



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2024 – 01:05 PM JST

PDB ID : 8IR5
Title : XFEL structure of cyanobacterial photosystem II under dark conditions
Authors : Li, H.; Suga, M.; Shen, J.R.
Deposited on : 2023-03-17
Resolution : 2.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

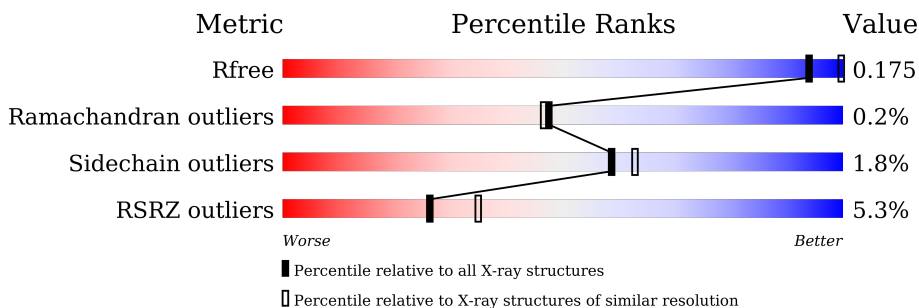
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	2% 97%
1	a	344	2% 97%
2	B	505	3% 99%
2	b	505	8% 99%
3	C	455	2% 98%
3	c	455	3% 99%
4	D	342	% 99%

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Mol	Chain	Length	Quality of chain
4	d	342	99%
5	E	84	94%
5	e	84	92% 6%
6	F	44	77% 23%
6	f	44	70% 30%
7	H	65	95%
7	h	65	94% 5%
8	I	38	89% 11%
8	i	38	97%
9	J	39	95%
9	j	39	97%
10	K	37	89% 11%
10	k	37	92% 8%
11	L	37	97%
11	l	37	97%
12	M	36	89% 8%
12	m	36	89% 6% 6%
13	O	244	97%
13	o	244	98%
14	T	32	88% 6% 6%
14	t	32	91% 6%
15	U	104	90% 8%
15	u	104	92% 7%
16	V	137	99%
16	v	137	96%

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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	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	501	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	D	402	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	406	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	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	c	514	X	-	-	-
23	CLA	d	401	X	-	-	-
23	CLA	d	402	X	-	-	-
27	GOL	A	418	-	-	-	X
27	GOL	a	419	-	-	-	X
27	GOL	a	420	-	-	-	X
27	GOL	l	102	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	UNL	B	626	-	-	-	X
31	LMT	F	101	-	-	-	X
31	LMT	e	101	-	-	-	X
34	HTG	b	623	-	-	-	X

2 Entry composition [i](#)

There are 41 unique types of molecules in this entry. The entry contains 52978 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	Total 2628	C 1722	N 432	O 459	S 15	0	1	0
1	a	334	Total 2629	C 1721	N 432	O 461	S 15	0	2	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	Total 4029	C 2639	N 674	O 703	S 13	0	7	0
2	b	504	Total 4017	C 2636	N 669	O 699	S 13	0	6	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	Total 3497	C 2287	N 588	O 609	S 13	0	1	0
3	c	455	Total 3555	C 2327	N 595	O 620	S 13	0	5	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	1	0
			2732	1808	446	466	12			
4	d	341	Total	C	N	O	S	0	2	0
			2732	1808	447	465	12			

- 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
			Total	C	N	O	S			
8	I	38	314	211	48	54	1	0	0	0
8	i	38	314	211	48	54	1	0	0	0

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

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

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

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

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
			Total	C	N	O			
11	L	36	296	197	47	52	0	0	0
11	l	36	296	197	47	52	0	0	0

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

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

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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	3	0
			1894	1181	321	388	4			
13	o	243	Total	C	N	O	S	0	0	0
			1865	1165	315	381	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	1	0
			267	186	37	42	2			
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	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	1	0
			774	491	129	154			
15	u	97	Total	C	N	O	0	1	0
			781	496	130	155			

- 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	2	0
			1082	685	179	214	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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

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

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

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

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

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

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

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

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

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

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

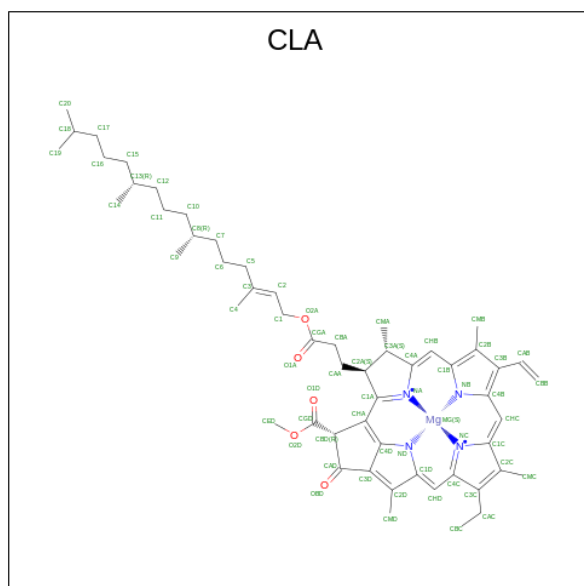
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		

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

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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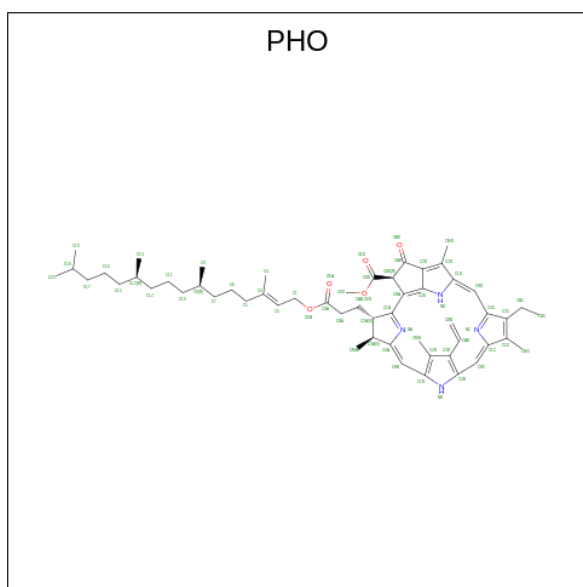
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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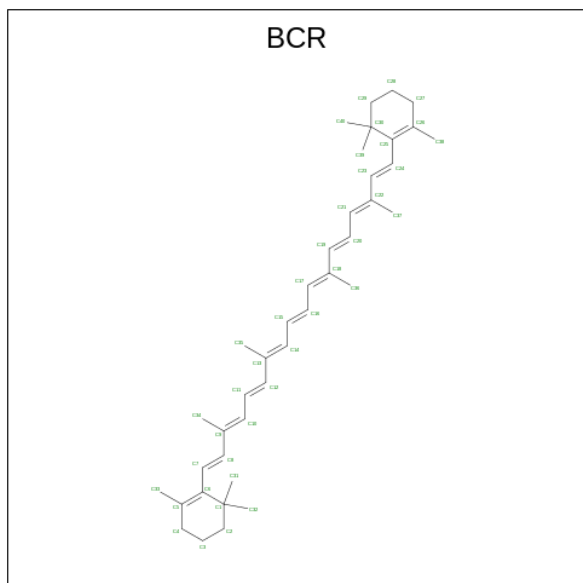
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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



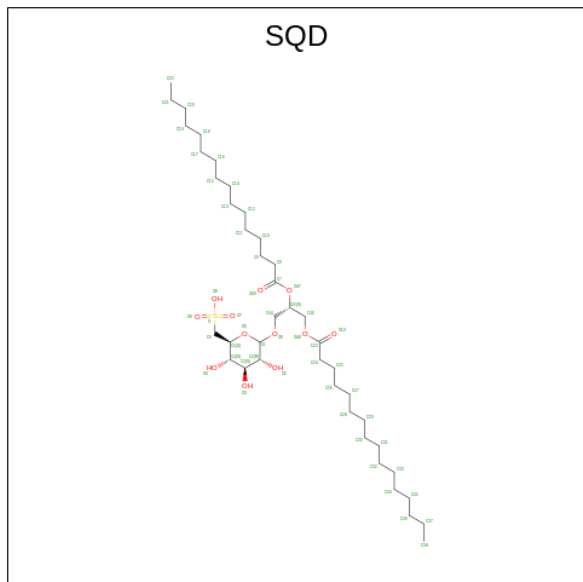
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
24	A	1	64	55	4	5	0	0
24	A	1	64	55	4	5	0	0
24	a	1	64	55	4	5	0	0
24	a	1	64	55	4	5	0	0

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



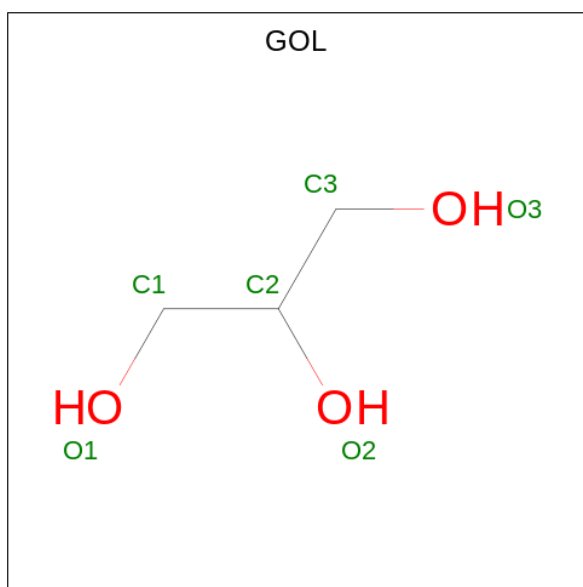
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total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

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



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

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



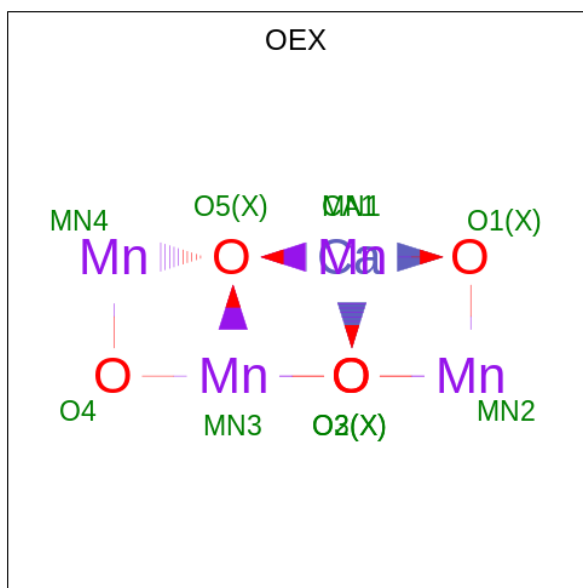
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 6 3 3	0	0
27	A	1	Total C O 6 3 3	0	0
27	B	1	Total C O 6 3 3	0	0
27	B	1	Total C O 6 3 3	0	0
27	B	1	Total C O 6 3 3	0	0
27	C	1	Total C O 6 3 3	0	0
27	O	1	Total C O 6 3 3	0	0
27	O	1	Total C O 6 3 3	0	0
27	V	1	Total C O 6 3 3	0	0
27	a	1	Total C O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

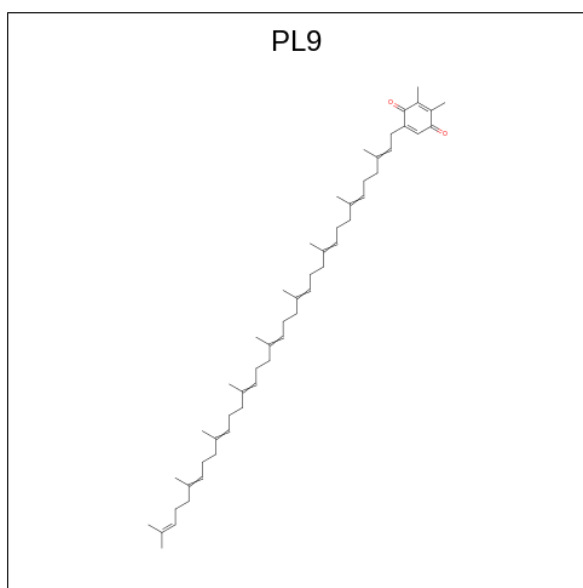
- Molecule 28 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
28	a	1	Total	Ca	Mn	O	0	0
			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	0
			55	53	2		
29	D	1	Total	C	O	0	0
			55	53	2		
29	a	1	Total	C	O	0	0
			55	53	2		
29	d	1	Total	C	O	0	0
			55	53	2		

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

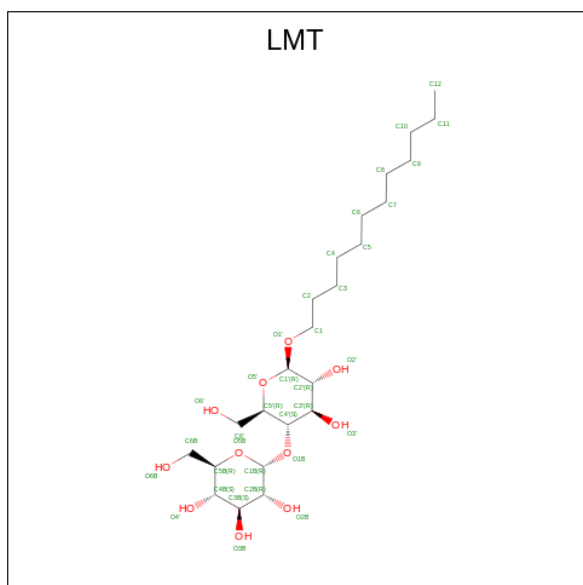
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			28	23	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	I	1	Total	C	O	0	0
			40	35	5		
30	J	1	Total	C		0	0
			10	10			
30	K	1	Total	C	O	0	0
			34	29	5		
30	X	1	Total	C	O	0	0
			18	16	2		

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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	0
			32	27	5		
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: $C_{24}H_{46}O_{11}$).



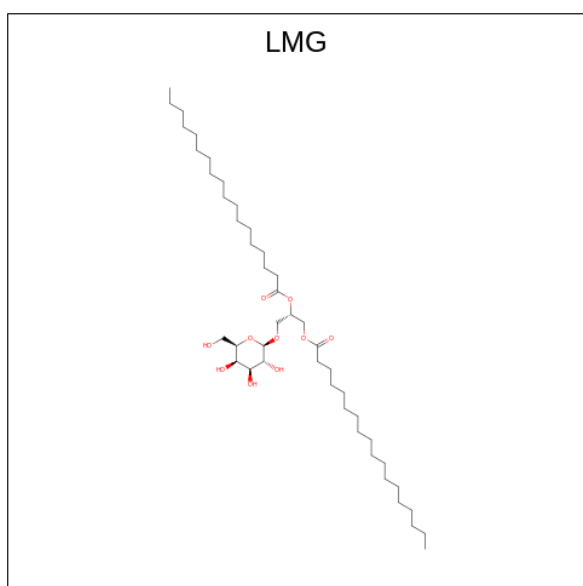
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			35	24	11		
31	A	1	Total	C	O	0	0
			35	24	11		

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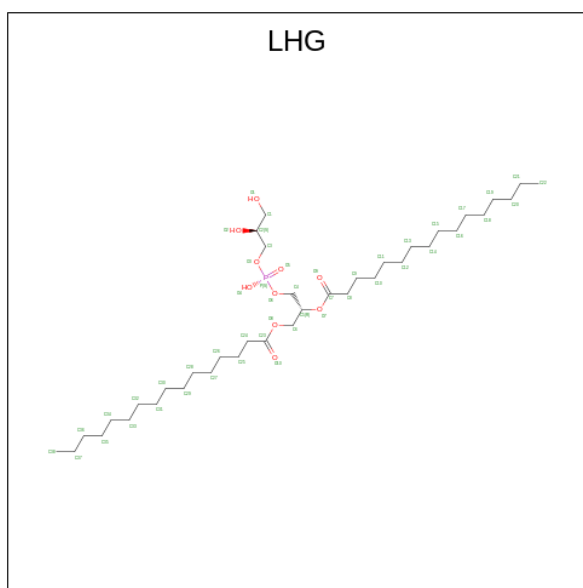
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			25	19	6		
31	F	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total	C	O	0	0
			35	24	11		
31	T	1	Total	C	O	0	0
			35	24	11		
31	b	1	Total	C	O	0	0
			25	19	6		
31	b	1	Total	C	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-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



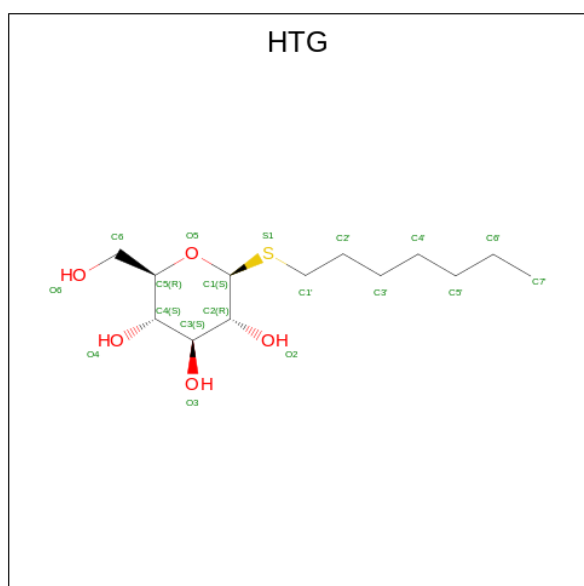
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			51	41	10		
32	B	1	Total	C	O	0	0
			51	41	10		
32	C	1	Total	C	O	0	0
			51	41	10		
32	C	1	Total	C	O	0	0
			51	41	10		
32	D	1	Total	C	O	0	0
			51	41	10		
32	a	1	Total	C	O	0	0
			51	41	10		
32	c	1	Total	C	O	0	0
			51	41	10		
32	c	1	Total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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	A	1	Total	C	O	P	0	0
			49	38	10	1		
33	D	1	Total	C	O	P	0	0
			49	38	10	1		
33	D	1	Total	C	O	P	0	0
			49	38	10	1		
33	E	1	Total	C	O	P	0	0
			42	31	10	1		
33	L	1	Total	C	O	P	0	0
			49	38	10	1		
33	a	1	Total	C	O	P	0	0
			42	31	10	1		
33	b	1	Total	C	O	P	0	0
			49	38	10	1		
33	d	1	Total	C	O	P	0	0
			49	38	10	1		
33	d	1	Total	C	O	P	0	0
			49	38	10	1		
33	d	1	Total	C	O	P	0	0
			49	38	10	1		

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



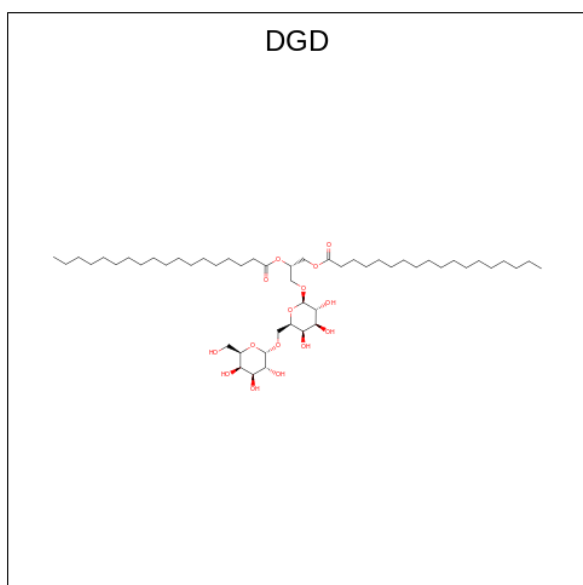
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	O	S	0	0
			19	13	5	1		

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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
35	C	1	Total 62	C 47	O 15	0	0

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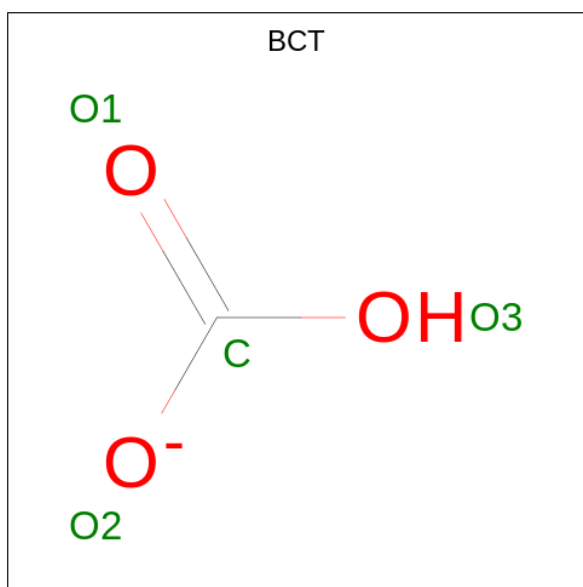
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	C	1	Total C O 62 47 15	0	0
35	C	1	Total C O 62 47 15	0	0
35	H	1	Total C O 62 47 15	0	0
35	c	1	Total C O 62 47 15	0	0
35	c	1	Total C O 62 47 15	0	0
35	c	1	Total C O 62 47 15	0	0
35	h	1	Total C O 62 47 15	0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

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

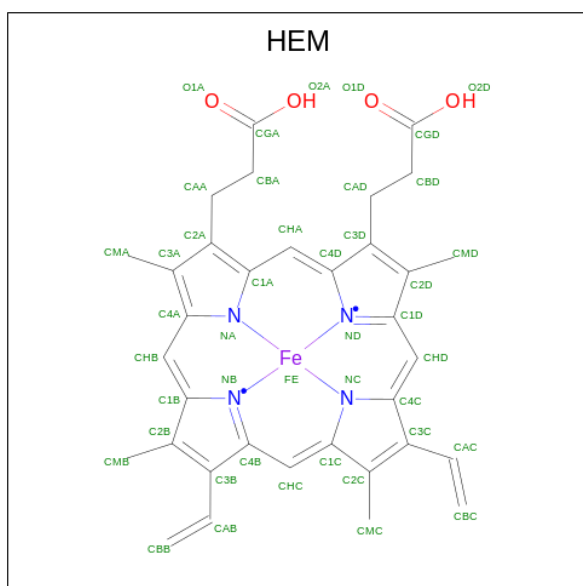
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	C	1	Total Ca 1 1	0	0
36	F	1	Total Ca 1 1	0	0
36	O	1	Total Ca 1 1	0	0
36	c	2	Total Ca 2 2	0	0
36	f	1	Total Ca 1 1	0	0
36	o	1	Total Ca 1 1	0	0

- Molecule 37 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	D	1	Total	C	O	0	0
			4	1	3		
37	a	1	Total	C	O	0	0
			4	1	3		

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



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

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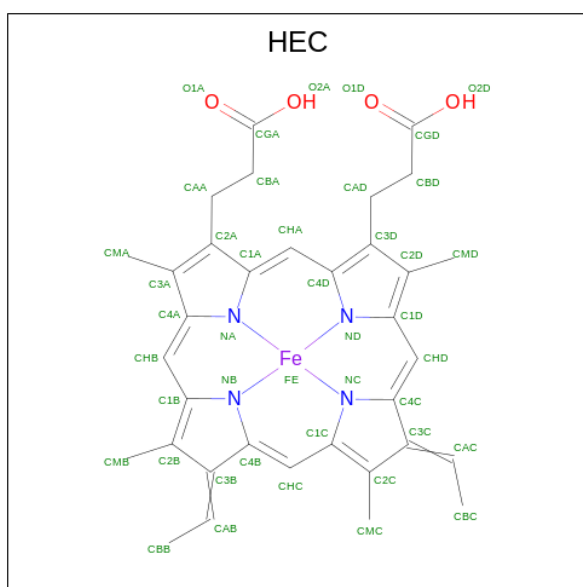
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
38	f	1	43	34	1	4	4	0	0

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

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

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



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
41	A	139	140	140	0	1
41	B	188	188	188	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	C	167	Total O 167 167	0	0
41	D	123	Total O 123 123	0	0
41	E	13	Total O 13 13	0	0
41	F	7	Total O 7 7	0	0
41	H	21	Total O 21 21	0	0
41	I	5	Total O 5 5	0	0
41	J	8	Total O 8 8	0	0
41	K	5	Total O 5 5	0	0
41	L	9	Total O 9 9	0	0
41	M	5	Total O 5 5	0	0
41	O	105	Total O 105 105	0	0
41	T	10	Total O 10 10	0	0
41	U	44	Total O 44 44	0	0
41	V	82	Total O 82 82	0	0
41	X	7	Total O 7 7	0	0
41	a	130	Total O 130 130	0	0
41	b	202	Total O 202 202	0	0
41	c	161	Total O 161 161	0	0
41	d	111	Total O 111 111	0	0
41	e	9	Total O 9 9	0	0
41	f	3	Total O 3 3	0	0

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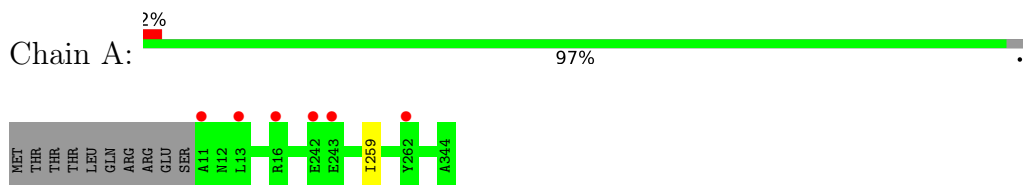
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	h	17	Total O 17 17	0	0
41	i	2	Total O 2 2	0	0
41	j	2	Total O 2 2	0	0
41	k	3	Total O 3 3	0	0
41	l	8	Total O 8 8	0	0
41	m	13	Total O 13 13	0	0
41	o	103	Total O 103 103	0	0
41	t	7	Total O 7 7	0	0
41	u	49	Total O 49 49	0	0
41	v	57	Total O 57 57	0	0
41	x	8	Total O 8 8	0	0
41	y	2	Total O 2 2	0	0

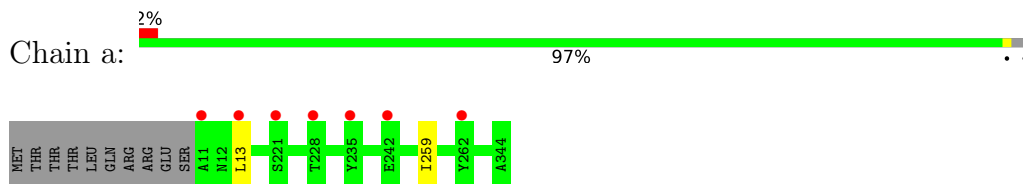
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

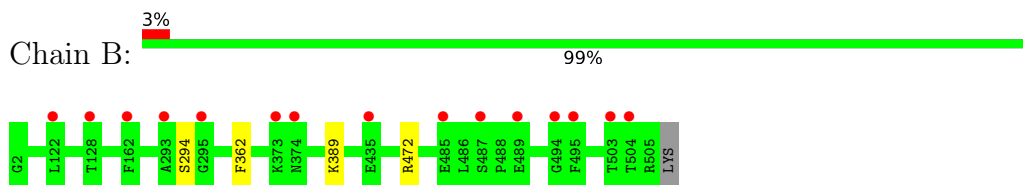
- Molecule 1: Photosystem II protein D1



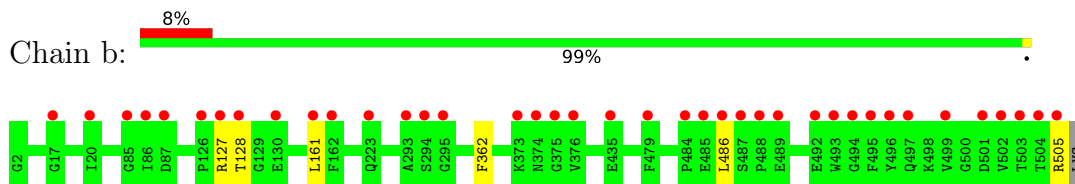
- Molecule 1: Photosystem II protein D1



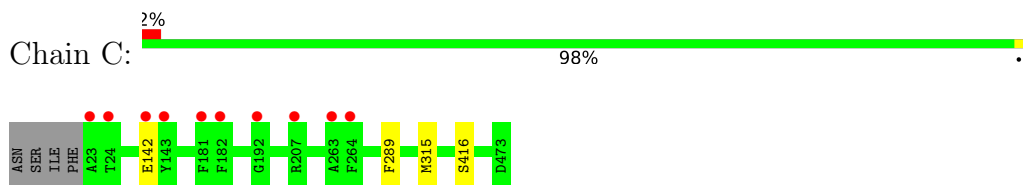
- Molecule 2: Photosystem II CP47 reaction center protein



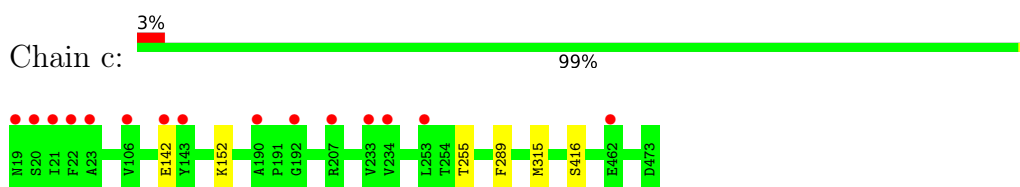
- Molecule 2: Photosystem II CP47 reaction center protein



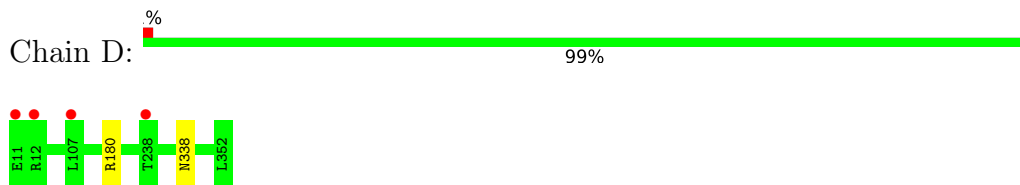
- Molecule 3: Photosystem II CP43 reaction center protein



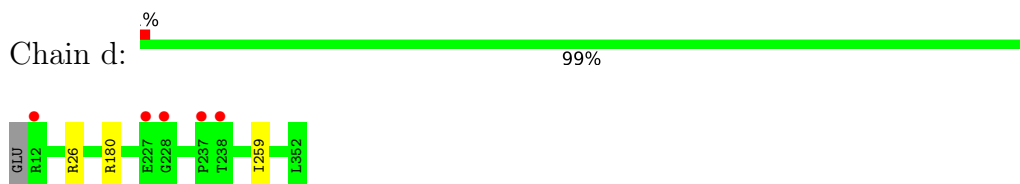
- Molecule 3: Photosystem II CP43 reaction center protein



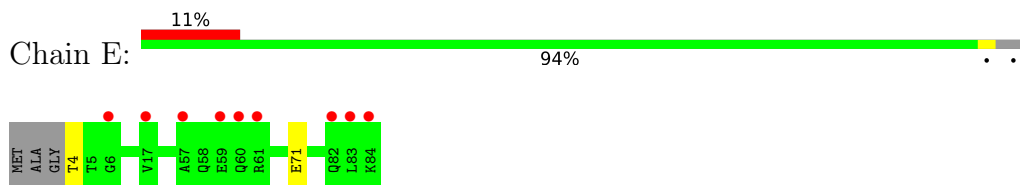
- Molecule 4: Photosystem II D2 protein



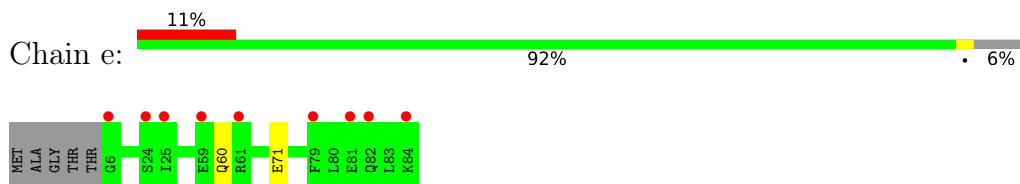
- Molecule 4: Photosystem II D2 protein



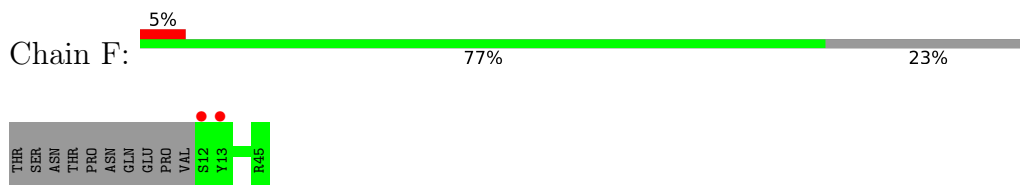
- Molecule 5: Cytochrome b559 subunit alpha



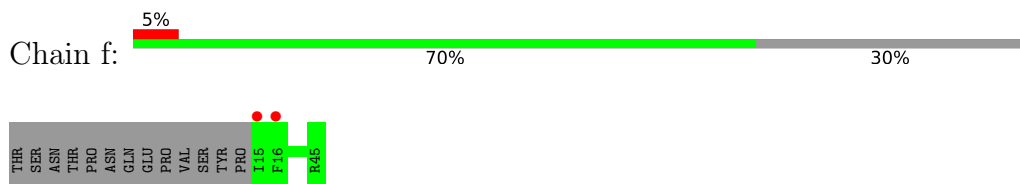
- Molecule 5: Cytochrome b559 subunit alpha



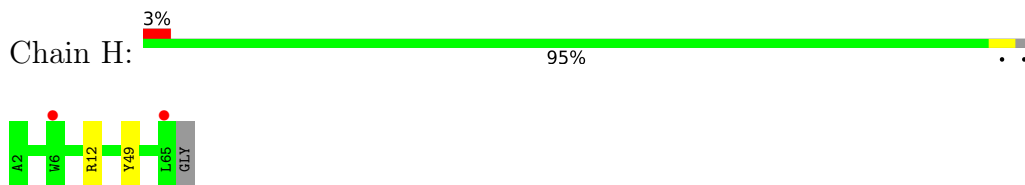
- Molecule 6: Cytochrome b559 subunit beta



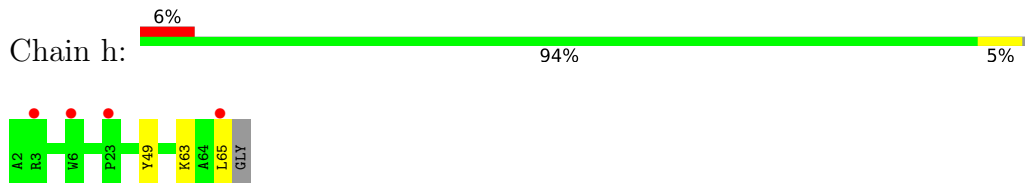
- Molecule 6: Cytochrome b559 subunit beta



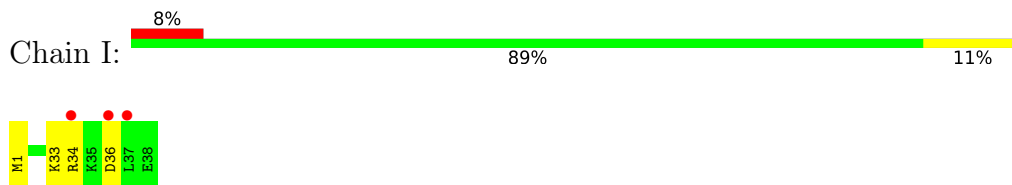
- Molecule 7: Photosystem II reaction center protein H



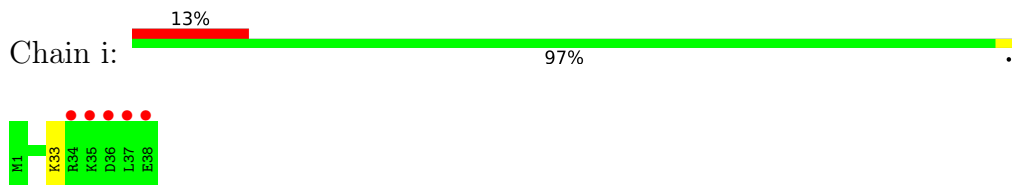
- Molecule 7: Photosystem II reaction center protein H



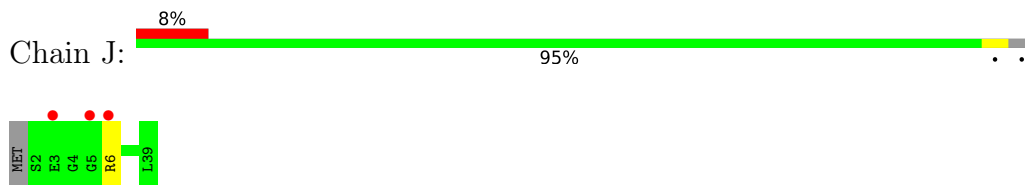
- Molecule 8: Photosystem II reaction center protein I



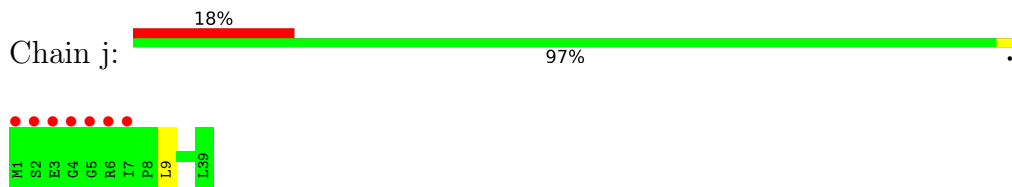
- Molecule 8: Photosystem II reaction center protein I



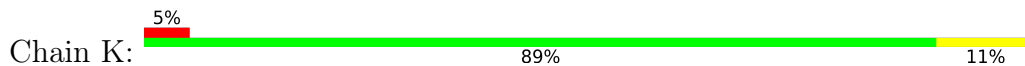
- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K

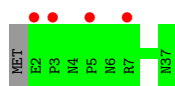




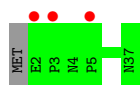
- Molecule 10: Photosystem II reaction center protein K



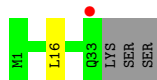
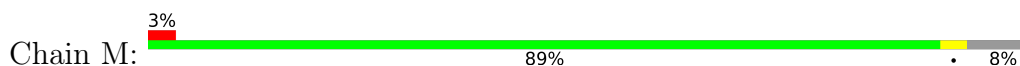
- Molecule 11: Photosystem II reaction center protein L



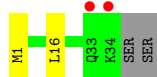
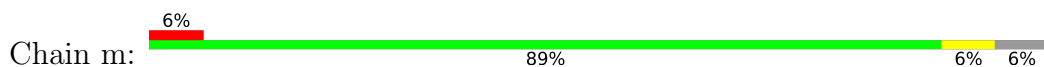
- Molecule 11: Photosystem II reaction center protein L



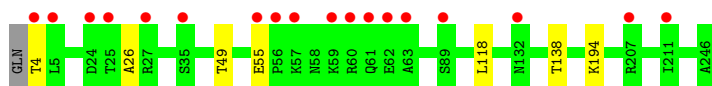
- Molecule 12: Photosystem II reaction center protein M



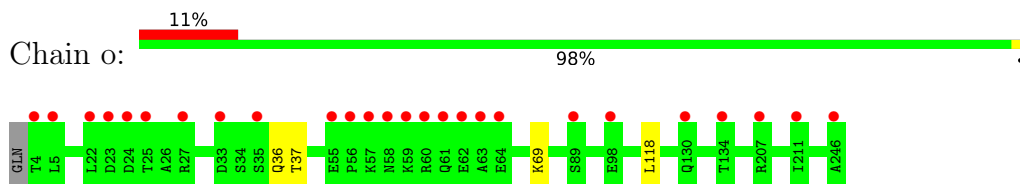
- Molecule 12: Photosystem II reaction center protein M



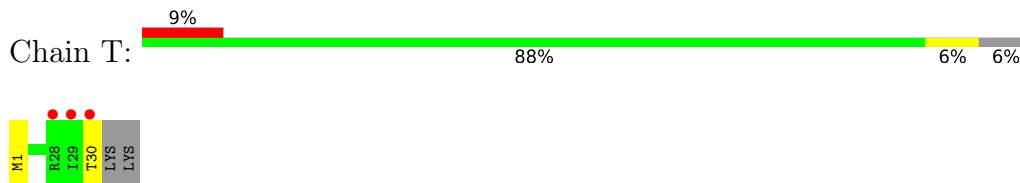
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



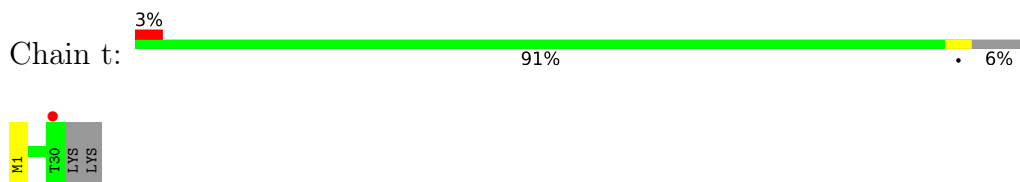
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



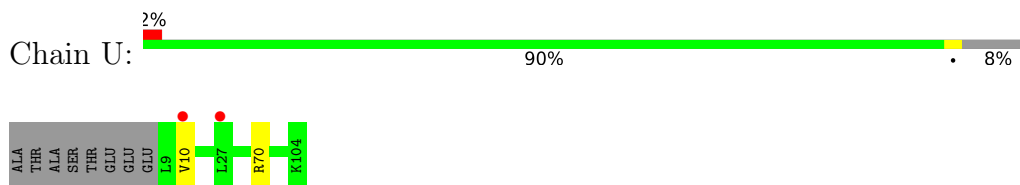
- Molecule 14: Photosystem II reaction center protein T



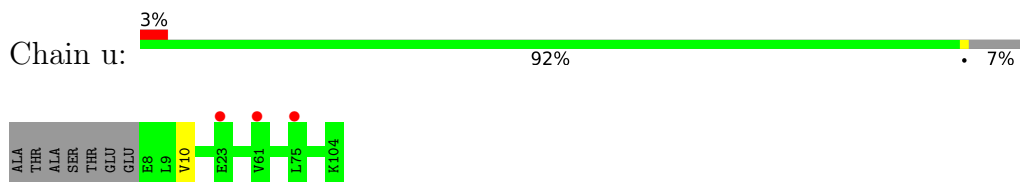
- Molecule 14: Photosystem II reaction center protein T



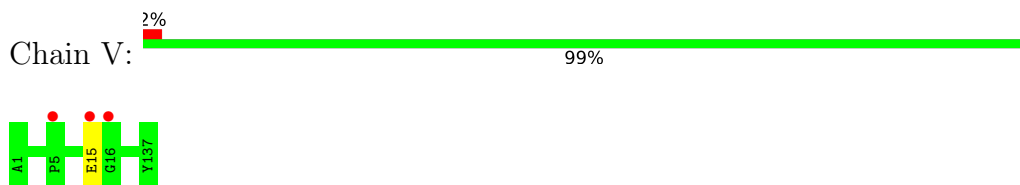
- Molecule 15: Photosystem II 12 kDa extrinsic protein



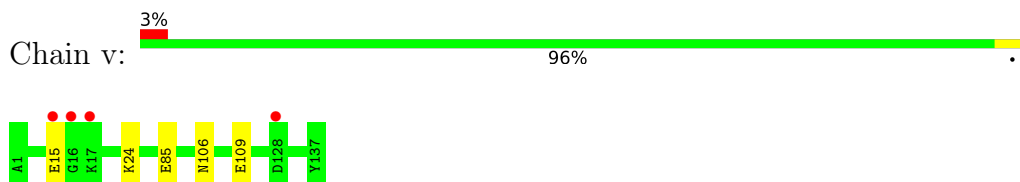
- Molecule 15: Photosystem II 12 kDa extrinsic protein



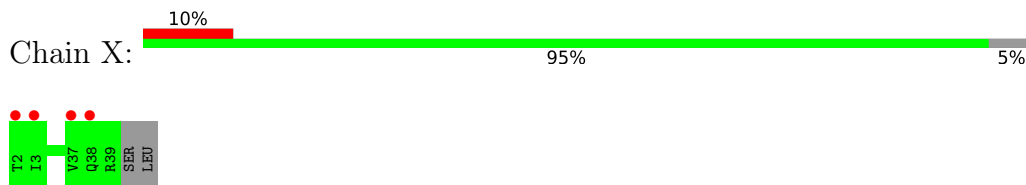
- Molecule 16: Cytochrome c-550



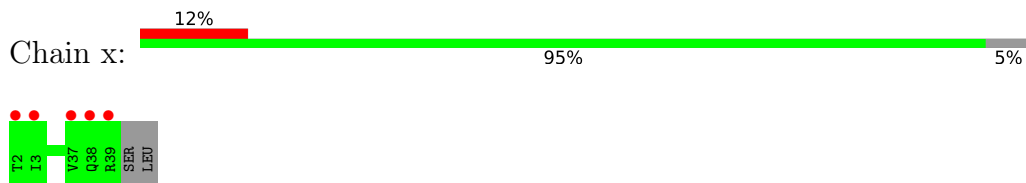
- Molecule 16: Cytochrome c-550



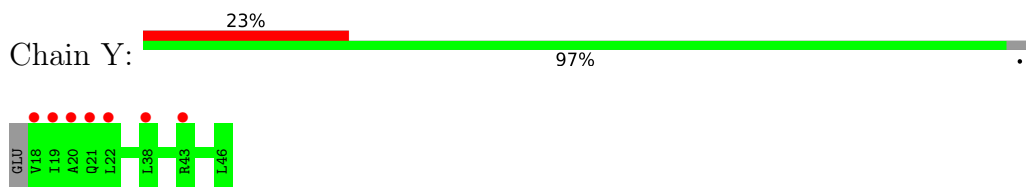
- Molecule 17: Photosystem II reaction center protein X



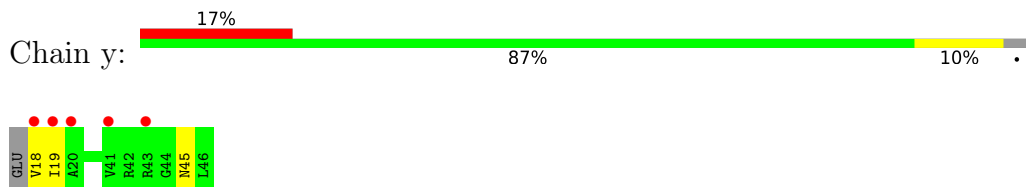
- Molecule 17: Photosystem II reaction center protein X



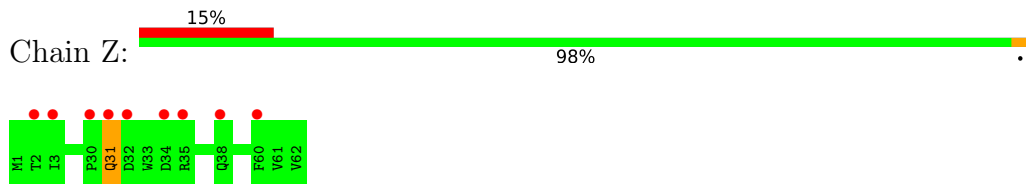
- Molecule 18: Photosystem II reaction center protein Ycf12



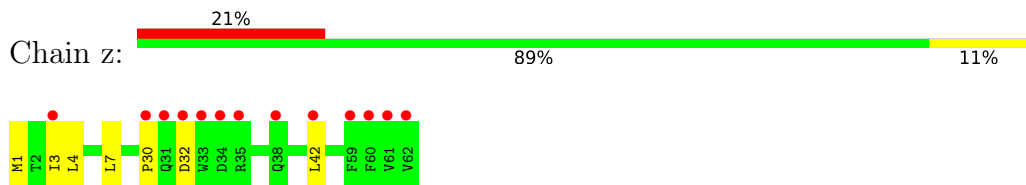
- Molecule 18: Photosystem II reaction center protein Ycf12



- Molecule 19: Photosystem II reaction center protein Z

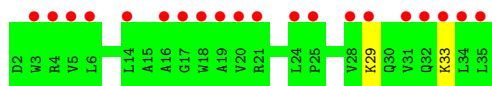


- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	125.75Å 231.60Å 288.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.15 19.98 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.98-2.15) 99.9 (19.98-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.15Å)	Xtrriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.144 , 0.175 0.144 , 0.175	Depositor DCC
R_{free} test set	22612 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtrriage
Anisotropy	0.493	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 84.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	52978	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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: CLA, CA, LMT, LHG, FE2, HTG, LMG, SQD, MG, UNL, HEM, GOL, BCR, CL, BCT, PHO, OEX, DGD, PL9, HEC, FME

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.42	0/2713	0.57	0/3700
1	a	0.41	0/2717	0.55	0/3705
2	B	0.41	0/4169	0.57	0/5679
2	b	0.38	0/4161	0.56	0/5669
3	C	0.37	0/3610	0.54	0/4914
3	c	0.37	0/3675	0.52	0/5002
4	D	0.44	0/2827	0.59	0/3852
4	d	0.43	0/2827	0.56	0/3852
5	E	0.36	0/681	0.56	0/928
5	e	0.36	0/690	0.53	0/939
6	F	0.37	0/284	0.52	0/387
6	f	0.34	0/269	0.51	0/365
7	H	0.36	0/519	0.58	0/708
7	h	0.35	0/530	0.55	0/722
8	I	0.33	0/311	0.53	0/419
8	i	0.38	0/311	0.53	0/419
9	J	0.37	0/278	0.51	0/376
9	j	0.32	0/283	0.52	0/383
10	K	0.36	0/303	0.49	0/416
10	k	0.35	0/303	0.49	0/416
11	L	0.37	0/303	0.53	0/412
11	l	0.40	0/303	0.52	0/412
12	M	0.39	0/261	0.48	0/357
12	m	0.37	0/279	0.49	0/380
13	O	0.38	0/1925	0.61	0/2609
13	o	0.37	0/1896	0.61	0/2571
14	T	0.45	0/266	0.54	0/362
14	t	0.43	0/257	0.51	0/349
15	U	0.40	0/785	0.59	0/1064
15	u	0.39	0/792	0.60	0/1074
16	V	0.37	0/1103	0.56	0/1497

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.33	0/1085	0.53	0/1473
17	X	0.31	0/292	0.47	0/395
17	x	0.30	0/284	0.46	0/384
18	Y	0.31	0/216	0.51	0/289
18	y	0.28	0/216	0.48	0/289
19	Z	0.29	0/490	0.43	0/669
19	z	0.30	0/490	0.41	0/669
20	R	0.29	0/279	0.52	0/383
All	All	0.39	0/42983	0.55	0/58489

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	328 (98%)	4 (1%)	1 (0%)	41	37
1	a	334/344 (97%)	327 (98%)	6 (2%)	1 (0%)	41	37
2	B	509/505 (101%)	501 (98%)	8 (2%)	0	100	100
2	b	508/505 (101%)	496 (98%)	12 (2%)	0	100	100
3	C	450/455 (99%)	443 (98%)	6 (1%)	1 (0%)	47	46
3	c	458/455 (101%)	449 (98%)	8 (2%)	1 (0%)	47	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	341/342 (100%)	327 (96%)	14 (4%)	0	100	100
4	d	341/342 (100%)	334 (98%)	7 (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%)	60 (95%)	2 (3%)	1 (2%)	9	4
8	I	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	5	1
8	i	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	37 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	34/37 (92%)	34 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (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	244/244 (100%)	237 (97%)	5 (2%)	2 (1%)	19	12
13	o	241/244 (99%)	237 (98%)	4 (2%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
15	u	96/104 (92%)	94 (98%)	2 (2%)	0	100	100
16	V	137/137 (100%)	133 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
17	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
17	x	36/40 (90%)	36 (100%)	0	0	100	100
18	Y	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
18	y	27/30 (90%)	27 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	9	3
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	5252/5384 (98%)	5138 (98%)	104 (2%)	10 (0%)	47	46

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
8	I	36	ASP
13	O	26	ALA
3	c	416	SER
19	Z	31	GLN
19	z	30	PRO
13	O	138	THR
7	h	63	LYS
1	a	259	ILE
1	A	259	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	270/279 (97%)	270 (100%)	0	100	100
1	a	271/279 (97%)	270 (100%)	1 (0%)	91	93
2	B	409/403 (102%)	405 (99%)	4 (1%)	76	81
2	b	408/403 (101%)	402 (98%)	6 (2%)	65	69
3	C	353/356 (99%)	350 (99%)	3 (1%)	81	86
3	c	361/356 (101%)	356 (99%)	5 (1%)	67	72
4	D	278/277 (100%)	276 (99%)	2 (1%)	84	89
4	d	278/277 (100%)	275 (99%)	3 (1%)	73	78
5	E	72/73 (99%)	70 (97%)	2 (3%)	43	44
5	e	72/73 (99%)	70 (97%)	2 (3%)	43	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	26/38 (68%)	26 (100%)	0	100	100
7	H	54/54 (100%)	52 (96%)	2 (4%)	34	32
7	h	55/54 (102%)	53 (96%)	2 (4%)	35	33
8	I	34/34 (100%)	32 (94%)	2 (6%)	19	15
8	i	34/34 (100%)	33 (97%)	1 (3%)	42	42
9	J	26/27 (96%)	25 (96%)	1 (4%)	33	31
9	j	26/27 (96%)	25 (96%)	1 (4%)	33	31
10	K	30/30 (100%)	26 (87%)	4 (13%)	4	1
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	4
11	L	34/35 (97%)	34 (100%)	0	100	100
11	l	34/35 (97%)	34 (100%)	0	100	100
12	M	30/32 (94%)	28 (93%)	2 (7%)	16	11
12	m	32/32 (100%)	30 (94%)	2 (6%)	18	13
13	O	209/207 (101%)	204 (98%)	5 (2%)	49	51
13	o	206/207 (100%)	202 (98%)	4 (2%)	57	61
14	T	27/28 (96%)	26 (96%)	1 (4%)	34	32
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	84/89 (94%)	82 (98%)	2 (2%)	49	51
15	u	85/89 (96%)	83 (98%)	2 (2%)	49	51
16	V	119/117 (102%)	118 (99%)	1 (1%)	81	86
16	v	117/117 (100%)	112 (96%)	5 (4%)	29	27
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	1
19	Z	52/52 (100%)	51 (98%)	1 (2%)	57	61
19	z	52/52 (100%)	46 (88%)	6 (12%)	5	2
20	R	29/29 (100%)	27 (93%)	2 (7%)	15	10
All	All	4358/4403 (99%)	4278 (98%)	80 (2%)	59	63

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	294	SER
2	B	362	PHE
2	B	389	LYS
2	B	472	ARG
3	C	142	GLU
3	C	289	PHE
3	C	315	MET
4	D	180	ARG
4	D	338	ASN
5	E	4	THR
5	E	71	GLU
7	H	12	ARG
7	H	49	TYR
8	I	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	194	LYS
14	T	30	THR
15	U	10	VAL
15	U	70	ARG
16	V	15	GLU
1	a	13	LEU
2	b	127	ARG
2	b	128	THR
2	b	161	LEU
2	b	362	PHE
2	b	486	LEU
2	b	505	ARG
3	c	142	GLU
3	c	152	LYS
3	c	255	THR
3	c	289	PHE
3	c	315	MET

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Mol	Chain	Res	Type
4	d	26	ARG
4	d	180	ARG
4	d	259	ILE
5	e	60	GLN
5	e	71	GLU
7	h	49	TYR
7	h	65	LEU
8	i	33	LYS
9	j	9	LEU
10	k	10	LYS
10	k	17	ILE
10	k	24	VAL
12	m	16[A]	LEU
12	m	16[B]	LEU
13	o	36	GLN
13	o	37	THR
13	o	69	LYS
13	o	118	LEU
15	u	10[A]	VAL
15	u	10[B]	VAL
16	v	15	GLU
16	v	24	LYS
16	v	85	GLU
16	v	106	ASN
16	v	109	GLU
18	y	18	VAL
18	y	19	ILE
18	y	45	ASN
19	Z	31	GLN
20	R	29	LYS
20	R	33	LYS
19	z	1	MET
19	z	3	ILE
19	z	4	LEU
19	z	7	LEU
19	z	32	ASP
19	z	42	LEU

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

Mol	Chain	Res	Type
4	D	61	HIS

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Mol	Chain	Res	Type
5	E	60	GLN
13	o	58	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	FME	m	1	12	8,9,10	0.56	0	7,9,11	1.38	1 (14%)
14	FME	t	1	14	8,9,10	0.62	0	7,9,11	1.63	2 (28%)
12	FME	M	1	12	8,9,10	0.66	0	7,9,11	1.24	0
8	FME	i	1	8	8,9,10	0.63	0	7,9,11	1.28	0
8	FME	I	1	8	8,9,10	0.55	0	7,9,11	1.24	1 (14%)
14	FME	T	1	14	8,9,10	0.71	0	7,9,11	1.68	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. '2' 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	-	0/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
14	FME	T	1	14	-	0/7/9/11	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	CA-N-CN	-2.69	118.69	122.82
14	T	1	FME	CG-CB-CA	2.51	119.91	112.95
14	T	1	FME	CA-N-CN	2.43	126.55	122.82
14	t	1	FME	O-C-CA	-2.42	118.42	124.78
12	m	1	FME	O1-CN-N	-2.26	119.31	125.27
8	I	1	FME	O-C-CA	-2.19	119.04	124.78

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

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 225 ligands modelled in this entry, 15 are monoatomic and 18 are unknown - leaving 192 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	616	-	65,73,73	1.99	15 (23%)	76,113,113	2.90	26 (34%)
25	BCR	H	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.36	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	604	-	65,73,73	2.00	18 (27%)	76,113,113	2.67	28 (36%)
24	PHO	A	416	-	51,69,69	1.87	8 (15%)	47,99,99	1.93	12 (25%)
27	GOL	b	628	-	5,5,5	0.40	0	5,5,5	1.38	1 (20%)
25	BCR	A	409	-	41,41,41	1.01	1 (2%)	56,56,56	1.41	9 (16%)
32	LMG	c	521	-	51,51,55	0.99	2 (3%)	59,59,63	1.36	7 (11%)
23	CLA	B	601	41	65,73,73	2.09	17 (26%)	76,113,113	2.76	27 (35%)
26	SQD	A	410	-	53,54,54	0.93	3 (5%)	62,65,65	1.81	10 (16%)
25	BCR	C	514	-	41,41,41	1.03	1 (2%)	56,56,56	1.38	8 (14%)
33	LHG	d	406	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	3 (5%)
23	CLA	C	513	-	65,73,73	2.07	15 (23%)	76,113,113	2.72	28 (36%)
23	CLA	c	507	-	65,73,73	2.05	17 (26%)	76,113,113	2.77	28 (36%)
31	LMT	c	501	-	36,36,36	1.03	1 (2%)	47,47,47	1.02	1 (2%)
33	LHG	L	101	-	48,48,48	0.89	2 (4%)	51,54,54	1.15	3 (5%)
32	LMG	Z	101	-	37,37,55	0.99	2 (5%)	45,45,63	1.42	5 (11%)
23	CLA	b	612	-	65,73,73	2.00	15 (23%)	76,113,113	2.79	27 (35%)
31	LMT	B	630	-	36,36,36	1.00	3 (8%)	47,47,47	1.14	3 (6%)
33	LHG	d	411	-	48,48,48	0.89	2 (4%)	51,54,54	1.12	4 (7%)
35	DGD	c	518	-	63,63,67	0.84	2 (3%)	77,77,81	0.97	5 (6%)
23	CLA	a	409	-	65,73,73	1.97	16 (24%)	76,113,113	2.84	28 (36%)
34	HTG	d	409	-	16,16,19	0.98	1 (6%)	20,21,24	1.59	1 (5%)
23	CLA	D	403	-	65,73,73	2.07	16 (24%)	76,113,113	2.75	29 (38%)
35	DGD	C	517	-	63,63,67	0.87	3 (4%)	77,77,81	0.93	3 (3%)
25	BCR	h	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.32	8 (14%)
32	LMG	A	419	-	51,51,55	0.92	2 (3%)	59,59,63	1.43	8 (13%)
34	HTG	B	622	-	19,19,19	1.16	2 (10%)	23,24,24	1.52	5 (21%)
27	GOL	a	419	-	5,5,5	1.02	0	5,5,5	0.97	0
29	PL9	a	415	-	55,55,55	0.65	2 (3%)	68,69,69	2.00	22 (32%)
27	GOL	B	624	-	5,5,5	0.88	0	5,5,5	1.13	1 (20%)
27	GOL	v	202	-	5,5,5	1.27	0	5,5,5	0.72	0
23	CLA	B	606	-	65,73,73	1.98	16 (24%)	76,113,113	2.93	28 (36%)
31	LMT	b	627	-	25,25,36	0.89	2 (8%)	30,30,47	1.10	1 (3%)
23	CLA	C	506	-	65,73,73	2.05	17 (26%)	76,113,113	2.73	29 (38%)
31	LMT	F	101	-	36,36,36	1.08	3 (8%)	47,47,47	1.02	2 (4%)
25	BCR	Y	101	-	41,41,41	0.98	1 (2%)	56,56,56	1.72	14 (25%)
23	CLA	B	607	41	65,73,73	1.93	17 (26%)	76,113,113	2.80	26 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	GOL	l	102	-	5,5,5	0.96	0	5,5,5	0.97	0
28	OEX	a	414	41,1,3	0,15,15	-	-	-	-	-
26	SQD	a	413	-	53,54,54	1.05	3 (5%)	62,65,65	1.19	8 (12%)
25	BCR	B	619	-	41,41,41	1.06	1 (2%)	56,56,56	1.30	7 (12%)
35	DGD	H	102	-	63,63,67	0.85	4 (6%)	77,77,81	0.97	6 (7%)
27	GOL	A	418	-	5,5,5	1.58	2 (40%)	5,5,5	1.02	1 (20%)
23	CLA	b	601	41	65,73,73	2.12	16 (24%)	76,113,113	2.75	27 (35%)
23	CLA	c	504	-	65,73,73	2.00	16 (24%)	76,113,113	2.79	25 (32%)
23	CLA	b	615	-	65,73,73	1.99	16 (24%)	76,113,113	2.77	28 (36%)
23	CLA	B	613	-	65,73,73	2.02	15 (23%)	76,113,113	2.76	29 (38%)
27	GOL	a	412	-	5,5,5	0.88	0	5,5,5	1.02	0
27	GOL	b	629	-	5,5,5	1.07	0	5,5,5	0.91	0
33	LHG	a	421	-	41,41,48	1.04	2 (4%)	44,47,54	0.92	2 (4%)
35	DGD	c	519	-	63,63,67	0.87	3 (4%)	77,77,81	1.00	5 (6%)
27	GOL	C	521	-	5,5,5	1.18	0	5,5,5	0.83	0
23	CLA	c	512	3	65,73,73	2.10	16 (24%)	76,113,113	2.74	30 (39%)
31	LMT	T	101	-	36,36,36	1.09	3 (8%)	47,47,47	1.07	2 (4%)
32	LMG	a	418	-	51,51,55	0.92	2 (3%)	59,59,63	1.17	4 (6%)
23	CLA	b	610	41	65,73,73	2.02	16 (24%)	76,113,113	2.80	28 (36%)
23	CLA	b	607	41	65,73,73	1.95	19 (29%)	76,113,113	2.76	27 (35%)
25	BCR	k	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.52	12 (21%)
32	LMG	C	519	-	51,51,55	1.05	3 (5%)	59,59,63	1.31	5 (8%)
25	BCR	b	619	-	41,41,41	1.07	1 (2%)	56,56,56	1.29	6 (10%)
27	GOL	O	303	-	5,5,5	0.85	0	5,5,5	1.14	1 (20%)
35	DGD	h	102	-	63,63,67	0.86	3 (4%)	77,77,81	1.07	6 (7%)
23	CLA	b	602	-	65,73,73	2.04	16 (24%)	76,113,113	2.87	35 (46%)
23	CLA	c	511	-	65,73,73	1.99	16 (24%)	76,113,113	2.82	30 (39%)
37	BCT	a	404	21	2,3,3	0.57	0	2,3,3	1.58	1 (50%)
23	CLA	A	408	-	65,73,73	2.00	16 (24%)	76,113,113	2.87	34 (44%)
23	CLA	b	613	-	65,73,73	1.96	15 (23%)	76,113,113	2.76	29 (38%)
23	CLA	C	503	-	65,73,73	1.98	16 (24%)	76,113,113	2.82	27 (35%)
27	GOL	c	526	-	5,5,5	0.94	0	5,5,5	0.95	0
25	BCR	D	404	-	41,41,41	1.07	1 (2%)	56,56,56	1.80	15 (26%)
23	CLA	B	611	-	65,73,73	2.61	18 (27%)	76,113,113	3.13	27 (35%)
23	CLA	D	402	-	65,73,73	1.99	16 (24%)	76,113,113	2.87	29 (38%)
38	HEM	f	101	6,5	41,50,50	1.30	5 (12%)	45,82,82	1.78	10 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	608	-	65,73,73	1.93	15 (23%)	76,113,113	2.78	31 (40%)
31	LMT	A	421	-	36,36,36	1.06	4 (11%)	47,47,47	1.14	4 (8%)
23	CLA	a	407	41	65,73,73	1.94	16 (24%)	76,113,113	2.81	27 (35%)
25	BCR	a	410	-	41,41,41	1.03	1 (2%)	56,56,56	1.39	9 (16%)
26	SQD	F	103	-	42,43,54	1.19	4 (9%)	51,54,65	2.02	12 (23%)
23	CLA	b	614	-	65,73,73	1.99	16 (24%)	76,113,113	2.85	28 (36%)
26	SQD	b	620	-	53,54,54	1.04	3 (5%)	62,65,65	1.61	11 (17%)
23	CLA	c	506	-	65,73,73	1.98	16 (24%)	76,113,113	2.69	26 (34%)
32	LMG	c	520	-	51,51,55	0.90	2 (3%)	59,59,63	1.12	6 (10%)
23	CLA	B	605	-	65,73,73	1.96	15 (23%)	76,113,113	2.92	28 (36%)
23	CLA	a	405	-	65,73,73	1.99	15 (23%)	76,113,113	2.87	32 (42%)
23	CLA	C	512	-	65,73,73	2.06	16 (24%)	76,113,113	2.78	32 (42%)
23	CLA	B	610	41	65,73,73	2.06	16 (24%)	76,113,113	2.90	28 (36%)
23	CLA	C	505	-	65,73,73	1.97	16 (24%)	76,113,113	2.73	28 (36%)
27	GOL	o	302	-	5,5,5	0.94	0	5,5,5	0.95	0
32	LMG	m	101	-	51,51,55	0.87	2 (3%)	59,59,63	1.22	5 (8%)
38	HEM	F	102	6,5	41,50,50	1.29	6 (14%)	45,82,82	2.00	13 (28%)
23	CLA	c	514	-	65,73,73	2.11	17 (26%)	76,113,113	2.77	28 (36%)
31	LMT	t	101	-	26,26,36	0.93	2 (7%)	31,31,47	1.31	2 (6%)
23	CLA	b	611	-	65,73,73	1.93	16 (24%)	76,113,113	2.86	27 (35%)
23	CLA	C	507	41	65,73,73	2.00	15 (23%)	76,113,113	2.77	27 (35%)
34	HTG	B	625	-	19,19,19	1.04	2 (10%)	23,24,24	1.22	3 (13%)
27	GOL	o	303	-	5,5,5	1.04	0	5,5,5	1.04	0
23	CLA	b	608	-	65,73,73	1.98	16 (24%)	76,113,113	2.84	31 (40%)
27	GOL	O	302	-	5,5,5	0.92	0	5,5,5	0.95	0
34	HTG	C	520	-	19,19,19	0.89	1 (5%)	23,24,24	1.33	2 (8%)
33	LHG	D	407	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	4 (7%)
27	GOL	B	629	-	5,5,5	1.32	1 (20%)	5,5,5	0.90	0
27	GOL	a	420	-	5,5,5	1.26	1 (20%)	5,5,5	0.87	0
23	CLA	c	509	-	65,73,73	2.11	16 (24%)	76,113,113	2.71	26 (34%)
34	HTG	B	623	-	19,19,19	0.79	1 (5%)	23,24,24	1.47	2 (8%)
25	BCR	B	617	-	41,41,41	1.04	1 (2%)	56,56,56	1.25	3 (5%)
35	DGD	C	516	-	63,63,67	0.89	3 (4%)	77,77,81	1.02	5 (6%)
40	HEC	V	201	16	32,50,50	2.00	4 (12%)	24,82,82	2.02	6 (25%)
25	BCR	c	516	-	41,41,41	1.03	1 (2%)	56,56,56	1.35	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	605	-	65,73,73	1.96	17 (26%)	76,113,113	3.00	25 (32%)
33	LHG	D	406	-	48,48,48	0.86	2 (4%)	51,54,54	0.99	3 (5%)
23	CLA	B	614	-	65,73,73	2.00	17 (26%)	76,113,113	2.91	30 (39%)
23	CLA	B	612	-	65,73,73	2.03	16 (24%)	76,113,113	2.87	30 (39%)
23	CLA	c	502	-	65,73,73	2.00	17 (26%)	76,113,113	2.78	27 (35%)
23	CLA	c	503	-	65,73,73	2.01	15 (23%)	76,113,113	2.70	24 (31%)
23	CLA	B	602	-	65,73,73	2.03	16 (24%)	76,113,113	2.83	27 (35%)
25	BCR	y	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.66	12 (21%)
23	CLA	A	405	41	65,73,73	1.90	16 (24%)	76,113,113	2.85	30 (39%)
34	HTG	b	625	-	19,19,19	1.01	2 (10%)	23,24,24	1.61	5 (21%)
23	CLA	A	406	41	65,73,73	1.96	16 (24%)	76,113,113	2.81	29 (38%)
27	GOL	b	624	-	5,5,5	1.15	1 (20%)	5,5,5	0.81	0
23	CLA	C	510	-	65,73,73	2.09	17 (26%)	76,113,113	2.85	30 (39%)
24	PHO	a	417	-	51,69,69	1.86	9 (17%)	47,99,99	1.99	13 (27%)
31	LMT	m	103	-	36,36,36	1.10	4 (11%)	47,47,47	1.06	3 (6%)
23	CLA	A	404	-	65,73,73	2.02	16 (24%)	76,113,113	2.77	32 (42%)
31	LMT	A	417	-	36,36,36	0.96	3 (8%)	47,47,47	1.01	1 (2%)
34	HTG	b	623	-	19,19,19	1.05	1 (5%)	23,24,24	1.87	2 (8%)
25	BCR	d	403	-	41,41,41	1.11	1 (2%)	56,56,56	1.89	18 (32%)
25	BCR	c	515	-	41,41,41	1.02	1 (2%)	56,56,56	1.61	12 (21%)
25	BCR	K	103	-	41,41,41	1.03	1 (2%)	56,56,56	1.44	9 (16%)
31	LMT	e	101	-	36,36,36	1.04	4 (11%)	47,47,47	0.97	1 (2%)
27	GOL	c	527	-	5,5,5	0.97	0	5,5,5	0.98	0
35	DGD	c	517	-	63,63,67	0.85	2 (3%)	77,77,81	1.12	6 (7%)
35	DGD	C	515	-	63,63,67	0.81	2 (3%)	77,77,81	1.21	8 (10%)
34	HTG	c	522	-	19,19,19	0.97	2 (10%)	23,24,24	1.54	2 (8%)
26	SQD	B	620	-	53,54,54	1.06	3 (5%)	62,65,65	1.75	14 (22%)
25	BCR	b	618	-	41,41,41	0.99	1 (2%)	56,56,56	1.23	7 (12%)
25	BCR	t	102	-	41,41,41	1.03	1 (2%)	56,56,56	1.58	12 (21%)
23	CLA	B	615	-	65,73,73	2.01	17 (26%)	76,113,113	2.79	27 (35%)
29	PL9	D	405	-	55,55,55	0.62	2 (3%)	68,69,69	1.64	18 (26%)
23	CLA	C	504	41	65,73,73	2.02	16 (24%)	76,113,113	2.74	27 (35%)
23	CLA	C	509	-	65,73,73	2.08	17 (26%)	76,113,113	2.88	28 (36%)
32	LMG	B	621	-	51,51,55	0.91	2 (3%)	59,59,63	1.28	4 (6%)
33	LHG	b	630	-	48,48,48	0.85	3 (6%)	51,54,54	1.03	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	d	401	-	65,73,73	1.94	17 (26%)	76,113,113	2.79	29 (38%)
37	BCT	D	401	21	2,3,3	0.54	0	2,3,3	1.81	1 (50%)
23	CLA	c	508	41	65,73,73	2.02	15 (23%)	76,113,113	2.79	26 (34%)
33	LHG	d	405	-	48,48,48	0.86	2 (4%)	51,54,54	1.08	4 (7%)
25	BCR	b	617	-	41,41,41	1.06	1 (2%)	56,56,56	1.33	5 (8%)
23	CLA	d	402	-	65,73,73	2.04	16 (24%)	76,113,113	2.79	29 (38%)
26	SQD	f	102	-	42,43,54	1.18	3 (7%)	51,54,65	1.57	10 (19%)
27	GOL	B	627	-	5,5,5	0.95	0	5,5,5	0.99	0
27	GOL	A	411	-	5,5,5	1.14	0	5,5,5	0.71	0
29	PL9	d	404	-	55,55,55	0.65	1 (1%)	68,69,69	1.63	17 (25%)
25	BCR	T	102	-	41,41,41	1.02	1 (2%)	56,56,56	1.55	12 (21%)
26	SQD	A	412	-	53,54,54	1.04	3 (5%)	62,65,65	1.16	6 (9%)
32	LMG	C	518	-	51,51,55	0.93	2 (3%)	59,59,63	1.11	4 (6%)
32	LMG	D	411	39	51,51,55	0.84	2 (3%)	59,59,63	1.01	3 (5%)
23	CLA	b	604	-	65,73,73	2.02	15 (23%)	76,113,113	2.73	25 (32%)
23	CLA	B	609	-	65,73,73	2.02	16 (24%)	76,113,113	2.75	26 (34%)
26	SQD	a	411	-	53,54,54	0.95	3 (5%)	62,65,65	1.77	13 (20%)
33	LHG	E	101	-	41,41,48	1.06	2 (4%)	44,47,54	1.11	3 (6%)
33	LHG	A	420	-	48,48,48	0.84	2 (4%)	51,54,54	1.31	6 (11%)
25	BCR	K	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.40	6 (10%)
23	CLA	c	510	-	65,73,73	2.06	15 (23%)	76,113,113	2.79	29 (38%)
23	CLA	a	406	41	65,73,73	2.00	14 (21%)	76,113,113	2.75	26 (34%)
31	LMT	b	621	-	25,25,36	0.97	2 (8%)	30,30,47	1.17	1 (3%)
23	CLA	B	603	-	65,73,73	2.02	16 (24%)	76,113,113	2.96	27 (35%)
25	BCR	B	618	-	41,41,41	0.97	1 (2%)	56,56,56	1.33	7 (12%)
23	CLA	C	511	3	65,73,73	2.03	16 (24%)	76,113,113	2.71	24 (31%)
23	CLA	b	603	-	65,73,73	1.99	15 (23%)	76,113,113	2.86	29 (38%)
31	LMT	B	631	-	25,25,36	0.90	2 (8%)	30,30,47	1.12	3 (10%)
23	CLA	B	616	-	65,73,73	2.01	16 (24%)	76,113,113	2.85	25 (32%)
23	CLA	c	513	-	65,73,73	2.06	16 (24%)	76,113,113	2.72	29 (38%)
31	LMT	M	101	-	36,36,36	1.15	3 (8%)	47,47,47	1.21	4 (8%)
24	PHO	A	407	-	51,69,69	1.78	8 (15%)	47,99,99	1.77	11 (23%)
23	CLA	b	609	-	65,73,73	2.01	16 (24%)	76,113,113	2.72	29 (38%)
28	OEX	A	413	41,1,3	0,15,15	-	-	-	-	-
32	LMG	d	410	39	51,51,55	0.90	2 (3%)	59,59,63	1.10	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PL9	A	414	-	55,55,55	0.68	2 (3%)	68,69,69	2.08	25 (36%)
24	PHO	a	408	-	51,69,69	1.83	8 (15%)	47,99,99	1.71	10 (21%)
27	GOL	V	203	-	5,5,5	1.22	0	5,5,5	0.91	0
34	HTG	V	202	-	11,11,19	0.23	0	15,15,24	1.08	1 (6%)
34	HTG	D	410	-	16,16,19	1.08	2 (12%)	20,21,24	1.50	1 (5%)
23	CLA	c	505	41	65,73,73	2.07	17 (26%)	76,113,113	2.74	26 (34%)
23	CLA	C	508	-	65,73,73	2.11	15 (23%)	76,113,113	2.72	26 (34%)
34	HTG	b	622	-	19,19,19	1.20	2 (10%)	23,24,24	1.94	7 (30%)
40	HEC	v	201	16	32,50,50	2.02	3 (9%)	24,82,82	1.94	6 (25%)
32	LMG	z	101	-	39,39,55	1.08	2 (5%)	47,47,63	1.07	3 (6%)
23	CLA	C	502	-	65,73,73	2.04	16 (24%)	76,113,113	2.64	25 (32%)
31	LMT	B	628	-	36,36,36	1.17	4 (11%)	47,47,47	1.30	5 (10%)
23	CLA	C	501	-	65,73,73	1.98	16 (24%)	76,113,113	2.78	27 (35%)
23	CLA	b	606	-	65,73,73	2.01	15 (23%)	76,113,113	2.84	29 (38%)

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	616	-	1/1/15/20	10/37/115/115	-
25	BCR	H	101	-	-	2/29/63/63	0/2/2/2
23	CLA	B	604	-	1/1/15/20	2/37/115/115	-
24	PHO	A	416	-	-	1/37/103/103	0/5/6/6
27	GOL	b	628	-	-	0/4/4/4	-
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
32	LMG	c	521	-	-	7/46/66/70	0/1/1/1
23	CLA	B	601	41	1/1/15/20	12/37/115/115	-
26	SQD	A	410	-	-	12/49/69/69	0/1/1/1
25	BCR	C	514	-	-	0/29/63/63	0/2/2/2
33	LHG	d	406	-	-	11/53/53/53	-
23	CLA	C	513	-	1/1/15/20	7/37/115/115	-
23	CLA	c	507	-	1/1/15/20	8/37/115/115	-
31	LMT	c	501	-	-	11/21/61/61	0/2/2/2
33	LHG	L	101	-	-	19/53/53/53	-
32	LMG	Z	101	-	-	10/31/51/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	612	-	1/1/15/20	2/37/115/115	-
31	LMT	B	630	-	-	11/21/61/61	0/2/2/2
33	LHG	d	411	-	-	13/53/53/53	-
35	DGD	c	518	-	-	17/51/91/95	0/2/2/2
23	CLA	a	409	-	1/1/15/20	9/37/115/115	-
34	HTG	d	409	-	-	1/7/27/30	0/1/1/1
23	CLA	D	403	-	1/1/15/20	14/37/115/115	-
35	DGD	C	517	-	-	16/51/91/95	0/2/2/2
25	BCR	h	101	-	-	2/29/63/63	0/2/2/2
32	LMG	A	419	-	-	13/46/66/70	0/1/1/1
34	HTG	B	622	-	-	4/10/30/30	0/1/1/1
27	GOL	a	419	-	-	2/4/4/4	-
29	PL9	a	415	-	-	14/53/73/73	0/1/1/1
27	GOL	B	624	-	-	4/4/4/4	-
27	GOL	v	202	-	-	1/4/4/4	-
23	CLA	B	606	-	1/1/15/20	10/37/115/115	-
31	LMT	b	627	-	-	11/17/37/61	0/1/1/2
23	CLA	C	506	-	1/1/15/20	11/37/115/115	-
31	LMT	F	101	-	-	9/21/61/61	0/2/2/2
25	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
23	CLA	B	607	41	1/1/15/20	5/37/115/115	-
27	GOL	l	102	-	-	2/4/4/4	-
26	SQD	a	413	-	-	15/49/69/69	0/1/1/1
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
35	DGD	H	102	-	-	9/51/91/95	0/2/2/2
27	GOL	A	418	-	-	2/4/4/4	-
23	CLA	b	601	41	1/1/15/20	19/37/115/115	-
23	CLA	c	504	-	1/1/15/20	1/37/115/115	-
23	CLA	b	615	-	1/1/15/20	7/37/115/115	-
23	CLA	B	613	-	1/1/15/20	8/37/115/115	-
27	GOL	a	412	-	-	4/4/4/4	-
27	GOL	b	629	-	-	1/4/4/4	-
33	LHG	a	421	-	-	16/46/46/53	-
35	DGD	c	519	-	-	8/51/91/95	0/2/2/2
27	GOL	C	521	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	512	3	1/1/15/20	4/37/115/115	-
31	LMT	T	101	-	-	8/21/61/61	0/2/2/2
32	LMG	a	418	-	-	13/46/66/70	0/1/1/1
23	CLA	b	610	41	1/1/15/20	7/37/115/115	-
23	CLA	b	607	41	1/1/15/20	2/37/115/115	-
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
32	LMG	C	519	-	-	11/46/66/70	0/1/1/1
25	BCR	b	619	-	-	3/29/63/63	0/2/2/2
27	GOL	O	303	-	-	2/4/4/4	-
35	DGD	h	102	-	-	15/51/91/95	0/2/2/2
23	CLA	b	602	-	1/1/15/20	5/37/115/115	-
23	CLA	c	511	-	1/1/15/20	11/37/115/115	-
23	CLA	A	408	-	1/1/15/20	8/37/115/115	-
23	CLA	b	613	-	1/1/15/20	3/37/115/115	-
23	CLA	C	503	-	-	3/37/115/115	-
27	GOL	c	526	-	-	0/4/4/4	-
25	BCR	D	404	-	-	4/29/63/63	0/2/2/2
23	CLA	B	611	-	1/1/15/20	3/37/115/115	-
23	CLA	D	402	-	1/1/15/20	0/37/115/115	-
38	HEM	f	101	6,5	-	4/12/54/54	-
23	CLA	B	608	-	-	3/37/115/115	-
31	LMT	A	421	-	-	15/21/61/61	0/2/2/2
23	CLA	a	407	41	-	5/37/115/115	-
25	BCR	a	410	-	-	1/29/63/63	0/2/2/2
26	SQD	F	103	-	-	15/38/58/69	0/1/1/1
23	CLA	b	614	-	1/1/15/20	15/37/115/115	-
26	SQD	b	620	-	-	18/49/69/69	0/1/1/1
23	CLA	c	506	-	1/1/15/20	7/37/115/115	-
32	LMG	c	520	-	-	11/46/66/70	0/1/1/1
23	CLA	B	605	-	1/1/15/20	6/37/115/115	-
23	CLA	a	405	-	1/1/15/20	3/37/115/115	-
23	CLA	C	512	-	1/1/15/20	11/37/115/115	-
23	CLA	B	610	41	1/1/15/20	7/37/115/115	-
23	CLA	C	505	-	1/1/15/20	6/37/115/115	-
27	GOL	o	302	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LMG	m	101	-	-	10/46/66/70	0/1/1/1
38	HEM	F	102	6,5	-	4/12/54/54	-
23	CLA	c	514	-	1/1/15/20	8/37/115/115	-
31	LMT	t	101	-	-	8/17/38/61	0/1/1/2
23	CLA	b	611	-	1/1/15/20	3/37/115/115	-
23	CLA	C	507	41	1/1/15/20	6/37/115/115	-
34	HTG	B	625	-	-	4/10/30/30	0/1/1/1
27	GOL	o	303	-	-	4/4/4/4	-
23	CLA	b	608	-	-	5/37/115/115	-
27	GOL	O	302	-	-	2/4/4/4	-
34	HTG	C	520	-	-	0/10/30/30	0/1/1/1
33	LHG	D	407	-	-	14/53/53/53	-
27	GOL	B	629	-	-	4/4/4/4	-
27	GOL	a	420	-	-	0/4/4/4	-
23	CLA	c	509	-	1/1/15/20	5/37/115/115	-
34	HTG	B	623	-	-	1/10/30/30	0/1/1/1
25	BCR	B	617	-	-	2/29/63/63	0/2/2/2
35	DGD	C	516	-	-	15/51/91/95	0/2/2/2
40	HEC	V	201	16	-	2/10/54/54	-
25	BCR	c	516	-	-	0/29/63/63	0/2/2/2
23	CLA	b	605	-	1/1/15/20	7/37/115/115	-
33	LHG	D	406	-	-	16/53/53/53	-
23	CLA	B	614	-	1/1/15/20	14/37/115/115	-
23	CLA	B	612	-	1/1/15/20	5/37/115/115	-
23	CLA	c	502	-	1/1/15/20	1/37/115/115	-
23	CLA	c	503	-	1/1/15/20	7/37/115/115	-
23	CLA	B	602	-	1/1/15/20	8/37/115/115	-
25	BCR	y	101	-	-	5/29/63/63	0/2/2/2
23	CLA	A	405	41	-	4/37/115/115	-
34	HTG	b	625	-	-	3/10/30/30	0/1/1/1
23	CLA	A	406	41	-	5/37/115/115	-
27	GOL	b	624	-	-	2/4/4/4	-
23	CLA	C	510	-	1/1/15/20	13/37/115/115	-
24	PHO	a	417	-	-	2/37/103/103	0/5/6/6
31	LMT	m	103	-	-	5/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	A	404	-	1/1/15/20	5/37/115/115	-
31	LMT	A	417	-	-	8/21/61/61	0/2/2/2
34	HTG	b	623	-	-	4/10/30/30	0/1/1/1
25	BCR	d	403	-	-	5/29/63/63	0/2/2/2
25	BCR	c	515	-	-	1/29/63/63	0/2/2/2
25	BCR	K	103	-	-	2/29/63/63	0/2/2/2
31	LMT	e	101	-	-	14/21/61/61	0/2/2/2
27	GOL	c	527	-	-	4/4/4/4	-
35	DGD	c	517	-	-	20/51/91/95	0/2/2/2
35	DGD	C	515	-	-	11/51/91/95	0/2/2/2
34	HTG	c	522	-	-	2/10/30/30	0/1/1/1
26	SQD	B	620	-	-	13/49/69/69	0/1/1/1
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
25	BCR	t	102	-	-	1/29/63/63	0/2/2/2
23	CLA	B	615	-	1/1/15/20	5/37/115/115	-
29	PL9	D	405	-	-	8/53/73/73	0/1/1/1
23	CLA	C	504	41	1/1/15/20	6/37/115/115	-
23	CLA	C	509	-	1/1/15/20	2/37/115/115	-
32	LMG	B	621	-	-	19/46/66/70	0/1/1/1
33	LHG	b	630	-	-	20/53/53/53	-
23	CLA	d	401	-	1/1/15/20	2/37/115/115	-
23	CLA	c	508	41	1/1/15/20	7/37/115/115	-
33	LHG	d	405	-	-	13/53/53/53	-
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
23	CLA	d	402	-	1/1/15/20	8/37/115/115	-
26	SQD	f	102	-	-	12/38/58/69	0/1/1/1
27	GOL	B	627	-	-	2/4/4/4	-
27	GOL	A	411	-	-	2/4/4/4	-
29	PL9	d	404	-	-	6/53/73/73	0/1/1/1
25	BCR	T	102	-	-	1/29/63/63	0/2/2/2
26	SQD	A	412	-	-	13/49/69/69	0/1/1/1
32	LMG	C	518	-	-	8/46/66/70	0/1/1/1
32	LMG	D	411	39	-	10/46/66/70	0/1/1/1
23	CLA	b	604	-	1/1/15/20	8/37/115/115	-
23	CLA	B	609	-	1/1/15/20	1/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	SQD	a	411	-	-	10/49/69/69	0/1/1/1
33	LHG	E	101	-	-	22/46/46/53	-
33	LHG	A	420	-	-	10/53/53/53	-
25	BCR	K	101	-	-	1/29/63/63	0/2/2/2
23	CLA	c	510	-	1/1/15/20	14/37/115/115	-
23	CLA	a	406	41	1/1/15/20	8/37/115/115	-
31	LMT	b	621	-	-	8/17/37/61	0/1/1/2
23	CLA	B	603	-	1/1/15/20	8/37/115/115	-
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
23	CLA	C	511	3	1/1/15/20	3/37/115/115	-
23	CLA	b	603	-	1/1/15/20	5/37/115/115	-
31	LMT	B	631	-	-	10/17/37/61	0/1/1/2
23	CLA	B	616	-	1/1/15/20	5/37/115/115	-
23	CLA	c	513	-	1/1/15/20	11/37/115/115	-
31	LMT	M	101	-	-	4/21/61/61	0/2/2/2
24	PHO	A	407	-	-	4/37/103/103	0/5/6/6
23	CLA	b	609	-	1/1/15/20	3/37/115/115	-
32	LMG	d	410	39	-	11/46/66/70	0/1/1/1
29	PL9	A	414	-	-	15/53/73/73	0/1/1/1
24	PHO	a	408	-	-	6/37/103/103	0/5/6/6
27	GOL	V	203	-	-	2/4/4/4	-
34	HTG	V	202	-	-	0/2/19/30	0/1/1/1
34	HTG	D	410	-	-	3/7/27/30	0/1/1/1
23	CLA	c	505	41	1/1/15/20	7/37/115/115	-
23	CLA	C	508	-	-	3/37/115/115	-
34	HTG	b	622	-	-	5/10/30/30	0/1/1/1
40	HEC	v	201	16	-	2/10/54/54	-
32	LMG	z	101	-	-	9/34/54/70	0/1/1/1
23	CLA	C	502	-	1/1/15/20	9/37/115/115	-
31	LMT	B	628	-	-	11/21/61/61	0/2/2/2
23	CLA	C	501	-	1/1/15/20	6/37/115/115	-
23	CLA	b	606	-	1/1/15/20	12/37/115/115	-

