-CHC	2.35	1.47	1.41
24	A	405[B]	CLA	C1C-C2C	2.35	1.49	1.44
24	B	616	CLA	C1B-CHB	2.35	1.47	1.41
24	C	504	CLA	C4B-CHC	2.34	1.47	1.41
24	C	512	CLA	C4B-CHC	2.34	1.47	1.41
24	b	609	CLA	C3D-C4D	-2.34	1.38	1.44
24	A	407[A]	CLA	C1B-CHB	2.34	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	M	104	LMT	O2'-C2'	-2.34	1.37	1.43
24	a	407[B]	CLA	C3D-C4D	-2.34	1.38	1.44
24	B	609	CLA	C4C-C3C	2.33	1.49	1.45
24	B	604	CLA	MG-NA	2.33	2.11	2.06
32	B	630	LMT	O3'-C3'	-2.33	1.37	1.43
24	c	505	CLA	C1B-CHB	2.33	1.47	1.41
24	C	502	CLA	C4C-C3C	2.33	1.49	1.45
30	d	406[A]	PL9	C6-C5	2.33	1.47	1.35
24	d	403[B]	CLA	C4B-CHC	2.32	1.47	1.41
24	c	505	CLA	C1C-C2C	2.32	1.49	1.44
24	B	609	CLA	C1C-C2C	2.32	1.49	1.44
32	B	627	LMT	O3'-C3'	-2.32	1.37	1.43
24	b	604	CLA	C1B-NB	-2.32	1.33	1.35
24	b	606	CLA	C1B-CHB	2.32	1.47	1.41
24	b	614	CLA	C4C-C3C	2.32	1.49	1.45
24	c	502	CLA	C4C-C3C	2.32	1.49	1.45
24	B	608	CLA	C3D-C4D	-2.32	1.38	1.44
24	C	512	CLA	C4B-NB	-2.32	1.33	1.35
24	b	601	CLA	C1B-CHB	2.32	1.47	1.41
24	c	505	CLA	C1B-NB	-2.31	1.33	1.35
24	d	404	CLA	C1B-CHB	2.31	1.47	1.41
24	b	613	CLA	C1B-NB	-2.31	1.33	1.35
24	C	514	CLA	C1B-CHB	2.31	1.47	1.41
24	B	607	CLA	C4B-CHC	2.31	1.47	1.41
24	c	507	CLA	C4C-C3C	2.30	1.49	1.45
24	C	508	CLA	C3D-C4D	-2.30	1.39	1.44
24	a	405[B]	CLA	C1B-CHB	2.30	1.47	1.41
24	C	514	CLA	C3D-C4D	-2.30	1.39	1.44
24	a	405[A]	CLA	C4B-CHC	2.30	1.47	1.41
24	C	502	CLA	C1B-CHB	2.30	1.47	1.41
24	c	507	CLA	C4B-CHC	2.30	1.47	1.41
24	a	407[A]	CLA	C1B-CHB	2.29	1.47	1.41
24	B	610	CLA	C1C-C2C	2.29	1.49	1.44
24	A	407[B]	CLA	C1B-CHB	2.29	1.47	1.41
24	A	409	CLA	C1C-C2C	2.29	1.49	1.44
24	b	605	CLA	C4C-C3C	2.29	1.49	1.45
24	B	606	CLA	C4B-CHC	2.29	1.47	1.41
24	b	608	CLA	C1B-CHB	2.29	1.47	1.41
24	C	514	CLA	C1C-NC	-2.29	1.34	1.37
32	A	421	LMT	O2'-C2'	-2.28	1.37	1.43
32	F	101	LMT	O3'-C3'	-2.28	1.37	1.43
27	X	101	SQD	C6-S	-2.28	1.69	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	e	102	LMT	O3'-C3'	-2.28	1.37	1.43
24	c	507	CLA	C1C-C2C	2.28	1.49	1.44
24	C	511	CLA	C4C-C3C	2.27	1.49	1.45
24	C	512	CLA	C4C-C3C	2.27	1.48	1.45
24	b	608	CLA	C1B-NB	-2.27	1.33	1.35
24	d	403[B]	CLA	C3D-C4D	-2.27	1.39	1.44
24	C	503	CLA	C1B-CHB	2.26	1.47	1.41
24	B	616	CLA	C1C-NC	-2.26	1.34	1.37
32	M	102	LMT	O2B-C2B	-2.26	1.37	1.43
24	A	405[B]	CLA	C3D-C4D	-2.26	1.39	1.44
24	A	407[B]	CLA	C3D-C4D	-2.26	1.39	1.44
24	B	603	CLA	C4B-CHC	2.25	1.47	1.41
24	D	402[A]	CLA	C4B-CHC	2.25	1.47	1.41
24	A	406[A]	CLA	C3D-C4D	-2.25	1.39	1.44
24	B	616	CLA	C3D-C4D	-2.25	1.39	1.44
24	c	513	CLA	C3D-C4D	-2.25	1.39	1.44
24	b	605	CLA	C1B-NB	-2.24	1.33	1.35
24	B	616	CLA	C4C-C3C	2.24	1.48	1.45
24	b	611	CLA	C1D-C2D	2.24	1.49	1.45
24	c	514	CLA	C4B-CHC	2.24	1.47	1.41
24	a	409	CLA	C4C-C3C	2.24	1.48	1.45
24	a	406[A]	CLA	C1B-CHB	2.24	1.47	1.41
24	C	510	CLA	C4B-NB	-2.24	1.33	1.35
26	B	619	BCR	C30-C25	-2.24	1.50	1.53
24	b	615	CLA	C4C-C3C	2.23	1.48	1.45
24	b	607	CLA	C3D-C4D	-2.23	1.39	1.44
24	C	503	CLA	C3D-C4D	-2.23	1.39	1.44
24	c	505	CLA	C3D-C4D	-2.23	1.39	1.44
24	b	611	CLA	C4D-CHA	2.23	1.46	1.38
24	b	606	CLA	C1C-C2C	2.23	1.48	1.44
24	b	606	CLA	C4C-C3C	2.23	1.48	1.45
24	c	508	CLA	C3D-C4D	-2.23	1.39	1.44
24	c	513	CLA	C1C-C2C	2.23	1.48	1.44
36	C	518[A]	DGD	O5D-C1E	2.22	1.44	1.40
24	C	502	CLA	C3D-C4D	-2.22	1.39	1.44
24	b	605	CLA	C3D-C4D	-2.21	1.39	1.44
24	c	514	CLA	C3D-C4D	-2.21	1.39	1.44
24	b	609	CLA	C1C-C2C	2.21	1.48	1.44
25	A	408[B]	PHO	CHA-CBD	-2.21	1.49	1.52
24	b	605	CLA	C1B-CHB	2.21	1.47	1.41
24	a	405[B]	CLA	C3D-C4D	-2.21	1.39	1.44
24	B	611	CLA	C3D-C4D	-2.20	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	512	CLA	MG-NA	2.20	2.11	2.06
24	B	603	CLA	C3D-C4D	-2.20	1.39	1.44
24	b	611	CLA	C4B-CHC	2.20	1.47	1.41
39	e	101	HEM	C1D-ND	-2.20	1.34	1.38
24	B	615	CLA	MG-NA	2.19	2.11	2.06
24	b	608	CLA	C3D-C4D	-2.19	1.39	1.44
25	A	408[A]	PHO	CHA-CBD	-2.19	1.49	1.52
32	B	628	LMT	O2'-C2'	-2.19	1.37	1.43
24	b	603	CLA	C3D-C4D	-2.18	1.39	1.44
24	c	512	CLA	C4B-CHC	2.18	1.47	1.41
24	B	601	CLA	C4C-C3C	2.18	1.48	1.45
24	a	405[B]	CLA	C1C-C2C	2.18	1.48	1.44
24	a	406[B]	CLA	C1B-CHB	2.18	1.47	1.41
24	c	504	CLA	C4C-C3C	2.18	1.48	1.45
24	D	402[A]	CLA	C4C-C3C	2.18	1.48	1.45
24	B	604	CLA	C4B-CHC	2.18	1.47	1.41
24	B	615	CLA	C4B-CHC	2.18	1.47	1.41
24	c	509	CLA	C3D-C4D	-2.17	1.39	1.44
24	C	509	CLA	C3D-C4D	-2.17	1.39	1.44
32	m	102	LMT	O2B-C2B	-2.17	1.37	1.43
24	b	608	CLA	C1C-NC	-2.16	1.34	1.37
24	B	601	CLA	C3D-C4D	-2.16	1.39	1.44
24	c	513	CLA	C4C-C3C	2.16	1.48	1.45
24	B	612	CLA	C3D-C4D	-2.16	1.39	1.44
24	b	601	CLA	C4C-C3C	2.16	1.48	1.45
24	B	611	CLA	C1C-NC	-2.15	1.34	1.37
24	d	403[A]	CLA	C4B-CHC	2.15	1.47	1.41
24	A	406[B]	CLA	C1C-C2C	2.15	1.48	1.44
32	t	101	LMT	O2'-C2'	-2.15	1.37	1.43
24	A	406[B]	CLA	C1B-CHB	2.15	1.47	1.41
27	B	620	SQD	O6-C1	2.15	1.43	1.40
24	b	604	CLA	C4C-C3C	2.14	1.48	1.45
24	b	607	CLA	C4B-CHC	2.14	1.46	1.41
24	B	603	CLA	C4C-C3C	2.13	1.48	1.45
24	b	604	CLA	MG-NA	2.13	2.11	2.06
32	e	102	LMT	O2'-C2'	-2.13	1.38	1.43
24	b	602	CLA	C1B-CHB	2.13	1.46	1.41
25	a	408[B]	PHO	C3A-C2A	-2.13	1.52	1.54
26	a	410	BCR	C19-C18	2.13	1.50	1.45
24	A	407[B]	CLA	C4C-C3C	2.13	1.48	1.45
24	b	614	CLA	C3D-C4D	-2.12	1.39	1.44
24	C	504	CLA	C4C-C3C	2.12	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	510	CLA	C1C-NC	-2.12	1.34	1.37
30	a	415[A]	PL9	C2-C3	2.12	1.40	1.34
32	M	104	LMT	O3B-C3B	-2.12	1.38	1.43
24	a	406[A]	CLA	C1C-C2C	2.12	1.48	1.44
24	B	607	CLA	C1A-CHA	2.12	1.51	1.43
24	A	407[A]	CLA	C1C-NC	-2.12	1.34	1.37
25	A	408[B]	PHO	C3A-C2A	-2.11	1.52	1.54
24	A	407[A]	CLA	C3D-C4D	-2.11	1.39	1.44
24	C	508	CLA	C4C-C3C	2.11	1.48	1.45
28	a	419	GOL	C1-C2	2.10	1.60	1.51
39	F	102	HEM	CHB-C1B	2.10	1.40	1.35
32	e	102	LMT	O2B-C2B	-2.10	1.38	1.43
24	B	613	CLA	C1A-CHA	2.10	1.51	1.43
39	F	102	HEM	C3B-C4B	2.10	1.49	1.44
24	a	405[A]	CLA	C3D-C4D	-2.10	1.39	1.44
24	a	407[A]	CLA	C4C-C3C	2.10	1.48	1.45
24	d	404	CLA	C1D-C2D	2.10	1.49	1.45
24	C	506	CLA	C3D-C4D	-2.09	1.39	1.44
24	C	510	CLA	C4B-CHC	2.09	1.46	1.41
24	B	605	CLA	C4C-C3C	2.09	1.48	1.45
24	C	511	CLA	C4B-CHC	2.09	1.46	1.41
24	A	409	CLA	C1B-CHB	2.09	1.46	1.41
24	B	612	CLA	C4C-C3C	2.09	1.48	1.45
32	B	628	LMT	O2B-C2B	-2.09	1.38	1.43
24	B	608	CLA	C1B-CHB	2.08	1.46	1.41
24	c	505	CLA	C4B-CHC	2.08	1.46	1.41
24	a	406[B]	CLA	C1C-C2C	2.08	1.48	1.44
24	c	510	CLA	C3D-C4D	-2.08	1.39	1.44
24	b	613	CLA	OBD-CAD	2.08	1.26	1.22
24	a	406[B]	CLA	C4B-CHC	2.08	1.46	1.41
24	b	603	CLA	C4C-C3C	2.08	1.48	1.45
32	B	630	LMT	O2'-C2'	-2.08	1.38	1.43
24	B	601	CLA	C1C-NC	-2.08	1.34	1.37
24	a	407[B]	CLA	C4C-C3C	2.08	1.48	1.45
24	C	513	CLA	C4C-C3C	2.07	1.48	1.45
24	c	512	CLA	C1C-NC	-2.07	1.34	1.37
24	C	513	CLA	C1B-CHB	2.07	1.46	1.41
36	c	518[A]	DGD	O2G-C2G	-2.07	1.41	1.46
32	m	102	LMT	O3B-C3B	-2.07	1.38	1.43
25	A	417[B]	PHO	C3A-C2A	-2.07	1.52	1.54
24	b	615	CLA	C1B-NB	-2.07	1.33	1.35
24	B	612	CLA	C1C-NC	-2.07	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	407[A]	CLA	C4B-CHC	2.07	1.46	1.41
24	B	604	CLA	C4C-C3C	2.06	1.48	1.45
36	H	102	DGD	O5D-C1E	2.06	1.43	1.40
24	b	609	CLA	C1C-NC	-2.06	1.34	1.37
24	C	512	CLA	C1C-NC	-2.05	1.34	1.37
24	B	606	CLA	MG-NA	2.05	2.11	2.06
24	C	514	CLA	C4B-CHC	2.05	1.46	1.41
32	b	626	LMT	O2'-C2'	-2.05	1.38	1.43
39	e	101	HEM	CHB-C1B	2.05	1.40	1.35
24	C	508	CLA	C1B-CHB	2.05	1.46	1.41
30	a	415[B]	PL9	C2-C3	2.04	1.40	1.34
41	v	201	HEC	C3C-C4C	2.04	1.46	1.43
32	B	627	LMT	O5'-C5'	-2.04	1.39	1.44
32	m	102	LMT	C3'-C2'	2.04	1.57	1.52
24	b	616	CLA	C1B-CHB	2.04	1.46	1.41
24	a	406[A]	CLA	C4B-CHC	2.04	1.46	1.41
24	C	509	CLA	C4B-CHC	2.04	1.46	1.41
30	A	415[A]	PL9	C2-C1	-2.04	1.39	1.44
24	C	503	CLA	C4C-C3C	2.04	1.48	1.45
24	A	405[A]	CLA	C3D-C4D	-2.03	1.39	1.44
24	c	508	CLA	C1D-C2D	2.03	1.49	1.45
24	B	611	CLA	C1D-C2D	2.03	1.49	1.45
24	b	608	CLA	C4B-NB	-2.03	1.33	1.35
24	B	614	CLA	C1C-C2C	2.02	1.48	1.44
32	B	628	LMT	O3'-C3'	-2.02	1.38	1.43
24	A	405[A]	CLA	C4B-NB	-2.02	1.33	1.35
24	a	407[B]	CLA	C1B-CHB	2.02	1.46	1.41
24	b	605	CLA	C1D-C2D	2.01	1.49	1.45
24	C	507	CLA	C4B-CHC	2.01	1.46	1.41
24	c	503	CLA	C4B-CHC	2.01	1.46	1.41
24	c	511	CLA	C3D-C4D	-2.00	1.39	1.44
32	B	627	LMT	O4'-C4B	-2.00	1.38	1.43
30	d	406[B]	PL9	C2-C3	2.00	1.39	1.34
27	a	413	SQD	O6-C1	2.00	1.43	1.40
24	B	609	CLA	C1B-NB	-2.00	1.33	1.35
24	b	604	CLA	C1A-CHA	2.00	1.51	1.43
32	c	501	LMT	O3'-C3'	-2.00	1.38	1.43

All (3105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	611	CLA	C1D-ND-C4D	-11.73	98.00	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	612	CLA	C1D-ND-C4D	-10.43	98.93	106.33
24	b	605	CLA	C1D-ND-C4D	-10.31	99.01	106.33
24	a	409	CLA	C1D-ND-C4D	-9.92	99.28	106.33
24	B	615	CLA	C1D-ND-C4D	-9.87	99.33	106.33
24	B	611	CLA	C2D-C1D-ND	9.86	117.37	110.10
24	d	403[B]	CLA	C1D-ND-C4D	-9.81	99.36	106.33
24	c	512	CLA	C1D-ND-C4D	-9.77	99.39	106.33
24	C	506	CLA	C1D-ND-C4D	-9.73	99.43	106.33
24	a	405[B]	CLA	C1D-ND-C4D	-9.70	99.45	106.33
24	B	607	CLA	C1D-ND-C4D	-9.69	99.45	106.33
24	b	615	CLA	C1D-ND-C4D	-9.69	99.45	106.33
24	a	407[B]	CLA	C1D-ND-C4D	-9.66	99.47	106.33
24	B	601	CLA	C1D-ND-C4D	-9.62	99.50	106.33
24	C	511	CLA	C1D-ND-C4D	-9.59	99.52	106.33
24	b	614	CLA	C1D-ND-C4D	-9.58	99.53	106.33
24	b	611	CLA	C1D-ND-C4D	-9.58	99.53	106.33
24	C	504	CLA	C1D-ND-C4D	-9.55	99.55	106.33
24	d	404	CLA	C1D-ND-C4D	-9.54	99.55	106.33
24	A	407[B]	CLA	C1D-ND-C4D	-9.50	99.58	106.33
24	B	606	CLA	C1D-ND-C4D	-9.47	99.61	106.33
24	c	514	CLA	C1D-ND-C4D	-9.46	99.61	106.33
24	B	615	CLA	C2D-C1D-ND	9.40	117.03	110.10
24	C	507	CLA	C1D-ND-C4D	-9.39	99.67	106.33
24	c	507	CLA	C1D-ND-C4D	-9.35	99.70	106.33
24	D	402[B]	CLA	C1D-ND-C4D	-9.33	99.71	106.33
24	C	514	CLA	C1D-ND-C4D	-9.31	99.72	106.33
24	c	506	CLA	C1D-ND-C4D	-9.25	99.77	106.33
24	C	502	CLA	C1D-ND-C4D	-9.24	99.77	106.33
24	b	601	CLA	C1D-ND-C4D	-9.22	99.78	106.33
24	B	614	CLA	C1D-ND-C4D	-9.22	99.79	106.33
24	A	405[B]	CLA	C1D-ND-C4D	-9.21	99.79	106.33
24	B	605	CLA	C1D-ND-C4D	-9.20	99.80	106.33
24	B	608	CLA	C1D-ND-C4D	-9.20	99.80	106.33
24	a	407[A]	CLA	C1D-ND-C4D	-9.17	99.82	106.33
24	D	402[A]	CLA	C1D-ND-C4D	-9.16	99.83	106.33
24	B	612	CLA	C2D-C1D-ND	9.15	116.85	110.10
24	a	409	CLA	C2D-C1D-ND	9.13	116.83	110.10
24	B	607	CLA	C2D-C1D-ND	9.13	116.83	110.10
24	B	603	CLA	C1D-ND-C4D	-9.11	99.86	106.33
24	d	403[A]	CLA	C1D-ND-C4D	-9.09	99.88	106.33
24	A	409	CLA	C2D-C1D-ND	9.09	116.80	110.10
24	b	614	CLA	C2D-C1D-ND	9.09	116.80	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	407[A]	CLA	C1D-ND-C4D	-9.08	99.89	106.33
24	c	502	CLA	C1D-ND-C4D	-9.07	99.89	106.33
24	b	615	CLA	C2D-C1D-ND	9.06	116.78	110.10
24	A	409	CLA	C1D-ND-C4D	-9.05	99.91	106.33
24	a	406[A]	CLA	C1D-ND-C4D	-9.04	99.91	106.33
24	b	607	CLA	C1D-ND-C4D	-9.00	99.94	106.33
24	C	505	CLA	C2D-C1D-ND	8.97	116.72	110.10
24	B	616	CLA	C2D-C1D-ND	8.97	116.71	110.10
24	b	606	CLA	C1D-ND-C4D	-8.96	99.97	106.33
24	C	510	CLA	C1D-ND-C4D	-8.95	99.98	106.33
24	c	510	CLA	C1D-ND-C4D	-8.95	99.98	106.33
24	c	504	CLA	C1D-ND-C4D	-8.95	99.98	106.33
24	A	406[A]	CLA	C1D-ND-C4D	-8.91	100.01	106.33
24	b	605	CLA	C2D-C1D-ND	8.89	116.66	110.10
24	A	406[B]	CLA	C1D-ND-C4D	-8.89	100.02	106.33
24	C	513	CLA	C1D-ND-C4D	-8.86	100.04	106.33
24	a	406[B]	CLA	C1D-ND-C4D	-8.85	100.05	106.33
24	b	603	CLA	C1D-ND-C4D	-8.85	100.05	106.33
24	b	611	CLA	C2D-C1D-ND	8.84	116.61	110.10
24	a	405[A]	CLA	C1D-ND-C4D	-8.83	100.06	106.33
24	B	614	CLA	C2D-C1D-ND	8.83	116.61	110.10
24	b	610	CLA	C1D-ND-C4D	-8.81	100.08	106.33
24	c	509	CLA	C2D-C1D-ND	8.80	116.59	110.10
24	B	606	CLA	C2D-C1D-ND	8.78	116.58	110.10
24	b	609	CLA	C1D-ND-C4D	-8.78	100.10	106.33
24	c	503	CLA	C1D-ND-C4D	-8.78	100.10	106.33
24	c	505	CLA	C1D-ND-C4D	-8.78	100.10	106.33
24	a	406[A]	CLA	C2D-C1D-ND	8.75	116.56	110.10
24	C	505	CLA	C1D-ND-C4D	-8.74	100.13	106.33
24	D	403	CLA	C1D-ND-C4D	-8.72	100.14	106.33
24	a	407[A]	CLA	C2D-C1D-ND	8.65	116.48	110.10
24	c	509	CLA	C1D-ND-C4D	-8.62	100.21	106.33
24	C	510	CLA	C2D-C1D-ND	8.61	116.45	110.10
24	c	508	CLA	C1D-ND-C4D	-8.60	100.23	106.33
24	B	613	CLA	C1D-ND-C4D	-8.59	100.23	106.33
24	b	602	CLA	C1D-ND-C4D	-8.56	100.25	106.33
24	b	607	CLA	C2D-C1D-ND	8.54	116.40	110.10
24	c	513	CLA	C1D-ND-C4D	-8.54	100.27	106.33
24	B	613	CLA	C2D-C1D-ND	8.54	116.39	110.10
24	b	613	CLA	C2D-C1D-ND	8.51	116.38	110.10
24	b	608	CLA	C1D-ND-C4D	-8.51	100.29	106.33
24	B	602	CLA	C1D-ND-C4D	-8.51	100.29	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	402[A]	CLA	C2D-C1D-ND	8.50	116.37	110.10
24	A	405[A]	CLA	C1D-ND-C4D	-8.50	100.30	106.33
24	B	608	CLA	C2D-C1D-ND	8.49	116.36	110.10
24	b	616	CLA	C1D-ND-C4D	-8.45	100.33	106.33
24	B	616	CLA	C1D-ND-C4D	-8.42	100.35	106.33
24	c	505	CLA	C2D-C1D-ND	8.39	116.28	110.10
24	c	510	CLA	C2D-C1D-ND	8.38	116.28	110.10
24	b	612	CLA	C1D-ND-C4D	-8.38	100.38	106.33
24	B	601	CLA	C2D-C1D-ND	8.38	116.28	110.10
24	a	406[B]	CLA	C2D-C1D-ND	8.38	116.28	110.10
24	C	512	CLA	C1D-ND-C4D	-8.35	100.40	106.33
24	c	512	CLA	C2D-C1D-ND	8.34	116.25	110.10
24	C	504	CLA	C2D-C1D-ND	8.32	116.24	110.10
24	c	511	CLA	C1D-ND-C4D	-8.25	100.47	106.33
24	A	406[A]	CLA	C2D-C1D-ND	8.25	116.18	110.10
24	B	609	CLA	C1D-ND-C4D	-8.23	100.48	106.33
24	B	610	CLA	C2D-C1D-ND	8.19	116.14	110.10
24	a	407[B]	CLA	C2D-C1D-ND	8.16	116.12	110.10
24	b	601	CLA	C2D-C1D-ND	8.16	116.12	110.10
24	A	407[A]	CLA	C2D-C1D-ND	8.15	116.11	110.10
25	a	408[A]	PHO	O2D-CGD-CBD	8.14	121.31	111.00
24	A	407[B]	CLA	C2D-C1D-ND	8.14	116.10	110.10
24	B	603	CLA	C2D-C1D-ND	8.14	116.10	110.10
24	c	503	CLA	C2D-C1D-ND	8.12	116.09	110.10
24	B	605	CLA	C2D-C1D-ND	8.12	116.09	110.10
24	C	514	CLA	C2D-C1D-ND	8.11	116.08	110.10
24	B	610	CLA	C1D-ND-C4D	-8.10	100.58	106.33
24	C	503	CLA	C1D-ND-C4D	-8.06	100.61	106.33
24	b	613	CLA	C1D-ND-C4D	-8.05	100.61	106.33
24	c	507	CLA	C2D-C1D-ND	8.05	116.04	110.10
24	c	508	CLA	C2D-C1D-ND	8.05	116.03	110.10
24	d	404	CLA	C2D-C1D-ND	8.03	116.02	110.10
24	d	403[B]	CLA	C2D-C1D-ND	8.02	116.01	110.10
24	C	507	CLA	C2D-C1D-ND	8.00	116.00	110.10
24	C	502	CLA	C2D-C1D-ND	7.99	115.99	110.10
24	b	604	CLA	C1D-ND-C4D	-7.95	100.69	106.33
24	C	509	CLA	C1D-ND-C4D	-7.95	100.69	106.33
24	a	405[B]	CLA	C2D-C1D-ND	7.93	115.95	110.10
24	D	403	CLA	C2D-C1D-ND	7.92	115.94	110.10
24	c	514	CLA	C2D-C1D-ND	7.90	115.93	110.10
24	c	506	CLA	C2D-C1D-ND	7.90	115.92	110.10
24	D	402[B]	CLA	C4A-NA-C1A	-7.87	103.17	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	402[A]	PHO	O2D-CGD-CBD	7.83	120.91	111.00
24	d	403[A]	CLA	C2D-C1D-ND	7.82	115.87	110.10
24	C	508	CLA	C2D-C1D-ND	7.80	115.85	110.10
24	B	609	CLA	C4A-NA-C1A	-7.80	103.20	106.71
24	b	602	CLA	C4A-NA-C1A	-7.79	103.21	106.71
25	a	408[B]	PHO	O2D-CGD-CBD	7.78	120.85	111.00
24	b	608	CLA	C2D-C1D-ND	7.77	115.83	110.10
24	b	603	CLA	C2D-C1D-ND	7.73	115.80	110.10
24	b	610	CLA	C2D-C1D-ND	7.71	115.78	110.10
24	A	406[B]	CLA	C2D-C1D-ND	7.69	115.77	110.10
24	D	402[B]	CLA	C2D-C1D-ND	7.69	115.77	110.10
24	b	616	CLA	C2D-C1D-ND	7.68	115.76	110.10
24	C	511	CLA	C2D-C1D-ND	7.67	115.76	110.10
24	B	604	CLA	C1D-ND-C4D	-7.66	100.89	106.33
24	C	508	CLA	C1D-ND-C4D	-7.65	100.90	106.33
24	b	604	CLA	C2D-C1D-ND	7.65	115.74	110.10
24	A	405[A]	CLA	C2D-C1D-ND	7.64	115.73	110.10
24	b	609	CLA	C2D-C1D-ND	7.64	115.73	110.10
24	C	506	CLA	C2D-C1D-ND	7.61	115.71	110.10
24	b	606	CLA	C2D-C1D-ND	7.57	115.69	110.10
24	c	513	CLA	C2D-C1D-ND	7.57	115.68	110.10
24	c	504	CLA	C2D-C1D-ND	7.55	115.67	110.10
24	C	512	CLA	C2D-C1D-ND	7.54	115.66	110.10
24	C	513	CLA	C2D-C1D-ND	7.54	115.66	110.10
25	A	408[B]	PHO	O2D-CGD-CBD	7.51	120.52	111.00
24	c	511	CLA	C2D-C1D-ND	7.51	115.64	110.10
24	c	502	CLA	C2D-C1D-ND	7.49	115.62	110.10
24	c	504	CLA	C4A-NA-C1A	-7.49	103.34	106.71
25	A	417[A]	PHO	O2D-CGD-CBD	7.46	120.44	111.00
24	B	602	CLA	C2D-C1D-ND	7.44	115.59	110.10
27	X	101	SQD	O6-C1-C2	7.44	119.92	108.30
24	C	509	CLA	C2D-C1D-ND	7.40	115.56	110.10
24	b	612	CLA	C2D-C1D-ND	7.37	115.53	110.10
24	a	405[A]	CLA	C2D-C1D-ND	7.32	115.50	110.10
25	d	402[B]	PHO	O2D-CGD-CBD	7.31	120.26	111.00
24	B	611	CLA	CHD-C4C-C3C	-7.29	114.12	124.84
24	A	405[B]	CLA	C2D-C1D-ND	7.21	115.42	110.10
24	D	402[A]	CLA	C4A-NA-C1A	-7.21	103.46	106.71
24	b	616	CLA	C4A-NA-C1A	-7.21	103.46	106.71
24	C	503	CLA	C2D-C1D-ND	7.21	115.42	110.10
24	B	606	CLA	CMD-C2D-C1D	7.20	137.41	124.71
24	B	606	CLA	C4A-NA-C1A	-7.16	103.49	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	407[B]	CLA	CHD-C1D-ND	-7.15	117.89	124.45
24	B	614	CLA	CMD-C2D-C1D	7.12	137.27	124.71
25	A	417[B]	PHO	O2D-CGD-CBD	7.09	119.98	111.00
24	b	606	CLA	C4A-NA-C1A	-7.06	103.53	106.71
24	B	609	CLA	C2D-C1D-ND	7.03	115.28	110.10
24	B	605	CLA	CHD-C4C-C3C	-7.02	114.52	124.84
24	C	511	CLA	CMD-C2D-C1D	7.02	137.08	124.71
24	B	610	CLA	O2D-CGD-CBD	6.97	123.65	111.27
34	b	622	HTG	C1'-S1-C1	6.97	113.12	100.09
24	c	502	CLA	CMD-C2D-C1D	6.93	136.93	124.71
24	C	504	CLA	C4A-NA-C1A	-6.92	103.59	106.71
24	B	615	CLA	CHD-C4C-C3C	-6.90	114.70	124.84
24	C	513	CLA	C4A-NA-C1A	-6.88	103.61	106.71
24	c	504	CLA	CMD-C2D-C1D	6.85	136.79	124.71
24	B	612	CLA	CHD-C4C-C3C	-6.85	114.78	124.84
24	B	605	CLA	CMD-C2D-C1D	6.85	136.78	124.71
24	d	403[B]	CLA	CMD-C2D-C1D	6.85	136.78	124.71
24	B	616	CLA	O2D-CGD-CBD	6.82	123.39	111.27
24	B	611	CLA	CMD-C2D-C1D	6.79	136.68	124.71
24	b	605	CLA	CHD-C1D-ND	-6.79	118.21	124.45
24	c	508	CLA	CMD-C2D-C1D	6.79	136.68	124.71
24	a	405[B]	CLA	CMD-C2D-C1D	6.79	136.68	124.71
24	b	616	CLA	O2D-CGD-CBD	6.77	123.31	111.27
24	b	607	CLA	C2C-C1C-NC	6.77	116.32	109.97
24	b	611	CLA	CMD-C2D-C1D	6.75	136.61	124.71
24	B	616	CLA	CHD-C4C-C3C	-6.73	114.95	124.84
24	c	503	CLA	C2C-C1C-NC	6.72	116.27	109.97
24	b	602	CLA	C2D-C1D-ND	6.71	115.05	110.10
24	D	402[B]	CLA	CMD-C2D-C1D	6.71	136.53	124.71
24	A	405[A]	CLA	CMD-C2D-C1D	6.70	136.53	124.71
24	A	405[B]	CLA	CMD-C2D-C1D	6.65	136.43	124.71
24	b	601	CLA	O2D-CGD-CBD	6.64	123.06	111.27
24	B	615	CLA	C4A-NA-C1A	-6.63	103.73	106.71
24	c	513	CLA	C4A-NA-C1A	-6.62	103.73	106.71
24	a	407[B]	CLA	C4A-NA-C1A	-6.62	103.73	106.71
24	c	505	CLA	CHD-C1D-ND	-6.61	118.38	124.45
24	c	507	CLA	CMD-C2D-C1D	6.61	136.36	124.71
24	a	406[A]	CLA	CHD-C4C-C3C	-6.61	115.12	124.84
24	C	508	CLA	O2D-CGD-CBD	6.61	123.01	111.27
24	d	404	CLA	CHD-C1D-ND	-6.60	118.39	124.45
24	C	505	CLA	C2C-C1C-NC	6.59	116.14	109.97
24	b	606	CLA	CMD-C2D-C1D	6.58	136.31	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	613	CLA	CHD-C4C-C3C	-6.57	115.18	124.84
24	B	606	CLA	CHD-C1D-ND	-6.55	118.44	124.45
24	c	502	CLA	CHD-C1D-ND	-6.55	118.44	124.45
24	b	605	CLA	CMD-C2D-C1D	6.54	136.25	124.71
24	C	507	CLA	CMD-C2D-C1D	6.54	136.24	124.71
24	a	409	CLA	CHD-C4C-C3C	-6.54	115.23	124.84
34	D	410	HTG	C1'-S1-C1	6.49	112.24	100.09
24	d	403[A]	CLA	C2C-C1C-NC	6.49	116.05	109.97
24	b	616	CLA	CMD-C2D-C1D	6.49	136.15	124.71
24	B	607	CLA	CHD-C4C-C3C	-6.48	115.32	124.84
24	C	509	CLA	C2C-C1C-NC	6.47	116.03	109.97
24	B	610	CLA	CHD-C4C-C3C	-6.47	115.33	124.84
24	C	503	CLA	C4A-NA-C1A	-6.45	103.81	106.71
24	C	511	CLA	CHD-C1D-ND	-6.45	118.53	124.45
24	a	409	CLA	O2D-CGD-CBD	6.44	122.72	111.27
24	A	405[A]	CLA	C4A-NA-C1A	-6.44	103.81	106.71
27	A	411[A]	SQD	O6-C1-C2	6.44	118.36	108.30
24	b	605	CLA	CHD-C4C-C3C	-6.43	115.38	124.84
24	c	510	CLA	C1-C2-C3	-6.43	114.93	126.04
24	a	407[A]	CLA	CHD-C4C-C3C	-6.40	115.43	124.84
24	B	603	CLA	O2D-CGD-CBD	6.39	122.62	111.27
24	B	604	CLA	C2D-C1D-ND	6.39	114.81	110.10
24	C	504	CLA	CMD-C2D-C1D	6.38	135.96	124.71
24	b	601	CLA	C4A-NA-C1A	-6.38	103.84	106.71
24	C	508	CLA	CMD-C2D-C1D	6.37	135.94	124.71
24	B	601	CLA	CHD-C4C-C3C	-6.37	115.48	124.84
24	D	402[B]	CLA	CHD-C1D-ND	-6.36	118.61	124.45
24	c	514	CLA	CHD-C1D-ND	-6.36	118.61	124.45
24	B	603	CLA	CHD-C4C-C3C	-6.36	115.50	124.84
24	c	509	CLA	CHD-C4C-C3C	-6.35	115.50	124.84
24	B	601	CLA	CMD-C2D-C1D	6.35	135.91	124.71
24	C	507	CLA	CHD-C1D-ND	-6.34	118.63	124.45
24	b	610	CLA	CHD-C4C-C3C	-6.33	115.53	124.84
24	b	603	CLA	CHD-C4C-C3C	-6.32	115.54	124.84
24	A	409	CLA	CHD-C1D-ND	-6.32	118.65	124.45
24	c	508	CLA	CHD-C1D-ND	-6.32	118.65	124.45
24	b	611	CLA	CHD-C1D-ND	-6.31	118.65	124.45
24	B	605	CLA	C4A-NA-C1A	-6.31	103.87	106.71
24	B	610	CLA	CMD-C2D-C1D	6.31	135.83	124.71
24	c	514	CLA	CMD-C2D-C1D	6.30	135.82	124.71
24	c	508	CLA	O2D-CGD-CBD	6.30	122.47	111.27
24	C	507	CLA	C2C-C1C-NC	6.30	115.87	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	615	CLA	C4A-NA-C1A	-6.29	103.88	106.71
24	b	614	CLA	CMD-C2D-C1D	6.29	135.80	124.71
24	d	404	CLA	CMD-C2D-C1D	6.29	135.79	124.71
24	c	507	CLA	CHD-C1D-ND	-6.27	118.69	124.45
24	c	505	CLA	CMD-C2D-C1D	6.25	135.73	124.71
24	A	409	CLA	CHD-C4C-C3C	-6.25	115.66	124.84
24	c	511	CLA	CHD-C4C-C3C	-6.25	115.66	124.84
24	c	512	CLA	CHD-C4C-C3C	-6.25	115.66	124.84
24	d	403[B]	CLA	C4A-NA-C1A	-6.24	103.90	106.71
25	A	408[A]	PHO	O2D-CGD-CBD	6.23	118.89	111.00
24	d	403[B]	CLA	CHD-C1D-ND	-6.22	118.73	124.45
24	c	508	CLA	CHD-C4C-C3C	-6.22	115.70	124.84
24	b	601	CLA	CHD-C4C-C3C	-6.22	115.70	124.84
24	a	405[A]	CLA	C2C-C1C-NC	6.21	115.79	109.97
24	B	606	CLA	CHD-C4C-C3C	-6.20	115.73	124.84
24	B	611	CLA	O2D-CGD-CBD	6.19	122.27	111.27
24	b	616	CLA	CHD-C4C-C3C	-6.19	115.75	124.84
34	c	522	HTG	C1'-S1-C1	6.19	111.66	100.09
24	B	615	CLA	CHD-C1D-ND	-6.19	118.77	124.45
24	C	502	CLA	O2D-CGD-CBD	6.19	122.26	111.27
24	a	405[A]	CLA	C4A-NA-C1A	-6.18	103.93	106.71
24	A	405[B]	CLA	CHD-C1D-ND	-6.17	118.78	124.45
24	a	407[A]	CLA	C4A-NA-C1A	-6.17	103.93	106.71
24	B	606	CLA	O2D-CGD-CBD	6.16	122.21	111.27
24	b	609	CLA	CHD-C4C-C3C	-6.15	115.80	124.84
24	A	407[A]	CLA	CHD-C1D-ND	-6.14	118.81	124.45
24	A	407[B]	CLA	CHD-C1D-ND	-6.14	118.81	124.45
24	B	614	CLA	CHD-C1D-ND	-6.14	118.81	124.45
24	C	511	CLA	CHD-C4C-C3C	-6.14	115.82	124.84
34	B	622	HTG	C1'-S1-C1	6.14	111.57	100.09
24	c	513	CLA	CMD-C2D-C1D	6.14	135.53	124.71
24	a	407[A]	CLA	CHD-C1D-ND	-6.14	118.81	124.45
24	C	502	CLA	CMD-C2D-C1D	6.13	135.52	124.71
24	A	406[B]	CLA	CHD-C1D-ND	-6.13	118.82	124.45
24	B	605	CLA	CHD-C1D-ND	-6.13	118.82	124.45
24	b	615	CLA	CHD-C1D-ND	-6.12	118.83	124.45
24	a	407[B]	CLA	CMD-C2D-C1D	6.12	135.50	124.71
24	A	405[A]	CLA	CHD-C1D-ND	-6.11	118.83	124.45
24	b	604	CLA	C2C-C1C-NC	6.11	115.70	109.97
24	A	407[B]	CLA	CMD-C2D-C1D	6.11	135.48	124.71
24	C	510	CLA	CHD-C4C-C3C	-6.11	115.86	124.84
24	D	402[A]	CLA	CMD-C2D-C1D	6.10	135.47	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	513	CLA	CHD-C4C-C3C	-6.09	115.89	124.84
24	B	608	CLA	C2C-C1C-NC	6.08	115.67	109.97
24	a	405[A]	CLA	CMD-C2D-C1D	6.07	135.41	124.71
24	c	514	CLA	C4A-NA-C1A	-6.06	103.98	106.71
24	c	510	CLA	C2C-C1C-NC	6.06	115.65	109.97
24	C	504	CLA	CHD-C1D-ND	-6.05	118.89	124.45
24	B	602	CLA	C2C-C1C-NC	6.05	115.64	109.97
24	b	602	CLA	CHD-C4C-C3C	-6.04	115.96	124.84
24	D	403	CLA	C4A-NA-C1A	-6.04	103.99	106.71
24	C	506	CLA	CHD-C1D-ND	-6.03	118.91	124.45
24	A	406[B]	CLA	CMD-C2D-C1D	6.03	135.34	124.71
24	C	512	CLA	CHD-C4C-C3C	-6.03	115.98	124.84
24	c	510	CLA	CHD-C4C-C3C	-6.03	115.98	124.84
41	V	201	HEC	CBD-CAD-C3D	-6.03	102.34	112.62
24	C	504	CLA	CHD-C4C-C3C	-6.02	115.98	124.84
24	C	514	CLA	CHD-C1D-ND	-6.00	118.94	124.45
24	c	511	CLA	C4A-NA-C1A	-5.99	104.02	106.71
24	b	602	CLA	O2D-CGD-CBD	5.98	121.90	111.27
24	b	606	CLA	CHD-C1D-ND	-5.97	118.97	124.45
24	c	504	CLA	CHD-C4C-C3C	-5.97	116.06	124.84
24	a	406[B]	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
24	b	614	CLA	O2D-CGD-CBD	5.96	121.85	111.27
27	A	411[B]	SQD	O6-C1-C2	5.95	117.59	108.30
24	C	508	CLA	CHD-C4C-C3C	-5.95	116.10	124.84
24	B	611	CLA	CHD-C1D-ND	-5.94	118.99	124.45
24	C	514	CLA	CMD-C2D-C1D	5.94	135.18	124.71
24	A	409	CLA	C2C-C1C-NC	5.93	115.53	109.97
24	b	614	CLA	CHD-C1D-ND	-5.93	119.00	124.45
27	B	620	SQD	O6-C1-C2	5.93	117.56	108.30
24	a	406[A]	CLA	CMD-C2D-C1D	5.93	135.16	124.71
24	c	506	CLA	CHD-C4C-C3C	-5.93	116.12	124.84
24	b	608	CLA	C2C-C1C-NC	5.93	115.53	109.97
24	C	510	CLA	CHD-C1D-ND	-5.92	119.02	124.45
24	C	503	CLA	CMD-C2D-C1D	5.92	135.14	124.71
24	a	405[B]	CLA	CHD-C1D-ND	-5.92	119.02	124.45
24	A	407[A]	CLA	C4A-NA-C1A	-5.91	104.05	106.71
24	D	402[A]	CLA	CHD-C1D-ND	-5.91	119.02	124.45
27	L	102	SQD	O6-C1-C2	5.91	117.53	108.30
24	b	601	CLA	CMD-C2D-C1D	5.91	135.13	124.71
24	c	513	CLA	O2D-CGD-CBD	5.91	121.77	111.27
24	a	407[B]	CLA	CHD-C4C-C3C	-5.89	116.17	124.84
24	A	407[A]	CLA	CMD-C2D-C1D	5.89	135.10	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	616	CLA	C3C-C4C-NC	5.89	117.17	110.57
24	A	407[B]	CLA	C4A-NA-C1A	-5.89	104.06	106.71
24	b	612	CLA	CHD-C4C-C3C	-5.89	116.19	124.84
24	c	513	CLA	CHD-C1D-ND	-5.88	119.05	124.45
24	b	607	CLA	CMD-C2D-C1D	5.88	135.08	124.71
24	b	613	CLA	CMD-C2D-C1D	5.88	135.07	124.71
24	D	402[A]	CLA	C2C-C1C-NC	5.88	115.48	109.97
24	B	609	CLA	CHD-C4C-C3C	-5.87	116.22	124.84
24	C	502	CLA	CHD-C4C-C3C	-5.86	116.23	124.84
24	A	407[A]	CLA	CHD-C4C-C3C	-5.85	116.25	124.84
24	b	607	CLA	CHD-C4C-C3C	-5.85	116.25	124.84
24	A	405[A]	CLA	C2C-C1C-NC	5.84	115.44	109.97
24	B	602	CLA	CHD-C4C-C3C	-5.84	116.26	124.84
24	c	509	CLA	CMD-C2D-C1D	5.84	135.00	124.71
24	b	611	CLA	CHD-C4C-C3C	-5.83	116.27	124.84
24	a	406[B]	CLA	C2C-C1C-NC	5.83	115.43	109.97
24	c	504	CLA	CHD-C1D-ND	-5.82	119.10	124.45
24	C	506	CLA	CMD-C2D-C1D	5.82	134.98	124.71
24	B	608	CLA	CHD-C4C-C3C	-5.82	116.28	124.84
24	C	505	CLA	CHD-C1D-ND	-5.82	119.11	124.45
24	b	606	CLA	CHD-C4C-C3C	-5.82	116.29	124.84
24	A	407[B]	CLA	CHD-C4C-C3C	-5.81	116.30	124.84
24	b	614	CLA	CHD-C4C-C3C	-5.81	116.30	124.84
24	B	601	CLA	O2D-CGD-CBD	5.81	121.59	111.27
24	D	402[B]	CLA	CHD-C4C-C3C	-5.80	116.31	124.84
24	B	602	CLA	O2D-CGD-CBD	5.80	121.57	111.27
24	b	601	CLA	CHD-C1D-ND	-5.79	119.13	124.45
24	C	513	CLA	CMD-C2D-C1D	5.79	134.91	124.71
24	C	508	CLA	CHD-C1D-ND	-5.79	119.14	124.45
24	C	506	CLA	CHD-C4C-C3C	-5.78	116.34	124.84
24	b	603	CLA	C4A-NA-C1A	-5.78	104.11	106.71
24	B	612	CLA	C3C-C4C-NC	5.78	117.05	110.57
24	C	514	CLA	CHD-C4C-C3C	-5.77	116.35	124.84
24	B	614	CLA	C2C-C1C-NC	5.77	115.38	109.97
24	C	510	CLA	CMD-C2D-C1D	5.77	134.88	124.71
24	A	406[A]	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
24	b	606	CLA	O2D-CGD-CBD	5.77	121.51	111.27
26	D	404	BCR	C7-C8-C9	-5.75	117.54	126.23
24	c	509	CLA	C4A-NA-C1A	-5.75	104.12	106.71
24	B	613	CLA	C2C-C1C-NC	5.75	115.36	109.97
24	C	511	CLA	O2D-CGD-CBD	5.74	121.47	111.27
24	D	403	CLA	CHD-C4C-C3C	-5.74	116.41	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	F	102	HEM	CAD-CBD-CGD	5.73	125.93	113.60
24	c	507	CLA	CHD-C4C-C3C	-5.73	116.42	124.84
24	A	406[B]	CLA	CHD-C4C-C3C	-5.72	116.43	124.84
24	B	614	CLA	CHD-C4C-C3C	-5.72	116.43	124.84
24	C	509	CLA	CHD-C4C-C3C	-5.72	116.44	124.84
24	B	604	CLA	C2C-C1C-NC	5.72	115.33	109.97
24	A	409	CLA	CMD-C2D-C1D	5.71	134.78	124.71
24	b	604	CLA	C1-C2-C3	-5.70	116.18	126.04
24	C	512	CLA	CMD-C2D-C1D	5.70	134.76	124.71
27	a	411[A]	SQD	O6-C1-C2	5.69	117.19	108.30
24	B	611	CLA	C3D-C2D-C1D	-5.69	98.07	105.83
24	B	614	CLA	C3D-C2D-C1D	-5.69	98.07	105.83
24	B	607	CLA	C2C-C1C-NC	5.69	115.30	109.97
24	C	507	CLA	CHD-C4C-C3C	-5.69	116.48	124.84
27	X	101	SQD	O47-C7-C8	5.68	123.75	111.50
24	B	601	CLA	CHD-C1D-ND	-5.68	119.23	124.45
24	c	502	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
24	b	611	CLA	C2C-C1C-NC	5.67	115.28	109.97
24	B	604	CLA	O2D-CGD-CBD	5.66	121.33	111.27
24	b	609	CLA	CMD-C2D-C1D	5.66	134.69	124.71
24	B	616	CLA	C2C-C1C-NC	5.66	115.27	109.97
24	C	502	CLA	C4A-NA-C1A	-5.66	104.16	106.71
24	c	505	CLA	CHD-C4C-C3C	-5.65	116.53	124.84
24	C	511	CLA	C2C-C1C-NC	5.65	115.26	109.97
24	d	403[B]	CLA	C2C-C1C-NC	5.65	115.26	109.97
24	C	506	CLA	O2D-CGD-CBD	5.65	121.30	111.27
24	b	613	CLA	C2C-C1C-NC	5.64	115.26	109.97
27	A	411[A]	SQD	C1-O5-C5	-5.64	102.61	113.69
24	d	403[B]	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
24	A	406[B]	CLA	C2C-C1C-NC	5.63	115.25	109.97
24	D	403	CLA	CMD-C2D-C1D	5.63	134.64	124.71
24	b	610	CLA	C2C-C1C-NC	5.63	115.25	109.97
24	b	608	CLA	CHD-C1D-ND	-5.63	119.28	124.45
24	A	406[B]	CLA	O2D-CGD-CBD	5.63	121.27	111.27
24	B	604	CLA	CMD-C2D-C1D	5.62	134.61	124.71
24	B	614	CLA	O2D-CGD-CBD	5.61	121.24	111.27
24	a	405[B]	CLA	C2C-C1C-NC	5.61	115.23	109.97
24	c	511	CLA	CMD-C2D-C1D	5.60	134.59	124.71
24	c	507	CLA	C4A-NA-C1A	-5.60	104.19	106.71
24	a	409	CLA	C4A-NA-C1A	-5.59	104.19	106.71
24	c	509	CLA	C2C-C1C-NC	5.58	115.20	109.97
24	B	612	CLA	O2D-CGD-CBD	5.58	121.18	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	603	CLA	CMD-C2D-C1D	5.58	134.54	124.71
24	b	613	CLA	C4A-NA-C1A	-5.57	104.20	106.71
24	C	512	CLA	C2C-C1C-NC	5.57	115.19	109.97
24	a	406[B]	CLA	CHD-C1D-ND	-5.56	119.34	124.45
24	C	503	CLA	CHD-C1D-ND	-5.56	119.35	124.45
24	b	605	CLA	C2C-C1C-NC	5.56	115.18	109.97
24	b	604	CLA	O2D-CGD-CBD	5.55	121.14	111.27
24	d	404	CLA	O2D-CGD-CBD	5.55	121.14	111.27
24	C	513	CLA	O2D-CGD-CBD	5.55	121.13	111.27
24	b	611	CLA	C3D-C2D-C1D	-5.54	98.26	105.83
24	A	406[A]	CLA	C2C-C1C-NC	5.54	115.17	109.97
24	C	512	CLA	O2D-CGD-CBD	5.54	121.12	111.27
24	c	503	CLA	CHD-C4C-C3C	-5.54	116.70	124.84
24	c	510	CLA	CMD-C2D-C1D	5.54	134.47	124.71
24	D	402[A]	CLA	CHD-C4C-C3C	-5.54	116.70	124.84
27	B	620	SQD	O47-C7-C8	5.54	123.43	111.50
24	B	614	CLA	C4A-NA-C1A	-5.53	104.22	106.71
24	C	502	CLA	CHD-C1D-ND	-5.53	119.37	124.45
24	C	513	CLA	CHD-C1D-ND	-5.53	119.37	124.45
24	b	615	CLA	CHD-C4C-C3C	-5.53	116.72	124.84
24	b	612	CLA	C4A-NA-C1A	-5.52	104.22	106.71
24	C	505	CLA	CMD-C2D-C1D	5.52	134.45	124.71
24	B	609	CLA	C2C-C1C-NC	5.52	115.14	109.97
24	c	509	CLA	C3D-C2D-C1D	-5.51	98.31	105.83
24	B	603	CLA	CMD-C2D-C1D	5.51	134.43	124.71
24	B	603	CLA	C2C-C1C-NC	5.51	115.13	109.97
24	a	405[A]	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
24	a	406[A]	CLA	C2C-C1C-NC	5.50	115.13	109.97
24	b	607	CLA	CHD-C1D-ND	-5.50	119.40	124.45
24	A	406[B]	CLA	C4A-NA-C1A	-5.50	104.23	106.71
35	C	501	LMG	C7-O1-C1	-5.50	103.00	113.74
24	c	507	CLA	C2C-C1C-NC	5.50	115.12	109.97
24	d	403[A]	CLA	CHD-C4C-C3C	-5.50	116.76	124.84
24	C	504	CLA	C2C-C1C-NC	5.49	115.12	109.97
24	C	506	CLA	C2C-C1C-NC	5.49	115.11	109.97
24	C	505	CLA	C3D-C2D-C1D	-5.49	98.34	105.83
24	a	406[A]	CLA	CHD-C1D-ND	-5.49	119.41	124.45
24	b	610	CLA	O2D-CGD-CBD	5.49	121.02	111.27
24	C	503	CLA	C2C-C1C-NC	5.49	115.11	109.97
24	c	513	CLA	CHD-C4C-C3C	-5.49	116.78	124.84
24	a	407[A]	CLA	CMD-C2D-C1D	5.49	134.38	124.71
24	c	514	CLA	CHD-C4C-C3C	-5.48	116.78	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	d	411	HTG	C1'-S1-C1	5.48	110.34	100.09
24	c	512	CLA	CMD-C2D-C1D	5.47	134.36	124.71
24	b	612	CLA	C2C-C1C-NC	5.47	115.10	109.97
24	B	602	CLA	CMD-C2D-C1D	5.46	134.34	124.71
24	b	608	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
24	B	603	CLA	CHD-C1D-ND	-5.46	119.44	124.45
24	b	604	CLA	CHD-C4C-C3C	-5.46	116.82	124.84
39	F	102	HEM	CBA-CAA-C2A	-5.45	103.32	112.62
24	B	609	CLA	CHD-C1D-ND	-5.44	119.46	124.45
24	C	508	CLA	C2C-C1C-NC	5.44	115.07	109.97
24	d	403[A]	CLA	CMD-C2D-C1D	5.44	134.30	124.71
24	a	406[B]	CLA	O2D-CGD-CBD	5.44	120.93	111.27
24	B	606	CLA	C2C-C1C-NC	5.43	115.06	109.97
24	B	605	CLA	O2D-CGD-CBD	5.43	120.92	111.27
24	c	508	CLA	C2C-C1C-NC	5.42	115.05	109.97
24	c	506	CLA	O2D-CGD-CBD	5.42	120.90	111.27
24	c	506	CLA	C4A-NA-C1A	-5.41	104.27	106.71
24	A	406[A]	CLA	CHD-C1D-ND	-5.41	119.48	124.45
24	C	510	CLA	C2C-C1C-NC	5.40	115.03	109.97
24	B	603	CLA	C4A-NA-C1A	-5.40	104.28	106.71
24	C	508	CLA	C4A-NA-C1A	-5.40	104.28	106.71
24	c	511	CLA	C2C-C1C-NC	5.40	115.03	109.97
24	c	505	CLA	O2D-CGD-CBD	5.39	120.85	111.27
25	d	402[A]	PHO	C1-C2-C3	-5.39	116.72	126.04
24	b	611	CLA	O2D-CGD-CBD	5.38	120.84	111.27
24	b	603	CLA	C2C-C1C-NC	5.38	115.02	109.97
24	c	508	CLA	C4A-NA-C1A	-5.38	104.29	106.71
24	c	502	CLA	C2C-C1C-NC	5.38	115.01	109.97
26	t	102	BCR	C33-C5-C6	-5.38	118.49	124.53
24	B	615	CLA	CMD-C2D-C1D	5.38	134.19	124.71
24	A	406[A]	CLA	C4A-NA-C1A	-5.38	104.29	106.71
24	A	409	CLA	C3D-C2D-C1D	-5.37	98.50	105.83
24	a	405[B]	CLA	CHD-C4C-C3C	-5.37	116.95	124.84
24	C	506	CLA	C4A-NA-C1A	-5.37	104.29	106.71
24	C	505	CLA	O2D-CGD-CBD	5.37	120.80	111.27
24	B	616	CLA	C3D-C2D-C1D	-5.36	98.52	105.83
24	b	605	CLA	O2D-CGD-CBD	5.36	120.78	111.27
24	c	512	CLA	CHD-C1D-ND	-5.35	119.53	124.45
24	b	608	CLA	CMD-C2D-C1D	5.35	134.14	124.71
24	a	409	CLA	C2C-C1C-NC	5.35	114.98	109.97
27	A	411[A]	SQD	C1-C2-C3	-5.35	98.86	110.00
24	a	405[A]	CLA	CHD-C1D-ND	-5.34	119.55	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	607	CLA	O2D-CGD-CBD	5.34	120.75	111.27
24	b	616	CLA	CHD-C1D-ND	-5.33	119.56	124.45
24	a	406[B]	CLA	CMD-C2D-C1D	5.33	134.11	124.71
24	B	611	CLA	CMB-C2B-C1B	5.33	136.65	128.46
24	c	514	CLA	C2C-C1C-NC	5.32	114.96	109.97
24	B	615	CLA	C2C-C1C-NC	5.32	114.95	109.97
24	B	613	CLA	C1-C2-C3	-5.32	116.85	126.04
24	c	509	CLA	O2D-CGD-CBD	5.32	120.71	111.27
24	a	409	CLA	CMD-C2D-C1D	5.31	134.07	124.71
24	b	603	CLA	CHD-C1D-ND	-5.30	119.58	124.45
24	B	606	CLA	C3D-C2D-C1D	-5.30	98.60	105.83
24	B	604	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
24	a	409	CLA	CHD-C1D-ND	-5.29	119.59	124.45
30	A	415[B]	PL9	C7-C8-C9	-5.29	117.99	126.79
24	A	405[B]	CLA	C2C-C1C-NC	5.28	114.92	109.97
24	B	607	CLA	CMD-C2D-C1D	5.28	134.01	124.71
24	C	514	CLA	C2C-C1C-NC	5.27	114.91	109.97
24	C	503	CLA	CHD-C4C-C3C	-5.27	117.09	124.84
24	A	405[B]	CLA	C4A-NA-C1A	-5.27	104.34	106.71
24	b	614	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
25	d	402[B]	PHO	C1-C2-C3	-5.25	116.96	126.04
24	c	505	CLA	C2C-C1C-NC	5.25	114.89	109.97
24	C	510	CLA	C4A-NA-C1A	-5.25	104.34	106.71
24	B	607	CLA	CHD-C1D-ND	-5.25	119.63	124.45
24	A	409	CLA	C3C-C4C-NC	5.24	116.45	110.57
24	A	405[B]	CLA	CHD-C4C-C3C	-5.23	117.15	124.84
24	B	610	CLA	C4A-NA-C1A	-5.23	104.36	106.71
26	Y	101	BCR	C33-C5-C6	-5.20	118.69	124.53
24	B	605	CLA	C3D-C2D-C1D	-5.19	98.74	105.83
24	C	509	CLA	O2D-CGD-CBD	5.19	120.49	111.27
24	D	403	CLA	CHD-C1D-ND	-5.19	119.69	124.45
24	C	505	CLA	CHD-C4C-C3C	-5.19	117.22	124.84
24	c	505	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
26	d	405	BCR	C7-C8-C9	-5.18	118.40	126.23
24	d	403[A]	CLA	CHD-C1D-ND	-5.18	119.69	124.45
24	b	613	CLA	C3D-C2D-C1D	-5.18	98.77	105.83
24	b	609	CLA	C2C-C1C-NC	5.15	114.80	109.97
24	c	510	CLA	O2D-CGD-CBD	5.15	120.42	111.27
24	B	612	CLA	CMD-C2D-C1D	5.15	133.79	124.71
24	c	506	CLA	C2C-C1C-NC	5.15	114.79	109.97
24	c	503	CLA	CHD-C1D-ND	-5.14	119.73	124.45
24	b	610	CLA	CMD-C2D-C1D	5.14	133.77	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	404	CLA	CHD-C4C-C3C	-5.14	117.29	124.84
24	b	610	CLA	C3C-C4C-NC	5.14	116.33	110.57
24	b	616	CLA	C3D-C2D-C1D	-5.13	98.82	105.83
24	b	614	CLA	C2C-C1C-NC	5.13	114.78	109.97
24	A	405[A]	CLA	CHD-C4C-C3C	-5.13	117.30	124.84
24	B	607	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
24	D	402[B]	CLA	C2C-C1C-NC	5.12	114.77	109.97
24	B	615	CLA	C3D-C2D-C1D	-5.11	98.85	105.83
24	C	505	CLA	C1C-C2C-C3C	-5.11	101.58	106.96
24	B	610	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
24	B	610	CLA	CHD-C1D-ND	-5.11	119.76	124.45
24	b	615	CLA	CMD-C2D-C1D	5.09	133.69	124.71
27	L	102	SQD	O47-C7-C8	5.09	122.47	111.50
24	B	604	CLA	C3C-C4C-NC	5.09	116.28	110.57
24	B	613	CLA	CHD-C1D-ND	-5.09	119.78	124.45
27	a	411[A]	SQD	O47-C7-C8	5.08	122.45	111.50
24	a	406[A]	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
24	b	607	CLA	C3C-C4C-NC	5.08	116.27	110.57
24	B	608	CLA	CHD-C1D-ND	-5.07	119.80	124.45
24	D	402[A]	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
24	C	502	CLA	C2C-C1C-NC	5.06	114.72	109.97
26	y	101	BCR	C33-C5-C6	-5.06	118.85	124.53
24	A	407[B]	CLA	C2C-C1C-NC	5.06	114.71	109.97
24	c	503	CLA	C1C-C2C-C3C	-5.05	101.64	106.96
24	b	614	CLA	C4A-NA-C1A	-5.05	104.44	106.71
24	c	506	CLA	C3C-C4C-NC	5.05	116.23	110.57
24	c	512	CLA	C2C-C1C-NC	5.05	114.70	109.97
24	B	608	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
24	c	502	CLA	O2D-CGD-CBD	5.05	120.23	111.27
34	b	621	HTG	C1-O5-C5	5.04	121.88	112.58
24	b	613	CLA	CHD-C1D-ND	-5.04	119.82	124.45
24	b	605	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
34	C	522	HTG	C1'-S1-C1	5.04	109.51	100.09
24	b	615	CLA	C2C-C1C-NC	5.03	114.69	109.97
27	a	411[B]	SQD	O47-C7-C8	5.02	122.33	111.50
24	a	405[B]	CLA	C4A-NA-C1A	-5.02	104.45	106.71
24	a	409	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
24	B	604	CLA	C1-C2-C3	-5.02	117.37	126.04
24	A	406[A]	CLA	O2D-CGD-CBD	5.01	120.17	111.27
24	b	611	CLA	C4A-NA-C1A	-5.01	104.45	106.71
24	b	605	CLA	C4A-NA-C1A	-5.00	104.46	106.71
24	D	402[A]	CLA	C3C-C4C-NC	5.00	116.18	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	613	CLA	C3C-C4C-NC	5.00	116.18	110.57
24	b	606	CLA	C2C-C1C-NC	5.00	114.66	109.97
24	b	607	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
24	c	506	CLA	CHD-C1D-ND	-4.99	119.87	124.45
24	b	609	CLA	CHD-C1D-ND	-4.99	119.87	124.45
24	B	605	CLA	C2C-C1C-NC	4.98	114.64	109.97
30	a	415[A]	PL9	C7-C8-C9	-4.98	118.50	126.79
24	b	612	CLA	CMD-C2D-C1D	4.98	133.48	124.71
24	b	612	CLA	C3C-C4C-NC	4.98	116.15	110.57
27	f	101	SQD	O47-C7-C8	4.97	122.22	111.50
24	C	509	CLA	C3C-C4C-NC	4.97	116.15	110.57
24	C	512	CLA	CHD-C1D-ND	-4.97	119.89	124.45
24	a	407[A]	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
24	c	509	CLA	C3C-C4C-NC	4.96	116.13	110.57
24	c	511	CLA	O2D-CGD-CBD	4.96	120.08	111.27
24	B	612	CLA	CHD-C1D-ND	-4.96	119.90	124.45
24	C	509	CLA	CMD-C2D-C1D	4.95	133.44	124.71
24	c	511	CLA	CHD-C1D-ND	-4.95	119.90	124.45
24	C	504	CLA	O2D-CGD-CBD	4.95	120.07	111.27
24	D	403	CLA	O2D-CGD-CBD	4.95	120.06	111.27
30	A	415[A]	PL9	C7-C8-C9	-4.94	118.56	126.79
24	B	609	CLA	CMD-C2D-C1D	4.94	133.42	124.71
24	c	504	CLA	C2C-C1C-NC	4.94	114.60	109.97
24	B	608	CLA	CMD-C2D-C1D	4.93	133.40	124.71
24	d	404	CLA	C2C-C1C-NC	4.92	114.58	109.97
24	B	602	CLA	C3C-C4C-NC	4.92	116.09	110.57
24	D	403	CLA	C2C-C1C-NC	4.91	114.57	109.97
24	b	602	CLA	CHD-C1D-ND	-4.91	119.94	124.45
24	B	610	CLA	C2C-C1C-NC	4.91	114.57	109.97
27	a	411[A]	SQD	C1-O5-C5	-4.91	104.05	113.69
24	C	514	CLA	O2D-CGD-CBD	4.90	119.98	111.27
24	b	612	CLA	O2D-CGD-CBD	4.90	119.97	111.27
24	d	403[A]	CLA	C4A-NA-C1A	-4.89	104.51	106.71
24	B	613	CLA	O2D-CGD-CBD	4.89	119.95	111.27
24	B	613	CLA	CHD-C4C-C3C	-4.89	117.66	124.84
24	b	609	CLA	C4A-NA-C1A	-4.87	104.52	106.71
24	c	508	CLA	C3D-C2D-C1D	-4.87	99.19	105.83
24	C	510	CLA	C3D-C2D-C1D	-4.86	99.19	105.83
24	b	608	CLA	O2D-CGD-CBD	4.86	119.90	111.27
24	b	603	CLA	O2D-CGD-CBD	4.86	119.90	111.27
24	c	509	CLA	CHD-C1D-ND	-4.86	119.99	124.45
24	B	601	CLA	C2C-C1C-NC	4.85	114.52	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	613	CLA	C3C-C4C-NC	4.85	116.01	110.57
24	c	511	CLA	C1-C2-C3	-4.85	117.66	126.04
24	b	602	CLA	CMD-C2D-C1D	4.85	133.25	124.71
24	b	604	CLA	C3C-C4C-NC	4.84	116.00	110.57
24	B	613	CLA	CMD-C2D-C1D	4.84	133.24	124.71
24	A	407[A]	CLA	C2C-C1C-NC	4.83	114.50	109.97
24	A	407[B]	CLA	O2D-CGD-CBD	4.83	119.85	111.27
24	C	502	CLA	O2D-CGD-O1D	-4.82	114.41	123.84
24	a	407[A]	CLA	C2C-C1C-NC	4.82	114.49	109.97
24	B	602	CLA	C4A-NA-C1A	-4.82	104.54	106.71
24	c	504	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
24	C	504	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
24	b	605	CLA	C3D-C4D-ND	4.81	118.02	110.24
24	a	406[B]	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
24	b	605	CLA	O2D-CGD-O1D	-4.81	114.44	123.84
24	b	615	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
24	c	514	CLA	O2D-CGD-CBD	4.80	119.80	111.27
24	B	612	CLA	C2C-C1C-NC	4.80	114.47	109.97
24	B	607	CLA	C4A-NA-C1A	-4.80	104.55	106.71
24	B	601	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
24	c	507	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
24	a	407[B]	CLA	C3D-C4D-ND	4.79	117.98	110.24
24	B	616	CLA	CMD-C2D-C1D	4.79	133.15	124.71
24	C	508	CLA	C3D-C2D-C1D	-4.78	99.30	105.83
24	D	403	CLA	C3D-C2D-C1D	-4.78	99.30	105.83
24	A	406[A]	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
27	A	411[B]	SQD	C1-O5-C5	-4.77	104.32	113.69
24	A	406[A]	CLA	CMD-C2D-C1D	4.77	133.12	124.71
24	c	511	CLA	C3C-C4C-NC	4.77	115.92	110.57
24	C	510	CLA	C1-C2-C3	-4.77	117.80	126.04
24	b	601	CLA	C2C-C1C-NC	4.76	114.43	109.97
24	b	607	CLA	C1C-C2C-C3C	-4.76	101.95	106.96
24	C	503	CLA	O2D-CGD-CBD	4.75	119.72	111.27
24	B	611	CLA	C3D-C4D-ND	4.75	117.92	110.24
24	C	502	CLA	C3D-C2D-C1D	-4.75	99.36	105.83
24	c	503	CLA	C4A-NA-C1A	-4.74	104.57	106.71
24	b	603	CLA	C3C-C4C-NC	4.74	115.89	110.57
24	C	508	CLA	C3C-C4C-NC	4.74	115.88	110.57
24	B	608	CLA	O2D-CGD-CBD	4.72	119.65	111.27
24	B	616	CLA	CHD-C1D-ND	-4.71	120.12	124.45
24	c	508	CLA	C3C-C4C-NC	4.71	115.85	110.57
26	H	101	BCR	C38-C26-C25	-4.70	119.25	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	605	CLA	C3C-C4C-NC	4.70	115.84	110.57
24	b	602	CLA	C3D-C4D-ND	4.69	117.83	110.24
24	A	407[B]	CLA	C3D-C4D-ND	4.68	117.80	110.24
24	C	507	CLA	O2D-CGD-CBD	4.67	119.57	111.27
24	C	514	CLA	C4A-NA-C1A	-4.67	104.61	106.71
24	c	513	CLA	C2C-C1C-NC	4.66	114.34	109.97
24	C	510	CLA	C3C-C4C-NC	4.66	115.80	110.57
24	C	507	CLA	C1C-C2C-C3C	-4.66	102.06	106.96
24	D	402[B]	CLA	O2D-CGD-CBD	4.66	119.55	111.27
24	C	506	CLA	C3D-C4D-ND	4.64	117.75	110.24
24	B	613	CLA	C3D-C2D-C1D	-4.64	99.49	105.83
24	c	513	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
24	C	514	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
24	b	604	CLA	CMD-C2D-C1D	4.64	132.88	124.71
24	A	406[B]	CLA	C1C-C2C-C3C	-4.64	102.08	106.96
24	a	406[A]	CLA	O2D-CGD-CBD	4.63	119.49	111.27
24	C	506	CLA	C3C-C4C-NC	4.62	115.75	110.57
27	a	411[B]	SQD	O6-C1-C2	4.62	115.51	108.30
39	e	101	HEM	CHC-C4B-NB	4.61	129.44	124.43
24	c	512	CLA	O2D-CGD-CBD	4.61	119.46	111.27
24	B	608	CLA	C3C-C4C-NC	4.61	115.74	110.57
24	b	611	CLA	C3C-C4C-NC	4.61	115.74	110.57
26	b	617	BCR	C7-C8-C9	-4.61	119.27	126.23
24	c	510	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
24	B	610	CLA	O2A-CGA-CBA	4.61	126.36	111.91
24	C	511	CLA	C1C-C2C-C3C	-4.61	102.11	106.96
24	C	505	CLA	C3C-C4C-NC	4.60	115.73	110.57
24	b	604	CLA	CHD-C1D-ND	-4.60	120.22	124.45
24	C	510	CLA	O2D-CGD-CBD	4.60	119.44	111.27
24	C	511	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
24	B	603	CLA	C3C-C4C-NC	4.60	115.72	110.57
24	b	609	CLA	C3C-C4C-NC	4.59	115.72	110.57
24	A	405[A]	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
24	B	615	CLA	C3C-C4C-NC	4.59	115.72	110.57
24	b	612	CLA	CHD-C1D-ND	-4.59	120.24	124.45
24	C	512	CLA	C3C-C4C-NC	4.58	115.71	110.57
24	a	406[B]	CLA	C1C-C2C-C3C	-4.58	102.14	106.96
24	c	510	CLA	CHD-C1D-ND	-4.58	120.24	124.45
24	c	507	CLA	O2D-CGD-CBD	4.58	119.40	111.27
24	C	507	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
24	b	604	CLA	C4A-NA-C1A	-4.57	104.65	106.71
24	A	406[A]	CLA	C1C-C2C-C3C	-4.57	102.15	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	407[B]	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
24	a	405[B]	CLA	C3D-C4D-ND	4.57	117.63	110.24
24	b	606	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
24	C	505	CLA	C4A-NA-C1A	-4.56	104.66	106.71
24	c	506	CLA	C3D-C4D-ND	4.56	117.61	110.24
24	c	506	CLA	CMD-C2D-C1D	4.56	132.74	124.71
24	a	409	CLA	CMC-C2C-C1C	4.56	131.98	125.04
24	c	510	CLA	C3C-C4C-NC	4.56	115.68	110.57
24	c	503	CLA	O2D-CGD-CBD	4.55	119.36	111.27
24	b	610	CLA	CHD-C1D-ND	-4.55	120.27	124.45
24	c	507	CLA	C3D-C4D-ND	4.55	117.60	110.24
24	d	403[B]	CLA	C3D-C4D-ND	4.55	117.59	110.24
24	a	407[B]	CLA	O2D-CGD-CBD	4.55	119.35	111.27
24	c	512	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
24	d	403[A]	CLA	C3C-C4C-NC	4.54	115.66	110.57
24	b	609	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
24	C	513	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
24	B	607	CLA	C3C-C4C-NC	4.53	115.65	110.57
24	A	407[A]	CLA	C3D-C4D-ND	4.53	117.56	110.24
26	Y	101	BCR	C16-C17-C18	-4.53	120.85	127.31
24	A	406[B]	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
24	B	601	CLA	C4A-NA-C1A	-4.52	104.67	106.71
24	c	514	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
24	d	404	CLA	C3D-C4D-ND	4.51	117.54	110.24
24	b	611	CLA	C3D-C4D-ND	4.51	117.54	110.24
24	A	407[A]	CLA	O2D-CGD-CBD	4.51	119.28	111.27
24	a	409	CLA	C3C-C4C-NC	4.51	115.62	110.57
35	M	101	LMG	O7-C10-C11	4.51	121.21	111.50
27	X	101	SQD	C1-O5-C5	-4.51	104.84	113.69
24	B	612	CLA	C3D-C4D-ND	4.50	117.52	110.24
24	a	405[B]	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
24	b	604	CLA	C1C-C2C-C3C	-4.49	102.23	106.96
24	c	502	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
24	C	511	CLA	C1-C2-C3	-4.49	118.27	126.04
24	B	609	CLA	C3C-C4C-NC	4.49	115.61	110.57
27	A	413	SQD	O8-S-C6	4.49	112.89	105.74
24	d	403[A]	CLA	C3D-C4D-ND	4.49	117.50	110.24
24	B	603	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
24	B	616	CLA	C4A-NA-C1A	-4.49	104.69	106.71
24	D	402[B]	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
24	b	615	CLA	C3D-C4D-ND	4.48	117.49	110.24
24	C	511	CLA	C3B-C4B-NB	4.48	115.00	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	612	CLA	C1-C2-C3	-4.47	118.30	126.04
24	C	511	CLA	C3D-C4D-ND	4.47	117.47	110.24
27	X	101	SQD	O8-S-C6	4.47	112.86	105.74
24	c	514	CLA	C3D-C4D-ND	4.47	117.46	110.24
24	C	513	CLA	C2C-C1C-NC	4.46	114.15	109.97
24	b	601	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
24	D	403	CLA	C3C-C4C-NC	4.46	115.57	110.57
24	c	505	CLA	C4A-NA-C1A	-4.46	104.70	106.71
24	C	503	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
24	C	507	CLA	C3D-C4D-ND	4.46	117.45	110.24
24	C	509	CLA	C3D-C2D-C1D	-4.45	99.75	105.83
24	c	503	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
24	c	502	CLA	O2D-CGD-O1D	-4.44	115.15	123.84
24	a	407[A]	CLA	O2D-CGD-CBD	4.44	119.17	111.27
24	c	502	CLA	C3D-C4D-ND	4.44	117.43	110.24
24	b	609	CLA	C1-C2-C3	-4.44	118.36	126.04
24	a	407[B]	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
24	d	404	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
24	B	601	CLA	C3C-C4C-NC	4.43	115.54	110.57
24	a	405[B]	CLA	C1D-CHD-C4C	-4.43	116.50	126.06
24	C	507	CLA	C4A-NA-C1A	-4.43	104.72	106.71
24	A	405[B]	CLA	C3D-C4D-ND	4.43	117.40	110.24
24	B	606	CLA	C3C-C4C-NC	4.42	115.53	110.57
24	B	602	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
24	C	509	CLA	C4A-NA-C1A	-4.42	104.72	106.71
24	c	504	CLA	C1D-CHD-C4C	-4.42	116.53	126.06
24	B	607	CLA	C1C-C2C-C3C	-4.42	102.31	106.96
26	K	102	BCR	C7-C8-C9	-4.42	119.56	126.23
24	A	405[B]	CLA	C1D-CHD-C4C	-4.41	116.55	126.06
24	c	505	CLA	C3B-C4B-NB	4.41	114.91	109.21
24	A	409	CLA	O2D-CGD-CBD	4.40	119.09	111.27
27	L	102	SQD	C1-O5-C5	-4.40	105.05	113.69
24	b	610	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
24	B	603	CLA	O2D-CGD-O1D	-4.40	115.24	123.84
24	a	405[A]	CLA	C1C-C2C-C3C	-4.39	102.34	106.96
24	a	406[A]	CLA	C1C-C2C-C3C	-4.39	102.34	106.96
24	c	503	CLA	CMD-C2D-C1D	4.39	132.44	124.71
24	B	610	CLA	C3C-C4C-NC	4.38	115.49	110.57
24	C	514	CLA	C3C-C4C-NC	4.38	115.49	110.57
24	A	409	CLA	C4A-NA-C1A	-4.38	104.73	106.71
24	C	504	CLA	C3C-C4C-NC	4.38	115.48	110.57
24	a	406[A]	CLA	C4A-NA-C1A	-4.38	104.74	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	601	CLA	C3D-C4D-ND	4.38	117.32	110.24
24	b	603	CLA	C3D-C4D-ND	4.38	117.32	110.24
24	a	407[B]	CLA	C2C-C1C-NC	4.37	114.07	109.97
24	A	407[A]	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
30	a	415[B]	PL9	C7-C8-C9	-4.37	119.52	126.79
24	D	402[B]	CLA	C3D-C4D-ND	4.37	117.30	110.24
24	C	509	CLA	C1-C2-C3	-4.37	118.49	126.04
24	A	406[A]	CLA	C3D-C4D-ND	4.36	117.30	110.24
33	E	101[A]	LHG	O7-C7-C8	4.36	120.90	111.50
33	E	101[B]	LHG	O7-C7-C8	4.36	120.90	111.50
24	b	608	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
24	B	612	CLA	C3D-C2D-C1D	-4.36	99.89	105.83
24	a	407[A]	CLA	C3C-C4C-NC	4.35	115.45	110.57
24	c	502	CLA	C4A-NA-C1A	-4.35	104.75	106.71
24	D	402[B]	CLA	C3C-C4C-NC	4.35	115.45	110.57
24	c	504	CLA	C3C-C4C-NC	4.35	115.45	110.57
24	b	602	CLA	C2C-C1C-NC	4.35	114.05	109.97
24	C	514	CLA	C3D-C4D-ND	4.34	117.26	110.24
24	d	403[A]	CLA	C1C-C2C-C3C	-4.34	102.39	106.96
24	C	513	CLA	C1-C2-C3	-4.34	118.54	126.04
24	C	504	CLA	C3D-C4D-ND	4.33	117.25	110.24
24	c	503	CLA	C3D-C4D-ND	4.33	117.24	110.24
33	b	628[B]	LHG	O7-C7-C8	4.33	120.83	111.50
24	C	511	CLA	C4A-NA-C1A	-4.33	104.76	106.71
39	e	101	HEM	CAD-CBD-CGD	4.32	122.91	113.60
24	b	604	CLA	C3D-C2D-C1D	-4.32	99.93	105.83
24	b	616	CLA	C1D-CHD-C4C	-4.32	116.73	126.06
24	B	613	CLA	C3B-C4B-NB	4.32	114.80	109.21
24	B	609	CLA	C3D-C4D-ND	4.32	117.23	110.24
30	A	415[B]	PL9	C32-C33-C34	-4.32	117.25	127.66
24	A	409	CLA	C1-C2-C3	-4.32	118.57	126.04
24	C	509	CLA	CHD-C1D-ND	-4.32	120.48	124.45
24	b	610	CLA	C1-C2-C3	-4.32	118.57	126.04
35	C	501	LMG	O1-C1-C2	4.32	115.04	108.30
24	B	601	CLA	C3D-C4D-ND	4.31	117.22	110.24
35	a	417	LMG	O7-C10-C11	4.31	120.80	111.50
24	C	512	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
27	a	411[A]	SQD	C1-C2-C3	-4.31	101.02	110.00
35	C	501	LMG	O7-C10-C11	4.31	120.78	111.50
24	b	612	CLA	C4-C3-C5	4.30	122.50	115.27
30	A	415[A]	PL9	C32-C33-C34	-4.30	117.31	127.66
24	b	605	CLA	C3C-C4C-NC	4.30	115.39	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	F	102	HEM	C1B-NB-C4B	4.30	109.51	105.07
24	B	615	CLA	C3D-C4D-ND	4.30	117.19	110.24
41	v	201	HEC	CBD-CAD-C3D	-4.30	105.29	112.62
24	a	409	CLA	C1C-C2C-C3C	-4.29	102.44	106.96
24	B	603	CLA	C3D-C4D-ND	4.29	117.19	110.24
24	C	502	CLA	C1D-CHD-C4C	-4.29	116.80	126.06
24	a	407[A]	CLA	C3D-C4D-ND	4.29	117.17	110.24
24	a	405[A]	CLA	C3D-C4D-ND	4.28	117.17	110.24
24	c	510	CLA	C4A-NA-C1A	-4.28	104.78	106.71
24	B	611	CLA	C1-C2-C3	-4.28	118.64	126.04
27	a	411[A]	SQD	O9-S-C6	4.27	112.01	106.94
24	a	405[A]	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
24	c	504	CLA	O2D-CGD-CBD	4.26	118.84	111.27
39	F	102	HEM	CHC-C4B-NB	4.26	129.06	124.43
24	A	405[B]	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
24	C	503	CLA	C1C-C2C-C3C	-4.26	102.48	106.96
35	Z	101	LMG	O7-C10-C11	4.25	120.67	111.50
34	b	624	HTG	C1-O5-C5	4.25	120.42	112.58
24	a	405[B]	CLA	C3B-C4B-NB	4.25	114.70	109.21
24	d	403[B]	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
24	b	616	CLA	C2C-C1C-NC	4.25	113.95	109.97
24	C	508	CLA	O2D-CGD-O1D	-4.24	115.54	123.84
24	C	513	CLA	C3D-C4D-ND	4.24	117.10	110.24
24	b	607	CLA	C3D-C4D-ND	4.24	117.10	110.24
24	B	611	CLA	C1D-CHD-C4C	-4.24	116.92	126.06
24	B	602	CLA	CMC-C2C-C1C	4.23	131.48	125.04
24	b	603	CLA	C1D-CHD-C4C	-4.23	116.93	126.06
24	c	512	CLA	C3D-C4D-ND	4.23	117.08	110.24
27	A	411[B]	SQD	C1-C2-C3	-4.23	101.19	110.00
24	a	409	CLA	C3D-C4D-ND	4.23	117.08	110.24
24	b	608	CLA	C1C-C2C-C3C	-4.22	102.52	106.96
24	d	403[A]	CLA	C3D-C2D-C1D	-4.22	100.07	105.83
24	b	612	CLA	C3D-C4D-ND	4.22	117.06	110.24
24	a	406[B]	CLA	C4A-NA-C1A	-4.22	104.81	106.71
24	b	603	CLA	C3D-C2D-C1D	-4.22	100.08	105.83
24	a	409	CLA	O2D-CGD-O1D	-4.21	115.60	123.84
32	t	101	LMT	C3'-C4'-C5'	-4.21	101.27	110.93
24	a	406[A]	CLA	C3C-C4C-NC	4.21	115.29	110.57
24	B	603	CLA	C1D-CHD-C4C	-4.21	116.98	126.06
24	D	403	CLA	C3D-C4D-ND	4.21	117.04	110.24
24	c	514	CLA	C3C-C4C-NC	4.21	115.29	110.57
26	B	617	BCR	C33-C5-C6	-4.21	119.80	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	616	CLA	C3B-C4B-NB	4.21	114.65	109.21
24	b	615	CLA	C3C-C4C-NC	4.20	115.29	110.57
24	B	605	CLA	C4-C3-C5	4.20	122.33	115.27
24	B	611	CLA	CMB-C2B-C3B	4.20	132.53	124.68
24	b	606	CLA	O2D-CGD-O1D	-4.19	115.64	123.84
24	b	609	CLA	C3D-C4D-ND	4.19	117.02	110.24
24	b	602	CLA	O2D-CGD-O1D	-4.19	115.65	123.84
24	b	614	CLA	C3C-C4C-NC	4.19	115.27	110.57
24	b	610	CLA	C3D-C4D-ND	4.18	117.01	110.24
24	A	406[B]	CLA	C3D-C4D-ND	4.18	117.01	110.24
24	d	403[B]	CLA	C3C-C4C-NC	4.18	115.26	110.57
33	A	420[A]	LHG	O8-C23-O10	-4.18	113.04	123.59
41	v	201	HEC	CMB-C2B-C1B	-4.18	122.04	128.46
24	c	507	CLA	C1-C2-C3	-4.17	118.83	126.04
24	b	614	CLA	C3D-C4D-ND	4.17	116.98	110.24
24	B	607	CLA	C3D-C4D-ND	4.17	116.98	110.24
24	C	503	CLA	C3D-C4D-ND	4.17	116.98	110.24
24	B	611	CLA	C3C-C4C-NC	4.16	115.24	110.57
24	c	512	CLA	C1D-CHD-C4C	-4.16	117.09	126.06
24	c	511	CLA	C3D-C2D-C1D	-4.15	100.16	105.83
24	b	608	CLA	C3B-C4B-NB	4.15	114.58	109.21
24	b	611	CLA	C1-C2-C3	-4.15	118.87	126.04
24	d	404	CLA	O2D-CGD-O1D	-4.15	115.73	123.84
24	b	610	CLA	C4A-NA-C1A	-4.15	104.84	106.71
35	b	629	LMG	O7-C10-C11	4.14	120.43	111.50
26	d	405	BCR	C15-C14-C13	-4.14	121.39	127.31
24	B	605	CLA	C3D-C4D-ND	4.14	116.94	110.24
24	a	405[A]	CLA	C1D-CHD-C4C	-4.14	117.12	126.06
24	B	602	CLA	CAC-C3C-C4C	4.14	130.18	124.81
24	C	502	CLA	C3D-C4D-ND	4.14	116.93	110.24
24	b	610	CLA	O2A-CGA-CBA	4.14	124.89	111.91
24	d	403[B]	CLA	O2D-CGD-CBD	4.14	118.62	111.27
30	a	415[A]	PL9	C7-C3-C4	4.13	120.24	116.88
24	B	606	CLA	O2D-CGD-O1D	-4.13	115.77	123.84
24	C	507	CLA	C1-C2-C3	-4.13	118.90	126.04
26	d	405	BCR	C40-C30-C25	-4.13	103.61	110.30
24	b	606	CLA	C3D-C4D-ND	4.13	116.91	110.24
24	c	510	CLA	C1D-CHD-C4C	-4.12	117.16	126.06
24	a	406[A]	CLA	C3D-C4D-ND	4.12	116.91	110.24
34	b	621	HTG	C1'-S1-C1	4.12	107.80	100.09
24	C	512	CLA	C4A-NA-C1A	-4.12	104.86	106.71
24	B	615	CLA	C1C-C2C-C3C	-4.12	102.63	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	513	CLA	C1D-CHD-C4C	-4.12	117.18	126.06
24	B	608	CLA	C3D-C4D-ND	4.11	116.89	110.24
24	b	604	CLA	CMC-C2C-C1C	4.11	131.30	125.04
24	B	615	CLA	C1D-CHD-C4C	-4.11	117.20	126.06
24	b	607	CLA	C4A-NA-C1A	-4.11	104.86	106.71
24	D	403	CLA	O2D-CGD-O1D	-4.11	115.81	123.84
24	b	601	CLA	C3C-C4C-NC	4.10	115.17	110.57
24	c	512	CLA	C3C-C4C-NC	4.10	115.17	110.57
24	c	502	CLA	C3C-C4C-NC	4.10	115.17	110.57
24	b	608	CLA	C3D-C4D-ND	4.10	116.86	110.24
24	d	403[A]	CLA	O2D-CGD-CBD	4.09	118.53	111.27
24	B	613	CLA	CAC-C3C-C4C	4.09	130.11	124.81
24	a	406[A]	CLA	CAA-C2A-C3A	-4.09	101.59	112.78
24	B	611	CLA	CHD-C4C-NC	4.08	130.64	124.20
24	C	509	CLA	C3B-C4B-NB	4.08	114.49	109.21
24	B	602	CLA	CHD-C1D-ND	-4.08	120.70	124.45
24	c	502	CLA	C1C-C2C-C3C	-4.08	102.67	106.96
25	A	408[A]	PHO	C1A-C2A-C3A	-4.08	98.96	102.84
24	D	402[A]	CLA	C3D-C4D-ND	4.07	116.82	110.24
25	A	417[A]	PHO	C1-C2-C3	-4.07	119.00	126.04
24	b	616	CLA	O2D-CGD-O1D	-4.07	115.89	123.84
24	D	402[A]	CLA	O2D-CGD-CBD	4.06	118.49	111.27
24	a	405[A]	CLA	CAA-C2A-C3A	-4.06	101.65	112.78
24	C	512	CLA	C3D-C4D-ND	4.06	116.81	110.24
24	a	406[A]	CLA	C1D-CHD-C4C	-4.06	117.30	126.06
24	B	613	CLA	C4A-NA-C1A	-4.06	104.88	106.71
24	a	406[B]	CLA	C3D-C4D-ND	4.06	116.80	110.24
27	A	413	SQD	O47-C7-C8	4.05	120.24	111.50
35	c	521	LMG	O7-C10-C11	4.05	120.24	111.50
24	a	409	CLA	C1D-CHD-C4C	-4.05	117.32	126.06
24	c	504	CLA	C3D-C4D-ND	4.05	116.79	110.24
24	B	614	CLA	O2D-CGD-O1D	-4.04	115.93	123.84
24	B	604	CLA	C4A-NA-C1A	-4.04	104.89	106.71
27	a	411[A]	SQD	C44-O6-C1	-4.04	105.84	113.74
24	b	602	CLA	C3D-C2D-C1D	-4.04	100.32	105.83
24	B	601	CLA	C1D-CHD-C4C	-4.04	117.34	126.06
24	b	609	CLA	O2D-CGD-CBD	4.04	118.44	111.27
24	C	507	CLA	CMC-C2C-C1C	4.04	131.19	125.04
24	d	404	CLA	C4A-NA-C1A	-4.03	104.89	106.71
24	b	601	CLA	C1D-CHD-C4C	-4.03	117.36	126.06
24	A	405[A]	CLA	C3D-C4D-ND	4.03	116.75	110.24
24	a	405[A]	CLA	C3C-C4C-NC	4.03	115.09	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	608	CLA	C4A-NA-C1A	-4.03	104.89	106.71
26	k	101	BCR	C7-C8-C9	-4.03	120.15	126.23
24	c	510	CLA	C3D-C4D-ND	4.03	116.75	110.24
30	a	415[A]	PL9	C32-C33-C34	-4.03	117.96	127.66
24	b	606	CLA	C1D-CHD-C4C	-4.02	117.38	126.06
24	B	616	CLA	C4C-C3C-C2C	-4.02	101.04	106.90
24	C	511	CLA	C1D-CHD-C4C	-4.02	117.39	126.06
24	B	606	CLA	C3D-C4D-ND	4.02	116.73	110.24
24	C	510	CLA	C3D-C4D-ND	4.02	116.73	110.24
24	B	614	CLA	C3C-C4C-NC	4.01	115.07	110.57
24	C	513	CLA	C3C-C4C-NC	4.01	115.07	110.57
24	B	602	CLA	C3D-C4D-ND	4.01	116.73	110.24
24	b	616	CLA	O2A-CGA-CBA	4.01	124.50	111.91
27	B	620	SQD	C1-O5-C5	-4.01	105.82	113.69
24	A	405[A]	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
24	B	606	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
24	B	602	CLA	C1D-CHD-C4C	-4.00	117.42	126.06
24	b	612	CLA	C3D-C2D-C1D	-4.00	100.37	105.83
24	c	513	CLA	C3D-C4D-ND	4.00	116.71	110.24
24	C	507	CLA	C3C-C4C-NC	4.00	115.06	110.57
36	C	518[A]	DGD	O2G-C1B-C2B	4.00	120.12	111.50
24	c	513	CLA	C1-C2-C3	-4.00	119.13	126.04
24	A	405[A]	CLA	C3B-C4B-NB	4.00	114.38	109.21
24	b	614	CLA	O2D-CGD-O1D	-4.00	116.02	123.84
24	b	607	CLA	O2D-CGD-CBD	4.00	118.37	111.27
24	C	509	CLA	C1C-C2C-C3C	-3.99	102.76	106.96
35	d	412	LMG	O7-C10-C11	3.99	120.11	111.50
24	c	510	CLA	C1C-C2C-C3C	-3.99	102.76	106.96
24	C	505	CLA	C3B-C4B-NB	3.99	114.37	109.21
24	C	509	CLA	C3D-C4D-ND	3.99	116.70	110.24
24	b	602	CLA	C3C-C4C-NC	3.99	115.05	110.57
24	c	514	CLA	C1D-CHD-C4C	-3.99	117.45	126.06
26	D	404	BCR	C37-C22-C23	3.98	124.34	118.08
27	B	620	SQD	C3-C4-C5	3.98	117.33	110.24
24	b	616	CLA	C3D-C4D-ND	3.97	116.67	110.24
26	A	410	BCR	C24-C23-C22	-3.97	120.24	126.23
26	b	617	BCR	C33-C5-C6	-3.97	120.07	124.53
36	C	517[A]	DGD	O2G-C1B-C2B	3.97	120.05	111.50
36	C	518[B]	DGD	O2G-C1B-C2B	3.96	120.05	111.50
24	A	407[A]	CLA	C3C-C4C-NC	3.96	115.02	110.57
35	C	521	LMG	O6-C5-C4	3.96	116.89	109.69
27	X	101	SQD	C44-O6-C1	-3.96	106.01	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	602	CLA	C1D-CHD-C4C	-3.96	117.52	126.06
27	A	411[A]	SQD	O9-S-C6	3.96	111.64	106.94
24	B	610	CLA	C1D-CHD-C4C	-3.95	117.53	126.06
24	B	602	CLA	O2D-CGD-O1D	-3.95	116.11	123.84
24	B	605	CLA	C1D-CHD-C4C	-3.95	117.53	126.06
24	A	406[A]	CLA	CMC-C2C-C1C	3.94	131.04	125.04
24	A	409	CLA	C3D-C4D-ND	3.94	116.61	110.24
24	B	608	CLA	C3B-C4B-NB	3.94	114.30	109.21
35	C	520	LMG	O7-C10-C11	3.93	119.98	111.50
35	c	521	LMG	C3-C4-C5	3.93	117.25	110.24
24	B	611	CLA	O2D-CGD-O1D	-3.93	116.15	123.84
36	c	517[B]	DGD	O2G-C1B-C2B	3.93	119.97	111.50
24	A	405[A]	CLA	C3C-C4C-NC	3.93	114.98	110.57
24	b	602	CLA	CMC-C2C-C1C	3.93	131.02	125.04
35	C	521	LMG	O7-C10-C11	3.93	119.96	111.50
24	c	505	CLA	C1-O2A-CGA	3.92	126.74	116.44
24	c	508	CLA	C3D-C4D-ND	3.92	116.58	110.24
24	C	503	CLA	C3C-C4C-NC	3.92	114.97	110.57
24	B	612	CLA	C4C-C3C-C2C	-3.92	101.19	106.90
24	B	609	CLA	C3D-C2D-C1D	-3.92	100.48	105.83
26	B	618	BCR	C29-C30-C25	3.92	116.51	110.48
24	B	606	CLA	C1D-CHD-C4C	-3.92	117.61	126.06
24	B	605	CLA	C1-C2-C3	-3.91	119.27	126.04
24	c	505	CLA	C3D-C4D-ND	3.91	116.57	110.24
24	b	613	CLA	C1C-C2C-C3C	-3.91	102.84	106.96
24	C	512	CLA	C1D-CHD-C4C	-3.90	117.64	126.06
27	A	411[B]	SQD	C44-O6-C1	-3.90	106.12	113.74
35	c	521	LMG	O6-C5-C4	3.90	116.78	109.69
24	b	616	CLA	C3C-C4C-NC	3.90	114.94	110.57
24	C	506	CLA	C1-C2-C3	-3.89	119.31	126.04
24	b	612	CLA	C3B-C4B-NB	3.89	114.24	109.21
24	A	407[A]	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
24	b	606	CLA	C3C-C4C-NC	3.89	114.93	110.57
24	C	514	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
24	d	403[B]	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
24	b	608	CLA	C3C-C4C-NC	3.88	114.92	110.57
24	c	505	CLA	C3C-C4C-NC	3.88	114.92	110.57
24	a	405[A]	CLA	O2D-CGD-CBD	3.88	118.16	111.27
24	C	510	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
24	c	511	CLA	CMC-C2C-C1C	3.87	130.93	125.04
24	A	405[B]	CLA	C3B-C4B-NB	3.87	114.21	109.21
24	A	407[B]	CLA	C3C-C4C-NC	3.86	114.90	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	608	CLA	C4A-NA-C1A	-3.86	104.97	106.71
26	d	405	BCR	C38-C26-C25	-3.85	120.20	124.53
24	c	506	CLA	C3D-C2D-C1D	-3.85	100.57	105.83
24	c	507	CLA	C3C-C4C-NC	3.85	114.89	110.57
24	c	512	CLA	C3B-C4B-NB	3.85	114.19	109.21
24	b	601	CLA	O2D-CGD-O1D	-3.85	116.31	123.84
24	A	405[B]	CLA	O2D-CGD-CBD	3.85	118.10	111.27
24	A	409	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
24	c	509	CLA	C3D-C4D-ND	3.84	116.45	110.24
24	B	612	CLA	O2D-CGD-O1D	-3.84	116.33	123.84
24	B	616	CLA	CMB-C2B-C3B	3.84	131.86	124.68
24	a	406[B]	CLA	C3C-C4C-NC	3.83	114.87	110.57
24	A	405[B]	CLA	CAA-C2A-C3A	-3.83	102.28	112.78
24	b	604	CLA	C3B-C4B-NB	3.83	114.16	109.21
30	A	415[A]	PL9	C7-C3-C4	3.83	119.99	116.88
24	A	405[A]	CLA	CAA-C2A-C3A	-3.83	102.30	112.78
24	A	406[A]	CLA	C3C-C4C-NC	3.83	114.86	110.57
24	B	604	CLA	C1D-CHD-C4C	-3.82	117.81	126.06
24	a	406[B]	CLA	C1D-CHD-C4C	-3.82	117.81	126.06
24	b	608	CLA	C1D-CHD-C4C	-3.82	117.81	126.06
24	C	506	CLA	C3D-C2D-C1D	-3.82	100.62	105.83
24	C	512	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
24	B	611	CLA	CMC-C2C-C1C	3.82	130.85	125.04
24	b	610	CLA	CAA-C2A-C3A	-3.81	102.34	112.78
25	A	417[B]	PHO	C1-C2-C3	-3.81	119.45	126.04
24	b	613	CLA	C3B-C4B-NB	3.81	114.14	109.21
30	A	415[B]	PL9	C15-C14-C16	3.81	121.68	115.27
24	B	610	CLA	C3D-C4D-ND	3.80	116.39	110.24
24	b	612	CLA	O2D-CGD-O1D	-3.80	116.41	123.84
24	C	514	CLA	C3B-C4B-NB	3.80	114.12	109.21
24	b	605	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
24	C	502	CLA	C3C-C4C-NC	3.80	114.83	110.57
24	c	503	CLA	O2D-CGD-O1D	-3.79	116.42	123.84
24	c	513	CLA	C1D-CHD-C4C	-3.79	117.87	126.06
24	A	405[A]	CLA	O2A-CGA-CBA	3.79	123.81	111.91
24	c	512	CLA	O2D-CGD-O1D	-3.79	116.42	123.84
24	c	512	CLA	C4A-NA-C1A	-3.79	105.00	106.71
35	Z	101	LMG	C1-C2-C3	3.79	117.88	110.00
24	c	508	CLA	CMC-C2C-C1C	3.79	130.81	125.04
24	b	613	CLA	C1-C2-C3	-3.78	119.50	126.04
41	V	201	HEC	CMB-C2B-C1B	-3.78	122.65	128.46
26	d	405	BCR	C29-C30-C25	3.78	116.30	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	405[B]	CLA	C3C-C4C-NC	3.78	114.81	110.57
35	C	521	LMG	C3-C4-C5	3.78	116.97	110.24
24	A	405[A]	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
36	c	518[B]	DGD	O2G-C1B-C2B	3.77	119.63	111.50
24	B	607	CLA	CMC-C2C-C1C	3.77	130.78	125.04
24	A	409	CLA	C3B-C4B-NB	3.77	114.08	109.21
24	B	612	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
24	A	407[B]	CLA	C1C-C2C-C3C	-3.77	103.00	106.96
24	b	602	CLA	CAA-C2A-C3A	-3.76	102.47	112.78
30	a	415[A]	PL9	C15-C14-C16	3.76	121.60	115.27
24	b	613	CLA	O2A-CGA-O1A	-3.76	114.10	123.59
24	b	603	CLA	CAA-C2A-C3A	-3.76	102.47	112.78
24	B	614	CLA	C3D-C4D-ND	3.76	116.32	110.24
24	D	402[A]	CLA	C1-C2-C3	-3.76	119.54	126.04
24	d	403[B]	CLA	C1D-CHD-C4C	-3.76	117.95	126.06
24	a	407[B]	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
24	b	608	CLA	CAC-C3C-C4C	3.75	129.68	124.81
24	B	607	CLA	C1D-CHD-C4C	-3.75	117.97	126.06
24	c	514	CLA	C1C-C2C-C3C	-3.75	103.02	106.96
24	A	406[A]	CLA	CBC-CAC-C3C	-3.75	102.10	112.43
27	a	413	SQD	O47-C7-C8	3.75	119.58	111.50
24	A	406[B]	CLA	CAA-C2A-C3A	-3.75	102.52	112.78
24	b	604	CLA	C3D-C4D-ND	3.74	116.29	110.24
24	B	613	CLA	C1C-C2C-C3C	-3.74	103.03	106.96
24	C	505	CLA	C3D-C4D-ND	3.74	116.28	110.24
33	d	414[A]	LHG	O8-C23-O10	-3.73	114.17	123.59
24	c	511	CLA	C3D-C4D-ND	3.73	116.28	110.24
24	c	508	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
27	A	411[B]	SQD	O47-C7-C8	3.73	119.54	111.50
24	B	614	CLA	C1D-CHD-C4C	-3.73	118.01	126.06
24	b	612	CLA	CAC-C3C-C4C	3.73	129.65	124.81
24	c	509	CLA	C1-C2-C3	-3.73	119.60	126.04
24	B	604	CLA	C3B-C4B-NB	3.73	114.03	109.21
24	D	403	CLA	CAC-C3C-C4C	3.72	129.64	124.81
24	D	403	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
24	c	506	CLA	O2D-CGD-O1D	-3.72	116.56	123.84
32	B	628	LMT	O1'-C1'-C2'	3.72	114.11	108.30
24	B	608	CLA	CMA-C3A-C4A	-3.72	101.78	111.77
24	B	615	CLA	CMC-C2C-C1C	3.72	130.70	125.04
24	b	611	CLA	C3B-C4B-NB	3.72	114.02	109.21
24	A	405[A]	CLA	O2D-CGD-CBD	3.72	117.88	111.27
24	B	613	CLA	C3D-C4D-ND	3.72	116.25	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	604	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
24	B	616	CLA	C3D-C4D-ND	3.71	116.25	110.24
24	D	402[A]	CLA	C3B-C4B-NB	3.71	114.01	109.21
33	L	101[A]	LHG	O7-C7-C8	3.71	119.50	111.50
24	C	512	CLA	O2D-CGD-O1D	-3.71	116.58	123.84
30	a	415[A]	PL9	C7-C3-C2	-3.71	118.42	123.30
24	b	609	CLA	C1D-CHD-C4C	-3.71	118.06	126.06
24	B	615	CLA	O2D-CGD-CBD	3.71	117.85	111.27
24	a	407[B]	CLA	C3C-C4C-NC	3.70	114.72	110.57
24	B	613	CLA	O2A-CGA-O1A	-3.70	114.25	123.59
24	c	510	CLA	C3B-C4B-NB	3.70	114.00	109.21
33	L	101[B]	LHG	O7-C7-C8	3.70	119.48	111.50
24	a	405[B]	CLA	C1C-C2C-C3C	-3.70	103.06	106.96
24	C	507	CLA	O2D-CGD-O1D	-3.70	116.60	123.84
24	c	507	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
24	C	504	CLA	C1D-CHD-C4C	-3.70	118.08	126.06
24	A	405[B]	CLA	C1C-C2C-C3C	-3.69	103.07	106.96
24	b	604	CLA	CAC-C3C-C4C	3.69	129.60	124.81
24	b	615	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
24	C	508	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
24	B	610	CLA	O2A-CGA-O1A	-3.68	114.29	123.59
24	B	605	CLA	O2D-CGD-O1D	-3.68	116.64	123.84
24	c	506	CLA	CAC-C3C-C4C	3.68	129.59	124.81
24	d	404	CLA	C3C-C4C-NC	3.68	114.70	110.57
41	V	201	HEC	C1D-C2D-C3D	-3.68	104.44	107.00
24	A	406[B]	CLA	C1D-CHD-C4C	-3.68	118.12	126.06
26	C	516	BCR	C7-C8-C9	-3.68	120.68	126.23
24	d	404	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
24	c	503	CLA	C1D-CHD-C4C	-3.68	118.13	126.06
24	B	616	CLA	O2D-CGD-O1D	-3.68	116.65	123.84
27	A	411[A]	SQD	C44-O6-C1	-3.67	106.57	113.74
24	B	607	CLA	CBC-CAC-C3C	-3.67	102.31	112.43
30	a	415[A]	PL9	C30-C29-C31	3.67	121.44	115.27
30	D	405[A]	PL9	C42-C43-C44	-3.67	118.83	127.66
24	a	405[A]	CLA	CMB-C2B-C3B	3.67	131.54	124.68
24	B	603	CLA	C3B-C4B-NB	3.67	113.95	109.21
24	c	511	CLA	C1D-CHD-C4C	-3.66	118.16	126.06
24	B	609	CLA	O2D-CGD-CBD	3.66	117.78	111.27
24	D	402[A]	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
24	b	613	CLA	C1D-CHD-C4C	-3.66	118.16	126.06
39	e	101	HEM	C1B-NB-C4B	3.66	108.85	105.07
30	A	415[A]	PL9	C15-C14-C16	3.65	121.41	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	v	201	HEC	CMC-C2C-C1C	-3.65	122.86	128.46
24	c	506	CLA	C4C-C3C-C2C	-3.65	101.58	106.90
24	C	507	CLA	C3B-C4B-NB	3.65	113.93	109.21
24	b	614	CLA	C1D-CHD-C4C	-3.65	118.19	126.06
24	B	611	CLA	CHB-C4A-NA	3.64	129.55	124.51
24	B	604	CLA	C3D-C4D-ND	3.64	116.13	110.24
24	c	503	CLA	C3C-C4C-NC	3.64	114.66	110.57
24	B	614	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
24	B	609	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
24	a	407[A]	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
24	b	610	CLA	C1D-CHD-C4C	-3.64	118.20	126.06
24	C	503	CLA	C1-C2-C3	-3.64	119.75	126.04
36	c	517[A]	DGD	O2G-C1B-C2B	3.64	119.34	111.50
24	B	611	CLA	C4C-C3C-C2C	-3.64	101.59	106.90
24	b	609	CLA	CAC-C3C-C4C	3.64	129.53	124.81
24	C	502	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
24	B	602	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
24	a	407[A]	CLA	C1D-CHD-C4C	-3.63	118.23	126.06
24	B	604	CLA	C3D-C2D-C1D	-3.63	100.88	105.83
24	b	613	CLA	O2D-CGD-CBD	3.62	117.71	111.27
24	A	409	CLA	C4C-C3C-C2C	-3.62	101.62	106.90
24	b	604	CLA	O2D-CGD-O1D	-3.62	116.76	123.84
24	a	405[A]	CLA	O2A-CGA-O1A	-3.62	114.47	123.59
26	T	101	BCR	C15-C16-C17	-3.61	116.07	123.47
24	A	407[B]	CLA	C1D-CHD-C4C	-3.61	118.26	126.06
35	C	520	LMG	O8-C28-C29	3.61	123.24	111.91
30	a	415[B]	PL9	C15-C14-C16	3.61	121.34	115.27
35	a	417	LMG	C7-O1-C1	-3.61	106.69	113.74
26	D	404	BCR	C38-C26-C25	-3.61	120.48	124.53
24	B	603	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
24	b	606	CLA	C4-C3-C5	3.61	121.34	115.27
24	c	509	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
33	d	414[A]	LHG	O8-C23-C24	3.60	123.21	111.91
30	a	415[B]	PL9	C32-C33-C34	-3.60	118.99	127.66
24	A	406[B]	CLA	O2D-CGD-O1D	-3.60	116.80	123.84
24	b	608	CLA	C1-C2-C3	-3.60	119.82	126.04
24	d	403[B]	CLA	C3B-C4B-NB	3.59	113.86	109.21
35	a	417	LMG	C8-O7-C10	-3.59	108.95	117.79
30	d	406[A]	PL9	C42-C43-C44	-3.59	119.02	127.66
24	c	511	CLA	C1C-C2C-C3C	-3.59	103.19	106.96
24	a	406[B]	CLA	CAA-C2A-C3A	-3.58	102.97	112.78
24	c	505	CLA	C1D-CHD-C4C	-3.58	118.33	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	615	CLA	O2D-CGD-CBD	3.58	117.63	111.27
30	A	415[A]	PL9	C22-C23-C24	-3.57	119.05	127.66
26	h	101	BCR	C38-C26-C25	-3.57	120.52	124.53
24	b	611	CLA	O2D-CGD-O1D	-3.57	116.85	123.84
30	d	406[A]	PL9	C40-C39-C41	3.57	121.28	115.27
36	c	518[A]	DGD	O2G-C1B-C2B	3.57	119.19	111.50
24	b	609	CLA	C3B-C4B-NB	3.56	113.82	109.21
24	C	504	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
24	A	406[A]	CLA	C1D-CHD-C4C	-3.56	118.38	126.06
24	a	405[B]	CLA	C1-C2-C3	-3.56	119.89	126.04
24	c	514	CLA	C3B-C4B-NB	3.56	113.81	109.21
24	c	509	CLA	C1D-CHD-C4C	-3.56	118.38	126.06
27	A	411[A]	SQD	O47-C7-C8	3.55	119.16	111.50
24	C	514	CLA	C1D-CHD-C4C	-3.55	118.39	126.06
24	c	507	CLA	O2D-CGD-O1D	-3.55	116.90	123.84
30	A	415[A]	PL9	C7-C3-C2	-3.55	118.63	123.30
24	b	603	CLA	C3B-C4B-NB	3.55	113.80	109.21
24	b	608	CLA	CMC-C2C-C1C	3.55	130.44	125.04
24	b	605	CLA	O2A-CGA-O1A	-3.54	114.65	123.59
24	B	610	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
35	c	520	LMG	O7-C10-C11	3.54	119.13	111.50
24	C	511	CLA	CHD-C4C-NC	3.54	129.78	124.20
24	B	608	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
24	C	506	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
24	b	611	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
24	A	407[A]	CLA	C1D-CHD-C4C	-3.54	118.42	126.06
24	C	504	CLA	O2A-CGA-O1A	-3.54	114.67	123.59
33	A	420[B]	LHG	O7-C7-C8	3.54	119.12	111.50
24	D	402[B]	CLA	C1C-C2C-C3C	-3.53	103.24	106.96
24	C	508	CLA	C1D-CHD-C4C	-3.53	118.44	126.06
24	C	502	CLA	C1-C2-C3	-3.53	119.94	126.04
24	A	406[A]	CLA	CAA-C2A-C3A	-3.52	103.13	112.78
24	b	610	CLA	C4C-C3C-C2C	-3.52	101.76	106.90
26	c	515	BCR	C15-C14-C13	-3.52	122.28	127.31
25	d	402[B]	PHO	C4-C3-C5	3.52	121.19	115.27
24	B	614	CLA	C1-C2-C3	-3.52	119.96	126.04
30	D	405[B]	PL9	C25-C24-C26	3.52	121.19	115.27
24	C	509	CLA	C1D-CHD-C4C	-3.52	118.47	126.06
24	B	605	CLA	C1C-C2C-C3C	-3.52	103.26	106.96
24	c	504	CLA	O2D-CGD-O1D	-3.52	116.96	123.84
24	B	616	CLA	C1D-CHD-C4C	-3.52	118.47	126.06
24	B	607	CLA	O2D-CGD-O1D	-3.52	116.97	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	409	CLA	CAA-C2A-C3A	-3.51	103.16	112.78
24	B	610	CLA	O2D-CGD-O1D	-3.51	116.97	123.84
25	A	408[B]	PHO	C1A-C2A-C3A	-3.51	99.50	102.84
24	C	508	CLA	C3D-C4D-ND	3.51	115.91	110.24
24	b	613	CLA	O2A-CGA-CBA	3.51	122.92	111.91
24	b	607	CLA	C3B-C4B-NB	3.51	113.74	109.21
39	F	102	HEM	CBD-CAD-C3D	-3.50	102.90	112.63
24	d	403[A]	CLA	C3B-C4B-NB	3.50	113.73	109.21
24	A	405[B]	CLA	C3C-C4C-NC	3.50	114.50	110.57
33	A	420[A]	LHG	O7-C7-C8	3.50	119.04	111.50
24	b	612	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
36	C	517[B]	DGD	O2G-C1B-C2B	3.50	119.04	111.50
24	C	513	CLA	C4-C3-C5	3.49	121.15	115.27
24	B	614	CLA	C3B-C4B-NB	3.49	113.73	109.21
24	C	509	CLA	O2D-CGD-O1D	-3.49	117.01	123.84
24	b	612	CLA	CMB-C2B-C3B	3.49	131.21	124.68
35	b	629	LMG	C7-O1-C1	-3.48	106.93	113.74
24	d	403[B]	CLA	C1-C2-C3	-3.48	120.02	126.04
24	b	606	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
24	d	403[A]	CLA	O2A-CGA-CBA	3.48	122.83	111.91
24	B	608	CLA	C1D-CHD-C4C	-3.48	118.56	126.06
24	b	612	CLA	C1D-CHD-C4C	-3.47	118.56	126.06
41	v	201	HEC	C1D-C2D-C3D	-3.47	104.58	107.00
24	b	603	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
24	b	614	CLA	C1-C2-C3	-3.47	120.05	126.04
39	F	102	HEM	CHB-C1B-NB	3.47	128.66	124.38
25	A	417[A]	PHO	C1A-C2A-C3A	-3.46	99.54	102.84
24	B	602	CLA	C3B-C4B-NB	3.46	113.69	109.21
30	d	406[A]	PL9	C37-C38-C39	-3.46	119.33	127.66
34	V	202	HTG	C1-O5-C5	3.46	116.88	112.19
24	c	511	CLA	CAC-C3C-C4C	3.46	129.30	124.81
24	b	609	CLA	C4C-C3C-C2C	-3.46	101.86	106.90
24	A	409	CLA	O2D-CGD-O1D	-3.46	117.08	123.84
24	c	507	CLA	C3B-C4B-NB	3.45	113.67	109.21
33	D	407[B]	LHG	O7-C7-C8	3.45	118.94	111.50
24	c	513	CLA	C3C-C4C-NC	3.45	114.44	110.57
24	A	405[A]	CLA	O2A-CGA-O1A	-3.45	114.89	123.59
25	a	408[B]	PHO	C1A-C2A-C3A	-3.45	99.56	102.84
34	b	624	HTG	O5-C5-C4	3.45	115.95	109.69
24	B	615	CLA	C4-C3-C5	3.45	121.07	115.27
24	B	605	CLA	CHD-C4C-NC	3.44	129.63	124.20
24	c	502	CLA	C1-C2-C3	-3.44	120.09	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	605	CLA	C1D-CHD-C4C	-3.44	118.64	126.06
24	C	507	CLA	C1D-CHD-C4C	-3.44	118.64	126.06
24	a	405[B]	CLA	CHC-C1C-C2C	-3.44	117.20	126.72
24	b	604	CLA	C1D-CHD-C4C	-3.44	118.64	126.06
24	b	610	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
24	b	612	CLA	C4C-C3C-C2C	-3.44	101.89	106.90
24	c	507	CLA	C1D-CHD-C4C	-3.44	118.65	126.06
24	B	610	CLA	C3B-C4B-NB	3.44	113.65	109.21
24	a	406[A]	CLA	C3B-C4B-NB	3.43	113.65	109.21
24	b	607	CLA	C1D-CHD-C4C	-3.43	118.66	126.06
30	d	406[B]	PL9	C10-C9-C11	3.43	121.04	115.27
24	c	510	CLA	CAC-C3C-C4C	3.43	129.26	124.81
25	a	408[A]	PHO	C1A-C2A-C3A	-3.43	99.58	102.84
24	c	513	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
26	Y	101	BCR	C15-C14-C13	-3.42	122.43	127.31
33	d	408[A]	LHG	O7-C7-C8	3.42	118.86	111.50
24	B	615	CLA	CHD-C4C-NC	3.42	129.59	124.20
26	t	102	BCR	C28-C27-C26	-3.42	107.98	114.08
24	a	406[A]	CLA	CHD-C4C-NC	3.41	129.58	124.20
24	B	603	CLA	CAA-C2A-C3A	-3.41	103.43	112.78
24	C	506	CLA	C4-C3-C5	3.41	121.01	115.27
24	A	406[B]	CLA	C3C-C4C-NC	3.41	114.40	110.57
24	B	609	CLA	C3B-C4B-NB	3.41	113.62	109.21
24	C	510	CLA	C1D-CHD-C4C	-3.41	118.70	126.06
24	a	405[B]	CLA	CAA-C2A-C3A	-3.41	103.44	112.78
24	C	511	CLA	C3C-C4C-NC	3.41	114.39	110.57
24	b	610	CLA	O2A-CGA-O1A	-3.41	114.99	123.59
27	B	620	SQD	O7-S-C6	3.41	110.99	106.94
25	a	408[A]	PHO	O1D-CGD-CBD	-3.41	119.07	124.74
24	C	510	CLA	CMC-C2C-C1C	3.40	130.22	125.04
30	A	415[B]	PL9	C27-C28-C29	-3.40	119.47	127.66
25	A	417[B]	PHO	C1A-C2A-C3A	-3.40	99.61	102.84
24	B	607	CLA	C3B-C4B-NB	3.40	113.60	109.21
24	A	405[B]	CLA	C1-C2-C3	-3.40	120.17	126.04
24	b	615	CLA	C1D-CHD-C4C	-3.39	118.74	126.06
24	a	405[B]	CLA	O2D-CGD-CBD	3.39	117.30	111.27
34	b	621	HTG	O5-C5-C4	3.39	115.85	109.69
24	A	407[B]	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
41	V	201	HEC	CBA-CAA-C2A	-3.39	106.89	112.60
30	A	415[B]	PL9	C22-C23-C24	-3.39	119.50	127.66
24	a	409	CLA	C4-C3-C5	3.39	120.97	115.27
24	B	611	CLA	C2A-C1A-CHA	-3.39	117.94	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	607	CLA	C4-C3-C5	3.39	120.97	115.27
27	a	413	SQD	O48-C23-C24	3.38	122.53	111.91
35	Z	101	LMG	O6-C1-C2	3.38	117.51	110.35
32	B	627	LMT	C1'-O5'-C5'	-3.38	107.05	113.69
24	c	514	CLA	CAC-C3C-C4C	3.38	129.20	124.81
24	c	508	CLA	C1D-CHD-C4C	-3.38	118.77	126.06
24	b	612	CLA	CMC-C2C-C1C	3.38	130.19	125.04
24	c	509	CLA	C4C-C3C-C2C	-3.38	101.97	106.90
24	a	406[B]	CLA	C3B-C4B-NB	3.38	113.58	109.21
24	C	506	CLA	C1D-CHD-C4C	-3.38	118.77	126.06
30	d	406[B]	PL9	C37-C38-C39	-3.38	119.53	127.66
24	a	405[A]	CLA	C3B-C4B-NB	3.38	113.58	109.21
30	a	415[A]	PL9	C27-C28-C29	-3.38	119.53	127.66
24	B	609	CLA	C1D-CHD-C4C	-3.37	118.78	126.06
26	H	101	BCR	C16-C17-C18	-3.37	122.49	127.31
30	A	415[A]	PL9	C37-C38-C39	-3.37	119.54	127.66
24	C	512	CLA	C3B-C4B-NB	3.37	113.57	109.21
30	A	415[B]	PL9	C37-C38-C39	-3.37	119.55	127.66
24	b	616	CLA	O2A-CGA-O1A	-3.37	115.09	123.59
24	A	407[A]	CLA	C3B-C4B-NB	3.37	113.56	109.21
24	B	610	CLA	C4C-C3C-C2C	-3.37	101.99	106.90
24	b	603	CLA	C4C-C3C-C2C	-3.36	101.99	106.90
30	A	415[A]	PL9	C27-C28-C29	-3.36	119.56	127.66
24	D	403	CLA	CMC-C2C-C1C	3.36	130.16	125.04
33	d	408[B]	LHG	O7-C7-C8	3.36	118.74	111.50
24	a	405[A]	CLA	O2A-CGA-CBA	3.36	122.45	111.91
35	z	101	LMG	O7-C10-C11	3.36	118.73	111.50
24	D	402[A]	CLA	C4C-C3C-C2C	-3.35	102.01	106.90
24	A	405[A]	CLA	CAC-C3C-C4C	3.35	129.15	124.81
33	b	628[A]	LHG	O7-C7-C8	3.35	118.72	111.50
25	d	402[A]	PHO	C4-C3-C5	3.35	120.90	115.27
24	c	505	CLA	C1C-C2C-C3C	-3.35	103.44	106.96
30	a	415[B]	PL9	C27-C28-C29	-3.34	119.61	127.66
26	k	101	BCR	C24-C23-C22	-3.34	121.19	126.23
24	d	403[A]	CLA	C4-C3-C5	3.34	120.89	115.27
27	L	102	SQD	C3-C4-C5	3.34	116.19	110.24
24	B	601	CLA	C4C-C3C-C2C	-3.33	102.04	106.90
24	a	405[A]	CLA	C1-C2-C3	-3.33	120.28	126.04
24	A	405[A]	CLA	CAA-C2A-C1A	-3.33	101.05	111.97
24	B	614	CLA	CAC-C3C-C4C	3.33	129.13	124.81
24	C	504	CLA	C4-C3-C5	3.33	120.87	115.27
24	B	616	CLA	C1C-C2C-C3C	-3.33	103.46	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	608	CLA	CAC-C3C-C4C	3.32	129.12	124.81
24	D	402[B]	CLA	C1D-CHD-C4C	-3.32	118.89	126.06
24	B	604	CLA	CHD-C1D-ND	-3.32	121.40	124.45
24	a	405[A]	CLA	CAA-C2A-C1A	-3.32	101.10	111.97
24	c	506	CLA	C1D-CHD-C4C	-3.32	118.90	126.06
24	A	406[B]	CLA	C4-C3-C5	3.32	120.85	115.27
24	B	614	CLA	CMB-C2B-C3B	3.31	130.88	124.68
24	c	503	CLA	C3B-C4B-NB	3.31	113.49	109.21
24	B	602	CLA	CAA-C2A-C3A	-3.31	103.71	112.78
26	h	101	BCR	C16-C17-C18	-3.31	122.58	127.31
39	e	101	HEM	CHA-C4D-ND	3.31	128.47	124.38
24	C	511	CLA	C4-C3-C5	3.31	120.84	115.27
24	a	405[B]	CLA	O2A-CGA-CBA	3.31	122.29	111.91
35	c	521	LMG	C9-C8-C7	-3.30	103.97	111.79
33	A	420[A]	LHG	O8-C23-C24	3.30	122.28	111.91
36	C	519	DGD	O1G-C1A-C2A	3.30	122.28	111.91
24	c	505	CLA	C4C-C3C-C2C	-3.30	102.08	106.90
24	C	503	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
30	a	415[A]	PL9	C37-C38-C39	-3.30	119.71	127.66
27	L	102	SQD	O8-S-C6	3.30	111.00	105.74
24	c	504	CLA	C1C-C2C-C3C	-3.30	103.49	106.96
24	a	407[B]	CLA	C1-C2-C3	-3.30	120.34	126.04
24	d	403[A]	CLA	C1D-CHD-C4C	-3.29	118.95	126.06
24	b	614	CLA	O2A-CGA-O1A	-3.29	115.28	123.59
34	b	621	HTG	O2-C2-C1	3.29	116.32	110.27
30	D	405[A]	PL9	C25-C24-C26	3.29	120.81	115.27
24	A	405[A]	CLA	CMB-C2B-C3B	3.29	130.84	124.68
24	c	510	CLA	C4-C3-C5	3.29	120.81	115.27
30	d	406[B]	PL9	C42-C43-C44	-3.29	119.74	127.66
24	C	505	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
24	C	514	CLA	CMC-C2C-C1C	3.29	130.05	125.04
24	b	603	CLA	C1C-C2C-C3C	-3.29	103.50	106.96
24	C	504	CLA	C4C-C3C-C2C	-3.28	102.11	106.90
24	A	407[A]	CLA	CAA-C2A-C3A	-3.28	103.78	112.78
24	c	511	CLA	C3B-C4B-NB	3.28	113.45	109.21
34	B	621	HTG	C1'-S1-C1	3.28	106.23	100.09
24	C	502	CLA	CMC-C2C-C1C	3.28	130.04	125.04
24	B	612	CLA	CAC-C3C-C4C	3.28	129.06	124.81
24	D	403	CLA	C4C-C3C-C2C	-3.28	102.12	106.90
24	a	405[A]	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
24	b	612	CLA	O2A-CGA-O1A	-3.28	115.33	123.59
24	c	511	CLA	C4-C3-C5	3.27	120.78	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	405[B]	PL9	C53-C6-C1	3.27	121.68	114.99
24	A	406[B]	CLA	CBC-CAC-C3C	-3.27	103.42	112.43
24	C	506	CLA	C4C-C3C-C2C	-3.27	102.14	106.90
24	C	509	CLA	C4C-C3C-C2C	-3.27	102.14	106.90
24	B	610	CLA	CAA-C2A-C3A	-3.26	103.84	112.78
30	D	405[B]	PL9	C10-C9-C11	3.26	120.76	115.27
33	d	414[B]	LHG	O7-C7-C8	3.26	118.53	111.50
24	b	608	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
24	b	607	CLA	C4-C3-C5	3.26	120.75	115.27
24	d	404	CLA	C3B-C4B-NB	3.26	113.42	109.21
30	d	406[B]	PL9	C7-C8-C9	-3.26	121.37	126.79
24	c	512	CLA	C4C-C3C-C2C	-3.25	102.15	106.90
24	C	502	CLA	CBC-CAC-C3C	-3.25	103.46	112.43
26	c	516	BCR	C32-C1-C6	-3.25	105.02	110.30
32	b	626	LMT	C3'-C4'-C5'	-3.25	103.47	110.93
24	B	603	CLA	CMB-C2B-C3B	3.25	130.76	124.68
24	b	614	CLA	CAC-C3C-C4C	3.25	129.03	124.81
24	a	407[B]	CLA	C1D-CHD-C4C	-3.25	119.05	126.06
24	B	615	CLA	C3B-C4B-NB	3.25	113.41	109.21
24	c	512	CLA	C1-C2-C3	-3.25	120.42	126.04
24	c	503	CLA	CHC-C1C-C2C	-3.25	117.74	126.72
36	h	102	DGD	O2G-C1B-C2B	3.25	118.50	111.50
24	d	403[A]	CLA	C1-C2-C3	-3.24	120.43	126.04
24	b	614	CLA	C3B-C4B-NB	3.24	113.40	109.21
24	b	616	CLA	CHD-C4C-NC	3.24	129.31	124.20
34	B	621	HTG	O5-C1-C2	3.24	114.39	110.31
24	b	612	CLA	C2A-C1A-CHA	-3.24	118.19	123.86
26	C	516	BCR	C11-C10-C9	-3.24	122.69	127.31
35	C	521	LMG	O8-C28-C29	3.24	122.07	111.91
24	b	613	CLA	C3D-C4D-ND	3.24	115.47	110.24
30	A	415[B]	PL9	C20-C19-C21	3.23	120.71	115.27
24	b	611	CLA	C1D-CHD-C4C	-3.23	119.09	126.06
24	C	505	CLA	CMC-C2C-C1C	3.23	129.96	125.04
24	b	611	CLA	CAC-C3C-C4C	3.23	129.00	124.81
24	A	407[A]	CLA	O2A-CGA-O1A	-3.23	115.45	123.59
24	B	601	CLA	C1C-C2C-C3C	-3.23	103.56	106.96
24	C	510	CLA	C3B-C4B-NB	3.23	113.38	109.21
24	c	513	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
24	A	409	CLA	C1D-CHD-C4C	-3.22	119.10	126.06
24	A	405[B]	CLA	O2A-CGA-CBA	3.22	122.02	111.91
24	C	508	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
27	a	411[B]	SQD	C1-C2-C3	-3.22	103.29	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	405	BCR	C10-C11-C12	-3.22	113.17	123.22
24	A	405[B]	CLA	CHC-C1C-C2C	-3.22	117.82	126.72
24	B	612	CLA	C3B-C4B-NB	3.22	113.37	109.21
24	a	407[A]	CLA	C3B-C4B-NB	3.22	113.37	109.21
27	a	411[A]	SQD	C45-O47-C7	-3.21	109.88	117.79
27	f	101	SQD	O7-S-C6	3.21	110.75	106.94
30	a	415[A]	PL9	C17-C18-C19	-3.21	119.94	127.66
24	C	513	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
25	a	408[A]	PHO	O2A-CGA-O1A	-3.20	115.51	123.59
30	a	415[A]	PL9	C25-C24-C26	3.20	120.65	115.27
24	b	610	CLA	CMC-C2C-C1C	3.20	129.91	125.04
24	d	404	CLA	CAC-C3C-C4C	3.20	128.96	124.81
30	D	405[A]	PL9	C17-C18-C19	-3.20	119.96	127.66
24	c	508	CLA	C4-C3-C5	3.20	120.65	115.27
30	a	415[B]	PL9	C37-C38-C39	-3.20	119.97	127.66
30	a	415[B]	PL9	C25-C24-C26	3.19	120.64	115.27
39	F	102	HEM	CHA-C4D-ND	3.19	128.33	124.38
24	b	601	CLA	C4C-C3C-C2C	-3.19	102.24	106.90
24	b	611	CLA	C2A-C1A-CHA	-3.19	118.28	123.86
25	A	417[A]	PHO	C4-C3-C5	3.19	120.64	115.27
30	a	415[B]	PL9	C30-C29-C31	3.19	120.64	115.27
24	d	404	CLA	C4-C3-C5	3.19	120.64	115.27
24	C	503	CLA	C3B-C4B-NB	3.19	113.33	109.21
24	b	615	CLA	C3B-C4B-NB	3.19	113.33	109.21
26	k	101	BCR	C29-C30-C25	3.19	115.39	110.48
24	b	605	CLA	CHD-C4C-NC	3.19	129.22	124.20
26	A	410	BCR	C33-C5-C6	-3.19	120.95	124.53
24	B	613	CLA	O2A-CGA-CBA	3.18	121.90	111.91
24	d	403[B]	CLA	O2A-CGA-CBA	3.18	121.90	111.91
24	A	407[B]	CLA	O2A-CGA-O1A	-3.18	115.56	123.59
24	c	512	CLA	C4-C3-C5	3.18	120.62	115.27
24	B	609	CLA	CBC-CAC-C3C	-3.18	103.66	112.43
24	C	502	CLA	C3B-C4B-NB	3.18	113.32	109.21
24	b	601	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
24	A	406[A]	CLA	C3B-C4B-NB	3.18	113.32	109.21
24	d	403[A]	CLA	O2A-CGA-O1A	-3.18	115.57	123.59
24	c	507	CLA	CAC-C3C-C4C	3.18	128.93	124.81
24	B	613	CLA	C4-C3-C5	3.18	120.61	115.27
27	A	411[B]	SQD	O9-S-C6	3.17	110.71	106.94
26	D	404	BCR	C28-C27-C26	-3.17	108.41	114.08
26	C	515	BCR	C7-C8-C9	-3.17	121.44	126.23
24	b	601	CLA	C4-C3-C5	3.17	120.60	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	617	BCR	C29-C30-C25	3.17	115.36	110.48
24	B	602	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
26	D	404	BCR	C10-C11-C12	-3.17	113.33	123.22
34	b	621	HTG	O5-C1-C2	3.17	114.30	110.31
24	c	513	CLA	O2A-CGA-CBA	3.17	121.85	111.91
24	b	614	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
24	B	608	CLA	C4C-C3C-C2C	-3.16	102.29	106.90
26	H	101	BCR	C11-C10-C9	-3.16	122.80	127.31
26	b	618	BCR	C15-C14-C13	-3.16	122.80	127.31
27	B	620	SQD	O48-C23-C24	3.16	121.83	111.91
24	b	602	CLA	C1C-C2C-C3C	-3.16	103.63	106.96
24	b	610	CLA	CAA-CBA-CGA	-3.16	104.02	113.25
24	B	608	CLA	CMB-C2B-C3B	3.16	130.59	124.68
25	A	408[B]	PHO	C1-C2-C3	-3.16	120.58	126.04
24	B	610	CLA	CHD-C4C-NC	3.16	129.18	124.20
24	D	402[B]	CLA	C1-C2-C3	-3.16	120.58	126.04
24	B	613	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
24	B	613	CLA	C4C-C3C-C2C	-3.15	102.30	106.90
24	c	503	CLA	CMC-C2C-C1C	3.15	129.84	125.04
26	c	515	BCR	C11-C10-C9	-3.15	122.81	127.31
24	c	510	CLA	C1-O2A-CGA	3.15	124.71	116.44
24	b	611	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
24	c	512	CLA	CHD-C4C-NC	3.15	129.17	124.20
24	C	507	CLA	CBC-CAC-C3C	-3.15	103.75	112.43
24	a	405[A]	CLA	C4-C3-C5	3.15	120.57	115.27
24	A	406[B]	CLA	CHD-C4C-NC	3.15	129.16	124.20
24	C	512	CLA	C4-C3-C5	3.15	120.56	115.27
26	b	619	BCR	C11-C10-C9	-3.15	122.82	127.31
24	C	506	CLA	CAC-C3C-C4C	3.15	128.89	124.81
24	d	404	CLA	C1D-CHD-C4C	-3.15	119.27	126.06
30	a	415[B]	PL9	C42-C43-C44	-3.14	120.09	127.66
24	C	506	CLA	O2A-CGA-O1A	-3.14	115.66	123.59
24	B	603	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
26	c	515	BCR	C16-C17-C18	-3.14	122.82	127.31
32	A	418	LMT	O5B-C5B-C4B	3.14	115.40	109.69
24	c	502	CLA	C3B-C4B-NB	3.14	113.27	109.21
24	A	405[B]	CLA	CAC-C3C-C4C	3.14	128.89	124.81
24	C	503	CLA	C1D-CHD-C4C	-3.14	119.28	126.06
24	C	505	CLA	C1D-CHD-C4C	-3.14	119.29	126.06
24	B	612	CLA	CMB-C2B-C3B	3.14	130.55	124.68
26	h	101	BCR	C7-C8-C9	-3.14	121.50	126.23
24	B	614	CLA	O2A-CGA-O1A	-3.13	115.68	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	409	CLA	CHD-C4C-NC	3.13	129.14	124.20
24	B	605	CLA	C4C-C3C-C2C	-3.13	102.33	106.90
24	d	403[B]	CLA	C4-C3-C5	3.13	120.54	115.27
24	C	514	CLA	C1-C2-C3	-3.13	120.63	126.04
24	A	405[A]	CLA	C1-C2-C3	-3.13	120.63	126.04
24	c	512	CLA	C1C-C2C-C3C	-3.12	103.67	106.96
27	X	101	SQD	C1-C2-C3	-3.12	103.49	110.00
26	A	410	BCR	C11-C10-C9	-3.12	122.85	127.31
24	b	601	CLA	CHD-C4C-NC	3.12	129.12	124.20
24	A	406[A]	CLA	CAC-C3C-C4C	3.12	128.86	124.81
24	B	606	CLA	C3B-C4B-NB	3.12	113.24	109.21
24	A	406[B]	CLA	C3B-C4B-NB	3.12	113.24	109.21
24	a	407[A]	CLA	CHD-C4C-NC	3.12	129.12	124.20
24	B	611	CLA	C3B-C4B-NB	3.12	113.24	109.21
24	B	609	CLA	O2D-CGD-O1D	-3.12	117.75	123.84
24	b	605	CLA	C4-C3-C5	3.12	120.51	115.27
41	V	201	HEC	CMC-C2C-C1C	-3.11	123.68	128.46
24	c	506	CLA	C1C-C2C-C3C	-3.11	103.68	106.96
24	b	606	CLA	C3B-C4B-NB	3.11	113.23	109.21
24	c	510	CLA	C4C-C3C-C2C	-3.11	102.36	106.90
24	B	609	CLA	CHC-C1C-C2C	-3.11	118.11	126.72
24	B	608	CLA	CHC-C1C-C2C	-3.11	118.11	126.72
24	C	513	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
24	B	610	CLA	CAA-CBA-CGA	-3.11	104.17	113.25
24	c	509	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
24	a	407[B]	CLA	CHD-C4C-NC	3.11	129.10	124.20
24	D	402[A]	CLA	C1D-CHD-C4C	-3.11	119.36	126.06
24	D	403	CLA	C1C-C2C-C3C	-3.11	103.69	106.96
24	C	504	CLA	O2D-CGD-O1D	-3.11	117.77	123.84
30	a	415[A]	PL9	C35-C34-C36	3.10	120.49	115.27
33	D	407[A]	LHG	O7-C7-C8	3.10	118.19	111.50
24	C	510	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
24	C	512	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
25	a	408[A]	PHO	O2A-CGA-CBA	3.10	121.63	111.91
24	b	605	CLA	C3B-C4B-NB	3.10	113.22	109.21
39	e	101	HEM	CHD-C1D-ND	3.10	127.80	124.43
27	a	411[B]	SQD	C44-O6-C1	-3.10	107.69	113.74
24	C	503	CLA	CMC-C2C-C1C	3.10	129.75	125.04
24	b	612	CLA	O2A-CGA-CBA	3.10	121.62	111.91
24	B	604	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
24	b	616	CLA	CBC-CAC-C3C	-3.09	103.90	112.43
24	c	505	CLA	CHC-C1C-C2C	-3.09	118.16	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	407[A]	CLA	CAA-C2A-C3A	-3.09	104.31	112.78
24	c	504	CLA	C3B-C4B-NB	3.09	113.21	109.21
24	C	506	CLA	C3B-C4B-NB	3.09	113.20	109.21
35	c	520	LMG	O1-C7-C8	-3.09	103.45	110.90
27	B	620	SQD	O9-S-C6	3.09	110.61	106.94
33	d	414[B]	LHG	O8-C23-C24	3.09	121.60	111.91
24	c	504	CLA	C4C-C3C-C2C	-3.09	102.40	106.90
24	C	512	CLA	C1-O2A-CGA	3.09	124.54	116.44
36	h	102	DGD	O1G-C1A-C2A	3.09	121.59	111.91
24	b	608	CLA	CMB-C2B-C3B	3.08	130.45	124.68
24	b	614	CLA	C1C-C2C-C3C	-3.08	103.72	106.96
24	C	503	CLA	CAC-C3C-C4C	3.08	128.81	124.81
33	D	406[A]	LHG	O8-C23-O10	-3.08	115.82	123.59
24	a	406[B]	CLA	CHD-C4C-NC	3.08	129.05	124.20
30	A	415[B]	PL9	C17-C18-C19	-3.07	120.26	127.66
26	d	405	BCR	C37-C22-C23	3.07	122.92	118.08
24	a	406[B]	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
24	D	402[B]	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
24	c	510	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
24	C	513	CLA	CHD-C4C-NC	3.07	129.03	124.20
24	C	511	CLA	CHC-C1C-C2C	-3.07	118.24	126.72
35	b	629	LMG	C8-O7-C10	-3.06	110.25	117.79
24	C	507	CLA	CAC-C3C-C4C	3.06	128.78	124.81
24	a	409	CLA	CAA-C2A-C3A	-3.06	104.39	112.78
24	b	613	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
24	B	616	CLA	CAC-C3C-C4C	3.06	128.78	124.81
24	d	403[B]	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
24	B	606	CLA	CMC-C2C-C1C	3.06	129.70	125.04
24	b	614	CLA	CHC-C1C-C2C	-3.06	118.27	126.72
24	a	405[B]	CLA	C4-C3-C5	3.06	120.41	115.27
24	B	607	CLA	CHD-C4C-NC	3.06	129.02	124.20
36	c	518[B]	DGD	C1D-O6D-C5D	3.06	119.69	113.69
33	a	420[A]	LHG	O7-C7-C8	3.05	118.08	111.50
24	b	615	CLA	C11-C10-C8	-3.05	106.05	115.92
24	a	407[B]	CLA	CMC-C2C-C1C	3.05	129.69	125.04
24	c	511	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
33	d	414[B]	LHG	O8-C23-O10	-3.05	115.90	123.59
24	b	613	CLA	CMC-C2C-C1C	3.05	129.68	125.04
24	A	405[A]	CLA	CMC-C2C-C1C	3.05	129.68	125.04
24	D	403	CLA	O2A-CGA-O1A	-3.05	115.91	123.59
33	D	407[A]	LHG	O8-C23-C24	3.05	121.46	111.91
30	A	415[A]	PL9	O1-C4-C3	-3.05	117.37	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	614	CLA	C4C-C3C-C2C	-3.04	102.46	106.90
30	a	415[A]	PL9	C10-C9-C11	3.04	120.39	115.27
24	b	602	CLA	CHD-C4C-NC	3.04	128.99	124.20
26	D	404	BCR	C40-C30-C25	-3.04	105.37	110.30
30	A	415[A]	PL9	C20-C19-C21	3.04	120.38	115.27
24	B	607	CLA	O2A-CGA-O1A	-3.04	115.93	123.59
24	c	510	CLA	CHC-C1C-C2C	-3.04	118.32	126.72
25	A	417[A]	PHO	CMC-C2C-C3C	3.03	130.66	124.94
24	C	512	CLA	CMC-C2C-C1C	3.03	129.66	125.04
30	D	405[B]	PL9	C17-C18-C19	-3.03	120.36	127.66
33	d	414[A]	LHG	O7-C7-C8	3.03	118.04	111.50
24	b	609	CLA	CBC-CAC-C3C	-3.03	104.07	112.43
30	a	415[B]	PL9	C17-C18-C19	-3.03	120.36	127.66
26	c	516	BCR	C7-C8-C9	-3.03	121.65	126.23
24	b	616	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
24	B	601	CLA	CHD-C4C-NC	3.03	128.97	124.20
24	B	614	CLA	CHC-C1C-C2C	-3.03	118.35	126.72
24	c	507	CLA	CHC-C1C-C2C	-3.03	118.35	126.72
24	b	615	CLA	C4-C3-C5	3.03	120.36	115.27
24	c	504	CLA	C1-C2-C3	-3.02	120.81	126.04
24	C	513	CLA	O2A-CGA-CBA	3.02	121.39	111.91
24	B	603	CLA	C4-C3-C5	3.02	120.35	115.27
30	d	406[B]	PL9	C40-C39-C41	3.02	120.35	115.27
24	A	407[B]	CLA	C3B-C4B-NB	3.02	113.11	109.21
24	b	611	CLA	CHC-C1C-C2C	-3.02	118.38	126.72
25	d	402[A]	PHO	CBA-CAA-C2A	-3.02	105.00	113.81
27	A	413	SQD	O48-C23-C24	3.01	121.36	111.91
24	D	402[B]	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
24	A	407[A]	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
33	D	407[A]	LHG	O8-C23-O10	-3.01	115.99	123.59
24	a	406[B]	CLA	CHC-C1C-C2C	-3.01	118.40	126.72
25	d	402[A]	PHO	CMB-C2B-C3B	3.01	130.30	124.68
24	C	502	CLA	CHD-C4C-NC	3.01	128.94	124.20
24	c	510	CLA	O2A-CGA-CBA	3.01	121.34	111.91
24	c	508	CLA	C4C-C3C-C2C	-3.01	102.52	106.90
24	C	507	CLA	CHC-C1C-C2C	-3.00	118.41	126.72
30	D	405[A]	PL9	C53-C6-C1	3.00	121.13	114.99
24	a	405[A]	CLA	CHC-C1C-C2C	-3.00	118.43	126.72
30	d	406[A]	PL9	C22-C23-C24	-3.00	120.44	127.66
24	c	514	CLA	C1-C2-C3	-3.00	120.86	126.04
30	d	406[A]	PL9	C36-C34-C33	-3.00	115.05	121.12
24	B	613	CLA	CHC-C1C-C2C	-3.00	118.43	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	407[A]	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
24	b	608	CLA	CHC-C1C-C2C	-3.00	118.43	126.72
24	C	505	CLA	C1-O2A-CGA	3.00	124.31	116.44
24	B	612	CLA	O2A-CGA-CBA	2.99	121.31	111.91
35	Z	101	LMG	C4-C3-C2	2.99	116.05	110.82
30	A	415[A]	PL9	C17-C18-C19	-2.99	120.45	127.66
24	b	602	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
24	B	601	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
36	c	519	DGD	O2G-C1B-C2B	2.99	117.94	111.50
39	F	102	HEM	CHD-C1D-ND	2.99	127.67	124.43
26	C	516	BCR	C33-C5-C6	-2.99	121.17	124.53
24	b	607	CLA	CHC-C1C-C2C	-2.99	118.46	126.72
32	B	627	LMT	C4B-C3B-C2B	2.98	116.03	110.82
33	a	420[B]	LHG	O7-C7-C8	2.98	117.93	111.50
24	c	504	CLA	C4-C3-C5	2.98	120.29	115.27
24	B	609	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
24	c	512	CLA	CAC-C3C-C4C	2.98	128.68	124.81
24	d	403[A]	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
33	D	406[B]	LHG	O7-C7-C8	2.98	117.93	111.50
27	B	620	SQD	C4-C3-C2	2.98	116.03	110.82
24	b	610	CLA	C4-C3-C5	2.98	120.28	115.27
24	a	405[A]	CLA	CMA-C3A-C4A	-2.98	103.77	111.77
24	C	509	CLA	CHC-C1C-C2C	-2.98	118.48	126.72
24	A	407[A]	CLA	CMC-C2C-C1C	2.98	129.57	125.04
24	C	502	CLA	C4-C3-C5	2.97	120.28	115.27
24	C	508	CLA	CBC-CAC-C3C	-2.97	104.23	112.43
24	c	502	CLA	C1D-CHD-C4C	-2.97	119.64	126.06
36	C	517[A]	DGD	C2G-O2G-C1B	-2.97	110.47	117.79
24	d	403[A]	CLA	C4C-C3C-C2C	-2.97	102.56	106.90
30	a	415[A]	PL9	C42-C43-C44	-2.97	120.50	127.66
24	a	405[A]	CLA	CMC-C2C-C1C	2.97	129.56	125.04
24	c	510	CLA	CMB-C2B-C3B	2.97	130.23	124.68
30	d	406[A]	PL9	C10-C9-C11	2.97	120.27	115.27
24	C	510	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
24	A	405[B]	CLA	O2A-CGA-O1A	-2.97	116.11	123.59
35	c	520	LMG	O8-C28-C29	2.96	121.21	111.91
27	A	411[A]	SQD	O8-S-C6	2.96	110.46	105.74
25	d	402[A]	PHO	O2D-CGD-O1D	-2.96	118.05	123.84
24	D	403	CLA	C4-C3-C5	2.96	120.25	115.27
24	b	616	CLA	C1C-C2C-C3C	-2.96	103.84	106.96
26	a	410	BCR	C38-C26-C25	-2.96	121.20	124.53
36	C	518[B]	DGD	C2G-O2G-C1B	-2.96	110.51	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	612	CLA	O2A-CGA-O1A	-2.96	116.13	123.59
24	a	405[B]	CLA	C4C-C3C-C2C	-2.95	102.59	106.90
25	a	408[B]	PHO	CMB-C2B-C3B	2.95	130.20	124.68
24	D	402[A]	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
24	c	514	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
35	M	101	LMG	O8-C28-C29	2.95	121.17	111.91
24	B	612	CLA	C1C-C2C-C3C	-2.95	103.85	106.96
32	A	421	LMT	O5B-C5B-C4B	2.95	115.05	109.69
27	a	411[B]	SQD	C45-O47-C7	-2.95	110.53	117.79
24	b	616	CLA	C3B-C4B-NB	2.95	113.02	109.21
24	c	508	CLA	C3B-C4B-NB	2.95	113.02	109.21
24	b	603	CLA	O2A-CGA-O1A	-2.94	116.16	123.59
24	b	601	CLA	C3B-C4B-NB	2.94	113.02	109.21
24	A	407[B]	CLA	C2A-C1A-CHA	-2.94	118.71	123.86
27	a	411[B]	SQD	C1-O5-C5	-2.94	107.91	113.69
24	b	603	CLA	O2A-CGA-CBA	2.94	121.14	111.91
24	b	607	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
24	d	403[B]	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
27	A	411[B]	SQD	O48-C23-C24	2.94	121.13	111.91
24	B	614	CLA	CMC-C2C-C1C	2.94	129.51	125.04
24	B	609	CLA	O2A-CGA-O1A	-2.94	116.18	123.59
39	e	101	HEM	CBD-CAD-C3D	-2.94	104.47	112.63
30	d	406[B]	PL9	C27-C28-C29	-2.94	120.59	127.66
41	v	201	HEC	CMB-C2B-C3B	2.94	129.27	125.82
24	C	503	CLA	CBC-CAC-C3C	-2.94	104.34	112.43
24	a	409	CLA	O2A-CGA-CBA	2.94	121.12	111.91
24	c	504	CLA	CAC-C3C-C4C	2.93	128.62	124.81
24	b	602	CLA	C2A-C1A-CHA	-2.93	118.73	123.86
24	B	609	CLA	O2A-CGA-CBA	2.93	121.11	111.91
30	D	405[A]	PL9	C10-C9-C11	2.93	120.20	115.27
30	D	405[B]	PL9	C42-C43-C44	-2.93	120.61	127.66
24	D	402[B]	CLA	C3B-C4B-NB	2.93	113.00	109.21
24	B	601	CLA	O2A-CGA-CBA	2.93	121.10	111.91
24	A	406[A]	CLA	CMA-C3A-C4A	-2.93	103.90	111.77
26	D	404	BCR	C29-C30-C25	2.93	114.99	110.48
24	b	605	CLA	CHC-C1C-C2C	-2.93	118.62	126.72
24	A	406[B]	CLA	CHC-C1C-C2C	-2.93	118.63	126.72
33	A	420[B]	LHG	C5-O7-C7	-2.93	110.59	117.79
24	A	405[A]	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
24	c	514	CLA	C2A-C1A-CHA	-2.92	118.75	123.86
24	a	406[A]	CLA	CMA-C3A-C2A	-2.92	102.03	113.83
24	A	409	CLA	CMC-C2C-C1C	2.92	129.49	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	516	BCR	C37-C22-C21	-2.92	118.83	122.92
24	c	514	CLA	CMC-C2C-C1C	2.92	129.48	125.04
24	B	615	CLA	C11-C10-C8	-2.92	106.49	115.92
26	B	618	BCR	C2-C1-C6	2.92	114.97	110.48
33	E	101[A]	LHG	O8-C23-C24	2.92	121.06	111.91
24	c	513	CLA	CHC-C1C-C2C	-2.91	118.66	126.72
24	D	402[A]	CLA	C4-C3-C5	2.91	120.17	115.27
24	b	609	CLA	CHC-C1C-C2C	-2.91	118.66	126.72
24	c	508	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
24	b	606	CLA	CHC-C1C-C2C	-2.91	118.67	126.72
24	A	407[B]	CLA	CHD-C4C-NC	2.91	128.79	124.20
26	Y	101	BCR	C37-C22-C23	2.91	122.66	118.08
24	A	405[A]	CLA	C2A-C1A-CHA	-2.91	118.77	123.86
25	d	402[B]	PHO	O2D-CGD-O1D	-2.91	118.15	123.84
24	B	605	CLA	CMC-C2C-C1C	2.91	129.47	125.04
24	a	407[B]	CLA	CAA-C2A-C3A	-2.91	104.82	112.78
24	c	513	CLA	CHD-C4C-NC	2.91	128.78	124.20
24	A	407[B]	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
26	A	410	BCR	C8-C7-C6	-2.90	119.05	127.20
26	H	101	BCR	C7-C8-C9	-2.90	121.85	126.23
24	B	608	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
24	b	606	CLA	CHD-C4C-NC	2.90	128.78	124.20
24	A	406[A]	CLA	CHD-C4C-NC	2.90	128.78	124.20
24	C	514	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
33	d	407[B]	LHG	O7-C7-C8	2.90	117.75	111.50
24	B	603	CLA	CHD-C4C-NC	2.90	128.77	124.20
24	D	402[A]	CLA	O2A-CGA-CBA	2.90	121.00	111.91
24	d	403[A]	CLA	CHC-C1C-C2C	-2.90	118.71	126.72
24	c	511	CLA	O2A-CGA-O1A	-2.90	116.28	123.59
24	A	406[B]	CLA	CMC-C2C-C1C	2.90	129.45	125.04
24	B	615	CLA	CED-O2D-CGD	2.89	122.48	115.94
24	b	605	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
35	D	411	LMG	O7-C10-C11	2.89	117.73	111.50
33	A	420[B]	LHG	O8-C23-O10	-2.89	116.30	123.59
24	D	403	CLA	C3B-C4B-NB	2.89	112.94	109.21
24	b	605	CLA	CMC-C2C-C1C	2.89	129.44	125.04
27	X	101	SQD	O48-C23-C24	2.89	120.97	111.91
24	C	506	CLA	CHC-C1C-C2C	-2.89	118.74	126.72
24	B	606	CLA	C4-C3-C5	2.89	120.12	115.27
24	b	607	CLA	CBC-CAC-C3C	-2.88	104.48	112.43
26	B	617	BCR	C15-C14-C13	-2.88	123.20	127.31
33	d	407[A]	LHG	O7-C7-C8	2.88	117.71	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	402[A]	CLA	CAA-C2A-C3A	-2.88	104.89	112.78
24	c	514	CLA	CAA-C2A-C3A	-2.88	104.89	112.78
24	B	616	CLA	C1-O2A-CGA	2.88	124.00	116.44
35	b	629	LMG	O8-C28-C29	2.88	120.94	111.91
24	b	607	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
24	D	402[B]	CLA	O2A-CGA-CBA	2.88	120.94	111.91
24	B	612	CLA	C4A-NA-C1A	-2.88	105.41	106.71
25	d	402[A]	PHO	C4A-C3A-C2A	-2.88	100.10	102.84
24	b	602	CLA	C1-C2-C3	-2.88	121.07	126.04
24	c	510	CLA	O2A-C1-C2	2.88	116.20	108.64
30	d	406[B]	PL9	C17-C18-C19	-2.88	120.73	127.66
24	c	505	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
24	A	407[A]	CLA	CHD-C4C-NC	2.88	128.73	124.20
27	a	411[A]	SQD	O47-C7-O49	-2.87	116.75	123.70
24	B	606	CLA	CHD-C4C-NC	2.87	128.73	124.20
24	B	608	CLA	CHB-C4A-NA	2.87	128.49	124.51
24	C	509	CLA	CAC-C3C-C4C	2.87	128.54	124.81
25	A	417[A]	PHO	O2D-CGD-O1D	-2.87	118.22	123.84
24	b	603	CLA	C4-C3-C5	2.87	120.10	115.27
26	T	101	BCR	C11-C10-C9	-2.87	123.21	127.31
24	b	601	CLA	CMB-C2B-C3B	2.87	130.05	124.68
24	A	409	CLA	CHC-C1C-C2C	-2.87	118.79	126.72
24	a	405[A]	CLA	CAC-C3C-C4C	2.87	128.53	124.81
24	B	603	CLA	CHC-C1C-C2C	-2.87	118.79	126.72
33	A	420[A]	LHG	C5-O7-C7	-2.87	110.73	117.79
24	B	606	CLA	O2A-CGA-O1A	-2.87	116.36	123.59
24	B	612	CLA	CMC-C2C-C1C	2.87	129.40	125.04
24	C	512	CLA	CAC-C3C-C4C	2.87	128.53	124.81
24	c	502	CLA	CHC-C1C-C2C	-2.86	118.80	126.72
26	B	618	BCR	C37-C22-C21	-2.86	118.91	122.92
25	d	402[B]	PHO	CMB-C2B-C3B	2.86	130.04	124.68
24	a	406[B]	CLA	CBC-CAC-C3C	-2.86	104.54	112.43
24	B	605	CLA	O2A-CGA-O1A	-2.86	116.37	123.59
24	b	601	CLA	C1-O2A-CGA	2.86	123.95	116.44
24	a	406[A]	CLA	CHC-C1C-C2C	-2.86	118.81	126.72
33	D	406[B]	LHG	O8-C23-O10	-2.86	116.37	123.59
33	E	101[B]	LHG	O8-C23-C24	2.86	120.88	111.91
30	D	405[A]	PL9	C51-C49-C50	2.86	120.92	114.60
35	z	101	LMG	O8-C28-C29	2.86	120.88	111.91
34	B	624	HTG	C1'-S1-C1	2.86	105.44	100.09
24	C	513	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
24	C	514	CLA	CAC-C3C-C4C	2.85	128.51	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	608	CLA	C11-C12-C13	-2.85	106.69	115.92
24	c	507	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
24	C	507	CLA	C4-C3-C5	2.85	120.07	115.27
30	a	415[A]	PL9	C53-C6-C1	2.85	120.82	114.99
24	C	511	CLA	O2A-CGA-CBA	2.85	120.85	111.91
26	c	515	BCR	C37-C22-C21	-2.85	118.93	122.92
24	b	609	CLA	C1C-C2C-C3C	-2.85	103.96	106.96
24	b	605	CLA	C2A-C1A-CHA	-2.85	118.88	123.86
24	b	615	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
24	B	614	CLA	C2A-C1A-CHA	-2.85	118.88	123.86
26	b	618	BCR	C37-C22-C21	-2.85	118.94	122.92
39	e	101	HEM	CHB-C1B-NB	2.85	127.90	124.38
24	C	502	CLA	CAC-C3C-C4C	2.85	128.50	124.81
24	c	507	CLA	CHD-C4C-NC	2.85	128.69	124.20
36	C	517[A]	DGD	O6D-C1D-O3G	-2.85	103.24	109.97
36	c	517[B]	DGD	O3G-C3G-C2G	-2.84	104.04	110.90
24	C	504	CLA	C3B-C4B-NB	2.84	112.89	109.21
24	A	405[B]	CLA	C2A-C1A-CHA	-2.84	118.89	123.86
24	c	504	CLA	CMC-C2C-C1C	2.84	129.37	125.04
24	c	502	CLA	CBC-CAC-C3C	-2.84	104.60	112.43
24	C	511	CLA	O2A-CGA-O1A	-2.84	116.42	123.59
27	A	411[A]	SQD	O48-C23-C24	2.84	120.82	111.91
24	C	514	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
24	d	404	CLA	CHC-C1C-C2C	-2.84	118.87	126.72
24	b	609	CLA	O2A-CGA-O1A	-2.84	116.43	123.59
27	L	102	SQD	O7-S-C6	2.84	110.31	106.94
24	a	405[B]	CLA	CAA-C2A-C1A	-2.84	102.68	111.97
24	c	502	CLA	CMC-C2C-C1C	2.84	129.36	125.04
24	C	508	CLA	CMC-C2C-C1C	2.84	129.36	125.04
24	a	407[A]	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
24	A	407[A]	CLA	O2A-CGA-CBA	2.83	120.80	111.91
24	A	409	CLA	CAC-C3C-C4C	2.83	128.49	124.81
25	A	408[A]	PHO	CMC-C2C-C3C	2.83	130.28	124.94
24	c	510	CLA	CMC-C2C-C1C	2.83	129.35	125.04
24	d	404	CLA	CAA-C2A-C3A	-2.83	105.03	112.78
24	c	513	CLA	C3B-C4B-NB	2.83	112.87	109.21
24	B	614	CLA	O2A-CGA-CBA	2.83	120.78	111.91
26	b	619	BCR	C38-C26-C25	-2.83	121.35	124.53
30	D	405[A]	PL9	C37-C38-C39	-2.83	120.85	127.66
24	c	512	CLA	CMC-C2C-C1C	2.83	129.34	125.04
24	C	502	CLA	CHC-C1C-C2C	-2.82	118.91	126.72
24	B	606	CLA	CBC-CAC-C3C	-2.82	104.64	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	M	102	LMT	C3'-C4'-C5'	-2.82	104.45	110.93
26	d	405	BCR	C16-C17-C18	-2.82	123.28	127.31
24	A	405[A]	CLA	CHC-C1C-C2C	-2.82	118.92	126.72
24	B	604	CLA	CHC-C1C-C2C	-2.82	118.92	126.72
24	C	511	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
30	A	415[A]	PL9	C35-C34-C36	2.82	120.01	115.27
30	a	415[B]	PL9	C35-C34-C36	2.82	120.01	115.27
26	c	516	BCR	C11-C10-C9	-2.82	123.29	127.31
24	C	514	CLA	CMB-C2B-C3B	2.82	129.95	124.68
24	b	610	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
33	L	101[A]	LHG	O8-C23-C24	2.82	120.75	111.91
24	b	602	CLA	CAC-C3C-C4C	2.82	128.46	124.81
24	c	503	CLA	CHD-C4C-NC	2.81	128.64	124.20
24	a	407[B]	CLA	O2D-CGD-O1D	-2.81	118.33	123.84
24	b	613	CLA	CHD-C4C-NC	2.81	128.64	124.20
24	B	612	CLA	C11-C12-C13	-2.81	106.83	115.92
24	B	601	CLA	C3B-C4B-NB	2.81	112.85	109.21
35	C	501	LMG	C8-O7-C10	-2.81	110.87	117.79
24	A	407[A]	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
24	C	503	CLA	CHC-C1C-C2C	-2.81	118.95	126.72
24	C	510	CLA	CMB-C2B-C3B	2.81	129.94	124.68
24	C	504	CLA	CHC-C1C-C2C	-2.81	118.95	126.72
24	A	407[A]	CLA	C4-C3-C5	2.81	119.99	115.27
30	A	415[A]	PL9	C30-C29-C31	2.81	119.99	115.27
24	D	403	CLA	O2A-CGA-CBA	2.81	120.72	111.91
30	a	415[B]	PL9	C22-C23-C24	-2.81	120.90	127.66
24	c	507	CLA	O2A-CGA-O1A	-2.81	116.51	123.59
24	c	506	CLA	CHC-C1C-C2C	-2.81	118.96	126.72
26	t	102	BCR	C21-C20-C19	-2.81	114.46	123.22
26	k	101	BCR	C39-C30-C25	-2.80	105.75	110.30
24	d	403[B]	CLA	C2A-C1A-CHA	-2.80	118.96	123.86
24	A	406[A]	CLA	CHC-C1C-C2C	-2.80	118.97	126.72
24	d	404	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
24	C	511	CLA	CBC-CAC-C3C	-2.80	104.71	112.43
30	A	415[B]	PL9	C35-C34-C36	2.80	119.98	115.27
24	D	402[B]	CLA	C2A-C1A-CHA	-2.80	118.96	123.86
30	a	415[A]	PL9	C22-C23-C24	-2.80	120.92	127.66
24	A	405[B]	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
24	c	509	CLA	C3B-C4B-NB	2.80	112.83	109.21
27	B	620	SQD	O48-C23-O10	-2.80	116.53	123.59
24	c	513	CLA	CAC-C3C-C4C	2.80	128.44	124.81
26	t	102	BCR	C19-C18-C17	-2.80	114.65	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	407[A]	CLA	CHC-C1C-C2C	-2.80	118.98	126.72
24	a	409	CLA	CBC-CAC-C3C	-2.79	104.73	112.43
24	B	613	CLA	CMB-C2B-C3B	2.79	129.90	124.68
24	A	407[B]	CLA	CAA-C2A-C3A	-2.79	105.14	112.78
27	A	413	SQD	C1-C2-C3	-2.79	104.19	110.00
36	C	517[B]	DGD	O3G-C3G-C2G	-2.79	104.17	110.90
35	C	501	LMG	C6-C5-C4	2.79	119.54	113.00
24	c	509	CLA	O2A-CGA-CBA	2.79	120.66	111.91
24	B	610	CLA	CHC-C1C-C2C	-2.79	119.01	126.72
24	A	409	CLA	C4-C3-C5	2.79	119.96	115.27
33	d	408[B]	LHG	O8-C23-C24	2.78	120.64	111.91
24	b	605	CLA	C1-C2-C3	-2.78	121.23	126.04
24	b	613	CLA	CBC-CAC-C3C	-2.78	104.77	112.43
25	a	408[B]	PHO	O1D-CGD-CBD	-2.78	120.11	124.74
24	a	409	CLA	C3B-C4B-NB	2.78	112.80	109.21
24	c	513	CLA	C4C-C3C-C2C	-2.78	102.85	106.90
24	a	405[B]	CLA	CAC-C3C-C4C	2.78	128.41	124.81
27	L	102	SQD	C1-C2-C3	-2.77	104.22	110.00
24	c	514	CLA	O2A-CGA-CBA	2.77	120.61	111.91
24	C	514	CLA	C2A-C1A-CHA	-2.77	119.01	123.86
24	A	406[A]	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
25	a	408[A]	PHO	CMB-C2B-C3B	2.77	129.86	124.68
24	d	403[B]	CLA	CHC-C1C-C2C	-2.77	119.06	126.72
36	H	102	DGD	O1G-C1A-C2A	2.77	120.59	111.91
24	a	407[B]	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
24	A	409	CLA	CMA-C3A-C2A	-2.77	102.67	113.83
26	Y	101	BCR	C28-C27-C26	-2.77	109.14	114.08
24	C	505	CLA	CHC-C1C-C2C	-2.77	119.07	126.72
26	A	410	BCR	C15-C14-C13	-2.76	123.36	127.31
24	C	510	CLA	O2A-CGA-O1A	-2.76	116.61	123.59
24	c	513	CLA	C4-C3-C5	2.76	119.92	115.27
24	a	406[A]	CLA	O2A-CGA-CBA	2.76	120.58	111.91
24	b	613	CLA	CHC-C1C-C2C	-2.76	119.08	126.72
24	b	615	CLA	CHC-C1C-C2C	-2.76	119.08	126.72
24	a	407[A]	CLA	O2A-CGA-O1A	-2.76	116.62	123.59
26	H	101	BCR	C37-C22-C21	-2.76	119.06	122.92
24	B	615	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
24	b	603	CLA	CHD-C4C-NC	2.76	128.55	124.20
24	c	505	CLA	CHD-C4C-NC	2.76	128.55	124.20
24	B	606	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
33	D	406[A]	LHG	O7-C7-C8	2.75	117.44	111.50
26	y	101	BCR	C24-C23-C22	-2.75	122.08	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	L	101[B]	LHG	O8-C23-C24	2.75	120.54	111.91
26	t	102	BCR	C2-C1-C6	2.75	114.72	110.48
24	c	512	CLA	CMA-C3A-C4A	2.75	119.16	111.77
24	a	407[B]	CLA	C4-C3-C5	2.75	119.89	115.27
24	b	608	CLA	CBC-CAC-C3C	-2.75	104.85	112.43
32	B	627	LMT	C2'-C3'-C4'	2.75	115.96	109.68
24	C	504	CLA	CHD-C4C-NC	2.75	128.53	124.20
24	A	409	CLA	O2A-CGA-CBA	2.75	120.52	111.91
30	d	406[A]	PL9	C36-C37-C38	-2.74	102.86	111.88
24	C	509	CLA	C4-C3-C5	2.74	119.89	115.27
34	c	522	HTG	O5-C1-C2	2.74	113.76	110.31
36	H	102	DGD	O2G-C1B-C2B	2.74	117.41	111.50
26	C	515	BCR	C15-C14-C13	-2.74	123.40	127.31
36	h	102	DGD	O3G-C1D-C2D	2.74	112.58	108.30
24	C	513	CLA	C3B-C4B-NB	2.74	112.75	109.21
24	B	607	CLA	C2A-C1A-CHA	-2.74	119.07	123.86
24	B	612	CLA	C1-C2-C3	-2.74	121.31	126.04
24	B	616	CLA	CHC-C1C-C2C	-2.74	119.15	126.72
24	B	608	CLA	CMC-C2C-C1C	2.73	129.20	125.04
24	b	613	CLA	CMB-C2B-C3B	2.73	129.79	124.68
24	B	602	CLA	C11-C12-C13	-2.73	107.08	115.92
24	B	603	CLA	O2A-CGA-O1A	-2.73	116.70	123.59
24	c	509	CLA	C4-C3-C5	2.73	119.87	115.27
24	d	404	CLA	CBC-CAC-C3C	-2.73	104.90	112.43
24	A	407[B]	CLA	O2A-CGA-CBA	2.73	120.48	111.91
24	b	603	CLA	C2A-C1A-CHA	-2.73	119.08	123.86
33	D	407[B]	LHG	O8-C23-C24	2.73	120.47	111.91
24	C	514	CLA	CBC-CAC-C3C	-2.73	104.91	112.43
24	c	503	CLA	O2A-CGA-CBA	2.73	120.47	111.91
24	B	603	CLA	O2A-CGA-CBA	2.73	120.47	111.91
24	b	606	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
24	c	505	CLA	CAC-C3C-C4C	2.73	128.35	124.81
24	B	606	CLA	C1-C2-C3	-2.72	121.33	126.04
24	a	407[B]	CLA	C3B-C4B-NB	2.72	112.73	109.21
26	D	404	BCR	C37-C22-C21	-2.72	119.11	122.92
24	c	502	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
30	d	406[A]	PL9	C27-C28-C29	-2.72	121.11	127.66
32	m	102	LMT	C3'-C4'-C5'	-2.72	104.69	110.93
35	c	521	LMG	O8-C28-C29	2.72	120.44	111.91
24	C	507	CLA	C2A-C1A-CHA	-2.72	119.11	123.86
24	c	512	CLA	CHC-C1C-C2C	-2.72	119.21	126.72
24	C	513	CLA	CBA-CAA-C2A	-2.72	105.85	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	405[B]	PL9	C40-C39-C41	2.72	119.84	115.27
27	f	101	SQD	C1-O5-C5	2.71	119.02	113.69
39	e	101	HEM	C4D-ND-C1D	2.71	107.88	105.07
26	h	101	BCR	C37-C22-C21	-2.71	119.12	122.92
27	a	413	SQD	C3-C4-C5	2.71	115.08	110.24
26	B	618	BCR	C38-C26-C25	-2.71	121.48	124.53
24	b	614	CLA	O2A-CGA-CBA	2.71	120.42	111.91
24	C	511	CLA	CMB-C2B-C3B	2.71	129.75	124.68
30	a	415[B]	PL9	C10-C9-C11	2.71	119.83	115.27
30	a	415[B]	PL9	C7-C3-C4	2.71	119.08	116.88
35	c	520	LMG	C8-O7-C10	-2.71	111.12	117.79
30	a	415[B]	PL9	C53-C6-C1	2.71	120.53	114.99
24	a	407[B]	CLA	C2A-C1A-CHA	-2.71	119.12	123.86
24	c	504	CLA	CHD-C4C-NC	2.71	128.47	124.20
30	A	415[B]	PL9	C30-C29-C31	2.71	119.83	115.27
24	C	514	CLA	O2A-CGA-CBA	2.71	120.40	111.91
24	C	504	CLA	O2A-CGA-CBA	2.71	120.40	111.91
24	b	609	CLA	CHD-C4C-NC	2.71	128.47	124.20
24	D	403	CLA	CMA-C3A-C2A	-2.70	102.92	113.83
30	a	415[B]	PL9	C20-C19-C21	2.70	119.82	115.27
24	a	405[B]	CLA	O2A-CGA-O1A	-2.70	116.77	123.59
24	b	607	CLA	CMC-C2C-C1C	2.70	129.16	125.04
34	b	622	HTG	O5-C1-C2	2.70	113.71	110.31
24	c	514	CLA	CHC-C1C-C2C	-2.70	119.25	126.72
26	t	102	BCR	C11-C10-C9	-2.70	123.46	127.31
24	B	614	CLA	CHD-C4C-NC	2.70	128.46	124.20
24	C	507	CLA	CHD-C4C-NC	2.70	128.46	124.20
24	a	409	CLA	CAC-C3C-C4C	2.70	128.31	124.81
36	c	519	DGD	O1G-C1A-C2A	2.70	120.38	111.91
24	c	508	CLA	O2A-CGA-CBA	2.70	120.37	111.91
24	B	605	CLA	CHC-C1C-C2C	-2.70	119.26	126.72
24	a	405[A]	CLA	C2A-C1A-CHA	-2.69	119.15	123.86
24	b	608	CLA	O2A-CGA-CBA	2.69	120.36	111.91
24	B	603	CLA	CMC-C2C-C1C	2.69	129.14	125.04
26	b	618	BCR	C29-C30-C25	2.69	114.62	110.48
24	B	615	CLA	C4C-C3C-C2C	-2.69	102.97	106.90
33	L	101[A]	LHG	O8-C23-O10	-2.69	116.80	123.59
24	c	511	CLA	O2A-CGA-CBA	2.69	120.35	111.91
24	D	402[A]	CLA	CAC-C3C-C4C	2.69	128.30	124.81
24	C	506	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
24	c	506	CLA	C3B-C4B-NB	2.69	112.69	109.21
24	A	407[B]	CLA	CMC-C2C-C1C	2.69	129.13	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	508	CLA	CHD-C4C-NC	2.69	128.44	124.20
24	C	513	CLA	CHB-C4A-NA	2.69	128.23	124.51
24	c	509	CLA	CMC-C2C-C1C	2.69	129.13	125.04
30	d	406[B]	PL9	C53-C6-C1	2.69	120.48	114.99
24	B	613	CLA	C1D-CHD-C4C	-2.69	120.26	126.06
24	B	606	CLA	CHC-C1C-C2C	-2.69	119.29	126.72
33	D	406[B]	LHG	O8-C23-C24	2.69	120.33	111.91
24	b	614	CLA	CHD-C4C-NC	2.68	128.43	124.20
24	C	506	CLA	O2A-CGA-CBA	2.68	120.33	111.91
26	d	405	BCR	C21-C20-C19	-2.68	114.84	123.22
24	C	503	CLA	CMB-C2B-C3B	2.68	129.70	124.68
33	b	628[A]	LHG	O8-C23-C24	2.68	120.32	111.91
24	C	502	CLA	CAA-C2A-C3A	-2.68	105.44	112.78
24	C	508	CLA	C4-C3-C5	2.68	119.78	115.27
24	B	607	CLA	C4C-C3C-C2C	-2.68	103.00	106.90
24	b	616	CLA	CAC-C3C-C4C	2.68	128.28	124.81
24	C	504	CLA	C1-C2-C3	-2.67	121.42	126.04
24	c	511	CLA	CHD-C4C-NC	2.67	128.42	124.20
24	B	608	CLA	O2A-CGA-O1A	-2.67	116.85	123.59
24	A	405[A]	CLA	CMA-C3A-C2A	-2.67	103.05	113.83
26	Y	101	BCR	C10-C11-C12	-2.67	114.88	123.22
30	D	405[B]	PL9	C12-C13-C14	-2.67	121.23	127.66
30	a	415[B]	PL9	C7-C3-C2	-2.67	119.79	123.30
26	T	101	BCR	C2-C1-C6	2.67	114.59	110.48
35	D	411	LMG	O8-C28-C29	2.67	120.28	111.91
24	B	614	CLA	CBC-CAC-C3C	-2.67	105.08	112.43
24	a	406[A]	CLA	C4C-C3C-C2C	-2.67	103.01	106.90
24	B	601	CLA	C1-O2A-CGA	2.67	123.44	116.44
24	B	603	CLA	CAC-C3C-C4C	2.66	128.27	124.81
24	B	606	CLA	O2A-CGA-CBA	2.66	120.27	111.91
26	c	515	BCR	C34-C9-C10	-2.66	119.19	122.92
30	D	405[B]	PL9	C45-C44-C46	2.66	119.75	115.27
24	B	605	CLA	OBD-CAD-C3D	-2.66	122.11	128.52
24	D	402[A]	CLA	CHC-C1C-C2C	-2.66	119.36	126.72
24	C	511	CLA	CHB-C4A-NA	2.66	128.19	124.51
33	a	420[A]	LHG	O8-C23-C24	2.66	120.25	111.91
24	C	503	CLA	O2A-CGA-CBA	2.66	120.25	111.91
36	C	518[B]	DGD	O1G-C1A-C2A	2.66	120.25	111.91
30	D	405[B]	PL9	C27-C28-C29	-2.66	121.26	127.66
25	A	408[A]	PHO	C1-C2-C3	-2.66	121.45	126.04
26	a	410	BCR	C29-C30-C25	2.66	114.57	110.48
27	A	413	SQD	C4-C3-C2	-2.66	106.19	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	511	CLA	CHC-C1C-C2C	-2.65	119.38	126.72
35	b	629	LMG	C3-C4-C5	2.65	114.97	110.24
24	C	506	CLA	CMC-C2C-C1C	2.65	129.08	125.04
24	a	406[A]	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
24	d	403[A]	CLA	CAC-C3C-C4C	2.65	128.25	124.81
26	h	101	BCR	C24-C23-C22	-2.65	122.23	126.23
36	C	518[A]	DGD	O1G-C1A-O1A	-2.65	116.90	123.59
36	c	518[B]	DGD	O1G-C1A-C2A	2.65	120.22	111.91
24	d	403[A]	CLA	C2A-C1A-CHA	-2.65	119.23	123.86
24	A	406[A]	CLA	C4-C3-C5	2.65	119.73	115.27
34	B	621	HTG	C1-O5-C5	2.65	117.47	112.58
24	b	607	CLA	O2A-CGA-O1A	-2.65	116.91	123.59
25	A	408[B]	PHO	O1D-CGD-CBD	-2.65	120.33	124.74
26	c	515	BCR	C36-C18-C17	-2.65	119.22	122.92
30	a	415[A]	PL9	C40-C39-C41	2.65	119.72	115.27
24	D	402[A]	CLA	C2A-C1A-CHA	-2.64	119.24	123.86
24	b	611	CLA	CBC-CAC-C3C	-2.64	105.14	112.43
33	D	406[A]	LHG	O8-C23-C24	2.64	120.20	111.91
25	a	408[B]	PHO	O2A-CGA-CBA	2.64	120.20	111.91
27	a	411[B]	SQD	O9-S-C6	2.64	110.08	106.94
24	c	509	CLA	CHD-C4C-NC	2.64	128.36	124.20
24	a	406[B]	CLA	C1-O2A-CGA	2.64	123.36	116.44
24	b	610	CLA	CHC-C1C-C2C	-2.64	119.43	126.72
24	B	616	CLA	O2A-CGA-CBA	2.64	120.18	111.91
24	C	502	CLA	C1-O2A-CGA	2.63	123.36	116.44
24	A	405[B]	CLA	CHD-C4C-NC	2.63	128.35	124.20
26	C	516	BCR	C37-C22-C23	2.63	122.23	118.08
24	b	611	CLA	O2A-CGA-O1A	-2.63	116.95	123.59
24	b	613	CLA	CED-O2D-CGD	2.63	121.89	115.94
30	A	415[A]	PL9	C40-C39-C41	2.63	119.70	115.27
24	B	611	CLA	C1-O2A-CGA	2.63	123.35	116.44
24	D	402[B]	CLA	CHC-C1C-C2C	-2.63	119.44	126.72
24	b	607	CLA	CAA-C2A-C3A	-2.63	105.58	112.78
24	c	502	CLA	CHD-C4C-NC	2.63	128.35	124.20
24	C	512	CLA	CHC-C1C-C2C	-2.63	119.45	126.72
24	b	610	CLA	CAC-C3C-C4C	2.63	128.22	124.81
33	b	628[B]	LHG	O8-C23-C24	2.62	120.14	111.91
24	b	611	CLA	CMB-C2B-C3B	2.62	129.59	124.68
25	a	408[B]	PHO	CMA-C3A-C4A	-2.62	108.63	114.38
30	A	415[B]	PL9	C40-C39-C41	2.62	119.68	115.27
24	c	507	CLA	CMC-C2C-C1C	2.62	129.03	125.04
24	a	406[B]	CLA	O2A-CGA-CBA	2.62	120.14	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	606	CLA	CAC-C3C-C4C	2.62	128.21	124.81
33	a	420[B]	LHG	O8-C23-C24	2.62	120.14	111.91
24	c	510	CLA	CHD-C4C-NC	2.62	128.34	124.20
24	A	407[B]	CLA	CHC-C1C-C2C	-2.62	119.47	126.72
24	C	510	CLA	CHD-C4C-NC	2.62	128.33	124.20
25	A	417[B]	PHO	O2D-CGD-O1D	-2.62	118.71	123.84
24	c	503	CLA	CBC-CAC-C3C	-2.62	105.21	112.43
24	d	403[B]	CLA	CMB-C2B-C3B	2.62	129.58	124.68
32	c	501	LMT	C3'-C4'-C5'	-2.62	104.92	110.93
26	k	101	BCR	C3-C4-C5	-2.62	109.40	114.08
24	b	609	CLA	CMC-C2C-C1C	2.62	129.03	125.04
36	h	102	DGD	O1G-C1A-O1A	-2.62	116.98	123.59
36	H	102	DGD	C2G-O2G-C1B	-2.62	111.34	117.79
36	h	102	DGD	O4D-C4D-C3D	-2.62	104.30	110.35
26	K	102	BCR	C11-C10-C9	-2.62	123.57	127.31
24	c	511	CLA	CMB-C2B-C3B	2.62	129.58	124.68
26	t	102	BCR	C1-C6-C7	2.62	123.19	115.78
24	c	506	CLA	CMC-C2C-C1C	2.62	129.03	125.04
24	C	513	CLA	CHC-C1C-C2C	-2.62	119.48	126.72
24	C	503	CLA	C2A-C1A-CHA	-2.62	119.28	123.86
41	v	201	HEC	CBA-CAA-C2A	-2.61	108.20	112.60
30	a	415[A]	PL9	C47-C48-C49	-2.61	118.83	127.75
24	a	407[A]	CLA	O2A-CGA-CBA	2.61	120.10	111.91
33	d	408[A]	LHG	O8-C23-C24	2.61	120.09	111.91
24	B	605	CLA	C3B-C4B-NB	2.61	112.58	109.21
24	b	603	CLA	CBC-CAC-C3C	-2.61	105.25	112.43
27	L	102	SQD	C44-O6-C1	-2.61	108.65	113.74
24	c	509	CLA	CAA-C2A-C3A	-2.61	105.64	112.78
24	B	614	CLA	OBD-CAD-C3D	-2.60	122.25	128.52
27	a	411[B]	SQD	O47-C7-O49	-2.60	117.41	123.70
26	k	101	BCR	C15-C14-C13	-2.60	123.59	127.31
24	A	406[A]	CLA	CMA-C3A-C2A	-2.60	103.33	113.83
24	a	405[B]	CLA	C2A-C1A-CHA	-2.60	119.31	123.86
30	a	415[A]	PL9	C10-C9-C8	-2.60	117.01	123.68
24	C	514	CLA	CAA-C2A-C3A	-2.60	105.66	112.78
24	C	502	CLA	O2A-CGA-O1A	-2.60	117.03	123.59
24	C	512	CLA	CHD-C4C-NC	2.60	128.30	124.20
27	f	101	SQD	O48-C23-C24	2.60	120.06	111.91
24	c	502	CLA	O2A-CGA-O1A	-2.60	117.04	123.59
24	a	407[A]	CLA	CMC-C2C-C1C	2.60	128.99	125.04
24	b	608	CLA	C4C-C3C-C2C	-2.60	103.11	106.90
34	C	522	HTG	C1-O5-C5	2.60	117.37	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	408[A]	PHO	O2A-CGA-CBA	2.59	120.05	111.91
32	M	104	LMT	C3'-C4'-C5'	-2.59	104.98	110.93
24	b	603	CLA	CMA-C3A-C2A	-2.59	103.37	113.83
26	c	515	BCR	C38-C26-C25	-2.59	121.62	124.53
24	b	604	CLA	CHC-C1C-C2C	-2.59	119.55	126.72
26	h	101	BCR	C34-C9-C8	2.59	122.16	118.08
36	c	519	DGD	O2D-C2D-C1D	-2.59	103.76	110.05
24	a	406[A]	CLA	O2A-CGA-O1A	-2.59	117.06	123.59
24	b	615	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
24	c	505	CLA	CBC-CAC-C3C	-2.59	105.30	112.43
30	D	405[B]	PL9	C51-C49-C50	2.59	120.32	114.60
24	c	508	CLA	CAC-C3C-C4C	2.59	128.17	124.81
24	A	407[A]	CLA	CHC-C1C-C2C	-2.59	119.57	126.72
26	K	102	BCR	C37-C22-C21	-2.58	119.30	122.92
26	K	102	BCR	C3-C4-C5	-2.58	109.46	114.08
24	c	512	CLA	O2A-CGA-CBA	2.58	120.01	111.91
24	d	403[B]	CLA	O2A-CGA-O1A	-2.58	117.07	123.59
24	c	506	CLA	O2A-CGA-O1A	-2.58	117.08	123.59
24	b	616	CLA	CMC-C2C-C1C	2.58	128.97	125.04
24	b	608	CLA	CHD-C4C-NC	2.58	128.27	124.20
24	b	615	CLA	O2A-CGA-CBA	2.58	120.00	111.91
24	c	513	CLA	CHB-C4A-NA	2.58	128.07	124.51
24	A	406[A]	CLA	C2A-C1A-CHA	-2.58	119.35	123.86
24	b	616	CLA	CHC-C1C-C2C	-2.58	119.59	126.72
30	d	406[B]	PL9	C45-C44-C46	2.58	119.60	115.27
24	C	510	CLA	O2A-CGA-CBA	2.58	119.99	111.91
26	H	101	BCR	C16-C15-C14	-2.58	118.20	123.47
27	a	411[B]	SQD	O48-C23-C24	2.57	119.98	111.91
24	D	402[A]	CLA	O2A-CGA-O1A	-2.57	117.10	123.59
24	b	606	CLA	CMC-C2C-C1C	2.57	128.96	125.04
25	A	408[A]	PHO	O1D-CGD-CBD	-2.57	120.46	124.74
26	K	102	BCR	C2-C1-C6	2.57	114.44	110.48
27	A	411[A]	SQD	O48-C23-O10	-2.57	117.11	123.59
25	A	408[A]	PHO	O2A-CGA-O1A	-2.57	117.12	123.59
26	K	102	BCR	C29-C30-C25	2.57	114.43	110.48
33	D	407[B]	LHG	O8-C23-O10	-2.57	117.12	123.59
24	b	615	CLA	CMC-C2C-C1C	2.56	128.94	125.04
24	B	602	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
24	b	601	CLA	CHC-C1C-C2C	-2.56	119.63	126.72
30	A	415[B]	PL9	O1-C4-C3	-2.56	117.90	120.72
24	A	406[B]	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
26	D	404	BCR	C15-C14-C13	-2.56	123.65	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	d	407[B]	LHG	O8-C23-O10	-2.56	117.13	123.59
26	C	515	BCR	C40-C30-C25	-2.56	106.14	110.30
24	a	405[B]	CLA	CHD-C4C-NC	2.56	128.24	124.20
30	A	415[A]	PL9	C10-C9-C8	-2.56	117.11	123.68
24	b	604	CLA	C4C-C3C-C2C	-2.56	103.17	106.90
24	b	603	CLA	CHC-C1C-C2C	-2.56	119.64	126.72
41	V	201	HEC	CMB-C2B-C3B	2.56	128.83	125.82
24	a	407[B]	CLA	O2A-CGA-O1A	-2.56	117.14	123.59
24	D	402[B]	CLA	CHD-C4C-NC	2.56	128.23	124.20
30	A	415[B]	PL9	C53-C6-C1	2.56	120.22	114.99
24	C	508	CLA	C3B-C4B-NB	2.56	112.51	109.21
27	a	413	SQD	O8-S-C6	2.55	109.81	105.74
36	C	519	DGD	O2G-C1B-C2B	2.55	117.00	111.50
32	A	421	LMT	O5'-C5'-C6'	2.55	112.78	106.44
32	M	104	LMT	C1'-O5'-C5'	-2.55	108.68	113.69
24	a	407[B]	CLA	O2A-CGA-CBA	2.55	119.91	111.91
24	c	505	CLA	O2A-CGA-O1A	-2.55	117.16	123.59
26	a	410	BCR	C7-C8-C9	-2.55	122.39	126.23
26	C	515	BCR	C33-C5-C6	-2.55	121.67	124.53
26	y	101	BCR	C21-C20-C19	-2.55	115.27	123.22
24	c	506	CLA	O2A-CGA-CBA	2.55	119.90	111.91
24	c	514	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
24	A	406[A]	CLA	O2A-CGA-O1A	-2.54	117.17	123.59
24	c	504	CLA	CHC-C1C-C2C	-2.54	119.68	126.72
24	C	506	CLA	CMB-C2B-C1B	2.54	132.38	128.46
24	d	403[A]	CLA	CAA-C2A-C3A	-2.54	105.81	112.78
30	A	415[A]	PL9	C47-C48-C49	-2.54	119.05	127.75
27	a	411[B]	SQD	O8-S-C6	2.54	109.79	105.74
30	a	415[B]	PL9	C40-C39-C41	2.54	119.55	115.27
24	a	409	CLA	C4C-C3C-C2C	-2.54	103.19	106.90
36	C	517[B]	DGD	C2G-O2G-C1B	-2.54	111.53	117.79
24	b	609	CLA	O2A-CGA-CBA	2.54	119.88	111.91
24	c	509	CLA	CHC-C1C-C2C	-2.54	119.69	126.72
30	A	415[B]	PL9	C42-C43-C44	-2.54	121.55	127.66
36	C	517[B]	DGD	C3G-C2G-C1G	-2.54	105.78	111.79
26	B	619	BCR	C7-C8-C9	-2.54	122.40	126.23
30	d	406[B]	PL9	C12-C13-C14	-2.54	121.55	127.66
30	a	415[B]	PL9	C47-C48-C49	-2.54	119.08	127.75
25	A	417[B]	PHO	C4-C3-C5	2.54	119.54	115.27
24	c	511	CLA	C4-C3-C2	-2.54	117.17	123.68
24	c	502	CLA	O2A-CGA-CBA	2.54	119.86	111.91
24	b	606	CLA	C1-C2-C3	-2.54	121.66	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	413	SQD	O48-C23-O10	-2.53	117.19	123.59
24	c	502	CLA	CAC-C3C-C4C	2.53	128.10	124.81
24	C	505	CLA	OBD-CAD-C3D	-2.53	122.43	128.52
24	c	513	CLA	CMA-C3A-C4A	-2.53	104.98	111.77
24	d	403[B]	CLA	CHD-C4C-NC	2.53	128.19	124.20
25	A	417[B]	PHO	CED-O2D-CGD	2.53	121.66	115.94
24	c	507	CLA	C2A-C1A-CHA	-2.53	119.44	123.86
25	A	408[B]	PHO	CMB-C2B-C3B	2.53	129.40	124.68
24	B	604	CLA	O1D-CGD-CBD	-2.52	119.32	124.48
24	B	603	CLA	CMA-C3A-C2A	-2.52	103.65	113.83
26	T	101	BCR	C7-C8-C9	-2.52	122.42	126.23
24	B	608	CLA	C11-C10-C8	-2.52	107.77	115.92
24	B	608	CLA	C1-C2-C3	-2.52	121.68	126.04
24	b	602	CLA	C11-C12-C13	-2.52	107.77	115.92
35	C	501	LMG	O6-C1-O1	-2.52	104.01	109.97
24	C	514	CLA	CHC-C1C-C2C	-2.52	119.75	126.72
24	B	615	CLA	CHC-C1C-C2C	-2.52	119.75	126.72
24	a	407[B]	CLA	CHC-C1C-C2C	-2.52	119.76	126.72
27	a	413	SQD	C1-O5-C5	2.52	118.63	113.69
24	B	606	CLA	C2A-C1A-CHA	-2.52	119.46	123.86
24	B	603	CLA	C2A-C1A-CHA	-2.51	119.46	123.86
24	a	406[A]	CLA	CAA-CBA-CGA	2.51	120.59	113.25
24	a	407[B]	CLA	CBC-CAC-C3C	-2.51	105.51	112.43
24	D	403	CLA	CMA-C3A-C4A	-2.51	105.02	111.77
24	b	610	CLA	C3B-C4B-NB	2.51	112.46	109.21
24	d	403[A]	CLA	CMC-C2C-C1C	2.51	128.86	125.04
24	C	514	CLA	CHD-C4C-NC	2.51	128.16	124.20
24	d	404	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
24	c	508	CLA	O1D-CGD-CBD	-2.51	119.35	124.48
24	B	609	CLA	CHD-C4C-NC	2.51	128.16	124.20
26	c	516	BCR	C37-C22-C23	2.51	122.03	118.08
24	A	407[A]	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
24	B	604	CLA	C6-C5-C3	-2.51	106.88	113.45
24	a	405[A]	CLA	CHD-C4C-NC	2.51	128.15	124.20
32	B	630	LMT	C3'-C4'-C5'	-2.51	105.18	110.93
24	A	409	CLA	O2A-CGA-O1A	-2.51	117.27	123.59
24	B	612	CLA	CHD-C4C-NC	2.51	128.15	124.20
24	B	602	CLA	CHC-C1C-C2C	-2.50	119.79	126.72
30	A	415[B]	PL9	C12-C13-C14	-2.50	121.63	127.66
33	A	420[B]	LHG	O8-C23-C24	2.50	119.76	111.91
30	D	405[A]	PL9	C42-C41-C39	-2.50	104.75	112.98
36	C	519	DGD	O3G-C3G-C2G	-2.50	104.86	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	607	CLA	C2A-C1A-CHA	-2.50	119.49	123.86
24	C	512	CLA	C1-C2-C3	-2.50	121.72	126.04
36	C	518[B]	DGD	O1G-C1A-O1A	-2.50	117.28	123.59
34	b	621	HTG	C6-C5-C4	-2.50	107.15	113.00
26	a	410	BCR	C33-C5-C6	-2.50	121.72	124.53
24	b	603	CLA	C7-C6-C5	-2.50	106.57	113.36
26	Y	101	BCR	C15-C16-C17	-2.50	118.36	123.47
36	c	518[A]	DGD	O1G-C1A-C2A	2.50	119.74	111.91
30	A	415[B]	PL9	C10-C9-C11	2.50	119.47	115.27
24	a	409	CLA	CMA-C3A-C2A	-2.50	103.76	113.83
24	B	610	CLA	O1D-CGD-CBD	-2.50	119.38	124.48
24	b	616	CLA	C4-C3-C5	2.49	119.47	115.27
24	a	405[A]	CLA	C4C-C3C-C2C	-2.49	103.26	106.90
24	C	503	CLA	O2A-CGA-O1A	-2.49	117.30	123.59
26	B	619	BCR	C2-C1-C6	2.49	114.32	110.48
24	b	610	CLA	CHD-C4C-NC	2.49	128.13	124.20
24	c	502	CLA	C4-C3-C5	2.49	119.46	115.27
24	C	509	CLA	CMC-C2C-C1C	2.49	128.83	125.04
35	C	501	LMG	C1-O6-C5	-2.49	108.80	113.69
36	c	517[B]	DGD	C2G-O2G-C1B	-2.49	111.66	117.79
24	b	601	CLA	C2A-C1A-CHA	-2.49	119.50	123.86
24	c	503	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
32	M	102	LMT	C1'-O5'-C5'	-2.49	108.80	113.69
24	C	513	CLA	CMA-C3A-C4A	-2.49	105.08	111.77
24	C	513	CLA	CBC-CAC-C3C	-2.49	105.57	112.43
24	b	611	CLA	CMC-C2C-C1C	2.49	128.83	125.04
24	A	406[B]	CLA	OBD-CAD-C3D	-2.49	122.53	128.52
24	B	609	CLA	CMC-C2C-C1C	2.49	128.83	125.04
24	b	601	CLA	CMC-C2C-C1C	2.49	128.82	125.04
27	a	411[A]	SQD	O8-S-C6	2.49	109.70	105.74
26	D	404	BCR	C29-C28-C27	-2.48	105.83	111.38
24	c	513	CLA	CBA-CAA-C2A	-2.48	106.53	113.86
24	D	403	CLA	C2A-C1A-CHA	-2.48	119.52	123.86
24	a	406[B]	CLA	C4C-C3C-C2C	-2.48	103.28	106.90
24	a	406[A]	CLA	CBC-CAC-C3C	-2.48	105.59	112.43
24	c	513	CLA	CMC-C2C-C1C	2.48	128.82	125.04
24	b	615	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
33	A	420[B]	LHG	O7-C7-O9	-2.48	117.71	123.70
24	b	614	CLA	C4-C3-C5	2.48	119.44	115.27
30	d	406[B]	PL9	C15-C14-C16	2.48	119.44	115.27
24	A	407[A]	CLA	CMB-C2B-C1B	2.48	132.27	128.46
24	c	504	CLA	CBC-CAC-C3C	-2.48	105.60	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B	630	LMT	O1'-C1'-C2'	2.48	112.17	108.30
24	d	403[B]	CLA	CAC-C3C-C4C	2.48	128.02	124.81
24	C	507	CLA	O2A-CGA-CBA	2.48	119.68	111.91
27	X	101	SQD	O47-C7-O49	-2.48	117.72	123.70
30	D	405[A]	PL9	C20-C19-C21	2.47	119.43	115.27
24	b	602	CLA	C1-O2A-CGA	2.47	122.93	116.44
24	C	502	CLA	C4C-C3C-C2C	-2.47	103.29	106.90
36	c	517[A]	DGD	C2G-O2G-C1B	-2.47	111.70	117.79
24	C	505	CLA	CMB-C2B-C3B	2.47	129.30	124.68
26	C	515	BCR	C16-C17-C18	-2.47	123.78	127.31
33	d	407[B]	LHG	O8-C23-C24	2.47	119.66	111.91
35	D	411	LMG	O8-C28-O10	-2.47	117.36	123.59
24	A	405[B]	CLA	C4-C3-C5	2.47	119.42	115.27
24	A	407[B]	CLA	CMA-C3A-C2A	-2.47	103.87	113.83
24	B	607	CLA	CHC-C1C-C2C	-2.47	119.90	126.72
26	K	102	BCR	C20-C21-C22	-2.47	123.79	127.31
24	c	507	CLA	O2A-CGA-CBA	2.47	119.65	111.91
24	C	510	CLA	CHC-C1C-C2C	-2.47	119.90	126.72
24	D	403	CLA	CHC-C1C-C2C	-2.47	119.90	126.72
26	D	404	BCR	C30-C25-C24	2.46	122.75	115.78
24	b	608	CLA	CHB-C4A-NA	2.46	127.92	124.51
25	A	408[A]	PHO	CMB-C2B-C3B	2.46	129.29	124.68
26	T	101	BCR	C33-C5-C6	-2.46	121.76	124.53
24	d	404	CLA	CMC-C2C-C1C	2.46	128.79	125.04
39	F	102	HEM	C4D-ND-C1D	2.46	107.61	105.07
24	B	607	CLA	CMA-C3A-C2A	-2.46	103.90	113.83
24	B	609	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
25	a	408[B]	PHO	O2D-CGD-O1D	-2.46	119.03	123.84
24	B	609	CLA	CED-O2D-CGD	2.46	121.50	115.94
24	b	606	CLA	O2A-CGA-O1A	-2.46	117.39	123.59
24	A	405[A]	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
36	C	519	DGD	O1G-C1A-O1A	-2.46	117.39	123.59
30	A	415[B]	PL9	C25-C24-C26	2.46	119.40	115.27
26	h	101	BCR	C11-C10-C9	-2.45	123.81	127.31
24	C	512	CLA	O2A-CGA-CBA	2.45	119.61	111.91
24	B	611	CLA	C4A-NA-C1A	-2.45	105.60	106.71
24	b	608	CLA	CMA-C3A-C4A	-2.45	105.18	111.77
26	B	617	BCR	C37-C22-C23	2.45	121.94	118.08
32	b	620	LMT	C1'-O5'-C5'	-2.45	108.88	113.69
24	b	607	CLA	C1-O2A-CGA	2.45	122.88	116.44
35	c	521	LMG	O8-C28-O10	-2.45	117.40	123.59
24	C	510	CLA	CAC-C3C-C4C	2.45	127.99	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	408[B]	PHO	CMA-C3A-C4A	-2.45	109.01	114.38
24	A	405[A]	CLA	CAA-CBA-CGA	-2.45	106.09	113.25
24	B	601	CLA	CHC-C1C-C2C	-2.45	119.95	126.72
25	a	408[B]	PHO	O2A-CGA-O1A	-2.45	117.41	123.59
30	D	405[A]	PL9	C40-C39-C41	2.45	119.39	115.27
24	C	508	CLA	CHC-C1C-C2C	-2.45	119.95	126.72
24	C	509	CLA	CMB-C2B-C3B	2.44	129.25	124.68
24	D	402[B]	CLA	O2A-CGA-O1A	-2.44	117.42	123.59
24	B	602	CLA	CMA-C3A-C4A	-2.44	105.21	111.77
24	b	612	CLA	CHC-C1C-C2C	-2.44	119.96	126.72
24	b	614	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
35	Z	101	LMG	C9-C8-C7	-2.44	106.01	111.79
24	c	505	CLA	C4-C3-C5	2.44	119.38	115.27
24	a	407[B]	CLA	CMB-C2B-C3B	2.44	129.24	124.68
30	D	405[B]	PL9	C7-C8-C9	-2.44	122.73	126.79
30	A	415[B]	PL9	C45-C44-C46	2.44	119.37	115.27
24	B	612	CLA	CHC-C1C-C2C	-2.44	119.98	126.72
32	B	627	LMT	O1'-C1'-C2'	2.44	112.11	108.30
24	c	504	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
24	C	511	CLA	C4-C3-C2	-2.43	117.44	123.68
26	H	101	BCR	C24-C23-C22	-2.43	122.56	126.23
24	C	505	CLA	CBC-CAC-C3C	-2.43	105.72	112.43
24	B	604	CLA	C4-C3-C5	2.43	119.36	115.27
24	B	604	CLA	C11-C12-C13	-2.43	108.06	115.92
24	C	510	CLA	C4-C3-C5	2.43	119.36	115.27
26	D	404	BCR	C16-C17-C18	-2.43	123.84	127.31
24	C	506	CLA	CBC-CAC-C3C	-2.43	105.73	112.43
24	C	513	CLA	C2A-C1A-CHA	-2.43	119.61	123.86
24	B	607	CLA	CAA-C2A-C3A	-2.43	106.13	112.78
24	a	409	CLA	CHC-C1C-C2C	-2.43	120.01	126.72
24	b	602	CLA	CMA-C3A-C4A	-2.43	105.25	111.77
24	b	604	CLA	O2A-CGA-O1A	-2.43	117.47	123.59
24	A	406[A]	CLA	CAA-CBA-CGA	2.42	120.34	113.25
24	b	607	CLA	CMB-C2B-C3B	2.42	129.21	124.68
24	C	510	CLA	C11-C12-C13	-2.42	108.09	115.92
24	b	607	CLA	CAC-C3C-C4C	2.42	127.95	124.81
26	B	618	BCR	C37-C22-C23	2.42	121.89	118.08
27	f	101	SQD	O8-S-C6	2.42	109.60	105.74
26	d	405	BCR	C28-C27-C26	-2.42	109.76	114.08
24	D	403	CLA	CHD-C4C-NC	2.42	128.01	124.20
24	A	407[A]	CLA	C1-C2-C3	-2.42	121.86	126.04
26	b	619	BCR	C24-C23-C22	-2.42	122.58	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	409	CLA	C2A-C1A-CHA	-2.42	119.63	123.86
27	A	413	SQD	O48-C23-O10	-2.42	117.49	123.59
30	D	405[A]	PL9	C7-C8-C9	-2.41	122.77	126.79
33	A	420[A]	LHG	O7-C7-O9	-2.41	117.87	123.70
24	b	615	CLA	C6-C7-C8	-2.41	108.12	115.92
24	C	508	CLA	CHD-C4C-NC	2.41	128.01	124.20
24	d	404	CLA	CHD-C4C-NC	2.41	128.01	124.20
24	b	609	CLA	CMA-C3A-C4A	-2.41	105.29	111.77
26	B	617	BCR	C7-C8-C9	-2.41	122.59	126.23
24	B	601	CLA	CAC-C3C-C4C	2.41	127.94	124.81
24	C	512	CLA	CMB-C2B-C3B	2.41	129.19	124.68
32	F	101	LMT	C3B-C4B-C5B	-2.41	105.94	110.24
24	b	605	CLA	O2A-CGA-CBA	2.41	119.47	111.91
26	Y	101	BCR	C1-C6-C7	2.41	122.59	115.78
24	b	609	CLA	C16-C15-C13	-2.41	108.14	115.92
24	b	608	CLA	CAA-C2A-C3A	-2.41	106.19	112.78
25	A	408[A]	PHO	CMA-C3A-C4A	-2.41	109.11	114.38
24	b	615	CLA	CHD-C4C-NC	2.41	128.00	124.20
26	Y	101	BCR	C36-C18-C19	2.41	121.87	118.08
24	A	406[B]	CLA	O2A-CGA-O1A	-2.41	117.52	123.59
24	c	512	CLA	O2A-CGA-O1A	-2.41	117.52	123.59
39	F	102	HEM	O2A-CGA-CBA	2.41	121.76	114.03
24	b	604	CLA	O2A-CGA-CBA	2.40	119.45	111.91
24	c	514	CLA	CMB-C2B-C3B	2.40	129.17	124.68
33	b	628[A]	LHG	O8-C23-O10	-2.40	117.53	123.59
26	T	101	BCR	C16-C17-C18	-2.40	123.89	127.31
24	d	403[B]	CLA	CMC-C2C-C1C	2.40	128.69	125.04
24	A	405[B]	CLA	CMA-C3A-C2A	-2.40	104.15	113.83
33	d	408[A]	LHG	O8-C23-O10	-2.40	117.54	123.59
32	B	628	LMT	O5'-C5'-C4'	2.40	114.81	109.75
35	d	412	LMG	O8-C28-C29	2.40	119.43	111.91
30	d	406[A]	PL9	C17-C18-C19	-2.40	121.89	127.66
24	b	611	CLA	CHD-C4C-NC	2.40	127.98	124.20
25	A	417[B]	PHO	CMC-C2C-C3C	2.40	129.46	124.94
24	c	508	CLA	CMB-C2B-C1B	2.40	132.15	128.46
27	f	101	SQD	C4-C3-C2	-2.40	106.64	110.82
25	A	408[B]	PHO	O2D-CGD-O1D	-2.40	119.15	123.84
27	a	413	SQD	O7-S-C6	2.39	109.78	106.94
27	A	413	SQD	O7-S-C6	2.39	109.78	106.94
24	B	608	CLA	CHD-C4C-NC	2.39	127.97	124.20
30	d	406[A]	PL9	C7-C8-C9	-2.39	122.81	126.79
24	b	615	CLA	CAC-C3C-C4C	2.39	127.91	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T	101	BCR	C12-C13-C14	-2.39	115.27	118.94
32	B	628	LMT	O5'-C5'-C6'	2.39	112.38	106.44
27	f	101	SQD	O47-C7-O49	-2.39	117.93	123.70
26	y	101	BCR	C10-C11-C12	-2.39	115.77	123.22
24	c	508	CLA	CHC-C1C-C2C	-2.38	120.13	126.72
25	A	417[B]	PHO	CMB-C2B-C3B	2.38	129.14	124.68
26	c	515	BCR	C20-C21-C22	-2.38	123.91	127.31
24	D	402[A]	CLA	CMC-C2C-C1C	2.38	128.67	125.04
24	a	405[A]	CLA	CMA-C3A-C2A	-2.38	104.22	113.83
30	a	415[A]	PL9	C20-C19-C21	2.38	119.28	115.27
39	e	101	HEM	CMD-C2D-C1D	2.38	128.66	125.04
26	b	618	BCR	C8-C7-C6	-2.38	120.52	127.20
36	c	517[B]	DGD	O6D-C1D-O3G	-2.38	104.34	109.97
30	D	405[A]	PL9	C36-C37-C38	-2.38	104.07	111.88
24	c	509	CLA	CMB-C2B-C3B	2.38	129.12	124.68
24	B	605	CLA	C2A-C1A-CHA	-2.38	119.71	123.86
24	b	609	CLA	O2D-CGD-O1D	-2.37	119.19	123.84
26	c	516	BCR	C33-C5-C6	-2.37	121.86	124.53
30	A	415[B]	PL9	C47-C48-C49	-2.37	119.64	127.75
24	C	505	CLA	C4C-C3C-C2C	-2.37	103.44	106.90
24	A	407[A]	CLA	CAC-C3C-C4C	2.37	127.89	124.81
24	A	409	CLA	CHB-C4A-NA	2.37	127.79	124.51
24	C	503	CLA	CHD-C4C-NC	2.37	127.94	124.20
24	a	405[A]	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
24	B	602	CLA	CHB-C4A-NA	2.37	127.79	124.51
24	C	502	CLA	O2A-CGA-CBA	2.37	119.34	111.91
25	A	417[B]	PHO	O2A-CGA-CBA	2.37	119.34	111.91
39	F	102	HEM	O2D-CGD-CBD	2.37	121.64	114.03
24	D	403	CLA	CAA-C2A-C3A	-2.37	106.29	112.78
25	A	408[B]	PHO	O2A-CGA-CBA	2.37	119.34	111.91
24	a	407[B]	CLA	C1-O2A-CGA	2.37	122.66	116.44
32	A	421	LMT	O5'-C5'-C4'	2.37	114.74	109.75
24	B	608	CLA	C4-C3-C5	2.37	119.25	115.27
26	y	101	BCR	C11-C10-C9	-2.37	123.93	127.31
30	d	406[B]	PL9	C30-C29-C31	2.37	119.25	115.27
26	h	101	BCR	C36-C18-C17	-2.36	119.61	122.92
33	d	408[B]	LHG	O8-C23-O10	-2.36	117.63	123.59
26	B	617	BCR	C16-C17-C18	-2.36	123.94	127.31
25	d	402[A]	PHO	C1A-C2A-C3A	-2.36	100.59	102.84
24	c	508	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
24	C	507	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
24	b	602	CLA	C1B-CHB-C4A	-2.36	125.44	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	c	517[A]	DGD	C3G-C2G-C1G	-2.36	106.21	111.79
27	L	102	SQD	O48-C23-C24	2.36	119.31	111.91
26	T	101	BCR	C16-C15-C14	2.36	128.31	123.47
24	c	514	CLA	CHD-C4C-NC	2.36	127.92	124.20
24	B	611	CLA	C2C-C1C-NC	2.36	112.18	109.97
24	c	504	CLA	C2A-C1A-CHA	-2.36	119.74	123.86
26	c	516	BCR	C21-C20-C19	-2.36	115.86	123.22
24	A	407[B]	CLA	CAC-C3C-C4C	2.36	127.87	124.81
27	f	101	SQD	O6-C1-C2	2.36	111.98	108.30
30	d	406[A]	PL9	C12-C13-C14	-2.36	121.99	127.66
24	b	608	CLA	C4-C3-C5	2.35	119.23	115.27
24	c	503	CLA	C1-C2-C3	-2.35	121.97	126.04
33	A	420[B]	LHG	O8-C6-C5	-2.35	101.58	108.43
26	T	101	BCR	C3-C4-C5	-2.35	109.88	114.08
24	a	407[A]	CLA	C1-C2-C3	-2.35	121.98	126.04
24	C	509	CLA	O2A-CGA-CBA	2.35	119.28	111.91
35	C	520	LMG	C8-O7-C10	-2.35	112.01	117.79
24	C	511	CLA	C2A-C1A-CHA	-2.35	119.75	123.86
30	A	415[A]	PL9	C45-C44-C46	2.35	119.22	115.27
24	B	609	CLA	CAC-C3C-C4C	2.35	127.86	124.81
26	C	515	BCR	C38-C26-C25	-2.35	121.89	124.53
24	C	508	CLA	CAC-C3C-C4C	2.35	127.86	124.81
24	b	608	CLA	C11-C12-C13	-2.35	108.33	115.92
24	c	503	CLA	C2A-C1A-CHA	-2.35	119.76	123.86
24	b	606	CLA	C2A-C1A-CHA	-2.35	119.76	123.86
24	c	505	CLA	CMB-C2B-C3B	2.34	129.06	124.68
24	d	404	CLA	O2A-CGA-CBA	2.34	119.27	111.91
24	A	406[B]	CLA	CMA-C3A-C2A	-2.34	104.37	113.83
26	b	618	BCR	C16-C17-C18	-2.34	123.97	127.31
24	A	409	CLA	CHD-C4C-NC	2.34	127.90	124.20
24	C	506	CLA	CHD-C4C-NC	2.34	127.90	124.20
27	X	101	SQD	O5-C1-C2	-2.34	105.39	110.35
24	A	407[A]	CLA	CMA-C3A-C2A	-2.34	104.38	113.83
25	d	402[B]	PHO	CMA-C3A-C4A	-2.34	109.25	114.38
26	H	101	BCR	C10-C11-C12	-2.34	115.91	123.22
25	A	417[B]	PHO	C6-C5-C3	-2.34	107.32	113.45
24	c	514	CLA	C4-C3-C5	2.34	119.21	115.27
24	A	405[B]	CLA	CMB-C2B-C3B	2.34	129.06	124.68
26	C	516	BCR	C29-C30-C25	2.34	114.08	110.48
24	b	602	CLA	C11-C10-C8	-2.34	108.36	115.92
28	b	627	GOL	C3-C2-C1	-2.34	102.61	111.70
30	A	415[A]	PL9	C42-C43-C44	-2.34	122.03	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	405[B]	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
24	B	610	CLA	CAC-C3C-C2C	2.34	131.53	127.53
39	F	102	HEM	C4B-C3B-C2B	-2.34	105.26	107.11
24	d	403[B]	CLA	C1B-CHB-C4A	-2.33	125.49	130.12
33	d	407[A]	LHG	C6-C5-C4	-2.33	106.27	111.79
30	d	406[A]	PL9	C20-C19-C21	2.33	119.20	115.27
36	H	102	DGD	O6E-C5E-C6E	2.33	112.24	106.44
25	d	402[B]	PHO	CBA-CAA-C2A	-2.33	107.00	113.81
25	d	402[B]	PHO	CMC-C2C-C3C	2.33	129.34	124.94
24	B	605	CLA	CAC-C3C-C4C	2.33	127.83	124.81
33	b	628[B]	LHG	O7-C7-O9	-2.33	118.07	123.70
24	c	509	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
36	C	518[B]	DGD	O2G-C1B-O1B	-2.33	118.08	123.70
24	C	510	CLA	C16-C15-C13	-2.33	108.40	115.92
35	C	520	LMG	O8-C28-O10	-2.33	117.72	123.59
24	C	503	CLA	C4C-C3C-C2C	-2.33	103.51	106.90
27	L	102	SQD	O47-C7-O49	-2.33	118.08	123.70
26	c	515	BCR	C35-C13-C14	-2.33	119.67	122.92
24	B	614	CLA	CAA-C2A-C3A	-2.33	106.41	112.78
26	y	101	BCR	C16-C17-C18	-2.32	123.99	127.31
24	B	616	CLA	CHD-C4C-NC	2.32	127.87	124.20
24	C	505	CLA	CAC-C3C-C4C	2.32	127.82	124.81
24	C	507	CLA	C4C-C3C-C2C	-2.32	103.51	106.90
24	B	601	CLA	CHB-C4A-NA	2.32	127.72	124.51
26	h	101	BCR	C10-C11-C12	-2.32	115.97	123.22
24	B	611	CLA	OBD-CAD-C3D	-2.32	122.94	128.52
24	c	514	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
32	b	626	LMT	O1'-C1'-C2'	2.32	111.92	108.30
24	C	508	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
36	c	519	DGD	O3G-C1D-C2D	-2.32	104.69	108.30
24	C	508	CLA	O2A-CGA-CBA	2.32	119.18	111.91
36	H	102	DGD	O1G-C1A-O1A	-2.32	117.75	123.59
24	A	405[B]	CLA	CMC-C2C-C1C	2.32	128.57	125.04
26	c	516	BCR	C29-C30-C25	2.31	114.04	110.48
39	e	101	HEM	C3C-C4C-NC	-2.31	106.58	110.94
26	c	515	BCR	C28-C27-C26	-2.31	109.95	114.08
24	C	502	CLA	C11-C12-C13	-2.31	108.44	115.92
24	b	606	CLA	C1-O2A-CGA	2.31	122.51	116.44
26	y	101	BCR	C32-C1-C6	-2.31	106.55	110.30
24	a	406[A]	CLA	CMC-C2C-C1C	2.31	128.56	125.04
26	b	617	BCR	C32-C1-C6	-2.31	106.55	110.30
24	B	601	CLA	CMC-C2C-C1C	2.31	128.56	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T	101	BCR	C1-C6-C7	2.31	122.31	115.78
26	H	101	BCR	C36-C18-C17	-2.31	119.69	122.92
36	C	518[A]	DGD	C2G-O2G-C1B	-2.31	112.11	117.79
24	C	510	CLA	C2A-C1A-CHA	-2.31	119.83	123.86
35	c	520	LMG	O8-C28-O10	-2.31	117.77	123.59
35	C	501	LMG	C9-C8-C7	-2.31	106.33	111.79
26	K	102	BCR	C38-C26-C25	-2.31	121.94	124.53
24	c	507	CLA	C4-C3-C5	2.31	119.15	115.27
24	c	505	CLA	C1-C2-C3	-2.30	122.06	126.04
30	D	405[B]	PL9	C37-C38-C39	-2.30	122.11	127.66
36	C	517[A]	DGD	O6E-C5E-C4E	2.30	113.88	109.69
32	b	620	LMT	C2'-C3'-C4'	2.30	114.94	109.68
24	b	613	CLA	OBD-CAD-C3D	-2.30	122.98	128.52
24	B	604	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
24	B	604	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
26	c	515	BCR	C36-C18-C19	2.30	121.70	118.08
24	C	511	CLA	CMA-C3A-C4A	-2.30	105.59	111.77
27	a	411[B]	SQD	C3-C4-C5	2.30	114.34	110.24
24	b	602	CLA	C4-C3-C5	2.30	119.14	115.27
24	d	403[B]	CLA	CBC-CAC-C3C	-2.30	106.09	112.43
24	A	409	CLA	CMA-C3A-C4A	-2.30	105.59	111.77
24	B	606	CLA	CMB-C2B-C3B	2.30	128.98	124.68
32	b	626	LMT	C1'-O5'-C5'	-2.30	109.18	113.69
24	b	613	CLA	CAC-C3C-C4C	2.30	127.79	124.81
24	B	602	CLA	CAA-CBA-CGA	-2.30	106.54	113.25
36	c	518[B]	DGD	O1G-C1A-O1A	-2.30	117.80	123.59
27	a	411[A]	SQD	O48-C23-C24	2.30	119.11	111.91
24	B	613	CLA	CHB-C4A-NA	2.30	127.69	124.51
24	b	613	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
27	B	620	SQD	C44-O6-C1	-2.30	109.25	113.74
24	B	613	CLA	CMA-C3A-C4A	-2.29	105.61	111.77
24	B	601	CLA	C2A-C1A-CHA	-2.29	119.85	123.86
26	d	405	BCR	C40-C30-C39	2.29	115.56	108.53
24	b	606	CLA	CMB-C2B-C3B	2.29	128.97	124.68
32	m	102	LMT	O5B-C5B-C6B	2.29	112.13	106.44
24	C	507	CLA	CMB-C2B-C3B	2.29	128.97	124.68
32	A	421	LMT	O1'-C1'-C2'	2.29	111.88	108.30
24	c	509	CLA	CAC-C3C-C4C	2.29	127.78	124.81
24	b	606	CLA	CAA-C2A-C3A	-2.29	106.51	112.78
24	d	403[B]	CLA	CAA-C2A-C3A	-2.29	106.52	112.78
24	c	511	CLA	C11-C10-C8	-2.29	108.53	115.92
36	C	517[A]	DGD	C3G-C2G-C1G	-2.29	106.38	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	410	BCR	C8-C7-C6	-2.28	120.79	127.20
24	a	407[B]	CLA	CAC-C3C-C4C	2.28	127.77	124.81
24	C	509	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
26	Y	101	BCR	C36-C18-C17	-2.28	119.73	122.92
24	c	512	CLA	CMB-C2B-C3B	2.28	128.95	124.68
26	y	101	BCR	C38-C26-C25	-2.28	121.97	124.53
34	B	621	HTG	O2-C2-C3	-2.28	105.08	110.35
24	C	513	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
26	y	101	BCR	C28-C27-C26	-2.28	110.01	114.08
24	D	402[A]	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
27	A	411[B]	SQD	O8-S-C6	2.28	109.37	105.74
26	T	101	BCR	C21-C20-C19	-2.28	116.11	123.22
30	d	406[A]	PL9	C51-C49-C50	2.28	119.63	114.60
30	a	415[B]	PL9	C51-C49-C50	2.27	119.62	114.60
24	a	409	CLA	OBD-CAD-C3D	-2.27	123.05	128.52
24	a	407[B]	CLA	CHB-C4A-NA	2.27	127.66	124.51
24	B	606	CLA	C1-O2A-CGA	2.27	122.41	116.44
24	A	406[B]	CLA	O2A-CGA-CBA	2.27	119.04	111.91
24	b	605	CLA	CHB-C4A-NA	2.27	127.65	124.51
25	d	402[A]	PHO	O2A-CGA-CBA	2.27	119.03	111.91
24	C	508	CLA	CHA-C1A-NA	-2.27	121.20	126.40
27	A	411[B]	SQD	O48-C23-O10	-2.27	117.87	123.59
36	H	102	DGD	C3E-C4E-C5E	-2.27	106.19	110.24
24	B	616	CLA	C2A-C1A-CHA	-2.27	119.89	123.86
24	c	505	CLA	C2A-C1A-CHA	-2.27	119.89	123.86
30	A	415[A]	PL9	C35-C34-C33	-2.27	117.86	123.68
26	K	102	BCR	C15-C14-C13	-2.27	124.07	127.31
24	b	603	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
24	a	405[A]	CLA	C7-C6-C5	-2.27	107.20	113.36
24	B	612	CLA	C2A-C1A-CHA	-2.27	119.90	123.86
24	d	404	CLA	CHB-C4A-NA	2.26	127.64	124.51
24	B	604	CLA	C6-C7-C8	-2.26	108.60	115.92
32	F	101	LMT	C1'-O5'-C5'	-2.26	109.25	113.69
24	c	511	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
24	b	613	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
36	C	518[A]	DGD	O2G-C1B-O1B	-2.26	118.24	123.70
24	c	512	CLA	C1-O2A-CGA	2.26	122.37	116.44
24	C	508	CLA	C1-C2-C3	-2.26	122.14	126.04
26	t	102	BCR	C36-C18-C19	2.26	121.64	118.08
25	d	402[B]	PHO	O2A-CGA-CBA	2.26	118.99	111.91
24	B	612	CLA	C4-C3-C5	2.26	119.07	115.27
24	D	402[A]	CLA	CMB-C2B-C3B	2.26	128.90	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	406[B]	CLA	C1-C2-C3	-2.26	122.14	126.04
33	L	101[B]	LHG	O8-C23-O10	-2.26	117.90	123.59
26	a	410	BCR	C40-C30-C25	-2.26	106.64	110.30
24	C	509	CLA	C2A-C1A-CHA	-2.26	119.92	123.86
24	D	402[B]	CLA	CAA-C2A-C3A	-2.25	106.60	112.78
24	B	615	CLA	CHA-C1A-NA	-2.25	121.23	126.40
25	a	408[B]	PHO	C1-C2-C3	-2.25	122.14	126.04
25	A	408[A]	PHO	C4-C3-C5	2.25	119.06	115.27
24	b	611	CLA	CHB-C4A-NA	2.25	127.63	124.51
24	b	609	CLA	C7-C6-C5	-2.25	107.24	113.36
24	D	402[A]	CLA	CED-O2D-CGD	2.25	121.03	115.94
25	a	408[A]	PHO	CMA-C3A-C4A	-2.25	109.45	114.38
24	a	406[A]	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
24	a	407[B]	CLA	CMA-C3A-C4A	-2.25	105.73	111.77
32	m	102	LMT	C3B-C4B-C5B	-2.25	106.23	110.24
24	B	616	CLA	CMC-C2C-C1C	2.25	128.46	125.04
32	e	102	LMT	O1'-C1'-C2'	2.25	111.81	108.30
24	B	615	CLA	C2A-C1A-CHA	-2.25	119.93	123.86
35	C	521	LMG	O1-C1-C2	2.25	111.81	108.30
36	c	517[A]	DGD	O3G-C3G-C2G	-2.24	105.48	110.90
24	c	513	CLA	CBC-CAC-C3C	-2.24	106.24	112.43
26	B	617	BCR	C37-C22-C21	-2.24	119.78	122.92
30	d	406[A]	PL9	C47-C48-C49	-2.24	120.08	127.75
26	Y	101	BCR	C3-C4-C5	-2.24	110.07	114.08
33	b	628[B]	LHG	C5-O7-C7	-2.24	112.27	117.79
24	c	510	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
33	d	407[B]	LHG	C6-C5-C4	-2.24	106.49	111.79
35	a	417	LMG	O7-C10-O9	-2.24	118.29	123.70
30	d	406[B]	PL9	C51-C49-C50	2.24	119.55	114.60
35	Z	101	LMG	C1-O6-C5	2.24	118.08	113.69
24	b	608	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
36	c	517[B]	DGD	C3G-C2G-C1G	-2.24	106.49	111.79
26	K	102	BCR	C36-C18-C19	2.24	121.60	118.08
25	d	402[B]	PHO	C1A-C2A-C3A	-2.24	100.71	102.84
24	b	602	CLA	CMB-C2B-C3B	2.24	128.86	124.68
25	d	402[B]	PHO	C4A-C3A-C2A	-2.24	100.71	102.84
24	a	405[B]	CLA	CMA-C3A-C2A	-2.24	104.81	113.83
24	C	507	CLA	CAA-C2A-C3A	-2.23	106.66	112.78
27	f	101	SQD	O48-C23-O10	-2.23	117.95	123.59
32	c	501	LMT	C1'-O5'-C5'	-2.23	109.31	113.69
24	B	608	CLA	O2A-CGA-CBA	2.23	118.91	111.91
26	c	516	BCR	C38-C26-C25	-2.23	122.02	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	505	CLA	O2A-CGA-CBA	2.23	118.91	111.91
30	a	415[A]	PL9	C35-C34-C33	-2.23	117.95	123.68
24	B	611	CLA	CAC-C3C-C2C	2.23	131.34	127.53
30	A	415[A]	PL9	C25-C24-C26	2.23	119.02	115.27
30	A	415[A]	PL9	C12-C13-C14	-2.23	122.30	127.66
25	A	417[A]	PHO	CED-O2D-CGD	2.22	120.97	115.94
24	C	511	CLA	CMC-C2C-C1C	2.22	128.43	125.04
30	A	415[A]	PL9	C53-C6-C1	2.22	119.54	114.99
27	A	411[A]	SQD	O9-S-O7	-2.22	106.25	113.95
24	A	405[A]	CLA	CHD-C4C-NC	2.22	127.71	124.20
24	B	610	CLA	CHB-C4A-NA	2.22	127.59	124.51
24	b	605	CLA	CED-O2D-CGD	2.22	120.96	115.94
24	B	616	CLA	CBC-CAC-C3C	-2.22	106.30	112.43
25	d	402[A]	PHO	O1D-CGD-CBD	-2.22	121.04	124.74
39	F	102	HEM	CMD-C2D-C1D	2.22	128.42	125.04
24	A	406[A]	CLA	C4C-C3C-C2C	-2.22	103.66	106.90
26	c	516	BCR	C16-C17-C18	-2.22	124.14	127.31
24	B	606	CLA	CAC-C3C-C4C	2.22	127.69	124.81
33	d	407[A]	LHG	O8-C23-O10	-2.22	117.99	123.59
24	B	602	CLA	CAA-C2A-C1A	-2.22	104.71	111.97
30	A	415[B]	PL9	C7-C3-C2	-2.22	120.38	123.30
26	t	102	BCR	C7-C6-C5	-2.22	116.09	121.46
24	B	602	CLA	C4-C3-C5	2.21	119.00	115.27
24	D	402[A]	CLA	CMA-C3A-C4A	-2.21	105.82	111.77
24	A	407[B]	CLA	C1-C2-C3	-2.21	122.21	126.04
36	c	518[B]	DGD	C2G-O2G-C1B	-2.21	112.34	117.79
24	c	503	CLA	C4C-C3C-C2C	-2.21	103.67	106.90
24	a	405[B]	CLA	CHC-C1C-NC	2.21	127.56	124.20
24	B	612	CLA	CMA-C3A-C2A	-2.21	104.90	113.83
24	b	611	CLA	O2A-CGA-CBA	2.21	118.85	111.91
26	y	101	BCR	C1-C6-C7	2.21	122.04	115.78
26	h	101	BCR	C16-C15-C14	-2.21	118.94	123.47
24	B	616	CLA	O1D-CGD-CBD	-2.21	119.96	124.48
24	B	611	CLA	C1C-C2C-C3C	-2.21	104.63	106.96
24	C	513	CLA	CMB-C2B-C3B	2.21	128.81	124.68
24	b	601	CLA	CAC-C3C-C4C	2.21	127.68	124.81
24	B	605	CLA	CMB-C2B-C1B	2.21	131.86	128.46
39	F	102	HEM	C3C-C4C-NC	-2.21	106.78	110.94
30	D	405[B]	PL9	C15-C14-C16	2.21	118.98	115.27
24	b	608	CLA	CMA-C3A-C2A	-2.21	104.93	113.83
30	a	415[B]	PL9	C45-C44-C46	2.21	118.98	115.27
33	E	101[A]	LHG	O7-C7-O9	-2.21	118.37	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	409	CLA	CMB-C2B-C3B	2.21	128.81	124.68
24	C	511	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
24	c	507	CLA	CAA-C2A-C3A	-2.20	106.74	112.78
32	B	628	LMT	O5B-C5B-C6B	2.20	111.91	106.44
32	B	630	LMT	O5'-C5'-C4'	2.20	114.39	109.75
24	c	504	CLA	O2A-CGA-CBA	2.20	118.82	111.91
24	C	503	CLA	CED-O2D-CGD	2.20	120.92	115.94
36	C	517[A]	DGD	O3G-C3G-C2G	-2.20	105.59	110.90
27	a	413	SQD	O5-C5-C4	2.20	113.69	109.69
35	d	412	LMG	O8-C28-O10	-2.20	118.04	123.59
24	B	614	CLA	C4-C3-C5	2.20	118.97	115.27
24	B	611	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
26	B	617	BCR	C11-C10-C9	-2.20	124.17	127.31
27	a	411[A]	SQD	O9-S-O7	-2.20	106.34	113.95
24	B	610	CLA	C1-C2-C3	-2.20	122.24	126.04
24	C	511	CLA	C4C-C3C-C2C	-2.20	103.69	106.90
24	b	608	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
26	y	101	BCR	C36-C18-C19	2.19	121.53	118.08
24	B	603	CLA	C5-C3-C2	-2.19	116.68	121.12
24	b	612	CLA	CHD-C4C-NC	2.19	127.66	124.20
24	b	604	CLA	C4-C3-C5	2.19	118.96	115.27
36	c	518[A]	DGD	O1G-C1A-O1A	-2.19	118.06	123.59
26	d	405	BCR	C37-C22-C21	-2.19	119.85	122.92
30	D	405[B]	PL9	C20-C19-C21	2.19	118.96	115.27
25	a	408[B]	PHO	C4A-C3A-C2A	-2.19	100.75	102.84
24	C	504	CLA	CBC-CAC-C3C	-2.19	106.39	112.43
24	b	616	CLA	C2A-C1A-CHA	-2.19	120.03	123.86
24	c	503	CLA	CAC-C3C-C4C	2.19	127.65	124.81
30	d	406[B]	PL9	C35-C34-C36	2.19	118.95	115.27
26	C	515	BCR	C29-C30-C25	2.19	113.85	110.48
36	H	102	DGD	O3G-C3G-C2G	-2.19	105.62	110.90
24	B	615	CLA	CMB-C2B-C1B	2.19	131.83	128.46
34	b	624	HTG	C1'-S1-C1	2.19	104.18	100.09
25	d	402[A]	PHO	C4-C3-C2	-2.19	118.07	123.68
24	b	602	CLA	CHB-C4A-NA	2.19	127.54	124.51
27	X	101	SQD	O7-S-C6	2.19	109.54	106.94
24	C	505	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
33	E	101[B]	LHG	O7-C7-O9	-2.19	118.42	123.70
30	A	415[B]	PL9	C51-C49-C50	2.19	119.43	114.60
36	h	102	DGD	C3B-C2B-C1B	-2.19	105.67	113.62
24	b	603	CLA	CMB-C2B-C3B	2.19	128.77	124.68
24	b	605	CLA	C1-O2A-CGA	2.19	122.18	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	510	CLA	C4-C3-C2	-2.19	118.07	123.68
24	B	602	CLA	CHD-C4C-NC	2.18	127.65	124.20
24	b	601	CLA	CAA-C2A-C3A	-2.18	106.80	112.78
25	A	408[B]	PHO	C4-C3-C5	2.18	118.94	115.27
24	B	614	CLA	CMA-C3A-C2A	-2.18	105.03	113.83
24	C	511	CLA	C6-C7-C8	-2.18	108.87	115.92
32	t	101	LMT	C1-O1'-C1'	2.18	117.45	113.84
27	X	101	SQD	O5-C1-O6	2.18	115.13	109.97
24	b	601	CLA	O2A-CGA-CBA	2.18	118.74	111.91
26	b	618	BCR	C7-C8-C9	-2.18	122.95	126.23
24	a	406[B]	CLA	C1-C2-C3	-2.18	122.28	126.04
36	c	518[B]	DGD	O2G-C1B-O1B	-2.18	118.44	123.70
35	d	412	LMG	O7-C10-O9	-2.17	118.45	123.70
24	C	502	CLA	OBD-CAD-C3D	-2.17	123.29	128.52
24	B	615	CLA	C6-C7-C8	-2.17	108.89	115.92
24	b	615	CLA	C6-C5-C3	-2.17	107.75	113.45
24	c	506	CLA	CHD-C4C-NC	2.17	127.63	124.20
26	b	619	BCR	C7-C6-C5	2.17	126.73	121.46
24	d	403[A]	CLA	CMB-C2B-C3B	2.17	128.74	124.68
24	a	407[A]	CLA	C4-C3-C5	2.17	118.92	115.27
26	B	617	BCR	C31-C1-C6	-2.17	106.78	110.30
32	M	102	LMT	O5B-C5B-C6B	2.17	111.84	106.44
24	b	605	CLA	CAC-C3C-C4C	2.17	127.63	124.81
24	b	601	CLA	CBC-CAC-C3C	-2.17	106.45	112.43
26	B	619	BCR	C3-C4-C5	-2.17	110.20	114.08
35	C	521	LMG	C9-C8-C7	-2.17	106.66	111.79
24	c	510	CLA	C2A-C1A-CHA	-2.17	120.06	123.86
33	A	420[A]	LHG	O4-P-O5	2.17	122.96	112.24
24	b	602	CLA	CHC-C1C-C2C	-2.17	120.73	126.72
24	B	607	CLA	CED-O2D-CGD	2.17	120.84	115.94
24	A	407[B]	CLA	C4-C3-C5	2.17	118.92	115.27
30	a	415[A]	PL9	C45-C44-C46	2.16	118.91	115.27
32	B	627	LMT	C1B-C2B-C3B	2.16	114.50	110.00
24	D	402[B]	CLA	CMB-C2B-C3B	2.16	128.72	124.68
24	c	511	CLA	C2A-C1A-CHA	-2.16	120.08	123.86
24	C	514	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
24	A	406[A]	CLA	O2A-CGA-CBA	2.16	118.68	111.91
25	a	408[A]	PHO	O2D-CGD-O1D	-2.16	119.62	123.84
24	D	403	CLA	C1-C2-C3	-2.16	122.31	126.04
24	C	507	CLA	CGD-CBD-CAD	-2.15	103.76	110.73
24	B	609	CLA	C16-C15-C13	-2.15	108.96	115.92
36	C	517[B]	DGD	O1G-C1A-O1A	-2.15	118.16	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	618	BCR	C37-C22-C23	2.15	121.47	118.08
26	T	101	BCR	C34-C9-C10	-2.15	119.91	122.92
25	a	408[B]	PHO	CBA-CAA-C2A	-2.15	107.53	113.81
30	D	405[A]	PL9	C12-C13-C14	-2.15	122.48	127.66
24	B	608	CLA	CMA-C3A-C2A	-2.15	105.16	113.83
24	B	607	CLA	OBD-CAD-C3D	-2.15	123.35	128.52
36	H	102	DGD	O2G-C1B-O1B	-2.15	118.51	123.70
24	B	602	CLA	C11-C10-C8	-2.15	108.97	115.92
24	C	508	CLA	C7-C6-C5	-2.15	107.52	113.36
26	k	101	BCR	C10-C11-C12	-2.15	116.51	123.22
33	d	414[A]	LHG	O7-C7-O9	-2.15	118.51	123.70
24	c	508	CLA	C1-C2-C3	-2.15	122.33	126.04
26	c	515	BCR	C37-C22-C23	2.15	121.46	118.08
24	b	614	CLA	CMB-C2B-C3B	2.15	128.69	124.68
27	a	411[B]	SQD	O4-C4-C3	-2.15	105.39	110.35
24	B	605	CLA	CAA-C2A-C3A	-2.15	106.90	112.78
34	c	522	HTG	C1-O5-C5	2.15	116.54	112.58
24	b	616	CLA	OBD-CAD-C3D	-2.15	123.36	128.52
26	t	102	BCR	C29-C30-C25	2.14	113.78	110.48
30	d	406[B]	PL9	C36-C37-C38	-2.14	104.84	111.88
24	b	614	CLA	CMC-C2C-C1C	2.14	128.30	125.04
24	c	514	CLA	CBC-CAC-C3C	-2.14	106.52	112.43
30	d	406[A]	PL9	C45-C44-C46	2.14	118.87	115.27
24	b	616	CLA	CHA-C1A-NA	-2.14	121.49	126.40
26	T	101	BCR	C10-C11-C12	-2.14	116.53	123.22
24	D	402[A]	CLA	OBD-CAD-C3D	-2.14	123.37	128.52
32	A	418	LMT	O1'-C1'-C2'	2.14	111.64	108.30
24	b	609	CLA	CHB-C4A-NA	2.14	127.47	124.51
24	C	513	CLA	C4-C3-C2	-2.14	118.19	123.68
26	c	516	BCR	C15-C16-C17	-2.14	119.09	123.47
30	A	415[B]	PL9	C35-C34-C33	-2.14	118.20	123.68
24	C	506	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
24	A	409	CLA	C2A-C1A-CHA	-2.14	120.12	123.86
24	a	406[B]	CLA	C2A-C1A-CHA	-2.13	120.13	123.86
24	B	601	CLA	C1B-CHB-C4A	-2.13	125.89	130.12
26	y	101	BCR	C29-C28-C27	-2.13	106.61	111.38
24	c	513	CLA	CHA-C1A-NA	-2.13	121.51	126.40
34	b	622	HTG	C1-C2-C3	2.13	114.80	110.59
24	B	608	CLA	CAA-C2A-C3A	-2.13	106.94	112.78
24	b	602	CLA	O2A-CGA-CBA	2.13	118.60	111.91
24	c	506	CLA	CMA-C3A-C4A	-2.13	106.05	111.77
24	A	407[B]	CLA	CBC-CAC-C3C	-2.13	106.56	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	c	517[A]	DGD	O6D-C1D-O3G	-2.13	104.93	109.97
24	A	407[A]	CLA	CHB-C4A-NA	2.13	127.46	124.51
36	C	517[A]	DGD	O5D-C6D-C5D	-2.13	105.11	109.05
26	T	101	BCR	C7-C6-C5	-2.13	116.31	121.46
33	d	407[A]	LHG	O8-C23-C24	2.13	118.59	111.91
27	X	101	SQD	O9-S-C6	-2.13	104.41	106.94
24	b	602	CLA	CAA-CBA-CGA	-2.13	107.03	113.25
24	A	406[B]	CLA	CED-O2D-CGD	2.13	120.75	115.94
24	b	610	CLA	C4-C3-C2	-2.13	118.23	123.68
24	a	409	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
24	a	407[A]	CLA	CBC-CAC-C3C	-2.12	106.57	112.43
24	d	403[A]	CLA	CHD-C4C-NC	2.12	127.55	124.20
24	b	606	CLA	O2A-CGA-CBA	2.12	118.57	111.91
24	C	502	CLA	C2A-C1A-CHA	-2.12	120.15	123.86
26	B	618	BCR	C40-C30-C25	-2.12	106.86	110.30
24	A	406[A]	CLA	CHB-C4A-NA	2.12	127.44	124.51
26	d	405	BCR	C38-C26-C27	2.12	117.69	113.62
26	t	102	BCR	C39-C30-C25	-2.12	106.86	110.30
24	c	504	CLA	OBD-CAD-C3D	-2.12	123.42	128.52
26	b	618	BCR	C21-C20-C19	-2.12	116.61	123.22
26	b	619	BCR	C15-C14-C13	-2.12	124.29	127.31
24	a	405[B]	CLA	C1B-CHB-C4A	-2.12	125.93	130.12
24	b	603	CLA	CGD-CBD-CAD	-2.12	103.88	110.73
24	A	405[B]	CLA	CAA-C2A-C1A	-2.11	105.05	111.97
35	b	629	LMG	O8-C28-O10	-2.11	118.26	123.59
26	b	619	BCR	C37-C22-C23	2.11	121.41	118.08
36	c	517[A]	DGD	O1G-C1A-O1A	-2.11	118.26	123.59
24	a	406[A]	CLA	CHB-C4A-NA	2.11	127.43	124.51
24	B	602	CLA	CMB-C2B-C3B	2.11	128.63	124.68
36	C	518[B]	DGD	O6E-C5E-C6E	2.11	111.69	106.44
24	b	615	CLA	CHA-C1A-NA	-2.11	121.56	126.40
24	c	502	CLA	CMB-C2B-C1B	2.11	131.71	128.46
24	d	403[A]	CLA	CMA-C3A-C2A	-2.11	105.31	113.83
26	k	101	BCR	C20-C21-C22	-2.11	124.30	127.31
36	C	518[A]	DGD	O1G-C1A-C2A	2.11	118.53	111.91
26	C	516	BCR	C21-C20-C19	-2.11	116.64	123.22
27	a	411[A]	SQD	C3-C4-C5	2.11	114.00	110.24
24	B	605	CLA	O2A-CGA-CBA	2.11	118.52	111.91
26	k	101	BCR	C2-C1-C6	2.11	113.72	110.48
24	c	509	CLA	CHA-C1A-NA	-2.11	121.58	126.40
24	b	607	CLA	C11-C10-C8	-2.10	109.12	115.92
30	d	406[A]	PL9	C31-C32-C33	-2.10	104.97	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	510	CLA	OBD-CAD-C3D	-2.10	123.46	128.52
24	a	406[A]	CLA	CAC-C3C-C2C	2.10	131.13	127.53
34	b	621	HTG	C3-C4-C5	2.10	113.99	110.24
30	D	405[B]	PL9	C35-C34-C36	2.10	118.81	115.27
35	z	101	LMG	C8-O7-C10	-2.10	112.61	117.79
27	X	101	SQD	C3-C4-C5	2.10	113.99	110.24
24	c	510	CLA	CAA-C2A-C3A	-2.10	107.02	112.78
30	a	415[A]	PL9	C51-C49-C50	2.10	119.25	114.60
24	A	405[A]	CLA	C7-C6-C5	-2.10	107.65	113.36
28	B	623	GOL	C3-C2-C1	-2.10	103.54	111.70
24	A	406[B]	CLA	C4C-C3C-C2C	-2.10	103.84	106.90
24	C	504	CLA	CMB-C2B-C3B	2.10	128.60	124.68
24	B	610	CLA	C2A-C1A-CHA	-2.10	120.19	123.86
24	c	502	CLA	C2A-C1A-CHA	-2.09	120.20	123.86
25	d	402[B]	PHO	C4-C3-C2	-2.09	118.31	123.68
26	B	618	BCR	C28-C27-C26	-2.09	110.34	114.08
26	A	410	BCR	C31-C1-C6	-2.09	106.90	110.30
24	b	613	CLA	C4-C3-C5	2.09	118.79	115.27
24	A	405[B]	CLA	C7-C6-C5	-2.09	107.67	113.36
24	B	604	CLA	CED-O2D-CGD	2.09	120.67	115.94
30	A	415[A]	PL9	C51-C49-C50	2.09	119.22	114.60
24	C	502	CLA	CMB-C2B-C3B	2.09	128.59	124.68
24	b	605	CLA	CBC-CAC-C3C	-2.09	106.66	112.43
26	B	618	BCR	C36-C18-C17	-2.09	119.99	122.92
24	C	511	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
24	d	404	CLA	C1-O2A-CGA	2.09	121.93	116.44
26	K	102	BCR	C24-C23-C22	-2.09	123.08	126.23
26	T	101	BCR	C35-C13-C12	2.09	121.37	118.08
26	B	618	BCR	C15-C14-C13	-2.09	124.33	127.31
24	b	614	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
24	C	513	CLA	CMC-C2C-C1C	2.09	128.22	125.04
39	e	101	HEM	CHA-C4D-C3D	-2.09	121.41	125.33
24	a	407[A]	CLA	CAC-C3C-C4C	2.08	127.52	124.81
27	X	101	SQD	O48-C23-O10	-2.08	118.33	123.59
26	c	515	BCR	C29-C30-C25	2.08	113.69	110.48
30	d	406[B]	PL9	C36-C34-C33	-2.08	116.90	121.12
24	C	512	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
24	b	607	CLA	CHD-C4C-NC	2.08	127.48	124.20
24	b	611	CLA	C7-C6-C5	-2.08	107.71	113.36
24	c	507	CLA	C1-O2A-CGA	2.08	121.90	116.44
24	B	613	CLA	CED-O2D-CGD	2.08	120.64	115.94
26	c	516	BCR	C20-C21-C22	-2.08	124.34	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	415[A]	PL9	C10-C9-C11	2.08	118.77	115.27
24	a	409	CLA	CMB-C2B-C3B	2.08	128.56	124.68
36	h	102	DGD	O6D-C1D-O3G	-2.08	105.06	109.97
26	Y	101	BCR	C37-C22-C21	-2.08	120.01	122.92
26	B	618	BCR	C11-C10-C9	-2.08	124.35	127.31
24	D	402[A]	CLA	CBC-CAC-C3C	-2.07	106.71	112.43
34	B	622	HTG	C1-C2-C3	2.07	114.68	110.59
24	b	610	CLA	CHB-C4A-NA	2.07	127.38	124.51
26	K	102	BCR	C32-C1-C6	-2.07	106.94	110.30
24	B	613	CLA	C7-C6-C5	-2.07	107.73	113.36
34	B	624	HTG	C3-C4-C5	2.07	113.93	110.24
30	d	406[A]	PL9	C40-C39-C38	-2.07	118.37	123.68
30	a	415[B]	PL9	C12-C13-C14	-2.07	122.68	127.66
24	B	602	CLA	OBD-CAD-C3D	-2.07	123.54	128.52
24	c	513	CLA	CAA-C2A-C3A	-2.07	107.12	112.78
26	y	101	BCR	C16-C15-C14	-2.06	119.25	123.47
24	C	512	CLA	C2A-C1A-CHA	-2.06	120.25	123.86
24	D	402[B]	CLA	CMC-C2C-C1C	2.06	128.18	125.04
26	Y	101	BCR	C7-C6-C5	-2.06	116.46	121.46
25	A	417[B]	PHO	O1D-CGD-CBD	-2.06	121.30	124.74
24	b	613	CLA	C16-C15-C13	-2.06	109.25	115.92
24	C	514	CLA	C4-C3-C5	2.06	118.74	115.27
30	D	405[B]	PL9	C7-C3-C4	2.06	118.55	116.88
24	c	513	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
24	c	506	CLA	C1-C2-C3	-2.06	122.48	126.04
24	b	605	CLA	OBD-CAD-C3D	-2.06	123.56	128.52
26	B	618	BCR	C34-C9-C8	2.06	121.32	118.08
26	C	516	BCR	C32-C1-C6	-2.06	106.96	110.30
24	d	403[A]	CLA	CBC-CAC-C3C	-2.06	106.75	112.43
34	d	411	HTG	C4-C3-C2	-2.06	107.23	110.82
33	L	101[B]	LHG	C5-O7-C7	-2.06	112.72	117.79
24	B	611	CLA	C11-C12-C13	-2.06	109.27	115.92
30	D	405[A]	PL9	C27-C28-C29	-2.06	122.71	127.66
24	b	604	CLA	C11-C12-C13	-2.05	109.28	115.92
25	A	408[B]	PHO	O2A-CGA-O1A	-2.05	118.41	123.59
30	d	406[A]	PL9	O2-C1-C6	-2.05	117.04	120.59
26	B	619	BCR	C2-C3-C4	-2.05	106.79	111.38
27	A	413	SQD	O47-C7-O49	-2.05	118.75	123.70
25	A	417[A]	PHO	O1D-CGD-CBD	-2.05	121.33	124.74
30	D	405[A]	PL9	C45-C44-C46	2.05	118.72	115.27
24	B	604	CLA	CHB-C4A-NA	2.05	127.34	124.51
24	c	511	CLA	CBC-CAC-C3C	-2.05	106.78	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	D	411	LMG	O7-C10-O9	-2.05	118.75	123.70
24	c	505	CLA	OBD-CAD-C3D	-2.05	123.59	128.52
24	b	609	CLA	C4-C3-C5	2.05	118.71	115.27
33	L	101[A]	LHG	O4-P-O5	2.05	122.36	112.24
26	B	619	BCR	C24-C23-C22	-2.05	123.14	126.23
24	c	506	CLA	C2A-C1A-CHA	-2.05	120.28	123.86
35	b	629	LMG	O7-C10-O9	-2.04	118.76	123.70
24	A	407[A]	CLA	CBC-CAC-C3C	-2.04	106.79	112.43
36	c	518[B]	DGD	O6E-C5E-C6E	2.04	111.52	106.44
30	d	406[B]	PL9	C20-C19-C21	2.04	118.71	115.27
35	b	629	LMG	O6-C1-C2	2.04	114.68	110.35
35	M	101	LMG	C3-C4-C5	2.04	113.88	110.24
24	b	609	CLA	CHA-C1A-NA	-2.04	121.72	126.40
25	d	402[A]	PHO	O2A-CGA-O1A	-2.04	118.44	123.59
25	a	408[A]	PHO	C1-C2-C3	-2.04	122.51	126.04
24	C	509	CLA	CHD-C4C-NC	2.04	127.42	124.20
24	a	406[A]	CLA	CMB-C2B-C1B	2.04	131.60	128.46
33	b	628[A]	LHG	O7-C7-O9	-2.04	118.77	123.70
24	B	610	CLA	CHA-C1A-NA	-2.04	121.73	126.40
35	z	101	LMG	C7-O1-C1	-2.04	109.76	113.74
24	B	605	CLA	CED-O2D-CGD	2.04	120.55	115.94
24	B	601	CLA	O2A-C1-C2	2.04	113.98	108.64
35	c	520	LMG	O7-C10-O9	-2.04	118.78	123.70
33	L	101[B]	LHG	O4-P-O5	2.03	122.29	112.24
39	e	101	HEM	O2A-CGA-CBA	2.03	120.56	114.03
26	b	618	BCR	C35-C13-C14	-2.03	120.08	122.92
30	D	405[A]	PL9	C47-C48-C49	-2.03	120.81	127.75
34	B	621	HTG	C2'-C1'-S1	-2.03	105.84	112.40
26	c	515	BCR	C21-C20-C19	-2.03	116.88	123.22
30	D	405[A]	PL9	C21-C22-C23	-2.03	105.21	111.88
24	d	403[B]	CLA	CMA-C3A-C4A	-2.03	106.31	111.77
24	B	609	CLA	C7-C6-C5	-2.03	107.84	113.36
36	C	519	DGD	O6E-C5E-C6E	2.03	111.48	106.44
26	b	619	BCR	C7-C8-C9	-2.03	123.17	126.23
24	c	508	CLA	C1-O2A-CGA	2.03	121.77	116.44
24	C	506	CLA	C11-C10-C8	-2.02	109.38	115.92
26	Y	101	BCR	C24-C23-C22	-2.02	123.18	126.23
27	B	620	SQD	C9-C8-C7	-2.02	106.26	113.62
24	c	507	CLA	CMB-C2B-C3B	2.02	128.46	124.68
24	B	605	CLA	CHA-C1A-NA	-2.02	121.76	126.40
36	c	519	DGD	O4D-C4D-C3D	-2.02	105.67	110.35
24	C	513	CLA	C1B-CHB-C4A	-2.02	126.11	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	508	CLA	CHA-C1A-NA	-2.02	121.77	126.40
24	C	505	CLA	C2A-C1A-CHA	-2.02	120.33	123.86
35	d	412	LMG	C7-O1-C1	-2.02	109.79	113.74
24	a	407[A]	CLA	CHA-C1A-NA	-2.02	121.77	126.40
30	d	406[B]	PL9	C25-C24-C26	2.02	118.67	115.27
26	B	619	BCR	C31-C1-C6	-2.02	107.03	110.30
27	a	411[A]	SQD	O4-C4-C3	-2.02	105.68	110.35
24	A	405[B]	CLA	CHC-C1C-NC	2.02	127.27	124.20
24	B	601	CLA	CMB-C2B-C3B	2.02	128.45	124.68
24	B	608	CLA	C1B-CHB-C4A	-2.02	126.12	130.12
24	b	602	CLA	CMA-C3A-C2A	-2.02	105.69	113.83
27	B	620	SQD	O47-C7-O49	-2.02	118.83	123.70
24	a	406[B]	CLA	CMC-C2C-C1C	2.02	128.11	125.04
24	a	406[B]	CLA	CHB-C4A-NA	2.01	127.30	124.51
24	A	407[B]	CLA	CED-O2D-CGD	2.01	120.49	115.94
24	c	509	CLA	C2A-C1A-CHA	-2.01	120.34	123.86
36	c	517[A]	DGD	O1G-C1A-C2A	2.01	118.23	111.91
24	c	513	CLA	CMB-C2B-C3B	2.01	128.44	124.68
24	B	606	CLA	C7-C6-C5	-2.01	107.89	113.36
24	B	604	CLA	C4-C3-C2	-2.01	118.52	123.68
24	B	608	CLA	CBC-CAC-C3C	-2.01	106.88	112.43
24	a	406[B]	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
24	A	405[B]	CLA	CBC-CAC-C3C	-2.01	106.89	112.43
24	a	405[B]	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
24	c	512	CLA	C2A-C1A-CHA	-2.01	120.35	123.86
35	z	101	LMG	O8-C28-O10	-2.01	118.53	123.59
35	C	501	LMG	O7-C10-O9	-2.01	118.86	123.70
26	B	617	BCR	C2-C1-C6	2.01	113.57	110.48
32	c	501	LMT	O5B-C5B-C4B	2.00	113.33	109.69
26	b	617	BCR	C11-C12-C13	-2.00	120.78	126.42
24	a	405[B]	CLA	CMB-C2B-C3B	2.00	128.43	124.68
24	B	603	CLA	C2A-C3A-C4A	-2.00	98.63	101.87
24	B	607	CLA	CAA-CBA-CGA	2.00	119.11	113.25
25	A	417[A]	PHO	CMB-C2B-C3B	2.00	128.43	124.68
27	a	411[B]	SQD	O48-C23-O10	-2.00	118.54	123.59
24	B	604	CLA	CAC-C3C-C4C	2.00	127.41	124.81
36	C	517[A]	DGD	C4E-C3E-C2E	-2.00	107.33	110.82
24	b	615	CLA	CBC-CAC-C3C	-2.00	106.91	112.43

