



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2024 – 02:28 PM JST

PDB ID : 8IRI
Title : XFEL structure of cyanobacterial photosystem II following two flashes (2F)
with a 5-millisecond 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)
Xtrriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

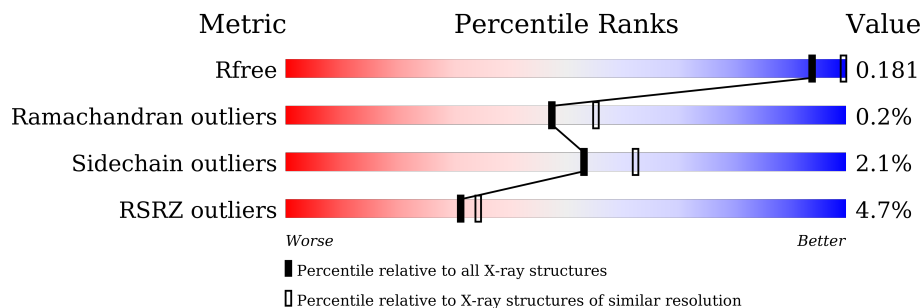
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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.



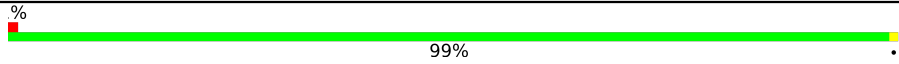
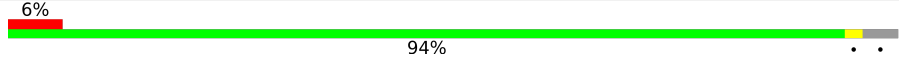
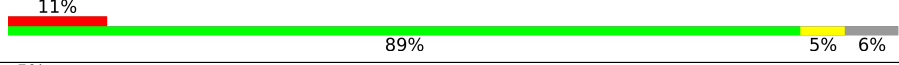

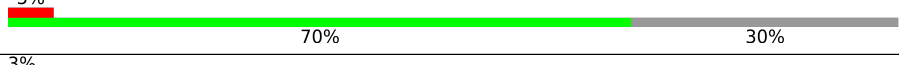
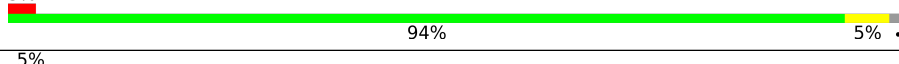
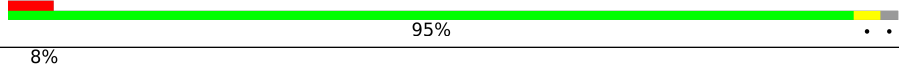
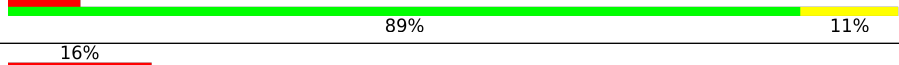
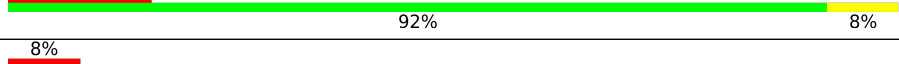
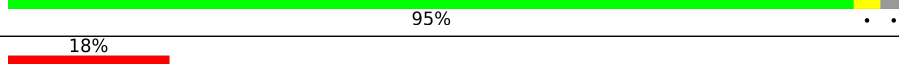
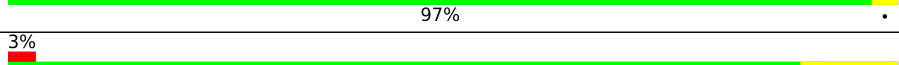
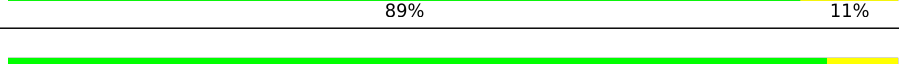
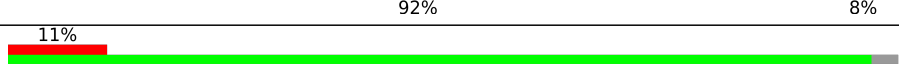
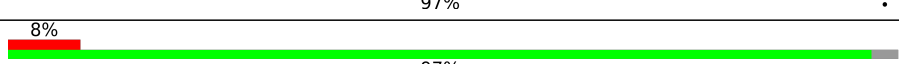
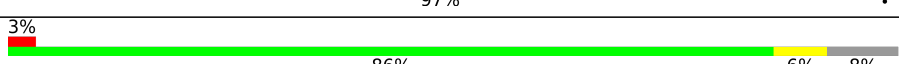
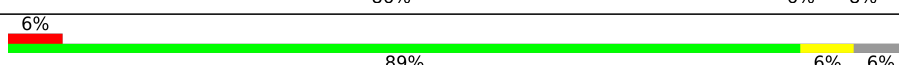
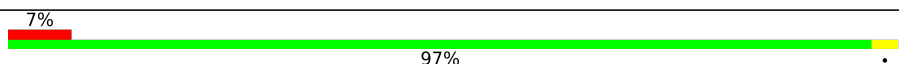
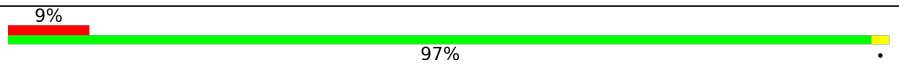
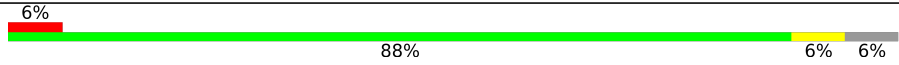
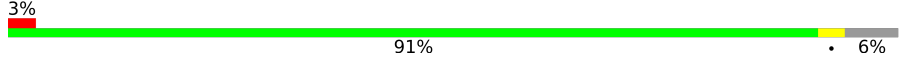
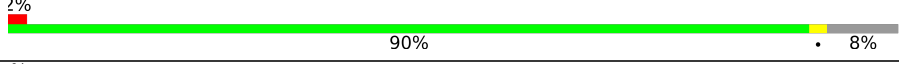
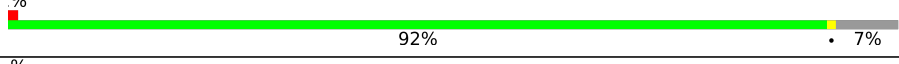
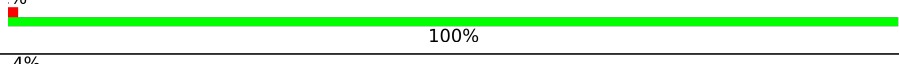
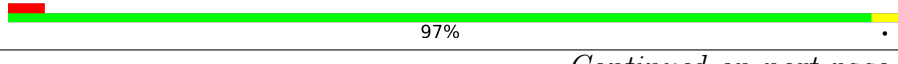

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1377 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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

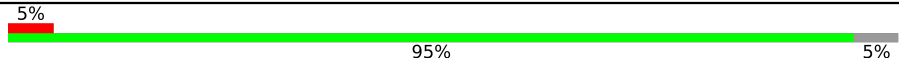
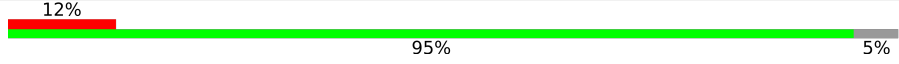
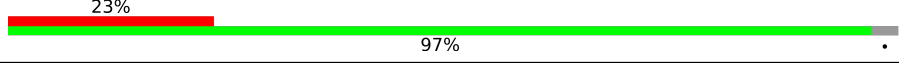
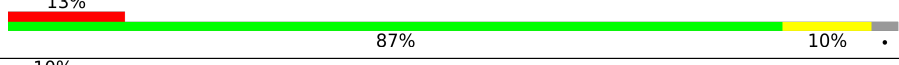
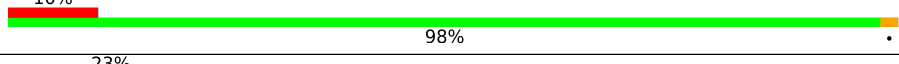
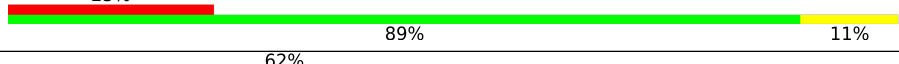
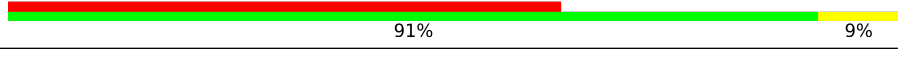
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Mol	Chain	Length	Quality of chain
4	d	342	 99%
5	E	84	 94%
5	e	84	 89%
6	F	44	 77%
6	f	44	 70%
7	H	65	 94%
7	h	65	 95%
8	I	38	 89%
8	i	38	 92%
9	J	39	 95%
9	j	39	 97%
10	K	37	 89%
10	k	37	 92%
11	L	37	 97%
11	l	37	 97%
12	M	36	 86%
12	m	36	 89%
13	O	244	 97%
13	o	244	 97%
14	T	32	 88%
14	t	32	 91%
15	U	104	 90%
15	u	104	 92%
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
23	CLA	A	404[A]	X	-	-	-
23	CLA	A	404[B]	X	-	-	-
23	CLA	A	405[A]	X	-	-	-
23	CLA	A	405[B]	X	-	-	-
23	CLA	A	408	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	D	404[A]	X	-	-	-
23	CLA	D	404[B]	X	-	-	-
23	CLA	D	405	X	-	-	-
23	CLA	a	405[A]	X	-	-	-
23	CLA	a	405[B]	X	-	-	-
23	CLA	a	406[A]	X	-	-	-
23	CLA	a	406[B]	X	-	-	-
23	CLA	a	409	X	-	-	-
23	CLA	b	601	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
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23	CLA	b	614	X	-	-	-
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23	CLA	b	616	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	c	514	X	-	-	-
23	CLA	d	402[A]	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	d	402[B]	X	-	-	-
23	CLA	d	403	X	-	-	-
27	GOL	a	418	-	-	-	X
31	LMT	F	101	-	-	-	X
31	LMT	c	501	-	-	-	X
31	LMT	e	101	-	-	-	X
32	LHG	a	420[A]	-	-	-	X
32	LHG	a	420[B]	-	-	-	X
34	HTG	b	623	-	-	-	X

2 Entry composition [i](#)

There are 42 unique types of molecules in this entry. The entry contains 62604 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			

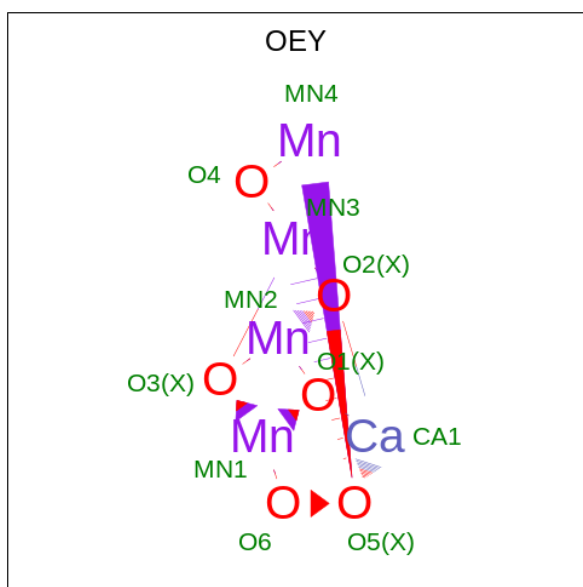
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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) (labeled as "Ligand of Interest" by depositor).

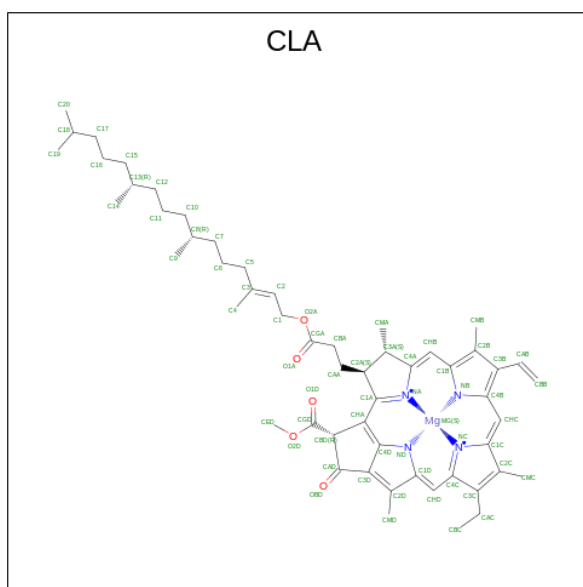


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Ca	Mn	O		
21	A	1	11	1	4	6	0	1
21	a	1	11	1	4	6	0	1

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

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

- Molecule 23 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		
23	A	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	A	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	A	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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

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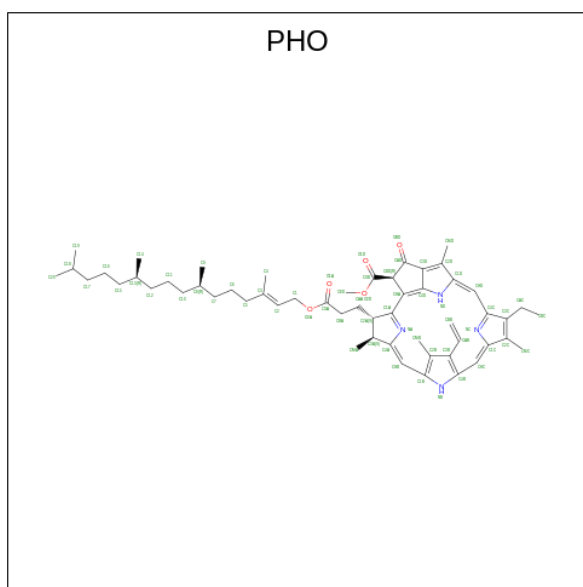
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	a	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	a	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	a	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65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

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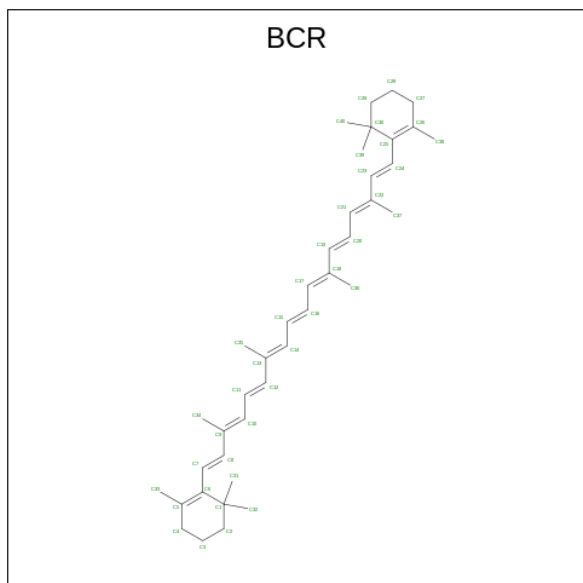
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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



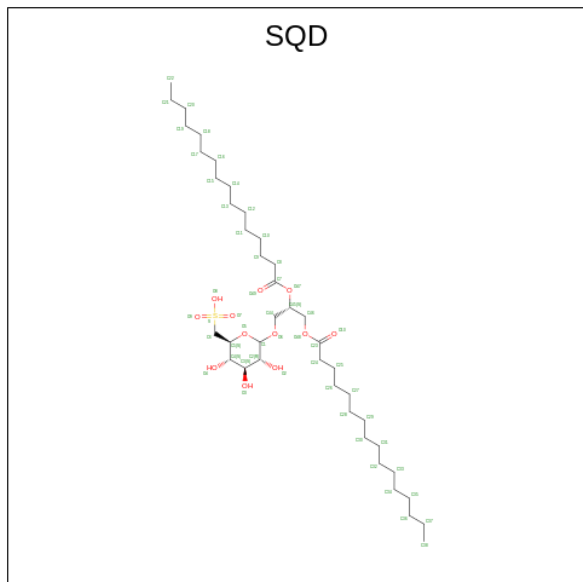
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
24	A	1	Total 128	C 110	N 8	O 10	0	1
24	A	1	Total 128	C 110	N 8	O 10	0	1
24	a	1	Total 128	C 110	N 8	O 10	0	1
24	a	1	Total 128	C 110	N 8	O 10	0	1

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



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

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



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

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



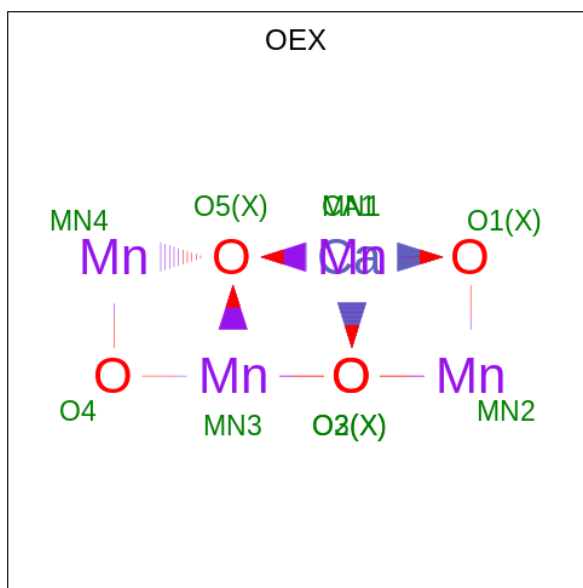
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 6 3 3	0	0
27	B	1	Total C O 6 3 3	0	0
27	B	1	Total C O 6 3 3	0	0
27	B	1	Total C O 6 3 3	0	0
27	C	1	Total C O 12 6 6	0	1
27	D	1	Total C O 6 3 3	0	0
27	D	1	Total C O 6 3 3	0	0
27	O	1	Total C O 6 3 3	0	0
27	O	1	Total C O 6 3 3	0	0
27	V	1	Total C O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

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

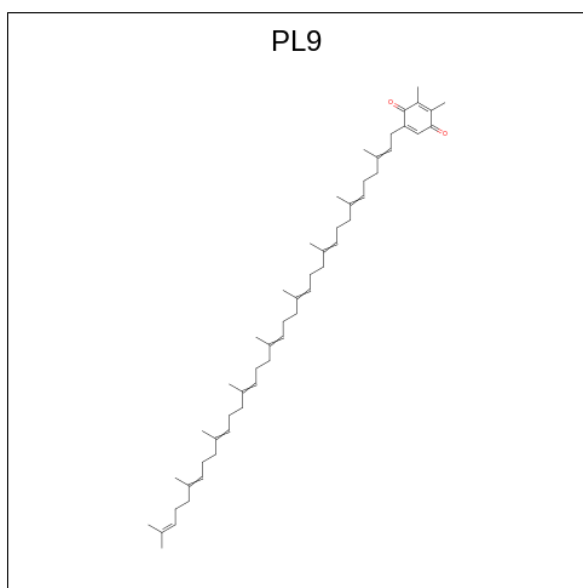
- Molecule 28 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:

C₅₃H₈₀O₂) (labeled as "Ligand of Interest" by depositor).



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

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

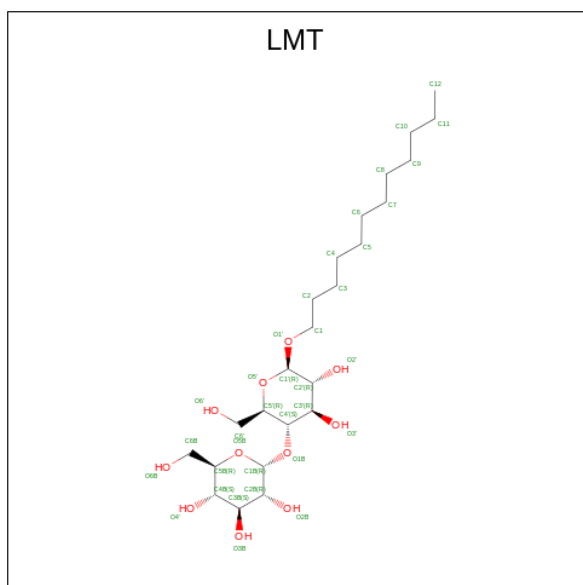
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			28	23	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	I	1	Total	C	O	0	0
			40	35	5		
30	J	1	Total	C		0	0
			10	10			
30	K	1	Total	C	O	0	1
			68	58	10		
30	X	1	Total	C	O	0	0
			18	16	2		

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

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



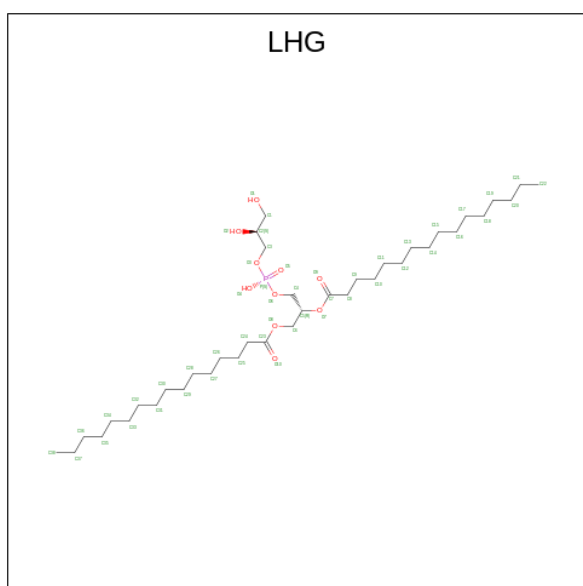
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			35	24	11		
31	A	1	Total	C	O	0	0
			35	24	11		

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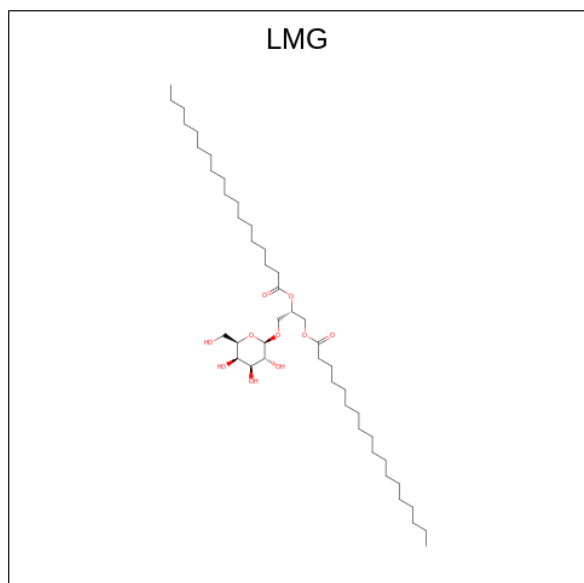
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			25	19	6		
31	F	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total	C	O	0	0
			35	24	11		
31	b	1	Total	C	O	0	0
			25	19	6		
31	b	1	Total	C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

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



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

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



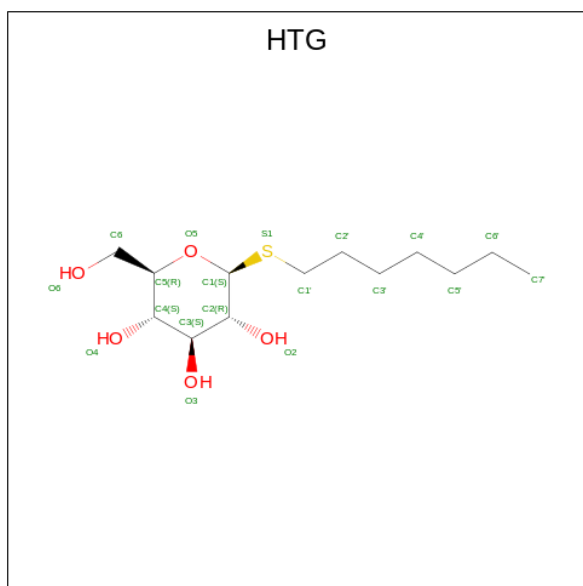
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
33	B	1	51	41	10	0	0

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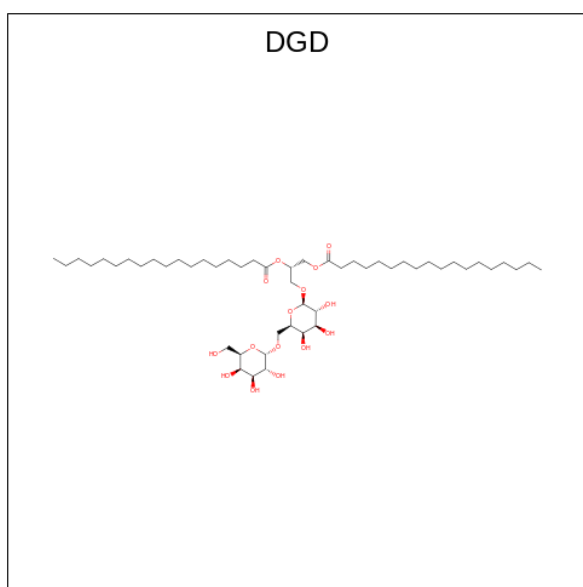
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	D	1	Total	C	O	0	0
			51	41	10		
33	a	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	d	1	Total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

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



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

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



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

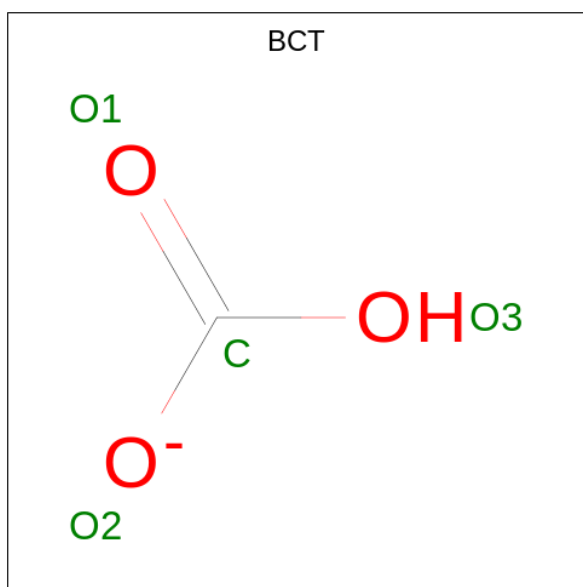
- Molecule 36 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 37 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

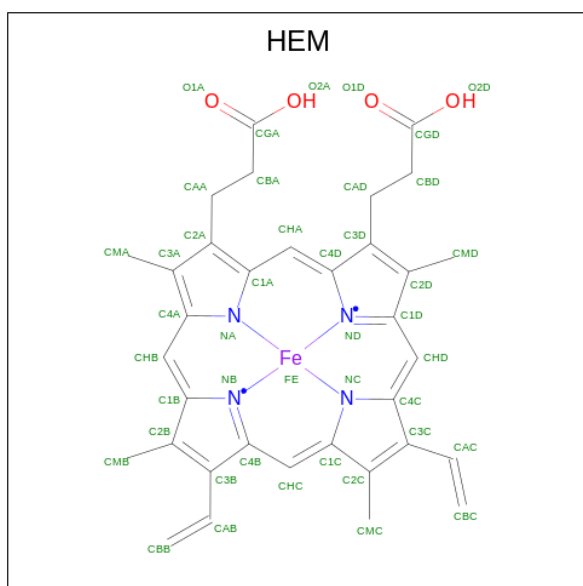
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	D	1	Total Fe 2 2	0	1
37	a	1	Total Fe 2 2	0	1

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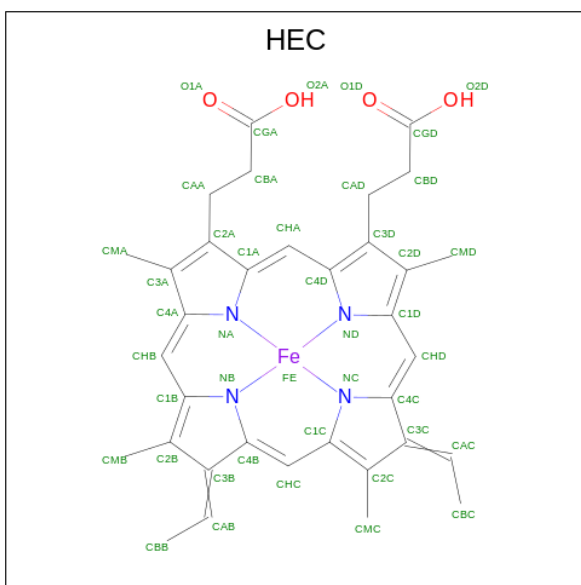
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
39	f	1	43	34	1	4	4	0	0

- 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	83
42	B	196	199	199	0	3

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
42	C	170	Total O 207 207	0	38
42	D	122	Total O 157 157	0	35
42	E	17	Total O 17 17	0	0
42	F	5	Total O 5 5	0	0
42	H	18	Total O 18 18	0	0
42	I	4	Total O 4 4	0	0
42	J	7	Total O 7 7	0	0
42	K	6	Total O 6 6	0	0
42	L	8	Total O 9 9	0	1
42	M	5	Total O 5 5	0	0
42	O	102	Total O 106 106	0	4
42	T	11	Total O 14 14	0	3
42	U	46	Total O 49 49	0	3
42	V	78	Total O 80 80	0	2
42	X	8	Total O 8 8	0	0
42	a	130	Total O 208 208	0	79
42	b	200	Total O 203 203	0	3
42	c	159	Total O 192 192	0	33
42	d	120	Total O 154 154	0	34
42	e	8	Total O 8 8	0	0
42	f	3	Total O 3 3	0	0

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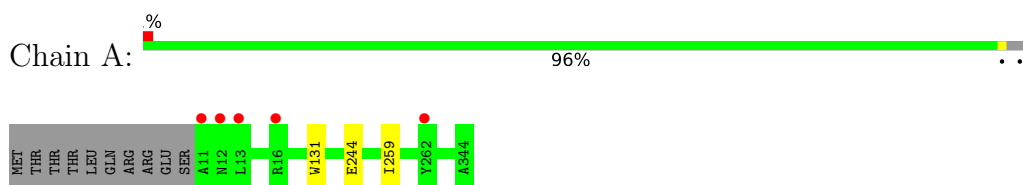
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
42	h	17	Total O 17 17	0	0
42	i	2	Total O 2 2	0	0
42	j	2	Total O 2 2	0	0
42	k	3	Total O 3 3	0	0
42	l	7	Total O 8 8	0	1
42	m	13	Total O 13 13	0	0
42	o	98	Total O 102 102	0	4
42	t	8	Total O 11 11	0	3
42	u	49	Total O 50 50	0	1
42	v	58	Total O 61 61	0	3
42	x	6	Total O 6 6	0	0
42	y	2	Total O 2 2	0	0

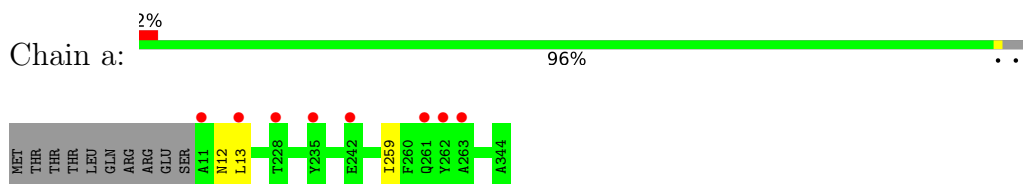
3 Residue-property plots [i](#)

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.

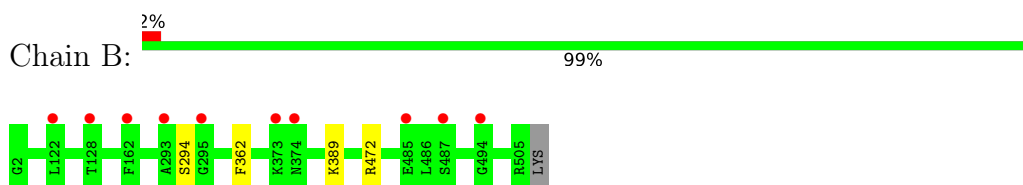
- Molecule 1: Photosystem II protein D1



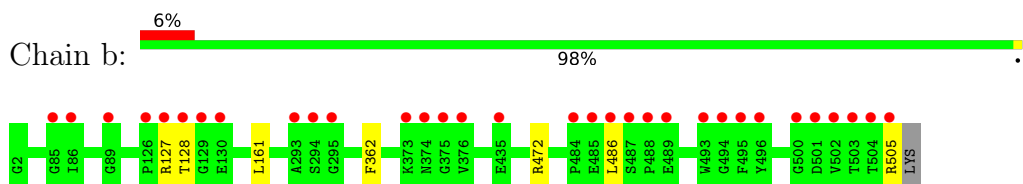
- Molecule 1: Photosystem II protein D1



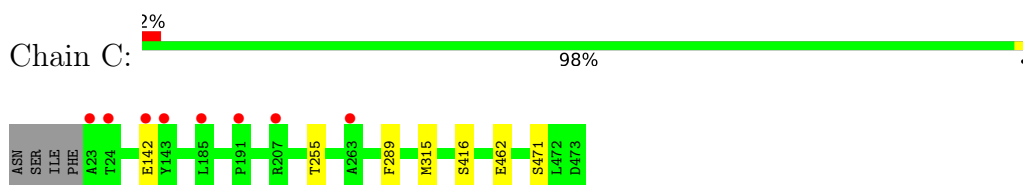
- Molecule 2: Photosystem II CP47 reaction center protein



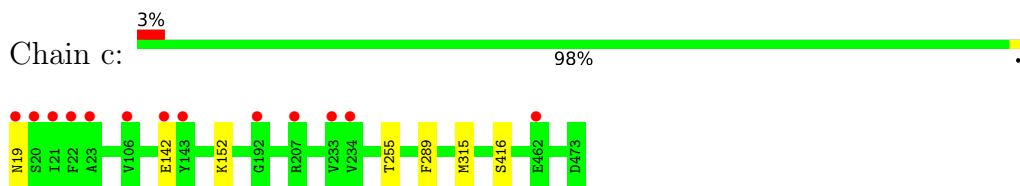
- Molecule 2: Photosystem II CP47 reaction center protein



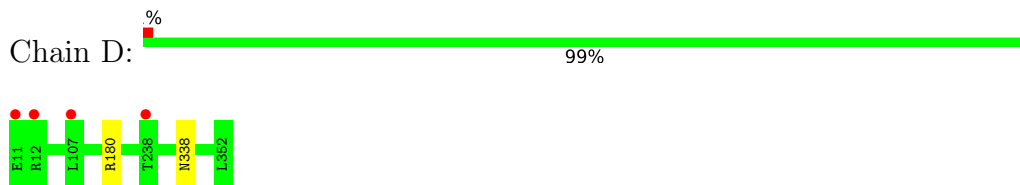
- Molecule 3: Photosystem II CP43 reaction center protein



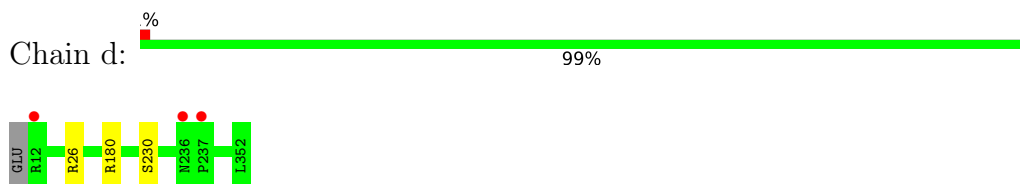
- Molecule 3: Photosystem II CP43 reaction center protein



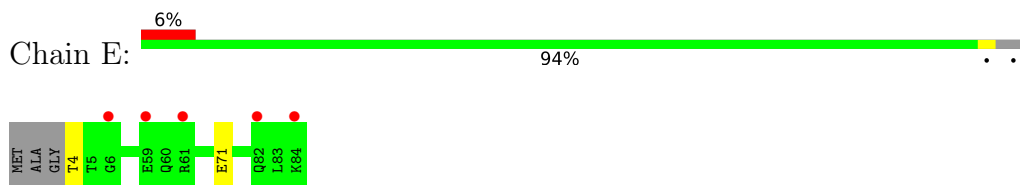
• Molecule 4: Photosystem II D2 protein



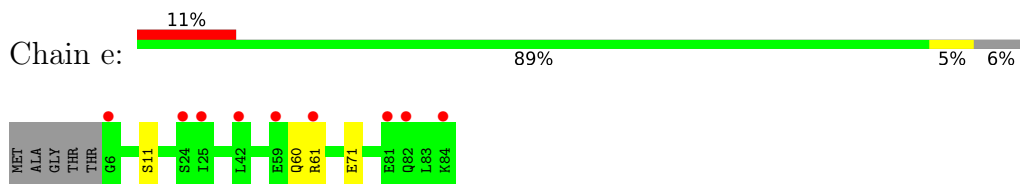
• Molecule 4: Photosystem II D2 protein



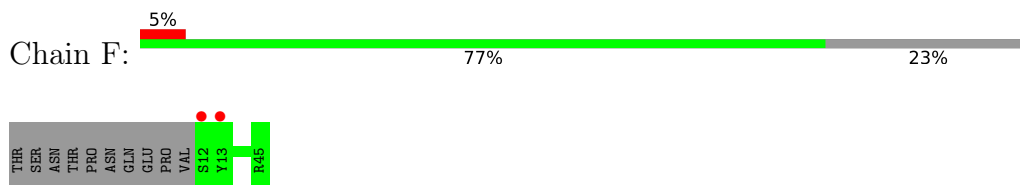
• Molecule 5: Cytochrome b559 subunit alpha



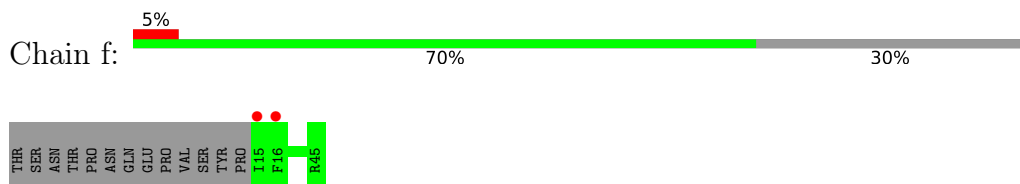
• Molecule 5: Cytochrome b559 subunit alpha



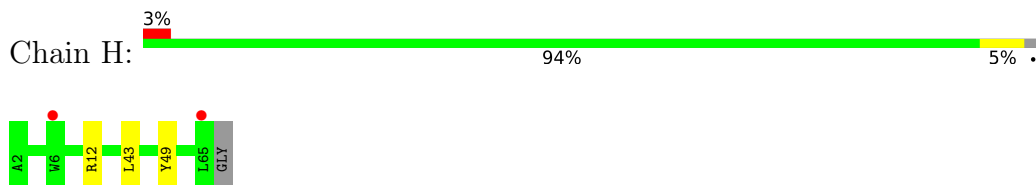
• Molecule 6: Cytochrome b559 subunit beta



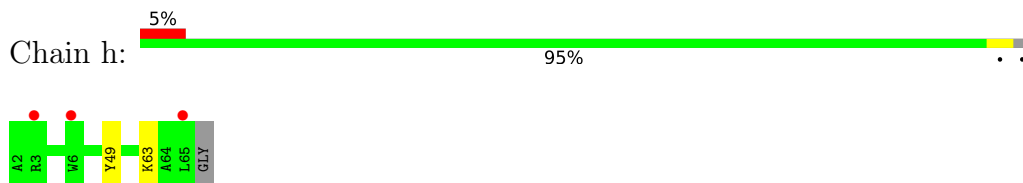
• Molecule 6: Cytochrome b559 subunit beta



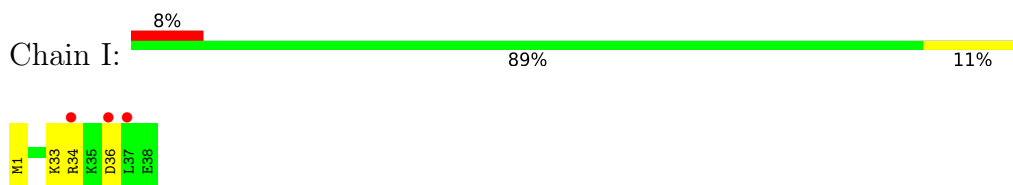
- Molecule 7: Photosystem II reaction center protein H



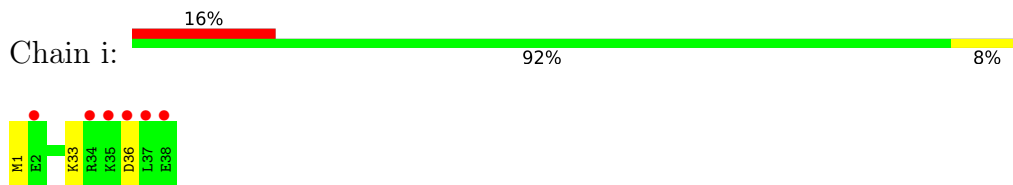
- Molecule 7: Photosystem II reaction center protein H



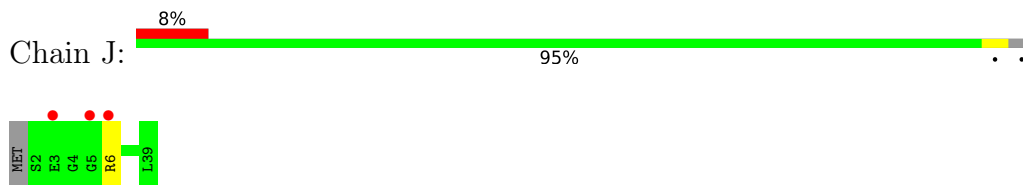
- Molecule 8: Photosystem II reaction center protein I



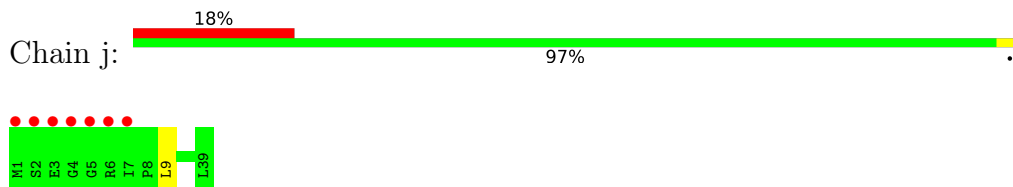
- Molecule 8: Photosystem II reaction center protein I



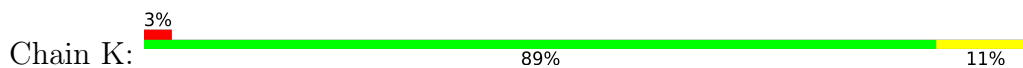
- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K

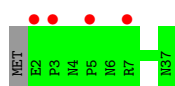




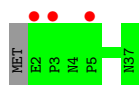
- Molecule 10: Photosystem II reaction center protein K



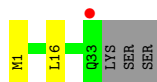
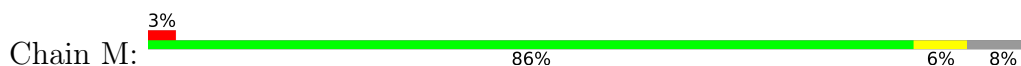
- Molecule 11: Photosystem II reaction center protein L



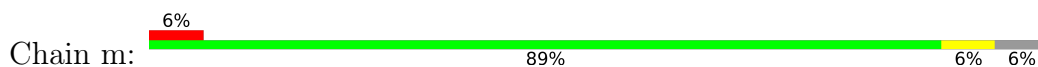
- Molecule 11: Photosystem II reaction center protein L



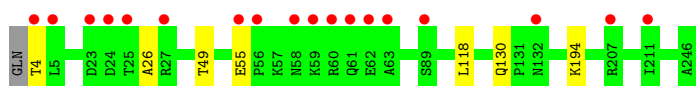
- Molecule 12: Photosystem II reaction center protein M



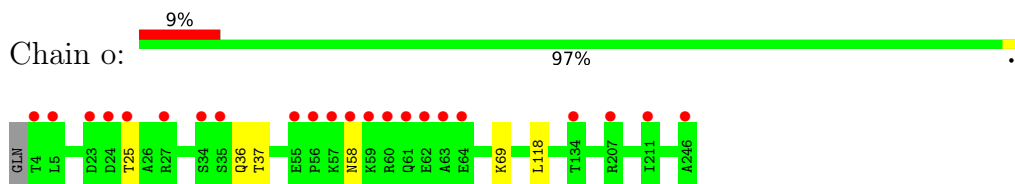
- Molecule 12: Photosystem II reaction center protein M



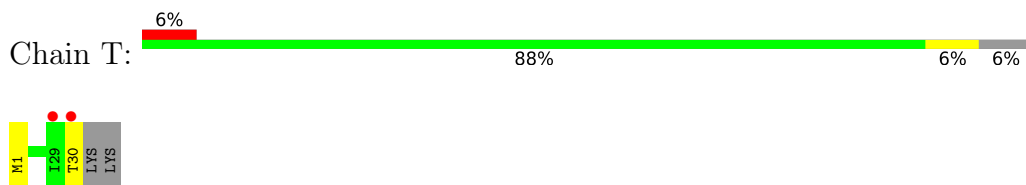
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



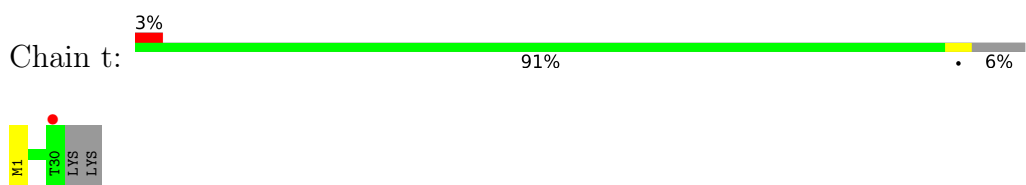
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



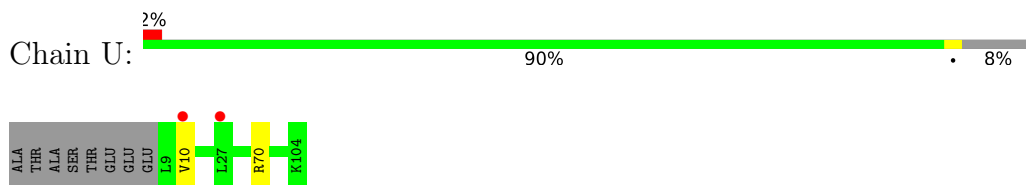
- Molecule 14: Photosystem II reaction center protein T



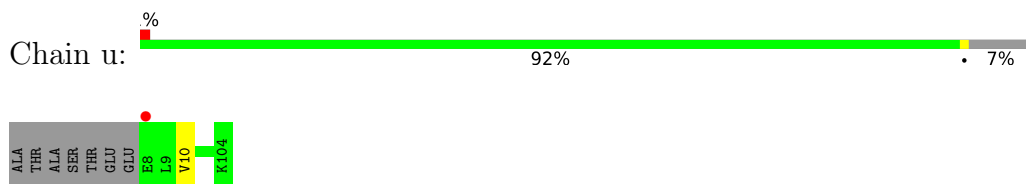
- Molecule 14: Photosystem II reaction center protein T



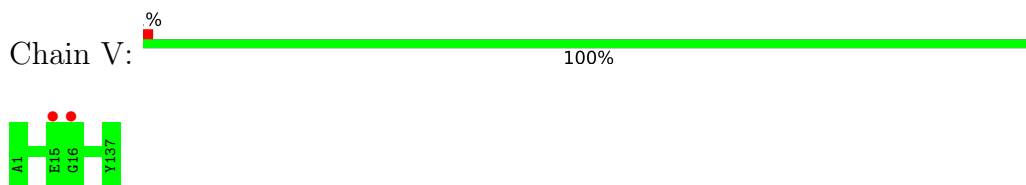
- Molecule 15: Photosystem II 12 kDa extrinsic protein



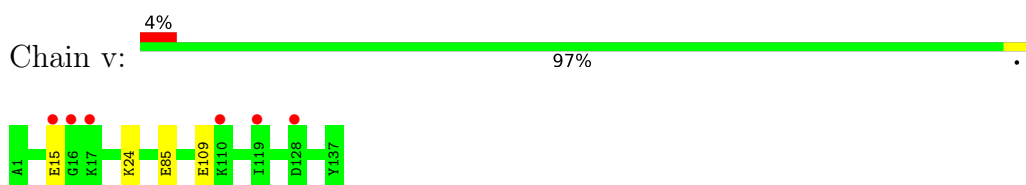
- Molecule 15: Photosystem II 12 kDa extrinsic protein



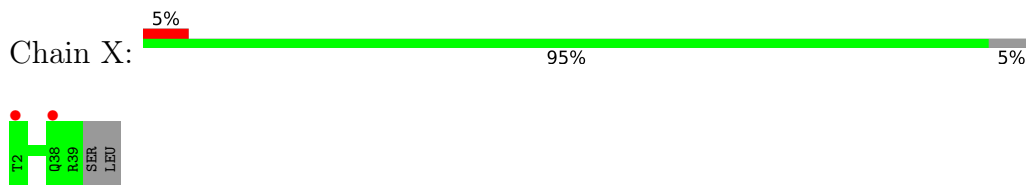
- Molecule 16: Cytochrome c-550



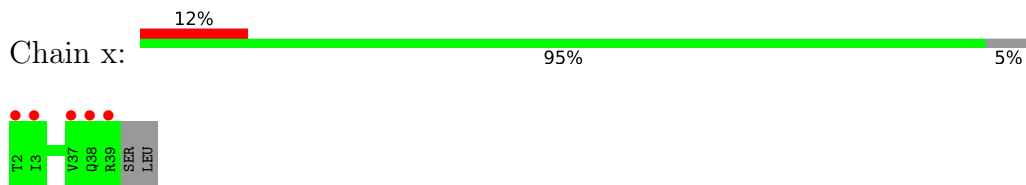
- Molecule 16: Cytochrome c-550



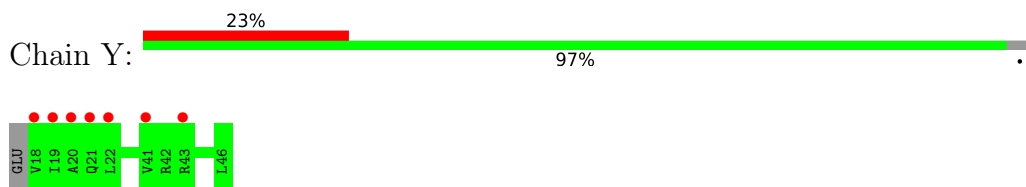
- Molecule 17: Photosystem II reaction center protein X



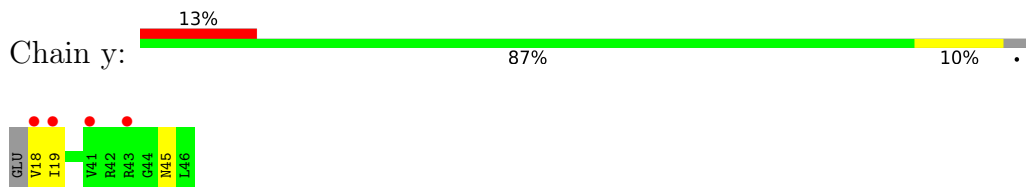
- Molecule 17: Photosystem II reaction center protein X



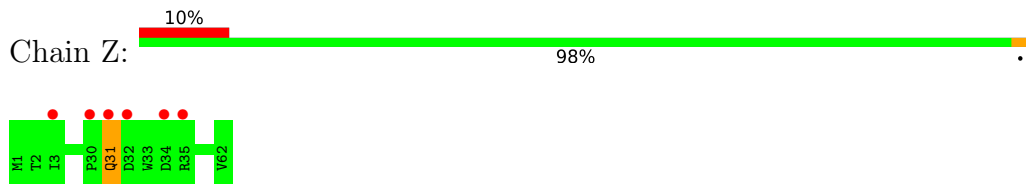
- Molecule 18: Photosystem II reaction center protein Ycf12



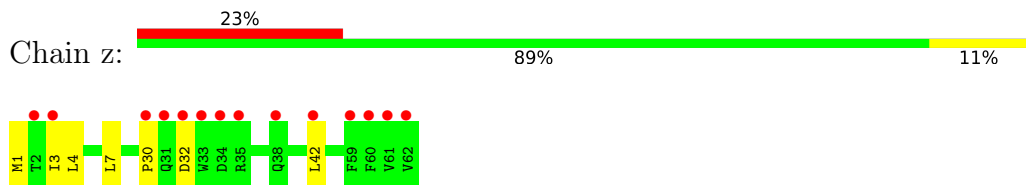
- Molecule 18: Photosystem II reaction center protein Ycf12



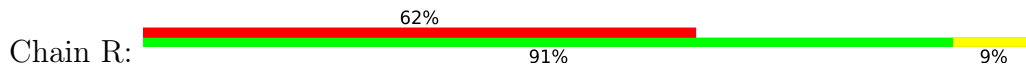
- Molecule 19: Photosystem II reaction center protein Z

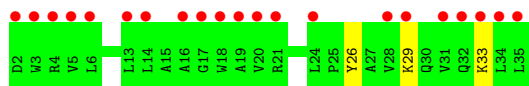


- Molecule 19: Photosystem II reaction center protein Z



- 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	1.66 (at 2.26Å)	Xtrriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.142 , 0.181 0.142 , 0.181	Depositor DCC
R_{free} test set	19873 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	50.6	Xtrriage
Anisotropy	0.465	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 86.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	62604	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 1.65% 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: LMT, CL, OEX, OEY, PL9, UNL, FE2, PHO, FME, BCT, DGD, MG, CLA, SQD, GOL, BCR, CA, HTG, LMG, HEM, LHG, HEC

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	0.45	0/4293	0.60	0/5851
2	b	0.44	0/4285	0.59	0/5841
3	C	0.40	0/4404	0.56	0/5997
3	c	0.40	0/4459	0.54	0/6071
4	D	0.48	0/3741	0.60	0/5095
4	d	0.46	0/3749	0.58	0/5106
5	E	0.43	0/681	0.59	0/928
5	e	0.40	0/690	0.54	0/939
6	F	0.43	0/284	0.58	0/387
6	f	0.39	0/269	0.53	0/365
7	H	0.40	0/519	0.61	0/708
7	h	0.36	0/530	0.59	0/722
8	I	0.42	0/311	0.55	0/419
8	i	0.43	0/311	0.54	0/419
9	J	0.40	0/278	0.52	0/376
9	j	0.39	0/283	0.56	0/383
10	K	0.38	0/303	0.51	0/416
10	k	0.39	0/303	0.54	0/416
11	L	0.44	0/318	0.56	0/433
11	l	0.46	0/318	0.53	0/433
12	M	0.46	0/261	0.50	0/357
12	m	0.42	0/279	0.54	0/380
13	O	0.43	0/1991	0.64	0/2698
13	o	0.42	0/1966	0.65	0/2665
14	T	0.46	0/310	0.63	0/419
14	t	0.42	0/301	0.59	0/406
15	U	0.46	0/811	0.61	0/1095
15	u	0.46	0/818	0.62	0/1105
16	V	0.43	0/1142	0.59	0/1545

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.36	0/1139	0.56	0/1542
17	X	0.33	0/292	0.49	0/395
17	x	0.32	0/284	0.50	0/384
18	Y	0.32	0/216	0.53	0/289
18	y	0.32	0/216	0.51	0/289
19	Z	0.33	0/490	0.47	0/669
19	z	0.33	0/490	0.43	0/669
20	R	0.32	0/279	0.51	0/383
All	All	0.43	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	131	TRP	CA-CB-CG	-5.24	103.75	113.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	553/344 (161%)	544 (98%)	7 (1%)	2 (0%)	34	37
1	a	552/344 (160%)	545 (99%)	5 (1%)	2 (0%)	34	37
2	B	522/505 (103%)	515 (99%)	7 (1%)	0	100	100
2	b	521/505 (103%)	511 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	546/455 (120%)	539 (99%)	6 (1%)	1 (0%)	47	55
3	c	553/455 (122%)	542 (98%)	10 (2%)	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%)	60 (97%)	2 (3%)	0	100	100
7	h	63/65 (97%)	59 (94%)	3 (5%)	1 (2%)	9	5
8	I	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	5	2
8	i	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
9	J	36/39 (92%)	36 (100%)	0	0	100	100
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	34/36 (94%)	34 (100%)	0	0	100	100
13	O	251/244 (103%)	242 (96%)	8 (3%)	1 (0%)	34	37
13	o	249/244 (102%)	243 (98%)	6 (2%)	0	100	100
14	T	33/32 (103%)	33 (100%)	0	0	100	100
14	t	32/32 (100%)	32 (100%)	0	0	100	100
15	U	97/104 (93%)	93 (96%)	4 (4%)	0	100	100
15	u	98/104 (94%)	93 (95%)	5 (5%)	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%)	37 (100%)	0	0	100	100
17	x	36/40 (90%)	36 (100%)	0	0	100	100
18	Y	27/30 (90%)	26 (96%)	1 (4%)	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%)	6040 (98%)	120 (2%)	11 (0%)	47	55

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	I	36	ASP
3	C	416	SER
3	c	416	SER
19	Z	31	GLN
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%)	423 (98%)	7 (2%)	62	73
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%)	365 (99%)	4 (1%)	73	82
5	E	72/73 (99%)	70 (97%)	2 (3%)	43	52
5	e	72/73 (99%)	68 (94%)	4 (6%)	21	21
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	26/38 (68%)	26 (100%)	0	100	100
7	H	54/54 (100%)	51 (94%)	3 (6%)	21	21
7	h	55/54 (102%)	54 (98%)	1 (2%)	59	68
8	I	34/34 (100%)	32 (94%)	2 (6%)	19	19
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%)	210 (97%)	6 (3%)	43	52
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%)	5005 (98%)	98 (2%)	53	66

All (98) 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	294	SER
2	B	362	PHE
2	B	389	LYS
2	B	472	ARG
3	C	142	GLU
3	C	255	THR
3	C	289	PHE
3	C	315[A]	MET
3	C	315[B]	MET
3	C	462	GLU
3	C	471	SER
4	D	180	ARG
4	D	338	ASN
5	E	4	THR
5	E	71	GLU
7	H	12	ARG
7	H	43	LEU
7	H	49	TYR
8	I	33	LYS
8	I	34	ARG
9	J	6	ARG
10	K	10	LYS
10	K	17	ILE
10	K	19	ASP
10	K	27	VAL
12	M	16[A]	LEU
12	M	16[B]	LEU
13	O	4	THR
13	O	49	THR
13	O	55	GLU
13	O	118	LEU
13	O	130	GLN
13	O	194	LYS
14	T	30[A]	THR

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Mol	Chain	Res	Type
14	T	30[B]	THR
15	U	10	VAL
15	U	70	ARG
1	a	12	ASN
1	a	13	LEU
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	180	ARG
4	d	230[A]	SER
4	d	230[B]	SER
5	e	11	SER
5	e	60	GLN
5	e	61	ARG
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	25	THR
13	o	36	GLN
13	o	37	THR
13	o	58	ASN
13	o	69	LYS

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Mol	Chain	Res	Type
13	o	118	LEU
15	u	10[A]	VAL
15	u	10[B]	VAL
16	v	15	GLU
16	v	24	LYS
16	v	85	GLU
16	v	109	GLU
18	y	18	VAL
18	y	19	ILE
18	y	45	ASN
19	Z	31	GLN
20	R	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 (3) such sidechains are listed below:

Mol	Chain	Res	Type
5	E	60	GLN
1	a	12	ASN
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
12	FME	m	1	12	8,9,10	0.49	0	7,9,11	1.45	2 (28%)
14	FME	T	1	14	8,9,10	0.59	0	7,9,11	1.43	1 (14%)
8	FME	i	1	8	8,9,10	0.68	0	7,9,11	1.23	1 (14%)
8	FME	I	1	8	8,9,10	0.62	0	7,9,11	1.38	2 (28%)
12	FME	M	1	12	8,9,10	0.71	0	7,9,11	1.23	1 (14%)
14	FME	t	1	14	8,9,10	0.67	0	7,9,11	1.80	2 (28%)

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

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

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	O-C-CA	-2.74	117.60	124.78
14	t	1	FME	CA-N-CN	-2.68	118.70	122.82
14	T	1	FME	CG-CB-CA	2.32	119.38	112.95
12	M	1	FME	O-C-CA	-2.29	118.77	124.78
8	I	1	FME	CA-N-CN	-2.26	119.34	122.82
12	m	1	FME	O1-CN-N	-2.26	119.32	125.27
8	I	1	FME	O-C-CA	-2.23	118.94	124.78
12	m	1	FME	O-C-CA	-2.18	119.07	124.78
8	i	1	FME	O-C-CA	-2.04	119.42	124.78

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

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$
23	CLA	B	601	42	65,73,73	2.10	17 (26%)	76,113,113	2.78	27 (35%)
29	PL9	d	405[A]	-	55,55,55	0.70	1 (1%)	68,69,69	1.63	18 (26%)
27	GOL	b	628	-	5,5,5	0.52	0	5,5,5	1.43	1 (20%)
29	PL9	D	407[B]	-	55,55,55	0.64	2 (3%)	68,69,69	1.56	14 (20%)
23	CLA	C	508	42	65,73,73	1.98	17 (26%)	76,113,113	2.81	27 (35%)
23	CLA	B	608	-	65,73,73	1.92	14 (21%)	76,113,113	2.79	33 (43%)
23	CLA	A	408	-	65,73,73	2.05	16 (24%)	76,113,113	2.84	35 (46%)
31	LMT	M	102	-	36,36,36	1.06	3 (8%)	47,47,47	1.06	3 (6%)
23	CLA	c	506	-	65,73,73	2.00	16 (24%)	76,113,113	2.74	25 (32%)
34	HTG	b	623	-	19,19,19	1.06	1 (5%)	23,24,24	1.84	2 (8%)
25	BCR	A	409	-	41,41,41	1.02	1 (2%)	56,56,56	1.38	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMT	B	628	-	36,36,36	1.17	3 (8%)	47,47,47	1.32	5 (10%)
23	CLA	B	602	-	65,73,73	2.06	17 (26%)	76,113,113	2.85	25 (32%)
34	HTG	V	202	-	11,11,19	0.32	0	15,15,24	1.31	1 (6%)
34	HTG	D	412	-	16,16,19	1.02	1 (6%)	20,21,24	1.56	1 (5%)
24	PHO	A	416[A]	-	51,69,69	1.92	8 (15%)	47,99,99	1.85	9 (19%)
27	GOL	V	203[B]	-	5,5,5	1.05	0	5,5,5	0.95	0
23	CLA	c	508	42	65,73,73	2.00	16 (24%)	76,113,113	2.80	28 (36%)
23	CLA	b	601	42	65,73,73	2.12	16 (24%)	76,113,113	2.76	25 (32%)
31	LMT	A	417	-	36,36,36	0.96	2 (5%)	47,47,47	1.07	3 (6%)
25	BCR	c	516	-	41,41,41	0.99	1 (2%)	56,56,56	1.36	10 (17%)
35	DGD	c	519	-	63,63,67	0.85	4 (6%)	77,77,81	1.06	4 (5%)
23	CLA	C	502	-	65,73,73	1.99	16 (24%)	76,113,113	2.79	29 (38%)
28	OEX	a	413[A]	42,1,3	0,15,15	-	-	-	-	-
23	CLA	b	607	42	65,73,73	1.92	17 (26%)	76,113,113	2.80	29 (38%)
32	LHG	A	418[B]	-	48,48,48	0.90	2 (4%)	51,54,54	1.16	5 (9%)
34	HTG	b	625	-	19,19,19	1.01	2 (10%)	23,24,24	1.46	3 (13%)
25	BCR	c	515	-	41,41,41	1.00	1 (2%)	56,56,56	1.61	15 (26%)
25	BCR	T	101	-	41,41,41	0.95	1 (2%)	56,56,56	1.69	14 (25%)
31	LMT	e	101	-	36,36,36	1.01	2 (5%)	47,47,47	1.00	1 (2%)
25	BCR	K	103	-	41,41,41	1.00	1 (2%)	56,56,56	1.77	12 (21%)
24	PHO	A	407[A]	-	51,69,69	1.77	8 (15%)	47,99,99	1.69	10 (21%)
23	CLA	b	606	-	65,73,73	2.02	15 (23%)	76,113,113	2.82	27 (35%)
32	LHG	D	409[B]	-	48,48,48	0.93	2 (4%)	51,54,54	1.02	3 (5%)
34	HTG	B	623	-	19,19,19	0.83	1 (5%)	23,24,24	1.44	2 (8%)
23	CLA	b	605	-	65,73,73	2.00	16 (24%)	76,113,113	3.04	25 (32%)
31	LMT	F	101	-	36,36,36	1.06	1 (2%)	47,47,47	1.05	3 (6%)
26	SQD	B	620	-	53,54,54	1.07	3 (5%)	62,65,65	1.83	13 (20%)
32	LHG	E	101[A]	-	41,41,48	1.08	2 (4%)	44,47,54	1.10	3 (6%)
38	BCT	D	402[A]	37	2,3,3	0.64	0	2,3,3	1.30	0
21	OEY	A	401[B]	42,1,3	0,16,16	-	-	-	-	-
31	LMT	A	419	-	36,36,36	1.03	2 (5%)	47,47,47	1.16	4 (8%)
27	GOL	D	414	-	5,5,5	1.41	1 (20%)	5,5,5	0.85	0
34	HTG	C	522	-	19,19,19	0.89	1 (5%)	23,24,24	1.39	1 (4%)
33	LMG	D	413	40	51,51,55	0.83	3 (5%)	59,59,63	1.07	4 (6%)
31	LMT	M	101	-	36,36,36	1.13	4 (11%)	47,47,47	1.23	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LMG	d	411	40	51,51,55	0.92	2 (3%)	59,59,63	1.19	6 (10%)
23	CLA	C	510	-	65,73,73	2.08	17 (26%)	76,113,113	2.80	28 (36%)
25	BCR	H	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.42	9 (16%)
24	PHO	A	407[B]	-	51,69,69	1.78	8 (15%)	47,99,99	1.73	8 (17%)
27	GOL	v	202[A]	-	5,5,5	1.20	0	5,5,5	0.82	0
23	CLA	c	502	-	65,73,73	2.01	18 (27%)	76,113,113	2.78	27 (35%)
27	GOL	C	523[A]	-	5,5,5	1.11	0	5,5,5	0.88	0
23	CLA	b	604	-	65,73,73	2.04	16 (24%)	76,113,113	2.72	23 (30%)
23	CLA	A	405[A]	42	65,73,73	1.99	15 (23%)	76,113,113	2.79	30 (39%)
27	GOL	B	629	-	5,5,5	0.98	0	5,5,5	1.02	0
32	LHG	E	101[B]	-	41,41,48	1.06	2 (4%)	44,47,54	1.11	4 (9%)
32	LHG	a	420[A]	-	41,41,48	1.06	2 (4%)	44,47,54	0.92	2 (4%)
23	CLA	C	504	-	65,73,73	1.97	16 (24%)	76,113,113	2.84	25 (32%)
35	DGD	c	518[B]	-	63,63,67	0.88	2 (3%)	77,77,81	0.94	4 (5%)
25	BCR	K	102	-	41,41,41	1.03	1 (2%)	56,56,56	1.49	12 (21%)
25	BCR	B	618	-	41,41,41	0.97	1 (2%)	56,56,56	1.42	9 (16%)
31	LMT	B	631	-	25,25,36	0.89	2 (8%)	30,30,47	1.20	3 (10%)
25	BCR	t	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.50	8 (14%)
33	LMG	a	417	-	51,51,55	0.91	2 (3%)	59,59,63	1.25	6 (10%)
23	CLA	B	616	-	65,73,73	2.07	17 (26%)	76,113,113	2.80	25 (32%)
31	LMT	b	621	-	25,25,36	0.97	1 (4%)	30,30,47	1.19	2 (6%)
23	CLA	d	402[A]	-	65,73,73	1.96	16 (24%)	76,113,113	2.74	29 (38%)
29	PL9	a	414[A]	-	55,55,55	0.65	2 (3%)	68,69,69	2.01	22 (32%)
23	CLA	B	605	-	65,73,73	2.04	16 (24%)	76,113,113	2.98	28 (36%)
27	GOL	l	102[A]	-	5,5,5	0.93	0	5,5,5	0.98	0
29	PL9	A	414[A]	-	55,55,55	0.69	2 (3%)	68,69,69	2.01	24 (35%)
23	CLA	b	602	-	65,73,73	2.04	16 (24%)	76,113,113	2.93	31 (40%)
35	DGD	C	518[A]	-	63,63,67	0.90	3 (4%)	77,77,81	1.03	5 (6%)
38	BCT	d	401[A]	37	2,3,3	0.59	0	2,3,3	1.49	0
39	HEM	f	101	6,5	41,50,50	1.28	5 (12%)	45,82,82	1.83	12 (26%)
23	CLA	a	406[A]	42	65,73,73	2.02	15 (23%)	76,113,113	2.80	29 (38%)
33	LMG	B	621	-	51,51,55	0.90	2 (3%)	59,59,63	1.29	5 (8%)
29	PL9	d	405[B]	-	55,55,55	0.67	1 (1%)	68,69,69	1.64	19 (27%)
25	BCR	y	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.48	9 (16%)
23	CLA	B	604	-	65,73,73	2.06	18 (27%)	76,113,113	2.60	24 (31%)
23	CLA	B	615	-	65,73,73	2.04	17 (26%)	76,113,113	2.87	28 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LHG	a	420[B]	-	41,41,48	1.04	2 (4%)	44,47,54	0.93	2 (4%)
35	DGD	C	517[A]	-	63,63,67	0.83	2 (3%)	77,77,81	1.20	8 (10%)
23	CLA	a	409	-	65,73,73	1.89	16 (24%)	76,113,113	2.97	31 (40%)
23	CLA	A	406[A]	42	65,73,73	1.98	17 (26%)	76,113,113	2.76	30 (39%)
23	CLA	C	503	-	65,73,73	2.06	15 (23%)	76,113,113	2.63	28 (36%)
24	PHO	a	408[A]	-	51,69,69	1.83	8 (15%)	47,99,99	1.87	9 (19%)
29	PL9	A	414[B]	-	55,55,55	0.64	1 (1%)	68,69,69	1.95	23 (33%)
33	LMG	Z	101	-	37,37,55	1.01	2 (5%)	45,45,63	1.43	7 (15%)
32	LHG	L	101[A]	-	48,48,48	0.88	2 (4%)	51,54,54	1.15	4 (7%)
23	CLA	C	511	-	65,73,73	2.04	16 (24%)	76,113,113	2.91	30 (39%)
23	CLA	b	613	-	65,73,73	2.02	16 (24%)	76,113,113	2.75	28 (36%)
31	LMT	t	101	-	26,26,36	0.92	2 (7%)	31,31,47	1.27	2 (6%)
35	DGD	C	518[B]	-	63,63,67	0.89	3 (4%)	77,77,81	0.99	4 (5%)
38	BCT	d	401[B]	37	2,3,3	0.65	0	2,3,3	0.88	0
24	PHO	A	416[B]	-	51,69,69	1.93	8 (15%)	47,99,99	1.94	12 (25%)
23	CLA	c	510	-	65,73,73	2.06	16 (24%)	76,113,113	2.75	29 (38%)
23	CLA	b	614	-	65,73,73	1.99	16 (24%)	76,113,113	2.93	28 (36%)
25	BCR	b	618	-	41,41,41	1.01	1 (2%)	56,56,56	1.25	7 (12%)
34	HTG	B	622	-	19,19,19	1.12	2 (10%)	23,24,24	1.69	5 (21%)
26	SQD	A	412	-	53,54,54	1.05	3 (5%)	62,65,65	1.28	6 (9%)
23	CLA	c	512	3	65,73,73	2.10	16 (24%)	76,113,113	2.82	28 (36%)
27	GOL	o	303	-	5,5,5	1.11	1 (20%)	5,5,5	1.06	0
23	CLA	b	603	-	65,73,73	1.99	14 (21%)	76,113,113	2.87	30 (39%)
23	CLA	b	615	-	65,73,73	1.98	15 (23%)	76,113,113	2.72	29 (38%)
23	CLA	c	514	-	65,73,73	2.12	17 (26%)	76,113,113	2.80	28 (36%)
24	PHO	a	408[B]	-	51,69,69	1.80	8 (15%)	47,99,99	1.73	11 (23%)
23	CLA	c	511	-	65,73,73	2.05	16 (24%)	76,113,113	2.76	32 (42%)
35	DGD	c	517[A]	-	63,63,67	0.85	2 (3%)	77,77,81	1.10	7 (9%)
23	CLA	b	608	-	65,73,73	2.01	17 (26%)	76,113,113	2.84	33 (43%)
23	CLA	C	513	-	65,73,73	2.08	15 (23%)	76,113,113	2.77	30 (39%)
23	CLA	c	509	-	65,73,73	2.17	16 (24%)	76,113,113	2.74	24 (31%)
23	CLA	D	405	-	65,73,73	2.10	16 (24%)	76,113,113	2.74	29 (38%)
25	BCR	b	619	-	41,41,41	1.07	1 (2%)	56,56,56	1.45	10 (17%)
32	LHG	b	629[A]	-	48,48,48	0.83	2 (4%)	51,54,54	1.04	4 (7%)
25	BCR	d	404	-	41,41,41	1.12	2 (4%)	56,56,56	1.96	20 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	BCT	D	402[B]	37	2,3,3	0.67	0	2,3,3	0.91	0
31	LMT	b	627	-	25,25,36	0.87	0	30,30,47	1.12	2 (6%)
27	GOL	A	411	-	5,5,5	1.04	0	5,5,5	0.89	0
23	CLA	D	404[A]	-	65,73,73	2.04	16 (24%)	76,113,113	2.87	31 (40%)
23	CLA	c	503	-	65,73,73	2.01	13 (20%)	76,113,113	2.66	25 (32%)
25	BCR	D	406	-	41,41,41	1.10	1 (2%)	56,56,56	1.83	16 (28%)
27	GOL	b	624	-	5,5,5	1.24	1 (20%)	5,5,5	0.73	0
23	CLA	a	407[A]	42	65,73,73	1.98	16 (24%)	76,113,113	2.77	27 (35%)
25	BCR	b	617	-	41,41,41	1.06	1 (2%)	56,56,56	1.45	5 (8%)
32	LHG	D	408[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.01	3 (5%)
27	GOL	a	418	-	5,5,5	1.15	0	5,5,5	1.00	0
21	OEY	a	401[B]	42,1,3	0,16,16	-	-	-	-	-
32	LHG	d	406[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.04	4 (7%)
32	LHG	d	413[A]	-	48,48,48	0.89	2 (4%)	51,54,54	1.11	4 (7%)
33	LMG	c	521	-	51,51,55	1.00	2 (3%)	59,59,63	1.36	6 (10%)
25	BCR	C	516	-	41,41,41	1.01	1 (2%)	56,56,56	1.27	6 (10%)
25	BCR	B	619	-	41,41,41	1.09	1 (2%)	56,56,56	1.29	5 (8%)
23	CLA	B	603	-	65,73,73	2.06	17 (26%)	76,113,113	2.92	30 (39%)
23	CLA	b	609	-	65,73,73	2.02	16 (24%)	76,113,113	2.69	29 (38%)
23	CLA	b	616	-	65,73,73	2.03	16 (24%)	76,113,113	2.87	27 (35%)
27	GOL	v	202[B]	-	5,5,5	1.03	0	5,5,5	0.94	0
23	CLA	A	404[A]	-	65,73,73	2.02	16 (24%)	76,113,113	2.85	30 (39%)
27	GOL	C	523[B]	-	5,5,5	1.06	0	5,5,5	0.86	0
27	GOL	o	302	-	5,5,5	1.04	0	5,5,5	0.99	0
25	BCR	a	410	-	41,41,41	1.08	1 (2%)	56,56,56	1.34	8 (14%)
33	LMG	C	520	-	51,51,55	0.94	2 (3%)	59,59,63	1.09	3 (5%)
23	CLA	A	405[B]	42	65,73,73	2.04	15 (23%)	76,113,113	2.76	31 (40%)
23	CLA	B	613	-	65,73,73	2.04	16 (24%)	76,113,113	2.78	29 (38%)
29	PL9	D	407[A]	-	55,55,55	0.63	1 (1%)	68,69,69	1.61	17 (25%)
32	LHG	b	629[B]	-	48,48,48	0.90	2 (4%)	51,54,54	1.04	4 (7%)
26	SQD	a	411[A]	-	53,54,54	0.96	3 (5%)	62,65,65	1.83	13 (20%)
23	CLA	C	514	-	65,73,73	2.08	15 (23%)	76,113,113	2.76	28 (36%)
41	HEC	v	201	16	32,50,50	1.98	4 (12%)	24,82,82	2.06	5 (20%)
23	CLA	b	611	-	65,73,73	1.95	15 (23%)	76,113,113	2.88	26 (34%)
34	HTG	d	410	-	16,16,19	0.91	1 (6%)	20,21,24	1.54	1 (5%)
23	CLA	D	404[B]	-	65,73,73	2.08	16 (24%)	76,113,113	2.82	27 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LHG	D	408[B]	-	48,48,48	0.90	2 (4%)	51,54,54	1.00	4 (7%)
32	LHG	d	406[B]	-	48,48,48	0.91	2 (4%)	51,54,54	1.06	4 (7%)
26	SQD	f	102	-	42,43,54	1.23	3 (7%)	51,54,65	1.48	10 (19%)
23	CLA	c	513	-	65,73,73	2.05	16 (24%)	76,113,113	2.72	29 (38%)
23	CLA	C	505	42	65,73,73	2.01	15 (23%)	76,113,113	2.78	25 (32%)
23	CLA	c	507	-	65,73,73	2.06	17 (26%)	76,113,113	2.85	29 (38%)
23	CLA	d	402[B]	-	65,73,73	2.04	16 (24%)	76,113,113	2.82	28 (36%)
29	PL9	a	414[B]	-	55,55,55	0.64	2 (3%)	68,69,69	1.95	21 (30%)
32	LHG	d	413[B]	-	48,48,48	0.91	2 (4%)	51,54,54	1.11	5 (9%)
33	LMG	C	521	-	51,51,55	1.09	3 (5%)	59,59,63	1.37	6 (10%)
27	GOL	a	419	-	5,5,5	1.21	1 (20%)	5,5,5	0.98	0
27	GOL	l	102[B]	-	5,5,5	0.94	0	5,5,5	0.96	0
23	CLA	B	609	-	65,73,73	2.04	15 (23%)	76,113,113	2.73	27 (35%)
23	CLA	b	612	-	65,73,73	2.02	18 (27%)	76,113,113	2.71	30 (39%)
31	LMT	m	103	-	36,36,36	1.03	3 (8%)	47,47,47	1.10	3 (6%)
25	BCR	B	617	-	41,41,41	1.13	1 (2%)	56,56,56	1.24	7 (12%)
23	CLA	a	406[B]	42	65,73,73	2.00	12 (18%)	76,113,113	2.80	27 (35%)
23	CLA	C	506	-	65,73,73	1.99	16 (24%)	76,113,113	2.78	27 (35%)
23	CLA	A	404[B]	-	65,73,73	2.08	17 (26%)	76,113,113	2.84	31 (40%)
23	CLA	C	509	-	65,73,73	2.13	16 (24%)	76,113,113	2.74	25 (32%)
25	BCR	h	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.38	10 (17%)
27	GOL	B	627	-	5,5,5	0.94	0	5,5,5	0.99	0
31	LMT	B	630	-	36,36,36	1.02	3 (8%)	47,47,47	1.15	4 (8%)
27	GOL	V	203[A]	-	5,5,5	1.34	0	5,5,5	0.80	0
33	LMG	c	520	-	51,51,55	0.91	2 (3%)	59,59,63	1.11	5 (8%)
23	CLA	C	512	3	65,73,73	2.08	17 (26%)	76,113,113	2.70	27 (35%)
34	HTG	b	622	-	19,19,19	1.20	2 (10%)	23,24,24	1.92	7 (30%)
35	DGD	C	517[B]	-	63,63,67	0.83	2 (3%)	77,77,81	1.06	6 (7%)
23	CLA	B	610	42	65,73,73	1.98	17 (26%)	76,113,113	2.87	31 (40%)
26	SQD	a	411[B]	-	53,54,54	0.94	3 (5%)	62,65,65	1.64	11 (17%)
26	SQD	a	412	-	53,54,54	1.08	4 (7%)	62,65,65	1.19	9 (14%)
27	GOL	d	412	-	5,5,5	1.30	1 (20%)	5,5,5	1.00	0
23	CLA	a	405[A]	-	65,73,73	2.01	16 (24%)	76,113,113	2.86	32 (42%)
23	CLA	c	505	42	65,73,73	2.08	17 (26%)	76,113,113	2.70	25 (32%)
27	GOL	B	624	-	5,5,5	0.79	0	5,5,5	1.12	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LHG	A	418[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.27	6 (11%)
23	CLA	A	406[B]	42	65,73,73	2.08	16 (24%)	76,113,113	2.79	29 (38%)
23	CLA	C	507	-	65,73,73	2.07	18 (27%)	76,113,113	2.79	29 (38%)
25	BCR	C	515	-	41,41,41	1.00	1 (2%)	56,56,56	1.42	6 (10%)
26	SQD	A	410[A]	-	53,54,54	0.93	3 (5%)	62,65,65	1.88	10 (16%)
23	CLA	B	612	-	65,73,73	2.09	15 (23%)	76,113,113	2.80	28 (36%)
32	LHG	D	409[A]	-	48,48,48	0.93	2 (4%)	51,54,54	1.02	3 (5%)
23	CLA	d	403	-	65,73,73	2.04	16 (24%)	76,113,113	2.79	29 (38%)
27	GOL	c	527	-	5,5,5	1.13	0	5,5,5	0.92	0
32	LHG	L	101[B]	-	48,48,48	0.92	2 (4%)	51,54,54	1.12	4 (7%)
32	LHG	d	407[A]	-	48,48,48	0.92	2 (4%)	51,54,54	1.01	3 (5%)
26	SQD	X	101	-	42,43,54	1.20	4 (9%)	51,54,65	2.16	13 (25%)
25	BCR	k	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.47	10 (17%)
33	LMG	m	101	-	51,51,55	0.87	2 (3%)	59,59,63	1.37	6 (10%)
35	DGD	H	102	-	63,63,67	0.89	4 (6%)	77,77,81	1.01	7 (9%)
35	DGD	C	519	-	63,63,67	0.86	3 (4%)	77,77,81	1.04	5 (6%)
24	PHO	a	416[A]	-	51,69,69	1.88	8 (15%)	47,99,99	1.99	12 (25%)
27	GOL	O	302	-	5,5,5	0.99	0	5,5,5	0.86	0
27	GOL	c	526[A]	-	5,5,5	1.00	0	5,5,5	0.98	0
23	CLA	a	405[B]	-	65,73,73	2.08	16 (24%)	76,113,113	2.85	32 (42%)
23	CLA	B	607	42	65,73,73	2.02	16 (24%)	76,113,113	2.84	28 (36%)
28	OEX	A	413[A]	42,1,3	0,15,15	-	-	-	-	-
23	CLA	b	610	42	65,73,73	2.05	16 (24%)	76,113,113	2.94	30 (39%)
34	HTG	B	625	-	19,19,19	1.13	2 (10%)	23,24,24	1.45	4 (17%)
26	SQD	A	410[B]	-	53,54,54	0.94	3 (5%)	62,65,65	1.67	11 (17%)
27	GOL	D	403	-	5,5,5	1.50	2 (40%)	5,5,5	0.98	1 (20%)
35	DGD	c	517[B]	-	63,63,67	0.86	2 (3%)	77,77,81	1.09	4 (5%)
34	HTG	c	522	-	19,19,19	0.94	1 (5%)	23,24,24	1.52	2 (8%)
23	CLA	B	606	-	65,73,73	1.95	17 (26%)	76,113,113	2.91	29 (38%)
32	LHG	d	407[B]	-	48,48,48	0.91	2 (4%)	51,54,54	0.96	3 (5%)
33	LMG	z	101	-	39,39,55	1.08	2 (5%)	47,47,63	1.05	2 (4%)
35	DGD	c	518[A]	-	63,63,67	0.85	3 (4%)	77,77,81	0.97	3 (3%)
23	CLA	c	504	-	65,73,73	2.01	16 (24%)	76,113,113	2.82	26 (34%)
23	CLA	a	407[B]	42	65,73,73	2.04	16 (24%)	76,113,113	2.78	29 (38%)
23	CLA	B	611	-	65,73,73	2.74	18 (27%)	76,113,113	3.15	29 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	614	-	65,73,73	2.03	16 (24%)	76,113,113	2.97	32 (42%)
27	GOL	O	303	-	5,5,5	0.91	0	5,5,5	1.09	1 (20%)
24	PHO	a	416[B]	-	51,69,69	1.88	8 (15%)	47,99,99	1.85	11 (23%)
35	DGD	h	102	-	63,63,67	0.88	3 (4%)	77,77,81	1.10	8 (10%)
27	GOL	c	526[B]	-	5,5,5	0.96	0	5,5,5	0.96	0
39	HEM	F	102	6,5	41,50,50	1.29	6 (14%)	45,82,82	2.11	13 (28%)
41	HEC	V	201	16	32,50,50	2.01	4 (12%)	24,82,82	2.13	7 (29%)
26	SQD	b	620	-	53,54,54	1.04	3 (5%)	62,65,65	1.72	13 (20%)
33	LMG	C	501	-	51,51,55	0.92	2 (3%)	59,59,63	1.55	6 (10%)
31	LMT	c	501	-	36,36,36	0.98	0	47,47,47	1.05	2 (4%)

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
23	CLA	B	601	42	1/1/15/20	13/37/115/115	-
29	PL9	d	405[A]	-	-	7/53/73/73	0/1/1/1
27	GOL	b	628	-	-	0/4/4/4	-
29	PL9	D	407[B]	-	-	9/53/73/73	0/1/1/1
23	CLA	C	508	42	1/1/15/20	9/37/115/115	-
23	CLA	B	608	-	-	3/37/115/115	-
23	CLA	A	408	-	1/1/15/20	9/37/115/115	-
31	LMT	M	102	-	-	8/21/61/61	0/2/2/2
23	CLA	c	506	-	1/1/15/20	7/37/115/115	-
34	HTG	b	623	-	-	4/10/30/30	0/1/1/1
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
31	LMT	B	628	-	-	12/21/61/61	0/2/2/2
23	CLA	B	602	-	1/1/15/20	9/37/115/115	-
34	HTG	V	202	-	-	0/2/19/30	0/1/1/1
34	HTG	D	412	-	-	3/7/27/30	0/1/1/1
24	PHO	A	416[A]	-	-	1/37/103/103	0/5/6/6
27	GOL	V	203[B]	-	-	3/4/4/4	-
23	CLA	c	508	42	1/1/15/20	8/37/115/115	-
23	CLA	b	601	42	1/1/15/20	20/37/115/115	-
31	LMT	A	417	-	-	8/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	c	516	-	-	1/29/63/63	0/2/2/2
35	DGD	c	519	-	-	7/51/91/95	0/2/2/2
23	CLA	C	502	-	1/1/15/20	3/37/115/115	-
23	CLA	b	607	42	1/1/15/20	2/37/115/115	-
32	LHG	A	418[B]	-	-	14/53/53/53	-
34	HTG	b	625	-	-	3/10/30/30	0/1/1/1
25	BCR	c	515	-	-	1/29/63/63	0/2/2/2
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
31	LMT	e	101	-	-	15/21/61/61	0/2/2/2
25	BCR	K	103	-	-	2/29/63/63	0/2/2/2
24	PHO	A	407[A]	-	-	3/37/103/103	0/5/6/6
23	CLA	b	606	-	1/1/15/20	13/37/115/115	-
32	LHG	D	409[B]	-	-	14/53/53/53	-
34	HTG	B	623	-	-	2/10/30/30	0/1/1/1
23	CLA	b	605	-	1/1/15/20	7/37/115/115	-
31	LMT	F	101	-	-	8/21/61/61	0/2/2/2
26	SQD	B	620	-	-	13/49/69/69	0/1/1/1
32	LHG	E	101[A]	-	-	22/46/46/53	-
31	LMT	A	419	-	-	16/21/61/61	0/2/2/2
27	GOL	D	414	-	-	3/4/4/4	-
34	HTG	C	522	-	-	1/10/30/30	0/1/1/1
33	LMG	D	413	40	-	8/46/66/70	0/1/1/1
31	LMT	M	101	-	-	5/21/61/61	0/2/2/2
33	LMG	d	411	40	-	10/46/66/70	0/1/1/1
23	CLA	C	510	-	1/1/15/20	5/37/115/115	-
25	BCR	H	101	-	-	2/29/63/63	0/2/2/2
24	PHO	A	407[B]	-	-	2/37/103/103	0/5/6/6
27	GOL	v	202[A]	-	-	2/4/4/4	-
23	CLA	c	502	-	1/1/15/20	4/37/115/115	-
27	GOL	C	523[A]	-	-	0/4/4/4	-
23	CLA	b	604	-	1/1/15/20	9/37/115/115	-
23	CLA	A	405[A]	42	1/1/15/20	3/37/115/115	-
27	GOL	B	629	-	-	4/4/4/4	-
32	LHG	E	101[B]	-	-	20/46/46/53	-
32	LHG	a	420[A]	-	-	16/46/46/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	504	-	-	1/37/115/115	-
35	DGD	c	518[B]	-	-	16/51/91/95	0/2/2/2
25	BCR	K	102	-	-	2/29/63/63	0/2/2/2
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
31	LMT	B	631	-	-	11/17/37/61	0/1/1/2
25	BCR	t	102	-	-	1/29/63/63	0/2/2/2
33	LMG	a	417	-	-	12/46/66/70	0/1/1/1
23	CLA	B	616	-	1/1/15/20	7/37/115/115	-
31	LMT	b	621	-	-	9/17/37/61	0/1/1/2
23	CLA	d	402[A]	-	1/1/15/20	4/37/115/115	-
29	PL9	a	414[A]	-	-	14/53/73/73	0/1/1/1
23	CLA	B	605	-	1/1/15/20	5/37/115/115	-
27	GOL	l	102[A]	-	-	1/4/4/4	-
29	PL9	A	414[A]	-	-	15/53/73/73	0/1/1/1
23	CLA	b	602	-	1/1/15/20	5/37/115/115	-
35	DGD	C	518[A]	-	-	13/51/91/95	0/2/2/2
39	HEM	f	101	6,5	-	6/12/54/54	-
23	CLA	a	406[A]	42	1/1/15/20	8/37/115/115	-
33	LMG	B	621	-	-	14/46/66/70	0/1/1/1
29	PL9	d	405[B]	-	-	7/53/73/73	0/1/1/1
25	BCR	y	101	-	-	5/29/63/63	0/2/2/2
23	CLA	B	604	-	1/1/15/20	3/37/115/115	-
23	CLA	B	615	-	1/1/15/20	8/37/115/115	-
32	LHG	a	420[B]	-	-	16/46/46/53	-
35	DGD	C	517[A]	-	-	14/51/91/95	0/2/2/2
23	CLA	a	409	-	1/1/15/20	9/37/115/115	-
23	CLA	A	406[A]	42	-	5/37/115/115	-
23	CLA	C	503	-	-	10/37/115/115	-
24	PHO	a	408[A]	-	-	6/37/103/103	0/5/6/6
29	PL9	A	414[B]	-	-	12/53/73/73	0/1/1/1
33	LMG	Z	101	-	-	10/31/51/70	0/1/1/1
32	LHG	L	101[A]	-	-	20/53/53/53	-
23	CLA	C	511	-	1/1/15/20	13/37/115/115	-
23	CLA	b	613	-	1/1/15/20	7/37/115/115	-
31	LMT	t	101	-	-	7/17/38/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	DGD	C	518[B]	-	-	13/51/91/95	0/2/2/2
24	PHO	A	416[B]	-	-	1/37/103/103	0/5/6/6
23	CLA	c	510	-	1/1/15/20	13/37/115/115	-
23	CLA	b	614	-	1/1/15/20	15/37/115/115	-
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
34	HTG	B	622	-	-	3/10/30/30	0/1/1/1
26	SQD	A	412	-	-	13/49/69/69	0/1/1/1
23	CLA	c	512	3	1/1/15/20	8/37/115/115	-
27	GOL	o	303	-	-	2/4/4/4	-
23	CLA	b	603	-	1/1/15/20	4/37/115/115	-
23	CLA	b	615	-	1/1/15/20	8/37/115/115	-
23	CLA	c	514	-	1/1/15/20	10/37/115/115	-
24	PHO	a	408[B]	-	-	6/37/103/103	0/5/6/6
23	CLA	c	511	-	1/1/15/20	12/37/115/115	-
35	DGD	c	517[A]	-	-	18/51/91/95	0/2/2/2
23	CLA	b	608	-	-	7/37/115/115	-
23	CLA	C	513	-	1/1/15/20	11/37/115/115	-
23	CLA	c	509	-	1/1/15/20	5/37/115/115	-
23	CLA	D	405	-	1/1/15/20	13/37/115/115	-
25	BCR	b	619	-	-	5/29/63/63	0/2/2/2
32	LHG	b	629[A]	-	-	14/53/53/53	-
25	BCR	d	404	-	-	5/29/63/63	0/2/2/2
31	LMT	b	627	-	-	11/17/37/61	0/1/1/2
27	GOL	A	411	-	-	2/4/4/4	-
23	CLA	D	404[A]	-	1/1/15/20	0/37/115/115	-
23	CLA	c	503	-	1/1/15/20	6/37/115/115	-
25	BCR	D	406	-	-	4/29/63/63	0/2/2/2
27	GOL	b	624	-	-	2/4/4/4	-
23	CLA	a	407[A]	42	-	6/37/115/115	-
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
32	LHG	D	408[A]	-	-	17/53/53/53	-
27	GOL	a	418	-	-	2/4/4/4	-
32	LHG	d	406[A]	-	-	13/53/53/53	-
32	LHG	d	413[A]	-	-	17/53/53/53	-
33	LMG	c	521	-	-	11/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
23	CLA	B	603	-	1/1/15/20	6/37/115/115	-
23	CLA	b	609	-	1/1/15/20	3/37/115/115	-
23	CLA	b	616	-	1/1/15/20	9/37/115/115	-
27	GOL	v	202[B]	-	-	2/4/4/4	-
23	CLA	A	404[A]	-	1/1/15/20	3/37/115/115	-
27	GOL	C	523[B]	-	-	0/4/4/4	-
27	GOL	o	302	-	-	2/4/4/4	-
25	BCR	a	410	-	-	2/29/63/63	0/2/2/2
33	LMG	C	520	-	-	10/46/66/70	0/1/1/1
23	CLA	A	405[B]	42	1/1/15/20	5/37/115/115	-
23	CLA	B	613	-	1/1/15/20	8/37/115/115	-
29	PL9	D	407[A]	-	-	6/53/73/73	0/1/1/1
32	LHG	b	629[B]	-	-	17/53/53/53	-
26	SQD	a	411[A]	-	-	9/49/69/69	0/1/1/1
23	CLA	C	514	-	1/1/15/20	7/37/115/115	-
41	HEC	v	201	16	-	2/10/54/54	-
23	CLA	b	611	-	1/1/15/20	2/37/115/115	-
34	HTG	d	410	-	-	1/7/27/30	0/1/1/1
23	CLA	D	404[B]	-	1/1/15/20	0/37/115/115	-
32	LHG	D	408[B]	-	-	16/53/53/53	-
32	LHG	d	406[B]	-	-	16/53/53/53	-
26	SQD	f	102	-	-	12/38/58/69	0/1/1/1
23	CLA	c	513	-	1/1/15/20	12/37/115/115	-
23	CLA	C	505	42	1/1/15/20	6/37/115/115	-
23	CLA	c	507	-	1/1/15/20	7/37/115/115	-
23	CLA	d	402[B]	-	1/1/15/20	4/37/115/115	-
29	PL9	a	414[B]	-	-	14/53/73/73	0/1/1/1
32	LHG	d	413[B]	-	-	14/53/53/53	-
33	LMG	C	521	-	-	14/46/66/70	0/1/1/1
27	GOL	a	419	-	-	2/4/4/4	-
27	GOL	l	102[B]	-	-	2/4/4/4	-
23	CLA	B	609	-	1/1/15/20	1/37/115/115	-
23	CLA	b	612	-	1/1/15/20	1/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	m	103	-	-	6/21/61/61	0/2/2/2
25	BCR	B	617	-	-	1/29/63/63	0/2/2/2
23	CLA	a	406[B]	42	1/1/15/20	7/37/115/115	-
23	CLA	C	506	-	1/1/15/20	7/37/115/115	-
23	CLA	A	404[B]	-	1/1/15/20	4/37/115/115	-
23	CLA	C	509	-	-	5/37/115/115	-
25	BCR	h	101	-	-	2/29/63/63	0/2/2/2
27	GOL	B	627	-	-	2/4/4/4	-
31	LMT	B	630	-	-	10/21/61/61	0/2/2/2
27	GOL	V	203[A]	-	-	2/4/4/4	-
33	LMG	c	520	-	-	13/46/66/70	0/1/1/1
23	CLA	C	512	3	1/1/15/20	4/37/115/115	-
34	HTG	b	622	-	-	4/10/30/30	0/1/1/1
35	DGD	C	517[B]	-	-	14/51/91/95	0/2/2/2
23	CLA	B	610	42	1/1/15/20	8/37/115/115	-
26	SQD	a	411[B]	-	-	8/49/69/69	0/1/1/1
26	SQD	a	412	-	-	15/49/69/69	0/1/1/1
27	GOL	d	412	-	-	4/4/4/4	-
23	CLA	a	405[A]	-	1/1/15/20	4/37/115/115	-
23	CLA	c	505	42	1/1/15/20	7/37/115/115	-
27	GOL	B	624	-	-	4/4/4/4	-
32	LHG	A	418[A]	-	-	14/53/53/53	-
23	CLA	C	507	-	1/1/15/20	12/37/115/115	-
23	CLA	A	406[B]	42	-	4/37/115/115	-
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
26	SQD	A	410[A]	-	-	12/49/69/69	0/1/1/1
23	CLA	B	612	-	1/1/15/20	7/37/115/115	-
32	LHG	D	409[A]	-	-	14/53/53/53	-
23	CLA	d	403	-	1/1/15/20	7/37/115/115	-
27	GOL	c	527	-	-	3/4/4/4	-
32	LHG	L	101[B]	-	-	17/53/53/53	-
32	LHG	d	407[A]	-	-	13/53/53/53	-
26	SQD	X	101	-	-	13/38/58/69	0/1/1/1
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
33	LMG	m	101	-	-	12/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	DGD	H	102	-	-	11/51/91/95	0/2/2/2
35	DGD	C	519	-	-	20/51/91/95	0/2/2/2
24	PHO	a	416[A]	-	-	1/37/103/103	0/5/6/6
27	GOL	O	302	-	-	2/4/4/4	-
27	GOL	c	526[A]	-	-	0/4/4/4	-
23	CLA	a	405[B]	-	1/1/15/20	3/37/115/115	-
23	CLA	B	607	42	1/1/15/20	2/37/115/115	-
23	CLA	b	610	42	1/1/15/20	9/37/115/115	-
34	HTG	B	625	-	-	4/10/30/30	0/1/1/1
26	SQD	A	410[B]	-	-	10/49/69/69	0/1/1/1
27	GOL	D	403	-	-	2/4/4/4	-
35	DGD	c	517[B]	-	-	16/51/91/95	0/2/2/2
34	HTG	c	522	-	-	2/10/30/30	0/1/1/1
23	CLA	B	606	-	1/1/15/20	7/37/115/115	-
32	LHG	d	407[B]	-	-	10/53/53/53	-
33	LMG	z	101	-	-	9/34/54/70	0/1/1/1
35	DGD	c	518[A]	-	-	16/51/91/95	0/2/2/2
23	CLA	c	504	-	1/1/15/20	2/37/115/115	-
23	CLA	a	407[B]	42	-	5/37/115/115	-
23	CLA	B	611	-	1/1/15/20	2/37/115/115	-
23	CLA	B	614	-	1/1/15/20	14/37/115/115	-
27	GOL	O	303	-	-	2/4/4/4	-
24	PHO	a	416[B]	-	-	2/37/103/103	0/5/6/6
35	DGD	h	102	-	-	14/51/91/95	0/2/2/2
27	GOL	c	526[B]	-	-	0/4/4/4	-
39	HEM	F	102	6,5	-	2/12/54/54	-
41	HEC	V	201	16	-	2/10/54/54	-
26	SQD	b	620	-	-	18/49/69/69	0/1/1/1
33	LMG	C	501	-	-	11/46/66/70	0/1/1/1
31	LMT	c	501	-	-	10/21/61/61	0/2/2/2

All (1550) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	611	CLA	C3B-C2B	11.24	1.56	1.40
23	B	611	CLA	CMB-C2B	7.50	1.67	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	C3B-C2B	7.13	1.50	1.40
23	c	503	CLA	C3B-C2B	6.98	1.50	1.40
23	C	510	CLA	C3B-C2B	6.94	1.50	1.40
23	C	509	CLA	C3B-C2B	6.89	1.49	1.40
23	B	603	CLA	C3B-C2B	6.85	1.49	1.40
23	B	612	CLA	C3B-C2B	6.83	1.49	1.40
23	C	512	CLA	C3B-C2B	6.77	1.49	1.40
23	c	509	CLA	C3B-C2B	6.64	1.49	1.40
24	A	416[B]	PHO	C3B-C2B	6.59	1.49	1.40
23	C	505	CLA	C3B-C2B	6.52	1.49	1.40
23	B	611	CLA	C1D-ND	6.50	1.45	1.37
23	c	512	CLA	C3B-C2B	6.47	1.49	1.40
23	B	608	CLA	C3B-C2B	6.45	1.49	1.40
23	C	514	CLA	C3B-C2B	6.43	1.49	1.40
23	b	612	CLA	C3B-C2B	6.41	1.49	1.40
23	D	404[B]	CLA	C3B-C2B	6.41	1.49	1.40
23	D	404[A]	CLA	C3B-C2B	6.40	1.49	1.40
23	b	601	CLA	C3B-C2B	6.39	1.49	1.40
23	A	408	CLA	C3B-C2B	6.39	1.49	1.40
24	a	408[A]	PHO	C3B-C2B	6.39	1.49	1.40
24	a	416[B]	PHO	C3B-C2B	6.36	1.49	1.40
23	a	405[B]	CLA	C3B-C2B	6.29	1.49	1.40
23	b	611	CLA	C3B-C2B	6.26	1.49	1.40
23	c	507	CLA	C3B-C2B	6.24	1.49	1.40
23	c	510	CLA	C3B-C2B	6.21	1.49	1.40
23	B	601	CLA	C3B-C2B	6.18	1.48	1.40
23	c	505	CLA	C3B-C2B	6.17	1.48	1.40
23	b	603	CLA	C3B-C2B	6.15	1.48	1.40
23	d	402[B]	CLA	C3B-C2B	6.14	1.48	1.40
24	A	407[A]	PHO	C3B-C2B	6.13	1.48	1.40
23	B	613	CLA	C3B-C2B	6.12	1.48	1.40
23	B	602	CLA	C3B-C2B	6.12	1.48	1.40
23	b	613	CLA	C3B-C2B	6.11	1.48	1.40
23	c	511	CLA	C3B-C2B	6.09	1.48	1.40
23	b	608	CLA	C3B-C2B	6.01	1.48	1.40
23	A	404[B]	CLA	C3B-C2B	6.01	1.48	1.40
23	C	511	CLA	C3B-C2B	6.00	1.48	1.40
41	V	201	HEC	C2B-C3B	-5.98	1.34	1.40
23	B	604	CLA	C3B-C2B	5.97	1.48	1.40
23	A	404[A]	CLA	C3B-C2B	5.96	1.48	1.40
23	C	507	CLA	C3B-C2B	5.96	1.48	1.40
24	A	416[A]	PHO	C3B-C2B	5.94	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	408[B]	PHO	C3B-C2B	5.93	1.48	1.40
23	b	605	CLA	C3B-C2B	5.93	1.48	1.40
23	C	508	CLA	C3B-C2B	5.89	1.48	1.40
24	a	416[A]	PHO	C3B-C2B	5.88	1.48	1.40
23	D	405	CLA	C1D-ND	5.87	1.45	1.37
23	a	405[A]	CLA	C3B-C2B	5.86	1.48	1.40
23	b	616	CLA	C3B-C2B	5.86	1.48	1.40
23	c	514	CLA	C3B-C2B	5.86	1.48	1.40
23	B	610	CLA	C3C-C2C	5.80	1.49	1.36
23	C	503	CLA	C3B-C2B	5.79	1.48	1.40
23	C	513	CLA	C3B-C2B	5.78	1.48	1.40
24	A	407[B]	PHO	C3B-C2B	5.77	1.48	1.40
41	v	201	HEC	C2B-C3B	-5.75	1.34	1.40
23	B	607	CLA	C3B-C2B	5.72	1.48	1.40
23	B	611	CLA	CHC-C1C	5.69	1.49	1.35
23	B	614	CLA	C3B-C2B	5.68	1.48	1.40
23	d	402[A]	CLA	C3B-C2B	5.68	1.48	1.40
23	b	606	CLA	C3B-C2B	5.67	1.48	1.40
23	B	605	CLA	C3C-C2C	5.65	1.48	1.36
23	b	604	CLA	C3B-C2B	5.65	1.48	1.40
23	C	504	CLA	C3C-C2C	5.64	1.48	1.36
23	c	509	CLA	O2D-CGD	5.63	1.46	1.33
23	a	405[B]	CLA	C1D-ND	5.59	1.44	1.37
23	a	406[A]	CLA	C3C-C2C	5.58	1.48	1.36
23	c	514	CLA	C1D-ND	5.57	1.44	1.37
23	B	612	CLA	CHC-C1C	5.57	1.49	1.35
23	b	614	CLA	C3B-C2B	5.56	1.48	1.40
23	C	503	CLA	C1D-ND	5.56	1.44	1.37
23	c	509	CLA	C3C-C2C	5.54	1.48	1.36
23	C	506	CLA	CHC-C1C	5.54	1.49	1.35
23	B	606	CLA	C3B-C2B	5.52	1.48	1.40
23	C	513	CLA	C3C-C2C	5.52	1.48	1.36
24	A	416[B]	PHO	C3D-C2D	5.52	1.49	1.39
23	b	607	CLA	C3B-C2B	5.51	1.48	1.40
23	b	610	CLA	C3B-C2B	5.50	1.48	1.40
23	b	610	CLA	C3C-C2C	5.50	1.48	1.36
23	d	402[B]	CLA	C3C-C2C	5.50	1.48	1.36
23	B	611	CLA	C3C-C2C	5.49	1.48	1.36
23	C	511	CLA	C1D-ND	5.49	1.44	1.37
23	c	505	CLA	C1D-ND	5.49	1.44	1.37
23	b	605	CLA	C3C-C2C	5.48	1.48	1.36
23	C	502	CLA	C3B-C2B	5.47	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	513	CLA	CHC-C1C	5.47	1.49	1.35
24	a	416[A]	PHO	C3D-C2D	5.46	1.49	1.39
23	c	504	CLA	C3C-C2C	5.46	1.48	1.36
24	a	408[A]	PHO	C3D-C2D	5.46	1.49	1.39
23	b	612	CLA	C3C-C2C	5.45	1.48	1.36
23	b	606	CLA	C1D-ND	5.44	1.44	1.37
23	c	513	CLA	C3C-C2C	5.44	1.48	1.36
23	a	406[B]	CLA	C3C-C2C	5.44	1.48	1.36
23	c	510	CLA	C1D-ND	5.44	1.44	1.37
23	A	406[B]	CLA	C3C-C2C	5.43	1.48	1.36
23	A	404[B]	CLA	CHC-C1C	5.43	1.48	1.35
23	A	404[A]	CLA	C3C-C2C	5.43	1.48	1.36
23	a	407[B]	CLA	C3B-C2B	5.43	1.47	1.40
23	b	609	CLA	O2D-CGD	5.42	1.46	1.33
23	d	403	CLA	C3C-C2C	5.42	1.48	1.36
23	c	510	CLA	C3C-C2C	5.42	1.48	1.36
23	a	406[A]	CLA	C1D-ND	5.42	1.44	1.37
23	a	407[A]	CLA	C3B-C2B	5.42	1.47	1.40
23	b	601	CLA	C3C-C2C	5.41	1.48	1.36
23	B	613	CLA	CHC-C1C	5.41	1.48	1.35
23	b	602	CLA	CHC-C1C	5.41	1.48	1.35
23	b	609	CLA	C3B-C2B	5.41	1.47	1.40
23	a	409	CLA	C3B-C2B	5.40	1.47	1.40
23	A	408	CLA	C3C-C2C	5.40	1.48	1.36
23	c	513	CLA	C1D-ND	5.40	1.44	1.37
23	B	601	CLA	C3C-C2C	5.40	1.48	1.36
23	d	403	CLA	C1D-ND	5.39	1.44	1.37
23	c	509	CLA	C1D-ND	5.39	1.44	1.37
23	C	504	CLA	C3B-C2B	5.39	1.47	1.40
23	c	504	CLA	CHC-C1C	5.38	1.48	1.35
23	A	406[B]	CLA	C3B-C2B	5.38	1.47	1.40
23	b	613	CLA	C1D-ND	5.38	1.44	1.37
24	a	408[B]	PHO	C3D-C2D	5.37	1.49	1.39
23	B	609	CLA	CHC-C1C	5.37	1.48	1.35
23	b	616	CLA	C3C-C2C	5.37	1.48	1.36
23	C	511	CLA	C3C-C2C	5.37	1.48	1.36
23	A	406[B]	CLA	CHC-C1C	5.37	1.48	1.35
23	b	603	CLA	O2D-CGD	5.37	1.46	1.33
23	A	405[B]	CLA	C3B-C2B	5.36	1.47	1.40
23	c	513	CLA	CHC-C1C	5.36	1.48	1.35
23	c	504	CLA	C1D-ND	5.36	1.44	1.37
23	B	604	CLA	C3C-C2C	5.36	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	505	CLA	CHC-C1C	5.36	1.48	1.35
23	b	610	CLA	CHC-C1C	5.36	1.48	1.35
23	c	502	CLA	C3B-C2B	5.34	1.47	1.40
24	A	416[A]	PHO	C3D-C2D	5.33	1.49	1.39
41	v	201	HEC	C3D-C2D	5.33	1.53	1.37
23	b	602	CLA	C3C-C2C	5.33	1.48	1.36
23	D	405	CLA	C3C-C2C	5.33	1.48	1.36
23	b	605	CLA	C1D-ND	5.33	1.44	1.37
23	a	407[B]	CLA	C3C-C2C	5.32	1.48	1.36
24	a	416[B]	PHO	C3D-C2D	5.32	1.49	1.39
23	C	503	CLA	C3C-C2C	5.32	1.48	1.36
23	B	615	CLA	C1D-ND	5.32	1.44	1.37
23	b	601	CLA	C1D-ND	5.32	1.44	1.37
23	c	506	CLA	CHC-C1C	5.32	1.48	1.35
23	A	404[B]	CLA	C3C-C2C	5.32	1.48	1.36
23	c	506	CLA	C3C-C2C	5.32	1.48	1.36
23	c	503	CLA	C3C-C2C	5.32	1.48	1.36
23	A	404[B]	CLA	C1D-ND	5.31	1.44	1.37
23	C	513	CLA	C1D-ND	5.31	1.44	1.37
23	c	506	CLA	C3B-C2B	5.31	1.47	1.40
23	a	407[A]	CLA	C3C-C2C	5.31	1.48	1.36
23	b	615	CLA	C3C-C2C	5.30	1.48	1.36
23	D	404[A]	CLA	C3C-C2C	5.30	1.48	1.36
23	A	406[A]	CLA	CHC-C1C	5.30	1.48	1.35
24	a	416[A]	PHO	OBD-CAD	5.30	1.29	1.22
23	c	507	CLA	C1D-ND	5.30	1.44	1.37
23	c	511	CLA	C1D-ND	5.30	1.44	1.37
23	D	405	CLA	CHC-C1C	5.29	1.48	1.35
23	d	403	CLA	C3B-C2B	5.29	1.47	1.40
23	c	509	CLA	CHC-C1C	5.29	1.48	1.35
23	b	614	CLA	CHC-C1C	5.29	1.48	1.35
24	A	416[A]	PHO	OBD-CAD	5.28	1.29	1.22
23	B	605	CLA	CHC-C1C	5.28	1.48	1.35
23	b	606	CLA	C3C-C2C	5.28	1.47	1.36
23	B	615	CLA	O2D-CGD	5.27	1.46	1.33
23	D	405	CLA	C3B-C2B	5.27	1.47	1.40
23	D	404[B]	CLA	C3C-C2C	5.27	1.47	1.36
23	c	514	CLA	C3C-C2C	5.27	1.47	1.36
23	C	502	CLA	CHC-C1C	5.26	1.48	1.35
23	d	403	CLA	CHC-C1C	5.26	1.48	1.35
23	B	605	CLA	C1D-ND	5.26	1.44	1.37
23	B	609	CLA	C3B-C2B	5.25	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	406[B]	CLA	C1D-ND	5.25	1.44	1.37
23	b	614	CLA	C3C-C2C	5.25	1.47	1.36
23	c	512	CLA	CHC-C1C	5.25	1.48	1.35
23	C	503	CLA	O2D-CGD	5.24	1.46	1.33
23	C	514	CLA	C1D-ND	5.24	1.44	1.37
23	c	512	CLA	C1D-ND	5.24	1.44	1.37
24	a	408[A]	PHO	O2D-CGD	5.24	1.46	1.33
23	c	507	CLA	O2D-CGD	5.23	1.46	1.33
23	B	605	CLA	O2D-CGD	5.23	1.46	1.33
23	a	406[B]	CLA	C3B-C2B	5.22	1.47	1.40
23	c	514	CLA	O2D-CGD	5.22	1.45	1.33
23	b	615	CLA	C3B-C2B	5.22	1.47	1.40
23	a	405[B]	CLA	CHC-C1C	5.21	1.48	1.35
23	B	601	CLA	C1D-ND	5.21	1.44	1.37
23	A	405[B]	CLA	C3C-C2C	5.20	1.47	1.36
23	B	607	CLA	C3C-C2C	5.20	1.47	1.36
23	B	612	CLA	C3C-C2C	5.20	1.47	1.36
23	B	616	CLA	C3C-C2C	5.19	1.47	1.36
23	C	509	CLA	C1D-ND	5.19	1.44	1.37
23	c	510	CLA	O2D-CGD	5.18	1.45	1.33
23	a	409	CLA	CHC-C1C	5.18	1.48	1.35
23	b	603	CLA	C3C-C2C	5.18	1.47	1.36
23	B	603	CLA	C3C-C2C	5.17	1.47	1.36
23	c	512	CLA	C3C-C2C	5.17	1.47	1.36
23	C	507	CLA	O2D-CGD	5.17	1.45	1.33
23	b	604	CLA	C3C-C2C	5.16	1.47	1.36
23	B	615	CLA	CHC-C1C	5.16	1.48	1.35
23	a	405[B]	CLA	C3C-C2C	5.16	1.47	1.36
23	A	406[B]	CLA	O2D-CGD	5.15	1.45	1.33
23	C	510	CLA	C3C-C2C	5.15	1.47	1.36
23	A	405[A]	CLA	O2D-CGD	5.14	1.45	1.33
23	C	511	CLA	CHC-C1C	5.14	1.48	1.35
23	A	406[A]	CLA	C3C-C2C	5.13	1.47	1.36
23	A	405[B]	CLA	CHC-C1C	5.13	1.48	1.35
23	C	509	CLA	C3C-C2C	5.13	1.47	1.36
23	B	601	CLA	CHC-C1C	5.13	1.48	1.35
23	a	405[A]	CLA	C1D-ND	5.13	1.44	1.37
23	B	609	CLA	O2D-CGD	5.13	1.45	1.33
23	A	404[A]	CLA	C1D-ND	5.13	1.44	1.37
23	b	616	CLA	C1D-ND	5.12	1.44	1.37
41	V	201	HEC	C3C-C2C	-5.12	1.35	1.40
23	c	505	CLA	O2D-CGD	5.12	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	408[B]	PHO	O2D-CGD	5.12	1.45	1.33
23	b	613	CLA	CHC-C1C	5.11	1.48	1.35
23	c	502	CLA	C3C-C2C	5.11	1.47	1.36
23	B	609	CLA	C3C-C2C	5.11	1.47	1.36
23	b	607	CLA	C3C-C2C	5.09	1.47	1.36
24	a	416[B]	PHO	OBD-CAD	5.09	1.29	1.22
23	c	502	CLA	C1D-ND	5.09	1.44	1.37
23	d	402[A]	CLA	C3C-C2C	5.09	1.47	1.36
23	a	406[B]	CLA	CHC-C1C	5.09	1.48	1.35
23	b	616	CLA	CHC-C1C	5.09	1.48	1.35
24	A	407[B]	PHO	C3D-C2D	5.08	1.48	1.39
23	B	614	CLA	C1D-ND	5.08	1.44	1.37
23	a	407[B]	CLA	CHC-C1C	5.08	1.48	1.35
23	c	508	CLA	CHC-C1C	5.08	1.48	1.35
23	b	601	CLA	CHC-C1C	5.08	1.48	1.35
23	C	506	CLA	C3C-C2C	5.07	1.47	1.36
23	C	506	CLA	C3B-C2B	5.07	1.47	1.40
23	A	405[B]	CLA	O2D-CGD	5.06	1.45	1.33
23	c	508	CLA	C3C-C2C	5.06	1.47	1.36
23	C	512	CLA	O2D-CGD	5.06	1.45	1.33
23	a	405[A]	CLA	CHC-C1C	5.06	1.47	1.35
23	b	608	CLA	C3C-C2C	5.06	1.47	1.36
23	C	512	CLA	CHC-C1C	5.06	1.47	1.35
23	C	502	CLA	C3C-C2C	5.06	1.47	1.36
23	b	602	CLA	C3B-C2B	5.05	1.47	1.40
23	b	604	CLA	CHC-C1C	5.04	1.47	1.35
23	C	508	CLA	C3C-C2C	5.04	1.47	1.36
23	b	615	CLA	CHC-C1C	5.04	1.47	1.35
23	C	514	CLA	CHC-C1C	5.04	1.47	1.35
23	A	405[A]	CLA	CHC-C1C	5.04	1.47	1.35
23	a	407[A]	CLA	CHC-C1C	5.04	1.47	1.35
23	A	404[B]	CLA	O2D-CGD	5.03	1.45	1.33
23	C	512	CLA	C3C-C2C	5.03	1.47	1.36
23	B	606	CLA	CHC-C1C	5.02	1.47	1.35
23	a	407[B]	CLA	O2D-CGD	5.02	1.45	1.33
23	a	405[A]	CLA	C3C-C2C	5.02	1.47	1.36
23	A	406[B]	CLA	C1D-ND	5.02	1.44	1.37
23	c	513	CLA	C3B-C2B	5.02	1.47	1.40
24	a	416[B]	PHO	O2D-CGD	5.02	1.45	1.33
23	B	606	CLA	C3C-C2C	5.02	1.47	1.36
23	C	505	CLA	C3C-C2C	5.01	1.47	1.36
23	b	613	CLA	C3C-C2C	5.01	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	504	CLA	CHC-C1C	5.01	1.47	1.35
23	B	610	CLA	CHC-C1C	5.01	1.47	1.35
25	k	101	BCR	C23-C22	-5.01	1.35	1.45
23	C	509	CLA	CHC-C1C	5.01	1.47	1.35
24	A	416[B]	PHO	O2D-CGD	5.01	1.45	1.33
23	C	508	CLA	CHC-C1C	5.01	1.47	1.35
23	b	611	CLA	CHC-C1C	5.00	1.47	1.35
23	b	602	CLA	O2D-CGD	5.00	1.45	1.33
23	c	511	CLA	C3C-C2C	5.00	1.47	1.36
23	b	606	CLA	CHC-C1C	4.98	1.47	1.35
23	D	404[A]	CLA	CHC-C1C	4.98	1.47	1.35
23	C	514	CLA	C3C-C2C	4.98	1.47	1.36
41	V	201	HEC	C3D-C2D	4.98	1.52	1.37
23	B	603	CLA	C1D-ND	4.98	1.43	1.37
23	B	613	CLA	O2D-CGD	4.98	1.45	1.33
23	B	611	CLA	O2D-CGD	4.97	1.45	1.33
23	c	514	CLA	CHC-C1C	4.97	1.47	1.35
23	B	601	CLA	O2A-CGA	4.97	1.47	1.33
23	B	616	CLA	CHC-C1C	4.96	1.47	1.35
23	b	615	CLA	O2D-CGD	4.96	1.45	1.33
23	A	405[A]	CLA	C3C-C2C	4.96	1.47	1.36
23	A	408	CLA	O2D-CGD	4.96	1.45	1.33
23	C	507	CLA	C3C-C2C	4.95	1.47	1.36
23	B	613	CLA	C3C-C2C	4.95	1.47	1.36
23	a	406[A]	CLA	O2D-CGD	4.95	1.45	1.33
24	A	416[A]	PHO	O2D-CGD	4.95	1.45	1.33
23	b	607	CLA	CHC-C1C	4.95	1.47	1.35
23	c	507	CLA	C3C-C2C	4.94	1.47	1.36
23	B	604	CLA	CHC-C1C	4.94	1.47	1.35
23	B	602	CLA	C1D-ND	4.94	1.43	1.37
23	B	607	CLA	CHC-C1C	4.94	1.47	1.35
23	c	508	CLA	C3B-C2B	4.94	1.47	1.40
23	A	404[A]	CLA	CHC-C1C	4.93	1.47	1.35
24	A	416[B]	PHO	OBD-CAD	4.93	1.29	1.22
25	B	617	BCR	C23-C22	-4.93	1.35	1.45
23	b	609	CLA	C3C-C2C	4.93	1.47	1.36
23	A	405[A]	CLA	C3B-C2B	4.92	1.47	1.40
23	D	404[B]	CLA	O2D-CGD	4.92	1.45	1.33
23	b	616	CLA	O2D-CGD	4.91	1.45	1.33
23	b	610	CLA	C1D-ND	4.91	1.43	1.37
23	B	610	CLA	C3B-C2B	4.91	1.47	1.40
23	c	503	CLA	C1D-ND	4.91	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	610	CLA	O2D-CGD	4.91	1.45	1.33
23	c	505	CLA	C3C-C2C	4.91	1.47	1.36
23	A	405[B]	CLA	C1D-ND	4.91	1.43	1.37
24	A	407[A]	PHO	O2D-CGD	4.91	1.45	1.33
23	D	405	CLA	O2D-CGD	4.91	1.45	1.33
23	C	509	CLA	O2D-CGD	4.91	1.45	1.33
23	a	406[A]	CLA	CHC-C1C	4.90	1.47	1.35
23	B	602	CLA	CHC-C1C	4.90	1.47	1.35
23	B	608	CLA	C3C-C2C	4.90	1.47	1.36
23	B	602	CLA	C3C-C2C	4.90	1.47	1.36
23	c	502	CLA	CHC-C1C	4.90	1.47	1.35
23	b	611	CLA	O2D-CGD	4.89	1.45	1.33
23	d	402[B]	CLA	O2D-CGD	4.89	1.45	1.33
23	d	402[B]	CLA	CHC-C1C	4.89	1.47	1.35
23	C	503	CLA	CHC-C1C	4.88	1.47	1.35
23	c	508	CLA	O2D-CGD	4.88	1.45	1.33
23	c	511	CLA	O2D-CGD	4.88	1.45	1.33
23	B	605	CLA	C3B-C2B	4.88	1.47	1.40
23	D	404[A]	CLA	O2D-CGD	4.88	1.45	1.33
23	B	601	CLA	O2D-CGD	4.88	1.45	1.33
24	A	407[B]	PHO	O2D-CGD	4.87	1.45	1.33
23	C	511	CLA	O2D-CGD	4.87	1.45	1.33
23	c	512	CLA	O2D-CGD	4.86	1.45	1.33
23	b	611	CLA	C3C-C2C	4.86	1.47	1.36
23	b	609	CLA	CHC-C1C	4.86	1.47	1.35
25	a	410	BCR	C23-C22	-4.85	1.35	1.45
23	b	603	CLA	CHC-C1C	4.85	1.47	1.35
23	B	615	CLA	C3B-C2B	4.85	1.47	1.40
23	B	614	CLA	CHC-C1C	4.85	1.47	1.35
23	a	405[B]	CLA	O2D-CGD	4.84	1.45	1.33
24	a	416[A]	PHO	O2D-CGD	4.84	1.45	1.33
23	C	504	CLA	C1D-ND	4.84	1.43	1.37
23	C	507	CLA	CHC-C1C	4.84	1.47	1.35
23	b	604	CLA	C1D-ND	4.84	1.43	1.37
23	b	601	CLA	O2A-CGA	4.84	1.47	1.33
23	B	603	CLA	CHC-C1C	4.84	1.47	1.35
23	a	409	CLA	C3C-C2C	4.84	1.47	1.36
23	D	404[B]	CLA	CHC-C1C	4.83	1.47	1.35
23	B	614	CLA	C3C-C2C	4.83	1.47	1.36
23	a	406[B]	CLA	O2D-CGD	4.82	1.45	1.33
23	B	604	CLA	O2D-CGD	4.82	1.45	1.33
23	D	404[B]	CLA	C1D-ND	4.82	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	515	BCR	C23-C22	-4.82	1.35	1.45
23	B	613	CLA	C1D-ND	4.82	1.43	1.37
25	b	619	BCR	C23-C22	-4.81	1.35	1.45
25	d	404	BCR	C23-C22	-4.81	1.35	1.45
23	B	603	CLA	O2D-CGD	4.81	1.44	1.33
23	c	503	CLA	O2D-CGD	4.81	1.44	1.33
23	c	505	CLA	CHC-C1C	4.81	1.47	1.35
23	b	608	CLA	CHC-C1C	4.80	1.47	1.35
24	A	407[A]	PHO	C3D-C2D	4.79	1.48	1.39
23	C	510	CLA	C1D-ND	4.78	1.43	1.37
26	X	101	SQD	O47-C7	4.78	1.47	1.34
23	c	511	CLA	CHC-C1C	4.78	1.47	1.35
23	c	507	CLA	CHC-C1C	4.77	1.47	1.35
23	A	404[A]	CLA	O2D-CGD	4.77	1.44	1.33
25	K	102	BCR	C23-C22	-4.77	1.35	1.45
25	B	619	BCR	C23-C22	-4.77	1.35	1.45
23	b	602	CLA	CHD-C1D	4.76	1.47	1.38
23	B	615	CLA	C3C-C2C	4.76	1.46	1.36
23	B	602	CLA	O2D-CGD	4.76	1.44	1.33
23	b	612	CLA	CHC-C1C	4.76	1.47	1.35
23	C	514	CLA	O2D-CGD	4.76	1.44	1.33
23	c	508	CLA	C1D-ND	4.75	1.43	1.37
23	b	605	CLA	O2D-CGD	4.75	1.44	1.33
23	B	609	CLA	CHD-C1D	4.75	1.47	1.38
23	C	502	CLA	C1D-ND	4.75	1.43	1.37
23	a	407[B]	CLA	C1D-ND	4.74	1.43	1.37
23	A	406[A]	CLA	O2D-CGD	4.73	1.44	1.33
26	f	102	SQD	O47-C7	4.72	1.47	1.34
23	d	402[A]	CLA	CHC-C1C	4.72	1.47	1.35
33	c	521	LMG	O7-C10	4.72	1.47	1.34
23	c	506	CLA	O2D-CGD	4.71	1.44	1.33
23	B	604	CLA	C1D-ND	4.71	1.43	1.37
23	C	510	CLA	O2D-CGD	4.71	1.44	1.33
25	t	102	BCR	C23-C22	-4.69	1.35	1.45
23	b	613	CLA	O2D-CGD	4.67	1.44	1.33
23	C	506	CLA	O2D-CGD	4.67	1.44	1.33
23	B	610	CLA	O2D-CGD	4.66	1.44	1.33
23	c	504	CLA	C3B-C2B	4.65	1.46	1.40
23	a	407[A]	CLA	O2D-CGD	4.65	1.44	1.33
33	C	521	LMG	O7-C10	4.64	1.47	1.34
23	c	513	CLA	O2D-CGD	4.64	1.44	1.33
26	A	412	SQD	O48-C23	4.64	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	604	CLA	O2D-CGD	4.63	1.44	1.33
23	b	608	CLA	O2D-CGD	4.63	1.44	1.33
41	v	201	HEC	C3C-C2C	-4.63	1.35	1.40
23	C	507	CLA	C1D-ND	4.63	1.43	1.37
33	C	521	LMG	O8-C28	4.62	1.46	1.33
25	D	406	BCR	C23-C22	-4.62	1.36	1.45
23	B	616	CLA	O2D-CGD	4.62	1.44	1.33
23	C	505	CLA	O2D-CGD	4.62	1.44	1.33
23	c	510	CLA	CHC-C1C	4.62	1.46	1.35
23	B	606	CLA	C1D-ND	4.61	1.43	1.37
25	C	516	BCR	C23-C22	-4.61	1.36	1.45
23	b	601	CLA	O2D-CGD	4.60	1.44	1.33
23	A	408	CLA	C1D-ND	4.59	1.43	1.37
23	b	605	CLA	CHC-C1C	4.59	1.46	1.35
23	d	402[A]	CLA	O2D-CGD	4.59	1.44	1.33
23	a	406[A]	CLA	C3B-C2B	4.58	1.46	1.40
23	B	610	CLA	C1D-ND	4.58	1.43	1.37
23	B	609	CLA	C1D-ND	4.58	1.43	1.37
25	A	409	BCR	C23-C22	-4.57	1.36	1.45
32	E	101[A]	LHG	O8-C23	4.57	1.46	1.33
23	A	408	CLA	CHC-C1C	4.57	1.46	1.35
23	B	616	CLA	C1D-ND	4.57	1.43	1.37
23	B	614	CLA	O2D-CGD	4.57	1.44	1.33
26	a	412	SQD	O48-C23	4.56	1.46	1.33
26	B	620	SQD	O47-C7	4.56	1.47	1.34
23	B	607	CLA	O2D-CGD	4.55	1.44	1.33
23	A	405[B]	CLA	CHD-C1D	4.55	1.47	1.38
23	C	507	CLA	CHD-C1D	4.55	1.47	1.38
23	A	405[A]	CLA	C1D-ND	4.55	1.43	1.37
23	C	506	CLA	CHD-C1D	4.55	1.47	1.38
23	b	612	CLA	O2D-CGD	4.54	1.44	1.33
23	B	615	CLA	CHD-C1D	4.54	1.47	1.38
23	b	607	CLA	C1D-ND	4.53	1.43	1.37
23	B	608	CLA	CHC-C1C	4.53	1.46	1.35
23	B	606	CLA	O2D-CGD	4.52	1.44	1.33
32	E	101[B]	LHG	O8-C23	4.51	1.46	1.33
23	C	502	CLA	CHD-C1D	4.50	1.47	1.38
32	a	420[A]	LHG	O8-C23	4.50	1.46	1.33
25	c	516	BCR	C23-C22	-4.50	1.36	1.45
23	d	403	CLA	O2D-CGD	4.49	1.44	1.33
25	c	515	BCR	C23-C22	-4.49	1.36	1.45
23	A	406[B]	CLA	CHD-C1D	4.49	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	406[A]	CLA	C3B-C2B	4.48	1.46	1.40
23	a	407[A]	CLA	C1D-ND	4.48	1.43	1.37
23	b	614	CLA	O2D-CGD	4.48	1.44	1.33
23	C	510	CLA	CHC-C1C	4.47	1.46	1.35
24	A	407[B]	PHO	OBD-CAD	4.47	1.28	1.22
23	c	514	CLA	O2A-CGA	4.46	1.46	1.33
23	C	513	CLA	CHD-C1D	4.46	1.47	1.38
25	b	617	BCR	C23-C22	-4.46	1.36	1.45
23	c	514	CLA	CHD-C1D	4.45	1.47	1.38
23	C	513	CLA	O2D-CGD	4.44	1.44	1.33
23	D	404[B]	CLA	CHD-C1D	4.44	1.47	1.38
23	c	503	CLA	CHC-C1C	4.44	1.46	1.35
33	z	101	LMG	O8-C28	4.43	1.46	1.33
23	b	606	CLA	O2D-CGD	4.42	1.44	1.33
25	y	101	BCR	C23-C22	-4.41	1.36	1.45
23	b	609	CLA	C1D-ND	4.40	1.43	1.37
23	C	508	CLA	O2D-CGD	4.39	1.43	1.33
23	b	609	CLA	CHD-C1D	4.39	1.46	1.38
23	c	504	CLA	CHD-C1D	4.39	1.46	1.38
23	b	611	CLA	C1D-ND	4.39	1.43	1.37
23	a	405[A]	CLA	O2D-CGD	4.38	1.43	1.33
25	K	103	BCR	C23-C22	-4.38	1.36	1.45
32	a	420[B]	LHG	O8-C23	4.37	1.46	1.33
23	C	510	CLA	CHD-C1D	4.37	1.46	1.38
23	a	409	CLA	O2D-CGD	4.37	1.43	1.33
23	b	603	CLA	C1D-ND	4.36	1.43	1.37
26	b	620	SQD	O48-C23	4.36	1.46	1.33
23	C	506	CLA	C1D-ND	4.36	1.43	1.37
23	c	502	CLA	CHD-C1D	4.36	1.46	1.38
23	d	402[B]	CLA	C1D-ND	4.35	1.43	1.37
26	b	620	SQD	O47-C7	4.35	1.46	1.34
26	f	102	SQD	O48-C23	4.34	1.46	1.33
25	h	101	BCR	C23-C22	-4.34	1.36	1.45
23	C	503	CLA	CHD-C1D	4.34	1.46	1.38
23	b	604	CLA	CHD-C1D	4.34	1.46	1.38
23	c	508	CLA	O2A-CGA	4.33	1.46	1.33
23	b	614	CLA	C1D-ND	4.33	1.43	1.37
24	A	416[A]	PHO	CHA-CBD	-4.32	1.47	1.52
23	c	513	CLA	CHD-C1D	4.32	1.46	1.38
23	c	513	CLA	O2A-CGA	4.32	1.46	1.33
25	H	101	BCR	C23-C22	-4.32	1.36	1.45
23	B	615	CLA	O2A-CGA	4.32	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	612	CLA	CHD-C1D	4.32	1.46	1.38
23	b	612	CLA	C1D-ND	4.32	1.43	1.37
23	d	403	CLA	CHD-C1D	4.31	1.46	1.38
23	a	406[A]	CLA	C3D-C2D	4.30	1.50	1.39
25	b	618	BCR	C23-C22	-4.30	1.36	1.45
33	C	520	LMG	O8-C28	4.30	1.45	1.33
23	C	509	CLA	O2A-CGA	4.30	1.45	1.33
23	a	407[B]	CLA	O2A-CGA	4.30	1.45	1.33
23	C	514	CLA	O2A-CGA	4.30	1.45	1.33
23	b	602	CLA	C1D-ND	4.30	1.43	1.37
33	B	621	LMG	O8-C28	4.29	1.45	1.33
23	C	508	CLA	C1D-ND	4.29	1.43	1.37
32	a	420[A]	LHG	O7-C7	4.28	1.46	1.34
23	D	404[B]	CLA	O2A-CGA	4.28	1.45	1.33
23	C	512	CLA	C1D-ND	4.28	1.43	1.37
23	B	604	CLA	CHD-C1D	4.28	1.46	1.38
26	B	620	SQD	O48-C23	4.28	1.45	1.33
23	B	611	CLA	C1C-C2C	4.27	1.52	1.44
23	C	505	CLA	C1D-ND	4.27	1.43	1.37
23	d	403	CLA	C3D-C2D	4.27	1.50	1.39
23	C	514	CLA	CHD-C1D	4.27	1.46	1.38
23	d	402[B]	CLA	O2A-CGA	4.26	1.45	1.33
23	b	607	CLA	CHD-C1D	4.26	1.46	1.38
23	b	601	CLA	CHD-C1D	4.26	1.46	1.38
23	b	602	CLA	CHD-C4C	4.25	1.48	1.39
23	B	614	CLA	C4B-NB	-4.25	1.31	1.35
24	a	408[B]	PHO	OBD-CAD	4.25	1.28	1.22
23	D	404[A]	CLA	C1D-ND	4.25	1.43	1.37
23	A	408	CLA	CHD-C4C	4.25	1.48	1.39
23	B	602	CLA	CHD-C1D	4.24	1.46	1.38
23	b	607	CLA	O2D-CGD	4.24	1.43	1.33
23	A	408	CLA	O2A-CGA	4.24	1.45	1.33
23	B	610	CLA	C3D-C2D	4.24	1.50	1.39
23	A	406[B]	CLA	C3D-C2D	4.24	1.50	1.39
23	a	406[B]	CLA	O2A-CGA	4.24	1.45	1.33
23	B	612	CLA	O2D-CGD	4.23	1.43	1.33
23	c	504	CLA	O2A-CGA	4.23	1.45	1.33
23	c	512	CLA	O2A-CGA	4.22	1.45	1.33
32	a	420[B]	LHG	O7-C7	4.22	1.46	1.34
23	a	407[B]	CLA	CHD-C1D	4.22	1.46	1.38
32	E	101[A]	LHG	O7-C7	4.22	1.46	1.34
23	C	513	CLA	O2A-CGA	4.21	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	508	CLA	CHD-C1D	4.21	1.46	1.38
23	a	409	CLA	O2A-CGA	4.21	1.45	1.33
33	m	101	LMG	O8-C28	4.21	1.45	1.33
35	c	519	DGD	O1G-C1A	4.21	1.45	1.33
25	T	101	BCR	C23-C22	-4.21	1.36	1.45
23	a	405[B]	CLA	CHD-C4C	4.20	1.48	1.39
23	c	503	CLA	C3D-C2D	4.20	1.50	1.39
23	b	608	CLA	C3D-C2D	4.20	1.50	1.39
23	a	405[B]	CLA	CHD-C1D	4.20	1.46	1.38
32	d	407[A]	LHG	O8-C23	4.19	1.45	1.33
23	b	610	CLA	CHD-C1D	4.19	1.46	1.38
23	D	404[A]	CLA	CHD-C1D	4.19	1.46	1.38
23	b	615	CLA	O2A-CGA	4.18	1.45	1.33
23	D	404[A]	CLA	O2A-CGA	4.18	1.45	1.33
23	b	616	CLA	O2A-CGA	4.18	1.45	1.33
23	b	611	CLA	O2A-CGA	4.18	1.45	1.33
23	D	405	CLA	CHD-C1D	4.18	1.46	1.38
35	c	518[B]	DGD	O1G-C1A	4.17	1.45	1.33
23	B	608	CLA	C3D-C2D	4.17	1.50	1.39
23	A	406[B]	CLA	CHD-C4C	4.17	1.48	1.39
23	c	507	CLA	O2A-CGA	4.16	1.45	1.33
33	c	521	LMG	O8-C28	4.16	1.45	1.33
23	d	403	CLA	O2A-CGA	4.16	1.45	1.33
23	b	616	CLA	CHD-C1D	4.16	1.46	1.38
32	E	101[B]	LHG	O7-C7	4.16	1.46	1.34
23	C	512	CLA	CHD-C1D	4.16	1.46	1.38
23	C	508	CLA	O2A-CGA	4.16	1.45	1.33
23	C	509	CLA	C3D-C2D	4.15	1.50	1.39
23	C	512	CLA	O2A-CGA	4.15	1.45	1.33
23	C	504	CLA	O2D-CGD	4.14	1.43	1.33
23	c	505	CLA	CHD-C1D	4.14	1.46	1.38
23	D	404[B]	CLA	CHD-C4C	4.14	1.48	1.39
33	d	411	LMG	O7-C10	4.14	1.46	1.34
23	c	512	CLA	CHD-C1D	4.13	1.46	1.38
23	c	511	CLA	C3D-C2D	4.13	1.50	1.39
23	C	503	CLA	C3D-C2D	4.13	1.50	1.39
35	C	517[A]	DGD	O2G-C1B	4.13	1.46	1.34
24	A	407[A]	PHO	OBD-CAD	4.13	1.28	1.22
23	A	405[B]	CLA	O2A-CGA	4.13	1.45	1.33
23	b	610	CLA	CHD-C4C	4.13	1.48	1.39
26	A	412	SQD	O47-C7	4.13	1.45	1.34
23	a	406[A]	CLA	O2A-CGA	4.12	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	502	CLA	CHD-C4C	4.12	1.48	1.39
23	a	405[A]	CLA	CHD-C1D	4.11	1.46	1.38
23	c	514	CLA	CHD-C4C	4.11	1.48	1.39
23	d	402[B]	CLA	CHD-C1D	4.11	1.46	1.38
32	d	407[B]	LHG	O8-C23	4.11	1.45	1.33
23	c	509	CLA	C3D-C2D	4.11	1.50	1.39
32	L	101[B]	LHG	O8-C23	4.11	1.45	1.33
23	A	406[A]	CLA	CHD-C1D	4.10	1.46	1.38
33	Z	101	LMG	O7-C10	4.10	1.45	1.34
23	A	405[A]	CLA	C3D-C2D	4.10	1.50	1.39
23	a	405[A]	CLA	CHD-C4C	4.10	1.48	1.39
23	c	508	CLA	CHD-C4C	4.10	1.48	1.39
23	b	606	CLA	CHD-C1D	4.10	1.46	1.38
23	C	506	CLA	CHD-C4C	4.10	1.48	1.39
23	C	511	CLA	CHD-C4C	4.09	1.48	1.39
24	a	416[B]	PHO	O2A-CGA	4.09	1.45	1.33
26	a	412	SQD	O47-C7	4.09	1.45	1.34
33	c	520	LMG	O7-C10	4.09	1.45	1.34
23	B	604	CLA	CHD-C4C	4.09	1.48	1.39
23	A	406[A]	CLA	C1D-ND	4.09	1.42	1.37
23	A	408	CLA	CHD-C1D	4.09	1.46	1.38
23	B	608	CLA	C1D-ND	4.08	1.42	1.37
23	b	601	CLA	C3D-C2D	4.08	1.50	1.39
32	D	409[B]	LHG	O7-C7	4.08	1.45	1.34
23	c	507	CLA	CHD-C1D	4.08	1.46	1.38
23	c	513	CLA	C3D-C2D	4.08	1.50	1.39
23	c	509	CLA	CHD-C1D	4.08	1.46	1.38
23	C	507	CLA	O2A-CGA	4.08	1.45	1.33
23	b	608	CLA	CHD-C1D	4.07	1.46	1.38
23	A	405[A]	CLA	O2A-CGA	4.07	1.45	1.33
33	C	520	LMG	O7-C10	4.07	1.45	1.34
23	c	506	CLA	C1D-ND	4.07	1.42	1.37
23	c	504	CLA	O2D-CGD	4.07	1.43	1.33
35	C	519	DGD	O1G-C1A	4.06	1.45	1.33
23	B	611	CLA	C1B-NB	4.06	1.38	1.35
32	D	409[B]	LHG	O8-C23	4.06	1.45	1.33
33	c	520	LMG	O8-C28	4.06	1.45	1.33
23	b	615	CLA	CHD-C1D	4.06	1.46	1.38
23	B	601	CLA	CHD-C1D	4.05	1.46	1.38
26	a	411[A]	SQD	O47-C7	4.05	1.45	1.34
23	C	509	CLA	CHD-C1D	4.05	1.46	1.38
23	c	509	CLA	O2A-CGA	4.04	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	d	406[B]	LHG	O7-C7	4.04	1.45	1.34
23	C	507	CLA	CHD-C4C	4.04	1.48	1.39
33	C	501	LMG	O8-C28	4.04	1.45	1.33
23	B	609	CLA	O2A-CGA	4.04	1.45	1.33
23	c	505	CLA	C3D-C2D	4.03	1.50	1.39
23	B	609	CLA	C3D-C2D	4.03	1.50	1.39
23	c	504	CLA	CHD-C4C	4.02	1.48	1.39
33	a	417	LMG	O8-C28	4.02	1.45	1.33
23	b	605	CLA	CHD-C4C	4.02	1.48	1.39
35	C	518[B]	DGD	O1G-C1A	4.02	1.45	1.33
24	A	416[A]	PHO	O2A-CGA	4.02	1.45	1.33
35	c	517[B]	DGD	O2G-C1B	4.01	1.45	1.34
23	b	601	CLA	CHD-C4C	4.01	1.48	1.39
23	b	610	CLA	OBD-CAD	4.00	1.29	1.22
35	c	518[A]	DGD	O1G-C1A	4.00	1.45	1.33
26	X	101	SQD	O48-C23	4.00	1.45	1.33
23	b	608	CLA	O2A-CGA	4.00	1.45	1.33
23	B	611	CLA	CHD-C1D	4.00	1.46	1.38
23	A	404[B]	CLA	CHD-C1D	4.00	1.46	1.38
23	a	407[B]	CLA	C3D-C2D	3.99	1.50	1.39
23	C	504	CLA	CHD-C1D	3.99	1.46	1.38
33	z	101	LMG	O7-C10	3.99	1.45	1.34
26	a	411[B]	SQD	O48-C23	3.99	1.45	1.33
23	B	609	CLA	CHD-C4C	3.99	1.48	1.39
35	C	518[B]	DGD	O2G-C1B	3.99	1.45	1.34
33	C	501	LMG	O7-C10	3.98	1.45	1.34
23	C	514	CLA	CHD-C4C	3.98	1.48	1.39
23	D	405	CLA	C3D-C2D	3.98	1.50	1.39
33	a	417	LMG	O7-C10	3.98	1.45	1.34
35	c	518[B]	DGD	O2G-C1B	3.98	1.45	1.34
23	C	503	CLA	O2A-CGA	3.98	1.45	1.33
23	A	406[B]	CLA	O2A-CGA	3.98	1.45	1.33
23	C	511	CLA	O2A-CGA	3.97	1.45	1.33
23	A	405[B]	CLA	CHD-C4C	3.97	1.48	1.39
23	A	405[A]	CLA	CHD-C1D	3.97	1.46	1.38
26	a	411[A]	SQD	O48-C23	3.97	1.44	1.33
23	c	506	CLA	CHD-C4C	3.97	1.48	1.39
23	b	604	CLA	CHD-C4C	3.97	1.48	1.39
23	a	406[B]	CLA	C3D-C2D	3.97	1.50	1.39
23	A	404[B]	CLA	CHD-C4C	3.97	1.48	1.39
23	C	510	CLA	OBD-CAD	3.96	1.29	1.22
32	A	418[B]	LHG	O8-C23	3.96	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	407[A]	CLA	O2A-CGA	3.96	1.44	1.33
23	a	407[A]	CLA	C3D-C2D	3.96	1.49	1.39
24	A	416[B]	PHO	CHA-CBD	-3.96	1.47	1.52
23	B	602	CLA	CHD-C4C	3.96	1.48	1.39
23	B	613	CLA	C3D-C2D	3.96	1.49	1.39
34	B	625	HTG	C1'-S1	-3.96	1.76	1.81
23	d	402[A]	CLA	O2A-CGA	3.96	1.44	1.33
23	B	602	CLA	O2A-CGA	3.96	1.44	1.33
24	A	407[B]	PHO	O2A-CGA	3.95	1.44	1.33
23	C	502	CLA	O2D-CGD	3.95	1.42	1.33
23	b	608	CLA	C1D-ND	3.95	1.42	1.37
35	C	517[B]	DGD	O2G-C1B	3.95	1.45	1.34
23	c	502	CLA	O2D-CGD	3.95	1.42	1.33
23	A	406[A]	CLA	OBD-CAD	3.95	1.29	1.22
23	a	407[B]	CLA	CHD-C4C	3.95	1.48	1.39
23	A	406[A]	CLA	C3D-C2D	3.95	1.49	1.39
23	A	408	CLA	C3D-C2D	3.95	1.49	1.39
26	A	410[B]	SQD	O48-C23	3.94	1.44	1.33
23	b	614	CLA	CHD-C1D	3.94	1.46	1.38
23	c	511	CLA	CHD-C4C	3.93	1.48	1.39
32	L	101[B]	LHG	O7-C7	3.93	1.45	1.34
23	a	407[B]	CLA	OBD-CAD	3.93	1.29	1.22
23	C	505	CLA	CHD-C1D	3.93	1.46	1.38
23	B	613	CLA	OBD-CAD	3.93	1.29	1.22
23	c	505	CLA	O2A-CGA	3.93	1.44	1.33
23	C	510	CLA	C3D-C2D	3.93	1.49	1.39
23	C	508	CLA	CHD-C1D	3.93	1.46	1.38
23	d	402[A]	CLA	CHD-C1D	3.93	1.46	1.38
23	c	511	CLA	CHD-C1D	3.92	1.46	1.38
23	b	615	CLA	C1D-ND	3.92	1.42	1.37
23	B	606	CLA	CHD-C1D	3.92	1.46	1.38
33	d	411	LMG	O8-C28	3.92	1.44	1.33
23	C	514	CLA	C3D-C2D	3.92	1.49	1.39
23	c	502	CLA	C3D-C2D	3.92	1.49	1.39
32	L	101[A]	LHG	O8-C23	3.92	1.44	1.33
23	B	605	CLA	CHD-C4C	3.91	1.48	1.39
23	C	502	CLA	O2A-CGA	3.91	1.44	1.33
35	c	517[B]	DGD	O1G-C1A	3.91	1.44	1.33
23	b	614	CLA	CHD-C4C	3.91	1.48	1.39
24	A	416[B]	PHO	O2A-CGA	3.91	1.44	1.33
32	D	409[A]	LHG	O8-C23	3.91	1.44	1.33
32	d	406[A]	LHG	O7-C7	3.90	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	d	413[B]	LHG	O8-C23	3.90	1.44	1.33
23	B	615	CLA	CHD-C4C	3.90	1.48	1.39
23	B	616	CLA	C3D-C2D	3.90	1.49	1.39
23	c	502	CLA	O2A-CGA	3.89	1.44	1.33
23	B	607	CLA	OBD-CAD	3.89	1.29	1.22
23	c	511	CLA	O2A-CGA	3.89	1.44	1.33
26	a	411[B]	SQD	O47-C7	3.89	1.45	1.34
32	D	409[A]	LHG	O7-C7	3.89	1.45	1.34
32	b	629[B]	LHG	O8-C23	3.89	1.44	1.33
24	a	416[A]	PHO	C3C-C2C	3.89	1.49	1.37
23	B	614	CLA	CHD-C4C	3.89	1.48	1.39
23	B	616	CLA	O2A-CGA	3.88	1.44	1.33
23	b	613	CLA	CHD-C1D	3.88	1.45	1.38
23	c	503	CLA	O2A-CGA	3.88	1.44	1.33
23	c	507	CLA	CHD-C4C	3.88	1.48	1.39
24	a	408[A]	PHO	OBD-CAD	3.87	1.27	1.22
23	c	509	CLA	CHD-C4C	3.87	1.48	1.39
32	b	629[B]	LHG	O7-C7	3.87	1.45	1.34
25	B	618	BCR	C23-C22	-3.87	1.37	1.45
23	b	606	CLA	O2A-CGA	3.87	1.44	1.33
23	c	513	CLA	CHD-C4C	3.86	1.48	1.39
23	a	406[B]	CLA	CHD-C1D	3.86	1.45	1.38
23	c	510	CLA	C3D-C2D	3.86	1.49	1.39
23	b	605	CLA	CHD-C1D	3.85	1.45	1.38
23	b	603	CLA	CHD-C1D	3.85	1.45	1.38
23	c	506	CLA	C3D-C2D	3.85	1.49	1.39
23	B	611	CLA	C4B-NB	-3.85	1.31	1.35
23	B	613	CLA	CHD-C1D	3.85	1.45	1.38
24	a	416[B]	PHO	C3C-C2C	3.85	1.49	1.37
23	c	507	CLA	C3D-C2D	3.85	1.49	1.39
24	a	416[A]	PHO	O2A-CGA	3.84	1.44	1.33
35	C	518[A]	DGD	O2G-C1B	3.84	1.45	1.34
23	a	406[A]	CLA	OBD-CAD	3.84	1.29	1.22
35	C	517[B]	DGD	O1G-C1A	3.84	1.44	1.33
23	b	606	CLA	CHD-C4C	3.84	1.48	1.39
23	b	605	CLA	OBD-CAD	3.84	1.29	1.22
23	B	608	CLA	O2D-CGD	3.83	1.42	1.33
23	C	513	CLA	CHD-C4C	3.83	1.48	1.39
23	b	614	CLA	C3D-C2D	3.83	1.49	1.39
23	B	605	CLA	CHD-C1D	3.82	1.45	1.38
23	A	405[B]	CLA	C3D-C2D	3.82	1.49	1.39
23	C	504	CLA	CHD-C4C	3.81	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	D	408[B]	LHG	O8-C23	3.81	1.44	1.33
35	c	517[A]	DGD	O2G-C1B	3.81	1.45	1.34
23	B	601	CLA	CHD-C4C	3.81	1.47	1.39
23	b	604	CLA	OBD-CAD	3.81	1.29	1.22
23	A	404[A]	CLA	C3D-C2D	3.81	1.49	1.39
23	B	614	CLA	O2A-CGA	3.80	1.44	1.33
23	c	510	CLA	CHD-C1D	3.80	1.45	1.38
23	c	514	CLA	C3D-C2D	3.80	1.49	1.39
23	b	612	CLA	OBD-CAD	3.80	1.29	1.22
23	B	606	CLA	O2A-CGA	3.80	1.44	1.33
23	B	607	CLA	O2A-CGA	3.80	1.44	1.33
23	C	512	CLA	CHD-C4C	3.80	1.47	1.39
23	b	609	CLA	C3D-C2D	3.79	1.49	1.39
35	C	518[A]	DGD	O1G-C1A	3.79	1.44	1.33
23	c	506	CLA	O2A-CGA	3.79	1.44	1.33
23	A	405[A]	CLA	CHD-C4C	3.79	1.47	1.39
23	a	407[A]	CLA	CHD-C4C	3.79	1.47	1.39
24	A	416[A]	PHO	C3C-C2C	3.78	1.48	1.37
23	b	615	CLA	C3D-C2D	3.78	1.49	1.39
23	C	512	CLA	C3D-C2D	3.78	1.49	1.39
24	A	407[A]	PHO	C3C-C2C	3.78	1.48	1.37
32	D	408[B]	LHG	O7-C7	3.78	1.45	1.34
35	c	517[A]	DGD	O1G-C1A	3.78	1.44	1.33
23	c	510	CLA	O2A-CGA	3.78	1.44	1.33
35	h	102	DGD	O2G-C1B	3.77	1.44	1.34
23	d	402[B]	CLA	CHD-C4C	3.77	1.47	1.39
34	b	623	HTG	C1'-S1	-3.77	1.76	1.81
24	A	407[A]	PHO	O2A-CGA	3.77	1.44	1.33
23	b	616	CLA	C3D-C2D	3.76	1.49	1.39
23	b	601	CLA	OBD-CAD	3.76	1.29	1.22
26	A	410[A]	SQD	O48-C23	3.76	1.44	1.33
23	a	405[B]	CLA	O2A-CGA	3.76	1.44	1.33
23	c	508	CLA	C3D-C2D	3.76	1.49	1.39
34	B	622	HTG	C1'-S1	-3.75	1.76	1.81
32	d	406[B]	LHG	O8-C23	3.75	1.44	1.33
23	c	509	CLA	OBD-CAD	3.75	1.28	1.22
23	a	406[B]	CLA	CHD-C4C	3.75	1.47	1.39
23	c	503	CLA	CHD-C1D	3.74	1.45	1.38
23	D	405	CLA	CHD-C4C	3.74	1.47	1.39
23	c	506	CLA	CHD-C1D	3.74	1.45	1.38
23	b	614	CLA	O2A-CGA	3.74	1.44	1.33
32	d	407[B]	LHG	O7-C7	3.74	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	405[A]	CLA	OBD-CAD	3.74	1.28	1.22
33	B	621	LMG	O7-C10	3.74	1.44	1.34
23	c	512	CLA	OBD-CAD	3.73	1.28	1.22
23	b	609	CLA	OBD-CAD	3.73	1.28	1.22
23	A	406[A]	CLA	O2A-CGA	3.73	1.44	1.33
23	B	616	CLA	CHD-C1D	3.73	1.45	1.38
23	B	611	CLA	OBD-CAD	3.73	1.28	1.22
23	C	510	CLA	CHD-C4C	3.73	1.47	1.39
23	C	513	CLA	C3D-C2D	3.73	1.49	1.39
26	A	410[B]	SQD	O47-C7	3.72	1.44	1.34
23	D	405	CLA	O2A-CGA	3.72	1.44	1.33
23	B	611	CLA	O2A-CGA	3.71	1.44	1.33
23	b	612	CLA	C3D-C2D	3.71	1.49	1.39
23	B	603	CLA	CHD-C1D	3.71	1.45	1.38
23	B	601	CLA	C3D-C2D	3.71	1.49	1.39
23	C	514	CLA	OBD-CAD	3.71	1.28	1.22
23	a	406[B]	CLA	OBD-CAD	3.71	1.28	1.22
23	b	609	CLA	O2A-CGA	3.71	1.44	1.33
35	h	102	DGD	O1G-C1A	3.71	1.44	1.33
23	B	612	CLA	O2A-CGA	3.71	1.44	1.33
23	c	512	CLA	CHD-C4C	3.71	1.47	1.39
23	C	507	CLA	C3D-C2D	3.70	1.49	1.39
23	A	406[A]	CLA	CHD-C4C	3.70	1.47	1.39
23	C	506	CLA	O2A-CGA	3.70	1.44	1.33
23	a	409	CLA	CHD-C1D	3.70	1.45	1.38
23	B	606	CLA	C3D-C2D	3.70	1.49	1.39
23	A	404[A]	CLA	CHD-C1D	3.70	1.45	1.38
35	H	102	DGD	O1G-C1A	3.69	1.44	1.33
23	B	615	CLA	OBD-CAD	3.69	1.28	1.22
23	C	502	CLA	CHD-C4C	3.69	1.47	1.39
23	b	609	CLA	CHD-C4C	3.69	1.47	1.39
23	b	615	CLA	CHD-C4C	3.69	1.47	1.39
32	d	413[B]	LHG	O7-C7	3.69	1.44	1.34
23	B	603	CLA	C3D-C2D	3.69	1.49	1.39
23	B	615	CLA	C3D-C2D	3.69	1.49	1.39
24	A	407[B]	PHO	C3C-C2C	3.68	1.48	1.37
23	C	505	CLA	C3D-C2D	3.68	1.49	1.39
23	b	612	CLA	O2A-CGA	3.68	1.44	1.33
32	L	101[A]	LHG	O7-C7	3.68	1.44	1.34
26	A	410[A]	SQD	O47-C7	3.68	1.44	1.34
23	b	616	CLA	CHD-C4C	3.68	1.47	1.39
23	B	602	CLA	C3D-C2D	3.68	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	603	CLA	O2A-CGA	3.68	1.44	1.33
23	B	611	CLA	CHD-C4C	3.68	1.47	1.39
32	d	407[A]	LHG	O7-C7	3.68	1.44	1.34
23	C	509	CLA	OBD-CAD	3.67	1.28	1.22
23	a	405[A]	CLA	C3D-C2D	3.67	1.49	1.39
23	A	404[A]	CLA	CHD-C4C	3.67	1.47	1.39
23	c	513	CLA	OBD-CAD	3.66	1.28	1.22
32	D	408[A]	LHG	O7-C7	3.66	1.44	1.34
23	C	510	CLA	O2A-CGA	3.66	1.44	1.33
23	c	510	CLA	CHD-C4C	3.65	1.47	1.39
23	b	602	CLA	OBD-CAD	3.65	1.28	1.22
23	B	612	CLA	C1B-NB	-3.65	1.32	1.35
35	C	517[A]	DGD	O1G-C1A	3.65	1.44	1.33
23	a	406[A]	CLA	CHD-C1D	3.65	1.45	1.38
23	b	602	CLA	O2A-CGA	3.65	1.44	1.33
32	d	413[A]	LHG	O8-C23	3.64	1.44	1.33
23	D	404[A]	CLA	CHD-C4C	3.64	1.47	1.39
23	b	604	CLA	O2A-CGA	3.64	1.44	1.33
23	B	604	CLA	OBD-CAD	3.64	1.28	1.22
23	b	603	CLA	C3D-C2D	3.64	1.49	1.39
23	C	503	CLA	CHD-C4C	3.64	1.47	1.39
23	B	605	CLA	O2A-CGA	3.63	1.43	1.33
23	b	608	CLA	OBD-CAD	3.63	1.28	1.22
23	C	504	CLA	O2A-CGA	3.63	1.43	1.33
23	b	607	CLA	C3D-C2D	3.63	1.49	1.39
35	c	519	DGD	O2G-C1B	3.62	1.44	1.34
24	a	408[B]	PHO	O2A-CGA	3.62	1.43	1.33
23	d	402[A]	CLA	C1D-ND	3.61	1.42	1.37
23	A	404[B]	CLA	C3D-C2D	3.61	1.49	1.39
23	a	407[A]	CLA	CHD-C1D	3.61	1.45	1.38
23	b	608	CLA	CHD-C4C	3.61	1.47	1.39
23	A	406[B]	CLA	OBD-CAD	3.61	1.28	1.22
23	b	604	CLA	C3D-C2D	3.61	1.49	1.39
23	d	402[A]	CLA	OBD-CAD	3.61	1.28	1.22
23	B	608	CLA	CHD-C1D	3.61	1.45	1.38
33	D	413	LMG	O8-C28	3.61	1.43	1.33
32	b	629[A]	LHG	O7-C7	3.60	1.44	1.34
23	c	505	CLA	CHD-C4C	3.60	1.47	1.39
32	D	408[A]	LHG	O8-C23	3.60	1.43	1.33
23	d	402[A]	CLA	CHD-C4C	3.60	1.47	1.39
24	A	416[B]	PHO	C3C-C2C	3.60	1.48	1.37
32	A	418[A]	LHG	O7-C7	3.60	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	404[B]	CLA	C3D-C2D	3.60	1.48	1.39
23	b	606	CLA	C3D-C2D	3.59	1.48	1.39
23	B	607	CLA	CHD-C4C	3.59	1.47	1.39
23	b	613	CLA	CHD-C4C	3.59	1.47	1.39
23	B	610	CLA	CHD-C1D	3.59	1.45	1.38
23	B	612	CLA	OBD-CAD	3.59	1.28	1.22
23	A	404[B]	CLA	O2A-CGA	3.59	1.43	1.33
32	d	406[A]	LHG	O8-C23	3.58	1.43	1.33
23	B	607	CLA	C1D-ND	3.58	1.42	1.37
34	b	622	HTG	C1'-S1	-3.58	1.76	1.81
23	b	606	CLA	OBD-CAD	3.57	1.28	1.22
23	B	608	CLA	O2A-CGA	3.57	1.43	1.33
23	B	603	CLA	CHD-C4C	3.56	1.47	1.39
23	B	614	CLA	CHD-C1D	3.56	1.45	1.38
23	C	508	CLA	C3D-C2D	3.56	1.48	1.39
23	B	616	CLA	CHD-C4C	3.56	1.47	1.39
23	b	613	CLA	C3D-C2D	3.56	1.48	1.39
23	C	511	CLA	C3D-C2D	3.55	1.48	1.39
23	C	507	CLA	OBD-CAD	3.55	1.28	1.22
23	b	602	CLA	C3D-C2D	3.55	1.48	1.39
32	A	418[B]	LHG	O7-C7	3.55	1.44	1.34
23	D	404[A]	CLA	C3D-C2D	3.55	1.48	1.39
23	b	615	CLA	OBD-CAD	3.55	1.28	1.22
23	b	611	CLA	C3D-C2D	3.54	1.48	1.39
23	B	606	CLA	CHD-C4C	3.54	1.47	1.39
23	b	610	CLA	C3D-C2D	3.54	1.48	1.39
23	c	506	CLA	OBD-CAD	3.54	1.28	1.22
35	c	518[A]	DGD	O2G-C1B	3.54	1.44	1.34
23	d	402[A]	CLA	C3D-C2D	3.53	1.48	1.39
23	B	612	CLA	C1C-C2C	3.53	1.51	1.44
35	H	102	DGD	O2G-C1B	3.53	1.44	1.34
24	a	408[A]	PHO	C3C-C2C	3.52	1.48	1.37
23	D	405	CLA	OBD-CAD	3.52	1.28	1.22
24	a	408[B]	PHO	C3C-C2C	3.52	1.48	1.37
23	a	406[A]	CLA	CHD-C4C	3.52	1.47	1.39
23	d	403	CLA	CHD-C4C	3.52	1.47	1.39
23	c	512	CLA	C3D-C2D	3.52	1.48	1.39
32	d	413[A]	LHG	O7-C7	3.50	1.44	1.34
23	B	613	CLA	CHD-C4C	3.50	1.47	1.39
23	a	405[B]	CLA	OBD-CAD	3.50	1.28	1.22
23	d	402[B]	CLA	C3D-C2D	3.50	1.48	1.39
23	b	613	CLA	O2A-CGA	3.50	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	610	CLA	CHD-C4C	3.50	1.47	1.39
23	C	505	CLA	O2A-CGA	3.50	1.43	1.33
23	a	405[B]	CLA	C3D-C2D	3.50	1.48	1.39
23	a	407[A]	CLA	OBD-CAD	3.50	1.28	1.22
35	C	519	DGD	O2G-C1B	3.50	1.44	1.34
32	A	418[A]	LHG	O8-C23	3.49	1.43	1.33
23	B	607	CLA	CHD-C1D	3.49	1.45	1.38
23	c	503	CLA	CHD-C4C	3.49	1.47	1.39
23	d	402[B]	CLA	OBD-CAD	3.49	1.28	1.22
23	C	508	CLA	CHD-C4C	3.49	1.47	1.39
23	B	605	CLA	C3D-C2D	3.48	1.48	1.39
23	B	612	CLA	C3D-C2D	3.48	1.48	1.39
23	C	502	CLA	C3D-C2D	3.48	1.48	1.39
23	B	604	CLA	O2A-CGA	3.48	1.43	1.33
23	b	603	CLA	OBD-CAD	3.48	1.28	1.22
23	B	611	CLA	C3D-C2D	3.47	1.48	1.39
23	C	504	CLA	OBD-CAD	3.46	1.28	1.22
23	b	605	CLA	O2A-CGA	3.46	1.43	1.33
33	m	101	LMG	O7-C10	3.45	1.44	1.34
23	c	503	CLA	OBD-CAD	3.45	1.28	1.22
23	b	612	CLA	CHD-C1D	3.45	1.45	1.38
23	C	505	CLA	CHD-C4C	3.45	1.47	1.39
23	B	601	CLA	OBD-CAD	3.45	1.28	1.22
23	b	611	CLA	CHD-C4C	3.44	1.47	1.39
23	D	404[B]	CLA	OBD-CAD	3.44	1.28	1.22
23	a	409	CLA	C1D-ND	3.44	1.42	1.37
23	B	612	CLA	CHD-C4C	3.44	1.47	1.39
23	C	504	CLA	C3D-C2D	3.44	1.48	1.39
23	C	503	CLA	OBD-CAD	3.43	1.28	1.22
23	B	607	CLA	C3D-C2D	3.42	1.48	1.39
23	C	509	CLA	CHD-C4C	3.41	1.47	1.39
23	C	511	CLA	CHD-C1D	3.40	1.45	1.38
23	B	611	CLA	C4B-CHC	3.40	1.50	1.41
23	c	514	CLA	OBD-CAD	3.40	1.28	1.22
32	b	629[A]	LHG	O8-C23	3.39	1.43	1.33
33	D	413	LMG	O7-C10	3.39	1.43	1.34
23	c	504	CLA	C3D-C2D	3.39	1.48	1.39
23	A	405[B]	CLA	OBD-CAD	3.38	1.28	1.22
23	c	508	CLA	OBD-CAD	3.38	1.28	1.22
23	b	607	CLA	CHD-C4C	3.37	1.46	1.39
23	b	614	CLA	OBD-CAD	3.36	1.28	1.22
23	A	405[A]	CLA	OBD-CAD	3.36	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	408[A]	PHO	O2A-CGA	3.35	1.43	1.33
23	b	603	CLA	CHD-C4C	3.35	1.46	1.39
23	A	404[B]	CLA	OBD-CAD	3.35	1.28	1.22
23	a	409	CLA	CHD-C4C	3.34	1.46	1.39
23	B	614	CLA	C3D-C2D	3.34	1.48	1.39
23	b	611	CLA	CHD-C1D	3.34	1.44	1.38
23	A	404[A]	CLA	OBD-CAD	3.33	1.28	1.22
23	B	610	CLA	OBD-CAD	3.33	1.28	1.22
39	f	101	HEM	C1B-NB	-3.32	1.34	1.40
23	B	607	CLA	C1B-NB	-3.31	1.32	1.35
23	B	613	CLA	O2A-CGA	3.31	1.43	1.33
23	C	506	CLA	C3D-C2D	3.30	1.48	1.39
23	b	612	CLA	CHD-C4C	3.30	1.46	1.39
23	B	612	CLA	C1D-ND	3.30	1.41	1.37
39	f	101	HEM	C4D-ND	-3.30	1.34	1.40
23	C	506	CLA	OBD-CAD	3.28	1.28	1.22
23	B	604	CLA	C3D-C2D	3.28	1.48	1.39
23	B	603	CLA	OBD-CAD	3.28	1.28	1.22
23	A	404[A]	CLA	O2A-CGA	3.28	1.42	1.33
23	B	610	CLA	O2A-CGA	3.28	1.42	1.33
23	C	513	CLA	OBD-CAD	3.26	1.28	1.22
39	F	102	HEM	C1B-NB	-3.26	1.34	1.40
23	c	505	CLA	OBD-CAD	3.25	1.28	1.22
23	C	502	CLA	OBD-CAD	3.24	1.28	1.22
23	D	404[A]	CLA	OBD-CAD	3.24	1.28	1.22
23	B	608	CLA	OBD-CAD	3.24	1.28	1.22
23	b	602	CLA	C1C-C2C	3.21	1.50	1.44
23	D	405	CLA	C1C-C2C	3.21	1.50	1.44
23	d	403	CLA	OBD-CAD	3.20	1.28	1.22
23	B	602	CLA	C1C-C2C	3.20	1.50	1.44
23	a	405[A]	CLA	O2A-CGA	3.19	1.42	1.33
23	B	614	CLA	OBD-CAD	3.17	1.27	1.22
23	b	603	CLA	O2A-CGA	3.16	1.42	1.33
34	b	625	HTG	C1'-S1	-3.16	1.77	1.81
34	D	412	HTG	C1'-S1	-3.16	1.77	1.81
23	C	505	CLA	OBD-CAD	3.16	1.27	1.22
39	F	102	HEM	C4D-ND	-3.14	1.34	1.40
23	B	602	CLA	OBD-CAD	3.14	1.27	1.22
23	b	616	CLA	OBD-CAD	3.13	1.27	1.22
23	B	608	CLA	CHD-C4C	3.13	1.46	1.39
23	c	510	CLA	OBD-CAD	3.13	1.27	1.22
23	c	502	CLA	OBD-CAD	3.13	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	507	CLA	OBD-CAD	3.13	1.27	1.22
23	B	609	CLA	OBD-CAD	3.12	1.27	1.22
23	b	610	CLA	O2A-CGA	3.12	1.42	1.33
34	C	522	HTG	C1'-S1	-3.11	1.77	1.81
23	c	509	CLA	C1C-C2C	3.11	1.50	1.44
23	a	409	CLA	C3D-C2D	3.10	1.47	1.39
23	A	406[A]	CLA	C1B-NB	-3.09	1.32	1.35
34	c	522	HTG	C1'-S1	-3.07	1.77	1.81
23	b	602	CLA	C4B-CHC	3.06	1.49	1.41
23	b	605	CLA	C3D-C2D	3.05	1.47	1.39
23	B	612	CLA	C1B-CHB	3.05	1.49	1.41
23	C	512	CLA	OBD-CAD	3.04	1.27	1.22
23	c	511	CLA	OBD-CAD	3.04	1.27	1.22
23	C	513	CLA	C1C-C2C	3.04	1.50	1.44
23	c	505	CLA	C4C-C3C	3.04	1.50	1.45
23	c	511	CLA	C1C-C2C	3.03	1.50	1.44
23	B	605	CLA	C4B-CHC	3.03	1.49	1.41
23	C	511	CLA	OBD-CAD	3.01	1.27	1.22
23	C	502	CLA	C1C-C2C	3.01	1.50	1.44
23	B	606	CLA	OBD-CAD	3.00	1.27	1.22
23	a	409	CLA	OBD-CAD	2.97	1.27	1.22
23	C	508	CLA	C1C-C2C	2.97	1.50	1.44
23	A	408	CLA	OBD-CAD	2.97	1.27	1.22
23	b	607	CLA	O2A-CGA	2.96	1.42	1.33
23	B	613	CLA	C4C-C3C	2.94	1.50	1.45
23	B	614	CLA	C1B-CHB	2.93	1.49	1.41
23	c	512	CLA	C1B-CHB	2.93	1.49	1.41
23	B	616	CLA	C1C-NC	-2.93	1.33	1.37
23	B	607	CLA	C1C-C2C	2.92	1.50	1.44
34	d	410	HTG	C1'-S1	-2.92	1.77	1.81
23	b	604	CLA	C4B-CHC	2.92	1.49	1.41
23	b	614	CLA	C1B-CHB	2.92	1.49	1.41
23	c	511	CLA	C4D-CHA	2.92	1.48	1.38
23	b	609	CLA	C4D-CHA	2.92	1.48	1.38
23	B	616	CLA	OBD-CAD	2.91	1.27	1.22
23	C	512	CLA	C1C-C2C	2.91	1.50	1.44
23	B	604	CLA	C1B-CHB	2.91	1.49	1.41
23	a	407[A]	CLA	C1C-C2C	2.91	1.50	1.44
23	C	505	CLA	C1B-CHB	2.90	1.49	1.41
23	B	605	CLA	OBD-CAD	2.90	1.27	1.22
23	C	512	CLA	C4D-CHA	2.90	1.48	1.38
23	B	607	CLA	C1B-CHB	2.89	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	509	CLA	C4C-C3C	2.89	1.50	1.45
23	D	405	CLA	C4B-CHC	2.89	1.49	1.41
23	C	514	CLA	C1C-C2C	2.88	1.50	1.44
23	B	607	CLA	C4D-CHA	2.87	1.48	1.38
23	B	601	CLA	C1C-C2C	2.86	1.50	1.44
23	B	616	CLA	C4D-CHA	2.86	1.48	1.38
23	A	405[B]	CLA	C4D-CHA	2.86	1.48	1.38
23	D	405	CLA	C1B-CHB	2.86	1.48	1.41
23	B	611	CLA	C1B-CHB	2.84	1.48	1.41
23	C	508	CLA	C4D-CHA	2.84	1.48	1.38
23	A	404[A]	CLA	C4C-C3C	2.84	1.49	1.45
23	C	513	CLA	C4B-CHC	2.83	1.48	1.41
23	B	604	CLA	C4D-CHA	2.82	1.48	1.38
23	C	502	CLA	C4D-CHA	2.82	1.48	1.38
23	a	405[B]	CLA	C4C-C3C	2.81	1.49	1.45
29	A	414[A]	PL9	C6-C5	2.81	1.49	1.35
23	C	511	CLA	C1C-C2C	2.81	1.50	1.44
23	c	506	CLA	C1C-C2C	2.80	1.50	1.44
23	C	507	CLA	C4C-C3C	2.80	1.49	1.45
23	b	613	CLA	C1C-C2C	2.80	1.50	1.44
23	d	402[A]	CLA	C4C-C3C	2.79	1.49	1.45
23	C	508	CLA	OBD-CAD	2.79	1.27	1.22
23	C	507	CLA	C4D-CHA	2.78	1.48	1.38
23	B	606	CLA	C1C-C2C	2.78	1.50	1.44
23	B	614	CLA	C4D-CHA	2.78	1.48	1.38
23	b	610	CLA	C1B-CHB	2.78	1.48	1.41
31	B	628	LMT	C3'-C2'	2.78	1.59	1.52
23	c	508	CLA	C4D-CHA	2.78	1.48	1.38
23	A	408	CLA	C4D-CHA	2.78	1.48	1.38
23	c	504	CLA	C1C-C2C	2.77	1.49	1.44
23	a	406[A]	CLA	C1B-NB	-2.77	1.32	1.35
26	A	410[B]	SQD	C6-S	-2.77	1.67	1.77
23	B	605	CLA	C4D-CHA	2.76	1.48	1.38
23	C	505	CLA	C4D-CHA	2.76	1.48	1.38
24	A	407[A]	PHO	CBD-CGD	-2.76	1.48	1.52
23	B	605	CLA	C1C-C2C	2.76	1.49	1.44
26	A	410[A]	SQD	C6-S	-2.76	1.67	1.77
23	c	510	CLA	C1B-CHB	2.75	1.48	1.41
23	B	610	CLA	C4D-CHA	2.75	1.48	1.38
23	c	512	CLA	C1C-C2C	2.75	1.49	1.44
23	b	607	CLA	C1B-NB	-2.74	1.32	1.35
26	a	411[B]	SQD	C6-S	-2.74	1.67	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	414[A]	PL9	C6-C5	2.74	1.49	1.35
23	C	503	CLA	C4B-CHC	2.74	1.48	1.41
23	b	610	CLA	C4C-C3C	2.74	1.49	1.45
23	b	603	CLA	C4D-CHA	2.74	1.48	1.38
23	B	613	CLA	C4D-CHA	2.74	1.48	1.38
26	a	411[A]	SQD	C6-S	-2.73	1.67	1.77
23	C	506	CLA	C4D-CHA	2.73	1.48	1.38
23	c	510	CLA	C4C-C3C	2.73	1.49	1.45
23	c	511	CLA	C1B-CHB	2.73	1.48	1.41
23	A	405[A]	CLA	C1C-C2C	2.73	1.49	1.44
23	c	502	CLA	C4C-C3C	2.73	1.49	1.45
23	b	611	CLA	OBD-CAD	2.72	1.27	1.22
29	a	414[B]	PL9	C6-C5	2.72	1.49	1.35
23	B	615	CLA	C1B-CHB	2.72	1.48	1.41
23	b	613	CLA	OBD-CAD	2.72	1.27	1.22
23	C	512	CLA	C1B-CHB	2.71	1.48	1.41
23	C	513	CLA	C4D-CHA	2.71	1.48	1.38
34	B	625	HTG	C1-S1	-2.71	1.76	1.80
23	c	513	CLA	C4B-CHC	2.71	1.48	1.41
39	f	101	HEM	FE-NB	2.71	2.10	1.96
34	b	622	HTG	O5-C1	2.70	1.46	1.42
23	B	606	CLA	C4D-CHA	2.70	1.48	1.38
23	B	605	CLA	C1B-CHB	2.70	1.48	1.41
26	f	102	SQD	C6-S	-2.70	1.67	1.77
23	a	409	CLA	C1C-C2C	2.70	1.49	1.44
23	c	509	CLA	C4D-CHA	2.70	1.48	1.38
23	C	509	CLA	C1C-C2C	2.70	1.49	1.44
23	b	613	CLA	C4D-CHA	2.69	1.48	1.38
33	Z	101	LMG	O8-C28	2.69	1.46	1.33
23	B	603	CLA	C4D-CHA	2.69	1.48	1.38
23	B	604	CLA	C4C-C3C	2.69	1.49	1.45
23	d	403	CLA	C4D-CHA	2.69	1.48	1.38
23	A	405[A]	CLA	C4D-CHA	2.69	1.48	1.38
23	b	611	CLA	C1B-CHB	2.69	1.48	1.41
23	c	513	CLA	C4D-CHA	2.69	1.47	1.38
23	C	509	CLA	C1B-CHB	2.68	1.48	1.41
23	B	602	CLA	C4C-C3C	2.68	1.49	1.45
23	D	404[A]	CLA	C1B-CHB	2.68	1.48	1.41
23	a	407[A]	CLA	C4D-CHA	2.67	1.47	1.38
23	a	405[B]	CLA	C4D-CHA	2.67	1.47	1.38
23	b	615	CLA	C4D-CHA	2.67	1.47	1.38
23	c	504	CLA	C4B-CHC	2.67	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	405[A]	CLA	C1B-CHB	2.67	1.48	1.41
34	b	625	HTG	C1-S1	-2.67	1.76	1.80
23	c	514	CLA	C1C-C2C	2.67	1.49	1.44
39	F	102	HEM	FE-NB	2.67	2.10	1.96
26	a	412	SQD	C6-S	-2.66	1.67	1.77
23	B	612	CLA	C4D-CHA	2.66	1.47	1.38
23	c	504	CLA	OBD-CAD	2.66	1.27	1.22
23	a	407[B]	CLA	C4D-CHA	2.66	1.47	1.38
23	C	511	CLA	C1B-CHB	2.66	1.48	1.41
23	c	504	CLA	C1B-CHB	2.66	1.48	1.41
23	c	506	CLA	C4C-C3C	2.66	1.49	1.45
23	B	610	CLA	C1C-C2C	2.65	1.49	1.44
23	B	607	CLA	C4B-CHC	2.65	1.48	1.41
29	A	414[B]	PL9	C6-C5	2.65	1.49	1.35
23	b	607	CLA	C4D-CHA	2.65	1.47	1.38
23	d	402[A]	CLA	C1B-CHB	2.65	1.48	1.41
23	d	403	CLA	C1C-C2C	2.65	1.49	1.44
23	b	606	CLA	C4D-CHA	2.65	1.47	1.38
23	A	404[B]	CLA	C4D-CHA	2.65	1.47	1.38
23	c	511	CLA	C4B-CHC	2.65	1.48	1.41
23	b	601	CLA	C1C-C2C	2.64	1.49	1.44
23	C	510	CLA	C4D-CHA	2.64	1.47	1.38
24	a	408[B]	PHO	CHA-CBD	-2.64	1.49	1.52
23	d	402[B]	CLA	C1B-CHB	2.64	1.48	1.41
23	B	606	CLA	C1B-CHB	2.64	1.48	1.41
23	b	604	CLA	C4D-CHA	2.64	1.47	1.38
23	B	601	CLA	C4B-CHC	2.64	1.48	1.41
35	H	102	DGD	O5D-C1E	2.63	1.44	1.40
23	C	508	CLA	C4B-CHC	2.63	1.48	1.41
33	C	521	LMG	O1-C1	2.63	1.44	1.40
23	b	605	CLA	C4D-CHA	2.63	1.47	1.38
23	C	506	CLA	C4B-CHC	2.63	1.48	1.41
23	B	611	CLA	C4D-CHA	2.63	1.47	1.38
23	c	506	CLA	C4D-CHA	2.63	1.47	1.38
23	b	612	CLA	C1B-CHB	2.63	1.48	1.41
23	B	602	CLA	C1B-CHB	2.62	1.48	1.41
23	C	510	CLA	C1B-CHB	2.62	1.48	1.41
23	B	615	CLA	C4D-CHA	2.62	1.47	1.38
23	c	508	CLA	C1C-C2C	2.62	1.49	1.44
23	B	609	CLA	C4B-CHC	2.62	1.48	1.41
23	B	614	CLA	C4C-C3C	2.61	1.49	1.45
23	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)
23	D	404[A]	CLA	C4D-CHA	2.61	1.47	1.38
23	C	513	CLA	C3D-C4D	-2.61	1.38	1.44
31	t	101	LMT	O3'-C3'	-2.61	1.36	1.43
26	A	412	SQD	C6-S	-2.61	1.67	1.77
23	b	610	CLA	C4B-CHC	2.61	1.48	1.41
23	C	505	CLA	C3D-C4D	-2.60	1.38	1.44
23	d	402[A]	CLA	C4D-CHA	2.60	1.47	1.38
23	c	506	CLA	C1B-CHB	2.59	1.48	1.41
23	c	512	CLA	C4D-CHA	2.59	1.47	1.38
23	c	505	CLA	C4D-CHA	2.59	1.47	1.38
23	b	614	CLA	C4B-CHC	2.59	1.48	1.41
23	D	405	CLA	C4C-C3C	2.59	1.49	1.45
24	a	408[A]	PHO	CHA-CBD	-2.59	1.49	1.52
23	c	502	CLA	C1C-C2C	2.58	1.49	1.44
23	B	602	CLA	C4D-CHA	2.58	1.47	1.38
23	b	606	CLA	C1B-CHB	2.58	1.48	1.41
23	A	406[A]	CLA	C4D-CHA	2.58	1.47	1.38
23	b	616	CLA	C1C-C2C	2.58	1.49	1.44
24	a	408[A]	PHO	CBD-CGD	-2.58	1.49	1.52
23	B	613	CLA	C1B-CHB	2.58	1.48	1.41
35	h	102	DGD	O5D-C1E	2.57	1.44	1.40
23	C	502	CLA	C4B-CHC	2.57	1.48	1.41
23	C	511	CLA	C4D-CHA	2.57	1.47	1.38
23	a	409	CLA	C1B-CHB	2.57	1.48	1.41
23	C	504	CLA	C4B-CHC	2.57	1.48	1.41
23	c	509	CLA	C4C-C3C	2.56	1.49	1.45
23	c	502	CLA	C4B-CHC	2.56	1.48	1.41
23	C	509	CLA	C4D-CHA	2.56	1.47	1.38
23	B	616	CLA	C1B-CHB	2.56	1.48	1.41
23	D	404[B]	CLA	C4C-C3C	2.56	1.49	1.45
23	c	514	CLA	C4C-C3C	2.56	1.49	1.45
23	B	609	CLA	C4D-CHA	2.56	1.47	1.38
23	C	510	CLA	C1C-C2C	2.56	1.49	1.44
23	d	402[B]	CLA	C4C-C3C	2.56	1.49	1.45
24	a	416[A]	PHO	CHA-CBD	-2.56	1.49	1.52
23	a	405[A]	CLA	C4D-CHA	2.55	1.47	1.38
23	C	504	CLA	C3D-C4D	-2.55	1.38	1.44
23	b	611	CLA	C1C-C2C	2.55	1.49	1.44
23	d	402[A]	CLA	C1C-C2C	2.55	1.49	1.44
23	c	509	CLA	C4B-CHC	2.55	1.48	1.41
23	b	605	CLA	C1D-C2D	2.54	1.50	1.45
23	A	404[A]	CLA	C4D-CHA	2.54	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	608	CLA	C4D-CHA	2.54	1.47	1.38
23	b	602	CLA	C3D-C4D	-2.54	1.38	1.44
23	b	610	CLA	C4D-CHA	2.54	1.47	1.38
23	B	603	CLA	C1B-NB	-2.54	1.32	1.35
23	b	609	CLA	C1B-CHB	2.54	1.48	1.41
23	C	505	CLA	C1C-C2C	2.54	1.49	1.44
23	b	615	CLA	C1B-CHB	2.54	1.48	1.41
23	B	603	CLA	C1C-C2C	2.53	1.49	1.44
23	b	601	CLA	C4D-CHA	2.53	1.47	1.38
23	C	514	CLA	C1B-CHB	2.53	1.48	1.41
23	b	610	CLA	C3D-C4D	-2.53	1.38	1.44
23	D	404[B]	CLA	C4D-CHA	2.53	1.47	1.38
23	C	504	CLA	C1C-C2C	2.53	1.49	1.44
23	c	510	CLA	C1C-C2C	2.53	1.49	1.44
23	A	406[B]	CLA	C4B-CHC	2.53	1.48	1.41
23	C	514	CLA	C4D-CHA	2.53	1.47	1.38
23	b	604	CLA	C1C-C2C	2.52	1.49	1.44
29	d	405[B]	PL9	C6-C5	2.52	1.48	1.35
29	D	407[B]	PL9	C6-C5	2.52	1.48	1.35
23	a	406[A]	CLA	C4D-CHA	2.52	1.47	1.38
23	B	610	CLA	C3D-C4D	-2.52	1.38	1.44
24	a	416[A]	PHO	C3A-C2A	-2.52	1.52	1.54
23	B	616	CLA	C1C-C2C	2.52	1.49	1.44
23	C	503	CLA	C1C-C2C	2.52	1.49	1.44
23	B	606	CLA	C3D-C4D	-2.51	1.38	1.44
23	B	604	CLA	C3D-C4D	-2.51	1.38	1.44
23	b	607	CLA	C1C-C2C	2.51	1.49	1.44
23	b	609	CLA	C3D-C4D	-2.51	1.38	1.44
23	b	612	CLA	C4D-CHA	2.51	1.47	1.38
23	B	615	CLA	C1C-C2C	2.51	1.49	1.44
26	X	101	SQD	O6-C1	2.50	1.44	1.40
23	b	604	CLA	C1B-CHB	2.50	1.48	1.41
23	c	507	CLA	C1B-CHB	2.50	1.48	1.41
23	B	605	CLA	C3D-C4D	-2.50	1.38	1.44
23	b	610	CLA	C1C-C2C	2.50	1.49	1.44
23	c	513	CLA	C1C-C2C	2.50	1.49	1.44
23	C	502	CLA	C3D-C4D	-2.50	1.38	1.44
31	b	621	LMT	C3'-C2'	2.50	1.58	1.52
23	c	502	CLA	C1B-CHB	2.50	1.47	1.41
29	D	407[A]	PL9	C6-C5	2.50	1.48	1.35
23	A	404[A]	CLA	C1B-CHB	2.49	1.47	1.41
23	b	603	CLA	C4B-CHC	2.49	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	507	CLA	C4C-C3C	2.49	1.49	1.45
23	b	608	CLA	C1B-CHB	2.49	1.47	1.41
23	b	616	CLA	C3D-C4D	-2.49	1.38	1.44
23	b	614	CLA	C4D-CHA	2.48	1.47	1.38
23	A	408	CLA	C3D-C4D	-2.48	1.38	1.44
23	A	406[B]	CLA	C4D-CHA	2.48	1.47	1.38
23	c	504	CLA	C3D-C4D	-2.48	1.38	1.44
23	C	507	CLA	C3D-C4D	-2.48	1.38	1.44
23	B	602	CLA	C4B-CHC	2.48	1.47	1.41
23	C	502	CLA	C1B-CHB	2.48	1.47	1.41
23	b	609	CLA	C1C-NC	-2.47	1.34	1.37
23	B	602	CLA	C3D-C4D	-2.47	1.38	1.44
23	a	405[A]	CLA	C1C-C2C	2.47	1.49	1.44
23	c	504	CLA	C4D-CHA	2.47	1.47	1.38
23	A	405[A]	CLA	C4B-CHC	2.47	1.47	1.41
31	B	630	LMT	O2B-C2B	-2.47	1.37	1.43
23	D	404[A]	CLA	C1C-C2C	2.46	1.49	1.44
23	B	608	CLA	C3D-C4D	-2.46	1.38	1.44
23	b	615	CLA	C3D-C4D	-2.46	1.38	1.44
23	D	404[B]	CLA	C1B-CHB	2.46	1.47	1.41
23	c	514	CLA	C1B-CHB	2.46	1.47	1.41
23	C	510	CLA	C4B-NB	-2.46	1.33	1.35
23	C	506	CLA	C4C-C3C	2.46	1.49	1.45
23	b	613	CLA	C4B-CHC	2.46	1.47	1.41
23	A	405[B]	CLA	C1C-C2C	2.46	1.49	1.44
23	d	402[B]	CLA	C4D-CHA	2.46	1.47	1.38
23	b	605	CLA	C1B-CHB	2.45	1.47	1.41
23	C	511	CLA	C4C-C3C	2.45	1.49	1.45
23	c	502	CLA	C4D-CHA	2.45	1.47	1.38
23	c	510	CLA	C4D-CHA	2.45	1.47	1.38
24	a	416[B]	PHO	CHA-CBD	-2.45	1.49	1.52
23	b	602	CLA	C4D-CHA	2.45	1.47	1.38
23	d	402[A]	CLA	C3D-C4D	-2.45	1.38	1.44
23	c	506	CLA	C4B-CHC	2.44	1.47	1.41
23	c	513	CLA	C1B-CHB	2.44	1.47	1.41
26	B	620	SQD	C6-S	-2.44	1.68	1.77
23	c	504	CLA	C4C-C3C	2.44	1.49	1.45
23	b	606	CLA	C1C-C2C	2.44	1.49	1.44
23	b	612	CLA	C4C-C3C	2.44	1.49	1.45
23	c	503	CLA	C4D-CHA	2.44	1.47	1.38
23	b	613	CLA	C1B-CHB	2.43	1.47	1.41
23	b	614	CLA	C1C-C2C	2.43	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	610	CLA	C1B-NB	-2.43	1.33	1.35
23	B	609	CLA	C1C-C2C	2.43	1.49	1.44
23	A	404[B]	CLA	C4C-C3C	2.43	1.49	1.45
31	B	628	LMT	O3'-C3'	-2.43	1.37	1.43
23	b	603	CLA	C1C-C2C	2.43	1.49	1.44
23	D	404[A]	CLA	C3D-C4D	-2.43	1.38	1.44
23	d	402[B]	CLA	C1C-C2C	2.43	1.49	1.44
23	c	505	CLA	C1C-C2C	2.42	1.49	1.44
23	b	601	CLA	C1B-CHB	2.42	1.47	1.41
23	B	616	CLA	C3D-C4D	-2.42	1.38	1.44
23	b	611	CLA	C3D-C4D	-2.42	1.38	1.44
23	b	616	CLA	C4B-CHC	2.42	1.47	1.41
23	b	615	CLA	C4C-C3C	2.42	1.49	1.45
23	b	607	CLA	OBD-CAD	2.42	1.26	1.22
23	A	404[A]	CLA	C1C-C2C	2.42	1.49	1.44
23	b	616	CLA	C4D-CHA	2.41	1.47	1.38
23	a	409	CLA	C4B-CHC	2.41	1.47	1.41
23	C	512	CLA	C4B-CHC	2.41	1.47	1.41
23	c	514	CLA	C4D-CHA	2.41	1.47	1.38
23	C	504	CLA	C4D-CHA	2.41	1.47	1.38
23	B	604	CLA	C1C-C2C	2.41	1.49	1.44
23	B	613	CLA	C1C-C2C	2.41	1.49	1.44
23	a	409	CLA	C4D-CHA	2.41	1.47	1.38
23	B	601	CLA	C4D-CHA	2.40	1.46	1.38
23	a	405[B]	CLA	C1B-CHB	2.40	1.47	1.41
26	b	620	SQD	C6-S	-2.40	1.68	1.77
23	b	608	CLA	C1B-NB	-2.40	1.33	1.35
23	C	502	CLA	C4C-C3C	2.40	1.49	1.45
31	A	419	LMT	O3'-C3'	-2.40	1.37	1.43
23	b	614	CLA	C3D-C4D	-2.39	1.38	1.44
26	X	101	SQD	C6-S	-2.39	1.68	1.77
24	A	407[B]	PHO	CHA-CBD	-2.39	1.49	1.52
23	b	604	CLA	MG-NA	2.39	2.11	2.06
23	B	608	CLA	C1B-CHB	2.39	1.47	1.41
23	B	608	CLA	C4D-CHA	2.39	1.46	1.38
23	A	406[A]	CLA	C1C-C2C	2.39	1.49	1.44
31	M	101	LMT	O3'-C3'	-2.39	1.37	1.43
23	A	404[B]	CLA	C4B-CHC	2.39	1.47	1.41
34	B	623	HTG	C1'-S1	-2.38	1.78	1.81
23	A	405[B]	CLA	C1B-CHB	2.38	1.47	1.41
23	B	610	CLA	C1B-CHB	2.38	1.47	1.41
23	A	405[B]	CLA	C3D-C4D	-2.38	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	414	GOL	O2-C2	-2.38	1.36	1.43
23	c	508	CLA	C4B-CHC	2.38	1.47	1.41
23	A	405[A]	CLA	C1B-CHB	2.37	1.47	1.41
23	c	507	CLA	C1C-C2C	2.37	1.49	1.44
23	a	407[B]	CLA	C1B-CHB	2.37	1.47	1.41
23	a	407[B]	CLA	C4C-C3C	2.37	1.49	1.45
23	b	613	CLA	C1B-NB	-2.37	1.33	1.35
31	A	419	LMT	O2'-C2'	-2.37	1.37	1.43
23	A	406[A]	CLA	C4B-CHC	2.37	1.47	1.41
31	B	631	LMT	O3'-C3'	-2.37	1.37	1.43
23	B	603	CLA	C1B-CHB	2.37	1.47	1.41
23	C	504	CLA	C4C-C3C	2.37	1.49	1.45
23	a	407[A]	CLA	C3D-C4D	-2.36	1.38	1.44
24	A	416[A]	PHO	C3A-C2A	-2.36	1.52	1.54
23	C	505	CLA	C4B-CHC	2.36	1.47	1.41
23	b	602	CLA	C4C-C3C	2.36	1.49	1.45
31	e	101	LMT	O3'-C3'	-2.36	1.37	1.43
23	c	503	CLA	C1B-CHB	2.36	1.47	1.41
23	C	507	CLA	C1C-C2C	2.36	1.49	1.44
23	a	405[A]	CLA	C4C-C3C	2.36	1.49	1.45
23	c	509	CLA	C1B-CHB	2.36	1.47	1.41
23	A	406[B]	CLA	C1B-CHB	2.36	1.47	1.41
23	C	503	CLA	C1B-CHB	2.36	1.47	1.41
27	d	412	GOL	O2-C2	-2.35	1.36	1.43
23	B	614	CLA	C3D-C4D	-2.35	1.38	1.44
31	M	102	LMT	O3'-C3'	-2.35	1.37	1.43
23	D	404[B]	CLA	C1C-C2C	2.35	1.49	1.44
23	b	612	CLA	C3D-C4D	-2.35	1.38	1.44
34	B	622	HTG	O5-C1	2.34	1.46	1.42
23	C	506	CLA	C1B-CHB	2.34	1.47	1.41
23	D	404[B]	CLA	C4B-CHC	2.34	1.47	1.41
23	C	512	CLA	C3D-C4D	-2.34	1.38	1.44
23	b	613	CLA	C4C-C3C	2.34	1.49	1.45
23	A	404[B]	CLA	C1C-C2C	2.34	1.49	1.44
23	A	406[A]	CLA	C1B-CHB	2.34	1.47	1.41
23	C	508	CLA	C1B-CHB	2.34	1.47	1.41
23	b	609	CLA	C1C-C2C	2.33	1.49	1.44
23	A	405[B]	CLA	C4B-CHC	2.33	1.47	1.41
23	A	404[B]	CLA	C1B-CHB	2.33	1.47	1.41
23	c	507	CLA	C4D-CHA	2.33	1.46	1.38
23	b	614	CLA	C4C-C3C	2.33	1.49	1.45
27	D	403	GOL	C3-C2	2.33	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	C	519	DGD	O2G-C2G	-2.33	1.40	1.46
23	C	511	CLA	C3D-C4D	-2.33	1.38	1.44
29	d	405[A]	PL9	C6-C5	2.33	1.47	1.35
23	C	507	CLA	C1B-CHB	2.32	1.47	1.41
23	C	506	CLA	C1C-C2C	2.32	1.49	1.44
23	b	608	CLA	C1C-C2C	2.32	1.49	1.44
23	d	403	CLA	C4B-CHC	2.32	1.47	1.41
23	c	502	CLA	C3D-C4D	-2.32	1.38	1.44
23	c	514	CLA	C3D-C4D	-2.32	1.38	1.44
23	B	604	CLA	MG-NA	2.32	2.11	2.06
23	A	406[B]	CLA	C1C-C2C	2.32	1.49	1.44
39	f	101	HEM	C1D-ND	-2.32	1.34	1.38
23	a	406[B]	CLA	C4D-CHA	2.31	1.46	1.38
23	B	615	CLA	C4B-CHC	2.31	1.47	1.41
23	D	405	CLA	C4D-CHA	2.31	1.46	1.38
23	B	610	CLA	C4B-CHC	2.31	1.47	1.41
31	M	102	LMT	O2'-C2'	-2.31	1.37	1.43
23	B	606	CLA	C4C-C3C	2.30	1.49	1.45
23	A	408	CLA	C1C-C2C	2.30	1.49	1.44
23	a	409	CLA	C4C-C3C	2.30	1.49	1.45
23	c	510	CLA	C1B-NB	-2.30	1.33	1.35
23	b	601	CLA	C4B-CHC	2.30	1.47	1.41
23	a	405[A]	CLA	C4B-CHC	2.30	1.47	1.41
23	b	607	CLA	C1B-CHB	2.30	1.47	1.41
23	a	407[A]	CLA	C1B-CHB	2.29	1.47	1.41
23	C	504	CLA	C1B-CHB	2.29	1.47	1.41
23	c	505	CLA	C1B-CHB	2.29	1.47	1.41
23	C	509	CLA	C4B-CHC	2.29	1.47	1.41
31	A	417	LMT	O2'-C2'	-2.29	1.37	1.43
27	a	419	GOL	C1-C2	2.29	1.61	1.51
23	d	402[B]	CLA	C3D-C4D	-2.29	1.39	1.44
23	b	611	CLA	C4D-CHA	2.29	1.46	1.38
24	a	416[B]	PHO	C3A-C2A	-2.29	1.52	1.54
23	C	508	CLA	C3D-C4D	-2.29	1.39	1.44
23	A	404[B]	CLA	C1B-NB	-2.29	1.33	1.35
24	A	416[B]	PHO	C3A-C2A	-2.28	1.52	1.54
27	b	624	GOL	C3-C2	2.28	1.61	1.51
23	b	612	CLA	C4B-CHC	2.28	1.47	1.41
23	A	404[B]	CLA	C3D-C4D	-2.28	1.39	1.44
23	b	606	CLA	C4B-CHC	2.28	1.47	1.41
23	c	512	CLA	C4C-C3C	2.27	1.49	1.45
23	B	606	CLA	C4B-CHC	2.27	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	505	CLA	C1C-NC	-2.27	1.34	1.37
23	C	507	CLA	C4B-NB	-2.27	1.33	1.35
23	C	507	CLA	C4B-CHC	2.27	1.47	1.41
31	A	417	LMT	O3'-C3'	-2.26	1.37	1.43
23	C	512	CLA	C4C-C3C	2.26	1.48	1.45
23	B	604	CLA	C1A-CHA	2.26	1.52	1.43
23	b	608	CLA	C3D-C4D	-2.26	1.39	1.44
23	A	406[B]	CLA	C4C-C3C	2.25	1.48	1.45
23	D	404[B]	CLA	C3D-C4D	-2.25	1.39	1.44
23	D	404[A]	CLA	C4B-CHC	2.25	1.47	1.41
31	m	103	LMT	O2B-C2B	-2.25	1.37	1.43
23	A	405[A]	CLA	C3D-C4D	-2.25	1.39	1.44
31	M	101	LMT	O2B-C2B	-2.25	1.37	1.43
23	b	608	CLA	C4B-CHC	2.25	1.47	1.41
23	B	609	CLA	C3D-C4D	-2.25	1.39	1.44
31	F	101	LMT	O3'-C3'	-2.25	1.37	1.43
23	b	606	CLA	C3D-C4D	-2.25	1.39	1.44
23	b	611	CLA	C4B-CHC	2.25	1.47	1.41
23	B	609	CLA	C1B-CHB	2.25	1.47	1.41
23	d	403	CLA	C1B-CHB	2.24	1.47	1.41
27	D	403	GOL	O2-C2	-2.24	1.36	1.43
23	B	612	CLA	C4C-C3C	2.24	1.48	1.45
23	D	405	CLA	C3D-C4D	-2.24	1.39	1.44
23	b	603	CLA	C1B-CHB	2.24	1.47	1.41
23	B	613	CLA	C4B-CHC	2.24	1.47	1.41
23	d	402[B]	CLA	C4B-CHC	2.24	1.47	1.41
23	a	406[A]	CLA	C1B-CHB	2.24	1.47	1.41
23	b	605	CLA	C1C-C2C	2.24	1.48	1.44
23	a	407[B]	CLA	C4B-CHC	2.23	1.47	1.41
23	a	407[B]	CLA	C3D-C4D	-2.23	1.39	1.44
31	m	103	LMT	O3'-C3'	-2.23	1.37	1.43
23	B	614	CLA	C4B-CHC	2.23	1.47	1.41
35	C	518[A]	DGD	O5D-C1E	2.22	1.44	1.40
23	C	511	CLA	C4B-CHC	2.22	1.47	1.41
23	C	513	CLA	C1B-CHB	2.22	1.47	1.41
35	H	102	DGD	O2G-C2G	-2.22	1.41	1.46
23	c	514	CLA	C4B-CHC	2.21	1.47	1.41
23	a	405[B]	CLA	C3D-C4D	-2.21	1.39	1.44
41	V	201	HEC	C3C-C4C	2.21	1.47	1.43
23	B	601	CLA	C1B-CHB	2.21	1.47	1.41
23	c	507	CLA	C3D-C4D	-2.21	1.39	1.44
23	c	513	CLA	C3D-C4D	-2.21	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	601	CLA	C4C-C3C	2.21	1.48	1.45
23	B	603	CLA	C3D-C4D	-2.20	1.39	1.44
23	C	509	CLA	C3D-C4D	-2.20	1.39	1.44
23	C	512	CLA	C1C-NC	-2.20	1.34	1.37
23	A	408	CLA	C4B-CHC	2.20	1.47	1.41
39	F	102	HEM	CHB-C1B	2.20	1.40	1.35
23	c	508	CLA	C1B-CHB	2.20	1.47	1.41
23	C	514	CLA	C3D-C4D	-2.20	1.39	1.44
23	b	602	CLA	C1B-CHB	2.19	1.47	1.41
24	A	407[A]	PHO	CHA-CBD	-2.19	1.49	1.52
23	B	604	CLA	C4B-CHC	2.19	1.47	1.41
23	B	603	CLA	C4B-CHC	2.19	1.47	1.41
23	b	601	CLA	C4C-C3C	2.19	1.48	1.45
23	c	508	CLA	C3D-C4D	-2.18	1.39	1.44
23	C	507	CLA	C1D-C2D	2.18	1.49	1.45
31	M	101	LMT	O1'-C1'	-2.18	1.36	1.40
23	c	507	CLA	C4B-CHC	2.18	1.47	1.41
23	D	404[A]	CLA	C4C-C3C	2.18	1.48	1.45
23	b	615	CLA	C4B-CHC	2.18	1.47	1.41
23	c	511	CLA	C3D-C4D	-2.17	1.39	1.44
39	f	101	HEM	CHB-C1B	2.17	1.40	1.35
23	B	615	CLA	C3D-C4D	-2.17	1.39	1.44
23	b	607	CLA	C3D-C4D	-2.16	1.39	1.44
23	c	506	CLA	C3D-C4D	-2.16	1.39	1.44
23	B	601	CLA	C3D-C4D	-2.16	1.39	1.44
23	C	506	CLA	C3D-C4D	-2.16	1.39	1.44
23	B	602	CLA	C1B-NB	-2.16	1.33	1.35
23	c	510	CLA	C3D-C4D	-2.16	1.39	1.44
23	d	402[A]	CLA	C4B-CHC	2.15	1.47	1.41
29	D	407[B]	PL9	C2-C3	2.15	1.40	1.34
23	c	505	CLA	C3D-C4D	-2.15	1.39	1.44
31	B	631	LMT	O2'-C2'	-2.15	1.37	1.43
39	F	102	HEM	C3B-C4B	2.15	1.49	1.44
23	B	607	CLA	C1A-CHA	2.14	1.52	1.43
23	B	611	CLA	C3D-C4D	-2.14	1.39	1.44
23	a	406[B]	CLA	C1B-CHB	2.14	1.46	1.41
23	c	509	CLA	C3D-C4D	-2.13	1.39	1.44
23	C	510	CLA	C4B-CHC	2.13	1.46	1.41
31	M	102	LMT	O3B-C3B	-2.13	1.38	1.43
23	a	409	CLA	C1D-C2D	2.13	1.49	1.45
23	C	503	CLA	C4D-CHA	2.13	1.46	1.38
23	b	616	CLA	C1B-CHB	2.12	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	414[A]	PL9	C2-C3	2.12	1.40	1.34
23	b	608	CLA	C1C-NC	-2.12	1.34	1.37
23	a	406[A]	CLA	C1C-C2C	2.12	1.48	1.44
23	A	406[A]	CLA	C1C-NC	-2.12	1.34	1.37
39	F	102	HEM	C1D-ND	-2.11	1.34	1.38
23	A	406[A]	CLA	C3D-C4D	-2.11	1.39	1.44
23	B	615	CLA	MG-NA	2.11	2.11	2.06
23	A	406[B]	CLA	C3D-C4D	-2.11	1.39	1.44
23	d	403	CLA	C3D-C4D	-2.10	1.39	1.44
23	c	512	CLA	C4B-CHC	2.10	1.46	1.41
23	C	503	CLA	C3D-C4D	-2.10	1.39	1.44
23	C	514	CLA	C4B-CHC	2.10	1.46	1.41
23	B	616	CLA	C4B-CHC	2.10	1.46	1.41
23	a	405[A]	CLA	C3D-C4D	-2.10	1.39	1.44
23	B	615	CLA	C4C-C3C	2.10	1.48	1.45
23	a	407[A]	CLA	C4C-C3C	2.10	1.48	1.45
23	A	408	CLA	C1C-NC	-2.10	1.34	1.37
31	B	630	LMT	O3'-C3'	-2.09	1.38	1.43
23	b	604	CLA	C1A-CHA	2.09	1.51	1.43
23	C	510	CLA	C4C-C3C	2.09	1.48	1.45
23	c	502	CLA	C1C-NC	-2.09	1.34	1.37
23	C	510	CLA	C1C-NC	-2.09	1.34	1.37
23	a	407[B]	CLA	C1C-C2C	2.09	1.48	1.44
35	c	519	DGD	O2G-C2G	-2.09	1.41	1.46
23	B	613	CLA	C1A-CHA	2.09	1.51	1.43
23	b	609	CLA	C4B-CHC	2.08	1.46	1.41
23	b	605	CLA	C1B-NB	-2.08	1.33	1.35
23	C	508	CLA	C4C-C3C	2.08	1.48	1.45
27	o	303	GOL	C1-C2	2.08	1.60	1.51
23	c	511	CLA	C4C-C3C	2.08	1.48	1.45
31	e	101	LMT	O2B-C2B	-2.07	1.38	1.43
35	c	518[A]	DGD	O2G-C2G	-2.07	1.41	1.46
23	b	612	CLA	C4B-NB	-2.07	1.33	1.35
23	c	505	CLA	C4B-CHC	2.07	1.46	1.41
31	M	101	LMT	O2'-C2'	-2.07	1.38	1.43
23	B	610	CLA	C4C-C3C	2.07	1.48	1.45
23	B	608	CLA	C1C-C2C	2.07	1.48	1.44
23	a	405[B]	CLA	C1C-C2C	2.07	1.48	1.44
23	a	407[A]	CLA	C4B-CHC	2.07	1.46	1.41
41	v	201	HEC	C3C-C4C	2.06	1.46	1.43
31	m	103	LMT	C3'-C2'	2.06	1.57	1.52
23	c	508	CLA	C1D-C2D	2.05	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	408[B]	PHO	C3A-C2A	-2.05	1.52	1.54
23	c	502	CLA	C1D-C2D	2.05	1.49	1.45
31	B	630	LMT	O2'-C2'	-2.05	1.38	1.43
23	b	607	CLA	C4B-CHC	2.05	1.46	1.41
23	b	616	CLA	C1B-NB	-2.04	1.33	1.35
23	B	606	CLA	MG-NA	2.04	2.11	2.06
23	A	408	CLA	C4C-C3C	2.04	1.48	1.45
33	D	413	LMG	O7-C8	-2.04	1.41	1.46
31	t	101	LMT	O2'-C2'	-2.04	1.38	1.43
25	d	404	BCR	C30-C25	-2.04	1.51	1.53
26	a	412	SQD	O6-C1	2.04	1.43	1.40
23	a	406[A]	CLA	C4B-CHC	2.04	1.46	1.41
23	B	601	CLA	C1C-NC	-2.04	1.34	1.37
29	A	414[A]	PL9	C2-C1	-2.04	1.39	1.44
31	B	628	LMT	O5'-C5'	-2.03	1.39	1.44
23	A	404[A]	CLA	C3D-C4D	-2.03	1.39	1.44
23	b	605	CLA	C4C-C3C	2.03	1.48	1.45
23	c	514	CLA	C1D-C2D	2.03	1.49	1.45
24	A	407[B]	PHO	CBD-CGD	-2.03	1.49	1.52
23	c	512	CLA	MG-NA	2.03	2.11	2.06
23	c	507	CLA	C1C-NC	-2.03	1.34	1.37
23	C	508	CLA	C1C-NC	-2.02	1.34	1.37
29	a	414[B]	PL9	C2-C3	2.02	1.40	1.34
23	c	513	CLA	C4C-C3C	2.02	1.48	1.45
23	b	612	CLA	C4D-ND	2.02	1.40	1.37
23	b	607	CLA	C4C-C3C	2.02	1.48	1.45
35	c	519	DGD	O5D-C1E	2.02	1.43	1.40
23	B	605	CLA	MG-NA	2.02	2.11	2.06
23	B	603	CLA	C4C-C3C	2.02	1.48	1.45
35	C	518[B]	DGD	O5D-C1E	2.02	1.43	1.40
23	A	404[A]	CLA	C4B-NB	-2.02	1.33	1.35
23	a	405[B]	CLA	C4B-CHC	2.01	1.46	1.41
23	c	503	CLA	C4B-CHC	2.01	1.46	1.41
23	B	616	CLA	C4C-C3C	2.01	1.48	1.45
23	d	403	CLA	C4C-C3C	2.00	1.48	1.45
23	b	601	CLA	C3D-C4D	-2.00	1.39	1.44