All (1356) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	611	CLA	C3B-C2B	10.63	1.55	1.40
23	B	611	CLA	CMB-C2B	6.82	1.65	1.51
23	B	616	CLA	C3B-C2B	6.65	1.49	1.40
23	B	612	CLA	C3B-C2B	6.62	1.49	1.40
23	b	612	CLA	C3B-C2B	6.57	1.49	1.40
23	C	508	CLA	C3B-C2B	6.56	1.49	1.40
23	b	603	CLA	C3B-C2B	6.46	1.49	1.40
23	C	513	CLA	C3B-C2B	6.38	1.49	1.40
23	c	503	CLA	C3B-C2B	6.37	1.49	1.40
24	a	408	PHO	C3B-C2B	6.36	1.49	1.40
23	c	512	CLA	C3B-C2B	6.29	1.49	1.40
23	B	603	CLA	C3B-C2B	6.28	1.49	1.40
23	a	405	CLA	C3B-C2B	6.26	1.49	1.40
23	A	404	CLA	C3B-C2B	6.26	1.49	1.40
23	A	408	CLA	C3B-C2B	6.24	1.49	1.40
23	C	509	CLA	C3B-C2B	6.23	1.49	1.40
23	C	504	CLA	C3B-C2B	6.21	1.49	1.40
23	C	511	CLA	C3B-C2B	6.20	1.49	1.40
23	c	509	CLA	C3B-C2B	6.20	1.49	1.40
24	A	407	PHO	C3B-C2B	6.19	1.49	1.40
23	B	611	CLA	C1D-ND	6.14	1.45	1.37
23	B	604	CLA	C3B-C2B	6.14	1.48	1.40
24	A	416	PHO	C3B-C2B	6.12	1.48	1.40
23	b	610	CLA	C3B-C2B	6.10	1.48	1.40
23	B	613	CLA	C3B-C2B	6.10	1.48	1.40
23	B	608	CLA	C3B-C2B	6.09	1.48	1.40
23	c	510	CLA	C3B-C2B	6.07	1.48	1.40
23	b	613	CLA	C3B-C2B	6.07	1.48	1.40
23	b	604	CLA	C3B-C2B	6.05	1.48	1.40
23	c	507	CLA	C3B-C2B	6.04	1.48	1.40
23	C	510	CLA	C3B-C2B	6.04	1.48	1.40
23	B	602	CLA	C3B-C2B	6.04	1.48	1.40
23	C	506	CLA	C3B-C2B	6.04	1.48	1.40
23	b	608	CLA	C3B-C2B	6.02	1.48	1.40
23	a	409	CLA	C3B-C2B	5.99	1.48	1.40
23	b	601	CLA	C3B-C2B	5.98	1.48	1.40
40	v	201	HEC	C2B-C3B	-5.95	1.34	1.40
23	D	402	CLA	C3B-C2B	5.94	1.48	1.40
24	a	417	PHO	C3B-C2B	5.90	1.48	1.40
23	C	502	CLA	C3B-C2B	5.90	1.48	1.40
23	c	505	CLA	C3B-C2B	5.90	1.48	1.40
23	C	510	CLA	C1D-ND	5.89	1.45	1.37
23	c	511	CLA	C3B-C2B	5.86	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	606	CLA	C3B-C2B	5.86	1.48	1.40
23	B	611	CLA	CHC-C1C	5.85	1.50	1.35
23	B	601	CLA	C3B-C2B	5.84	1.48	1.40
23	c	514	CLA	C3B-C2B	5.79	1.48	1.40
23	C	512	CLA	C3B-C2B	5.78	1.48	1.40
23	b	614	CLA	C3B-C2B	5.78	1.48	1.40
23	b	611	CLA	C3B-C2B	5.76	1.48	1.40
40	V	201	HEC	C2B-C3B	-5.71	1.34	1.40
23	B	606	CLA	C3B-C2B	5.67	1.48	1.40
23	d	401	CLA	C3B-C2B	5.65	1.48	1.40
23	C	507	CLA	C3B-C2B	5.64	1.48	1.40
23	C	501	CLA	C3B-C2B	5.59	1.48	1.40
23	B	610	CLA	C3C-C2C	5.59	1.48	1.36
23	B	611	CLA	C3C-C2C	5.57	1.48	1.36
23	d	402	CLA	C1D-ND	5.55	1.44	1.37
23	c	502	CLA	C3B-C2B	5.55	1.48	1.40
23	C	503	CLA	C3C-C2C	5.53	1.48	1.36
23	B	607	CLA	C3B-C2B	5.53	1.48	1.40
23	c	509	CLA	C3C-C2C	5.53	1.48	1.36
23	d	402	CLA	C3B-C2B	5.53	1.48	1.40
23	c	510	CLA	C3C-C2C	5.53	1.48	1.36
23	c	513	CLA	C3C-C2C	5.51	1.48	1.36
23	c	513	CLA	C3B-C2B	5.51	1.48	1.40
23	c	512	CLA	C1D-ND	5.50	1.44	1.37
23	b	605	CLA	C3C-C2C	5.47	1.48	1.36
23	b	601	CLA	C1D-ND	5.45	1.44	1.37
23	A	404	CLA	C3C-C2C	5.45	1.48	1.36
23	D	403	CLA	C3C-C2C	5.42	1.48	1.36
23	C	512	CLA	C3C-C2C	5.42	1.48	1.36
23	B	610	CLA	C3B-C2B	5.42	1.47	1.40
24	a	408	PHO	C3D-C2D	5.41	1.49	1.39
23	C	510	CLA	C3C-C2C	5.40	1.48	1.36
23	c	506	CLA	C3C-C2C	5.40	1.48	1.36
23	C	508	CLA	C3C-C2C	5.39	1.48	1.36
23	B	612	CLA	CHC-C1C	5.38	1.48	1.35
23	B	609	CLA	C3B-C2B	5.37	1.47	1.40
23	b	607	CLA	C3B-C2B	5.37	1.47	1.40
23	c	504	CLA	C3C-C2C	5.36	1.48	1.36
23	a	406	CLA	C3C-C2C	5.35	1.48	1.36
23	B	616	CLA	CHC-C1C	5.35	1.48	1.35
23	a	407	CLA	C3C-C2C	5.34	1.48	1.36
23	b	605	CLA	C3B-C2B	5.34	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	403	CLA	C1D-ND	5.32	1.44	1.37
23	c	509	CLA	O2D-CGD	5.32	1.46	1.33
23	C	512	CLA	CHC-C1C	5.32	1.48	1.35
23	b	616	CLA	C3B-C2B	5.31	1.47	1.40
23	b	602	CLA	CHC-C1C	5.31	1.48	1.35
23	B	614	CLA	C3C-C2C	5.31	1.48	1.36
23	b	602	CLA	C3B-C2B	5.31	1.47	1.40
23	c	514	CLA	C1D-ND	5.30	1.44	1.37
23	d	402	CLA	C3C-C2C	5.30	1.48	1.36
23	B	613	CLA	CHC-C1C	5.30	1.48	1.35
23	b	609	CLA	C3B-C2B	5.30	1.47	1.40
23	B	610	CLA	C1D-ND	5.30	1.44	1.37
23	B	616	CLA	C3C-C2C	5.30	1.48	1.36
23	b	607	CLA	C3C-C2C	5.30	1.48	1.36
23	b	601	CLA	C3C-C2C	5.30	1.48	1.36
23	c	508	CLA	C3B-C2B	5.28	1.47	1.40
23	c	513	CLA	CHC-C1C	5.28	1.48	1.35
23	B	614	CLA	C3B-C2B	5.28	1.47	1.40
23	B	605	CLA	C3C-C2C	5.28	1.48	1.36
24	a	417	PHO	C3D-C2D	5.28	1.48	1.39
23	b	616	CLA	C3C-C2C	5.27	1.47	1.36
23	B	601	CLA	C3C-C2C	5.27	1.47	1.36
23	C	509	CLA	C3C-C2C	5.27	1.47	1.36
23	c	502	CLA	C1D-ND	5.27	1.44	1.37
23	C	502	CLA	C3C-C2C	5.26	1.47	1.36
23	b	616	CLA	CHC-C1C	5.26	1.48	1.35
23	C	503	CLA	CHC-C1C	5.26	1.48	1.35
23	A	408	CLA	C3C-C2C	5.25	1.47	1.36
24	A	416	PHO	C3D-C2D	5.25	1.48	1.39
23	D	403	CLA	C3B-C2B	5.25	1.47	1.40
23	c	514	CLA	CHC-C1C	5.25	1.48	1.35
23	c	505	CLA	O2D-CGD	5.24	1.46	1.33
23	B	610	CLA	CHC-C1C	5.24	1.48	1.35
23	C	505	CLA	CHC-C1C	5.24	1.48	1.35
23	b	606	CLA	C3C-C2C	5.23	1.47	1.36
23	d	401	CLA	C3C-C2C	5.23	1.47	1.36
23	b	614	CLA	C3C-C2C	5.23	1.47	1.36
23	c	514	CLA	C3C-C2C	5.23	1.47	1.36
23	B	609	CLA	O2D-CGD	5.23	1.46	1.33
40	v	201	HEC	C3D-C2D	5.23	1.53	1.37
23	C	507	CLA	C3C-C2C	5.23	1.47	1.36
23	a	407	CLA	C3B-C2B	5.22	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	402	CLA	C3C-C2C	5.22	1.47	1.36
23	D	403	CLA	CHC-C1C	5.22	1.48	1.35
23	a	405	CLA	C3C-C2C	5.22	1.47	1.36
23	a	409	CLA	CHC-C1C	5.22	1.48	1.35
23	b	615	CLA	C3C-C2C	5.21	1.47	1.36
23	b	609	CLA	O2D-CGD	5.21	1.45	1.33
23	C	507	CLA	CHC-C1C	5.21	1.48	1.35
23	b	603	CLA	C3C-C2C	5.21	1.47	1.36
23	c	510	CLA	O2D-CGD	5.19	1.45	1.33
23	b	610	CLA	C3C-C2C	5.18	1.47	1.36
23	A	405	CLA	C3B-C2B	5.18	1.47	1.40
23	c	504	CLA	CHC-C1C	5.18	1.48	1.35
23	B	601	CLA	C1D-ND	5.18	1.44	1.37
23	b	615	CLA	C3B-C2B	5.18	1.47	1.40
23	B	615	CLA	C1D-ND	5.18	1.44	1.37
23	C	502	CLA	C1D-ND	5.17	1.44	1.37
23	c	505	CLA	C3C-C2C	5.16	1.47	1.36
23	a	406	CLA	C1D-ND	5.16	1.44	1.37
23	d	402	CLA	CHC-C1C	5.16	1.48	1.35
23	B	612	CLA	C3C-C2C	5.16	1.47	1.36
23	C	510	CLA	CHC-C1C	5.15	1.48	1.35
23	C	503	CLA	C3B-C2B	5.15	1.47	1.40
23	b	604	CLA	C1D-ND	5.15	1.44	1.37
23	c	502	CLA	C3C-C2C	5.14	1.47	1.36
23	B	614	CLA	C1D-ND	5.14	1.44	1.37
23	C	508	CLA	C1D-ND	5.14	1.44	1.37
23	c	507	CLA	O2D-CGD	5.14	1.45	1.33
23	b	616	CLA	C1D-ND	5.14	1.44	1.37
23	b	602	CLA	C3C-C2C	5.14	1.47	1.36
23	c	507	CLA	C1D-ND	5.13	1.44	1.37
23	c	509	CLA	CHC-C1C	5.13	1.48	1.35
23	b	603	CLA	O2D-CGD	5.13	1.45	1.33
23	c	513	CLA	C1D-ND	5.13	1.44	1.37
23	b	614	CLA	CHC-C1C	5.13	1.48	1.35
23	C	501	CLA	C3C-C2C	5.12	1.47	1.36
23	A	406	CLA	CHC-C1C	5.12	1.48	1.35
23	B	606	CLA	CHC-C1C	5.12	1.48	1.35
23	b	612	CLA	C3C-C2C	5.12	1.47	1.36
23	B	615	CLA	CHC-C1C	5.12	1.48	1.35
23	B	601	CLA	CHC-C1C	5.11	1.48	1.35
23	c	509	CLA	C1D-ND	5.11	1.44	1.37
23	c	506	CLA	C3B-C2B	5.11	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	602	CLA	O2D-CGD	5.11	1.45	1.33
23	C	501	CLA	CHC-C1C	5.11	1.48	1.35
23	b	603	CLA	CHC-C1C	5.10	1.48	1.35
23	B	605	CLA	C1D-ND	5.10	1.44	1.37
23	c	507	CLA	C3C-C2C	5.10	1.47	1.36
23	b	601	CLA	CHC-C1C	5.09	1.48	1.35
23	B	609	CLA	C3C-C2C	5.09	1.47	1.36
23	c	514	CLA	O2D-CGD	5.09	1.45	1.33
23	c	503	CLA	C3C-C2C	5.08	1.47	1.36
23	B	606	CLA	C3C-C2C	5.08	1.47	1.36
23	B	602	CLA	C3C-C2C	5.08	1.47	1.36
23	C	504	CLA	C3C-C2C	5.08	1.47	1.36
23	B	609	CLA	CHC-C1C	5.08	1.48	1.35
23	c	506	CLA	CHC-C1C	5.08	1.48	1.35
23	C	509	CLA	C1D-ND	5.08	1.44	1.37
23	C	506	CLA	O2D-CGD	5.07	1.45	1.33
23	B	602	CLA	CHC-C1C	5.06	1.48	1.35
23	C	512	CLA	C1D-ND	5.06	1.44	1.37
23	b	609	CLA	CHC-C1C	5.06	1.47	1.35
23	c	508	CLA	CHC-C1C	5.06	1.47	1.35
23	c	508	CLA	C1D-ND	5.06	1.44	1.37
23	B	613	CLA	O2D-CGD	5.05	1.45	1.33
23	A	406	CLA	C3C-C2C	5.05	1.47	1.36
23	C	505	CLA	C3B-C2B	5.05	1.47	1.40
23	b	604	CLA	CHC-C1C	5.05	1.47	1.35
23	c	502	CLA	CHC-C1C	5.05	1.47	1.35
23	C	513	CLA	C1D-ND	5.05	1.44	1.37
23	b	613	CLA	C1D-ND	5.05	1.44	1.37
23	b	610	CLA	O2D-CGD	5.05	1.45	1.33
23	C	513	CLA	C3C-C2C	5.04	1.47	1.36
23	C	511	CLA	O2D-CGD	5.04	1.45	1.33
23	c	512	CLA	C3C-C2C	5.04	1.47	1.36
25	K	101	BCR	C23-C22	-5.03	1.35	1.45
23	b	613	CLA	CHC-C1C	5.03	1.47	1.35
24	a	408	PHO	O2D-CGD	5.03	1.45	1.33
23	B	603	CLA	C3C-C2C	5.03	1.47	1.36
25	d	403	BCR	C23-C22	-5.03	1.35	1.45
23	C	508	CLA	CHC-C1C	5.03	1.47	1.35
23	b	610	CLA	CHC-C1C	5.03	1.47	1.35
23	B	613	CLA	C1D-ND	5.02	1.44	1.37
23	B	601	CLA	O2D-CGD	5.02	1.45	1.33
23	c	504	CLA	C1D-ND	5.02	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	511	CLA	C3C-C2C	5.02	1.47	1.36
23	B	604	CLA	C3C-C2C	5.02	1.47	1.36
23	a	407	CLA	CHC-C1C	5.01	1.47	1.35
23	a	406	CLA	C3B-C2B	5.01	1.47	1.40
23	C	508	CLA	O2D-CGD	5.00	1.45	1.33
23	a	409	CLA	C3C-C2C	4.99	1.47	1.36
40	V	201	HEC	C3C-C2C	-4.99	1.35	1.40
23	b	605	CLA	CHC-C1C	4.99	1.47	1.35
23	A	405	CLA	CHC-C1C	4.99	1.47	1.35
23	b	606	CLA	C1D-ND	4.98	1.43	1.37
23	C	513	CLA	CHC-C1C	4.98	1.47	1.35
23	a	406	CLA	O2D-CGD	4.98	1.45	1.33
23	B	605	CLA	CHC-C1C	4.97	1.47	1.35
23	b	615	CLA	O2D-CGD	4.97	1.45	1.33
25	k	101	BCR	C23-C22	-4.97	1.35	1.45
23	c	505	CLA	C1D-ND	4.96	1.43	1.37
23	b	606	CLA	CHC-C1C	4.96	1.47	1.35
23	c	505	CLA	CHC-C1C	4.96	1.47	1.35
23	C	502	CLA	O2D-CGD	4.96	1.45	1.33
40	V	201	HEC	C3D-C2D	4.95	1.52	1.37
23	b	613	CLA	O2D-CGD	4.95	1.45	1.33
23	B	601	CLA	O2A-CGA	4.95	1.47	1.33
23	b	607	CLA	CHC-C1C	4.95	1.47	1.35
24	a	417	PHO	O2D-CGD	4.95	1.45	1.33
23	C	509	CLA	O2D-CGD	4.95	1.45	1.33
23	C	504	CLA	O2D-CGD	4.94	1.45	1.33
23	c	508	CLA	O2D-CGD	4.94	1.45	1.33
23	c	512	CLA	CHC-C1C	4.94	1.47	1.35
23	B	604	CLA	CHC-C1C	4.94	1.47	1.35
23	c	511	CLA	O2D-CGD	4.94	1.45	1.33
23	c	508	CLA	C3C-C2C	4.93	1.47	1.36
23	B	615	CLA	O2D-CGD	4.93	1.45	1.33
23	A	406	CLA	C3B-C2B	4.93	1.47	1.40
23	C	506	CLA	C3C-C2C	4.92	1.47	1.36
23	B	615	CLA	C3C-C2C	4.92	1.47	1.36
23	B	606	CLA	C1D-ND	4.92	1.43	1.37
23	b	609	CLA	C3C-C2C	4.92	1.47	1.36
23	b	613	CLA	C3C-C2C	4.92	1.47	1.36
23	b	608	CLA	C3C-C2C	4.91	1.47	1.36
23	b	601	CLA	O2D-CGD	4.91	1.45	1.33
23	D	403	CLA	O2D-CGD	4.91	1.45	1.33
24	A	416	PHO	O2D-CGD	4.91	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	511	CLA	C1D-ND	4.90	1.43	1.37
23	B	603	CLA	C1D-ND	4.90	1.43	1.37
24	A	407	PHO	O2D-CGD	4.90	1.45	1.33
23	A	406	CLA	O2D-CGD	4.90	1.45	1.33
23	C	505	CLA	C3C-C2C	4.89	1.47	1.36
23	B	603	CLA	CHC-C1C	4.88	1.47	1.35
23	b	615	CLA	CHC-C1C	4.88	1.47	1.35
24	A	407	PHO	C3D-C2D	4.88	1.48	1.39
40	v	201	HEC	C3C-C2C	-4.88	1.35	1.40
25	T	102	BCR	C23-C22	-4.88	1.35	1.45
23	b	611	CLA	CHC-C1C	4.88	1.47	1.35
23	a	406	CLA	CHC-C1C	4.87	1.47	1.35
23	c	512	CLA	O2D-CGD	4.87	1.45	1.33
23	A	405	CLA	C3C-C2C	4.87	1.47	1.36
23	C	513	CLA	O2D-CGD	4.87	1.45	1.33
23	c	503	CLA	O2D-CGD	4.86	1.45	1.33
23	B	614	CLA	CHC-C1C	4.86	1.47	1.35
23	b	608	CLA	CHC-C1C	4.85	1.47	1.35
23	a	409	CLA	O2D-CGD	4.85	1.45	1.33
23	b	604	CLA	C3C-C2C	4.84	1.47	1.36
23	b	614	CLA	C1D-ND	4.84	1.43	1.37
24	a	417	PHO	OBD-CAD	4.84	1.29	1.22
23	B	602	CLA	C1D-ND	4.84	1.43	1.37
23	a	405	CLA	CHC-C1C	4.84	1.47	1.35
25	b	617	BCR	C23-C22	-4.84	1.35	1.45
23	C	511	CLA	CHC-C1C	4.83	1.47	1.35
23	B	605	CLA	O2D-CGD	4.82	1.45	1.33
23	c	507	CLA	CHC-C1C	4.82	1.47	1.35
23	B	613	CLA	C3C-C2C	4.82	1.47	1.36
25	K	103	BCR	C23-C22	-4.82	1.35	1.45
25	c	516	BCR	C23-C22	-4.81	1.35	1.45
23	C	510	CLA	O2D-CGD	4.80	1.44	1.33
23	B	604	CLA	O2D-CGD	4.80	1.44	1.33
23	D	402	CLA	O2D-CGD	4.80	1.44	1.33
23	A	404	CLA	CHC-C1C	4.80	1.47	1.35
23	c	511	CLA	CHC-C1C	4.80	1.47	1.35
23	A	408	CLA	CHC-C1C	4.80	1.47	1.35
23	C	501	CLA	C1D-ND	4.79	1.43	1.37
23	B	607	CLA	CHC-C1C	4.79	1.47	1.35
23	b	611	CLA	C3C-C2C	4.79	1.46	1.36
23	b	605	CLA	O2D-CGD	4.79	1.44	1.33
23	C	505	CLA	O2D-CGD	4.78	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	514	BCR	C23-C22	-4.78	1.35	1.45
23	C	512	CLA	O2D-CGD	4.78	1.44	1.33
23	C	511	CLA	C3C-C2C	4.78	1.46	1.36
23	b	616	CLA	O2D-CGD	4.78	1.44	1.33
23	B	610	CLA	O2D-CGD	4.77	1.44	1.33
23	b	605	CLA	C1D-ND	4.77	1.43	1.37
23	C	502	CLA	CHC-C1C	4.77	1.47	1.35
23	B	607	CLA	C3C-C2C	4.77	1.46	1.36
23	C	504	CLA	CHC-C1C	4.76	1.47	1.35
23	B	603	CLA	O2D-CGD	4.76	1.44	1.33
25	D	404	BCR	C23-C22	-4.76	1.35	1.45
23	A	408	CLA	O2D-CGD	4.76	1.44	1.33
23	c	513	CLA	O2D-CGD	4.75	1.44	1.33
23	B	605	CLA	C3B-C2B	4.75	1.47	1.40
23	D	402	CLA	CHC-C1C	4.75	1.47	1.35
26	F	103	SQD	O47-C7	4.75	1.47	1.34
23	b	601	CLA	O2A-CGA	4.75	1.47	1.33
23	b	614	CLA	O2D-CGD	4.75	1.44	1.33
23	c	503	CLA	C1D-ND	4.74	1.43	1.37
23	b	602	CLA	CHD-C1D	4.73	1.47	1.38
23	A	404	CLA	O2D-CGD	4.73	1.44	1.33
23	c	504	CLA	C3B-C2B	4.73	1.46	1.40
23	C	509	CLA	CHC-C1C	4.72	1.47	1.35
25	c	515	BCR	C23-C22	-4.72	1.35	1.45
23	b	611	CLA	O2D-CGD	4.71	1.44	1.33
25	t	102	BCR	C23-C22	-4.71	1.35	1.45
23	C	503	CLA	C1D-ND	4.70	1.43	1.37
23	C	505	CLA	C1D-ND	4.70	1.43	1.37
23	C	506	CLA	CHC-C1C	4.69	1.47	1.35
23	B	611	CLA	O2D-CGD	4.69	1.44	1.33
23	b	612	CLA	CHC-C1C	4.68	1.47	1.35
23	b	615	CLA	C1D-ND	4.68	1.43	1.37
25	b	619	BCR	C23-C22	-4.67	1.35	1.45
25	B	619	BCR	C23-C22	-4.67	1.35	1.45
23	d	401	CLA	O2D-CGD	4.66	1.44	1.33
25	A	409	BCR	C23-C22	-4.66	1.35	1.45
23	C	504	CLA	C1D-ND	4.66	1.43	1.37
23	d	401	CLA	CHC-C1C	4.66	1.46	1.35
23	C	506	CLA	C1D-ND	4.65	1.43	1.37
23	b	612	CLA	O2D-CGD	4.65	1.44	1.33
23	B	608	CLA	C1D-ND	4.64	1.43	1.37
23	B	615	CLA	C3B-C2B	4.64	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	608	CLA	O2D-CGD	4.64	1.44	1.33
23	c	510	CLA	CHC-C1C	4.64	1.46	1.35
23	c	510	CLA	C1D-ND	4.63	1.43	1.37
23	C	506	CLA	CHD-C1D	4.62	1.47	1.38
23	a	405	CLA	C1D-ND	4.62	1.43	1.37
23	B	616	CLA	O2D-CGD	4.62	1.44	1.33
25	y	101	BCR	C23-C22	-4.61	1.36	1.45
23	B	606	CLA	O2D-CGD	4.61	1.44	1.33
23	b	606	CLA	O2D-CGD	4.60	1.44	1.33
23	b	609	CLA	C1D-ND	4.60	1.43	1.37
25	a	410	BCR	C23-C22	-4.60	1.36	1.45
23	B	602	CLA	O2D-CGD	4.59	1.44	1.33
32	c	521	LMG	O7-C10	4.58	1.47	1.34
23	C	507	CLA	O2D-CGD	4.58	1.44	1.33
23	c	503	CLA	CHC-C1C	4.58	1.46	1.35
23	B	608	CLA	C3C-C2C	4.56	1.46	1.36
23	C	507	CLA	C1D-ND	4.55	1.43	1.37
23	B	614	CLA	O2D-CGD	4.55	1.44	1.33
32	C	519	LMG	O7-C10	4.54	1.47	1.34
23	a	405	CLA	O2D-CGD	4.54	1.44	1.33
23	c	514	CLA	CHD-C1D	4.52	1.47	1.38
23	B	609	CLA	C1D-ND	4.52	1.43	1.37
23	b	607	CLA	O2D-CGD	4.51	1.44	1.33
23	C	511	CLA	C1D-ND	4.51	1.43	1.37
23	B	604	CLA	CHD-C1D	4.50	1.47	1.38
23	B	615	CLA	CHD-C1D	4.50	1.47	1.38
23	a	407	CLA	O2D-CGD	4.50	1.44	1.33
26	A	412	SQD	O48-C23	4.49	1.46	1.33
32	C	519	LMG	O8-C28	4.49	1.46	1.33
23	c	504	CLA	CHD-C1D	4.49	1.47	1.38
25	h	101	BCR	C23-C22	-4.48	1.36	1.45
25	H	101	BCR	C23-C22	-4.48	1.36	1.45
25	B	617	BCR	C23-C22	-4.48	1.36	1.45
33	E	101	LHG	O8-C23	4.48	1.46	1.33
23	b	604	CLA	O2D-CGD	4.47	1.44	1.33
26	f	102	SQD	O47-C7	4.47	1.46	1.34
23	b	601	CLA	CHD-C1D	4.46	1.47	1.38
26	a	413	SQD	O48-C23	4.46	1.46	1.33
23	b	612	CLA	C1D-ND	4.45	1.43	1.37
26	B	620	SQD	O47-C7	4.44	1.46	1.34
23	B	607	CLA	O2D-CGD	4.44	1.44	1.33
23	d	402	CLA	O2A-CGA	4.43	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	408	CLA	O2A-CGA	4.43	1.46	1.33
23	c	513	CLA	O2A-CGA	4.42	1.46	1.33
32	z	101	LMG	O8-C28	4.42	1.46	1.33
23	c	506	CLA	O2D-CGD	4.42	1.44	1.33
23	B	609	CLA	CHD-C1D	4.40	1.46	1.38
23	b	602	CLA	C1D-ND	4.40	1.43	1.37
33	a	421	LHG	O8-C23	4.39	1.46	1.33
23	D	403	CLA	CHD-C1D	4.38	1.46	1.38
23	a	406	CLA	C3D-C2D	4.38	1.51	1.39
23	B	610	CLA	OBD-CAD	4.38	1.30	1.22
23	c	512	CLA	CHD-C1D	4.37	1.46	1.38
23	C	512	CLA	CHD-C1D	4.37	1.46	1.38
23	c	506	CLA	C1D-ND	4.36	1.43	1.37
24	a	408	PHO	OBD-CAD	4.36	1.28	1.22
23	B	616	CLA	C1D-ND	4.35	1.43	1.37
23	B	608	CLA	CHC-C1C	4.35	1.46	1.35
23	A	405	CLA	O2D-CGD	4.35	1.43	1.33
23	b	611	CLA	O2A-CGA	4.34	1.46	1.33
23	A	408	CLA	C1D-ND	4.34	1.43	1.37
23	c	514	CLA	O2A-CGA	4.34	1.46	1.33
32	C	518	LMG	O8-C28	4.33	1.46	1.33
32	B	621	LMG	O8-C28	4.33	1.46	1.33
23	b	608	CLA	C1D-ND	4.32	1.43	1.37
23	c	513	CLA	CHD-C1D	4.31	1.46	1.38
23	C	513	CLA	CHD-C1D	4.31	1.46	1.38
24	A	416	PHO	OBD-CAD	4.31	1.28	1.22
23	B	602	CLA	CHD-C1D	4.31	1.46	1.38
25	Y	101	BCR	C23-C22	-4.31	1.36	1.45
26	b	620	SQD	O48-C23	4.31	1.45	1.33
33	d	406	LHG	O8-C23	4.31	1.45	1.33
26	b	620	SQD	O47-C7	4.31	1.46	1.34
23	C	502	CLA	CHD-C1D	4.31	1.46	1.38
23	B	608	CLA	O2D-CGD	4.30	1.43	1.33
23	C	503	CLA	O2D-CGD	4.30	1.43	1.33
23	c	506	CLA	CHD-C1D	4.30	1.46	1.38
23	a	409	CLA	O2A-CGA	4.29	1.45	1.33
26	B	620	SQD	O48-C23	4.28	1.45	1.33
23	d	402	CLA	CHD-C1D	4.28	1.46	1.38
23	c	502	CLA	O2D-CGD	4.27	1.43	1.33
35	c	519	DGD	O1G-C1A	4.27	1.45	1.33
23	C	509	CLA	CHD-C1D	4.27	1.46	1.38
23	D	402	CLA	C1D-ND	4.27	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	512	CLA	O2A-CGA	4.27	1.45	1.33
23	c	508	CLA	O2A-CGA	4.26	1.45	1.33
23	b	609	CLA	CHD-C1D	4.26	1.46	1.38
23	C	508	CLA	C3D-C2D	4.25	1.50	1.39
23	b	614	CLA	CHD-C1D	4.25	1.46	1.38
26	f	102	SQD	O48-C23	4.25	1.45	1.33
25	b	618	BCR	C23-C22	-4.24	1.36	1.45
32	c	521	LMG	O8-C28	4.23	1.45	1.33
23	c	510	CLA	CHD-C1D	4.23	1.46	1.38
32	m	101	LMG	O8-C28	4.23	1.45	1.33
23	b	611	CLA	C1D-ND	4.23	1.43	1.37
23	B	604	CLA	C1D-ND	4.22	1.43	1.37
23	A	404	CLA	C1D-ND	4.22	1.43	1.37
23	D	402	CLA	O2A-CGA	4.22	1.45	1.33
26	A	412	SQD	O47-C7	4.22	1.46	1.34
23	c	505	CLA	C3D-C2D	4.21	1.50	1.39
23	b	607	CLA	CHD-C1D	4.20	1.46	1.38
23	C	508	CLA	O2A-CGA	4.19	1.45	1.33
33	E	101	LHG	O7-C7	4.19	1.46	1.34
34	B	622	HTG	C1'-S1	-4.19	1.76	1.81
23	A	406	CLA	CHD-C1D	4.18	1.46	1.38
23	c	503	CLA	O2A-CGA	4.18	1.45	1.33
26	F	103	SQD	O48-C23	4.18	1.45	1.33
23	b	602	CLA	CHD-C4C	4.18	1.48	1.39
23	C	513	CLA	O2A-CGA	4.18	1.45	1.33
23	c	507	CLA	O2A-CGA	4.18	1.45	1.33
23	C	511	CLA	CHD-C1D	4.17	1.46	1.38
34	b	622	HTG	C1'-S1	-4.17	1.76	1.81
23	C	512	CLA	O2A-CGA	4.17	1.45	1.33
23	C	505	CLA	CHD-C1D	4.16	1.46	1.38
23	b	603	CLA	C1D-ND	4.16	1.42	1.37
23	b	601	CLA	C3D-C2D	4.16	1.50	1.39
23	b	616	CLA	O2A-CGA	4.15	1.45	1.33
23	a	407	CLA	C1D-ND	4.15	1.42	1.37
23	c	509	CLA	O2A-CGA	4.15	1.45	1.33
23	d	402	CLA	O2D-CGD	4.15	1.43	1.33
32	Z	101	LMG	O7-C10	4.15	1.46	1.34
23	C	501	CLA	CHD-C1D	4.15	1.46	1.38
23	B	601	CLA	CHD-C1D	4.15	1.46	1.38
24	A	407	PHO	OBD-CAD	4.14	1.28	1.22
23	c	514	CLA	CHD-C4C	4.14	1.48	1.39
23	b	610	CLA	CHD-C1D	4.13	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	a	421	LHG	O7-C7	4.13	1.46	1.34
23	b	606	CLA	CHD-C1D	4.13	1.46	1.38
23	c	509	CLA	CHD-C1D	4.13	1.46	1.38
23	c	503	CLA	CHD-C1D	4.13	1.46	1.38
23	b	601	CLA	CHD-C4C	4.12	1.48	1.39
23	a	407	CLA	O2A-CGA	4.12	1.45	1.33
23	C	510	CLA	CHD-C4C	4.12	1.48	1.39
23	b	610	CLA	C1D-ND	4.12	1.42	1.37
23	c	504	CLA	O2D-CGD	4.11	1.43	1.33
23	b	615	CLA	CHD-C1D	4.11	1.46	1.38
23	C	503	CLA	CHD-C1D	4.11	1.46	1.38
23	c	510	CLA	O2A-CGA	4.11	1.45	1.33
23	b	604	CLA	CHD-C1D	4.11	1.46	1.38
32	z	101	LMG	O7-C10	4.10	1.45	1.34
23	b	607	CLA	C1D-ND	4.10	1.42	1.37
23	C	507	CLA	O2A-CGA	4.10	1.45	1.33
32	d	410	LMG	O8-C28	4.10	1.45	1.33
32	c	520	LMG	O7-C10	4.09	1.45	1.34
23	c	508	CLA	CHD-C1D	4.09	1.46	1.38
35	c	517	DGD	O2G-C1B	4.09	1.45	1.34
23	B	612	CLA	O2D-CGD	4.09	1.43	1.33
23	B	609	CLA	O2A-CGA	4.08	1.45	1.33
23	C	503	CLA	CHD-C4C	4.08	1.48	1.39
23	B	608	CLA	C3D-C2D	4.08	1.50	1.39
23	B	608	CLA	CHD-C1D	4.08	1.46	1.38
23	a	406	CLA	O2A-CGA	4.08	1.45	1.33
23	B	615	CLA	O2A-CGA	4.08	1.45	1.33
23	C	511	CLA	O2A-CGA	4.08	1.45	1.33
35	C	517	DGD	O1G-C1A	4.08	1.45	1.33
32	a	418	LMG	O8-C28	4.07	1.45	1.33
23	c	513	CLA	CHD-C4C	4.07	1.48	1.39
23	B	606	CLA	CHD-C1D	4.07	1.46	1.38
23	C	501	CLA	O2D-CGD	4.07	1.43	1.33
26	a	411	SQD	O47-C7	4.07	1.45	1.34
23	c	504	CLA	O2A-CGA	4.06	1.45	1.33
23	c	504	CLA	CHD-C4C	4.06	1.48	1.39
23	b	608	CLA	CHD-C1D	4.06	1.46	1.38
35	C	515	DGD	O2G-C1B	4.06	1.45	1.34
32	c	520	LMG	O8-C28	4.06	1.45	1.33
32	a	418	LMG	O7-C10	4.05	1.45	1.34
23	A	405	CLA	C3D-C2D	4.05	1.50	1.39
23	C	506	CLA	CHD-C4C	4.05	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	401	CLA	O2A-CGA	4.05	1.45	1.33
23	C	502	CLA	O2A-CGA	4.05	1.45	1.33
23	C	508	CLA	CHD-C1D	4.04	1.46	1.38
32	A	419	LMG	O7-C10	4.04	1.45	1.34
24	A	416	PHO	C3C-C2C	4.04	1.49	1.37
23	A	404	CLA	CHD-C1D	4.03	1.46	1.38
23	c	502	CLA	O2A-CGA	4.03	1.45	1.33
23	C	502	CLA	C3D-C2D	4.03	1.50	1.39
23	B	611	CLA	O2A-CGA	4.03	1.45	1.33
23	c	507	CLA	CHD-C1D	4.03	1.46	1.38
23	A	406	CLA	C1D-ND	4.02	1.42	1.37
23	C	513	CLA	CHD-C4C	4.02	1.48	1.39
26	a	413	SQD	O47-C7	4.01	1.45	1.34
23	c	507	CLA	CHD-C4C	4.01	1.48	1.39
23	A	408	CLA	CHD-C1D	4.01	1.46	1.38
23	C	506	CLA	O2A-CGA	4.01	1.45	1.33
23	B	616	CLA	O2A-CGA	4.01	1.45	1.33
23	B	610	CLA	CHD-C1D	4.00	1.46	1.38
32	A	419	LMG	O8-C28	4.00	1.45	1.33
23	C	511	CLA	CHD-C4C	4.00	1.48	1.39
23	c	509	CLA	C3D-C2D	3.99	1.50	1.39
23	B	609	CLA	C3D-C2D	3.99	1.50	1.39
23	a	405	CLA	CHD-C1D	3.99	1.46	1.38
23	b	608	CLA	O2A-CGA	3.99	1.45	1.33
32	C	518	LMG	O7-C10	3.99	1.45	1.34
23	B	615	CLA	OBD-CAD	3.99	1.29	1.22
23	C	501	CLA	O2A-CGA	3.98	1.45	1.33
23	B	605	CLA	O2A-CGA	3.98	1.45	1.33
33	D	407	LHG	O7-C7	3.98	1.45	1.34
26	a	411	SQD	O48-C23	3.98	1.45	1.33
24	a	417	PHO	C3C-C2C	3.97	1.49	1.37
23	B	614	CLA	O2A-CGA	3.97	1.44	1.33
23	B	602	CLA	CHD-C4C	3.97	1.48	1.39
23	b	615	CLA	O2A-CGA	3.97	1.44	1.33
23	c	510	CLA	C3D-C2D	3.97	1.50	1.39
23	c	512	CLA	CHD-C4C	3.96	1.48	1.39
23	C	513	CLA	C3D-C2D	3.96	1.49	1.39
23	C	510	CLA	CHD-C1D	3.96	1.46	1.38
23	b	606	CLA	O2A-CGA	3.96	1.44	1.33
23	C	504	CLA	C3D-C2D	3.96	1.49	1.39
32	d	410	LMG	O7-C10	3.96	1.45	1.34
23	a	405	CLA	CHD-C4C	3.96	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	614	CLA	CHD-C4C	3.95	1.48	1.39
23	c	511	CLA	C3D-C2D	3.95	1.49	1.39
23	b	615	CLA	CHD-C4C	3.95	1.48	1.39
23	c	503	CLA	C3D-C2D	3.95	1.49	1.39
23	c	505	CLA	CHD-C1D	3.95	1.46	1.38
23	B	611	CLA	OBD-CAD	3.95	1.29	1.22
23	B	613	CLA	C3D-C2D	3.95	1.49	1.39
23	c	503	CLA	CHD-C4C	3.94	1.48	1.39
23	B	614	CLA	CHD-C1D	3.93	1.46	1.38
23	c	505	CLA	O2A-CGA	3.93	1.44	1.33
23	B	601	CLA	CHD-C4C	3.93	1.48	1.39
23	b	609	CLA	C3D-C2D	3.93	1.49	1.39
23	b	616	CLA	CHD-C1D	3.93	1.46	1.38
23	d	402	CLA	C3D-C2D	3.92	1.49	1.39
23	c	508	CLA	CHD-C4C	3.92	1.48	1.39
23	B	611	CLA	CHD-C1D	3.92	1.46	1.38
23	D	402	CLA	CHD-C1D	3.92	1.46	1.38
23	c	508	CLA	C3D-C2D	3.92	1.49	1.39
23	B	609	CLA	CHD-C4C	3.92	1.48	1.39
23	b	612	CLA	C3D-C2D	3.91	1.49	1.39
23	B	613	CLA	CHD-C1D	3.91	1.46	1.38
23	b	603	CLA	CHD-C1D	3.91	1.46	1.38
33	D	407	LHG	O8-C23	3.90	1.44	1.33
23	B	616	CLA	C3D-C2D	3.90	1.49	1.39
35	h	102	DGD	O2G-C1B	3.90	1.45	1.34
23	a	407	CLA	C3D-C2D	3.90	1.49	1.39
23	D	402	CLA	CHD-C4C	3.89	1.48	1.39
25	B	618	BCR	C23-C22	-3.89	1.37	1.45
23	C	509	CLA	O2A-CGA	3.89	1.44	1.33
23	A	405	CLA	C1D-ND	3.89	1.42	1.37
23	B	615	CLA	CHD-C4C	3.89	1.48	1.39
23	B	606	CLA	O2A-CGA	3.89	1.44	1.33
23	C	512	CLA	CHD-C4C	3.89	1.48	1.39
32	B	621	LMG	O7-C10	3.88	1.45	1.34
23	c	502	CLA	CHD-C1D	3.88	1.45	1.38
23	b	614	CLA	CHD-C4C	3.88	1.48	1.39
23	C	504	CLA	CHD-C1D	3.88	1.45	1.38
23	b	602	CLA	C3D-C2D	3.87	1.49	1.39
23	c	506	CLA	CHD-C4C	3.87	1.48	1.39
23	b	610	CLA	CHD-C4C	3.87	1.48	1.39
23	c	507	CLA	C3D-C2D	3.87	1.49	1.39
23	C	512	CLA	C3D-C2D	3.87	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	610	CLA	C3D-C2D	3.87	1.49	1.39
23	C	509	CLA	CHD-C4C	3.86	1.48	1.39
24	A	416	PHO	O2A-CGA	3.86	1.44	1.33
35	h	102	DGD	O1G-C1A	3.86	1.44	1.33
23	C	505	CLA	O2A-CGA	3.85	1.44	1.33
23	B	603	CLA	CHD-C1D	3.85	1.45	1.38
23	b	615	CLA	C3D-C2D	3.85	1.49	1.39
35	C	516	DGD	O2G-C1B	3.85	1.45	1.34
23	B	615	CLA	C3D-C2D	3.85	1.49	1.39
23	C	505	CLA	CHD-C4C	3.85	1.48	1.39
26	A	410	SQD	O48-C23	3.85	1.44	1.33
23	A	408	CLA	CHD-C4C	3.84	1.48	1.39
23	b	609	CLA	OBD-CAD	3.84	1.29	1.22
33	L	101	LHG	O8-C23	3.84	1.44	1.33
23	A	406	CLA	C3D-C2D	3.84	1.49	1.39
35	c	518	DGD	O1G-C1A	3.83	1.44	1.33
23	B	610	CLA	CHD-C4C	3.83	1.48	1.39
23	A	405	CLA	O2A-CGA	3.83	1.44	1.33
24	a	417	PHO	O2A-CGA	3.83	1.44	1.33
23	b	611	CLA	CHD-C1D	3.83	1.45	1.38
23	c	514	CLA	C3D-C2D	3.82	1.49	1.39
33	L	101	LHG	O7-C7	3.82	1.45	1.34
23	B	607	CLA	CHD-C1D	3.82	1.45	1.38
23	B	603	CLA	C3D-C2D	3.82	1.49	1.39
23	D	403	CLA	OBD-CAD	3.82	1.29	1.22
23	B	604	CLA	CHD-C4C	3.82	1.47	1.39
23	D	403	CLA	O2A-CGA	3.82	1.44	1.33
23	c	502	CLA	C3D-C2D	3.81	1.49	1.39
23	b	604	CLA	C3D-C2D	3.81	1.49	1.39
23	b	610	CLA	C3D-C2D	3.81	1.49	1.39
23	C	507	CLA	C3D-C2D	3.81	1.49	1.39
35	C	517	DGD	O2G-C1B	3.81	1.45	1.34
23	d	401	CLA	CHD-C1D	3.81	1.45	1.38
23	b	612	CLA	CHD-C1D	3.80	1.45	1.38
23	C	509	CLA	C3D-C2D	3.80	1.49	1.39
23	C	508	CLA	OBD-CAD	3.80	1.29	1.22
23	A	406	CLA	O2A-CGA	3.80	1.44	1.33
23	c	511	CLA	CHD-C4C	3.80	1.47	1.39
23	b	613	CLA	C3D-C2D	3.80	1.49	1.39
23	c	511	CLA	CHD-C1D	3.80	1.45	1.38
23	a	406	CLA	CHD-C1D	3.80	1.45	1.38
23	C	503	CLA	O2A-CGA	3.79	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	616	CLA	C3D-C2D	3.79	1.49	1.39
24	A	416	PHO	CHA-CBD	-3.79	1.47	1.52
23	C	511	CLA	C3D-C2D	3.79	1.49	1.39
23	c	509	CLA	CHD-C4C	3.79	1.47	1.39
23	B	605	CLA	C3D-C2D	3.79	1.49	1.39
23	b	608	CLA	CHD-C4C	3.78	1.47	1.39
23	b	604	CLA	CHD-C4C	3.78	1.47	1.39
23	B	602	CLA	O2A-CGA	3.78	1.44	1.33
23	c	509	CLA	OBD-CAD	3.78	1.29	1.22
23	c	511	CLA	O2A-CGA	3.78	1.44	1.33
23	C	507	CLA	CHD-C1D	3.77	1.45	1.38
23	a	406	CLA	OBD-CAD	3.77	1.29	1.22
23	c	512	CLA	OBD-CAD	3.77	1.29	1.22
23	D	403	CLA	C3D-C2D	3.77	1.49	1.39
23	B	607	CLA	C1D-ND	3.76	1.42	1.37
23	B	612	CLA	C1D-ND	3.76	1.42	1.37
23	c	510	CLA	CHD-C4C	3.76	1.47	1.39
23	b	605	CLA	CHD-C1D	3.75	1.45	1.38
23	B	611	CLA	C1C-C2C	3.75	1.51	1.44
23	c	506	CLA	O2A-CGA	3.75	1.44	1.33
34	b	623	HTG	C1'-S1	-3.75	1.76	1.81
23	b	614	CLA	C3D-C2D	3.75	1.49	1.39
23	C	501	CLA	CHD-C4C	3.75	1.47	1.39
33	d	411	LHG	O8-C23	3.75	1.44	1.33
23	b	606	CLA	CHD-C4C	3.75	1.47	1.39
23	c	512	CLA	C3D-C2D	3.74	1.49	1.39
23	b	603	CLA	CHD-C4C	3.74	1.47	1.39
23	c	513	CLA	C3D-C2D	3.74	1.49	1.39
23	C	504	CLA	O2A-CGA	3.74	1.44	1.33
23	A	406	CLA	OBD-CAD	3.74	1.28	1.22
23	b	607	CLA	C3D-C2D	3.73	1.49	1.39
23	C	510	CLA	O2A-CGA	3.73	1.44	1.33
23	b	610	CLA	OBD-CAD	3.73	1.28	1.22
23	A	404	CLA	CHD-C4C	3.73	1.47	1.39
23	C	506	CLA	C3D-C2D	3.73	1.49	1.39
23	b	605	CLA	CHD-C4C	3.73	1.47	1.39
23	B	603	CLA	O2A-CGA	3.73	1.44	1.33
23	d	402	CLA	CHD-C4C	3.72	1.47	1.39
33	d	405	LHG	O7-C7	3.72	1.44	1.34
23	A	405	CLA	CHD-C1D	3.72	1.45	1.38
23	B	601	CLA	C3D-C2D	3.72	1.49	1.39
23	a	409	CLA	C1D-ND	3.72	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	505	CLA	CHD-C4C	3.72	1.47	1.39
35	C	516	DGD	O1G-C1A	3.71	1.44	1.33
23	B	605	CLA	CHD-C1D	3.70	1.45	1.38
23	b	608	CLA	C3D-C2D	3.70	1.49	1.39
23	C	510	CLA	C3D-C2D	3.70	1.49	1.39
23	b	615	CLA	OBD-CAD	3.70	1.28	1.22
23	B	601	CLA	OBD-CAD	3.70	1.28	1.22
23	B	611	CLA	CHD-C4C	3.70	1.47	1.39
23	C	509	CLA	OBD-CAD	3.69	1.28	1.22
23	B	602	CLA	C3D-C2D	3.69	1.49	1.39
23	b	613	CLA	O2A-CGA	3.68	1.44	1.33
24	A	407	PHO	C3C-C2C	3.68	1.48	1.37
23	c	513	CLA	OBD-CAD	3.68	1.28	1.22
26	A	410	SQD	O47-C7	3.68	1.44	1.34
23	a	407	CLA	OBD-CAD	3.68	1.28	1.22
23	b	612	CLA	O2A-CGA	3.68	1.44	1.33
23	C	504	CLA	CHD-C4C	3.68	1.47	1.39
23	b	601	CLA	OBD-CAD	3.68	1.28	1.22
32	m	101	LMG	O7-C10	3.67	1.44	1.34
23	b	616	CLA	CHD-C4C	3.67	1.47	1.39
23	b	609	CLA	CHD-C4C	3.67	1.47	1.39
23	A	406	CLA	CHD-C4C	3.67	1.47	1.39
35	H	102	DGD	O1G-C1A	3.66	1.44	1.33
23	B	612	CLA	O2A-CGA	3.66	1.44	1.33
23	b	611	CLA	CHD-C4C	3.66	1.47	1.39
23	a	405	CLA	C3D-C2D	3.66	1.49	1.39
23	B	613	CLA	OBD-CAD	3.66	1.28	1.22
33	d	406	LHG	O7-C7	3.66	1.44	1.34
23	b	606	CLA	OBD-CAD	3.66	1.28	1.22
23	C	502	CLA	CHD-C4C	3.65	1.47	1.39
23	c	506	CLA	OBD-CAD	3.65	1.28	1.22
23	B	612	CLA	CHD-C1D	3.65	1.45	1.38
23	a	409	CLA	CHD-C1D	3.65	1.45	1.38
23	C	501	CLA	C3D-C2D	3.65	1.49	1.39
23	c	502	CLA	CHD-C4C	3.65	1.47	1.39
23	C	502	CLA	OBD-CAD	3.65	1.28	1.22
23	C	513	CLA	OBD-CAD	3.65	1.28	1.22
23	b	609	CLA	O2A-CGA	3.65	1.44	1.33
23	B	607	CLA	O2A-CGA	3.65	1.44	1.33
24	A	407	PHO	O2A-CGA	3.64	1.44	1.33
23	c	506	CLA	C3D-C2D	3.64	1.49	1.39
23	D	403	CLA	CHD-C4C	3.64	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	603	CLA	C3D-C2D	3.64	1.49	1.39
23	c	508	CLA	OBD-CAD	3.64	1.28	1.22
23	A	404	CLA	C3D-C2D	3.63	1.49	1.39
23	B	604	CLA	O2A-CGA	3.63	1.43	1.33
23	b	611	CLA	C3D-C2D	3.63	1.49	1.39
23	B	607	CLA	CHD-C4C	3.63	1.47	1.39
23	B	604	CLA	OBD-CAD	3.62	1.28	1.22
24	a	408	PHO	C3C-C2C	3.62	1.48	1.37
35	c	517	DGD	O1G-C1A	3.62	1.43	1.33
23	B	606	CLA	C3D-C2D	3.62	1.49	1.39
23	B	613	CLA	CHD-C4C	3.62	1.47	1.39
23	a	406	CLA	CHD-C4C	3.62	1.47	1.39
33	b	630	LHG	O7-C7	3.62	1.44	1.34
23	a	405	CLA	OBD-CAD	3.61	1.28	1.22
23	B	606	CLA	CHD-C4C	3.61	1.47	1.39
32	D	411	LMG	O8-C28	3.61	1.43	1.33
23	b	614	CLA	O2A-CGA	3.61	1.43	1.33
23	B	603	CLA	CHD-C4C	3.60	1.47	1.39
23	B	612	CLA	C3D-C2D	3.60	1.49	1.39
23	b	606	CLA	C3D-C2D	3.60	1.48	1.39
33	D	406	LHG	O7-C7	3.60	1.44	1.34
23	a	409	CLA	C3D-C2D	3.60	1.48	1.39
23	C	508	CLA	CHD-C4C	3.60	1.47	1.39
32	D	411	LMG	O7-C10	3.58	1.44	1.34
23	a	407	CLA	CHD-C4C	3.58	1.47	1.39
34	B	625	HTG	C1'-S1	-3.58	1.76	1.81
23	b	604	CLA	O2A-CGA	3.57	1.43	1.33
23	d	401	CLA	CHD-C4C	3.57	1.47	1.39
23	b	604	CLA	OBD-CAD	3.57	1.28	1.22
23	A	405	CLA	CHD-C4C	3.56	1.47	1.39
23	b	602	CLA	OBD-CAD	3.56	1.28	1.22
23	C	507	CLA	CHD-C4C	3.56	1.47	1.39
35	C	515	DGD	O1G-C1A	3.55	1.43	1.33
23	b	612	CLA	OBD-CAD	3.55	1.28	1.22
23	d	401	CLA	C3D-C2D	3.55	1.48	1.39
23	B	614	CLA	C3D-C2D	3.54	1.48	1.39
23	a	407	CLA	CHD-C1D	3.54	1.45	1.38
35	c	518	DGD	O2G-C1B	3.53	1.44	1.34
23	A	408	CLA	C3D-C2D	3.53	1.48	1.39
23	c	507	CLA	OBD-CAD	3.53	1.28	1.22
33	d	405	LHG	O8-C23	3.53	1.43	1.33
33	D	406	LHG	O8-C23	3.53	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	A	420	LHG	O8-C23	3.52	1.43	1.33
23	C	512	CLA	OBD-CAD	3.52	1.28	1.22
23	c	514	CLA	OBD-CAD	3.52	1.28	1.22
35	c	519	DGD	O2G-C1B	3.51	1.44	1.34
23	B	605	CLA	CHD-C4C	3.51	1.47	1.39
23	b	602	CLA	O2A-CGA	3.51	1.43	1.33
23	C	503	CLA	C3D-C2D	3.51	1.48	1.39
33	d	411	LHG	O7-C7	3.50	1.44	1.34
23	C	506	CLA	OBD-CAD	3.50	1.28	1.22
33	A	420	LHG	O7-C7	3.49	1.44	1.34
33	b	630	LHG	O8-C23	3.49	1.43	1.33
23	B	616	CLA	CHD-C1D	3.48	1.45	1.38
23	b	605	CLA	OBD-CAD	3.48	1.28	1.22
23	c	503	CLA	OBD-CAD	3.48	1.28	1.22
23	b	613	CLA	CHD-C1D	3.47	1.45	1.38
23	b	605	CLA	C3D-C2D	3.46	1.48	1.39
23	b	608	CLA	OBD-CAD	3.45	1.28	1.22
23	B	610	CLA	O2A-CGA	3.45	1.43	1.33
23	b	605	CLA	O2A-CGA	3.44	1.43	1.33
23	D	402	CLA	C3D-C2D	3.43	1.48	1.39
23	C	505	CLA	OBD-CAD	3.43	1.28	1.22
23	B	611	CLA	C3D-C2D	3.42	1.48	1.39
23	d	401	CLA	OBD-CAD	3.41	1.28	1.22
23	B	608	CLA	CHD-C4C	3.41	1.47	1.39
23	c	510	CLA	OBD-CAD	3.41	1.28	1.22
23	B	608	CLA	OBD-CAD	3.40	1.28	1.22
23	C	505	CLA	C3D-C2D	3.40	1.48	1.39
23	c	504	CLA	C3D-C2D	3.40	1.48	1.39
23	c	505	CLA	OBD-CAD	3.40	1.28	1.22
23	C	501	CLA	OBD-CAD	3.39	1.28	1.22
24	a	408	PHO	O2A-CGA	3.39	1.43	1.33
23	b	607	CLA	CHD-C4C	3.39	1.47	1.39
23	b	603	CLA	OBD-CAD	3.39	1.28	1.22
38	f	101	HEM	C4D-ND	-3.39	1.34	1.40
23	B	607	CLA	OBD-CAD	3.38	1.28	1.22
23	B	612	CLA	OBD-CAD	3.37	1.28	1.22
23	B	608	CLA	O2A-CGA	3.37	1.43	1.33
35	H	102	DGD	O2G-C1B	3.37	1.43	1.34
34	D	410	HTG	C1'-S1	-3.36	1.77	1.81
23	b	616	CLA	OBD-CAD	3.36	1.28	1.22
23	B	613	CLA	O2A-CGA	3.35	1.43	1.33
23	A	404	CLA	OBD-CAD	3.34	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	607	CLA	C3D-C2D	3.34	1.48	1.39
23	b	610	CLA	O2A-CGA	3.33	1.43	1.33
23	C	510	CLA	OBD-CAD	3.33	1.28	1.22
23	B	612	CLA	CHD-C4C	3.32	1.46	1.39
23	b	603	CLA	O2A-CGA	3.31	1.43	1.33
23	C	507	CLA	OBD-CAD	3.30	1.28	1.22
38	F	102	HEM	C1B-NB	-3.30	1.34	1.40
23	C	504	CLA	OBD-CAD	3.29	1.28	1.22
23	B	616	CLA	CHD-C4C	3.29	1.46	1.39
38	f	101	HEM	C1B-NB	-3.28	1.34	1.40
23	d	401	CLA	C1D-ND	3.27	1.41	1.37
34	c	522	HTG	C1'-S1	-3.27	1.77	1.81
23	D	402	CLA	OBD-CAD	3.26	1.28	1.22
23	B	611	CLA	C4B-CHC	3.26	1.50	1.41
23	B	612	CLA	C1B-NB	-3.26	1.32	1.35
23	B	603	CLA	OBD-CAD	3.26	1.28	1.22
23	B	604	CLA	C3D-C2D	3.26	1.48	1.39
38	F	102	HEM	C4D-ND	-3.26	1.34	1.40
23	B	611	CLA	C4B-NB	-3.26	1.32	1.35
23	b	607	CLA	O2A-CGA	3.24	1.42	1.33
23	d	402	CLA	OBD-CAD	3.24	1.28	1.22
23	a	409	CLA	CHD-C4C	3.21	1.46	1.39
23	b	613	CLA	CHD-C4C	3.20	1.46	1.39
23	A	404	CLA	O2A-CGA	3.19	1.42	1.33
34	b	625	HTG	C1'-S1	-3.19	1.77	1.81
23	B	609	CLA	OBD-CAD	3.18	1.28	1.22
23	D	403	CLA	C1C-C2C	3.18	1.50	1.44
23	C	503	CLA	OBD-CAD	3.18	1.28	1.22
23	B	612	CLA	C1C-C2C	3.17	1.50	1.44
23	b	611	CLA	OBD-CAD	3.17	1.27	1.22
23	B	611	CLA	C1B-NB	3.17	1.38	1.35
23	c	502	CLA	OBD-CAD	3.17	1.27	1.22
23	c	511	CLA	OBD-CAD	3.16	1.27	1.22
23	b	612	CLA	CHD-C4C	3.16	1.46	1.39
23	B	606	CLA	OBD-CAD	3.15	1.27	1.22
34	d	409	HTG	C1'-S1	-3.15	1.77	1.81
23	B	602	CLA	OBD-CAD	3.14	1.27	1.22
23	A	405	CLA	OBD-CAD	3.12	1.27	1.22
23	a	405	CLA	O2A-CGA	3.07	1.42	1.33
23	b	614	CLA	OBD-CAD	3.07	1.27	1.22
34	C	520	HTG	C1'-S1	-3.06	1.77	1.81
23	a	409	CLA	C1C-C2C	3.05	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	511	CLA	OBD-CAD	3.05	1.27	1.22
23	a	409	CLA	OBD-CAD	3.04	1.27	1.22
23	B	616	CLA	OBD-CAD	3.02	1.27	1.22
23	B	612	CLA	C1B-CHB	3.01	1.49	1.41
23	B	602	CLA	C1C-C2C	2.99	1.50	1.44
23	B	614	CLA	OBD-CAD	2.98	1.27	1.22
23	A	404	CLA	C4C-C3C	2.96	1.50	1.45
23	A	408	CLA	OBD-CAD	2.95	1.27	1.22
23	B	605	CLA	OBD-CAD	2.95	1.27	1.22
23	c	504	CLA	OBD-CAD	2.94	1.27	1.22
23	b	602	CLA	C1C-C2C	2.91	1.50	1.44
23	b	607	CLA	OBD-CAD	2.91	1.27	1.22
23	c	508	CLA	C1C-C2C	2.90	1.50	1.44
23	C	511	CLA	C4D-CHA	2.90	1.48	1.38
23	C	501	CLA	C1C-C2C	2.90	1.50	1.44
23	c	504	CLA	C1C-C2C	2.89	1.50	1.44
23	B	607	CLA	C4D-CHA	2.88	1.48	1.38
23	C	512	CLA	C1C-C2C	2.87	1.50	1.44
23	b	604	CLA	C4D-CHA	2.86	1.48	1.38
24	A	407	PHO	CBD-CGD	-2.83	1.48	1.52
23	c	510	CLA	C1B-NB	-2.83	1.32	1.35
23	b	602	CLA	C4B-CHC	2.81	1.48	1.41
23	C	504	CLA	C1B-CHB	2.81	1.48	1.41
23	C	507	CLA	C4D-CHA	2.81	1.48	1.38
35	H	102	DGD	O5D-C1E	2.81	1.45	1.40
23	B	614	CLA	C4D-CHA	2.80	1.48	1.38
23	B	613	CLA	C4D-CHA	2.80	1.48	1.38
23	B	611	CLA	C1B-CHB	2.79	1.48	1.41
23	D	403	CLA	C4B-CHC	2.79	1.48	1.41
23	c	512	CLA	C1B-CHB	2.79	1.48	1.41
23	C	504	CLA	C4D-CHA	2.79	1.48	1.38
23	b	612	CLA	C1C-C2C	2.78	1.49	1.44
23	b	613	CLA	C4D-CHA	2.77	1.48	1.38
29	A	414	PL9	C6-C5	2.76	1.49	1.35
23	b	609	CLA	C4D-CHA	2.76	1.48	1.38
23	B	610	CLA	C4D-CHA	2.75	1.48	1.38
29	a	415	PL9	C6-C5	2.75	1.49	1.35
23	d	401	CLA	C1B-CHB	2.75	1.48	1.41
23	B	605	CLA	C4B-CHC	2.74	1.48	1.41
23	C	512	CLA	C4B-CHC	2.74	1.48	1.41
23	c	509	CLA	C4D-CHA	2.74	1.48	1.38
34	b	625	HTG	C1-S1	-2.74	1.76	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	411	SQD	C6-S	-2.73	1.67	1.77
23	c	513	CLA	C4D-CHA	2.73	1.48	1.38
23	c	505	CLA	C1C-C2C	2.73	1.49	1.44
23	c	506	CLA	C1C-C2C	2.73	1.49	1.44
26	A	410	SQD	C6-S	-2.73	1.67	1.77
23	c	504	CLA	C4B-CHC	2.73	1.48	1.41
23	A	406	CLA	C4D-CHA	2.72	1.48	1.38
23	a	407	CLA	C1C-C2C	2.72	1.49	1.44
23	c	508	CLA	C4D-CHA	2.72	1.48	1.38
23	c	512	CLA	C4D-CHA	2.72	1.48	1.38
23	b	615	CLA	C4D-CHA	2.72	1.48	1.38
23	c	511	CLA	C1B-CHB	2.72	1.48	1.41
23	D	402	CLA	C4D-CHA	2.71	1.48	1.38
23	c	514	CLA	C1C-C2C	2.71	1.49	1.44
23	c	506	CLA	C4C-C3C	2.71	1.49	1.45
23	c	510	CLA	C4D-CHA	2.71	1.48	1.38
23	B	613	CLA	C4C-C3C	2.70	1.49	1.45
23	D	402	CLA	C1B-CHB	2.70	1.48	1.41
26	A	412	SQD	C6-S	-2.70	1.67	1.77
23	B	607	CLA	C1B-NB	-2.70	1.32	1.35
23	c	511	CLA	C4D-CHA	2.70	1.48	1.38
26	f	102	SQD	C6-S	-2.70	1.67	1.77
23	B	607	CLA	C1B-CHB	2.70	1.48	1.41
23	B	605	CLA	C1C-C2C	2.69	1.49	1.44
23	c	511	CLA	C1C-C2C	2.69	1.49	1.44
23	C	501	CLA	C4D-CHA	2.69	1.48	1.38
23	B	610	CLA	C1C-C2C	2.69	1.49	1.44
23	A	405	CLA	C4D-CHA	2.68	1.47	1.38
38	f	101	HEM	FE-NB	2.68	2.10	1.96
23	B	612	CLA	C4D-CHA	2.68	1.47	1.38
32	Z	101	LMG	O8-C28	2.68	1.46	1.33
23	c	509	CLA	C1C-C2C	2.68	1.49	1.44
23	B	608	CLA	C4C-C3C	2.67	1.49	1.45
23	B	606	CLA	C1C-C2C	2.67	1.49	1.44
23	B	615	CLA	C1C-C2C	2.67	1.49	1.44
23	A	408	CLA	C4D-CHA	2.67	1.47	1.38
23	b	609	CLA	C1B-CHB	2.67	1.48	1.41
23	C	510	CLA	C1C-C2C	2.66	1.49	1.44
23	B	601	CLA	C1C-C2C	2.66	1.49	1.44
23	B	616	CLA	C4D-CHA	2.66	1.47	1.38
26	a	413	SQD	C6-S	-2.65	1.67	1.77
23	C	504	CLA	C1C-C2C	2.65	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	502	CLA	C1B-CHB	2.65	1.48	1.41
23	C	506	CLA	C4C-C3C	2.65	1.49	1.45
23	B	605	CLA	C1B-CHB	2.65	1.48	1.41
38	F	102	HEM	FE-NB	2.65	2.10	1.96
23	b	610	CLA	C1C-C2C	2.64	1.49	1.44
23	C	505	CLA	C4D-CHA	2.64	1.47	1.38
23	C	507	CLA	C1C-C2C	2.64	1.49	1.44
23	c	502	CLA	C1C-C2C	2.64	1.49	1.44
31	t	101	LMT	O3'-C3'	-2.64	1.36	1.43
23	c	504	CLA	C4D-CHA	2.63	1.47	1.38
23	c	506	CLA	C4B-CHC	2.63	1.48	1.41
23	b	607	CLA	C1B-NB	-2.62	1.32	1.35
23	c	508	CLA	C4B-CHC	2.62	1.48	1.41
23	c	509	CLA	C4C-C3C	2.62	1.49	1.45
23	a	407	CLA	C4D-CHA	2.62	1.47	1.38
23	c	502	CLA	C4D-CHA	2.62	1.47	1.38
27	A	418	GOL	O2-C2	-2.62	1.35	1.43
23	b	616	CLA	C1C-C2C	2.62	1.49	1.44
23	c	504	CLA	C1B-CHB	2.62	1.48	1.41
23	C	506	CLA	C4D-CHA	2.62	1.47	1.38
23	b	607	CLA	C4D-CHA	2.61	1.47	1.38
23	B	607	CLA	C4C-C3C	2.61	1.49	1.45
23	C	503	CLA	C1C-C2C	2.61	1.49	1.44
23	D	403	CLA	C4C-C3C	2.61	1.49	1.45
23	c	510	CLA	C4C-C3C	2.61	1.49	1.45
23	c	505	CLA	C4D-CHA	2.61	1.47	1.38
23	b	612	CLA	C1B-CHB	2.61	1.48	1.41
23	C	511	CLA	C3D-C4D	-2.60	1.38	1.44
23	C	508	CLA	C4D-CHA	2.60	1.47	1.38
23	B	604	CLA	C4D-CHA	2.60	1.47	1.38
23	C	505	CLA	C1C-C2C	2.60	1.49	1.44
23	B	610	CLA	C1B-CHB	2.60	1.48	1.41
23	b	616	CLA	C4B-CHC	2.59	1.48	1.41
23	C	513	CLA	C4D-CHA	2.59	1.47	1.38
23	B	614	CLA	C1B-CHB	2.59	1.48	1.41
23	c	504	CLA	C3D-C4D	-2.59	1.38	1.44
31	m	103	LMT	O2B-C2B	-2.59	1.36	1.43
23	C	505	CLA	C1B-CHB	2.59	1.48	1.41
23	B	603	CLA	C4D-CHA	2.59	1.47	1.38
23	c	502	CLA	C4B-CHC	2.59	1.48	1.41
23	B	609	CLA	C1C-C2C	2.58	1.49	1.44
23	b	610	CLA	C4D-CHA	2.58	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	512	CLA	C4D-CHA	2.58	1.47	1.38
23	C	509	CLA	C1C-C2C	2.57	1.49	1.44
23	A	404	CLA	C4D-CHA	2.57	1.47	1.38
34	B	623	HTG	C1'-S1	-2.57	1.78	1.81
23	b	614	CLA	C4C-C3C	2.57	1.49	1.45
23	B	603	CLA	C1B-NB	-2.57	1.32	1.35
23	B	601	CLA	C4B-CHC	2.56	1.48	1.41
23	B	607	CLA	C1C-C2C	2.56	1.49	1.44
23	C	509	CLA	C4D-CHA	2.56	1.47	1.38
23	b	604	CLA	C4B-CHC	2.56	1.48	1.41
23	d	401	CLA	C4C-C3C	2.56	1.49	1.45
23	B	609	CLA	C4B-CHC	2.56	1.48	1.41
23	a	409	CLA	C1B-CHB	2.55	1.48	1.41
23	B	615	CLA	C1B-CHB	2.55	1.48	1.41
23	C	501	CLA	C4B-CHC	2.55	1.48	1.41
23	a	409	CLA	C4D-CHA	2.55	1.47	1.38
23	c	503	CLA	C1B-CHB	2.55	1.48	1.41
34	b	622	HTG	O5-C1	2.55	1.46	1.42
23	d	402	CLA	C4D-CHA	2.55	1.47	1.38
31	A	421	LMT	O3'-C3'	-2.55	1.37	1.43
23	c	513	CLA	C4B-CHC	2.55	1.48	1.41
23	B	607	CLA	C3D-C4D	-2.55	1.38	1.44
23	B	608	CLA	C4D-CHA	2.55	1.47	1.38
24	a	417	PHO	C3A-C2A	-2.55	1.52	1.54
23	d	402	CLA	C1C-C2C	2.55	1.49	1.44
23	b	614	CLA	C4B-CHC	2.54	1.48	1.41
23	b	607	CLA	C1C-C2C	2.54	1.49	1.44
23	C	507	CLA	C4B-CHC	2.54	1.48	1.41
23	B	616	CLA	C1B-CHB	2.54	1.48	1.41
23	c	506	CLA	C4D-CHA	2.54	1.47	1.38
23	B	602	CLA	C4C-C3C	2.54	1.49	1.45
23	b	610	CLA	C4C-C3C	2.54	1.49	1.45
23	B	615	CLA	C4D-CHA	2.54	1.47	1.38
23	b	606	CLA	C4D-CHA	2.54	1.47	1.38
23	c	503	CLA	C4D-CHA	2.54	1.47	1.38
23	C	510	CLA	C4D-CHA	2.54	1.47	1.38
23	B	602	CLA	C4D-CHA	2.53	1.47	1.38
23	C	511	CLA	C4C-C3C	2.53	1.49	1.45
23	B	604	CLA	C4C-C3C	2.53	1.49	1.45
23	C	503	CLA	C4B-CHC	2.53	1.48	1.41
23	c	510	CLA	C1B-CHB	2.53	1.48	1.41
23	B	605	CLA	C4D-CHA	2.53	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	511	CLA	C1B-CHB	2.53	1.48	1.41
23	b	601	CLA	C4D-CHA	2.53	1.47	1.38
26	b	620	SQD	C6-S	-2.52	1.68	1.77
23	B	606	CLA	C4D-CHA	2.52	1.47	1.38
26	B	620	SQD	C6-S	-2.52	1.68	1.77
23	B	609	CLA	C4D-CHA	2.52	1.47	1.38
31	e	101	LMT	O3'-C3'	-2.52	1.37	1.43
23	D	403	CLA	C1B-CHB	2.52	1.48	1.41
34	B	625	HTG	C1-S1	-2.52	1.76	1.80
23	C	510	CLA	C4C-C3C	2.52	1.49	1.45
23	b	608	CLA	C4D-CHA	2.52	1.47	1.38
31	c	501	LMT	O3'-C3'	-2.51	1.37	1.43
31	B	631	LMT	O3'-C3'	-2.51	1.37	1.43
24	a	408	PHO	CHA-CBD	-2.51	1.49	1.52
23	B	602	CLA	C1B-CHB	2.51	1.48	1.41
23	b	610	CLA	C1B-CHB	2.51	1.48	1.41
31	M	101	LMT	O2'-C2'	-2.51	1.37	1.43
23	b	613	CLA	C4C-C3C	2.51	1.49	1.45
23	B	616	CLA	C1C-C2C	2.51	1.49	1.44
23	C	511	CLA	C1C-C2C	2.51	1.49	1.44
23	B	606	CLA	C1B-CHB	2.51	1.48	1.41
23	b	603	CLA	C1C-C2C	2.51	1.49	1.44
23	b	610	CLA	C4B-CHC	2.51	1.48	1.41
23	b	614	CLA	C4D-CHA	2.50	1.47	1.38
23	C	505	CLA	C4C-C3C	2.50	1.49	1.45
23	C	507	CLA	C1B-CHB	2.50	1.47	1.41
23	B	614	CLA	C3D-C4D	-2.50	1.38	1.44
23	b	612	CLA	C4D-CHA	2.50	1.47	1.38
23	C	502	CLA	C1B-CHB	2.50	1.47	1.41
23	A	404	CLA	C1C-C2C	2.49	1.49	1.44
23	a	405	CLA	C4C-C3C	2.49	1.49	1.45
23	A	406	CLA	C4B-CHC	2.49	1.47	1.41
23	B	603	CLA	C1B-CHB	2.49	1.47	1.41
23	b	616	CLA	C3D-C4D	-2.48	1.38	1.44
23	A	405	CLA	C1B-CHB	2.48	1.47	1.41
23	C	503	CLA	C3D-C4D	-2.48	1.38	1.44
23	c	507	CLA	C4D-CHA	2.48	1.47	1.38
23	C	505	CLA	C4B-CHC	2.48	1.47	1.41
23	C	509	CLA	C4B-NB	-2.48	1.33	1.35
23	a	405	CLA	C4D-CHA	2.48	1.47	1.38
23	B	604	CLA	C1B-CHB	2.48	1.47	1.41
23	a	406	CLA	C4D-CHA	2.48	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	514	CLA	C4D-CHA	2.47	1.47	1.38
23	B	603	CLA	C1C-C2C	2.47	1.49	1.44
23	c	512	CLA	C1C-C2C	2.47	1.49	1.44
23	c	509	CLA	C4B-CHC	2.47	1.47	1.41
23	B	610	CLA	C4B-CHC	2.47	1.47	1.41
26	F	103	SQD	C6-S	-2.47	1.68	1.77
23	C	508	CLA	C1B-CHB	2.46	1.47	1.41
23	b	602	CLA	C3D-C4D	-2.46	1.38	1.44
23	a	407	CLA	C1B-CHB	2.46	1.47	1.41
23	C	502	CLA	C4D-CHA	2.46	1.47	1.38
23	c	502	CLA	C3D-C4D	-2.46	1.38	1.44
23	b	616	CLA	C4D-CHA	2.46	1.47	1.38
23	C	513	CLA	C1C-C2C	2.46	1.49	1.44
23	C	509	CLA	C1B-CHB	2.46	1.47	1.41
23	B	613	CLA	C1C-C2C	2.45	1.49	1.44
23	c	502	CLA	C4C-C3C	2.45	1.49	1.45
23	C	506	CLA	C1C-C2C	2.45	1.49	1.44
23	B	606	CLA	C3D-C4D	-2.45	1.38	1.44
23	d	401	CLA	C1B-NB	-2.44	1.33	1.35
23	b	607	CLA	C4C-C3C	2.44	1.49	1.45
23	B	602	CLA	C3D-C4D	-2.44	1.38	1.44
23	C	506	CLA	C3D-C4D	-2.44	1.38	1.44
23	a	407	CLA	C3D-C4D	-2.44	1.38	1.44
23	b	602	CLA	C4C-C3C	2.44	1.49	1.45
23	b	609	CLA	C1C-C2C	2.44	1.49	1.44
31	T	101	LMT	O3'-C3'	-2.43	1.37	1.43
23	B	601	CLA	C4D-CHA	2.43	1.47	1.38
31	M	101	LMT	O3'-C3'	-2.43	1.37	1.43
23	C	503	CLA	C4D-CHA	2.43	1.47	1.38
23	b	605	CLA	C1B-CHB	2.43	1.47	1.41
23	C	510	CLA	C1B-CHB	2.43	1.47	1.41
23	b	606	CLA	C1B-CHB	2.43	1.47	1.41
23	C	509	CLA	C4C-C3C	2.43	1.49	1.45
23	A	408	CLA	C3D-C4D	-2.43	1.38	1.44
23	c	507	CLA	C1B-CHB	2.43	1.47	1.41
23	b	602	CLA	C4D-CHA	2.42	1.47	1.38
23	c	504	CLA	C4C-C3C	2.42	1.49	1.45
23	B	613	CLA	C1B-CHB	2.42	1.47	1.41
23	c	514	CLA	C1B-CHB	2.42	1.47	1.41
31	F	101	LMT	O3'-C3'	-2.42	1.37	1.43
31	M	101	LMT	O2B-C2B	-2.42	1.37	1.43
24	A	407	PHO	CHA-CBD	-2.42	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	611	CLA	C1B-CHB	2.42	1.47	1.41
23	b	614	CLA	C3D-C4D	-2.41	1.38	1.44
23	b	604	CLA	C1B-CHB	2.41	1.47	1.41
23	B	614	CLA	C4B-CHC	2.41	1.47	1.41
23	A	405	CLA	C1C-C2C	2.41	1.49	1.44
23	b	604	CLA	C1C-C2C	2.41	1.49	1.44
23	d	402	CLA	C4B-CHC	2.41	1.47	1.41
23	A	406	CLA	C1C-C2C	2.41	1.49	1.44
23	a	405	CLA	C1B-CHB	2.41	1.47	1.41
23	C	508	CLA	C4B-CHC	2.41	1.47	1.41
23	B	614	CLA	C4C-C3C	2.41	1.49	1.45
23	C	508	CLA	C1C-C2C	2.41	1.49	1.44
23	D	403	CLA	C4D-CHA	2.41	1.47	1.38
23	C	503	CLA	C1B-CHB	2.40	1.47	1.41
23	b	603	CLA	C4D-CHA	2.40	1.46	1.38
23	b	612	CLA	C4C-C3C	2.40	1.49	1.45
23	b	605	CLA	C1C-C2C	2.40	1.49	1.44
23	b	603	CLA	C4B-CHC	2.40	1.47	1.41
23	b	605	CLA	C4D-CHA	2.40	1.46	1.38
23	C	513	CLA	C1B-CHB	2.40	1.47	1.41
23	b	615	CLA	C3D-C4D	-2.40	1.38	1.44
40	V	201	HEC	C3C-C4C	2.39	1.47	1.43
23	D	402	CLA	C3D-C4D	-2.39	1.38	1.44
23	b	608	CLA	C3D-C4D	-2.39	1.38	1.44
23	c	506	CLA	C1B-CHB	2.39	1.47	1.41
23	a	409	CLA	C4B-CHC	2.38	1.47	1.41
23	b	605	CLA	C4B-CHC	2.38	1.47	1.41
23	c	511	CLA	C4B-CHC	2.38	1.47	1.41
23	b	610	CLA	C3D-C4D	-2.38	1.38	1.44
23	d	401	CLA	C4D-CHA	2.38	1.46	1.38
23	c	514	CLA	C3D-C4D	-2.38	1.38	1.44
23	b	601	CLA	C4B-CHC	2.38	1.47	1.41
23	C	501	CLA	C1B-CHB	2.37	1.47	1.41
23	b	615	CLA	C1B-CHB	2.37	1.47	1.41
23	B	611	CLA	C4D-CHA	2.37	1.46	1.38
23	b	606	CLA	C3D-C4D	-2.37	1.38	1.44
31	B	630	LMT	O2'-C2'	-2.36	1.37	1.43
23	C	510	CLA	C3D-C4D	-2.36	1.38	1.44
23	b	601	CLA	C1C-C2C	2.36	1.49	1.44
32	C	519	LMG	O1-C1	2.36	1.44	1.40
23	c	505	CLA	C1C-NC	-2.36	1.34	1.37
23	B	605	CLA	C3D-C4D	-2.36	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402	CLA	C1B-CHB	2.36	1.47	1.41
23	b	613	CLA	C4B-CHC	2.35	1.47	1.41
23	b	613	CLA	OBD-CAD	2.35	1.26	1.22
29	d	404	PL9	C6-C5	2.35	1.47	1.35
23	C	504	CLA	C4B-CHC	2.35	1.47	1.41
24	a	417	PHO	CHA-CBD	-2.35	1.49	1.52
23	c	512	CLA	C4C-C3C	2.35	1.49	1.45
23	c	514	CLA	C4B-CHC	2.35	1.47	1.41
38	f	101	HEM	C1D-ND	-2.35	1.34	1.38
23	b	614	CLA	C1C-C2C	2.35	1.49	1.44
31	B	628	LMT	C3'-C2'	2.35	1.58	1.52
23	c	505	CLA	C4C-C3C	2.35	1.49	1.45
24	A	416	PHO	C3A-C2A	-2.34	1.52	1.54
23	A	405	CLA	C3D-C4D	-2.34	1.38	1.44
23	b	613	CLA	C1C-C2C	2.34	1.49	1.44
23	b	605	CLA	C1B-NB	-2.34	1.33	1.35
23	B	606	CLA	C4B-CHC	2.34	1.47	1.41
23	C	506	CLA	C1B-CHB	2.34	1.47	1.41
23	b	611	CLA	C4D-CHA	2.34	1.46	1.38
29	D	405	PL9	C6-C5	2.34	1.47	1.35
23	B	602	CLA	C4B-CHC	2.34	1.47	1.41
35	c	519	DGD	O2G-C2G	-2.34	1.40	1.46
23	B	604	CLA	C3D-C4D	-2.34	1.38	1.44
31	B	628	LMT	O3'-C3'	-2.34	1.37	1.43
24	a	408	PHO	CBD-CGD	-2.33	1.49	1.52
23	b	611	CLA	C4B-CHC	2.33	1.47	1.41
23	b	615	CLA	C4C-C3C	2.33	1.49	1.45
23	c	514	CLA	C4C-C3C	2.33	1.49	1.45
23	C	501	CLA	C3D-C4D	-2.32	1.38	1.44
23	b	608	CLA	C1B-CHB	2.32	1.47	1.41
23	C	510	CLA	C4B-CHC	2.31	1.47	1.41
23	c	507	CLA	C3D-C4D	-2.31	1.39	1.44
31	A	417	LMT	O3'-C3'	-2.31	1.37	1.43
23	C	502	CLA	C1C-C2C	2.31	1.49	1.44
23	c	505	CLA	C4B-CHC	2.31	1.47	1.41
23	C	512	CLA	C3D-C4D	-2.31	1.39	1.44
23	d	401	CLA	C1C-C2C	2.30	1.49	1.44
23	d	401	CLA	C3D-C4D	-2.30	1.39	1.44
23	c	509	CLA	C1B-CHB	2.30	1.47	1.41
23	c	513	CLA	C1B-CHB	2.30	1.47	1.41
23	A	405	CLA	C4B-CHC	2.30	1.47	1.41
23	A	404	CLA	C1B-CHB	2.30	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	612	CLA	C4B-CHC	2.30	1.47	1.41
35	C	517	DGD	O2G-C2G	-2.30	1.40	1.46
23	b	614	CLA	C1B-CHB	2.30	1.47	1.41
23	B	613	CLA	C4B-CHC	2.29	1.47	1.41
23	B	607	CLA	C4B-CHC	2.29	1.47	1.41
23	B	614	CLA	C4B-NB	-2.29	1.33	1.35
23	B	614	CLA	C1C-C2C	2.29	1.49	1.44
31	m	103	LMT	O3'-C3'	-2.28	1.37	1.43
23	b	606	CLA	C1C-C2C	2.28	1.49	1.44
23	b	609	CLA	C3D-C4D	-2.28	1.39	1.44
23	C	509	CLA	C4B-CHC	2.27	1.47	1.41
31	A	421	LMT	O2'-C2'	-2.27	1.37	1.43
23	d	402	CLA	C3D-C4D	-2.27	1.39	1.44
31	B	630	LMT	O2B-C2B	-2.27	1.37	1.43
23	C	513	CLA	C3D-C4D	-2.27	1.39	1.44
23	b	607	CLA	C1B-CHB	2.27	1.47	1.41
27	A	418	GOL	C3-C2	2.27	1.61	1.51
23	B	609	CLA	C1B-CHB	2.27	1.47	1.41
23	b	606	CLA	C4B-CHC	2.27	1.47	1.41
23	C	504	CLA	C3D-C4D	-2.26	1.39	1.44
23	B	601	CLA	C3D-C4D	-2.26	1.39	1.44
23	C	502	CLA	C3D-C4D	-2.26	1.39	1.44
23	c	513	CLA	C1C-C2C	2.26	1.48	1.44
23	b	601	CLA	C1B-CHB	2.26	1.47	1.41
31	T	101	LMT	O2'-C2'	-2.25	1.37	1.43
23	b	601	CLA	C4C-C3C	2.25	1.48	1.45
31	T	101	LMT	O3B-C3B	-2.25	1.37	1.43
23	C	512	CLA	C1B-CHB	2.25	1.47	1.41
23	c	508	CLA	C1B-CHB	2.25	1.47	1.41
23	a	405	CLA	C1C-C2C	2.25	1.48	1.44
27	a	420	GOL	C1-C2	2.25	1.61	1.51
23	c	511	CLA	C4C-C3C	2.25	1.48	1.45
23	c	505	CLA	C1B-CHB	2.25	1.47	1.41
31	b	621	LMT	C3'-C2'	2.25	1.58	1.52
23	b	609	CLA	C4B-CHC	2.25	1.47	1.41
23	A	406	CLA	C3D-C4D	-2.24	1.39	1.44
23	B	612	CLA	C4C-C3C	2.24	1.48	1.45
31	B	630	LMT	O3'-C3'	-2.24	1.37	1.43
23	C	502	CLA	C4C-C3C	2.24	1.48	1.45
23	D	402	CLA	C1B-NB	-2.24	1.33	1.35
35	h	102	DGD	O5D-C1E	2.24	1.44	1.40
23	B	615	CLA	C4C-C3C	2.24	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	608	CLA	C1B-CHB	2.24	1.47	1.41
23	a	406	CLA	C1B-CHB	2.24	1.47	1.41
23	C	508	CLA	C3D-C4D	-2.24	1.39	1.44
23	C	503	CLA	C4C-C3C	2.24	1.48	1.45
34	D	410	HTG	C1-S1	-2.23	1.77	1.80
23	B	616	CLA	C3D-C4D	-2.23	1.39	1.44
34	B	622	HTG	O5-C1	2.23	1.45	1.42
23	a	406	CLA	C4B-CHC	2.23	1.47	1.41
35	H	102	DGD	O2G-C2G	-2.23	1.41	1.46
23	C	505	CLA	C3D-C4D	-2.23	1.39	1.44
23	B	601	CLA	C1B-CHB	2.22	1.47	1.41
23	b	613	CLA	C1B-CHB	2.22	1.47	1.41
23	A	408	CLA	C4C-C3C	2.22	1.48	1.45
23	d	402	CLA	C4C-C3C	2.22	1.48	1.45
23	b	605	CLA	C3D-C4D	-2.22	1.39	1.44
23	c	513	CLA	C4C-C3C	2.22	1.48	1.45
23	B	610	CLA	C4C-C3C	2.21	1.48	1.45
23	c	505	CLA	C3D-C4D	-2.21	1.39	1.44
23	c	513	CLA	C3D-C4D	-2.21	1.39	1.44
35	C	516	DGD	O5D-C1E	2.21	1.44	1.40
23	D	402	CLA	C4C-C3C	2.21	1.48	1.45
23	B	604	CLA	C1A-CHA	2.21	1.52	1.43
23	b	602	CLA	C1B-CHB	2.21	1.47	1.41
31	A	417	LMT	O2'-C2'	-2.20	1.37	1.43
23	c	507	CLA	C4B-CHC	2.20	1.47	1.41
23	B	616	CLA	C4B-CHC	2.20	1.47	1.41
23	b	611	CLA	C4C-C3C	2.20	1.48	1.45
23	a	409	CLA	C4C-C3C	2.20	1.48	1.45
23	c	503	CLA	C4B-CHC	2.20	1.47	1.41
23	A	406	CLA	C1B-CHB	2.20	1.47	1.41
29	a	415	PL9	C2-C3	2.19	1.40	1.34
23	d	401	CLA	C4B-CHC	2.19	1.47	1.41
23	C	507	CLA	C3D-C4D	-2.19	1.39	1.44
23	c	509	CLA	C3D-C4D	-2.19	1.39	1.44
23	C	501	CLA	C4C-C3C	2.19	1.48	1.45
23	b	611	CLA	C3D-C4D	-2.19	1.39	1.44
23	c	510	CLA	C3D-C4D	-2.19	1.39	1.44
31	t	101	LMT	O2'-C2'	-2.19	1.37	1.43
23	B	612	CLA	C4B-CHC	2.18	1.47	1.41
23	A	408	CLA	C1B-CHB	2.18	1.47	1.41
23	A	404	CLA	C4B-NB	-2.18	1.33	1.35
31	B	628	LMT	O4'-C4B	-2.17	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	512	CLA	MG-NA	2.17	2.11	2.06
27	b	624	GOL	C3-C2	2.17	1.60	1.51
23	A	406	CLA	C1B-NB	-2.17	1.33	1.35
23	B	608	CLA	C3D-C4D	-2.17	1.39	1.44
23	b	607	CLA	C4B-CHC	2.17	1.47	1.41
23	C	502	CLA	C4B-CHC	2.17	1.47	1.41
23	b	603	CLA	C1B-CHB	2.16	1.47	1.41
23	c	508	CLA	C3D-C4D	-2.16	1.39	1.44
31	b	627	LMT	O3'-C3'	-2.16	1.37	1.43
23	b	611	CLA	C1C-C2C	2.16	1.48	1.44
23	C	506	CLA	C1D-C2D	2.16	1.49	1.45
23	c	512	CLA	C4B-CHC	2.15	1.47	1.41
23	A	405	CLA	C1B-NB	-2.15	1.33	1.35
23	B	610	CLA	C3D-C4D	-2.15	1.39	1.44
23	B	603	CLA	C4B-CHC	2.14	1.47	1.41
23	B	609	CLA	C3D-C4D	-2.14	1.39	1.44
23	b	605	CLA	C1D-C2D	2.14	1.49	1.45
23	B	601	CLA	C4C-C3C	2.14	1.48	1.45
23	a	405	CLA	C4B-CHC	2.14	1.46	1.41
23	B	604	CLA	C1C-C2C	2.14	1.48	1.44
31	m	103	LMT	O3B-C3B	-2.14	1.37	1.43
23	C	513	CLA	C4B-CHC	2.14	1.46	1.41
23	c	511	CLA	C3D-C4D	-2.13	1.39	1.44
23	a	409	CLA	C1B-NB	-2.13	1.33	1.35
31	b	621	LMT	O3'-C3'	-2.13	1.38	1.43
23	C	511	CLA	C4B-CHC	2.13	1.46	1.41
23	b	608	CLA	C1C-C2C	2.13	1.48	1.44
29	A	414	PL9	C2-C1	-2.12	1.39	1.44
23	B	604	CLA	C4B-CHC	2.12	1.46	1.41
26	F	103	SQD	O6-C1	2.12	1.43	1.40
23	D	402	CLA	C4B-CHC	2.12	1.46	1.41
23	B	616	CLA	C1C-NC	-2.12	1.34	1.37
31	A	417	LMT	O2B-C2B	-2.12	1.38	1.43
23	a	406	CLA	C1C-C2C	2.12	1.48	1.44
23	b	607	CLA	C3D-C4D	-2.12	1.39	1.44
38	f	101	HEM	CHB-C1B	2.12	1.40	1.35
23	A	408	CLA	C4B-CHC	2.12	1.46	1.41
31	B	631	LMT	O2'-C2'	-2.11	1.38	1.43
23	D	403	CLA	C3D-C4D	-2.11	1.39	1.44
31	e	101	LMT	O2'-C2'	-2.11	1.38	1.43
23	B	604	CLA	MG-NA	2.11	2.11	2.06
31	e	101	LMT	O2B-C2B	-2.11	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	628	LMT	O5'-C5'	-2.11	1.39	1.44
23	b	615	CLA	C4B-CHC	2.11	1.46	1.41
31	b	627	LMT	O2'-C2'	-2.10	1.38	1.43
38	F	102	HEM	CHB-C1B	2.10	1.40	1.35
23	c	506	CLA	C3D-C4D	-2.10	1.39	1.44
23	c	507	CLA	C1C-NC	-2.10	1.34	1.37
23	C	506	CLA	C4B-CHC	2.09	1.46	1.41
23	B	615	CLA	C3D-C4D	-2.08	1.39	1.44
23	a	407	CLA	C4C-C3C	2.08	1.48	1.45
23	c	514	CLA	C1D-C2D	2.08	1.49	1.45
23	b	604	CLA	C1A-CHA	2.08	1.51	1.43
23	B	603	CLA	C4C-C3C	2.08	1.48	1.45
23	B	608	CLA	C1C-NC	-2.07	1.34	1.37
23	C	510	CLA	C1B-NB	-2.07	1.33	1.35
23	c	502	CLA	C1C-NC	-2.07	1.34	1.37
23	b	603	CLA	C4C-C3C	2.06	1.48	1.45
23	c	503	CLA	C3D-C4D	-2.06	1.39	1.44
31	e	101	LMT	O3B-C3B	-2.06	1.38	1.43
23	b	607	CLA	C1D-C2D	2.06	1.49	1.45
23	C	509	CLA	C3D-C4D	-2.05	1.39	1.44
38	F	102	HEM	C3B-C4B	2.05	1.49	1.44
23	c	507	CLA	C4C-C3C	2.05	1.48	1.45
23	b	608	CLA	C4B-CHC	2.05	1.46	1.41
23	b	616	CLA	C1B-CHB	2.05	1.46	1.41
23	b	609	CLA	C1C-NC	-2.04	1.34	1.37
23	b	615	CLA	C1B-NB	-2.04	1.33	1.35
23	a	407	CLA	C4B-CHC	2.04	1.46	1.41
23	B	606	CLA	C4C-C3C	2.04	1.48	1.45
23	b	601	CLA	C3D-C4D	-2.04	1.39	1.44
34	c	522	HTG	C1-S1	-2.04	1.77	1.80
29	D	405	PL9	C2-C3	2.04	1.40	1.34
38	F	102	HEM	C1D-ND	-2.04	1.34	1.38
23	b	608	CLA	C1B-NB	-2.04	1.33	1.35
23	c	503	CLA	C1C-C2C	2.03	1.48	1.44
23	B	611	CLA	C3D-C4D	-2.03	1.39	1.44
23	c	507	CLA	C1C-C2C	2.03	1.48	1.44
31	F	101	LMT	O3B-C3B	-2.03	1.38	1.43
33	b	630	LHG	O7-C5	-2.02	1.41	1.46
23	B	609	CLA	C4C-C3C	2.02	1.48	1.45
31	m	103	LMT	C3'-C2'	2.02	1.57	1.52
23	b	607	CLA	C1A-CHA	2.02	1.51	1.43
23	A	408	CLA	C1C-C2C	2.02	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	615	CLA	C4B-CHC	2.02	1.46	1.41
23	A	404	CLA	C3D-C4D	-2.02	1.39	1.44
27	B	629	GOL	O2-C2	-2.02	1.37	1.43
23	B	615	CLA	C1C-NC	-2.01	1.34	1.37
23	C	512	CLA	C4C-C3C	2.01	1.48	1.45
31	A	421	LMT	O2B-C2B	-2.01	1.38	1.43
23	C	504	CLA	C4C-C3C	2.01	1.48	1.45
23	B	601	CLA	C1C-NC	-2.01	1.34	1.37
31	A	421	LMT	O3B-C3B	-2.00	1.38	1.43
31	F	101	LMT	O2B-C2B	-2.00	1.38	1.43
24	a	417	PHO	CBD-CGD	-2.00	1.49	1.52