All (71) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
24	A	405[A]	CLA	ND
24	A	405[B]	CLA	ND
24	A	406[A]	CLA	ND
24	A	406[B]	CLA	ND
24	A	409	CLA	ND
24	B	601	CLA	ND
24	B	602	CLA	ND
24	B	603	CLA	ND
24	B	604	CLA	ND
24	B	605	CLA	ND
24	B	606	CLA	ND
24	B	607	CLA	ND
24	B	609	CLA	ND
24	B	610	CLA	ND
24	B	611	CLA	ND
24	B	612	CLA	ND
24	B	613	CLA	ND
24	B	614	CLA	ND
24	B	615	CLA	ND
24	B	616	CLA	ND
24	C	502	CLA	ND
24	C	503	CLA	ND
24	C	505	CLA	ND
24	C	506	CLA	ND
24	C	507	CLA	ND
24	C	508	CLA	ND
24	C	509	CLA	ND
24	C	510	CLA	ND
24	C	511	CLA	ND
24	C	512	CLA	ND
24	C	513	CLA	ND
24	C	514	CLA	ND
24	D	402[A]	CLA	ND
24	D	402[B]	CLA	ND
24	D	403	CLA	ND
24	a	405[A]	CLA	ND
24	a	405[B]	CLA	ND
24	a	406[A]	CLA	ND
24	a	406[B]	CLA	ND
24	a	409	CLA	ND
24	b	601	CLA	ND

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Mol	Chain	Res	Type	Atom
24	b	602	CLA	ND
24	b	603	CLA	ND
24	b	604	CLA	ND
24	b	605	CLA	ND
24	b	606	CLA	ND
24	b	607	CLA	ND
24	b	609	CLA	ND
24	b	610	CLA	ND
24	b	611	CLA	ND
24	b	612	CLA	ND
24	b	613	CLA	ND
24	b	614	CLA	ND
24	b	615	CLA	ND
24	b	616	CLA	ND
24	c	502	CLA	ND
24	c	503	CLA	ND
24	c	504	CLA	ND
24	c	505	CLA	ND
24	c	506	CLA	ND
24	c	507	CLA	ND
24	c	508	CLA	ND
24	c	509	CLA	ND
24	c	510	CLA	ND
24	c	511	CLA	ND
24	c	512	CLA	ND
24	c	513	CLA	ND
24	c	514	CLA	ND
24	d	403[A]	CLA	ND
24	d	403[B]	CLA	ND
24	d	404	CLA	ND

All (1643) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	614	CLA	CHA-CBD-CGD-O1D
24	B	614	CLA	CHA-CBD-CGD-O2D
24	B	614	CLA	CAD-CBD-CGD-O1D
24	B	614	CLA	CAD-CBD-CGD-O2D
24	C	505	CLA	C2-C3-C5-C6
24	C	505	CLA	C4-C3-C5-C6
24	C	508	CLA	C4-C3-C5-C6
24	C	509	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	C	509	CLA	CHA-CBD-CGD-O2D
24	b	604	CLA	C6-C7-C8-C9
24	b	614	CLA	CHA-CBD-CGD-O1D
24	b	614	CLA	CHA-CBD-CGD-O2D
24	b	614	CLA	CAD-CBD-CGD-O1D
24	b	614	CLA	CAD-CBD-CGD-O2D
24	c	509	CLA	CHA-CBD-CGD-O1D
24	c	509	CLA	CHA-CBD-CGD-O2D
24	c	510	CLA	C2-C1-O2A-CGA
24	c	510	CLA	C11-C10-C8-C9
24	d	404	CLA	C2-C3-C5-C6
24	d	404	CLA	C4-C3-C5-C6
26	D	404	BCR	C21-C22-C23-C24
26	D	404	BCR	C37-C22-C23-C24
26	D	404	BCR	C23-C24-C25-C30
26	K	102	BCR	C7-C8-C9-C10
26	K	102	BCR	C7-C8-C9-C34
26	T	101	BCR	C13-C14-C15-C16
26	b	617	BCR	C1-C6-C7-C8
26	y	101	BCR	C5-C6-C7-C8
27	A	411[B]	SQD	C8-C7-O47-C45
27	A	413	SQD	O6-C44-C45-O47
27	B	620	SQD	O49-C7-O47-C45
27	L	102	SQD	C8-C7-O47-C45
27	X	101	SQD	C2-C1-O6-C44
27	X	101	SQD	O49-C7-O47-C45
27	X	101	SQD	C8-C7-O47-C45
27	a	413	SQD	O6-C44-C45-O47
27	a	413	SQD	C5-C6-S-O7
27	a	413	SQD	C5-C6-S-O8
27	a	413	SQD	C5-C6-S-O9
27	f	101	SQD	O6-C44-C45-O47
27	f	101	SQD	O49-C7-O47-C45
27	f	101	SQD	C8-C7-O47-C45
28	A	412	GOL	O1-C1-C2-C3
28	B	623	GOL	C1-C2-C3-O3
28	D	412	GOL	O1-C1-C2-C3
28	D	412	GOL	C1-C2-C3-O3
28	V	203[A]	GOL	C1-C2-C3-O3
28	V	203[B]	GOL	O1-C1-C2-C3
28	V	203[B]	GOL	C1-C2-C3-O3
28	V	203[B]	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
28	a	412	GOL	O1-C1-C2-C3
28	a	419	GOL	C1-C2-C3-O3
28	b	623	GOL	C1-C2-C3-O3
28	c	527	GOL	C1-C2-C3-O3
28	o	302	GOL	C1-C2-C3-O3
28	o	303	GOL	C1-C2-C3-O3
30	A	415[A]	PL9	C9-C11-C12-C13
30	A	415[A]	PL9	C15-C14-C16-C17
30	A	415[A]	PL9	C14-C16-C17-C18
30	A	415[B]	PL9	C14-C16-C17-C18
30	a	415[A]	PL9	C9-C11-C12-C13
30	a	415[A]	PL9	C14-C16-C17-C18
30	a	415[A]	PL9	C23-C24-C26-C27
30	a	415[A]	PL9	C25-C24-C26-C27
30	a	415[B]	PL9	C9-C11-C12-C13
30	a	415[B]	PL9	C14-C16-C17-C18
32	A	418	LMT	C2'-C1'-O1'-C1
32	A	418	LMT	O5'-C1'-O1'-C1
32	A	421	LMT	C2'-C1'-O1'-C1
32	A	421	LMT	O5'-C1'-O1'-C1
32	A	421	LMT	C2-C1-O1'-C1'
32	B	627	LMT	C2-C1-O1'-C1'
32	B	628	LMT	C2'-C1'-O1'-C1
32	B	630	LMT	O5'-C1'-O1'-C1
32	B	630	LMT	C2-C1-O1'-C1'
32	F	101	LMT	C2'-C1'-O1'-C1
32	F	101	LMT	O5'-C1'-O1'-C1
32	M	104	LMT	C2-C1-O1'-C1'
32	b	620	LMT	C2'-C1'-O1'-C1
32	b	626	LMT	C2'-C1'-O1'-C1
32	b	626	LMT	O5'-C1'-O1'-C1
32	e	102	LMT	C2'-C1'-O1'-C1
32	e	102	LMT	O5'-C1'-O1'-C1
32	t	101	LMT	O5'-C1'-O1'-C1
32	t	101	LMT	C2-C1-O1'-C1'
33	D	406[A]	LHG	O2-C2-C3-O3
33	D	406[A]	LHG	C3-O3-P-O4
33	D	406[A]	LHG	C3-O3-P-O5
33	D	406[A]	LHG	C3-O3-P-O6
33	D	406[A]	LHG	C4-O6-P-O4
33	D	406[B]	LHG	C3-O3-P-O4
33	D	406[B]	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
33	D	406[B]	LHG	C4-O6-P-O4
33	D	406[B]	LHG	C4-O6-P-O5
33	E	101[A]	LHG	C3-O3-P-O4
33	E	101[A]	LHG	C3-O3-P-O5
33	E	101[A]	LHG	O10-C23-O8-C6
33	E	101[A]	LHG	C24-C23-O8-C6
33	E	101[B]	LHG	C3-O3-P-O4
33	E	101[B]	LHG	C3-O3-P-O5
33	E	101[B]	LHG	C4-O6-P-O3
33	E	101[B]	LHG	C4-O6-P-O5
33	E	101[B]	LHG	O10-C23-O8-C6
33	E	101[B]	LHG	C24-C23-O8-C6
33	L	101[A]	LHG	C4-O6-P-O4
33	L	101[A]	LHG	C4-O6-P-O5
33	L	101[B]	LHG	C4-O6-P-O3
33	L	101[B]	LHG	C4-O6-P-O4
33	L	101[B]	LHG	C4-O6-P-O5
33	a	420[A]	LHG	C3-O3-P-O4
33	a	420[A]	LHG	C4-O6-P-O5
33	a	420[A]	LHG	O10-C23-O8-C6
33	a	420[A]	LHG	C24-C23-O8-C6
33	a	420[B]	LHG	C3-O3-P-O4
33	a	420[B]	LHG	C4-O6-P-O5
33	a	420[B]	LHG	O10-C23-O8-C6
33	a	420[B]	LHG	C24-C23-O8-C6
33	b	628[A]	LHG	C4-O6-P-O4
33	b	628[A]	LHG	C4-O6-P-O5
33	b	628[B]	LHG	C4-O6-P-O3
33	b	628[B]	LHG	C4-O6-P-O4
33	b	628[B]	LHG	C4-O6-P-O5
33	d	407[A]	LHG	C3-O3-P-O4
33	d	407[A]	LHG	C3-O3-P-O5
33	d	407[A]	LHG	C4-O6-P-O4
33	d	407[B]	LHG	O2-C2-C3-O3
33	d	407[B]	LHG	C3-O3-P-O6
33	d	407[B]	LHG	C4-O6-P-O4
33	d	407[B]	LHG	C4-O6-P-O5
33	d	408[B]	LHG	C4-O6-P-O4
33	d	414[A]	LHG	C3-O3-P-O5
34	B	621	HTG	C2'-C1'-S1-C1
35	C	521	LMG	C11-C10-O7-C8
35	c	521	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
35	c	521	LMG	C11-C10-O7-C8
35	Z	101	LMG	O9-C10-O7-C8
35	Z	101	LMG	C11-C10-O7-C8
35	z	101	LMG	O6-C1-O1-C7
32	A	421	LMT	O5B-C1B-O1B-C4'
32	B	628	LMT	C4'-C5'-C6'-O6'
27	A	411[A]	SQD	O49-C7-O47-C45
27	A	411[B]	SQD	O49-C7-O47-C45
27	L	102	SQD	O49-C7-O47-C45
35	C	521	LMG	O9-C10-O7-C8
35	z	101	LMG	O9-C10-O7-C8
32	M	104	LMT	C4B-C5B-C6B-O6B
24	b	616	CLA	C3-C5-C6-C7
24	c	513	CLA	C3-C5-C6-C7
24	d	404	CLA	C3-C5-C6-C7
27	B	620	SQD	C8-C7-O47-C45
32	F	101	LMT	O5'-C5'-C6'-O6'
24	D	403	CLA	C4-C3-C5-C6
24	a	409	CLA	C4-C3-C5-C6
30	A	415[A]	PL9	C20-C19-C21-C22
30	a	415[B]	PL9	C25-C24-C26-C27
24	C	508	CLA	C2-C3-C5-C6
24	D	403	CLA	C2-C3-C5-C6
30	A	415[A]	PL9	C18-C19-C21-C22
24	B	606	CLA	C2A-CAA-CBA-CGA
24	B	614	CLA	C3-C5-C6-C7
24	D	403	CLA	CBD-CGD-O2D-CED
32	c	501	LMT	O5B-C5B-C6B-O6B
35	C	521	LMG	O6-C5-C6-O5
33	A	420[B]	LHG	O2-C2-C3-O3
33	d	407[A]	LHG	O2-C2-C3-O3
24	A	409	CLA	C3-C5-C6-C7
24	D	403	CLA	C3-C5-C6-C7
32	B	627	LMT	C6-C7-C8-C9
32	B	628	LMT	O5B-C5B-C6B-O6B
32	M	104	LMT	O5'-C5'-C6'-O6'
27	A	411[A]	SQD	C8-C7-O47-C45
35	z	101	LMG	C11-C10-O7-C8
24	C	513	CLA	CBD-CGD-O2D-CED
32	B	627	LMT	C4'-C5'-C6'-O6'
34	D	410	HTG	O5-C5-C6-O6
34	b	624	HTG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
34	D	410	HTG	S1-C1'-C2'-C3'
34	b	621	HTG	S1-C1'-C2'-C3'
34	b	624	HTG	S1-C1'-C2'-C3'
32	A	421	LMT	O5B-C5B-C6B-O6B
32	M	104	LMT	O5B-C5B-C6B-O6B
35	c	521	LMG	C4-C5-C6-O5
32	B	630	LMT	O5'-C5'-C6'-O6'
32	e	102	LMT	O5B-C5B-C6B-O6B
24	A	409	CLA	C4-C3-C5-C6
24	B	605	CLA	C4-C3-C5-C6
24	b	603	CLA	C4-C3-C5-C6
24	b	605	CLA	C4-C3-C5-C6
24	b	614	CLA	C4-C3-C5-C6
24	c	508	CLA	C4-C3-C5-C6
30	A	415[B]	PL9	C15-C14-C16-C17
30	A	415[B]	PL9	C20-C19-C21-C22
30	a	415[A]	PL9	C15-C14-C16-C17
30	a	415[A]	PL9	C30-C29-C31-C32
30	a	415[B]	PL9	C15-C14-C16-C17
30	a	415[B]	PL9	C30-C29-C31-C32
32	c	501	LMT	C4B-C5B-C6B-O6B
24	A	409	CLA	C2-C3-C5-C6
24	B	605	CLA	C2-C3-C5-C6
24	b	603	CLA	C2-C3-C5-C6
24	b	605	CLA	C2-C3-C5-C6
24	b	614	CLA	C2-C3-C5-C6
24	c	508	CLA	C2-C3-C5-C6
30	A	415[A]	PL9	C13-C14-C16-C17
30	A	415[B]	PL9	C13-C14-C16-C17
30	A	415[B]	PL9	C18-C19-C21-C22
30	a	415[A]	PL9	C13-C14-C16-C17
30	a	415[A]	PL9	C28-C29-C31-C32
30	a	415[B]	PL9	C13-C14-C16-C17
30	a	415[B]	PL9	C28-C29-C31-C32
24	b	606	CLA	C2A-CAA-CBA-CGA
32	B	628	LMT	C1-C2-C3-C4
32	A	421	LMT	O5'-C5'-C6'-O6'
32	B	627	LMT	O5B-C5B-C6B-O6B
32	B	628	LMT	O5'-C5'-C6'-O6'
32	b	620	LMT	O5'-C5'-C6'-O6'
32	b	620	LMT	O5'-C1'-O1'-C1
30	A	415[A]	PL9	C44-C46-C47-C48

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Mol	Chain	Res	Type	Atoms
30	A	415[B]	PL9	C9-C11-C12-C13
30	A	415[B]	PL9	C44-C46-C47-C48
30	D	405[A]	PL9	C39-C41-C42-C43
35	M	101	LMG	C39-C40-C41-C42
32	e	102	LMT	C4'-C5'-C6'-O6'
24	c	514	CLA	CBD-CGD-O2D-CED
35	d	412	LMG	C10-C11-C12-C13
33	A	420[B]	LHG	C1-C2-C3-O3
33	d	407[A]	LHG	C1-C2-C3-O3
32	B	628	LMT	C4B-C5B-C6B-O6B
32	F	101	LMT	C4'-C5'-C6'-O6'
24	c	510	CLA	C3-C5-C6-C7
24	a	409	CLA	CBA-CGA-O2A-C1
24	C	514	CLA	CBD-CGD-O2D-CED
32	A	421	LMT	C4B-C5B-C6B-O6B
35	a	417	LMG	C4-C5-C6-O5
35	M	101	LMG	C15-C16-C17-C18
36	C	519	DGD	C6B-C7B-C8B-C9B
32	b	626	LMT	O5'-C5'-C6'-O6'
32	M	104	LMT	C4'-C5'-C6'-O6'
32	b	626	LMT	C4'-C5'-C6'-O6'
34	D	410	HTG	C4-C5-C6-O6
32	B	627	LMT	C4B-C5B-C6B-O6B
24	B	602	CLA	C13-C15-C16-C17
24	b	601	CLA	C10-C11-C12-C13
24	b	606	CLA	C10-C11-C12-C13
32	B	630	LMT	C2'-C1'-O1'-C1
32	t	101	LMT	C2'-C1'-O1'-C1
32	B	627	LMT	O5'-C5'-C6'-O6'
30	A	415[A]	PL9	C30-C29-C31-C32
24	C	503	CLA	C14-C13-C15-C16
24	C	507	CLA	C14-C13-C15-C16
24	b	601	CLA	C11-C10-C8-C9
24	b	610	CLA	C11-C12-C13-C14
24	b	616	CLA	C6-C7-C8-C9
24	c	505	CLA	C11-C12-C13-C14
24	c	513	CLA	C6-C7-C8-C9
32	A	418	LMT	O5B-C5B-C6B-O6B
32	e	102	LMT	C4B-C5B-C6B-O6B
27	X	101	SQD	C23-C24-C25-C26
33	E	101[A]	LHG	C23-C24-C25-C26
24	B	606	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	b	605	CLA	C8-C10-C11-C12
32	b	620	LMT	C4'-C5'-C6'-O6'
24	A	409	CLA	C5-C6-C7-C8
24	B	603	CLA	C13-C15-C16-C17
24	B	614	CLA	C8-C10-C11-C12
24	b	611	CLA	C15-C16-C17-C18
24	B	601	CLA	C5-C6-C7-C8
24	B	601	CLA	C10-C11-C12-C13
24	C	508	CLA	C5-C6-C7-C8
24	b	604	CLA	C8-C10-C11-C12
24	b	614	CLA	C8-C10-C11-C12
28	D	412	GOL	O1-C1-C2-O2
28	D	412	GOL	O2-C2-C3-O3
28	O	302	GOL	O1-C1-C2-O2
28	c	527	GOL	O2-C2-C3-O3
28	o	303	GOL	O2-C2-C3-O3
28	v	202[B]	GOL	O1-C1-C2-O2
27	B	620	SQD	C7-C8-C9-C10
35	Z	101	LMG	C10-C11-C12-C13
36	c	518[A]	DGD	C1B-C2B-C3B-C4B
24	B	616	CLA	C3-C5-C6-C7
32	A	421	LMT	O1'-C1-C2-C3
35	D	411	LMG	O6-C5-C6-O5
24	B	616	CLA	C2-C1-O2A-CGA
33	D	407[A]	LHG	C33-C34-C35-C36
24	C	511	CLA	C10-C11-C12-C13
27	X	101	SQD	C7-C8-C9-C10
36	c	518[B]	DGD	C1B-C2B-C3B-C4B
24	C	502	CLA	CBD-CGD-O2D-CED
24	B	614	CLA	C10-C11-C12-C13
24	D	403	CLA	C10-C11-C12-C13
24	b	606	CLA	C13-C15-C16-C17
24	A	409	CLA	C12-C13-C15-C16
24	C	511	CLA	C11-C12-C13-C15
24	D	403	CLA	C11-C10-C8-C7
24	b	606	CLA	C12-C13-C15-C16
24	c	503	CLA	C11-C12-C13-C15
24	C	503	CLA	C15-C16-C17-C18
24	C	509	CLA	C10-C11-C12-C13
32	A	418	LMT	O1'-C1-C2-C3
34	b	622	HTG	C1'-C2'-C3'-C4'
27	X	101	SQD	O5-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
24	a	405[A]	CLA	C15-C16-C17-C18
24	c	513	CLA	C15-C16-C17-C18
30	D	405[B]	PL9	C39-C41-C42-C43
30	d	406[A]	PL9	C39-C41-C42-C43
30	d	406[B]	PL9	C39-C41-C42-C43
32	c	501	LMT	O1'-C1-C2-C3
32	t	101	LMT	O5'-C5'-C6'-O6'
24	B	608	CLA	C13-C15-C16-C17
24	b	611	CLA	C8-C10-C11-C12
24	b	614	CLA	C10-C11-C12-C13
24	c	514	CLA	C10-C11-C12-C13
36	C	519	DGD	C2B-C3B-C4B-C5B
36	c	519	DGD	C2B-C3B-C4B-C5B
24	a	409	CLA	O1A-CGA-O2A-C1
24	A	406[B]	CLA	C15-C16-C17-C18
24	b	601	CLA	C8-C10-C11-C12
32	B	630	LMT	O1'-C1-C2-C3
32	m	102	LMT	O5'-C5'-C6'-O6'
27	B	620	SQD	C30-C31-C32-C33
33	D	407[B]	LHG	C33-C34-C35-C36
24	b	604	CLA	C5-C6-C7-C8
33	D	406[B]	LHG	C3-O3-P-O6
33	E	101[A]	LHG	C3-O3-P-O6
33	E	101[A]	LHG	C4-O6-P-O3
33	E	101[B]	LHG	C3-O3-P-O6
33	L	101[A]	LHG	C4-O6-P-O3
33	a	420[A]	LHG	C3-O3-P-O6
33	a	420[A]	LHG	C4-O6-P-O3
33	a	420[B]	LHG	C3-O3-P-O6
33	a	420[B]	LHG	C4-O6-P-O3
33	b	628[A]	LHG	C4-O6-P-O3
33	d	407[A]	LHG	C3-O3-P-O6
33	d	407[B]	LHG	C4-O6-P-O3
27	A	411[A]	SQD	C7-C8-C9-C10
33	D	406[A]	LHG	C1-C2-C3-O3
32	m	102	LMT	C4B-C5B-C6B-O6B
24	a	409	CLA	C2-C3-C5-C6
30	a	415[B]	PL9	C23-C24-C26-C27
27	A	411[A]	SQD	C12-C13-C14-C15
32	M	102	LMT	O1'-C1-C2-C3
24	B	610	CLA	C2A-CAA-CBA-CGA
27	L	102	SQD	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
35	a	417	LMG	C10-C11-C12-C13
36	C	518[B]	DGD	CCB-CDB-CEB-CFB
24	c	513	CLA	CBD-CGD-O2D-CED
24	b	604	CLA	C15-C16-C17-C18
27	X	101	SQD	C30-C31-C32-C33
27	a	413	SQD	C25-C26-C27-C28
27	f	101	SQD	C32-C33-C34-C35
32	B	630	LMT	C11-C10-C9-C8
33	D	406[B]	LHG	C16-C17-C18-C19
33	L	101[A]	LHG	C15-C16-C17-C18
33	L	101[A]	LHG	C17-C18-C19-C20
33	d	408[B]	LHG	C25-C26-C27-C28
35	C	501	LMG	C36-C37-C38-C39
35	M	101	LMG	C34-C35-C36-C37
35	b	629	LMG	C35-C36-C37-C38
36	H	102	DGD	C5B-C6B-C7B-C8B
36	c	517[A]	DGD	C9A-CAA-CBA-CCA
36	c	518[A]	DGD	C9A-CAA-CBA-CCA
24	B	615	CLA	C16-C17-C18-C19
24	b	614	CLA	C16-C17-C18-C20
24	c	510	CLA	C16-C17-C18-C20
24	c	510	CLA	CBA-CGA-O2A-C1
34	B	624	HTG	S1-C1'-C2'-C3'
32	A	421	LMT	C5'-C4'-O1B-C1B
32	b	626	LMT	C7-C8-C9-C10
33	L	101[B]	LHG	C17-C18-C19-C20
33	b	628[B]	LHG	C14-C15-C16-C17
33	d	414[A]	LHG	C16-C17-C18-C19
35	C	501	LMG	C12-C13-C14-C15
34	B	624	HTG	O5-C5-C6-O6
27	a	413	SQD	C31-C32-C33-C34
32	B	630	LMT	C4-C5-C6-C7
33	d	414[B]	LHG	C16-C17-C18-C19
35	C	521	LMG	C18-C19-C20-C21
35	D	411	LMG	C19-C20-C21-C22
36	c	517[B]	DGD	C2B-C3B-C4B-C5B
36	c	518[B]	DGD	C9A-CAA-CBA-CCA
36	h	102	DGD	C9A-CAA-CBA-CCA
33	A	420[B]	LHG	C34-C35-C36-C37
33	D	406[A]	LHG	C16-C17-C18-C19
33	d	414[A]	LHG	C32-C33-C34-C35
35	a	417	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
36	C	517[A]	DGD	C5B-C6B-C7B-C8B
33	E	101[B]	LHG	O2-C2-C3-O3
27	X	101	SQD	C29-C30-C31-C32
32	t	101	LMT	C2-C3-C4-C5
33	D	407[B]	LHG	C32-C33-C34-C35
33	E	101[B]	LHG	C24-C25-C26-C27
33	a	420[A]	LHG	C26-C27-C28-C29
33	a	420[B]	LHG	C26-C27-C28-C29
36	c	517[A]	DGD	C5A-C6A-C7A-C8A
36	c	518[A]	DGD	CBA-CCA-CDA-CEA
35	c	521	LMG	O6-C5-C6-O5
27	A	413	SQD	C2-C1-O6-C44
35	M	101	LMG	C2-C1-O1-C7
36	C	518[A]	DGD	C2E-C1E-O5D-C6D
27	A	411[B]	SQD	O6-C44-C45-O47
27	a	413	SQD	C16-C17-C18-C19
32	B	627	LMT	C5'-C4'-O1B-C1B
36	C	517[A]	DGD	C4B-C5B-C6B-C7B
36	c	517[A]	DGD	C2B-C3B-C4B-C5B
36	c	518[A]	DGD	CAA-CBA-CCA-CDA
36	c	518[B]	DGD	CBA-CCA-CDA-CEA
32	b	620	LMT	C3'-C4'-O1B-C1B
24	B	603	CLA	C16-C17-C18-C20
24	b	615	CLA	C16-C17-C18-C19
24	c	509	CLA	C16-C17-C18-C19
24	d	404	CLA	C16-C17-C18-C20
32	m	102	LMT	O5B-C5B-C6B-O6B
30	a	415[B]	PL9	C12-C11-C9-C10
32	B	628	LMT	C5-C6-C7-C8
33	L	101[A]	LHG	C13-C14-C15-C16
34	b	621	HTG	C2'-C3'-C4'-C5'
24	B	602	CLA	C6-C7-C8-C9
24	B	603	CLA	C11-C12-C13-C14
24	B	610	CLA	C11-C12-C13-C14
24	B	610	CLA	C14-C13-C15-C16
24	C	513	CLA	C11-C10-C8-C9
24	a	407[A]	CLA	C11-C12-C13-C14
24	a	407[B]	CLA	C11-C12-C13-C14
24	c	503	CLA	C11-C12-C13-C14
24	c	505	CLA	C14-C13-C15-C16
24	c	506	CLA	C11-C12-C13-C14
24	d	404	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	C	510	CLA	CBD-CGD-O2D-CED
27	A	411[A]	SQD	C15-C16-C17-C18
27	A	411[B]	SQD	C15-C16-C17-C18
32	B	628	LMT	C2-C3-C4-C5
32	b	626	LMT	C3-C4-C5-C6
35	C	521	LMG	C13-C14-C15-C16
35	d	412	LMG	C29-C30-C31-C32
36	C	518[A]	DGD	CCB-CDB-CEB-CFB
24	C	503	CLA	C13-C15-C16-C17
32	B	630	LMT	C4'-C5'-C6'-O6'
24	c	510	CLA	O1A-CGA-O2A-C1
26	b	619	BCR	C7-C8-C9-C34
32	A	421	LMT	C3-C4-C5-C6
32	e	102	LMT	C5-C6-C7-C8
33	b	628[B]	LHG	C27-C28-C29-C30
28	B	623	GOL	O1-C1-C2-C3
28	O	302	GOL	O1-C1-C2-C3
28	a	412	GOL	C1-C2-C3-O3
28	a	418	GOL	O1-C1-C2-C3
28	d	413	GOL	O1-C1-C2-C3
28	o	302	GOL	O1-C1-C2-C3
28	v	202[A]	GOL	O1-C1-C2-C3
28	v	202[B]	GOL	O1-C1-C2-C3
33	A	420[B]	LHG	O1-C1-C2-C3
26	b	619	BCR	C7-C8-C9-C10
27	A	413	SQD	C26-C27-C28-C29
33	D	407[A]	LHG	C32-C33-C34-C35
33	b	628[A]	LHG	C14-C15-C16-C17
36	c	517[B]	DGD	C9A-CAA-CBA-CCA
36	c	518[B]	DGD	CAA-CBA-CCA-CDA
32	b	626	LMT	C5-C6-C7-C8
33	L	101[A]	LHG	C12-C13-C14-C15
33	d	414[A]	LHG	C29-C30-C31-C32
35	C	501	LMG	C19-C20-C21-C22
35	D	411	LMG	C12-C13-C14-C15
35	D	411	LMG	C35-C36-C37-C38
35	M	101	LMG	C17-C18-C19-C20
36	c	517[B]	DGD	O6D-C5D-C6D-O5D
24	a	409	CLA	C16-C17-C18-C20
24	b	602	CLA	C16-C17-C18-C19
24	b	602	CLA	C16-C17-C18-C20
24	d	403[A]	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
32	B	628	LMT	O5'-C1'-O1'-C1
35	M	101	LMG	O6-C1-O1-C7
24	A	406[A]	CLA	C15-C16-C17-C18
24	B	613	CLA	C13-C15-C16-C17
32	B	627	LMT	C5-C6-C7-C8
33	b	628[A]	LHG	C16-C17-C18-C19
24	D	403	CLA	O1D-CGD-O2D-CED
32	e	102	LMT	C4-C5-C6-C7
35	b	629	LMG	C39-C40-C41-C42
35	c	520	LMG	C10-C11-C12-C13
24	B	601	CLA	C13-C15-C16-C17
24	B	615	CLA	C10-C11-C12-C13
24	a	405[B]	CLA	C15-C16-C17-C18
24	c	508	CLA	C5-C6-C7-C8
27	B	620	SQD	C11-C10-C9-C8
33	D	407[B]	LHG	C29-C30-C31-C32
33	d	408[A]	LHG	C27-C28-C29-C30
34	B	622	HTG	C3'-C4'-C5'-C6'
36	C	517[A]	DGD	C9A-CAA-CBA-CCA
32	B	627	LMT	C1-C2-C3-C4
32	c	501	LMT	C1-C2-C3-C4
32	M	104	LMT	C7-C8-C9-C10
33	E	101[A]	LHG	C24-C25-C26-C27
35	c	520	LMG	C34-C35-C36-C37
36	c	519	DGD	CBB-CCB-CDB-CEB
36	h	102	DGD	CCB-CDB-CEB-CFB
33	E	101[B]	LHG	C23-C24-C25-C26
24	B	615	CLA	C16-C17-C18-C20
24	a	409	CLA	C16-C17-C18-C19
24	c	510	CLA	C16-C17-C18-C19
27	X	101	SQD	C24-C25-C26-C27
33	L	101[A]	LHG	C25-C26-C27-C28
36	C	517[B]	DGD	C5B-C6B-C7B-C8B
36	h	102	DGD	C9B-CAB-CBB-CCB
32	e	102	LMT	O5'-C5'-C6'-O6'
35	Z	101	LMG	O6-C5-C6-O5
33	b	628[A]	LHG	C27-C28-C29-C30
36	c	517[A]	DGD	O6D-C5D-C6D-O5D
24	c	513	CLA	C10-C11-C12-C13
30	D	405[B]	PL9	C15-C14-C16-C17
25	A	408[B]	PHO	C2-C3-C5-C6
30	A	415[A]	PL9	C12-C11-C9-C8

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Mol	Chain	Res	Type	Atoms
30	D	405[A]	PL9	C13-C14-C16-C17
35	b	629	LMG	C11-C10-O7-C8
33	D	406[B]	LHG	C12-C13-C14-C15
24	C	508	CLA	C2A-CAA-CBA-CGA
28	A	412	GOL	O1-C1-C2-O2
28	B	623	GOL	O2-C2-C3-O3
28	V	203[A]	GOL	O2-C2-C3-O3
28	a	412	GOL	O1-C1-C2-O2
28	a	418	GOL	O1-C1-C2-O2
28	b	623	GOL	O2-C2-C3-O3
33	d	414[A]	LHG	C24-C25-C26-C27
35	c	520	LMG	C31-C32-C33-C34
24	b	614	CLA	C16-C17-C18-C19
33	A	420[B]	LHG	C12-C13-C14-C15
33	D	406[B]	LHG	O2-C2-C3-O3
33	E	101[A]	LHG	O2-C2-C3-O3
33	D	406[A]	LHG	C12-C13-C14-C15
33	L	101[B]	LHG	C12-C13-C14-C15
35	C	520	LMG	C16-C17-C18-C19
35	C	521	LMG	C17-C18-C19-C20
35	a	417	LMG	C21-C22-C23-C24
32	b	626	LMT	C1-C2-C3-C4
27	L	102	SQD	C27-C28-C29-C30
32	m	102	LMT	C7-C8-C9-C10
33	d	407[B]	LHG	C1-C2-C3-O3
36	C	517[B]	DGD	C4B-C5B-C6B-C7B
35	M	101	LMG	O9-C10-O7-C8
35	b	629	LMG	O9-C10-O7-C8
24	C	510	CLA	C2-C1-O2A-CGA
24	b	601	CLA	C2-C1-O2A-CGA
36	C	517[A]	DGD	O6D-C5D-C6D-O5D
27	L	102	SQD	C28-C29-C30-C31
32	B	630	LMT	C3-C4-C5-C6
32	t	101	LMT	C4-C5-C6-C7
33	d	408[B]	LHG	C27-C28-C29-C30
33	d	414[B]	LHG	C32-C33-C34-C35
35	C	501	LMG	C17-C18-C19-C20
27	L	102	SQD	C18-C19-C20-C21
33	A	420[A]	LHG	C34-C35-C36-C37
35	D	411	LMG	C30-C31-C32-C33
36	c	517[B]	DGD	C5A-C6A-C7A-C8A
26	D	404	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
26	Y	101	BCR	C1-C6-C7-C8
26	Y	101	BCR	C5-C6-C7-C8
26	b	617	BCR	C5-C6-C7-C8
26	b	619	BCR	C1-C6-C7-C8
26	b	619	BCR	C5-C6-C7-C8
26	y	101	BCR	C1-C6-C7-C8
27	f	101	SQD	C25-C26-C27-C28
33	d	407[B]	LHG	C13-C14-C15-C16
36	c	517[A]	DGD	C7A-C8A-C9A-CAA
24	b	601	CLA	C13-C15-C16-C17
24	c	507	CLA	C15-C16-C17-C18
35	M	101	LMG	C11-C10-O7-C8
27	A	413	SQD	C17-C18-C19-C20
33	L	101[B]	LHG	C25-C26-C27-C28
33	d	408[A]	LHG	C29-C30-C31-C32
36	c	517[B]	DGD	CAA-CBA-CCA-CDA
33	d	407[A]	LHG	C34-C35-C36-C37
36	c	518[A]	DGD	C6A-C7A-C8A-C9A
33	d	407[B]	LHG	C34-C35-C36-C37
36	c	518[B]	DGD	C4A-C5A-C6A-C7A
30	A	415[A]	PL9	C45-C44-C46-C47
30	a	415[A]	PL9	C12-C11-C9-C10
24	B	602	CLA	C11-C12-C13-C15
24	B	603	CLA	C11-C12-C13-C15
24	B	610	CLA	C12-C13-C15-C16
24	B	614	CLA	C11-C10-C8-C7
24	C	513	CLA	C11-C10-C8-C7
24	a	407[A]	CLA	C11-C12-C13-C15
24	a	407[B]	CLA	C11-C12-C13-C15
24	b	606	CLA	C11-C10-C8-C7
24	c	506	CLA	C2-C3-C5-C6
24	c	506	CLA	C11-C12-C13-C15
25	a	408[B]	PHO	C2-C3-C5-C6
30	d	406[A]	PL9	C13-C14-C16-C17
33	A	420[A]	LHG	C12-C13-C14-C15
36	c	518[A]	DGD	C4A-C5A-C6A-C7A
36	h	102	DGD	C7B-C8B-C9B-CAB
24	a	406[B]	CLA	CBD-CGD-O2D-CED
24	B	603	CLA	C16-C17-C18-C19
24	b	615	CLA	C16-C17-C18-C20
24	c	509	CLA	C16-C17-C18-C20
35	D	411	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	B	601	CLA	CBA-CGA-O2A-C1
27	L	102	SQD	C24-C23-O48-C46
35	C	520	LMG	C17-C18-C19-C20
35	C	521	LMG	C19-C20-C21-C22
24	b	610	CLA	C2A-CAA-CBA-CGA
36	c	517[B]	DGD	C4D-C5D-C6D-O5D
24	A	407[B]	CLA	C13-C15-C16-C17
27	a	411[B]	SQD	C12-C13-C14-C15
35	M	101	LMG	C29-C30-C31-C32
35	a	417	LMG	O6-C5-C6-O5
27	X	101	SQD	C34-C35-C36-C37
33	d	408[A]	LHG	C25-C26-C27-C28
35	C	501	LMG	C39-C40-C41-C42
27	A	411[B]	SQD	C7-C8-C9-C10
36	C	517[B]	DGD	O6D-C5D-C6D-O5D
33	D	407[A]	LHG	C13-C14-C15-C16
36	c	517[A]	DGD	CAA-CBA-CCA-CDA
35	a	417	LMG	C34-C35-C36-C37
35	b	629	LMG	C38-C39-C40-C41
27	A	413	SQD	O5-C1-O6-C44
36	C	518[A]	DGD	O6E-C1E-O5D-C6D
36	C	518[B]	DGD	O6E-C1E-O5D-C6D
27	L	102	SQD	C26-C27-C28-C29
33	D	407[A]	LHG	C15-C16-C17-C18
33	d	408[B]	LHG	C34-C35-C36-C37
32	A	421	LMT	C4'-C5'-C6'-O6'
32	A	421	LMT	C1-C2-C3-C4
35	Z	101	LMG	C11-C12-C13-C14
32	e	102	LMT	C9-C10-C11-C12
36	C	518[B]	DGD	C2E-C1E-O5D-C6D
27	A	411[A]	SQD	O6-C44-C45-O47
34	b	622	HTG	O5-C5-C6-O6
33	d	407[B]	LHG	C16-C17-C18-C19
33	d	408[A]	LHG	C34-C35-C36-C37
33	d	414[A]	LHG	C25-C26-C27-C28
35	b	629	LMG	C11-C12-C13-C14
36	C	517[B]	DGD	C9A-CAA-CBA-CCA
27	A	413	SQD	C27-C28-C29-C30
35	C	501	LMG	C13-C14-C15-C16
36	C	517[B]	DGD	C8A-C9A-CAA-CBA
36	C	517[B]	DGD	O6E-C5E-C6E-O5E
24	C	507	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	c	506	CLA	C4-C3-C5-C6
25	A	408[B]	PHO	C4-C3-C5-C6
25	a	408[B]	PHO	C4-C3-C5-C6
30	A	415[B]	PL9	C30-C29-C31-C32
30	A	415[B]	PL9	C45-C44-C46-C47
30	d	406[B]	PL9	C15-C14-C16-C17
30	D	405[B]	PL9	C13-C14-C16-C17
30	d	406[B]	PL9	C13-C14-C16-C17
33	d	414[B]	LHG	C25-C26-C27-C28
35	C	520	LMG	C31-C32-C33-C34
24	B	606	CLA	C11-C10-C8-C9
24	C	505	CLA	C14-C13-C15-C16
24	D	403	CLA	C11-C10-C8-C9
24	D	403	CLA	C14-C13-C15-C16
24	b	606	CLA	C11-C10-C8-C9
36	c	518[A]	DGD	C2B-C3B-C4B-C5B
24	C	502	CLA	C2A-CAA-CBA-CGA
33	L	101[B]	LHG	C13-C14-C15-C16
24	A	407[A]	CLA	C13-C15-C16-C17
24	c	511	CLA	CBD-CGD-O2D-CED
24	C	502	CLA	C1A-C2A-CAA-CBA
24	c	514	CLA	C1A-C2A-CAA-CBA
27	a	411[A]	SQD	C9-C10-C11-C12
32	M	102	LMT	C3-C4-C5-C6
32	b	620	LMT	C11-C10-C9-C8
32	t	101	LMT	C7-C8-C9-C10
33	A	420[A]	LHG	C26-C27-C28-C29
35	c	520	LMG	C33-C34-C35-C36
34	b	624	HTG	C4-C5-C6-O6
24	b	606	CLA	C15-C16-C17-C18
33	D	406[A]	LHG	C4-O6-P-O3
34	b	621	HTG	C3'-C4'-C5'-C6'
33	E	101[B]	LHG	C13-C14-C15-C16
32	e	102	LMT	C1-C2-C3-C4
24	C	509	CLA	C5-C6-C7-C8
32	b	620	LMT	C3-C4-C5-C6
33	d	408[A]	LHG	C28-C29-C30-C31
24	d	404	CLA	C16-C17-C18-C19
32	A	421	LMT	C4-C5-C6-C7
32	M	102	LMT	O5'-C5'-C6'-O6'
35	d	412	LMG	O6-C5-C6-O5
36	c	517[B]	DGD	CAB-CBB-CCB-CDB