All (3089) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	C1D-ND-C4D	-11.62	98.08	106.33
23	b	605	CLA	C1D-ND-C4D	-11.12	98.43	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	409	CLA	C1D-ND-C4D	-10.51	98.87	106.33
23	c	512	CLA	C1D-ND-C4D	-10.31	99.01	106.33
23	B	612	CLA	C1D-ND-C4D	-10.23	99.07	106.33
23	B	615	CLA	C1D-ND-C4D	-10.09	99.17	106.33
23	b	614	CLA	C1D-ND-C4D	-10.03	99.21	106.33
23	C	504	CLA	C1D-ND-C4D	-9.92	99.28	106.33
23	a	405[B]	CLA	C1D-ND-C4D	-9.90	99.30	106.33
23	C	511	CLA	C1D-ND-C4D	-9.89	99.31	106.33
23	c	504	CLA	C1D-ND-C4D	-9.86	99.33	106.33
23	B	611	CLA	C2D-C1D-ND	9.85	117.36	110.10
23	b	611	CLA	C1D-ND-C4D	-9.85	99.34	106.33
23	C	506	CLA	C1D-ND-C4D	-9.70	99.45	106.33
23	B	605	CLA	C1D-ND-C4D	-9.67	99.47	106.33
23	b	603	CLA	C1D-ND-C4D	-9.66	99.48	106.33
23	B	601	CLA	C1D-ND-C4D	-9.65	99.48	106.33
23	A	406[B]	CLA	C1D-ND-C4D	-9.65	99.48	106.33
23	b	602	CLA	C1D-ND-C4D	-9.64	99.49	106.33
23	B	607	CLA	C2D-C1D-ND	9.54	117.14	110.10
23	a	407[B]	CLA	C1D-ND-C4D	-9.52	99.58	106.33
23	a	406[B]	CLA	C1D-ND-C4D	-9.51	99.58	106.33
23	A	404[B]	CLA	C1D-ND-C4D	-9.50	99.58	106.33
23	b	610	CLA	C1D-ND-C4D	-9.48	99.60	106.33
23	d	402[B]	CLA	C1D-ND-C4D	-9.47	99.60	106.33
23	b	607	CLA	C1D-ND-C4D	-9.47	99.61	106.33
23	B	614	CLA	C1D-ND-C4D	-9.43	99.63	106.33
23	C	505	CLA	C1D-ND-C4D	-9.43	99.64	106.33
23	B	607	CLA	C1D-ND-C4D	-9.40	99.66	106.33
23	c	514	CLA	C1D-ND-C4D	-9.37	99.68	106.33
23	c	507	CLA	C1D-ND-C4D	-9.37	99.68	106.33
23	B	603	CLA	C1D-ND-C4D	-9.36	99.69	106.33
23	d	403	CLA	C1D-ND-C4D	-9.35	99.69	106.33
23	C	514	CLA	C1D-ND-C4D	-9.35	99.69	106.33
23	b	601	CLA	C1D-ND-C4D	-9.31	99.72	106.33
23	C	510	CLA	C1D-ND-C4D	-9.30	99.73	106.33
23	C	502	CLA	C1D-ND-C4D	-9.22	99.78	106.33
23	a	409	CLA	C2D-C1D-ND	9.20	116.88	110.10
23	a	407[A]	CLA	C1D-ND-C4D	-9.17	99.82	106.33
23	D	404[B]	CLA	C1D-ND-C4D	-9.17	99.82	106.33
23	D	404[A]	CLA	C1D-ND-C4D	-9.16	99.83	106.33
23	c	506	CLA	C1D-ND-C4D	-9.16	99.83	106.33
23	B	602	CLA	C1D-ND-C4D	-9.15	99.84	106.33
23	B	606	CLA	C1D-ND-C4D	-9.14	99.84	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	605	CLA	C2D-C1D-ND	9.12	116.83	110.10
23	d	402[A]	CLA	C1D-ND-C4D	-9.09	99.88	106.33
23	A	406[A]	CLA	C1D-ND-C4D	-9.08	99.89	106.33
23	a	406[A]	CLA	C1D-ND-C4D	-9.04	99.91	106.33
23	b	614	CLA	C2D-C1D-ND	9.04	116.77	110.10
23	B	613	CLA	C1D-ND-C4D	-9.03	99.92	106.33
23	b	607	CLA	C2D-C1D-ND	9.03	116.76	110.10
23	A	405[B]	CLA	C1D-ND-C4D	-9.03	99.92	106.33
23	b	615	CLA	C1D-ND-C4D	-8.99	99.95	106.33
23	b	611	CLA	C2D-C1D-ND	8.94	116.69	110.10
23	C	512	CLA	C1D-ND-C4D	-8.91	100.00	106.33
23	A	405[A]	CLA	C1D-ND-C4D	-8.91	100.01	106.33
23	A	408	CLA	C1D-ND-C4D	-8.90	100.01	106.33
23	B	612	CLA	C2D-C1D-ND	8.90	116.67	110.10
23	B	615	CLA	C2D-C1D-ND	8.90	116.67	110.10
23	B	608	CLA	C1D-ND-C4D	-8.90	100.01	106.33
23	c	512	CLA	C2D-C1D-ND	8.87	116.64	110.10
23	a	405[A]	CLA	C1D-ND-C4D	-8.83	100.06	106.33
23	c	502	CLA	C1D-ND-C4D	-8.82	100.07	106.33
23	b	608	CLA	C1D-ND-C4D	-8.80	100.08	106.33
23	B	610	CLA	C2D-C1D-ND	8.79	116.58	110.10
23	b	612	CLA	C1D-ND-C4D	-8.78	100.09	106.33
23	C	505	CLA	C2D-C1D-ND	8.76	116.56	110.10
23	a	406[A]	CLA	C2D-C1D-ND	8.75	116.56	110.10
23	c	513	CLA	C1D-ND-C4D	-8.74	100.12	106.33
23	c	510	CLA	C1D-ND-C4D	-8.73	100.13	106.33
23	d	403	CLA	C2D-C1D-ND	8.72	116.53	110.10
23	c	503	CLA	C1D-ND-C4D	-8.69	100.16	106.33
23	b	603	CLA	C2D-C1D-ND	8.69	116.51	110.10
23	A	408	CLA	C2D-C1D-ND	8.68	116.50	110.10
23	B	614	CLA	C2D-C1D-ND	8.67	116.50	110.10
23	c	503	CLA	C2D-C1D-ND	8.67	116.49	110.10
23	b	606	CLA	C1D-ND-C4D	-8.66	100.19	106.33
23	B	613	CLA	C2D-C1D-ND	8.65	116.48	110.10
23	a	407[A]	CLA	C2D-C1D-ND	8.65	116.48	110.10
23	D	405	CLA	C1D-ND-C4D	-8.64	100.20	106.33
23	B	605	CLA	C2D-C1D-ND	8.62	116.46	110.10
23	C	508	CLA	C1D-ND-C4D	-8.61	100.22	106.33
23	b	616	CLA	C1D-ND-C4D	-8.59	100.23	106.33
23	B	609	CLA	C1D-ND-C4D	-8.56	100.25	106.33
23	B	603	CLA	C2D-C1D-ND	8.55	116.41	110.10
23	c	509	CLA	C1D-ND-C4D	-8.55	100.26	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	508	CLA	C1D-ND-C4D	-8.54	100.27	106.33
23	b	608	CLA	C2D-C1D-ND	8.53	116.39	110.10
23	a	406[B]	CLA	C2D-C1D-ND	8.53	116.39	110.10
23	D	404[A]	CLA	C2D-C1D-ND	8.50	116.37	110.10
23	A	404[A]	CLA	C1D-ND-C4D	-8.50	100.30	106.33
23	b	613	CLA	C1D-ND-C4D	-8.49	100.30	106.33
23	C	504	CLA	C2D-C1D-ND	8.47	116.35	110.10
23	c	504	CLA	C2D-C1D-ND	8.47	116.34	110.10
23	c	505	CLA	C1D-ND-C4D	-8.46	100.32	106.33
23	C	513	CLA	C1D-ND-C4D	-8.46	100.32	106.33
23	C	507	CLA	C1D-ND-C4D	-8.46	100.33	106.33
23	B	606	CLA	C2D-C1D-ND	8.44	116.32	110.10
23	C	509	CLA	C1D-ND-C4D	-8.42	100.35	106.33
23	C	510	CLA	C2D-C1D-ND	8.41	116.30	110.10
23	B	608	CLA	C2D-C1D-ND	8.41	116.30	110.10
23	c	509	CLA	C2D-C1D-ND	8.40	116.29	110.10
23	B	616	CLA	C1D-ND-C4D	-8.39	100.38	106.33
23	C	503	CLA	C1D-ND-C4D	-8.35	100.40	106.33
23	b	610	CLA	C2D-C1D-ND	8.35	116.26	110.10
23	b	609	CLA	C1D-ND-C4D	-8.31	100.44	106.33
23	A	404[B]	CLA	C2D-C1D-ND	8.28	116.20	110.10
23	A	405[A]	CLA	C2D-C1D-ND	8.25	116.18	110.10
23	c	506	CLA	C2D-C1D-ND	8.21	116.15	110.10
23	B	601	CLA	C2D-C1D-ND	8.21	116.15	110.10
23	C	509	CLA	C2D-C1D-ND	8.16	116.12	110.10
23	c	507	CLA	C2D-C1D-ND	8.16	116.12	110.10
23	C	508	CLA	C2D-C1D-ND	8.16	116.12	110.10
23	A	406[A]	CLA	C2D-C1D-ND	8.15	116.11	110.10
23	b	616	CLA	C2D-C1D-ND	8.15	116.11	110.10
24	a	408[A]	PHO	O2D-CGD-CBD	8.14	121.31	111.00
23	C	512	CLA	C2D-C1D-ND	8.11	116.08	110.10
23	B	610	CLA	C1D-ND-C4D	-8.10	100.58	106.33
23	b	601	CLA	C2D-C1D-ND	8.09	116.07	110.10
23	D	404[B]	CLA	C2D-C1D-ND	8.08	116.06	110.10
23	c	511	CLA	C1D-ND-C4D	-8.06	100.61	106.33
23	a	405[B]	CLA	C2D-C1D-ND	8.03	116.02	110.10
23	C	514	CLA	C2D-C1D-ND	8.03	116.02	110.10
23	b	613	CLA	C2D-C1D-ND	8.02	116.02	110.10
23	C	511	CLA	C2D-C1D-ND	8.02	116.01	110.10
23	c	505	CLA	C2D-C1D-ND	8.00	116.00	110.10
23	b	602	CLA	C2D-C1D-ND	8.00	116.00	110.10
23	A	406[B]	CLA	C2D-C1D-ND	7.97	115.98	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	602	CLA	C2D-C1D-ND	7.94	115.95	110.10
23	d	402[B]	CLA	C2D-C1D-ND	7.94	115.95	110.10
23	C	513	CLA	C4A-NA-C1A	-7.92	103.14	106.71
23	A	405[B]	CLA	C2D-C1D-ND	7.92	115.94	110.10
23	D	405	CLA	C2D-C1D-ND	7.92	115.94	110.10
23	b	604	CLA	C1D-ND-C4D	-7.89	100.73	106.33
23	c	510	CLA	C2D-C1D-ND	7.89	115.92	110.10
23	a	407[B]	CLA	C2D-C1D-ND	7.89	115.92	110.10
23	B	616	CLA	C2D-C1D-ND	7.88	115.91	110.10
23	C	506	CLA	C2D-C1D-ND	7.85	115.89	110.10
23	c	513	CLA	C2D-C1D-ND	7.84	115.88	110.10
24	a	416[A]	PHO	O2D-CGD-CBD	7.83	120.91	111.00
23	d	402[A]	CLA	C2D-C1D-ND	7.82	115.87	110.10
23	b	615	CLA	C2D-C1D-ND	7.79	115.85	110.10
23	c	508	CLA	C2D-C1D-ND	7.79	115.84	110.10
23	c	502	CLA	C2D-C1D-ND	7.75	115.82	110.10
23	C	504	CLA	C4A-NA-C1A	-7.75	103.22	106.71
23	B	611	CLA	CHD-C4C-C3C	-7.75	113.45	124.84
23	C	502	CLA	C2D-C1D-ND	7.73	115.80	110.10
23	C	503	CLA	C2D-C1D-ND	7.70	115.78	110.10
24	A	416[B]	PHO	O2D-CGD-CBD	7.67	120.72	111.00
23	c	514	CLA	C2D-C1D-ND	7.66	115.75	110.10
23	A	404[A]	CLA	C2D-C1D-ND	7.64	115.73	110.10
24	a	408[B]	PHO	O2D-CGD-CBD	7.60	120.63	111.00
23	b	605	CLA	CHD-C1D-ND	-7.54	117.53	124.45
23	B	609	CLA	C2D-C1D-ND	7.51	115.64	110.10
23	c	502	CLA	CHD-C1D-ND	-7.50	117.56	124.45
23	b	606	CLA	C2D-C1D-ND	7.49	115.62	110.10
26	X	101	SQD	O6-C1-C2	7.49	119.99	108.30
24	A	416[A]	PHO	O2D-CGD-CBD	7.46	120.44	111.00
23	B	604	CLA	C1D-ND-C4D	-7.38	101.09	106.33
23	c	511	CLA	C2D-C1D-ND	7.35	115.52	110.10
24	a	416[B]	PHO	O2D-CGD-CBD	7.34	120.30	111.00
23	c	502	CLA	CMD-C2D-C1D	7.32	137.62	124.71
23	a	405[A]	CLA	C2D-C1D-ND	7.32	115.50	110.10
23	b	605	CLA	CMD-C2D-C1D	7.32	137.61	124.71
23	B	605	CLA	CHD-C4C-C3C	-7.30	114.11	124.84
23	b	609	CLA	C2D-C1D-ND	7.21	115.42	110.10
23	b	612	CLA	C2D-C1D-ND	7.21	115.42	110.10
23	D	404[A]	CLA	C4A-NA-C1A	-7.21	103.46	106.71
23	b	604	CLA	C2D-C1D-ND	7.20	115.41	110.10
23	B	614	CLA	CMD-C2D-C1D	7.17	137.35	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	407[B]	PHO	O2D-CGD-CBD	7.14	120.05	111.00
23	B	609	CLA	C4A-NA-C1A	-7.14	103.50	106.71
23	C	508	CLA	CMD-C2D-C1D	7.12	137.26	124.71
23	c	508	CLA	O2D-CGD-CBD	7.12	123.92	111.27
34	b	623	HTG	C1'-S1-C1	7.10	113.37	100.09
23	a	405[B]	CLA	CMD-C2D-C1D	7.10	137.22	124.71
23	b	606	CLA	C4A-NA-C1A	-7.10	103.52	106.71
23	B	610	CLA	O2D-CGD-CBD	7.08	123.86	111.27
23	C	507	CLA	C2D-C1D-ND	7.07	115.32	110.10
23	b	602	CLA	C4A-NA-C1A	-7.04	103.54	106.71
23	B	611	CLA	CMD-C2D-C1D	6.96	136.98	124.71
23	C	513	CLA	C2D-C1D-ND	6.96	115.23	110.10
23	C	502	CLA	O2D-CGD-CBD	6.94	123.60	111.27
23	c	504	CLA	C4A-NA-C1A	-6.94	103.59	106.71
23	B	615	CLA	C4A-NA-C1A	-6.94	103.59	106.71
23	b	616	CLA	O2D-CGD-CBD	6.93	123.58	111.27
23	C	504	CLA	CMD-C2D-C1D	6.90	136.88	124.71
23	C	511	CLA	CMD-C2D-C1D	6.87	136.82	124.71
23	b	615	CLA	C4A-NA-C1A	-6.86	103.62	106.71
23	b	611	CLA	CMD-C2D-C1D	6.86	136.81	124.71
23	b	616	CLA	CMD-C2D-C1D	6.84	136.77	124.71
23	b	616	CLA	CHD-C4C-C3C	-6.84	114.78	124.84
23	B	605	CLA	C4A-NA-C1A	-6.83	103.64	106.71
23	a	407[B]	CLA	CHD-C1D-ND	-6.82	118.19	124.45
23	b	611	CLA	CHD-C4C-C3C	-6.81	114.82	124.84
23	b	614	CLA	O2D-CGD-CBD	6.80	123.36	111.27
23	A	404[B]	CLA	CMD-C2D-C1D	6.80	136.70	124.71
23	c	512	CLA	CHD-C4C-C3C	-6.79	114.86	124.84
23	B	606	CLA	CMD-C2D-C1D	6.76	136.63	124.71
23	B	616	CLA	O2D-CGD-CBD	6.74	123.25	111.27
23	c	507	CLA	CMD-C2D-C1D	6.74	136.59	124.71
23	b	606	CLA	CMD-C2D-C1D	6.73	136.57	124.71
23	A	406[B]	CLA	CHD-C1D-ND	-6.72	118.27	124.45
23	B	606	CLA	O2D-CGD-CBD	6.72	123.22	111.27
23	c	508	CLA	CHD-C1D-ND	-6.72	118.28	124.45
23	c	514	CLA	CMD-C2D-C1D	6.71	136.54	124.71
23	B	605	CLA	CMD-C2D-C1D	6.71	136.53	124.71
23	A	404[A]	CLA	CMD-C2D-C1D	6.70	136.53	124.71
23	b	610	CLA	CHD-C4C-C3C	-6.68	115.02	124.84
23	C	507	CLA	CMD-C2D-C1D	6.67	136.47	124.71
23	D	404[B]	CLA	C4A-NA-C1A	-6.66	103.71	106.71
23	B	616	CLA	CHD-C4C-C3C	-6.65	115.06	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	508	CLA	CMD-C2D-C1D	6.63	136.41	124.71
23	b	610	CLA	O2D-CGD-CBD	6.63	123.05	111.27
23	B	603	CLA	CHD-C4C-C3C	-6.61	115.12	124.84
23	a	406[A]	CLA	CHD-C4C-C3C	-6.61	115.12	124.84
23	B	604	CLA	C2C-C1C-NC	6.61	116.17	109.97
23	c	514	CLA	CHD-C1D-ND	-6.59	118.40	124.45
23	b	603	CLA	CHD-C4C-C3C	-6.58	115.17	124.84
23	C	507	CLA	C2C-C1C-NC	6.57	116.12	109.97
23	b	605	CLA	CHD-C4C-C3C	-6.56	115.19	124.84
23	C	509	CLA	C2C-C1C-NC	6.56	116.11	109.97
23	C	513	CLA	CHD-C4C-C3C	-6.54	115.22	124.84
23	b	616	CLA	C4A-NA-C1A	-6.53	103.77	106.71
23	A	408	CLA	CHD-C1D-ND	-6.51	118.47	124.45
23	B	606	CLA	C4A-NA-C1A	-6.51	103.78	106.71
23	c	504	CLA	CMD-C2D-C1D	6.51	136.18	124.71
23	C	507	CLA	CHD-C1D-ND	-6.51	118.48	124.45
23	C	508	CLA	O2D-CGD-CBD	6.50	122.83	111.27
23	b	604	CLA	O2D-CGD-CBD	6.49	122.81	111.27
23	d	402[A]	CLA	C2C-C1C-NC	6.49	116.05	109.97
23	c	511	CLA	C4A-NA-C1A	-6.46	103.80	106.71
23	C	504	CLA	CHD-C4C-C3C	-6.45	115.36	124.84
23	c	505	CLA	CHD-C1D-ND	-6.44	118.53	124.45
23	B	601	CLA	CMD-C2D-C1D	6.44	136.07	124.71
23	A	404[A]	CLA	C4A-NA-C1A	-6.44	103.81	106.71
26	A	410[A]	SQD	O6-C1-C2	6.44	118.36	108.30
23	b	610	CLA	CMD-C2D-C1D	6.43	136.04	124.71
23	d	402[B]	CLA	C4A-NA-C1A	-6.42	103.82	106.71
23	B	602	CLA	O2D-CGD-CBD	6.41	122.66	111.27
23	a	406[B]	CLA	CMD-C2D-C1D	6.41	136.00	124.71
23	c	513	CLA	C4A-NA-C1A	-6.40	103.83	106.71
23	a	407[A]	CLA	CHD-C4C-C3C	-6.40	115.43	124.84
23	b	613	CLA	C4A-NA-C1A	-6.40	103.83	106.71
23	C	511	CLA	CHD-C1D-ND	-6.39	118.58	124.45
23	c	507	CLA	CHD-C1D-ND	-6.37	118.60	124.45
23	a	409	CLA	CHD-C4C-C3C	-6.37	115.48	124.84
23	C	512	CLA	CHD-C4C-C3C	-6.36	115.50	124.84
23	B	606	CLA	CHD-C1D-ND	-6.35	118.62	124.45
23	b	602	CLA	CHD-C4C-C3C	-6.35	115.50	124.84
23	c	503	CLA	C2C-C1C-NC	6.35	115.92	109.97
23	B	604	CLA	CMD-C2D-C1D	6.34	135.88	124.71
23	a	406[B]	CLA	CHD-C1D-ND	-6.34	118.63	124.45
23	B	610	CLA	CHD-C4C-C3C	-6.34	115.52	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	606	CLA	CHD-C4C-C3C	-6.33	115.53	124.84
23	C	513	CLA	CMD-C2D-C1D	6.33	135.87	124.71
23	B	616	CLA	C2C-C1C-NC	6.30	115.88	109.97
23	b	613	CLA	CMD-C2D-C1D	6.30	135.82	124.71
23	B	615	CLA	CHD-C4C-C3C	-6.30	115.58	124.84
23	b	601	CLA	CMD-C2D-C1D	6.29	135.80	124.71
26	X	101	SQD	O47-C7-C8	6.27	125.02	111.50
23	c	509	CLA	CHD-C4C-C3C	-6.27	115.63	124.84
23	C	506	CLA	CMD-C2D-C1D	6.26	135.75	124.71
34	D	412	HTG	C1'-S1-C1	6.25	111.78	100.09
23	B	614	CLA	C2C-C1C-NC	6.25	115.82	109.97
23	B	614	CLA	CHD-C1D-ND	-6.24	118.72	124.45
23	B	601	CLA	CHD-C1D-ND	-6.24	118.72	124.45
24	A	407[A]	PHO	O2D-CGD-CBD	6.23	118.89	111.00
23	d	402[B]	CLA	CMD-C2D-C1D	6.22	135.68	124.71
23	c	505	CLA	CMD-C2D-C1D	6.21	135.66	124.71
23	c	504	CLA	CHD-C4C-C3C	-6.21	115.72	124.84
23	C	505	CLA	CMD-C2D-C1D	6.21	135.65	124.71
23	a	405[A]	CLA	C2C-C1C-NC	6.21	115.79	109.97
23	c	503	CLA	CHD-C4C-C3C	-6.20	115.72	124.84
23	b	604	CLA	C2C-C1C-NC	6.20	115.78	109.97
23	D	405	CLA	CHD-C4C-C3C	-6.20	115.73	124.84
34	c	522	HTG	C1'-S1-C1	6.19	111.67	100.09
23	D	404[B]	CLA	CMD-C2D-C1D	6.19	135.63	124.71
23	B	606	CLA	CHD-C4C-C3C	-6.19	115.75	124.84
23	b	607	CLA	CHD-C4C-C3C	-6.19	115.75	124.84
23	a	405[A]	CLA	C4A-NA-C1A	-6.18	103.93	106.71
23	a	407[B]	CLA	CMD-C2D-C1D	6.17	135.59	124.71
23	a	407[A]	CLA	C4A-NA-C1A	-6.17	103.93	106.71
23	a	406[B]	CLA	CHD-C4C-C3C	-6.17	115.78	124.84
23	b	601	CLA	CHD-C4C-C3C	-6.16	115.79	124.84
23	A	406[B]	CLA	C4A-NA-C1A	-6.16	103.94	106.71
23	c	510	CLA	CMD-C2D-C1D	6.15	135.55	124.71
23	A	406[A]	CLA	CHD-C1D-ND	-6.14	118.81	124.45
23	B	601	CLA	CHD-C4C-C3C	-6.14	115.81	124.84
23	b	602	CLA	O2D-CGD-CBD	6.14	122.18	111.27
23	C	506	CLA	CHD-C1D-ND	-6.14	118.81	124.45
23	a	407[A]	CLA	CHD-C1D-ND	-6.14	118.81	124.45
23	A	404[B]	CLA	CHD-C1D-ND	-6.13	118.82	124.45
23	c	513	CLA	CHD-C4C-C3C	-6.13	115.83	124.84
23	c	506	CLA	C4A-NA-C1A	-6.13	103.95	106.71
23	B	609	CLA	CHD-C1D-ND	-6.12	118.83	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	511	CLA	CHD-C4C-C3C	-6.12	115.84	124.84
23	C	508	CLA	CHD-C4C-C3C	-6.12	115.84	124.84
23	b	607	CLA	CMD-C2D-C1D	6.12	135.50	124.71
23	A	404[A]	CLA	CHD-C1D-ND	-6.11	118.83	124.45
23	C	505	CLA	CHD-C1D-ND	-6.11	118.84	124.45
23	d	403	CLA	CHD-C1D-ND	-6.11	118.84	124.45
23	c	511	CLA	CHD-C4C-C3C	-6.11	115.86	124.84
23	C	514	CLA	CHD-C4C-C3C	-6.11	115.86	124.84
23	D	404[A]	CLA	CMD-C2D-C1D	6.10	135.47	124.71
23	C	502	CLA	CMD-C2D-C1D	6.09	135.45	124.71
23	b	613	CLA	CHD-C4C-C3C	-6.08	115.90	124.84
23	B	612	CLA	CHD-C4C-C3C	-6.08	115.91	124.84
23	a	405[A]	CLA	CMD-C2D-C1D	6.07	135.41	124.71
23	C	505	CLA	C2C-C1C-NC	6.05	115.64	109.97
23	b	601	CLA	O2D-CGD-CBD	6.05	122.02	111.27
23	A	408	CLA	C2C-C1C-NC	6.04	115.63	109.97
23	b	615	CLA	CMD-C2D-C1D	6.04	135.36	124.71
23	a	405[B]	CLA	CHD-C1D-ND	-6.04	118.90	124.45
23	b	602	CLA	CMD-C2D-C1D	6.04	135.35	124.71
23	C	508	CLA	CHD-C1D-ND	-6.03	118.91	124.45
23	C	509	CLA	CHD-C4C-C3C	-6.02	115.99	124.84
23	A	404[B]	CLA	CHD-C4C-C3C	-6.02	115.99	124.84
23	c	507	CLA	C2C-C1C-NC	6.02	115.61	109.97
23	B	609	CLA	CMD-C2D-C1D	6.01	135.30	124.71
23	B	603	CLA	O2D-CGD-CBD	6.01	121.94	111.27
23	b	612	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
23	D	405	CLA	CMD-C2D-C1D	6.00	135.29	124.71
23	d	402[B]	CLA	C2C-C1C-NC	5.99	115.58	109.97
23	b	602	CLA	CHD-C1D-ND	-5.99	118.95	124.45
23	B	603	CLA	CMD-C2D-C1D	5.98	135.26	124.71
23	B	604	CLA	C2D-C1D-ND	5.98	114.51	110.10
26	B	620	SQD	O6-C1-C2	5.97	117.63	108.30
23	B	602	CLA	C2C-C1C-NC	5.95	115.54	109.97
23	a	407[B]	CLA	C4A-NA-C1A	-5.94	104.03	106.71
23	b	614	CLA	CHD-C4C-C3C	-5.94	116.11	124.84
23	c	511	CLA	CMD-C2D-C1D	5.93	135.17	124.71
23	c	502	CLA	C4A-NA-C1A	-5.93	104.04	106.71
23	a	406[A]	CLA	CMD-C2D-C1D	5.93	135.16	124.71
23	C	505	CLA	CHD-C4C-C3C	-5.93	116.13	124.84
23	b	613	CLA	C2C-C1C-NC	5.93	115.52	109.97
23	B	613	CLA	C2C-C1C-NC	5.92	115.52	109.97
25	K	103	BCR	C33-C5-C6	-5.92	117.89	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406[A]	CLA	C4A-NA-C1A	-5.91	104.05	106.71
23	D	404[A]	CLA	CHD-C1D-ND	-5.91	119.02	124.45
23	B	609	CLA	CHD-C4C-C3C	-5.91	116.15	124.84
23	c	505	CLA	C2C-C1C-NC	5.91	115.50	109.97
23	c	510	CLA	CHD-C4C-C3C	-5.90	116.16	124.84
23	A	405[B]	CLA	CMD-C2D-C1D	5.90	135.12	124.71
23	D	405	CLA	O2D-CGD-CBD	5.90	121.74	111.27
23	D	404[B]	CLA	C2C-C1C-NC	5.89	115.49	109.97
23	B	602	CLA	C4A-NA-C1A	-5.89	104.06	106.71
23	A	406[A]	CLA	CMD-C2D-C1D	5.89	135.10	124.71
23	B	603	CLA	C4A-NA-C1A	-5.88	104.06	106.71
23	b	608	CLA	CHD-C4C-C3C	-5.88	116.20	124.84
23	c	504	CLA	CHD-C1D-ND	-5.88	119.05	124.45
23	d	403	CLA	O2D-CGD-CBD	5.88	121.71	111.27
23	D	404[A]	CLA	C2C-C1C-NC	5.88	115.48	109.97
23	b	601	CLA	CHD-C1D-ND	-5.87	119.06	124.45
23	A	408	CLA	CHD-C4C-C3C	-5.87	116.21	124.84
23	C	502	CLA	CHD-C4C-C3C	-5.87	116.21	124.84
23	B	607	CLA	CHD-C4C-C3C	-5.87	116.22	124.84
23	B	608	CLA	CHD-C4C-C3C	-5.86	116.23	124.84
23	D	405	CLA	C4A-NA-C1A	-5.85	104.08	106.71
23	B	605	CLA	CHD-C1D-ND	-5.85	119.08	124.45
23	A	406[A]	CLA	CHD-C4C-C3C	-5.85	116.25	124.84
23	B	602	CLA	CHD-C4C-C3C	-5.84	116.25	124.84
23	A	404[A]	CLA	C2C-C1C-NC	5.84	115.44	109.97
23	c	509	CLA	C2C-C1C-NC	5.84	115.44	109.97
34	d	410	HTG	C1'-S1-C1	5.84	111.01	100.09
41	V	201	HEC	CBD-CAD-C3D	-5.83	102.67	112.62
23	b	609	CLA	C4A-NA-C1A	-5.83	104.09	106.71
23	d	403	CLA	CMD-C2D-C1D	5.83	134.98	124.71
23	a	406[B]	CLA	C2C-C1C-NC	5.82	115.43	109.97
23	C	510	CLA	CHD-C1D-ND	-5.82	119.10	124.45
23	c	507	CLA	CHD-C4C-C3C	-5.82	116.28	124.84
23	b	604	CLA	CMD-C2D-C1D	5.82	134.97	124.71
26	A	410[B]	SQD	O6-C1-C2	5.82	117.39	108.30
23	C	504	CLA	CHD-C1D-ND	-5.82	119.11	124.45
23	A	405[B]	CLA	CHD-C4C-C3C	-5.81	116.30	124.84
33	C	501	LMG	C7-O1-C1	-5.81	102.39	113.74
23	c	506	CLA	CHD-C4C-C3C	-5.80	116.31	124.84
23	C	511	CLA	O2D-CGD-CBD	5.80	121.57	111.27
23	B	608	CLA	CHD-C1D-ND	-5.80	119.13	124.45
23	A	408	CLA	CMD-C2D-C1D	5.79	134.92	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	404[B]	CLA	CHD-C1D-ND	-5.79	119.13	124.45
23	b	607	CLA	CHD-C1D-ND	-5.78	119.15	124.45
23	b	611	CLA	CHD-C1D-ND	-5.77	119.15	124.45
23	C	503	CLA	CHD-C4C-C3C	-5.77	116.35	124.84
23	A	405[A]	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
23	a	409	CLA	C2C-C1C-NC	5.76	115.37	109.97
23	C	514	CLA	CHD-C1D-ND	-5.76	119.16	124.45
23	b	609	CLA	CHD-C4C-C3C	-5.76	116.38	124.84
23	C	510	CLA	CHD-C4C-C3C	-5.76	116.38	124.84
23	A	405[B]	CLA	CHD-C1D-ND	-5.75	119.17	124.45
23	C	506	CLA	CHD-C4C-C3C	-5.75	116.39	124.84
23	C	510	CLA	CMD-C2D-C1D	5.75	134.84	124.71
23	d	403	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
25	D	406	BCR	C7-C8-C9	-5.74	117.57	126.23
23	C	506	CLA	C4A-NA-C1A	-5.73	104.13	106.71
23	C	514	CLA	CMD-C2D-C1D	5.73	134.81	124.71
23	b	609	CLA	C2C-C1C-NC	5.72	115.33	109.97
23	B	613	CLA	CHD-C1D-ND	-5.71	119.20	124.45
23	b	605	CLA	O2D-CGD-CBD	5.71	121.42	111.27
23	b	603	CLA	C2C-C1C-NC	5.71	115.32	109.97
23	c	508	CLA	C2C-C1C-NC	5.71	115.32	109.97
23	c	514	CLA	C4A-NA-C1A	-5.70	104.14	106.71
23	d	402[B]	CLA	CHD-C1D-ND	-5.70	119.22	124.45
26	a	411[A]	SQD	O6-C1-C2	5.69	117.19	108.30
23	b	611	CLA	O2D-CGD-CBD	5.69	121.38	111.27
23	B	606	CLA	C2C-C1C-NC	5.69	115.30	109.97
23	C	510	CLA	C2C-C1C-NC	5.68	115.29	109.97
23	B	604	CLA	CHD-C4C-C3C	-5.68	116.50	124.84
23	B	604	CLA	C1-C2-C3	-5.67	116.23	126.04
23	b	601	CLA	C4A-NA-C1A	-5.67	104.16	106.71
23	c	512	CLA	CHD-C1D-ND	-5.66	119.25	124.45
23	C	503	CLA	CHD-C1D-ND	-5.66	119.25	124.45
23	C	512	CLA	CMD-C2D-C1D	5.66	134.69	124.71
23	a	409	CLA	O2D-CGD-CBD	5.64	121.30	111.27
23	d	402[B]	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
26	b	620	SQD	O6-C1-C2	5.64	117.11	108.30
26	A	410[A]	SQD	C1-O5-C5	-5.64	102.61	113.69
23	B	602	CLA	CMD-C2D-C1D	5.64	134.65	124.71
39	F	102	HEM	CAD-CBD-CGD	5.63	125.72	113.60
34	C	522	HTG	C1'-S1-C1	5.63	110.62	100.09
23	B	611	CLA	CMB-C2B-C1B	5.62	137.11	128.46
23	B	611	CLA	C3D-C2D-C1D	-5.62	98.16	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	509	CLA	O2D-CGD-CBD	5.62	121.25	111.27
23	c	514	CLA	C2C-C1C-NC	5.62	115.23	109.97
23	C	509	CLA	C3C-C4C-NC	5.61	116.86	110.57
23	C	511	CLA	C2C-C1C-NC	5.60	115.22	109.97
23	B	612	CLA	CHD-C1D-ND	-5.60	119.31	124.45
23	b	604	CLA	CHD-C1D-ND	-5.60	119.31	124.45
23	b	615	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
23	c	506	CLA	O2D-CGD-CBD	5.59	121.20	111.27
23	b	608	CLA	CHD-C1D-ND	-5.59	119.32	124.45
23	c	512	CLA	CMD-C2D-C1D	5.58	134.55	124.71
23	c	508	CLA	CHD-C4C-C3C	-5.58	116.63	124.84
23	B	601	CLA	O2D-CGD-CBD	5.58	121.18	111.27
23	b	607	CLA	C2C-C1C-NC	5.57	115.19	109.97
34	B	623	HTG	C1'-S1-C1	5.56	110.50	100.09
23	D	404[B]	CLA	CHD-C4C-C3C	-5.55	116.68	124.84
23	B	607	CLA	O2D-CGD-CBD	5.55	121.13	111.27
23	A	405[A]	CLA	C2C-C1C-NC	5.54	115.17	109.97
23	b	615	CLA	C2C-C1C-NC	5.54	115.17	109.97
23	D	404[A]	CLA	CHD-C4C-C3C	-5.54	116.70	124.84
23	b	604	CLA	CHD-C4C-C3C	-5.54	116.70	124.84
23	B	605	CLA	O2D-CGD-CBD	5.53	121.10	111.27
23	A	406[B]	CLA	CMD-C2D-C1D	5.53	134.46	124.71
23	A	406[B]	CLA	CHD-C4C-C3C	-5.53	116.72	124.84
23	B	603	CLA	C2C-C1C-NC	5.52	115.14	109.97
23	C	503	CLA	C2C-C1C-NC	5.51	115.14	109.97
23	a	405[A]	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
23	a	406[A]	CLA	C2C-C1C-NC	5.50	115.13	109.97
23	b	606	CLA	CHD-C1D-ND	-5.50	119.40	124.45
23	b	611	CLA	C2C-C1C-NC	5.50	115.12	109.97
23	b	608	CLA	C4A-NA-C1A	-5.50	104.23	106.71
23	d	402[A]	CLA	CHD-C4C-C3C	-5.50	116.76	124.84
23	a	409	CLA	CMD-C2D-C1D	5.49	134.39	124.71
23	a	406[A]	CLA	CHD-C1D-ND	-5.49	119.41	124.45
23	B	611	CLA	CHD-C1D-ND	-5.49	119.41	124.45
23	b	614	CLA	CHD-C1D-ND	-5.49	119.41	124.45
23	a	407[A]	CLA	CMD-C2D-C1D	5.49	134.38	124.71
23	b	608	CLA	O2D-CGD-CBD	5.48	121.00	111.27
23	C	513	CLA	O2D-CGD-CBD	5.47	121.00	111.27
23	c	506	CLA	CHD-C1D-ND	-5.47	119.42	124.45
23	B	615	CLA	CMD-C2D-C1D	5.46	134.34	124.71
23	c	506	CLA	C2C-C1C-NC	5.46	115.08	109.97
23	c	513	CLA	O2D-CGD-CBD	5.46	120.96	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	616	CLA	C3C-C4C-NC	5.46	116.69	110.57
23	B	607	CLA	C2C-C1C-NC	5.45	115.08	109.97
23	B	610	CLA	C4A-NA-C1A	-5.45	104.25	106.71
23	c	511	CLA	CHD-C1D-ND	-5.45	119.45	124.45
23	B	614	CLA	C3D-C2D-C1D	-5.45	98.40	105.83
23	B	610	CLA	CMD-C2D-C1D	5.44	134.31	124.71
23	B	601	CLA	C4A-NA-C1A	-5.44	104.26	106.71
23	d	402[A]	CLA	CMD-C2D-C1D	5.44	134.30	124.71
23	B	614	CLA	CHD-C4C-C3C	-5.44	116.85	124.84
23	b	603	CLA	C4A-NA-C1A	-5.43	104.26	106.71
23	A	408	CLA	C3D-C2D-C1D	-5.43	98.43	105.83
23	C	506	CLA	C2C-C1C-NC	5.42	115.05	109.97
23	B	613	CLA	CMD-C2D-C1D	5.42	134.26	124.71
23	C	503	CLA	O2D-CGD-CBD	5.42	120.90	111.27
23	C	514	CLA	C4A-NA-C1A	-5.42	104.27	106.71
23	B	603	CLA	CHD-C1D-ND	-5.42	119.47	124.45
23	C	503	CLA	CMD-C2D-C1D	5.42	134.26	124.71
23	B	609	CLA	C2C-C1C-NC	5.41	115.04	109.97
23	b	614	CLA	O2D-CGD-O1D	-5.41	113.26	123.84
23	B	615	CLA	CHD-C1D-ND	-5.41	119.48	124.45
23	b	607	CLA	C3D-C2D-C1D	-5.41	98.45	105.83
23	C	502	CLA	O2D-CGD-O1D	-5.41	113.26	123.84
23	A	405[A]	CLA	CHD-C1D-ND	-5.41	119.48	124.45
23	b	613	CLA	CHD-C1D-ND	-5.41	119.48	124.45
23	B	602	CLA	CHD-C1D-ND	-5.40	119.49	124.45
23	B	608	CLA	CMD-C2D-C1D	5.39	134.22	124.71
24	a	416[A]	PHO	C1-C2-C3	-5.39	116.72	126.04
23	A	405[A]	CLA	C4A-NA-C1A	-5.38	104.29	106.71
26	B	620	SQD	O47-C7-C8	5.38	123.09	111.50
23	c	514	CLA	CHD-C4C-C3C	-5.38	116.94	124.84
23	B	607	CLA	CHD-C1D-ND	-5.37	119.52	124.45
23	B	608	CLA	O2D-CGD-CBD	5.37	120.81	111.27
23	b	616	CLA	C3D-C2D-C1D	-5.37	98.50	105.83
23	A	405[B]	CLA	C2C-C1C-NC	5.37	115.00	109.97
23	B	610	CLA	C3D-C2D-C1D	-5.36	98.52	105.83
23	C	512	CLA	C2C-C1C-NC	5.36	114.99	109.97
23	b	608	CLA	C2C-C1C-NC	5.36	114.99	109.97
23	b	612	CLA	C2C-C1C-NC	5.35	114.99	109.97
23	c	510	CLA	C2C-C1C-NC	5.35	114.99	109.97
23	B	612	CLA	O2D-CGD-CBD	5.35	120.78	111.27
26	A	410[A]	SQD	C1-C2-C3	-5.35	98.86	110.00
23	a	409	CLA	CHD-C1D-ND	-5.34	119.54	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	608	CLA	C2C-C1C-NC	5.34	114.98	109.97
23	c	505	CLA	CHD-C4C-C3C	-5.34	116.99	124.84
23	a	405[A]	CLA	CHD-C1D-ND	-5.34	119.55	124.45
25	t	102	BCR	C33-C5-C6	-5.34	118.53	124.53
23	b	610	CLA	C2C-C1C-NC	5.33	114.96	109.97
23	C	506	CLA	O2D-CGD-CBD	5.32	120.73	111.27
23	B	604	CLA	C3C-C4C-NC	5.32	116.54	110.57
23	b	605	CLA	C2C-C1C-NC	5.32	114.96	109.97
23	C	514	CLA	C2C-C1C-NC	5.32	114.95	109.97
23	B	613	CLA	CHD-C4C-C3C	-5.32	117.03	124.84
23	C	502	CLA	C4A-NA-C1A	-5.32	104.32	106.71
23	b	606	CLA	C2C-C1C-NC	5.30	114.94	109.97
23	b	603	CLA	CMD-C2D-C1D	5.29	134.04	124.71
23	b	605	CLA	C3D-C2D-C1D	-5.28	98.62	105.83
23	a	407[B]	CLA	CHD-C4C-C3C	-5.27	117.09	124.84
23	a	405[B]	CLA	CHD-C4C-C3C	-5.27	117.09	124.84
23	B	614	CLA	O2D-CGD-CBD	5.27	120.63	111.27
23	b	615	CLA	CHD-C1D-ND	-5.26	119.62	124.45
23	B	605	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
23	b	611	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
23	C	507	CLA	CHD-C4C-C3C	-5.26	117.11	124.84
23	c	503	CLA	O2D-CGD-CBD	5.26	120.61	111.27
23	c	506	CLA	CMD-C2D-C1D	5.26	133.97	124.71
26	b	620	SQD	O47-C7-C8	5.25	122.82	111.50
29	A	414[B]	PL9	C7-C8-C9	-5.24	118.07	126.79
23	B	612	CLA	C3C-C4C-NC	5.23	116.44	110.57
23	b	616	CLA	CHD-C1D-ND	-5.22	119.66	124.45
23	c	513	CLA	CMD-C2D-C1D	5.22	133.90	124.71
23	c	508	CLA	C4A-NA-C1A	-5.21	104.36	106.71
23	b	609	CLA	CMD-C2D-C1D	5.21	133.89	124.71
23	A	404[B]	CLA	C4A-NA-C1A	-5.21	104.36	106.71
23	B	614	CLA	C4A-NA-C1A	-5.20	104.37	106.71
23	c	511	CLA	C2C-C1C-NC	5.20	114.84	109.97
23	b	614	CLA	C4A-NA-C1A	-5.19	104.37	106.71
23	C	502	CLA	CHD-C1D-ND	-5.19	119.69	124.45
23	c	507	CLA	C4A-NA-C1A	-5.19	104.37	106.71
23	d	402[A]	CLA	CHD-C1D-ND	-5.18	119.69	124.45
23	C	509	CLA	CMD-C2D-C1D	5.18	133.84	124.71
23	C	508	CLA	C2C-C1C-NC	5.16	114.81	109.97
23	c	504	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
23	B	607	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
23	C	512	CLA	CHD-C1D-ND	-5.14	119.73	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	507	CLA	C4A-NA-C1A	-5.14	104.39	106.71
23	C	512	CLA	O2D-CGD-CBD	5.14	120.40	111.27
23	B	610	CLA	C3C-C4C-NC	5.14	116.33	110.57
23	A	404[A]	CLA	CHD-C4C-C3C	-5.13	117.30	124.84
23	A	404[B]	CLA	C2C-C1C-NC	5.13	114.78	109.97
26	f	102	SQD	O47-C7-C8	5.13	122.55	111.50
23	c	505	CLA	O2D-CGD-CBD	5.12	120.37	111.27
23	B	607	CLA	CMD-C2D-C1D	5.11	133.72	124.71
23	B	607	CLA	C4A-NA-C1A	-5.10	104.41	106.71
23	b	609	CLA	CHD-C1D-ND	-5.10	119.77	124.45
23	C	505	CLA	C3D-C2D-C1D	-5.09	98.88	105.83
23	c	504	CLA	C2C-C1C-NC	5.09	114.74	109.97
23	c	509	CLA	C3D-C2D-C1D	-5.08	98.89	105.83
23	b	612	CLA	CMD-C2D-C1D	5.08	133.67	124.71
26	a	411[A]	SQD	O47-C7-C8	5.08	122.45	111.50
23	a	406[A]	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
23	b	612	CLA	C1-C2-C3	-5.07	117.28	126.04
23	D	404[A]	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
23	A	406[B]	CLA	C2C-C1C-NC	5.06	114.71	109.97
23	d	403	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
23	a	405[B]	CLA	C2C-C1C-NC	5.05	114.70	109.97
23	b	614	CLA	CMD-C2D-C1D	5.05	133.60	124.71
23	c	513	CLA	CHD-C1D-ND	-5.04	119.82	124.45
23	c	502	CLA	C2C-C1C-NC	5.04	114.69	109.97
23	B	603	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
23	D	405	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
39	F	102	HEM	CBA-CAA-C2A	-5.03	104.04	112.62
26	b	620	SQD	C1-O5-C5	-5.02	103.83	113.69
23	B	606	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
23	C	513	CLA	CHD-C1D-ND	-5.02	119.84	124.45
23	b	614	CLA	C2C-C1C-NC	5.02	114.67	109.97
23	c	505	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
23	A	405[A]	CLA	O2D-CGD-CBD	5.01	120.17	111.27
23	c	510	CLA	CHD-C1D-ND	-5.01	119.85	124.45
23	D	404[A]	CLA	C3C-C4C-NC	5.00	116.18	110.57
23	C	508	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
23	b	610	CLA	CHD-C1D-ND	-4.99	119.86	124.45
29	a	414[B]	PL9	C7-C3-C4	4.99	120.93	116.88
23	B	611	CLA	CMC-C2C-C1C	4.98	132.63	125.04
29	a	414[A]	PL9	C7-C8-C9	-4.98	118.50	126.79
23	b	613	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
23	b	611	CLA	C3C-C4C-NC	4.97	116.14	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	509	CLA	CMD-C2D-C1D	4.96	133.46	124.71
23	B	616	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
23	a	407[A]	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
23	B	615	CLA	C2C-C1C-NC	4.96	114.62	109.97
23	B	615	CLA	C3D-C2D-C1D	-4.96	99.07	105.83
23	C	507	CLA	C1C-C2C-C3C	-4.95	101.75	106.96
23	b	603	CLA	CHD-C1D-ND	-4.95	119.91	124.45
23	B	613	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
23	b	612	CLA	C3C-C4C-NC	4.95	116.12	110.57
41	v	201	HEC	CBD-CAD-C3D	-4.94	104.18	112.62
29	A	414[A]	PL9	C7-C8-C9	-4.94	118.56	126.79
34	b	622	HTG	C1-O5-C5	4.94	121.69	112.58
23	c	502	CLA	CHD-C4C-C3C	-4.94	117.58	124.84
23	B	613	CLA	C1-C2-C3	-4.93	117.51	126.04
23	B	607	CLA	C3C-C4C-NC	4.93	116.10	110.57
23	c	509	CLA	C4A-NA-C1A	-4.93	104.49	106.71
23	c	506	CLA	C3C-C4C-NC	4.93	116.10	110.57
23	b	610	CLA	C3D-C2D-C1D	-4.92	99.11	105.83
23	c	510	CLA	C1-C2-C3	-4.91	117.55	126.04
23	A	406[B]	CLA	C3D-C4D-ND	4.91	118.18	110.24
25	b	617	BCR	C7-C8-C9	-4.91	118.82	126.23
26	a	411[A]	SQD	C1-O5-C5	-4.91	104.05	113.69
23	B	612	CLA	CMD-C2D-C1D	4.90	133.35	124.71
23	D	405	CLA	CHD-C1D-ND	-4.90	119.95	124.45
23	B	611	CLA	O2D-CGD-CBD	4.89	119.97	111.27
23	B	616	CLA	C4A-NA-C1A	-4.89	104.51	106.71
23	C	504	CLA	C2C-C1C-NC	4.89	114.56	109.97
23	a	407[B]	CLA	C2C-C1C-NC	4.89	114.56	109.97
23	d	402[A]	CLA	C4A-NA-C1A	-4.89	104.51	106.71
23	B	604	CLA	O2D-CGD-CBD	4.89	119.96	111.27
23	C	504	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
23	d	403	CLA	C4A-NA-C1A	-4.88	104.51	106.71
26	a	411[B]	SQD	O6-C1-C2	4.88	115.92	108.30
23	b	606	CLA	O2D-CGD-CBD	4.88	119.93	111.27
23	b	605	CLA	C3D-C4D-ND	4.86	118.10	110.24
23	c	502	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
23	C	510	CLA	C4A-NA-C1A	-4.86	104.52	106.71
39	f	101	HEM	CHC-C4B-NB	4.86	129.71	124.43
23	c	511	CLA	O2D-CGD-CBD	4.85	119.88	111.27
25	T	101	BCR	C11-C10-C9	-4.84	120.40	127.31
23	A	406[B]	CLA	O2D-CGD-CBD	4.84	119.86	111.27
23	C	502	CLA	C2C-C1C-NC	4.83	114.50	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	404[B]	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
23	A	406[A]	CLA	C2C-C1C-NC	4.83	114.50	109.97
23	C	509	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
26	X	101	SQD	C1-O5-C5	-4.83	104.21	113.69
23	c	507	CLA	C3D-C2D-C1D	-4.83	99.25	105.83
23	B	610	CLA	C2C-C1C-NC	4.82	114.49	109.97
23	a	407[A]	CLA	C2C-C1C-NC	4.82	114.49	109.97
26	a	411[B]	SQD	O47-C7-C8	4.82	121.89	111.50
23	a	406[B]	CLA	C3D-C2D-C1D	-4.81	99.26	105.83
23	C	508	CLA	C4A-NA-C1A	-4.81	104.54	106.71
23	D	405	CLA	C3C-C4C-NC	4.81	115.97	110.57
23	b	604	CLA	C1C-C2C-C3C	-4.81	101.90	106.96
23	c	503	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
23	a	407[B]	CLA	C3D-C4D-ND	4.80	118.00	110.24
23	B	608	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
23	c	512	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
23	c	508	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
23	b	604	CLA	C1-C2-C3	-4.79	117.76	126.04
23	B	610	CLA	CHD-C1D-ND	-4.79	120.05	124.45
23	c	510	CLA	O2D-CGD-CBD	4.79	119.78	111.27
23	b	608	CLA	CMD-C2D-C1D	4.79	133.15	124.71
23	A	408	CLA	C3C-C4C-NC	4.78	115.94	110.57
23	c	510	CLA	C3D-C2D-C1D	-4.78	99.30	105.83
23	a	409	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
23	A	405[A]	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
23	B	605	CLA	C3C-C4C-NC	4.78	115.93	110.57
23	B	613	CLA	O2D-CGD-CBD	4.78	119.76	111.27
23	B	616	CLA	CMD-C2D-C1D	4.78	133.13	124.71
25	d	404	BCR	C7-C8-C9	-4.77	119.02	126.23
23	A	408	CLA	C4A-NA-C1A	-4.77	104.56	106.71
23	A	405[A]	CLA	CMD-C2D-C1D	4.77	133.12	124.71
23	C	509	CLA	O2D-CGD-CBD	4.77	119.74	111.27
23	b	604	CLA	C4A-NA-C1A	-4.76	104.56	106.71
23	D	404[B]	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
23	b	603	CLA	C3C-C4C-NC	4.76	115.91	110.57
23	b	607	CLA	C3C-C4C-NC	4.76	115.91	110.57
23	b	616	CLA	C1D-CHD-C4C	-4.76	115.80	126.06
23	a	405[B]	CLA	C4A-NA-C1A	-4.76	104.57	106.71
23	C	505	CLA	C3C-C4C-NC	4.75	115.90	110.57
23	b	614	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
23	B	603	CLA	C3C-C4C-NC	4.75	115.89	110.57
23	c	507	CLA	O2D-CGD-CBD	4.75	119.70	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	507	CLA	O2D-CGD-CBD	4.74	119.70	111.27
23	b	606	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
23	d	403	CLA	C2C-C1C-NC	4.73	114.40	109.97
23	a	409	CLA	C3D-C4D-ND	4.73	117.88	110.24
23	B	605	CLA	C2C-C1C-NC	4.73	114.40	109.97
23	a	406[B]	CLA	C1C-C2C-C3C	-4.72	101.99	106.96
23	a	405[B]	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
23	D	405	CLA	C2C-C1C-NC	4.71	114.38	109.97
23	b	608	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
23	b	609	CLA	C3C-C4C-NC	4.71	115.85	110.57
23	C	511	CLA	C1C-C2C-C3C	-4.71	102.01	106.96
23	c	511	CLA	C1-C2-C3	-4.70	117.91	126.04
23	b	603	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
23	A	405[B]	CLA	C3D-C2D-C1D	-4.69	99.42	105.83
23	C	511	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
23	B	601	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
23	A	405[B]	CLA	C4A-NA-C1A	-4.67	104.61	106.71
23	c	513	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
23	b	602	CLA	C3D-C4D-ND	4.66	117.78	110.24
26	B	620	SQD	O7-S-C6	4.65	112.47	106.94
23	B	609	CLA	C3C-C4C-NC	4.64	115.78	110.57
23	C	505	CLA	C1C-C2C-C3C	-4.64	102.08	106.96
23	b	601	CLA	C2C-C1C-NC	4.63	114.31	109.97
23	B	612	CLA	C3D-C4D-ND	4.63	117.73	110.24
23	c	509	CLA	C3C-C4C-NC	4.63	115.77	110.57
23	a	406[A]	CLA	O2D-CGD-CBD	4.63	119.49	111.27
23	B	616	CLA	C3B-C4B-NB	4.63	115.19	109.21
23	C	508	CLA	C3C-C4C-NC	4.63	115.76	110.57
23	B	608	CLA	C3C-C4C-NC	4.63	115.76	110.57
23	b	604	CLA	C3C-C4C-NC	4.62	115.76	110.57
23	C	510	CLA	O2D-CGD-CBD	4.62	119.48	111.27
23	C	514	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
23	B	611	CLA	C3C-C4C-NC	4.61	115.74	110.57
23	b	602	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
23	C	510	CLA	C3C-C4C-NC	4.60	115.73	110.57
23	b	613	CLA	C3C-C4C-NC	4.60	115.73	110.57
23	b	610	CLA	O2A-CGA-CBA	4.59	126.33	111.91
23	b	603	CLA	C1D-CHD-C4C	-4.59	116.15	126.06
23	B	611	CLA	C3D-C4D-ND	4.59	117.67	110.24
23	c	514	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
23	A	404[A]	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
23	b	611	CLA	C4A-NA-C1A	-4.59	104.64	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	510	CLA	C4A-NA-C1A	-4.59	104.64	106.71
23	B	615	CLA	O2D-CGD-CBD	4.59	119.42	111.27
23	c	512	CLA	C2C-C1C-NC	4.59	114.27	109.97
25	b	617	BCR	C33-C5-C6	-4.59	119.38	124.53
23	d	402[B]	CLA	C3C-C4C-NC	4.58	115.71	110.57
23	a	407[B]	CLA	O2D-CGD-CBD	4.58	119.40	111.27
23	c	508	CLA	C1C-C2C-C3C	-4.58	102.15	106.96
23	C	503	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
23	A	405[A]	CLA	C1C-C2C-C3C	-4.57	102.15	106.96
23	d	402[B]	CLA	O2D-CGD-CBD	4.57	119.39	111.27
23	c	502	CLA	O2D-CGD-O1D	-4.57	114.91	123.84
24	a	416[B]	PHO	C1-C2-C3	-4.57	118.14	126.04
23	b	606	CLA	C1D-CHD-C4C	-4.57	116.21	126.06
23	C	507	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
23	B	610	CLA	O2A-CGA-CBA	4.56	126.23	111.91
23	B	602	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
23	C	511	CLA	C3D-C4D-ND	4.56	117.61	110.24
23	c	504	CLA	C3C-C4C-NC	4.55	115.67	110.57
23	d	402[A]	CLA	C3C-C4C-NC	4.54	115.66	110.57
23	a	409	CLA	C4A-NA-C1A	-4.53	104.67	106.71
23	b	606	CLA	C4-C3-C5	4.53	122.89	115.27
23	A	406[A]	CLA	C3D-C4D-ND	4.53	117.56	110.24
23	B	615	CLA	C3C-C4C-NC	4.53	115.65	110.57
23	C	503	CLA	C4A-NA-C1A	-4.53	104.67	106.71
23	b	614	CLA	C3D-C4D-ND	4.53	117.56	110.24
23	B	606	CLA	C3C-C4C-NC	4.52	115.64	110.57
23	C	512	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
23	d	402[B]	CLA	C3D-C4D-ND	4.52	117.55	110.24
23	c	514	CLA	O2D-CGD-CBD	4.52	119.30	111.27
23	B	601	CLA	C2C-C1C-NC	4.52	114.20	109.97
23	A	406[A]	CLA	O2D-CGD-CBD	4.51	119.28	111.27
23	b	610	CLA	C3C-C4C-NC	4.51	115.63	110.57
23	c	502	CLA	O2D-CGD-CBD	4.51	119.28	111.27
23	B	612	CLA	C2C-C1C-NC	4.51	114.19	109.97
23	C	512	CLA	C3C-C4C-NC	4.51	115.62	110.57
23	C	505	CLA	O2D-CGD-CBD	4.50	119.26	111.27
39	F	102	HEM	CHC-C4B-NB	4.50	129.32	124.43
33	d	411	LMG	O7-C10-C11	4.49	121.18	111.50
23	a	409	CLA	C3C-C4C-NC	4.49	115.61	110.57
23	C	502	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
23	d	402[A]	CLA	C3D-C4D-ND	4.49	117.50	110.24
33	B	621	LMG	O7-C10-C11	4.49	121.18	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	603	CLA	O2D-CGD-CBD	4.49	119.25	111.27
23	c	512	CLA	O2D-CGD-CBD	4.49	119.24	111.27
23	C	506	CLA	C3D-C4D-ND	4.49	117.50	110.24
23	b	601	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
23	b	615	CLA	C3D-C4D-ND	4.48	117.49	110.24
23	a	405[B]	CLA	C3D-C4D-ND	4.48	117.49	110.24
23	B	611	CLA	C1D-CHD-C4C	-4.48	116.39	126.06
23	C	506	CLA	C3C-C4C-NC	4.48	115.60	110.57
23	c	509	CLA	CHD-C1D-ND	-4.47	120.34	124.45
23	b	608	CLA	C1C-C2C-C3C	-4.47	102.26	106.96
23	a	409	CLA	CMC-C2C-C1C	4.47	131.84	125.04
23	C	513	CLA	C3D-C2D-C1D	-4.47	99.74	105.83
23	B	607	CLA	C1C-C2C-C3C	-4.46	102.27	106.96
23	a	407[A]	CLA	O2D-CGD-CBD	4.44	119.17	111.27
23	b	612	CLA	O2D-CGD-CBD	4.44	119.15	111.27
23	c	503	CLA	C3C-C4C-NC	4.44	115.55	110.57
23	C	504	CLA	C3C-C4C-NC	4.43	115.54	110.57
23	D	404[B]	CLA	C3C-C4C-NC	4.43	115.54	110.57
23	B	609	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
23	b	603	CLA	C3D-C4D-ND	4.43	117.41	110.24
23	B	606	CLA	O2D-CGD-O1D	-4.43	115.18	123.84
39	F	102	HEM	C1B-NB-C4B	4.43	109.65	105.07
23	b	609	CLA	O2D-CGD-CBD	4.43	119.14	111.27
23	b	601	CLA	C3D-C4D-ND	4.42	117.39	110.24
23	B	601	CLA	C3C-C4C-NC	4.42	115.53	110.57
25	K	103	BCR	C16-C17-C18	-4.42	121.00	127.31
23	B	602	CLA	C3C-C4C-NC	4.42	115.53	110.57
23	a	406[B]	CLA	C4A-NA-C1A	-4.42	104.72	106.71
23	A	405[B]	CLA	O2D-CGD-CBD	4.41	119.11	111.27
23	C	514	CLA	C3C-C4C-NC	4.41	115.52	110.57
23	a	406[B]	CLA	C3D-C4D-ND	4.41	117.37	110.24
23	C	513	CLA	C3C-C4C-NC	4.41	115.51	110.57
23	c	512	CLA	C3D-C4D-ND	4.40	117.36	110.24
23	C	514	CLA	C3D-C4D-ND	4.40	117.35	110.24
23	c	507	CLA	C3D-C4D-ND	4.39	117.35	110.24
23	c	504	CLA	O2D-CGD-CBD	4.39	119.08	111.27
23	a	405[A]	CLA	C1C-C2C-C3C	-4.39	102.34	106.96
23	b	615	CLA	C3D-C2D-C1D	-4.39	99.84	105.83
23	B	601	CLA	C3D-C4D-ND	4.39	117.34	110.24
23	a	406[A]	CLA	C1C-C2C-C3C	-4.39	102.34	106.96
24	A	416[B]	PHO	C1-C2-C3	-4.39	118.46	126.04
23	c	514	CLA	C3D-C4D-ND	4.39	117.33	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	CMB-C2B-C3B	4.38	132.88	124.68
23	C	514	CLA	O2D-CGD-CBD	4.38	119.05	111.27
29	A	414[B]	PL9	C32-C33-C34	-4.38	117.12	127.66
23	b	602	CLA	C3C-C4C-NC	4.38	115.48	110.57
23	a	406[A]	CLA	C4A-NA-C1A	-4.38	104.74	106.71
23	a	405[B]	CLA	C3B-C4B-NB	4.38	114.87	109.21
23	A	406[A]	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
23	b	607	CLA	C3D-C4D-ND	4.37	117.30	110.24
33	m	101	LMG	O7-C10-C11	4.36	120.91	111.50
23	A	405[A]	CLA	C3D-C4D-ND	4.36	117.30	110.24
23	A	405[B]	CLA	C1C-C2C-C3C	-4.36	102.37	106.96
23	B	615	CLA	C3D-C4D-ND	4.36	117.30	110.24
23	c	511	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
32	E	101[A]	LHG	O7-C7-C8	4.36	120.90	111.50
23	a	409	CLA	C1C-C2C-C3C	-4.36	102.37	106.96
23	a	407[B]	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
23	b	612	CLA	CHD-C1D-ND	-4.36	120.45	124.45
23	b	611	CLA	C3D-C4D-ND	4.36	117.28	110.24
23	C	511	CLA	C1-C2-C3	-4.35	118.51	126.04
23	B	609	CLA	C3D-C4D-ND	4.35	117.28	110.24
23	a	407[A]	CLA	C3C-C4C-NC	4.35	115.45	110.57
23	C	503	CLA	C3C-C4C-NC	4.35	115.45	110.57
23	d	402[A]	CLA	C1C-C2C-C3C	-4.34	102.39	106.96
23	C	504	CLA	C3D-C4D-ND	4.34	117.26	110.24
23	c	512	CLA	C4A-NA-C1A	-4.34	104.76	106.71
33	C	501	LMG	O1-C1-C2	4.33	115.07	108.30
23	c	503	CLA	O2D-CGD-O1D	-4.33	115.37	123.84
23	b	615	CLA	C3C-C4C-NC	4.32	115.42	110.57
23	b	605	CLA	O2D-CGD-O1D	-4.32	115.38	123.84
23	B	616	CLA	C1D-CHD-C4C	-4.32	116.74	126.06
23	b	612	CLA	C4A-NA-C1A	-4.32	104.77	106.71
23	b	616	CLA	C2C-C1C-NC	4.32	114.02	109.97
23	B	609	CLA	O2D-CGD-CBD	4.31	118.93	111.27
23	c	506	CLA	C3D-C4D-ND	4.31	117.21	110.24
26	a	411[A]	SQD	C1-C2-C3	-4.31	101.02	110.00
23	C	503	CLA	C1C-C2C-C3C	-4.30	102.44	106.96
29	A	414[A]	PL9	C32-C33-C34	-4.30	117.31	127.66
23	B	608	CLA	C4A-NA-C1A	-4.30	104.77	106.71
23	B	603	CLA	C1D-CHD-C4C	-4.30	116.79	126.06
23	A	408	CLA	O2D-CGD-CBD	4.29	118.90	111.27
26	A	410[B]	SQD	C1-C2-C3	-4.29	101.05	110.00
33	a	417	LMG	O7-C10-C11	4.29	120.75	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	504	CLA	C1D-CHD-C4C	-4.29	116.81	126.06
23	C	505	CLA	C4A-NA-C1A	-4.29	104.78	106.71
23	a	407[A]	CLA	C3D-C4D-ND	4.29	117.17	110.24
23	B	614	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
24	A	416[B]	PHO	C1A-C2A-C3A	-4.29	98.76	102.84
23	c	506	CLA	C3D-C2D-C1D	-4.28	99.98	105.83
23	a	405[A]	CLA	C3D-C4D-ND	4.28	117.17	110.24
23	C	507	CLA	C3D-C4D-ND	4.28	117.16	110.24
23	c	502	CLA	C3D-C4D-ND	4.28	117.16	110.24
23	b	602	CLA	C2C-C1C-NC	4.28	113.98	109.97
23	b	614	CLA	C3C-C4C-NC	4.28	115.37	110.57
23	C	510	CLA	C3D-C2D-C1D	-4.28	100.00	105.83
23	c	513	CLA	C2C-C1C-NC	4.28	113.98	109.97
23	b	609	CLA	C3D-C2D-C1D	-4.27	100.00	105.83
23	C	509	CLA	CHD-C1D-ND	-4.27	120.53	124.45
26	a	411[A]	SQD	O9-S-C6	4.27	112.01	106.94
31	t	101	LMT	C3'-C4'-C5'	-4.27	101.14	110.93
23	B	602	CLA	C1C-C2C-C3C	-4.27	102.47	106.96
23	c	511	CLA	C3C-C4C-NC	4.26	115.35	110.57
23	d	403	CLA	C3D-C4D-ND	4.26	117.13	110.24
23	a	405[A]	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
32	E	101[B]	LHG	O7-C7-C8	4.26	120.68	111.50
23	b	604	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
23	C	502	CLA	C3C-C4C-NC	4.25	115.34	110.57
26	X	101	SQD	O8-S-C6	4.25	112.51	105.74
23	A	406[B]	CLA	C3D-C2D-C1D	-4.24	100.04	105.83
25	H	101	BCR	C38-C26-C25	-4.24	119.76	124.53
23	A	404[B]	CLA	C1D-CHD-C4C	-4.24	116.91	126.06
23	d	402[B]	CLA	C3D-C2D-C1D	-4.24	100.05	105.83
23	B	608	CLA	C3D-C4D-ND	4.23	117.08	110.24
23	c	504	CLA	C3D-C4D-ND	4.23	117.08	110.24
23	B	602	CLA	C3D-C4D-ND	4.22	117.07	110.24
23	d	402[A]	CLA	C3D-C2D-C1D	-4.22	100.07	105.83
23	C	502	CLA	C3D-C4D-ND	4.22	117.07	110.24
23	c	502	CLA	C1-C2-C3	-4.22	118.74	126.04
33	c	521	LMG	O7-C10-C11	4.22	120.59	111.50
23	C	510	CLA	C3D-C4D-ND	4.21	117.06	110.24
23	b	607	CLA	C4A-NA-C1A	-4.21	104.81	106.71
23	a	406[A]	CLA	C3C-C4C-NC	4.21	115.29	110.57
23	c	503	CLA	C1C-C2C-C3C	-4.21	102.53	106.96
26	A	412	SQD	O8-S-C6	4.21	112.44	105.74
23	D	404[B]	CLA	C3D-C4D-ND	4.20	117.04	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	506	CLA	C3D-C2D-C1D	-4.20	100.10	105.83
23	b	610	CLA	C1-C2-C3	-4.19	118.79	126.04
23	B	613	CLA	C3C-C4C-NC	4.19	115.28	110.57
23	B	611	CLA	CHD-C4C-NC	4.19	130.80	124.20
23	b	616	CLA	C3C-C4C-NC	4.19	115.27	110.57
23	c	510	CLA	C3C-C4C-NC	4.19	115.27	110.57
33	c	521	LMG	O6-C5-C4	4.18	117.29	109.69
32	A	418[A]	LHG	O8-C23-O10	-4.18	113.04	123.59
23	b	606	CLA	C3C-C4C-NC	4.18	115.26	110.57
23	c	512	CLA	C1D-CHD-C4C	-4.18	117.04	126.06
23	b	602	CLA	O2D-CGD-O1D	-4.18	115.66	123.84
23	d	403	CLA	C3C-C4C-NC	4.18	115.26	110.57
23	A	408	CLA	C1C-C2C-C3C	-4.18	102.57	106.96
23	A	405[B]	CLA	C3D-C4D-ND	4.17	116.99	110.24
23	b	608	CLA	C3D-C4D-ND	4.17	116.99	110.24
41	v	201	HEC	CMC-C2C-C1C	-4.17	122.05	128.46
23	C	505	CLA	C3D-C4D-ND	4.17	116.98	110.24
23	b	610	CLA	C3D-C4D-ND	4.17	116.98	110.24
23	c	507	CLA	C1C-C2C-C3C	-4.16	102.58	106.96
23	B	605	CLA	C4-C3-C5	4.16	122.27	115.27
23	c	503	CLA	C3D-C4D-ND	4.16	116.96	110.24
25	B	619	BCR	C24-C23-C22	-4.15	119.96	126.23
23	c	505	CLA	C3B-C4B-NB	4.15	114.57	109.21
23	a	405[A]	CLA	C1D-CHD-C4C	-4.14	117.12	126.06
23	c	512	CLA	C3C-C4C-NC	4.14	115.22	110.57
25	k	101	BCR	C29-C30-C25	4.14	116.86	110.48
23	b	612	CLA	C3D-C4D-ND	4.14	116.94	110.24
29	a	414[B]	PL9	C32-C33-C34	-4.14	117.70	127.66
23	c	513	CLA	C1D-CHD-C4C	-4.14	117.13	126.06
29	a	414[A]	PL9	C7-C3-C4	4.13	120.24	116.88
23	c	505	CLA	C1-O2A-CGA	4.13	127.28	116.44
23	B	606	CLA	C1C-C2C-C3C	-4.13	102.61	106.96
23	c	509	CLA	C1C-C2C-C3C	-4.13	102.61	106.96
23	b	605	CLA	C4A-NA-C1A	-4.13	104.85	106.71
24	A	407[B]	PHO	C1A-C2A-C3A	-4.12	98.91	102.84
23	a	406[A]	CLA	C3D-C4D-ND	4.12	116.91	110.24
23	B	604	CLA	C4A-NA-C1A	-4.12	104.85	106.71
33	C	501	LMG	O7-C10-C11	4.11	120.36	111.50
23	B	602	CLA	CMC-C2C-C1C	4.11	131.30	125.04
23	A	404[B]	CLA	C3D-C4D-ND	4.11	116.88	110.24
23	B	616	CLA	C3D-C4D-ND	4.10	116.88	110.24
23	B	613	CLA	C1C-C2C-C3C	-4.10	102.64	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	412	SQD	O47-C7-C8	4.10	120.34	111.50
23	C	513	CLA	C1D-CHD-C4C	-4.10	117.21	126.06
23	c	508	CLA	C3C-C4C-NC	4.10	115.17	110.57
23	C	504	CLA	C1D-CHD-C4C	-4.10	117.22	126.06
23	c	513	CLA	C3D-C4D-ND	4.10	116.86	110.24
23	b	601	CLA	C3C-C4C-NC	4.09	115.16	110.57
25	d	404	BCR	C40-C30-C25	-4.09	103.66	110.30
23	d	402[A]	CLA	O2D-CGD-CBD	4.09	118.53	111.27
23	b	612	CLA	C4-C3-C5	4.09	122.15	115.27
23	a	406[A]	CLA	CAA-C2A-C3A	-4.09	101.59	112.78
23	B	602	CLA	O2D-CGD-O1D	-4.09	115.85	123.84
23	C	509	CLA	C4A-NA-C1A	-4.09	104.87	106.71
23	B	612	CLA	C3D-C2D-C1D	-4.08	100.26	105.83
23	A	405[B]	CLA	CAA-C2A-C3A	-4.08	101.59	112.78
33	C	521	LMG	O6-C5-C4	4.08	117.11	109.69
23	B	605	CLA	C3D-C4D-ND	4.08	116.84	110.24
23	B	613	CLA	C3D-C4D-ND	4.08	116.84	110.24
23	D	405	CLA	O2D-CGD-O1D	-4.08	115.87	123.84
24	A	407[A]	PHO	C1A-C2A-C3A	-4.08	98.96	102.84
23	B	603	CLA	C3D-C4D-ND	4.08	116.83	110.24
25	C	515	BCR	C7-C8-C9	-4.07	120.08	126.23
23	B	605	CLA	C1D-CHD-C4C	-4.07	117.27	126.06
23	B	616	CLA	O2D-CGD-O1D	-4.07	115.88	123.84
23	D	404[A]	CLA	C3D-C4D-ND	4.07	116.82	110.24
24	A	416[A]	PHO	C1-C2-C3	-4.07	119.00	126.04
26	a	412	SQD	O47-C7-C8	4.07	120.27	111.50
23	D	404[A]	CLA	O2D-CGD-CBD	4.06	118.49	111.27
23	a	405[A]	CLA	CAA-C2A-C3A	-4.06	101.65	112.78
23	a	406[A]	CLA	C1D-CHD-C4C	-4.06	117.30	126.06
23	c	507	CLA	C1-C2-C3	-4.06	119.02	126.04
23	C	512	CLA	C3D-C4D-ND	4.06	116.80	110.24
23	c	514	CLA	C3C-C4C-NC	4.06	115.12	110.57
25	K	102	BCR	C7-C8-C9	-4.06	120.11	126.23
26	B	620	SQD	C3-C4-C5	4.06	117.47	110.24
23	c	514	CLA	C3B-C4B-NB	4.05	114.45	109.21
26	X	101	SQD	C44-O6-C1	-4.05	105.82	113.74
23	A	408	CLA	C3D-C4D-ND	4.05	116.80	110.24
23	B	615	CLA	C1D-CHD-C4C	-4.05	117.32	126.06
23	D	404[B]	CLA	O2D-CGD-CBD	4.04	118.45	111.27
23	C	503	CLA	C3D-C4D-ND	4.04	116.78	110.24
26	a	411[A]	SQD	C44-O6-C1	-4.04	105.84	113.74
23	C	513	CLA	C3D-C4D-ND	4.04	116.77	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	608	CLA	C3B-C4B-NB	4.04	114.43	109.21
23	C	512	CLA	C4A-NA-C1A	-4.03	104.89	106.71
23	A	404[B]	CLA	C3B-C4B-NB	4.03	114.42	109.21
23	A	404[A]	CLA	C3D-C4D-ND	4.03	116.75	110.24
23	b	610	CLA	C1D-CHD-C4C	-4.03	117.37	126.06
23	a	405[A]	CLA	C3C-C4C-NC	4.03	115.09	110.57
23	B	604	CLA	C1D-CHD-C4C	-4.03	117.37	126.06
29	a	414[A]	PL9	C32-C33-C34	-4.03	117.96	127.66
23	B	612	CLA	C1-C2-C3	-4.03	119.08	126.04
23	C	511	CLA	C4A-NA-C1A	-4.02	104.90	106.71
23	b	614	CLA	C1-C2-C3	-4.02	119.09	126.04
33	C	521	LMG	O7-C10-C11	4.02	120.16	111.50
39	f	101	HEM	CAD-CBD-CGD	4.01	122.23	113.60
23	c	503	CLA	C1D-CHD-C4C	-4.01	117.41	126.06
23	c	514	CLA	C1D-CHD-C4C	-4.01	117.41	126.06
23	A	404[A]	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
23	A	404[B]	CLA	C3C-C4C-NC	4.01	115.06	110.57
23	c	511	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
23	b	609	CLA	C3D-C4D-ND	4.00	116.72	110.24
23	a	406[B]	CLA	O2D-CGD-CBD	4.00	118.38	111.27
23	C	509	CLA	C3B-C4B-NB	4.00	114.38	109.21
35	C	518[A]	DGD	O2G-C1B-C2B	4.00	120.12	111.50
23	C	511	CLA	C3B-C4B-NB	4.00	114.38	109.21
23	B	614	CLA	C3D-C4D-ND	4.00	116.71	110.24
23	A	404[A]	CLA	C3B-C4B-NB	4.00	114.38	109.21
23	C	502	CLA	C1D-CHD-C4C	-3.99	117.44	126.06
34	B	622	HTG	O5-C1-C2	3.99	115.34	110.31
34	V	202	HTG	C1-O5-C5	3.99	117.60	112.19
23	B	614	CLA	CAC-C3C-C4C	3.99	129.99	124.81
32	b	629[B]	LHG	O7-C7-C8	3.98	120.08	111.50
23	b	613	CLA	C1C-C2C-C3C	-3.98	102.77	106.96
23	B	607	CLA	C3D-C4D-ND	3.98	116.68	110.24
26	A	410[B]	SQD	C1-O5-C5	-3.98	105.88	113.69
23	C	511	CLA	C1D-CHD-C4C	-3.97	117.48	126.06
23	b	606	CLA	O2D-CGD-O1D	-3.97	116.07	123.84
23	b	601	CLA	C1D-CHD-C4C	-3.97	117.50	126.06
35	C	517[A]	DGD	O2G-C1B-C2B	3.97	120.05	111.50
23	A	406[A]	CLA	C3C-C4C-NC	3.96	115.02	110.57
23	A	408	CLA	C3B-C4B-NB	3.96	114.33	109.21
23	B	614	CLA	C1-C2-C3	-3.96	119.19	126.04
23	a	405[B]	CLA	C1D-CHD-C4C	-3.96	117.52	126.06
25	d	404	BCR	C15-C14-C13	-3.96	121.66	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	410[A]	SQD	O9-S-C6	3.96	111.64	106.94
23	c	508	CLA	CMC-C2C-C1C	3.95	131.06	125.04
23	c	503	CLA	CMD-C2D-C1D	3.95	131.68	124.71
23	D	404[B]	CLA	C1-C2-C3	-3.95	119.22	126.04
23	d	403	CLA	O2D-CGD-O1D	-3.94	116.12	123.84
23	C	508	CLA	C1D-CHD-C4C	-3.94	117.55	126.06
23	B	613	CLA	C4A-NA-C1A	-3.94	104.93	106.71
23	C	509	CLA	C3D-C4D-ND	3.94	116.62	110.24
23	b	602	CLA	CMC-C2C-C1C	3.94	131.04	125.04
23	A	405[A]	CLA	CMC-C2C-C1C	3.94	131.04	125.04
23	c	510	CLA	C3D-C4D-ND	3.94	116.61	110.24
23	a	406[B]	CLA	C1D-CHD-C4C	-3.93	117.57	126.06
23	c	509	CLA	C1D-CHD-C4C	-3.93	117.57	126.06
23	A	404[A]	CLA	C3C-C4C-NC	3.93	114.98	110.57
23	c	507	CLA	C3B-C4B-NB	3.93	114.29	109.21
23	C	510	CLA	C1-C2-C3	-3.92	119.26	126.04
25	B	618	BCR	C29-C30-C25	3.92	116.52	110.48
25	d	404	BCR	C29-C30-C25	3.92	116.51	110.48
23	b	615	CLA	C1D-CHD-C4C	-3.92	117.61	126.06
23	A	406[B]	CLA	C1C-C2C-C3C	-3.92	102.84	106.96
23	B	606	CLA	C3D-C4D-ND	3.91	116.57	110.24
23	c	509	CLA	C3D-C4D-ND	3.91	116.57	110.24
23	c	506	CLA	C1C-C2C-C3C	-3.91	102.84	106.96
25	C	515	BCR	C33-C5-C6	-3.91	120.14	124.53
23	A	404[B]	CLA	CAA-C2A-C3A	-3.91	102.07	112.78
23	c	508	CLA	C3D-C4D-ND	3.91	116.56	110.24
23	c	505	CLA	C3C-C4C-NC	3.91	114.95	110.57
23	B	616	CLA	C4C-C3C-C2C	-3.91	101.21	106.90
33	Z	101	LMG	O7-C10-C11	3.90	119.92	111.50
23	C	514	CLA	C1C-C2C-C3C	-3.90	102.85	106.96
23	B	603	CLA	C1C-C2C-C3C	-3.90	102.86	106.96
23	c	503	CLA	CHD-C1D-ND	-3.90	120.87	124.45
33	c	521	LMG	C3-C4-C5	3.90	117.20	110.24
23	C	509	CLA	CAC-C3C-C4C	3.90	129.87	124.81
32	L	101[B]	LHG	O7-C7-C8	3.89	119.89	111.50
23	A	406[A]	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
23	b	613	CLA	O2A-CGA-O1A	-3.89	113.77	123.59
23	C	514	CLA	C1D-CHD-C4C	-3.88	117.68	126.06
35	C	518[B]	DGD	O2G-C1B-C2B	3.88	119.86	111.50
23	B	611	CLA	C4A-NA-C1A	-3.88	104.96	106.71
23	a	405[A]	CLA	O2D-CGD-CBD	3.88	118.16	111.27
23	B	610	CLA	O2A-CGA-O1A	-3.88	113.81	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	606	CLA	C3D-C4D-ND	3.87	116.50	110.24
33	Z	101	LMG	C1-C2-C3	3.87	118.06	110.00
23	B	615	CLA	CED-O2D-CGD	3.87	124.69	115.94
41	V	201	HEC	CMB-C2B-C1B	-3.87	122.51	128.46
23	D	405	CLA	C3D-C4D-ND	3.87	116.49	110.24
23	C	512	CLA	C1D-CHD-C4C	-3.87	117.72	126.06
23	C	507	CLA	CMC-C2C-C1C	3.87	130.93	125.04
23	c	505	CLA	C3D-C4D-ND	3.86	116.49	110.24
23	b	605	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
39	f	101	HEM	C1B-NB-C4B	3.86	109.06	105.07
23	b	610	CLA	O2D-CGD-O1D	-3.86	116.29	123.84
23	c	510	CLA	C1D-CHD-C4C	-3.86	117.73	126.06
23	B	606	CLA	C1D-CHD-C4C	-3.86	117.74	126.06
23	B	613	CLA	C3B-C4B-NB	3.86	114.19	109.21
23	b	612	CLA	C3B-C4B-NB	3.86	114.19	109.21
23	C	512	CLA	O2D-CGD-O1D	-3.85	116.30	123.84
23	a	409	CLA	C1D-CHD-C4C	-3.85	117.76	126.06
29	a	414[B]	PL9	C7-C3-C2	-3.85	118.24	123.30
23	b	607	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
23	C	513	CLA	C1-C2-C3	-3.84	119.41	126.04
23	b	616	CLA	C3D-C4D-ND	3.83	116.44	110.24
23	b	610	CLA	O2A-CGA-O1A	-3.83	113.92	123.59
23	b	609	CLA	CAC-C3C-C4C	3.83	129.78	124.81
23	b	616	CLA	O2A-CGA-CBA	3.83	123.93	111.91
23	b	608	CLA	O2D-CGD-O1D	-3.83	116.36	123.84
29	A	414[A]	PL9	C7-C3-C4	3.83	119.99	116.88
23	b	604	CLA	O2D-CGD-O1D	-3.83	116.36	123.84
23	A	404[A]	CLA	CAA-C2A-C3A	-3.83	102.30	112.78
23	b	610	CLA	C4A-NA-C1A	-3.83	104.99	106.71
23	A	405[A]	CLA	C3C-C4C-NC	3.83	114.86	110.57
23	c	507	CLA	C3C-C4C-NC	3.82	114.86	110.57
23	B	604	CLA	C3D-C2D-C1D	-3.82	100.62	105.83
25	A	409	BCR	C24-C23-C22	-3.81	120.48	126.23
23	c	511	CLA	C3D-C4D-ND	3.81	116.40	110.24
23	b	612	CLA	O2D-CGD-O1D	-3.81	116.39	123.84
23	a	405[B]	CLA	CAC-C3C-C4C	3.80	129.75	124.81
23	B	614	CLA	CMC-C2C-C1C	3.80	130.83	125.04
23	A	405[B]	CLA	C1D-CHD-C4C	-3.80	117.86	126.06
23	B	614	CLA	C1D-CHD-C4C	-3.80	117.86	126.06
23	b	604	CLA	C3D-C4D-ND	3.80	116.38	110.24
23	c	514	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
23	C	513	CLA	C2C-C1C-NC	3.80	113.53	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	f	102	SQD	C1-O5-C5	3.79	121.14	113.69
23	A	404[A]	CLA	O2A-CGA-CBA	3.79	123.81	111.91
23	c	513	CLA	C3C-C4C-NC	3.78	114.81	110.57
23	a	405[B]	CLA	C1-C2-C3	-3.78	119.50	126.04
23	c	511	CLA	CMC-C2C-C1C	3.78	130.79	125.04
23	A	404[A]	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
23	b	605	CLA	C3C-C4C-NC	3.77	114.80	110.57
23	b	602	CLA	CAA-C2A-C3A	-3.77	102.46	112.78
23	C	514	CLA	C3B-C4B-NB	3.77	114.08	109.21
23	B	603	CLA	O2D-CGD-O1D	-3.77	116.47	123.84
23	B	609	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
23	d	402[B]	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
29	a	414[A]	PL9	C15-C14-C16	3.76	121.60	115.27
23	b	611	CLA	C1D-CHD-C4C	-3.76	117.94	126.06
23	C	510	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
23	D	404[A]	CLA	C1-C2-C3	-3.76	119.54	126.04
23	b	603	CLA	C1C-C2C-C3C	-3.75	103.01	106.96
23	b	616	CLA	O2D-CGD-O1D	-3.75	116.50	123.84
23	A	405[A]	CLA	CBC-CAC-C3C	-3.75	102.10	112.43
23	d	402[B]	CLA	C1D-CHD-C4C	-3.74	117.99	126.06
23	B	608	CLA	C3B-C4B-NB	3.74	114.04	109.21
23	C	510	CLA	C3B-C4B-NB	3.74	114.04	109.21
23	b	606	CLA	C1C-C2C-C3C	-3.74	103.03	106.96
23	C	509	CLA	C4C-C3C-C2C	-3.74	101.45	106.90
23	b	601	CLA	O2D-CGD-O1D	-3.74	116.53	123.84
23	B	611	CLA	C1-C2-C3	-3.74	119.58	126.04
32	d	413[A]	LHG	O8-C23-O10	-3.73	114.17	123.59
29	a	414[B]	PL9	C7-C8-C9	-3.73	120.58	126.79
23	C	508	CLA	C3D-C4D-ND	3.73	116.27	110.24
23	a	409	CLA	O2D-CGD-O1D	-3.73	116.56	123.84
23	C	504	CLA	O2D-CGD-CBD	3.72	117.88	111.27
23	b	607	CLA	C3B-C4B-NB	3.72	114.02	109.21
23	A	404[A]	CLA	O2D-CGD-CBD	3.72	117.88	111.27
23	b	613	CLA	C3D-C4D-ND	3.72	116.25	110.24
41	V	201	HEC	C1D-C2D-C3D	-3.72	104.41	107.00
23	A	404[B]	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
23	D	404[A]	CLA	C3B-C4B-NB	3.71	114.01	109.21
32	L	101[A]	LHG	O7-C7-C8	3.71	119.50	111.50
23	b	603	CLA	CAA-C2A-C3A	-3.71	102.62	112.78
29	a	414[A]	PL9	C7-C3-C2	-3.71	118.42	123.30
23	b	608	CLA	C1D-CHD-C4C	-3.71	118.06	126.06
23	B	605	CLA	O2A-CGA-O1A	-3.71	114.24	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	612	CLA	C3D-C2D-C1D	-3.70	100.78	105.83
23	b	613	CLA	C3B-C4B-NB	3.70	113.99	109.21
23	d	402[B]	CLA	C1-C2-C3	-3.70	119.65	126.04
23	B	601	CLA	C1D-CHD-C4C	-3.69	118.09	126.06
25	y	101	BCR	C33-C5-C6	-3.69	120.38	124.53
32	d	413[B]	LHG	O7-C7-C8	3.69	119.46	111.50
23	B	608	CLA	CMA-C3A-C4A	-3.69	101.86	111.77
23	C	507	CLA	C1-C2-C3	-3.69	119.66	126.04
35	c	517[B]	DGD	O2G-C1B-C2B	3.69	119.44	111.50
23	D	405	CLA	C1D-CHD-C4C	-3.69	118.11	126.06
23	b	605	CLA	CHD-C4C-NC	3.68	130.01	124.20
23	b	611	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
35	c	518[B]	DGD	O2G-C1B-C2B	3.68	119.43	111.50
23	c	502	CLA	C3C-C4C-NC	3.68	114.70	110.57
23	C	509	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
23	b	608	CLA	C3C-C4C-NC	3.67	114.69	110.57
25	D	406	BCR	C29-C30-C25	3.67	116.13	110.48
25	D	406	BCR	C38-C26-C25	-3.67	120.41	124.53
26	A	410[A]	SQD	C44-O6-C1	-3.67	106.57	113.74
26	A	410[B]	SQD	C44-O6-C1	-3.67	106.57	113.74
23	B	610	CLA	C4C-C3C-C2C	-3.67	101.55	106.90
29	a	414[A]	PL9	C30-C29-C31	3.67	121.44	115.27
29	D	407[A]	PL9	C42-C43-C44	-3.67	118.83	127.66
23	a	405[A]	CLA	CMB-C2B-C3B	3.67	131.54	124.68
23	D	404[A]	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
23	B	610	CLA	C3D-C4D-ND	3.66	116.16	110.24
23	c	513	CLA	C1-C2-C3	-3.66	119.72	126.04
29	A	414[A]	PL9	C15-C14-C16	3.65	121.41	115.27
34	b	625	HTG	C1-O5-C5	3.65	119.31	112.58
23	b	607	CLA	C1D-CHD-C4C	-3.65	118.18	126.06
23	c	503	CLA	C4A-NA-C1A	-3.65	105.06	106.71
23	b	609	CLA	C3B-C4B-NB	3.65	113.93	109.21
23	b	605	CLA	C1D-CHD-C4C	-3.65	118.19	126.06
23	B	605	CLA	CHD-C4C-NC	3.65	129.95	124.20
23	b	616	CLA	CHD-C4C-NC	3.65	129.95	124.20
26	B	620	SQD	O9-S-C6	3.64	111.27	106.94
23	c	510	CLA	C3B-C4B-NB	3.64	113.92	109.21
23	A	404[B]	CLA	O2D-CGD-CBD	3.64	117.74	111.27
23	a	407[A]	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
23	a	406[B]	CLA	C3C-C4C-NC	3.64	114.65	110.57
23	c	507	CLA	C1D-CHD-C4C	-3.64	118.21	126.06
35	c	517[A]	DGD	O2G-C1B-C2B	3.64	119.34	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	512	CLA	CHD-C4C-NC	3.63	129.93	124.20
23	C	510	CLA	CAC-C3C-C4C	3.63	129.52	124.81
23	a	407[A]	CLA	C1D-CHD-C4C	-3.63	118.23	126.06
23	B	604	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
23	a	405[A]	CLA	O2A-CGA-O1A	-3.62	114.47	123.59
23	C	508	CLA	O2D-CGD-O1D	-3.61	116.77	123.84
23	B	616	CLA	CHD-C1D-ND	-3.61	121.13	124.45
23	c	505	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
23	b	613	CLA	O2A-CGA-CBA	3.61	123.24	111.91
41	v	201	HEC	C1D-C2D-C3D	-3.61	104.48	107.00
23	a	407[B]	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
23	c	502	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
26	A	410[B]	SQD	O47-C7-C8	3.61	119.28	111.50
23	b	612	CLA	C4C-C3C-C2C	-3.61	101.64	106.90
23	d	402[B]	CLA	C3B-C4B-NB	3.61	113.87	109.21
23	C	502	CLA	CAC-C3C-C4C	3.61	129.49	124.81
32	d	413[A]	LHG	O8-C23-C24	3.60	123.21	111.91
23	c	509	CLA	C1-C2-C3	-3.60	119.82	126.04
33	C	520	LMG	O8-C28-C29	3.59	123.18	111.91
33	a	417	LMG	C7-O1-C1	-3.59	106.72	113.74
23	b	604	CLA	CMC-C2C-C1C	3.59	130.50	125.04
23	c	509	CLA	O2D-CGD-O1D	-3.59	116.82	123.84
29	d	405[A]	PL9	C42-C43-C44	-3.59	119.02	127.66
33	C	521	LMG	C3-C4-C5	3.59	116.63	110.24
23	B	608	CLA	CAC-C3C-C4C	3.58	129.46	124.81
23	b	614	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
23	A	406[B]	CLA	C1D-CHD-C4C	-3.58	118.33	126.06
23	C	509	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
29	A	414[A]	PL9	C22-C23-C24	-3.57	119.05	127.66
29	d	405[A]	PL9	C40-C39-C41	3.57	121.28	115.27
23	C	508	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
35	c	518[A]	DGD	O2G-C1B-C2B	3.57	119.19	111.50
23	B	602	CLA	C1D-CHD-C4C	-3.56	118.37	126.06
23	C	506	CLA	C1-C2-C3	-3.56	119.88	126.04
26	a	411[B]	SQD	C1-O5-C5	-3.56	106.70	113.69
23	b	612	CLA	CAC-C3C-C4C	3.56	129.43	124.81
23	A	405[A]	CLA	C1D-CHD-C4C	-3.56	118.38	126.06
23	b	603	CLA	C3B-C4B-NB	3.56	113.81	109.21
25	C	516	BCR	C7-C8-C9	-3.56	120.86	126.23
23	B	604	CLA	C3D-C4D-ND	3.56	115.99	110.24
23	B	612	CLA	O2D-CGD-O1D	-3.56	116.89	123.84
23	B	613	CLA	O2A-CGA-O1A	-3.55	114.62	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	410[A]	SQD	O47-C7-C8	3.55	119.16	111.50
23	C	510	CLA	CMC-C2C-C1C	3.55	130.45	125.04
33	c	520	LMG	O7-C10-C11	3.55	119.15	111.50
29	A	414[A]	PL9	C7-C3-C2	-3.55	118.63	123.30
25	b	619	BCR	C24-C23-C22	-3.55	120.87	126.23
23	b	614	CLA	C1D-CHD-C4C	-3.54	118.41	126.06
23	b	608	CLA	CBC-CAC-C3C	-3.54	102.67	112.43
23	b	610	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
23	A	406[A]	CLA	C1D-CHD-C4C	-3.54	118.42	126.06
23	B	614	CLA	C3B-C4B-NB	3.54	113.78	109.21
23	C	503	CLA	O2D-CGD-O1D	-3.54	116.92	123.84
23	C	505	CLA	C3B-C4B-NB	3.54	113.78	109.21
23	B	607	CLA	C4-C3-C5	3.54	121.22	115.27
23	B	608	CLA	O2D-CGD-O1D	-3.54	116.93	123.84
23	A	406[B]	CLA	C3C-C4C-NC	3.53	114.53	110.57
23	C	503	CLA	C1-C2-C3	-3.53	119.93	126.04
23	b	615	CLA	C1C-C2C-C3C	-3.53	103.24	106.96
23	C	506	CLA	C1C-C2C-C3C	-3.53	103.25	106.96
23	b	609	CLA	C1C-C2C-C3C	-3.53	103.25	106.96
23	B	612	CLA	CAC-C3C-C4C	3.53	129.39	124.81
23	B	604	CLA	C4C-C3C-C2C	-3.53	101.76	106.90
23	C	507	CLA	C3C-C4C-NC	3.52	114.52	110.57
23	b	604	CLA	C3B-C4B-NB	3.52	113.77	109.21
23	c	502	CLA	CAC-C3C-C4C	3.52	129.38	124.81
23	A	405[A]	CLA	CAA-C2A-C3A	-3.52	103.13	112.78
25	c	515	BCR	C11-C10-C9	-3.52	122.28	127.31
35	C	517[B]	DGD	O2G-C1B-C2B	3.52	119.09	111.50
23	C	505	CLA	CMC-C2C-C1C	3.52	130.40	125.04
23	D	404[B]	CLA	C1C-C2C-C3C	-3.52	103.26	106.96
23	c	510	CLA	C1C-C2C-C3C	-3.52	103.26	106.96
29	a	414[B]	PL9	C15-C14-C16	3.51	121.18	115.27
23	B	612	CLA	C4C-C3C-C2C	-3.51	101.78	106.90
23	B	603	CLA	CAA-C2A-C3A	-3.51	103.17	112.78
23	D	404[B]	CLA	C1D-CHD-C4C	-3.51	118.49	126.06
32	D	408[B]	LHG	O7-C7-C8	3.51	119.06	111.50
23	D	404[B]	CLA	CAC-C3C-C4C	3.51	129.36	124.81
23	b	608	CLA	CMC-C2C-C1C	3.51	130.38	125.04
23	b	611	CLA	C3B-C4B-NB	3.51	113.74	109.21
23	A	405[B]	CLA	C3C-C4C-NC	3.51	114.50	110.57
26	a	411[B]	SQD	C1-C2-C3	-3.51	102.70	110.00
32	D	409[B]	LHG	O7-C7-C8	3.50	119.05	111.50
23	d	402[A]	CLA	C3B-C4B-NB	3.50	113.73	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	612	CLA	C1D-CHD-C4C	-3.50	118.51	126.06
23	b	613	CLA	C1D-CHD-C4C	-3.50	118.51	126.06
32	A	418[A]	LHG	O7-C7-C8	3.50	119.04	111.50
23	C	511	CLA	CHD-C4C-NC	3.50	129.71	124.20
33	m	101	LMG	C8-O7-C10	-3.50	109.18	117.79
29	A	414[B]	PL9	C15-C14-C16	3.49	121.15	115.27
23	b	606	CLA	C3B-C4B-NB	3.49	113.72	109.21
23	B	614	CLA	O2A-CGA-O1A	-3.49	114.78	123.59
23	B	604	CLA	CAC-C3C-C4C	3.49	129.34	124.81
23	b	614	CLA	C3B-C4B-NB	3.49	113.72	109.21
23	B	610	CLA	C1D-CHD-C4C	-3.49	118.54	126.06
23	B	607	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
23	b	609	CLA	C1-C2-C3	-3.48	120.02	126.04
23	d	402[A]	CLA	O2A-CGA-CBA	3.48	122.83	111.91
23	b	609	CLA	C1D-CHD-C4C	-3.48	118.56	126.06
23	d	403	CLA	C1C-C2C-C3C	-3.47	103.30	106.96
26	b	620	SQD	O8-S-C6	3.47	111.28	105.74
29	a	414[B]	PL9	C27-C28-C29	-3.47	119.30	127.66
23	B	610	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
25	d	404	BCR	C38-C26-C25	-3.47	120.63	124.53
23	a	405[B]	CLA	C3C-C4C-NC	3.47	114.46	110.57
25	b	619	BCR	C38-C26-C25	-3.47	120.63	124.53
23	b	611	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
24	A	416[A]	PHO	C1A-C2A-C3A	-3.46	99.54	102.84
29	d	405[A]	PL9	C37-C38-C39	-3.46	119.33	127.66
25	k	101	BCR	C7-C8-C9	-3.46	121.01	126.23
23	B	613	CLA	O2D-CGD-O1D	-3.46	117.08	123.84
23	c	512	CLA	C3B-C4B-NB	3.46	113.68	109.21
23	B	613	CLA	C4-C3-C5	3.45	121.08	115.27
23	c	511	CLA	C1D-CHD-C4C	-3.45	118.61	126.06
25	h	101	BCR	C38-C26-C25	-3.45	120.65	124.53
23	b	613	CLA	O2D-CGD-CBD	3.45	117.40	111.27
23	A	404[A]	CLA	O2A-CGA-O1A	-3.45	114.89	123.59
34	B	625	HTG	C1'-S1-C1	3.45	106.54	100.09
23	C	509	CLA	O2D-CGD-O1D	-3.45	117.10	123.84
23	c	514	CLA	CAC-C3C-C4C	3.45	129.28	124.81
39	f	101	HEM	CHA-C4D-ND	3.44	128.63	124.38
23	B	610	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
23	C	507	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
23	C	511	CLA	C3C-C4C-NC	3.44	114.43	110.57
23	b	602	CLA	C1D-CHD-C4C	-3.44	118.64	126.06
25	T	101	BCR	C15-C16-C17	-3.44	116.43	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	A	418[B]	LHG	O7-C7-C8	3.44	118.91	111.50
23	a	406[A]	CLA	C3B-C4B-NB	3.43	113.65	109.21
23	c	512	CLA	O2D-CGD-O1D	-3.43	117.12	123.84
24	a	408[A]	PHO	C1A-C2A-C3A	-3.43	99.58	102.84
23	B	605	CLA	C1-C2-C3	-3.43	120.12	126.04
29	A	414[B]	PL9	C22-C23-C24	-3.42	119.43	127.66
25	T	101	BCR	C12-C13-C14	-3.42	113.69	118.94
32	d	407[A]	LHG	O7-C7-C8	3.42	118.86	111.50
23	C	512	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
23	b	610	CLA	C4C-C3C-C2C	-3.42	101.92	106.90
23	a	406[A]	CLA	CHD-C4C-NC	3.41	129.58	124.20
23	b	610	CLA	CAA-C2A-C3A	-3.41	103.43	112.78
23	B	601	CLA	C4C-C3C-C2C	-3.41	101.92	106.90
23	a	407[B]	CLA	C1D-CHD-C4C	-3.41	118.70	126.06
23	B	610	CLA	CAA-C2A-C3A	-3.41	103.44	112.78
34	b	622	HTG	O2-C2-C1	3.41	116.53	110.27
23	c	505	CLA	C1D-CHD-C4C	-3.41	118.71	126.06
23	a	406[B]	CLA	CHD-C4C-NC	3.41	129.57	124.20
24	a	408[A]	PHO	O1D-CGD-CBD	-3.41	119.07	124.74
29	D	407[B]	PL9	C25-C24-C26	3.40	121.00	115.27
29	A	414[B]	PL9	C27-C28-C29	-3.40	119.46	127.66
33	a	417	LMG	C8-O7-C10	-3.40	109.42	117.79
23	C	506	CLA	C1D-CHD-C4C	-3.40	118.73	126.06
31	B	628	LMT	C1'-O5'-C5'	-3.39	107.03	113.69
23	D	404[B]	CLA	C3B-C4B-NB	3.39	113.59	109.21
23	b	608	CLA	CMB-C2B-C3B	3.39	131.01	124.68
29	D	407[B]	PL9	C42-C43-C44	-3.38	119.51	127.66
23	B	611	CLA	C2A-C1A-CHA	-3.38	117.95	123.86
23	B	614	CLA	C3C-C4C-NC	3.38	114.36	110.57
39	F	102	HEM	CHB-C1B-NB	3.38	128.56	124.38
23	a	405[A]	CLA	C3B-C4B-NB	3.38	113.58	109.21
29	a	414[A]	PL9	C27-C28-C29	-3.38	119.53	127.66
23	a	406[B]	CLA	C3B-C4B-NB	3.38	113.58	109.21
23	c	512	CLA	C4-C3-C5	3.37	120.95	115.27
29	A	414[A]	PL9	C37-C38-C39	-3.37	119.54	127.66
23	b	607	CLA	O2D-CGD-CBD	3.37	117.26	111.27
23	a	407[B]	CLA	C3C-C4C-NC	3.37	114.35	110.57
23	B	615	CLA	CMC-C2C-C1C	3.37	130.17	125.04
23	A	406[A]	CLA	C3B-C4B-NB	3.37	113.56	109.21
29	A	414[A]	PL9	C27-C28-C29	-3.36	119.56	127.66
23	C	513	CLA	C4-C3-C5	3.36	120.92	115.27
23	a	405[A]	CLA	O2A-CGA-CBA	3.36	122.45	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	512	CLA	C3B-C4B-NB	3.36	113.55	109.21
23	A	405[B]	CLA	C3B-C4B-NB	3.36	113.55	109.21
23	B	611	CLA	CHB-C4A-NA	3.36	129.15	124.51
23	b	615	CLA	O2D-CGD-CBD	3.36	117.23	111.27
23	D	404[A]	CLA	C4C-C3C-C2C	-3.35	102.01	106.90
23	c	506	CLA	CAC-C3C-C4C	3.35	129.16	124.81
23	c	511	CLA	C3B-C4B-NB	3.35	113.55	109.21
23	a	409	CLA	C4-C3-C5	3.35	120.91	115.27
23	A	404[A]	CLA	CAC-C3C-C4C	3.35	129.15	124.81
32	b	629[A]	LHG	O7-C7-C8	3.35	118.72	111.50
24	a	416[A]	PHO	C4-C3-C5	3.35	120.90	115.27
26	X	101	SQD	C1-C2-C3	-3.34	103.03	110.00
26	a	411[B]	SQD	C44-O6-C1	-3.34	107.20	113.74
23	B	616	CLA	C1C-C2C-C3C	-3.34	103.44	106.96
31	b	627	LMT	C3'-C4'-C5'	-3.34	103.26	110.93
32	A	418[B]	LHG	C5-O7-C7	-3.34	109.57	117.79
23	d	402[A]	CLA	C4-C3-C5	3.34	120.89	115.27
29	A	414[B]	PL9	C37-C38-C39	-3.34	119.62	127.66
23	C	510	CLA	C1D-CHD-C4C	-3.34	118.86	126.06
23	a	405[B]	CLA	CHC-C1C-C2C	-3.34	117.49	126.72
23	a	405[A]	CLA	C1-C2-C3	-3.33	120.28	126.04
23	A	404[A]	CLA	CAA-C2A-C1A	-3.33	101.05	111.97
23	c	510	CLA	C4-C3-C5	3.33	120.87	115.27
23	a	407[B]	CLA	CBC-CAC-C3C	-3.33	103.25	112.43
25	h	101	BCR	C7-C8-C9	-3.33	121.20	126.23
33	C	520	LMG	O7-C10-C11	3.33	118.67	111.50
23	B	608	CLA	C4C-C3C-C2C	-3.33	102.05	106.90
23	C	504	CLA	C4C-C3C-C2C	-3.33	102.05	106.90
23	c	506	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
25	K	103	BCR	C15-C14-C13	-3.33	122.56	127.31
23	b	609	CLA	CBC-CAC-C3C	-3.32	103.27	112.43
23	C	506	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
23	a	405[A]	CLA	CAA-C2A-C1A	-3.32	101.10	111.97
41	v	201	HEC	CBA-CAA-C2A	-3.32	107.02	112.60
23	d	403	CLA	C1D-CHD-C4C	-3.32	118.90	126.06
23	B	604	CLA	C3B-C4B-NB	3.31	113.49	109.21
26	A	412	SQD	O48-C23-C24	3.31	122.30	111.91
31	B	630	LMT	O1'-C1'-C2'	3.31	113.47	108.30
23	C	510	CLA	CMB-C2B-C3B	3.31	130.87	124.68
23	B	607	CLA	C3B-C4B-NB	3.31	113.49	109.21
32	A	418[A]	LHG	O8-C23-C24	3.30	122.28	111.91
23	C	507	CLA	C3B-C4B-NB	3.30	113.48	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	414[A]	PL9	C37-C38-C39	-3.30	119.71	127.66
23	B	608	CLA	C1C-C2C-C3C	-3.30	103.49	106.96
33	B	621	LMG	O8-C28-C29	3.30	122.26	111.91
23	B	602	CLA	C3B-C4B-NB	3.30	113.47	109.21
23	b	602	CLA	C1C-C2C-C3C	-3.30	103.49	106.96
23	c	513	CLA	C1C-C2C-C3C	-3.30	103.49	106.96
23	d	402[A]	CLA	C1D-CHD-C4C	-3.29	118.95	126.06
39	f	101	HEM	CHD-C1D-ND	3.29	128.01	124.43
29	D	407[A]	PL9	C25-C24-C26	3.29	120.81	115.27
23	c	503	CLA	C3B-C4B-NB	3.29	113.47	109.21
23	A	404[A]	CLA	CMB-C2B-C3B	3.29	130.84	124.68
23	c	508	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
29	A	414[B]	PL9	C17-C18-C19	-3.29	119.75	127.66
23	A	406[A]	CLA	CAA-C2A-C3A	-3.28	103.78	112.78
23	c	511	CLA	C4-C3-C5	3.28	120.79	115.27
25	B	617	BCR	C33-C5-C6	-3.28	120.85	124.53
23	B	602	CLA	CAA-C2A-C3A	-3.28	103.80	112.78
23	a	405[A]	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
23	c	504	CLA	C4C-C3C-C2C	-3.28	102.12	106.90
23	b	609	CLA	C4C-C3C-C2C	-3.28	102.12	106.90
23	b	601	CLA	C1C-C2C-C3C	-3.28	103.51	106.96
25	D	406	BCR	C28-C27-C26	-3.27	108.23	114.08
23	c	505	CLA	CAC-C3C-C4C	3.27	129.06	124.81
23	c	513	CLA	CHD-C4C-NC	3.27	129.36	124.20
23	B	605	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
23	d	402[B]	CLA	C4C-C3C-C2C	-3.26	102.14	106.90
23	B	615	CLA	O2D-CGD-O1D	-3.26	117.45	123.84
23	b	610	CLA	CHD-C4C-NC	3.26	129.35	124.20
23	c	512	CLA	C1C-C2C-C3C	-3.26	103.53	106.96
23	c	506	CLA	CMC-C2C-C1C	3.26	130.00	125.04
23	B	613	CLA	CAC-C3C-C4C	3.26	129.04	124.81
23	B	614	CLA	CHC-C1C-C2C	-3.26	117.71	126.72
23	c	510	CLA	C1-O2A-CGA	3.26	124.99	116.44
23	B	601	CLA	CMB-C2B-C3B	3.26	130.77	124.68
23	d	402[B]	CLA	O2A-CGA-CBA	3.26	122.12	111.91
23	B	612	CLA	C1C-C2C-C3C	-3.25	103.53	106.96
23	B	604	CLA	CHD-C1D-ND	-3.25	121.47	124.45
23	c	510	CLA	C4C-C3C-C2C	-3.24	102.17	106.90
23	d	402[A]	CLA	C1-C2-C3	-3.24	120.43	126.04
23	B	605	CLA	O2D-CGD-O1D	-3.24	117.49	123.84
23	a	409	CLA	C3B-C4B-NB	3.24	113.40	109.21
23	B	608	CLA	C1D-CHD-C4C	-3.24	119.06	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	615	CLA	C11-C10-C8	-3.24	105.44	115.92
23	a	405[B]	CLA	O2D-CGD-CBD	3.24	117.03	111.27
23	c	505	CLA	CHC-C1C-C2C	-3.24	117.76	126.72
23	c	504	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
23	B	611	CLA	C4C-C3C-C2C	-3.24	102.18	106.90
26	B	620	SQD	O48-C23-C24	3.24	122.06	111.91
23	c	513	CLA	O2A-CGA-CBA	3.24	122.06	111.91
23	C	505	CLA	C1D-CHD-C4C	-3.24	119.08	126.06
29	a	414[B]	PL9	C30-C29-C31	3.23	120.70	115.27
23	b	612	CLA	C1C-C2C-C3C	-3.23	103.56	106.96
26	a	411[B]	SQD	O9-S-C6	3.23	110.78	106.94
23	A	406[A]	CLA	O2A-CGA-O1A	-3.23	115.45	123.59
24	A	416[B]	PHO	C4-C3-C5	3.23	120.70	115.27
23	B	614	CLA	O2A-CGA-CBA	3.23	122.03	111.91
32	d	407[B]	LHG	O7-C7-C8	3.22	118.44	111.50
23	A	408	CLA	C1D-CHD-C4C	-3.22	119.11	126.06
23	C	512	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
33	c	521	LMG	C9-C8-C7	-3.22	104.17	111.79
41	V	201	HEC	CBA-CAA-C2A	-3.22	107.18	112.60
23	D	405	CLA	C1C-C2C-C3C	-3.22	103.58	106.96
23	a	407[A]	CLA	C3B-C4B-NB	3.22	113.37	109.21
23	B	605	CLA	C4C-C3C-C2C	-3.22	102.21	106.90
23	b	605	CLA	O2A-CGA-O1A	-3.21	115.48	123.59
26	a	411[A]	SQD	C45-O47-C7	-3.21	109.88	117.79
23	C	509	CLA	C1-C2-C3	-3.21	120.49	126.04
23	C	513	CLA	CHD-C4C-NC	3.21	129.27	124.20
23	A	405[B]	CLA	CBC-CAC-C3C	-3.21	103.58	112.43
23	C	514	CLA	CMC-C2C-C1C	3.21	129.93	125.04
32	d	406[B]	LHG	O7-C7-C8	3.21	118.42	111.50
23	C	502	CLA	C1C-C2C-C3C	-3.21	103.58	106.96
23	C	511	CLA	C4-C3-C5	3.21	120.67	115.27
23	A	408	CLA	C4C-C3C-C2C	-3.21	102.22	106.90
29	a	414[A]	PL9	C17-C18-C19	-3.21	119.94	127.66
23	a	406[B]	CLA	CAA-C2A-C3A	-3.20	104.00	112.78
24	a	408[A]	PHO	O2A-CGA-O1A	-3.20	115.51	123.59
26	b	620	SQD	C3-C4-C5	3.20	115.95	110.24
29	a	414[A]	PL9	C25-C24-C26	3.20	120.65	115.27
23	B	612	CLA	C3B-C4B-NB	3.20	113.34	109.21
34	b	622	HTG	C1'-S1-C1	3.20	106.07	100.09
23	A	406[B]	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
29	D	407[A]	PL9	C17-C18-C19	-3.20	119.96	127.66
26	a	412	SQD	O48-C23-C24	3.19	121.93	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	414[B]	PL9	C25-C24-C26	3.19	120.64	115.27
24	A	416[A]	PHO	C4-C3-C5	3.19	120.64	115.27
23	a	407[B]	CLA	C3B-C4B-NB	3.19	113.33	109.21
23	B	614	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
33	Z	101	LMG	C4-C3-C2	3.19	116.39	110.82
23	D	404[B]	CLA	O2A-CGA-CBA	3.19	121.91	111.91
23	B	612	CLA	CMC-C2C-C1C	3.19	129.89	125.04
23	B	615	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
23	b	603	CLA	C4-C3-C5	3.18	120.62	115.27
23	D	404[B]	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
23	b	606	CLA	CHD-C4C-NC	3.18	129.21	124.20
23	B	601	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
23	b	615	CLA	C4C-C3C-C2C	-3.18	102.27	106.90
23	A	405[A]	CLA	C3B-C4B-NB	3.18	113.32	109.21
23	d	402[A]	CLA	O2A-CGA-O1A	-3.18	115.57	123.59
23	c	509	CLA	C3B-C4B-NB	3.18	113.32	109.21
23	D	405	CLA	C4C-C3C-C2C	-3.18	102.27	106.90
23	B	610	CLA	CAA-CBA-CGA	-3.17	103.98	113.25
31	M	101	LMT	C1'-O5'-C5'	-3.17	107.46	113.69
23	B	609	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
23	A	405[B]	CLA	CHD-C4C-NC	3.17	129.20	124.20
23	C	513	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
23	C	510	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
29	a	414[B]	PL9	C17-C18-C19	-3.17	120.04	127.66
25	d	404	BCR	C37-C22-C23	3.16	123.06	118.08
39	F	102	HEM	CBD-CAD-C3D	-3.16	103.84	112.63
23	C	504	CLA	C4-C3-C5	3.16	120.59	115.27
23	B	616	CLA	CHC-C1C-C2C	-3.16	117.98	126.72
23	C	510	CLA	C4C-C3C-C2C	-3.16	102.29	106.90
23	B	609	CLA	C3B-C4B-NB	3.16	113.29	109.21
23	c	505	CLA	C4A-NA-C1A	-3.16	105.29	106.71
23	a	409	CLA	CAA-C2A-C3A	-3.16	104.14	112.78
23	c	506	CLA	C4C-C3C-C2C	-3.16	102.30	106.90
23	c	513	CLA	C4-C3-C5	3.15	120.58	115.27
25	K	102	BCR	C20-C21-C22	-3.15	122.81	127.31
29	d	405[B]	PL9	C40-C39-C41	3.15	120.58	115.27
29	d	405[B]	PL9	C10-C9-C11	3.15	120.58	115.27
41	v	201	HEC	CMB-C2B-C1B	-3.15	123.62	128.46
23	a	405[A]	CLA	C4-C3-C5	3.15	120.57	115.27
23	B	609	CLA	C1D-CHD-C4C	-3.15	119.26	126.06
23	b	603	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
23	C	511	CLA	CBC-CAC-C3C	-3.15	103.75	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	612	CLA	C1D-CHD-C4C	-3.15	119.27	126.06
23	b	603	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
23	B	613	CLA	O2A-CGA-CBA	3.14	121.78	111.91
23	B	603	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
23	C	507	CLA	C1D-CHD-C4C	-3.14	119.28	126.06
23	B	612	CLA	C11-C12-C13	-3.14	105.77	115.92
33	m	101	LMG	O8-C28-C29	3.14	121.76	111.91
23	c	507	CLA	CHC-C1C-C2C	-3.14	118.04	126.72
23	C	508	CLA	C4C-C3C-C2C	-3.14	102.33	106.90
23	b	614	CLA	C2A-C1A-CHA	-3.14	118.37	123.86
23	B	615	CLA	C3B-C4B-NB	3.14	113.27	109.21
25	D	406	BCR	C10-C11-C12	-3.14	113.43	123.22
23	b	607	CLA	CBC-CAC-C3C	-3.13	103.79	112.43
29	d	405[B]	PL9	C42-C43-C44	-3.13	120.12	127.66
23	d	402[B]	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
23	c	505	CLA	C4C-C3C-C2C	-3.13	102.33	106.90
23	A	406[B]	CLA	CAA-C2A-C3A	-3.13	104.20	112.78
23	a	407[B]	CLA	CAC-C3C-C4C	3.13	128.87	124.81
23	b	614	CLA	O2A-CGA-O1A	-3.13	115.69	123.59
23	b	605	CLA	C3B-C4B-NB	3.13	113.26	109.21
23	b	603	CLA	CMA-C3A-C2A	-3.13	101.21	113.83
23	C	502	CLA	CMC-C2C-C1C	3.13	129.80	125.04
23	A	404[A]	CLA	C1-C2-C3	-3.13	120.63	126.04
33	Z	101	LMG	O6-C1-C2	3.13	116.97	110.35
25	b	619	BCR	C11-C10-C9	-3.13	122.85	127.31
34	b	622	HTG	O5-C5-C4	3.13	115.37	109.69
23	c	513	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
23	b	615	CLA	C3B-C4B-NB	3.13	113.25	109.21
23	C	504	CLA	C1C-C2C-C3C	-3.12	103.67	106.96
32	d	413[B]	LHG	O8-C23-C24	3.12	121.71	111.91
23	b	609	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
23	c	508	CLA	C1D-CHD-C4C	-3.12	119.32	126.06
23	C	508	CLA	CMC-C2C-C1C	3.12	129.79	125.04
26	B	620	SQD	C1-O5-C5	-3.12	107.56	113.69
23	C	506	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
23	A	405[A]	CLA	CAC-C3C-C4C	3.12	128.86	124.81
23	B	615	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
23	a	407[A]	CLA	CHD-C4C-NC	3.12	129.12	124.20
23	a	409	CLA	CBC-CAC-C3C	-3.12	103.84	112.43
23	b	608	CLA	CHD-C4C-NC	3.11	129.11	124.20
23	C	504	CLA	C1-C2-C3	-3.11	120.67	126.04
25	b	618	BCR	C37-C22-C21	-3.11	118.57	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402[B]	CLA	C4-C3-C5	3.11	120.50	115.27
25	b	617	BCR	C29-C30-C25	3.11	115.26	110.48
23	C	504	CLA	CHD-C4C-NC	3.11	129.10	124.20
23	D	404[A]	CLA	C1D-CHD-C4C	-3.11	119.36	126.06
23	B	614	CLA	C2A-C1A-CHA	-3.11	118.43	123.86
23	b	615	CLA	C4-C3-C5	3.11	120.50	115.27
29	a	414[A]	PL9	C35-C34-C36	3.10	120.49	115.27
23	a	409	CLA	O2A-CGA-CBA	3.10	121.65	111.91
32	D	409[A]	LHG	O7-C7-C8	3.10	118.19	111.50
33	C	521	LMG	O8-C28-C29	3.10	121.64	111.91
23	b	616	CLA	C1C-C2C-C3C	-3.10	103.70	106.96
24	a	408[A]	PHO	O2A-CGA-CBA	3.10	121.63	111.91
23	B	607	CLA	CMC-C2C-C1C	3.10	129.76	125.04
23	D	404[B]	CLA	O2D-CGD-O1D	-3.10	117.79	123.84
23	c	509	CLA	C4C-C3C-C2C	-3.10	102.39	106.90
23	B	616	CLA	CAC-C3C-C4C	3.09	128.82	124.81
23	b	601	CLA	CMB-C2B-C3B	3.09	130.47	124.68
23	a	407[A]	CLA	CAA-C2A-C3A	-3.09	104.31	112.78
23	D	404[B]	CLA	CMB-C2B-C3B	3.09	130.46	124.68
29	A	414[B]	PL9	C7-C3-C2	-3.09	119.24	123.30
23	b	601	CLA	C4C-C3C-C2C	-3.09	102.40	106.90
25	d	404	BCR	C3-C4-C5	-3.09	108.56	114.08
34	B	625	HTG	O5-C5-C4	3.09	115.30	109.69
23	B	616	CLA	O2A-CGA-CBA	3.09	121.59	111.91
23	b	613	CLA	C1-C2-C3	-3.09	120.71	126.04
23	c	504	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
41	V	201	HEC	CMC-C2C-C1C	-3.08	123.72	128.46
23	B	606	CLA	C3B-C4B-NB	3.08	113.20	109.21
32	D	408[A]	LHG	O8-C23-O10	-3.08	115.82	123.59
23	c	503	CLA	CHC-C1C-C2C	-3.08	118.20	126.72
23	b	601	CLA	C4-C3-C5	3.08	120.45	115.27
31	B	628	LMT	C4B-C3B-C2B	3.08	116.20	110.82
25	B	618	BCR	C15-C14-C13	-3.08	122.92	127.31
23	b	601	CLA	CHD-C4C-NC	3.08	129.05	124.20
33	z	101	LMG	O7-C10-C11	3.08	118.14	111.50
23	c	510	CLA	CAC-C3C-C4C	3.08	128.80	124.81
23	d	403	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
23	b	614	CLA	CAC-C3C-C4C	3.08	128.80	124.81
23	B	603	CLA	CMB-C2B-C3B	3.07	130.43	124.68
23	C	507	CLA	CHC-C1C-C2C	-3.07	118.23	126.72
23	A	408	CLA	C1-C2-C3	-3.07	120.73	126.04
39	F	102	HEM	CHD-C1D-ND	3.07	127.77	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	605	CLA	CHC-C1C-C2C	-3.07	118.23	126.72
23	C	506	CLA	C4-C3-C5	3.07	120.43	115.27
23	b	611	CLA	CHD-C4C-NC	3.07	129.04	124.20
23	B	601	CLA	C1C-C2C-C3C	-3.07	103.73	106.96
25	y	101	BCR	C38-C26-C25	-3.07	121.09	124.53
23	c	509	CLA	O2A-CGA-CBA	3.06	121.53	111.91
23	a	405[B]	CLA	CAA-C2A-C3A	-3.06	104.39	112.78
23	c	504	CLA	C3B-C4B-NB	3.06	113.17	109.21
25	D	406	BCR	C37-C22-C23	3.06	122.90	118.08
23	b	614	CLA	CMC-C2C-C1C	3.06	129.70	125.04
29	A	414[B]	PL9	C20-C19-C21	3.06	120.42	115.27
23	c	507	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
23	b	611	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
23	A	408	CLA	CAA-C2A-C3A	-3.06	104.41	112.78
32	a	420[A]	LHG	O7-C7-C8	3.05	118.08	111.50
23	b	602	CLA	CHD-C4C-NC	3.05	129.01	124.20
39	f	101	HEM	CBD-CAD-C3D	-3.05	104.14	112.63
23	C	502	CLA	C3B-C4B-NB	3.05	113.16	109.21
23	b	616	CLA	C3B-C4B-NB	3.05	113.16	109.21
23	c	506	CLA	C1D-CHD-C4C	-3.05	119.48	126.06
24	A	416[B]	PHO	O2D-CGD-O1D	-3.05	117.88	123.84
23	C	503	CLA	C1D-CHD-C4C	-3.05	119.48	126.06
23	a	407[B]	CLA	CAA-C2A-C3A	-3.05	104.44	112.78
23	A	404[A]	CLA	CMC-C2C-C1C	3.05	129.68	125.04
32	D	409[A]	LHG	O8-C23-C24	3.05	121.46	111.91
29	A	414[A]	PL9	O1-C4-C3	-3.05	117.37	120.72
29	a	414[A]	PL9	C10-C9-C11	3.04	120.39	115.27
23	a	407[B]	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
23	b	602	CLA	C4C-C3C-C2C	-3.04	102.46	106.90
23	A	406[B]	CLA	C3B-C4B-NB	3.04	113.14	109.21
23	C	508	CLA	CBC-CAC-C3C	-3.04	104.05	112.43
23	A	406[B]	CLA	C2A-C1A-CHA	-3.04	118.55	123.86
23	B	603	CLA	O2A-CGA-CBA	3.04	121.44	111.91
29	A	414[A]	PL9	C20-C19-C21	3.04	120.38	115.27
23	B	606	CLA	CMC-C2C-C1C	3.04	129.66	125.04
23	a	406[B]	CLA	CHC-C1C-C2C	-3.04	118.32	126.72
23	C	507	CLA	CBC-CAC-C3C	-3.04	104.06	112.43
23	a	405[B]	CLA	CAA-C2A-C1A	-3.04	102.03	111.97
24	A	416[A]	PHO	CMC-C2C-C3C	3.03	130.66	124.94
23	a	405[B]	CLA	C4C-C3C-C2C	-3.03	102.47	106.90
32	d	413[A]	LHG	O7-C7-C8	3.03	118.04	111.50
23	b	612	CLA	C2A-C1A-CHA	-3.03	118.56	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	603	CLA	CHD-C4C-NC	3.03	128.98	124.20
23	b	607	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
25	B	618	BCR	C38-C26-C25	-3.03	121.13	124.53
26	a	411[B]	SQD	C45-O47-C7	-3.03	110.34	117.79
25	c	516	BCR	C7-C8-C9	-3.03	121.66	126.23
25	c	515	BCR	C15-C14-C13	-3.02	123.00	127.31
29	a	414[B]	PL9	C37-C38-C39	-3.02	120.38	127.66
23	A	406[B]	CLA	O2A-CGA-O1A	-3.02	115.97	123.59
23	B	609	CLA	CHC-C1C-C2C	-3.02	118.36	126.72
29	D	407[B]	PL9	C17-C18-C19	-3.02	120.39	127.66
23	a	405[B]	CLA	C1C-C2C-C3C	-3.02	103.78	106.96
23	B	609	CLA	CBC-CAC-C3C	-3.02	104.11	112.43
23	c	512	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
23	B	603	CLA	O2A-CGA-O1A	-3.02	115.98	123.59
26	A	410[B]	SQD	O9-S-C6	3.02	110.53	106.94
24	a	416[A]	PHO	CBA-CAA-C2A	-3.02	105.00	113.81
23	A	408	CLA	CHC-C1C-C2C	-3.02	118.38	126.72
23	b	601	CLA	C1-O2A-CGA	3.01	124.35	116.44
23	B	603	CLA	C3B-C4B-NB	3.01	113.10	109.21
23	A	406[A]	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
32	D	409[A]	LHG	O8-C23-O10	-3.01	115.99	123.59
23	A	404[B]	CLA	CHC-C1C-C2C	-3.01	118.40	126.72
23	A	408	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
23	B	614	CLA	CBC-CAC-C3C	-3.01	104.14	112.43
24	a	416[A]	PHO	CMB-C2B-C3B	3.01	130.30	124.68
35	h	102	DGD	O1G-C1A-O1A	-3.01	116.00	123.59
23	b	616	CLA	C4C-C3C-C2C	-3.00	102.52	106.90
23	d	403	CLA	CAA-C2A-C3A	-3.00	104.55	112.78
23	A	405[B]	CLA	CMC-C2C-C1C	3.00	129.61	125.04
23	B	601	CLA	C3B-C4B-NB	3.00	113.09	109.21
29	D	407[A]	PL9	C53-C6-C1	3.00	121.13	114.99
23	b	605	CLA	C4-C3-C5	3.00	120.32	115.27
23	b	604	CLA	C1D-CHD-C4C	-3.00	119.59	126.06
25	c	516	BCR	C32-C1-C6	-3.00	105.44	110.30
23	B	607	CLA	CAA-C2A-C3A	-3.00	104.57	112.78
23	a	405[A]	CLA	CHC-C1C-C2C	-3.00	118.43	126.72
29	d	405[A]	PL9	C22-C23-C24	-3.00	120.44	127.66
29	d	405[A]	PL9	C36-C34-C33	-3.00	115.05	121.12
23	B	613	CLA	CMC-C2C-C1C	3.00	129.60	125.04
23	c	510	CLA	CHC-C1C-C2C	-3.00	118.43	126.72
23	C	507	CLA	CMB-C2B-C3B	3.00	130.29	124.68
24	a	416[B]	PHO	CMB-C2B-C3B	3.00	130.29	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	407[A]	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
23	A	404[B]	CLA	CHD-C4C-NC	3.00	128.93	124.20
32	a	420[B]	LHG	O7-C7-C8	3.00	117.96	111.50
23	b	614	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
25	T	101	BCR	C16-C17-C18	-2.99	123.04	127.31
31	B	628	LMT	C2'-C3'-C4'	2.99	116.52	109.68
29	A	414[A]	PL9	C17-C18-C19	-2.99	120.45	127.66
24	a	416[B]	PHO	C4-C3-C5	2.99	120.30	115.27
23	b	603	CLA	CHD-C4C-NC	2.99	128.92	124.20
23	B	609	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
23	a	409	CLA	CHD-C4C-NC	2.99	128.91	124.20
25	C	516	BCR	C32-C1-C6	-2.98	105.46	110.30
23	D	405	CLA	CMC-C2C-C1C	2.98	129.58	125.04
25	c	515	BCR	C28-C27-C26	-2.98	108.75	114.08
23	d	402[A]	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
23	C	509	CLA	C4-C3-C5	2.98	120.29	115.27
23	C	512	CLA	C4-C3-C5	2.98	120.29	115.27
25	H	101	BCR	C11-C10-C9	-2.98	123.06	127.31
23	c	502	CLA	CHC-C1C-C2C	-2.98	118.48	126.72
23	a	405[A]	CLA	CMA-C3A-C4A	-2.98	103.77	111.77
23	C	507	CLA	C4-C3-C5	2.98	120.28	115.27
23	A	406[A]	CLA	CMC-C2C-C1C	2.98	129.57	125.04
35	c	519	DGD	O2G-C1B-C2B	2.98	117.91	111.50
23	C	512	CLA	C1-C2-C3	-2.97	120.90	126.04
23	b	609	CLA	CHC-C1C-C2C	-2.97	118.50	126.72
35	C	517[A]	DGD	C2G-O2G-C1B	-2.97	110.47	117.79
23	d	402[A]	CLA	C4C-C3C-C2C	-2.97	102.56	106.90
32	D	409[B]	LHG	O8-C23-C24	2.97	121.23	111.91
23	c	502	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
23	B	607	CLA	CBC-CAC-C3C	-2.97	104.24	112.43
29	a	414[A]	PL9	C42-C43-C44	-2.97	120.50	127.66
23	a	405[A]	CLA	CMC-C2C-C1C	2.97	129.56	125.04
23	B	615	CLA	CAC-C3C-C4C	2.97	128.66	124.81
23	B	607	CLA	C1D-CHD-C4C	-2.97	119.65	126.06
29	d	405[A]	PL9	C10-C9-C11	2.97	120.27	115.27
34	B	625	HTG	C3-C4-C5	2.97	115.53	110.24
23	b	606	CLA	CAA-C2A-C3A	-2.97	104.65	112.78
23	b	602	CLA	C2A-C1A-CHA	-2.97	118.67	123.86
23	c	502	CLA	C3B-C4B-NB	2.97	113.05	109.21
32	E	101[B]	LHG	O8-C23-C24	2.97	121.21	111.91
35	h	102	DGD	O2G-C1B-C2B	2.96	117.89	111.50
26	A	410[A]	SQD	O8-S-C6	2.96	110.46	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	405[B]	CLA	C4-C3-C5	2.96	120.25	115.27
23	c	507	CLA	CAC-C3C-C4C	2.96	128.65	124.81
24	a	416[A]	PHO	O2D-CGD-O1D	-2.96	118.05	123.84
23	b	613	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
25	A	409	BCR	C11-C10-C9	-2.96	123.08	127.31
23	B	603	CLA	C4-C3-C5	2.96	120.25	115.27
23	B	604	CLA	CHC-C1C-C2C	-2.96	118.54	126.72
32	d	413[B]	LHG	O8-C23-O10	-2.96	116.13	123.59
25	T	101	BCR	C2-C1-C6	2.96	115.03	110.48
23	a	407[B]	CLA	CHC-C1C-C2C	-2.96	118.54	126.72
23	c	504	CLA	C1-C2-C3	-2.96	120.93	126.04
23	C	512	CLA	CHD-C4C-NC	2.96	128.86	124.20
35	C	519	DGD	O1G-C1A-C2A	2.95	121.18	111.91
23	c	512	CLA	C1-C2-C3	-2.95	120.93	126.04
23	A	404[B]	CLA	O2A-CGA-CBA	2.95	121.17	111.91
23	a	405[B]	CLA	O2A-CGA-CBA	2.95	121.17	111.91
29	A	414[B]	PL9	C30-C29-C31	2.95	120.24	115.27
23	D	404[A]	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
29	d	405[B]	PL9	C37-C38-C39	-2.95	120.56	127.66
23	c	506	CLA	C3B-C4B-NB	2.95	113.02	109.21
23	c	507	CLA	CHD-C4C-NC	2.95	128.85	124.20
23	C	510	CLA	O2A-CGA-CBA	2.95	121.16	111.91
23	B	610	CLA	C3B-C4B-NB	2.95	113.02	109.21
31	m	103	LMT	C3'-C4'-C5'	-2.95	104.17	110.93
23	C	506	CLA	CMC-C2C-C1C	2.94	129.52	125.04
23	C	502	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
25	c	515	BCR	C16-C17-C18	-2.94	123.11	127.31
23	B	613	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
34	B	622	HTG	C1'-S1-C1	2.94	105.59	100.09
23	b	602	CLA	C1-C2-C3	-2.94	120.96	126.04
29	a	414[B]	PL9	C35-C34-C36	2.94	120.22	115.27
23	c	514	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
23	a	405[B]	CLA	C2A-C1A-CHA	-2.94	118.72	123.86
23	D	405	CLA	C4-C3-C5	2.94	120.21	115.27
31	A	419	LMT	O5B-C5B-C4B	2.93	115.02	109.69
29	D	407[A]	PL9	C10-C9-C11	2.93	120.20	115.27
23	A	405[B]	CLA	CHC-C1C-C2C	-2.93	118.61	126.72
33	C	501	LMG	C8-O7-C10	-2.93	110.58	117.79
23	A	405[A]	CLA	CMA-C3A-C4A	-2.93	103.90	111.77
23	c	512	CLA	CMC-C2C-C1C	2.93	129.50	125.04
23	A	404[A]	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
23	a	406[A]	CLA	CMA-C3A-C2A	-2.92	102.03	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	614	CLA	CHC-C1C-C2C	-2.92	118.64	126.72
25	d	404	BCR	C10-C11-C12	-2.92	114.10	123.22
23	C	506	CLA	CAC-C3C-C4C	2.92	128.60	124.81
23	b	603	CLA	CBC-CAC-C3C	-2.92	104.38	112.43
23	c	503	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
23	C	509	CLA	CHC-C1C-C2C	-2.92	118.64	126.72
25	c	515	BCR	C37-C22-C21	-2.92	118.83	122.92
23	b	615	CLA	CHC-C1C-C2C	-2.92	118.64	126.72
32	d	413[B]	LHG	C5-O7-C7	-2.92	110.60	117.79
23	A	405[B]	CLA	CED-O2D-CGD	2.92	122.53	115.94
23	C	511	CLA	CHC-C1C-C2C	-2.92	118.65	126.72
32	E	101[A]	LHG	O8-C23-C24	2.92	121.06	111.91
23	C	507	CLA	CAA-C2A-C3A	-2.91	104.80	112.78
23	D	404[A]	CLA	C4-C3-C5	2.91	120.17	115.27
23	A	404[B]	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
29	d	405[B]	PL9	C17-C18-C19	-2.91	120.64	127.66
23	c	509	CLA	CAA-C2A-C3A	-2.91	104.80	112.78
23	b	606	CLA	CHC-C1C-C2C	-2.91	118.67	126.72
23	a	409	CLA	O2A-CGA-O1A	-2.91	116.25	123.59
23	A	404[A]	CLA	C2A-C1A-CHA	-2.91	118.77	123.86
23	b	608	CLA	C1-C2-C3	-2.91	121.01	126.04
23	C	512	CLA	CMC-C2C-C1C	2.91	129.47	125.04
23	C	513	CLA	CMC-C2C-C1C	2.91	129.47	125.04
26	B	620	SQD	C4-C3-C2	2.91	115.89	110.82
23	A	405[A]	CLA	CHD-C4C-NC	2.90	128.78	124.20
23	B	608	CLA	CHB-C4A-NA	2.90	128.52	124.51
23	c	511	CLA	CHD-C4C-NC	2.90	128.77	124.20
23	D	404[A]	CLA	O2A-CGA-CBA	2.90	121.00	111.91
29	D	407[B]	PL9	C10-C9-C11	2.90	120.14	115.27
23	b	616	CLA	CBC-CAC-C3C	-2.90	104.44	112.43
23	d	402[A]	CLA	CHC-C1C-C2C	-2.90	118.71	126.72
23	C	514	CLA	CMB-C2B-C3B	2.90	130.10	124.68
23	B	615	CLA	CHD-C4C-NC	2.89	128.76	124.20
23	C	510	CLA	C16-C15-C13	-2.89	106.57	115.92
23	C	511	CLA	CMC-C2C-C1C	2.89	129.44	125.04
23	b	607	CLA	CHC-C1C-C2C	-2.89	118.73	126.72
23	c	514	CLA	O2A-CGA-CBA	2.89	120.98	111.91
23	A	406[B]	CLA	CHD-C4C-NC	2.89	128.75	124.20
23	a	406[B]	CLA	CBC-CAC-C3C	-2.88	104.48	112.43
23	C	511	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
34	B	622	HTG	C1-O5-C5	2.88	117.90	112.58
32	d	406[A]	LHG	O7-C7-C8	2.88	117.71	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	404[A]	CLA	CAA-C2A-C3A	-2.88	104.89	112.78
34	b	623	HTG	O5-C1-C2	2.88	113.94	110.31
23	a	406[B]	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
23	B	612	CLA	CMB-C2B-C3B	2.88	130.07	124.68
24	a	408[B]	PHO	O1D-CGD-CBD	-2.88	119.94	124.74
23	c	510	CLA	O2A-C1-C2	2.88	116.20	108.64
23	B	611	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
29	a	414[B]	PL9	C22-C23-C24	-2.88	120.73	127.66
23	C	505	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
24	a	416[A]	PHO	C4A-C3A-C2A	-2.88	100.10	102.84
23	c	503	CLA	CHD-C4C-NC	2.88	128.74	124.20
23	A	406[A]	CLA	CHD-C4C-NC	2.88	128.73	124.20
26	a	411[A]	SQD	O47-C7-O49	-2.87	116.75	123.70
23	b	611	CLA	CHC-C1C-C2C	-2.87	118.77	126.72
23	C	508	CLA	C4-C3-C5	2.87	120.10	115.27
24	A	416[A]	PHO	O2D-CGD-O1D	-2.87	118.22	123.84
26	A	412	SQD	C4-C3-C2	-2.87	105.81	110.82
29	A	414[B]	PL9	C10-C9-C11	2.87	120.10	115.27
23	C	513	CLA	O2A-CGA-CBA	2.87	120.91	111.91
23	B	606	CLA	CHC-C1C-C2C	-2.87	118.78	126.72
23	B	602	CLA	CAC-C3C-C4C	2.87	128.53	124.81
23	d	403	CLA	C3B-C4B-NB	2.87	112.92	109.21
23	a	405[A]	CLA	CAC-C3C-C4C	2.87	128.53	124.81
23	B	614	CLA	CHD-C4C-NC	2.87	128.72	124.20
32	A	418[B]	LHG	O8-C23-O10	-2.87	116.36	123.59
25	C	515	BCR	C15-C14-C13	-2.87	123.22	127.31
32	A	418[A]	LHG	C5-O7-C7	-2.87	110.73	117.79
23	c	511	CLA	CBC-CAC-C3C	-2.87	104.53	112.43
35	h	102	DGD	O1G-C1A-C2A	2.87	120.90	111.91
24	A	407[B]	PHO	O1D-CGD-CBD	-2.87	119.97	124.74
23	b	611	CLA	C2A-C1A-CHA	-2.86	118.85	123.86
23	B	614	CLA	CMB-C2B-C3B	2.86	130.03	124.68
33	z	101	LMG	O8-C28-C29	2.86	120.89	111.91
23	C	510	CLA	O2A-CGA-O1A	-2.86	116.37	123.59
23	a	406[A]	CLA	CHC-C1C-C2C	-2.86	118.81	126.72
34	b	625	HTG	O5-C5-C4	2.86	114.89	109.69
29	D	407[A]	PL9	C51-C49-C50	2.86	120.92	114.60
23	C	503	CLA	C3B-C4B-NB	2.86	112.90	109.21
23	B	609	CLA	CMC-C2C-C1C	2.86	129.39	125.04
23	D	404[B]	CLA	O2A-CGA-O1A	-2.85	116.39	123.59
33	d	411	LMG	O8-C28-O10	-2.85	116.39	123.59
23	C	504	CLA	O2A-CGA-O1A	-2.85	116.40	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	414[A]	PL9	C53-C6-C1	2.85	120.82	114.99
23	C	503	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
23	B	605	CLA	CMC-C2C-C1C	2.85	129.38	125.04
23	b	604	CLA	C6-C5-C3	-2.85	105.98	113.45
23	c	508	CLA	O1D-CGD-CBD	-2.85	118.66	124.48
26	X	101	SQD	O48-C23-C24	2.85	120.84	111.91
23	d	402[B]	CLA	CMB-C2B-C3B	2.85	130.00	124.68
23	B	615	CLA	C4-C3-C5	2.85	120.06	115.27
35	C	517[A]	DGD	O6D-C1D-O3G	-2.85	103.24	109.97
23	B	607	CLA	C4C-C3C-C2C	-2.84	102.75	106.90
23	b	610	CLA	CAA-CBA-CGA	-2.84	104.94	113.25
23	c	510	CLA	CMB-C2B-C3B	2.84	130.00	124.68
23	c	514	CLA	CHC-C1C-C2C	-2.84	118.86	126.72
32	A	418[B]	LHG	O8-C23-C24	2.84	120.82	111.91
26	A	410[A]	SQD	O48-C23-C24	2.84	120.82	111.91
23	c	512	CLA	O2A-CGA-CBA	2.84	120.82	111.91
23	c	506	CLA	CHC-C1C-C2C	-2.84	118.87	126.72
23	A	406[B]	CLA	O2A-CGA-CBA	2.84	120.81	111.91
35	C	519	DGD	O2G-C1B-C2B	2.84	117.62	111.50
23	B	613	CLA	CHC-C1C-C2C	-2.84	118.87	126.72
25	h	101	BCR	C37-C22-C21	-2.84	118.95	122.92
23	A	406[B]	CLA	CHC-C1C-C2C	-2.84	118.88	126.72
23	a	407[A]	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
23	d	403	CLA	C4-C3-C5	2.83	120.04	115.27
23	A	406[A]	CLA	O2A-CGA-CBA	2.83	120.80	111.91
23	b	616	CLA	O2A-CGA-O1A	-2.83	116.44	123.59
23	b	613	CLA	CHC-C1C-C2C	-2.83	118.89	126.72
23	D	404[B]	CLA	CHC-C1C-C2C	-2.83	118.89	126.72
23	B	615	CLA	C2A-C1A-CHA	-2.83	118.91	123.86
24	A	407[A]	PHO	CMC-C2C-C3C	2.83	130.28	124.94
23	B	610	CLA	C1-C2-C3	-2.83	121.15	126.04
39	f	101	HEM	CHB-C1B-NB	2.83	127.88	124.38
23	C	505	CLA	C1-O2A-CGA	2.83	123.86	116.44
31	M	102	LMT	C1'-O5'-C5'	-2.83	108.14	113.69
23	d	402[B]	CLA	CHC-C1C-C2C	-2.83	118.90	126.72
29	D	407[A]	PL9	C37-C38-C39	-2.83	120.85	127.66
29	a	414[B]	PL9	C53-C6-C1	2.82	120.76	114.99
23	B	601	CLA	CHD-C4C-NC	2.82	128.65	124.20
25	K	103	BCR	C10-C11-C12	-2.82	114.41	123.22
31	b	621	LMT	C1'-O5'-C5'	-2.82	108.15	113.69
23	A	404[A]	CLA	CHC-C1C-C2C	-2.82	118.92	126.72
29	A	414[A]	PL9	C35-C34-C36	2.82	120.01	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	410	BCR	C29-C30-C25	2.82	114.82	110.48
26	A	410[B]	SQD	O48-C23-C24	2.82	120.75	111.91
23	D	405	CLA	CAC-C3C-C4C	2.82	128.46	124.81
32	L	101[A]	LHG	O8-C23-C24	2.82	120.75	111.91
25	a	410	BCR	C7-C8-C9	-2.82	121.98	126.23
25	D	406	BCR	C40-C30-C25	-2.81	105.73	110.30
25	K	103	BCR	C28-C27-C26	-2.81	109.05	114.08
23	c	514	CLA	C2A-C1A-CHA	-2.81	118.94	123.86
23	B	611	CLA	C3B-C4B-NB	2.81	112.85	109.21
23	A	406[A]	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
25	k	101	BCR	C39-C30-C25	-2.81	105.74	110.30
29	D	407[B]	PL9	C20-C19-C21	2.81	120.00	115.27
33	c	521	LMG	O8-C28-C29	2.81	120.72	111.91
39	F	102	HEM	CHA-C4D-ND	2.81	127.85	124.38
33	D	413	LMG	O8-C28-O10	-2.81	116.50	123.59
23	B	608	CLA	CHC-C1C-C2C	-2.81	118.95	126.72
25	H	101	BCR	C16-C17-C18	-2.81	123.30	127.31
23	C	513	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
25	B	619	BCR	C38-C26-C25	-2.81	121.38	124.53
23	A	406[A]	CLA	C4-C3-C5	2.81	119.99	115.27
29	A	414[A]	PL9	C30-C29-C31	2.81	119.99	115.27
23	C	506	CLA	C3B-C4B-NB	2.81	112.84	109.21
23	b	608	CLA	O2A-CGA-CBA	2.81	120.71	111.91
34	B	622	HTG	O2-C2-C3	-2.80	103.87	110.35
23	A	404[B]	CLA	C2A-C1A-CHA	-2.80	118.96	123.86
23	C	514	CLA	CHD-C4C-NC	2.80	128.62	124.20
23	A	405[A]	CLA	CHC-C1C-C2C	-2.80	118.97	126.72
29	a	414[A]	PL9	C22-C23-C24	-2.80	120.92	127.66
23	b	605	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
23	C	508	CLA	CAC-C3C-C4C	2.80	128.44	124.81
23	a	407[A]	CLA	CHC-C1C-C2C	-2.80	118.98	126.72
29	A	414[B]	PL9	C53-C6-C1	2.80	120.71	114.99
26	f	102	SQD	O48-C23-C24	2.80	120.68	111.91
23	c	514	CLA	CMC-C2C-C1C	2.80	129.30	125.04
23	B	606	CLA	CHD-C4C-NC	2.80	128.61	124.20
23	b	608	CLA	CHC-C1C-C2C	-2.80	118.99	126.72
29	a	414[B]	PL9	C42-C43-C44	-2.79	120.93	127.66
23	c	514	CLA	CAA-C2A-C3A	-2.79	105.13	112.78
23	D	405	CLA	CMA-C3A-C2A	-2.79	102.56	113.83
25	A	409	BCR	C33-C5-C6	-2.79	121.39	124.53
23	d	402[B]	CLA	C2A-C1A-CHA	-2.79	118.97	123.86
33	c	520	LMG	O8-C28-C29	2.79	120.67	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	K	103	BCR	C36-C18-C17	-2.79	119.01	122.92
23	c	509	CLA	CHD-C4C-NC	2.79	128.60	124.20
25	H	101	BCR	C16-C15-C14	-2.79	117.76	123.47
24	A	407[B]	PHO	CMA-C3A-C4A	-2.79	108.27	114.38
23	a	409	CLA	CMA-C3A-C2A	-2.79	102.58	113.83
23	b	612	CLA	O2A-CGA-CBA	2.79	120.66	111.91
35	c	519	DGD	O1G-C1A-C2A	2.79	120.65	111.91
23	D	404[B]	CLA	CMC-C2C-C1C	2.78	129.28	125.04
23	b	612	CLA	CHC-C1C-C2C	-2.78	119.03	126.72
31	B	631	LMT	C3'-C4'-C5'	-2.78	104.55	110.93
23	C	514	CLA	C1-C2-C3	-2.78	121.23	126.04
23	c	504	CLA	CHD-C4C-NC	2.78	128.58	124.20
23	B	616	CLA	CMB-C2B-C3B	2.78	129.88	124.68
23	C	514	CLA	C4C-C3C-C2C	-2.78	102.85	106.90
23	C	506	CLA	CHC-C1C-C2C	-2.78	119.05	126.72
23	B	605	CLA	C2A-C1A-CHA	-2.77	119.01	123.86
23	b	603	CLA	CHC-C1C-C2C	-2.77	119.05	126.72
26	a	411[B]	SQD	O47-C7-O49	-2.77	117.00	123.70
23	b	607	CLA	C4-C3-C5	2.77	119.94	115.27
23	c	507	CLA	CMC-C2C-C1C	2.77	129.26	125.04
23	b	605	CLA	C1-C2-C3	-2.77	121.25	126.04
23	B	601	CLA	CAC-C3C-C4C	2.77	128.41	124.81
23	A	405[A]	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
25	C	515	BCR	C38-C26-C25	-2.77	121.42	124.53
23	B	603	CLA	CMC-C2C-C1C	2.77	129.26	125.04
24	a	408[A]	PHO	CMB-C2B-C3B	2.77	129.86	124.68
23	c	510	CLA	CHD-C4C-NC	2.77	128.57	124.20
29	D	407[B]	PL9	C27-C28-C29	-2.77	121.00	127.66
23	a	407[B]	CLA	CHD-C4C-NC	2.77	128.56	124.20
23	c	513	CLA	CHC-C1C-C2C	-2.77	119.07	126.72
41	V	201	HEC	CMB-C2B-C3B	2.76	129.07	125.82
25	k	101	BCR	C24-C23-C22	-2.76	122.06	126.23
23	a	406[A]	CLA	O2A-CGA-CBA	2.76	120.58	111.91
35	C	517[B]	DGD	C2G-O2G-C1B	-2.76	110.99	117.79
23	a	407[A]	CLA	O2A-CGA-O1A	-2.76	116.62	123.59
23	B	608	CLA	C1-C2-C3	-2.76	121.27	126.04
23	B	606	CLA	C4-C3-C5	2.76	119.92	115.27
23	c	508	CLA	C3B-C4B-NB	2.76	112.78	109.21
23	b	601	CLA	C3B-C4B-NB	2.76	112.77	109.21
23	C	506	CLA	O2A-CGA-CBA	2.76	120.56	111.91
23	c	509	CLA	CHC-C1C-C2C	-2.76	119.10	126.72
32	D	408[A]	LHG	O7-C7-C8	2.75	117.44	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	602	CLA	C2A-C1A-CHA	-2.75	119.04	123.86
39	f	101	HEM	C4D-ND-C1D	2.75	107.92	105.07
23	B	616	CLA	C1-O2A-CGA	2.75	123.66	116.44
25	B	618	BCR	C40-C30-C25	-2.75	105.84	110.30
23	c	508	CLA	C4-C3-C5	2.75	119.89	115.27
23	c	508	CLA	O2A-CGA-CBA	2.75	120.53	111.91
23	b	601	CLA	CHC-C1C-C2C	-2.75	119.12	126.72
23	b	602	CLA	C1-O2A-CGA	2.75	123.65	116.44
25	D	406	BCR	C16-C17-C18	-2.75	123.39	127.31
23	b	611	CLA	CMC-C2C-C1C	2.74	129.22	125.04
25	A	409	BCR	C8-C7-C6	-2.74	119.50	127.20
29	d	405[A]	PL9	C36-C37-C38	-2.74	102.86	111.88
23	d	402[B]	CLA	CAC-C3C-C4C	2.74	128.37	124.81
29	A	414[B]	PL9	C7-C3-C4	2.74	119.11	116.88
23	a	407[B]	CLA	C4C-C3C-C2C	-2.74	102.91	106.90
23	b	614	CLA	CHD-C4C-NC	2.74	128.52	124.20
23	b	606	CLA	C4C-C3C-C2C	-2.74	102.91	106.90
23	b	616	CLA	CHC-C1C-C2C	-2.74	119.15	126.72
23	B	608	CLA	CMB-C2B-C3B	2.74	129.80	124.68
23	b	607	CLA	CMB-C2B-C3B	2.74	129.80	124.68
23	c	511	CLA	CMB-C2B-C3B	2.73	129.79	124.68
23	D	404[B]	CLA	C2A-C1A-CHA	-2.73	119.08	123.86
23	c	504	CLA	O2A-CGA-CBA	2.73	120.48	111.91
23	B	603	CLA	CHC-C1C-C2C	-2.73	119.16	126.72
23	C	504	CLA	CHC-C1C-C2C	-2.73	119.17	126.72
32	b	629[B]	LHG	O8-C23-C24	2.73	120.48	111.91
23	a	407[B]	CLA	C4-C3-C5	2.73	119.86	115.27
33	c	520	LMG	O1-C7-C8	-2.73	104.32	110.90
23	b	614	CLA	CBC-CAC-C3C	-2.73	104.92	112.43
26	b	620	SQD	C44-O6-C1	-2.72	108.42	113.74
26	X	101	SQD	O5-C1-O6	2.72	116.42	109.97
29	d	405[A]	PL9	C27-C28-C29	-2.72	121.11	127.66
29	d	405[B]	PL9	C7-C8-C9	-2.72	122.26	126.79
23	C	503	CLA	CMC-C2C-C1C	2.72	129.18	125.04
23	b	604	CLA	CHC-C1C-C2C	-2.72	119.21	126.72
23	C	512	CLA	CAC-C3C-C4C	2.71	128.33	124.81
23	c	504	CLA	C4-C3-C5	2.71	119.83	115.27
25	K	103	BCR	C15-C16-C17	-2.71	117.92	123.47
23	A	406[B]	CLA	CBC-CAC-C3C	-2.71	104.96	112.43
33	D	413	LMG	O7-C10-C11	2.71	117.34	111.50
23	c	513	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
23	B	606	CLA	C4C-C3C-C2C	-2.71	102.95	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	610	CLA	CHC-C1C-C2C	-2.71	119.24	126.72
23	A	406[B]	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
39	F	102	HEM	O2A-CGA-CBA	2.71	122.72	114.03
23	C	507	CLA	CAC-C3C-C4C	2.70	128.31	124.81
35	c	518[B]	DGD	O1G-C1A-C2A	2.70	120.38	111.91
23	C	502	CLA	CHC-C1C-C2C	-2.70	119.26	126.72
23	c	513	CLA	CMC-C2C-C1C	2.70	129.15	125.04
23	b	612	CLA	O2A-CGA-O1A	-2.70	116.78	123.59
23	b	605	CLA	CMC-C2C-C1C	2.70	129.15	125.04
24	a	408[B]	PHO	C1A-C2A-C3A	-2.70	100.27	102.84
23	a	405[A]	CLA	C2A-C1A-CHA	-2.69	119.15	123.86
23	A	408	CLA	CHB-C4A-NA	2.69	128.24	124.51
23	C	502	CLA	CHD-C4C-NC	2.69	128.45	124.20
23	b	603	CLA	C2A-C1A-CHA	-2.69	119.15	123.86
23	c	507	CLA	C4C-C3C-C2C	-2.69	102.97	106.90
32	L	101[A]	LHG	O8-C23-O10	-2.69	116.80	123.59
23	b	602	CLA	C11-C12-C13	-2.69	107.22	115.92
24	a	408[B]	PHO	CMA-C3A-C4A	-2.69	108.49	114.38
31	A	417	LMT	O5B-C5B-C4B	2.69	114.58	109.69
23	B	604	CLA	C6-C5-C3	-2.69	106.40	113.45
23	D	404[A]	CLA	CAC-C3C-C4C	2.69	128.30	124.81
23	a	405[B]	CLA	CHD-C4C-NC	2.69	128.44	124.20
26	f	102	SQD	O7-S-C6	2.69	110.13	106.94
23	c	503	CLA	O2A-CGA-CBA	2.69	120.34	111.91
23	B	612	CLA	O2A-CGA-CBA	2.69	120.33	111.91
29	d	405[B]	PL9	C22-C23-C24	-2.68	121.20	127.66
23	b	612	CLA	CMB-C2B-C3B	2.68	129.69	124.68
23	c	507	CLA	CBC-CAC-C3C	-2.68	105.04	112.43
32	b	629[A]	LHG	O8-C23-C24	2.68	120.32	111.91
23	B	601	CLA	O2A-CGA-CBA	2.68	120.31	111.91
23	c	513	CLA	C3B-C4B-NB	2.68	112.67	109.21
29	D	407[B]	PL9	C37-C38-C39	-2.67	121.22	127.66
23	A	404[A]	CLA	CMA-C3A-C2A	-2.67	103.05	113.83
23	c	512	CLA	O2A-CGA-O1A	-2.67	116.85	123.59
23	B	608	CLA	O2A-CGA-O1A	-2.67	116.85	123.59
23	B	609	CLA	CAC-C3C-C4C	2.67	128.28	124.81
23	C	514	CLA	CBC-CAC-C3C	-2.67	105.07	112.43
23	B	613	CLA	C1D-CHD-C4C	-2.67	120.30	126.06
33	d	411	LMG	O8-C28-C29	2.67	120.28	111.91
23	a	406[A]	CLA	C4C-C3C-C2C	-2.67	103.01	106.90
23	b	610	CLA	C3B-C4B-NB	2.67	112.66	109.21
23	b	603	CLA	O2A-CGA-O1A	-2.67	116.87	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	504	CLA	O2A-CGA-O1A	-2.66	116.88	123.59
23	D	404[A]	CLA	CHC-C1C-C2C	-2.66	119.36	126.72
27	b	628	GOL	C3-C2-C1	-2.66	101.36	111.70
24	a	416[B]	PHO	O2D-CGD-O1D	-2.66	118.64	123.84
32	a	420[A]	LHG	O8-C23-C24	2.66	120.25	111.91
23	C	508	CLA	CHD-C4C-NC	2.66	128.39	124.20
35	c	517[B]	DGD	C2G-O2G-C1B	-2.66	111.25	117.79
23	d	403	CLA	CBC-CAC-C3C	-2.66	105.10	112.43
23	A	404[B]	CLA	CMC-C2C-C1C	2.66	129.09	125.04
24	A	407[A]	PHO	C1-C2-C3	-2.66	121.45	126.04
31	M	101	LMT	C3'-C4'-C5'	-2.66	104.84	110.93
23	C	511	CLA	O2A-CGA-CBA	2.65	120.23	111.91
23	a	406[A]	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
23	c	511	CLA	O2A-CGA-O1A	-2.65	116.90	123.59
23	d	402[A]	CLA	CAC-C3C-C4C	2.65	128.25	124.81
35	C	518[A]	DGD	O1G-C1A-O1A	-2.65	116.90	123.59
23	d	402[A]	CLA	C2A-C1A-CHA	-2.65	119.23	123.86
23	A	405[A]	CLA	C4-C3-C5	2.65	119.73	115.27
31	B	628	LMT	O1'-C1'-C2'	2.65	112.44	108.30
33	C	521	LMG	O1-C1-C2	2.65	112.44	108.30
23	A	408	CLA	CMA-C3A-C2A	-2.65	103.14	113.83
23	a	409	CLA	CAC-C3C-C4C	2.65	128.25	124.81
23	C	514	CLA	CHC-C1C-C2C	-2.65	119.40	126.72
29	a	414[A]	PL9	C40-C39-C41	2.65	119.72	115.27
23	b	613	CLA	CHD-C4C-NC	2.64	128.37	124.20
23	D	404[A]	CLA	C2A-C1A-CHA	-2.64	119.24	123.86
23	B	609	CLA	O2A-CGA-CBA	2.64	120.20	111.91
32	D	408[A]	LHG	O8-C23-C24	2.64	120.20	111.91
26	X	101	SQD	O7-S-C6	2.64	110.08	106.94
23	b	609	CLA	CMC-C2C-C1C	2.64	129.06	125.04
23	C	507	CLA	CHD-C4C-NC	2.64	128.36	124.20
23	b	608	CLA	C11-C12-C13	-2.64	107.39	115.92
25	a	410	BCR	C38-C26-C25	-2.64	121.57	124.53
23	d	402[B]	CLA	CAA-C2A-C3A	-2.64	105.56	112.78
29	a	414[B]	PL9	C40-C39-C41	2.64	119.70	115.27
23	B	610	CLA	O1D-CGD-CBD	-2.64	119.09	124.48
33	D	413	LMG	O8-C28-C29	2.64	120.18	111.91
25	H	101	BCR	C37-C22-C21	-2.64	119.23	122.92
25	c	515	BCR	C36-C18-C17	-2.63	119.23	122.92
25	K	102	BCR	C38-C26-C25	-2.63	121.57	124.53
33	C	501	LMG	C6-C5-C4	2.63	119.17	113.00
26	a	412	SQD	O8-S-C6	2.63	109.94	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	414[A]	PL9	C40-C39-C41	2.63	119.70	115.27
35	H	102	DGD	O6E-C5E-C6E	2.63	112.98	106.44
23	B	602	CLA	C4C-C3C-C2C	-2.63	103.06	106.90
23	b	604	CLA	CAC-C3C-C4C	2.63	128.22	124.81
23	a	406[B]	CLA	C2A-C1A-CHA	-2.63	119.26	123.86
23	A	408	CLA	O2A-CGA-CBA	2.63	120.16	111.91
25	h	101	BCR	C33-C5-C6	-2.63	121.58	124.53
23	C	510	CLA	CHC-C1C-C2C	-2.63	119.45	126.72
29	a	414[B]	PL9	C20-C19-C21	2.63	119.69	115.27
35	h	102	DGD	O3G-C1D-C2D	2.63	112.40	108.30
23	C	514	CLA	CAC-C3C-C4C	2.63	128.22	124.81
29	d	405[B]	PL9	C35-C34-C36	2.63	119.69	115.27
23	D	405	CLA	C2A-C1A-CHA	-2.63	119.27	123.86
29	D	407[B]	PL9	C45-C44-C46	2.63	119.69	115.27
23	C	511	CLA	O2A-CGA-O1A	-2.63	116.97	123.59
23	b	610	CLA	C4-C3-C5	2.62	119.69	115.27
23	c	504	CLA	CHC-C1C-C2C	-2.62	119.47	126.72
23	C	514	CLA	C2A-C1A-CHA	-2.62	119.27	123.86
23	d	403	CLA	CHD-C4C-NC	2.62	128.34	124.20
23	b	608	CLA	O2A-CGA-O1A	-2.62	116.98	123.59
25	B	618	BCR	C2-C1-C6	2.62	114.51	110.48
23	b	607	CLA	CHD-C4C-NC	2.62	128.33	124.20
23	C	504	CLA	CAC-C3C-C4C	2.62	128.21	124.81
23	B	603	CLA	C5-C3-C2	-2.62	115.82	121.12
25	c	515	BCR	C20-C21-C22	-2.61	123.58	127.31
29	a	414[B]	PL9	C10-C9-C11	2.61	119.67	115.27
23	D	404[B]	CLA	CAA-C2A-C3A	-2.61	105.62	112.78
29	a	414[A]	PL9	C47-C48-C49	-2.61	118.83	127.75
33	m	101	LMG	C7-O1-C1	-2.61	108.64	113.74
23	a	407[A]	CLA	O2A-CGA-CBA	2.61	120.10	111.91
23	c	508	CLA	CHC-C1C-C2C	-2.61	119.50	126.72
23	b	607	CLA	CAA-C2A-C3A	-2.61	105.63	112.78
32	d	407[A]	LHG	O8-C23-C24	2.61	120.09	111.91
25	B	618	BCR	C37-C22-C23	2.61	122.18	118.08
25	b	618	BCR	C15-C14-C13	-2.60	123.59	127.31
23	B	608	CLA	CMC-C2C-C1C	2.60	129.00	125.04
23	C	514	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
23	A	405[A]	CLA	CMA-C3A-C2A	-2.60	103.33	113.83
29	A	414[B]	PL9	C45-C44-C46	2.60	119.65	115.27
23	D	405	CLA	CHD-C4C-NC	2.60	128.30	124.20
29	a	414[A]	PL9	C10-C9-C8	-2.60	117.01	123.68
23	D	405	CLA	CAA-C2A-C3A	-2.60	105.66	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	514	CLA	O2A-CGA-CBA	2.60	120.07	111.91
29	D	407[B]	PL9	C40-C39-C41	2.60	119.64	115.27
23	A	404[B]	CLA	C4-C3-C5	2.60	119.64	115.27
25	B	617	BCR	C7-C8-C9	-2.60	122.31	126.23
23	A	404[B]	CLA	CAA-C2A-C1A	-2.60	103.46	111.97
32	a	420[B]	LHG	O8-C23-C24	2.60	120.06	111.91
23	c	510	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
25	T	101	BCR	C15-C14-C13	2.60	131.02	127.31
23	C	503	CLA	CAC-C3C-C4C	2.60	128.18	124.81
23	a	407[A]	CLA	CMC-C2C-C1C	2.60	128.99	125.04
23	C	512	CLA	O2A-CGA-CBA	2.60	120.05	111.91
24	A	407[A]	PHO	O2A-CGA-CBA	2.59	120.05	111.91
31	A	419	LMT	O5'-C5'-C4'	2.59	115.22	109.75
23	A	404[B]	CLA	CAC-C3C-C4C	2.59	128.17	124.81
23	B	615	CLA	C11-C10-C8	-2.59	107.54	115.92
23	c	511	CLA	CHC-C1C-C2C	-2.59	119.56	126.72
23	c	512	CLA	CHC-C1C-C2C	-2.59	119.56	126.72
23	b	609	CLA	C16-C15-C13	-2.59	107.55	115.92
23	a	406[A]	CLA	O2A-CGA-O1A	-2.59	117.06	123.59
29	d	405[B]	PL9	C27-C28-C29	-2.59	121.43	127.66
23	A	406[A]	CLA	CHC-C1C-C2C	-2.59	119.57	126.72
23	b	611	CLA	C1-C2-C3	-2.59	121.57	126.04
29	A	414[B]	PL9	C12-C13-C14	-2.59	121.43	127.66
23	C	503	CLA	CBC-CAC-C3C	-2.59	105.30	112.43
23	C	503	CLA	C2A-C1A-CHA	-2.58	119.34	123.86
29	A	414[B]	PL9	C35-C34-C36	2.58	119.62	115.27
23	A	408	CLA	CMB-C2B-C3B	2.58	129.51	124.68
23	d	403	CLA	O2A-CGA-CBA	2.58	120.01	111.91
23	c	508	CLA	CAC-C3C-C4C	2.58	128.16	124.81
32	L	101[B]	LHG	O8-C23-C24	2.58	120.01	111.91
23	a	405[B]	CLA	C4-C3-C5	2.58	119.61	115.27
23	A	405[B]	CLA	C1-C2-C3	-2.58	121.59	126.04
23	A	405[A]	CLA	C2A-C1A-CHA	-2.58	119.35	123.86
23	a	409	CLA	C2A-C1A-CHA	-2.58	119.35	123.86
29	A	414[B]	PL9	C42-C43-C44	-2.58	121.46	127.66
25	T	101	BCR	C35-C13-C12	2.57	122.13	118.08
23	B	602	CLA	C11-C12-C13	-2.57	107.60	115.92
26	X	101	SQD	O47-C7-O49	-2.57	117.48	123.70
23	b	615	CLA	C6-C7-C8	-2.57	107.60	115.92
23	D	404[A]	CLA	O2A-CGA-O1A	-2.57	117.10	123.59
31	A	419	LMT	O5'-C5'-C6'	2.57	112.83	106.44
23	a	407[B]	CLA	C1-C2-C3	-2.57	121.60	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	407[A]	PHO	O1D-CGD-CBD	-2.57	120.46	124.74
26	A	410[A]	SQD	O48-C23-O10	-2.57	117.11	123.59
23	d	403	CLA	CHC-C1C-C2C	-2.57	119.62	126.72
23	a	406[B]	CLA	C1-O2A-CGA	2.57	123.18	116.44
24	A	407[A]	PHO	O2A-CGA-O1A	-2.57	117.12	123.59
23	B	603	CLA	CMA-C3A-C2A	-2.56	103.49	113.83
25	C	516	BCR	C33-C5-C6	-2.56	121.65	124.53
25	B	618	BCR	C37-C22-C21	-2.56	119.33	122.92
23	a	406[B]	CLA	C1-C2-C3	-2.56	121.61	126.04
25	K	102	BCR	C24-C23-C22	-2.56	122.36	126.23
23	B	616	CLA	CHD-C4C-NC	2.56	128.24	124.20
29	A	414[A]	PL9	C10-C9-C8	-2.56	117.11	123.68
25	b	619	BCR	C7-C8-C9	-2.56	122.37	126.23
23	B	608	CLA	C11-C12-C13	-2.56	107.65	115.92
23	B	606	CLA	O2A-CGA-O1A	-2.55	117.14	123.59
23	C	513	CLA	CMA-C3A-C4A	-2.55	104.91	111.77
23	c	505	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
23	C	509	CLA	O2A-CGA-CBA	2.55	119.92	111.91
23	c	509	CLA	C4-C3-C5	2.55	119.56	115.27
25	d	404	BCR	C40-C30-C39	2.55	116.36	108.53
23	C	512	CLA	CHC-C1C-C2C	-2.55	119.67	126.72
23	c	504	CLA	C2A-C1A-CHA	-2.55	119.40	123.86
23	B	606	CLA	O2A-CGA-CBA	2.55	119.91	111.91
23	B	602	CLA	CHD-C4C-NC	2.55	128.22	124.20
23	c	507	CLA	CMB-C2B-C3B	2.55	129.45	124.68
23	D	404[B]	CLA	C4-C3-C5	2.55	119.56	115.27
23	C	511	CLA	CMB-C2B-C3B	2.55	129.44	124.68
23	b	604	CLA	C1-O2A-CGA	2.55	123.12	116.44
25	B	619	BCR	C7-C8-C9	-2.55	122.39	126.23
23	A	405[A]	CLA	O2A-CGA-O1A	-2.54	117.17	123.59
23	d	402[A]	CLA	CAA-C2A-C3A	-2.54	105.81	112.78
23	a	407[B]	CLA	O2A-CGA-CBA	2.54	119.89	111.91
35	C	518[B]	DGD	O1G-C1A-C2A	2.54	119.89	111.91
29	A	414[A]	PL9	C47-C48-C49	-2.54	119.05	127.75
23	B	615	CLA	CMB-C2B-C1B	2.54	132.37	128.46
25	t	102	BCR	C1-C6-C7	2.54	122.97	115.78
23	B	615	CLA	CHC-C1C-C2C	-2.54	119.69	126.72
23	c	503	CLA	C1-C2-C3	-2.54	121.65	126.04
23	b	603	CLA	C7-C6-C5	-2.54	106.47	113.36
23	b	608	CLA	CMA-C3A-C4A	-2.54	104.95	111.77
25	c	515	BCR	C36-C18-C19	2.54	122.08	118.08
23	c	511	CLA	O2A-CGA-CBA	2.54	119.86	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	502	CLA	C1D-CHD-C4C	-2.53	120.59	126.06
23	B	602	CLA	CHC-C1C-C2C	-2.53	119.72	126.72
23	c	511	CLA	C4C-C3C-C2C	-2.53	103.21	106.90
23	a	407[B]	CLA	CMC-C2C-C1C	2.53	128.90	125.04
23	c	508	CLA	CHD-C4C-NC	2.53	128.19	124.20
24	A	407[B]	PHO	C1-C2-C3	-2.53	121.67	126.04
23	b	602	CLA	CMA-C3A-C4A	-2.53	104.97	111.77
25	t	102	BCR	C21-C20-C19	-2.53	115.33	123.22
23	b	605	CLA	C2A-C1A-CHA	-2.53	119.44	123.86
23	C	503	CLA	CHD-C4C-NC	2.53	128.19	124.20
23	C	505	CLA	C4C-C3C-C2C	-2.53	103.21	106.90
24	A	416[B]	PHO	CMB-C2B-C3B	2.52	129.40	124.68
33	a	417	LMG	O6-C5-C4	2.52	114.28	109.69
23	b	611	CLA	O2A-CGA-O1A	-2.52	117.22	123.59
23	b	614	CLA	O2A-CGA-CBA	2.52	119.82	111.91
35	C	519	DGD	O5E-C6E-C5E	-2.52	102.64	111.29
32	d	406[B]	LHG	O8-C23-O10	-2.52	117.23	123.59
23	C	506	CLA	O2A-CGA-O1A	-2.52	117.23	123.59
25	K	103	BCR	C3-C4-C5	-2.52	109.58	114.08
23	B	601	CLA	CHC-C1C-C2C	-2.52	119.76	126.72
23	C	513	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
23	c	509	CLA	O2A-CGA-O1A	-2.51	117.25	123.59
23	C	511	CLA	C2A-C1A-CHA	-2.51	119.46	123.86
25	H	101	BCR	C24-C23-C22	-2.51	122.44	126.23
23	C	505	CLA	CHC-C1C-C2C	-2.51	119.77	126.72
23	a	406[A]	CLA	CAA-CBA-CGA	2.51	120.59	113.25
23	b	615	CLA	C6-C5-C3	-2.51	106.87	113.45
23	b	613	CLA	CMB-C2B-C3B	2.51	129.37	124.68
23	A	405[B]	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
23	d	402[A]	CLA	CMC-C2C-C1C	2.51	128.86	125.04
25	B	617	BCR	C31-C1-C6	-2.51	106.23	110.30
23	c	506	CLA	O2A-CGA-CBA	2.51	119.78	111.91
32	d	406[B]	LHG	O8-C23-C24	2.51	119.78	111.91
23	A	406[A]	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
31	m	103	LMT	C3B-C4B-C5B	-2.51	105.77	110.24
23	C	509	CLA	CMB-C2B-C3B	2.51	129.37	124.68
23	a	405[A]	CLA	CHD-C4C-NC	2.51	128.15	124.20
23	D	405	CLA	CHC-C1C-C2C	-2.51	119.79	126.72
23	C	513	CLA	CMB-C2B-C3B	2.51	129.37	124.68
23	B	610	CLA	CHC-C1C-C2C	-2.51	119.79	126.72
25	d	404	BCR	C16-C17-C18	-2.51	123.73	127.31
23	C	505	CLA	CBC-CAC-C3C	-2.50	105.53	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	610	CLA	CHD-C4C-NC	2.50	128.15	124.20
29	D	407[A]	PL9	C42-C41-C39	-2.50	104.75	112.98
26	B	620	SQD	O48-C23-O10	-2.50	117.28	123.59
34	B	622	HTG	C6-C5-C4	-2.50	107.15	113.00
23	B	601	CLA	C1-O2A-CGA	2.50	123.00	116.44
24	A	416[B]	PHO	O2A-CGA-CBA	2.50	119.75	111.91
24	a	408[B]	PHO	O2A-CGA-CBA	2.50	119.75	111.91
35	c	518[A]	DGD	O1G-C1A-C2A	2.50	119.74	111.91
23	B	608	CLA	CMA-C3A-C2A	-2.50	103.76	113.83
23	a	409	CLA	CHC-C1C-C2C	-2.50	119.82	126.72
23	a	409	CLA	C4C-C3C-C2C	-2.49	103.26	106.90
32	D	409[B]	LHG	O8-C23-O10	-2.49	117.30	123.59
23	a	405[A]	CLA	C4C-C3C-C2C	-2.49	103.26	106.90
26	f	102	SQD	C4-C3-C2	-2.49	106.47	110.82
25	D	406	BCR	C37-C22-C21	-2.49	119.43	122.92
24	a	408[B]	PHO	CMB-C2B-C3B	2.49	129.34	124.68
23	b	601	CLA	C2A-C1A-CHA	-2.49	119.50	123.86
25	C	516	BCR	C2-C1-C6	2.49	114.31	110.48
23	b	607	CLA	C2A-C1A-CHA	-2.49	119.50	123.86
23	c	506	CLA	C1-C2-C3	-2.49	121.74	126.04
23	c	507	CLA	C2A-C1A-CHA	-2.49	119.51	123.86
23	B	607	CLA	C2A-C1A-CHA	-2.49	119.51	123.86
23	B	603	CLA	C2A-C1A-CHA	-2.49	119.51	123.86
26	a	412	SQD	C1-O5-C5	2.49	118.57	113.69
23	A	404[B]	CLA	CBC-CAC-C3C	-2.49	105.57	112.43
23	D	405	CLA	C3B-C4B-NB	2.49	112.43	109.21
23	C	503	CLA	C4C-C3C-C2C	-2.49	103.27	106.90
23	A	408	CLA	CAC-C3C-C4C	2.49	128.03	124.81
23	B	611	CLA	C1-O2A-CGA	2.49	122.97	116.44
25	c	516	BCR	C33-C5-C6	-2.49	121.74	124.53
26	a	411[A]	SQD	O8-S-C6	2.49	109.70	105.74
35	C	517[B]	DGD	O1G-C1A-O1A	-2.48	117.32	123.59
26	b	620	SQD	O48-C23-C24	2.48	119.70	111.91
23	a	406[A]	CLA	CBC-CAC-C3C	-2.48	105.59	112.43
23	B	604	CLA	CMC-C2C-C1C	2.48	128.82	125.04
32	d	407[B]	LHG	O8-C23-C24	2.48	119.70	111.91
23	C	510	CLA	C2A-C1A-CHA	-2.48	119.52	123.86
26	B	620	SQD	C44-O6-C1	-2.48	108.89	113.74
25	b	618	BCR	C37-C22-C23	2.48	121.99	118.08
23	a	405[B]	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
23	B	612	CLA	CHC-C1C-C2C	-2.48	119.86	126.72
23	d	403	CLA	C1-O2A-CGA	2.48	122.95	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406[A]	CLA	CMB-C2B-C1B	2.48	132.27	128.46
23	C	503	CLA	O2A-CGA-CBA	2.48	119.68	111.91
33	C	520	LMG	O8-C28-O10	-2.48	117.34	123.59
23	C	512	CLA	CMB-C2B-C3B	2.48	129.31	124.68
23	B	605	CLA	OBD-CAD-C3D	-2.47	122.56	128.52
29	D	407[A]	PL9	C20-C19-C21	2.47	119.43	115.27
23	A	404[B]	CLA	C1-C2-C3	-2.47	121.77	126.04
23	C	507	CLA	O2A-CGA-CBA	2.47	119.67	111.91
35	H	102	DGD	O1G-C1A-C2A	2.47	119.67	111.91
29	d	405[B]	PL9	C51-C49-C50	2.47	120.06	114.60
35	c	517[A]	DGD	C2G-O2G-C1B	-2.47	111.70	117.79
25	y	101	BCR	C15-C14-C13	-2.47	123.78	127.31
23	b	608	CLA	CAC-C3C-C4C	2.47	128.02	124.81
23	C	509	CLA	C2A-C1A-CHA	-2.47	119.54	123.86
23	b	614	CLA	CAA-C2A-C3A	-2.47	106.02	112.78
23	B	613	CLA	CMB-C2B-C3B	2.47	129.29	124.68
26	f	102	SQD	O5-C1-C2	2.47	115.57	110.35
23	b	608	CLA	CHB-C4A-NA	2.47	127.92	124.51
35	h	102	DGD	O4D-C4D-C3D	-2.47	104.65	110.35
25	B	619	BCR	C21-C20-C19	-2.47	115.52	123.22
23	b	603	CLA	C1B-CHB-C4A	-2.46	125.23	130.12
29	d	405[B]	PL9	C12-C13-C14	-2.46	121.73	127.66
23	c	511	CLA	CAC-C3C-C4C	2.46	128.01	124.81
24	A	407[A]	PHO	CMB-C2B-C3B	2.46	129.29	124.68
23	C	514	CLA	C4-C3-C5	2.46	119.41	115.27
35	H	102	DGD	O1G-C1A-O1A	-2.46	117.38	123.59
23	b	612	CLA	OBD-CAD-C3D	-2.46	122.60	128.52
23	C	502	CLA	C4-C3-C5	2.46	119.41	115.27
25	h	101	BCR	C10-C11-C12	-2.46	115.54	123.22
25	K	102	BCR	C33-C5-C6	-2.46	121.77	124.53
35	C	519	DGD	O3G-C3G-C2G	-2.46	104.97	110.90
25	K	102	BCR	C29-C30-C25	2.46	114.27	110.48
23	A	408	CLA	C4-C3-C5	2.46	119.41	115.27
34	b	625	HTG	C1'-S1-C1	2.46	104.69	100.09
23	A	404[A]	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
25	b	618	BCR	C8-C7-C6	-2.46	120.30	127.20
26	b	620	SQD	O47-C7-O49	-2.46	117.77	123.70
26	A	412	SQD	O48-C23-O10	-2.46	117.39	123.59
23	b	603	CLA	O2A-CGA-CBA	2.46	119.61	111.91
25	K	102	BCR	C37-C22-C21	-2.46	119.48	122.92
33	c	521	LMG	O8-C28-O10	-2.46	117.39	123.59
23	c	507	CLA	O2A-CGA-O1A	-2.45	117.40	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	609	CLA	CHD-C4C-NC	2.45	128.07	124.20
25	y	101	BCR	C37-C22-C23	2.45	121.94	118.08
23	a	406[B]	CLA	C4C-C3C-C2C	-2.45	103.32	106.90
23	B	611	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
23	A	404[A]	CLA	CAA-CBA-CGA	-2.45	106.09	113.25
23	B	604	CLA	C6-C7-C8	-2.45	108.00	115.92
26	a	411[B]	SQD	O48-C23-C24	2.45	119.59	111.91
23	B	615	CLA	C6-C7-C8	-2.45	108.00	115.92
29	D	407[A]	PL9	C40-C39-C41	2.45	119.39	115.27
26	A	410[B]	SQD	O7-S-C6	2.45	109.85	106.94
23	c	504	CLA	CAC-C3C-C4C	2.45	127.98	124.81
25	k	101	BCR	C36-C18-C19	2.45	121.93	118.08
23	b	613	CLA	C4-C3-C5	2.45	119.39	115.27
23	c	504	CLA	CMB-C2B-C1B	2.45	132.22	128.46
25	K	103	BCR	C37-C22-C23	2.44	121.93	118.08
23	D	405	CLA	O2A-CGA-O1A	-2.44	117.42	123.59
33	d	411	LMG	C7-O1-C1	-2.44	108.96	113.74
23	B	604	CLA	C11-C12-C13	-2.44	108.02	115.92
32	A	418[B]	LHG	O7-C7-O9	-2.44	117.80	123.70
23	B	614	CLA	CED-O2D-CGD	2.44	121.46	115.94
23	c	505	CLA	CHD-C4C-NC	2.44	128.05	124.20
23	A	404[B]	CLA	O2A-CGA-O1A	-2.44	117.43	123.59
25	t	102	BCR	C29-C30-C25	2.44	114.24	110.48
23	a	405[B]	CLA	O2A-CGA-O1A	-2.44	117.43	123.59
23	C	502	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
26	a	411[B]	SQD	O8-S-C6	2.44	109.63	105.74
23	b	609	CLA	C1-O2A-CGA	2.44	122.84	116.44
23	C	502	CLA	C1-C2-C3	-2.44	121.83	126.04
25	c	516	BCR	C21-C20-C19	-2.44	115.61	123.22
29	d	405[B]	PL9	C20-C19-C21	2.44	119.37	115.27
34	b	622	HTG	O5-C1-C2	2.44	113.38	110.31
23	a	409	CLA	CMB-C2B-C3B	2.44	129.23	124.68
23	B	614	CLA	C4C-C3C-C2C	-2.44	103.35	106.90
23	c	507	CLA	CAA-C2A-C3A	-2.43	106.11	112.78
31	A	419	LMT	O1'-C1'-C2'	2.43	112.10	108.30
23	b	615	CLA	C11-C12-C13	-2.43	108.05	115.92
25	k	101	BCR	C2-C1-C6	2.43	114.23	110.48
23	b	607	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
23	d	402[B]	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
35	c	517[B]	DGD	O6D-C1D-O3G	-2.43	104.22	109.97
31	e	101	LMT	O1'-C1'-C2'	2.43	112.09	108.30
23	B	614	CLA	C4-C3-C5	2.42	119.35	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	405[A]	CLA	CAA-CBA-CGA	2.42	120.34	113.25
23	b	602	CLA	C11-C10-C8	-2.42	108.09	115.92
23	b	606	CLA	C1-C2-C3	-2.42	121.86	126.04
23	b	606	CLA	CMC-C2C-C1C	2.42	128.72	125.04
23	A	406[A]	CLA	C1-C2-C3	-2.42	121.86	126.04
23	b	604	CLA	C4C-C3C-C2C	-2.42	103.37	106.90
23	B	607	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
23	C	506	CLA	CHD-C4C-NC	2.42	128.01	124.20
23	B	609	CLA	C16-C15-C13	-2.42	108.11	115.92
23	b	612	CLA	CMC-C2C-C1C	2.42	128.72	125.04
23	C	514	CLA	CAA-C2A-C3A	-2.42	106.16	112.78
23	A	408	CLA	C2A-C1A-CHA	-2.42	119.63	123.86
24	a	408[B]	PHO	O2A-CGA-O1A	-2.42	117.49	123.59
23	B	611	CLA	O2A-CGA-O1A	-2.42	117.50	123.59
29	D	407[A]	PL9	C7-C8-C9	-2.41	122.77	126.79
32	L	101[B]	LHG	C5-O7-C7	-2.41	111.85	117.79
32	A	418[A]	LHG	O7-C7-O9	-2.41	117.87	123.70
31	c	501	LMT	C3'-C4'-C5'	-2.41	105.40	110.93
25	T	101	BCR	C33-C5-C6	-2.41	121.82	124.53
23	B	613	CLA	CHB-C4A-NA	2.41	127.85	124.51
23	c	505	CLA	CED-O2D-CGD	2.41	121.39	115.94
23	B	605	CLA	CHC-C1C-C2C	-2.41	120.05	126.72
33	C	501	LMG	O6-C1-O1	-2.41	104.27	109.97
25	d	404	BCR	C33-C5-C6	-2.41	121.82	124.53
25	K	102	BCR	C2-C1-C6	2.41	114.19	110.48
25	T	101	BCR	C34-C9-C10	-2.41	119.55	122.92
23	c	508	CLA	C4C-C3C-C2C	-2.41	103.39	106.90
24	A	407[A]	PHO	CMA-C3A-C4A	-2.41	109.11	114.38
23	b	616	CLA	CMC-C2C-C1C	2.41	128.70	125.04
32	d	406[B]	LHG	C5-O7-C7	-2.41	111.87	117.79
25	d	404	BCR	C29-C28-C27	-2.40	106.00	111.38
23	c	512	CLA	C2A-C1A-CHA	-2.40	119.66	123.86
23	d	403	CLA	CMB-C2B-C3B	2.40	129.17	124.68
23	C	509	CLA	CMC-C2C-C1C	2.40	128.70	125.04
25	c	515	BCR	C31-C1-C6	-2.40	106.40	110.30
23	b	608	CLA	CAA-C2A-C3A	-2.40	106.20	112.78
32	b	629[A]	LHG	O8-C23-O10	-2.40	117.53	123.59
23	b	608	CLA	C4C-C3C-C2C	-2.40	103.40	106.90
23	c	511	CLA	C11-C10-C8	-2.40	108.17	115.92
23	b	607	CLA	CAC-C3C-C4C	2.40	127.92	124.81
32	d	407[A]	LHG	O8-C23-O10	-2.40	117.54	123.59
29	d	405[A]	PL9	C17-C18-C19	-2.40	121.89	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	608	CLA	CHD-C4C-NC	2.40	127.98	124.20
23	c	509	CLA	CMB-C2B-C3B	2.40	129.16	124.68
23	b	616	CLA	OBD-CAD-C3D	-2.39	122.76	128.52
29	d	405[A]	PL9	C7-C8-C9	-2.39	122.81	126.79
29	D	407[B]	PL9	C53-C6-C1	2.39	119.88	114.99
23	D	405	CLA	CMA-C3A-C4A	-2.39	105.34	111.77
23	C	505	CLA	CHD-C4C-NC	2.39	127.97	124.20
23	b	615	CLA	C2A-C1A-CHA	-2.39	119.68	123.86
23	b	615	CLA	C1-C2-C3	-2.39	121.91	126.04
29	a	414[B]	PL9	C47-C48-C49	-2.39	119.58	127.75
34	b	622	HTG	O2-C2-C3	-2.39	104.83	110.35
23	b	610	CLA	CMC-C2C-C1C	2.39	128.68	125.04
23	A	408	CLA	CMA-C3A-C4A	-2.39	105.36	111.77
23	C	504	CLA	C3B-C4B-NB	2.38	112.29	109.21
33	m	101	LMG	O7-C10-O9	-2.38	117.94	123.70
31	B	631	LMT	O1'-C1'-C2'	2.38	112.03	108.30
23	b	615	CLA	CHD-C4C-NC	2.38	127.96	124.20
23	c	507	CLA	C4-C3-C5	2.38	119.28	115.27
25	a	410	BCR	C40-C30-C25	-2.38	106.43	110.30
23	D	404[A]	CLA	CMC-C2C-C1C	2.38	128.67	125.04
23	a	405[A]	CLA	CMA-C3A-C2A	-2.38	104.22	113.83
35	C	517[B]	DGD	O1G-C1A-C2A	2.38	119.38	111.91
23	b	612	CLA	C4D-CHA-C1A	-2.38	118.35	121.25
29	a	414[A]	PL9	C20-C19-C21	2.38	119.28	115.27
25	y	101	BCR	C10-C11-C12	-2.38	115.79	123.22
23	C	509	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
25	C	516	BCR	C11-C10-C9	-2.38	123.91	127.31
31	F	101	LMT	C3B-C4B-C5B	-2.38	106.00	110.24
23	B	605	CLA	CBC-CAC-C3C	-2.38	105.88	112.43
29	D	407[A]	PL9	C36-C37-C38	-2.38	104.07	111.88
23	A	405[B]	CLA	CMA-C3A-C4A	-2.38	105.39	111.77
31	F	101	LMT	C1'-O5'-C5'	-2.38	109.03	113.69
23	C	512	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
23	a	405[B]	CLA	CHC-C1C-NC	2.37	127.80	124.20
23	A	408	CLA	C1-O2A-CGA	2.37	122.67	116.44
23	a	405[B]	CLA	CMA-C3A-C2A	-2.37	104.26	113.83
23	A	406[A]	CLA	CAC-C3C-C4C	2.37	127.89	124.81
23	b	615	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
23	d	403	CLA	CMC-C2C-C1C	2.37	128.65	125.04
25	D	406	BCR	C30-C25-C24	2.37	122.49	115.78
23	c	514	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
23	a	405[A]	CLA	C1B-CHB-C4A	-2.37	125.42	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	c	520	LMG	C8-O7-C10	-2.37	111.96	117.79
26	X	101	SQD	O6-C44-C45	2.37	116.61	110.90
23	C	507	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
23	c	514	CLA	CHD-C4C-NC	2.37	127.94	124.20
31	B	630	LMT	O5'-C5'-C6'	2.37	112.32	106.44
23	c	508	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
23	b	611	CLA	CAC-C3C-C4C	2.37	127.88	124.81
23	B	608	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
25	b	619	BCR	C15-C14-C13	-2.36	123.94	127.31
29	d	405[B]	PL9	C7-C3-C4	2.36	118.80	116.88
23	a	407[B]	CLA	CMB-C2B-C3B	2.36	129.10	124.68
23	a	405[B]	CLA	CMA-C3A-C4A	-2.36	105.42	111.77
25	k	101	BCR	C3-C4-C5	-2.36	109.86	114.08
25	k	101	BCR	C20-C21-C22	-2.36	123.94	127.31
24	a	416[A]	PHO	C1A-C2A-C3A	-2.36	100.59	102.84
23	B	605	CLA	C7-C6-C5	-2.36	106.95	113.36
23	A	406[B]	CLA	CAC-C3C-C4C	2.36	127.87	124.81
35	c	517[A]	DGD	C3G-C2G-C1G	-2.36	106.21	111.79
23	B	611	CLA	C2C-C1C-NC	2.36	112.18	109.97
24	a	416[B]	PHO	CMC-C2C-C3C	2.36	129.39	124.94
23	a	407[B]	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
29	A	414[B]	PL9	C40-C39-C41	2.36	119.24	115.27
23	B	605	CLA	C3B-C4B-NB	2.36	112.26	109.21
29	d	405[A]	PL9	C12-C13-C14	-2.36	121.99	127.66
23	D	405	CLA	OBD-CAD-C3D	-2.35	122.85	128.52
23	b	607	CLA	C1-C2-C3	-2.35	121.97	126.04
25	c	516	BCR	C37-C22-C21	-2.35	119.62	122.92
23	B	610	CLA	CAC-C3C-C4C	2.35	127.86	124.81
23	a	406[B]	CLA	O2A-CGA-CBA	2.35	119.29	111.91
26	a	412	SQD	C3-C4-C5	2.35	114.43	110.24
23	a	407[A]	CLA	C1-C2-C3	-2.35	121.98	126.04
35	C	518[B]	DGD	C2G-O2G-C1B	-2.35	112.00	117.79
25	t	102	BCR	C7-C6-C5	-2.35	115.77	121.46
23	C	513	CLA	C2A-C1A-CHA	-2.35	119.75	123.86
31	M	102	LMT	C3'-C4'-C5'	-2.35	105.54	110.93
23	c	502	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
23	B	614	CLA	CAA-C2A-C3A	-2.35	106.35	112.78
29	A	414[A]	PL9	C45-C44-C46	2.35	119.22	115.27
25	y	101	BCR	C24-C23-C22	-2.35	122.69	126.23
23	C	504	CLA	CMC-C2C-C1C	2.35	128.61	125.04
26	f	102	SQD	O47-C7-O49	-2.35	118.03	123.70
32	D	408[B]	LHG	O8-C23-C24	2.34	119.27	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	414[B]	PL9	C25-C24-C26	2.34	119.21	115.27
25	c	516	BCR	C11-C10-C9	-2.34	123.97	127.31
32	D	408[B]	LHG	O8-C23-O10	-2.34	117.68	123.59
23	A	406[A]	CLA	CMA-C3A-C2A	-2.34	104.38	113.83
23	B	607	CLA	CHC-C1C-C2C	-2.34	120.25	126.72
23	C	510	CLA	CHD-C4C-NC	2.34	127.89	124.20
29	d	405[B]	PL9	C36-C37-C38	-2.34	104.19	111.88
23	B	608	CLA	CAA-C2A-C3A	-2.34	106.37	112.78
25	c	516	BCR	C38-C26-C25	-2.34	121.90	124.53
23	C	502	CLA	C1-O2A-CGA	2.34	122.58	116.44
29	A	414[A]	PL9	C42-C43-C44	-2.34	122.03	127.66
23	C	513	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
23	B	603	CLA	C7-C6-C5	-2.34	107.01	113.36
23	C	508	CLA	O2A-CGA-CBA	2.33	119.23	111.91
32	d	406[A]	LHG	C6-C5-C4	-2.33	106.27	111.79
23	A	404[B]	CLA	CAA-CBA-CGA	-2.33	106.43	113.25
29	d	405[A]	PL9	C20-C19-C21	2.33	119.20	115.27
23	B	601	CLA	CMC-C2C-C1C	2.33	128.59	125.04
23	A	405[B]	CLA	CHB-C4A-NA	2.33	127.73	124.51
25	y	101	BCR	C21-C20-C19	-2.33	115.95	123.22
23	b	615	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
25	b	618	BCR	C3-C4-C5	-2.33	109.92	114.08
23	B	612	CLA	C2A-C1A-CHA	-2.33	119.79	123.86
23	C	505	CLA	C2A-C1A-CHA	-2.33	119.79	123.86
24	A	407[B]	PHO	O2A-CGA-CBA	2.33	119.21	111.91
23	c	502	CLA	C4-C3-C5	2.33	119.19	115.27
23	B	610	CLA	CMA-C3A-C2A	-2.33	104.44	113.83
23	b	609	CLA	O2A-CGA-CBA	2.32	119.20	111.91
23	c	511	CLA	O2D-CGD-O1D	-2.32	119.29	123.84
23	b	612	CLA	CHD-C4C-NC	2.32	127.86	124.20
26	b	620	SQD	C1-C2-C3	-2.32	105.16	110.00
35	c	517[B]	DGD	O3G-C3G-C2G	-2.32	105.29	110.90
23	C	502	CLA	CBC-CAC-C3C	-2.32	106.03	112.43
29	d	405[B]	PL9	C47-C48-C49	-2.32	119.81	127.75
23	a	407[B]	CLA	C2A-C1A-CHA	-2.32	119.80	123.86
31	A	417	LMT	O1'-C1'-C2'	2.32	111.92	108.30
23	b	613	CLA	CAC-C3C-C4C	2.32	127.82	124.81
23	A	408	CLA	CHD-C4C-NC	2.32	127.86	124.20
23	A	408	CLA	CMC-C2C-C1C	2.31	128.56	125.04
24	a	408[B]	PHO	C1-C2-C3	-2.31	122.04	126.04
23	B	608	CLA	C2A-C1A-CHA	-2.31	119.81	123.86
23	A	405[B]	CLA	OBD-CAD-C3D	-2.31	122.95	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	515	BCR	C15-C16-C17	-2.31	118.73	123.47
23	d	403	CLA	C2A-C1A-CHA	-2.31	119.81	123.86
29	D	407[B]	PL9	C51-C49-C50	2.31	119.71	114.60
23	c	510	CLA	C2A-C1A-CHA	-2.31	119.82	123.86
23	a	406[A]	CLA	CMC-C2C-C1C	2.31	128.56	125.04
23	B	608	CLA	O2A-CGA-CBA	2.31	119.16	111.91
23	c	513	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
23	c	510	CLA	CMC-C2C-C1C	2.31	128.56	125.04
25	K	102	BCR	C36-C18-C19	2.31	121.72	118.08
23	B	605	CLA	O2A-CGA-CBA	2.31	119.15	111.91
35	C	518[A]	DGD	C2G-O2G-C1B	-2.31	112.11	117.79
24	a	416[B]	PHO	C4A-C3A-C2A	-2.31	100.64	102.84
23	b	607	CLA	C1-O2A-CGA	2.31	122.50	116.44
23	C	508	CLA	CHC-C1C-C2C	-2.31	120.34	126.72
23	C	513	CLA	CHB-C4A-NA	2.30	127.70	124.51
35	C	517[A]	DGD	O6E-C5E-C4E	2.30	113.88	109.69
23	B	612	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
25	t	102	BCR	C11-C10-C9	-2.30	124.03	127.31
23	c	513	CLA	CAC-C3C-C4C	2.30	127.80	124.81
23	B	610	CLA	CMC-C2C-C1C	2.30	128.54	125.04
23	b	611	CLA	CMB-C2B-C3B	2.30	128.98	124.68
23	b	607	CLA	CMC-C2C-C1C	2.30	128.54	125.04
25	h	101	BCR	C20-C21-C22	-2.30	124.03	127.31
26	a	411[A]	SQD	O48-C23-C24	2.30	119.11	111.91
25	T	101	BCR	C21-C20-C19	-2.30	116.05	123.22
23	C	510	CLA	O2A-C1-C2	2.30	114.67	108.64
23	C	502	CLA	O2A-CGA-CBA	2.29	119.11	111.91
25	b	619	BCR	C34-C9-C10	-2.29	119.71	122.92
23	c	508	CLA	CMB-C2B-C1B	2.29	131.99	128.46
23	D	405	CLA	O2A-CGA-CBA	2.29	119.10	111.91
23	B	601	CLA	CHB-C4A-NA	2.29	127.68	124.51
25	k	101	BCR	C15-C14-C13	-2.29	124.04	127.31
25	t	102	BCR	C35-C13-C12	2.29	121.69	118.08
26	X	101	SQD	O48-C23-O10	-2.29	117.81	123.59
23	b	606	CLA	C1-O2A-CGA	2.29	122.45	116.44
23	C	511	CLA	CHB-C4A-NA	2.29	127.68	124.51
29	a	414[B]	PL9	C45-C44-C46	2.29	119.12	115.27
35	C	517[A]	DGD	C3G-C2G-C1G	-2.29	106.38	111.79
23	b	606	CLA	OBD-CAD-C3D	-2.28	123.02	128.52
23	b	605	CLA	CBC-CAC-C3C	-2.28	106.13	112.43
23	B	611	CLA	CMA-C3A-C2A	-2.28	104.61	113.83
24	A	407[B]	PHO	C4-C3-C5	2.28	119.11	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	609	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
26	f	102	SQD	O48-C23-O10	-2.28	117.84	123.59
25	c	515	BCR	C38-C26-C25	-2.28	121.97	124.53
23	D	404[A]	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
23	C	503	CLA	CMB-C2B-C3B	2.28	128.94	124.68
29	d	405[A]	PL9	C51-C49-C50	2.28	119.63	114.60
23	c	503	CLA	O2A-CGA-O1A	-2.27	117.85	123.59
23	b	608	CLA	C2A-C1A-CHA	-2.27	119.88	123.86
23	b	611	CLA	O2A-CGA-CBA	2.27	119.04	111.91
23	C	503	CLA	C4-C3-C5	2.27	119.10	115.27
23	B	610	CLA	CHB-C4A-NA	2.27	127.66	124.51
25	T	101	BCR	C38-C26-C25	-2.27	121.98	124.53
25	b	617	BCR	C37-C22-C21	-2.27	119.74	122.92
23	D	404[B]	CLA	CHD-C4C-NC	2.27	127.78	124.20
32	b	629[B]	LHG	O7-C7-O9	-2.27	118.21	123.70
23	C	502	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
23	b	602	CLA	CHB-C4A-NA	2.27	127.65	124.51
25	A	409	BCR	C16-C17-C18	-2.27	124.07	127.31
23	c	513	CLA	CHB-C4A-NA	2.27	127.65	124.51
32	d	413[B]	LHG	O7-C7-O9	-2.27	118.22	123.70
23	c	507	CLA	O2A-CGA-CBA	2.27	119.03	111.91
24	a	416[A]	PHO	O2A-CGA-CBA	2.27	119.03	111.91
23	B	604	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
23	b	606	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
23	B	601	CLA	CAA-C2A-C3A	-2.27	106.57	112.78
29	A	414[A]	PL9	C35-C34-C33	-2.27	117.86	123.68
25	K	102	BCR	C3-C4-C5	-2.27	110.03	114.08
23	a	405[A]	CLA	C7-C6-C5	-2.27	107.20	113.36
23	B	601	CLA	C2A-C1A-CHA	-2.26	119.90	123.86
26	a	411[B]	SQD	C3-C4-C5	2.26	114.28	110.24
23	b	614	CLA	CMA-C3A-C2A	-2.26	104.70	113.83
29	a	414[B]	PL9	C51-C49-C50	2.26	119.60	114.60
23	B	612	CLA	C4A-NA-C1A	-2.26	105.69	106.71
31	B	630	LMT	C3B-C4B-C5B	-2.26	106.20	110.24
23	c	512	CLA	CBC-CAC-C3C	-2.26	106.20	112.43
23	b	609	CLA	CHD-C4C-NC	2.26	127.77	124.20
35	C	518[A]	DGD	O2G-C1B-O1B	-2.26	118.24	123.70
24	a	408[B]	PHO	O2D-CGD-O1D	-2.26	119.42	123.84
31	B	631	LMT	O5'-C5'-C4'	2.26	114.52	109.75
26	B	620	SQD	O5-C1-C2	-2.26	105.57	110.35
23	D	404[A]	CLA	CMB-C2B-C3B	2.26	128.90	124.68
29	d	405[B]	PL9	C36-C34-C33	-2.25	116.55	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	609	CLA	C1-O2A-CGA	2.25	122.36	116.44
23	b	615	CLA	O2A-CGA-CBA	2.25	118.98	111.91
25	K	103	BCR	C38-C26-C25	-2.25	122.00	124.53
24	A	407[A]	PHO	C4-C3-C5	2.25	119.06	115.27
23	C	505	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
23	C	511	CLA	C4C-C3C-C2C	-2.25	103.61	106.90
23	b	601	CLA	O2A-CGA-CBA	2.25	118.97	111.91
23	D	404[A]	CLA	CED-O2D-CGD	2.25	121.03	115.94
24	a	408[A]	PHO	CMA-C3A-C4A	-2.25	109.45	114.38
31	B	628	LMT	C1B-C2B-C3B	2.25	114.68	110.00
23	a	406[A]	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
23	C	505	CLA	CMB-C2B-C3B	2.25	128.88	124.68
23	c	514	CLA	CMB-C2B-C3B	2.25	128.88	124.68
23	C	510	CLA	C11-C12-C13	-2.25	108.66	115.92
35	C	518[B]	DGD	O1G-C1A-O1A	-2.25	117.92	123.59
35	c	517[A]	DGD	O3G-C3G-C2G	-2.24	105.48	110.90
23	d	402[B]	CLA	CHD-C4C-NC	2.24	127.74	124.20
23	B	606	CLA	C1-C2-C3	-2.24	122.16	126.04
39	F	102	HEM	C4B-C3B-C2B	-2.24	105.33	107.11
29	d	405[A]	PL9	C47-C48-C49	-2.24	120.08	127.75
25	H	101	BCR	C36-C18-C17	-2.24	119.78	122.92
23	B	606	CLA	CAC-C3C-C4C	2.24	127.72	124.81
23	B	604	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
23	B	614	CLA	OBD-CAD-C3D	-2.24	123.13	128.52
39	F	102	HEM	C3C-C4C-NC	-2.24	106.71	110.94
23	B	610	CLA	C2A-C1A-CHA	-2.24	119.94	123.86
35	C	517[B]	DGD	O3G-C3G-C2G	-2.24	105.50	110.90
33	d	411	LMG	C8-O7-C10	-2.24	112.28	117.79
25	D	406	BCR	C21-C20-C19	-2.24	116.23	123.22
25	C	515	BCR	C16-C17-C18	-2.24	124.12	127.31
25	D	406	BCR	C11-C10-C9	-2.24	124.12	127.31
26	A	410[B]	SQD	C45-O47-C7	-2.24	112.29	117.79
23	B	614	CLA	CMA-C3A-C2A	-2.24	104.81	113.83
31	F	101	LMT	C2'-C3'-C4'	2.24	114.79	109.68
23	A	405[B]	CLA	C4C-C3C-C2C	-2.23	103.64	106.90
35	c	519	DGD	O3G-C3G-C2G	-2.23	105.51	110.90
23	c	502	CLA	CHD-C4C-NC	2.23	127.72	124.20
23	b	616	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
29	A	414[B]	PL9	C10-C9-C8	-2.23	117.95	123.68
29	a	414[A]	PL9	C35-C34-C33	-2.23	117.95	123.68
26	A	410[B]	SQD	O8-S-C6	2.23	109.30	105.74
23	a	405[B]	CLA	C7-C6-C5	-2.23	107.30	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402[B]	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
29	A	414[A]	PL9	C25-C24-C26	2.23	119.02	115.27
24	a	416[B]	PHO	C1A-C2A-C3A	-2.23	100.72	102.84
25	d	404	BCR	C30-C25-C26	-2.23	119.48	122.61
23	C	508	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
29	A	414[A]	PL9	C12-C13-C14	-2.23	122.30	127.66
23	b	610	CLA	CAC-C3C-C2C	2.23	131.34	127.53
23	B	616	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
24	A	416[A]	PHO	CED-O2D-CGD	2.22	120.97	115.94
29	A	414[A]	PL9	C53-C6-C1	2.22	119.54	114.99
26	A	410[A]	SQD	O9-S-O7	-2.22	106.25	113.95
23	A	404[A]	CLA	CHD-C4C-NC	2.22	127.71	124.20
23	a	406[B]	CLA	C4-C3-C5	2.22	119.01	115.27
23	c	514	CLA	C1-C2-C3	-2.22	122.20	126.04
25	d	404	BCR	C28-C27-C26	-2.22	110.11	114.08
24	a	416[A]	PHO	O1D-CGD-CBD	-2.22	121.04	124.74
23	A	405[A]	CLA	C4C-C3C-C2C	-2.22	103.66	106.90
23	c	513	CLA	CMA-C3A-C4A	-2.22	105.80	111.77
23	A	405[B]	CLA	CMA-C3A-C2A	-2.22	104.87	113.83
23	B	612	CLA	C4-C3-C5	2.22	119.01	115.27
41	V	201	HEC	CAD-CBD-CGD	-2.22	107.53	113.76
23	B	608	CLA	C11-C10-C8	-2.22	108.74	115.92
23	A	406[B]	CLA	CHB-C4A-NA	2.22	127.58	124.51
32	d	406[A]	LHG	O8-C23-O10	-2.22	117.99	123.59
23	B	613	CLA	CHD-C4C-NC	2.22	127.70	124.20
35	H	102	DGD	O2G-C1B-C2B	2.22	116.28	111.50
23	D	404[A]	CLA	CMA-C3A-C4A	-2.21	105.82	111.77
23	c	511	CLA	C4-C3-C2	-2.21	118.00	123.68
29	A	414[B]	PL9	C35-C34-C33	-2.21	118.00	123.68
31	b	627	LMT	C1'-O5'-C5'	-2.21	109.35	113.69
23	b	609	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
23	B	611	CLA	OBD-CAD-C3D	-2.21	123.20	128.52
24	a	416[B]	PHO	O2A-CGA-CBA	2.21	118.85	111.91
23	c	503	CLA	C2A-C1A-CHA	-2.21	120.00	123.86
23	d	403	CLA	CGD-CBD-CAD	-2.21	103.58	110.73
23	a	409	CLA	C1-O2A-CGA	2.21	122.24	116.44
25	c	515	BCR	C34-C9-C10	-2.21	119.83	122.92
23	a	405[B]	CLA	CMB-C2B-C3B	2.21	128.81	124.68
23	c	512	CLA	CMB-C2B-C3B	2.21	128.81	124.68
24	a	416[B]	PHO	O1D-CGD-CBD	-2.21	121.06	124.74
23	A	406[B]	CLA	CMC-C2C-C1C	2.21	128.40	125.04
23	b	603	CLA	C1-C2-C3	-2.21	122.23	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	613	CLA	C4-C3-C2	-2.21	118.02	123.68
32	E	101[A]	LHG	O7-C7-O9	-2.21	118.37	123.70
23	b	610	CLA	CMA-C3A-C2A	-2.20	104.94	113.83
25	d	404	BCR	C30-C25-C24	2.20	122.01	115.78
23	c	510	CLA	O2A-CGA-CBA	2.20	118.82	111.91
23	B	607	CLA	CHD-C4C-NC	2.20	127.67	124.20
23	B	606	CLA	CAA-C2A-C3A	-2.20	106.75	112.78
25	d	404	BCR	C35-C13-C14	-2.20	119.84	122.92
39	F	102	HEM	O2D-CGD-CBD	2.20	121.11	114.03
23	C	506	CLA	CMB-C2B-C1B	2.20	131.85	128.46
35	C	517[A]	DGD	O3G-C3G-C2G	-2.20	105.59	110.90
23	c	505	CLA	CBC-CAC-C3C	-2.20	106.36	112.43
23	C	502	CLA	OBD-CAD-C3D	-2.20	123.22	128.52
25	T	101	BCR	C36-C18-C19	2.20	121.54	118.08
26	a	411[A]	SQD	O9-S-O7	-2.20	106.34	113.95
25	k	101	BCR	C10-C11-C12	-2.20	116.36	123.22
23	b	615	CLA	CAC-C3C-C4C	2.20	127.66	124.81
26	a	412	SQD	O48-C23-O10	-2.20	118.05	123.59
29	d	405[B]	PL9	C15-C14-C16	2.20	118.97	115.27
25	T	101	BCR	C1-C6-C7	2.20	121.99	115.78
23	C	513	CLA	C3B-C4B-NB	2.20	112.05	109.21
25	K	102	BCR	C32-C1-C6	-2.19	106.74	110.30
35	c	518[A]	DGD	O1G-C1A-O1A	-2.19	118.06	123.59
23	d	403	CLA	CHB-C4A-NA	2.19	127.54	124.51
26	f	102	SQD	O5-C5-C4	2.19	113.67	109.69
23	c	506	CLA	CBC-CAC-C3C	-2.19	106.39	112.43
23	d	403	CLA	CAC-C3C-C4C	2.19	127.65	124.81
23	b	613	CLA	CED-O2D-CGD	2.19	120.89	115.94
24	a	416[A]	PHO	C4-C3-C2	-2.19	118.07	123.68
23	c	514	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
31	b	621	LMT	C2'-C3'-C4'	2.19	114.67	109.68
25	y	101	BCR	C1-C6-C7	2.18	121.96	115.78
23	B	612	CLA	CHD-C4C-NC	2.18	127.64	124.20
29	D	407[B]	PL9	C7-C8-C9	-2.18	123.16	126.79
23	c	505	CLA	C4-C3-C5	2.18	118.94	115.27
23	A	405[B]	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
23	C	504	CLA	CBC-CAC-C3C	-2.18	106.42	112.43
25	B	617	BCR	C28-C27-C26	-2.18	110.18	114.08
23	B	605	CLA	CED-O2D-CGD	2.18	120.87	115.94
23	c	513	CLA	CBA-CAA-C2A	-2.18	107.43	113.86
33	B	621	LMG	O8-C28-O10	-2.18	118.09	123.59
34	b	622	HTG	C6-C5-C4	-2.18	107.90	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	508	CLA	CBC-CAC-C3C	-2.18	106.43	112.43
23	a	405[B]	CLA	CMC-C2C-C1C	2.18	128.35	125.04
23	B	607	CLA	C6-C7-C8	-2.18	108.88	115.92
25	d	404	BCR	C36-C18-C17	-2.18	119.88	122.92
29	D	407[B]	PL9	C22-C23-C24	-2.18	122.42	127.66
23	A	404[B]	CLA	CMA-C3A-C2A	-2.18	105.05	113.83
23	c	503	CLA	CBC-CAC-C3C	-2.18	106.43	112.43
23	b	609	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
25	B	617	BCR	C24-C23-C22	-2.17	122.95	126.23
23	d	402[A]	CLA	CMB-C2B-C3B	2.17	128.74	124.68
23	a	407[A]	CLA	C4-C3-C5	2.17	118.92	115.27
23	b	602	CLA	C4-C3-C5	2.17	118.92	115.27
23	B	601	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
23	b	613	CLA	CMC-C2C-C1C	2.17	128.34	125.04
24	A	416[B]	PHO	CMA-C3A-C4A	-2.17	109.62	114.38
29	A	414[B]	PL9	C47-C48-C49	-2.17	120.33	127.75
32	A	418[A]	LHG	O4-P-O5	2.17	122.96	112.24
23	A	406[B]	CLA	C1-C2-C3	-2.17	122.29	126.04
23	c	502	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
33	c	520	LMG	O8-C28-O10	-2.17	118.12	123.59
23	b	605	CLA	O2A-CGA-CBA	2.17	118.70	111.91
23	b	610	CLA	CMA-C3A-C4A	-2.17	105.95	111.77
29	a	414[A]	PL9	C45-C44-C46	2.16	118.91	115.27
23	a	409	CLA	CHB-C4A-NA	2.16	127.50	124.51
23	c	503	CLA	CMC-C2C-C1C	2.16	128.34	125.04
31	c	501	LMT	O5B-C1B-C2B	2.16	114.93	110.35
32	E	101[B]	LHG	C5-O7-C7	-2.16	112.47	117.79
23	B	613	CLA	C2A-C1A-CHA	-2.16	120.08	123.86
25	K	102	BCR	C39-C30-C25	-2.16	106.79	110.30
23	A	405[B]	CLA	C2A-C1A-CHA	-2.16	120.08	123.86
23	A	405[A]	CLA	O2A-CGA-CBA	2.16	118.68	111.91
23	C	511	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
24	a	408[A]	PHO	O2D-CGD-O1D	-2.16	119.62	123.84
23	C	513	CLA	O1D-CGD-CBD	-2.16	120.07	124.48
23	c	502	CLA	CMC-C2C-C1C	2.16	128.32	125.04
39	f	101	HEM	CMD-C2D-C1D	2.16	128.32	125.04
25	a	410	BCR	C33-C5-C6	-2.16	122.11	124.53
23	B	606	CLA	C11-C10-C8	-2.16	108.95	115.92
24	a	408[B]	PHO	CBA-CAA-C2A	-2.16	107.51	113.81
23	B	602	CLA	C1-C2-C3	-2.15	122.32	126.04
23	A	408	CLA	O2A-CGA-O1A	-2.15	118.15	123.59
25	A	409	BCR	C15-C14-C13	-2.15	124.23	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	606	CLA	CMB-C2B-C3B	2.15	128.71	124.68
23	C	504	CLA	C2A-C1A-CHA	-2.15	120.09	123.86
27	B	624	GOL	C3-C2-C1	-2.15	103.33	111.70
23	b	608	CLA	C4-C3-C5	2.15	118.89	115.27
33	C	521	LMG	C9-C8-C7	-2.15	106.70	111.79
29	D	407[B]	PL9	C15-C14-C16	2.15	118.89	115.27
29	D	407[A]	PL9	C12-C13-C14	-2.15	122.48	127.66
33	d	411	LMG	O7-C10-O9	-2.15	118.50	123.70
23	A	405[B]	CLA	O2A-CGA-CBA	2.15	118.65	111.91
35	H	102	DGD	C3E-C4E-C5E	-2.15	106.41	110.24
32	d	413[A]	LHG	O7-C7-O9	-2.15	118.51	123.70
26	f	102	SQD	O8-S-C6	2.15	109.16	105.74
34	c	522	HTG	O5-C1-C2	2.15	113.02	110.31
35	C	519	DGD	O2G-C1B-O1B	-2.15	118.51	123.70
23	b	616	CLA	C4-C3-C5	2.15	118.88	115.27
25	b	619	BCR	C16-C17-C18	-2.15	124.25	127.31
23	c	506	CLA	CHD-C4C-NC	2.15	127.58	124.20
23	c	510	CLA	C4-C3-C2	-2.14	118.18	123.68
23	b	610	CLA	C4-C3-C2	-2.14	118.18	123.68
29	d	405[A]	PL9	C45-C44-C46	2.14	118.87	115.27
33	m	101	LMG	O8-C28-O10	-2.14	118.19	123.59
23	D	404[A]	CLA	OBD-CAD-C3D	-2.14	123.37	128.52
23	C	503	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
23	a	409	CLA	C1-C2-C3	-2.14	122.35	126.04
26	X	101	SQD	O5-C1-C2	-2.14	105.83	110.35
25	T	101	BCR	C7-C6-C5	-2.13	116.29	121.46
23	A	408	CLA	C11-C12-C13	-2.13	109.03	115.92
33	Z	101	LMG	C3-C4-C5	2.13	114.04	110.24
25	c	515	BCR	C35-C13-C14	-2.13	119.94	122.92
23	B	606	CLA	OBD-CAD-C3D	-2.13	123.39	128.52
35	h	102	DGD	O2G-C1B-O1B	-2.13	118.55	123.70
35	c	517[A]	DGD	O6D-C1D-O3G	-2.13	104.93	109.97
23	A	406[A]	CLA	CHB-C4A-NA	2.13	127.46	124.51
25	h	101	BCR	C16-C17-C18	-2.13	124.27	127.31
35	C	517[A]	DGD	O5D-C6D-C5D	-2.13	105.11	109.05
23	c	502	CLA	O2A-CGA-CBA	2.13	118.59	111.91
32	d	406[A]	LHG	O8-C23-C24	2.13	118.59	111.91
23	c	503	CLA	CMB-C2B-C3B	2.13	128.66	124.68
25	b	619	BCR	C21-C20-C19	-2.13	116.58	123.22
23	b	607	CLA	CMA-C3A-C2A	-2.13	105.25	113.83
25	d	404	BCR	C39-C30-C25	-2.13	106.85	110.30
23	b	613	CLA	C2A-C1A-CHA	-2.13	120.14	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	b	629[B]	LHG	C5-O7-C7	-2.13	112.56	117.79
23	C	505	CLA	CAA-C2A-C3A	-2.13	106.96	112.78
23	C	506	CLA	C11-C10-C8	-2.13	109.05	115.92
23	C	504	CLA	O2A-CGA-CBA	2.12	118.58	111.91
23	a	407[A]	CLA	CBC-CAC-C3C	-2.12	106.57	112.43
23	C	512	CLA	C1-O2A-CGA	2.12	122.02	116.44
23	b	614	CLA	C4D-CHA-C1A	-2.12	118.66	121.25
23	d	402[A]	CLA	CHD-C4C-NC	2.12	127.55	124.20
23	c	505	CLA	C2A-C1A-CHA	-2.12	120.15	123.86
25	a	410	BCR	C3-C4-C5	-2.12	110.29	114.08
39	f	101	HEM	CHA-C4D-C3D	-2.12	121.34	125.33
23	A	405[A]	CLA	CHB-C4A-NA	2.12	127.44	124.51
26	B	620	SQD	C9-C8-C7	-2.12	105.91	113.62
23	B	616	CLA	CBC-CAC-C3C	-2.12	106.59	112.43
23	b	610	CLA	CHB-C4A-NA	2.12	127.44	124.51
39	f	101	HEM	C3C-C4C-NC	-2.12	106.95	110.94
23	C	507	CLA	C2A-C1A-CHA	-2.12	120.16	123.86
25	A	409	BCR	C38-C26-C25	-2.11	122.15	124.53
25	b	618	BCR	C29-C28-C27	-2.11	106.65	111.38
23	c	502	CLA	CBC-CAC-C3C	-2.11	106.60	112.43
23	b	604	CLA	CHD-C4C-NC	2.11	127.54	124.20
32	D	408[B]	LHG	O7-C7-O9	-2.11	118.59	123.70
26	b	620	SQD	O7-S-C6	2.11	109.45	106.94
35	c	518[B]	DGD	O1G-C1A-O1A	-2.11	118.26	123.59
25	d	404	BCR	C21-C20-C19	-2.11	116.62	123.22
35	c	517[A]	DGD	O1G-C1A-O1A	-2.11	118.26	123.59
23	a	406[A]	CLA	CHB-C4A-NA	2.11	127.43	124.51
25	C	515	BCR	C37-C22-C23	2.11	121.41	118.08
34	B	625	HTG	C6-C5-C4	-2.11	108.06	113.00
23	C	507	CLA	C4C-C3C-C2C	-2.11	103.82	106.90
23	b	602	CLA	C7-C6-C5	-2.11	107.63	113.36
25	D	406	BCR	C3-C4-C5	-2.11	110.31	114.08
32	E	101[B]	LHG	O7-C7-O9	-2.11	118.60	123.70
23	d	402[A]	CLA	CMA-C3A-C2A	-2.11	105.31	113.83
25	H	101	BCR	C31-C1-C6	-2.11	106.88	110.30
35	C	518[A]	DGD	O1G-C1A-C2A	2.11	118.53	111.91
25	K	103	BCR	C1-C6-C7	2.11	121.75	115.78
33	Z	101	LMG	C1-O6-C5	2.11	117.83	113.69
24	A	416[B]	PHO	O2A-CGA-O1A	-2.11	118.27	123.59
26	a	411[A]	SQD	C3-C4-C5	2.11	114.00	110.24
23	c	511	CLA	C2A-C1A-CHA	-2.11	120.18	123.86
26	a	412	SQD	O7-S-C6	2.11	109.44	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	d	405[A]	PL9	C31-C32-C33	-2.10	104.97	111.88
23	a	406[A]	CLA	CAC-C3C-C2C	2.10	131.13	127.53
23	C	507	CLA	CGD-CBD-CAD	-2.10	103.92	110.73
23	B	607	CLA	CMB-C2B-C3B	2.10	128.61	124.68
31	M	101	LMT	O5B-C5B-C6B	2.10	111.67	106.44
23	c	507	CLA	C1-O2A-CGA	2.10	121.96	116.44
23	B	611	CLA	C4D-CHA-C1A	-2.10	118.69	121.25
29	a	414[A]	PL9	C51-C49-C50	2.10	119.25	114.60
25	b	618	BCR	C35-C13-C14	-2.10	119.98	122.92
23	B	609	CLA	C2A-C1A-CHA	-2.10	120.18	123.86
23	A	404[A]	CLA	C7-C6-C5	-2.10	107.65	113.36
23	b	608	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
23	c	513	CLA	CBC-CAC-C3C	-2.10	106.64	112.43
33	B	621	LMG	O6-C5-C4	2.10	113.51	109.69
23	C	511	CLA	C4-C3-C2	-2.10	118.30	123.68
23	A	406[B]	CLA	CMA-C3A-C2A	-2.10	105.37	113.83
26	b	620	SQD	O5-C1-C2	-2.10	105.91	110.35
29	d	405[B]	PL9	C31-C32-C33	-2.10	104.99	111.88
23	b	615	CLA	CHA-C1A-NA	-2.10	121.60	126.40
23	c	514	CLA	C4-C3-C5	2.10	118.80	115.27
35	H	102	DGD	C2G-O2G-C1B	-2.09	112.64	117.79
23	C	514	CLA	C1-O2A-CGA	2.09	121.94	116.44
33	a	417	LMG	O8-C28-C29	2.09	118.48	111.91
29	A	414[A]	PL9	C51-C49-C50	2.09	119.22	114.60
23	B	603	CLA	CAC-C3C-C4C	2.09	127.52	124.81
25	h	101	BCR	C36-C18-C17	-2.09	119.99	122.92
23	C	513	CLA	OBD-CAD-C3D	-2.09	123.49	128.52
26	A	410[B]	SQD	O48-C23-O10	-2.09	118.31	123.59
23	b	603	CLA	CMC-C2C-C1C	2.09	128.22	125.04
25	b	617	BCR	C20-C21-C22	-2.09	124.33	127.31
23	B	608	CLA	C6-C7-C8	-2.09	109.17	115.92
23	B	607	CLA	CMA-C3A-C2A	-2.09	105.40	113.83
23	a	406[B]	CLA	CHB-C4A-NA	2.09	127.40	124.51
23	b	601	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
23	b	602	CLA	CHC-C1C-C2C	-2.09	120.95	126.72
25	B	617	BCR	C16-C17-C18	-2.09	124.33	127.31
23	B	616	CLA	C2A-C1A-CHA	-2.09	120.21	123.86
23	A	408	CLA	OBD-CAD-C3D	-2.09	123.50	128.52
23	c	502	CLA	C1-O2A-CGA	2.09	121.92	116.44
23	b	609	CLA	CGD-CBD-CAD	-2.09	103.98	110.73
25	K	103	BCR	C7-C6-C5	-2.09	116.41	121.46
23	a	407[A]	CLA	CAC-C3C-C4C	2.08	127.52	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	h	101	BCR	C34-C9-C8	2.08	121.36	118.08
33	B	621	LMG	C4-C3-C2	-2.08	107.19	110.82
23	C	502	CLA	C11-C12-C13	-2.08	109.19	115.92
23	c	506	CLA	C4-C3-C5	2.08	118.77	115.27
23	B	615	CLA	O2A-CGA-CBA	2.08	118.44	111.91
23	C	511	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
23	A	404[B]	CLA	CMB-C2B-C3B	2.08	128.57	124.68
29	A	414[A]	PL9	C10-C9-C11	2.08	118.77	115.27
25	B	618	BCR	C24-C23-C22	-2.08	123.09	126.23
23	C	513	CLA	CHC-C1C-C2C	-2.08	120.97	126.72
23	a	407[B]	CLA	CHB-C4A-NA	2.08	127.38	124.51
25	D	406	BCR	C39-C30-C25	-2.08	106.93	110.30
23	D	404[A]	CLA	CBC-CAC-C3C	-2.07	106.71	112.43
33	Z	101	LMG	C9-C8-C7	-2.07	106.88	111.79
25	t	102	BCR	C2-C1-C6	2.07	113.67	110.48
25	C	516	BCR	C37-C22-C23	2.07	121.34	118.08
25	c	515	BCR	C37-C22-C23	2.07	121.34	118.08
23	C	503	CLA	CED-O2D-CGD	2.07	120.62	115.94
31	A	417	LMT	C4B-C3B-C2B	-2.07	107.21	110.82
29	d	405[A]	PL9	C40-C39-C38	-2.07	118.37	123.68
23	c	514	CLA	C1-O2A-CGA	2.07	121.88	116.44
29	a	414[B]	PL9	C35-C34-C33	-2.07	118.37	123.68
32	d	407[B]	LHG	O8-C23-O10	-2.07	118.37	123.59
23	c	513	CLA	CHA-C1A-NA	-2.07	121.66	126.40
35	h	102	DGD	C6D-C5D-C4D	2.07	116.41	112.09
23	b	616	CLA	C2A-C1A-CHA	-2.07	120.24	123.86
25	B	617	BCR	C15-C14-C13	-2.07	124.36	127.31
32	L	101[B]	LHG	O8-C23-O10	-2.07	118.38	123.59
23	b	603	CLA	CMB-C2B-C3B	2.07	128.54	124.68
23	A	408	CLA	C1B-CHB-C4A	-2.06	126.03	130.12
23	b	602	CLA	C1B-CHB-C4A	-2.06	126.03	130.12
23	C	508	CLA	C3B-C4B-NB	2.06	111.88	109.21
23	c	512	CLA	CAC-C3C-C4C	2.06	127.49	124.81
25	b	619	BCR	C16-C15-C14	-2.06	119.25	123.47
23	b	602	CLA	CAC-C3C-C4C	2.06	127.48	124.81
23	B	612	CLA	C6-C5-C3	-2.06	108.05	113.45
23	C	512	CLA	C2A-C1A-CHA	-2.06	120.26	123.86
23	c	511	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
23	d	402[A]	CLA	CBC-CAC-C3C	-2.06	106.75	112.43
23	c	504	CLA	CMC-C2C-C1C	2.06	128.17	125.04
33	a	417	LMG	O7-C10-O9	-2.06	118.73	123.70
29	D	407[A]	PL9	C27-C28-C29	-2.06	122.71	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	619	BCR	C39-C30-C25	-2.06	106.96	110.30
23	A	404[B]	CLA	CED-O2D-CGD	2.06	120.59	115.94
23	b	606	CLA	C2A-C1A-CHA	-2.05	120.27	123.86
31	M	101	LMT	C3B-C4B-C5B	-2.05	106.57	110.24
23	c	511	CLA	C7-C6-C5	-2.05	107.78	113.36
29	d	405[A]	PL9	O2-C1-C6	-2.05	117.04	120.59
24	A	407[B]	PHO	CMC-C2C-C3C	2.05	128.81	124.94
23	C	508	CLA	C7-C6-C5	-2.05	107.79	113.36
29	A	414[B]	PL9	C2-C3-C4	2.05	121.62	118.80
24	A	416[B]	PHO	CMC-C2C-C3C	2.05	128.81	124.94
23	d	402[B]	CLA	CMC-C2C-C1C	2.05	128.16	125.04
24	A	416[A]	PHO	O1D-CGD-CBD	-2.05	121.33	124.74
23	B	611	CLA	CAC-C3C-C4C	2.05	127.47	124.81
29	D	407[A]	PL9	C45-C44-C46	2.05	118.72	115.27
27	O	303	GOL	C3-C2-C1	-2.05	103.74	111.70
32	L	101[A]	LHG	O4-P-O5	2.05	122.36	112.24
25	c	516	BCR	C29-C30-C25	2.05	113.63	110.48
23	C	506	CLA	CHA-C1A-NA	-2.05	121.71	126.40
23	A	406[A]	CLA	CBC-CAC-C3C	-2.04	106.79	112.43
25	D	406	BCR	C30-C25-C26	-2.04	119.73	122.61
23	b	613	CLA	CBC-CAC-C3C	-2.04	106.80	112.43
24	a	408[B]	PHO	C4A-C3A-C2A	-2.04	100.89	102.84
23	c	505	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
23	B	614	CLA	C4-C3-C2	-2.04	118.44	123.68
24	a	416[A]	PHO	O2A-CGA-O1A	-2.04	118.44	123.59
39	F	102	HEM	C4D-ND-C1D	2.04	107.18	105.07
23	B	607	CLA	OBD-CAD-C3D	-2.04	123.61	128.52
24	a	408[A]	PHO	C1-C2-C3	-2.04	122.51	126.04
23	a	406[A]	CLA	CMB-C2B-C1B	2.04	131.60	128.46
32	b	629[A]	LHG	O7-C7-O9	-2.04	118.77	123.70
25	c	516	BCR	C37-C22-C23	2.04	121.29	118.08
23	b	602	CLA	CAA-CBA-CGA	-2.04	107.29	113.25
23	B	606	CLA	C2A-C1A-CHA	-2.04	120.30	123.86
26	b	620	SQD	C4-C3-C2	2.04	114.38	110.82
23	A	408	CLA	CBC-CAC-C3C	-2.04	106.81	112.43
25	c	516	BCR	C15-C14-C13	-2.04	124.40	127.31
25	c	515	BCR	C33-C5-C6	-2.04	122.24	124.53
35	c	518[B]	DGD	O2G-C1B-O1B	-2.03	118.78	123.70
35	C	517[B]	DGD	O6D-C1D-O3G	-2.03	105.16	109.97
33	D	413	LMG	C7-O1-C1	-2.03	109.76	113.74
23	a	406[B]	CLA	CAA-CBA-CGA	2.03	119.20	113.25
31	M	101	LMT	O1'-C1'-C2'	2.03	111.48	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	511	CLA	CHA-C1A-NA	-2.03	121.74	126.40
35	c	519	DGD	O2G-C1B-O1B	-2.03	118.79	123.70
23	b	613	CLA	CHA-C1A-NA	-2.03	121.74	126.40
25	a	410	BCR	C24-C23-C22	-2.03	123.16	126.23
23	b	616	CLA	CHA-C1A-NA	-2.03	121.74	126.40
23	B	615	CLA	OBD-CAD-C3D	-2.03	123.63	128.52
29	D	407[A]	PL9	C47-C48-C49	-2.03	120.81	127.75
25	d	404	BCR	C37-C22-C21	-2.03	120.08	122.92
23	B	606	CLA	CBC-CAC-C3C	-2.03	106.83	112.43
29	D	407[A]	PL9	C21-C22-C23	-2.03	105.21	111.88
29	d	405[B]	PL9	C45-C44-C46	2.03	118.69	115.27
25	y	101	BCR	C28-C27-C26	-2.03	110.45	114.08
23	c	510	CLA	CED-O2D-CGD	2.03	120.53	115.94
26	a	412	SQD	O47-C7-O49	-2.03	118.80	123.70
23	B	603	CLA	CBC-CAC-C3C	-2.03	106.84	112.43
23	b	611	CLA	OBD-CAD-C3D	-2.03	123.64	128.52
35	h	102	DGD	C3B-C2B-C1B	-2.03	106.25	113.62
23	A	406[B]	CLA	C1B-CHB-C4A	-2.03	126.10	130.12
23	D	405	CLA	CBC-CAC-C3C	-2.03	106.84	112.43
23	b	601	CLA	CAC-C3C-C4C	2.03	127.44	124.81
23	b	612	CLA	C4-C3-C2	-2.02	118.48	123.68
31	m	103	LMT	O1'-C1'-C2'	2.02	111.46	108.30
23	C	513	CLA	CHA-C1A-NA	-2.02	121.77	126.40
23	a	407[A]	CLA	CHA-C1A-NA	-2.02	121.77	126.40
25	B	618	BCR	C7-C8-C9	-2.02	123.18	126.23
23	B	610	CLA	C4-C3-C5	2.02	118.67	115.27
26	a	411[A]	SQD	O4-C4-C3	-2.02	105.68	110.35
26	a	412	SQD	O5-C5-C4	2.02	113.36	109.69
23	b	612	CLA	O2A-C1-C2	-2.02	103.33	108.64
23	b	607	CLA	C6-C7-C8	-2.02	109.40	115.92
23	B	609	CLA	CHA-C1A-NA	-2.02	121.78	126.40
23	c	506	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
23	c	512	CLA	CMA-C3A-C4A	2.02	117.19	111.77
31	B	630	LMT	O5'-C5'-C4'	2.02	114.00	109.75
23	B	602	CLA	CMA-C3A-C2A	-2.02	105.70	113.83
23	C	508	CLA	CHB-C4A-NA	2.02	127.30	124.51
26	b	620	SQD	O4-C4-C3	-2.01	105.69	110.35
25	h	101	BCR	C16-C15-C14	-2.01	119.35	123.47
26	B	620	SQD	O9-S-O7	-2.01	106.98	113.95
23	b	609	CLA	CHB-C4A-NA	2.01	127.30	124.51
35	c	517[A]	DGD	O1G-C1A-C2A	2.01	118.23	111.91
27	D	403	GOL	C3-C2-C1	-2.01	103.88	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	M	102	LMT	C3B-C4B-C5B	-2.01	106.65	110.24
23	C	508	CLA	CMB-C2B-C1B	2.01	131.56	128.46
26	A	412	SQD	O6-C44-C45	-2.01	106.05	110.90
25	D	406	BCR	C40-C30-C39	2.01	114.70	108.53
25	a	410	BCR	C10-C11-C12	-2.01	116.94	123.22
34	B	623	HTG	O5-C1-C2	2.01	112.84	110.31
35	H	102	DGD	C1E-O6E-C5E	-2.01	109.74	113.69
39	f	101	HEM	O2D-CGD-CBD	2.01	120.48	114.03
23	B	610	CLA	CMA-C3A-C4A	-2.01	106.37	111.77
25	B	619	BCR	C10-C11-C12	-2.01	116.95	123.22
24	A	416[B]	PHO	O1D-CGD-CBD	-2.01	121.39	124.74
25	H	101	BCR	C10-C11-C12	-2.01	116.95	123.22
24	A	416[B]	PHO	CED-O2D-CGD	2.01	120.47	115.94
24	a	416[B]	PHO	CMA-C3A-C4A	-2.01	109.98	114.38
23	B	613	CLA	CBC-CAC-C3C	-2.01	106.90	112.43
24	A	416[A]	PHO	CMB-C2B-C3B	2.00	128.43	124.68
31	t	101	LMT	O5'-C5'-C6'	2.00	111.42	106.44
35	C	517[A]	DGD	C4E-C3E-C2E	-2.00	107.33	110.82
23	b	608	CLA	C11-C10-C8	-2.00	109.45	115.92
23	c	508	CLA	C1-C2-C3	-2.00	122.58	126.04
23	c	508	CLA	CHA-C1A-NA	-2.00	121.82	126.40