All (2626) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	C1D-ND-C4D	-11.66	98.05	106.33
23	B	612	CLA	C1D-ND-C4D	-10.41	98.94	106.33
23	b	605	CLA	C1D-ND-C4D	-10.31	99.01	106.33
23	B	611	CLA	C2D-C1D-ND	9.92	117.42	110.10
23	a	409	CLA	C1D-ND-C4D	-9.84	99.34	106.33
23	C	503	CLA	C1D-ND-C4D	-9.77	99.40	106.33
23	B	615	CLA	C1D-ND-C4D	-9.72	99.43	106.33
23	a	407	CLA	C1D-ND-C4D	-9.69	99.45	106.33
23	B	605	CLA	C1D-ND-C4D	-9.66	99.47	106.33
23	b	611	CLA	C1D-ND-C4D	-9.64	99.49	106.33
23	B	606	CLA	C1D-ND-C4D	-9.62	99.50	106.33
23	B	612	CLA	C2D-C1D-ND	9.59	117.17	110.10
23	b	603	CLA	C1D-ND-C4D	-9.56	99.54	106.33
23	A	408	CLA	C1D-ND-C4D	-9.54	99.56	106.33
23	c	504	CLA	C1D-ND-C4D	-9.54	99.56	106.33
23	B	601	CLA	C1D-ND-C4D	-9.48	99.60	106.33
23	c	502	CLA	C1D-ND-C4D	-9.47	99.61	106.33
23	C	501	CLA	C1D-ND-C4D	-9.45	99.62	106.33
23	C	509	CLA	C1D-ND-C4D	-9.41	99.65	106.33
23	A	406	CLA	C1D-ND-C4D	-9.41	99.65	106.33
23	d	402	CLA	C1D-ND-C4D	-9.39	99.66	106.33
23	C	510	CLA	C1D-ND-C4D	-9.38	99.67	106.33
23	B	603	CLA	C1D-ND-C4D	-9.37	99.68	106.33
23	c	512	CLA	C1D-ND-C4D	-9.36	99.68	106.33
23	C	505	CLA	C1D-ND-C4D	-9.36	99.69	106.33
23	B	610	CLA	C1D-ND-C4D	-9.33	99.71	106.33
23	c	514	CLA	C1D-ND-C4D	-9.30	99.73	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	607	CLA	C1D-ND-C4D	-9.30	99.73	106.33
23	B	614	CLA	C1D-ND-C4D	-9.29	99.73	106.33
23	b	616	CLA	C1D-ND-C4D	-9.23	99.78	106.33
23	b	606	CLA	C1D-ND-C4D	-9.21	99.79	106.33
23	B	616	CLA	C1D-ND-C4D	-9.17	99.82	106.33
23	B	605	CLA	C2D-C1D-ND	9.16	116.85	110.10
23	a	409	CLA	C2D-C1D-ND	9.14	116.84	110.10
23	c	506	CLA	C1D-ND-C4D	-9.14	99.84	106.33
23	D	402	CLA	C1D-ND-C4D	-9.14	99.84	106.33
23	b	602	CLA	C1D-ND-C4D	-9.12	99.86	106.33
23	C	513	CLA	C1D-ND-C4D	-9.09	99.87	106.33
23	b	601	CLA	C1D-ND-C4D	-9.09	99.88	106.33
23	b	611	CLA	C2D-C1D-ND	9.09	116.80	110.10
23	A	405	CLA	C2D-C1D-ND	9.08	116.79	110.10
23	A	405	CLA	C1D-ND-C4D	-9.06	99.90	106.33
23	B	616	CLA	C2D-C1D-ND	9.06	116.78	110.10
23	b	615	CLA	C1D-ND-C4D	-9.05	99.91	106.33
23	d	401	CLA	C1D-ND-C4D	-9.03	99.92	106.33
23	c	507	CLA	C1D-ND-C4D	-9.02	99.93	106.33
23	D	403	CLA	C1D-ND-C4D	-9.01	99.93	106.33
23	B	602	CLA	C1D-ND-C4D	-9.01	99.94	106.33
23	b	614	CLA	C1D-ND-C4D	-9.01	99.94	106.33
23	b	608	CLA	C1D-ND-C4D	-9.01	99.94	106.33
23	a	405	CLA	C1D-ND-C4D	-8.97	99.96	106.33
23	b	605	CLA	C2D-C1D-ND	8.95	116.70	110.10
23	c	510	CLA	C1D-ND-C4D	-8.94	99.98	106.33
23	c	505	CLA	C1D-ND-C4D	-8.94	99.99	106.33
23	b	610	CLA	C1D-ND-C4D	-8.89	100.02	106.33
23	b	613	CLA	C2D-C1D-ND	8.88	116.65	110.10
23	c	513	CLA	C1D-ND-C4D	-8.88	100.03	106.33
23	C	512	CLA	C1D-ND-C4D	-8.86	100.04	106.33
23	A	408	CLA	C2D-C1D-ND	8.86	116.63	110.10
23	c	503	CLA	C1D-ND-C4D	-8.85	100.05	106.33
23	C	508	CLA	C1D-ND-C4D	-8.84	100.06	106.33
23	b	607	CLA	C1D-ND-C4D	-8.84	100.06	106.33
23	C	504	CLA	C1D-ND-C4D	-8.82	100.07	106.33
23	a	407	CLA	C2D-C1D-ND	8.81	116.60	110.10
23	B	610	CLA	C2D-C1D-ND	8.78	116.58	110.10
23	b	609	CLA	C1D-ND-C4D	-8.78	100.10	106.33
23	B	603	CLA	C2D-C1D-ND	8.76	116.56	110.10
23	B	613	CLA	C2D-C1D-ND	8.76	116.56	110.10
23	B	608	CLA	C1D-ND-C4D	-8.76	100.11	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	504	CLA	C2D-C1D-ND	8.72	116.53	110.10
23	c	502	CLA	C2D-C1D-ND	8.72	116.53	110.10
23	B	606	CLA	C2D-C1D-ND	8.71	116.52	110.10
23	B	615	CLA	C2D-C1D-ND	8.67	116.49	110.10
23	a	406	CLA	C1D-ND-C4D	-8.67	100.18	106.33
23	b	612	CLA	C1D-ND-C4D	-8.66	100.18	106.33
23	B	607	CLA	C2D-C1D-ND	8.63	116.47	110.10
23	B	614	CLA	C2D-C1D-ND	8.63	116.47	110.10
23	c	511	CLA	C1D-ND-C4D	-8.62	100.21	106.33
23	A	406	CLA	C2D-C1D-ND	8.61	116.45	110.10
23	B	608	CLA	C2D-C1D-ND	8.56	116.41	110.10
23	c	509	CLA	C1D-ND-C4D	-8.54	100.27	106.33
23	B	613	CLA	C1D-ND-C4D	-8.53	100.28	106.33
23	b	614	CLA	C2D-C1D-ND	8.53	116.39	110.10
23	a	406	CLA	C2D-C1D-ND	8.52	116.39	110.10
23	C	511	CLA	C1D-ND-C4D	-8.52	100.28	106.33
23	D	402	CLA	C2D-C1D-ND	8.48	116.35	110.10
23	C	509	CLA	C2D-C1D-ND	8.48	116.35	110.10
23	C	507	CLA	C1D-ND-C4D	-8.47	100.32	106.33
23	C	503	CLA	C2D-C1D-ND	8.46	116.34	110.10
23	B	609	CLA	C1D-ND-C4D	-8.46	100.33	106.33
23	c	509	CLA	C2D-C1D-ND	8.41	116.30	110.10
23	c	503	CLA	C2D-C1D-ND	8.37	116.27	110.10
23	C	506	CLA	C1D-ND-C4D	-8.36	100.39	106.33
23	b	603	CLA	C2D-C1D-ND	8.36	116.27	110.10
23	C	501	CLA	C2D-C1D-ND	8.34	116.25	110.10
23	b	607	CLA	C2D-C1D-ND	8.29	116.21	110.10
23	b	608	CLA	C2D-C1D-ND	8.29	116.21	110.10
23	C	508	CLA	C2D-C1D-ND	8.29	116.21	110.10
23	c	505	CLA	C2D-C1D-ND	8.28	116.21	110.10
23	b	613	CLA	C1D-ND-C4D	-8.28	100.45	106.33
23	d	402	CLA	C2D-C1D-ND	8.28	116.20	110.10
23	c	512	CLA	C2D-C1D-ND	8.26	116.19	110.10
23	b	610	CLA	C2D-C1D-ND	8.25	116.19	110.10
23	c	504	CLA	C2D-C1D-ND	8.22	116.16	110.10
23	C	502	CLA	C1D-ND-C4D	-8.21	100.50	106.33
23	b	612	CLA	C2D-C1D-ND	8.18	116.13	110.10
23	b	604	CLA	C1D-ND-C4D	-8.15	100.55	106.33
23	b	615	CLA	C2D-C1D-ND	8.12	116.09	110.10
23	c	511	CLA	C2D-C1D-ND	8.12	116.09	110.10
23	c	508	CLA	C1D-ND-C4D	-8.12	100.57	106.33
23	b	616	CLA	C2D-C1D-ND	8.11	116.08	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	507	CLA	C2D-C1D-ND	8.10	116.07	110.10
23	C	513	CLA	C2D-C1D-ND	8.08	116.06	110.10
23	b	602	CLA	C4A-NA-C1A	-8.03	103.09	106.71
23	a	405	CLA	C2D-C1D-ND	8.03	116.02	110.10
23	B	601	CLA	C2D-C1D-ND	7.98	115.98	110.10
23	b	609	CLA	C2D-C1D-ND	7.96	115.97	110.10
23	c	507	CLA	C2D-C1D-ND	7.96	115.97	110.10
23	d	401	CLA	C2D-C1D-ND	7.92	115.94	110.10
23	C	511	CLA	C2D-C1D-ND	7.92	115.94	110.10
23	c	510	CLA	C2D-C1D-ND	7.88	115.91	110.10
23	D	403	CLA	C2D-C1D-ND	7.85	115.89	110.10
23	b	606	CLA	C2D-C1D-ND	7.85	115.89	110.10
23	B	602	CLA	C2D-C1D-ND	7.83	115.87	110.10
23	b	601	CLA	C2D-C1D-ND	7.83	115.87	110.10
23	C	512	CLA	C2D-C1D-ND	7.81	115.86	110.10
23	C	503	CLA	C4A-NA-C1A	-7.76	103.22	106.71
23	B	611	CLA	CHD-C4C-C3C	-7.75	113.45	124.84
23	C	505	CLA	C2D-C1D-ND	7.70	115.78	110.10
23	A	404	CLA	C1D-ND-C4D	-7.69	100.87	106.33
23	B	604	CLA	C1D-ND-C4D	-7.68	100.88	106.33
23	c	513	CLA	C2D-C1D-ND	7.67	115.76	110.10
23	c	508	CLA	C2D-C1D-ND	7.66	115.75	110.10
23	c	506	CLA	C2D-C1D-ND	7.65	115.74	110.10
23	c	514	CLA	C2D-C1D-ND	7.64	115.74	110.10
23	B	609	CLA	C2D-C1D-ND	7.58	115.69	110.10
23	b	604	CLA	C2D-C1D-ND	7.54	115.66	110.10
23	A	404	CLA	C2D-C1D-ND	7.53	115.66	110.10
23	C	502	CLA	C2D-C1D-ND	7.47	115.61	110.10
23	C	510	CLA	C2D-C1D-ND	7.45	115.59	110.10
34	b	623	HTG	C1'-S1-C1	7.40	113.94	100.09
23	B	605	CLA	CHD-C4C-C3C	-7.39	113.97	124.84
23	b	602	CLA	C2D-C1D-ND	7.39	115.55	110.10
24	A	416	PHO	O2D-CGD-CBD	7.38	120.34	111.00
23	B	606	CLA	CMD-C2D-C1D	7.34	137.65	124.71
23	C	510	CLA	CMD-C2D-C1D	7.29	137.57	124.71
24	a	417	PHO	O2D-CGD-CBD	7.21	120.13	111.00
23	B	609	CLA	C4A-NA-C1A	-7.20	103.47	106.71
24	a	408	PHO	O2D-CGD-CBD	7.16	120.07	111.00
23	B	614	CLA	CMD-C2D-C1D	7.13	137.28	124.71
23	c	508	CLA	O2D-CGD-CBD	7.13	123.93	111.27
23	b	616	CLA	C4A-NA-C1A	-7.05	103.53	106.71
23	C	506	CLA	C2D-C1D-ND	7.00	115.27	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	610	CLA	CMD-C2D-C1D	6.98	137.02	124.71
23	B	604	CLA	C2D-C1D-ND	6.97	115.24	110.10
23	B	606	CLA	CHD-C1D-ND	-6.96	118.06	124.45
26	F	103	SQD	O6-C1-C2	6.95	119.16	108.30
23	b	605	CLA	CHD-C1D-ND	-6.95	118.06	124.45
23	b	605	CLA	CHD-C4C-C3C	-6.94	114.63	124.84
24	A	407	PHO	O2D-CGD-CBD	6.91	119.75	111.00
23	b	616	CLA	O2D-CGD-CBD	6.83	123.40	111.27
23	b	606	CLA	C4A-NA-C1A	-6.82	103.64	106.71
23	b	605	CLA	CMD-C2D-C1D	6.82	136.73	124.71
23	c	502	CLA	CMD-C2D-C1D	6.81	136.72	124.71
23	B	616	CLA	CHD-C4C-C3C	-6.80	114.85	124.84
23	b	616	CLA	CHD-C4C-C3C	-6.79	114.86	124.84
23	c	508	CLA	CMD-C2D-C1D	6.79	136.68	124.71
23	c	514	CLA	CMD-C2D-C1D	6.79	136.67	124.71
23	b	606	CLA	CMD-C2D-C1D	6.78	136.67	124.71
23	B	616	CLA	O2D-CGD-CBD	6.77	123.30	111.27
23	c	507	CLA	CMD-C2D-C1D	6.76	136.62	124.71
23	B	603	CLA	O2D-CGD-CBD	6.75	123.27	111.27
23	b	611	CLA	CMD-C2D-C1D	6.73	136.58	124.71
23	B	611	CLA	CMD-C2D-C1D	6.73	136.58	124.71
23	d	402	CLA	CMD-C2D-C1D	6.72	136.56	124.71
23	C	507	CLA	CHD-C4C-C3C	-6.68	115.02	124.84
23	C	509	CLA	CMD-C2D-C1D	6.65	136.43	124.71
23	A	404	CLA	CMD-C2D-C1D	6.62	136.38	124.71
23	c	504	CLA	CMD-C2D-C1D	6.62	136.38	124.71
23	C	512	CLA	C4A-NA-C1A	-6.62	103.73	106.71
23	b	616	CLA	CMD-C2D-C1D	6.59	136.32	124.71
23	B	606	CLA	C4A-NA-C1A	-6.57	103.75	106.71
23	C	506	CLA	CMD-C2D-C1D	6.57	136.29	124.71
23	a	409	CLA	CHD-C4C-C3C	-6.56	115.19	124.84
23	b	606	CLA	CHD-C1D-ND	-6.55	118.44	124.45
23	c	504	CLA	C4A-NA-C1A	-6.53	103.77	106.71
23	D	402	CLA	C4A-NA-C1A	-6.52	103.77	106.71
23	d	401	CLA	C2C-C1C-NC	6.51	116.07	109.97
23	b	615	CLA	C4A-NA-C1A	-6.50	103.78	106.71
23	b	601	CLA	O2D-CGD-CBD	6.49	122.81	111.27
23	B	603	CLA	CHD-C4C-C3C	-6.49	115.30	124.84
23	C	507	CLA	CMD-C2D-C1D	6.47	136.11	124.71
23	D	402	CLA	CMD-C2D-C1D	6.46	136.10	124.71
23	B	612	CLA	CHD-C4C-C3C	-6.45	115.36	124.84
23	c	505	CLA	CHD-C1D-ND	-6.45	118.53	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	503	CLA	C2C-C1C-NC	6.45	116.01	109.97
23	C	503	CLA	CMD-C2D-C1D	6.44	136.07	124.71
23	C	512	CLA	CHD-C4C-C3C	-6.44	115.37	124.84
23	B	604	CLA	C2C-C1C-NC	6.43	116.00	109.97
23	c	514	CLA	CHD-C1D-ND	-6.43	118.54	124.45
23	B	601	CLA	CMD-C2D-C1D	6.43	136.04	124.71
23	c	513	CLA	C4A-NA-C1A	-6.41	103.83	106.71
23	B	614	CLA	CHD-C1D-ND	-6.39	118.58	124.45
23	b	611	CLA	CHD-C1D-ND	-6.39	118.59	124.45
23	B	604	CLA	CMD-C2D-C1D	6.36	135.93	124.71
23	B	608	CLA	C2C-C1C-NC	6.36	115.93	109.97
23	c	508	CLA	CHD-C1D-ND	-6.35	118.61	124.45
23	c	507	CLA	CHD-C1D-ND	-6.34	118.63	124.45
23	a	407	CLA	CHD-C4C-C3C	-6.34	115.52	124.84
23	C	507	CLA	O2D-CGD-CBD	6.33	122.52	111.27
34	D	410	HTG	C1'-S1-C1	6.33	111.93	100.09
23	C	508	CLA	CHD-C4C-C3C	-6.32	115.55	124.84
23	C	503	CLA	CHD-C1D-ND	-6.32	118.65	124.45
23	b	610	CLA	CHD-C4C-C3C	-6.31	115.56	124.84
23	a	407	CLA	CHD-C1D-ND	-6.31	118.66	124.45
23	b	607	CLA	C2C-C1C-NC	6.30	115.88	109.97
23	C	510	CLA	CHD-C1D-ND	-6.30	118.66	124.45
23	B	610	CLA	CHD-C4C-C3C	-6.29	115.59	124.84
23	C	506	CLA	CHD-C1D-ND	-6.29	118.68	124.45
23	c	502	CLA	CHD-C1D-ND	-6.28	118.69	124.45
23	b	614	CLA	CMD-C2D-C1D	6.27	135.76	124.71
23	D	402	CLA	C2C-C1C-NC	6.26	115.84	109.97
23	b	612	CLA	CHD-C4C-C3C	-6.26	115.64	124.84
23	a	405	CLA	C2C-C1C-NC	6.26	115.83	109.97
23	b	614	CLA	O2D-CGD-CBD	6.22	122.32	111.27
23	b	601	CLA	CMD-C2D-C1D	6.22	135.67	124.71
23	a	406	CLA	CHD-C4C-C3C	-6.22	115.70	124.84
23	B	605	CLA	CMD-C2D-C1D	6.20	135.65	124.71
23	b	613	CLA	CHD-C4C-C3C	-6.20	115.72	124.84
23	C	501	CLA	CMD-C2D-C1D	6.20	135.65	124.71
23	d	402	CLA	CHD-C1D-ND	-6.20	118.76	124.45
23	a	405	CLA	C4A-NA-C1A	-6.19	103.92	106.71
23	C	501	CLA	CHD-C4C-C3C	-6.19	115.74	124.84
23	b	609	CLA	CHD-C4C-C3C	-6.18	115.75	124.84
23	C	502	CLA	C2C-C1C-NC	6.17	115.76	109.97
23	c	503	CLA	CHD-C4C-C3C	-6.17	115.77	124.84
23	B	609	CLA	CHD-C4C-C3C	-6.17	115.77	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	402	CLA	CHD-C1D-ND	-6.16	118.79	124.45
23	c	511	CLA	CHD-C4C-C3C	-6.16	115.78	124.84
23	b	603	CLA	CHD-C4C-C3C	-6.16	115.78	124.84
23	c	504	CLA	CHD-C4C-C3C	-6.15	115.80	124.84
23	A	408	CLA	CHD-C1D-ND	-6.15	118.81	124.45
23	c	512	CLA	CHD-C4C-C3C	-6.14	115.81	124.84
23	D	403	CLA	CMD-C2D-C1D	6.14	135.53	124.71
23	C	503	CLA	CHD-C4C-C3C	-6.13	115.83	124.84
23	C	506	CLA	C2C-C1C-NC	6.13	115.72	109.97
23	C	509	CLA	CHD-C1D-ND	-6.12	118.83	124.45
23	C	505	CLA	CMD-C2D-C1D	6.12	135.50	124.71
23	c	512	CLA	CMD-C2D-C1D	6.12	135.50	124.71
23	C	504	CLA	C2C-C1C-NC	6.12	115.70	109.97
23	B	610	CLA	O2D-CGD-CBD	6.10	122.11	111.27
23	b	607	CLA	CMD-C2D-C1D	6.10	135.46	124.71
23	A	404	CLA	C2C-C1C-NC	6.08	115.67	109.97
26	F	103	SQD	O47-C7-C8	6.08	124.60	111.50
23	b	601	CLA	CHD-C1D-ND	-6.08	118.87	124.45
23	A	408	CLA	C2C-C1C-NC	6.06	115.65	109.97
23	B	615	CLA	CHD-C4C-C3C	-6.06	115.93	124.84
23	D	403	CLA	CHD-C4C-C3C	-6.05	115.94	124.84
23	c	506	CLA	O2D-CGD-CBD	6.05	122.02	111.27
23	b	601	CLA	C4A-NA-C1A	-6.05	103.99	106.71
23	b	615	CLA	CMD-C2D-C1D	6.04	135.36	124.71
34	c	522	HTG	C1'-S1-C1	6.04	111.39	100.09
26	A	410	SQD	O6-C1-C2	6.03	117.72	108.30
23	b	602	CLA	O2D-CGD-CBD	6.03	121.99	111.27
23	b	613	CLA	C2C-C1C-NC	6.03	115.62	109.97
23	B	601	CLA	CHD-C4C-C3C	-6.03	115.98	124.84
23	c	513	CLA	CMD-C2D-C1D	6.03	135.34	124.71
23	d	401	CLA	C4A-NA-C1A	-6.03	104.00	106.71
23	B	613	CLA	C2C-C1C-NC	6.02	115.61	109.97
23	b	606	CLA	CHD-C4C-C3C	-6.02	116.00	124.84
23	C	509	CLA	CHD-C4C-C3C	-6.01	116.00	124.84
23	b	604	CLA	O2D-CGD-CBD	6.01	121.95	111.27
23	A	408	CLA	CMD-C2D-C1D	6.01	135.30	124.71
23	B	611	CLA	CHD-C1D-ND	-6.01	118.93	124.45
23	B	609	CLA	CHD-C1D-ND	-6.00	118.94	124.45
23	B	602	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
23	C	505	CLA	CHD-C4C-C3C	-5.99	116.03	124.84
23	B	606	CLA	CHD-C4C-C3C	-5.99	116.04	124.84
23	A	406	CLA	CHD-C4C-C3C	-5.98	116.05	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	d	409	HTG	C1'-S1-C1	5.98	111.28	100.09
23	B	615	CLA	C4A-NA-C1A	-5.97	104.02	106.71
23	A	408	CLA	CHD-C4C-C3C	-5.96	116.07	124.84
23	b	612	CLA	C2C-C1C-NC	5.96	115.56	109.97
23	b	604	CLA	C2C-C1C-NC	5.96	115.55	109.97
23	C	510	CLA	CHD-C4C-C3C	-5.95	116.09	124.84
23	b	611	CLA	CHD-C4C-C3C	-5.94	116.11	124.84
23	B	607	CLA	C2C-C1C-NC	5.93	115.53	109.97
23	c	505	CLA	CHD-C4C-C3C	-5.93	116.13	124.84
23	c	507	CLA	C2C-C1C-NC	5.92	115.52	109.97
23	B	609	CLA	CMD-C2D-C1D	5.92	135.14	124.71
23	b	608	CLA	CMD-C2D-C1D	5.92	135.14	124.71
23	b	610	CLA	O2D-CGD-CBD	5.91	121.77	111.27
23	A	405	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
23	c	502	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
29	A	414	PL9	C7-C8-C9	-5.89	116.99	126.79
23	A	404	CLA	C4A-NA-C1A	-5.89	104.06	106.71
23	B	613	CLA	CMD-C2D-C1D	5.89	135.09	124.71
23	c	505	CLA	CMD-C2D-C1D	5.88	135.08	124.71
23	A	406	CLA	CHD-C1D-ND	-5.88	119.05	124.45
23	C	509	CLA	C2C-C1C-NC	5.88	115.48	109.97
23	B	603	CLA	C4A-NA-C1A	-5.88	104.06	106.71
23	B	614	CLA	CHD-C4C-C3C	-5.87	116.20	124.84
23	b	615	CLA	C2C-C1C-NC	5.87	115.47	109.97
23	c	509	CLA	CHD-C4C-C3C	-5.86	116.22	124.84
23	c	510	CLA	C2C-C1C-NC	5.86	115.46	109.97
23	D	403	CLA	C4A-NA-C1A	-5.85	104.07	106.71
23	b	608	CLA	C2C-C1C-NC	5.85	115.45	109.97
23	B	601	CLA	CHD-C1D-ND	-5.85	119.08	124.45
23	C	511	CLA	C2C-C1C-NC	5.85	115.45	109.97
23	c	511	CLA	CMD-C2D-C1D	5.84	135.01	124.71
23	B	613	CLA	CHD-C4C-C3C	-5.84	116.26	124.84
23	b	607	CLA	CHD-C1D-ND	-5.84	119.09	124.45
23	c	508	CLA	CHD-C4C-C3C	-5.84	116.26	124.84
23	C	510	CLA	O2D-CGD-CBD	5.83	121.63	111.27
23	b	608	CLA	CHD-C1D-ND	-5.83	119.10	124.45
23	C	513	CLA	CHD-C1D-ND	-5.83	119.10	124.45
23	b	613	CLA	CMD-C2D-C1D	5.82	134.97	124.71
23	b	614	CLA	CHD-C4C-C3C	-5.82	116.28	124.84
23	A	404	CLA	CHD-C1D-ND	-5.81	119.11	124.45
23	c	506	CLA	CHD-C4C-C3C	-5.81	116.31	124.84
23	C	511	CLA	CHD-C4C-C3C	-5.80	116.31	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	511	CLA	CMD-C2D-C1D	5.79	134.93	124.71
23	C	509	CLA	C4A-NA-C1A	-5.79	104.10	106.71
23	c	509	CLA	C2C-C1C-NC	5.79	115.40	109.97
26	B	620	SQD	O6-C1-C2	5.79	117.35	108.30
23	B	601	CLA	O2D-CGD-CBD	5.78	121.55	111.27
23	d	402	CLA	CHD-C4C-C3C	-5.78	116.35	124.84
23	c	504	CLA	CHD-C1D-ND	-5.77	119.16	124.45
23	B	615	CLA	CMD-C2D-C1D	5.76	134.86	124.71
23	B	602	CLA	C4A-NA-C1A	-5.76	104.12	106.71
23	C	501	CLA	O2D-CGD-CBD	5.75	121.49	111.27
23	B	607	CLA	CHD-C4C-C3C	-5.75	116.39	124.84
23	a	405	CLA	CMD-C2D-C1D	5.75	134.84	124.71
23	a	406	CLA	C4A-NA-C1A	-5.75	104.12	106.71
23	C	512	CLA	CMD-C2D-C1D	5.74	134.83	124.71
23	B	615	CLA	CHD-C1D-ND	-5.74	119.18	124.45
23	A	406	CLA	C4A-NA-C1A	-5.72	104.13	106.71
23	c	507	CLA	CHD-C4C-C3C	-5.72	116.43	124.84
23	b	604	CLA	CMD-C2D-C1D	5.71	134.78	124.71
23	B	602	CLA	O2D-CGD-CBD	5.71	121.42	111.27
23	b	601	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
23	B	602	CLA	C2C-C1C-NC	5.70	115.32	109.97
23	C	513	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
23	C	502	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
23	b	602	CLA	CHD-C4C-C3C	-5.70	116.47	124.84
23	b	615	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
23	B	606	CLA	O2D-CGD-CBD	5.69	121.38	111.27
23	b	602	CLA	CHD-C1D-ND	-5.69	119.22	124.45
23	c	513	CLA	CHD-C1D-ND	-5.68	119.23	124.45
23	B	614	CLA	C2C-C1C-NC	5.66	115.27	109.97
23	b	603	CLA	CMD-C2D-C1D	5.65	134.67	124.71
23	C	504	CLA	CHD-C1D-ND	-5.64	119.27	124.45
23	b	607	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
23	d	401	CLA	CMD-C2D-C1D	5.64	134.65	124.71
23	B	608	CLA	CHD-C4C-C3C	-5.64	116.56	124.84
23	B	603	CLA	C2C-C1C-NC	5.63	115.25	109.97
23	c	506	CLA	CMD-C2D-C1D	5.63	134.64	124.71
23	b	602	CLA	CMD-C2D-C1D	5.63	134.64	124.71
23	c	513	CLA	CHD-C4C-C3C	-5.63	116.57	124.84
23	b	611	CLA	O2D-CGD-CBD	5.61	121.23	111.27
23	a	406	CLA	C2C-C1C-NC	5.61	115.22	109.97
23	B	602	CLA	CMD-C2D-C1D	5.60	134.58	124.71
23	b	616	CLA	CHD-C1D-ND	-5.59	119.31	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	610	CLA	CHD-C1D-ND	-5.59	119.31	124.45
23	b	615	CLA	CHD-C1D-ND	-5.59	119.32	124.45
26	a	411	SQD	O6-C1-C2	5.58	117.02	108.30
23	b	603	CLA	C4A-NA-C1A	-5.58	104.20	106.71
23	c	514	CLA	C4A-NA-C1A	-5.58	104.20	106.71
23	C	508	CLA	C2C-C1C-NC	5.58	115.20	109.97
23	A	405	CLA	C2C-C1C-NC	5.58	115.19	109.97
23	C	507	CLA	CHD-C1D-ND	-5.57	119.33	124.45
26	A	410	SQD	C1-O5-C5	-5.56	102.77	113.69
23	c	514	CLA	CHD-C4C-C3C	-5.56	116.67	124.84
23	d	401	CLA	CHD-C1D-ND	-5.56	119.35	124.45
23	b	608	CLA	CHD-C4C-C3C	-5.56	116.67	124.84
23	a	407	CLA	C4A-NA-C1A	-5.55	104.21	106.71
23	C	502	CLA	CMD-C2D-C1D	5.55	134.50	124.71
40	V	201	HEC	CBD-CAD-C3D	-5.55	103.15	112.62
23	d	401	CLA	CHD-C4C-C3C	-5.55	116.69	124.84
23	b	603	CLA	C2C-C1C-NC	5.54	115.16	109.97
23	b	609	CLA	CHD-C1D-ND	-5.54	119.36	124.45
23	c	511	CLA	CHD-C1D-ND	-5.54	119.37	124.45
23	b	605	CLA	C4A-NA-C1A	-5.54	104.22	106.71
23	B	607	CLA	O2D-CGD-CBD	5.53	121.10	111.27
23	D	402	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
23	A	405	CLA	CHD-C1D-ND	-5.53	119.37	124.45
23	B	614	CLA	C3D-C2D-C1D	-5.53	98.28	105.83
23	c	508	CLA	C2C-C1C-NC	5.53	115.15	109.97
23	c	503	CLA	O2D-CGD-CBD	5.53	121.10	111.27
25	D	404	BCR	C7-C8-C9	-5.52	117.89	126.23
23	B	603	CLA	CMD-C2D-C1D	5.52	134.45	124.71
23	B	607	CLA	CMD-C2D-C1D	5.52	134.44	124.71
23	C	513	CLA	C2C-C1C-NC	5.52	115.14	109.97
23	d	402	CLA	O2D-CGD-CBD	5.51	121.06	111.27
23	B	616	CLA	C4A-NA-C1A	-5.51	104.23	106.71
23	B	614	CLA	O2D-CGD-CBD	5.51	121.06	111.27
23	B	612	CLA	CHD-C1D-ND	-5.51	119.39	124.45
23	C	513	CLA	CMD-C2D-C1D	5.51	134.42	124.71
23	B	612	CLA	O2D-CGD-CBD	5.50	121.05	111.27
23	b	603	CLA	CHD-C1D-ND	-5.50	119.40	124.45
23	b	614	CLA	CHD-C1D-ND	-5.50	119.40	124.45
34	B	623	HTG	C1'-S1-C1	5.50	110.37	100.09
23	c	512	CLA	C2C-C1C-NC	5.49	115.12	109.97
23	C	505	CLA	O2D-CGD-CBD	5.49	121.03	111.27
23	c	509	CLA	CMD-C2D-C1D	5.49	134.38	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	511	CLA	C4A-NA-C1A	-5.49	104.24	106.71
23	b	612	CLA	O2D-CGD-CBD	5.48	121.01	111.27
23	c	510	CLA	C1-C2-C3	-5.47	116.57	126.04
23	b	609	CLA	CMD-C2D-C1D	5.47	134.35	124.71
25	Y	101	BCR	C33-C5-C6	-5.47	118.39	124.53
23	c	510	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
23	C	501	CLA	C4A-NA-C1A	-5.46	104.25	106.71
23	B	609	CLA	C2C-C1C-NC	5.46	115.08	109.97
23	b	613	CLA	C3D-C2D-C1D	-5.46	98.38	105.83
23	b	611	CLA	C4A-NA-C1A	-5.45	104.25	106.71
23	B	604	CLA	CHD-C4C-C3C	-5.45	116.84	124.84
23	a	406	CLA	CHD-C1D-ND	-5.44	119.46	124.45
23	B	611	CLA	C3D-C2D-C1D	-5.43	98.42	105.83
23	b	614	CLA	C2C-C1C-NC	5.42	115.05	109.97
23	C	504	CLA	CHD-C4C-C3C	-5.42	116.87	124.84
23	B	604	CLA	O2D-CGD-CBD	5.42	120.90	111.27
23	B	605	CLA	C3D-C2D-C1D	-5.42	98.43	105.83
23	B	605	CLA	CHD-C1D-ND	-5.42	119.47	124.45
23	c	506	CLA	C2C-C1C-NC	5.41	115.04	109.97
23	C	505	CLA	C2C-C1C-NC	5.40	115.03	109.97
23	c	510	CLA	CMD-C2D-C1D	5.40	134.23	124.71
23	b	605	CLA	O2D-CGD-CBD	5.39	120.85	111.27
23	a	405	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
23	c	512	CLA	CHD-C1D-ND	-5.38	119.51	124.45
23	B	603	CLA	CHD-C1D-ND	-5.38	119.51	124.45
23	B	607	CLA	CHD-C1D-ND	-5.37	119.52	124.45
23	C	512	CLA	O2D-CGD-CBD	5.37	120.81	111.27
23	C	504	CLA	CMD-C2D-C1D	5.37	134.17	124.71
24	a	417	PHO	C1-C2-C3	-5.37	116.76	126.04
23	b	603	CLA	O2D-CGD-CBD	5.37	120.80	111.27
38	F	102	HEM	CAD-CBD-CGD	5.36	125.14	113.60
23	B	616	CLA	C3C-C4C-NC	5.36	116.58	110.57
23	b	609	CLA	C4A-NA-C1A	-5.36	104.30	106.71
23	A	405	CLA	O2D-CGD-CBD	5.35	120.78	111.27
23	b	604	CLA	CHD-C4C-C3C	-5.35	116.98	124.84
23	a	407	CLA	CMD-C2D-C1D	5.34	134.12	124.71
23	A	406	CLA	C2C-C1C-NC	5.33	114.97	109.97
23	b	608	CLA	C4A-NA-C1A	-5.33	104.31	106.71
23	C	501	CLA	CHD-C1D-ND	-5.33	119.56	124.45
26	B	620	SQD	O47-C7-C8	5.32	122.97	111.50
23	C	510	CLA	C2C-C1C-NC	5.32	114.95	109.97
23	c	504	CLA	C2C-C1C-NC	5.32	114.95	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	506	CLA	C4A-NA-C1A	-5.32	104.32	106.71
23	b	610	CLA	C2C-C1C-NC	5.31	114.95	109.97
23	B	611	CLA	O2D-CGD-CBD	5.31	120.70	111.27
23	b	609	CLA	C2C-C1C-NC	5.30	114.94	109.97
23	c	511	CLA	C2C-C1C-NC	5.30	114.94	109.97
23	a	409	CLA	C2C-C1C-NC	5.29	114.93	109.97
23	c	510	CLA	O2D-CGD-CBD	5.29	120.67	111.27
23	a	405	CLA	CHD-C1D-ND	-5.29	119.59	124.45
23	C	511	CLA	O2D-CGD-CBD	5.28	120.66	111.27
23	B	602	CLA	CHD-C1D-ND	-5.28	119.60	124.45
23	b	604	CLA	CHD-C1D-ND	-5.28	119.61	124.45
23	c	508	CLA	C4A-NA-C1A	-5.27	104.34	106.71
23	C	507	CLA	C2C-C1C-NC	5.27	114.91	109.97
23	A	408	CLA	C3D-C2D-C1D	-5.27	98.65	105.83
23	B	612	CLA	C3C-C4C-NC	5.26	116.47	110.57
23	c	513	CLA	O2D-CGD-CBD	5.25	120.60	111.27
26	A	410	SQD	C1-C2-C3	-5.25	99.07	110.00
23	B	605	CLA	C4A-NA-C1A	-5.24	104.35	106.71
23	b	610	CLA	CMD-C2D-C1D	5.24	133.94	124.71
23	b	612	CLA	C3C-C4C-NC	5.24	116.44	110.57
23	B	608	CLA	CHD-C1D-ND	-5.23	119.64	124.45
23	C	506	CLA	CHD-C4C-C3C	-5.23	117.15	124.84
23	c	510	CLA	CHD-C1D-ND	-5.22	119.65	124.45
23	C	508	CLA	CMD-C2D-C1D	5.22	133.91	124.71
25	t	102	BCR	C33-C5-C6	-5.22	118.67	124.53
23	b	606	CLA	C2C-C1C-NC	5.21	114.86	109.97
23	b	611	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
26	a	411	SQD	O47-C7-C8	5.21	122.73	111.50
23	C	504	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
23	C	502	CLA	CHD-C1D-ND	-5.20	119.67	124.45
23	b	614	CLA	C4A-NA-C1A	-5.20	104.37	106.71
23	B	610	CLA	C3D-C2D-C1D	-5.20	98.74	105.83
23	B	606	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
23	c	502	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
23	c	502	CLA	O2D-CGD-CBD	5.19	120.49	111.27
23	A	405	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
23	b	605	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
23	a	406	CLA	CMD-C2D-C1D	5.19	133.85	124.71
23	C	505	CLA	CHD-C1D-ND	-5.18	119.69	124.45
23	B	608	CLA	CMD-C2D-C1D	5.17	133.83	124.71
23	a	409	CLA	C3C-C4C-NC	5.16	116.35	110.57
23	c	505	CLA	O2D-CGD-CBD	5.15	120.41	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	604	CLA	C4A-NA-C1A	-5.14	104.40	106.71
23	c	505	CLA	C2C-C1C-NC	5.14	114.78	109.97
23	B	616	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
23	B	613	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
23	D	402	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
23	A	406	CLA	CMD-C2D-C1D	5.12	133.74	124.71
23	D	403	CLA	O2D-CGD-CBD	5.12	120.36	111.27
23	C	512	CLA	CHD-C1D-ND	-5.12	119.75	124.45
23	C	511	CLA	CHD-C1D-ND	-5.11	119.76	124.45
23	b	614	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
23	c	509	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
23	c	506	CLA	C4A-NA-C1A	-5.09	104.42	106.71
23	c	502	CLA	C2C-C1C-NC	5.09	114.74	109.97
23	C	508	CLA	O2D-CGD-CBD	5.09	120.31	111.27
23	C	508	CLA	C3C-C4C-NC	5.09	116.28	110.57
23	B	615	CLA	C2C-C1C-NC	5.09	114.74	109.97
23	C	501	CLA	C2C-C1C-NC	5.08	114.73	109.97
23	a	409	CLA	O2D-CGD-CBD	5.07	120.28	111.27
23	b	607	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
23	B	613	CLA	C1-C2-C3	-5.06	117.30	126.04
26	b	620	SQD	O6-C1-C2	5.05	116.19	108.30
23	b	605	CLA	C2C-C1C-NC	5.05	114.70	109.97
23	b	608	CLA	O2D-CGD-CBD	5.04	120.22	111.27
23	b	613	CLA	C4A-NA-C1A	-5.04	104.44	106.71
23	B	611	CLA	CMB-C2B-C1B	5.04	136.21	128.46
23	D	403	CLA	CHD-C1D-ND	-5.03	119.83	124.45
23	B	616	CLA	C2C-C1C-NC	5.03	114.69	109.97
23	a	409	CLA	CHD-C1D-ND	-5.03	119.83	124.45
23	B	614	CLA	C4A-NA-C1A	-5.00	104.46	106.71
23	b	606	CLA	O2D-CGD-CBD	4.99	120.14	111.27
23	d	402	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
23	B	606	CLA	C2C-C1C-NC	4.99	114.65	109.97
23	B	605	CLA	C3C-C4C-NC	4.99	116.16	110.57
23	c	514	CLA	C2C-C1C-NC	4.98	114.64	109.97
23	B	608	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
32	A	419	LMG	C7-O1-C1	-4.97	104.02	113.74
23	B	605	CLA	C2C-C1C-NC	4.97	114.63	109.97
23	B	603	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
23	B	613	CLA	CHD-C1D-ND	-4.96	119.89	124.45
23	c	504	CLA	C3D-C2D-C1D	-4.96	99.07	105.83
23	c	506	CLA	CHD-C1D-ND	-4.95	119.91	124.45
34	b	622	HTG	C1-O5-C5	4.94	121.69	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	407	CLA	C2C-C1C-NC	4.94	114.60	109.97
23	c	505	CLA	C4A-NA-C1A	-4.93	104.49	106.71
23	b	611	CLA	C2C-C1C-NC	4.93	114.59	109.97
23	b	607	CLA	C3C-C4C-NC	4.93	116.10	110.57
23	C	507	CLA	C4A-NA-C1A	-4.92	104.49	106.71
23	b	613	CLA	CHD-C1D-ND	-4.92	119.94	124.45
23	B	607	CLA	C3D-C2D-C1D	-4.92	99.12	105.83
23	a	407	CLA	C3D-C2D-C1D	-4.91	99.12	105.83
23	B	608	CLA	O2D-CGD-CBD	4.91	119.99	111.27
23	c	504	CLA	O2D-CGD-CBD	4.90	119.98	111.27
26	b	620	SQD	O47-C7-C8	4.90	122.05	111.50
23	C	507	CLA	C3C-C4C-NC	4.89	116.06	110.57
23	c	507	CLA	C4A-NA-C1A	-4.89	104.51	106.71
23	a	406	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
23	B	615	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
23	b	616	CLA	C3D-C2D-C1D	-4.87	99.19	105.83
23	c	509	CLA	CHD-C1D-ND	-4.87	119.98	124.45
23	c	505	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
23	c	509	CLA	C4A-NA-C1A	-4.86	104.52	106.71
23	a	409	CLA	C3D-C2D-C1D	-4.86	99.21	105.83
26	f	102	SQD	O47-C7-C8	4.85	121.96	111.50
23	A	405	CLA	C4A-NA-C1A	-4.85	104.53	106.71
23	d	402	CLA	C2C-C1C-NC	4.85	114.51	109.97
23	C	502	CLA	C4A-NA-C1A	-4.84	104.53	106.71
23	C	507	CLA	C3D-C2D-C1D	-4.84	99.22	105.83
23	A	404	CLA	CHD-C4C-C3C	-4.84	117.73	124.84
23	B	610	CLA	C2C-C1C-NC	4.83	114.50	109.97
23	C	504	CLA	O2D-CGD-CBD	4.83	119.85	111.27
23	c	509	CLA	O2D-CGD-CBD	4.83	119.85	111.27
23	b	613	CLA	C3C-C4C-NC	4.83	115.98	110.57
23	c	508	CLA	C3D-C2D-C1D	-4.83	99.25	105.83
23	b	608	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
23	C	510	CLA	C4A-NA-C1A	-4.82	104.54	106.71
23	C	509	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
23	B	603	CLA	C3C-C4C-NC	4.82	115.97	110.57
23	b	601	CLA	C2C-C1C-NC	4.82	114.48	109.97
23	c	507	CLA	C3D-C2D-C1D	-4.81	99.26	105.83
23	b	604	CLA	C1-C2-C3	-4.81	117.72	126.04
23	C	503	CLA	C3D-C2D-C1D	-4.81	99.26	105.83
23	c	506	CLA	C3C-C4C-NC	4.81	115.97	110.57
23	C	511	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
23	B	601	CLA	C4A-NA-C1A	-4.80	104.55	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	409	CLA	C4A-NA-C1A	-4.80	104.55	106.71
23	C	504	CLA	C3C-C4C-NC	4.80	115.95	110.57
34	C	520	HTG	C1'-S1-C1	4.80	109.06	100.09
23	B	601	CLA	C2C-C1C-NC	4.80	114.47	109.97
23	B	611	CLA	CMC-C2C-C1C	4.78	132.33	125.04
26	f	102	SQD	C1-O5-C5	4.78	123.06	113.69
23	b	612	CLA	CMD-C2D-C1D	4.77	133.12	124.71
23	b	610	CLA	C4A-NA-C1A	-4.76	104.56	106.71
23	C	505	CLA	C3C-C4C-NC	4.75	115.90	110.57
23	C	508	CLA	CHD-C1D-ND	-4.74	120.10	124.45
23	A	406	CLA	O2D-CGD-CBD	4.74	119.69	111.27
23	B	616	CLA	CMD-C2D-C1D	4.74	133.06	124.71
23	B	611	CLA	C3C-C4C-NC	4.74	115.88	110.57
23	C	502	CLA	O2D-CGD-CBD	4.74	119.69	111.27
38	f	101	HEM	CHC-C4B-NB	4.73	129.57	124.43
23	B	610	CLA	C3C-C4C-NC	4.73	115.88	110.57
23	c	510	CLA	C4A-NA-C1A	-4.73	104.58	106.71
23	C	501	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
23	c	512	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
23	B	612	CLA	CMD-C2D-C1D	4.72	133.04	124.71
23	C	508	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
23	b	602	CLA	C3D-C4D-ND	4.72	117.87	110.24
23	C	509	CLA	O2D-CGD-CBD	4.72	119.65	111.27
23	C	505	CLA	C4A-NA-C1A	-4.71	104.59	106.71
23	A	405	CLA	C1C-C2C-C3C	-4.71	102.00	106.96
23	A	404	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
23	c	503	CLA	C1C-C2C-C3C	-4.70	102.02	106.96
23	b	615	CLA	C3D-C2D-C1D	-4.69	99.42	105.83
23	c	511	CLA	O2D-CGD-CBD	4.69	119.61	111.27
23	B	604	CLA	C3C-C4C-NC	4.69	115.83	110.57
23	a	407	CLA	C3D-C4D-ND	4.68	117.81	110.24
23	b	602	CLA	C2C-C1C-NC	4.68	114.35	109.97
25	d	403	BCR	C15-C14-C13	-4.67	120.64	127.31
23	B	605	CLA	O2D-CGD-CBD	4.67	119.56	111.27
23	C	513	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
23	d	401	CLA	C3C-C4C-NC	4.67	115.80	110.57
23	b	610	CLA	C3C-C4C-NC	4.65	115.79	110.57
23	B	612	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
23	c	511	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
23	D	403	CLA	C2C-C1C-NC	4.64	114.32	109.97
23	b	605	CLA	C3D-C4D-ND	4.64	117.75	110.24
23	B	611	CLA	C3D-C4D-ND	4.64	117.74	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	614	CLA	O2D-CGD-O1D	-4.64	114.77	123.84
23	B	613	CLA	C3C-C4C-NC	4.63	115.77	110.57
23	b	606	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
23	b	610	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
23	D	403	CLA	C3D-C2D-C1D	-4.63	99.52	105.83
23	c	502	CLA	O2D-CGD-O1D	-4.63	114.80	123.84
23	A	406	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
23	c	514	CLA	O2D-CGD-CBD	4.62	119.48	111.27
23	B	601	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
23	b	610	CLA	CHD-C1D-ND	-4.61	120.22	124.45
23	C	503	CLA	C2C-C1C-NC	4.60	114.29	109.97
29	a	415	PL9	C7-C8-C9	-4.60	119.13	126.79
23	B	608	CLA	C3C-C4C-NC	4.60	115.73	110.57
23	c	511	CLA	C1-C2-C3	-4.60	118.08	126.04
23	c	509	CLA	C3C-C4C-NC	4.60	115.73	110.57
23	B	609	CLA	C3C-C4C-NC	4.60	115.73	110.57
23	c	513	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
23	c	514	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
23	B	602	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
23	c	503	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
23	b	603	CLA	C3D-C4D-ND	4.58	117.65	110.24
23	C	512	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
23	a	405	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
23	C	511	CLA	C4A-NA-C1A	-4.58	104.65	106.71
23	a	407	CLA	O2D-CGD-CBD	4.58	119.40	111.27
23	b	609	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
23	C	513	CLA	O2D-CGD-CBD	4.57	119.38	111.27
23	B	604	CLA	C1-C2-C3	-4.57	118.15	126.04
32	B	621	LMG	O7-C10-C11	4.56	121.34	111.50
23	B	612	CLA	C2C-C1C-NC	4.56	114.25	109.97
23	D	403	CLA	C3C-C4C-NC	4.56	115.69	110.57
23	c	504	CLA	C3C-C4C-NC	4.56	115.68	110.57
23	D	402	CLA	O2D-CGD-CBD	4.55	119.36	111.27
23	A	406	CLA	C3D-C4D-ND	4.55	117.61	110.24
23	b	609	CLA	C3C-C4C-NC	4.55	115.68	110.57
23	A	405	CLA	CMD-C2D-C1D	4.55	132.73	124.71
23	b	601	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
23	C	506	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
23	A	408	CLA	O2D-CGD-CBD	4.53	119.31	111.27
24	A	416	PHO	C1-C2-C3	-4.53	118.22	126.04
25	d	403	BCR	C7-C8-C9	-4.52	119.40	126.23
23	b	605	CLA	C3C-C4C-NC	4.52	115.64	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	510	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
32	c	521	LMG	O6-C5-C4	4.51	117.88	109.69
23	d	402	CLA	C4A-NA-C1A	-4.51	104.68	106.71
23	B	610	CLA	C4A-NA-C1A	-4.50	104.68	106.71
23	b	604	CLA	C3C-C4C-NC	4.50	115.62	110.57
23	a	406	CLA	C1C-C2C-C3C	-4.49	102.24	106.96
23	C	504	CLA	C4A-NA-C1A	-4.48	104.69	106.71
23	b	603	CLA	C3C-C4C-NC	4.48	115.59	110.57
23	B	613	CLA	O2D-CGD-CBD	4.48	119.22	111.27
23	B	612	CLA	C3D-C4D-ND	4.47	117.47	110.24
23	C	506	CLA	C1C-C2C-C3C	-4.47	102.26	106.96
23	a	409	CLA	C3D-C4D-ND	4.47	117.46	110.24
23	b	604	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
23	c	503	CLA	C1D-CHD-C4C	-4.45	116.45	126.06
32	d	410	LMG	O7-C10-C11	4.45	121.09	111.50
23	c	513	CLA	C2C-C1C-NC	4.45	114.14	109.97
23	d	401	CLA	C1C-C2C-C3C	-4.45	102.28	106.96
23	C	502	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
26	B	620	SQD	C3-C4-C5	4.44	118.17	110.24
23	c	508	CLA	C3C-C4C-NC	4.44	115.55	110.57
23	B	609	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
23	d	401	CLA	C3D-C4D-ND	4.44	117.42	110.24
23	b	601	CLA	C3D-C4D-ND	4.44	117.42	110.24
23	C	510	CLA	C1-C2-C3	-4.44	118.37	126.04
23	c	503	CLA	CMD-C2D-C1D	4.44	132.53	124.71
23	C	512	CLA	C2C-C1C-NC	4.43	114.12	109.97
23	b	607	CLA	O2D-CGD-CBD	4.42	119.13	111.27
23	c	514	CLA	C3D-C4D-ND	4.42	117.39	110.24
23	B	615	CLA	C3D-C4D-ND	4.42	117.38	110.24
23	c	510	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
26	F	103	SQD	C1-O5-C5	-4.41	105.03	113.69
23	c	503	CLA	CHD-C1D-ND	-4.41	120.40	124.45
31	t	101	LMT	C3'-C4'-C5'	-4.40	100.83	110.93
23	B	613	CLA	C4A-NA-C1A	-4.40	104.73	106.71
38	F	102	HEM	CHC-C4B-NB	4.40	129.21	124.43
23	b	608	CLA	C1C-C2C-C3C	-4.40	102.33	106.96
23	C	510	CLA	C3D-C4D-ND	4.39	117.35	110.24
23	c	506	CLA	C3D-C4D-ND	4.39	117.34	110.24
23	a	406	CLA	O2D-CGD-CBD	4.39	119.07	111.27
23	B	610	CLA	O2A-CGA-CBA	4.39	125.67	111.91
23	B	601	CLA	C3D-C4D-ND	4.38	117.33	110.24
29	a	415	PL9	C7-C3-C4	4.38	120.44	116.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	617	BCR	C33-C5-C6	-4.38	119.61	124.53
23	c	512	CLA	O2D-CGD-CBD	4.38	119.05	111.27
25	y	101	BCR	C33-C5-C6	-4.38	119.61	124.53
38	F	102	HEM	C1B-NB-C4B	4.37	109.59	105.07
32	A	419	LMG	O7-C10-C11	4.36	120.90	111.50
23	B	603	CLA	C1D-CHD-C4C	-4.36	116.66	126.06
23	b	611	CLA	C3D-C4D-ND	4.36	117.28	110.24
23	B	602	CLA	C3C-C4C-NC	4.35	115.45	110.57
23	C	506	CLA	O2D-CGD-CBD	4.34	118.99	111.27
32	a	418	LMG	O7-C10-C11	4.34	120.86	111.50
23	b	616	CLA	C1D-CHD-C4C	-4.34	116.70	126.06
23	B	604	CLA	C4A-NA-C1A	-4.33	104.76	106.71
23	b	607	CLA	C3D-C4D-ND	4.33	117.25	110.24
23	C	511	CLA	C3C-C4C-NC	4.33	115.43	110.57
23	C	512	CLA	C3C-C4C-NC	4.33	115.42	110.57
23	c	510	CLA	C3D-C4D-ND	4.33	117.23	110.24
33	E	101	LHG	O7-C7-C8	4.32	120.82	111.50
23	A	404	CLA	C1C-C2C-C3C	-4.32	102.41	106.96
23	b	612	CLA	C1-C2-C3	-4.32	118.57	126.04
23	B	607	CLA	C1C-C2C-C3C	-4.32	102.41	106.96
23	C	502	CLA	C3C-C4C-NC	4.32	115.41	110.57
23	a	409	CLA	CMD-C2D-C1D	4.32	132.32	124.71
23	B	616	CLA	CHD-C1D-ND	-4.32	120.49	124.45
23	D	402	CLA	C3C-C4C-NC	4.31	115.41	110.57
23	b	603	CLA	C3D-C2D-C1D	-4.31	99.94	105.83
23	C	509	CLA	C3C-C4C-NC	4.31	115.41	110.57
23	b	612	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
29	A	414	PL9	C32-C33-C34	-4.30	117.31	127.66
23	C	506	CLA	C3D-C4D-ND	4.30	117.19	110.24
23	B	609	CLA	O2D-CGD-CBD	4.29	118.89	111.27
23	c	507	CLA	C3D-C4D-ND	4.29	117.18	110.24
23	C	504	CLA	C1C-C2C-C3C	-4.29	102.44	106.96
23	b	603	CLA	C1D-CHD-C4C	-4.29	116.81	126.06
23	a	405	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
23	C	505	CLA	C3D-C4D-ND	4.28	117.17	110.24
23	b	616	CLA	C3C-C4C-NC	4.28	115.37	110.57
23	C	503	CLA	C3D-C4D-ND	4.28	117.16	110.24
23	c	505	CLA	C3C-C4C-NC	4.27	115.36	110.57
23	d	402	CLA	C3D-C4D-ND	4.27	117.14	110.24
23	c	505	CLA	C3D-C4D-ND	4.26	117.14	110.24
23	b	611	CLA	C3C-C4C-NC	4.26	115.35	110.57
23	b	612	CLA	C4A-NA-C1A	-4.26	104.79	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	601	CLA	C3C-C4C-NC	4.25	115.34	110.57
23	c	502	CLA	C3C-C4C-NC	4.25	115.34	110.57
23	a	407	CLA	C3C-C4C-NC	4.25	115.34	110.57
23	B	609	CLA	C3D-C4D-ND	4.25	117.12	110.24
23	C	513	CLA	C3D-C4D-ND	4.25	117.12	110.24
23	B	611	CLA	CMB-C2B-C3B	4.25	132.63	124.68
23	c	508	CLA	C1C-C2C-C3C	-4.25	102.49	106.96
23	B	616	CLA	O2D-CGD-O1D	-4.25	115.53	123.84
23	C	502	CLA	C1C-C2C-C3C	-4.25	102.49	106.96
23	A	408	CLA	C3C-C4C-NC	4.25	115.33	110.57
23	C	501	CLA	C3D-C4D-ND	4.25	117.11	110.24
23	B	605	CLA	C1D-CHD-C4C	-4.24	116.91	126.06
23	b	604	CLA	C1C-C2C-C3C	-4.24	102.50	106.96
23	B	602	CLA	C3D-C4D-ND	4.23	117.07	110.24
23	b	610	CLA	C3D-C4D-ND	4.22	117.07	110.24
23	B	611	CLA	C1D-CHD-C4C	-4.22	116.95	126.06
23	a	405	CLA	C3D-C4D-ND	4.22	117.06	110.24
23	b	606	CLA	C3D-C4D-ND	4.22	117.06	110.24
23	c	504	CLA	C1D-CHD-C4C	-4.21	116.97	126.06
25	H	101	BCR	C38-C26-C25	-4.21	119.80	124.53
23	b	614	CLA	C3C-C4C-NC	4.21	115.29	110.57
23	a	405	CLA	C1D-CHD-C4C	-4.21	116.98	126.06
23	B	606	CLA	C3C-C4C-NC	4.20	115.28	110.57
23	C	501	CLA	C3C-C4C-NC	4.20	115.28	110.57
23	B	615	CLA	C3C-C4C-NC	4.20	115.28	110.57
23	c	511	CLA	C3C-C4C-NC	4.20	115.28	110.57
23	C	509	CLA	C3D-C4D-ND	4.20	117.03	110.24
23	C	513	CLA	C4A-NA-C1A	-4.20	104.82	106.71
23	b	607	CLA	C1C-C2C-C3C	-4.19	102.55	106.96
23	b	612	CLA	CHD-C1D-ND	-4.19	120.60	124.45
23	b	602	CLA	C3C-C4C-NC	4.19	115.27	110.57
23	B	604	CLA	C3D-C2D-C1D	-4.19	100.11	105.83
23	B	612	CLA	O2D-CGD-O1D	-4.19	115.65	123.84
26	a	411	SQD	C1-C2-C3	-4.19	101.27	110.00
23	B	603	CLA	C3D-C4D-ND	4.19	117.01	110.24
23	b	602	CLA	C3D-C2D-C1D	-4.19	100.12	105.83
23	B	607	CLA	C3C-C4C-NC	4.18	115.26	110.57
23	b	610	CLA	C1-C2-C3	-4.18	118.81	126.04
23	C	503	CLA	O2D-CGD-CBD	4.18	118.69	111.27
23	a	405	CLA	CAA-C2A-C3A	-4.18	101.34	112.78
23	b	615	CLA	C3D-C4D-ND	4.17	116.98	110.24
32	Z	101	LMG	O7-C10-C11	4.17	120.48	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	408	CLA	C3D-C4D-ND	4.17	116.98	110.24
23	B	607	CLA	C3D-C4D-ND	4.16	116.97	110.24
25	b	617	BCR	C7-C8-C9	-4.16	119.95	126.23
23	A	406	CLA	C1C-C2C-C3C	-4.16	102.59	106.96
23	b	616	CLA	C3D-C4D-ND	4.16	116.96	110.24
23	A	408	CLA	C1C-C2C-C3C	-4.15	102.59	106.96
23	B	610	CLA	C3D-C4D-ND	4.15	116.95	110.24
23	C	512	CLA	C1D-CHD-C4C	-4.15	117.10	126.06
23	C	505	CLA	C3D-C2D-C1D	-4.15	100.17	105.83
23	C	503	CLA	C3C-C4C-NC	4.15	115.22	110.57
23	c	512	CLA	C1D-CHD-C4C	-4.15	117.12	126.06
23	c	504	CLA	C3D-C4D-ND	4.14	116.94	110.24
23	D	402	CLA	C1C-C2C-C3C	-4.14	102.60	106.96
23	C	507	CLA	C1D-CHD-C4C	-4.14	117.14	126.06
23	b	609	CLA	C3D-C4D-ND	4.13	116.92	110.24
23	B	605	CLA	C3D-C4D-ND	4.13	116.92	110.24
23	c	510	CLA	C3B-C4B-NB	4.13	114.54	109.21
23	c	512	CLA	C3D-C4D-ND	4.13	116.91	110.24
23	c	513	CLA	C3D-C4D-ND	4.12	116.91	110.24
23	C	512	CLA	C3D-C4D-ND	4.12	116.90	110.24
23	D	403	CLA	C3D-C4D-ND	4.12	116.90	110.24
23	a	406	CLA	C3D-C4D-ND	4.12	116.90	110.24
29	A	414	PL9	C7-C3-C2	-4.12	117.89	123.30
23	d	401	CLA	O2D-CGD-CBD	4.11	118.58	111.27
23	C	508	CLA	C3D-C4D-ND	4.11	116.89	110.24
23	C	513	CLA	C3C-C4C-NC	4.11	115.18	110.57
23	B	604	CLA	C1D-CHD-C4C	-4.11	117.19	126.06
23	d	401	CLA	C3D-C2D-C1D	-4.11	100.22	105.83
23	B	616	CLA	C3D-C4D-ND	4.11	116.89	110.24
23	B	608	CLA	C3B-C4B-NB	4.11	114.52	109.21
23	A	404	CLA	C3B-C4B-NB	4.11	114.52	109.21
23	B	608	CLA	C3D-C4D-ND	4.11	116.88	110.24
23	B	611	CLA	C4A-NA-C1A	-4.10	104.86	106.71
23	B	611	CLA	CHD-C4C-NC	4.10	130.67	124.20
23	c	503	CLA	C3D-C4D-ND	4.10	116.87	110.24
23	A	405	CLA	C3D-C4D-ND	4.10	116.87	110.24
23	c	503	CLA	O2D-CGD-O1D	-4.09	115.84	123.84
23	B	606	CLA	C3D-C4D-ND	4.09	116.86	110.24
26	b	620	SQD	C1-O5-C5	-4.09	105.66	113.69
23	b	610	CLA	O2A-CGA-CBA	4.09	124.74	111.91
23	C	509	CLA	C1C-C2C-C3C	-4.09	102.66	106.96
32	c	521	LMG	O7-C10-C11	4.09	120.31	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	404	CLA	CAA-C2A-C3A	-4.08	101.61	112.78
23	A	405	CLA	CAA-C2A-C3A	-4.08	101.61	112.78
35	C	515	DGD	O2G-C1B-C2B	4.08	120.29	111.50
23	b	607	CLA	C3B-C4B-NB	4.08	114.48	109.21
26	a	411	SQD	C1-O5-C5	-4.07	105.69	113.69
23	b	615	CLA	C1D-CHD-C4C	-4.07	117.27	126.06
23	c	502	CLA	C3D-C4D-ND	4.07	116.82	110.24
23	c	503	CLA	C4A-NA-C1A	-4.07	104.88	106.71
23	b	616	CLA	O2D-CGD-O1D	-4.07	115.88	123.84
23	C	508	CLA	C4A-NA-C1A	-4.07	104.88	106.71
23	D	402	CLA	C3D-C4D-ND	4.07	116.82	110.24
38	F	102	HEM	CBA-CAA-C2A	-4.06	105.69	112.62
23	A	406	CLA	C3C-C4C-NC	4.06	115.13	110.57
23	b	616	CLA	C2C-C1C-NC	4.06	113.78	109.97
23	c	507	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
23	b	609	CLA	O2D-CGD-CBD	4.06	118.48	111.27
23	a	406	CLA	C3C-C4C-NC	4.06	115.12	110.57
25	Y	101	BCR	C16-C17-C18	-4.05	121.53	127.31
23	b	614	CLA	C3D-C4D-ND	4.05	116.79	110.24
23	B	604	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
23	b	613	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
23	C	511	CLA	C1D-CHD-C4C	-4.05	117.33	126.06
23	b	608	CLA	C3D-C4D-ND	4.04	116.78	110.24
23	c	512	CLA	C3C-C4C-NC	4.04	115.10	110.57
23	C	510	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
23	c	507	CLA	O2D-CGD-CBD	4.04	118.44	111.27
23	B	613	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
23	C	502	CLA	C3D-C4D-ND	4.03	116.76	110.24
23	c	506	CLA	C3D-C2D-C1D	-4.02	100.34	105.83
23	A	408	CLA	C4A-NA-C1A	-4.01	104.90	106.71
23	B	614	CLA	C3C-C4C-NC	4.01	115.07	110.57
32	C	519	LMG	O6-C5-C4	4.01	116.98	109.69
23	a	406	CLA	C1D-CHD-C4C	-4.01	117.41	126.06
23	C	501	CLA	C1D-CHD-C4C	-4.01	117.41	126.06
23	C	512	CLA	C1-C2-C3	-4.00	119.12	126.04
32	C	519	LMG	O7-C10-C11	4.00	120.12	111.50
23	C	505	CLA	C1D-CHD-C4C	-4.00	117.43	126.06
23	b	606	CLA	C3C-C4C-NC	4.00	115.05	110.57
23	c	514	CLA	C1D-CHD-C4C	-4.00	117.44	126.06
25	C	514	BCR	C7-C8-C9	-3.99	120.20	126.23
23	c	514	CLA	C3C-C4C-NC	3.99	115.05	110.57
23	B	607	CLA	C4A-NA-C1A	-3.99	104.91	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	409	CLA	CMC-C2C-C1C	3.99	131.11	125.04
25	c	515	BCR	C11-C10-C9	-3.98	121.63	127.31
23	B	615	CLA	C1D-CHD-C4C	-3.98	117.48	126.06
23	b	602	CLA	O2D-CGD-O1D	-3.97	116.07	123.84
23	c	503	CLA	C3C-C4C-NC	3.97	115.03	110.57
23	c	505	CLA	C1-O2A-CGA	3.97	126.86	116.44
23	C	513	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
23	B	602	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
23	b	615	CLA	C1C-C2C-C3C	-3.97	102.79	106.96
23	b	612	CLA	C3B-C4B-NB	3.96	114.34	109.21
23	C	513	CLA	C3B-C4B-NB	3.96	114.33	109.21
23	C	509	CLA	C1-C2-C3	-3.95	119.20	126.04
23	b	615	CLA	C3C-C4C-NC	3.95	115.00	110.57
23	a	405	CLA	C3C-C4C-NC	3.95	115.00	110.57
23	B	604	CLA	CAC-C3C-C4C	3.95	129.93	124.81
23	c	510	CLA	C1D-CHD-C4C	-3.95	117.54	126.06
23	a	405	CLA	C3B-C4B-NB	3.95	114.31	109.21
23	c	511	CLA	C3D-C4D-ND	3.95	116.62	110.24
23	B	603	CLA	O2D-CGD-O1D	-3.95	116.12	123.84
23	A	404	CLA	C3C-C4C-NC	3.95	115.00	110.57
32	c	520	LMG	O7-C10-C11	3.94	120.00	111.50
23	c	508	CLA	O2D-CGD-O1D	-3.94	116.13	123.84
32	m	101	LMG	O7-C10-C11	3.94	120.00	111.50
23	C	504	CLA	C3D-C4D-ND	3.94	116.61	110.24
23	b	604	CLA	C3B-C4B-NB	3.94	114.30	109.21
23	b	612	CLA	C3D-C4D-ND	3.94	116.61	110.24
29	d	404	PL9	C42-C43-C44	-3.93	118.19	127.66
38	f	101	HEM	CAD-CBD-CGD	3.93	122.07	113.60
23	b	601	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
23	c	512	CLA	C3B-C4B-NB	3.93	114.29	109.21
23	D	402	CLA	C1-C2-C3	-3.93	119.25	126.04
23	B	614	CLA	C3D-C4D-ND	3.93	116.59	110.24
23	a	407	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
23	c	502	CLA	C4A-NA-C1A	-3.93	104.94	106.71
25	d	403	BCR	C29-C30-C25	3.92	116.52	110.48
23	b	605	CLA	O2D-CGD-O1D	-3.92	116.17	123.84
23	B	610	CLA	CAA-CBA-CGA	-3.92	101.80	113.25
26	a	411	SQD	C44-O6-C1	-3.91	106.09	113.74
40	v	201	HEC	CBD-CAD-C3D	-3.91	105.95	112.62
23	C	501	CLA	O2D-CGD-O1D	-3.91	116.19	123.84
29	A	414	PL9	C7-C3-C4	3.91	120.05	116.88
23	c	508	CLA	CMC-C2C-C1C	3.91	130.99	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	511	CLA	C1C-C2C-C3C	-3.91	102.85	106.96
23	b	610	CLA	C1D-CHD-C4C	-3.91	117.63	126.06
23	A	408	CLA	C3B-C4B-NB	3.91	114.26	109.21
34	b	625	HTG	C1-O5-C5	3.90	119.78	112.58
23	c	509	CLA	C3D-C4D-ND	3.90	116.55	110.24
23	b	606	CLA	C1D-CHD-C4C	-3.90	117.65	126.06
29	a	415	PL9	C32-C33-C34	-3.89	118.28	127.66
23	B	602	CLA	C1D-CHD-C4C	-3.89	117.66	126.06
23	B	604	CLA	CHD-C1D-ND	-3.89	120.88	124.45
23	b	609	CLA	C1-C2-C3	-3.89	119.31	126.04
23	b	608	CLA	C3B-C4B-NB	3.89	114.24	109.21
31	B	628	LMT	C1'-O5'-C5'	-3.89	106.05	113.69
23	D	403	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
23	c	510	CLA	C3C-C4C-NC	3.89	114.93	110.57
23	B	608	CLA	CAC-C3C-C4C	3.89	129.85	124.81
33	A	420	LHG	O8-C23-O10	-3.88	113.79	123.59
35	c	517	DGD	O2G-C1B-C2B	3.88	119.87	111.50
23	b	605	CLA	C4-C3-C5	3.88	121.80	115.27
23	b	612	CLA	CAC-C3C-C4C	3.88	129.85	124.81
23	A	405	CLA	CMC-C2C-C1C	3.88	130.95	125.04
23	b	614	CLA	C1D-CHD-C4C	-3.88	117.69	126.06
23	C	508	CLA	C3B-C4B-NB	3.88	114.22	109.21
23	c	510	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
23	a	406	CLA	CAA-C2A-C3A	-3.87	102.19	112.78
24	A	407	PHO	C1A-C2A-C3A	-3.87	99.16	102.84
23	C	510	CLA	C3B-C4B-NB	3.87	114.21	109.21
32	c	521	LMG	C3-C4-C5	3.86	117.13	110.24
23	B	602	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	612	CLA	O2D-CGD-O1D	-3.86	116.30	123.84
23	C	502	CLA	C3B-C4B-NB	3.86	114.20	109.21
23	C	503	CLA	C1D-CHD-C4C	-3.86	117.74	126.06
23	c	509	CLA	C1-C2-C3	-3.86	119.38	126.04
23	A	405	CLA	C3C-C4C-NC	3.85	114.89	110.57
23	c	509	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
23	B	609	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
23	B	601	CLA	C1D-CHD-C4C	-3.84	117.77	126.06
23	B	610	CLA	CAA-C2A-C3A	-3.84	102.26	112.78
23	b	607	CLA	C4A-NA-C1A	-3.84	104.98	106.71
29	a	415	PL9	C7-C3-C2	-3.84	118.25	123.30
23	b	603	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
23	c	507	CLA	C3C-C4C-NC	3.84	114.87	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	513	CLA	C1D-CHD-C4C	-3.83	117.79	126.06
23	C	501	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
23	C	511	CLA	C3D-C4D-ND	3.83	116.43	110.24
40	v	201	HEC	CMB-C2B-C1B	-3.83	122.58	128.46
23	B	616	CLA	C4C-C3C-C2C	-3.83	101.32	106.90
32	C	518	LMG	O7-C10-C11	3.83	119.75	111.50
23	C	511	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
23	C	504	CLA	C3B-C4B-NB	3.82	114.15	109.21
23	B	614	CLA	O2D-CGD-O1D	-3.81	116.38	123.84
23	B	614	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
23	B	606	CLA	C1C-C2C-C3C	-3.81	102.96	106.96
23	B	602	CLA	CMC-C2C-C1C	3.80	130.83	125.04
25	k	101	BCR	C29-C30-C25	3.80	116.33	110.48
33	A	420	LHG	O7-C7-C8	3.80	119.69	111.50
24	A	416	PHO	C1A-C2A-C3A	-3.80	99.22	102.84
23	c	507	CLA	C3B-C4B-NB	3.80	114.12	109.21
23	B	614	CLA	C1-C2-C3	-3.80	119.47	126.04
23	d	402	CLA	C3C-C4C-NC	3.79	114.82	110.57
23	B	616	CLA	C1D-CHD-C4C	-3.79	117.89	126.06
23	b	606	CLA	C1C-C2C-C3C	-3.79	102.98	106.96
23	C	507	CLA	C3D-C4D-ND	3.78	116.35	110.24
26	A	410	SQD	C44-O6-C1	-3.78	106.36	113.74
23	B	606	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
23	a	409	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
23	b	606	CLA	O2D-CGD-O1D	-3.77	116.46	123.84
23	A	405	CLA	CBC-CAC-C3C	-3.77	102.04	112.43
23	C	511	CLA	C3B-C4B-NB	3.77	114.08	109.21
24	a	417	PHO	C4-C3-C5	3.76	121.59	115.27
23	B	608	CLA	C4A-NA-C1A	-3.75	105.02	106.71
23	b	604	CLA	C3D-C4D-ND	3.75	116.31	110.24
23	b	608	CLA	CMC-C2C-C1C	3.75	130.75	125.04
23	D	403	CLA	O2D-CGD-O1D	-3.75	116.51	123.84
23	b	604	CLA	CMC-C2C-C1C	3.75	130.75	125.04
23	c	512	CLA	C4A-NA-C1A	-3.75	105.02	106.71
23	b	608	CLA	C3C-C4C-NC	3.75	114.77	110.57
23	C	508	CLA	C1-C2-C3	-3.75	119.56	126.04
32	Z	101	LMG	C1-C2-C3	3.75	117.80	110.00
25	d	403	BCR	C38-C26-C25	-3.74	120.32	124.53
23	b	616	CLA	O2A-CGA-CBA	3.74	123.65	111.91
23	B	603	CLA	C1C-C2C-C3C	-3.74	103.02	106.96
26	A	410	SQD	O47-C7-C8	3.74	119.56	111.50
29	a	415	PL9	C15-C14-C16	3.74	121.56	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	F	103	SQD	O8-S-C6	3.74	111.69	105.74
23	A	406	CLA	C1D-CHD-C4C	-3.73	118.01	126.06
23	b	611	CLA	C3B-C4B-NB	3.73	114.03	109.21
23	b	612	CLA	CMC-C2C-C1C	3.73	130.72	125.04
23	b	612	CLA	C4-C3-C5	3.72	121.53	115.27
23	A	404	CLA	C3D-C4D-ND	3.72	116.25	110.24
23	C	513	CLA	C1D-CHD-C4C	-3.72	118.04	126.06
23	b	612	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
23	B	615	CLA	O2D-CGD-CBD	3.71	117.87	111.27
23	c	512	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
23	B	613	CLA	C4-C3-C5	3.71	121.51	115.27
23	C	511	CLA	O2D-CGD-O1D	-3.71	116.59	123.84
23	B	605	CLA	C4-C3-C5	3.71	121.50	115.27
23	D	403	CLA	CAC-C3C-C4C	3.70	129.62	124.81
23	B	607	CLA	C3B-C4B-NB	3.70	114.00	109.21
23	B	604	CLA	C3B-C4B-NB	3.70	113.99	109.21
35	C	516	DGD	O2G-C1B-C2B	3.69	119.46	111.50
23	c	508	CLA	C3D-C4D-ND	3.69	116.21	110.24
23	C	508	CLA	C1D-CHD-C4C	-3.69	118.10	126.06
23	c	511	CLA	C1D-CHD-C4C	-3.69	118.10	126.06
23	b	613	CLA	O2D-CGD-CBD	3.69	117.82	111.27
23	C	507	CLA	O2D-CGD-O1D	-3.68	116.64	123.84
23	b	605	CLA	C1D-CHD-C4C	-3.68	118.12	126.06
33	L	101	LHG	O7-C7-C8	3.68	119.43	111.50
26	A	412	SQD	O47-C7-C8	3.68	119.43	111.50
23	c	503	CLA	C3B-C4B-NB	3.68	113.97	109.21
23	B	612	CLA	C4C-C3C-C2C	-3.67	101.55	106.90
29	A	414	PL9	C37-C38-C39	-3.67	118.82	127.66
23	d	402	CLA	O2D-CGD-O1D	-3.67	116.66	123.84
23	b	602	CLA	CMC-C2C-C1C	3.67	130.62	125.04
23	B	616	CLA	C3B-C4B-NB	3.67	113.95	109.21
25	d	403	BCR	C40-C30-C25	-3.67	104.35	110.30
23	a	405	CLA	O2A-CGA-O1A	-3.67	114.34	123.59
23	B	613	CLA	C3B-C4B-NB	3.66	113.95	109.21
40	v	201	HEC	CMC-C2C-C1C	-3.66	122.84	128.46
23	b	614	CLA	C1-C2-C3	-3.65	119.73	126.04
23	a	405	CLA	CMB-C2B-C3B	3.65	131.51	124.68
23	b	602	CLA	CAA-C2A-C3A	-3.65	102.79	112.78
23	c	504	CLA	O2D-CGD-O1D	-3.65	116.71	123.84
23	c	505	CLA	C3B-C4B-NB	3.64	113.92	109.21
23	b	604	CLA	CAC-C3C-C4C	3.64	129.54	124.81
23	B	611	CLA	C1-C2-C3	-3.64	119.75	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	603	CLA	O2D-CGD-O1D	-3.64	116.72	123.84
23	B	603	CLA	CAA-C2A-C3A	-3.64	102.81	112.78
23	B	614	CLA	C3B-C4B-NB	3.64	113.91	109.21
23	d	402	CLA	C1D-CHD-C4C	-3.64	118.21	126.06
23	B	612	CLA	CMC-C2C-C1C	3.64	130.57	125.04
23	b	612	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
23	b	602	CLA	C1D-CHD-C4C	-3.63	118.22	126.06
23	b	601	CLA	O2D-CGD-O1D	-3.63	116.74	123.84
26	a	411	SQD	O9-S-C6	3.63	111.25	106.94
23	b	608	CLA	C1D-CHD-C4C	-3.63	118.23	126.06
25	Y	101	BCR	C15-C14-C13	-3.62	122.14	127.31
23	D	402	CLA	C3B-C4B-NB	3.62	113.89	109.21
23	B	607	CLA	O2D-CGD-O1D	-3.62	116.76	123.84
23	A	405	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
25	y	101	BCR	C15-C14-C13	-3.62	122.15	127.31
23	d	402	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
23	B	614	CLA	C1D-CHD-C4C	-3.61	118.27	126.06
26	F	103	SQD	C44-O6-C1	-3.61	106.69	113.74
23	B	616	CLA	CAC-C3C-C4C	3.60	129.48	124.81
32	A	419	LMG	O1-C1-C2	3.60	113.92	108.30
23	b	613	CLA	C3B-C4B-NB	3.60	113.86	109.21
23	B	610	CLA	C1D-CHD-C4C	-3.60	118.30	126.06
23	C	506	CLA	C3C-C4C-NC	3.60	114.61	110.57
23	B	605	CLA	CHD-C4C-NC	3.59	129.86	124.20
23	C	510	CLA	C3C-C4C-NC	3.59	114.59	110.57
23	A	405	CLA	O2D-CGD-O1D	-3.58	116.83	123.84
23	c	502	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
25	B	618	BCR	C29-C30-C25	3.58	116.00	110.48
34	b	625	HTG	O5-C5-C4	3.58	116.20	109.69
23	c	514	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
26	a	413	SQD	O47-C7-C8	3.58	119.22	111.50
25	T	102	BCR	C11-C10-C9	-3.58	122.20	127.31
25	h	101	BCR	C38-C26-C25	-3.58	120.51	124.53
23	d	401	CLA	C3B-C4B-NB	3.58	113.84	109.21
23	B	611	CLA	C4C-C3C-C2C	-3.58	101.68	106.90
23	c	507	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
23	c	509	CLA	C1D-CHD-C4C	-3.57	118.35	126.06
23	c	511	CLA	C3B-C4B-NB	3.57	113.83	109.21
23	B	613	CLA	C3D-C4D-ND	3.57	116.01	110.24
23	b	605	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
23	b	608	CLA	C1-C2-C3	-3.57	119.87	126.04
23	b	609	CLA	C1D-CHD-C4C	-3.57	118.36	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	513	CLA	C1-C2-C3	-3.57	119.87	126.04
25	B	617	BCR	C33-C5-C6	-3.57	120.52	124.53
23	C	508	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
25	K	101	BCR	C7-C8-C9	-3.56	120.85	126.23
23	B	615	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
23	d	401	CLA	C1-C2-C3	-3.56	119.89	126.04
23	C	505	CLA	CAC-C3C-C4C	3.56	129.42	124.81
23	B	611	CLA	C2A-C1A-CHA	-3.56	117.64	123.86
23	C	509	CLA	C1D-CHD-C4C	-3.55	118.39	126.06
23	b	610	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
25	D	404	BCR	C28-C27-C26	-3.55	107.74	114.08
23	C	502	CLA	C1D-CHD-C4C	-3.55	118.41	126.06
29	d	404	PL9	C40-C39-C41	3.55	121.23	115.27
29	a	415	PL9	C27-C28-C29	-3.54	119.13	127.66
38	f	101	HEM	C1B-NB-C4B	3.54	108.73	105.07
23	C	502	CLA	O2D-CGD-O1D	-3.54	116.92	123.84
23	b	616	CLA	CHD-C4C-NC	3.53	129.77	124.20
23	A	404	CLA	O2D-CGD-CBD	3.53	117.54	111.27
23	c	514	CLA	C3B-C4B-NB	3.53	113.77	109.21
23	b	614	CLA	C1C-C2C-C3C	-3.53	103.25	106.96
23	c	513	CLA	C3C-C4C-NC	3.53	114.53	110.57
23	b	601	CLA	C3C-C4C-NC	3.53	114.53	110.57
23	c	505	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
23	b	603	CLA	C3B-C4B-NB	3.52	113.77	109.21
23	a	409	CLA	C1D-CHD-C4C	-3.52	118.46	126.06
23	c	509	CLA	C3B-C4B-NB	3.52	113.76	109.21
23	A	408	CLA	C1D-CHD-C4C	-3.52	118.46	126.06
23	b	615	CLA	O2D-CGD-CBD	3.52	117.52	111.27
23	B	608	CLA	O2D-CGD-O1D	-3.52	116.96	123.84
23	C	507	CLA	C1C-C2C-C3C	-3.52	103.26	106.96
29	A	414	PL9	C22-C23-C24	-3.52	119.19	127.66
23	B	612	CLA	CMB-C2B-C3B	3.51	131.25	124.68
29	A	414	PL9	C15-C14-C16	3.51	121.18	115.27
23	B	608	CLA	C1C-C2C-C3C	-3.51	103.27	106.96
23	A	404	CLA	C1D-CHD-C4C	-3.51	118.49	126.06
23	b	605	CLA	CHD-C4C-NC	3.50	129.72	124.20
25	K	101	BCR	C15-C14-C13	-3.50	122.31	127.31
23	c	508	CLA	C4-C3-C5	3.50	121.16	115.27
29	D	405	PL9	C53-C6-C1	3.50	122.15	114.99
23	c	507	CLA	C1-C2-C3	-3.50	119.99	126.04
32	C	519	LMG	C3-C4-C5	3.50	116.48	110.24
23	c	504	CLA	C1C-C2C-C3C	-3.49	103.29	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	407	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
23	c	505	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
23	C	508	CLA	C4C-C3C-C2C	-3.49	101.81	106.90
34	B	622	HTG	C1'-S1-C1	3.49	106.61	100.09
29	a	415	PL9	C30-C29-C31	3.48	121.13	115.27
23	A	404	CLA	O2A-CGA-CBA	3.48	122.83	111.91
25	D	404	BCR	C38-C26-C25	-3.48	120.62	124.53
29	D	405	PL9	C42-C43-C44	-3.47	119.29	127.66
23	c	512	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
23	c	511	CLA	CMC-C2C-C1C	3.47	130.33	125.04
23	a	409	CLA	CAA-C2A-C3A	-3.47	103.27	112.78
23	b	608	CLA	CAC-C3C-C4C	3.47	129.31	124.81
23	a	405	CLA	O2D-CGD-CBD	3.47	117.43	111.27
23	b	614	CLA	C3B-C4B-NB	3.47	113.69	109.21
23	B	607	CLA	C4-C3-C5	3.47	121.10	115.27
25	c	515	BCR	C15-C14-C13	-3.46	122.37	127.31
23	A	406	CLA	O2A-CGA-O1A	-3.46	114.85	123.59
23	d	401	CLA	O2A-CGA-CBA	3.46	122.77	111.91
23	B	602	CLA	CAA-C2A-C3A	-3.46	103.31	112.78
23	B	607	CLA	C1D-CHD-C4C	-3.46	118.60	126.06
23	B	609	CLA	C1D-CHD-C4C	-3.45	118.61	126.06
34	V	202	HTG	C1-O5-C5	3.45	116.87	112.19
23	B	606	CLA	O2D-CGD-O1D	-3.45	117.09	123.84
34	b	622	HTG	O2-C2-C1	3.45	116.60	110.27
23	C	502	CLA	C1-C2-C3	-3.44	120.09	126.04
23	B	604	CLA	C3D-C4D-ND	3.44	115.81	110.24
25	T	102	BCR	C15-C16-C17	-3.44	116.42	123.47
23	c	506	CLA	C1D-CHD-C4C	-3.44	118.64	126.06
23	C	506	CLA	C3B-C4B-NB	3.44	113.66	109.21
23	B	610	CLA	C4C-C3C-C2C	-3.43	101.89	106.90
23	B	616	CLA	CMB-C2B-C3B	3.43	131.10	124.68
23	b	613	CLA	C1D-CHD-C4C	-3.43	118.67	126.06
23	b	615	CLA	C3B-C4B-NB	3.43	113.64	109.21
34	b	622	HTG	C1'-S1-C1	3.42	106.50	100.09
23	c	511	CLA	C4-C3-C5	3.42	121.03	115.27
23	B	607	CLA	CBC-CAC-C3C	-3.42	103.00	112.43
23	b	603	CLA	CAA-C2A-C3A	-3.42	103.41	112.78
23	b	610	CLA	CAA-C2A-C3A	-3.42	103.41	112.78
23	B	611	CLA	O2D-CGD-O1D	-3.42	117.15	123.84
23	B	602	CLA	C3B-C4B-NB	3.41	113.62	109.21
23	a	405	CLA	O2A-CGA-CBA	3.41	122.61	111.91
23	b	604	CLA	O2D-CGD-O1D	-3.41	117.17	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	606	CLA	C4-C3-C5	3.41	121.01	115.27
29	a	415	PL9	C35-C34-C36	3.41	121.01	115.27
23	c	506	CLA	C1C-C2C-C3C	-3.41	103.37	106.96
23	C	506	CLA	C1D-CHD-C4C	-3.40	118.72	126.06
23	b	609	CLA	C3B-C4B-NB	3.40	113.61	109.21
40	V	201	HEC	CMC-C2C-C1C	-3.40	123.24	128.46
23	b	612	CLA	C4C-C3C-C2C	-3.40	101.95	106.90
23	b	609	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
23	b	613	CLA	C3D-C4D-ND	3.39	115.73	110.24
23	b	609	CLA	CAC-C3C-C4C	3.39	129.21	124.81
23	c	506	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
23	A	406	CLA	C3B-C4B-NB	3.39	113.59	109.21
29	D	405	PL9	C25-C24-C26	3.39	120.97	115.27
23	B	603	CLA	CMB-C2B-C3B	3.39	131.01	124.68
34	B	622	HTG	O5-C1-C2	3.39	114.57	110.31
23	B	613	CLA	C1D-CHD-C4C	-3.38	118.76	126.06
32	Z	101	LMG	O6-C1-C2	3.38	117.51	110.35
23	b	608	CLA	O2D-CGD-O1D	-3.38	117.23	123.84
23	c	506	CLA	CAC-C3C-C4C	3.38	129.19	124.81
23	B	615	CLA	C3B-C4B-NB	3.38	113.57	109.21
23	b	601	CLA	C1C-C2C-C3C	-3.38	103.41	106.96
32	z	101	LMG	O7-C10-C11	3.37	118.77	111.50
35	c	518	DGD	O2G-C1B-C2B	3.37	118.77	111.50
23	b	616	CLA	C4C-C3C-C2C	-3.37	101.99	106.90
23	B	601	CLA	C1C-C2C-C3C	-3.36	103.42	106.96
23	c	506	CLA	C4C-C3C-C2C	-3.36	102.00	106.90
23	C	512	CLA	C4-C3-C5	3.36	120.93	115.27
23	a	409	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
25	A	409	BCR	C24-C23-C22	-3.36	121.16	126.23
23	B	605	CLA	C4C-C3C-C2C	-3.36	102.00	106.90
23	B	608	CLA	C1D-CHD-C4C	-3.36	118.81	126.06
23	b	610	CLA	C4C-C3C-C2C	-3.36	102.01	106.90
23	C	509	CLA	C3B-C4B-NB	3.35	113.55	109.21
25	D	404	BCR	C29-C30-C25	3.35	115.64	110.48
25	D	404	BCR	C10-C11-C12	-3.35	112.76	123.22
24	A	416	PHO	CMC-C2C-C3C	3.35	131.26	124.94
23	b	612	CLA	O2A-CGA-O1A	-3.35	115.14	123.59
23	b	606	CLA	C3B-C4B-NB	3.34	113.53	109.21
23	C	508	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
25	B	617	BCR	C7-C8-C9	-3.34	121.19	126.23
23	b	611	CLA	O2D-CGD-O1D	-3.33	117.32	123.84
25	b	618	BCR	C15-C14-C13	-3.33	122.56	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	401	CLA	C1D-CHD-C4C	-3.33	118.87	126.06
23	B	608	CLA	C4C-C3C-C2C	-3.33	102.05	106.90
23	A	405	CLA	C3B-C4B-NB	3.33	113.51	109.21
23	C	506	CLA	C1-C2-C3	-3.32	120.30	126.04
23	B	615	CLA	CED-O2D-CGD	3.32	123.45	115.94
23	D	403	CLA	C4C-C3C-C2C	-3.32	102.06	106.90
23	C	510	CLA	C4-C3-C5	3.32	120.85	115.27
24	A	407	PHO	CMA-C3A-C4A	-3.32	107.11	114.38
23	b	615	CLA	C4-C3-C5	3.31	120.85	115.27
23	C	505	CLA	C1-C2-C3	-3.31	120.31	126.04
26	f	102	SQD	O5-C1-C2	3.31	117.36	110.35
23	C	507	CLA	C4C-C3C-C2C	-3.31	102.07	106.90
25	t	102	BCR	C11-C10-C9	-3.31	122.58	127.31
23	C	506	CLA	CMC-C2C-C1C	3.31	130.08	125.04
23	B	603	CLA	C3B-C4B-NB	3.31	113.48	109.21
23	b	608	CLA	CMB-C2B-C3B	3.30	130.86	124.68
23	B	610	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
23	C	509	CLA	CMC-C2C-C1C	3.30	130.07	125.04
35	h	102	DGD	O2G-C1B-C2B	3.30	118.61	111.50
26	F	103	SQD	C1-C2-C3	-3.30	103.13	110.00
23	b	602	CLA	C1C-C2C-C3C	-3.30	103.49	106.96
33	d	411	LHG	O8-C23-O10	-3.30	115.27	123.59
23	A	408	CLA	CAA-C2A-C3A	-3.30	103.75	112.78
33	d	406	LHG	O7-C7-C8	3.29	118.59	111.50
23	b	615	CLA	C11-C10-C8	-3.29	105.29	115.92
25	b	619	BCR	C24-C23-C22	-3.29	121.27	126.23
23	C	510	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
23	B	605	CLA	C1C-C2C-C3C	-3.29	103.50	106.96
23	c	509	CLA	C4C-C3C-C2C	-3.29	102.11	106.90
23	C	501	CLA	CMC-C2C-C1C	3.28	130.04	125.04
23	b	602	CLA	CAC-C3C-C4C	3.28	129.07	124.81
23	C	513	CLA	C1-C2-C3	-3.28	120.37	126.04
32	C	518	LMG	O8-C28-C29	3.28	122.20	111.91
23	C	511	CLA	C4-C3-C5	3.28	120.78	115.27
23	c	513	CLA	C1C-C2C-C3C	-3.28	103.51	106.96
23	B	611	CLA	CHB-C4A-NA	3.28	129.04	124.51
23	B	612	CLA	CAC-C3C-C4C	3.27	129.06	124.81
40	V	201	HEC	CMB-C2B-C1B	-3.27	123.43	128.46
26	b	620	SQD	C3-C4-C5	3.27	116.07	110.24
23	c	510	CLA	CAC-C3C-C4C	3.27	129.05	124.81
23	C	505	CLA	C4C-C3C-C2C	-3.26	102.14	106.90
23	b	613	CLA	C1-C2-C3	-3.26	120.40	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	604	CLA	C1D-CHD-C4C	-3.26	119.03	126.06
23	b	611	CLA	C1D-CHD-C4C	-3.26	119.03	126.06
26	B	620	SQD	O7-S-C6	3.26	110.81	106.94
23	b	607	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
23	B	606	CLA	C3B-C4B-NB	3.26	113.42	109.21
23	B	610	CLA	C1C-C2C-C3C	-3.26	103.53	106.96
23	a	406	CLA	C3B-C4B-NB	3.25	113.42	109.21
23	B	608	CLA	CHC-C1C-C2C	-3.25	117.72	126.72
23	b	603	CLA	C4-C3-C5	3.25	120.74	115.27
23	B	612	CLA	C4A-NA-C1A	-3.25	105.25	106.71
23	a	409	CLA	C4-C3-C5	3.25	120.74	115.27
23	A	404	CLA	CMB-C2B-C3B	3.25	130.75	124.68
33	d	411	LHG	O7-C7-C8	3.25	118.50	111.50
23	B	608	CLA	C1-C2-C3	-3.25	120.43	126.04
23	b	613	CLA	O2A-CGA-O1A	-3.25	115.40	123.59
32	B	621	LMG	O8-C28-C29	3.24	122.09	111.91
23	C	505	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
23	c	507	CLA	CHC-C1C-C2C	-3.24	117.75	126.72
32	a	418	LMG	C8-O7-C10	-3.24	109.81	117.79
25	a	410	BCR	C38-C26-C25	-3.24	120.89	124.53
23	C	503	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
23	C	510	CLA	CHD-C4C-NC	3.24	129.31	124.20
23	c	512	CLA	C4-C3-C5	3.24	120.72	115.27
23	B	614	CLA	CAC-C3C-C4C	3.24	129.01	124.81
23	a	409	CLA	C3B-C4B-NB	3.24	113.39	109.21
23	B	608	CLA	CMA-C3A-C4A	-3.24	103.07	111.77
23	c	505	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
23	b	613	CLA	O2A-CGA-CBA	3.23	122.05	111.91
23	B	607	CLA	CMC-C2C-C1C	3.23	129.96	125.04
23	A	408	CLA	C1-C2-C3	-3.22	120.47	126.04
25	k	101	BCR	C7-C8-C9	-3.22	121.36	126.23
24	a	417	PHO	C4A-C3A-C2A	-3.22	99.77	102.84
25	h	101	BCR	C7-C8-C9	-3.22	121.38	126.23
33	d	411	LHG	O8-C23-C24	3.22	122.00	111.91
25	y	101	BCR	C38-C26-C25	-3.22	120.92	124.53
23	B	610	CLA	C3B-C4B-NB	3.22	113.37	109.21
38	F	102	HEM	CBD-CAD-C3D	-3.21	103.70	112.63
23	c	502	CLA	C1D-CHD-C4C	-3.21	119.13	126.06
23	C	509	CLA	CMB-C2B-C3B	3.21	130.69	124.68
23	c	509	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
23	B	601	CLA	O2D-CGD-O1D	-3.20	117.57	123.84
23	a	405	CLA	CHC-C1C-C2C	-3.20	117.86	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	504	CLA	C1D-CHD-C4C	-3.20	119.15	126.06
23	B	615	CLA	CMC-C2C-C1C	3.20	129.91	125.04
23	a	407	CLA	C3B-C4B-NB	3.20	113.34	109.21
38	F	102	HEM	CHD-C1D-ND	3.20	127.90	124.43
23	c	503	CLA	CHC-C1C-C2C	-3.19	117.89	126.72
23	b	607	CLA	C4C-C3C-C2C	-3.19	102.24	106.90
23	C	504	CLA	CMC-C2C-C1C	3.19	129.90	125.04
23	b	615	CLA	CHC-C1C-C2C	-3.19	117.89	126.72
23	a	405	CLA	CAA-C2A-C1A	-3.19	101.52	111.97
23	B	601	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
23	B	614	CLA	O2A-CGA-O1A	-3.19	115.55	123.59
29	a	415	PL9	C17-C18-C19	-3.19	119.99	127.66
38	f	101	HEM	CHA-C4D-ND	3.19	128.32	124.38
23	B	603	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
23	A	408	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
26	A	412	SQD	O8-S-C6	3.18	110.81	105.74
25	a	410	BCR	C40-C30-C25	-3.18	105.14	110.30
23	c	502	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
23	A	406	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
23	b	603	CLA	C2A-C1A-CHA	-3.18	118.30	123.86
23	C	512	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
29	A	414	PL9	C27-C28-C29	-3.18	120.01	127.66
23	C	512	CLA	CHD-C4C-NC	3.18	129.21	124.20
23	B	609	CLA	CBC-CAC-C3C	-3.18	103.68	112.43
23	b	610	CLA	O2D-CGD-O1D	-3.17	117.63	123.84
23	C	502	CLA	CHC-C1C-C2C	-3.17	117.95	126.72