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Mol	Chain	Res	Type	Atoms
36	h	102	DGD	CAA-CBA-CCA-CDA
36	C	517[A]	DGD	C8A-C9A-CAA-CBA
36	c	517[A]	DGD	C4D-C5D-C6D-O5D
36	c	517[B]	DGD	O6E-C5E-C6E-O5E
35	z	101	LMG	C19-C20-C21-C22
24	c	512	CLA	C8-C10-C11-C12
27	L	102	SQD	C13-C14-C15-C16
33	D	407[B]	LHG	C17-C18-C19-C20
35	C	501	LMG	C10-C11-C12-C13
24	B	601	CLA	O1A-CGA-O2A-C1
27	L	102	SQD	O10-C23-O48-C46
27	B	620	SQD	C24-C25-C26-C27
33	D	406[A]	LHG	C10-C11-C12-C13
24	d	403[A]	CLA	C16-C17-C18-C19
27	A	411[B]	SQD	O6-C44-C45-C46
27	A	413	SQD	O6-C44-C45-C46
27	a	411[A]	SQD	O6-C44-C45-C46
27	f	101	SQD	O6-C44-C45-C46
27	f	101	SQD	C44-C45-C46-O48
33	E	101[A]	LHG	C4-C5-C6-O8
33	E	101[B]	LHG	C4-C5-C6-O8
35	C	501	LMG	C7-C8-C9-O8
35	a	417	LMG	C7-C8-C9-O8
36	C	518[A]	DGD	CDA-CEA-CFA-CGA
24	B	605	CLA	C5-C6-C7-C8
24	b	605	CLA	C5-C6-C7-C8
33	d	414[B]	LHG	C24-C25-C26-C27
36	C	518[B]	DGD	CDA-CEA-CFA-CGA
36	C	518[A]	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
32	A	421	LMT	C7-C8-C9-C10
36	H	102	DGD	C7A-C8A-C9A-CAA
24	b	615	CLA	C10-C11-C12-C13
32	F	101	LMT	C6-C7-C8-C9
32	c	501	LMT	C9-C10-C11-C12
33	b	628[A]	LHG	C9-C10-C11-C12
33	D	407[A]	LHG	C29-C30-C31-C32
32	B	630	LMT	C1-C2-C3-C4
30	A	415[B]	PL9	C39-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
33	d	414[A]	LHG	C33-C34-C35-C36
35	C	501	LMG	C29-C30-C31-C32
28	a	412	GOL	O2-C2-C3-O3
28	o	302	GOL	O2-C2-C3-O3
32	B	628	LMT	C6-C7-C8-C9
32	b	620	LMT	C7-C8-C9-C10
33	A	420[B]	LHG	C26-C27-C28-C29
35	C	501	LMG	C18-C19-C20-C21
36	C	517[B]	DGD	C7A-C8A-C9A-CAA
32	B	627	LMT	C3'-C4'-O1B-C1B
36	C	517[A]	DGD	O6E-C5E-C6E-O5E
36	c	517[A]	DGD	O6E-C5E-C6E-O5E
30	a	415[B]	PL9	C12-C11-C9-C8
24	B	610	CLA	C15-C16-C17-C18
24	a	406[A]	CLA	C2C-C3C-CAC-CBC
32	A	421	LMT	C3'-C4'-O1B-C1B
33	D	407[B]	LHG	C15-C16-C17-C18
33	b	628[B]	LHG	C17-C18-C19-C20
27	B	620	SQD	C46-C45-O47-C7
24	c	514	CLA	C2-C1-O2A-CGA
27	a	411[A]	SQD	C12-C13-C14-C15
24	c	514	CLA	O1D-CGD-O2D-CED
35	b	629	LMG	C37-C38-C39-C40
36	h	102	DGD	C6B-C7B-C8B-C9B
24	C	513	CLA	O1D-CGD-O2D-CED
33	d	408[B]	LHG	C9-C10-C11-C12
24	c	512	CLA	CBA-CGA-O2A-C1
33	D	407[B]	LHG	C24-C23-O8-C6
36	c	517[A]	DGD	C2A-C1A-O1G-C1G
27	f	101	SQD	C23-C24-C25-C26
27	B	620	SQD	C34-C35-C36-C37
32	A	418	LMT	C9-C10-C11-C12
33	D	407[A]	LHG	C17-C18-C19-C20
35	C	520	LMG	C34-C35-C36-C37
24	B	614	CLA	C5-C6-C7-C8
27	A	411[A]	SQD	C11-C10-C9-C8
35	D	411	LMG	C36-C37-C38-C39
36	c	518[B]	DGD	C6A-C7A-C8A-C9A
33	A	420[A]	LHG	O2-C2-C3-O3
24	c	512	CLA	O1A-CGA-O2A-C1
27	L	102	SQD	C11-C10-C9-C8
33	b	628[B]	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
35	d	412	LMG	C35-C36-C37-C38
33	E	101[A]	LHG	C25-C26-C27-C28
33	d	408[A]	LHG	C33-C34-C35-C36
24	c	513	CLA	CBA-CGA-O2A-C1
33	D	406[B]	LHG	C13-C14-C15-C16
33	E	101[A]	LHG	C13-C14-C15-C16
24	A	405[A]	CLA	C13-C15-C16-C17
24	B	602	CLA	C15-C16-C17-C18
36	H	102	DGD	CCB-CDB-CEB-CFB
24	C	511	CLA	C4-C3-C5-C6
35	c	520	LMG	C30-C31-C32-C33
24	A	407[B]	CLA	C12-C13-C15-C16
24	B	606	CLA	C11-C10-C8-C7
24	C	505	CLA	C12-C13-C15-C16
24	C	506	CLA	C12-C13-C15-C16
24	C	511	CLA	C2-C3-C5-C6
24	D	403	CLA	C12-C13-C15-C16
24	b	601	CLA	C11-C10-C8-C7
24	b	614	CLA	C12-C13-C15-C16
24	b	615	CLA	C12-C13-C15-C16
24	c	505	CLA	C11-C12-C13-C15
24	c	505	CLA	C12-C13-C15-C16
24	c	511	CLA	C11-C10-C8-C7
24	c	513	CLA	C12-C13-C15-C16
32	c	501	LMT	C2-C3-C4-C5
24	B	602	CLA	C11-C12-C13-C14
24	B	614	CLA	C14-C13-C15-C16
24	C	507	CLA	C6-C7-C8-C9
24	C	511	CLA	C11-C12-C13-C14
24	C	514	CLA	C11-C10-C8-C9
24	c	514	CLA	C6-C7-C8-C9
27	L	102	SQD	C30-C31-C32-C33
32	b	626	LMT	C6-C7-C8-C9
36	c	517[B]	DGD	C2A-C1A-O1G-C1G
28	l	801[A]	GOL	O1-C1-C2-C3
33	b	628[B]	LHG	C13-C14-C15-C16
36	h	102	DGD	CBA-CCA-CDA-CEA
35	c	521	LMG	C29-C28-O8-C9
27	L	102	SQD	C14-C15-C16-C17
33	a	420[A]	LHG	C23-C24-C25-C26
35	C	521	LMG	C4-C5-C6-O5
33	b	628[B]	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
24	B	615	CLA	C5-C6-C7-C8
33	D	406[B]	LHG	O6-C4-C5-C6
33	L	101[B]	LHG	O6-C4-C5-C6
33	b	628[B]	LHG	O6-C4-C5-C6
30	A	415[A]	PL9	C39-C41-C42-C43
33	D	407[B]	LHG	C13-C14-C15-C16
24	b	610	CLA	C15-C16-C17-C18
32	c	501	LMT	O5'-C5'-C6'-O6'
24	C	514	CLA	O1D-CGD-O2D-CED
30	D	405[A]	PL9	C45-C44-C46-C47
30	d	406[B]	PL9	C18-C19-C21-C22
33	D	407[B]	LHG	O10-C23-O8-C6
32	A	421	LMT	C5-C6-C7-C8
36	c	518[A]	DGD	CBB-CCB-CDB-CEB
36	c	518[B]	DGD	C2B-C3B-C4B-C5B
24	C	502	CLA	O1D-CGD-O2D-CED
36	C	517[B]	DGD	C4D-C5D-C6D-O5D
32	F	101	LMT	C4-C5-C6-C7
33	L	101[B]	LHG	C27-C28-C29-C30
35	C	520	LMG	C11-C12-C13-C14
24	B	601	CLA	C2A-CAA-CBA-CGA
24	C	513	CLA	CBA-CGA-O2A-C1
24	D	403	CLA	CBA-CGA-O2A-C1
36	C	517[A]	DGD	CCA-CDA-CEA-CFA
24	C	507	CLA	C3A-C2A-CAA-CBA
24	c	507	CLA	C3A-C2A-CAA-CBA
33	a	420[A]	LHG	C10-C11-C12-C13
35	a	417	LMG	C29-C30-C31-C32
35	a	417	LMG	C35-C36-C37-C38
32	b	626	LMT	C2-C1-O1'-C1'
32	e	102	LMT	C2-C1-O1'-C1'
32	m	102	LMT	C2-C1-O1'-C1'
24	B	601	CLA	C15-C16-C17-C18
24	b	612	CLA	C8-C10-C11-C12
24	b	606	CLA	C16-C17-C18-C19
36	c	519	DGD	C2A-C1A-O1G-C1G
24	c	507	CLA	C10-C11-C12-C13
27	A	411[A]	SQD	O6-C44-C45-C46
27	L	102	SQD	C44-C45-C46-O48
33	a	420[A]	LHG	C4-C5-C6-O8
33	a	420[B]	LHG	C4-C5-C6-O8
33	L	101[A]	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
36	C	517[A]	DGD	C1B-C2B-C3B-C4B
33	L	101[B]	LHG	C24-C25-C26-C27
32	c	501	LMT	C3-C4-C5-C6
36	H	102	DGD	C9B-CAB-CBB-CCB
24	C	510	CLA	C3-C5-C6-C7
36	c	517[A]	DGD	O1A-C1A-O1G-C1G
30	D	405[A]	PL9	C15-C14-C16-C17
24	B	610	CLA	C16-C17-C18-C19
30	D	405[A]	PL9	C43-C44-C46-C47
36	C	517[A]	DGD	C4D-C5D-C6D-O5D
36	C	517[A]	DGD	C7A-C8A-C9A-CAA
36	C	519	DGD	CBA-CCA-CDA-CEA
24	a	406[B]	CLA	C2C-C3C-CAC-CBC
35	C	521	LMG	C12-C13-C14-C15
33	d	414[A]	LHG	C3-O3-P-O6
35	C	521	LMG	C10-C11-C12-C13
35	Z	101	LMG	C29-C28-O8-C9
28	B	623	GOL	O1-C1-C2-O2
28	v	202[A]	GOL	O1-C1-C2-O2
27	a	411[B]	SQD	C35-C36-C37-C38
33	D	406[B]	LHG	C11-C10-C9-C8
33	E	101[B]	LHG	C25-C26-C27-C28
35	d	412	LMG	C18-C19-C20-C21
36	C	517[A]	DGD	C3B-C4B-C5B-C6B
24	d	404	CLA	CBA-CGA-O2A-C1
24	A	407[A]	CLA	C16-C17-C18-C20
24	c	513	CLA	C13-C15-C16-C17
36	H	102	DGD	O2G-C1B-C2B-C3B
36	c	517[B]	DGD	O1A-C1A-O1G-C1G
33	b	628[B]	LHG	C12-C13-C14-C15
36	C	519	DGD	CDB-CEB-CFB-CGB
27	a	411[A]	SQD	O6-C44-C45-O47
35	M	101	LMG	O1-C7-C8-O7
24	C	511	CLA	CBA-CGA-O2A-C1
35	C	520	LMG	C37-C38-C39-C40
35	z	101	LMG	C14-C15-C16-C17
24	B	610	CLA	C16-C17-C18-C20
33	L	101[B]	LHG	C15-C16-C17-C18
36	c	517[A]	DGD	O6E-C1E-O5D-C6D
30	a	415[A]	PL9	C24-C26-C27-C28
33	A	420[A]	LHG	C1-C2-C3-O3
27	a	411[B]	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
35	b	629	LMG	C14-C15-C16-C17
24	b	608	CLA	C2-C1-O2A-CGA
33	D	407[B]	LHG	C10-C11-C12-C13
35	M	101	LMG	C36-C37-C38-C39
24	B	612	CLA	C10-C11-C12-C13
24	b	601	CLA	C6-C7-C8-C9
27	A	411[B]	SQD	C18-C19-C20-C21
35	M	101	LMG	C20-C21-C22-C23
35	c	520	LMG	C32-C33-C34-C35
24	b	616	CLA	C5-C6-C7-C8
33	D	407[A]	LHG	C27-C28-C29-C30
33	b	628[A]	LHG	C34-C35-C36-C37
36	H	102	DGD	CAB-CBB-CCB-CDB
24	b	606	CLA	C16-C17-C18-C20
24	b	610	CLA	C16-C17-C18-C19
24	b	607	CLA	C3-C5-C6-C7
26	B	617	BCR	C1-C6-C7-C8
26	B	617	BCR	C5-C6-C7-C8
26	H	101	BCR	C23-C24-C25-C26
26	H	101	BCR	C23-C24-C25-C30
26	d	405	BCR	C23-C24-C25-C26
26	d	405	BCR	C23-C24-C25-C30
26	h	101	BCR	C23-C24-C25-C26
24	b	607	CLA	C8-C10-C11-C12
26	Y	101	BCR	C37-C22-C23-C24
34	d	411	HTG	S1-C1'-C2'-C3'
26	Y	101	BCR	C21-C22-C23-C24
26	d	405	BCR	C21-C22-C23-C24
27	a	411[B]	SQD	C9-C10-C11-C12
33	L	101[A]	LHG	C11-C10-C9-C8
24	D	403	CLA	O1A-CGA-O2A-C1
27	A	411[A]	SQD	C18-C19-C20-C21
33	a	420[A]	LHG	C7-C8-C9-C10
33	d	414[B]	LHG	C17-C18-C19-C20
24	C	513	CLA	C10-C11-C12-C13
36	C	518[A]	DGD	C5B-C6B-C7B-C8B
33	b	628[A]	LHG	C13-C14-C15-C16
33	L	101[A]	LHG	O6-C4-C5-C6
36	C	518[A]	DGD	C8B-C9B-CAB-CBB
24	B	614	CLA	C12-C13-C15-C16
24	C	507	CLA	C6-C7-C8-C10
24	C	514	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
24	a	409	CLA	C11-C10-C8-C7
24	b	601	CLA	C6-C7-C8-C10
24	b	601	CLA	C11-C12-C13-C15
24	b	603	CLA	C11-C10-C8-C7
24	b	604	CLA	C6-C7-C8-C10
24	c	507	CLA	C11-C10-C8-C7
24	c	510	CLA	C6-C7-C8-C10
24	c	510	CLA	C11-C10-C8-C7
24	c	514	CLA	C12-C13-C15-C16
30	a	415[A]	PL9	C12-C11-C9-C8
30	d	406[B]	PL9	C28-C29-C31-C32
35	c	521	LMG	O10-C28-O8-C9
33	D	406[A]	LHG	C11-C10-C9-C8
36	c	517[A]	DGD	CCB-CDB-CEB-CFB
36	c	518[B]	DGD	C9B-CAB-CBB-CCB
27	a	411[A]	SQD	C27-C28-C29-C30
33	L	101[A]	LHG	C24-C25-C26-C27
33	D	407[A]	LHG	C10-C11-C12-C13
33	d	407[A]	LHG	C13-C14-C15-C16
33	D	406[B]	LHG	C10-C11-C12-C13
36	C	518[A]	DGD	C7A-C8A-C9A-CAA
24	C	507	CLA	C15-C16-C17-C18
27	L	102	SQD	C16-C17-C18-C19
32	b	626	LMT	O1'-C1-C2-C3
34	B	621	HTG	C1'-C2'-C3'-C4'
36	c	519	DGD	CDA-CEA-CFA-CGA
24	b	610	CLA	C16-C17-C18-C20
24	b	601	CLA	CBA-CGA-O2A-C1
36	c	518[B]	DGD	C5B-C6B-C7B-C8B
36	C	518[B]	DGD	C3B-C4B-C5B-C6B
24	b	602	CLA	C10-C11-C12-C13
24	B	610	CLA	CAD-CBD-CGD-O2D
24	b	610	CLA	CAD-CBD-CGD-O2D
24	b	612	CLA	CAD-CBD-CGD-O2D
24	b	616	CLA	CAD-CBD-CGD-O2D
25	A	408[B]	PHO	CAD-CBD-CGD-O2D
25	a	408[A]	PHO	CAD-CBD-CGD-O2D
27	L	102	SQD	C46-C45-O47-C7
39	e	101	HEM	C2B-C3B-CAB-CBB
27	A	413	SQD	C15-C16-C17-C18
24	c	510	CLA	C8-C10-C11-C12
30	d	406[A]	PL9	C45-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
27	a	411[A]	SQD	C34-C35-C36-C37
36	c	517[B]	DGD	O6E-C1E-O5D-C6D
36	c	518[A]	DGD	O6E-C1E-O5D-C6D
25	A	417[A]	PHO	C2C-C3C-CAC-CBC
27	B	620	SQD	C44-C45-C46-O48
27	a	413	SQD	O6-C44-C45-C46
33	d	408[B]	LHG	C2-C3-O3-P
36	H	102	DGD	O1G-C1G-C2G-C3G
24	c	513	CLA	O1A-CGA-O2A-C1
33	D	406[B]	LHG	O6-C4-C5-O7
33	E	101[A]	LHG	O6-C4-C5-O7
33	L	101[A]	LHG	O6-C4-C5-O7
33	b	628[B]	LHG	O6-C4-C5-O7
24	B	615	CLA	C8-C10-C11-C12
24	b	610	CLA	C13-C15-C16-C17
24	b	605	CLA	C3-C5-C6-C7
24	B	601	CLA	CAA-CBA-CGA-O2A
24	b	601	CLA	CAA-CBA-CGA-O2A
33	a	420[B]	LHG	C10-C11-C12-C13
24	b	615	CLA	C13-C15-C16-C17
36	C	519	DGD	C7A-C8A-C9A-CAA
24	B	601	CLA	CHA-CBD-CGD-O1D
24	B	601	CLA	CHA-CBD-CGD-O2D
24	C	503	CLA	CHA-CBD-CGD-O1D
24	C	503	CLA	CHA-CBD-CGD-O2D
24	C	505	CLA	CHA-CBD-CGD-O1D
24	b	601	CLA	CHA-CBD-CGD-O1D
24	b	601	CLA	CHA-CBD-CGD-O2D
24	b	606	CLA	CHA-CBD-CGD-O1D
24	c	503	CLA	CHA-CBD-CGD-O1D
24	c	511	CLA	CHA-CBD-CGD-O1D
24	c	510	CLA	C10-C11-C12-C13
36	c	519	DGD	O1A-C1A-O1G-C1G
35	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
33	A	420[A]	LHG	C32-C33-C34-C35
27	L	102	SQD	O47-C45-C46-O48
27	a	411[B]	SQD	O6-C44-C45-O47
33	a	420[A]	LHG	O7-C5-C6-O8
35	C	501	LMG	O7-C8-C9-O8
36	H	102	DGD	O1G-C1G-C2G-O2G

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Mol	Chain	Res	Type	Atoms
27	A	411[A]	SQD	C34-C35-C36-C37
24	B	604	CLA	C5-C6-C7-C8
24	d	404	CLA	O1A-CGA-O2A-C1
24	A	407[B]	CLA	C16-C17-C18-C20
28	B	626	GOL	O1-C1-C2-O2
28	c	527	GOL	O1-C1-C2-O2
33	A	420[B]	LHG	O1-C1-C2-O2
27	B	620	SQD	C9-C10-C11-C12
33	d	407[A]	LHG	C11-C10-C9-C8
33	d	408[A]	LHG	C9-C10-C11-C12
34	b	622	HTG	S1-C1'-C2'-C3'
24	C	506	CLA	C4-C3-C5-C6
27	B	620	SQD	C29-C30-C31-C32
33	d	408[B]	LHG	C32-C33-C34-C35
24	C	511	CLA	O1A-CGA-O2A-C1
24	C	513	CLA	O1A-CGA-O2A-C1
24	C	506	CLA	C2-C3-C5-C6
30	D	405[B]	PL9	C4-C3-C7-C8
33	b	628[B]	LHG	C9-C10-C11-C12
24	b	603	CLA	C11-C10-C8-C9
24	b	601	CLA	O1A-CGA-O2A-C1
24	B	602	CLA	C8-C10-C11-C12
35	C	501	LMG	C20-C21-C22-C23
24	a	406[B]	CLA	C15-C16-C17-C18
24	C	512	CLA	C3-C5-C6-C7
33	d	414[A]	LHG	C18-C19-C20-C21
24	B	604	CLA	C1A-C2A-CAA-CBA
24	a	406[A]	CLA	C1A-C2A-CAA-CBA
33	d	407[A]	LHG	C16-C17-C18-C19
35	D	411	LMG	C18-C19-C20-C21
24	c	513	CLA	O1D-CGD-O2D-CED
27	B	620	SQD	C31-C32-C33-C34
27	a	411[A]	SQD	C35-C36-C37-C38
35	C	520	LMG	C36-C37-C38-C39
33	D	407[A]	LHG	C2-C3-O3-P
33	D	407[B]	LHG	C2-C3-O3-P
33	D	406[A]	LHG	C4-O6-P-O5
33	E	101[A]	LHG	C4-O6-P-O5
33	a	420[A]	LHG	C4-O6-P-O4
33	a	420[B]	LHG	C4-O6-P-O4
33	d	407[B]	LHG	C3-O3-P-O4
24	C	511	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
33	E	101[A]	LHG	O6-C4-C5-C6
33	D	407[B]	LHG	C28-C29-C30-C31
24	b	615	CLA	C5-C6-C7-C8
33	d	407[B]	LHG	C25-C26-C27-C28
36	c	517[B]	DGD	C8B-C9B-CAB-CBB
33	L	101[A]	LHG	C26-C27-C28-C29
35	C	501	LMG	C30-C31-C32-C33
24	B	608	CLA	C16-C17-C18-C20
34	B	624	HTG	C4'-C5'-C6'-C7'
36	C	518[B]	DGD	C7A-C8A-C9A-CAA
36	c	518[A]	DGD	C7B-C8B-C9B-CAB
24	B	601	CLA	CAD-CBD-CGD-O1D
24	B	609	CLA	CAD-CBD-CGD-O1D
24	C	503	CLA	CAD-CBD-CGD-O1D
24	C	505	CLA	CAD-CBD-CGD-O1D
24	b	601	CLA	CAD-CBD-CGD-O1D
24	c	503	CLA	CAD-CBD-CGD-O1D
24	c	507	CLA	CAD-CBD-CGD-O1D
36	C	517[A]	DGD	C6A-C7A-C8A-C9A
24	a	406[B]	CLA	O1D-CGD-O2D-CED
35	z	101	LMG	C10-C11-C12-C13
24	b	616	CLA	CBA-CGA-O2A-C1
36	C	517[B]	DGD	C3B-C4B-C5B-C6B
24	b	608	CLA	C16-C17-C18-C20
24	d	403[B]	CLA	C16-C17-C18-C20
30	A	415[B]	PL9	C25-C24-C26-C27
24	A	407[A]	CLA	C12-C13-C15-C16
24	B	616	CLA	C12-C13-C15-C16
24	C	503	CLA	C12-C13-C15-C16
24	C	506	CLA	C11-C12-C13-C15
24	C	511	CLA	C12-C13-C15-C16
24	C	514	CLA	C11-C12-C13-C15
24	b	616	CLA	C6-C7-C8-C10
24	c	506	CLA	C12-C13-C15-C16
24	d	403[A]	CLA	C11-C12-C13-C15
24	d	403[B]	CLA	C11-C12-C13-C15
33	L	101[B]	LHG	O6-C4-C5-O7
33	a	420[B]	LHG	C23-C24-C25-C26
27	A	411[A]	SQD	C13-C14-C15-C16
33	b	628[B]	LHG	C10-C11-C12-C13
33	D	406[A]	LHG	C34-C35-C36-C37
36	C	517[B]	DGD	C2A-C3A-C4A-C5A

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Mol	Chain	Res	Type	Atoms
36	C	519	DGD	CAB-CBB-CCB-CDB
35	C	501	LMG	C11-C12-C13-C14
36	c	518[A]	DGD	C5A-C6A-C7A-C8A
35	M	101	LMG	O1-C7-C8-C9
36	h	102	DGD	O1G-C1G-C2G-C3G
27	B	620	SQD	O47-C45-C46-O48
33	E	101[A]	LHG	O7-C5-C6-O8
33	E	101[B]	LHG	O7-C5-C6-O8
33	a	420[B]	LHG	O7-C5-C6-O8
35	a	417	LMG	O7-C8-C9-O8
33	d	408[A]	LHG	C32-C33-C34-C35
36	C	518[A]	DGD	C8A-C9A-CAA-CBA
27	A	411[B]	SQD	C12-C13-C14-C15
33	d	407[B]	LHG	C9-C10-C11-C12
35	M	101	LMG	C18-C19-C20-C21
36	C	518[A]	DGD	C5D-C6D-O5D-C1E
36	c	518[B]	DGD	C2G-C3G-O3G-C1D
36	H	102	DGD	CCA-CDA-CEA-CFA
33	d	408[A]	LHG	C2-C3-O3-P
24	C	512	CLA	O1A-CGA-O2A-C1
27	X	101	SQD	C24-C23-O48-C46
33	d	414[A]	LHG	C34-C35-C36-C37
24	C	507	CLA	C5-C6-C7-C8
24	C	506	CLA	C11-C12-C13-C14
24	a	409	CLA	C11-C10-C8-C9
24	b	615	CLA	C14-C13-C15-C16
24	c	510	CLA	C6-C7-C8-C9
24	c	511	CLA	C11-C10-C8-C9
33	D	406[A]	LHG	C26-C27-C28-C29
34	B	621	HTG	C2'-C3'-C4'-C5'
30	a	415[B]	PL9	C24-C26-C27-C28
27	a	411[B]	SQD	C34-C35-C36-C37
36	C	519	DGD	C4A-C5A-C6A-C7A
33	d	408[B]	LHG	O10-C23-O8-C6
24	c	508	CLA	C2A-CAA-CBA-CGA
36	C	518[A]	DGD	C7B-C8B-C9B-CAB
36	h	102	DGD	C5B-C6B-C7B-C8B
33	d	414[A]	LHG	C11-C12-C13-C14
36	h	102	DGD	CDA-CEA-CFA-CGA
33	b	628[B]	LHG	C34-C35-C36-C37
24	b	616	CLA	O1A-CGA-O2A-C1
24	C	511	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
32	c	501	LMT	C4'-C5'-C6'-O6'
27	a	413	SQD	C15-C16-C17-C18
32	e	102	LMT	C2-C3-C4-C5
30	d	406[B]	PL9	C45-C44-C46-C47
27	a	411[B]	SQD	C19-C20-C21-C22
30	a	415[A]	PL9	C43-C44-C46-C47
33	L	101[A]	LHG	C23-C24-C25-C26
33	D	406[A]	LHG	C13-C14-C15-C16
32	B	628	LMT	C3-C4-C5-C6
33	b	628[A]	LHG	C28-C29-C30-C31
33	A	420[B]	LHG	C17-C18-C19-C20
24	A	405[B]	CLA	C2-C1-O2A-CGA
24	A	409	CLA	C2-C1-O2A-CGA
24	a	405[B]	CLA	C2-C1-O2A-CGA
24	b	613	CLA	C2-C1-O2A-CGA
24	C	510	CLA	O1D-CGD-O2D-CED
33	D	406[B]	LHG	C9-C10-C11-C12
35	a	417	LMG	O8-C28-C29-C30
33	d	408[B]	LHG	C24-C23-O8-C6
36	C	517[B]	DGD	C6A-C7A-C8A-C9A
36	c	519	DGD	C6A-C7A-C8A-C9A
26	a	410	BCR	C1-C6-C7-C8
26	h	101	BCR	C23-C24-C25-C30
30	A	415[A]	PL9	C28-C29-C31-C32
35	a	417	LMG	C13-C14-C15-C16
36	c	519	DGD	CBA-CCA-CDA-CEA
33	d	408[A]	LHG	C10-C11-C12-C13
36	C	519	DGD	C8A-C9A-CAA-CBA
35	C	520	LMG	C30-C31-C32-C33
35	C	521	LMG	C38-C39-C40-C41
36	C	519	DGD	C6A-C7A-C8A-C9A
36	c	518[B]	DGD	O6E-C1E-O5D-C6D
32	A	418	LMT	C7-C8-C9-C10
35	d	412	LMG	C36-C37-C38-C39
36	C	518[B]	DGD	C8A-C9A-CAA-CBA
36	c	517[B]	DGD	C2E-C1E-O5D-C6D
34	B	622	HTG	S1-C1'-C2'-C3'
27	f	101	SQD	O47-C45-C46-O48
36	h	102	DGD	O1G-C1G-C2G-O2G
24	D	403	CLA	C15-C16-C17-C18
33	d	414[B]	LHG	C3-O3-P-O6
27	A	411[A]	SQD	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
35	c	521	LMG	C31-C32-C33-C34
27	L	102	SQD	C35-C36-C37-C38
24	B	605	CLA	C11-C12-C13-C15
24	C	507	CLA	C2-C3-C5-C6
33	d	407[B]	LHG	C12-C13-C14-C15
24	a	406[A]	CLA	C4C-C3C-CAC-CBC
32	B	628	LMT	C7-C8-C9-C10
32	B	630	LMT	C2-C3-C4-C5
36	C	517[B]	DGD	CCA-CDA-CEA-CFA
24	A	407[A]	CLA	C14-C13-C15-C16
24	A	407[B]	CLA	C14-C13-C15-C16
24	C	506	CLA	C14-C13-C15-C16
24	c	507	CLA	C11-C10-C8-C9
24	d	403[A]	CLA	C11-C12-C13-C14
24	C	502	CLA	C16-C17-C18-C20
33	D	406[A]	LHG	C28-C29-C30-C31
27	X	101	SQD	O10-C23-O48-C46
35	c	520	LMG	C29-C30-C31-C32
28	B	626	GOL	C1-C2-C3-O3
28	l	801[B]	GOL	O1-C1-C2-C3
33	A	420[A]	LHG	O1-C1-C2-C3
36	C	519	DGD	C2A-C3A-C4A-C5A
24	a	406[A]	CLA	C15-C16-C17-C18
36	c	518[B]	DGD	C1A-C2A-C3A-C4A
28	a	419	GOL	O2-C2-C3-O3
28	o	302	GOL	O1-C1-C2-O2
24	B	608	CLA	C16-C17-C18-C19
24	C	511	CLA	C16-C17-C18-C20
24	C	512	CLA	CBA-CGA-O2A-C1
33	d	407[B]	LHG	C24-C23-O8-C6
36	C	517[B]	DGD	C2A-C1A-O1G-C1G
27	A	411[B]	SQD	C11-C10-C9-C8
27	a	411[A]	SQD	C11-C12-C13-C14
36	h	102	DGD	O2G-C1B-C2B-C3B
24	B	611	CLA	C8-C10-C11-C12
33	D	407[A]	LHG	O10-C23-O8-C6
33	D	407[A]	LHG	C24-C23-O8-C6
27	B	620	SQD	O5-C1-O6-C44
36	h	102	DGD	C6A-C7A-C8A-C9A
33	d	407[B]	LHG	O6-C4-C5-C6
36	C	517[B]	DGD	O1A-C1A-O1G-C1G
34	B	624	HTG	C2'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
24	b	605	CLA	C16-C17-C18-C20
25	a	408[A]	PHO	C4-C3-C5-C6
36	c	518[B]	DGD	C5A-C6A-C7A-C8A
25	a	408[A]	PHO	C2-C3-C5-C6
24	A	405[B]	CLA	C13-C15-C16-C17
24	c	504	CLA	C8-C10-C11-C12
33	a	420[B]	LHG	C24-C25-C26-C27
24	b	614	CLA	C2-C1-O2A-CGA
24	d	403[B]	CLA	C16-C17-C18-C19
36	c	518[B]	DGD	C2E-C1E-O5D-C6D
24	A	405[B]	CLA	C2A-CAA-CBA-CGA
36	c	517[A]	DGD	C4B-C5B-C6B-C7B
33	a	420[B]	LHG	C7-C8-C9-C10
32	e	102	LMT	C3-C4-C5-C6
33	d	407[A]	LHG	C9-C10-C11-C12
33	D	406[A]	LHG	C17-C18-C19-C20
30	a	415[A]	PL9	C4-C3-C7-C8
30	a	415[B]	PL9	C4-C3-C7-C8
24	B	613	CLA	C11-C12-C13-C14
24	B	614	CLA	C11-C10-C8-C9
24	C	510	CLA	C6-C7-C8-C9
24	C	511	CLA	C14-C13-C15-C16
24	a	407[A]	CLA	C14-C13-C15-C16
24	c	506	CLA	C14-C13-C15-C16
24	c	507	CLA	C6-C7-C8-C9
24	c	512	CLA	C11-C10-C8-C9
33	d	414[B]	LHG	C33-C34-C35-C36
34	b	624	HTG	C4'-C5'-C6'-C7'
33	b	628[A]	LHG	C10-C11-C12-C13
27	a	411[B]	SQD	O6-C44-C45-C46
33	d	414[A]	LHG	C1-C2-C3-O3
27	a	411[A]	SQD	C10-C11-C12-C13
33	E	101[A]	LHG	C12-C13-C14-C15
25	A	408[A]	PHO	O2A-C1-C2-C3
25	a	408[A]	PHO	O2A-C1-C2-C3
25	a	408[B]	PHO	O2A-C1-C2-C3
32	M	102	LMT	O5'-C1'-O1'-C1
32	c	501	LMT	C7-C8-C9-C10
36	c	517[A]	DGD	CBA-CCA-CDA-CEA
36	c	519	DGD	C4A-C5A-C6A-C7A
26	d	405	BCR	C37-C22-C23-C24
24	D	403	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	b	601	CLA	C4-C3-C5-C6
30	a	415[A]	PL9	C45-C44-C46-C47
24	B	611	CLA	C1A-C2A-CAA-CBA
24	a	406[B]	CLA	C1A-C2A-CAA-CBA
24	a	407[A]	CLA	C1A-C2A-CAA-CBA
24	a	407[B]	CLA	C1A-C2A-CAA-CBA
36	h	102	DGD	CAB-CBB-CCB-CDB
24	B	613	CLA	C12-C13-C15-C16
24	B	615	CLA	C11-C12-C13-C15
24	b	605	CLA	C13-C15-C16-C17
36	C	518[B]	DGD	C7B-C8B-C9B-CAB
36	C	519	DGD	CAA-CBA-CCA-CDA
33	A	420[A]	LHG	C29-C30-C31-C32
33	L	101[A]	LHG	C10-C11-C12-C13
33	d	408[B]	LHG	C28-C29-C30-C31
24	b	612	CLA	C13-C15-C16-C17
36	c	517[B]	DGD	CBA-CCA-CDA-CEA
24	a	406[B]	CLA	C4C-C3C-CAC-CBC
24	b	612	CLA	C10-C11-C12-C13
24	c	507	CLA	C13-C15-C16-C17
35	z	101	LMG	O7-C10-C11-C12
33	E	101[B]	LHG	C11-C10-C9-C8
24	C	506	CLA	C8-C10-C11-C12
36	h	102	DGD	CDB-CEB-CFB-CGB
41	V	201	HEC	CAD-CBD-CGD-O1D
41	V	201	HEC	CAD-CBD-CGD-O2D
24	B	603	CLA	C4-C3-C5-C6
35	z	101	LMG	C13-C14-C15-C16
24	B	610	CLA	C13-C15-C16-C17
33	L	101[B]	LHG	C23-C24-C25-C26
35	c	520	LMG	C28-C29-C30-C31
30	A	415[B]	PL9	C12-C11-C9-C8
33	d	407[B]	LHG	O10-C23-O8-C6
36	C	519	DGD	C9A-CAA-CBA-CCA
27	X	101	SQD	O47-C45-C46-O48
24	c	511	CLA	O1D-CGD-O2D-CED
26	a	410	BCR	C19-C20-C21-C22
24	a	409	CLA	C8-C10-C11-C12
33	a	420[A]	LHG	C24-C25-C26-C27
33	d	414[A]	LHG	C27-C28-C29-C30
24	A	407[A]	CLA	C16-C17-C18-C19
33	d	414[A]	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
33	d	414[B]	LHG	C1-C2-C3-O3
33	d	407[A]	LHG	C25-C26-C27-C28
30	D	405[B]	PL9	C35-C34-C36-C37
24	B	613	CLA	C2-C1-O2A-CGA
24	a	405[A]	CLA	C2-C1-O2A-CGA
30	a	415[B]	PL9	C43-C44-C46-C47
30	d	406[A]	PL9	C43-C44-C46-C47
24	B	605	CLA	C11-C12-C13-C14
24	a	407[B]	CLA	C14-C13-C15-C16
24	b	603	CLA	C14-C13-C15-C16
24	b	614	CLA	C11-C12-C13-C14
27	A	413	SQD	C25-C26-C27-C28
27	a	413	SQD	C28-C29-C30-C31
33	A	420[B]	LHG	C18-C19-C20-C21
33	L	101[B]	LHG	C26-C27-C28-C29
24	b	608	CLA	C13-C15-C16-C17
24	c	503	CLA	C16-C17-C18-C19
36	c	519	DGD	C9B-CAB-CBB-CCB
26	c	515	BCR	C23-C24-C25-C30
32	A	418	LMT	C4B-C5B-C6B-O6B
39	F	102	HEM	CAD-CBD-CGD-O1D
28	O	303	GOL	O1-C1-C2-C3
33	D	406[B]	LHG	C28-C29-C30-C31
24	b	616	CLA	C4-C3-C5-C6
24	c	511	CLA	C4-C3-C5-C6
30	a	415[B]	PL9	C45-C44-C46-C47
26	b	619	BCR	C21-C22-C23-C24
24	b	608	CLA	C16-C17-C18-C19
33	d	414[A]	LHG	C9-C10-C11-C12
30	A	415[A]	PL9	C43-C44-C46-C47
36	C	518[B]	DGD	C1A-C2A-C3A-C4A
27	a	413	SQD	C18-C19-C20-C21
35	d	412	LMG	C13-C14-C15-C16
24	b	604	CLA	C10-C11-C12-C13
36	C	518[B]	DGD	C2G-C3G-O3G-C1D
33	A	420[A]	LHG	C17-C18-C19-C20
34	B	621	HTG	C3'-C4'-C5'-C6'
35	Z	101	LMG	O10-C28-O8-C9
36	c	517[A]	DGD	CDB-CEB-CFB-CGB
33	d	407[B]	LHG	O6-C4-C5-O7
27	f	101	SQD	C11-C10-C9-C8
33	d	414[B]	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
35	C	520	LMG	C15-C16-C17-C18
25	A	408[B]	PHO	CBA-CGA-O2A-C1
24	A	406[B]	CLA	C2C-C3C-CAC-CBC
32	c	501	LMT	C4-C5-C6-C7
36	C	517[B]	DGD	CDB-CEB-CFB-CGB
24	c	514	CLA	C3-C5-C6-C7
36	C	517[B]	DGD	O6E-C1E-O5D-C6D
36	c	518[A]	DGD	C1A-C2A-C3A-C4A
24	b	604	CLA	C4-C3-C5-C6
30	D	405[A]	PL9	C35-C34-C36-C37
30	d	406[B]	PL9	C20-C19-C21-C22
24	b	601	CLA	C2-C3-C5-C6
24	b	613	CLA	C11-C10-C8-C7
24	b	615	CLA	C11-C12-C13-C15
24	b	616	CLA	C2-C3-C5-C6
24	c	511	CLA	C12-C13-C15-C16
30	d	406[B]	PL9	C43-C44-C46-C47
24	a	409	CLA	C15-C16-C17-C18
28	V	203[B]	GOL	O1-C1-C2-O2
28	d	413	GOL	O1-C1-C2-O2
24	b	601	CLA	C3-C5-C6-C7
36	h	102	DGD	C2B-C3B-C4B-C5B
35	b	629	LMG	C2-C1-O1-C7
36	C	517[B]	DGD	C2E-C1E-O5D-C6D
33	b	628[A]	LHG	C25-C26-C27-C28
39	e	101	HEM	CAD-CBD-CGD-O1D
27	X	101	SQD	C31-C32-C33-C34
27	A	411[B]	SQD	C34-C35-C36-C37
39	e	101	HEM	CAA-CBA-CGA-O2A
41	v	201	HEC	CAD-CBD-CGD-O2D
33	A	420[A]	LHG	O8-C23-C24-C25
33	b	628[B]	LHG	O7-C7-C8-C9
36	H	102	DGD	C8A-C9A-CAA-CBA
35	M	101	LMG	C37-C38-C39-C40
35	c	520	LMG	C14-C15-C16-C17
24	c	510	CLA	C13-C15-C16-C17
25	A	417[B]	PHO	C4C-C3C-CAC-CBC
34	c	522	HTG	C2'-C1'-S1-C1
35	d	412	LMG	C28-C29-C30-C31
24	c	514	CLA	C4-C3-C5-C6
30	A	415[A]	PL9	C25-C24-C26-C27
35	c	521	LMG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
30	A	415[B]	PL9	C23-C24-C26-C27
24	b	605	CLA	C16-C17-C18-C19
27	A	413	SQD	C24-C23-O48-C46
36	C	519	DGD	O1G-C1A-C2A-C3A
33	d	408[B]	LHG	C24-C25-C26-C27
36	C	519	DGD	CDA-CEA-CFA-CGA
24	A	409	CLA	C11-C12-C13-C14
24	B	605	CLA	C11-C10-C8-C9
24	B	614	CLA	C6-C7-C8-C9
24	B	616	CLA	C14-C13-C15-C16
24	a	407[A]	CLA	C6-C7-C8-C9
24	b	601	CLA	C11-C12-C13-C14
24	b	605	CLA	C6-C7-C8-C9
24	c	511	CLA	C11-C12-C13-C14
24	c	514	CLA	C14-C13-C15-C16
24	d	403[B]	CLA	C11-C12-C13-C14
24	C	511	CLA	CAA-CBA-CGA-O2A
33	E	101[B]	LHG	O7-C7-C8-C9
33	a	420[A]	LHG	O8-C23-C24-C25
35	C	501	LMG	O8-C28-C29-C30
24	B	603	CLA	CAD-CBD-CGD-O2D
24	B	604	CLA	CAD-CBD-CGD-O2D
24	B	616	CLA	CAD-CBD-CGD-O2D
24	C	513	CLA	CAD-CBD-CGD-O2D
24	b	604	CLA	CAD-CBD-CGD-O2D
24	b	607	CLA	CAD-CBD-CGD-O2D
24	c	502	CLA	CAD-CBD-CGD-O2D
24	c	504	CLA	CAD-CBD-CGD-O2D
25	A	408[A]	PHO	CAD-CBD-CGD-O2D
25	a	408[B]	PHO	CAD-CBD-CGD-O2D
33	A	420[B]	LHG	C9-C10-C11-C12
24	c	512	CLA	C3-C5-C6-C7
36	C	518[B]	DGD	C8B-C9B-CAB-CBB
24	B	608	CLA	C2-C1-O2A-CGA
33	L	101[A]	LHG	C11-C12-C13-C14
33	L	101[A]	LHG	O7-C7-C8-C9
24	B	614	CLA	C15-C16-C17-C18
24	c	511	CLA	C2-C3-C5-C6
33	L	101[B]	LHG	O7-C7-C8-C9
33	b	628[A]	LHG	O7-C7-C8-C9
35	Z	101	LMG	O7-C10-C11-C12
32	B	628	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
35	M	101	LMG	C30-C31-C32-C33
26	d	405	BCR	C7-C8-C9-C10
32	m	102	LMT	C4-C5-C6-C7
25	A	417[B]	PHO	C2C-C3C-CAC-CBC
25	a	408[A]	PHO	C2C-C3C-CAC-CBC
25	d	402[A]	PHO	C2C-C3C-CAC-CBC
25	d	402[B]	PHO	C2C-C3C-CAC-CBC
24	c	504	CLA	C5-C6-C7-C8
24	B	602	CLA	O2A-C1-C2-C3
24	b	613	CLA	O2A-C1-C2-C3
25	A	408[B]	PHO	O2A-C1-C2-C3
39	e	101	HEM	C4B-C3B-CAB-CBB
24	a	405[B]	CLA	C2A-CAA-CBA-CGA
24	B	612	CLA	O1A-CGA-O2A-C1
39	F	102	HEM	CAD-CBD-CGD-O2D
39	e	101	HEM	CAA-CBA-CGA-O1A
24	a	405[A]	CLA	C2C-C3C-CAC-CBC
24	A	405[A]	CLA	C2C-C3C-CAC-CBC
24	A	406[A]	CLA	CHA-CBD-CGD-O1D
24	A	406[A]	CLA	CHA-CBD-CGD-O2D
24	A	406[B]	CLA	CHA-CBD-CGD-O1D
24	A	406[B]	CLA	CHA-CBD-CGD-O2D
24	A	407[B]	CLA	CHA-CBD-CGD-O1D
24	A	407[B]	CLA	CHA-CBD-CGD-O2D
24	B	606	CLA	CHA-CBD-CGD-O1D
24	B	606	CLA	CHA-CBD-CGD-O2D
24	B	607	CLA	CHA-CBD-CGD-O1D
24	B	607	CLA	CHA-CBD-CGD-O2D
24	C	505	CLA	CHA-CBD-CGD-O2D
24	C	510	CLA	CHA-CBD-CGD-O1D
24	C	510	CLA	CHA-CBD-CGD-O2D
24	a	406[A]	CLA	CHA-CBD-CGD-O1D
24	a	406[A]	CLA	CHA-CBD-CGD-O2D
24	b	606	CLA	CHA-CBD-CGD-O2D
24	b	612	CLA	CHA-CBD-CGD-O1D
24	c	503	CLA	CHA-CBD-CGD-O2D
24	c	508	CLA	CHA-CBD-CGD-O1D
24	c	508	CLA	CHA-CBD-CGD-O2D
24	c	510	CLA	CHA-CBD-CGD-O2D
35	D	411	LMG	O7-C10-C11-C12
35	C	501	LMG	C22-C23-C24-C25
41	v	201	HEC	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
32	t	101	LMT	C3-C4-C5-C6
27	a	411[B]	SQD	C11-C12-C13-C14
27	A	413	SQD	O10-C23-O48-C46
24	c	511	CLA	CAA-CBA-CGA-O2A
24	c	513	CLA	CAA-CBA-CGA-O2A
27	a	413	SQD	O48-C23-C24-C25
35	c	520	LMG	O7-C10-C11-C12
25	A	408[A]	PHO	CHA-CBD-CGD-O2D
25	A	417[B]	PHO	CHA-CBD-CGD-O1D
25	A	417[B]	PHO	CHA-CBD-CGD-O2D
25	a	408[A]	PHO	CHA-CBD-CGD-O1D
33	A	420[A]	LHG	O1-C1-C2-O2
35	d	412	LMG	C40-C41-C42-C43
35	c	520	LMG	C39-C40-C41-C42
24	b	613	CLA	CAA-CBA-CGA-O2A
35	b	629	LMG	C21-C22-C23-C24
24	a	406[A]	CLA	C11-C12-C13-C15
24	b	604	CLA	C11-C12-C13-C15
24	b	608	CLA	C6-C7-C8-C10
24	b	608	CLA	C12-C13-C15-C16
24	b	609	CLA	C2-C3-C5-C6
30	A	415[A]	PL9	C4-C3-C7-C8
33	d	414[B]	LHG	C18-C19-C20-C21
24	B	613	CLA	CAA-CBA-CGA-O2A
33	d	414[A]	LHG	C30-C31-C32-C33
24	A	409	CLA	C14-C13-C15-C16
24	a	407[B]	CLA	C6-C7-C8-C9
24	b	606	CLA	C14-C13-C15-C16
24	b	614	CLA	C14-C13-C15-C16
30	d	406[A]	PL9	C34-C36-C37-C38
24	b	603	CLA	C13-C15-C16-C17
27	a	413	SQD	C27-C28-C29-C30
35	M	101	LMG	C11-C12-C13-C14
24	a	405[A]	CLA	C4C-C3C-CAC-CBC
39	e	101	HEM	CAD-CBD-CGD-O2D
24	c	502	CLA	C2A-CAA-CBA-CGA
33	a	420[B]	LHG	O8-C23-C24-C25
33	b	628[B]	LHG	C32-C33-C34-C35
35	d	412	LMG	C19-C20-C21-C22
36	C	519	DGD	O1A-C1A-O1G-C1G
33	E	101[B]	LHG	O9-C7-C8-C9
33	b	628[B]	LHG	O9-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
26	k	101	BCR	C7-C8-C9-C10
26	y	101	BCR	C21-C22-C23-C24
33	A	420[B]	LHG	C11-C12-C13-C14
32	t	101	LMT	C4'-C5'-C6'-O6'
24	c	507	CLA	C1A-C2A-CAA-CBA
33	b	628[A]	LHG	O9-C7-C8-C9
24	B	604	CLA	C4C-C3C-CAC-CBC
27	A	411[B]	SQD	C13-C14-C15-C16
35	C	501	LMG	C38-C39-C40-C41
30	D	405[B]	PL9	C46-C47-C48-C49
24	C	507	CLA	C2-C1-O2A-CGA
24	C	514	CLA	C2-C1-O2A-CGA
24	A	405[A]	CLA	C4C-C3C-CAC-CBC
33	A	420[A]	LHG	O10-C23-C24-C25
33	L	101[A]	LHG	O9-C7-C8-C9
33	a	420[A]	LHG	O10-C23-C24-C25
35	Z	101	LMG	O9-C10-C11-C12
36	C	519	DGD	O1A-C1A-C2A-C3A
36	C	517[A]	DGD	C3A-C4A-C5A-C6A
27	X	101	SQD	C44-C45-C46-O48
35	C	520	LMG	O1-C7-C8-C9
33	E	101[A]	LHG	O7-C7-C8-C9
24	b	602	CLA	C2A-CAA-CBA-CGA
24	C	511	CLA	CAA-CBA-CGA-O1A
33	E	101[B]	LHG	C17-C18-C19-C20
32	F	101	LMT	C9-C10-C11-C12
24	c	513	CLA	CAA-CBA-CGA-O1A
24	B	603	CLA	C2-C3-C5-C6
33	d	407[A]	LHG	C4-O6-P-O5
33	d	408[B]	LHG	C4-O6-P-O5
24	B	613	CLA	CAA-CBA-CGA-O1A
33	a	420[B]	LHG	O10-C23-C24-C25
27	L	102	SQD	C15-C16-C17-C18
26	a	410	BCR	C5-C6-C7-C8
24	B	613	CLA	C10-C11-C12-C13
36	C	519	DGD	CCB-CDB-CEB-CFB
25	A	408[B]	PHO	O1A-CGA-O2A-C1
24	B	612	CLA	CBA-CGA-O2A-C1
24	b	603	CLA	C2A-CAA-CBA-CGA
33	L	101[B]	LHG	O9-C7-C8-C9
35	D	411	LMG	O9-C10-C11-C12
33	d	408[A]	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
24	C	504	CLA	CBD-CGD-O2D-CED
33	A	420[A]	LHG	C18-C19-C20-C21
34	c	522	HTG	C4'-C5'-C6'-C7'
35	d	412	LMG	C16-C17-C18-C19
36	c	517[B]	DGD	C7A-C8A-C9A-CAA
27	a	411[B]	SQD	C7-C8-C9-C10
30	D	405[B]	PL9	C45-C44-C46-C47
30	d	406[A]	PL9	C15-C14-C16-C17
33	d	408[A]	LHG	C30-C31-C32-C33
30	d	406[A]	PL9	C11-C12-C13-C14
35	a	417	LMG	C32-C33-C34-C35
36	c	518[A]	DGD	CDA-CEA-CFA-CGA
24	B	605	CLA	CAD-CBD-CGD-O1D
24	B	607	CLA	CAD-CBD-CGD-O1D
24	B	611	CLA	CAD-CBD-CGD-O1D
24	C	507	CLA	CAD-CBD-CGD-O1D
24	b	605	CLA	CAD-CBD-CGD-O1D
24	b	609	CLA	CAD-CBD-CGD-O1D
24	c	505	CLA	CAD-CBD-CGD-O1D
33	E	101[A]	LHG	O8-C23-C24-C25
36	C	518[A]	DGD	O2G-C1B-C2B-C3B
24	B	611	CLA	C11-C12-C13-C14
24	a	406[A]	CLA	C11-C12-C13-C14
24	b	603	CLA	C6-C7-C8-C9
24	b	608	CLA	C6-C7-C8-C9
24	c	509	CLA	C11-C10-C8-C9
24	c	512	CLA	C11-C12-C13-C14
33	A	420[A]	LHG	C30-C31-C32-C33
33	D	407[B]	LHG	C27-C28-C29-C30
33	D	407[A]	LHG	C28-C29-C30-C31
24	c	510	CLA	C15-C16-C17-C18
36	C	518[B]	DGD	O2G-C1B-C2B-C3B
36	C	517[A]	DGD	CBA-CCA-CDA-CEA
27	a	413	SQD	O10-C23-C24-C25
33	L	101[A]	LHG	C32-C33-C34-C35
33	D	407[A]	LHG	O8-C23-C24-C25
33	D	407[B]	LHG	O8-C23-C24-C25
33	E	101[B]	LHG	O8-C23-C24-C25
25	A	417[B]	PHO	C8-C10-C11-C12
35	c	520	LMG	O9-C10-C11-C12
24	C	502	CLA	C11-C12-C13-C15
24	C	504	CLA	C6-C7-C8-C10

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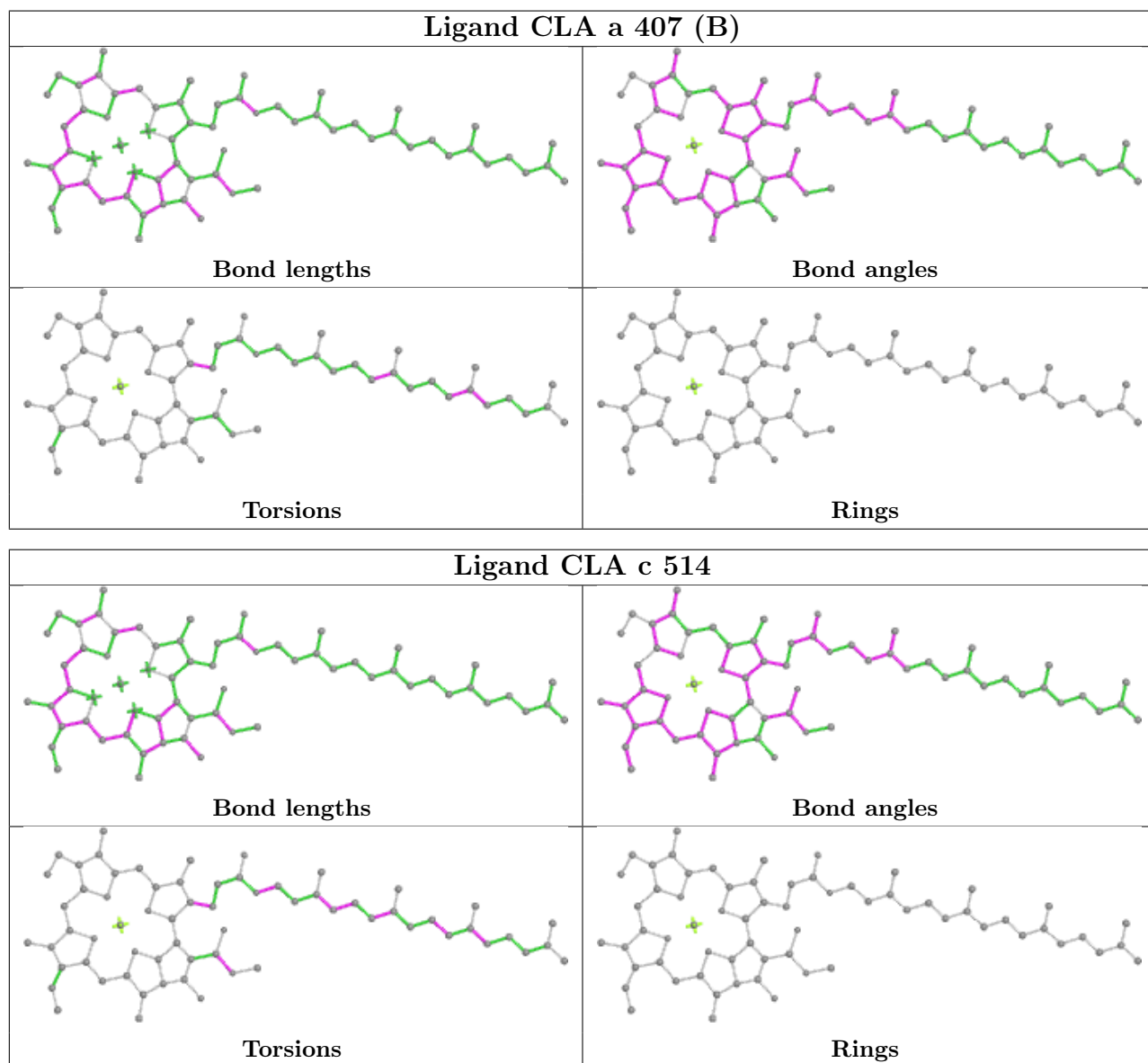
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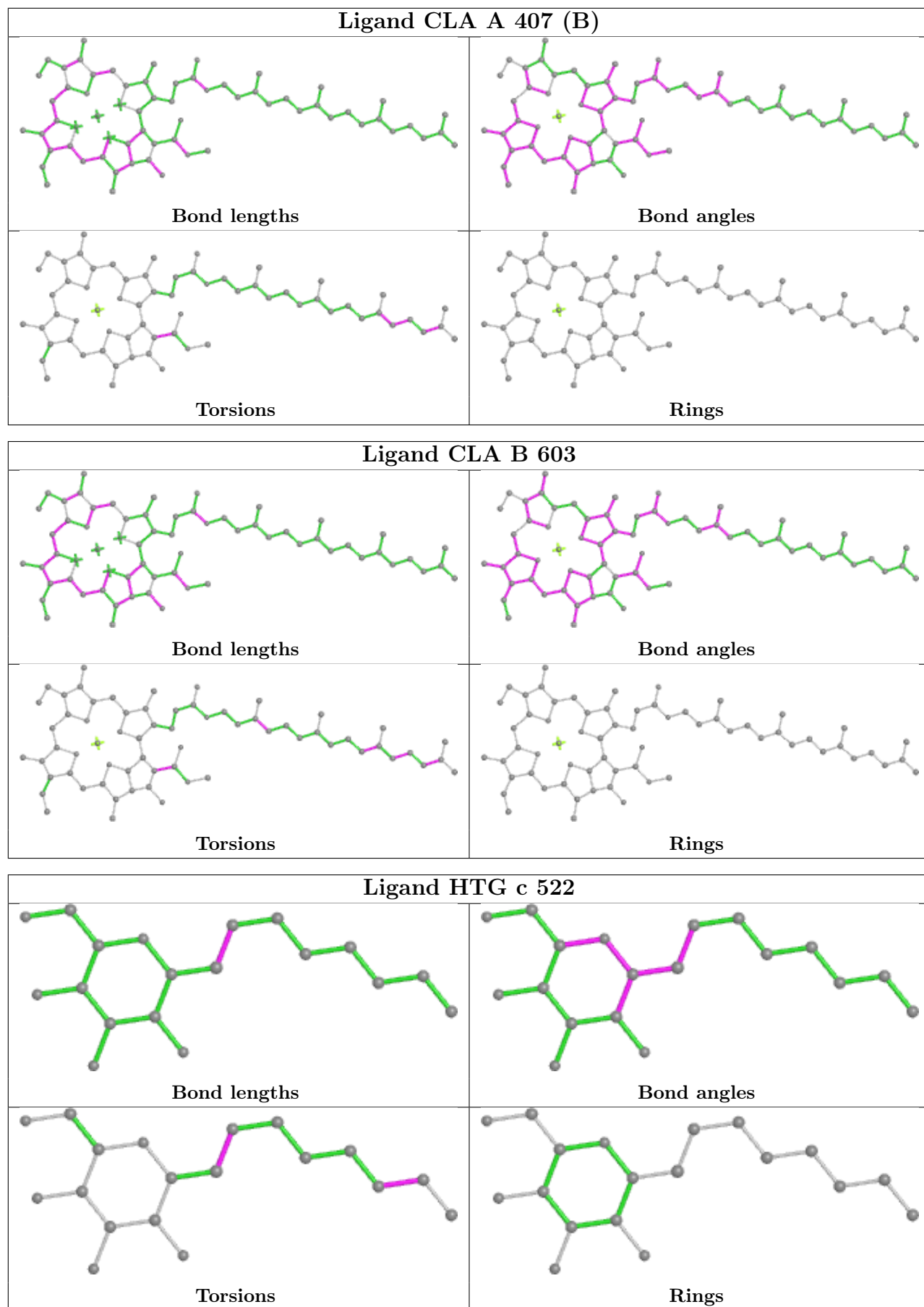
Mol	Chain	Res	Type	Atoms
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24	a	407[A]	CLA	C6-C7-C8-C10
24	a	407[B]	CLA	C6-C7-C8-C10
24	a	409	CLA	C6-C7-C8-C10
24	b	603	CLA	C6-C7-C8-C10
24	c	509	CLA	C12-C13-C15-C16
24	c	513	CLA	C6-C7-C8-C10
30	A	415[B]	PL9	C43-C44-C46-C47
33	E	101[A]	LHG	O9-C7-C8-C9
33	E	101[A]	LHG	O10-C23-C24-C25
24	C	513	CLA	CAA-CBA-CGA-O2A
27	A	413	SQD	O48-C23-C24-C25
27	a	411[B]	SQD	O47-C7-C8-C9
35	c	521	LMG	O7-C10-C11-C12
35	d	412	LMG	O7-C10-C11-C12
36	c	517[A]	DGD	O2G-C1B-C2B-C3B
33	D	407[A]	LHG	O10-C23-C24-C25
36	C	518[B]	DGD	O1B-C1B-C2B-C3B
36	c	517[A]	DGD	O1B-C1B-C2B-C3B
27	f	101	SQD	C28-C29-C30-C31
35	a	417	LMG	C31-C32-C33-C34
32	F	101	LMT	C2-C1-O1'-C1'
24	C	506	CLA	CAA-CBA-CGA-O2A
34	B	622	HTG	C1'-C2'-C3'-C4'
24	b	613	CLA	CAA-CBA-CGA-O1A
33	D	407[B]	LHG	O10-C23-C24-C25
36	C	518[A]	DGD	O1B-C1B-C2B-C3B
35	M	101	LMG	C14-C15-C16-C17
24	c	505	CLA	C5-C6-C7-C8
33	d	414[A]	LHG	C31-C32-C33-C34
33	A	420[B]	LHG	O8-C23-C24-C25
36	c	517[B]	DGD	O2G-C1B-C2B-C3B
32	e	102	LMT	C2B-C1B-O1B-C4'
24	C	509	CLA	C13-C15-C16-C17
24	c	511	CLA	CAA-CBA-CGA-O1A
35	c	521	LMG	C39-C40-C41-C42
35	c	521	LMG	O9-C10-C11-C12
33	E	101[A]	LHG	C11-C10-C9-C8
33	d	408[A]	LHG	O8-C23-C24-C25

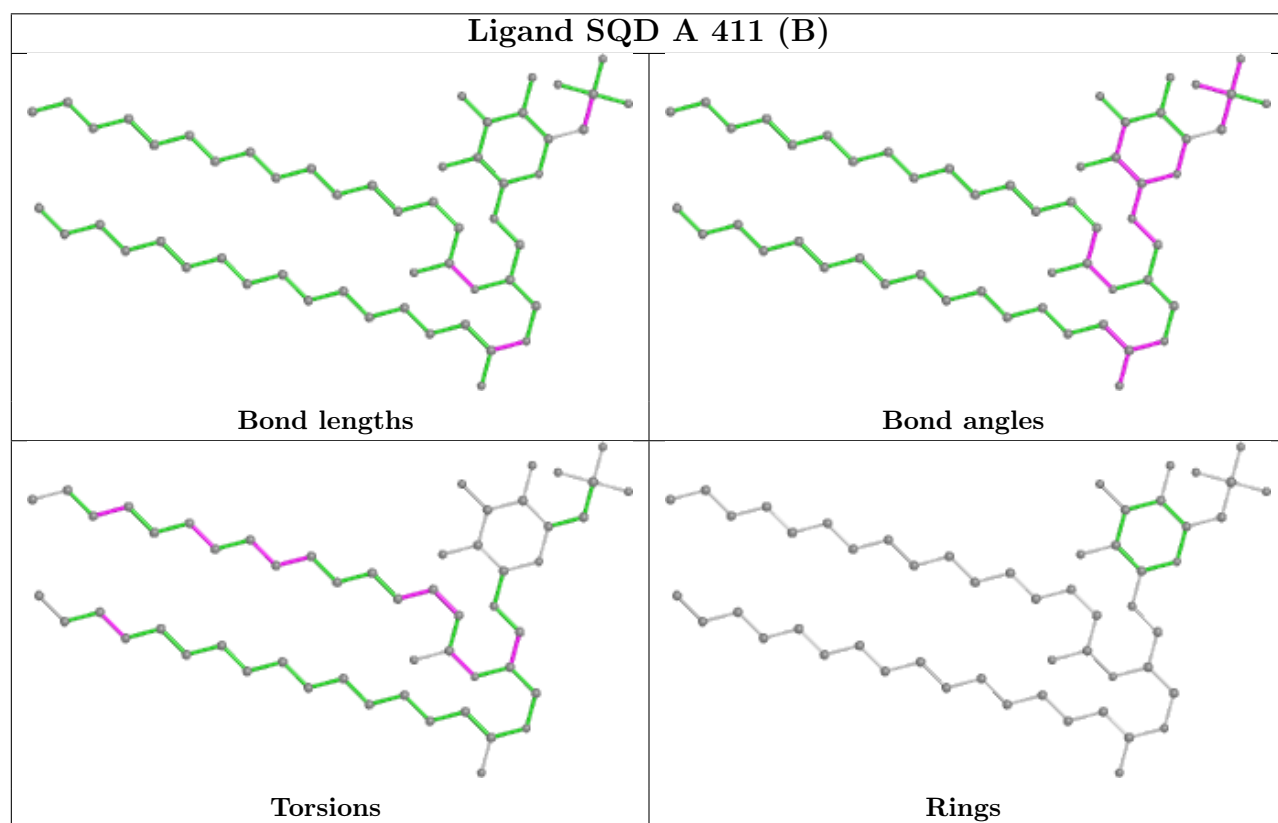
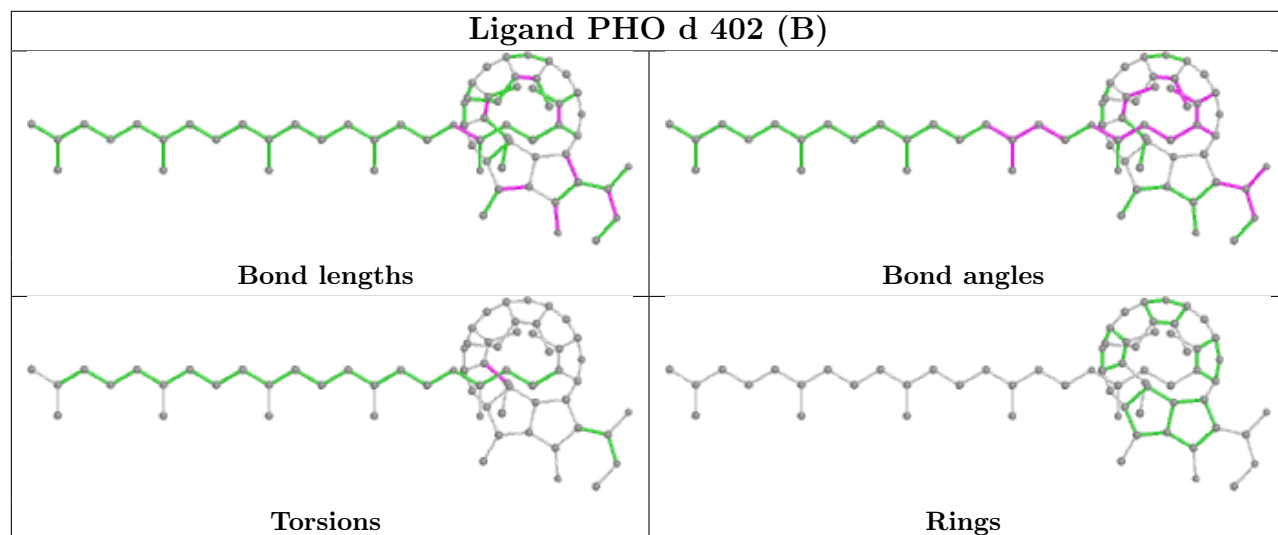
There are no ring outliers.

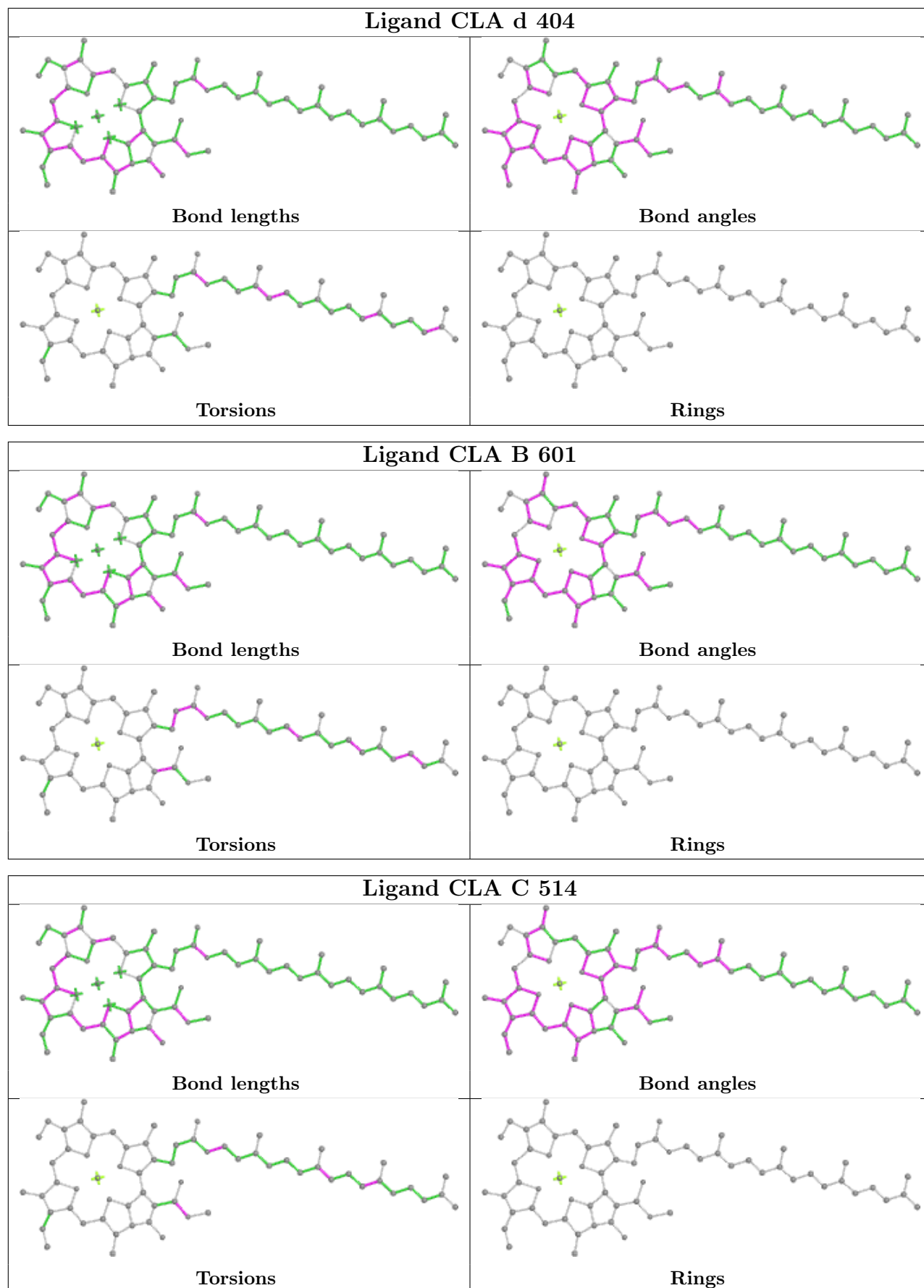
No monomer is involved in short contacts.

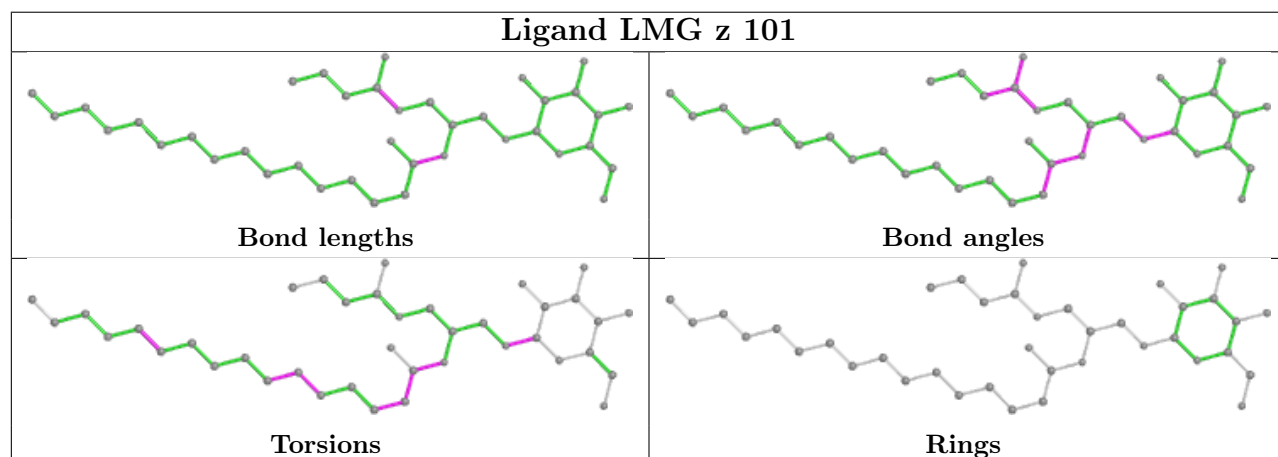
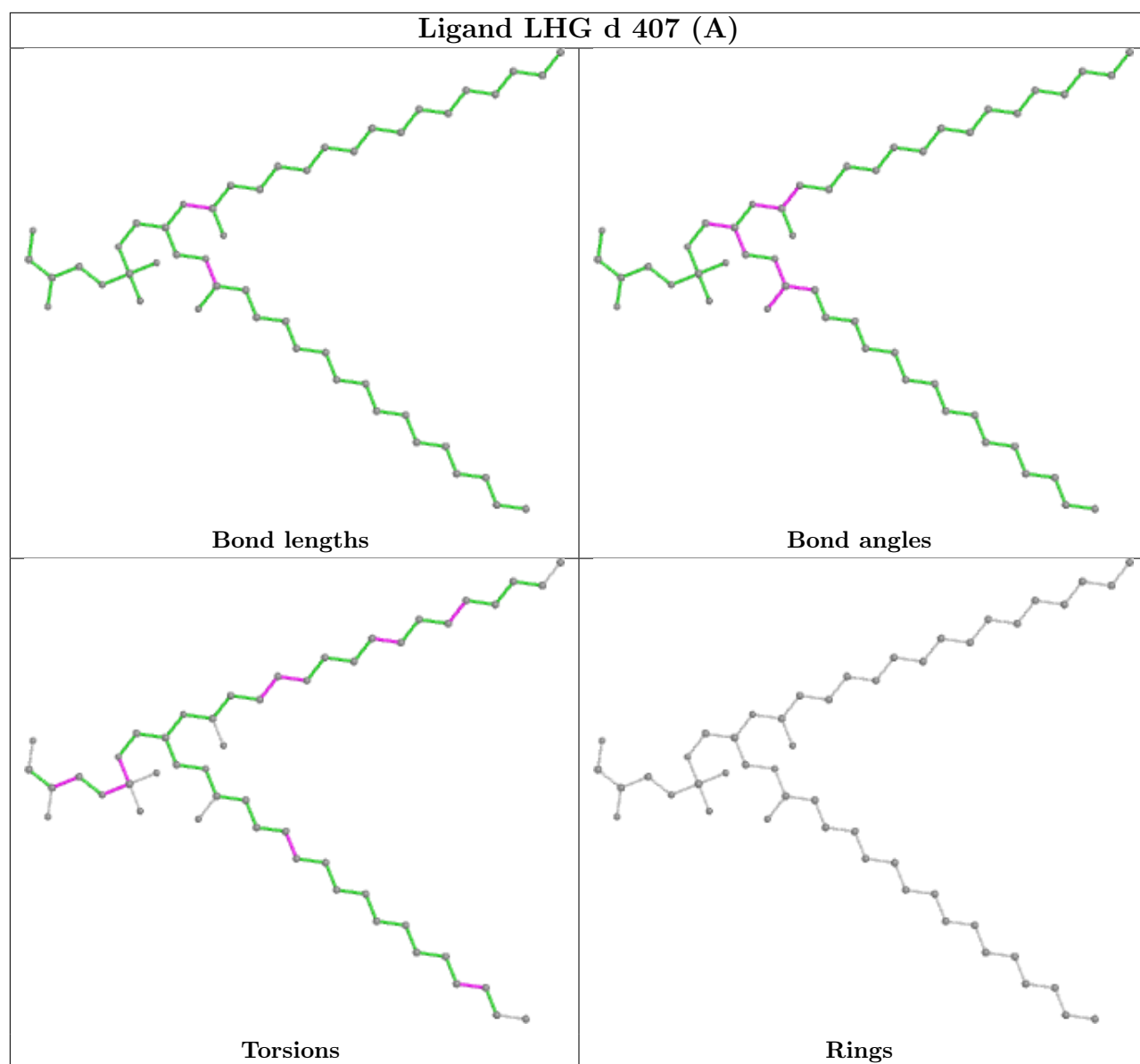
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

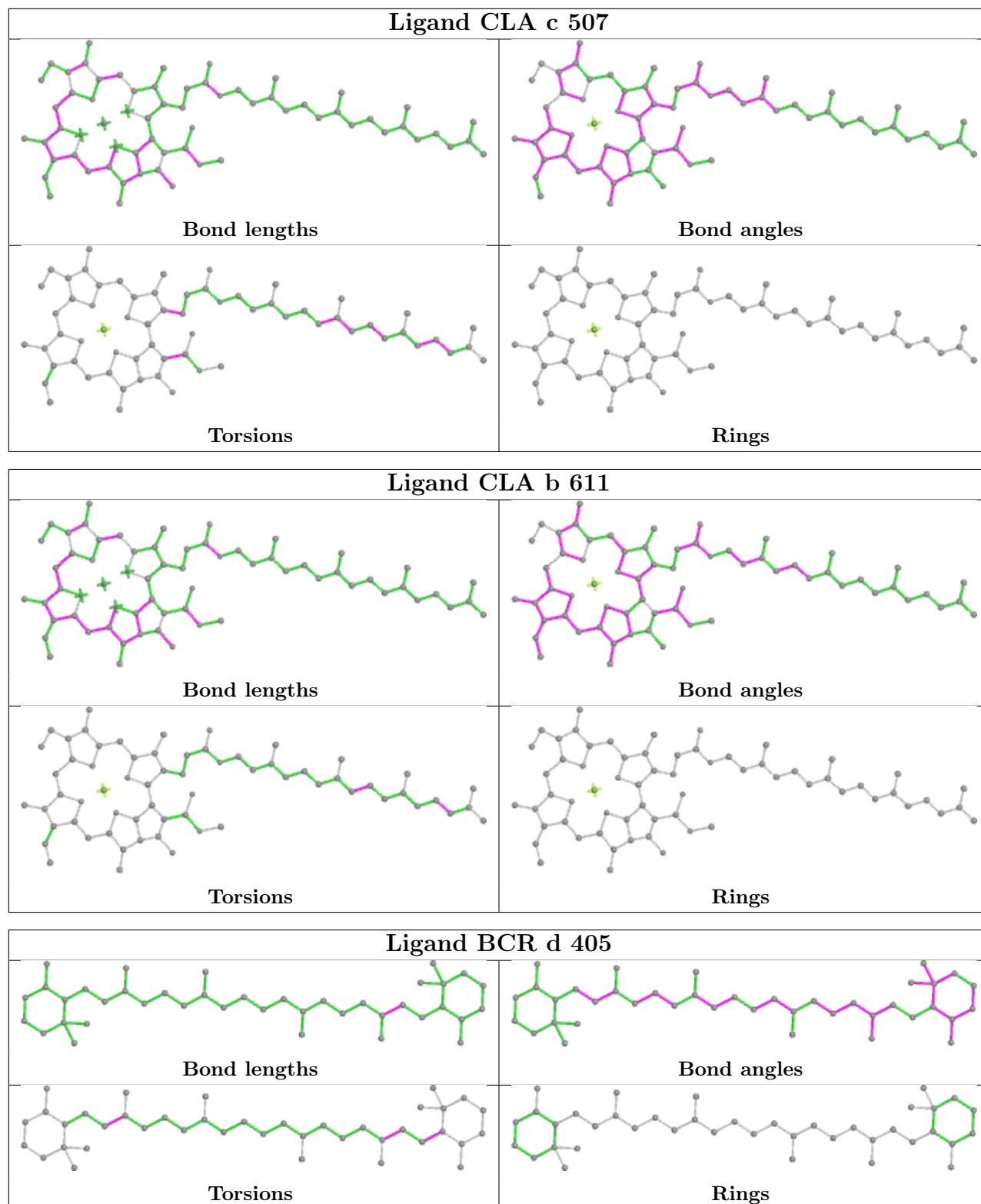


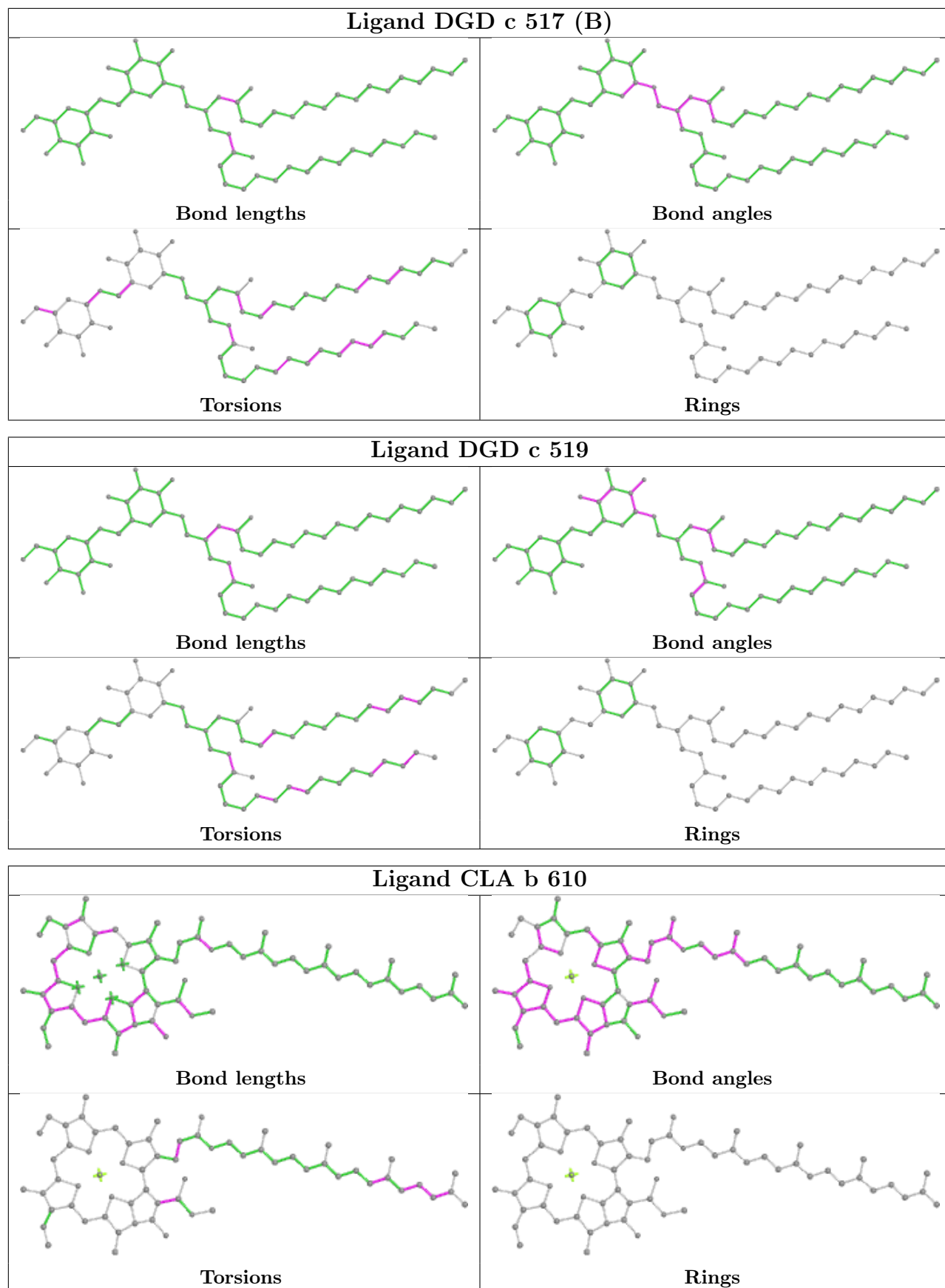


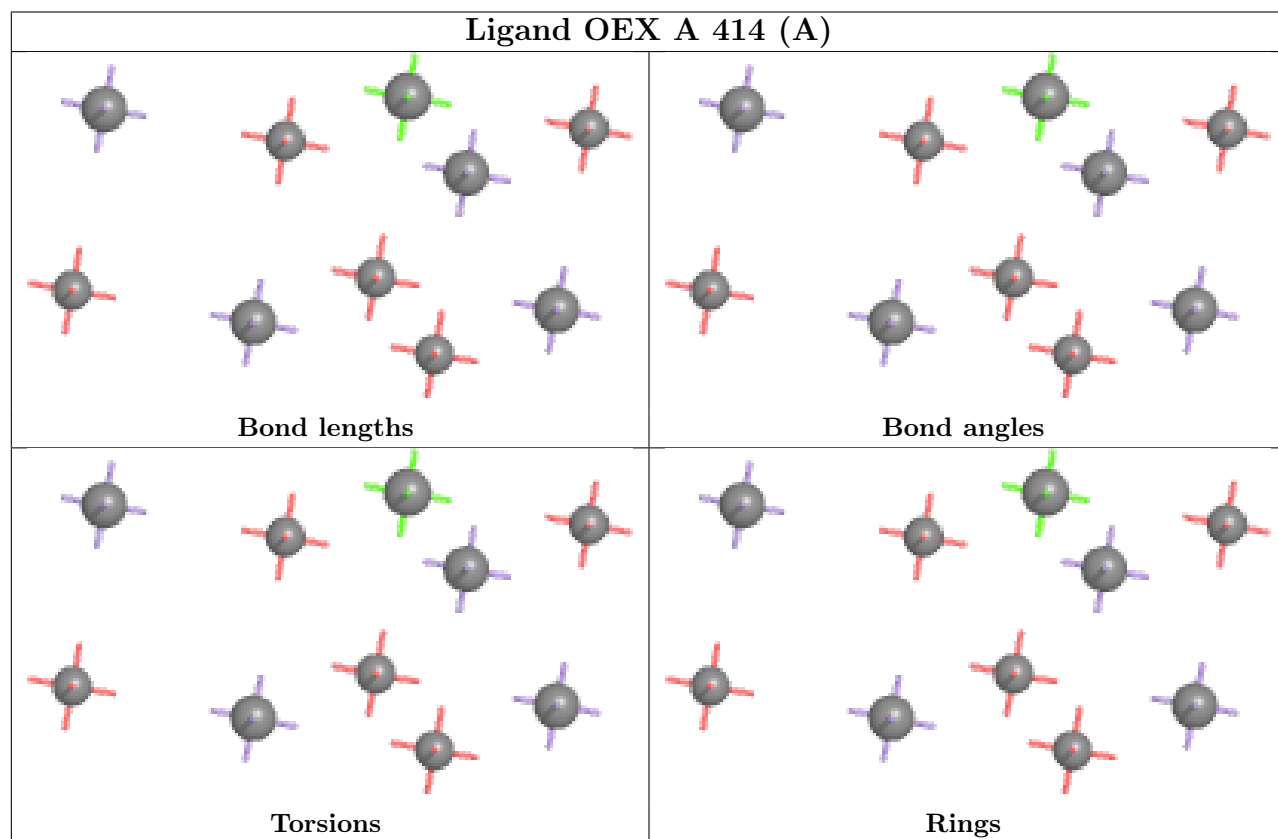
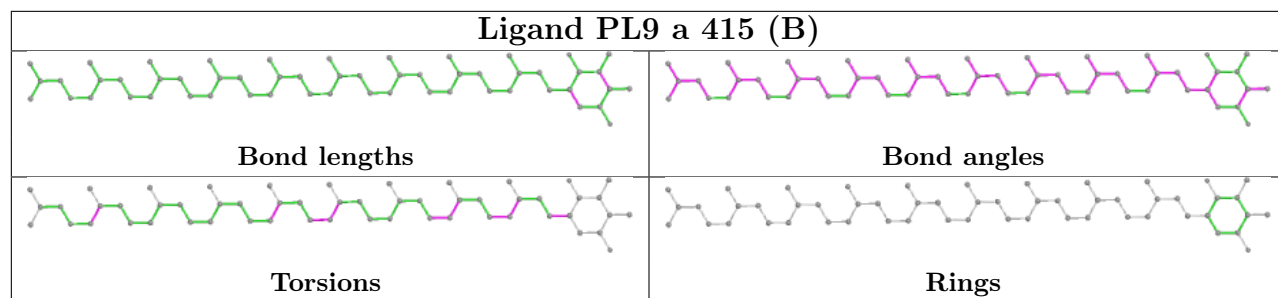
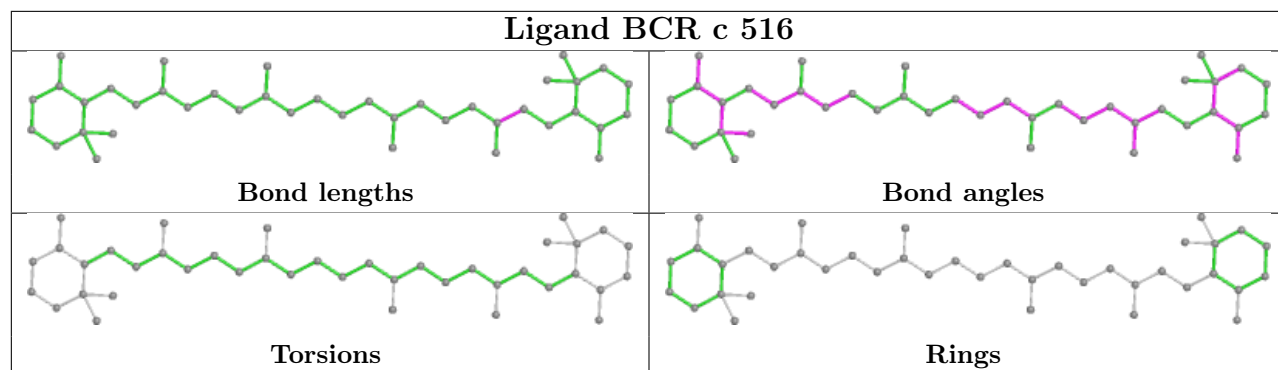


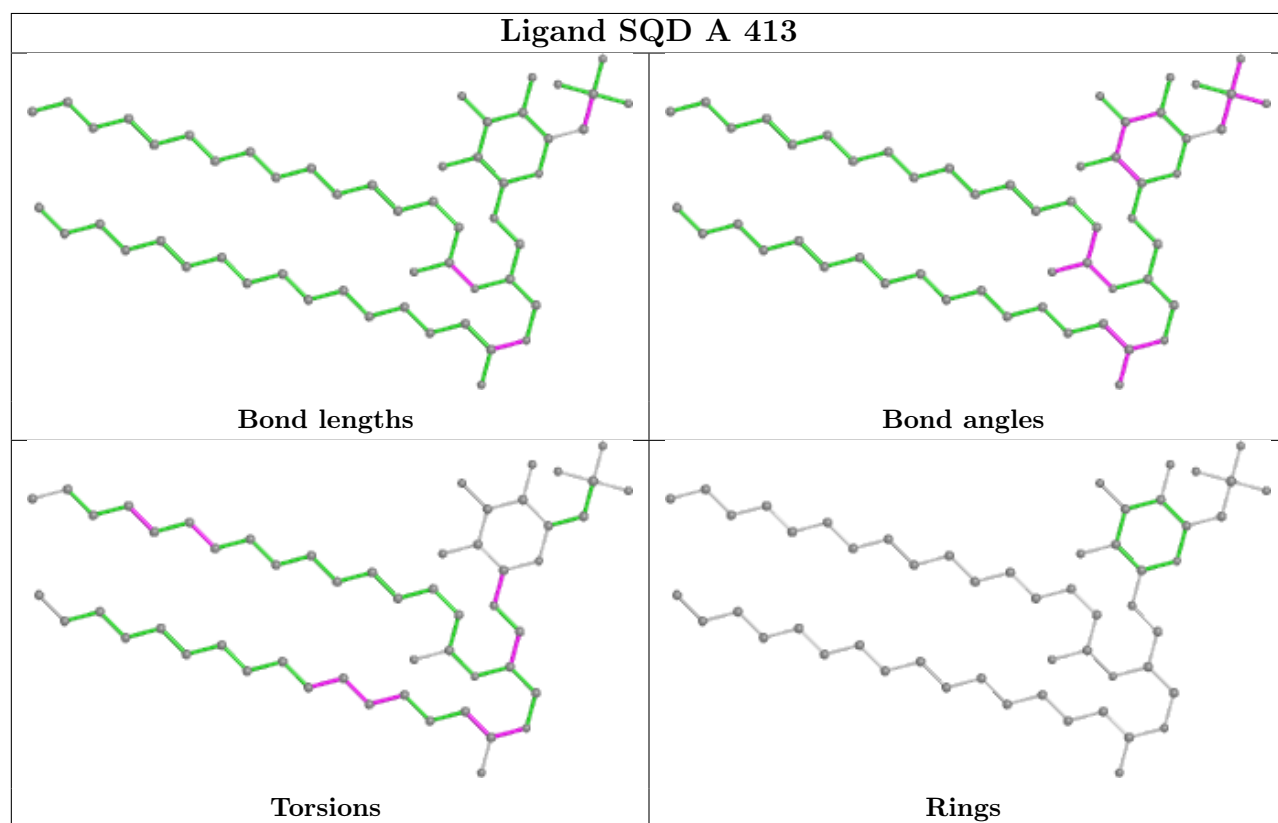
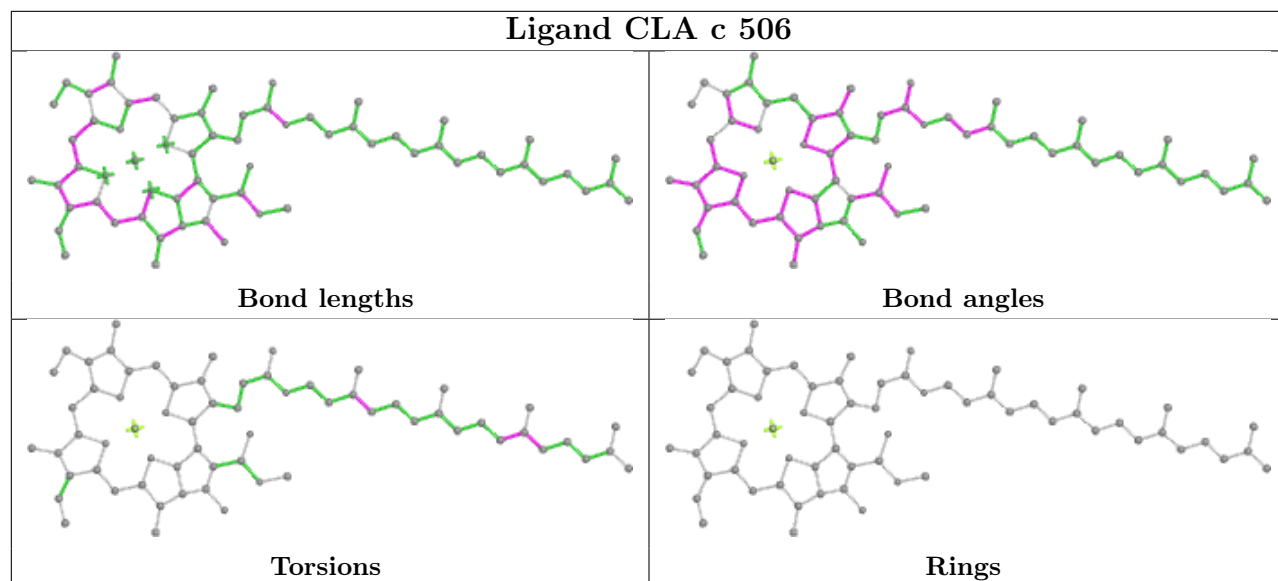
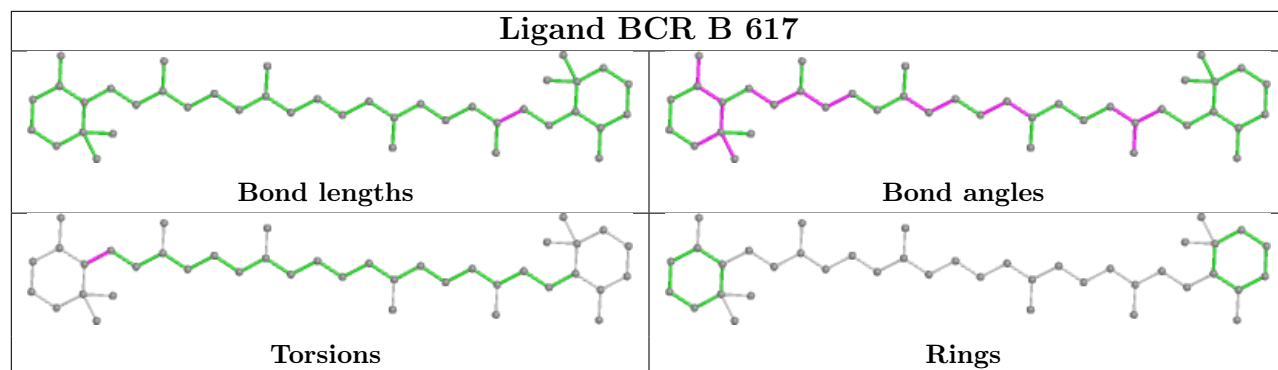


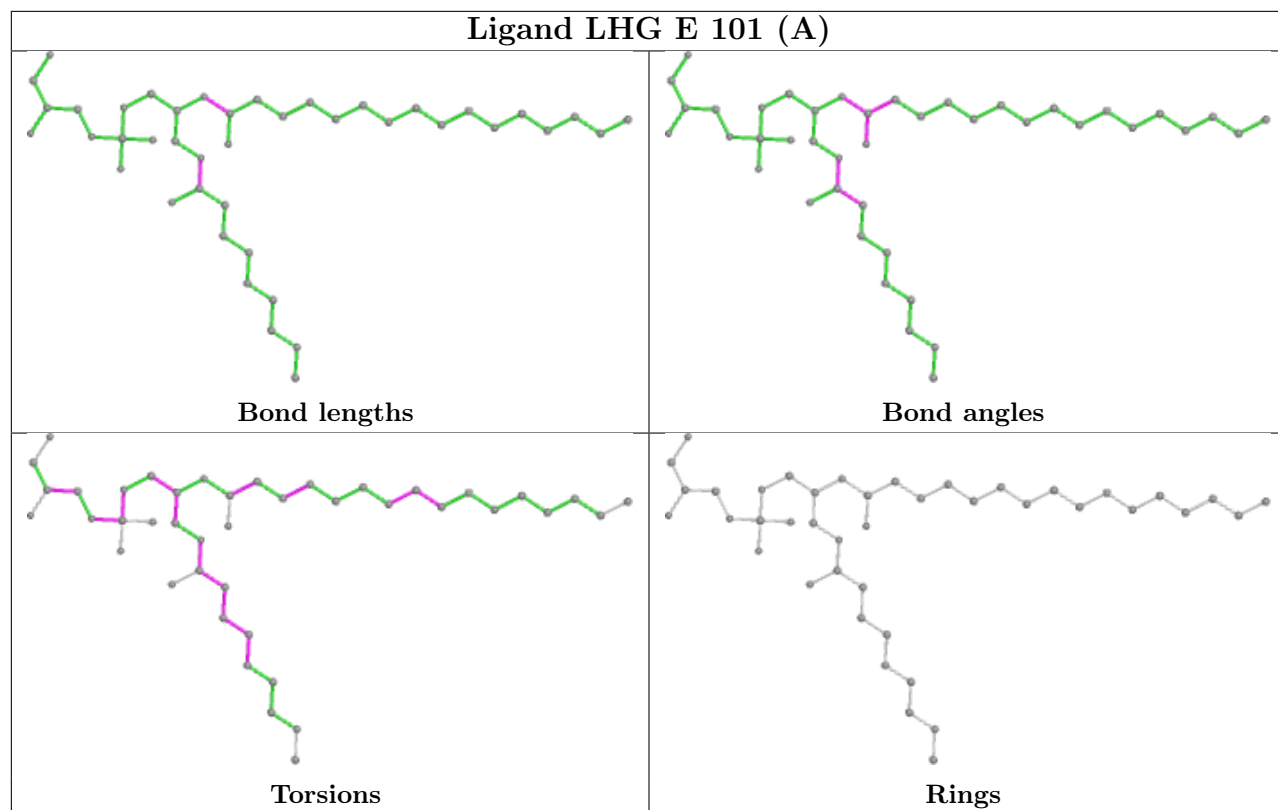


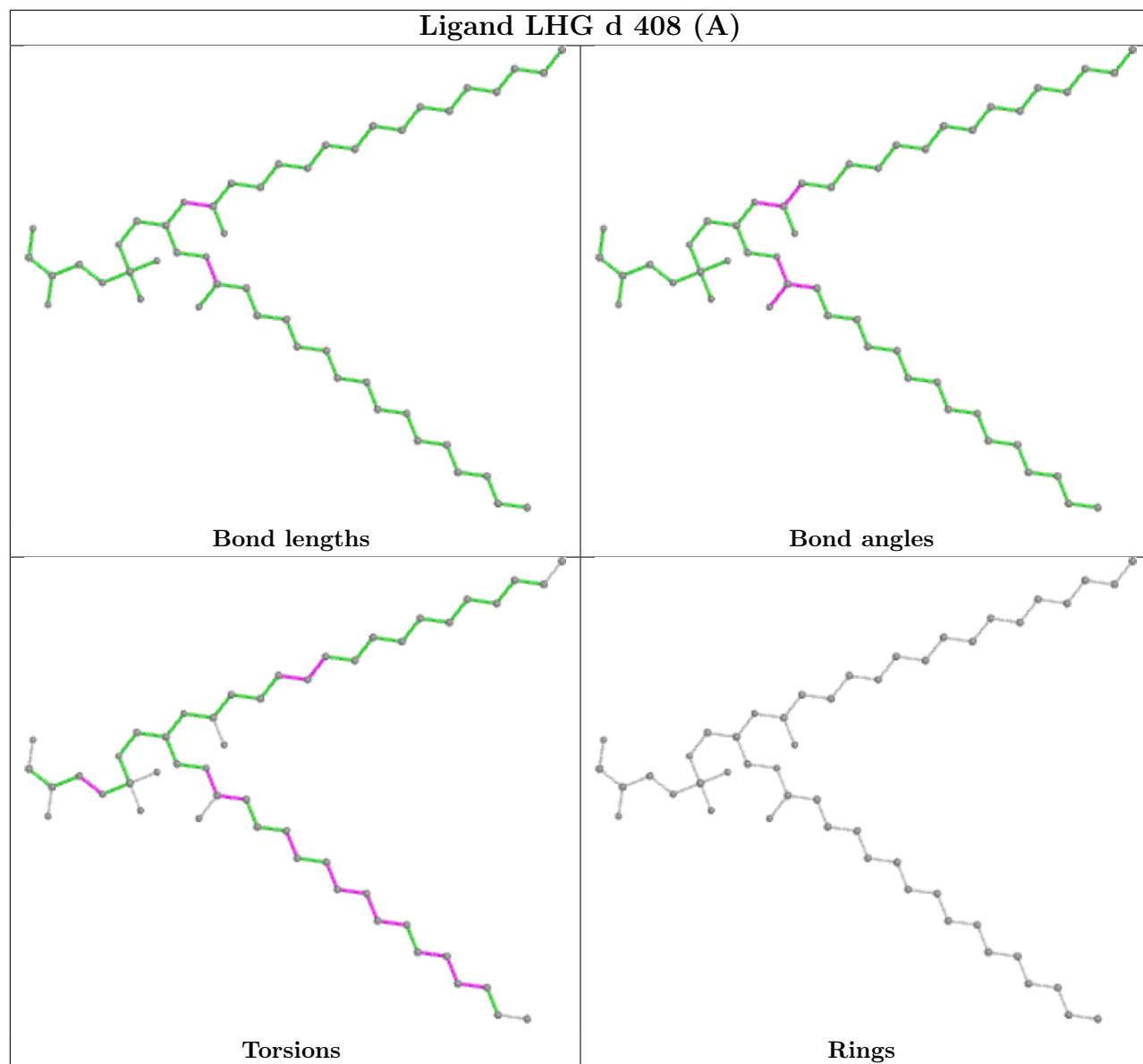


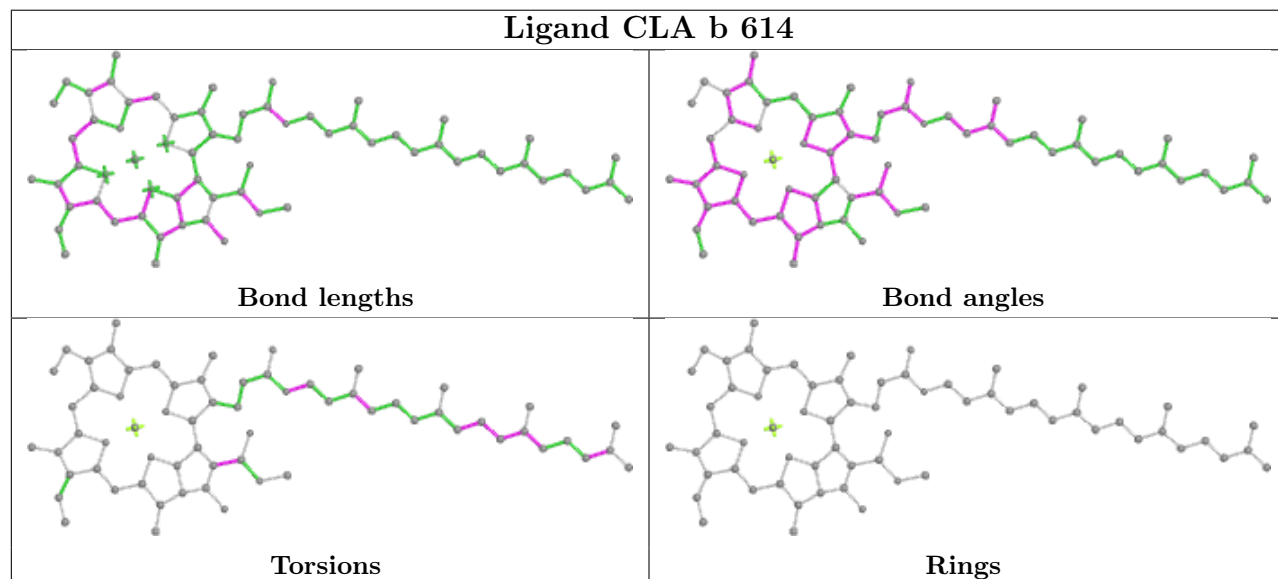
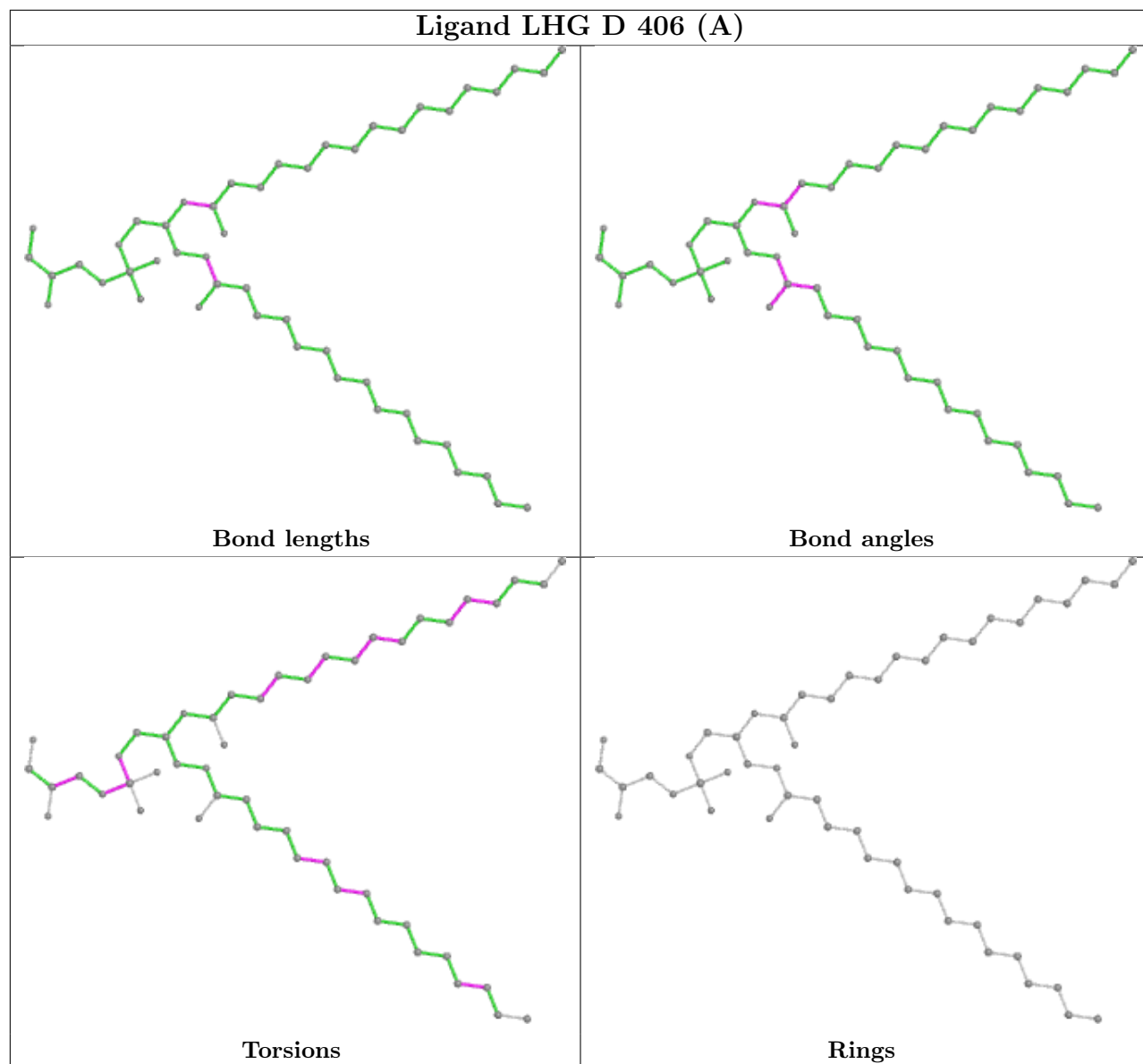


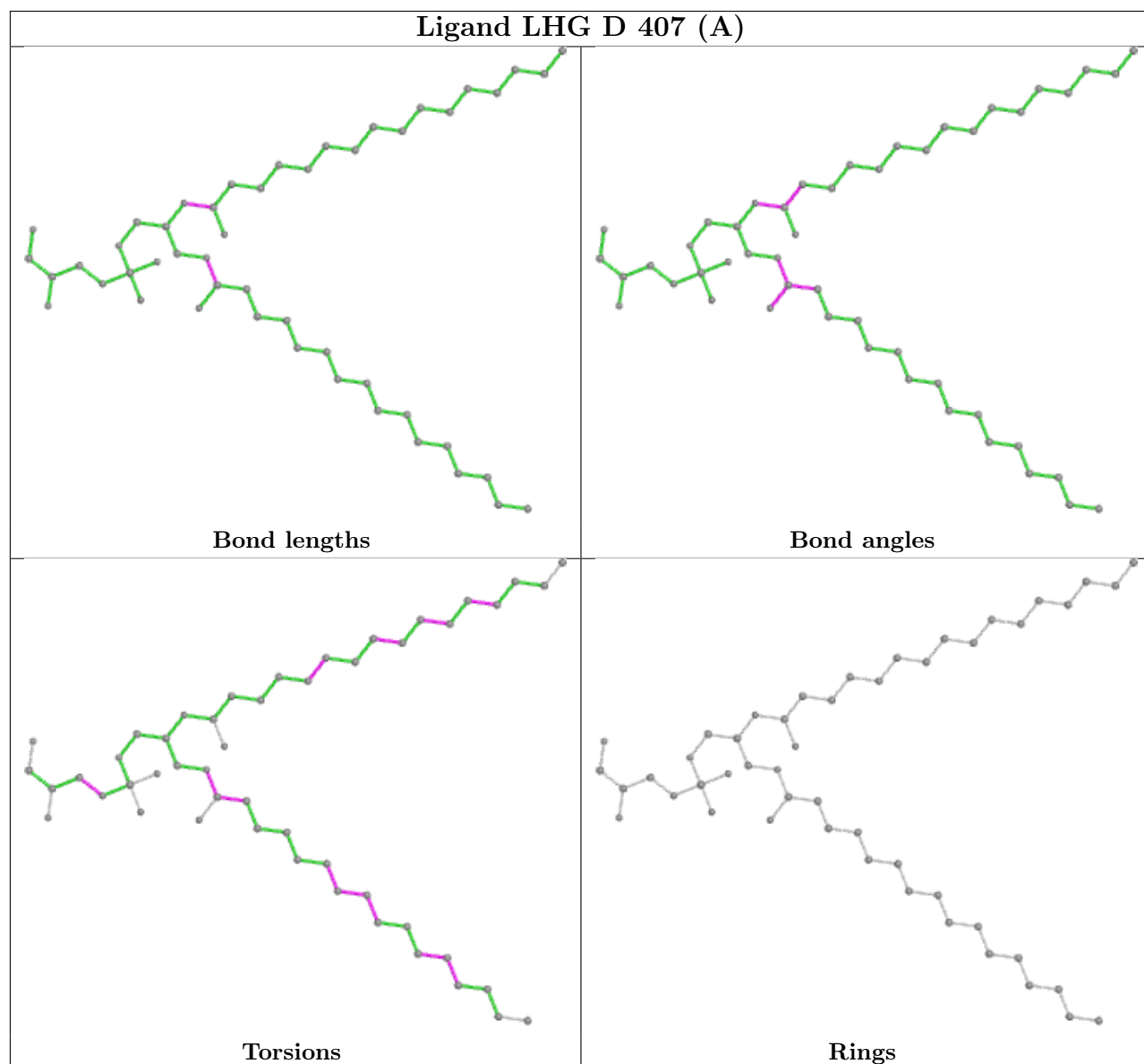
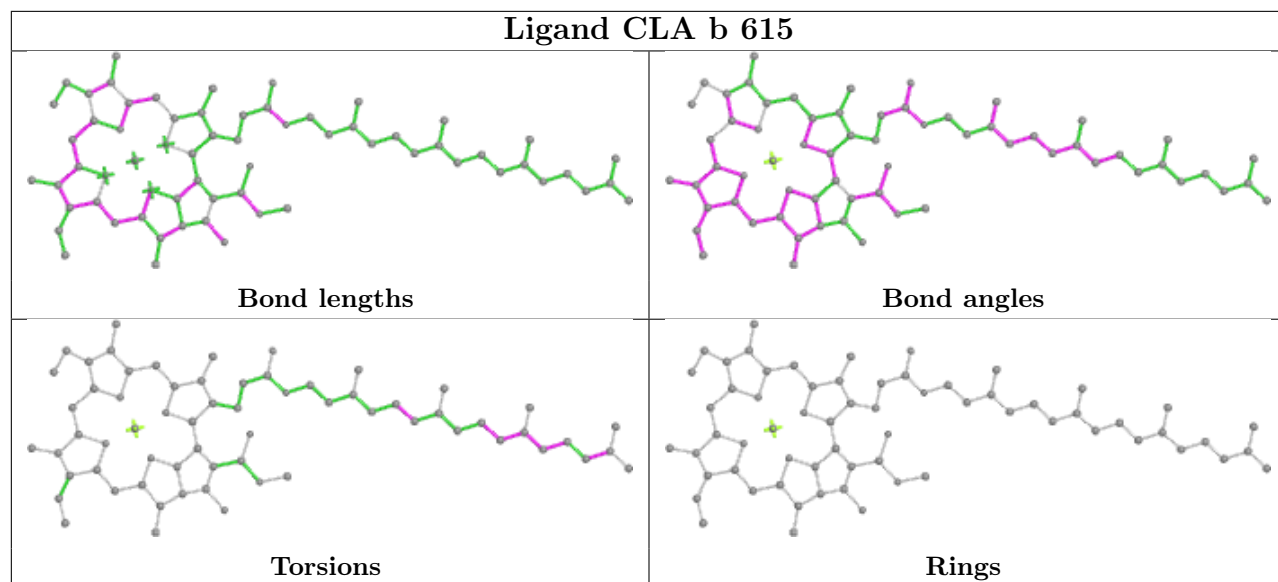


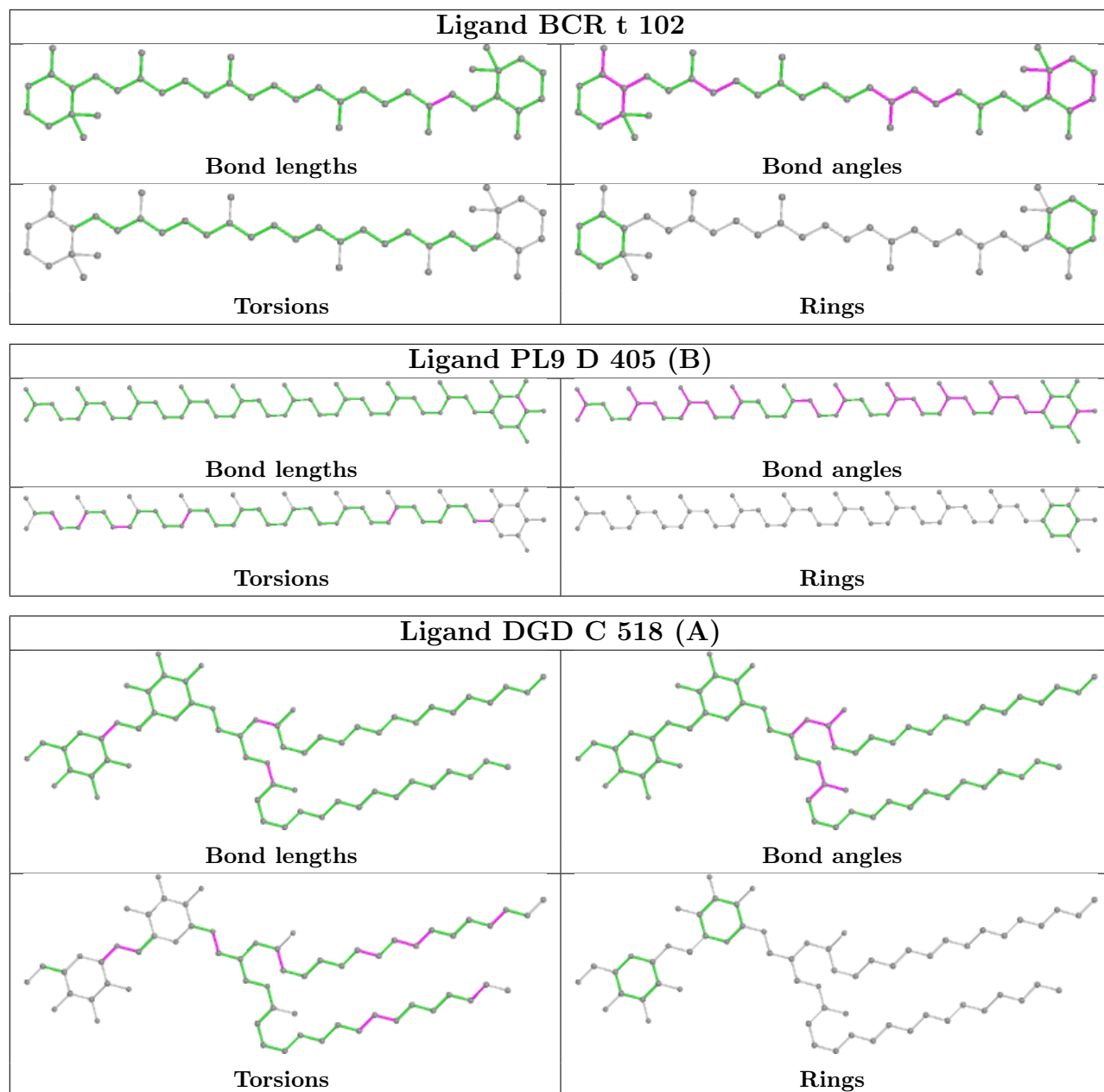


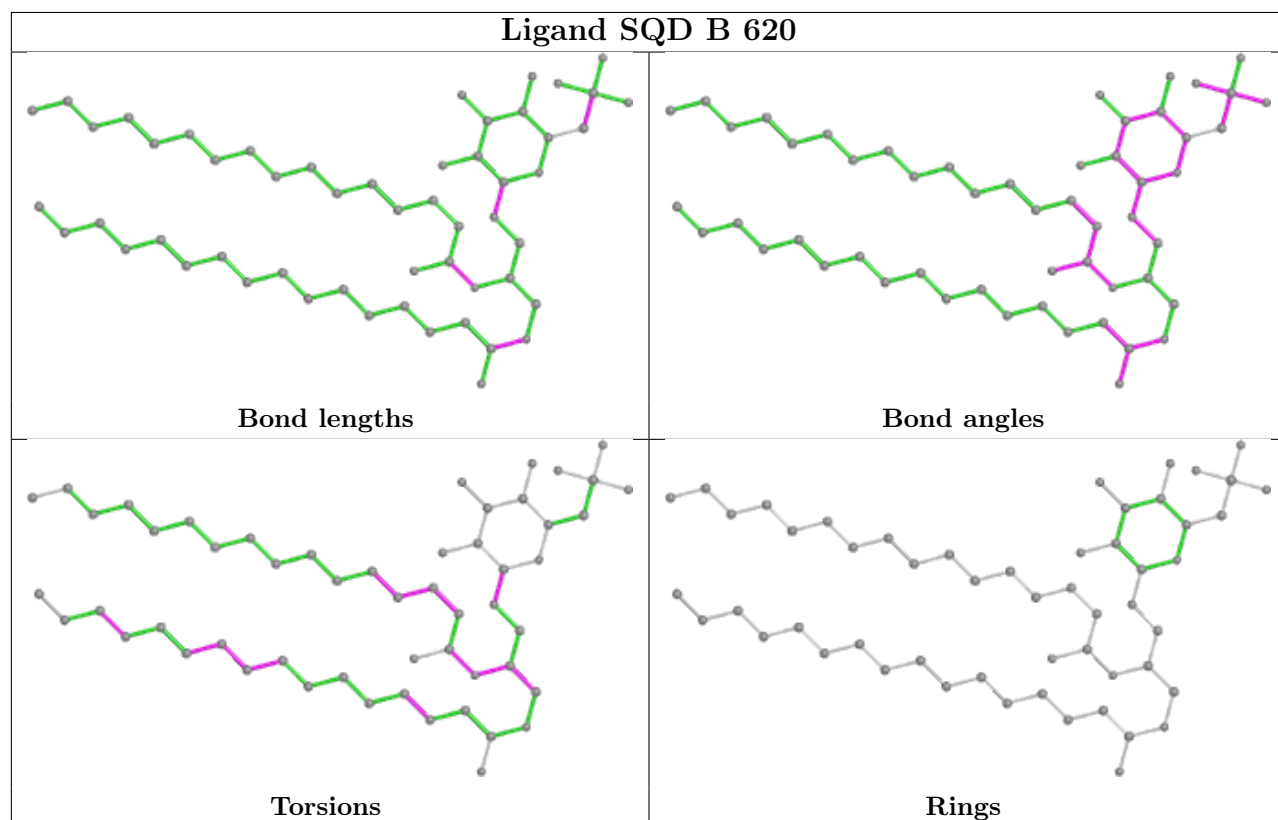
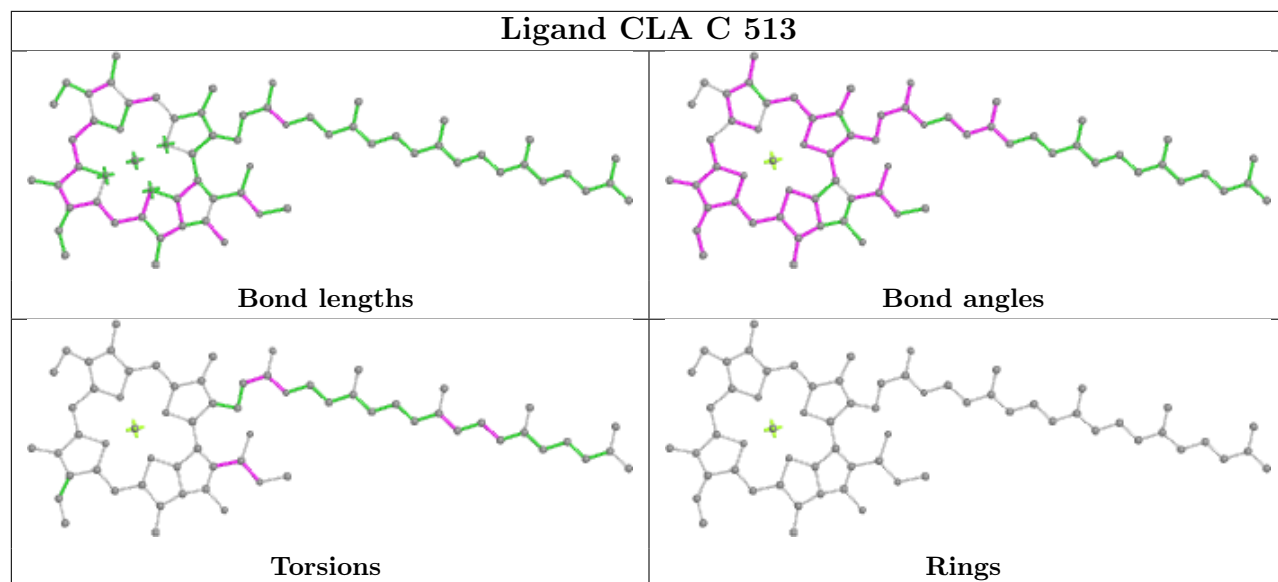


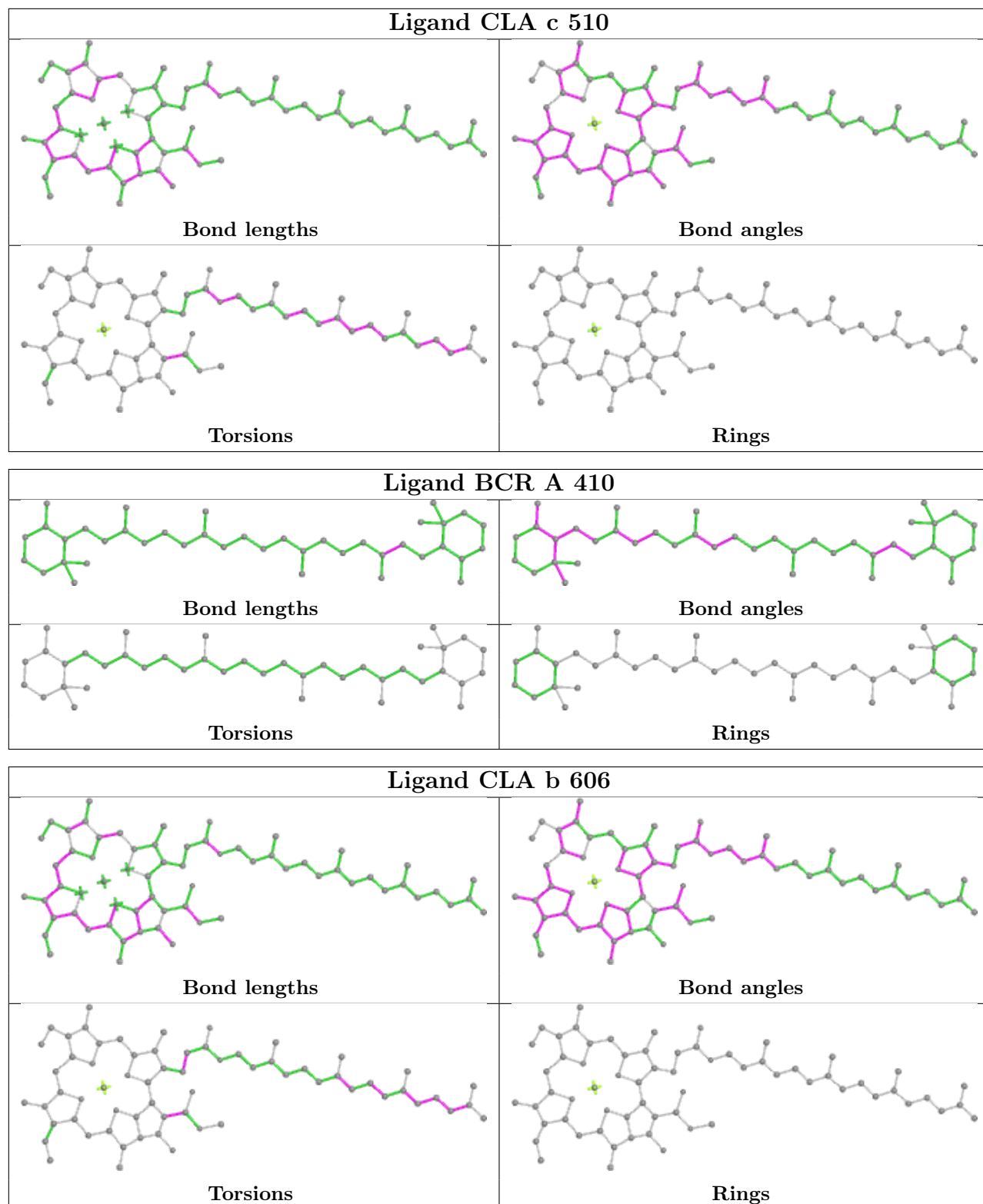


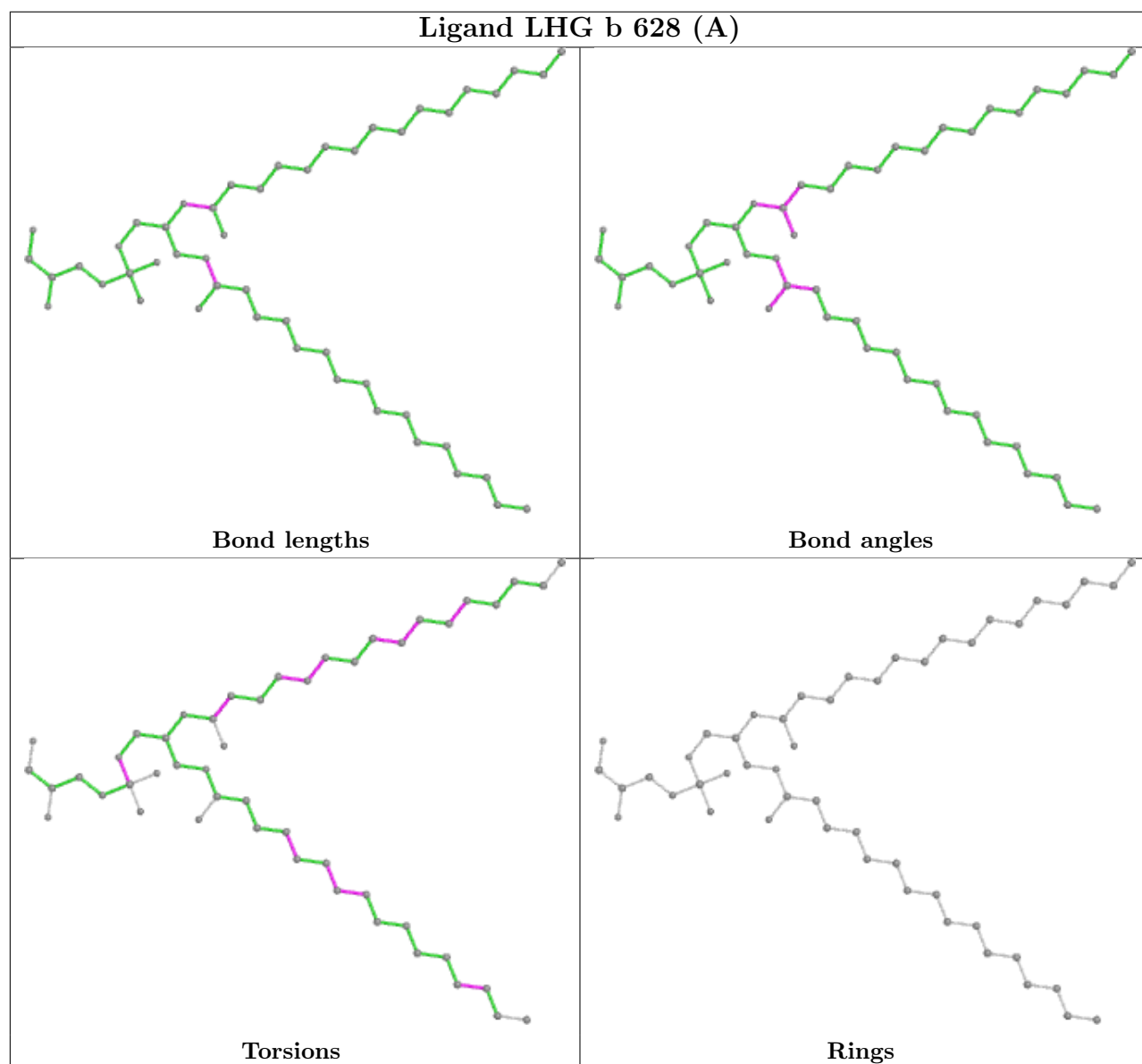
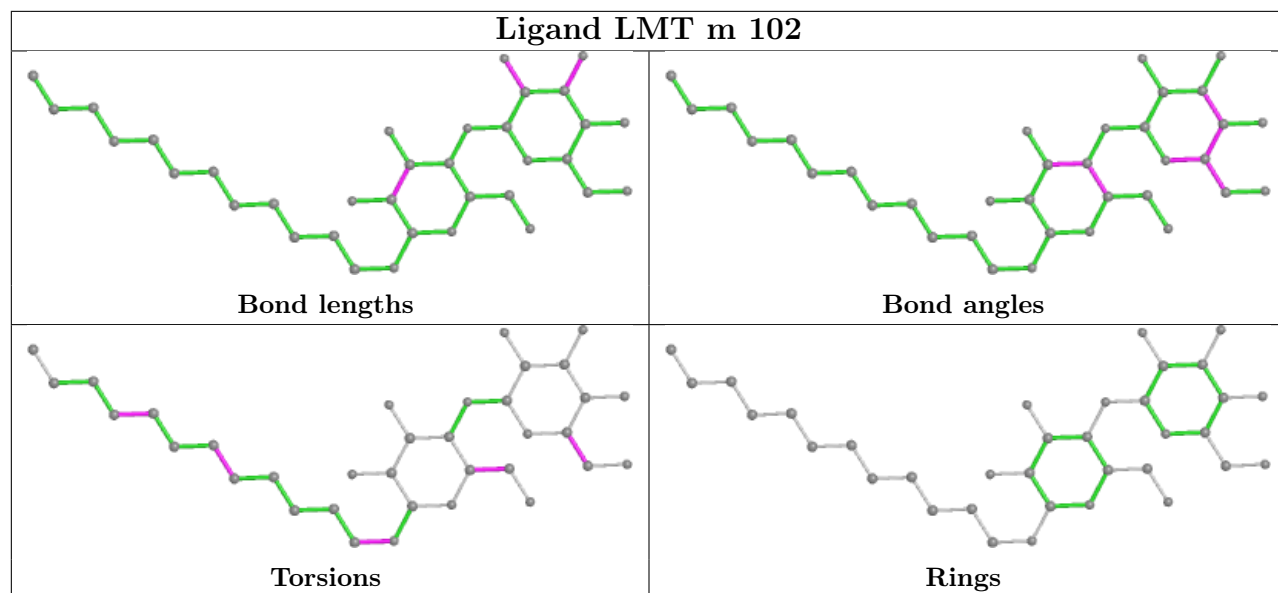


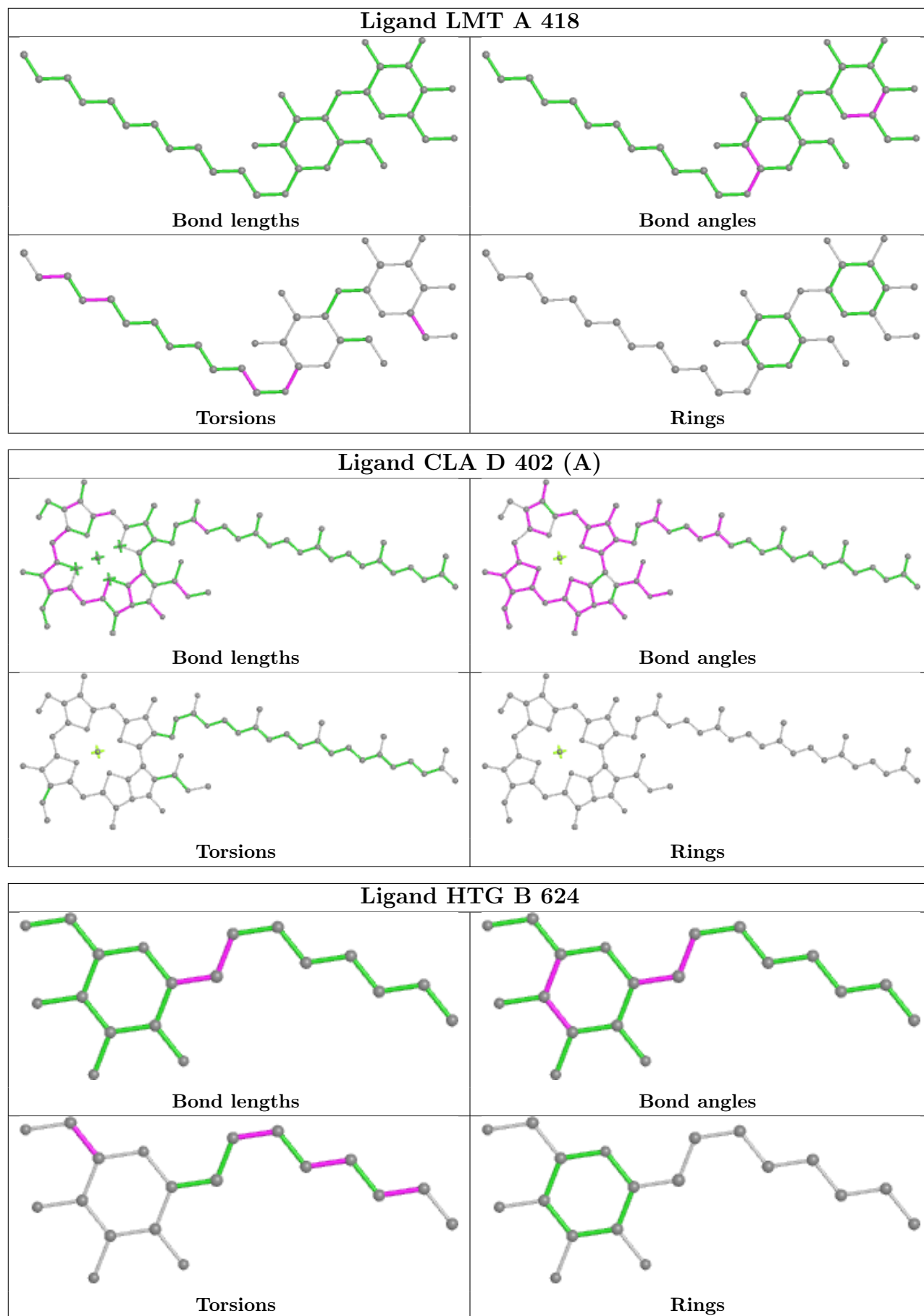


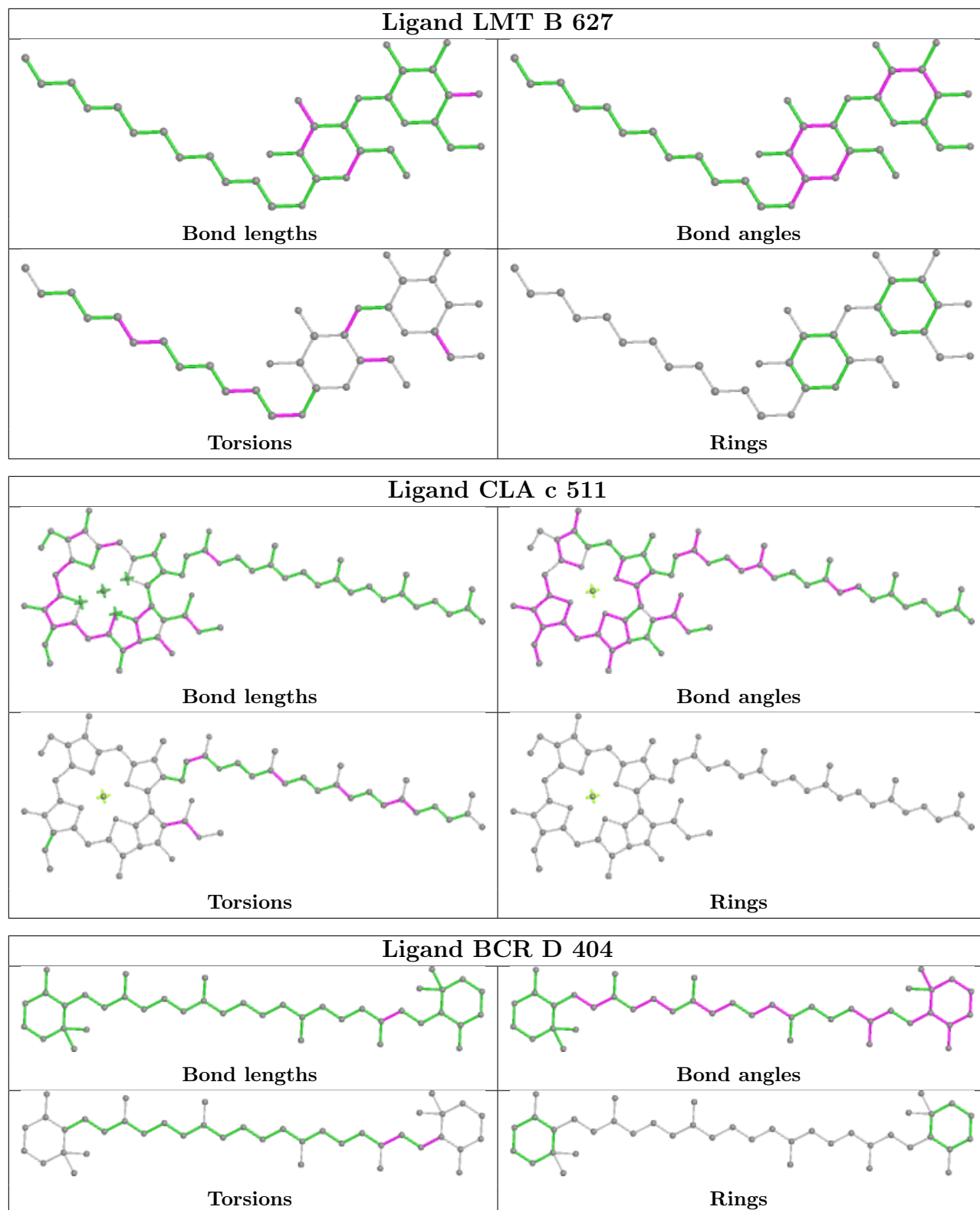


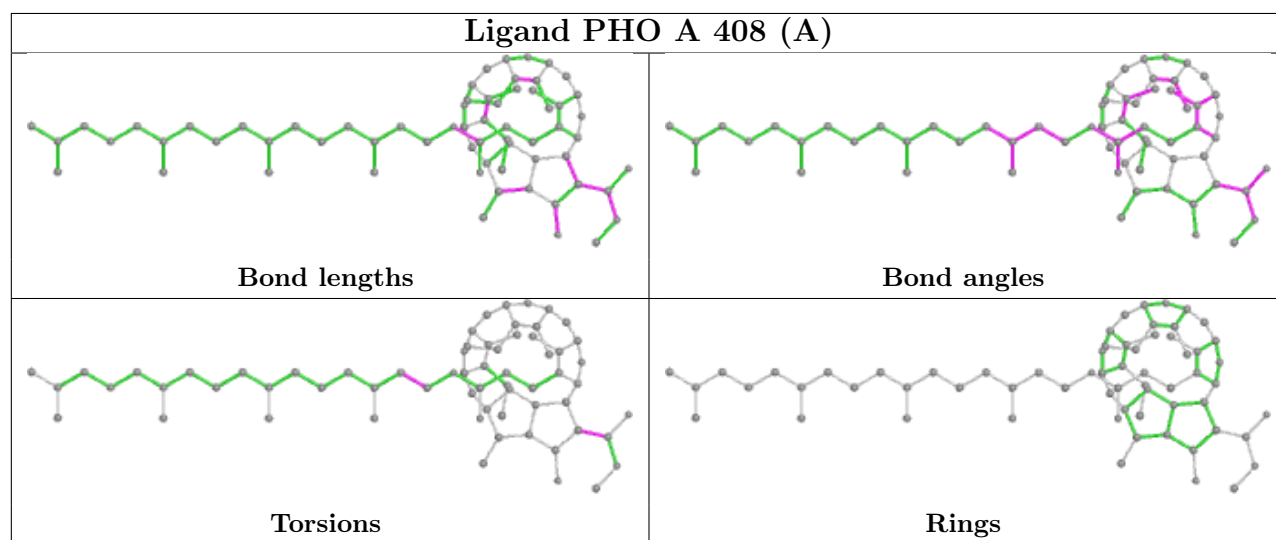
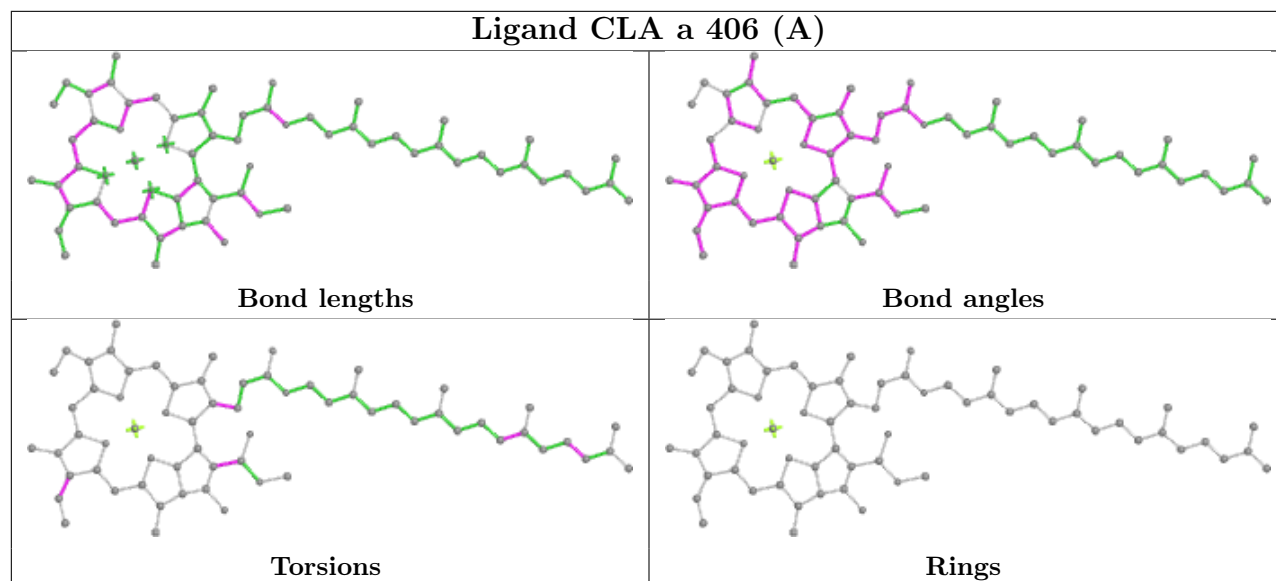
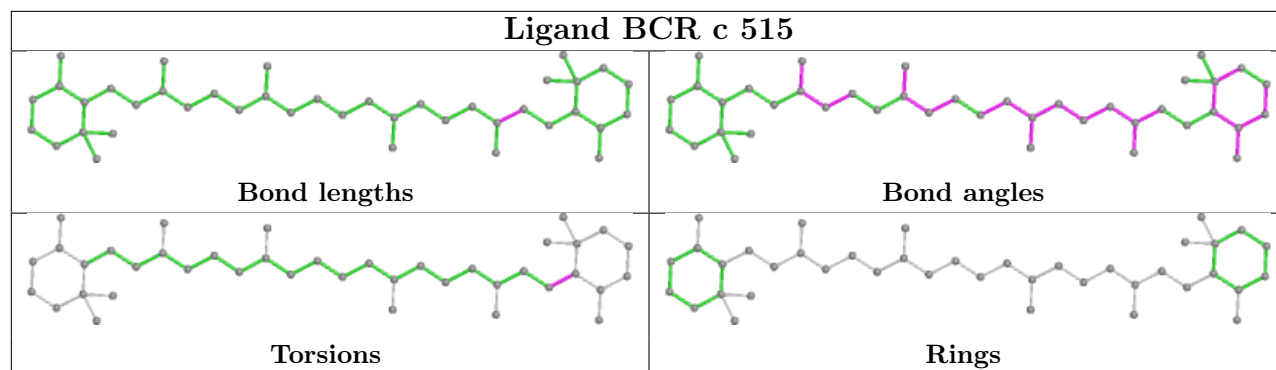