All (69) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404[A]	CLA	ND
23	A	404[B]	CLA	ND
23	A	405[A]	CLA	ND
23	A	405[B]	CLA	ND
23	A	408	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND
23	B	604	CLA	ND
23	B	605	CLA	ND
23	B	606	CLA	ND
23	B	607	CLA	ND
23	B	609	CLA	ND
23	B	610	CLA	ND
23	B	611	CLA	ND
23	B	612	CLA	ND
23	B	613	CLA	ND

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Mol	Chain	Res	Type	Atom
23	B	614	CLA	ND
23	B	615	CLA	ND
23	B	616	CLA	ND
23	C	502	CLA	ND
23	C	505	CLA	ND
23	C	506	CLA	ND
23	C	507	CLA	ND
23	C	508	CLA	ND
23	C	510	CLA	ND
23	C	511	CLA	ND
23	C	512	CLA	ND
23	C	513	CLA	ND
23	C	514	CLA	ND
23	D	404[A]	CLA	ND
23	D	404[B]	CLA	ND
23	D	405	CLA	ND
23	a	405[A]	CLA	ND
23	a	405[B]	CLA	ND
23	a	406[A]	CLA	ND
23	a	406[B]	CLA	ND
23	a	409	CLA	ND
23	b	601	CLA	ND
23	b	602	CLA	ND
23	b	603	CLA	ND
23	b	604	CLA	ND
23	b	605	CLA	ND
23	b	606	CLA	ND
23	b	607	CLA	ND
23	b	609	CLA	ND
23	b	610	CLA	ND
23	b	611	CLA	ND
23	b	612	CLA	ND
23	b	613	CLA	ND
23	b	614	CLA	ND
23	b	615	CLA	ND
23	b	616	CLA	ND
23	c	502	CLA	ND
23	c	503	CLA	ND
23	c	504	CLA	ND
23	c	505	CLA	ND
23	c	506	CLA	ND
23	c	507	CLA	ND

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Mol	Chain	Res	Type	Atom
23	c	508	CLA	ND
23	c	509	CLA	ND
23	c	510	CLA	ND
23	c	511	CLA	ND
23	c	512	CLA	ND
23	c	513	CLA	ND
23	c	514	CLA	ND
23	d	402[A]	CLA	ND
23	d	402[B]	CLA	ND
23	d	403	CLA	ND

All (1631) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	408	CLA	C2-C3-C5-C6
23	A	408	CLA	C4-C3-C5-C6
23	B	602	CLA	C6-C7-C8-C9
23	B	603	CLA	C2-C3-C5-C6
23	B	603	CLA	C4-C3-C5-C6
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	C	505	CLA	C2-C3-C5-C6
23	C	505	CLA	C4-C3-C5-C6
23	C	509	CLA	CHA-CBD-CGD-O1D
23	C	509	CLA	CHA-CBD-CGD-O2D
23	a	409	CLA	C2-C3-C5-C6
23	a	409	CLA	C4-C3-C5-C6
23	b	601	CLA	C11-C10-C8-C9
23	b	614	CLA	CHA-CBD-CGD-O1D
23	b	614	CLA	CHA-CBD-CGD-O2D
23	b	614	CLA	CAD-CBD-CGD-O1D
23	b	614	CLA	CAD-CBD-CGD-O2D
23	c	505	CLA	C11-C12-C13-C14
23	c	509	CLA	CHA-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O2D
23	c	510	CLA	C2-C1-O2A-CGA
23	c	510	CLA	C11-C10-C8-C9
23	d	403	CLA	C2-C3-C5-C6
23	d	403	CLA	C4-C3-C5-C6
25	D	406	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
25	K	103	BCR	C1-C6-C7-C8
25	K	103	BCR	C5-C6-C7-C8
25	d	404	BCR	C21-C22-C23-C24
26	A	410[B]	SQD	C8-C7-O47-C45
26	A	412	SQD	O6-C44-C45-O47
26	B	620	SQD	O49-C7-O47-C45
26	X	101	SQD	C2-C1-O6-C44
26	X	101	SQD	O49-C7-O47-C45
26	X	101	SQD	C8-C7-O47-C45
26	a	412	SQD	O6-C44-C45-O47
26	a	412	SQD	C5-C6-S-O7
26	a	412	SQD	C5-C6-S-O8
26	a	412	SQD	C5-C6-S-O9
26	b	620	SQD	C8-C7-O47-C45
26	f	102	SQD	O6-C44-C45-O47
26	f	102	SQD	O49-C7-O47-C45
26	f	102	SQD	C8-C7-O47-C45
27	B	624	GOL	C1-C2-C3-O3
27	B	624	GOL	O2-C2-C3-O3
27	B	629	GOL	O1-C1-C2-C3
27	D	414	GOL	C1-C2-C3-O3
27	O	302	GOL	O1-C1-C2-C3
27	O	303	GOL	O1-C1-C2-O2
27	V	203[A]	GOL	C1-C2-C3-O3
27	V	203[B]	GOL	C1-C2-C3-O3
27	V	203[B]	GOL	O2-C2-C3-O3
27	b	624	GOL	C1-C2-C3-O3
27	c	527	GOL	C1-C2-C3-O3
27	d	412	GOL	C1-C2-C3-O3
27	o	302	GOL	C1-C2-C3-O3
27	o	303	GOL	C1-C2-C3-O3
29	A	414[A]	PL9	C9-C11-C12-C13
29	A	414[A]	PL9	C15-C14-C16-C17
29	A	414[A]	PL9	C14-C16-C17-C18
29	A	414[B]	PL9	C14-C16-C17-C18
29	A	414[B]	PL9	C28-C29-C31-C32
29	A	414[B]	PL9	C30-C29-C31-C32
29	a	414[A]	PL9	C9-C11-C12-C13
29	a	414[A]	PL9	C14-C16-C17-C18
29	a	414[A]	PL9	C23-C24-C26-C27
29	a	414[A]	PL9	C25-C24-C26-C27
29	a	414[B]	PL9	C9-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
29	a	414[B]	PL9	C14-C16-C17-C18
31	A	417	LMT	C2'-C1'-O1'-C1
31	A	417	LMT	O5'-C1'-O1'-C1
31	A	419	LMT	C2'-C1'-O1'-C1
31	A	419	LMT	O5'-C1'-O1'-C1
31	A	419	LMT	C2-C1-O1'-C1'
31	B	628	LMT	C2-C1-O1'-C1'
31	B	631	LMT	O5'-C1'-O1'-C1
31	B	631	LMT	C2-C1-O1'-C1'
31	F	101	LMT	C2'-C1'-O1'-C1
31	F	101	LMT	O5'-C1'-O1'-C1
31	F	101	LMT	C2-C1-O1'-C1'
31	M	102	LMT	C2-C1-O1'-C1'
31	b	627	LMT	C2'-C1'-O1'-C1
31	b	627	LMT	O5'-C1'-O1'-C1
31	t	101	LMT	O5'-C1'-O1'-C1
31	t	101	LMT	C2-C1-O1'-C1'
32	A	418[B]	LHG	C4-O6-P-O5
32	D	408[A]	LHG	O2-C2-C3-O3
32	D	408[A]	LHG	C3-O3-P-O4
32	D	408[A]	LHG	C3-O3-P-O5
32	D	408[A]	LHG	C3-O3-P-O6
32	D	408[A]	LHG	C4-O6-P-O4
32	D	408[B]	LHG	O2-C2-C3-O3
32	D	408[B]	LHG	C3-O3-P-O4
32	D	408[B]	LHG	C4-O6-P-O4
32	D	408[B]	LHG	C4-O6-P-O5
32	E	101[A]	LHG	C3-O3-P-O4
32	E	101[A]	LHG	C3-O3-P-O5
32	E	101[A]	LHG	O10-C23-O8-C6
32	E	101[A]	LHG	C24-C23-O8-C6
32	E	101[B]	LHG	C3-O3-P-O4
32	E	101[B]	LHG	C3-O3-P-O5
32	E	101[B]	LHG	O10-C23-O8-C6
32	E	101[B]	LHG	C24-C23-O8-C6
32	L	101[A]	LHG	C4-O6-P-O4
32	L	101[A]	LHG	C4-O6-P-O5
32	L	101[B]	LHG	C4-O6-P-O3
32	L	101[B]	LHG	C4-O6-P-O4
32	L	101[B]	LHG	C4-O6-P-O5
32	a	420[A]	LHG	C3-O3-P-O4
32	a	420[A]	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
32	a	420[A]	LHG	O10-C23-O8-C6
32	a	420[A]	LHG	C24-C23-O8-C6
32	a	420[B]	LHG	C3-O3-P-O4
32	a	420[B]	LHG	C4-O6-P-O5
32	a	420[B]	LHG	O10-C23-O8-C6
32	a	420[B]	LHG	C24-C23-O8-C6
32	b	629[A]	LHG	C4-O6-P-O4
32	b	629[A]	LHG	C4-O6-P-O5
32	b	629[B]	LHG	C4-O6-P-O4
32	b	629[B]	LHG	C4-O6-P-O5
32	d	406[A]	LHG	C3-O3-P-O4
32	d	406[A]	LHG	C3-O3-P-O5
32	d	406[A]	LHG	C4-O6-P-O4
32	d	406[B]	LHG	O2-C2-C3-O3
32	d	406[B]	LHG	C3-O3-P-O4
32	d	406[B]	LHG	C3-O3-P-O5
32	d	406[B]	LHG	C3-O3-P-O6
32	d	406[B]	LHG	C4-O6-P-O4
32	d	413[A]	LHG	C3-O3-P-O5
32	d	413[B]	LHG	C3-O3-P-O5
33	C	521	LMG	C11-C10-O7-C8
33	c	521	LMG	O9-C10-O7-C8
33	Z	101	LMG	O9-C10-O7-C8
33	Z	101	LMG	C11-C10-O7-C8
33	z	101	LMG	O6-C1-O1-C7
34	B	622	HTG	C2'-C1'-S1-C1
31	A	419	LMT	O5B-C1B-O1B-C4'
31	B	630	LMT	C4'-C5'-C6'-O6'
31	M	102	LMT	C4B-C5B-C6B-O6B
23	D	405	CLA	CBD-CGD-O2D-CED
26	A	410[A]	SQD	O49-C7-O47-C45
26	A	410[B]	SQD	O49-C7-O47-C45
26	b	620	SQD	O49-C7-O47-C45
33	C	521	LMG	O9-C10-O7-C8
23	c	513	CLA	C3-C5-C6-C7
23	d	403	CLA	C3-C5-C6-C7
31	M	102	LMT	O5'-C5'-C6'-O6'
31	c	501	LMT	O5B-C5B-C6B-O6B
26	B	620	SQD	C8-C7-O47-C45
33	c	521	LMG	C11-C10-O7-C8
23	C	514	CLA	CBD-CGD-O2D-CED
31	B	630	LMT	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
34	D	412	HTG	O5-C5-C6-O6
23	D	405	CLA	C4-C3-C5-C6
29	A	414[A]	PL9	C20-C19-C21-C22
29	a	414[B]	PL9	C25-C24-C26-C27
29	A	414[A]	PL9	C18-C19-C21-C22
29	A	414[B]	PL9	C18-C19-C21-C22
23	B	606	CLA	C2A-CAA-CBA-CGA
23	B	614	CLA	C3-C5-C6-C7
23	b	616	CLA	C3-C5-C6-C7
34	D	412	HTG	S1-C1'-C2'-C3'
34	b	625	HTG	S1-C1'-C2'-C3'
31	B	628	LMT	C4'-C5'-C6'-O6'
31	m	103	LMT	C4B-C5B-C6B-O6B
25	T	101	BCR	C13-C14-C15-C16
31	b	621	LMT	O5'-C5'-C6'-O6'
33	C	521	LMG	O6-C5-C6-O5
23	c	502	CLA	CBD-CGD-O2D-CED
23	c	512	CLA	CBD-CGD-O2D-CED
32	d	406[A]	LHG	O2-C2-C3-O3
32	d	413[B]	LHG	O2-C2-C3-O3
23	A	408	CLA	C3-C5-C6-C7
23	B	616	CLA	C3-C5-C6-C7
23	D	405	CLA	C3-C5-C6-C7
31	F	101	LMT	O5'-C5'-C6'-O6'
31	m	103	LMT	O5B-C5B-C6B-O6B
31	c	501	LMT	C4B-C5B-C6B-O6B
26	A	410[A]	SQD	C8-C7-O47-C45
33	z	101	LMG	C11-C10-O7-C8
23	c	514	CLA	CBD-CGD-O2D-CED
31	B	628	LMT	O5B-C5B-C6B-O6B
34	B	625	HTG	O5-C5-C6-O6
33	c	521	LMG	C4-C5-C6-O5
31	A	419	LMT	O5B-C5B-C6B-O6B
31	M	102	LMT	O5B-C5B-C6B-O6B
31	M	102	LMT	C4'-C5'-C6'-O6'
31	B	630	LMT	O5'-C5'-C6'-O6'
31	B	630	LMT	C4B-C5B-C6B-O6B
23	B	605	CLA	C4-C3-C5-C6
23	C	508	CLA	C4-C3-C5-C6
23	b	603	CLA	C4-C3-C5-C6
23	b	605	CLA	C4-C3-C5-C6
23	b	614	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	c	508	CLA	C4-C3-C5-C6
29	A	414[B]	PL9	C15-C14-C16-C17
29	A	414[B]	PL9	C20-C19-C21-C22
29	a	414[A]	PL9	C15-C14-C16-C17
29	a	414[A]	PL9	C30-C29-C31-C32
29	a	414[B]	PL9	C15-C14-C16-C17
29	a	414[B]	PL9	C30-C29-C31-C32
34	D	412	HTG	C4-C5-C6-O6
23	B	605	CLA	C2-C3-C5-C6
23	C	508	CLA	C2-C3-C5-C6
23	b	603	CLA	C2-C3-C5-C6
23	b	605	CLA	C2-C3-C5-C6
23	b	614	CLA	C2-C3-C5-C6
23	c	508	CLA	C2-C3-C5-C6
29	A	414[A]	PL9	C13-C14-C16-C17
29	A	414[B]	PL9	C13-C14-C16-C17
29	a	414[A]	PL9	C13-C14-C16-C17
29	a	414[A]	PL9	C28-C29-C31-C32
29	a	414[B]	PL9	C13-C14-C16-C17
29	a	414[B]	PL9	C28-C29-C31-C32
23	b	606	CLA	C2A-CAA-CBA-CGA
31	A	419	LMT	O5'-C5'-C6'-O6'
31	B	631	LMT	O5'-C5'-C6'-O6'
31	b	621	LMT	C4'-C5'-C6'-O6'
26	B	620	SQD	O5-C1-O6-C44
29	A	414[A]	PL9	C44-C46-C47-C48
29	A	414[B]	PL9	C9-C11-C12-C13
29	A	414[B]	PL9	C44-C46-C47-C48
29	D	407[A]	PL9	C39-C41-C42-C43
35	h	102	DGD	C6B-C7B-C8B-C9B
31	e	101	LMT	C4'-C5'-C6'-O6'
33	B	621	LMG	C39-C40-C41-C42
31	B	628	LMT	O5'-C5'-C6'-O6'
32	d	406[A]	LHG	C1-C2-C3-O3
32	d	413[B]	LHG	C1-C2-C3-O3
33	z	101	LMG	O9-C10-O7-C8
31	b	627	LMT	C4'-C5'-C6'-O6'
35	C	519	DGD	C6B-C7B-C8B-C9B
23	a	409	CLA	CBA-CGA-O2A-C1
31	F	101	LMT	C4'-C5'-C6'-O6'
26	X	101	SQD	C23-C24-C25-C26
23	b	606	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	b	627	LMT	O5'-C5'-C6'-O6'
34	b	625	HTG	O5-C5-C6-O6
26	B	620	SQD	C30-C31-C32-C33
23	b	614	CLA	C8-C10-C11-C12
31	B	631	LMT	C2'-C1'-O1'-C1
31	t	101	LMT	C2'-C1'-O1'-C1
29	A	414[A]	PL9	C30-C29-C31-C32
31	A	419	LMT	C4B-C5B-C6B-O6B
23	D	405	CLA	C2-C3-C5-C6
23	C	503	CLA	C14-C13-C15-C16
23	C	507	CLA	C14-C13-C15-C16
23	b	604	CLA	C6-C7-C8-C9
23	b	616	CLA	C6-C7-C8-C9
23	c	513	CLA	C6-C7-C8-C9
23	D	405	CLA	O1D-CGD-O2D-CED
25	K	102	BCR	C7-C8-C9-C34
25	b	619	BCR	C7-C8-C9-C34
25	d	404	BCR	C37-C22-C23-C24
25	b	619	BCR	C7-C8-C9-C10
26	A	410[B]	SQD	C7-C8-C9-C10
32	E	101[A]	LHG	C23-C24-C25-C26
23	c	513	CLA	C15-C16-C17-C18
33	c	521	LMG	O6-C5-C6-O5
23	B	602	CLA	C13-C15-C16-C17
23	b	601	CLA	C10-C11-C12-C13
34	b	623	HTG	C1'-C2'-C3'-C4'
31	e	101	LMT	O5B-C5B-C6B-O6B
23	A	408	CLA	C5-C6-C7-C8
23	B	601	CLA	C5-C6-C7-C8
23	B	601	CLA	C10-C11-C12-C13
23	b	611	CLA	C8-C10-C11-C12
27	b	624	GOL	O2-C2-C3-O3
27	v	202[B]	GOL	O1-C1-C2-O2
33	Z	101	LMG	C10-C11-C12-C13
35	c	518[A]	DGD	C1B-C2B-C3B-C4B
35	c	518[B]	DGD	C1B-C2B-C3B-C4B
23	C	502	CLA	CBD-CGD-O2D-CED
23	C	510	CLA	CBD-CGD-O2D-CED
23	b	604	CLA	C8-C10-C11-C12
31	B	628	LMT	C5'-C4'-O1B-C1B
34	b	622	HTG	S1-C1'-C2'-C3'
32	D	409[A]	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
23	B	606	CLA	C10-C11-C12-C13
23	b	606	CLA	C13-C15-C16-C17
31	B	631	LMT	C4'-C5'-C6'-O6'
23	A	408	CLA	C12-C13-C15-C16
23	b	606	CLA	C12-C13-C15-C16
31	A	419	LMT	O1'-C1-C2-C3
23	B	610	CLA	C2A-CAA-CBA-CGA
23	B	603	CLA	C13-C15-C16-C17
23	D	405	CLA	C10-C11-C12-C13
23	a	409	CLA	O1A-CGA-O2A-C1
26	X	101	SQD	O5-C1-O6-C44
31	b	621	LMT	O5'-C1'-O1'-C1
31	e	101	LMT	O5'-C1'-O1'-C1
23	a	405[A]	CLA	C15-C16-C17-C18
23	a	405[B]	CLA	C15-C16-C17-C18
29	A	414[B]	PL9	C39-C41-C42-C43
29	D	407[B]	PL9	C39-C41-C42-C43
29	a	414[B]	PL9	C24-C26-C27-C28
29	d	405[A]	PL9	C39-C41-C42-C43
29	d	405[B]	PL9	C39-C41-C42-C43
32	E	101[B]	LHG	C23-C24-C25-C26
31	B	628	LMT	C4B-C5B-C6B-O6B
23	B	608	CLA	C13-C15-C16-C17
23	C	508	CLA	C5-C6-C7-C8
23	b	611	CLA	C15-C16-C17-C18
23	b	614	CLA	C10-C11-C12-C13
31	B	628	LMT	C6-C7-C8-C9
31	A	419	LMT	C4'-C5'-C6'-O6'
23	B	615	CLA	C5-C6-C7-C8
33	B	621	LMG	C37-C38-C39-C40
35	c	517[B]	DGD	O6D-C5D-C6D-O5D
23	C	503	CLA	C13-C15-C16-C17
23	b	604	CLA	C5-C6-C7-C8
23	c	507	CLA	C15-C16-C17-C18
32	D	408[B]	LHG	C3-O3-P-O6
32	D	408[B]	LHG	C4-O6-P-O3
32	E	101[A]	LHG	C3-O3-P-O6
32	E	101[A]	LHG	C4-O6-P-O3
32	E	101[B]	LHG	C3-O3-P-O6
32	E	101[B]	LHG	C4-O6-P-O3
32	L	101[A]	LHG	C4-O6-P-O3
32	a	420[A]	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
32	a	420[A]	LHG	C4-O6-P-O3
32	a	420[B]	LHG	C3-O3-P-O6
32	a	420[B]	LHG	C4-O6-P-O3
32	b	629[A]	LHG	C4-O6-P-O3
32	b	629[B]	LHG	C4-O6-P-O3
32	d	406[A]	LHG	C3-O3-P-O6
32	d	406[B]	LHG	C4-O6-P-O3
26	A	410[A]	SQD	C7-C8-C9-C10
31	c	501	LMT	O1'-C1-C2-C3
23	B	614	CLA	C10-C11-C12-C13
23	C	509	CLA	C10-C11-C12-C13
31	A	417	LMT	O1'-C1-C2-C3
26	B	620	SQD	C7-C8-C9-C10
31	e	101	LMT	O5'-C5'-C6'-O6'
32	D	408[A]	LHG	C1-C2-C3-O3
32	d	406[B]	LHG	C1-C2-C3-O3
23	C	511	CLA	C4-C3-C5-C6
29	d	405[B]	PL9	C15-C14-C16-C17
26	A	410[A]	SQD	C12-C13-C14-C15
26	A	410[B]	SQD	C11-C10-C9-C8
32	D	409[B]	LHG	C33-C34-C35-C36
31	B	631	LMT	O1'-C1-C2-C3
33	c	520	LMG	C10-C11-C12-C13
31	t	101	LMT	C4-C5-C6-C7
32	d	413[B]	LHG	C16-C17-C18-C19
33	C	501	LMG	C36-C37-C38-C39
35	h	102	DGD	C7B-C8B-C9B-CAB
23	B	614	CLA	C5-C6-C7-C8
23	B	615	CLA	C10-C11-C12-C13
34	B	622	HTG	C1'-C2'-C3'-C4'
26	X	101	SQD	C30-C31-C32-C33
26	b	620	SQD	C18-C19-C20-C21
26	f	102	SQD	C32-C33-C34-C35
32	L	101[A]	LHG	C15-C16-C17-C18
32	L	101[A]	LHG	C17-C18-C19-C20
32	L	101[B]	LHG	C12-C13-C14-C15
35	C	518[B]	DGD	CCB-CDB-CEB-CFB
35	H	102	DGD	CCB-CDB-CEB-CFB
35	c	517[A]	DGD	C9A-CAA-CBA-CCA
35	c	518[A]	DGD	C9A-CAA-CBA-CCA
23	b	615	CLA	C16-C17-C18-C19
23	d	403	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
26	A	410[B]	SQD	C15-C16-C17-C18
32	D	409[B]	LHG	C32-C33-C34-C35
32	d	413[A]	LHG	C16-C17-C18-C19
33	D	413	LMG	C19-C20-C21-C22
34	B	623	HTG	C3'-C4'-C5'-C6'
35	c	517[B]	DGD	C9A-CAA-CBA-CCA
23	c	514	CLA	C10-C11-C12-C13
31	b	627	LMT	C7-C8-C9-C10
32	d	407[B]	LHG	C27-C28-C29-C30
33	B	621	LMG	C17-C18-C19-C20
31	A	419	LMT	C3-C4-C5-C6
31	B	630	LMT	C5-C6-C7-C8
32	D	408[A]	LHG	C16-C17-C18-C19
32	b	629[B]	LHG	C14-C15-C16-C17
32	d	413[A]	LHG	C32-C33-C34-C35
35	C	517[A]	DGD	C5B-C6B-C7B-C8B
35	c	517[B]	DGD	C5A-C6A-C7A-C8A
35	c	518[B]	DGD	C9A-CAA-CBA-CCA
23	B	614	CLA	C8-C10-C11-C12
32	E	101[B]	LHG	O2-C2-C3-O3
31	b	627	LMT	C3-C4-C5-C6
32	a	420[A]	LHG	C26-C27-C28-C29
35	c	517[A]	DGD	C5A-C6A-C7A-C8A
35	c	518[A]	DGD	CBA-CCA-CDA-CEA
31	B	630	LMT	C2'-C1'-O1'-C1
31	b	621	LMT	C2'-C1'-O1'-C1
31	e	101	LMT	C2'-C1'-O1'-C1
35	C	518[A]	DGD	C2E-C1E-O5D-C6D
35	C	518[B]	DGD	C2E-C1E-O5D-C6D
35	c	517[B]	DGD	C2E-C1E-O5D-C6D
34	b	622	HTG	C2'-C3'-C4'-C5'
35	C	517[A]	DGD	C4B-C5B-C6B-C7B
35	c	517[A]	DGD	C2B-C3B-C4B-C5B
35	c	518[A]	DGD	CAA-CBA-CCA-CDA
23	B	603	CLA	C16-C17-C18-C19
23	a	409	CLA	C16-C17-C18-C19
23	c	509	CLA	C16-C17-C18-C19
23	c	510	CLA	C16-C17-C18-C20
23	C	514	CLA	O1D-CGD-O2D-CED
31	e	101	LMT	C4-C5-C6-C7
32	L	101[A]	LHG	C13-C14-C15-C16
32	L	101[B]	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
33	D	413	LMG	C35-C36-C37-C38
33	D	413	LMG	C36-C37-C38-C39
29	d	405[B]	PL9	C28-C29-C31-C32
23	B	602	CLA	C11-C12-C13-C14
23	a	407[A]	CLA	C11-C12-C13-C14
23	a	407[B]	CLA	C11-C12-C13-C14
23	b	606	CLA	C14-C13-C15-C16
23	c	502	CLA	O1D-CGD-O2D-CED
35	C	517[B]	DGD	O6D-C5D-C6D-O5D
26	A	410[A]	SQD	C15-C16-C17-C18
32	L	101[B]	LHG	C17-C18-C19-C20
32	a	420[B]	LHG	C26-C27-C28-C29
33	C	501	LMG	C12-C13-C14-C15
33	C	521	LMG	C18-C19-C20-C21
33	d	411	LMG	C29-C30-C31-C32
35	C	518[A]	DGD	CCB-CDB-CEB-CFB
35	H	102	DGD	C5B-C6B-C7B-C8B
23	b	605	CLA	C8-C10-C11-C12
34	B	625	HTG	C4-C5-C6-O6
35	c	517[B]	DGD	C4D-C5D-C6D-O5D
25	D	406	BCR	C37-C22-C23-C24
26	A	412	SQD	C17-C18-C19-C20
27	A	411	GOL	O1-C1-C2-C3
27	B	624	GOL	O1-C1-C2-C3
27	B	629	GOL	C1-C2-C3-O3
27	D	414	GOL	O1-C1-C2-C3
27	O	303	GOL	O1-C1-C2-C3
27	a	418	GOL	O1-C1-C2-C3
27	d	412	GOL	O1-C1-C2-C3
27	v	202[A]	GOL	O1-C1-C2-C3
27	v	202[B]	GOL	O1-C1-C2-C3
25	D	406	BCR	C21-C22-C23-C24
26	X	101	SQD	C29-C30-C31-C32
31	e	101	LMT	C5-C6-C7-C8
32	D	409[A]	LHG	C32-C33-C34-C35
32	b	629[A]	LHG	C14-C15-C16-C17
35	c	518[B]	DGD	CBA-CCA-CDA-CEA
33	C	501	LMG	C10-C11-C12-C13
26	b	620	SQD	C27-C28-C29-C30
31	M	101	LMT	C3-C4-C5-C6
32	D	408[B]	LHG	C16-C17-C18-C19
32	L	101[A]	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
32	d	413[A]	LHG	C29-C30-C31-C32
33	m	101	LMG	C35-C36-C37-C38
35	c	517[B]	DGD	C2B-C3B-C4B-C5B
35	c	518[B]	DGD	CAA-CBA-CCA-CDA
23	B	603	CLA	C16-C17-C18-C20
23	B	615	CLA	C16-C17-C18-C19
23	b	602	CLA	C16-C17-C18-C19
23	b	614	CLA	C16-C17-C18-C19
23	b	615	CLA	C16-C17-C18-C20
23	d	402[A]	CLA	C16-C17-C18-C20
31	B	630	LMT	O5'-C1'-O1'-C1
23	A	405[A]	CLA	C15-C16-C17-C18
31	B	628	LMT	C7-C8-C9-C10
31	B	631	LMT	C11-C10-C9-C8
32	b	629[A]	LHG	C16-C17-C18-C19
33	D	413	LMG	C30-C31-C32-C33
35	c	519	DGD	CBB-CCB-CDB-CEB
31	M	101	LMT	O5'-C5'-C6'-O6'
31	A	419	LMT	C5'-C4'-O1B-C1B
32	d	406[B]	LHG	C34-C35-C36-C37
33	a	417	LMG	C10-C11-C12-C13
31	B	631	LMT	C3-C4-C5-C6
33	C	501	LMG	C20-C21-C22-C23
33	C	521	LMG	C19-C20-C21-C22
31	M	102	LMT	C7-C8-C9-C10
32	d	407[A]	LHG	C27-C28-C29-C30
35	C	517[A]	DGD	C9A-CAA-CBA-CCA
23	c	512	CLA	O1D-CGD-O2D-CED
23	b	606	CLA	C15-C16-C17-C18
31	m	103	LMT	C2-C1-O1'-C1'
32	E	101[A]	LHG	C24-C25-C26-C27
23	B	615	CLA	C16-C17-C18-C20
23	b	602	CLA	C16-C17-C18-C20
23	b	614	CLA	C16-C17-C18-C20
23	d	403	CLA	C16-C17-C18-C19
31	B	628	LMT	C5-C6-C7-C8
32	L	101[A]	LHG	C25-C26-C27-C28
32	L	101[B]	LHG	C13-C14-C15-C16
32	L	101[B]	LHG	C25-C26-C27-C28
33	C	501	LMG	C17-C18-C19-C20
33	a	417	LMG	C30-C31-C32-C33
32	b	629[A]	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
35	c	517[A]	DGD	O6D-C5D-C6D-O5D
33	Z	101	LMG	O6-C5-C6-O5
33	C	501	LMG	C19-C20-C21-C22
23	c	506	CLA	C4-C3-C5-C6
23	c	506	CLA	C2-C3-C5-C6
24	a	408[B]	PHO	C2-C3-C5-C6
29	A	414[A]	PL9	C12-C11-C9-C8
29	A	414[B]	PL9	C12-C11-C9-C8
29	D	407[A]	PL9	C13-C14-C16-C17
33	B	621	LMG	C11-C10-O7-C8
33	m	101	LMG	C11-C10-O7-C8
26	X	101	SQD	C24-C25-C26-C27
33	C	520	LMG	C16-C17-C18-C19
35	c	518[B]	DGD	CBB-CCB-CDB-CEB
35	h	102	DGD	C9A-CAA-CBA-CCA
27	B	629	GOL	O1-C1-C2-O2
27	O	302	GOL	O1-C1-C2-O2
27	V	203[A]	GOL	O2-C2-C3-O3
27	c	527	GOL	O2-C2-C3-O3
26	a	412	SQD	C31-C32-C33-C34
31	b	627	LMT	C5-C6-C7-C8
32	A	418[B]	LHG	C34-C35-C36-C37
32	d	413[A]	LHG	C24-C25-C26-C27
33	C	521	LMG	C17-C18-C19-C20
33	c	520	LMG	C31-C32-C33-C34
33	c	520	LMG	C34-C35-C36-C37
31	c	501	LMT	O5'-C5'-C6'-O6'
31	B	631	LMT	C4-C5-C6-C7
35	h	102	DGD	CAA-CBA-CCA-CDA
31	A	419	LMT	C1-C2-C3-C4
32	E	101[A]	LHG	O2-C2-C3-O3
23	B	615	CLA	C13-C15-C16-C17
23	b	605	CLA	C5-C6-C7-C8
32	D	408[A]	LHG	C12-C13-C14-C15
32	D	408[B]	LHG	C1-C2-C3-O3
26	A	410[B]	SQD	C12-C13-C14-C15
32	E	101[B]	LHG	C24-C25-C26-C27
33	C	521	LMG	C13-C14-C15-C16
33	m	101	LMG	C39-C40-C41-C42
33	B	621	LMG	O9-C10-O7-C8
33	m	101	LMG	O9-C10-O7-C8
23	B	616	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
23	C	510	CLA	C2-C1-O2A-CGA
23	b	601	CLA	C2-C1-O2A-CGA
35	C	517[A]	DGD	O6D-C5D-C6D-O5D
35	C	517[B]	DGD	C4D-C5D-C6D-O5D
26	B	620	SQD	C11-C10-C9-C8
26	a	412	SQD	C25-C26-C27-C28
26	b	620	SQD	C31-C32-C33-C34
32	A	418[A]	LHG	C34-C35-C36-C37
32	b	629[B]	LHG	C16-C17-C18-C19
32	d	413[B]	LHG	C32-C33-C34-C35
33	a	417	LMG	C34-C35-C36-C37
23	a	409	CLA	C16-C17-C18-C20
25	D	406	BCR	C23-C24-C25-C26
25	b	617	BCR	C1-C6-C7-C8
25	b	617	BCR	C5-C6-C7-C8
25	y	101	BCR	C1-C6-C7-C8
25	y	101	BCR	C5-C6-C7-C8
26	A	412	SQD	C26-C27-C28-C29
32	d	407[B]	LHG	C25-C26-C27-C28
35	c	517[A]	DGD	C7A-C8A-C9A-CAA
35	h	102	DGD	CAB-CBB-CCB-CDB
23	c	513	CLA	CBA-CGA-O2A-C1
26	b	620	SQD	C24-C23-O48-C46
31	c	501	LMT	C1-C2-C3-C4
32	A	418[B]	LHG	C12-C13-C14-C15
32	d	407[A]	LHG	C29-C30-C31-C32
23	c	513	CLA	CBD-CGD-O2D-CED
32	d	406[A]	LHG	C34-C35-C36-C37
33	C	501	LMG	C39-C40-C41-C42
33	C	520	LMG	C34-C35-C36-C37
35	c	518[A]	DGD	C6A-C7A-C8A-C9A
23	A	406[B]	CLA	C13-C15-C16-C17
29	A	414[A]	PL9	C45-C44-C46-C47
29	D	407[B]	PL9	C15-C14-C16-C17
29	a	414[A]	PL9	C12-C11-C9-C10
23	B	602	CLA	C11-C12-C13-C15
23	B	606	CLA	C11-C10-C8-C7
23	C	511	CLA	C2-C3-C5-C6
23	C	511	CLA	C11-C12-C13-C15
23	a	407[A]	CLA	C11-C12-C13-C15
23	a	407[B]	CLA	C11-C12-C13-C15
23	c	505	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
29	d	405[A]	PL9	C13-C14-C16-C17
32	A	418[A]	LHG	C12-C13-C14-C15
32	D	409[B]	LHG	C29-C30-C31-C32
33	C	501	LMG	C29-C30-C31-C32
35	c	518[A]	DGD	C4A-C5A-C6A-C7A
23	B	610	CLA	C16-C17-C18-C19
23	c	510	CLA	C16-C17-C18-C19
32	D	409[B]	LHG	C24-C23-O8-C6
31	b	627	LMT	C1-C2-C3-C4
23	b	610	CLA	C2A-CAA-CBA-CGA
31	B	628	LMT	C3'-C4'-O1B-C1B
32	d	406[B]	LHG	C11-C10-C9-C8
33	d	411	LMG	C11-C12-C13-C14
32	d	407[A]	LHG	C25-C26-C27-C28
31	t	101	LMT	O5'-C5'-C6'-O6'
23	c	514	CLA	O1D-CGD-O2D-CED
23	A	404[B]	CLA	C13-C15-C16-C17
32	D	409[A]	LHG	C13-C14-C15-C16
35	C	519	DGD	C2B-C3B-C4B-C5B
35	c	517[A]	DGD	CAA-CBA-CCA-CDA
33	a	417	LMG	C29-C30-C31-C32
35	C	517[B]	DGD	C9A-CAA-CBA-CCA
23	c	503	CLA	C16-C17-C18-C19
33	a	417	LMG	C4-C5-C6-O5
26	A	412	SQD	O5-C1-O6-C44
31	M	101	LMT	O5'-C1'-O1'-C1
35	C	518[A]	DGD	O6E-C1E-O5D-C6D
35	C	518[B]	DGD	O6E-C1E-O5D-C6D
35	c	517[B]	DGD	O6E-C1E-O5D-C6D
32	D	409[A]	LHG	C15-C16-C17-C18
35	C	517[B]	DGD	C4B-C5B-C6B-C7B
35	H	102	DGD	C7A-C8A-C9A-CAA
35	c	517[B]	DGD	CAA-CBA-CCA-CDA
23	B	605	CLA	C5-C6-C7-C8
23	c	511	CLA	CBD-CGD-O2D-CED
35	h	102	DGD	CBA-CCA-CDA-CEA
32	D	409[B]	LHG	C15-C16-C17-C18
26	A	412	SQD	C2-C1-O6-C44
33	m	101	LMG	C2-C1-O1-C7
33	Z	101	LMG	C2-C1-O1-C7
26	A	410[A]	SQD	O6-C44-C45-O47
32	d	407[A]	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
32	d	413[A]	LHG	C25-C26-C27-C28
33	B	621	LMG	C34-C35-C36-C37
23	c	509	CLA	C16-C17-C18-C20
33	m	101	LMG	C14-C15-C16-C17
35	H	102	DGD	CAB-CBB-CCB-CDB
33	D	413	LMG	O6-C5-C6-O5
35	C	517[B]	DGD	O6E-C5E-C6E-O5E
23	b	601	CLA	C8-C10-C11-C12
24	a	408[B]	PHO	C4-C3-C5-C6
29	a	414[B]	PL9	C23-C24-C26-C27
31	B	630	LMT	C2-C3-C4-C5
23	B	606	CLA	C11-C10-C8-C9
23	C	510	CLA	C6-C7-C8-C9
23	C	514	CLA	C6-C7-C8-C9
23	D	405	CLA	C14-C13-C15-C16
23	b	606	CLA	C11-C10-C8-C9
23	c	505	CLA	C14-C13-C15-C16
31	b	621	LMT	C11-C10-C9-C8
32	b	629[B]	LHG	C27-C28-C29-C30
33	C	520	LMG	C17-C18-C19-C20
35	c	518[A]	DGD	C2B-C3B-C4B-C5B
31	B	630	LMT	C6-C7-C8-C9
33	m	101	LMG	C38-C39-C40-C41
23	A	406[A]	CLA	C13-C15-C16-C17
23	B	604	CLA	C5-C6-C7-C8
26	f	102	SQD	C25-C26-C27-C28
32	d	413[B]	LHG	C24-C25-C26-C27
35	H	102	DGD	C9B-CAB-CBB-CCB
23	A	405[B]	CLA	C1A-C2A-CAA-CBA
23	B	611	CLA	C1A-C2A-CAA-CBA
23	a	407[B]	CLA	C1A-C2A-CAA-CBA
23	c	512	CLA	C1A-C2A-CAA-CBA
23	c	514	CLA	C1A-C2A-CAA-CBA
33	d	411	LMG	O6-C5-C6-O5
23	B	610	CLA	C16-C17-C18-C20
26	a	411[A]	SQD	C9-C10-C11-C12
32	A	418[A]	LHG	C26-C27-C28-C29
32	D	408[B]	LHG	C12-C13-C14-C15
31	b	621	LMT	C3'-C4'-O1B-C1B
23	c	508	CLA	C5-C6-C7-C8
32	D	408[A]	LHG	C4-O6-P-O3
35	c	519	DGD	CBA-CCA-CDA-CEA

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Mol	Chain	Res	Type	Atoms
23	c	510	CLA	C3-C5-C6-C7
33	c	520	LMG	C4-C5-C6-O5
32	d	406[B]	LHG	C13-C14-C15-C16
32	D	409[B]	LHG	O10-C23-O8-C6
23	c	507	CLA	C10-C11-C12-C13
33	c	521	LMG	C29-C28-O8-C9
33	c	520	LMG	C33-C34-C35-C36
32	d	407[A]	LHG	C28-C29-C30-C31
35	c	518[B]	DGD	C2B-C3B-C4B-C5B
35	C	517[B]	DGD	C5B-C6B-C7B-C8B
31	e	101	LMT	C1-C2-C3-C4
35	c	517[B]	DGD	C7A-C8A-C9A-CAA
23	C	503	CLA	C15-C16-C17-C18
35	C	517[A]	DGD	C8A-C9A-CAA-CBA
35	c	517[A]	DGD	C4D-C5D-C6D-O5D
34	b	623	HTG	O5-C5-C6-O6
23	C	507	CLA	C4-C3-C5-C6
29	a	414[B]	PL9	C12-C11-C9-C10
31	A	419	LMT	C5-C6-C7-C8
32	d	413[B]	LHG	C29-C30-C31-C32
32	d	413[B]	LHG	C33-C34-C35-C36
33	d	411	LMG	C35-C36-C37-C38
33	z	101	LMG	C14-C15-C16-C17
33	C	520	LMG	C31-C32-C33-C34
33	a	417	LMG	C21-C22-C23-C24
35	c	518[B]	DGD	C6A-C7A-C8A-C9A
23	c	513	CLA	O1A-CGA-O2A-C1
26	b	620	SQD	O10-C23-O48-C46
32	D	408[A]	LHG	C10-C11-C12-C13
33	C	520	LMG	C11-C12-C13-C14
23	b	606	CLA	C16-C17-C18-C20
23	d	402[A]	CLA	C16-C17-C18-C19
23	C	512	CLA	C3-C5-C6-C7
26	A	412	SQD	O6-C44-C45-C46
26	a	411[A]	SQD	O6-C44-C45-C46
26	f	102	SQD	C44-C45-C46-O48
32	E	101[A]	LHG	C4-C5-C6-O8
32	E	101[B]	LHG	C4-C5-C6-O8
32	a	420[B]	LHG	C4-C5-C6-O8
35	C	518[A]	DGD	CDA-CEA-CFA-CGA
31	c	501	LMT	C2-C3-C4-C5
35	C	518[B]	DGD	CDA-CEA-CFA-CGA

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Mol	Chain	Res	Type	Atoms
35	C	518[A]	DGD	C2G-C3G-O3G-C1D
35	C	518[B]	DGD	C5D-C6D-O5D-C1E
35	c	518[A]	DGD	C2G-C3G-O3G-C1D
35	c	518[A]	DGD	C5D-C6D-O5D-C1E
35	c	518[B]	DGD	C5D-C6D-O5D-C1E
23	a	406[B]	CLA	C2C-C3C-CAC-CBC
26	X	101	SQD	C34-C35-C36-C37
32	L	101[B]	LHG	C27-C28-C29-C30
32	D	408[B]	LHG	C10-C11-C12-C13
32	b	629[A]	LHG	C9-C10-C11-C12
26	b	620	SQD	C26-C27-C28-C29
32	D	409[A]	LHG	C29-C30-C31-C32
35	c	518[B]	DGD	C4A-C5A-C6A-C7A
32	d	413[A]	LHG	C33-C34-C35-C36
35	c	517[B]	DGD	O6E-C5E-C6E-O5E
27	B	629	GOL	O2-C2-C3-O3
27	D	414	GOL	O2-C2-C3-O3
27	o	302	GOL	O2-C2-C3-O3
27	o	303	GOL	O2-C2-C3-O3
31	B	628	LMT	C1-C2-C3-C4
32	D	409[B]	LHG	C13-C14-C15-C16
32	D	409[B]	LHG	C17-C18-C19-C20
33	D	413	LMG	C12-C13-C14-C15
34	B	622	HTG	C2'-C3'-C4'-C5'
35	h	102	DGD	CDB-CEB-CFB-CGB
23	B	613	CLA	C13-C15-C16-C17
35	C	517[A]	DGD	O6E-C5E-C6E-O5E
35	c	517[A]	DGD	O6E-C5E-C6E-O5E
23	C	506	CLA	C4-C3-C5-C6
26	B	620	SQD	C34-C35-C36-C37
32	d	407[B]	LHG	C28-C29-C30-C31
31	c	501	LMT	C4'-C5'-C6'-O6'
35	c	517[B]	DGD	C2A-C1A-O1G-C1G
23	B	602	CLA	C15-C16-C17-C18
23	C	511	CLA	C10-C11-C12-C13
23	b	605	CLA	C13-C15-C16-C17
23	a	406[A]	CLA	C2C-C3C-CAC-CBC
26	B	620	SQD	C46-C45-O47-C7
26	b	620	SQD	C46-C45-O47-C7
23	C	507	CLA	C5-C6-C7-C8
26	a	411[A]	SQD	C12-C13-C14-C15
32	d	413[B]	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
31	B	628	LMT	C9-C10-C11-C12
31	c	501	LMT	C9-C10-C11-C12
23	B	601	CLA	CBA-CGA-O2A-C1
35	c	517[A]	DGD	C2A-C1A-O1G-C1G
26	b	620	SQD	C11-C10-C9-C8
32	D	409[A]	LHG	C17-C18-C19-C20
33	C	520	LMG	C37-C38-C39-C40
34	B	625	HTG	C2'-C3'-C4'-C5'
23	b	610	CLA	C15-C16-C17-C18
26	A	410[A]	SQD	C11-C10-C9-C8
31	A	419	LMT	C3'-C4'-O1B-C1B
32	A	418[A]	LHG	O2-C2-C3-O3
32	E	101[B]	LHG	C25-C26-C27-C28
23	c	512	CLA	C8-C10-C11-C12
31	M	101	LMT	C2'-C1'-O1'-C1
32	E	101[A]	LHG	C25-C26-C27-C28
32	d	407[A]	LHG	C33-C34-C35-C36
26	A	410[B]	SQD	O6-C44-C45-O47
26	X	101	SQD	O47-C45-C46-O48
32	E	101[A]	LHG	C13-C14-C15-C16
23	A	404[A]	CLA	C13-C15-C16-C17
23	A	405[B]	CLA	C15-C16-C17-C18
23	C	509	CLA	C5-C6-C7-C8
33	c	521	LMG	O10-C28-O8-C9
23	c	503	CLA	C16-C17-C18-C20
32	A	418[B]	LHG	C29-C30-C31-C32
33	a	417	LMG	C35-C36-C37-C38
31	m	103	LMT	O5'-C5'-C6'-O6'
23	B	614	CLA	C12-C13-C15-C16
23	C	505	CLA	C12-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C15
23	C	511	CLA	C12-C13-C15-C16
23	C	514	CLA	C11-C10-C8-C7
23	C	514	CLA	C11-C12-C13-C15
23	D	405	CLA	C11-C10-C8-C7
23	D	405	CLA	C12-C13-C15-C16
23	a	409	CLA	C11-C10-C8-C7
23	b	604	CLA	C6-C7-C8-C10
23	b	606	CLA	C11-C10-C8-C7
23	b	616	CLA	C6-C7-C8-C10
23	c	511	CLA	C11-C10-C8-C7
23	c	513	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
29	D	407[B]	PL9	C13-C14-C16-C17
29	d	405[B]	PL9	C13-C14-C16-C17
23	B	610	CLA	C11-C12-C13-C14
23	B	610	CLA	C14-C13-C15-C16
23	B	613	CLA	C11-C12-C13-C14
23	C	505	CLA	C14-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C14
23	C	507	CLA	C6-C7-C8-C9
23	C	514	CLA	C11-C10-C8-C9
23	D	405	CLA	C11-C10-C8-C9
23	c	506	CLA	C11-C12-C13-C14
23	c	514	CLA	C6-C7-C8-C9
23	c	512	CLA	CBA-CGA-O2A-C1
26	A	412	SQD	C24-C23-O48-C46
35	c	519	DGD	C2A-C1A-O1G-C1G
27	l	102[A]	GOL	O1-C1-C2-C3
23	C	513	CLA	C3-C5-C6-C7
23	b	615	CLA	C10-C11-C12-C13
32	d	407[B]	LHG	C9-C10-C11-C12
31	b	621	LMT	C3-C4-C5-C6
35	h	102	DGD	C9B-CAB-CBB-CCB
32	a	420[A]	LHG	C23-C24-C25-C26
26	B	620	SQD	C29-C30-C31-C32
35	C	517[B]	DGD	CCA-CDA-CEA-CFA
35	c	517[B]	DGD	O1A-C1A-O1G-C1G
33	C	501	LMG	C13-C14-C15-C16
23	B	612	CLA	C10-C11-C12-C13
23	C	508	CLA	C13-C15-C16-C17
32	L	101[B]	LHG	O6-C4-C5-C6
29	A	414[A]	PL9	C39-C41-C42-C43
29	D	407[A]	PL9	C45-C44-C46-C47
23	b	609	CLA	C2-C3-C5-C6
26	X	101	SQD	C7-C8-C9-C10
33	d	411	LMG	C28-C29-C30-C31
26	a	411[B]	SQD	C12-C13-C14-C15
35	C	517[B]	DGD	C8A-C9A-CAA-CBA
35	c	518[A]	DGD	CBB-CCB-CDB-CEB
23	b	601	CLA	C13-C15-C16-C17
23	C	513	CLA	CBA-CGA-O2A-C1
23	b	601	CLA	CBA-CGA-O2A-C1
32	d	406[B]	LHG	C24-C23-O8-C6
32	a	420[B]	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
33	z	101	LMG	C19-C20-C21-C22
35	C	517[A]	DGD	CCA-CDA-CEA-CFA
35	c	519	DGD	C2B-C3B-C4B-C5B
32	a	420[A]	LHG	C10-C11-C12-C13
34	b	622	HTG	C3'-C4'-C5'-C6'
35	C	517[B]	DGD	C7A-C8A-C9A-CAA
35	C	519	DGD	CDB-CEB-CFB-CGB
31	b	627	LMT	C2-C1-O1'-C1'
31	e	101	LMT	C2-C1-O1'-C1'
32	d	407[B]	LHG	C29-C30-C31-C32
33	B	621	LMG	C15-C16-C17-C18
23	C	502	CLA	O1D-CGD-O2D-CED
31	e	101	LMT	C9-C10-C11-C12
32	L	101[B]	LHG	C24-C25-C26-C27
23	b	602	CLA	C10-C11-C12-C13
23	c	513	CLA	C10-C11-C12-C13
26	A	410[A]	SQD	O6-C44-C45-C46
26	A	410[B]	SQD	O6-C44-C45-C46
26	B	620	SQD	C44-C45-C46-O48
26	a	411[B]	SQD	O6-C44-C45-C46
26	b	620	SQD	C44-C45-C46-O48
32	a	420[A]	LHG	C4-C5-C6-O8
32	L	101[A]	LHG	C27-C28-C29-C30
35	C	517[A]	DGD	C1B-C2B-C3B-C4B
31	t	101	LMT	C7-C8-C9-C10
26	b	620	SQD	C13-C14-C15-C16
35	c	517[A]	DGD	O1A-C1A-O1G-C1G
23	c	514	CLA	C4-C3-C5-C6
29	D	407[A]	PL9	C15-C14-C16-C17
23	C	506	CLA	C2-C3-C5-C6
29	D	407[A]	PL9	C43-C44-C46-C47
35	C	517[A]	DGD	C4D-C5D-C6D-O5D
35	C	517[A]	DGD	C7A-C8A-C9A-CAA
26	a	411[B]	SQD	C35-C36-C37-C38
32	d	413[A]	LHG	C3-O3-P-O6
32	d	413[B]	LHG	C3-O3-P-O6
26	f	102	SQD	C23-C24-C25-C26
23	B	601	CLA	O1A-CGA-O2A-C1
23	c	512	CLA	O1A-CGA-O2A-C1
31	b	627	LMT	C6-C7-C8-C9
32	b	629[B]	LHG	C9-C10-C11-C12
33	C	521	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
27	B	624	GOL	O1-C1-C2-O2
27	B	627	GOL	O1-C1-C2-O2
27	a	418	GOL	O1-C1-C2-O2
27	v	202[A]	GOL	O1-C1-C2-O2
23	b	615	CLA	C5-C6-C7-C8
26	A	412	SQD	C30-C31-C32-C33
35	C	517[A]	DGD	C3B-C4B-C5B-C6B
35	C	519	DGD	CAB-CBB-CCB-CDB
35	c	519	DGD	O1A-C1A-O1G-C1G
23	A	406[A]	CLA	C16-C17-C18-C20
23	b	606	CLA	C16-C17-C18-C19
23	b	601	CLA	CAA-CBA-CGA-O2A
26	A	412	SQD	C27-C28-C29-C30
26	a	411[A]	SQD	O6-C44-C45-O47
26	a	411[B]	SQD	O6-C44-C45-O47
33	c	521	LMG	O1-C7-C8-O7
23	C	511	CLA	CBA-CGA-O2A-C1
23	C	512	CLA	CBA-CGA-O2A-C1
35	h	102	DGD	C2B-C3B-C4B-C5B
26	a	412	SQD	C16-C17-C18-C19
35	c	517[A]	DGD	O6E-C1E-O5D-C6D
29	a	414[A]	PL9	C24-C26-C27-C28
32	A	418[A]	LHG	C1-C2-C3-O3
33	C	521	LMG	C12-C13-C14-C15
23	A	408	CLA	C2-C1-O2A-CGA
23	b	613	CLA	C2-C1-O2A-CGA
23	b	614	CLA	C2-C1-O2A-CGA
23	C	511	CLA	C14-C13-C15-C16
23	C	513	CLA	C6-C7-C8-C9
23	b	601	CLA	C6-C7-C8-C9
32	D	409[B]	LHG	C2-C3-O3-P
32	d	407[B]	LHG	C2-C3-O3-P
26	A	412	SQD	O10-C23-O48-C46
32	D	409[A]	LHG	C27-C28-C29-C30
32	b	629[A]	LHG	C34-C35-C36-C37
23	B	608	CLA	C16-C17-C18-C20
23	d	402[B]	CLA	C16-C17-C18-C20
25	H	101	BCR	C23-C24-C25-C26
25	d	404	BCR	C23-C24-C25-C26
25	d	404	BCR	C23-C24-C25-C30
25	h	101	BCR	C23-C24-C25-C26
25	h	101	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
25	K	102	BCR	C7-C8-C9-C10
32	L	101[A]	LHG	C11-C10-C9-C8
35	C	519	DGD	O6D-C5D-C6D-O5D
32	a	420[B]	LHG	C10-C11-C12-C13
33	B	621	LMG	C32-C33-C34-C35
26	A	410[A]	SQD	C18-C19-C20-C21
31	t	101	LMT	O1'-C1-C2-C3
32	a	420[A]	LHG	C7-C8-C9-C10
32	D	408[B]	LHG	C26-C27-C28-C29
33	C	501	LMG	C18-C19-C20-C21
23	C	510	CLA	O1D-CGD-O2D-CED
35	C	518[A]	DGD	C5B-C6B-C7B-C8B
32	b	629[A]	LHG	C13-C14-C15-C16
33	C	501	LMG	C11-C12-C13-C14
32	L	101[A]	LHG	O6-C4-C5-C6
33	d	411	LMG	C10-C11-C12-C13
31	M	102	LMT	C9-C10-C11-C12
35	C	518[A]	DGD	C8B-C9B-CAB-CBB
23	B	610	CLA	C12-C13-C15-C16
23	C	507	CLA	C6-C7-C8-C10
23	b	601	CLA	C6-C7-C8-C10
23	b	601	CLA	C11-C10-C8-C7
23	b	614	CLA	C12-C13-C15-C16
23	c	505	CLA	C11-C12-C13-C15
23	c	506	CLA	C11-C12-C13-C15
23	c	506	CLA	C12-C13-C15-C16
23	c	507	CLA	C11-C10-C8-C7
23	c	510	CLA	C11-C10-C8-C7
29	a	414[A]	PL9	C12-C11-C9-C8
33	B	621	LMG	O6-C5-C6-O5
32	D	408[A]	LHG	C11-C10-C9-C8
33	C	520	LMG	C30-C31-C32-C33
35	c	517[A]	DGD	CCB-CDB-CEB-CFB
33	C	521	LMG	C4-C5-C6-O5
26	a	411[A]	SQD	C27-C28-C29-C30
31	F	101	LMT	C4-C5-C6-C7
32	L	101[A]	LHG	C24-C25-C26-C27
33	z	101	LMG	C13-C14-C15-C16
32	D	409[A]	LHG	C10-C11-C12-C13
32	b	629[B]	LHG	C25-C26-C27-C28
32	d	406[A]	LHG	C13-C14-C15-C16
23	B	601	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
35	C	518[A]	DGD	C7A-C8A-C9A-CAA
35	c	518[B]	DGD	C1A-C2A-C3A-C4A
34	b	622	HTG	C1'-C2'-C3'-C4'
26	a	411[B]	SQD	C9-C10-C11-C12
31	F	101	LMT	C6-C7-C8-C9
35	c	517[B]	DGD	C4B-C5B-C6B-C7B
35	c	518[B]	DGD	C5A-C6A-C7A-C8A
31	b	621	LMT	C7-C8-C9-C10
33	Z	101	LMG	C11-C12-C13-C14
23	B	604	CLA	CAD-CBD-CGD-O2D
23	B	616	CLA	CAD-CBD-CGD-O2D
23	b	616	CLA	CAD-CBD-CGD-O2D
23	c	504	CLA	CAD-CBD-CGD-O2D
23	c	511	CLA	CAD-CBD-CGD-O2D
24	a	408[A]	PHO	CAD-CBD-CGD-O2D
39	f	101	HEM	C2B-C3B-CAB-CBB
23	B	601	CLA	C15-C16-C17-C18
23	C	513	CLA	C10-C11-C12-C13
29	d	405[A]	PL9	C45-C44-C46-C47
29	d	405[B]	PL9	C45-C44-C46-C47
26	a	411[A]	SQD	C34-C35-C36-C37
35	C	519	DGD	C8A-C9A-CAA-CBA
35	c	518[A]	DGD	O6E-C1E-O5D-C6D
35	c	518[B]	DGD	O6E-C1E-O5D-C6D
32	D	408[B]	LHG	C13-C14-C15-C16
24	A	416[A]	PHO	C2C-C3C-CAC-CBC
24	A	416[B]	PHO	C2C-C3C-CAC-CBC
26	a	412	SQD	O6-C44-C45-C46
26	f	102	SQD	O6-C44-C45-C46
23	b	613	CLA	CBD-CGD-O2D-CED
33	z	101	LMG	C20-C21-C22-C23
32	E	101[A]	LHG	O6-C4-C5-O7
32	L	101[A]	LHG	O6-C4-C5-O7
32	L	101[B]	LHG	O6-C4-C5-O7
35	c	519	DGD	O6D-C5D-C6D-O5D
32	E	101[B]	LHG	C13-C14-C15-C16
33	d	411	LMG	C18-C19-C20-C21
23	c	513	CLA	O1D-CGD-O2D-CED
23	B	601	CLA	CHA-CBD-CGD-O1D
23	B	601	CLA	CHA-CBD-CGD-O2D
23	C	503	CLA	CHA-CBD-CGD-O1D
23	b	601	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
26	b	620	SQD	C14-C15-C16-C17
23	C	511	CLA	O1A-CGA-O2A-C1
23	C	512	CLA	O1A-CGA-O2A-C1
23	C	513	CLA	O1A-CGA-O2A-C1
23	b	601	CLA	O1A-CGA-O2A-C1
32	d	406[B]	LHG	O10-C23-O8-C6
35	c	517[A]	DGD	C2E-C1E-O5D-C6D
35	c	518[A]	DGD	C2E-C1E-O5D-C6D
35	c	518[B]	DGD	C2E-C1E-O5D-C6D
32	A	418[A]	LHG	C32-C33-C34-C35
26	B	620	SQD	O47-C45-C46-O48
26	b	620	SQD	O47-C45-C46-O48
32	a	420[A]	LHG	O7-C5-C6-O8
26	A	410[A]	SQD	C34-C35-C36-C37
33	d	411	LMG	C16-C17-C18-C19
23	C	511	CLA	C13-C15-C16-C17
32	d	406[B]	LHG	C16-C17-C18-C19
35	H	102	DGD	CDB-CEB-CFB-CGB
23	A	406[B]	CLA	C16-C17-C18-C20
27	D	403	GOL	O1-C1-C2-O2
31	F	101	LMT	C2-C3-C4-C5
32	d	406[A]	LHG	C11-C10-C9-C8
32	d	407[A]	LHG	C9-C10-C11-C12
23	b	609	CLA	C4-C3-C5-C6
33	m	101	LMG	C37-C38-C39-C40
29	a	414[B]	PL9	C12-C11-C9-C8
29	a	414[B]	PL9	C4-C3-C7-C8
32	D	408[B]	LHG	C28-C29-C30-C31
23	C	513	CLA	C11-C10-C8-C9
31	A	417	LMT	O5B-C5B-C6B-O6B
33	m	101	LMG	C30-C31-C32-C33
23	C	511	CLA	C8-C10-C11-C12
26	b	620	SQD	C15-C16-C17-C18
31	e	101	LMT	C3-C4-C5-C6
32	L	101[B]	LHG	C26-C27-C28-C29
33	c	520	LMG	C32-C33-C34-C35
25	y	101	BCR	C21-C22-C23-C24
32	d	413[A]	LHG	C18-C19-C20-C21
33	c	521	LMG	C31-C32-C33-C34
23	a	406[A]	CLA	C1A-C2A-CAA-CBA
32	d	406[A]	LHG	C16-C17-C18-C19
32	L	101[B]	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
32	A	418[B]	LHG	C23-C24-C25-C26
26	a	411[A]	SQD	C35-C36-C37-C38
32	A	418[B]	LHG	C17-C18-C19-C20
32	D	409[B]	LHG	C10-C11-C12-C13
32	D	409[A]	LHG	C2-C3-O3-P
32	b	629[B]	LHG	C12-C13-C14-C15
32	b	629[B]	LHG	C13-C14-C15-C16
33	a	417	LMG	C33-C34-C35-C36
32	D	408[A]	LHG	C4-O6-P-O5
32	E	101[A]	LHG	C4-O6-P-O5
32	E	101[B]	LHG	C4-O6-P-O5
32	a	420[A]	LHG	C4-O6-P-O4
32	a	420[B]	LHG	C4-O6-P-O4
32	d	406[B]	LHG	C4-O6-P-O5
23	a	406[B]	CLA	C15-C16-C17-C18
23	b	604	CLA	C13-C15-C16-C17
32	E	101[A]	LHG	O6-C4-C5-C6
35	C	517[B]	DGD	C3B-C4B-C5B-C6B
31	c	501	LMT	C3-C4-C5-C6
26	a	411[B]	SQD	C27-C28-C29-C30
32	L	101[A]	LHG	C26-C27-C28-C29
26	X	101	SQD	C32-C33-C34-C35
35	c	518[A]	DGD	C7B-C8B-C9B-CAB
23	B	601	CLA	CAD-CBD-CGD-O1D
23	C	503	CLA	CAD-CBD-CGD-O1D
23	C	505	CLA	CAD-CBD-CGD-O1D
23	C	507	CLA	CAD-CBD-CGD-O1D
23	b	601	CLA	CAD-CBD-CGD-O1D
23	c	503	CLA	CAD-CBD-CGD-O1D
23	c	507	CLA	CAD-CBD-CGD-O1D
23	B	606	CLA	C8-C10-C11-C12
33	c	520	LMG	C30-C31-C32-C33
35	C	517[A]	DGD	C6A-C7A-C8A-C9A
23	d	403	CLA	O1A-CGA-O2A-C1
33	C	521	LMG	C38-C39-C40-C41
32	d	407[B]	LHG	C24-C23-O8-C6
23	A	406[A]	CLA	C12-C13-C15-C16
23	A	406[B]	CLA	C12-C13-C15-C16
23	B	616	CLA	C12-C13-C15-C16
23	C	503	CLA	C12-C13-C15-C16
23	C	513	CLA	C11-C10-C8-C7
23	b	608	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	b	615	CLA	C12-C13-C15-C16
23	c	510	CLA	C6-C7-C8-C10
23	d	402[A]	CLA	C11-C12-C13-C15
23	d	402[B]	CLA	C11-C12-C13-C15
26	A	410[A]	SQD	C13-C14-C15-C16
34	B	623	HTG	C4'-C5'-C6'-C7'
35	C	519	DGD	C7A-C8A-C9A-CAA
23	c	510	CLA	O1A-CGA-O2A-C1
32	d	407[B]	LHG	O10-C23-O8-C6
31	b	627	LMT	O1'-C1-C2-C3
32	D	408[A]	LHG	C34-C35-C36-C37
31	A	419	LMT	C4-C5-C6-C7
35	c	518[A]	DGD	C5A-C6A-C7A-C8A
23	b	604	CLA	C15-C16-C17-C18
23	B	601	CLA	C2A-CAA-CBA-CGA
26	X	101	SQD	C44-C45-C46-O48
31	A	417	LMT	C9-C10-C11-C12
33	B	621	LMG	C20-C21-C22-C23
32	E	101[A]	LHG	O7-C5-C6-O8
32	a	420[B]	LHG	O7-C5-C6-O8
32	d	407[A]	LHG	C32-C33-C34-C35
35	C	518[A]	DGD	C8A-C9A-CAA-CBA
35	C	518[A]	DGD	C5D-C6D-O5D-C1E
35	C	518[B]	DGD	C2G-C3G-O3G-C1D
35	H	102	DGD	O2G-C1B-C2B-C3B
23	d	402[B]	CLA	C16-C17-C18-C19
33	d	411	LMG	C36-C37-C38-C39
32	d	407[A]	LHG	C2-C3-O3-P
33	a	417	LMG	C36-C37-C38-C39
29	D	407[B]	PL9	C20-C19-C21-C22
23	d	403	CLA	CBA-CGA-O2A-C1
32	d	413[A]	LHG	C34-C35-C36-C37
23	B	614	CLA	C14-C13-C15-C16
23	a	406[B]	CLA	C11-C12-C13-C14
23	b	610	CLA	C11-C12-C13-C14
23	b	614	CLA	C11-C12-C13-C14
23	c	506	CLA	C14-C13-C15-C16
23	c	507	CLA	C11-C10-C8-C9
23	c	511	CLA	C11-C10-C8-C9
26	b	620	SQD	C16-C17-C18-C19
23	b	607	CLA	C3-C5-C6-C7
32	D	408[A]	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
35	C	519	DGD	O1A-C1A-O1G-C1G
23	C	507	CLA	C15-C16-C17-C18
35	C	518[A]	DGD	C7B-C8B-C9B-CAB
32	d	413[A]	LHG	C11-C12-C13-C14
33	B	621	LMG	C29-C30-C31-C32
23	b	608	CLA	C16-C17-C18-C20
26	b	620	SQD	C28-C29-C30-C31
31	c	501	LMT	C7-C8-C9-C10
35	C	519	DGD	CBA-CCA-CDA-CEA
33	B	621	LMG	C14-C15-C16-C17
26	A	412	SQD	C31-C32-C33-C34
32	D	408[B]	LHG	C11-C10-C9-C8
32	d	407[B]	LHG	C34-C35-C36-C37
29	a	414[A]	PL9	C43-C44-C46-C47
29	a	414[B]	PL9	C43-C44-C46-C47
23	b	616	CLA	C5-C6-C7-C8
32	L	101[A]	LHG	C23-C24-C25-C26
32	D	408[A]	LHG	C13-C14-C15-C16
26	a	411[B]	SQD	C34-C35-C36-C37
32	b	629[A]	LHG	C28-C29-C30-C31
32	b	629[B]	LHG	C34-C35-C36-C37
33	c	521	LMG	C39-C40-C41-C42
34	b	623	HTG	C4'-C5'-C6'-C7'
23	A	404[B]	CLA	C2A-CAA-CBA-CGA
23	c	508	CLA	C2A-CAA-CBA-CGA
23	B	613	CLA	C2-C1-O2A-CGA
23	a	405[B]	CLA	C2-C1-O2A-CGA
23	b	608	CLA	C2-C1-O2A-CGA
23	c	508	CLA	C2-C1-O2A-CGA
23	B	608	CLA	C16-C17-C18-C19
35	C	518[B]	DGD	C1A-C2A-C3A-C4A
23	c	508	CLA	C8-C10-C11-C12
35	C	519	DGD	CAA-CBA-CCA-CDA
35	H	102	DGD	CCA-CDA-CEA-CFA
32	D	408[B]	LHG	C34-C35-C36-C37
32	D	409[B]	LHG	C27-C28-C29-C30
29	D	407[B]	PL9	C45-C44-C46-C47
25	H	101	BCR	C23-C24-C25-C30
25	y	101	BCR	C23-C24-C25-C26
25	y	101	BCR	C23-C24-C25-C30
29	A	414[A]	PL9	C28-C29-C31-C32
32	A	418[B]	LHG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
32	d	413[B]	LHG	C27-C28-C29-C30
32	d	407[A]	LHG	C10-C11-C12-C13
23	c	510	CLA	CBA-CGA-O2A-C1
33	B	621	LMG	O8-C28-C29-C30
34	B	625	HTG	C4'-C5'-C6'-C7'
31	B	631	LMT	C2-C3-C4-C5
23	C	507	CLA	C16-C17-C18-C20
33	m	101	LMG	O6-C1-O1-C7
23	B	610	CLA	C13-C15-C16-C17
35	C	517[B]	DGD	C2E-C1E-O5D-C6D
26	f	102	SQD	O47-C45-C46-O48
32	E	101[B]	LHG	O7-C5-C6-O8
32	a	420[B]	LHG	C24-C25-C26-C27
23	b	613	CLA	O1D-CGD-O2D-CED
35	C	519	DGD	C8B-C9B-CAB-CBB
23	D	405	CLA	C8-C10-C11-C12
26	A	410[A]	SQD	C16-C17-C18-C19
35	C	518[B]	DGD	C8A-C9A-CAA-CBA
33	c	521	LMG	O1-C7-C8-C9
33	C	520	LMG	C36-C37-C38-C39
35	c	517[B]	DGD	CCB-CDB-CEB-CFB
34	b	625	HTG	C4-C5-C6-O6
23	B	613	CLA	C11-C12-C13-C15
23	B	614	CLA	C11-C10-C8-C7
23	C	507	CLA	C2-C3-C5-C6
23	C	510	CLA	C6-C7-C8-C10
23	a	406[B]	CLA	C11-C12-C13-C15
23	c	503	CLA	C11-C12-C13-C15
23	c	509	CLA	C12-C13-C15-C16
29	D	407[B]	PL9	C18-C19-C21-C22
23	a	406[A]	CLA	C4C-C3C-CAC-CBC
32	b	629[B]	LHG	C10-C11-C12-C13
23	A	406[A]	CLA	C14-C13-C15-C16
23	a	409	CLA	C11-C10-C8-C9
23	b	615	CLA	C14-C13-C15-C16
23	c	510	CLA	C6-C7-C8-C9
23	d	402[A]	CLA	C11-C12-C13-C14
32	D	408[A]	LHG	C28-C29-C30-C31
26	a	412	SQD	C26-C27-C28-C29
31	e	101	LMT	O1'-C1-C2-C3
31	e	101	LMT	C4B-C5B-C6B-O6B
35	C	519	DGD	C7B-C8B-C9B-CAB

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Mol	Chain	Res	Type	Atoms
35	H	102	DGD	C8A-C9A-CAA-CBA
32	L	101[B]	LHG	C11-C10-C9-C8
32	b	629[B]	LHG	C17-C18-C19-C20
32	d	413[B]	LHG	C17-C18-C19-C20
35	C	519	DGD	C6A-C7A-C8A-C9A
23	c	504	CLA	C8-C10-C11-C12
23	B	612	CLA	CBA-CGA-O2A-C1
27	l	102[B]	GOL	O1-C1-C2-C3
32	A	418[A]	LHG	O1-C1-C2-C3
35	C	519	DGD	C9A-CAA-CBA-CCA
23	a	406[A]	CLA	C15-C16-C17-C18
23	b	610	CLA	C13-C15-C16-C17
32	a	420[B]	LHG	C7-C8-C9-C10
27	A	411	GOL	O1-C1-C2-O2
29	D	407[B]	PL9	C28-C29-C31-C32
23	b	616	CLA	CBA-CGA-O2A-C1
31	M	101	LMT	C2-C3-C4-C5
23	c	512	CLA	C3-C5-C6-C7
26	a	411[A]	SQD	C11-C12-C13-C14
23	D	405	CLA	O1A-CGA-O2A-C1
23	b	616	CLA	O1A-CGA-O2A-C1
32	D	409[A]	LHG	O10-C23-O8-C6
32	D	409[A]	LHG	C24-C23-O8-C6
35	C	519	DGD	C2A-C1A-O1G-C1G
35	C	517[B]	DGD	O6E-C1E-O5D-C6D
23	a	406[B]	CLA	C4C-C3C-CAC-CBC
32	A	418[B]	LHG	C31-C32-C33-C34
23	B	612	CLA	O1A-CGA-O2A-C1
23	B	601	CLA	CAA-CBA-CGA-O2A
39	f	101	HEM	C4B-C3B-CAB-CBB
24	a	408[A]	PHO	C4-C3-C5-C6
32	D	409[B]	LHG	C28-C29-C30-C31
24	a	408[A]	PHO	C2-C3-C5-C6
23	C	507	CLA	C2-C1-O2A-CGA
35	C	517[B]	DGD	C2A-C3A-C4A-C5A
33	B	621	LMG	C18-C19-C20-C21
33	C	521	LMG	C20-C21-C22-C23
33	m	101	LMG	C32-C33-C34-C35
35	c	517[A]	DGD	C4B-C5B-C6B-C7B
33	c	520	LMG	C28-C29-C30-C31
35	h	102	DGD	O2G-C1B-C2B-C3B
32	d	406[A]	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
35	C	518[B]	DGD	C7A-C8A-C9A-CAA
32	D	408[A]	LHG	C17-C18-C19-C20
23	c	511	CLA	C4-C3-C5-C6
35	c	517[B]	DGD	CBA-CCA-CDA-CEA
23	C	503	CLA	C3-C5-C6-C7
29	a	414[A]	PL9	C4-C3-C7-C8
35	C	518[B]	DGD	C8B-C9B-CAB-CBB
23	A	406[B]	CLA	C14-C13-C15-C16
23	A	408	CLA	C11-C12-C13-C14
23	B	614	CLA	C6-C7-C8-C9
23	a	407[A]	CLA	C14-C13-C15-C16
23	d	402[B]	CLA	C11-C12-C13-C14
24	a	408[B]	PHO	C14-C13-C15-C16
23	a	409	CLA	C15-C16-C17-C18
26	A	410[B]	SQD	C34-C35-C36-C37
26	f	102	SQD	C11-C10-C9-C8
32	b	629[A]	LHG	C10-C11-C12-C13
32	d	413[A]	LHG	C1-C2-C3-O3
33	a	417	LMG	C7-C8-C9-O8
39	F	102	HEM	CAD-CBD-CGD-O1D
26	a	411[A]	SQD	C10-C11-C12-C13
32	E	101[A]	LHG	C12-C13-C14-C15
32	A	418[B]	LHG	C33-C34-C35-C36
24	A	407[A]	PHO	O2A-C1-C2-C3
24	a	408[A]	PHO	O2A-C1-C2-C3
24	a	408[B]	PHO	O2A-C1-C2-C3
23	D	405	CLA	CBA-CGA-O2A-C1
35	c	517[A]	DGD	CBA-CCA-CDA-CEA
39	f	101	HEM	CAD-CBD-CGD-O1D
23	B	614	CLA	C4-C3-C5-C6
29	a	414[A]	PL9	C45-C44-C46-C47
29	a	414[B]	PL9	C45-C44-C46-C47
23	B	604	CLA	C1A-C2A-CAA-CBA
23	C	514	CLA	C1A-C2A-CAA-CBA
23	a	407[A]	CLA	C1A-C2A-CAA-CBA
26	b	620	SQD	C33-C34-C35-C36
35	C	519	DGD	CDA-CEA-CFA-CGA
23	B	602	CLA	C6-C7-C8-C10
23	B	613	CLA	C12-C13-C15-C16
23	b	601	CLA	C11-C12-C13-C15
23	b	615	CLA	C11-C12-C13-C15
23	c	511	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
32	A	418[A]	LHG	C29-C30-C31-C32
32	L	101[A]	LHG	C10-C11-C12-C13
23	c	511	CLA	O1A-CGA-O2A-C1
23	C	508	CLA	C2A-CAA-CBA-CGA
27	c	527	GOL	O1-C1-C2-O2
33	z	101	LMG	O7-C10-C11-C12
32	D	408[B]	LHG	O6-C4-C5-C6
32	d	406[B]	LHG	O6-C4-C5-C6
33	d	411	LMG	C19-C20-C21-C22
23	b	608	CLA	C16-C17-C18-C19
23	c	513	CLA	C13-C15-C16-C17
32	b	629[B]	LHG	C28-C29-C30-C31
23	b	601	CLA	C4-C3-C5-C6
23	b	616	CLA	C4-C3-C5-C6
26	A	410[B]	SQD	C16-C17-C18-C19
31	m	103	LMT	C7-C8-C9-C10
32	d	413[B]	LHG	C23-C24-C25-C26
29	d	405[B]	PL9	C43-C44-C46-C47
31	A	417	LMT	C2B-C1B-O1B-C4'
35	C	519	DGD	C2A-C3A-C4A-C5A
23	b	608	CLA	C13-C15-C16-C17
23	b	610	CLA	C16-C17-C18-C19
23	B	611	CLA	C8-C10-C11-C12
35	H	102	DGD	O1G-C1G-C2G-O2G
32	a	420[A]	LHG	C24-C25-C26-C27
32	d	413[A]	LHG	C27-C28-C29-C30
35	H	102	DGD	C4E-C5E-C6E-O5E
23	A	406[A]	CLA	C16-C17-C18-C19
32	d	413[A]	LHG	C17-C18-C19-C20
32	d	406[A]	LHG	C25-C26-C27-C28
23	c	507	CLA	C13-C15-C16-C17
23	a	405[A]	CLA	C2-C1-O2A-CGA
23	c	514	CLA	C2-C1-O2A-CGA
23	c	511	CLA	C2-C3-C5-C6
29	D	407[B]	PL9	C43-C44-C46-C47
29	d	405[A]	PL9	C43-C44-C46-C47
23	B	616	CLA	C6-C7-C8-C9
23	c	503	CLA	C11-C12-C13-C14
33	C	520	LMG	C29-C30-C31-C32
23	C	502	CLA	C2A-CAA-CBA-CGA
25	B	617	BCR	C1-C6-C7-C8
25	a	410	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
25	b	619	BCR	C1-C6-C7-C8
25	b	619	BCR	C5-C6-C7-C8
25	c	515	BCR	C23-C24-C25-C30
23	c	510	CLA	C15-C16-C17-C18
27	B	627	GOL	O1-C1-C2-C3
27	D	403	GOL	O1-C1-C2-C3
27	a	419	GOL	C1-C2-C3-O3
23	A	405[B]	CLA	C2C-C3C-CAC-CBC
25	t	102	BCR	C13-C14-C15-C16
31	e	101	LMT	C2B-C1B-O1B-C4'
32	d	413[A]	LHG	C9-C10-C11-C12
29	A	414[A]	PL9	C43-C44-C46-C47
39	F	102	HEM	CAD-CBD-CGD-O2D
35	c	518[B]	DGD	C2G-C3G-O3G-C1D
32	A	418[A]	LHG	C17-C18-C19-C20
32	d	413[B]	LHG	C18-C19-C20-C21
35	C	519	DGD	C4A-C5A-C6A-C7A
41	V	201	HEC	CAD-CBD-CGD-O2D
41	v	201	HEC	CAD-CBD-CGD-O2D
33	a	417	LMG	O8-C28-C29-C30
23	A	404[B]	CLA	C16-C17-C18-C19
35	c	517[A]	DGD	CDB-CEB-CFB-CGB
32	E	101[B]	LHG	O6-C4-C5-O7
41	v	201	HEC	CAD-CBD-CGD-O1D
23	A	408	CLA	C16-C17-C18-C19
23	C	503	CLA	C16-C17-C18-C19
31	B	630	LMT	C7-C8-C9-C10
35	c	518[A]	DGD	C1A-C2A-C3A-C4A
29	D	407[A]	PL9	C35-C34-C36-C37
23	B	615	CLA	C12-C13-C15-C16
23	b	602	CLA	C8-C10-C11-C12
27	a	419	GOL	O2-C2-C3-O3
27	d	412	GOL	O1-C1-C2-O2
27	d	412	GOL	O2-C2-C3-O3
23	C	512	CLA	C8-C10-C11-C12
32	b	629[A]	LHG	C25-C26-C27-C28
23	b	605	CLA	C3-C5-C6-C7
32	A	418[A]	LHG	O8-C23-C24-C25
32	b	629[B]	LHG	O7-C7-C8-C9
33	Z	101	LMG	O7-C10-C11-C12
31	e	101	LMT	C2-C3-C4-C5
35	c	518[B]	DGD	C7B-C8B-C9B-CAB

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Mol	Chain	Res	Type	Atoms
32	E	101[B]	LHG	C11-C10-C9-C8
39	f	101	HEM	CAD-CBD-CGD-O2D
41	V	201	HEC	CAD-CBD-CGD-O1D
24	a	416[B]	PHO	C4C-C3C-CAC-CBC
34	c	522	HTG	C2'-C1'-S1-C1
23	c	505	CLA	C4-C3-C5-C6
29	A	414[A]	PL9	C25-C24-C26-C27
35	c	517[B]	DGD	C2A-C3A-C4A-C5A
23	b	601	CLA	C2-C3-C5-C6
23	b	616	CLA	C2-C3-C5-C6
23	c	514	CLA	C2-C3-C5-C6
23	C	511	CLA	CAA-CBA-CGA-O2A
23	c	511	CLA	CAA-CBA-CGA-O2A
23	B	605	CLA	C6-C7-C8-C9
23	B	615	CLA	C14-C13-C15-C16
23	B	616	CLA	C14-C13-C15-C16
23	C	506	CLA	C14-C13-C15-C16
23	a	407[A]	CLA	C6-C7-C8-C9
23	b	603	CLA	C11-C10-C8-C9
23	b	608	CLA	C14-C13-C15-C16
23	c	512	CLA	C11-C10-C8-C9
33	c	520	LMG	C29-C30-C31-C32
23	B	613	CLA	C15-C16-C17-C18
34	d	410	HTG	S1-C1'-C2'-C3'
23	c	507	CLA	C3A-C2A-CAA-CBA
26	a	412	SQD	O10-C23-O48-C46
32	a	420[A]	LHG	O8-C23-C24-C25
23	B	610	CLA	CAD-CBD-CGD-O2D
23	C	506	CLA	CAD-CBD-CGD-O2D
23	C	513	CLA	CAD-CBD-CGD-O2D
23	b	603	CLA	CAD-CBD-CGD-O2D
23	b	604	CLA	CAD-CBD-CGD-O2D
23	b	610	CLA	CAD-CBD-CGD-O2D
23	c	513	CLA	CAD-CBD-CGD-O2D
24	A	407[A]	PHO	CAD-CBD-CGD-O2D
24	A	407[B]	PHO	CAD-CBD-CGD-O2D
24	a	408[B]	PHO	CAD-CBD-CGD-O2D
23	b	610	CLA	C16-C17-C18-C20
32	b	629[B]	LHG	C32-C33-C34-C35
31	B	631	LMT	C1-C2-C3-C4
23	B	602	CLA	C8-C10-C11-C12
32	L	101[A]	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	B	613	CLA	CAA-CBA-CGA-O2A
32	L	101[A]	LHG	O7-C7-C8-C9
32	a	420[B]	LHG	O8-C23-C24-C25
34	b	623	HTG	S1-C1'-C2'-C3'
39	f	101	HEM	CAA-CBA-CGA-O2A
26	A	412	SQD	O48-C23-C24-C25
32	b	629[A]	LHG	O7-C7-C8-C9
31	m	103	LMT	C9-C10-C11-C12
25	b	619	BCR	C21-C22-C23-C24
25	d	404	BCR	C7-C8-C9-C10
24	a	408[A]	PHO	C2C-C3C-CAC-CBC
24	a	416[A]	PHO	C2C-C3C-CAC-CBC
24	a	416[B]	PHO	C2C-C3C-CAC-CBC
26	B	620	SQD	C12-C13-C14-C15
23	B	602	CLA	O2A-C1-C2-C3
23	b	613	CLA	O2A-C1-C2-C3
24	A	407[B]	PHO	O2A-C1-C2-C3
31	M	102	LMT	C3-C4-C5-C6
32	A	418[B]	LHG	C32-C33-C34-C35
26	a	412	SQD	C24-C23-O48-C46
23	a	405[B]	CLA	C2A-CAA-CBA-CGA
32	L	101[B]	LHG	O7-C7-C8-C9
23	a	405[A]	CLA	C2C-C3C-CAC-CBC
23	A	404[A]	CLA	C2C-C3C-CAC-CBC
23	b	601	CLA	CAA-CBA-CGA-O1A
23	A	405[A]	CLA	CHA-CBD-CGD-O1D
23	A	405[A]	CLA	CHA-CBD-CGD-O2D
23	A	405[B]	CLA	CHA-CBD-CGD-O1D
23	A	405[B]	CLA	CHA-CBD-CGD-O2D
23	B	606	CLA	CHA-CBD-CGD-O1D
23	B	606	CLA	CHA-CBD-CGD-O2D
23	B	607	CLA	CHA-CBD-CGD-O1D
23	C	503	CLA	CHA-CBD-CGD-O2D
23	C	505	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O2D
23	a	406[A]	CLA	CHA-CBD-CGD-O1D
23	a	406[A]	CLA	CHA-CBD-CGD-O2D
23	a	406[B]	CLA	CHA-CBD-CGD-O1D
23	a	406[B]	CLA	CHA-CBD-CGD-O2D
23	b	601	CLA	CHA-CBD-CGD-O2D
23	b	606	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	b	606	CLA	CHA-CBD-CGD-O2D
23	c	503	CLA	CHA-CBD-CGD-O1D
23	c	508	CLA	CHA-CBD-CGD-O1D
23	c	508	CLA	CHA-CBD-CGD-O2D
32	A	418[B]	LHG	O8-C23-C24-C25
32	E	101[B]	LHG	O7-C7-C8-C9
33	D	413	LMG	O7-C10-C11-C12
23	B	601	CLA	C3-C5-C6-C7
34	c	522	HTG	C4'-C5'-C6'-C7'
23	c	511	CLA	O1D-CGD-O2D-CED
23	B	612	CLA	CAA-CBA-CGA-O2A
24	A	407[A]	PHO	CHA-CBD-CGD-O2D
24	a	408[A]	PHO	CHA-CBD-CGD-O1D
24	a	408[B]	PHO	CHA-CBD-CGD-O2D
32	A	418[A]	LHG	O1-C1-C2-O2
23	c	511	CLA	CBA-CGA-O2A-C1
26	a	412	SQD	C18-C19-C20-C21
23	b	601	CLA	C3-C5-C6-C7
23	b	613	CLA	CAA-CBA-CGA-O2A
29	D	407[B]	PL9	C35-C34-C36-C37
23	C	506	CLA	C12-C13-C15-C16
23	a	406[A]	CLA	C11-C12-C13-C15
23	b	604	CLA	C11-C12-C13-C15
23	b	608	CLA	C6-C7-C8-C10
23	c	514	CLA	C12-C13-C15-C16
29	A	414[A]	PL9	C4-C3-C7-C8
29	A	414[B]	PL9	C4-C3-C7-C8
35	c	518[B]	DGD	C9B-CAB-CBB-CCB
35	h	102	DGD	C6A-C7A-C8A-C9A
23	b	607	CLA	C8-C10-C11-C12
23	C	513	CLA	CAA-CBA-CGA-O2A
33	c	520	LMG	O7-C10-C11-C12
35	C	519	DGD	O1G-C1A-C2A-C3A
32	d	413[A]	LHG	C30-C31-C32-C33
35	C	517[B]	DGD	C6A-C7A-C8A-C9A
23	A	408	CLA	C14-C13-C15-C16
23	B	612	CLA	C11-C10-C8-C9
23	C	511	CLA	C11-C12-C13-C14
23	a	407[B]	CLA	C6-C7-C8-C9
23	b	601	CLA	C11-C12-C13-C14
23	b	614	CLA	C14-C13-C15-C16
23	c	514	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
29	d	405[A]	PL9	C34-C36-C37-C38
39	f	101	HEM	CAA-CBA-CGA-O1A
34	C	522	HTG	S1-C1'-C2'-C3'
33	z	101	LMG	C10-C11-C12-C13
23	a	405[A]	CLA	C4C-C3C-CAC-CBC
33	Z	101	LMG	O9-C10-C11-C12
31	A	419	LMT	C7-C8-C9-C10
26	B	620	SQD	C24-C25-C26-C27
25	c	516	BCR	C7-C8-C9-C34
23	C	507	CLA	C16-C17-C18-C19
27	V	203[B]	GOL	O1-C1-C2-C3
27	l	102[B]	GOL	C1-C2-C3-O3
32	A	418[B]	LHG	O1-C1-C2-C3
33	c	520	LMG	C39-C40-C41-C42
35	h	102	DGD	C3B-C4B-C5B-C6B
35	C	518[B]	DGD	C5B-C6B-C7B-C8B
32	b	629[A]	LHG	O9-C7-C8-C9
23	A	404[A]	CLA	C4C-C3C-CAC-CBC
23	c	511	CLA	CAA-CBA-CGA-O1A
32	A	418[A]	LHG	O10-C23-C24-C25
32	L	101[A]	LHG	O9-C7-C8-C9
32	a	420[A]	LHG	O10-C23-C24-C25
35	C	517[A]	DGD	C3A-C4A-C5A-C6A
35	h	102	DGD	O1G-C1G-C2G-C3G
32	E	101[A]	LHG	O7-C7-C8-C9
26	f	102	SQD	C26-C27-C28-C29
31	A	417	LMT	O5B-C1B-O1B-C4'
23	c	505	CLA	C5-C6-C7-C8
33	C	521	LMG	C11-C12-C13-C14
29	d	405[B]	PL9	C30-C29-C31-C32
31	b	621	LMT	C5'-C4'-O1B-C1B
23	C	511	CLA	CAA-CBA-CGA-O1A
32	A	418[B]	LHG	O10-C23-C24-C25
32	a	420[B]	LHG	O10-C23-C24-C25
32	b	629[B]	LHG	O9-C7-C8-C9
32	d	406[B]	LHG	C11-C12-C13-C14
35	h	102	DGD	CCB-CDB-CEB-CFB
32	d	406[A]	LHG	C4-O6-P-O5
23	C	503	CLA	C16-C17-C18-C20
33	m	101	LMG	C11-C12-C13-C14
23	B	613	CLA	CAA-CBA-CGA-O1A
23	C	513	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
26	A	412	SQD	O10-C23-C24-C25
35	C	519	DGD	O1A-C1A-C2A-C3A
32	A	418[B]	LHG	C30-C31-C32-C33
25	a	410	BCR	C23-C24-C25-C26
23	b	610	CLA	C5-C6-C7-C8
23	b	613	CLA	C5-C6-C7-C8
23	c	510	CLA	C13-C15-C16-C17
32	E	101[B]	LHG	O9-C7-C8-C9
32	L	101[B]	LHG	O9-C7-C8-C9
33	c	520	LMG	O9-C10-C11-C12
32	d	407[A]	LHG	O10-C23-O8-C6
33	a	417	LMG	C14-C15-C16-C17
35	c	519	DGD	C2A-C3A-C4A-C5A
23	c	502	CLA	CAA-CBA-CGA-O2A
32	A	418[A]	LHG	C18-C19-C20-C21
29	d	405[A]	PL9	C15-C14-C16-C17
32	d	407[A]	LHG	C30-C31-C32-C33
29	d	405[A]	PL9	C11-C12-C13-C14
35	c	518[A]	DGD	CDA-CEA-CFA-CGA
23	B	603	CLA	CAD-CBD-CGD-O1D
23	B	605	CLA	CAD-CBD-CGD-O1D
23	B	607	CLA	CAD-CBD-CGD-O1D
23	B	609	CLA	CAD-CBD-CGD-O1D
23	b	605	CLA	CAD-CBD-CGD-O1D
23	b	606	CLA	CAD-CBD-CGD-O1D
23	b	609	CLA	CAD-CBD-CGD-O1D
23	c	505	CLA	CAD-CBD-CGD-O1D
26	f	102	SQD	O5-C5-C6-S
31	A	417	LMT	C7-C8-C9-C10
33	C	521	LMG	C33-C34-C35-C36
32	E	101[A]	LHG	O8-C23-C24-C25
35	C	518[A]	DGD	O2G-C1B-C2B-C3B
23	B	601	CLA	C8-C10-C11-C12
23	b	612	CLA	C10-C11-C12-C13
23	C	508	CLA	C11-C12-C13-C14
23	a	406[A]	CLA	C11-C12-C13-C14
23	b	604	CLA	C11-C12-C13-C14
32	A	418[A]	LHG	C30-C31-C32-C33
32	D	409[A]	LHG	C28-C29-C30-C31
32	D	409[B]	LHG	O8-C23-C24-C25
32	E	101[B]	LHG	O8-C23-C24-C25
33	c	521	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
23	B	615	CLA	C8-C10-C11-C12
23	c	510	CLA	C8-C10-C11-C12
35	C	517[A]	DGD	CBA-CCA-CDA-CEA
33	D	413	LMG	O9-C10-C11-C12
32	L	101[A]	LHG	C32-C33-C34-C35
23	B	602	CLA	C2A-CAA-CBA-CGA
23	c	506	CLA	CAA-CBA-CGA-O2A
32	D	409[A]	LHG	O8-C23-C24-C25
35	C	518[B]	DGD	O2G-C1B-C2B-C3B
23	C	513	CLA	C4-C3-C5-C6
23	B	612	CLA	C11-C10-C8-C7
23	B	614	CLA	C2-C3-C5-C6
23	B	616	CLA	C11-C12-C13-C15
23	C	507	CLA	C12-C13-C15-C16
23	C	508	CLA	C11-C12-C13-C15
23	a	407[A]	CLA	C6-C7-C8-C10
23	a	407[B]	CLA	C6-C7-C8-C10
23	b	614	CLA	C11-C12-C13-C15
32	E	101[A]	LHG	O9-C7-C8-C9
32	E	101[A]	LHG	O10-C23-C24-C25
32	E	101[B]	LHG	O10-C23-C24-C25
26	a	412	SQD	O48-C23-C24-C25
35	c	517[A]	DGD	O2G-C1B-C2B-C3B
23	b	615	CLA	C13-C15-C16-C17
23	b	610	CLA	C3-C5-C6-C7
33	c	520	LMG	C36-C37-C38-C39
23	B	612	CLA	CAA-CBA-CGA-O1A
23	c	502	CLA	CAA-CBA-CGA-O1A
32	D	409[A]	LHG	O10-C23-C24-C25
32	D	409[B]	LHG	O10-C23-C24-C25
35	C	518[B]	DGD	O1B-C1B-C2B-C3B
35	c	517[A]	DGD	O1B-C1B-C2B-C3B
23	c	513	CLA	CAA-CBA-CGA-O2A
26	a	411[B]	SQD	O47-C7-C8-C9
33	C	520	LMG	O7-C10-C11-C12
33	Z	101	LMG	O6-C1-O1-C7
26	a	412	SQD	C15-C16-C17-C18
26	a	412	SQD	O10-C23-C24-C25
35	C	518[A]	DGD	O1B-C1B-C2B-C3B
23	A	404[B]	CLA	C15-C16-C17-C18
23	C	509	CLA	C13-C15-C16-C17
32	d	413[A]	LHG	C31-C32-C33-C34

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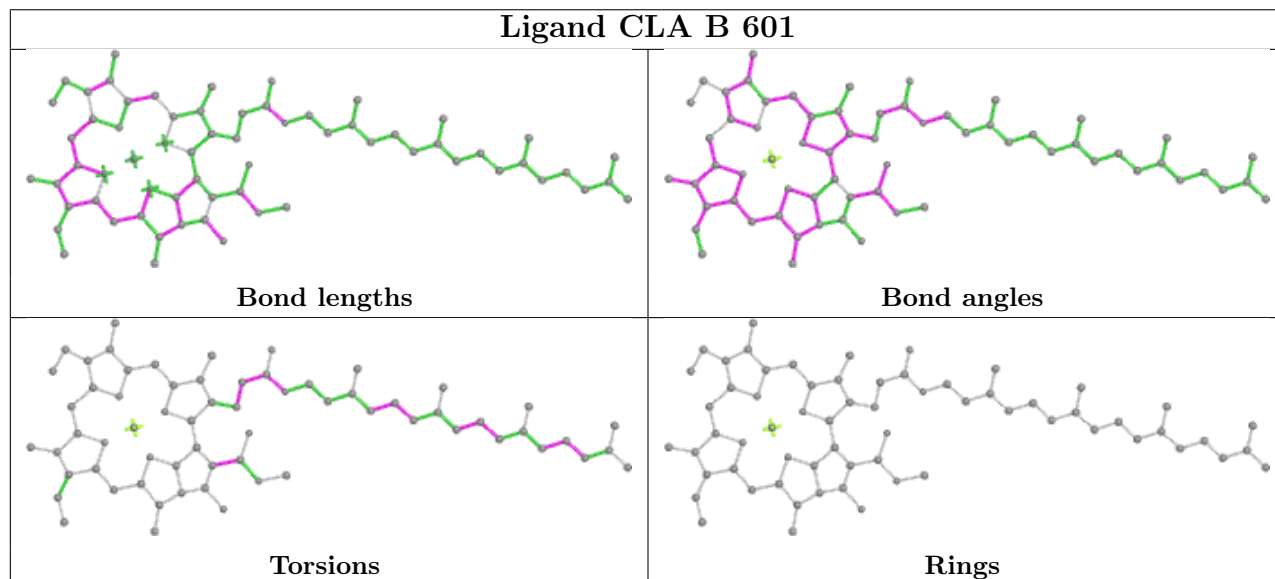
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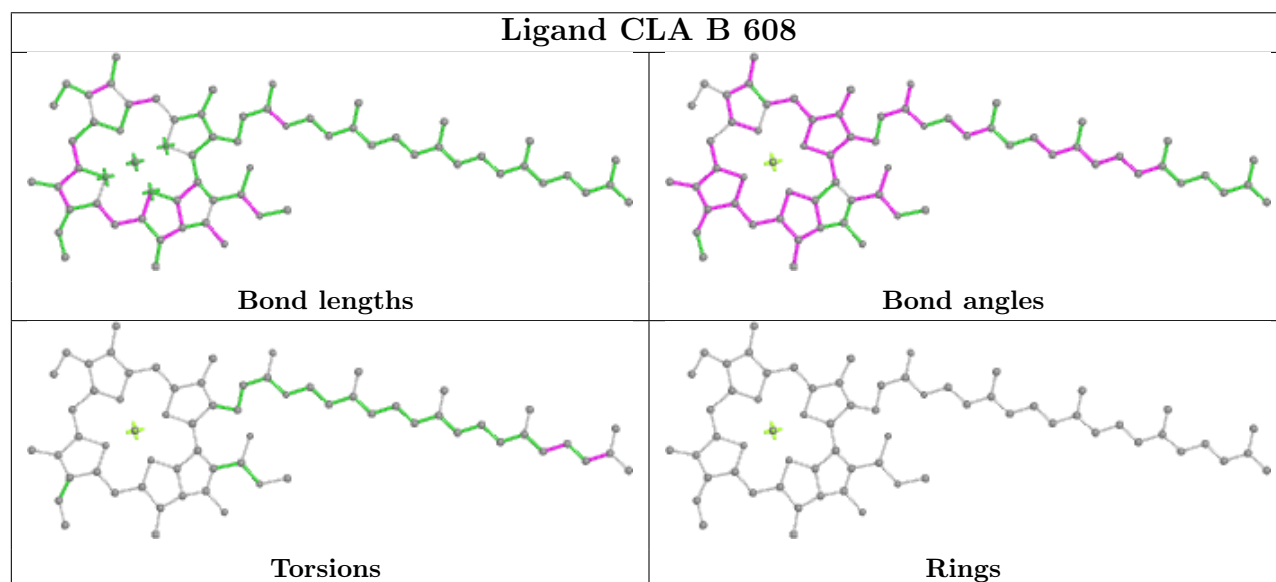
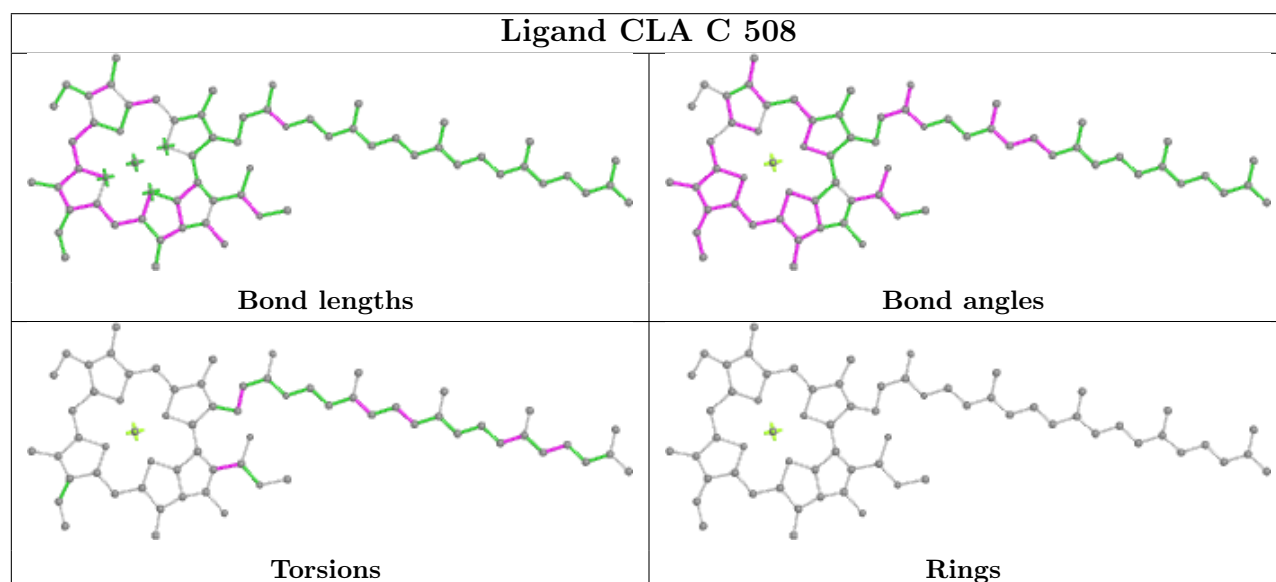
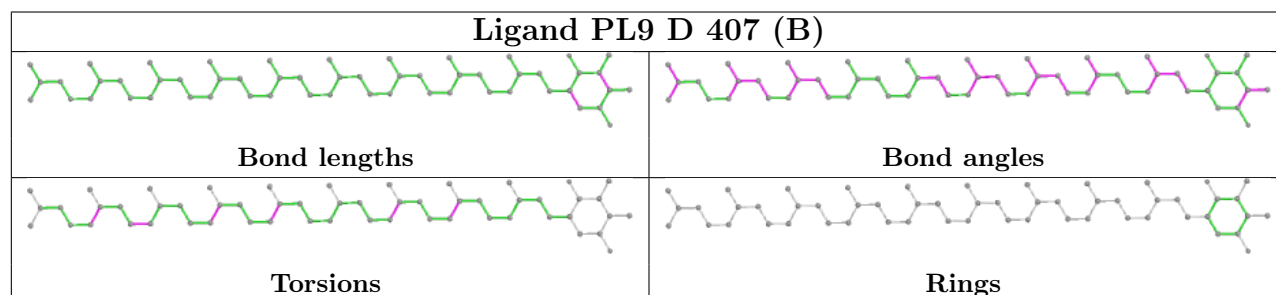
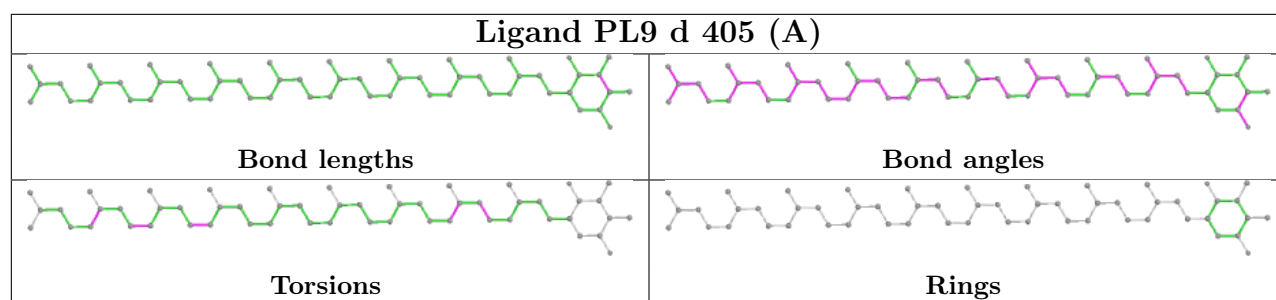
Mol	Chain	Res	Type	Atoms
33	Z	101	LMG	C19-C20-C21-C22
32	d	407[B]	LHG	O8-C23-C24-C25
23	b	613	CLA	CAA-CBA-CGA-O1A
23	C	504	CLA	C2A-CAA-CBA-CGA
23	b	602	CLA	C2A-CAA-CBA-CGA
32	E	101[A]	LHG	C11-C10-C9-C8
32	d	407[A]	LHG	O8-C23-C24-C25

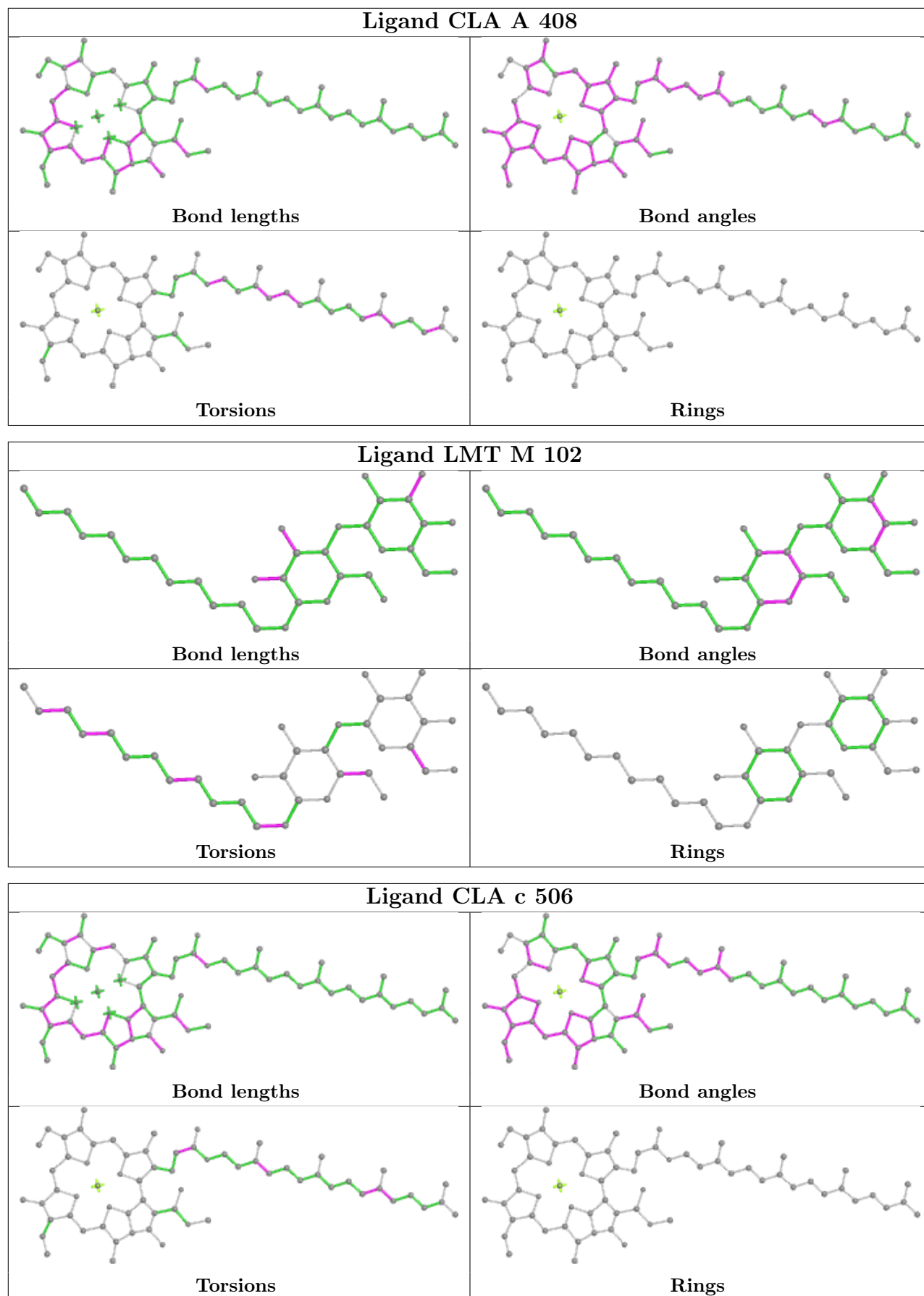
There are no ring outliers.