29	a	415	PL9	C25-C24-C26	3.17	120.61	115.27
23	A	404	CLA	O2A-CGA-O1A	-3.17	115.59	123.59
23	D	402	CLA	C1D-CHD-C4C	-3.17	119.22	126.06
23	c	503	CLA	CHD-C4C-NC	3.17	129.20	124.20
25	b	619	BCR	C11-C10-C9	-3.17	122.79	127.31
23	c	510	CLA	CHC-C1C-C2C	-3.17	117.96	126.72
23	C	504	CLA	CAC-C3C-C4C	3.16	128.92	124.81
31	A	417	LMT	O5B-C5B-C4B	3.16	115.44	109.69
23	B	612	CLA	C1D-CHD-C4C	-3.16	119.24	126.06
25	H	101	BCR	C16-C17-C18	-3.16	122.80	127.31
23	b	609	CLA	C4C-C3C-C2C	-3.16	102.30	106.90
23	b	613	CLA	C4C-C3C-C2C	-3.16	102.30	106.90
26	B	620	SQD	O9-S-C6	3.16	110.69	106.94
25	c	516	BCR	C7-C8-C9	-3.16	121.47	126.23
23	a	409	CLA	C4C-C3C-C2C	-3.15	102.30	106.90
23	C	506	CLA	O2D-CGD-O1D	-3.15	117.67	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	416	PHO	C4-C3-C5	3.15	120.58	115.27
23	b	605	CLA	C4C-C3C-C2C	-3.15	102.30	106.90
23	a	406	CLA	CHD-C4C-NC	3.15	129.17	124.20
33	A	420	LHG	C5-O7-C7	-3.15	110.03	117.79
33	A	420	LHG	O8-C23-C24	3.15	121.79	111.91
29	D	405	PL9	C17-C18-C19	-3.15	120.08	127.66
25	c	515	BCR	C16-C17-C18	-3.14	122.82	127.31
23	B	604	CLA	CHC-C1C-C2C	-3.14	118.03	126.72
23	B	606	CLA	O2A-CGA-O1A	-3.14	115.67	123.59
23	b	611	CLA	C1-C2-C3	-3.14	120.61	126.04
23	b	616	CLA	O2A-CGA-O1A	-3.14	115.67	123.59
23	B	616	CLA	CMC-C2C-C1C	3.14	129.82	125.04
23	c	504	CLA	C3B-C4B-NB	3.13	113.26	109.21
23	B	614	CLA	CMC-C2C-C1C	3.13	129.81	125.04
26	A	412	SQD	O48-C23-C24	3.13	121.74	111.91
23	C	506	CLA	CAC-C3C-C4C	3.13	128.87	124.81
23	b	611	CLA	C1C-C2C-C3C	-3.13	103.67	106.96
23	a	407	CLA	CHD-C4C-NC	3.13	129.13	124.20
23	c	504	CLA	C4C-C3C-C2C	-3.13	102.34	106.90
23	b	609	CLA	CBC-CAC-C3C	-3.13	103.81	112.43
23	a	407	CLA	C1-C2-C3	-3.13	120.64	126.04
23	d	401	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
26	a	413	SQD	O48-C23-C24	3.12	121.70	111.91
29	D	405	PL9	C51-C49-C50	3.12	121.49	114.60
23	C	503	CLA	C4C-C3C-C2C	-3.12	102.36	106.90
23	b	614	CLA	CHC-C1C-C2C	-3.11	118.11	126.72
23	c	510	CLA	O2A-CGA-CBA	3.11	121.67	111.91
23	C	503	CLA	C1-C2-C3	-3.11	120.66	126.04
23	C	506	CLA	CBC-CAC-C3C	-3.11	103.86	112.43
23	C	509	CLA	O2A-CGA-CBA	3.11	121.66	111.91
25	y	101	BCR	C24-C23-C22	-3.11	121.54	126.23
23	B	603	CLA	C4-C3-C5	3.11	120.50	115.27
29	D	405	PL9	C10-C9-C11	3.11	120.50	115.27
23	B	603	CLA	CMC-C2C-C1C	3.11	129.77	125.04
23	D	403	CLA	C1C-C2C-C3C	-3.10	103.69	106.96
31	b	627	LMT	C3'-C4'-C5'	-3.10	103.81	110.93
23	B	609	CLA	C3B-C4B-NB	3.10	113.22	109.21
23	D	403	CLA	CMC-C2C-C1C	3.10	129.76	125.04
23	c	513	CLA	O2A-CGA-CBA	3.10	121.64	111.91
23	c	512	CLA	CHD-C4C-NC	3.10	129.09	124.20
23	B	612	CLA	C1C-C2C-C3C	-3.10	103.70	106.96
40	V	201	HEC	C1D-C2D-C3D	-3.10	104.84	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	611	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
29	A	414	PL9	C10-C9-C11	3.10	120.48	115.27
38	F	102	HEM	CHB-C1B-NB	3.09	128.20	124.38
23	B	613	CLA	O2A-CGA-O1A	-3.09	115.78	123.59
33	b	630	LHG	O7-C7-C8	3.09	118.16	111.50
23	b	609	CLA	CMC-C2C-C1C	3.09	129.75	125.04
23	b	610	CLA	O2A-CGA-O1A	-3.09	115.79	123.59
23	c	502	CLA	C3B-C4B-NB	3.09	113.20	109.21
23	b	601	CLA	C3B-C4B-NB	3.09	113.20	109.21
23	C	505	CLA	C3B-C4B-NB	3.09	113.20	109.21
24	a	417	PHO	CMB-C2B-C3B	3.08	130.44	124.68
29	a	415	PL9	C10-C9-C11	3.08	120.45	115.27
23	b	614	CLA	O2A-CGA-O1A	-3.08	115.82	123.59
25	K	101	BCR	C33-C5-C6	-3.08	121.07	124.53
23	b	601	CLA	C4-C3-C5	3.08	120.45	115.27
23	C	506	CLA	CHC-C1C-C2C	-3.07	118.22	126.72
23	C	513	CLA	CMC-C2C-C1C	3.07	129.72	125.04
25	K	103	BCR	C38-C26-C25	-3.07	121.08	124.53
23	c	513	CLA	C4-C3-C5	3.07	120.44	115.27
23	a	405	CLA	C1-C2-C3	-3.07	120.73	126.04
23	b	605	CLA	C1-C2-C3	-3.07	120.73	126.04
23	c	508	CLA	C1D-CHD-C4C	-3.07	119.44	126.06
23	B	605	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
23	C	512	CLA	C4C-C3C-C2C	-3.06	102.43	106.90
23	b	614	CLA	C4C-C3C-C2C	-3.06	102.43	106.90
23	b	607	CLA	C1D-CHD-C4C	-3.06	119.45	126.06
32	C	519	LMG	O8-C28-C29	3.06	121.52	111.91
23	B	604	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
23	b	601	CLA	CHD-C4C-NC	3.06	129.03	124.20
23	B	605	CLA	CED-O2D-CGD	3.06	122.85	115.94
23	c	503	CLA	CMC-C2C-C1C	3.06	129.69	125.04
29	d	404	PL9	C10-C9-C11	3.05	120.41	115.27
23	C	505	CLA	CMC-C2C-C1C	3.05	129.69	125.04
32	a	418	LMG	C7-O1-C1	-3.05	107.77	113.74
23	a	405	CLA	C4-C3-C5	3.05	120.41	115.27
23	c	509	CLA	CHC-C1C-C2C	-3.05	118.28	126.72
23	c	510	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
23	B	612	CLA	O2A-CGA-CBA	3.05	121.48	111.91
23	D	402	CLA	O2A-CGA-CBA	3.05	121.48	111.91
23	a	407	CLA	CMC-C2C-C1C	3.05	129.68	125.04
23	d	401	CLA	C2A-C1A-CHA	-3.05	118.53	123.86
23	d	401	CLA	C4C-C3C-C2C	-3.04	102.46	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	602	CLA	C2A-C1A-CHA	-3.04	118.54	123.86
26	b	620	SQD	O8-S-C6	3.04	110.59	105.74
23	B	605	CLA	CMC-C2C-C1C	3.04	129.67	125.04
23	d	402	CLA	C3B-C4B-NB	3.04	113.14	109.21
23	C	509	CLA	O2A-CGA-O1A	-3.04	115.92	123.59
23	A	408	CLA	CHC-C1C-C2C	-3.04	118.32	126.72
25	d	403	BCR	C10-C11-C12	-3.04	113.73	123.22
29	A	414	PL9	C20-C19-C21	3.04	120.38	115.27
25	B	619	BCR	C24-C23-C22	-3.04	121.65	126.23
23	B	614	CLA	CHC-C1C-C2C	-3.03	118.33	126.72
23	b	607	CLA	CHC-C1C-C2C	-3.03	118.33	126.72
23	B	610	CLA	O2A-CGA-O1A	-3.03	115.94	123.59
23	B	609	CLA	O2A-CGA-CBA	3.03	121.42	111.91
23	d	401	CLA	O2A-CGA-O1A	-3.03	115.94	123.59
23	A	406	CLA	O2A-CGA-CBA	3.03	121.42	111.91
23	C	501	CLA	CHD-C4C-NC	3.03	128.97	124.20
26	B	620	SQD	O48-C23-C24	3.03	121.41	111.91
23	A	404	CLA	C1-C2-C3	-3.03	120.81	126.04
23	b	602	CLA	C4C-C3C-C2C	-3.02	102.49	106.90
23	d	401	CLA	C4-C3-C5	3.02	120.36	115.27
23	B	615	CLA	C4-C3-C5	3.02	120.36	115.27
29	d	404	PL9	C37-C38-C39	-3.02	120.38	127.66
25	K	103	BCR	C20-C21-C22	-3.02	123.00	127.31
34	B	625	HTG	C1'-S1-C1	3.02	105.74	100.09
23	b	613	CLA	CHC-C1C-C2C	-3.02	118.38	126.72
25	A	409	BCR	C38-C26-C25	-3.02	121.14	124.53
23	A	404	CLA	CAA-C2A-C1A	-3.01	102.09	111.97
23	C	504	CLA	O2D-CGD-O1D	-3.01	117.94	123.84
23	C	503	CLA	CHD-C4C-NC	3.01	128.95	124.20
23	C	510	CLA	CHC-C1C-C2C	-3.01	118.39	126.72
23	a	409	CLA	O2A-CGA-CBA	3.01	121.36	111.91
29	a	415	PL9	C42-C43-C44	-3.01	120.41	127.66
23	C	509	CLA	CAC-C3C-C4C	3.01	128.72	124.81
23	B	615	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
23	b	606	CLA	CHD-C4C-NC	3.01	128.95	124.20
33	d	405	LHG	O7-C7-C8	3.01	117.99	111.50
25	K	103	BCR	C24-C23-C22	-3.01	121.69	126.23
23	D	402	CLA	CAC-C3C-C4C	3.01	128.71	124.81
23	c	511	CLA	CMB-C2B-C3B	3.01	130.31	124.68
23	c	502	CLA	C1-C2-C3	-3.01	120.84	126.04
40	v	201	HEC	CBA-CAA-C2A	-3.01	107.54	112.60
23	D	403	CLA	C4-C3-C5	3.00	120.32	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	T	102	BCR	C15-C14-C13	3.00	131.59	127.31
23	c	511	CLA	CHD-C4C-NC	3.00	128.93	124.20
23	C	511	CLA	C4C-C3C-C2C	-3.00	102.52	106.90
23	A	404	CLA	CHC-C1C-C2C	-3.00	118.43	126.72
23	b	606	CLA	CHC-C1C-C2C	-3.00	118.43	126.72
23	A	405	CLA	CHD-C4C-NC	3.00	128.93	124.20
26	a	411	SQD	C45-O47-C7	-3.00	110.42	117.79
25	C	514	BCR	C33-C5-C6	-2.99	121.17	124.53
23	C	507	CLA	CHD-C4C-NC	2.99	128.92	124.20
23	c	512	CLA	CMC-C2C-C1C	2.99	129.60	125.04
23	b	608	CLA	CHC-C1C-C2C	-2.99	118.44	126.72
38	f	101	HEM	C4D-ND-C1D	2.99	108.16	105.07
32	Z	101	LMG	C4-C3-C2	2.99	116.04	110.82
23	B	614	CLA	CMB-C2B-C3B	2.99	130.26	124.68
23	c	513	CLA	CHD-C4C-NC	2.98	128.91	124.20
23	C	511	CLA	CAC-C3C-C4C	2.98	128.68	124.81
33	D	407	LHG	O8-C23-C24	2.98	121.27	111.91
31	M	101	LMT	C1'-O5'-C5'	-2.98	107.84	113.69
23	B	609	CLA	CHC-C1C-C2C	-2.98	118.49	126.72
32	c	521	LMG	C9-C8-C7	-2.98	104.75	111.79
26	a	413	SQD	O7-S-C6	2.97	110.47	106.94
33	E	101	LHG	O8-C23-C24	2.97	121.23	111.91
23	A	408	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
23	c	510	CLA	CMB-C2B-C3B	2.97	130.24	124.68
23	C	504	CLA	C1-O2A-CGA	2.97	124.23	116.44
23	B	602	CLA	CAC-C3C-C4C	2.97	128.66	124.81
23	C	501	CLA	C3B-C4B-NB	2.97	113.05	109.21
23	B	606	CLA	CMC-C2C-C1C	2.96	129.55	125.04
23	c	506	CLA	C3B-C4B-NB	2.96	113.04	109.21
23	b	605	CLA	O2A-CGA-O1A	-2.96	116.12	123.59
23	a	406	CLA	CHC-C1C-C2C	-2.96	118.53	126.72
23	b	613	CLA	CMA-C3A-C4A	-2.96	103.82	111.77
23	b	616	CLA	CBC-CAC-C3C	-2.96	104.27	112.43
32	m	101	LMG	O8-C28-C29	2.96	121.20	111.91
24	A	407	PHO	O1D-CGD-CBD	-2.96	119.81	124.74
23	C	503	CLA	C4-C3-C5	2.96	120.24	115.27
23	B	616	CLA	C1C-C2C-C3C	-2.96	103.85	106.96
23	D	403	CLA	C3B-C4B-NB	2.96	113.03	109.21
38	f	101	HEM	CHD-C1D-ND	2.95	127.64	124.43
23	C	511	CLA	CHC-C1C-C2C	-2.95	118.55	126.72
31	B	628	LMT	C4B-C3B-C2B	2.95	115.98	110.82
23	b	603	CLA	CMC-C2C-C1C	2.95	129.53	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	603	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
23	B	613	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
23	B	605	CLA	O2A-CGA-O1A	-2.95	116.16	123.59
23	C	503	CLA	O2A-CGA-O1A	-2.95	116.16	123.59
26	A	410	SQD	O9-S-C6	2.95	110.44	106.94
23	b	612	CLA	O2A-CGA-CBA	2.95	121.15	111.91
23	B	606	CLA	O2A-CGA-CBA	2.94	121.14	111.91
29	A	414	PL9	C30-C29-C31	2.94	120.22	115.27
25	k	101	BCR	C24-C23-C22	-2.94	121.79	126.23
23	b	616	CLA	C3B-C4B-NB	2.94	113.01	109.21
23	d	402	CLA	C4-C3-C5	2.94	120.22	115.27
25	c	516	BCR	C32-C1-C6	-2.94	105.53	110.30
23	d	402	CLA	CHD-C4C-NC	2.94	128.83	124.20
23	c	510	CLA	C1-O2A-CGA	2.94	124.15	116.44
33	a	421	LHG	O7-C7-C8	2.94	117.83	111.50
23	c	510	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
23	b	608	CLA	CBC-CAC-C3C	-2.94	104.34	112.43
23	A	406	CLA	CHD-C4C-NC	2.93	128.83	124.20
29	A	414	PL9	C17-C18-C19	-2.93	120.59	127.66
23	b	612	CLA	CMB-C2B-C3B	2.93	130.17	124.68
33	D	406	LHG	O8-C23-O10	-2.93	116.19	123.59
29	d	404	PL9	C22-C23-C24	-2.93	120.60	127.66
23	B	603	CLA	O2A-CGA-O1A	-2.93	116.19	123.59
23	C	508	CLA	CHC-C1C-C2C	-2.93	118.61	126.72
23	C	505	CLA	C4-C3-C5	2.93	120.20	115.27
25	C	514	BCR	C11-C10-C9	-2.93	123.13	127.31
29	d	404	PL9	C27-C28-C29	-2.93	120.61	127.66
23	d	402	CLA	CAA-C2A-C3A	-2.93	104.77	112.78
23	A	404	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
23	C	512	CLA	CMC-C2C-C1C	2.92	129.49	125.04
23	B	613	CLA	CMB-C2B-C3B	2.92	130.15	124.68
23	B	609	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
23	a	406	CLA	CBC-CAC-C3C	-2.92	104.38	112.43
23	B	607	CLA	CAA-C2A-C3A	-2.92	104.78	112.78
26	F	103	SQD	O7-S-C6	2.92	110.41	106.94
23	A	406	CLA	CAA-C2A-C3A	-2.92	104.78	112.78
35	h	102	DGD	O1G-C1A-C2A	2.92	121.06	111.91
25	K	103	BCR	C7-C8-C9	-2.92	121.83	126.23
29	d	404	PL9	C53-C6-C1	2.92	120.95	114.99
40	V	201	HEC	CBA-CAA-C2A	-2.92	107.69	112.60
29	a	415	PL9	C22-C23-C24	-2.92	120.64	127.66
23	b	613	CLA	C4-C3-C5	2.91	120.17	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	408	CLA	O2A-CGA-CBA	2.91	121.05	111.91
23	c	511	CLA	CBC-CAC-C3C	-2.91	104.40	112.43
23	c	504	CLA	CMC-C2C-C1C	2.91	129.47	125.04
23	c	514	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
26	A	410	SQD	O48-C23-C24	2.91	121.04	111.91
23	C	513	CLA	CMB-C2B-C3B	2.91	130.12	124.68
33	D	407	LHG	O8-C23-O10	-2.91	116.25	123.59
23	B	615	CLA	CHD-C4C-NC	2.91	128.79	124.20
23	C	509	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
23	A	405	CLA	C4-C3-C5	2.91	120.16	115.27
23	a	405	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
23	C	511	CLA	C1-O2A-CGA	2.90	124.06	116.44
23	a	407	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
23	B	604	CLA	CMC-C2C-C1C	2.90	129.46	125.04
35	c	519	DGD	O1G-C1A-C2A	2.90	121.00	111.91
23	a	406	CLA	CMA-C3A-C2A	-2.90	102.14	113.83
23	B	614	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
23	A	405	CLA	CHC-C1C-C2C	-2.89	118.72	126.72
23	D	402	CLA	CHC-C1C-C2C	-2.89	118.72	126.72
23	D	403	CLA	CAA-C2A-C3A	-2.89	104.87	112.78
25	D	404	BCR	C37-C22-C23	2.89	122.63	118.08
23	D	402	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
23	B	611	CLA	C3B-C4B-NB	2.89	112.94	109.21
23	c	506	CLA	CMC-C2C-C1C	2.88	129.43	125.04
25	T	102	BCR	C16-C17-C18	-2.88	123.20	127.31
25	b	619	BCR	C38-C26-C25	-2.88	121.29	124.53
23	C	501	CLA	CBC-CAC-C3C	-2.87	104.51	112.43
23	B	612	CLA	O2A-CGA-O1A	-2.87	116.34	123.59
24	a	408	PHO	O2A-CGA-CBA	2.87	120.92	111.91
23	D	402	CLA	O2A-CGA-O1A	-2.87	116.35	123.59
23	B	603	CLA	CHD-C4C-NC	2.87	128.72	124.20
31	A	421	LMT	O5B-C5B-C4B	2.87	114.90	109.69
23	c	514	CLA	CAC-C3C-C4C	2.87	128.53	124.81
23	B	614	CLA	O2A-CGA-CBA	2.87	120.91	111.91
23	b	611	CLA	CHC-C1C-C2C	-2.87	118.79	126.72
23	b	603	CLA	O2A-CGA-O1A	-2.87	116.36	123.59
29	a	415	PL9	C37-C38-C39	-2.86	120.77	127.66
23	B	606	CLA	C4-C3-C5	2.86	120.09	115.27
23	b	605	CLA	C2A-C1A-CHA	-2.86	118.86	123.86
23	c	513	CLA	CHC-C1C-C2C	-2.86	118.81	126.72
23	C	507	CLA	CBC-CAC-C3C	-2.86	104.55	112.43
23	C	505	CLA	CHC-C1C-C2C	-2.86	118.81	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	601	CLA	C3B-C4B-NB	2.86	112.90	109.21
23	c	514	CLA	C1-C2-C3	-2.86	121.10	126.04
23	B	616	CLA	O2A-CGA-CBA	2.86	120.87	111.91
23	b	601	CLA	CHC-C1C-C2C	-2.85	118.83	126.72
24	a	408	PHO	C1A-C2A-C3A	-2.85	100.13	102.84
34	b	622	HTG	O5-C5-C4	2.85	114.87	109.69
23	B	614	CLA	CHD-C4C-NC	2.85	128.69	124.20
23	B	601	CLA	O2A-CGA-CBA	2.85	120.85	111.91
35	h	102	DGD	O1G-C1A-O1A	-2.85	116.40	123.59
23	c	507	CLA	CHD-C4C-NC	2.85	128.69	124.20
33	b	630	LHG	O8-C23-C24	2.85	120.84	111.91
23	B	613	CLA	O2A-CGA-CBA	2.84	120.83	111.91
23	C	511	CLA	C1-C2-C3	-2.84	121.13	126.04
23	b	607	CLA	C4-C3-C5	2.84	120.05	115.27
24	a	408	PHO	O1D-CGD-CBD	-2.84	120.01	124.74
25	T	102	BCR	C33-C5-C6	-2.84	121.34	124.53
23	c	512	CLA	CHC-C1C-C2C	-2.84	118.86	126.72
23	B	601	CLA	CHD-C4C-NC	2.84	128.68	124.20
23	B	606	CLA	CHD-C4C-NC	2.84	128.68	124.20
23	b	609	CLA	CHC-C1C-C2C	-2.84	118.87	126.72
23	b	601	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
23	c	510	CLA	C4-C3-C5	2.84	120.05	115.27
23	d	402	CLA	C4C-C3C-C2C	-2.84	102.77	106.90
23	c	504	CLA	C1-C2-C3	-2.83	121.14	126.04
23	c	513	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
26	f	102	SQD	C4-C3-C2	-2.83	105.88	110.82
23	B	609	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
23	c	512	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
23	c	502	CLA	CHC-C1C-C2C	-2.83	118.90	126.72
23	b	605	CLA	C3B-C4B-NB	2.83	112.86	109.21
23	C	502	CLA	C4C-C3C-C2C	-2.82	102.78	106.90
23	c	505	CLA	CHC-C1C-C2C	-2.82	118.92	126.72
25	T	102	BCR	C12-C13-C14	-2.82	114.61	118.94
23	b	610	CLA	CHD-C4C-NC	2.82	128.65	124.20
23	B	609	CLA	CMC-C2C-C1C	2.82	129.33	125.04
23	C	504	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
23	b	615	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
26	B	620	SQD	C4-C3-C2	2.82	115.74	110.82
40	v	201	HEC	C1D-C2D-C3D	-2.82	105.04	107.00
35	c	517	DGD	O3G-C3G-C2G	-2.82	104.11	110.90
23	B	603	CLA	CHC-C1C-C2C	-2.81	118.95	126.72
38	f	101	HEM	CHB-C1B-NB	2.81	127.85	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	615	CLA	CAC-C3C-C4C	2.81	128.45	124.81
23	B	604	CLA	C6-C7-C8	-2.81	106.84	115.92
24	a	417	PHO	CMC-C2C-C3C	2.81	130.23	124.94
23	c	511	CLA	O2A-CGA-O1A	-2.81	116.51	123.59
23	d	401	CLA	CHC-C1C-C2C	-2.80	118.97	126.72
23	b	603	CLA	CHD-C4C-NC	2.80	128.62	124.20
23	c	514	CLA	O2A-CGA-CBA	2.80	120.70	111.91
25	D	404	BCR	C40-C30-C25	-2.80	105.76	110.30
23	B	616	CLA	C1-O2A-CGA	2.80	123.79	116.44
23	C	506	CLA	C4-C3-C5	2.80	119.98	115.27
23	b	603	CLA	O2A-CGA-CBA	2.80	120.69	111.91
23	C	512	CLA	O2A-CGA-CBA	2.80	120.69	111.91
23	b	605	CLA	CHC-C1C-C2C	-2.80	118.98	126.72
23	c	514	CLA	CAA-C2A-C3A	-2.80	105.12	112.78
23	c	507	CLA	CAC-C3C-C4C	2.80	128.44	124.81
23	A	406	CLA	CHC-C1C-C2C	-2.80	118.99	126.72
23	b	606	CLA	O2A-CGA-O1A	-2.79	116.54	123.59
32	c	520	LMG	O8-C28-C29	2.79	120.68	111.91
32	z	101	LMG	O8-C28-C29	2.79	120.67	111.91
35	C	515	DGD	O3G-C3G-C2G	-2.79	104.16	110.90
23	c	511	CLA	CHC-C1C-C2C	-2.79	118.99	126.72
23	d	402	CLA	CMC-C2C-C1C	2.79	129.29	125.04
24	A	407	PHO	CMC-C2C-C3C	2.79	130.21	124.94
31	T	101	LMT	C1'-O5'-C5'	-2.79	108.22	113.69
23	b	604	CLA	CHC-C1C-C2C	-2.79	119.01	126.72
33	D	407	LHG	O7-C7-C8	2.79	117.50	111.50
23	A	408	CLA	CHD-C4C-NC	2.78	128.59	124.20
23	B	603	CLA	O2A-CGA-CBA	2.78	120.64	111.91
23	B	608	CLA	CMC-C2C-C1C	2.78	129.28	125.04
26	a	411	SQD	O47-C7-O49	-2.78	116.98	123.70
23	A	408	CLA	CMB-C2B-C3B	2.78	129.88	124.68
23	B	612	CLA	C3B-C4B-NB	2.78	112.80	109.21
23	C	509	CLA	CHD-C4C-NC	2.78	128.58	124.20
23	A	404	CLA	CAA-CBA-CGA	-2.78	105.14	113.25
25	A	409	BCR	C33-C5-C6	-2.78	121.41	124.53
35	C	517	DGD	O1G-C1A-C2A	2.78	120.62	111.91
23	C	504	CLA	CHC-C1C-C2C	-2.78	119.05	126.72
23	b	602	CLA	CMA-C3A-C4A	-2.77	104.31	111.77
23	B	616	CLA	CHD-C4C-NC	2.77	128.57	124.20
25	K	101	BCR	C38-C26-C25	-2.77	121.41	124.53
23	C	504	CLA	CBC-CAC-C3C	-2.77	104.79	112.43
25	B	618	BCR	C2-C1-C6	2.77	114.74	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	509	CLA	C16-C15-C13	-2.77	106.98	115.92
25	b	618	BCR	C37-C22-C21	-2.77	119.05	122.92
23	c	513	CLA	C4C-C3C-C2C	-2.77	102.87	106.90
23	B	613	CLA	CHC-C1C-C2C	-2.77	119.07	126.72
32	m	101	LMG	C8-O7-C10	-2.76	110.99	117.79
23	b	609	CLA	CHD-C4C-NC	2.76	128.56	124.20
29	a	415	PL9	C53-C6-C1	2.76	120.64	114.99
23	c	512	CLA	C1-C2-C3	-2.76	121.27	126.04
23	b	608	CLA	CHD-C4C-NC	2.76	128.55	124.20
23	B	606	CLA	CHC-C1C-C2C	-2.76	119.10	126.72
25	B	618	BCR	C15-C14-C13	-2.76	123.38	127.31
23	b	611	CLA	C2A-C1A-CHA	-2.75	119.04	123.86
23	b	611	CLA	CHD-C4C-NC	2.75	128.54	124.20
23	d	402	CLA	CAC-C3C-C4C	2.75	128.38	124.81
23	B	608	CLA	CMB-C2B-C3B	2.75	129.83	124.68
23	c	514	CLA	C2A-C1A-CHA	-2.75	119.05	123.86
23	C	509	CLA	CHC-C1C-C2C	-2.75	119.11	126.72
23	c	509	CLA	C4-C3-C5	2.75	119.90	115.27
29	A	414	PL9	C40-C39-C41	2.75	119.90	115.27
23	C	513	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
23	c	512	CLA	CAC-C3C-C4C	2.75	128.38	124.81
23	b	610	CLA	CAA-CBA-CGA	-2.75	105.22	113.25
26	f	102	SQD	O8-S-C6	2.75	110.12	105.74
23	c	507	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
23	B	602	CLA	CHD-C4C-NC	2.75	128.53	124.20
26	f	102	SQD	O48-C23-C24	2.74	120.52	111.91
23	A	408	CLA	CMC-C2C-C1C	2.74	129.22	125.04
23	c	508	CLA	O2A-CGA-CBA	2.74	120.52	111.91
23	B	610	CLA	CHD-C4C-NC	2.74	128.53	124.20
23	c	513	CLA	C3B-C4B-NB	2.74	112.76	109.21
23	B	607	CLA	O2A-CGA-O1A	-2.74	116.67	123.59
23	C	513	CLA	CHC-C1C-C2C	-2.74	119.14	126.72
25	a	410	BCR	C11-C10-C9	-2.74	123.40	127.31
23	b	615	CLA	CHD-C4C-NC	2.74	128.52	124.20
23	B	602	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
23	C	508	CLA	CMB-C2B-C3B	2.74	129.80	124.68
25	k	101	BCR	C15-C14-C13	-2.74	123.40	127.31
23	b	610	CLA	C3B-C4B-NB	2.74	112.75	109.21
23	b	606	CLA	C4C-C3C-C2C	-2.74	102.91	106.90
29	A	414	PL9	C10-C9-C8	-2.74	116.66	123.68
25	c	515	BCR	C20-C21-C22	-2.74	123.41	127.31
32	c	520	LMG	O1-C7-C8	-2.73	104.30	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	404	CLA	CAC-C3C-C4C	2.73	128.36	124.81
23	C	501	CLA	C4C-C3C-C2C	-2.73	102.91	106.90
23	B	605	CLA	C1-C2-C3	-2.73	121.32	126.04
23	c	504	CLA	CHD-C4C-NC	2.73	128.51	124.20
23	c	505	CLA	CHD-C4C-NC	2.73	128.51	124.20
23	A	406	CLA	CBC-CAC-C3C	-2.73	104.90	112.43
23	B	605	CLA	C3B-C4B-NB	2.73	112.74	109.21
35	C	515	DGD	C2G-O2G-C1B	-2.73	111.07	117.79
33	d	406	LHG	O8-C23-C24	2.73	120.46	111.91
23	c	506	CLA	CHC-C1C-C2C	-2.72	119.19	126.72
23	B	606	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
23	C	506	CLA	CMB-C2B-C3B	2.72	129.77	124.68
23	a	406	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
23	b	603	CLA	CBC-CAC-C3C	-2.72	104.93	112.43
29	D	405	PL9	C42-C41-C39	-2.72	104.03	112.98
23	D	402	CLA	CAA-C2A-C3A	-2.72	105.33	112.78
23	B	608	CLA	CHB-C4A-NA	2.72	128.27	124.51
23	B	609	CLA	CHD-C4C-NC	2.72	128.49	124.20
34	b	623	HTG	O5-C1-C2	2.72	113.73	110.31
31	B	628	LMT	O1'-C1'-C2'	2.72	112.55	108.30
33	A	420	LHG	O7-C7-O9	-2.72	117.13	123.70
23	c	510	CLA	O2A-C1-C2	2.72	115.78	108.64
25	t	102	BCR	C15-C16-C17	-2.72	117.91	123.47
23	C	501	CLA	C1-O2A-CGA	2.71	123.57	116.44
40	v	201	HEC	CMB-C2B-C3B	2.71	129.01	125.82
23	c	502	CLA	CHD-C4C-NC	2.71	128.48	124.20
29	d	404	PL9	C36-C34-C33	-2.71	115.63	121.12
23	C	510	CLA	O2A-CGA-O1A	-2.71	116.75	123.59
26	B	620	SQD	C1-O5-C5	-2.71	108.37	113.69
23	b	614	CLA	CBC-CAC-C3C	-2.71	104.96	112.43
23	d	402	CLA	CHC-C1C-C2C	-2.71	119.23	126.72
23	a	407	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
24	a	408	PHO	CMA-C3A-C4A	-2.71	108.45	114.38
23	A	406	CLA	C2A-C1A-CHA	-2.71	119.13	123.86
23	A	404	CLA	C2A-C1A-CHA	-2.70	119.13	123.86
23	B	615	CLA	CHC-C1C-C2C	-2.70	119.24	126.72
32	D	411	LMG	O8-C28-C29	2.70	120.39	111.91
32	A	419	LMG	C8-O7-C10	-2.70	111.13	117.79
23	B	615	CLA	C11-C10-C8	-2.70	107.18	115.92
23	c	513	CLA	CAC-C3C-C4C	2.70	128.32	124.81
23	d	402	CLA	CBC-CAC-C3C	-2.70	104.98	112.43
23	c	511	CLA	O2A-CGA-CBA	2.70	120.38	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	y	101	BCR	C10-C11-C12	-2.70	114.80	123.22
31	c	501	LMT	C3'-C4'-C5'	-2.70	104.74	110.93
31	b	621	LMT	C1'-O5'-C5'	-2.70	108.39	113.69
35	C	516	DGD	O1G-C1A-O1A	-2.70	116.78	123.59
23	a	409	CLA	CHD-C4C-NC	2.70	128.45	124.20
23	D	402	CLA	CMC-C2C-C1C	2.70	129.15	125.04
32	c	521	LMG	O8-C28-C29	2.70	120.37	111.91
25	b	618	BCR	C29-C30-C25	2.70	114.63	110.48
23	B	609	CLA	O2A-CGA-O1A	-2.70	116.79	123.59
23	B	615	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
23	C	512	CLA	C3B-C4B-NB	2.69	112.69	109.21
23	a	405	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
23	B	604	CLA	O2A-CGA-O1A	-2.69	116.81	123.59
23	a	407	CLA	CHC-C1C-C2C	-2.69	119.29	126.72
23	b	610	CLA	CHC-C1C-C2C	-2.69	119.29	126.72
25	k	101	BCR	C2-C1-C6	2.68	114.61	110.48
23	A	408	CLA	CBC-CAC-C3C	-2.68	105.04	112.43
23	A	406	CLA	CMC-C2C-C1C	2.68	129.12	125.04
23	A	405	CLA	CAC-C3C-C4C	2.68	128.29	124.81
23	b	610	CLA	C4-C3-C5	2.68	119.78	115.27
23	B	607	CLA	CHC-C1C-C2C	-2.68	119.31	126.72
23	b	616	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
23	c	505	CLA	CAC-C3C-C4C	2.68	128.28	124.81
23	b	614	CLA	CHD-C4C-NC	2.68	128.42	124.20
25	H	101	BCR	C24-C23-C22	-2.68	122.19	126.23
33	a	421	LHG	O8-C23-C24	2.68	120.30	111.91
24	a	417	PHO	CBA-CAA-C2A	-2.68	105.99	113.81
35	c	517	DGD	C3G-C2G-C1G	-2.68	105.46	111.79
29	D	405	PL9	C37-C38-C39	-2.67	121.22	127.66
23	A	406	CLA	C1-C2-C3	-2.67	121.42	126.04
23	b	603	CLA	CHC-C1C-C2C	-2.67	119.33	126.72
23	c	511	CLA	CAC-C3C-C4C	2.67	128.28	124.81
35	c	519	DGD	O2G-C1B-C2B	2.67	117.25	111.50
23	c	505	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
25	t	102	BCR	C35-C13-C12	2.67	122.28	118.08
23	b	611	CLA	O2A-CGA-O1A	-2.67	116.86	123.59
23	B	608	CLA	C11-C12-C13	-2.67	107.30	115.92
23	b	607	CLA	C2A-C1A-CHA	-2.67	119.20	123.86
25	K	101	BCR	C16-C17-C18	-2.66	123.51	127.31
26	b	620	SQD	O9-S-C6	2.66	110.11	106.94
23	c	514	CLA	CMC-C2C-C1C	2.66	129.09	125.04
23	b	607	CLA	CAC-C3C-C4C	2.66	128.26	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	607	CLA	C1-C2-C3	-2.66	121.44	126.04
23	a	407	CLA	CAA-C2A-C3A	-2.66	105.50	112.78
31	B	630	LMT	O1'-C1'-C2'	2.66	112.45	108.30
23	b	612	CLA	CHC-C1C-C2C	-2.66	119.38	126.72
23	B	614	CLA	C4-C3-C5	2.66	119.74	115.27
34	b	622	HTG	O2-C2-C3	-2.66	104.21	110.35
23	c	508	CLA	CAC-C3C-C4C	2.65	128.25	124.81
26	A	410	SQD	O48-C23-O10	-2.65	116.89	123.59
23	c	504	CLA	C4-C3-C5	2.65	119.74	115.27
23	c	514	CLA	CHC-C1C-C2C	-2.65	119.38	126.72
23	C	513	CLA	CAC-C3C-C4C	2.65	128.25	124.81
23	a	405	CLA	CAC-C3C-C4C	2.65	128.25	124.81
23	C	507	CLA	CHC-C1C-C2C	-2.65	119.38	126.72
23	A	408	CLA	CAC-C3C-C4C	2.65	128.25	124.81
23	B	603	CLA	CAC-C3C-C4C	2.65	128.25	124.81
23	C	511	CLA	CMC-C2C-C1C	2.65	129.08	125.04
23	C	510	CLA	C4C-C3C-C2C	-2.65	103.03	106.90
25	B	619	BCR	C38-C26-C25	-2.65	121.55	124.53
23	C	513	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
25	a	410	BCR	C29-C30-C25	2.65	114.56	110.48
29	D	405	PL9	C40-C39-C41	2.65	119.72	115.27
32	c	520	LMG	C8-O7-C10	-2.65	111.28	117.79
38	F	102	HEM	CHA-C4D-ND	2.65	127.65	124.38
23	C	510	CLA	CMB-C2B-C3B	2.65	129.63	124.68
23	D	403	CLA	CHD-C4C-NC	2.65	128.37	124.20
23	C	509	CLA	O2D-CGD-O1D	-2.65	118.67	123.84
23	C	513	CLA	CBC-CAC-C3C	-2.64	105.14	112.43
23	b	607	CLA	CAA-C2A-C3A	-2.64	105.55	112.78
23	c	511	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
23	c	514	CLA	CMB-C2B-C3B	2.64	129.61	124.68
23	A	406	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
23	C	513	CLA	CHD-C4C-NC	2.64	128.36	124.20
23	B	608	CLA	O2A-CGA-O1A	-2.64	116.94	123.59
23	A	406	CLA	C4-C3-C5	2.63	119.70	115.27
31	T	101	LMT	C3'-C4'-C5'	-2.63	104.89	110.93
26	a	413	SQD	C3-C4-C5	2.63	114.94	110.24
24	A	416	PHO	O2D-CGD-O1D	-2.63	118.69	123.84
23	B	612	CLA	C2A-C1A-CHA	-2.63	119.26	123.86
23	B	610	CLA	CHC-C1C-C2C	-2.63	119.44	126.72
23	b	606	CLA	CAA-C2A-C3A	-2.63	105.57	112.78
25	t	102	BCR	C21-C20-C19	-2.63	115.01	123.22
23	B	607	CLA	CHD-C4C-NC	2.63	128.35	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	f	102	SQD	O5-C5-C4	2.63	114.47	109.69
23	C	506	CLA	C2A-C1A-CHA	-2.63	119.26	123.86
23	B	602	CLA	CHC-C1C-C2C	-2.63	119.45	126.72
23	c	512	CLA	O2A-CGA-CBA	2.63	120.15	111.91
23	c	503	CLA	CBC-CAC-C3C	-2.62	105.20	112.43
23	a	409	CLA	CAC-C3C-C4C	2.62	128.21	124.81
23	D	403	CLA	CHC-C1C-C2C	-2.62	119.47	126.72
23	B	605	CLA	C2A-C1A-CHA	-2.62	119.28	123.86
23	D	402	CLA	CMB-C2B-C3B	2.62	129.58	124.68
23	b	612	CLA	C2A-C1A-CHA	-2.62	119.28	123.86
23	d	401	CLA	CAA-C2A-C3A	-2.62	105.61	112.78
23	B	607	CLA	C4C-C3C-C2C	-2.62	103.08	106.90
23	B	614	CLA	C2A-C1A-CHA	-2.62	119.28	123.86
23	C	503	CLA	CMC-C2C-C1C	2.62	129.02	125.04
23	C	506	CLA	CAA-C2A-C3A	-2.61	105.62	112.78
23	B	606	CLA	CBC-CAC-C3C	-2.61	105.23	112.43
29	A	414	PL9	C53-C6-C1	2.61	120.33	114.99
23	C	505	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
33	D	406	LHG	O8-C23-C24	2.61	120.09	111.91
33	D	406	LHG	O7-C7-C8	2.61	117.12	111.50
23	c	508	CLA	C4C-C3C-C2C	-2.61	103.10	106.90
23	B	613	CLA	CMC-C2C-C1C	2.60	129.01	125.04
23	b	605	CLA	CMC-C2C-C1C	2.60	129.00	125.04
23	C	503	CLA	C3B-C4B-NB	2.60	112.58	109.21
23	C	513	CLA	O2A-CGA-CBA	2.60	120.08	111.91
23	B	601	CLA	CAC-C3C-C4C	2.60	128.19	124.81
23	C	510	CLA	CBC-CAC-C3C	-2.60	105.26	112.43
38	f	101	HEM	CBD-CAD-C3D	-2.60	105.40	112.63
32	D	411	LMG	O7-C10-C11	2.60	117.11	111.50
23	b	610	CLA	CMA-C3A-C4A	-2.60	104.79	111.77
23	C	501	CLA	CHC-C1C-C2C	-2.60	119.53	126.72
33	L	101	LHG	O8-C23-C24	2.60	120.06	111.91
23	c	508	CLA	C3B-C4B-NB	2.60	112.57	109.21
23	c	507	CLA	O2A-CGA-O1A	-2.60	117.04	123.59
23	b	613	CLA	CHD-C4C-NC	2.60	128.29	124.20
31	A	421	LMT	O5'-C5'-C6'	2.60	112.89	106.44
23	b	616	CLA	C4-C3-C5	2.60	119.64	115.27
23	C	503	CLA	CHC-C1C-C2C	-2.60	119.54	126.72
23	b	613	CLA	CAC-C3C-C4C	2.60	128.18	124.81
23	b	615	CLA	O2A-CGA-CBA	2.59	120.05	111.91
23	a	406	CLA	O2A-CGA-CBA	2.59	120.05	111.91
23	b	613	CLA	CMC-C2C-C1C	2.59	128.99	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	405	CLA	OBD-CAD-C3D	-2.59	122.28	128.52
23	C	513	CLA	C4-C3-C5	2.59	119.62	115.27
23	C	501	CLA	CAC-C3C-C4C	2.59	128.17	124.81
23	B	603	CLA	CMA-C3A-C2A	-2.59	103.39	113.83
23	C	512	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
23	B	602	CLA	CMB-C2B-C3B	2.59	129.52	124.68
25	d	403	BCR	C28-C27-C26	-2.59	109.46	114.08
23	a	405	CLA	C2A-C1A-CHA	-2.59	119.34	123.86
23	c	514	CLA	CHD-C4C-NC	2.59	128.28	124.20
23	b	614	CLA	C2A-C1A-CHA	-2.59	119.34	123.86
23	b	606	CLA	C1-O2A-CGA	2.59	123.23	116.44
32	D	411	LMG	O8-C28-O10	-2.59	117.07	123.59
23	c	509	CLA	O2A-CGA-CBA	2.59	120.02	111.91
23	b	601	CLA	CMB-C2B-C3B	2.58	129.51	124.68
23	b	615	CLA	O2A-CGA-O1A	-2.58	117.07	123.59
23	B	612	CLA	C11-C12-C13	-2.58	107.57	115.92
23	b	603	CLA	CMA-C3A-C2A	-2.58	103.41	113.83
29	d	404	PL9	C36-C37-C38	-2.58	103.40	111.88
23	b	613	CLA	CMB-C2B-C3B	2.58	129.50	124.68
23	C	513	CLA	C2A-C1A-CHA	-2.58	119.35	123.86
23	B	615	CLA	C2A-C1A-CHA	-2.58	119.35	123.86
23	b	611	CLA	CAC-C3C-C4C	2.58	128.15	124.81
23	c	508	CLA	CBC-CAC-C3C	-2.57	105.33	112.43
23	d	402	CLA	C2A-C1A-CHA	-2.57	119.36	123.86
23	B	601	CLA	CHC-C1C-C2C	-2.57	119.60	126.72
23	b	604	CLA	C4C-C3C-C2C	-2.57	103.15	106.90
23	b	602	CLA	CHD-C4C-NC	2.57	128.26	124.20
23	C	511	CLA	CHD-C4C-NC	2.57	128.26	124.20
23	b	604	CLA	O2A-CGA-CBA	2.57	119.98	111.91
25	c	515	BCR	C37-C22-C21	-2.57	119.32	122.92
23	c	510	CLA	CHD-C4C-NC	2.57	128.25	124.20
23	B	602	CLA	CMA-C3A-C4A	-2.57	104.87	111.77
23	a	405	CLA	CMA-C3A-C4A	-2.57	104.87	111.77
23	C	507	CLA	C4-C3-C5	2.57	119.59	115.27
31	m	103	LMT	C1'-O5'-C5'	-2.56	108.66	113.69
23	C	506	CLA	CHD-C4C-NC	2.56	128.24	124.20
23	D	402	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
23	C	502	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
23	D	402	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
35	c	517	DGD	O1G-C1A-O1A	-2.56	117.13	123.59
31	M	101	LMT	C3'-C4'-C5'	-2.56	105.06	110.93
25	d	403	BCR	C21-C20-C19	-2.56	115.23	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	612	CLA	C1-C2-C3	-2.56	121.62	126.04
23	b	606	CLA	C1-C2-C3	-2.56	121.62	126.04
23	b	609	CLA	O2A-CGA-O1A	-2.55	117.14	123.59
25	T	102	BCR	C2-C1-C6	2.55	114.41	110.48
23	D	403	CLA	CMA-C3A-C2A	-2.55	103.53	113.83
23	a	409	CLA	CMA-C3A-C2A	-2.55	103.53	113.83
23	b	608	CLA	O2A-CGA-CBA	2.55	119.92	111.91
23	b	606	CLA	CMC-C2C-C1C	2.55	128.92	125.04
23	c	511	CLA	C4-C3-C2	-2.55	117.14	123.68
23	b	614	CLA	O2A-CGA-CBA	2.55	119.90	111.91
23	C	508	CLA	C4-C3-C5	2.54	119.55	115.27
27	b	628	GOL	C3-C2-C1	-2.54	101.81	111.70
25	A	409	BCR	C15-C14-C13	-2.54	123.68	127.31
25	a	410	BCR	C24-C23-C22	-2.54	122.39	126.23
23	A	405	CLA	CMA-C3A-C2A	-2.54	103.58	113.83
23	C	507	CLA	O2A-CGA-CBA	2.54	119.88	111.91
23	C	510	CLA	O2A-CGA-CBA	2.54	119.88	111.91
23	C	503	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
23	B	616	CLA	C2A-C1A-CHA	-2.54	119.42	123.86
26	F	103	SQD	O47-C7-O49	-2.54	117.57	123.70
25	y	101	BCR	C21-C20-C19	-2.54	115.30	123.22
31	B	628	LMT	C2'-C3'-C4'	2.54	115.48	109.68
24	a	417	PHO	O1D-CGD-CBD	-2.54	120.51	124.74
23	D	403	CLA	O2A-CGA-O1A	-2.54	117.19	123.59
26	F	103	SQD	O48-C23-C24	2.53	119.86	111.91
26	b	620	SQD	O7-S-C6	2.53	109.95	106.94
29	A	414	PL9	C35-C34-C36	2.53	119.53	115.27
23	c	508	CLA	CHC-C1C-C2C	-2.53	119.72	126.72
23	A	405	CLA	C2A-C1A-CHA	-2.53	119.44	123.86
23	b	616	CLA	CHC-C1C-C2C	-2.53	119.73	126.72
23	B	613	CLA	CAC-C3C-C4C	2.53	128.09	124.81
35	h	102	DGD	O3G-C1D-C2D	2.53	112.25	108.30
25	c	515	BCR	C33-C5-C6	-2.53	121.69	124.53
25	t	102	BCR	C20-C21-C22	-2.52	123.71	127.31
23	c	508	CLA	CHD-C4C-NC	2.52	128.18	124.20
23	C	508	CLA	CHD-C4C-NC	2.52	128.18	124.20
23	a	407	CLA	C2A-C1A-CHA	-2.52	119.45	123.86
23	A	406	CLA	CMA-C3A-C2A	-2.52	103.66	113.83
23	d	401	CLA	CMB-C2B-C3B	2.52	129.39	124.68
23	c	505	CLA	C2A-C1A-CHA	-2.52	119.46	123.86
23	c	506	CLA	C1-C2-C3	-2.52	121.69	126.04
25	B	618	BCR	C37-C22-C23	2.52	122.04	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	507	CLA	CBC-CAC-C3C	-2.51	105.50	112.43
23	b	615	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
31	B	630	LMT	O5'-C5'-C6'	2.51	112.69	106.44
29	a	415	PL9	C47-C48-C49	-2.51	119.16	127.75
23	b	603	CLA	CMB-C2B-C3B	2.51	129.38	124.68
23	b	609	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
23	c	509	CLA	CAA-C2A-C3A	-2.51	105.90	112.78
23	a	406	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
24	A	407	PHO	O2A-CGA-CBA	2.51	119.78	111.91
24	A	407	PHO	CMB-C2B-C3B	2.51	129.37	124.68
23	B	611	CLA	C4-C3-C5	2.51	119.49	115.27
23	B	615	CLA	C6-C7-C8	-2.51	107.81	115.92
23	b	601	CLA	C1-O2A-CGA	2.51	123.03	116.44
23	a	409	CLA	CMB-C2B-C3B	2.51	129.37	124.68
23	B	612	CLA	CHD-C4C-NC	2.51	128.16	124.20
23	a	407	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
23	B	602	CLA	C11-C12-C13	-2.51	107.82	115.92
23	C	504	CLA	C4-C3-C5	2.50	119.48	115.27
23	c	507	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
23	b	601	CLA	CAC-C3C-C4C	2.50	128.05	124.81
23	a	405	CLA	CMC-C2C-C1C	2.50	128.84	125.04
23	C	507	CLA	C3B-C4B-NB	2.50	112.44	109.21
25	k	101	BCR	C39-C30-C25	-2.49	106.25	110.30
23	A	408	CLA	CHB-C4A-NA	2.49	127.96	124.51
25	Y	101	BCR	C36-C18-C17	-2.49	119.43	122.92
23	D	403	CLA	CMA-C3A-C4A	-2.49	105.08	111.77
23	c	513	CLA	CMC-C2C-C1C	2.49	128.83	125.04
23	a	407	CLA	O2A-CGA-CBA	2.49	119.72	111.91
23	B	604	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
23	c	514	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
23	b	602	CLA	C11-C12-C13	-2.49	107.88	115.92
23	C	502	CLA	CHD-C4C-NC	2.49	128.12	124.20
24	a	408	PHO	CMB-C2B-C3B	2.48	129.33	124.68
34	B	622	HTG	C1-O5-C5	2.48	117.16	112.58
23	C	512	CLA	CHC-C1C-C2C	-2.48	119.86	126.72
40	V	201	HEC	CAD-CBD-CGD	-2.48	106.81	113.76
35	C	515	DGD	O5D-C6D-C5D	-2.48	104.46	109.05
29	d	404	PL9	C17-C18-C19	-2.48	121.69	127.66
25	t	102	BCR	C1-C6-C7	2.48	122.79	115.78
25	d	403	BCR	C24-C23-C22	-2.48	122.49	126.23
23	A	408	CLA	C4-C3-C5	2.48	119.44	115.27
23	C	502	CLA	C4-C3-C5	2.48	119.44	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	507	CLA	C1-C2-C3	-2.48	121.76	126.04
23	B	616	CLA	CHC-C1C-C2C	-2.48	119.87	126.72
24	A	407	PHO	O2A-CGA-O1A	-2.48	117.34	123.59
23	A	404	CLA	CMA-C3A-C2A	-2.47	103.85	113.83
23	c	509	CLA	O2A-CGA-O1A	-2.47	117.35	123.59
23	a	409	CLA	O2A-CGA-O1A	-2.47	117.35	123.59
23	c	506	CLA	C4-C3-C5	2.47	119.43	115.27
23	C	503	CLA	C2A-C1A-CHA	-2.47	119.54	123.86
23	c	512	CLA	CBC-CAC-C3C	-2.47	105.62	112.43
23	B	608	CLA	O2A-CGA-CBA	2.47	119.66	111.91
25	H	101	BCR	C7-C8-C9	-2.47	122.50	126.23
23	C	505	CLA	O2A-CGA-CBA	2.47	119.66	111.91
26	B	620	SQD	C44-O6-C1	-2.47	108.91	113.74
23	C	509	CLA	C11-C12-C13	-2.47	107.94	115.92
34	b	622	HTG	O5-C1-C2	2.47	113.42	110.31
23	b	611	CLA	CMB-C2B-C3B	2.47	129.29	124.68
25	d	403	BCR	C16-C17-C18	-2.47	123.79	127.31
23	C	508	CLA	CAC-C3C-C4C	2.47	128.01	124.81
25	c	516	BCR	C33-C5-C6	-2.46	121.76	124.53
23	C	502	CLA	O2A-CGA-CBA	2.46	119.64	111.91
23	C	503	CLA	O2A-CGA-CBA	2.46	119.64	111.91
33	d	405	LHG	O8-C23-O10	-2.46	117.38	123.59
23	A	408	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
25	c	516	BCR	C21-C20-C19	-2.46	115.54	123.22
26	a	411	SQD	O7-S-C6	2.46	109.86	106.94
35	H	102	DGD	O1G-C1A-C2A	2.46	119.62	111.91
34	B	625	HTG	O5-C5-C4	2.46	114.16	109.69
25	h	101	BCR	C24-C23-C22	-2.46	122.52	126.23
25	B	619	BCR	C21-C20-C19	-2.46	115.56	123.22
23	C	505	CLA	CHD-C4C-NC	2.45	128.07	124.20
23	c	502	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
23	a	406	CLA	C4C-C3C-C2C	-2.45	103.32	106.90
23	b	613	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
25	Y	101	BCR	C15-C16-C17	-2.45	118.45	123.47
23	A	405	CLA	CMA-C3A-C4A	-2.45	105.19	111.77
26	a	413	SQD	O8-S-C6	2.45	109.64	105.74
23	c	506	CLA	O2A-CGA-CBA	2.45	119.59	111.91
29	a	415	PL9	C40-C39-C41	2.45	119.39	115.27
31	B	631	LMT	C3'-C4'-C5'	-2.45	105.32	110.93
23	c	507	CLA	C4-C3-C5	2.45	119.39	115.27
29	D	405	PL9	C27-C28-C29	-2.44	121.77	127.66
29	a	415	PL9	C20-C19-C21	2.44	119.38	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	h	101	BCR	C36-C18-C17	-2.44	119.50	122.92
31	m	103	LMT	C3'-C4'-C5'	-2.44	105.33	110.93
25	T	102	BCR	C21-C20-C19	-2.44	115.59	123.22
23	b	607	CLA	CBC-CAC-C3C	-2.44	105.70	112.43
23	C	503	CLA	CMB-C2B-C3B	2.44	129.25	124.68
23	b	615	CLA	CAC-C3C-C4C	2.44	127.98	124.81
34	C	520	HTG	C1-O5-C5	2.44	117.08	112.58
23	c	509	CLA	CHD-C4C-NC	2.44	128.05	124.20
23	A	405	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
23	a	405	CLA	CHD-C4C-NC	2.44	128.05	124.20
25	Y	101	BCR	C28-C27-C26	-2.44	109.73	114.08
34	b	625	HTG	C1'-S1-C1	2.43	104.64	100.09
25	Y	101	BCR	C37-C22-C23	2.43	121.91	118.08
25	K	103	BCR	C36-C18-C19	2.43	121.91	118.08
23	b	602	CLA	C1-C2-C3	-2.43	121.83	126.04
23	C	513	CLA	CAA-C2A-C3A	-2.43	106.12	112.78
23	b	602	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
23	c	504	CLA	CHC-C1C-C2C	-2.43	120.00	126.72
25	c	515	BCR	C38-C26-C25	-2.43	121.80	124.53
24	a	408	PHO	O2A-CGA-O1A	-2.43	117.46	123.59
23	A	408	CLA	CMA-C3A-C2A	-2.43	104.03	113.83
23	c	502	CLA	O2A-CGA-CBA	2.43	119.53	111.91
25	H	101	BCR	C37-C22-C21	-2.43	119.52	122.92
23	C	502	CLA	CAC-C3C-C4C	2.43	127.96	124.81
23	c	504	CLA	CAC-C3C-C4C	2.43	127.96	124.81
29	d	404	PL9	C47-C48-C49	-2.42	119.47	127.75
23	b	614	CLA	CAC-C3C-C4C	2.42	127.95	124.81
25	A	409	BCR	C16-C17-C18	-2.42	123.85	127.31
23	D	403	CLA	O2A-CGA-CBA	2.42	119.51	111.91
23	c	503	CLA	C1-C2-C3	-2.42	121.86	126.04
32	A	419	LMG	C6-C5-C4	2.42	118.67	113.00
23	B	606	CLA	CAC-C3C-C4C	2.42	127.95	124.81
23	B	601	CLA	CMC-C2C-C1C	2.42	128.72	125.04
23	C	510	CLA	C2A-C1A-CHA	-2.42	119.63	123.86
26	B	620	SQD	O48-C23-O10	-2.42	117.49	123.59
23	D	403	CLA	C2A-C1A-CHA	-2.42	119.63	123.86
26	a	411	SQD	O8-S-C6	2.41	109.59	105.74
29	A	414	PL9	C35-C34-C33	-2.41	117.49	123.68
31	A	421	LMT	O1'-C1'-C2'	2.41	112.07	108.30
23	B	605	CLA	CHC-C1C-C2C	-2.41	120.05	126.72
23	b	606	CLA	CMB-C2B-C3B	2.41	129.19	124.68
23	B	601	CLA	CMB-C2B-C3B	2.41	129.19	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	c	522	HTG	O5-C1-C2	2.41	113.34	110.31
23	B	607	CLA	C2A-C1A-CHA	-2.41	119.65	123.86
23	A	404	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
23	B	613	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
29	A	414	PL9	C42-C43-C44	-2.41	121.87	127.66
23	C	501	CLA	C4-C3-C5	2.40	119.31	115.27
23	B	602	CLA	C2A-C1A-CHA	-2.40	119.66	123.86
23	C	511	CLA	CMB-C2B-C3B	2.40	129.18	124.68
23	b	601	CLA	O2A-CGA-CBA	2.40	119.44	111.91
25	B	618	BCR	C37-C22-C21	-2.40	119.56	122.92
23	B	604	CLA	C11-C12-C13	-2.40	108.16	115.92
23	c	503	CLA	O2A-CGA-CBA	2.40	119.43	111.91
23	C	512	CLA	CHB-C4A-NA	2.40	127.83	124.51
23	b	611	CLA	O2A-CGA-CBA	2.40	119.43	111.91
23	c	511	CLA	C11-C10-C8	-2.40	108.18	115.92
25	C	514	BCR	C32-C1-C6	-2.40	106.41	110.30
32	B	621	LMG	C12-C11-C10	-2.39	104.91	113.62
26	f	102	SQD	O47-C7-O49	-2.39	117.92	123.70
23	B	613	CLA	CHD-C4C-NC	2.39	127.97	124.20
23	D	403	CLA	CBC-CAC-C3C	-2.39	105.84	112.43
25	y	101	BCR	C40-C30-C25	-2.39	106.42	110.30
26	a	413	SQD	C1-O5-C5	2.39	118.37	113.69
23	B	601	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
25	T	102	BCR	C3-C4-C5	-2.38	109.83	114.08
35	H	102	DGD	O1G-C1A-O1A	-2.38	117.58	123.59
23	A	408	CLA	OBD-CAD-C3D	-2.38	122.79	128.52
33	L	101	LHG	O8-C23-O10	-2.38	117.59	123.59
23	B	601	CLA	CHB-C4A-NA	2.38	127.80	124.51
25	b	617	BCR	C24-C23-C22	-2.38	122.64	126.23
23	C	506	CLA	C4C-C3C-C2C	-2.38	103.43	106.90
23	c	508	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
23	c	507	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
29	a	415	PL9	C10-C9-C8	-2.38	117.58	123.68
23	B	611	CLA	CAC-C3C-C4C	2.38	127.89	124.81
23	C	510	CLA	CMC-C2C-C1C	2.38	128.66	125.04
29	d	404	PL9	C7-C8-C9	-2.38	122.84	126.79
29	D	405	PL9	C45-C44-C46	2.38	119.27	115.27
25	D	404	BCR	C24-C23-C22	-2.37	122.65	126.23
23	b	603	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
25	H	101	BCR	C16-C15-C14	-2.37	118.62	123.47
38	F	102	HEM	O2A-CGA-CBA	2.37	121.65	114.03
23	b	608	CLA	C11-C10-C8	-2.37	108.26	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	507	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
23	c	510	CLA	CMC-C2C-C1C	2.37	128.65	125.04
26	a	413	SQD	O5-C5-C4	2.37	113.99	109.69
23	C	506	CLA	O2A-CGA-CBA	2.37	119.33	111.91
25	A	409	BCR	C40-C30-C25	-2.37	106.46	110.30
32	C	518	LMG	O8-C28-O10	-2.36	117.62	123.59
23	C	512	CLA	CAC-C3C-C4C	2.36	127.88	124.81
23	b	601	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
23	c	504	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
23	B	603	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
25	D	404	BCR	C3-C4-C5	-2.36	109.86	114.08
29	D	405	PL9	C22-C23-C24	-2.36	121.98	127.66
23	B	609	CLA	CAC-C3C-C4C	2.36	127.87	124.81
23	b	612	CLA	CHD-C4C-NC	2.36	127.92	124.20
25	c	515	BCR	C36-C18-C17	-2.36	119.62	122.92
25	c	516	BCR	C38-C26-C25	-2.36	121.88	124.53
23	b	615	CLA	CBC-CAC-C3C	-2.36	105.94	112.43
23	B	601	CLA	C1-O2A-CGA	2.35	122.62	116.44
23	b	610	CLA	CMB-C2B-C3B	2.35	129.08	124.68
24	A	416	PHO	CMA-C3A-C4A	-2.35	109.23	114.38
23	C	503	CLA	CAC-C3C-C4C	2.35	127.86	124.81
29	A	414	PL9	C45-C44-C46	2.35	119.22	115.27
35	C	516	DGD	O6E-C5E-C6E	2.35	112.28	106.44
29	a	415	PL9	C45-C44-C46	2.35	119.22	115.27
23	C	502	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
31	F	101	LMT	C1'-O5'-C5'	-2.35	109.08	113.69
23	B	609	CLA	C1-C2-C3	-2.35	121.98	126.04
23	a	406	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
23	C	512	CLA	CMA-C3A-C4A	-2.35	105.47	111.77
26	b	620	SQD	O48-C23-C24	2.34	119.27	111.91
23	B	611	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
23	B	612	CLA	C4-C3-C5	2.34	119.21	115.27
23	b	602	CLA	C4-C3-C5	2.34	119.21	115.27
23	c	514	CLA	C4-C3-C5	2.34	119.21	115.27
23	b	616	CLA	CMC-C2C-C1C	2.34	128.60	125.04
23	C	506	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
23	C	512	CLA	C2A-C1A-CHA	-2.34	119.77	123.86
23	c	507	CLA	O2A-CGA-CBA	2.34	119.25	111.91
24	a	408	PHO	CMC-C2C-C3C	2.34	129.35	124.94
23	d	402	CLA	O2A-CGA-CBA	2.34	119.24	111.91
23	b	609	CLA	CMA-C3A-C4A	-2.34	105.50	111.77
23	B	614	CLA	OBD-CAD-C3D	-2.34	122.90	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	403	BCR	C39-C30-C25	-2.33	106.51	110.30
23	c	507	CLA	CMC-C2C-C1C	2.33	128.59	125.04
23	D	402	CLA	CHD-C4C-NC	2.33	127.88	124.20
25	D	404	BCR	C15-C14-C13	-2.33	123.98	127.31
23	a	406	CLA	C1-O2A-CGA	2.33	122.56	116.44
25	b	618	BCR	C3-C4-C5	-2.33	109.92	114.08
25	T	102	BCR	C1-C6-C7	2.33	122.37	115.78
23	b	604	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
23	b	615	CLA	C6-C7-C8	-2.33	108.39	115.92
29	a	415	PL9	C35-C34-C33	-2.33	117.70	123.68
35	C	516	DGD	O1G-C1A-C2A	2.33	119.21	111.91
35	c	518	DGD	O1G-C1A-C2A	2.33	119.21	111.91
26	A	412	SQD	C4-C3-C2	-2.33	106.76	110.82
23	b	606	CLA	O2A-CGA-CBA	2.33	119.21	111.91
23	d	402	CLA	C1-O2A-CGA	2.33	122.55	116.44
26	b	620	SQD	C44-O6-C1	-2.33	109.19	113.74
33	d	405	LHG	O8-C23-C24	2.33	119.21	111.91
23	c	503	CLA	C4C-C3C-C2C	-2.33	103.51	106.90
23	b	610	CLA	CMC-C2C-C1C	2.32	128.58	125.04
35	c	519	DGD	O3G-C3G-C2G	-2.32	105.29	110.90
35	c	517	DGD	C2G-O2G-C1B	-2.32	112.07	117.79
25	k	101	BCR	C36-C18-C19	2.32	121.74	118.08
23	b	614	CLA	CMC-C2C-C1C	2.32	128.57	125.04
23	a	407	CLA	C4-C3-C5	2.32	119.17	115.27
23	B	602	CLA	CAA-CBA-CGA	-2.32	106.48	113.25
23	A	404	CLA	CMA-C3A-C4A	-2.32	105.54	111.77
23	b	604	CLA	C4-C3-C5	2.32	119.17	115.27
31	B	630	LMT	O5'-C5'-C4'	2.32	114.64	109.75
38	F	102	HEM	O2D-CGD-CBD	2.32	121.47	114.03
23	C	504	CLA	C2A-C1A-CHA	-2.32	119.81	123.86
26	a	411	SQD	O48-C23-C24	2.32	119.17	111.91
25	A	409	BCR	C11-C10-C9	-2.31	124.01	127.31
32	d	410	LMG	O8-C28-C29	2.31	119.17	111.91
25	k	101	BCR	C16-C17-C18	-2.31	124.01	127.31
25	d	403	BCR	C3-C4-C5	-2.31	109.95	114.08
23	c	509	CLA	CAC-C3C-C4C	2.31	127.81	124.81
23	B	613	CLA	CHB-C4A-NA	2.31	127.71	124.51
29	A	414	PL9	C37-C36-C34	-2.31	105.38	112.98
26	a	413	SQD	O48-C23-O10	-2.31	117.76	123.59
25	D	404	BCR	C15-C16-C17	-2.31	118.74	123.47
25	Y	101	BCR	C34-C9-C8	2.31	121.71	118.08
23	c	513	CLA	CMB-C2B-C3B	2.31	128.99	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	405	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
23	d	401	CLA	CMC-C2C-C1C	2.30	128.55	125.04
23	C	501	CLA	C2A-C1A-CHA	-2.30	119.83	123.86
23	d	402	CLA	CHB-C4A-NA	2.30	127.70	124.51
23	c	514	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
29	A	414	PL9	C2-C3-C4	2.30	121.97	118.80
25	b	617	BCR	C29-C30-C25	2.30	114.02	110.48
32	C	519	LMG	C9-C8-C7	-2.30	106.35	111.79
23	b	608	CLA	C4C-C3C-C2C	-2.30	103.54	106.90
23	C	504	CLA	CMB-C2B-C3B	2.30	128.98	124.68
23	c	510	CLA	C2A-C1A-CHA	-2.30	119.84	123.86
23	A	404	CLA	CMC-C2C-C1C	2.30	128.54	125.04
23	b	609	CLA	C7-C6-C5	-2.30	107.12	113.36
23	C	506	CLA	CGD-CBD-CAD	-2.30	103.30	110.73
23	b	602	CLA	CHC-C1C-C2C	-2.29	120.38	126.72
26	F	103	SQD	O5-C1-O6	2.29	115.41	109.97
23	B	615	CLA	O2A-CGA-O1A	-2.29	117.80	123.59
23	b	604	CLA	C6-C5-C3	-2.29	107.44	113.45
23	C	505	CLA	CBC-CAC-C3C	-2.29	106.11	112.43
32	C	518	LMG	C8-O7-C10	-2.29	112.15	117.79
29	A	414	PL9	C47-C48-C49	-2.29	119.92	127.75
24	a	417	PHO	O2D-CGD-O1D	-2.29	119.36	123.84
23	B	604	CLA	O2A-CGA-CBA	2.29	119.10	111.91
23	C	509	CLA	C2A-C1A-CHA	-2.29	119.85	123.86
23	B	610	CLA	CMC-C2C-C1C	2.29	128.53	125.04
32	d	410	LMG	O7-C10-O9	-2.29	118.17	123.70
23	b	608	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
33	d	406	LHG	O8-C23-O10	-2.29	117.82	123.59
23	a	407	CLA	CBC-CAC-C3C	-2.29	106.12	112.43
23	c	507	CLA	CAA-C2A-C3A	-2.29	106.52	112.78
23	b	601	CLA	CMC-C2C-C1C	2.29	128.52	125.04
23	b	602	CLA	CAA-CBA-CGA	-2.29	106.57	113.25
23	c	512	CLA	C1-O2A-CGA	2.28	122.44	116.44
31	B	631	LMT	O5'-C5'-C4'	2.28	114.57	109.75
25	c	516	BCR	C37-C22-C23	2.28	121.67	118.08
26	A	412	SQD	O48-C23-O10	-2.28	117.83	123.59
23	b	608	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
23	b	607	CLA	C1-O2A-CGA	2.28	122.43	116.44
23	b	606	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
23	C	510	CLA	CAC-C3C-C4C	2.28	127.77	124.81
25	y	101	BCR	C16-C17-C18	-2.28	124.06	127.31
34	b	625	HTG	O5-C1-S1	-2.28	104.38	109.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	606	CLA	C2A-C1A-CHA	-2.28	119.88	123.86
23	b	608	CLA	C11-C12-C13	-2.28	108.56	115.92
23	B	604	CLA	C4-C3-C5	2.28	119.10	115.27
25	a	410	BCR	C34-C9-C10	-2.28	119.74	122.92
23	B	610	CLA	CAC-C3C-C4C	2.27	127.76	124.81
23	a	405	CLA	CMA-C3A-C2A	-2.27	104.66	113.83
23	c	507	CLA	CMB-C2B-C3B	2.27	128.93	124.68
23	c	512	CLA	CMA-C3A-C4A	2.27	117.88	111.77
29	d	404	PL9	C31-C32-C33	-2.27	104.42	111.88
23	c	513	CLA	CHB-C4A-NA	2.27	127.65	124.51
26	b	620	SQD	O47-C7-O49	-2.27	118.22	123.70
23	c	511	CLA	C2A-C1A-CHA	-2.27	119.89	123.86
24	A	416	PHO	O1D-CGD-CBD	-2.27	120.96	124.74
23	B	613	CLA	CMA-C3A-C4A	-2.27	105.68	111.77
25	Y	101	BCR	C36-C18-C19	2.26	121.64	118.08
23	b	616	CLA	C2A-C1A-CHA	-2.26	119.90	123.86
25	a	410	BCR	C7-C8-C9	-2.26	122.82	126.23
25	y	101	BCR	C34-C9-C10	-2.26	119.75	122.92
23	B	616	CLA	CBC-CAC-C3C	-2.26	106.20	112.43
33	d	411	LHG	O7-C7-O9	-2.26	118.24	123.70
23	D	402	CLA	C4-C3-C5	2.26	119.07	115.27
23	C	508	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
33	d	405	LHG	C6-C5-C4	-2.26	106.44	111.79
23	C	501	CLA	O2A-CGA-CBA	2.26	119.00	111.91
35	C	517	DGD	O2G-C1B-C2B	2.26	116.37	111.50
23	B	614	CLA	CAA-C2A-C3A	-2.26	106.60	112.78
33	b	630	LHG	O8-C23-O10	-2.26	117.90	123.59
24	a	417	PHO	C4-C3-C2	-2.26	117.89	123.68
23	a	409	CLA	CHC-C1C-C2C	-2.25	120.49	126.72
23	c	510	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
25	k	101	BCR	C10-C11-C12	-2.25	116.19	123.22
23	b	611	CLA	CMC-C2C-C1C	2.25	128.47	125.04
32	d	410	LMG	C7-O1-C1	-2.25	109.34	113.74
23	B	612	CLA	C6-C5-C3	-2.25	107.55	113.45
23	B	610	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
25	Y	101	BCR	C38-C26-C25	-2.25	122.00	124.53
25	H	101	BCR	C10-C11-C12	-2.25	116.20	123.22
25	h	101	BCR	C37-C22-C21	-2.25	119.77	122.92
29	D	405	PL9	C20-C19-C21	2.25	119.05	115.27
25	b	619	BCR	C39-C30-C25	-2.25	106.65	110.30
23	c	505	CLA	CMC-C2C-C1C	2.25	128.46	125.04
24	A	416	PHO	CMB-C2B-C3B	2.25	128.88	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	508	CLA	O2A-CGA-CBA	2.25	118.96	111.91
23	c	514	CLA	CBC-CAC-C3C	-2.24	106.24	112.43
23	C	507	CLA	CMC-C2C-C1C	2.24	128.46	125.04
23	B	604	CLA	C6-C5-C3	-2.24	107.57	113.45
25	b	618	BCR	C37-C22-C23	2.24	121.61	118.08
23	d	402	CLA	CMA-C3A-C2A	-2.24	104.78	113.83
25	t	102	BCR	C34-C9-C10	-2.24	119.78	122.92
24	a	417	PHO	CED-O2D-CGD	2.24	121.00	115.94
23	C	504	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
25	K	103	BCR	C37-C22-C21	-2.24	119.79	122.92
32	B	621	LMG	O8-C28-O10	-2.24	117.94	123.59
23	c	508	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
23	c	512	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
25	c	515	BCR	C34-C9-C10	-2.24	119.79	122.92
23	c	506	CLA	CHD-C4C-NC	2.24	127.73	124.20
32	c	521	LMG	O8-C28-O10	-2.23	117.95	123.59
23	a	409	CLA	CBC-CAC-C3C	-2.23	106.28	112.43
29	D	405	PL9	C36-C37-C38	-2.23	104.54	111.88
23	b	609	CLA	O2A-CGA-CBA	2.23	118.91	111.91
31	B	631	LMT	O1'-C1'-C2'	2.23	111.79	108.30
23	b	616	CLA	CAC-C3C-C4C	2.23	127.70	124.81
31	A	421	LMT	O5'-C5'-C4'	2.23	114.45	109.75
23	B	608	CLA	C11-C10-C8	-2.23	108.72	115.92
23	a	405	CLA	C7-C6-C5	-2.22	107.32	113.36
23	B	608	CLA	CHD-C4C-NC	2.22	127.71	124.20
32	Z	101	LMG	C1-O6-C5	2.22	118.05	113.69
23	b	602	CLA	CMB-C2B-C3B	2.22	128.84	124.68
23	C	505	CLA	CHA-C1A-NA	-2.22	121.31	126.40
23	d	401	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
26	A	410	SQD	O8-S-C6	2.22	109.28	105.74
35	h	102	DGD	C6D-C5D-C4D	2.22	116.73	112.09
25	c	516	BCR	C20-C21-C22	-2.22	124.14	127.31
25	D	404	BCR	C21-C20-C19	-2.22	116.29	123.22
26	b	620	SQD	C1-C2-C3	-2.22	105.37	110.00
25	h	101	BCR	C33-C5-C6	-2.22	122.03	124.53
23	c	502	CLA	CAC-C3C-C4C	2.22	127.69	124.81
23	C	502	CLA	CMC-C2C-C1C	2.22	128.42	125.04
23	B	608	CLA	CMA-C3A-C2A	-2.22	104.88	113.83
23	A	405	CLA	CHB-C4A-NA	2.22	127.58	124.51
23	C	505	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
25	Y	101	BCR	C10-C11-C12	-2.22	116.30	123.22
23	b	613	CLA	CED-O2D-CGD	2.22	120.95	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	609	CLA	C16-C15-C13	-2.22	108.75	115.92
23	B	614	CLA	CBC-CAC-C3C	-2.22	106.32	112.43
35	C	515	DGD	C3G-C2G-C1G	-2.22	106.55	111.79
35	c	518	DGD	O4E-C4E-C3E	-2.22	105.23	110.35
23	b	605	CLA	O2A-C1-C2	-2.21	102.81	108.64
23	c	504	CLA	O2A-CGA-CBA	2.21	118.86	111.91
25	c	516	BCR	C37-C22-C21	-2.21	119.82	122.92
23	c	511	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
23	B	615	CLA	CMB-C2B-C1B	2.21	131.86	128.46
26	f	102	SQD	O48-C23-O10	-2.21	118.01	123.59
23	b	614	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
25	c	516	BCR	C15-C16-C17	-2.21	118.95	123.47
38	f	101	HEM	CMD-C2D-C1D	2.21	128.40	125.04
23	C	512	CLA	O2A-CGA-O1A	-2.21	118.03	123.59
26	F	103	SQD	O8-S-O7	-2.20	105.89	111.27
23	C	503	CLA	CBC-CAC-C3C	-2.20	106.36	112.43
24	A	407	PHO	C1-C2-C3	-2.20	122.24	126.04
23	a	407	CLA	CAC-C3C-C4C	2.20	127.67	124.81
23	b	601	CLA	CBC-CAC-C3C	-2.20	106.37	112.43
23	c	510	CLA	C4-C3-C2	-2.20	118.04	123.68
25	Y	101	BCR	C1-C6-C7	2.20	122.00	115.78
23	b	607	CLA	CMB-C2B-C3B	2.20	128.79	124.68
29	A	414	PL9	C51-C49-C50	2.20	119.46	114.60
25	C	514	BCR	C29-C30-C25	2.20	113.86	110.48
24	A	416	PHO	O2A-CGA-CBA	2.20	118.80	111.91
23	c	502	CLA	OBD-CAD-C3D	-2.19	123.24	128.52
23	c	506	CLA	CMA-C3A-C4A	-2.19	105.88	111.77
23	B	602	CLA	C4-C3-C5	2.19	118.96	115.27
23	B	601	CLA	CBC-CAC-C3C	-2.19	106.39	112.43
23	b	606	CLA	CAC-C3C-C4C	2.19	127.65	124.81
23	B	609	CLA	CHA-C1A-NA	-2.19	121.39	126.40
25	b	618	BCR	C8-C7-C6	-2.19	121.06	127.20
34	B	625	HTG	C3-C4-C5	2.19	114.14	110.24
23	D	402	CLA	CED-O2D-CGD	2.19	120.88	115.94
25	T	102	BCR	C35-C13-C12	2.18	121.52	118.08
26	a	411	SQD	O9-S-O7	-2.18	106.39	113.95
23	b	602	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
23	c	513	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
25	c	515	BCR	C28-C27-C26	-2.18	110.18	114.08
23	b	609	CLA	CHA-C1A-NA	-2.18	121.41	126.40
23	C	510	CLA	CHB-C4A-NA	2.18	127.53	124.51
38	f	101	HEM	C3C-C4C-NC	-2.18	106.83	110.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	d	404	PL9	C51-C49-C50	2.18	119.42	114.60
23	c	502	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
23	d	401	CLA	CAC-C3C-C4C	2.18	127.64	124.81
23	c	502	CLA	C4-C3-C5	2.18	118.93	115.27
25	k	101	BCR	C34-C9-C8	2.18	121.51	118.08
35	c	518	DGD	C2G-O2G-C1B	-2.18	112.43	117.79
35	H	102	DGD	O2G-C1B-C2B	2.17	116.18	111.50
23	b	615	CLA	CHA-C1A-NA	-2.17	121.42	126.40
23	B	612	CLA	CHC-C1C-C2C	-2.17	120.71	126.72
25	A	409	BCR	C8-C7-C6	-2.17	121.11	127.20
23	B	605	CLA	CBC-CAC-C3C	-2.17	106.45	112.43
23	b	615	CLA	C11-C12-C13	-2.17	108.90	115.92
25	d	403	BCR	C38-C26-C27	2.17	117.78	113.62
24	a	408	PHO	CBA-CAA-C2A	-2.17	107.47	113.81
23	c	505	CLA	CBC-CAC-C3C	-2.17	106.45	112.43
32	m	101	LMG	O8-C28-O10	-2.17	118.12	123.59
33	A	420	LHG	O4-P-O5	2.17	122.95	112.24
23	c	502	CLA	CBC-CAC-C3C	-2.17	106.46	112.43
31	e	101	LMT	O1'-C1'-C2'	2.17	111.69	108.30
23	c	512	CLA	CMB-C2B-C3B	2.16	128.73	124.68
25	K	103	BCR	C11-C10-C9	-2.16	124.22	127.31
23	A	405	CLA	C4C-C3C-C2C	-2.16	103.75	106.90
23	B	612	CLA	CMA-C3A-C2A	-2.16	105.11	113.83
23	B	606	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
25	c	515	BCR	C36-C18-C19	2.16	121.48	118.08
35	c	519	DGD	O3G-C1D-C2D	-2.16	104.93	108.30
26	A	410	SQD	O9-S-O7	-2.16	106.48	113.95
26	B	620	SQD	O5-C1-C2	-2.16	105.79	110.35
34	B	622	HTG	O2-C2-C3	-2.15	105.37	110.35
23	b	605	CLA	C1-O2A-CGA	2.15	122.09	116.44
25	d	403	BCR	C33-C5-C6	-2.15	122.11	124.53
23	A	408	CLA	CMA-C3A-C4A	-2.15	106.00	111.77
35	C	516	DGD	C2G-O2G-C1B	-2.15	112.50	117.79
23	b	602	CLA	C1-O2A-CGA	2.15	122.08	116.44
23	C	504	CLA	CAA-C2A-C3A	-2.15	106.89	112.78
35	c	517	DGD	O6D-C1D-O3G	-2.15	104.89	109.97
29	d	404	PL9	C35-C34-C36	2.15	118.88	115.27
23	D	403	CLA	C1-C2-C3	-2.15	122.33	126.04
23	B	605	CLA	OBD-CAD-C3D	-2.15	123.36	128.52
23	a	409	CLA	C2A-C1A-CHA	-2.14	120.11	123.86
25	B	617	BCR	C15-C14-C13	-2.14	124.25	127.31
23	b	602	CLA	CMA-C3A-C2A	-2.14	105.18	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	510	CLA	C4-C3-C2	-2.14	118.18	123.68
25	Y	101	BCR	C24-C23-C22	-2.14	123.00	126.23
23	b	607	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
23	B	610	CLA	C4-C3-C5	2.14	118.87	115.27
34	b	622	HTG	C6-C5-C4	-2.14	107.99	113.00
32	a	418	LMG	O8-C28-C29	2.14	118.62	111.91
29	A	414	PL9	C25-C24-C26	2.14	118.87	115.27
26	A	412	SQD	O7-S-C6	2.14	109.48	106.94
23	B	604	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
23	c	504	CLA	OBD-CAD-C3D	-2.14	123.38	128.52
31	m	103	LMT	C3B-C4B-C5B	-2.14	106.43	110.24
38	F	102	HEM	C4D-ND-C1D	2.14	107.28	105.07
23	C	504	CLA	OBD-CAD-C3D	-2.14	123.38	128.52
23	c	513	CLA	CBA-CAA-C2A	-2.14	107.56	113.86
24	A	407	PHO	CBA-CAA-C2A	-2.14	107.57	113.81
35	H	102	DGD	C3E-C4E-C5E	-2.13	106.43	110.24
38	F	102	HEM	C3C-C4C-NC	-2.13	106.92	110.94
23	b	603	CLA	CAC-C3C-C4C	2.13	127.58	124.81
23	B	605	CLA	CMB-C2B-C1B	2.13	131.74	128.46
23	b	608	CLA	C4-C3-C5	2.13	118.86	115.27
25	b	618	BCR	C33-C5-C6	-2.13	122.14	124.53
25	C	514	BCR	C21-C20-C19	-2.13	116.57	123.22
25	D	404	BCR	C38-C26-C27	2.13	117.70	113.62
35	C	515	DGD	O1G-C1A-O1A	-2.13	118.22	123.59
35	c	518	DGD	O1G-C1A-O1A	-2.13	118.23	123.59
25	D	404	BCR	C16-C17-C18	-2.12	124.28	127.31
31	F	101	LMT	C3B-C4B-C5B	-2.12	106.45	110.24
24	a	417	PHO	C1A-C2A-C3A	-2.12	100.82	102.84
25	A	409	BCR	C31-C1-C6	-2.12	106.86	110.30
23	C	505	CLA	CMB-C2B-C1B	2.12	131.73	128.46
25	y	101	BCR	C1-C6-C7	2.12	121.78	115.78
32	c	521	LMG	C1-C2-C3	-2.12	105.58	110.00
23	A	408	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
23	b	606	CLA	CBC-CAC-C3C	-2.12	106.58	112.43
35	C	515	DGD	O6D-C1D-O3G	-2.12	104.95	109.97
25	k	101	BCR	C20-C21-C22	-2.12	124.28	127.31
32	m	101	LMG	C7-O1-C1	-2.12	109.59	113.74
23	A	405	CLA	O2A-CGA-CBA	2.12	118.56	111.91
23	c	509	CLA	CMB-C2B-C3B	2.12	128.65	124.68
23	b	602	CLA	C3B-C4B-NB	2.12	111.95	109.21
23	C	509	CLA	C4-C3-C5	2.12	118.84	115.27
25	b	619	BCR	C16-C15-C14	-2.12	119.13	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	K	103	BCR	C2-C1-C6	2.12	113.74	110.48
29	A	414	PL9	C12-C13-C14	-2.12	122.56	127.66
27	A	418	GOL	C3-C2-C1	-2.12	103.47	111.70
23	b	613	CLA	CHA-C1A-NA	-2.12	121.55	126.40
25	K	101	BCR	C24-C23-C22	-2.12	123.04	126.23
23	B	611	CLA	OBD-CAD-C3D	-2.12	123.43	128.52
23	b	608	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
23	c	505	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
23	c	512	CLA	C11-C10-C8	-2.11	109.09	115.92
23	B	610	CLA	CMA-C3A-C2A	-2.11	105.31	113.83
34	b	625	HTG	C1-C2-C3	-2.11	106.42	110.59
25	T	102	BCR	C7-C6-C5	-2.11	116.35	121.46
23	C	510	CLA	CMD-C2D-C3D	-2.11	122.76	127.61
27	B	624	GOL	C3-C2-C1	-2.11	103.50	111.70
23	C	501	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
32	c	520	LMG	O7-C10-O9	-2.11	118.61	123.70
23	c	503	CLA	C2A-C1A-CHA	-2.11	120.17	123.86
23	b	607	CLA	CMC-C2C-C1C	2.11	128.25	125.04
26	f	102	SQD	C44-O6-C1	-2.11	109.62	113.74
24	A	416	PHO	C6-C5-C3	-2.11	107.94	113.45
25	c	516	BCR	C11-C10-C9	-2.10	124.31	127.31
29	d	404	PL9	C12-C13-C14	-2.10	122.60	127.66
25	y	101	BCR	C35-C13-C14	-2.10	119.98	122.92
25	B	619	BCR	C10-C11-C12	-2.10	116.66	123.22
25	H	101	BCR	C36-C18-C17	-2.10	119.98	122.92
23	b	615	CLA	CMC-C2C-C1C	2.10	128.24	125.04
25	B	618	BCR	C7-C8-C9	-2.10	123.06	126.23
33	b	630	LHG	O7-C7-O9	-2.10	118.63	123.70
23	B	608	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
25	k	101	BCR	C3-C4-C5	-2.10	110.33	114.08
23	b	613	CLA	OBD-CAD-C3D	-2.10	123.47	128.52
26	B	620	SQD	C9-C8-C7	-2.10	106.00	113.62
35	c	519	DGD	O2G-C1B-O1B	-2.10	118.64	123.70
23	c	506	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
25	t	102	BCR	C7-C6-C5	-2.10	116.39	121.46
23	c	503	CLA	C1-O2A-CGA	2.09	121.94	116.44
23	b	610	CLA	CHB-C4A-NA	2.09	127.41	124.51
23	c	513	CLA	CHA-C1A-NA	-2.09	121.60	126.40
33	E	101	LHG	O7-C7-O9	-2.09	118.64	123.70
23	B	608	CLA	C6-C7-C8	-2.09	109.15	115.92
25	B	619	BCR	C37-C22-C21	-2.09	119.99	122.92
25	d	403	BCR	C11-C10-C9	-2.09	124.33	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	620	SQD	O8-S-C6	2.09	109.07	105.74
23	b	602	CLA	O2A-CGA-CBA	2.09	118.46	111.91
26	F	103	SQD	C3-C4-C5	2.09	113.96	110.24
23	A	404	CLA	C7-C6-C5	-2.09	107.69	113.36
23	c	506	CLA	CBC-CAC-C3C	-2.09	106.68	112.43
23	c	513	CLA	CBC-CAC-C3C	-2.09	106.68	112.43
35	H	102	DGD	O6E-C5E-C6E	2.08	111.62	106.44
23	d	401	CLA	CHD-C4C-NC	2.08	127.49	124.20
25	Y	101	BCR	C3-C4-C5	-2.08	110.36	114.08
25	B	619	BCR	C7-C8-C9	-2.08	123.09	126.23
23	C	507	CLA	CHA-C1A-NA	-2.08	121.63	126.40
23	C	512	CLA	C4-C3-C2	-2.08	118.34	123.68
23	c	505	CLA	CED-O2D-CGD	2.08	120.64	115.94
23	B	612	CLA	C7-C6-C5	-2.08	107.72	113.36
38	F	102	HEM	O2D-CGD-O1D	-2.08	118.12	123.30
23	b	616	CLA	C11-C12-C13	-2.08	109.21	115.92
25	a	410	BCR	C33-C5-C6	-2.08	122.20	124.53
31	M	101	LMT	C3B-C4B-C5B	-2.07	106.54	110.24
34	B	622	HTG	C2'-C1'-S1	-2.07	105.70	112.40
23	C	505	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
35	H	102	DGD	C3B-C2B-C1B	-2.07	106.08	113.62
23	B	609	CLA	C7-C6-C5	-2.07	107.73	113.36
23	A	404	CLA	C4-C3-C5	2.07	118.75	115.27
29	D	405	PL9	C12-C13-C14	-2.07	122.68	127.66
23	A	408	CLA	C1-O2A-CGA	2.07	121.87	116.44
32	d	410	LMG	O8-C28-O10	-2.07	118.37	123.59
32	A	419	LMG	O6-C1-O1	-2.07	105.07	109.97
23	C	512	CLA	CBA-CAA-C2A	-2.07	107.76	113.86
25	y	101	BCR	C37-C22-C23	2.07	121.34	118.08
29	D	405	PL9	C30-C29-C31	2.07	118.75	115.27
29	a	415	PL9	C51-C49-C50	2.07	119.17	114.60
25	t	102	BCR	C28-C27-C26	-2.07	110.39	114.08
34	B	623	HTG	O5-C1-C2	2.07	112.91	110.31
29	D	405	PL9	C25-C24-C23	-2.06	118.38	123.68
23	B	613	CLA	CBC-CAC-C3C	-2.06	106.74	112.43
31	t	101	LMT	C1-O1'-C1'	2.06	117.26	113.84
26	B	620	SQD	O47-C7-O49	-2.06	118.72	123.70
23	b	614	CLA	C4-C3-C5	2.06	118.74	115.27
23	c	509	CLA	C2A-C1A-CHA	-2.06	120.25	123.86
23	C	512	CLA	CMB-C2B-C3B	2.06	128.53	124.68
25	C	514	BCR	C3-C4-C5	-2.06	110.40	114.08
32	z	101	LMG	C8-O7-C10	-2.06	112.72	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	619	BCR	C7-C8-C9	-2.06	123.12	126.23
35	h	102	DGD	C3B-C2B-C1B	-2.06	106.14	113.62
23	d	402	CLA	CMA-C3A-C4A	-2.05	106.25	111.77
23	C	513	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
31	B	628	LMT	C1B-C2B-C3B	2.05	114.27	110.00
25	d	403	BCR	C16-C15-C14	-2.05	119.27	123.47
23	c	512	CLA	C2A-C1A-CHA	-2.05	120.27	123.86
23	C	507	CLA	CMB-C2B-C3B	2.05	128.52	124.68
35	C	515	DGD	C3E-C4E-C5E	2.05	113.90	110.24
23	A	406	CLA	CMA-C3A-C4A	-2.05	106.26	111.77
23	B	607	CLA	O2A-CGA-CBA	2.05	118.34	111.91
23	c	505	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
23	b	612	CLA	OBD-CAD-C3D	-2.05	123.59	128.52
32	A	419	LMG	O8-C28-C29	2.05	118.34	111.91
23	A	404	CLA	CHB-C4A-NA	2.05	127.34	124.51
25	b	617	BCR	C21-C20-C19	-2.05	116.83	123.22
23	B	613	CLA	C4-C3-C2	-2.05	118.43	123.68
25	h	101	BCR	C10-C11-C12	-2.04	116.84	123.22
33	D	407	LHG	O4-P-O5	2.04	122.34	112.24
23	b	611	CLA	CBC-CAC-C3C	-2.04	106.80	112.43
23	B	610	CLA	CHB-C4A-NA	2.04	127.33	124.51
24	A	407	PHO	C4-C3-C5	2.04	118.70	115.27
23	b	611	CLA	C7-C6-C5	-2.04	107.82	113.36
23	B	607	CLA	C11-C10-C8	-2.04	109.33	115.92
27	O	303	GOL	C3-C2-C1	-2.04	103.78	111.70
25	B	618	BCR	C28-C27-C26	-2.04	110.44	114.08
25	B	619	BCR	C34-C9-C8	2.04	121.29	118.08
25	t	102	BCR	C2-C1-C6	2.04	113.62	110.48
23	b	602	CLA	C11-C10-C8	-2.04	109.33	115.92
23	B	611	CLA	C2C-C1C-NC	2.04	111.88	109.97
23	b	608	CLA	CMA-C3A-C4A	-2.04	106.30	111.77
31	M	101	LMT	O5B-C5B-C6B	2.03	111.50	106.44
25	d	403	BCR	C37-C22-C23	2.03	121.28	118.08
23	b	614	CLA	CMB-C2B-C3B	2.03	128.49	124.68
23	B	611	CLA	O2A-CGA-CBA	2.03	118.29	111.91
32	c	520	LMG	O8-C28-O10	-2.03	118.46	123.59
25	t	102	BCR	C37-C22-C23	2.03	121.28	118.08
23	c	508	CLA	C2A-C1A-CHA	-2.03	120.31	123.86
23	b	601	CLA	CAA-C2A-C3A	-2.03	107.21	112.78
23	C	508	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
23	a	406	CLA	CAC-C3C-C2C	2.03	131.00	127.53
23	B	614	CLA	CMA-C3A-C2A	-2.03	105.64	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	K	103	BCR	C15-C14-C13	-2.03	124.41	127.31
26	a	411	SQD	O48-C23-O10	-2.03	118.47	123.59
23	b	604	CLA	CHD-C4C-NC	2.03	127.40	124.20
23	B	606	CLA	C11-C10-C8	-2.03	109.36	115.92
23	b	602	CLA	CHB-C4A-NA	2.03	127.32	124.51
23	A	408	CLA	C11-C12-C13	-2.03	109.37	115.92
25	d	403	BCR	C40-C30-C39	2.03	114.75	108.53
29	d	404	PL9	C45-C44-C46	2.03	118.68	115.27
25	a	410	BCR	C15-C16-C17	-2.03	119.33	123.47
23	C	512	CLA	OBD-CAD-C3D	-2.02	123.65	128.52
23	B	606	CLA	C7-C6-C5	-2.02	107.86	113.36
23	C	508	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
24	a	417	PHO	O2A-CGA-CBA	2.02	118.25	111.91
23	B	601	CLA	C1-C2-C3	-2.02	122.55	126.04
23	c	511	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
23	A	406	CLA	CHB-C4A-NA	2.02	127.30	124.51
23	C	507	CLA	C6-C7-C8	-2.02	109.39	115.92
23	c	502	CLA	CMC-C2C-C1C	2.02	128.11	125.04
23	b	609	CLA	C4-C3-C5	2.02	118.66	115.27
23	C	512	CLA	CBC-CAC-C3C	-2.01	106.88	112.43
24	A	416	PHO	CED-O2D-CGD	2.01	120.49	115.94
23	d	401	CLA	CBC-CAC-C3C	-2.01	106.88	112.43
24	a	408	PHO	O2D-CGD-O1D	-2.01	119.90	123.84
25	C	514	BCR	C2-C1-C6	2.01	113.58	110.48
35	C	517	DGD	O3G-C3G-C2G	-2.01	106.04	110.90
25	h	101	BCR	C16-C15-C14	-2.01	119.35	123.47
37	D	401	BCT	O2-C-O1	2.01	124.76	119.55
23	D	402	CLA	CBC-CAC-C3C	-2.01	106.89	112.43
37	a	404	BCT	O2-C-O1	2.01	124.76	119.55
29	D	405	PL9	O2-C1-C6	-2.01	117.11	120.59
23	B	604	CLA	CHA-C1A-NA	-2.01	121.81	126.40
25	c	515	BCR	C31-C1-C6	-2.00	107.05	110.30
32	A	419	LMG	O7-C10-O9	-2.00	118.86	123.70
25	c	516	BCR	C2-C1-C6	2.00	113.56	110.48
23	C	501	CLA	C11-C12-C13	-2.00	109.45	115.92
25	D	404	BCR	C30-C25-C24	2.00	121.44	115.78
23	B	605	CLA	O2A-CGA-CBA	2.00	118.19	111.91