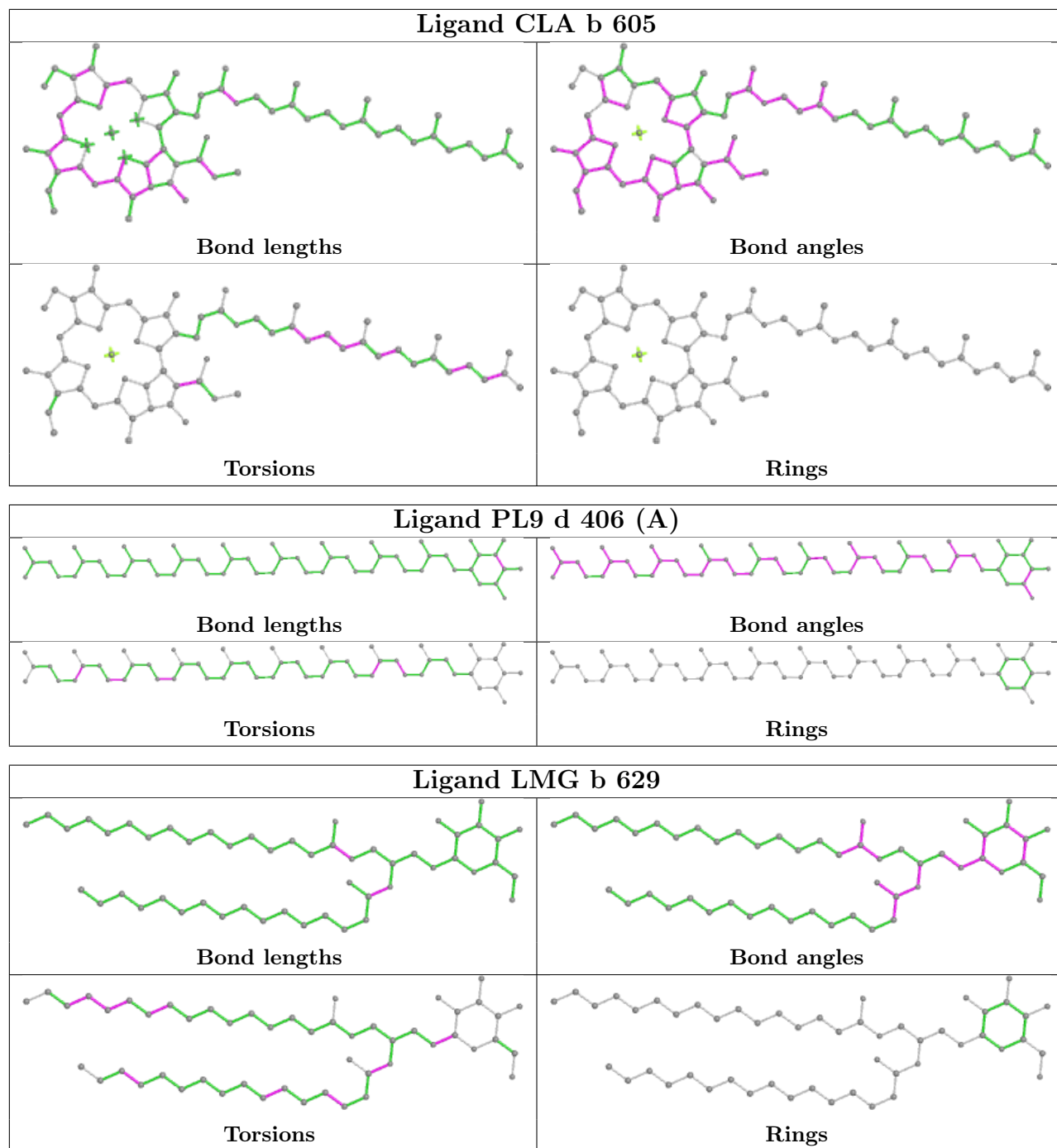


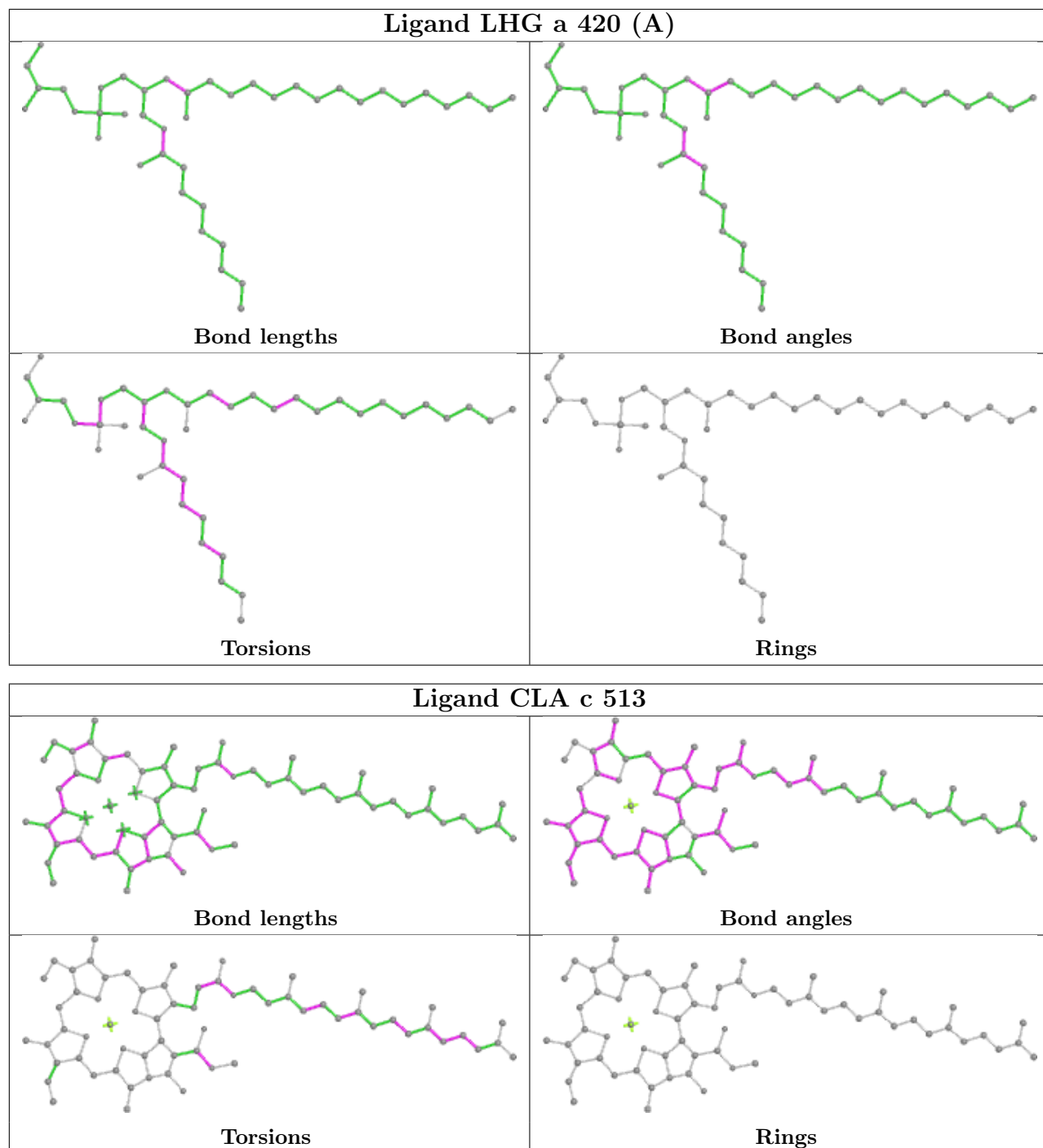


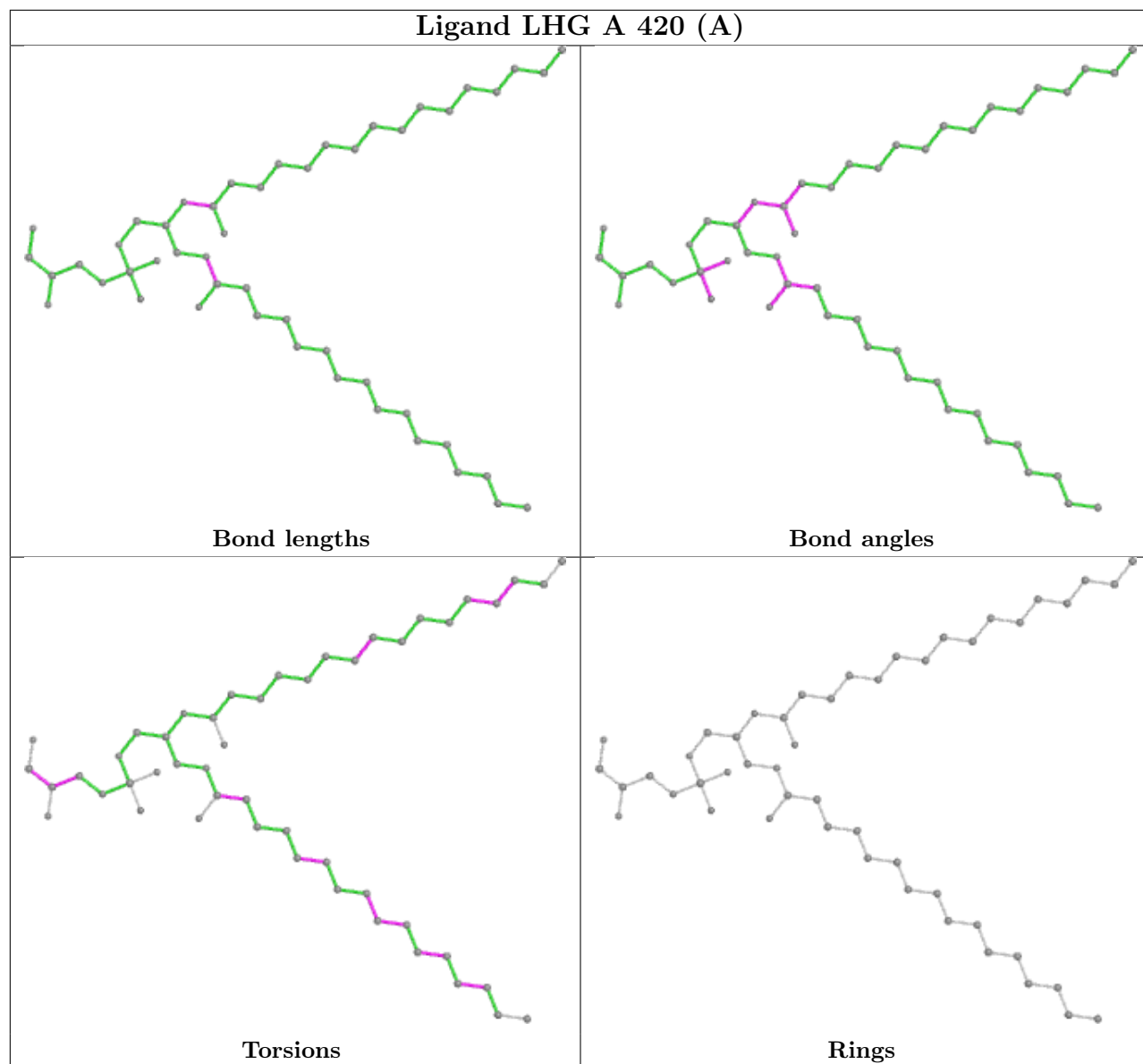


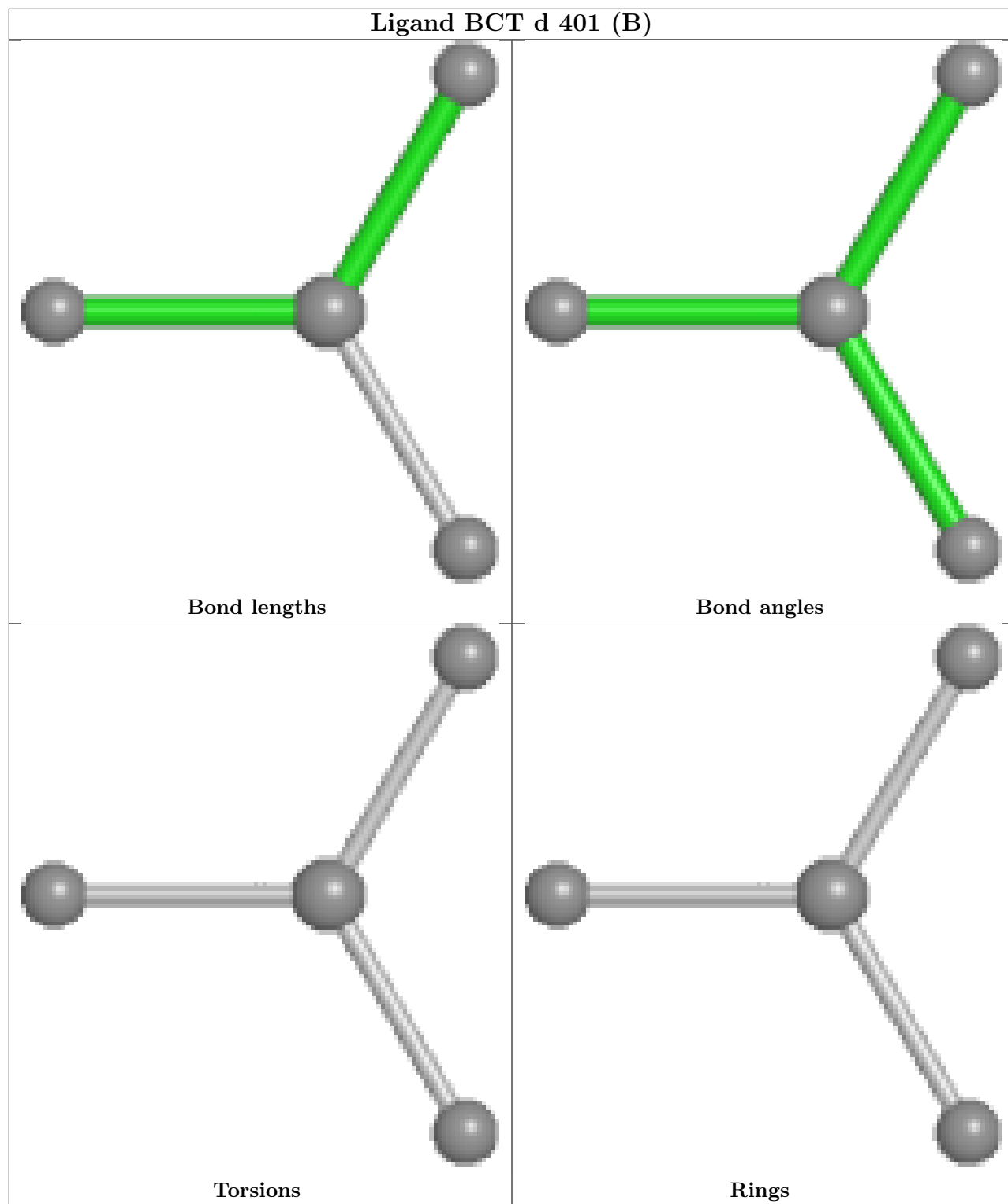


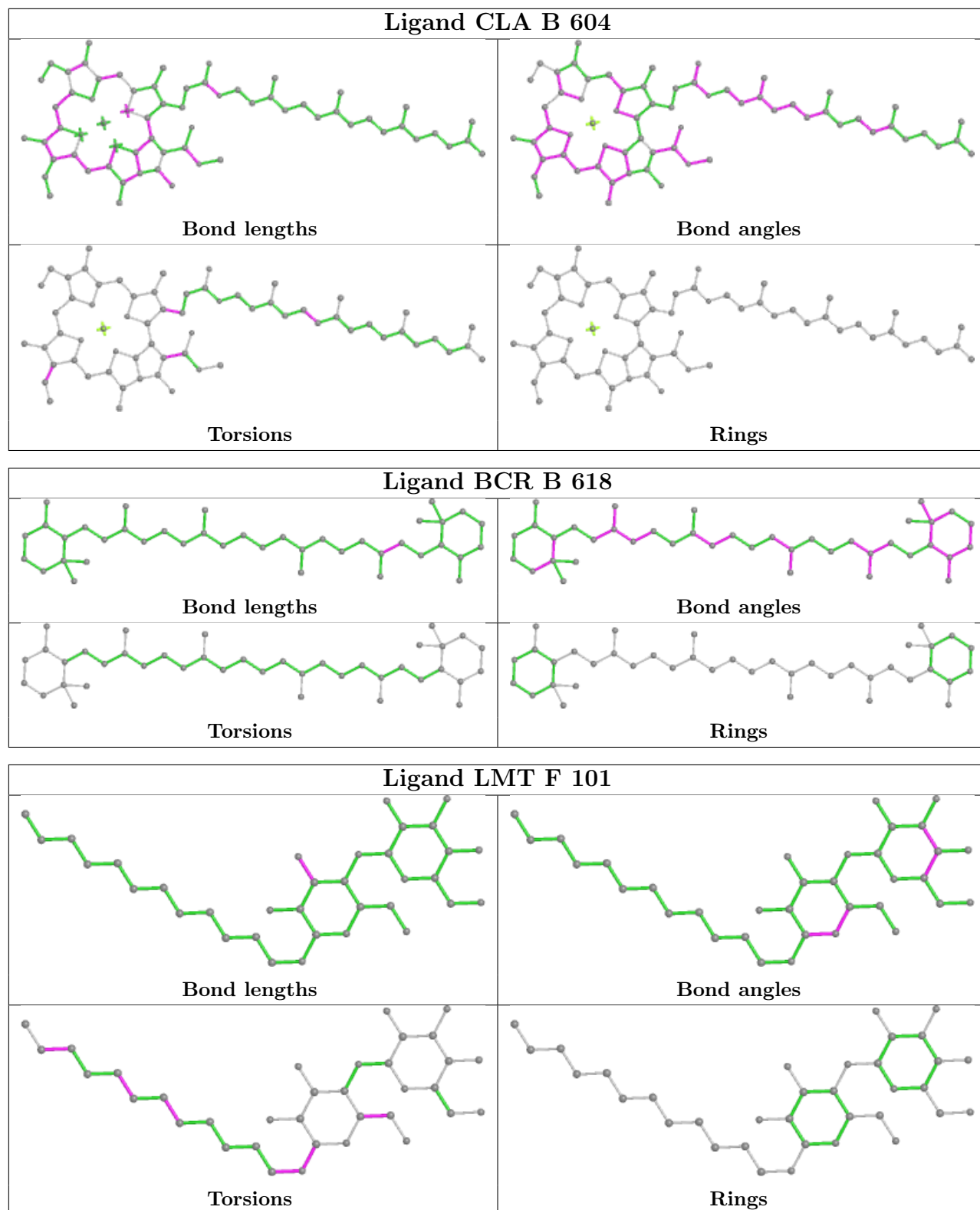


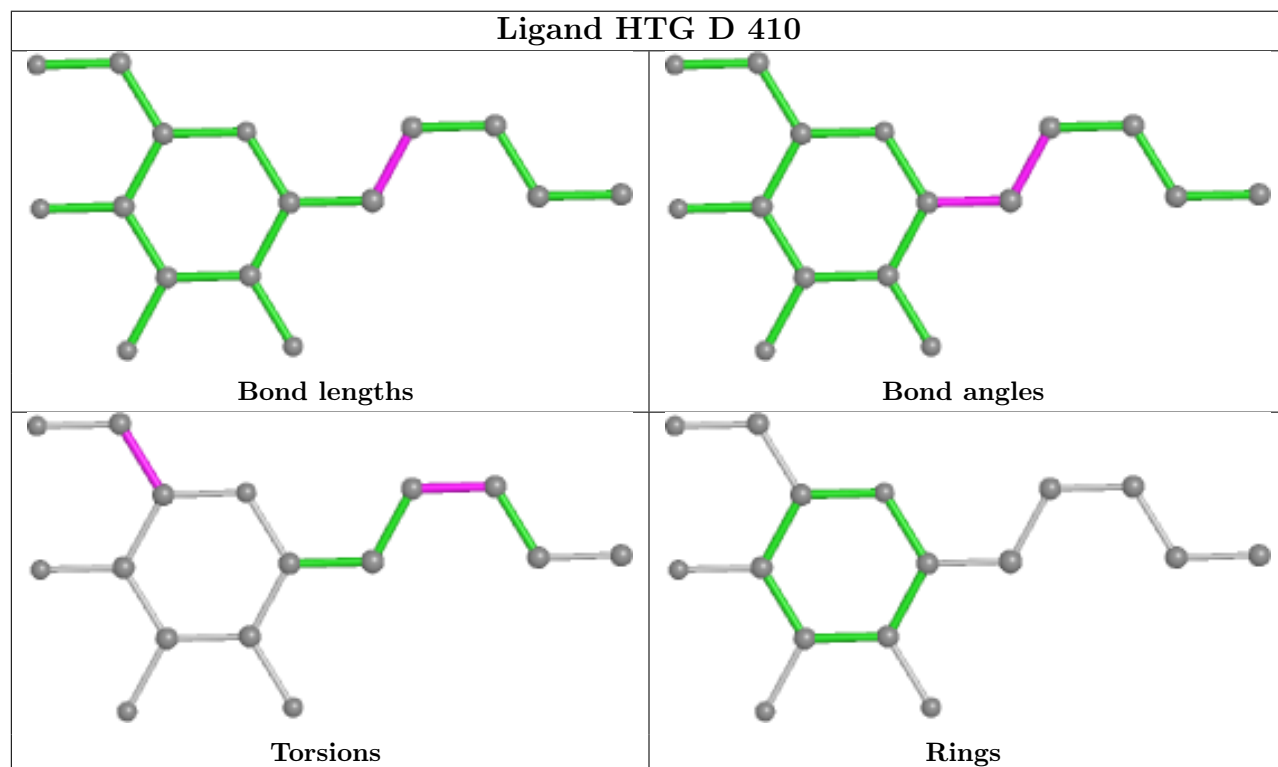
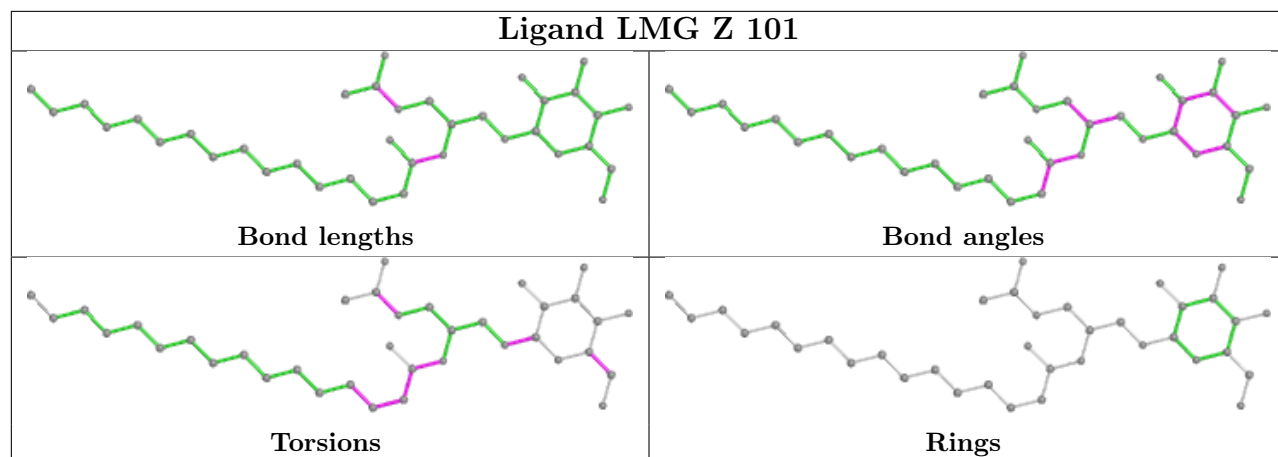


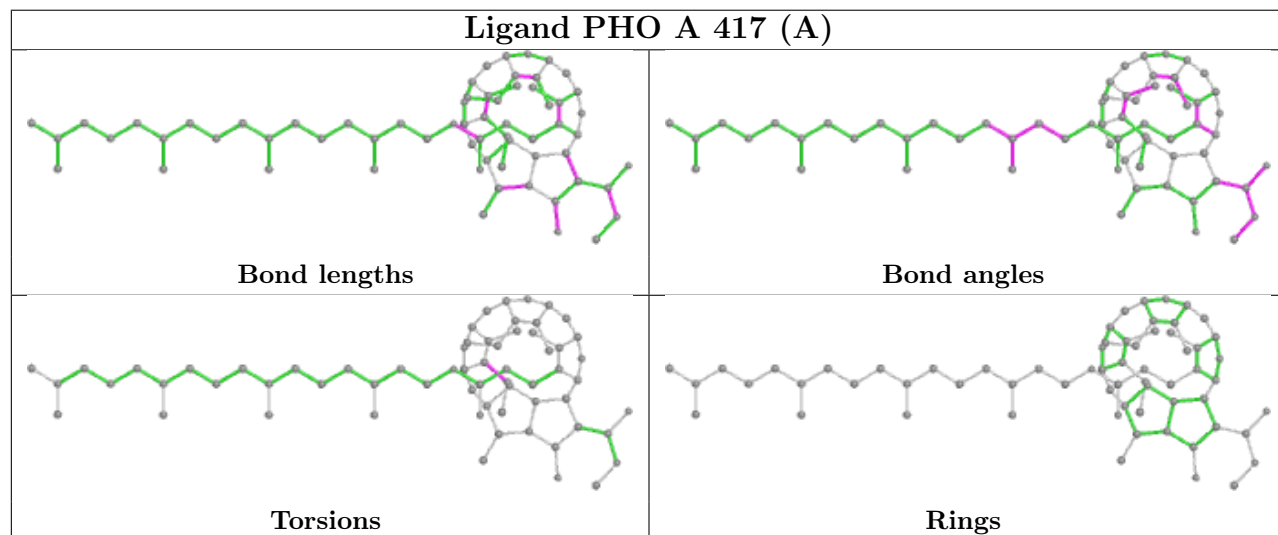
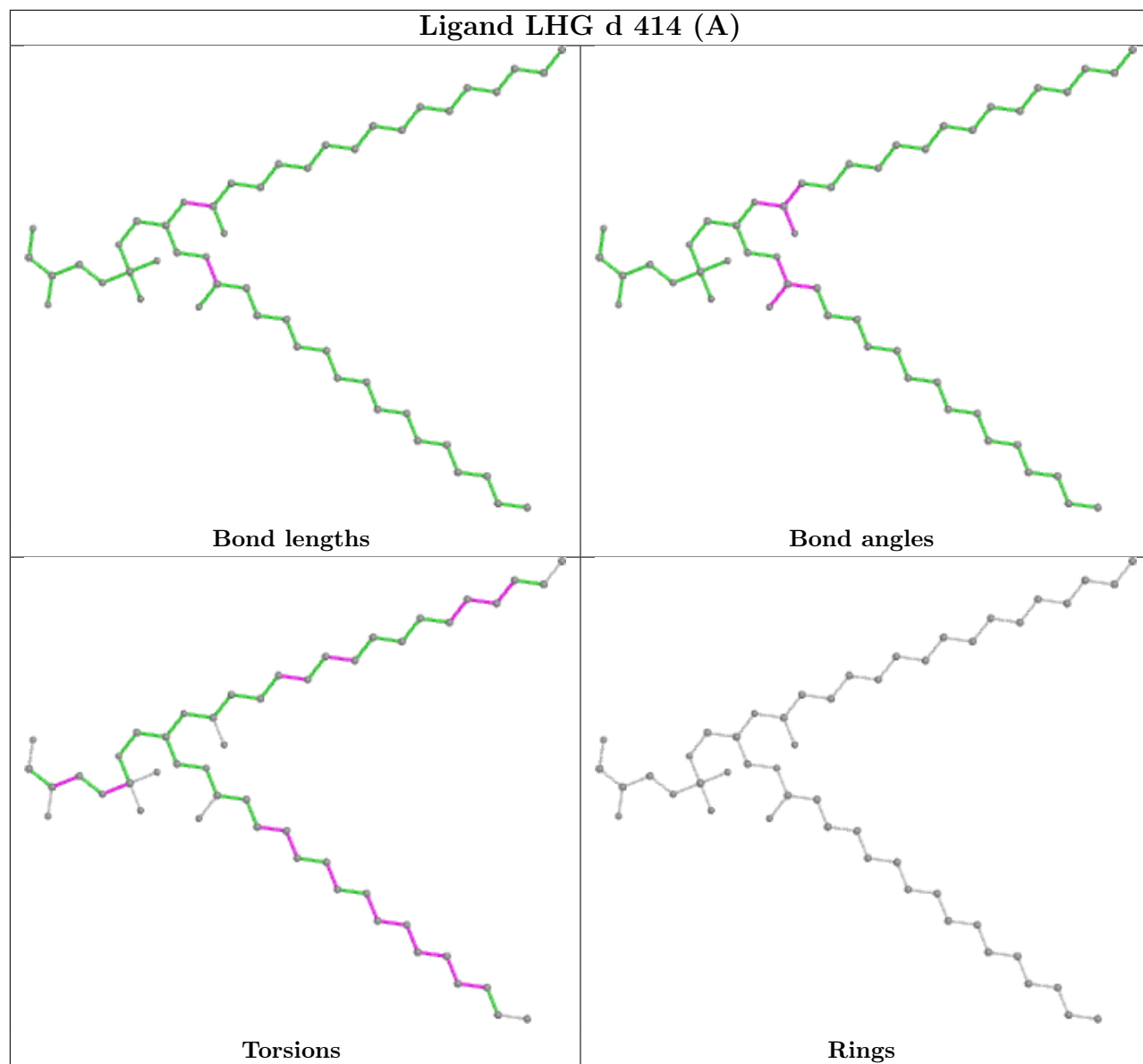


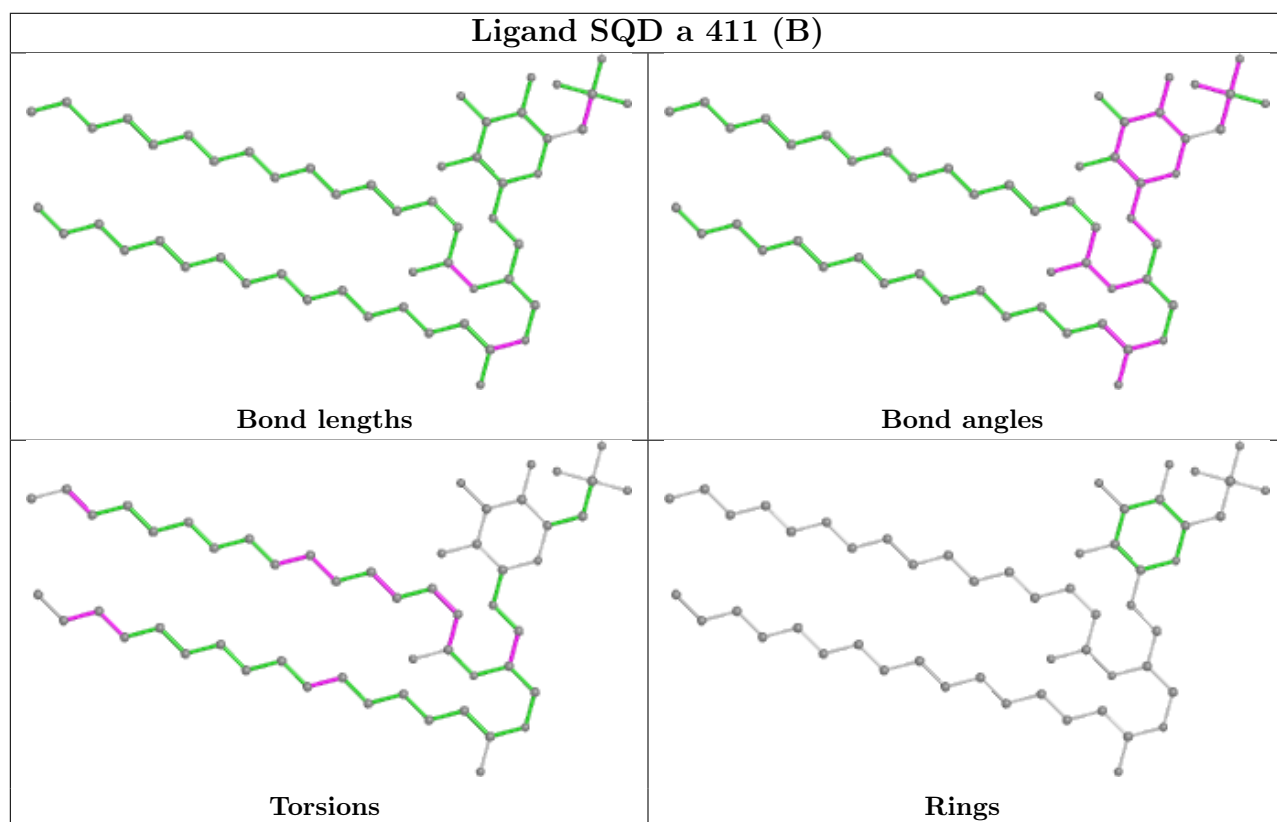
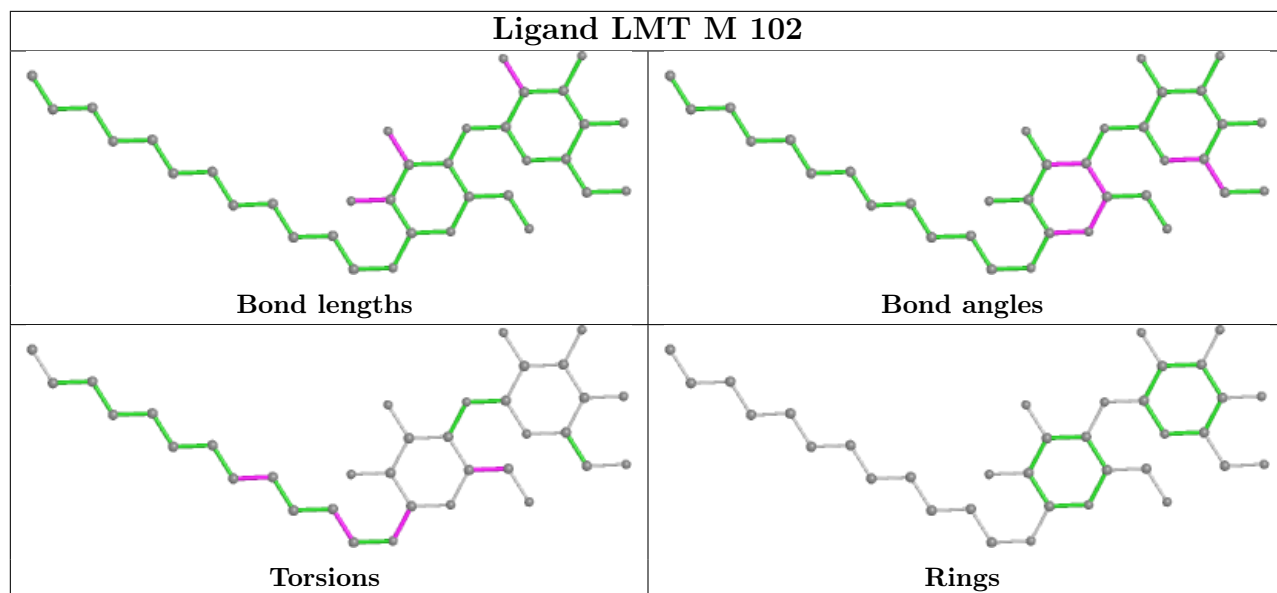


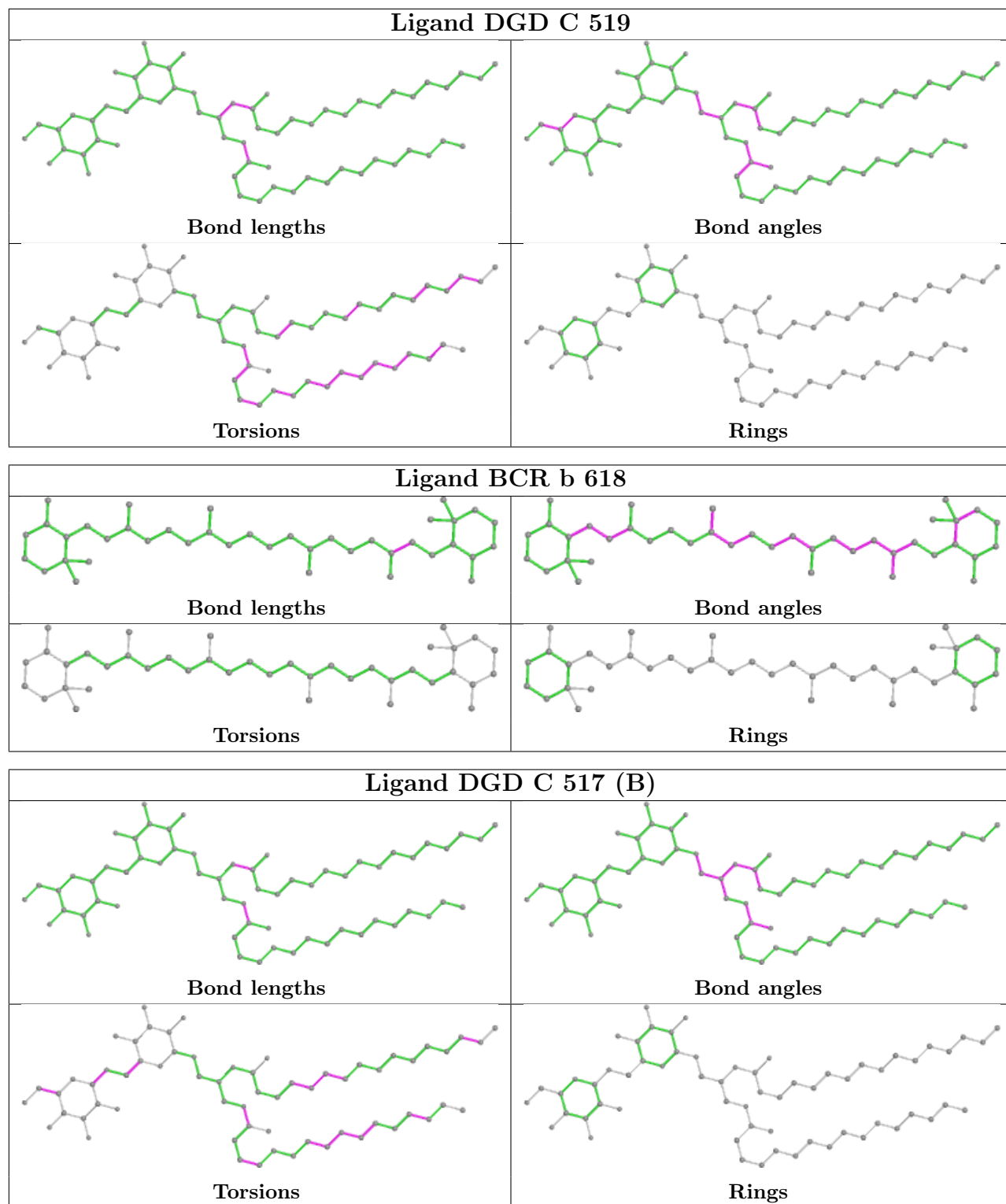


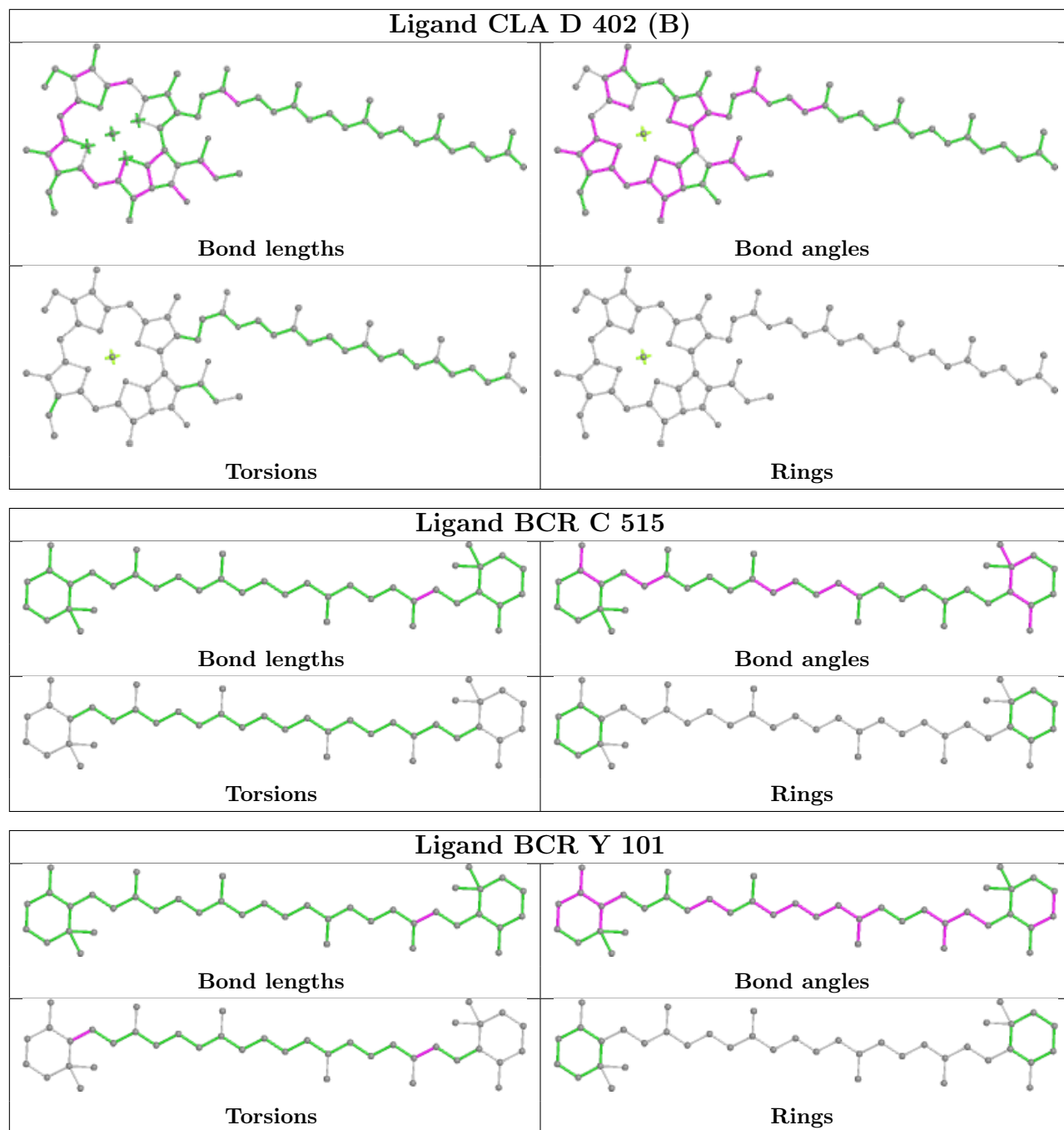


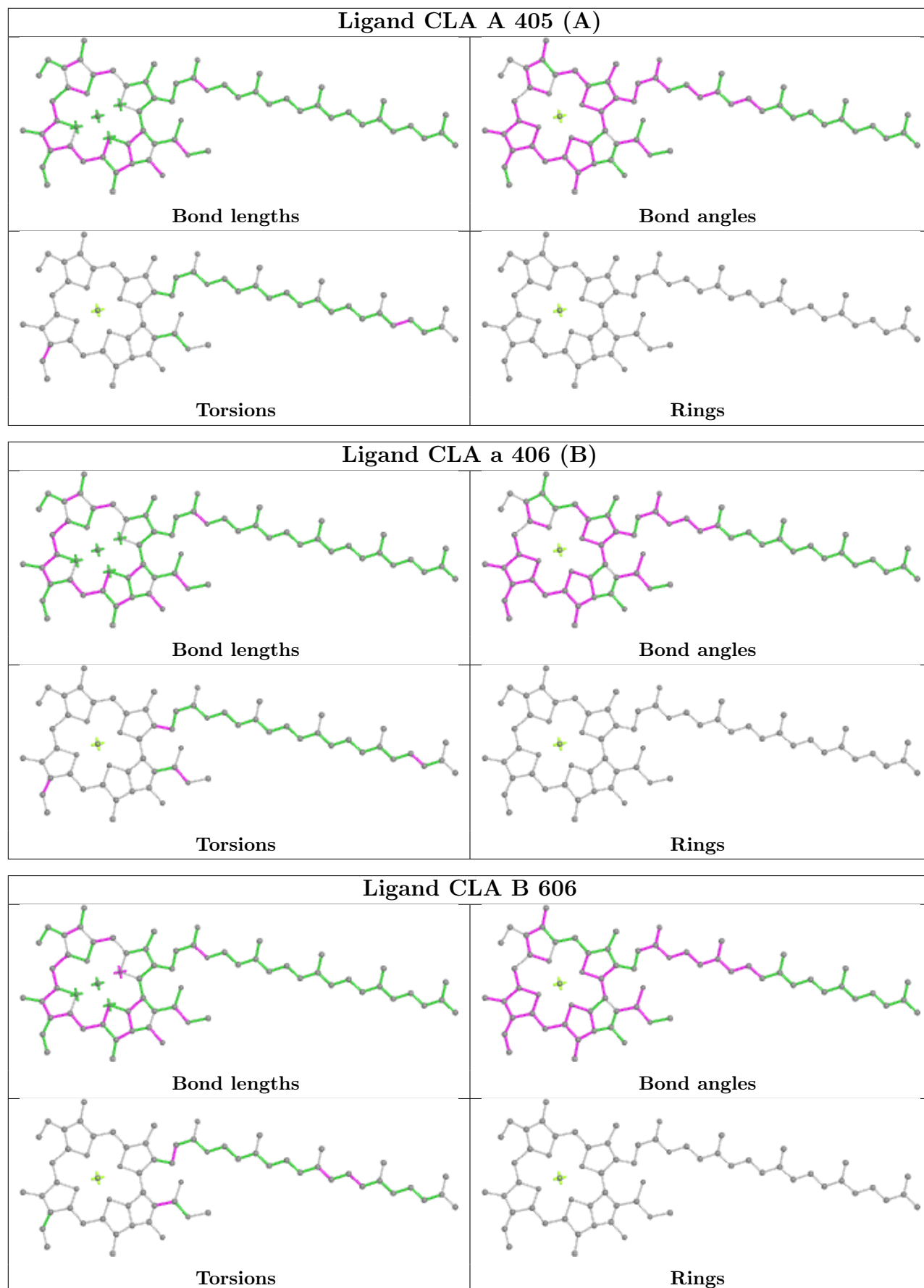


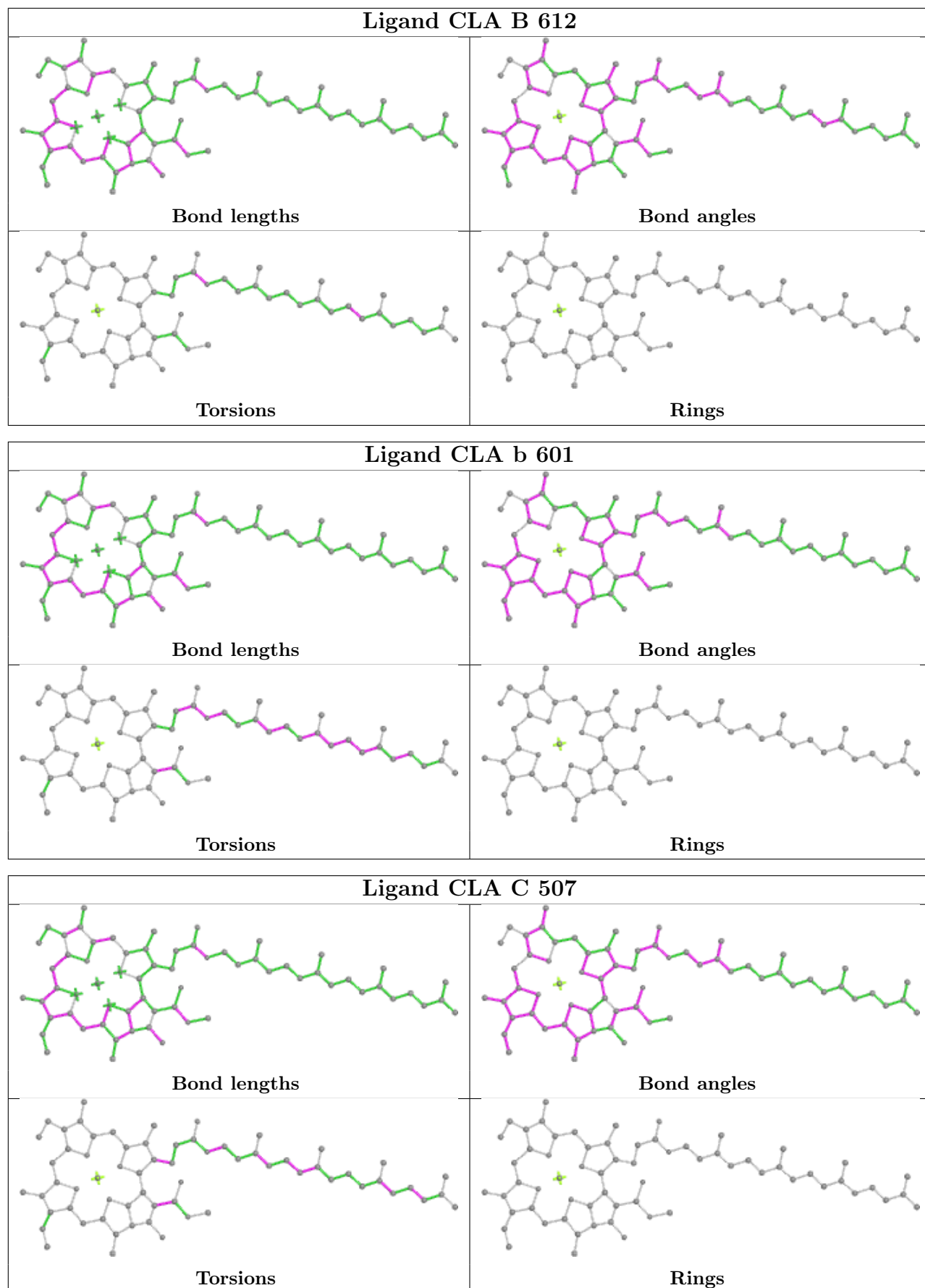


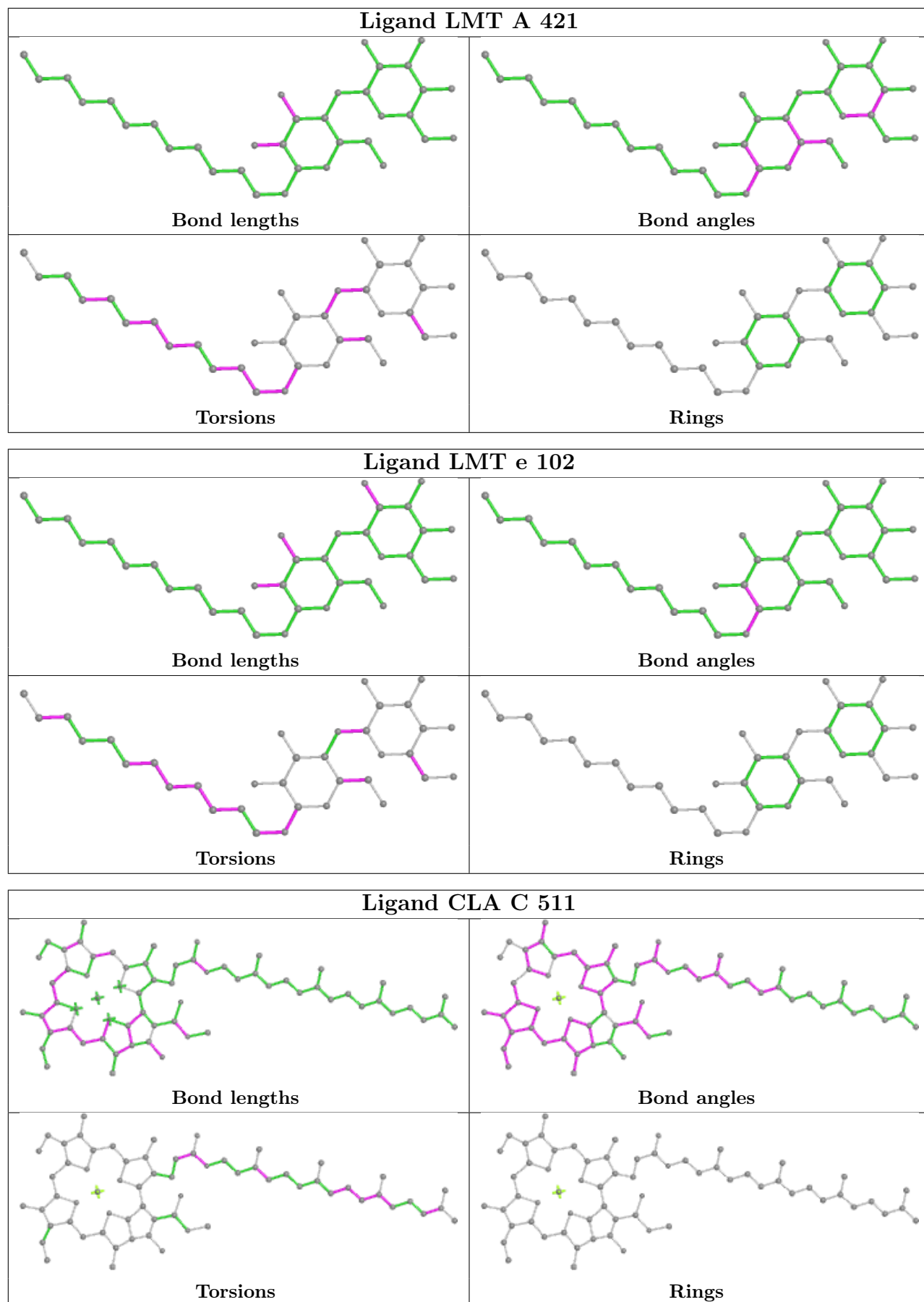


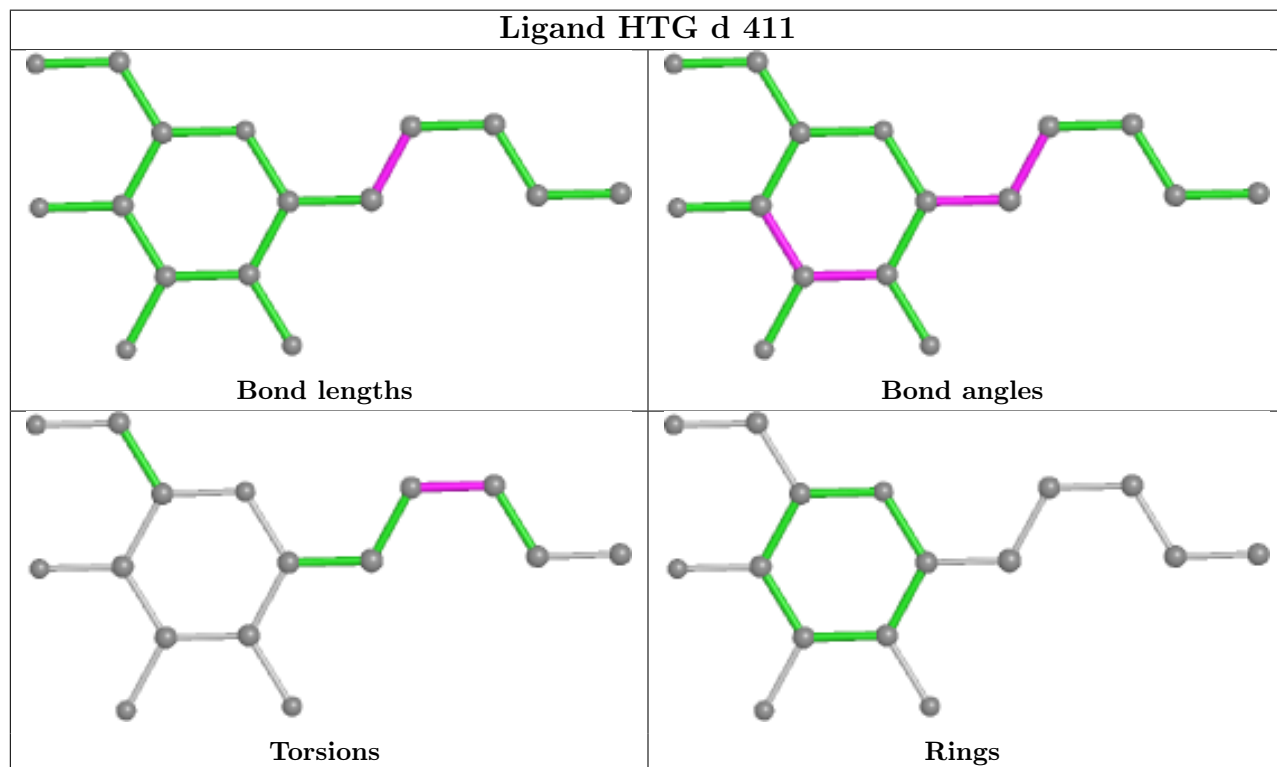
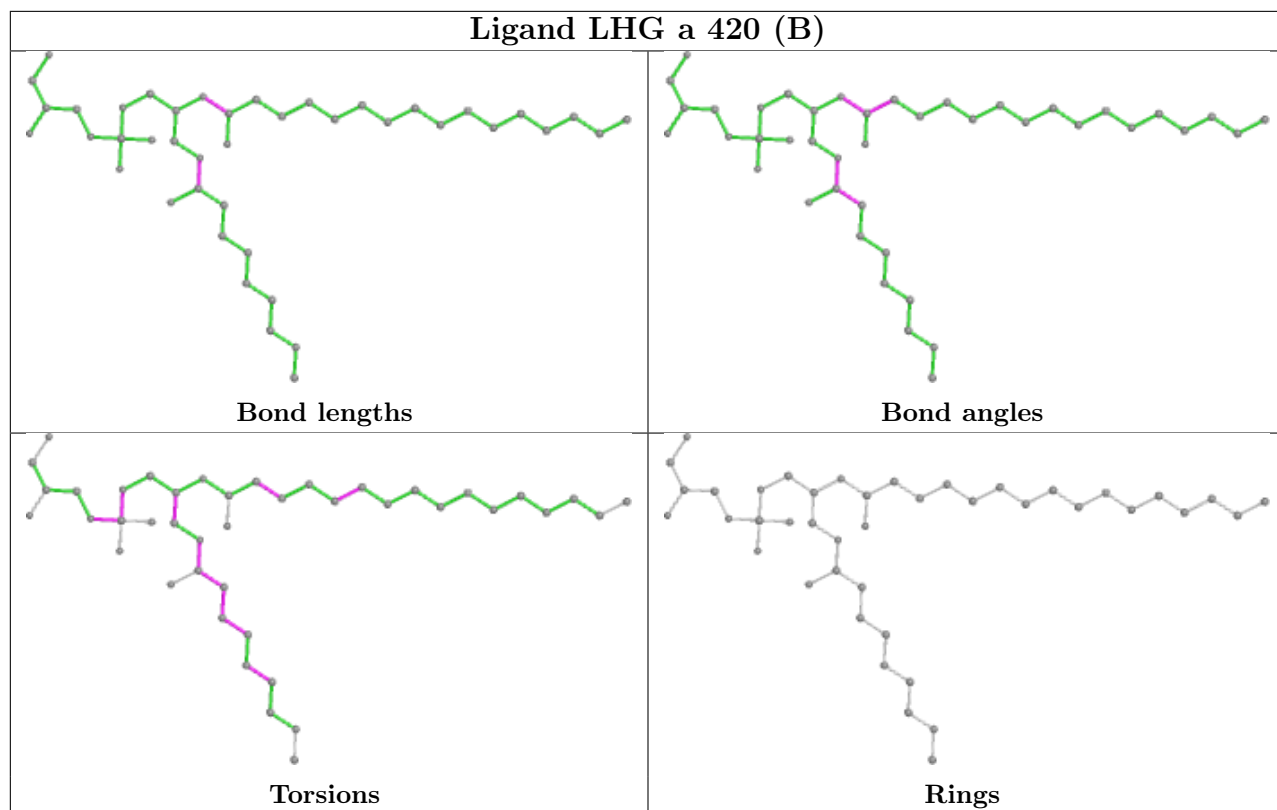


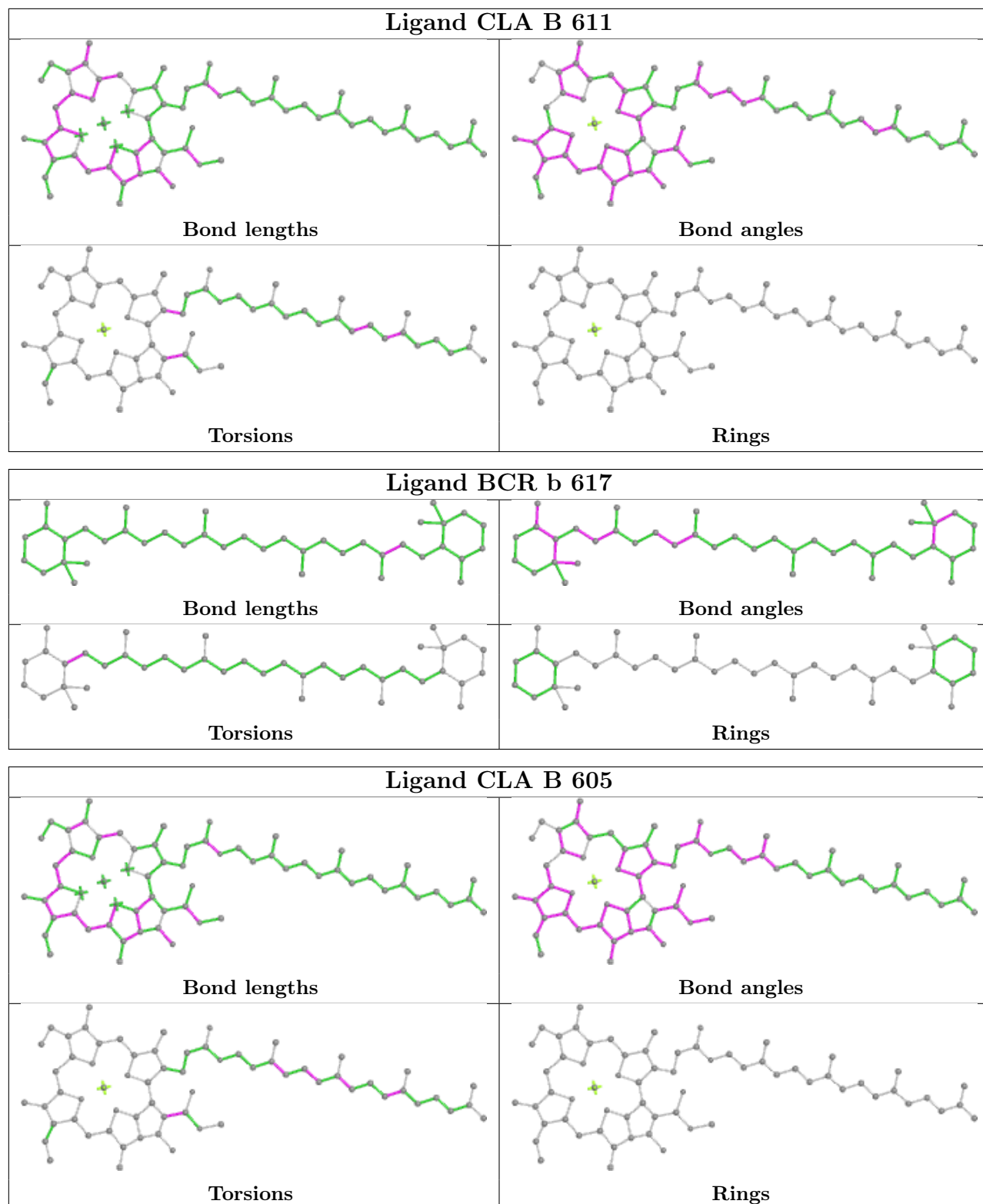


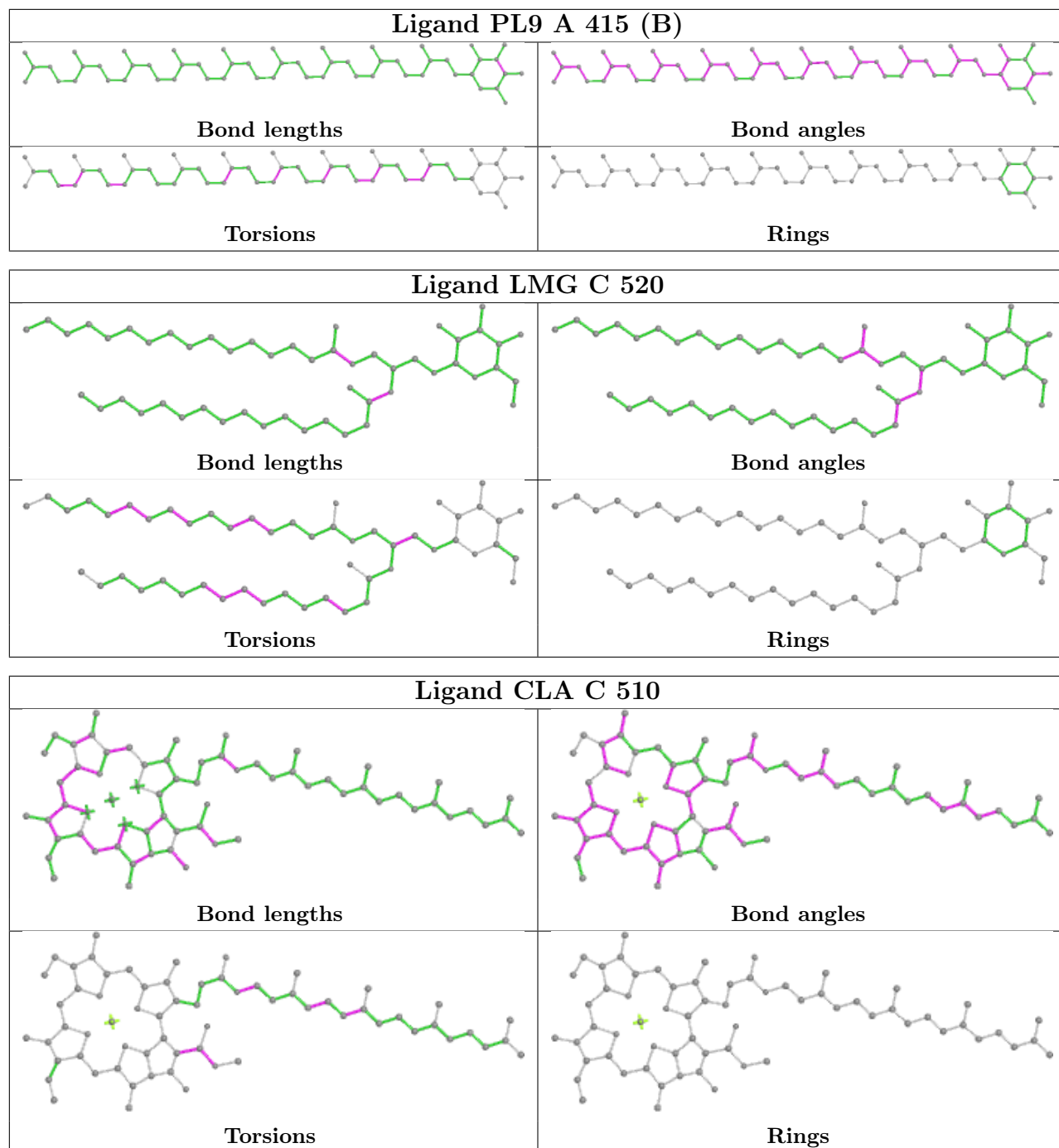


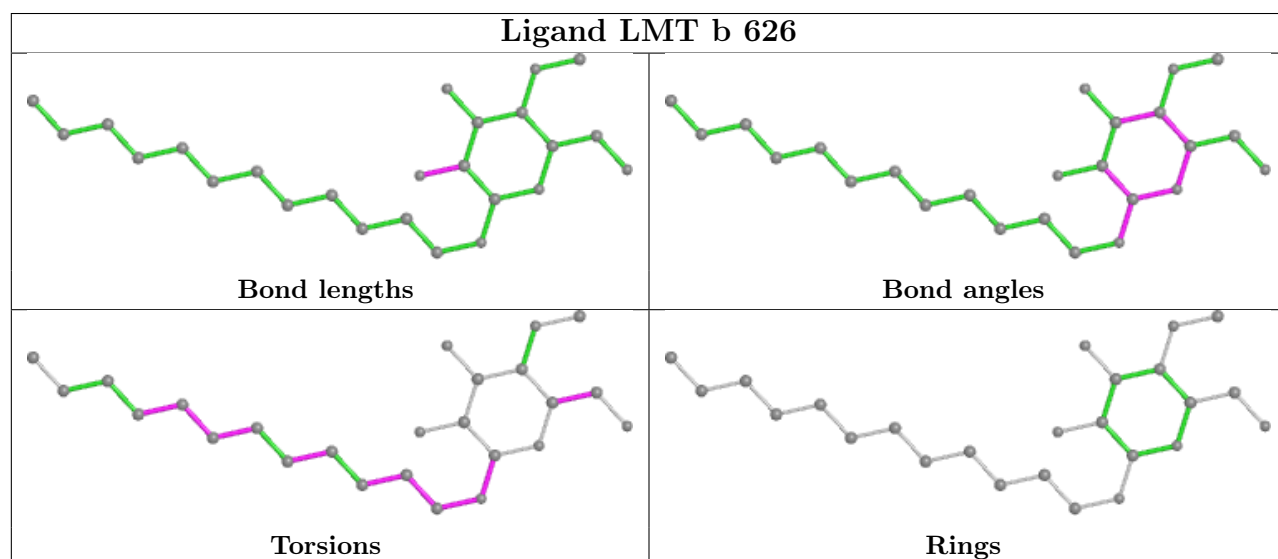
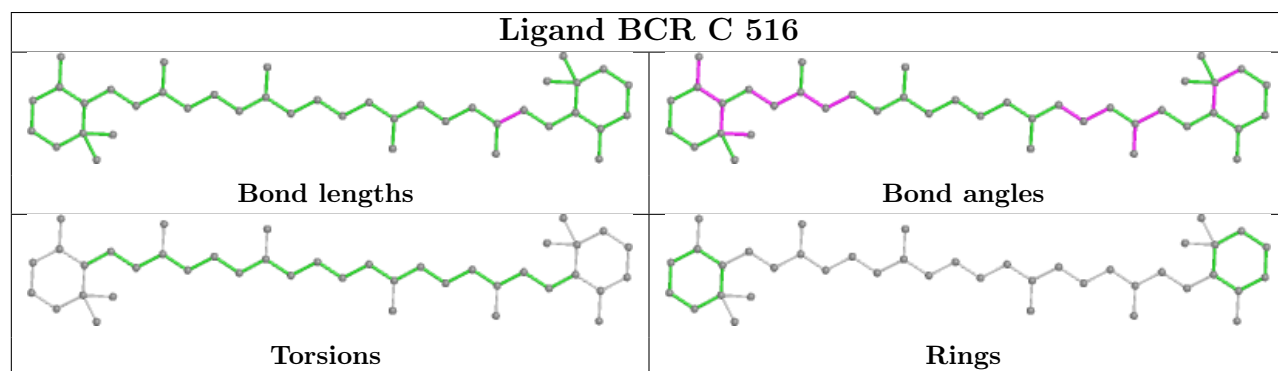
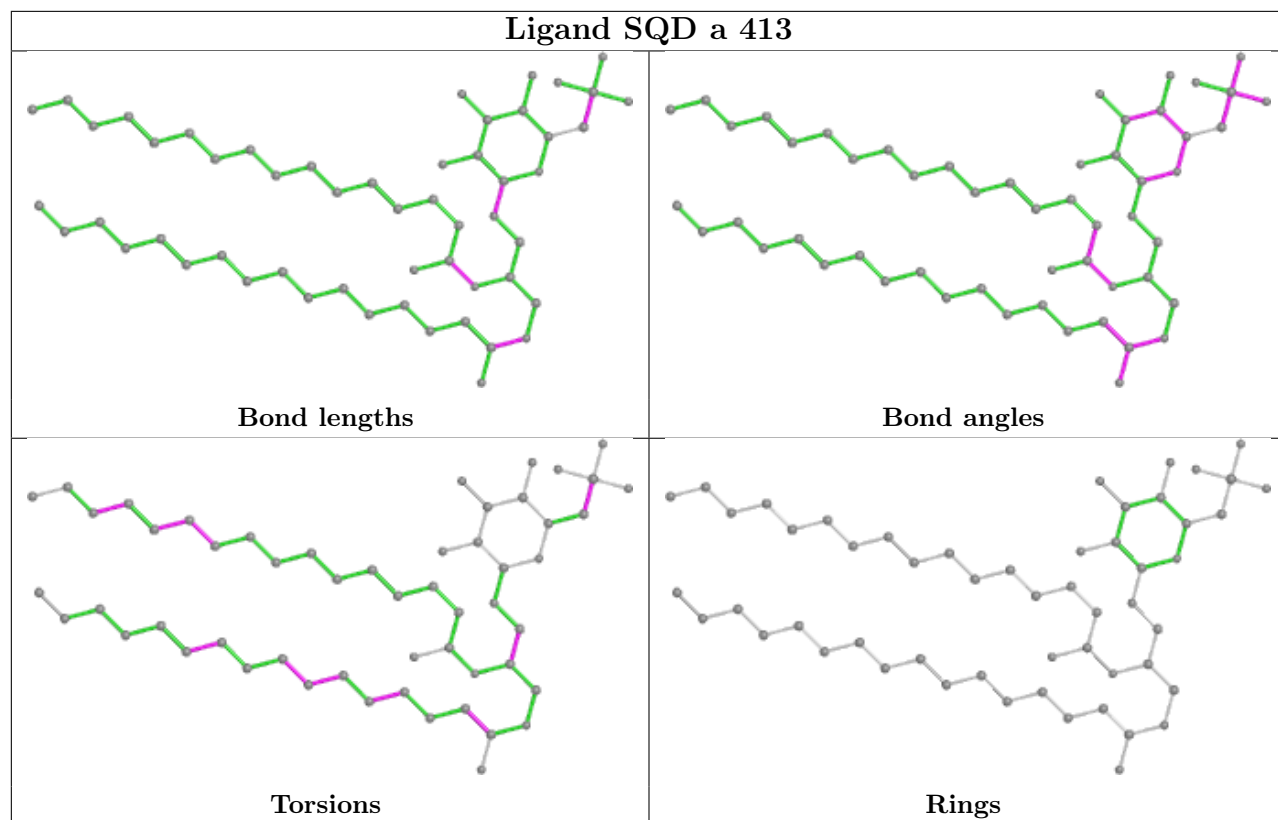


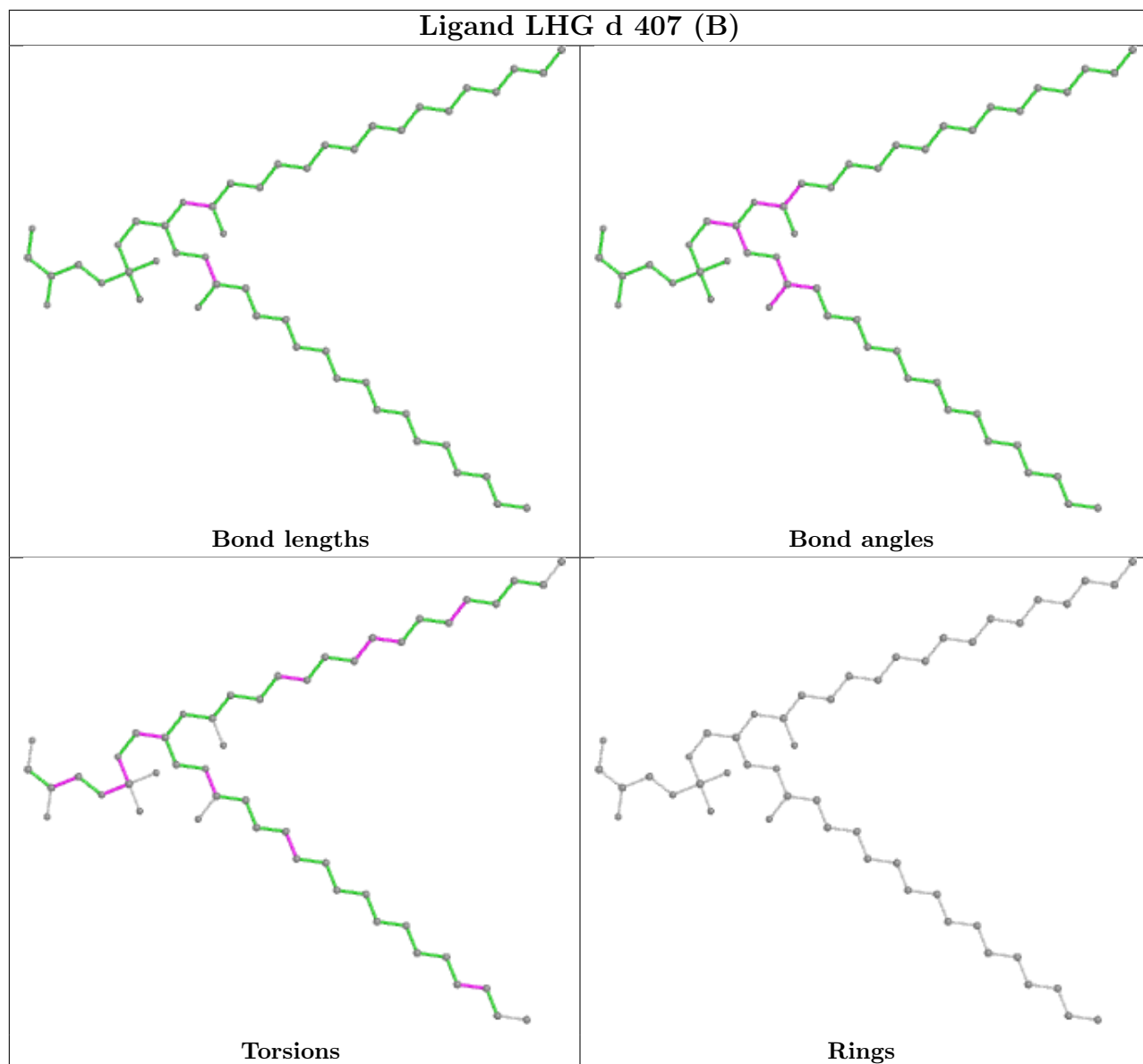
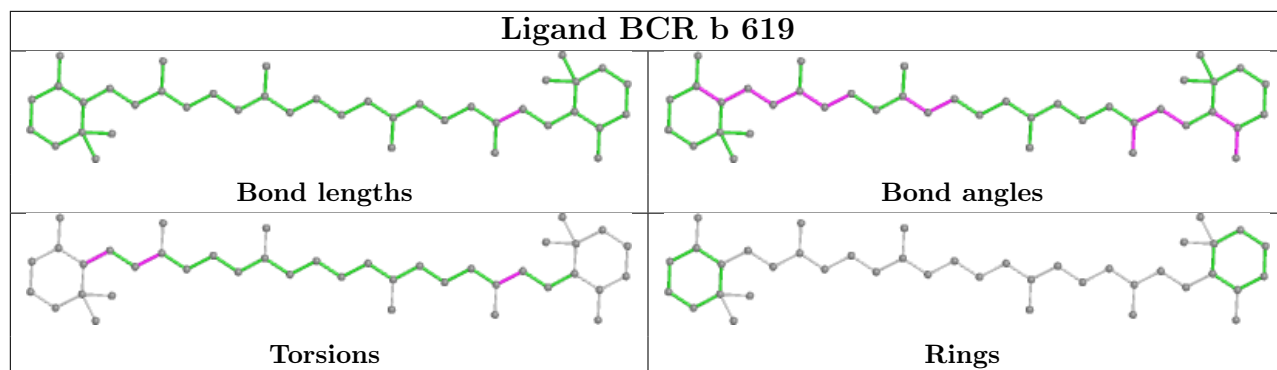


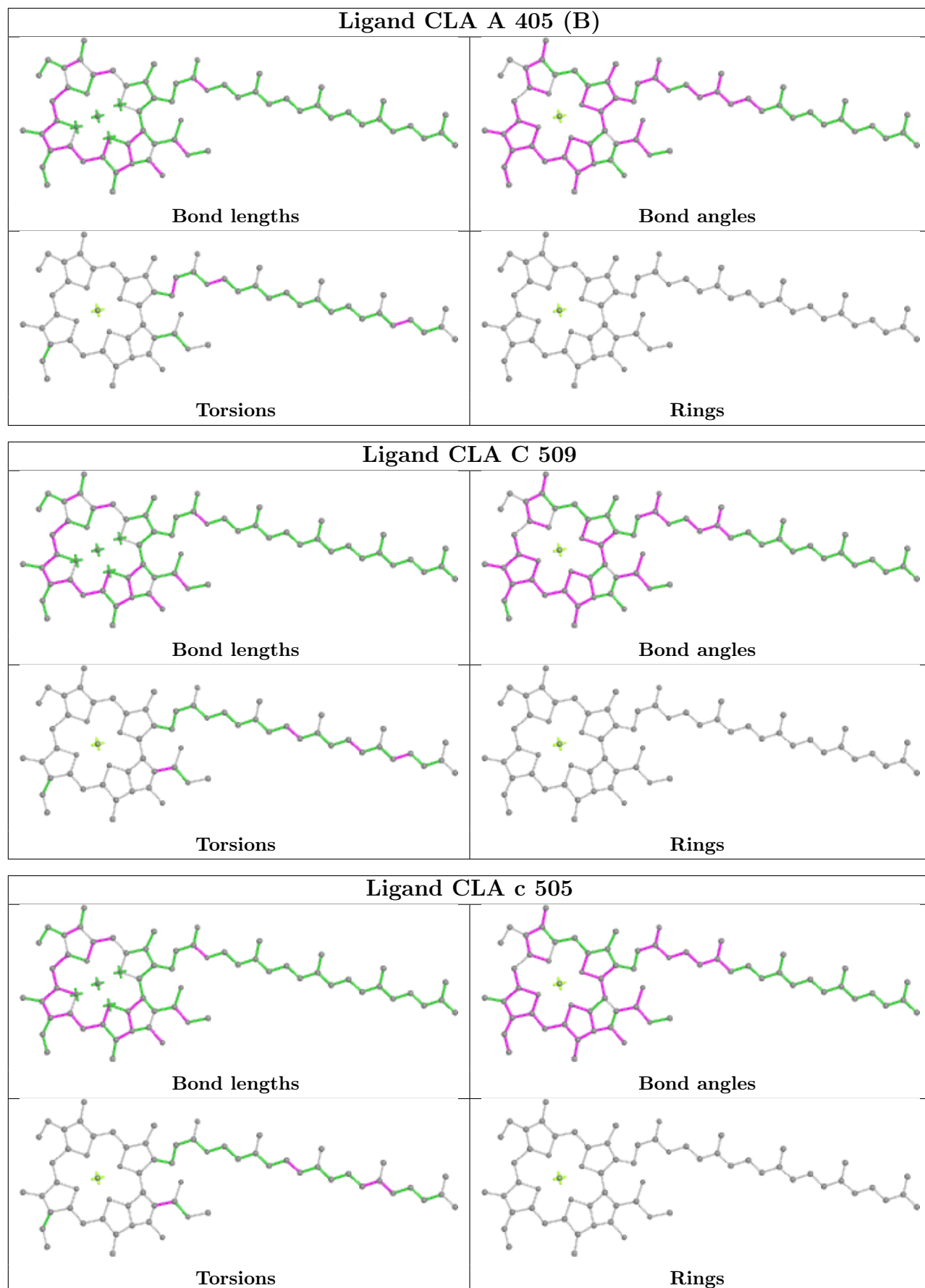


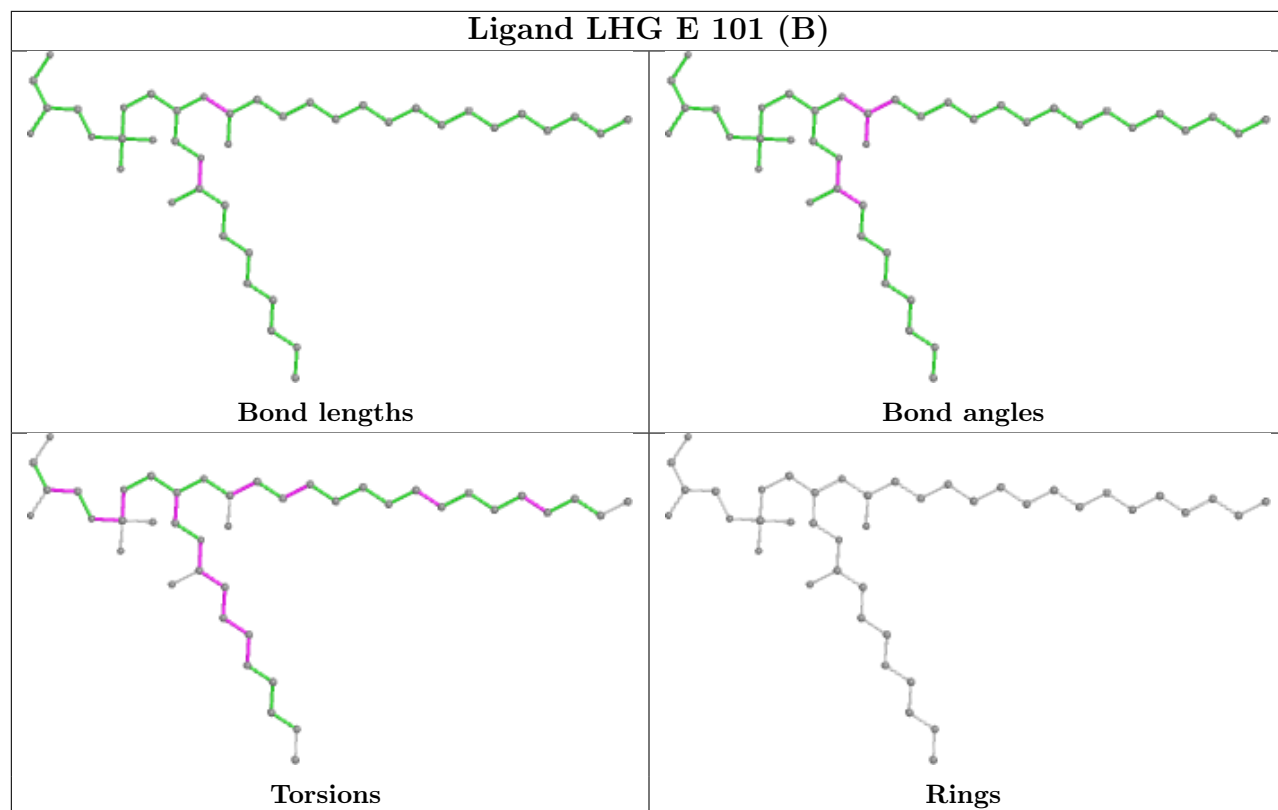


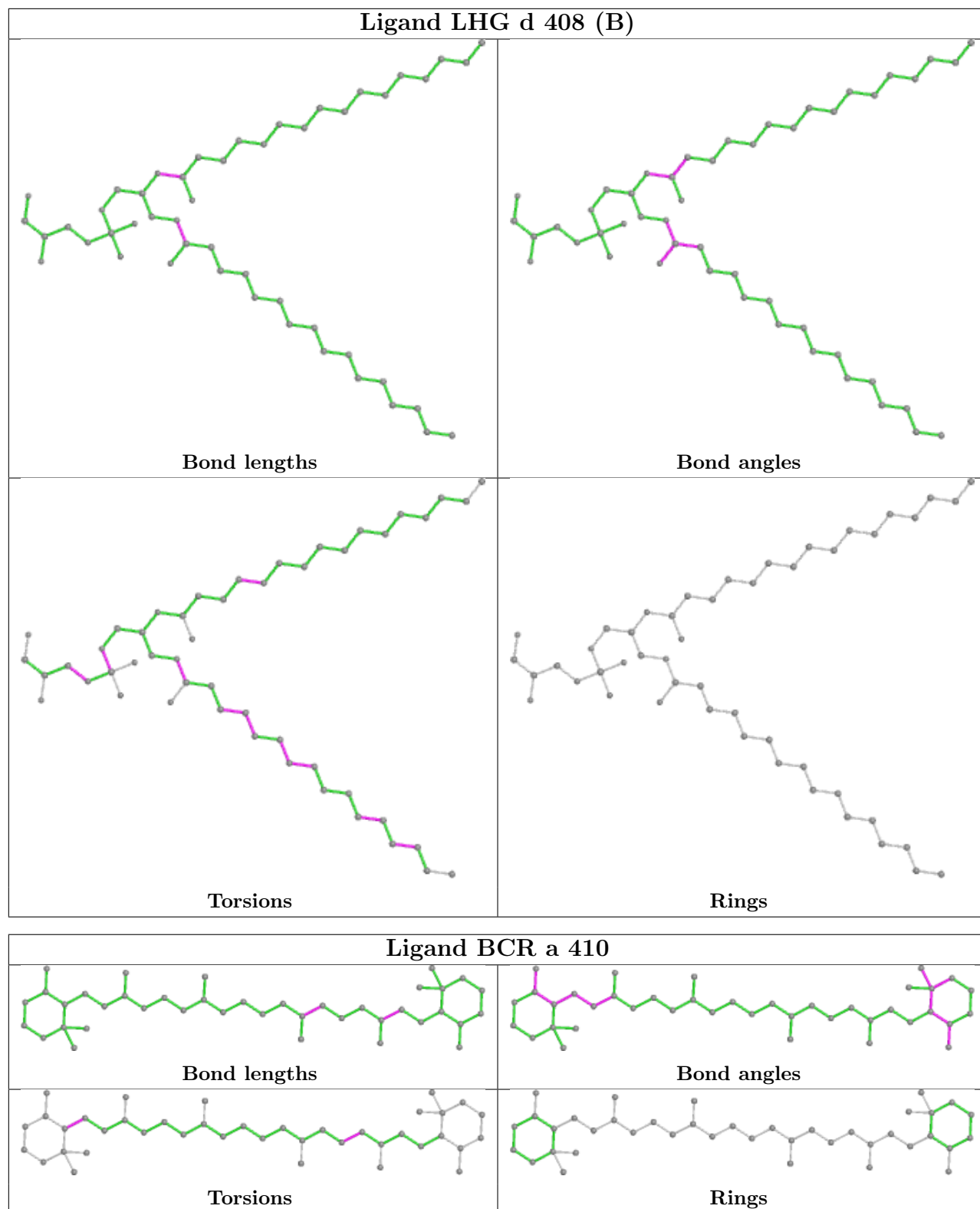


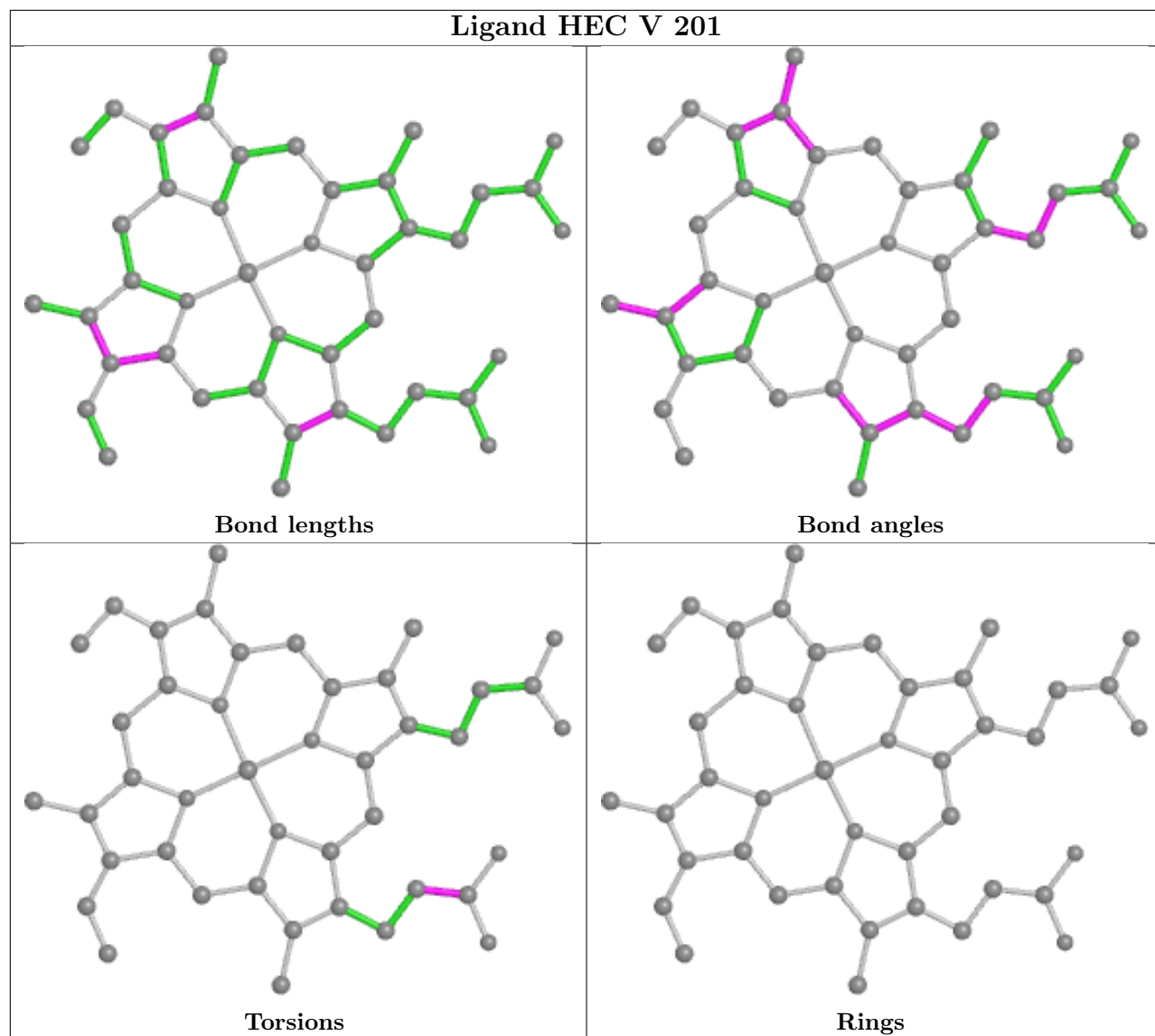


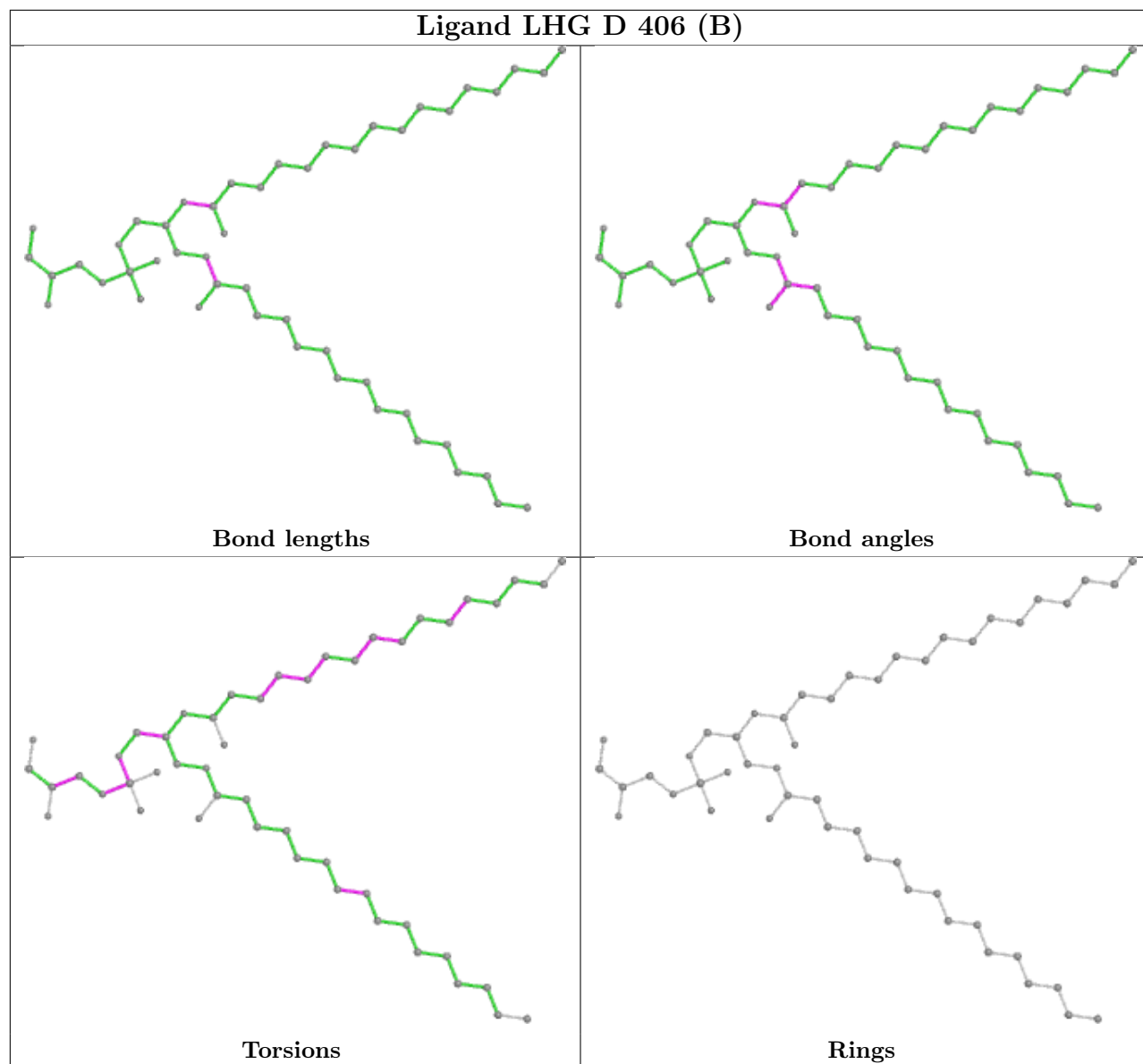


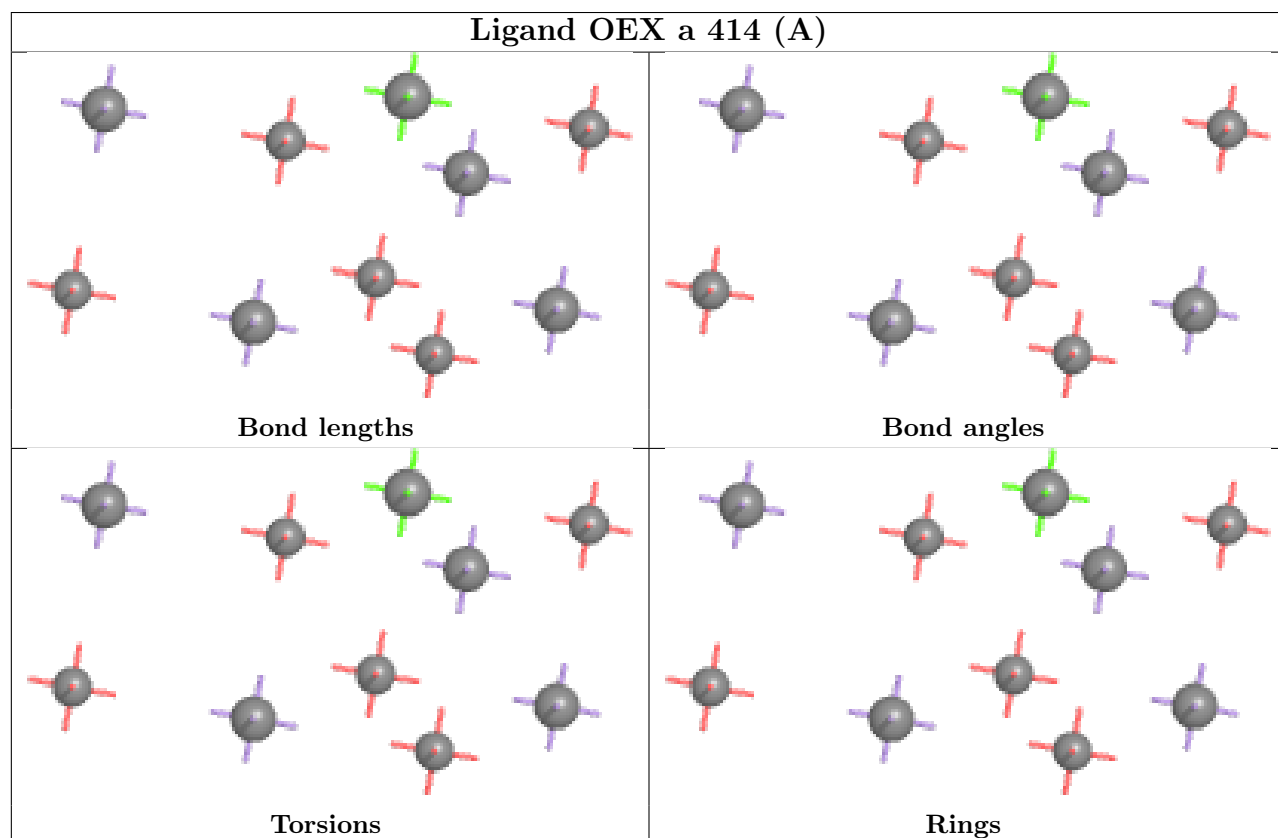
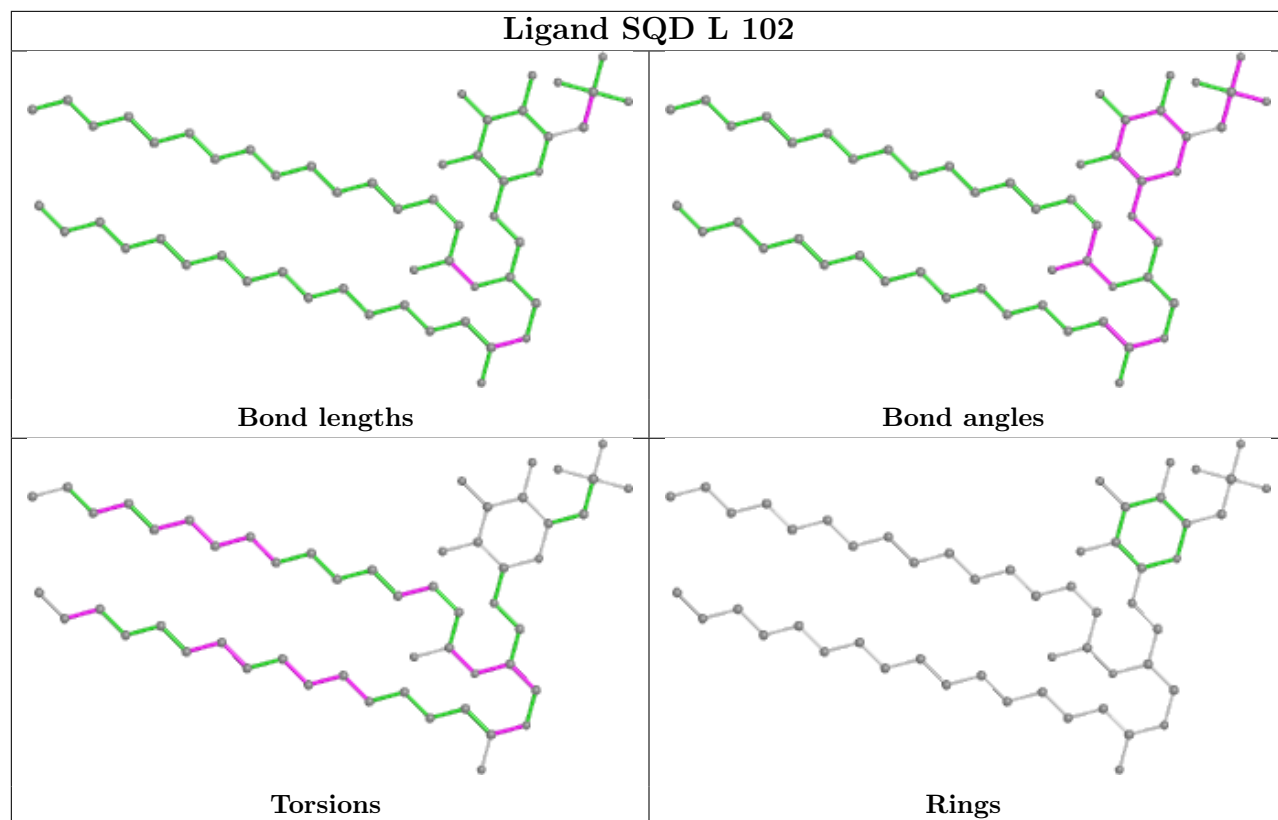


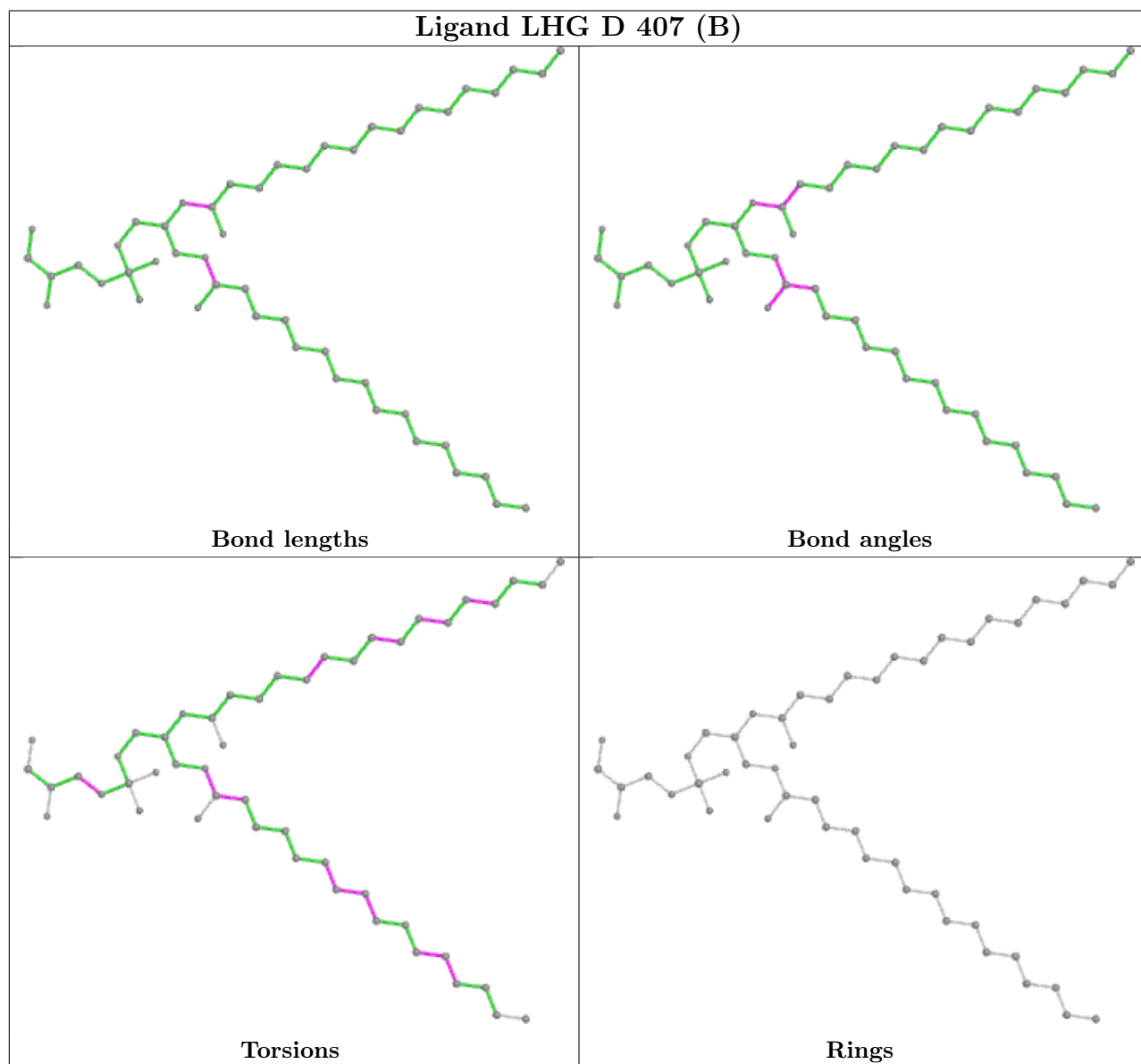
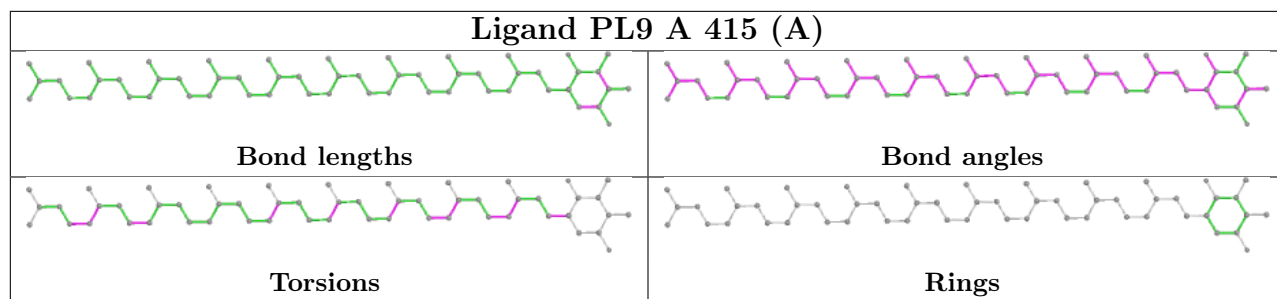


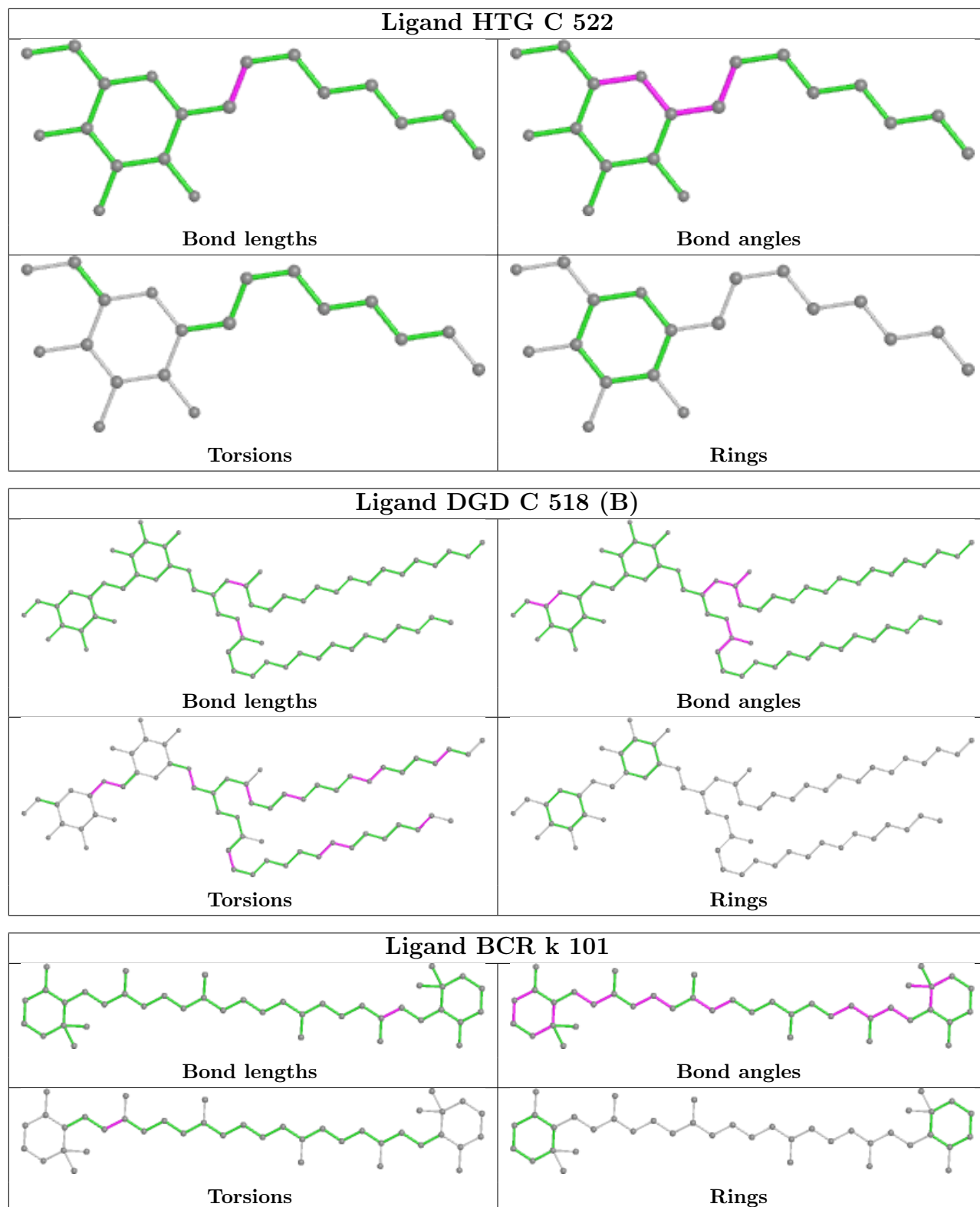


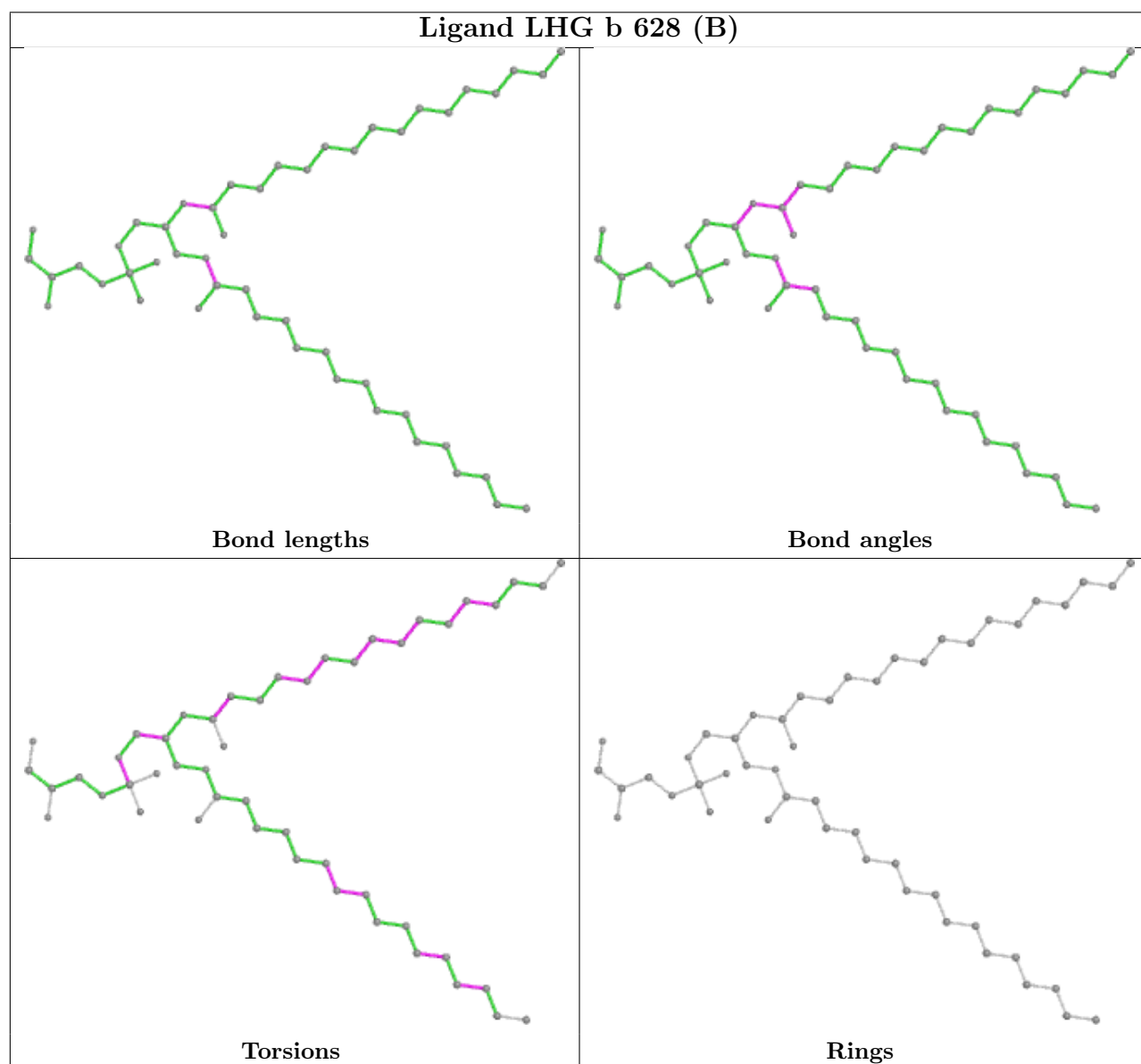
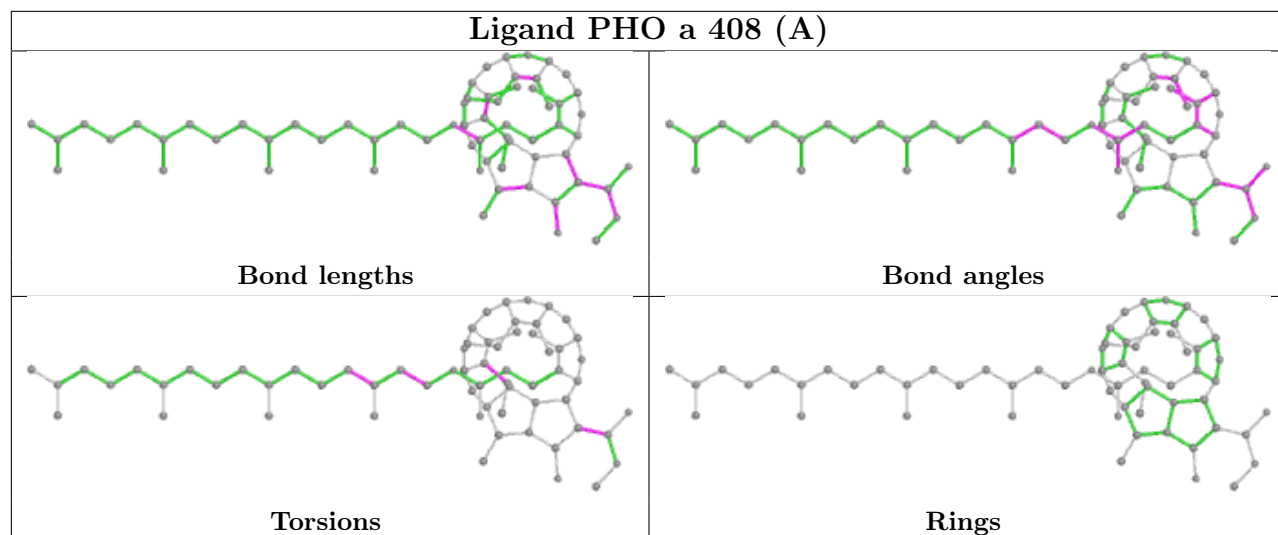


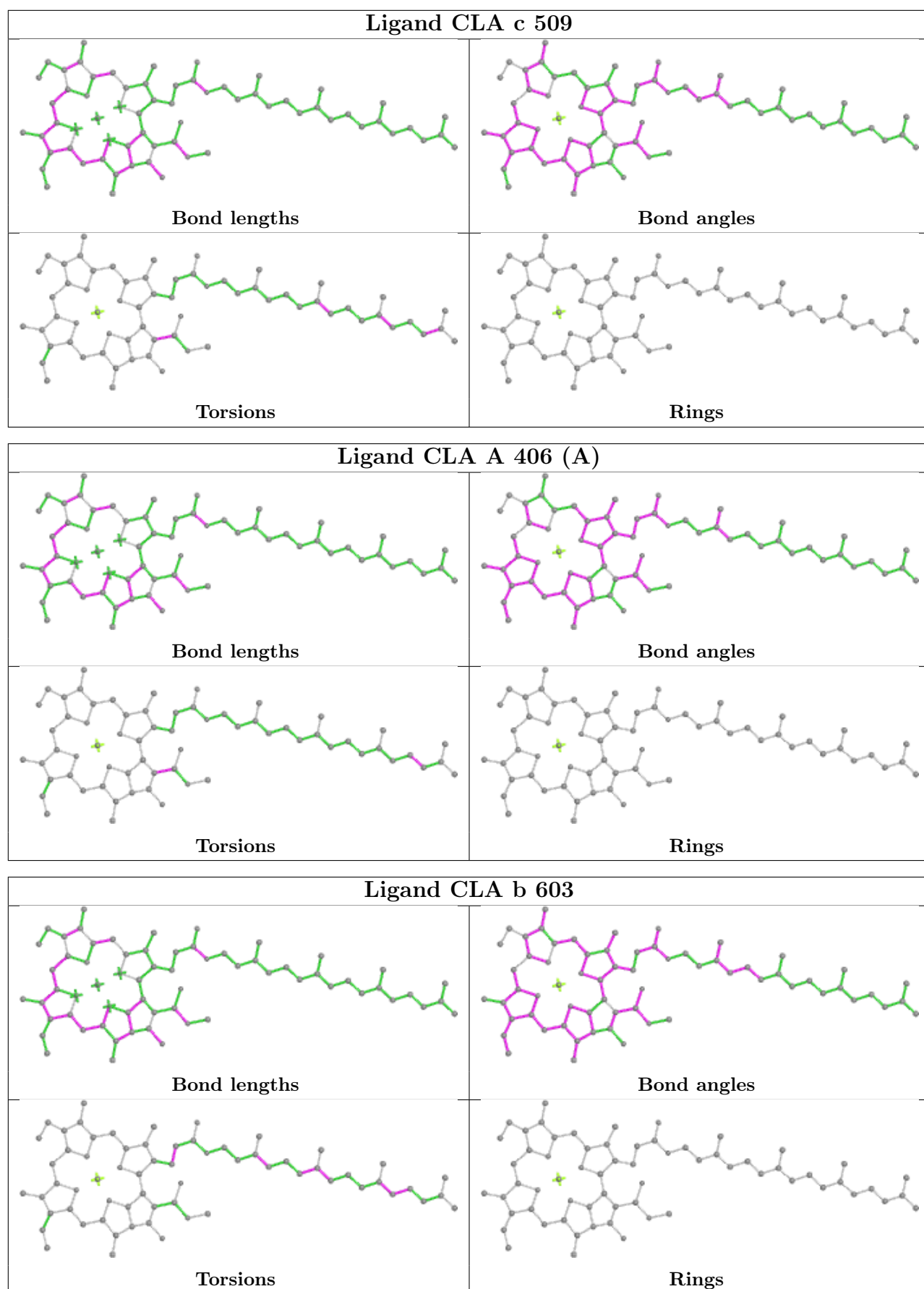


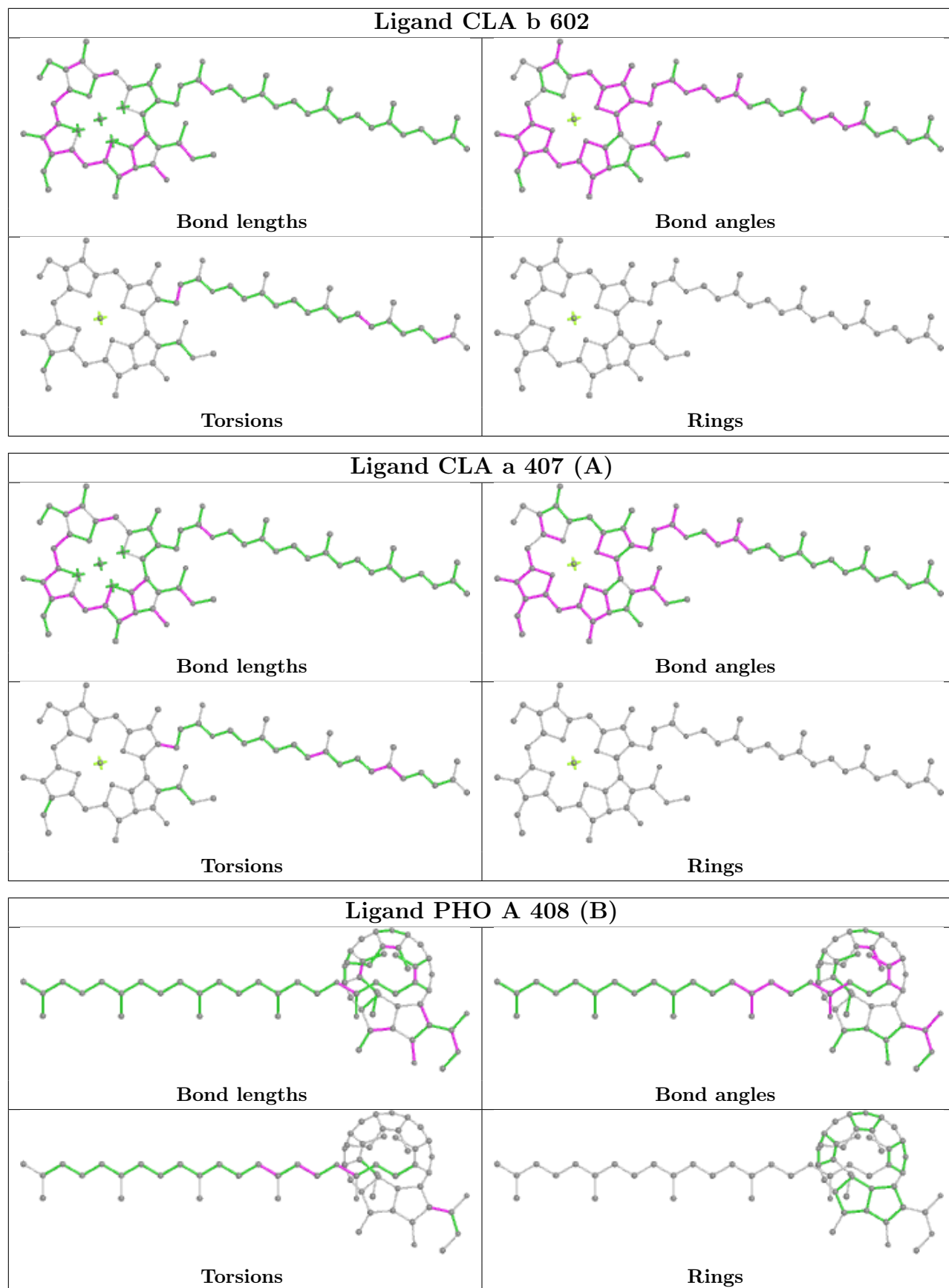


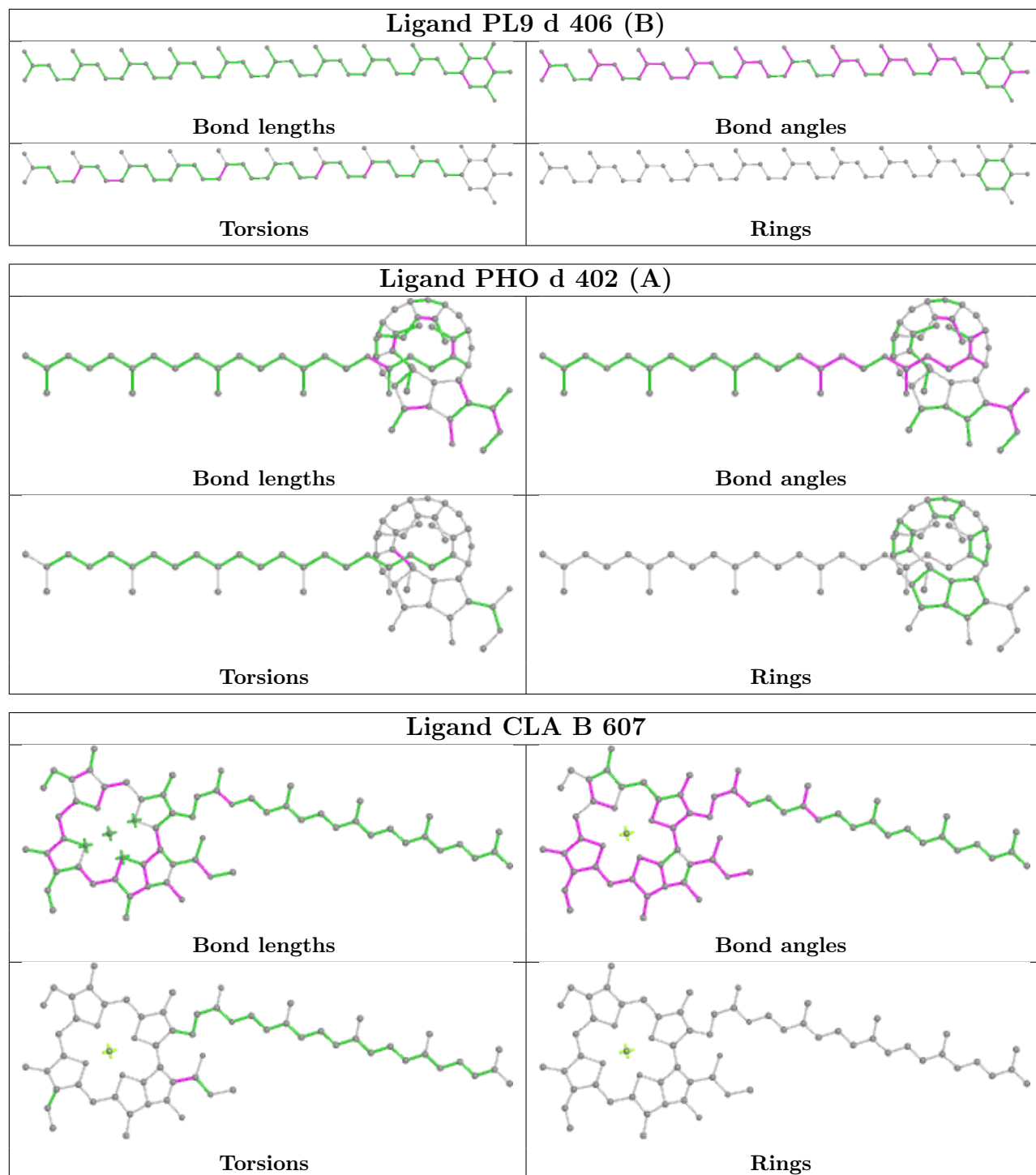


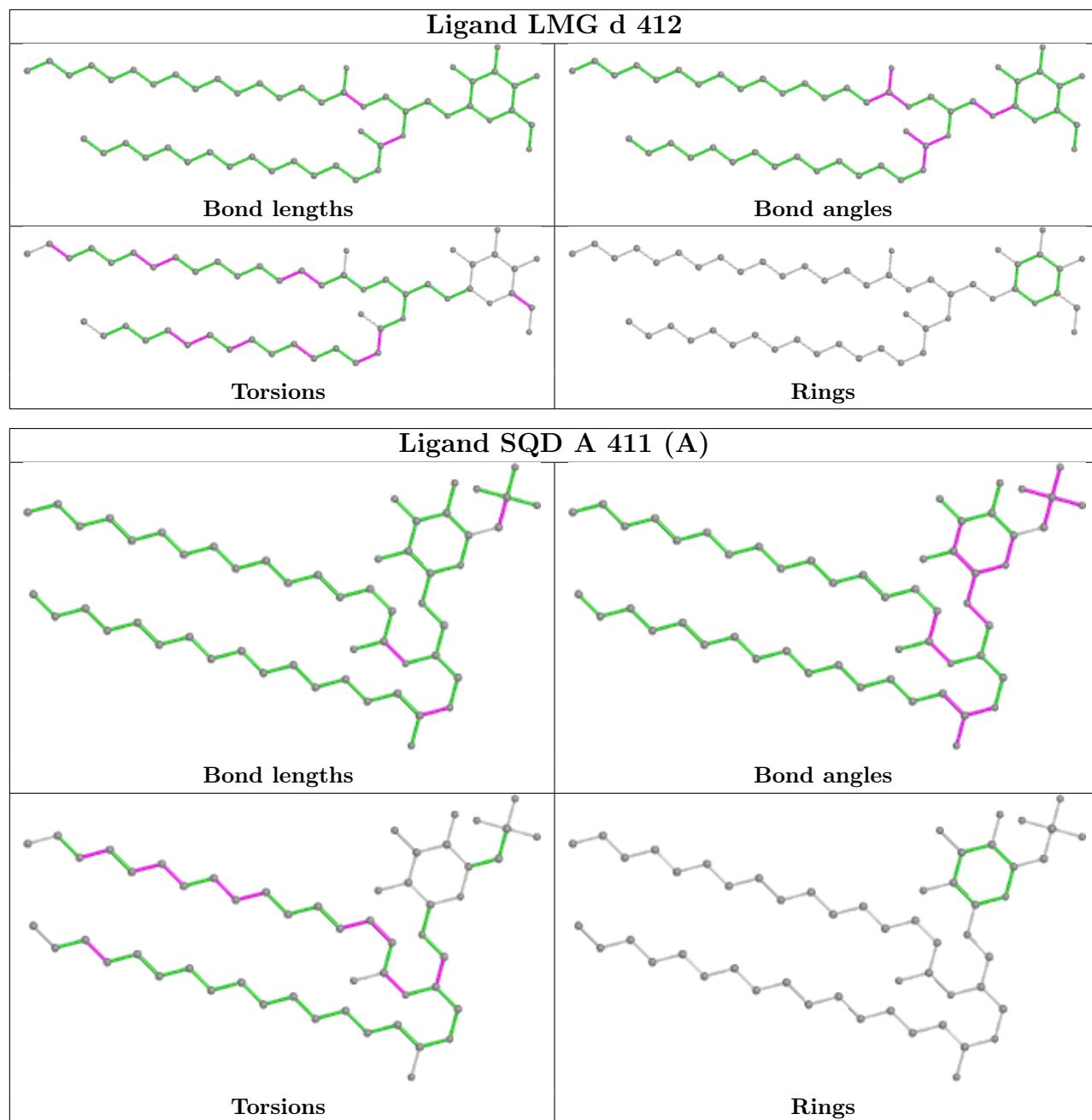


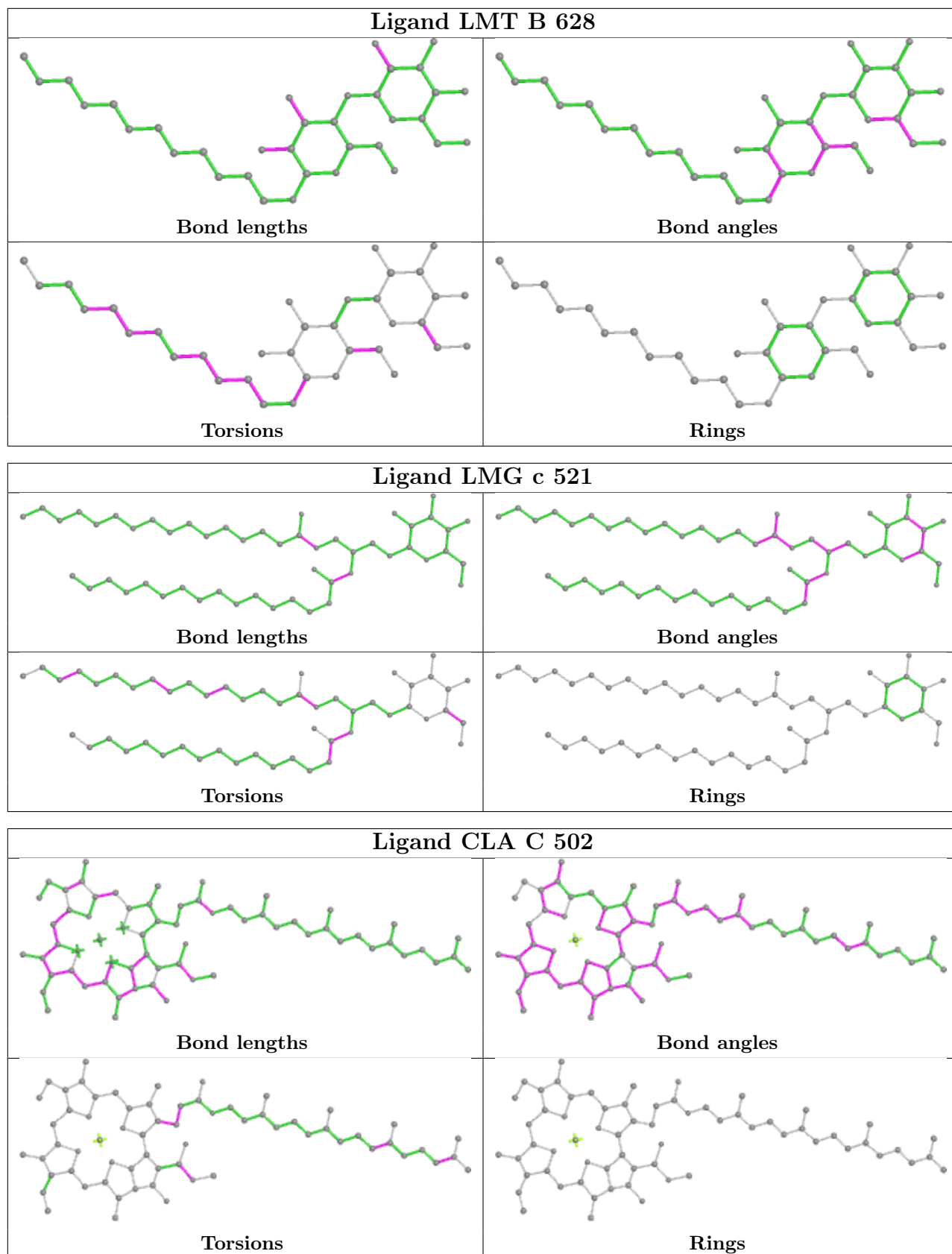


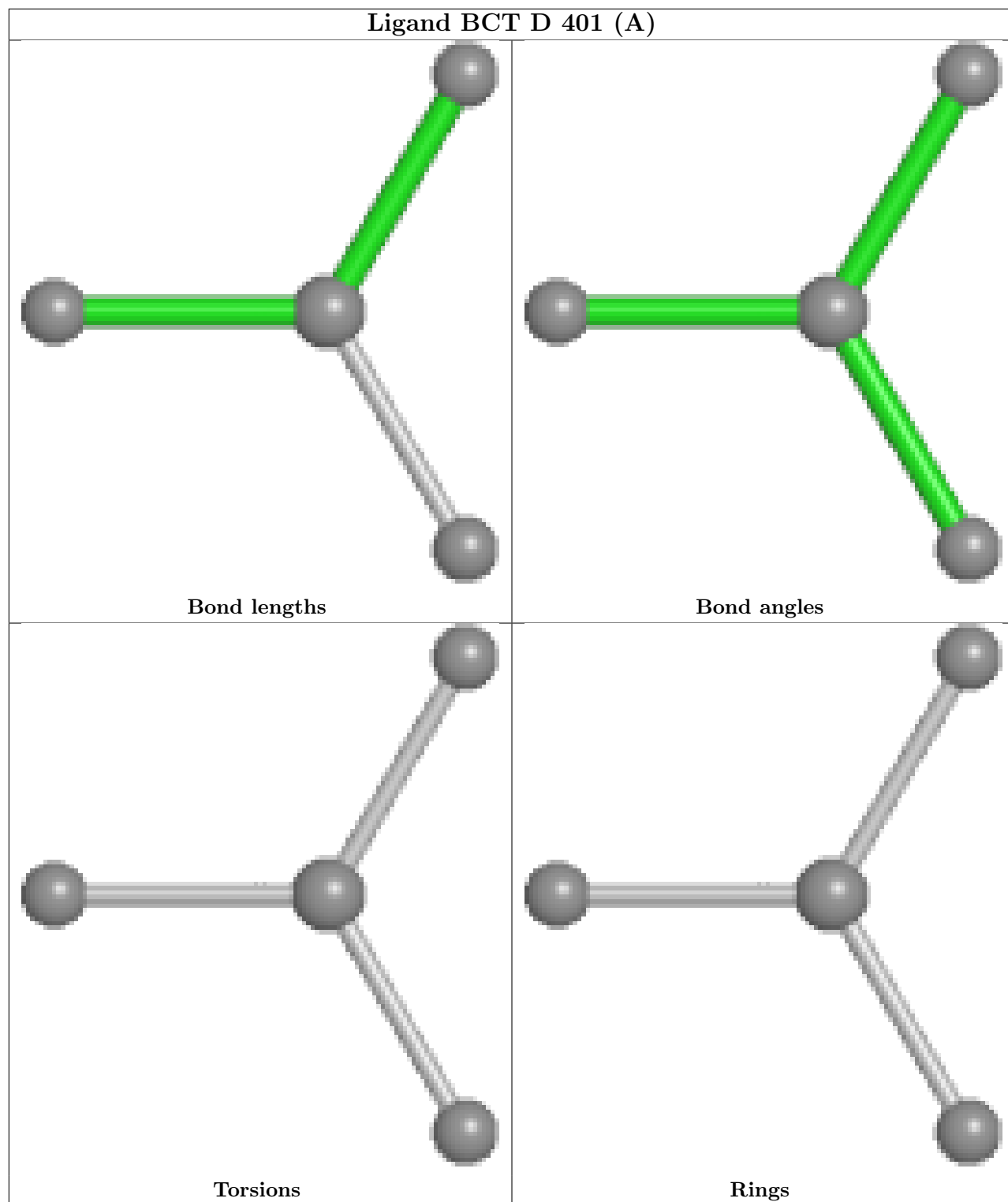


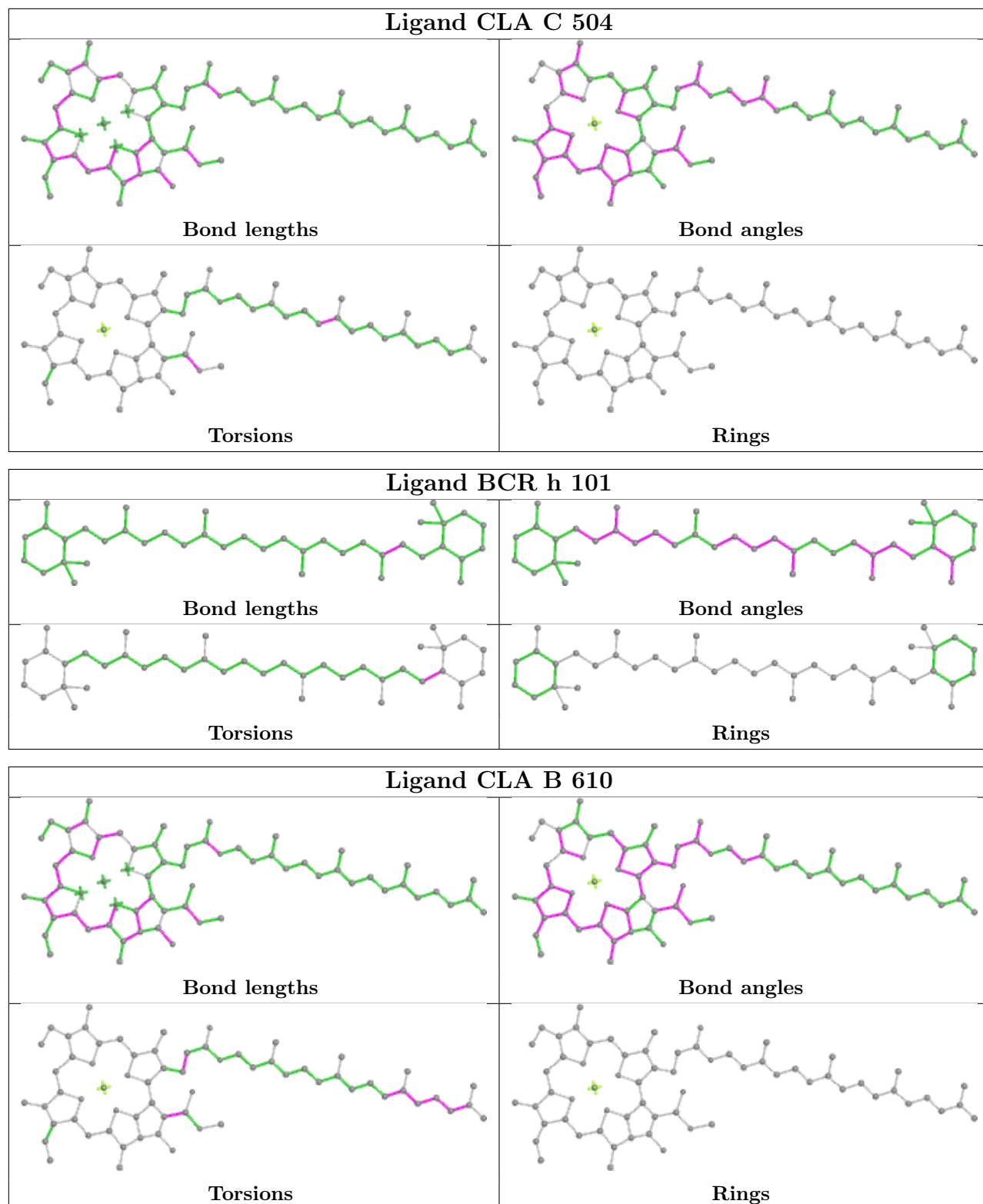


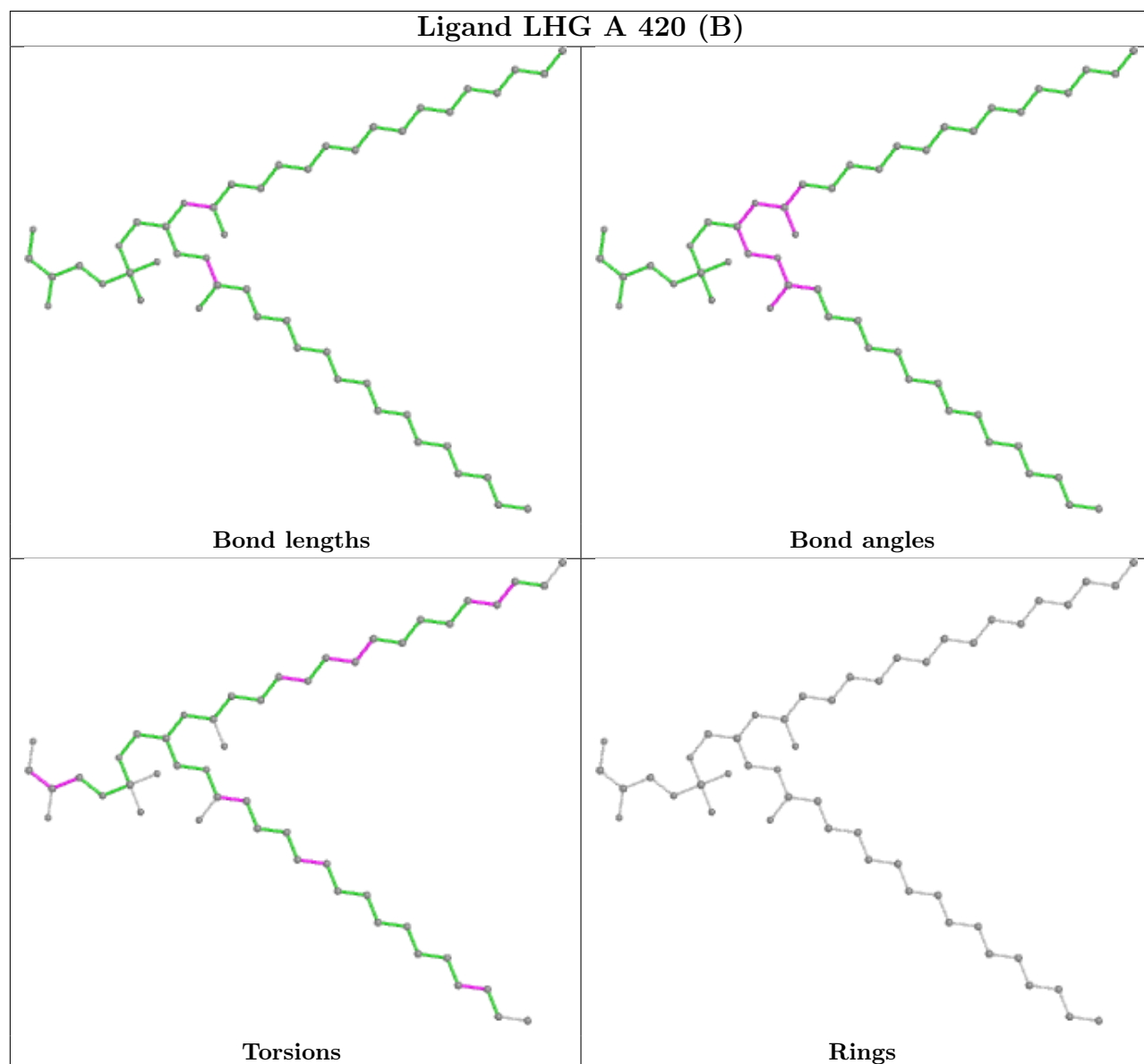
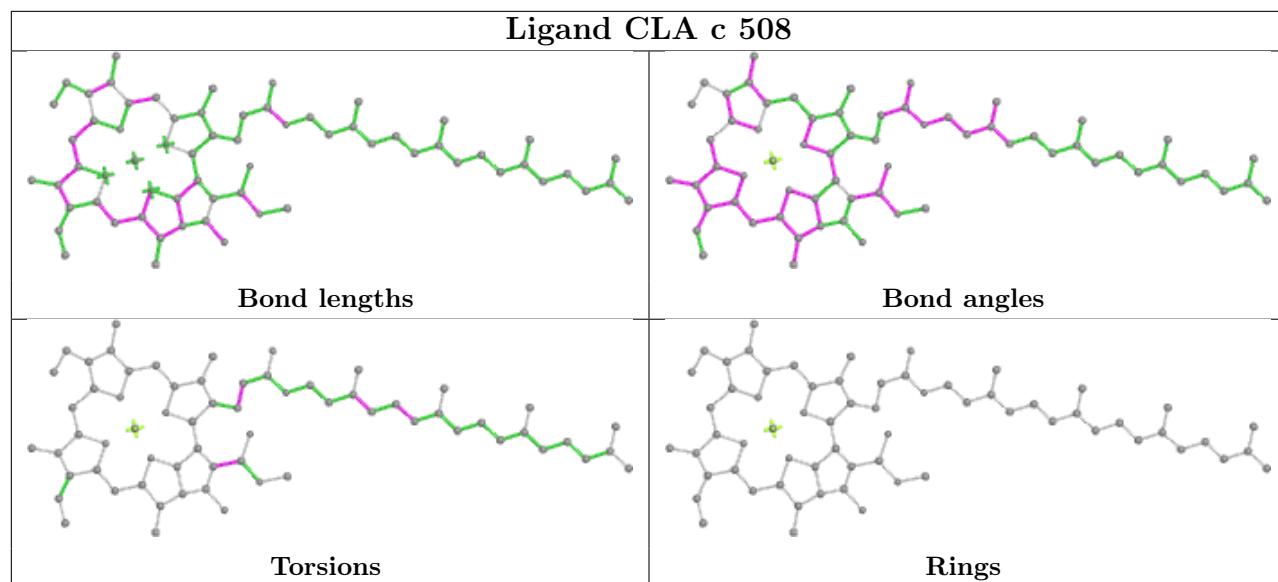