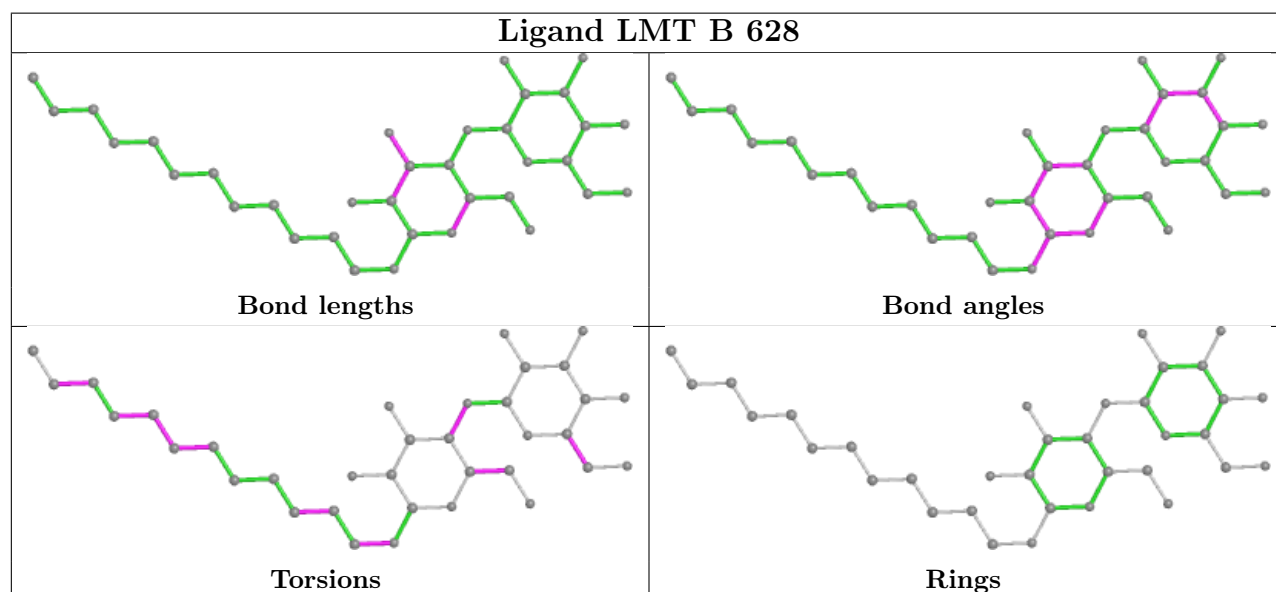
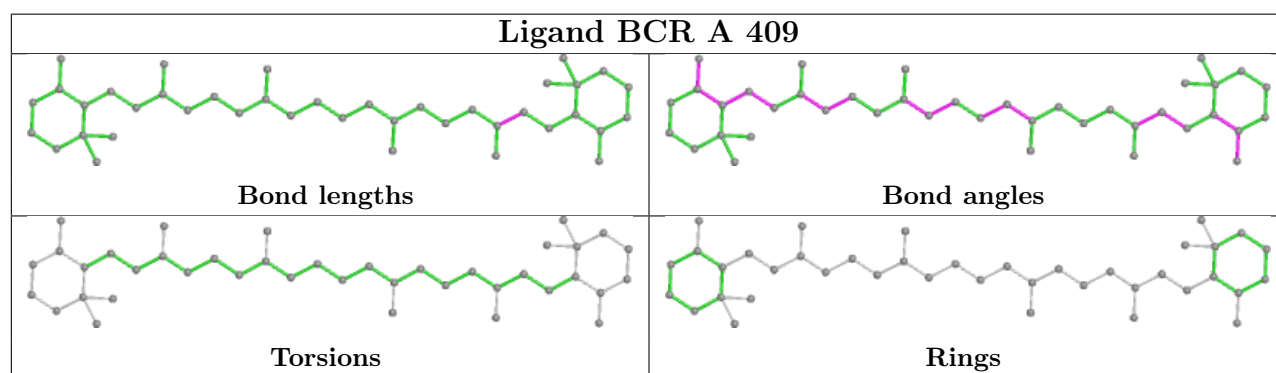
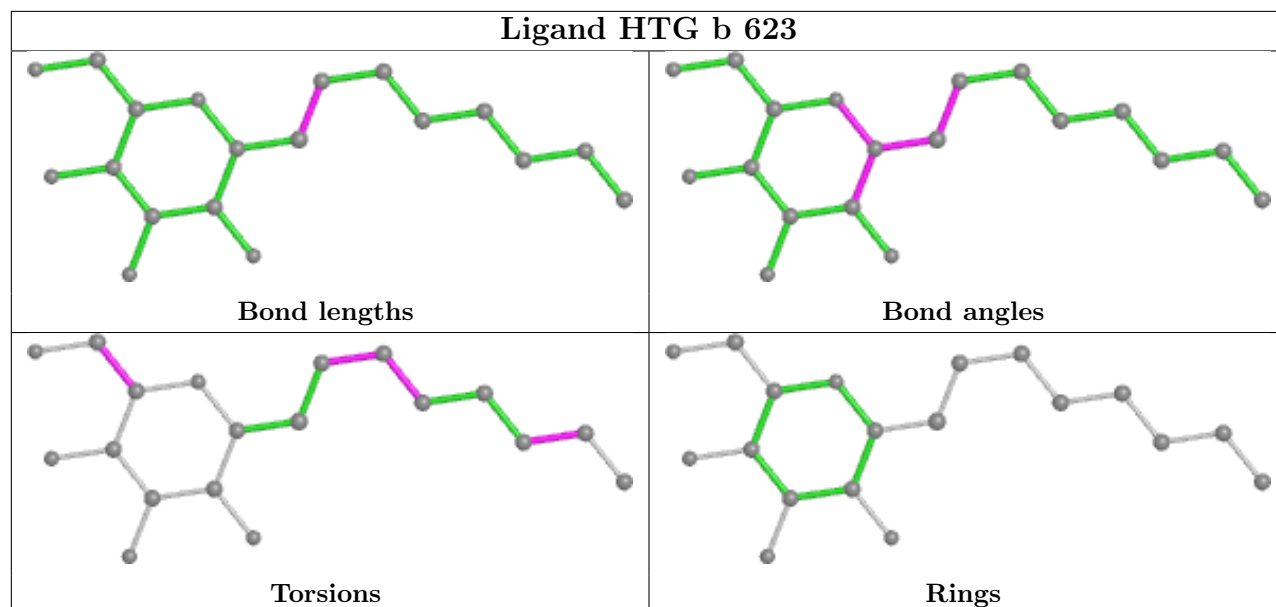
No monomer is involved in short contacts.

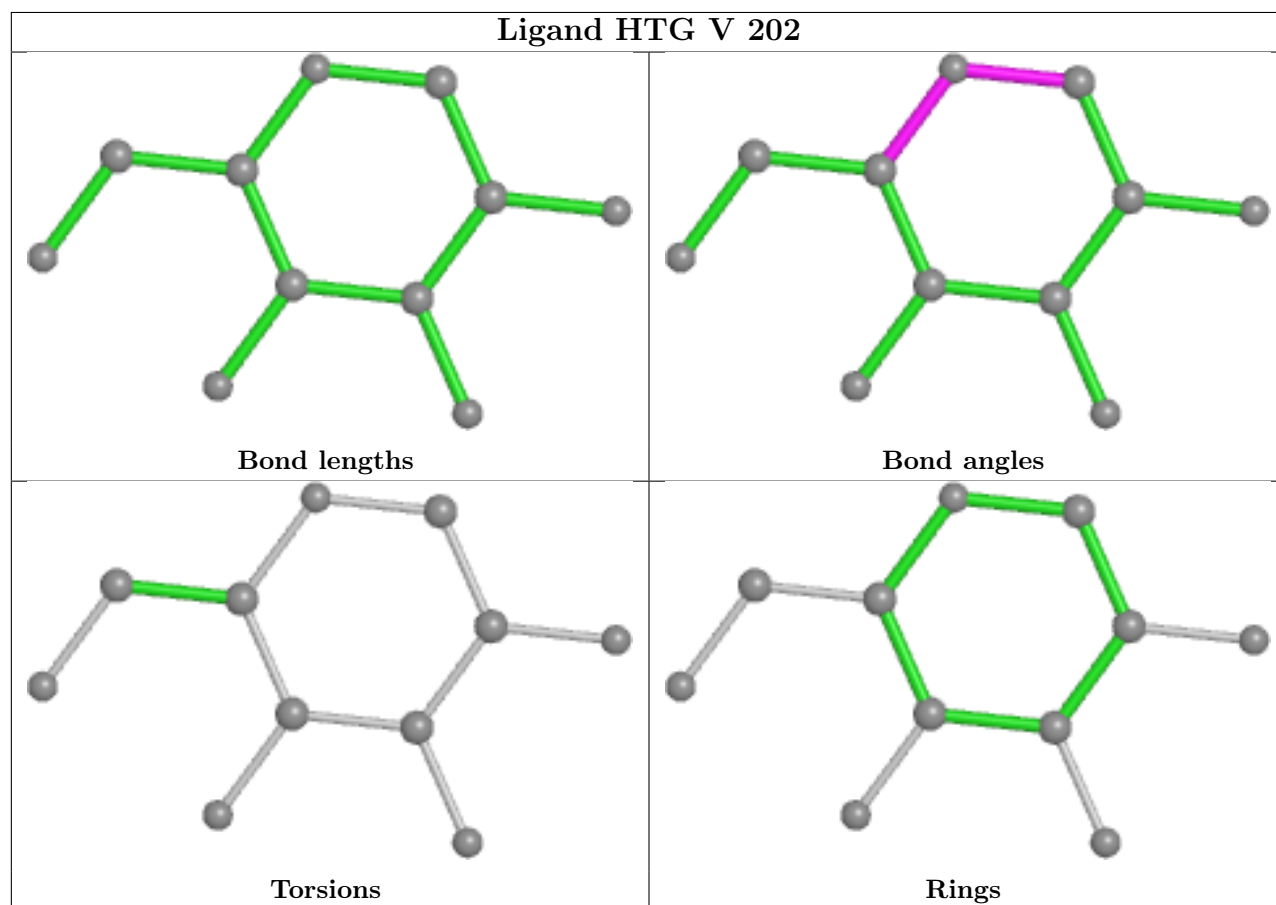
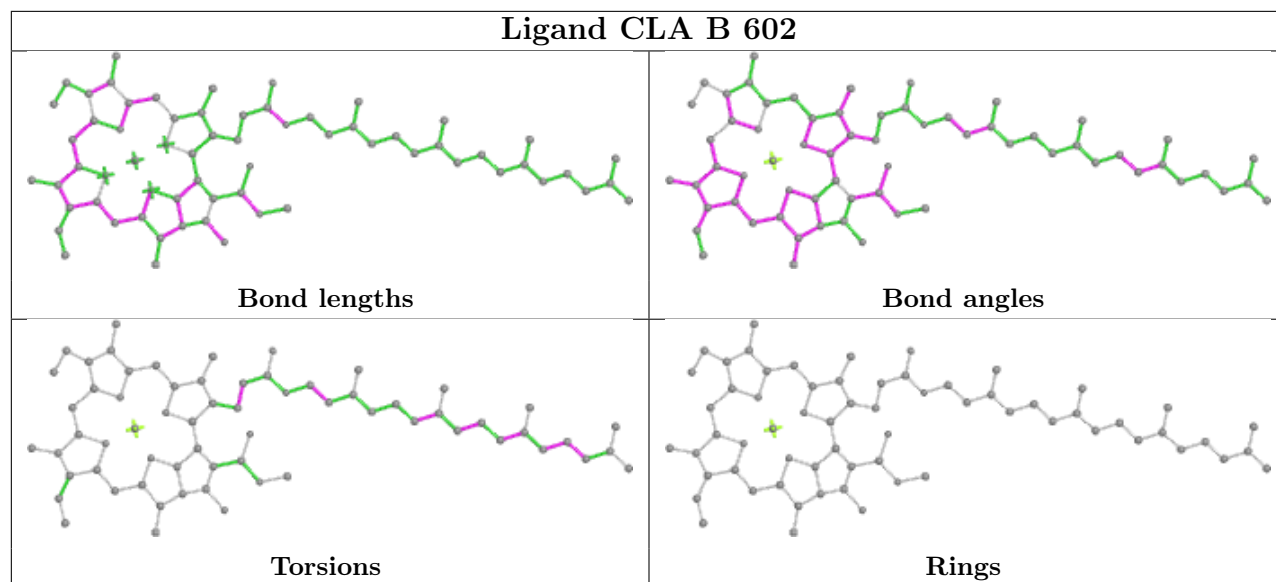
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

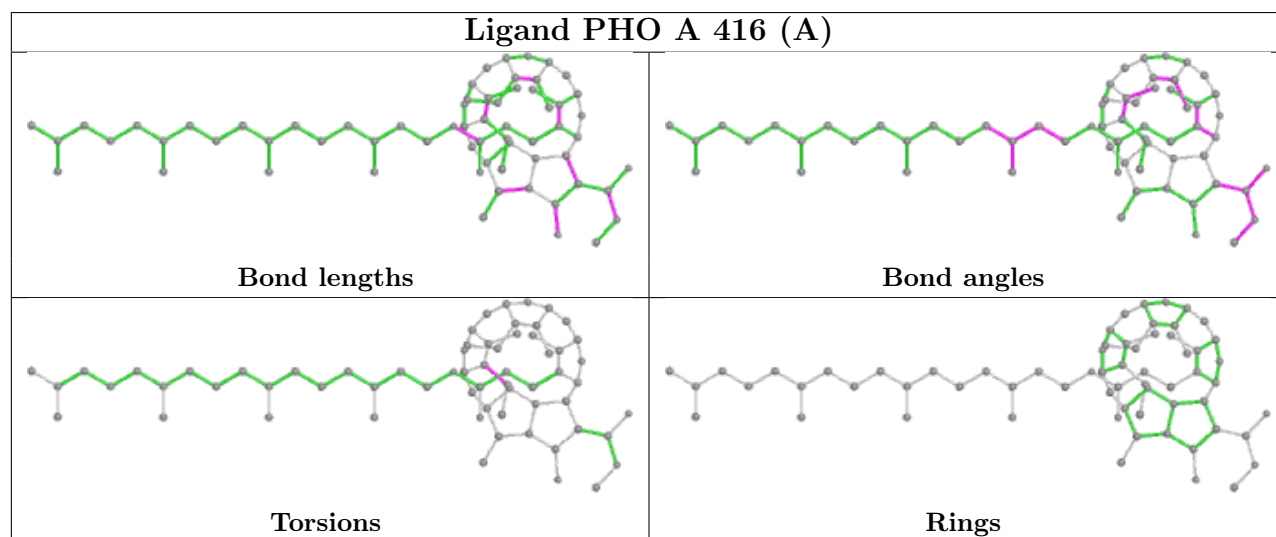
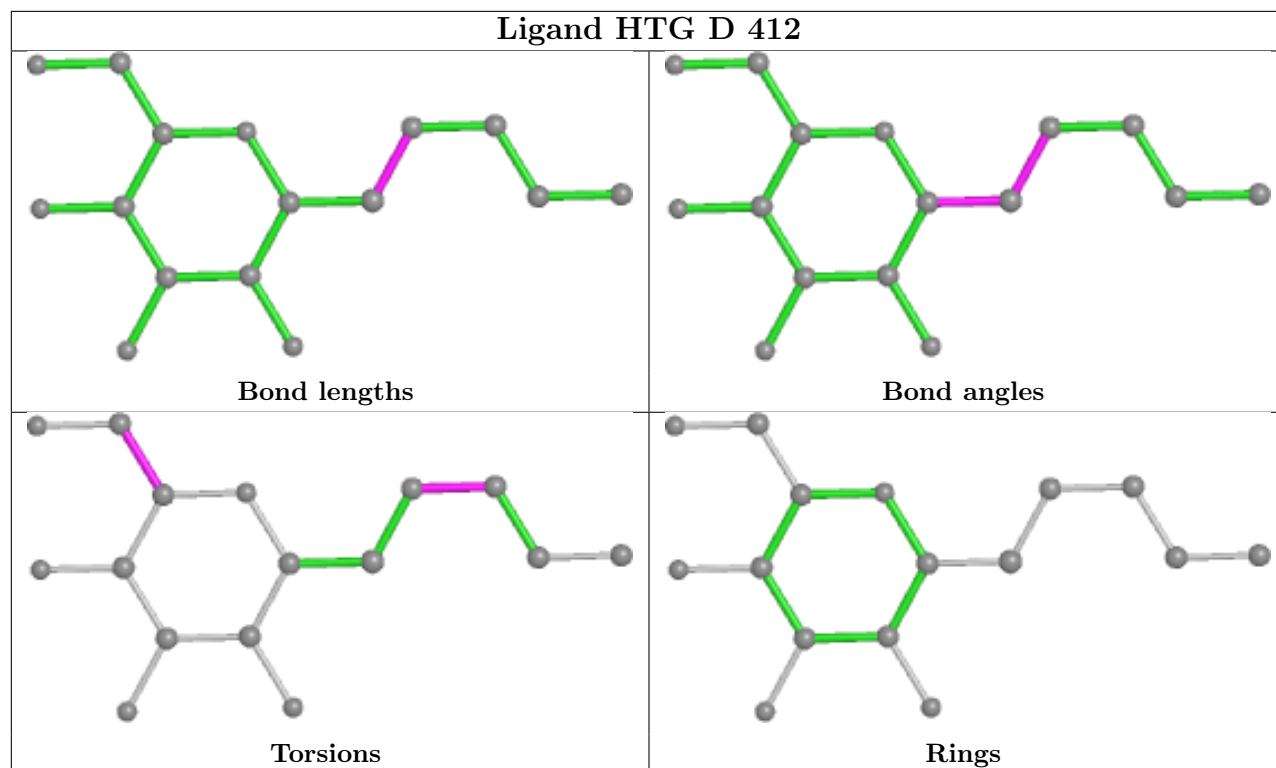


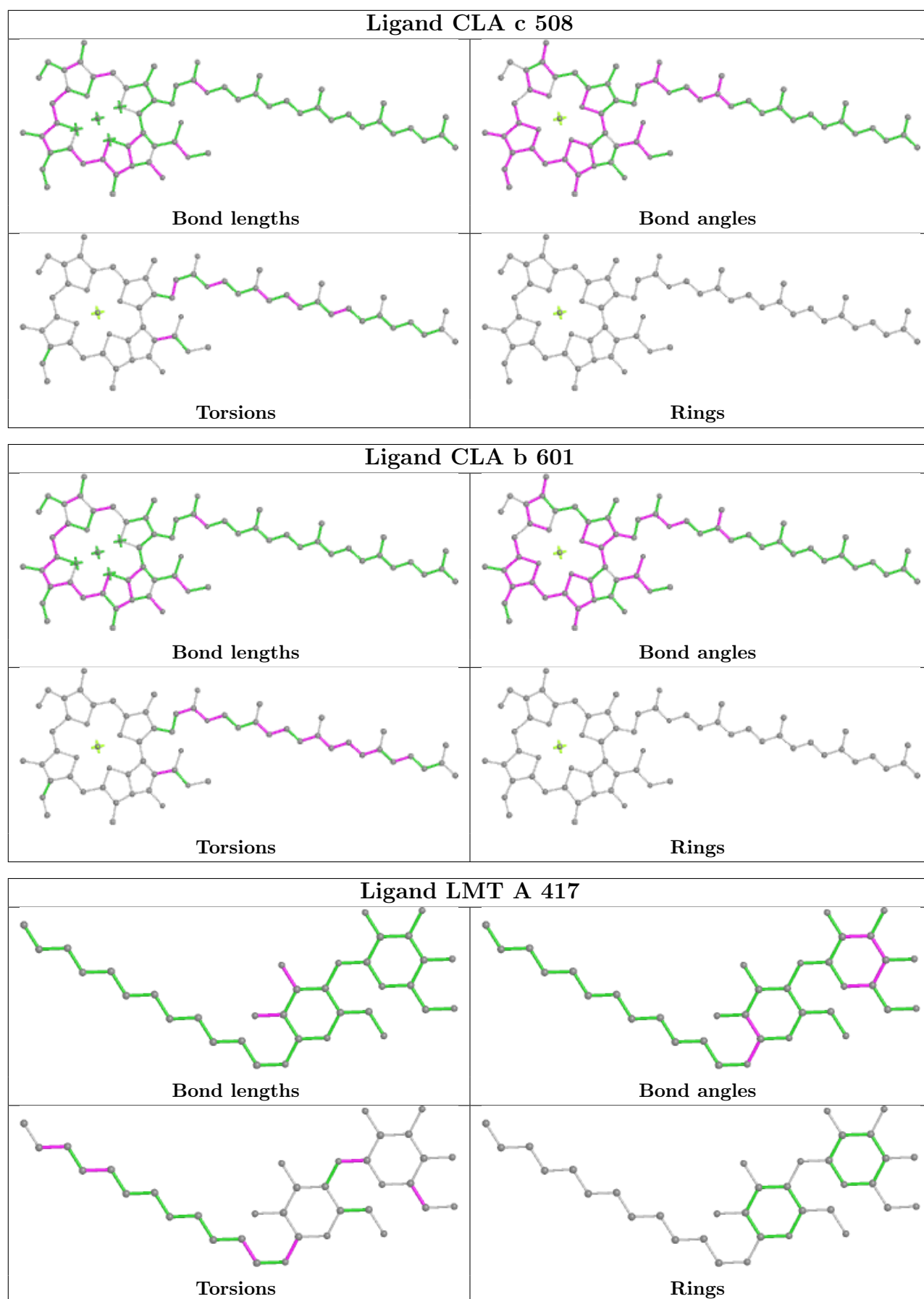


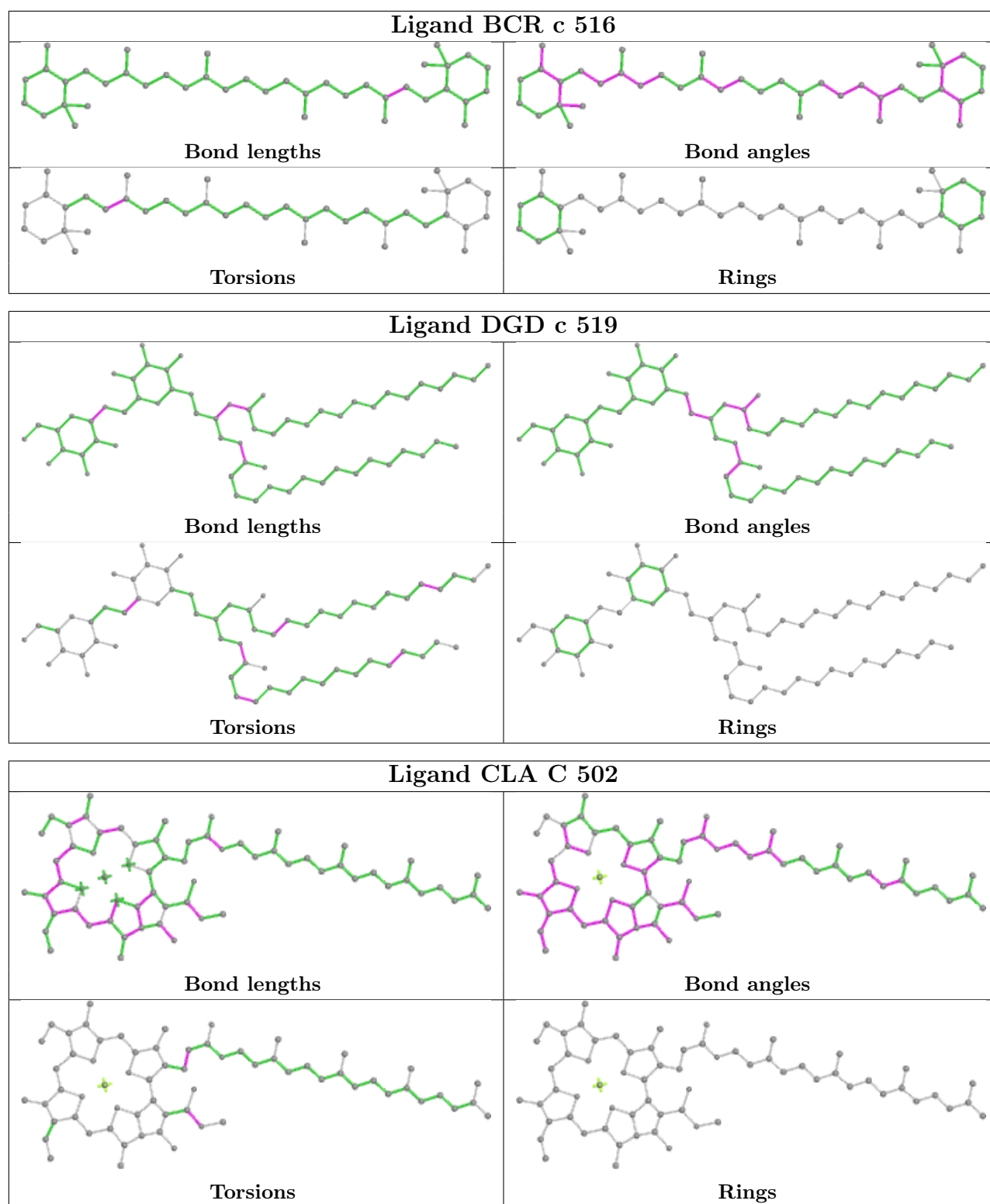


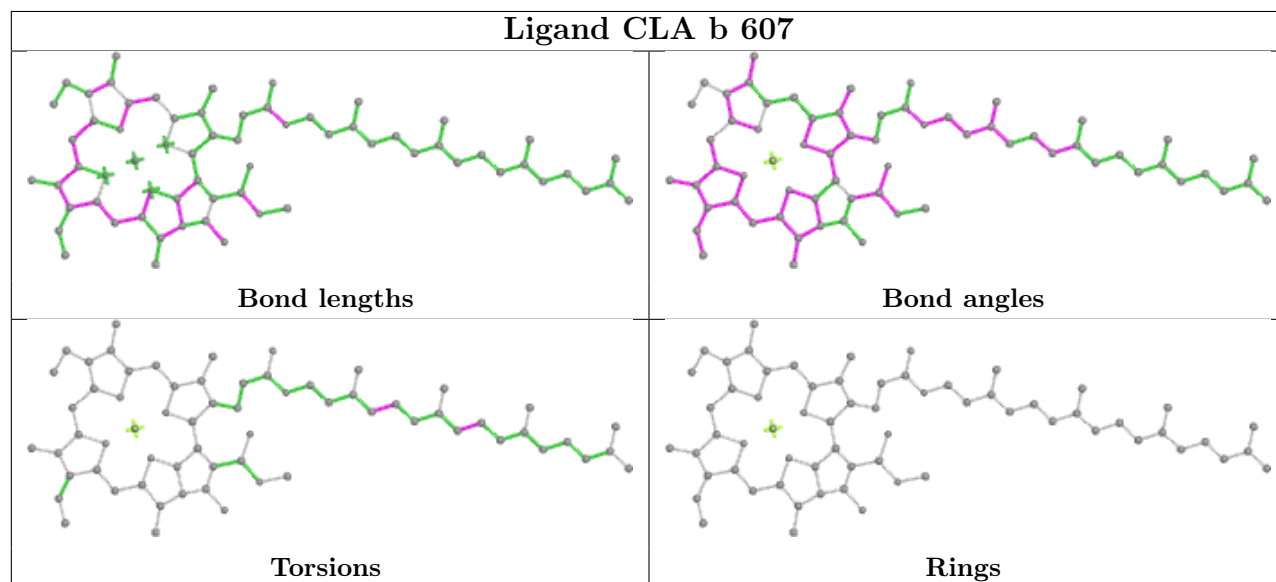
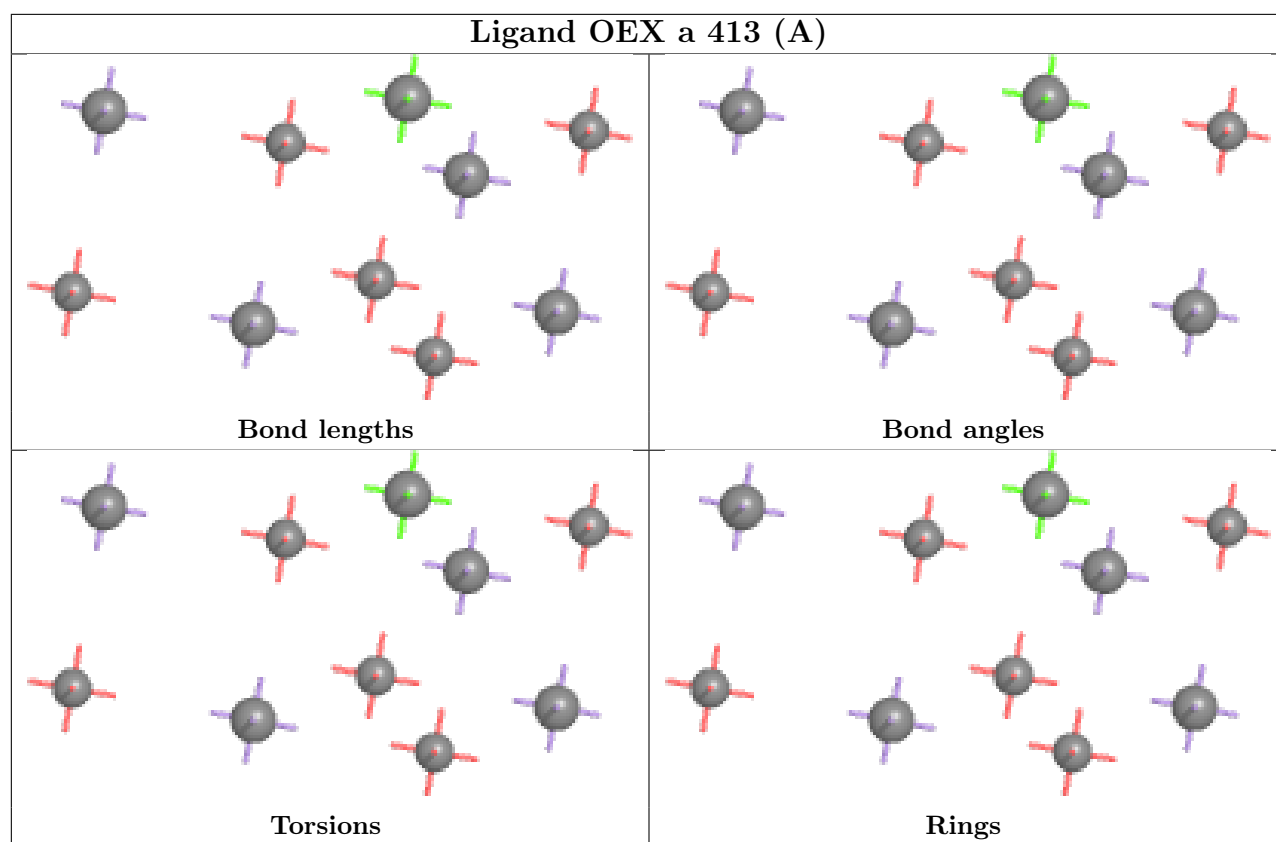


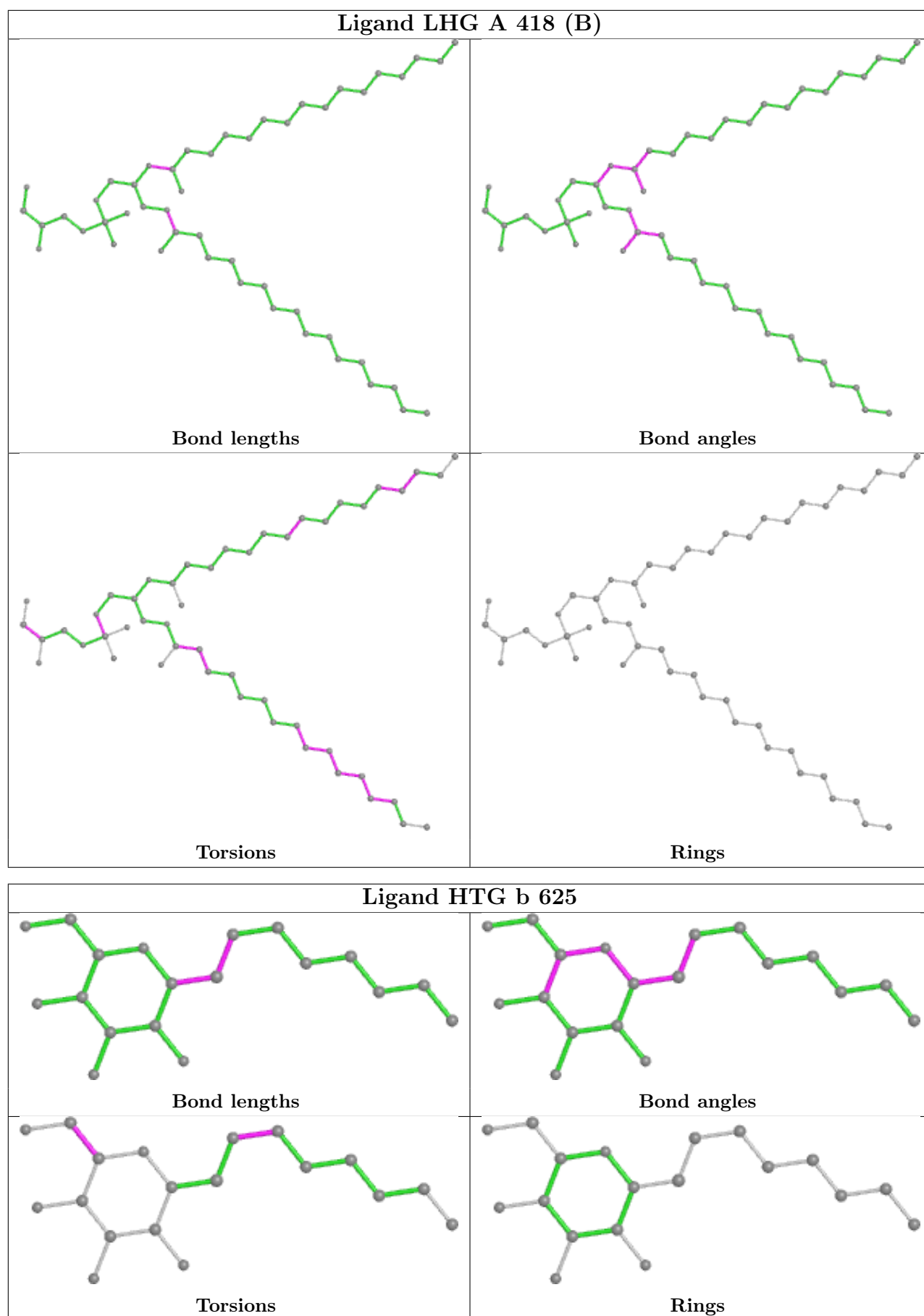


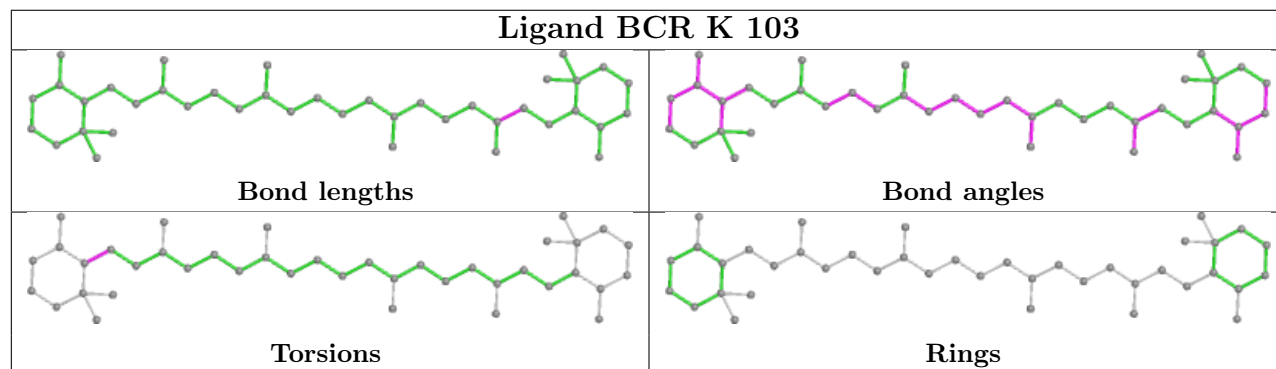
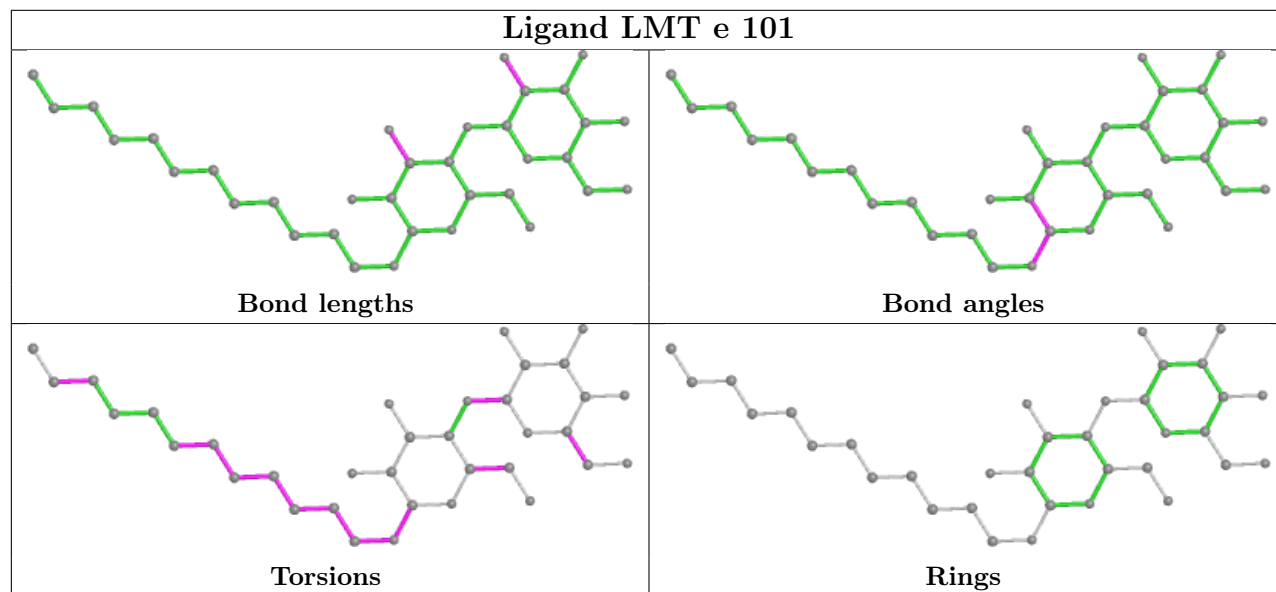
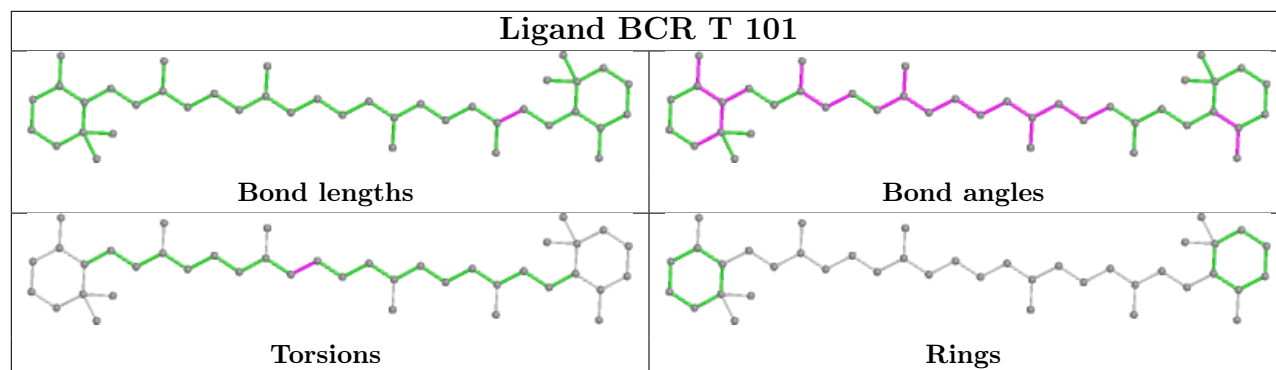
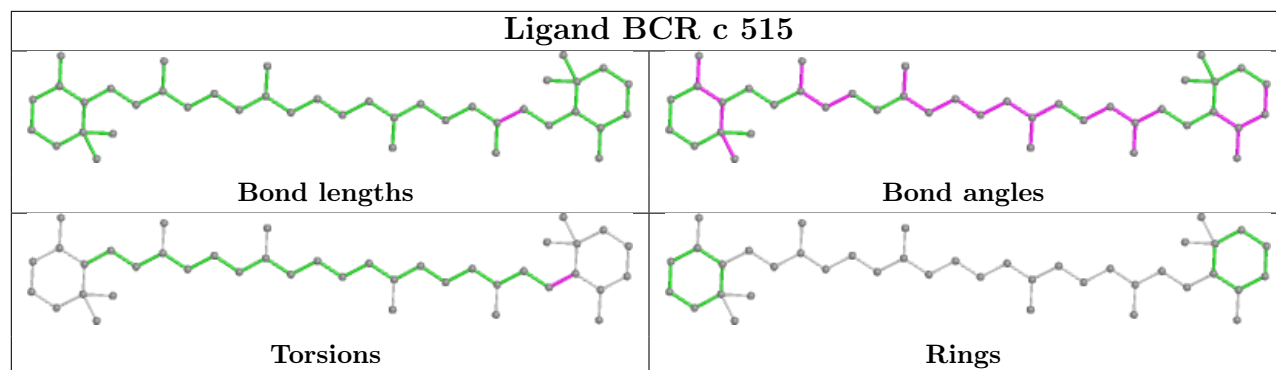


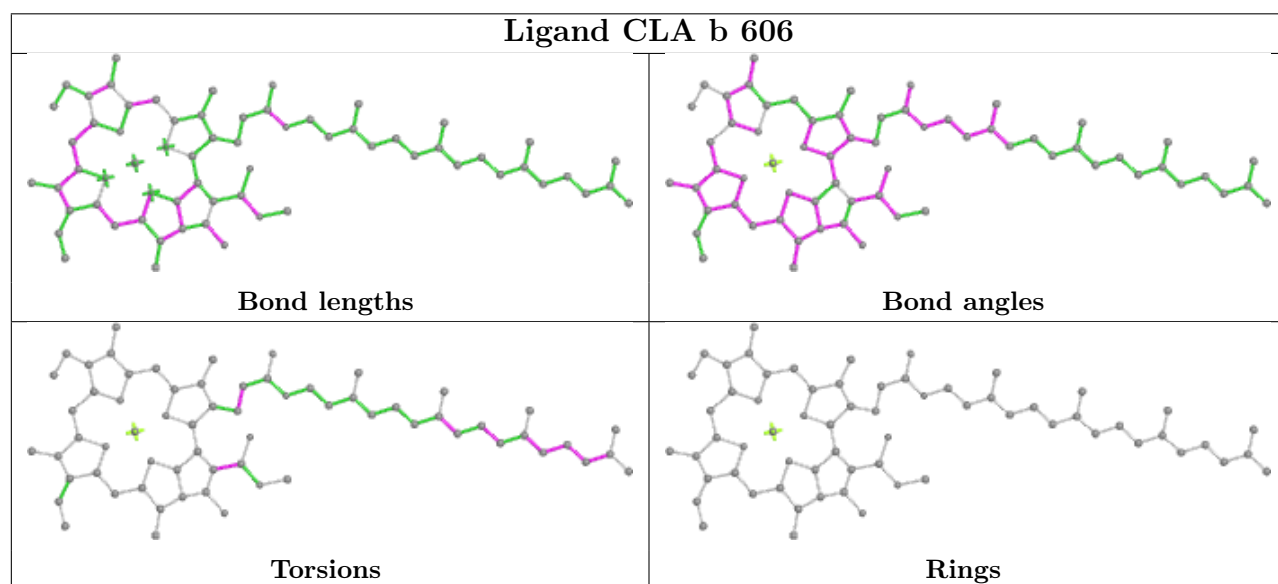
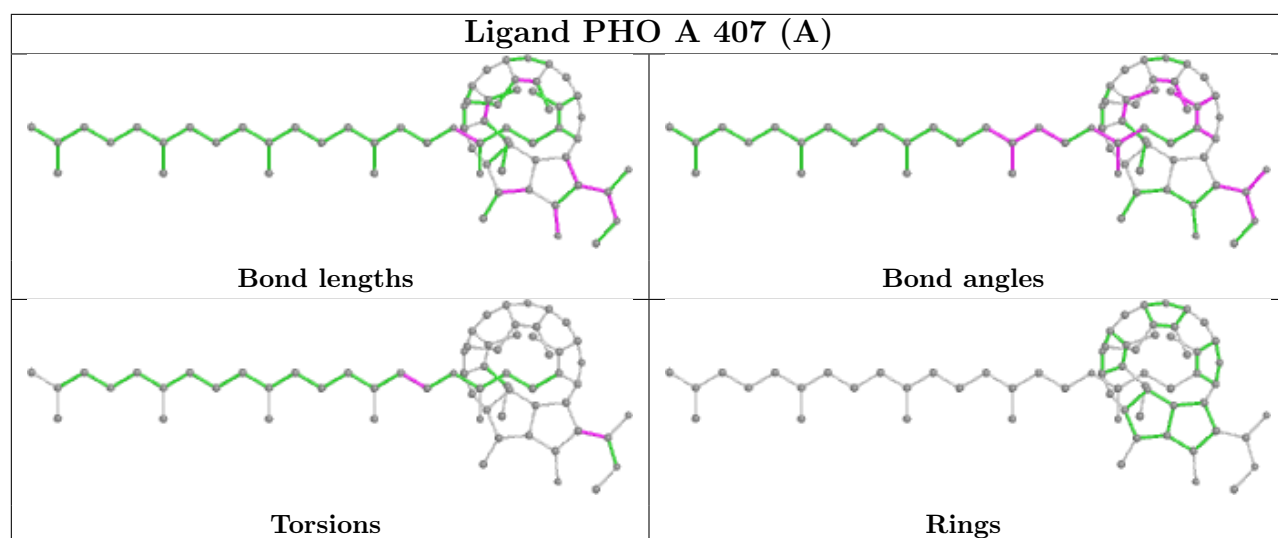


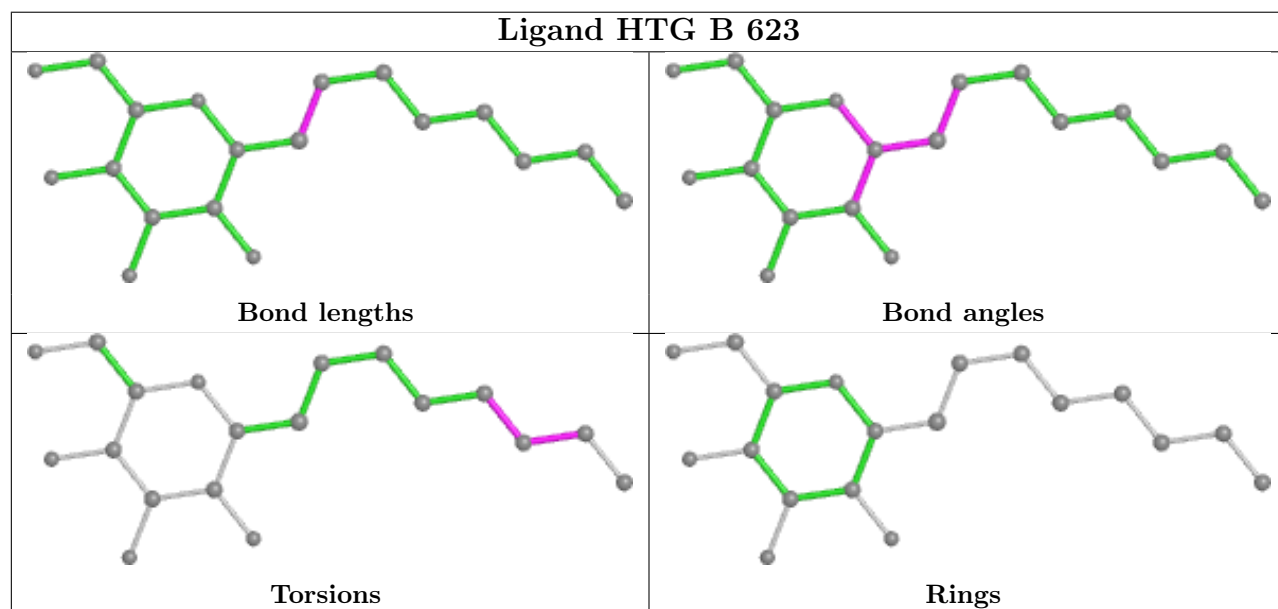
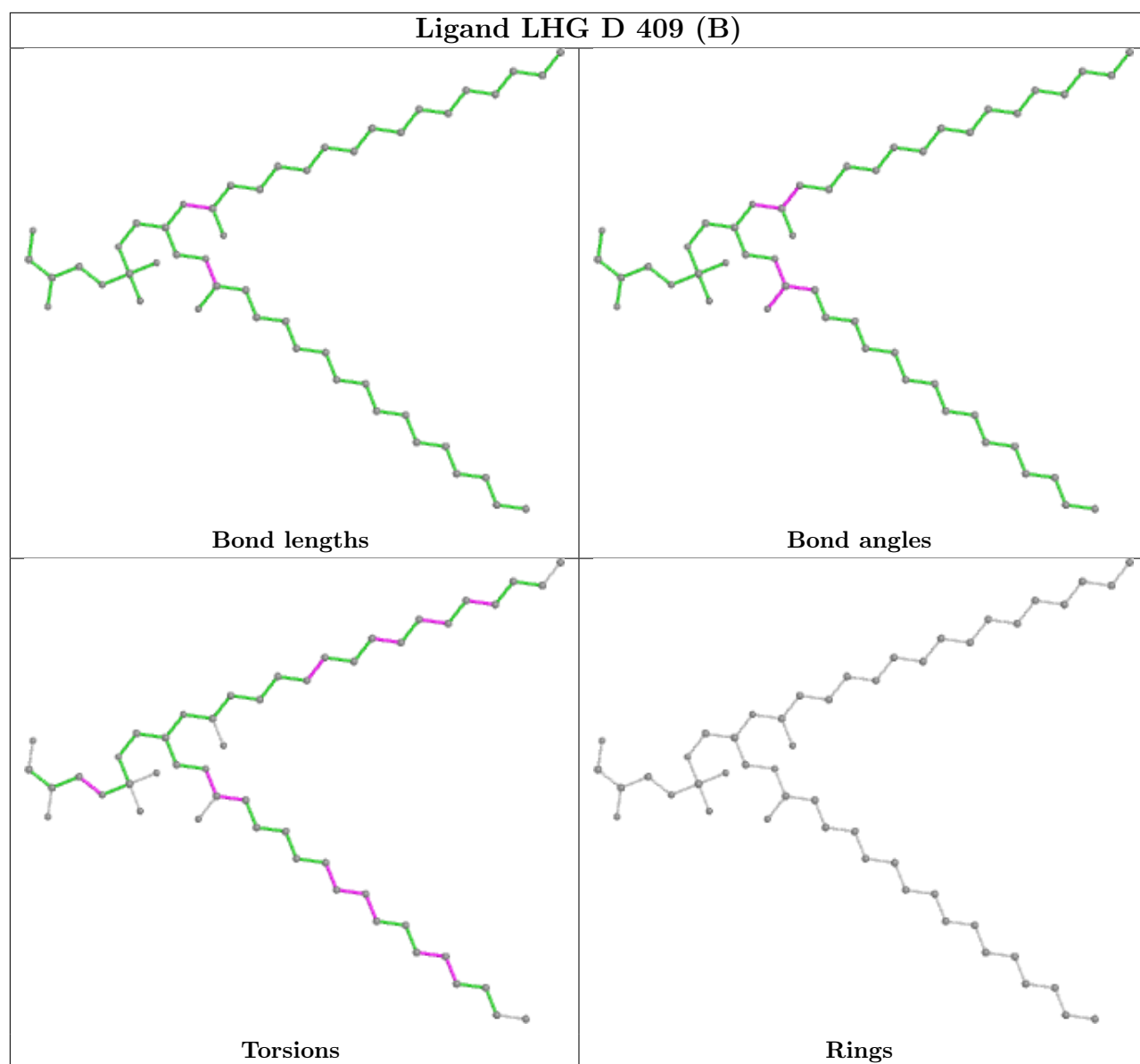


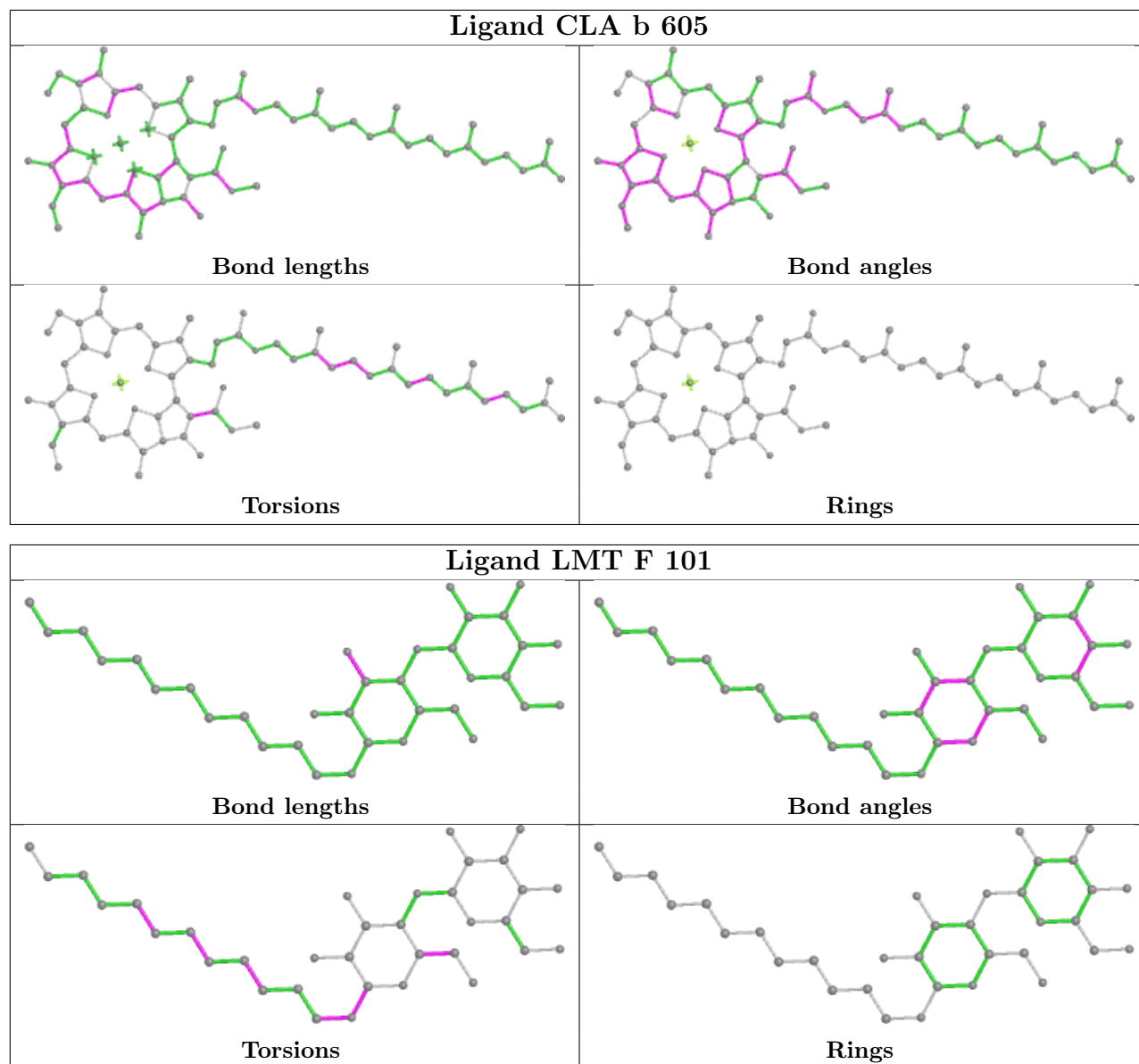


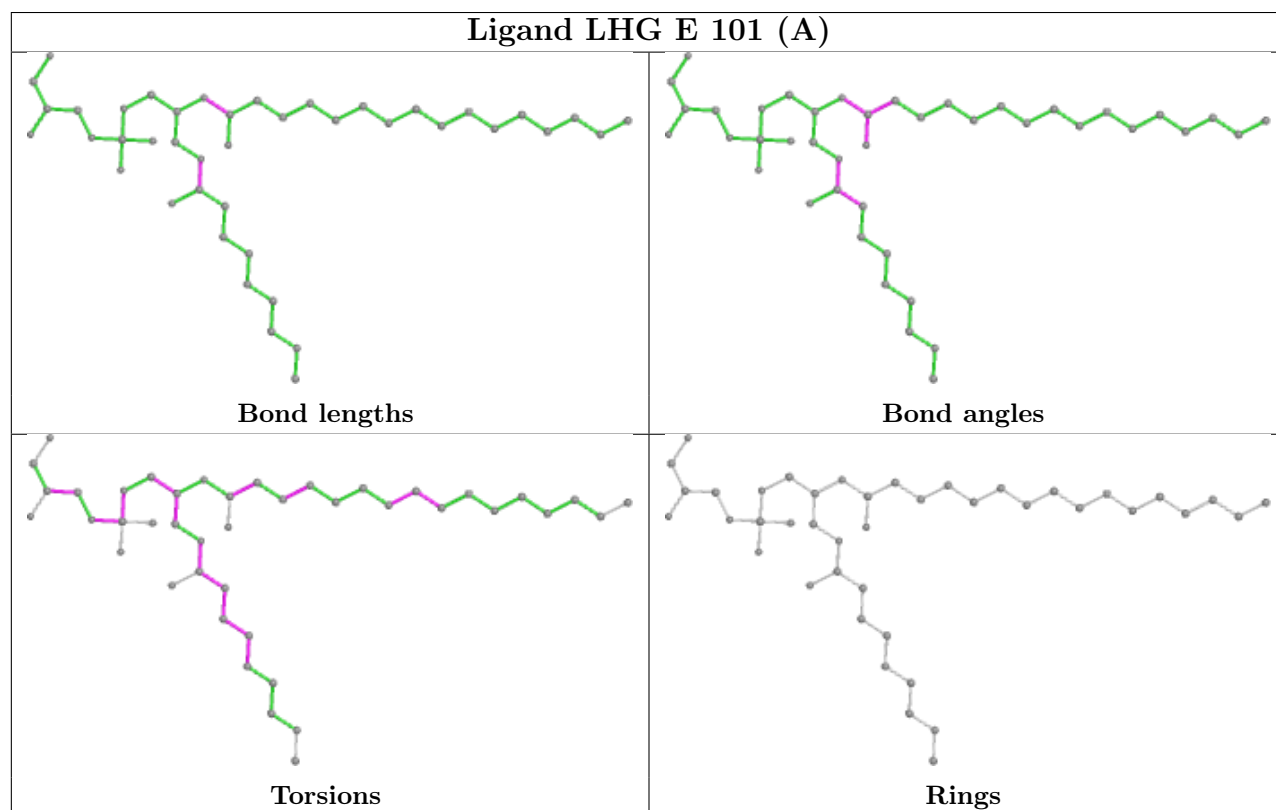
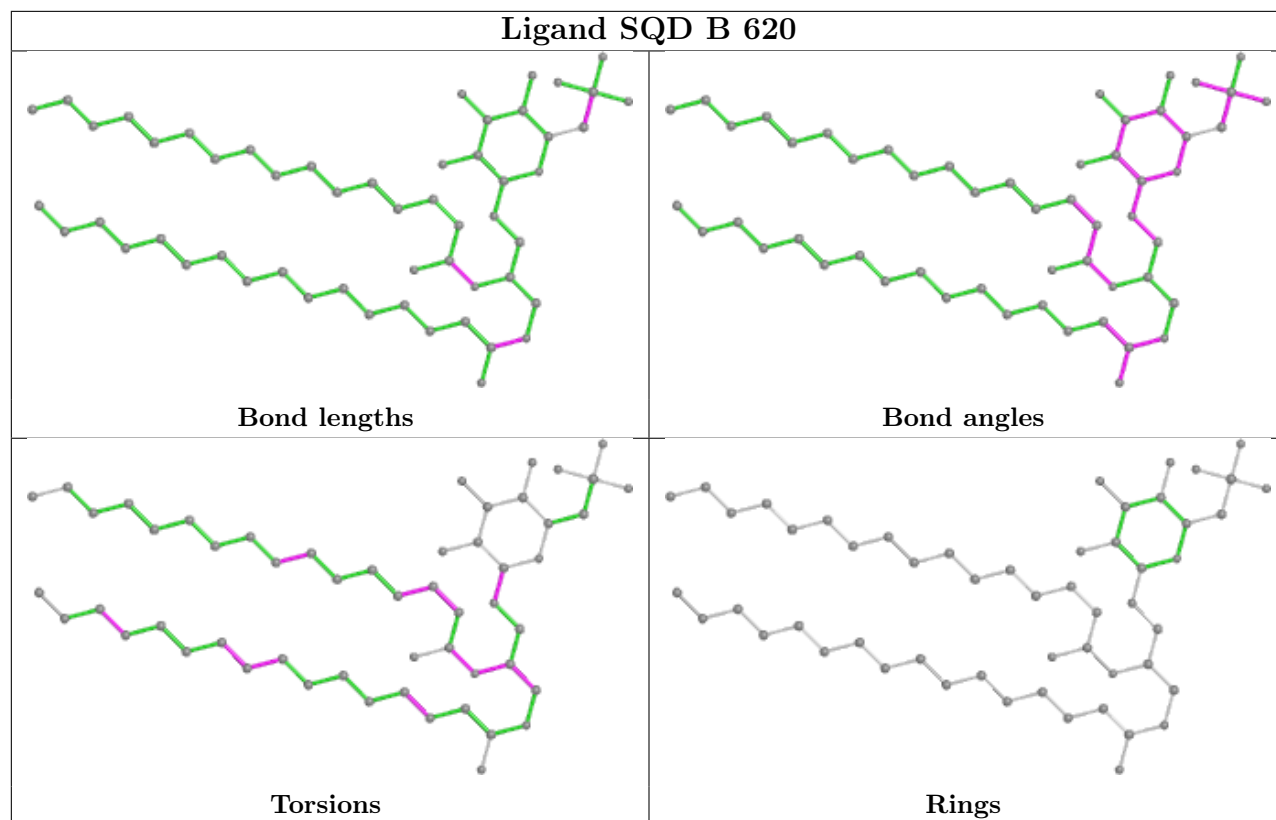


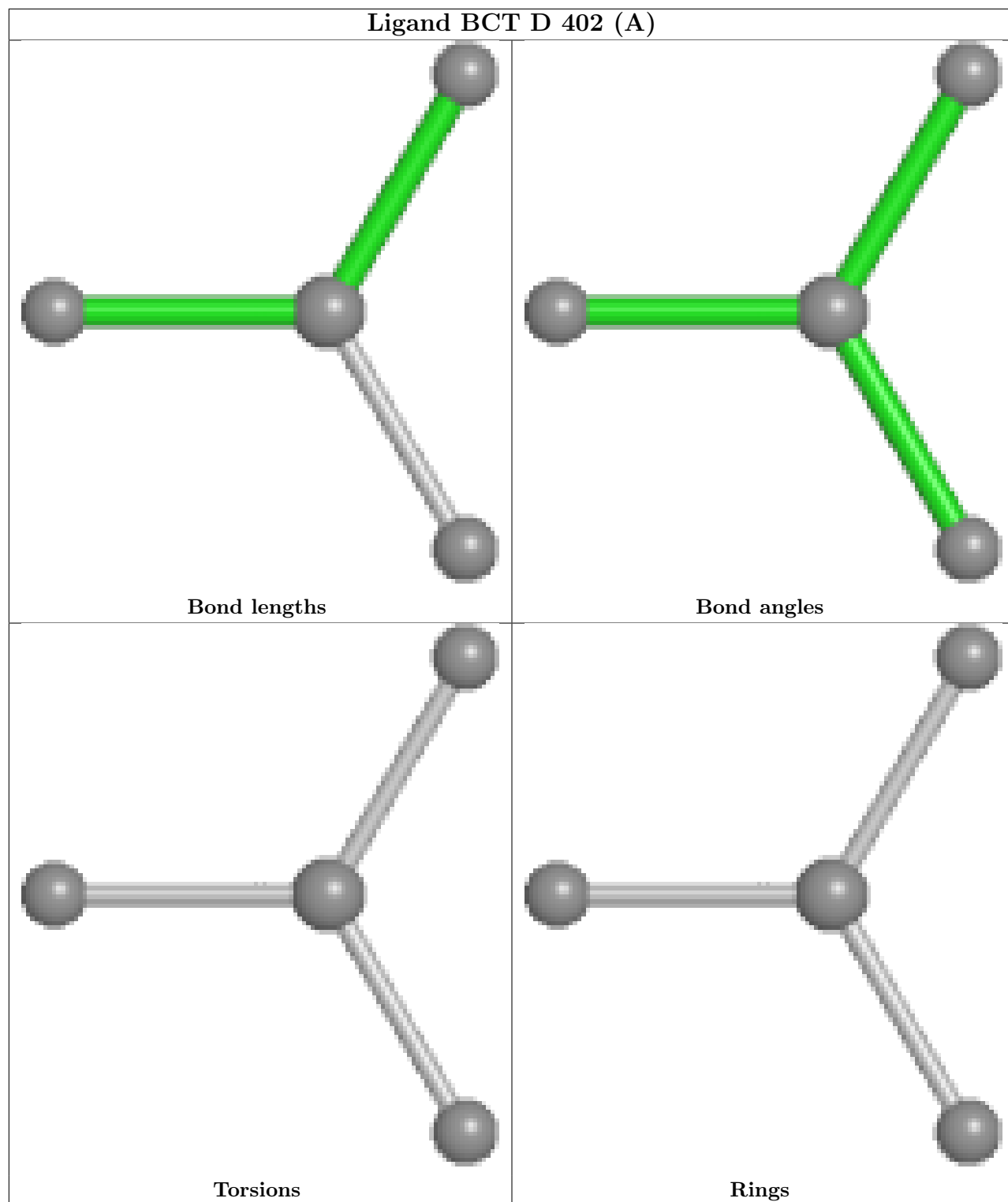


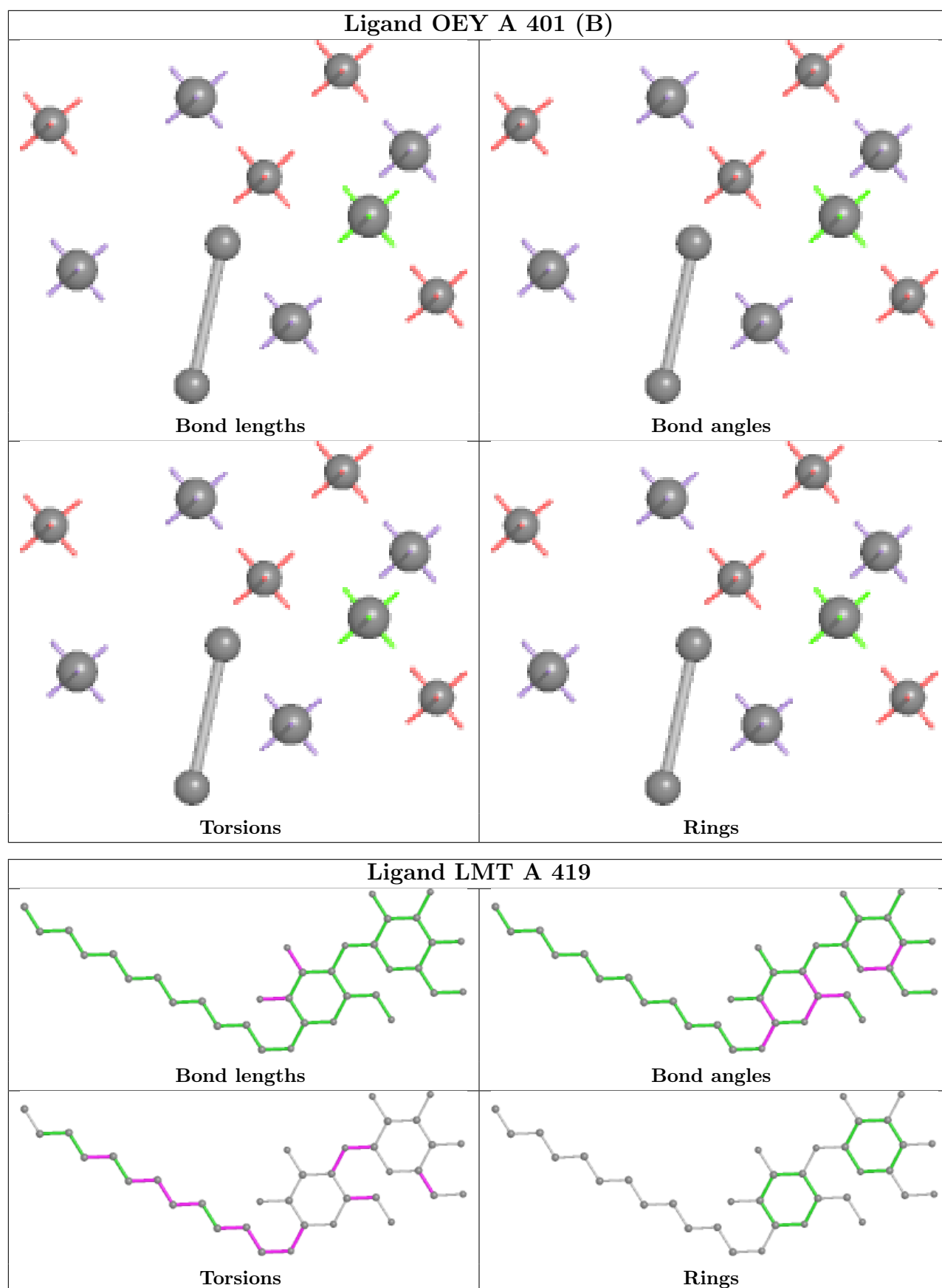


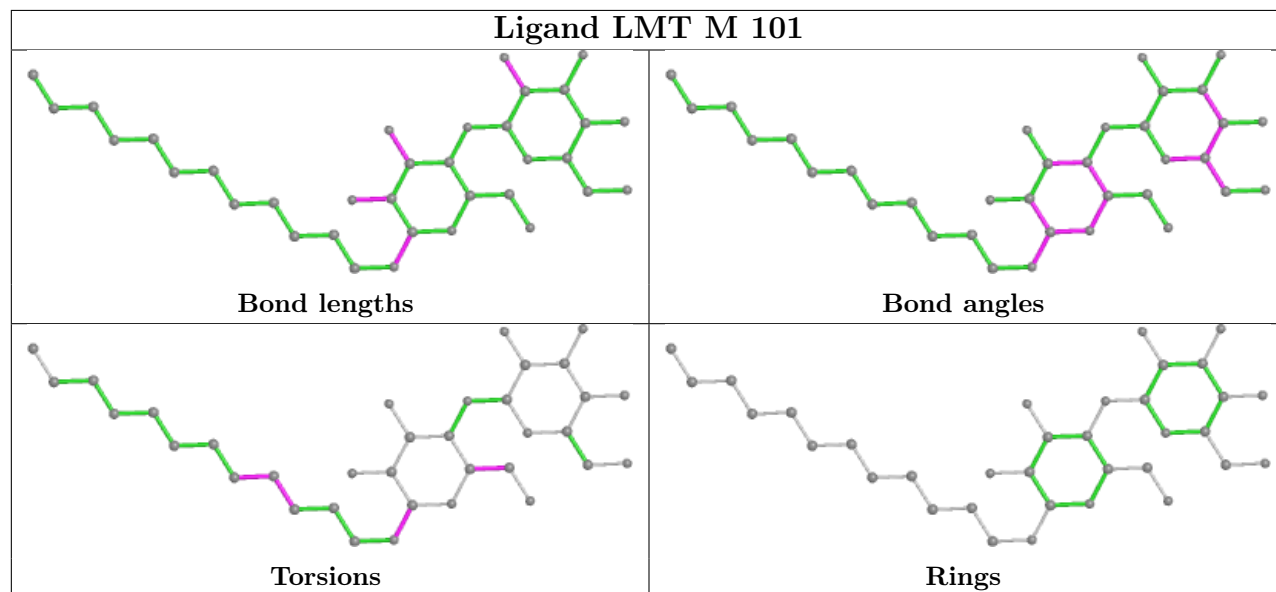
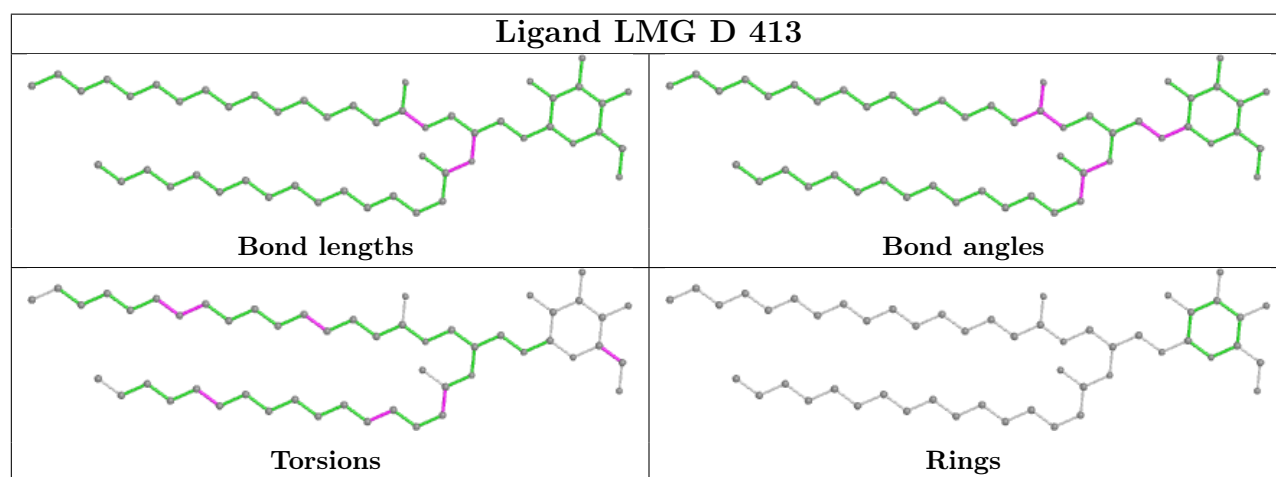
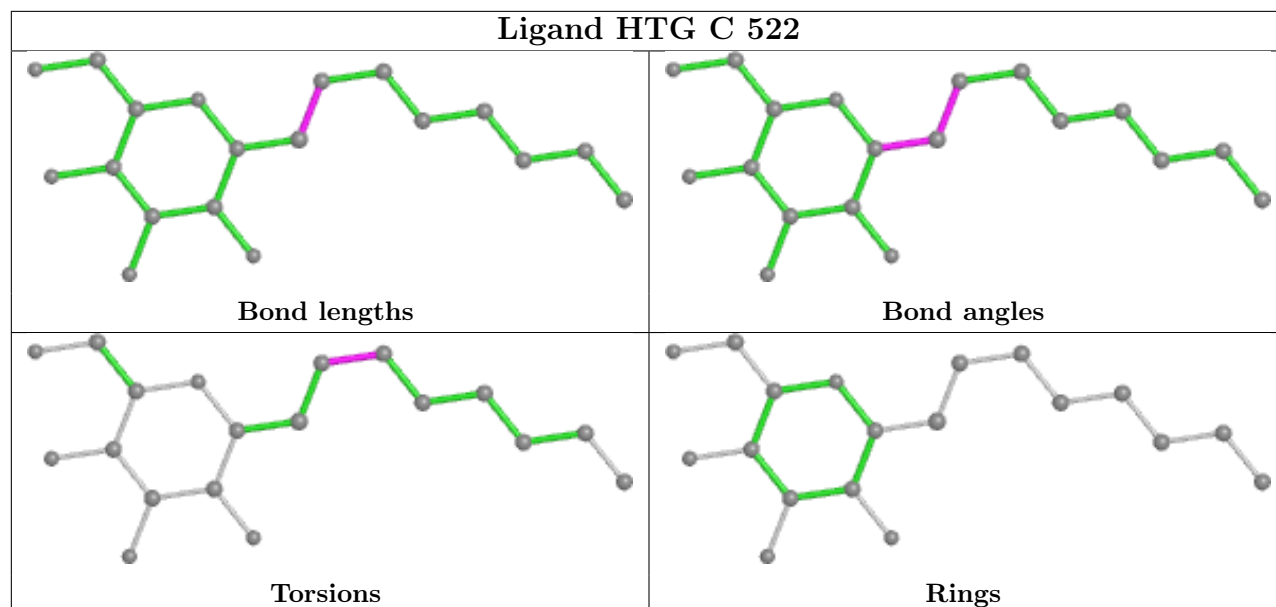


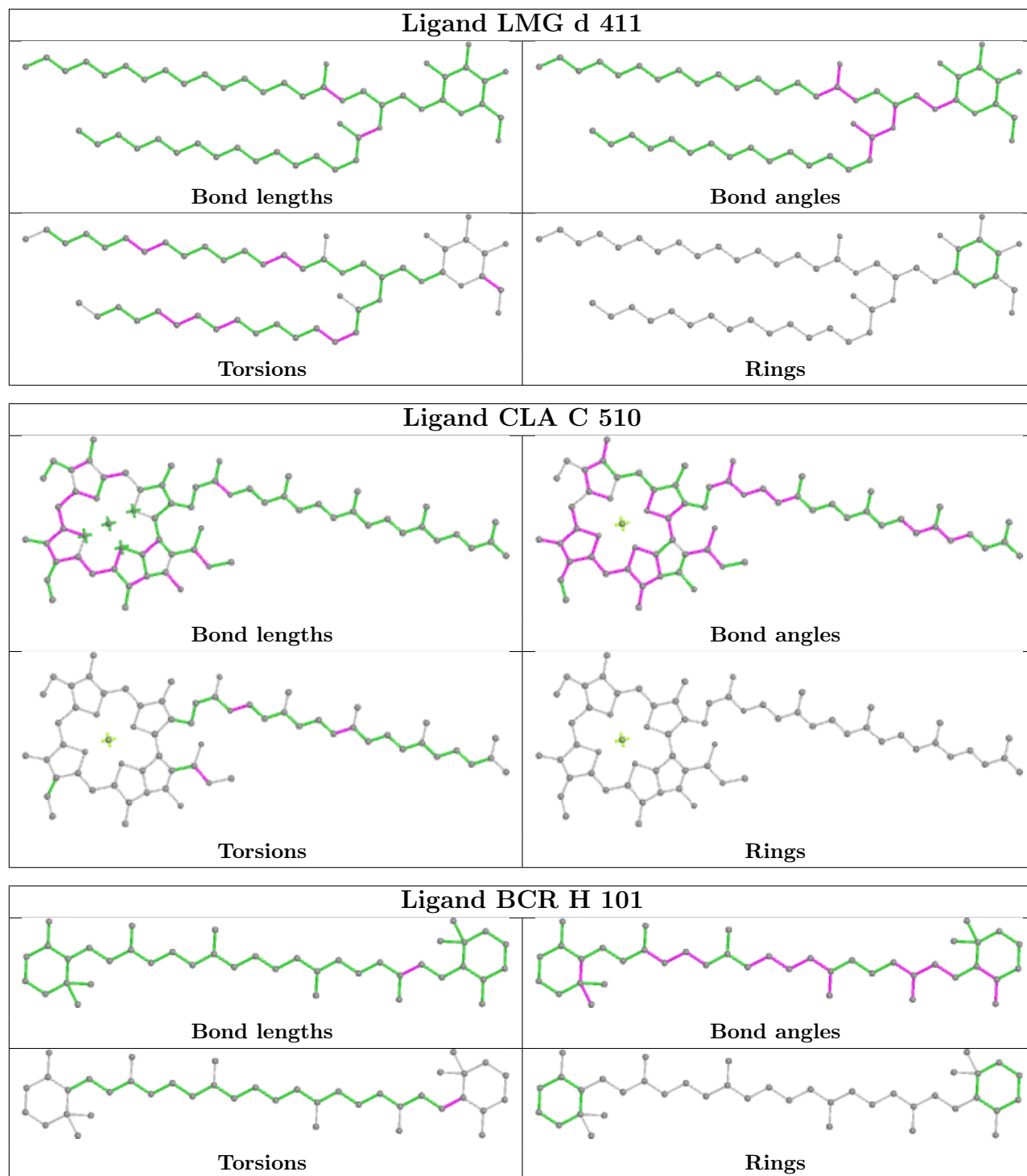


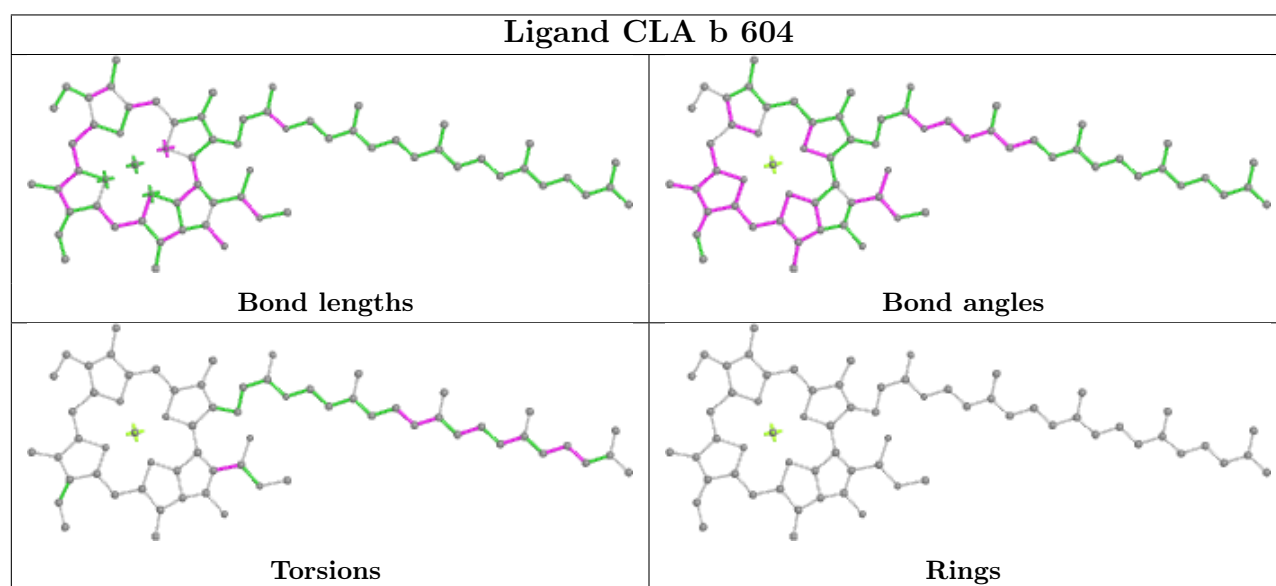
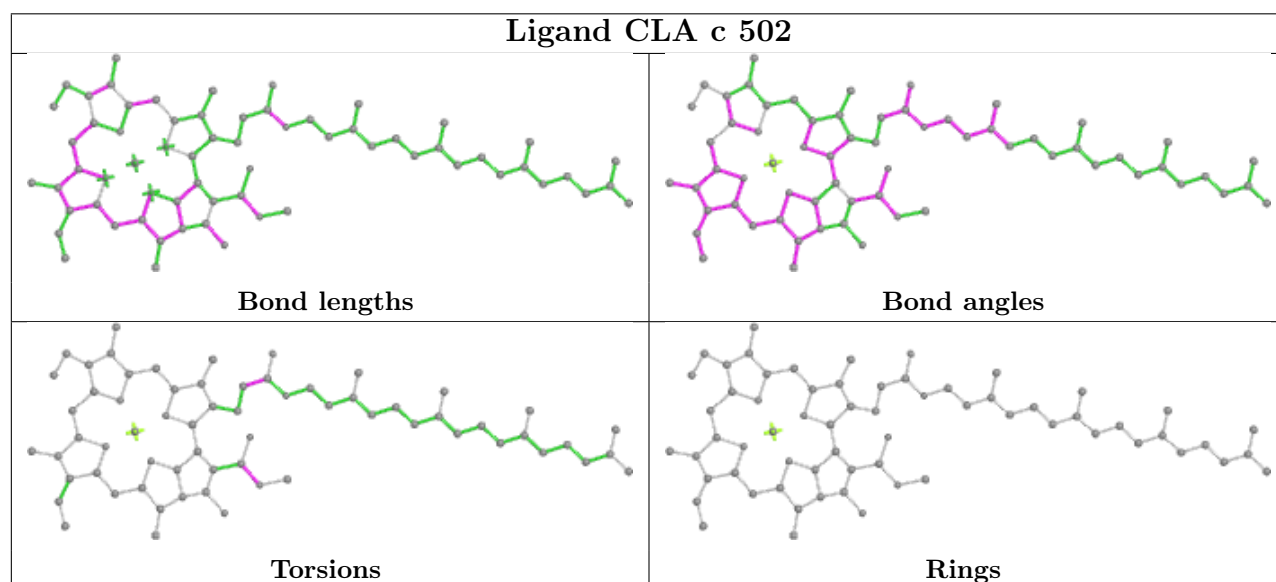
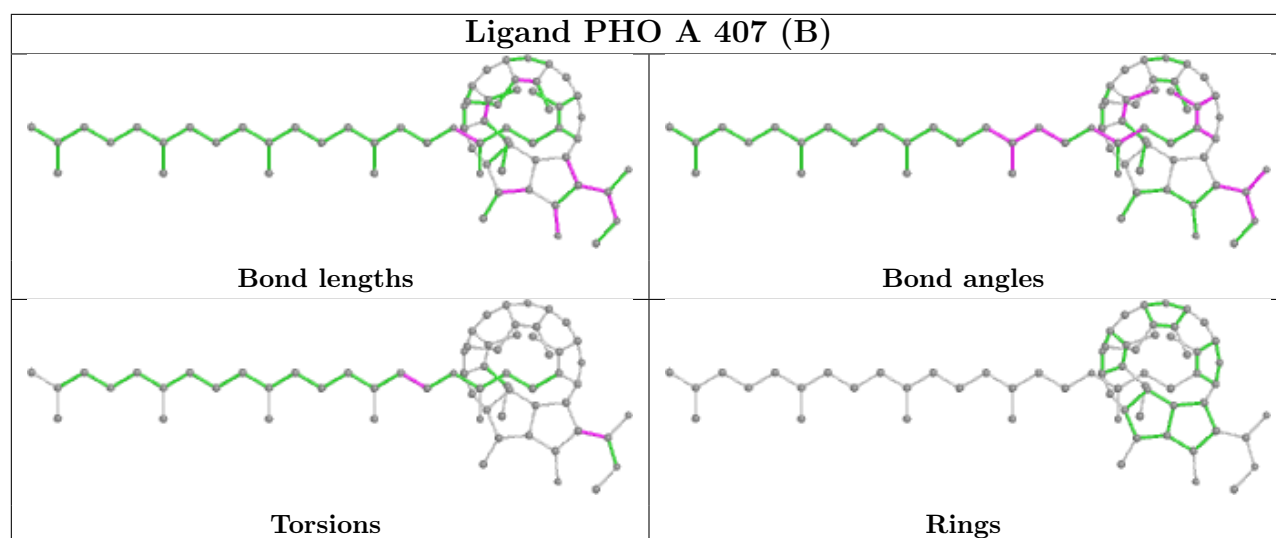


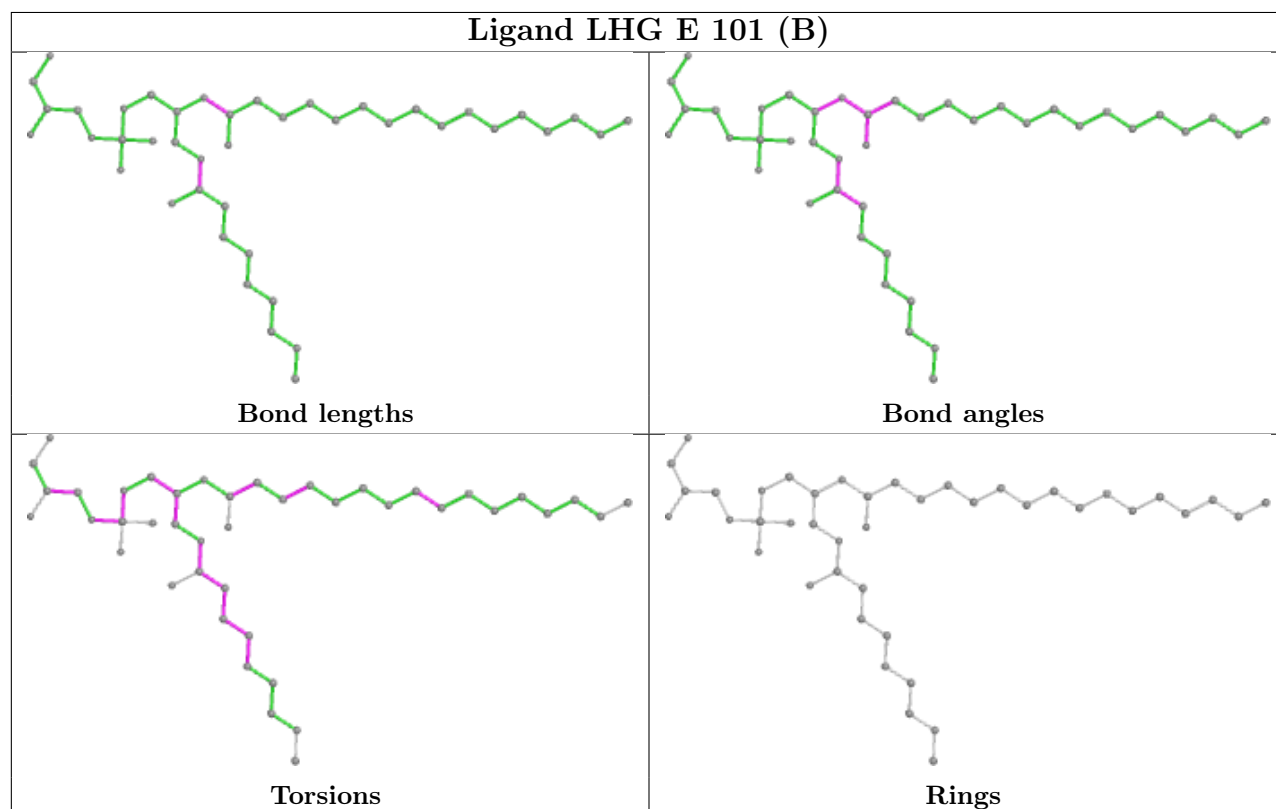
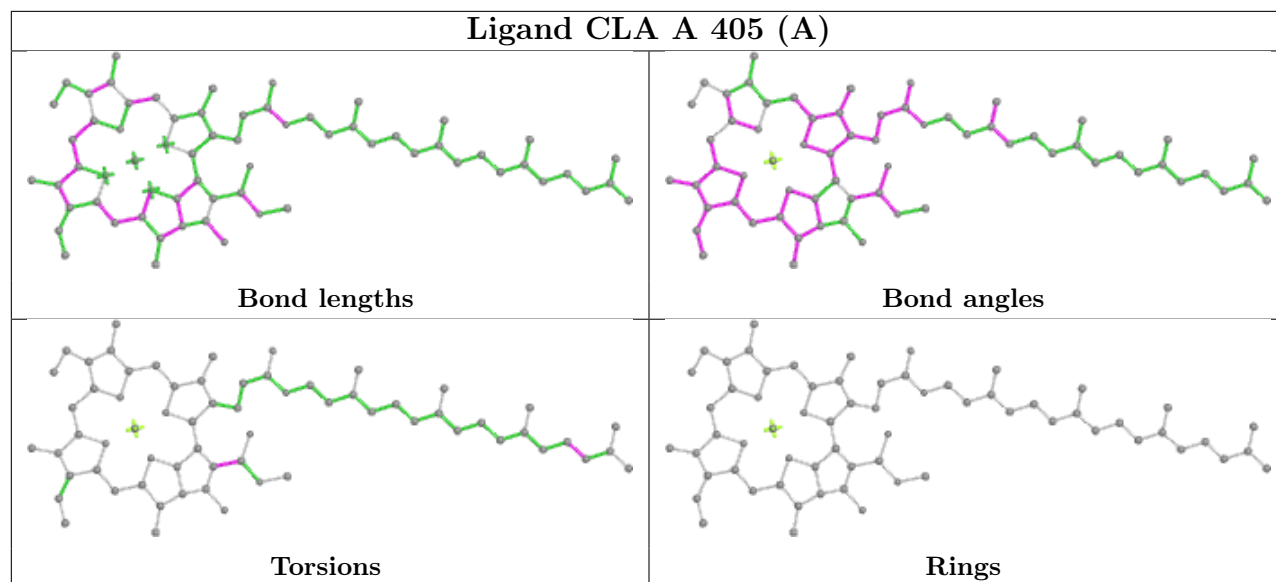


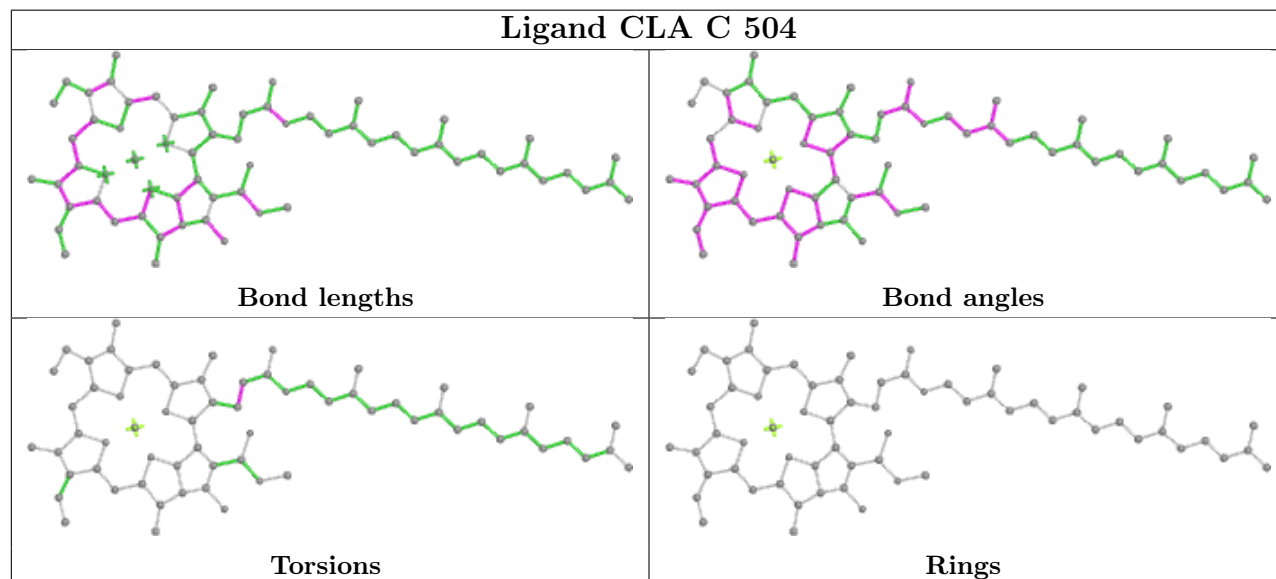
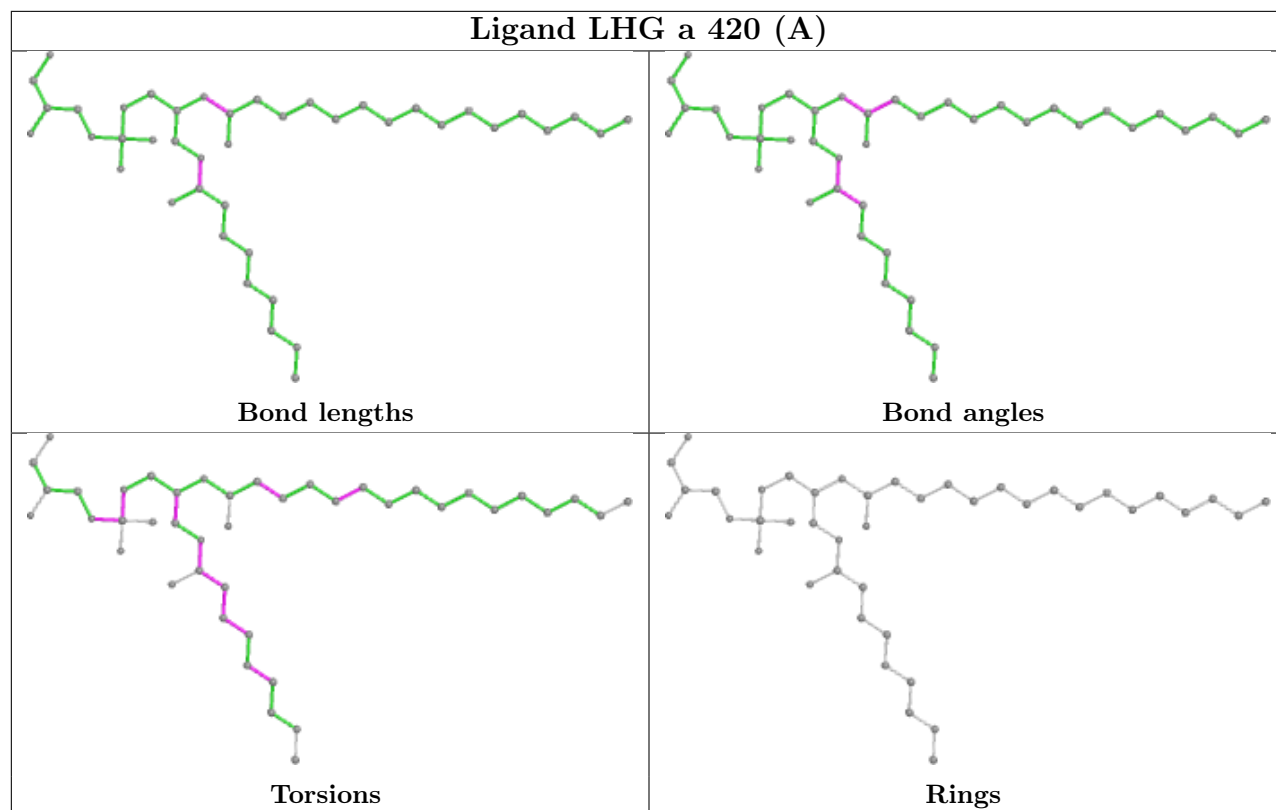


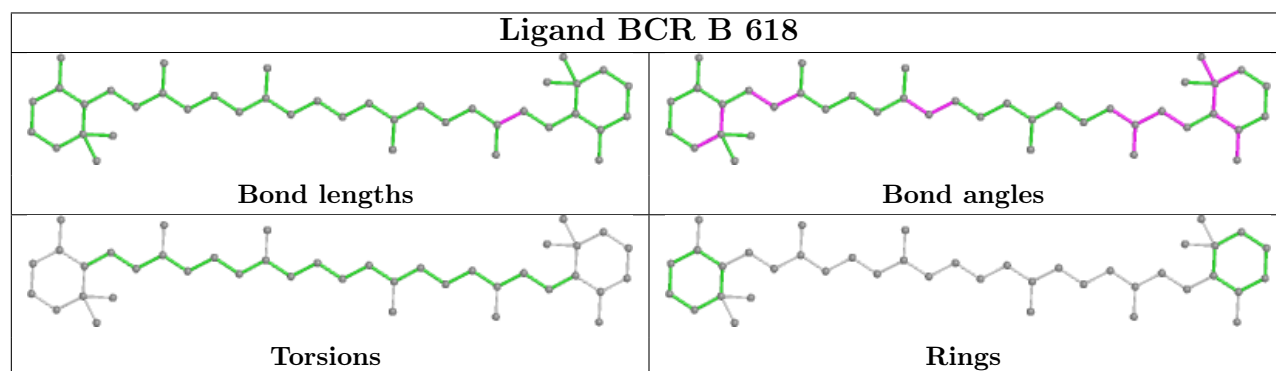
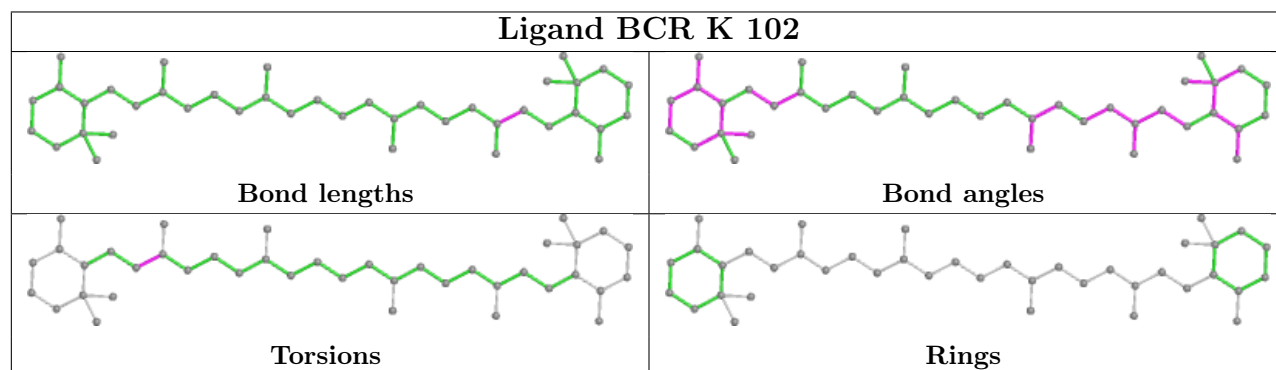
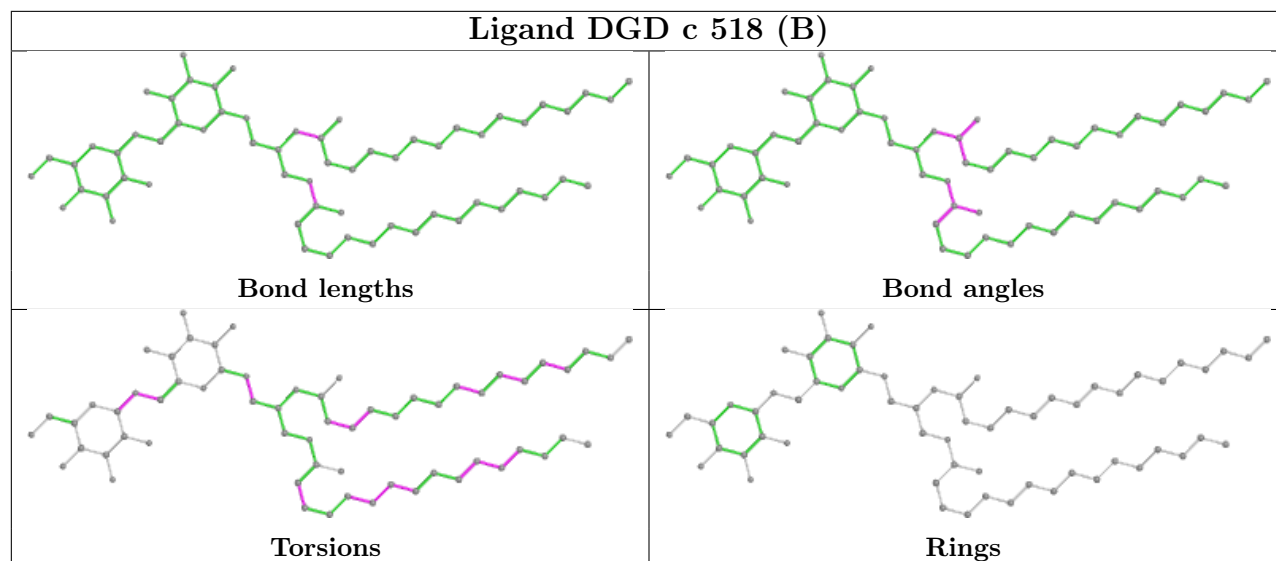


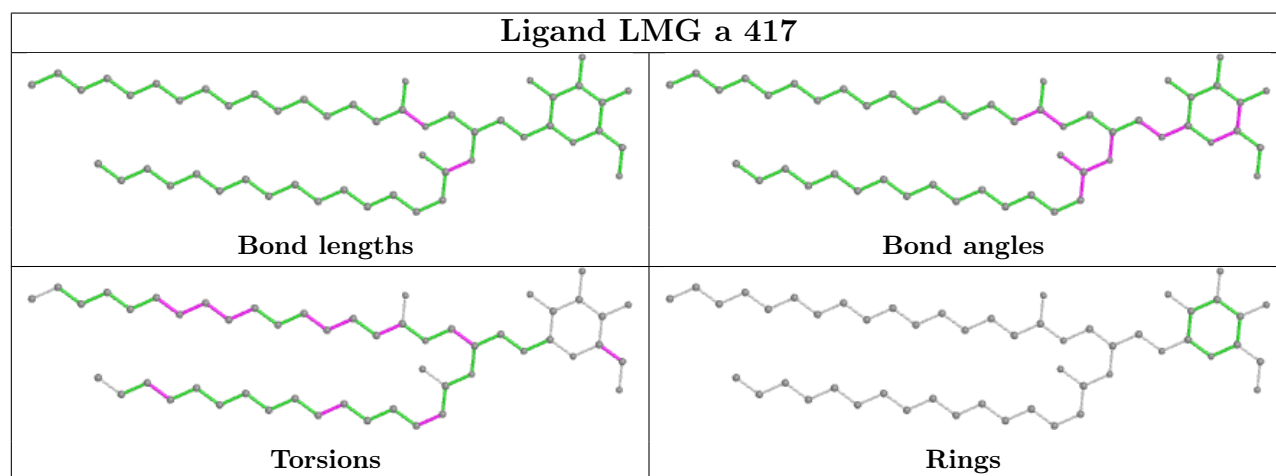
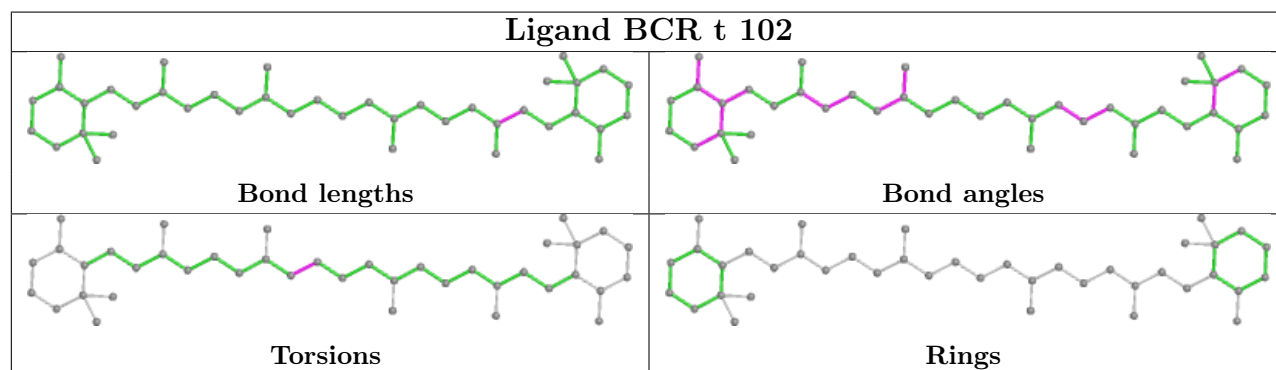
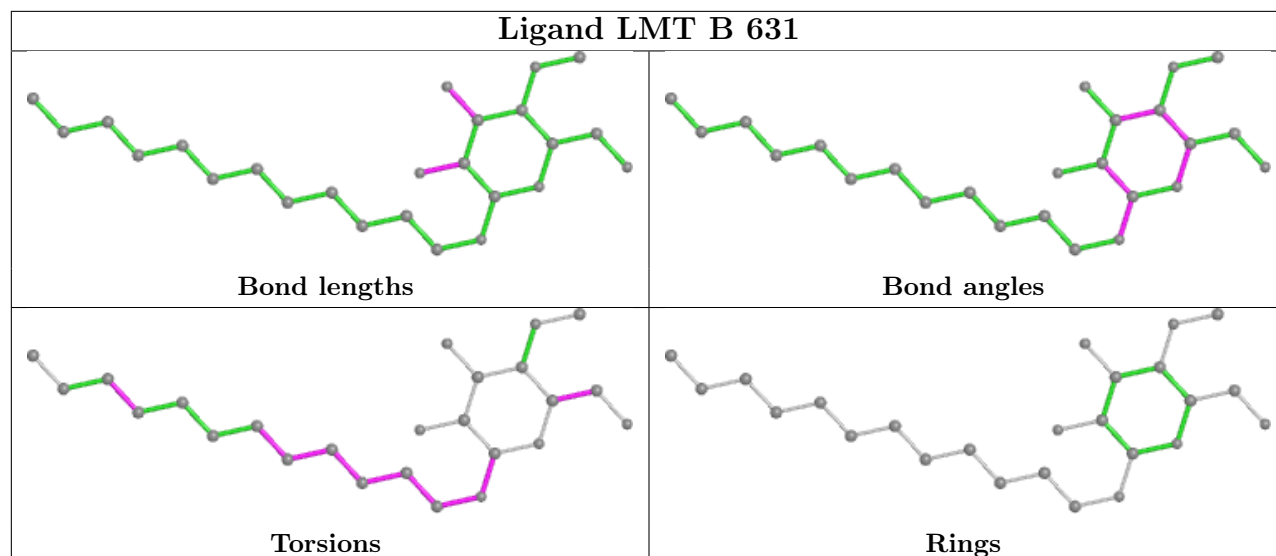


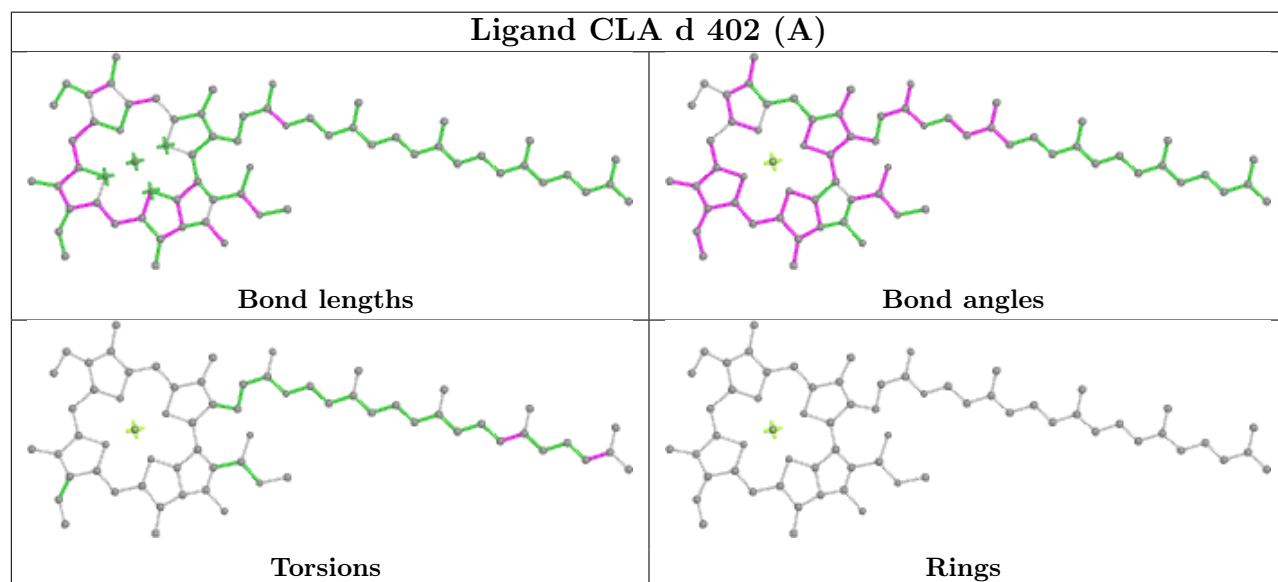
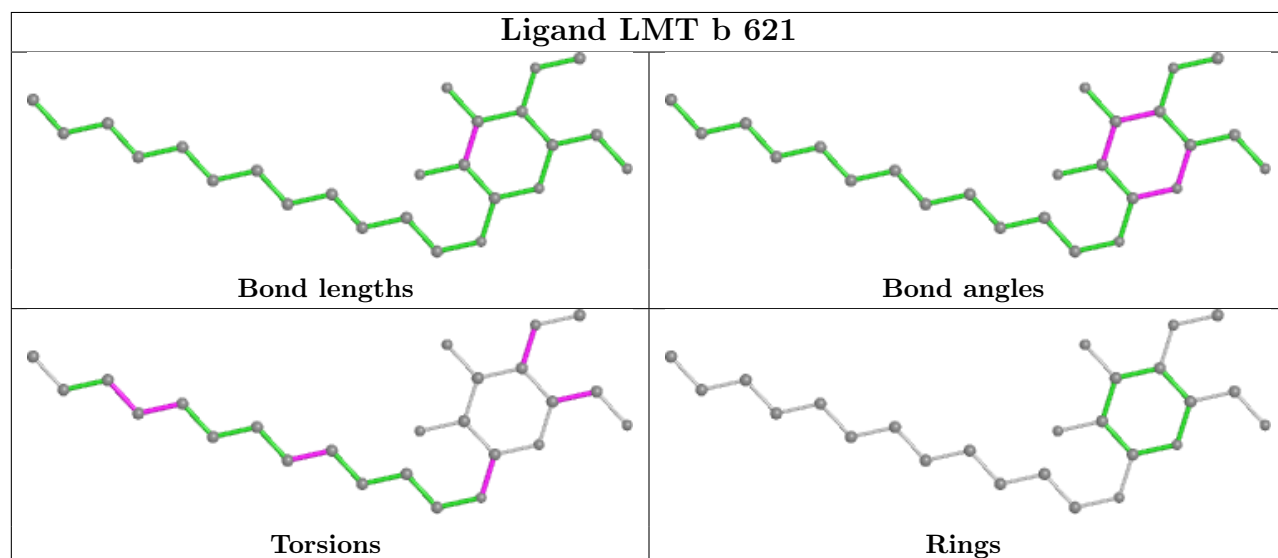
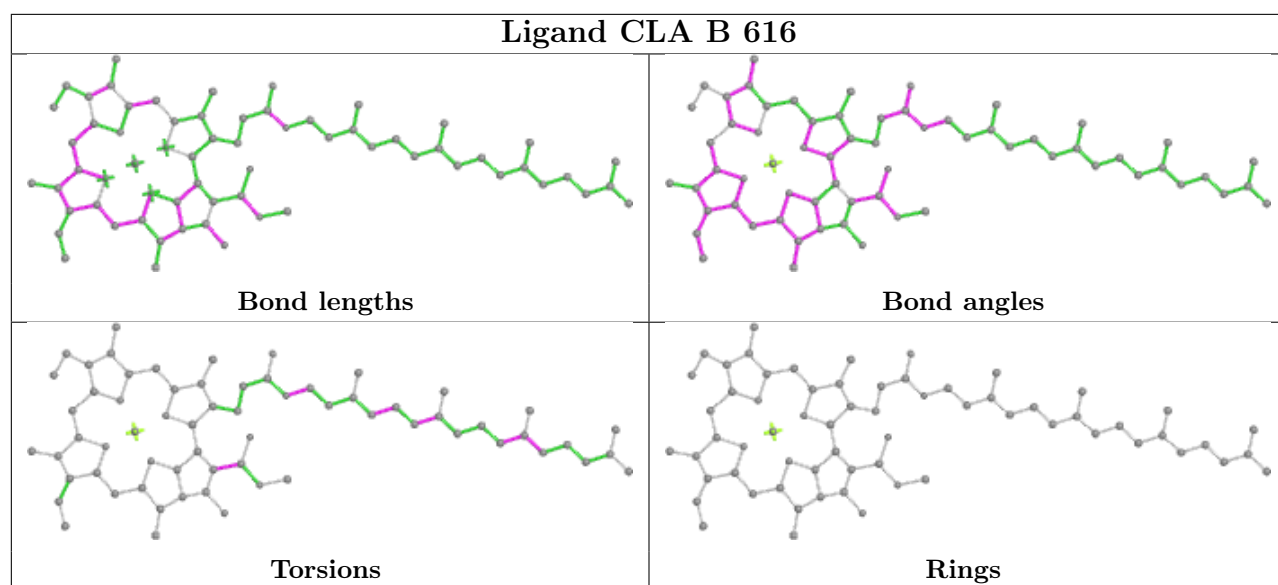


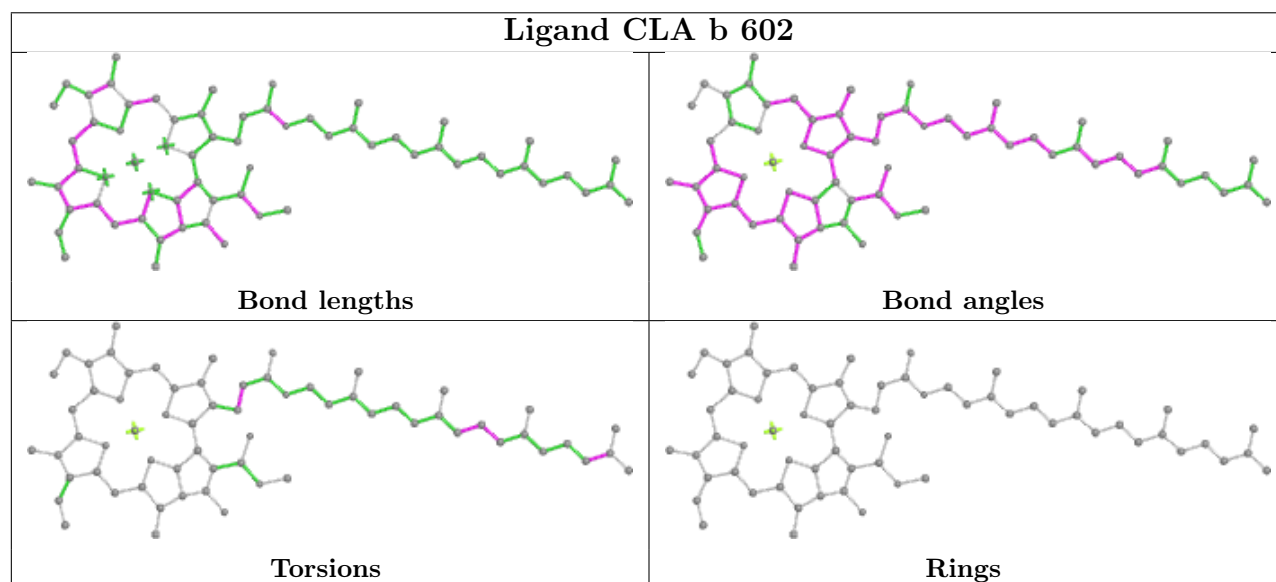
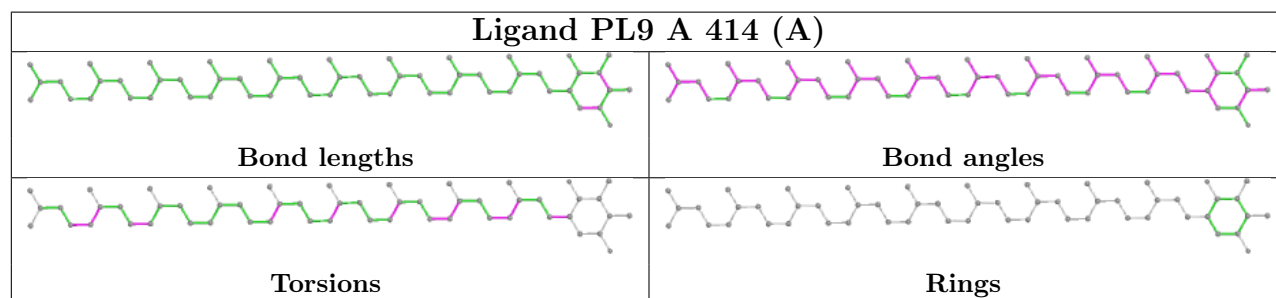
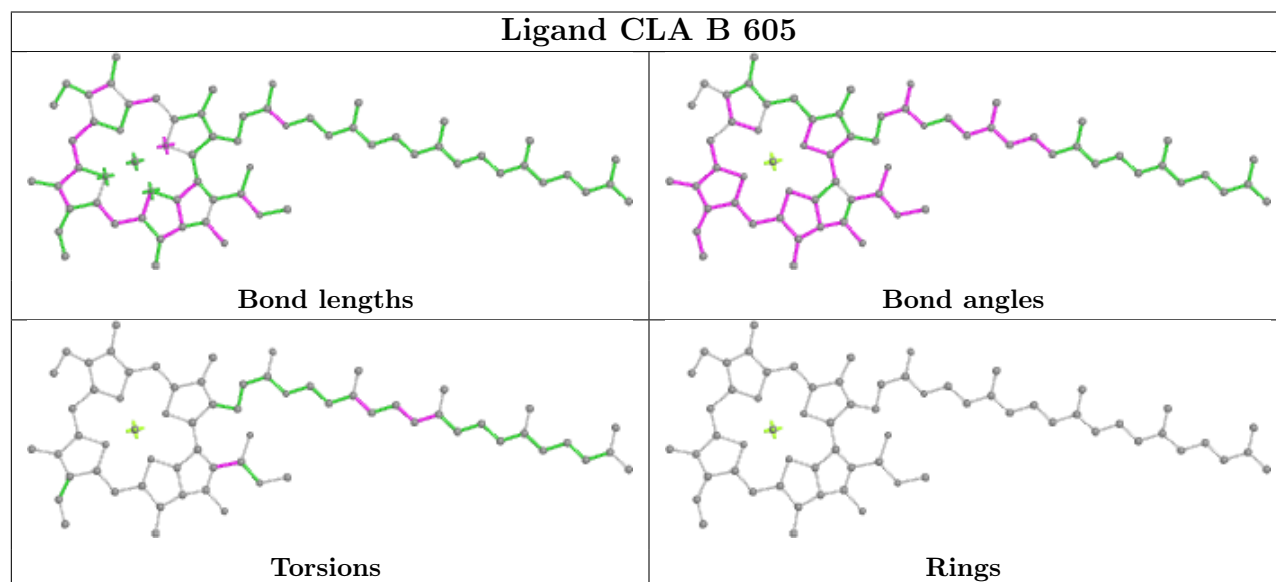
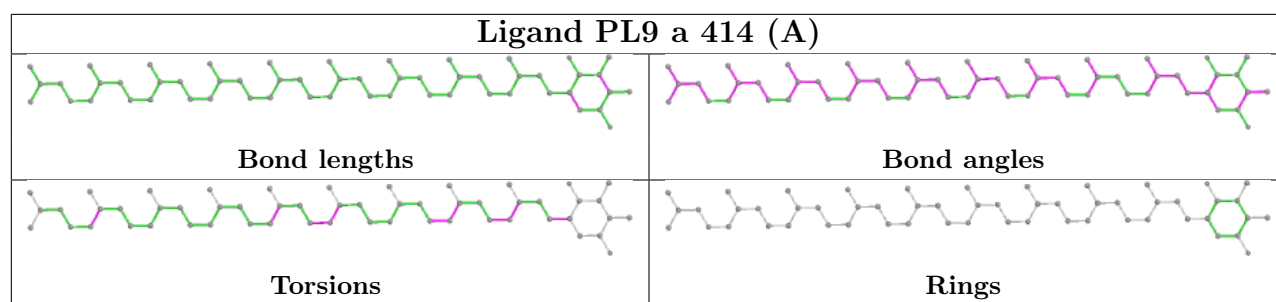


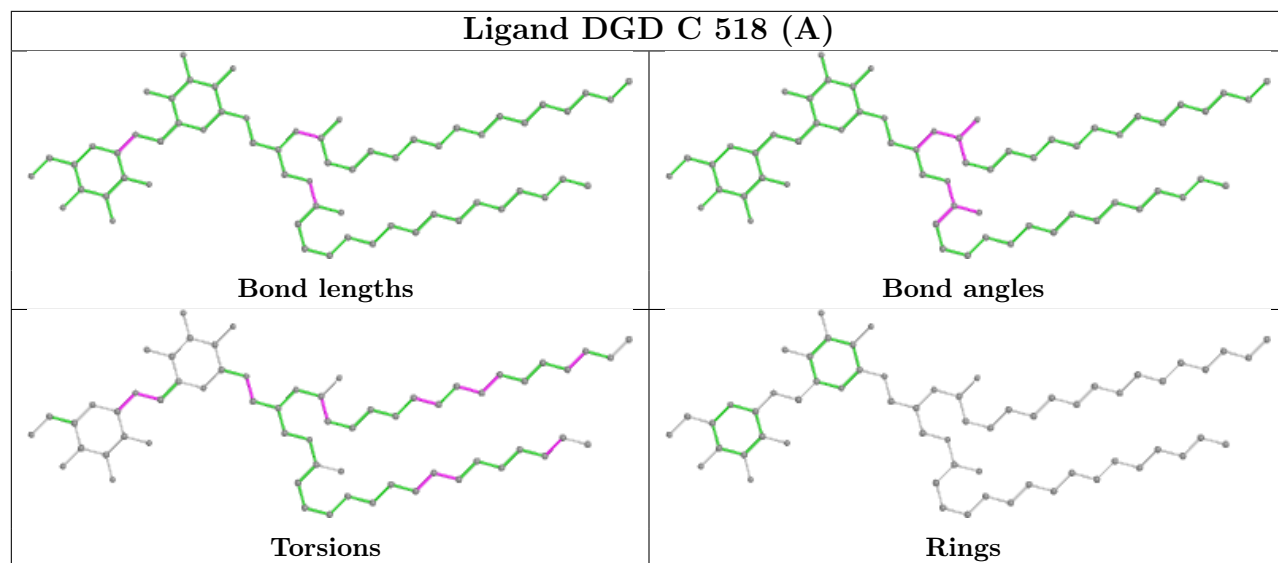


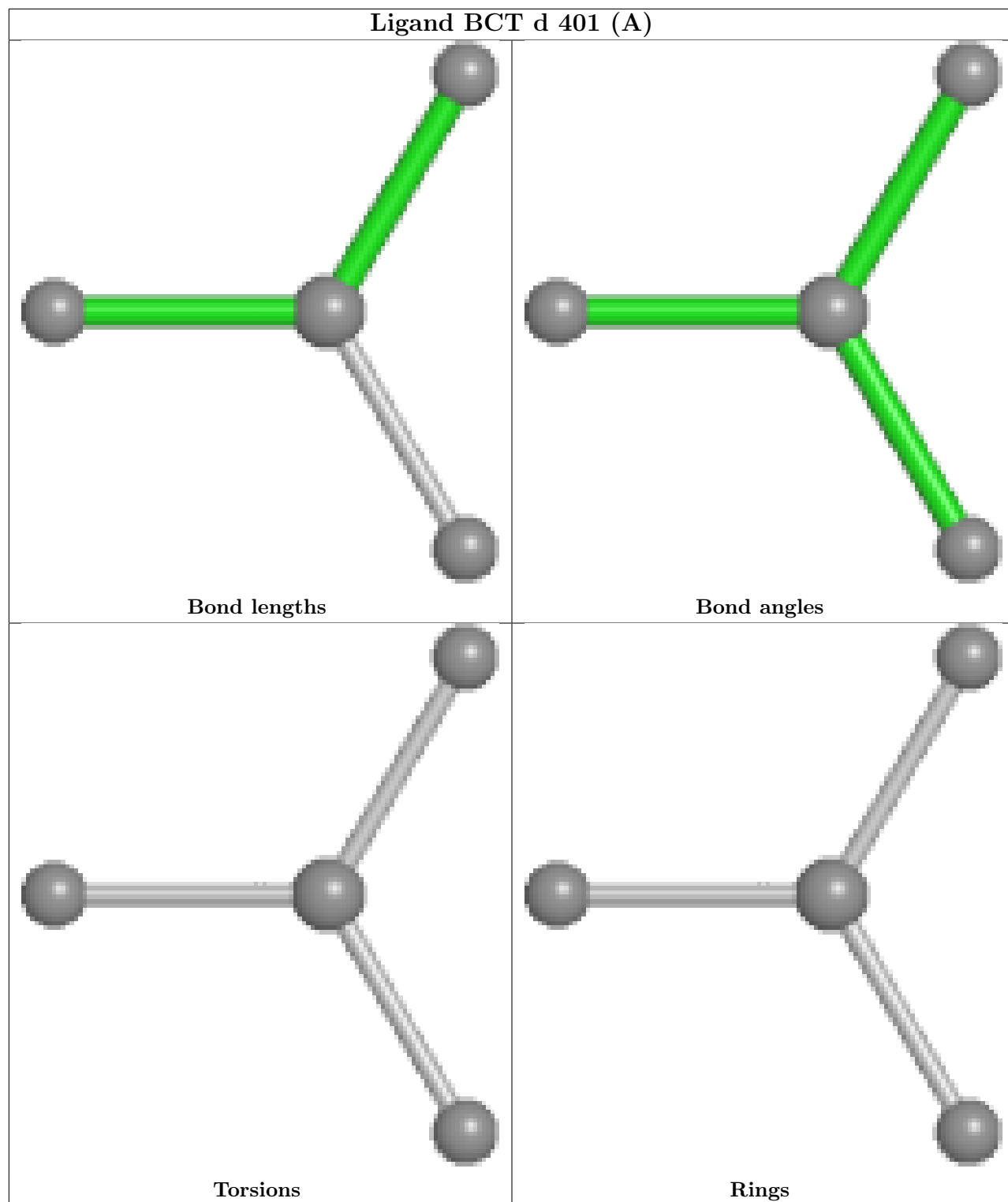


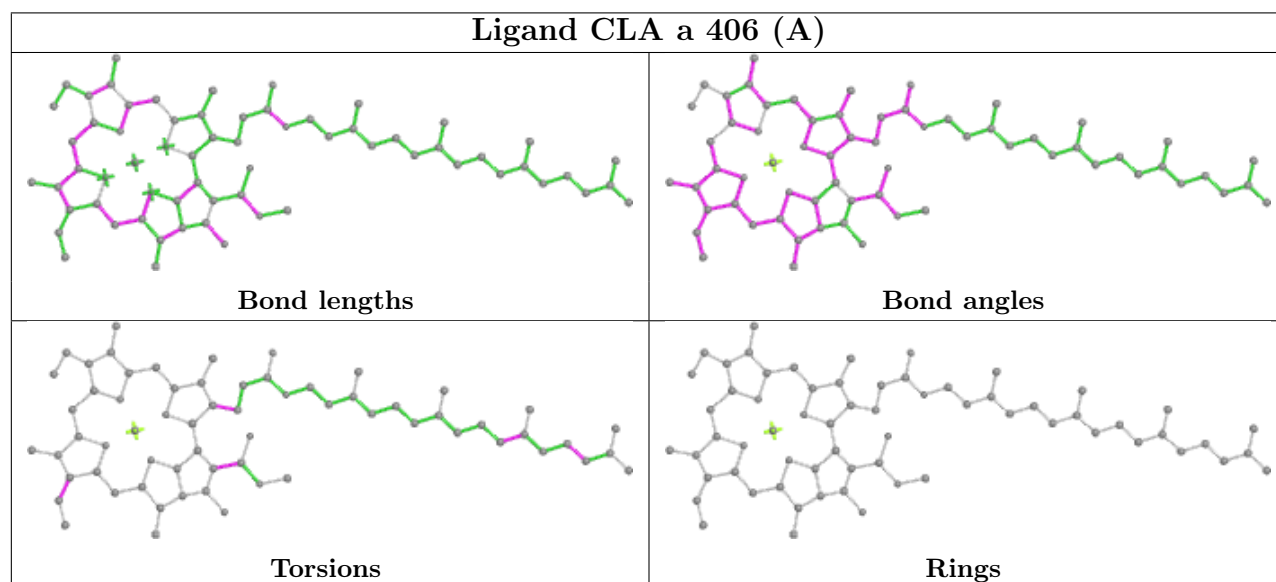
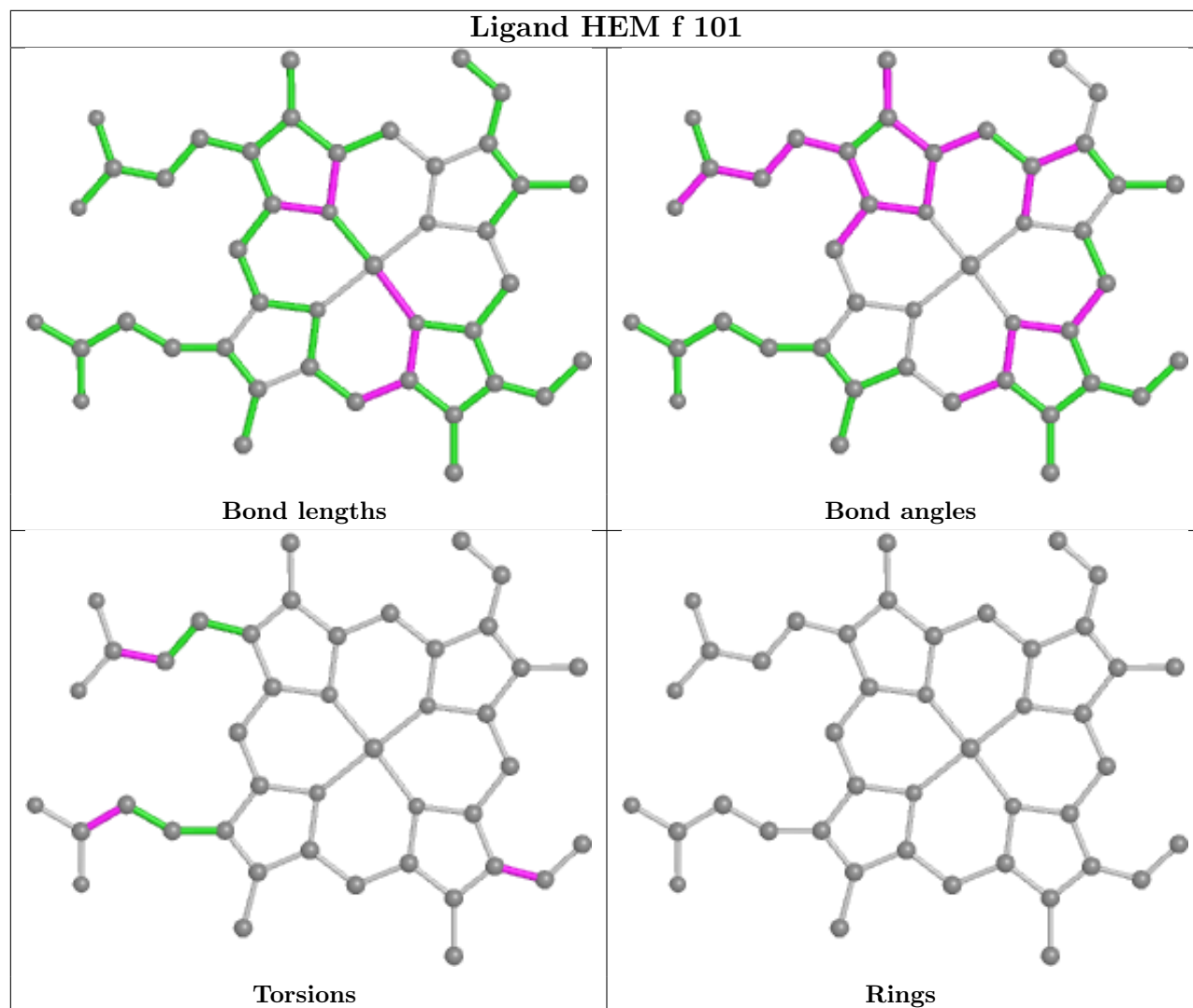


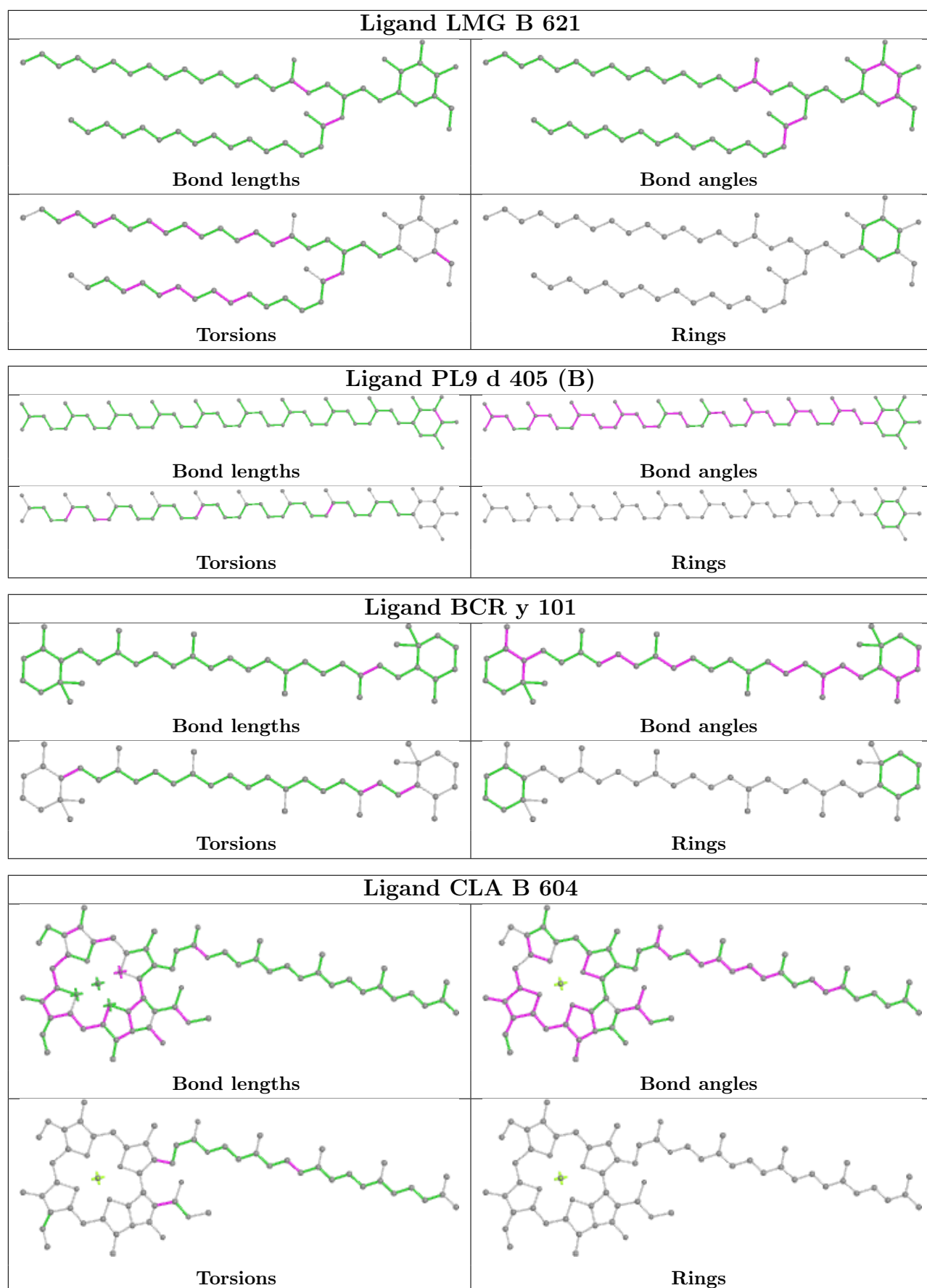


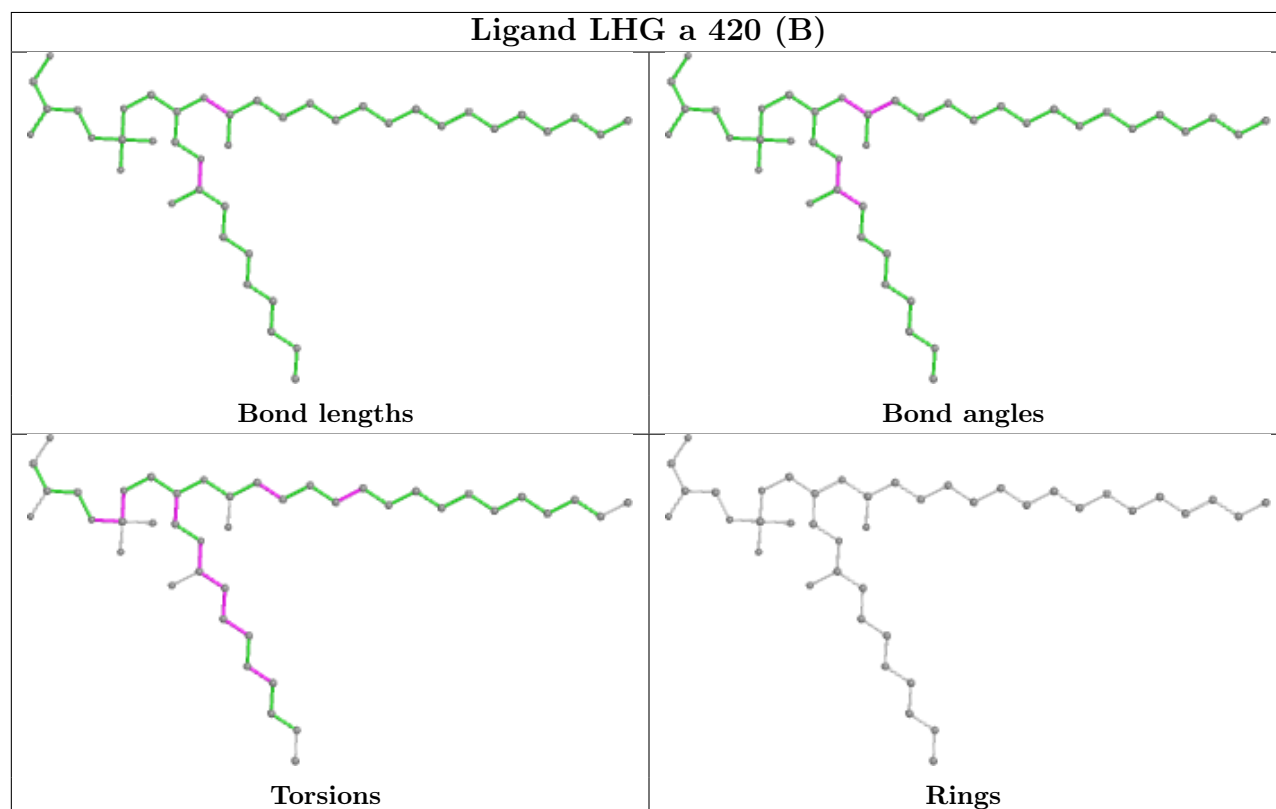
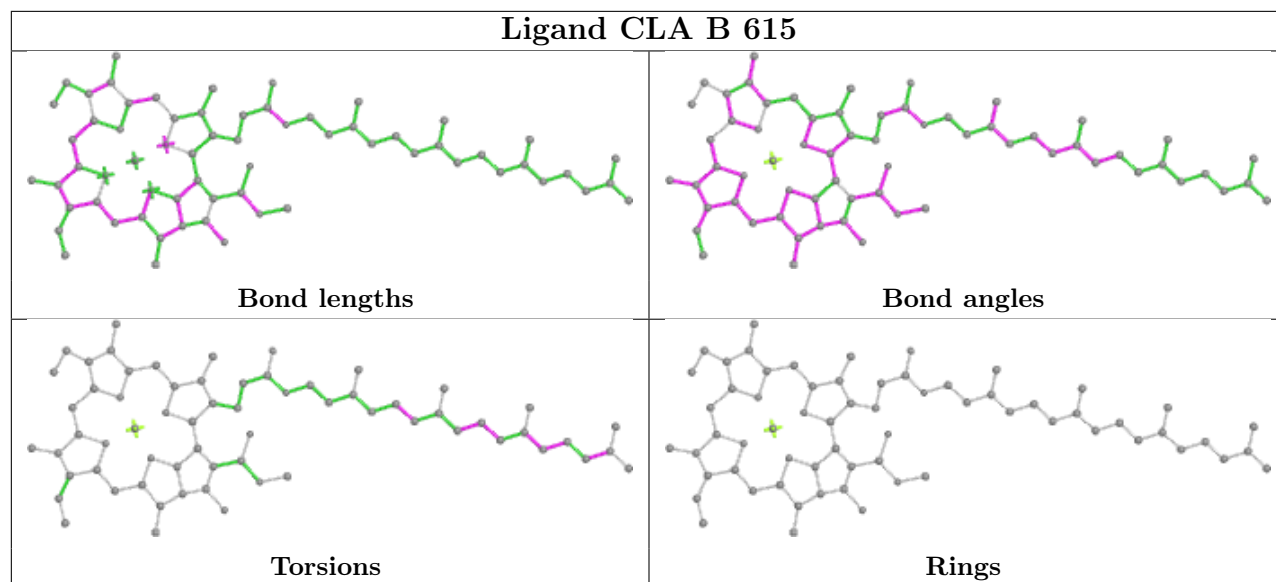


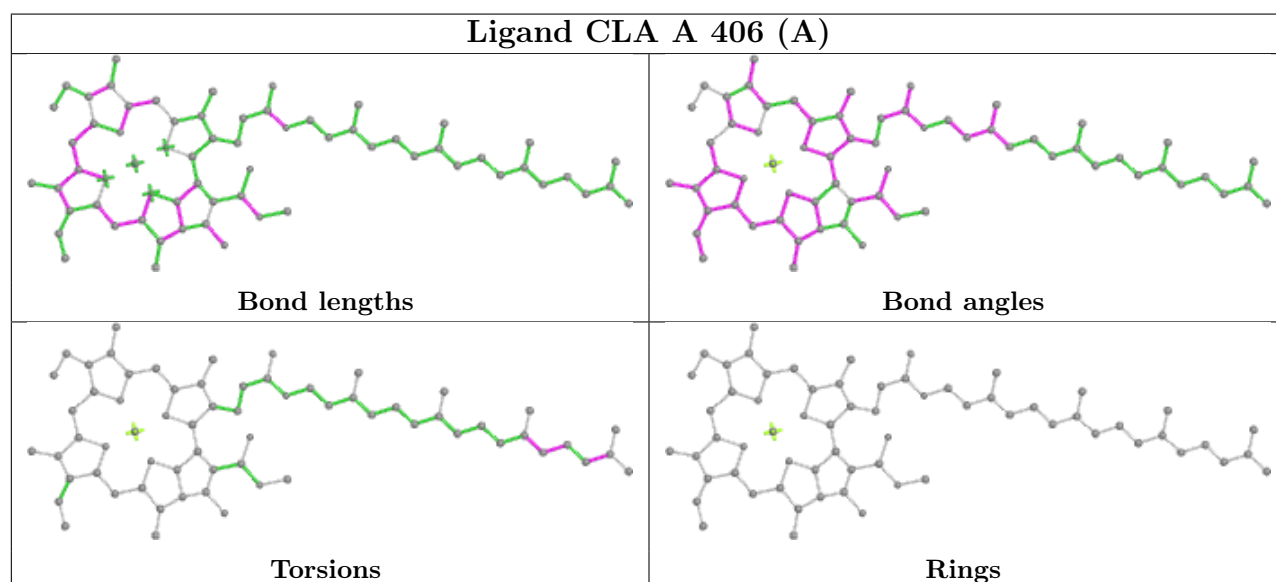
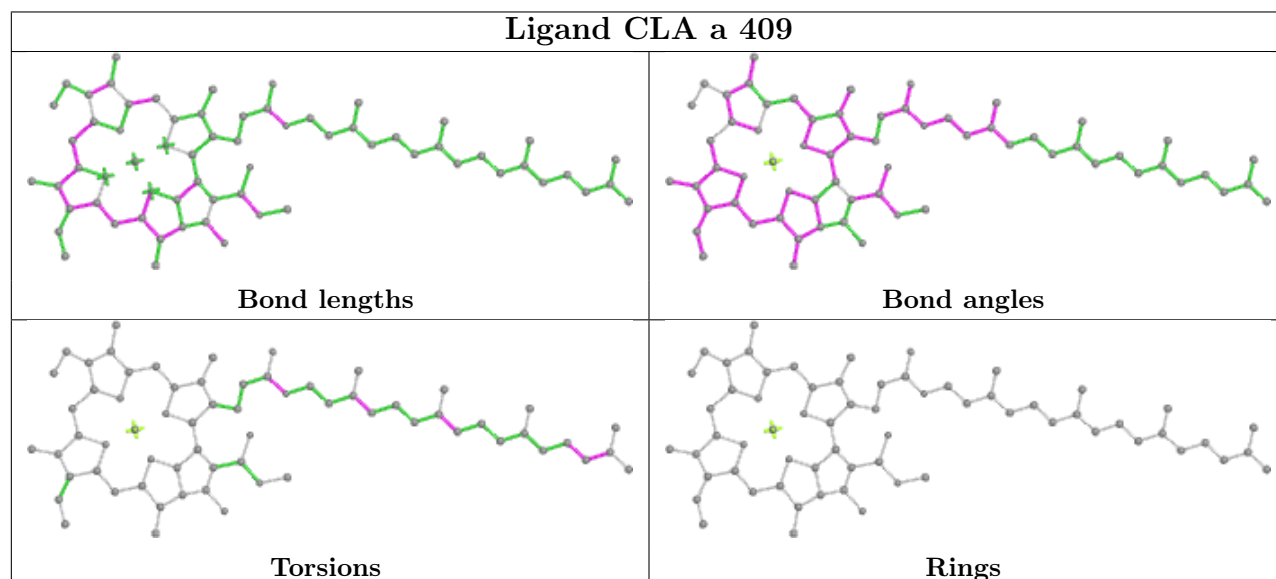
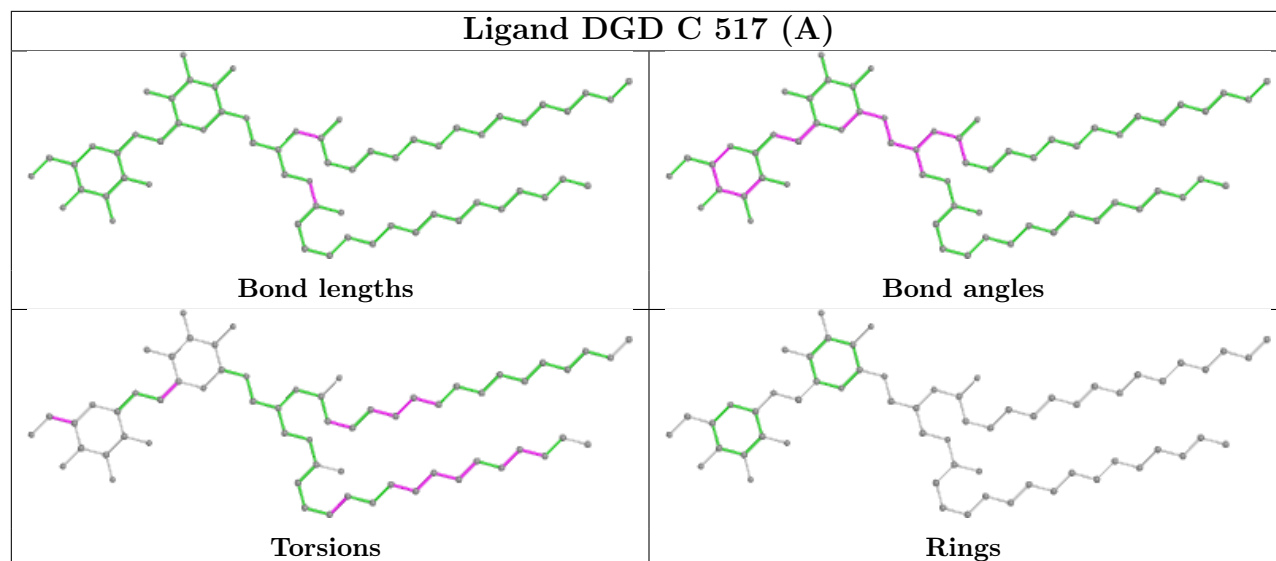


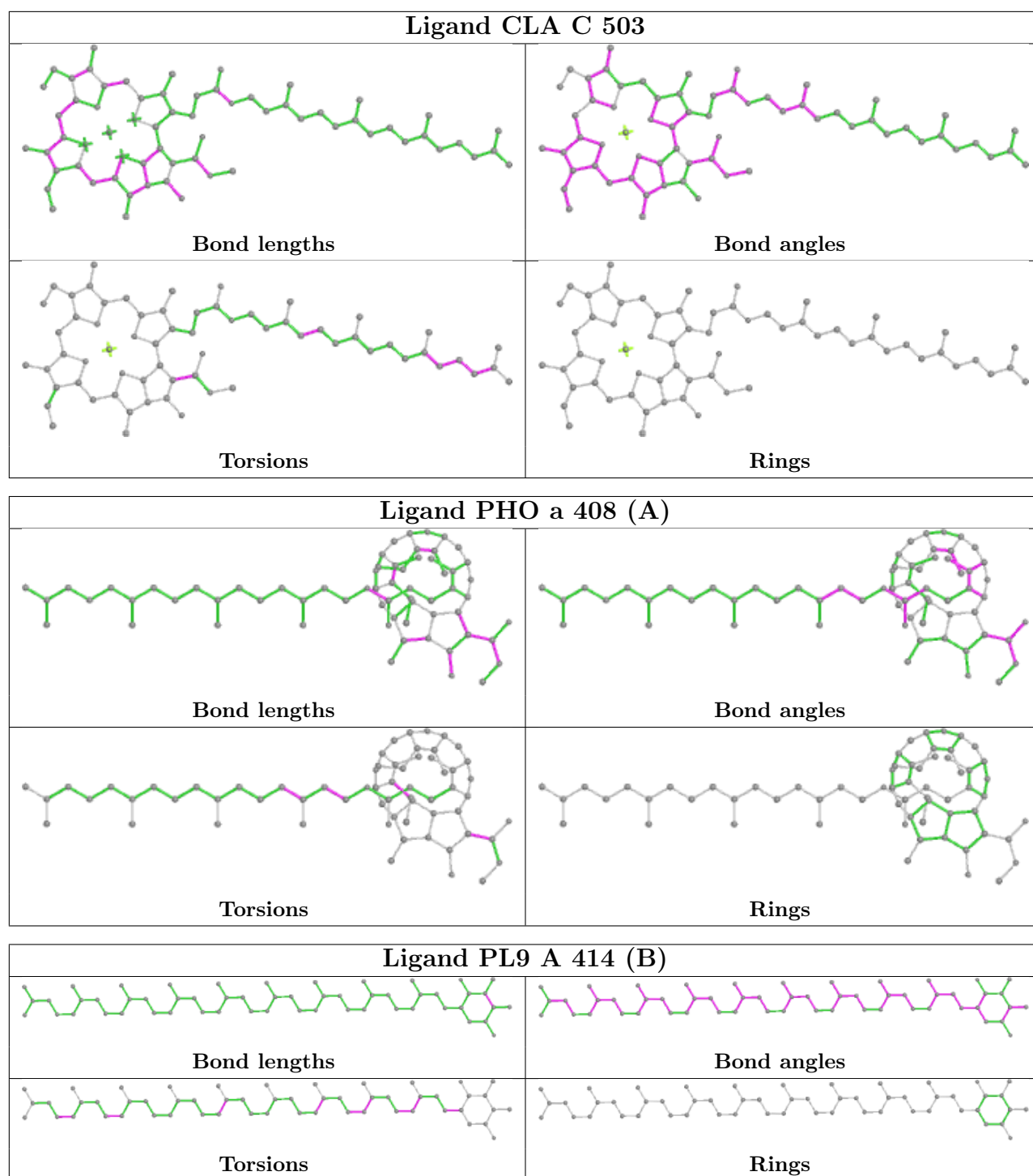


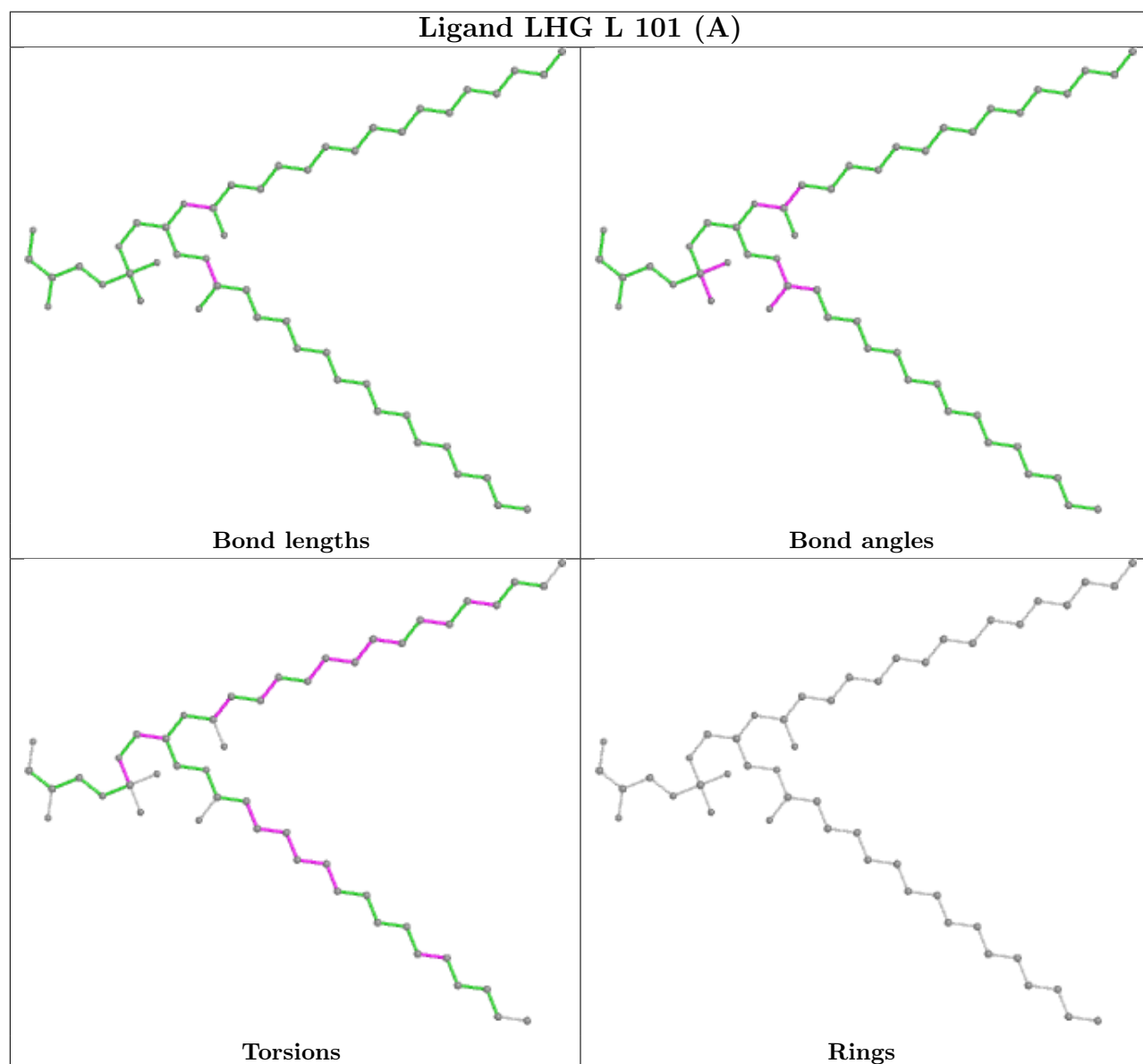
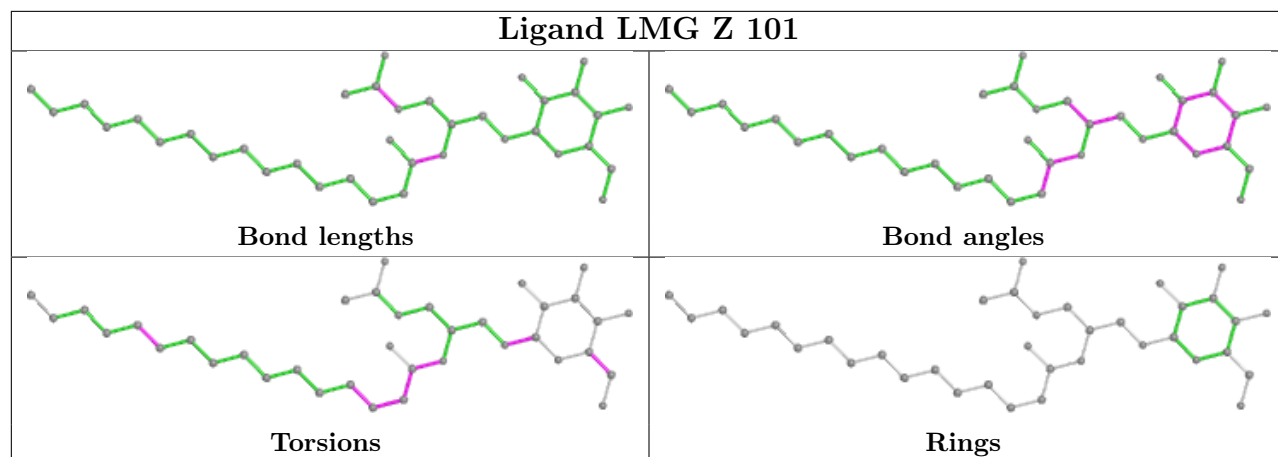