All (63) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404	CLA	ND

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Mol	Chain	Res	Type	Atom
23	A	408	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND
23	B	604	CLA	ND
23	B	605	CLA	ND
23	B	606	CLA	ND
23	B	607	CLA	ND
23	B	609	CLA	ND
23	B	610	CLA	ND
23	B	611	CLA	ND
23	B	612	CLA	ND
23	B	613	CLA	ND
23	B	614	CLA	ND
23	B	615	CLA	ND
23	B	616	CLA	ND
23	C	501	CLA	ND
23	C	502	CLA	ND
23	C	504	CLA	ND
23	C	505	CLA	ND
23	C	506	CLA	ND
23	C	507	CLA	ND
23	C	509	CLA	ND
23	C	510	CLA	ND
23	C	511	CLA	ND
23	C	512	CLA	ND
23	C	513	CLA	ND
23	D	402	CLA	ND
23	D	403	CLA	ND
23	a	405	CLA	ND
23	a	406	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

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Mol	Chain	Res	Type	Atom
23	b	612	CLA	ND
23	b	613	CLA	ND
23	b	614	CLA	ND
23	b	615	CLA	ND
23	b	616	CLA	ND
23	c	502	CLA	ND
23	c	503	CLA	ND
23	c	504	CLA	ND
23	c	505	CLA	ND
23	c	506	CLA	ND
23	c	507	CLA	ND
23	c	508	CLA	ND
23	c	509	CLA	ND
23	c	510	CLA	ND
23	c	511	CLA	ND
23	c	512	CLA	ND
23	c	513	CLA	ND
23	c	514	CLA	ND
23	d	401	CLA	ND
23	d	402	CLA	ND

All (1274) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	408	CLA	C2-C3-C5-C6
23	A	408	CLA	C4-C3-C5-C6
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	C	508	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O2D
23	b	605	CLA	C4-C3-C5-C6
23	b	606	CLA	CHA-CBD-CGD-O1D
23	b	606	CLA	CHA-CBD-CGD-O2D
23	b	614	CLA	CHA-CBD-CGD-O1D
23	b	614	CLA	CHA-CBD-CGD-O2D
23	b	614	CLA	CAD-CBD-CGD-O1D
23	b	614	CLA	CAD-CBD-CGD-O2D
23	c	509	CLA	CHA-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O2D
23	c	510	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
23	c	510	CLA	C11-C10-C8-C9
23	d	402	CLA	C2-C3-C5-C6
23	d	402	CLA	C4-C3-C5-C6
25	B	617	BCR	C1-C6-C7-C8
25	Y	101	BCR	C5-C6-C7-C8
25	b	617	BCR	C1-C6-C7-C8
25	y	101	BCR	C1-C6-C7-C8
25	y	101	BCR	C5-C6-C7-C8
26	A	410	SQD	O49-C7-O47-C45
26	A	412	SQD	O6-C44-C45-O47
26	B	620	SQD	O49-C7-O47-C45
26	F	103	SQD	C2-C1-O6-C44
26	F	103	SQD	O49-C7-O47-C45
26	F	103	SQD	C8-C7-O47-C45
26	a	413	SQD	O6-C44-C45-O47
26	a	413	SQD	C5-C6-S-O7
26	a	413	SQD	C5-C6-S-O8
26	a	413	SQD	C5-C6-S-O9
26	b	620	SQD	O49-C7-O47-C45
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	629	GOL	C1-C2-C3-O3
27	V	203	GOL	C1-C2-C3-O3
27	a	412	GOL	O1-C1-C2-C3
27	a	419	GOL	O1-C1-C2-C3
27	b	624	GOL	C1-C2-C3-O3
27	c	527	GOL	C1-C2-C3-O3
27	c	527	GOL	O2-C2-C3-O3
27	o	302	GOL	C1-C2-C3-O3
27	o	303	GOL	O1-C1-C2-C3
27	o	303	GOL	C1-C2-C3-O3
29	A	414	PL9	C9-C11-C12-C13
29	A	414	PL9	C15-C14-C16-C17
29	A	414	PL9	C14-C16-C17-C18
29	a	415	PL9	C9-C11-C12-C13
29	a	415	PL9	C14-C16-C17-C18
29	a	415	PL9	C25-C24-C26-C27
31	A	417	LMT	C2'-C1'-O1'-C1
31	A	417	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
31	A	421	LMT	O5'-C1'-O1'-C1
31	B	630	LMT	C2'-C1'-O1'-C1
31	B	631	LMT	O5'-C1'-O1'-C1
31	B	631	LMT	C2-C1-O1'-C1'
31	F	101	LMT	C2'-C1'-O1'-C1
31	F	101	LMT	O5'-C1'-O1'-C1
31	T	101	LMT	C2-C1-O1'-C1'
31	b	627	LMT	C2'-C1'-O1'-C1
31	b	627	LMT	O5'-C1'-O1'-C1
31	e	101	LMT	C2'-C1'-O1'-C1
31	e	101	LMT	O5'-C1'-O1'-C1
31	t	101	LMT	O5'-C1'-O1'-C1
31	t	101	LMT	C2-C1-O1'-C1'
32	C	519	LMG	C11-C10-O7-C8
32	c	521	LMG	O9-C10-O7-C8
32	c	521	LMG	C11-C10-O7-C8
32	Z	101	LMG	O9-C10-O7-C8
32	Z	101	LMG	C11-C10-O7-C8
32	z	101	LMG	O6-C1-O1-C7
33	D	406	LHG	O2-C2-C3-O3
33	D	406	LHG	C3-O3-P-O4
33	D	406	LHG	C3-O3-P-O5
33	D	406	LHG	C3-O3-P-O6
33	D	406	LHG	C4-O6-P-O4
33	E	101	LHG	C3-O3-P-O4
33	E	101	LHG	C3-O3-P-O5
33	E	101	LHG	O10-C23-O8-C6
33	E	101	LHG	C24-C23-O8-C6
33	L	101	LHG	C4-O6-P-O4
33	L	101	LHG	C4-O6-P-O5
33	a	421	LHG	C3-O3-P-O4
33	a	421	LHG	C4-O6-P-O5
33	a	421	LHG	O10-C23-O8-C6
33	a	421	LHG	C24-C23-O8-C6
33	b	630	LHG	C4-O6-P-O3
33	b	630	LHG	C4-O6-P-O4
33	b	630	LHG	C4-O6-P-O5
33	d	405	LHG	C3-O3-P-O5
33	d	405	LHG	C4-O6-P-O4
33	d	411	LHG	C3-O3-P-O5
34	B	622	HTG	C2'-C1'-S1-C1
31	A	421	LMT	O5B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
31	B	630	LMT	C4'-C5'-C6'-O6'
31	T	101	LMT	O5'-C5'-C6'-O6'
32	C	519	LMG	O9-C10-O7-C8
31	T	101	LMT	C4B-C5B-C6B-O6B
23	D	403	CLA	C3-C5-C6-C7
23	c	513	CLA	C3-C5-C6-C7
23	d	402	CLA	C3-C5-C6-C7
26	A	410	SQD	C8-C7-O47-C45
26	B	620	SQD	C8-C7-O47-C45
31	m	103	LMT	C4B-C5B-C6B-O6B
31	m	103	LMT	O5B-C5B-C6B-O6B
23	C	504	CLA	C4-C3-C5-C6
23	D	403	CLA	C4-C3-C5-C6
23	D	403	CLA	C2-C3-C5-C6
29	A	414	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
23	b	616	CLA	C3-C5-C6-C7
31	F	101	LMT	O5'-C5'-C6'-O6'
31	c	501	LMT	O5B-C5B-C6B-O6B
32	c	521	LMG	O6-C5-C6-O5
34	b	625	HTG	S1-C1'-C2'-C3'
31	B	628	LMT	C4'-C5'-C6'-O6'
31	B	628	LMT	O5B-C5B-C6B-O6B
31	B	630	LMT	O5B-C5B-C6B-O6B
23	C	501	CLA	CBD-CGD-O2D-CED
23	D	403	CLA	CBD-CGD-O2D-CED
33	E	101	LHG	O2-C2-C3-O3
33	d	405	LHG	O2-C2-C3-O3
23	A	408	CLA	C3-C5-C6-C7
32	C	519	LMG	O6-C5-C6-O5
34	b	625	HTG	O5-C5-C6-O6
31	T	101	LMT	C4'-C5'-C6'-O6'
34	D	410	HTG	C4-C5-C6-O6
32	z	101	LMG	C11-C10-O7-C8
31	B	628	LMT	O5'-C5'-C6'-O6'
34	D	410	HTG	O5-C5-C6-O6
31	B	628	LMT	C6-C7-C8-C9
31	b	621	LMT	O5'-C5'-C6'-O6'
34	D	410	HTG	S1-C1'-C2'-C3'
34	d	409	HTG	S1-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
31	A	421	LMT	O5B-C5B-C6B-O6B
31	A	421	LMT	O5'-C5'-C6'-O6'
31	B	630	LMT	O5'-C5'-C6'-O6'
31	B	631	LMT	O5'-C5'-C6'-O6'
31	T	101	LMT	O5B-C5B-C6B-O6B
31	e	101	LMT	C4'-C5'-C6'-O6'
23	B	605	CLA	C4-C3-C5-C6
23	C	507	CLA	C4-C3-C5-C6
23	b	603	CLA	C4-C3-C5-C6
23	b	614	CLA	C4-C3-C5-C6
23	c	508	CLA	C4-C3-C5-C6
29	A	414	PL9	C20-C19-C21-C22
29	a	415	PL9	C15-C14-C16-C17
29	a	415	PL9	C30-C29-C31-C32
31	c	501	LMT	C4B-C5B-C6B-O6B
23	B	605	CLA	C2-C3-C5-C6
23	C	507	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	PL9	C13-C14-C16-C17
29	a	415	PL9	C13-C14-C16-C17
29	a	415	PL9	C28-C29-C31-C32
23	b	606	CLA	C2A-CAA-CBA-CGA
31	b	627	LMT	O5'-C5'-C6'-O6'
31	t	101	LMT	O5'-C5'-C6'-O6'
31	B	630	LMT	C4B-C5B-C6B-O6B
31	F	101	LMT	C4'-C5'-C6'-O6'
26	B	620	SQD	O5-C1-O6-C44
29	D	405	PL9	C39-C41-C42-C43
34	B	625	HTG	O5-C5-C6-O6
31	A	421	LMT	C4B-C5B-C6B-O6B
23	C	513	CLA	CBD-CGD-O2D-CED
33	d	405	LHG	C1-C2-C3-O3
32	z	101	LMG	O9-C10-O7-C8
31	b	627	LMT	C4'-C5'-C6'-O6'
23	c	510	CLA	CBA-CGA-O2A-C1
32	c	521	LMG	C4-C5-C6-O5
25	T	102	BCR	C13-C14-C15-C16
26	F	103	SQD	C23-C24-C25-C26
23	b	614	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	e	101	LMT	O5B-C5B-C6B-O6B
32	B	621	LMG	C39-C40-C41-C42
32	B	621	LMG	C15-C16-C17-C18
33	D	407	LHG	C33-C34-C35-C36
31	B	631	LMT	C4'-C5'-C6'-O6'
31	A	421	LMT	C2'-C1'-O1'-C1
31	B	631	LMT	C2'-C1'-O1'-C1
31	t	101	LMT	C2'-C1'-O1'-C1
23	C	504	CLA	C2-C3-C5-C6
29	a	415	PL9	C23-C24-C26-C27
23	B	602	CLA	C6-C7-C8-C9
23	C	502	CLA	C14-C13-C15-C16
23	C	506	CLA	C14-C13-C15-C16
23	b	601	CLA	C11-C10-C8-C9
23	b	604	CLA	C6-C7-C8-C9
23	b	616	CLA	C6-C7-C8-C9
23	c	505	CLA	C11-C12-C13-C14
25	b	619	BCR	C7-C8-C9-C34
25	d	403	BCR	C37-C22-C23-C24
25	b	619	BCR	C7-C8-C9-C10
35	C	517	DGD	C6B-C7B-C8B-C9B
26	B	620	SQD	C7-C8-C9-C10
23	c	513	CLA	C15-C16-C17-C18
31	A	421	LMT	C5'-C4'-O1B-C1B
23	A	408	CLA	C5-C6-C7-C8
23	C	508	CLA	C10-C11-C12-C13
23	c	511	CLA	CBD-CGD-O2D-CED
34	b	623	HTG	C1'-C2'-C3'-C4'
31	B	628	LMT	C5'-C4'-O1B-C1B
23	B	601	CLA	C5-C6-C7-C8
23	B	601	CLA	C10-C11-C12-C13
23	C	507	CLA	C5-C6-C7-C8
23	b	601	CLA	C10-C11-C12-C13
31	A	421	LMT	C4'-C5'-C6'-O6'
27	O	302	GOL	O1-C1-C2-O2
27	V	203	GOL	O2-C2-C3-O3
27	a	412	GOL	O1-C1-C2-O2
27	a	419	GOL	O1-C1-C2-O2
31	e	101	LMT	O5'-C5'-C6'-O6'
23	B	606	CLA	C10-C11-C12-C13
23	B	608	CLA	C13-C15-C16-C17
34	b	622	HTG	S1-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
31	c	501	LMT	O1'-C1-C2-C3
23	B	603	CLA	C13-C15-C16-C17
23	b	604	CLA	C8-C10-C11-C12
32	Z	101	LMG	C10-C11-C12-C13
33	E	101	LHG	C23-C24-C25-C26
35	c	518	DGD	C1B-C2B-C3B-C4B
23	C	512	CLA	CBD-CGD-O2D-CED
23	B	602	CLA	C13-C15-C16-C17
23	B	614	CLA	C8-C10-C11-C12
23	B	606	CLA	C11-C10-C8-C7
23	C	510	CLA	C11-C12-C13-C15
23	D	403	CLA	C11-C10-C8-C7
23	b	606	CLA	C12-C13-C15-C16
23	B	610	CLA	C2A-CAA-CBA-CGA
23	c	514	CLA	C10-C11-C12-C13
35	h	102	DGD	C6B-C7B-C8B-C9B
23	c	510	CLA	O1A-CGA-O2A-C1
23	c	514	CLA	CBD-CGD-O2D-CED
31	b	621	LMT	C4'-C5'-C6'-O6'
26	F	103	SQD	O5-C1-O6-C44
31	B	630	LMT	O5'-C1'-O1'-C1
31	b	621	LMT	O5'-C1'-O1'-C1
23	C	512	CLA	C10-C11-C12-C13
29	A	414	PL9	C44-C46-C47-C48
29	d	404	PL9	C39-C41-C42-C43
31	A	421	LMT	O1'-C1-C2-C3
23	B	614	CLA	C10-C11-C12-C13
23	b	605	CLA	C8-C10-C11-C12
23	b	606	CLA	C13-C15-C16-C17
23	b	611	CLA	C15-C16-C17-C18
23	a	409	CLA	CBA-CGA-O2A-C1
31	B	628	LMT	C4B-C5B-C6B-O6B
23	b	606	CLA	C10-C11-C12-C13
23	b	611	CLA	C8-C10-C11-C12
26	b	620	SQD	C18-C19-C20-C21
31	A	417	LMT	O1'-C1-C2-C3
34	b	625	HTG	C4-C5-C6-O6
23	a	405	CLA	C15-C16-C17-C18
23	b	604	CLA	C5-C6-C7-C8
33	E	101	LHG	C3-O3-P-O6
33	E	101	LHG	C4-O6-P-O3
33	L	101	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
33	a	421	LHG	C3-O3-P-O6
33	a	421	LHG	C4-O6-P-O3
33	d	405	LHG	C3-O3-P-O6
26	A	410	SQD	C7-C8-C9-C10
33	D	406	LHG	C1-C2-C3-O3
32	B	621	LMG	O9-C10-O7-C8
23	B	615	CLA	C10-C11-C12-C13
23	D	403	CLA	C10-C11-C12-C13
26	A	410	SQD	C15-C16-C17-C18
26	F	103	SQD	C30-C31-C32-C33
33	L	101	LHG	C12-C13-C14-C15
32	B	621	LMG	C11-C10-O7-C8
23	c	507	CLA	C15-C16-C17-C18
34	B	622	HTG	C1'-C2'-C3'-C4'
26	F	103	SQD	C24-C25-C26-C27
31	A	421	LMT	C3-C4-C5-C6
31	b	627	LMT	C7-C8-C9-C10
32	B	621	LMG	C34-C35-C36-C37
32	D	411	LMG	C19-C20-C21-C22
32	a	418	LMG	C30-C31-C32-C33
33	L	101	LHG	C17-C18-C19-C20
33	d	411	LHG	C16-C17-C18-C19
34	B	623	HTG	C3'-C4'-C5'-C6'
35	c	518	DGD	CAA-CBA-CCA-CDA
31	t	101	LMT	C4'-C5'-C6'-O6'
23	c	510	CLA	C16-C17-C18-C20
34	b	622	HTG	C2'-C3'-C4'-C5'
35	c	518	DGD	C9A-CAA-CBA-CCA
23	C	503	CLA	CBD-CGD-O2D-CED
26	f	102	SQD	C32-C33-C34-C35
31	B	631	LMT	C3-C4-C5-C6
32	D	411	LMG	C35-C36-C37-C38
35	C	516	DGD	CCB-CDB-CEB-CFB
35	h	102	DGD	C7B-C8B-C9B-CAB
26	A	412	SQD	C17-C18-C19-C20
32	C	519	LMG	C18-C19-C20-C21
35	c	517	DGD	C2B-C3B-C4B-C5B
35	c	519	DGD	CBB-CCB-CDB-CEB
35	C	515	DGD	C4B-C5B-C6B-C7B
23	c	510	CLA	C3-C5-C6-C7
31	b	621	LMT	C2'-C1'-O1'-C1
35	C	516	DGD	C2E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
31	e	101	LMT	C4-C5-C6-C7
32	D	411	LMG	C12-C13-C14-C15
32	m	101	LMG	C35-C36-C37-C38
35	C	515	DGD	C5B-C6B-C7B-C8B
35	c	517	DGD	C9A-CAA-CBA-CCA
23	b	606	CLA	C15-C16-C17-C18
23	a	409	CLA	O1A-CGA-O2A-C1
23	B	603	CLA	C16-C17-C18-C19
23	a	409	CLA	C16-C17-C18-C19
23	b	602	CLA	C16-C17-C18-C19
23	b	614	CLA	C16-C17-C18-C20
23	b	615	CLA	C16-C17-C18-C19
23	c	509	CLA	C16-C17-C18-C19
23	d	402	CLA	C16-C17-C18-C20
29	A	414	PL9	C45-C44-C46-C47
33	D	406	LHG	C16-C17-C18-C19
33	a	421	LHG	C26-C27-C28-C29
33	b	630	LHG	C14-C15-C16-C17
35	h	102	DGD	C9A-CAA-CBA-CCA
29	d	404	PL9	C13-C14-C16-C17
23	B	613	CLA	C11-C12-C13-C14
23	a	407	CLA	C11-C12-C13-C14
32	C	519	LMG	C17-C18-C19-C20
33	D	407	LHG	C32-C33-C34-C35
33	L	101	LHG	C15-C16-C17-C18
32	A	419	LMG	C12-C13-C14-C15
33	d	411	LHG	C32-C33-C34-C35
35	c	518	DGD	CBA-CCA-CDA-CEA
27	A	411	GOL	O1-C1-C2-C3
27	B	624	GOL	O1-C1-C2-C3
27	B	629	GOL	O1-C1-C2-C3
27	O	302	GOL	O1-C1-C2-C3
27	O	303	GOL	O1-C1-C2-C3
27	a	412	GOL	C1-C2-C3-O3
31	c	501	LMT	C1-C2-C3-C4
32	Z	101	LMG	O6-C5-C6-O5
31	e	101	LMT	C5-C6-C7-C8
33	L	101	LHG	C25-C26-C27-C28
32	a	418	LMG	C10-C11-C12-C13
26	B	620	SQD	C11-C10-C9-C8
31	B	630	LMT	C5-C6-C7-C8
32	A	419	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
32	D	411	LMG	C30-C31-C32-C33
32	c	520	LMG	C34-C35-C36-C37
33	A	420	LHG	C34-C35-C36-C37
33	d	405	LHG	C11-C10-C9-C8
35	H	102	DGD	C5B-C6B-C7B-C8B
23	B	603	CLA	C16-C17-C18-C20
23	C	502	CLA	C15-C16-C17-C18
26	A	410	SQD	C12-C13-C14-C15
31	B	631	LMT	C11-C10-C9-C8
32	d	410	LMG	C29-C30-C31-C32
35	H	102	DGD	CCB-CDB-CEB-CFB
26	F	103	SQD	C29-C30-C31-C32
31	M	101	LMT	C3-C4-C5-C6
31	t	101	LMT	C4-C5-C6-C7
32	B	621	LMG	C17-C18-C19-C20
32	C	519	LMG	C13-C14-C15-C16
33	L	101	LHG	C13-C14-C15-C16
33	d	405	LHG	C34-C35-C36-C37
31	B	630	LMT	C2-C3-C4-C5
32	m	101	LMG	C39-C40-C41-C42
33	d	406	LHG	C27-C28-C29-C30
32	c	520	LMG	C33-C34-C35-C36
23	C	501	CLA	O1D-CGD-O2D-CED
23	B	615	CLA	C5-C6-C7-C8
23	C	502	CLA	C13-C15-C16-C17
31	A	421	LMT	C2-C1-O1'-C1'
31	F	101	LMT	C2-C1-O1'-C1'
31	b	627	LMT	C2-C1-O1'-C1'
31	T	101	LMT	C7-C8-C9-C10
32	a	418	LMG	C34-C35-C36-C37
34	b	622	HTG	C3'-C4'-C5'-C6'
23	b	602	CLA	C16-C17-C18-C20
23	c	510	CLA	C16-C17-C18-C19
26	a	413	SQD	C31-C32-C33-C34
32	C	518	LMG	C16-C17-C18-C19
33	A	420	LHG	C12-C13-C14-C15
33	b	630	LHG	C16-C17-C18-C19
32	C	519	LMG	C19-C20-C21-C22
33	E	101	LHG	C24-C25-C26-C27
35	c	517	DGD	O6D-C5D-C6D-O5D
23	C	511	CLA	C3-C5-C6-C7
31	A	421	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
29	d	404	PL9	C15-C14-C16-C17
35	c	517	DGD	C2A-C1A-O1G-C1G
23	C	505	CLA	C2-C3-C5-C6
29	A	414	PL9	C12-C11-C9-C8
29	A	414	PL9	C43-C44-C46-C47
29	D	405	PL9	C13-C14-C16-C17
32	m	101	LMG	C11-C10-O7-C8
26	b	620	SQD	C13-C14-C15-C16
23	c	508	CLA	C2A-CAA-CBA-CGA
27	B	624	GOL	O2-C2-C3-O3
27	B	629	GOL	O1-C1-C2-O2
27	a	412	GOL	O2-C2-C3-O3
27	b	624	GOL	O2-C2-C3-O3
26	b	620	SQD	C14-C15-C16-C17
26	f	102	SQD	C25-C26-C27-C28
31	B	631	LMT	C4-C5-C6-C7
32	C	518	LMG	C17-C18-C19-C20
35	c	518	DGD	CBB-CCB-CDB-CEB
31	m	103	LMT	O5'-C5'-C6'-O6'
23	a	409	CLA	C16-C17-C18-C20
23	b	615	CLA	C16-C17-C18-C20
23	d	402	CLA	C16-C17-C18-C19
33	D	407	LHG	C15-C16-C17-C18
35	c	517	DGD	C5A-C6A-C7A-C8A
31	e	101	LMT	C1-C2-C3-C4
32	c	520	LMG	C10-C11-C12-C13
31	b	627	LMT	C3-C4-C5-C6
35	H	102	DGD	C9B-CAB-CBB-CCB
35	c	517	DGD	CAA-CBA-CCA-CDA
32	m	101	LMG	O9-C10-O7-C8
23	B	616	CLA	C2-C1-O2A-CGA
23	b	601	CLA	C2-C1-O2A-CGA
32	D	411	LMG	C36-C37-C38-C39
33	d	411	LHG	C29-C30-C31-C32
23	C	510	CLA	C10-C11-C12-C13
31	b	627	LMT	C5-C6-C7-C8
32	c	520	LMG	C31-C32-C33-C34
35	c	517	DGD	C7A-C8A-C9A-CAA
23	b	614	CLA	C16-C17-C18-C19
32	A	419	LMG	C10-C11-C12-C13
25	D	404	BCR	C23-C24-C25-C26
25	D	404	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
25	Y	101	BCR	C1-C6-C7-C8
25	b	617	BCR	C5-C6-C7-C8
26	a	413	SQD	C25-C26-C27-C28
26	b	620	SQD	C27-C28-C29-C30
35	h	102	DGD	CAA-CBA-CCA-CDA
23	b	614	CLA	C10-C11-C12-C13
35	c	518	DGD	C6A-C7A-C8A-C9A
35	h	102	DGD	C3B-C4B-C5B-C6B
23	C	505	CLA	C4-C3-C5-C6
23	C	510	CLA	C4-C3-C5-C6
23	c	506	CLA	C4-C3-C5-C6
29	A	414	PL9	C30-C29-C31-C32
29	D	405	PL9	C15-C14-C16-C17
23	A	408	CLA	C12-C13-C15-C16
23	B	614	CLA	C11-C10-C8-C7
23	C	510	CLA	C2-C3-C5-C6
23	a	407	CLA	C11-C12-C13-C15
23	c	505	CLA	C12-C13-C15-C16
23	c	506	CLA	C2-C3-C5-C6
31	A	421	LMT	C3'-C4'-O1B-C1B
31	B	628	LMT	C3'-C4'-O1B-C1B
31	b	621	LMT	C3'-C4'-O1B-C1B
23	C	506	CLA	C5-C6-C7-C8
23	C	502	CLA	C16-C17-C18-C19
23	C	512	CLA	CBA-CGA-O2A-C1
32	A	419	LMG	C13-C14-C15-C16
32	m	101	LMG	C38-C39-C40-C41
33	D	407	LHG	C29-C30-C31-C32
23	b	610	CLA	C2A-CAA-CBA-CGA
31	t	101	LMT	O1'-C1-C2-C3
33	D	406	LHG	C13-C14-C15-C16
35	h	102	DGD	C2B-C3B-C4B-C5B
32	A	419	LMG	C36-C37-C38-C39
35	C	515	DGD	C8A-C9A-CAA-CBA
35	c	517	DGD	O1A-C1A-O1G-C1G
23	c	513	CLA	CBA-CGA-O2A-C1
23	b	606	CLA	C16-C17-C18-C20
35	C	516	DGD	O6E-C1E-O5D-C6D
23	D	403	CLA	O1D-CGD-O2D-CED
26	A	412	SQD	C26-C27-C28-C29
26	a	411	SQD	C9-C10-C11-C12
26	b	620	SQD	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
32	A	419	LMG	C19-C20-C21-C22
35	C	517	DGD	C2B-C3B-C4B-C5B
34	B	625	HTG	S1-C1'-C2'-C3'
23	B	601	CLA	C13-C15-C16-C17
23	B	614	CLA	C5-C6-C7-C8
26	B	620	SQD	C34-C35-C36-C37
31	e	101	LMT	C4B-C5B-C6B-O6B
26	A	410	SQD	O6-C44-C45-O47
34	B	622	HTG	C2'-C3'-C4'-C5'
23	c	509	CLA	C16-C17-C18-C20
31	B	630	LMT	C6-C7-C8-C9
35	C	515	DGD	C9A-CAA-CBA-CCA
35	c	518	DGD	C2B-C3B-C4B-C5B
34	b	623	HTG	O5-C5-C6-O6
23	c	514	CLA	C4-C3-C5-C6
32	A	419	LMG	C11-C12-C13-C14
23	B	606	CLA	C11-C10-C8-C9
23	D	403	CLA	C11-C10-C8-C9
23	b	606	CLA	C11-C10-C8-C9
23	c	505	CLA	C14-C13-C15-C16
35	C	515	DGD	O6E-C5E-C6E-O5E
33	b	630	LHG	C13-C14-C15-C16
32	m	101	LMG	C37-C38-C39-C40
32	z	101	LMG	C19-C20-C21-C22
35	c	519	DGD	CBA-CCA-CDA-CEA
25	d	403	BCR	C21-C22-C23-C24
23	A	405	CLA	C1A-C2A-CAA-CBA
32	d	410	LMG	O6-C5-C6-O5
23	B	610	CLA	C16-C17-C18-C20
23	C	502	CLA	C16-C17-C18-C20
31	b	621	LMT	C11-C10-C9-C8
33	D	407	LHG	C17-C18-C19-C20
23	A	406	CLA	C13-C15-C16-C17
26	b	620	SQD	C24-C23-O48-C46
32	a	418	LMG	C35-C36-C37-C38
32	c	520	LMG	C28-C29-C30-C31
31	B	628	LMT	C5-C6-C7-C8
32	A	419	LMG	C20-C21-C22-C23
23	A	404	CLA	C13-C15-C16-C17
23	B	610	CLA	C16-C17-C18-C19
23	d	401	CLA	C16-C17-C18-C20
33	d	406	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
31	B	631	LMT	O1'-C1-C2-C3
31	b	621	LMT	C3-C4-C5-C6
32	a	418	LMG	C29-C30-C31-C32
31	A	421	LMT	C4-C5-C6-C7
32	C	518	LMG	C34-C35-C36-C37
35	c	518	DGD	C4A-C5A-C6A-C7A
26	A	410	SQD	O6-C44-C45-C46
26	A	412	SQD	O6-C44-C45-C46
26	B	620	SQD	C44-C45-C46-O48
26	a	411	SQD	O6-C44-C45-C46
26	f	102	SQD	O6-C44-C45-C46
26	f	102	SQD	C44-C45-C46-O48
32	a	418	LMG	C7-C8-C9-O8
35	H	102	DGD	C7A-C8A-C9A-CAA
33	E	101	LHG	C25-C26-C27-C28
35	C	516	DGD	C2G-C3G-O3G-C1D
35	C	516	DGD	C5D-C6D-O5D-C1E
35	c	518	DGD	C2G-C3G-O3G-C1D
35	c	518	DGD	C5D-C6D-O5D-C1E
35	C	516	DGD	CDA-CEA-CFA-CGA
26	b	620	SQD	C11-C10-C9-C8
35	C	517	DGD	CAB-CBB-CCB-CDB
35	c	517	DGD	C4D-C5D-C6D-O5D
32	d	410	LMG	C10-C11-C12-C13
23	C	512	CLA	O1A-CGA-O2A-C1
35	C	515	DGD	C3B-C4B-C5B-C6B
34	c	522	HTG	C4'-C5'-C6'-C7'
27	A	411	GOL	O1-C1-C2-O2
27	B	629	GOL	O2-C2-C3-O3
27	O	303	GOL	O1-C1-C2-O2
27	o	302	GOL	O2-C2-C3-O3
27	o	303	GOL	O2-C2-C3-O3
23	A	405	CLA	C15-C16-C17-C18
35	c	517	DGD	O6E-C5E-C6E-O5E
29	a	415	PL9	C12-C11-C9-C10
23	B	615	CLA	C16-C17-C18-C19
35	h	102	DGD	CDB-CEB-CFB-CGB
23	c	513	CLA	C10-C11-C12-C13
31	B	628	LMT	C1-C2-C3-C4
34	b	623	HTG	S1-C1'-C2'-C3'
23	a	406	CLA	C2C-C3C-CAC-CBC
33	d	411	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
26	b	620	SQD	C46-C45-O47-C7
32	D	411	LMG	O6-C5-C6-O5
23	b	601	CLA	C8-C10-C11-C12
23	C	509	CLA	C2-C1-O2A-CGA
33	d	406	LHG	C34-C35-C36-C37
26	a	411	SQD	C12-C13-C14-C15
31	c	501	LMT	C3-C4-C5-C6
33	D	406	LHG	C12-C13-C14-C15
23	C	513	CLA	O1D-CGD-O2D-CED
26	B	620	SQD	C30-C31-C32-C33
31	c	501	LMT	C2-C3-C4-C5
23	B	615	CLA	C16-C17-C18-C20
23	B	613	CLA	C13-C15-C16-C17
23	B	610	CLA	C13-C15-C16-C17
23	b	601	CLA	C13-C15-C16-C17
35	h	102	DGD	C9B-CAB-CBB-CCB
35	C	515	DGD	O6D-C5D-C6D-O5D
23	c	513	CLA	C13-C15-C16-C17
23	d	401	CLA	C16-C17-C18-C19
33	d	406	LHG	C29-C30-C31-C32
23	a	409	CLA	C4-C3-C5-C6
23	b	604	CLA	C15-C16-C17-C18
23	A	406	CLA	C12-C13-C15-C16
23	C	504	CLA	C12-C13-C15-C16
23	C	510	CLA	C12-C13-C15-C16
23	C	513	CLA	C11-C10-C8-C7
23	a	409	CLA	C11-C10-C8-C7
23	b	601	CLA	C6-C7-C8-C10
23	b	601	CLA	C11-C10-C8-C7
23	b	606	CLA	C11-C10-C8-C7
23	b	614	CLA	C12-C13-C15-C16
23	c	503	CLA	C11-C12-C13-C15
23	c	505	CLA	C11-C12-C13-C15
23	B	602	CLA	C11-C12-C13-C14
23	C	504	CLA	C14-C13-C15-C16
23	C	505	CLA	C11-C12-C13-C14
23	C	510	CLA	C14-C13-C15-C16
23	C	513	CLA	C11-C10-C8-C9
23	D	403	CLA	C14-C13-C15-C16
23	b	601	CLA	C6-C7-C8-C9
23	c	506	CLA	C11-C12-C13-C14
23	d	402	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
32	A	419	LMG	C39-C40-C41-C42
33	d	406	LHG	C28-C29-C30-C31
23	B	601	CLA	CBA-CGA-O2A-C1
35	C	517	DGD	CAA-CBA-CCA-CDA
23	c	513	CLA	O1A-CGA-O2A-C1
26	a	413	SQD	C16-C17-C18-C19
31	c	501	LMT	C9-C10-C11-C12
31	e	101	LMT	C9-C10-C11-C12
32	B	621	LMG	C36-C37-C38-C39
33	b	630	LHG	C27-C28-C29-C30
26	b	620	SQD	O10-C23-O48-C46
23	c	512	CLA	CBA-CGA-O2A-C1
26	F	103	SQD	C7-C8-C9-C10
32	C	518	LMG	C36-C37-C38-C39
32	m	101	LMG	C14-C15-C16-C17
35	C	516	DGD	C5B-C6B-C7B-C8B
33	E	101	LHG	O6-C4-C5-C6
33	b	630	LHG	O6-C4-C5-C6
33	D	406	LHG	C10-C11-C12-C13
33	D	407	LHG	C13-C14-C15-C16
33	d	406	LHG	C9-C10-C11-C12
35	H	102	DGD	CAB-CBB-CCB-CDB
32	C	518	LMG	C31-C32-C33-C34
31	A	417	LMT	O5B-C5B-C6B-O6B
23	c	511	CLA	C4-C3-C5-C6
29	d	404	PL9	C45-C44-C46-C47
23	c	511	CLA	C2-C3-C5-C6
32	z	101	LMG	C10-C11-C12-C13
32	C	518	LMG	C37-C38-C39-C40
33	A	420	LHG	C26-C27-C28-C29
33	d	405	LHG	C13-C14-C15-C16
26	b	620	SQD	C31-C32-C33-C34
35	C	515	DGD	C7A-C8A-C9A-CAA
23	c	514	CLA	O1D-CGD-O2D-CED
23	c	507	CLA	C3A-C2A-CAA-CBA
35	h	102	DGD	CAB-CBB-CCB-CDB
31	e	101	LMT	C2-C1-O1'-C1'
23	B	612	CLA	C10-C11-C12-C13
35	c	518	DGD	CDA-CEA-CFA-CGA
26	a	413	SQD	O6-C44-C45-C46
26	b	620	SQD	C44-C45-C46-O48
33	a	421	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
33	L	101	LHG	C24-C25-C26-C27
33	a	421	LHG	C10-C11-C12-C13
31	M	101	LMT	O1'-C1-C2-C3
33	b	630	LHG	C12-C13-C14-C15
24	a	408	PHO	O2A-C1-C2-C3
23	B	602	CLA	C15-C16-C17-C18
31	e	101	LMT	C3-C4-C5-C6
32	A	419	LMG	C29-C30-C31-C32
26	A	412	SQD	C27-C28-C29-C30
35	c	518	DGD	C5A-C6A-C7A-C8A
24	a	408	PHO	C4-C3-C5-C6
29	D	405	PL9	C43-C44-C46-C47
32	B	621	LMG	C20-C21-C22-C23
33	L	101	LHG	C11-C12-C13-C14
33	a	421	LHG	C7-C8-C9-C10
34	B	625	HTG	C4'-C5'-C6'-C7'
23	C	512	CLA	O1D-CGD-O2D-CED
26	F	103	SQD	C32-C33-C34-C35
31	m	103	LMT	C7-C8-C9-C10
33	E	101	LHG	O6-C4-C5-O7
32	C	519	LMG	C12-C13-C14-C15
23	B	601	CLA	O1A-CGA-O2A-C1
23	A	406	CLA	C16-C17-C18-C20
33	b	630	LHG	C31-C32-C33-C34
26	a	411	SQD	C34-C35-C36-C37
26	a	411	SQD	O6-C44-C45-O47
26	f	102	SQD	O47-C45-C46-O48
26	F	103	SQD	C24-C23-O48-C46
23	C	503	CLA	O1D-CGD-O2D-CED
23	c	511	CLA	O1D-CGD-O2D-CED
23	b	601	CLA	CAA-CBA-CGA-O2A
35	C	516	DGD	C8B-C9B-CAB-CBB
32	z	101	LMG	C14-C15-C16-C17
33	E	101	LHG	C17-C18-C19-C20
23	b	610	CLA	C15-C16-C17-C18
29	a	415	PL9	C24-C26-C27-C28
33	D	407	LHG	C10-C11-C12-C13
35	h	102	DGD	CBA-CCA-CDA-CEA
23	b	608	CLA	C2-C1-O2A-CGA
23	b	614	CLA	C2-C1-O2A-CGA
32	d	410	LMG	C11-C12-C13-C14
23	C	513	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	b	610	CLA	C11-C12-C13-C14
23	c	503	CLA	C11-C12-C13-C14
23	c	511	CLA	C11-C10-C8-C9
23	c	514	CLA	C6-C7-C8-C9
35	C	517	DGD	CDB-CEB-CFB-CGB
23	C	510	CLA	C13-C15-C16-C17
23	b	615	CLA	C5-C6-C7-C8
23	c	512	CLA	O1A-CGA-O2A-C1
26	F	103	SQD	C34-C35-C36-C37
35	C	516	DGD	C8A-C9A-CAA-CBA
23	B	601	CLA	C2A-CAA-CBA-CGA
25	B	617	BCR	C5-C6-C7-C8
25	H	101	BCR	C23-C24-C25-C26
25	H	101	BCR	C23-C24-C25-C30
25	d	403	BCR	C23-C24-C25-C26
25	d	403	BCR	C23-C24-C25-C30
23	B	601	CLA	C15-C16-C17-C18
32	C	519	LMG	C35-C36-C37-C38
25	D	404	BCR	C37-C22-C23-C24
33	d	411	LHG	C25-C26-C27-C28
25	D	404	BCR	C21-C22-C23-C24
23	c	508	CLA	C5-C6-C7-C8
26	b	620	SQD	C33-C34-C35-C36
23	C	511	CLA	C8-C10-C11-C12
32	z	101	LMG	C20-C21-C22-C23
35	H	102	DGD	CCA-CDA-CEA-CFA
31	t	101	LMT	C7-C8-C9-C10
23	B	602	CLA	C11-C12-C13-C15
23	B	614	CLA	C12-C13-C15-C16
23	C	502	CLA	C12-C13-C15-C16
23	C	505	CLA	C11-C12-C13-C15
23	C	506	CLA	C6-C7-C8-C10
23	D	403	CLA	C12-C13-C15-C16
23	b	615	CLA	C12-C13-C15-C16
23	c	506	CLA	C11-C12-C13-C15
23	c	510	CLA	C11-C10-C8-C7
23	c	511	CLA	C11-C10-C8-C7
24	a	408	PHO	C2-C3-C5-C6
31	F	101	LMT	C2-C3-C4-C5
23	c	510	CLA	C15-C16-C17-C18
23	b	606	CLA	C16-C17-C18-C19
33	L	101	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
33	d	411	LHG	C24-C25-C26-C27
33	b	630	LHG	C34-C35-C36-C37
26	b	620	SQD	C28-C29-C30-C31
35	C	515	DGD	CCA-CDA-CEA-CFA
33	b	630	LHG	C9-C10-C11-C12
34	c	522	HTG	C2'-C1'-S1-C1
23	C	510	CLA	CBA-CGA-O2A-C1
23	b	601	CLA	CBA-CGA-O2A-C1
31	b	627	LMT	C6-C7-C8-C9
32	a	418	LMG	C21-C22-C23-C24
23	B	610	CLA	CAD-CBD-CGD-O2D
23	B	616	CLA	CAD-CBD-CGD-O2D
23	c	502	CLA	CAD-CBD-CGD-O2D
23	c	511	CLA	CAD-CBD-CGD-O2D
23	c	513	CLA	CAD-CBD-CGD-O2D
24	A	407	PHO	CAD-CBD-CGD-O2D
24	a	408	PHO	CAD-CBD-CGD-O2D
26	B	620	SQD	C46-C45-O47-C7
38	F	102	HEM	C2B-C3B-CAB-CBB
34	B	625	HTG	C4-C5-C6-O6
31	F	101	LMT	C4-C5-C6-C7
33	E	101	LHG	C13-C14-C15-C16
26	a	411	SQD	C27-C28-C29-C30
26	A	412	SQD	C24-C23-O48-C46
32	c	521	LMG	C29-C28-O8-C9
35	c	519	DGD	C2A-C1A-O1G-C1G
33	D	406	LHG	C34-C35-C36-C37
33	E	101	LHG	C4-C5-C6-O8
33	b	630	LHG	O6-C4-C5-O7
35	C	516	DGD	C7A-C8A-C9A-CAA
23	B	601	CLA	CHA-CBD-CGD-O1D
23	B	601	CLA	CHA-CBD-CGD-O2D
23	C	502	CLA	CHA-CBD-CGD-O1D
23	c	503	CLA	CHA-CBD-CGD-O1D
23	C	506	CLA	C15-C16-C17-C18
23	B	607	CLA	C3-C5-C6-C7
23	C	510	CLA	O1A-CGA-O2A-C1
26	b	620	SQD	O47-C45-C46-O48
32	a	418	LMG	O7-C8-C9-O8
33	a	421	LHG	O7-C5-C6-O8
27	B	624	GOL	O1-C1-C2-O2
27	B	627	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
27	c	527	GOL	O1-C1-C2-O2
31	A	421	LMT	C5-C6-C7-C8
32	C	518	LMG	C29-C30-C31-C32
29	D	405	PL9	C45-C44-C46-C47
26	B	620	SQD	C24-C25-C26-C27
35	c	518	DGD	C1A-C2A-C3A-C4A
35	C	517	DGD	C8A-C9A-CAA-CBA
23	B	611	CLA	C11-C12-C13-C14
35	C	515	DGD	C4D-C5D-C6D-O5D
23	b	601	CLA	O1A-CGA-O2A-C1
26	F	103	SQD	O10-C23-O48-C46
35	c	519	DGD	O1A-C1A-O1G-C1G
23	b	612	CLA	C8-C10-C11-C12
32	B	621	LMG	C29-C30-C31-C32
23	a	405	CLA	C2C-C3C-CAC-CBC
25	Y	101	BCR	C21-C22-C23-C24
23	a	406	CLA	C1A-C2A-CAA-CBA
33	d	406	LHG	C24-C23-O8-C6
33	A	420	LHG	C32-C33-C34-C35
35	c	519	DGD	C2B-C3B-C4B-C5B
35	h	102	DGD	C6A-C7A-C8A-C9A
31	b	627	LMT	C1-C2-C3-C4
33	D	406	LHG	C4-O6-P-O3
33	d	411	LHG	C3-O3-P-O6
33	a	421	LHG	C23-C24-C25-C26
26	a	411	SQD	C35-C36-C37-C38
23	c	505	CLA	C4-C3-C5-C6
33	D	407	LHG	C2-C3-O3-P
33	d	406	LHG	C2-C3-O3-P
32	C	519	LMG	C4-C5-C6-O5
31	b	621	LMT	C7-C8-C9-C10
32	c	521	LMG	O10-C28-O8-C9
33	D	406	LHG	C4-O6-P-O5
33	E	101	LHG	C4-O6-P-O5
33	a	421	LHG	C4-O6-P-O4
33	d	405	LHG	C3-O3-P-O4
35	C	517	DGD	C7B-C8B-C9B-CAB
31	c	501	LMT	O5'-C1'-O1'-C1
35	c	517	DGD	O6E-C1E-O5D-C6D
23	B	606	CLA	C15-C16-C17-C18
23	b	615	CLA	C10-C11-C12-C13
23	c	507	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
33	L	101	LHG	O6-C4-C5-C6
26	A	410	SQD	C18-C19-C20-C21
23	C	509	CLA	C3-C5-C6-C7
23	B	606	CLA	C16-C17-C18-C19
33	d	411	LHG	C27-C28-C29-C30
35	C	517	DGD	CDA-CEA-CFA-CGA
35	c	517	DGD	CCB-CDB-CEB-CFB
23	B	601	CLA	CAD-CBD-CGD-O1D
23	C	502	CLA	CAD-CBD-CGD-O1D
23	C	504	CLA	CAD-CBD-CGD-O1D
23	C	506	CLA	CAD-CBD-CGD-O1D
23	c	503	CLA	CAD-CBD-CGD-O1D
31	M	101	LMT	C2-C3-C4-C5
35	h	102	DGD	CDA-CEA-CFA-CGA
26	A	412	SQD	O10-C23-O48-C46
31	M	101	LMT	O5'-C5'-C6'-O6'
33	D	407	LHG	C24-C23-O8-C6
33	E	101	LHG	C1-C2-C3-O3
23	C	501	CLA	C16-C17-C18-C20
23	B	610	CLA	C12-C13-C15-C16
23	B	616	CLA	C12-C13-C15-C16
23	b	604	CLA	C6-C7-C8-C10
23	b	616	CLA	C6-C7-C8-C10
23	c	506	CLA	C12-C13-C15-C16
23	c	507	CLA	C11-C10-C8-C7
23	c	510	CLA	C6-C7-C8-C10
33	d	406	LHG	O10-C23-O8-C6
23	B	601	CLA	CAA-CBA-CGA-O2A
32	c	520	LMG	C29-C30-C31-C32
35	C	516	DGD	C1A-C2A-C3A-C4A
35	C	517	DGD	C6A-C7A-C8A-C9A
33	D	407	LHG	O10-C23-O8-C6
35	c	517	DGD	C8B-C9B-CAB-CBB
26	A	410	SQD	C34-C35-C36-C37
26	B	620	SQD	O47-C45-C46-O48
33	E	101	LHG	O7-C5-C6-O8
26	A	412	SQD	C30-C31-C32-C33
26	a	413	SQD	C26-C27-C28-C29
26	a	411	SQD	C11-C12-C13-C14
23	c	514	CLA	C2-C3-C5-C6
35	H	102	DGD	O2G-C1B-C2B-C3B
23	A	406	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	B	603	CLA	C11-C12-C13-C14
23	B	610	CLA	C14-C13-C15-C16
23	B	614	CLA	C14-C13-C15-C16
23	C	506	CLA	C6-C7-C8-C9
23	D	403	CLA	C6-C7-C8-C9
23	b	615	CLA	C14-C13-C15-C16
23	c	510	CLA	C8-C10-C11-C12
32	Z	101	LMG	C11-C12-C13-C14
23	d	402	CLA	O1A-CGA-O2A-C1
24	a	408	PHO	C8-C10-C11-C12
25	K	103	BCR	C7-C8-C9-C34
25	Y	101	BCR	C37-C22-C23-C24
23	C	506	CLA	C16-C17-C18-C20
34	b	622	HTG	C1'-C2'-C3'-C4'
29	a	415	PL9	C12-C11-C9-C8
23	c	507	CLA	C13-C15-C16-C17
33	d	411	LHG	C34-C35-C36-C37
23	B	611	CLA	C8-C10-C11-C12
26	B	620	SQD	C29-C30-C31-C32
33	d	406	LHG	C32-C33-C34-C35
23	b	601	CLA	C3-C5-C6-C7
23	C	501	CLA	C2A-CAA-CBA-CGA
23	A	408	CLA	C2-C1-O2A-CGA
23	B	613	CLA	C2-C1-O2A-CGA
23	C	506	CLA	C2-C1-O2A-CGA
23	c	514	CLA	C2-C1-O2A-CGA
26	A	410	SQD	C16-C17-C18-C19
23	B	606	CLA	C8-C10-C11-C12
32	C	518	LMG	C30-C31-C32-C33
33	d	405	LHG	O10-C23-O8-C6
33	L	101	LHG	O6-C4-C5-O7
31	B	628	LMT	C9-C10-C11-C12
23	C	512	CLA	C3-C5-C6-C7
29	A	414	PL9	C28-C29-C31-C32
33	d	405	LHG	C24-C23-O8-C6
23	a	406	CLA	C4C-C3C-CAC-CBC
23	b	602	CLA	C10-C11-C12-C13
26	A	412	SQD	O5-C1-O6-C44
35	c	518	DGD	O6E-C1E-O5D-C6D
35	C	515	DGD	C6A-C7A-C8A-C9A
23	b	612	CLA	C10-C11-C12-C13
26	A	412	SQD	C2-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
31	c	501	LMT	C2'-C1'-O1'-C1
35	c	517	DGD	C2E-C1E-O5D-C6D
35	c	518	DGD	C2E-C1E-O5D-C6D
33	L	101	LHG	C26-C27-C28-C29
23	c	510	CLA	C10-C11-C12-C13
33	L	101	LHG	C27-C28-C29-C30
23	a	409	CLA	C15-C16-C17-C18
23	B	603	CLA	C11-C12-C13-C15
23	B	613	CLA	C11-C12-C13-C15
23	C	505	CLA	C12-C13-C15-C16
23	a	409	CLA	C2-C3-C5-C6
23	b	608	CLA	C12-C13-C15-C16
23	B	614	CLA	C11-C10-C8-C9
23	C	510	CLA	C11-C12-C13-C14
23	a	409	CLA	C11-C10-C8-C9
23	c	506	CLA	C14-C13-C15-C16
23	c	507	CLA	C11-C10-C8-C9
23	c	510	CLA	C6-C7-C8-C9
23	B	606	CLA	C16-C17-C18-C20
32	a	418	LMG	C31-C32-C33-C34
23	c	508	CLA	C8-C10-C11-C12
23	a	405	CLA	C4C-C3C-CAC-CBC
32	a	418	LMG	O8-C28-C29-C30
33	D	407	LHG	C27-C28-C29-C30
23	B	613	CLA	C15-C16-C17-C18
35	c	517	DGD	C4B-C5B-C6B-C7B
33	d	411	LHG	C1-C2-C3-O3
34	b	622	HTG	O5-C5-C6-O6
23	B	603	CLA	C4-C3-C5-C6
32	d	410	LMG	C28-C29-C30-C31
27	o	303	GOL	O1-C1-C2-O2
35	H	102	DGD	CDB-CEB-CFB-CGB
23	d	402	CLA	CBA-CGA-O2A-C1
31	b	627	LMT	O1'-C1-C2-C3
31	c	501	LMT	C7-C8-C9-C10
33	d	406	LHG	C33-C34-C35-C36
23	C	507	CLA	C2A-CAA-CBA-CGA
35	c	519	DGD	CDA-CEA-CFA-CGA
38	F	102	HEM	CAD-CBD-CGD-O1D
32	d	410	LMG	C35-C36-C37-C38
23	b	609	CLA	C2-C3-C5-C6
26	A	410	SQD	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
32	z	101	LMG	C13-C14-C15-C16
33	b	630	LHG	C25-C26-C27-C28
23	B	608	CLA	C2-C1-O2A-CGA
23	C	513	CLA	C2-C1-O2A-CGA
23	c	504	CLA	C8-C10-C11-C12
23	c	503	CLA	C16-C17-C18-C19
33	D	406	LHG	C11-C10-C9-C8
32	Z	101	LMG	C2-C1-O1-C7
38	f	101	HEM	CAD-CBD-CGD-O1D
26	F	103	SQD	O47-C45-C46-O48
33	a	421	LHG	C24-C25-C26-C27
31	e	101	LMT	C2B-C1B-O1B-C4'
32	B	621	LMG	C32-C33-C34-C35
23	b	601	CLA	C4-C3-C5-C6
29	a	415	PL9	C4-C3-C7-C8
35	h	102	DGD	CCB-CDB-CEB-CFB
32	B	621	LMG	O8-C28-C29-C30
23	A	408	CLA	C11-C12-C13-C14
23	B	614	CLA	C6-C7-C8-C9
23	C	512	CLA	C6-C7-C8-C9
23	a	407	CLA	C6-C7-C8-C9
23	b	616	CLA	C11-C10-C8-C9
23	c	513	CLA	C6-C7-C8-C9
23	B	605	CLA	C5-C6-C7-C8
35	c	518	DGD	C7B-C8B-C9B-CAB
32	A	419	LMG	C7-C8-C9-O8
32	B	621	LMG	C14-C15-C16-C17
32	Z	101	LMG	C19-C20-C21-C22
33	L	101	LHG	C23-C24-C25-C26
23	c	512	CLA	C8-C10-C11-C12
32	C	519	LMG	C20-C21-C22-C23
35	H	102	DGD	C8A-C9A-CAA-CBA
32	B	621	LMG	O6-C1-O1-C7
23	a	406	CLA	C15-C16-C17-C18
31	A	417	LMT	C7-C8-C9-C10
26	A	410	SQD	C13-C14-C15-C16
32	d	410	LMG	C18-C19-C20-C21
35	C	517	DGD	C7A-C8A-C9A-CAA
23	B	604	CLA	C1A-C2A-CAA-CBA
23	B	611	CLA	C1A-C2A-CAA-CBA
23	C	501	CLA	C1A-C2A-CAA-CBA
23	c	514	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
35	c	519	DGD	CDB-CEB-CFB-CGB
23	C	513	CLA	C11-C12-C13-C15
23	b	601	CLA	C11-C12-C13-C15
23	b	603	CLA	C11-C10-C8-C7
23	b	614	CLA	C11-C10-C8-C7
23	c	513	CLA	C12-C13-C15-C16
23	A	404	CLA	C2C-C3C-CAC-CBC
33	A	420	LHG	C18-C19-C20-C21
33	b	630	LHG	C17-C18-C19-C20
31	B	631	LMT	C6-C7-C8-C9
32	a	418	LMG	C13-C14-C15-C16
38	f	101	HEM	CAD-CBD-CGD-O2D
40	V	201	HEC	CAD-CBD-CGD-O1D
23	C	510	CLA	C8-C10-C11-C12
26	a	413	SQD	C24-C23-O48-C46
33	D	406	LHG	C26-C27-C28-C29
33	d	405	LHG	C16-C17-C18-C19
23	b	616	CLA	C4-C3-C5-C6
29	d	404	PL9	C43-C44-C46-C47
35	c	519	DGD	O6D-C5D-C6D-O5D
38	F	102	HEM	CAD-CBD-CGD-O2D
34	B	622	HTG	C3'-C4'-C5'-C6'
32	z	101	LMG	O7-C10-C11-C12
25	t	102	BCR	C13-C14-C15-C16
23	b	613	CLA	C5-C6-C7-C8
31	T	101	LMT	C3-C4-C5-C6
26	f	102	SQD	C7-C8-C9-C10
23	A	406	CLA	C16-C17-C18-C19
32	B	621	LMG	C21-C22-C23-C24
26	a	413	SQD	O10-C23-O48-C46
29	A	414	PL9	C39-C41-C42-C43
32	Z	101	LMG	C29-C28-O8-C9
29	a	415	PL9	C45-C44-C46-C47
23	b	613	CLA	C2-C1-O2A-CGA
23	b	601	CLA	C2-C3-C5-C6
31	A	417	LMT	C2B-C1B-O1B-C4'
40	V	201	HEC	CAD-CBD-CGD-O2D
32	A	419	LMG	C18-C19-C20-C21
33	A	420	LHG	C29-C30-C31-C32
35	c	517	DGD	CAB-CBB-CCB-CDB
23	b	608	CLA	C16-C17-C18-C20
35	C	517	DGD	C3B-C4B-C5B-C6B

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Mol	Chain	Res	Type	Atoms
25	c	515	BCR	C23-C24-C25-C30
25	h	101	BCR	C23-C24-C25-C30
25	y	101	BCR	C23-C24-C25-C30
35	C	517	DGD	C4A-C5A-C6A-C7A
27	A	418	GOL	O1-C1-C2-C3
27	l	102	GOL	O1-C1-C2-C3
27	v	202	GOL	O1-C1-C2-C3
32	d	410	LMG	C19-C20-C21-C22
29	D	405	PL9	C35-C34-C36-C37
25	K	103	BCR	C7-C8-C9-C10
25	y	101	BCR	C21-C22-C23-C24
23	b	605	CLA	C5-C6-C7-C8
23	b	616	CLA	C5-C6-C7-C8
29	a	415	PL9	C43-C44-C46-C47
35	h	102	DGD	O2G-C1B-C2B-C3B
38	f	101	HEM	CAA-CBA-CGA-O2A
26	B	620	SQD	C31-C32-C33-C34
23	A	404	CLA	C16-C17-C18-C19
32	m	101	LMG	C32-C33-C34-C35
33	A	420	LHG	C35-C36-C37-C38
31	F	101	LMT	C9-C10-C11-C12
33	b	630	LHG	C10-C11-C12-C13
35	C	517	DGD	C9A-CAA-CBA-CCA
23	B	613	CLA	C11-C10-C8-C7
23	a	407	CLA	C6-C7-C8-C10
23	c	509	CLA	C12-C13-C15-C16
23	D	403	CLA	C8-C10-C11-C12
33	L	101	LHG	C16-C17-C18-C19
27	A	418	GOL	O1-C1-C2-O2
23	b	607	CLA	C3-C5-C6-C7
23	D	403	CLA	O1A-CGA-O2A-C1
31	T	101	LMT	C1-C2-C3-C4
23	C	512	CLA	CAA-CBA-CGA-O2A
32	B	621	LMG	C2-C1-O1-C7
32	m	101	LMG	C2-C1-O1-C7
26	a	413	SQD	C18-C19-C20-C21
31	e	101	LMT	C2-C3-C4-C5
32	d	410	LMG	C16-C17-C18-C19
23	b	611	CLA	C13-C15-C16-C17
31	B	630	LMT	C3-C4-C5-C6
33	A	420	LHG	O8-C23-C24-C25
23	c	512	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	B	603	CLA	C2-C3-C5-C6
23	c	505	CLA	C2-C3-C5-C6
35	c	518	DGD	C9B-CAB-CBB-CCB
35	h	102	DGD	CCA-CDA-CEA-CFA
23	B	616	CLA	C14-C13-C15-C16
23	C	505	CLA	C14-C13-C15-C16
23	a	407	CLA	C14-C13-C15-C16
23	b	601	CLA	C11-C12-C13-C14
23	b	603	CLA	C11-C10-C8-C9
23	b	614	CLA	C14-C13-C15-C16
23	C	506	CLA	C3A-C2A-CAA-CBA
23	B	613	CLA	CAA-CBA-CGA-O2A
32	a	418	LMG	C33-C34-C35-C36
40	v	201	HEC	CAD-CBD-CGD-O2D
23	B	603	CLA	CAD-CBD-CGD-O2D
23	B	604	CLA	CAD-CBD-CGD-O2D
23	B	612	CLA	CAD-CBD-CGD-O2D
23	C	512	CLA	CAD-CBD-CGD-O2D
23	b	604	CLA	CAD-CBD-CGD-O2D
23	b	607	CLA	CAD-CBD-CGD-O2D
23	b	610	CLA	CAD-CBD-CGD-O2D
23	b	616	CLA	CAD-CBD-CGD-O2D
23	c	506	CLA	CAD-CBD-CGD-O2D
24	a	417	PHO	CAD-CBD-CGD-O2D
33	D	407	LHG	C28-C29-C30-C31
33	b	630	LHG	C30-C31-C32-C33
32	Z	101	LMG	O7-C10-C11-C12
33	L	101	LHG	O7-C7-C8-C9
33	a	421	LHG	O8-C23-C24-C25
23	b	609	CLA	C4-C3-C5-C6
29	A	414	PL9	C25-C24-C26-C27
23	b	605	CLA	C3-C5-C6-C7
32	B	621	LMG	C30-C31-C32-C33
32	c	520	LMG	C32-C33-C34-C35
23	b	616	CLA	C2-C3-C5-C6
32	c	520	LMG	C30-C31-C32-C33
24	A	407	PHO	C2C-C3C-CAC-CBC
24	A	416	PHO	C2C-C3C-CAC-CBC
24	a	408	PHO	C2C-C3C-CAC-CBC
24	a	417	PHO	C2C-C3C-CAC-CBC
32	B	621	LMG	O1-C7-C8-C9
23	b	610	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
33	b	630	LHG	O7-C7-C8-C9
26	b	620	SQD	C30-C31-C32-C33
31	F	101	LMT	C6-C7-C8-C9
38	f	101	HEM	CAA-CBA-CGA-O1A
23	A	404	CLA	C15-C16-C17-C18
23	B	602	CLA	O2A-C1-C2-C3
24	A	407	PHO	O2A-C1-C2-C3
23	A	404	CLA	C4C-C3C-CAC-CBC
38	F	102	HEM	C4B-C3B-CAB-CBB
40	v	201	HEC	CAD-CBD-CGD-O1D
35	C	517	DGD	CBA-CCA-CDA-CEA
23	C	506	CLA	C16-C17-C18-C19
26	f	102	SQD	C26-C27-C28-C29
23	A	405	CLA	CHA-CBD-CGD-O1D
23	A	405	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	502	CLA	CHA-CBD-CGD-O2D
23	C	504	CLA	CHA-CBD-CGD-O1D
23	C	507	CLA	CHA-CBD-CGD-O1D
23	C	507	CLA	CHA-CBD-CGD-O2D
23	a	406	CLA	CHA-CBD-CGD-O1D
23	a	406	CLA	CHA-CBD-CGD-O2D
23	b	601	CLA	CHA-CBD-CGD-O1D
23	c	503	CLA	CHA-CBD-CGD-O2D
23	c	508	CLA	CHA-CBD-CGD-O1D
23	c	508	CLA	CHA-CBD-CGD-O2D
23	c	510	CLA	CHA-CBD-CGD-O2D
31	A	417	LMT	O5B-C1B-O1B-C4'
23	B	608	CLA	C16-C17-C18-C20
23	C	510	CLA	CAA-CBA-CGA-O2A
23	c	511	CLA	CAA-CBA-CGA-O2A
32	c	520	LMG	O7-C10-C11-C12
26	b	620	SQD	C10-C11-C12-C13
33	A	420	LHG	C17-C18-C19-C20
33	d	411	LHG	C13-C14-C15-C16
32	c	521	LMG	O1-C7-C8-O7
35	C	516	DGD	CAB-CBB-CCB-CDB
23	c	513	CLA	CAA-CBA-CGA-O2A
26	a	413	SQD	C15-C16-C17-C18
24	A	407	PHO	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	b	601	CLA	CAA-CBA-CGA-O1A
23	B	607	CLA	C12-C13-C15-C16
23	a	406	CLA	C11-C12-C13-C15
23	b	610	CLA	C16-C17-C18-C19
29	A	414	PL9	C4-C3-C7-C8
31	A	417	LMT	C9-C10-C11-C12
23	B	605	CLA	C11-C12-C13-C14
23	C	511	CLA	C11-C12-C13-C14
23	b	606	CLA	C14-C13-C15-C16
23	b	608	CLA	C14-C13-C15-C16
23	b	614	CLA	C11-C12-C13-C14
23	B	612	CLA	CBA-CGA-O2A-C1
23	B	612	CLA	O1A-CGA-O2A-C1
33	d	411	LHG	C18-C19-C20-C21
23	B	602	CLA	C2A-CAA-CBA-CGA
23	B	614	CLA	C2A-CAA-CBA-CGA
23	C	503	CLA	C2A-CAA-CBA-CGA
33	b	630	LHG	C24-C25-C26-C27
34	b	623	HTG	C4'-C5'-C6'-C7'
23	b	604	CLA	C13-C15-C16-C17
32	d	410	LMG	C40-C41-C42-C43
27	B	627	GOL	C1-C2-C3-O3
27	b	629	GOL	C1-C2-C3-O3
27	c	527	GOL	O1-C1-C2-C3
27	l	102	GOL	C1-C2-C3-O3
29	D	405	PL9	C28-C29-C31-C32
23	C	512	CLA	CAA-CBA-CGA-O1A
25	b	619	BCR	C21-C22-C23-C24
23	D	403	CLA	CBA-CGA-O2A-C1
23	b	616	CLA	CBA-CGA-O2A-C1
23	c	507	CLA	C1A-C2A-CAA-CBA
32	Z	101	LMG	O9-C10-C11-C12
33	A	420	LHG	O10-C23-C24-C25
23	b	616	CLA	O1A-CGA-O2A-C1
26	A	412	SQD	C31-C32-C33-C34
23	b	603	CLA	C5-C6-C7-C8
33	a	421	LHG	O10-C23-C24-C25
33	b	630	LHG	O9-C7-C8-C9
26	F	103	SQD	C44-C45-C46-O48
35	c	517	DGD	O2G-C1B-C2B-C3B
23	b	602	CLA	C2A-CAA-CBA-CGA
23	B	613	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
26	f	102	SQD	C34-C35-C36-C37
33	E	101	LHG	O7-C7-C8-C9
33	d	405	LHG	C4-O6-P-O5
23	A	408	CLA	C16-C17-C18-C19
23	b	610	CLA	C16-C17-C18-C20
23	c	511	CLA	O1A-CGA-O2A-C1
32	A	419	LMG	C15-C16-C17-C18
25	K	101	BCR	C23-C24-C25-C30
25	h	101	BCR	C23-C24-C25-C26
25	y	101	BCR	C23-C24-C25-C26
32	c	520	LMG	O9-C10-C11-C12
33	L	101	LHG	O9-C7-C8-C9
32	D	411	LMG	C34-C35-C36-C37
23	c	503	CLA	C16-C17-C18-C20
35	c	517	DGD	C1A-C2A-C3A-C4A
23	c	513	CLA	CAA-CBA-CGA-O1A
25	a	410	BCR	C19-C20-C21-C22
31	c	501	LMT	C4-C5-C6-C7
32	a	418	LMG	C14-C15-C16-C17
29	d	404	PL9	C11-C12-C13-C14
32	c	520	LMG	C4-C5-C6-O5
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	601	CLA	CAD-CBD-CGD-O1D
23	b	605	CLA	CAD-CBD-CGD-O1D
23	b	609	CLA	CAD-CBD-CGD-O1D
23	c	505	CLA	CAD-CBD-CGD-O1D
23	c	507	CLA	CAD-CBD-CGD-O1D
26	f	102	SQD	O5-C5-C6-S
26	a	411	SQD	C10-C11-C12-C13
23	b	613	CLA	CAA-CBA-CGA-O2A
23	b	608	CLA	C13-C15-C16-C17
23	B	607	CLA	C14-C13-C15-C16
23	B	615	CLA	C14-C13-C15-C16
23	C	512	CLA	C11-C10-C8-C9
23	a	406	CLA	C11-C12-C13-C14
23	B	612	CLA	C8-C10-C11-C12
23	b	605	CLA	C13-C15-C16-C17
35	C	517	DGD	O1A-C1A-O1G-C1G
32	B	621	LMG	C37-C38-C39-C40
32	D	411	LMG	C16-C17-C18-C19

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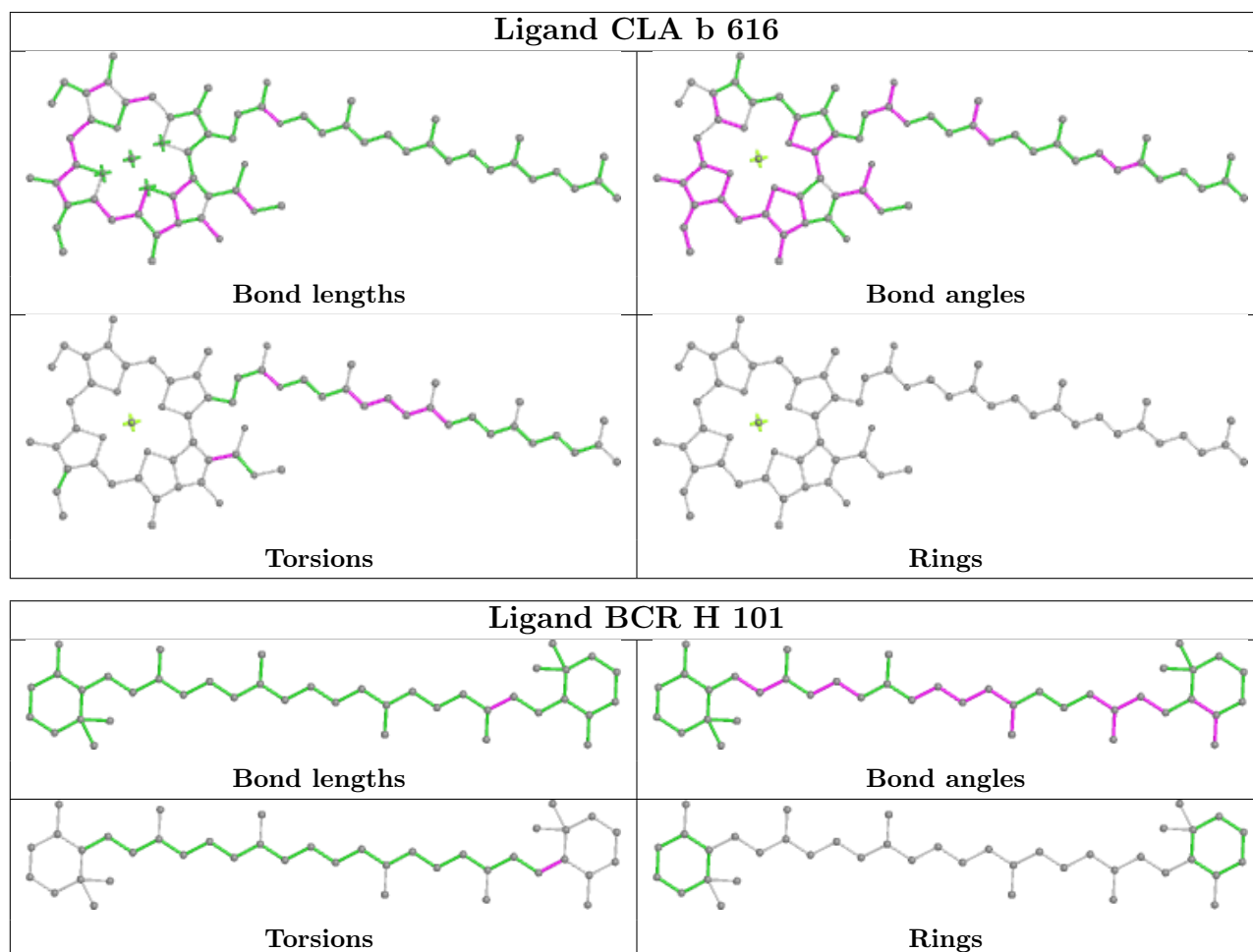
Mol	Chain	Res	Type	Atoms
26	A	412	SQD	O48-C23-C24-C25
26	a	413	SQD	O48-C23-C24-C25
33	D	407	LHG	O8-C23-C24-C25
35	C	517	DGD	O1G-C1A-C2A-C3A
32	d	410	LMG	C38-C39-C40-C41
32	D	411	LMG	O7-C10-C11-C12
26	a	411	SQD	C19-C20-C21-C22
31	B	630	LMT	C7-C8-C9-C10
29	D	405	PL9	C40-C39-C41-C42
23	b	604	CLA	C10-C11-C12-C13
32	B	621	LMG	C18-C19-C20-C21
35	c	517	DGD	CBA-CCA-CDA-CEA
23	B	601	CLA	C11-C12-C13-C15
23	B	602	CLA	C6-C7-C8-C10
23	B	605	CLA	C11-C12-C13-C15
23	C	501	CLA	C11-C12-C13-C15
23	C	506	CLA	C12-C13-C15-C16
23	b	615	CLA	C11-C12-C13-C15
23	c	511	CLA	C12-C13-C15-C16
33	E	101	LHG	O8-C23-C24-C25
35	C	516	DGD	O2G-C1B-C2B-C3B
33	D	406	LHG	C28-C29-C30-C31
25	d	403	BCR	C7-C8-C9-C10
33	D	407	LHG	O10-C23-C24-C25
35	c	517	DGD	O1B-C1B-C2B-C3B
35	C	516	DGD	C3A-C4A-C5A-C6A
31	B	628	LMT	C2-C1-O1'-C1'
31	m	103	LMT	C2-C1-O1'-C1'
32	m	101	LMG	O6-C1-O1-C7
23	C	510	CLA	CAA-CBA-CGA-O1A
23	c	511	CLA	CAA-CBA-CGA-O1A
26	a	413	SQD	O10-C23-C24-C25
32	D	411	LMG	O9-C10-C11-C12
26	A	412	SQD	O10-C23-C24-C25
33	E	101	LHG	O9-C7-C8-C9
33	E	101	LHG	O10-C23-C24-C25
23	b	602	CLA	C8-C10-C11-C12
35	C	516	DGD	O1B-C1B-C2B-C3B

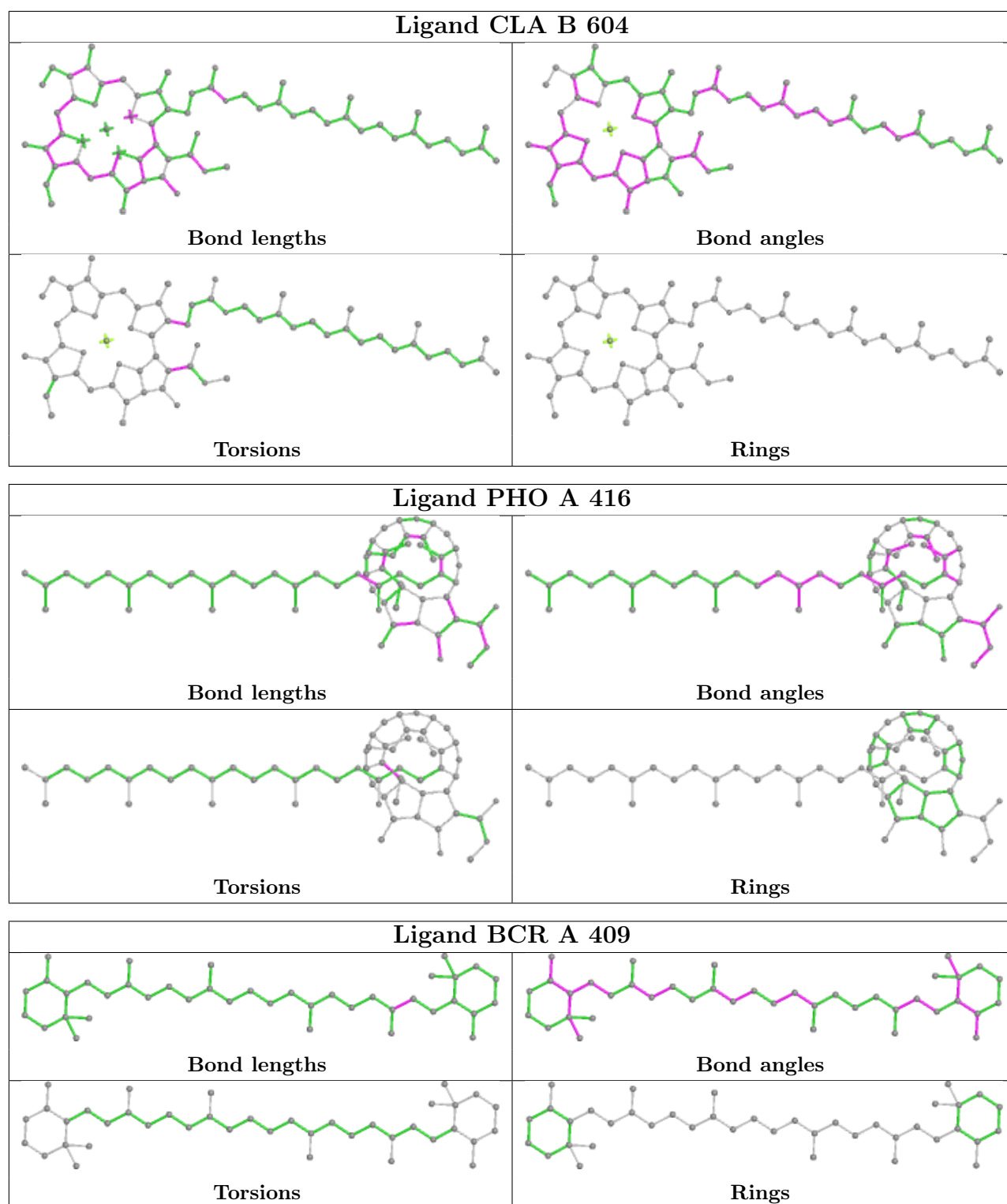
There are no ring outliers.