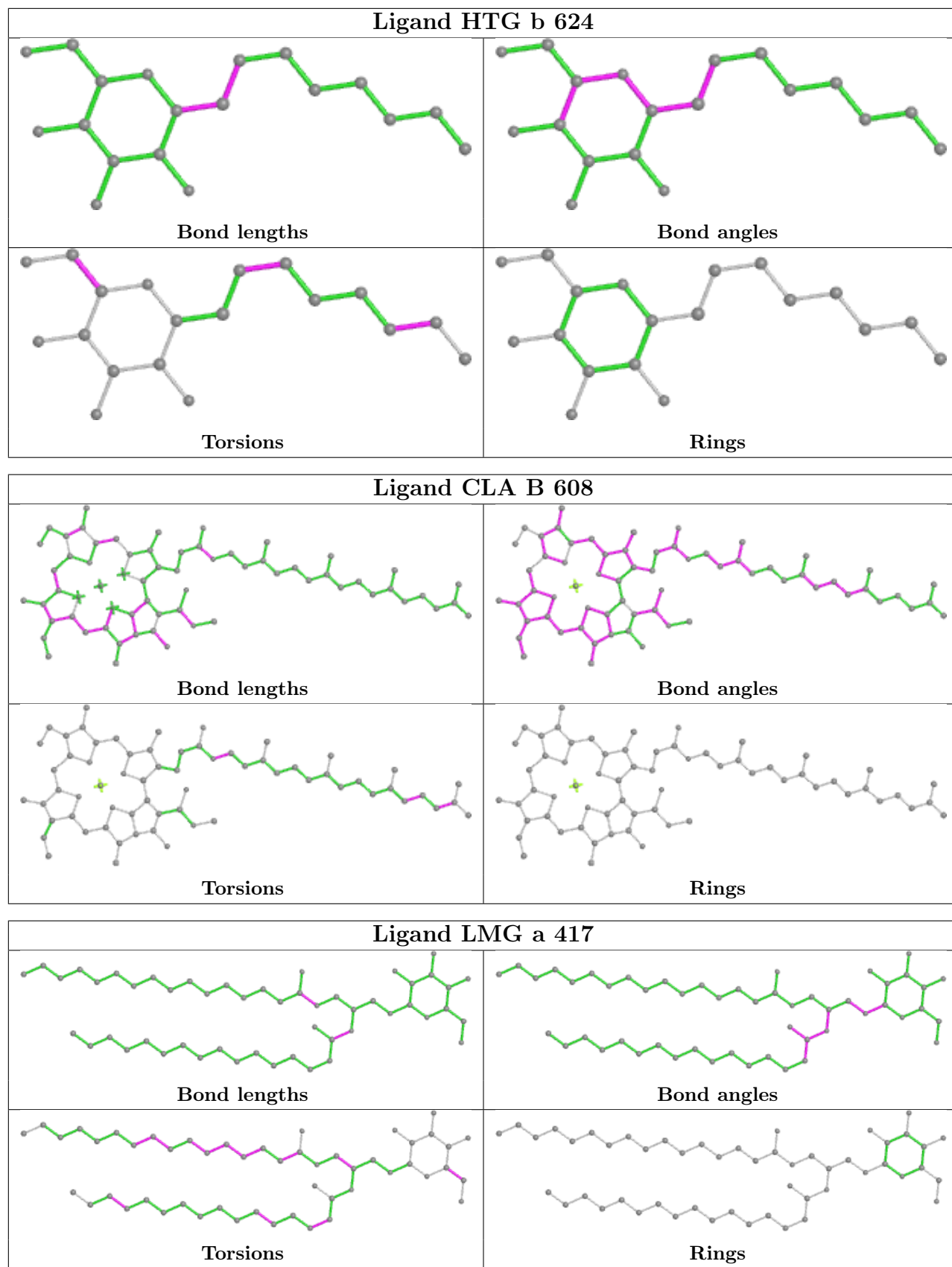


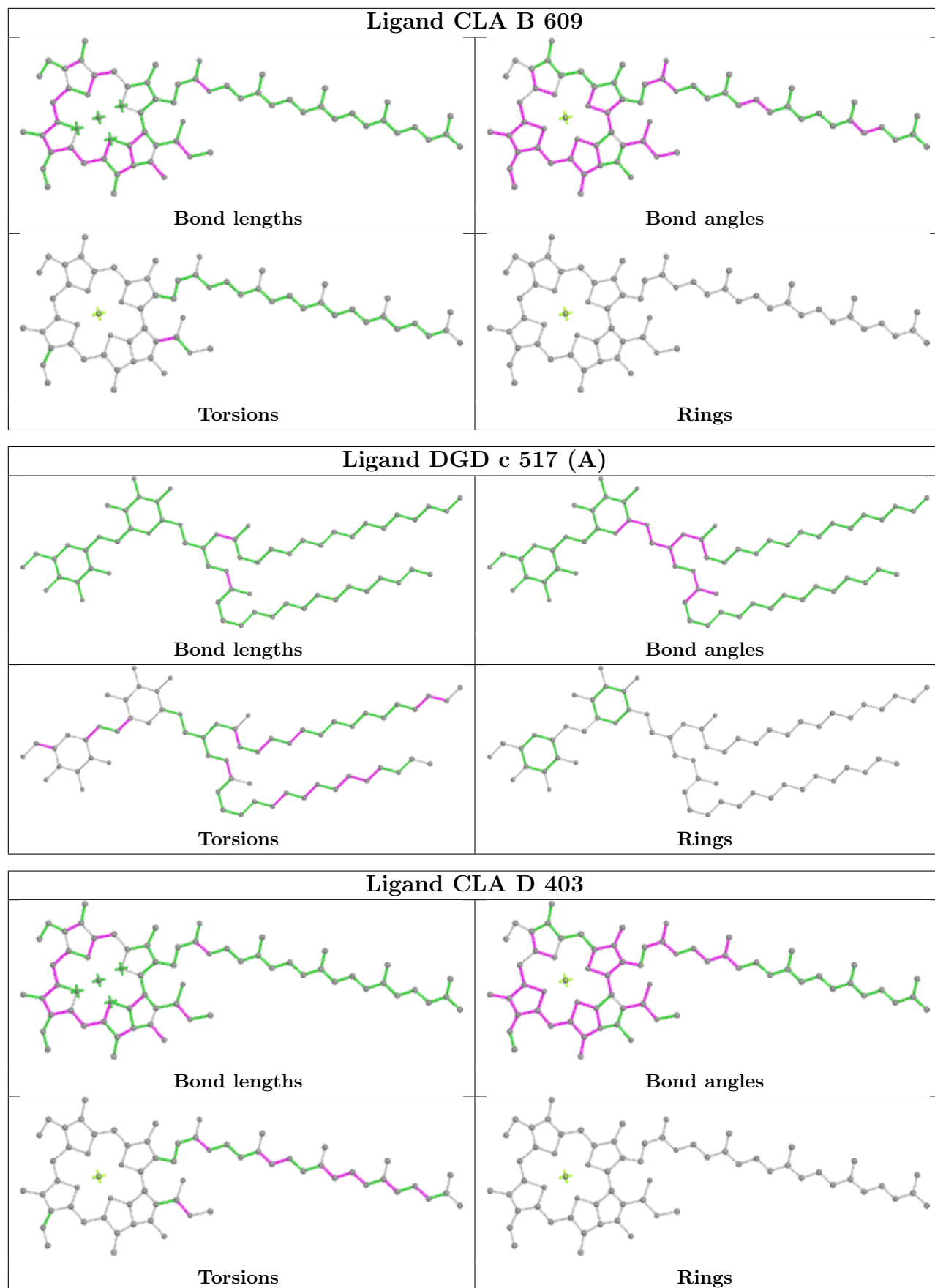


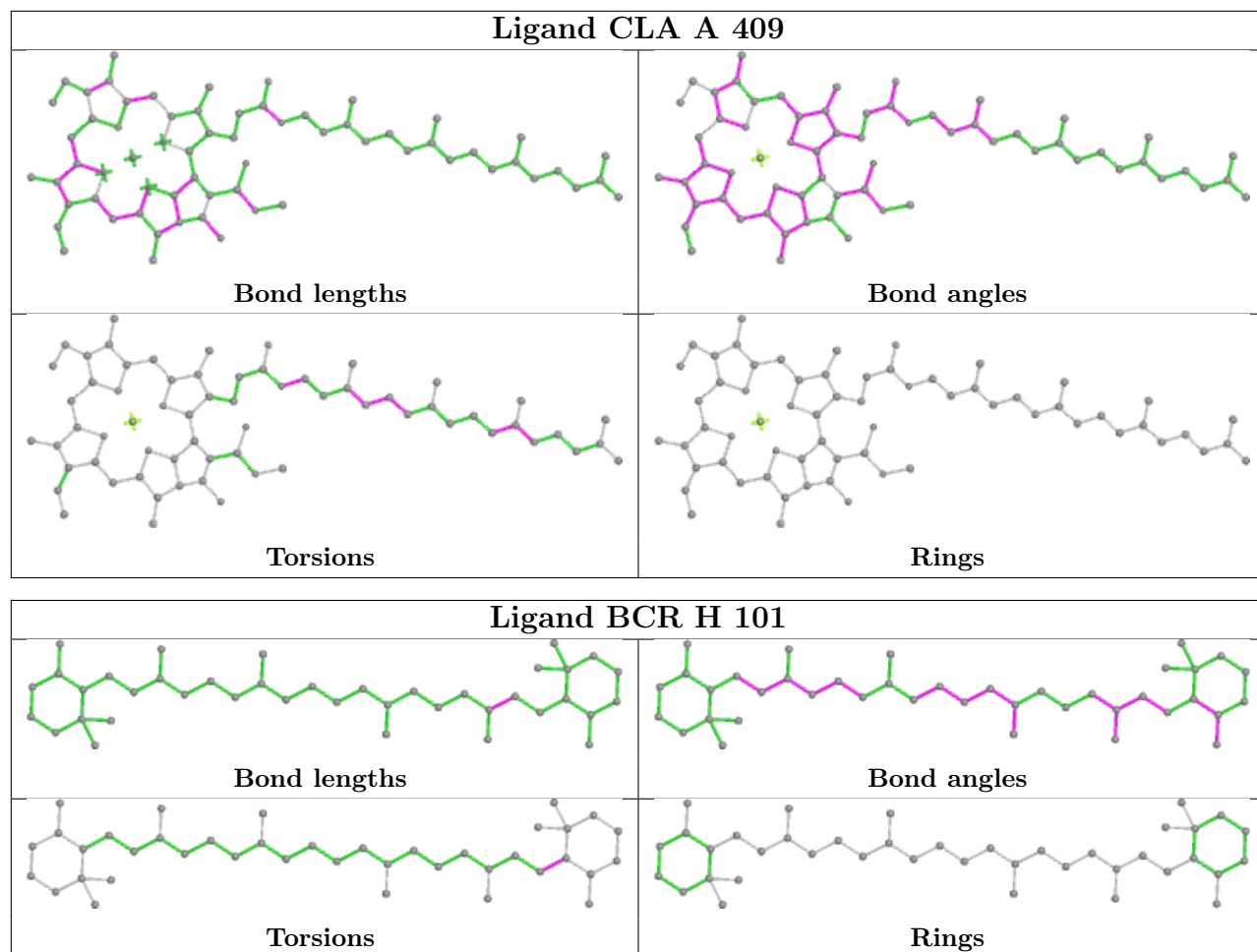


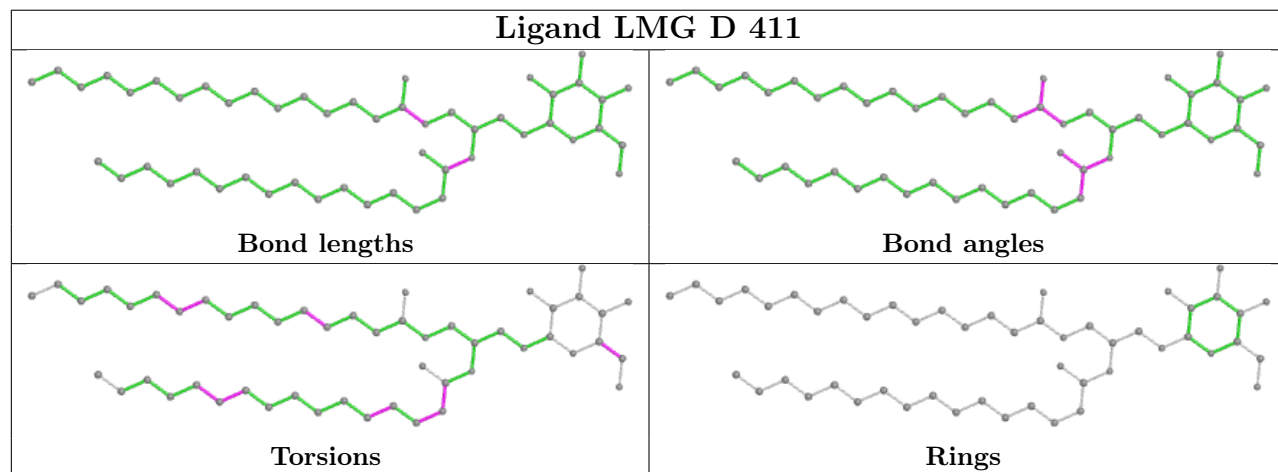
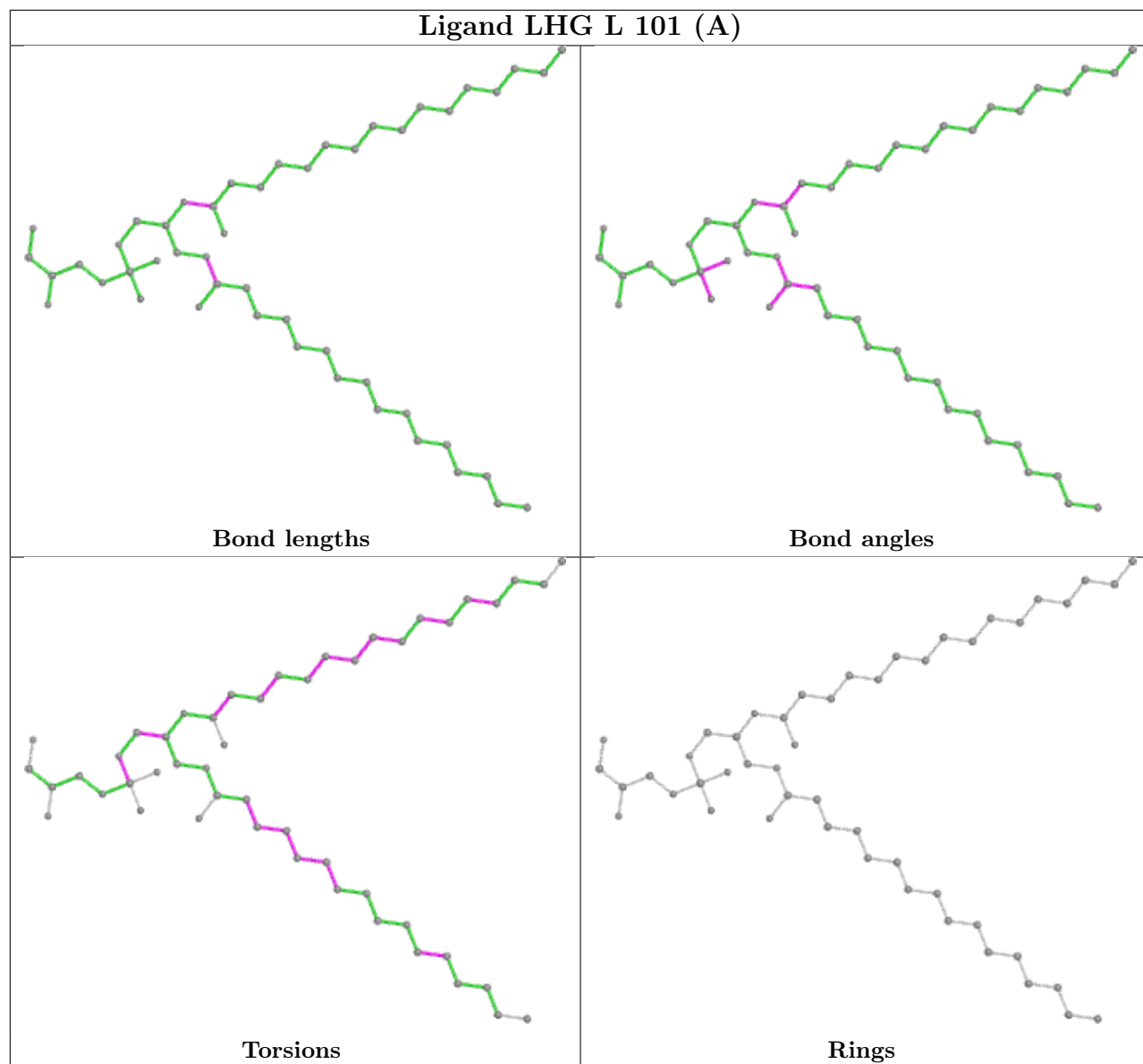


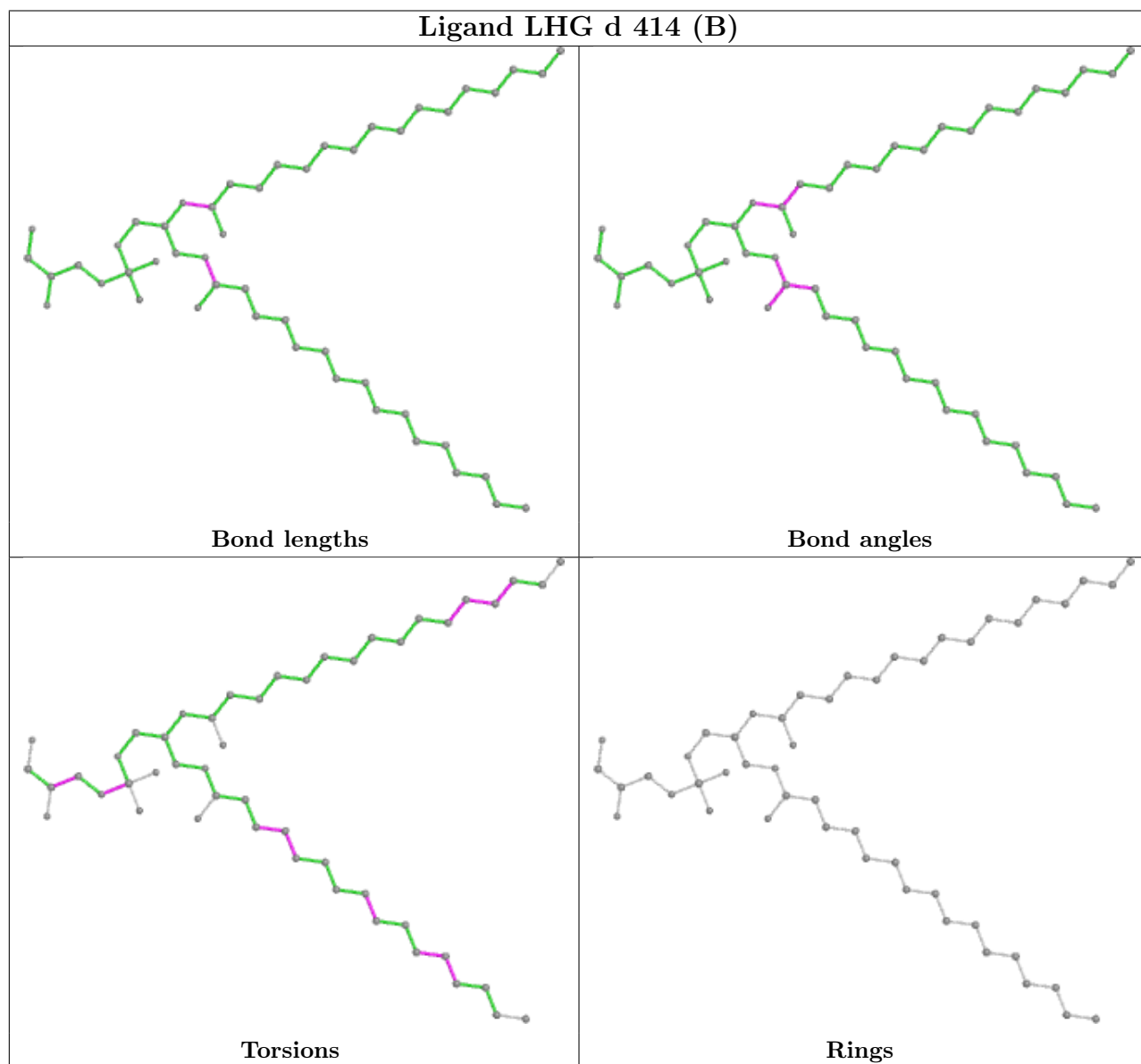
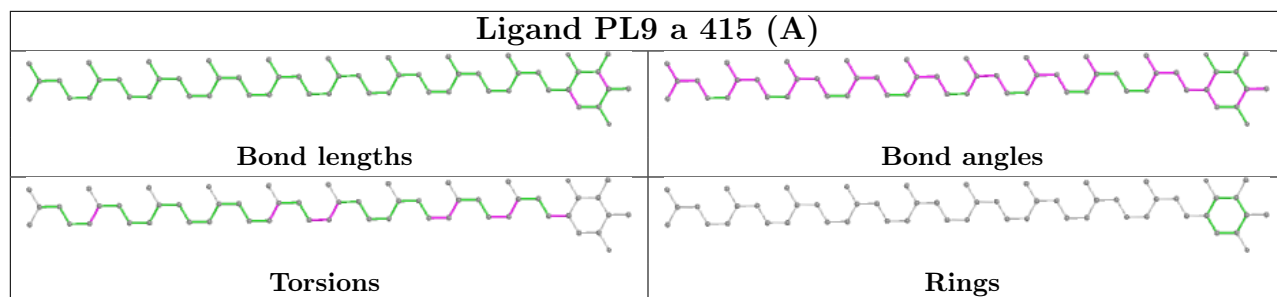


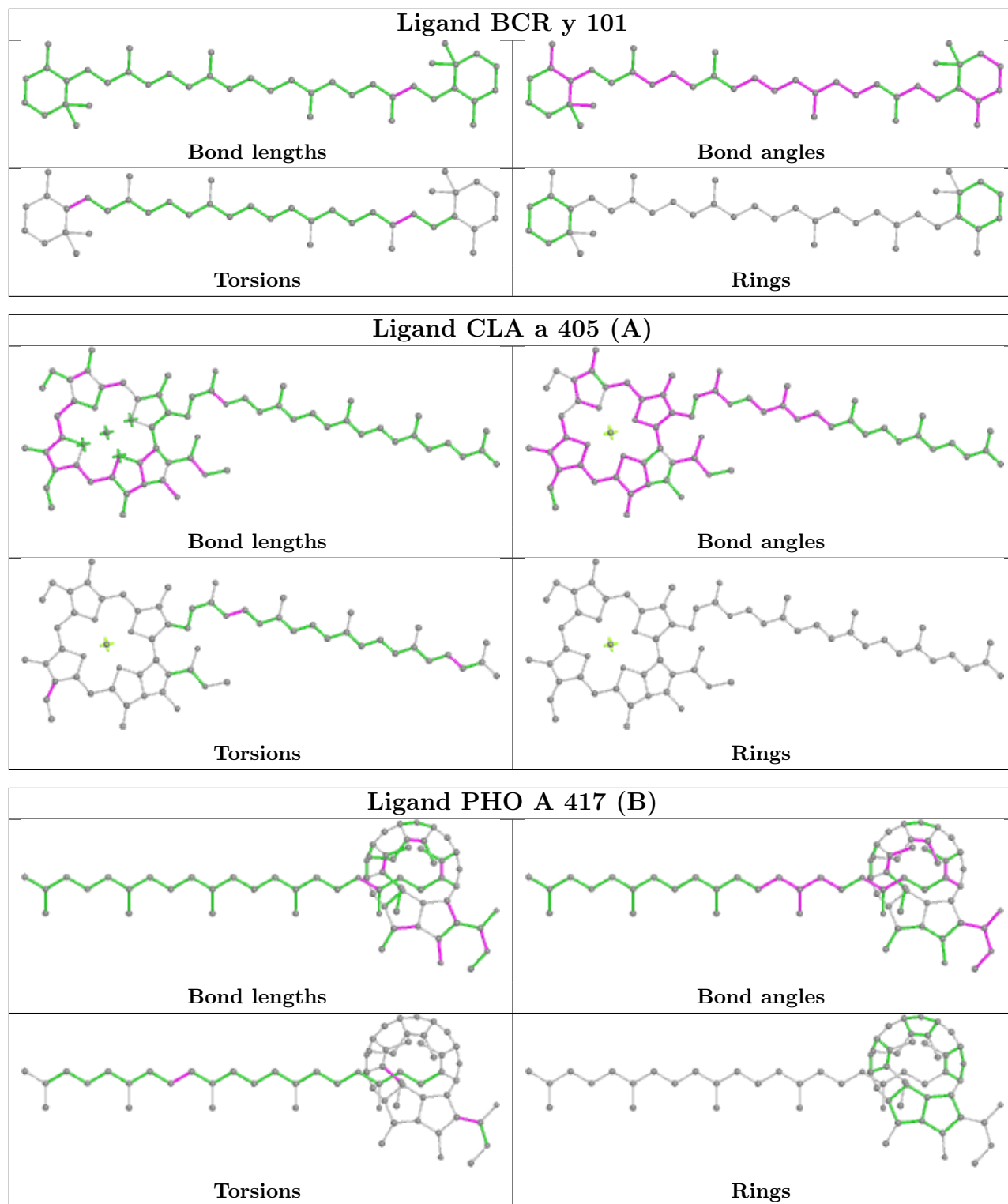


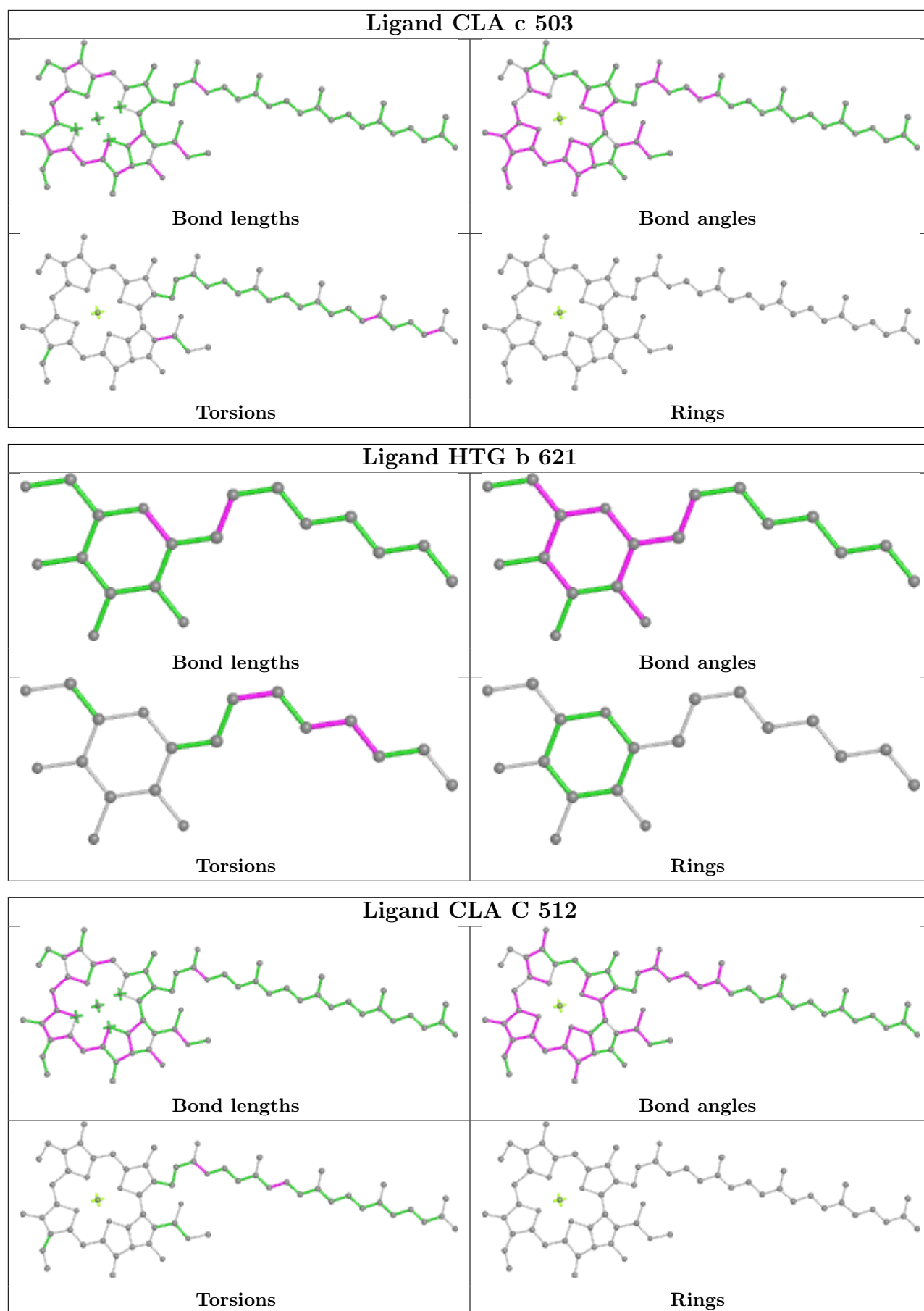


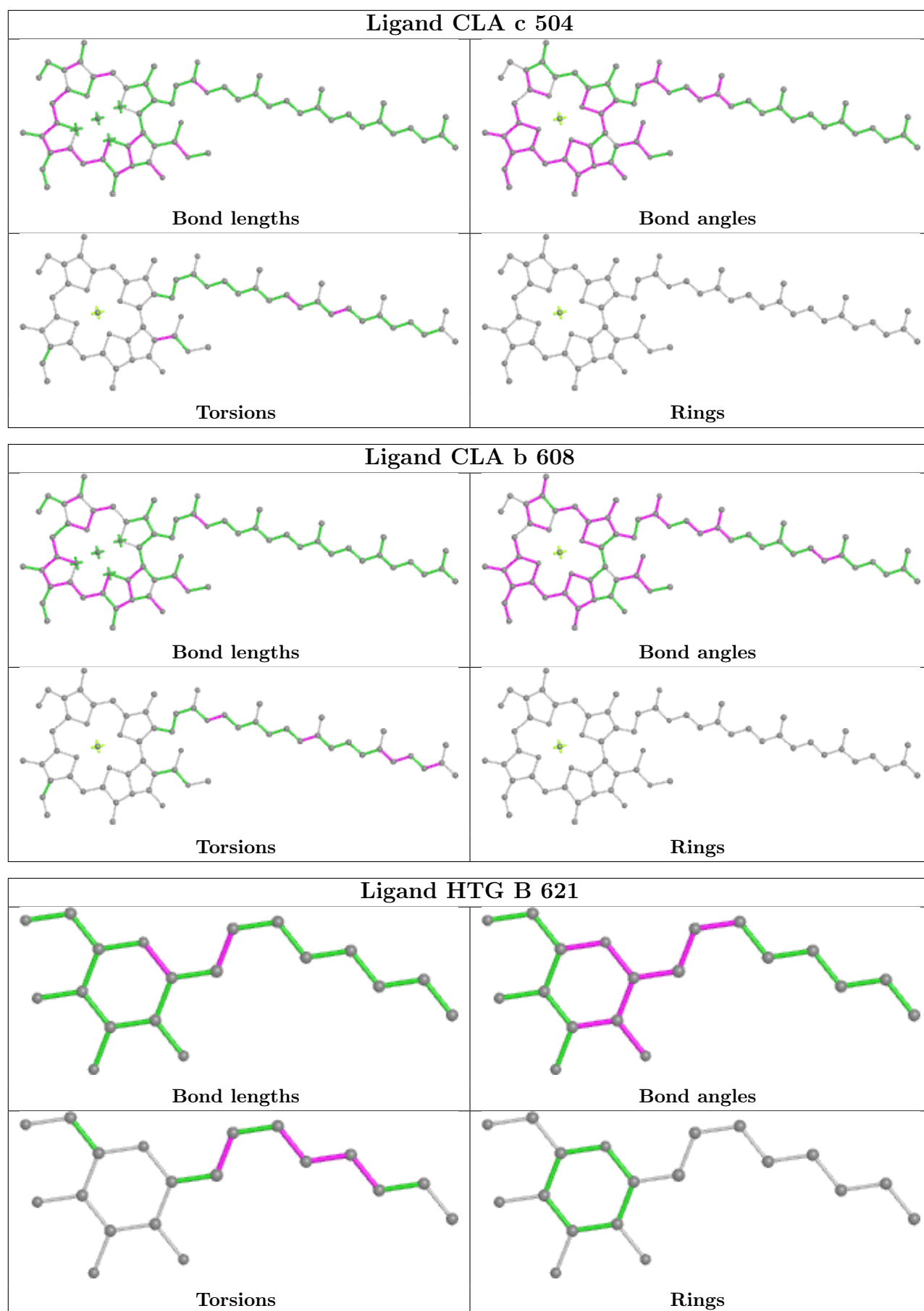


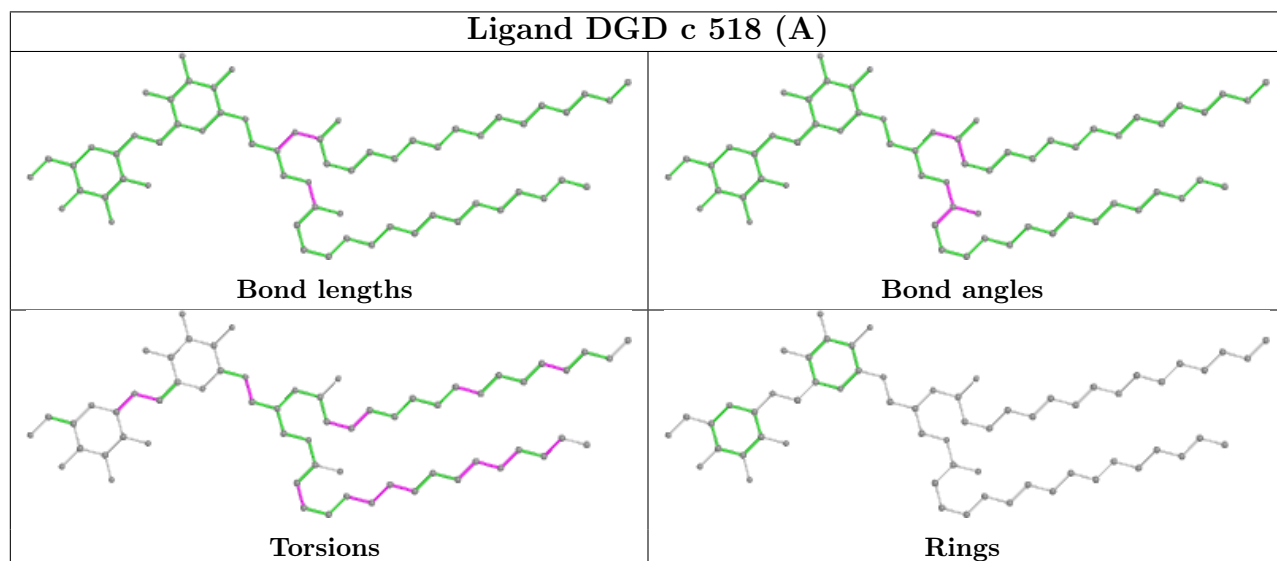
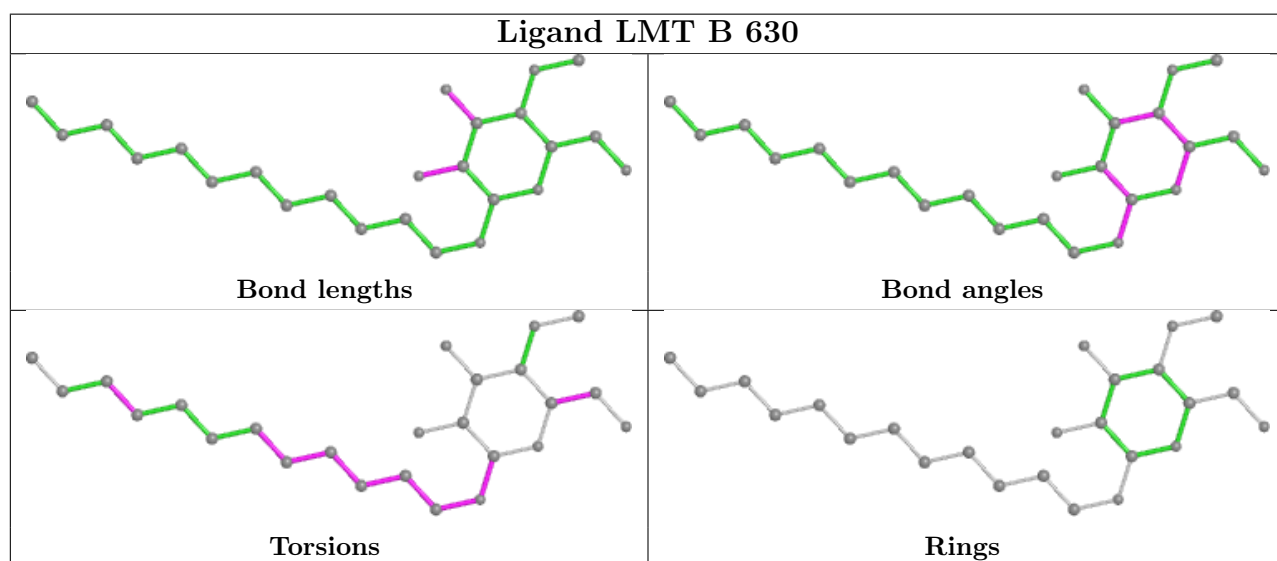
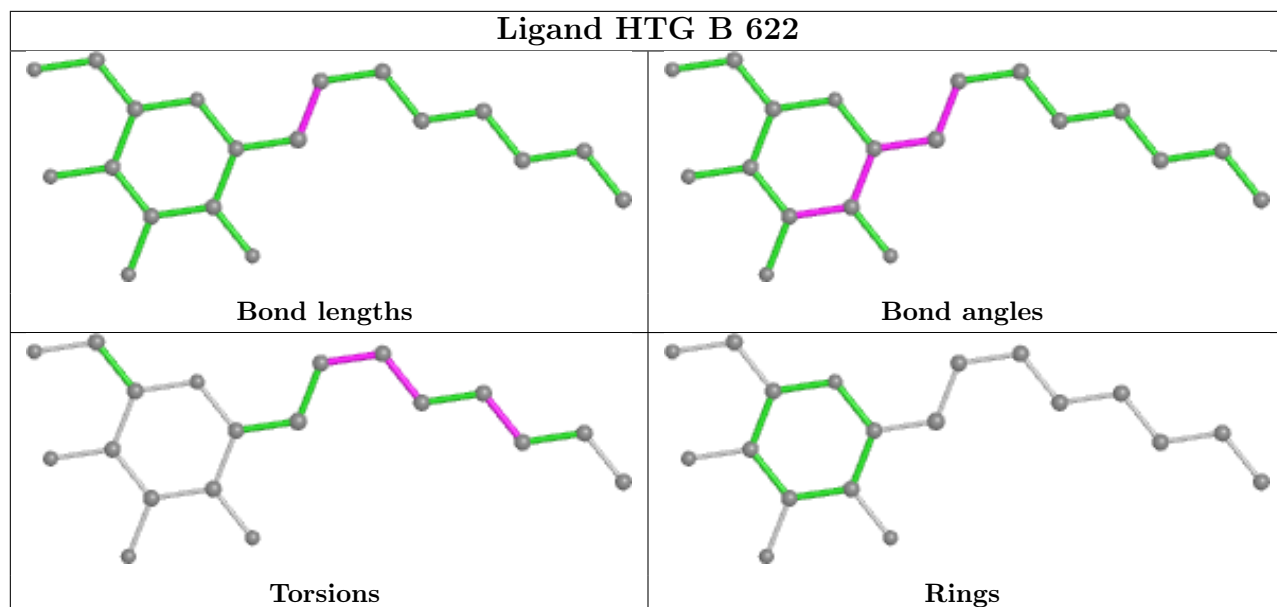


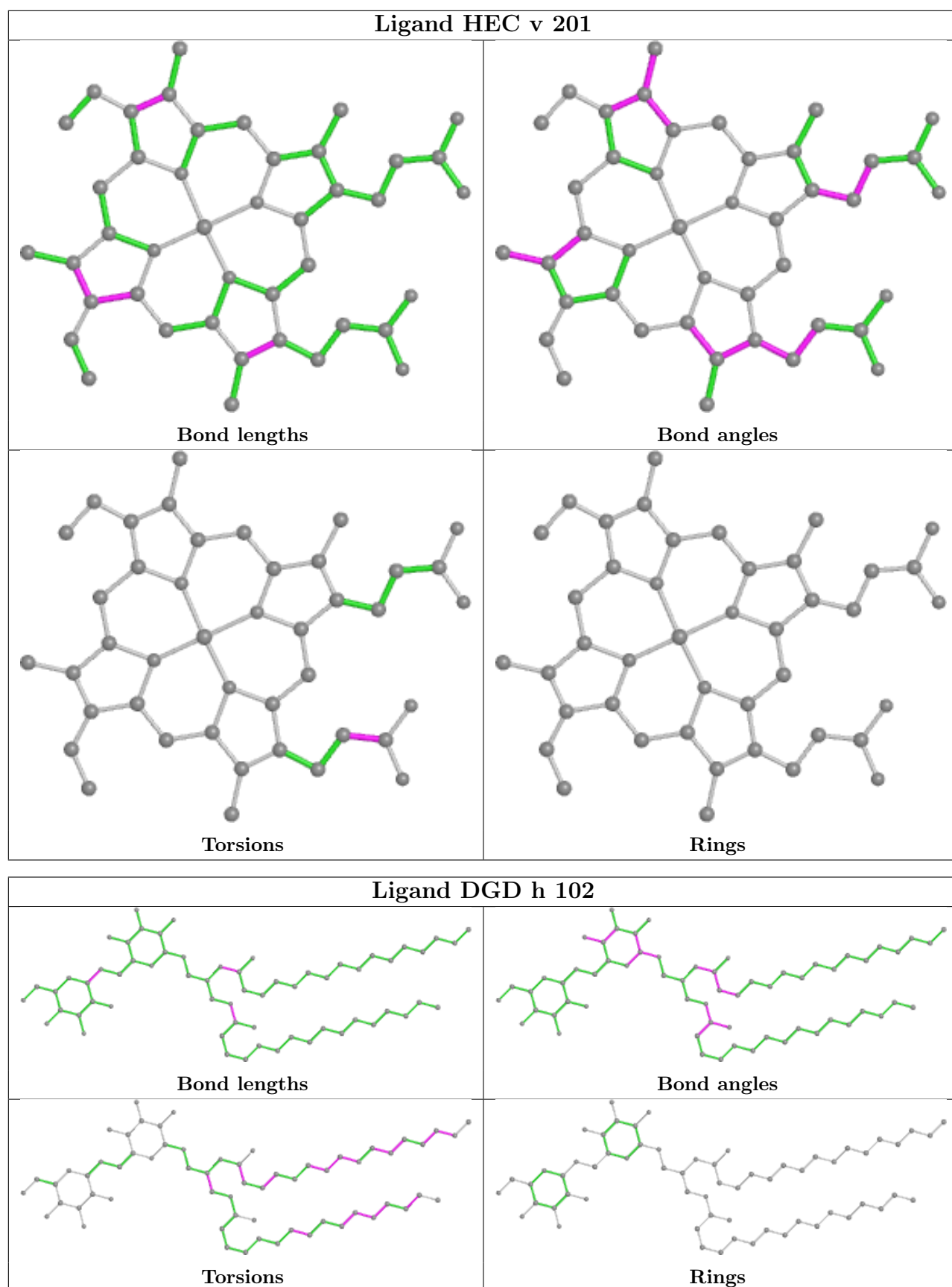


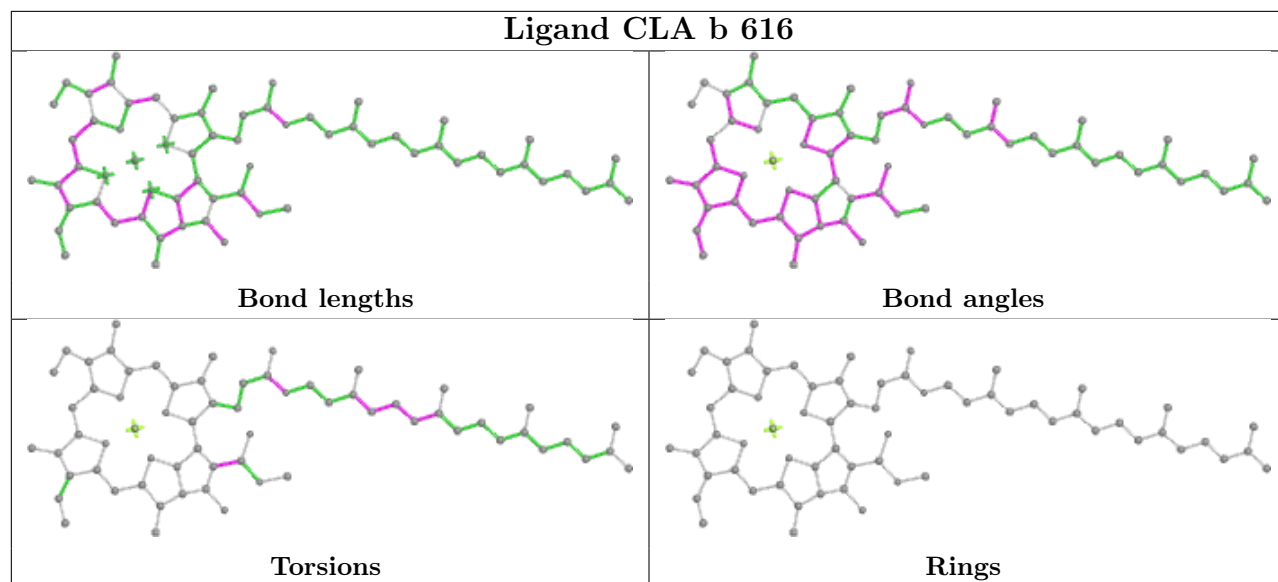


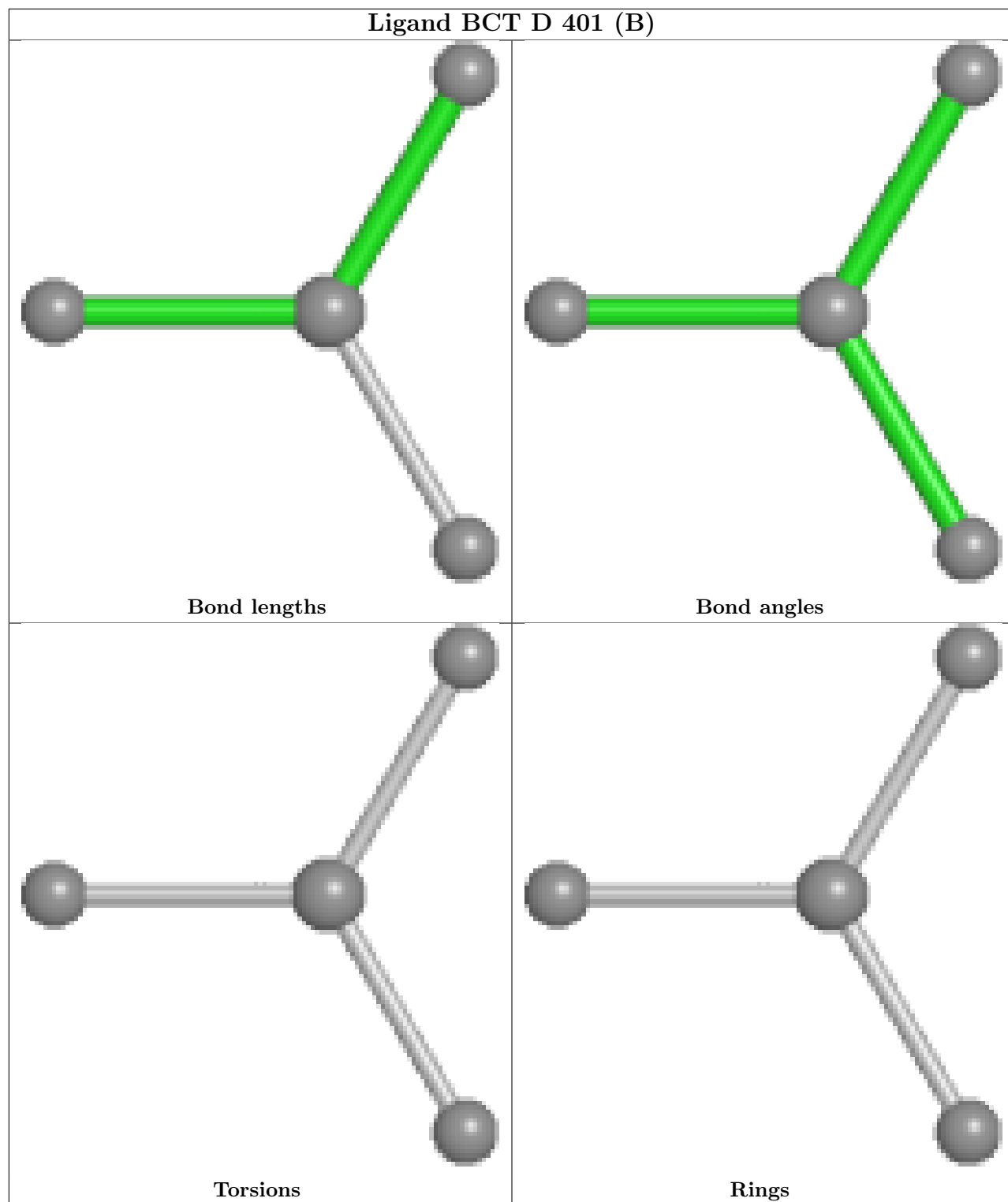


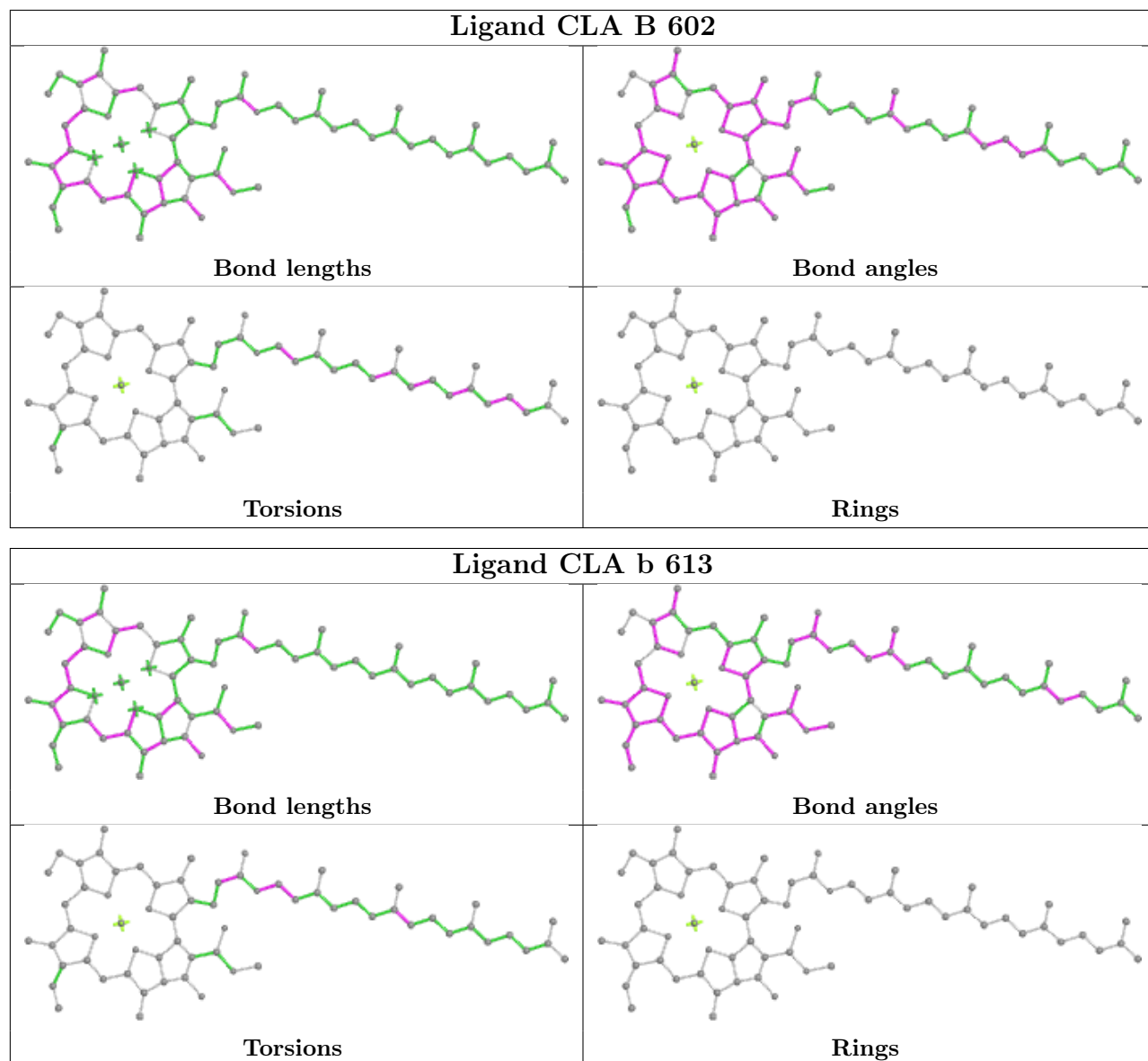


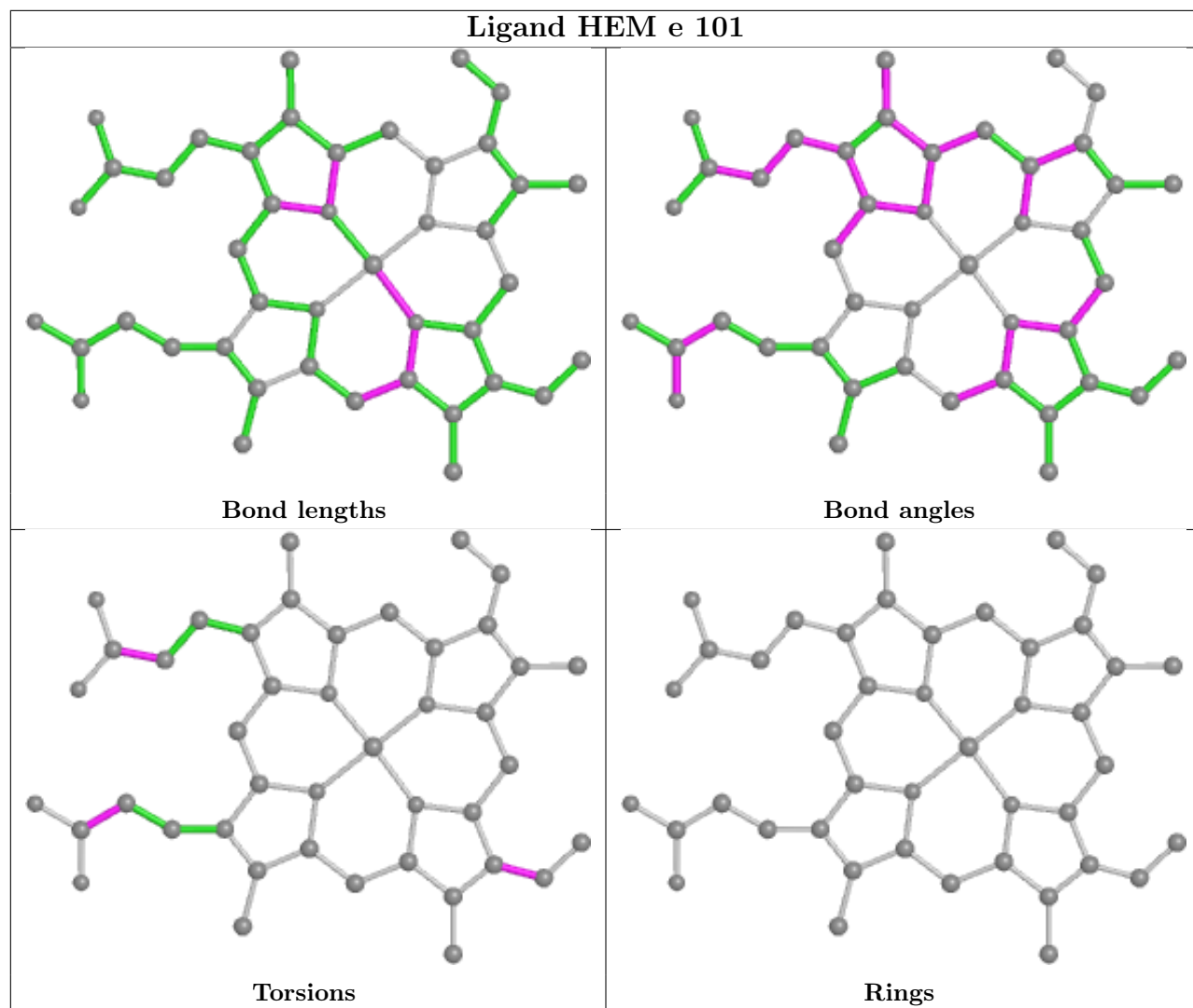


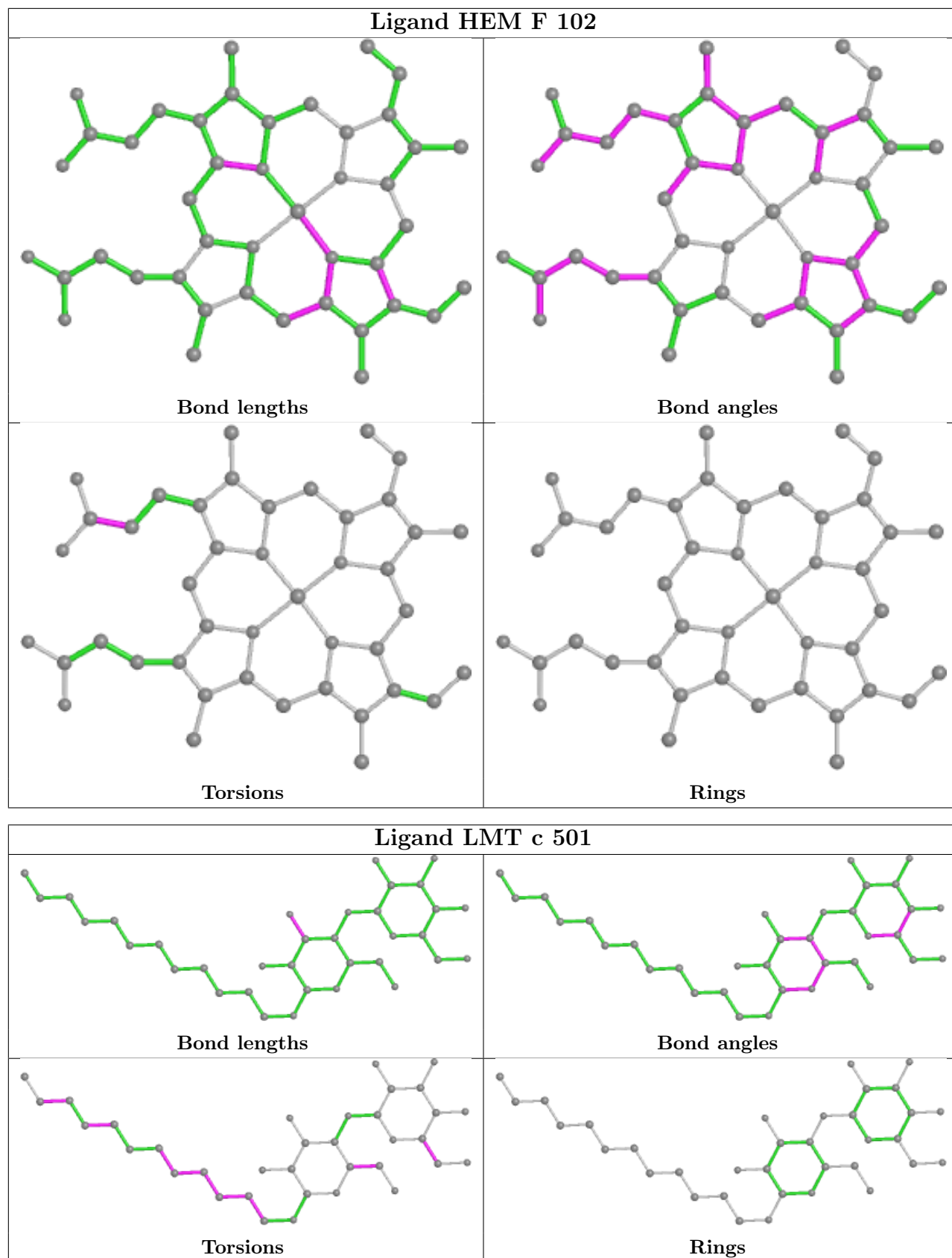


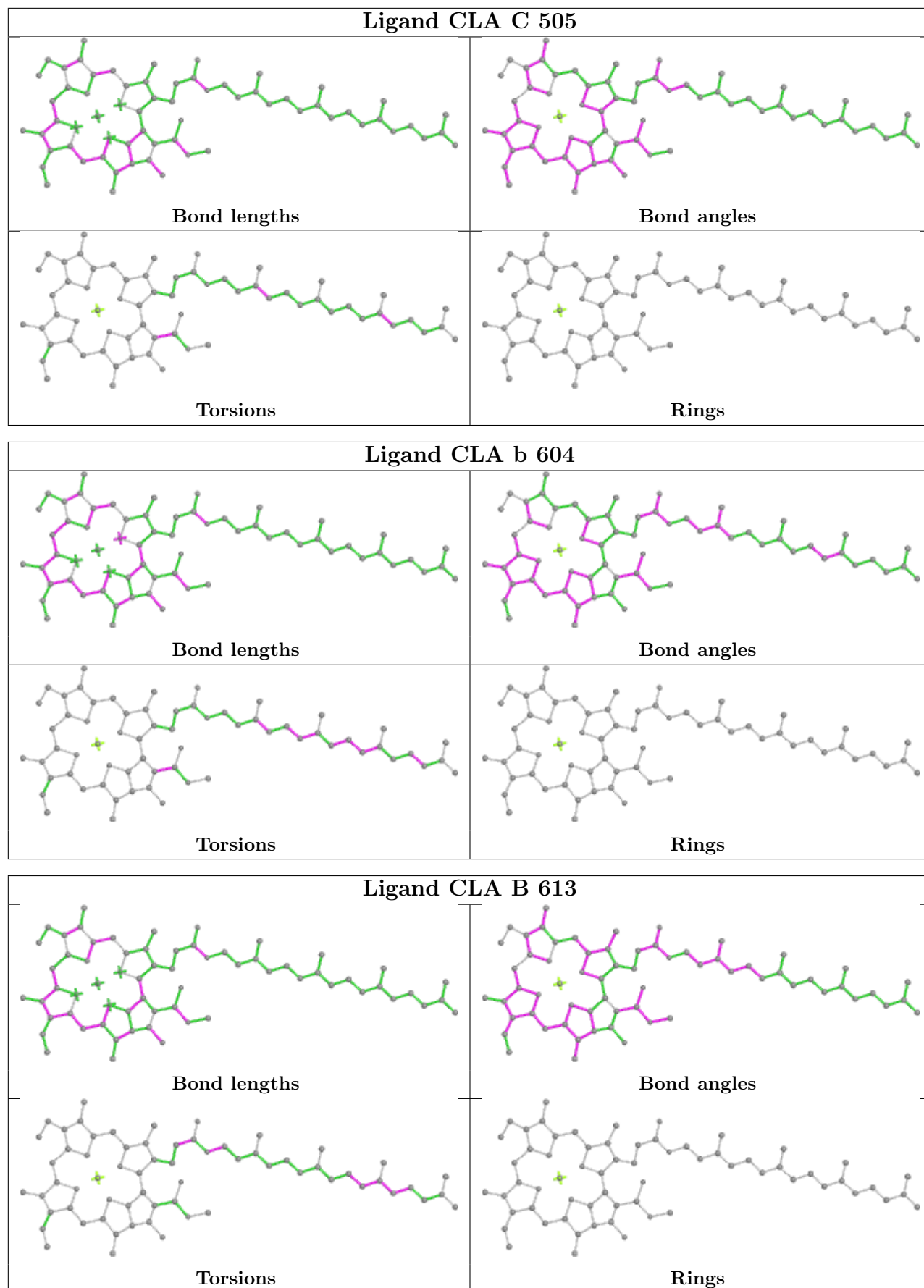


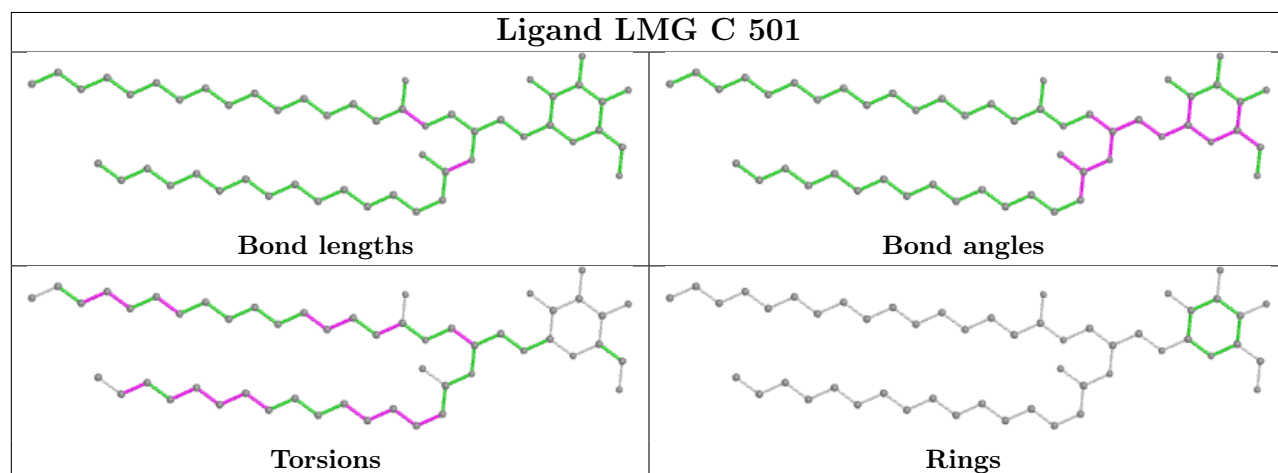
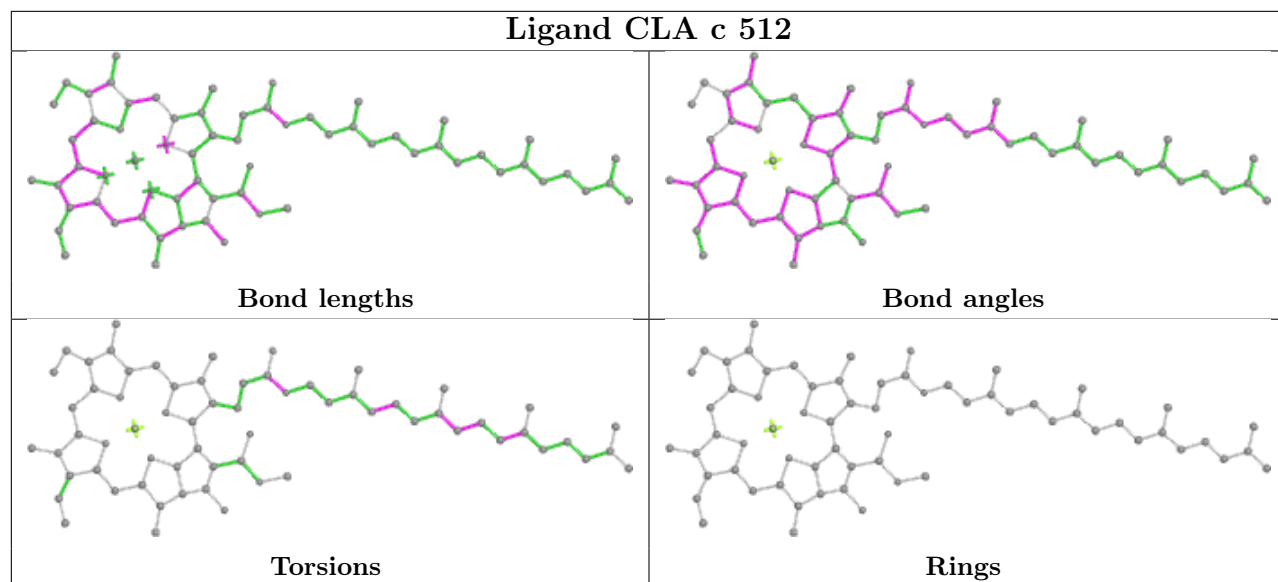


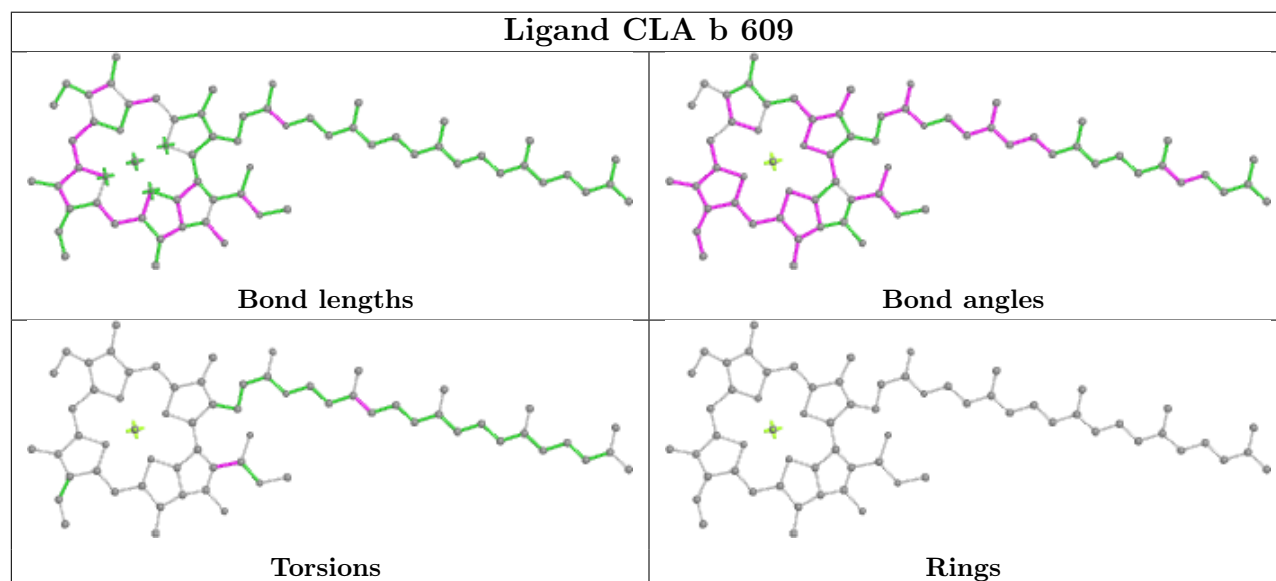
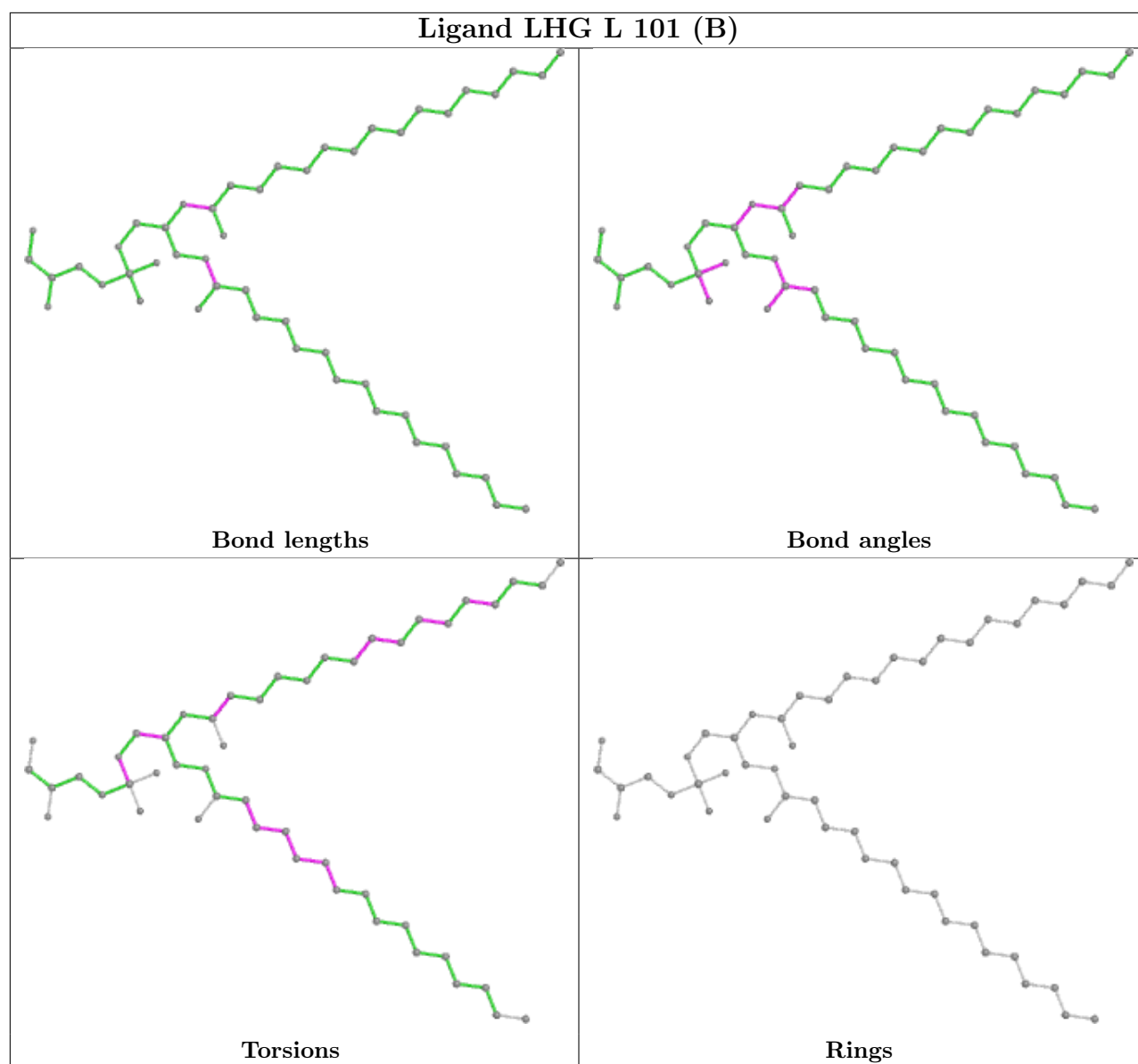


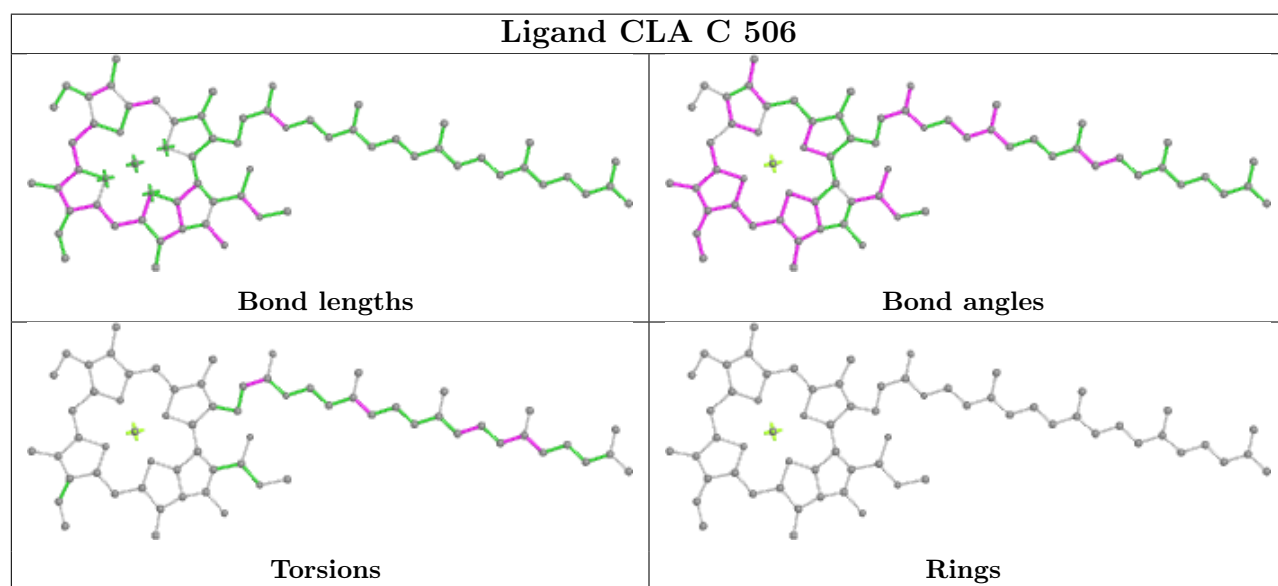
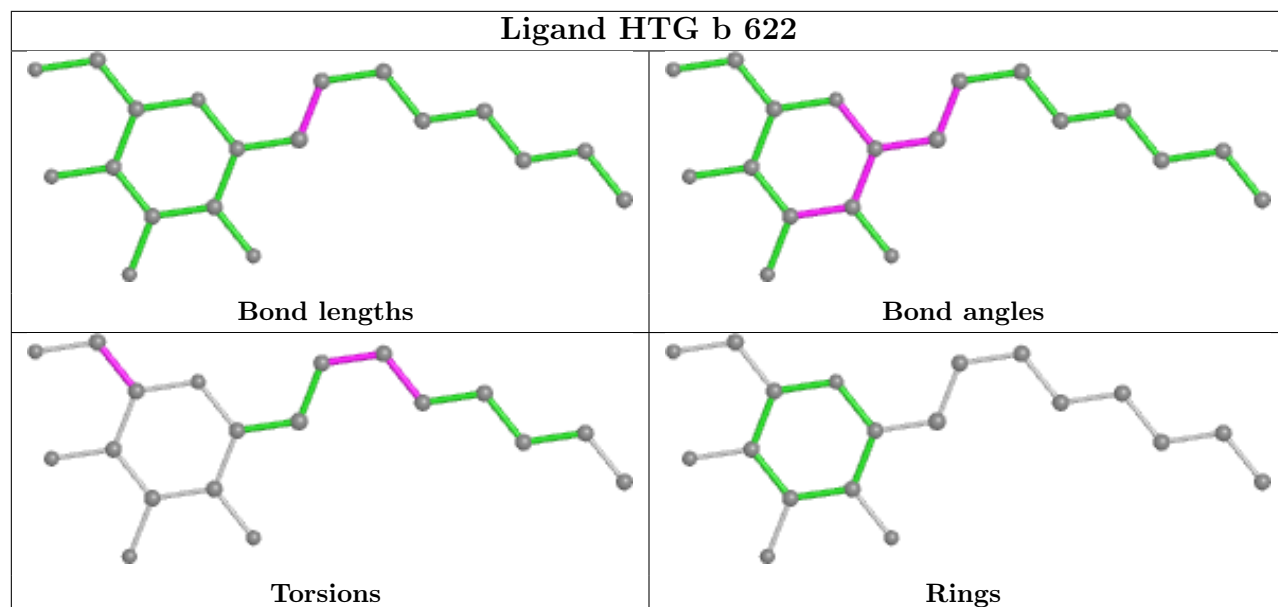


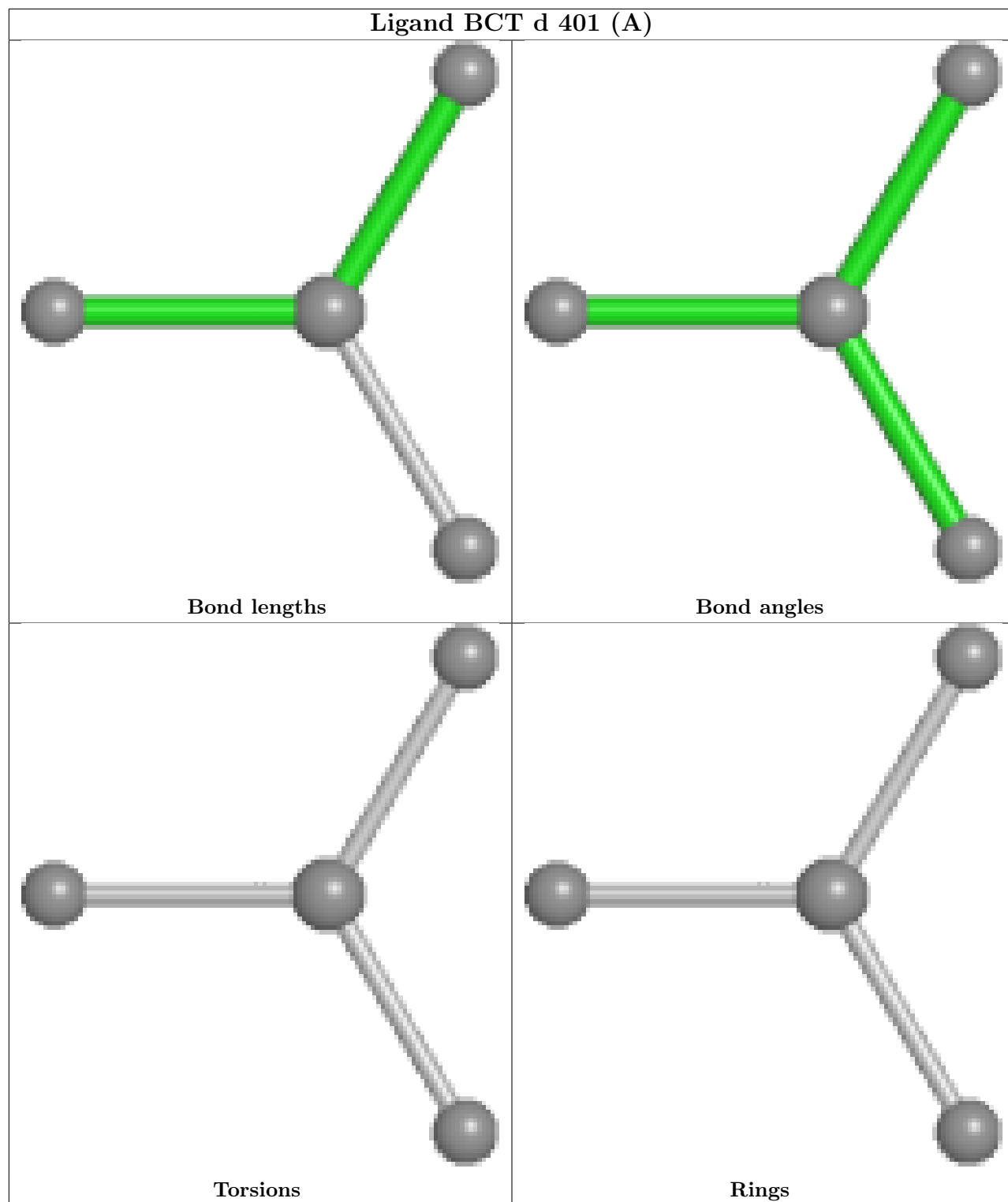


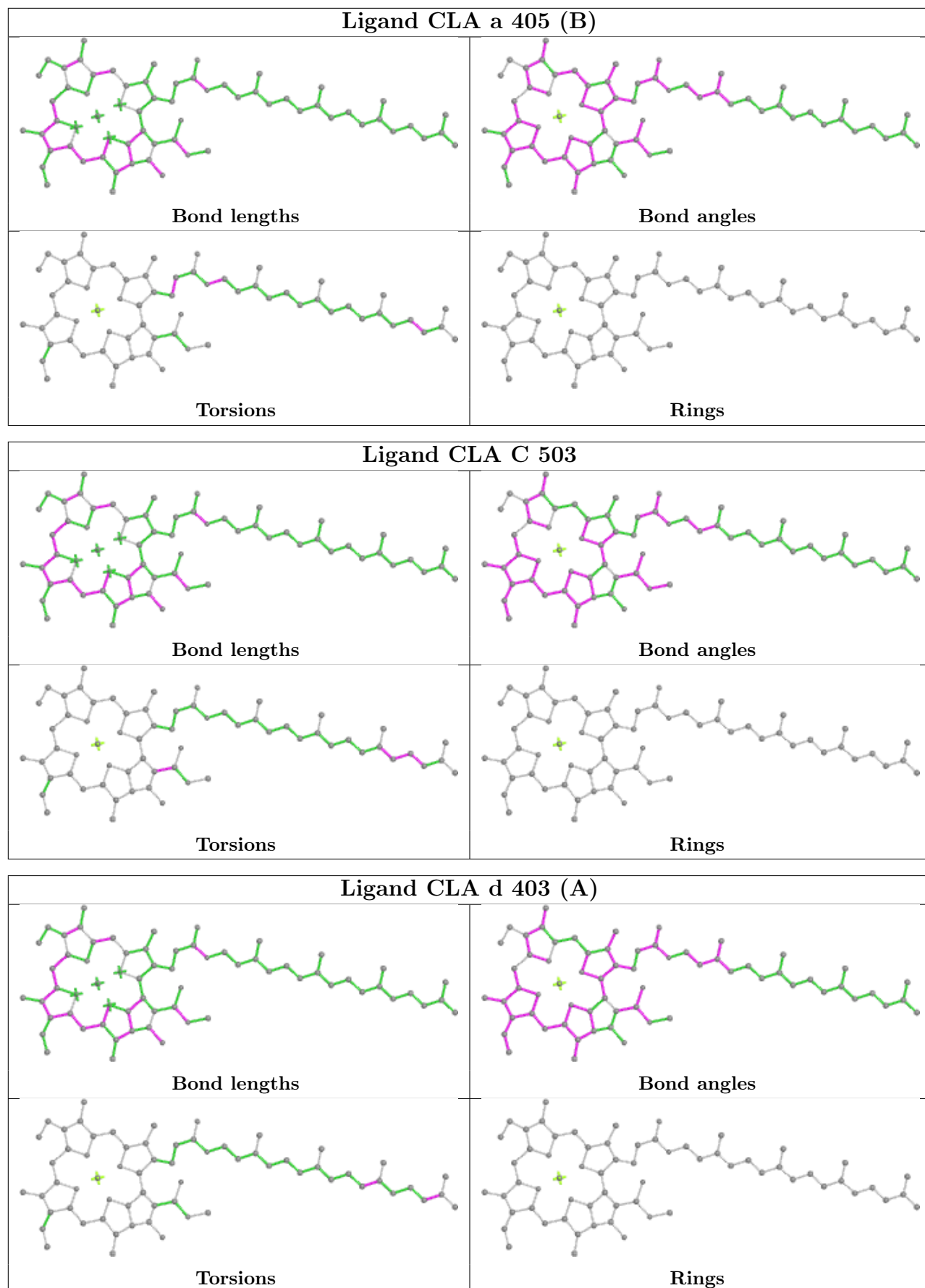


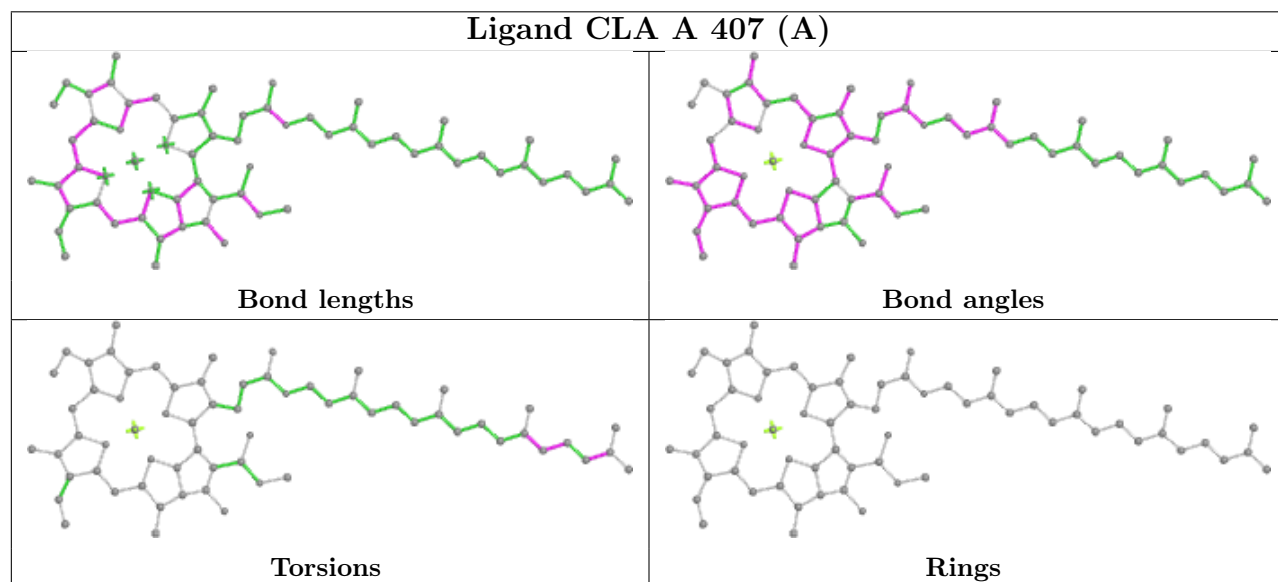
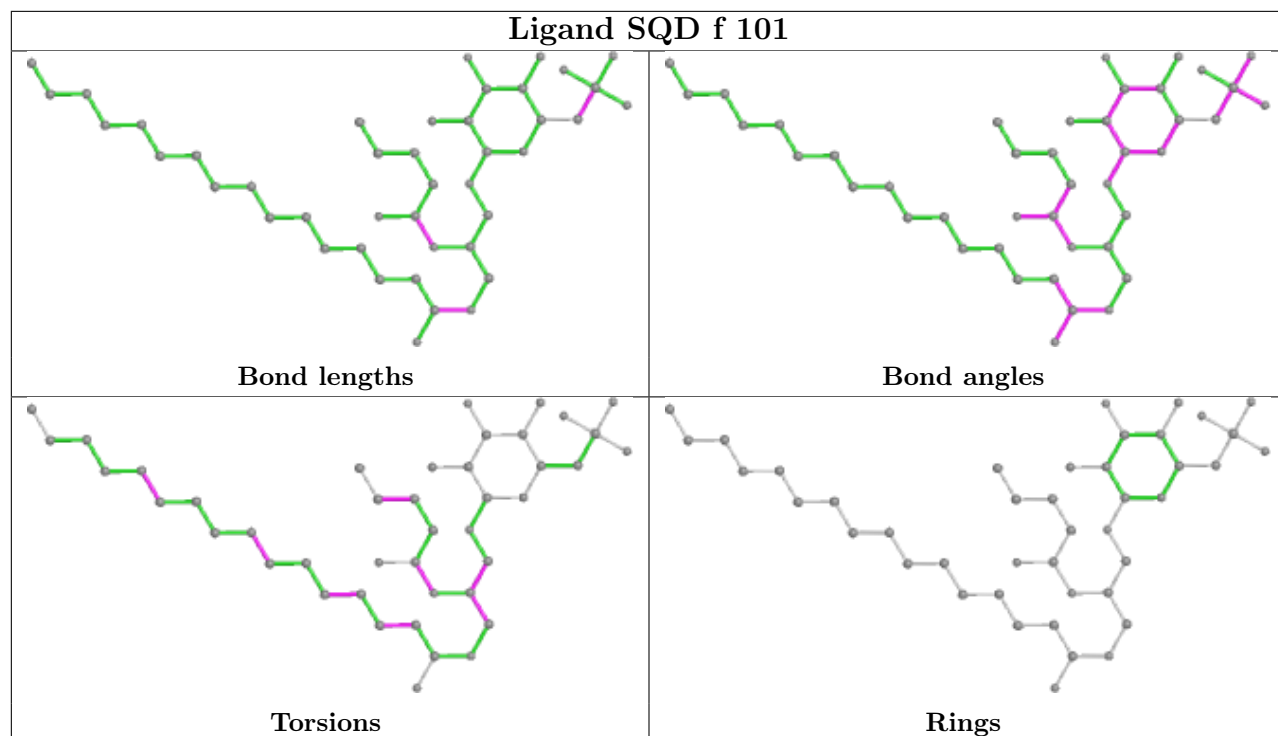


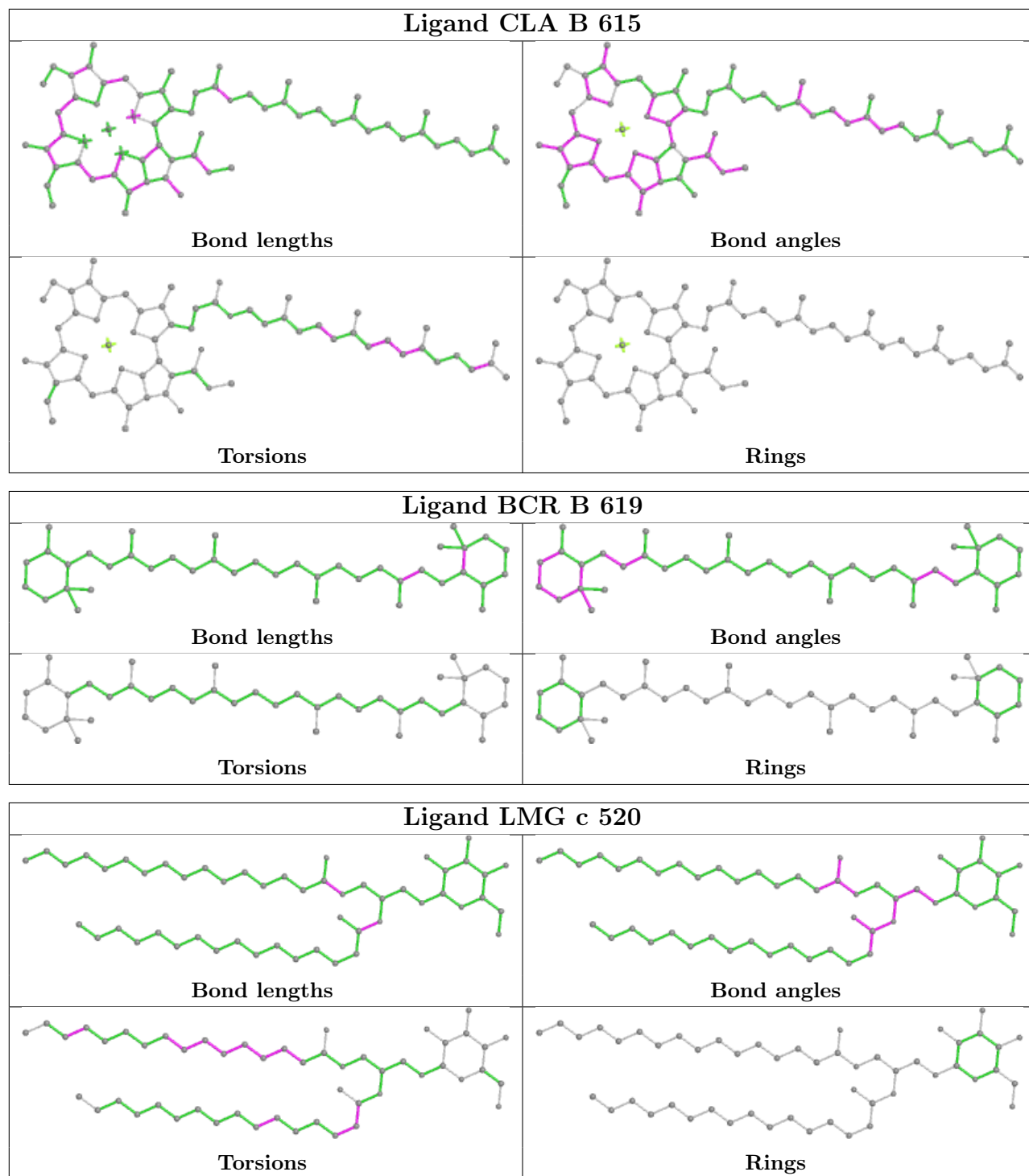


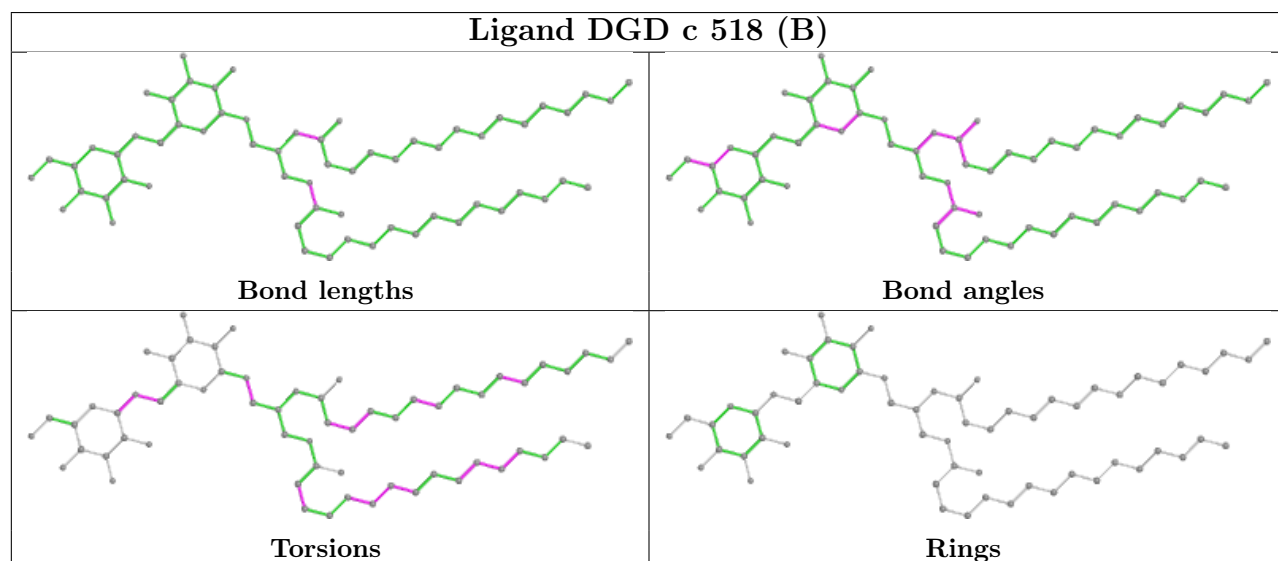
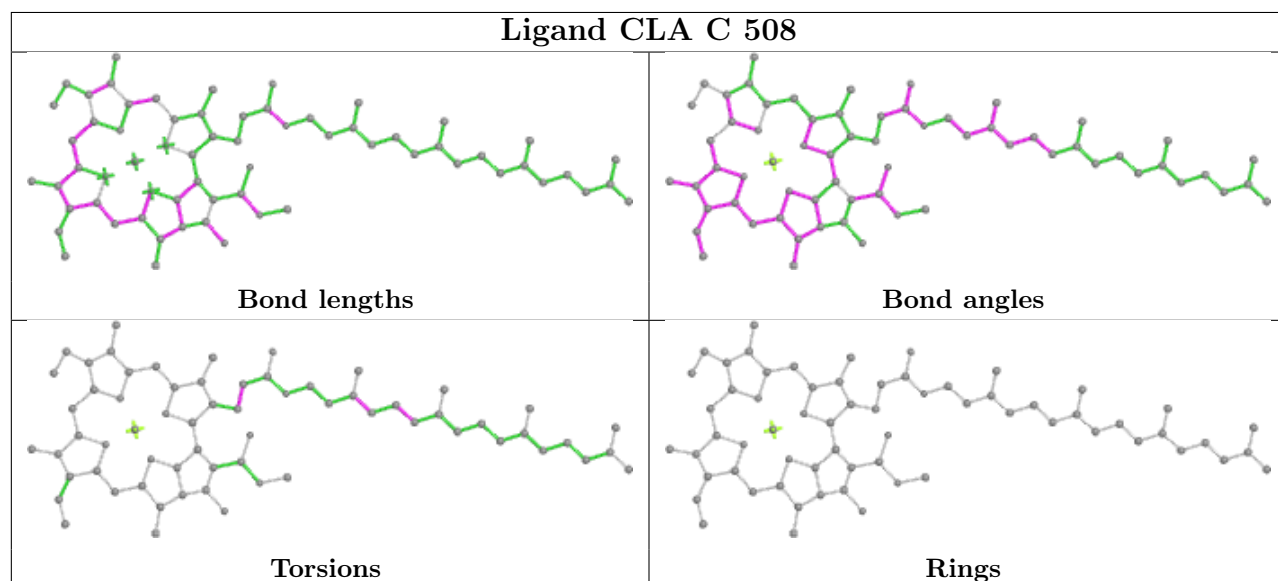
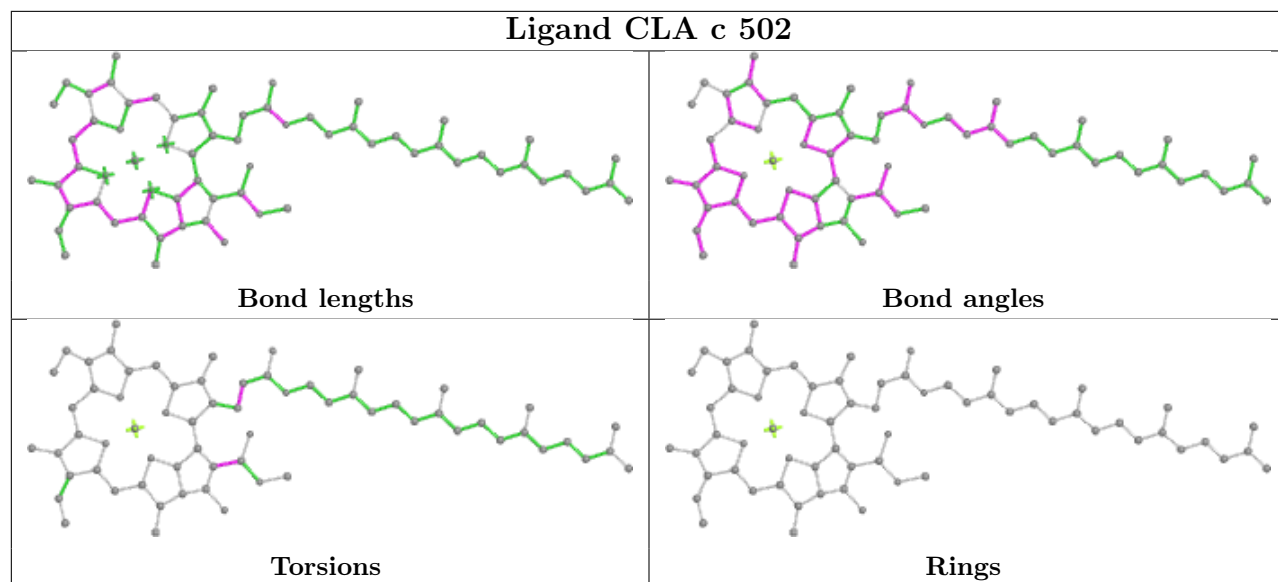


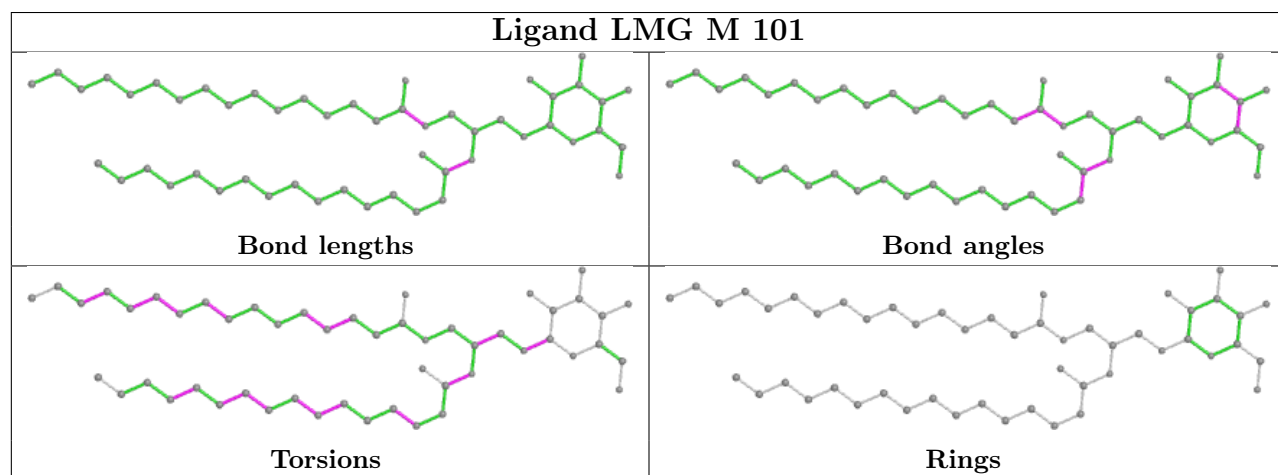
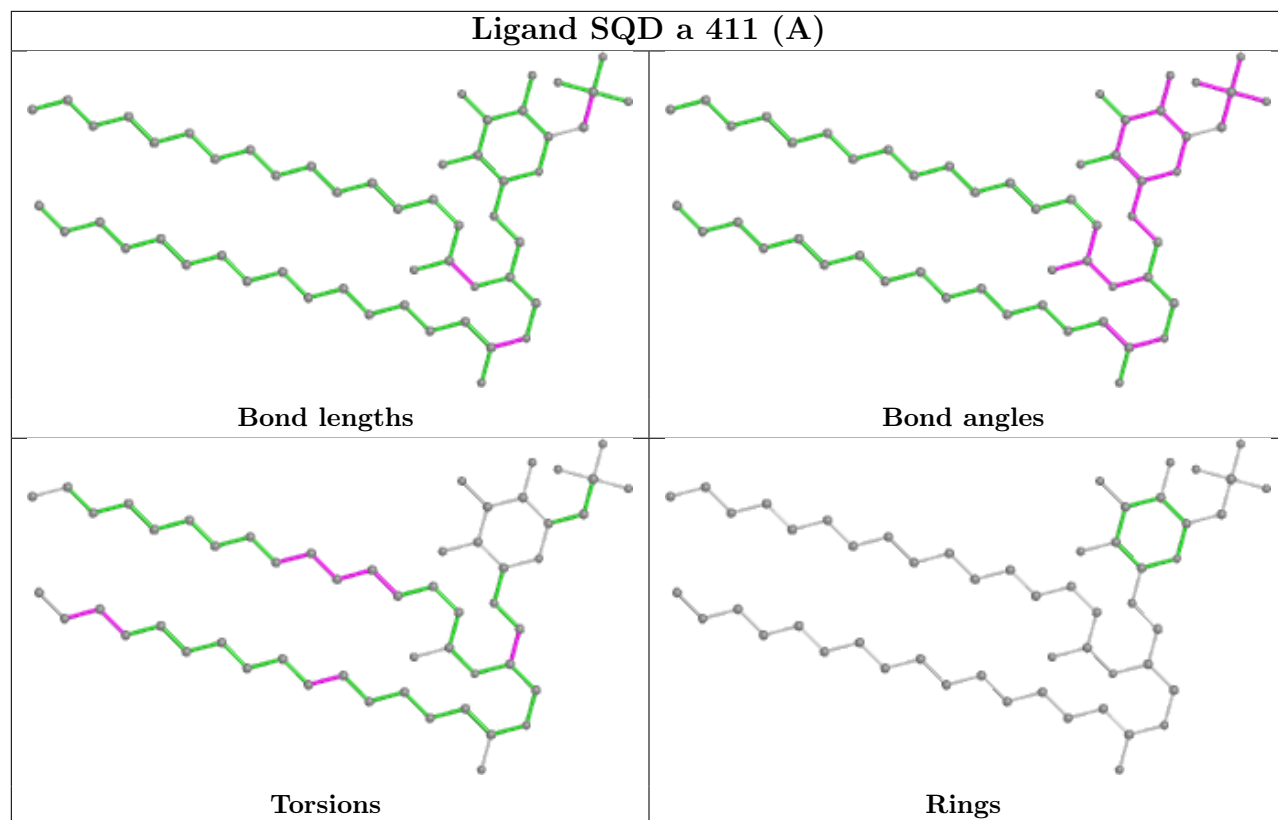


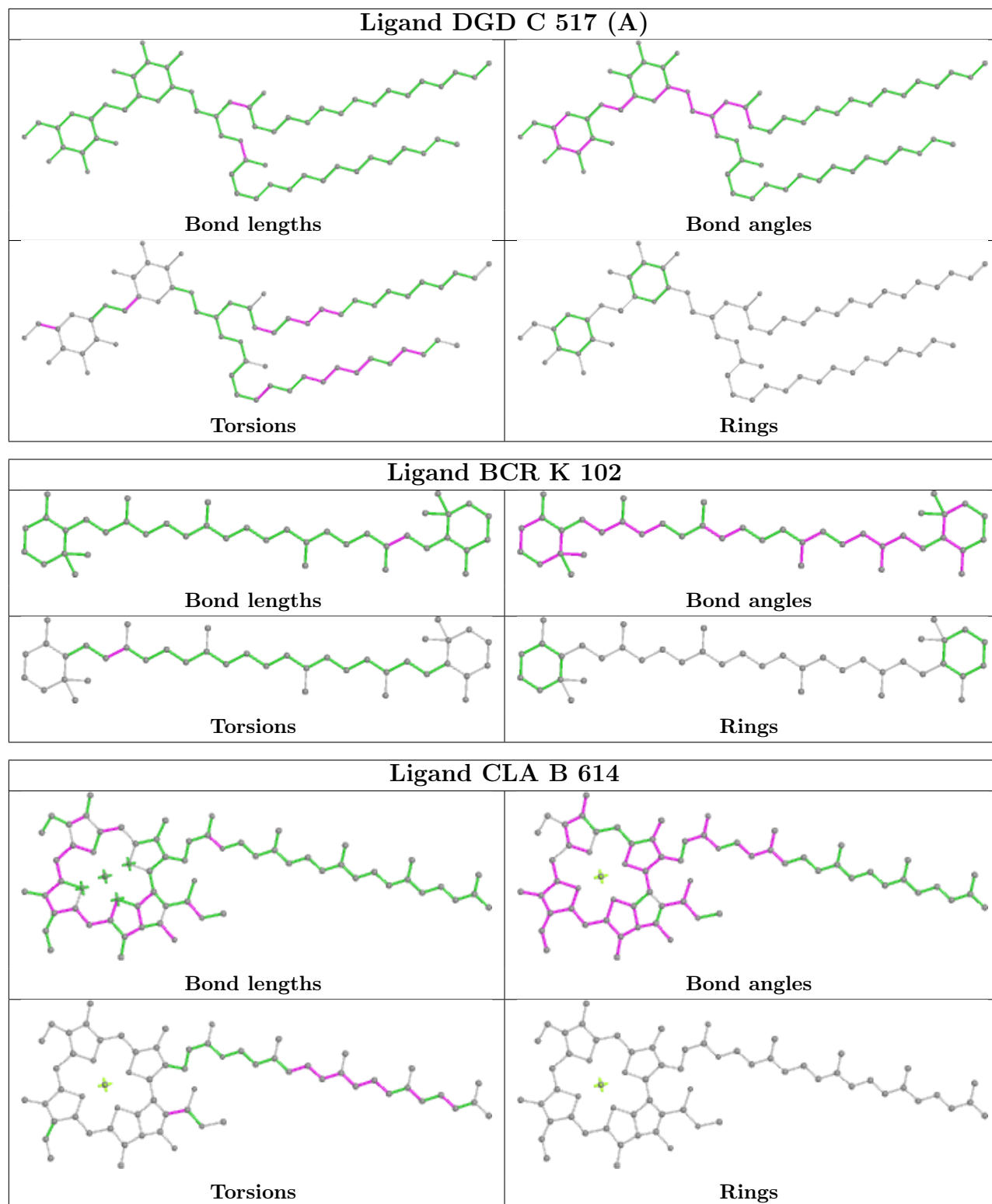


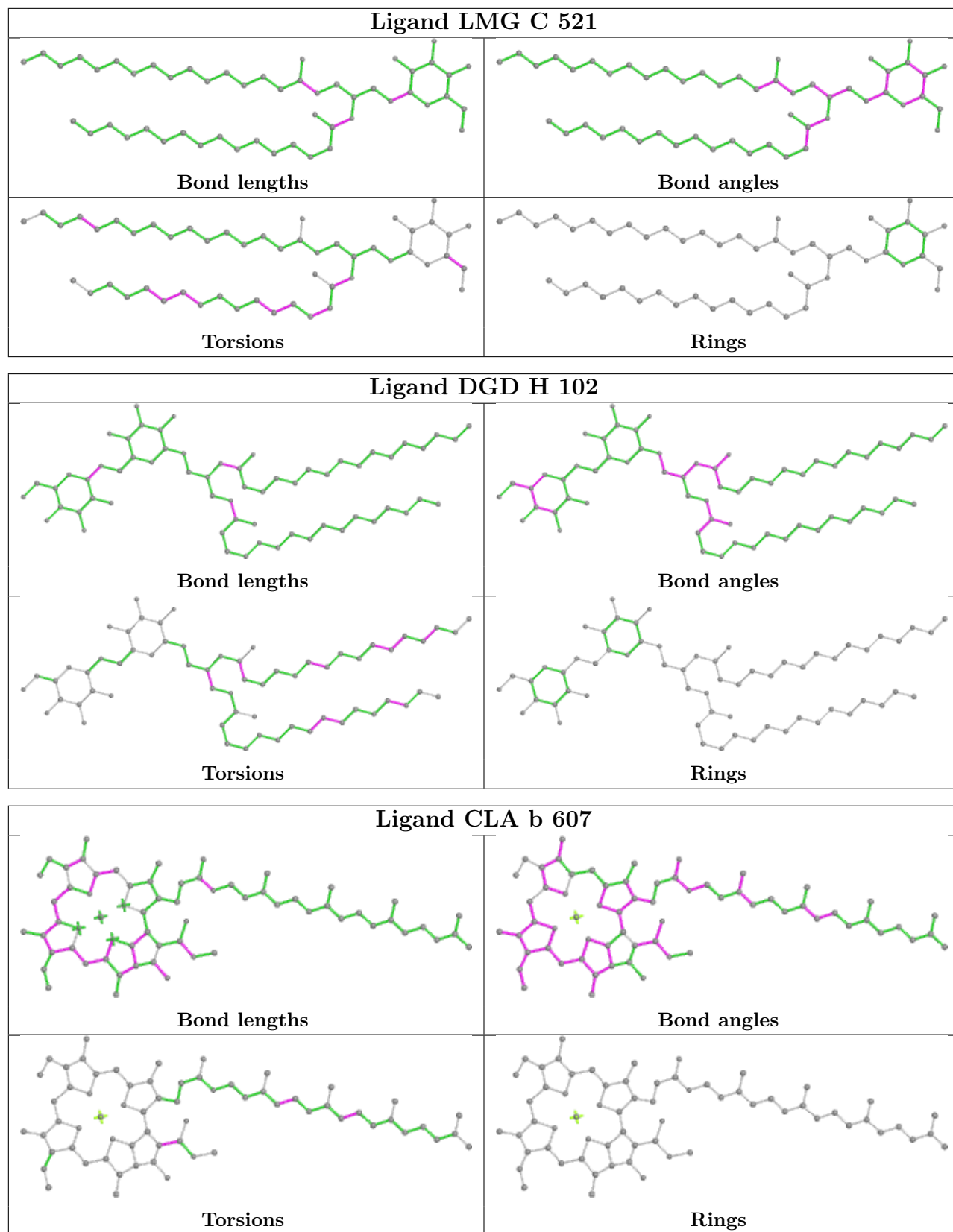


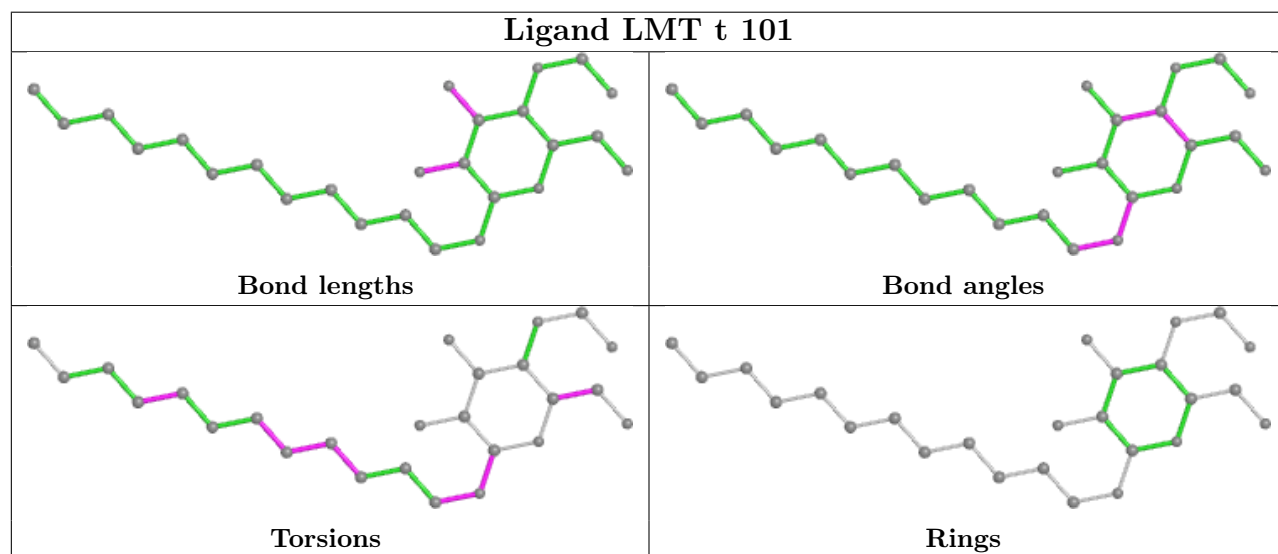
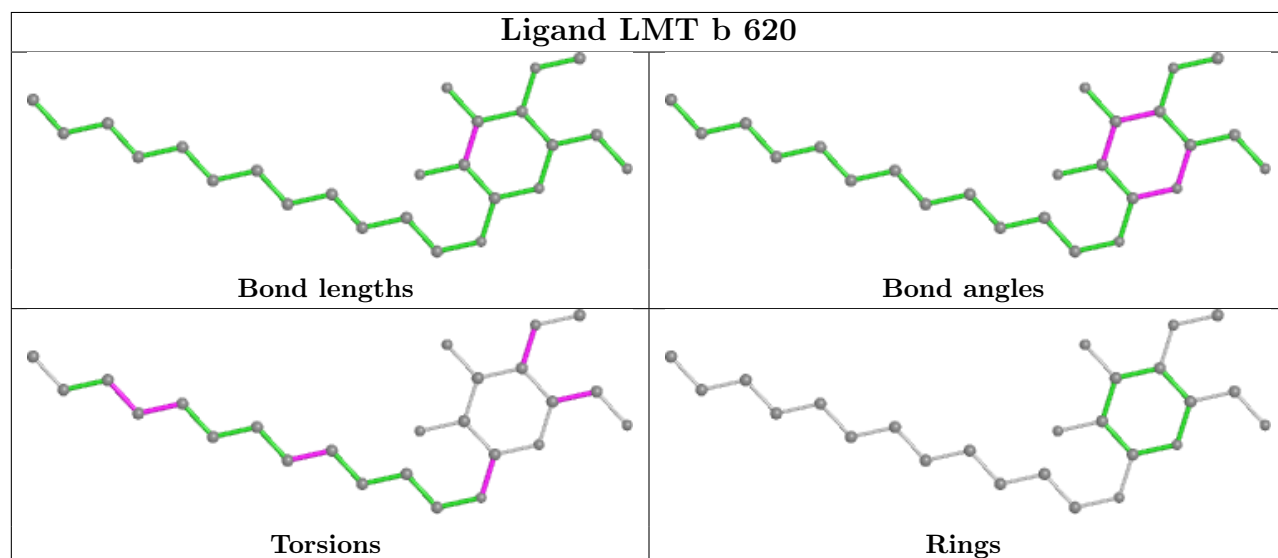
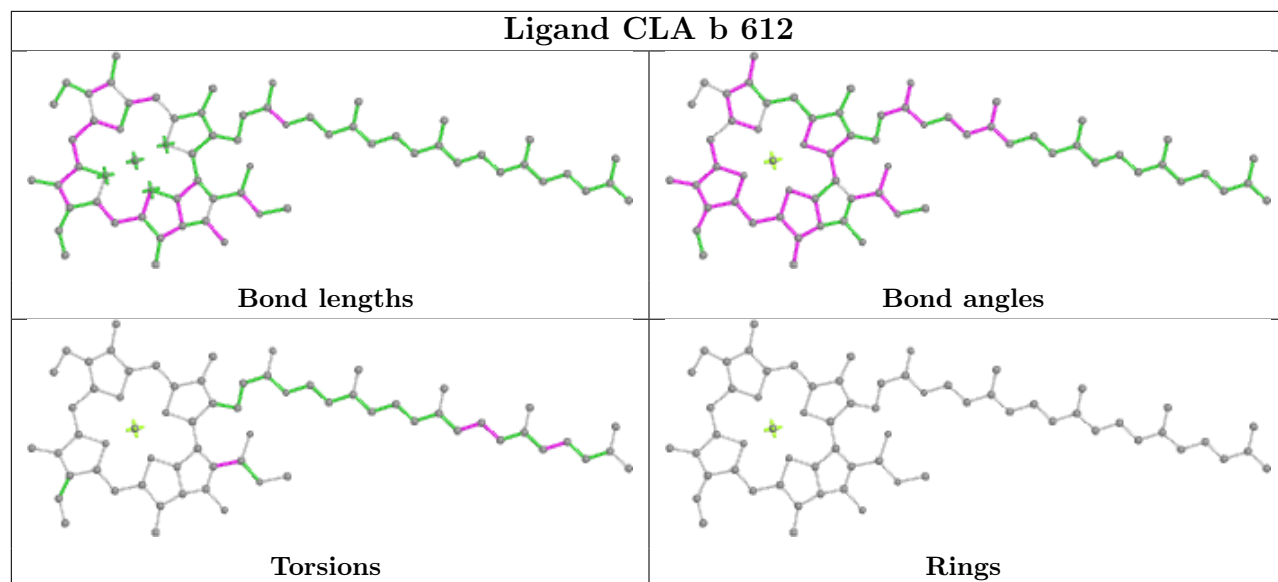


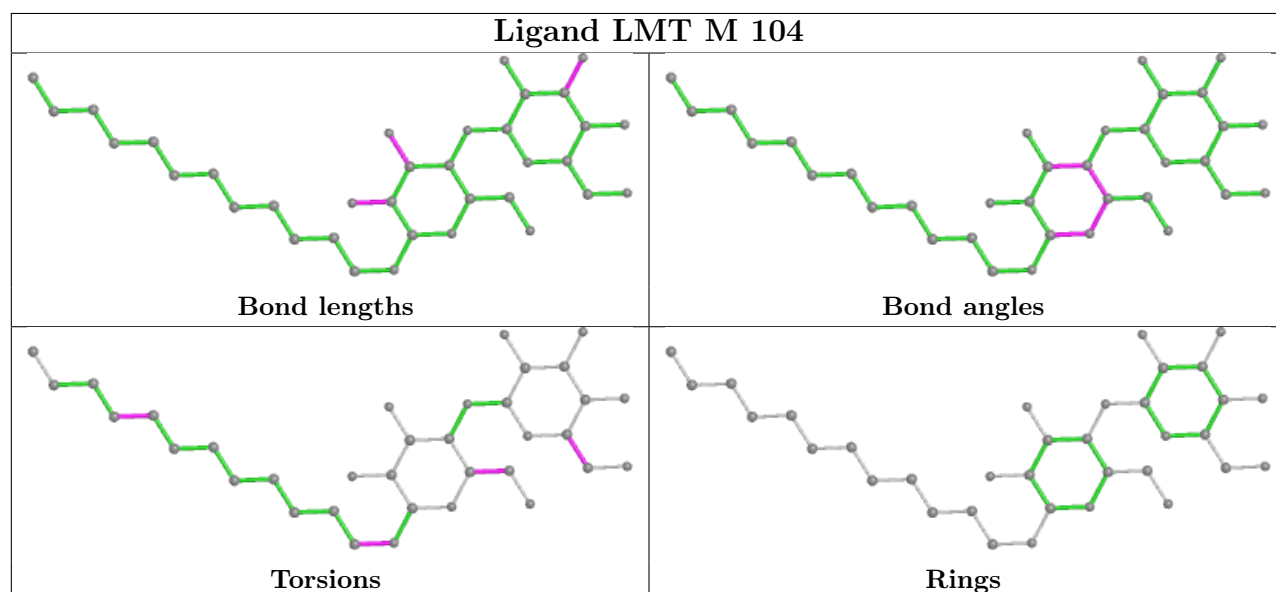
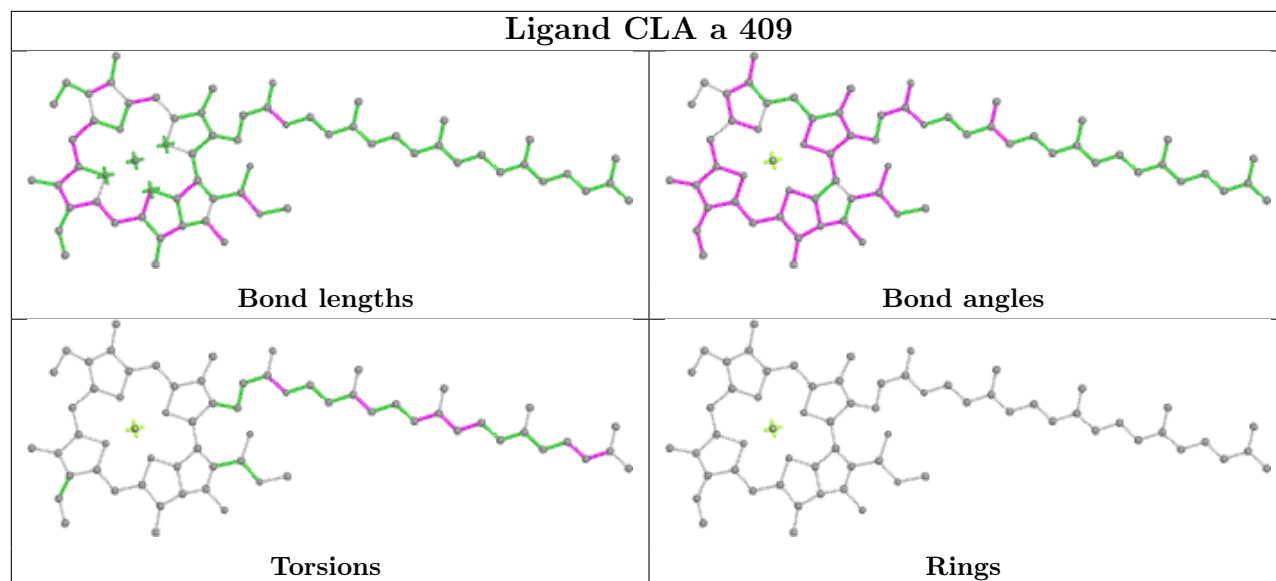
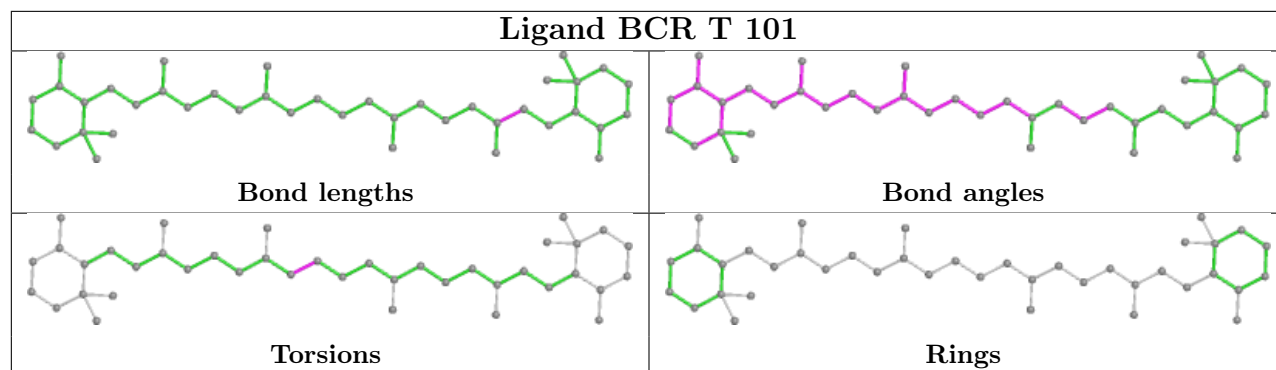


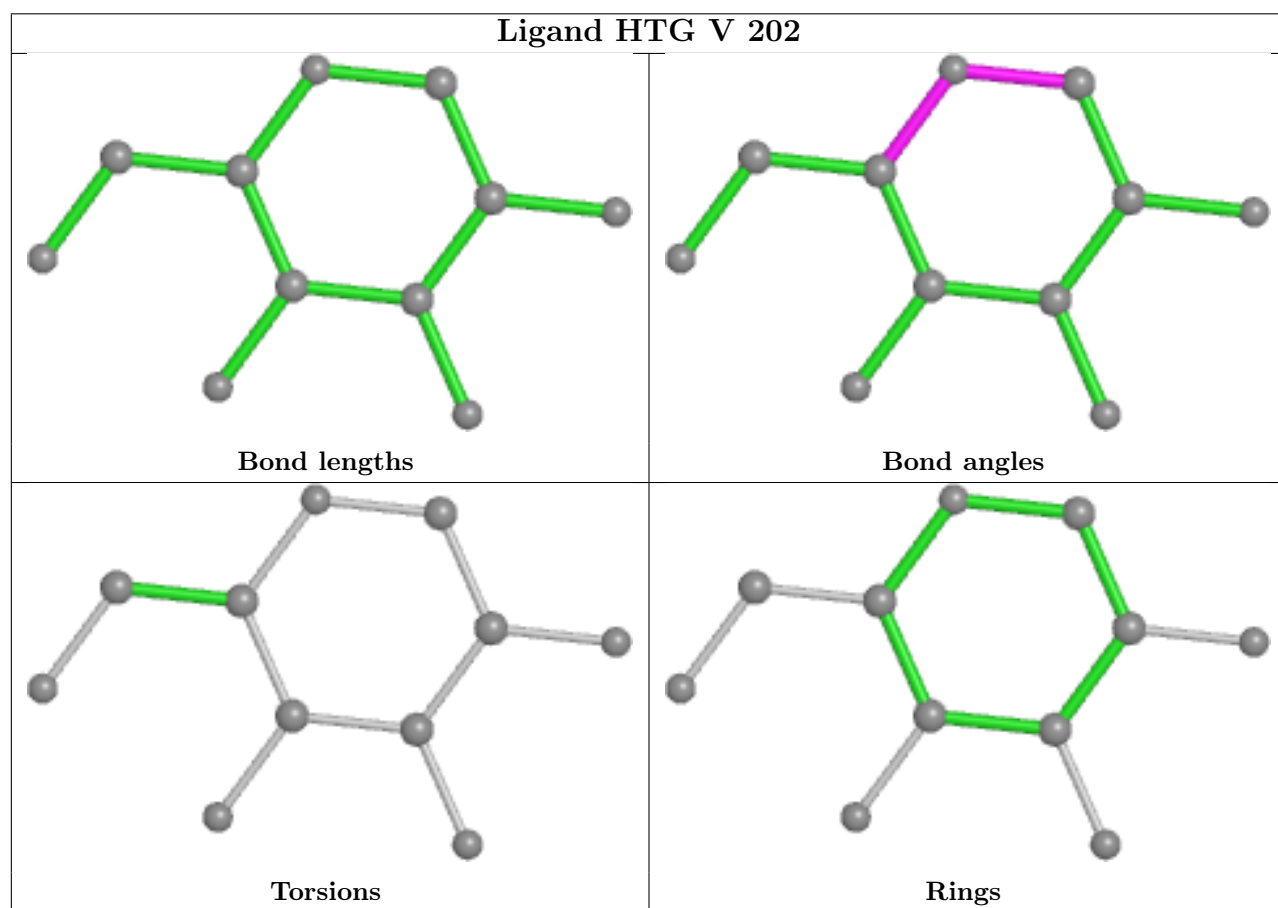
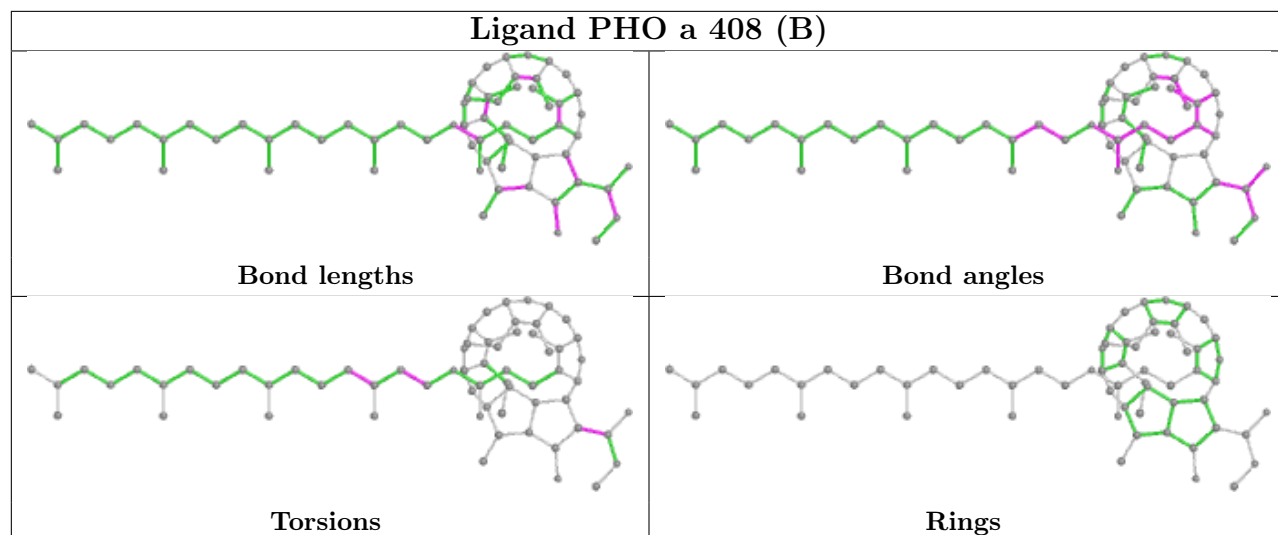


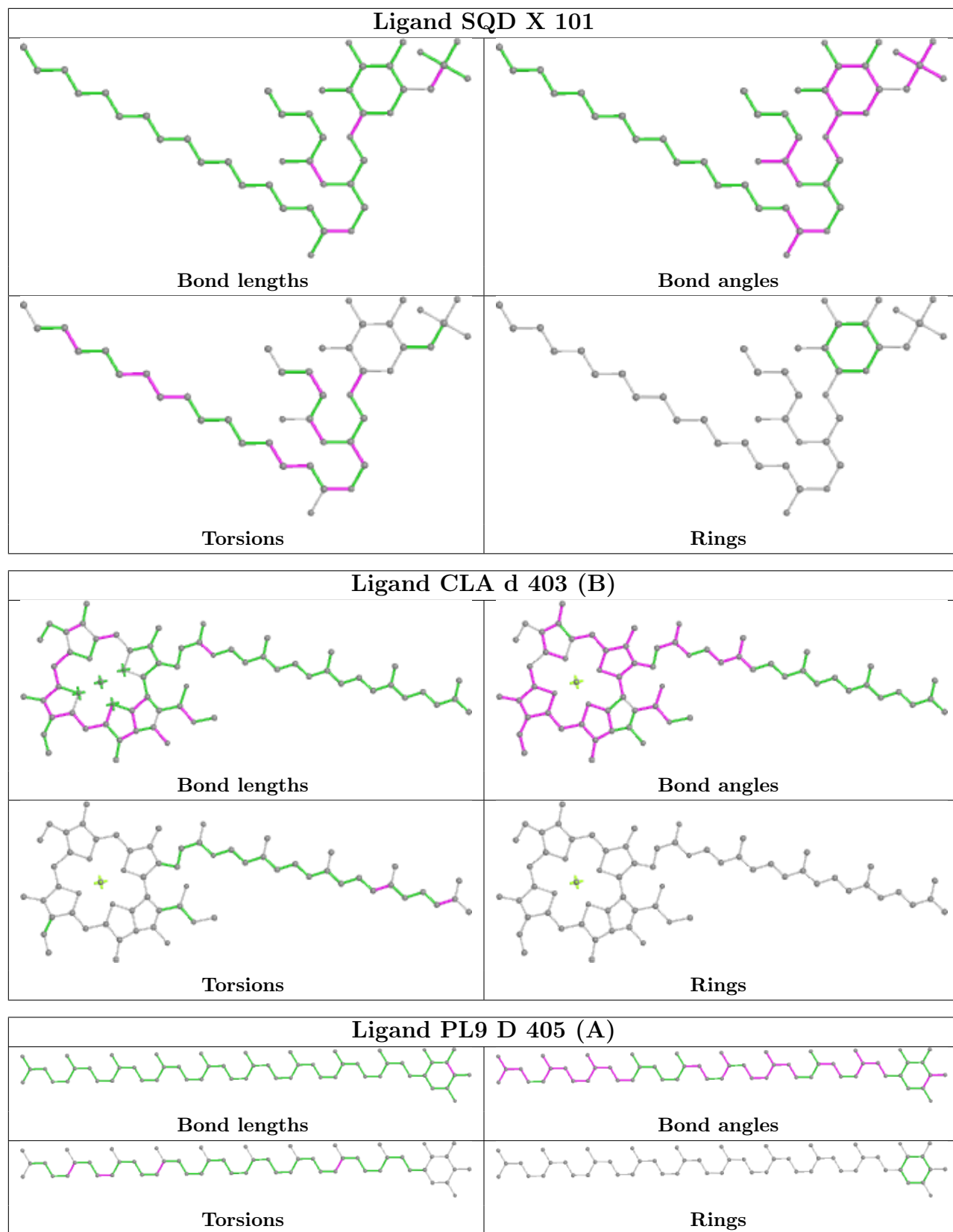


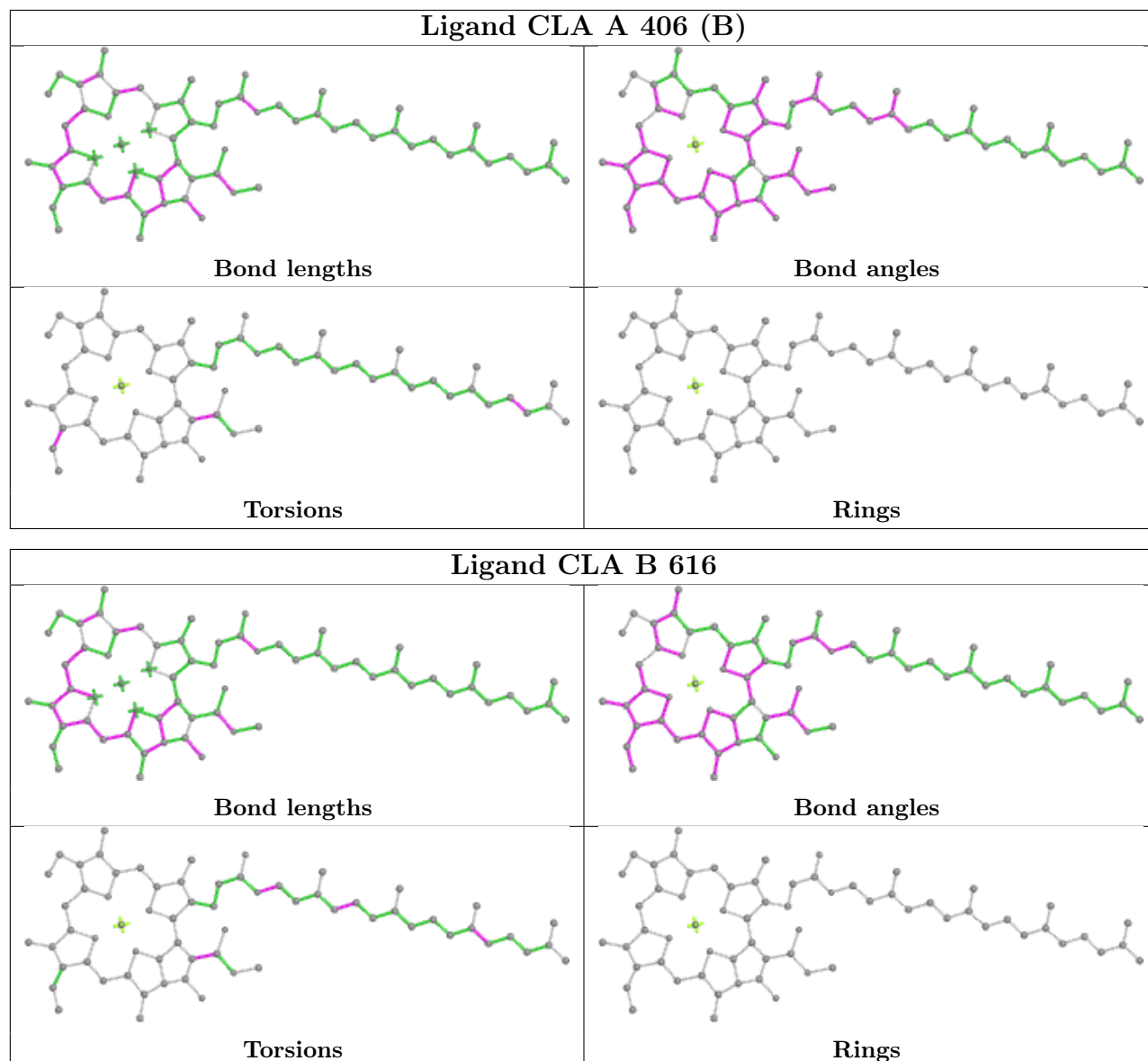












5.7 Other polymers [\(i\)](#)

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%)	-0.81	5 (1%) 73 75	38, 46, 67, 124	0
1	a	334/344 (97%)	-0.69	7 (2%) 63 66	40, 51, 78, 132	0
2	B	504/505 (99%)	-0.53	14 (2%) 53 55	40, 54, 83, 114	0
2	b	504/505 (99%)	-0.32	34 (6%) 17 19	43, 58, 101, 152	1 (0%)
3	C	451/455 (99%)	-0.57	6 (1%) 77 79	43, 59, 84, 137	0
3	c	455/455 (100%)	-0.44	15 (3%) 46 48	48, 65, 87, 125	2 (0%)
4	D	342/342 (100%)	-0.76	4 (1%) 79 81	36, 48, 67, 132	0
4	d	341/342 (99%)	-0.72	4 (1%) 79 81	41, 53, 78, 130	0
5	E	81/84 (96%)	-0.13	6 (7%) 14 15	52, 69, 101, 148	0
5	e	79/84 (94%)	0.24	9 (11%) 5 4	61, 75, 119, 146	0
6	F	34/44 (77%)	-0.46	2 (5%) 22 24	51, 60, 89, 113	0
6	f	31/44 (70%)	-0.26	2 (6%) 18 20	59, 68, 97, 139	0
7	H	64/65 (98%)	-0.28	2 (3%) 49 52	52, 63, 87, 106	0
7	h	64/65 (98%)	-0.26	4 (6%) 20 22	56, 73, 93, 104	0
8	I	37/38 (97%)	-0.17	3 (8%) 12 13	56, 65, 119, 143	0
8	i	37/38 (97%)	0.02	6 (16%) 1 1	54, 64, 113, 135	0
9	J	38/39 (97%)	-0.18	3 (7%) 12 14	48, 68, 115, 157	0
9	j	39/39 (100%)	0.34	7 (17%) 1 1	57, 76, 125, 156	0
10	K	37/37 (100%)	-0.64	1 (2%) 54 57	57, 67, 82, 105	0
10	k	37/37 (100%)	-0.49	0 100 100	66, 74, 96, 112	0
11	L	36/37 (97%)	-0.31	4 (11%) 5 5	38, 45, 113, 129	0
11	l	36/37 (97%)	-0.45	3 (8%) 11 12	40, 46, 102, 114	0
12	M	32/36 (88%)	-0.71	1 (3%) 49 52	42, 48, 73, 127	0
12	m	33/36 (91%)	-0.51	2 (6%) 21 23	42, 48, 70, 135	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.04	19 (7%) 13 14	41, 66, 120, 164	0
13	o	243/244 (99%)	0.06	23 (9%) 8 8	44, 68, 122, 155	0
14	T	29/32 (90%)	-0.71	3 (10%) 6 6	42, 48, 76, 98	0
14	t	29/32 (90%)	-0.70	1 (3%) 45 47	44, 48, 78, 106	0
15	U	96/104 (92%)	-0.41	1 (1%) 82 84	46, 58, 90, 100	0
15	u	97/104 (93%)	-0.39	2 (2%) 63 66	50, 61, 83, 122	0
16	V	137/137 (100%)	-0.53	2 (1%) 73 75	46, 56, 83, 106	0
16	v	137/137 (100%)	-0.11	5 (3%) 42 44	51, 71, 102, 131	0
17	X	38/40 (95%)	-0.33	2 (5%) 26 29	62, 71, 93, 113	0
17	x	38/40 (95%)	0.10	4 (10%) 6 6	67, 80, 124, 157	0
18	Y	29/30 (96%)	0.88	7 (24%) 0 0	64, 84, 117, 122	0
18	y	29/30 (96%)	0.43	5 (17%) 1 1	76, 88, 109, 113	0
19	Z	62/62 (100%)	0.10	6 (9%) 7 8	67, 80, 133, 150	0
19	z	62/62 (100%)	0.49	10 (16%) 1 1	79, 94, 141, 168	0
20	R	34/34 (100%)	2.25	21 (61%) 0 0	85, 109, 132, 142	0
All	All	5283/5384 (98%)	-0.40	255 (4%) 30 33	36, 59, 101, 168	3 (0%)

All (255) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	23	ALA	8.7
1	a	11	ALA	8.4
13	O	56	PRO	7.7
5	E	84	LYS	7.6
13	O	60	ARG	7.6
13	o	4	THR	7.6
3	c	20	SER	7.5
2	b	495	PHE	6.9
5	e	84	LYS	6.3
2	b	494	GLY	6.2
2	b	502	VAL	6.0
13	O	62	GLU	6.0
17	x	38	GLN	6.0
20	R	35	LEU	5.9
18	Y	19	ILE	5.9
13	o	62	GLU	5.7
12	m	34	LYS	5.7

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Mol	Chain	Res	Type	RSRZ
13	O	4	THR	5.6
19	Z	31	GLN	5.6
19	Z	32	ASP	5.6
1	A	11	ALA	5.4
13	O	63	ALA	5.4
13	O	59	LYS	5.3
13	o	56	PRO	5.3
19	z	32	ASP	5.2
3	c	19	ASN	5.2
13	o	60	ARG	5.2
9	j	3	GLU	5.1
19	z	31	GLN	5.1
18	Y	18	VAL	4.9
17	x	2	THR	4.9
13	o	63	ALA	4.8
6	f	15	ILE	4.8
13	o	58	ASN	4.8
2	b	293	ALA	4.8
14	T	30[A]	THR	4.8
19	Z	3	ILE	4.8
9	j	5	GLY	4.8
19	z	3	ILE	4.8
18	y	41	VAL	4.7
2	b	127	ARG	4.7
12	m	33	GLN	4.7
8	I	36	ASP	4.7
9	j	4	GLY	4.7
12	M	33	GLN	4.7
9	j	1	MET	4.6
13	o	61	GLN	4.6
11	L	3	PRO	4.6
11	l	3	PRO	4.5
6	F	12	SER	4.4
2	b	493[A]	TRP	4.4
13	o	59	LYS	4.4
20	R	3	TRP	4.4
20	R	32	GLN	4.4
4	D	11	GLU	4.4
13	O	5	LEU	4.3
2	b	505	ARG	4.2
11	L	7	ARG	4.2
6	f	16[A]	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
19	Z	30	PRO	4.2
3	c	143	TYR	4.2
13	o	24	ASP	4.2
9	J	3	GLU	4.1
20	R	33	LYS	4.1
20	R	24	LEU	4.1
14	t	30[A]	THR	4.1
2	b	489	GLU	4.1
13	O	61	GLN	4.0
1	a	262[A]	TYR	4.0
3	C	143	TYR	4.0
19	z	60	PHE	4.0
19	z	30	PRO	4.0
2	B	485	GLU	3.9
2	b	484[A]	PRO	3.9
19	z	35	ARG	3.9
2	B	494	GLY	3.9
16	v	15	GLU	3.9
2	b	486[A]	LEU	3.9
5	e	81	GLU	3.8
18	y	43	ARG	3.8
13	o	64	GLU	3.8
4	D	12	ARG	3.8
2	b	503	THR	3.7
2	b	487	SER	3.7
13	O	55	GLU	3.7
18	Y	20	ALA	3.7
20	R	20	VAL	3.7
3	c	21	ILE	3.6
2	b	485	GLU	3.6
13	o	57	LYS	3.6
18	y	18	VAL	3.6
7	H	6	TRP	3.5
20	R	4	ARG	3.5
8	i	38	GLU	3.5
13	o	134	THR	3.5
7	h	6	TRP	3.5
20	R	34	LEU	3.5
18	Y	43	ARG	3.5
19	z	34	ASP	3.5
19	z	42	LEU	3.4
3	C	207	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
13	o	23	ASP	3.4
9	j	6	ARG	3.4
13	o	35	SER	3.4
3	c	23	ALA	3.4
19	Z	34	ASP	3.3
2	b	496	TYR	3.3
13	o	207	ARG	3.3
8	I	34	ARG	3.3
19	z	38	GLN	3.3
4	d	12	ARG	3.3
9	J	6	ARG	3.3
8	i	36	ASP	3.3
3	c	22	PHE	3.2
2	b	376	VAL	3.2
13	O	25	THR	3.2
3	C	24	THR	3.2
13	O	207	ARG	3.2
18	y	19	ILE	3.2
2	B	293	ALA	3.2
8	i	34	ARG	3.2
13	o	25	THR	3.1
13	o	55	GLU	3.1
17	X	38	GLN	3.1
2	b	504	THR	3.1
6	F	13	TYR	3.1
13	o	5	LEU	3.1
11	l	2	GLU	3.1
20	R	21	ARG	3.1
16	v	17	LYS	3.0
20	R	6	LEU	3.0
2	b	374	ASN	3.0
3	c	207	ARG	3.0
2	b	85	GLY	3.0
3	c	192	GLY	2.9
13	o	211	ILE	2.9
1	A	13	LEU	2.9
13	O	211	ILE	2.9
20	R	31	VAL	2.9
11	L	5	PRO	2.9
2	B	295	GLY	2.9
1	a	263[A]	ALA	2.9
20	R	14	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
5	E	61	ARG	2.9
2	b	375	GLY	2.8
17	x	39	ARG	2.8
1	a	228	THR	2.8
13	O	58	ASN	2.8
17	x	3	ILE	2.8
3	C	191	PRO	2.8
4	d	236[A]	ASN	2.8
5	E	6	GLY	2.8
16	v	16	GLY	2.8
2	b	294	SER	2.7
2	b	373	LYS	2.7
8	I	37	LEU	2.7
19	Z	35	ARG	2.7
2	b	126	PRO	2.7
5	e	82	GLN	2.7
9	j	2	SER	2.7
2	B	487	SER	2.7
13	O	89	SER	2.7
2	b	295	GLY	2.7
5	E	59	GLU	2.7
20	R	29	LYS	2.7
5	e	6	GLY	2.7
1	A	12	ASN	2.6
11	L	2	GLU	2.6
1	a	261[A]	GLN	2.6
3	c	233	VAL	2.6
3	c	234	VAL	2.6
2	b	500	GLY	2.6
5	e	59	GLU	2.6
7	h	65	LEU	2.6
17	X	2	THR	2.5
15	u	8	GLU	2.5
2	B	505	ARG	2.5
4	D	107	LEU	2.5
1	A	16	ARG	2.5
8	i	35	LYS	2.5
7	h	3[A]	ARG	2.5
3	c	142	GLU	2.5
13	o	27	ARG	2.4
2	B	128	THR	2.4
13	O	132	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
20	R	18	TRP	2.4
14	T	29[A]	ILE	2.4
2	B	374	ASN	2.4
5	E	82	GLN	2.4
1	A	243[A]	GLU	2.4
9	J	5	GLY	2.4
2	b	86	ILE	2.4
2	b	501	ASP	2.4
2	B	495	PHE	2.4
2	B	489	GLU	2.4
13	O	24	ASP	2.4
20	R	2	ASP	2.4
2	b	350	GLU	2.3
2	b	435	GLU	2.3
9	j	7	ILE	2.3
5	E	60	GLN	2.3
11	l	5	PRO	2.3
3	c	145	SER	2.3
15	u	66	GLY	2.3
4	d	237[A]	PRO	2.3
1	a	235[A]	TYR	2.3
20	R	19	ALA	2.3
2	b	130	GLU	2.3
3	c	462[A]	GLU	2.3
16	v	14	SER	2.3
18	Y	41	VAL	2.3
18	Y	22	LEU	2.3
7	h	64	ALA	2.3
18	Y	21	GLN	2.2
2	B	86	ILE	2.2
3	C	142	GLU	2.2
20	R	17	GLY	2.2
2	B	162	PHE	2.2
1	a	13	LEU	2.2
3	c	201	ASN	2.2
13	O	85	LEU	2.2
2	b	488	PRO	2.2
20	R	25	PRO	2.2
13	o	34	SER	2.2
2	b	128	THR	2.2
5	e	61	ARG	2.2
10	K	13	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
16	V	15	GLU	2.2
4	D	238[A]	THR	2.2
4	d	238[A]	THR	2.2
16	v	110	LYS	2.1
18	y	20	ALA	2.1
15	U	70	ARG	2.1
5	e	25	ILE	2.1
3	c	106	VAL	2.1
13	o	136	ILE	2.1
20	R	5	VAL	2.1
20	R	16	ALA	2.1
14	T	28[A]	ARG	2.1
13	O	91	GLY	2.1
2	b	20	ILE	2.1
20	R	13	LEU	2.1
8	i	2	GLU	2.1
5	e	21	VAL	2.1
19	z	62	VAL	2.1
7	H	23	PRO	2.1
5	e	42	LEU	2.1
2	b	129	GLY	2.1
8	i	37	LEU	2.0
13	o	246	ALA	2.0
16	V	16	GLY	2.0
2	B	435[A]	GLU	2.0
13	O	27	ARG	2.0
2	b	223	GLN	2.0
2	B	373	LYS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	0.91	0.17	55,69,77,80	0
14	FME	T	1	10/11	0.95	0.08	39,57,65,70	0
12	FME	M	1	10/11	0.96	0.13	51,57,96,104	0
12	FME	m	1	10/11	0.97	0.14	50,63,91,114	0
14	FME	t	1	10/11	0.97	0.09	43,47,56,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	FME	I	1	10/11	0.98	0.08	59,70,76,78	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
31	UNL	b	625	33/-	0.41	0.35	68,99,153,163	0
31	UNL	B	625	33/-	0.46	0.37	59,111,142,148	0
32	LMT	M	104	35/35	0.47	0.31	69,121,170,178	0
31	UNL	I	101	40/-	0.51	0.32	72,99,151,161	0
32	LMT	b	620	25/35	0.51	0.28	76,114,160,172	0
28	GOL	a	418	6/6	0.56	0.53	78,93,107,112	0
35	LMG	C	521	51/55	0.56	0.30	59,115,159,173	0
32	LMT	B	628	35/35	0.59	0.34	68,115,140,152	0
31	UNL	B	629	40/-	0.59	0.29	71,106,143,163	0
32	LMT	A	418	35/35	0.65	0.33	64,110,132,141	0
32	LMT	F	101	35/35	0.65	0.51	85,132,174,181	0
32	LMT	M	102	35/35	0.65	0.27	57,93,123,126	0
35	LMG	c	521	51/55	0.65	0.29	71,132,161,181	0
32	LMT	B	630	25/35	0.66	0.26	58,82,147,160	0
34	HTG	b	622	19/19	0.66	0.46	83,129,157,161	0
35	LMG	Z	101	37/55	0.66	0.30	68,117,154,166	0
31	UNL	c	525[B]	32/-	0.67	0.41	86,104,118,129	32
31	UNL	c	525[A]	32/-	0.67	0.41	86,104,118,129	32
32	LMT	m	102	35/35	0.68	0.27	61,92,107,116	0
31	UNL	j	101	10/-	0.69	0.25	72,85,101,102	0
34	HTG	D	410	16/19	0.69	0.28	85,106,134,143	0
31	UNL	A	416	28/-	0.69	0.37	84,108,124,146	0
31	UNL	K	101[A]	34/-	0.70	0.36	77,101,118,120	34
32	LMT	b	626	25/35	0.70	0.24	51,93,149,157	0
31	UNL	K	101[B]	34/-	0.70	0.36	77,101,118,120	34
33	LHG	a	420[A]	42/49	0.70	0.40	87,129,143,148	42
33	LHG	a	420[B]	42/49	0.70	0.40	87,129,143,149	42