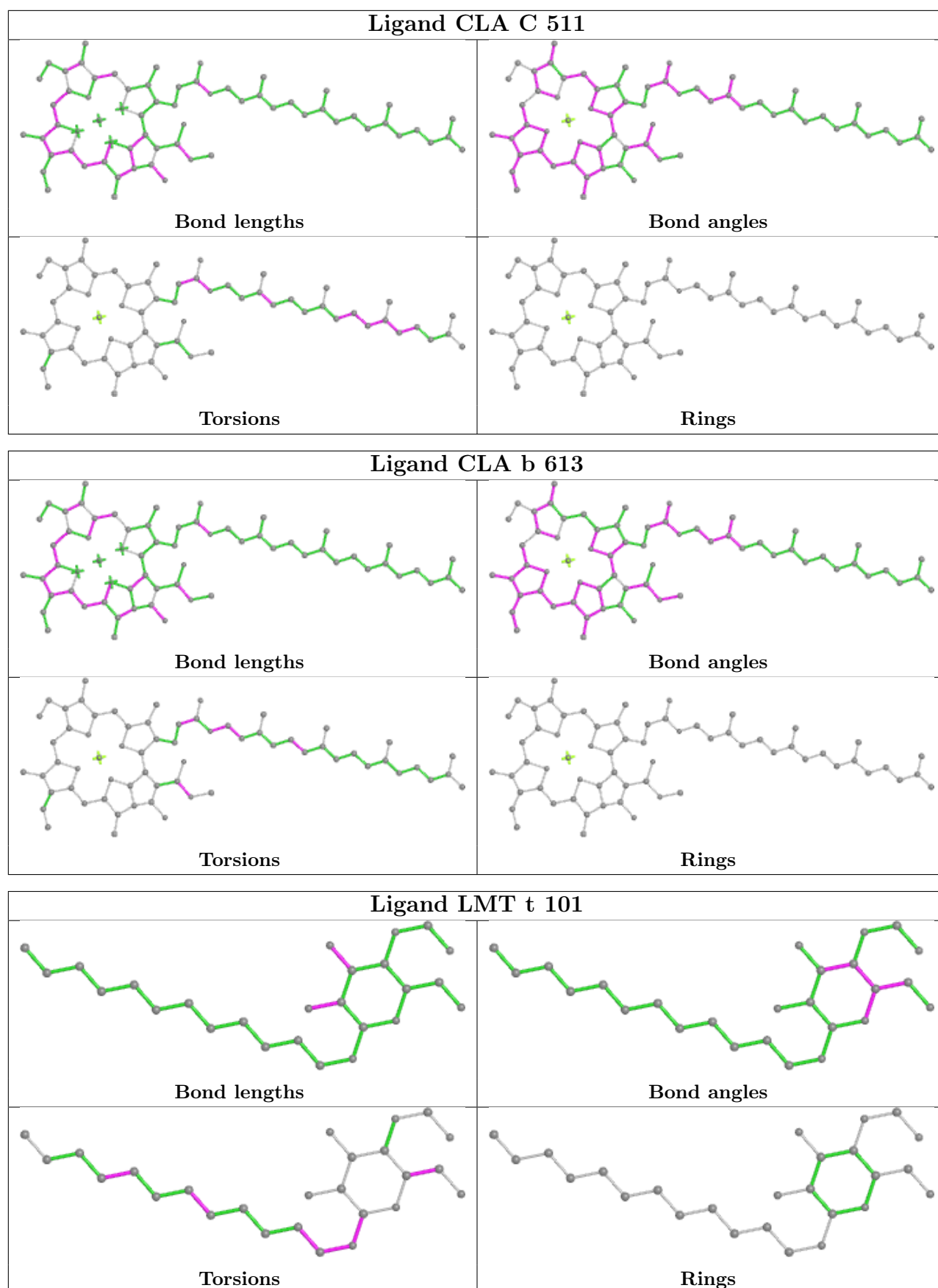


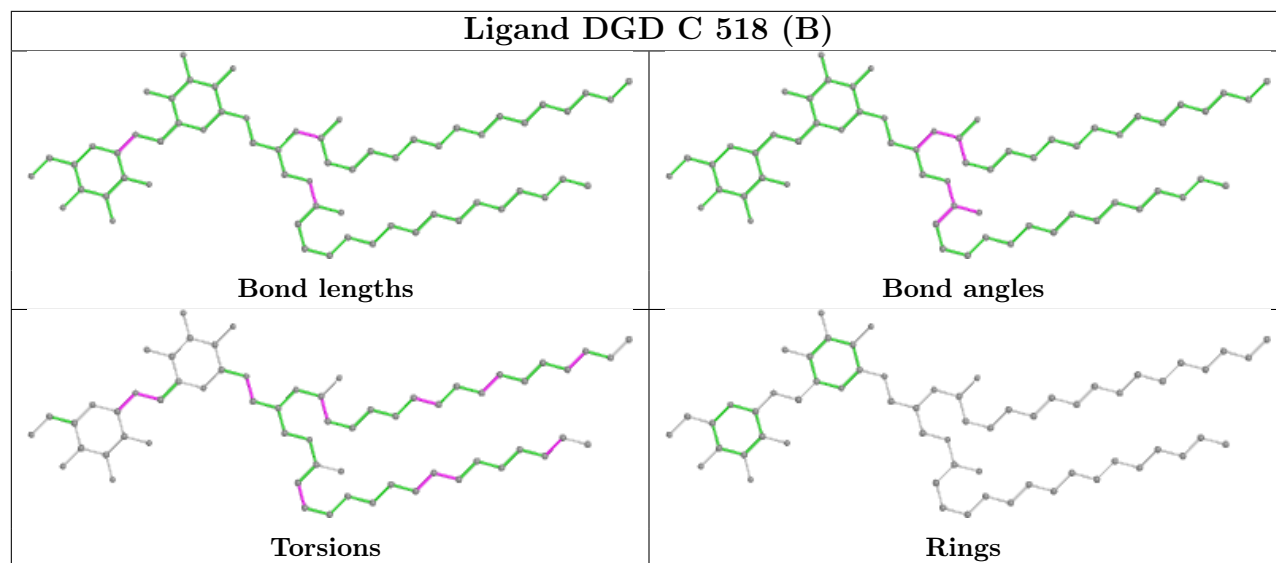


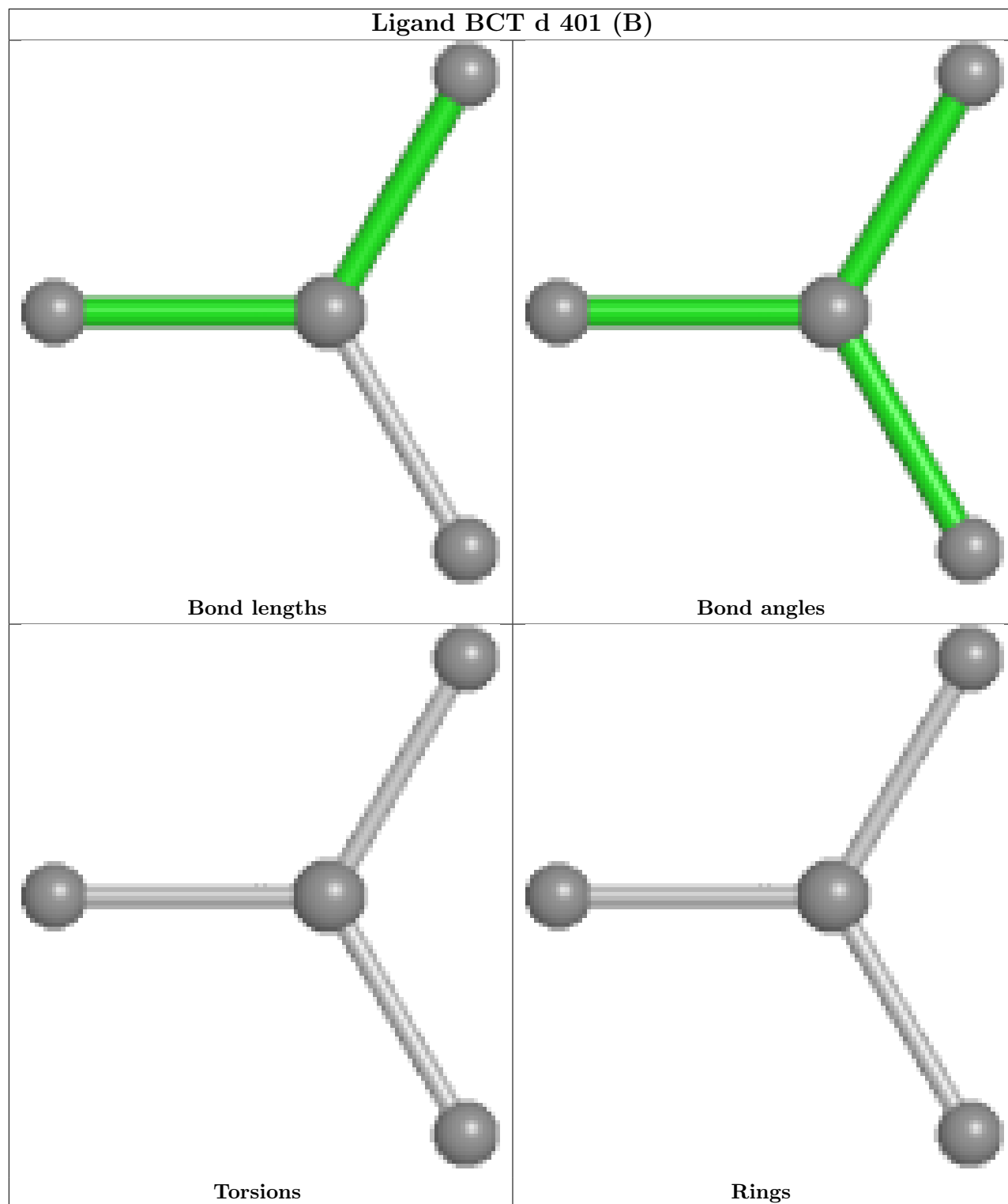


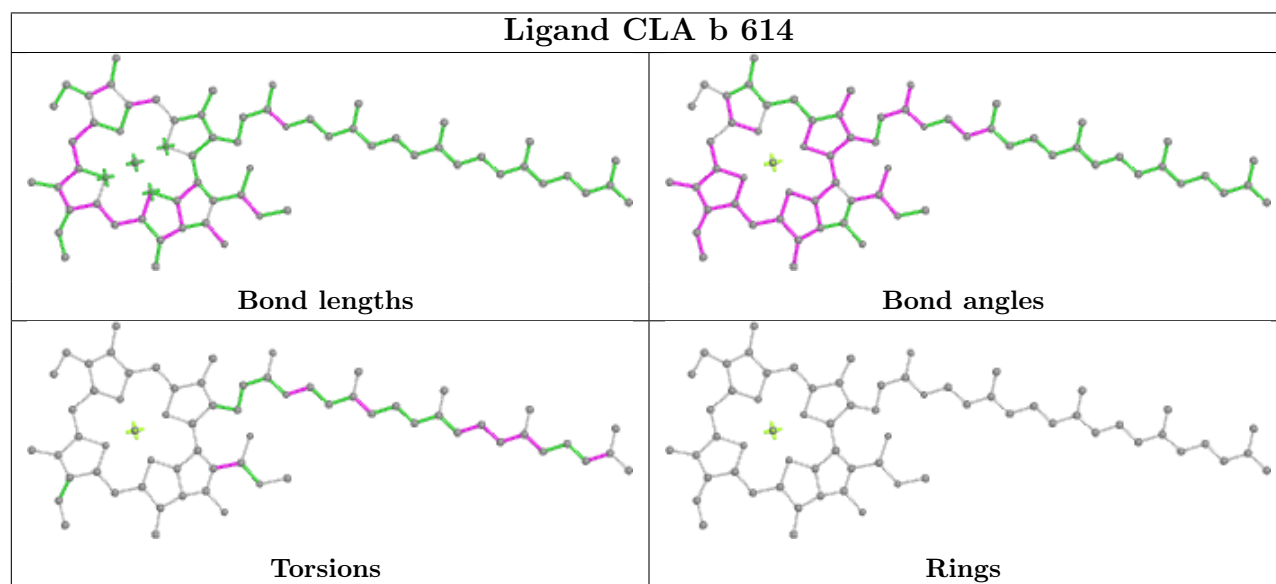
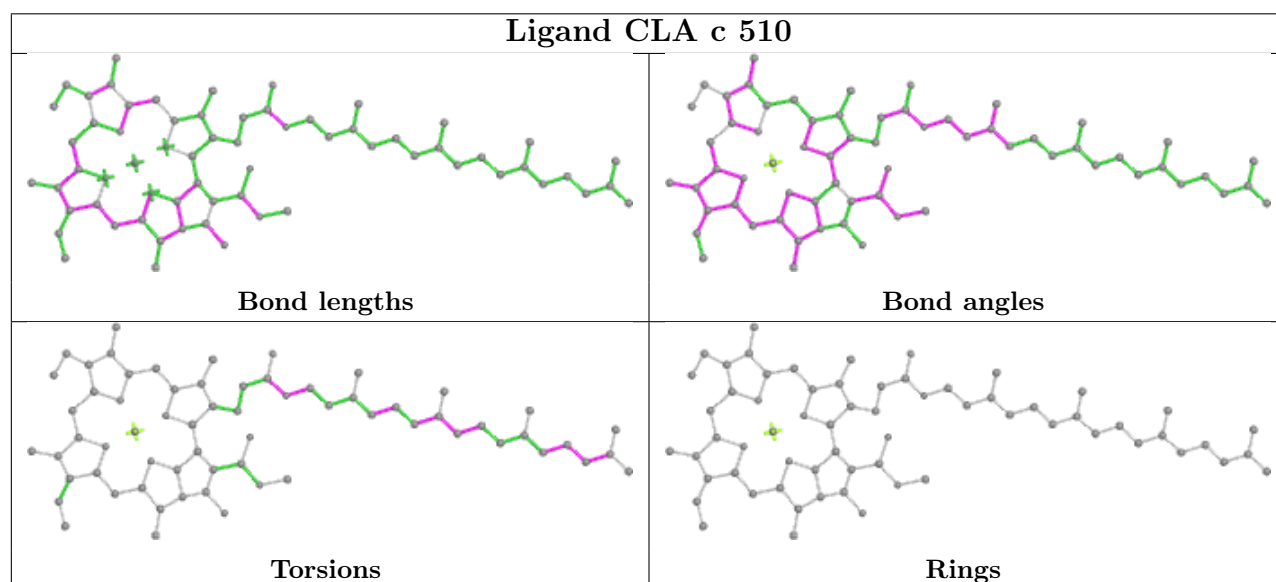
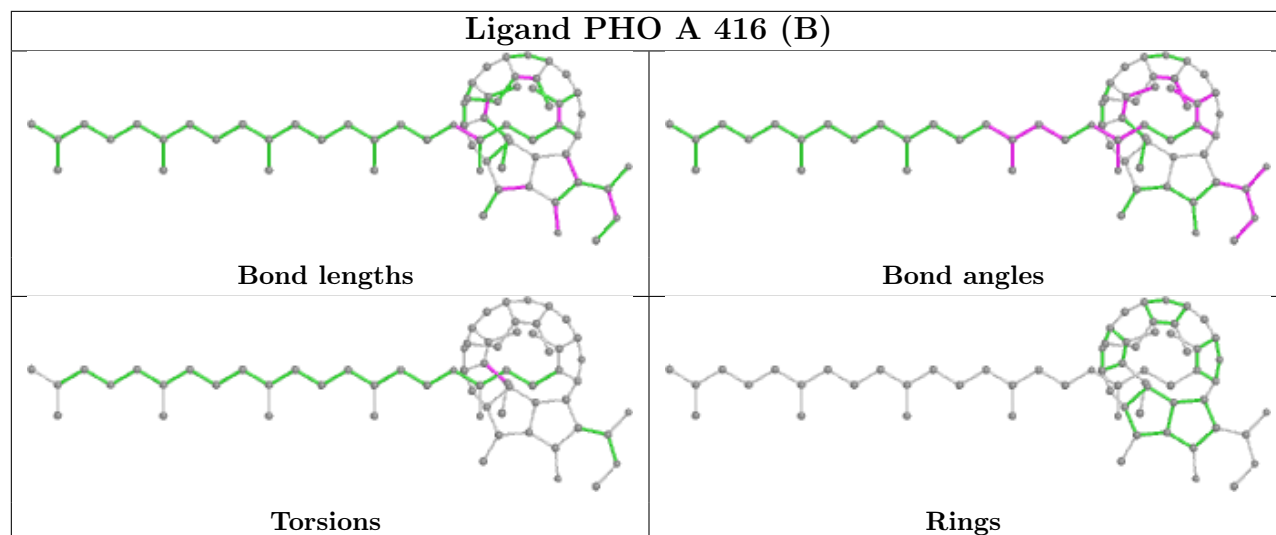


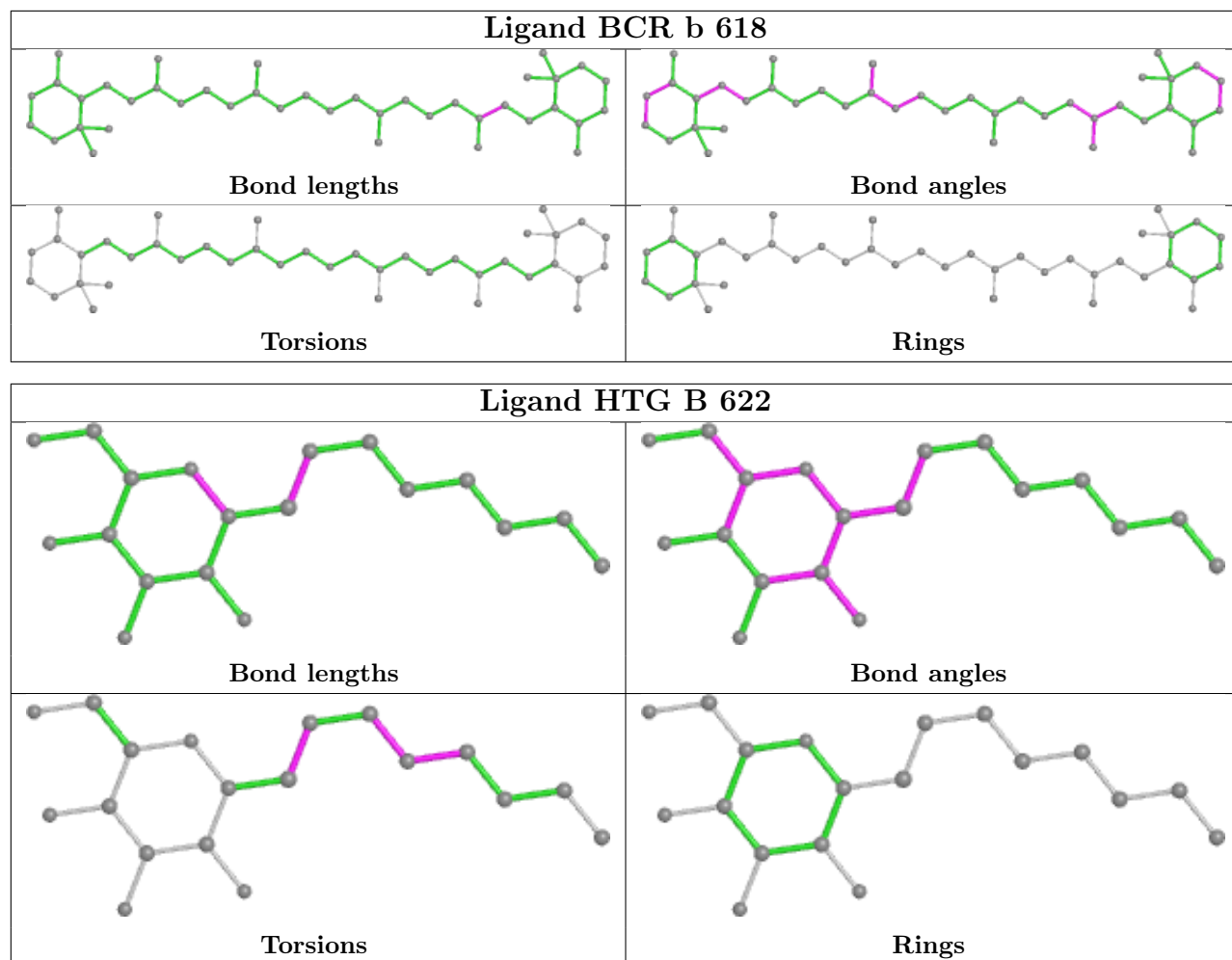


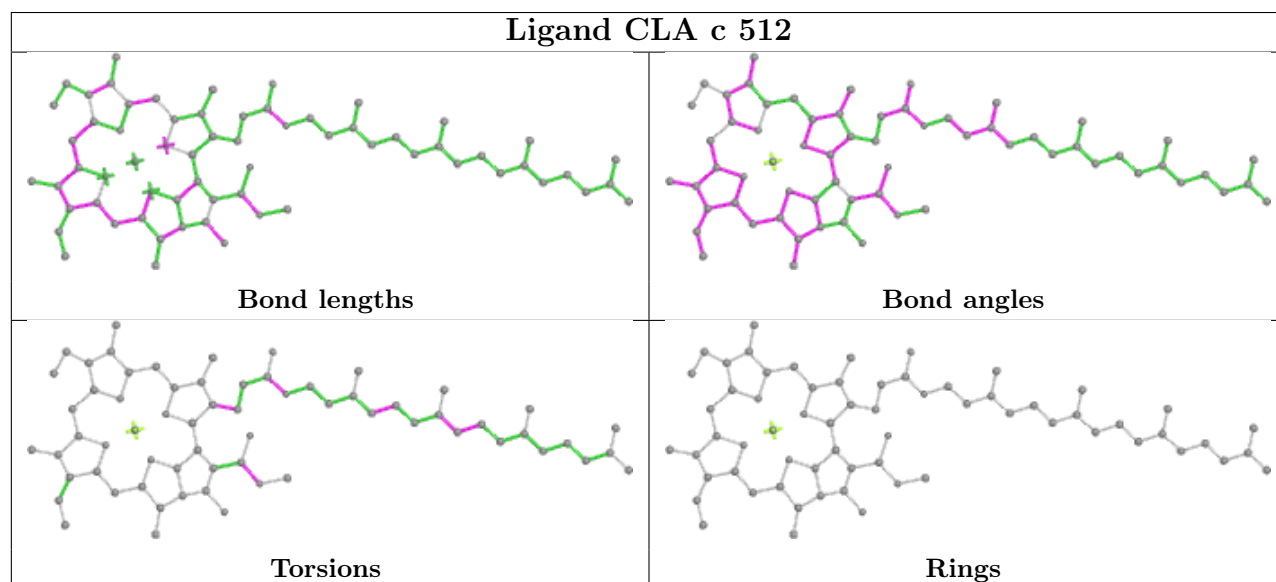
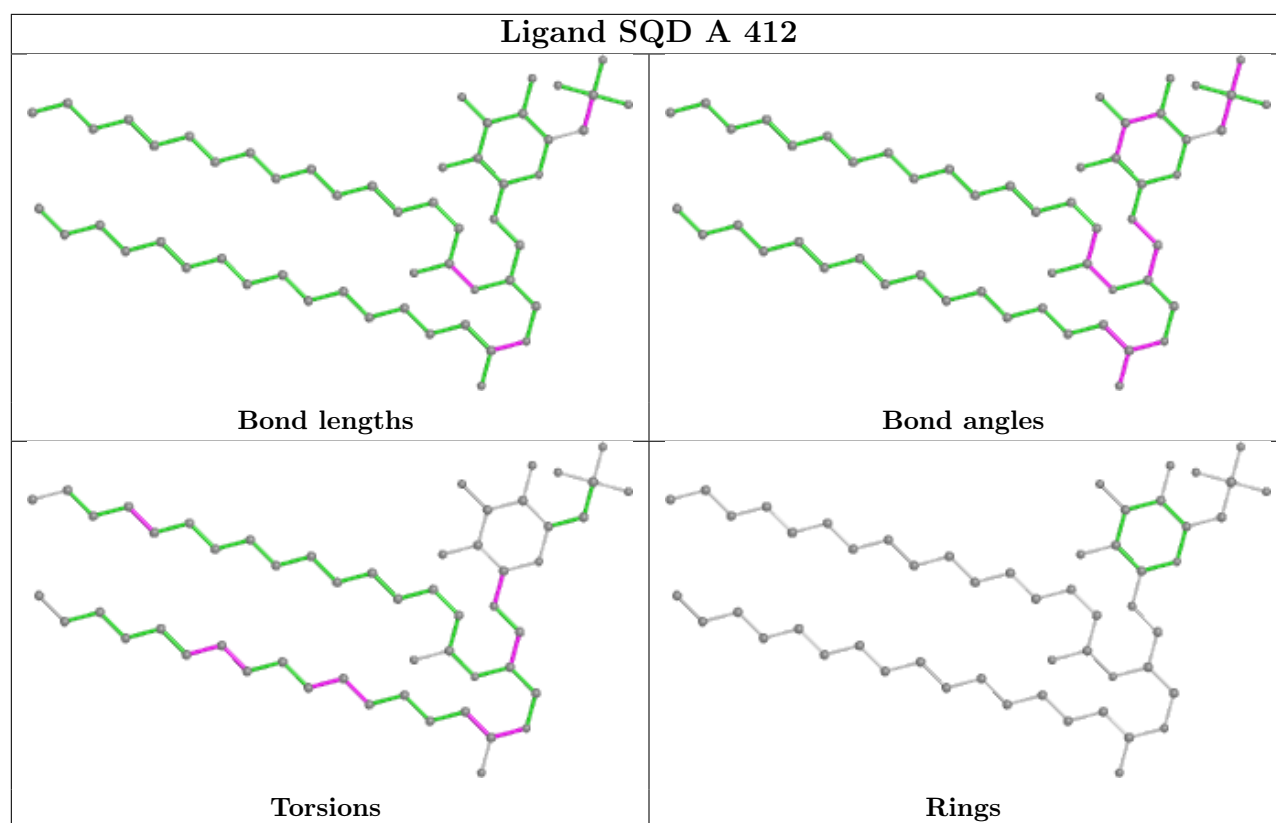


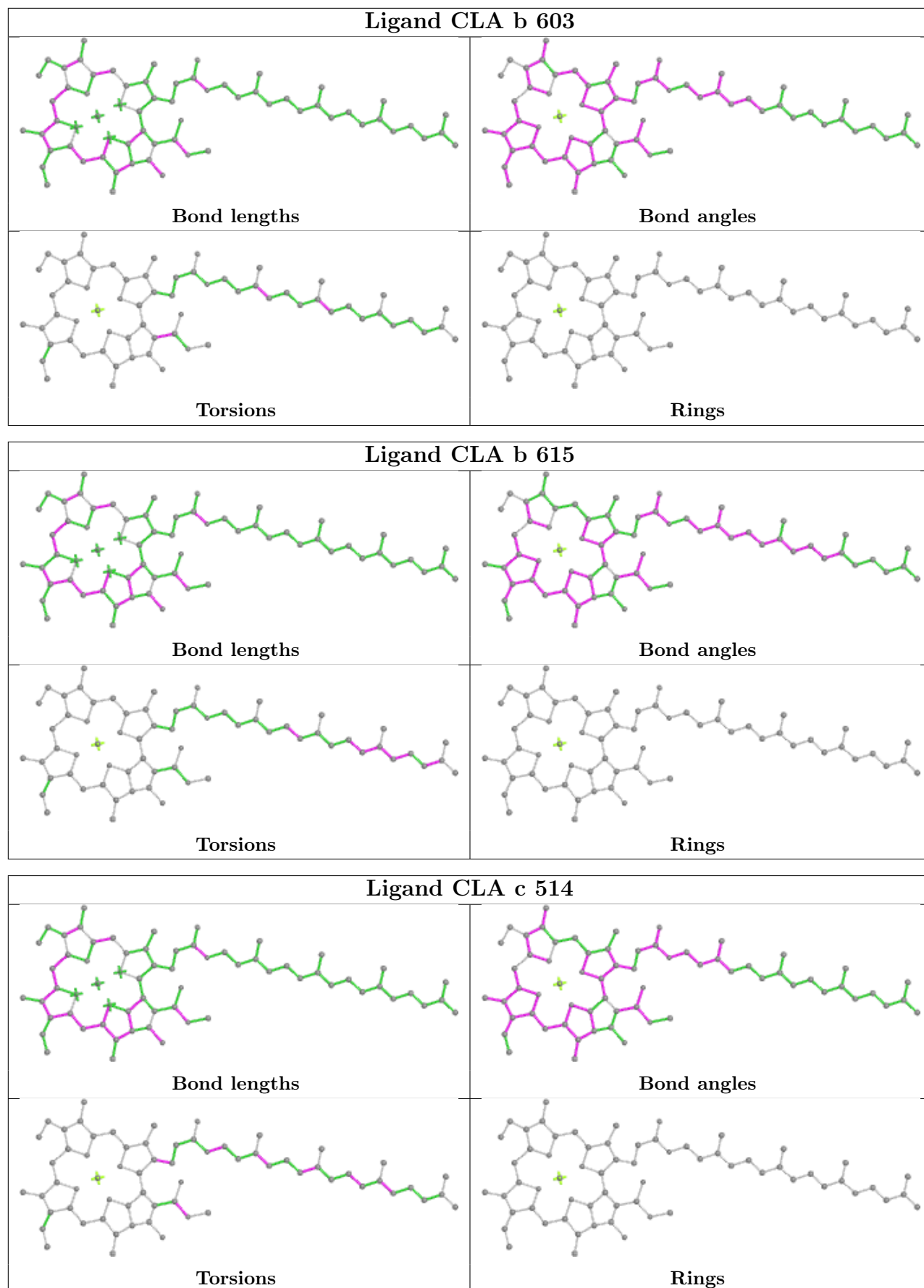


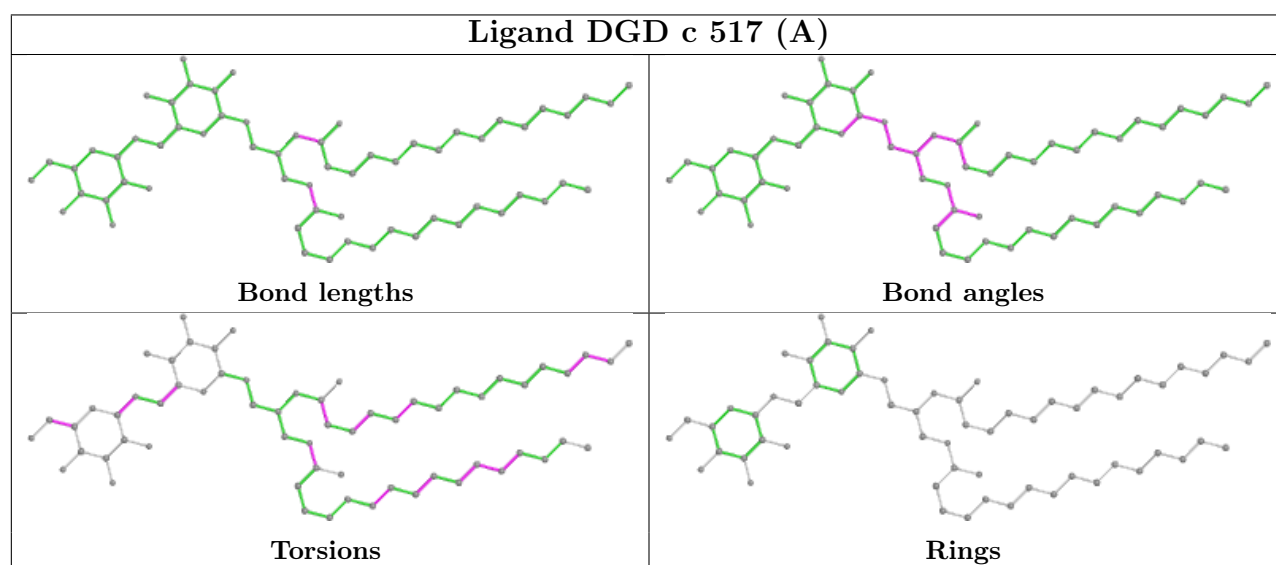
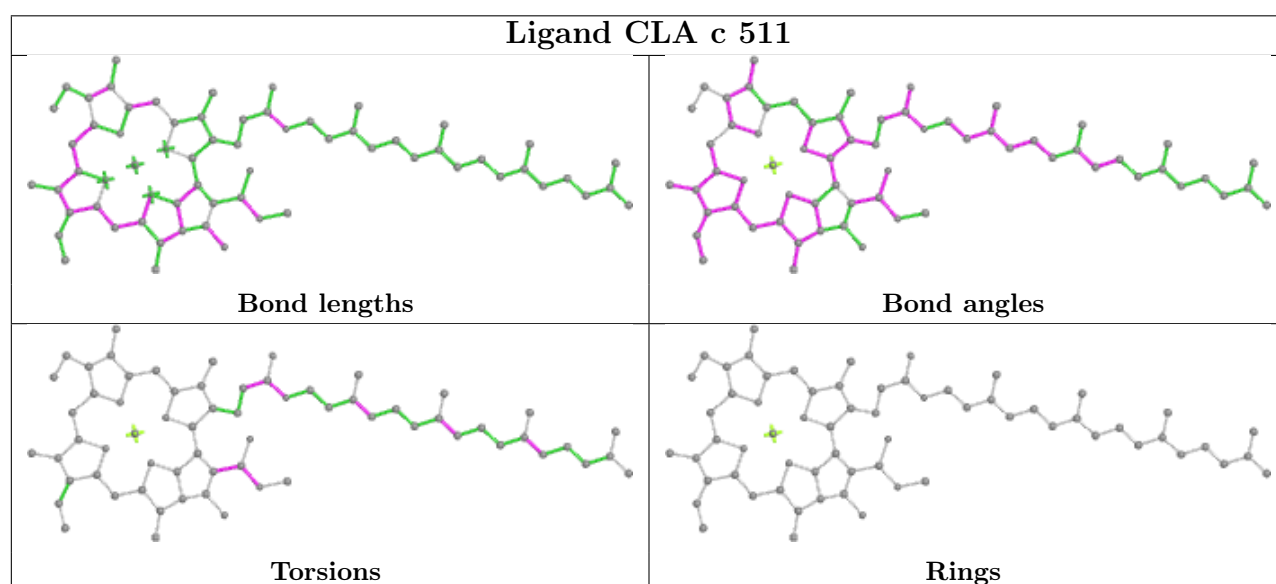
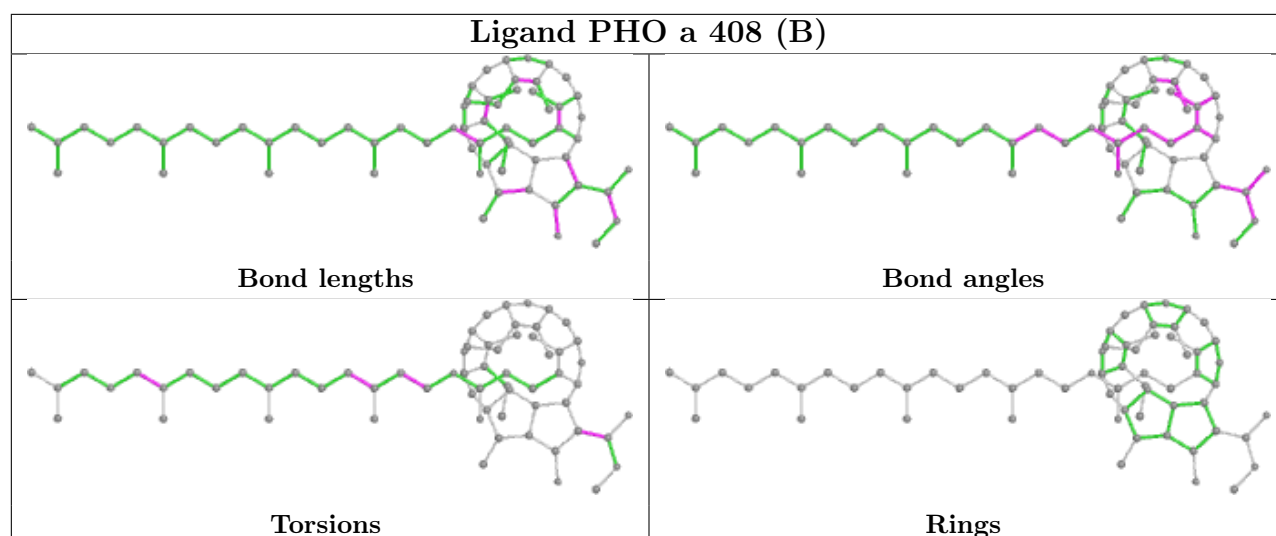


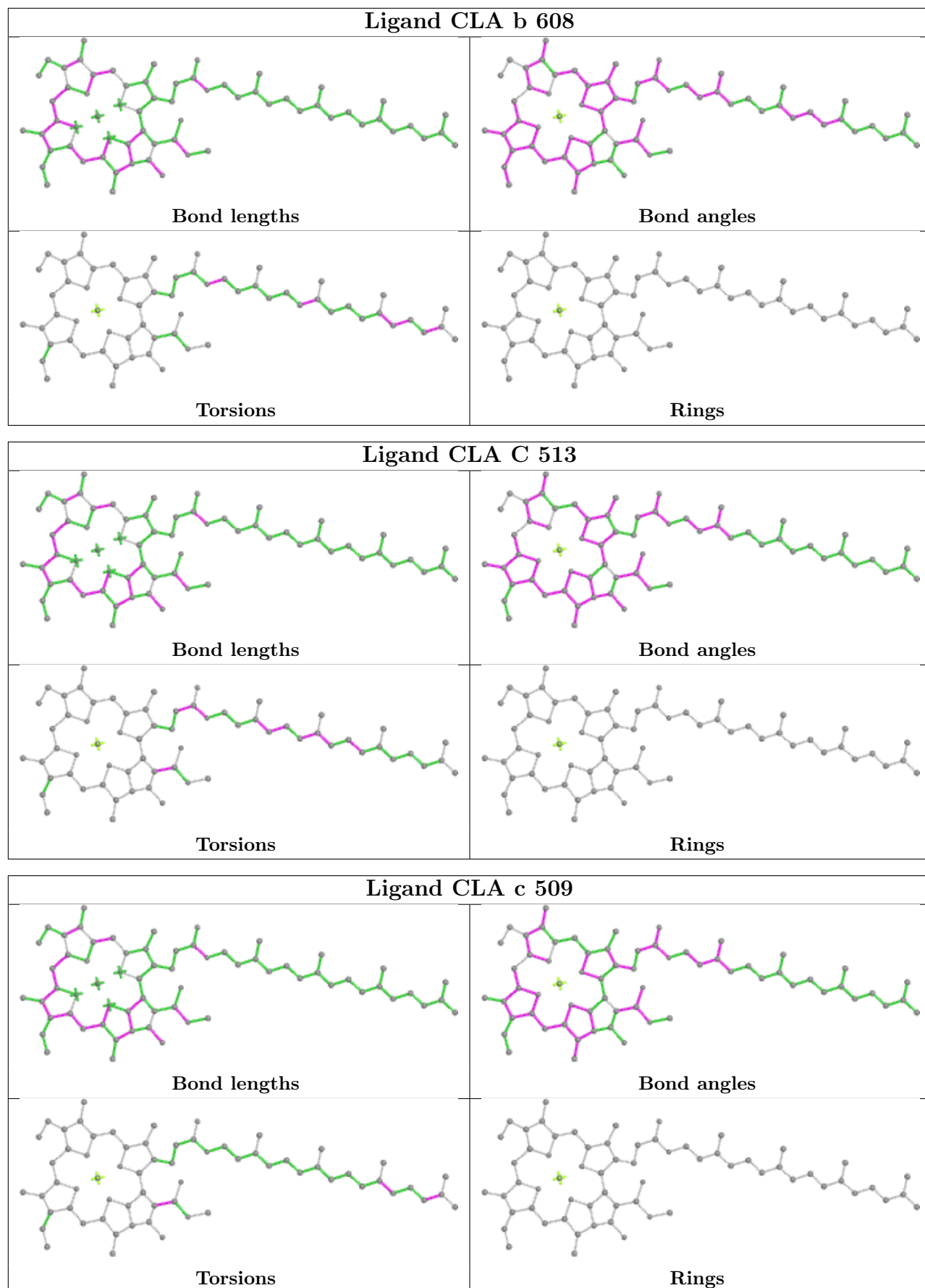


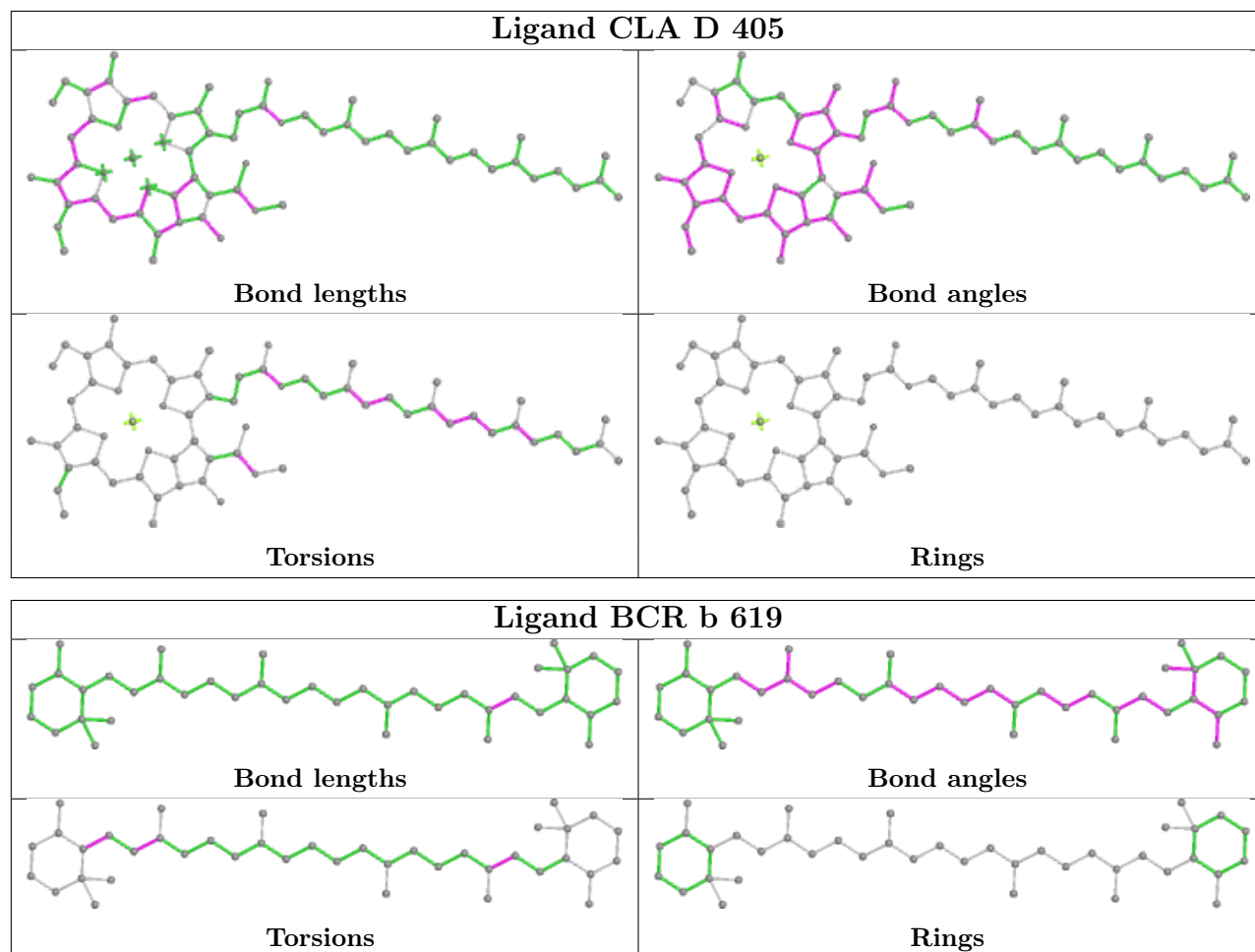


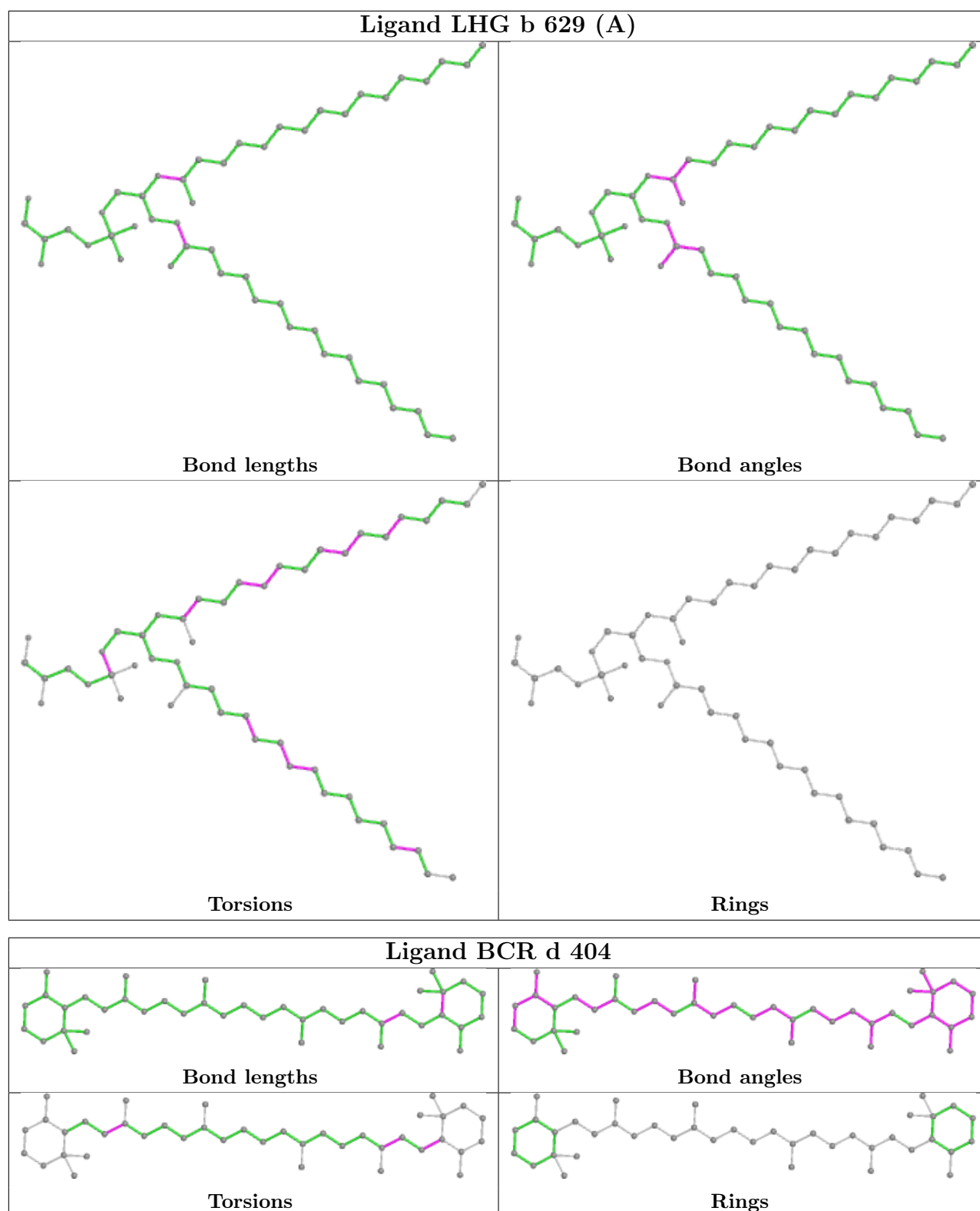


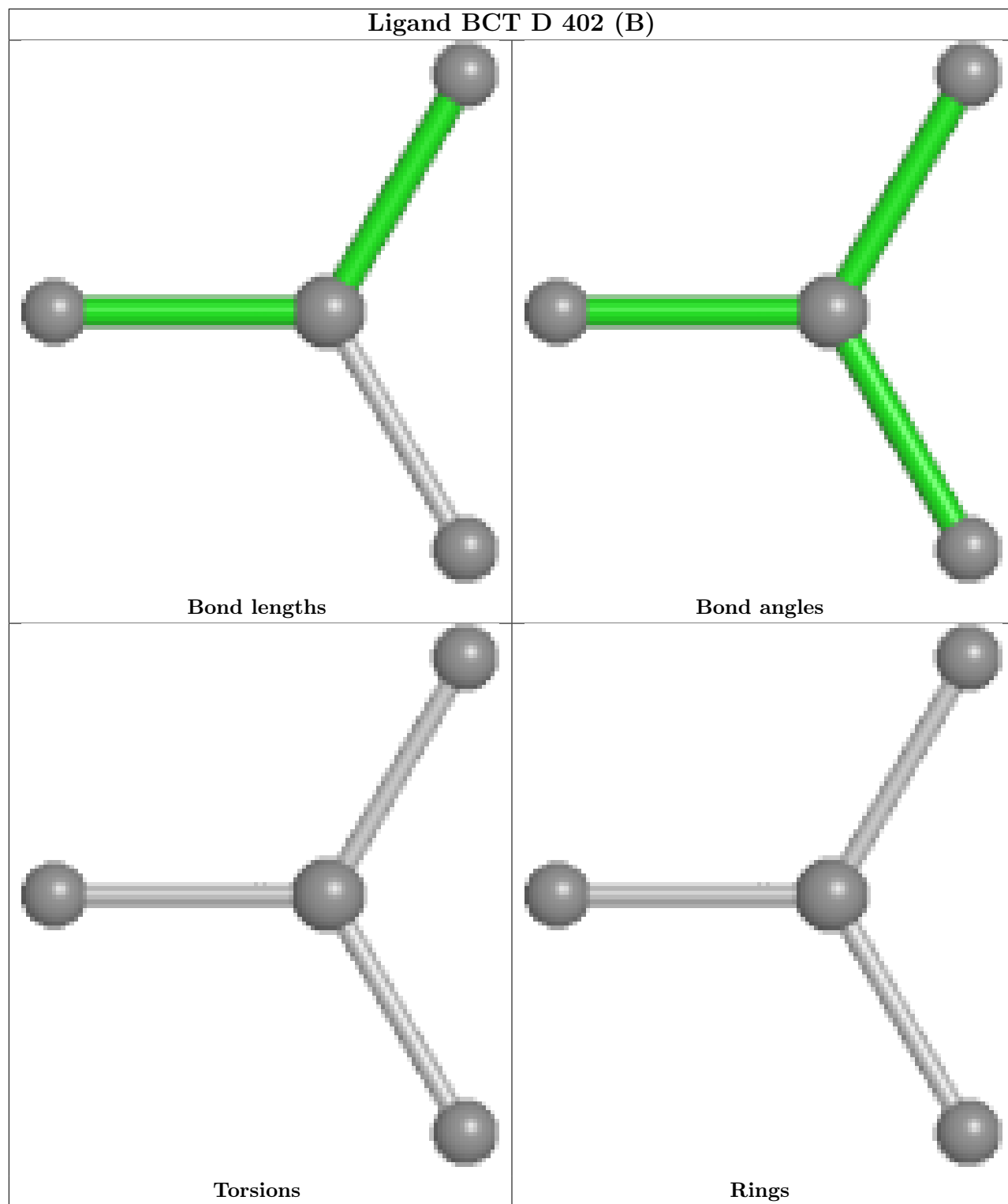


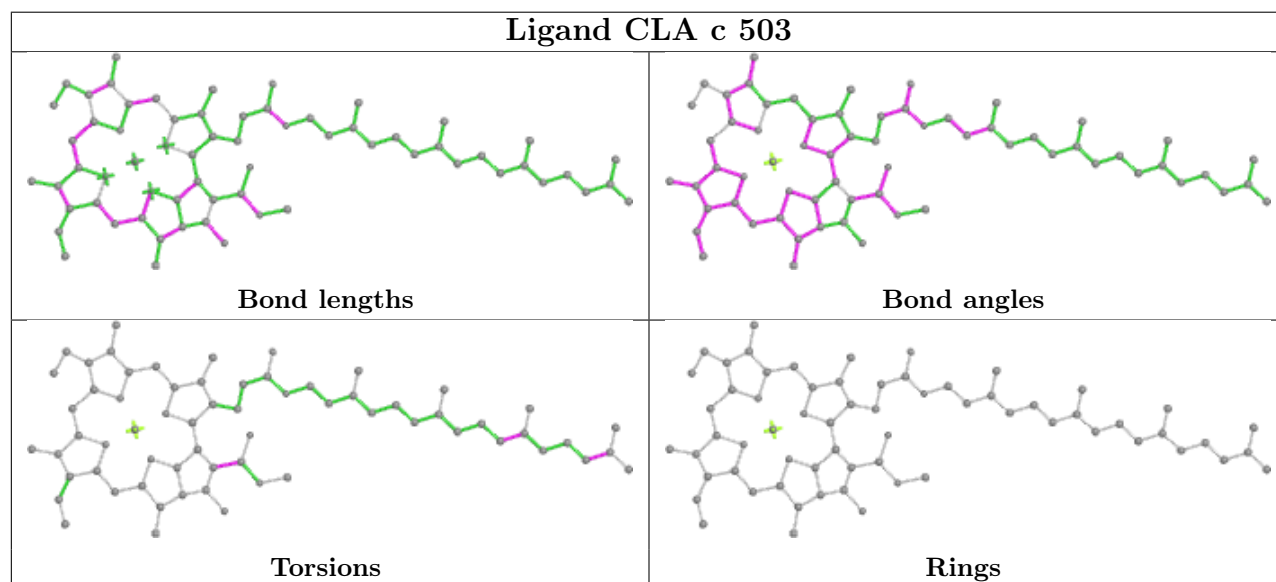
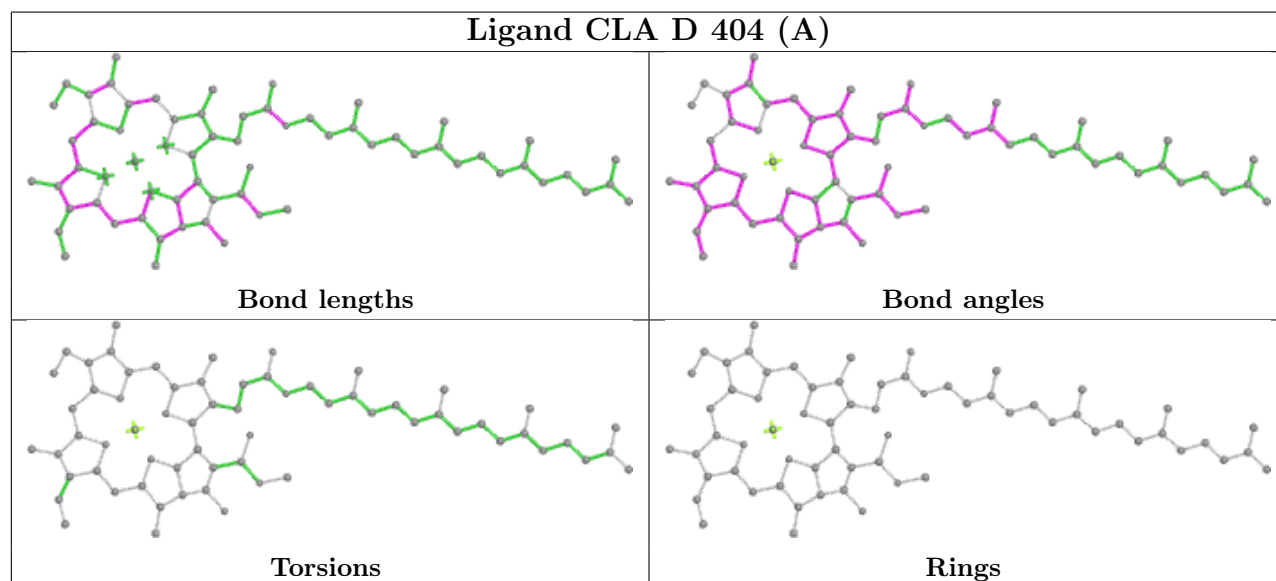
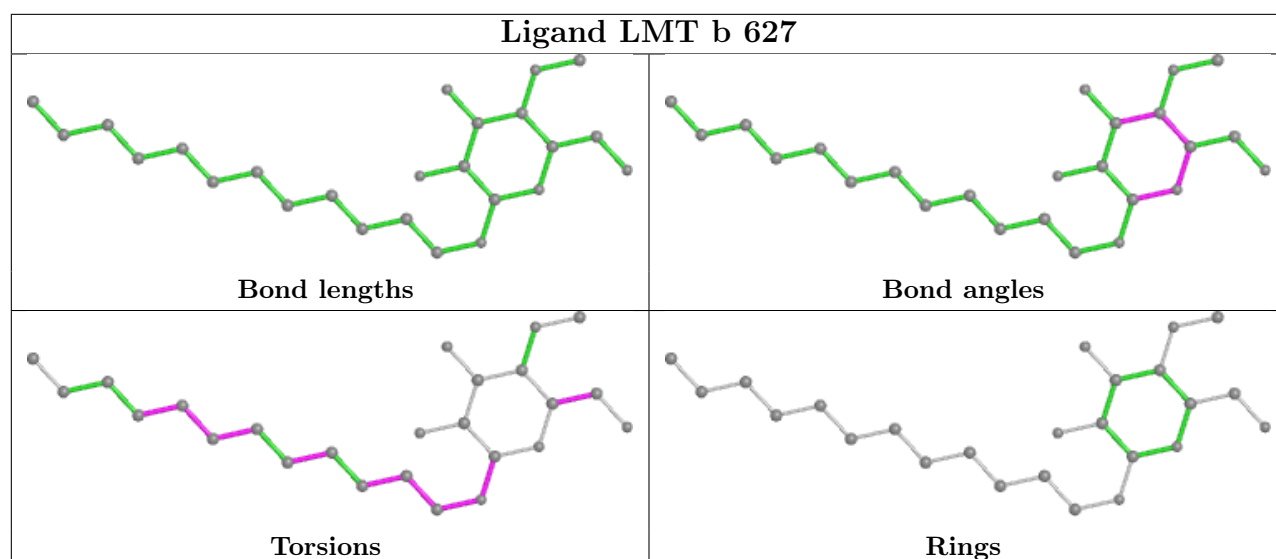


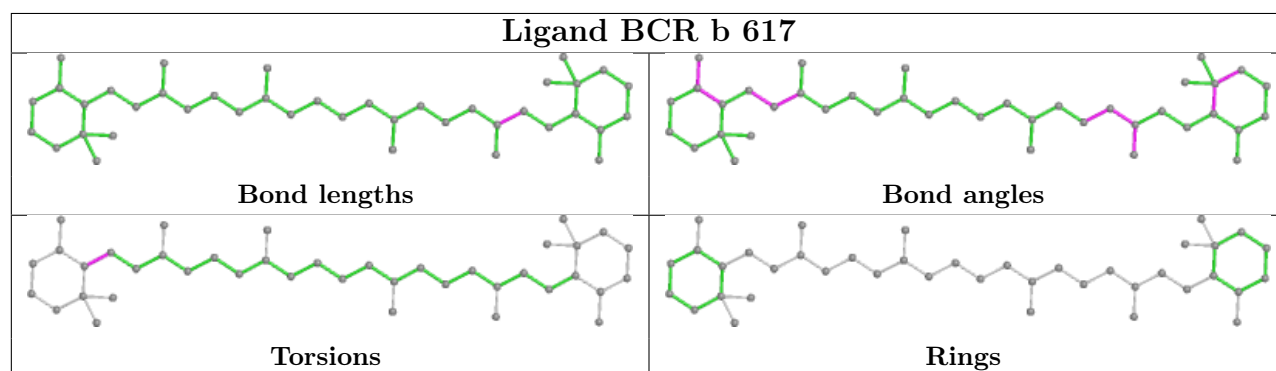
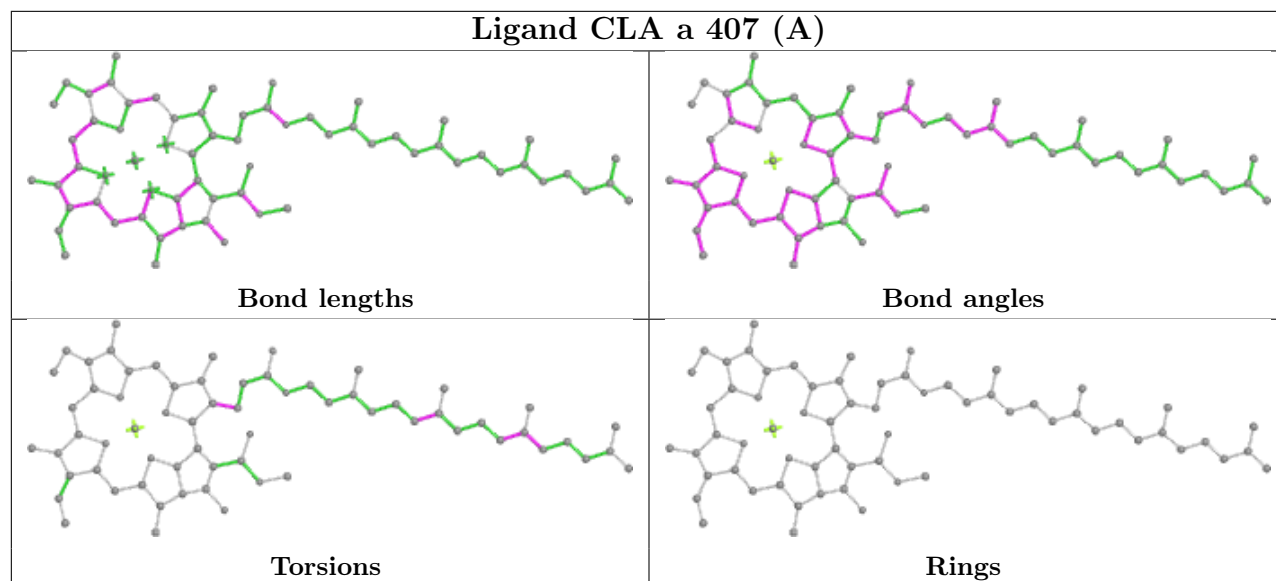
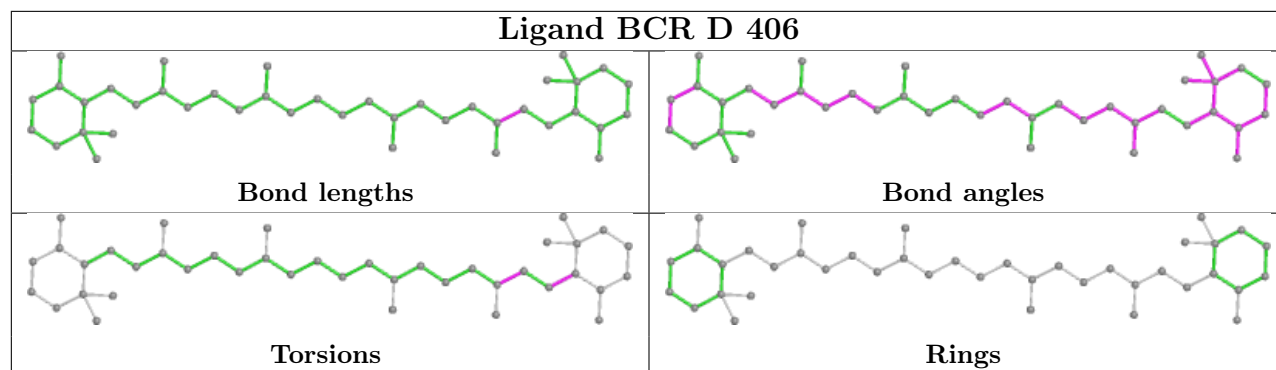


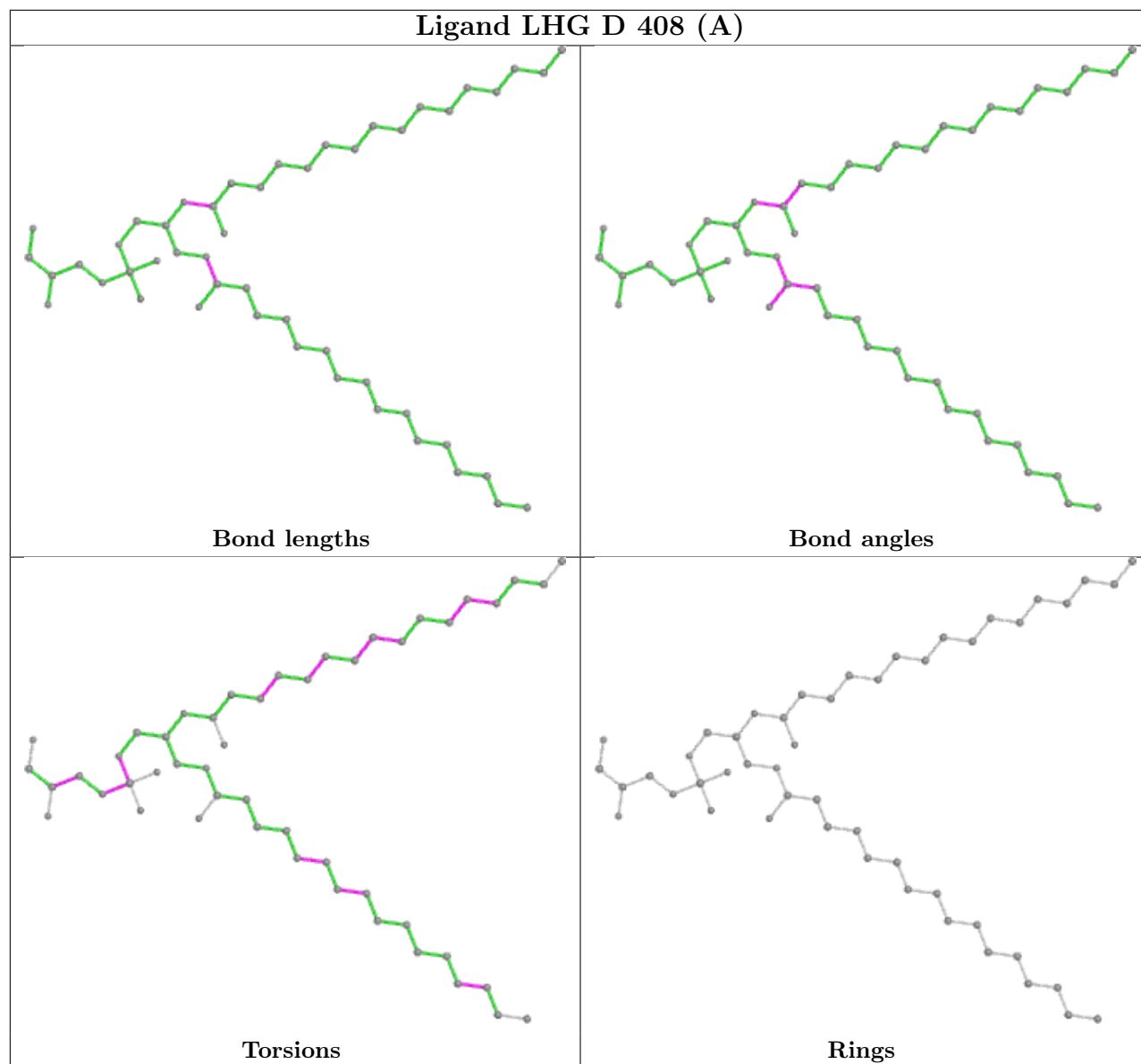


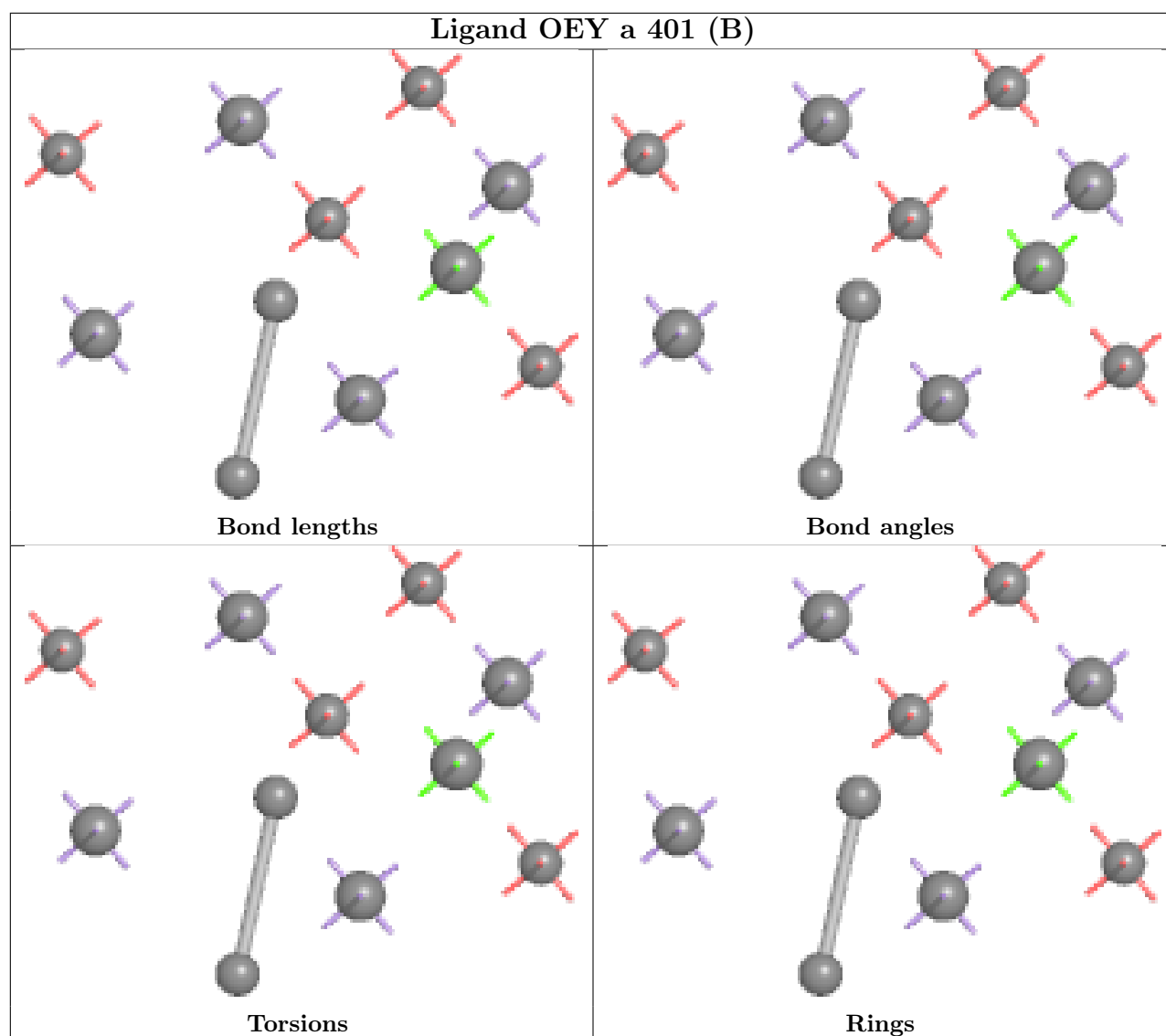


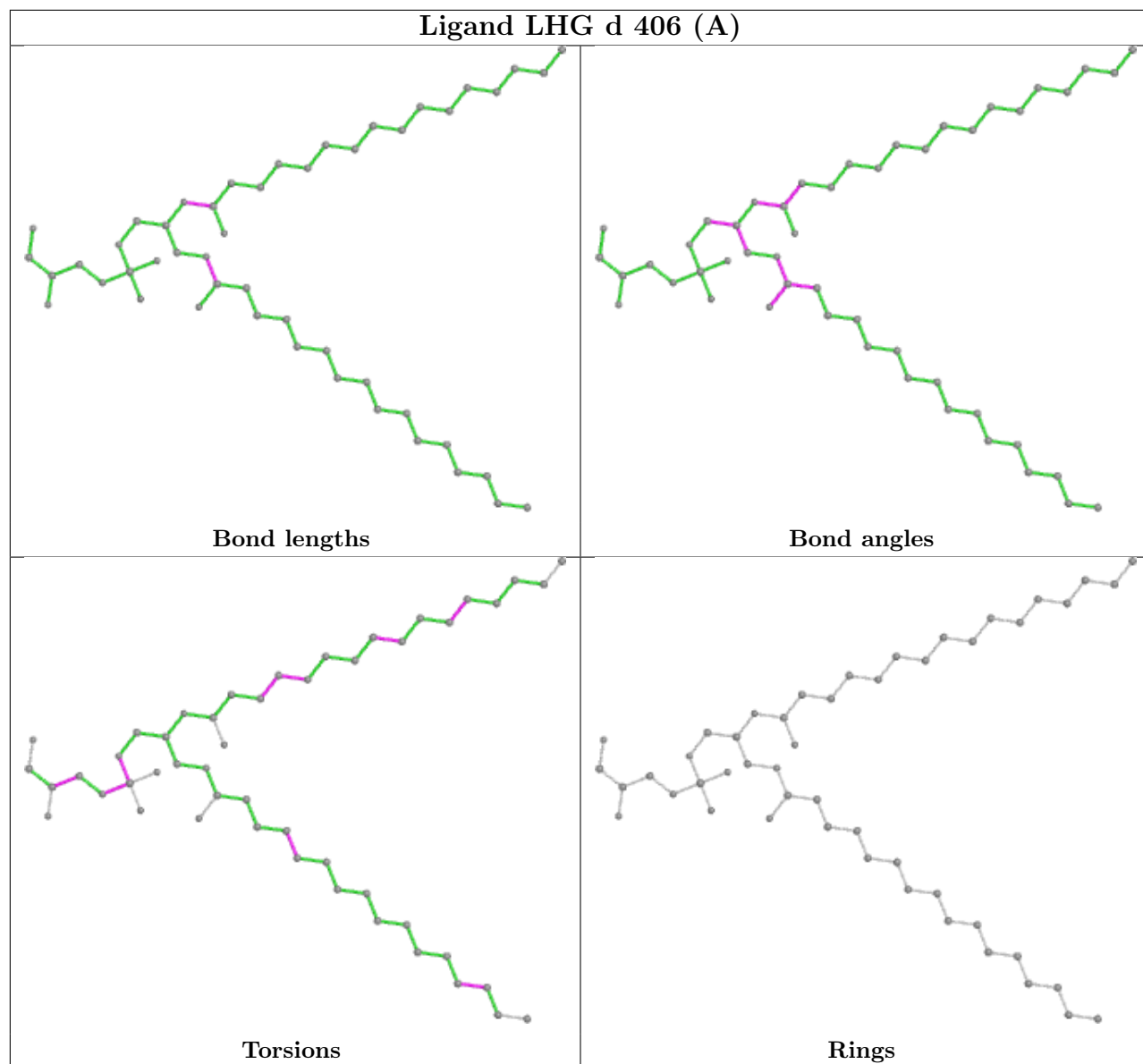


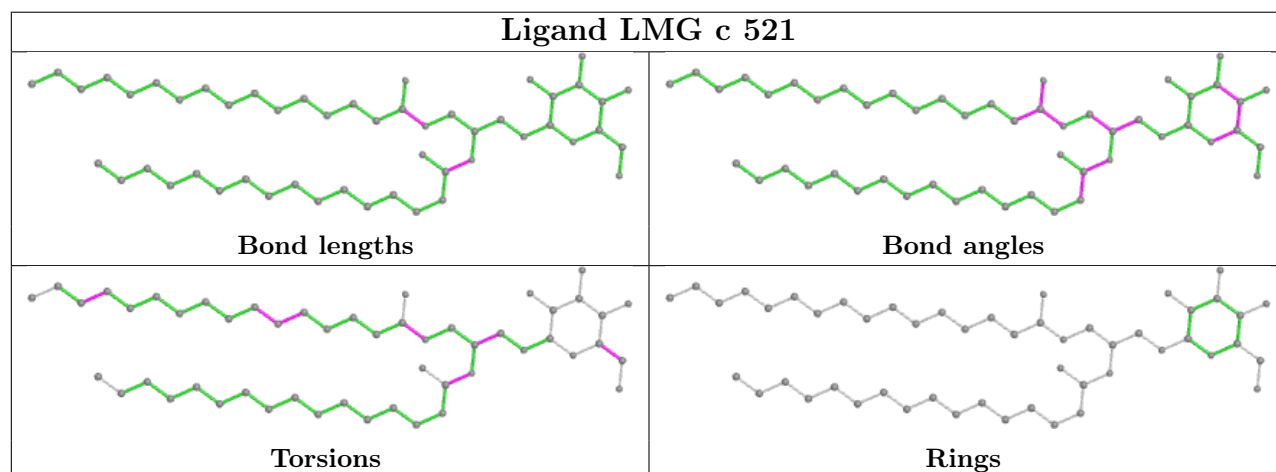
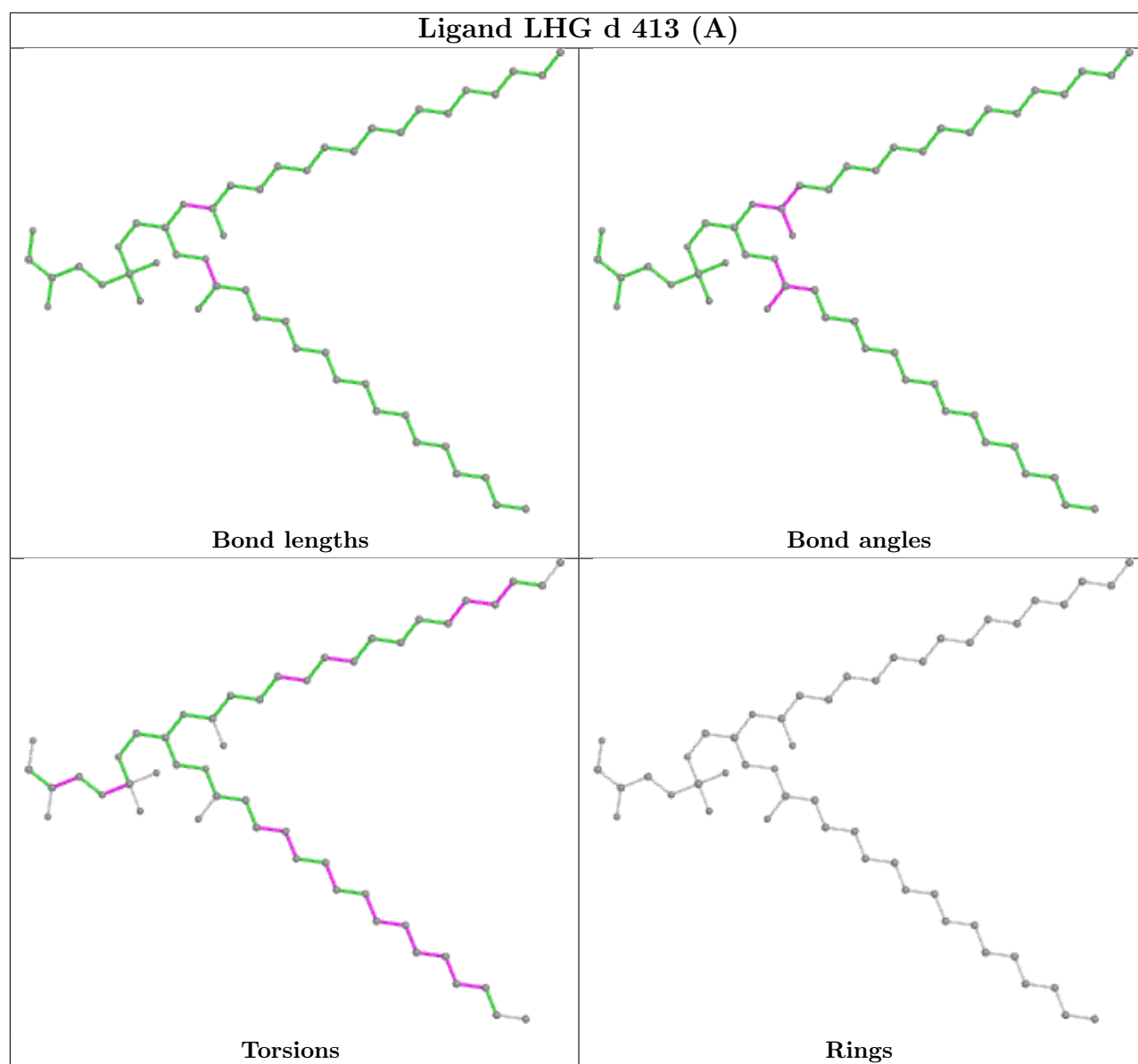


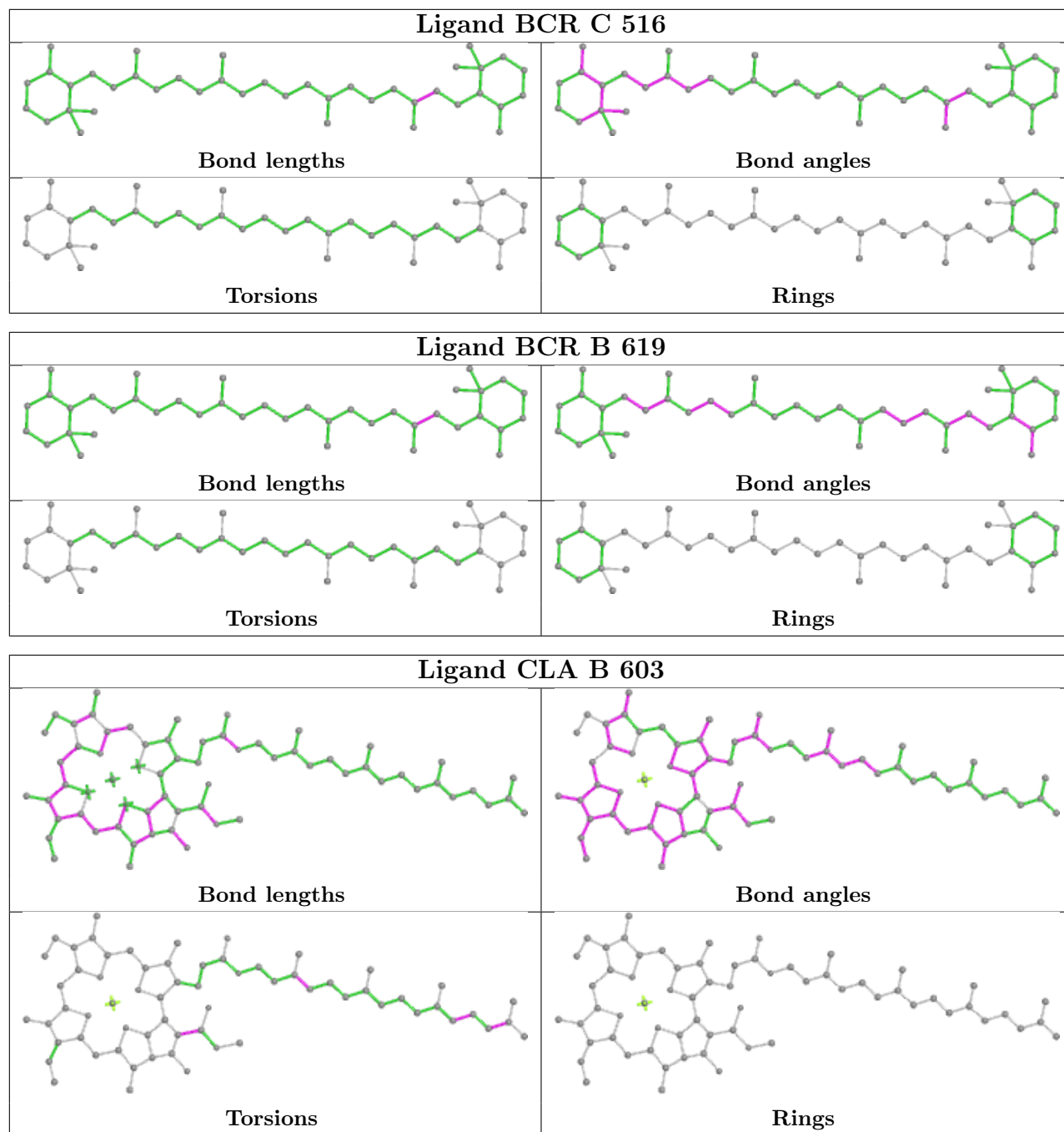


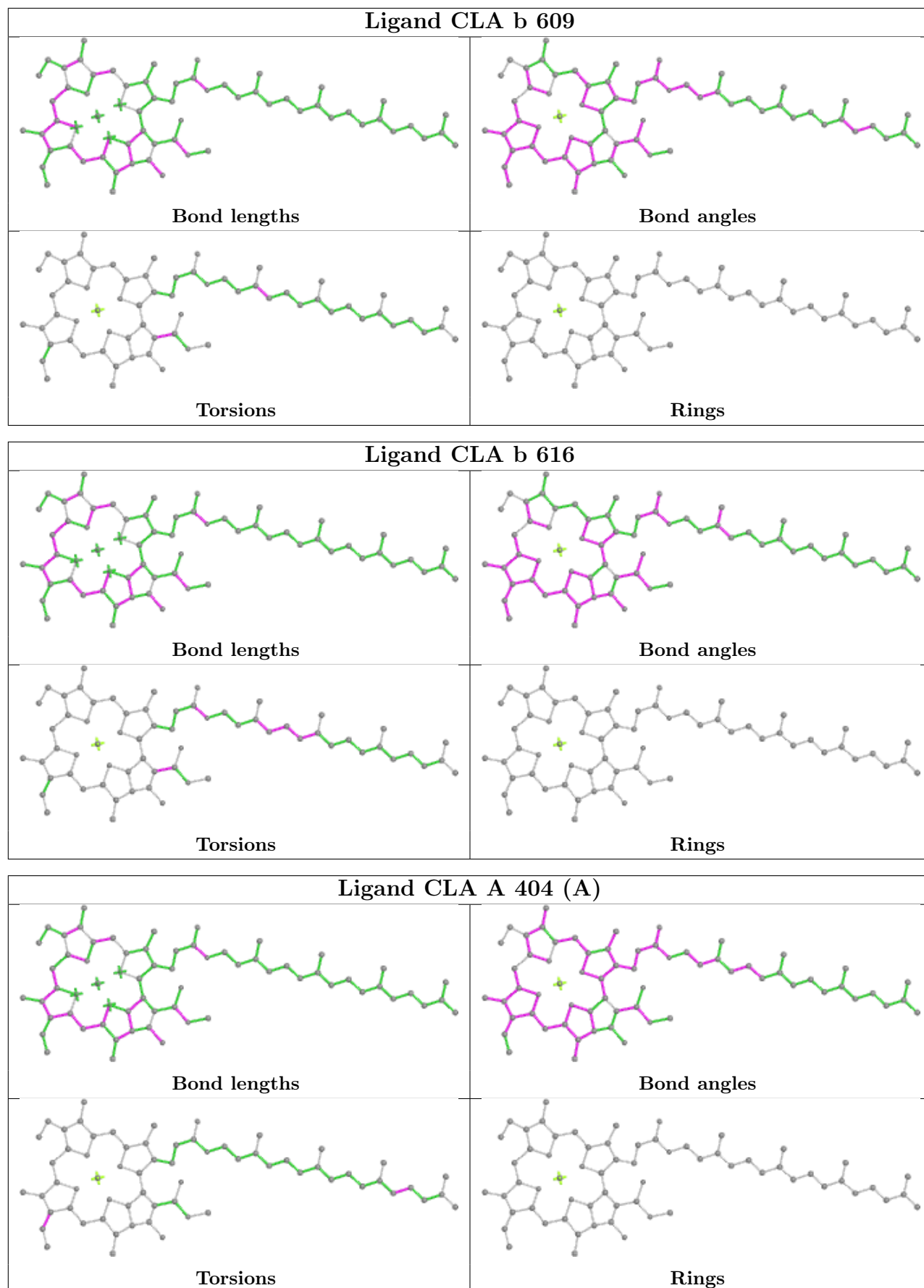


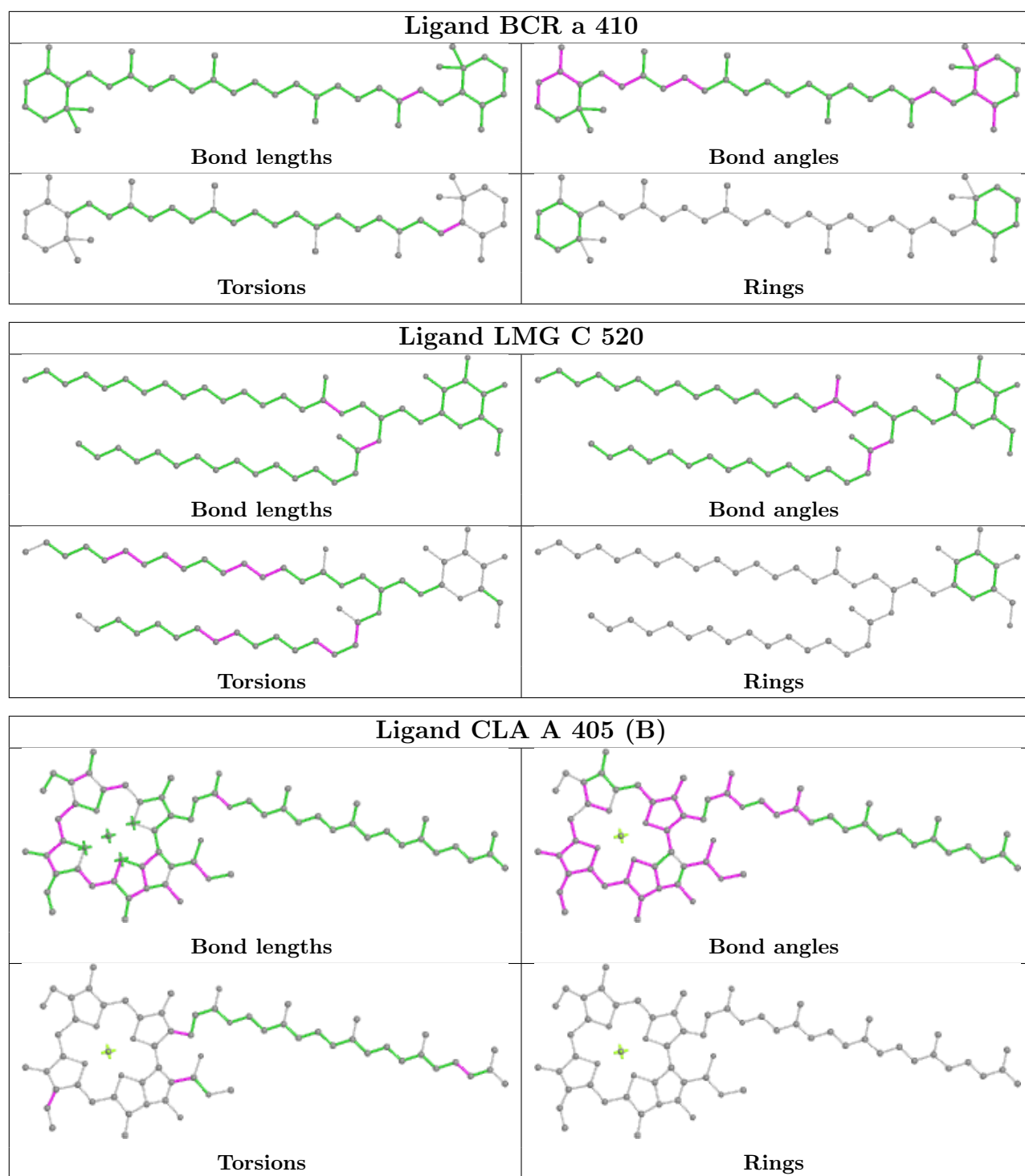


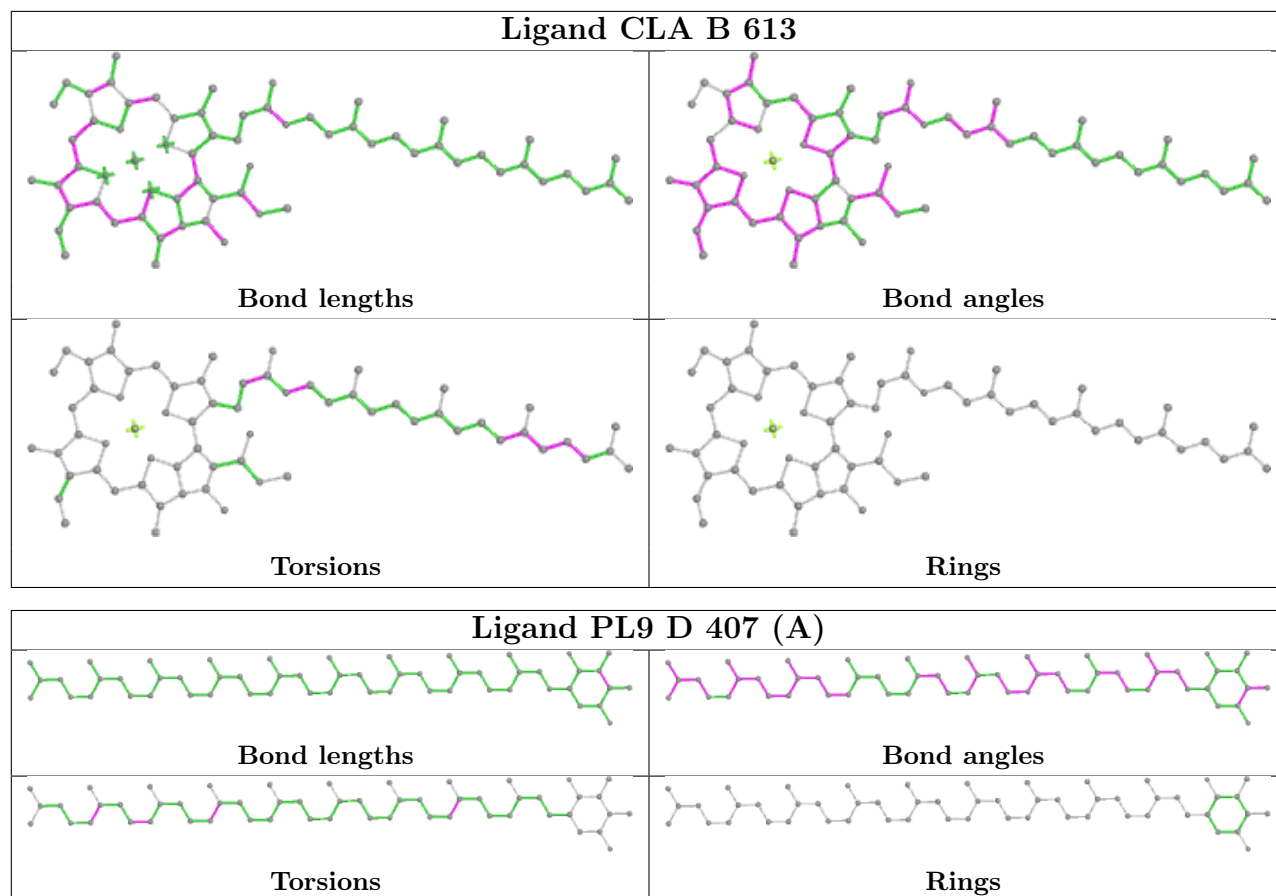


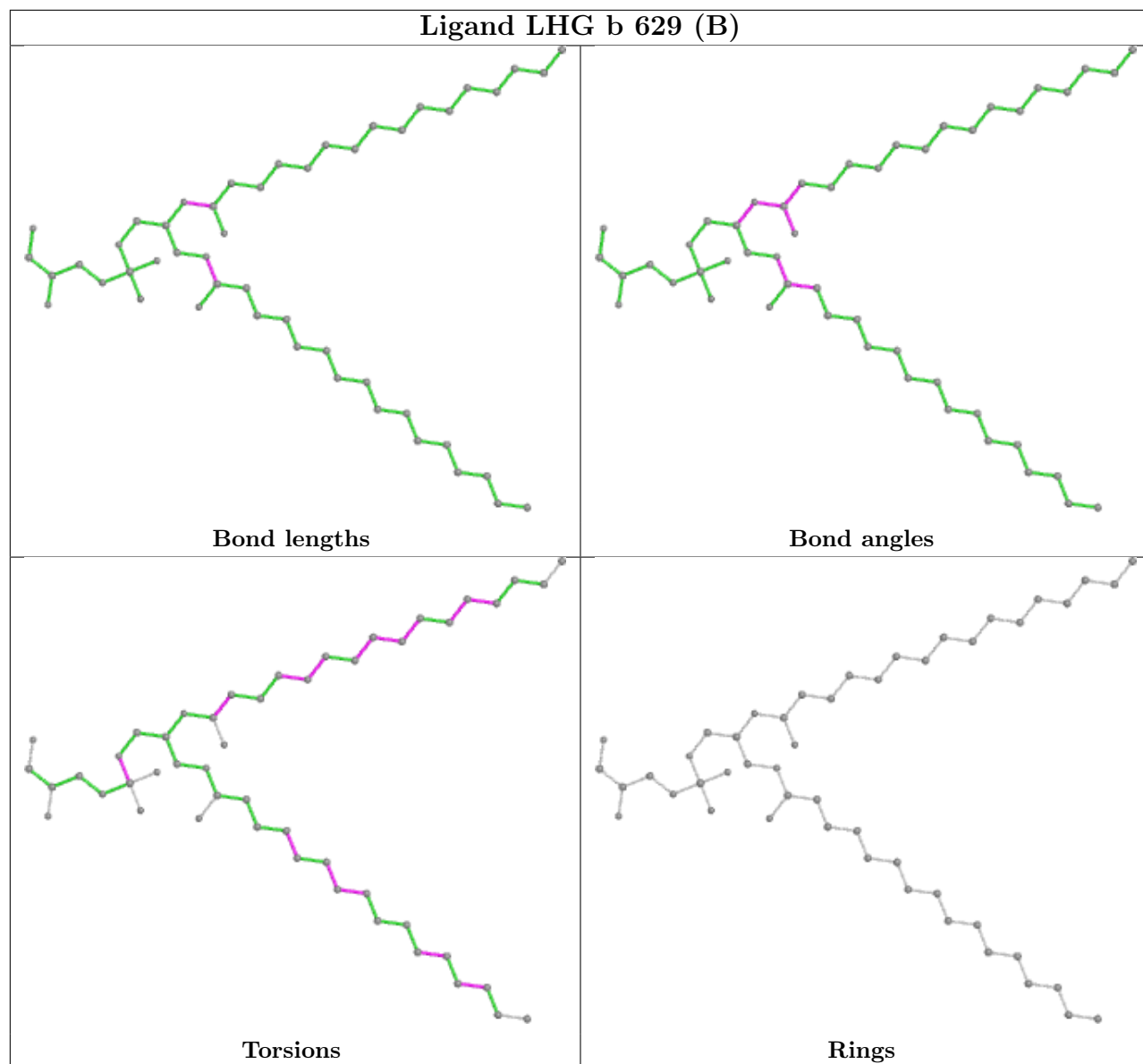


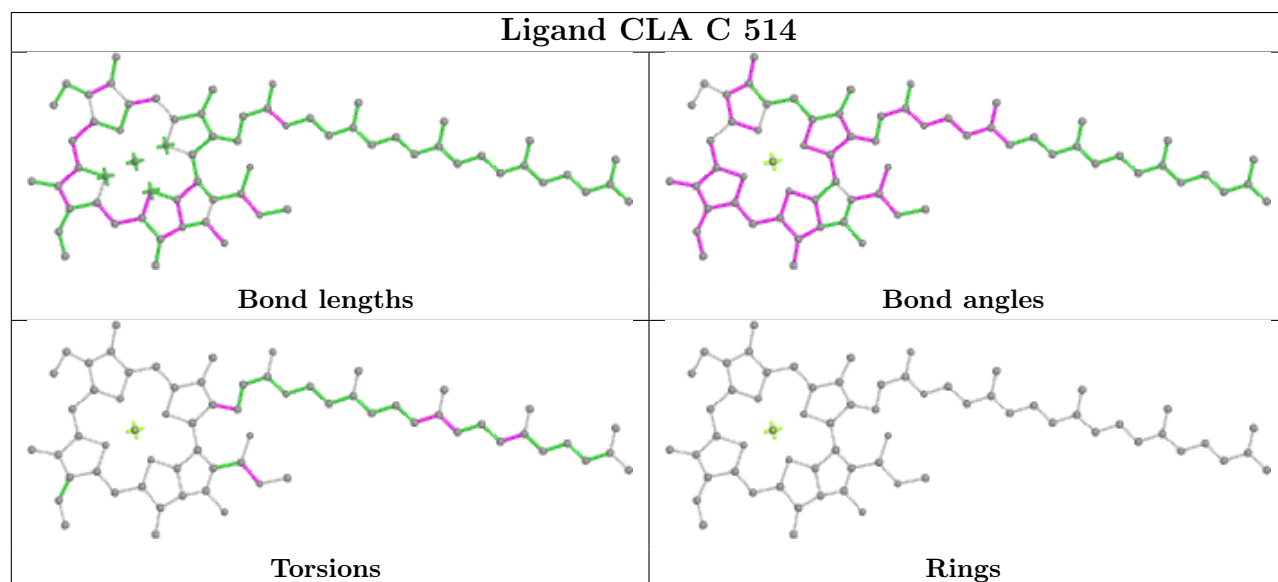
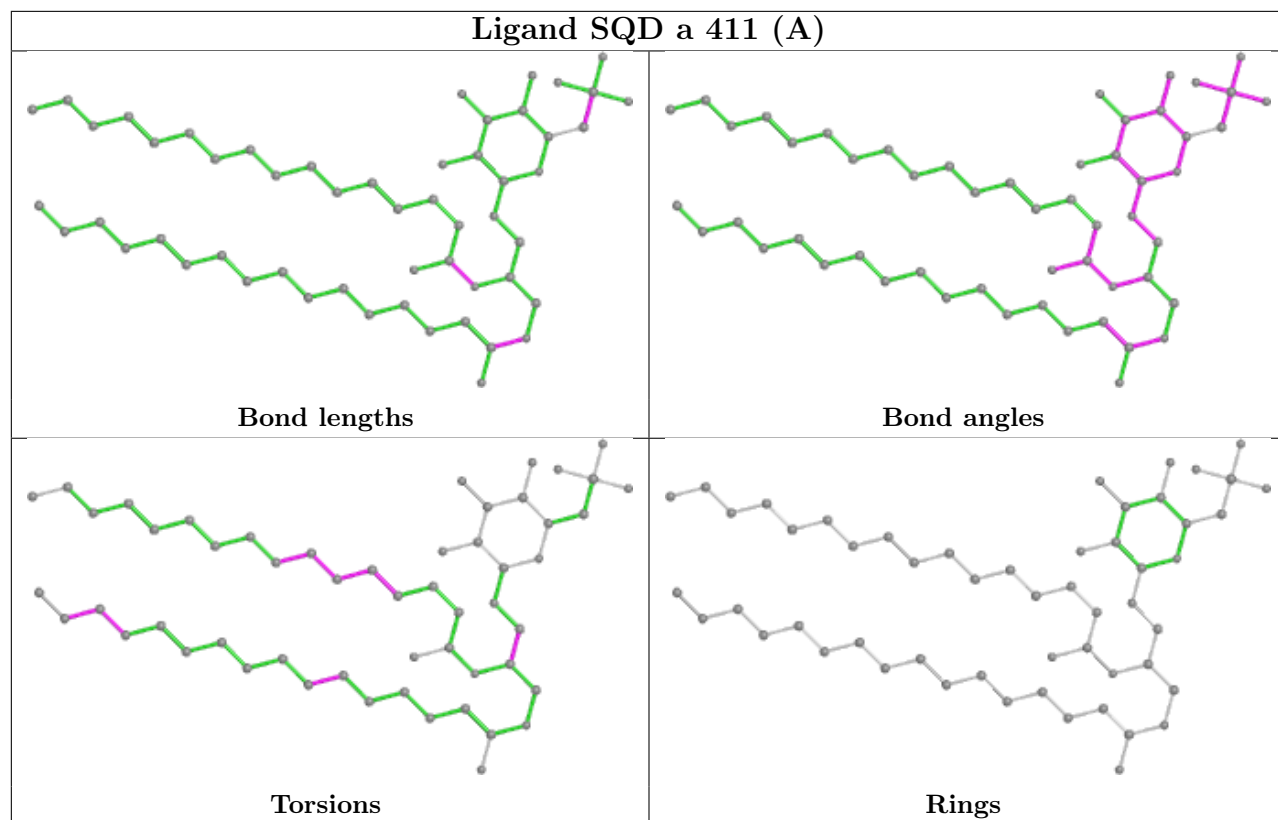


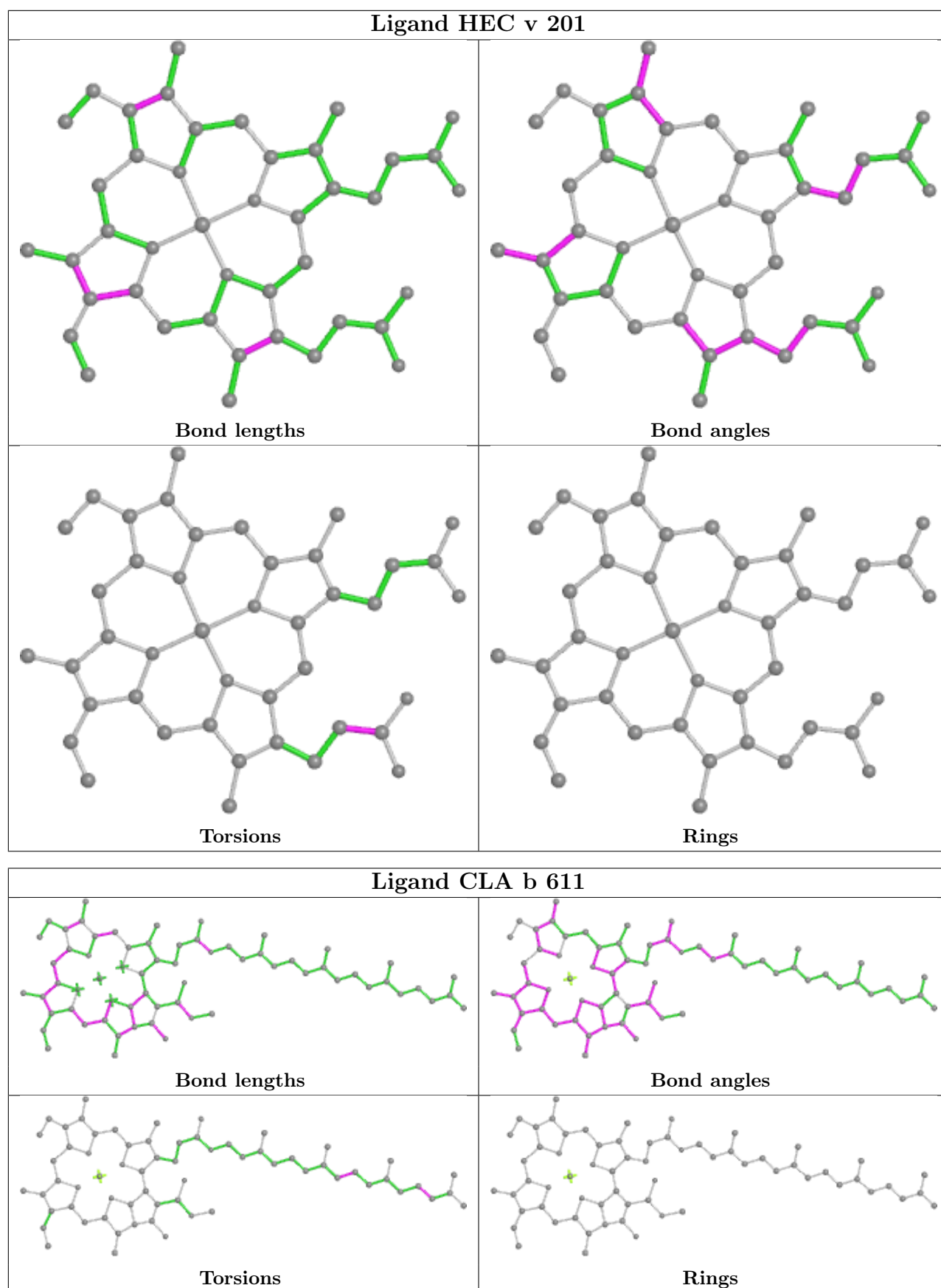


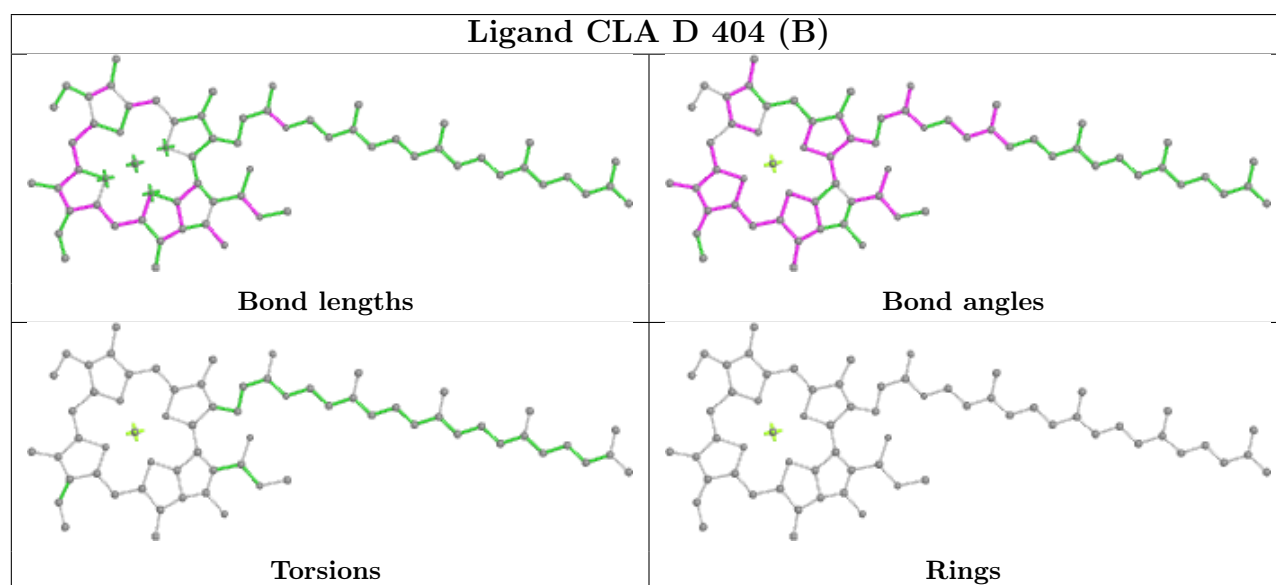
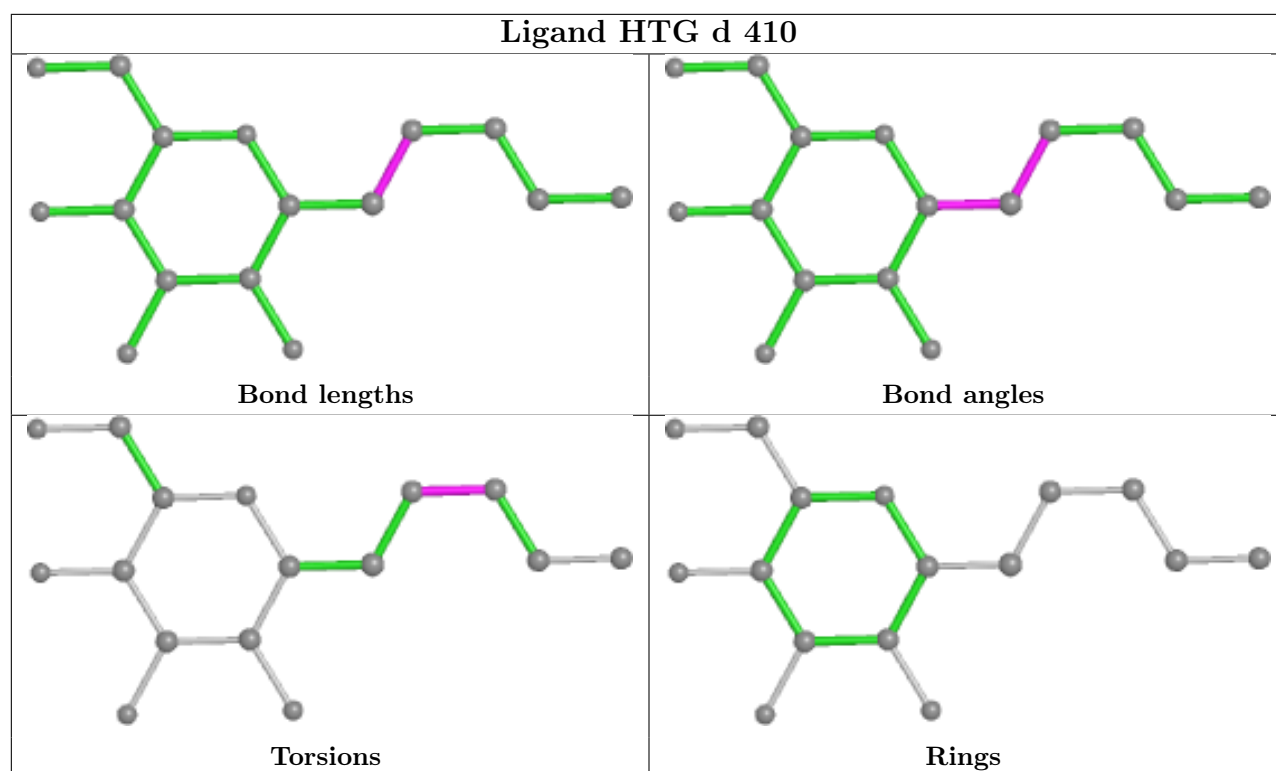


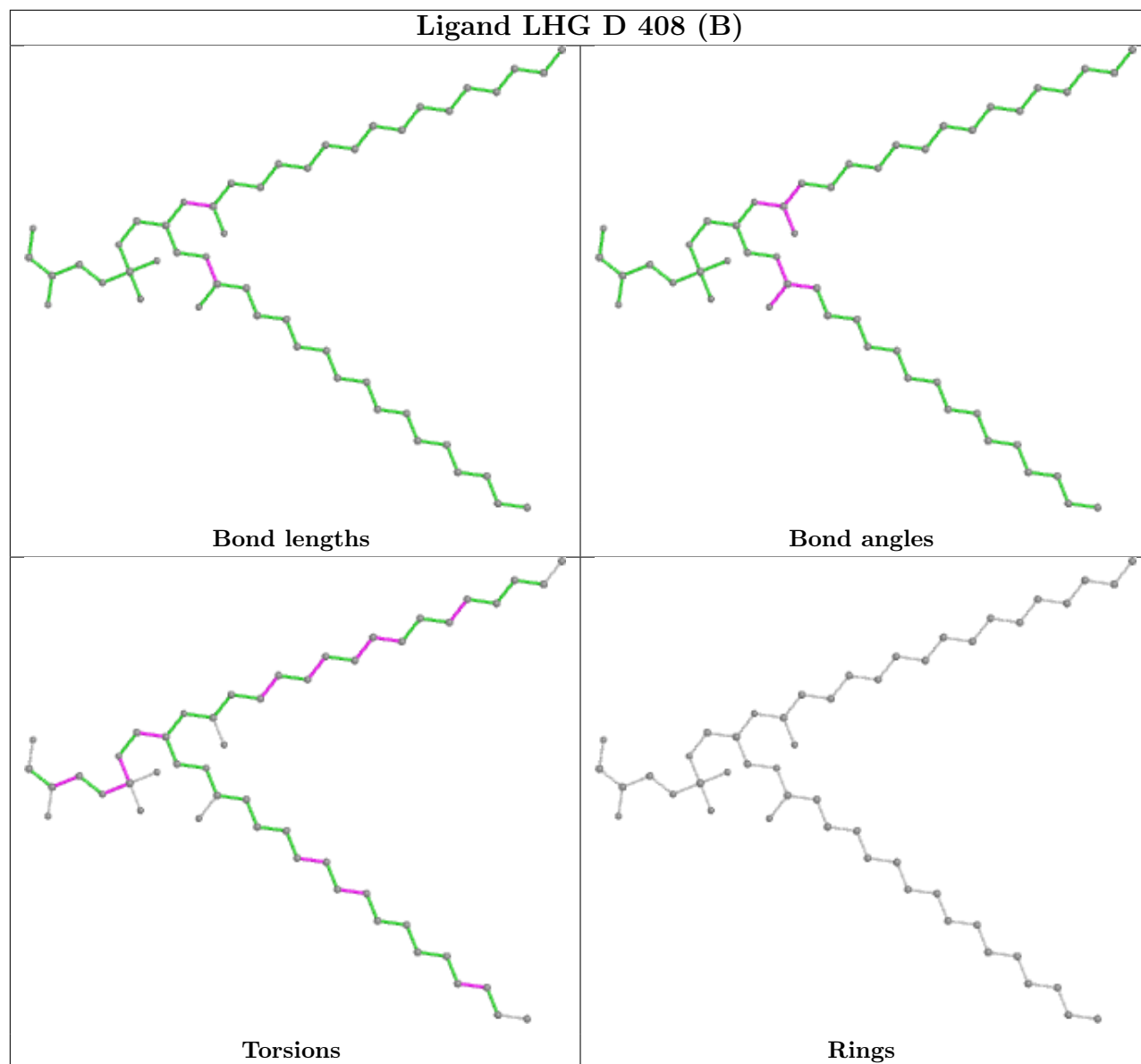


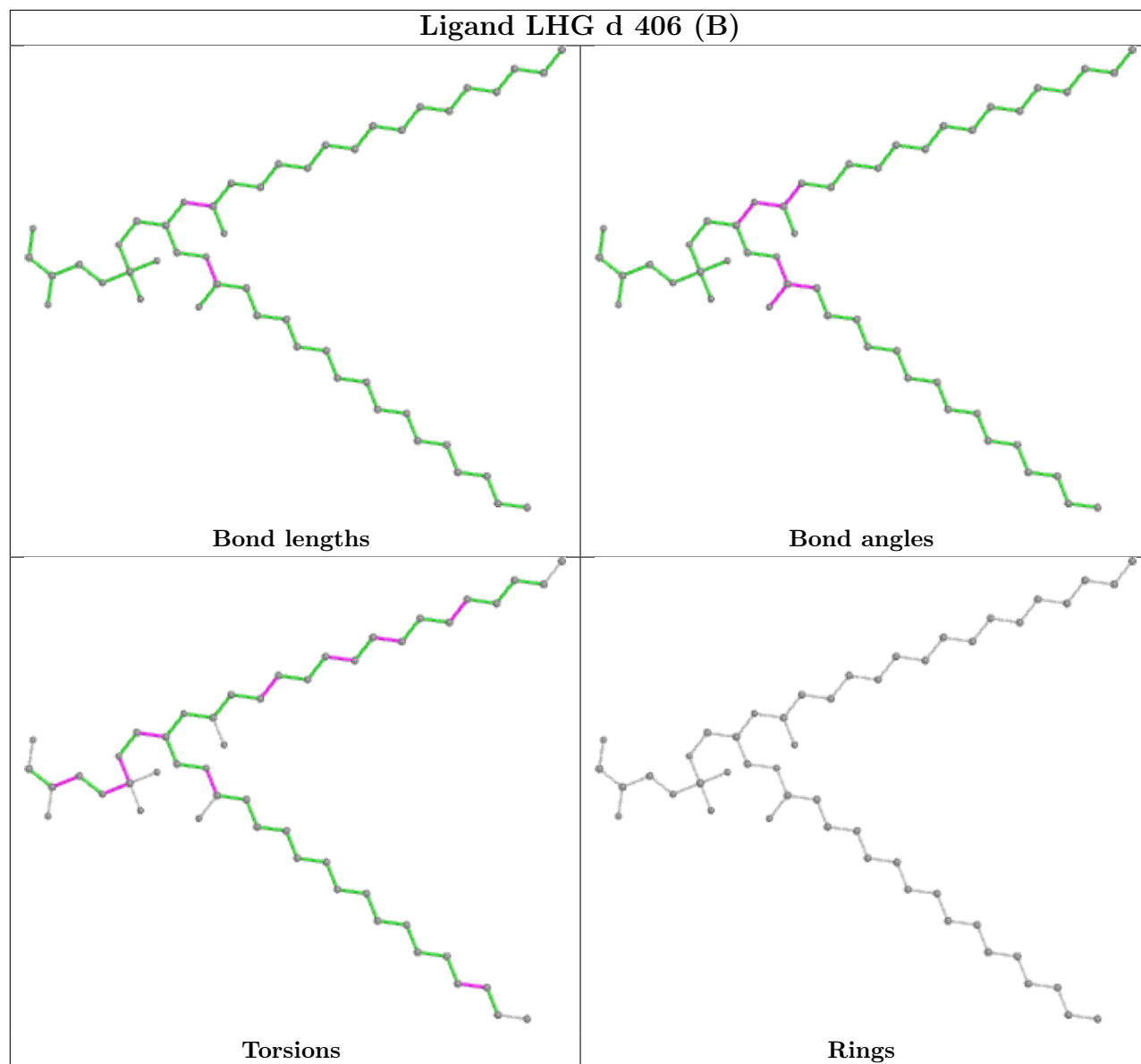


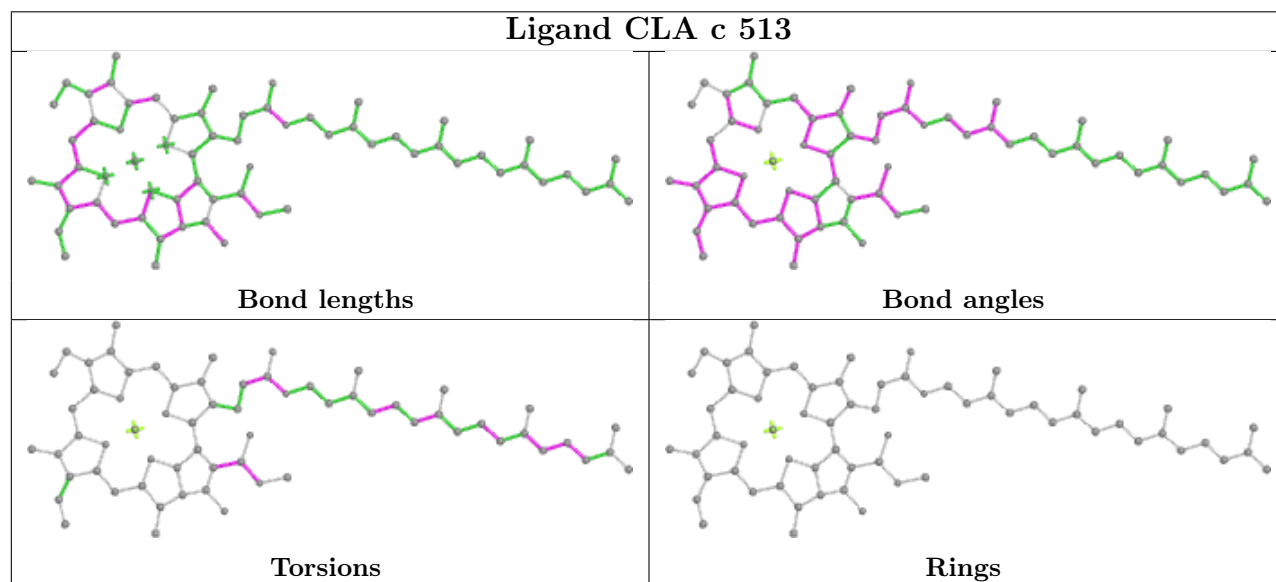
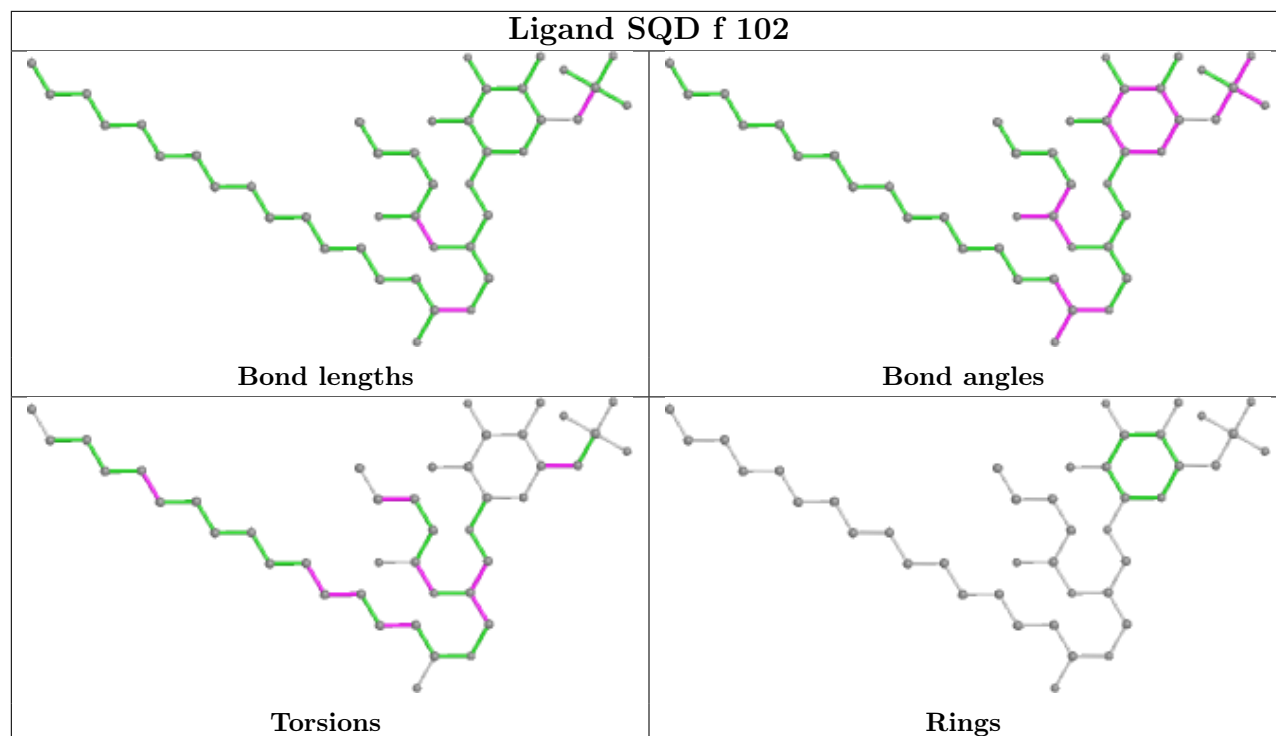


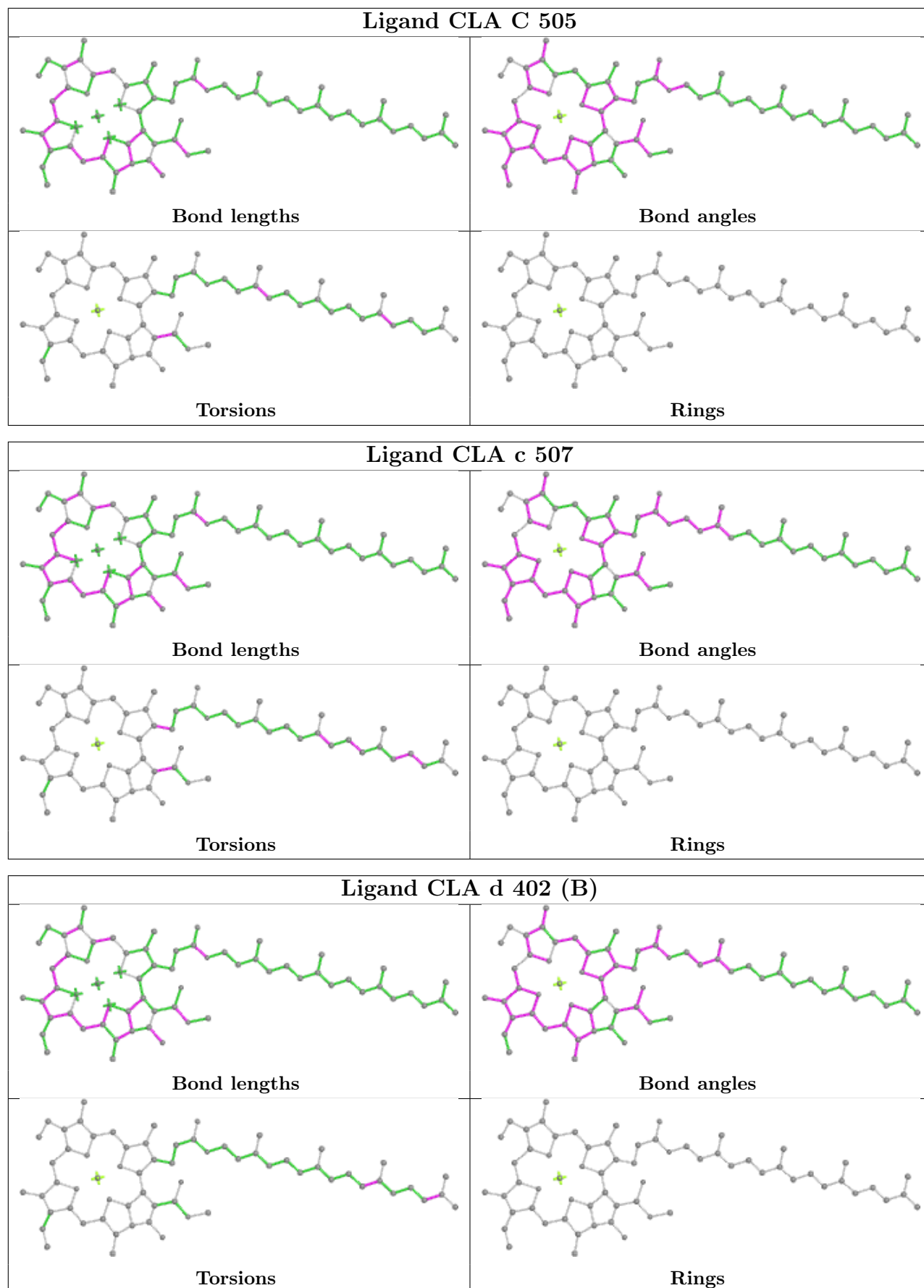


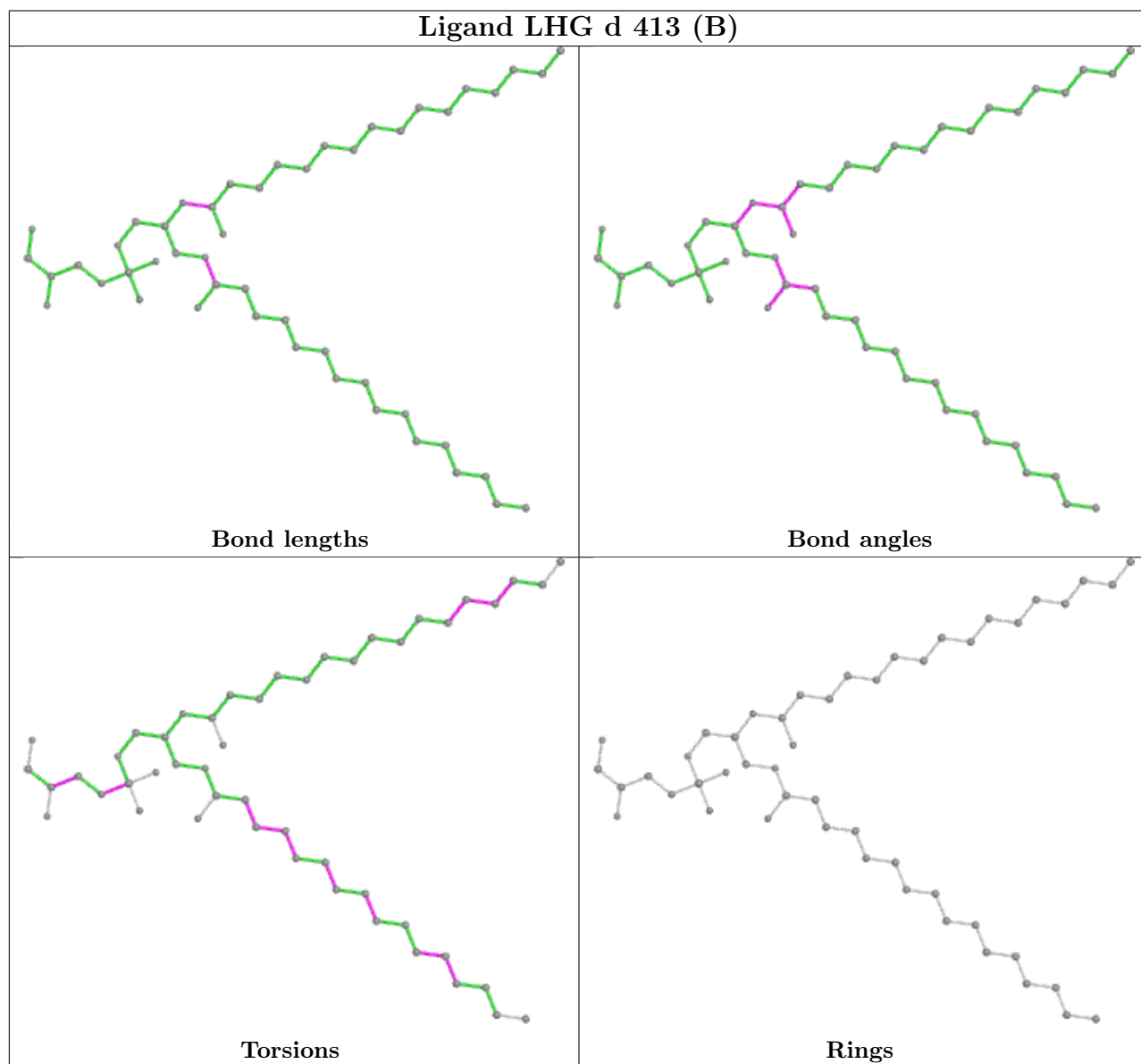
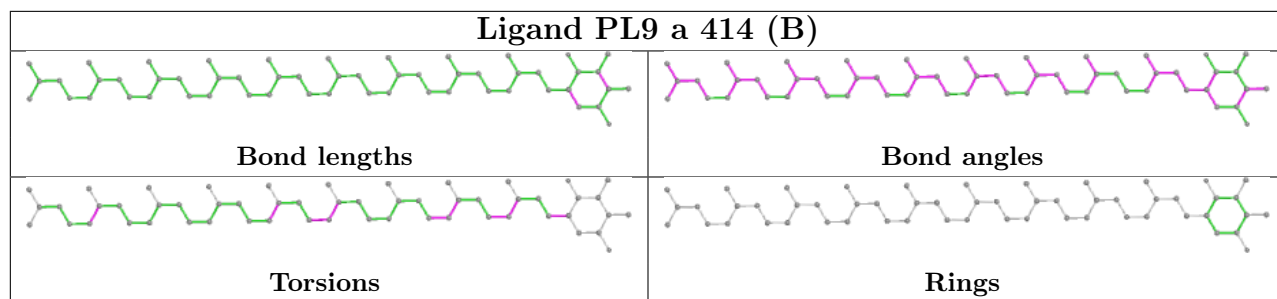


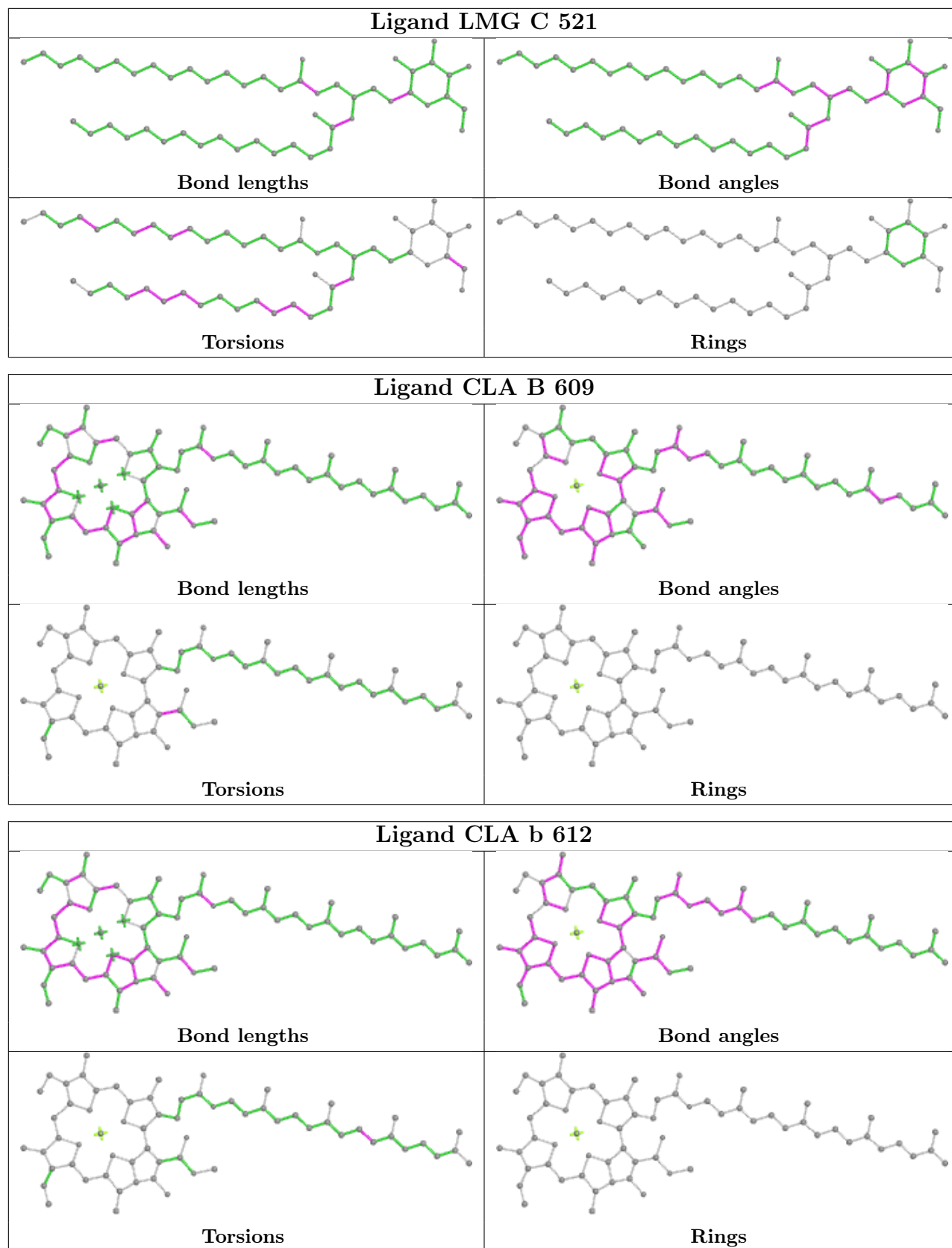


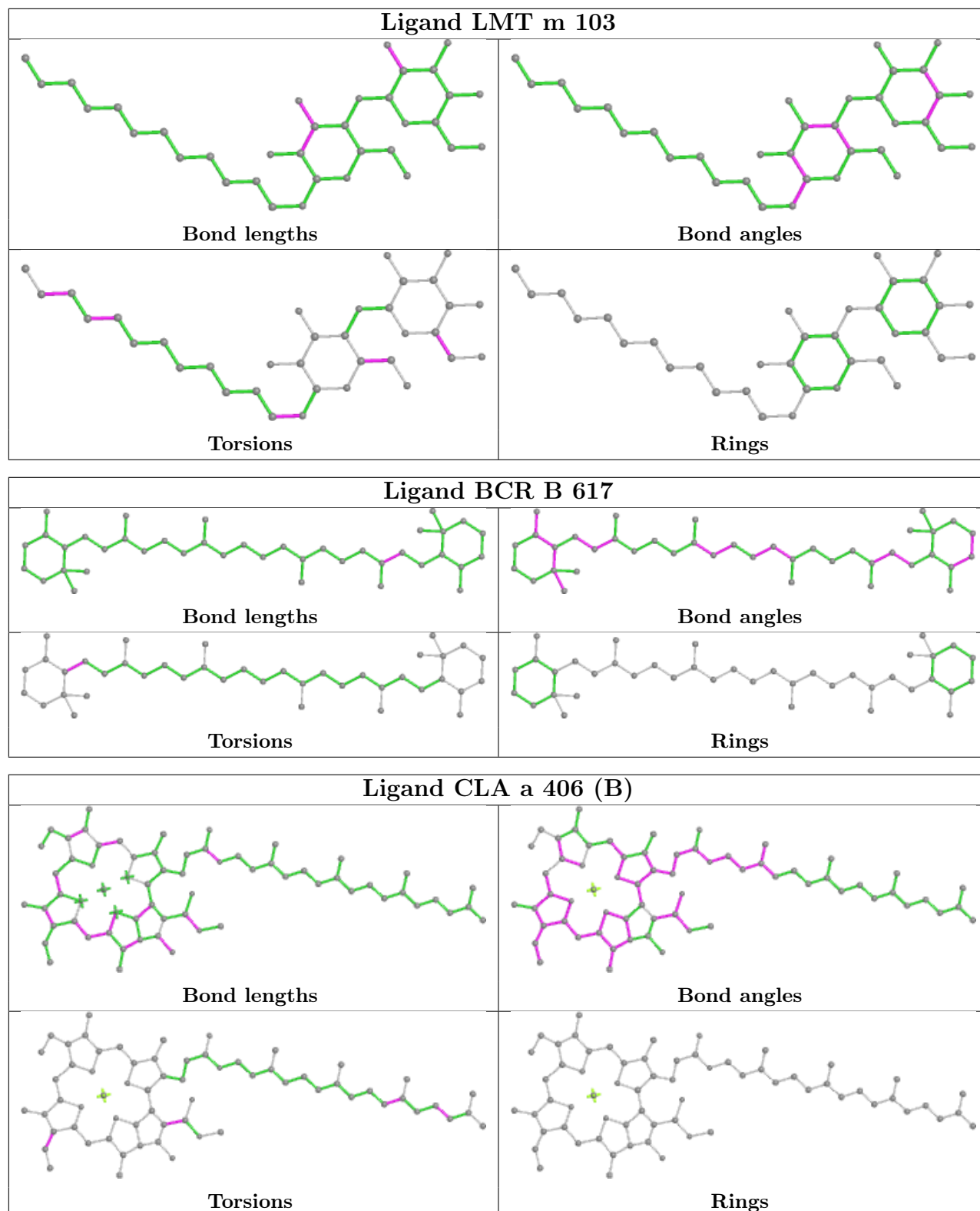


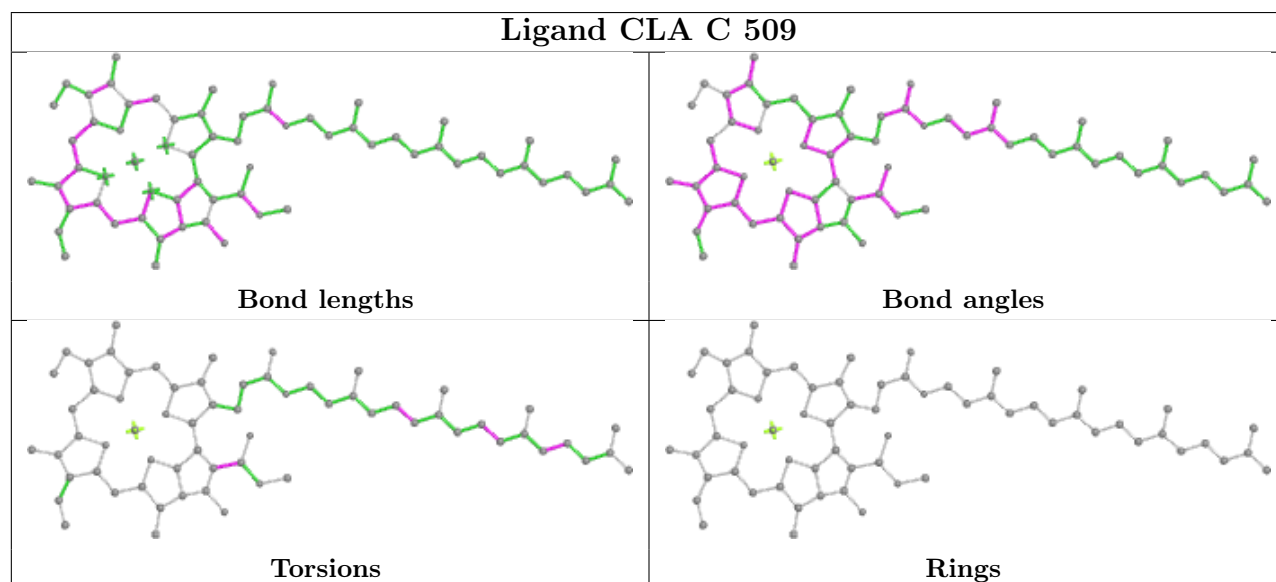
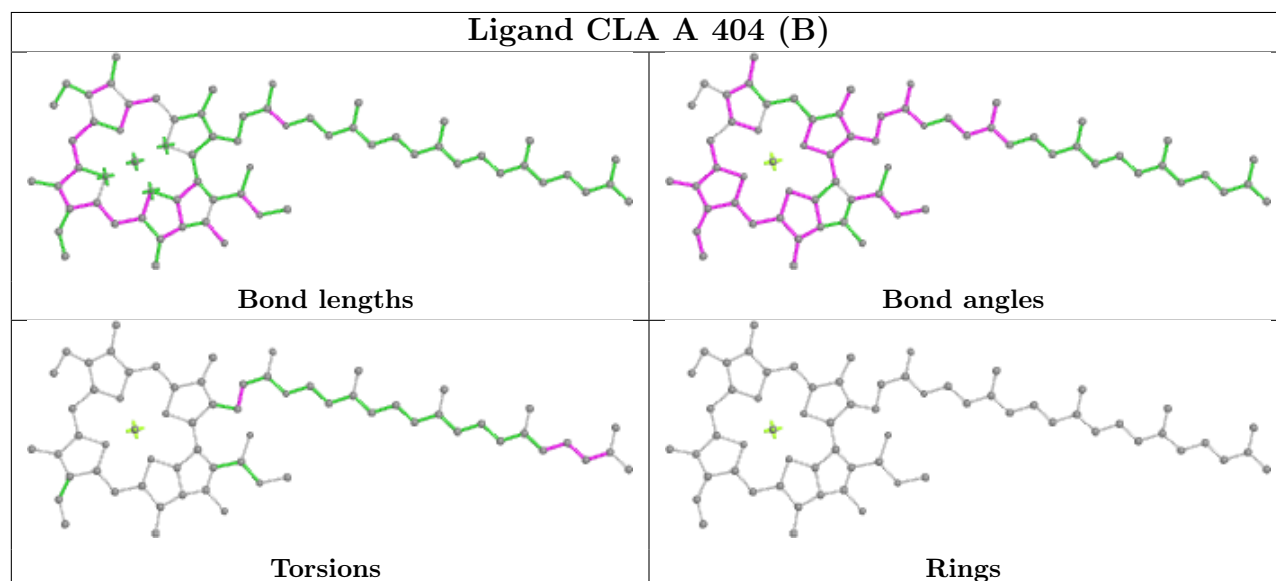
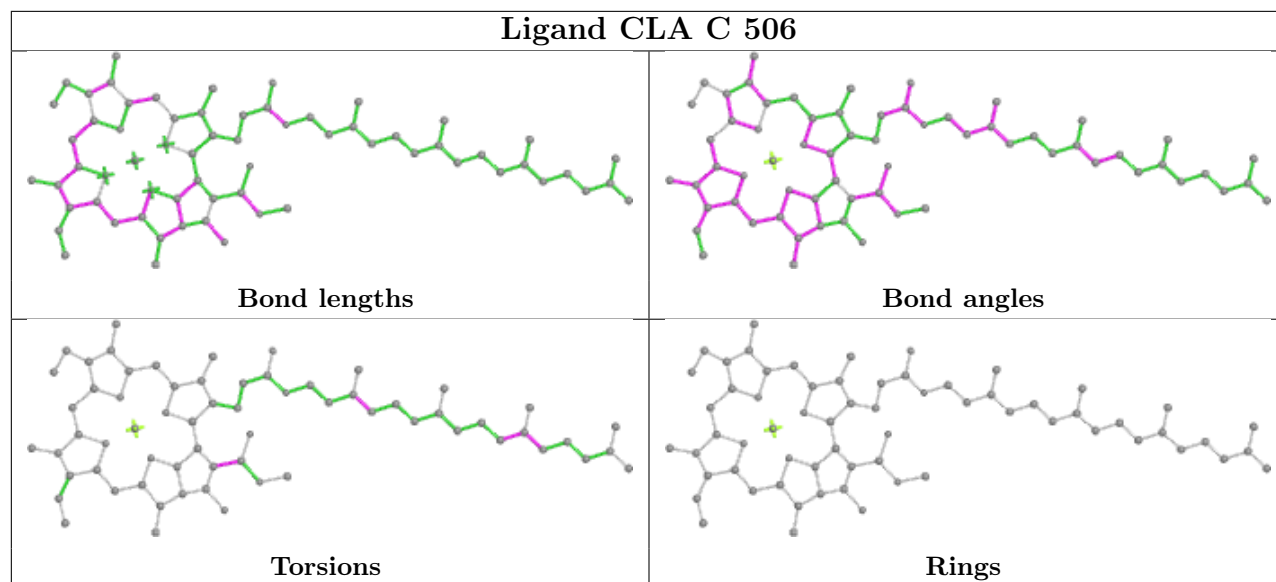


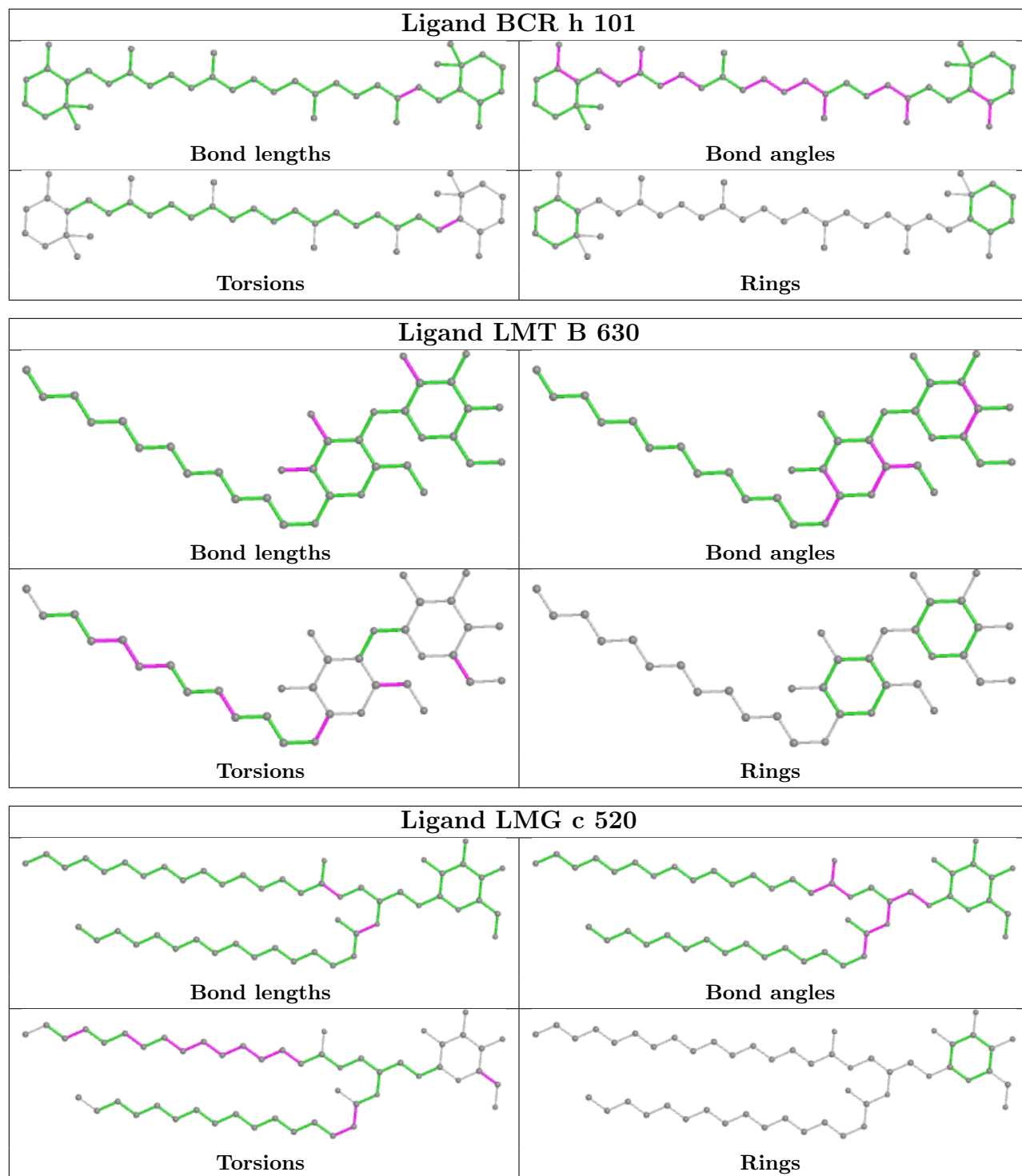


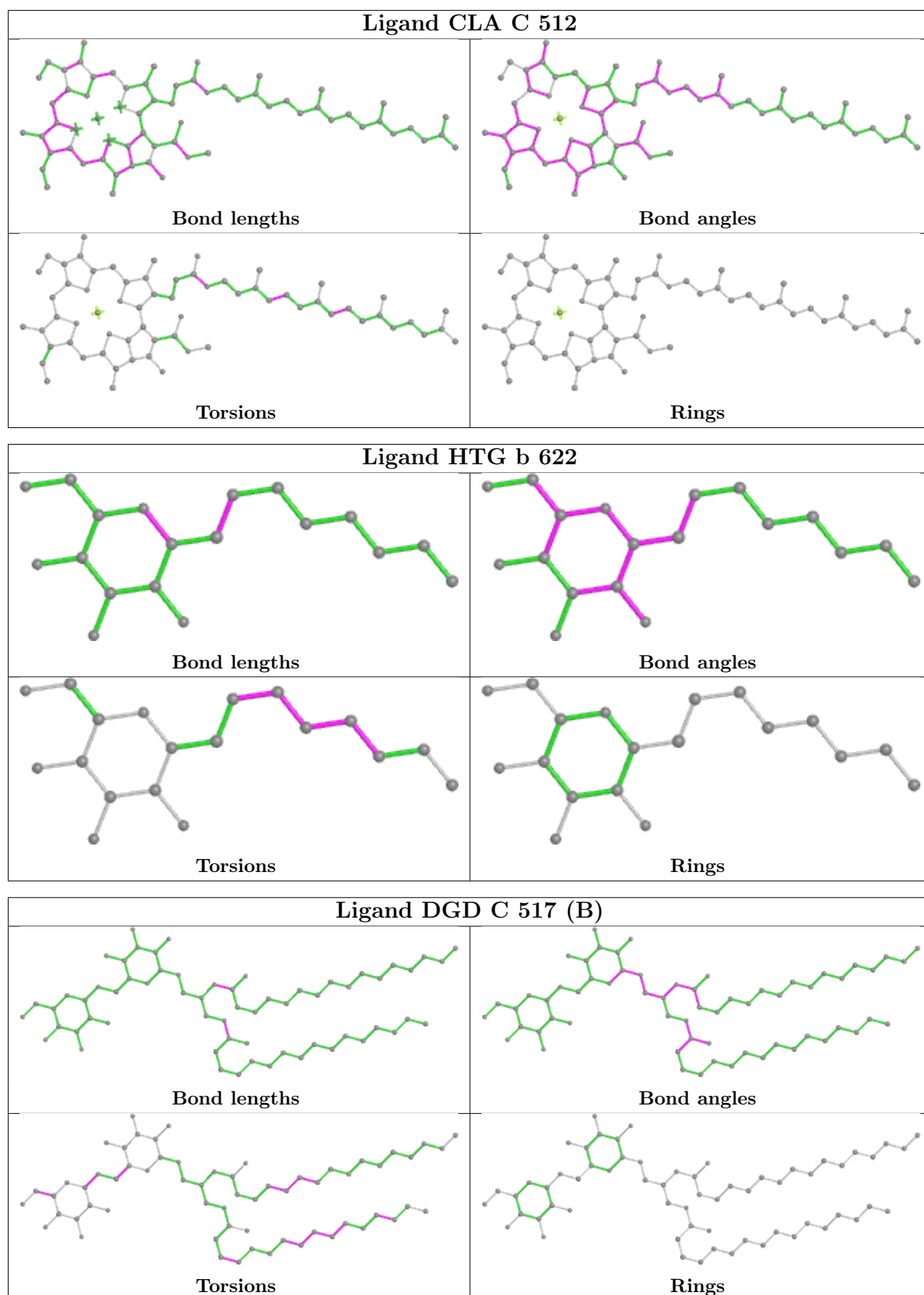


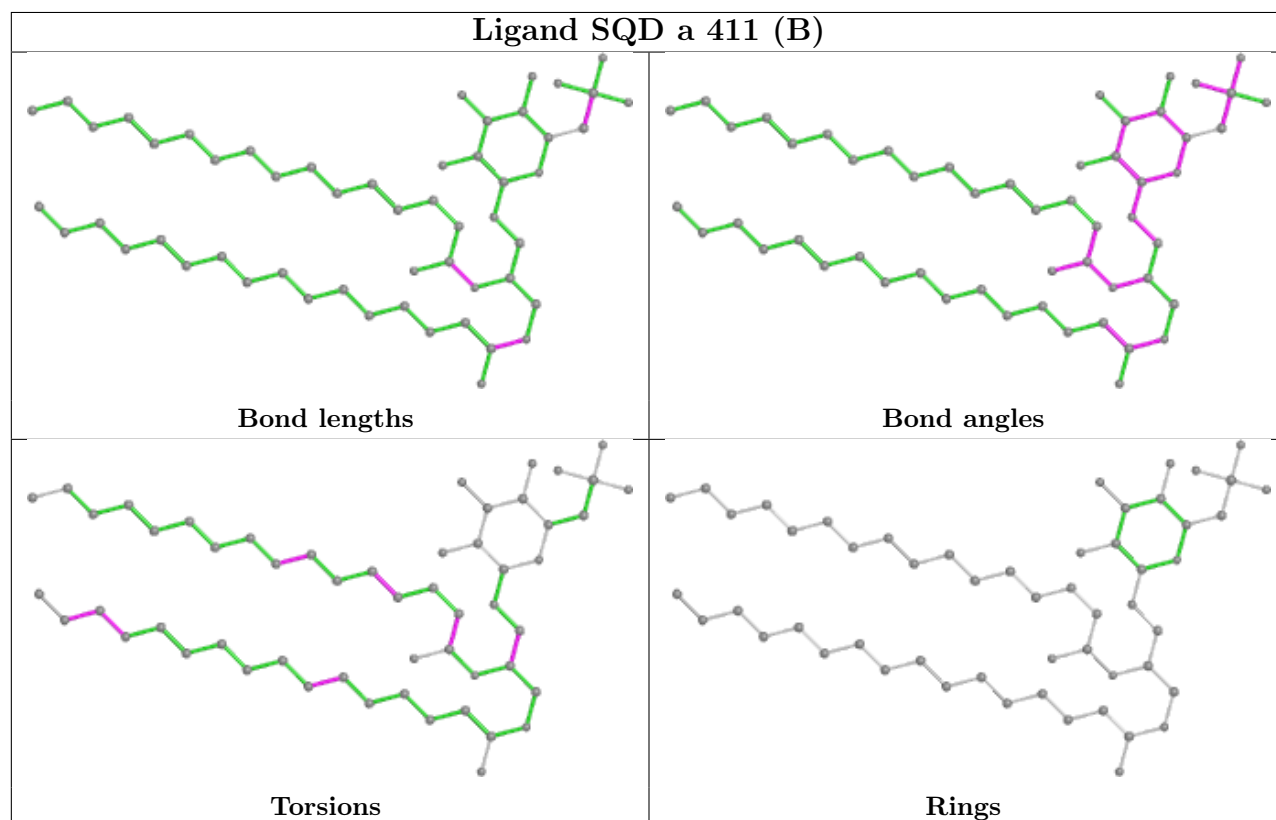
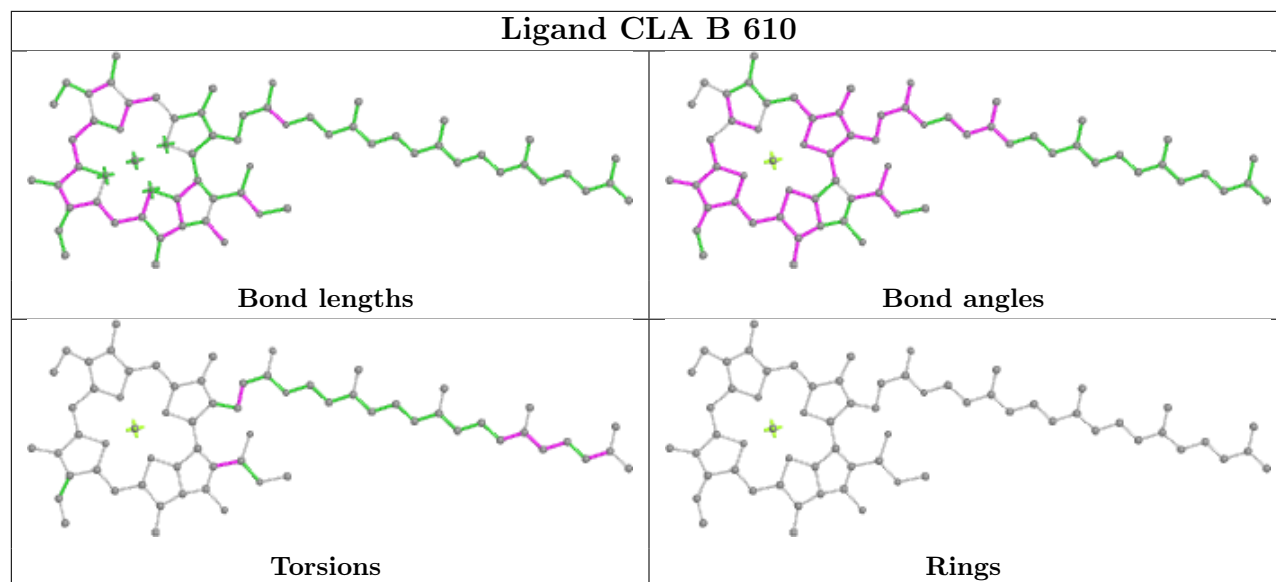


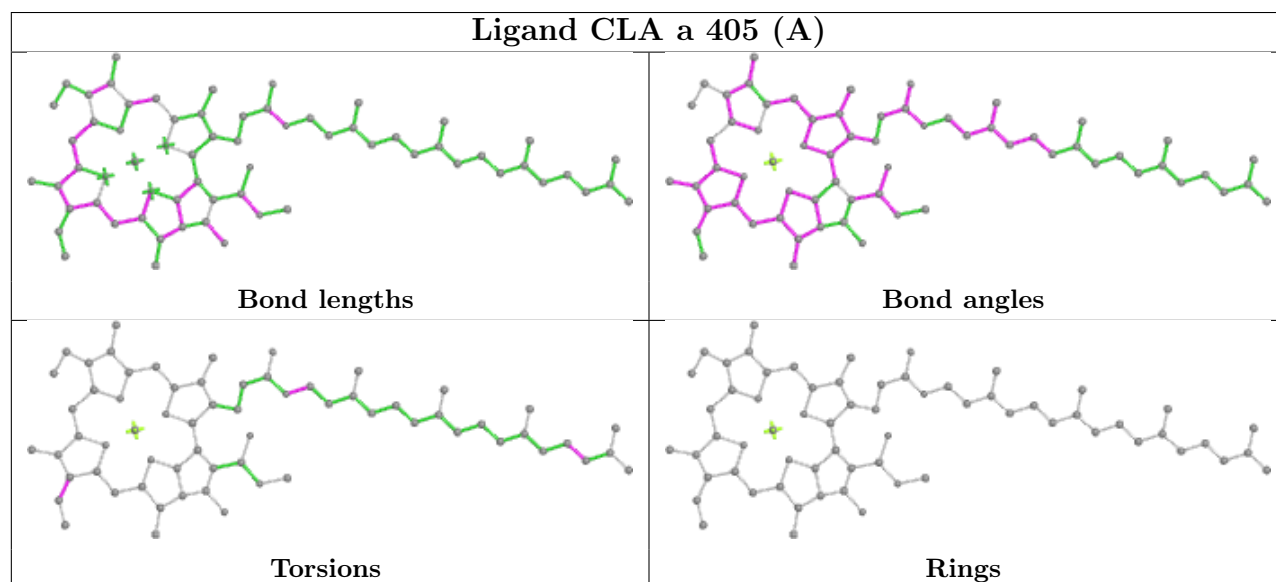
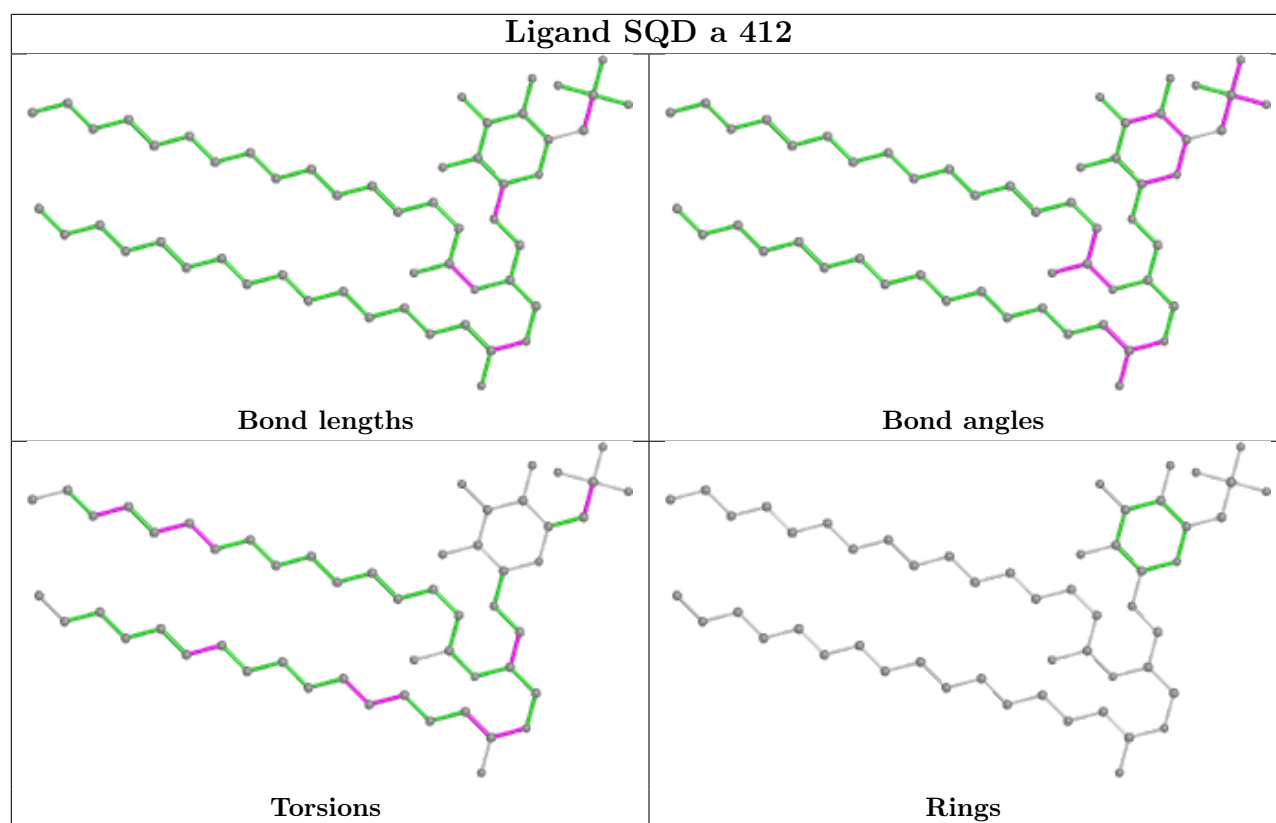


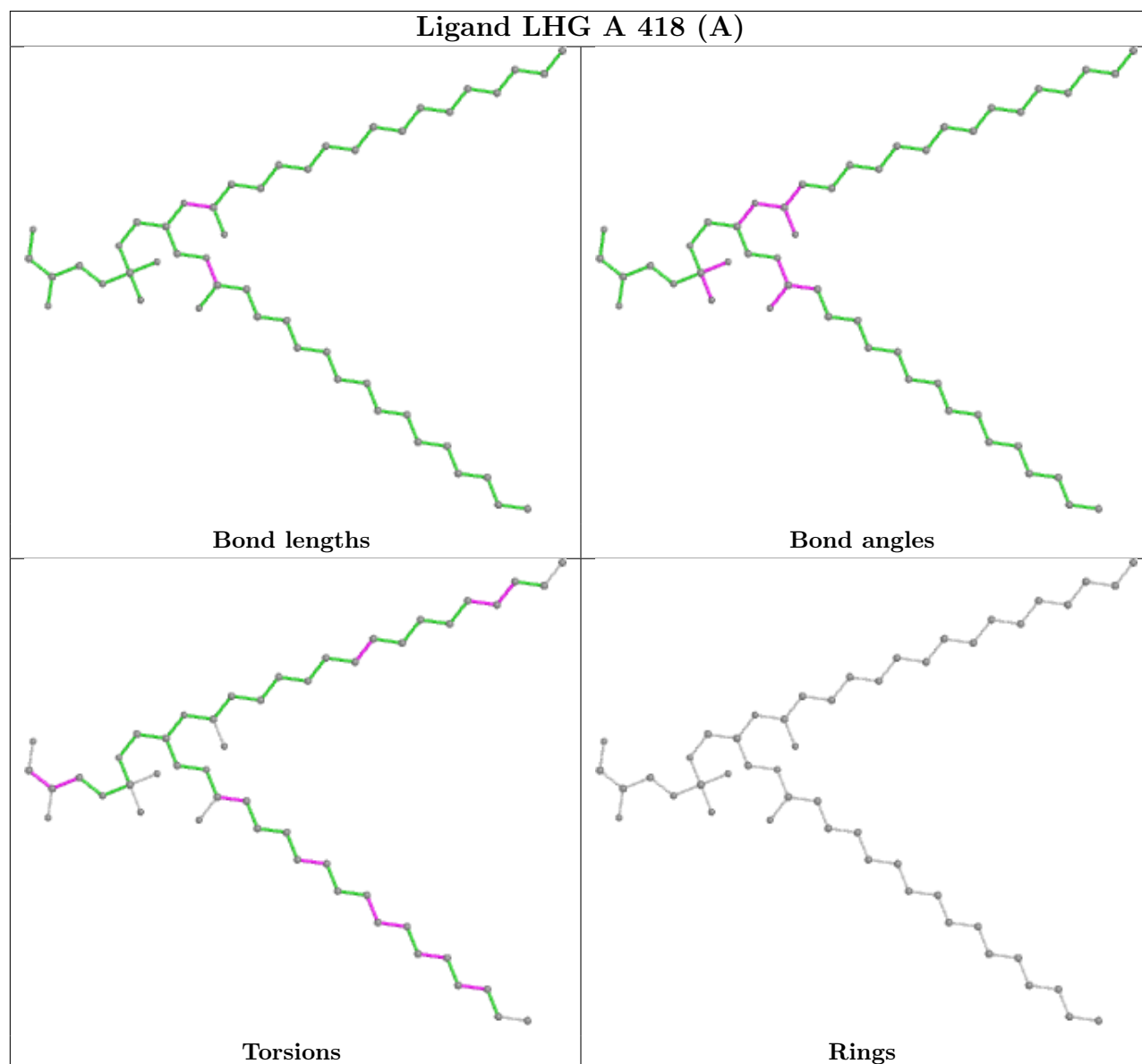
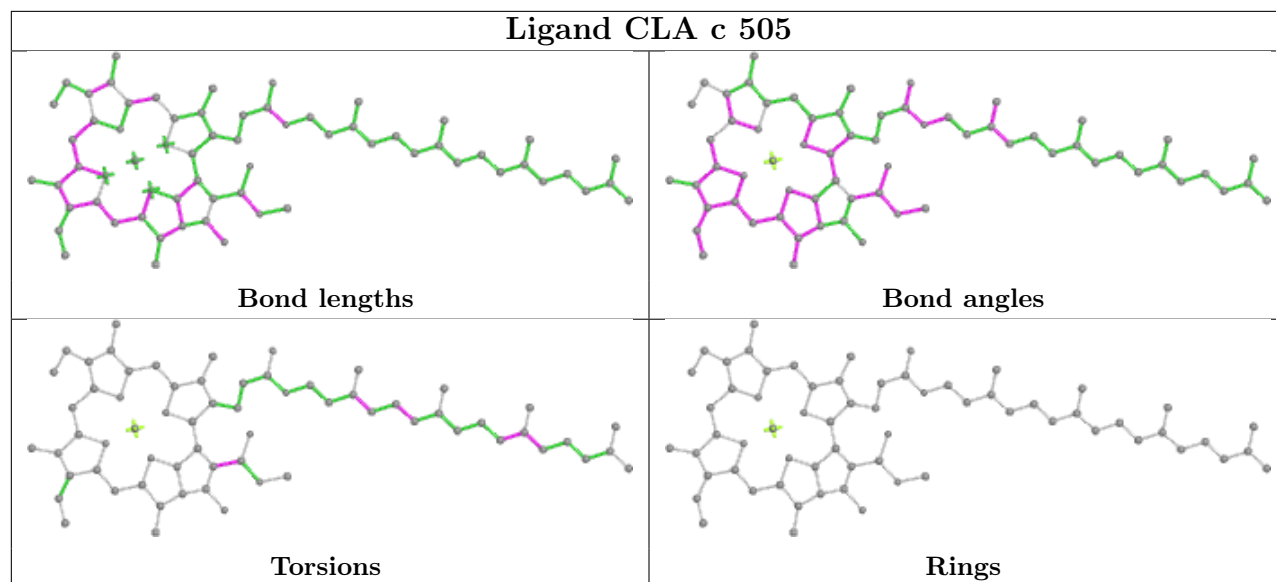


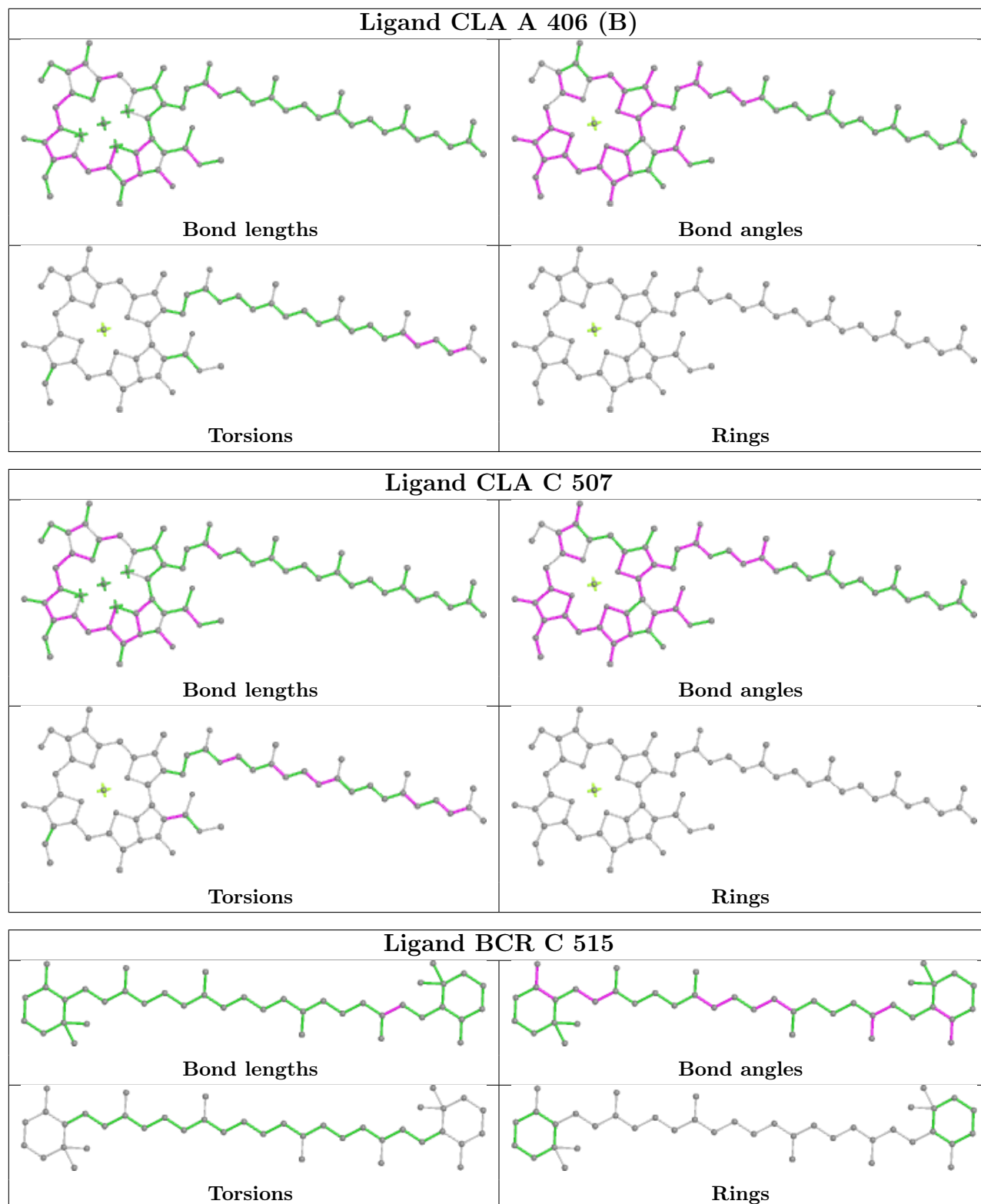


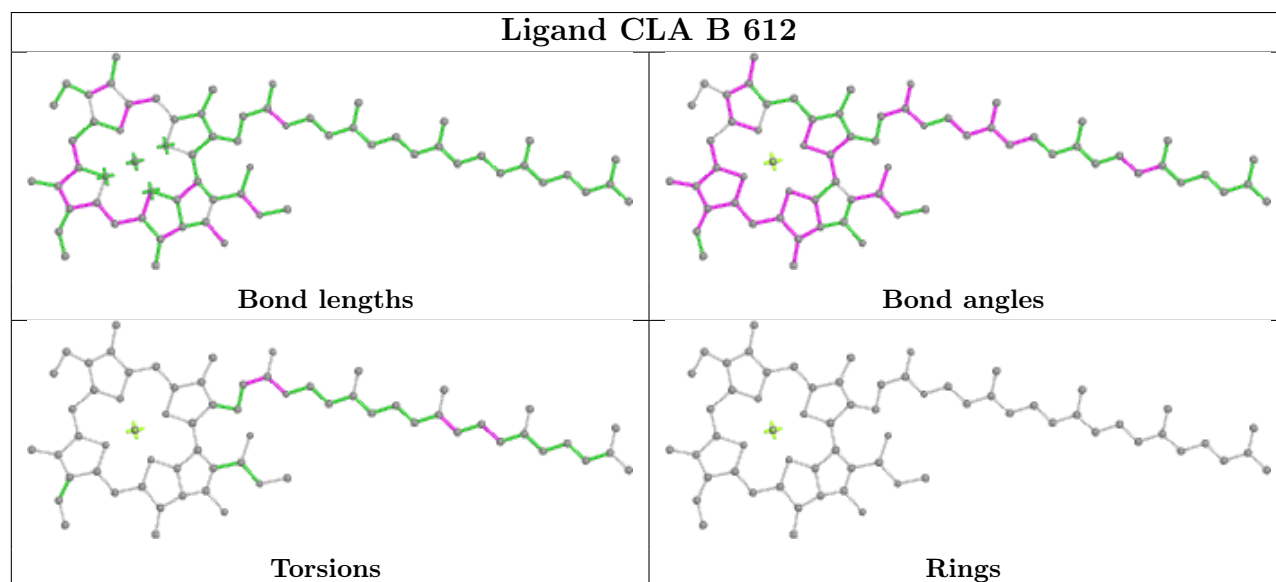
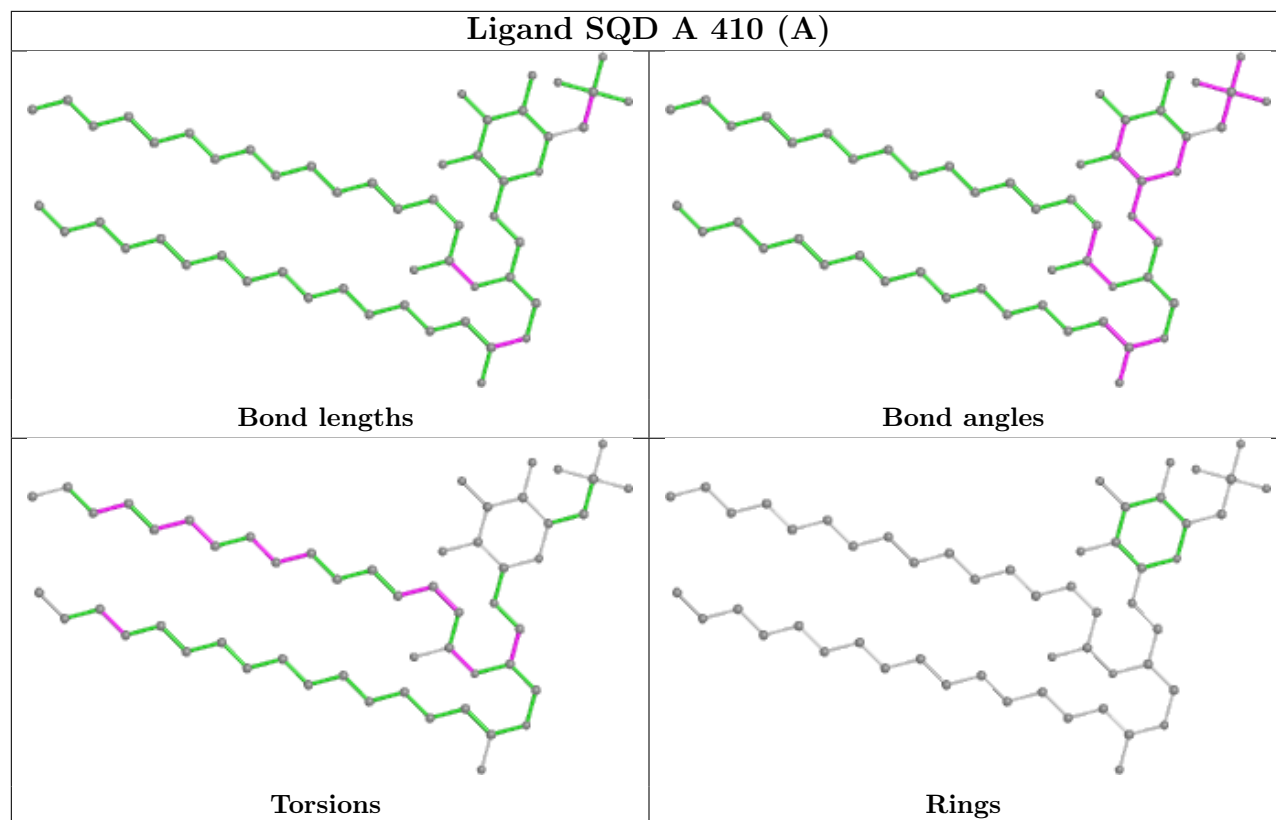