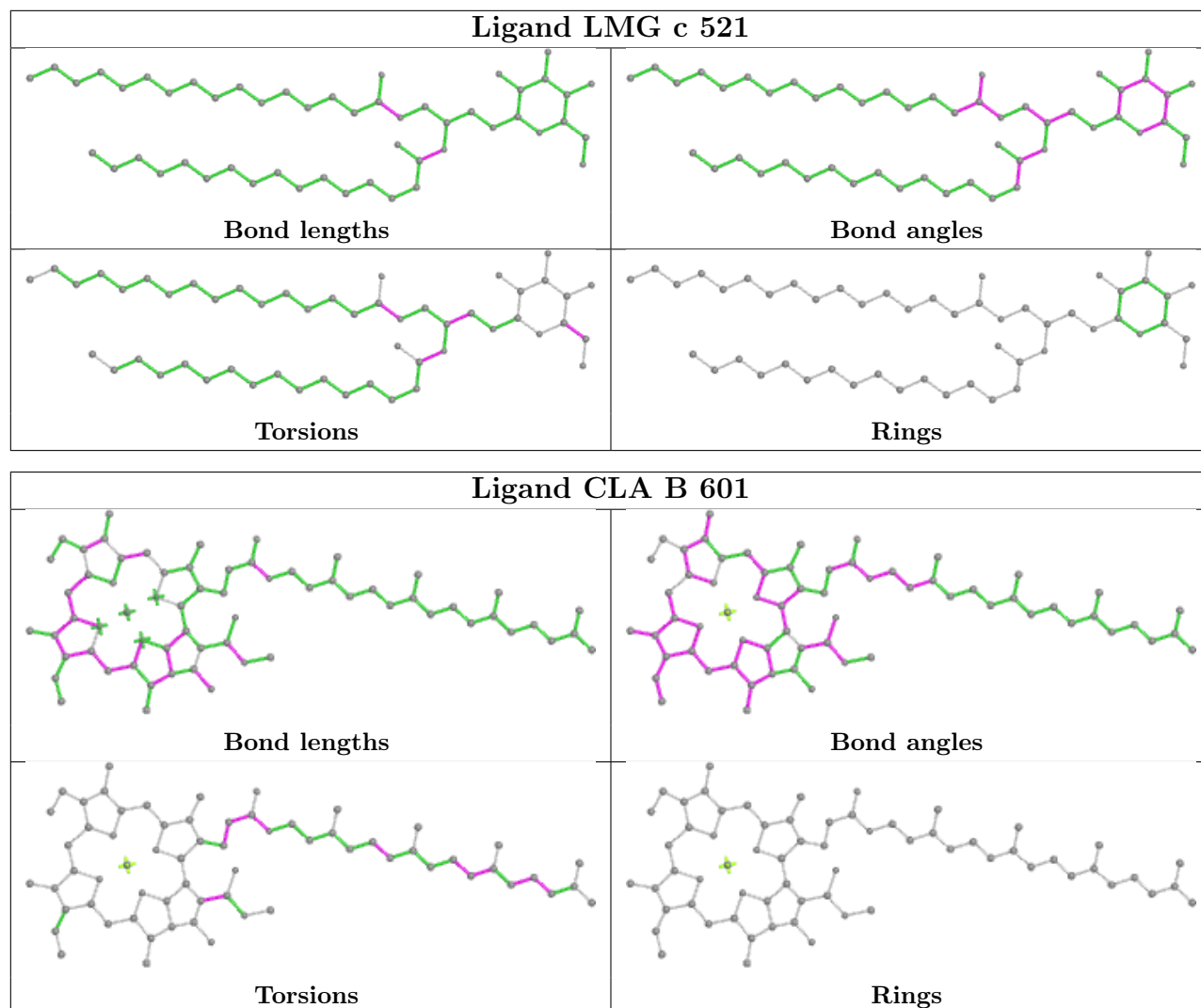
No monomer is involved in short contacts.

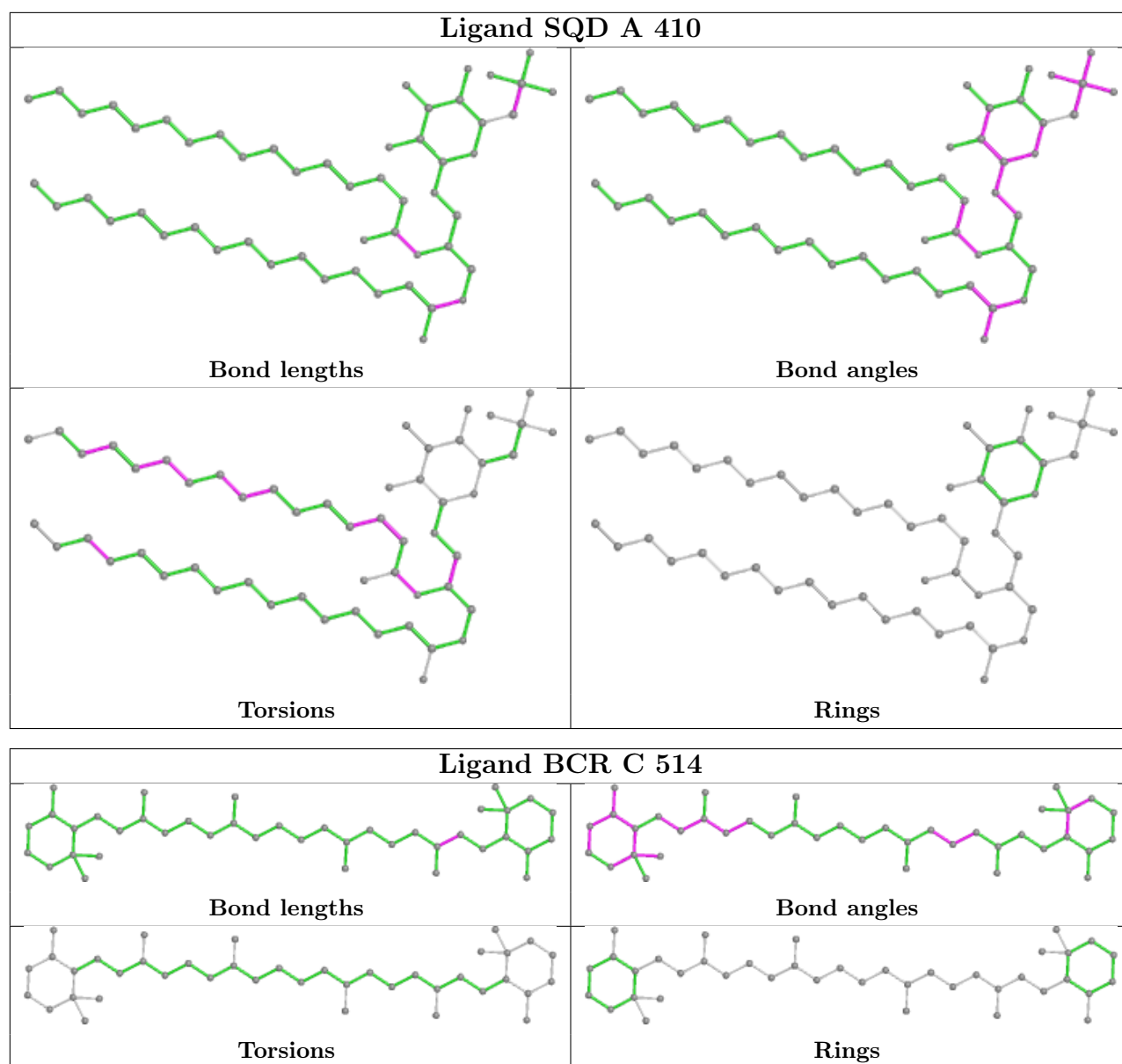
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

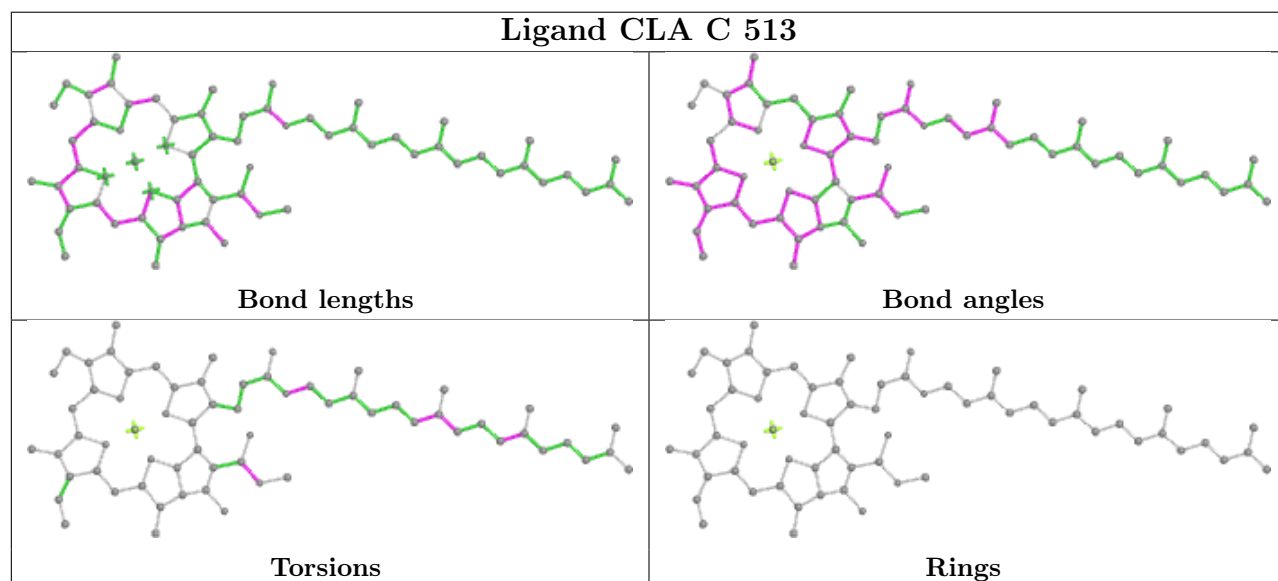
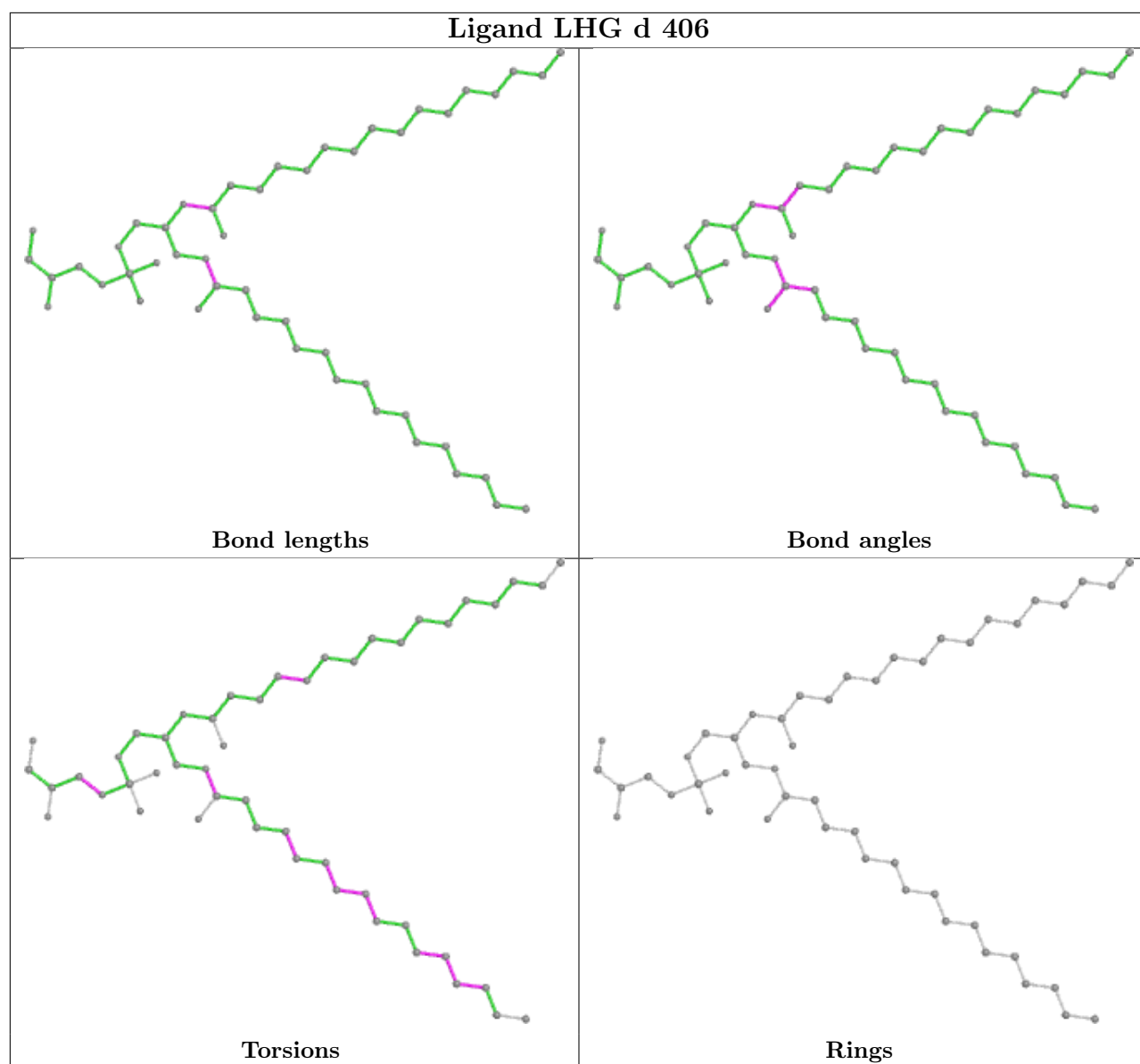
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

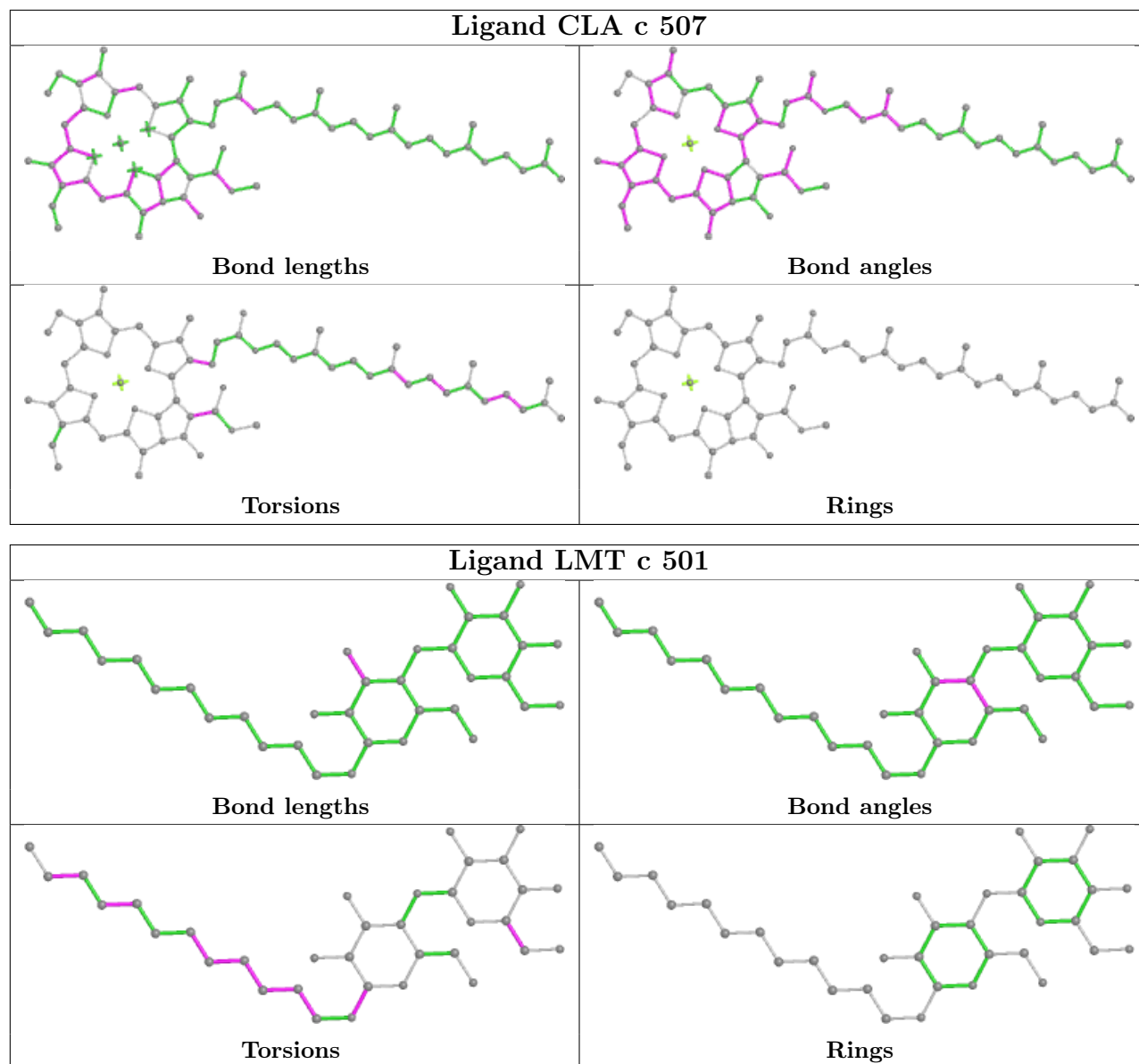


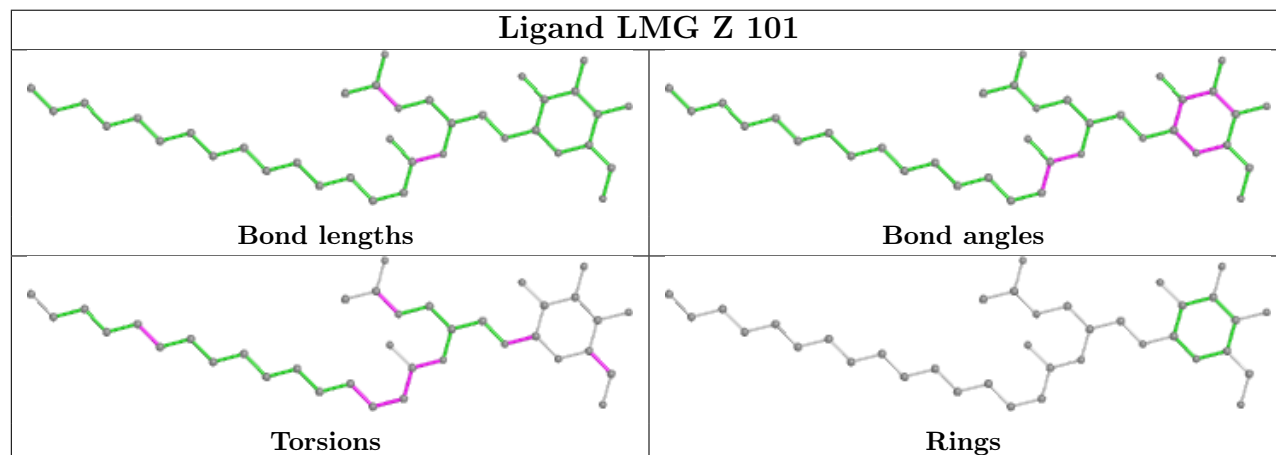
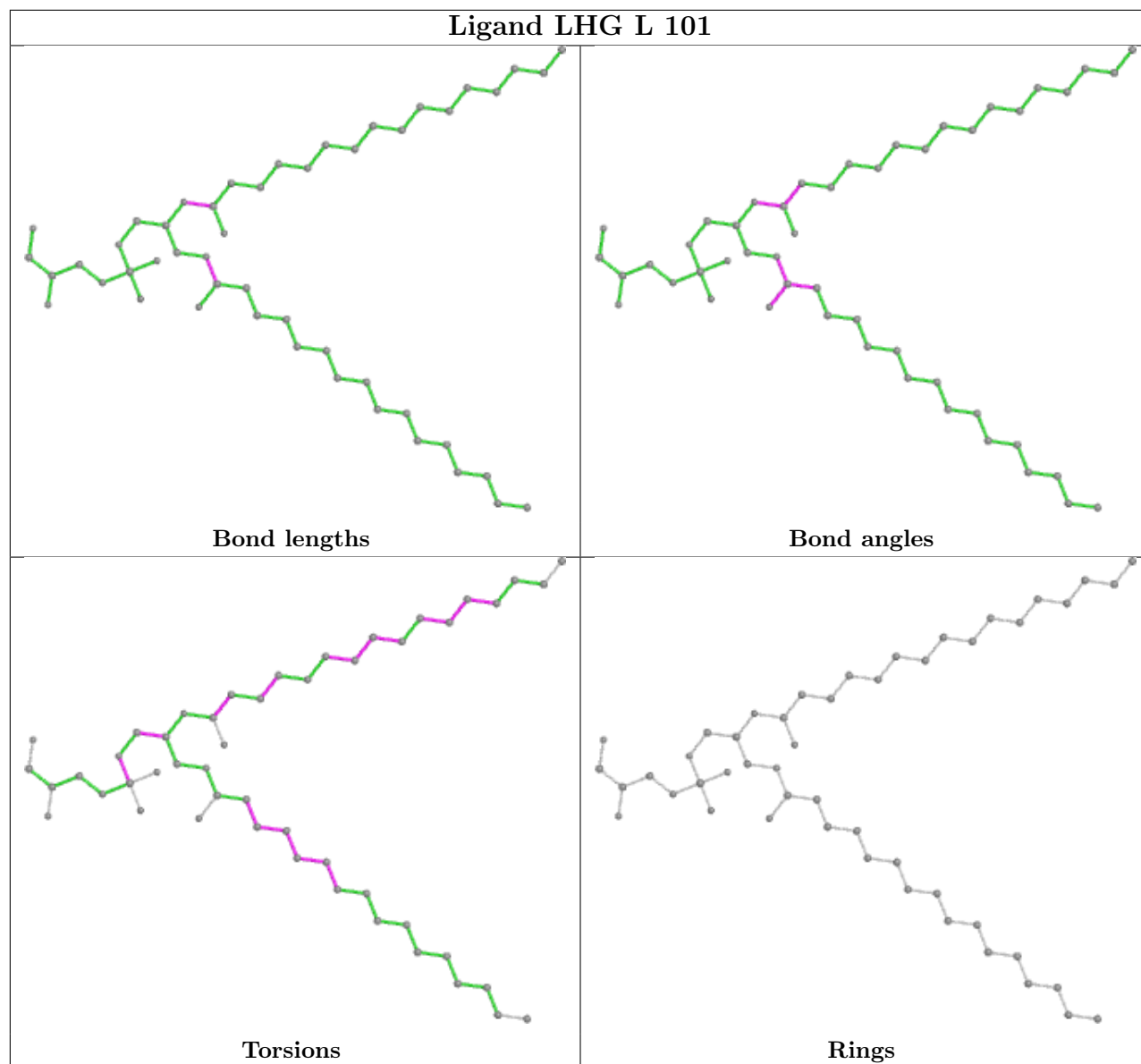


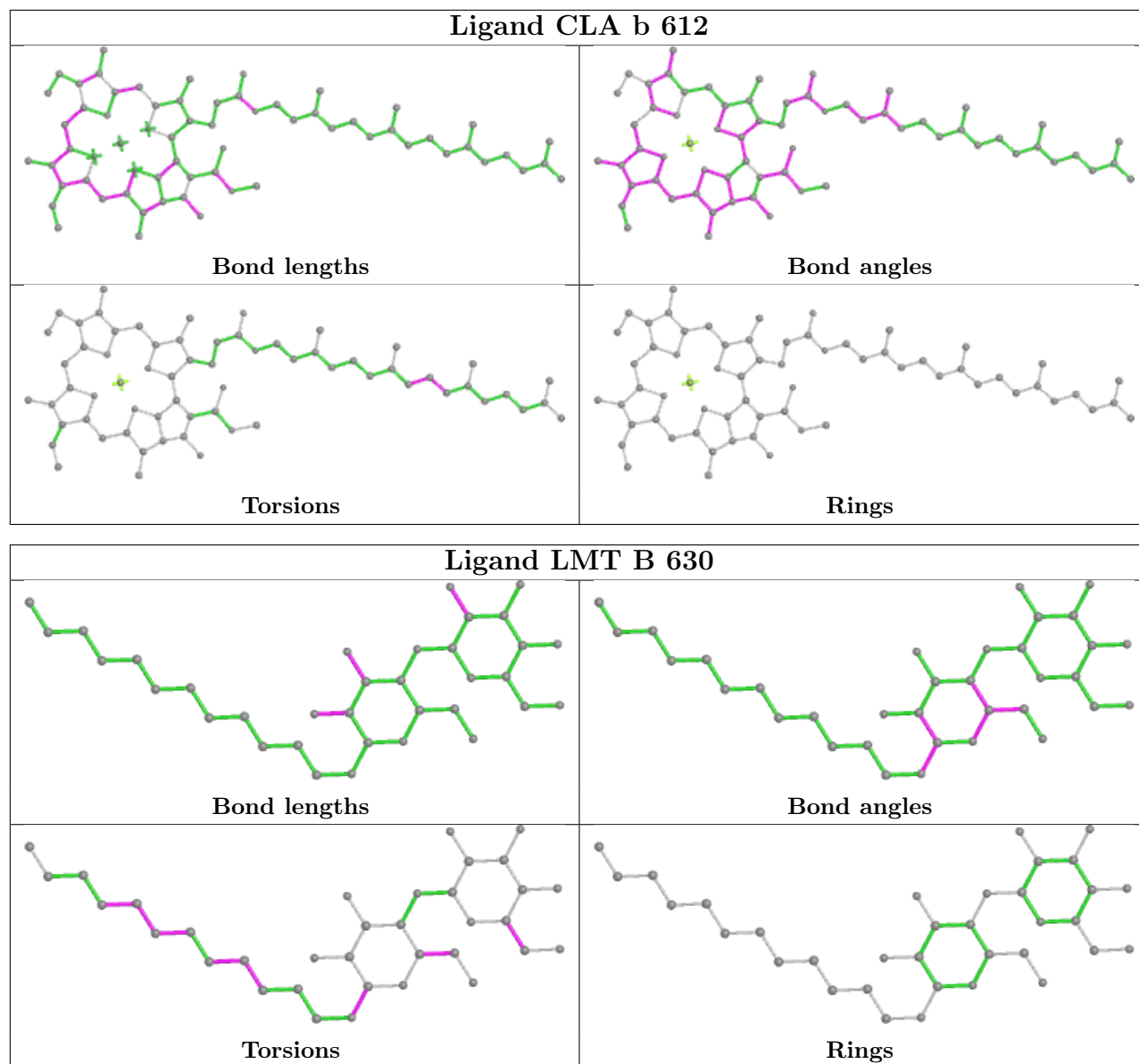


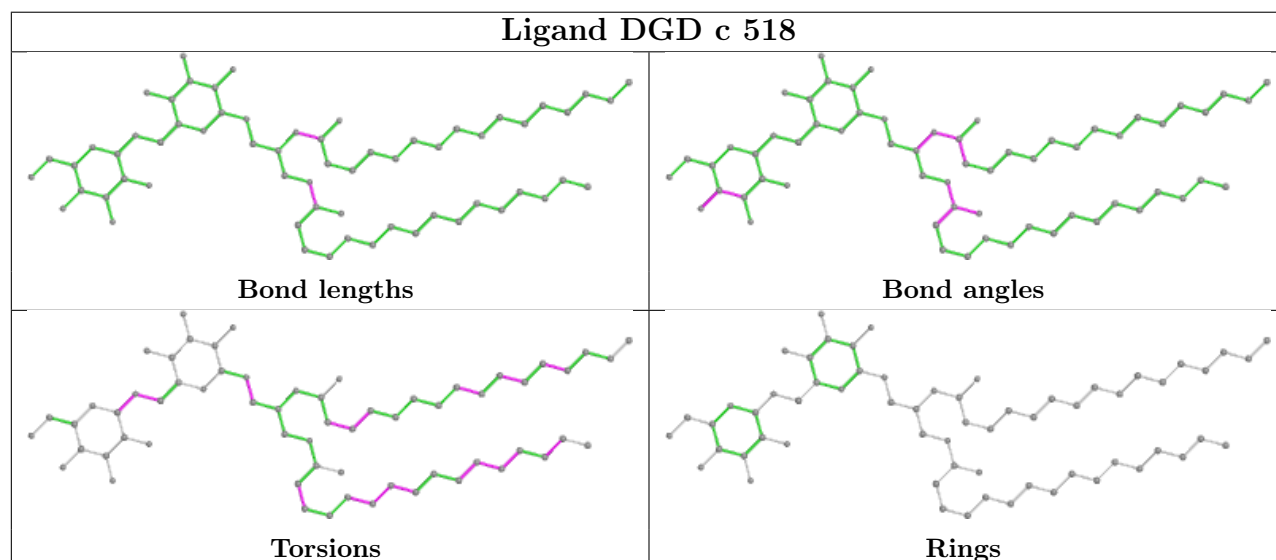
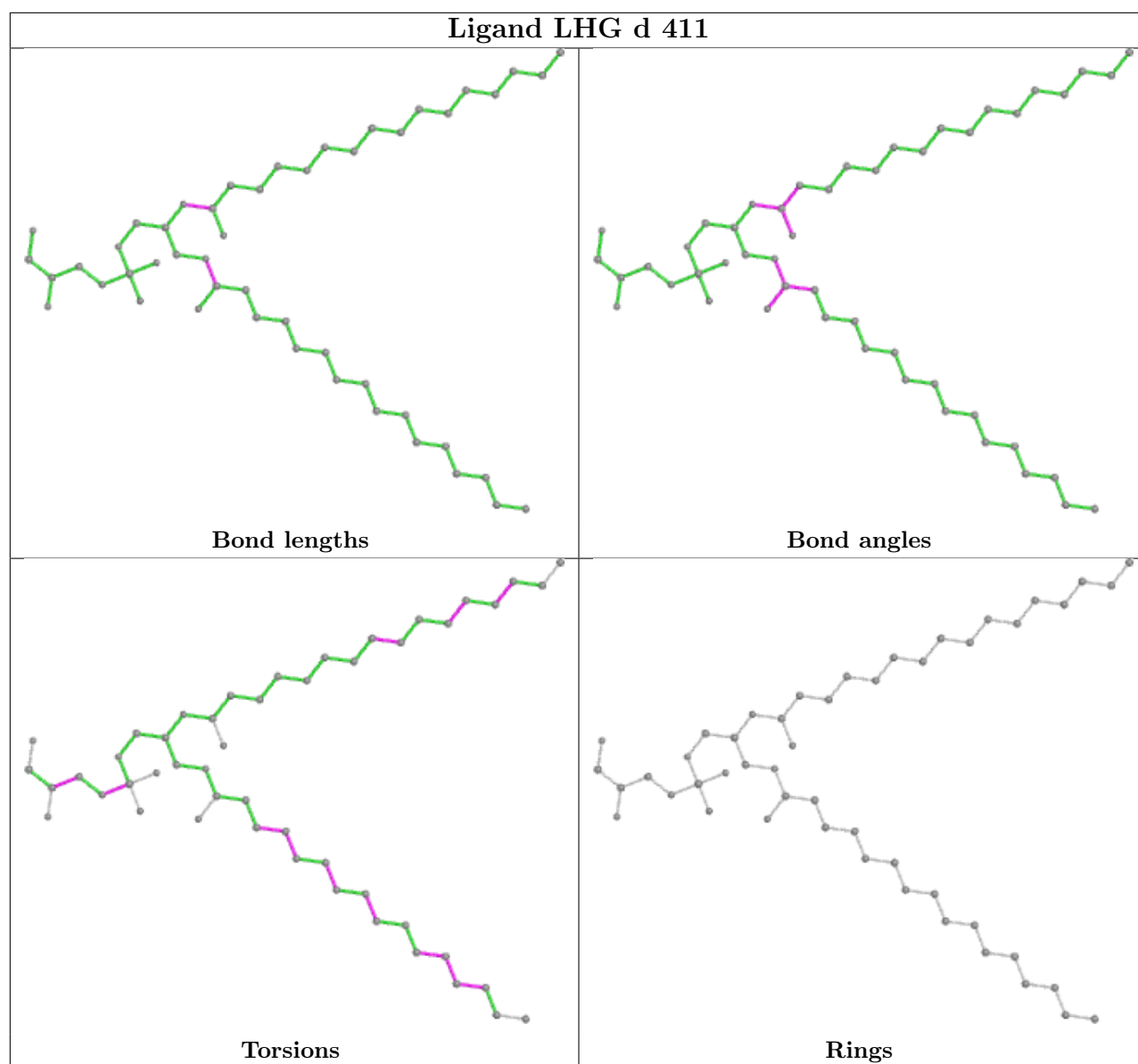


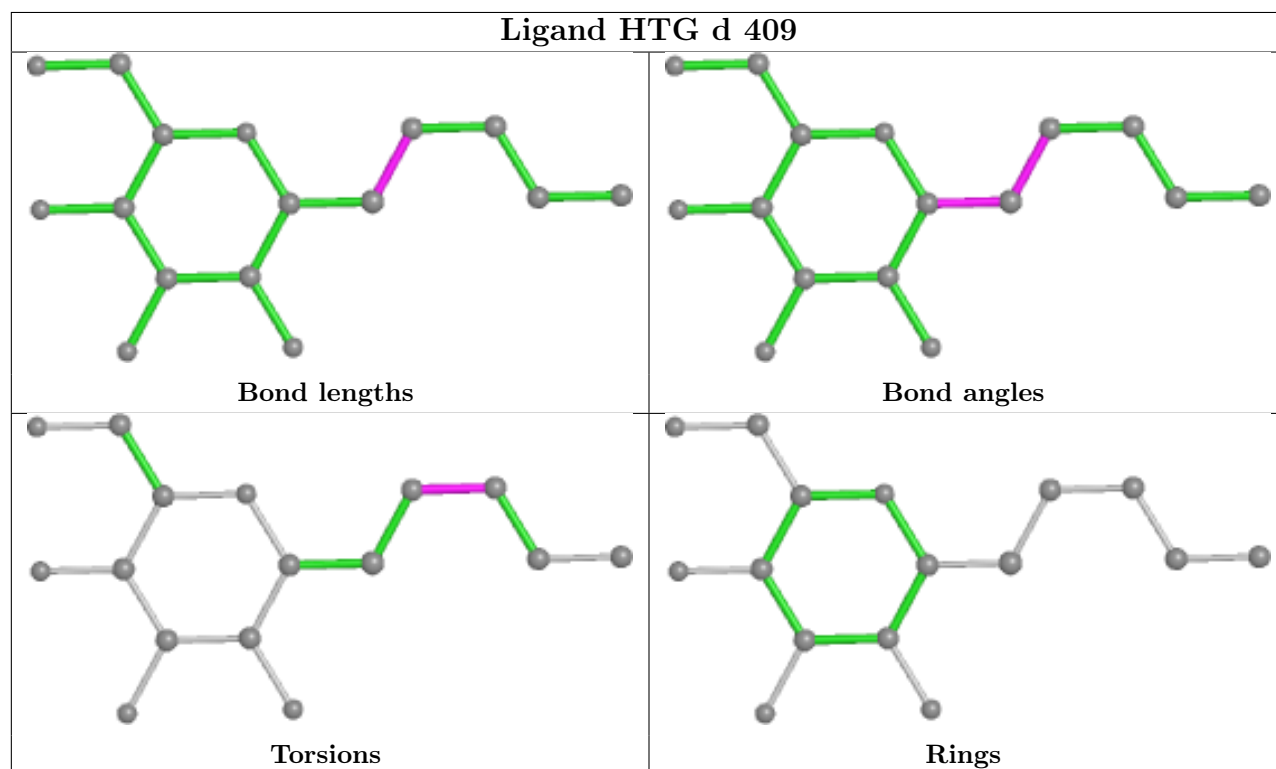
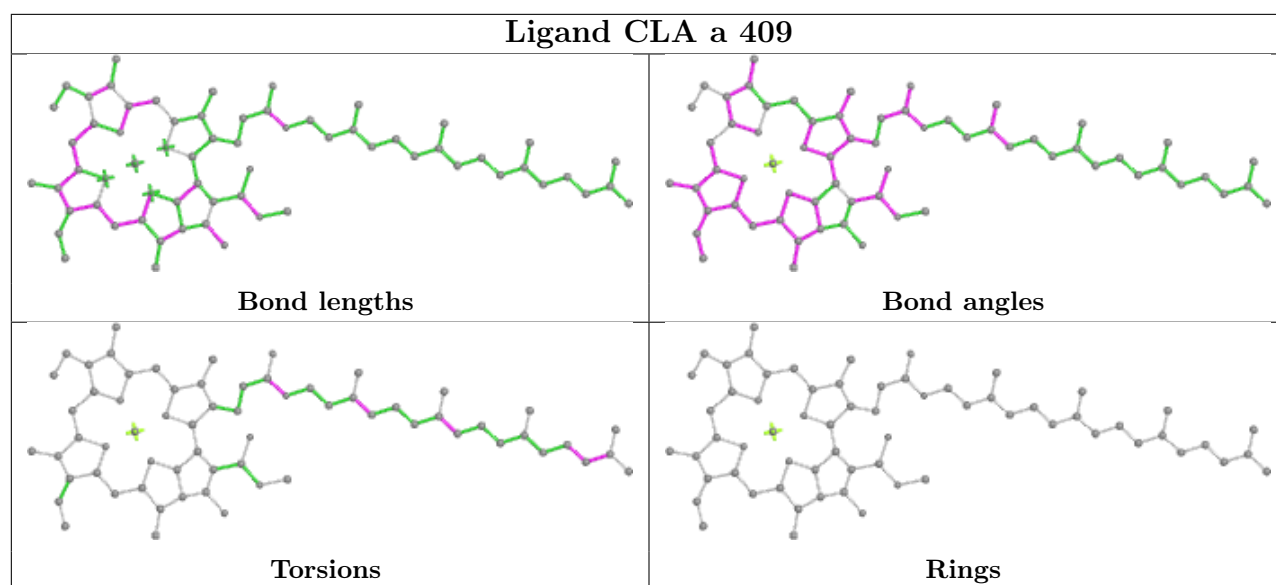


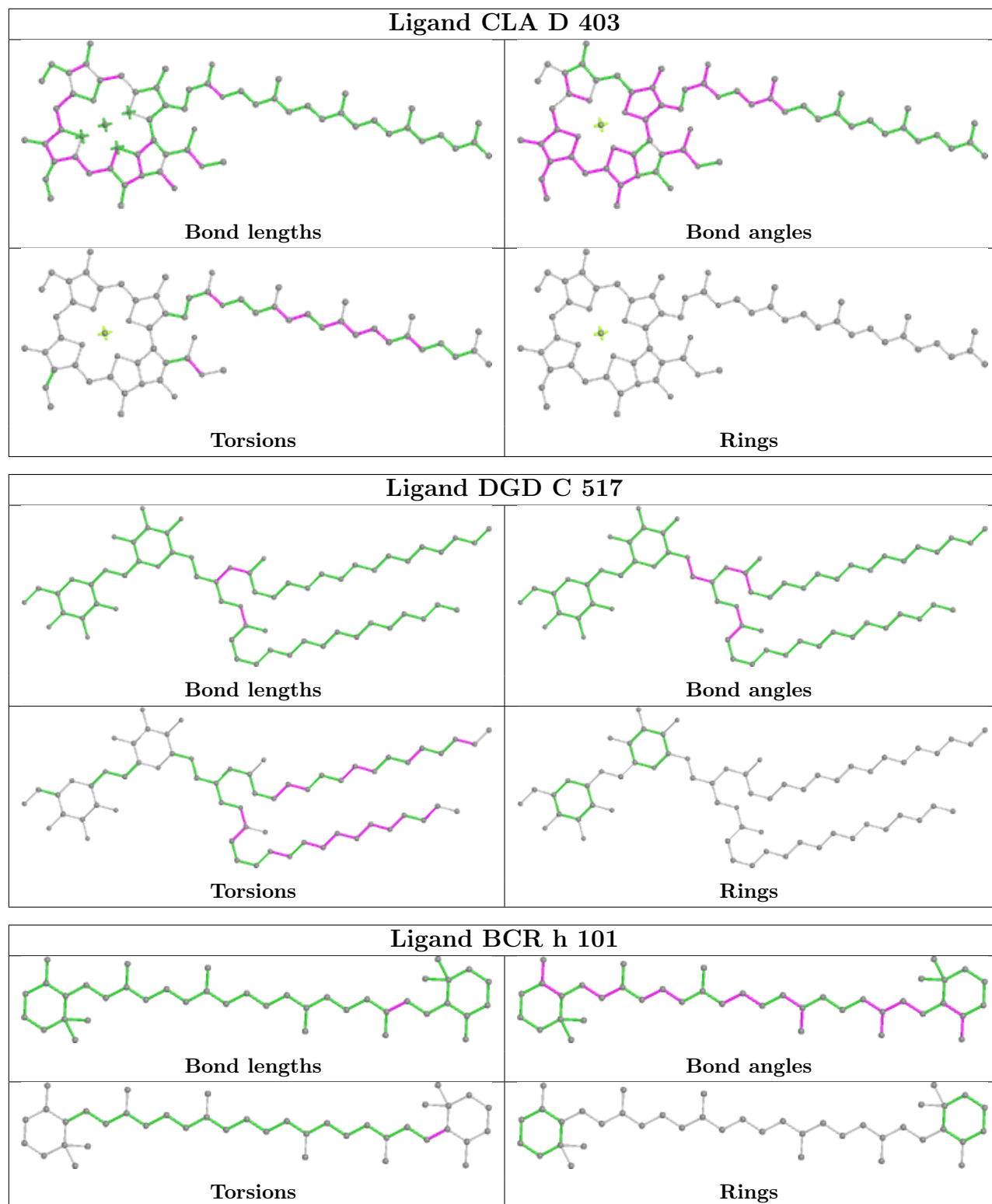


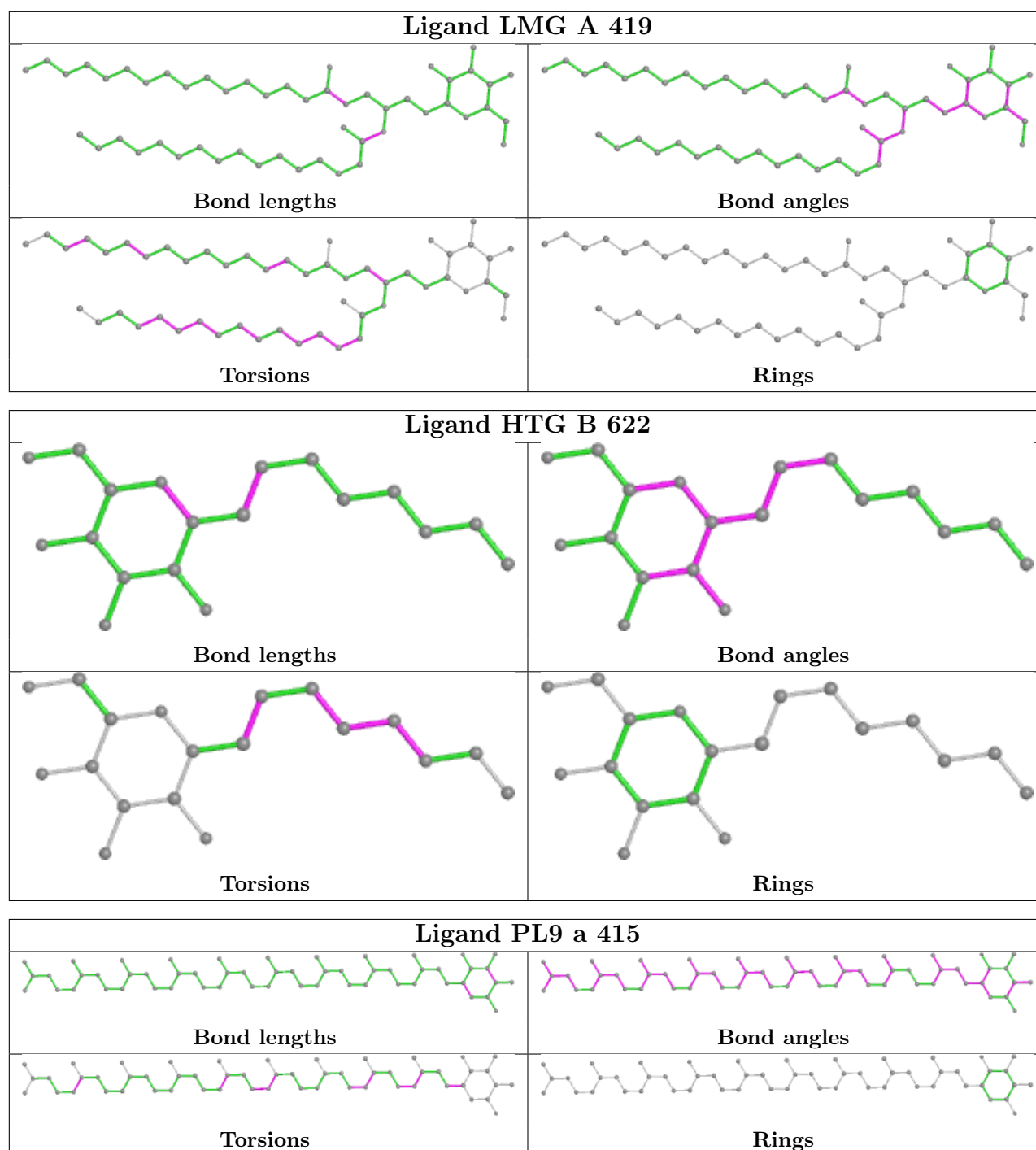


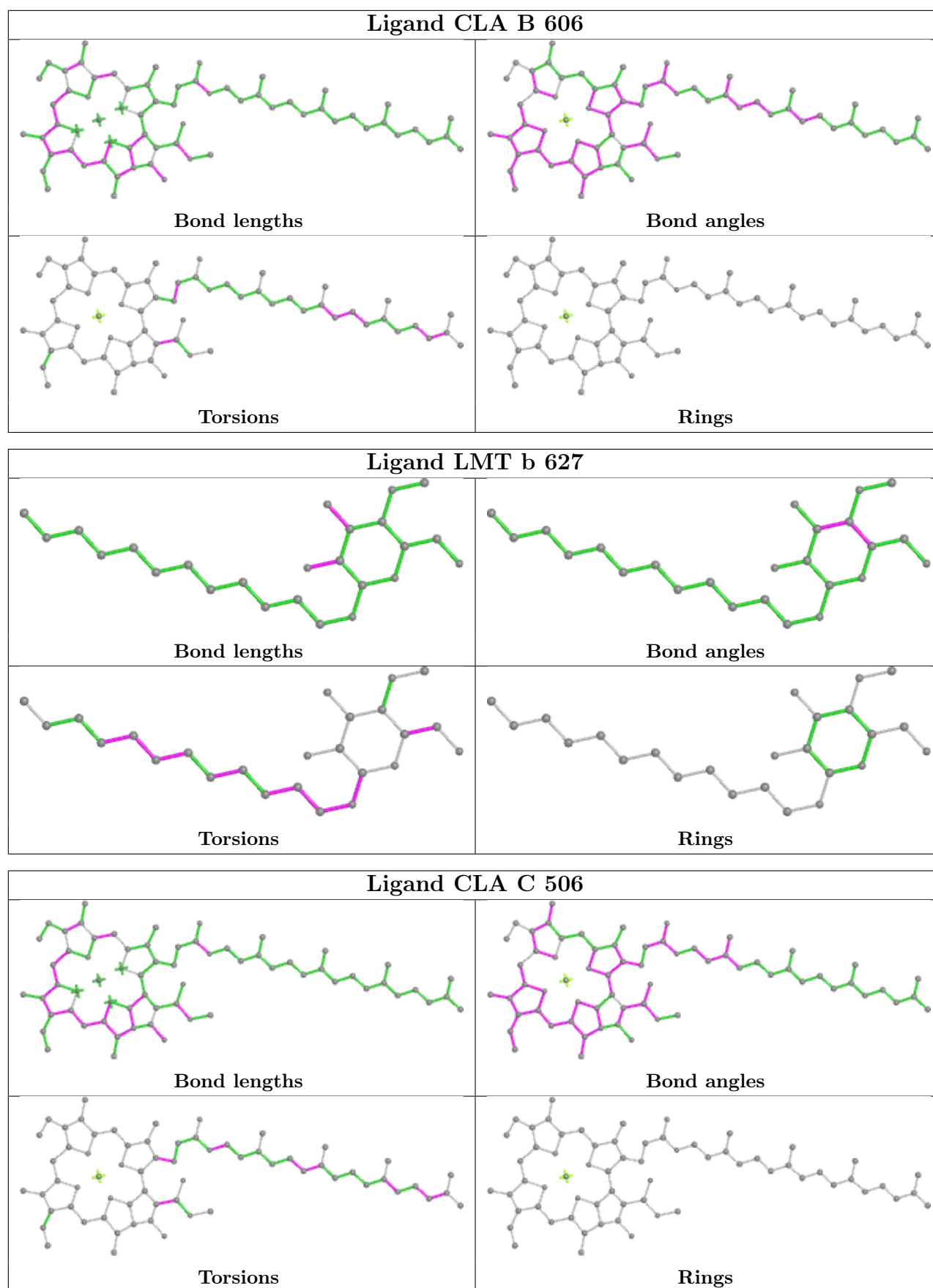


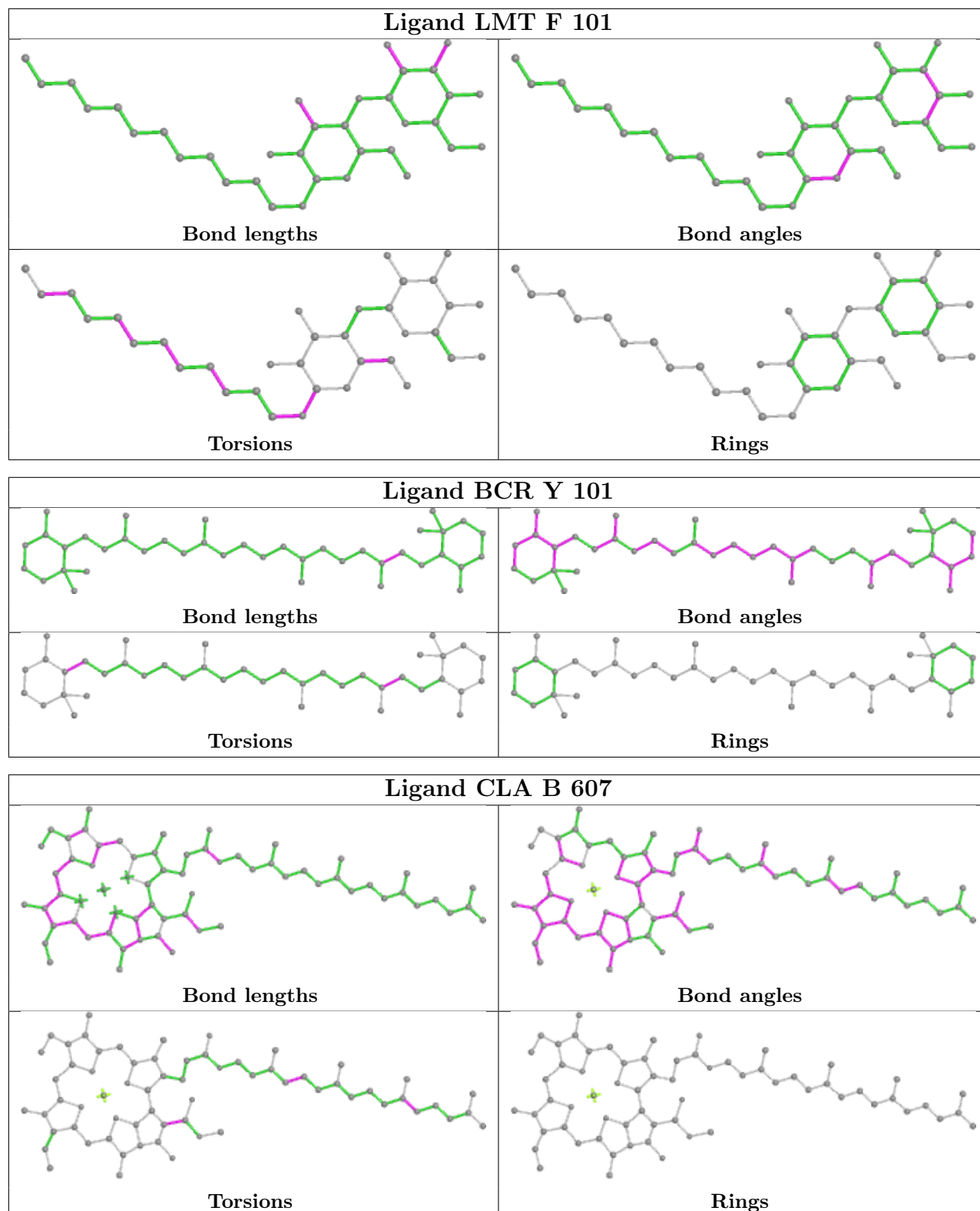


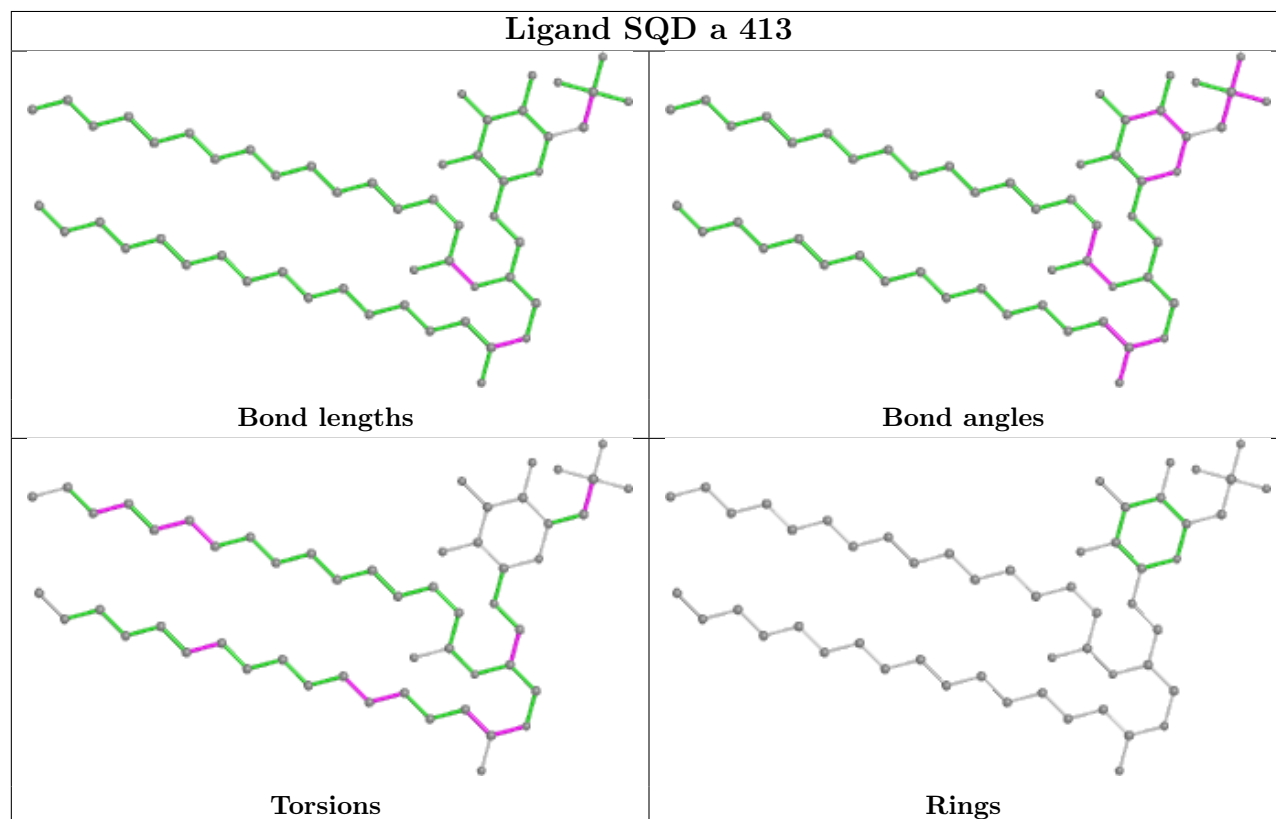
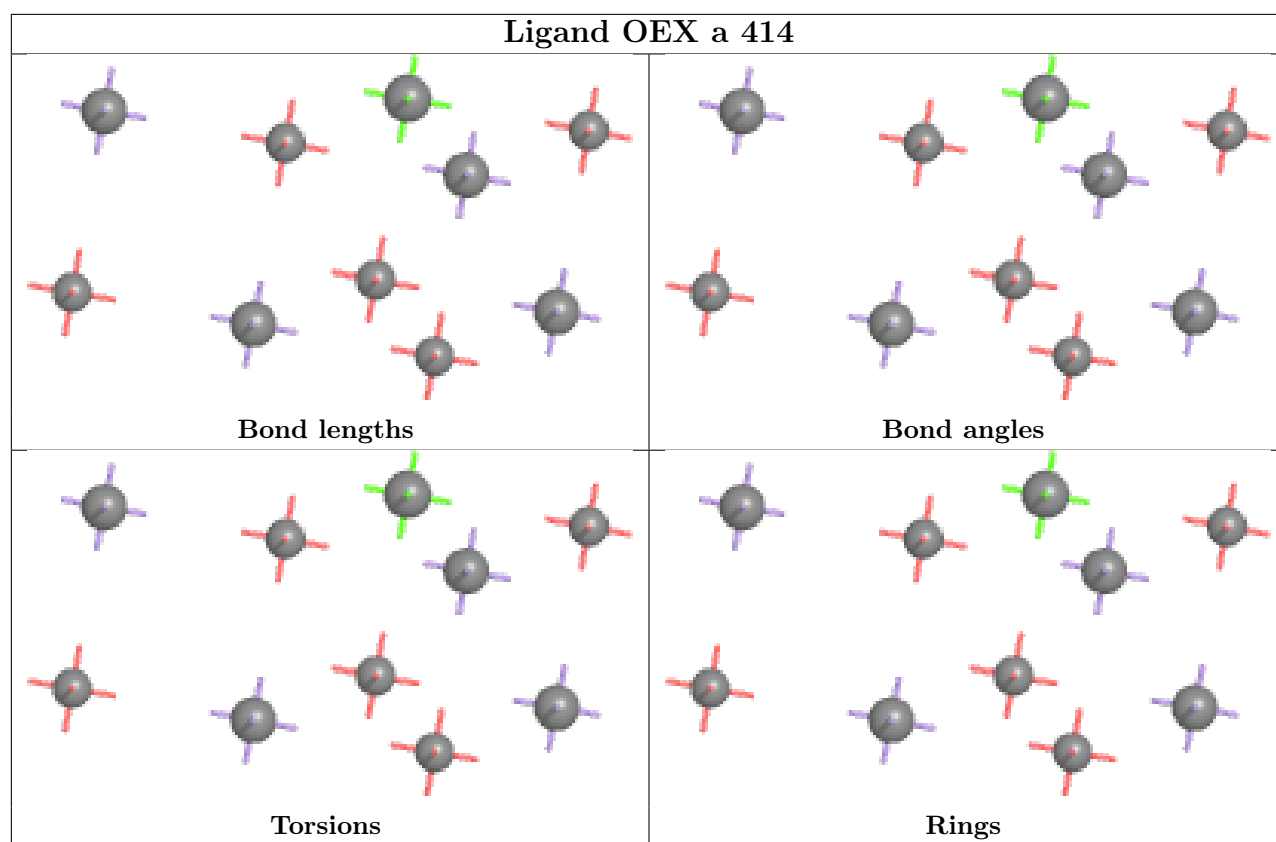


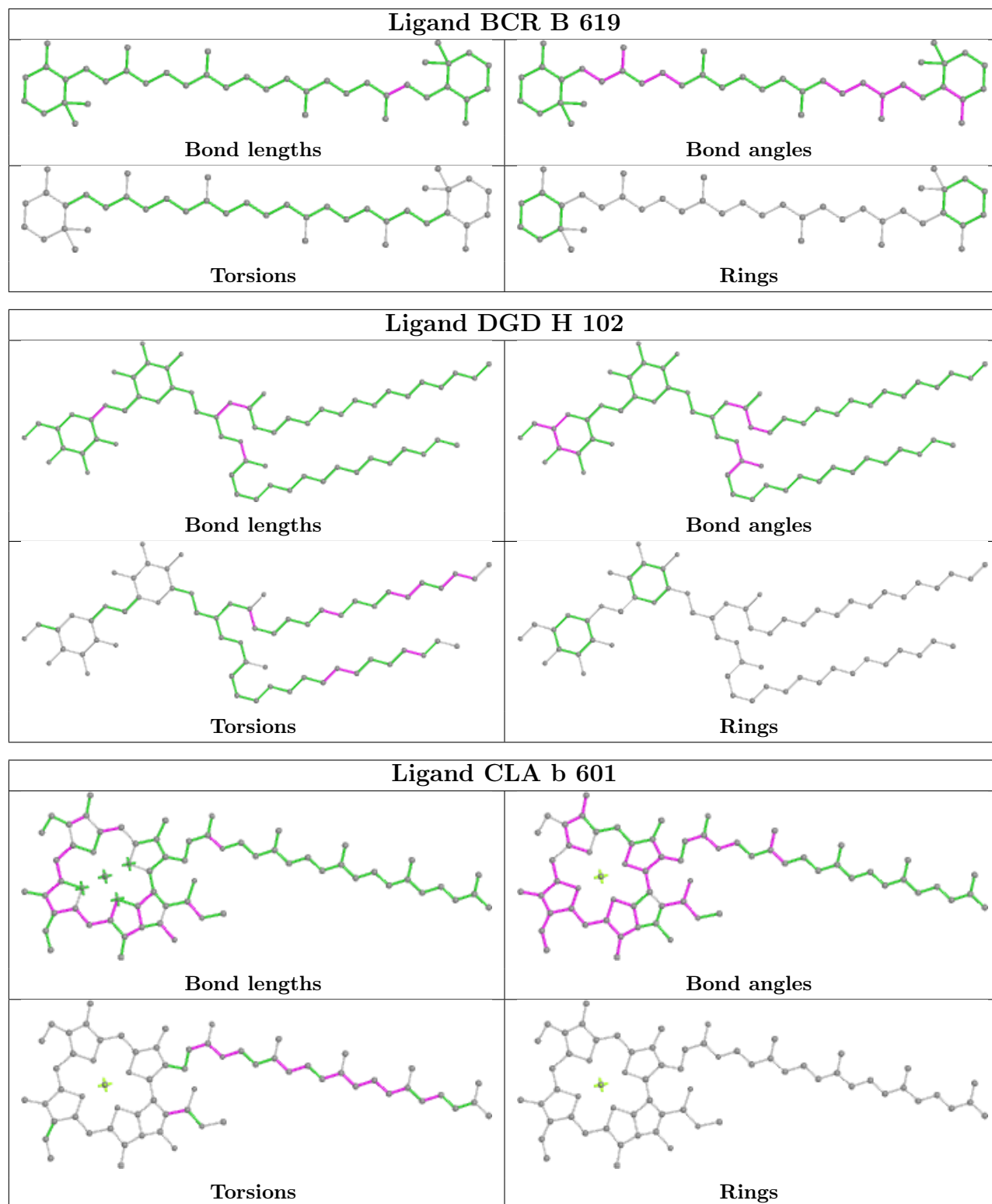


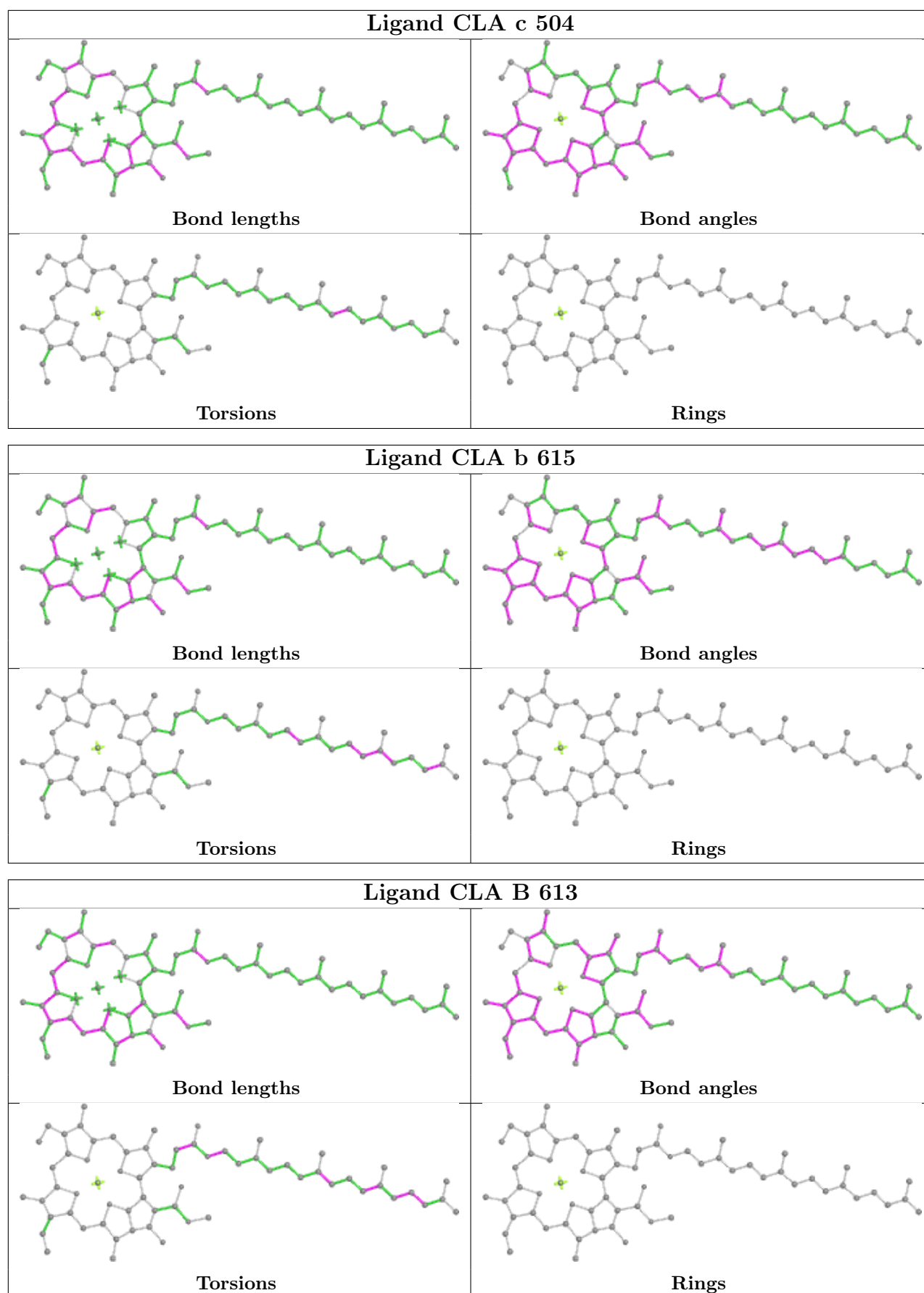


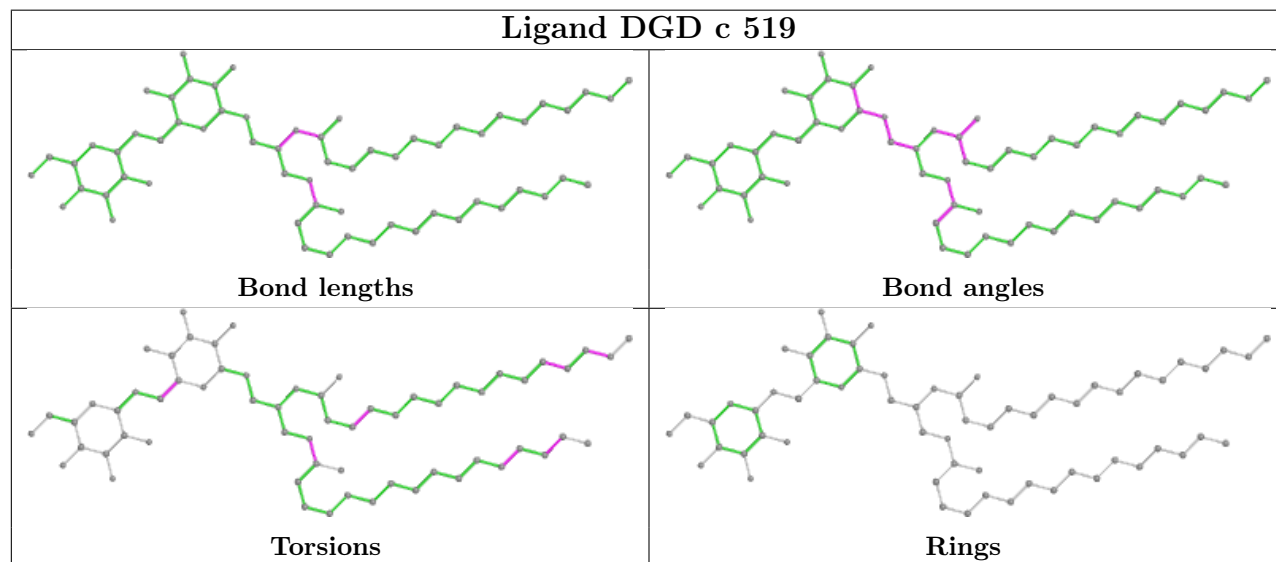
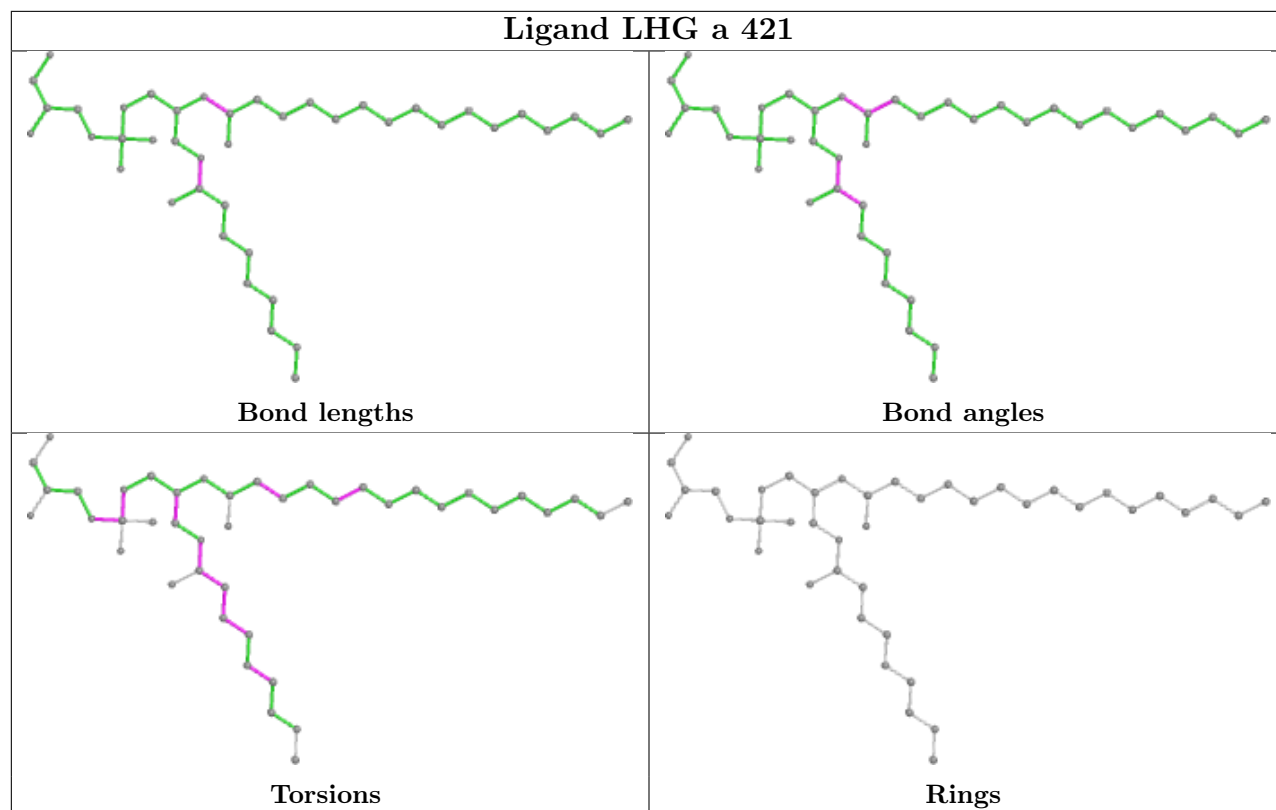