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
31	UNL	d	410	36/-	0.72	0.21	68,92,130,142	0
31	UNL	a	416	30/-	0.72	0.36	86,111,131,146	0
32	LMT	c	501	35/35	0.74	0.41	101,129,154,159	0
32	LMT	B	627	35/35	0.74	0.26	69,105,140,151	0
31	UNL	x	101	18/-	0.74	0.22	67,76,128,139	0
32	LMT	e	102	35/35	0.75	0.56	104,138,183,189	0
35	LMG	z	101	39/55	0.75	0.26	66,129,151,172	0
34	HTG	d	411	16/19	0.76	0.29	86,121,141,151	0
32	LMT	A	421	35/35	0.77	0.35	81,126,151,163	0
28	GOL	c	527	6/6	0.77	0.24	96,103,107,107	0
32	LMT	t	101	26/35	0.77	0.20	71,97,145,155	0
27	SQD	f	101	43/54	0.78	0.34	91,128,167,188	0
28	GOL	A	412	6/6	0.78	0.19	54,78,80,83	0
31	UNL	m	101	10/-	0.78	0.29	67,74,93,102	0
31	UNL	J	101	10/-	0.80	0.17	69,80,89,96	0
27	SQD	L	102	54/54	0.80	0.18	59,96,124,133	0
28	GOL	b	623	6/6	0.81	0.17	82,99,106,111	0
33	LHG	E	101[A]	42/49	0.81	0.26	68,97,110,116	42
33	LHG	E	101[B]	42/49	0.81	0.26	68,97,110,116	42
28	GOL	o	302	6/6	0.81	0.25	83,103,105,112	0
34	HTG	C	522	19/19	0.82	0.34	93,127,138,138	0
28	GOL	O	302	6/6	0.82	0.23	79,94,101,109	0
27	SQD	B	620	54/54	0.82	0.17	62,91,136,142	0
31	UNL	D	409	40/-	0.82	0.19	61,88,138,153	0
27	SQD	a	413	54/54	0.83	0.20	67,94,142,152	0
31	UNL	X	102	18/-	0.83	0.18	61,74,107,110	0
31	UNL	M	103	10/-	0.84	0.23	63,75,93,94	0
35	LMG	a	417	51/55	0.84	0.16	66,92,114,118	0
34	HTG	c	522	19/19	0.84	0.29	100,121,139,142	0
27	SQD	A	413	54/54	0.84	0.18	60,85,124,145	0
35	LMG	C	501	51/55	0.84	0.17	66,91,116,128	0
37	CA	f	102	1/1	0.84	0.11	117,117,117,117	0
28	GOL	B	626	6/6	0.85	0.21	69,85,107,119	0
28	GOL	O	303	6/6	0.85	0.22	78,86,96,98	0
28	GOL	o	303	6/6	0.85	0.22	79,83,97,100	0
30	PL9	a	415[B]	55/55	0.86	0.20	67,98,108,115	55
34	HTG	B	622	19/19	0.86	0.21	63,92,112,114	0
28	GOL	l	801[A]	6/6	0.86	0.63	64,92,95,96	6
28	GOL	l	801[B]	6/6	0.86	0.63	65,93,95,96	6
35	LMG	d	412	51/55	0.86	0.20	53,71,120,150	0
26	BCR	C	515	40/40	0.86	0.15	57,77,89,91	0
28	GOL	a	419	6/6	0.86	0.37	54,73,83,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	PL9	a	415[A]	55/55	0.86	0.20	68,98,108,115	55
34	HTG	b	621	19/19	0.87	0.17	61,79,113,124	0
28	GOL	d	413	6/6	0.87	0.25	50,69,83,83	0
34	HTG	B	621	19/19	0.87	0.16	60,85,115,119	0
30	PL9	A	415[A]	55/55	0.87	0.17	59,84,101,112	55
30	PL9	A	415[B]	55/55	0.87	0.17	60,84,101,112	55
37	CA	F	103	1/1	0.87	0.20	121,121,121,121	0
24	CLA	b	601	65/65	0.87	0.17	59,85,128,155	0
24	CLA	d	404	65/65	0.88	0.15	54,67,121,150	0
28	GOL	a	412	6/6	0.88	0.27	74,76,83,96	0
28	GOL	v	202[A]	6/6	0.88	0.17	65,78,80,80	6
28	GOL	v	202[B]	6/6	0.88	0.17	65,78,80,81	6
35	LMG	D	411	51/55	0.88	0.17	48,64,118,133	0
24	CLA	c	514	65/65	0.88	0.17	69,95,124,148	0
24	CLA	b	616	65/65	0.89	0.16	49,63,127,143	0
35	LMG	c	520	51/55	0.89	0.17	61,91,130,153	0
24	CLA	C	514	65/65	0.89	0.14	58,86,112,123	0
26	BCR	h	101	40/40	0.89	0.16	55,69,93,96	0
37	CA	o	301	1/1	0.89	0.06	114,114,114,114	0
28	GOL	A	419	6/6	0.90	0.30	50,74,76,82	0
26	BCR	K	102	40/40	0.90	0.17	55,63,77,82	0
26	BCR	d	405	40/40	0.90	0.13	48,63,109,111	0
24	CLA	B	601	65/65	0.90	0.14	56,78,110,153	0
28	GOL	V	203[A]	6/6	0.90	0.19	57,68,75,79	6
28	GOL	V	203[B]	6/6	0.90	0.19	57,69,75,79	6
35	LMG	M	101	51/55	0.91	0.12	53,70,89,116	0
26	BCR	Y	101	40/40	0.91	0.12	49,63,79,85	0
35	LMG	C	520	51/55	0.91	0.15	51,83,113,127	0
24	CLA	B	616	65/65	0.91	0.17	47,58,136,145	0
24	CLA	c	513	65/65	0.91	0.16	59,82,122,130	0
27	SQD	X	101	43/54	0.92	0.18	66,104,129,144	0
28	GOL	D	412	6/6	0.92	0.17	44,64,69,84	0
26	BCR	D	404	40/40	0.92	0.10	42,59,101,108	0
24	CLA	C	507	65/65	0.92	0.13	54,69,119,142	0
24	CLA	C	513	65/65	0.92	0.14	59,73,111,124	0
36	DGD	c	518[A]	62/66	0.92	0.12	53,66,117,133	62
36	DGD	c	518[B]	62/66	0.92	0.12	53,66,117,133	62
36	DGD	h	102	62/66	0.92	0.12	51,66,80,87	0
24	CLA	B	606	65/65	0.92	0.14	43,58,112,128	0
31	UNL	d	409	17/-	0.92	0.13	66,81,110,112	0
34	HTG	b	624	19/19	0.92	0.12	63,77,94,110	0
36	DGD	C	518[A]	62/66	0.93	0.13	46,62,115,120	62

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	DGD	C	518[B]	62/66	0.93	0.13	46,62,115,120	62
36	DGD	C	519	62/66	0.93	0.12	43,57,101,112	0
36	DGD	H	102	62/66	0.93	0.12	43,60,77,85	0
35	LMG	b	629	51/55	0.93	0.11	52,73,97,113	0
24	CLA	b	606	65/65	0.93	0.14	46,61,117,130	0
36	DGD	c	519	62/66	0.93	0.12	49,66,104,131	0
26	BCR	A	410	40/40	0.93	0.11	42,51,65,68	0
26	BCR	k	101	40/40	0.93	0.17	57,74,83,88	0
37	CA	O	301	1/1	0.93	0.08	107,107,107,107	0
24	CLA	c	507	65/65	0.93	0.13	53,68,119,143	0
26	BCR	c	515	40/40	0.93	0.12	67,81,93,97	0
28	GOL	C	523[A]	6/6	0.94	0.17	58,60,68,72	6
28	GOL	C	523[B]	6/6	0.94	0.17	58,61,68,72	6
28	GOL	c	526[A]	6/6	0.94	0.29	66,71,76,77	6
28	GOL	c	526[B]	6/6	0.94	0.29	66,70,76,77	6
26	BCR	C	516	40/40	0.94	0.14	53,64,79,83	0
24	CLA	C	509	65/65	0.94	0.11	45,55,114,143	0
24	CLA	D	403	65/65	0.94	0.14	47,58,124,137	0
27	SQD	A	411[A]	54/54	0.94	0.13	58,78,114,121	54
31	UNL	D	408	17/-	0.94	0.13	59,74,102,119	0
34	HTG	B	624	19/19	0.94	0.09	65,78,104,105	0
27	SQD	A	411[B]	54/54	0.94	0.13	58,78,114,121	54
24	CLA	a	409	65/65	0.94	0.17	42,56,133,155	0
34	HTG	V	202	11/19	0.94	0.44	81,117,124,129	0
24	CLA	B	609	65/65	0.94	0.15	46,59,73,85	0
24	CLA	c	508	65/65	0.95	0.12	49,69,84,91	0
33	LHG	d	408[A]	49/49	0.95	0.15	51,62,111,128	49
33	LHG	d	408[B]	49/49	0.95	0.15	51,63,111,128	49
26	BCR	b	618	40/40	0.95	0.09	39,55,74,86	0
26	BCR	b	619	40/40	0.95	0.08	48,63,86,91	0
24	CLA	a	407[A]	65/65	0.95	0.11	40,51,123,132	65
26	BCR	c	516	40/40	0.95	0.13	51,67,76,84	0
24	CLA	a	407[B]	65/65	0.95	0.11	40,51,123,132	65
24	CLA	C	508	65/65	0.95	0.14	52,63,83,93	0
24	CLA	A	409	65/65	0.95	0.12	39,52,130,147	0
26	BCR	t	102	40/40	0.95	0.08	42,61,78,84	0
36	DGD	c	517[A]	62/66	0.95	0.12	48,64,101,107	62
36	DGD	c	517[B]	62/66	0.95	0.12	48,64,101,107	62
26	BCR	y	101	40/40	0.95	0.09	56,69,85,103	0
26	BCR	B	618	40/40	0.95	0.08	39,51,69,78	0
24	CLA	C	502	65/65	0.95	0.10	50,61,71,78	0
24	CLA	b	612	65/65	0.95	0.10	42,53,68,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	CLA	C	505	65/65	0.95	0.09	41,55,102,133	0
26	BCR	H	101	40/40	0.95	0.11	51,66,91,92	0
24	CLA	B	611	65/65	0.95	0.10	33,45,69,78	0
28	GOL	b	627	6/6	0.95	0.20	80,85,86,90	0
24	CLA	C	510	65/65	0.96	0.12	46,58,82,102	0
24	CLA	b	609	65/65	0.96	0.15	50,65,80,94	0
24	CLA	C	511	65/65	0.96	0.09	47,57,78,86	0
24	CLA	b	615	65/65	0.96	0.10	47,60,80,86	0
26	BCR	B	619	40/40	0.96	0.08	46,59,91,99	0
24	CLA	C	512	65/65	0.96	0.14	49,63,78,90	0
24	CLA	c	502	65/65	0.96	0.11	54,68,79,85	0
24	CLA	c	504	65/65	0.96	0.09	52,70,83,97	0
24	CLA	c	505	65/65	0.96	0.10	49,62,106,138	0
24	CLA	c	506	65/65	0.96	0.10	47,63,96,105	0
27	SQD	a	411[A]	54/54	0.96	0.13	60,80,117,121	54
27	SQD	a	411[B]	54/54	0.96	0.13	60,80,117,121	54
26	BCR	T	101	40/40	0.96	0.07	41,58,71,79	0
33	LHG	A	420[A]	49/49	0.96	0.11	46,60,81,88	49
33	LHG	A	420[B]	49/49	0.96	0.11	46,60,81,88	49
33	LHG	D	407[A]	49/49	0.96	0.14	45,58,108,111	49
33	LHG	D	407[B]	49/49	0.96	0.14	44,58,108,110	49
24	CLA	B	602	65/65	0.96	0.12	46,56,74,89	0
26	BCR	a	410	40/40	0.96	0.08	44,54,64,65	0
24	CLA	B	614	65/65	0.96	0.09	37,50,102,127	0
28	GOL	B	623	6/6	0.96	0.19	68,74,81,82	0
33	LHG	b	628[A]	49/49	0.96	0.12	47,55,71,84	49
33	LHG	b	628[B]	49/49	0.96	0.12	47,55,72,84	49
33	LHG	d	407[A]	49/49	0.96	0.15	45,55,71,77	49
33	LHG	d	407[B]	49/49	0.96	0.15	45,55,71,77	49
24	CLA	c	509	65/65	0.96	0.11	47,62,119,153	0
24	CLA	c	510	65/65	0.96	0.11	42,59,88,95	0
33	LHG	d	414[A]	49/49	0.96	0.13	49,67,78,86	49
33	LHG	d	414[B]	49/49	0.96	0.13	50,67,82,86	49
37	CA	C	524	1/1	0.96	0.05	78,78,78,78	0
24	CLA	c	512	65/65	0.96	0.11	54,68,85,103	0
24	CLA	b	602	65/65	0.96	0.13	48,60,82,95	0
30	PL9	D	405[A]	55/55	0.96	0.11	39,47,58,69	55
30	PL9	D	405[B]	55/55	0.96	0.11	39,47,58,68	55
39	HEM	e	101	43/43	0.96	0.13	62,82,110,130	0
24	CLA	d	403[B]	65/65	0.97	0.10	38,46,75,89	65
24	CLA	b	604	65/65	0.97	0.11	40,53,97,117	0
25	PHO	d	402[A]	64/64	0.97	0.12	45,54,63,68	64

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	PHO	d	402[B]	64/64	0.97	0.12	45,54,63,68	64
24	CLA	b	605	65/65	0.97	0.11	38,49,73,82	0
24	CLA	A	405[B]	65/65	0.97	0.11	35,41,60,69	65
24	CLA	b	607	65/65	0.97	0.08	37,46,80,88	0
30	PL9	d	406[A]	55/55	0.97	0.11	37,49,60,68	55
30	PL9	d	406[B]	55/55	0.97	0.11	37,50,60,69	55
24	CLA	B	612	65/65	0.97	0.08	36,48,60,69	0
24	CLA	b	610	65/65	0.97	0.09	49,58,70,80	0
24	CLA	b	611	65/65	0.97	0.09	37,49,72,85	0
24	CLA	B	613	65/65	0.97	0.08	34,44,97,112	0
24	CLA	b	613	65/65	0.97	0.08	40,49,86,108	0
24	CLA	b	614	65/65	0.97	0.08	41,50,102,111	0
24	CLA	A	407[A]	65/65	0.97	0.08	35,46,104,120	65
24	CLA	B	615	65/65	0.97	0.10	42,53,79,91	0
33	LHG	L	101[A]	49/49	0.97	0.11	46,54,69,86	49
36	DGD	C	517[A]	62/66	0.97	0.11	44,58,95,100	62
36	DGD	C	517[B]	62/66	0.97	0.11	44,58,95,100	62
33	LHG	L	101[B]	49/49	0.97	0.11	46,54,70,86	49
26	BCR	b	617	40/40	0.97	0.08	43,52,62,66	0
24	CLA	B	603	65/65	0.97	0.10	43,52,71,82	0
24	CLA	c	503	65/65	0.97	0.08	43,58,82,100	0
24	CLA	B	605	65/65	0.97	0.10	37,48,65,83	0
24	CLA	a	405[A]	65/65	0.97	0.13	37,45,64,74	65
24	CLA	a	405[B]	65/65	0.97	0.13	37,45,64,74	65
24	CLA	a	406[A]	65/65	0.97	0.07	37,43,60,71	65
24	CLA	a	406[B]	65/65	0.97	0.07	37,43,60,71	65
24	CLA	C	504	65/65	0.97	0.09	47,61,72,87	0
24	CLA	A	407[B]	65/65	0.97	0.08	35,46,104,120	65
24	CLA	c	511	65/65	0.97	0.10	49,62,79,84	0
24	CLA	C	506	65/65	0.97	0.10	48,60,88,104	0
37	CA	c	523	1/1	0.97	0.03	79,79,79,79	0
24	CLA	A	405[A]	65/65	0.97	0.11	35,41,55,69	65
24	CLA	B	610	65/65	0.97	0.11	39,53,63,81	0
39	HEM	F	102	43/43	0.97	0.11	55,68,81,89	0
24	CLA	d	403[A]	65/65	0.97	0.10	38,46,76,89	65
40	MG	j	102	1/1	0.97	0.04	63,63,63,63	0
41	HEC	v	201	43/43	0.97	0.13	51,62,70,75	0
24	CLA	b	608	65/65	0.98	0.08	42,54,78,90	0
24	CLA	D	402[A]	65/65	0.98	0.11	33,42,65,73	65
24	CLA	D	402[B]	65/65	0.98	0.11	33,42,65,73	65
24	CLA	C	503	65/65	0.98	0.09	43,55,78,90	0
24	CLA	B	608	65/65	0.98	0.07	37,50,65,78	0

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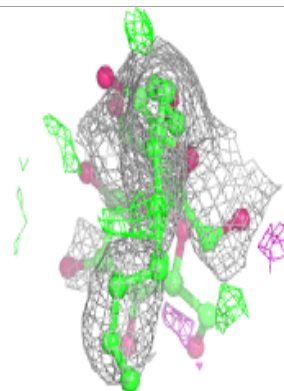
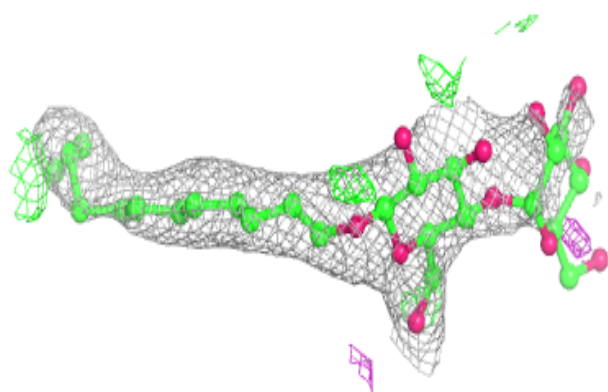
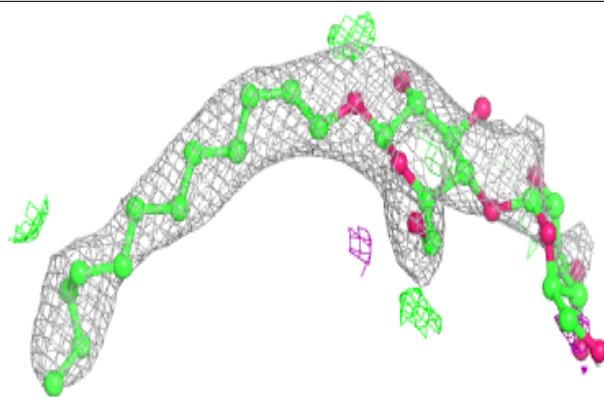
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	PHO	A	408[A]	64/64	0.98	0.08	35,44,51,56	64
25	PHO	A	408[B]	64/64	0.98	0.08	35,44,52,56	64
25	PHO	A	417[A]	64/64	0.98	0.09	35,48,53,61	64
25	PHO	A	417[B]	64/64	0.98	0.09	35,48,53,61	64
25	PHO	a	408[A]	64/64	0.98	0.08	40,48,53,54	64
25	PHO	a	408[B]	64/64	0.98	0.08	40,48,52,54	64
24	CLA	b	603	65/65	0.98	0.08	43,56,78,95	0
24	CLA	B	604	65/65	0.98	0.08	36,47,119,138	0
33	LHG	D	406[A]	49/49	0.98	0.13	44,52,66,77	49
33	LHG	D	406[B]	49/49	0.98	0.13	43,53,66,78	49
24	CLA	A	406[A]	65/65	0.98	0.08	34,42,55,70	65
26	BCR	B	617	40/40	0.98	0.09	41,52,62,64	0
24	CLA	A	406[B]	65/65	0.98	0.08	34,42,56,70	65
41	HEC	V	201	43/43	0.98	0.13	42,50,56,60	0
24	CLA	B	607	65/65	0.98	0.08	35,46,71,90	0
29	OEX	A	414[A]	10/10	0.99	0.04	39,45,49,49	10
23	CL	a	403[B]	1/1	0.99	0.06	49,49,49,49	1
38	BCT	D	401[A]	4/4	0.99	0.12	52,56,60,66	4
38	BCT	D	401[B]	4/4	0.99	0.12	52,56,60,66	4
38	BCT	d	401[A]	4/4	0.99	0.06	53,57,64,73	4
38	BCT	d	401[B]	4/4	0.99	0.06	53,57,64,70	4
21	OEY	A	401[B]	11/11	0.99	0.05	38,44,49,51	11
23	CL	A	404[A]	1/1	0.99	0.03	47,47,47,47	1
40	MG	J	102	1/1	0.99	0.08	54,54,54,54	0
23	CL	A	404[B]	1/1	0.99	0.03	47,47,47,47	1
23	CL	a	403[A]	1/1	0.99	0.06	49,49,49,49	1
37	CA	c	524	1/1	0.99	0.09	76,76,76,76	0
22	FE2	A	402[B]	1/1	1.00	0.05	51,51,51,51	1
22	FE2	a	402[A]	1/1	1.00	0.03	52,52,52,52	1
23	CL	a	404[A]	1/1	1.00	0.02	52,52,52,52	1
23	CL	a	404[B]	1/1	1.00	0.02	52,52,52,52	1
22	FE2	a	402[B]	1/1	1.00	0.03	53,53,53,53	1
29	OEX	a	414[A]	10/10	1.00	0.04	46,47,50,53	10
23	CL	A	403[A]	1/1	1.00	0.01	41,41,41,41	1
23	CL	A	403[B]	1/1	1.00	0.01	41,41,41,41	1
21	OEY	a	401[B]	11/11	1.00	0.04	46,48,51,53	11
22	FE2	A	402[A]	1/1	1.00	0.05	51,51,51,51	1

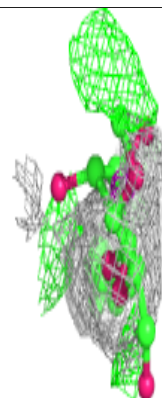
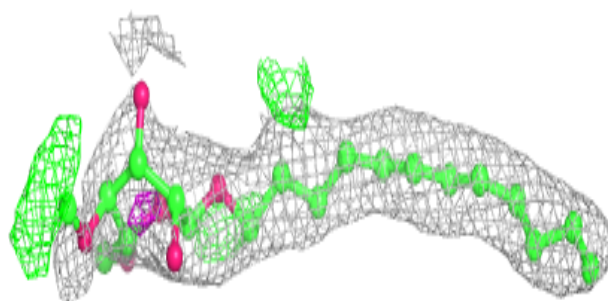
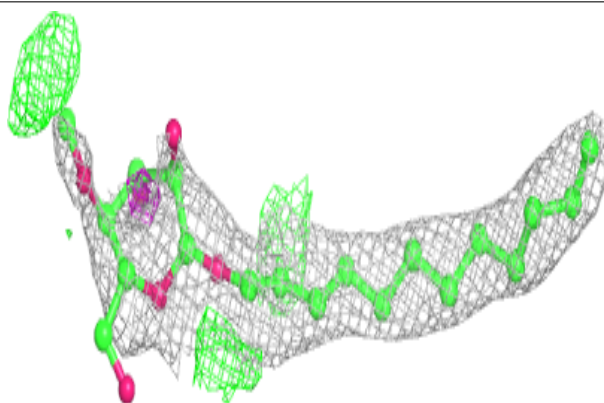
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT M 104:

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

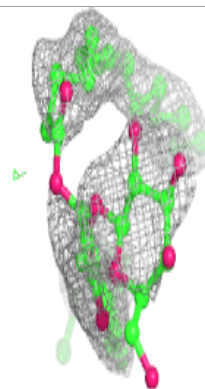
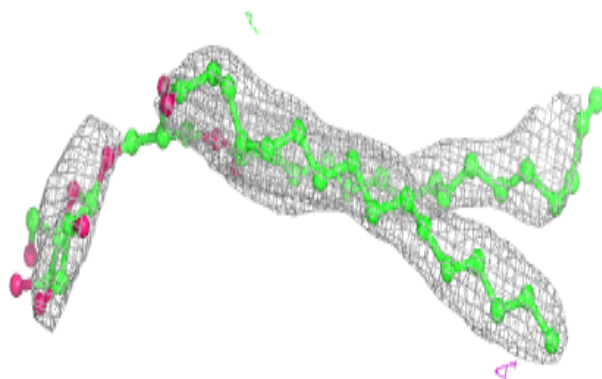
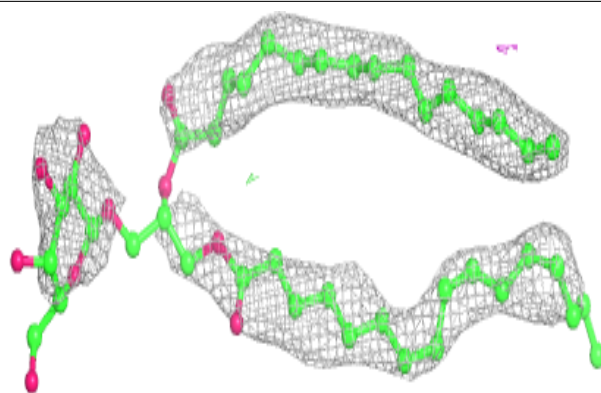
**Electron density around LMT b 620:**

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

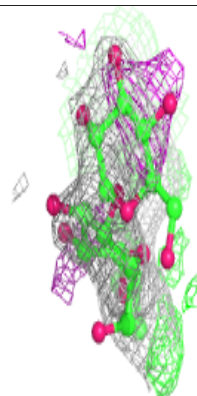
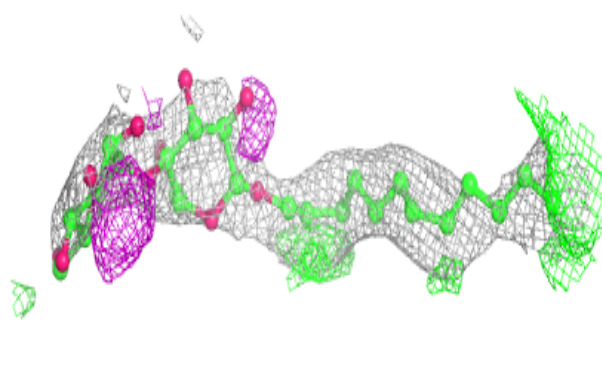
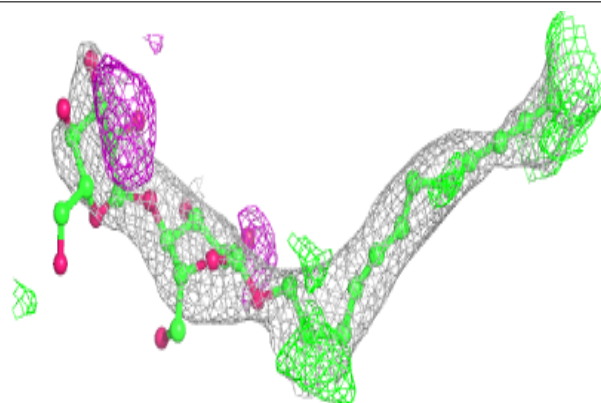


Electron density around LMG C 521:

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

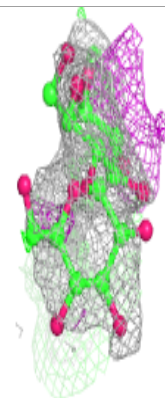
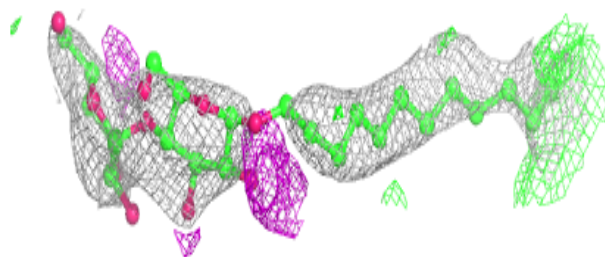
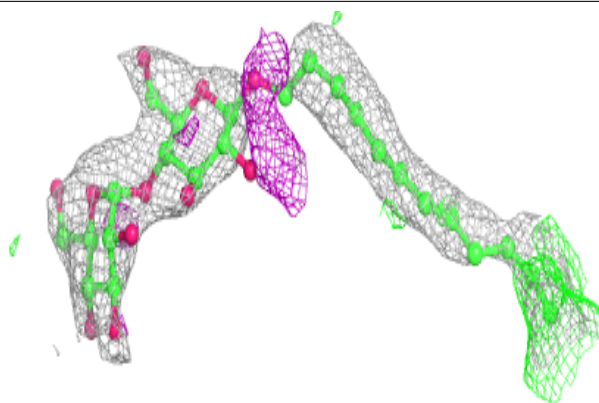
**Electron density around LMT B 628:**

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

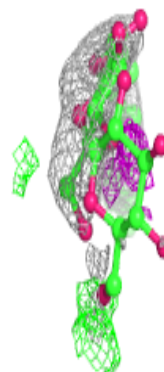
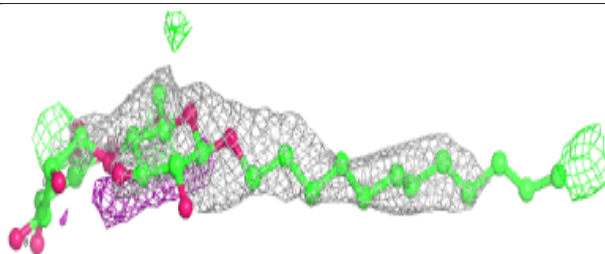
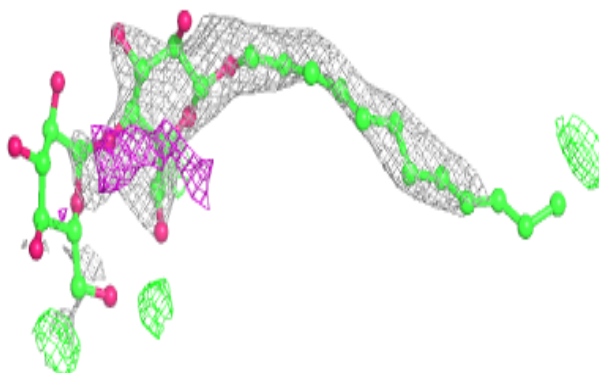


Electron density around LMT A 418:

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

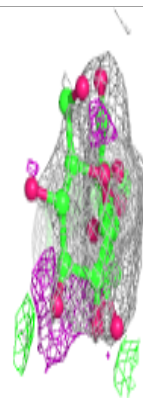
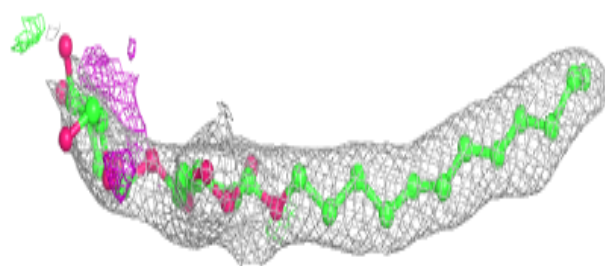
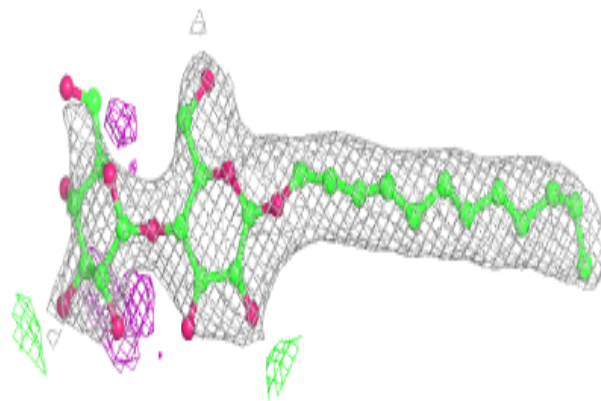
**Electron density around LMT F 101:**

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

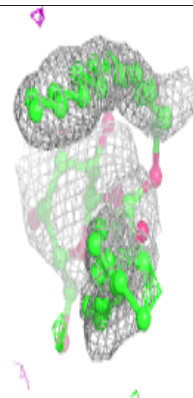
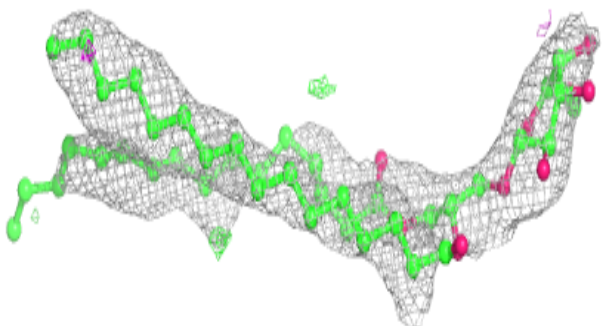
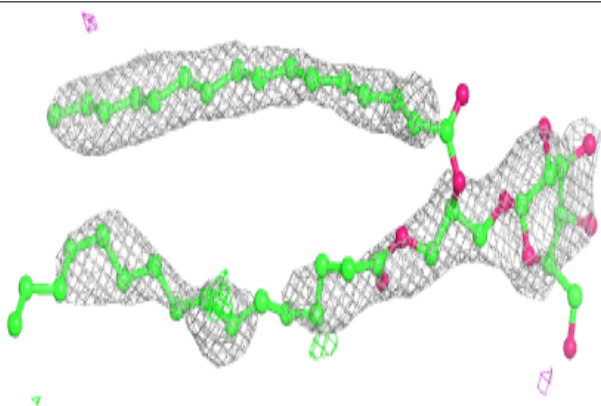


Electron density around LMT M 102:

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

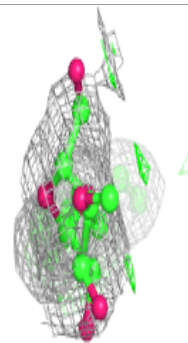
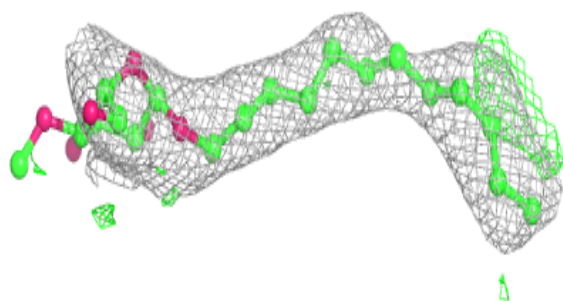
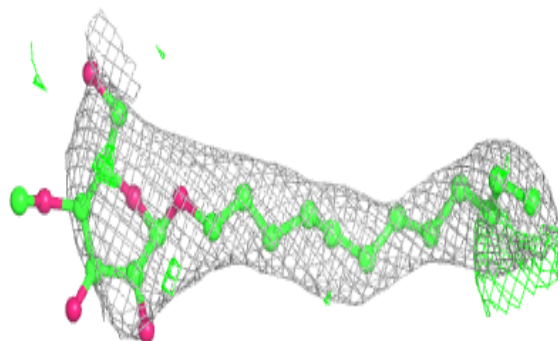
**Electron density around LMG c 521:**

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

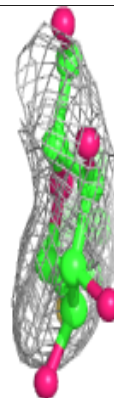
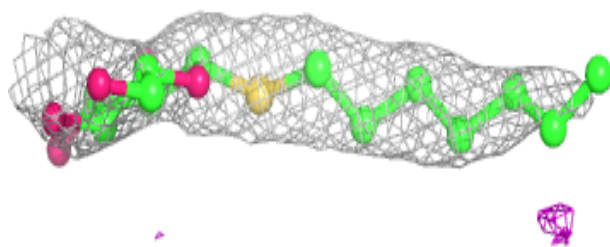
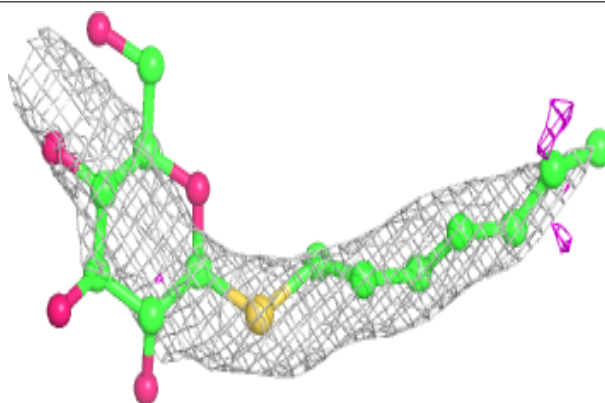


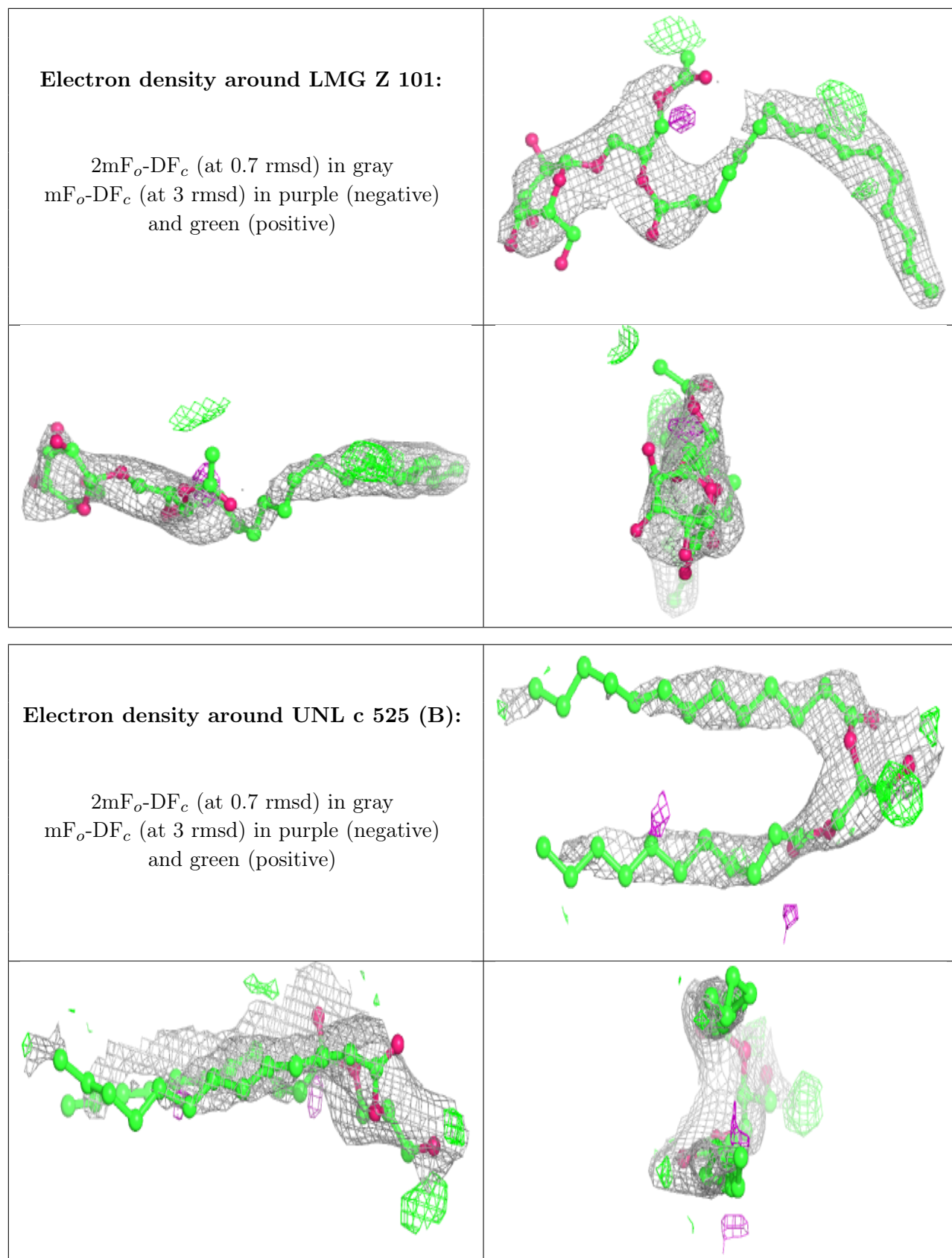
Electron density around LMT B 630:

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

**Electron density around HTG b 622:**

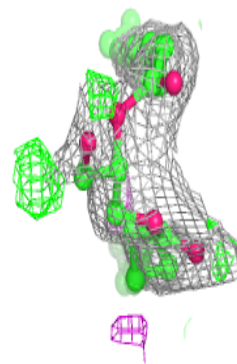
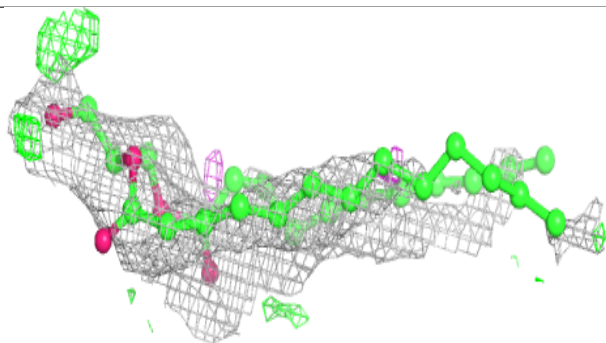
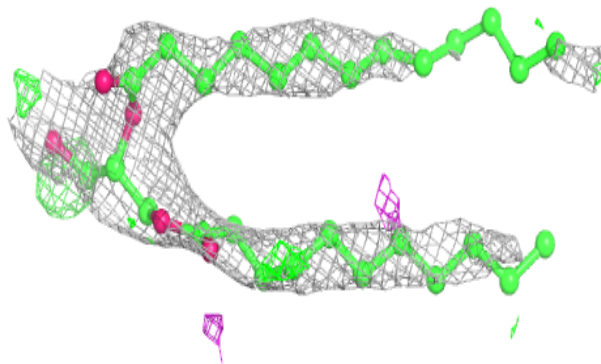
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



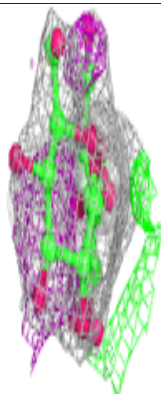
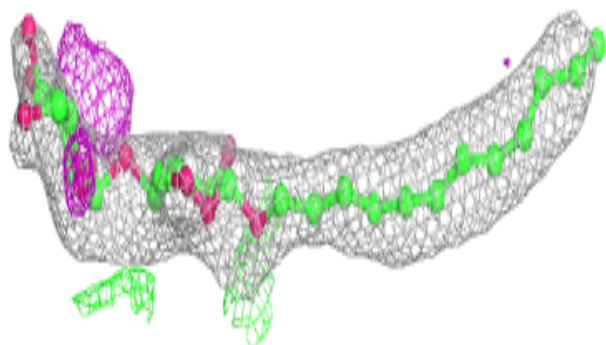
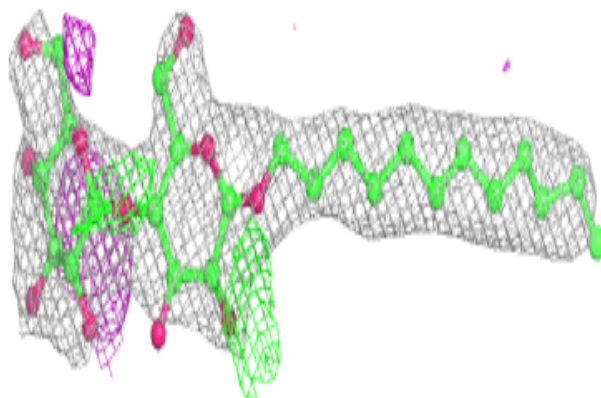


Electron density around UNL c 525 (A):

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

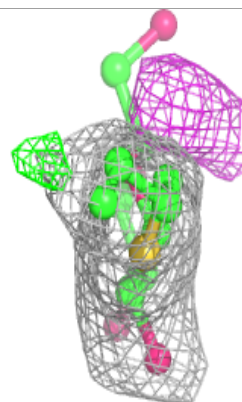
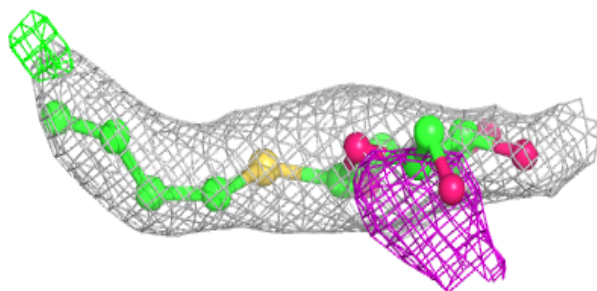
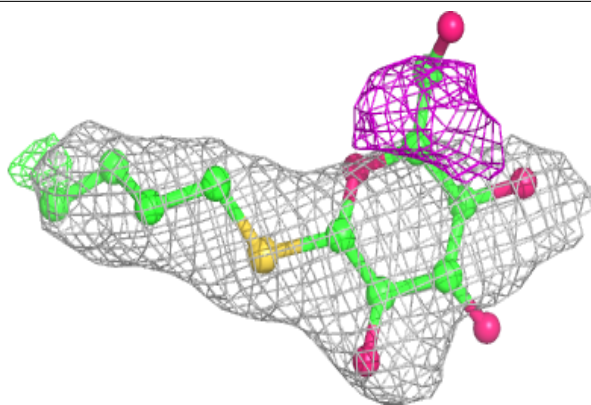
**Electron density around LMT m 102:**

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

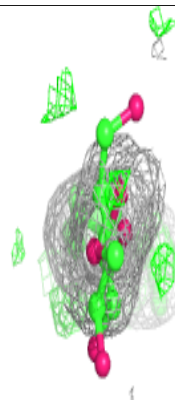
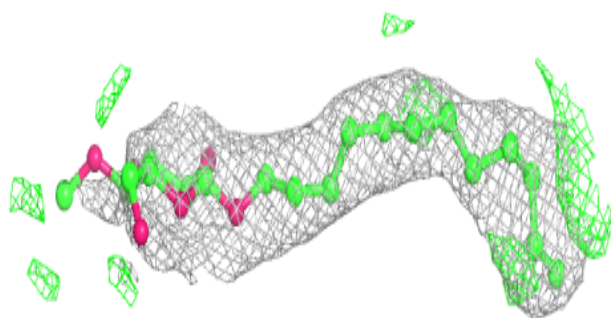
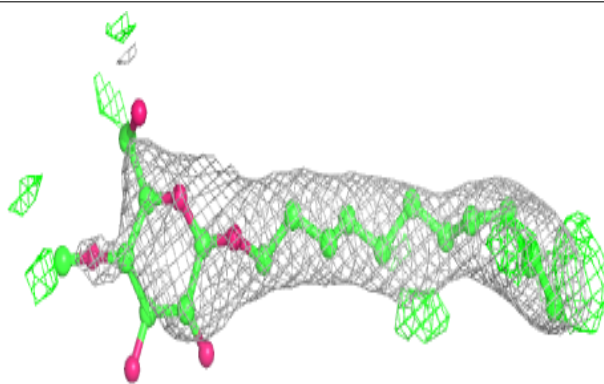


Electron density around HTG D 410:

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

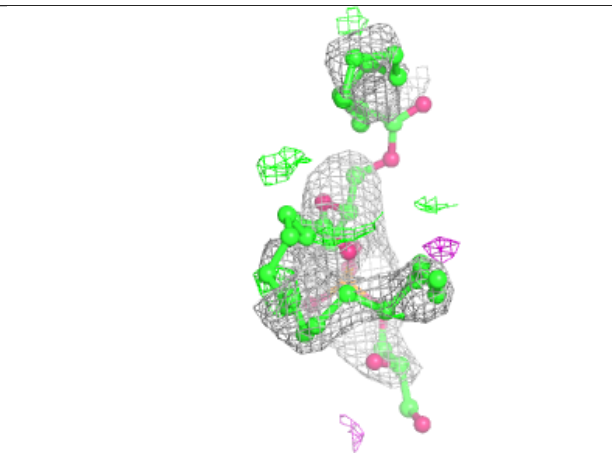
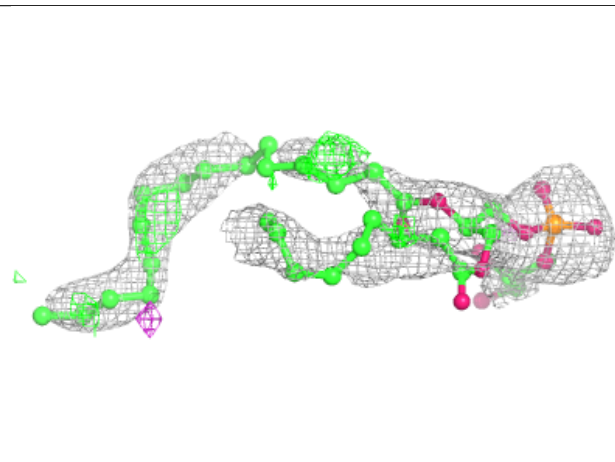
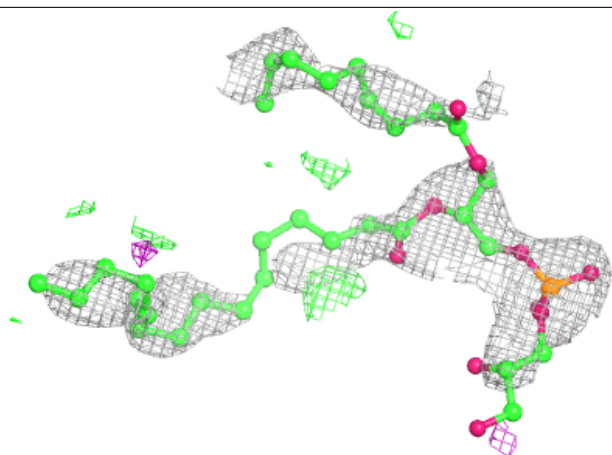
**Electron density around LMT b 626:**

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



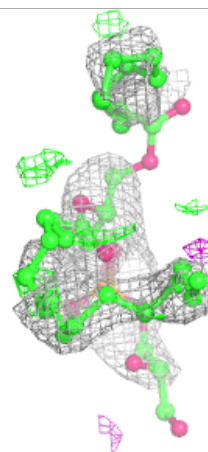
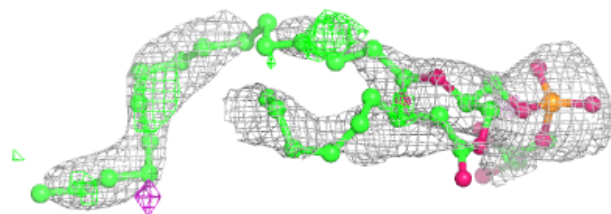
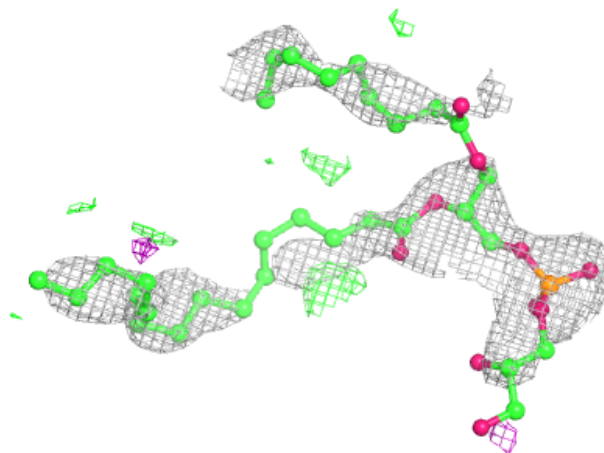
Electron density around LHG a 420 (A):

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



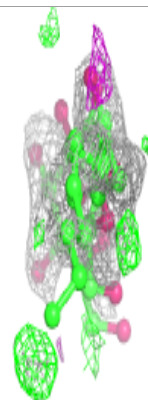
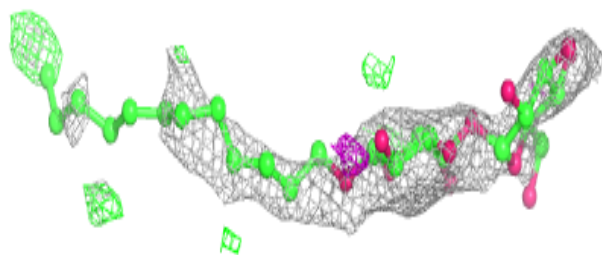
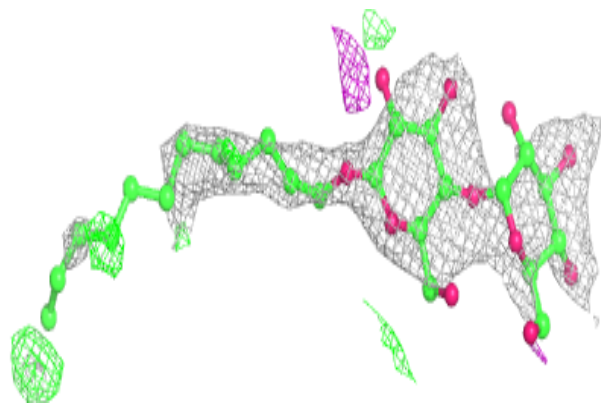
Electron density around LHG a 420 (B):

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

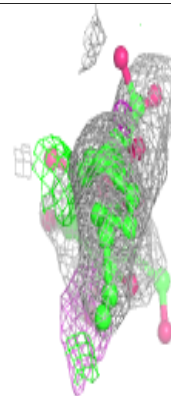
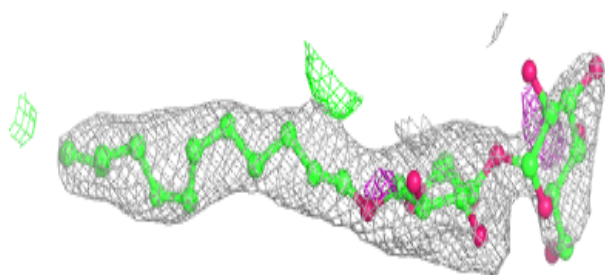
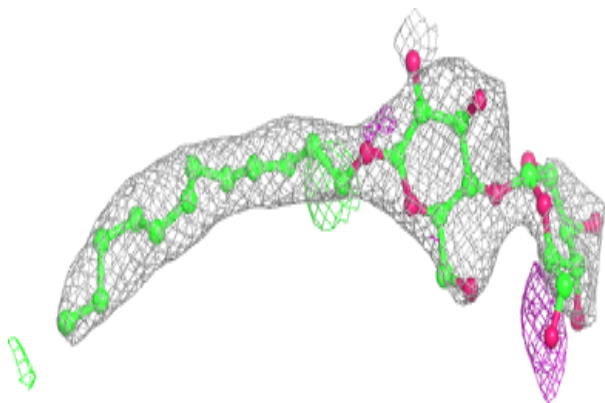


Electron density around LMT c 501:

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

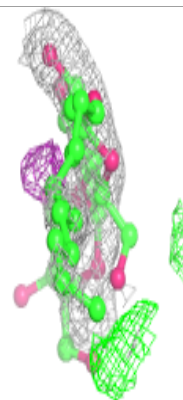
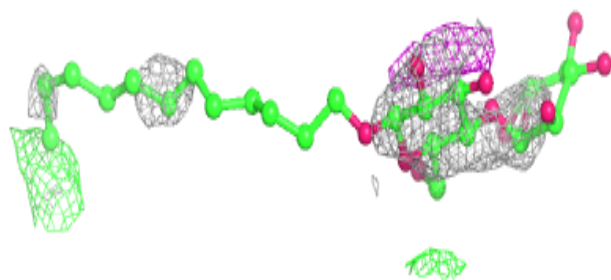
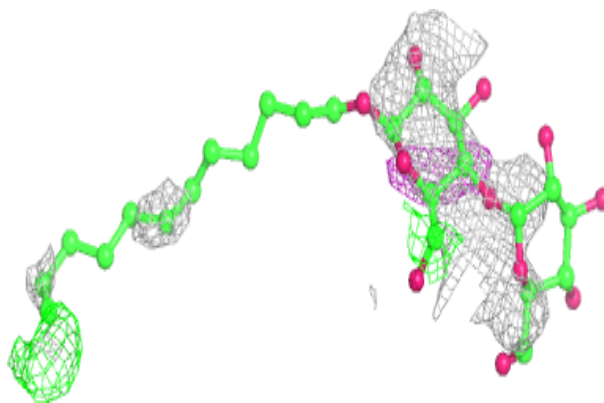
**Electron density around LMT B 627:**

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

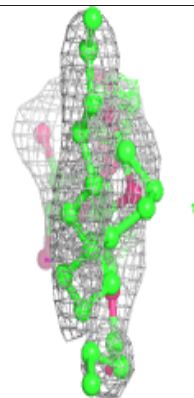
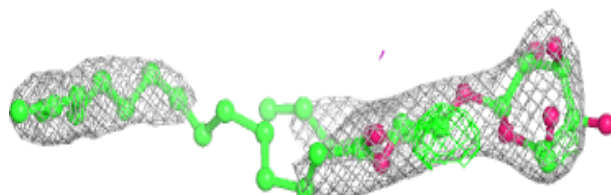
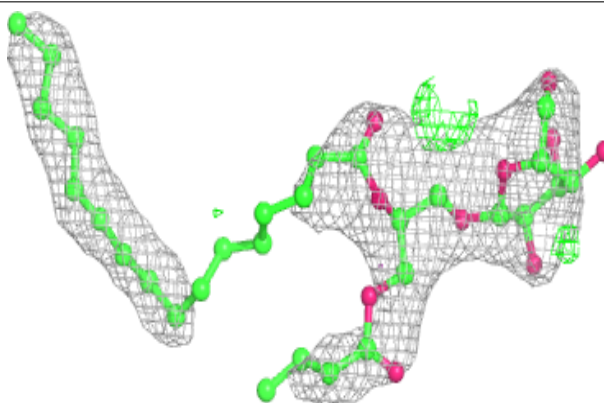


Electron density around LMT e 102:

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

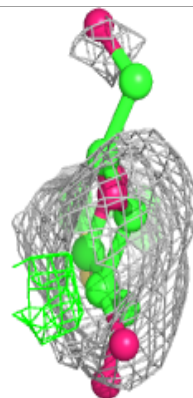
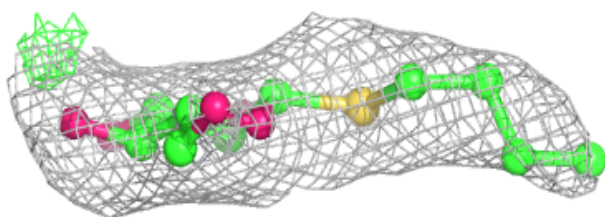
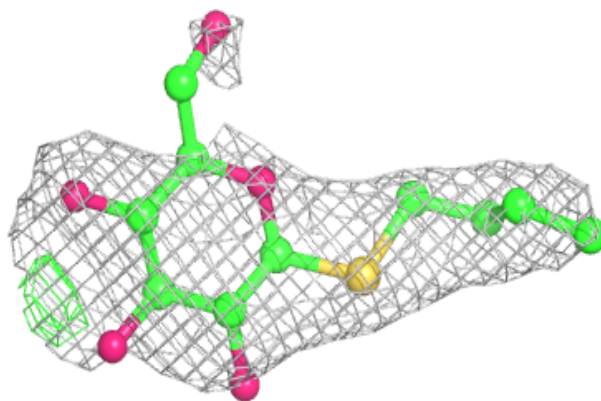
**Electron density around LMG z 101:**

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

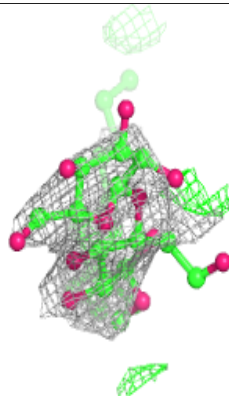
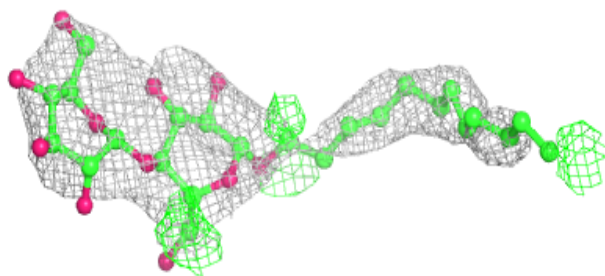
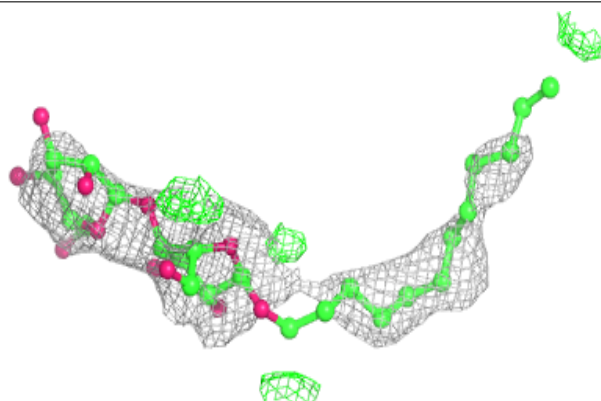


Electron density around HTG d 411:

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

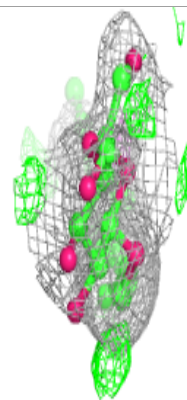
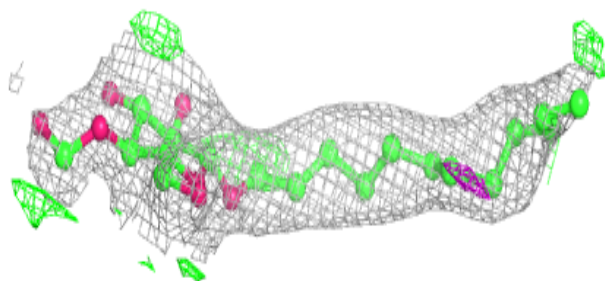
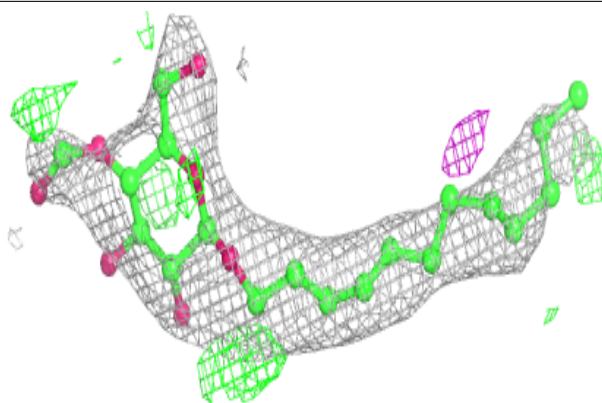
**Electron density around LMT A 421:**

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

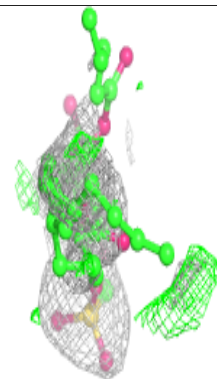
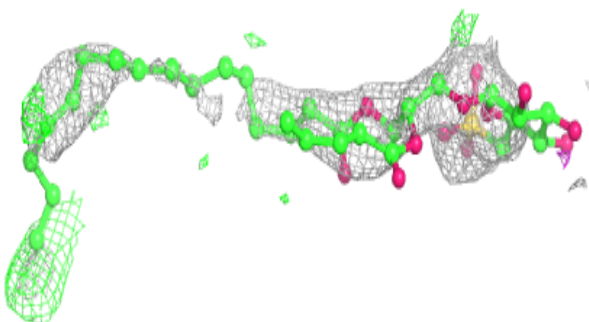
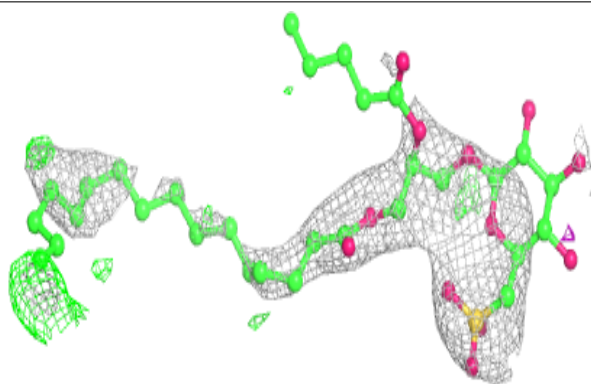


Electron density around LMT t 101:

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

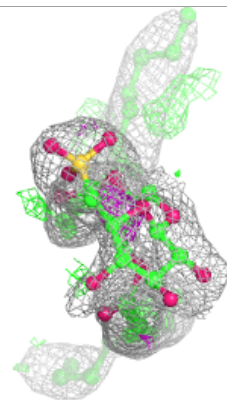
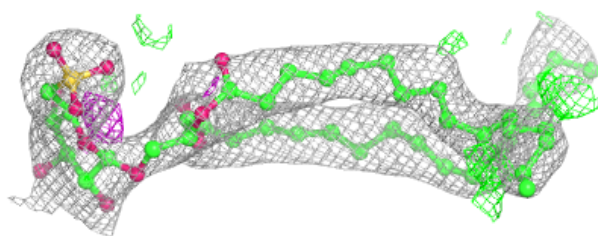
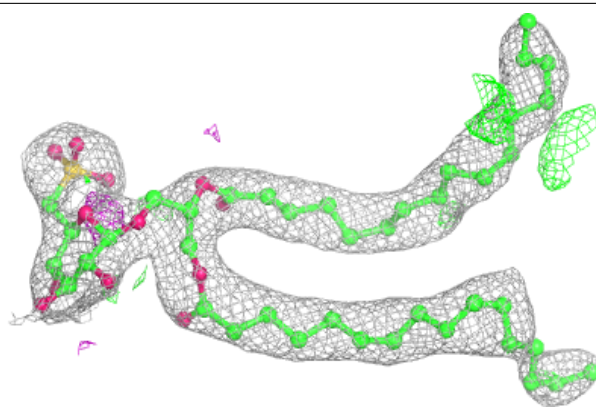
**Electron density around SQD f 101:**

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

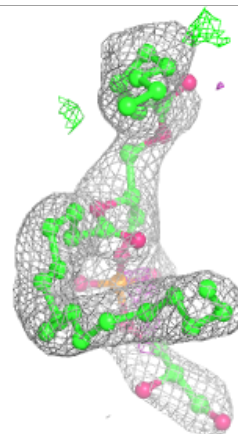
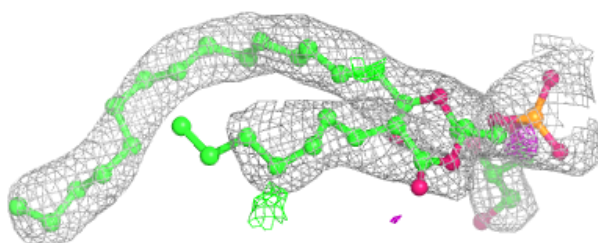
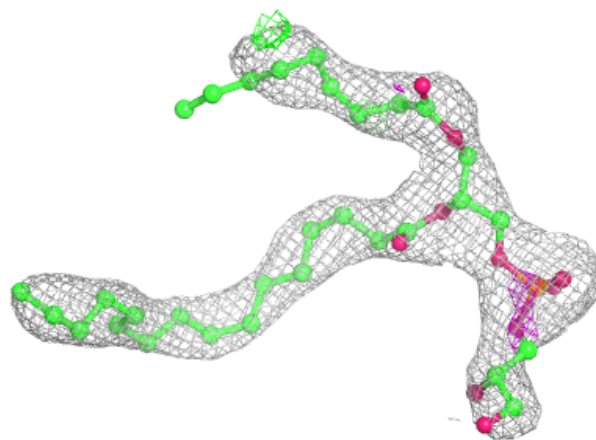


Electron density around SQD L 102:

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

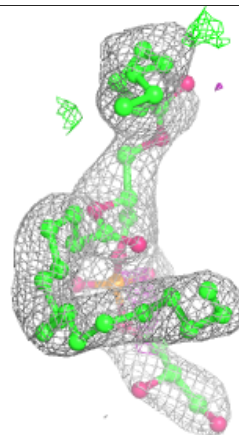
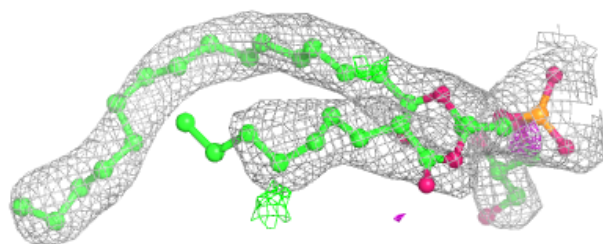
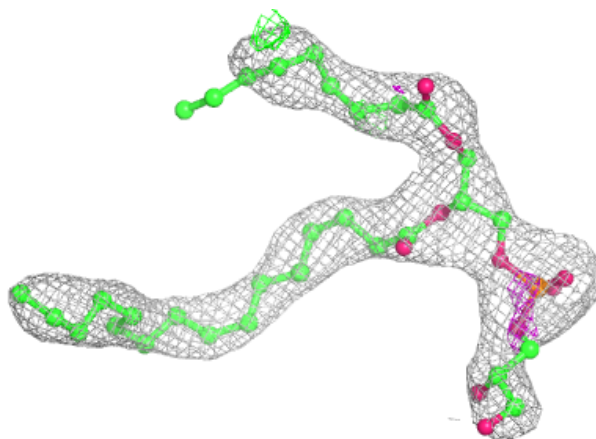
**Electron density around LHG E 101 (A):**

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

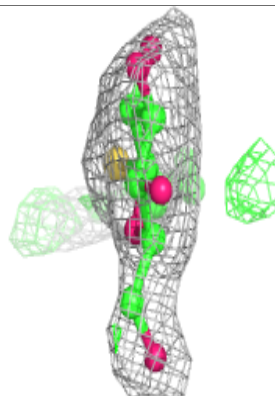
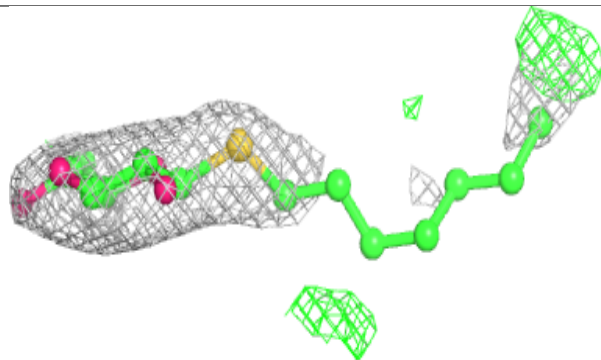
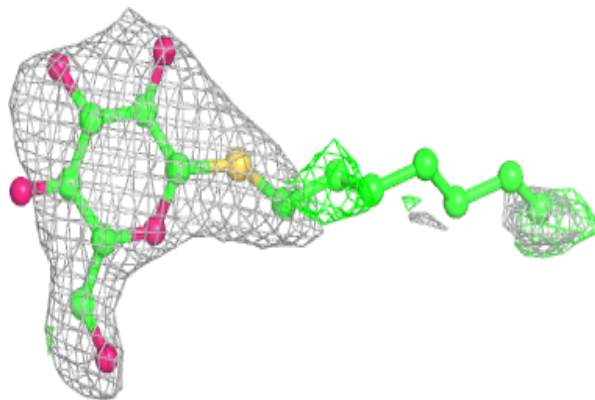


Electron density around LHG E 101 (B):

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

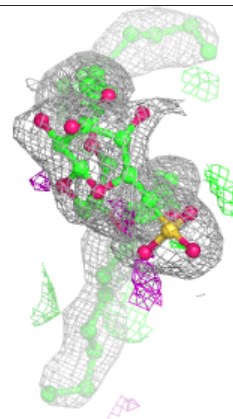
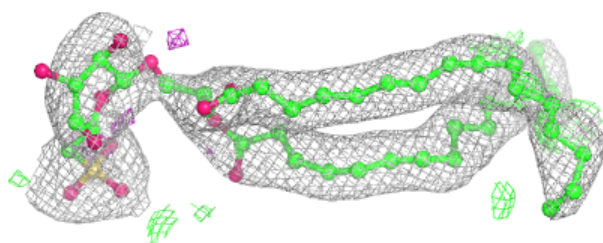
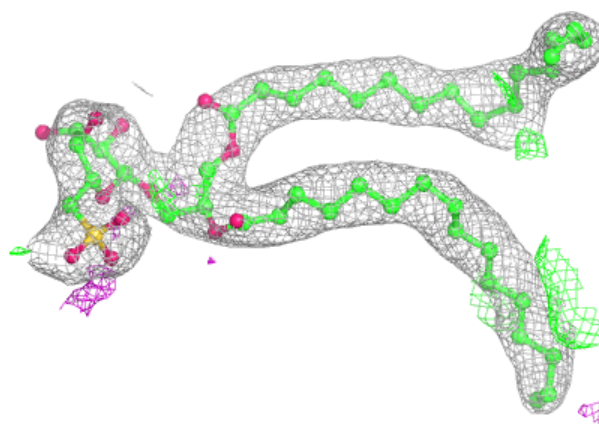
**Electron density around HTG C 522:**

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

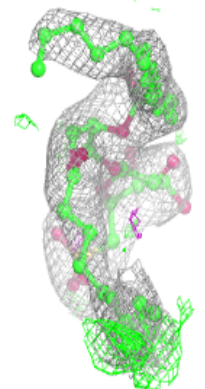
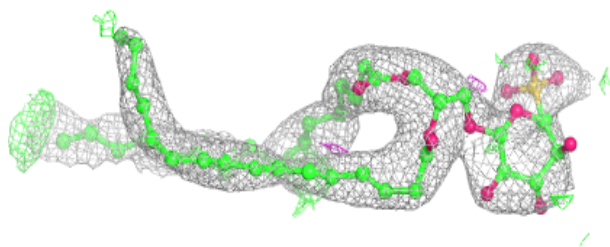
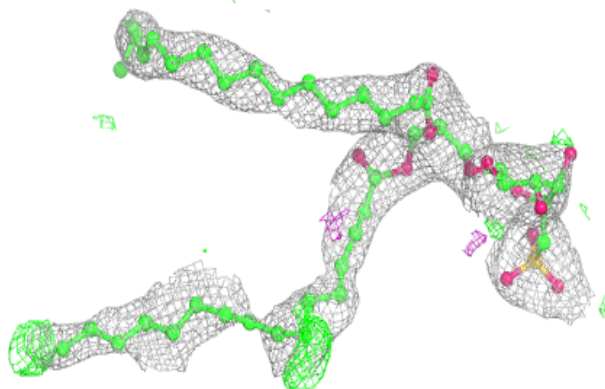


Electron density around SQD B 620:

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

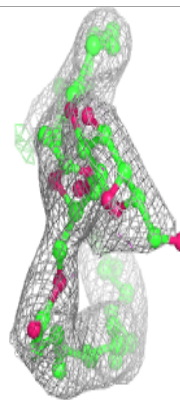
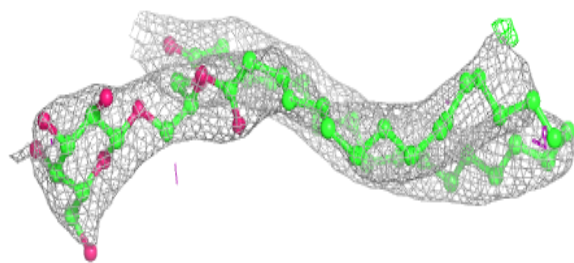
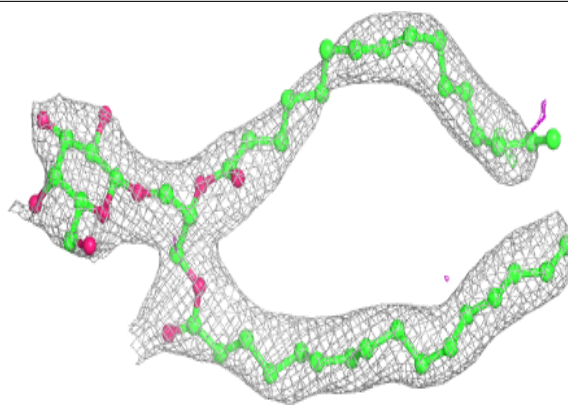
**Electron density around SQD a 413:**

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

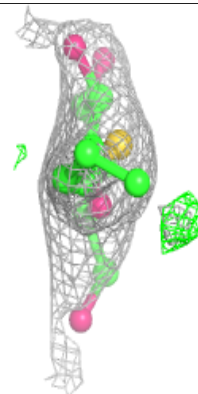
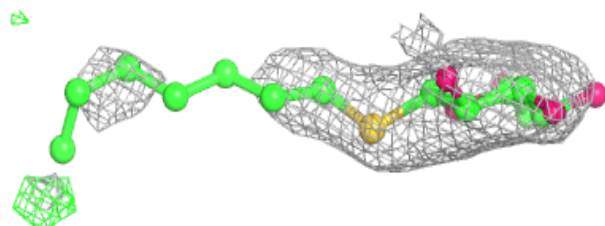
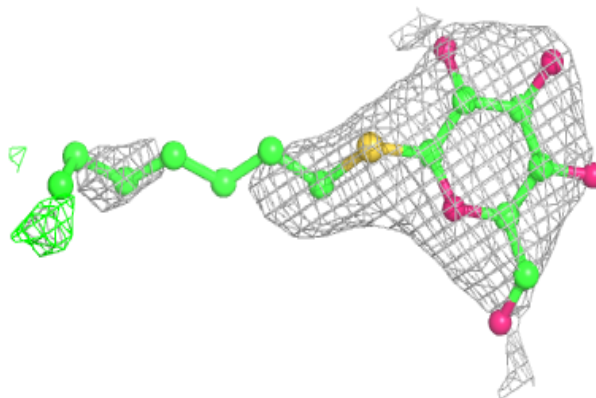


Electron density around LMG a 417:

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

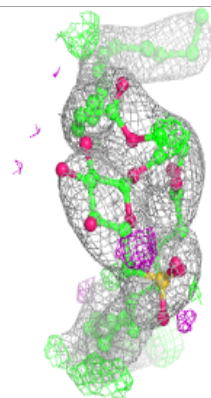
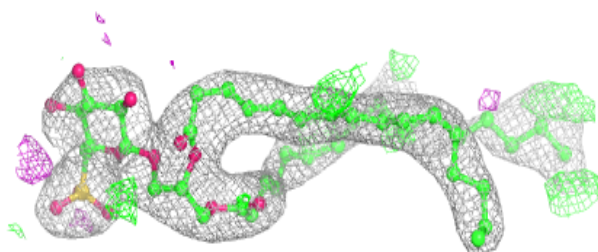
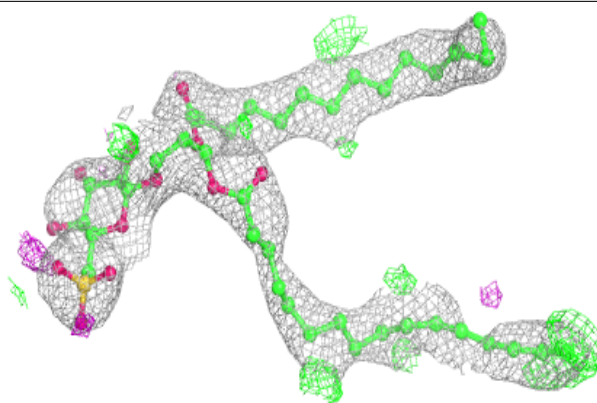
**Electron density around HTG c 522:**

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

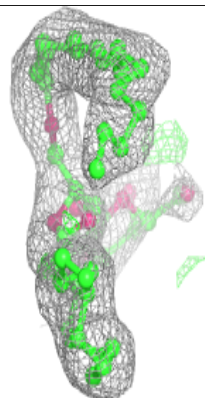
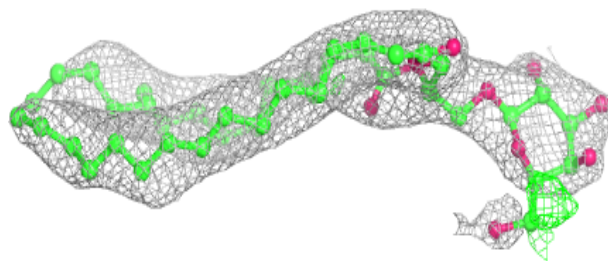
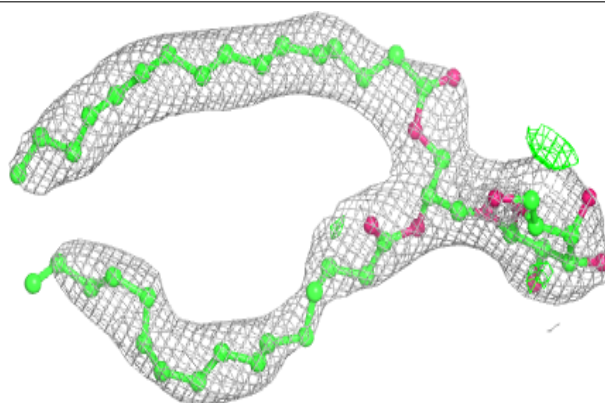


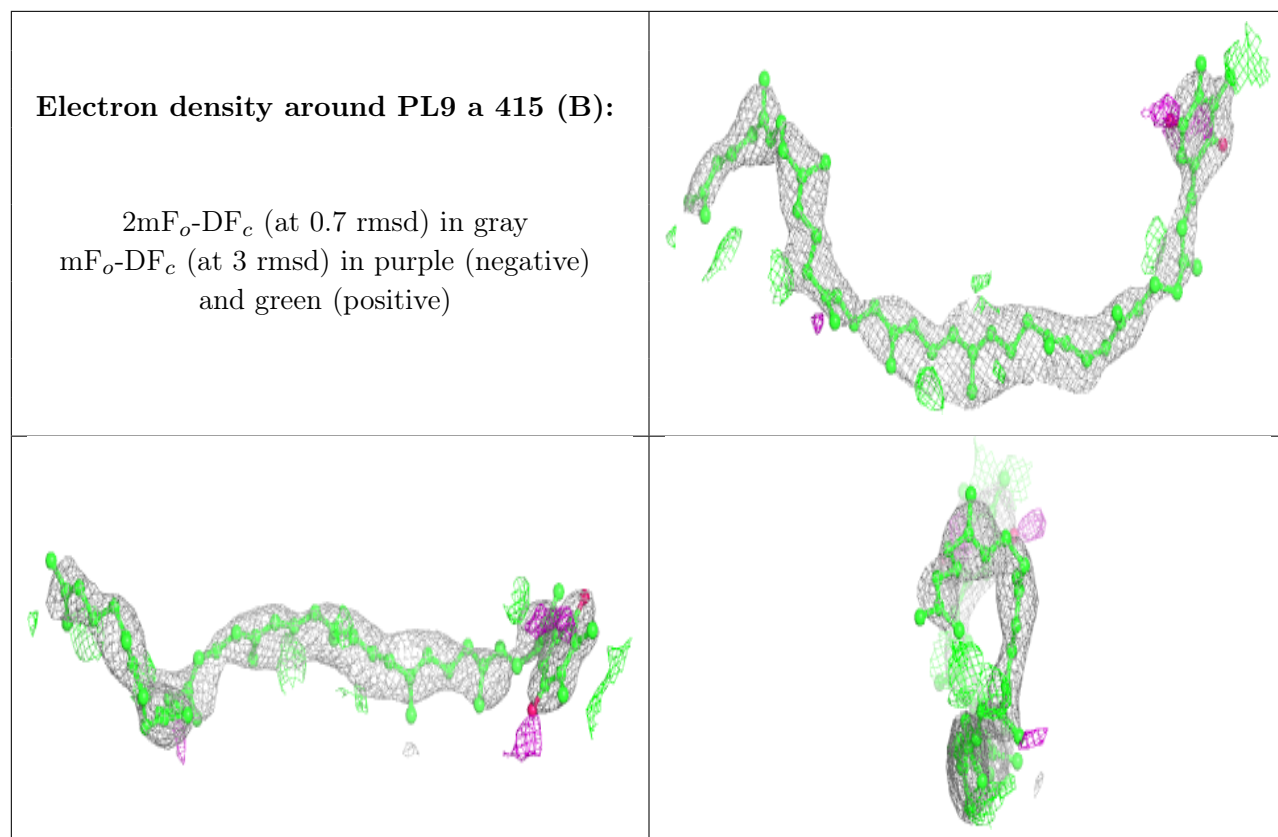
Electron density around SQD A 413:

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

**Electron density around LMG C 501:**

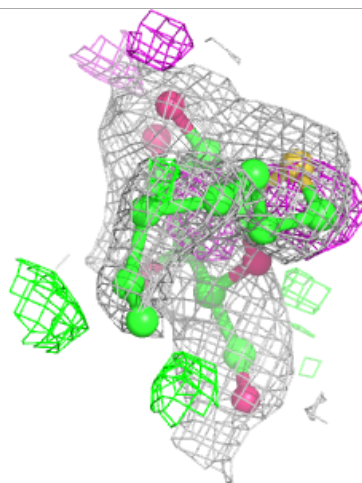
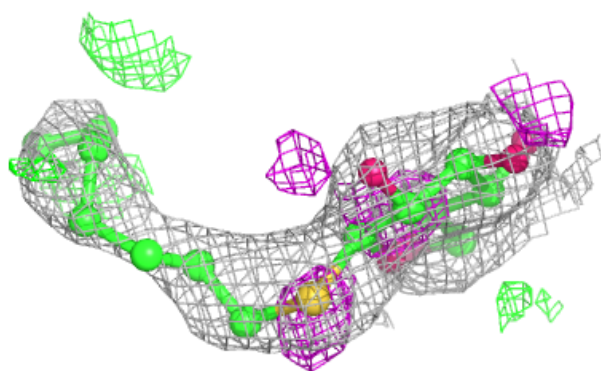
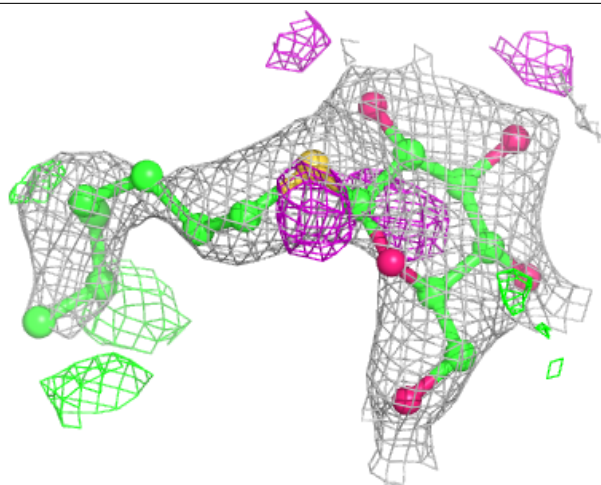
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

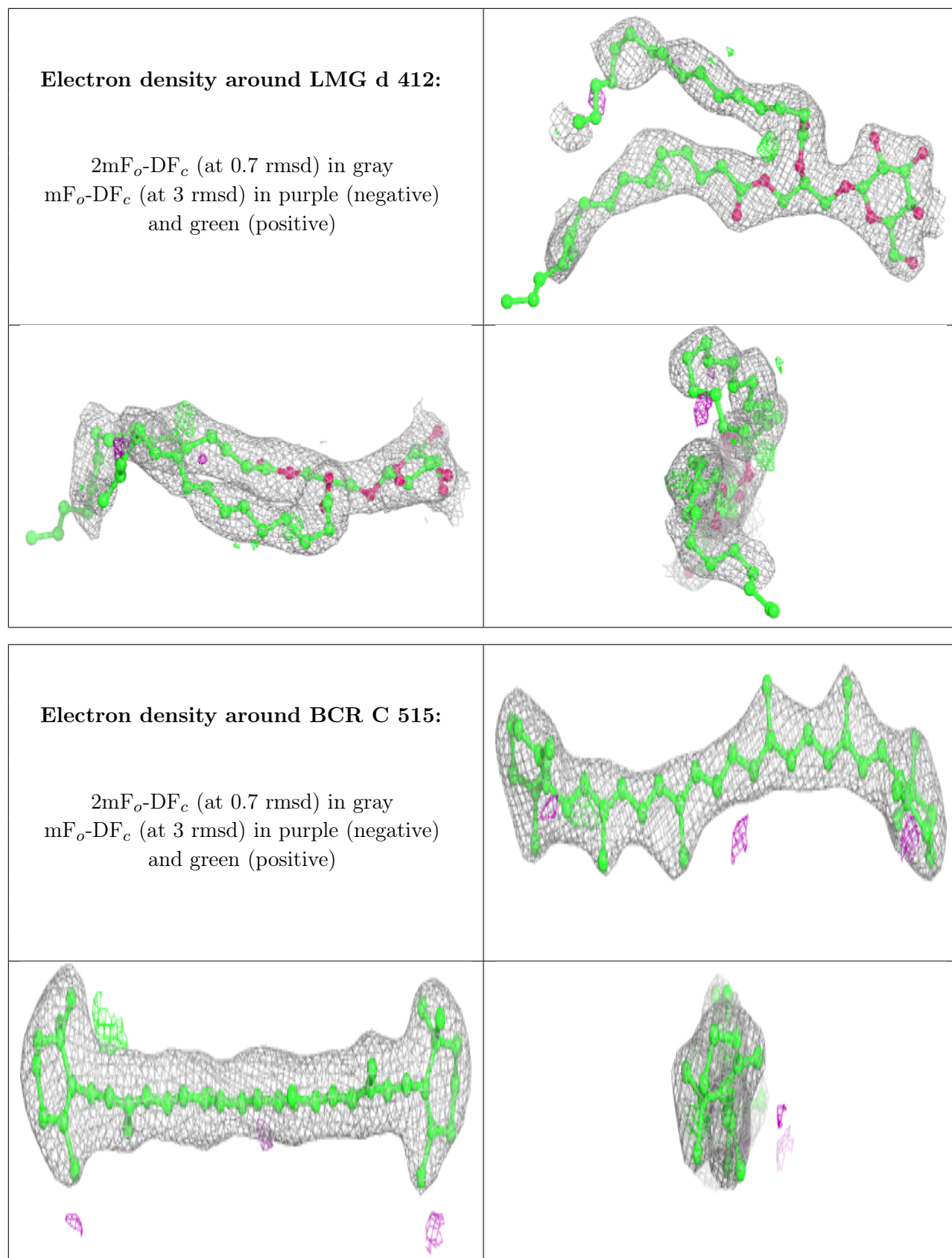




Electron density around HTG B 622:

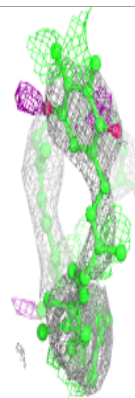
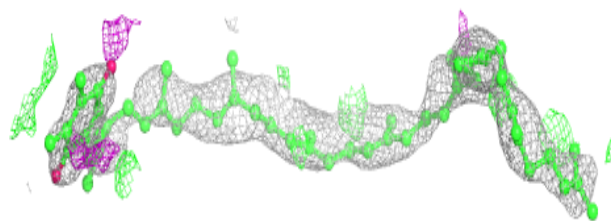
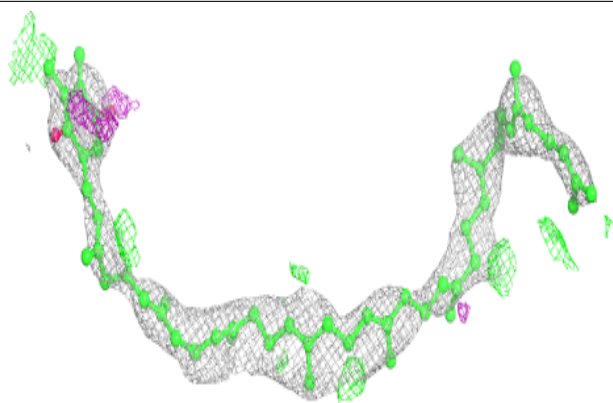
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



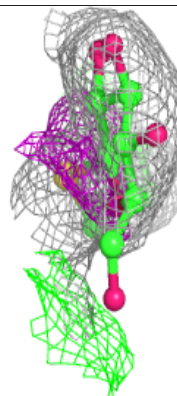
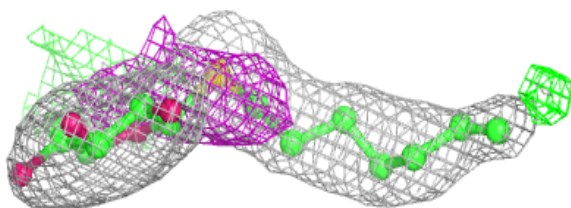
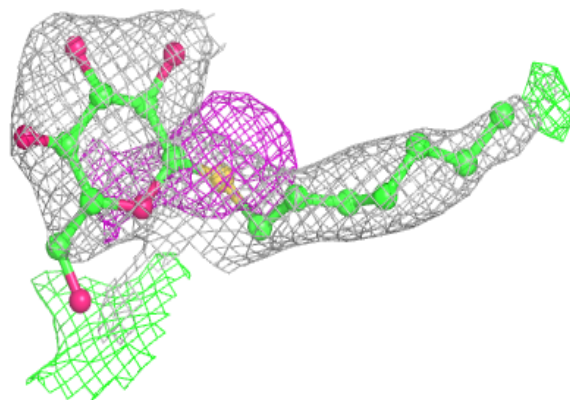


Electron density around PL9 a 415 (A):

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

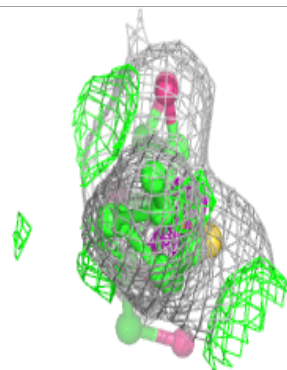
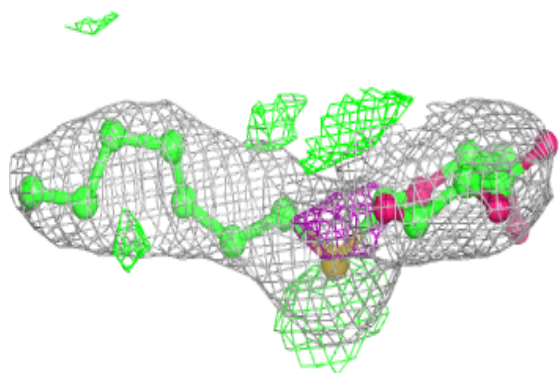
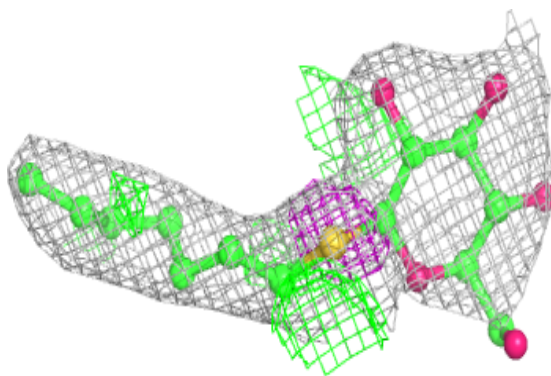
**Electron density around HTG b 621:**

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

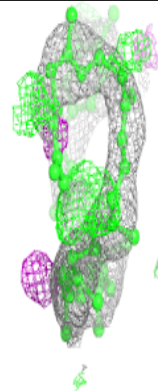
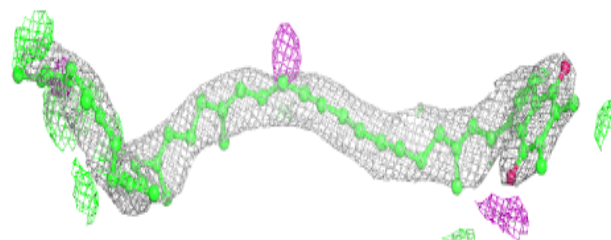
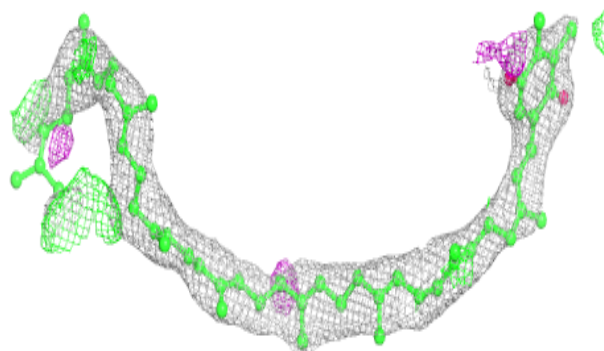


Electron density around HTG B 621:

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

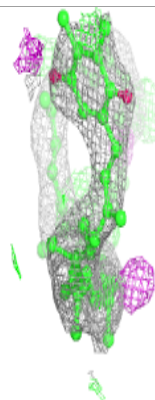
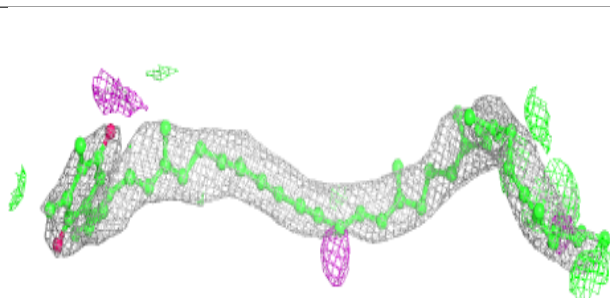
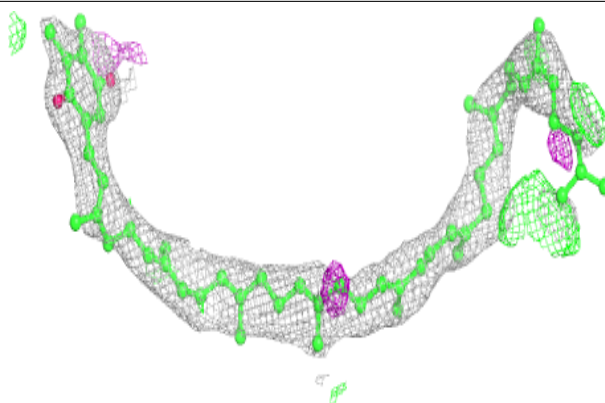
**Electron density around PL9 A 415 (A):**

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

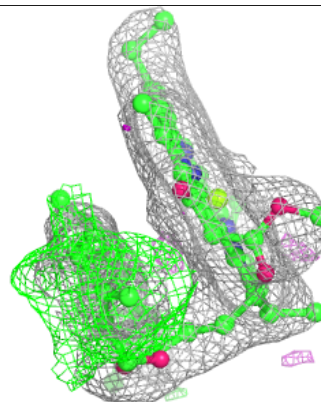
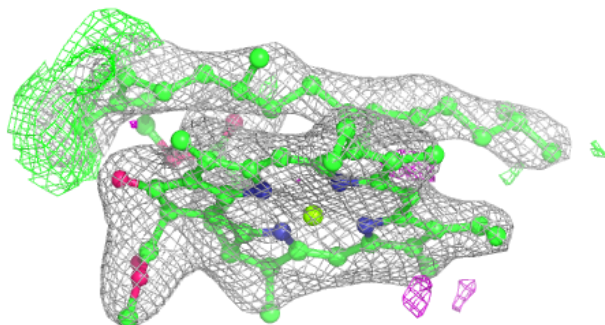
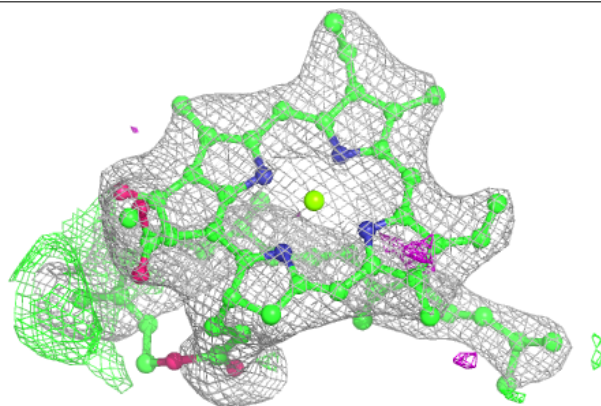


Electron density around PL9 A 415 (B):

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

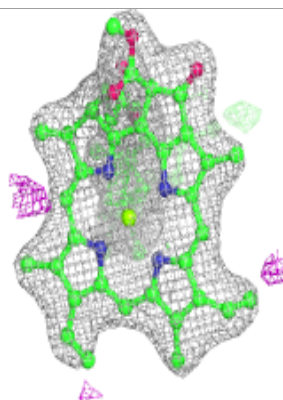
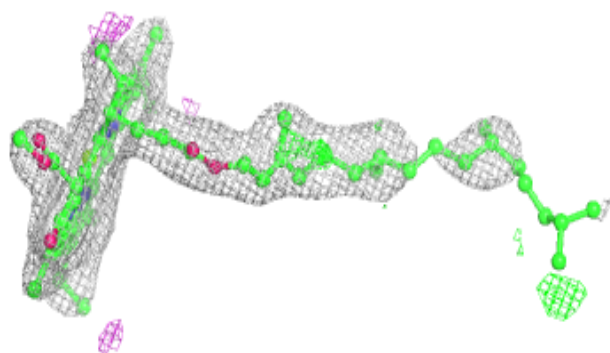
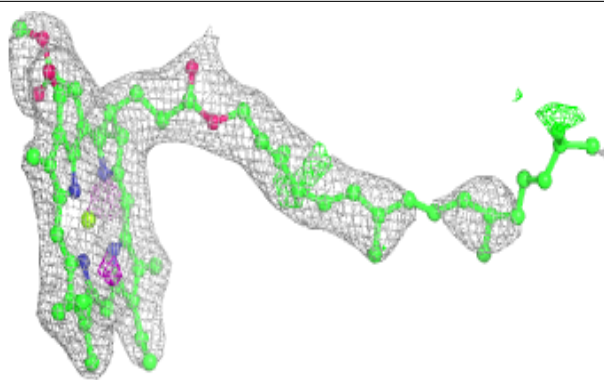
**Electron density around CLA b 601:**

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

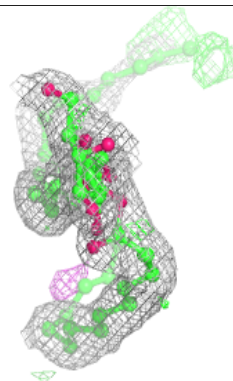
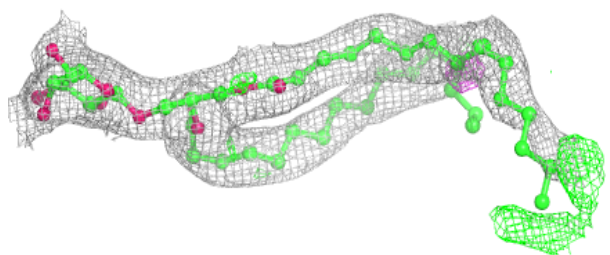
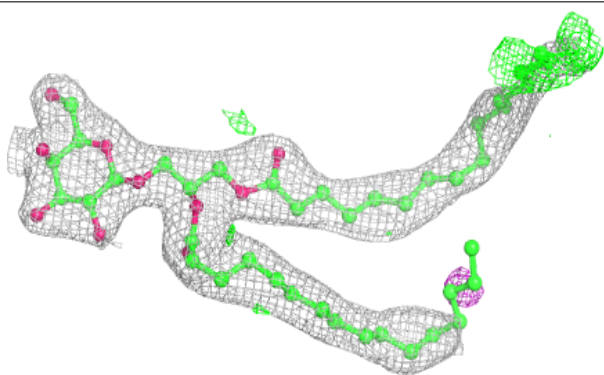


Electron density around CLA d 404:

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

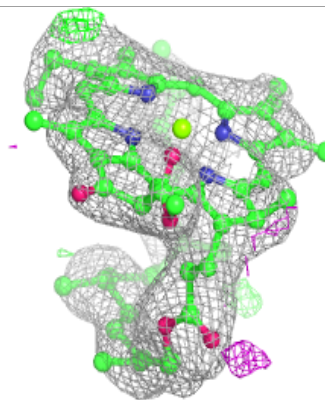
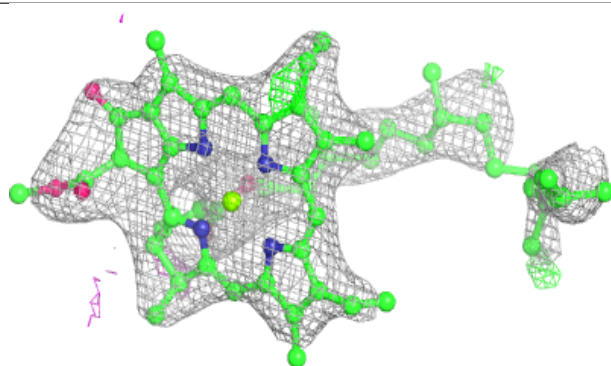
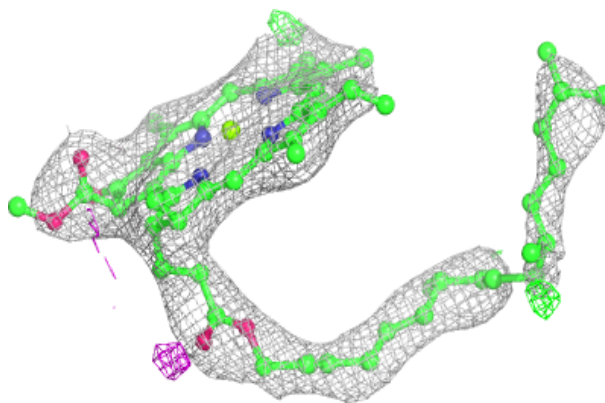
**Electron density around LMG D 411:**

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



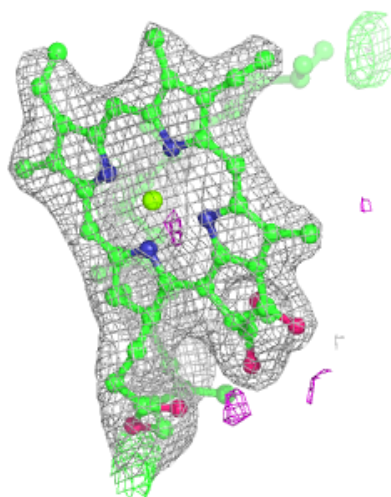
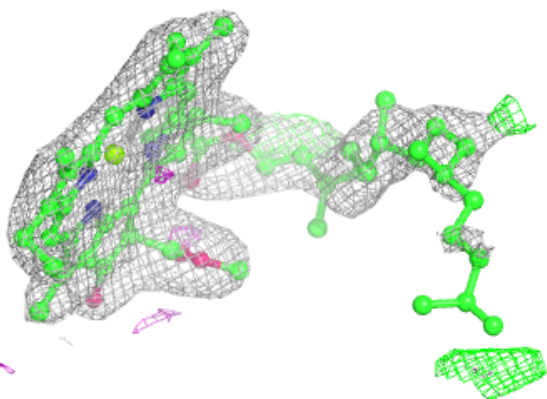
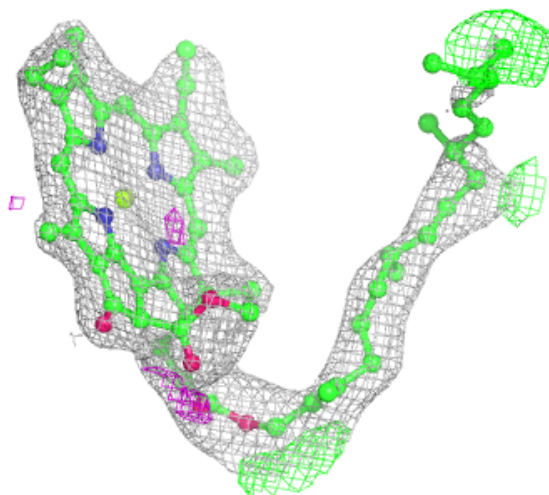
Electron density around CLA c 514:

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



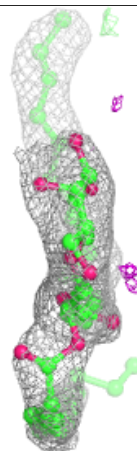
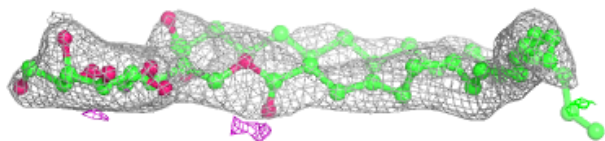
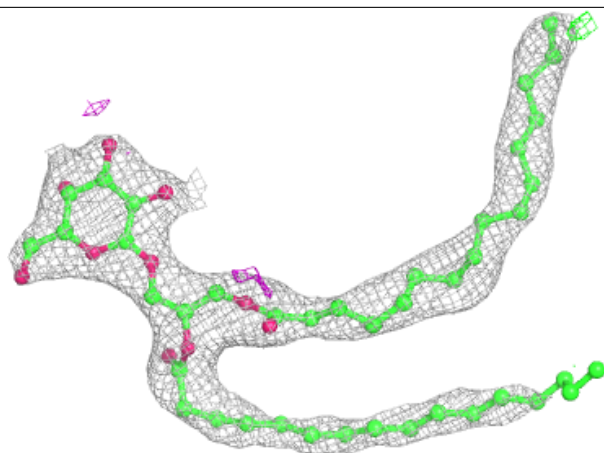
Electron density around CLA b 616:

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

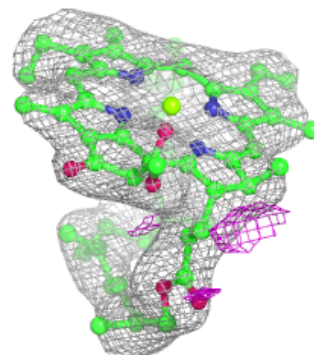
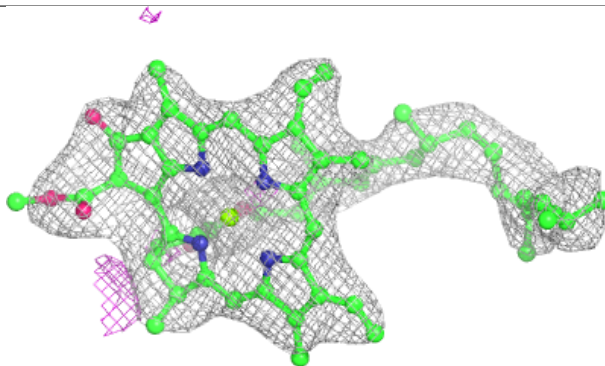
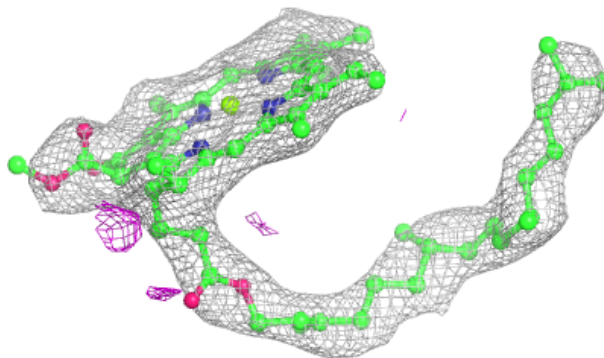


Electron density around LMG c 520:

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

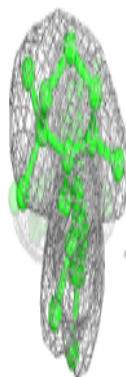
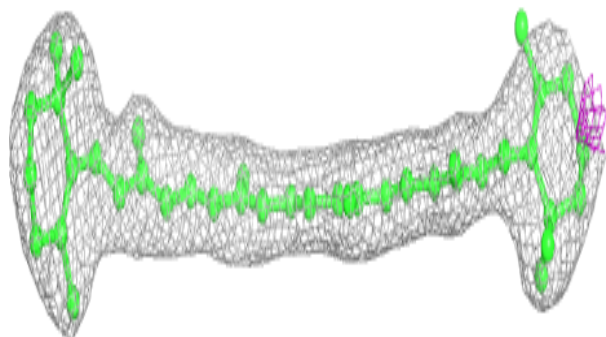
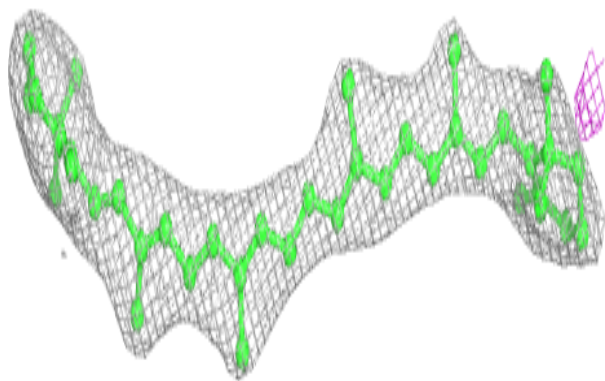
**Electron density around CLA C 514:**

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

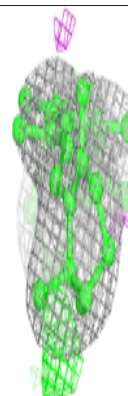
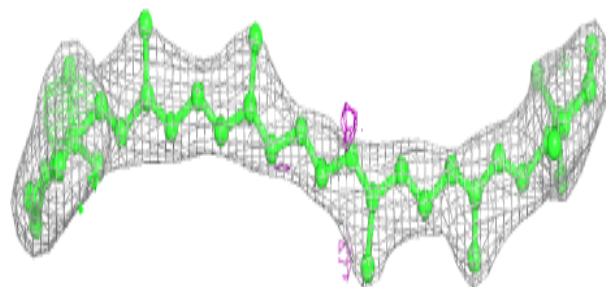
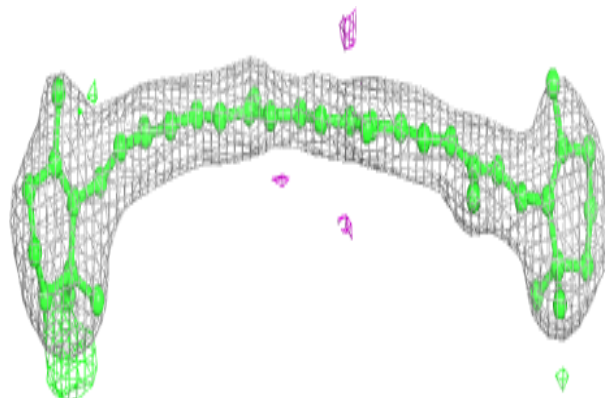


Electron density around BCR h 101:

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

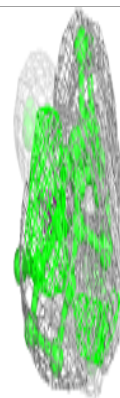
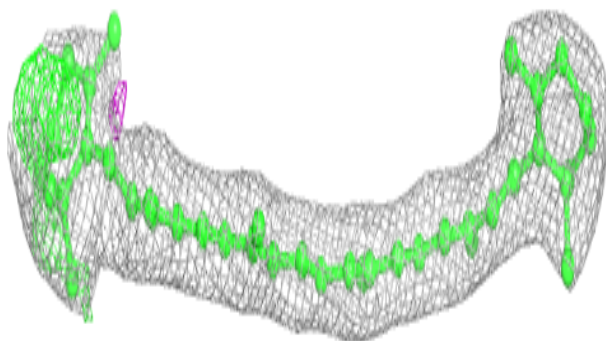
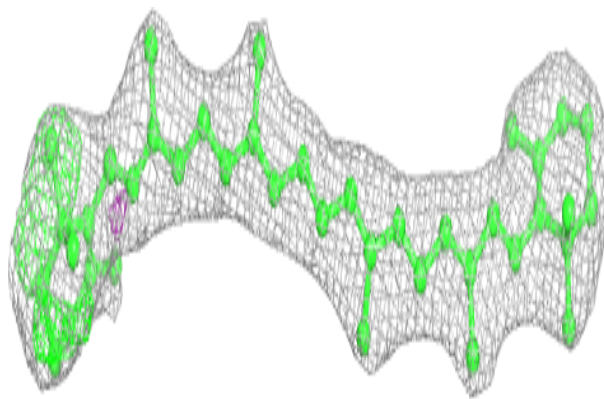
**Electron density around BCR K 102:**

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

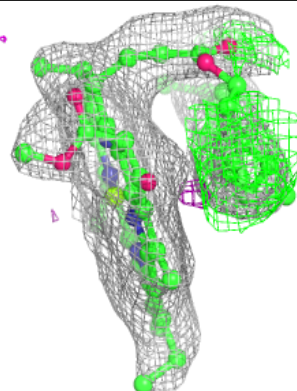
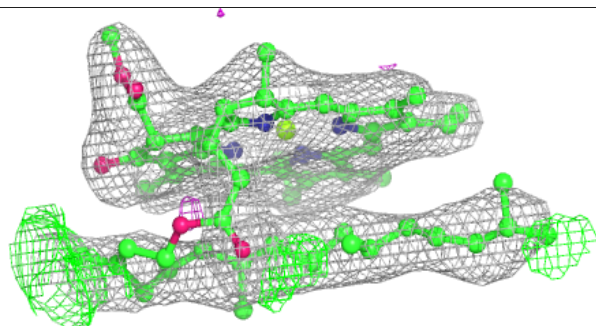
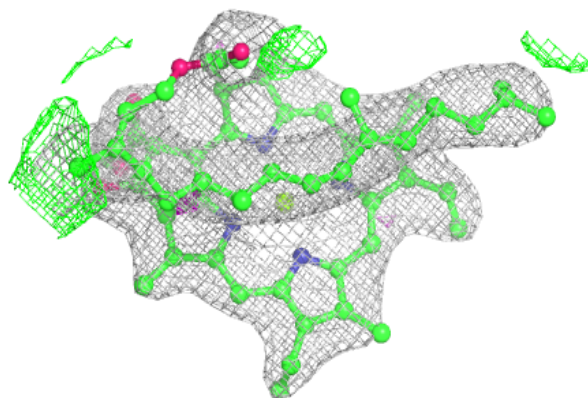


Electron density around BCR d 405:

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

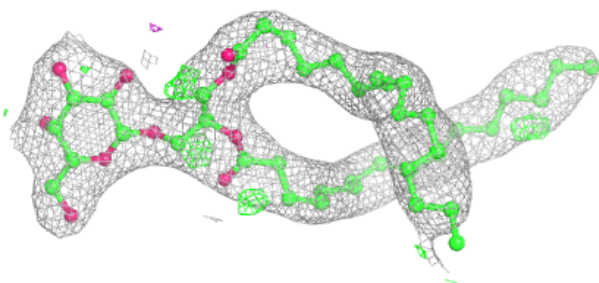
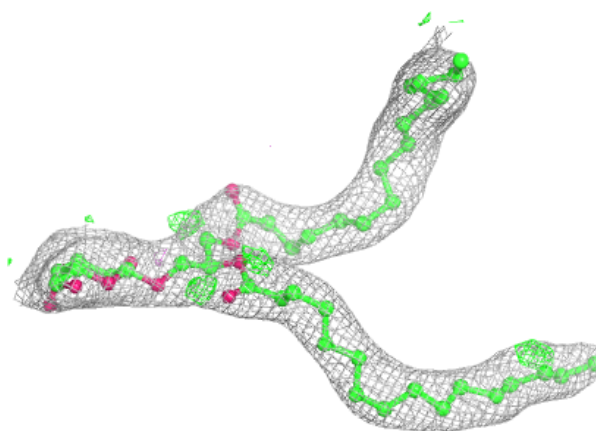
**Electron density around CLA B 601:**

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

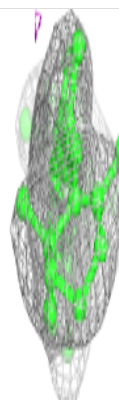
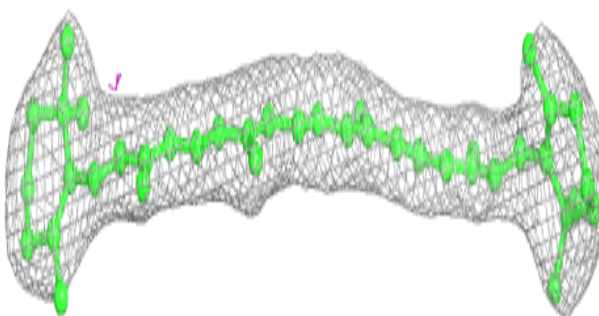
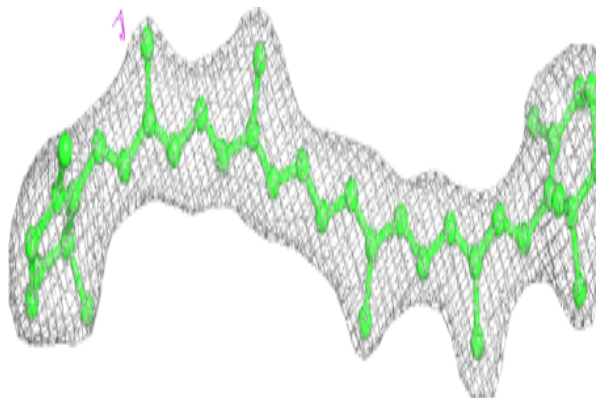


Electron density around LMG M 101:

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

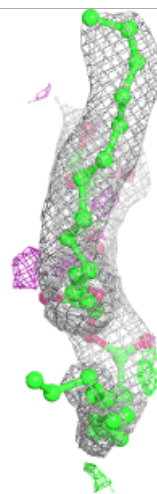
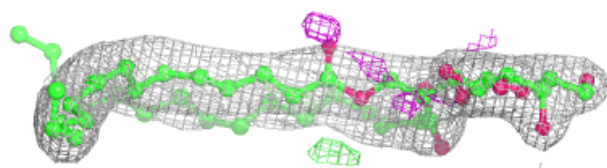
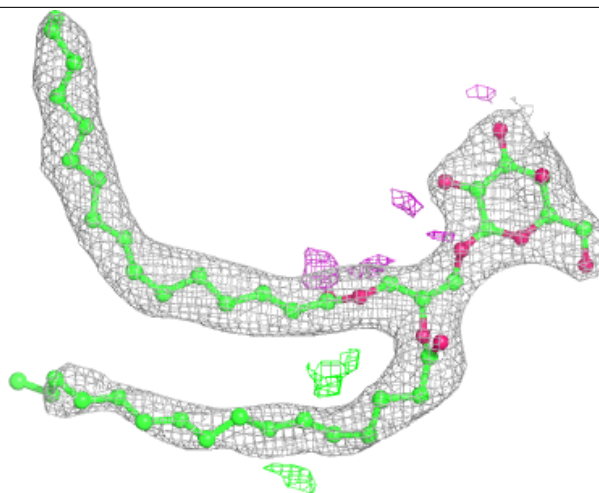
**Electron density around BCR Y 101:**

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



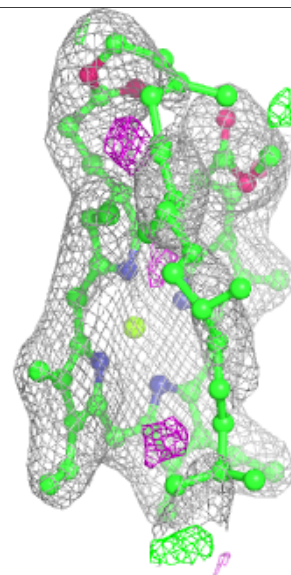
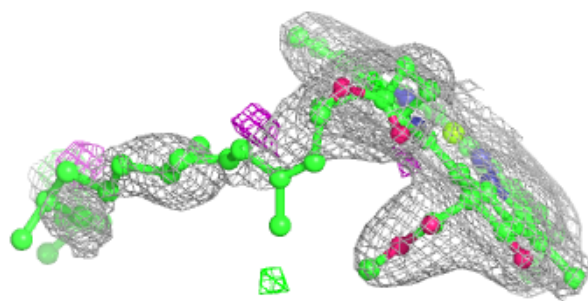
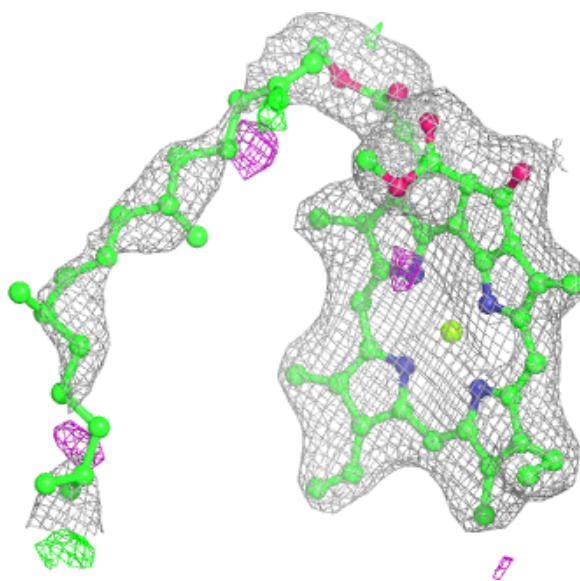
Electron density around LMG C 520:

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



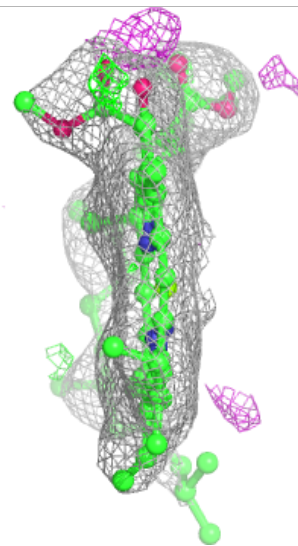
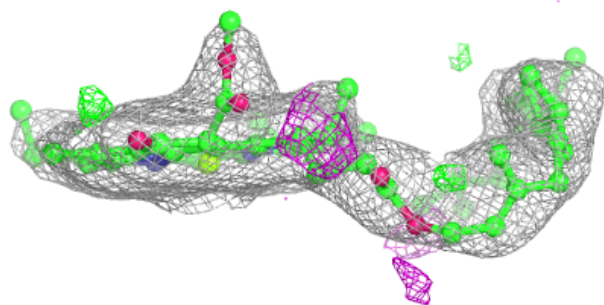
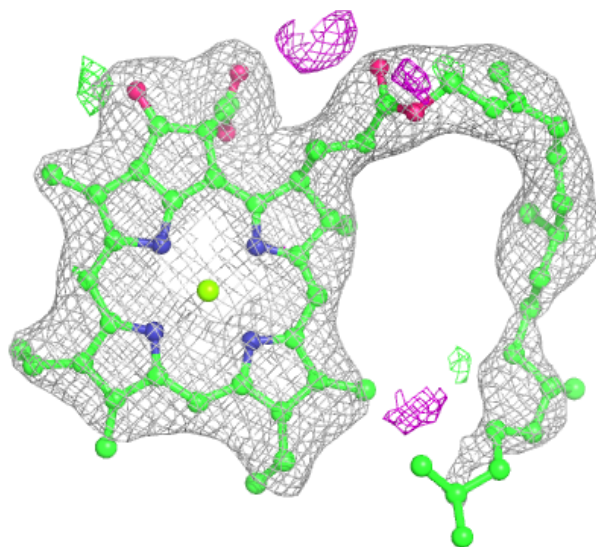
Electron density around CLA B 616:

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



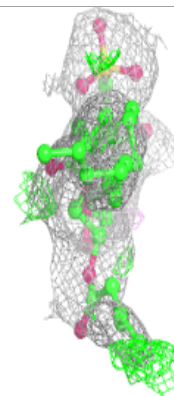
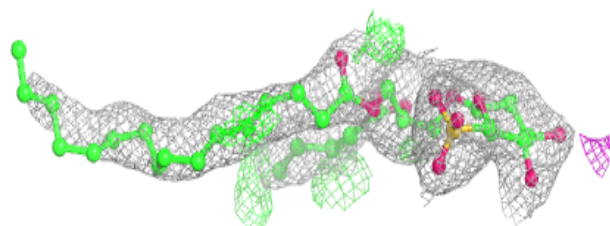
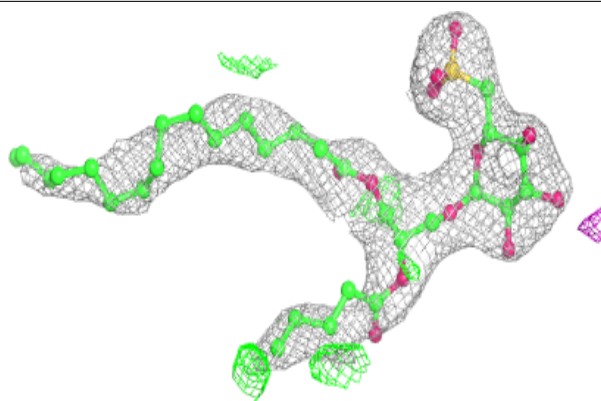
Electron density around CLA c 513:

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

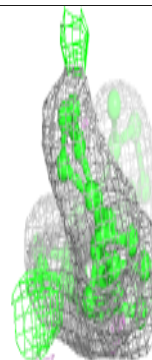
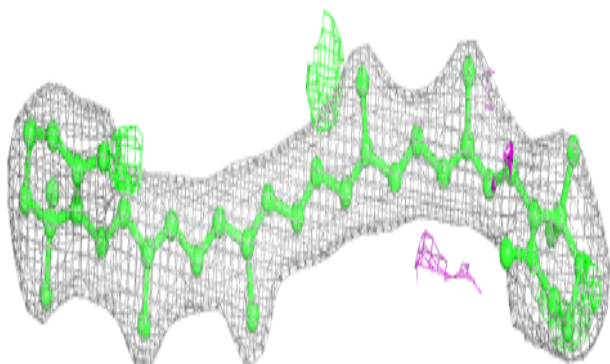
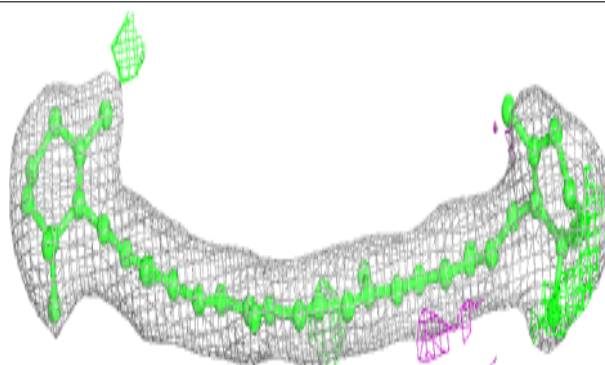


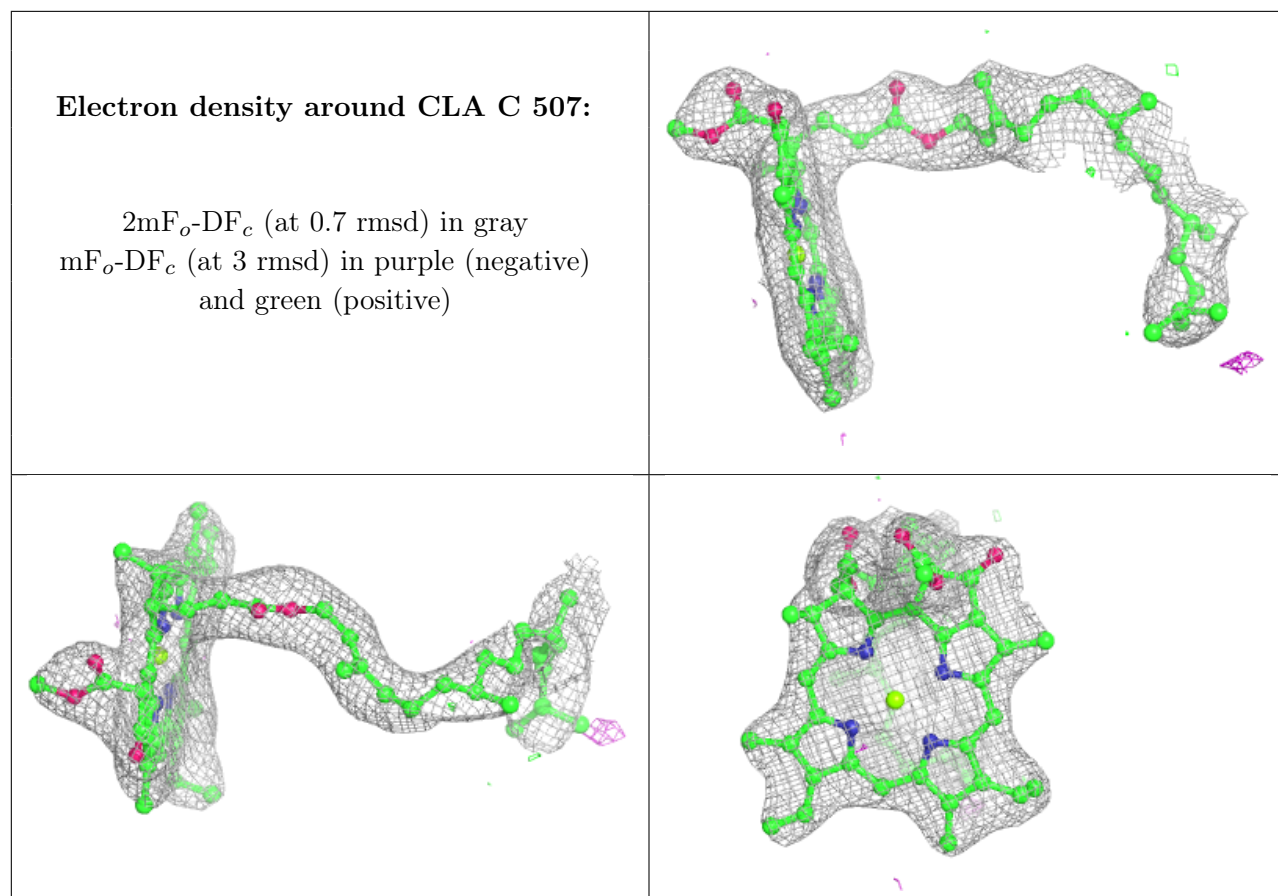
Electron density around SQD X 101:

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

**Electron density around BCR D 404:**

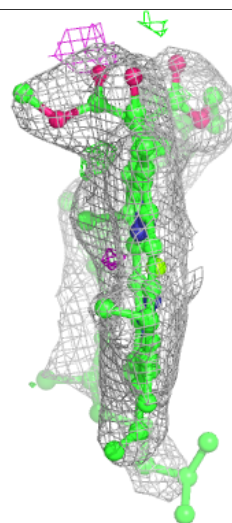
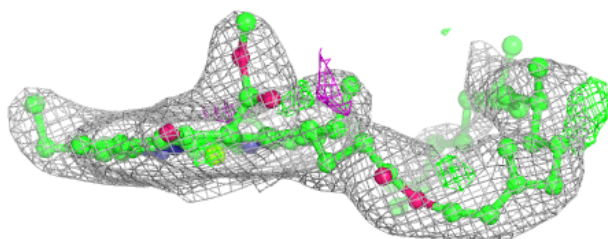
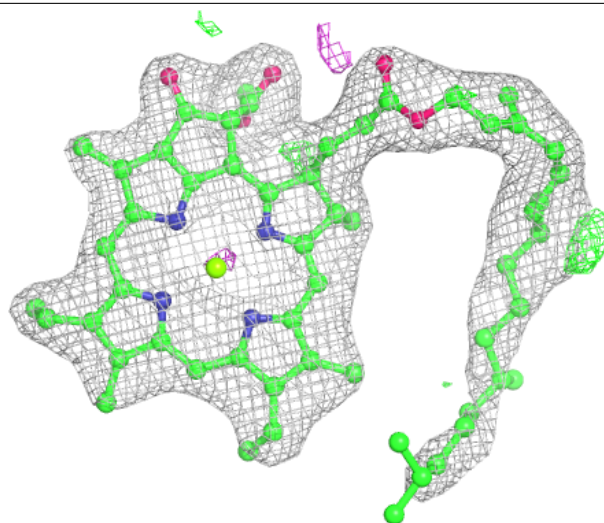
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





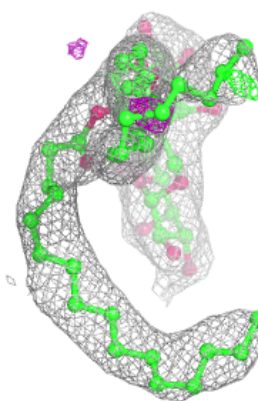
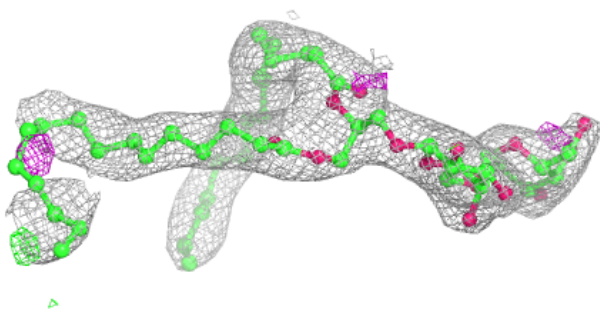
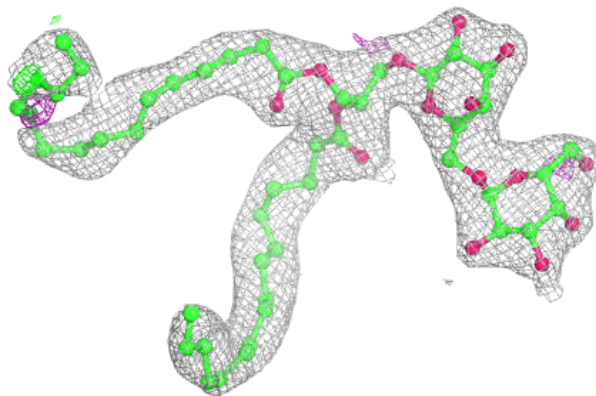
Electron density around CLA C 513:

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



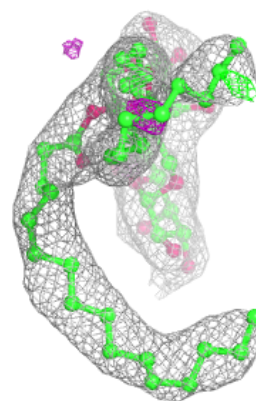
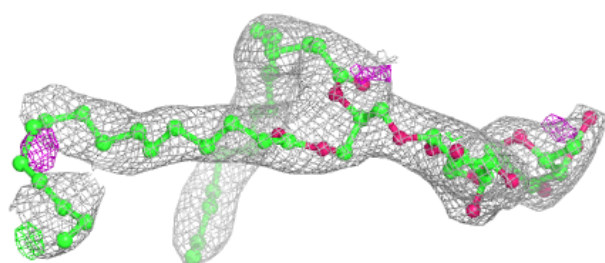
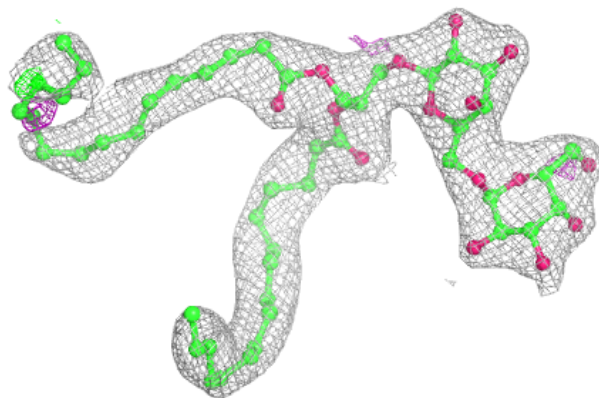
Electron density around DGD c 518 (A):

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

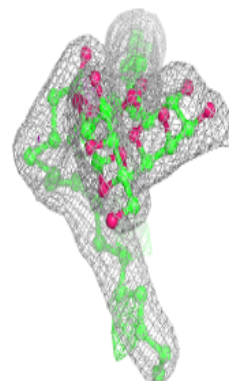
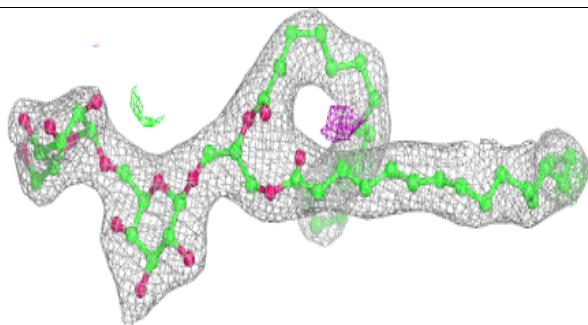
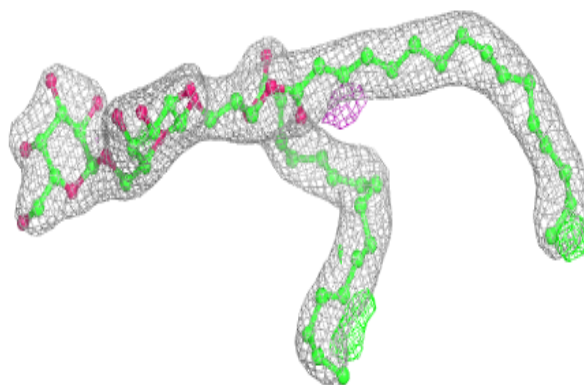


Electron density around DGD c 518 (B):

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

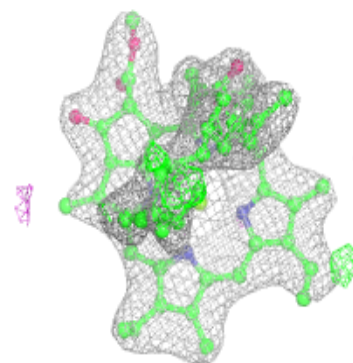
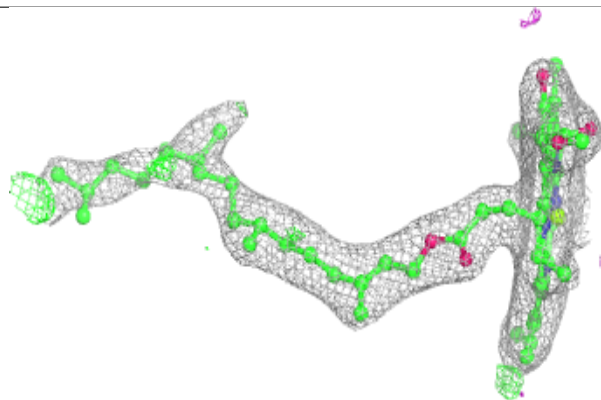
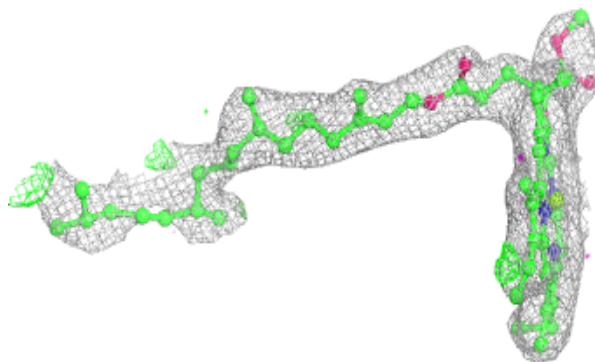
**Electron density around DGD h 102:**

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

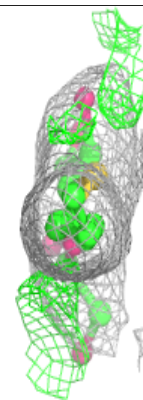
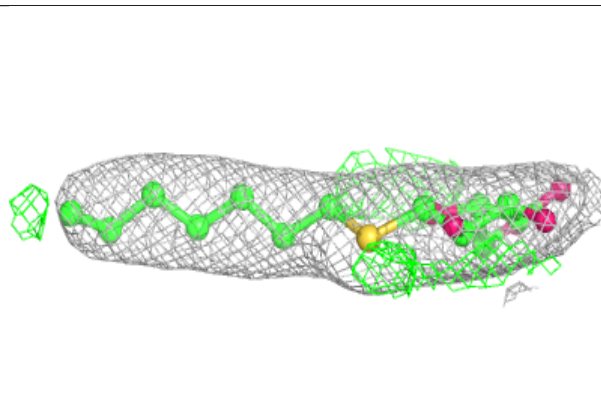
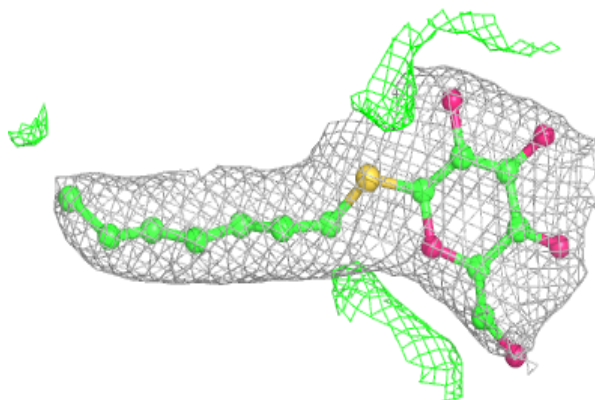


Electron density around CLA B 606:

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

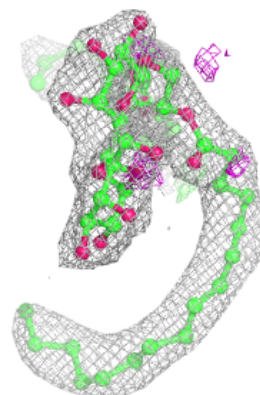
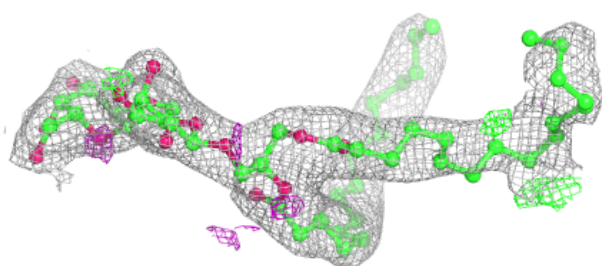
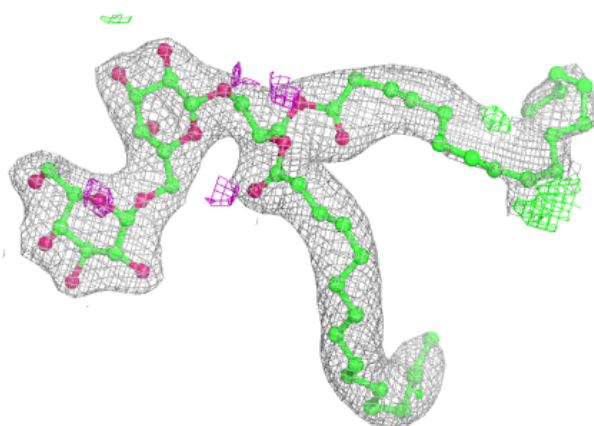
**Electron density around HTG b 624:**