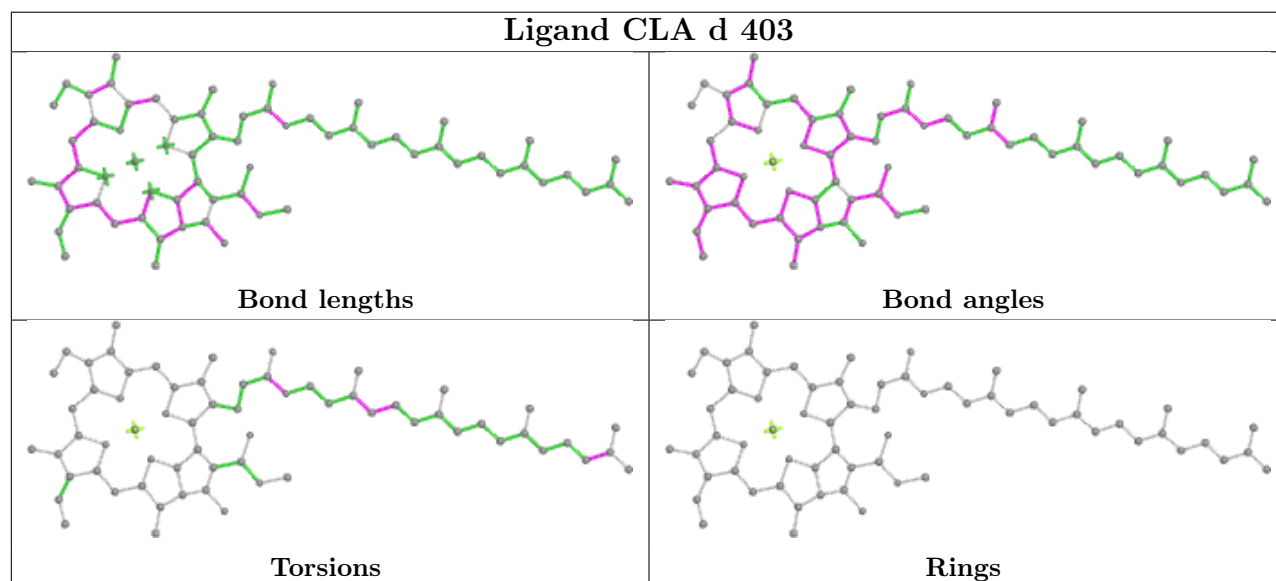
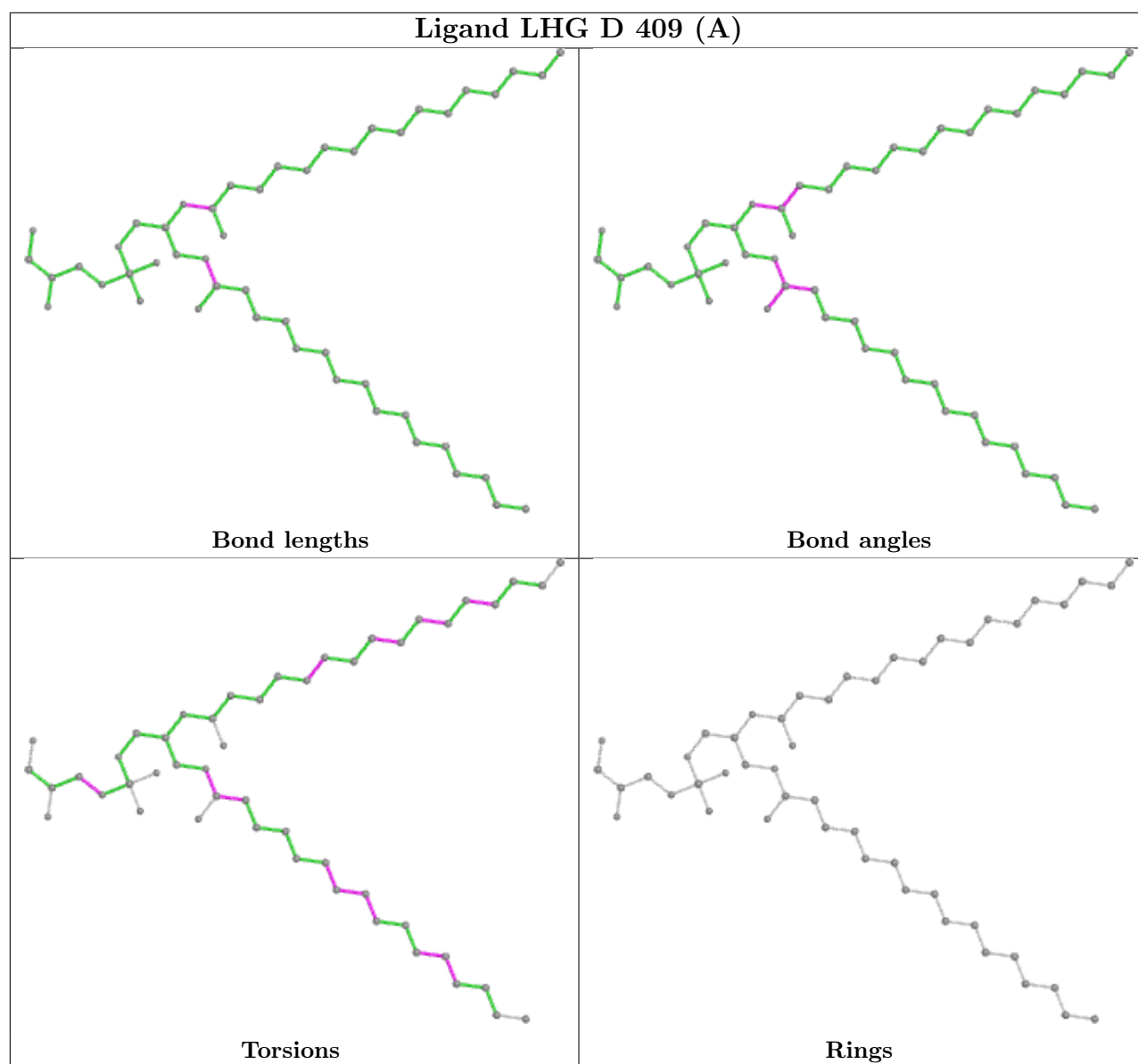


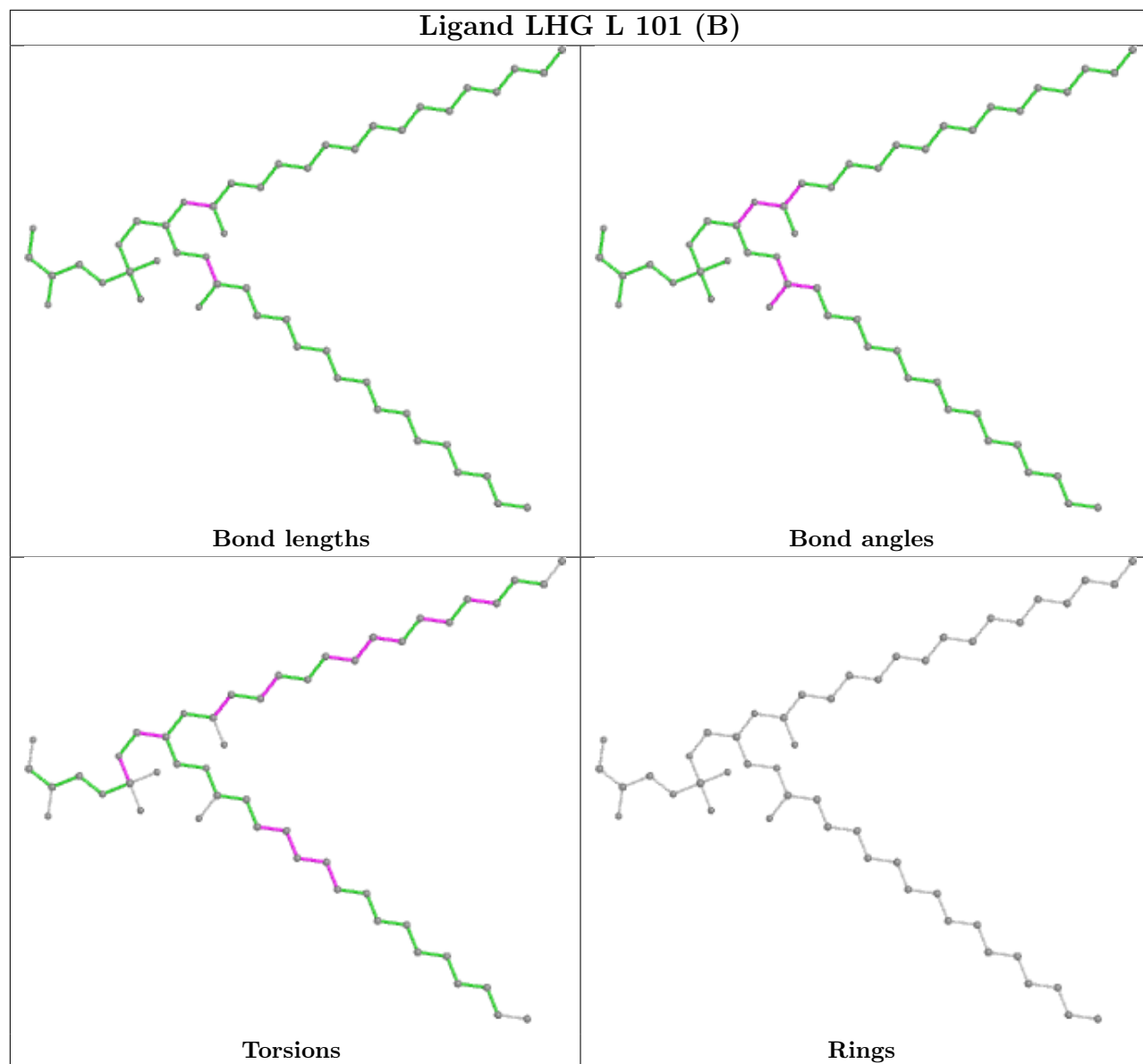


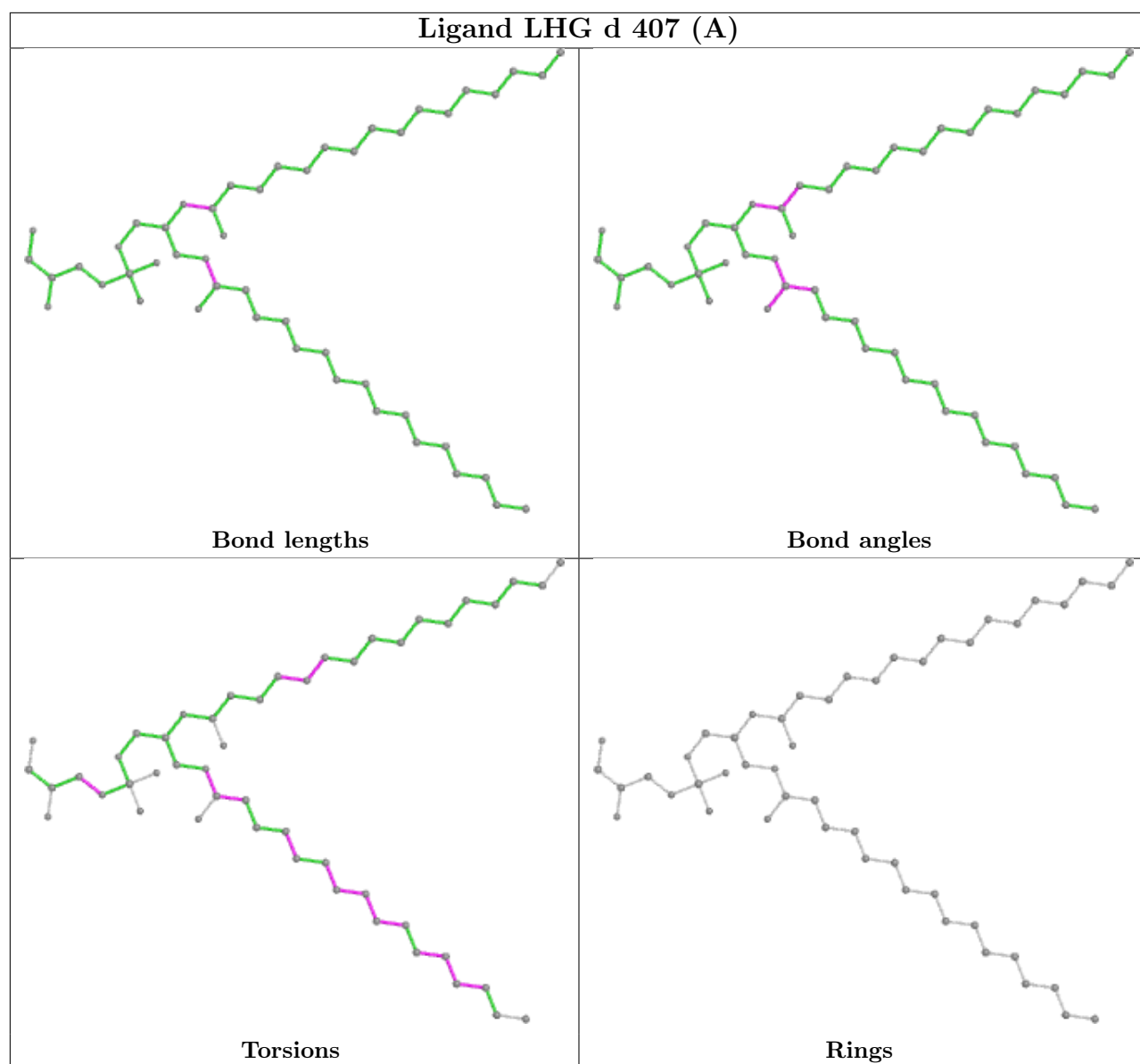


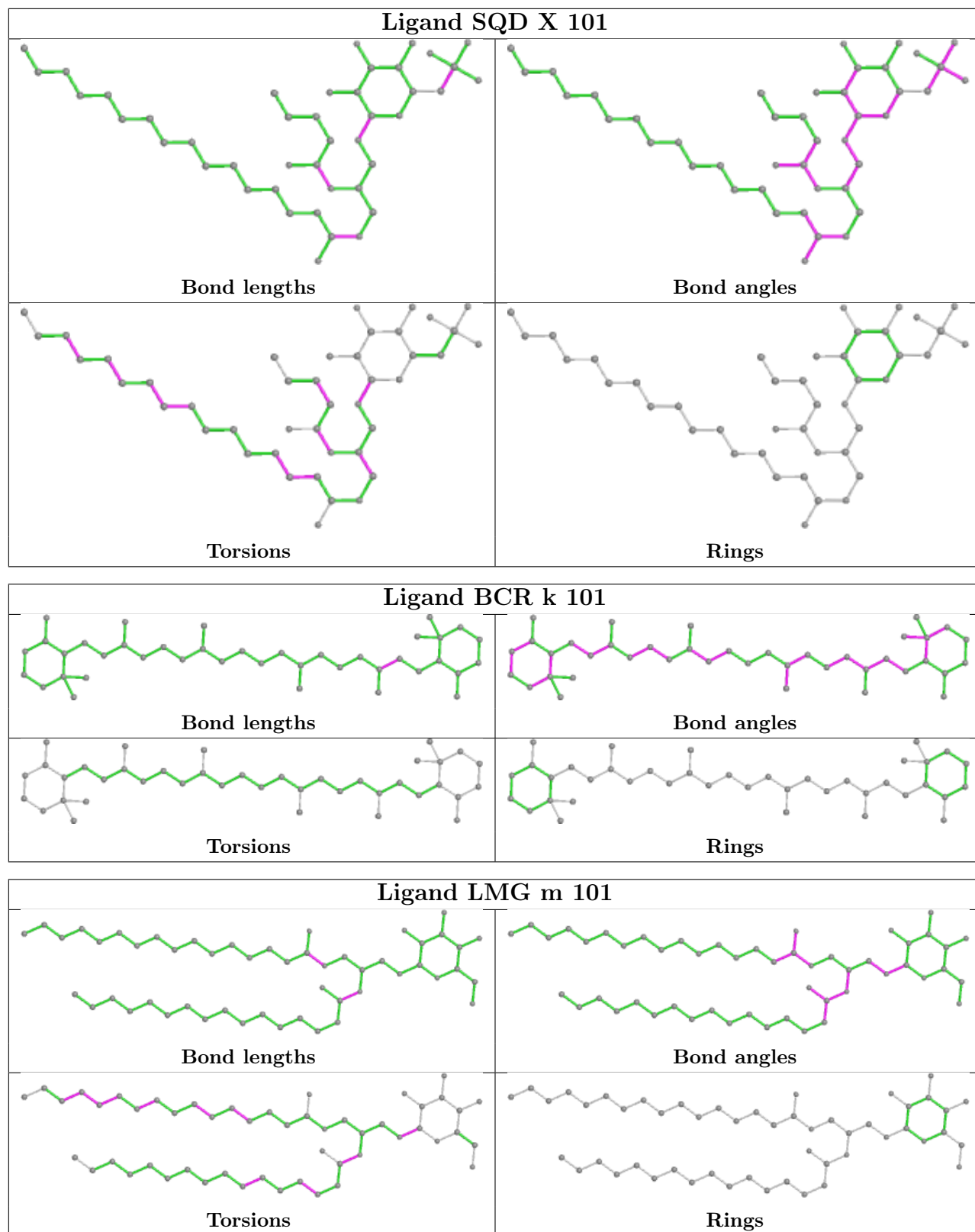


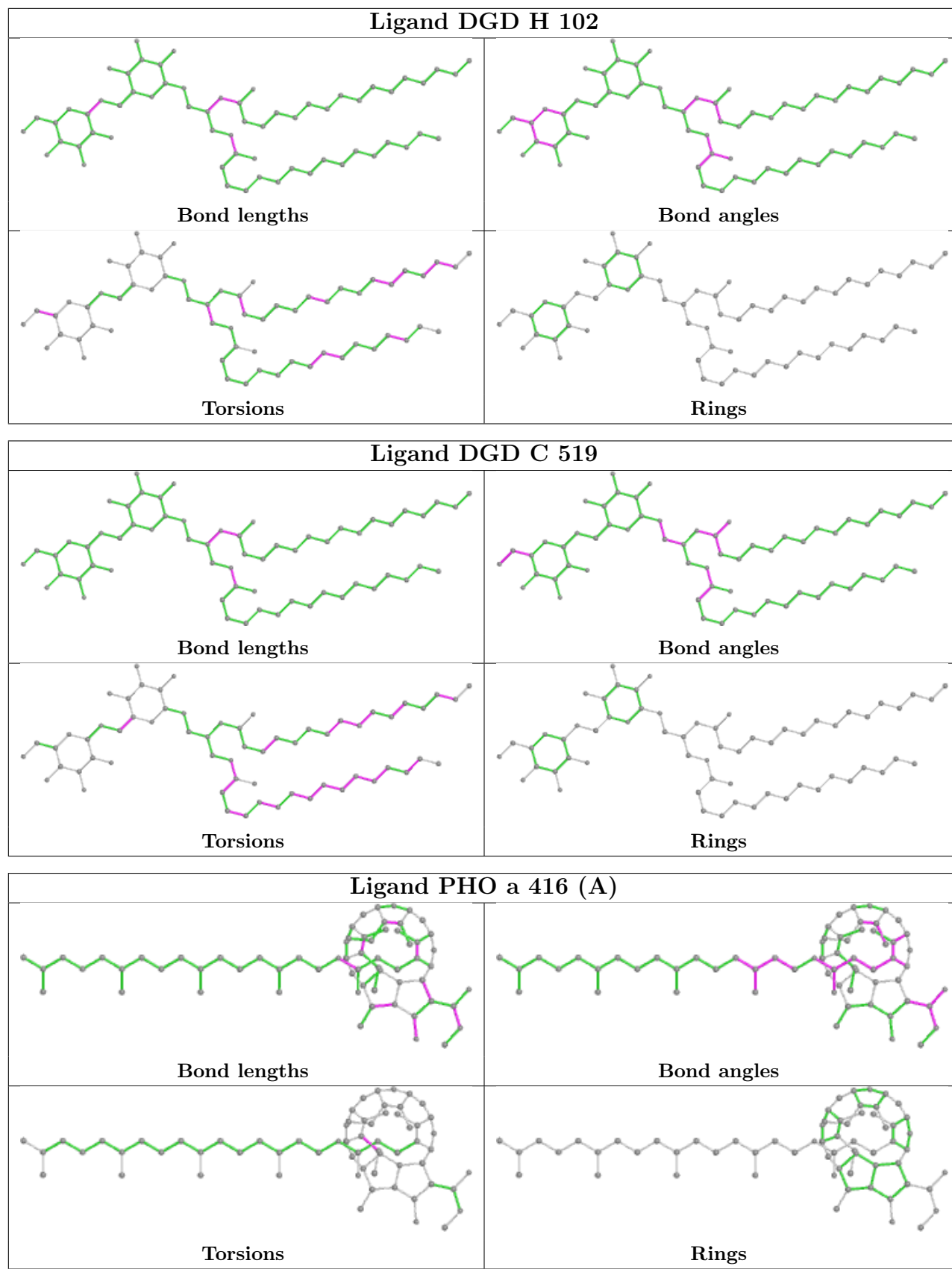


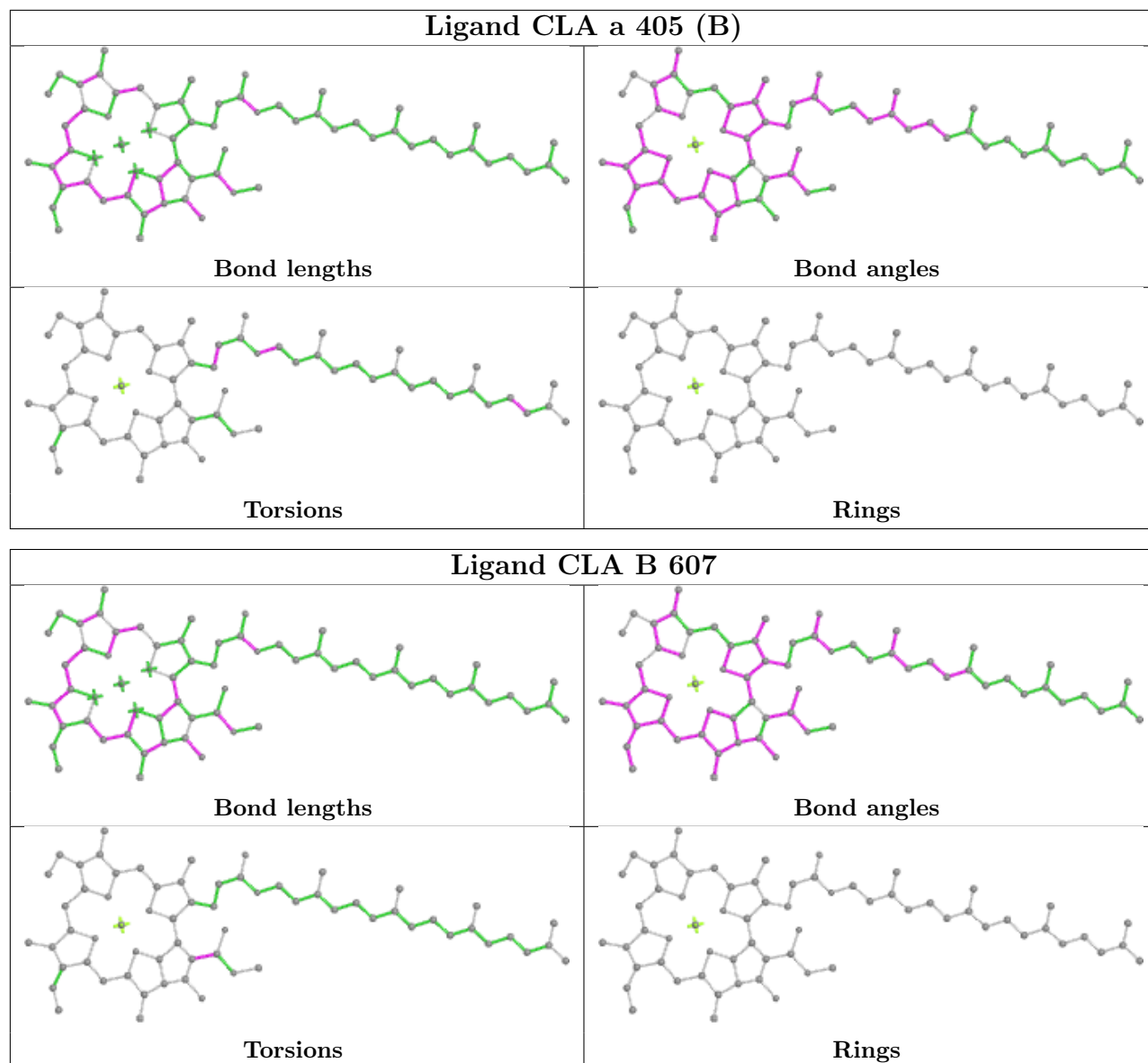


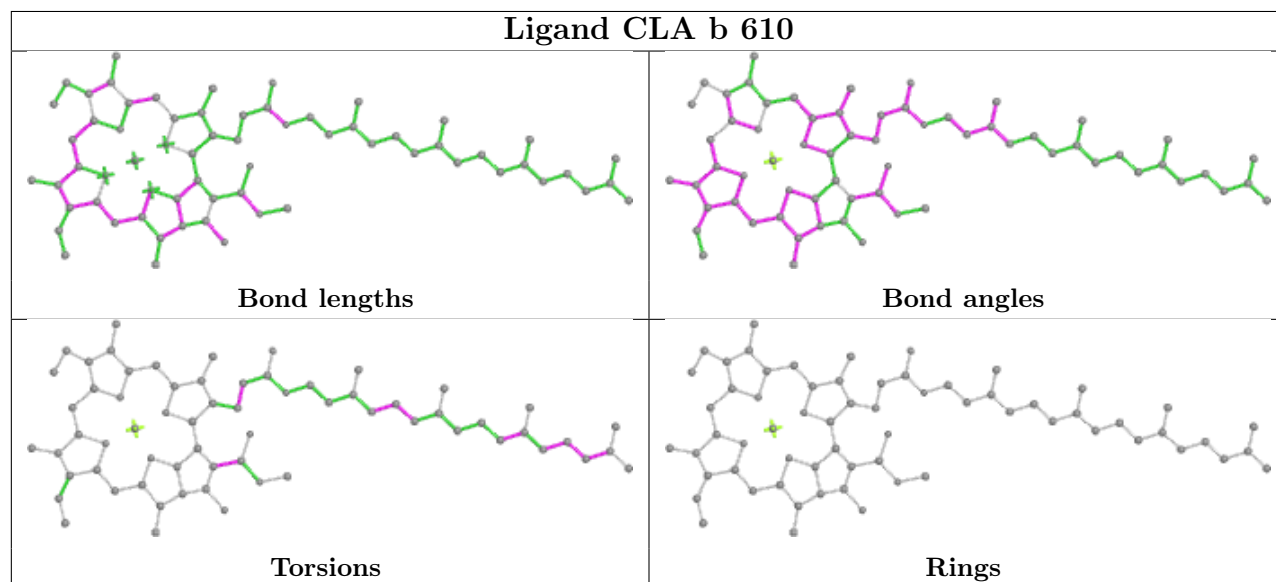
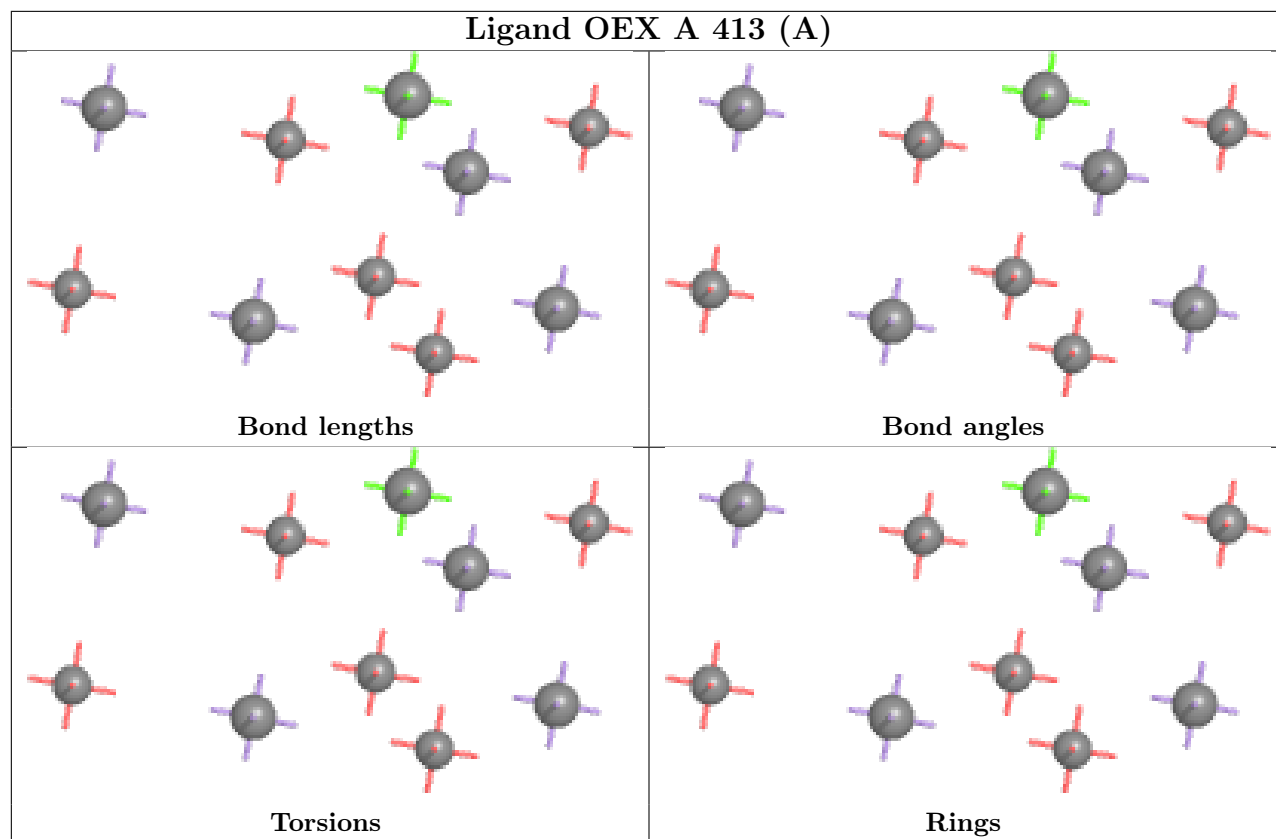


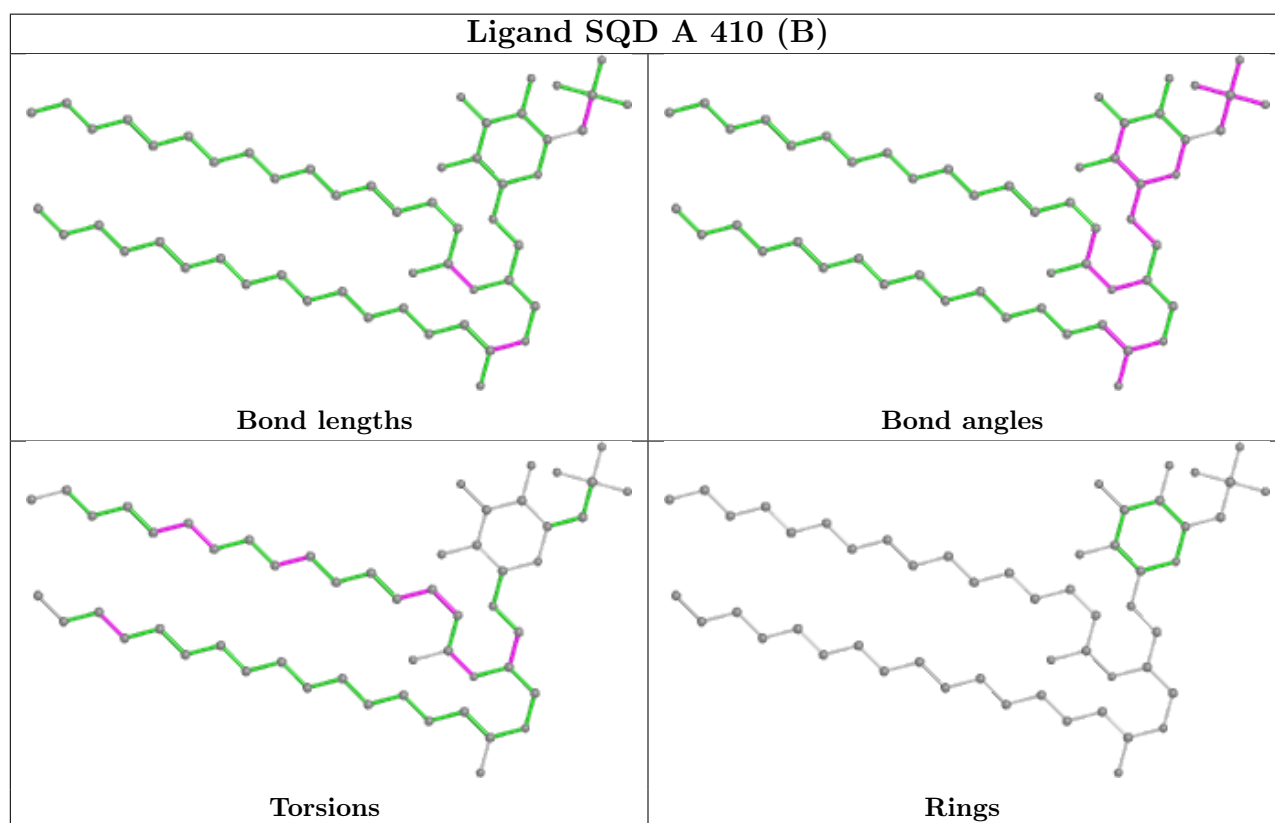
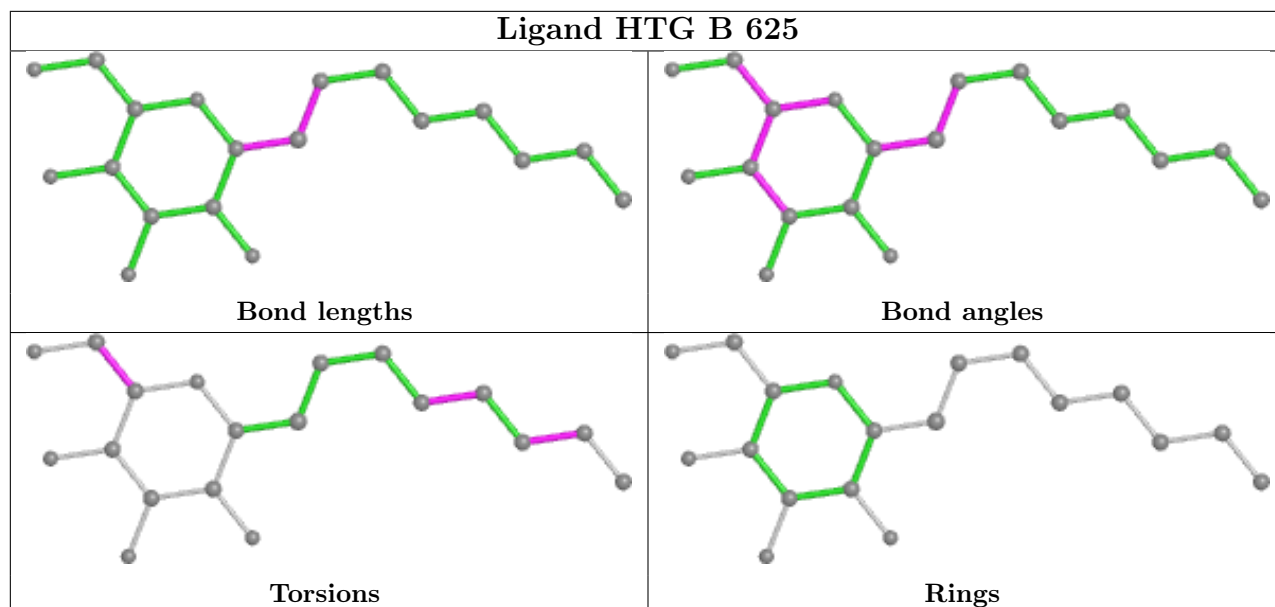


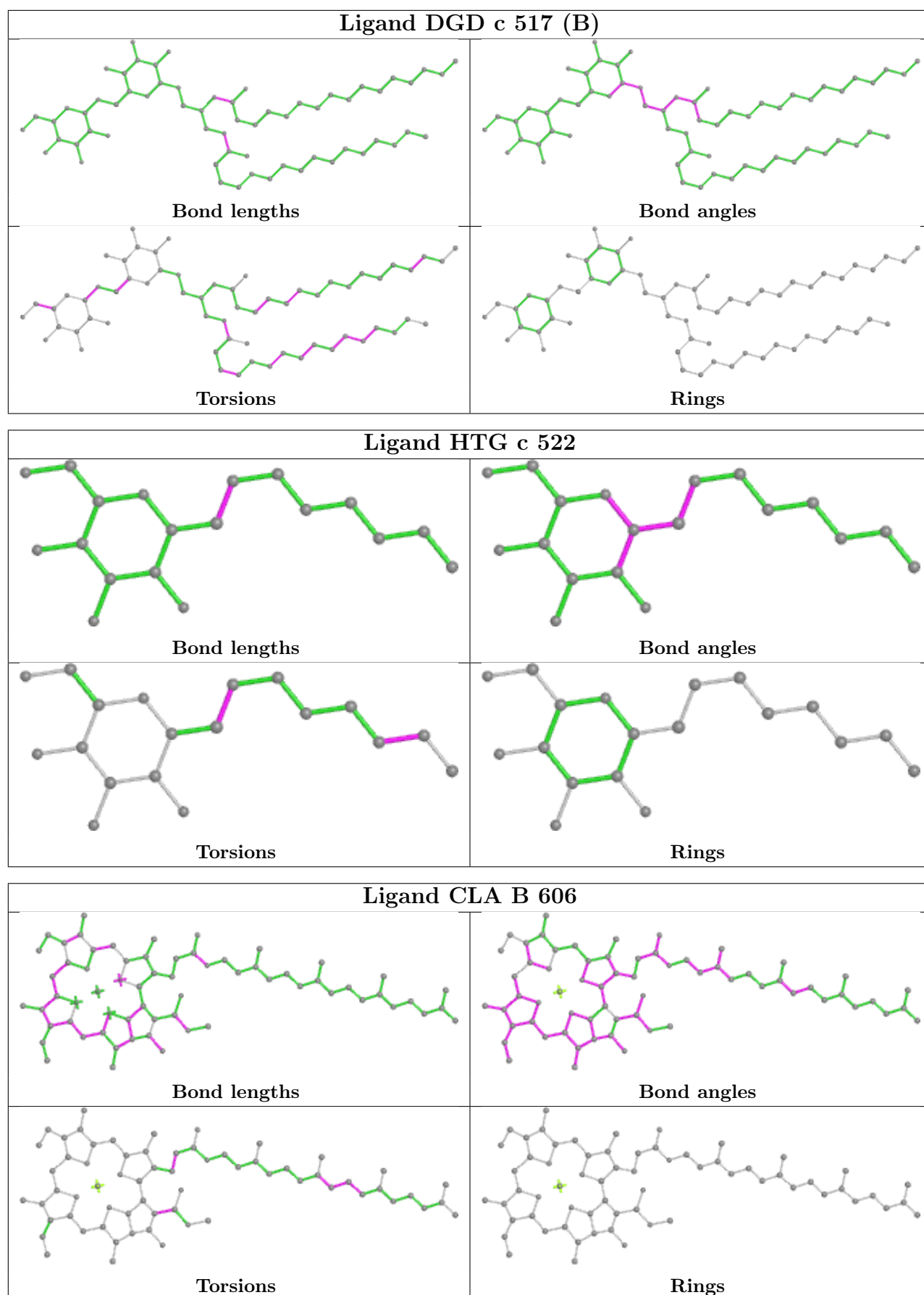


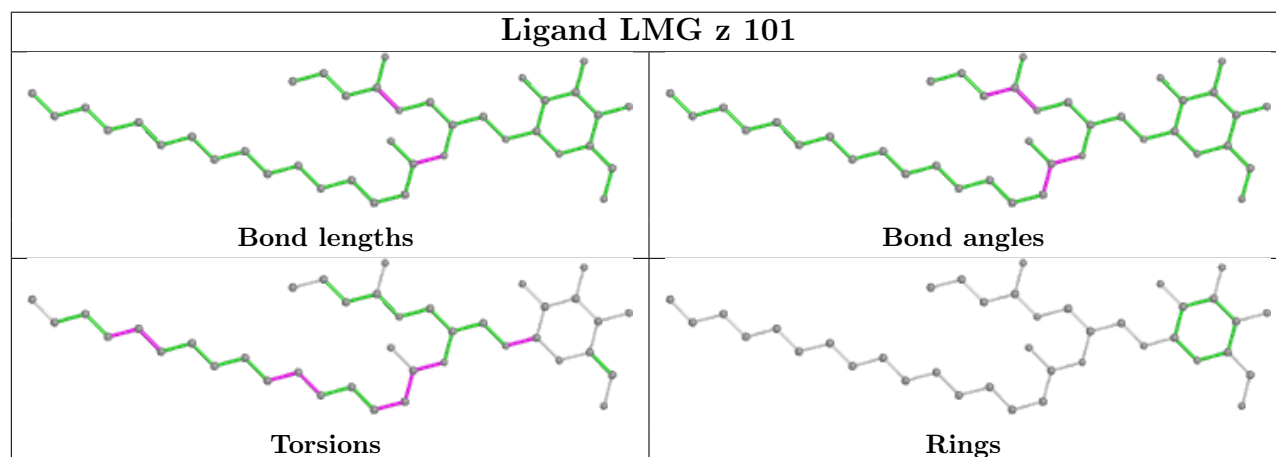
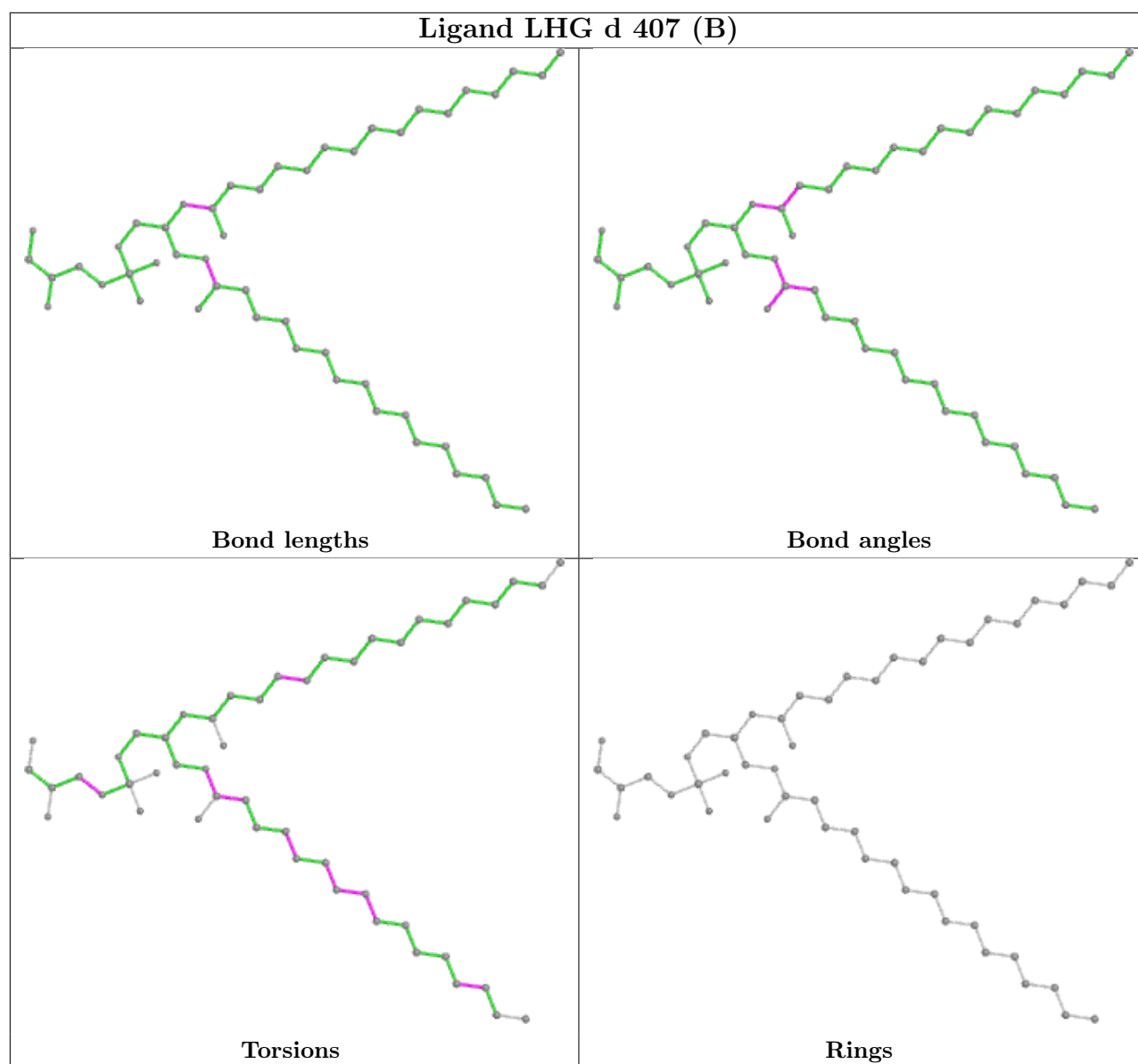


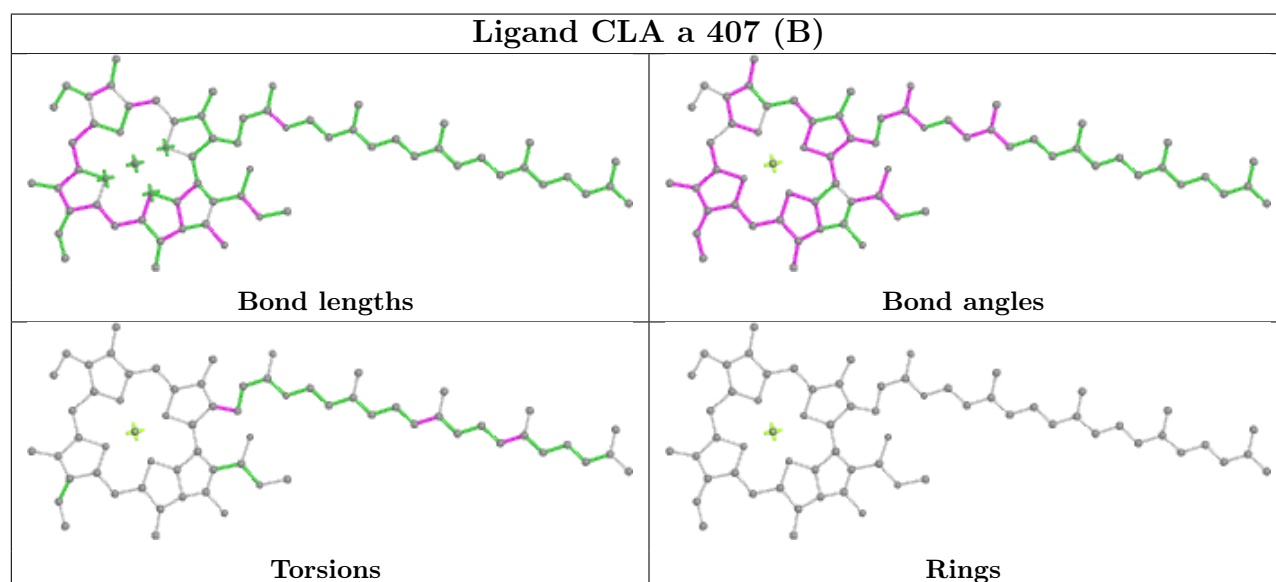
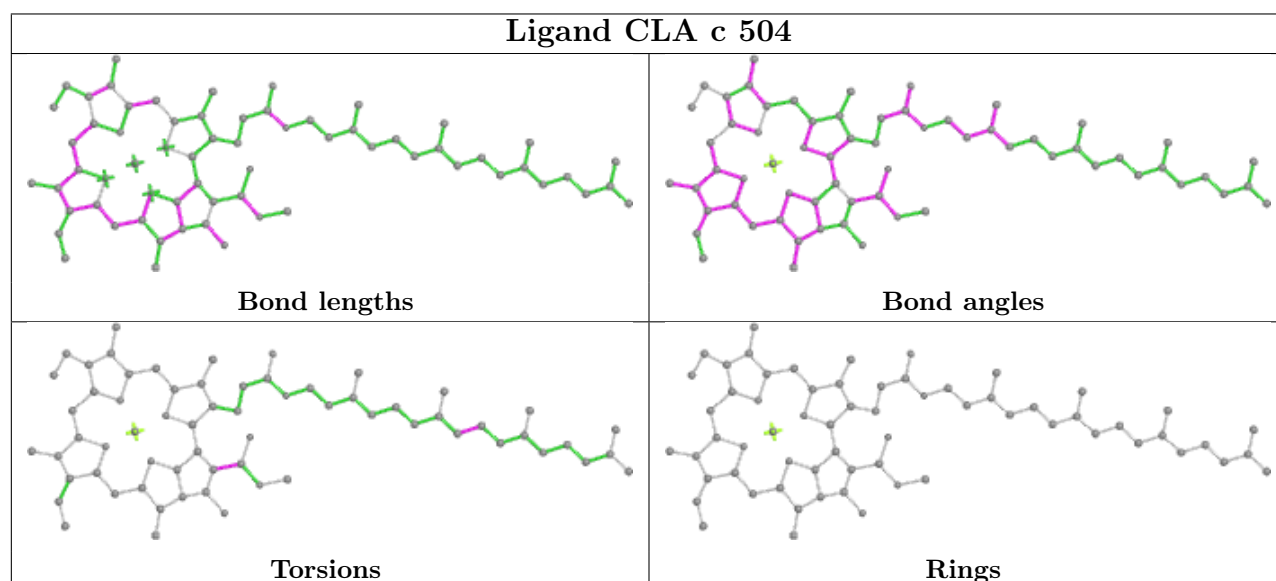
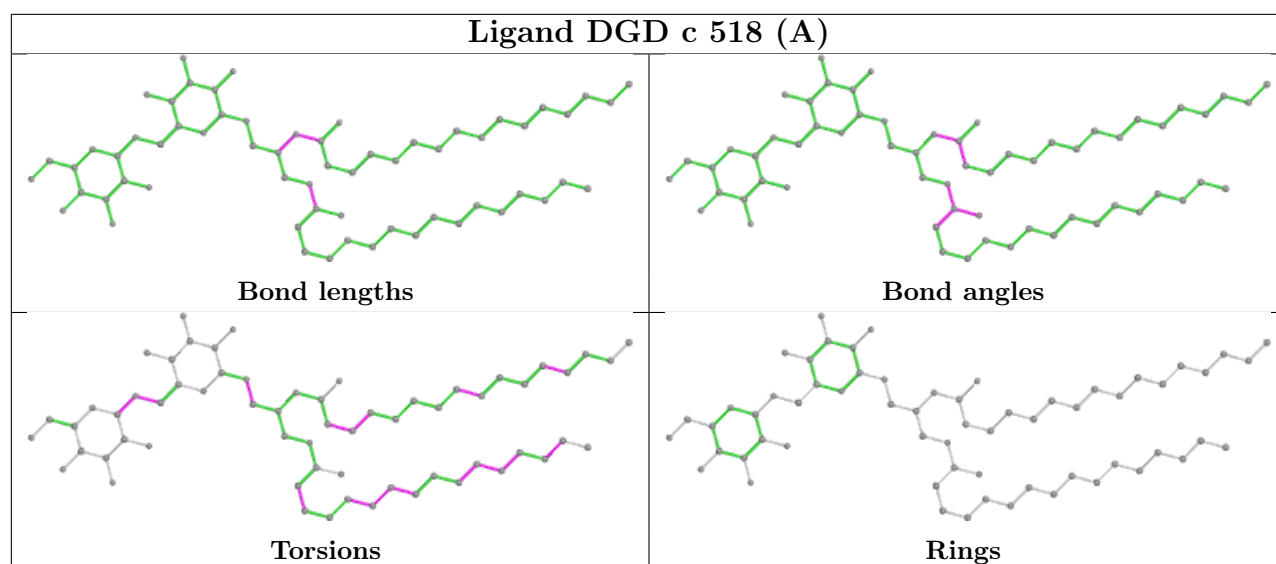


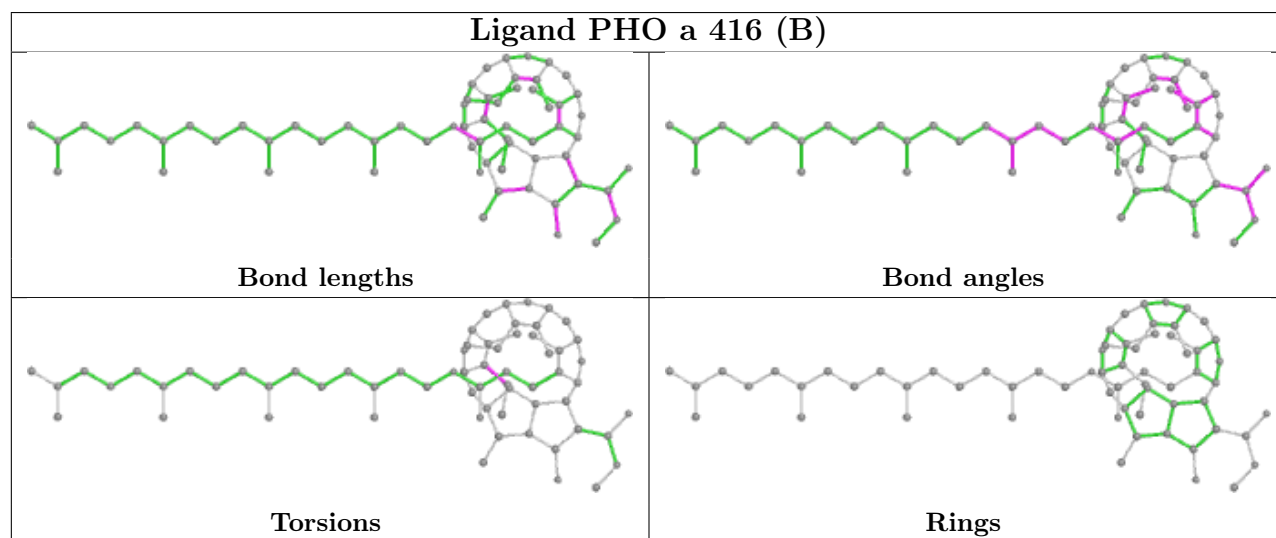
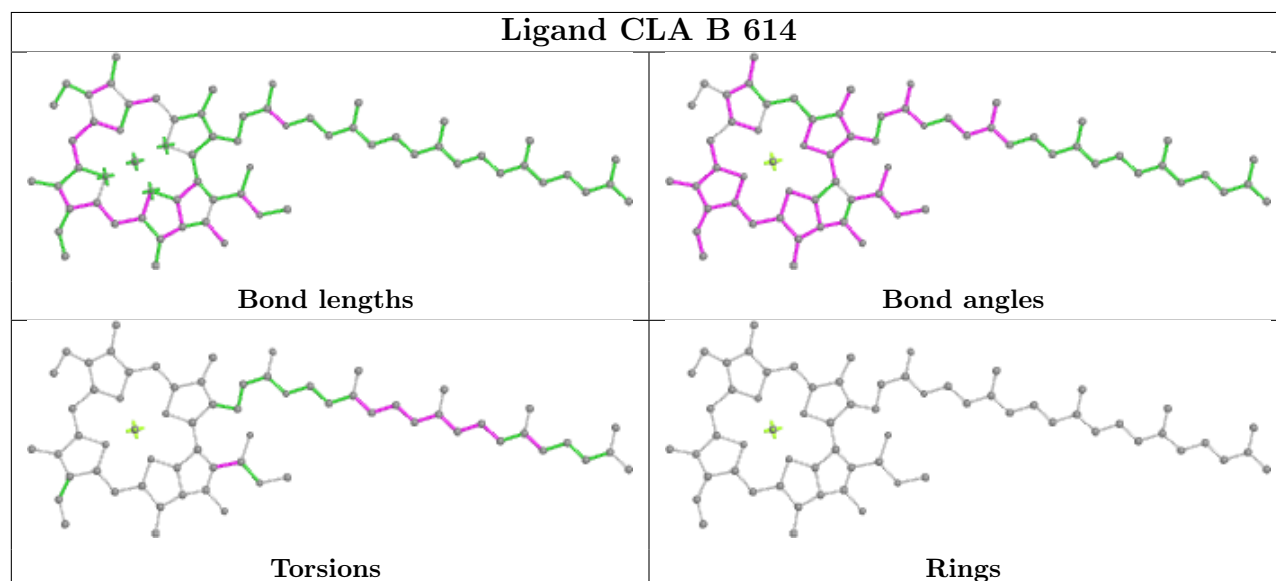
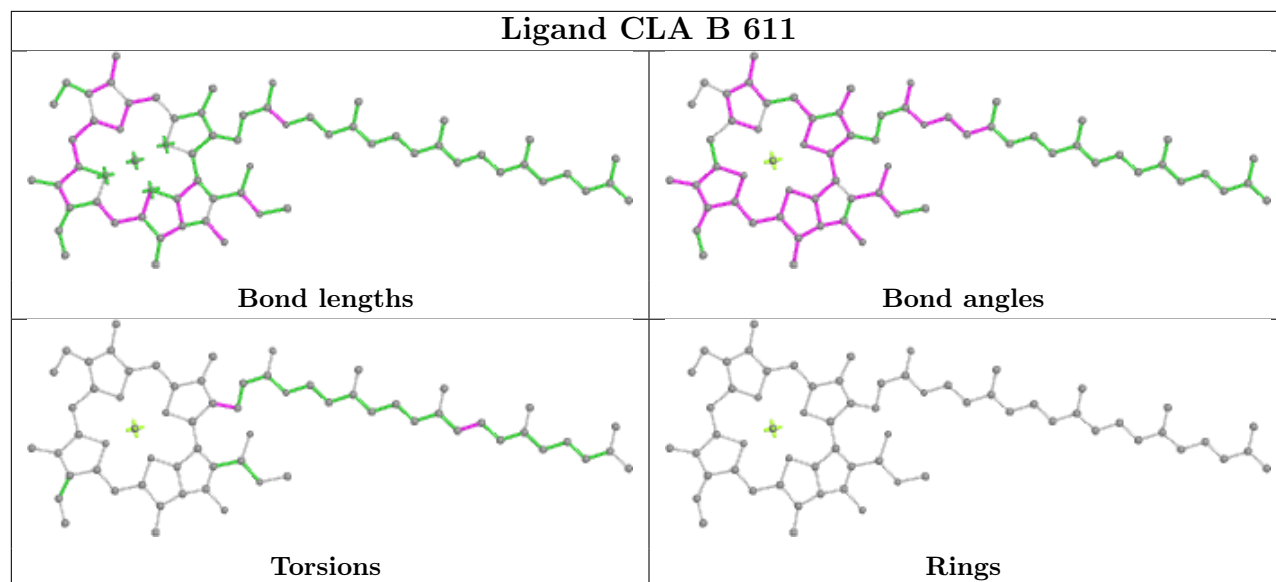


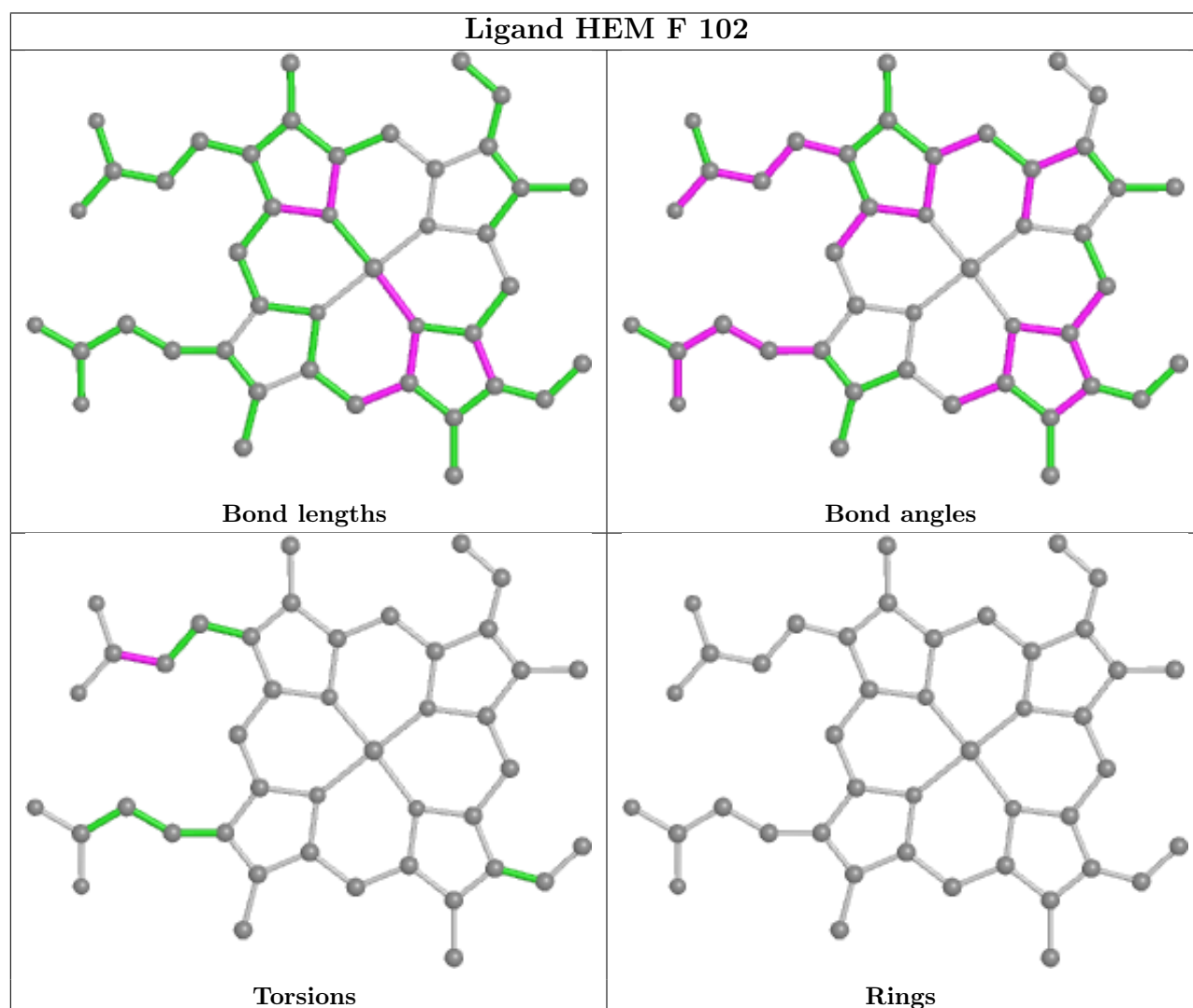
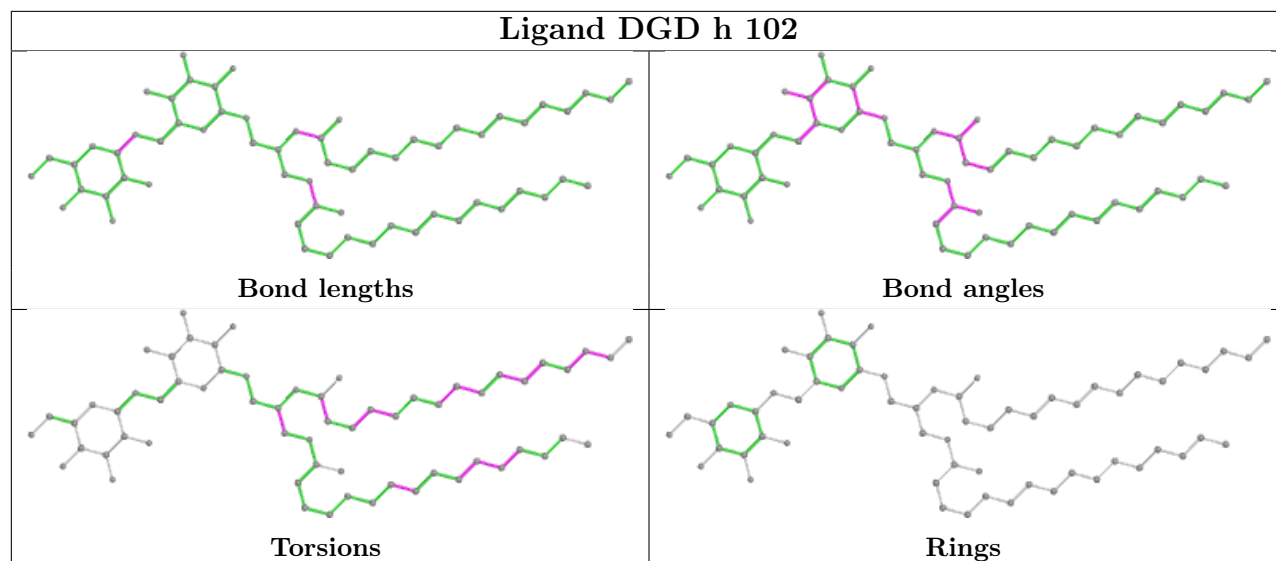


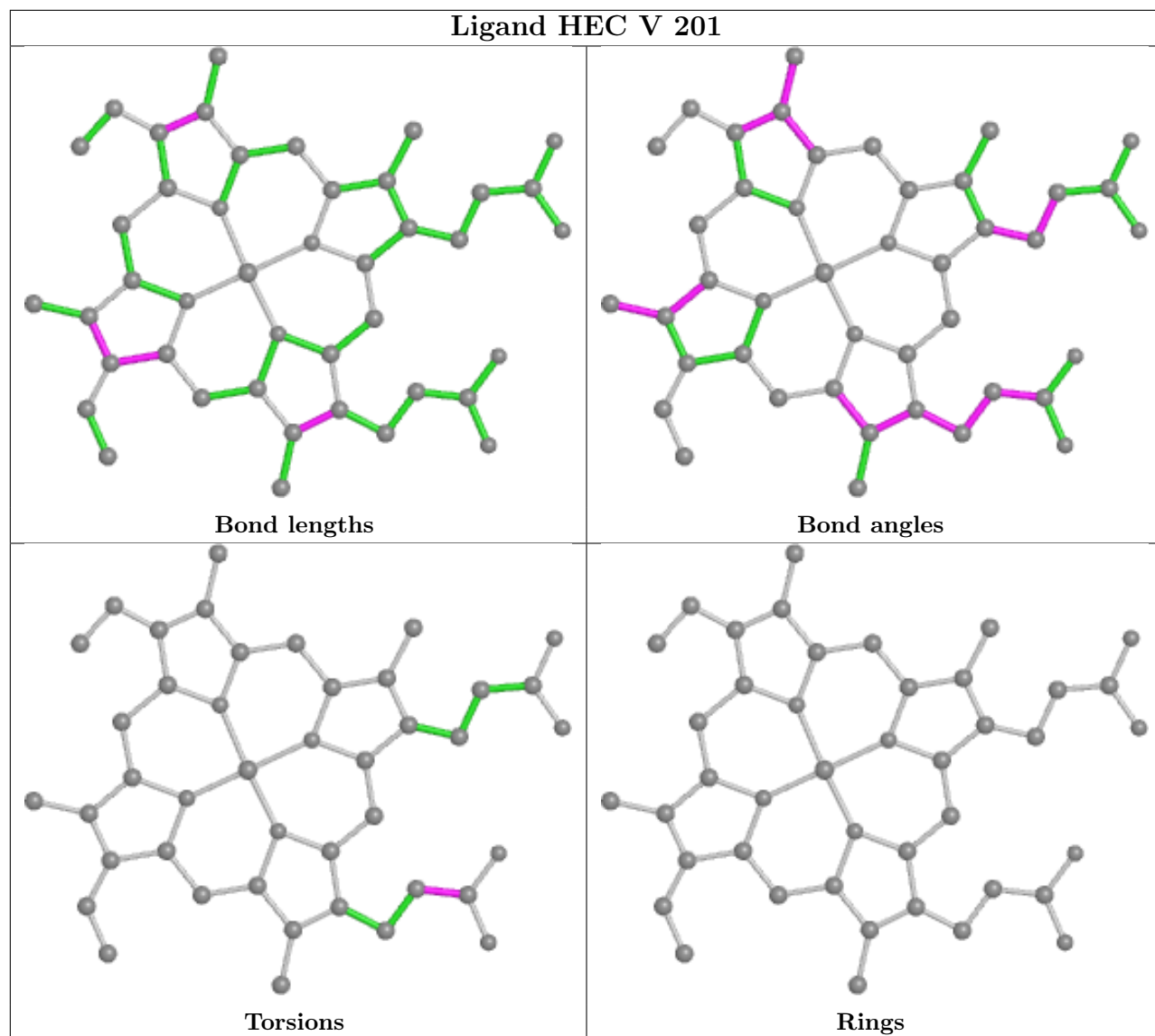


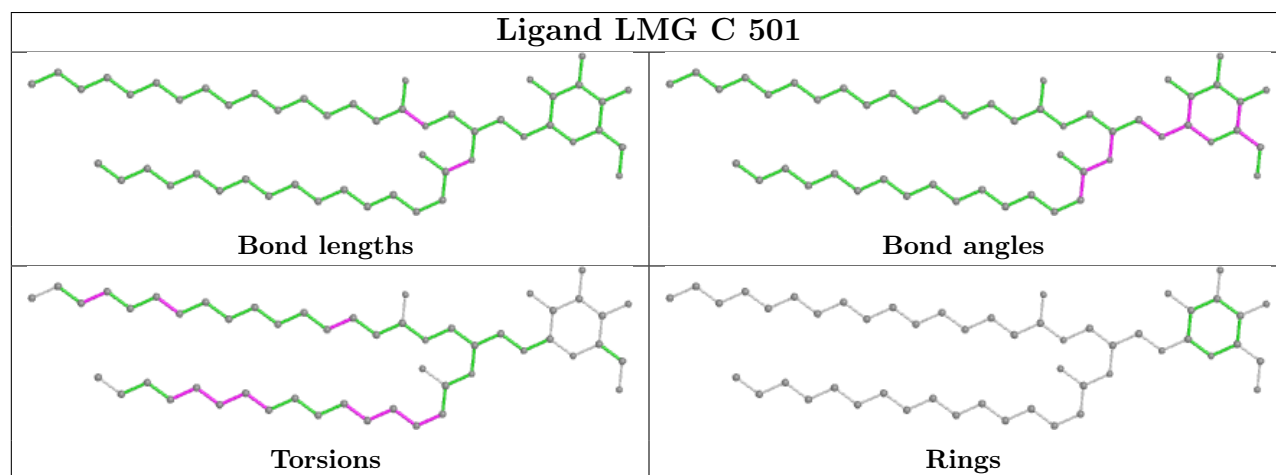
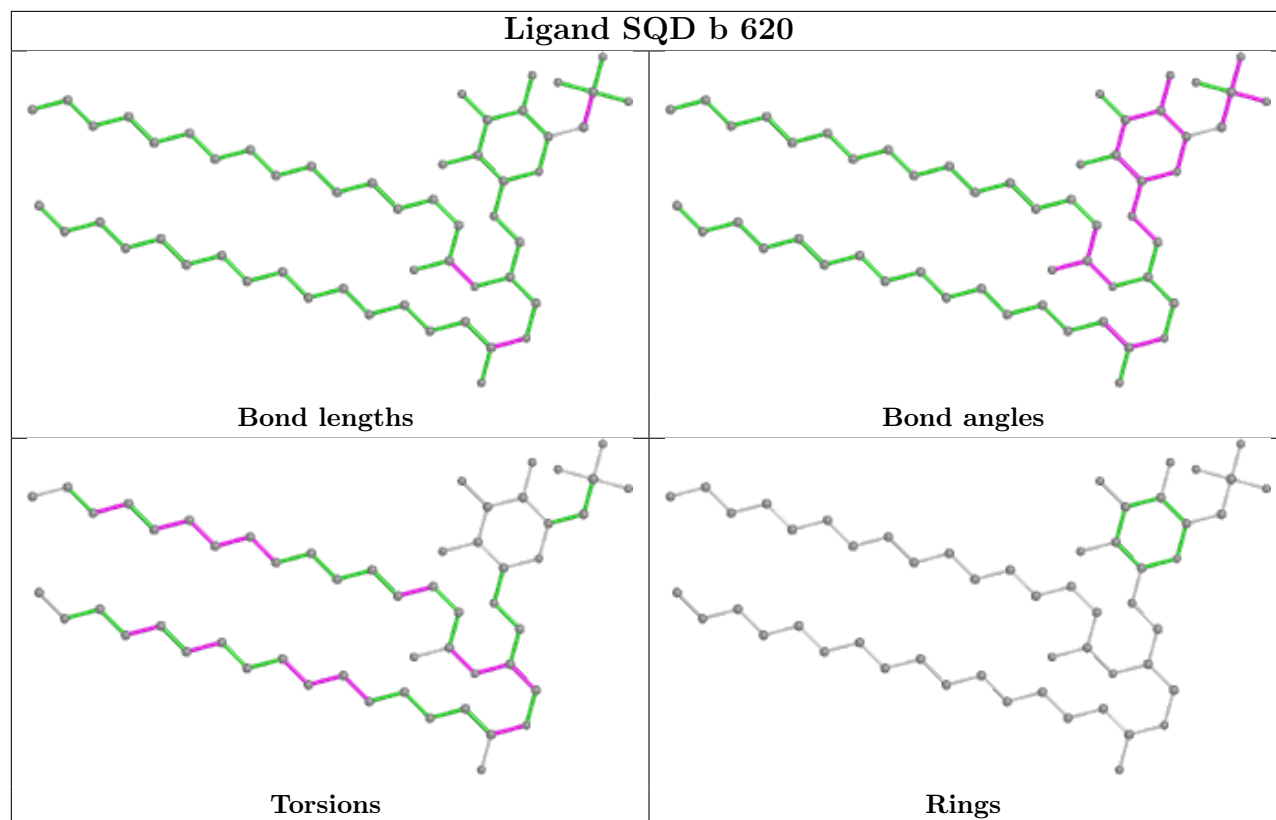


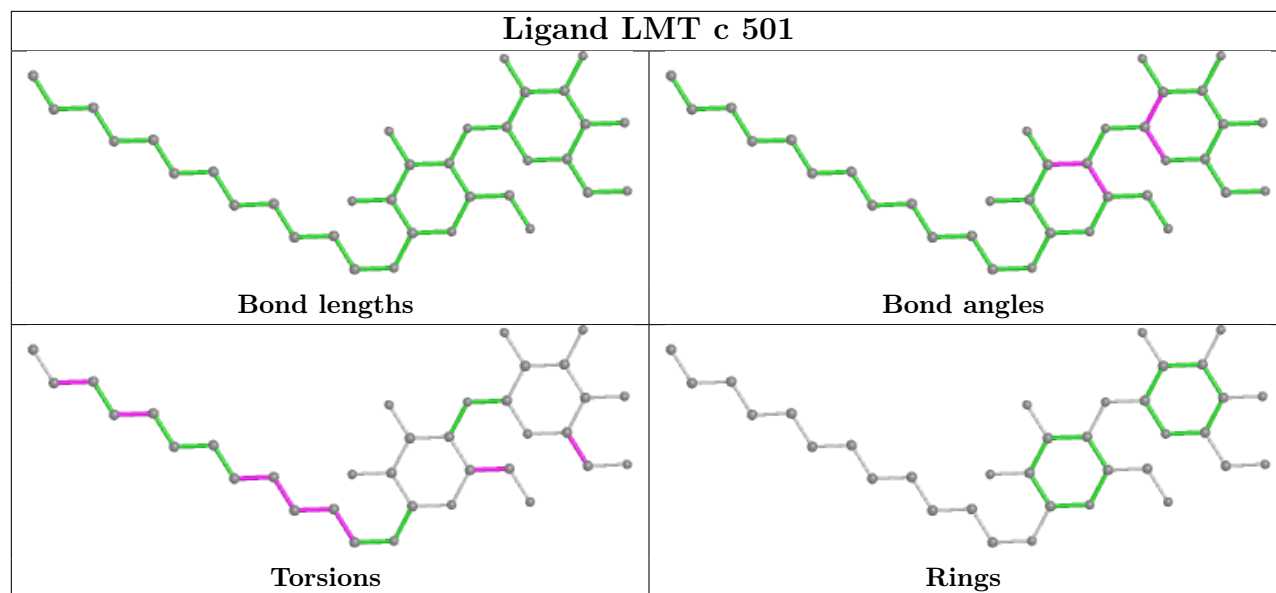












5.7 Other polymers [i](#)

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	37, 46, 67, 122	0
1	a	334/344 (97%)	-0.68	8 (2%) 59 62	38, 50, 82, 131	0
2	B	504/505 (99%)	-0.53	10 (1%) 65 68	39, 53, 82, 113	0
2	b	504/505 (99%)	-0.28	32 (6%) 20 22	42, 57, 100, 158	1 (0%)
3	C	451/455 (99%)	-0.56	8 (1%) 68 71	42, 58, 81, 134	0
3	c	455/455 (100%)	-0.43	13 (2%) 51 55	48, 65, 86, 121	2 (0%)
4	D	342/342 (100%)	-0.74	4 (1%) 79 81	37, 47, 66, 128	0
4	d	341/342 (99%)	-0.69	3 (0%) 84 85	40, 52, 79, 126	0
5	E	81/84 (96%)	-0.10	5 (6%) 20 22	51, 68, 98, 147	0
5	e	79/84 (94%)	0.27	9 (11%) 5 4	60, 76, 122, 142	0
6	F	34/44 (77%)	-0.42	2 (5%) 22 24	53, 61, 89, 111	0
6	f	31/44 (70%)	-0.19	2 (6%) 18 20	58, 67, 96, 134	0
7	H	64/65 (98%)	-0.29	2 (3%) 49 52	52, 61, 85, 107	0
7	h	64/65 (98%)	-0.28	3 (4%) 31 34	58, 72, 93, 105	0
8	I	37/38 (97%)	-0.17	3 (8%) 12 13	55, 63, 119, 145	0
8	i	37/38 (97%)	-0.01	6 (16%) 1 1	53, 63, 113, 130	0
9	J	38/39 (97%)	-0.19	3 (7%) 12 14	50, 66, 116, 159	0
9	j	39/39 (100%)	0.32	7 (17%) 1 1	56, 76, 128, 155	0
10	K	37/37 (100%)	-0.60	1 (2%) 54 57	56, 66, 84, 102	0
10	k	37/37 (100%)	-0.48	0 100 100	64, 74, 95, 111	0
11	L	36/37 (97%)	-0.33	4 (11%) 5 5	37, 44, 113, 128	0
11	l	36/37 (97%)	-0.40	3 (8%) 11 12	40, 47, 100, 117	0
12	M	32/36 (88%)	-0.75	1 (3%) 49 52	41, 47, 75, 125	0
12	m	33/36 (91%)	-0.46	2 (6%) 21 23	41, 47, 69, 139	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.06	18 (7%) 14 15	41, 65, 116, 165	0
13	o	243/244 (99%)	0.02	22 (9%) 9 10	41, 67, 121, 155	0
14	T	29/32 (90%)	-0.69	2 (6%) 16 18	42, 47, 76, 98	0
14	t	29/32 (90%)	-0.71	1 (3%) 45 47	43, 48, 76, 105	0
15	U	96/104 (92%)	-0.42	2 (2%) 63 66	45, 56, 88, 101	0
15	u	97/104 (93%)	-0.40	1 (1%) 82 84	50, 60, 82, 119	0
16	V	137/137 (100%)	-0.57	2 (1%) 73 75	44, 55, 78, 102	0
16	v	137/137 (100%)	-0.12	6 (4%) 34 37	52, 69, 101, 131	0
17	X	38/40 (95%)	-0.39	2 (5%) 26 29	60, 72, 92, 112	0
17	x	38/40 (95%)	0.11	5 (13%) 3 3	66, 78, 124, 154	0
18	Y	29/30 (96%)	0.87	7 (24%) 0 0	66, 82, 115, 121	0
18	y	29/30 (96%)	0.40	4 (13%) 2 2	75, 88, 107, 113	0
19	Z	62/62 (100%)	0.17	6 (9%) 7 8	65, 79, 131, 149	0
19	z	62/62 (100%)	0.43	14 (22%) 0 0	80, 92, 137, 164	0
20	R	34/34 (100%)	2.46	21 (61%) 0 0	89, 113, 135, 148	0
All	All	5283/5384 (98%)	-0.39	249 (4%) 31 34	37, 58, 101, 165	3 (0%)

All (249) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	23	ALA	8.8
5	E	84	LYS	8.7
1	a	11	ALA	8.7
2	b	495	PHE	7.5
3	c	20	SER	7.5
13	O	62	GLU	7.0
13	O	56	PRO	7.0
17	x	38	GLN	6.9
2	b	494	GLY	6.4
13	O	60	ARG	6.2
19	Z	32	ASP	6.1
13	o	56	PRO	6.0
19	Z	31	GLN	5.9
2	b	502	VAL	5.9
13	o	4	THR	5.6
12	m	34	LYS	5.6
20	R	32	GLN	5.5

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Mol	Chain	Res	Type	RSRZ
2	b	489	GLU	5.5
19	z	32	ASP	5.5
20	R	35	LEU	5.5
13	O	4	THR	5.4
18	Y	19	ILE	5.4
13	o	59	LYS	5.3
18	Y	18	VAL	5.3
5	e	84	LYS	5.2
12	M	33	GLN	5.2
13	o	58	ASN	5.2
9	j	3	GLU	5.2
8	I	36	ASP	5.2
13	O	59	LYS	5.1
19	z	31	GLN	5.1
19	Z	3	ILE	5.1
13	O	63	ALA	5.0
13	o	62	GLU	4.9
6	f	15	ILE	4.9
6	F	12	SER	4.8
14	T	30[A]	THR	4.8
1	A	11	ALA	4.8
6	f	16[A]	PHE	4.8
4	D	11	GLU	4.8
20	R	20	VAL	4.8
20	R	3	TRP	4.6
2	b	493[A]	TRP	4.6
13	o	60	ARG	4.6
17	x	2	THR	4.6
13	O	5	LEU	4.5
2	b	127	ARG	4.5
19	Z	30	PRO	4.5
11	l	3	PRO	4.4
13	o	25	THR	4.4
2	b	505	ARG	4.4
19	z	3	ILE	4.3
12	m	33	GLN	4.3
3	c	19	ASN	4.3
2	b	485	GLU	4.3
3	C	143	TYR	4.3
13	o	61	GLN	4.2
13	o	24	ASP	4.2
2	b	503	THR	4.2

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Mol	Chain	Res	Type	RSRZ
11	L	3	PRO	4.1
19	z	30	PRO	4.1
2	b	486[A]	LEU	4.1
13	O	61	GLN	4.1
9	j	5	GLY	4.1
1	a	262[A]	TYR	4.1
19	z	38	GLN	4.0
2	b	487	SER	4.0
13	o	63	ALA	4.0
19	z	60	PHE	4.0
18	y	41	VAL	4.0
19	Z	34	ASP	4.0
14	t	30[A]	THR	4.0
18	Y	20	ALA	3.9
2	B	494	GLY	3.9
7	h	6	TRP	3.9
2	b	504	THR	3.9
2	b	484[A]	PRO	3.9
3	C	207	ARG	3.9
2	b	293	ALA	3.9
9	J	3	GLU	3.9
3	c	143	TYR	3.8
20	R	33	LYS	3.8
4	D	12	ARG	3.8
19	z	35	ARG	3.8
3	c	21	ILE	3.8
20	R	31	VAL	3.7
17	x	39	ARG	3.7
20	R	4	ARG	3.7
13	O	55	GLU	3.6
11	L	7	ARG	3.6
2	b	496	TYR	3.6
18	y	18	VAL	3.6
18	y	43	ARG	3.5
16	v	17	LYS	3.5
8	I	34	ARG	3.5
13	o	35	SER	3.5
7	H	6	TRP	3.5
18	Y	43	ARG	3.5
2	B	293	ALA	3.5
1	A	13	LEU	3.4
20	R	21	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	a	263[A]	ALA	3.4
17	X	38	GLN	3.4
2	B	485	GLU	3.4
3	c	23	ALA	3.4
11	l	2	GLU	3.3
5	e	81	GLU	3.3
20	R	16	ALA	3.3
9	j	1	MET	3.3
8	i	34	ARG	3.3
13	o	57	LYS	3.3
9	j	6	ARG	3.3
13	o	55	GLU	3.3
16	v	15	GLU	3.3
13	o	207	ARG	3.2
20	R	34	LEU	3.2
20	R	24	LEU	3.2
17	X	2	THR	3.2
20	R	5	VAL	3.2
20	R	29	LYS	3.2
6	F	13	TYR	3.2
9	J	6	ARG	3.2
13	o	5	LEU	3.2
20	R	6	LEU	3.2
20	R	18	TRP	3.1
19	z	42	LEU	3.1
3	c	207	ARG	3.1
13	o	23	ASP	3.1
13	o	64	GLU	3.1
2	b	501	ASP	3.1
13	O	25	THR	3.1
11	L	5	PRO	3.1
5	E	61	ARG	3.0
2	b	375	GLY	3.0
9	j	4	GLY	3.0
4	d	236[A]	ASN	3.0
3	C	24	THR	2.9
19	Z	35	ARG	2.9
19	z	34	ASP	2.9
2	b	488	PRO	2.9
8	i	36	ASP	2.9
13	O	58	ASN	2.8
18	y	19	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
3	c	233	VAL	2.8
8	i	38	GLU	2.8
2	b	85	GLY	2.8
2	b	374	ASN	2.8
2	b	294	SER	2.8
9	j	2	SER	2.7
13	O	89	SER	2.7
2	b	373	LYS	2.7
15	u	8	GLU	2.7
17	x	3	ILE	2.7
13	o	134	THR	2.7
5	E	59	GLU	2.7
13	o	211	ILE	2.7
2	B	487	SER	2.7
13	O	207	ARG	2.7
16	v	16	GLY	2.7
1	a	261[A]	GLN	2.6
2	B	295	GLY	2.6
3	c	192	GLY	2.6
13	o	246	ALA	2.6
20	R	28	VAL	2.6
2	b	500	GLY	2.6
5	e	6	GLY	2.6
2	b	376	VAL	2.6
20	R	14	LEU	2.6
11	L	2	GLU	2.6
2	b	86	ILE	2.6
18	Y	22	LEU	2.5
3	c	22	PHE	2.5
5	e	82	GLN	2.5
20	R	2	ASP	2.5
5	e	25	ILE	2.5
20	R	19	ALA	2.5
1	a	228	THR	2.5
8	I	37	LEU	2.5
1	A	12	ASN	2.5
3	c	106	VAL	2.5
20	R	17	GLY	2.5
2	B	162	PHE	2.5
13	O	211	ILE	2.5
3	c	234	VAL	2.5
2	b	128	THR	2.4

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Mol	Chain	Res	Type	RSRZ
2	b	129	GLY	2.4
7	h	65	LEU	2.4
20	R	13	LEU	2.4
2	b	126	PRO	2.4
7	h	3[A]	ARG	2.4
2	B	373	LYS	2.4
2	b	295	GLY	2.4
8	i	35	LYS	2.4
5	e	24	SER	2.4
1	A	16	ARG	2.4
13	o	27	ARG	2.4
3	C	263	ALA	2.4
19	z	59	PHE	2.4
2	b	89	GLY	2.3
3	c	462[A]	GLU	2.3
14	T	29[A]	ILE	2.3
13	o	34	SER	2.3
18	Y	41	VAL	2.3
3	C	142	GLU	2.3
3	c	142	GLU	2.3
3	C	191	PRO	2.3
13	O	27	ARG	2.3
2	b	130	GLU	2.3
1	a	235[A]	TYR	2.3
5	e	61	ARG	2.3
5	e	59	GLU	2.3
16	v	119	ILE	2.3
13	O	23	ASP	2.2
2	b	435	GLU	2.2
10	K	13	GLU	2.2
4	D	107	LEU	2.2
4	D	238[A]	THR	2.2
8	i	37	LEU	2.2
13	O	24	ASP	2.2
16	v	128	ASP	2.2
4	d	237[A]	PRO	2.2
15	U	27	LEU	2.2
16	v	110	LYS	2.2
1	a	13	LEU	2.2
2	B	122	LEU	2.2
5	E	6	GLY	2.2
9	J	5	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
13	O	132	ASN	2.2
9	j	7	ILE	2.2
1	a	242[A]	GLU	2.2
16	V	15	GLU	2.2
2	B	374	ASN	2.1
1	A	262[A]	TYR	2.1
4	d	12	ARG	2.1
18	Y	21	GLN	2.1
19	z	33	TRP	2.1
16	V	16	GLY	2.1
19	z	62	VAL	2.1
15	U	10	VAL	2.1
17	x	37	VAL	2.1
5	E	82	GLN	2.1
2	B	128	THR	2.1
19	z	2	THR	2.1
8	i	2	GLU	2.1
19	z	61	VAL	2.1
11	l	5	PRO	2.1
5	e	42	LEU	2.0
3	C	185	LEU	2.0
7	H	65	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	FME	i	1	10/11	0.92	0.16	51,70,75,80	0
14	FME	T	1	10/11	0.96	0.09	44,52,66,69	0
12	FME	M	1	10/11	0.97	0.14	47,58,93,94	0
14	FME	t	1	10/11	0.97	0.09	41,47,64,74	0
12	FME	m	1	10/11	0.98	0.14	48,62,89,111	0
8	FME	I	1	10/11	0.98	0.07	58,70,80,82	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
30	UNL	b	626	33/-	0.47	0.36	66,92,150,160	0
36	CA	F	103	1/1	0.47	0.25	123,123,123,123	0
31	LMT	b	621	25/35	0.48	0.31	80,108,155,168	0
30	UNL	B	626	33/-	0.49	0.34	49,100,140,150	0
30	UNL	I	101	40/-	0.50	0.32	70,98,154,158	0
31	LMT	M	102	35/35	0.50	0.30	70,116,169,173	0
33	LMG	C	521	51/55	0.56	0.32	59,109,155,182	0
30	UNL	i	101	40/-	0.62	0.30	69,101,149,158	0
33	LMG	Z	101	37/55	0.65	0.31	73,119,150,165	0
31	LMT	F	101	35/35	0.65	0.53	99,125,174,181	0
31	LMT	B	630	35/35	0.66	0.33	64,112,141,149	0
31	LMT	m	103	35/35	0.67	0.27	59,91,105,123	0
31	LMT	M	101	35/35	0.67	0.25	59,95,122,132	0
31	LMT	B	631	25/35	0.67	0.25	56,79,145,158	0
30	UNL	x	101	18/-	0.67	0.24	64,80,124,134	0
31	LMT	e	101	35/35	0.68	0.56	101,141,173,185	0
30	UNL	K	101[B]	34/-	0.68	0.37	75,100,114,120	34
30	UNL	K	101[A]	34/-	0.68	0.37	76,100,114,120	34
30	UNL	c	525[A]	32/-	0.68	0.38	85,105,118,124	32
30	UNL	c	525[B]	32/-	0.68	0.38	85,105,118,125	32
31	LMT	A	417	35/35	0.69	0.31	63,110,133,143	0
34	HTG	D	412	16/19	0.69	0.27	86,106,131,142	0
34	HTG	b	623	19/19	0.69	0.45	77,129,156,158	0
30	UNL	j	101	10/-	0.69	0.26	74,84,94,103	0
30	UNL	d	409	36/-	0.70	0.20	68,91,127,139	0
33	LMG	c	521	51/55	0.70	0.28	74,127,151,183	0
32	LHG	a	420[A]	42/49	0.71	0.42	86,128,146,160	42
32	LHG	a	420[B]	42/49	0.71	0.42	86,128,146,161	42
30	UNL	A	415	28/-	0.71	0.37	75,106,122,143	0
31	LMT	b	627	25/35	0.71	0.24	49,93,146,152	0
36	CA	o	301	1/1	0.71	0.06	108,108,108,108	0
27	GOL	b	624	6/6	0.72	0.23	85,90,98,109	0
27	GOL	a	418	6/6	0.72	0.50	74,91,102,106	0
27	GOL	o	302	6/6	0.75	0.20	79,96,106,107	0
30	UNL	a	415	30/-	0.76	0.35	82,107,135,143	0
31	LMT	A	419	35/35	0.76	0.38	84,125,147,154	0
34	HTG	d	410	16/19	0.76	0.31	84,118,135,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
30	UNL	m	102	10/-	0.76	0.30	68,74,92,95	0
30	UNL	X	102	18/-	0.76	0.21	55,71,104,104	0
31	LMT	B	628	35/35	0.77	0.26	64,104,142,147	0
31	LMT	c	501	35/35	0.77	0.41	96,127,142,156	0
34	HTG	C	522	19/19	0.77	0.35	100,120,131,134	0
31	LMT	t	101	26/35	0.77	0.20	68,101,143,157	0
26	SQD	f	102	43/54	0.78	0.33	98,125,174,183	0
30	UNL	D	411	40/-	0.78	0.20	62,92,143,144	0
33	LMG	z	101	39/55	0.79	0.24	70,121,149,162	0
27	GOL	B	627	6/6	0.80	0.22	68,83,98,114	0
27	GOL	A	411	6/6	0.80	0.19	62,73,77,86	0
26	SQD	b	620	54/54	0.81	0.18	60,93,127,136	0
32	LHG	E	101[A]	42/49	0.81	0.26	71,96,110,120	42
32	LHG	E	101[B]	42/49	0.81	0.26	71,96,110,120	42
27	GOL	d	412	6/6	0.82	0.24	50,69,79,87	0
26	SQD	B	620	54/54	0.82	0.16	61,88,137,149	0
27	GOL	c	527	6/6	0.83	0.21	96,104,109,110	0
26	SQD	A	412	54/54	0.84	0.18	61,84,127,151	0
26	SQD	a	412	54/54	0.84	0.20	66,94,138,154	0
27	GOL	v	202[A]	6/6	0.84	0.17	65,79,82,84	6
30	UNL	J	101	10/-	0.84	0.14	62,77,82,84	0
33	LMG	C	501	51/55	0.84	0.17	70,86,112,128	0
34	HTG	c	522	19/19	0.84	0.25	99,118,138,139	0
27	GOL	v	202[B]	6/6	0.84	0.17	65,79,82,84	6
33	LMG	a	417	51/55	0.84	0.16	67,93,108,115	0
27	GOL	O	302	6/6	0.84	0.20	81,88,98,99	0
27	GOL	V	203[B]	6/6	0.85	0.19	57,65,72,73	6
36	CA	f	103	1/1	0.85	0.11	118,118,118,118	0
27	GOL	V	203[A]	6/6	0.85	0.19	57,64,72,73	6
30	UNL	l	101	10/-	0.86	0.23	65,71,90,94	0
27	GOL	o	303	6/6	0.86	0.17	76,84,95,96	0
27	GOL	a	419	6/6	0.86	0.36	51,78,82,88	0
34	HTG	B	623	19/19	0.86	0.20	61,90,112,112	0
29	PL9	A	414[A]	55/55	0.87	0.17	59,83,98,106	55
29	PL9	A	414[B]	55/55	0.87	0.17	59,83,98,106	55
29	PL9	a	414[A]	55/55	0.87	0.18	74,95,109,111	55
29	PL9	a	414[B]	55/55	0.87	0.18	73,95,109,111	55
25	BCR	C	515	40/40	0.87	0.14	54,73,89,94	0
27	GOL	D	403	6/6	0.88	0.30	47,76,78,81	0
23	CLA	C	514	65/65	0.88	0.15	59,85,113,121	0
33	LMG	d	411	51/55	0.88	0.18	52,74,116,144	0
23	CLA	b	601	65/65	0.88	0.16	60,85,120,153	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	b	616	65/65	0.88	0.16	48,63,121,133	0
23	CLA	d	403	65/65	0.88	0.16	50,66,117,142	0
33	LMG	D	413	51/55	0.88	0.17	47,67,117,134	0
23	CLA	c	514	65/65	0.89	0.17	69,94,124,151	0
27	GOL	l	102[A]	6/6	0.89	0.47	61,90,91,96	6
27	GOL	l	102[B]	6/6	0.89	0.47	61,90,91,96	6
34	HTG	b	622	19/19	0.89	0.14	55,79,115,117	0
33	LMG	c	520	51/55	0.89	0.17	61,88,133,163	0
25	BCR	h	101	40/40	0.90	0.15	59,72,94,97	0
23	CLA	c	513	65/65	0.90	0.17	60,79,121,133	0
27	GOL	O	303	6/6	0.90	0.20	73,86,96,96	0
23	CLA	C	513	65/65	0.91	0.15	58,74,116,126	0
34	HTG	V	202	11/19	0.91	0.40	75,108,122,129	0
23	CLA	B	601	65/65	0.91	0.13	56,76,108,146	0
25	BCR	K	102	40/40	0.91	0.17	56,64,76,79	0
27	GOL	B	629	6/6	0.91	0.24	71,76,90,96	0
25	BCR	K	103	40/40	0.91	0.13	54,63,84,87	0
34	HTG	B	622	19/19	0.91	0.13	60,85,119,121	0
25	BCR	d	404	40/40	0.91	0.13	50,64,99,110	0
30	UNL	d	408	17/-	0.91	0.13	64,78,111,121	0
23	CLA	B	616	65/65	0.92	0.17	41,57,131,139	0
23	CLA	C	507	65/65	0.92	0.14	52,70,118,141	0
33	LMG	B	621	51/55	0.92	0.12	48,68,90,106	0
33	LMG	m	101	51/55	0.92	0.12	50,72,94,107	0
34	HTG	b	625	19/19	0.92	0.10	61,78,94,103	0
26	SQD	X	101	43/54	0.92	0.17	71,104,131,133	0
33	LMG	C	520	51/55	0.92	0.14	53,83,109,128	0
35	DGD	c	518[A]	62/66	0.92	0.13	53,68,114,129	62
35	DGD	c	518[B]	62/66	0.92	0.13	54,68,114,129	62
23	CLA	b	606	65/65	0.92	0.13	44,59,112,127	0
23	CLA	B	606	65/65	0.92	0.14	44,57,111,135	0
27	GOL	D	414	6/6	0.92	0.17	46,63,67,82	0
25	BCR	D	406	40/40	0.93	0.11	43,57,102,106	0
35	DGD	c	519	62/66	0.93	0.12	49,61,101,125	0
35	DGD	h	102	62/66	0.93	0.12	52,64,77,86	0
30	UNL	D	410	17/-	0.93	0.13	56,71,101,118	0
35	DGD	H	102	62/66	0.93	0.12	43,61,76,93	0
23	CLA	c	507	65/65	0.93	0.12	46,70,118,131	0
23	CLA	D	405	65/65	0.94	0.13	46,59,121,138	0
35	DGD	C	518[A]	62/66	0.94	0.12	47,64,107,111	62
35	DGD	C	518[B]	62/66	0.94	0.12	47,63,107,111	62
35	DGD	C	519	62/66	0.94	0.11	42,59,95,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	HTG	B	625	19/19	0.94	0.10	65,76,101,101	0
25	BCR	c	515	40/40	0.94	0.10	65,78,91,96	0
23	CLA	a	409	65/65	0.94	0.17	43,56,138,157	0
23	CLA	B	609	65/65	0.94	0.15	46,58,72,81	0
25	BCR	k	101	40/40	0.94	0.17	58,73,86,88	0
26	SQD	A	410[A]	54/54	0.94	0.13	54,78,112,115	54
26	SQD	A	410[B]	54/54	0.94	0.13	54,78,112,115	54
23	CLA	C	509	65/65	0.94	0.10	45,54,113,140	0
23	CLA	C	502	65/65	0.95	0.10	48,60,71,76	0
25	BCR	y	101	40/40	0.95	0.10	56,70,83,96	0
32	LHG	D	409[A]	49/49	0.95	0.15	47,60,109,113	49
32	LHG	D	409[B]	49/49	0.95	0.15	47,60,109,113	49
25	BCR	A	409	40/40	0.95	0.10	37,51,65,67	0
25	BCR	B	618	40/40	0.95	0.09	39,55,70,78	0
23	CLA	C	505	65/65	0.95	0.10	41,56,107,134	0
25	BCR	C	516	40/40	0.95	0.14	52,64,80,85	0
32	LHG	d	407[A]	49/49	0.95	0.15	52,62,108,122	49
32	LHG	d	407[B]	49/49	0.95	0.15	52,62,108,122	49
23	CLA	b	612	65/65	0.95	0.10	41,53,69,76	0
25	BCR	H	101	40/40	0.95	0.10	48,65,85,89	0
27	GOL	c	526[A]	6/6	0.95	0.21	65,69,74,75	6
27	GOL	c	526[B]	6/6	0.95	0.21	65,69,74,75	6
23	CLA	B	611	65/65	0.95	0.09	33,42,64,68	0
23	CLA	a	407[A]	65/65	0.95	0.11	39,52,118,132	65
25	BCR	b	618	40/40	0.95	0.09	43,55,77,84	0
23	CLA	c	509	65/65	0.95	0.12	42,62,124,152	0
23	CLA	a	407[B]	65/65	0.95	0.11	39,52,118,132	65
27	GOL	C	523[A]	6/6	0.95	0.12	56,60,64,69	6
27	GOL	C	523[B]	6/6	0.95	0.12	56,60,65,69	6
23	CLA	A	408	65/65	0.95	0.12	37,49,126,140	0
23	CLA	C	508	65/65	0.96	0.12	50,61,84,92	0
25	BCR	t	102	40/40	0.96	0.08	42,62,75,83	0
29	PL9	d	405[A]	55/55	0.96	0.10	36,49,60,73	55
29	PL9	d	405[B]	55/55	0.96	0.10	36,49,60,73	55
23	CLA	b	615	65/65	0.96	0.11	47,61,82,92	0
23	CLA	C	510	65/65	0.96	0.11	48,58,80,86	0
23	CLA	c	502	65/65	0.96	0.11	51,67,81,95	0
23	CLA	c	504	65/65	0.96	0.10	52,70,82,98	0
23	CLA	c	506	65/65	0.96	0.10	49,64,90,97	0
23	CLA	C	511	65/65	0.96	0.09	46,57,76,81	0
26	SQD	a	411[A]	54/54	0.96	0.13	59,78,111,118	54
26	SQD	a	411[B]	54/54	0.96	0.13	59,78,111,118	54

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	c	508	65/65	0.96	0.10	49,67,83,90	0
23	CLA	b	604	65/65	0.96	0.11	40,52,102,119	0
32	LHG	A	418[A]	49/49	0.96	0.11	48,60,79,83	49
32	LHG	A	418[B]	49/49	0.96	0.11	48,60,80,83	49
25	BCR	T	101	40/40	0.96	0.07	40,57,73,80	0
23	CLA	c	510	65/65	0.96	0.11	42,60,84,98	0
27	GOL	B	624	6/6	0.96	0.22	63,69,80,88	0
25	BCR	b	619	40/40	0.96	0.07	46,63,86,89	0
23	CLA	c	512	65/65	0.96	0.11	53,68,86,97	0
25	BCR	c	516	40/40	0.96	0.12	56,64,78,81	0
32	LHG	b	629[A]	49/49	0.96	0.13	47,56,75,91	49
32	LHG	b	629[B]	49/49	0.96	0.13	47,56,75,92	49
32	LHG	d	406[A]	49/49	0.96	0.15	44,55,68,76	49
35	DGD	c	517[A]	62/66	0.96	0.11	46,63,97,105	62
35	DGD	c	517[B]	62/66	0.96	0.11	46,63,97,105	62
32	LHG	d	406[B]	49/49	0.96	0.15	44,55,68,76	49
23	CLA	C	512	65/65	0.96	0.14	49,62,80,89	0
23	CLA	b	609	65/65	0.96	0.15	49,64,77,92	0
32	LHG	d	413[A]	49/49	0.96	0.13	49,64,78,85	49
36	CA	C	524	1/1	0.96	0.04	77,77,77,77	0
32	LHG	d	413[B]	49/49	0.96	0.13	48,64,79,85	49
36	CA	O	301	1/1	0.96	0.11	104,104,104,104	0
29	PL9	D	407[A]	55/55	0.96	0.11	37,47,57,68	55
29	PL9	D	407[B]	55/55	0.96	0.11	37,47,57,68	55
39	HEM	f	101	43/43	0.96	0.13	65,85,116,138	0
23	CLA	B	613	65/65	0.97	0.07	35,44,93,108	0
23	CLA	B	614	65/65	0.97	0.09	36,47,102,121	0
23	CLA	a	405[A]	65/65	0.97	0.13	34,44,60,74	65
23	CLA	a	405[B]	65/65	0.97	0.13	36,44,63,74	65
23	CLA	c	511	65/65	0.97	0.09	47,61,80,91	0
23	CLA	B	615	65/65	0.97	0.10	44,54,76,83	0
23	CLA	A	404[B]	65/65	0.97	0.11	34,41,59,67	65
23	CLA	B	602	65/65	0.97	0.12	43,55,72,95	0
23	CLA	C	504	65/65	0.97	0.09	47,61,72,85	0
24	PHO	a	416[A]	64/64	0.97	0.12	44,55,61,65	64
24	PHO	a	416[B]	64/64	0.97	0.12	44,55,61,65	64
23	CLA	b	602	65/65	0.97	0.13	48,61,80,91	0
25	BCR	B	617	40/40	0.97	0.09	38,50,61,65	0
23	CLA	B	603	65/65	0.97	0.10	42,52,71,81	0
25	BCR	B	619	40/40	0.97	0.07	46,58,93,96	0
32	LHG	D	408[A]	49/49	0.97	0.13	43,53,64,73	49
32	LHG	D	408[B]	49/49	0.97	0.13	43,53,64,73	49

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	b	605	65/65	0.97	0.11	36,49,74,76	0
23	CLA	C	506	65/65	0.97	0.10	49,59,87,103	0
35	DGD	C	517[A]	62/66	0.97	0.11	46,57,97,102	62
35	DGD	C	517[B]	62/66	0.97	0.11	46,57,97,102	62
23	CLA	b	607	65/65	0.97	0.08	37,47,79,93	0
23	CLA	B	605	65/65	0.97	0.10	39,48,62,78	0
23	CLA	b	610	65/65	0.97	0.09	48,57,67,72	0
23	CLA	b	611	65/65	0.97	0.08	38,48,70,75	0
23	CLA	A	406[A]	65/65	0.97	0.08	37,45,105,116	65
25	BCR	a	410	40/40	0.97	0.08	42,53,63,67	0
25	BCR	b	617	40/40	0.97	0.08	43,54,60,67	0
23	CLA	b	613	65/65	0.97	0.08	40,48,85,98	0
23	CLA	b	614	65/65	0.97	0.08	40,50,98,117	0
27	GOL	b	628	6/6	0.97	0.15	72,79,85,88	0
23	CLA	B	607	65/65	0.97	0.08	36,44,74,81	0
23	CLA	A	406[B]	65/65	0.97	0.08	37,45,105,116	65
23	CLA	B	610	65/65	0.97	0.12	39,52,67,79	0
23	CLA	A	404[A]	65/65	0.97	0.11	34,41,59,67	65
23	CLA	c	505	65/65	0.97	0.09	47,63,102,132	0
39	HEM	F	102	43/43	0.97	0.11	54,70,82,90	0
23	CLA	B	612	65/65	0.97	0.07	31,47,58,74	0
41	HEC	V	201	43/43	0.97	0.14	38,50,58,66	0
41	HEC	v	201	43/43	0.97	0.12	48,62,68,75	0
23	CLA	a	406[B]	65/65	0.98	0.07	35,43,61,70	65
23	CLA	b	608	65/65	0.98	0.08	40,54,84,96	0
23	CLA	C	503	65/65	0.98	0.08	41,54,72,86	0
23	CLA	A	405[B]	65/65	0.98	0.09	33,41,58,69	65
23	CLA	D	404[A]	65/65	0.98	0.11	34,42,64,74	65
23	CLA	D	404[B]	65/65	0.98	0.11	34,42,64,75	65
23	CLA	B	604	65/65	0.98	0.07	37,45,117,138	0
23	CLA	b	603	65/65	0.98	0.08	46,55,82,93	0
23	CLA	B	608	65/65	0.98	0.07	37,48,67,73	0
23	CLA	A	405[A]	65/65	0.98	0.09	33,41,58,69	65
32	LHG	L	101[A]	49/49	0.98	0.10	45,54,69,88	49
32	LHG	L	101[B]	49/49	0.98	0.10	45,54,69,89	49
23	CLA	a	406[A]	65/65	0.98	0.07	35,42,61,70	65
23	CLA	d	402[A]	65/65	0.98	0.11	38,45,69,85	65
23	CLA	d	402[B]	65/65	0.98	0.11	38,45,69,85	65
23	CLA	c	503	65/65	0.98	0.07	41,57,81,96	0
36	CA	c	523	1/1	0.98	0.04	76,76,76,76	0
36	CA	c	524	1/1	0.98	0.08	76,76,76,76	0
24	PHO	A	407[A]	64/64	0.98	0.08	33,44,51,54	64

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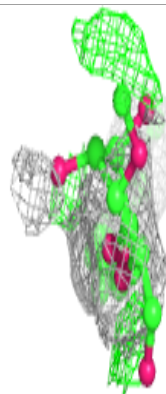
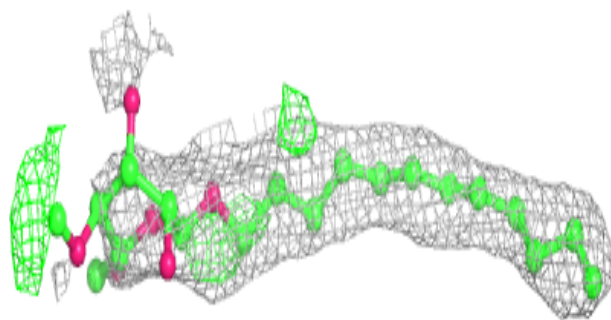
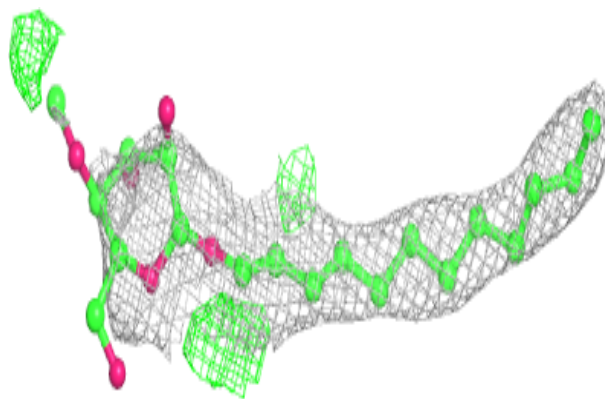
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	PHO	A	407[B]	64/64	0.98	0.08	33,44,51,54	64
38	BCT	d	401[A]	4/4	0.98	0.06	53,54,63,71	4
38	BCT	d	401[B]	4/4	0.98	0.06	53,53,63,70	4
24	PHO	A	416[A]	64/64	0.98	0.10	37,48,53,60	64
24	PHO	A	416[B]	64/64	0.98	0.10	37,47,53,60	64
40	MG	J	102	1/1	0.98	0.03	56,56,56,56	0
40	MG	j	102	1/1	0.98	0.04	63,63,63,63	0
24	PHO	a	408[A]	64/64	0.98	0.08	38,47,53,58	64
24	PHO	a	408[B]	64/64	0.98	0.08	38,47,52,58	64
22	CL	A	402[B]	1/1	0.99	0.03	41,41,41,41	1
22	CL	A	403[A]	1/1	0.99	0.03	45,45,45,45	1
22	CL	A	403[B]	1/1	0.99	0.03	45,45,45,45	1
37	FE2	D	401[A]	1/1	0.99	0.04	48,48,48,48	1
37	FE2	D	401[B]	1/1	0.99	0.04	48,48,48,48	1
38	BCT	D	402[A]	4/4	0.99	0.10	50,52,56,67	4
38	BCT	D	402[B]	4/4	0.99	0.10	50,52,56,68	4
22	CL	a	403[A]	1/1	0.99	0.06	47,47,47,47	1
22	CL	a	403[B]	1/1	0.99	0.06	47,47,47,47	1
22	CL	a	404[A]	1/1	0.99	0.02	52,52,52,52	1
22	CL	a	404[B]	1/1	0.99	0.02	52,52,52,52	1
28	OEX	A	413[A]	10/10	0.99	0.05	37,43,47,48	10
28	OEX	a	413[A]	10/10	0.99	0.04	47,48,51,52	10
21	OEY	A	401[B]	11/11	0.99	0.05	37,44,47,47	11
22	CL	A	402[A]	1/1	0.99	0.03	41,41,41,41	1
37	FE2	a	402[A]	1/1	1.00	0.04	52,52,52,52	1
37	FE2	a	402[B]	1/1	1.00	0.04	52,52,52,52	1
21	OEY	a	401[B]	11/11	1.00	0.05	45,48,52,55	11

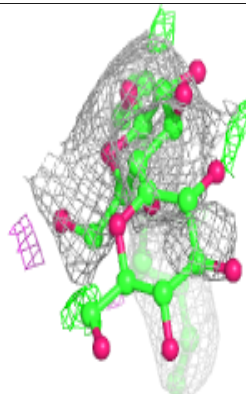
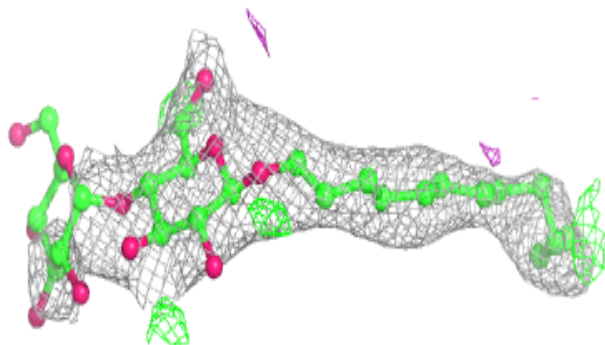
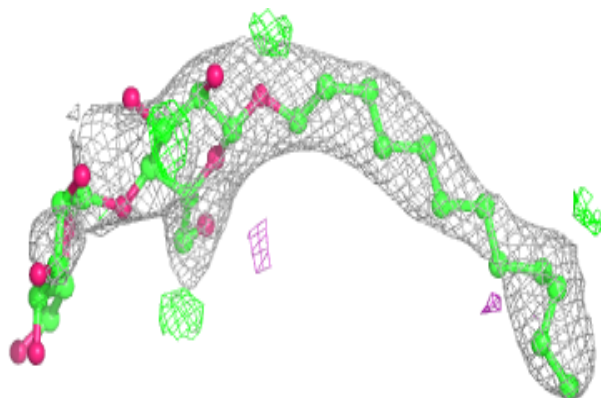
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT b 621:

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

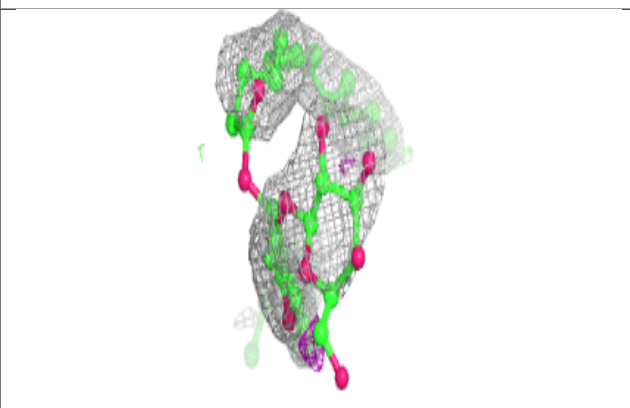
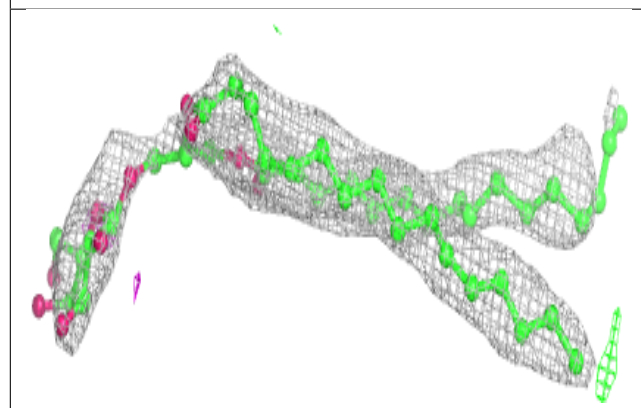
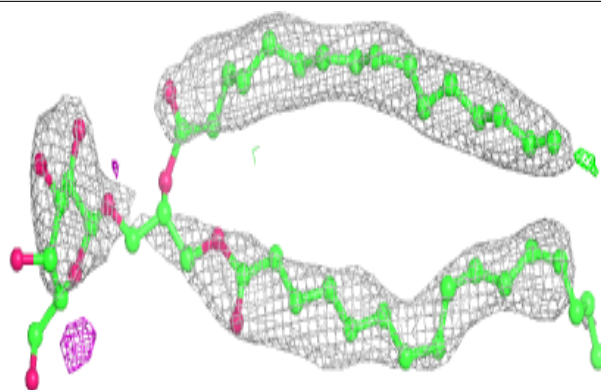
**Electron density around LMT M 102:**

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

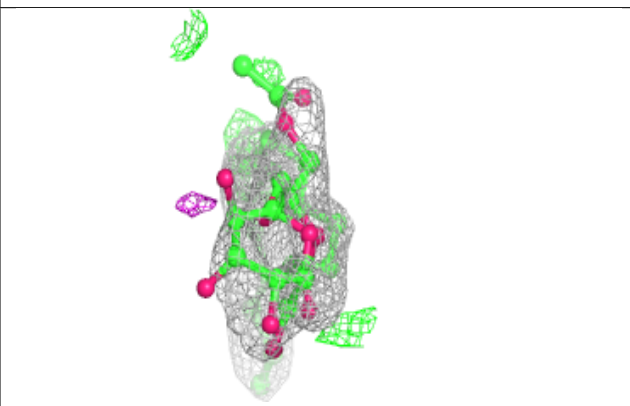
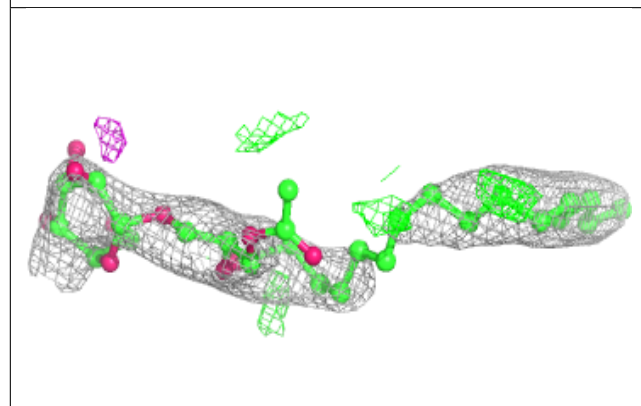
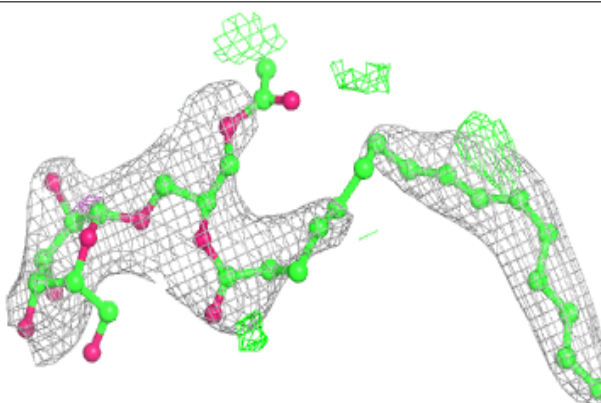


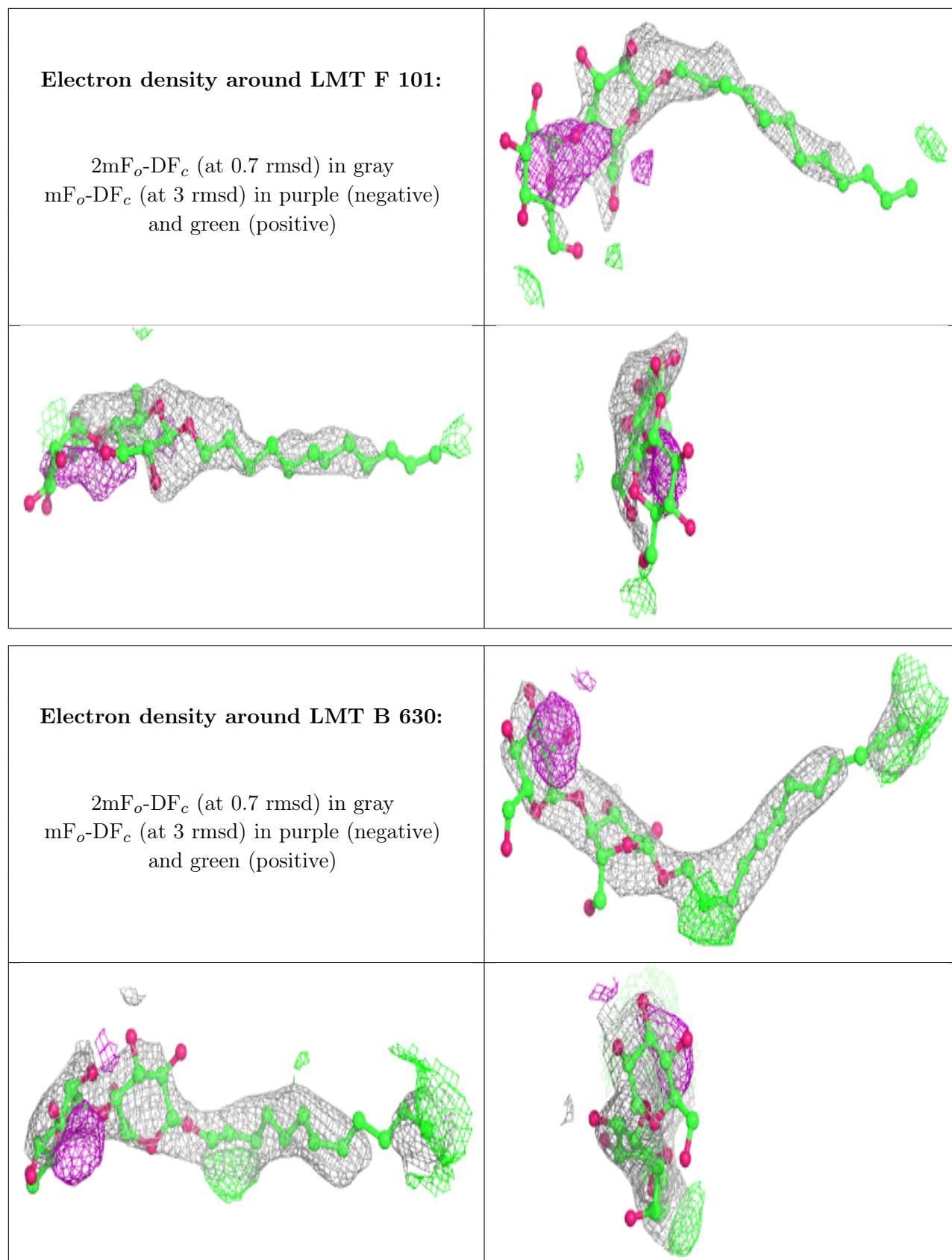
Electron density around LMG C 521:

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

**Electron density around LMG Z 101:**

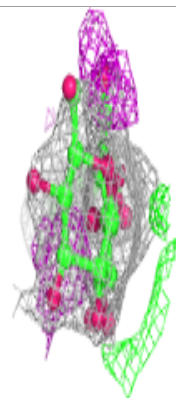
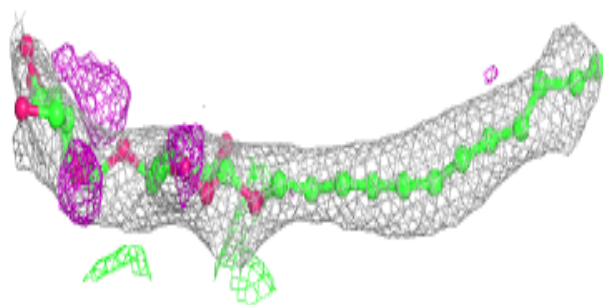
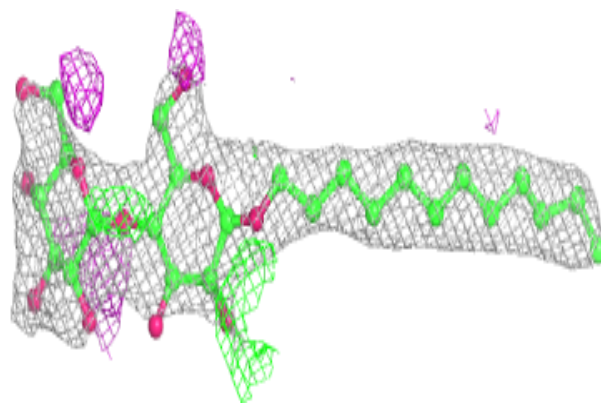
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



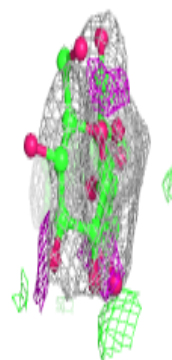
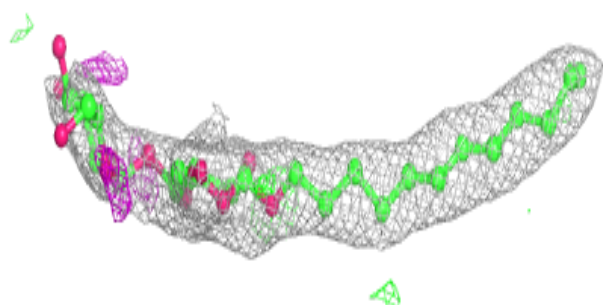
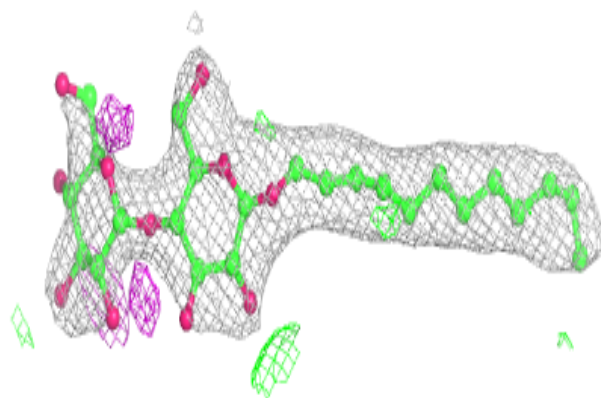


Electron density around LMT m 103:

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

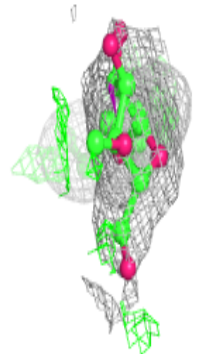
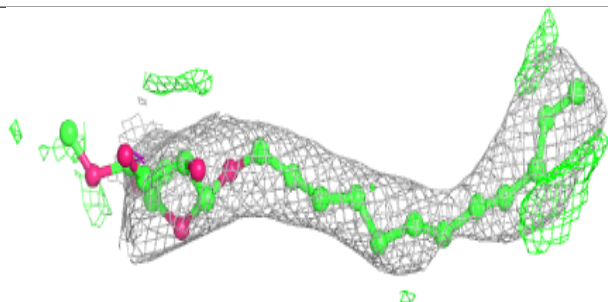
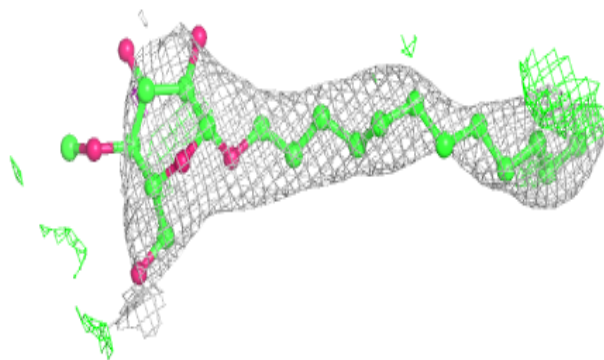
**Electron density around LMT M 101:**

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

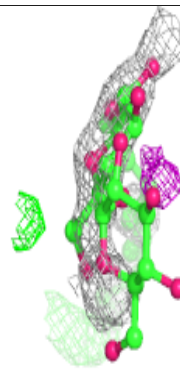
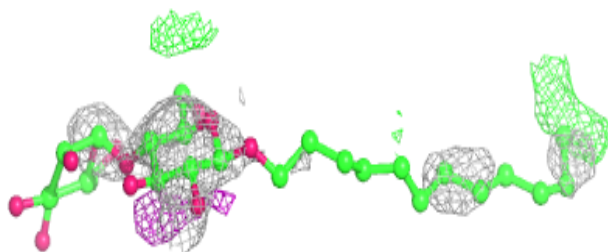
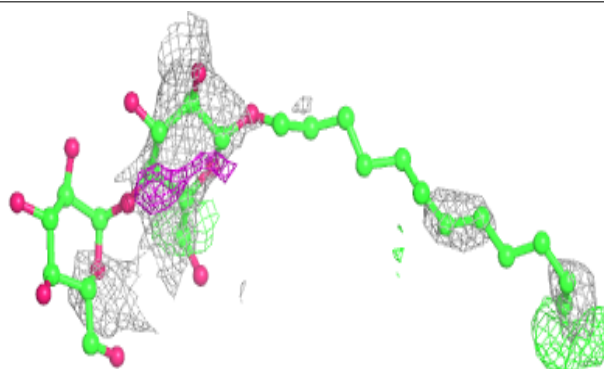


Electron density around LMT B 631:

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

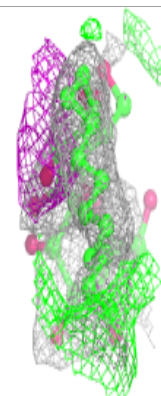
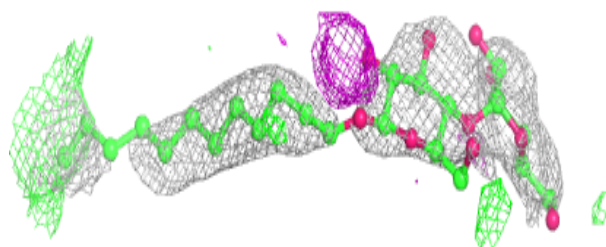
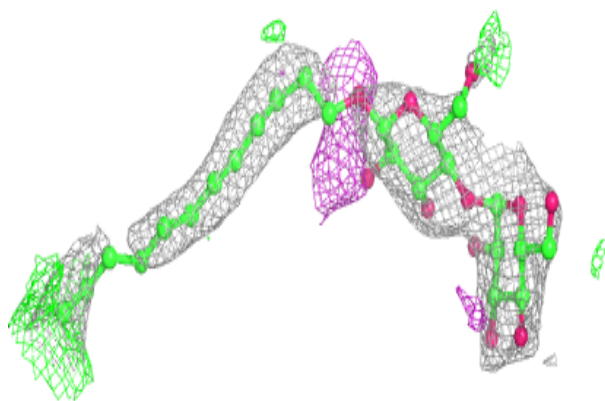
**Electron density around LMT e 101:**

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

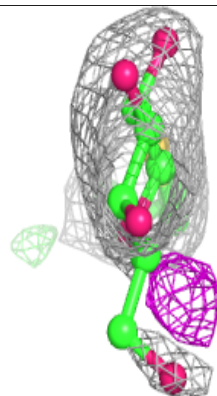
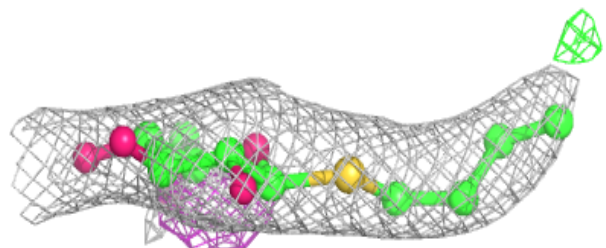
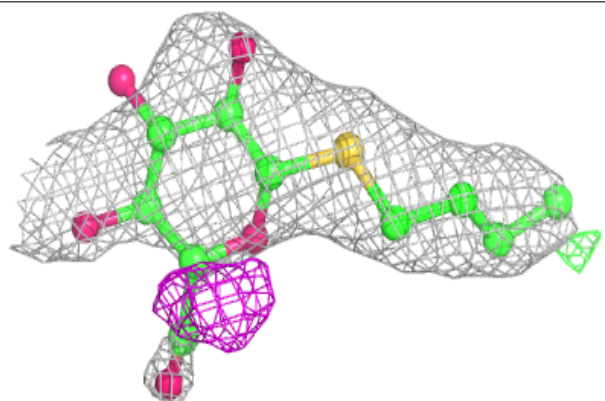


Electron density around LMT A 417:

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

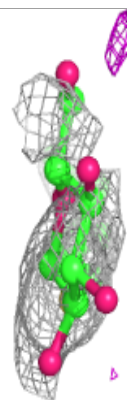
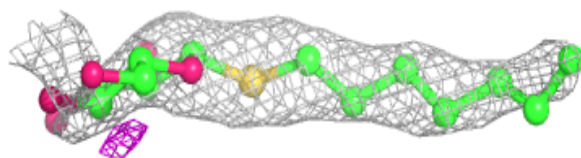
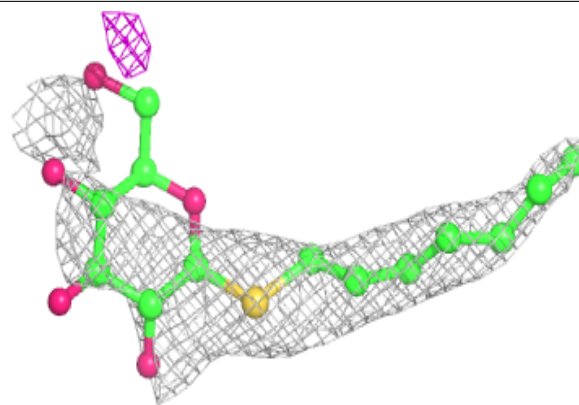
**Electron density around HTG D 412:**

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

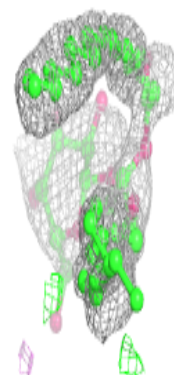
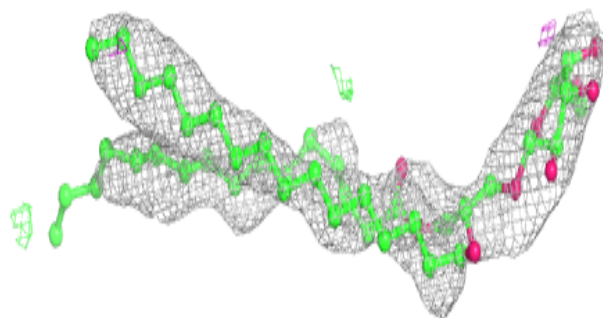
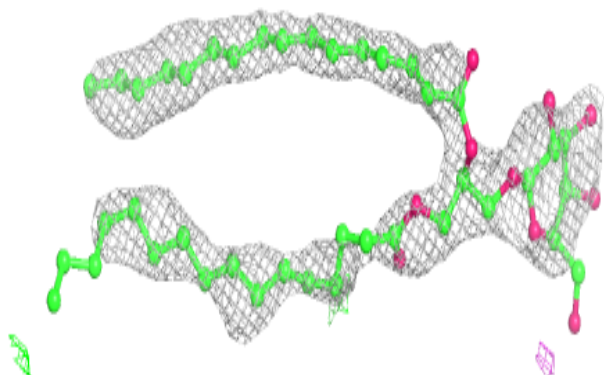


Electron density around HTG b 623:

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

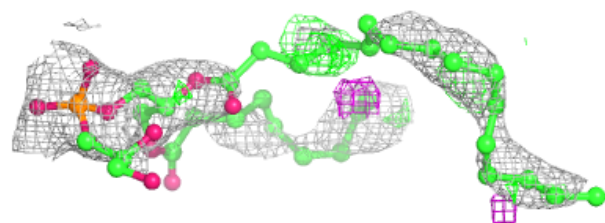
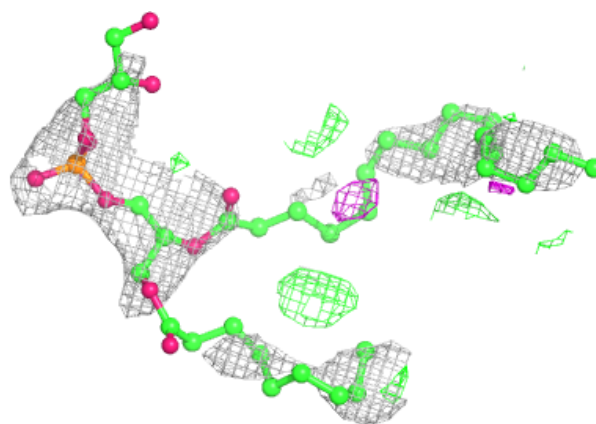
**Electron density around LMG c 521:**

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

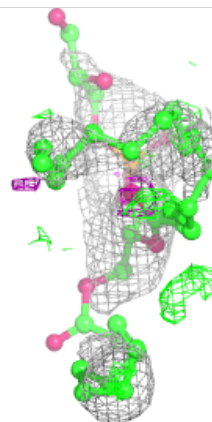
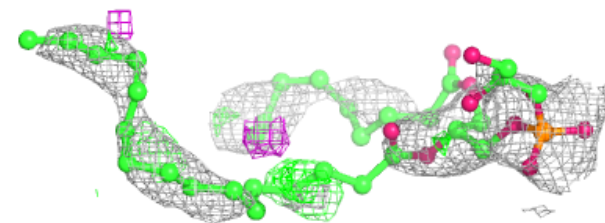
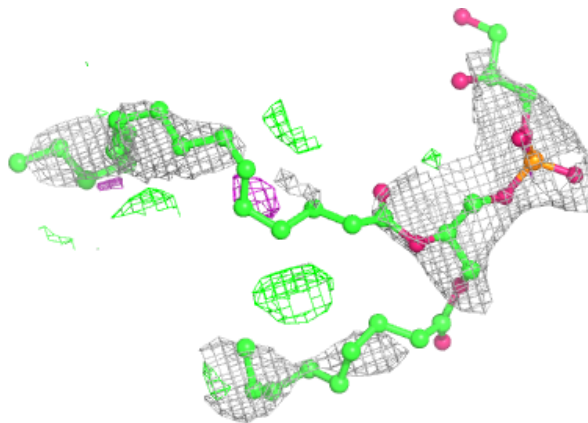


Electron density around LHG a 420 (A):

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

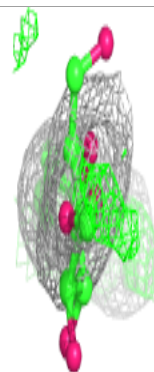
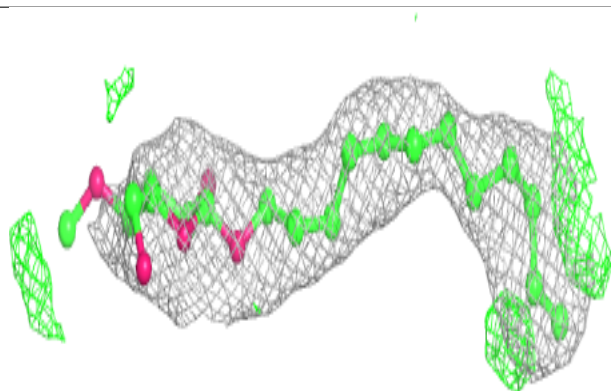
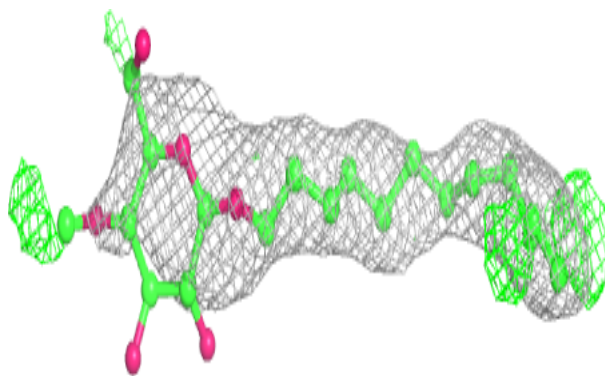
**Electron density around LHG a 420 (B):**

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

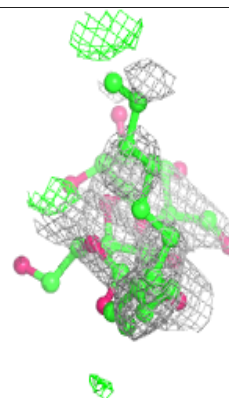
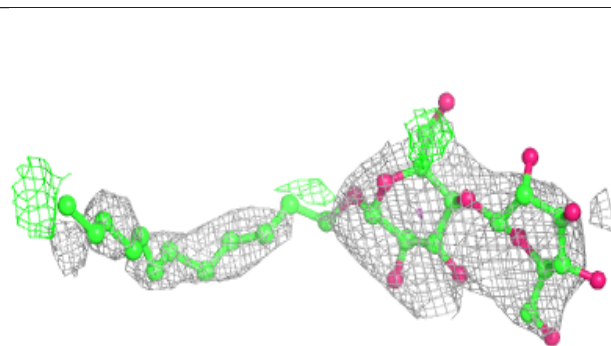
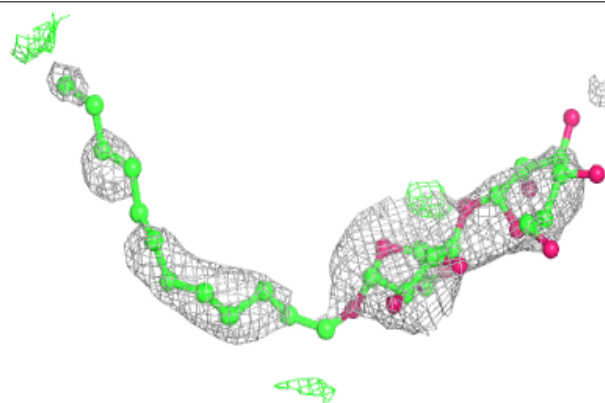


Electron density around LMT b 627:

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

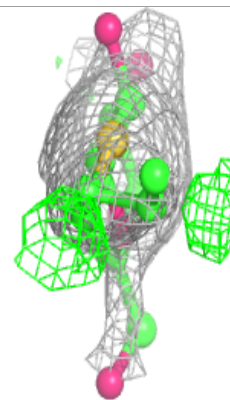
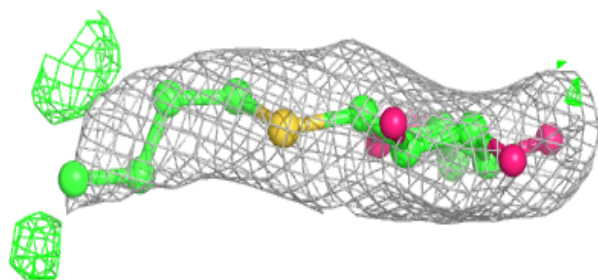
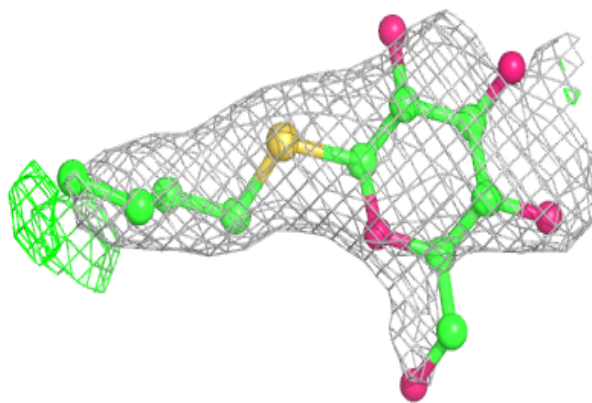
**Electron density around LMT A 419:**

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

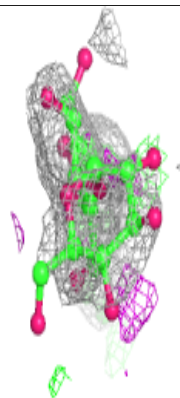
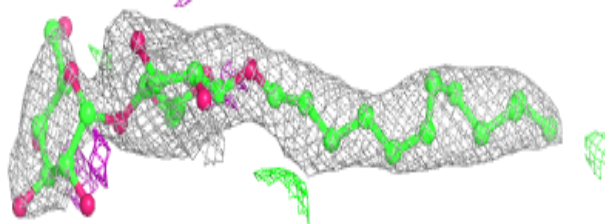
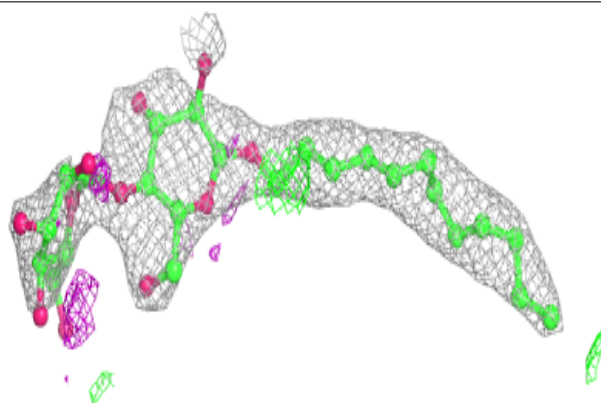


Electron density around HTG d 410:

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

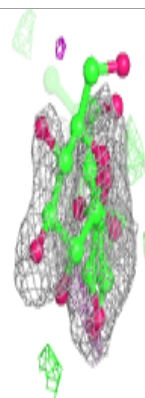
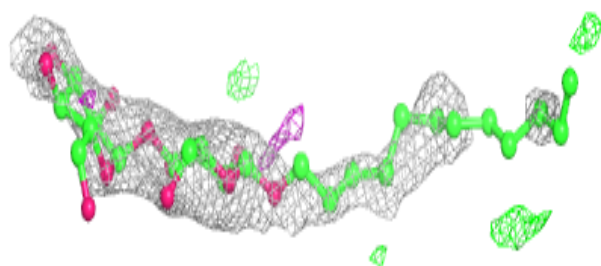
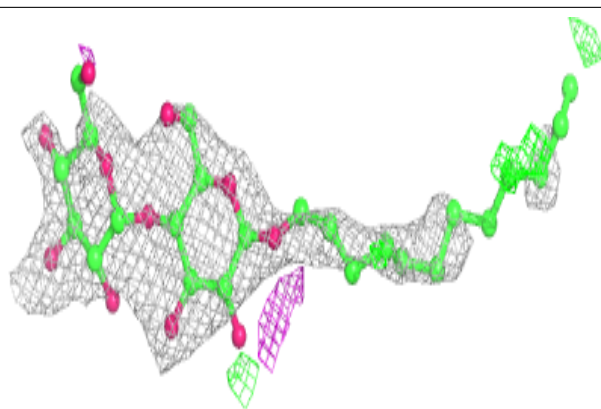
**Electron density around LMT B 628:**

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

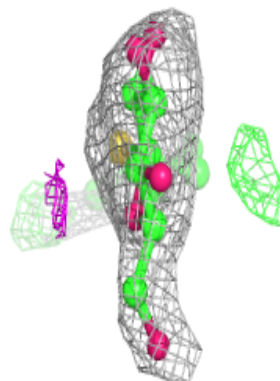
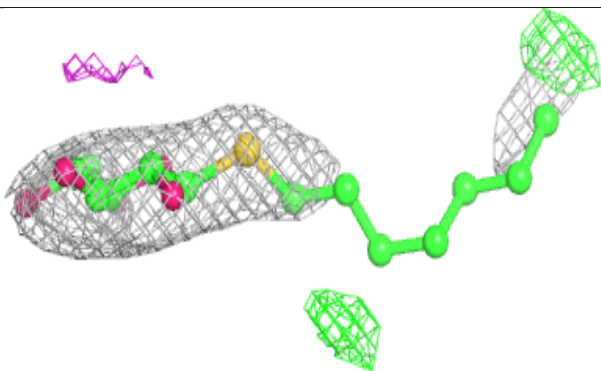
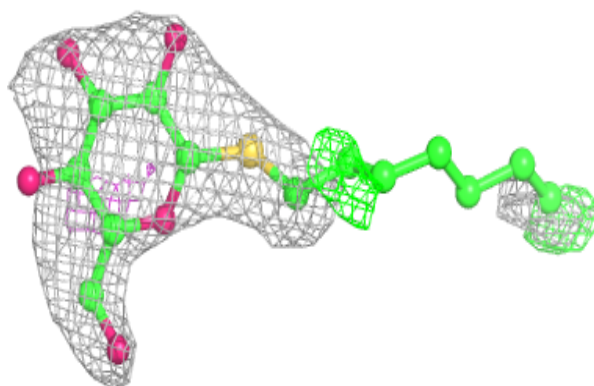


Electron density around LMT c 501:

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

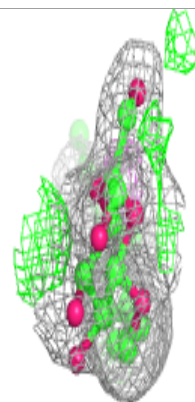
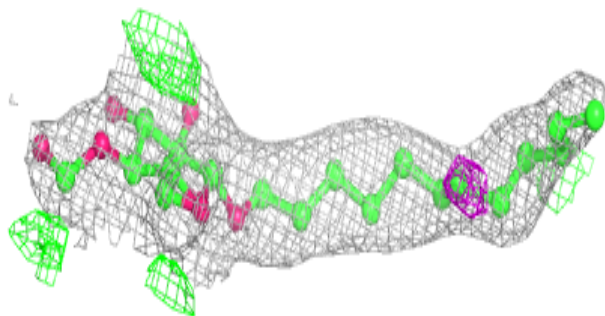
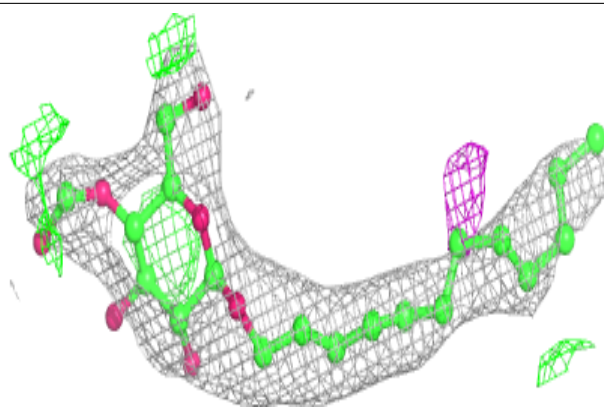
**Electron density around HTG C 522:**

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

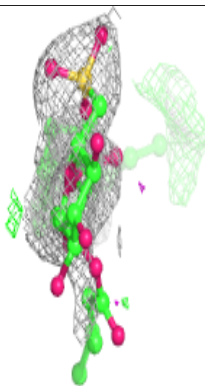
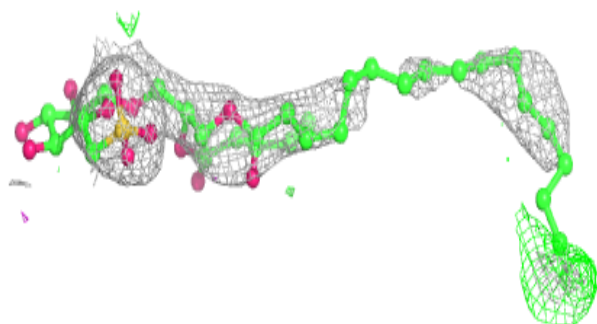
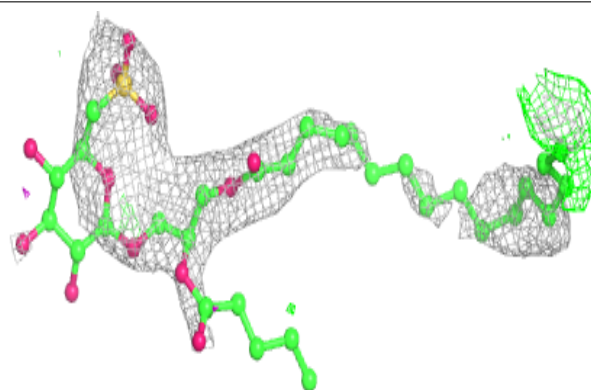


Electron density around LMT t 101:

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

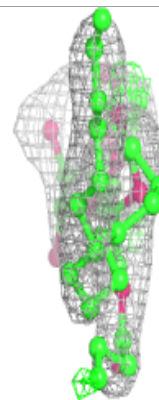
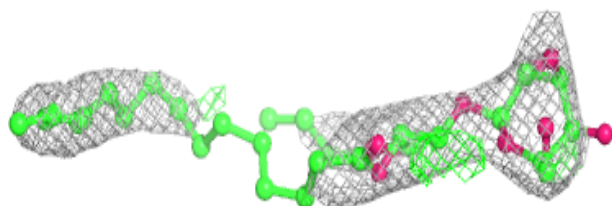
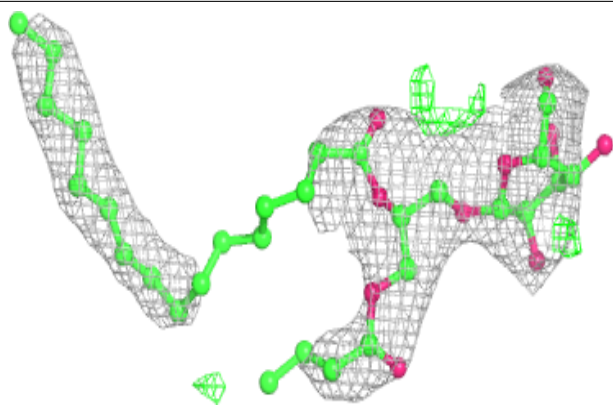
**Electron density around SQD f 102:**

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

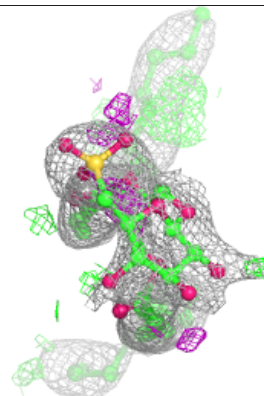
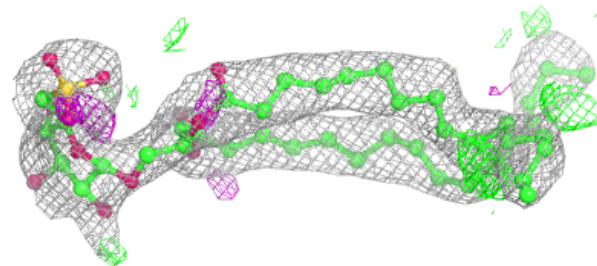
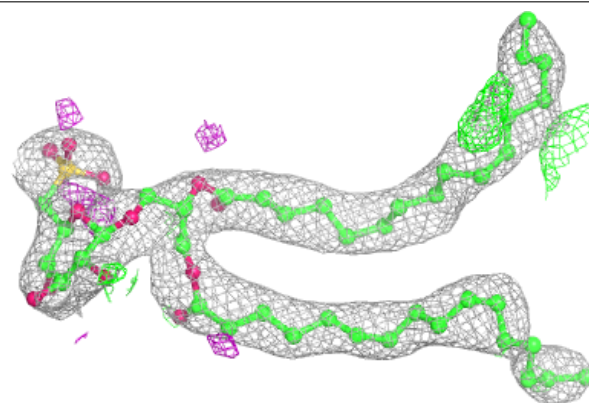


Electron density around LMG z 101:

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

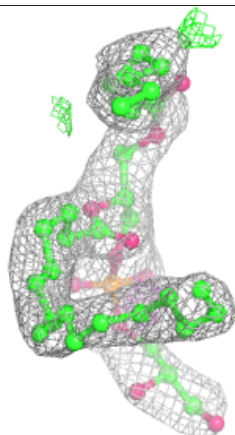
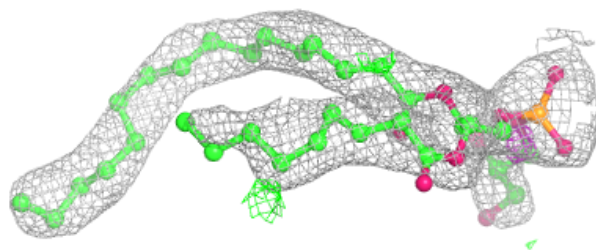
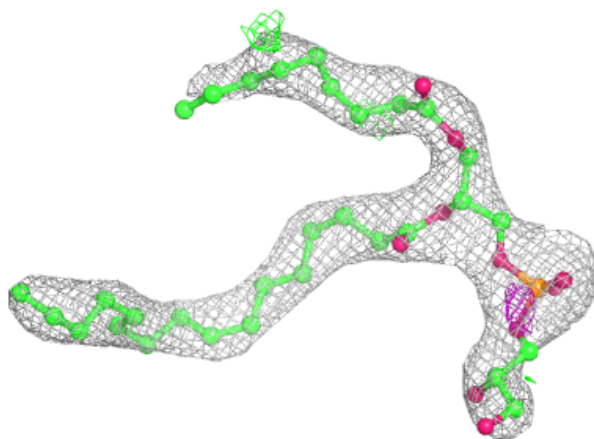
**Electron density around SQD b 620:**

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



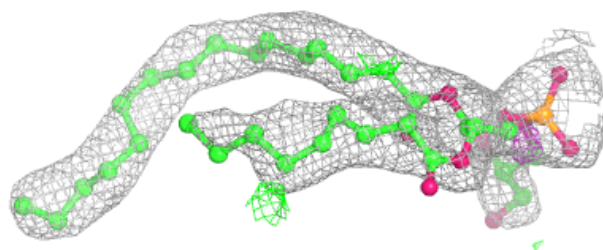
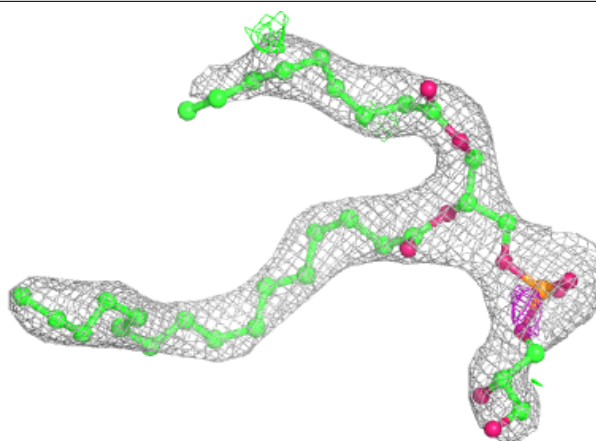
Electron density around LHG E 101 (A):

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

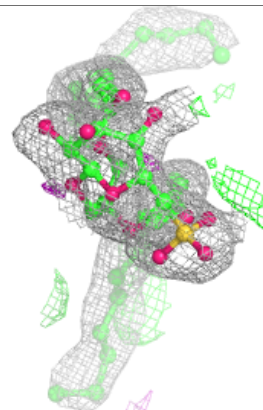
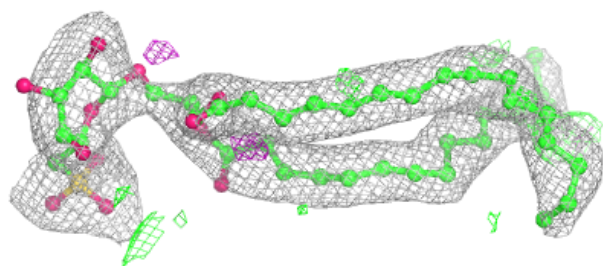
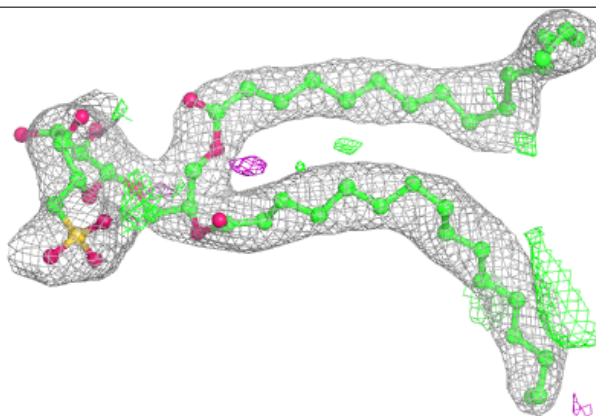


Electron density around LHG E 101 (B):

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

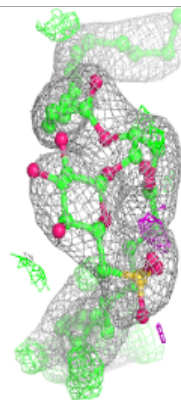
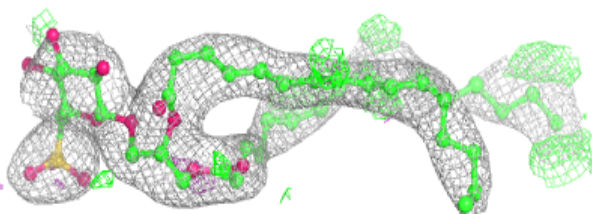
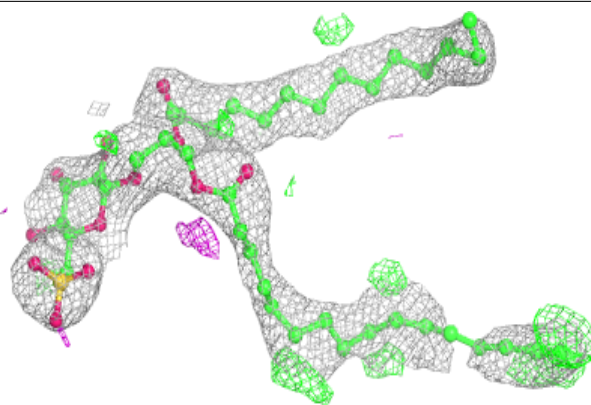
**Electron density around SQD B 620:**

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

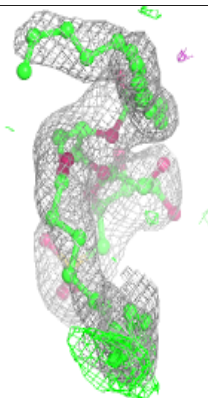
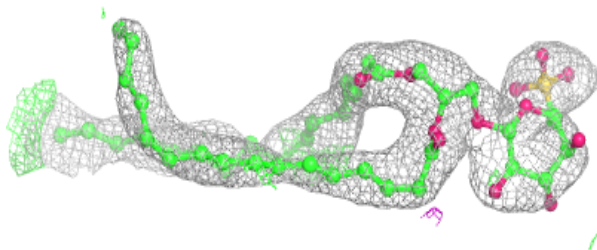
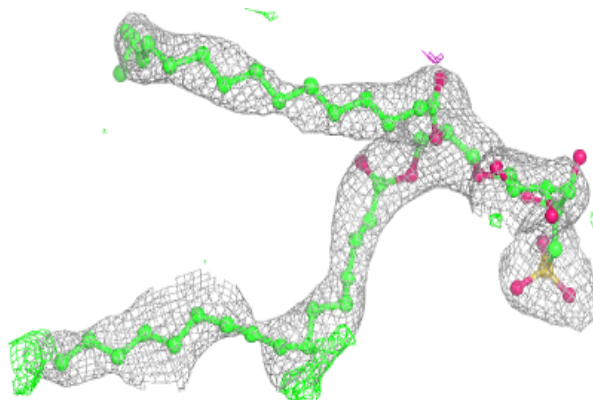


Electron density around SQD A 412:

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

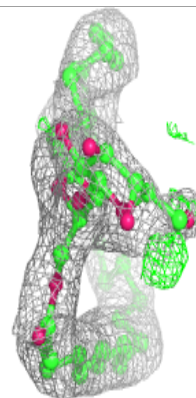
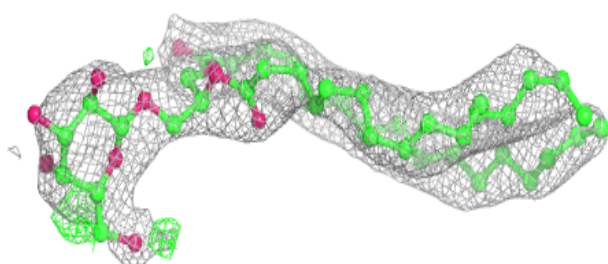
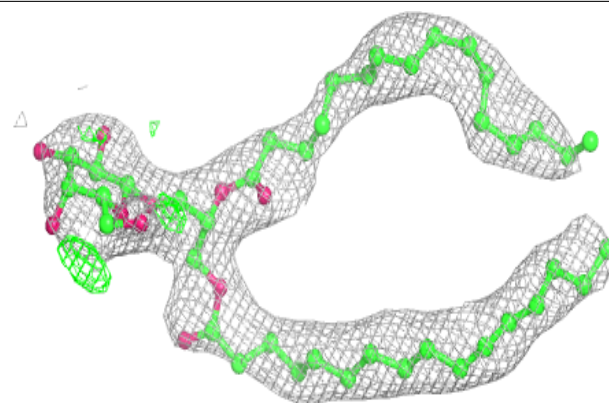
**Electron density around SQD a 412:**

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

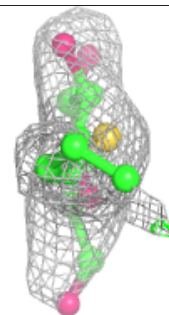
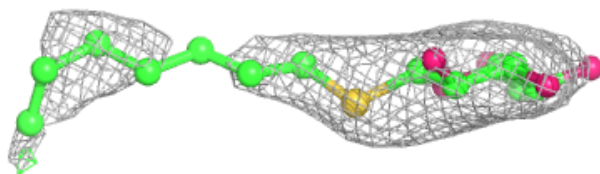
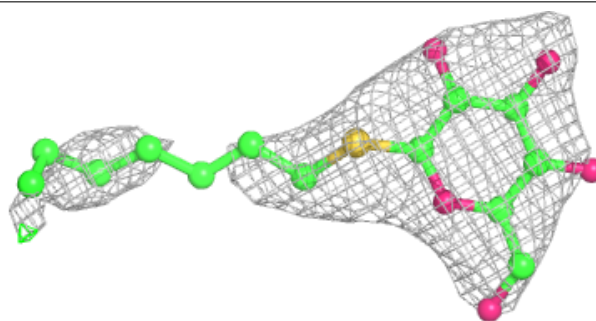


Electron density around LMG C 501:

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

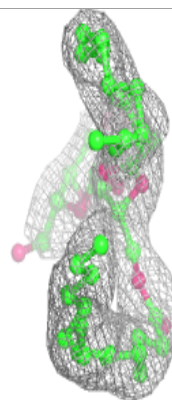
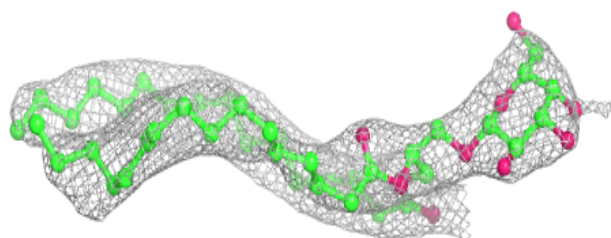
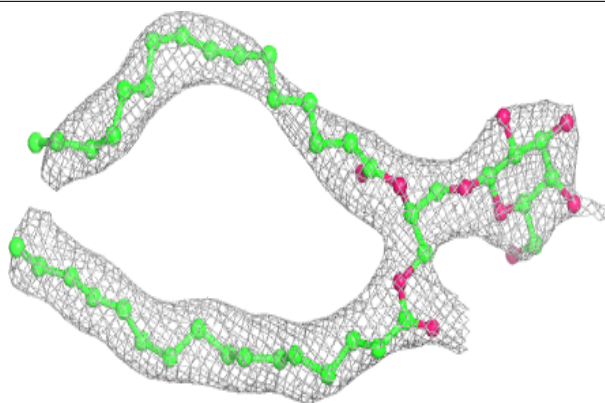
**Electron density around HTG c 522:**

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

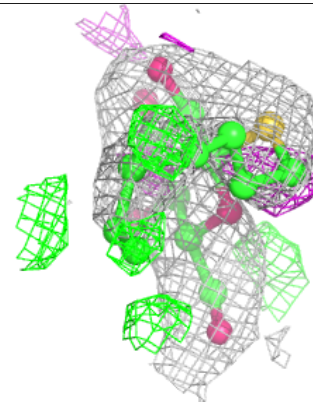
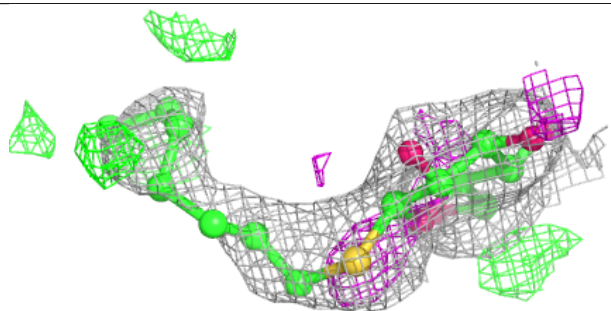
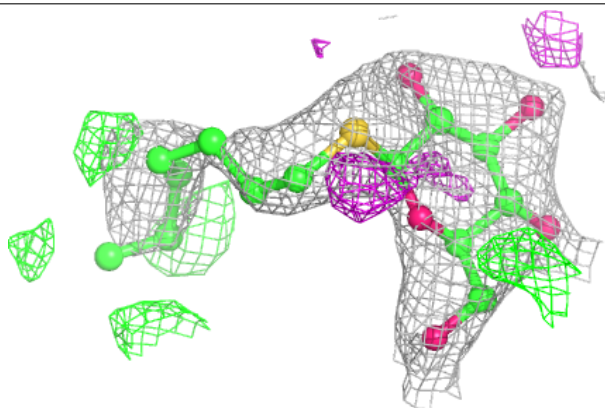


Electron density around LMG a 417:

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

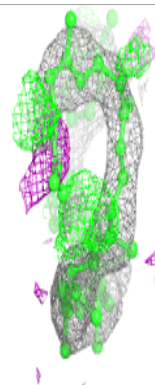
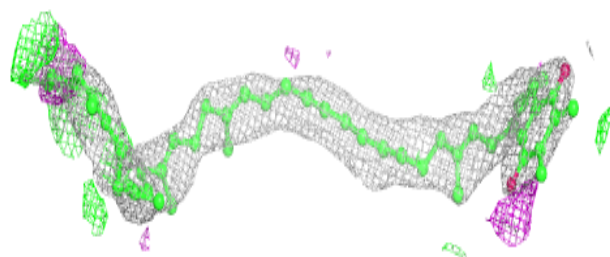
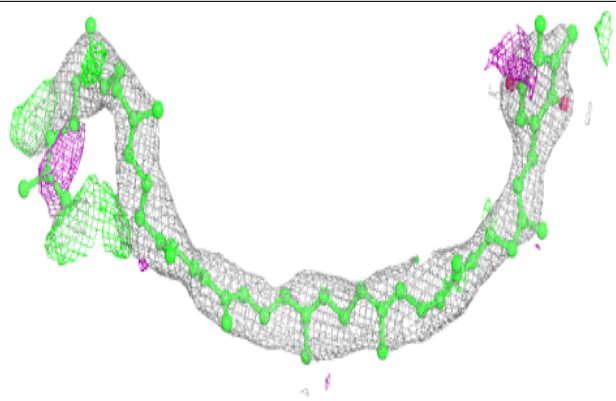
**Electron density around HTG B 623:**

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

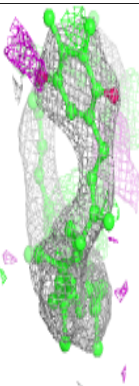
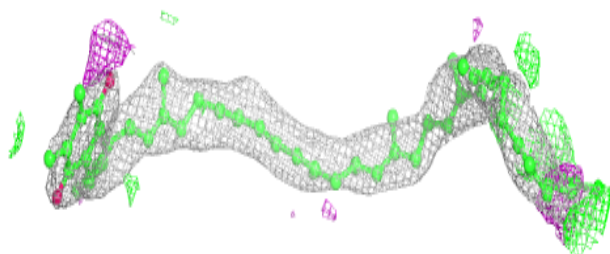
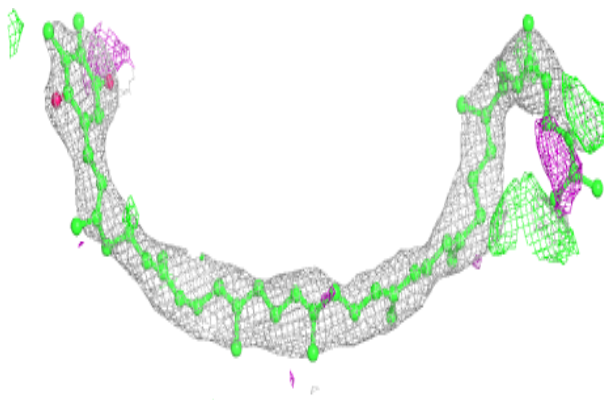


Electron density around PL9 A 414 (A):

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

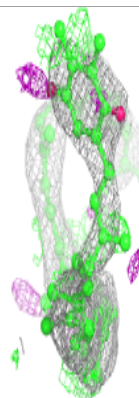
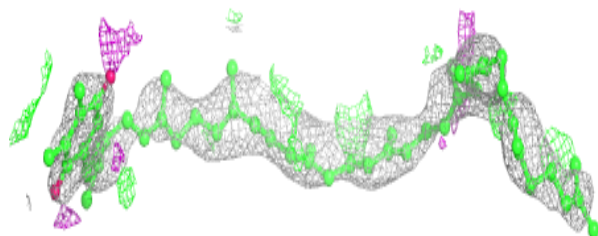
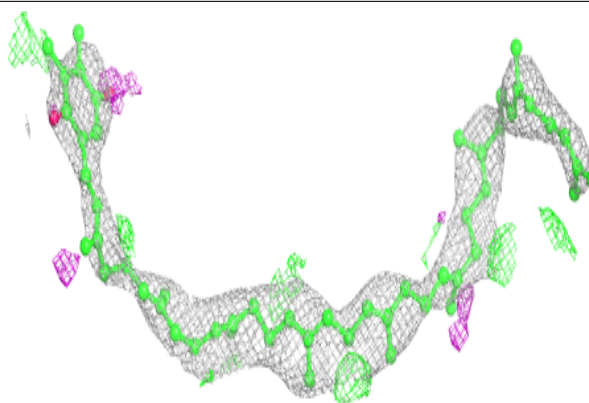
**Electron density around PL9 A 414 (B):**

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

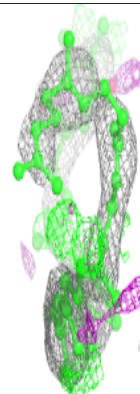
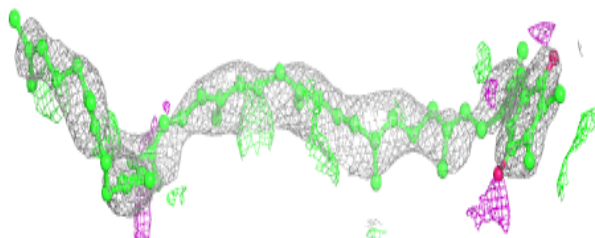
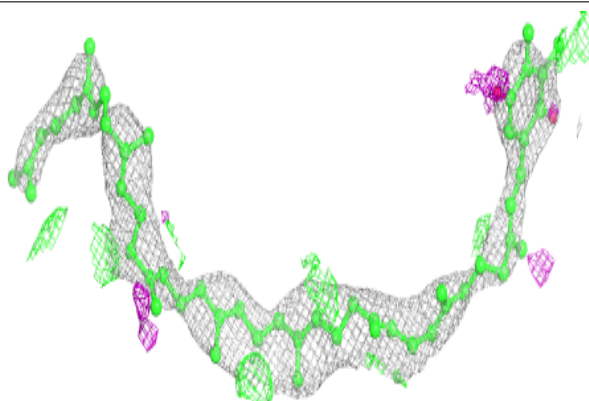


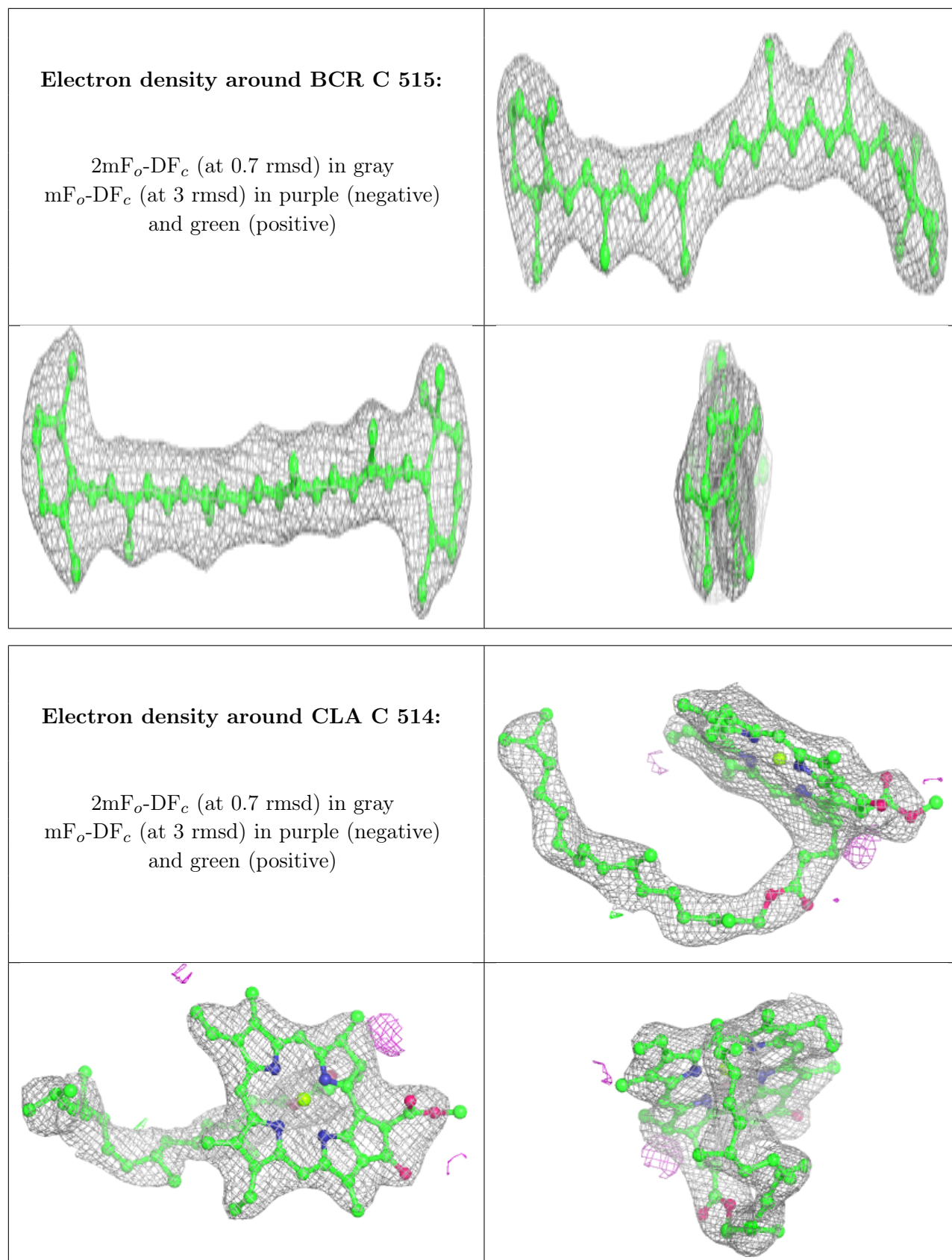
Electron density around PL9 a 414 (A):