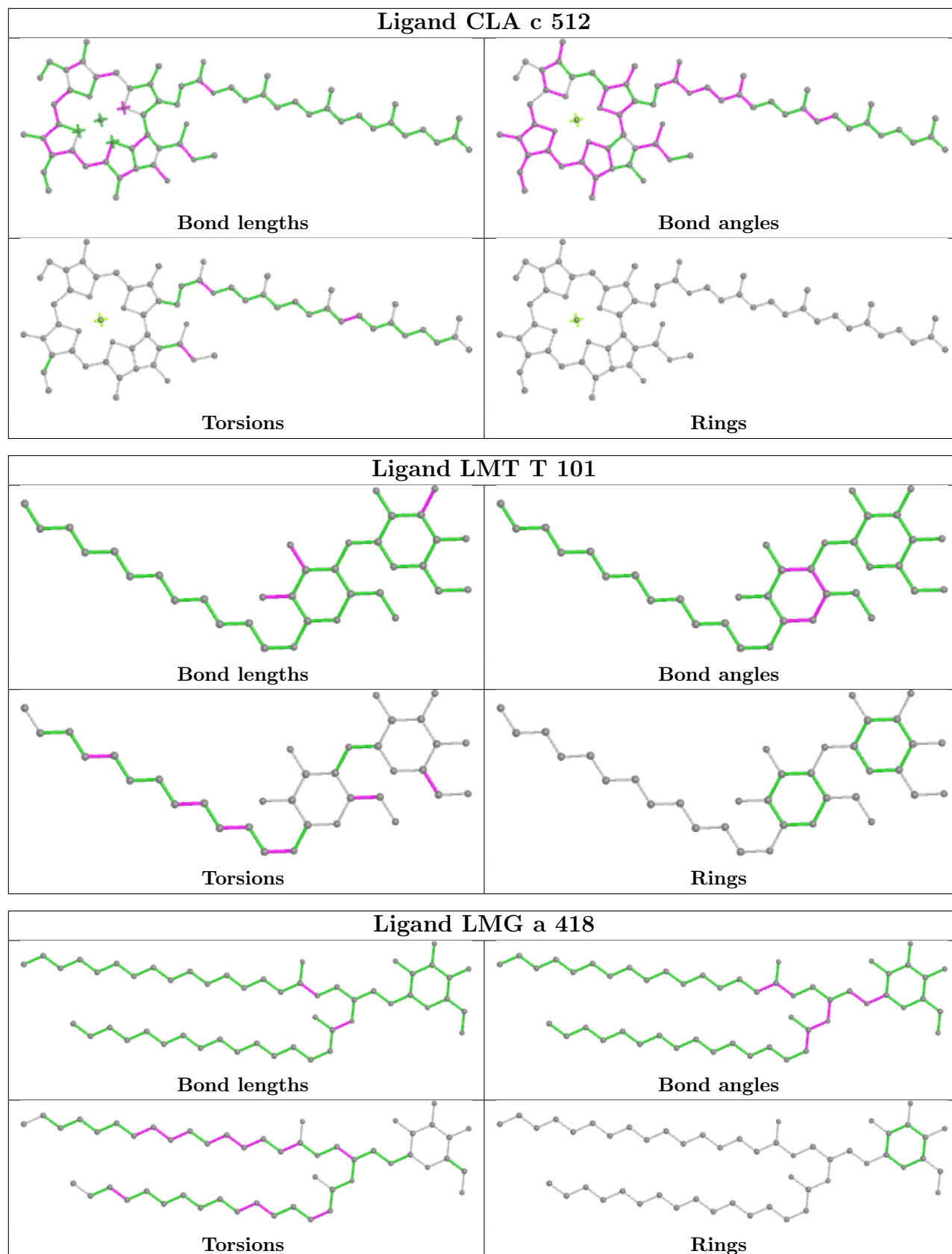


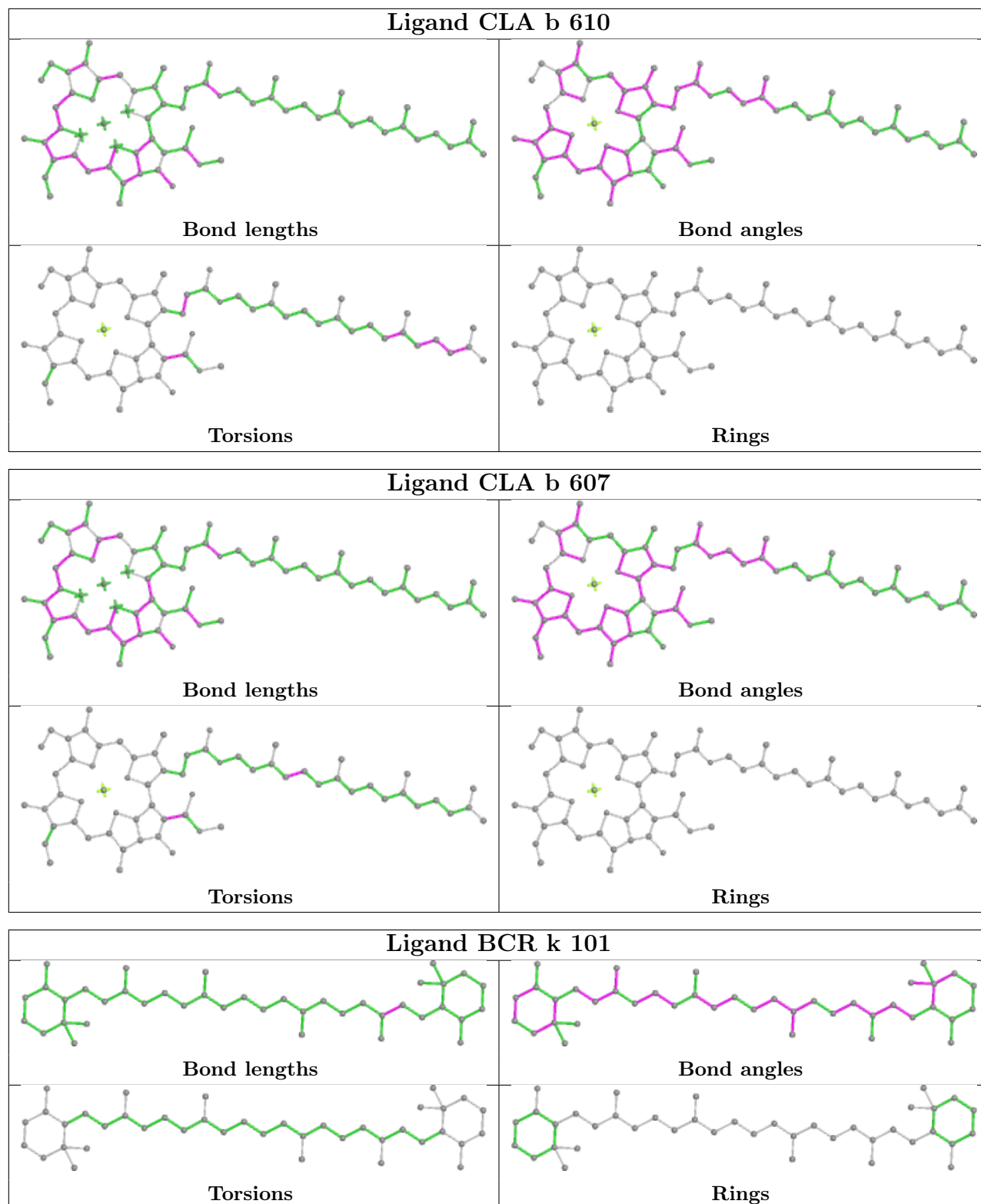


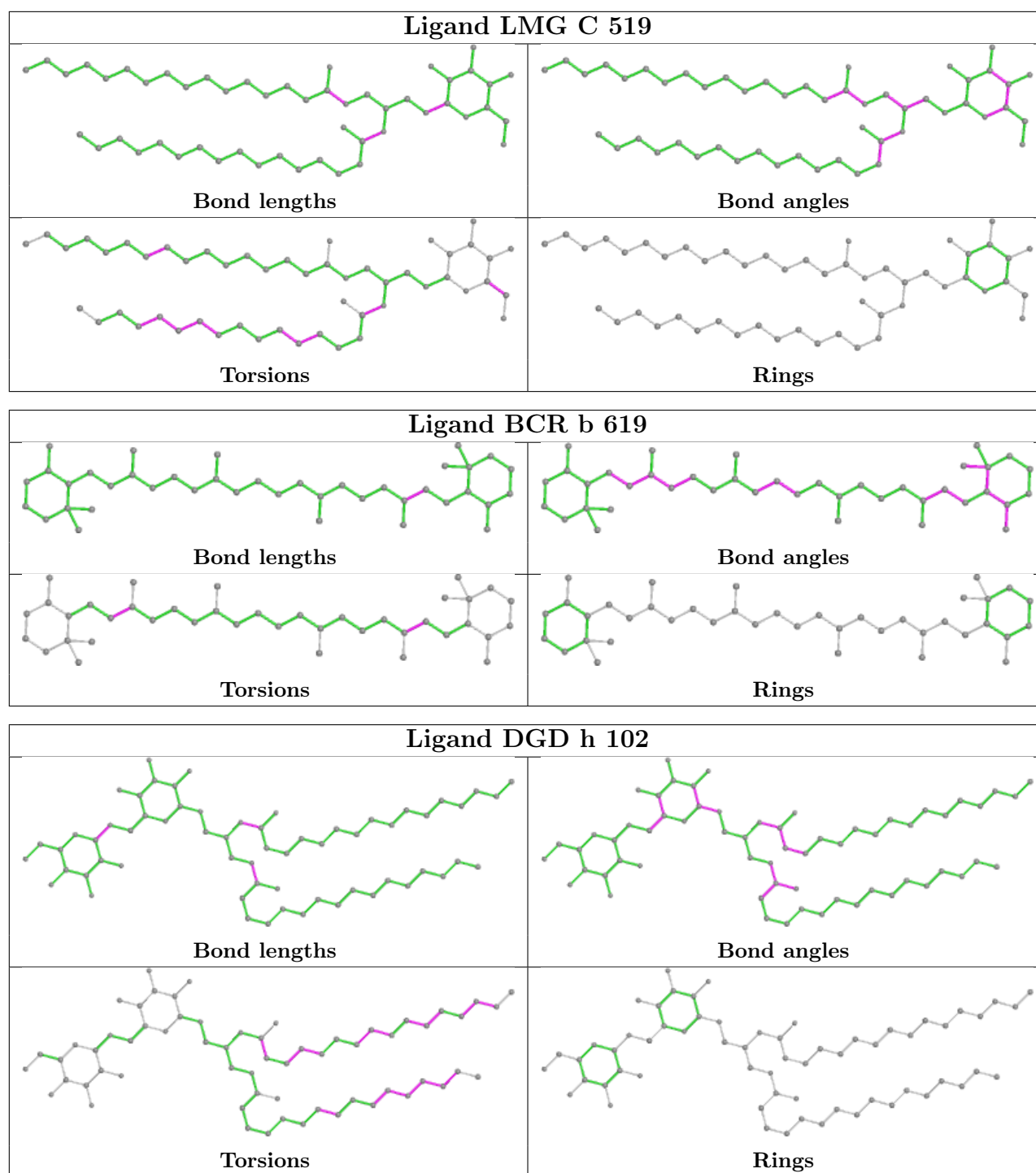


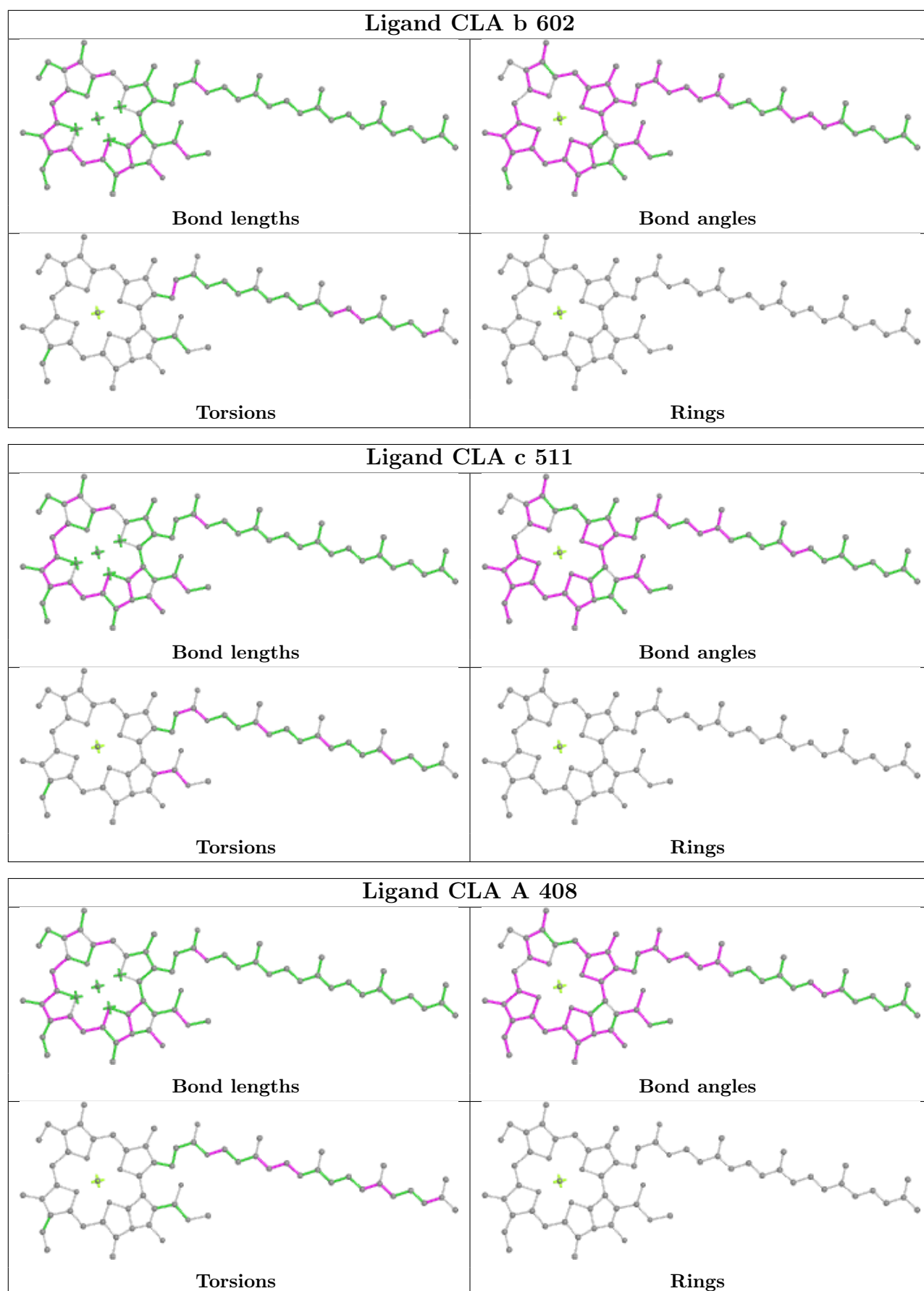


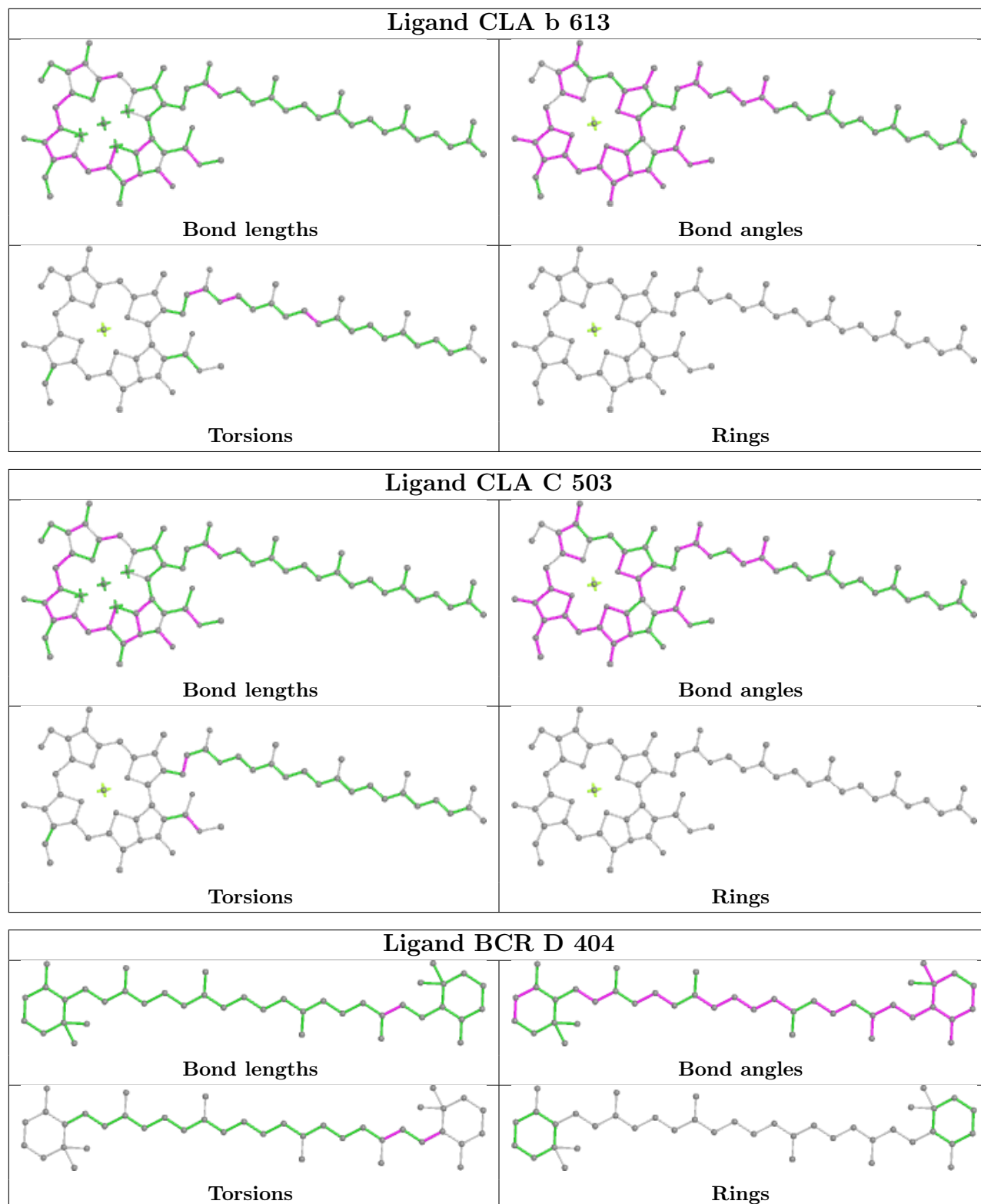


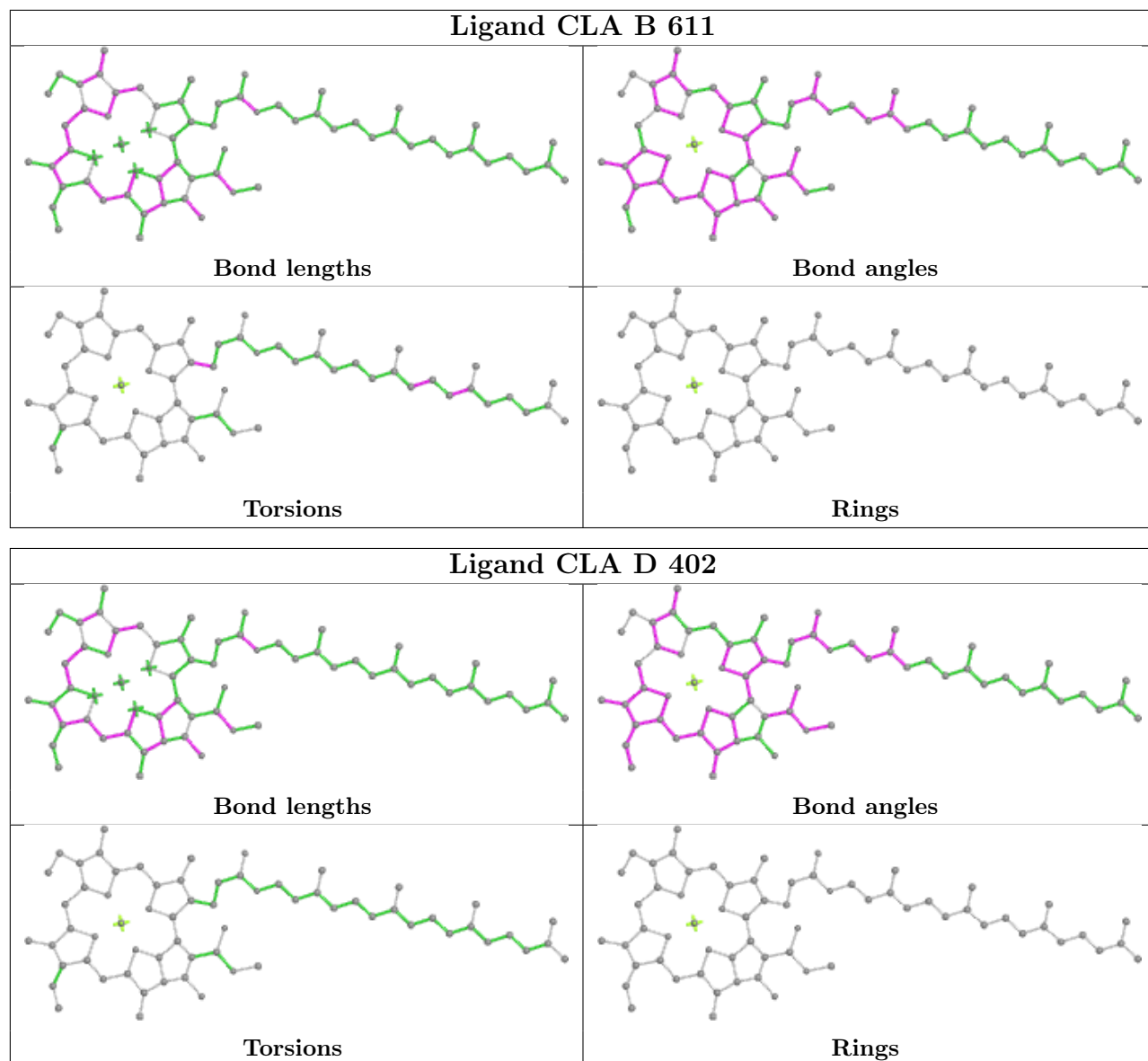


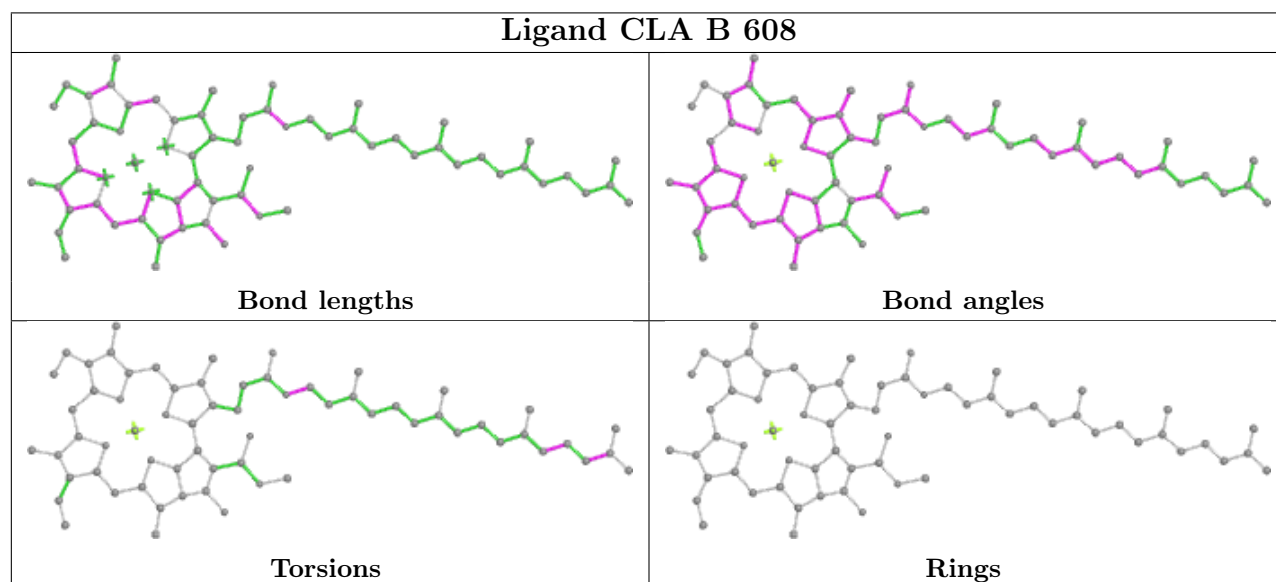
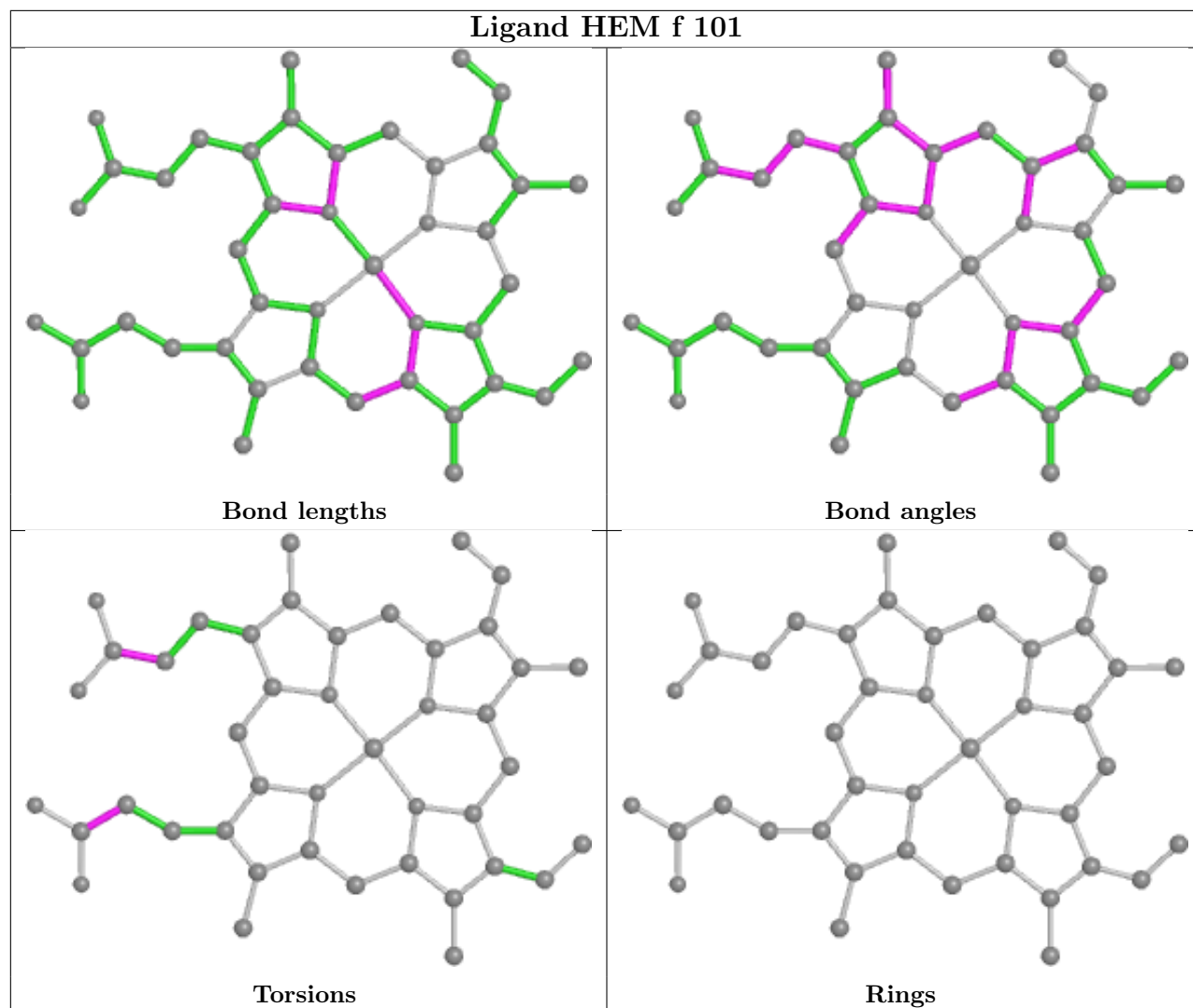


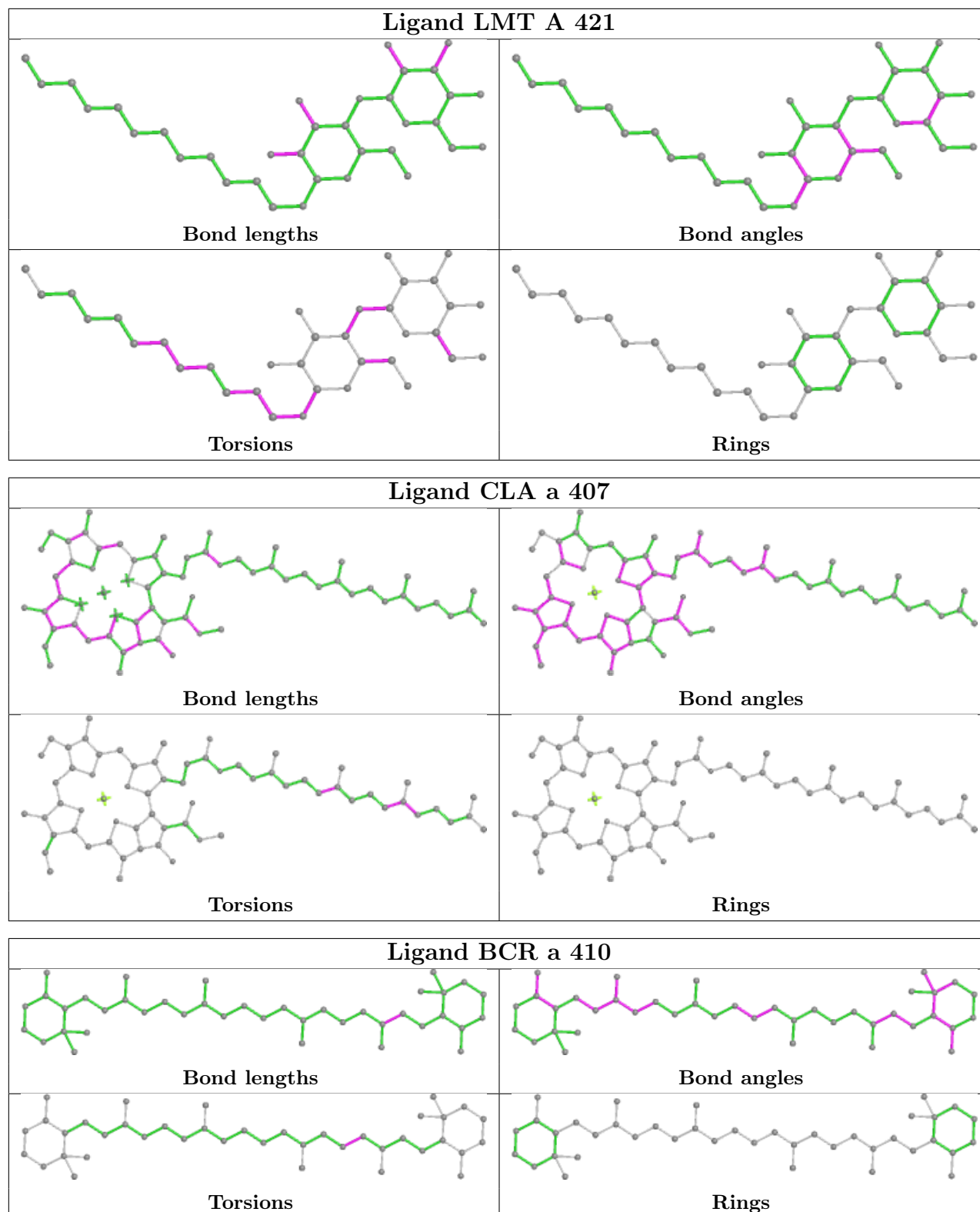


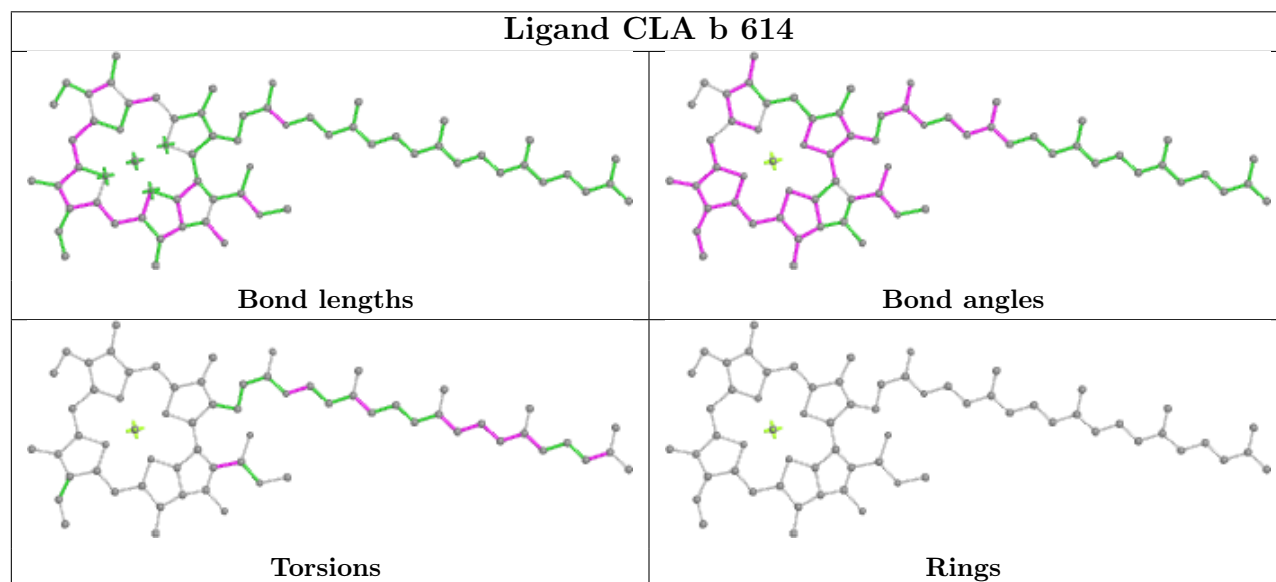
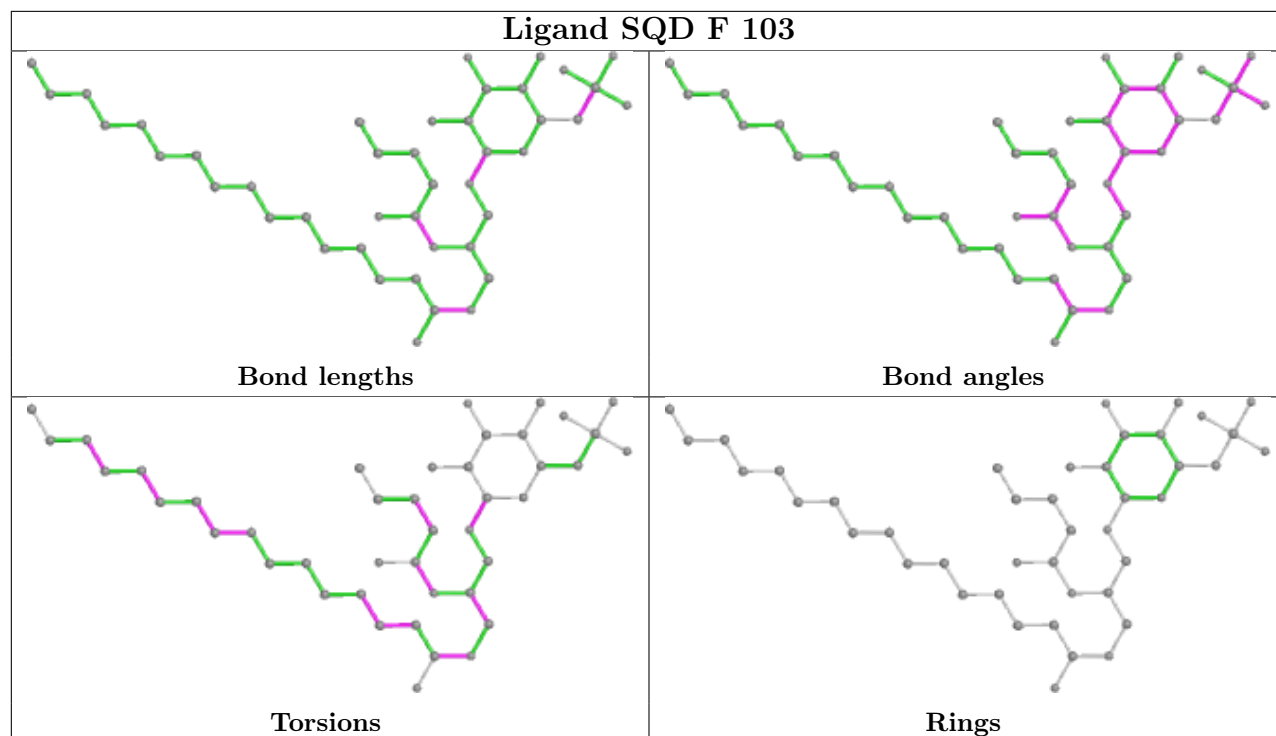


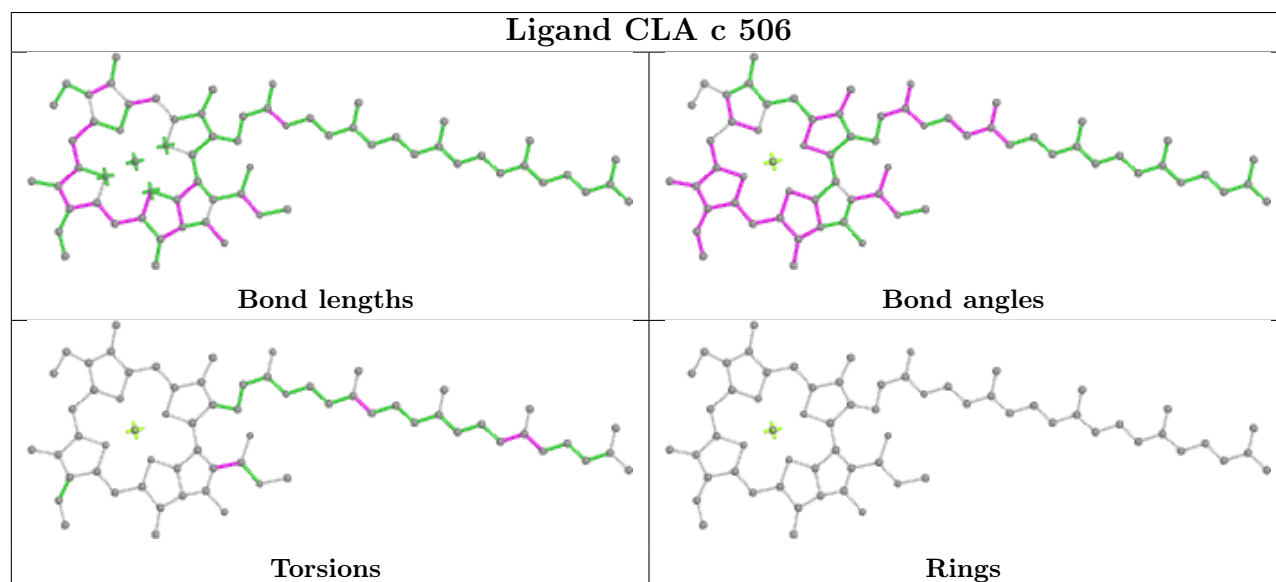
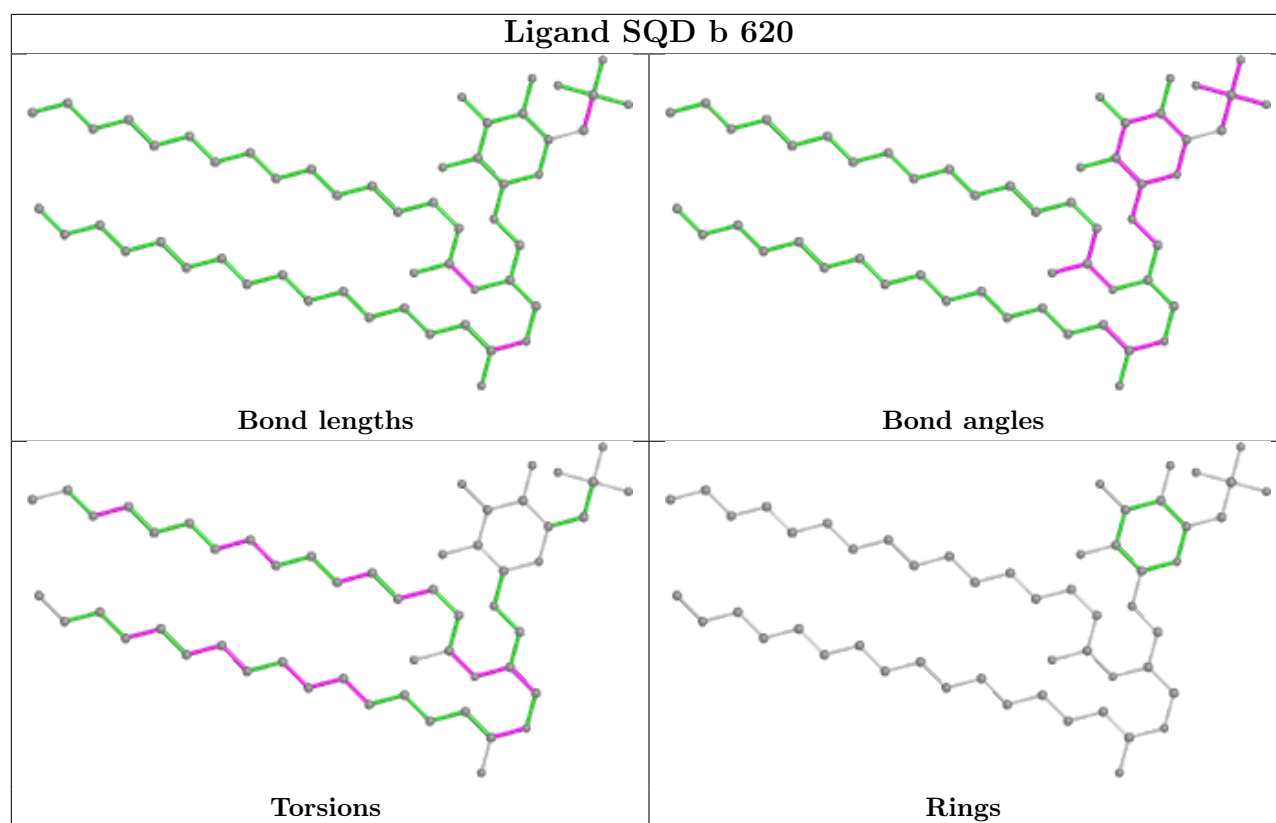


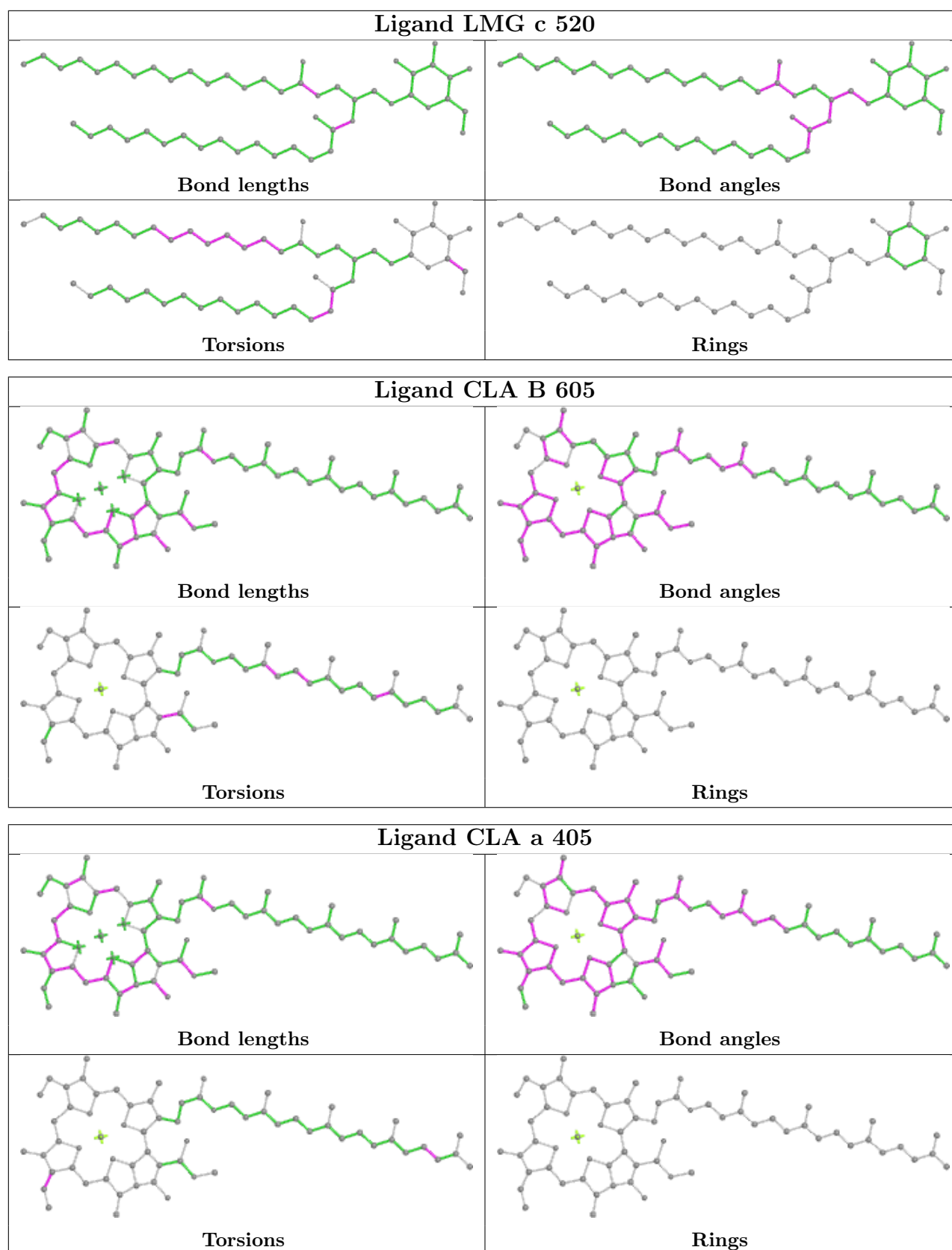


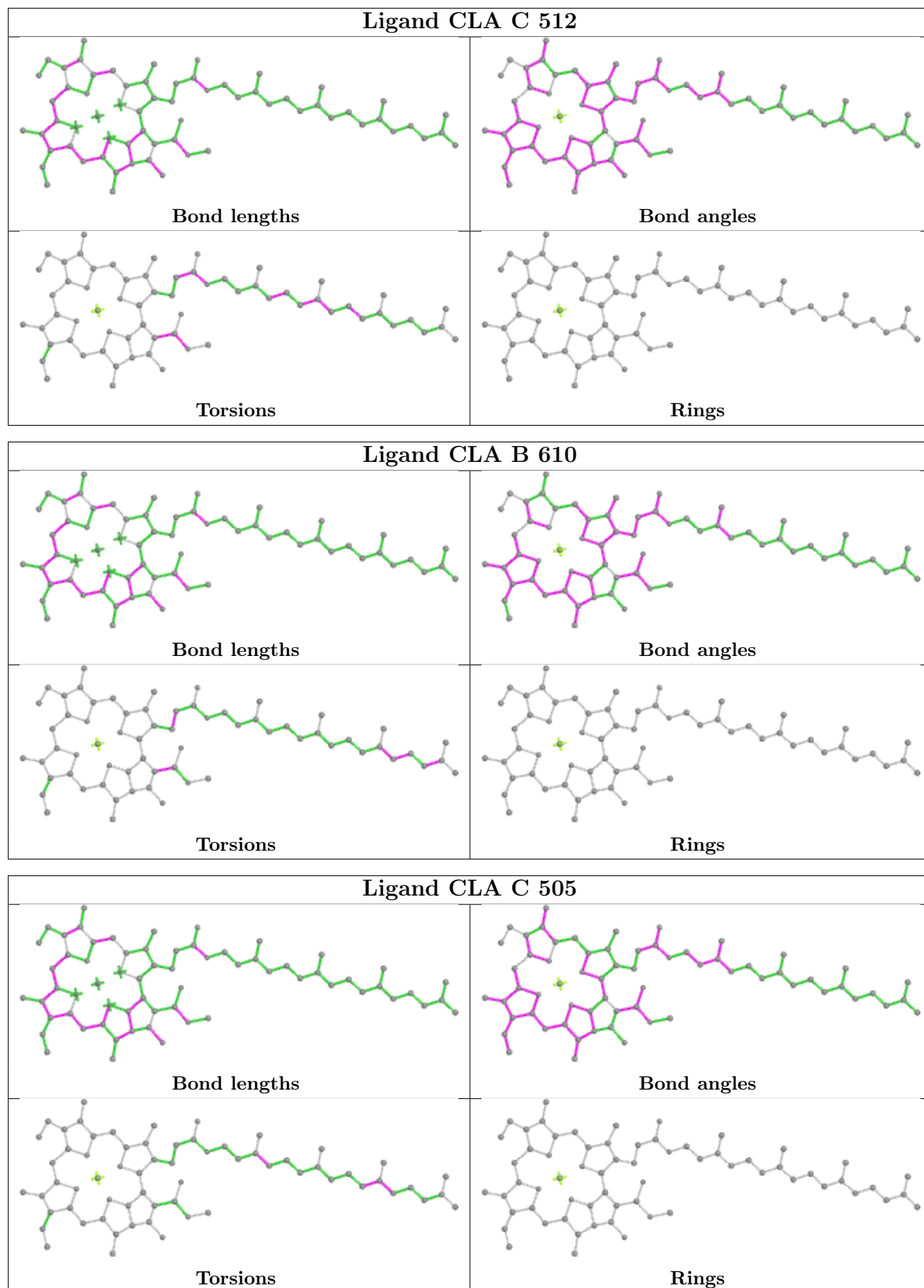


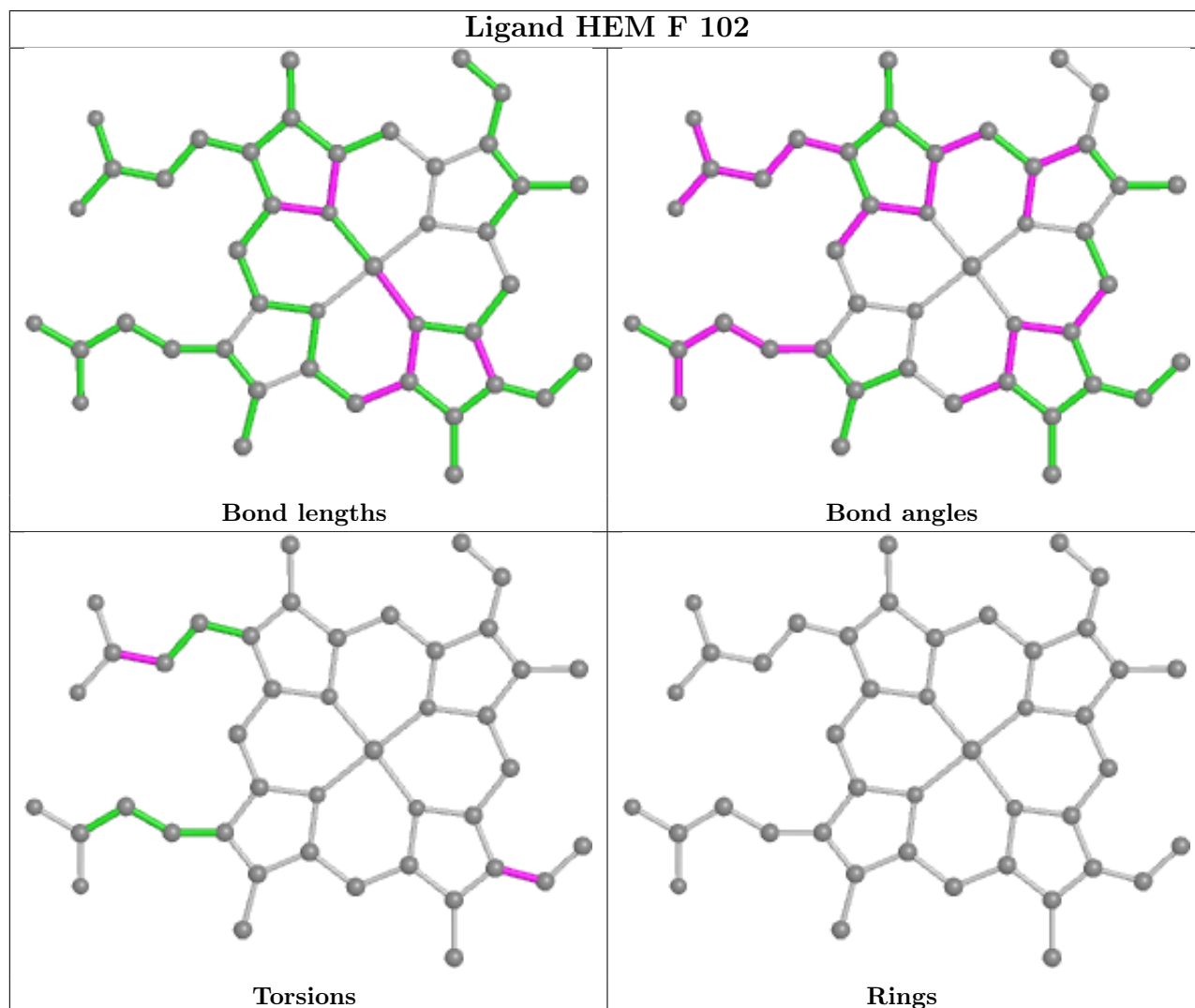
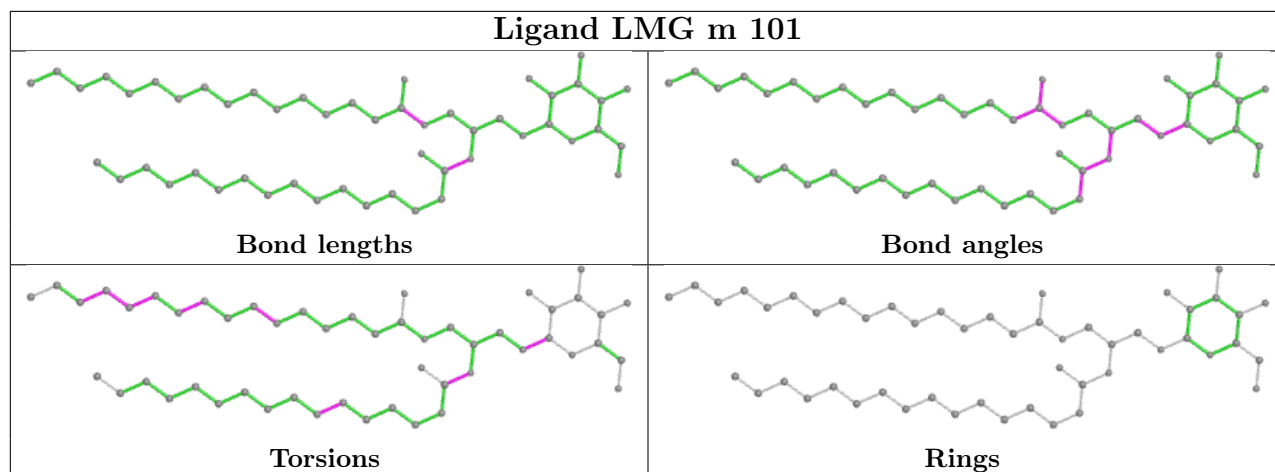


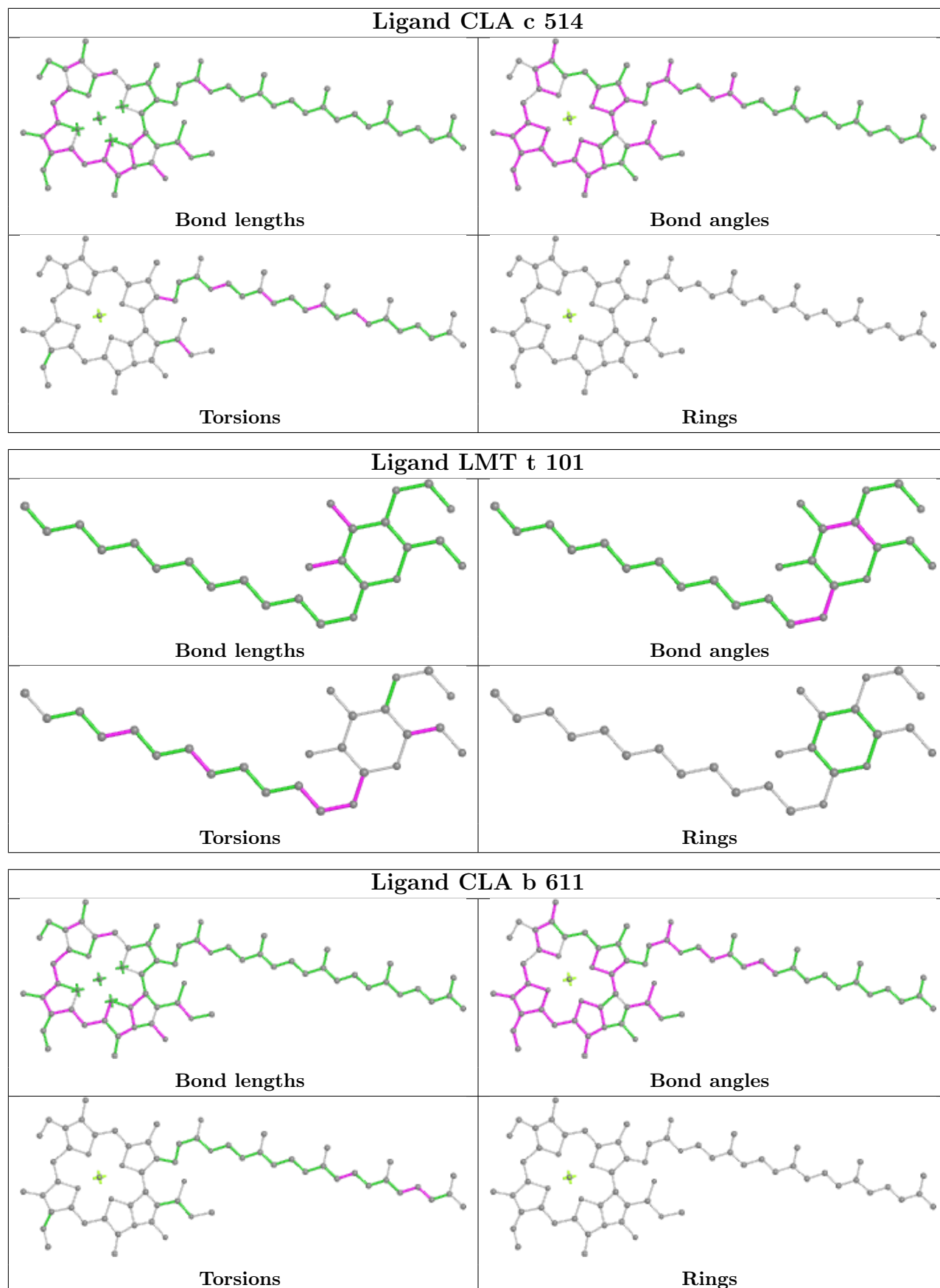


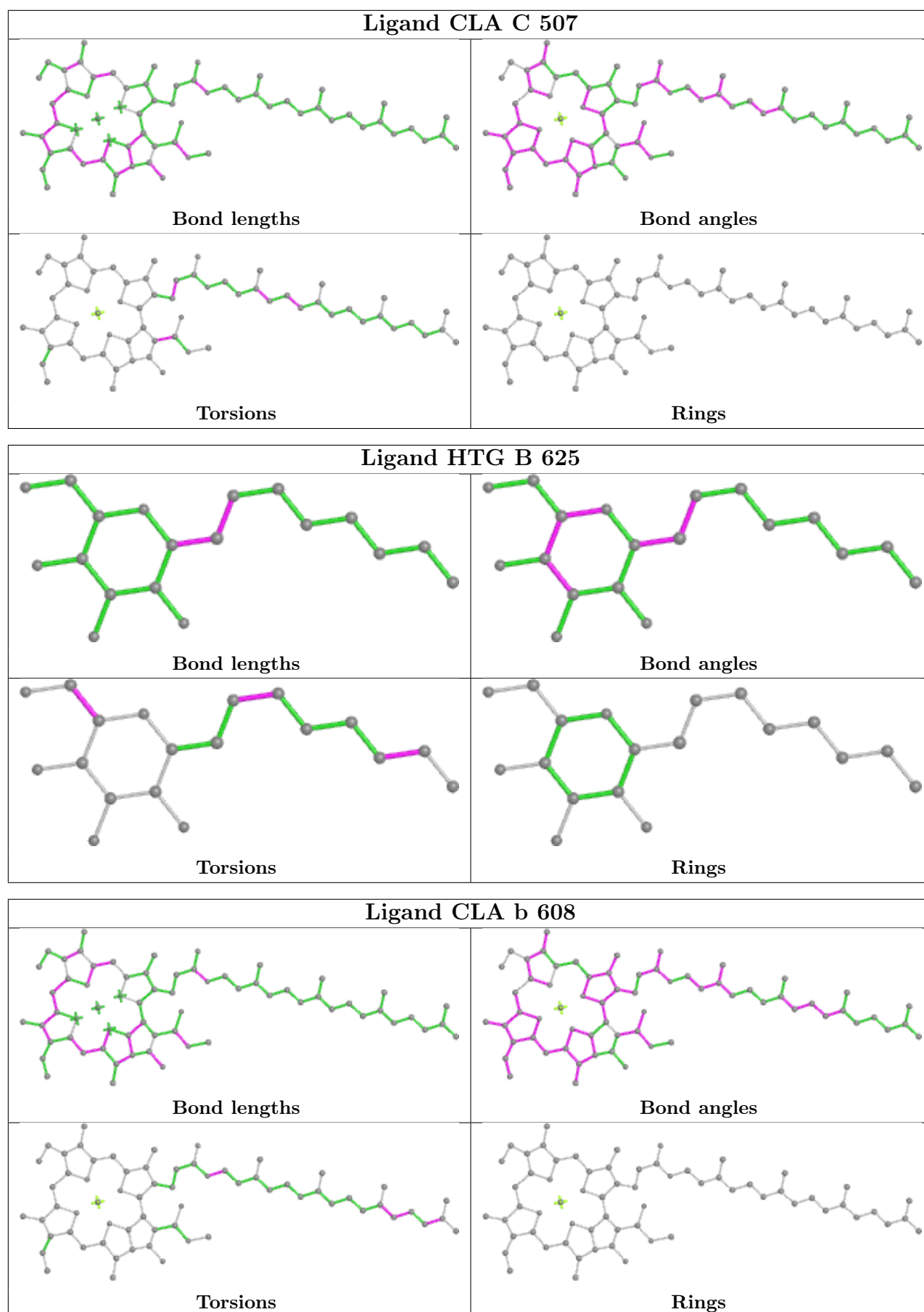


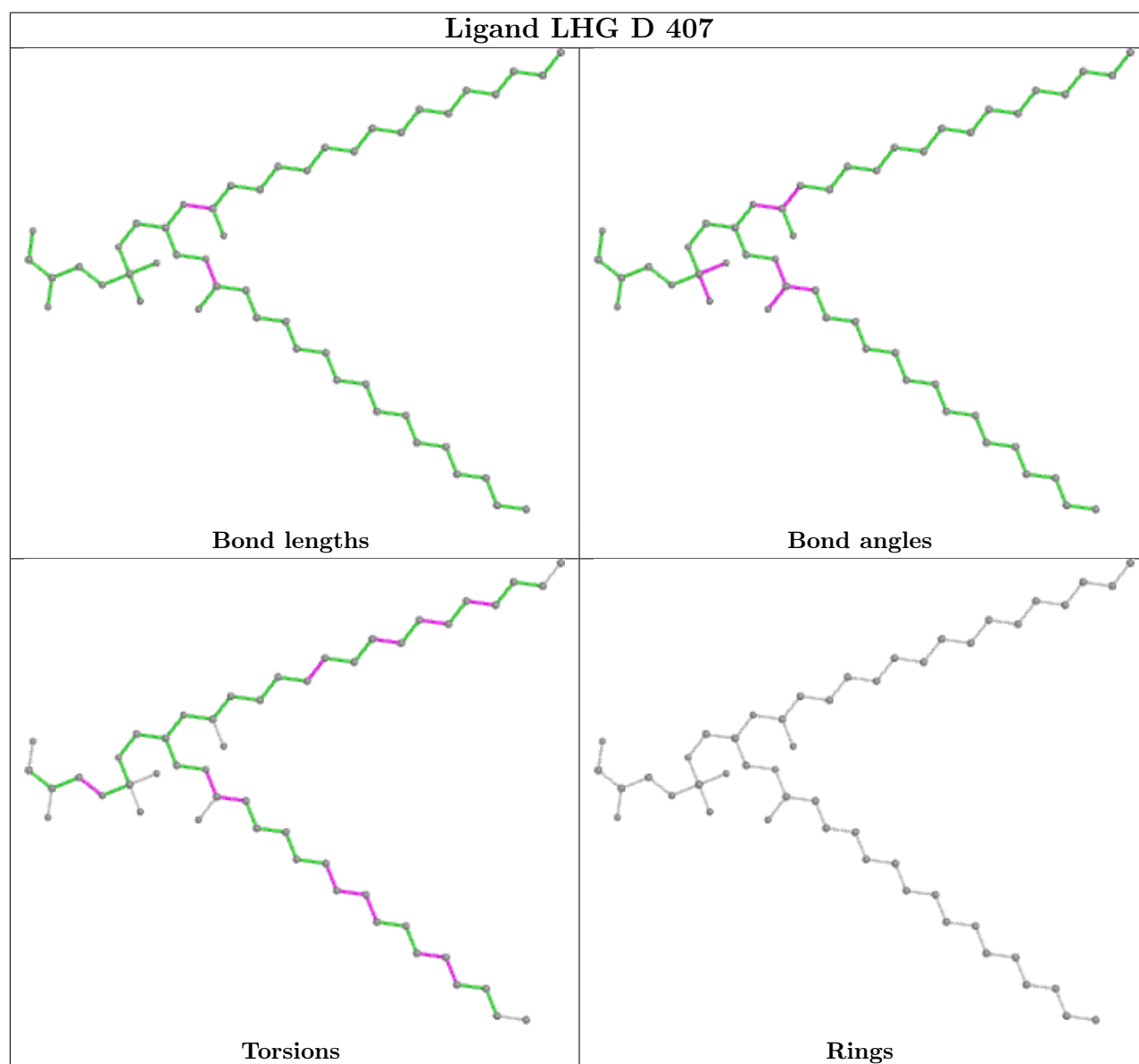
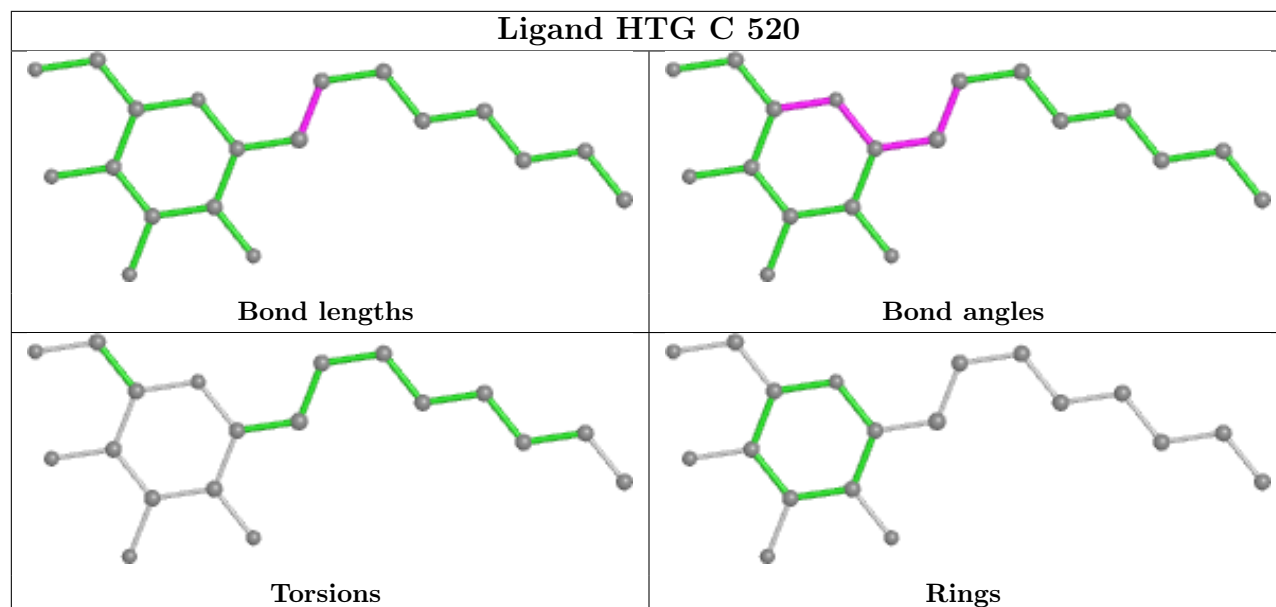


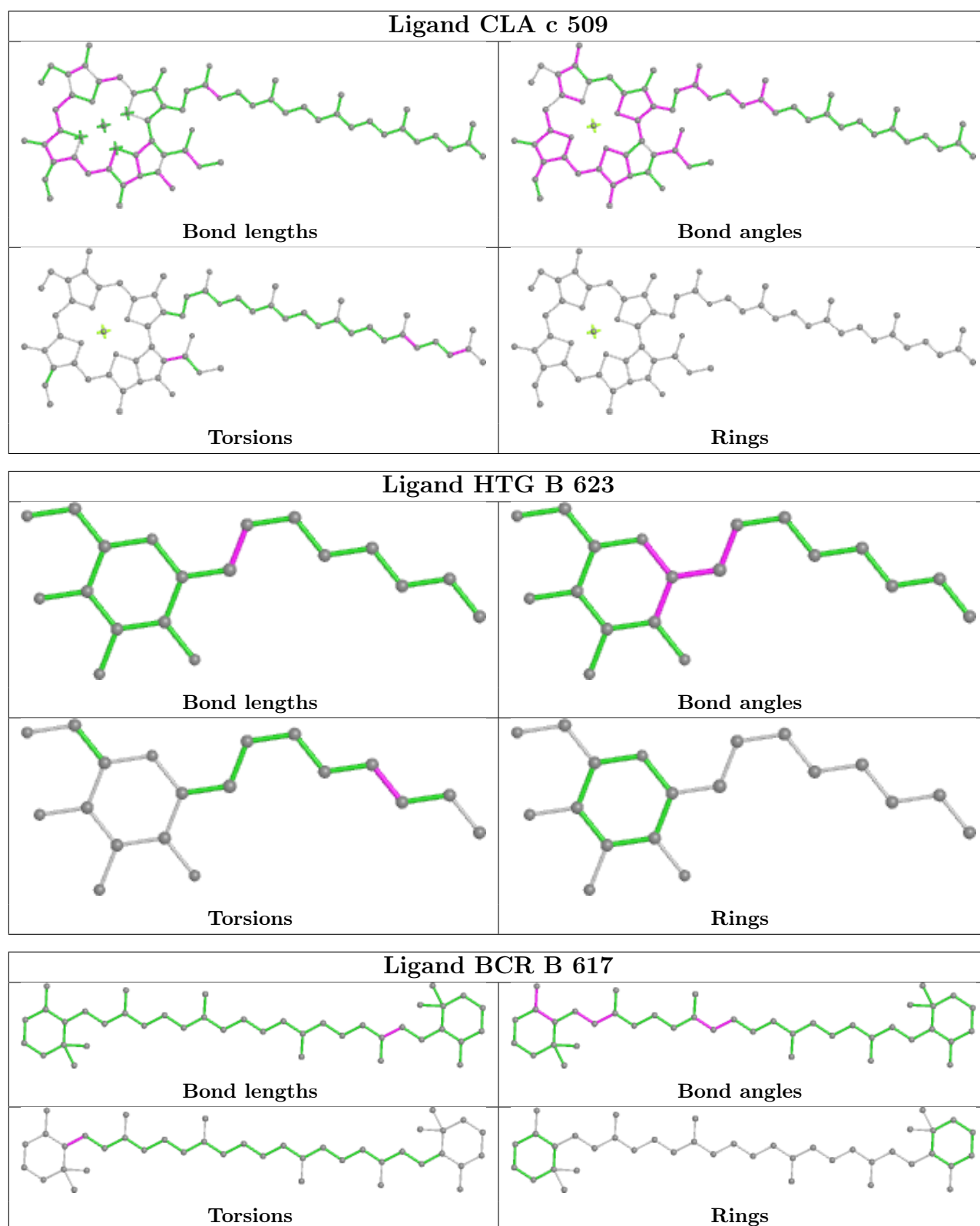


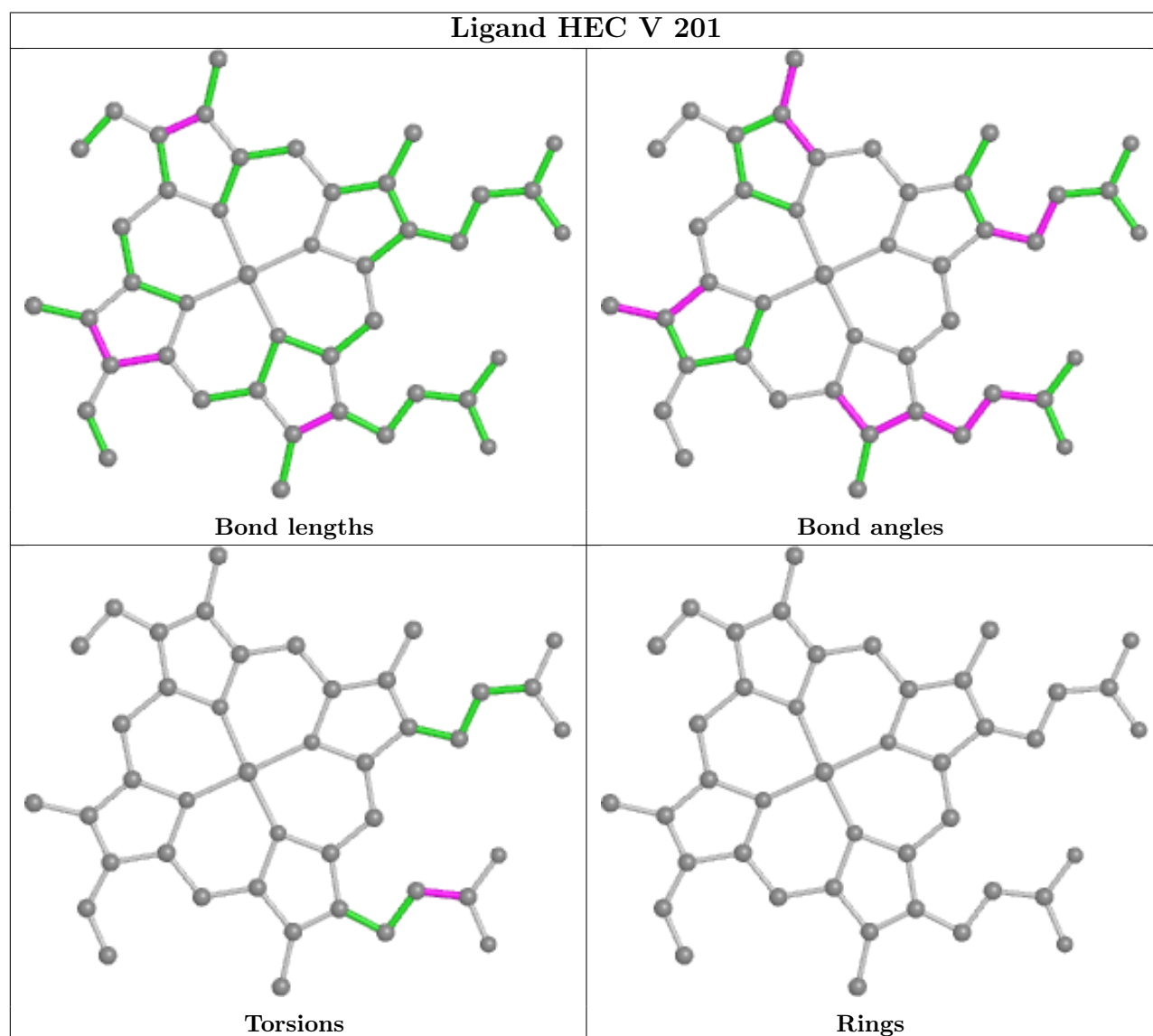
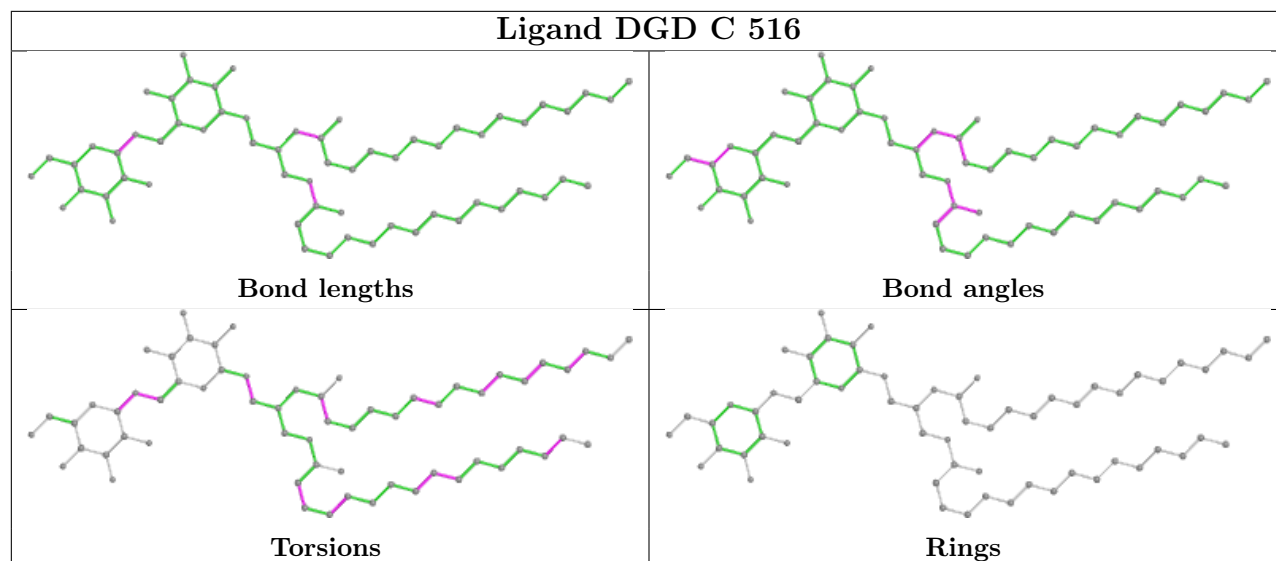


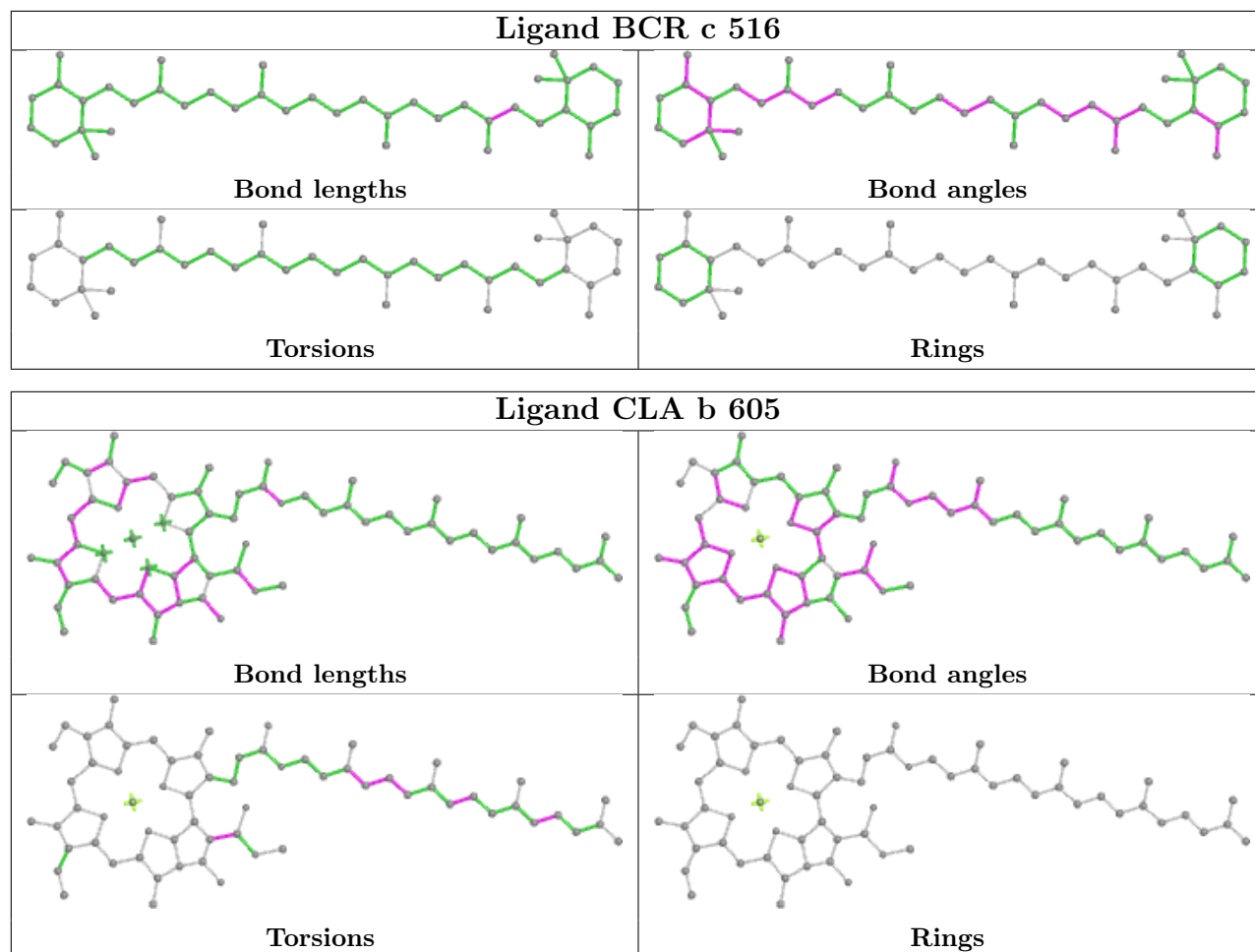


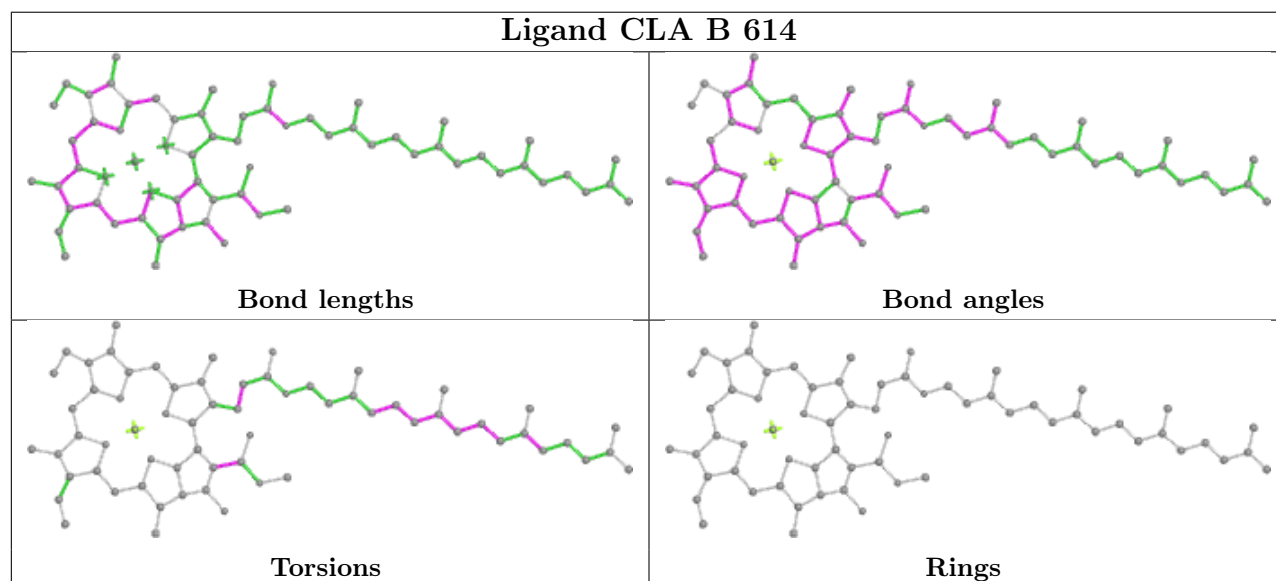
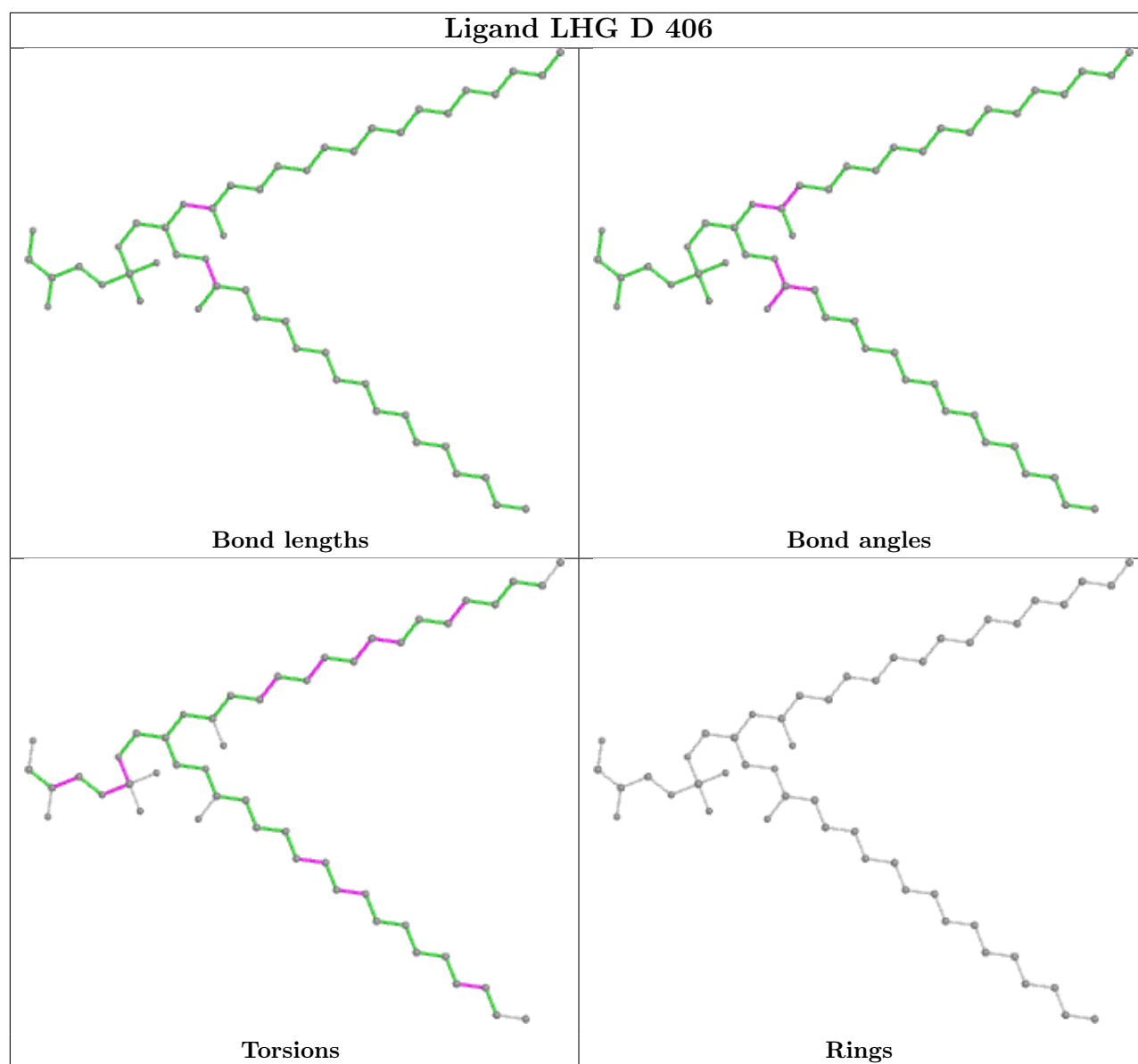