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

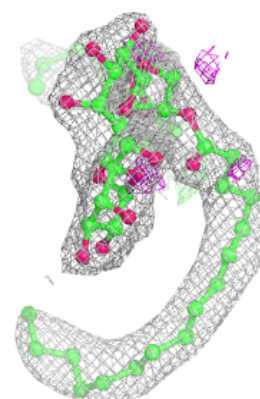
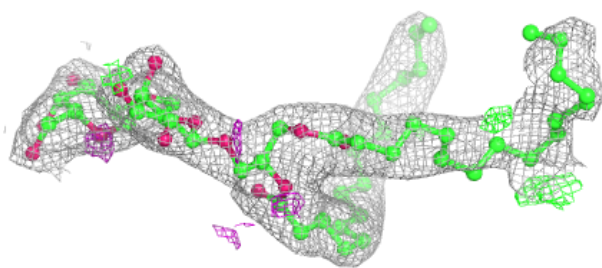
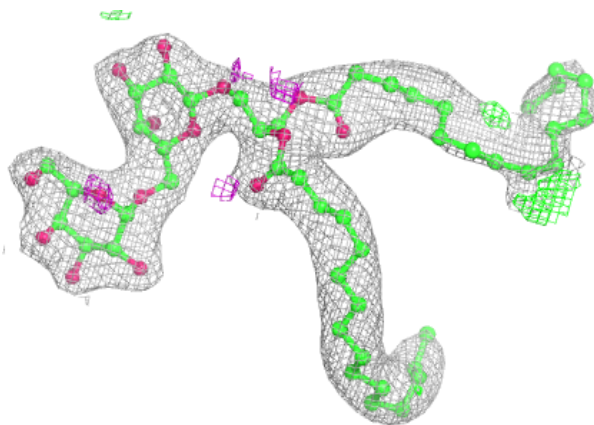


Electron density around DGD C 518 (A):

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

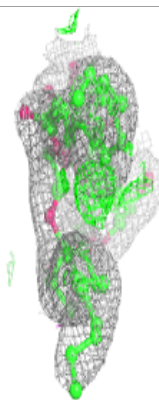
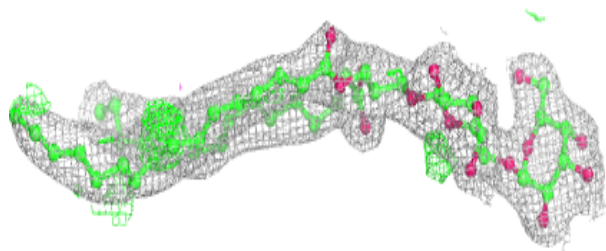
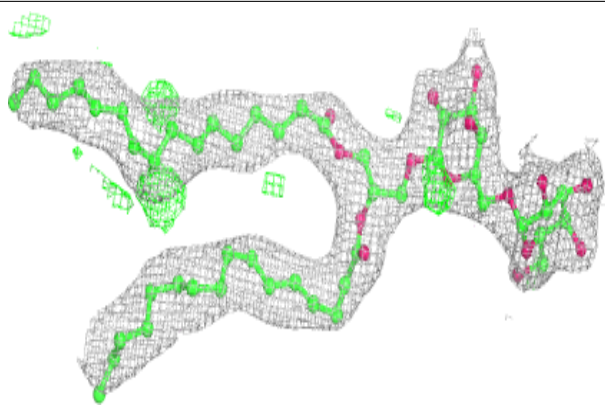
**Electron density around DGD C 518 (B):**

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

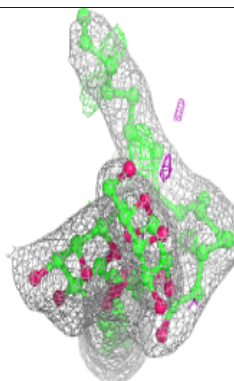
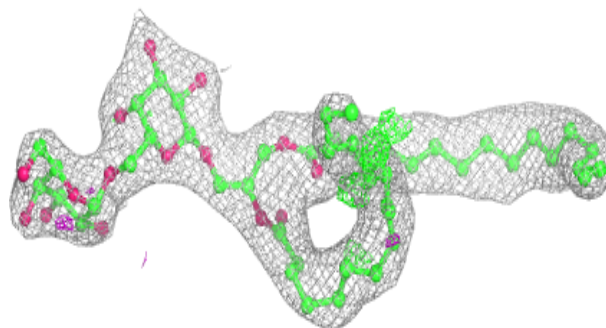
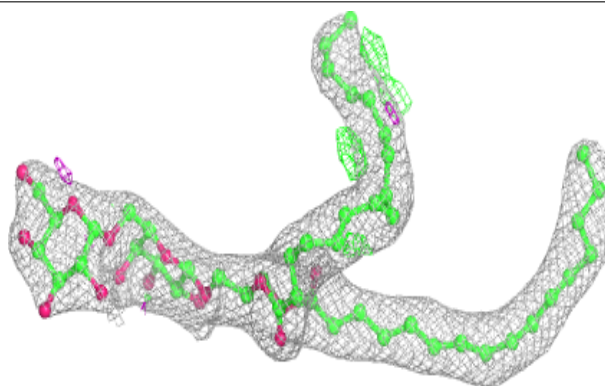


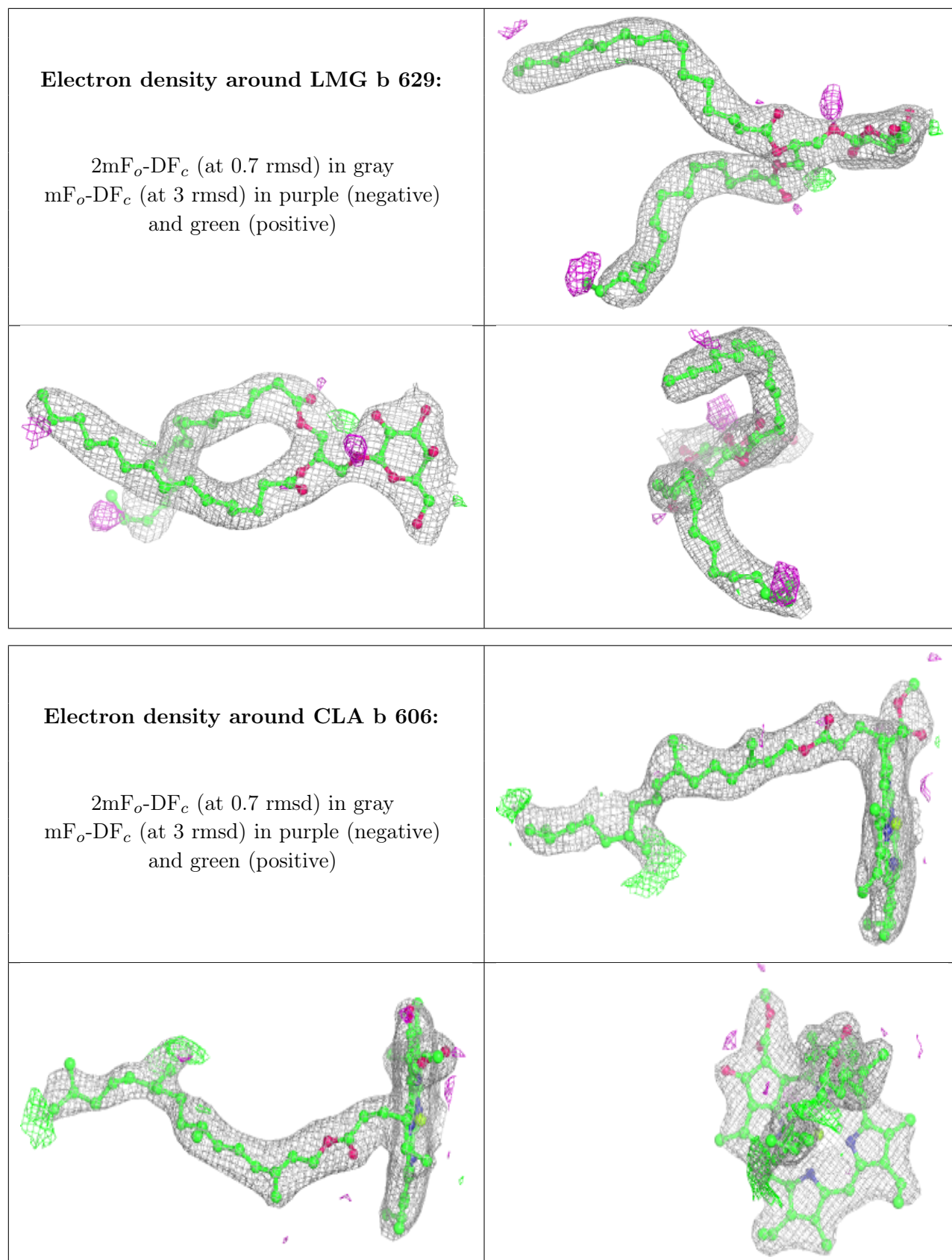
Electron density around DGD C 519:

$2mF_o-DF_c$ (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:**

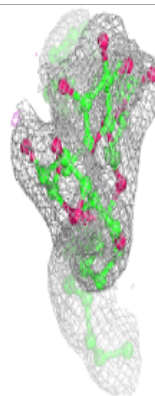
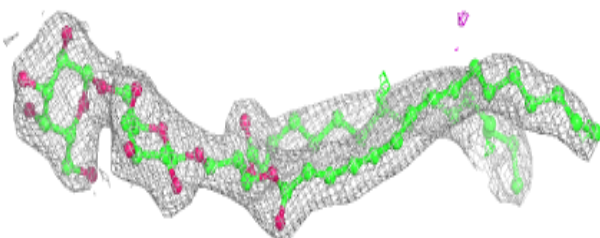
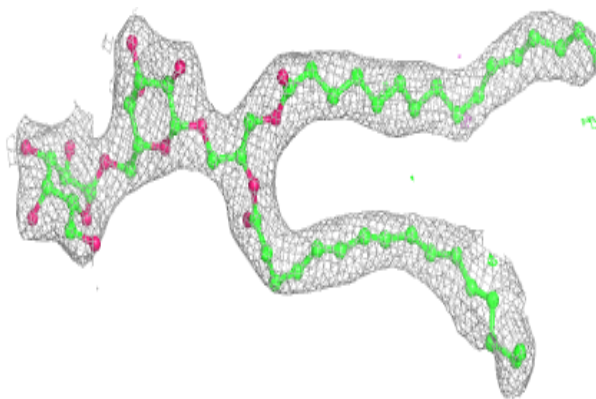
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



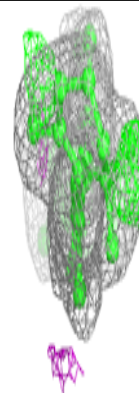
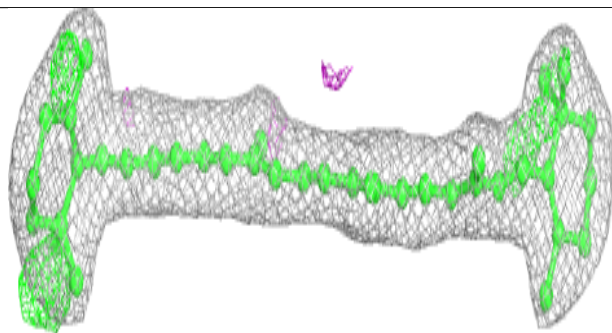
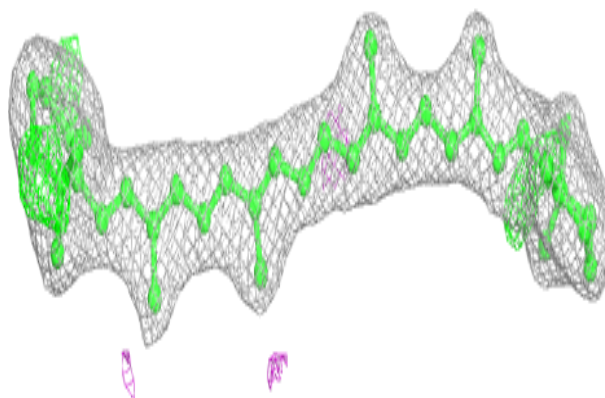


Electron density around DGD c 519:

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

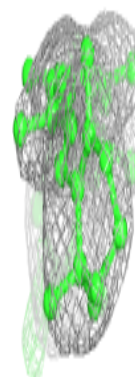
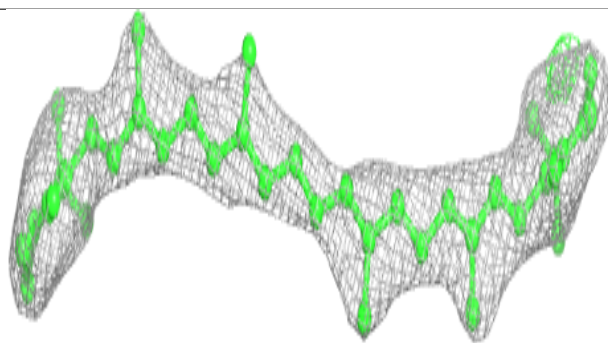
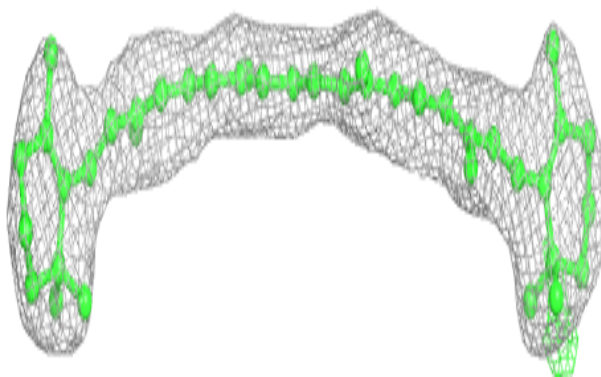
**Electron density around BCR A 410:**

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

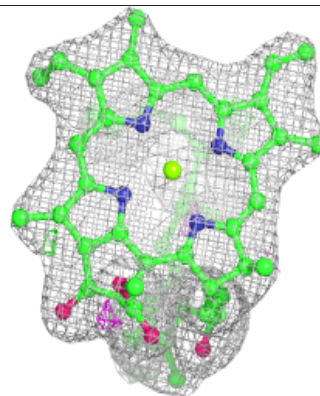
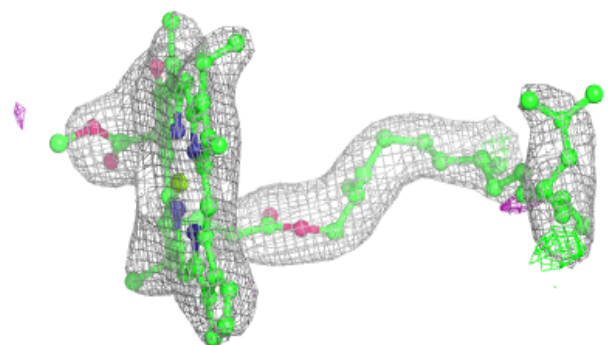
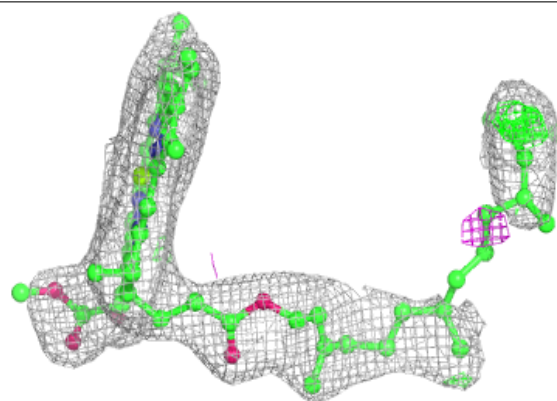


Electron density around BCR k 101:

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

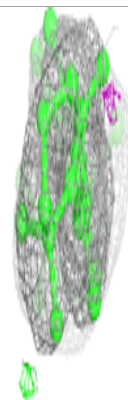
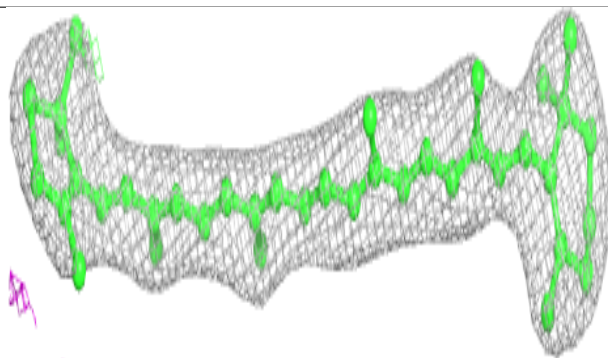
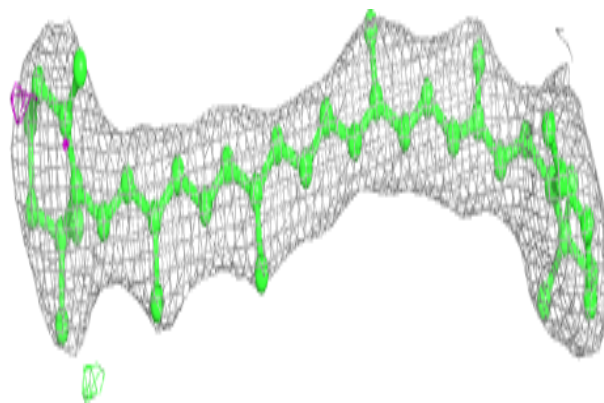
**Electron density around CLA c 507:**

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

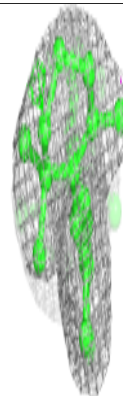
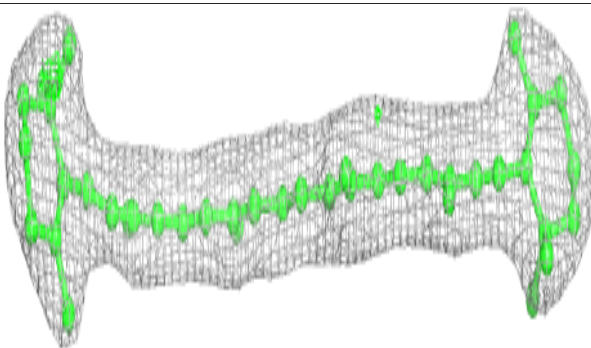
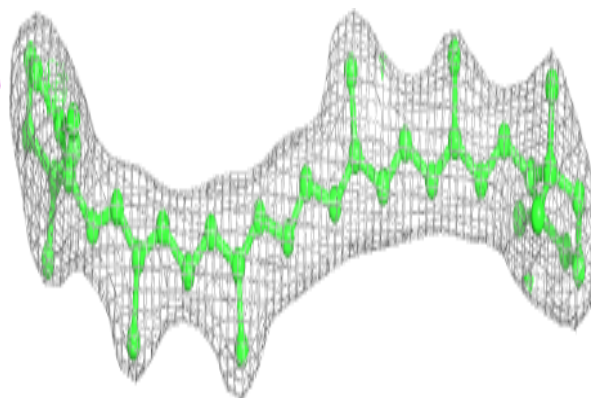


Electron density around BCR c 515:

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

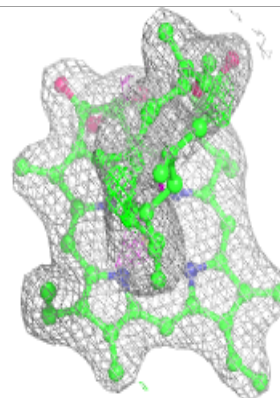
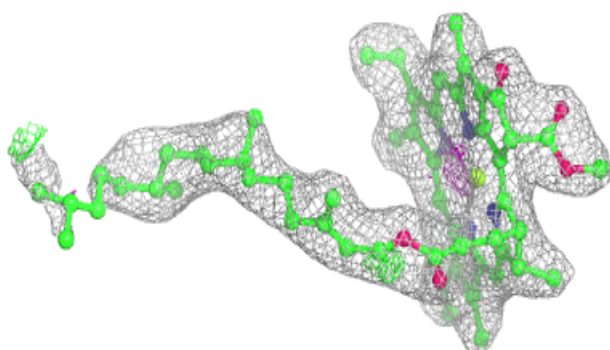
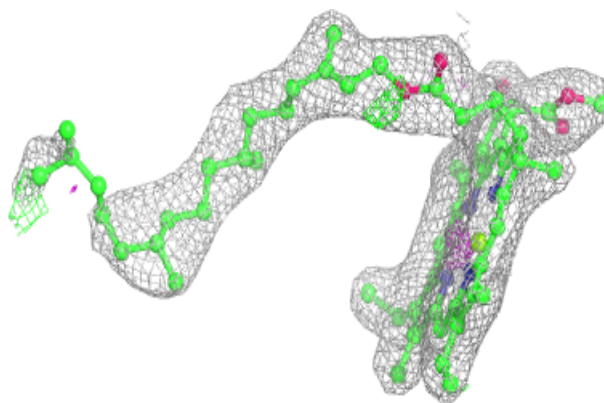
**Electron density around BCR C 516:**

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

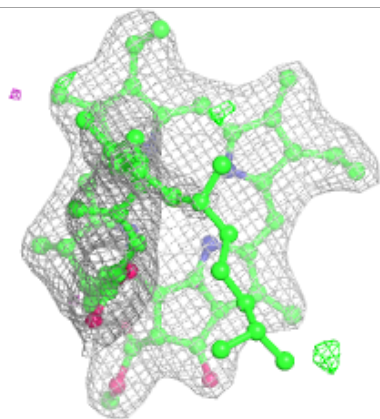
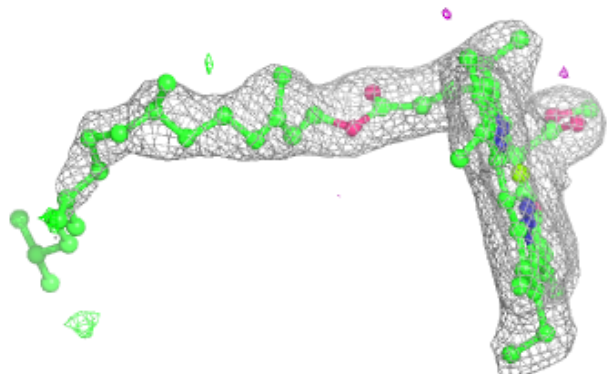
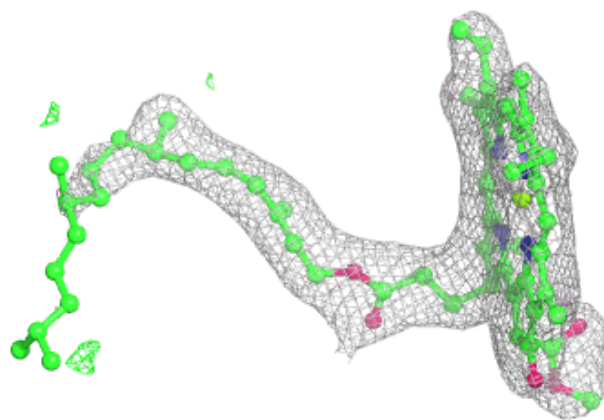


Electron density around CLA C 509:

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

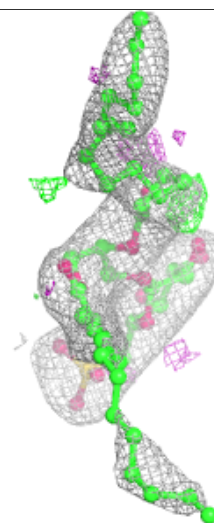
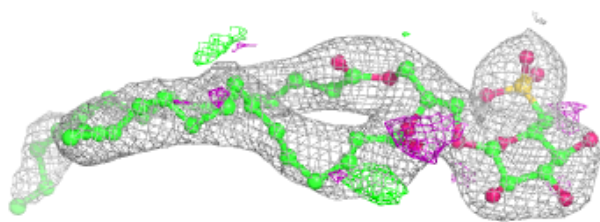
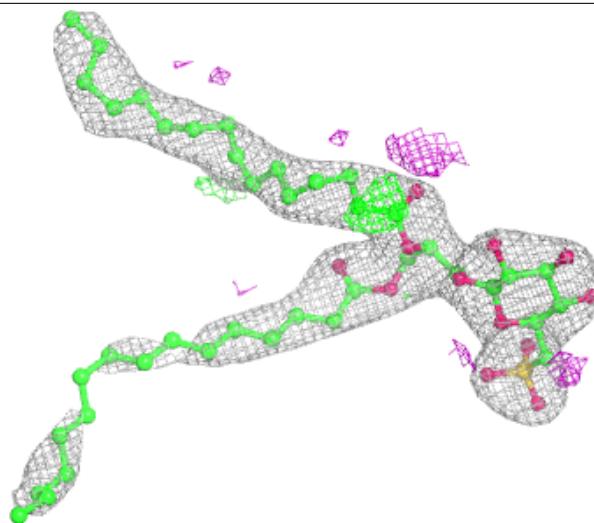
**Electron density around CLA D 403:**

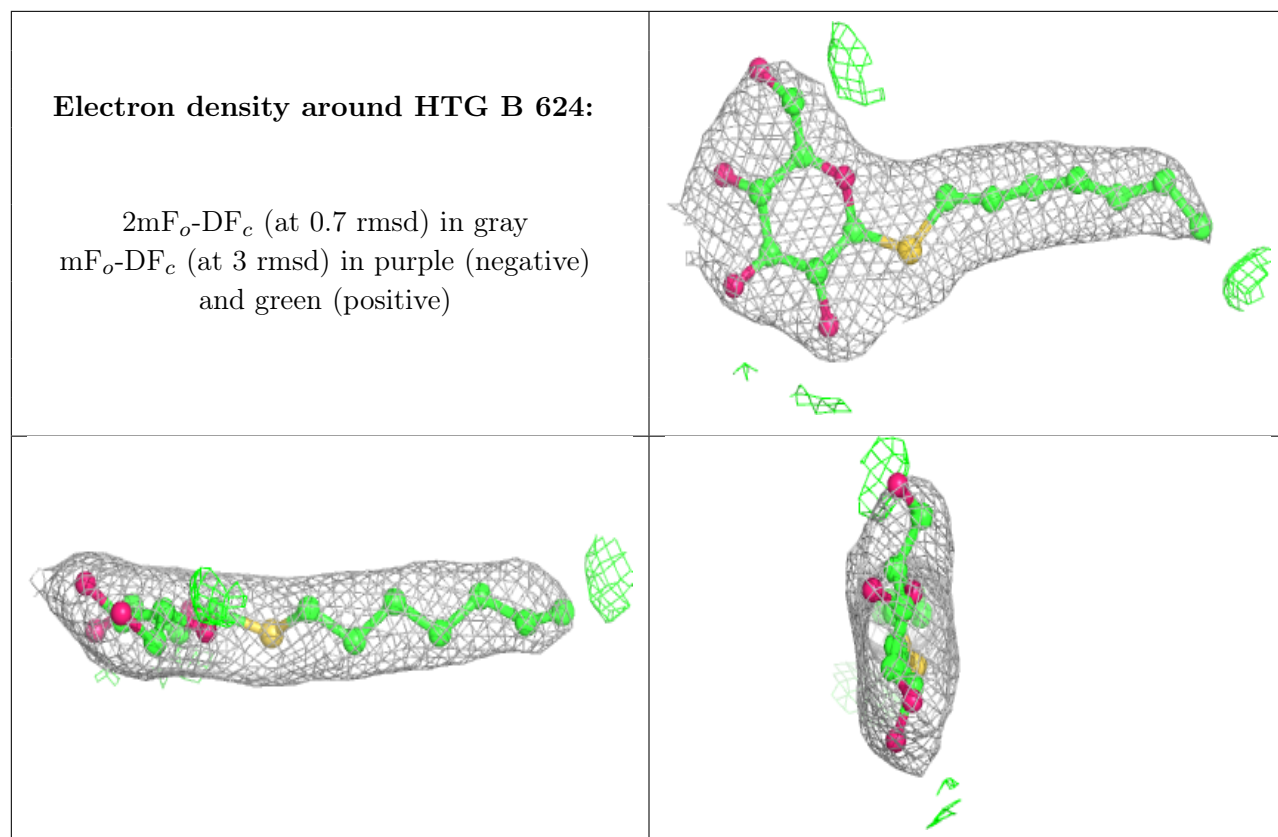
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SQD A 411 (A):

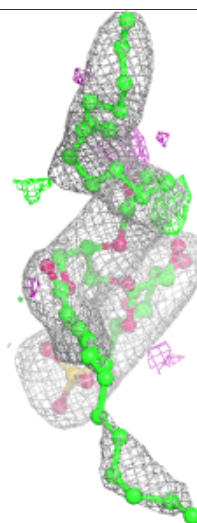
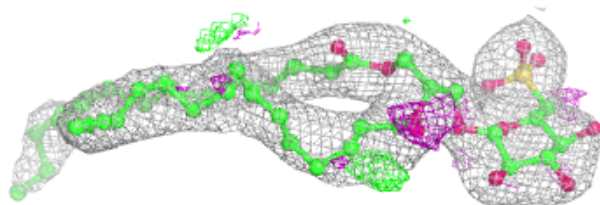
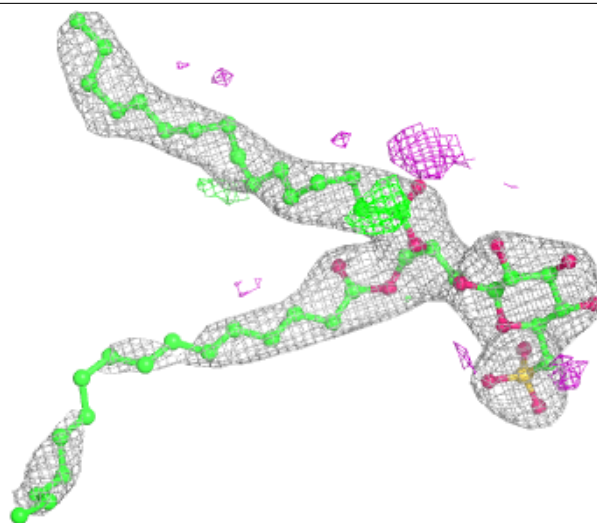
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





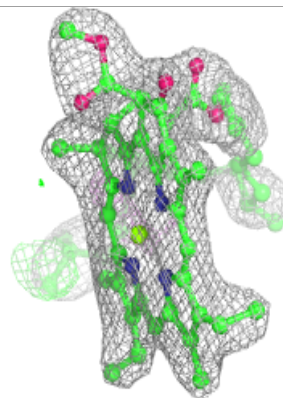
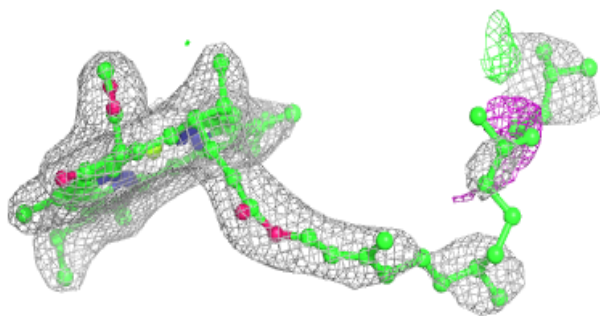
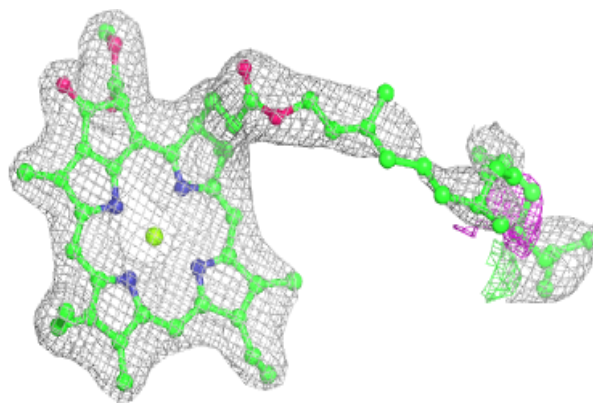
Electron density around SQD A 411 (B):

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



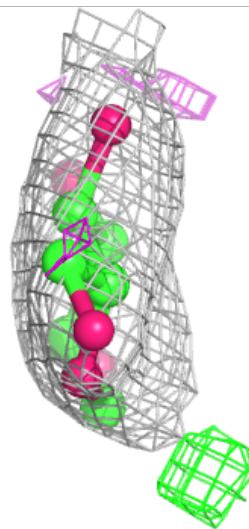
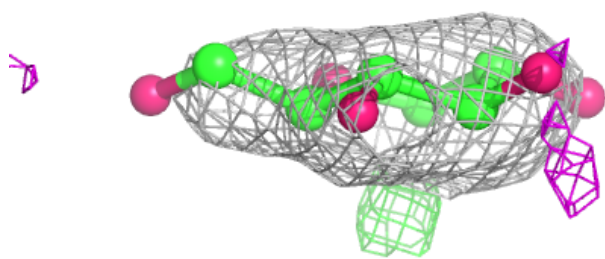
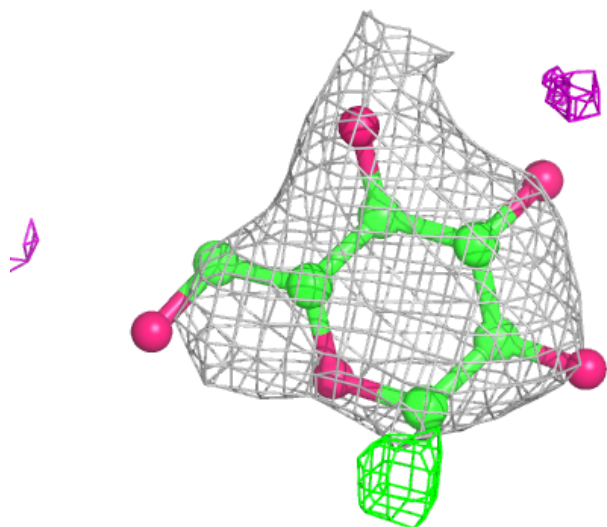
Electron density around CLA a 409:

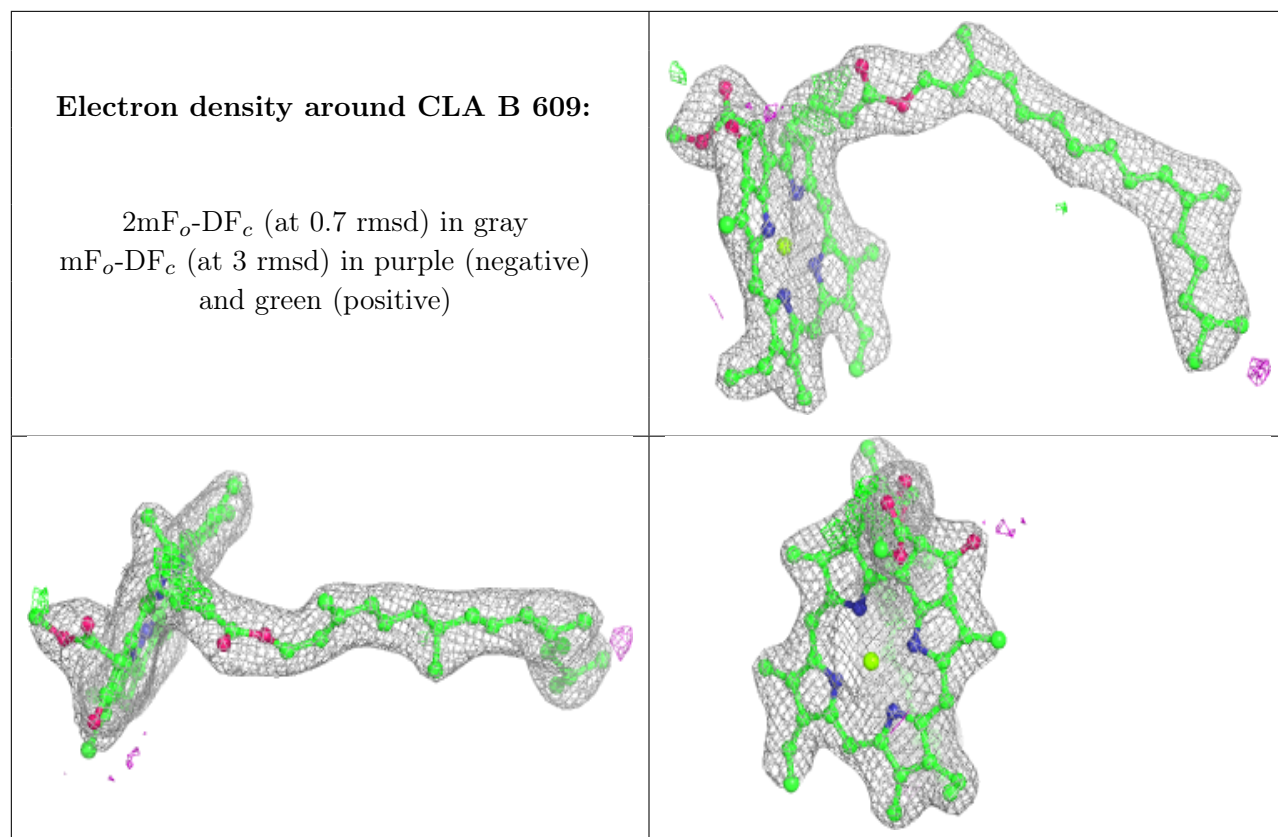
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HTG V 202:

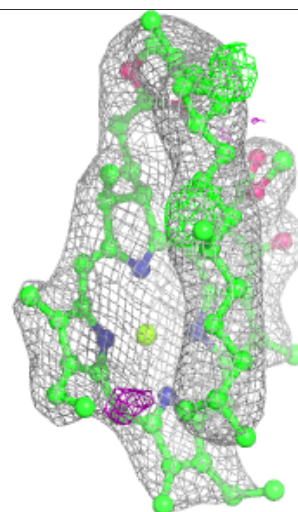
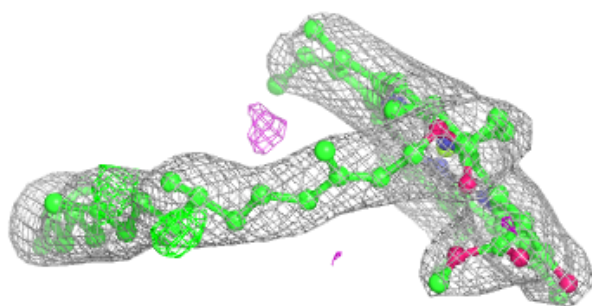
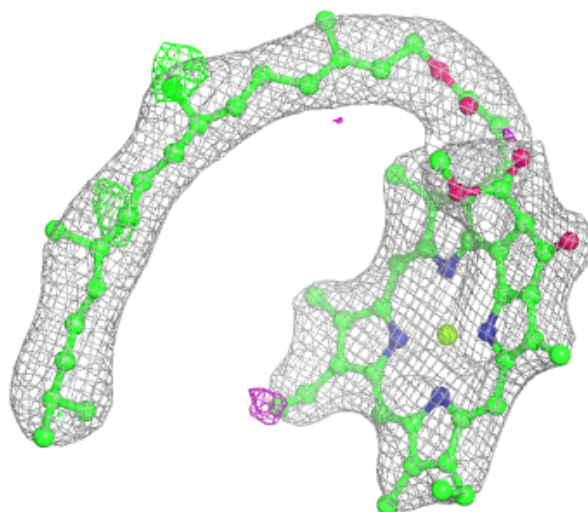
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





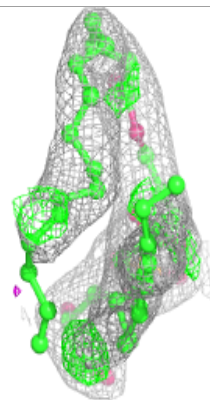
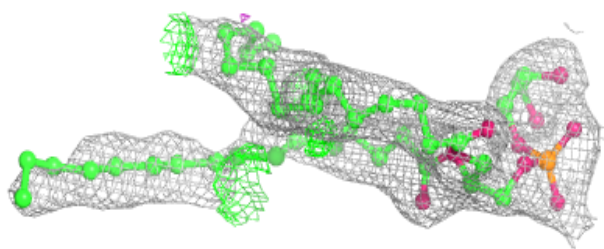
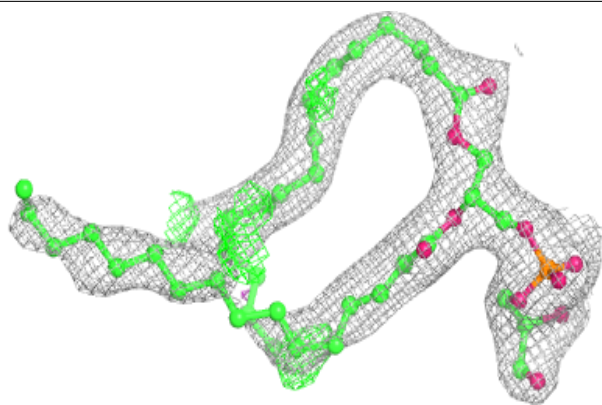
Electron density around CLA c 508:

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

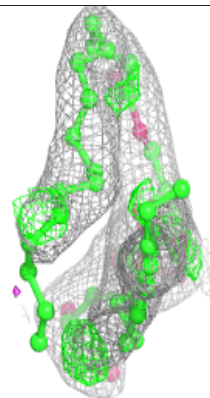
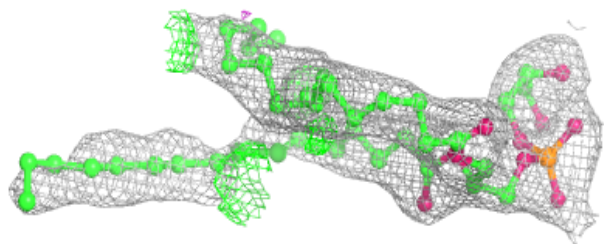
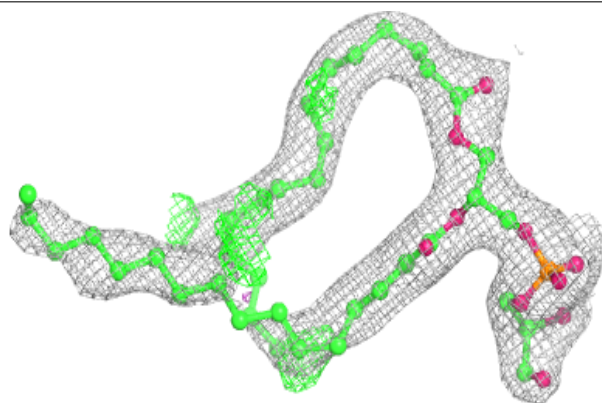


Electron density around LHG d 408 (A):

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

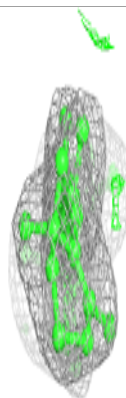
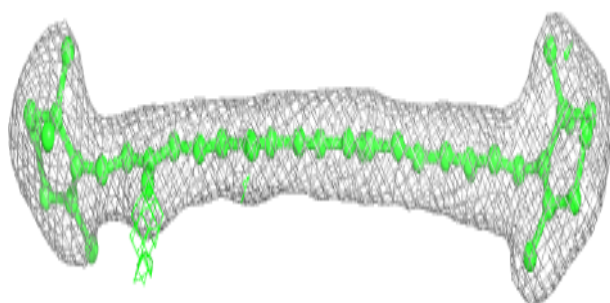
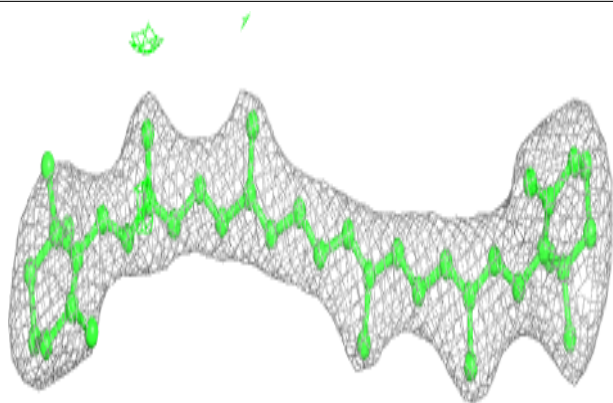
**Electron density around LHG d 408 (B):**

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

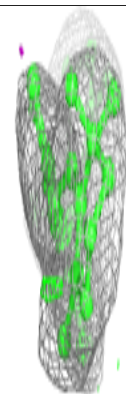
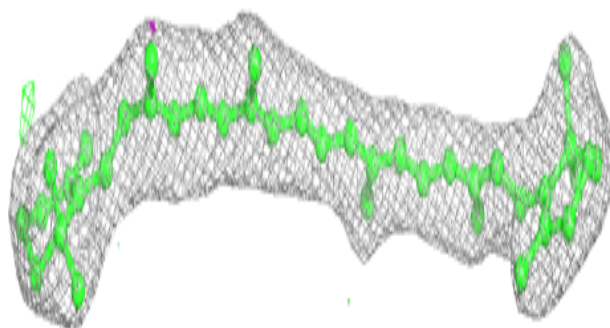
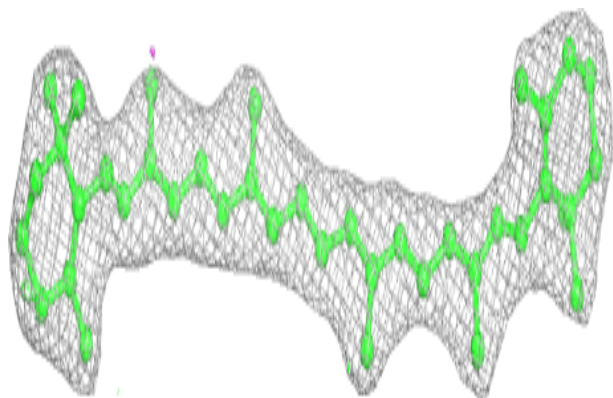


Electron density around BCR b 618:

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

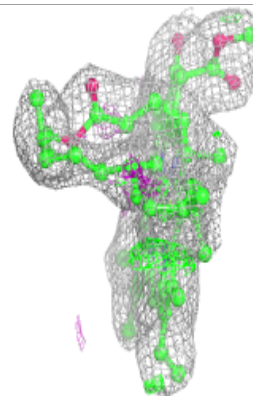
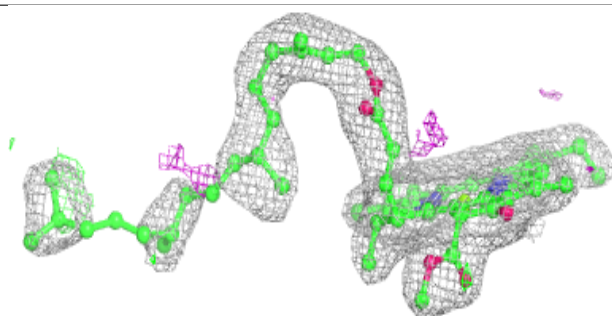
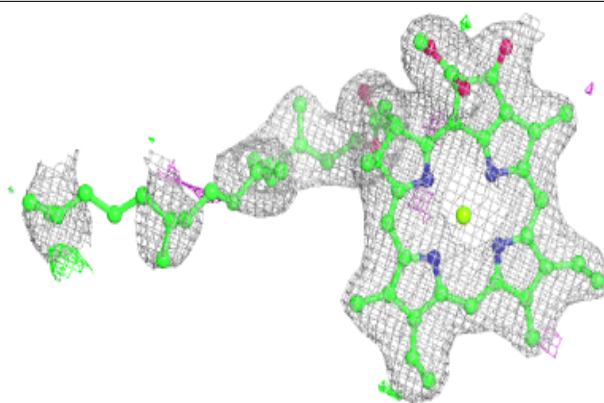
**Electron density around BCR b 619:**

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

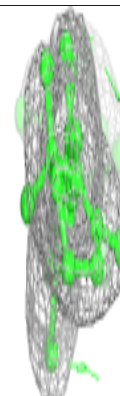
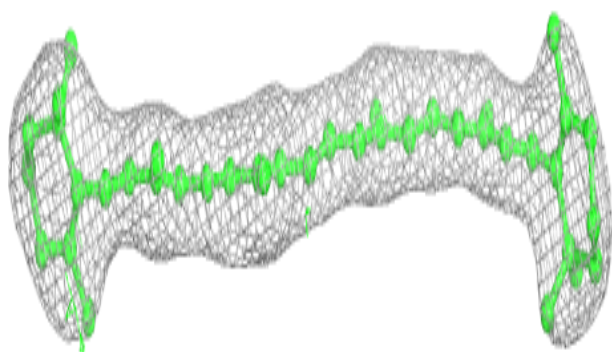
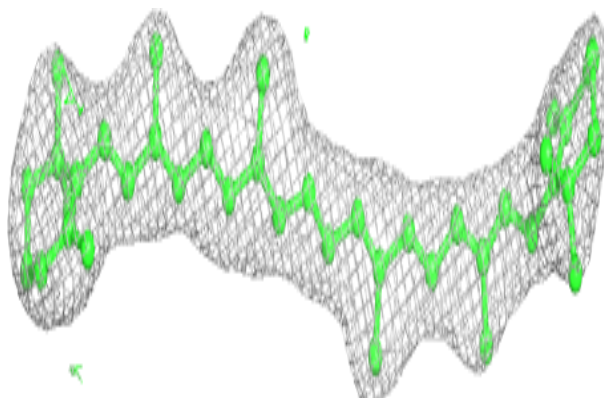


Electron density around CLA a 407 (A):

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

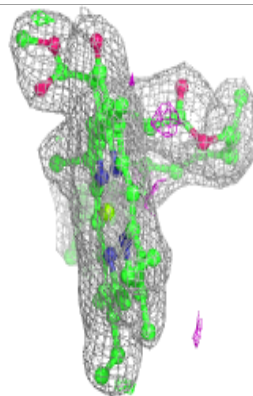
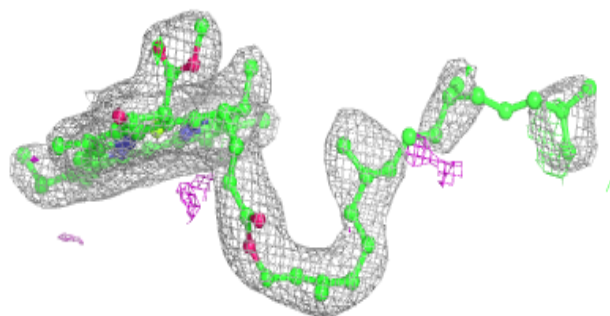
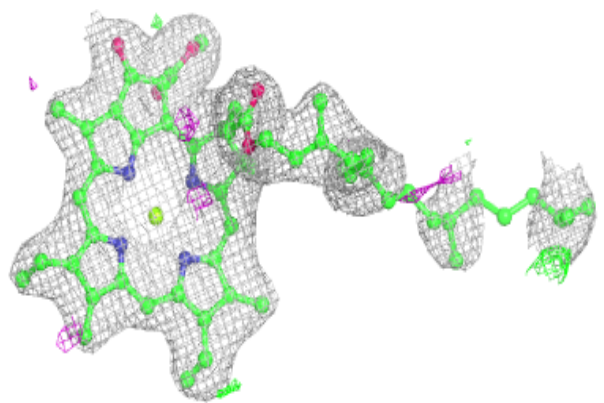
**Electron density around BCR c 516:**

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



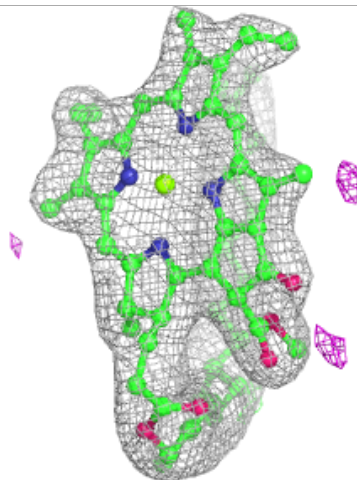
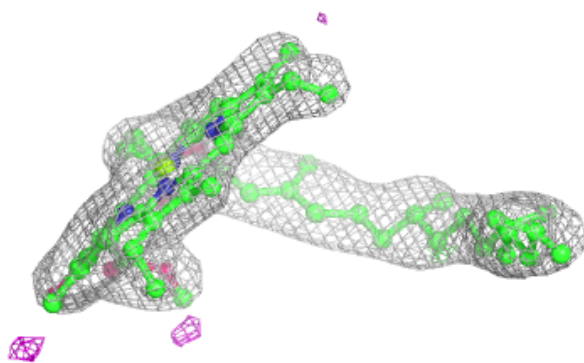
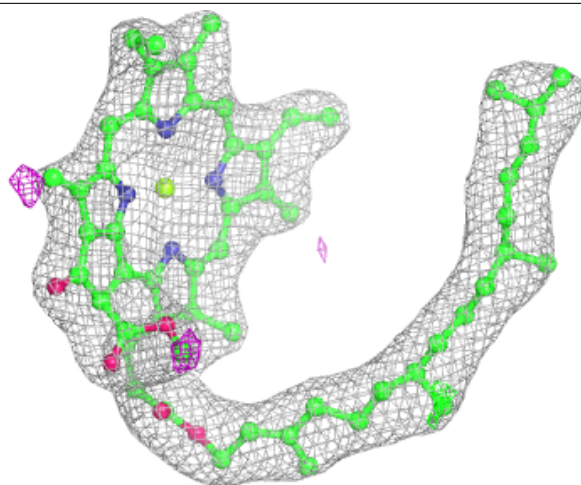
Electron density around CLA a 407 (B):

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



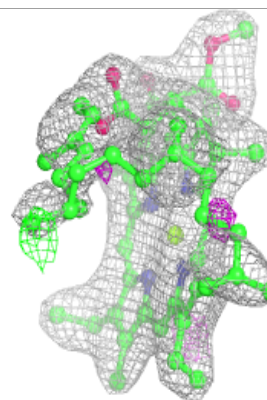
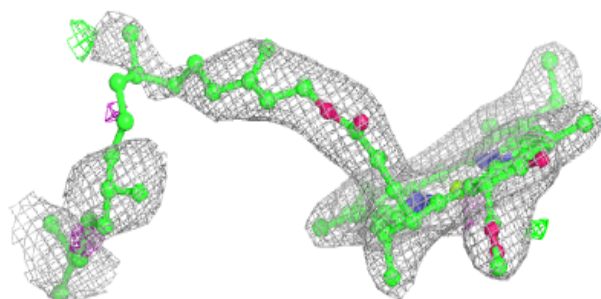
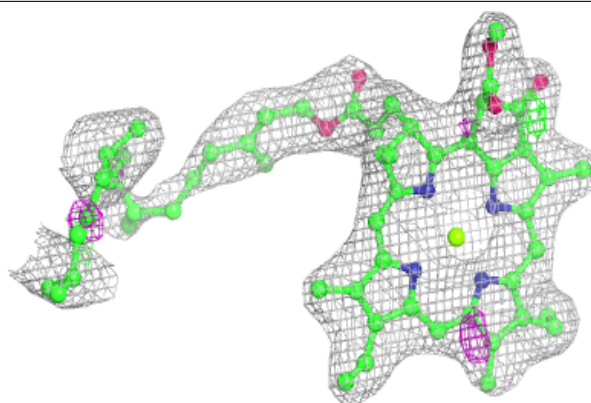
Electron density around CLA C 508:

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

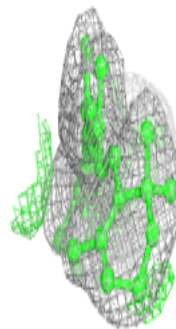
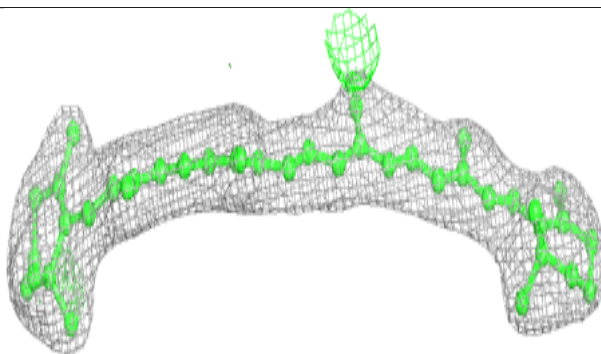
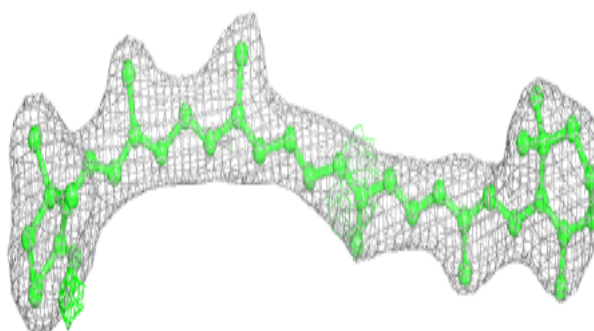


Electron density around CLA A 409:

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

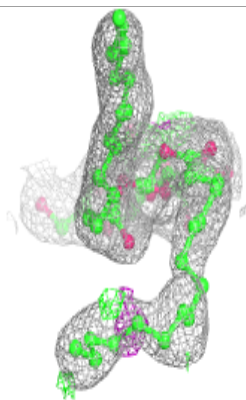
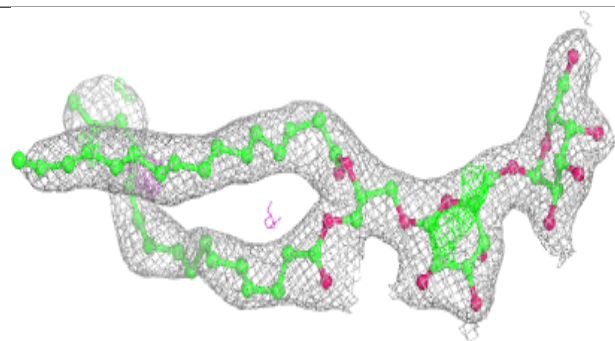
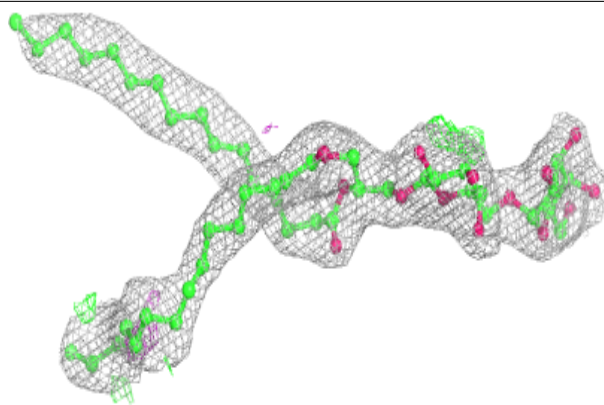
**Electron density around BCR t 102:**

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

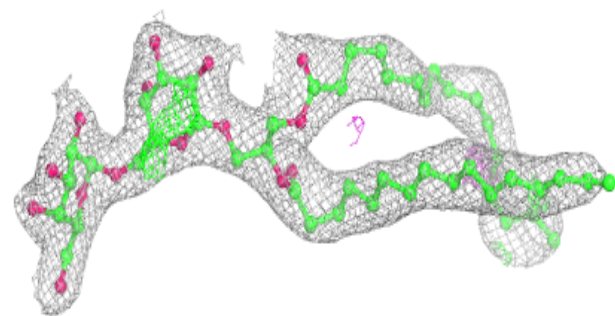
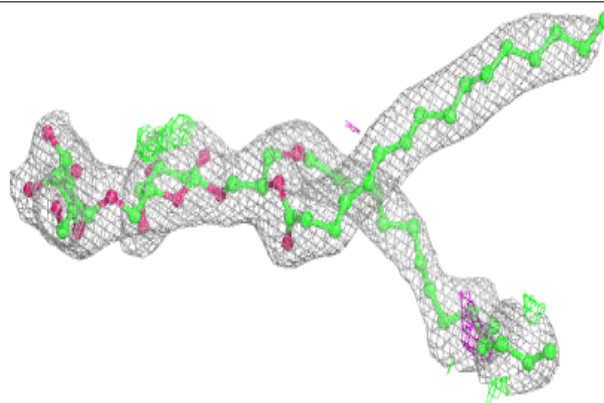


Electron density around DGD c 517 (A):

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

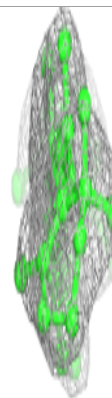
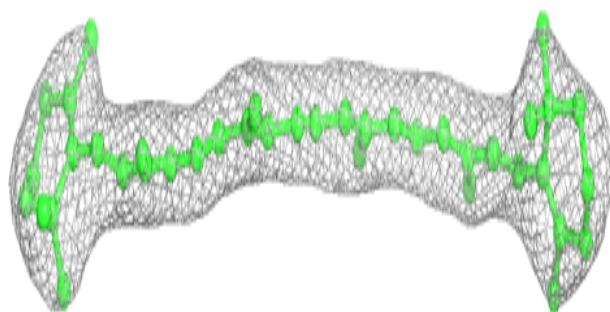
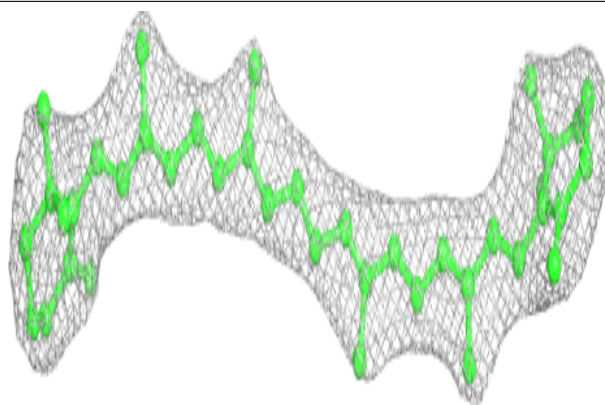
**Electron density around DGD c 517 (B):**

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

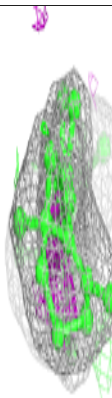
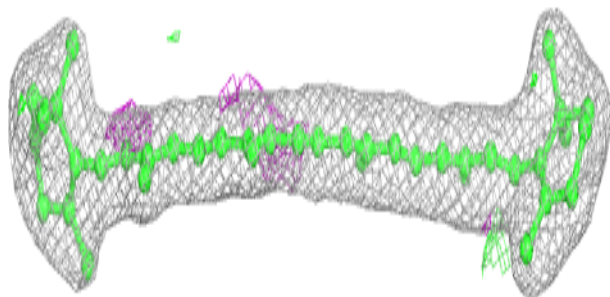
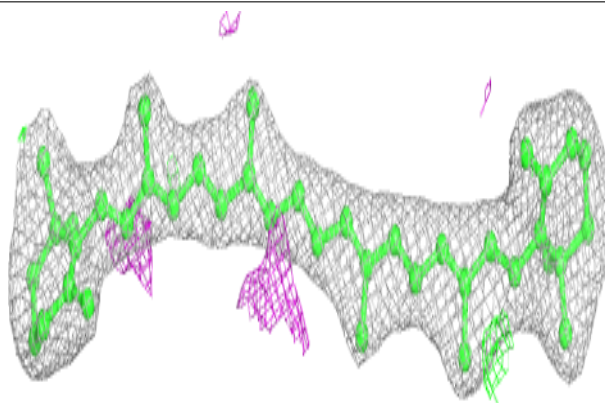


Electron density around BCR y 101:

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

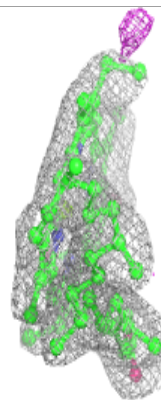
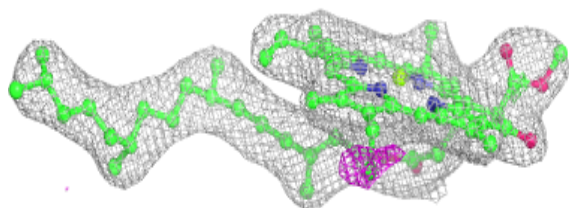
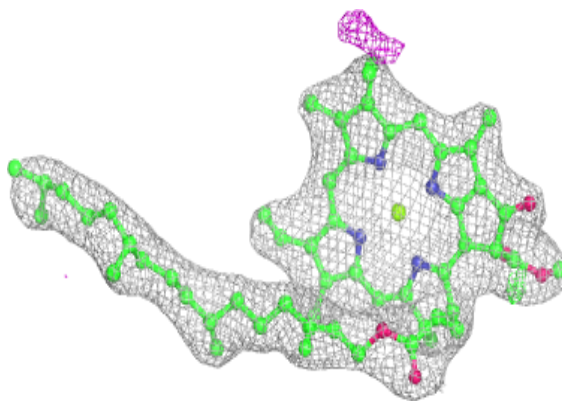
**Electron density around BCR B 618:**

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

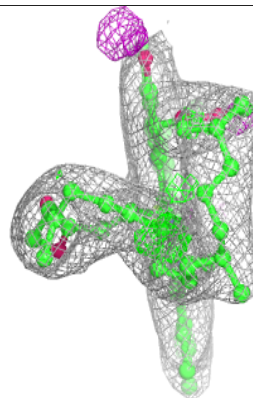
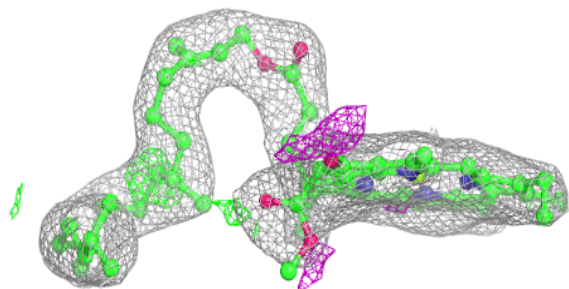
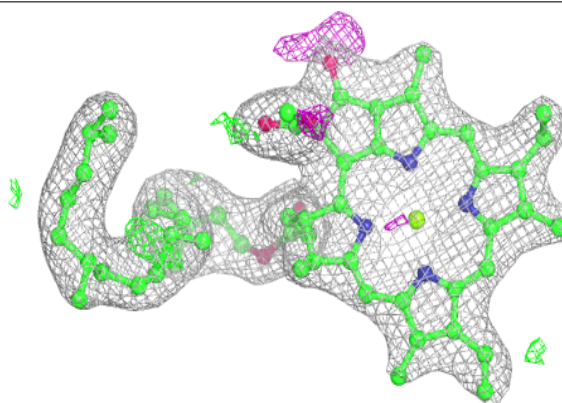


Electron density around CLA C 502:

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

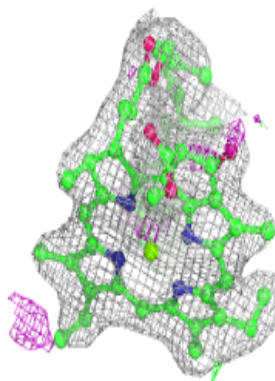
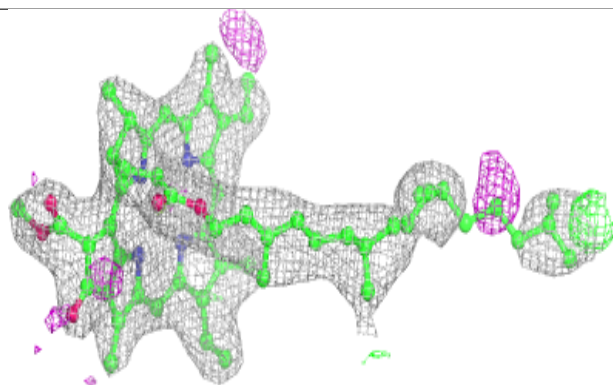
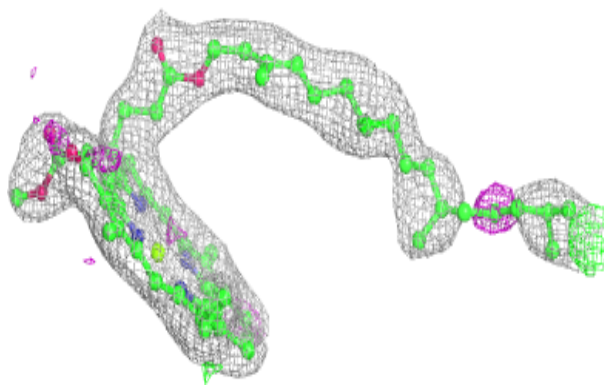
**Electron density around CLA b 612:**

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

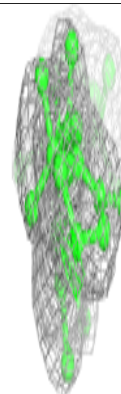
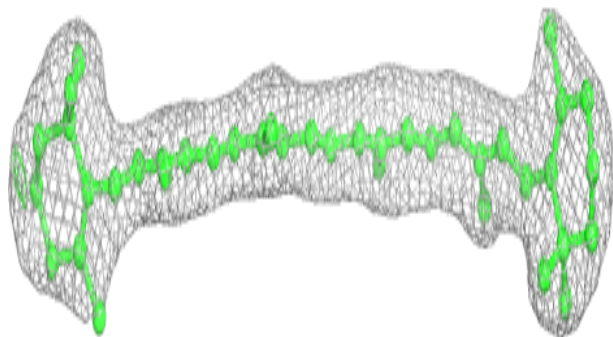
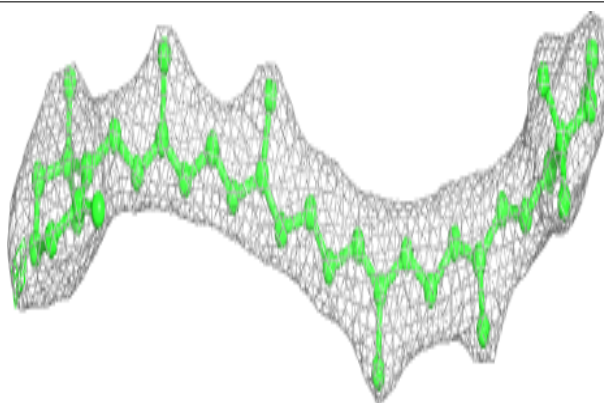


Electron density around CLA C 505:

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

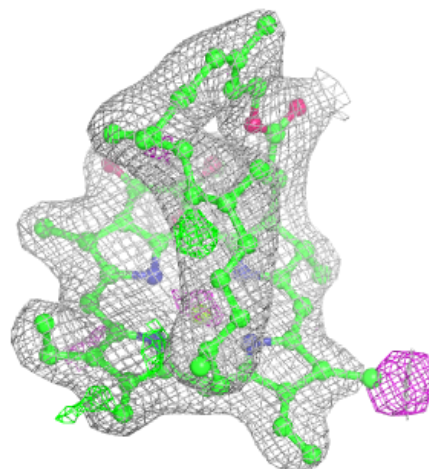
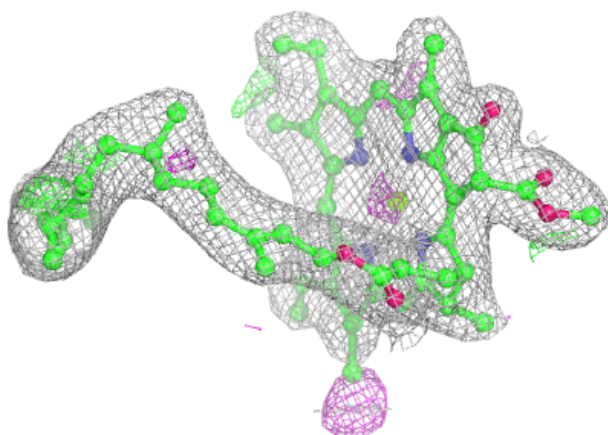
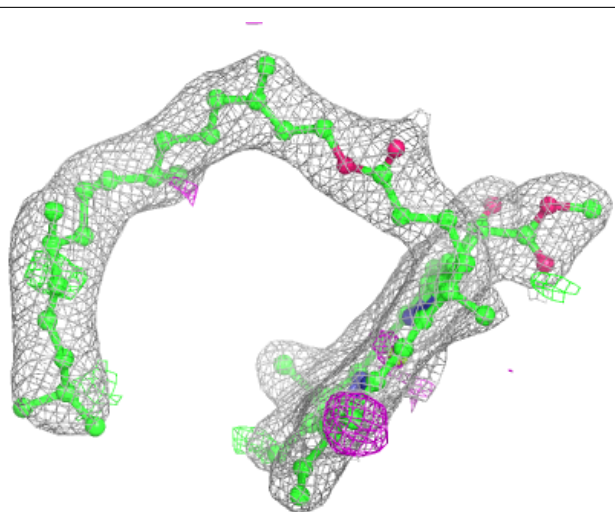
**Electron density around BCR H 101:**

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



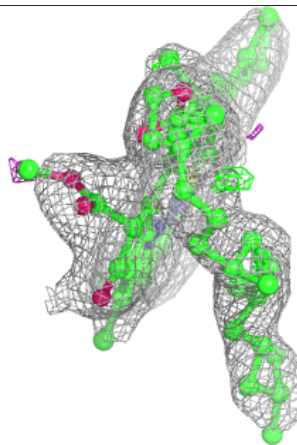
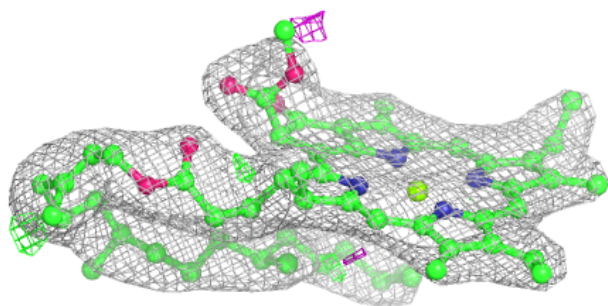
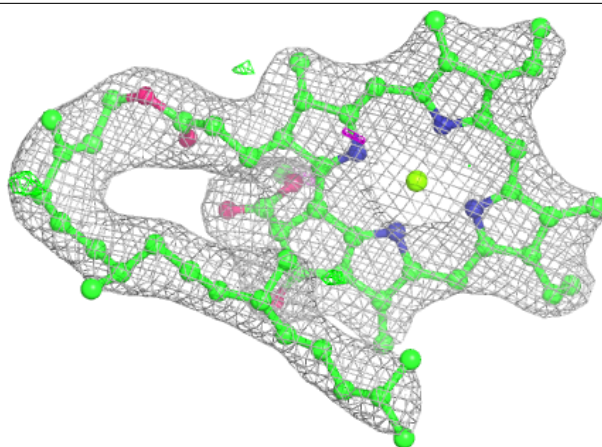
Electron density around CLA B 611:

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

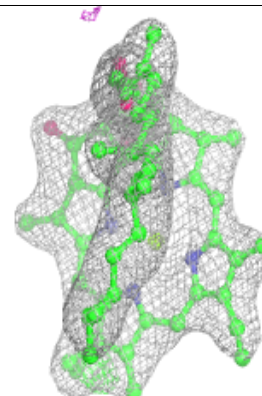
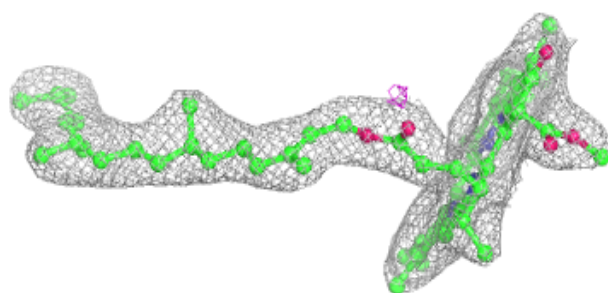
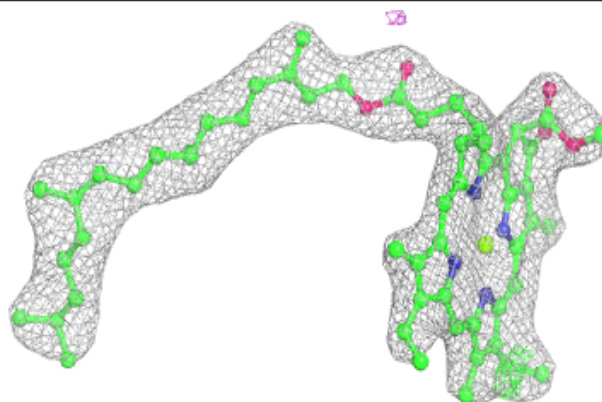


Electron density around CLA C 510:

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

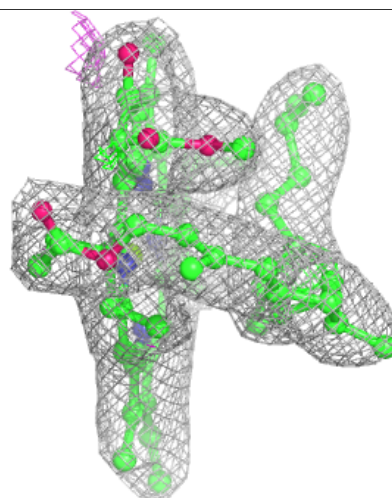
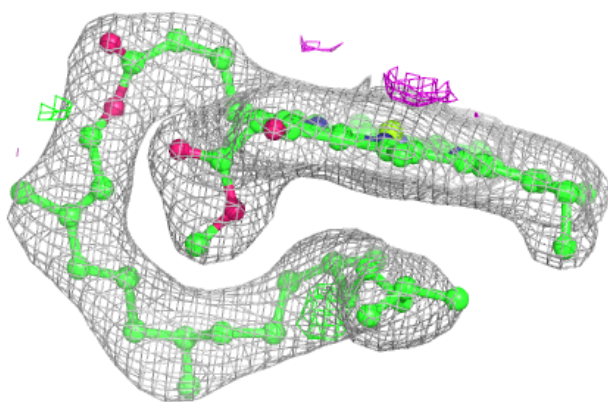
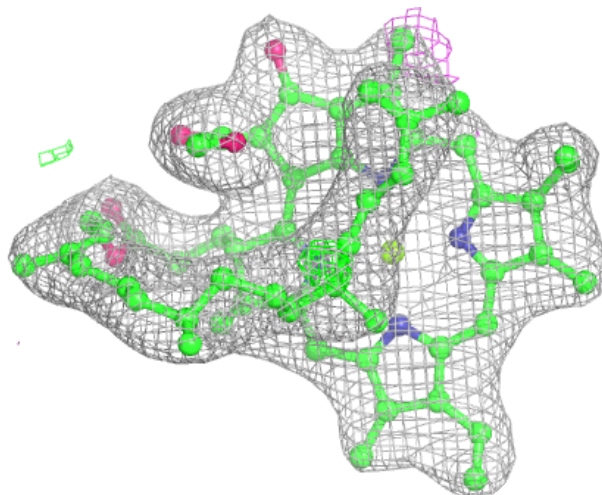
**Electron density around CLA b 609:**

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



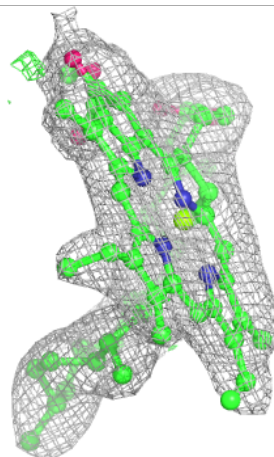
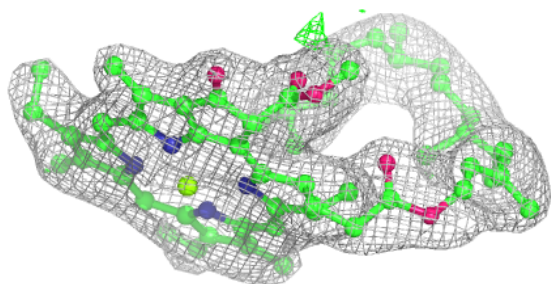
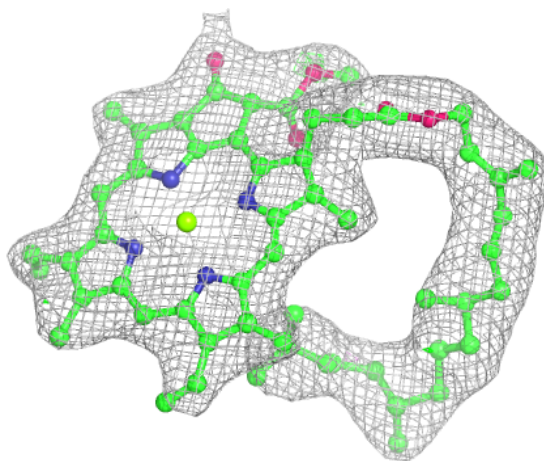
Electron density around CLA C 511:

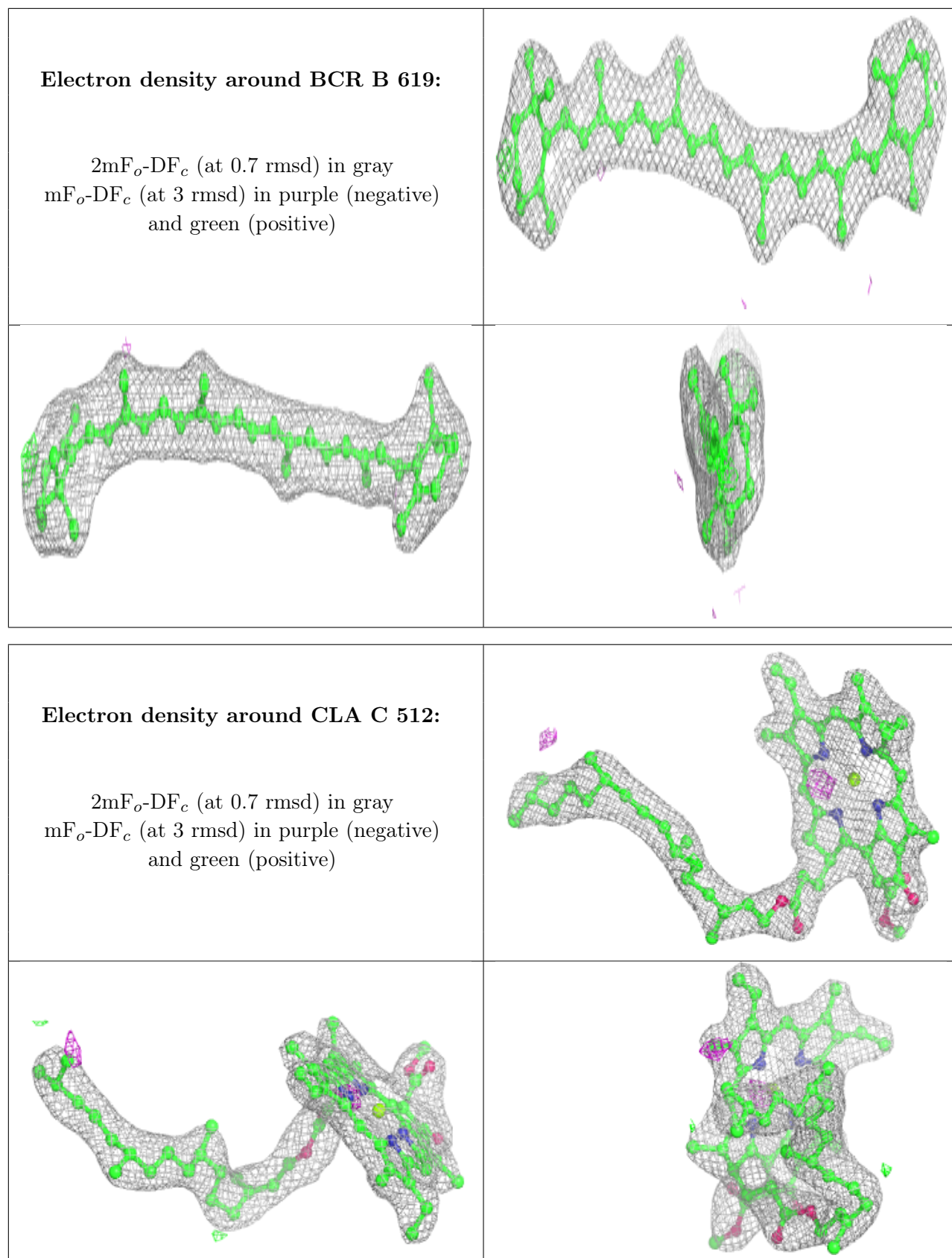
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA b 615:

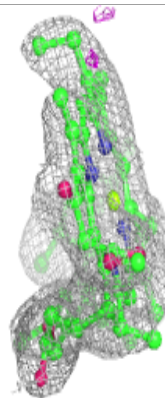
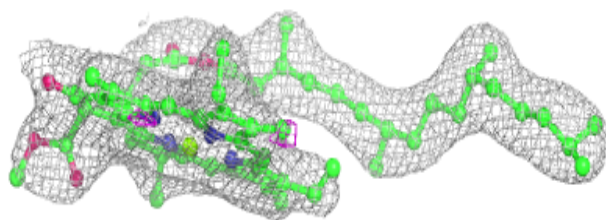
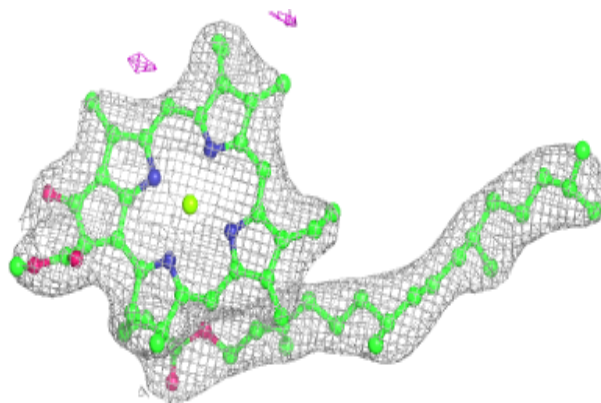
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





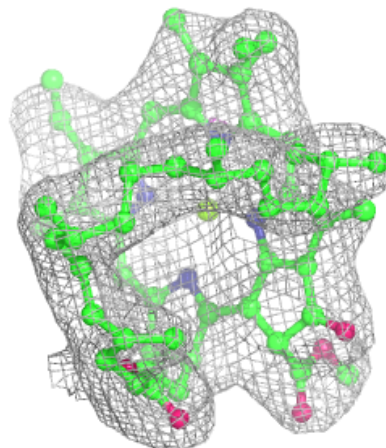
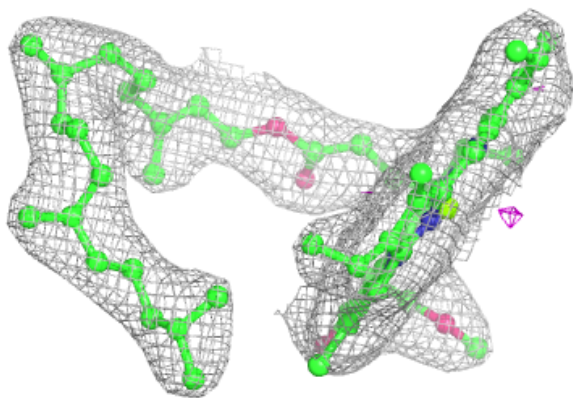
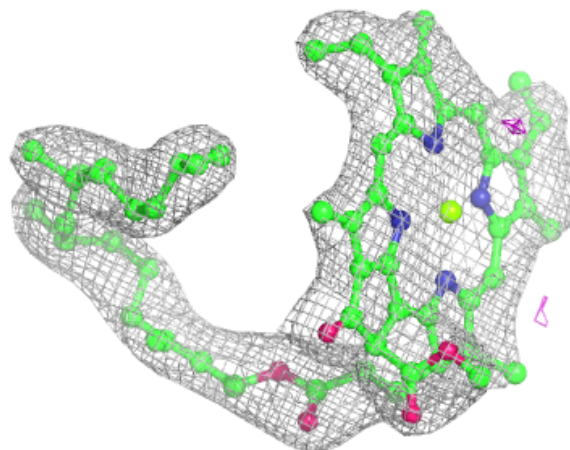
Electron density around CLA c 502:

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



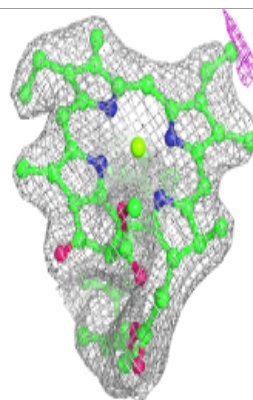
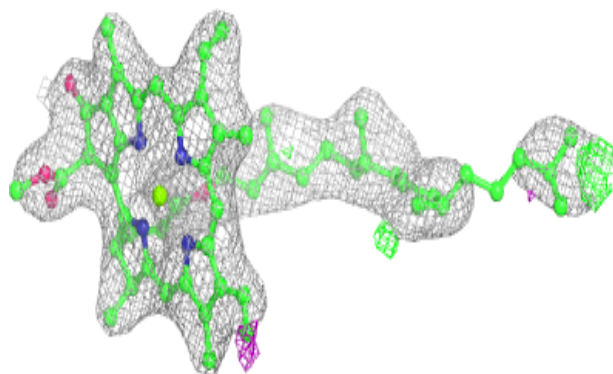
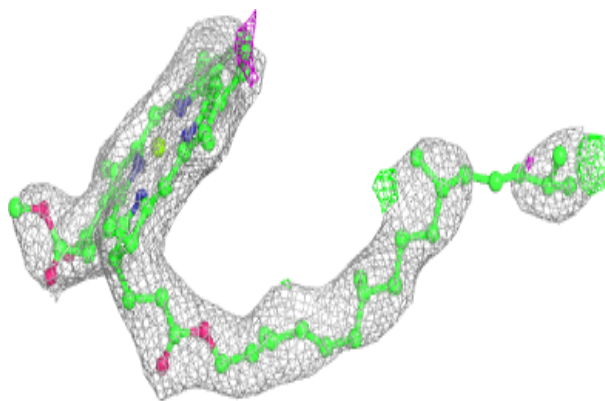
Electron density around CLA c 504:

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

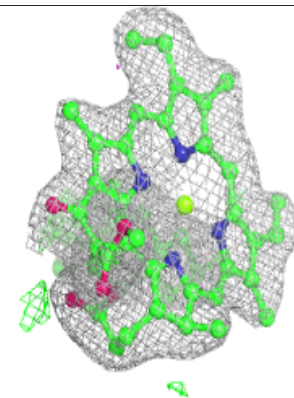
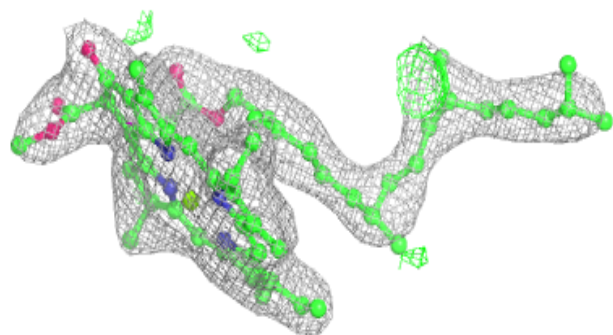
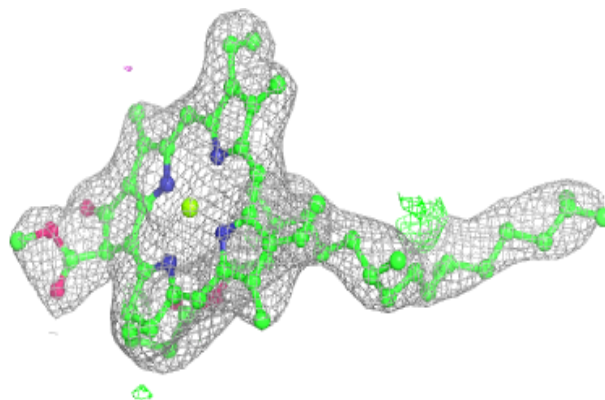


Electron density around CLA c 505:

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

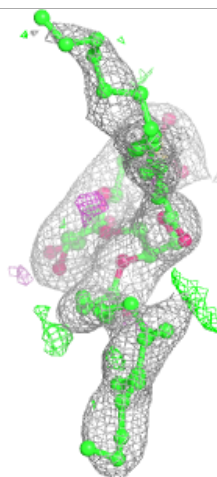
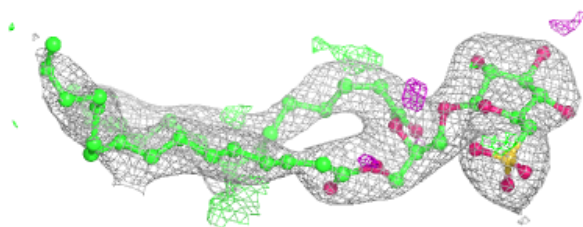
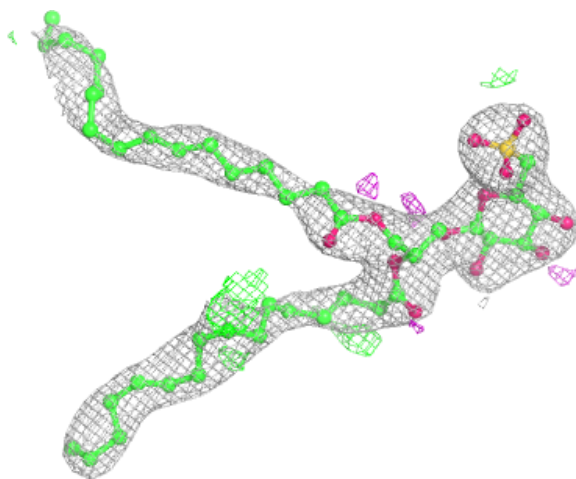
**Electron density around CLA c 506:**

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



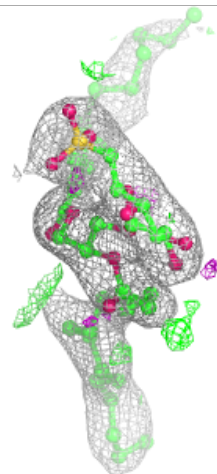
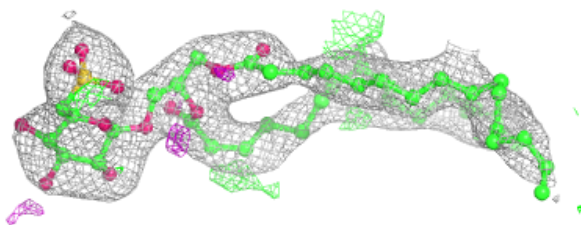
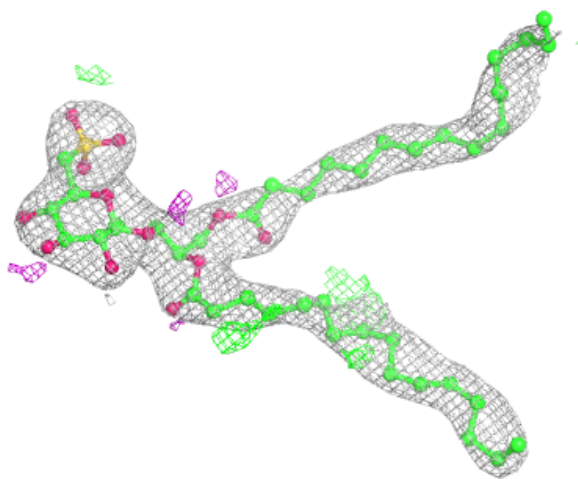
Electron density around SQD a 411 (A):

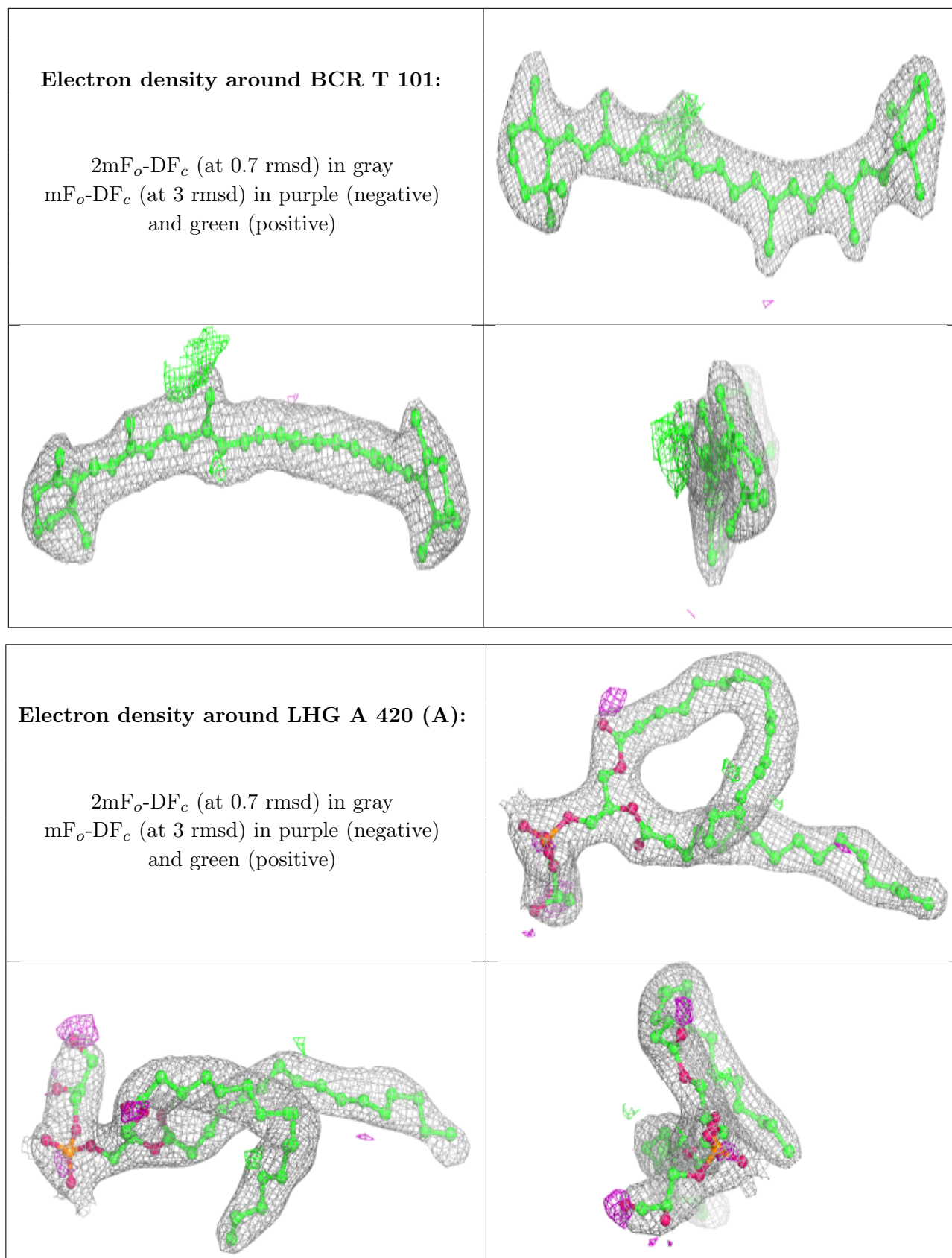
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SQD a 411 (B):

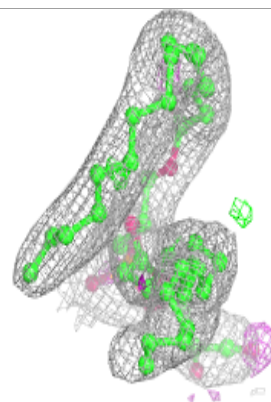
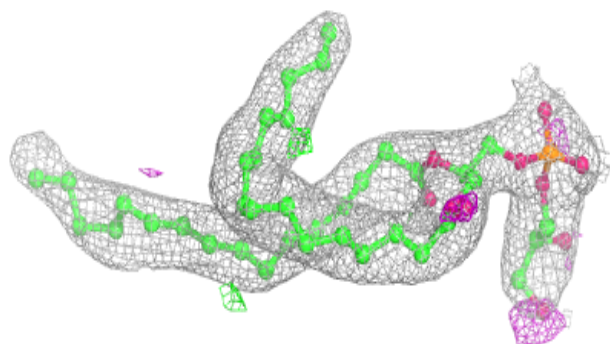
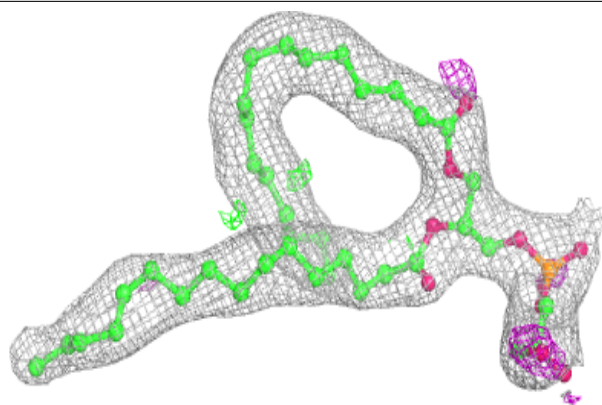
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



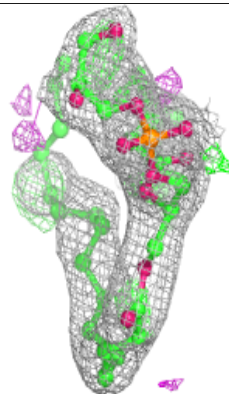
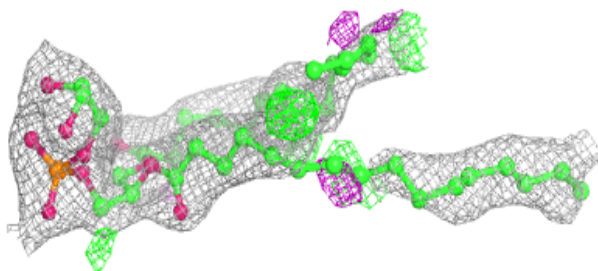
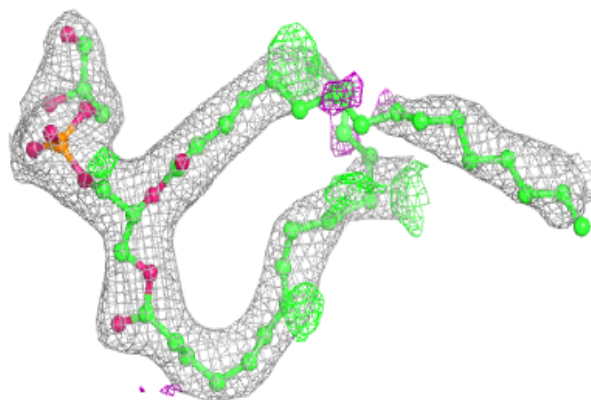


Electron density around LHG A 420 (B):

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

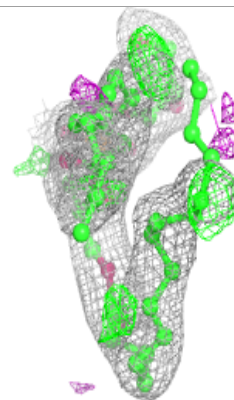
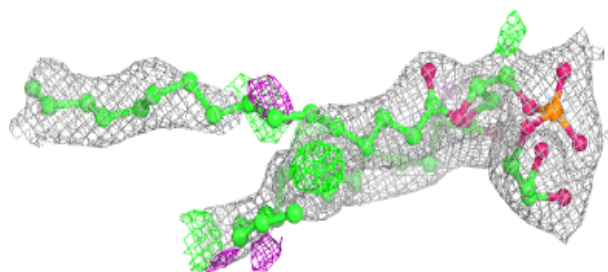
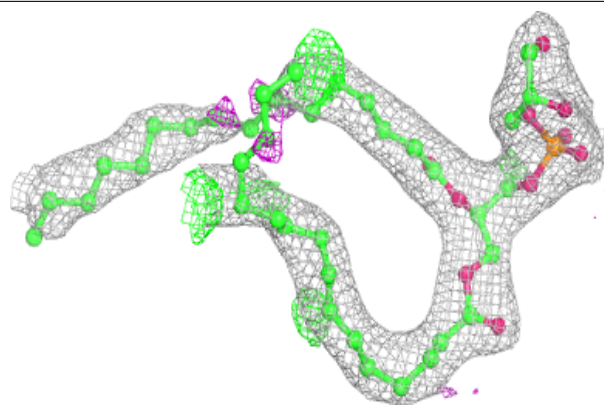
**Electron density around LHG D 407 (A):**

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

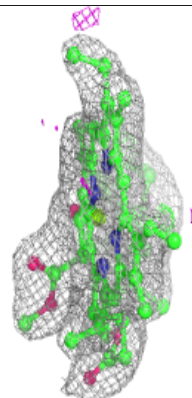
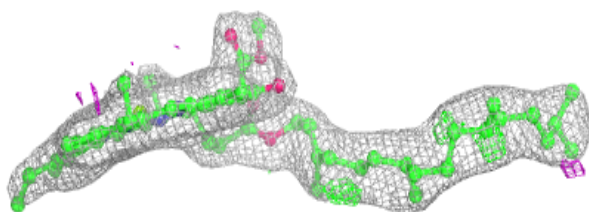
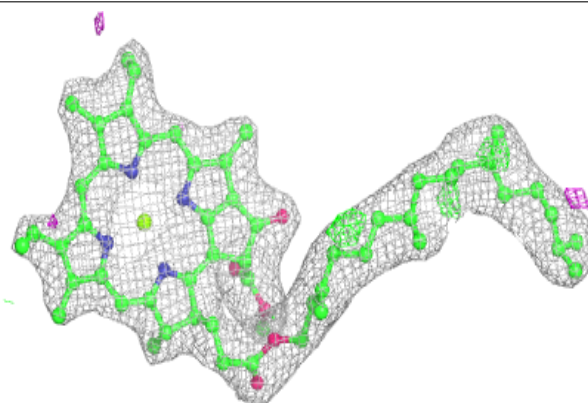


Electron density around LHG D 407 (B):

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

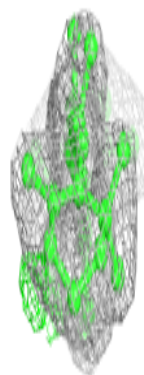
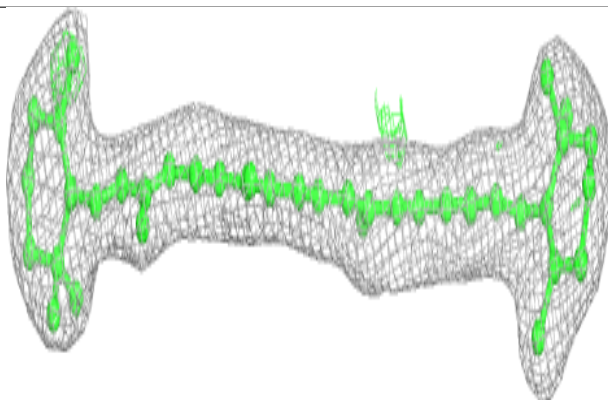
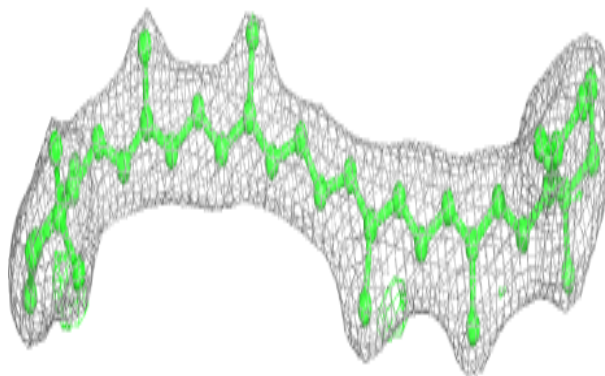
**Electron density around CLA B 602:**

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

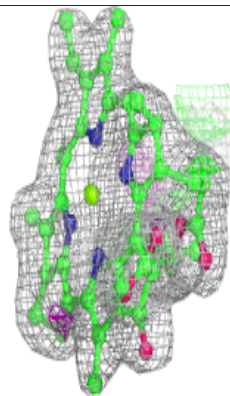
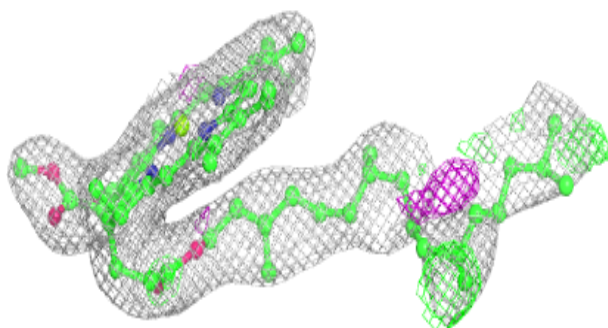
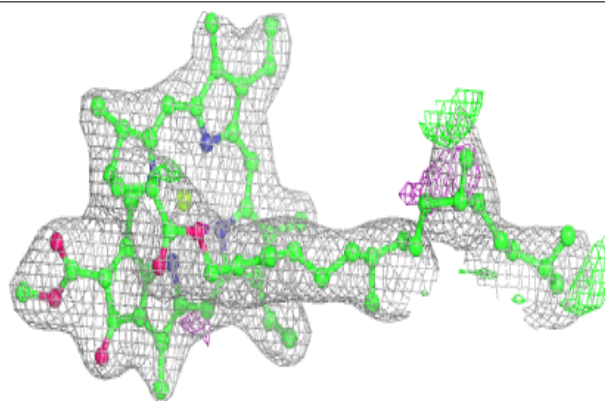


Electron density around BCR a 410:

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

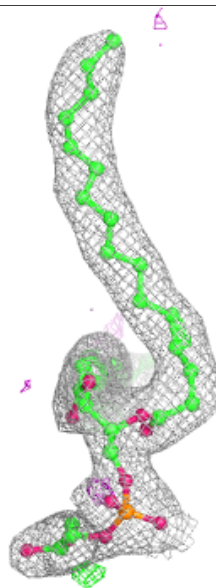
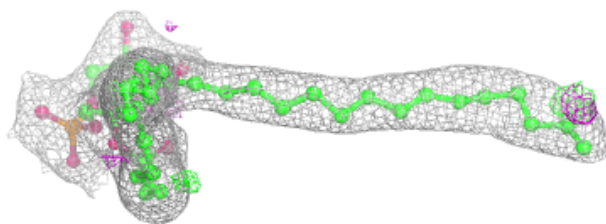
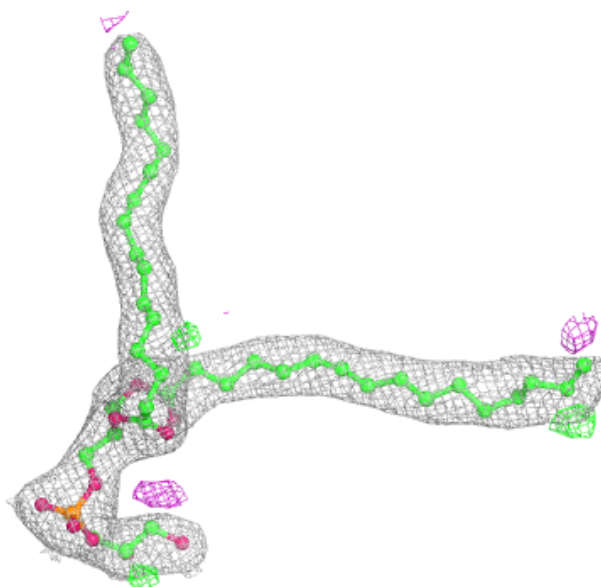
**Electron density around CLA B 614:**

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



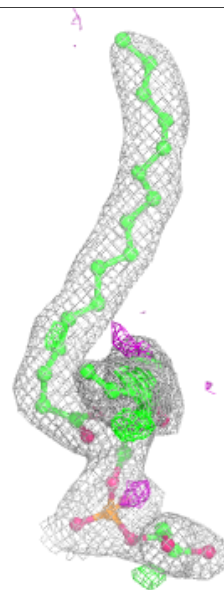
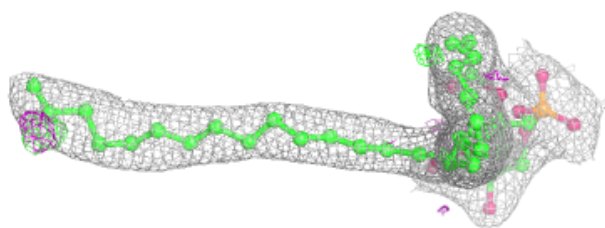
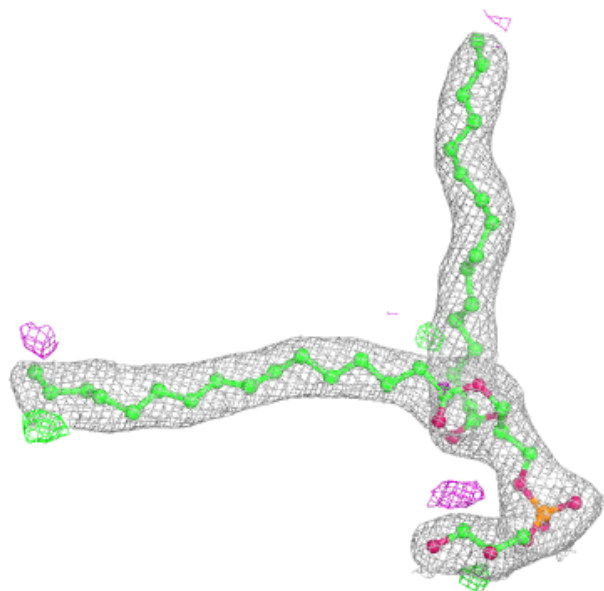
Electron density around LHG b 628 (A):

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



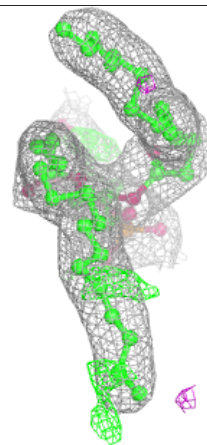
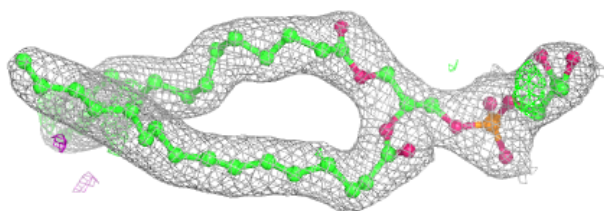
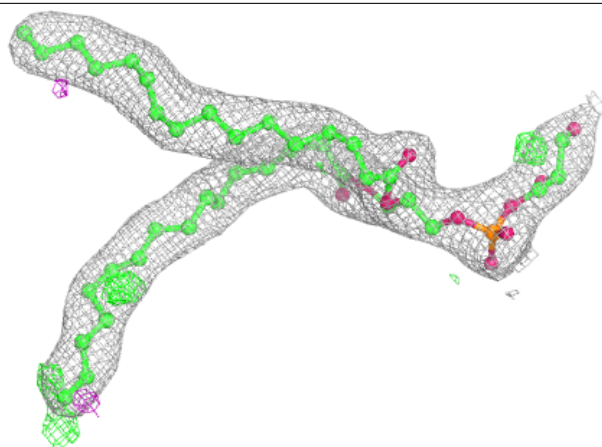
Electron density around LHG b 628 (B):

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



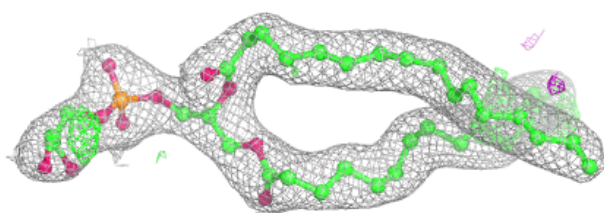
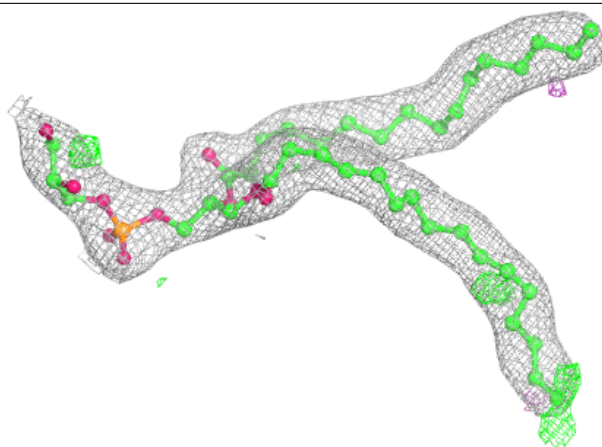
Electron density around LHG d 407 (A):

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

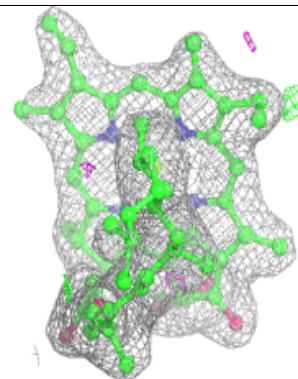
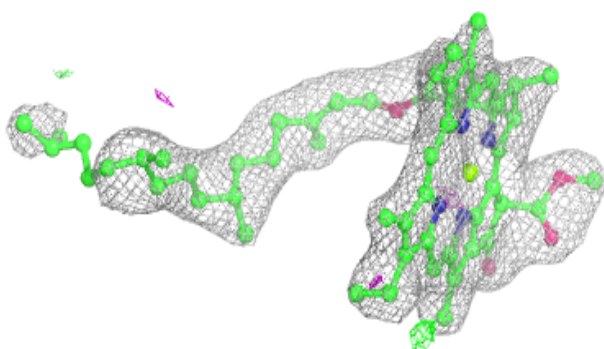
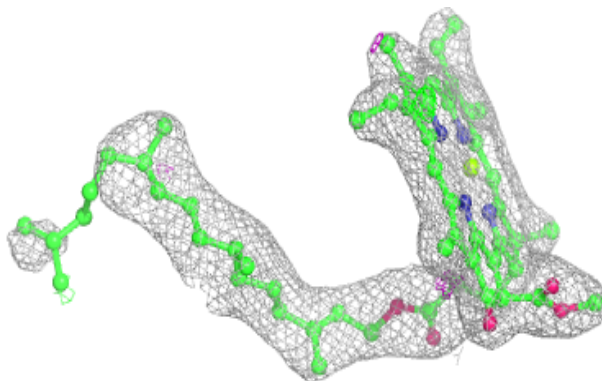


Electron density around LHG d 407 (B):

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

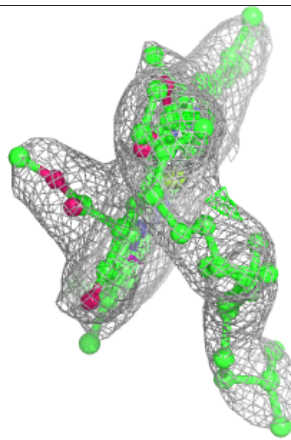
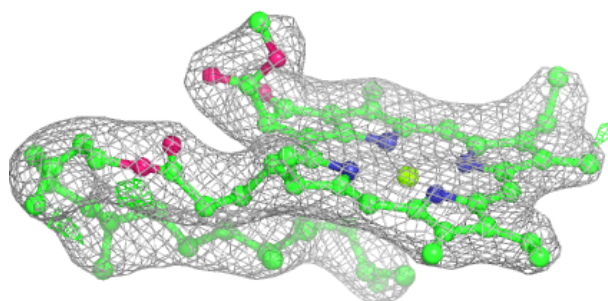
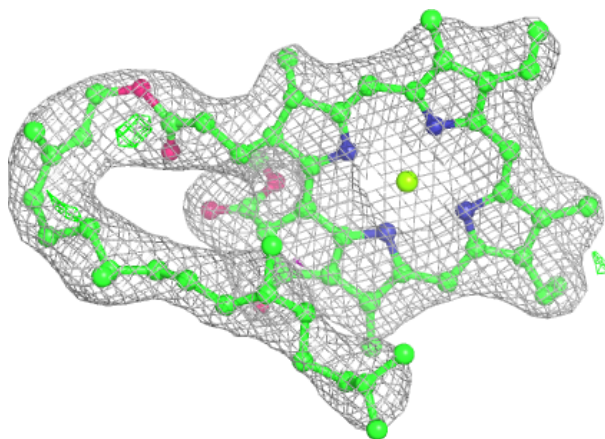
**Electron density around CLA c 509:**

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

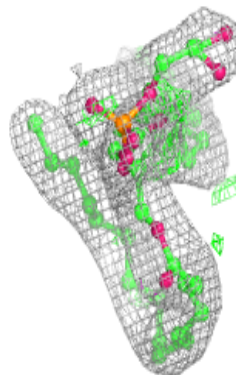
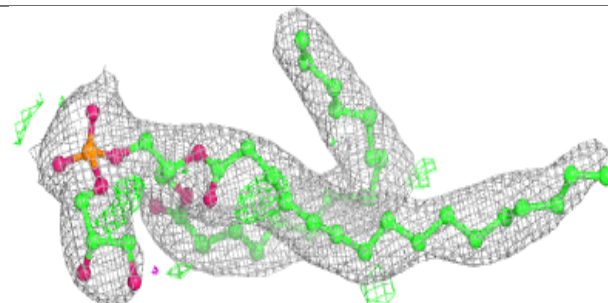
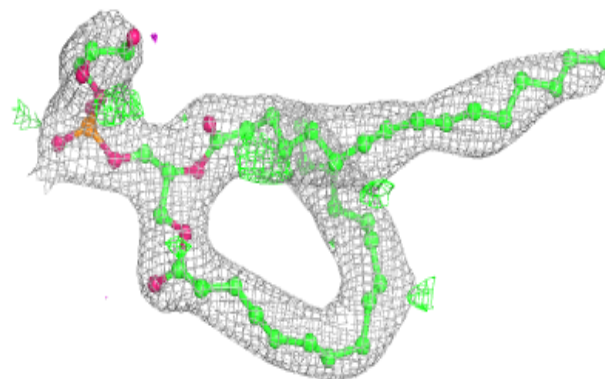


Electron density around CLA c 510:

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

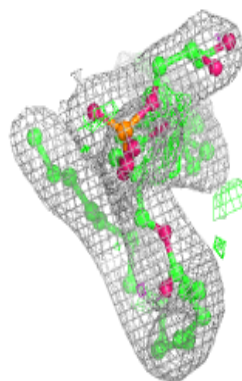
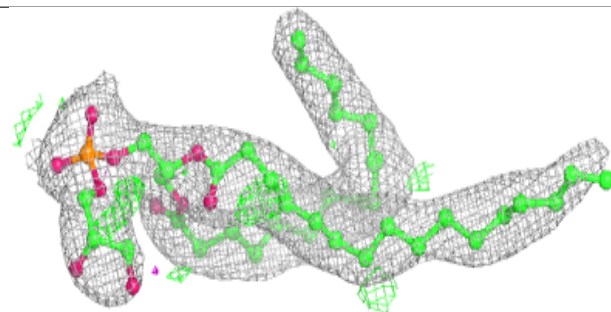
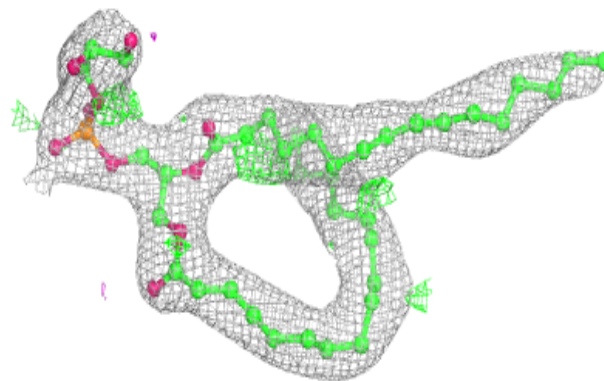
**Electron density around LHG d 414 (A):**

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

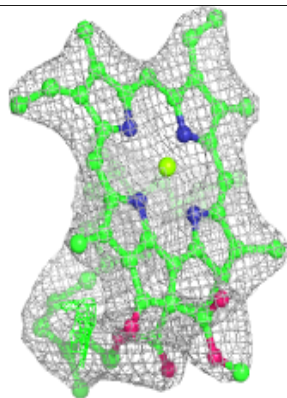
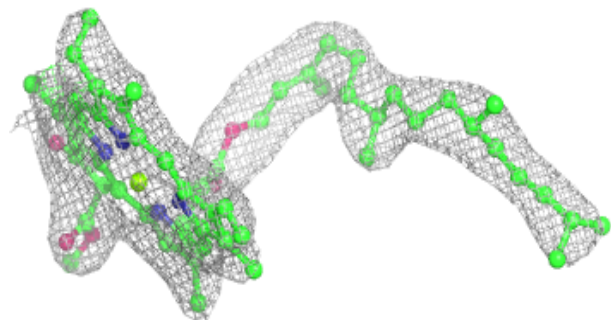
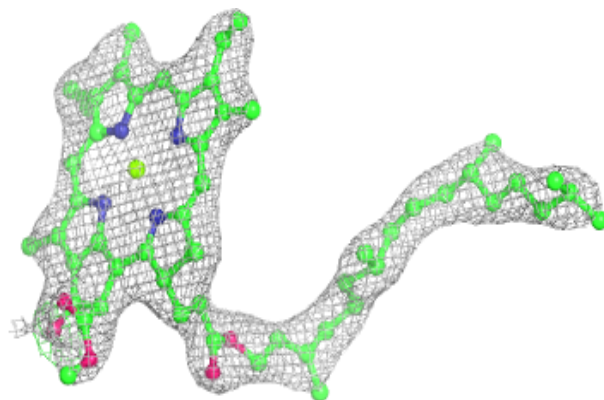


Electron density around LHG d 414 (B):

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

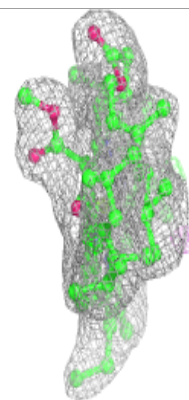
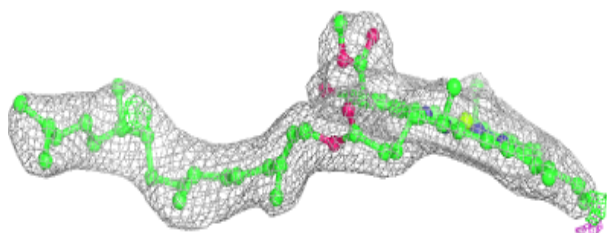
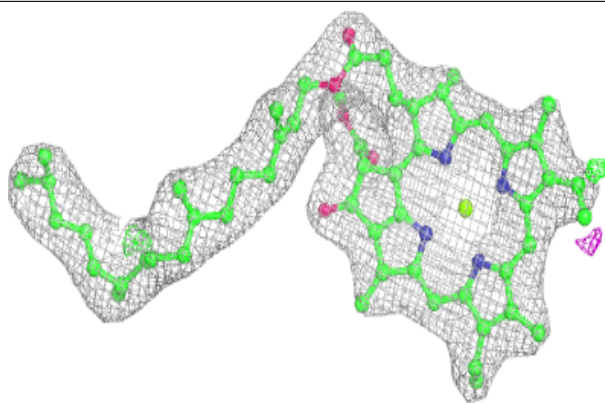
**Electron density around CLA c 512:**

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

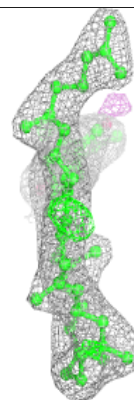
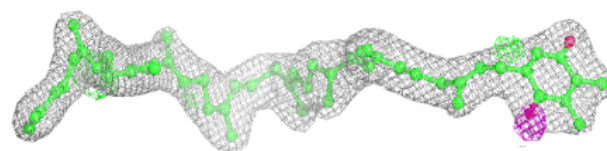
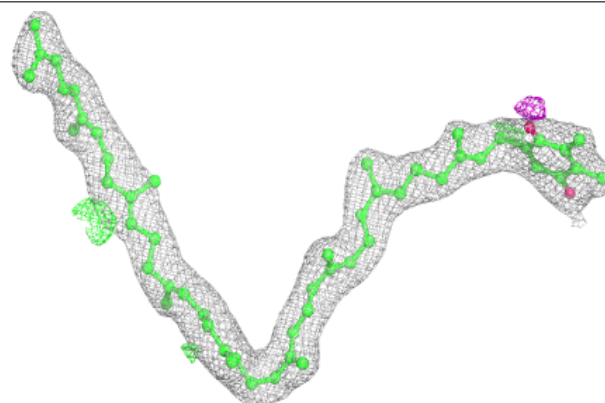


Electron density around CLA b 602:

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

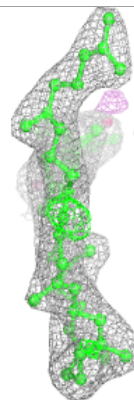
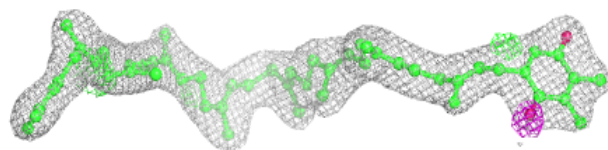
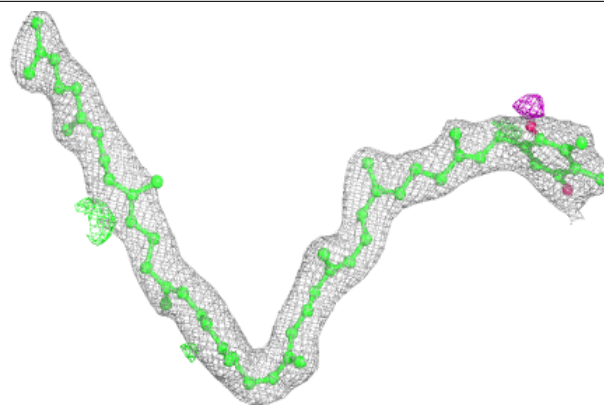
**Electron density around PL9 D 405 (A):**

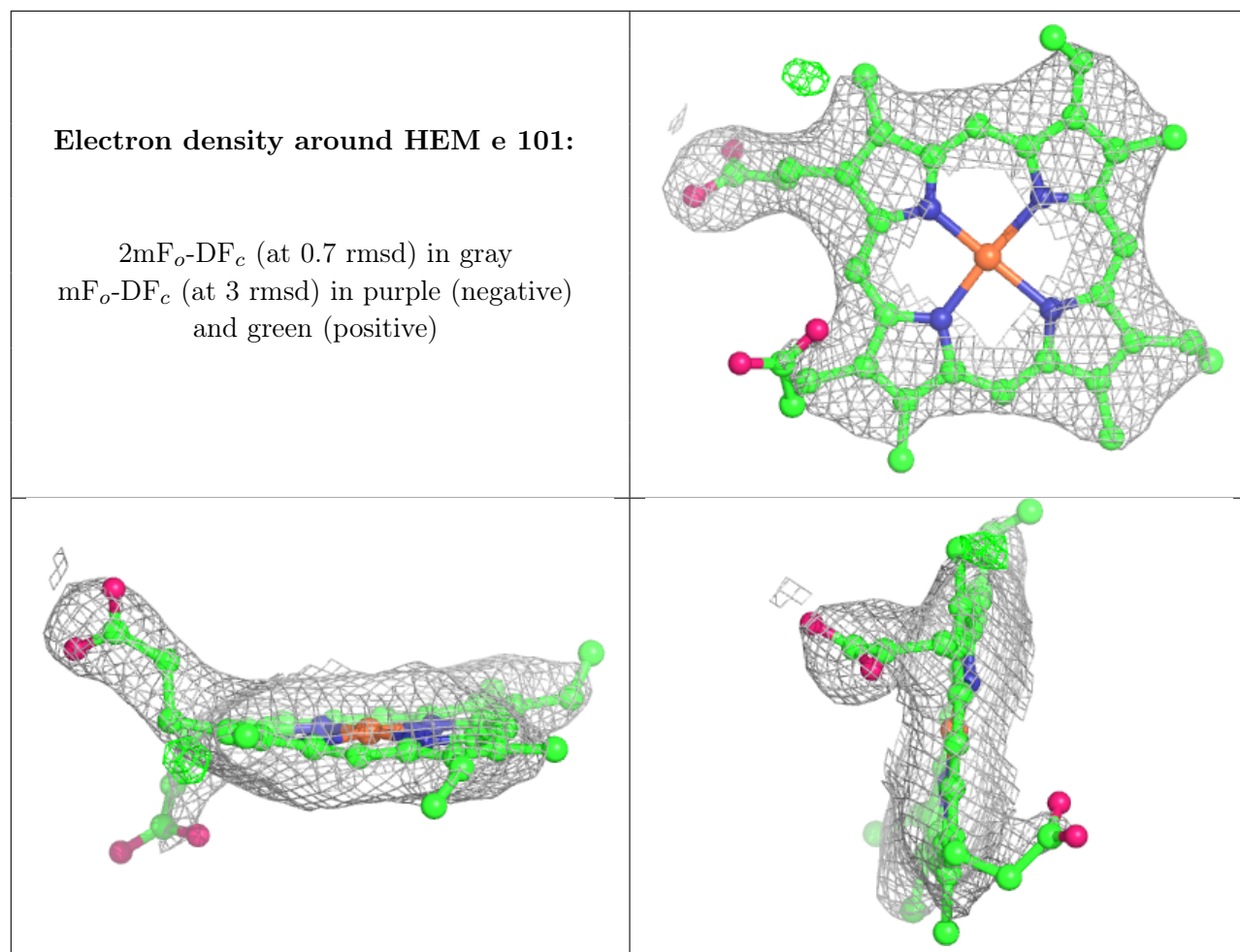
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PL9 D 405 (B):

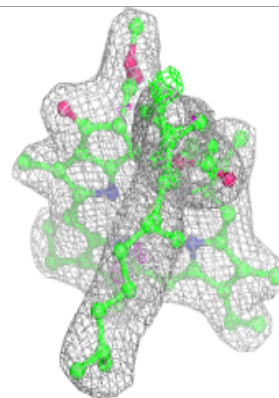
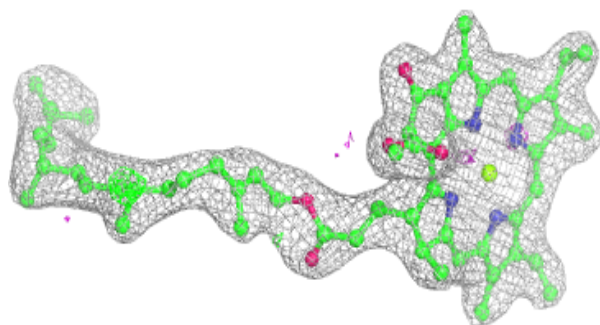
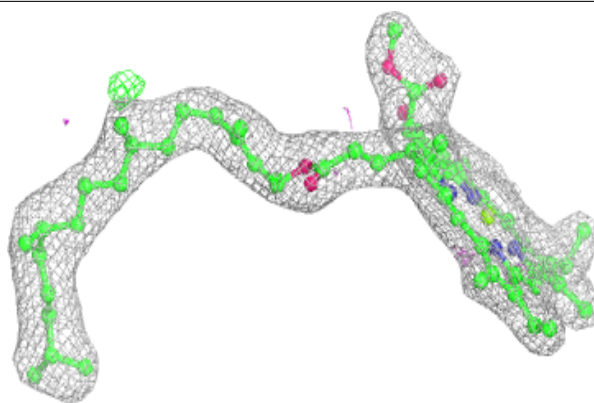
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



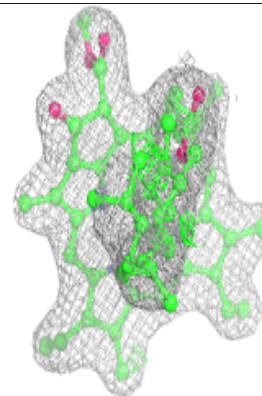
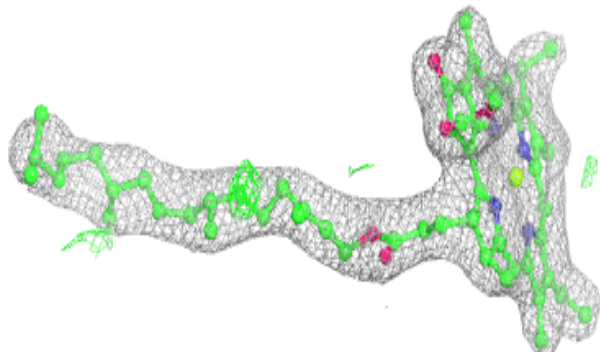
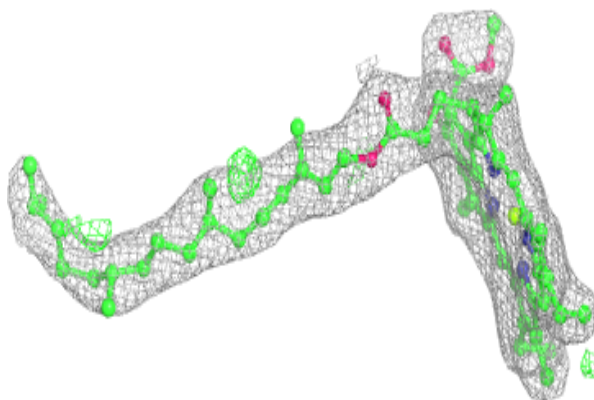


Electron density around CLA d 403 (B):

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

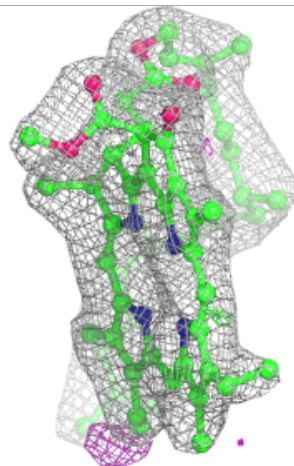
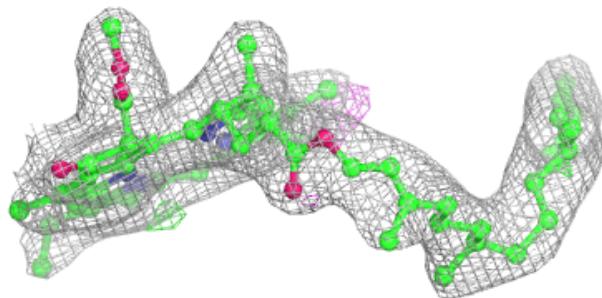
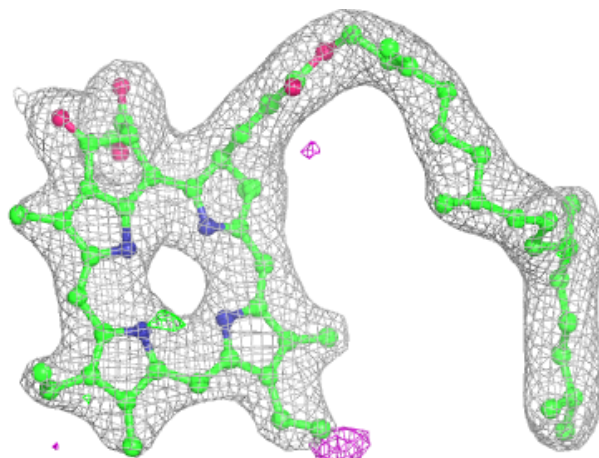
**Electron density around CLA b 604:**

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



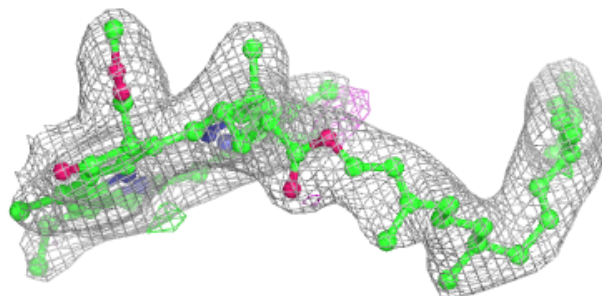
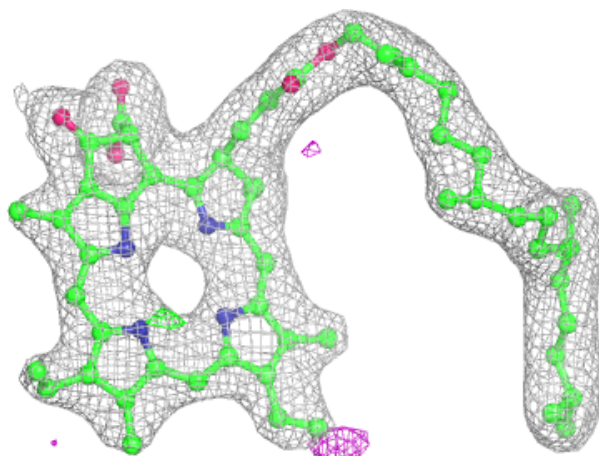
Electron density around PHO d 402 (A):

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



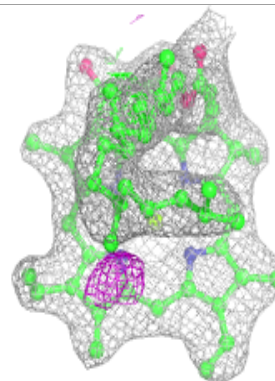
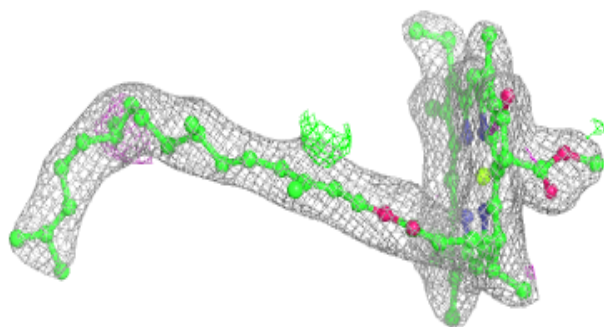
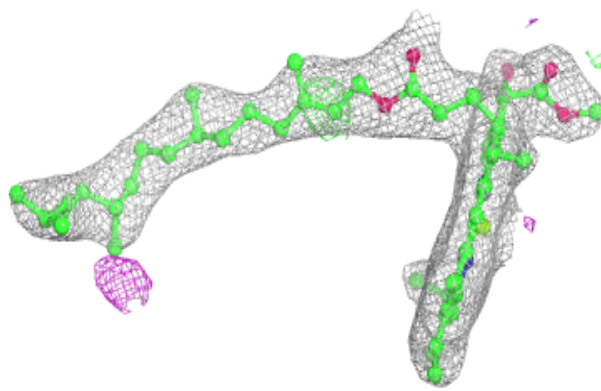
Electron density around PHO d 402 (B):

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

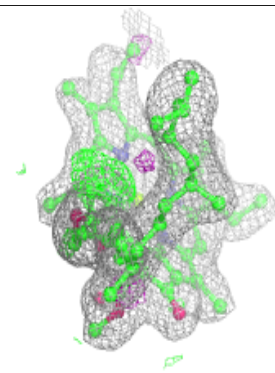
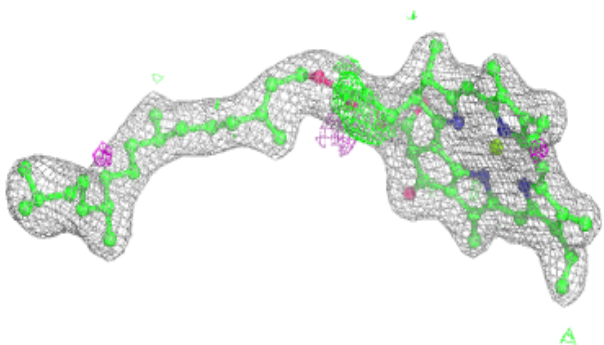
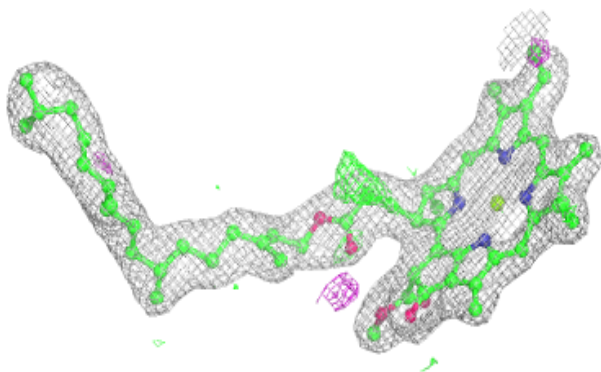


Electron density around CLA b 605:

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

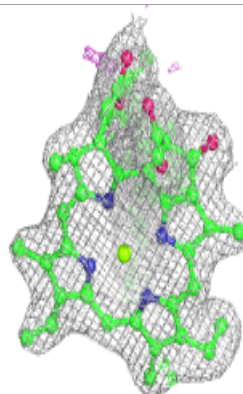
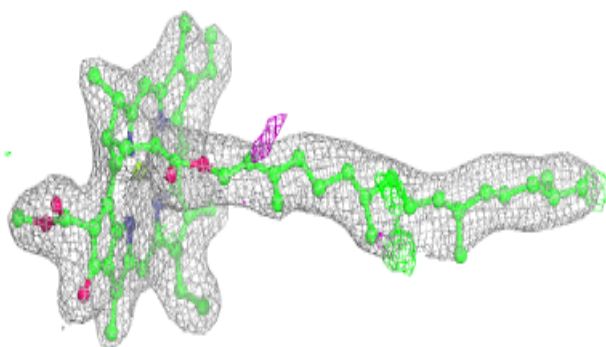
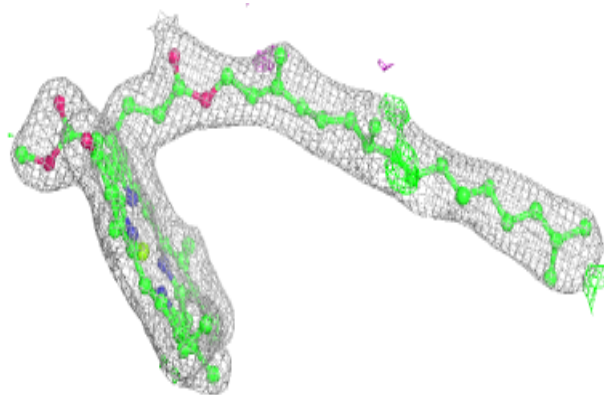
**Electron density around CLA A 405 (B):**

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

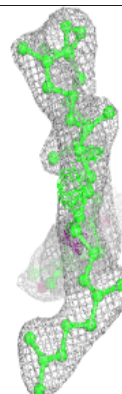
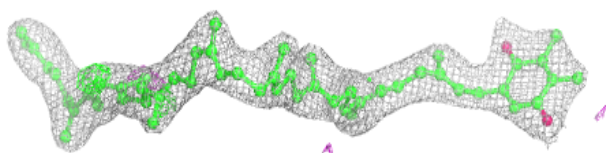
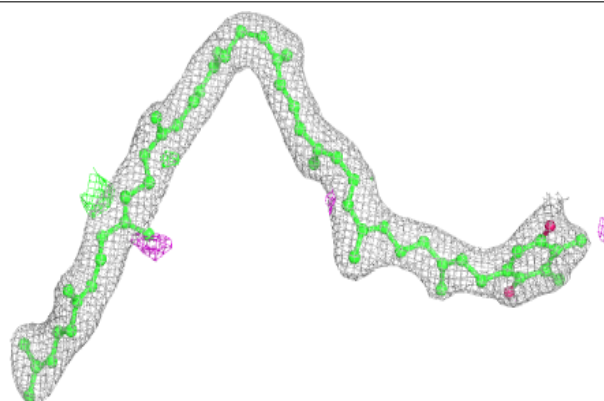


Electron density around CLA b 607:

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

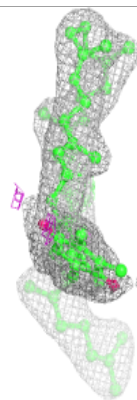
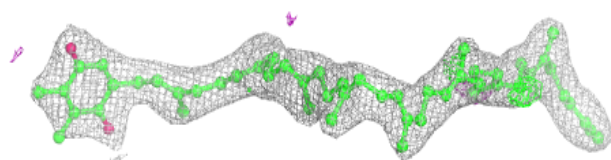
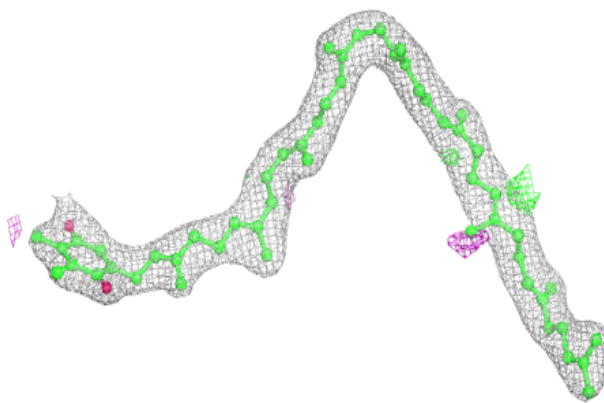
**Electron density around PL9 d 406 (A):**

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

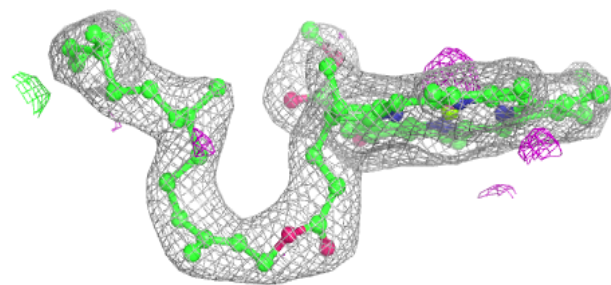
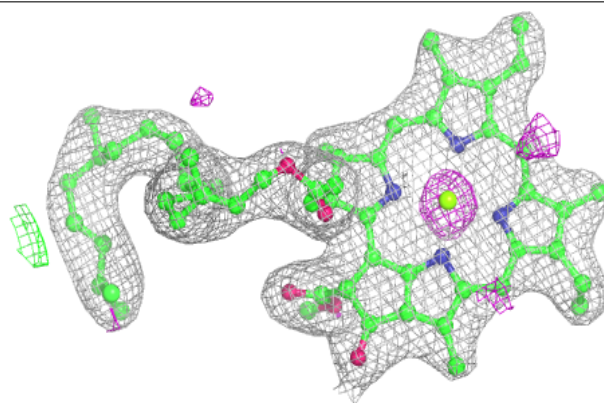


Electron density around PL9 d 406 (B):