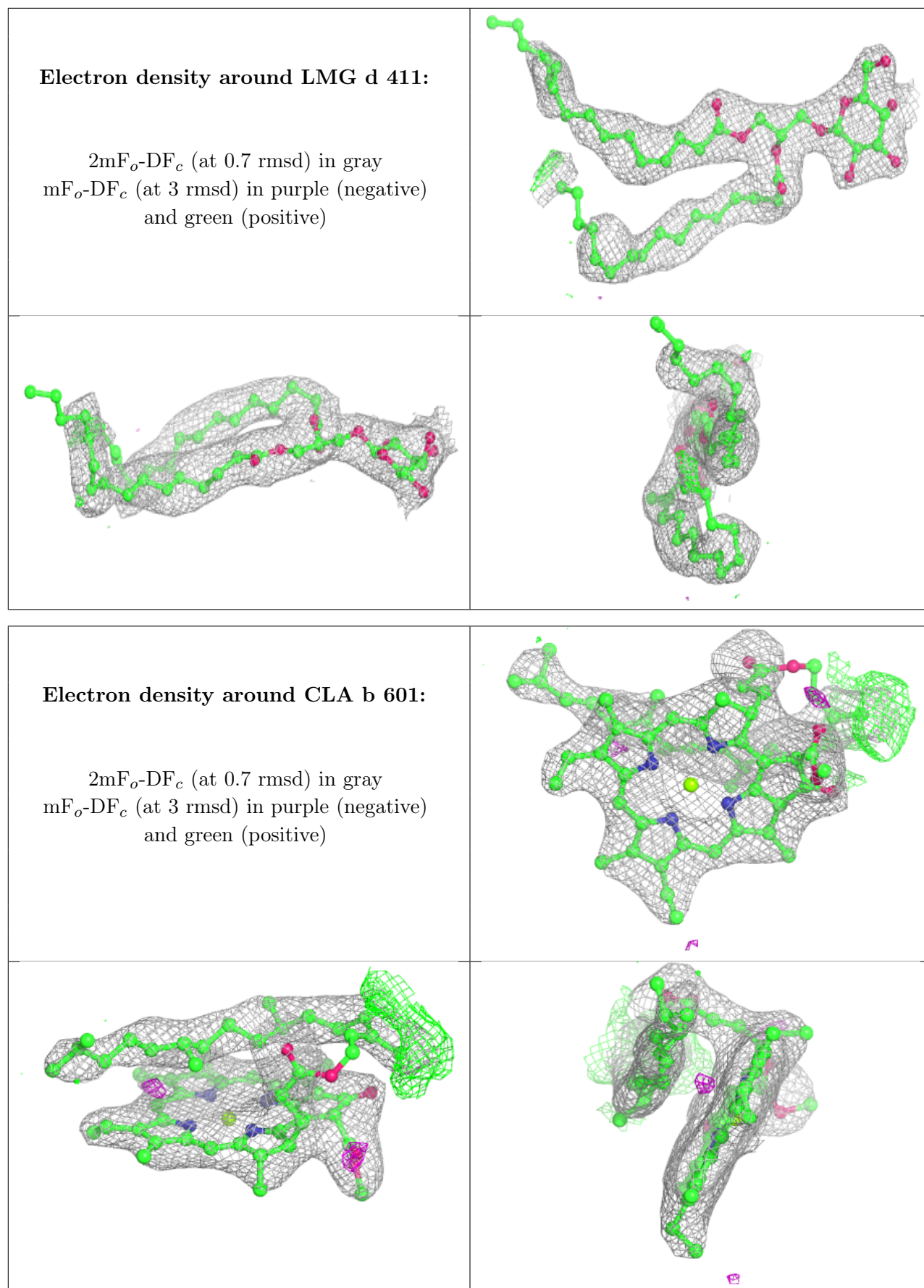
$2mF_o-DF_c$ (at 0.7 rnsd) in gray
 mF_o-DF_c (at 3 rnsd) in purple (negative)
and green (positive)

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

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

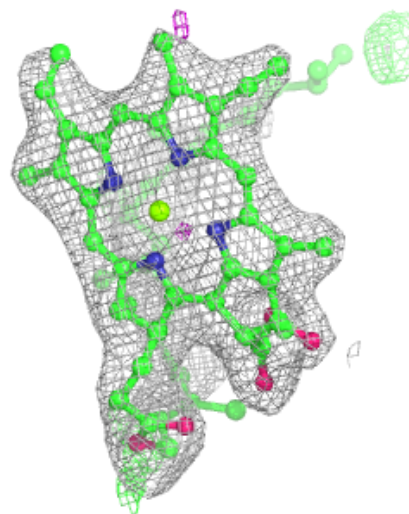
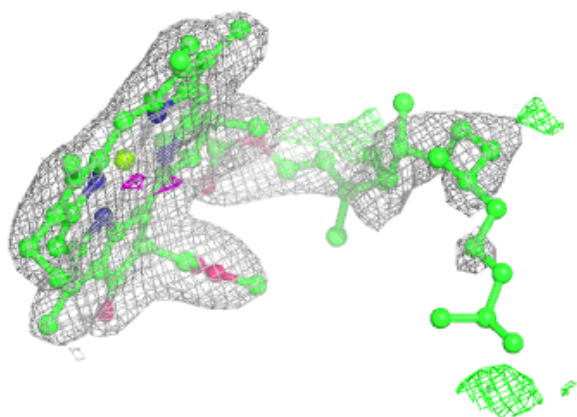
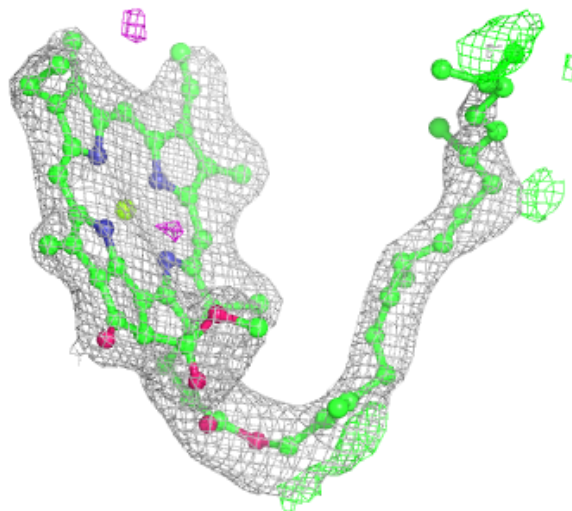






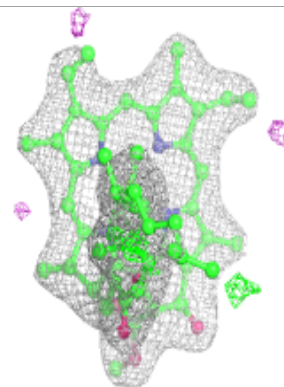
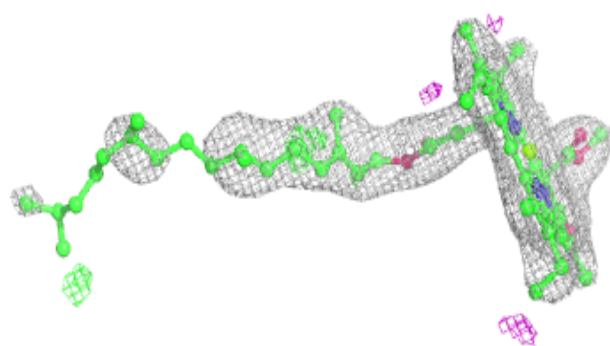
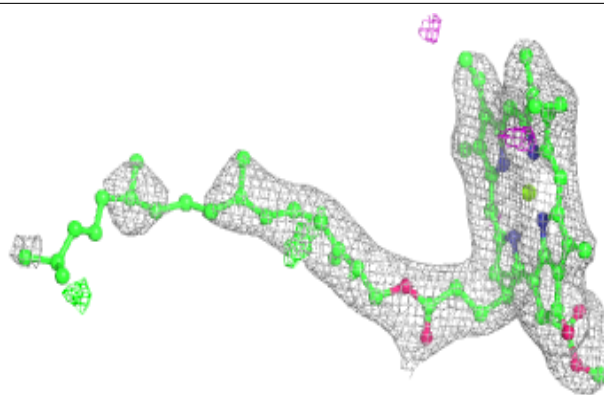
Electron density around CLA b 616:

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

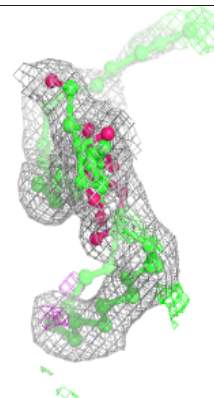
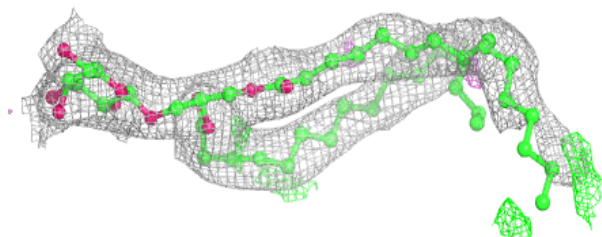
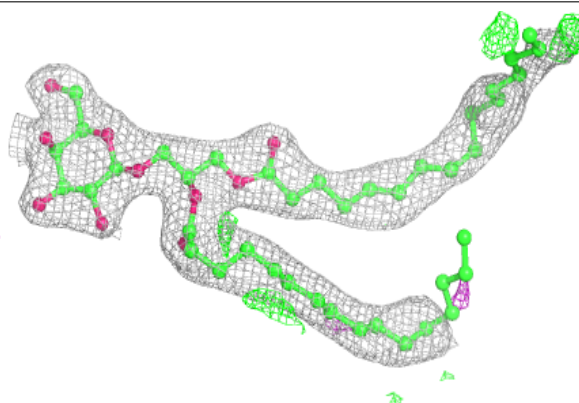


Electron density around CLA d 403:

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

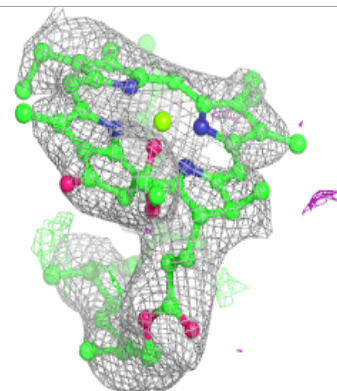
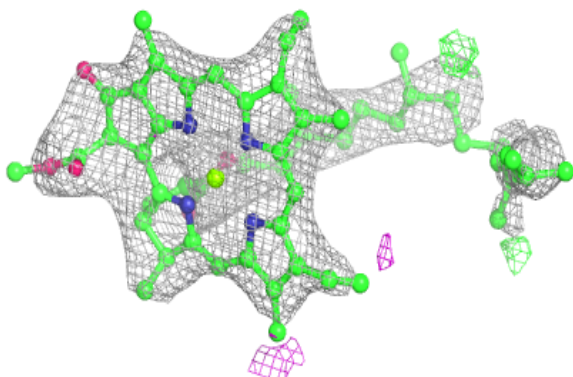
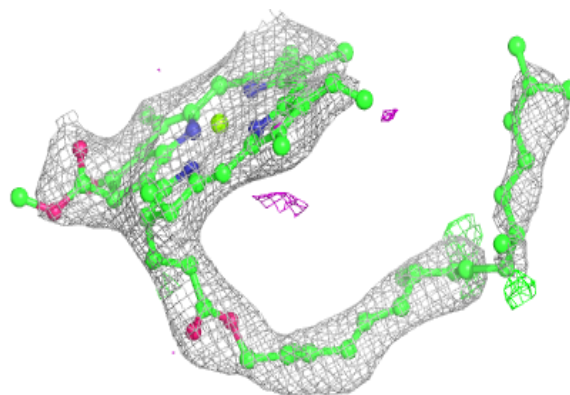
**Electron density around LMG D 413:**

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

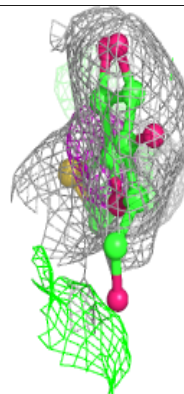
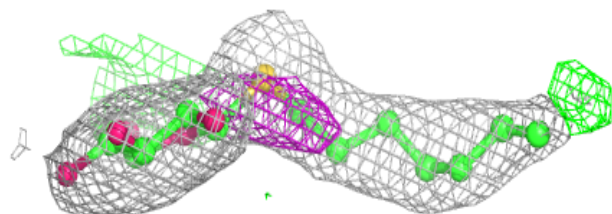
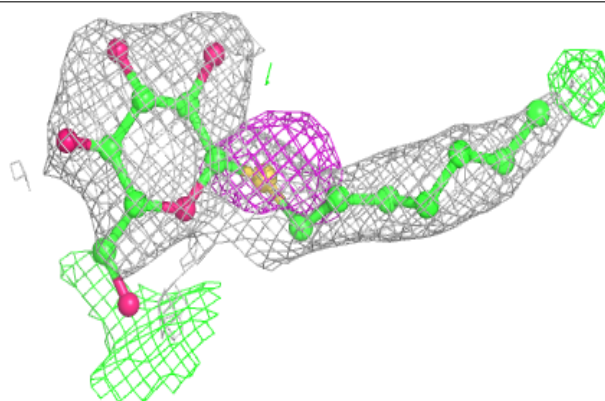


Electron density around CLA c 514:

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

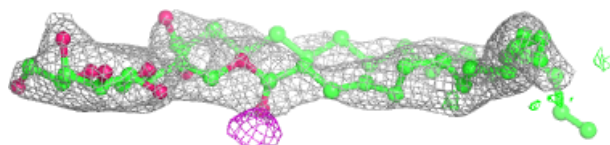
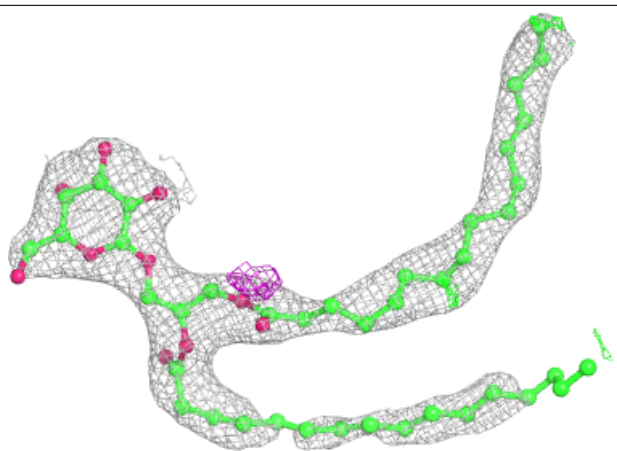
**Electron density around HTG b 622:**

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

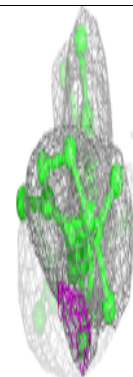
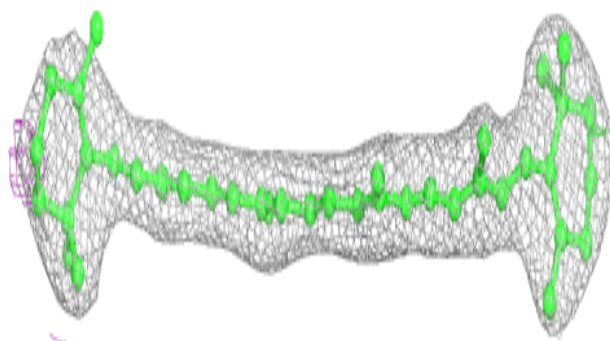
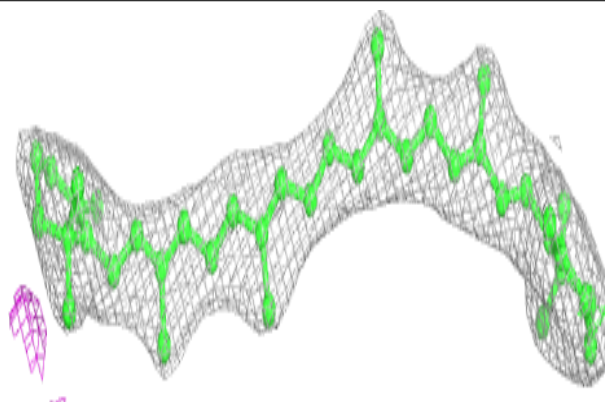


Electron density around LMG c 520:

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

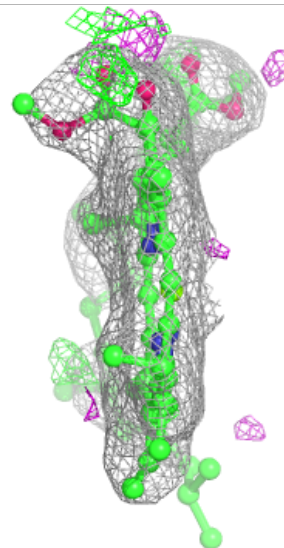
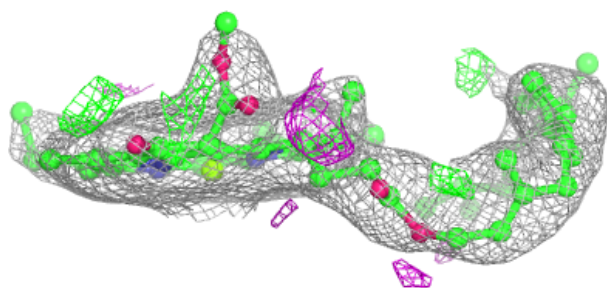
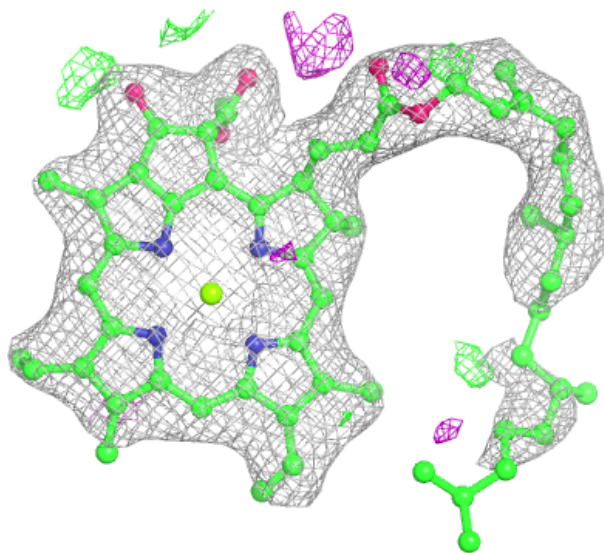
**Electron density around BCR h 101:**

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



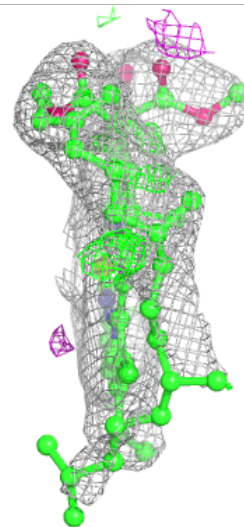
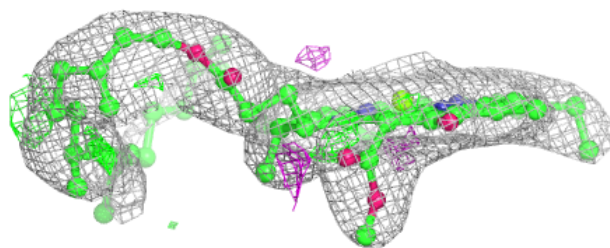
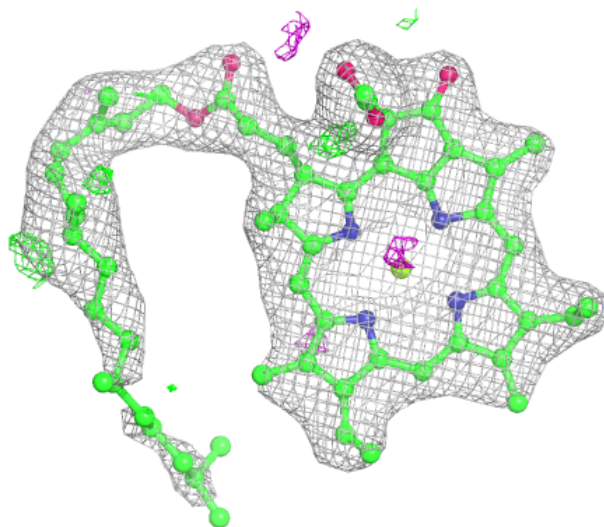
Electron density around CLA c 513:

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



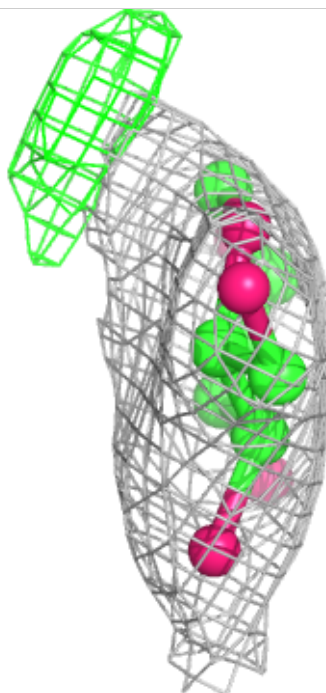
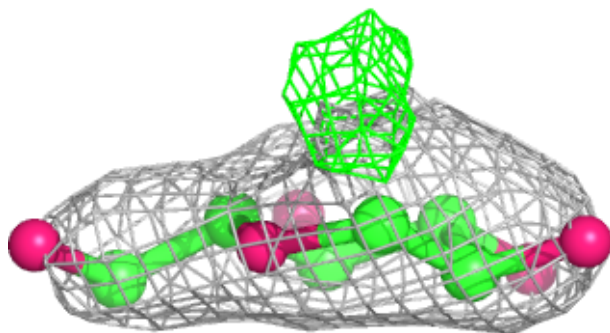
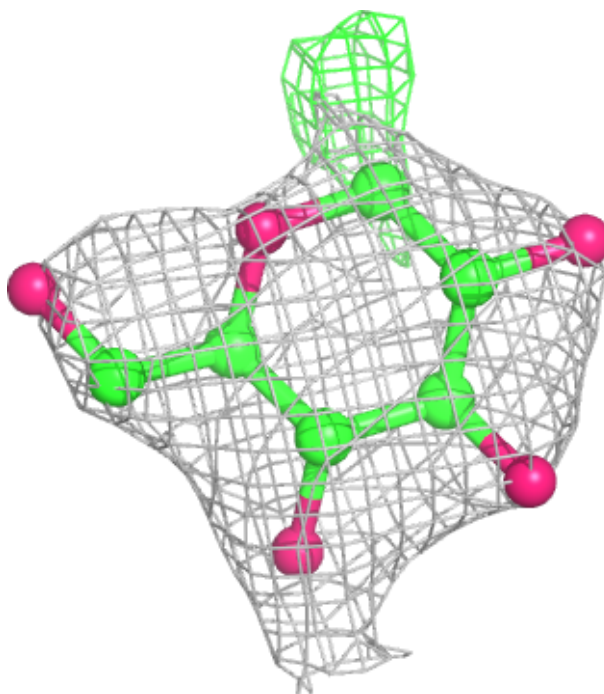
Electron density around CLA C 513:

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



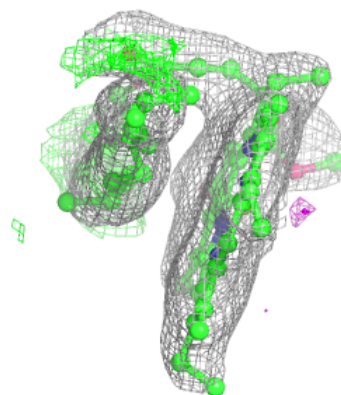
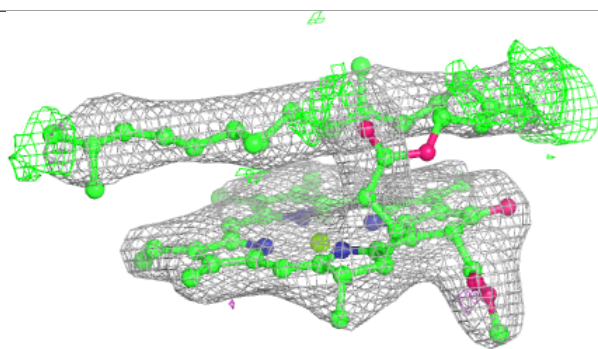
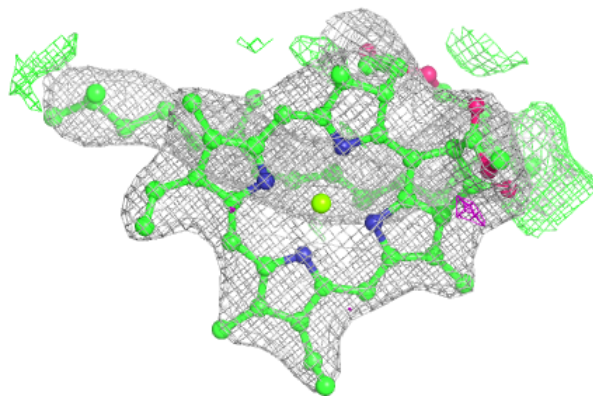
Electron density around HTG V 202:

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

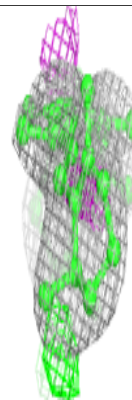
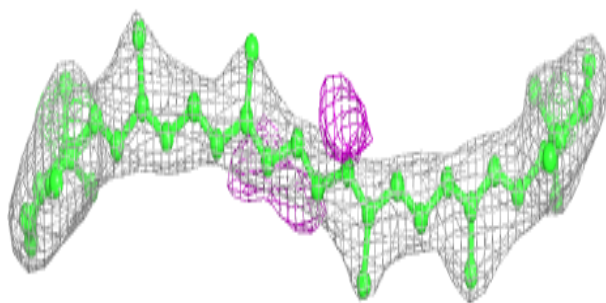
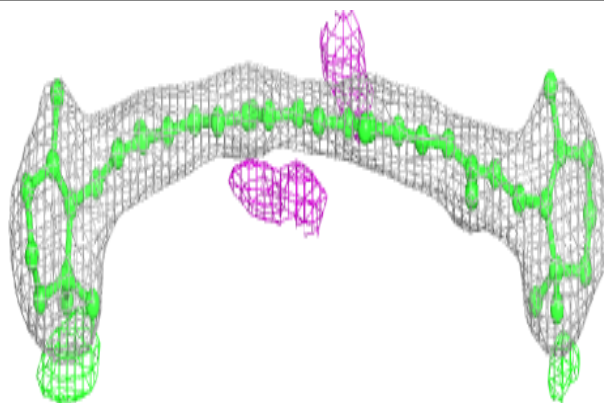


Electron density around CLA B 601:

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

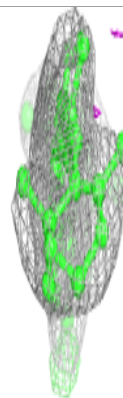
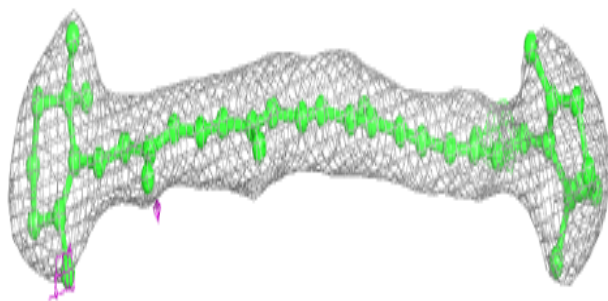
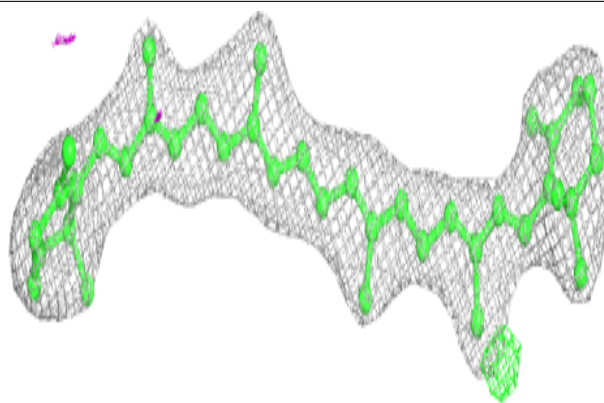
**Electron density around BCR K 102:**

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

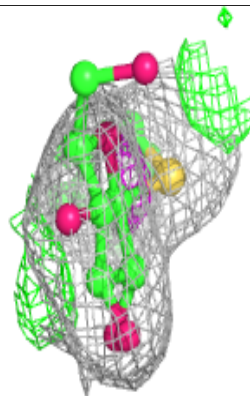
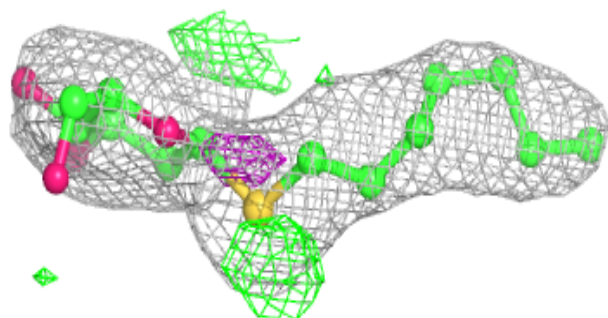
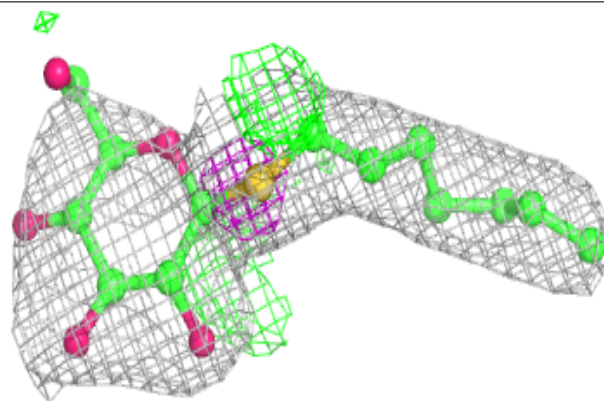


Electron density around BCR K 103:

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

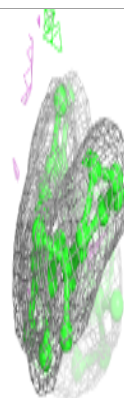
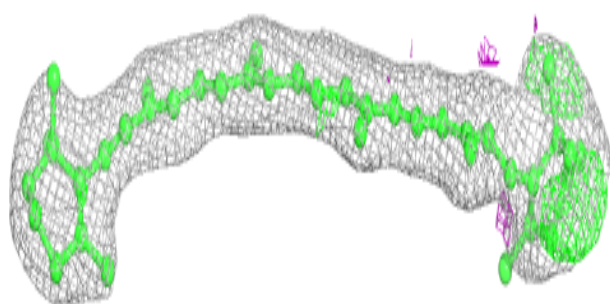
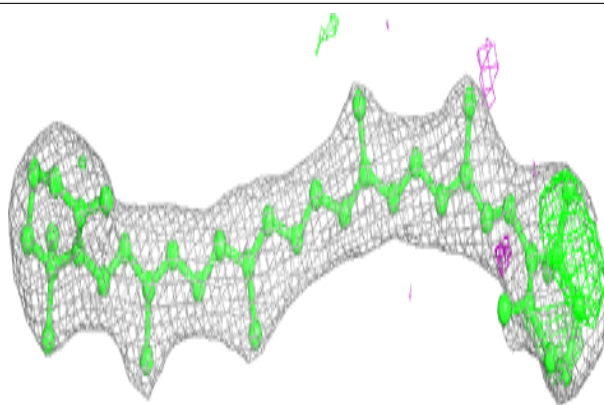
**Electron density around HTG B 622:**

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



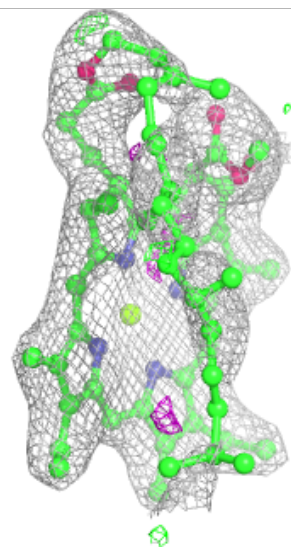
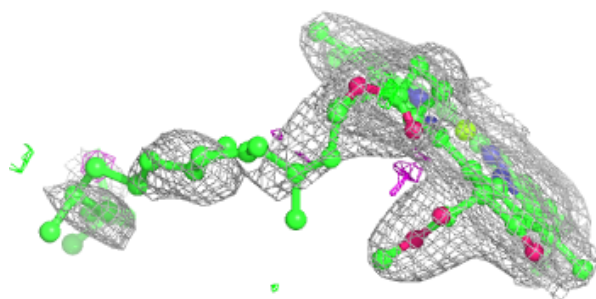
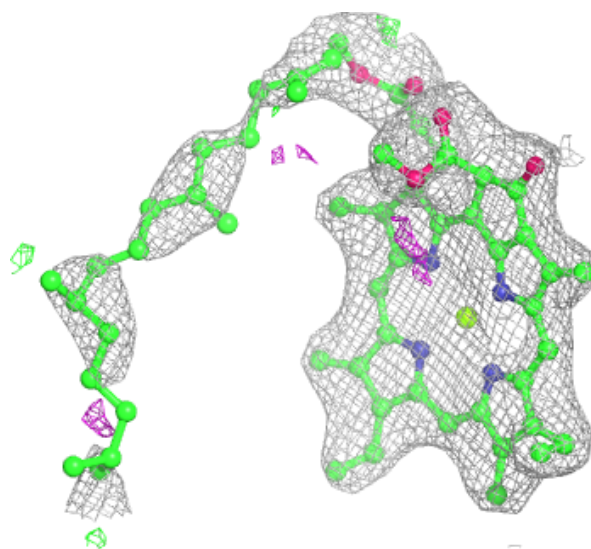
Electron density around BCR d 404:

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



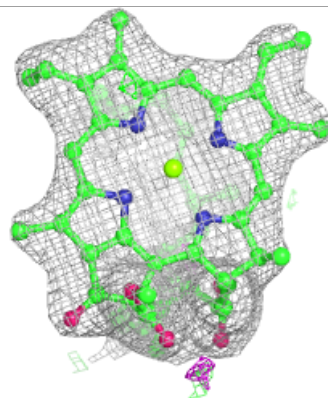
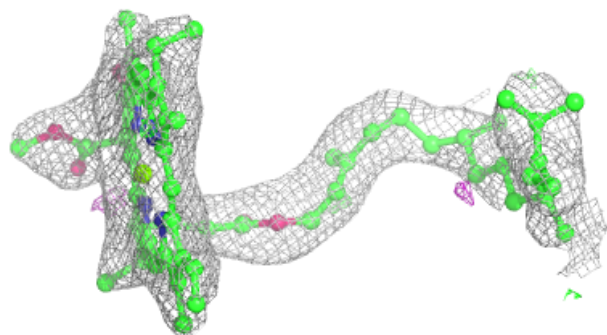
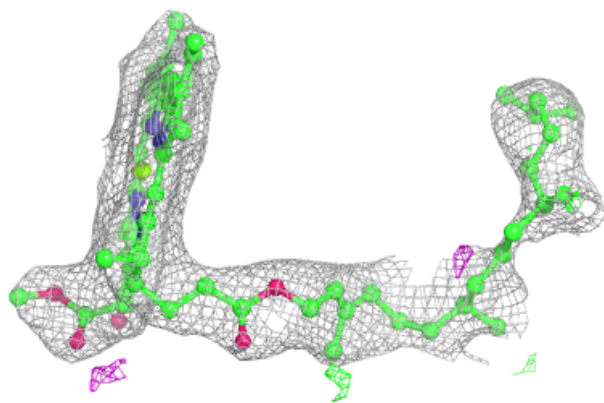
Electron density around CLA B 616:

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

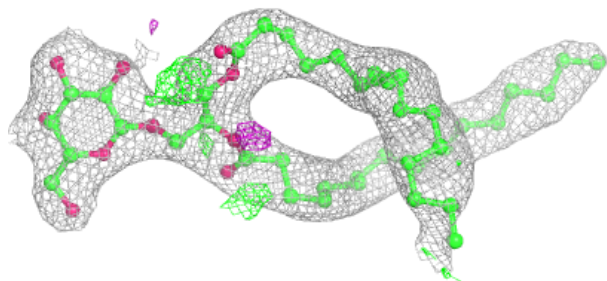
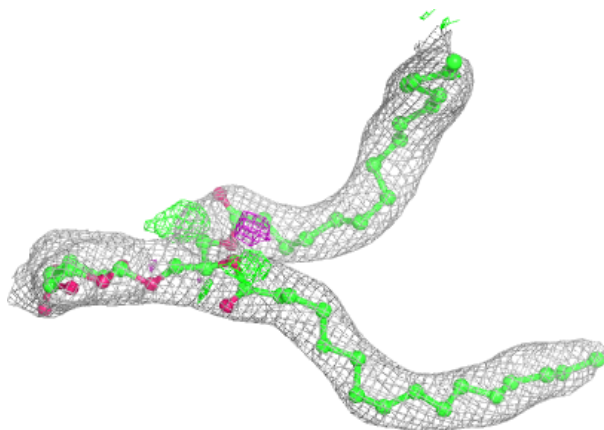


Electron density around CLA C 507:

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

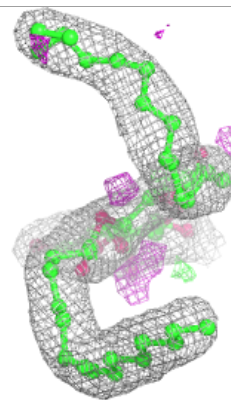
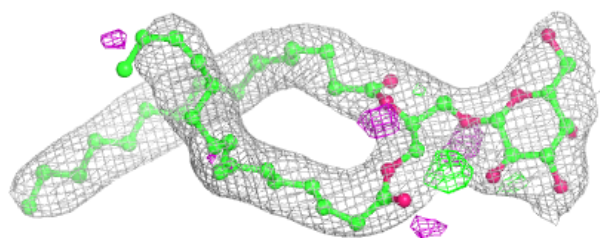
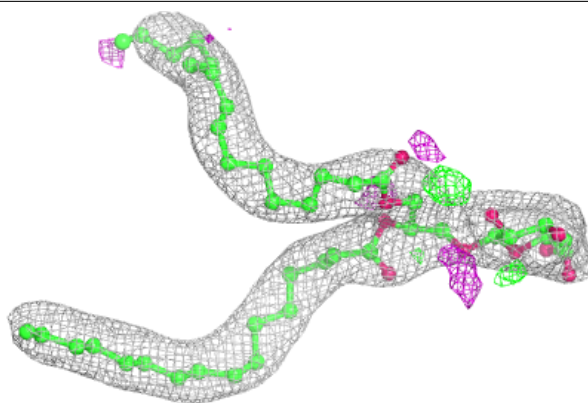
**Electron density around LMG B 621:**

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

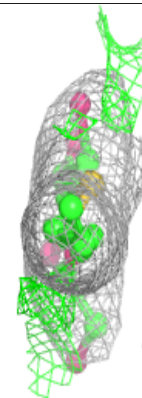
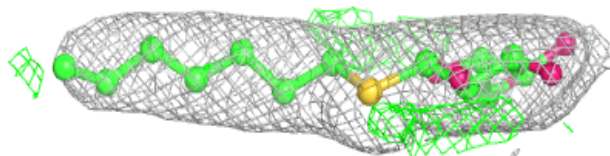
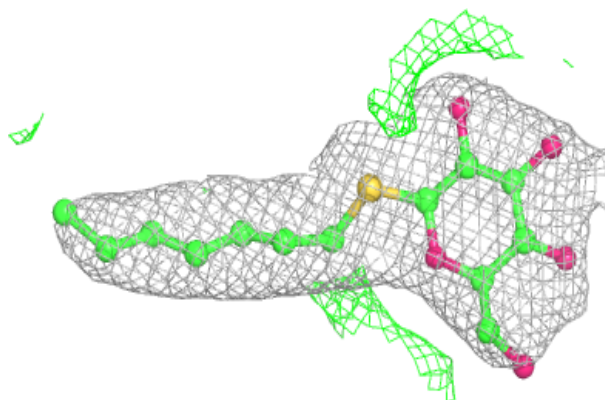


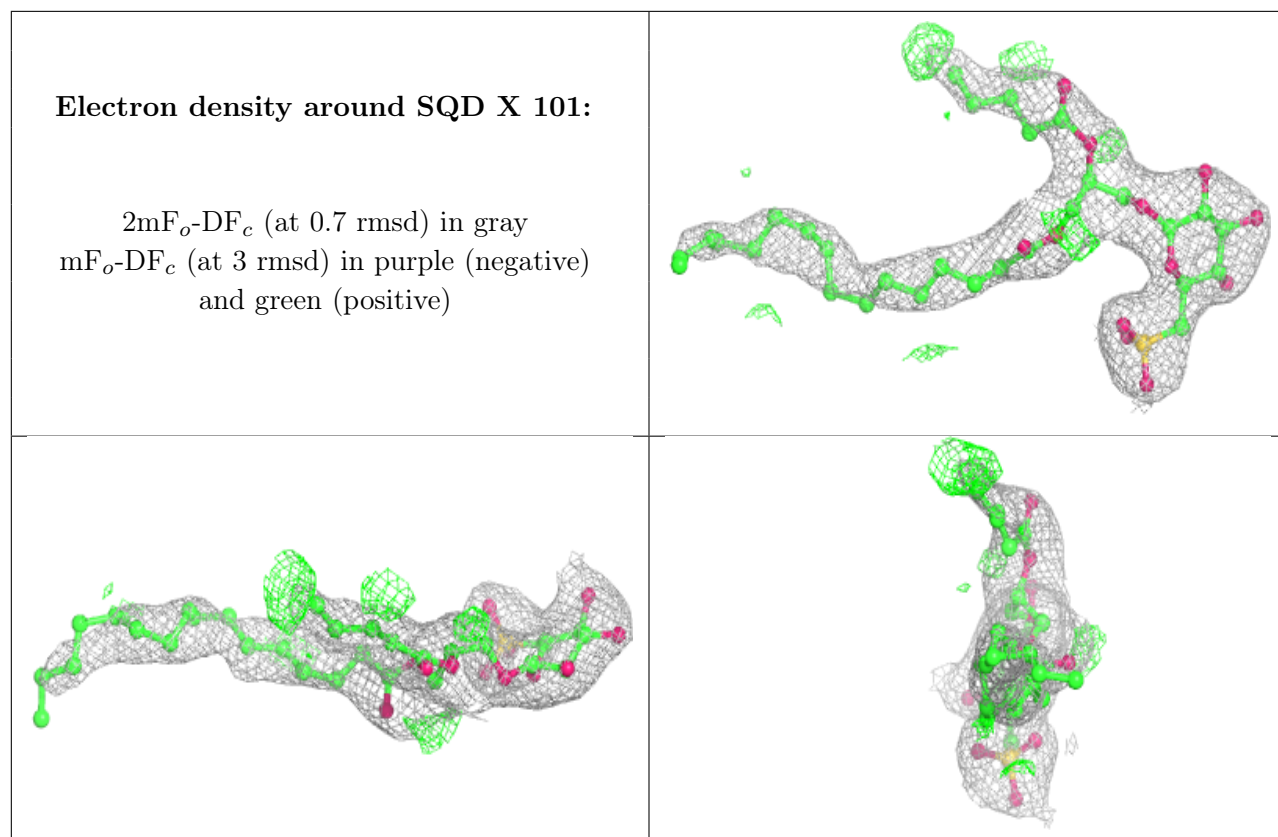
Electron density around LMG m 101:

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

**Electron density around HTG b 625:**

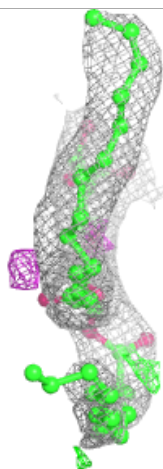
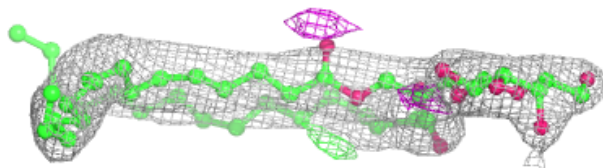
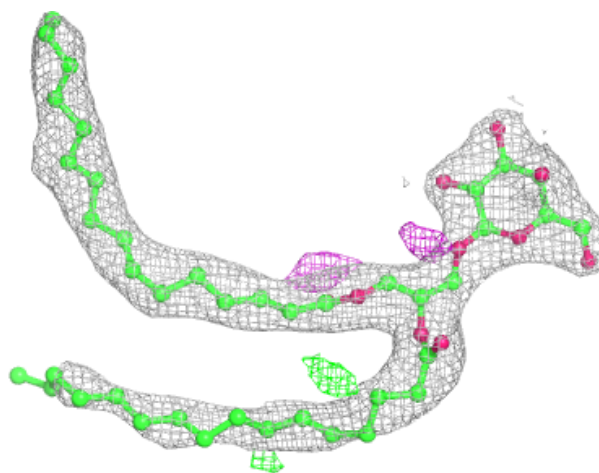
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





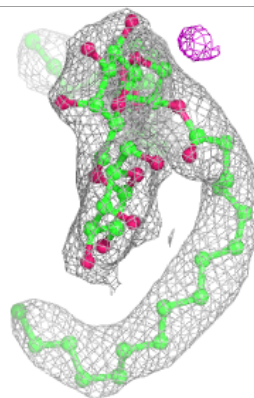
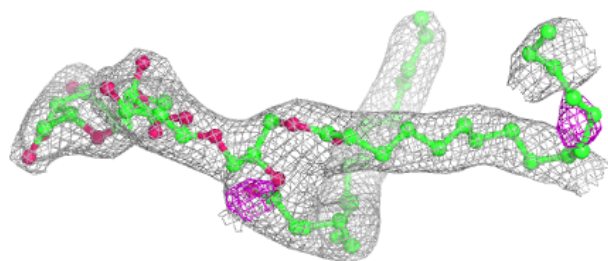
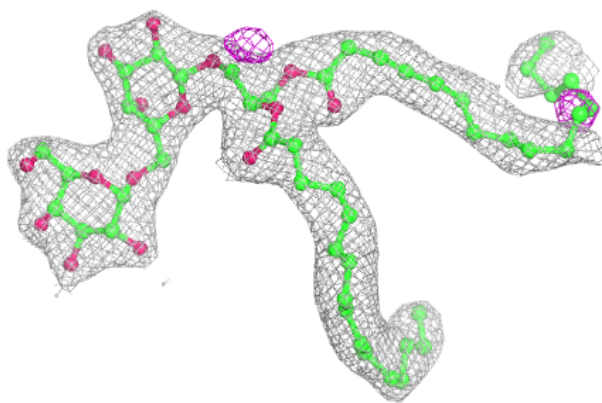
Electron density around LMG C 520:

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

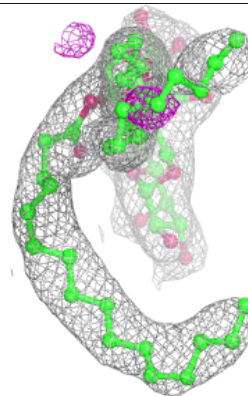
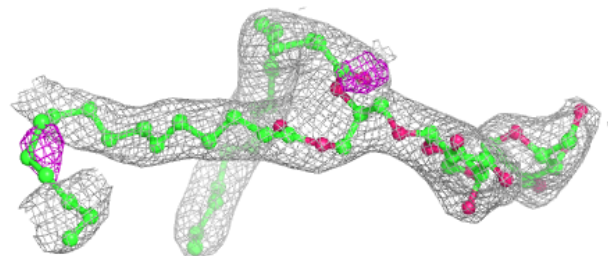
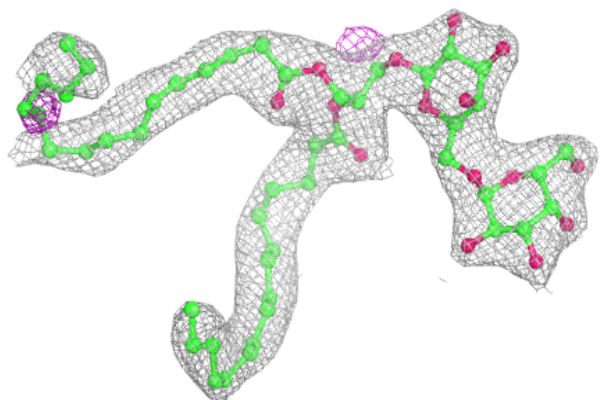


Electron density around DGD c 518 (A):

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

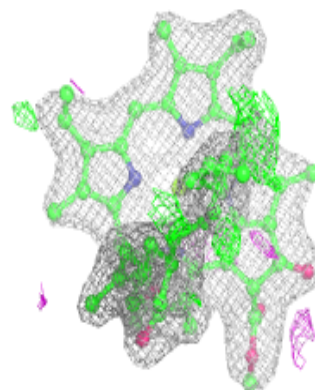
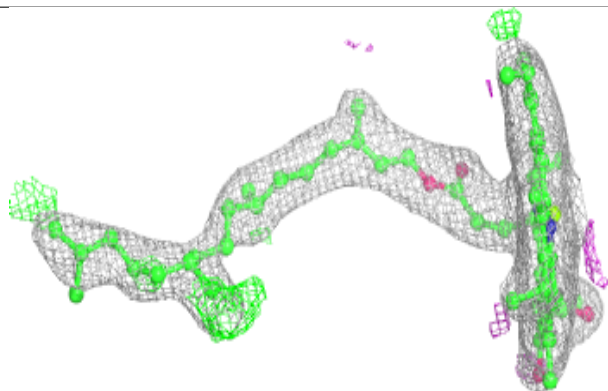
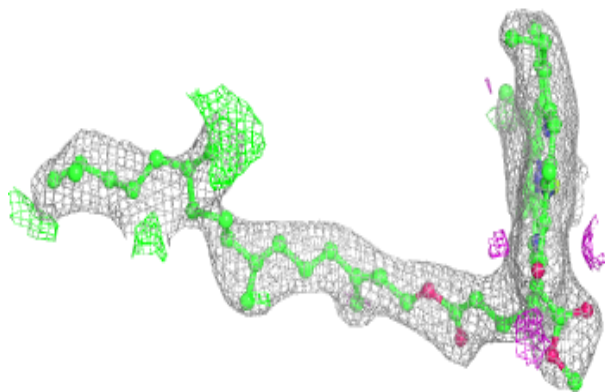
**Electron density around DGD c 518 (B):**

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

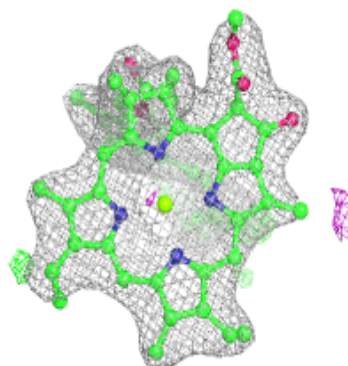
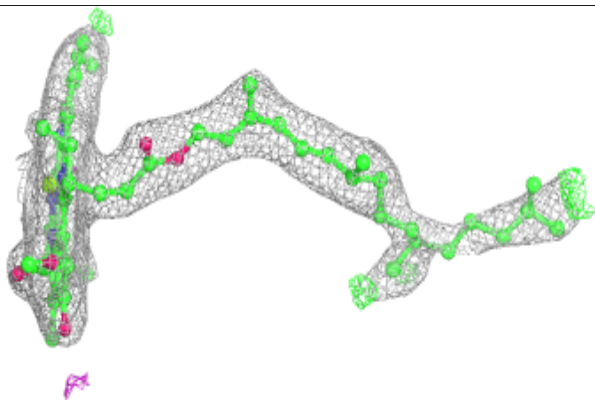
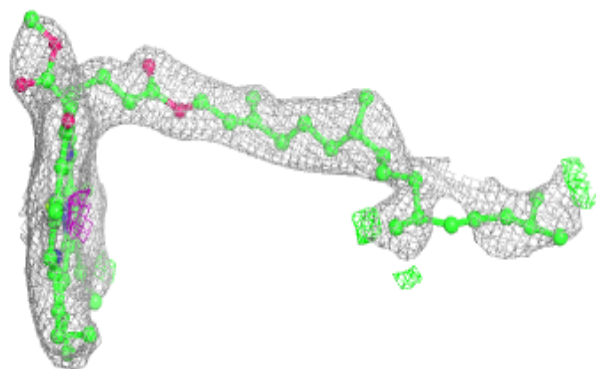


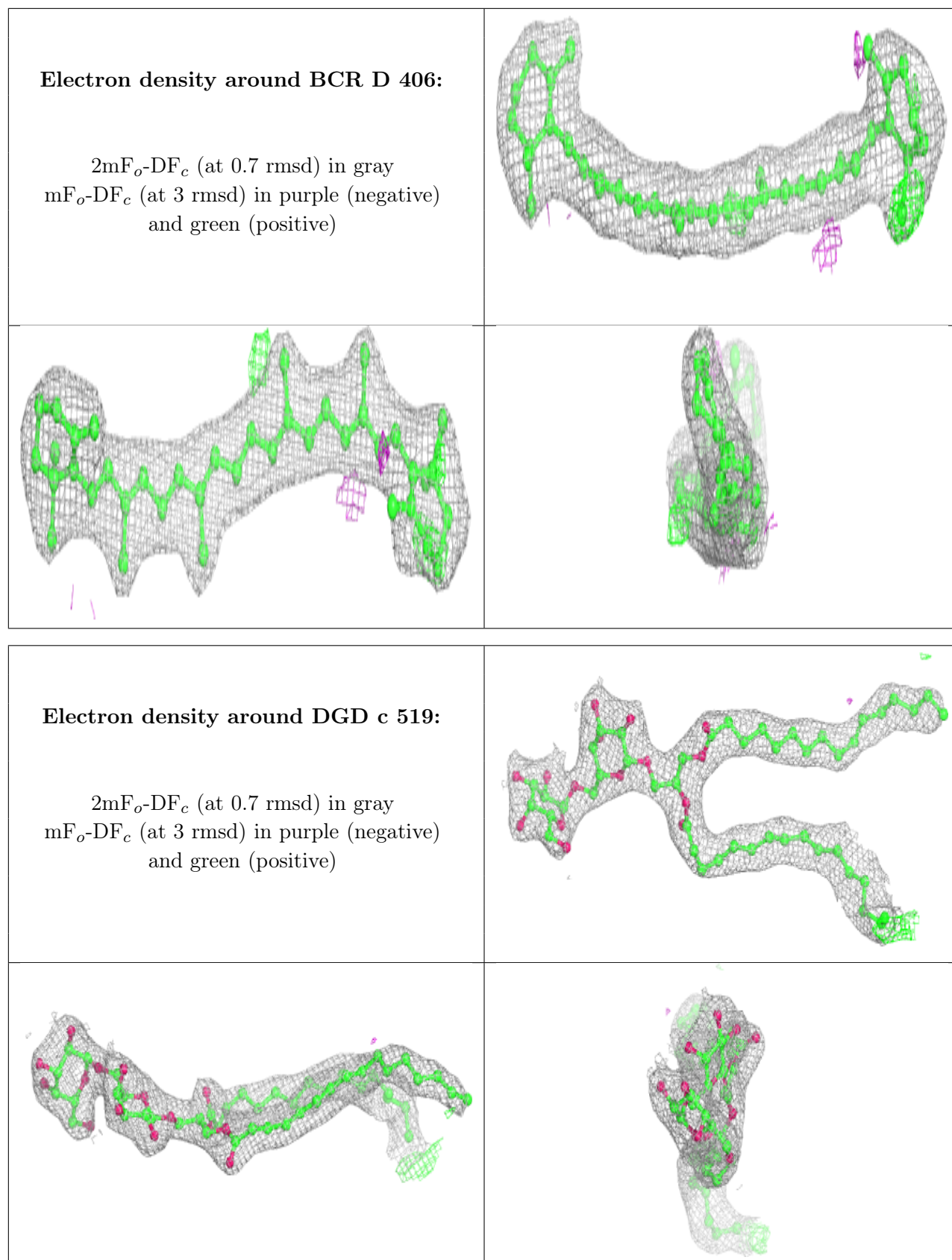
Electron density around CLA b 606:

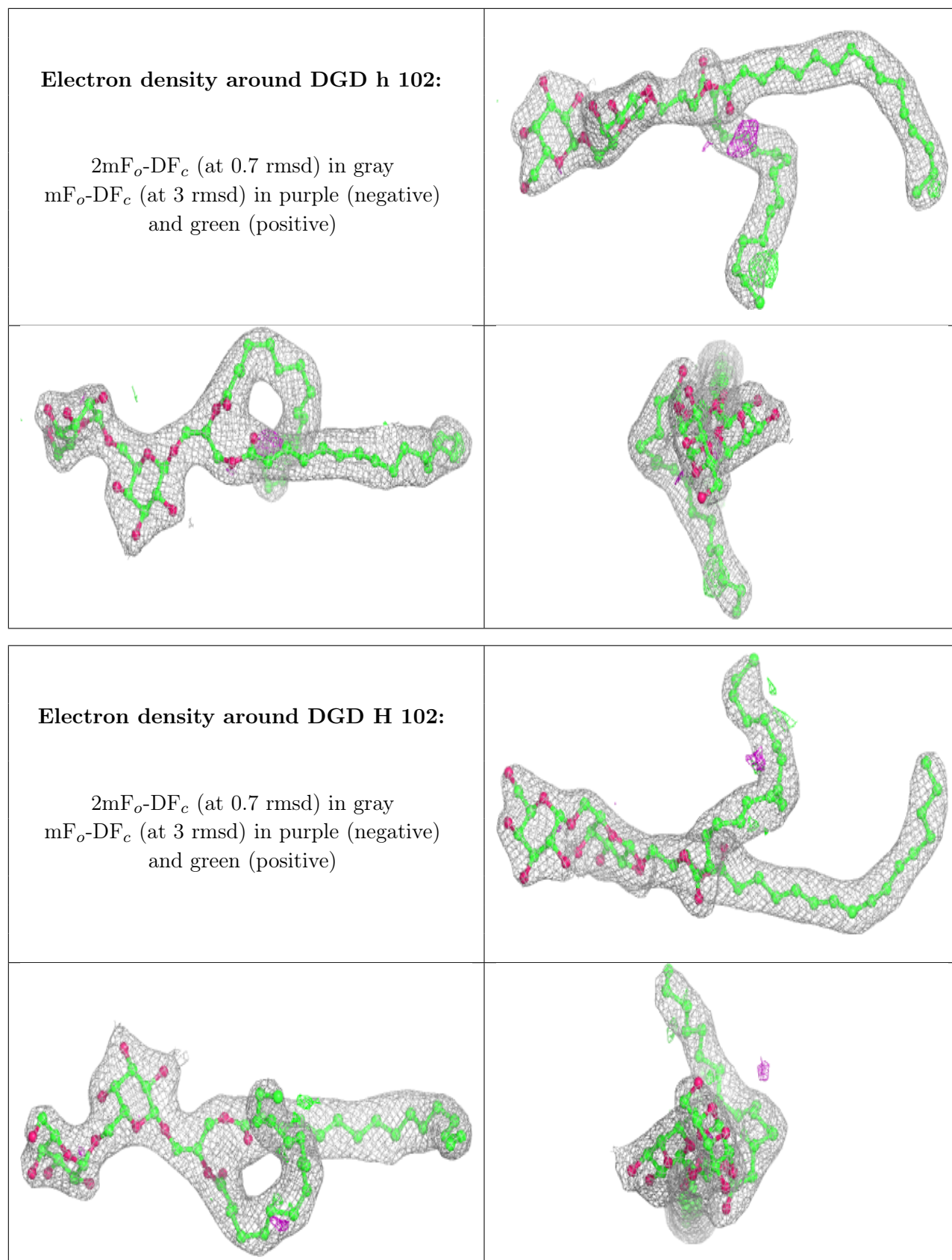
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around CLA B 606:**

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

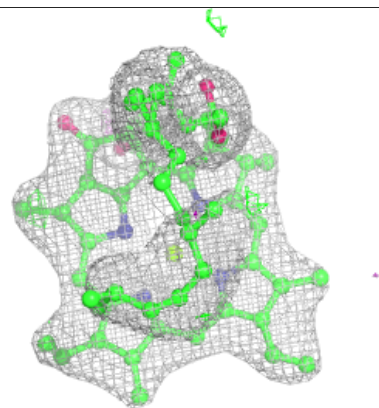
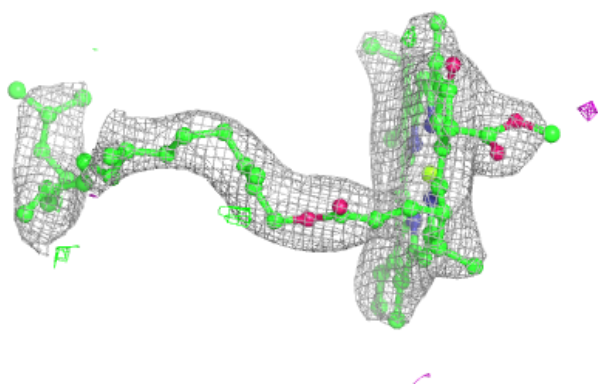
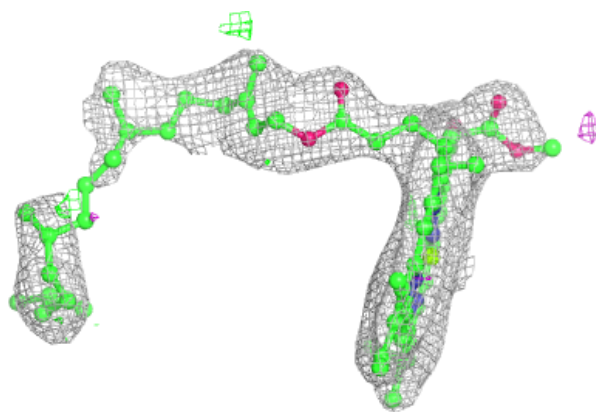






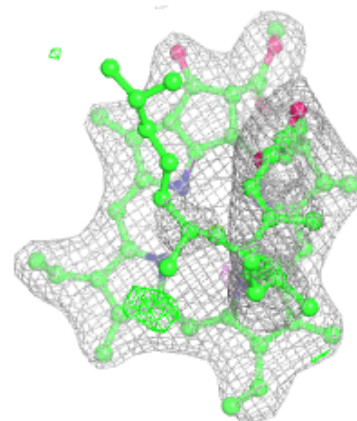
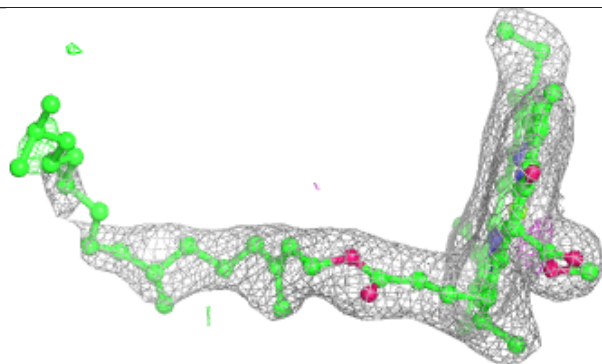
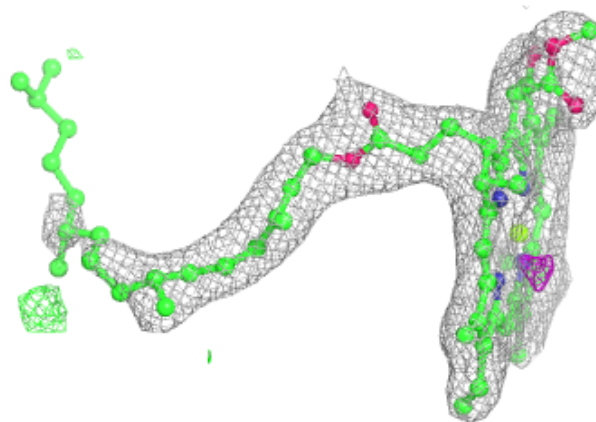
Electron density around CLA c 507:

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

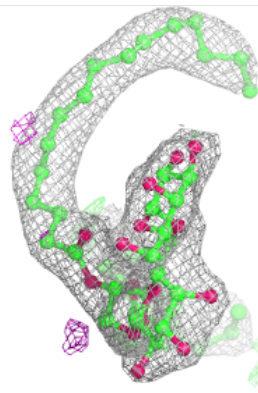
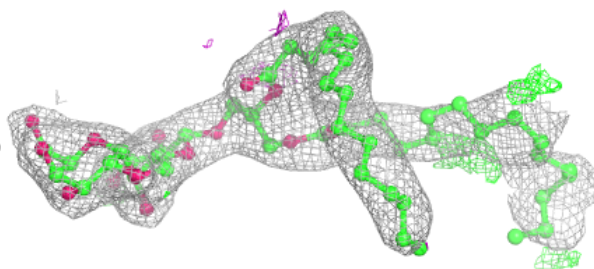
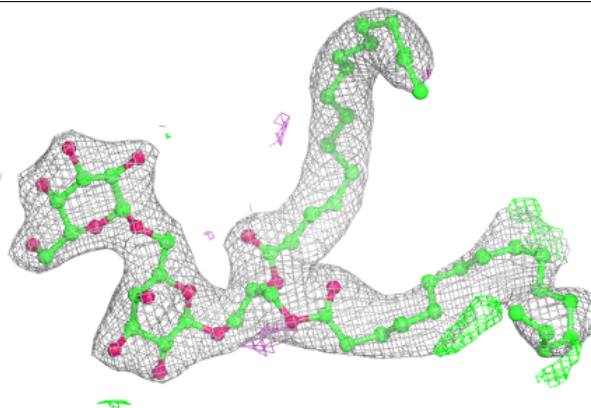


Electron density around CLA D 405:

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

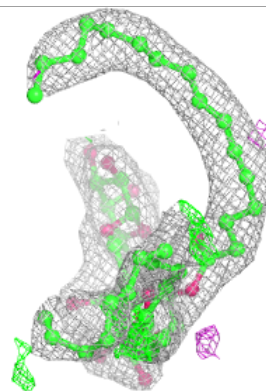
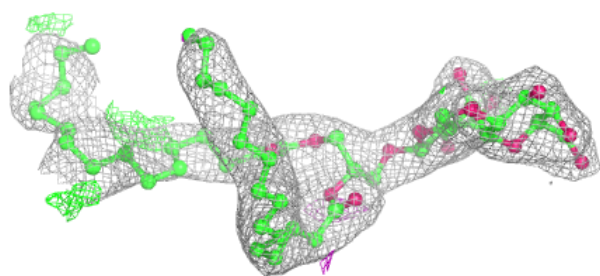
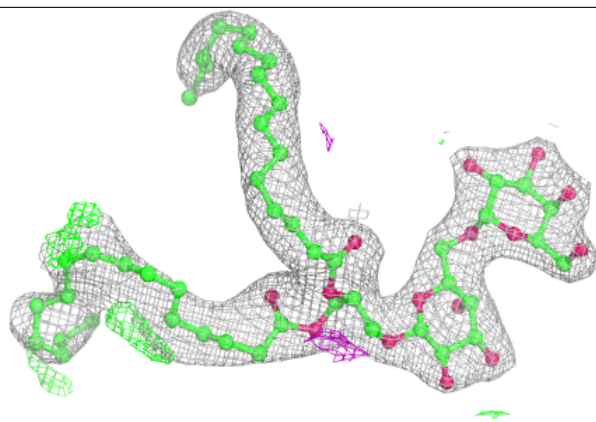
**Electron density around DGD C 518 (A):**

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

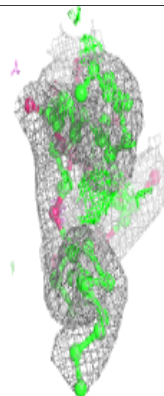
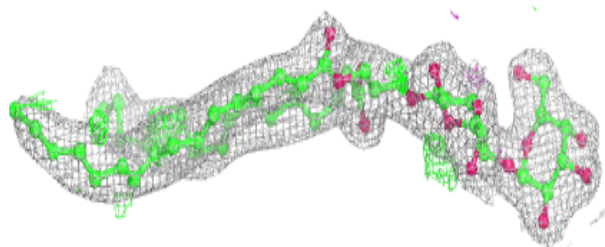
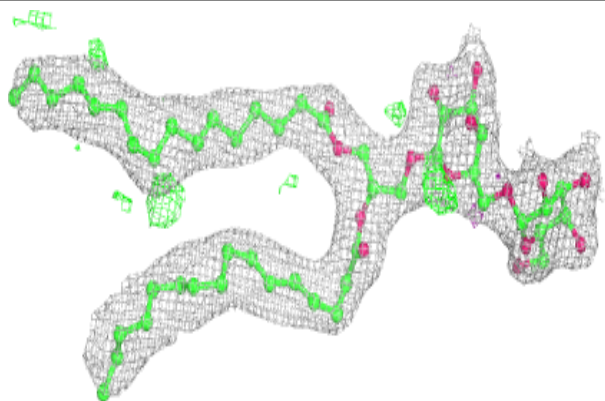


Electron density around DGD C 518 (B):

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

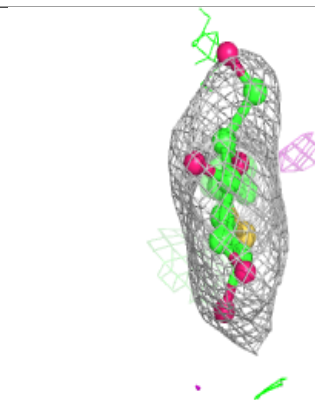
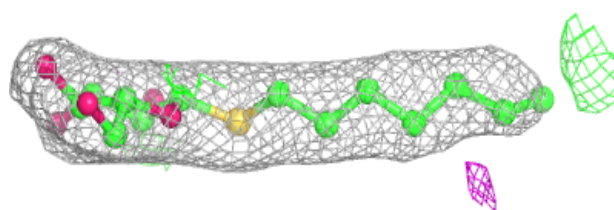
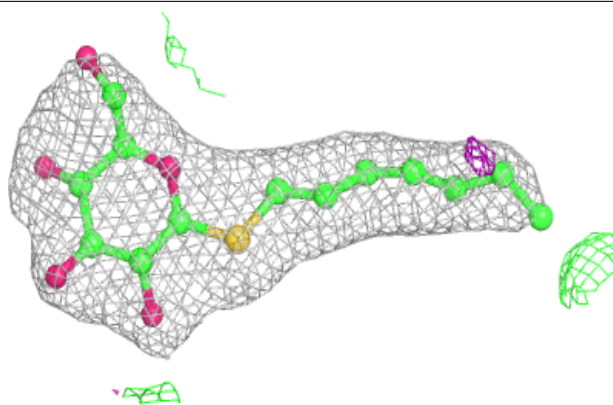
**Electron density around DGD C 519:**

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

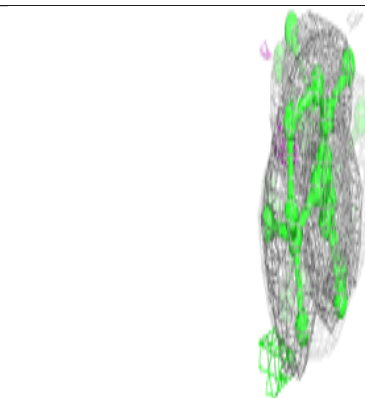
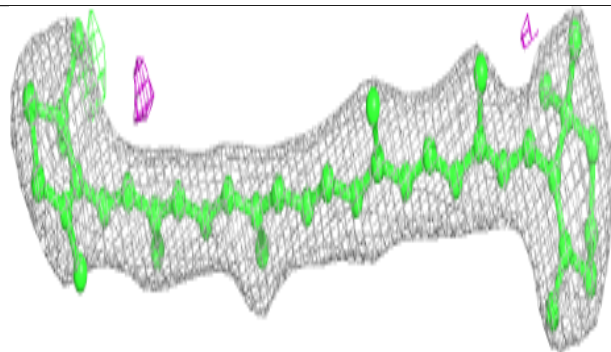
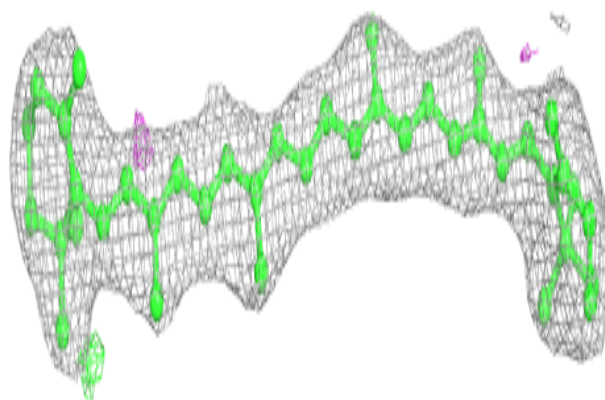


Electron density around HTG B 625:

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

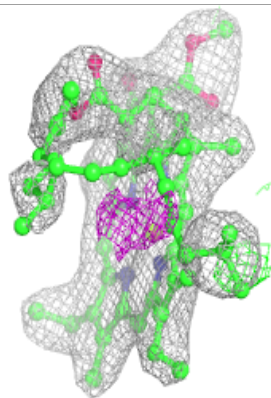
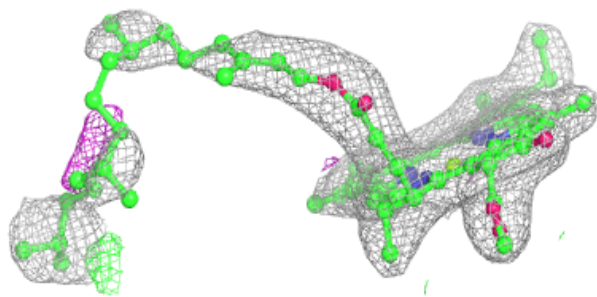
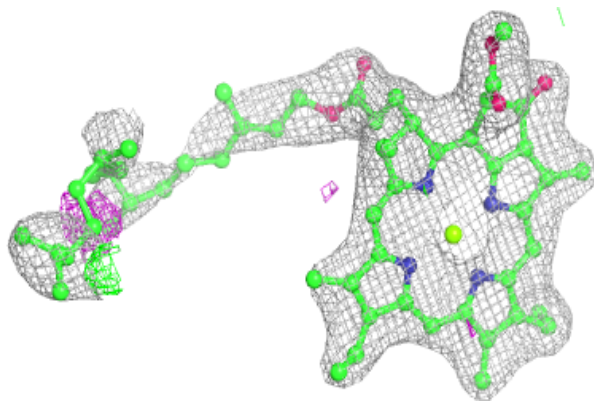
**Electron density around BCR c 515:**

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

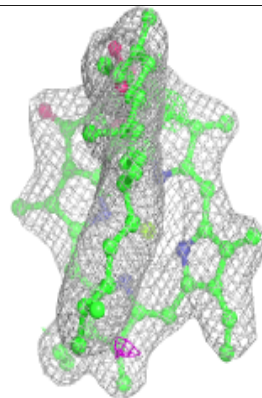
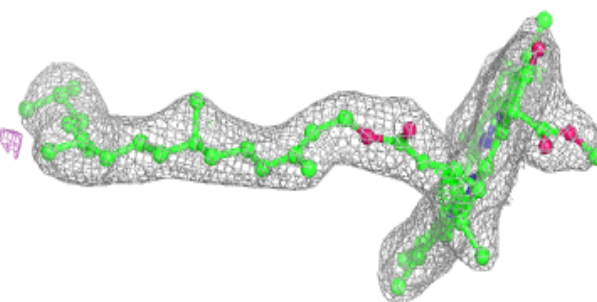
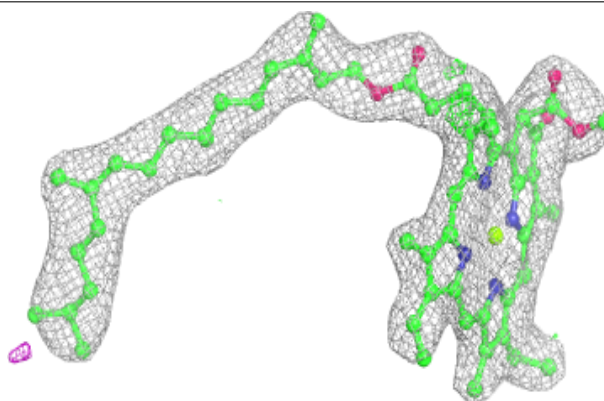


Electron density around CLA a 409:

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

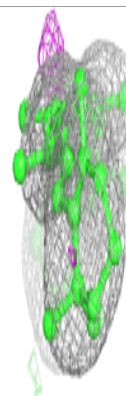
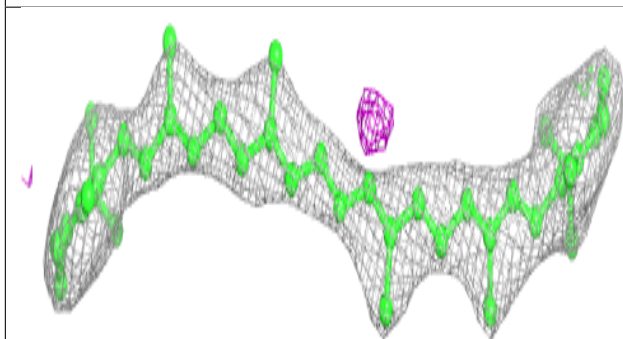
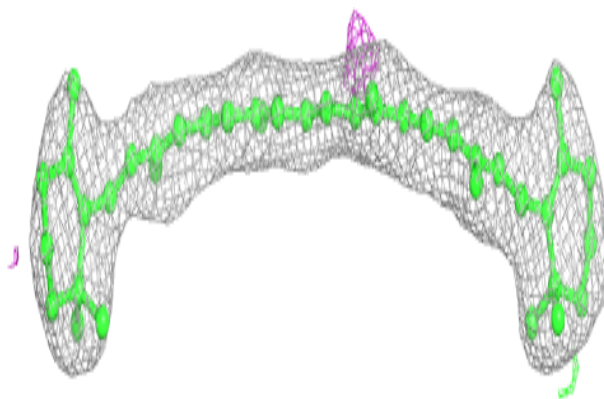
**Electron density around CLA B 609:**

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



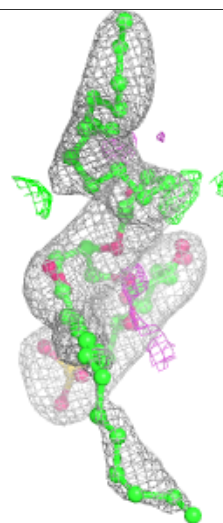
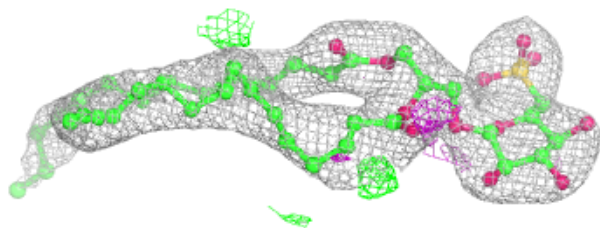
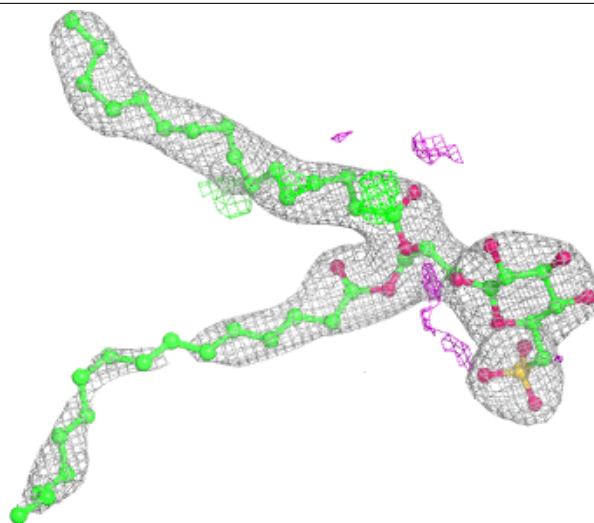
Electron density around BCR k 101:

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



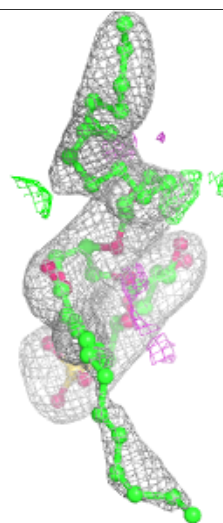
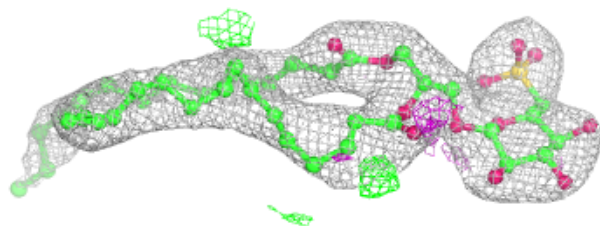
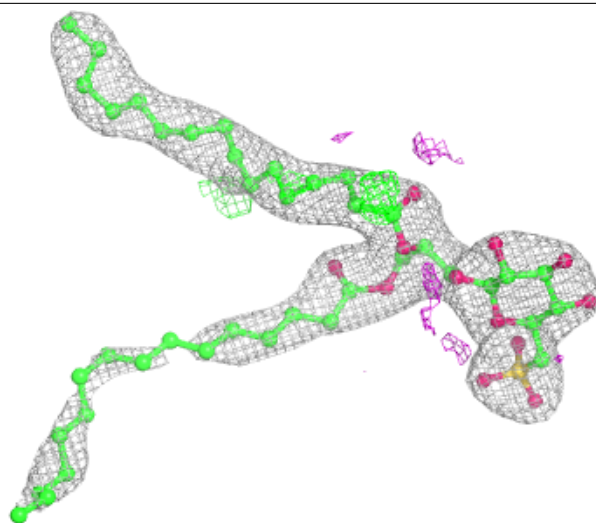
Electron density around SQD A 410 (A):

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



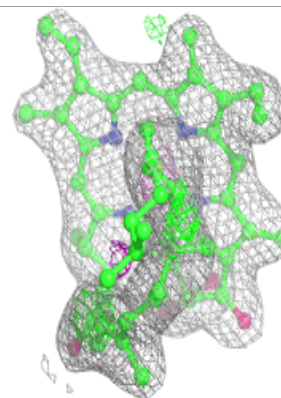
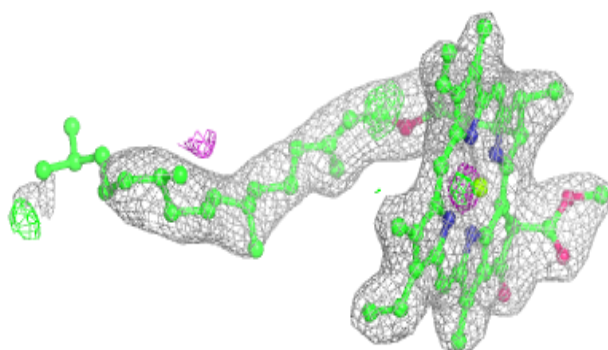
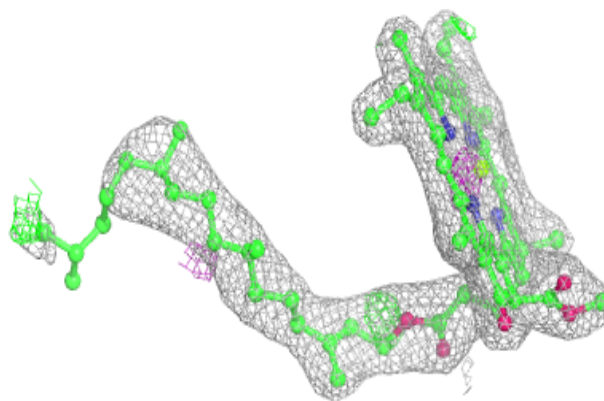
Electron density around SQD A 410 (B):

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

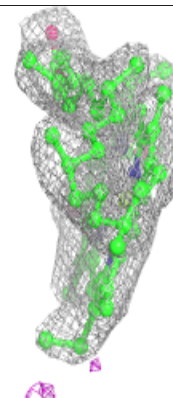
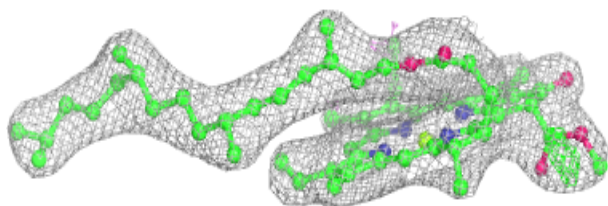
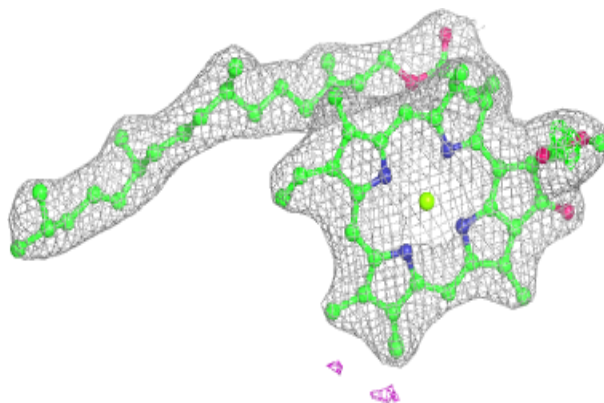


Electron density around CLA C 509:

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

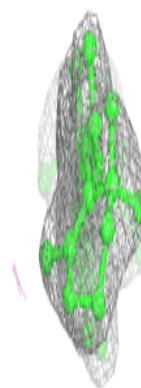
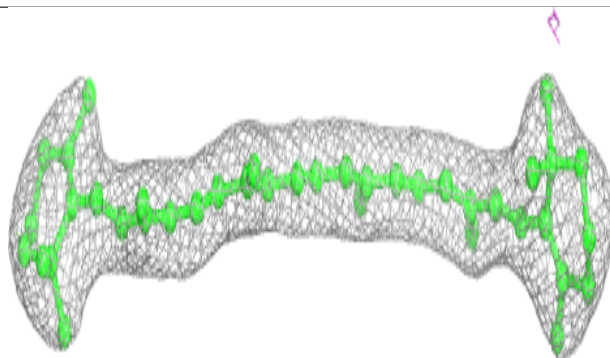
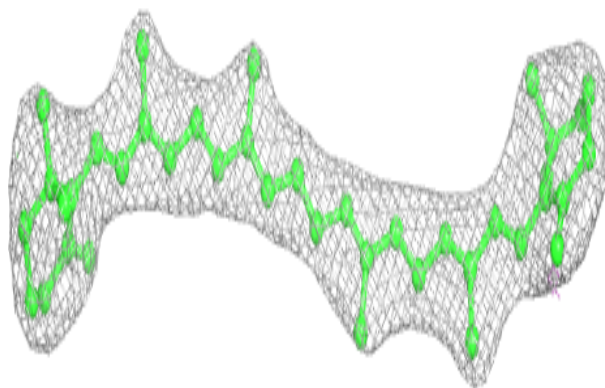
**Electron density around CLA C 502:**

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

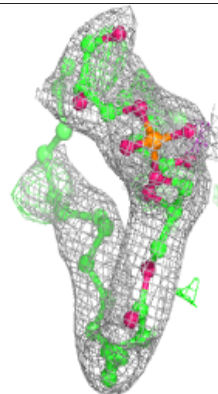
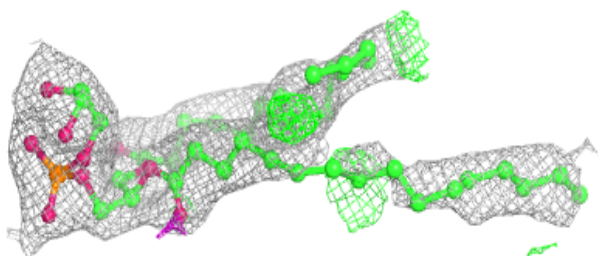
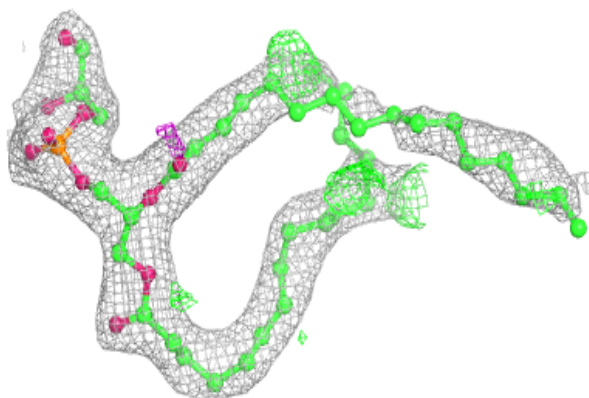


Electron density around BCR y 101:

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

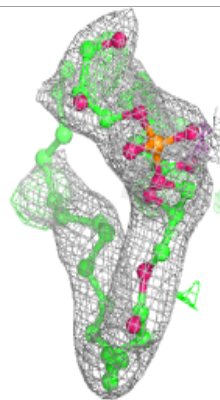
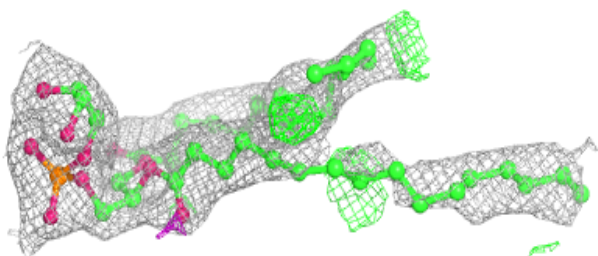
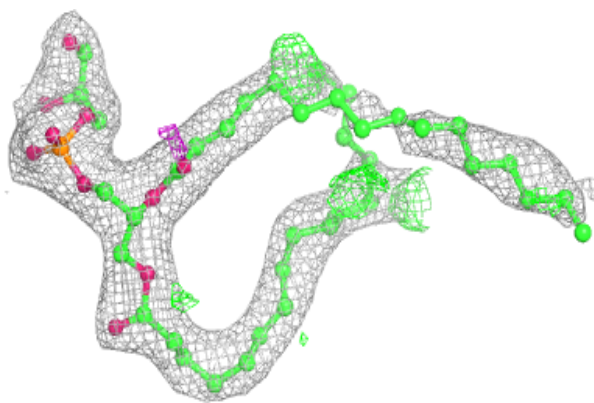
**Electron density around LHG D 409 (A):**

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

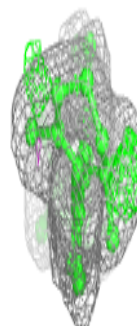
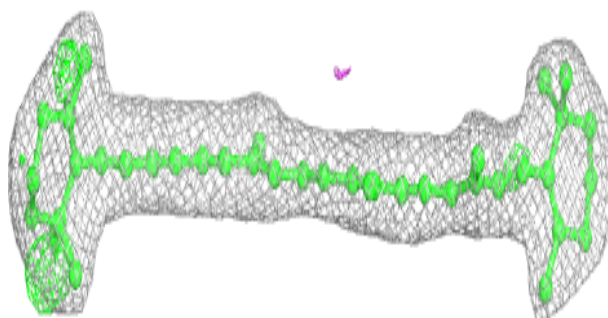
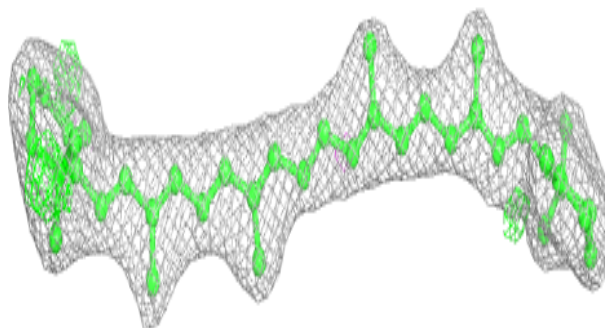


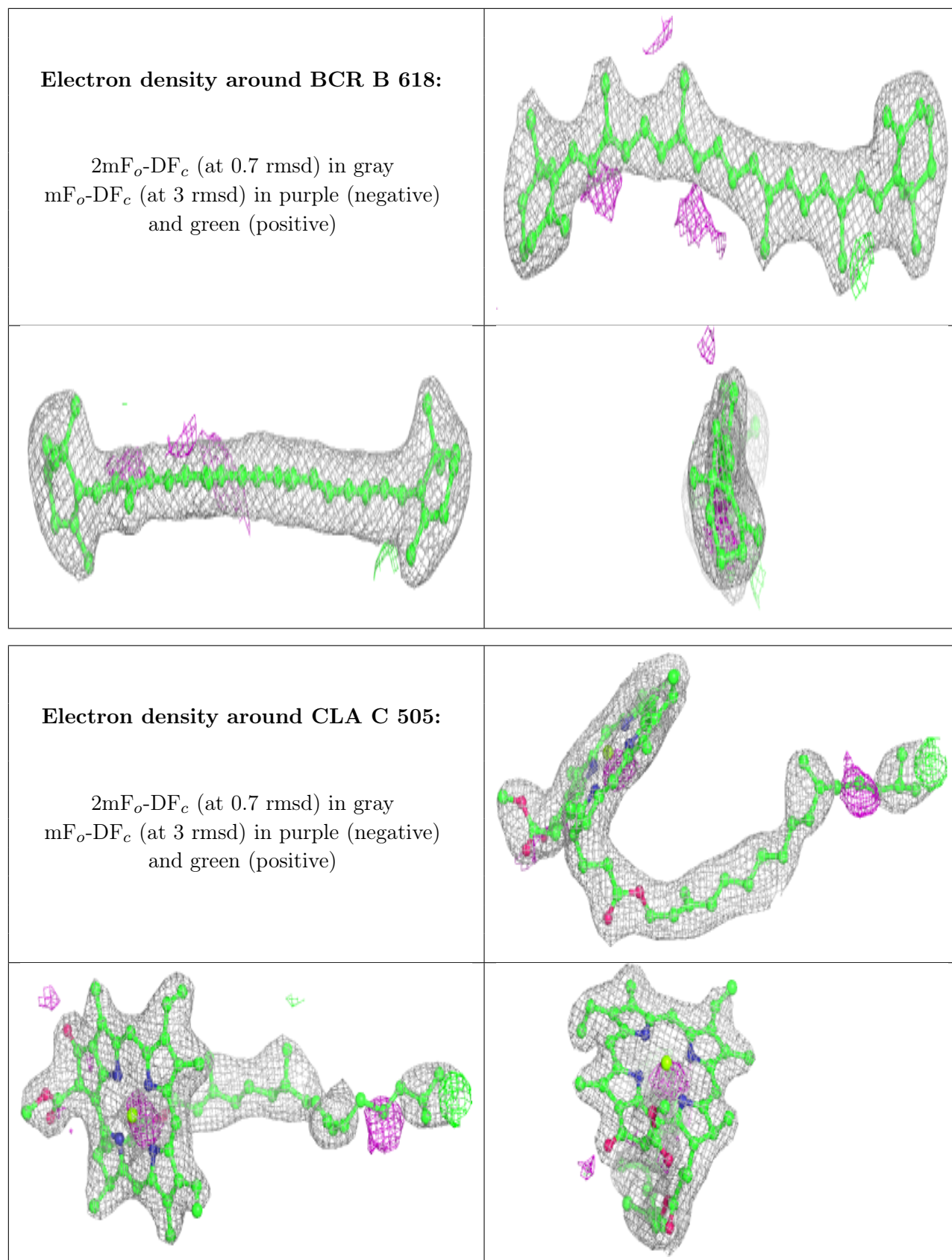
Electron density around LHG D 409 (B):

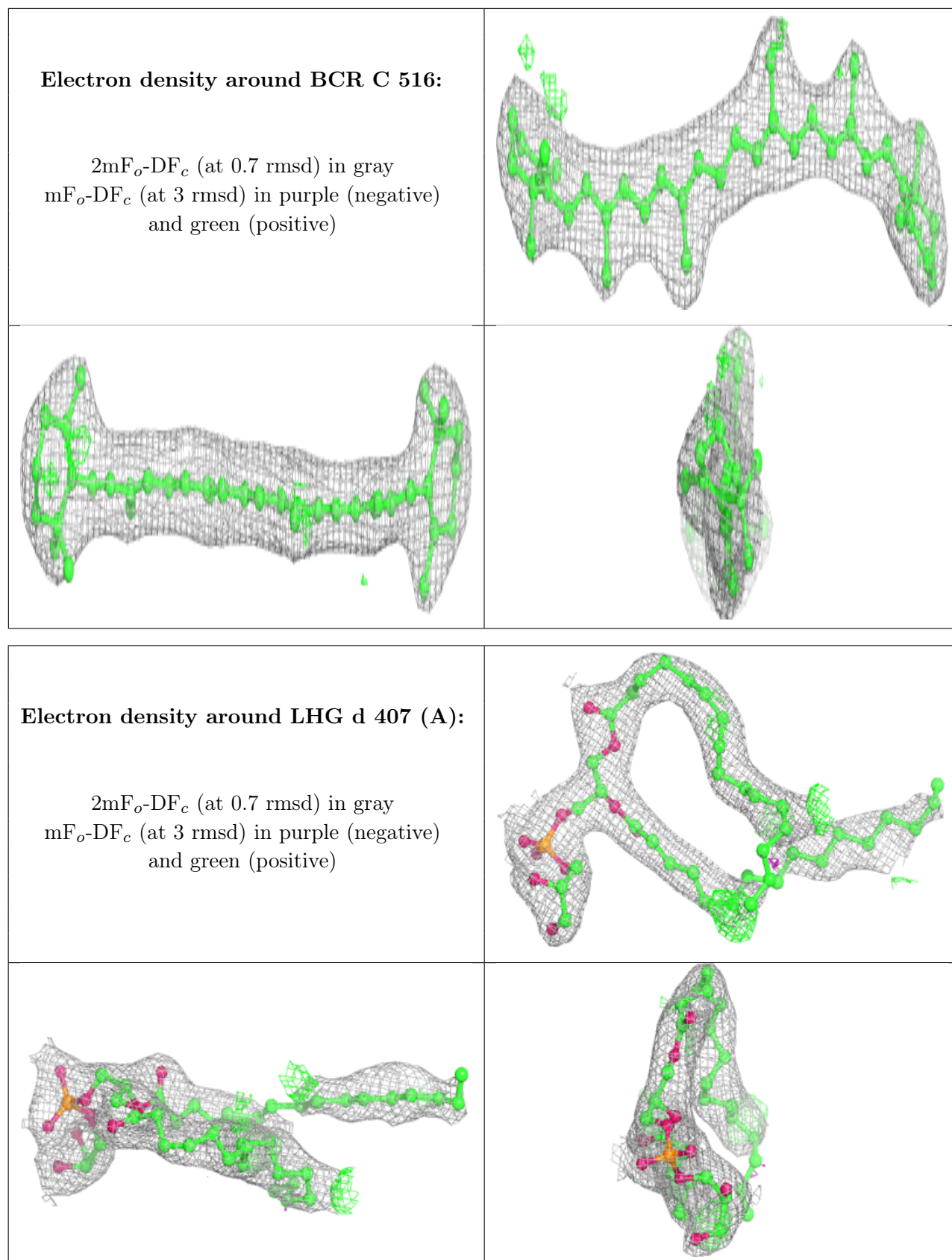
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around BCR A 409:**

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

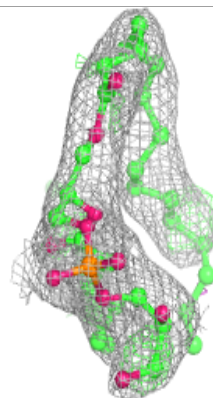
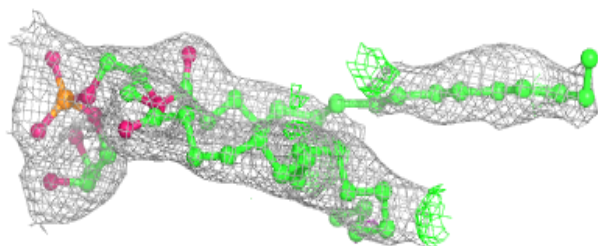
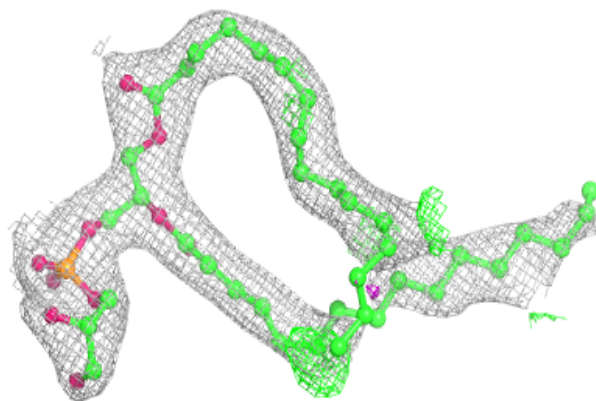




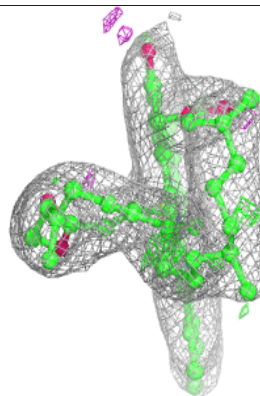
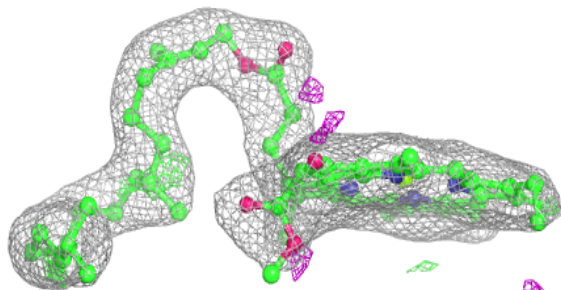
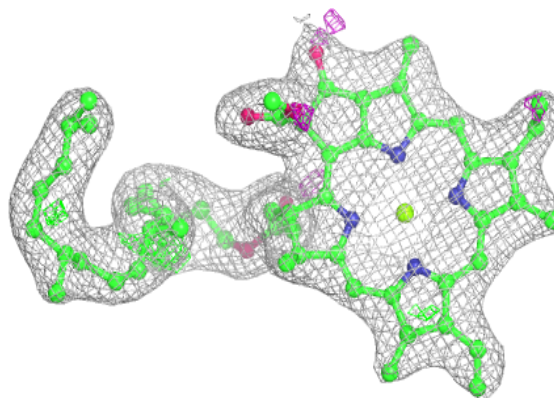


Electron density around LHG d 407 (B):

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

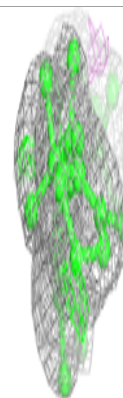
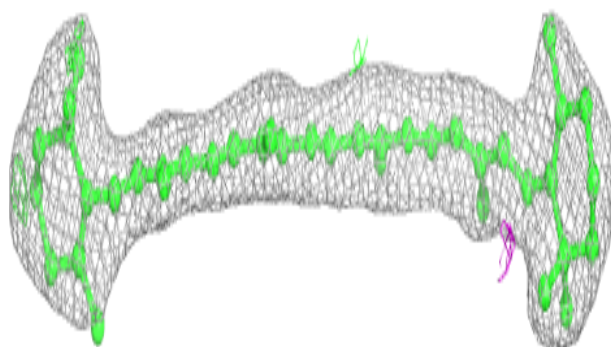
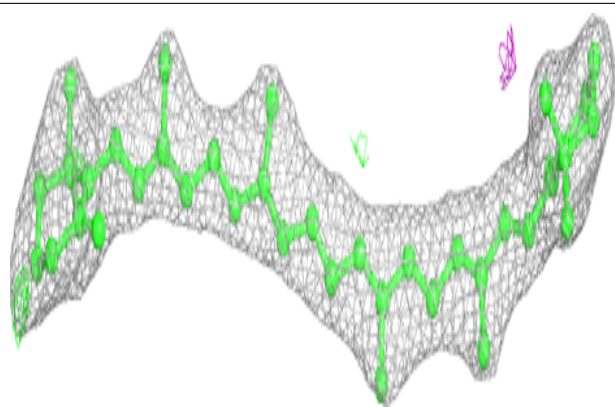
**Electron density around CLA b 612:**

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

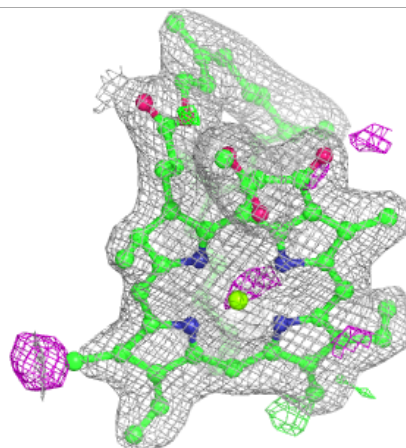
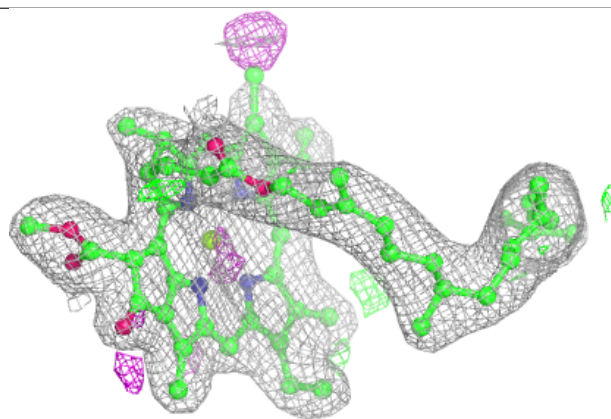
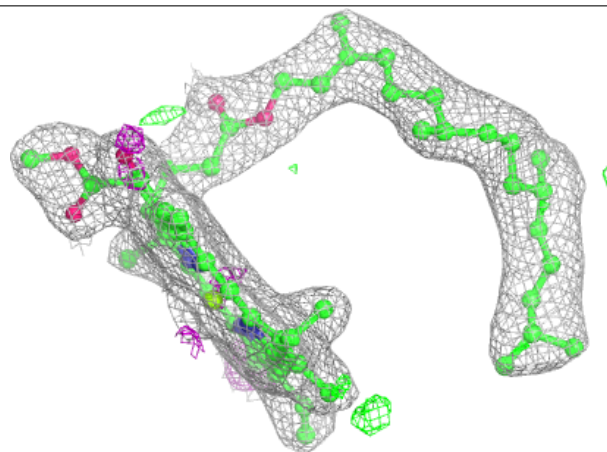


Electron density around BCR H 101:

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

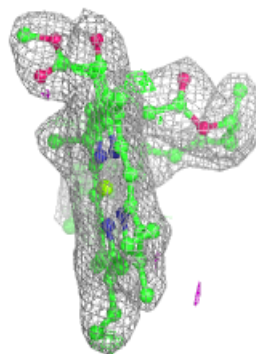
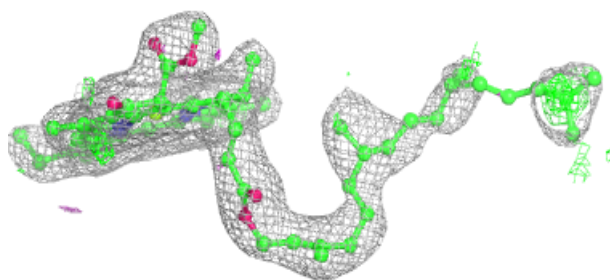
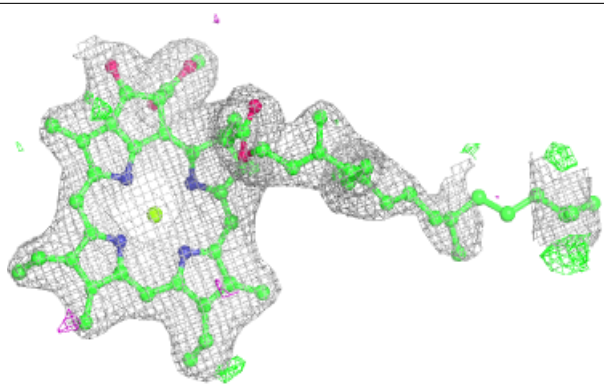
**Electron density around CLA B 611:**

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

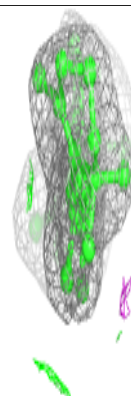
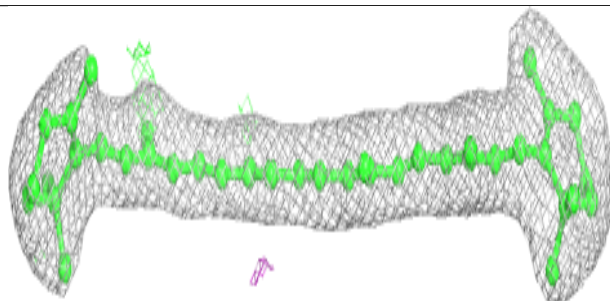
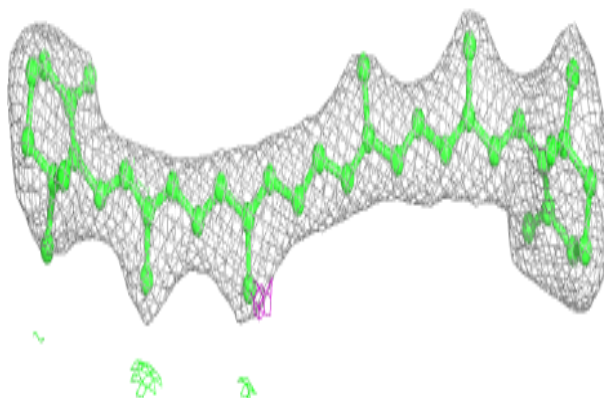


Electron density around CLA a 407 (A):

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

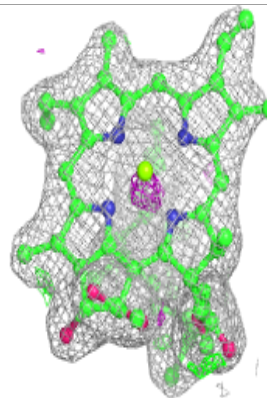
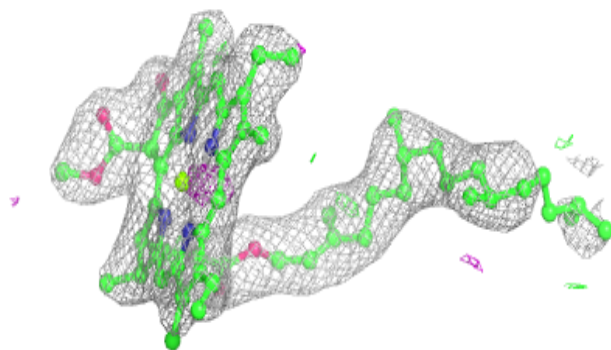
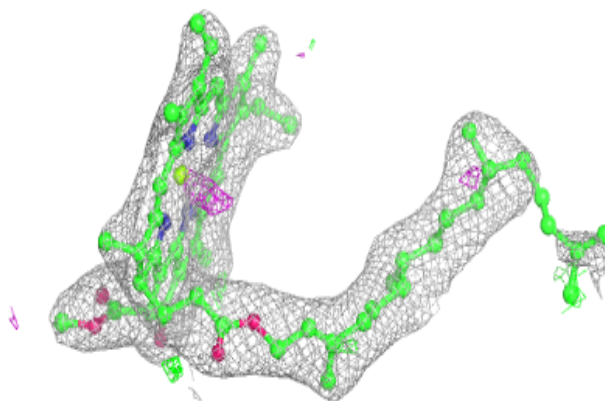
**Electron density around BCR b 618:**

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

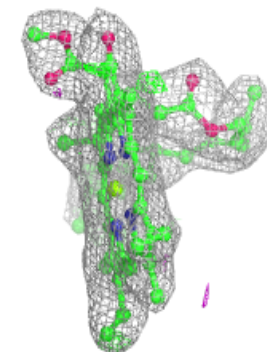
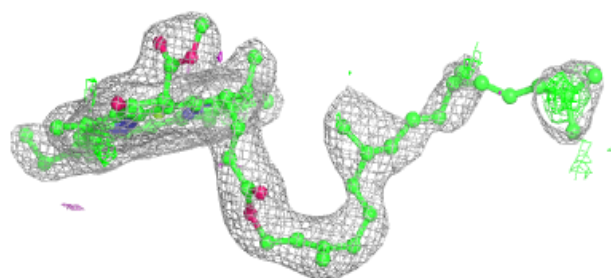
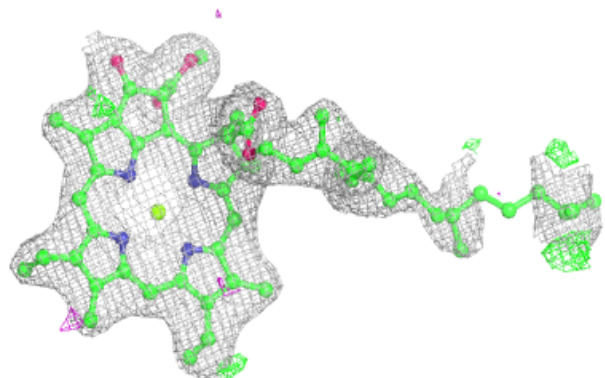


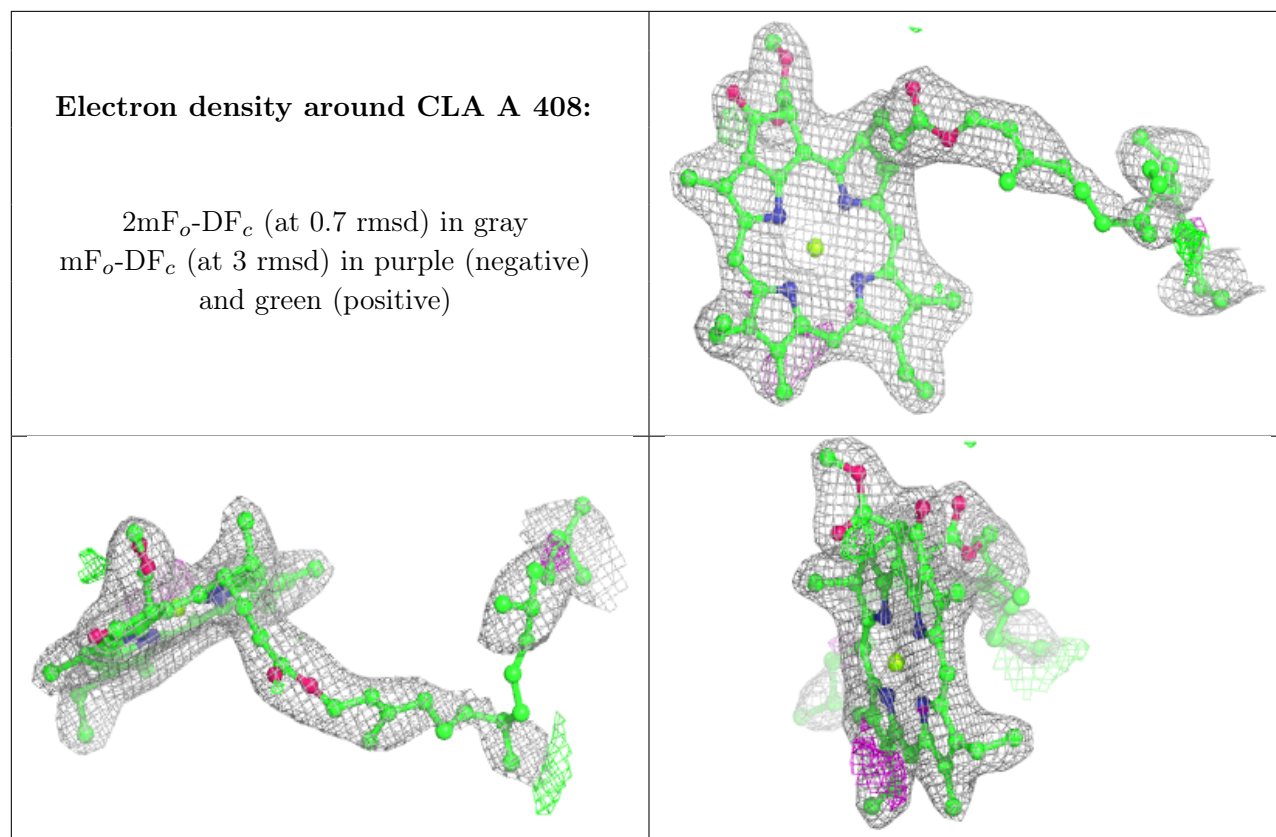
Electron density around CLA c 509:

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

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

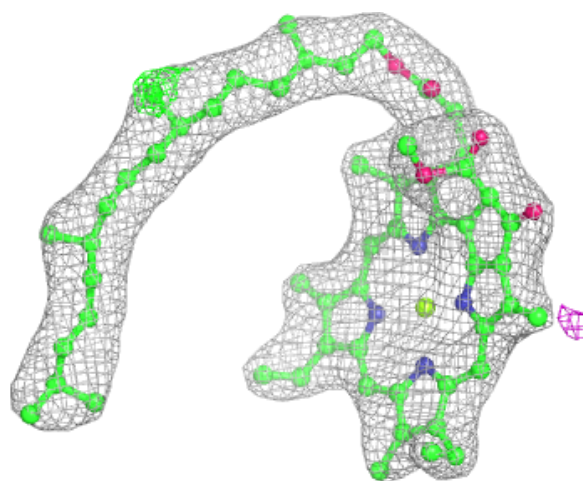
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



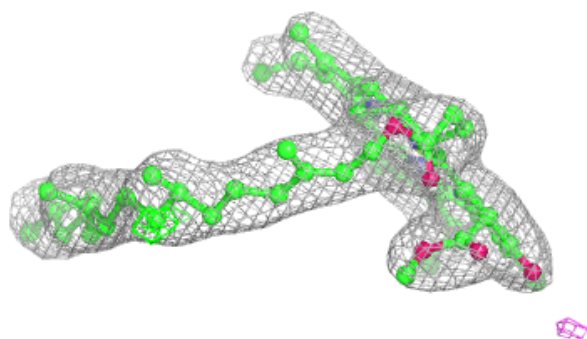


Electron density around CLA C 508:

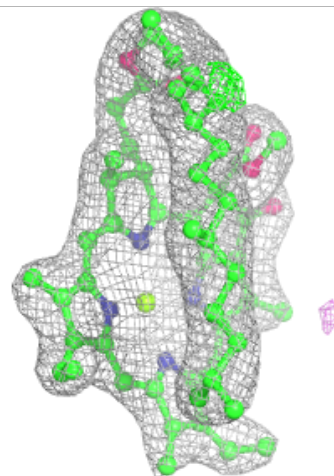
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



A



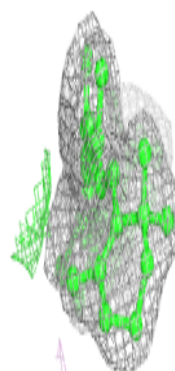
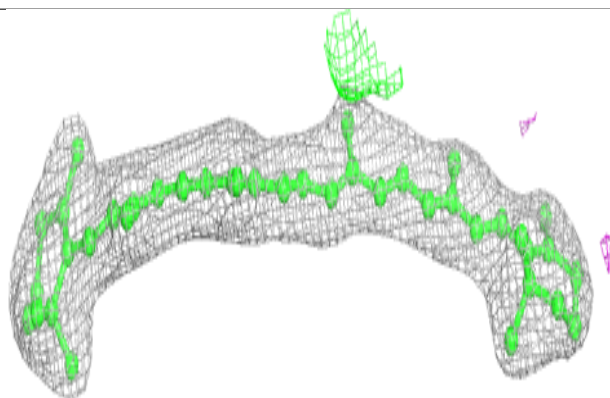
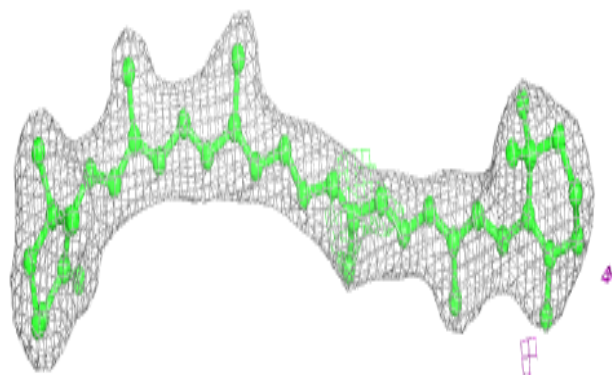
A



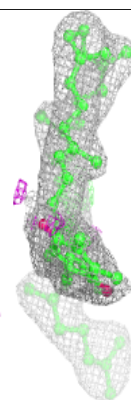
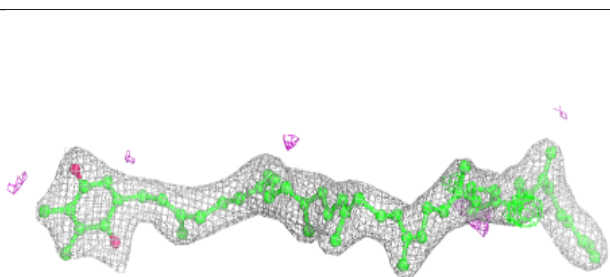
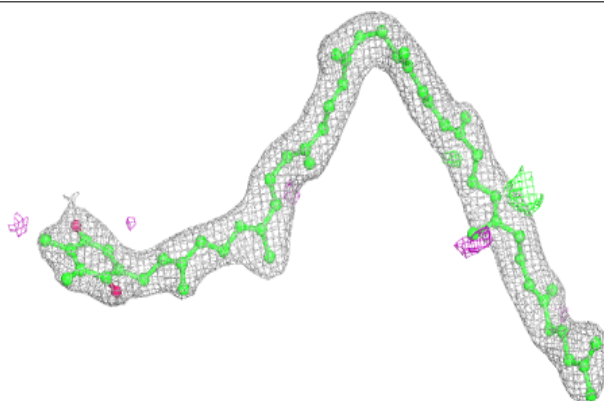
A

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)

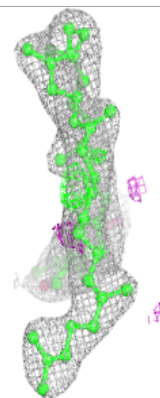
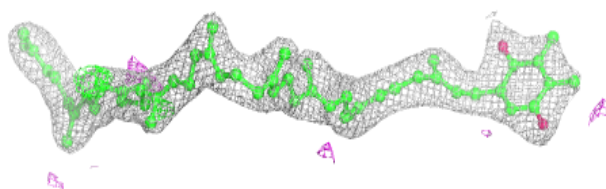
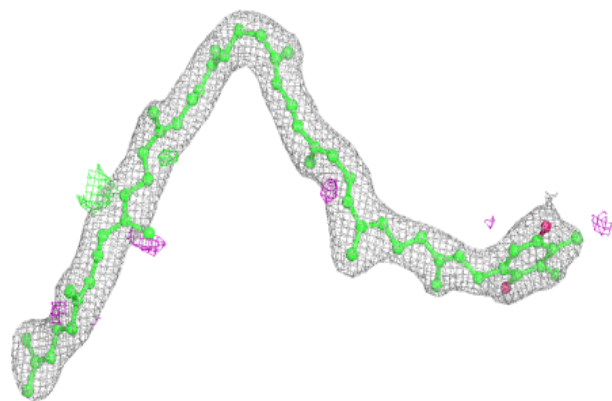
**Electron density around PL9 d 405 (A):**

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



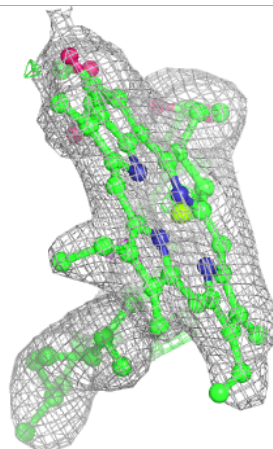
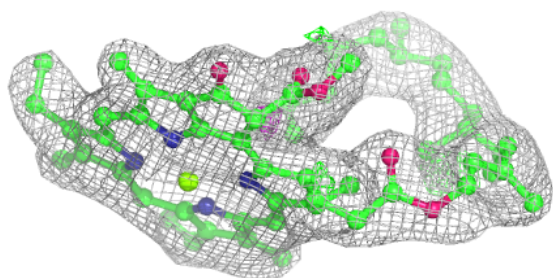
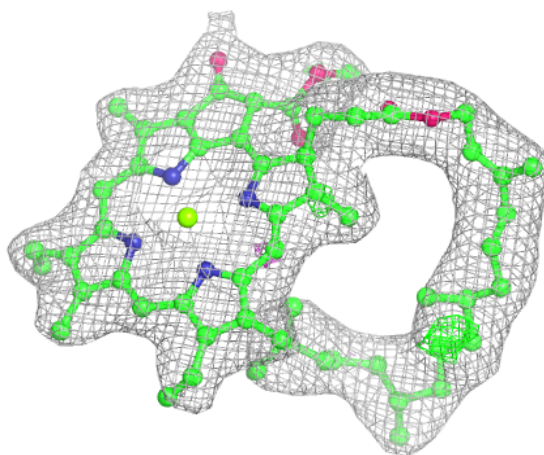
Electron density around PL9 d 405 (B):

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



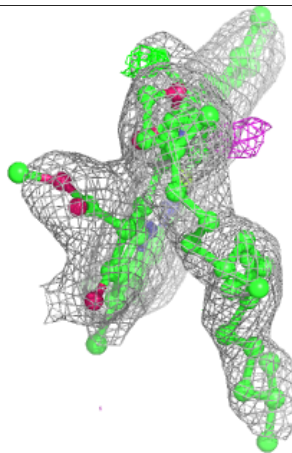
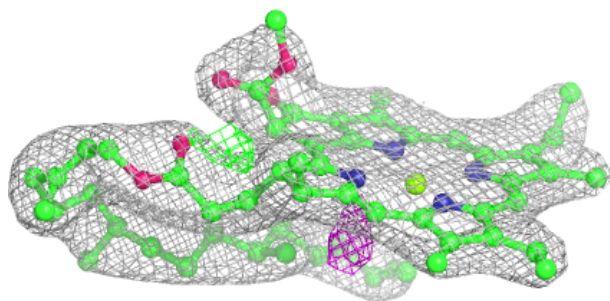
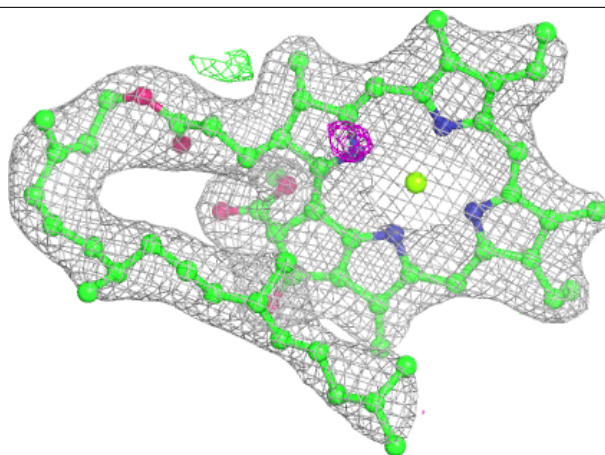
Electron density around CLA b 615:

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

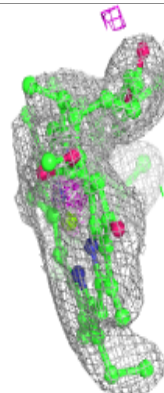
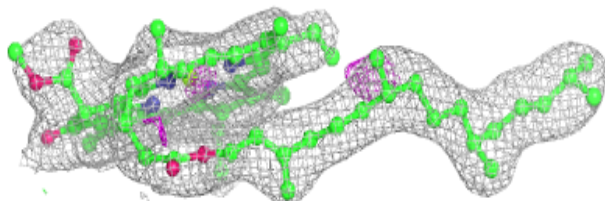
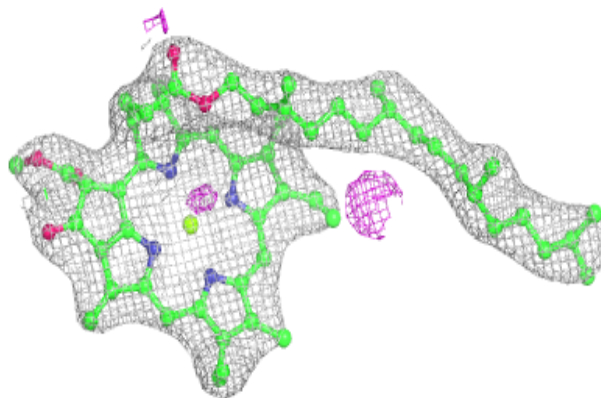


Electron density around CLA C 510:

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

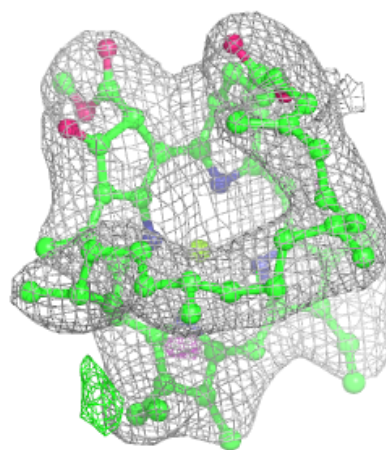
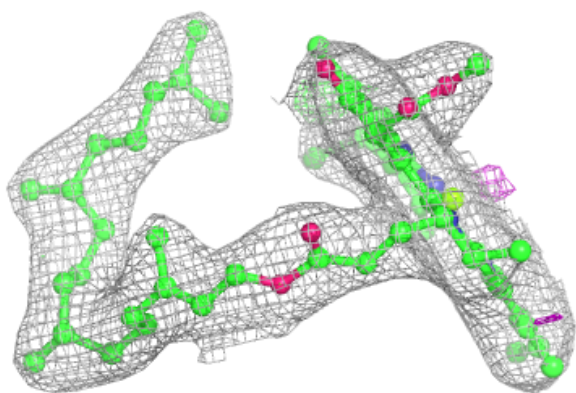
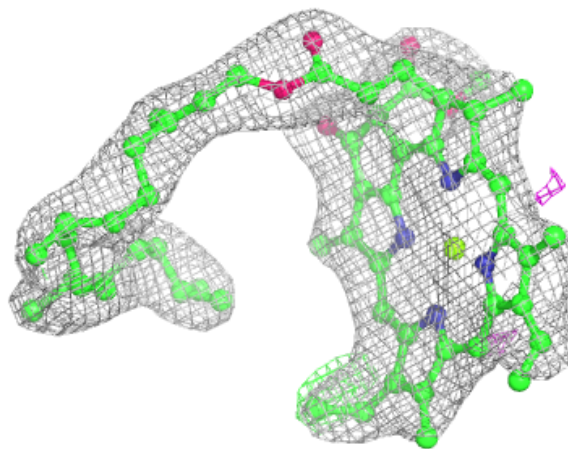
**Electron density around CLA c 502:**

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



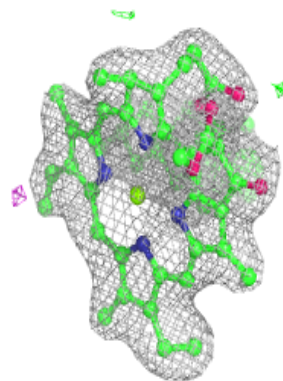
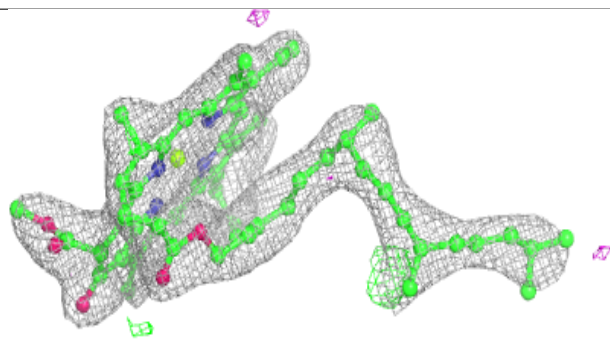
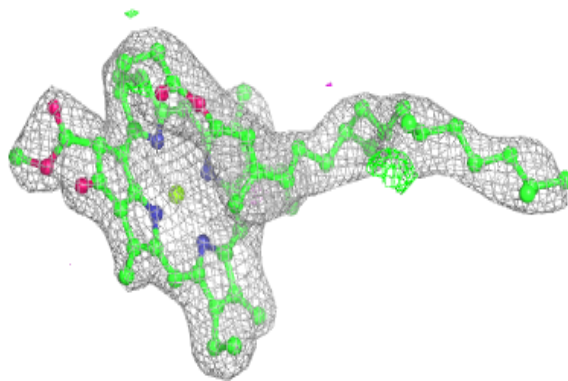
Electron density around CLA c 504:

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



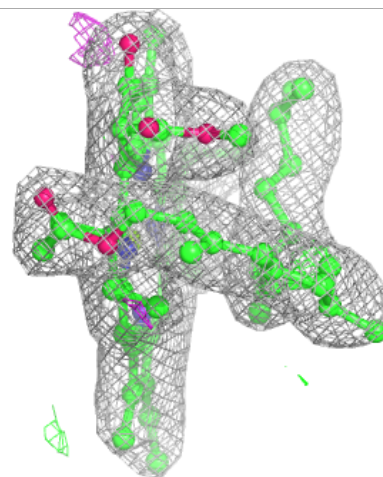
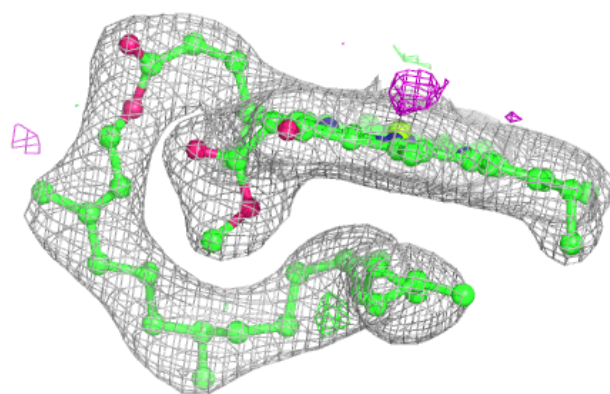
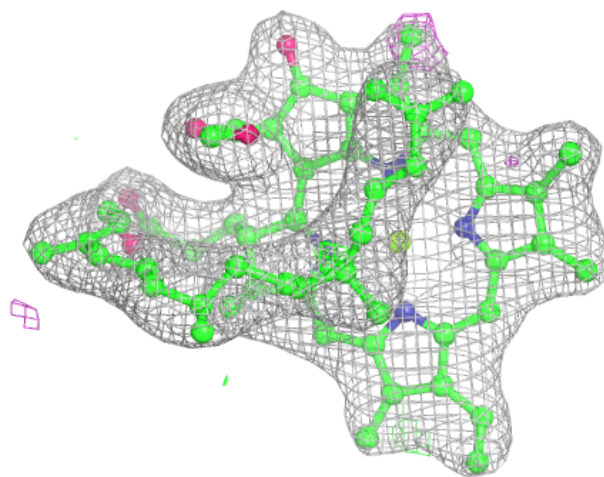
Electron density around CLA c 506:

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



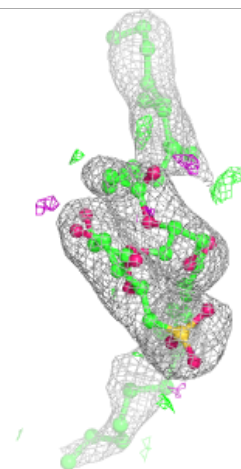
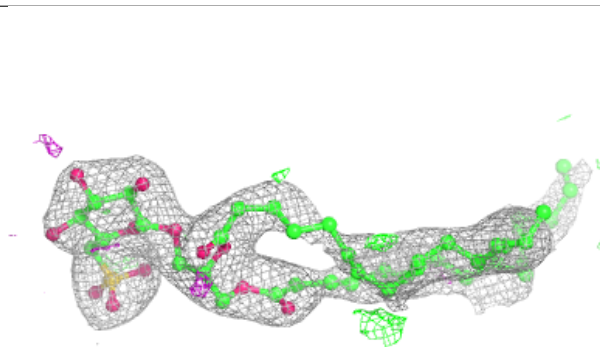
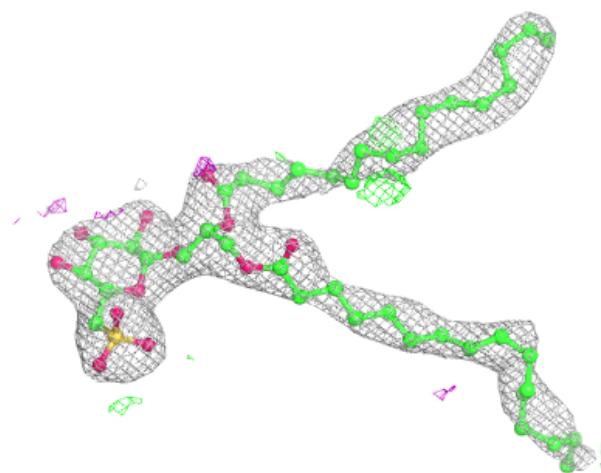
Electron density around CLA C 511:

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



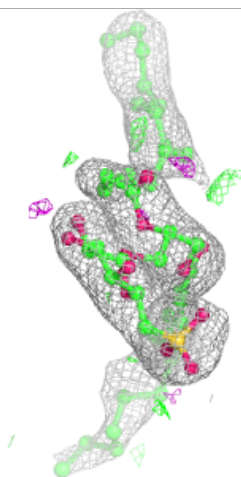
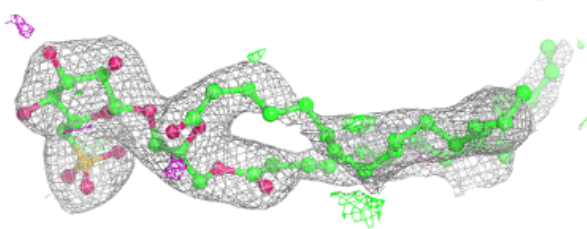
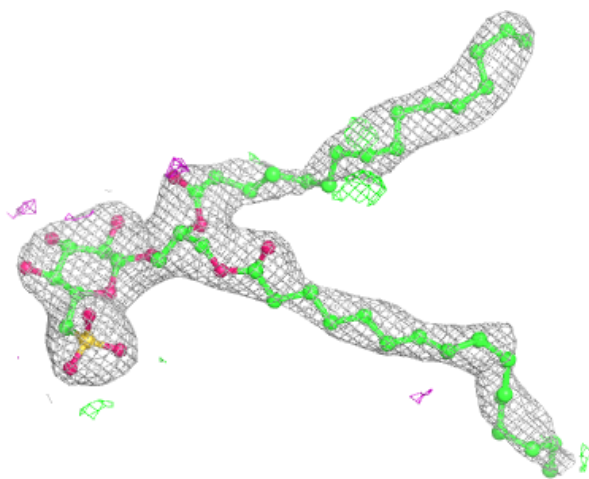
Electron density around SQD a 411 (A):

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



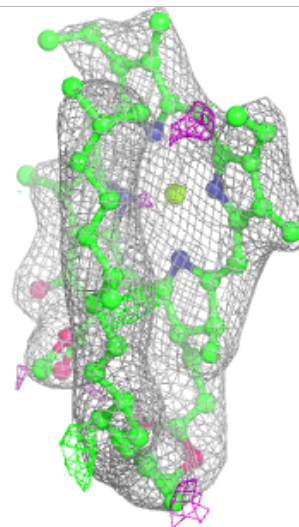
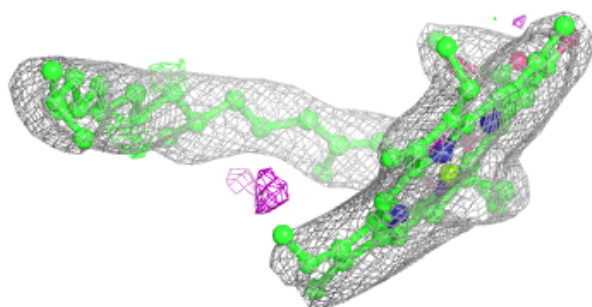
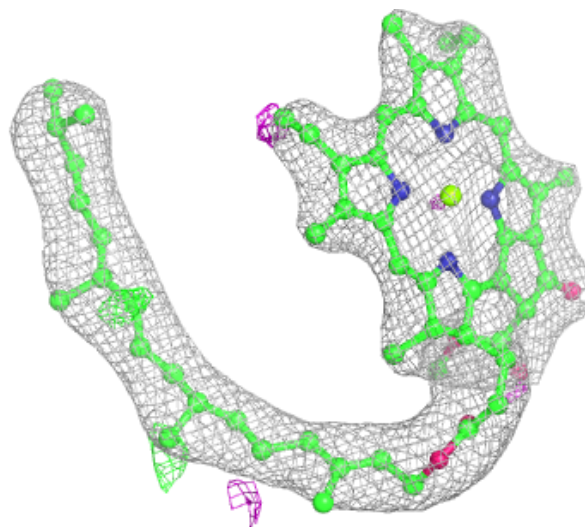
Electron density around SQD a 411 (B):

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



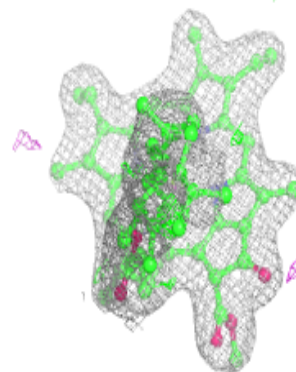
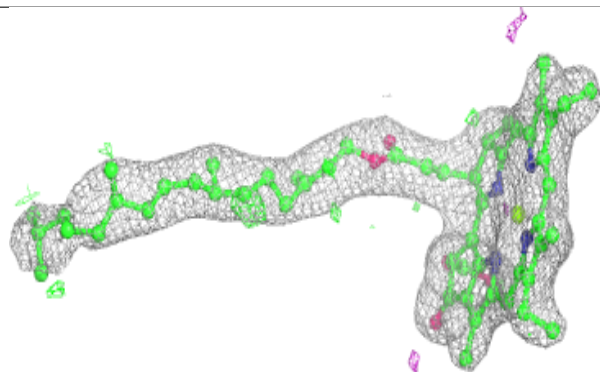
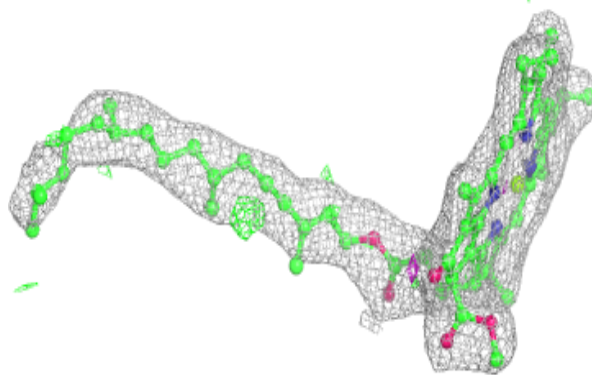
Electron density around CLA c 508:

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

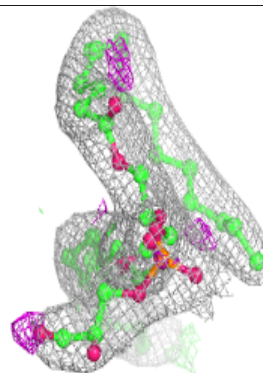
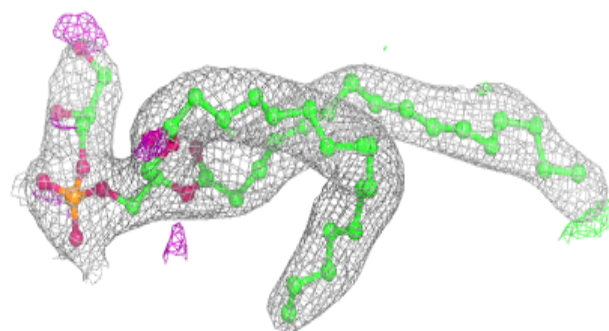
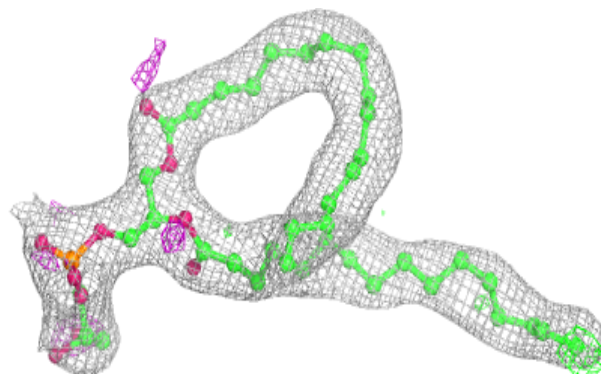


Electron density around CLA b 604:

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

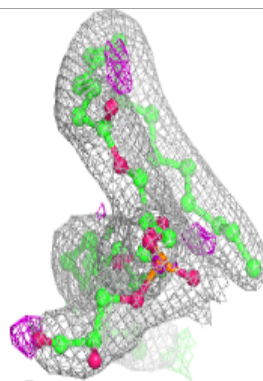
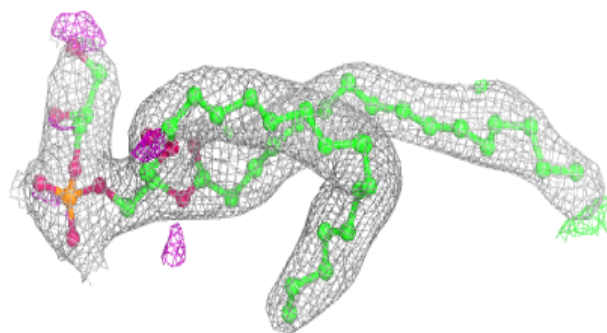
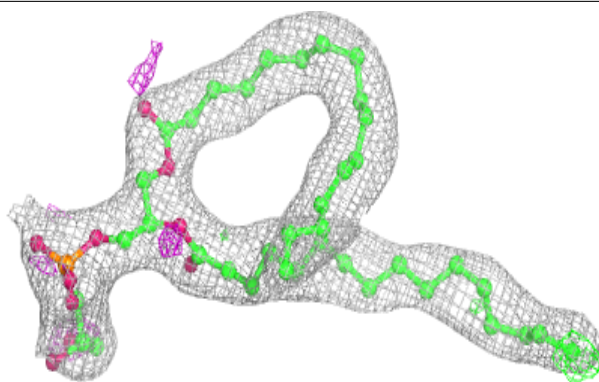
**Electron density around LHG A 418 (A):**

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

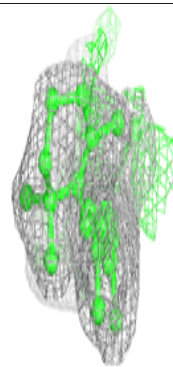
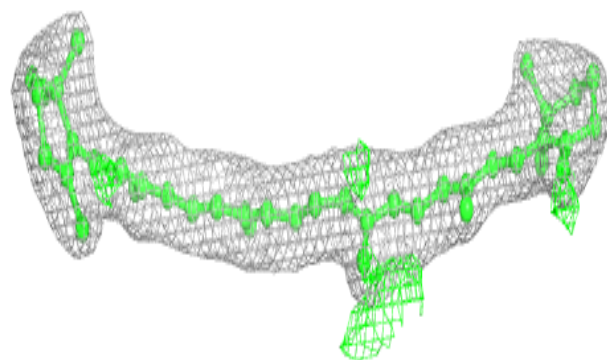
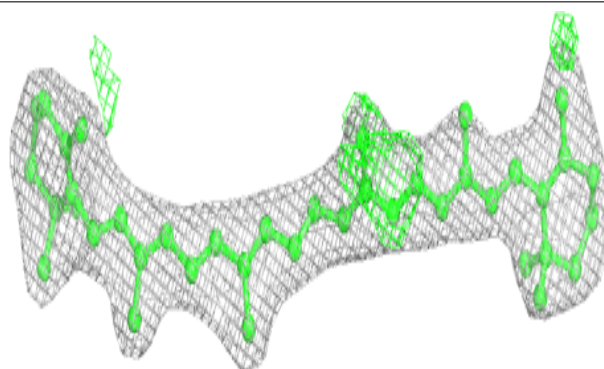


Electron density around LHG A 418 (B):

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

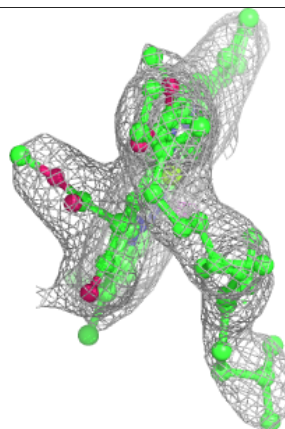
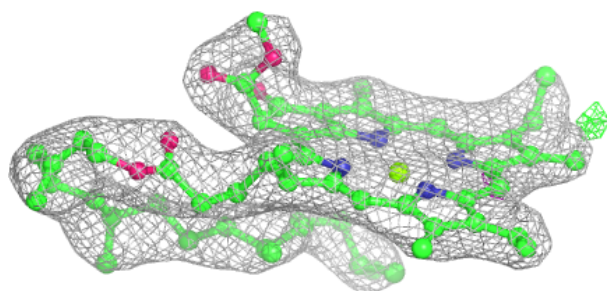
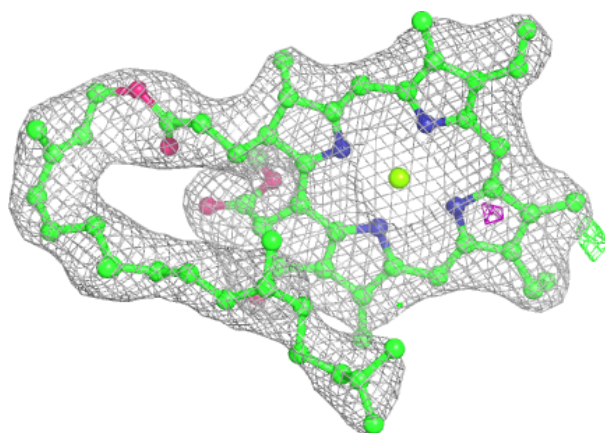
**Electron density around BCR T 101:**

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

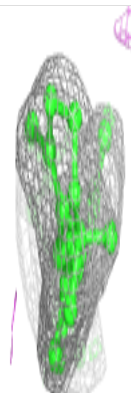
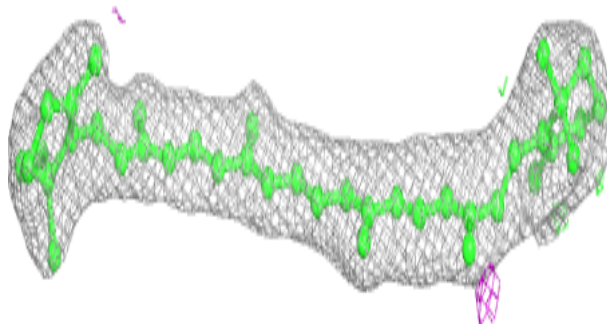
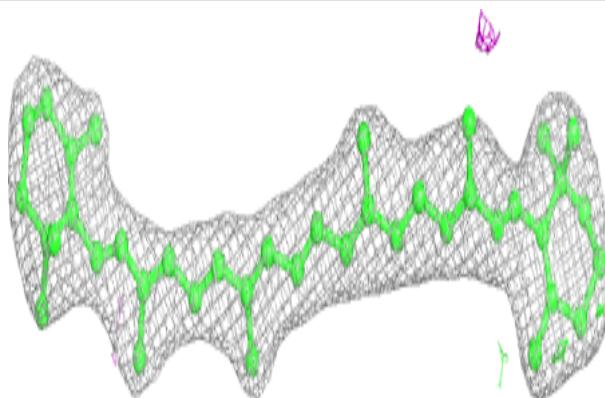


Electron density around CLA c 510:

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

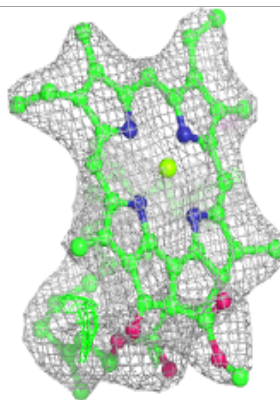
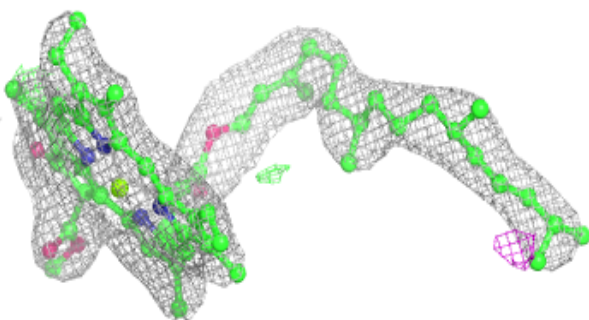
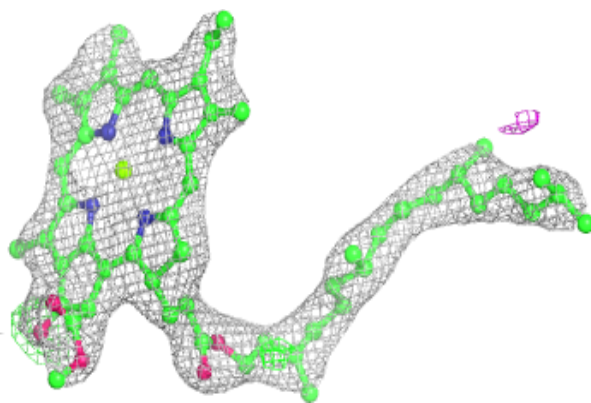
**Electron density around BCR b 619:**

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

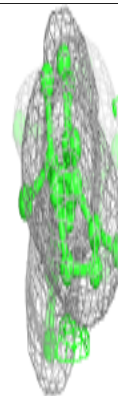
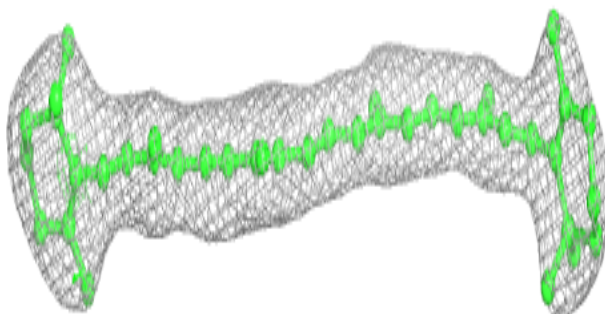
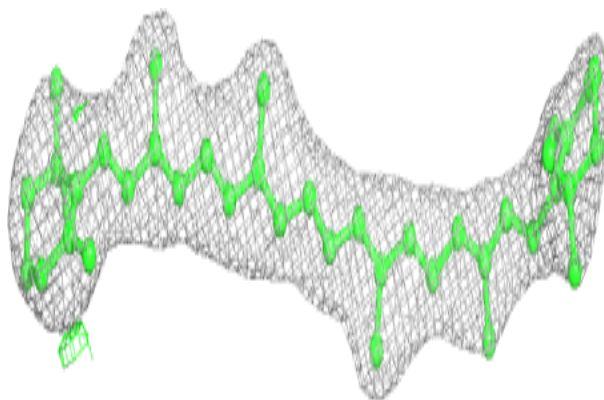


Electron density around CLA c 512:

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

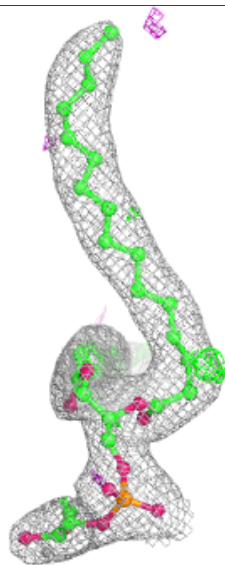
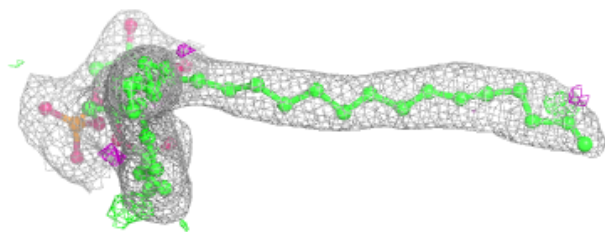
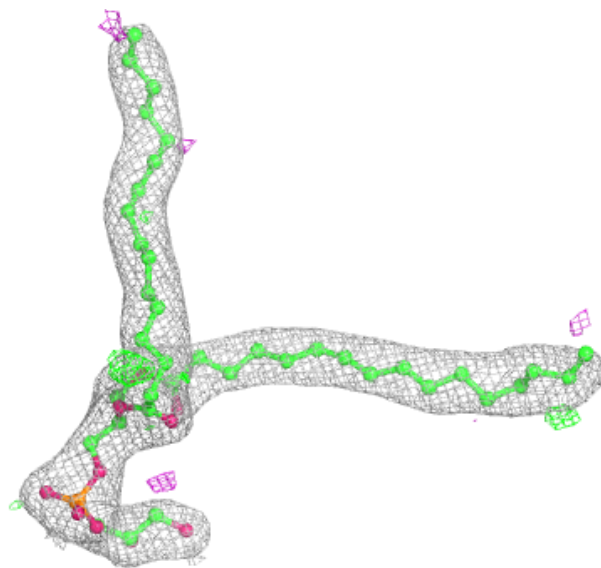
**Electron density around BCR c 516:**

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



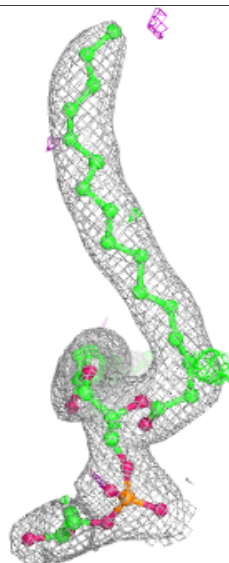
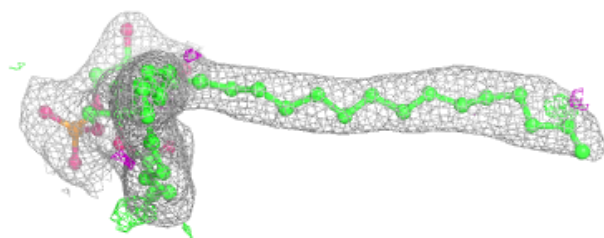
Electron density around LHG b 629 (A):

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



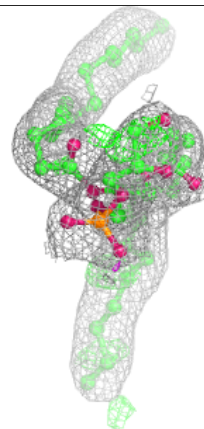
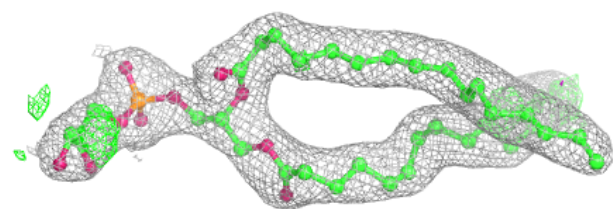
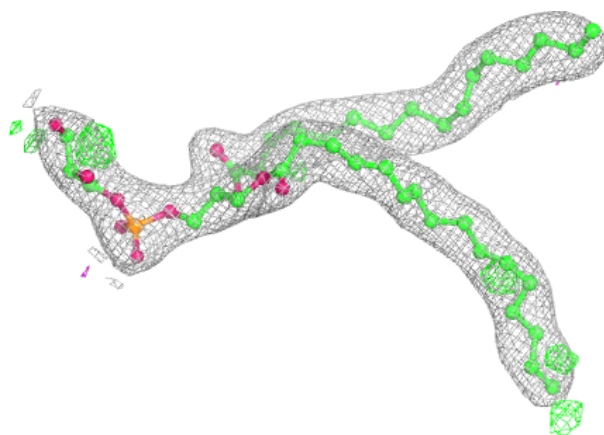
Electron density around LHG b 629 (B):

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

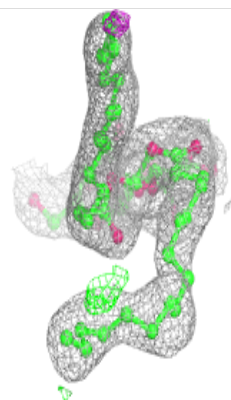
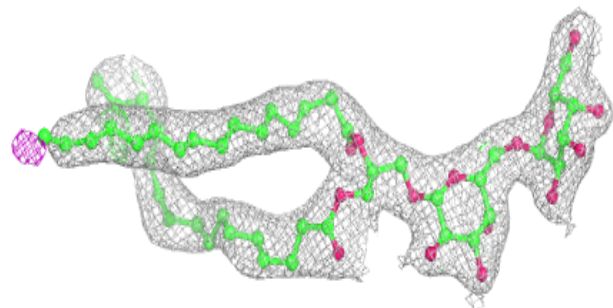
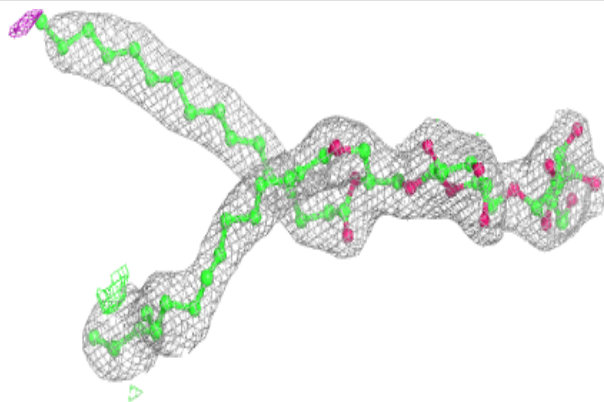


Electron density around LHG d 406 (A):

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

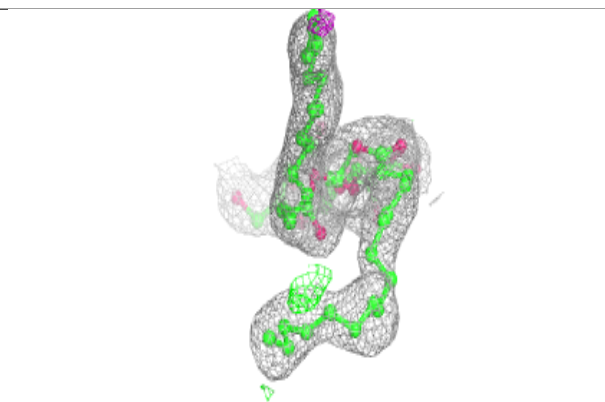
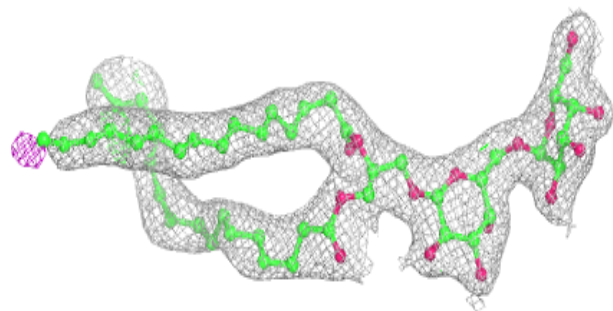
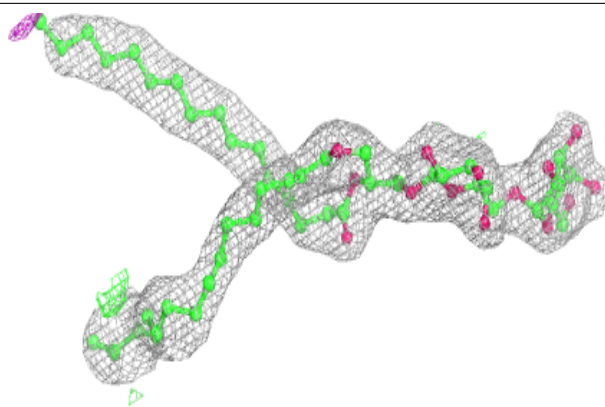
**Electron density around DGD c 517 (A):**

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

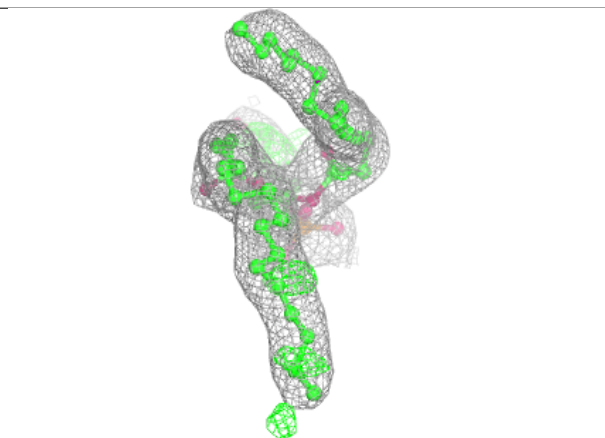
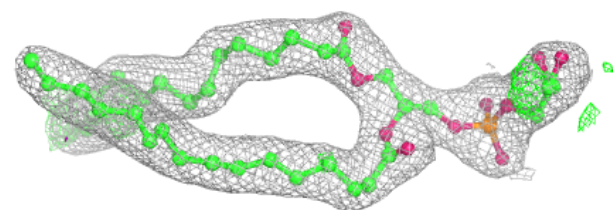
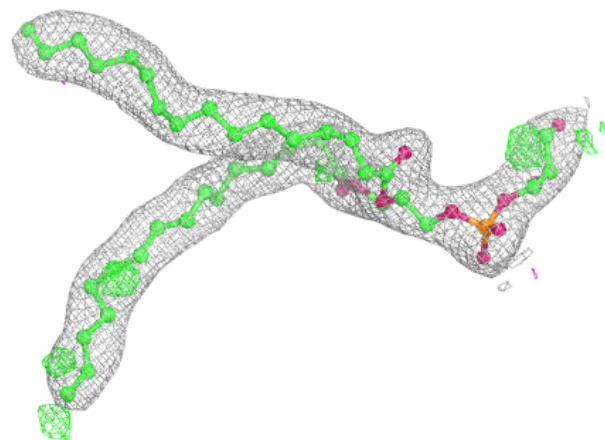


Electron density around DGD c 517 (B):

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

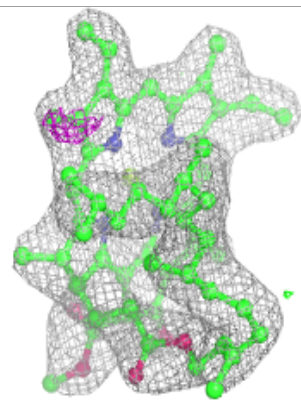
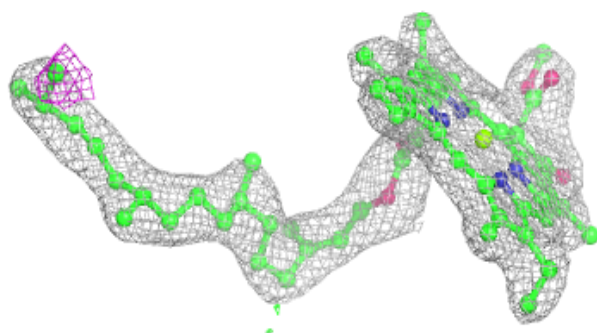
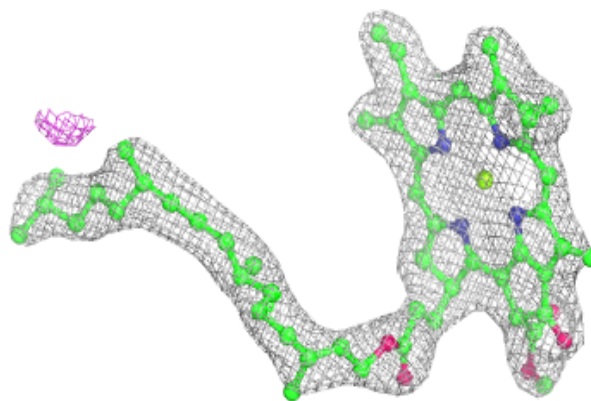
**Electron density around LHG d 406 (B):**

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

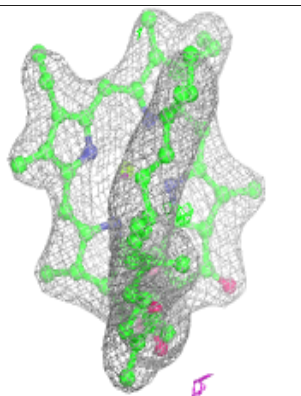
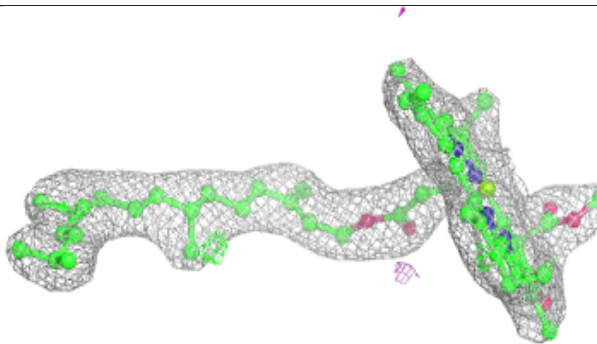
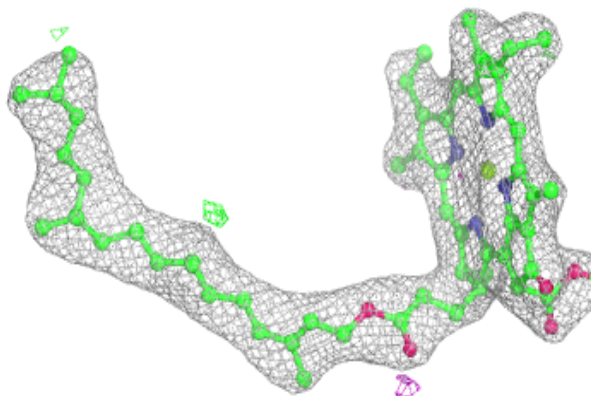


Electron density around CLA C 512:

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

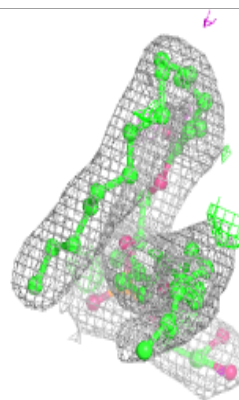
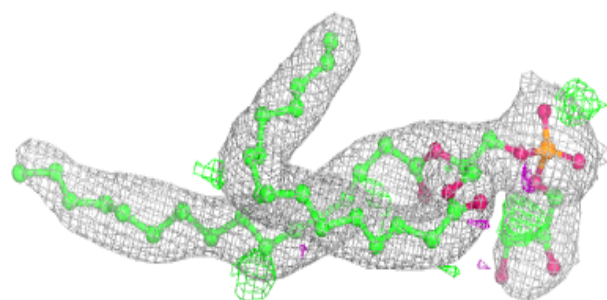
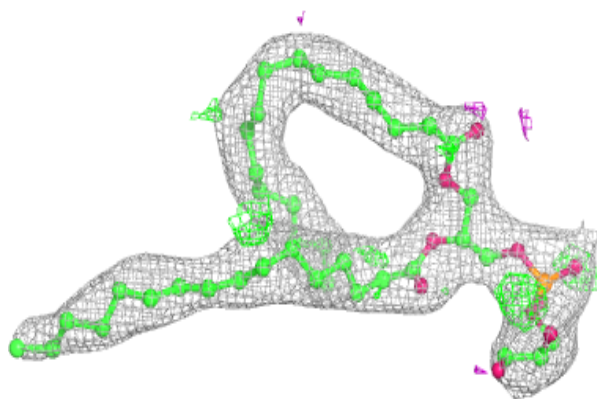
**Electron density around CLA b 609:**

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

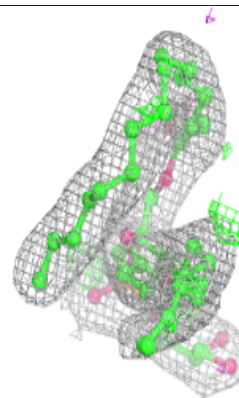
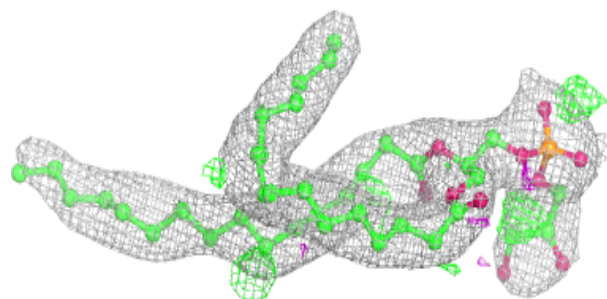
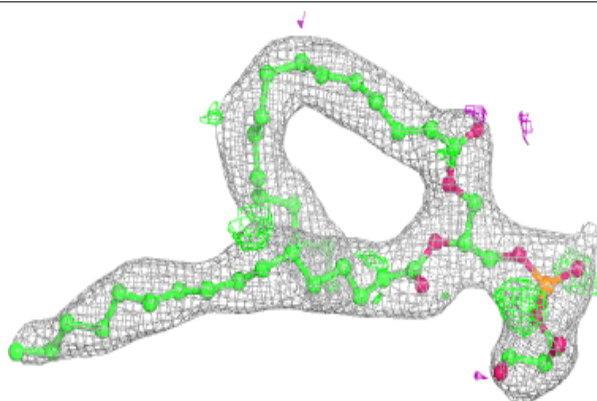


Electron density around LHG d 413 (A):

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

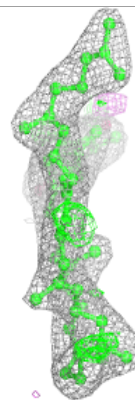
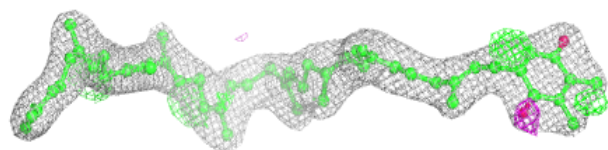
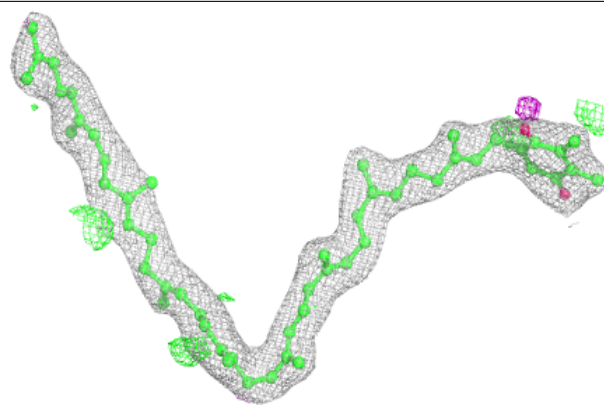
**Electron density around LHG d 413 (B):**

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

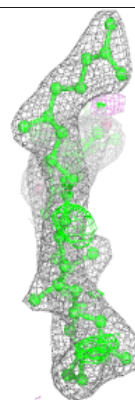
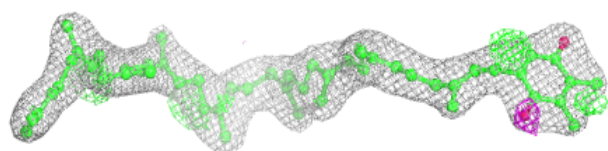
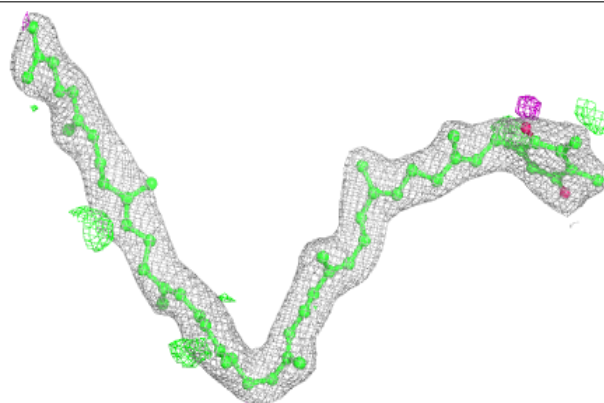


Electron density around PL9 D 407 (A):

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

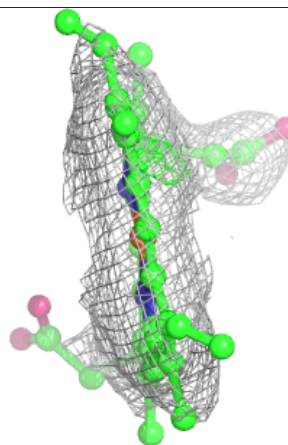
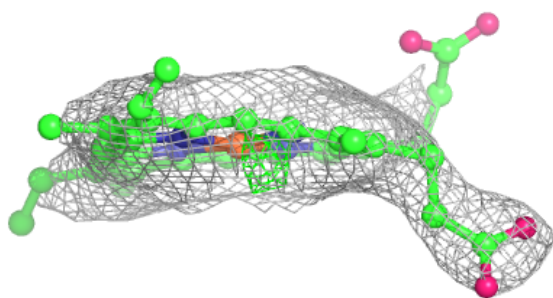
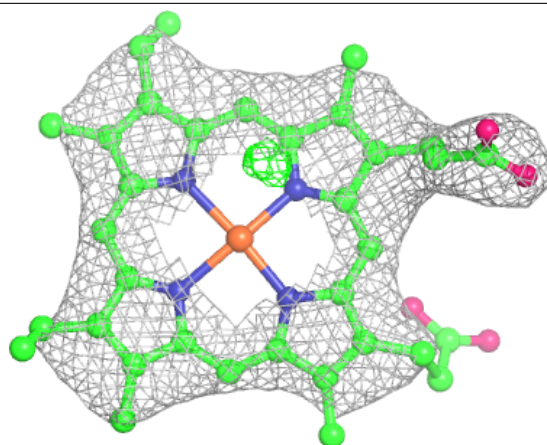
**Electron density around PL9 D 407 (B):**

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



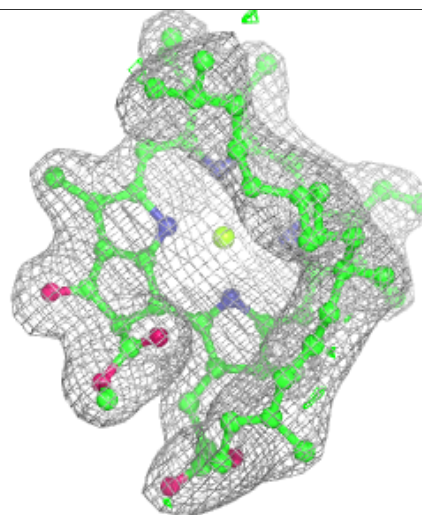
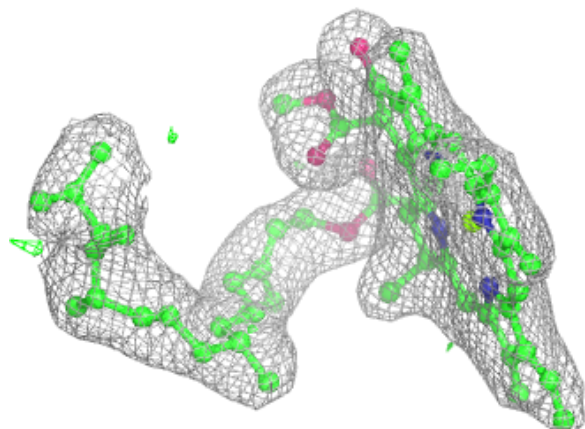
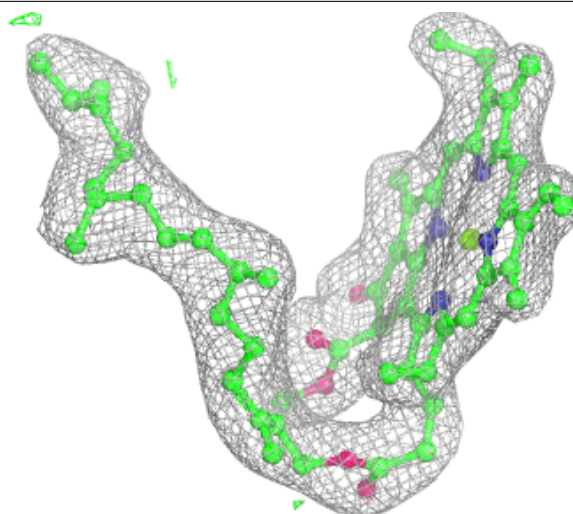
Electron density around HEM f 101:

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



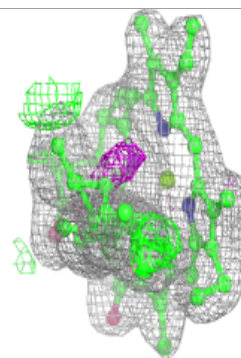
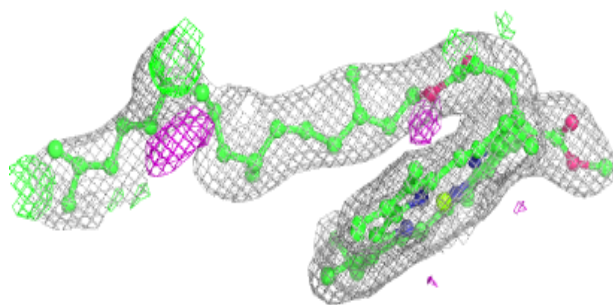
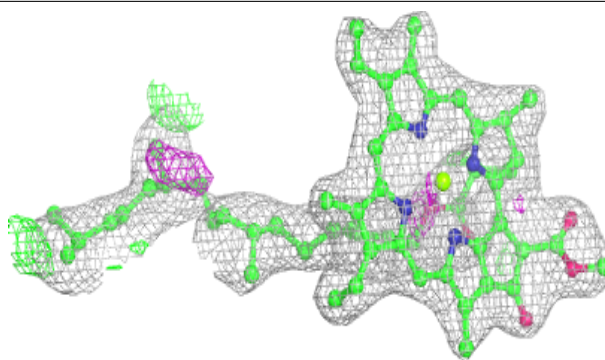
Electron density around CLA B 613:

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

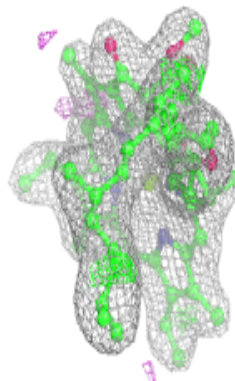
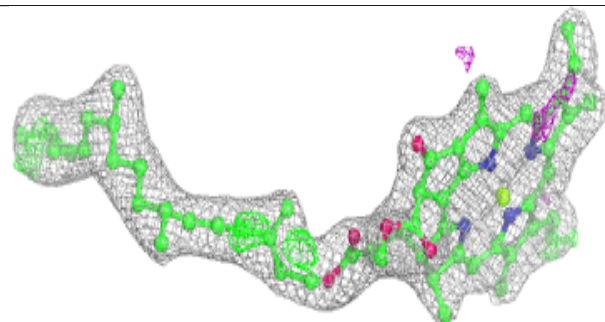
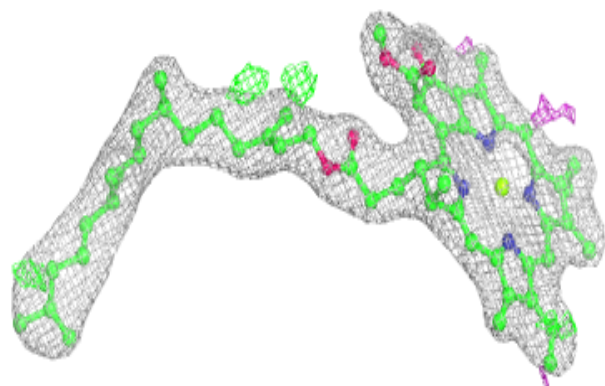


Electron density around CLA B 614:

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

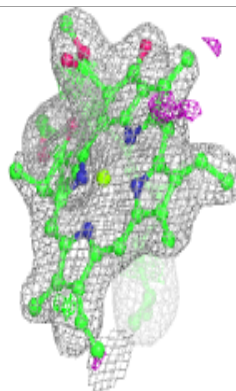
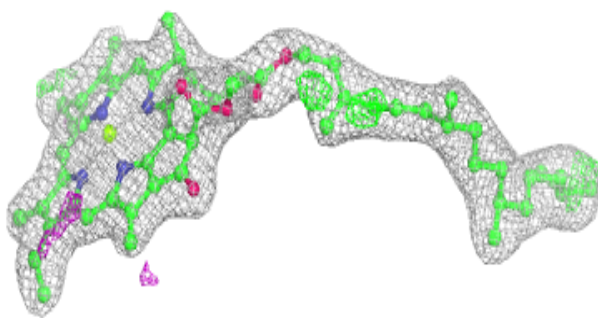
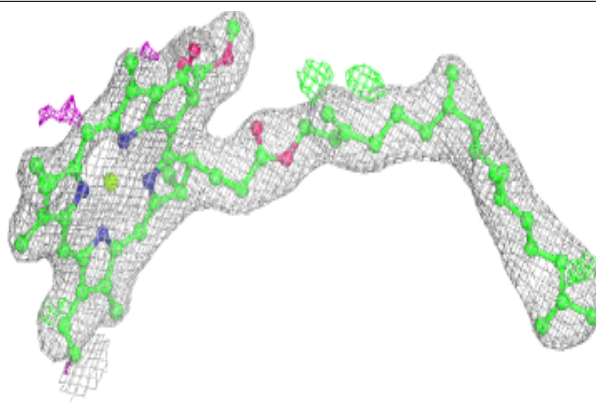
**Electron density around CLA a 405 (A):**

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



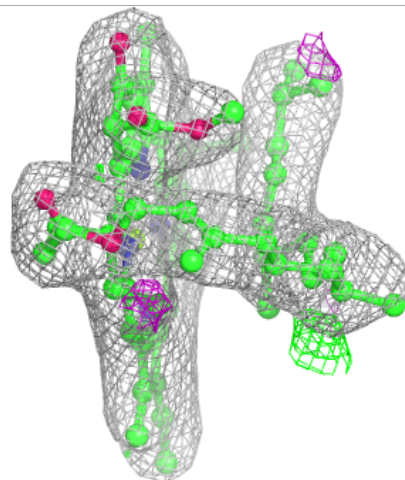
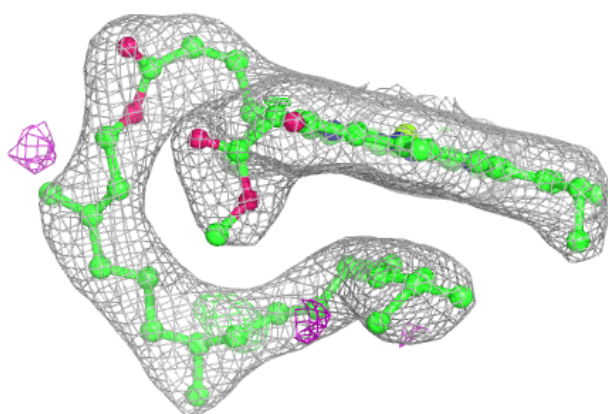
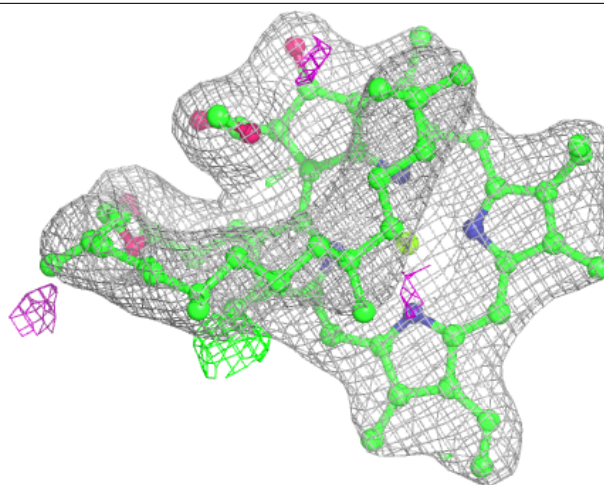
Electron density around CLA a 405 (B):

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



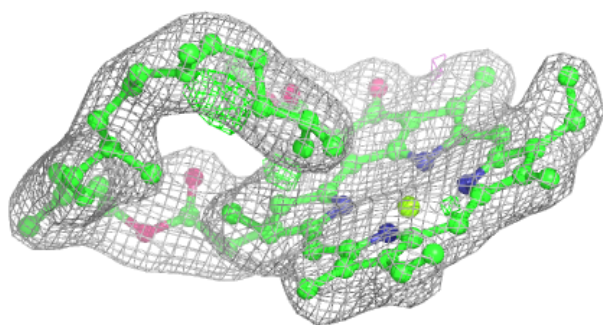
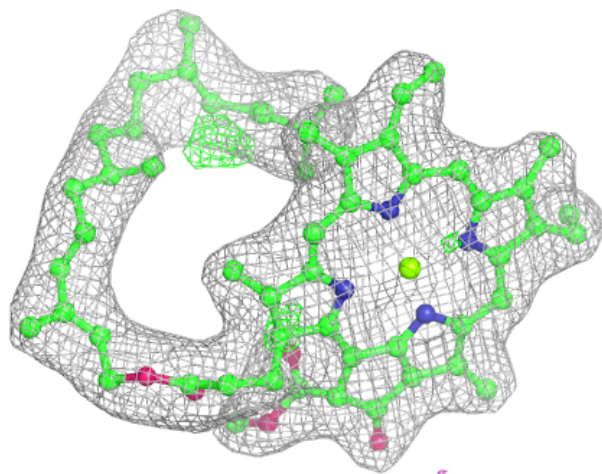
Electron density around CLA c 511:

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



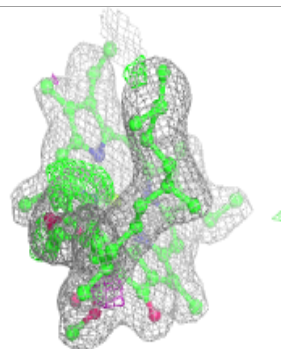
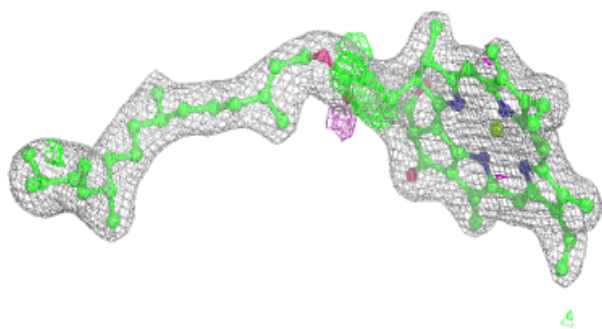
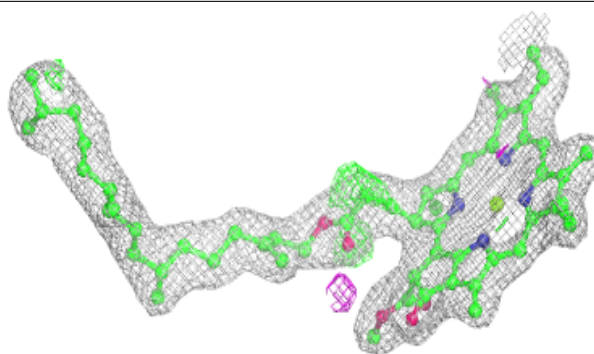
Electron density around CLA B 615:

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

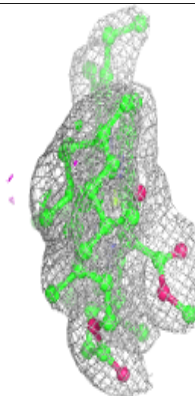
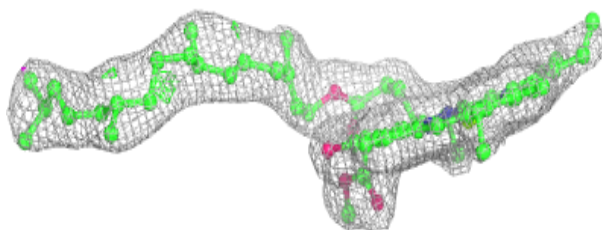
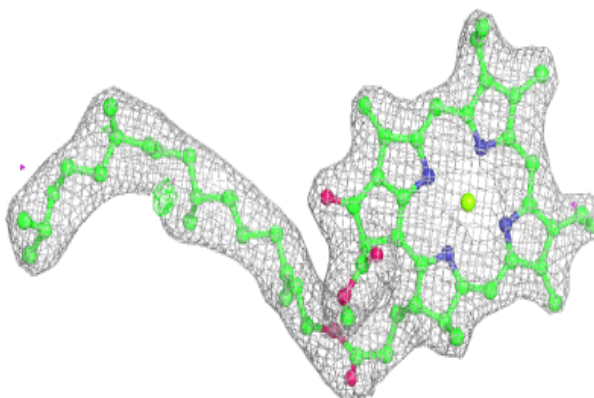


Electron density around CLA A 404 (B):

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

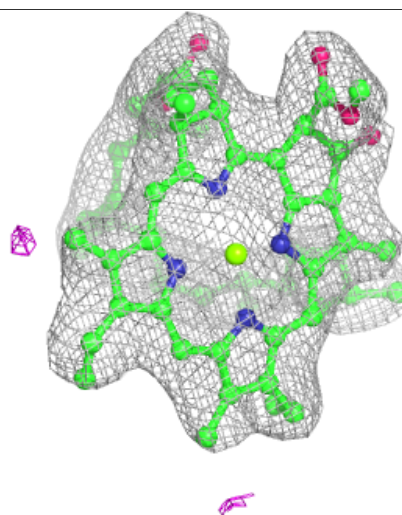
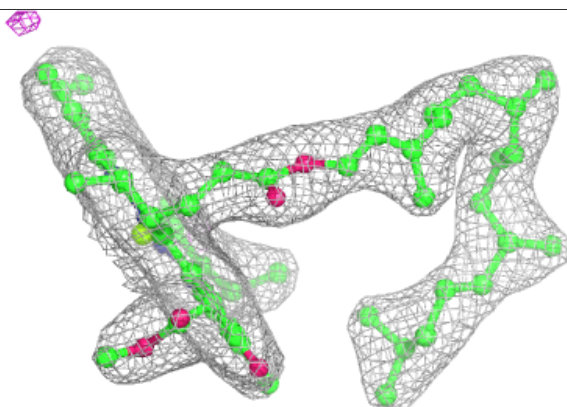
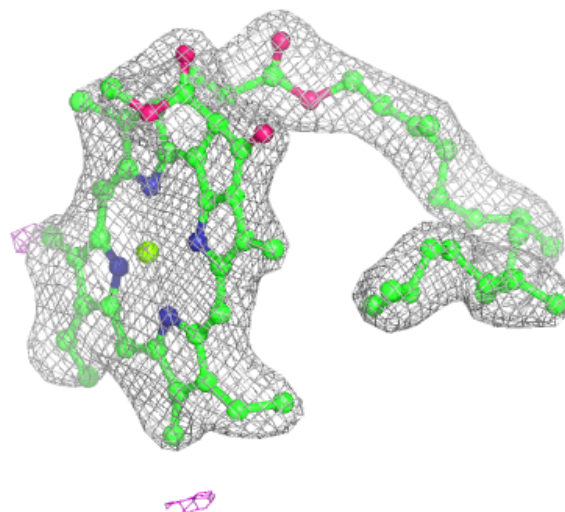
**Electron density around CLA B 602:**

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



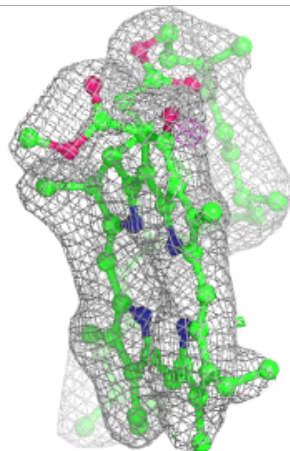
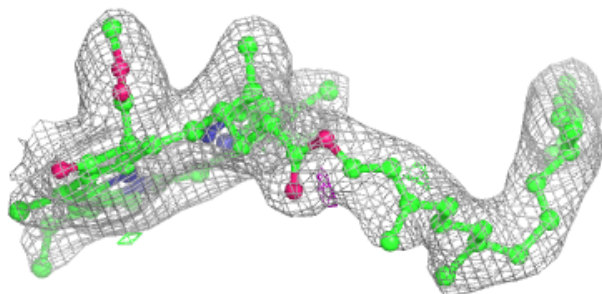
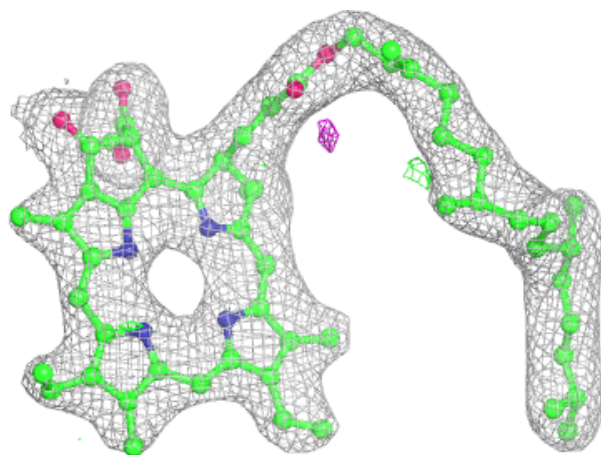
Electron density around CLA C 504:

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



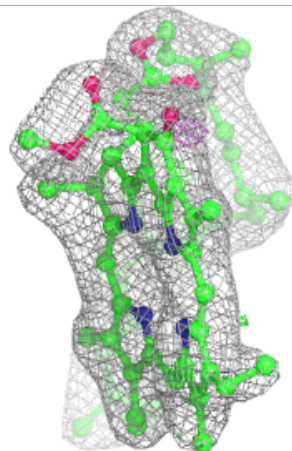
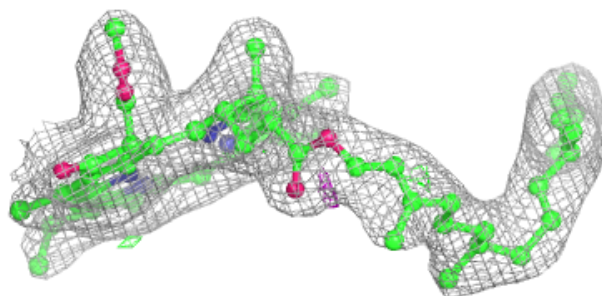
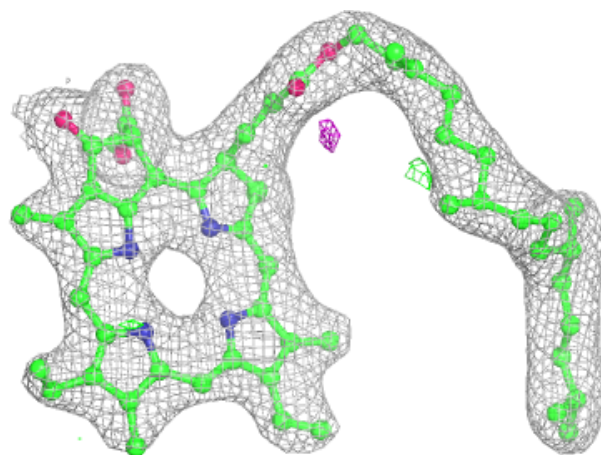
Electron density around PHO a 416 (A):

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



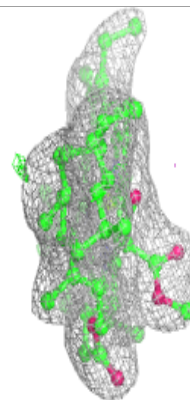
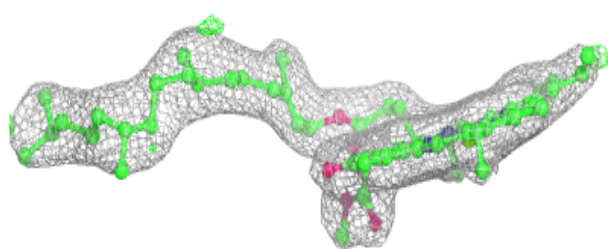
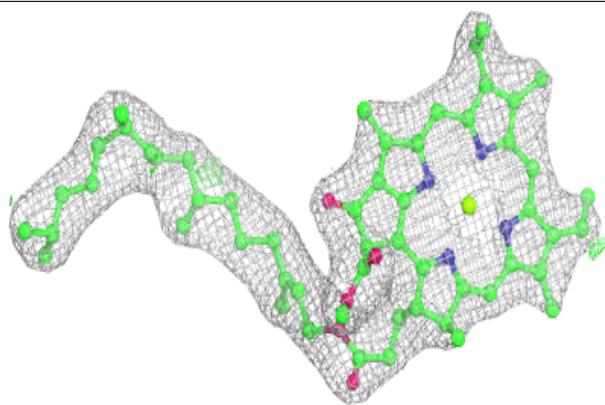
Electron density around PHO a 416 (B):

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

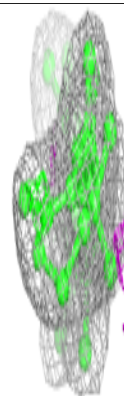
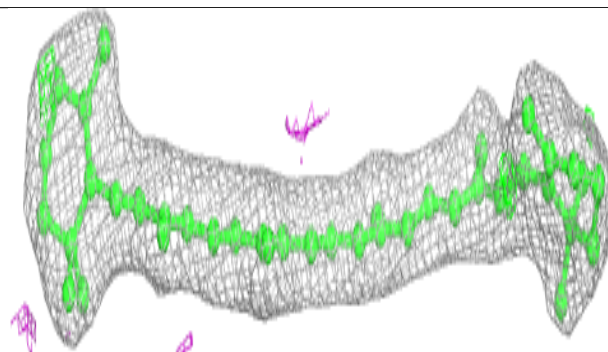
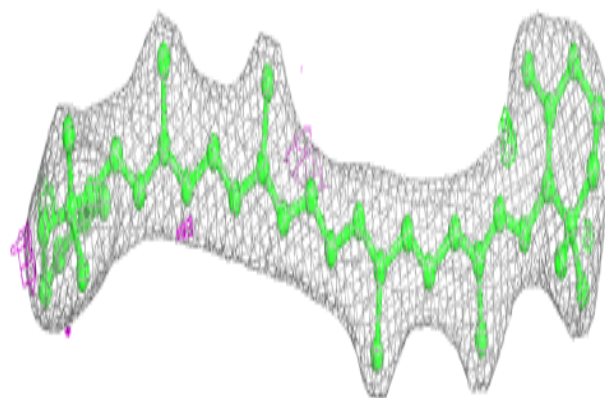


Electron density around CLA b 602:

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

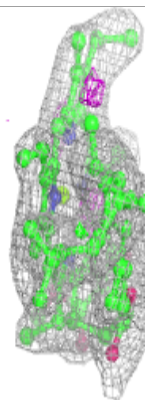
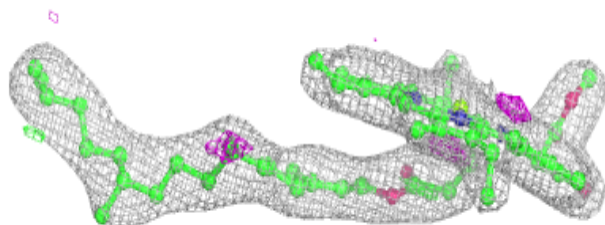
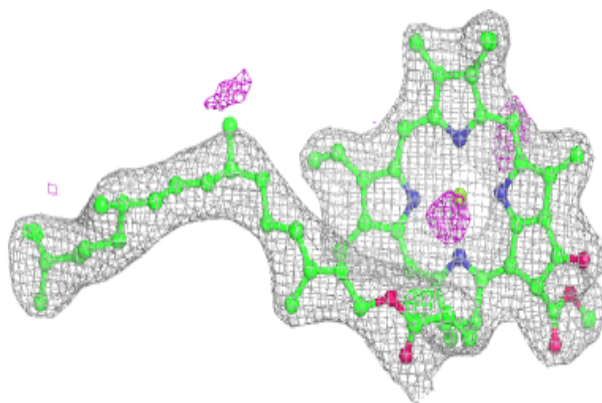
**Electron density around BCR B 617:**

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

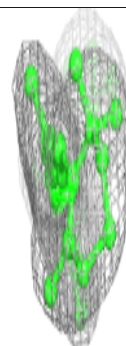
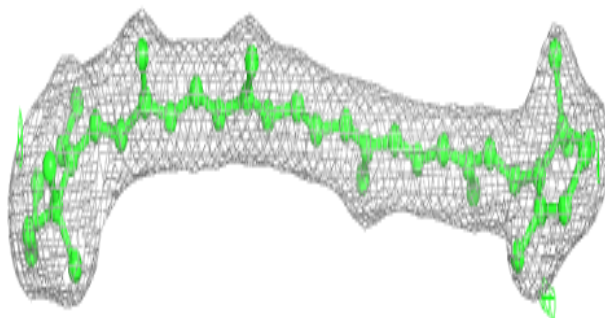
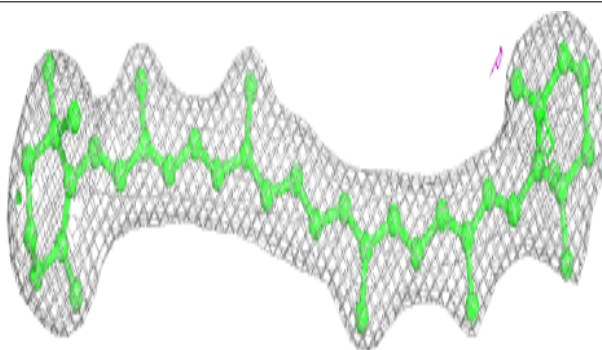


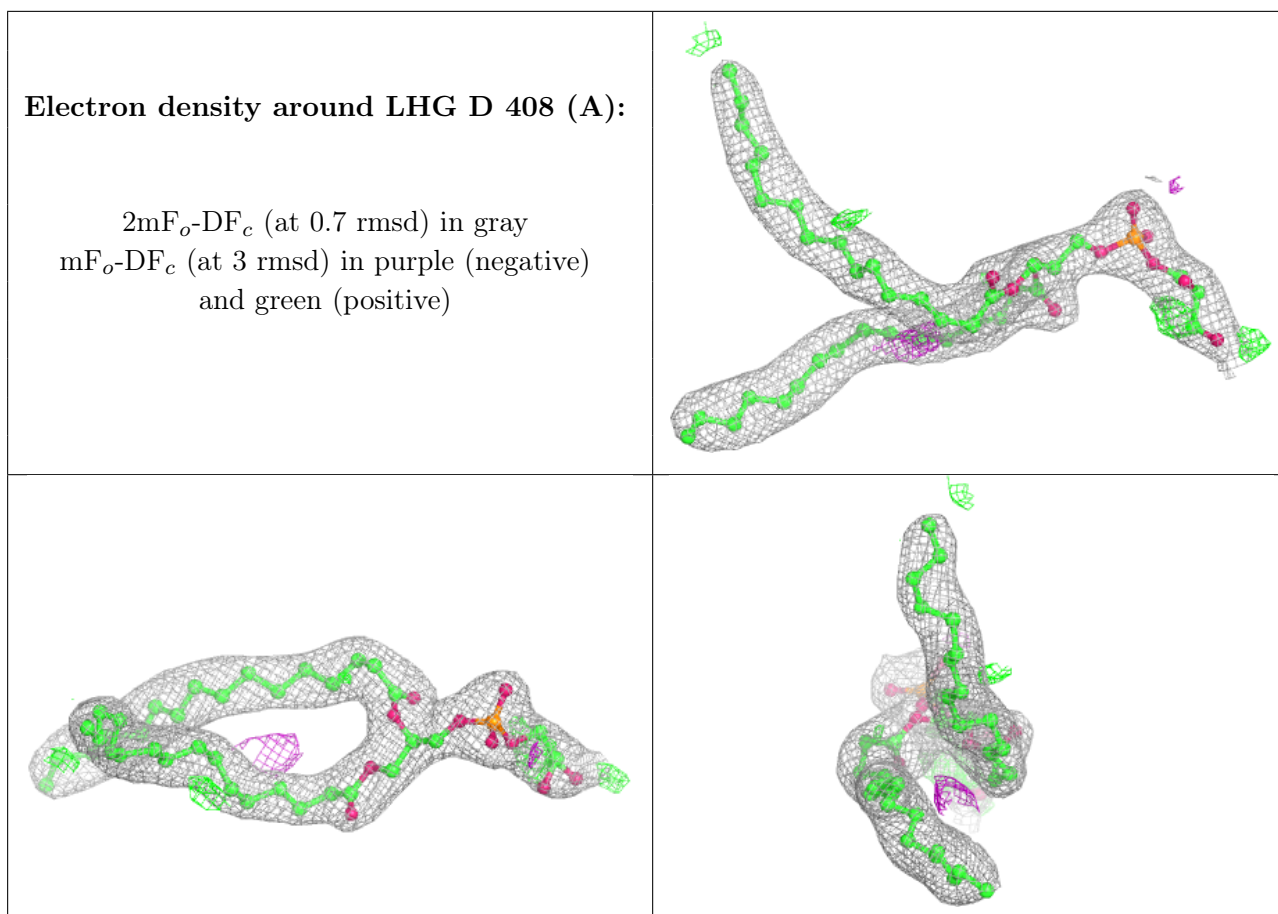
Electron density around CLA B 603:

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

**Electron density around BCR B 619:**

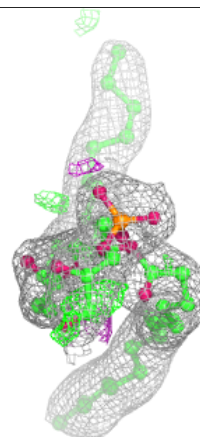
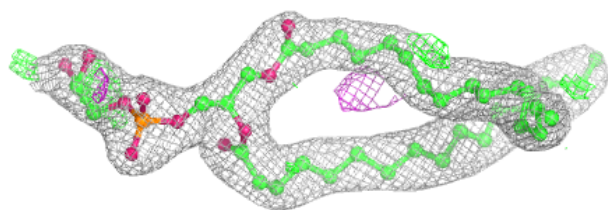
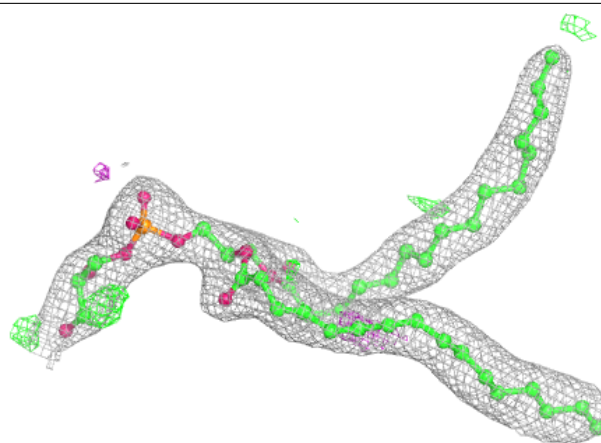
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



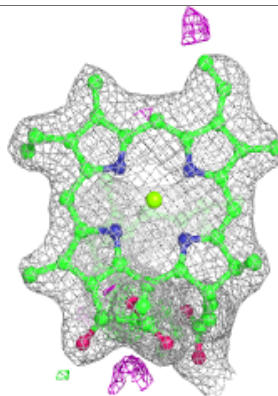
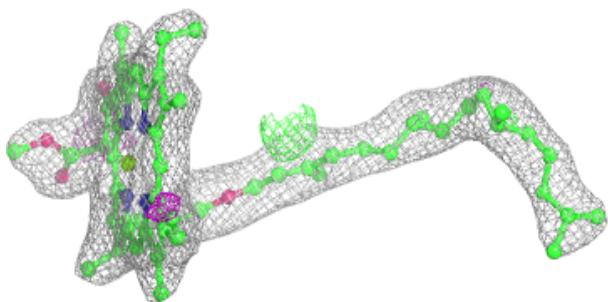
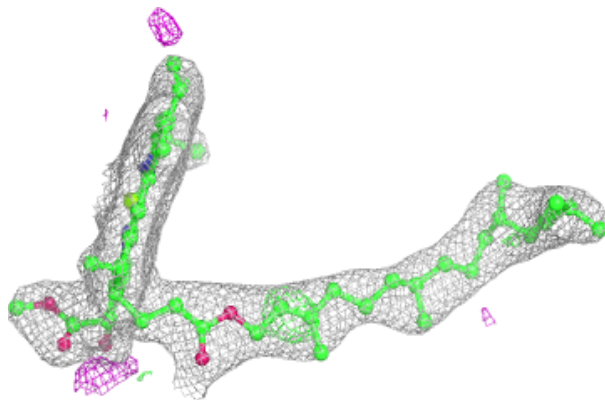


Electron density around LHG D 408 (B):

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

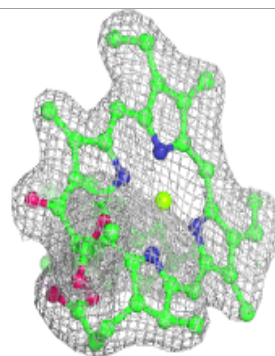
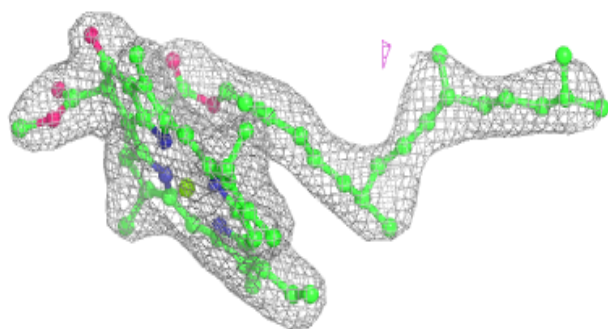
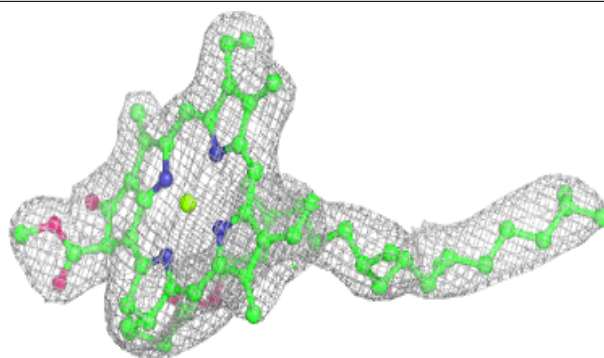
**Electron density around CLA b 605:**

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

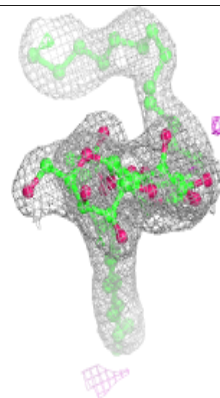
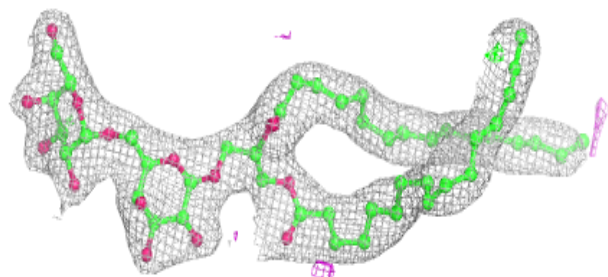
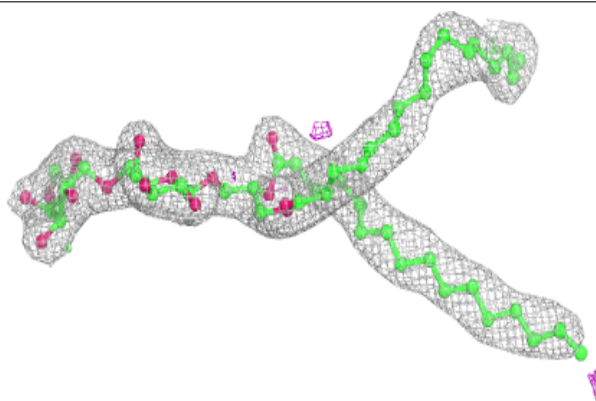


Electron density around CLA C 506:

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

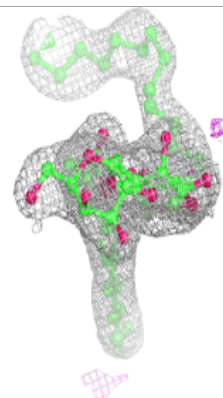
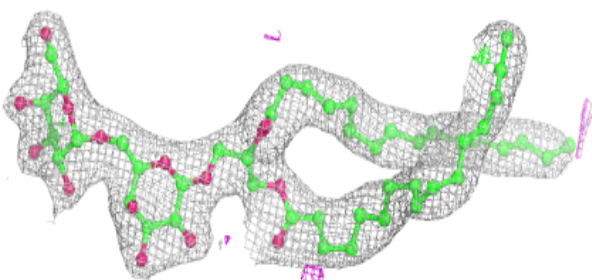
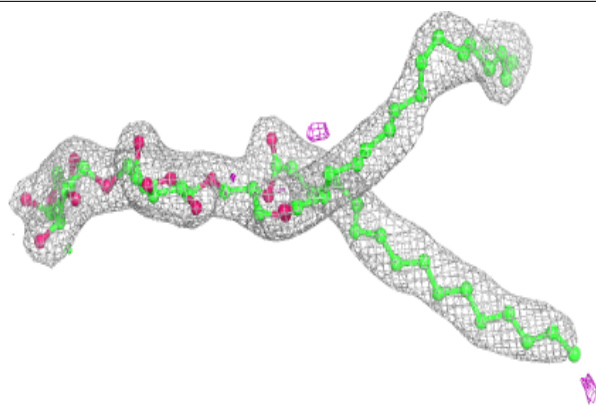
**Electron density around DGD C 517 (A):**

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

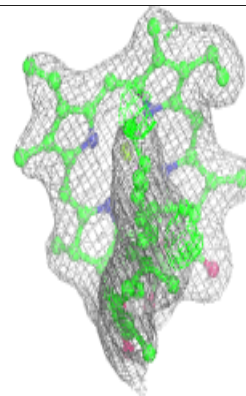
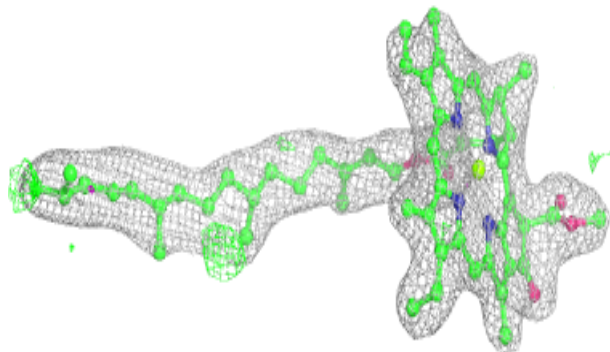
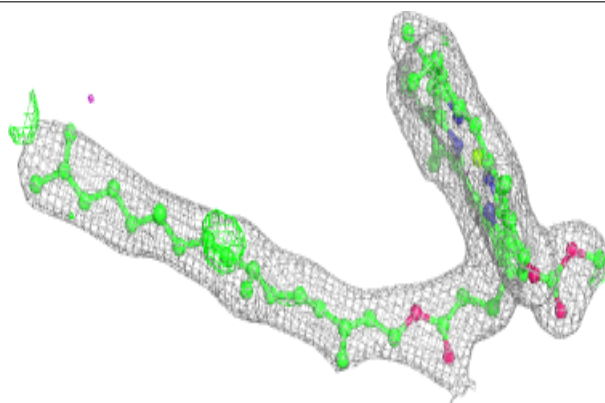


Electron density around DGD C 517 (B):

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

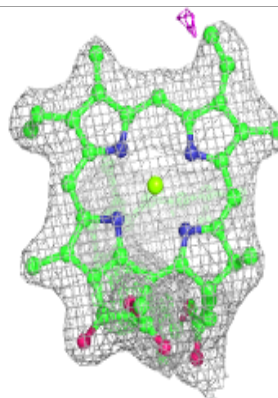
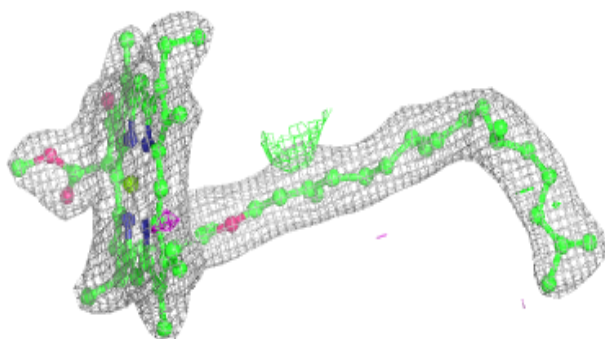
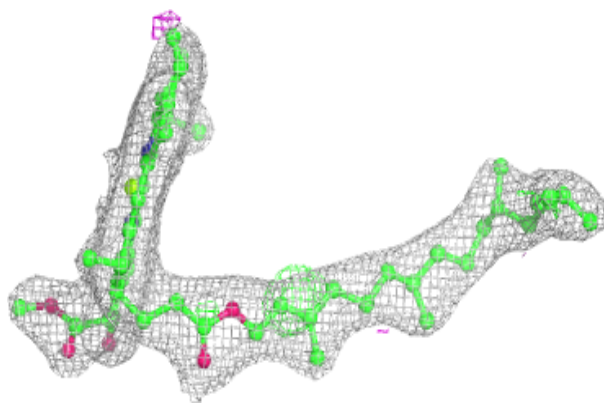
**Electron density around CLA b 607:**

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

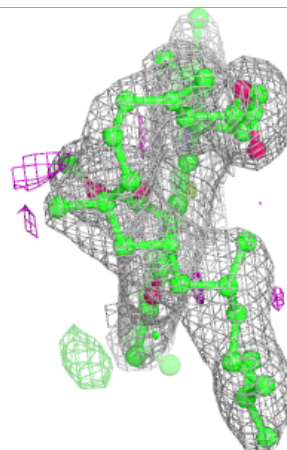
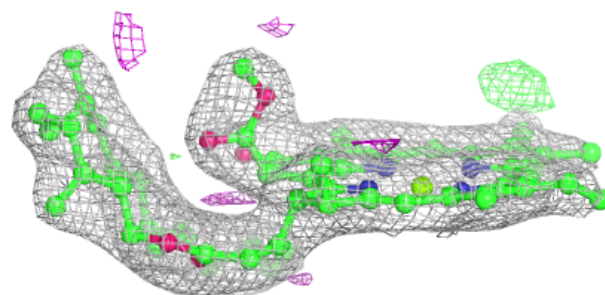
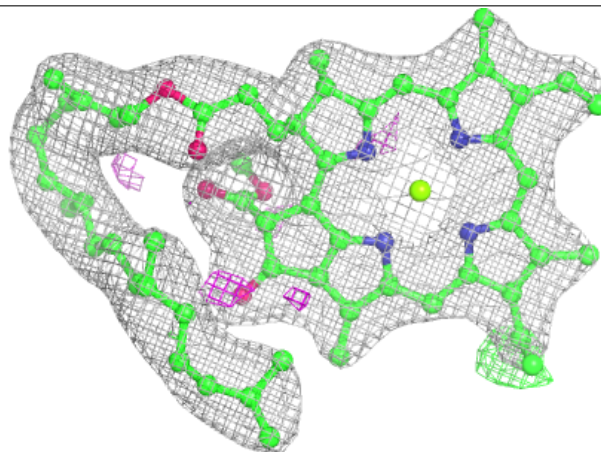


Electron density around CLA B 605:

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

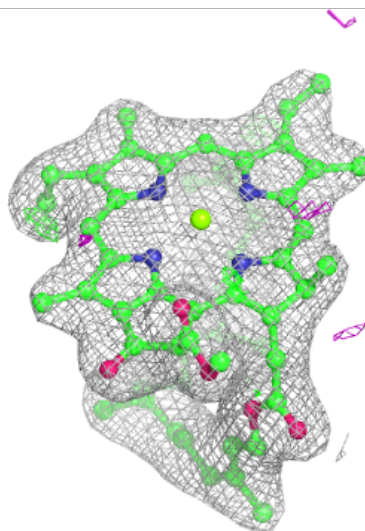
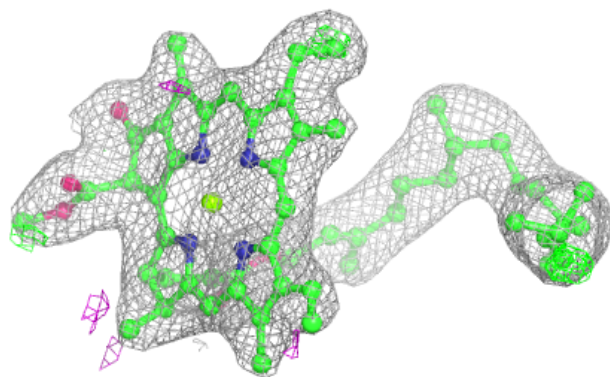
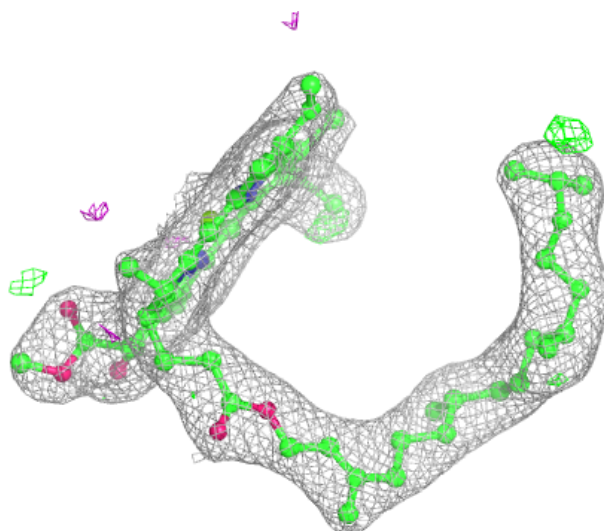
**Electron density around CLA b 610:**

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



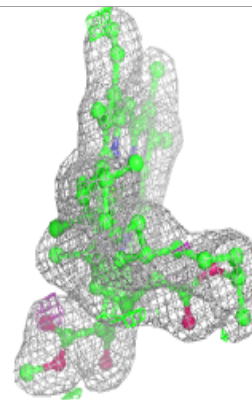
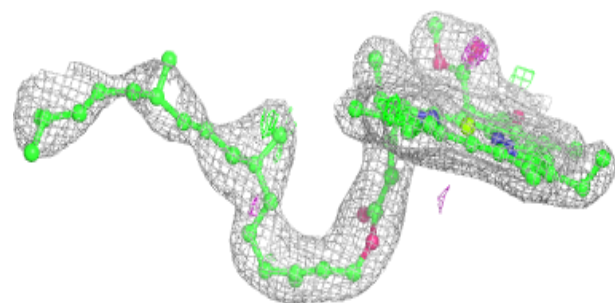
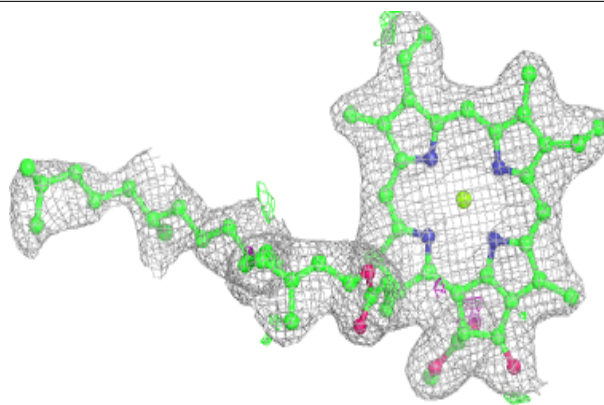
Electron density around CLA b 611:

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

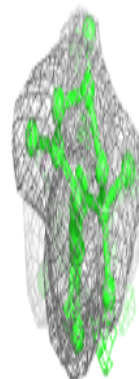
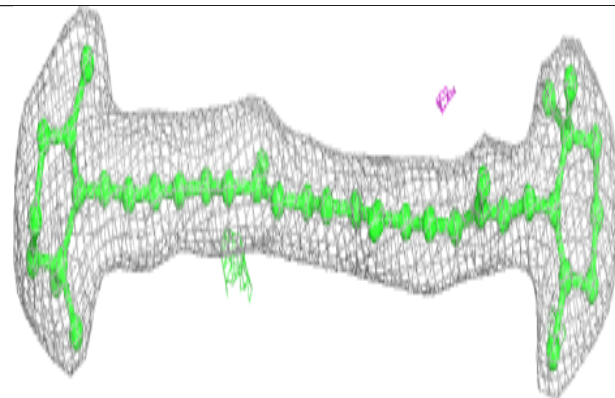
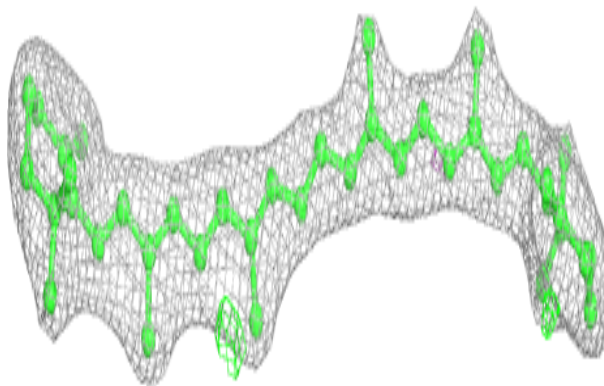


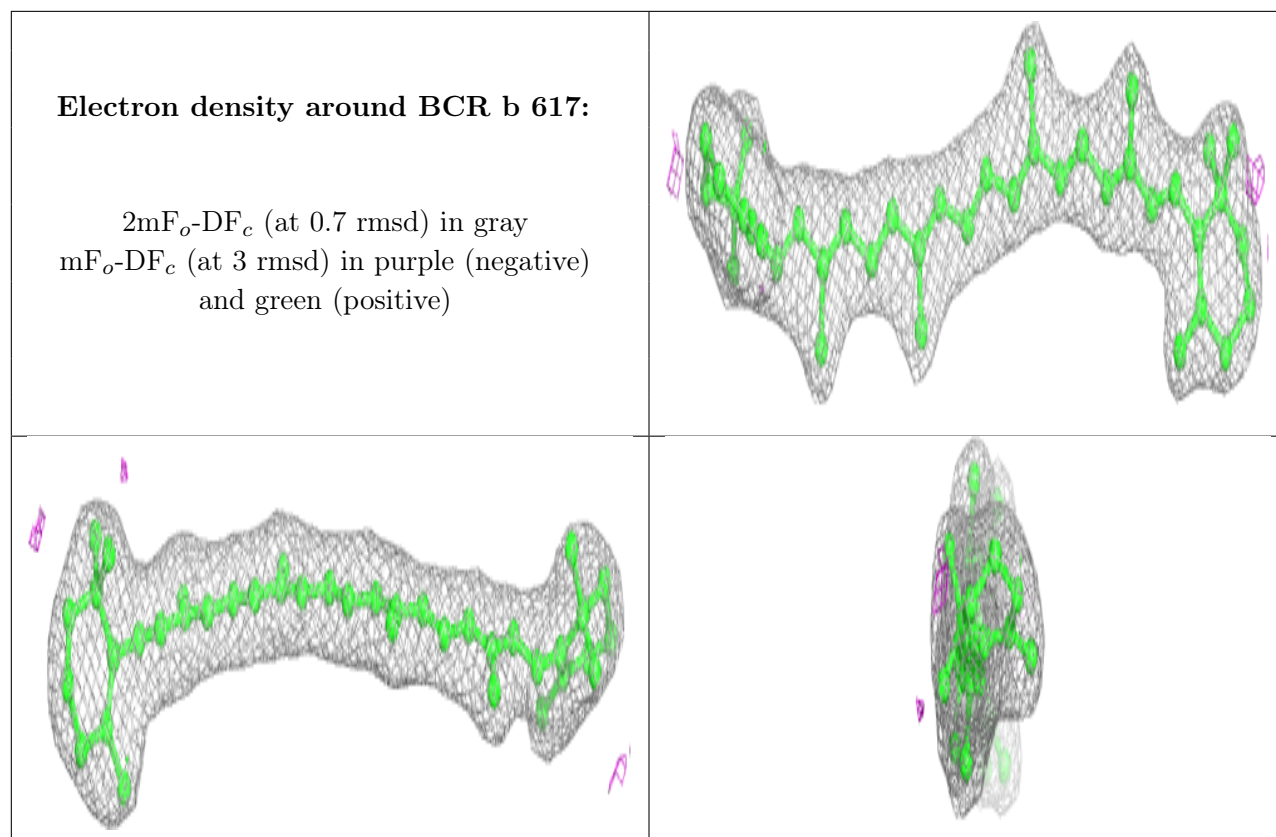
Electron density around CLA A 406 (A):

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

**Electron density around BCR a 410:**

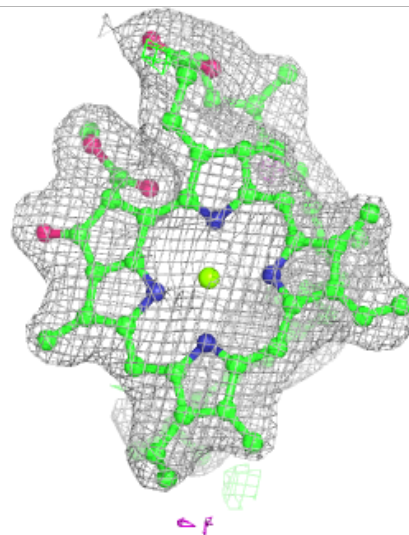
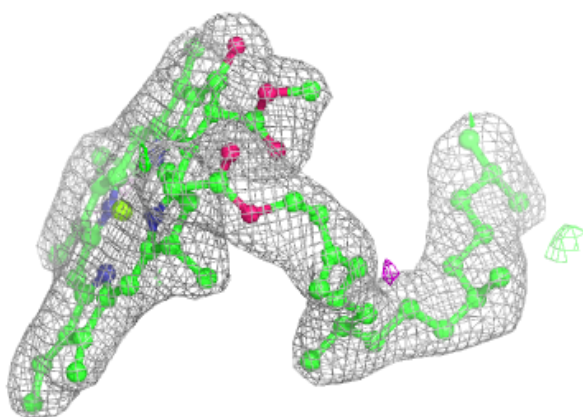
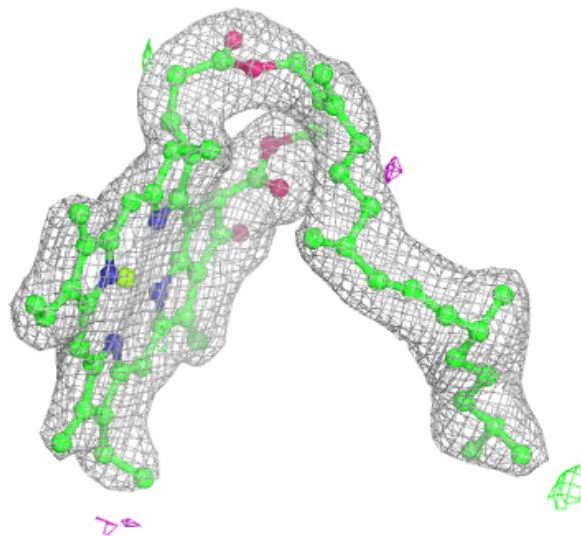
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





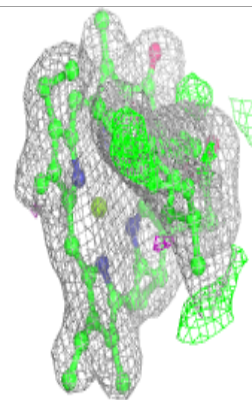
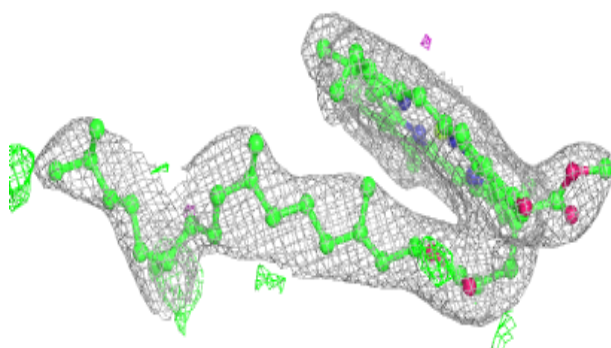
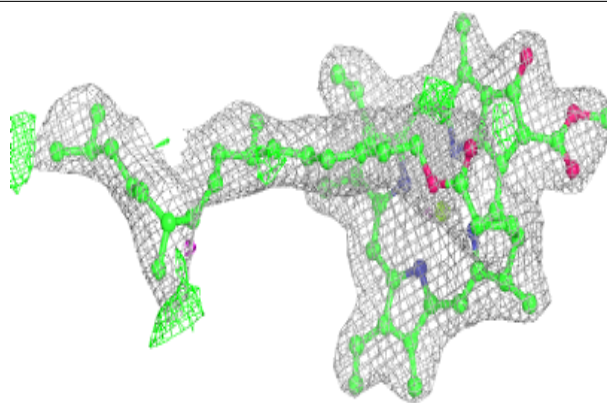
Electron density around CLA b 613:

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

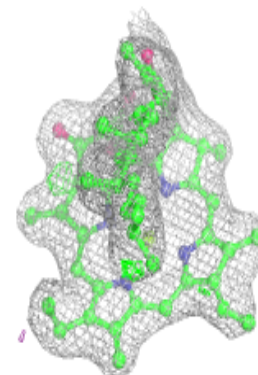
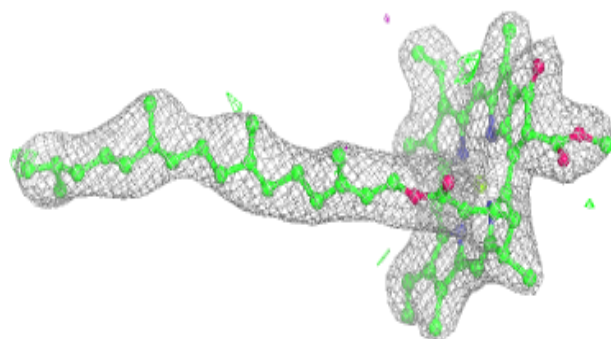
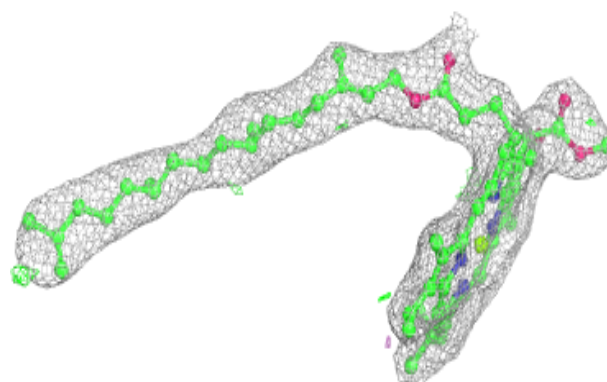


Electron density around CLA b 614:

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

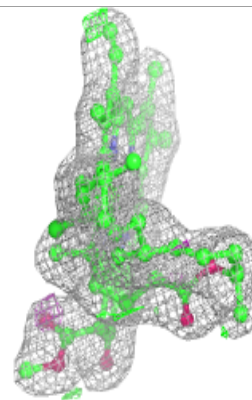
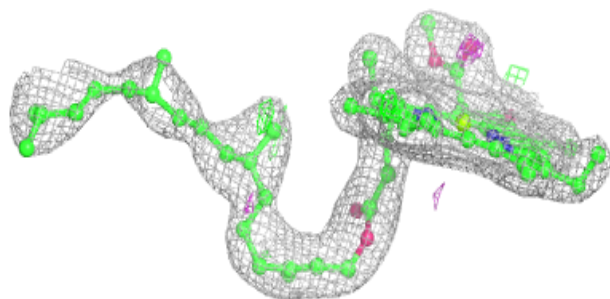
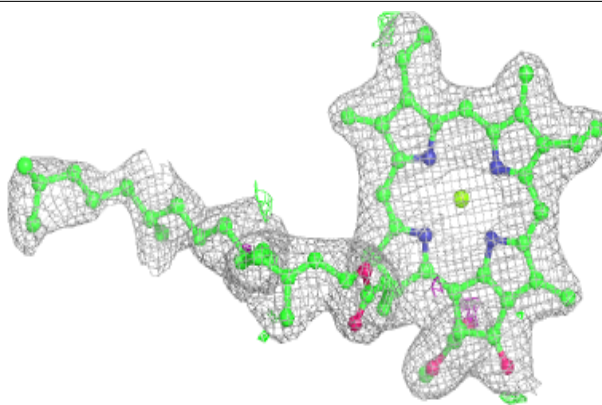
**Electron density around CLA B 607:**

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



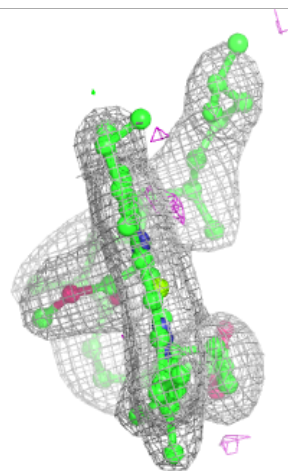
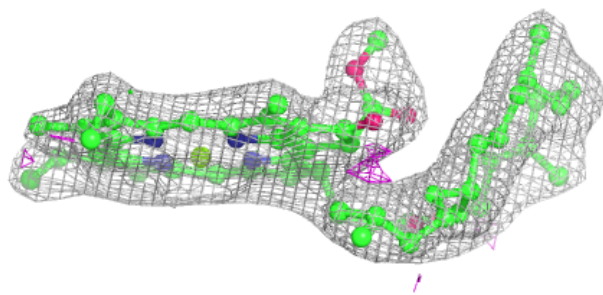
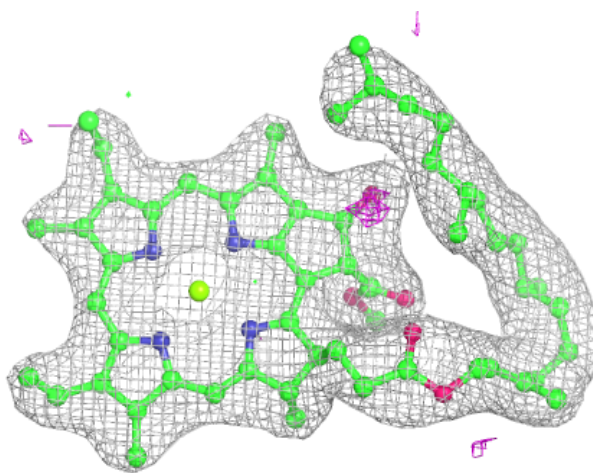
Electron density around CLA A 406 (B):

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



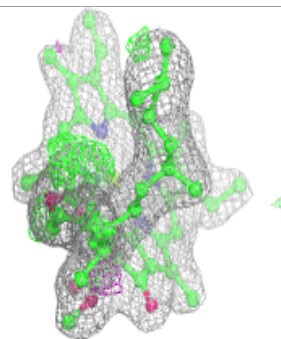
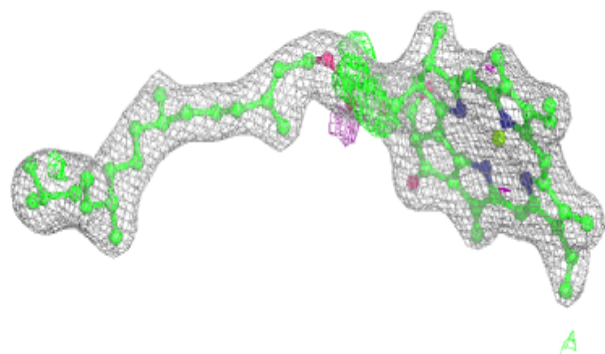
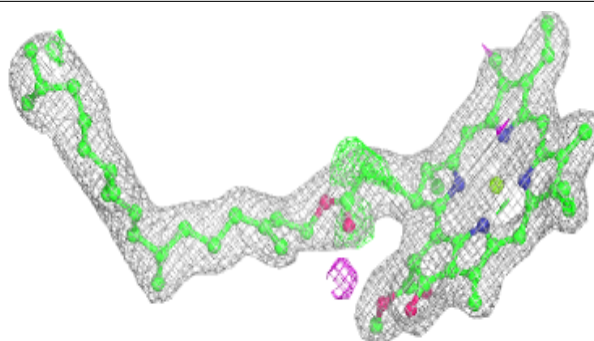
Electron density around CLA B 610:

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

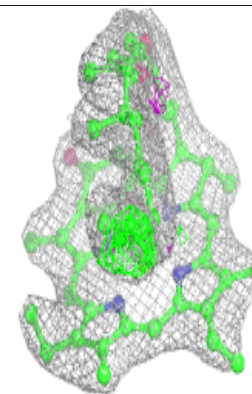
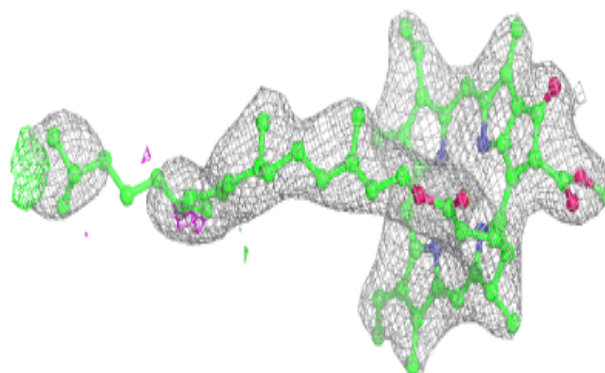
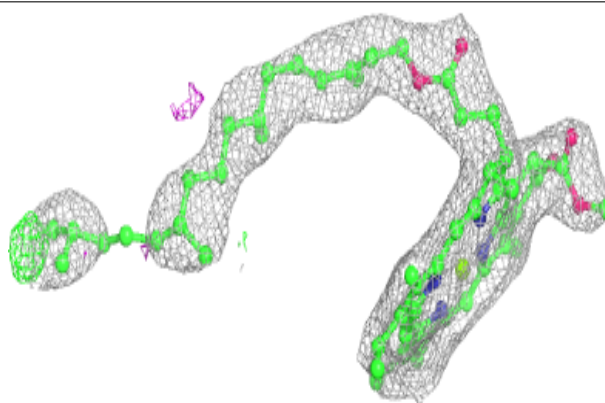


Electron density around CLA A 404 (A):

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

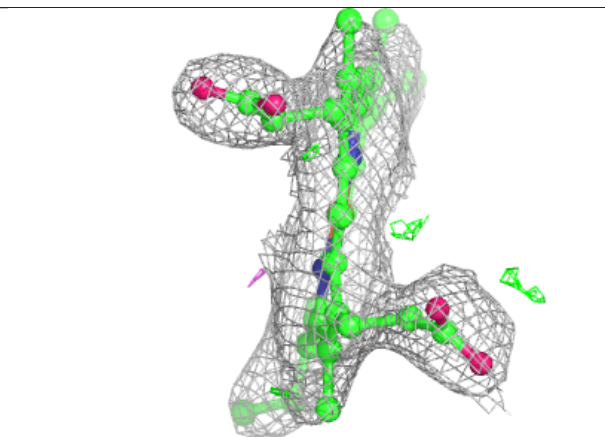
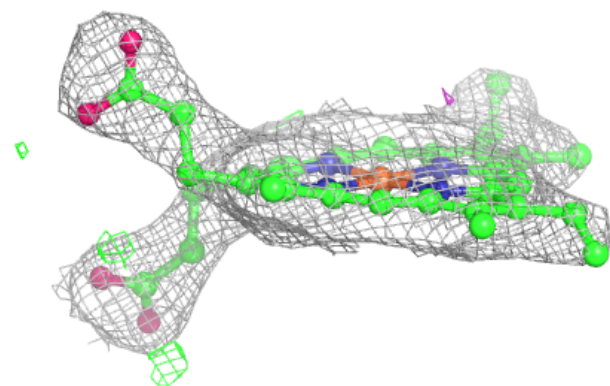
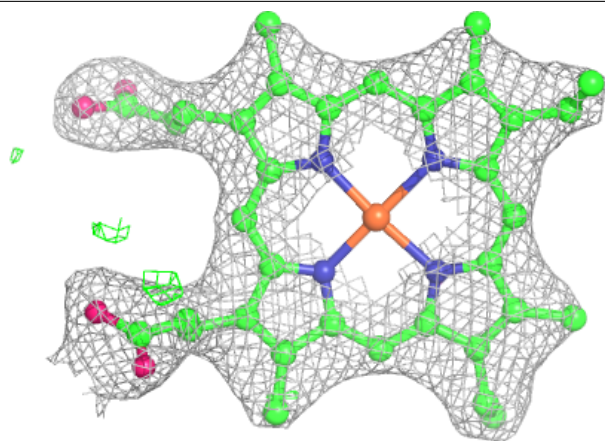
**Electron density around CLA c 505:**

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

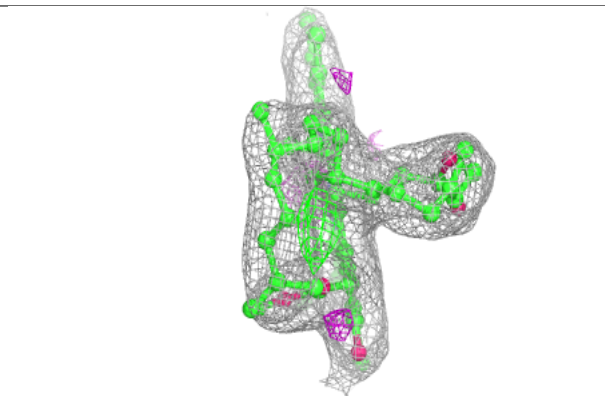
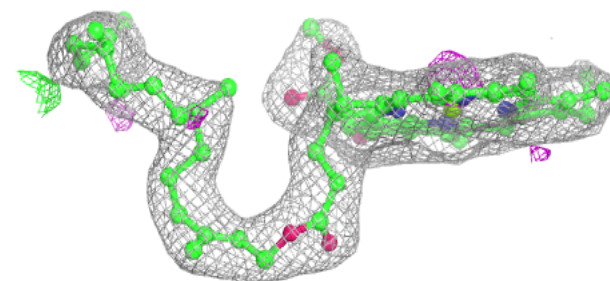
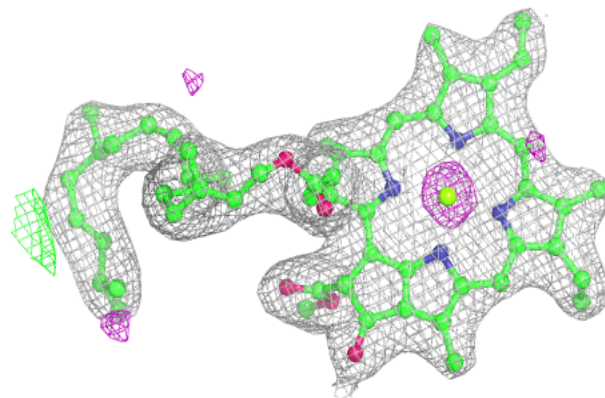


Electron density around HEM F 102:

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

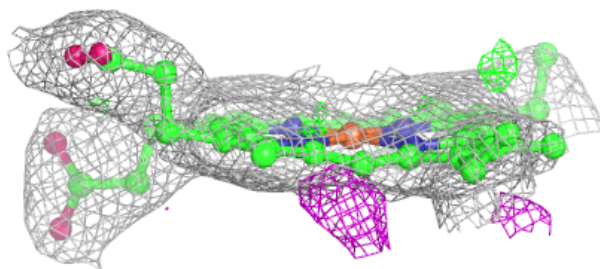
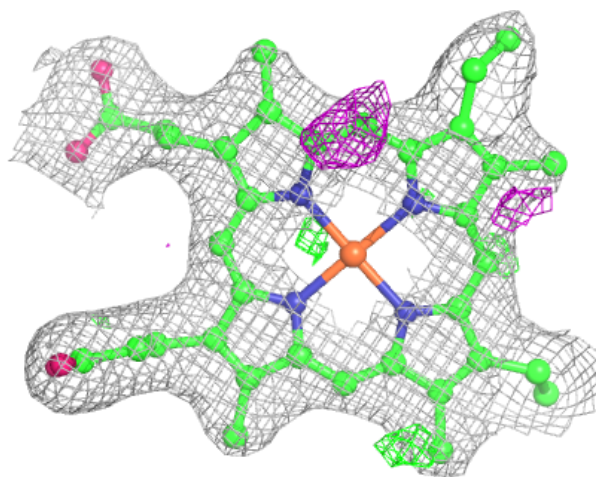
**Electron density around CLA B 612:**

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



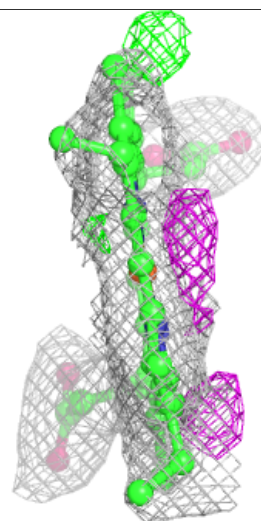
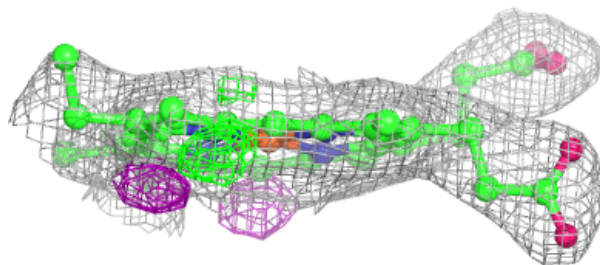
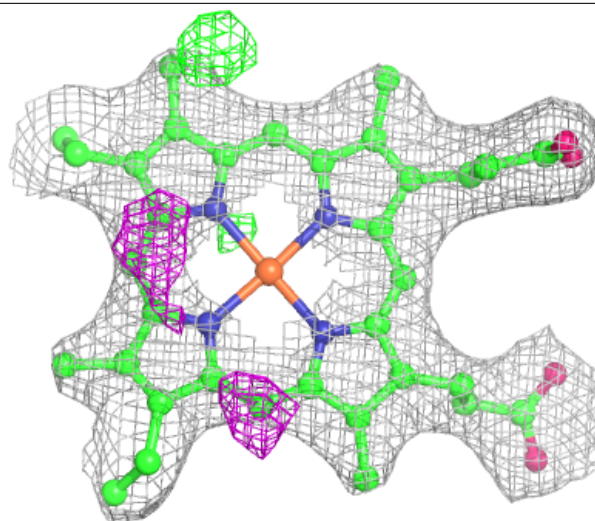
Electron density around HEC V 201:

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



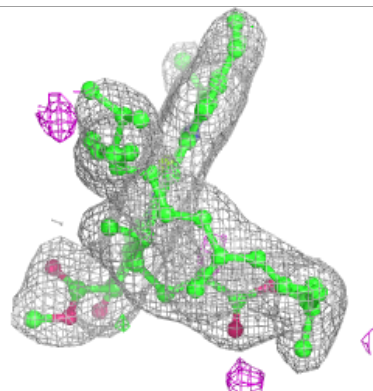
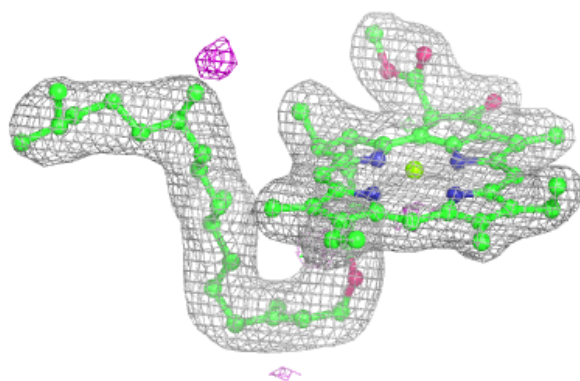
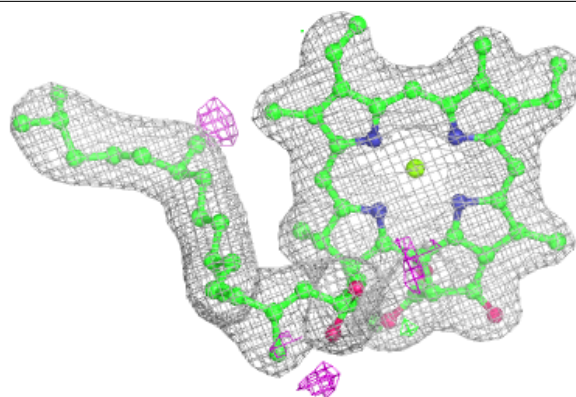
Electron density around HEC v 201:

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

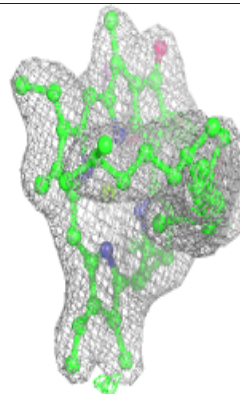
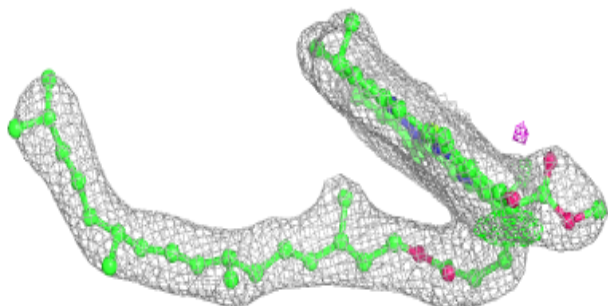
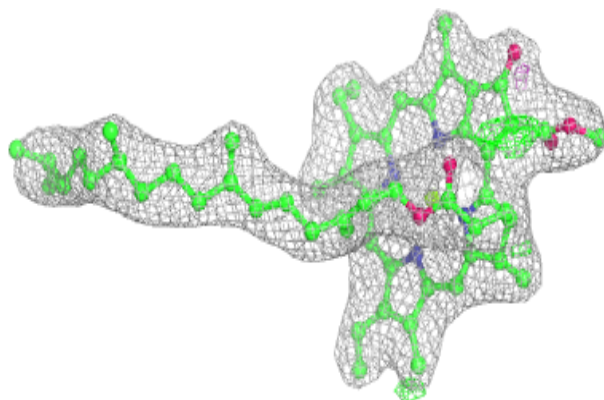


Electron density around CLA a 406 (B):

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

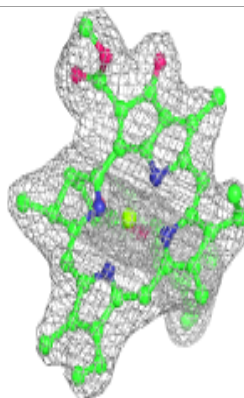
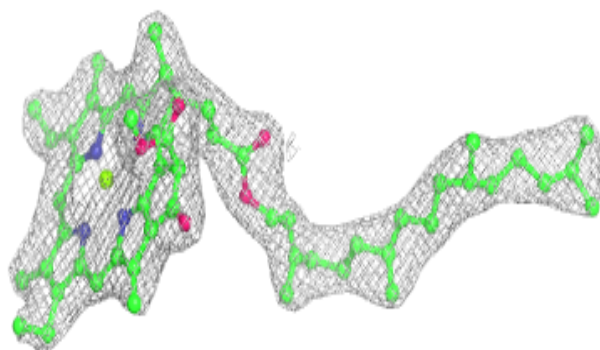
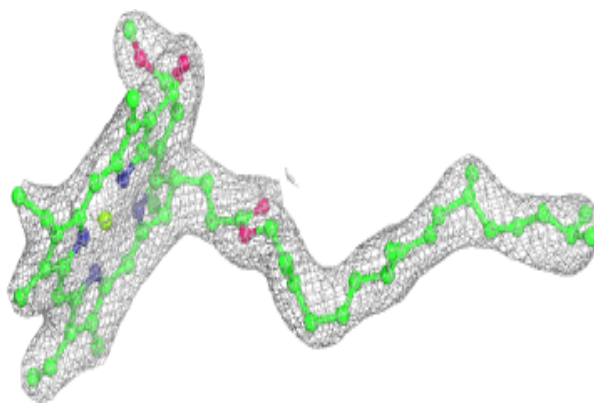
**Electron density around CLA b 608:**

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

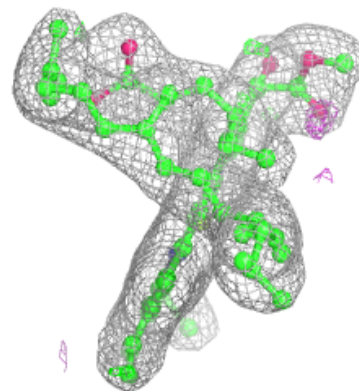
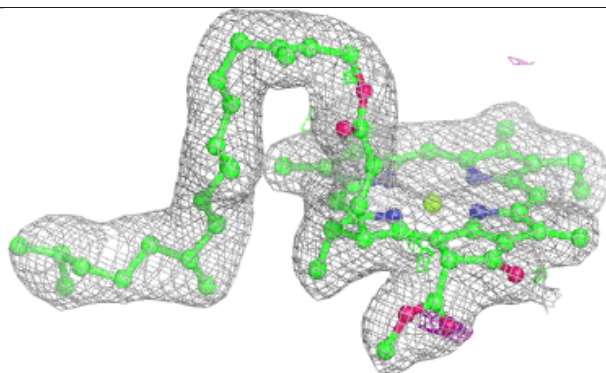
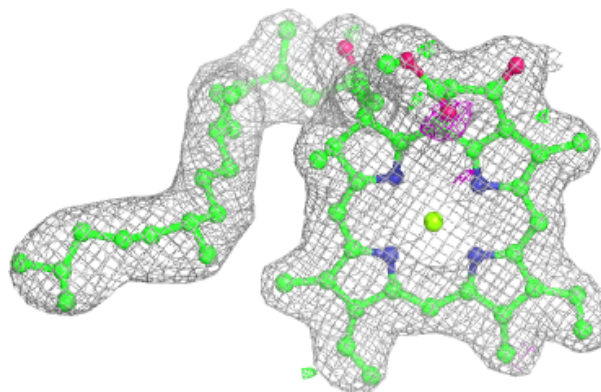


Electron density around CLA C 503:

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

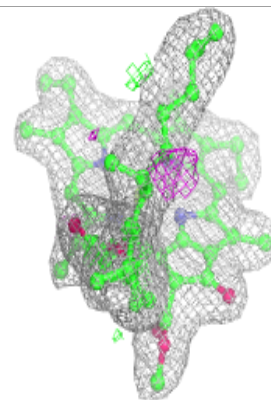
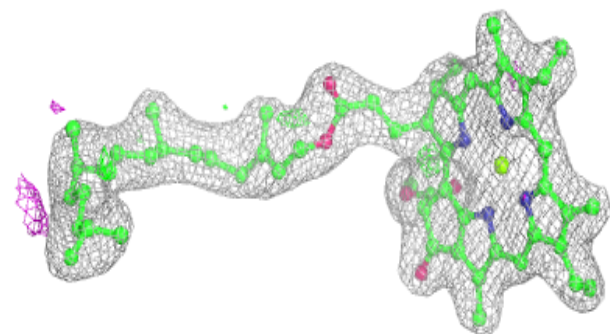
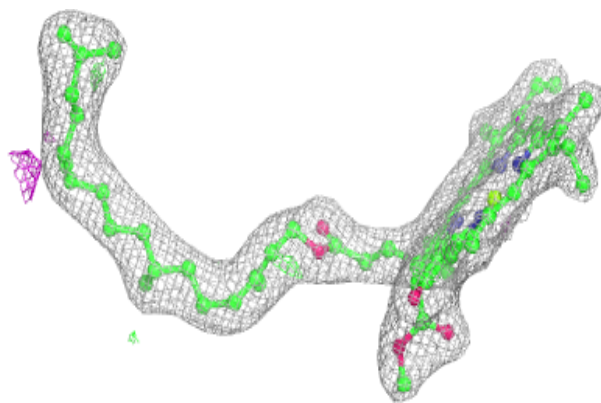
**Electron density around CLA A 405 (B):**

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

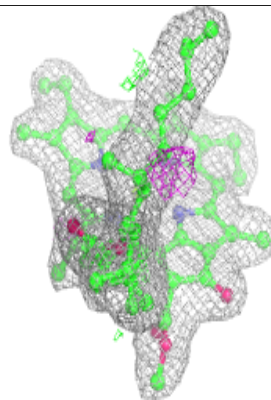
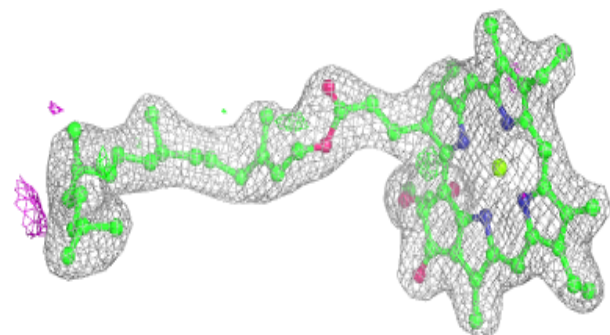
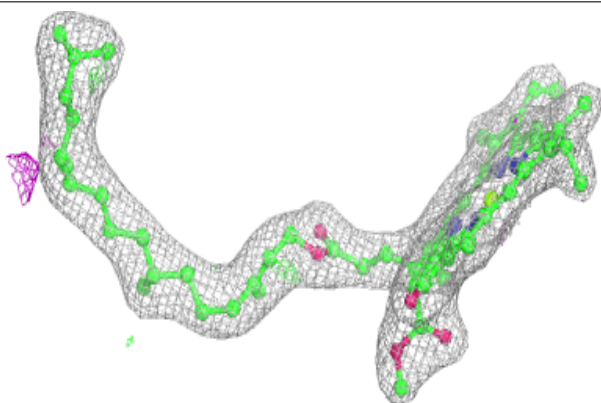


Electron density around CLA D 404 (A):

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

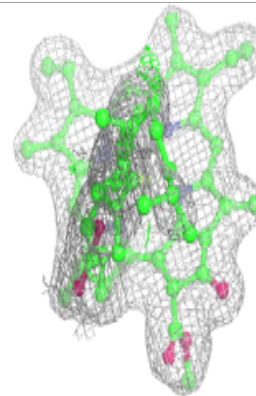
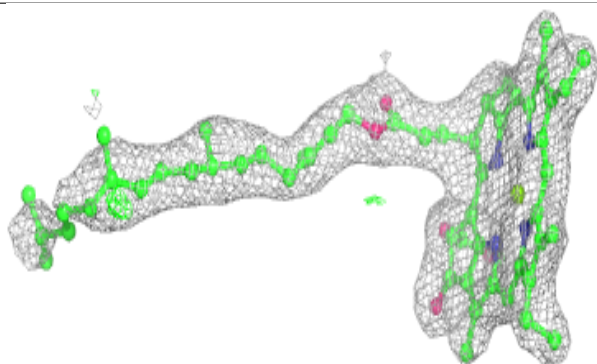
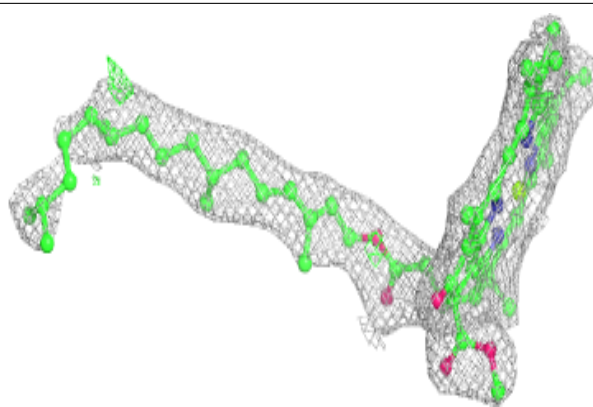
**Electron density around CLA D 404 (B):**

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

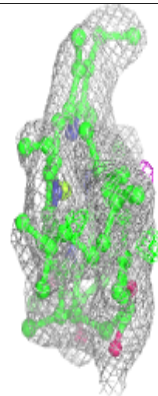
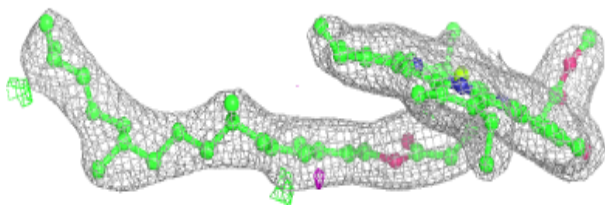
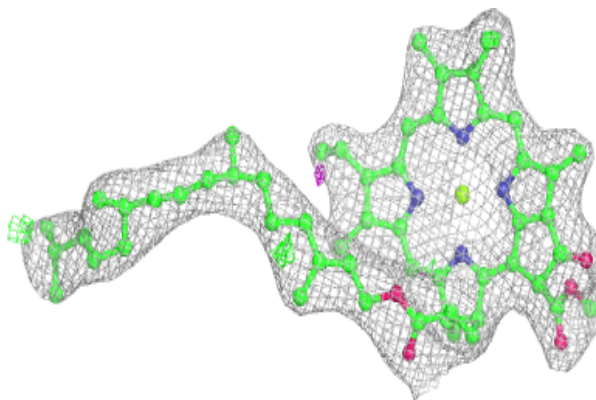


Electron density around CLA B 604:

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

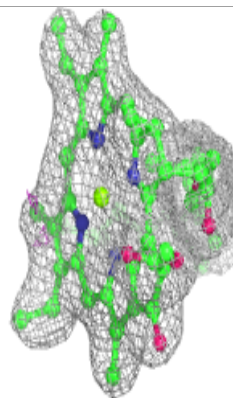
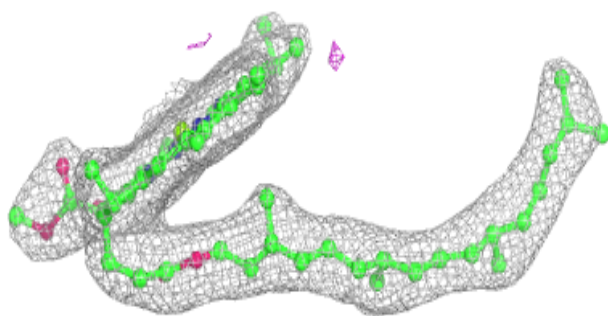
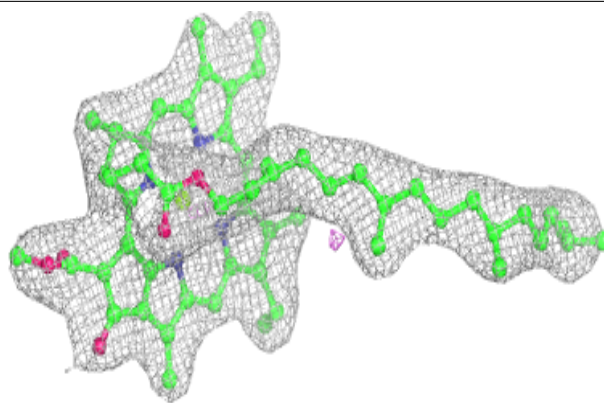
**Electron density around CLA b 603:**

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

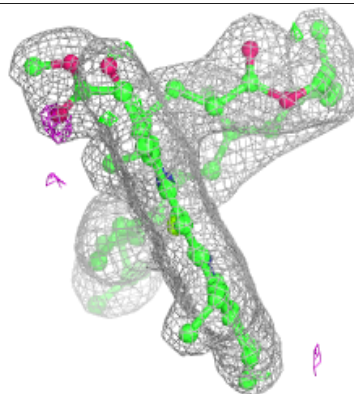
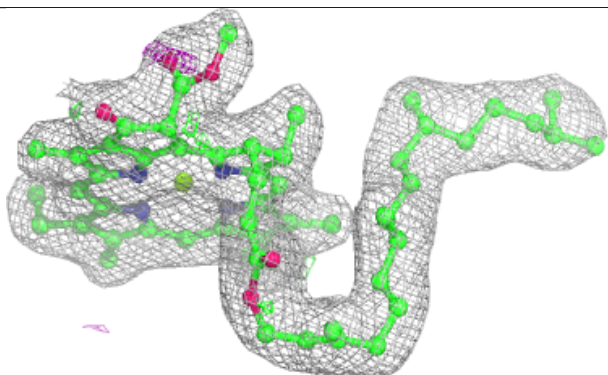
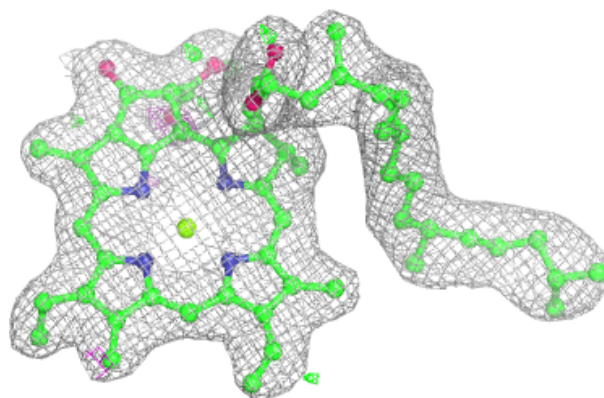


Electron density around CLA B 608:

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

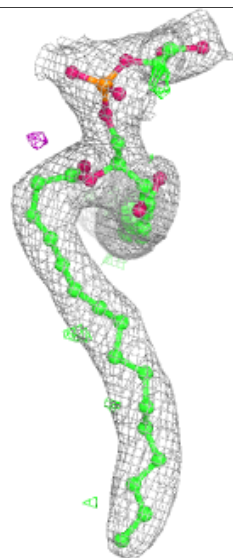
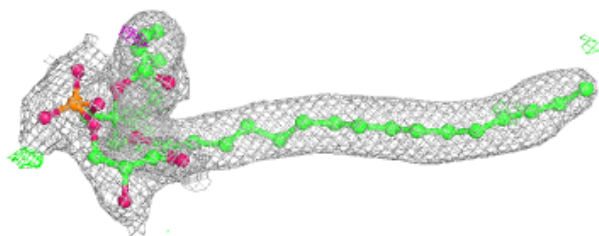
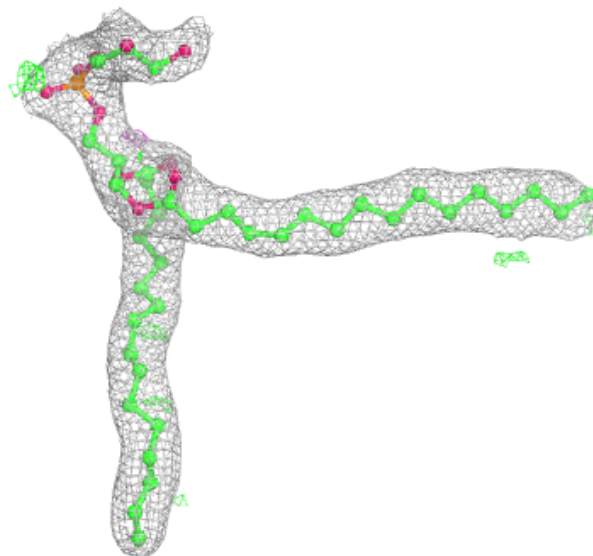
**Electron density around CLA A 405 (A):**

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



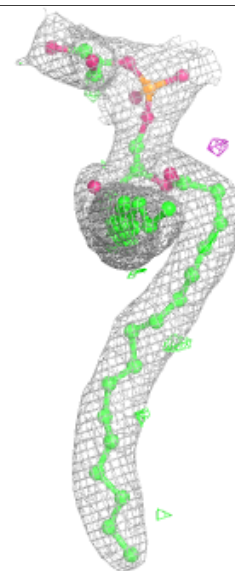
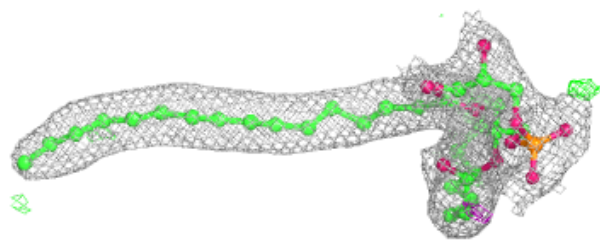
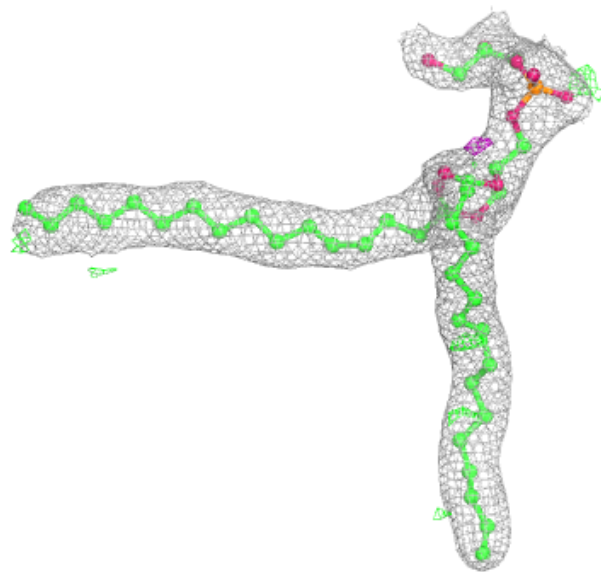
Electron density around LHG L 101 (A):

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



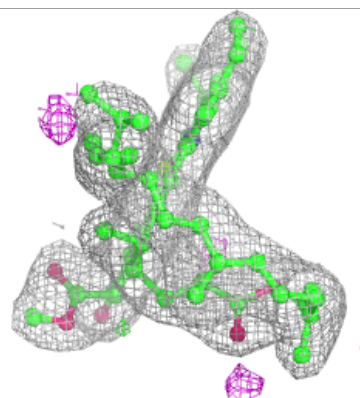
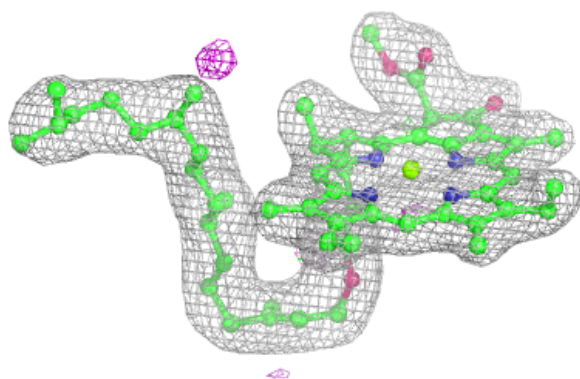
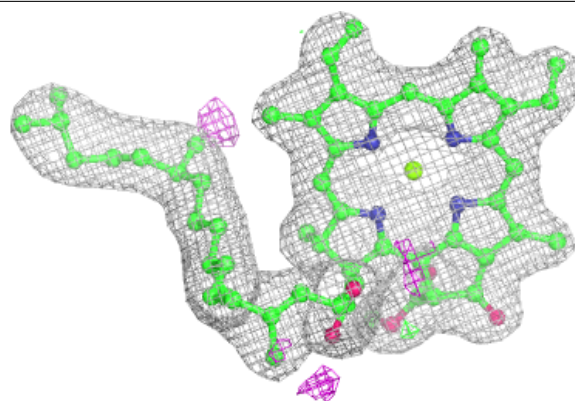
Electron density around LHG L 101 (B):

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

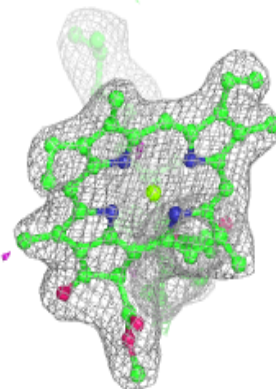
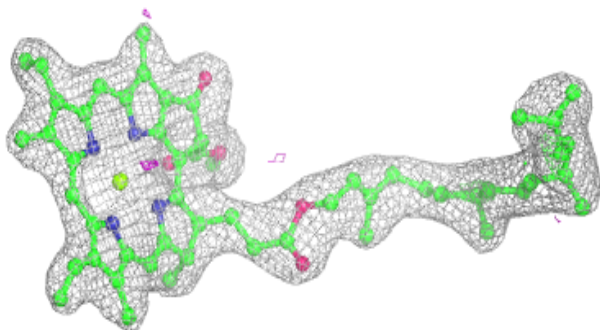
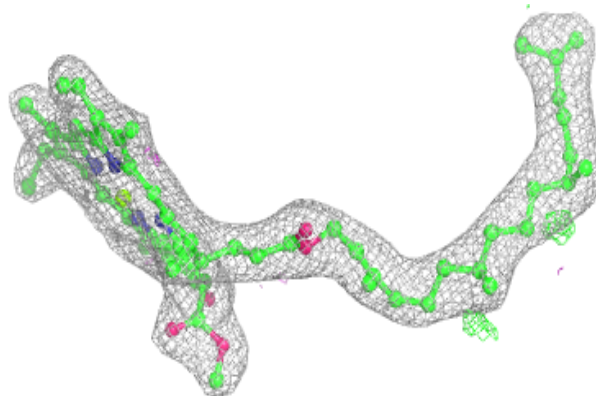


Electron density around CLA a 406 (A):

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

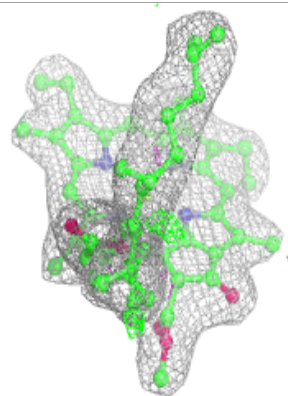
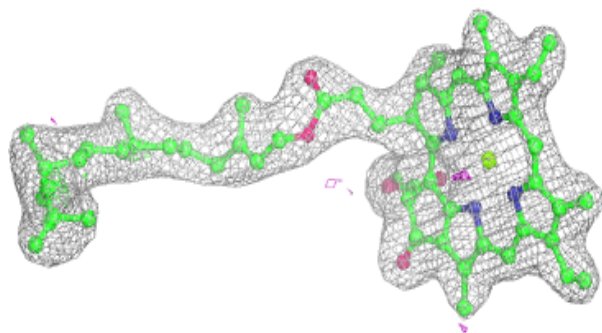
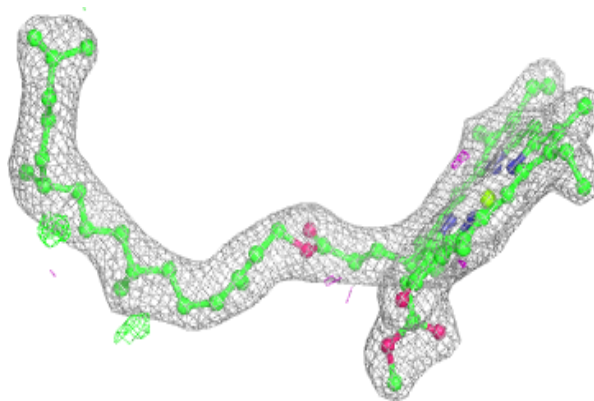
**Electron density around CLA d 402 (A):**

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

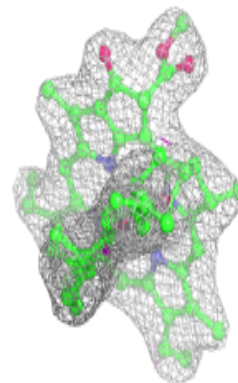
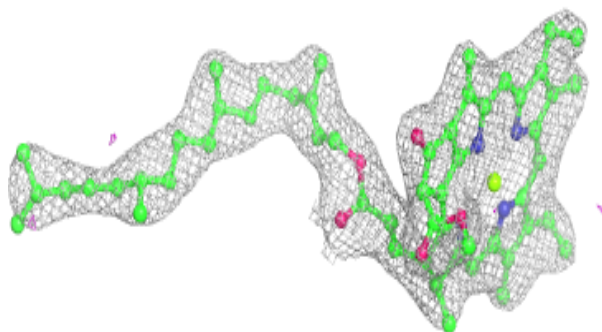
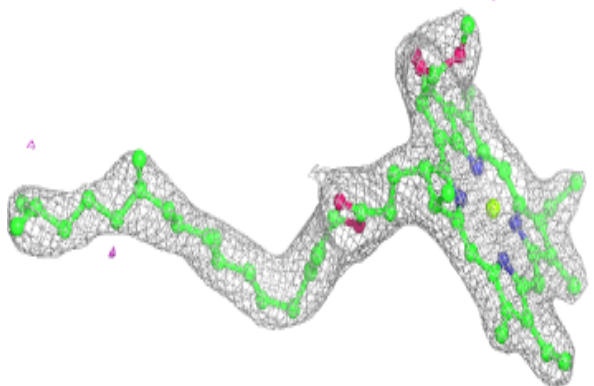


Electron density around CLA d 402 (B):

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

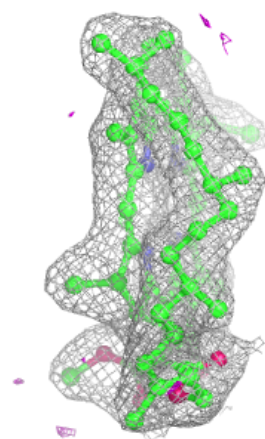
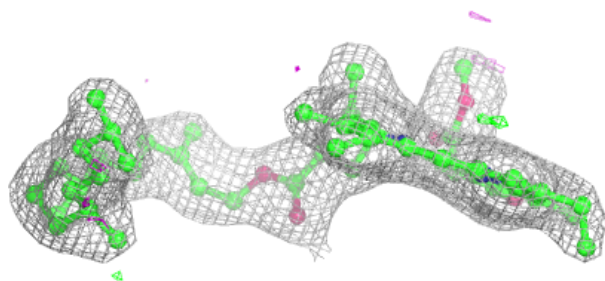
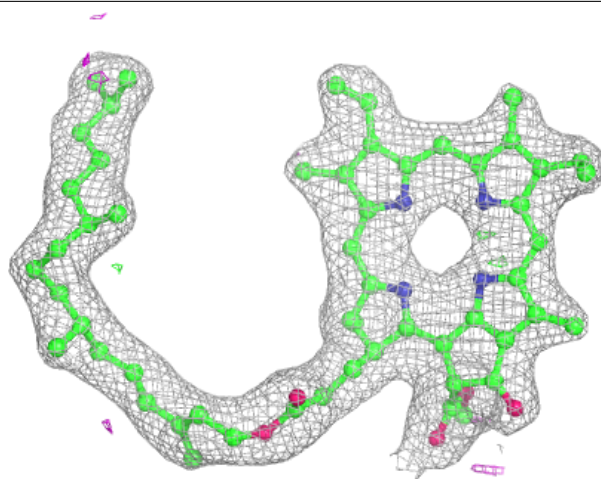
**Electron density around CLA c 503:**

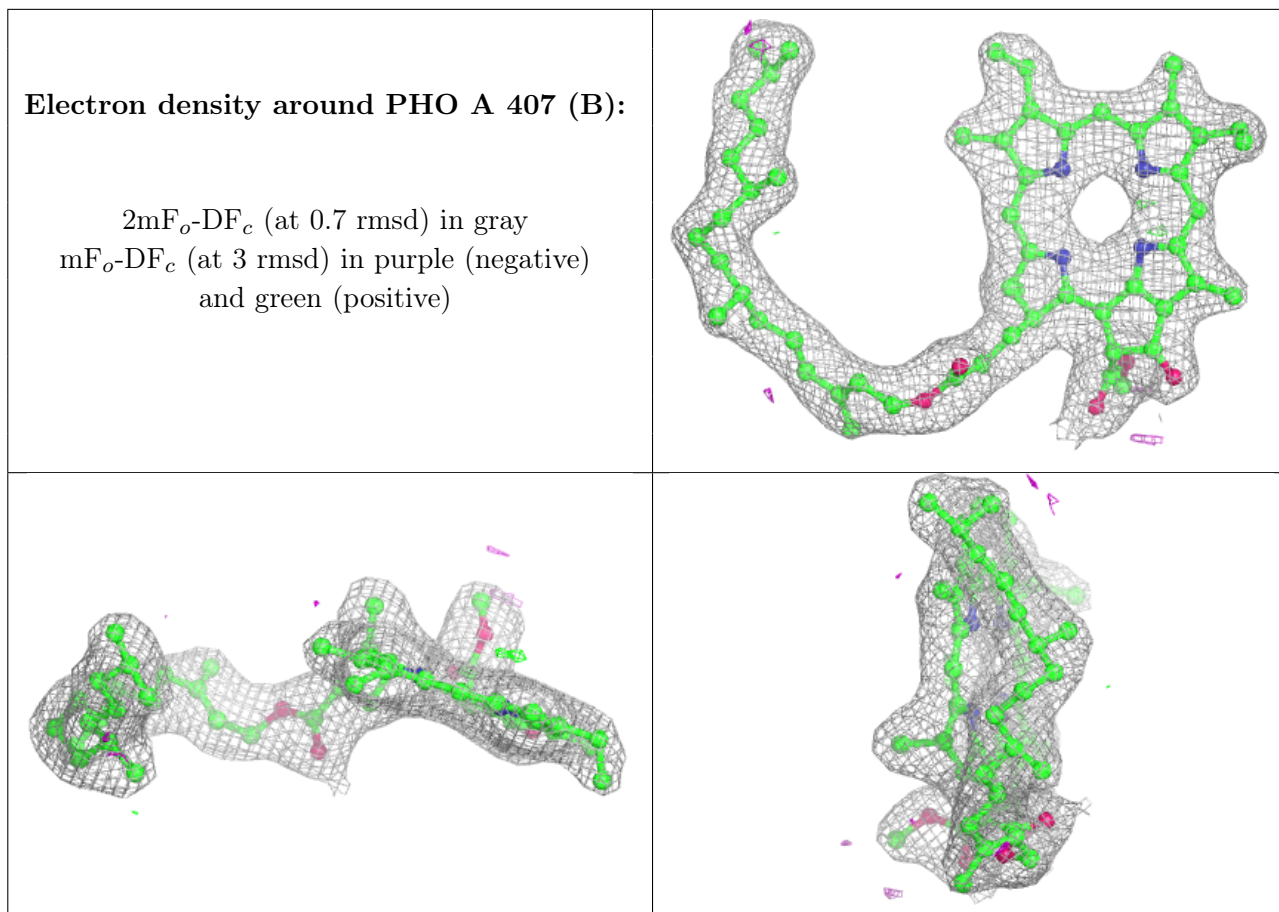
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PHO A 407 (A):

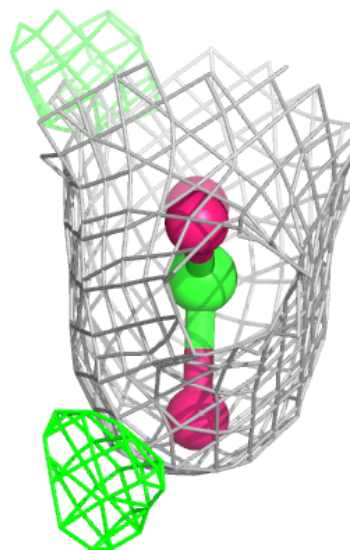
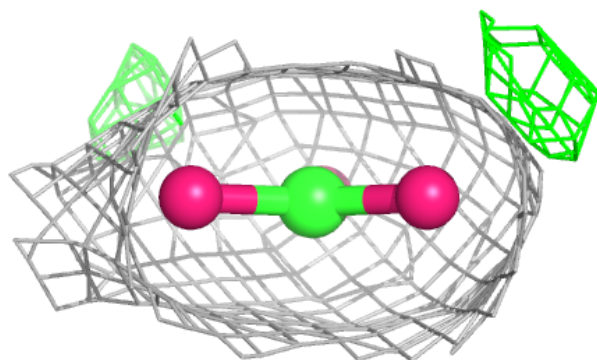
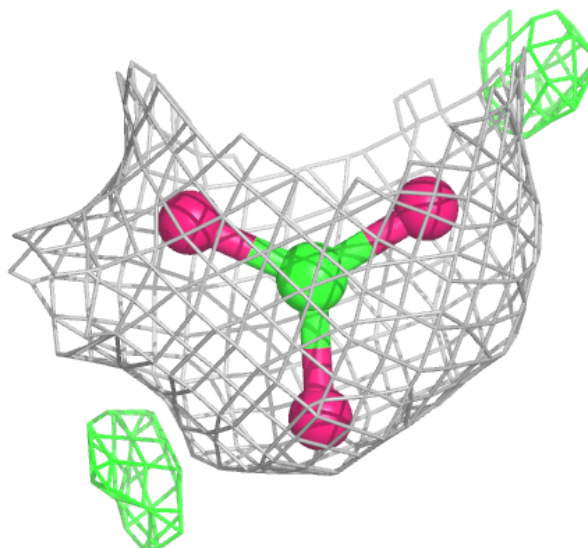
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





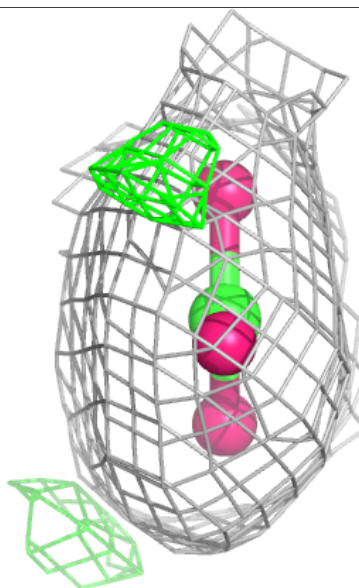
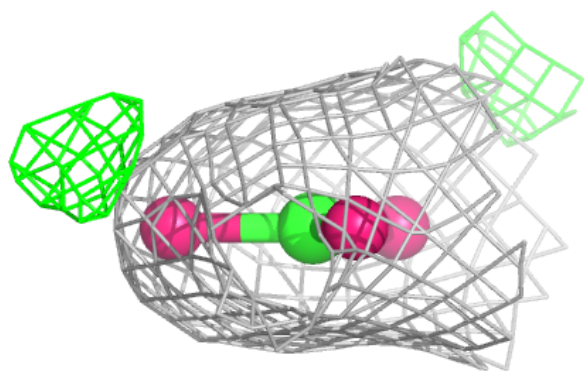
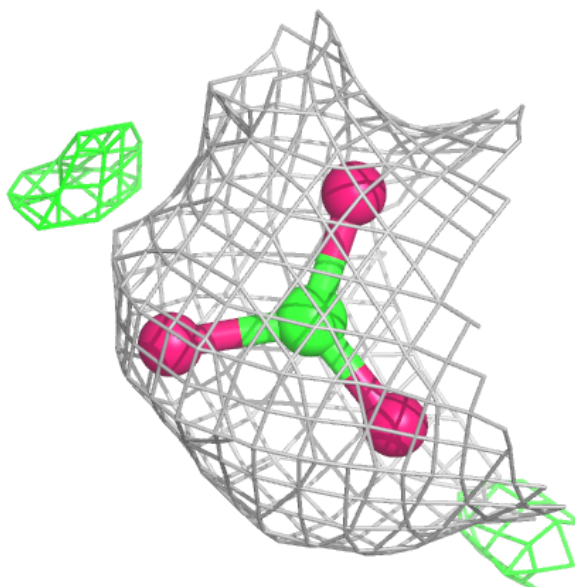
Electron density around BCT d 401 (A):

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



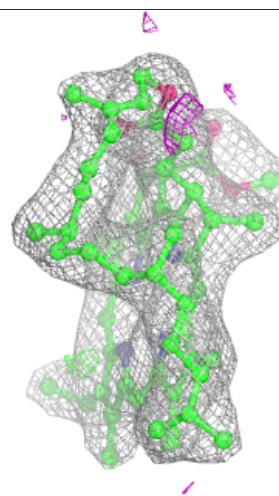
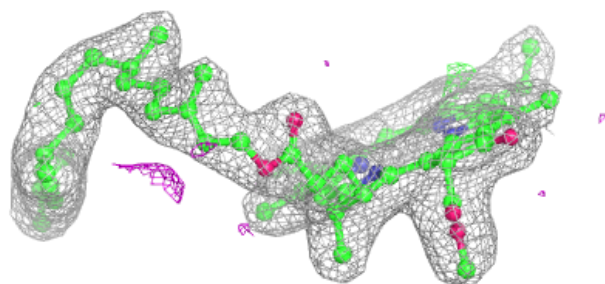
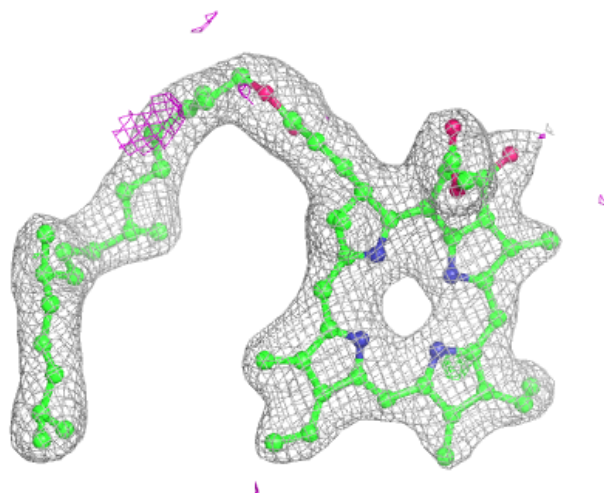
Electron density around BCT d 401 (B):

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



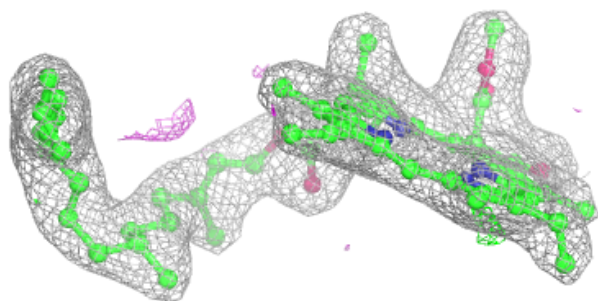
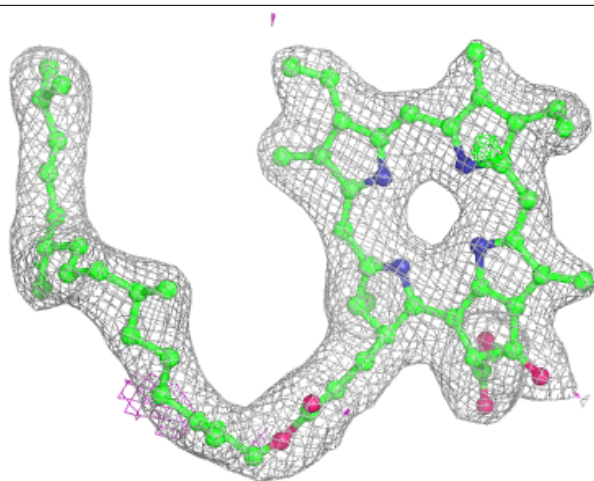
Electron density around PHO A 416 (A):

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



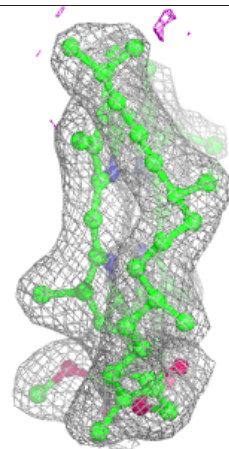
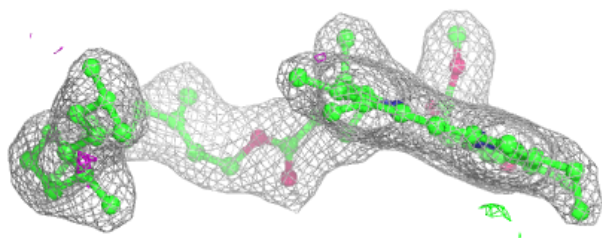
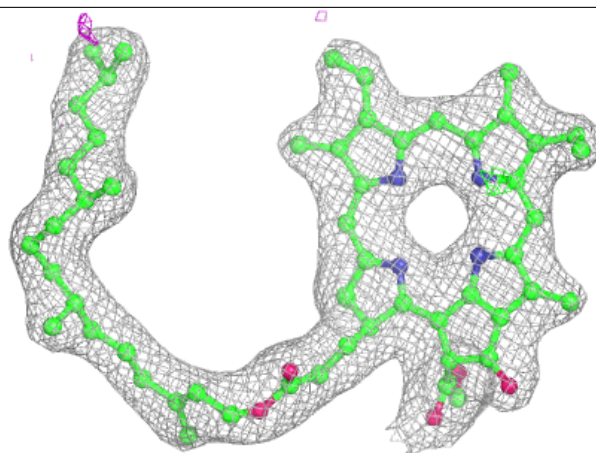
Electron density around PHO A 416 (B):

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



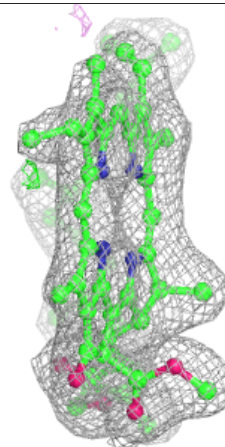
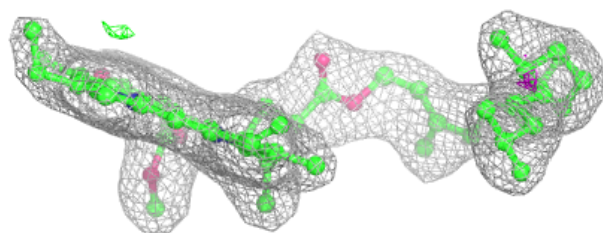
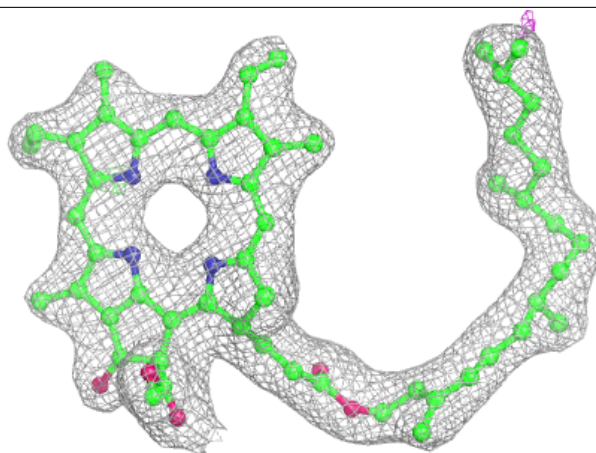
Electron density around PHO a 408 (A):

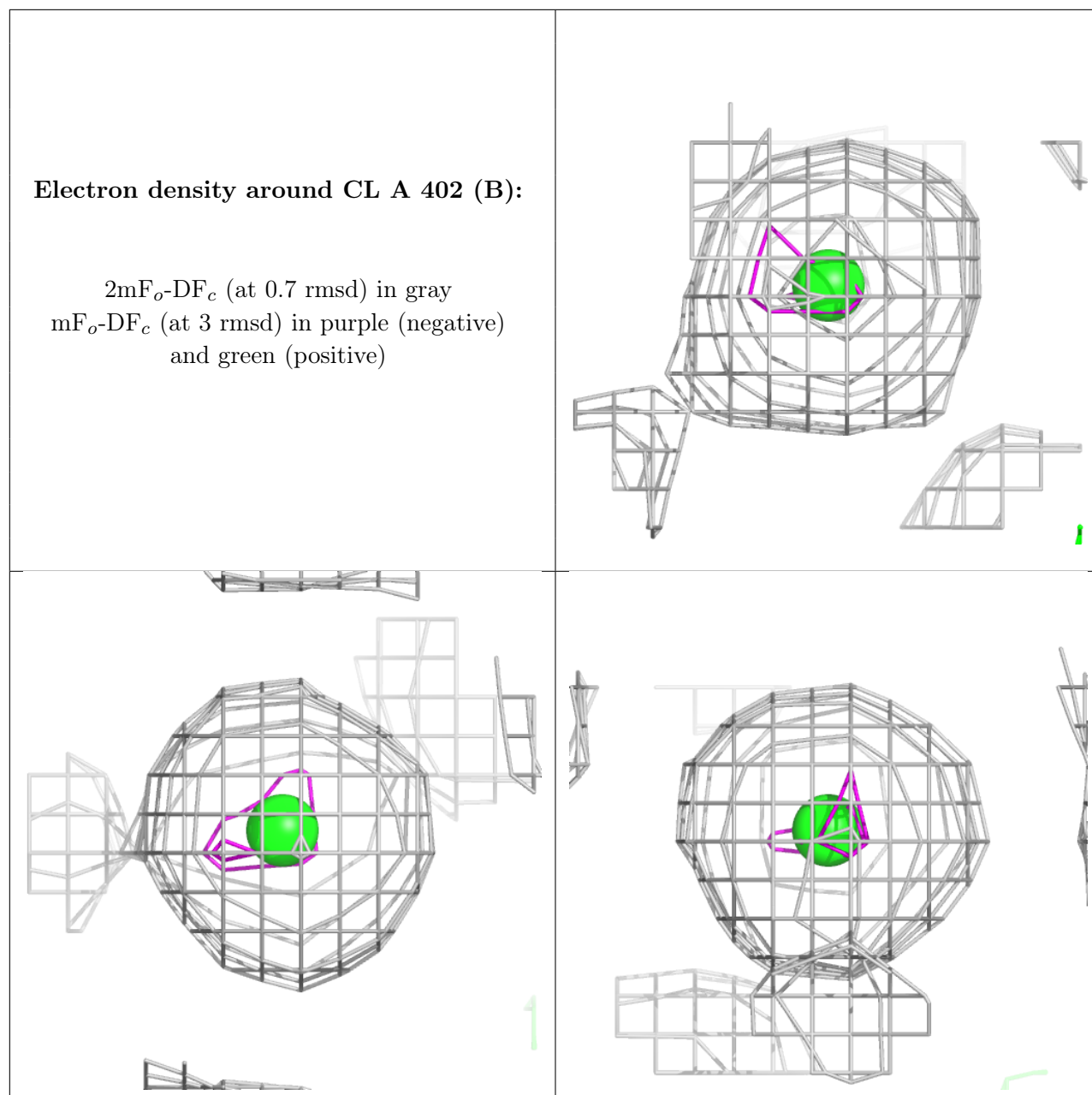
$2mF_o-DF_c$ (at 0.7 rnsd) in gray
 mF_o-DF_c (at 3 rnsd) in purple (negative)
and green (positive)

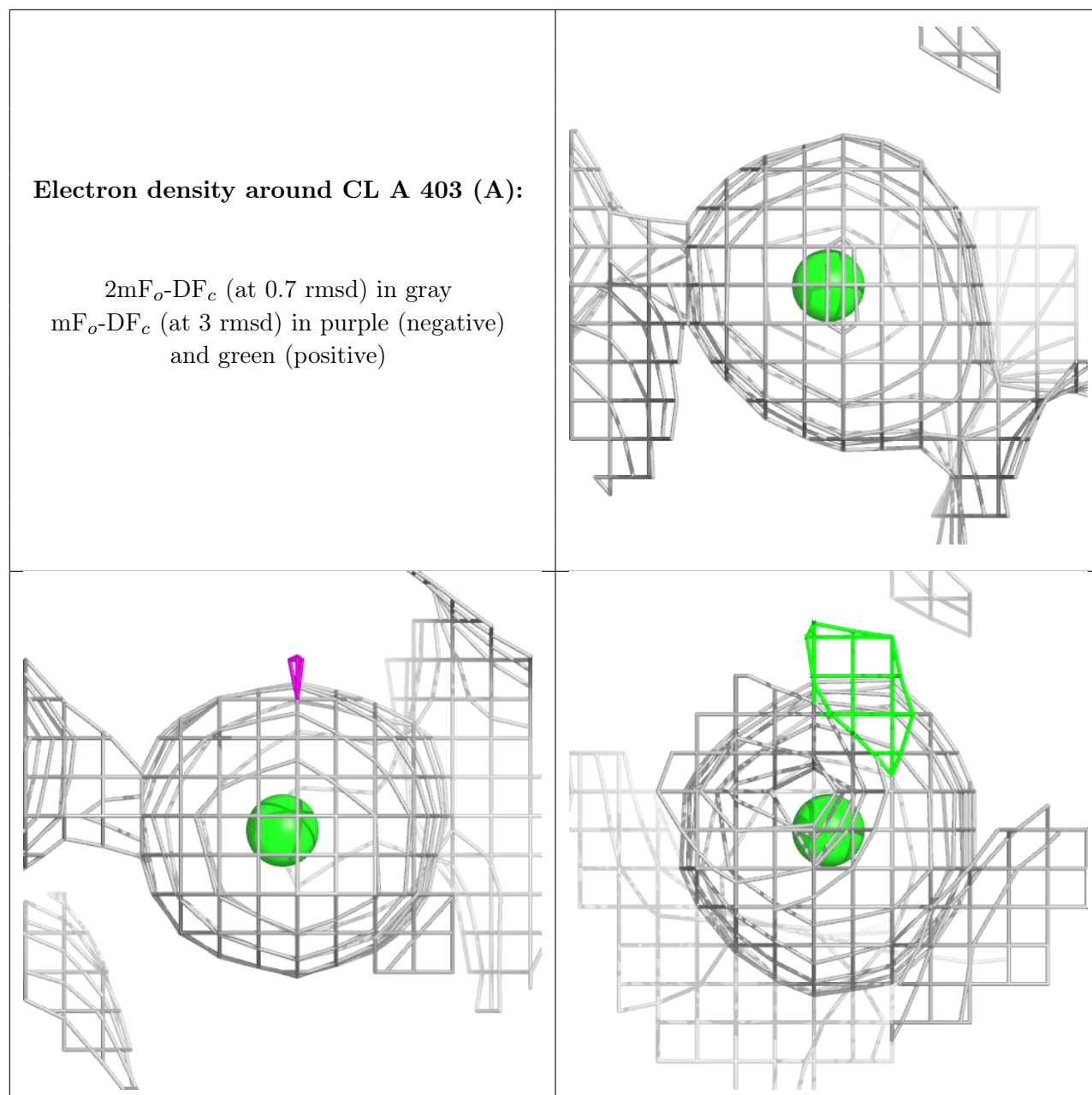


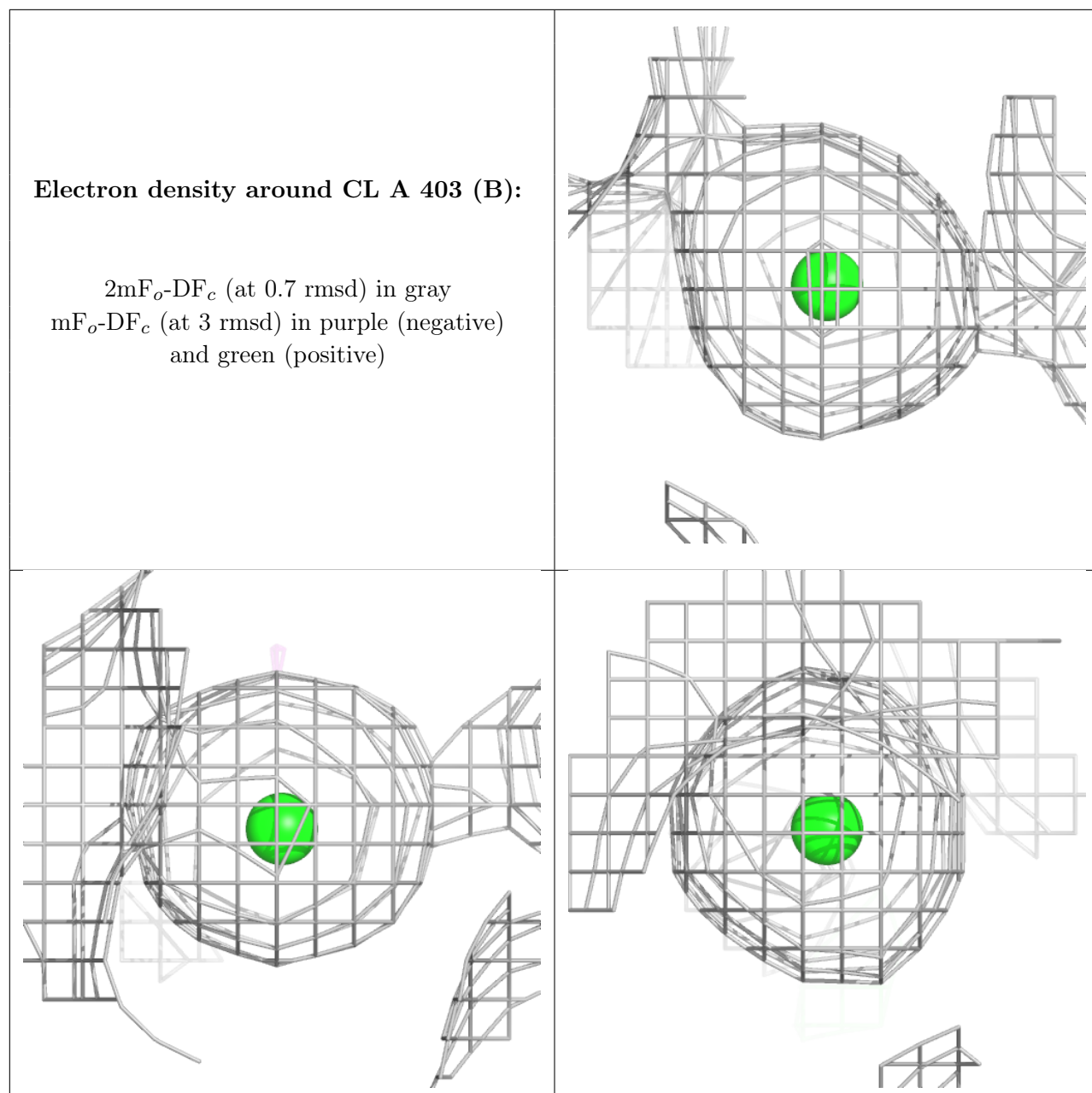
Electron density around PHO a 408 (B):

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



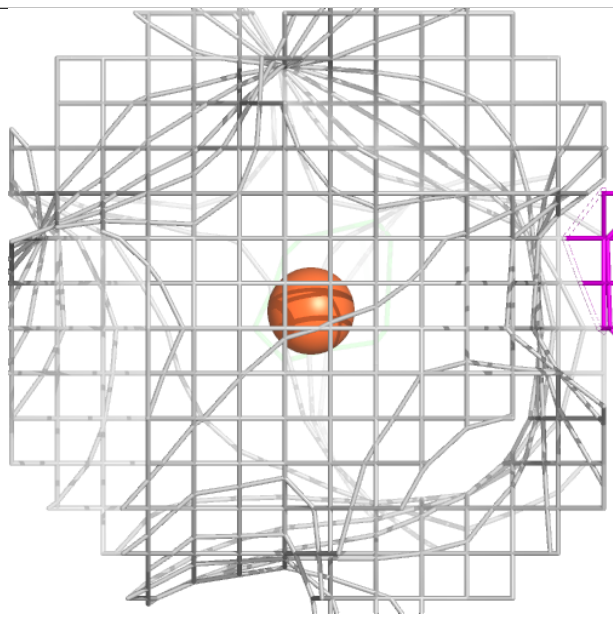
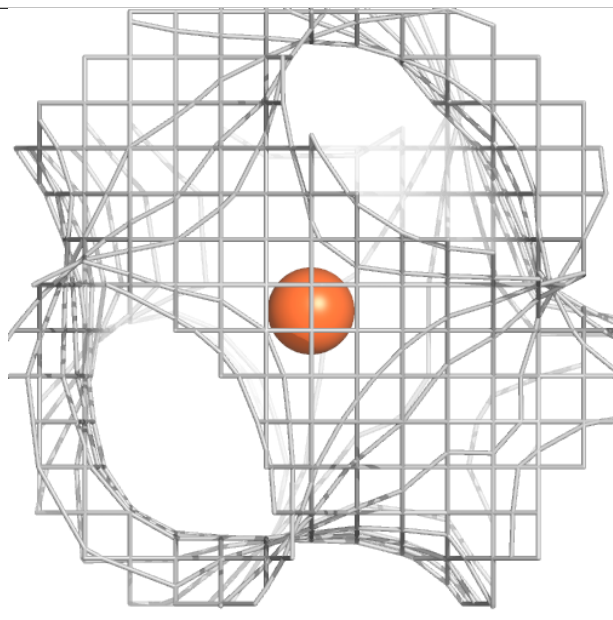
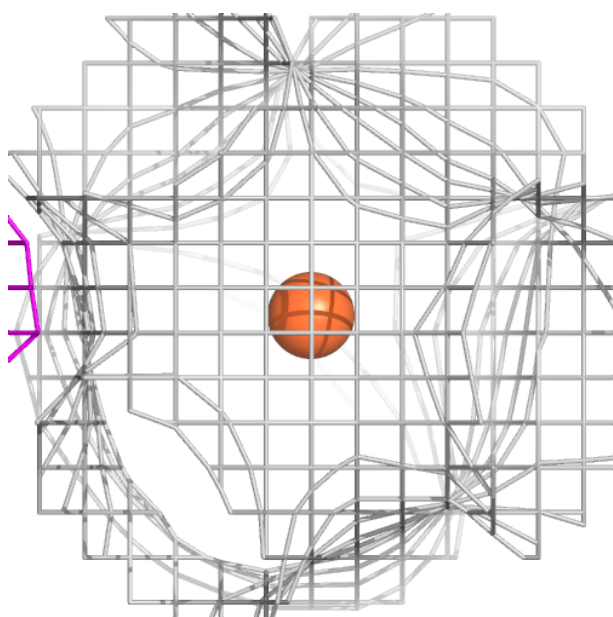






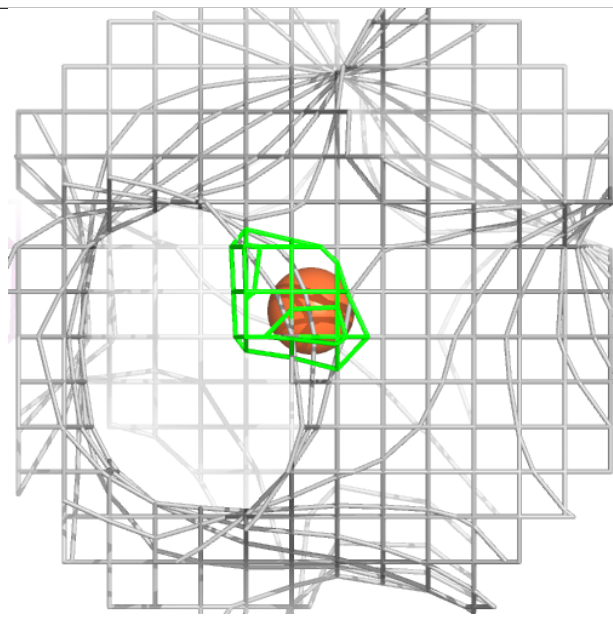
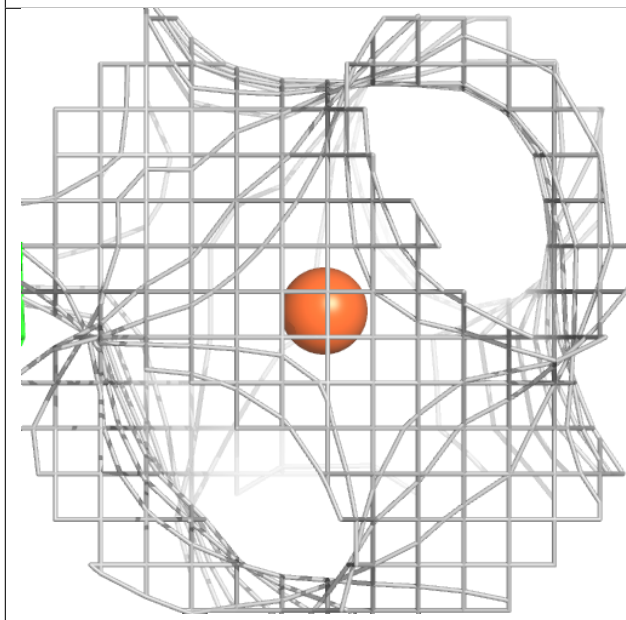
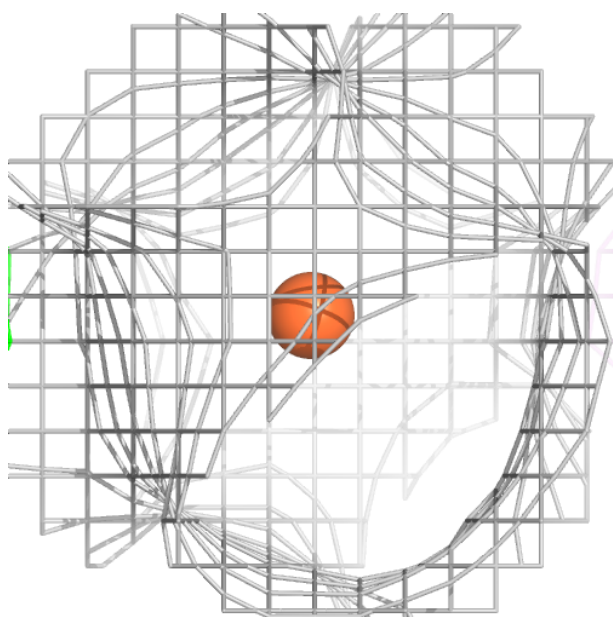
Electron density around FE2 D 401 (A):

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



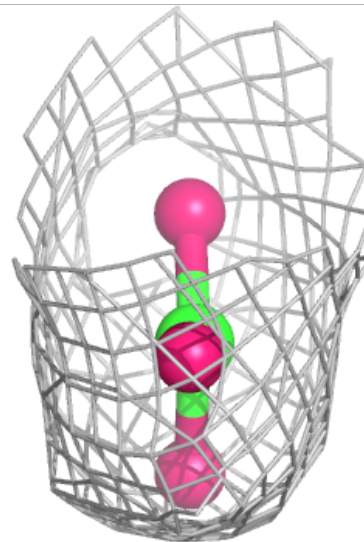
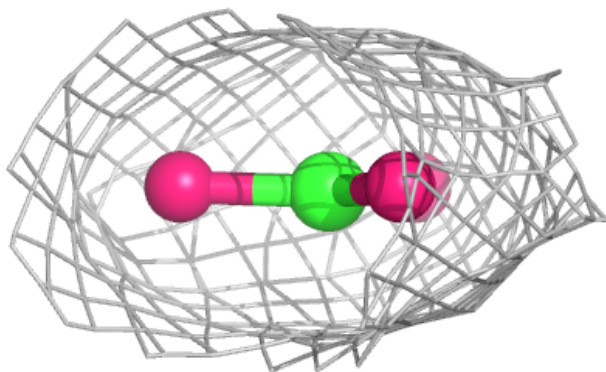
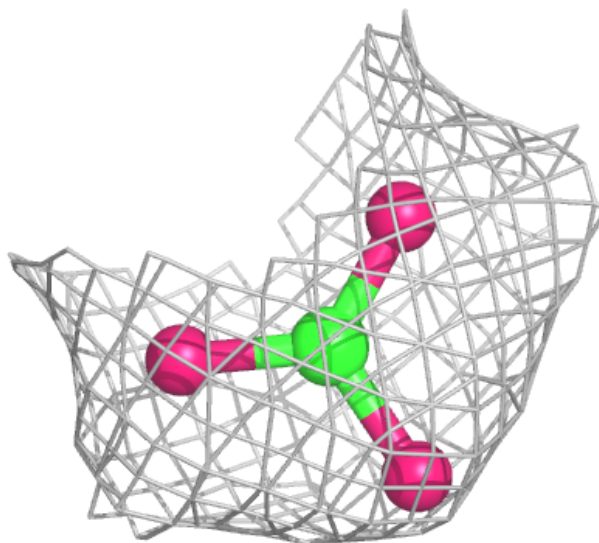
Electron density around FE2 D 401 (B):

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



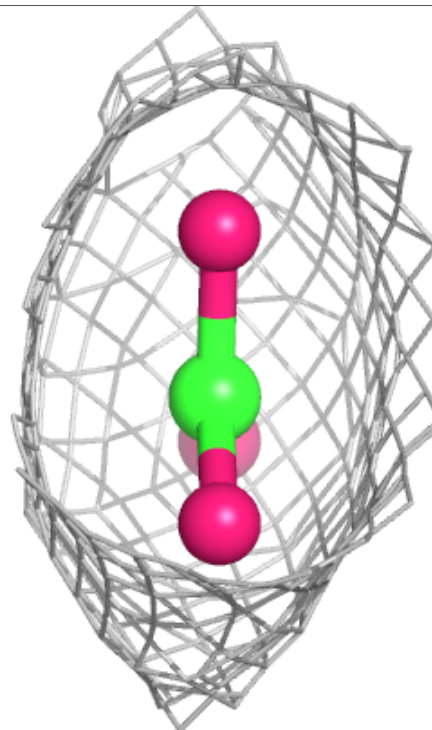
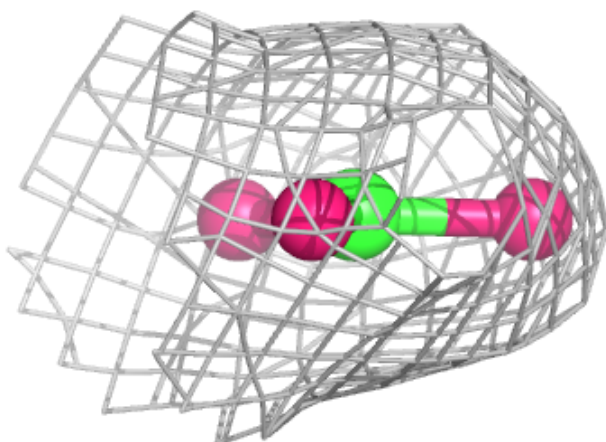
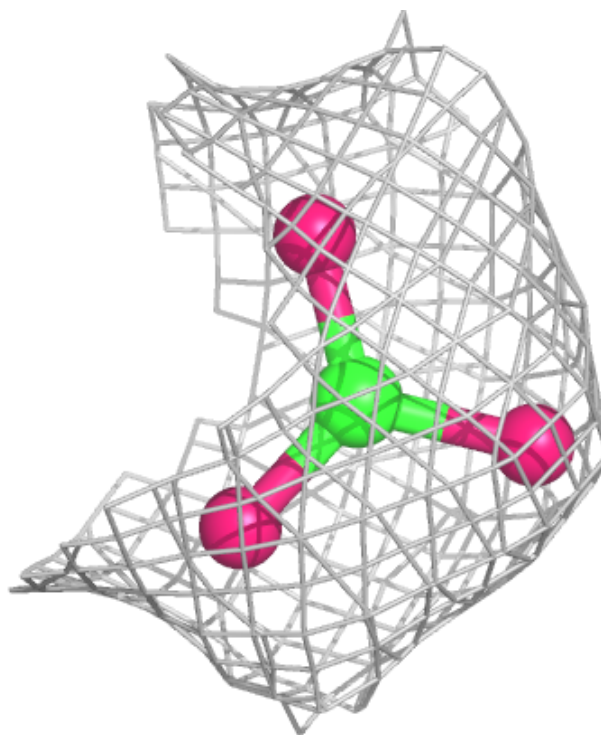
Electron density around BCT D 402 (A):

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



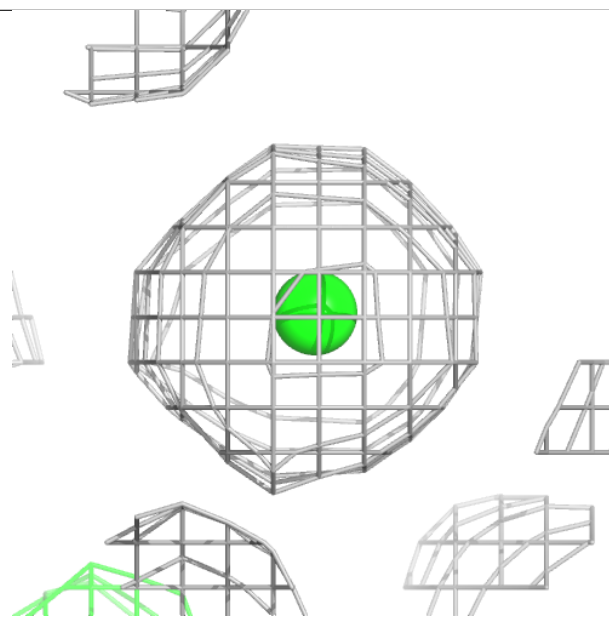
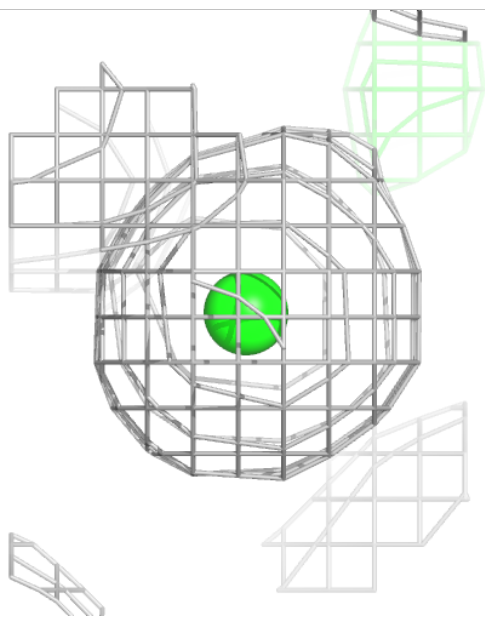
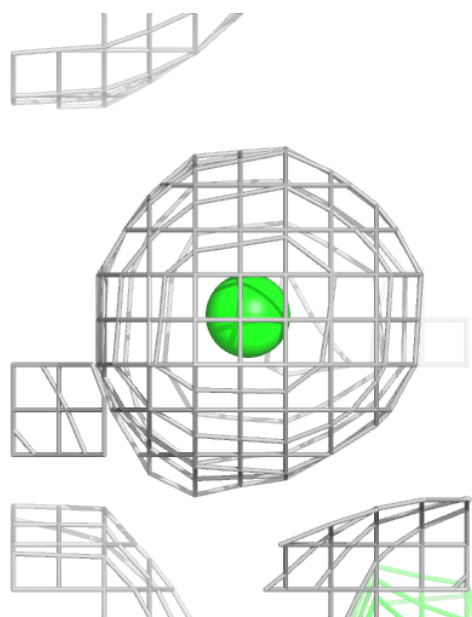
Electron density around BCT D 402 (B):

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



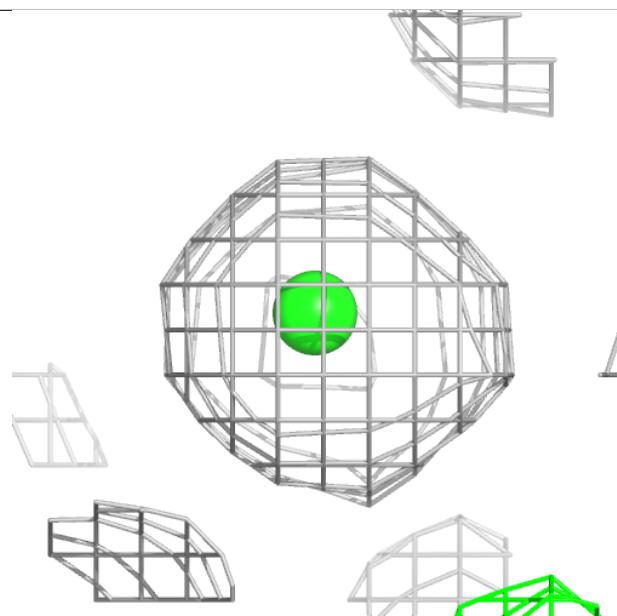
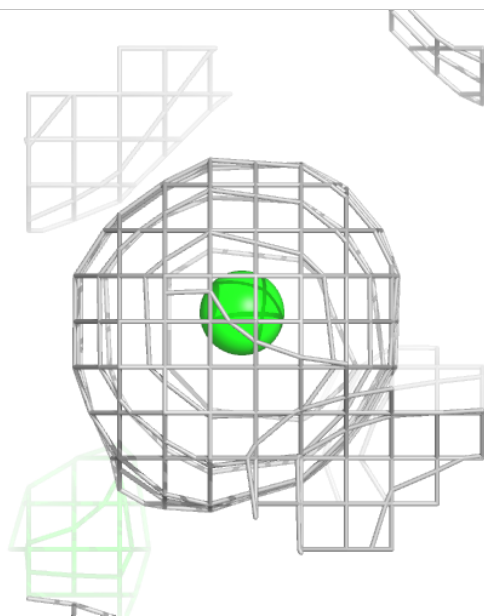
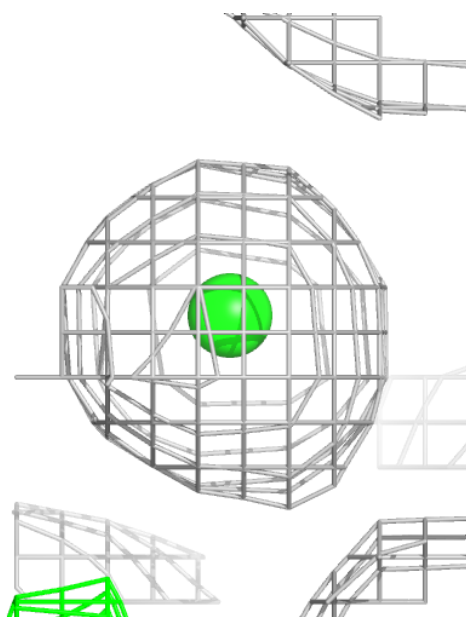
Electron density around CL a 403 (A):

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



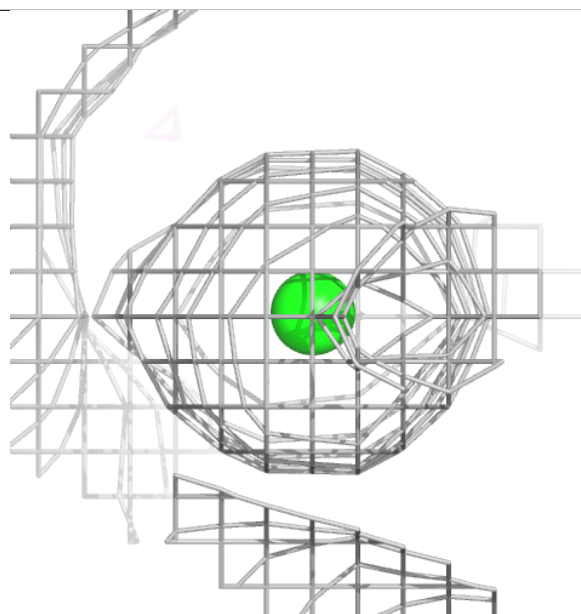
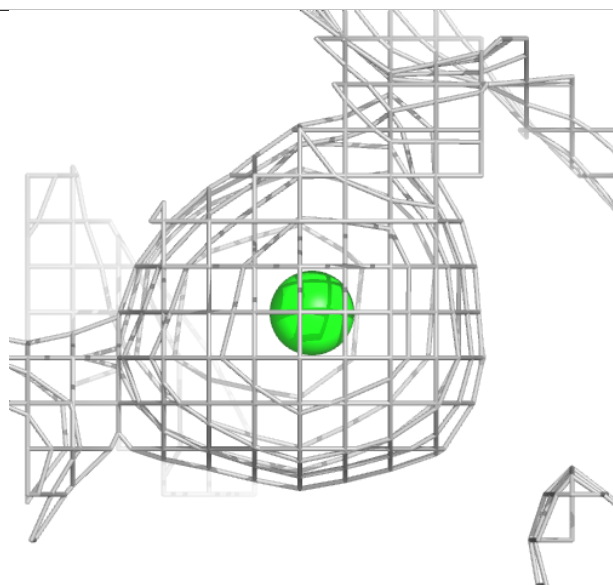
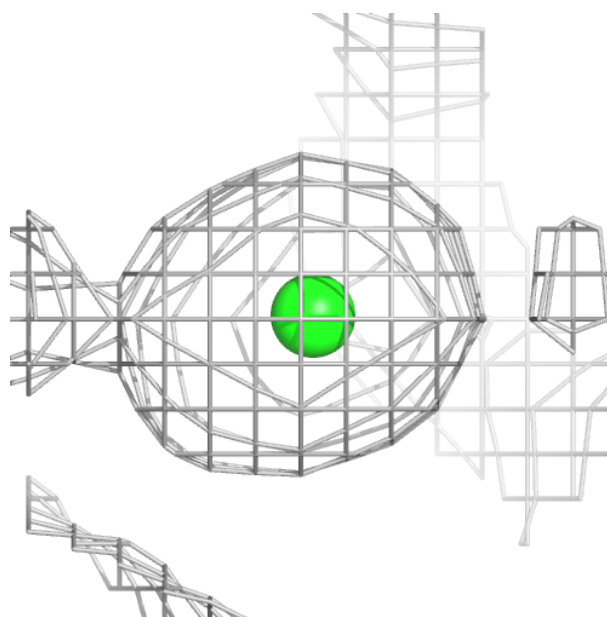
Electron density around CL a 403 (B):

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



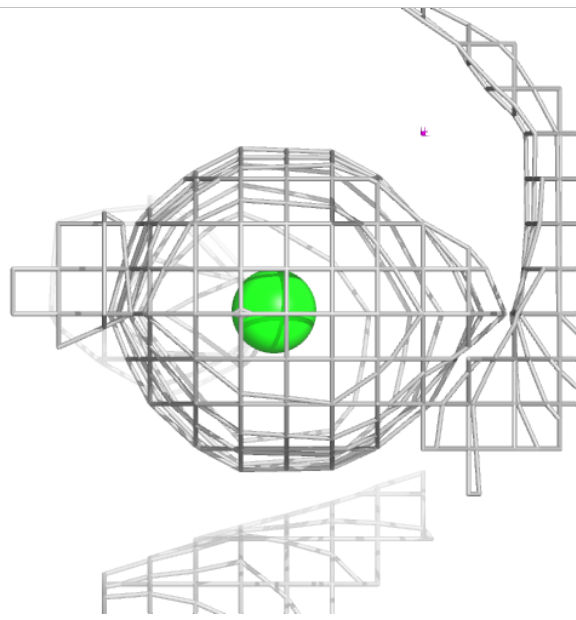
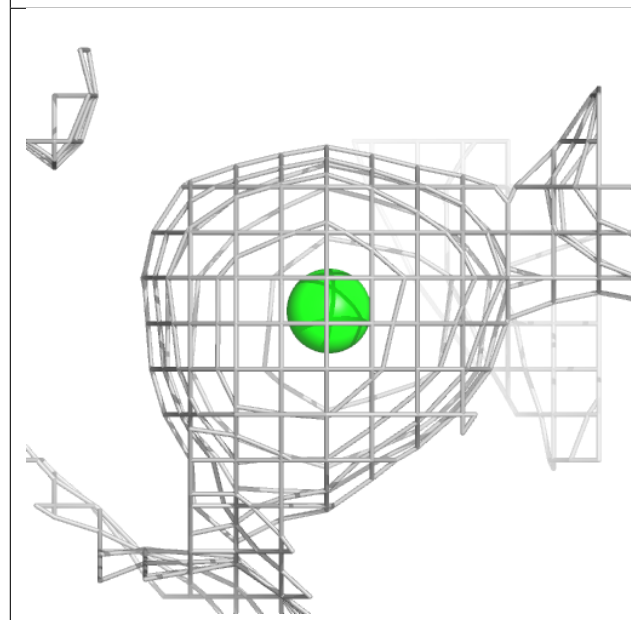
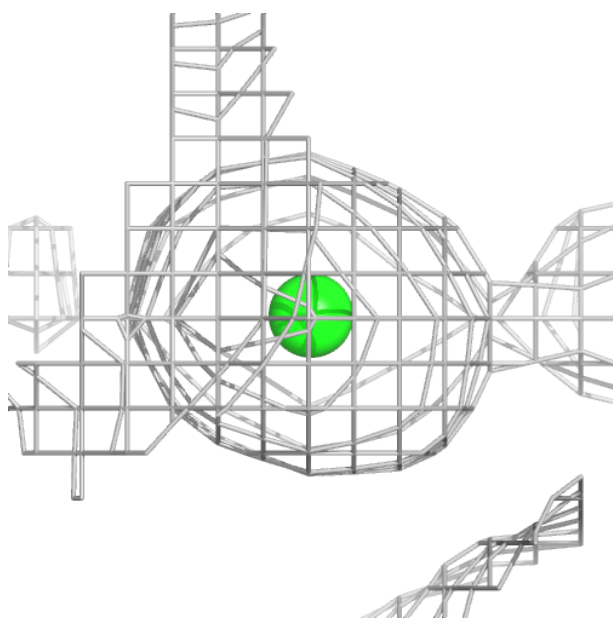
Electron density around CL a 404 (A):

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



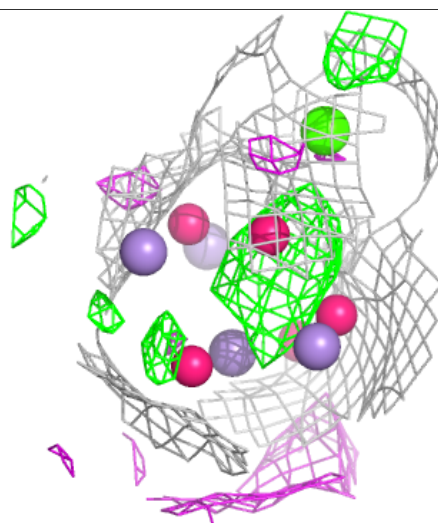
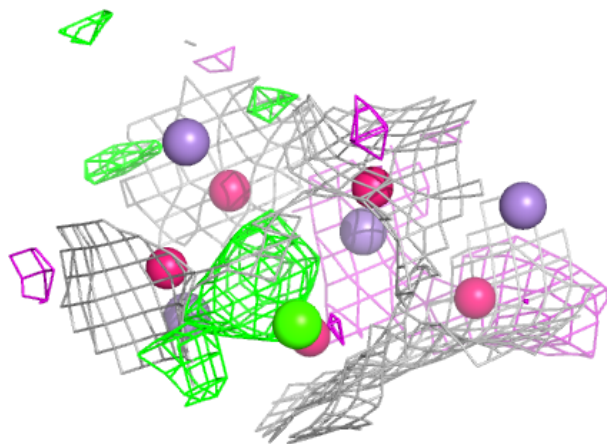
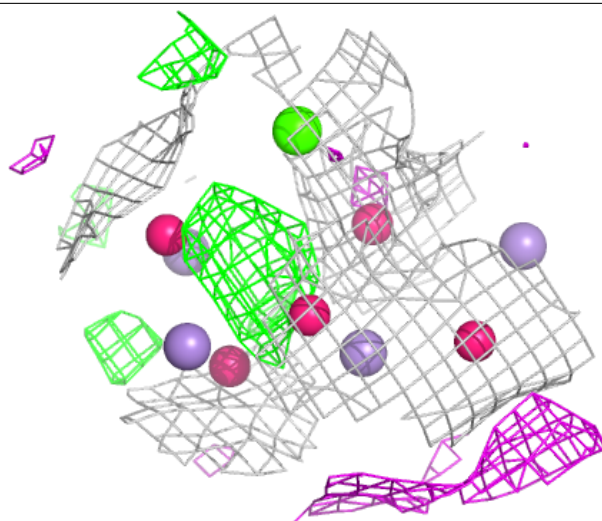
Electron density around CL a 404 (B):

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



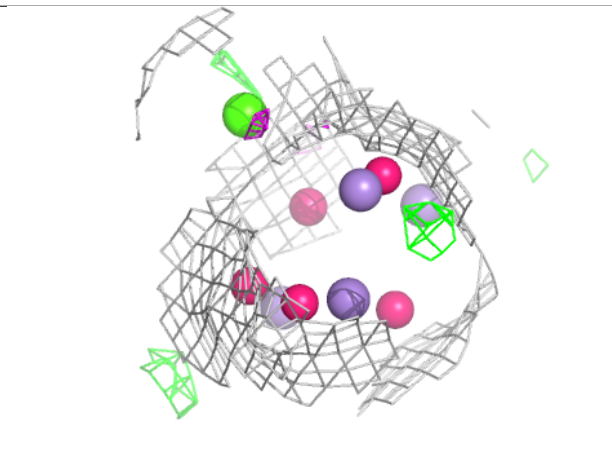
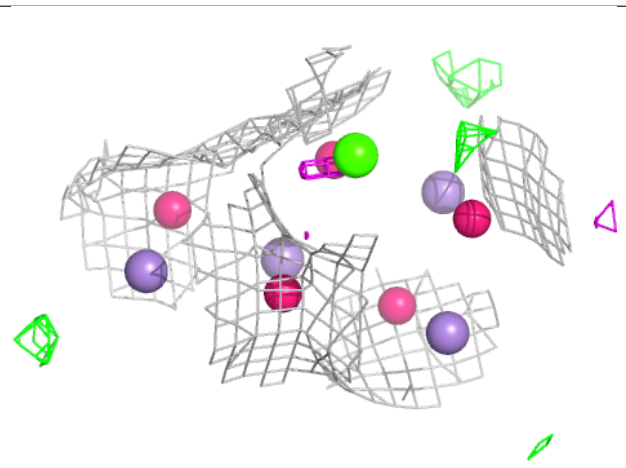
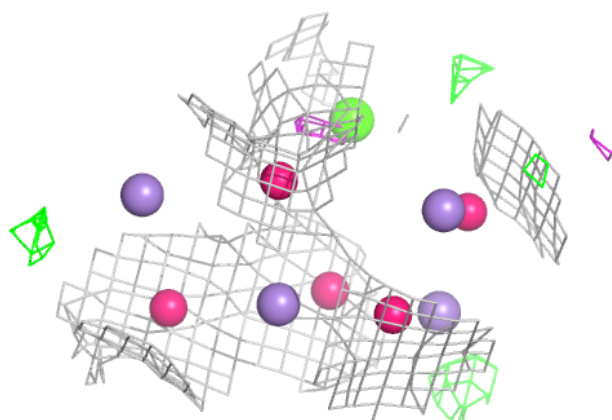
Electron density around OEX A 413 (A):

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



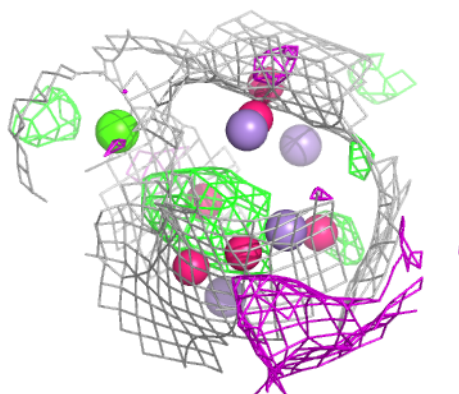
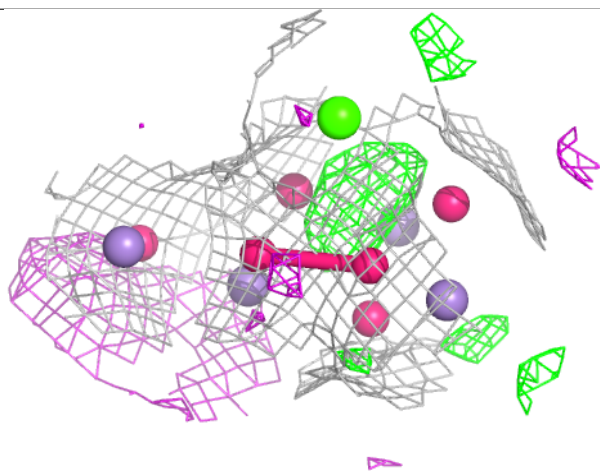
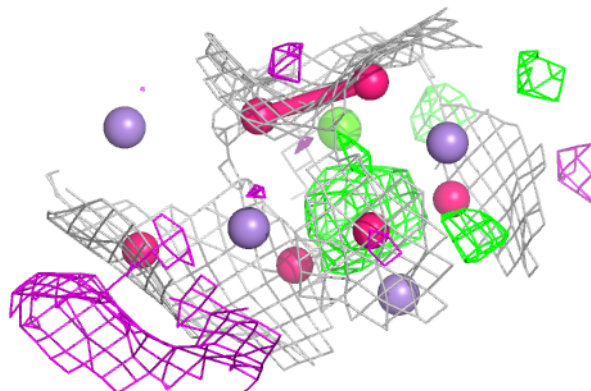
Electron density around OEX a 413 (A):

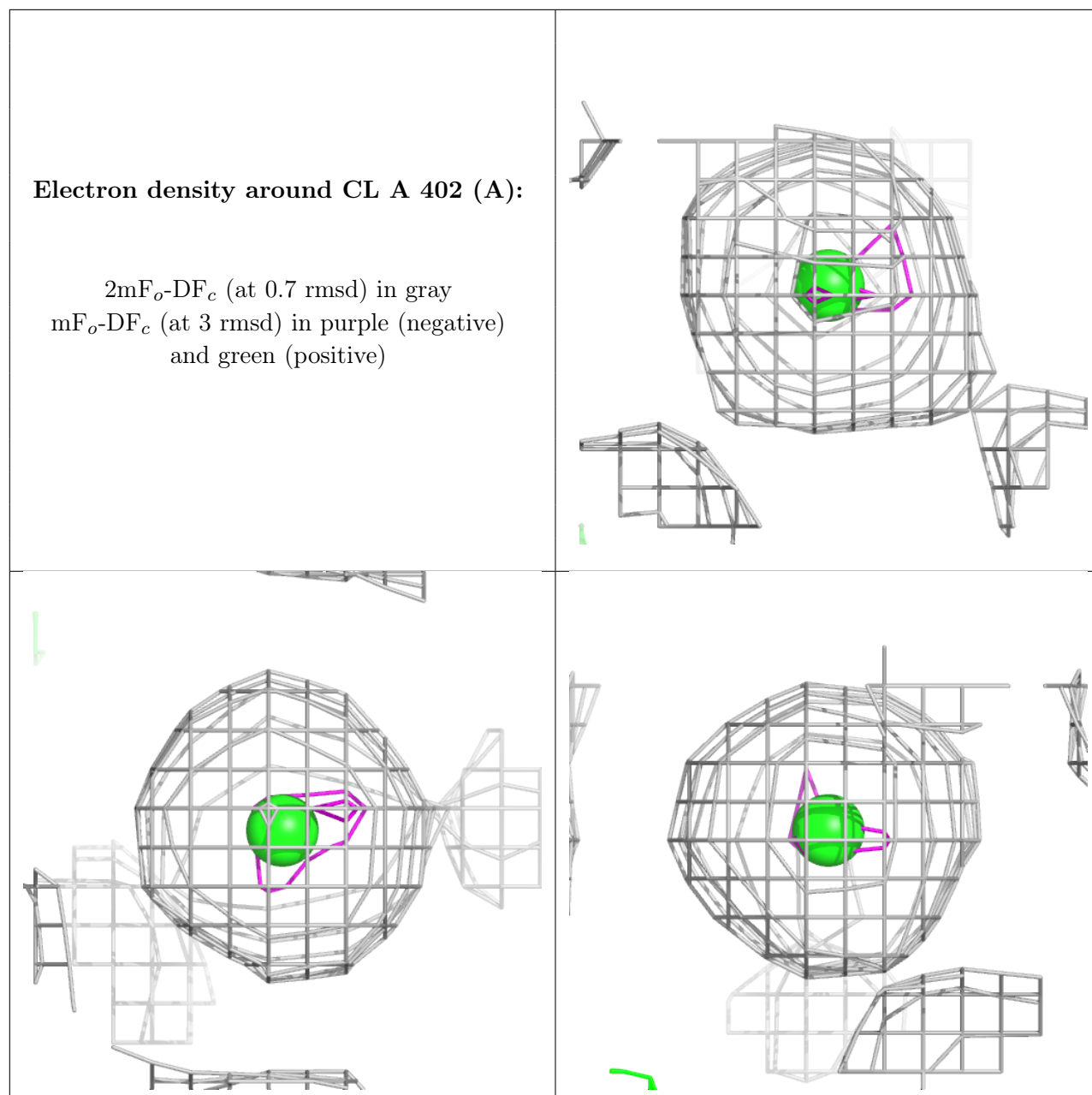
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OEY A 401 (B):

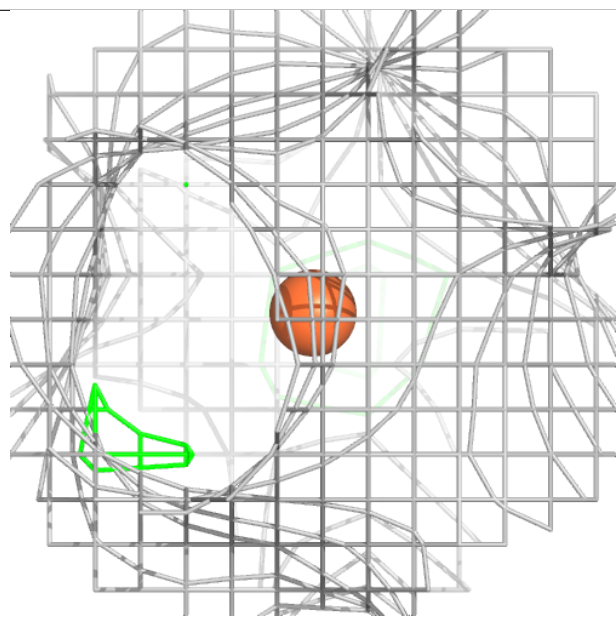
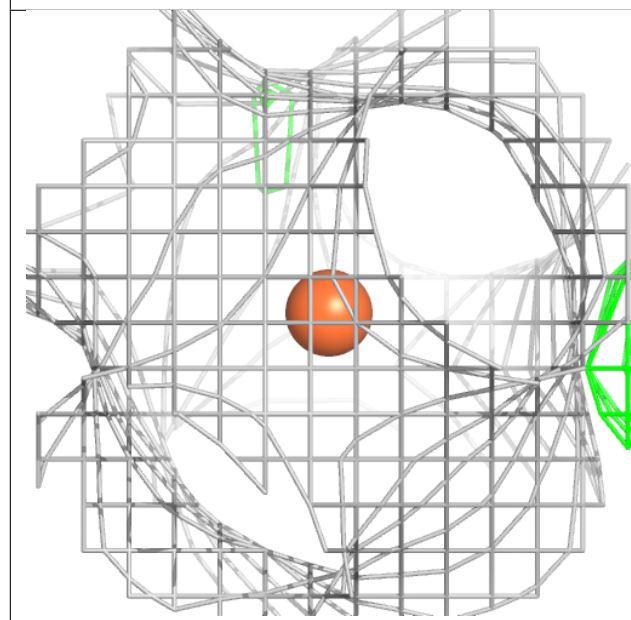
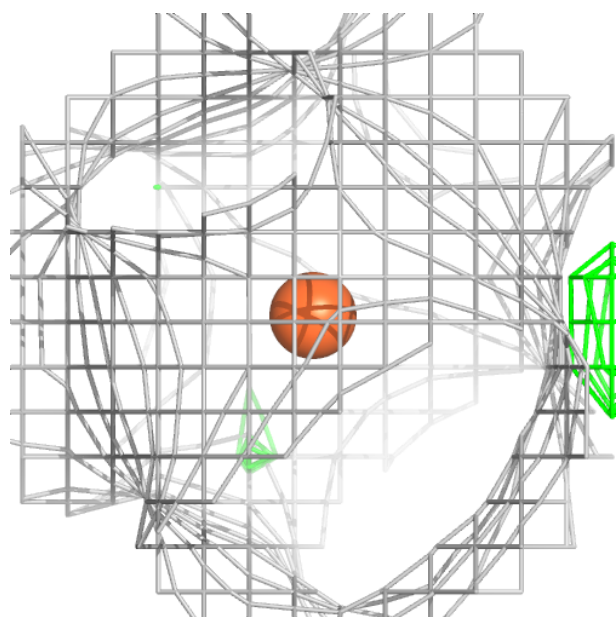
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





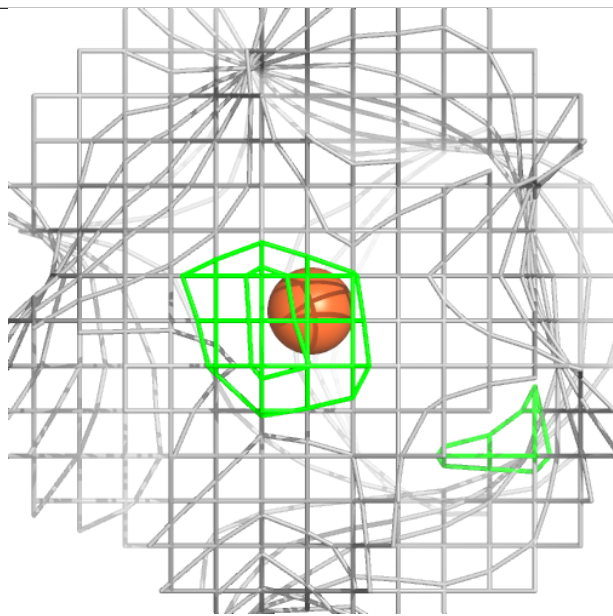
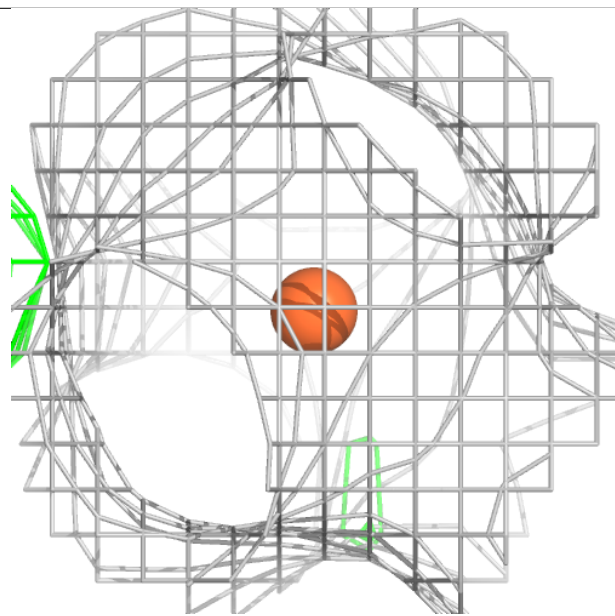
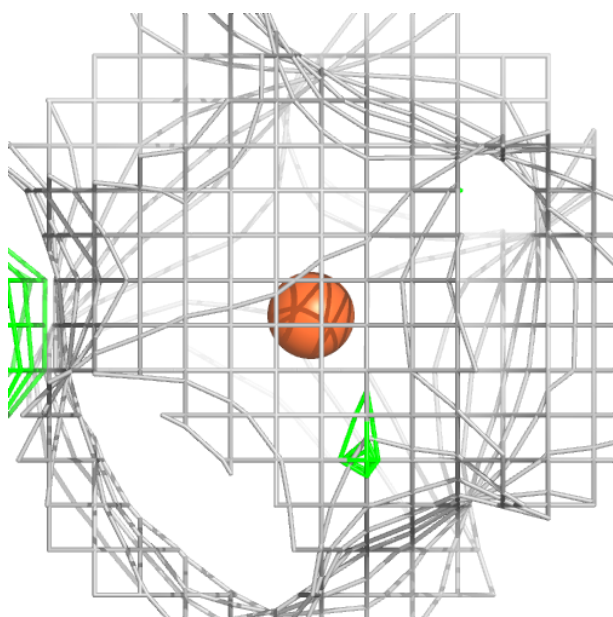
Electron density around FE2 a 402 (A):

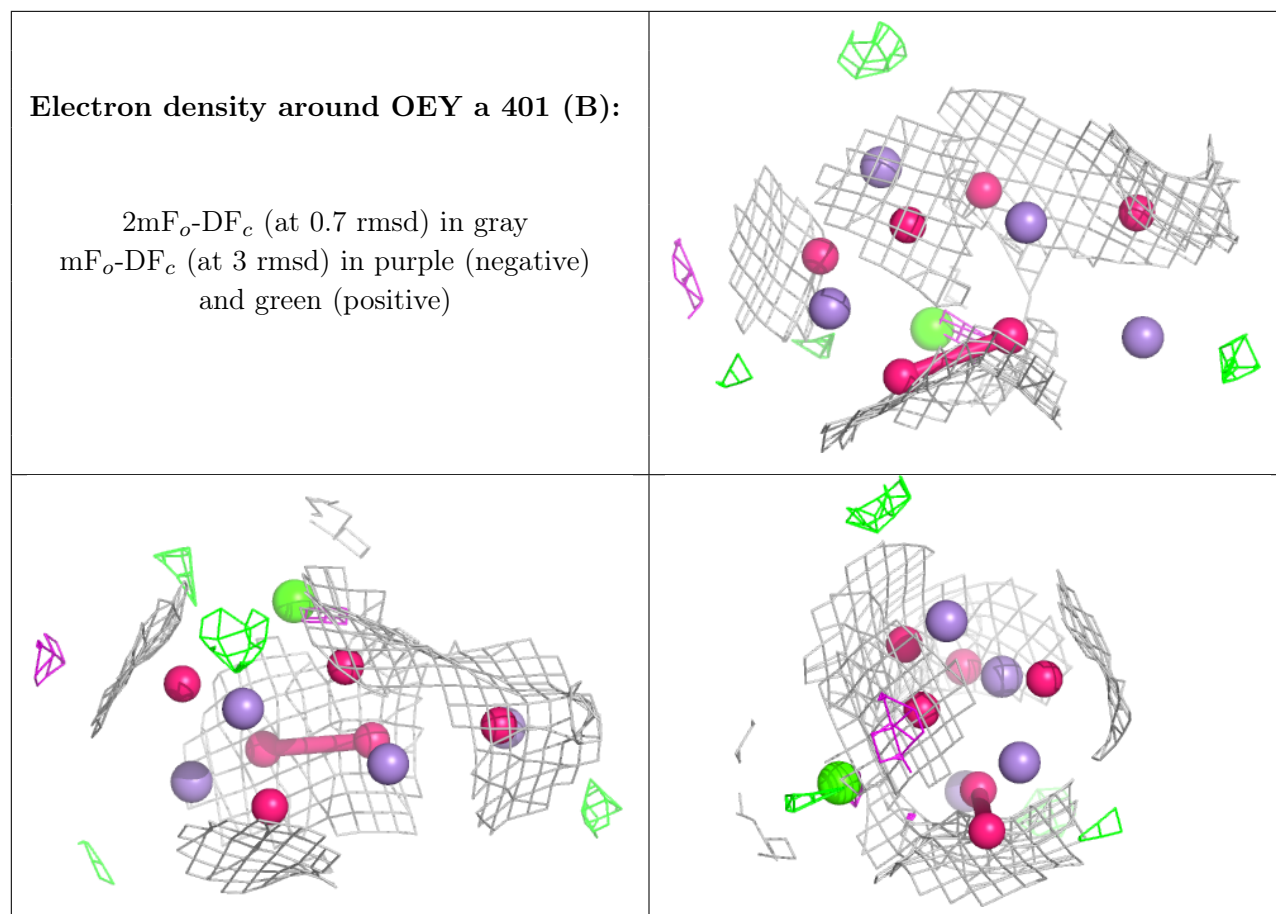
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.