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

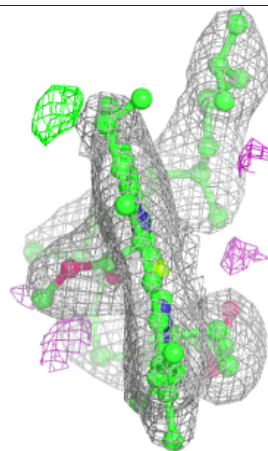
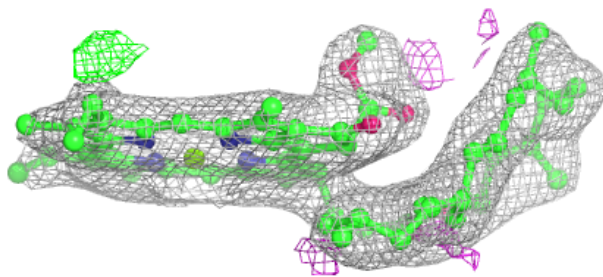
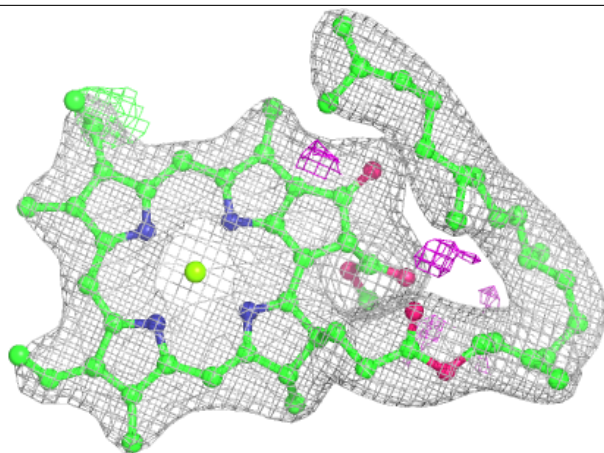
**Electron density around CLA B 612:**

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



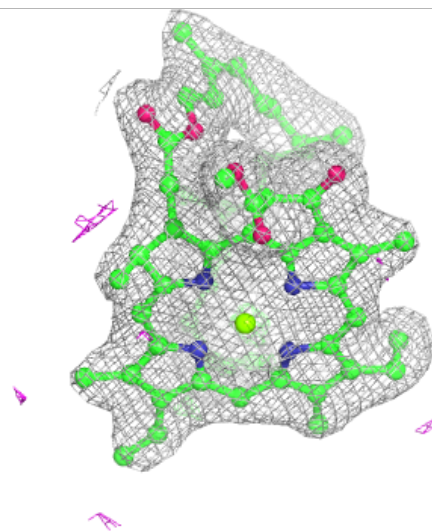
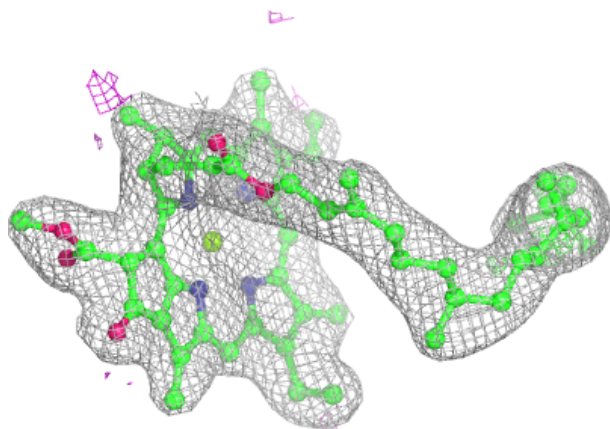
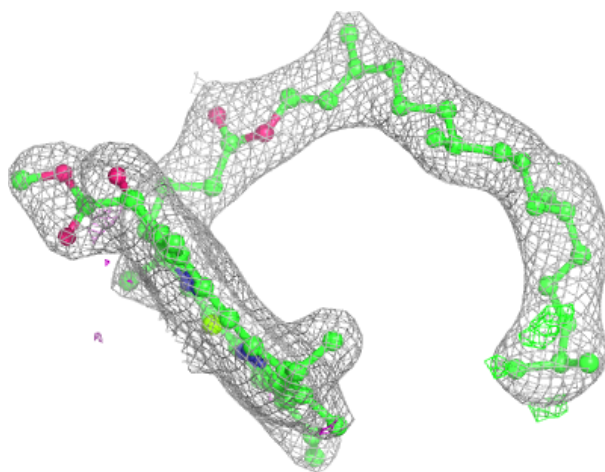
Electron density around CLA b 610:

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



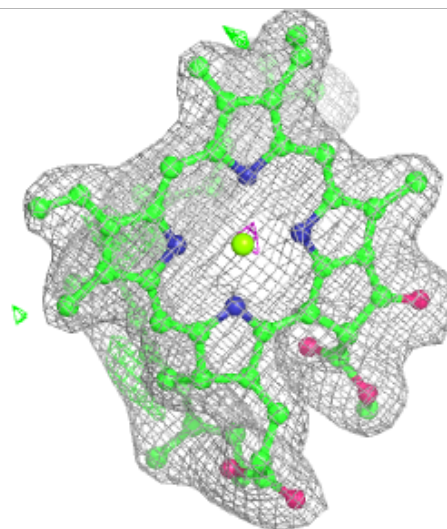
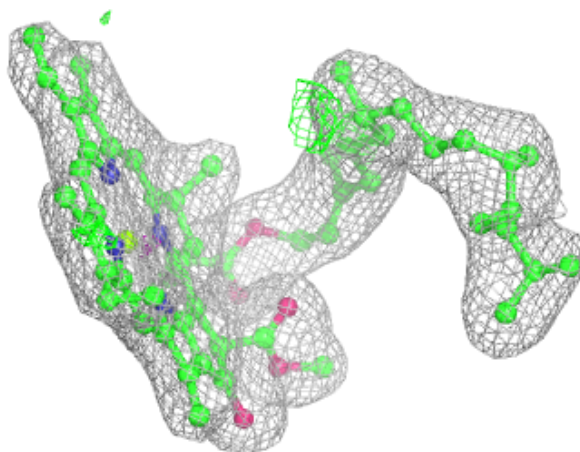
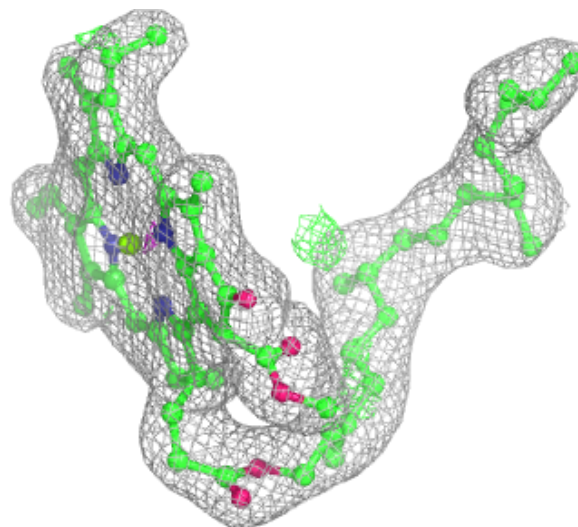
Electron density around CLA b 611:

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



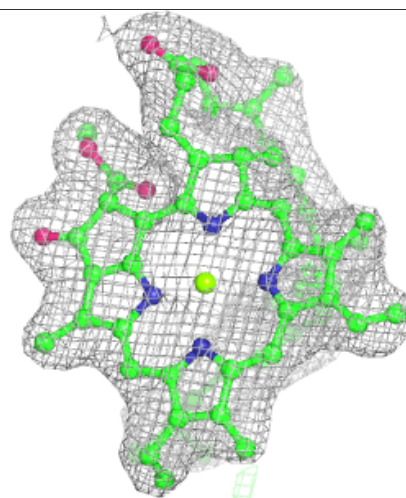
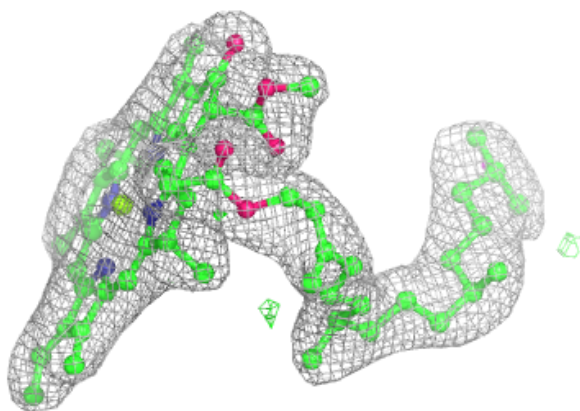
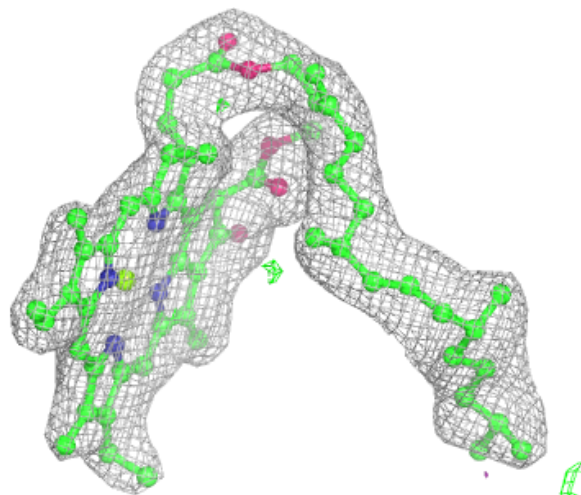
Electron density around CLA B 613:

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



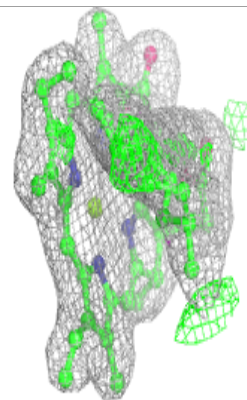
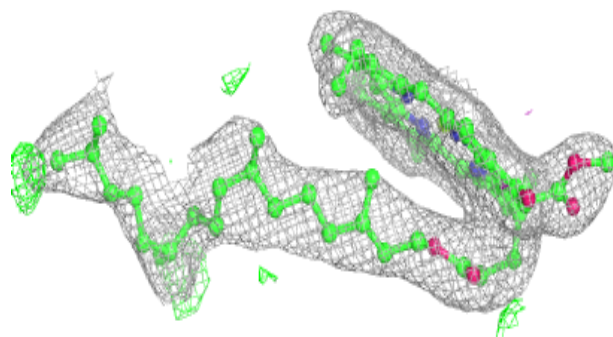
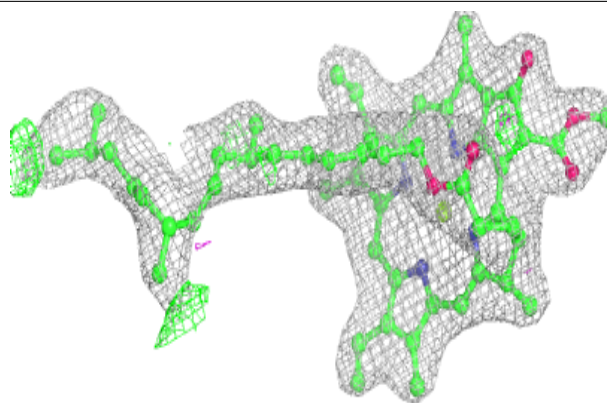
Electron density around CLA b 613:

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

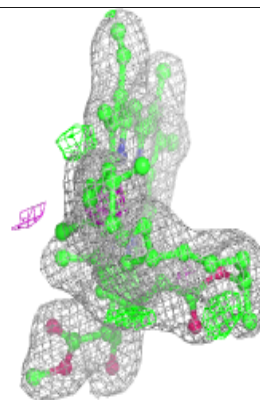
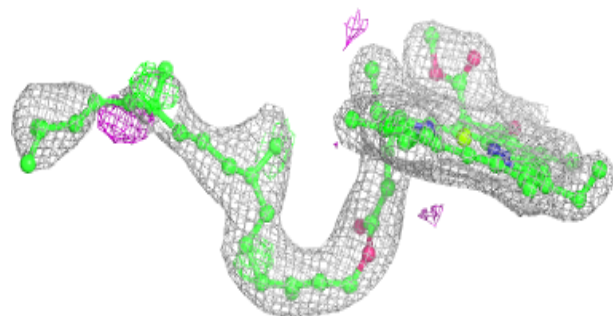
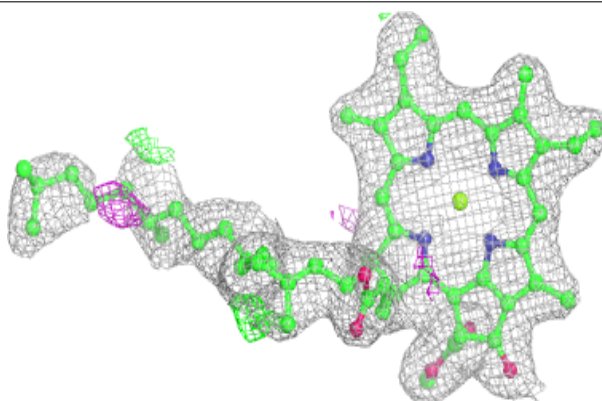


Electron density around CLA b 614:

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

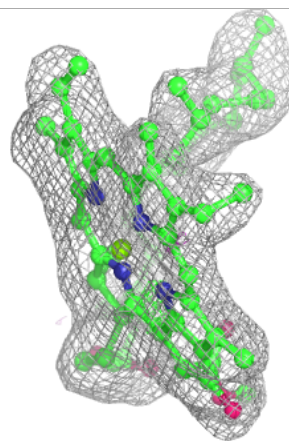
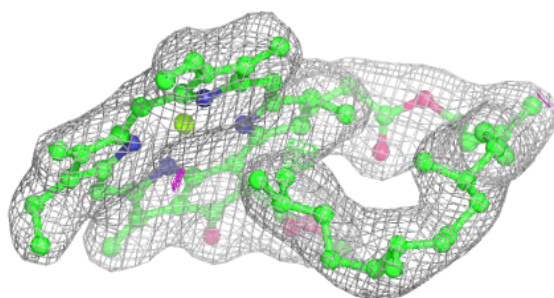
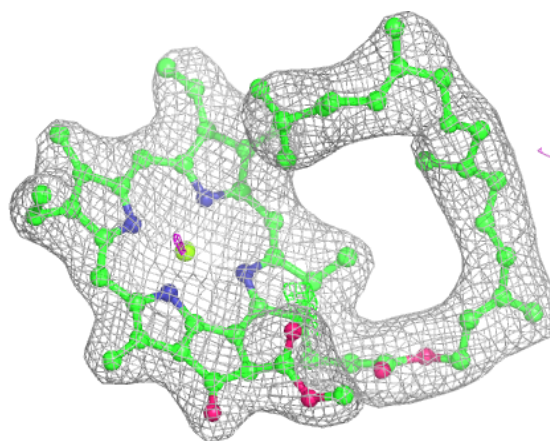
**Electron density around CLA A 407 (A):**

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



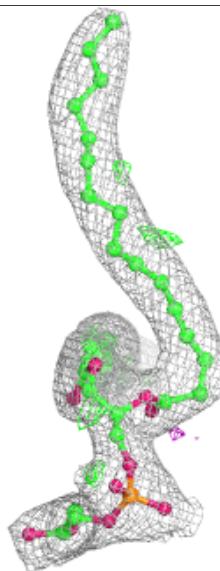
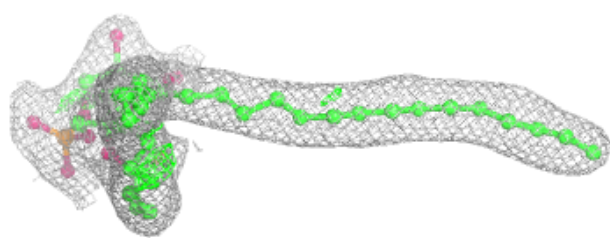
Electron density around CLA B 615:

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



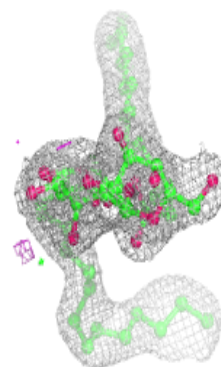
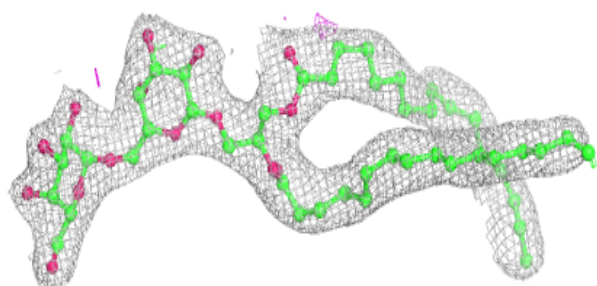
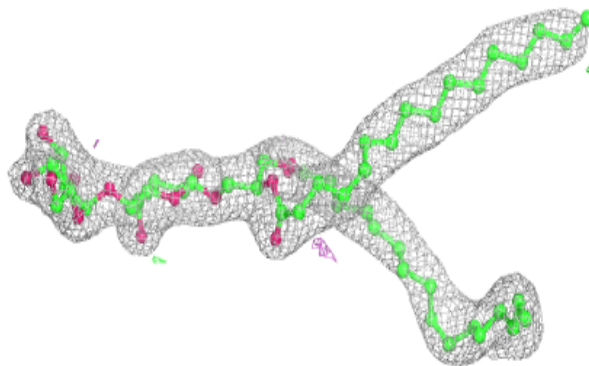
Electron density around LHG L 101 (A):

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

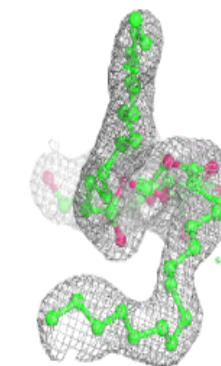
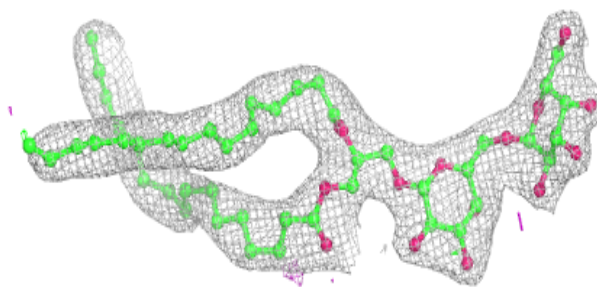
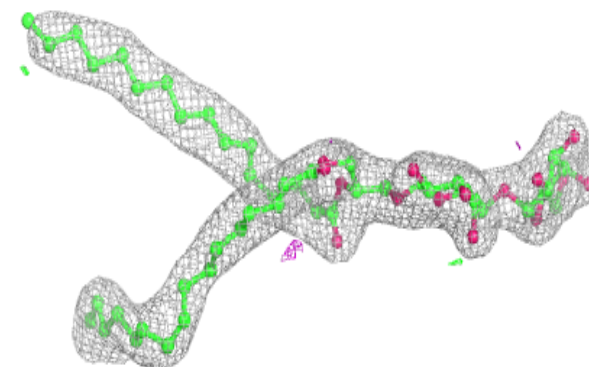


Electron density around DGD C 517 (A):

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

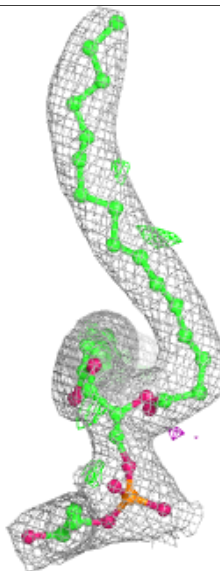
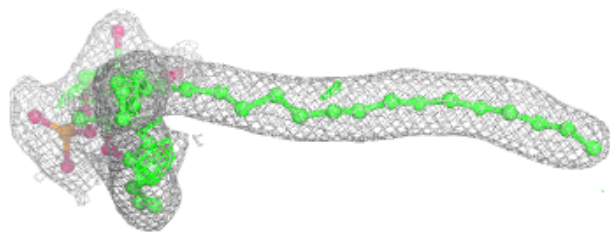
**Electron density around DGD C 517 (B):**

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



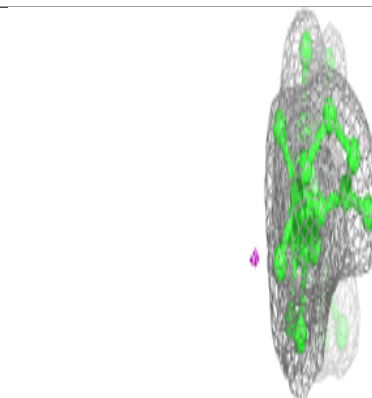
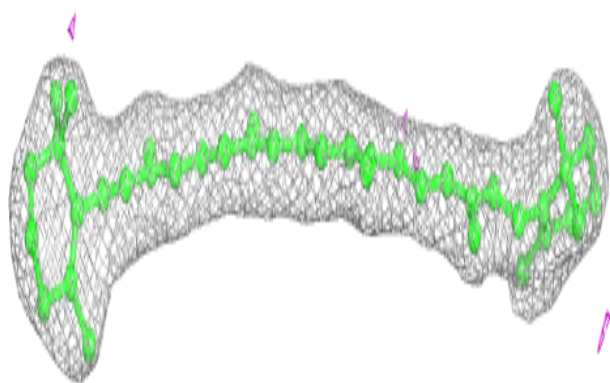
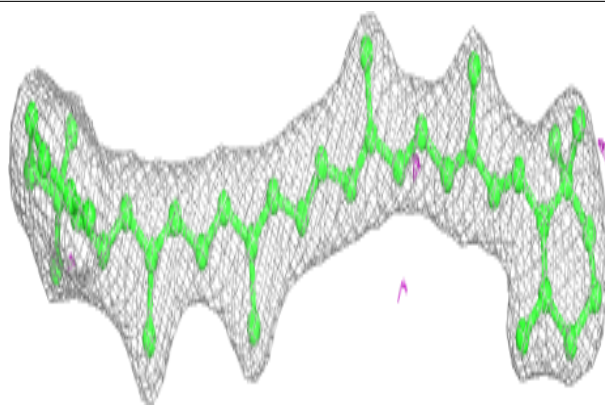
Electron density around LHG L 101 (B):

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

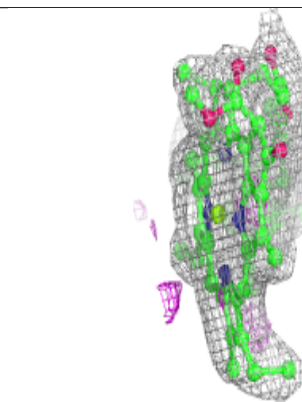
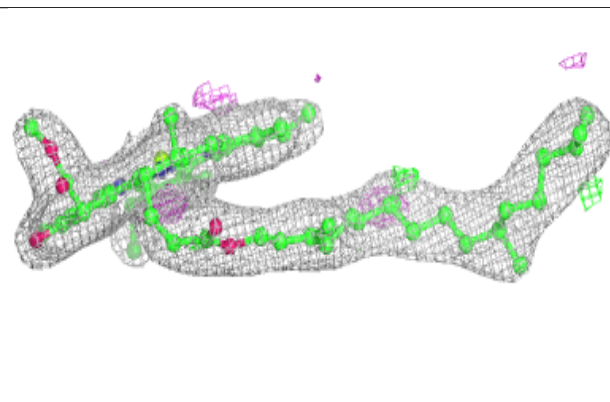
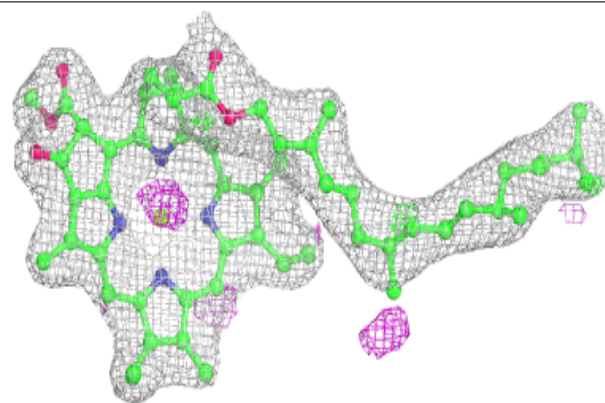


Electron density around BCR b 617:

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

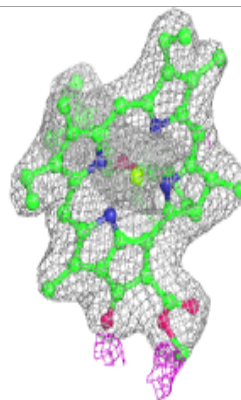
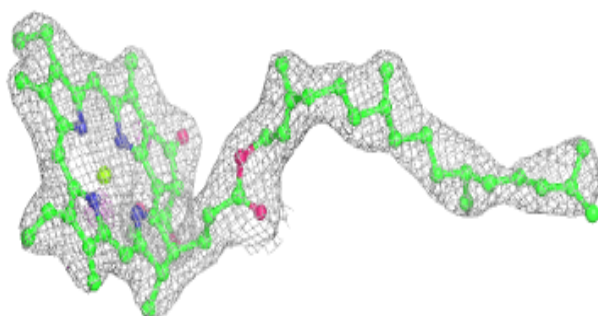
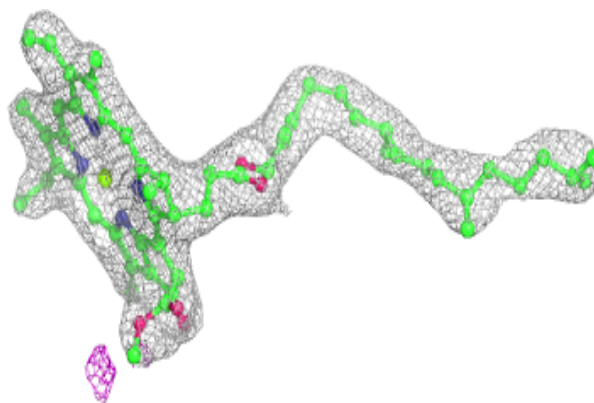
**Electron density around CLA B 603:**

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

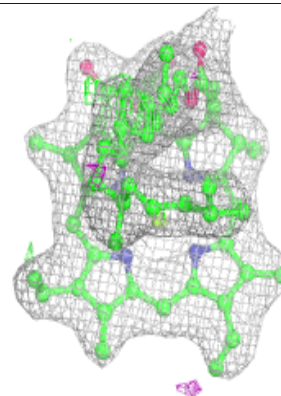
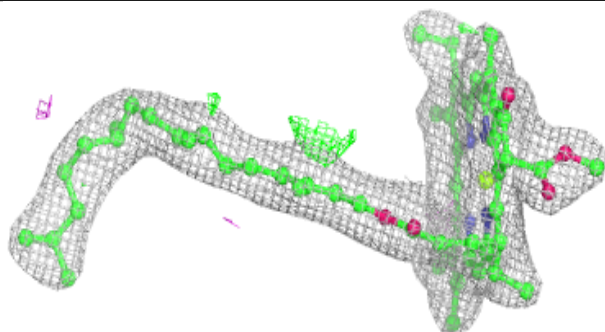
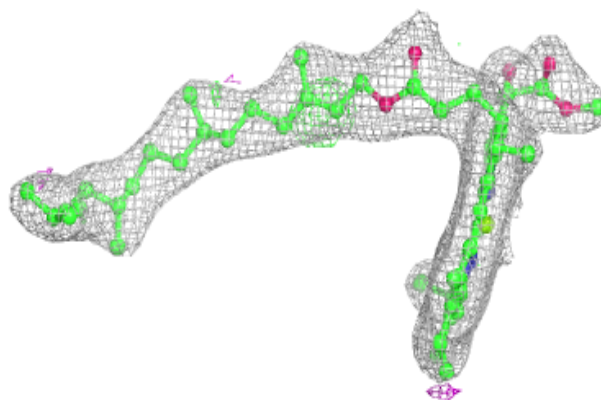


Electron density around CLA c 503:

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

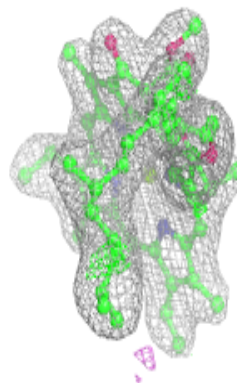
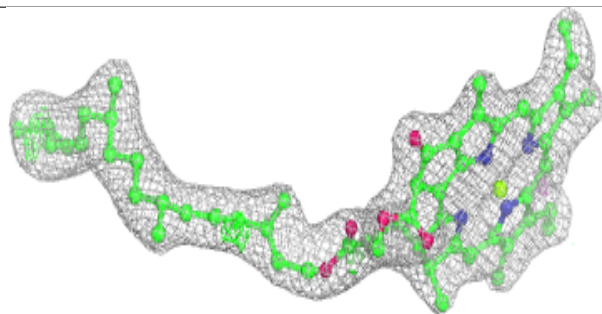
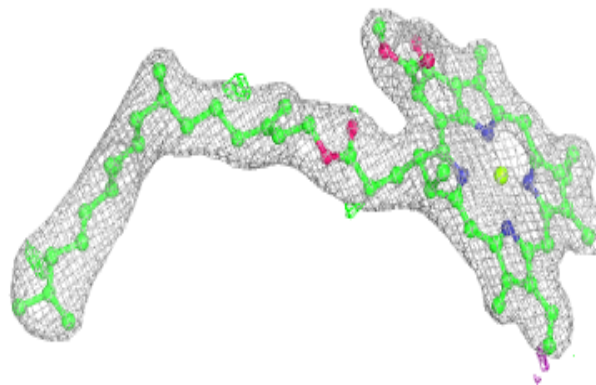
**Electron density around CLA B 605:**

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

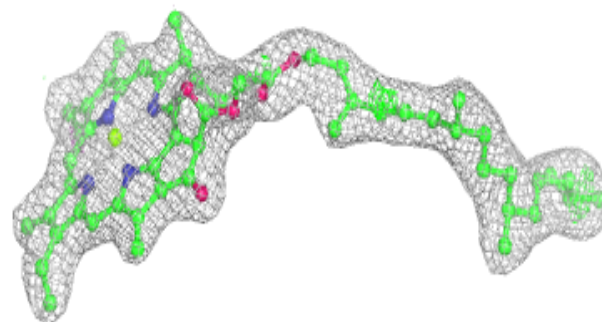
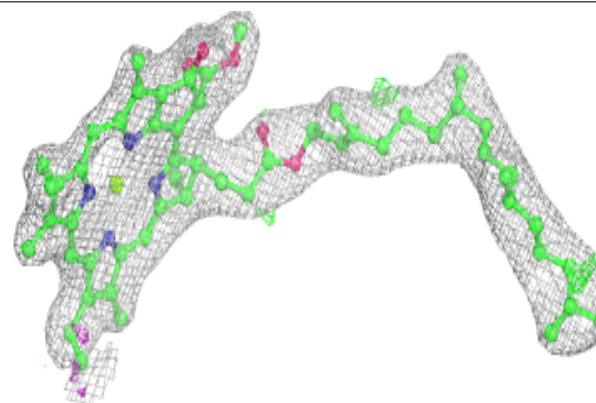


Electron density around CLA a 405 (A):

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

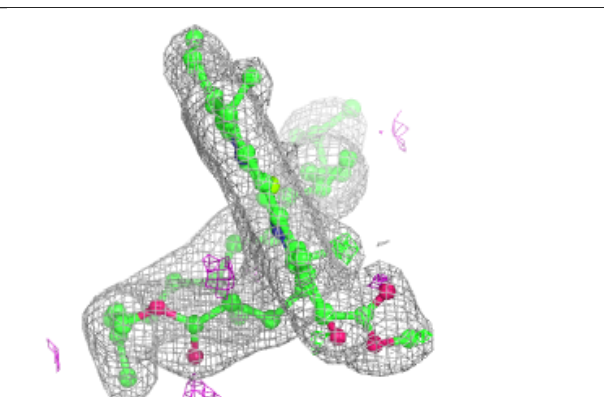
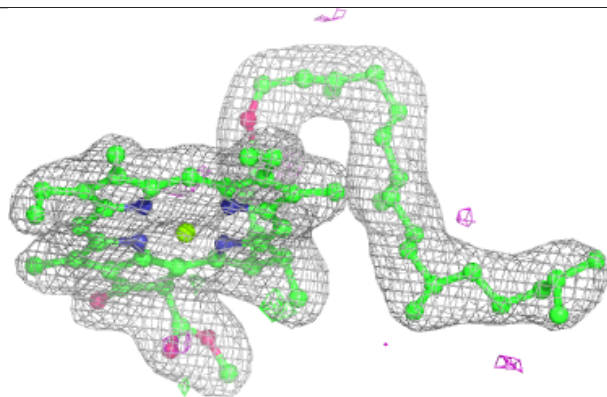
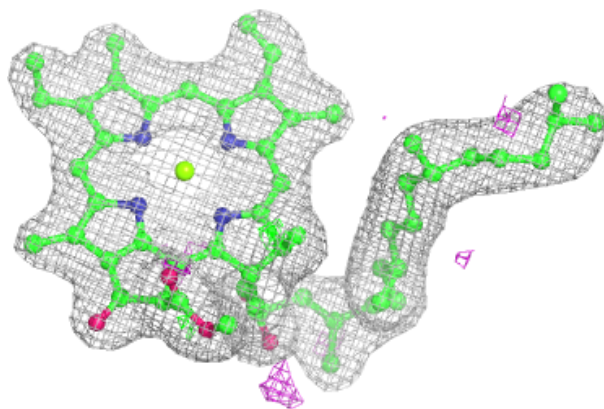
**Electron density around CLA a 405 (B):**

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

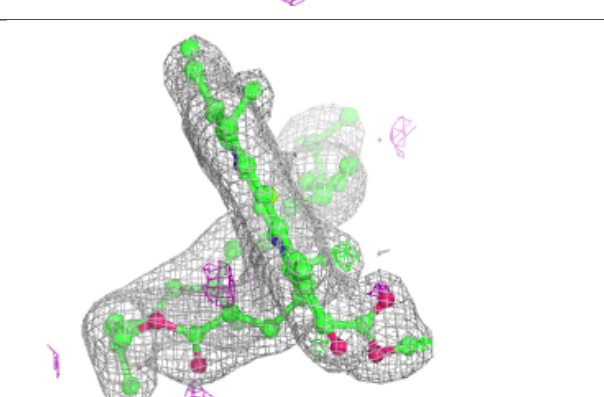
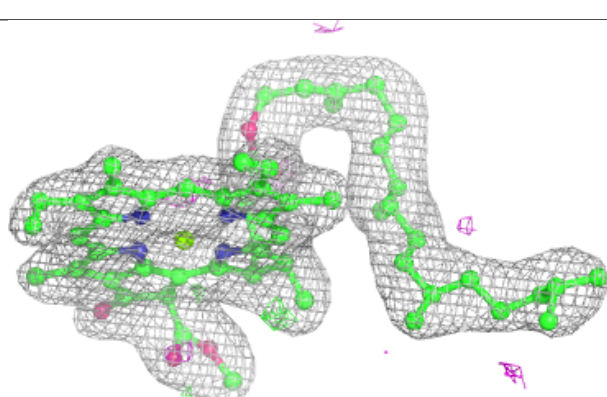
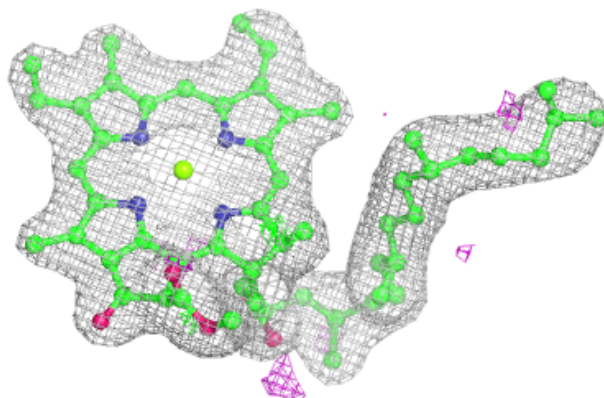


Electron density around CLA a 406 (A):

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

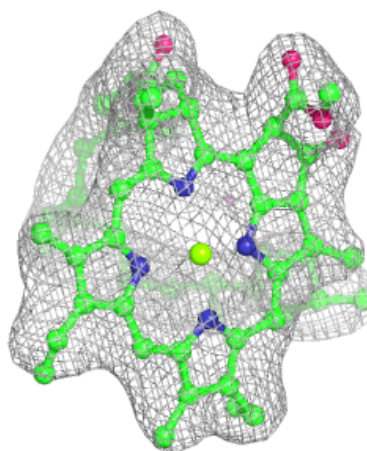
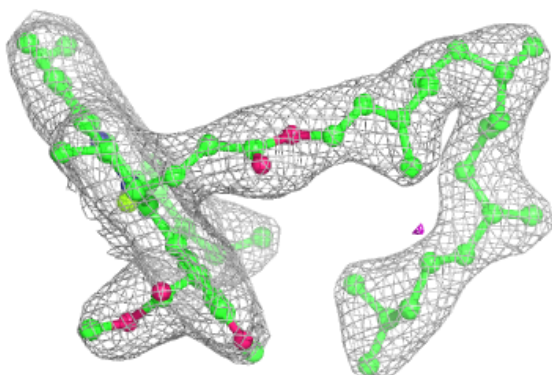
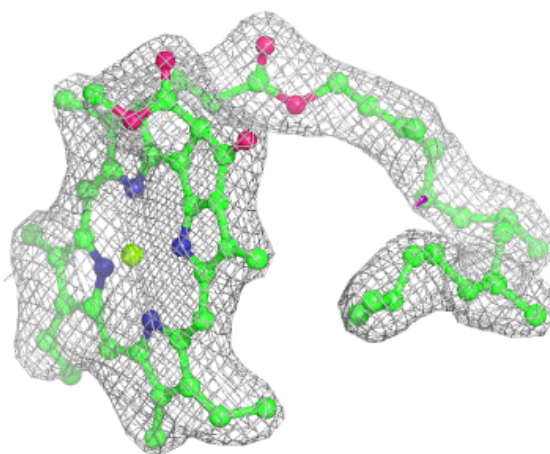
**Electron density around CLA a 406 (B):**

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



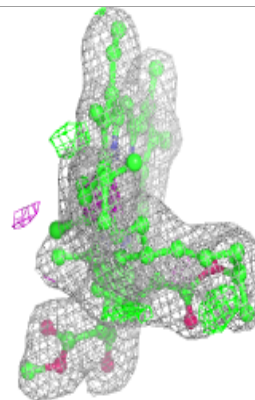
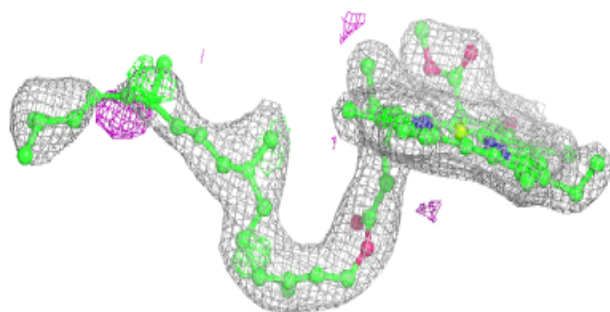
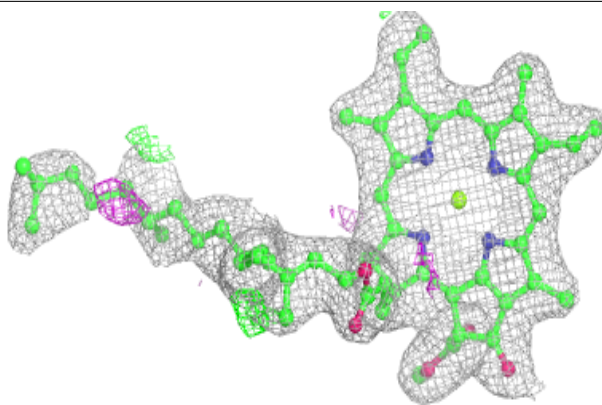
Electron density around CLA C 504:

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



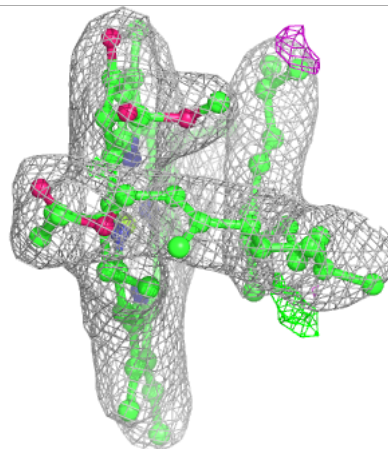
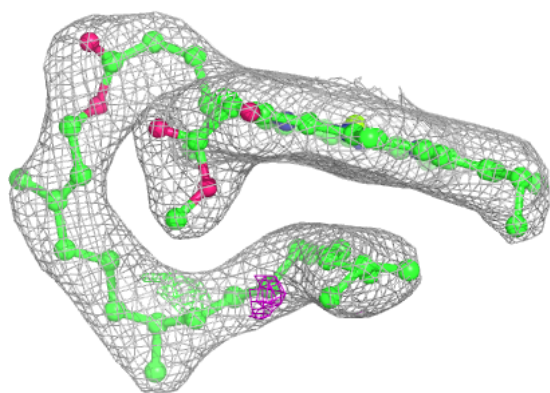
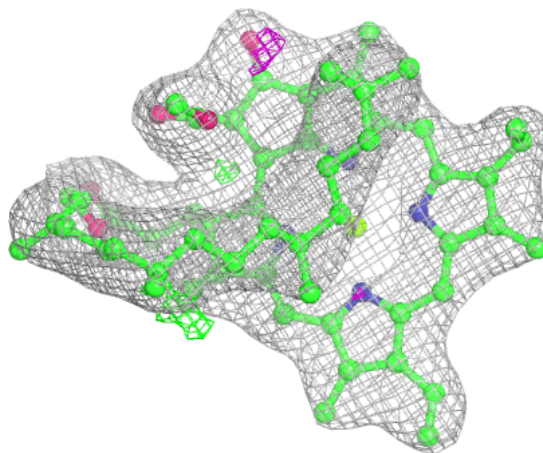
Electron density around CLA A 407 (B):

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



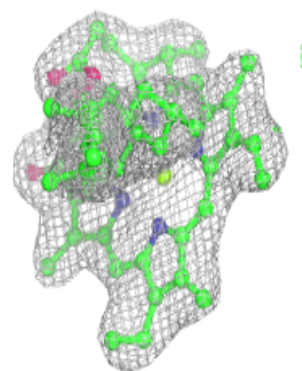
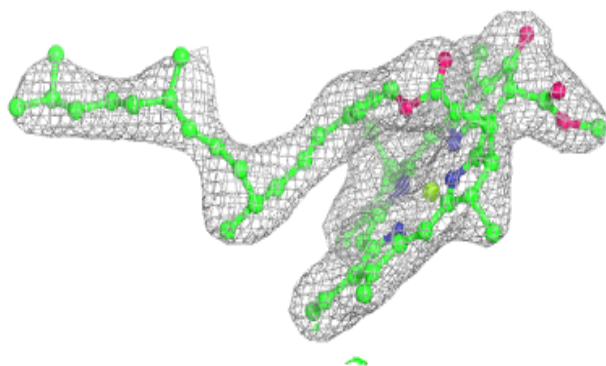
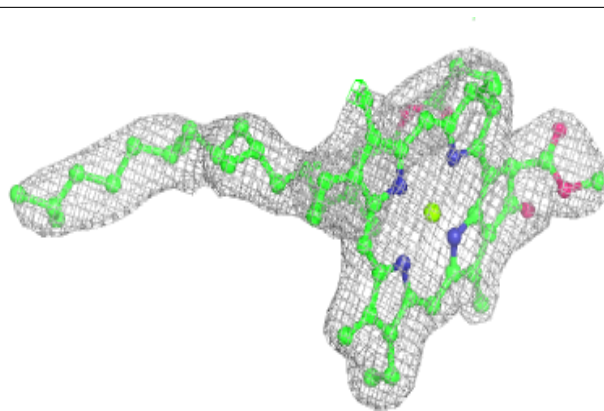
Electron density around CLA c 511:

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

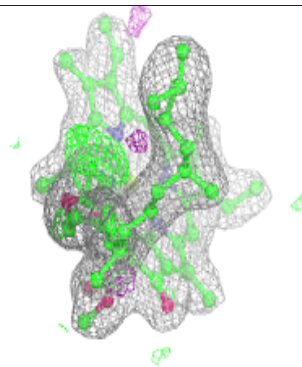
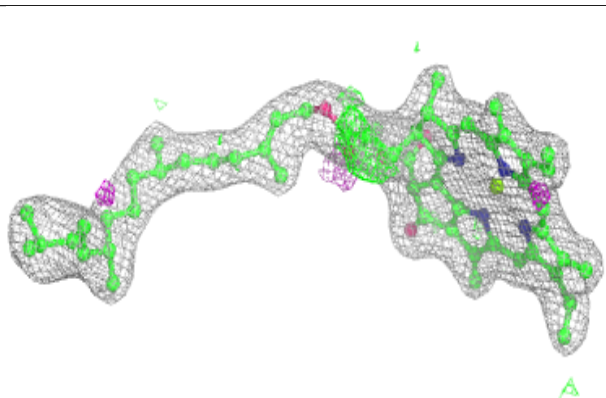
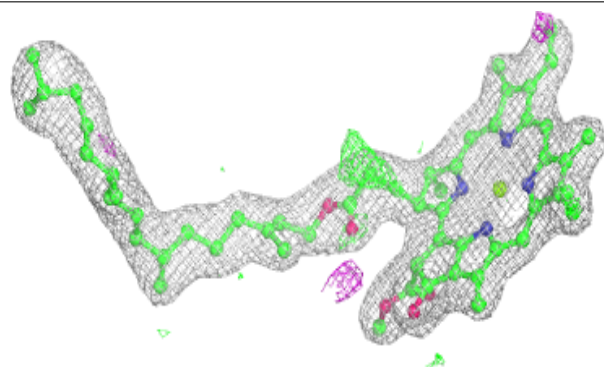


Electron density around CLA C 506:

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

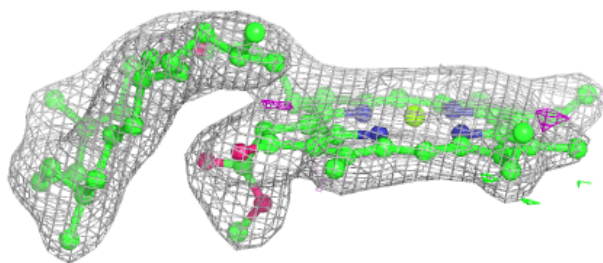
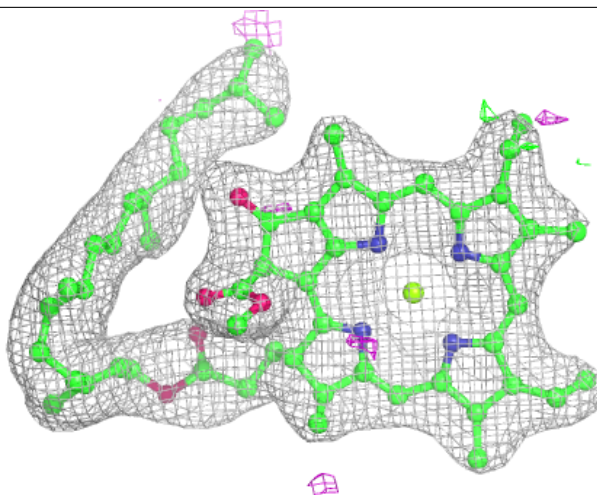
**Electron density around CLA A 405 (A):**

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



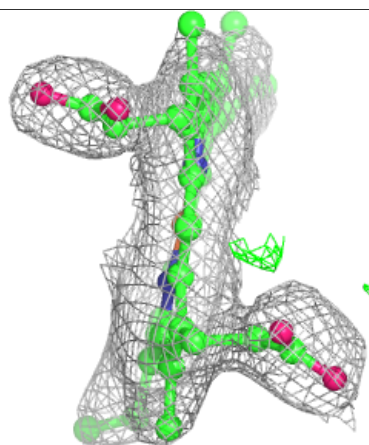
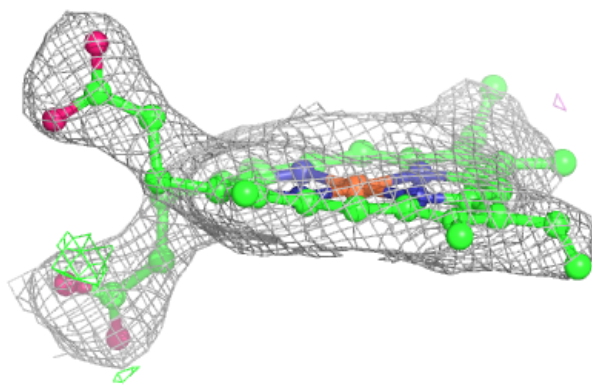
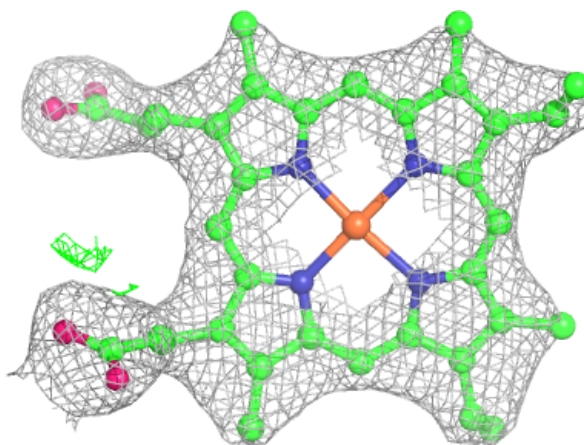
Electron density around CLA B 610:

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



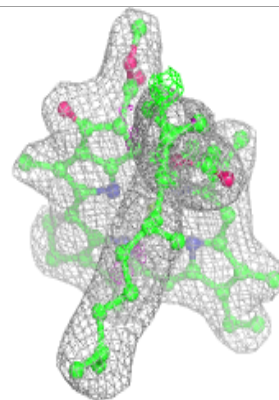
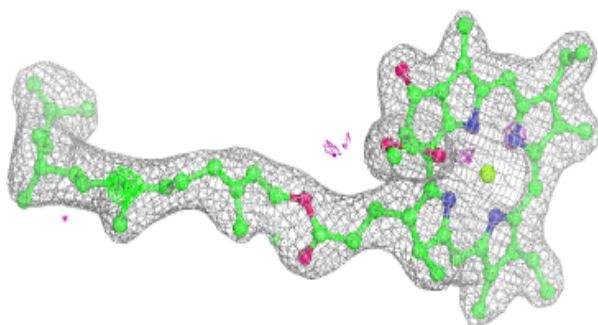
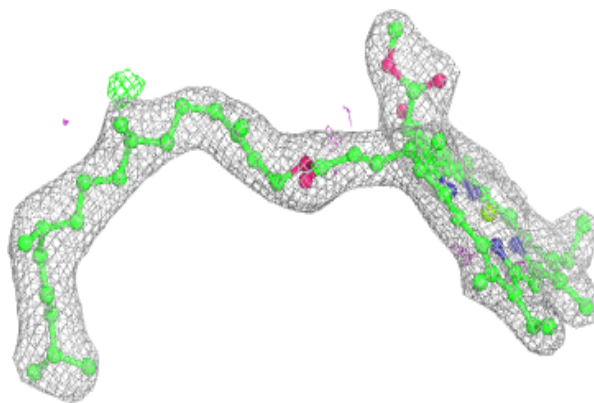
Electron density around HEM F 102:

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



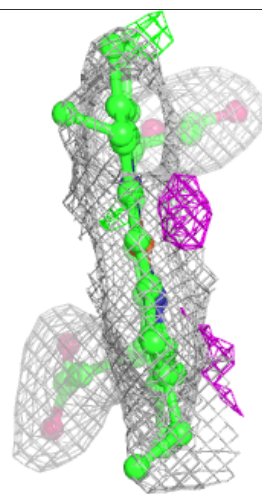
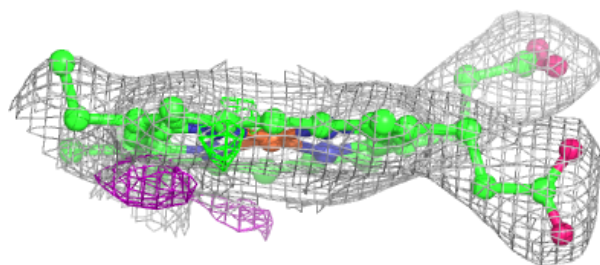
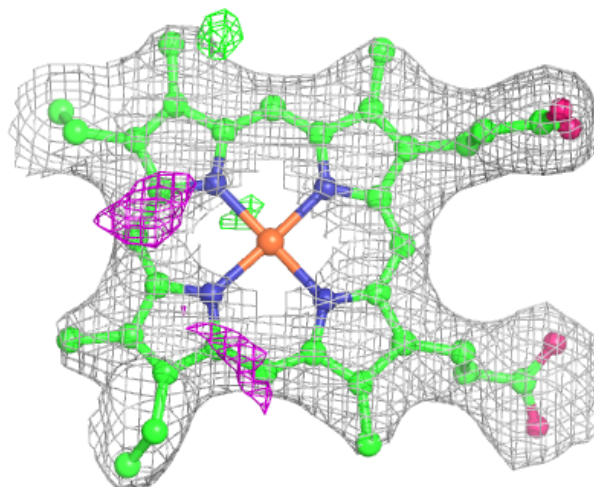
Electron density around CLA d 403 (A):

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



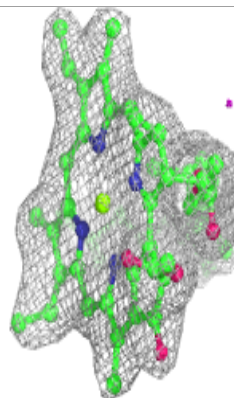
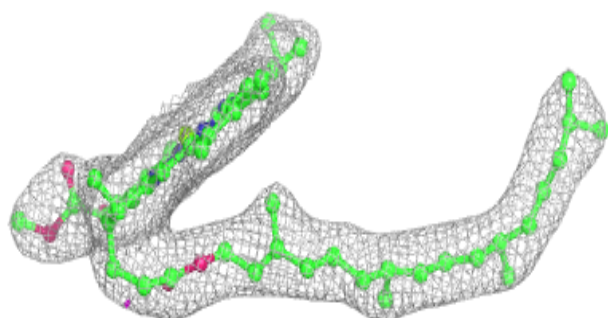
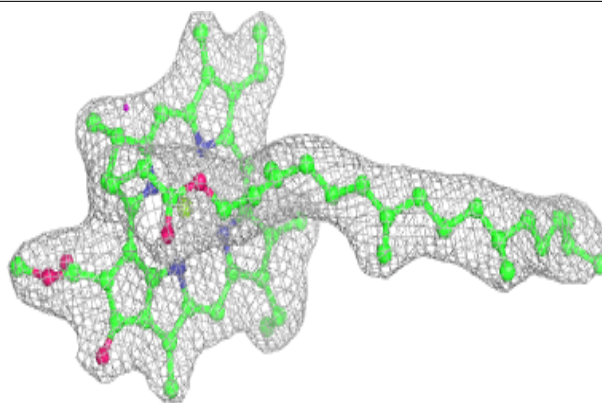
Electron density around HEC v 201:

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

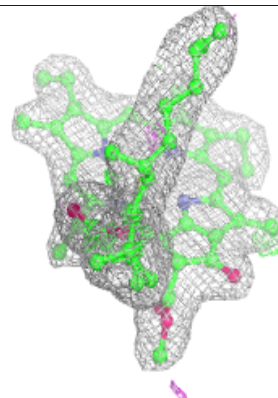
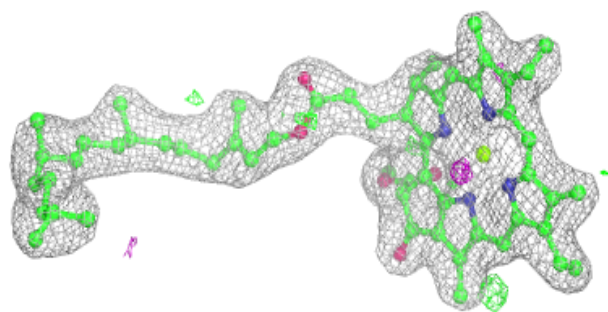
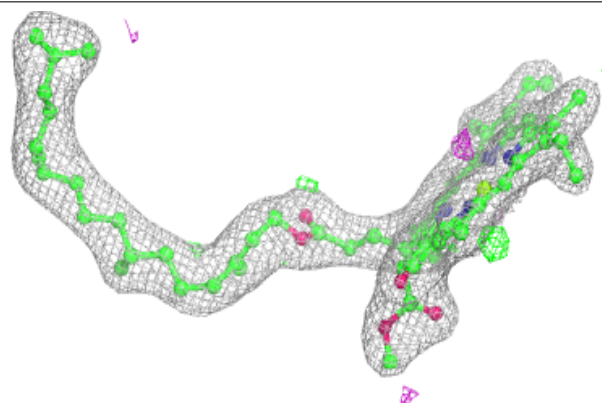


Electron density around CLA b 608:

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

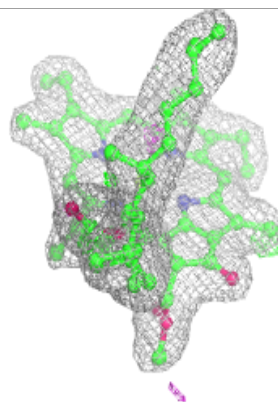
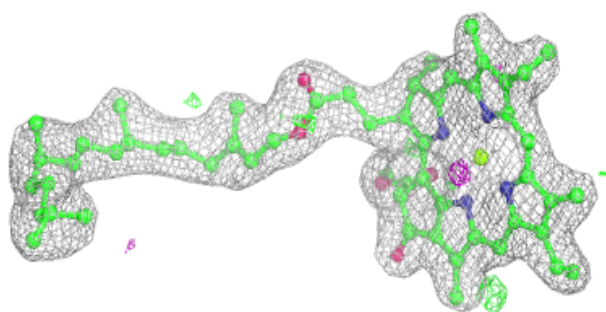
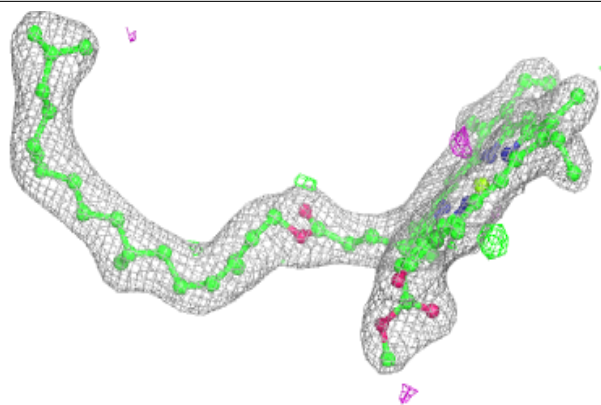
**Electron density around CLA D 402 (A):**

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

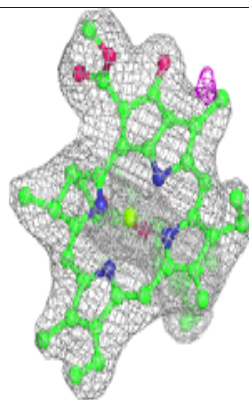
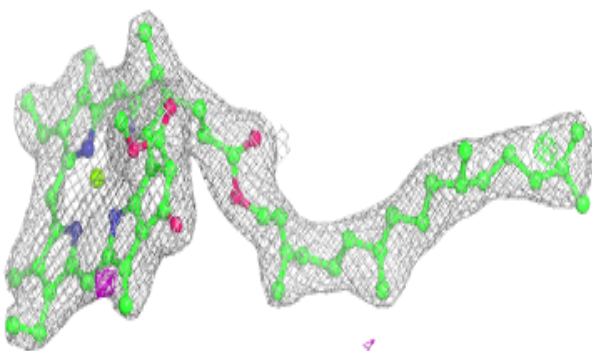
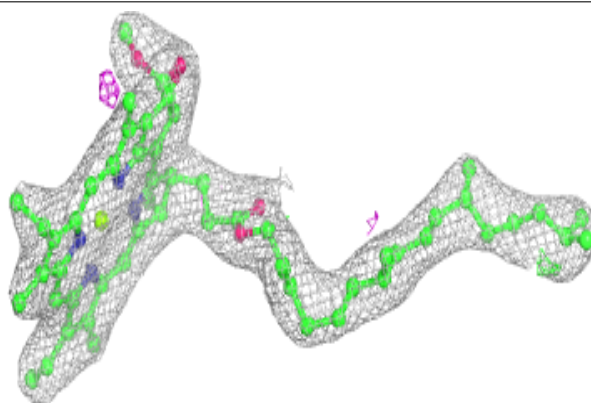


Electron density around CLA D 402 (B):

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

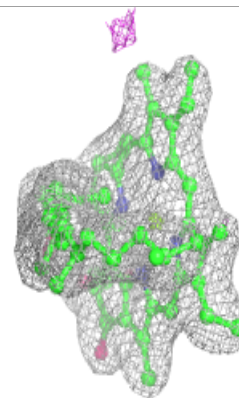
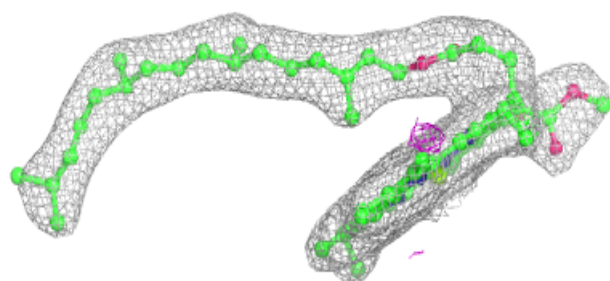
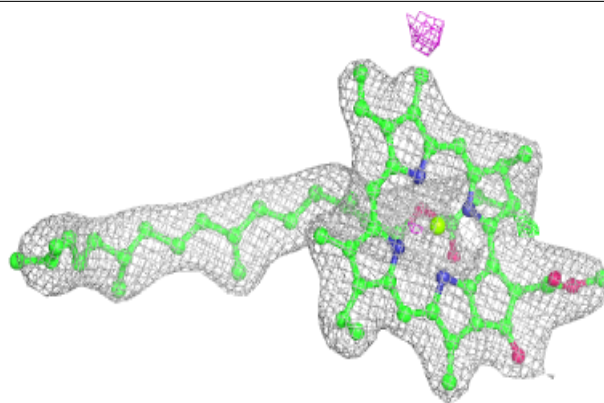
**Electron density around CLA C 503:**

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

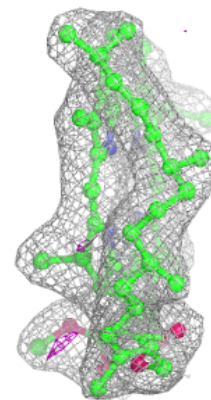
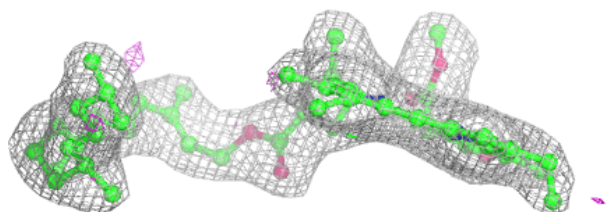
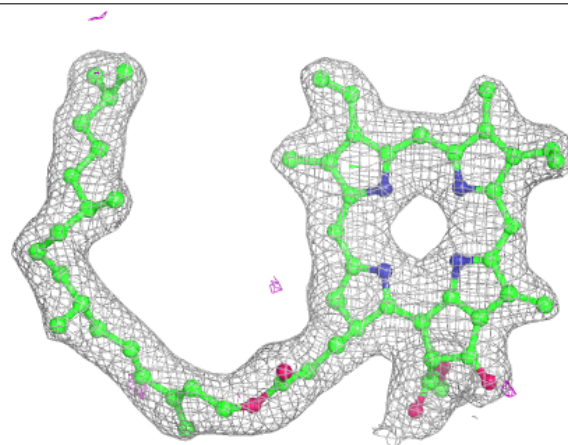


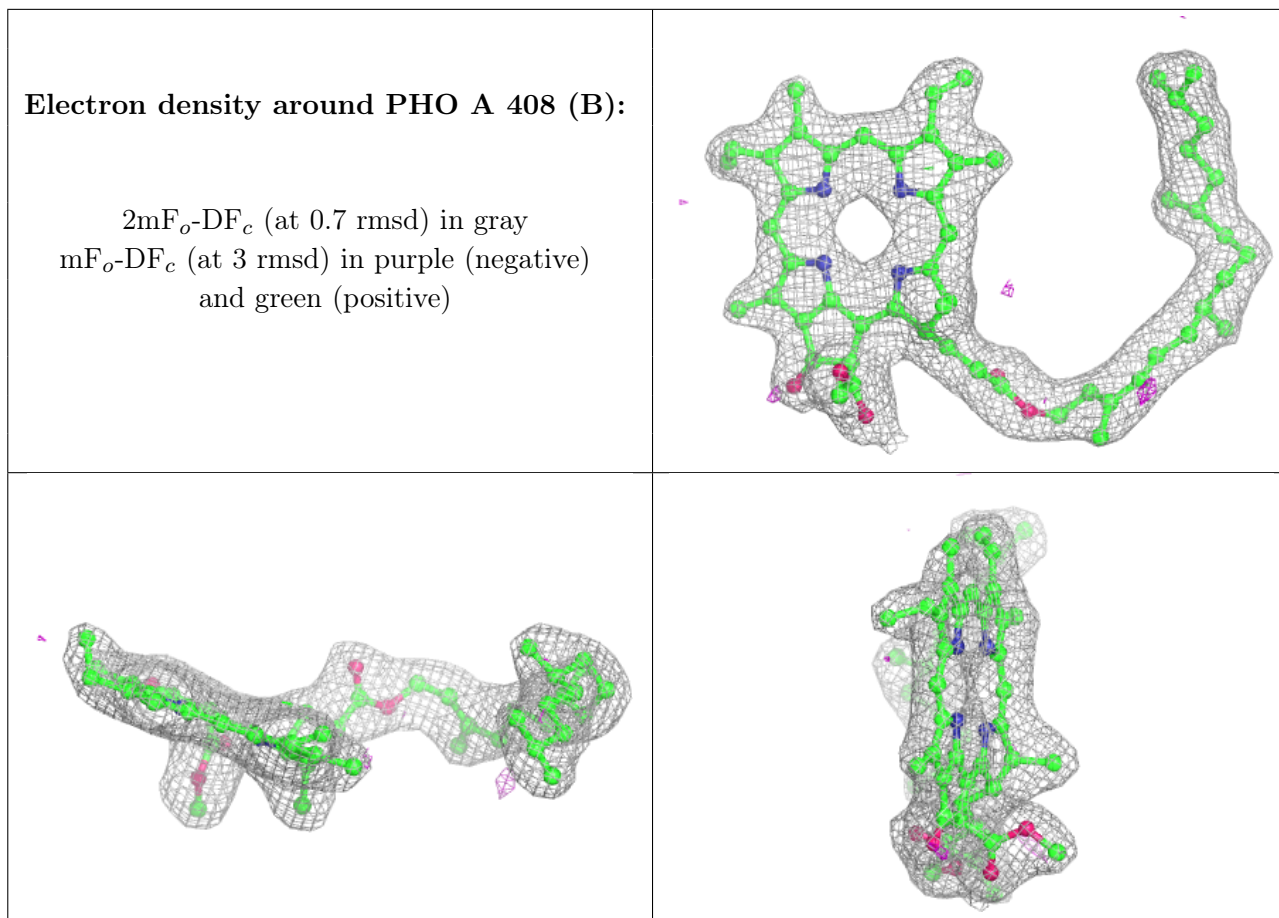
Electron density around CLA B 608:

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

**Electron density around PHO A 408 (A):**

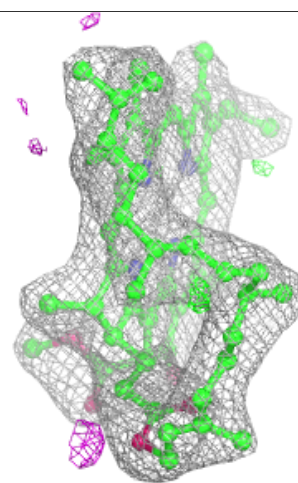
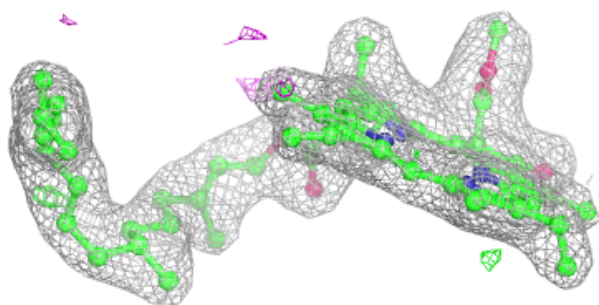
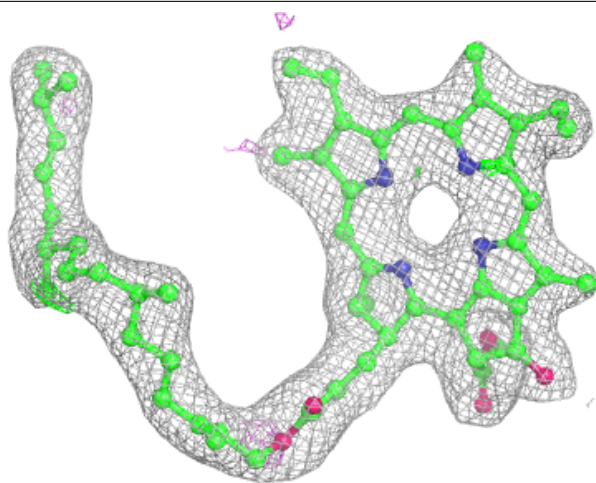
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





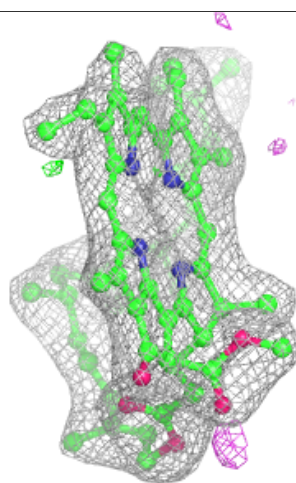
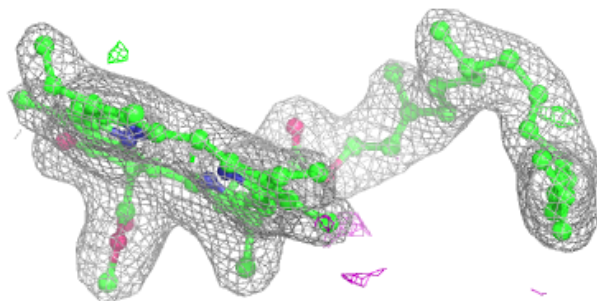
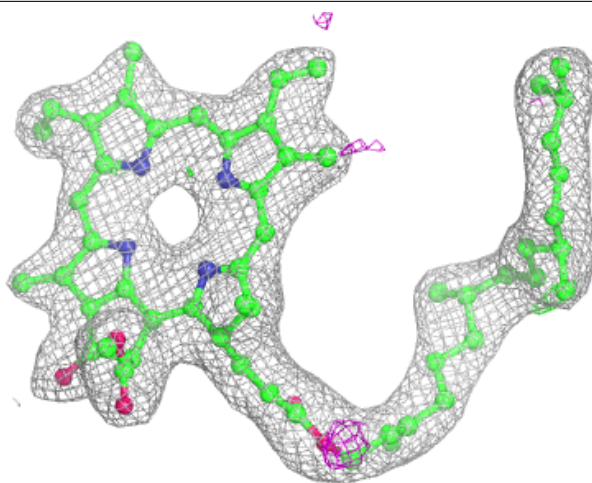
Electron density around PHO A 417 (A):

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



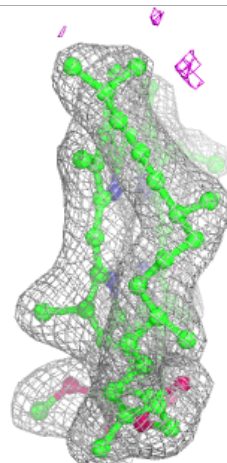
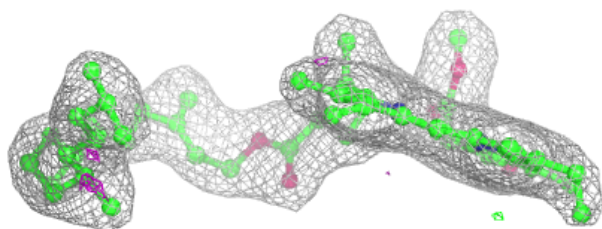
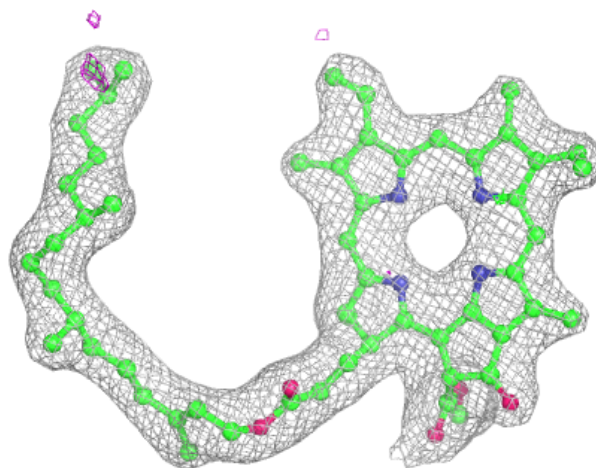
Electron density around PHO A 417 (B):

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



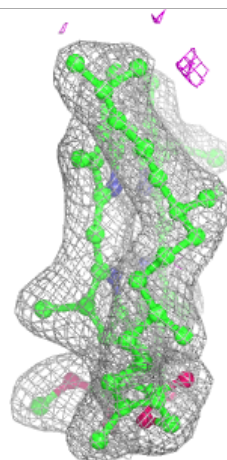
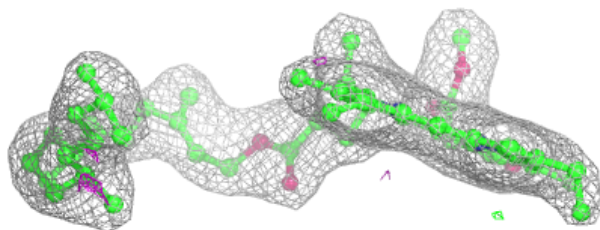
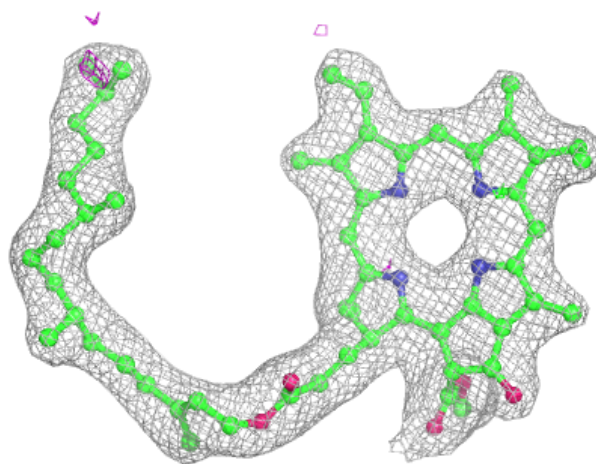
Electron density around PHO a 408 (A):

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



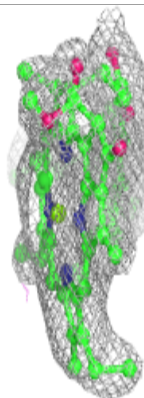
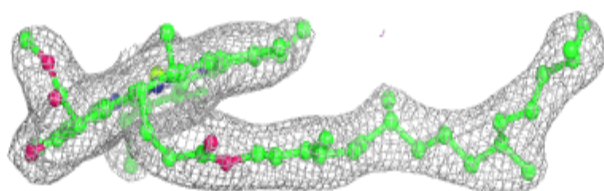
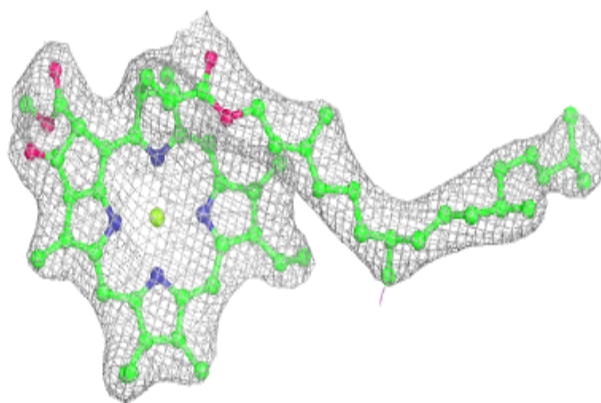
Electron density around PHO a 408 (B):

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

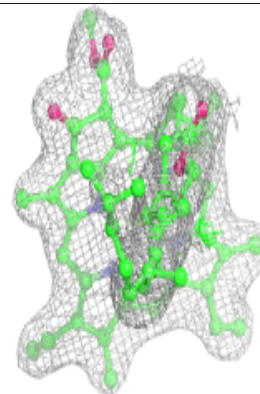
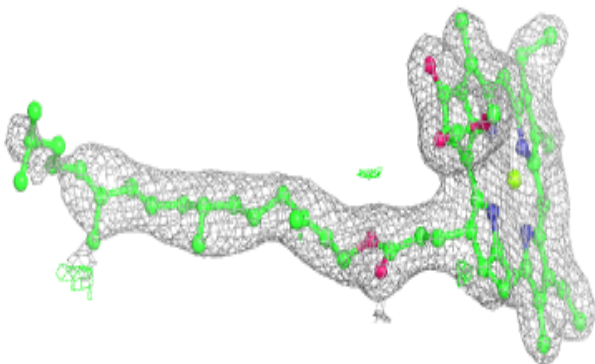
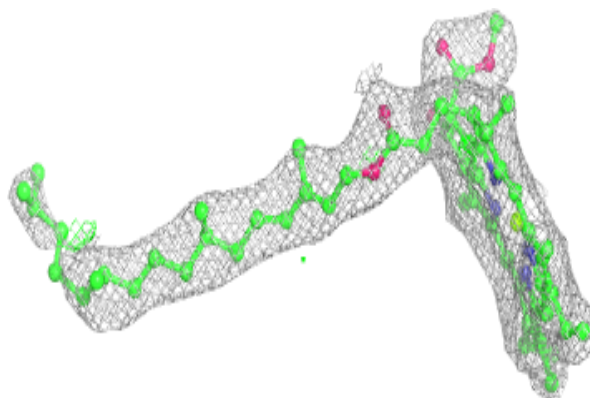


Electron density around CLA b 603:

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

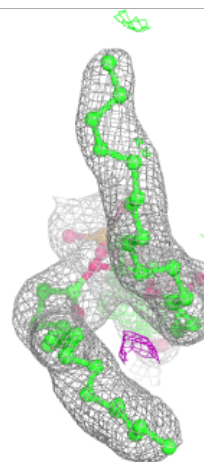
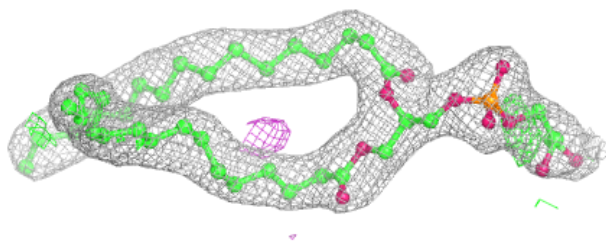
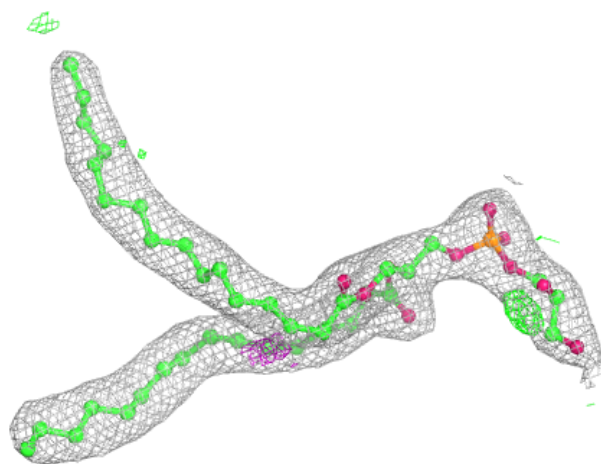
**Electron density around CLA B 604:**

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



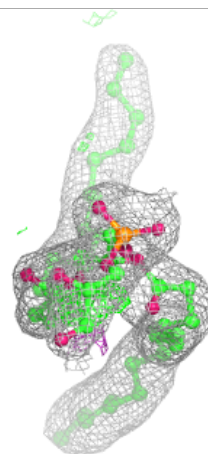
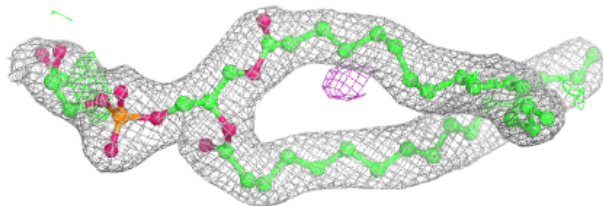
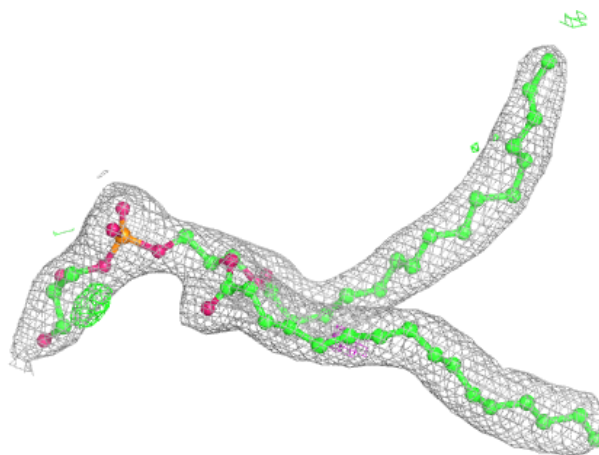
Electron density around LHG D 406 (A):

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



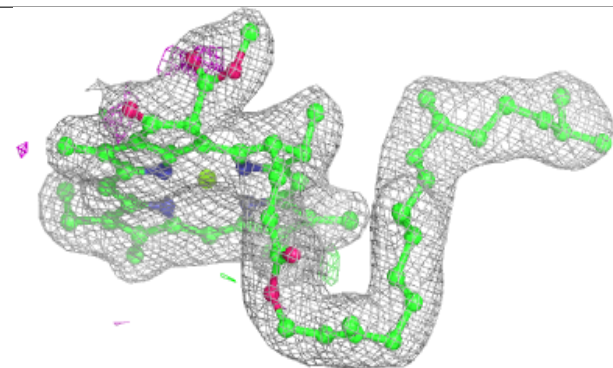
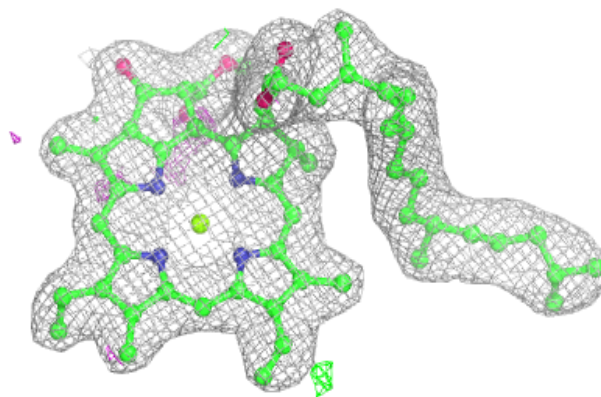
Electron density around LHG D 406 (B):

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

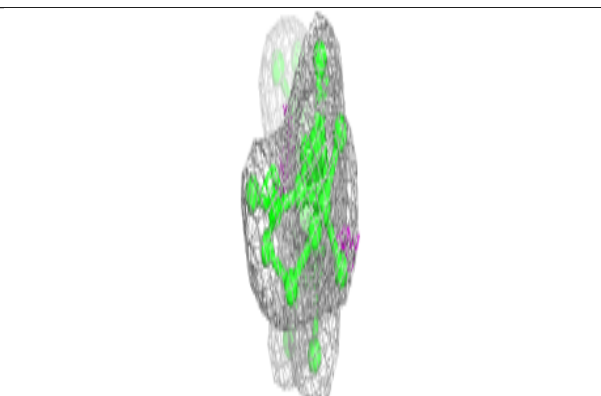
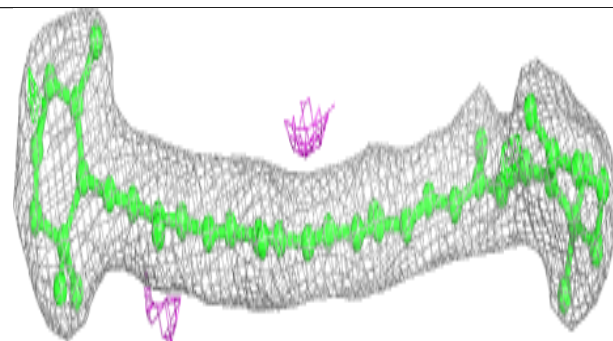
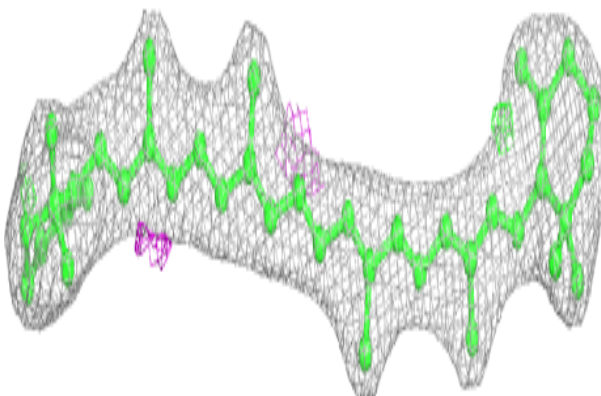


Electron density around CLA A 406 (A):

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

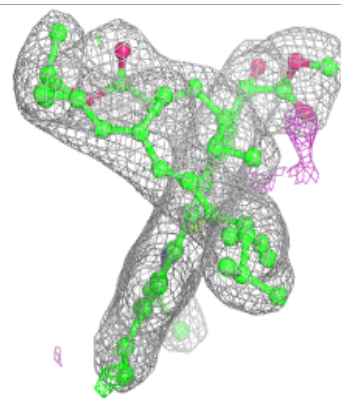
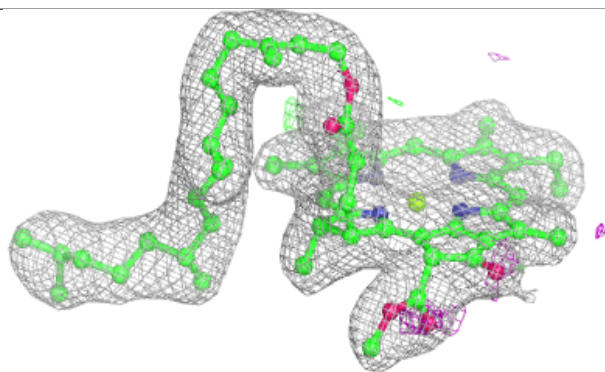
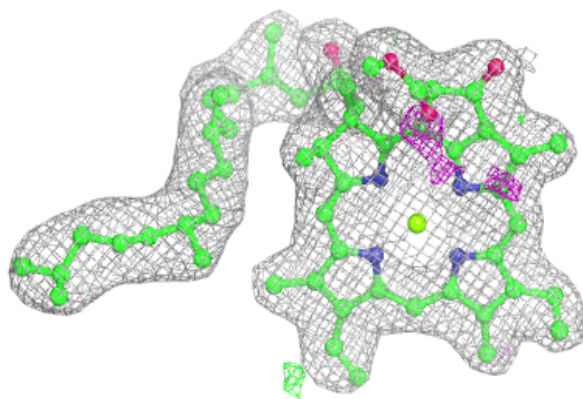
**Electron density around BCR B 617:**

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



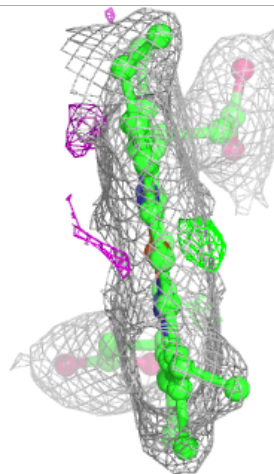
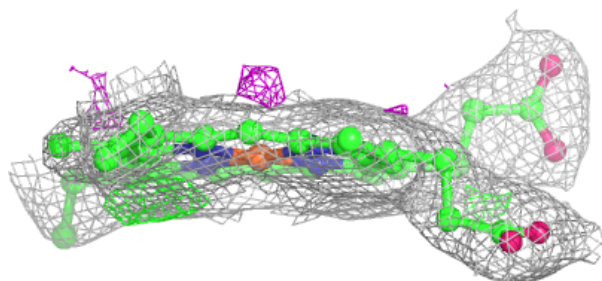
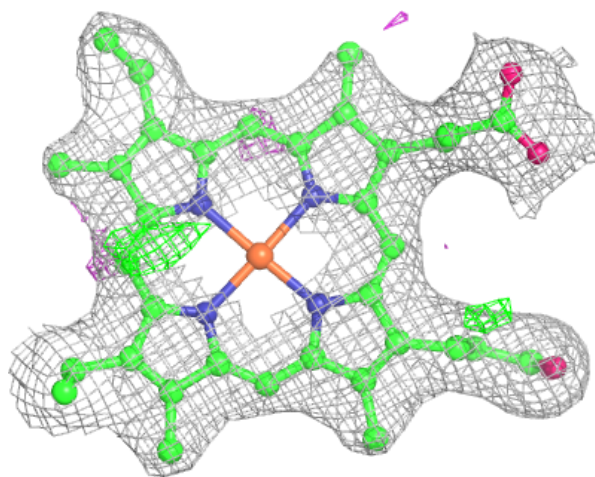
Electron density around CLA A 406 (B):

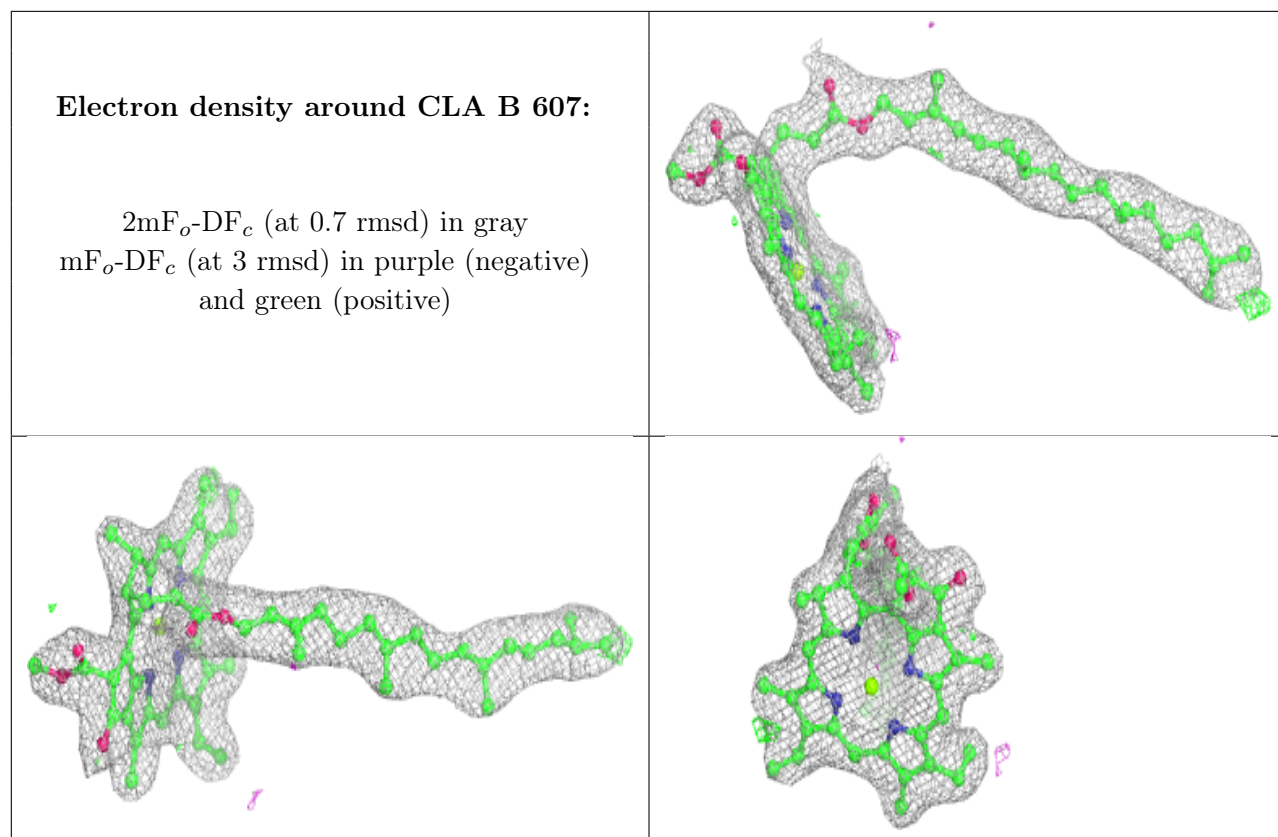
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC V 201:

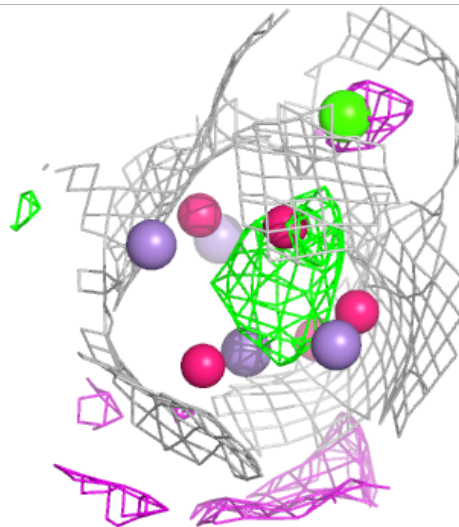
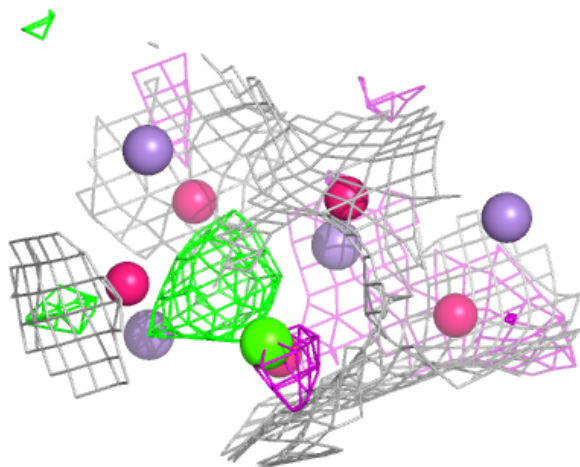
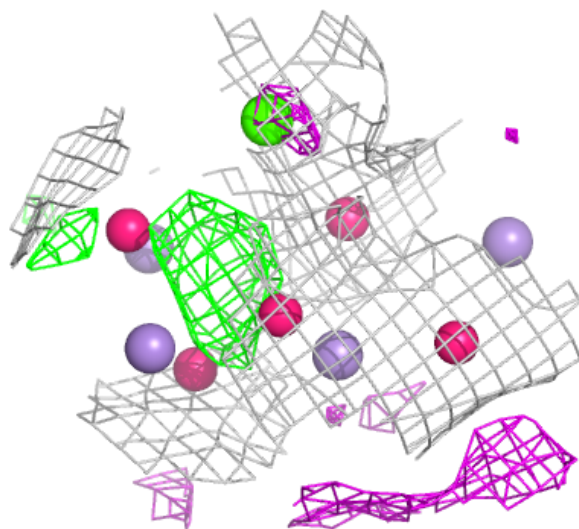
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





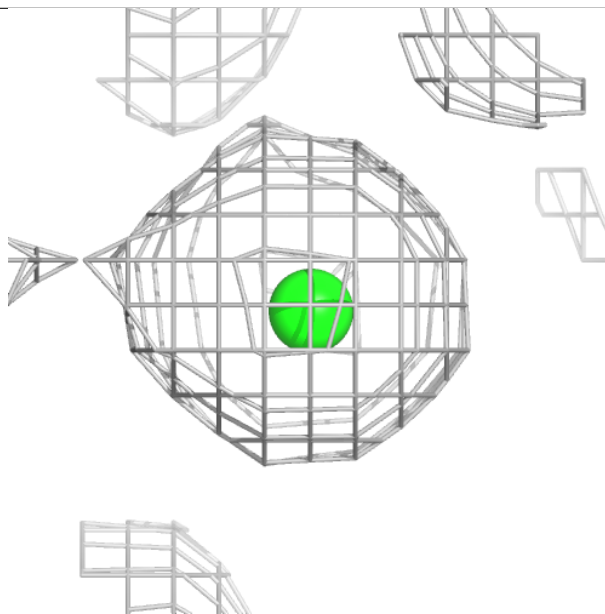
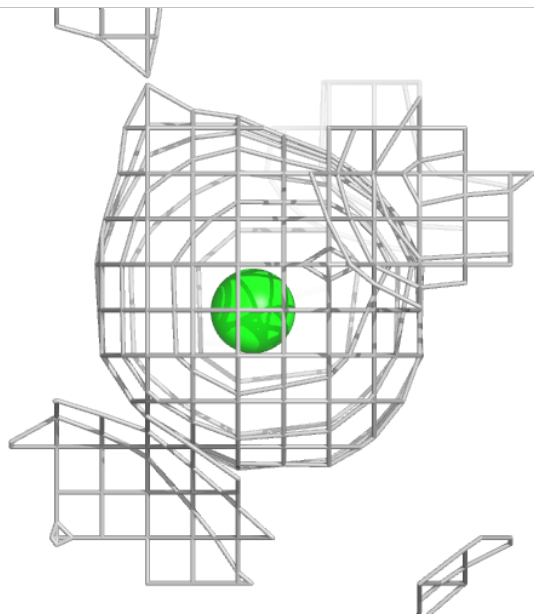
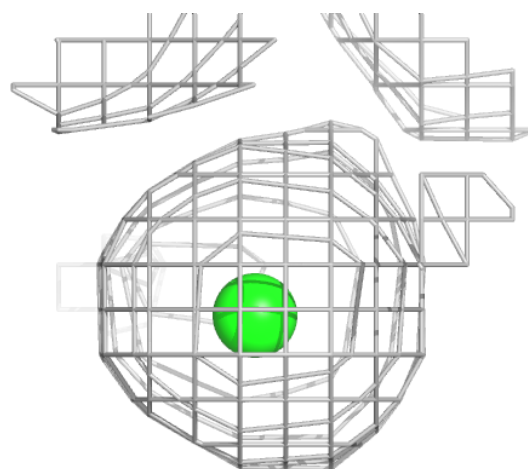
Electron density around OEX A 414 (A):

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



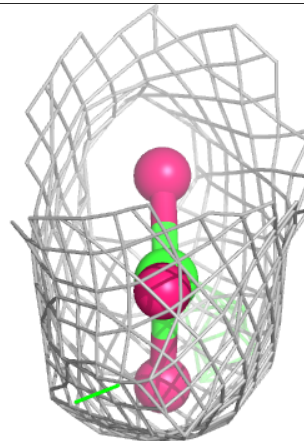
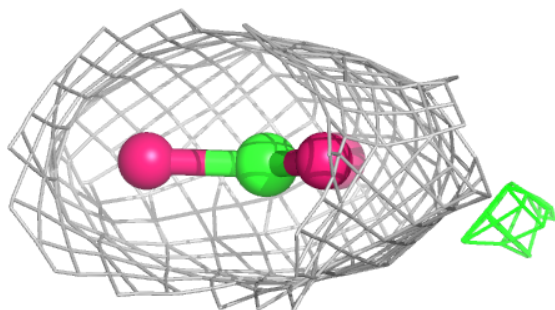
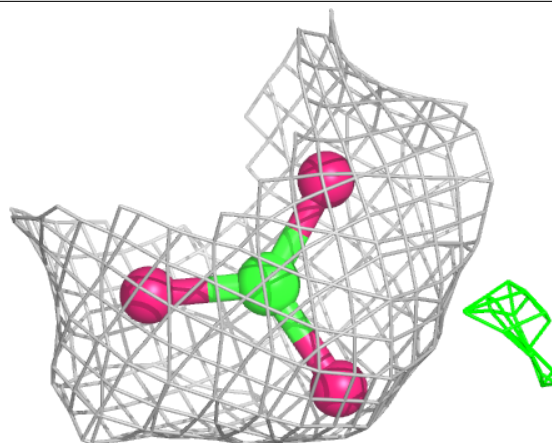
Electron density around CL a 403 (B):

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



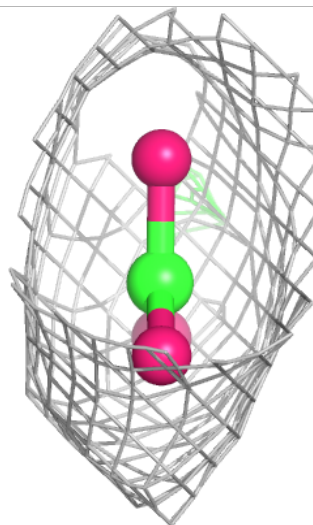
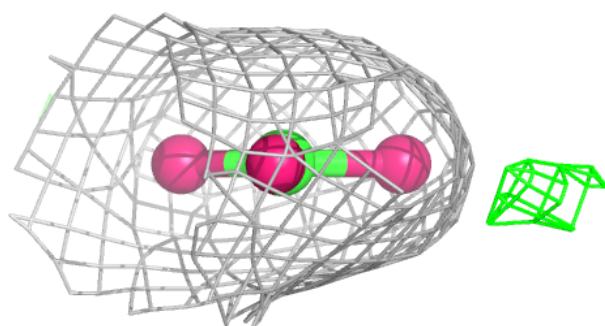
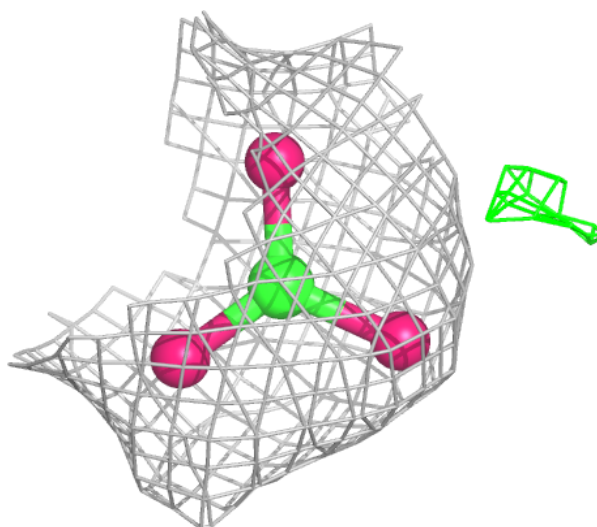
Electron density around BCT D 401 (A):

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



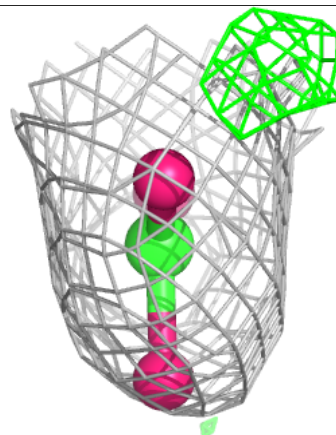
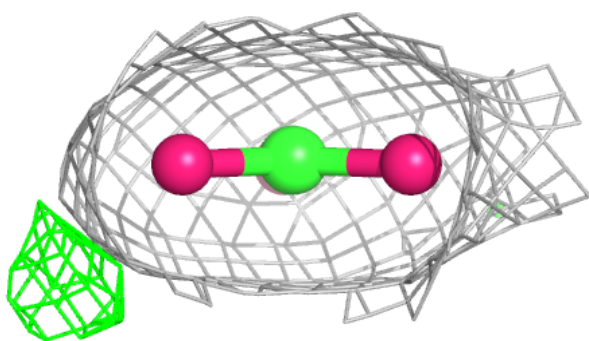
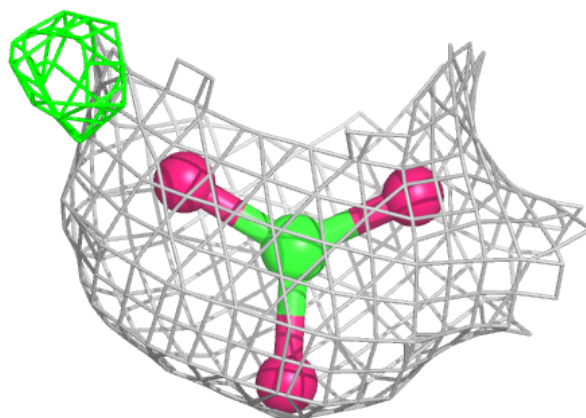
Electron density around BCT D 401 (B):

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



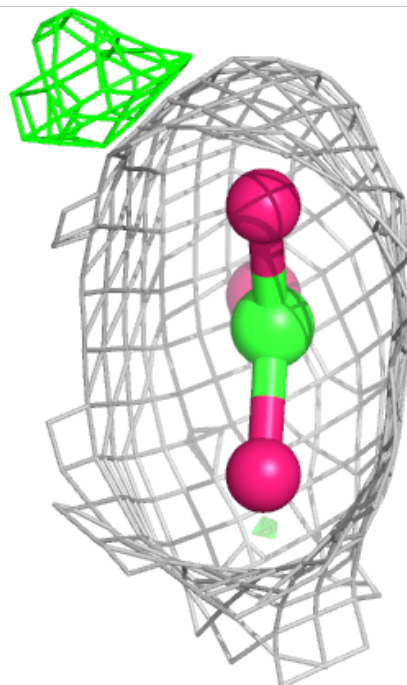
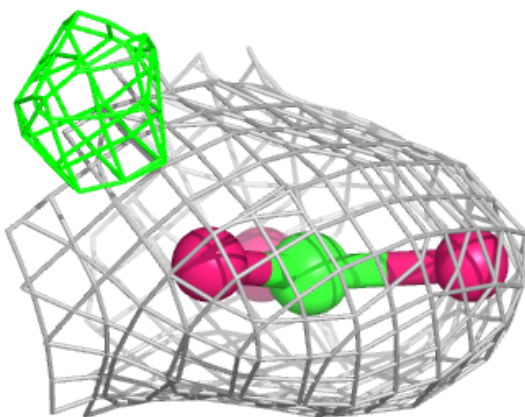
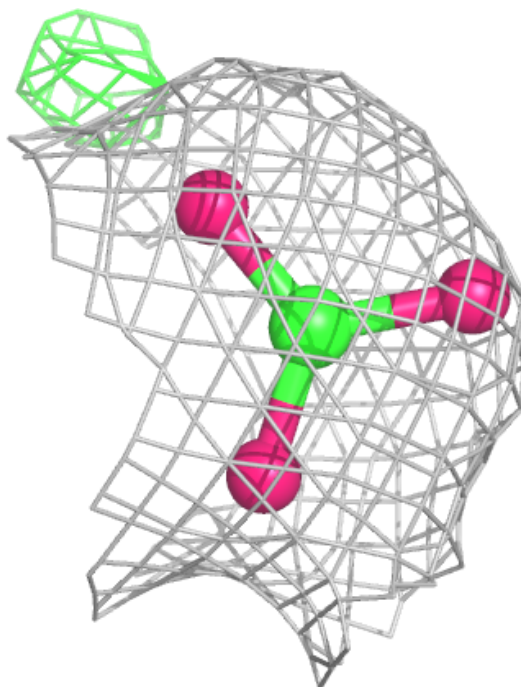
Electron density around BCT d 401 (A):

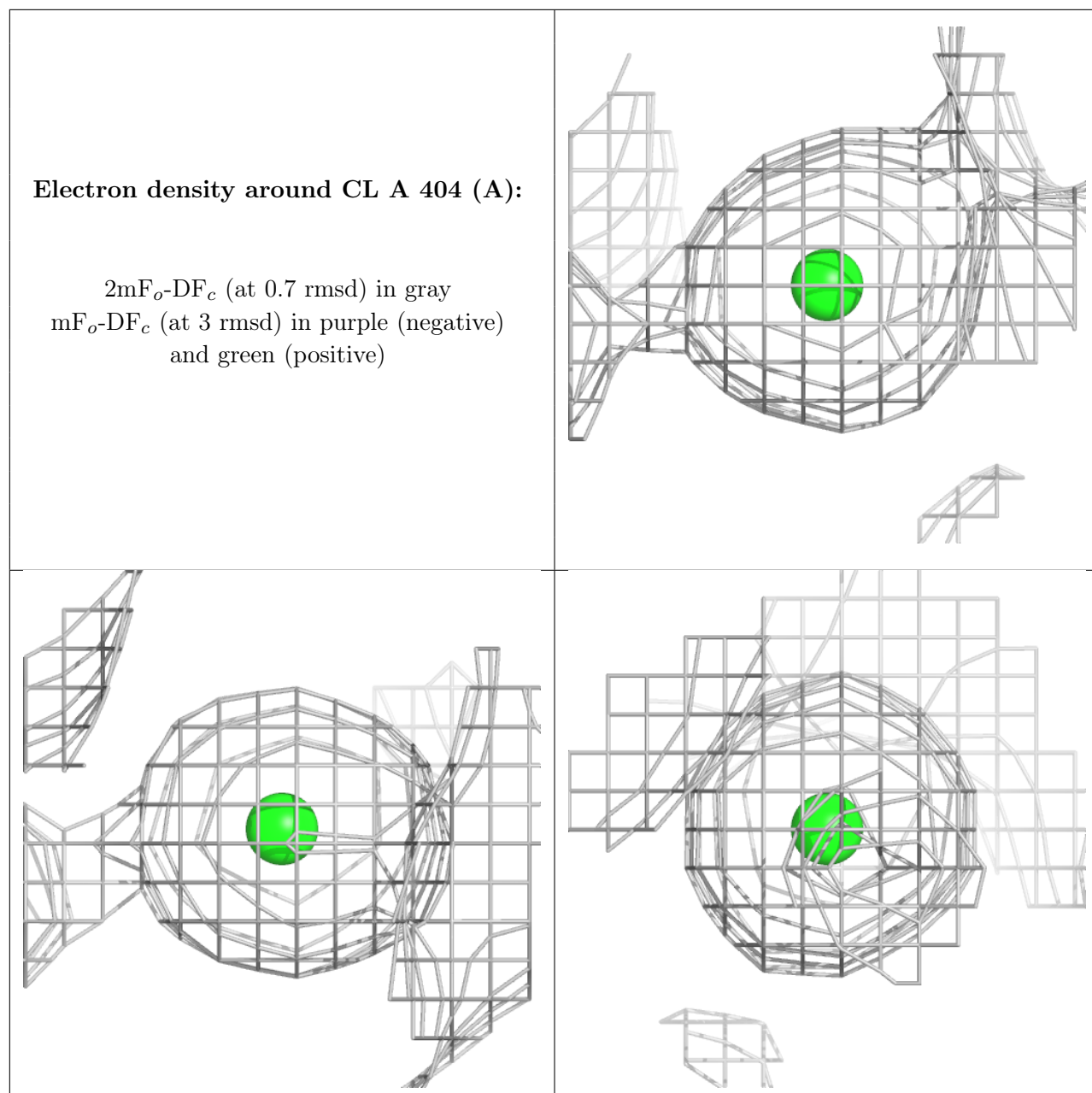
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

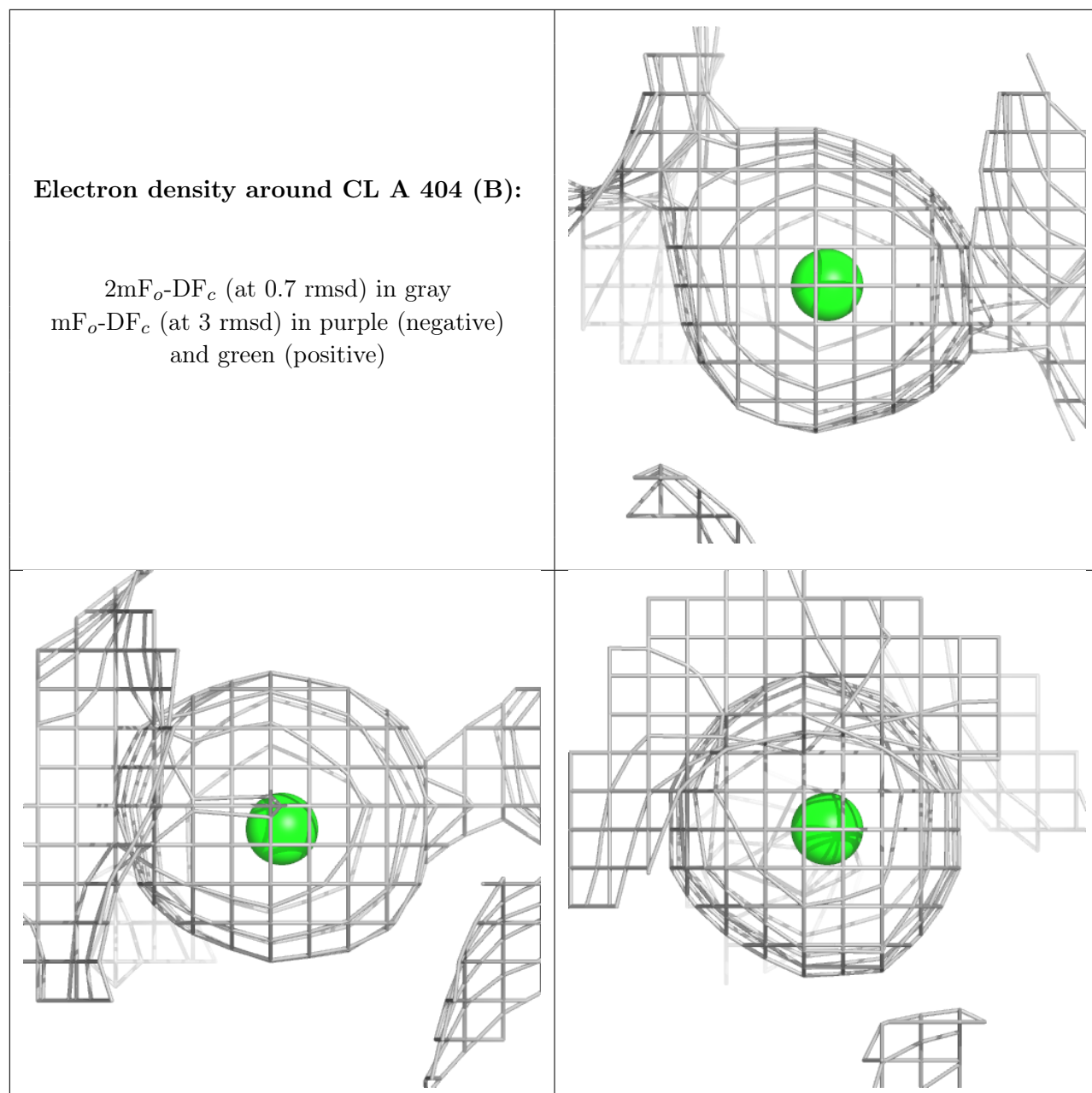


Electron density around BCT d 401 (B):

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

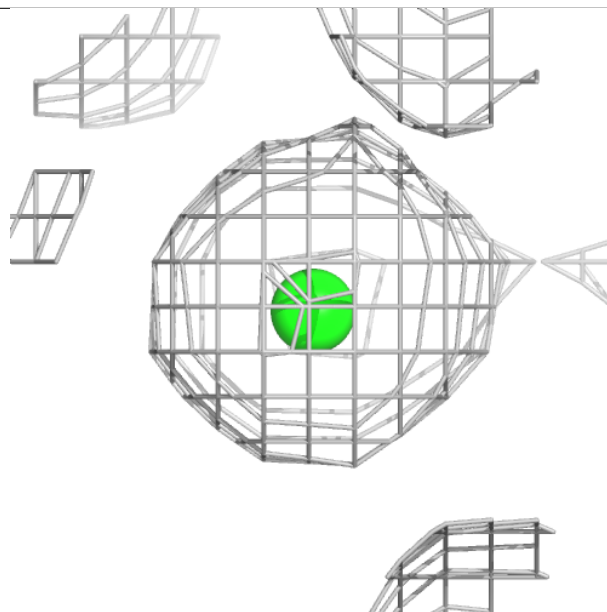
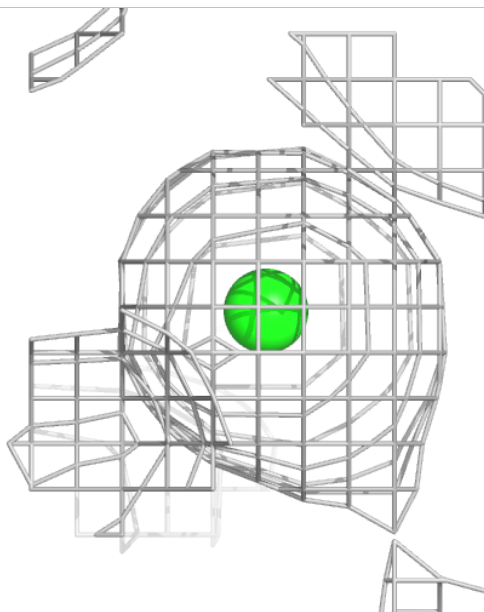
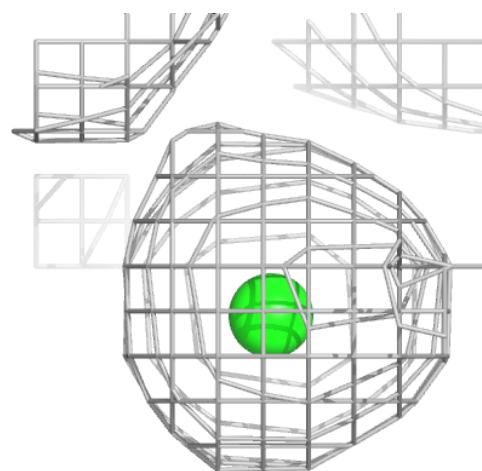






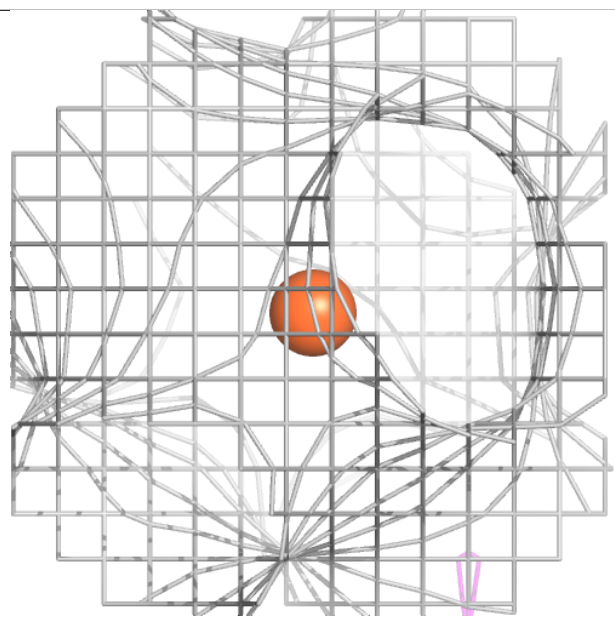
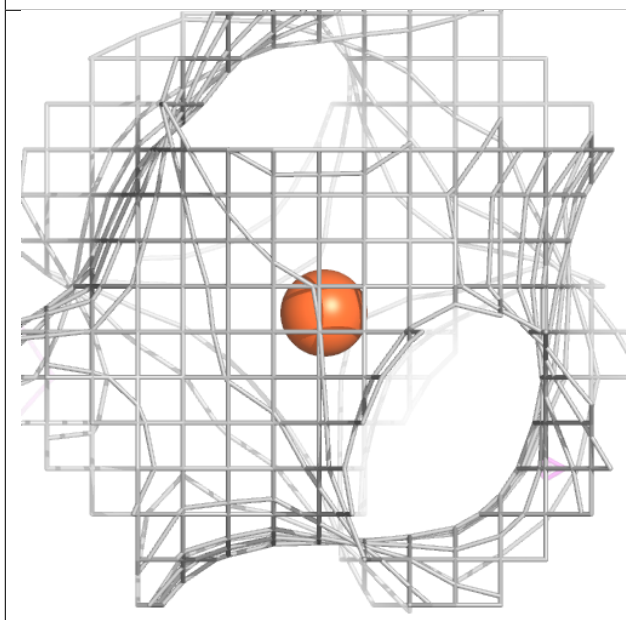
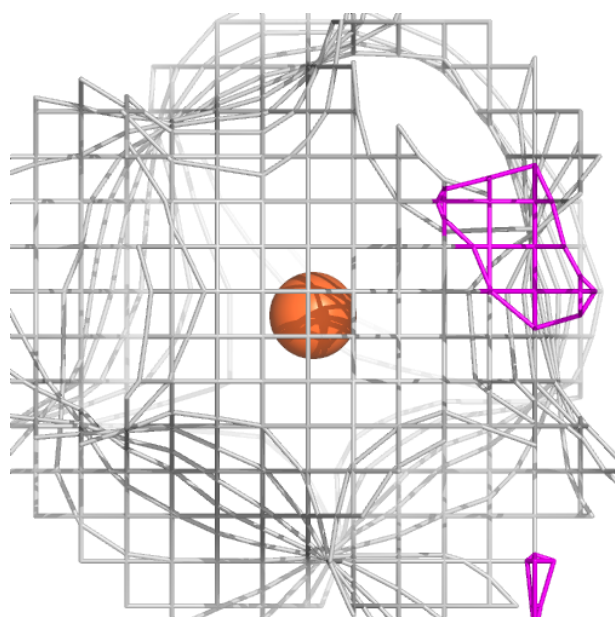
Electron density around CL a 403 (A):

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



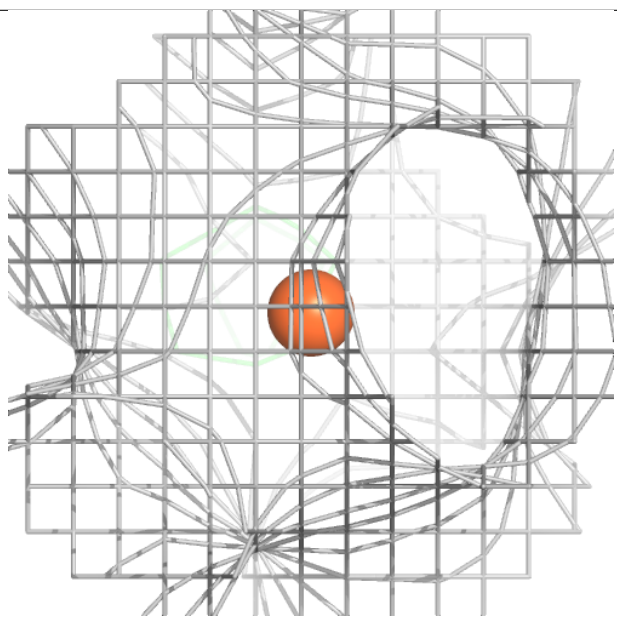
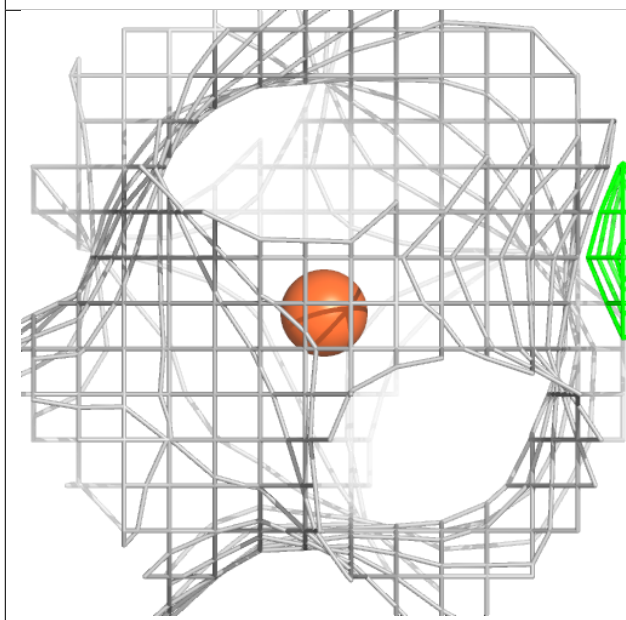
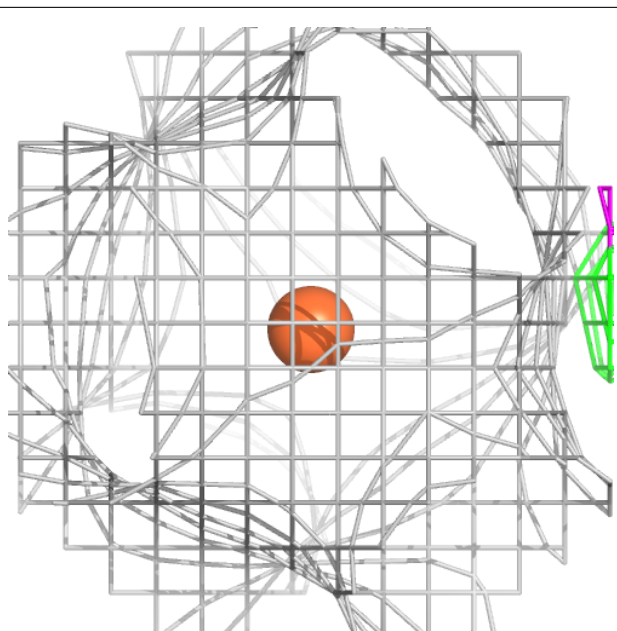
Electron density around FE2 A 402 (B):

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



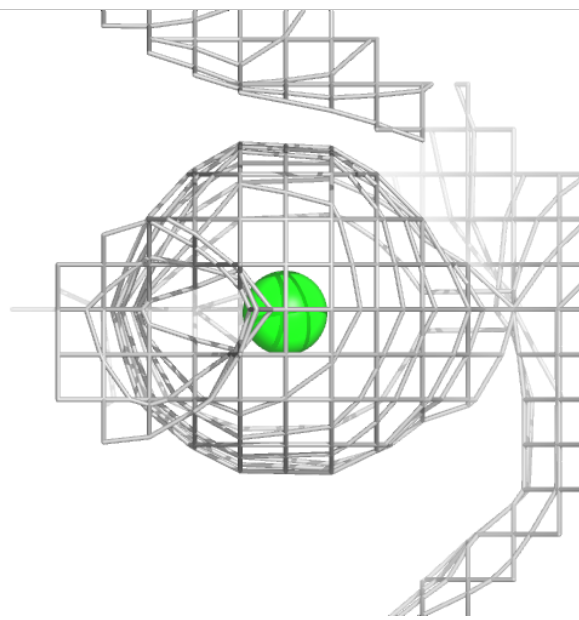
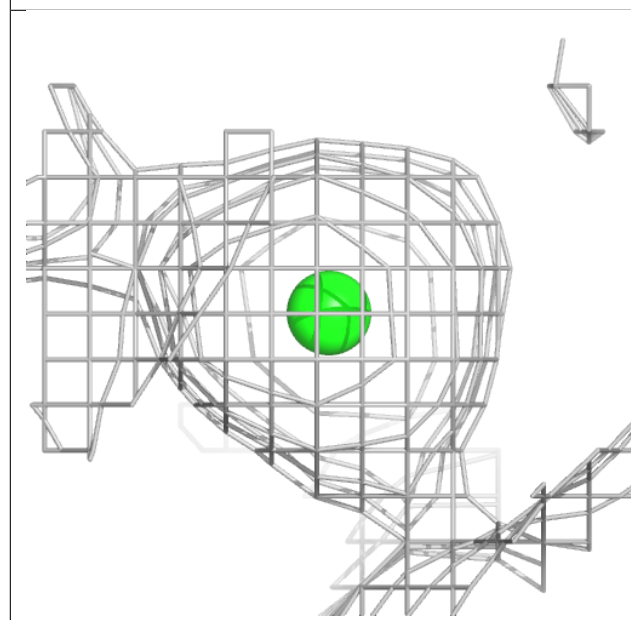
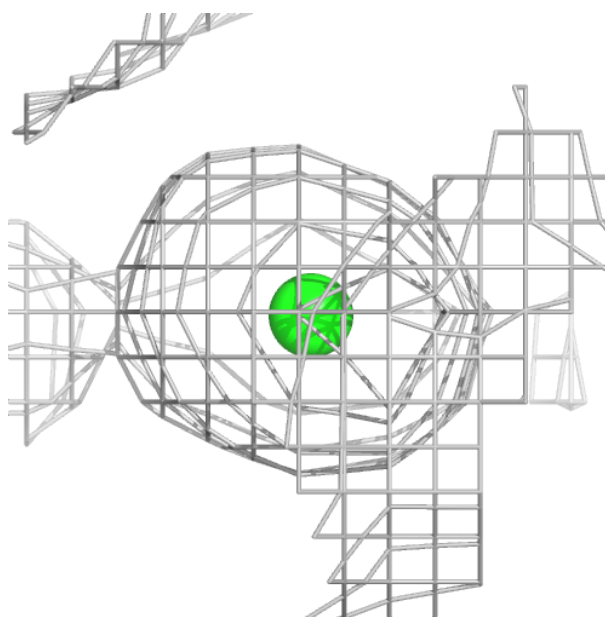
Electron density around FE2 a 402 (A):

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



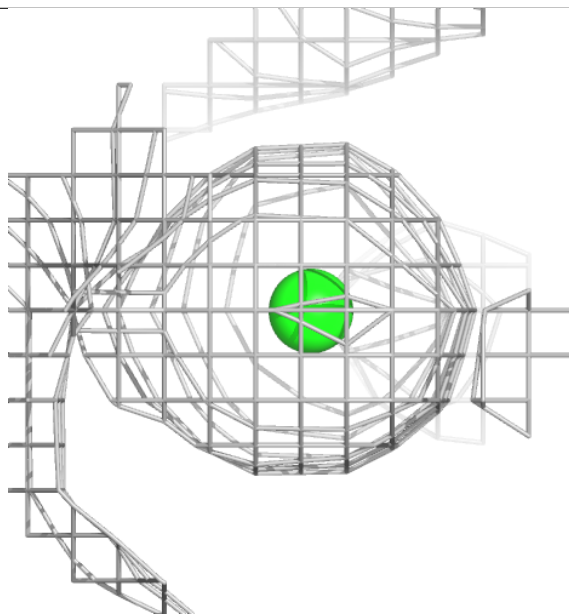
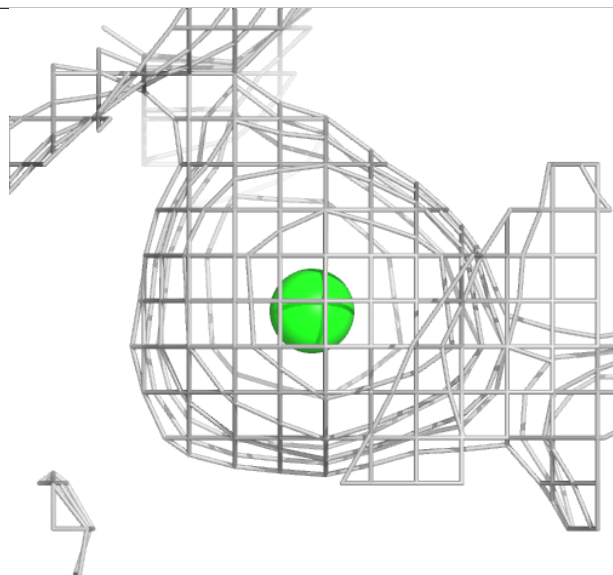
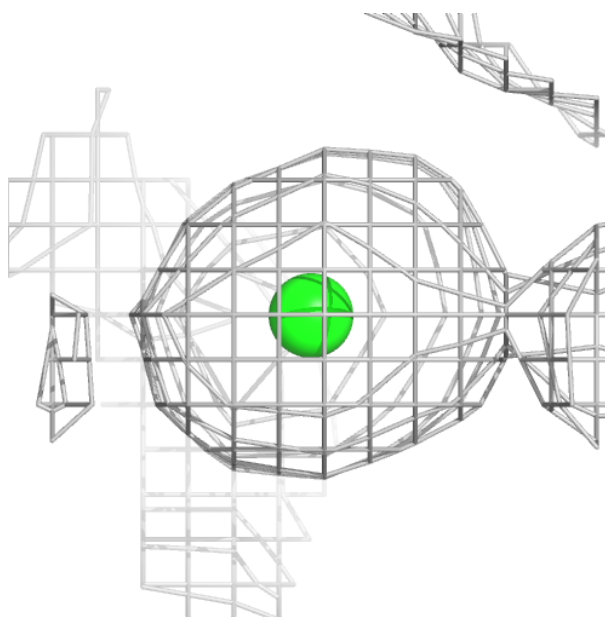
Electron density around CL a 404 (A):

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



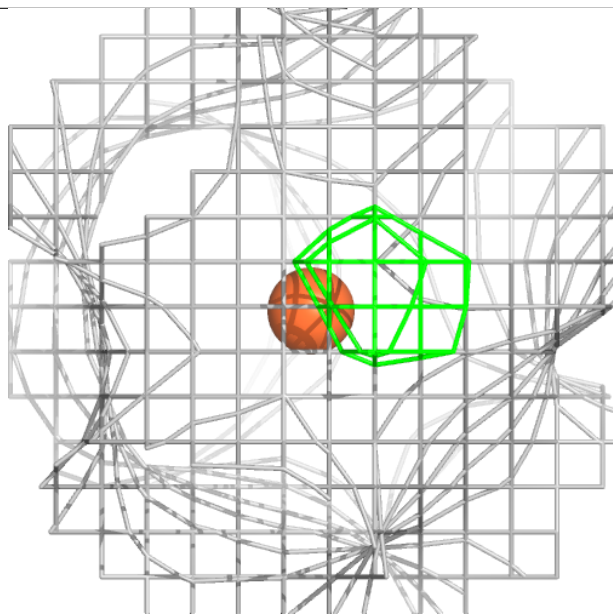
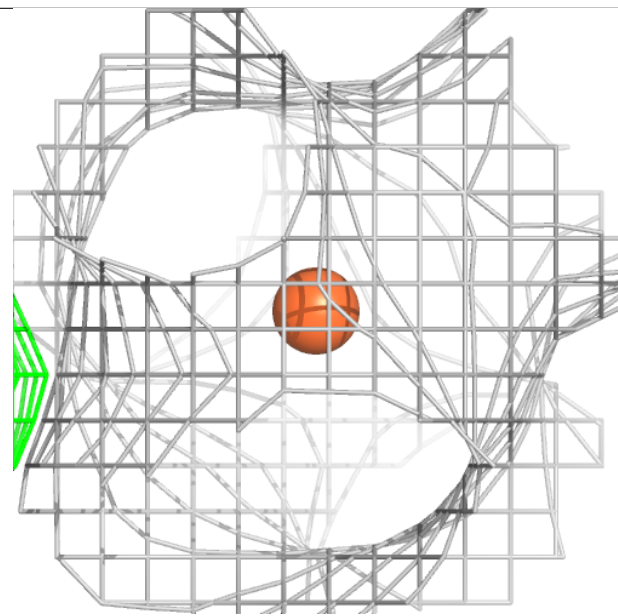
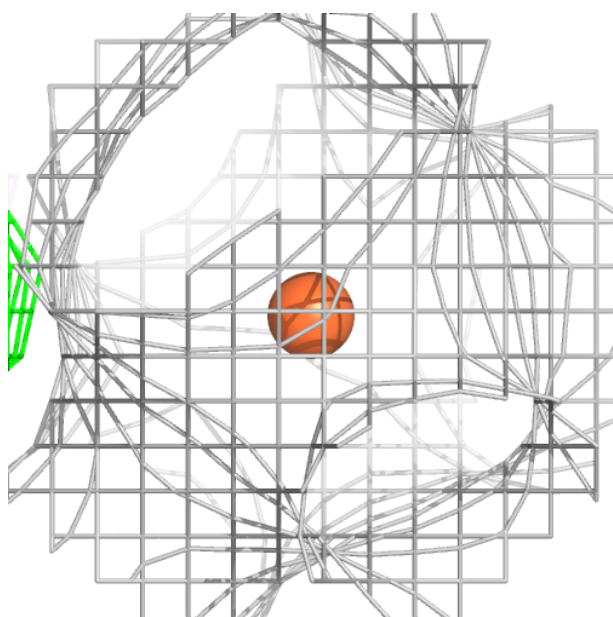
Electron density around CL a 404 (B):

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



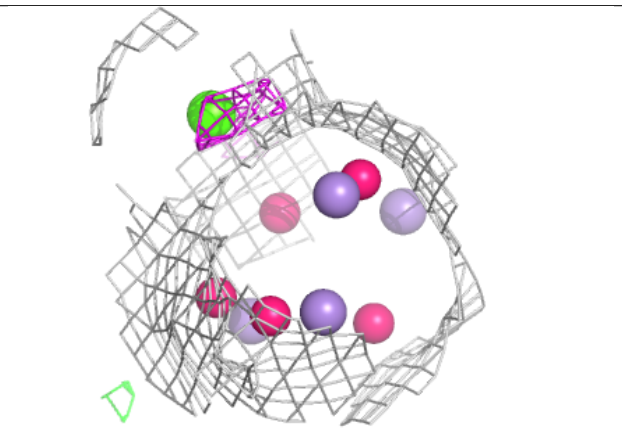
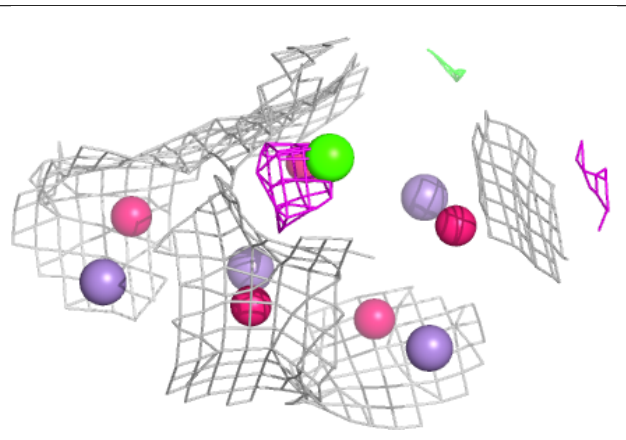
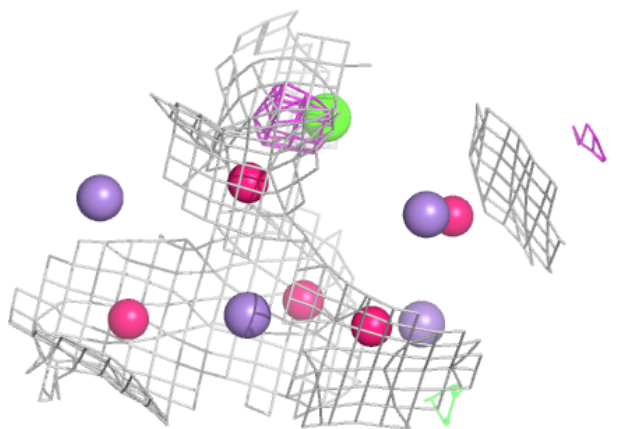
Electron density around FE2 a 402 (B):

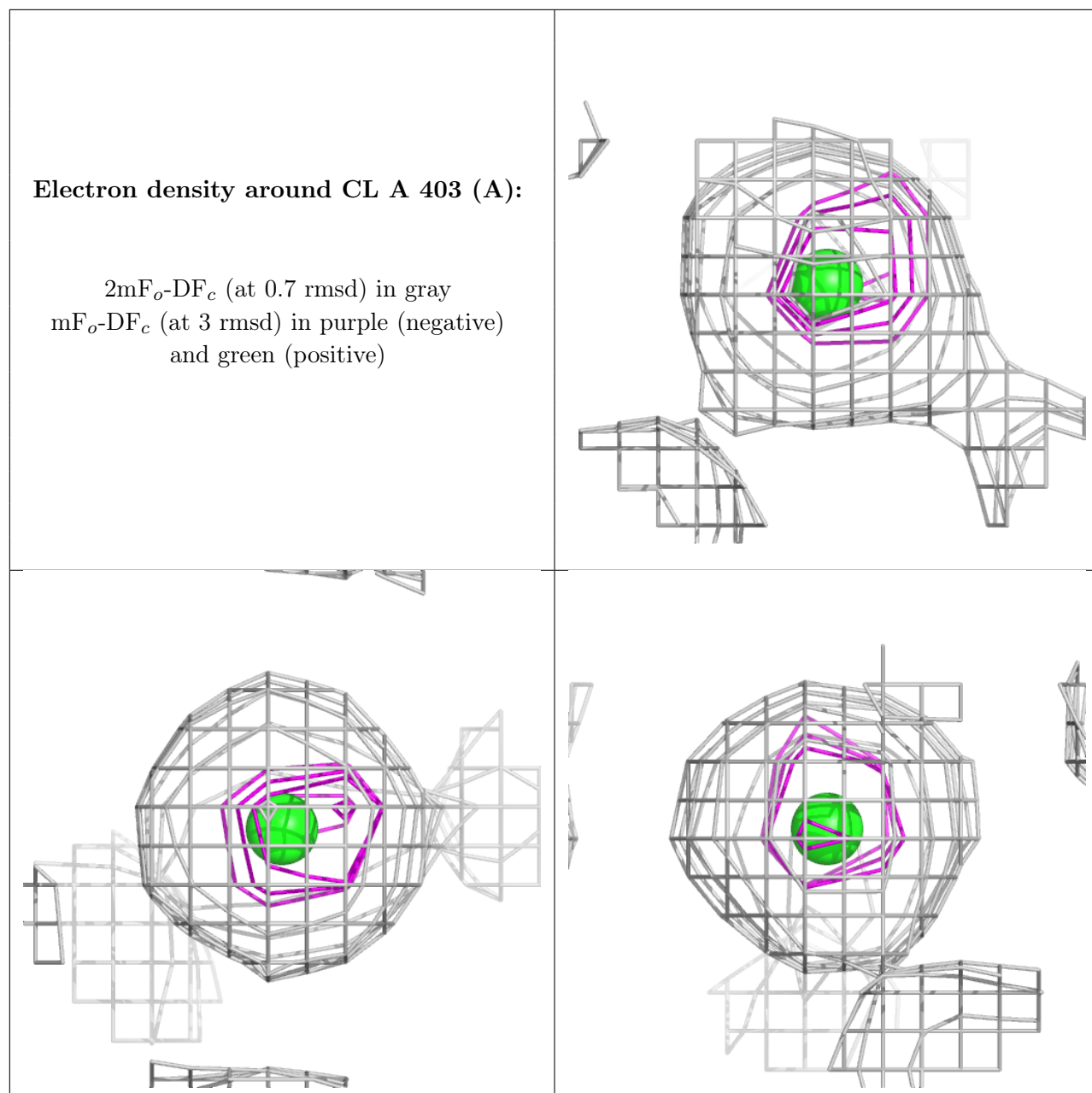
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

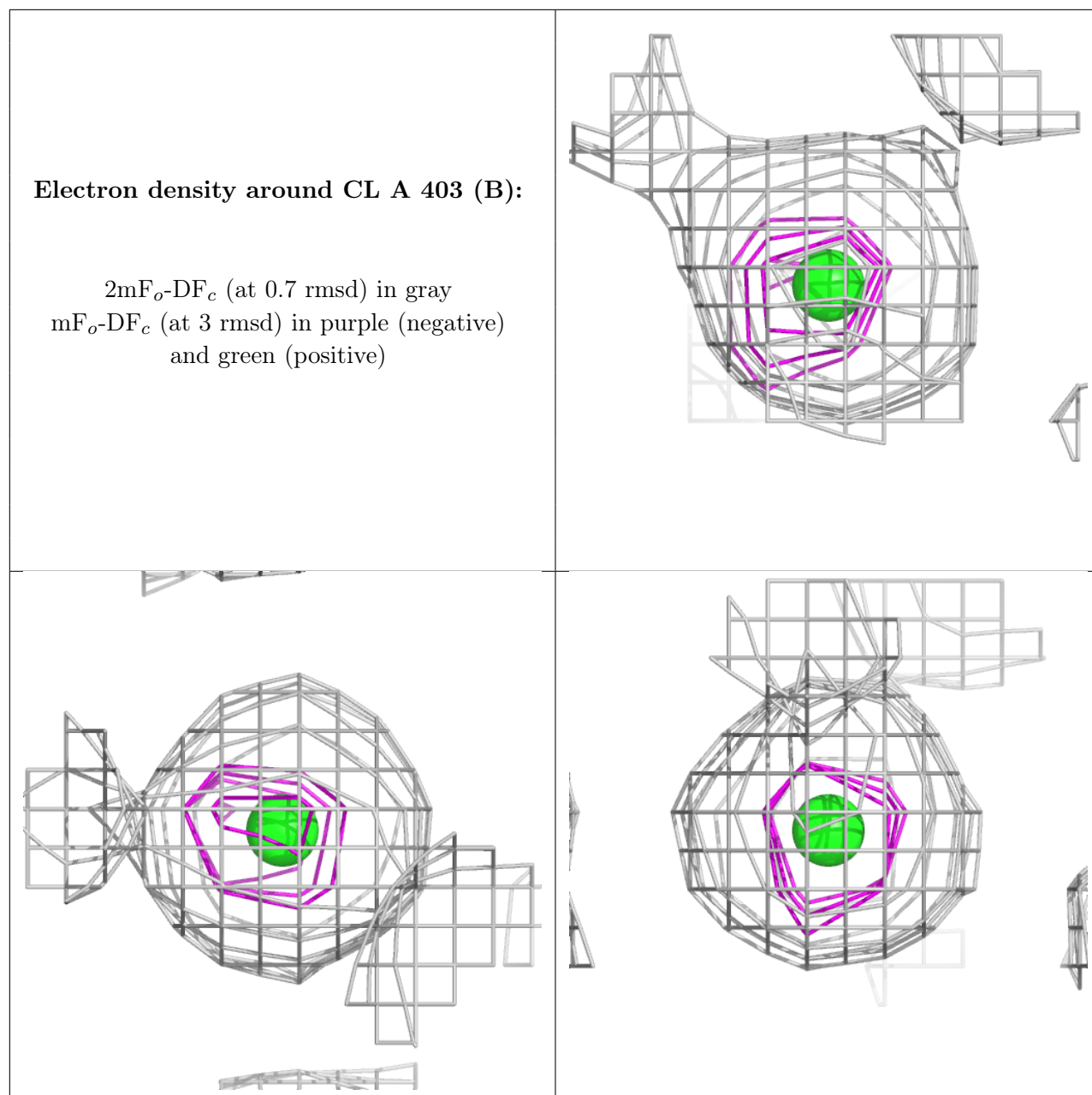


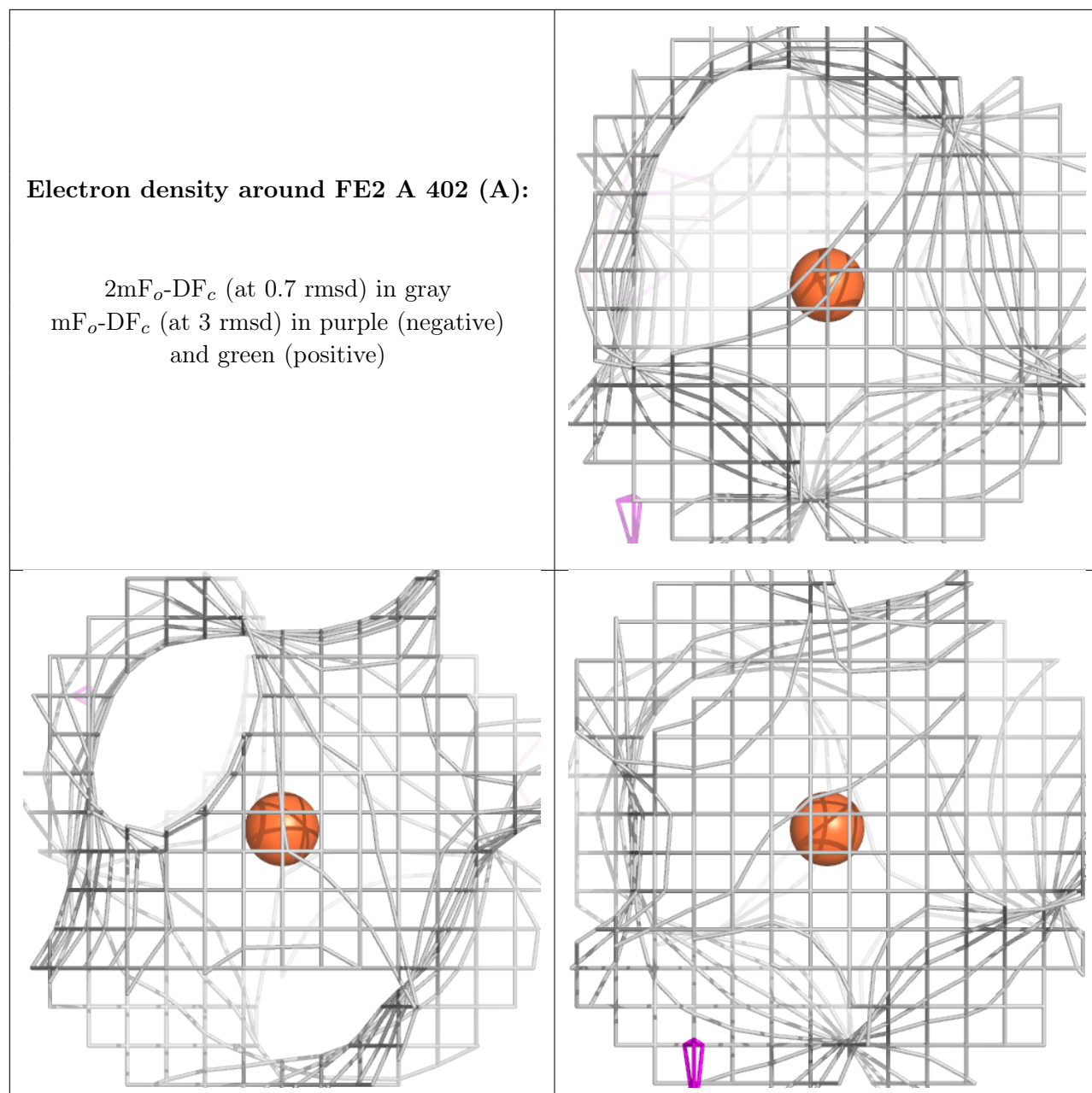
Electron density around OEX a 414 (A):

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









6.5 Other polymers [i](#)

There are no such residues in this entry.