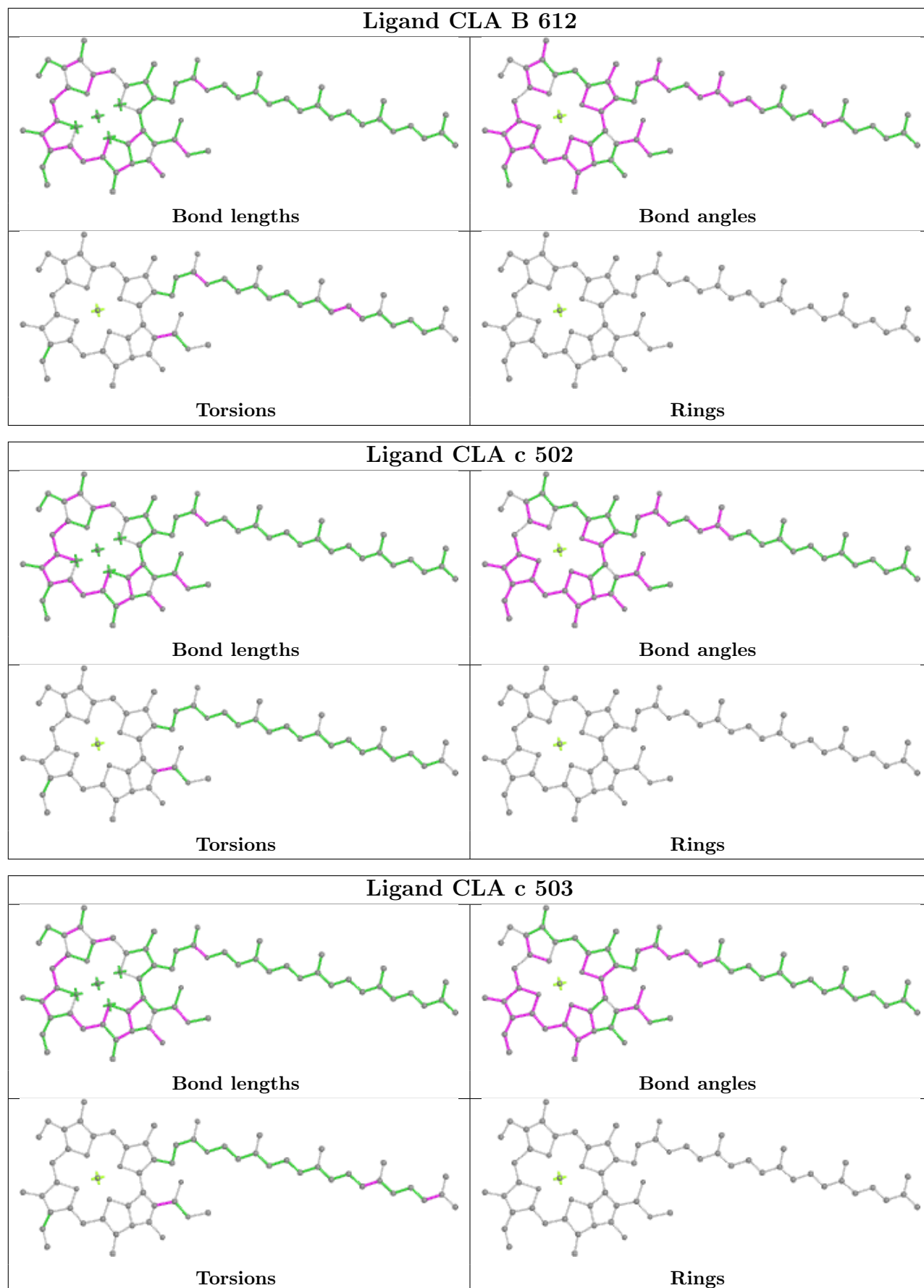


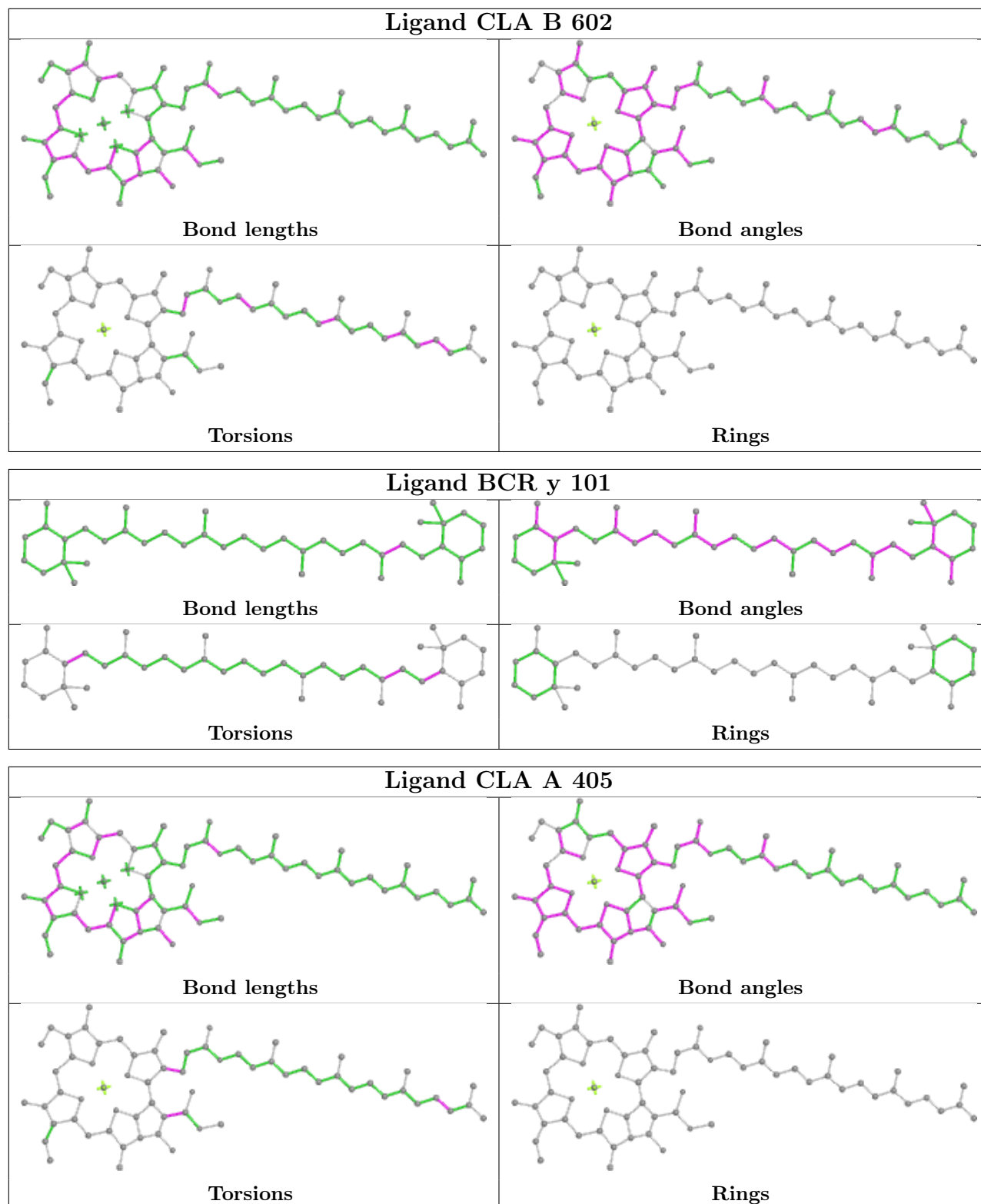


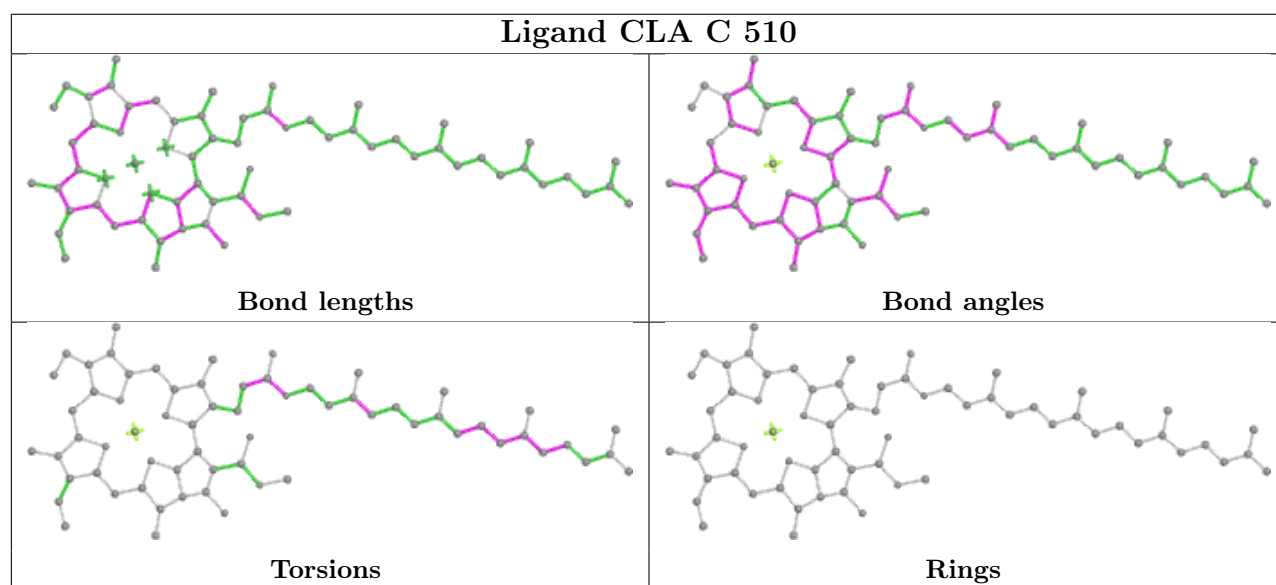
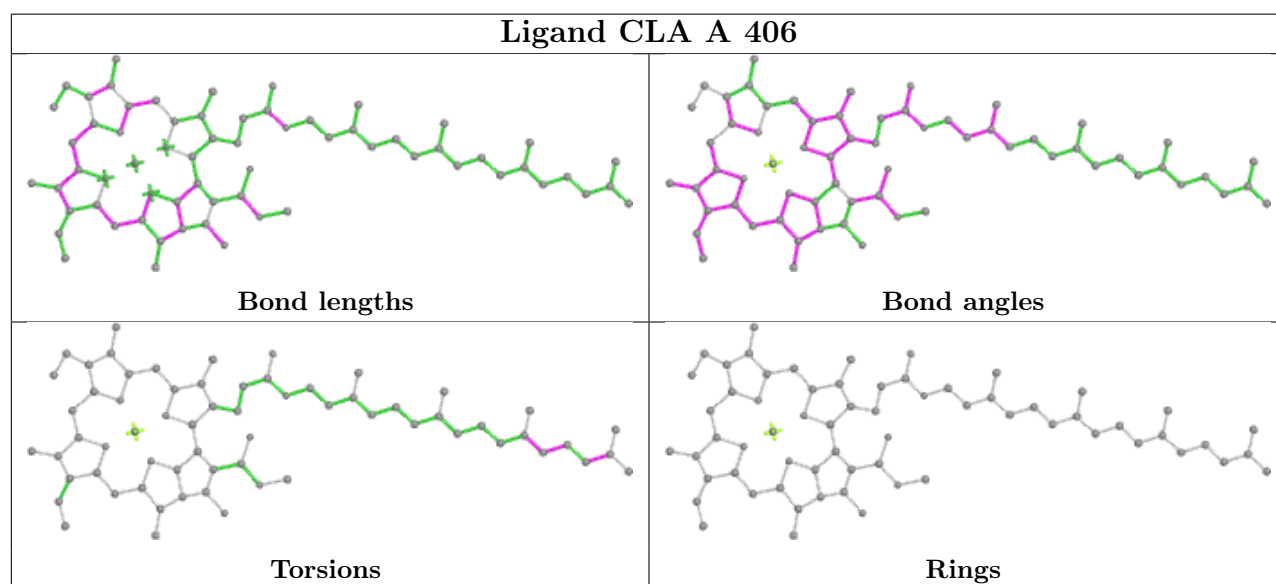
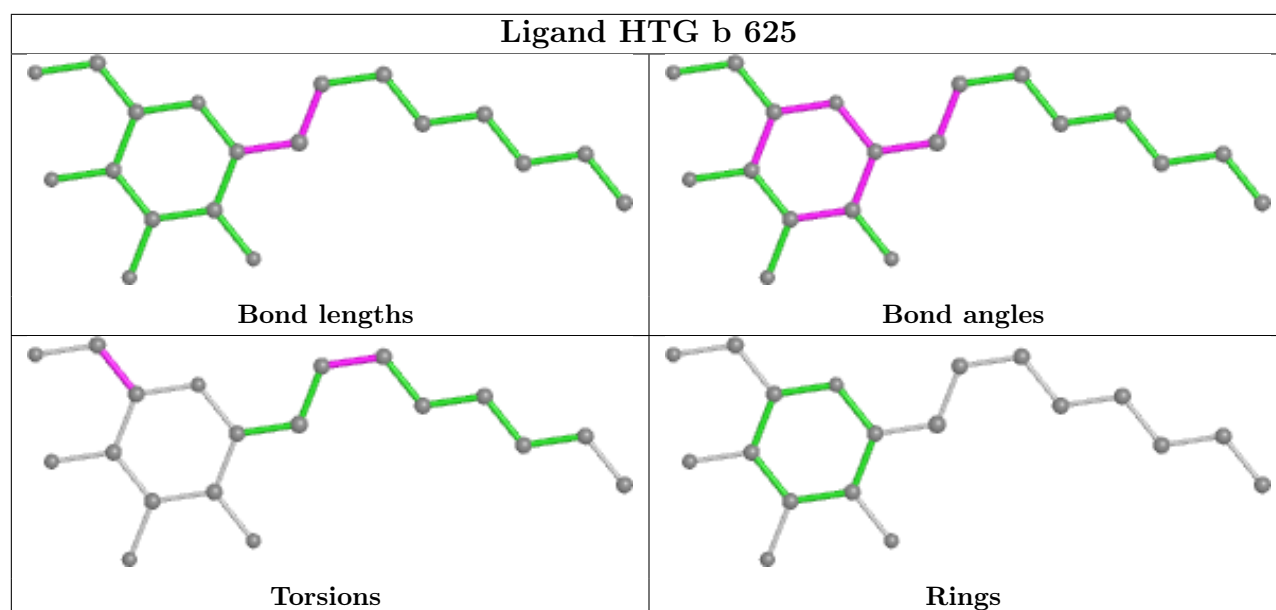


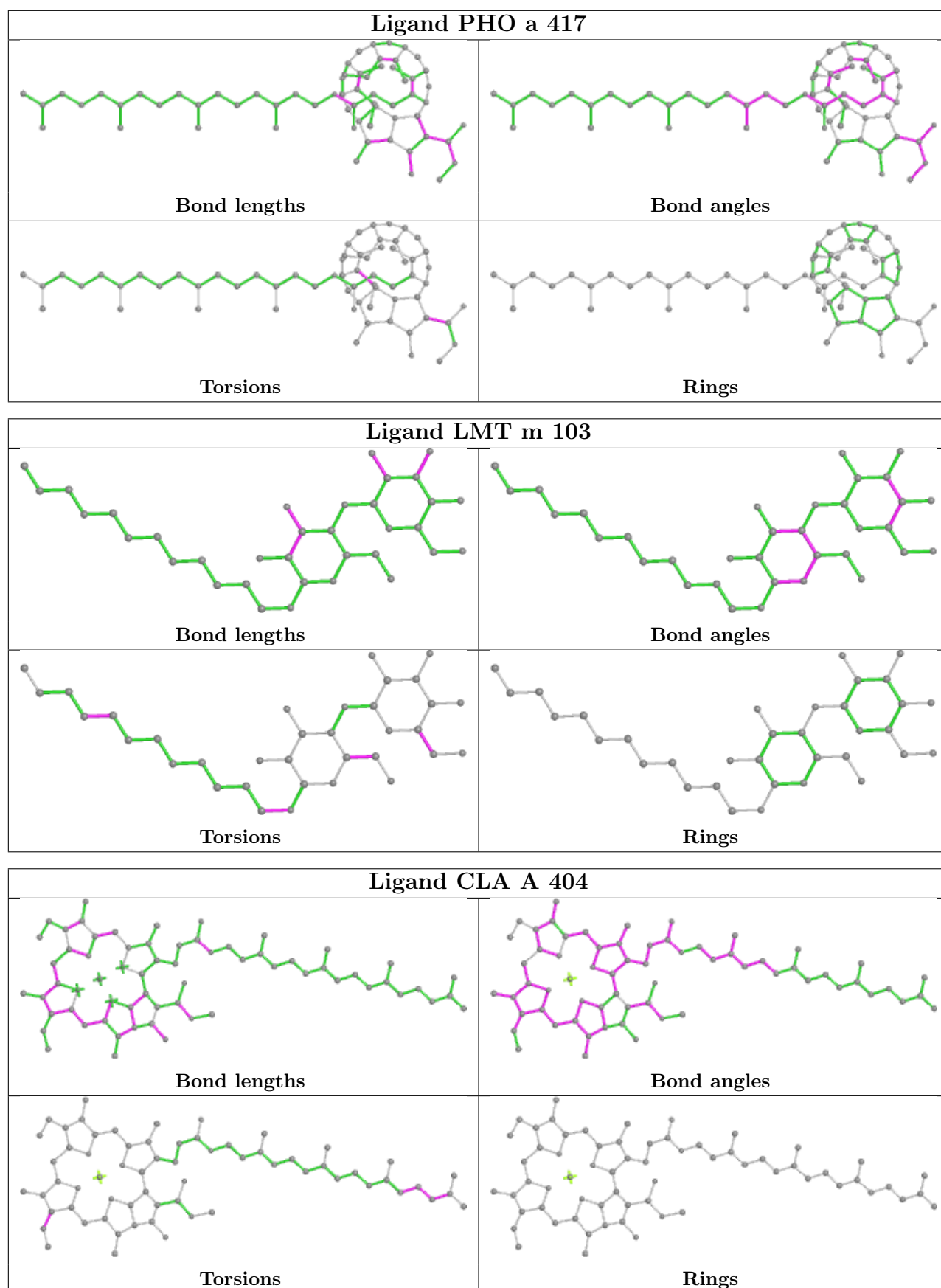


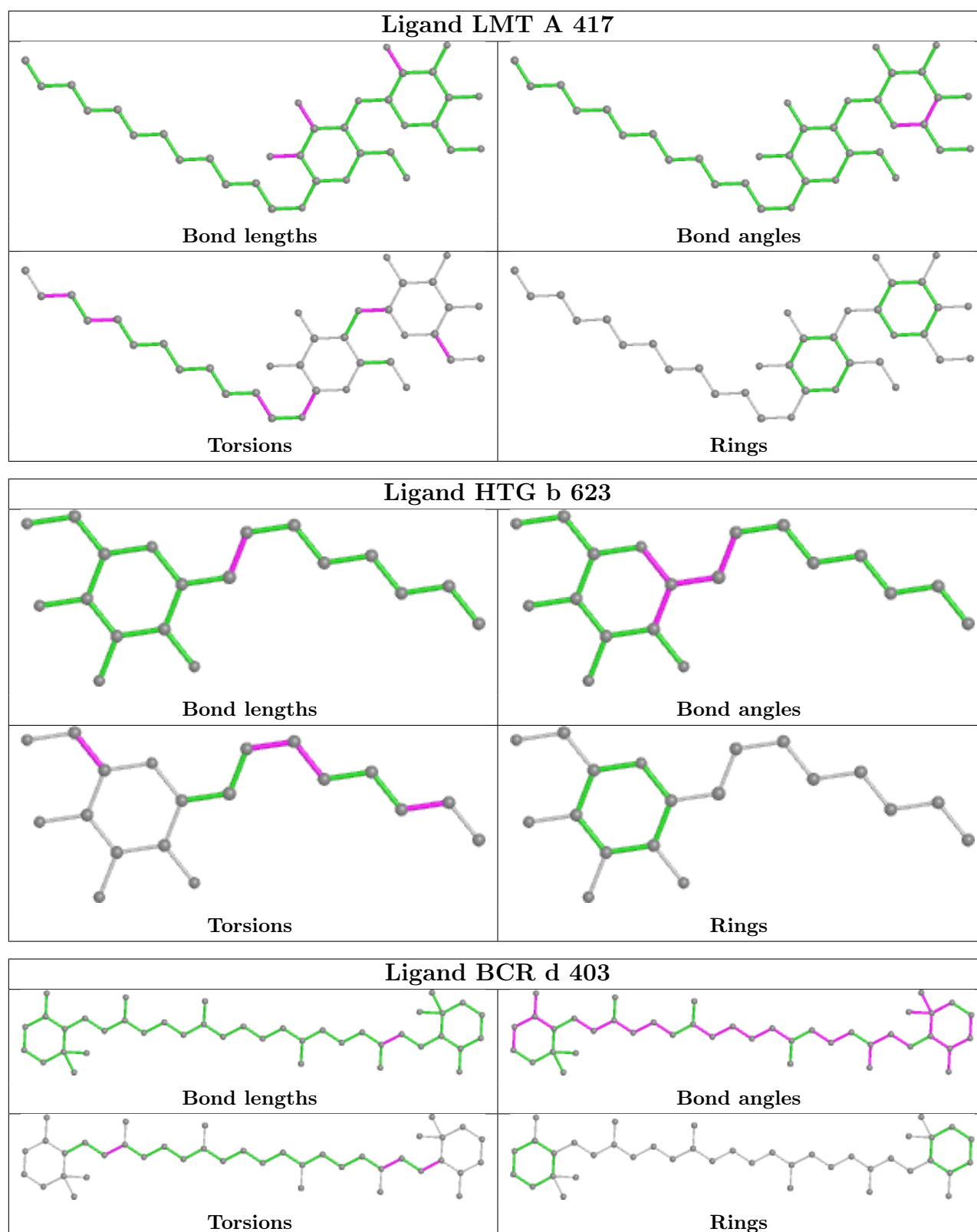


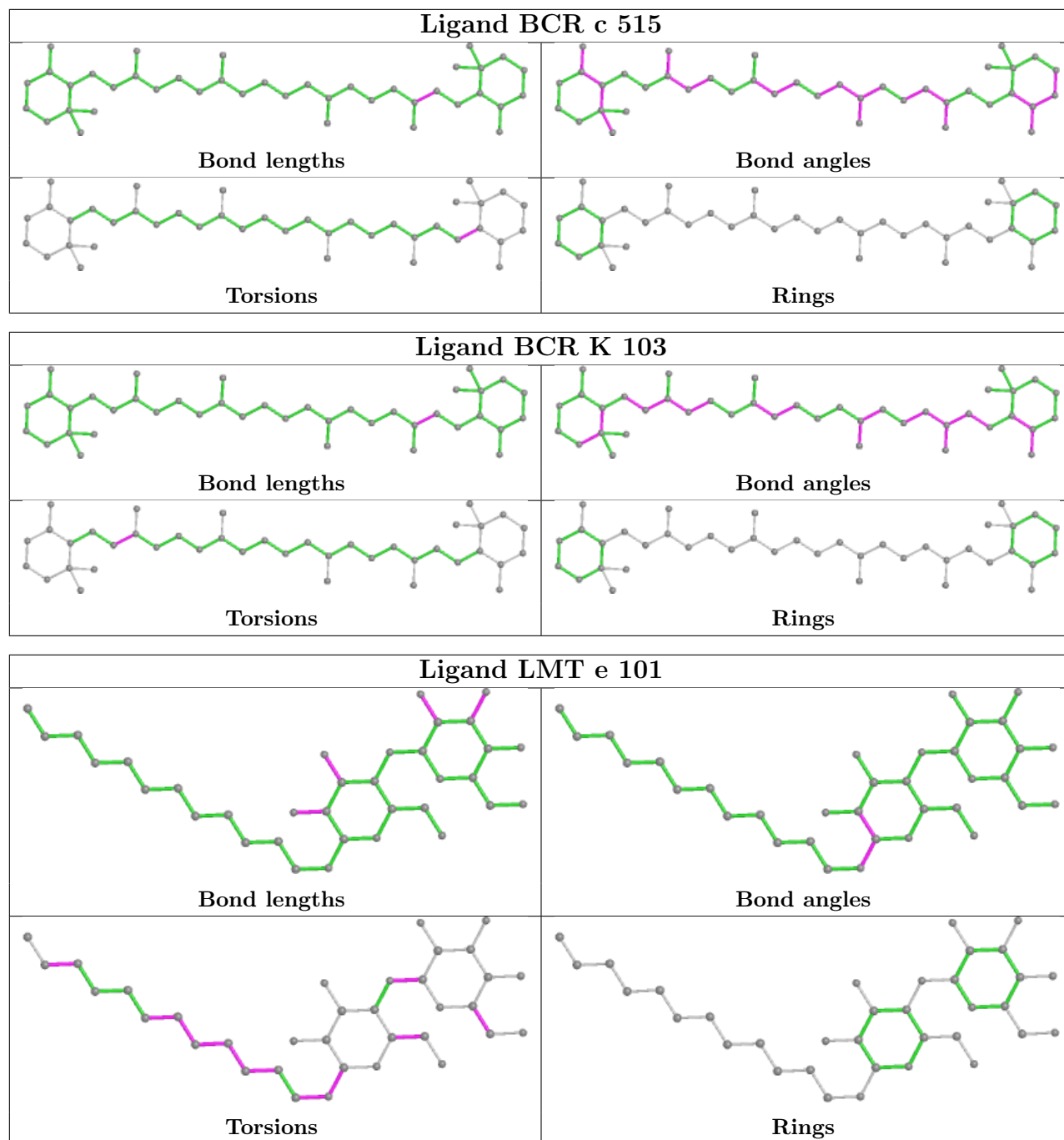


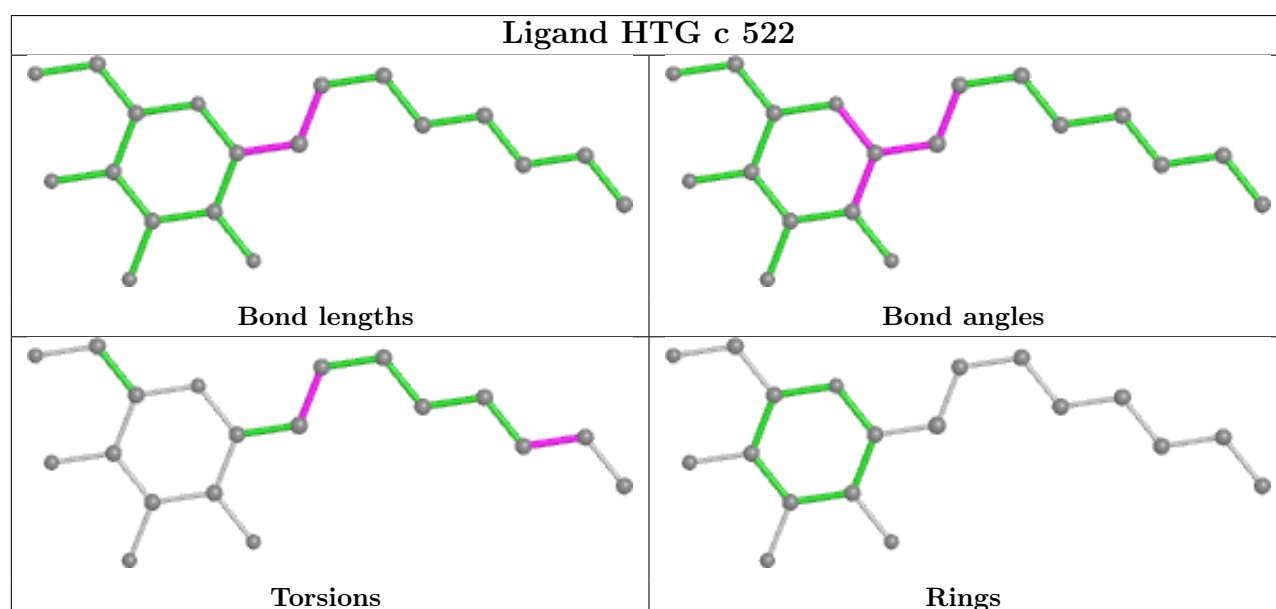
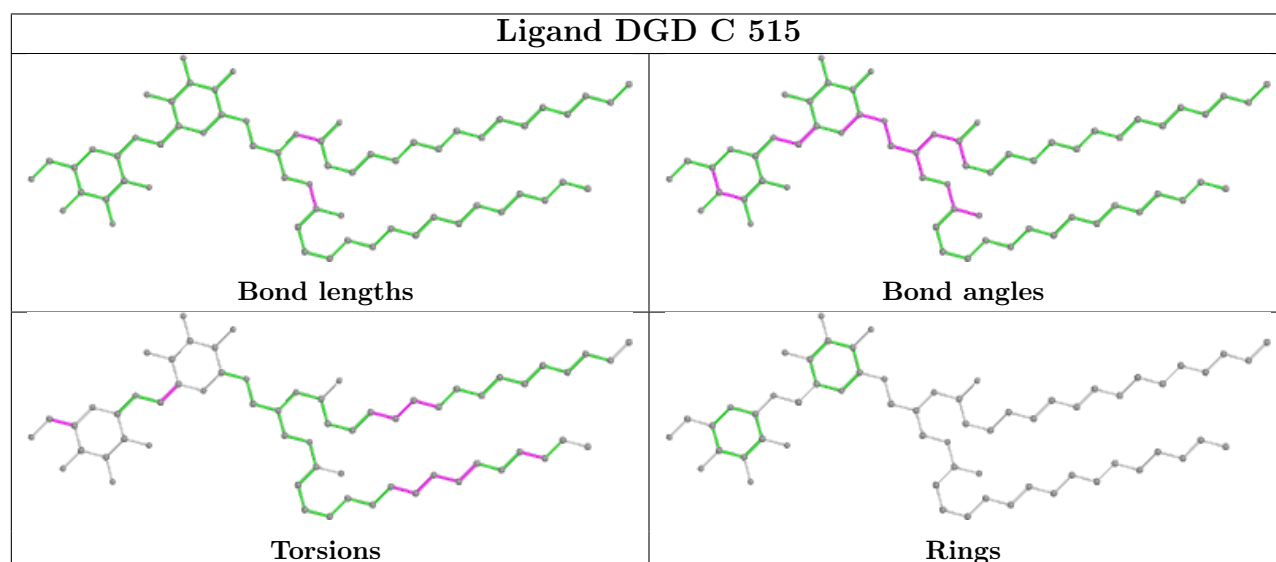
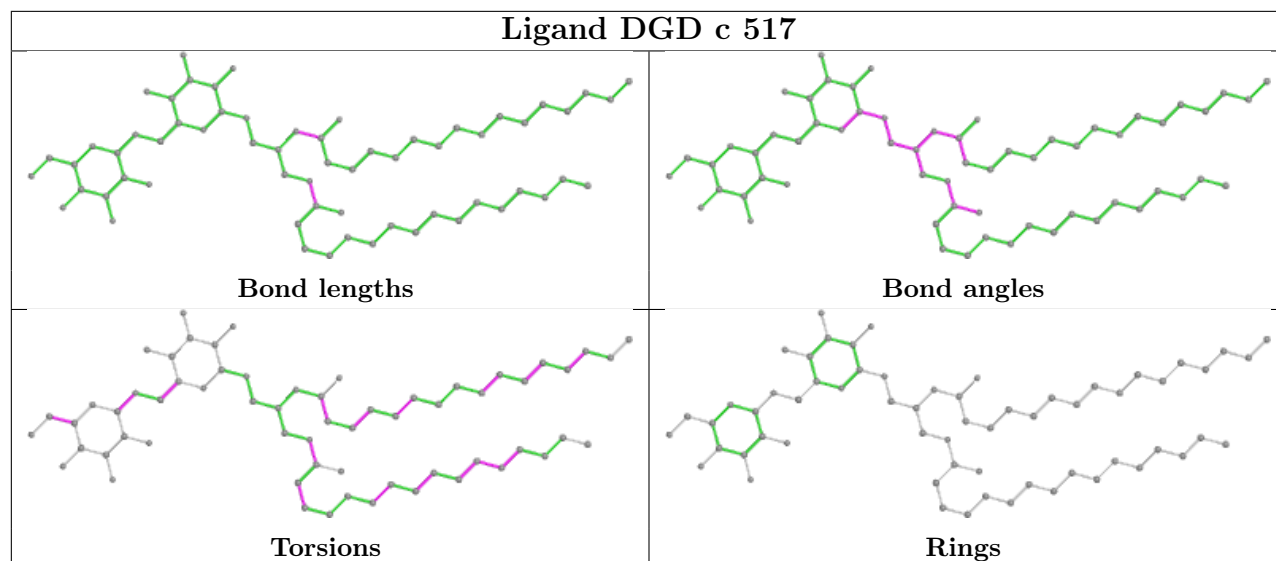


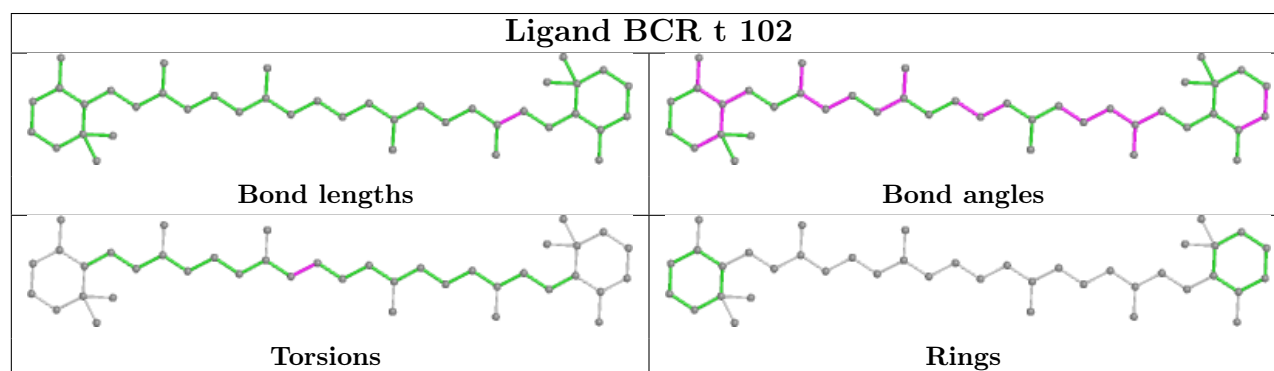
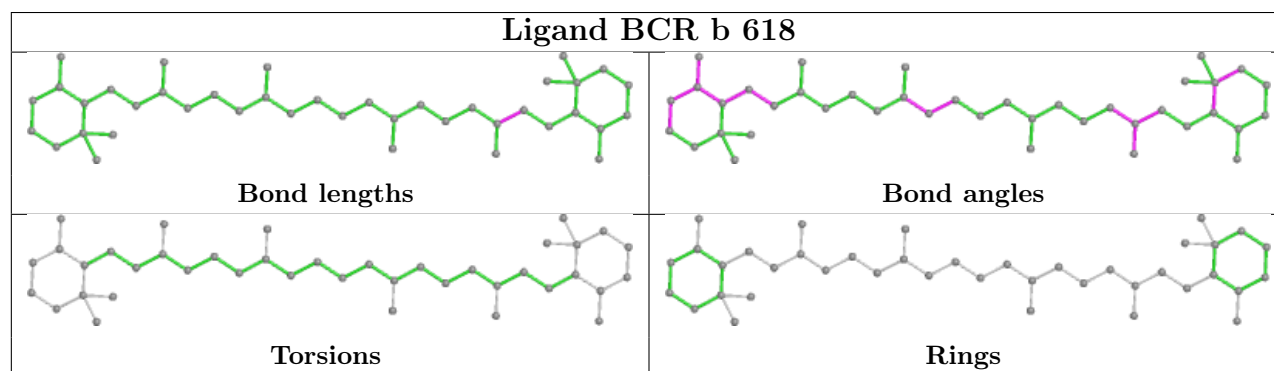
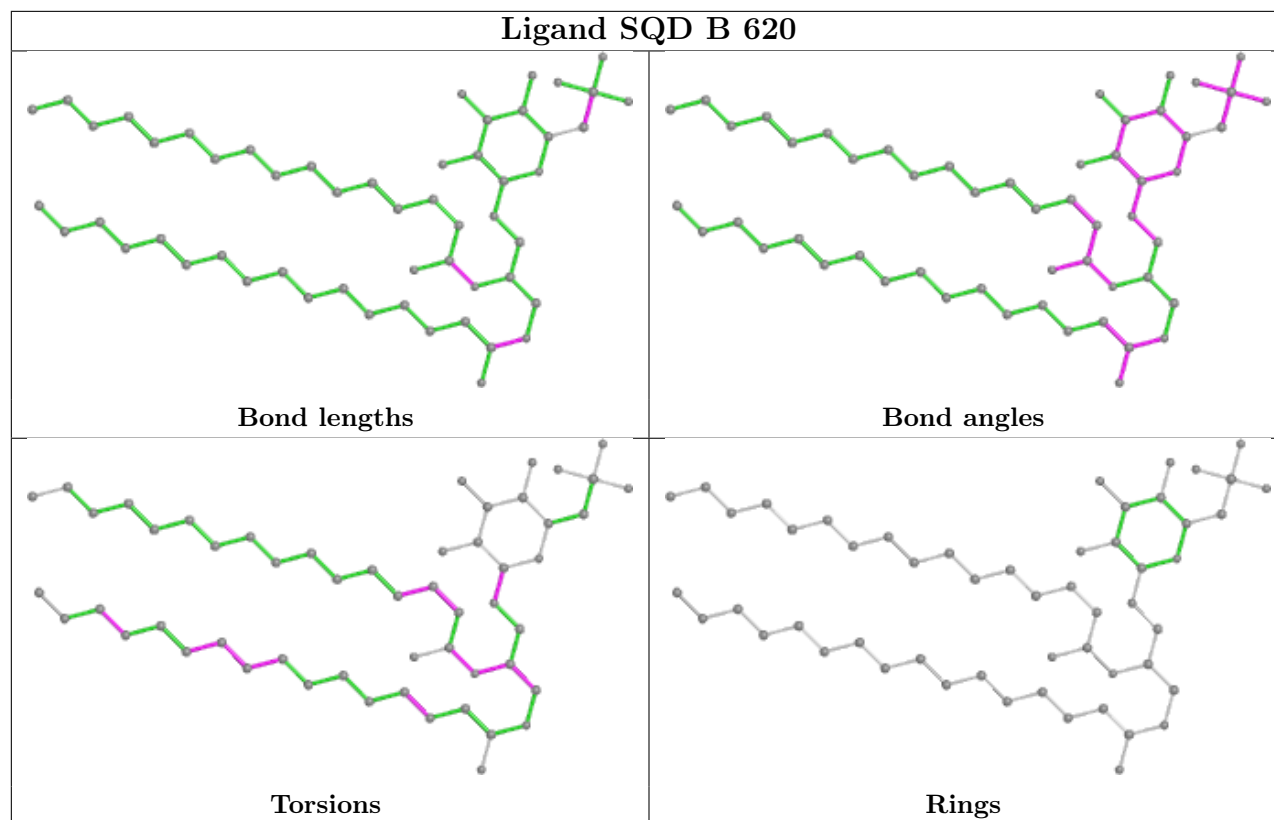


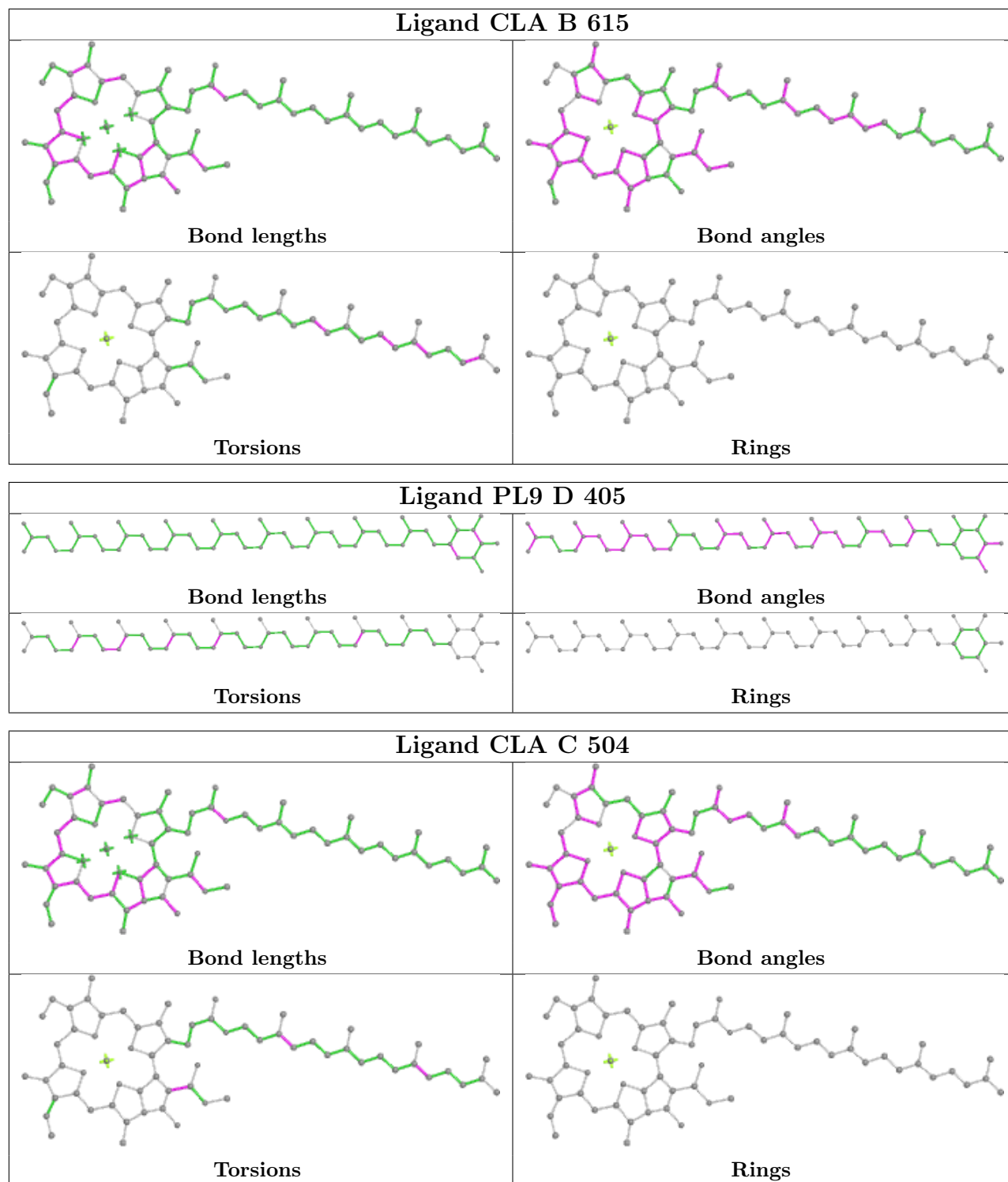


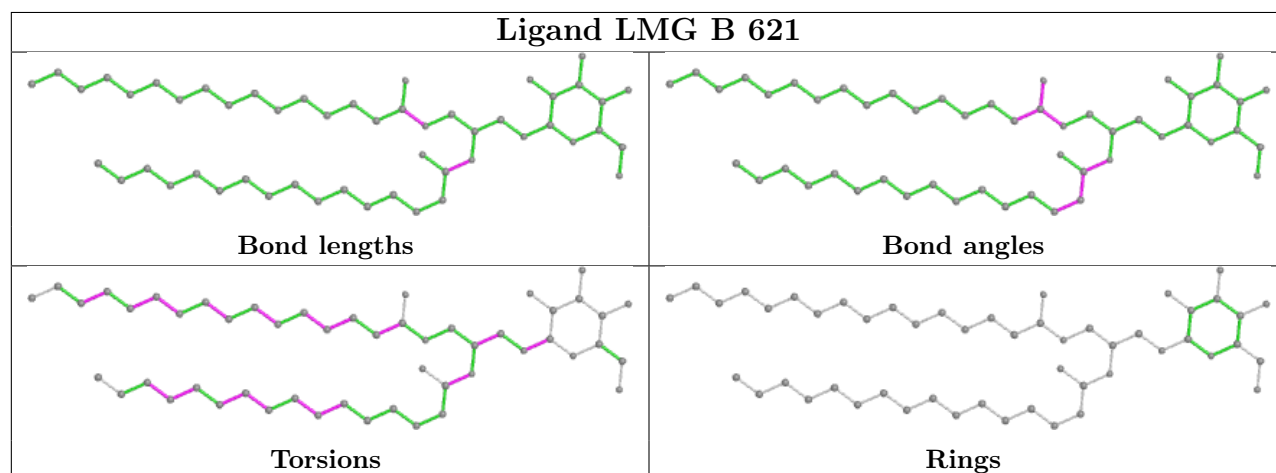
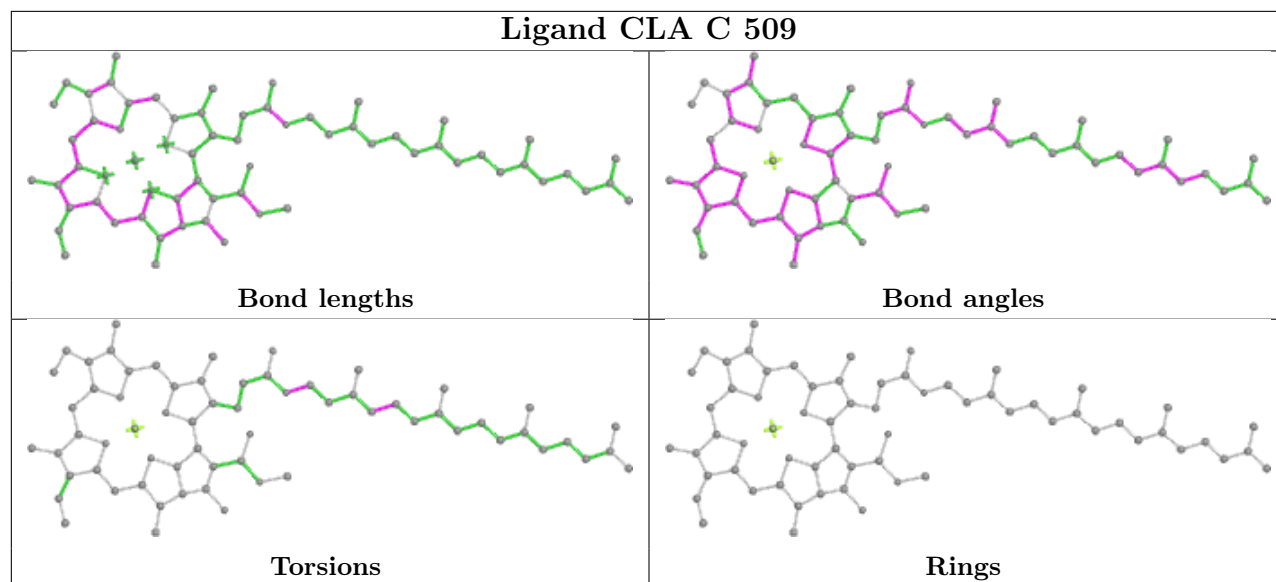


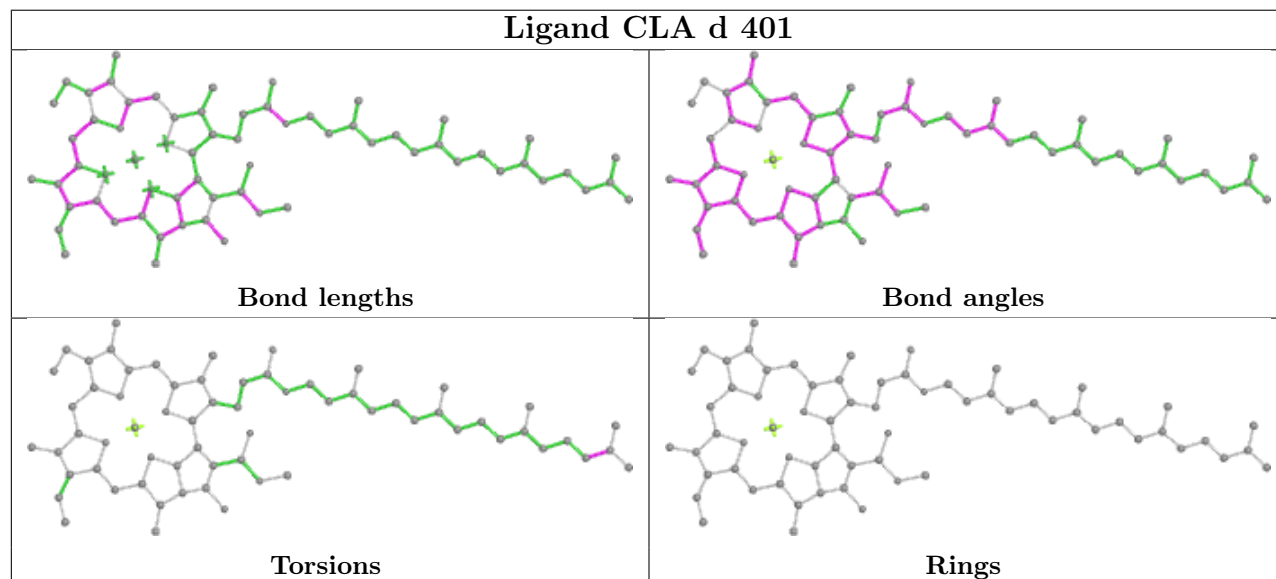
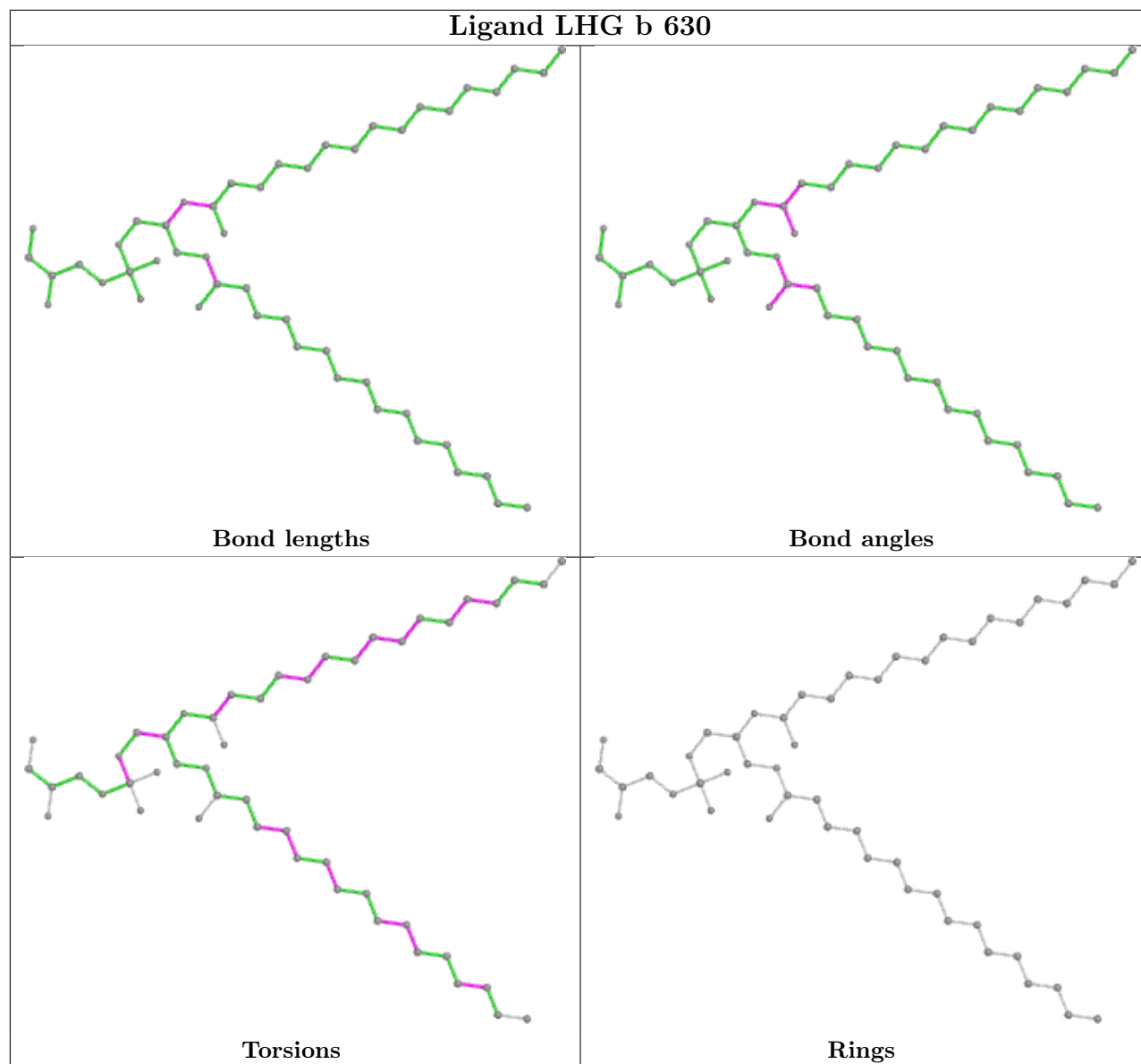


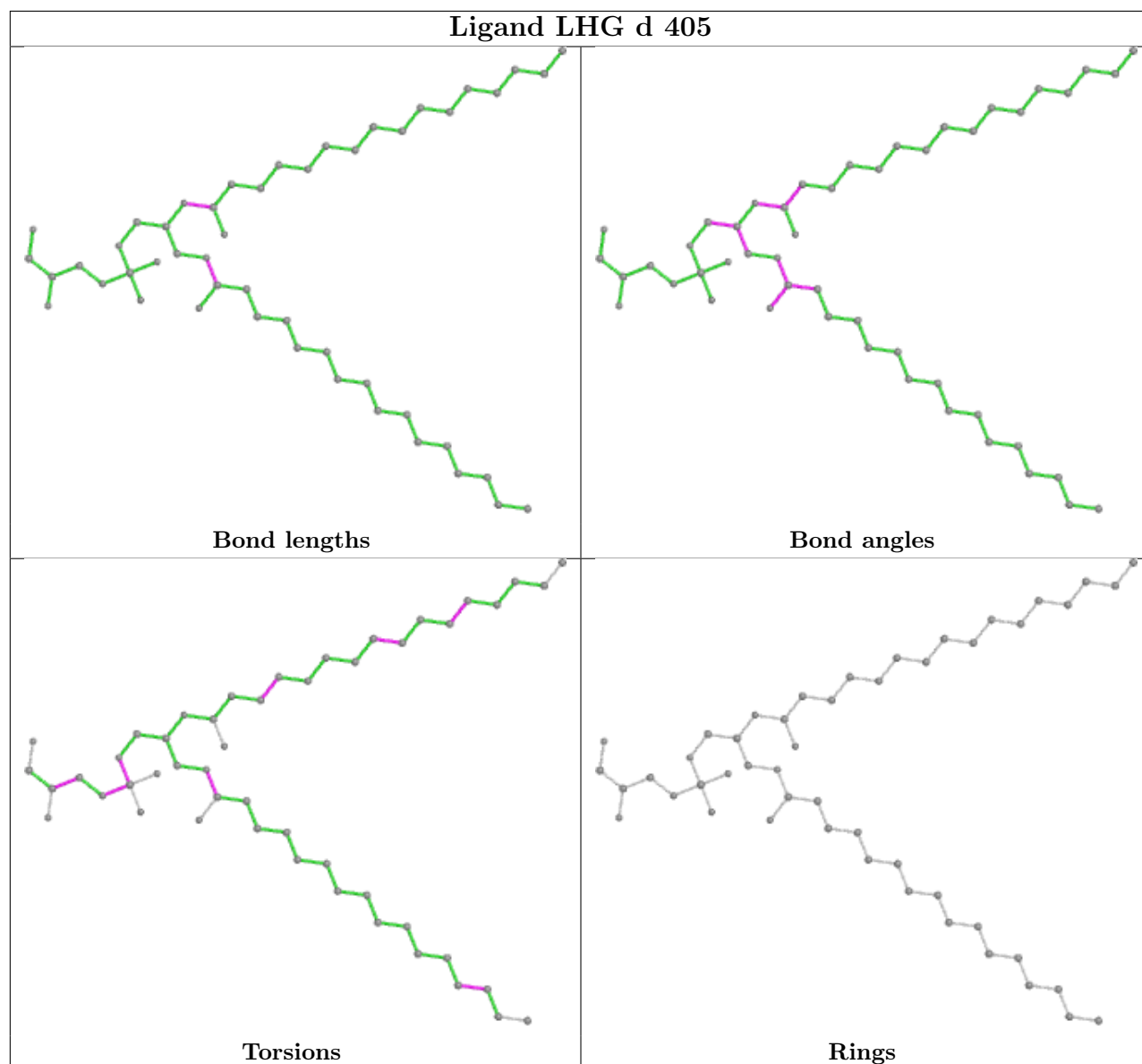
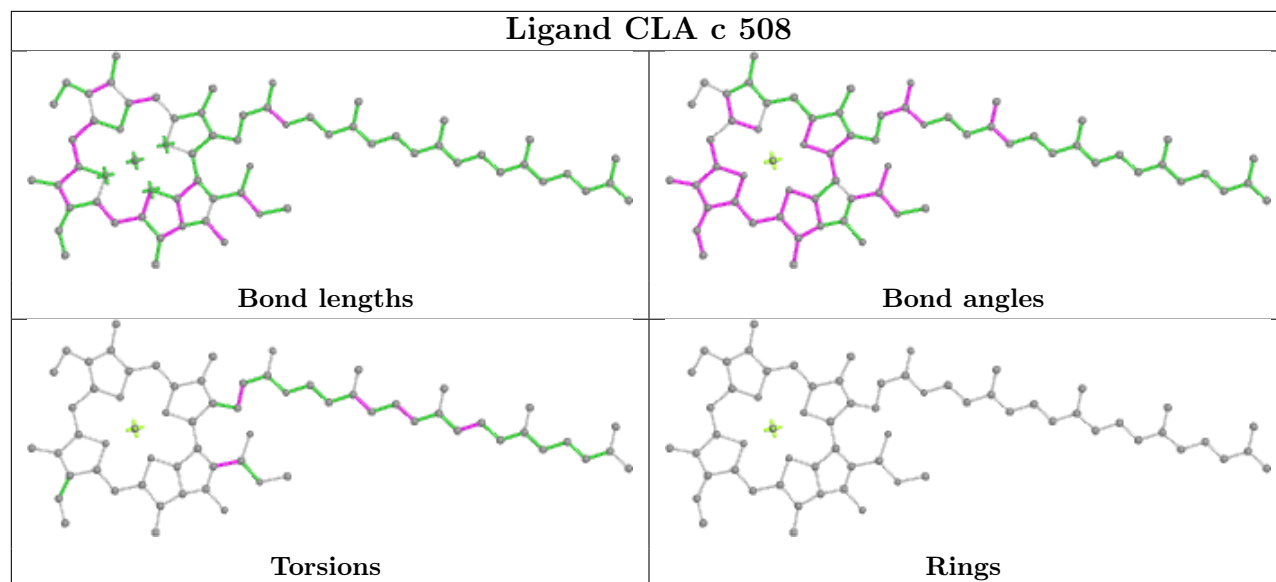


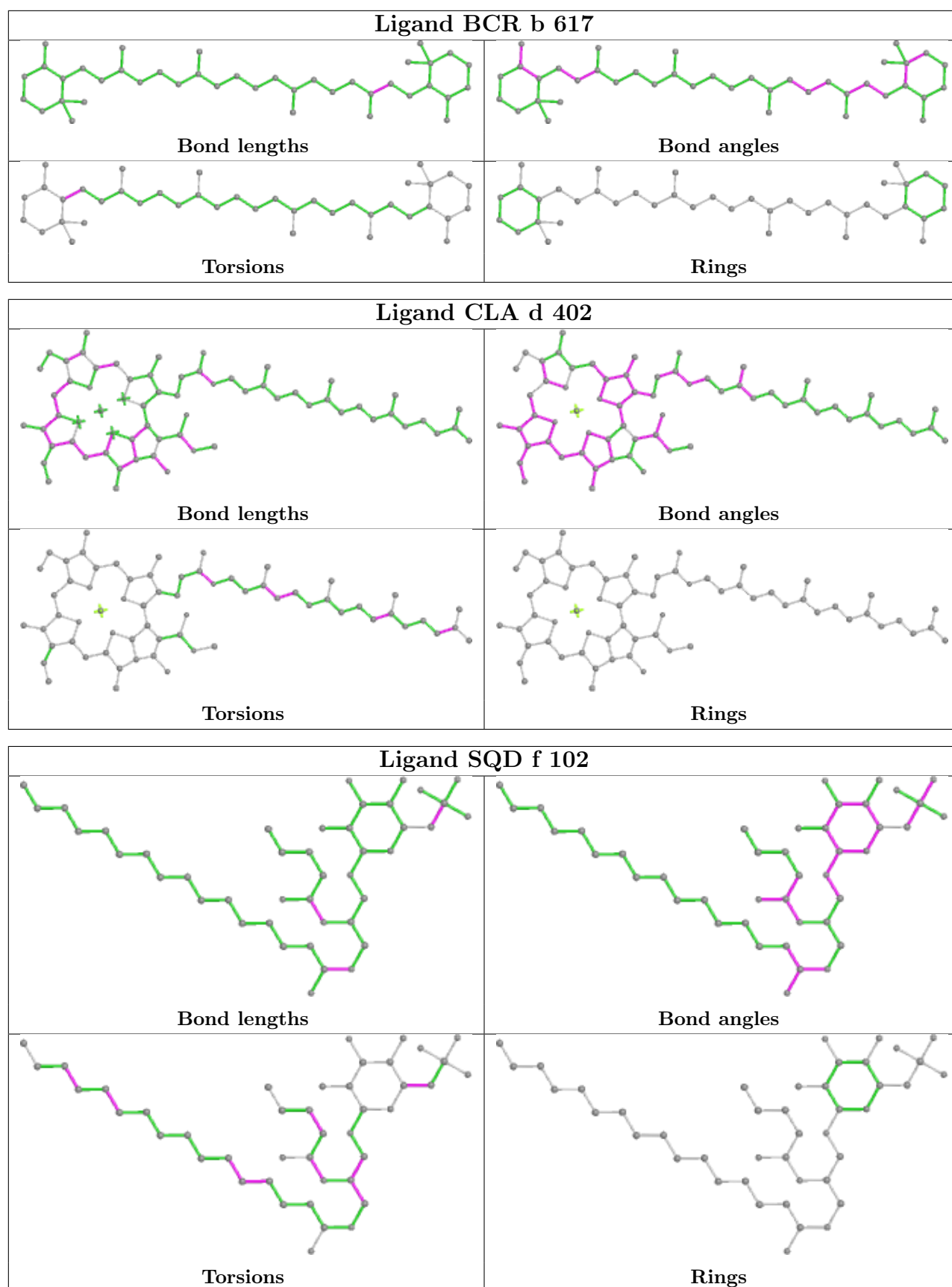


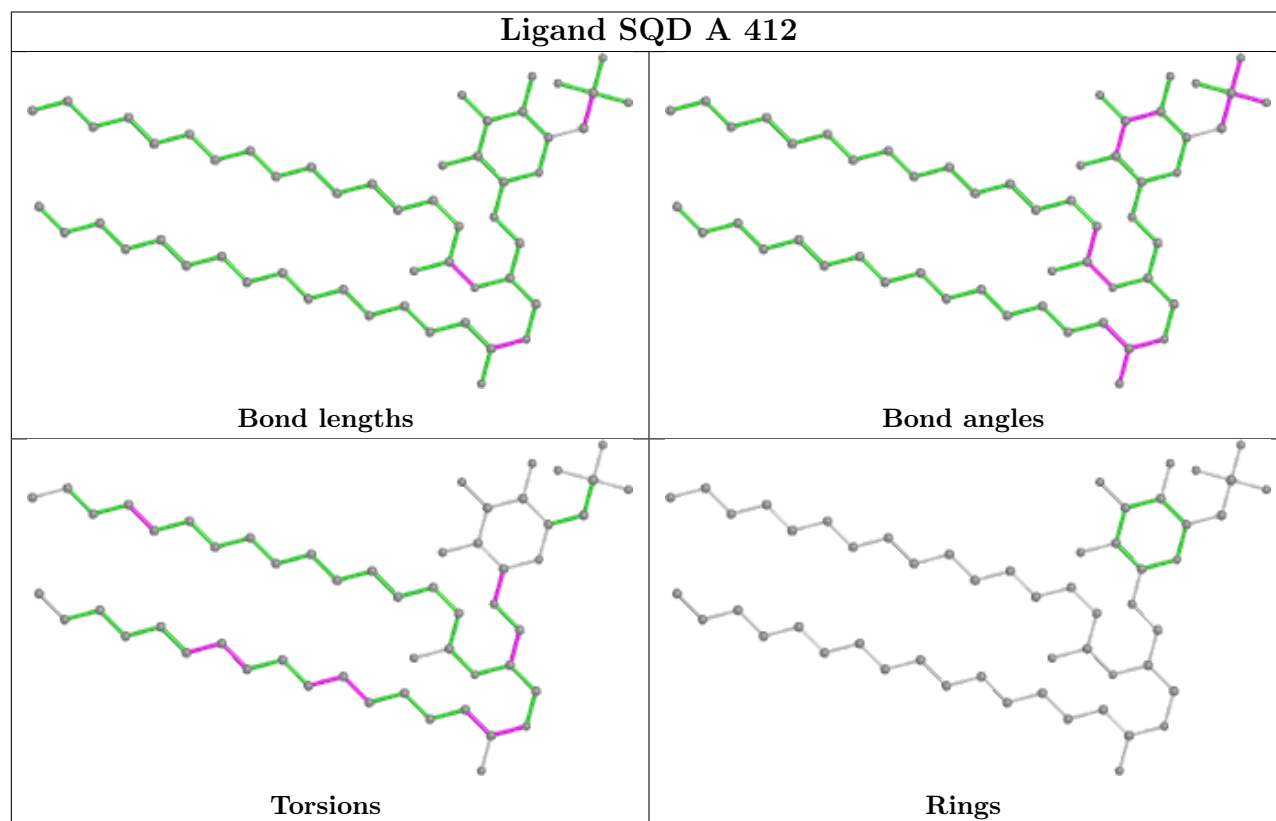
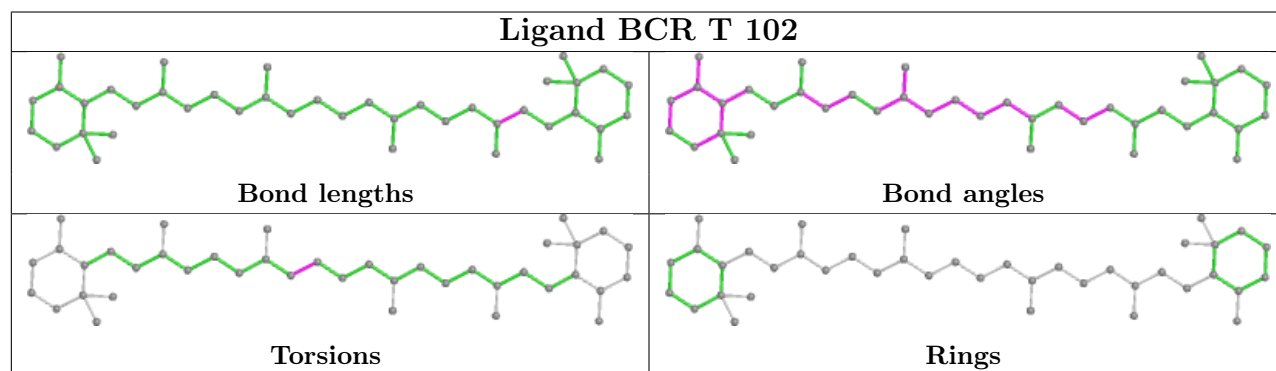
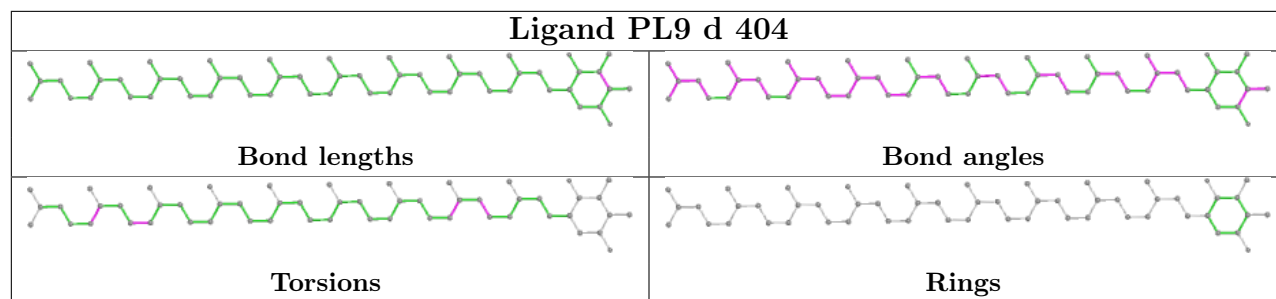


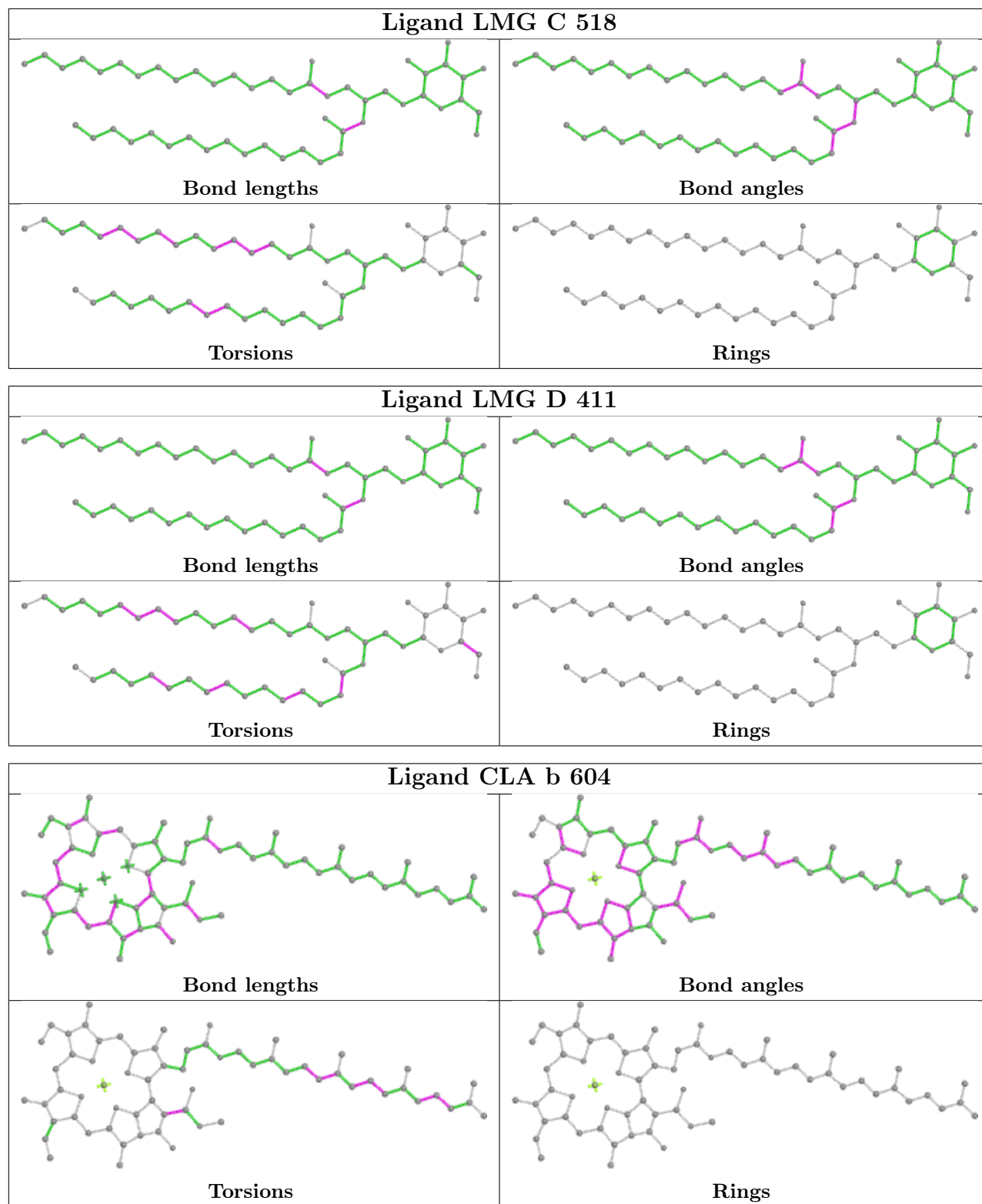


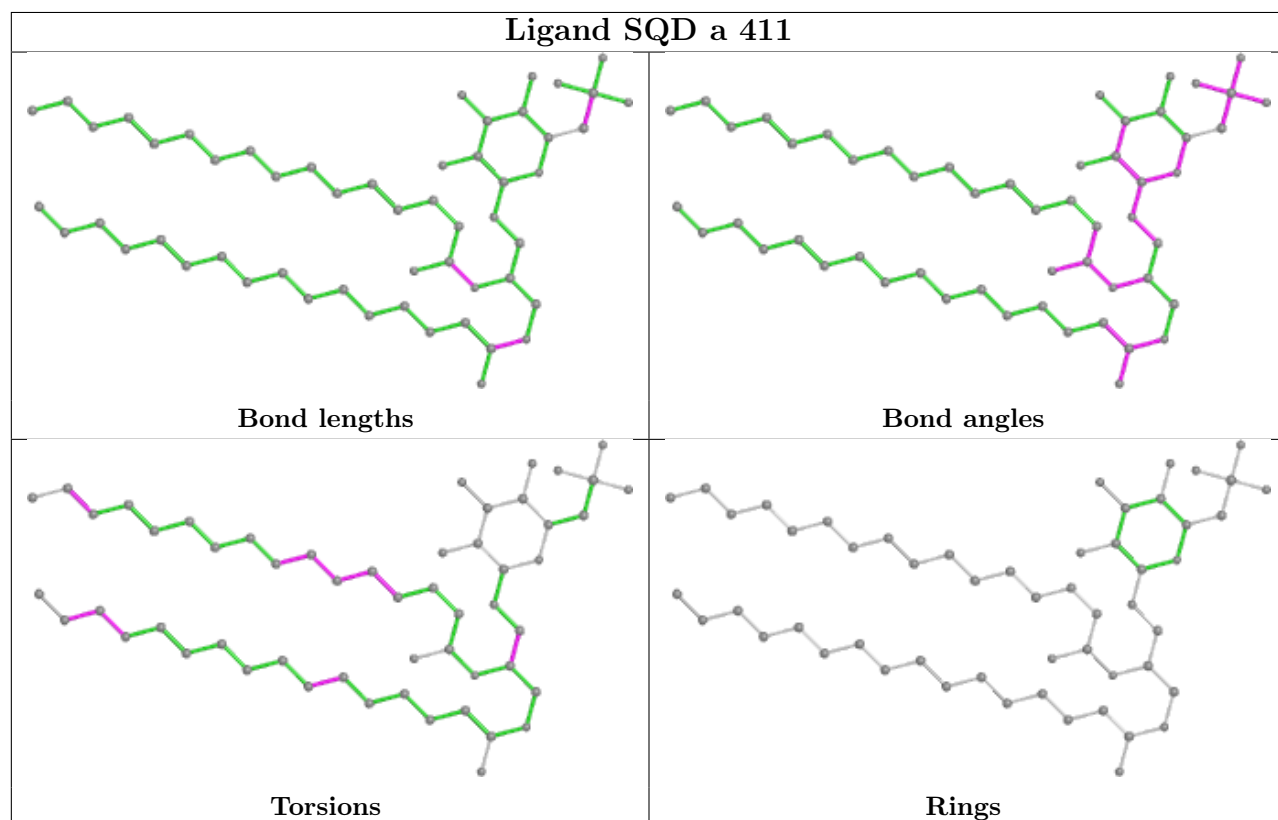
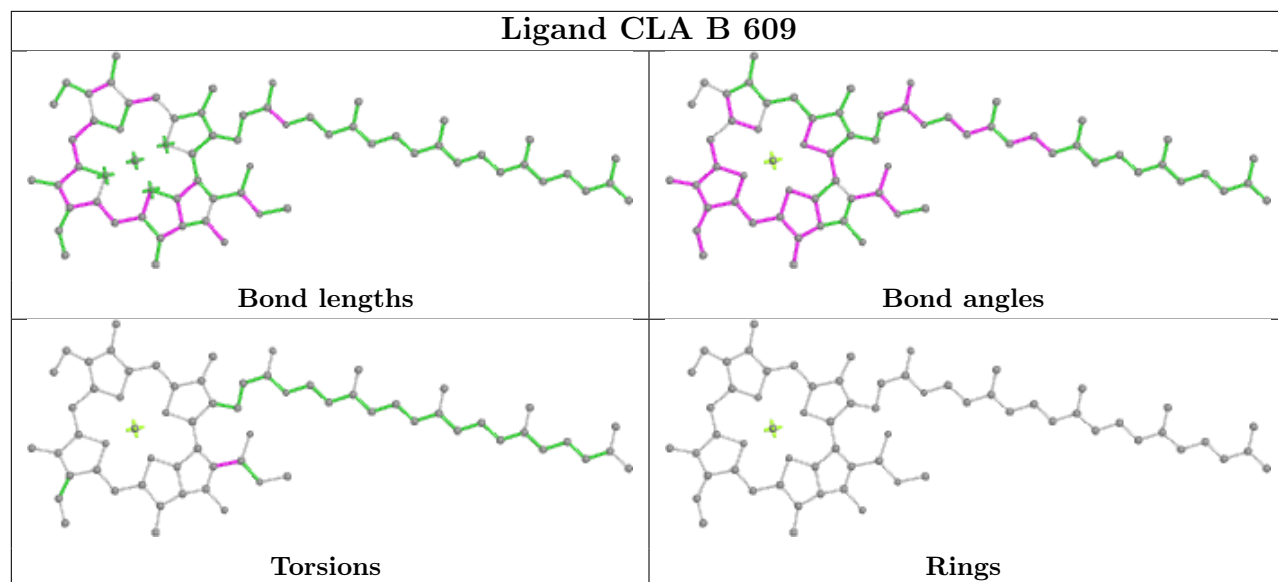


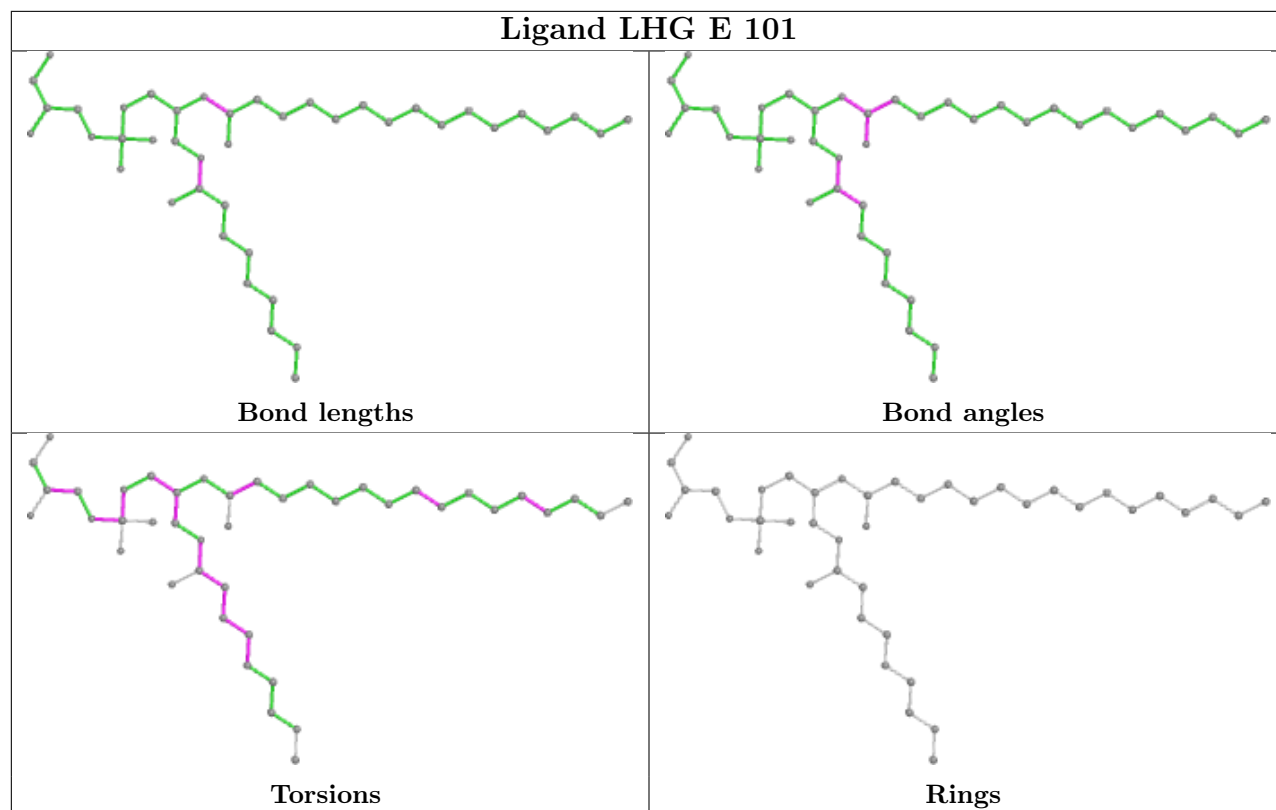


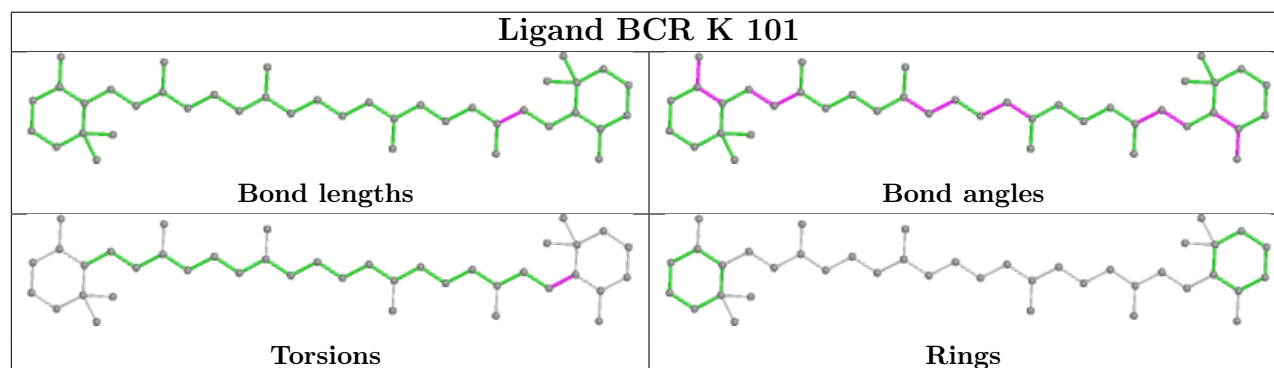
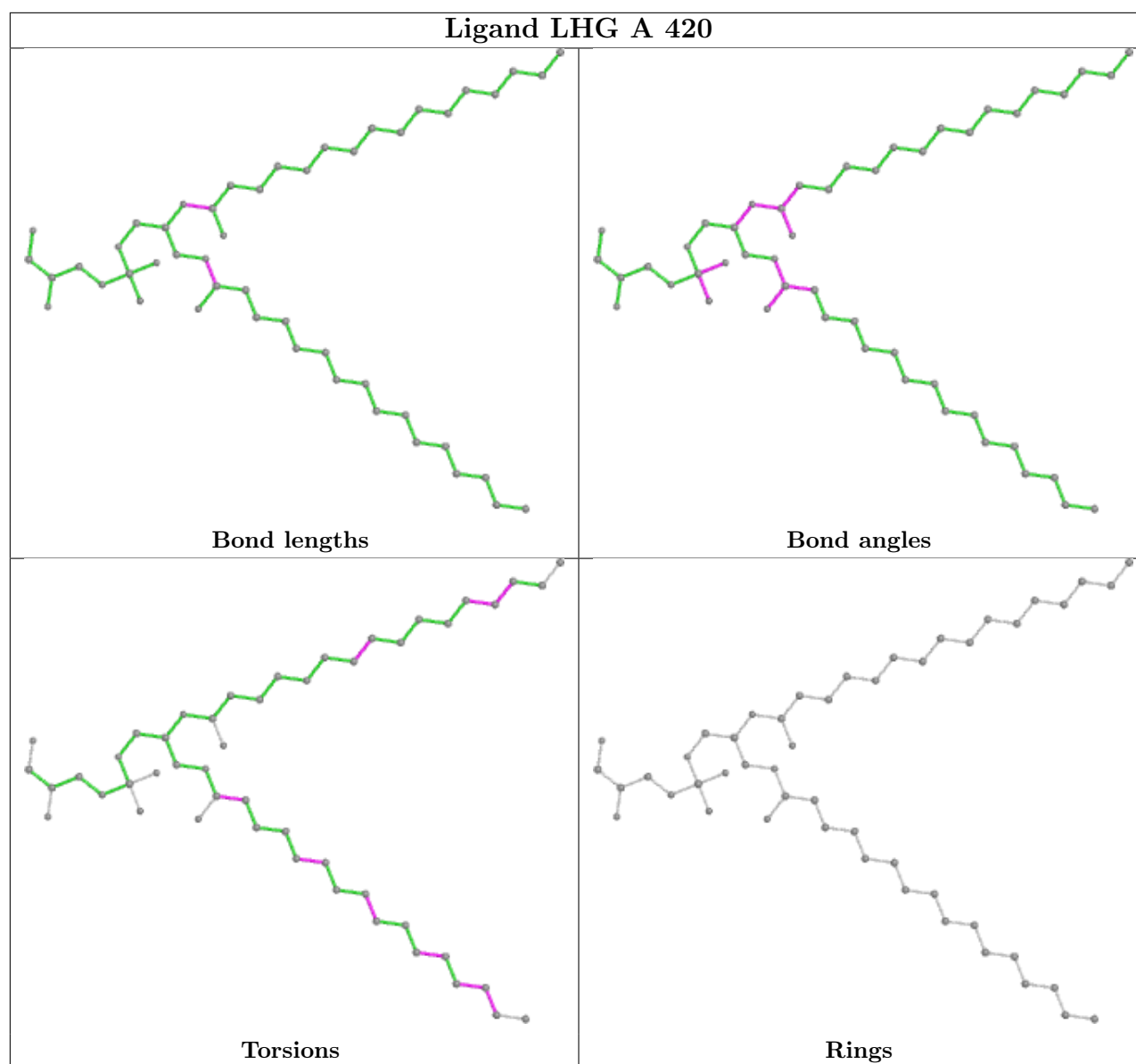


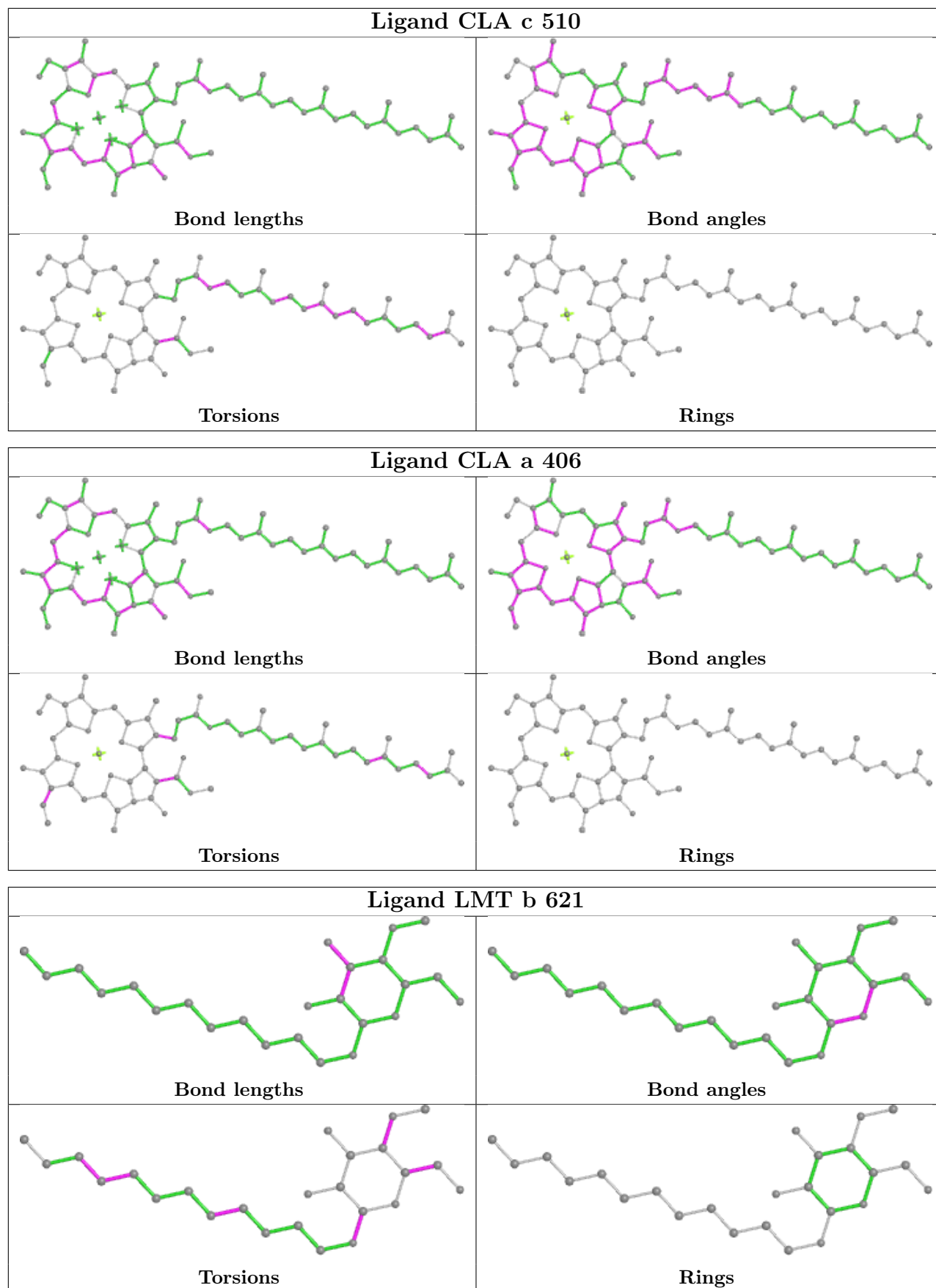


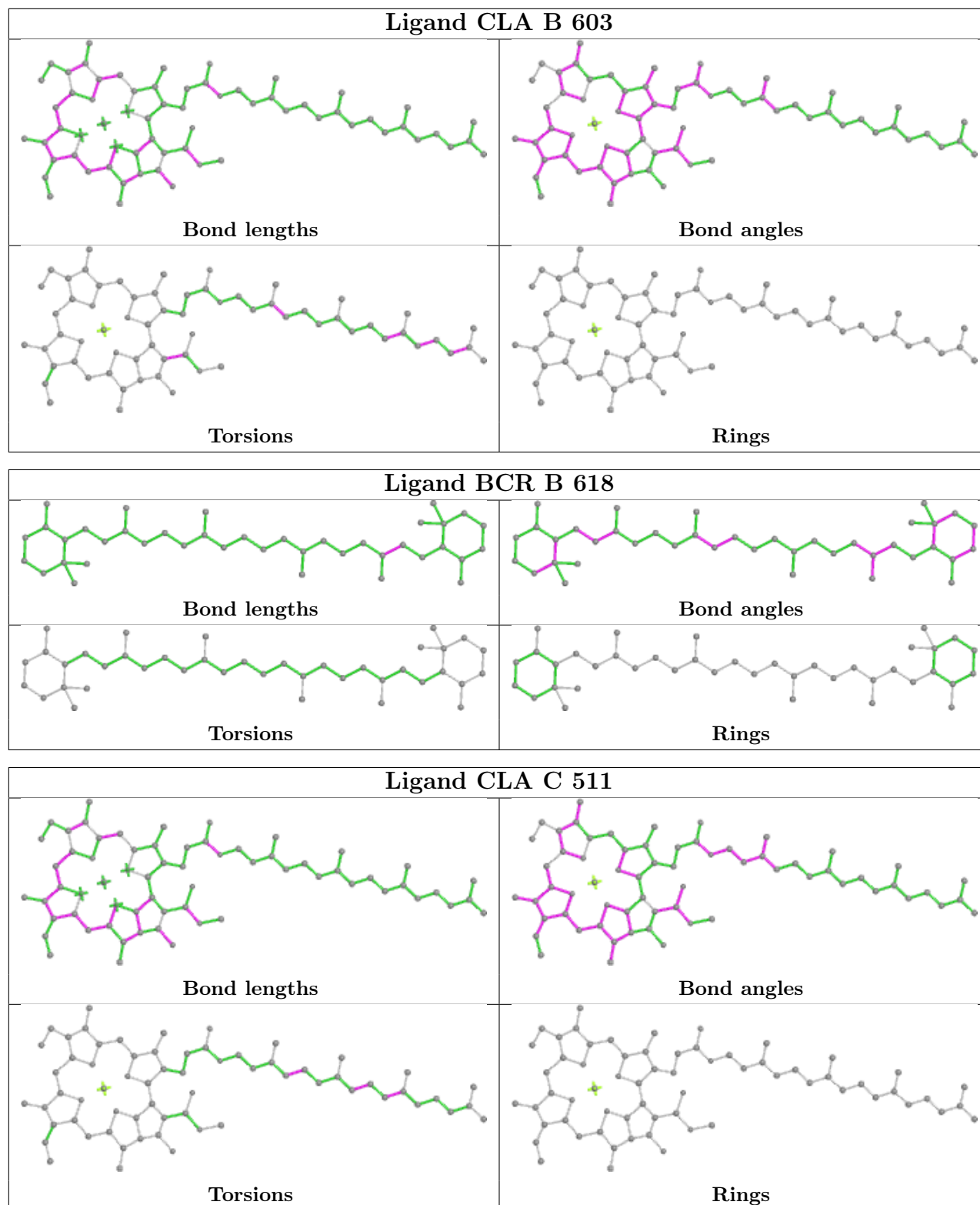


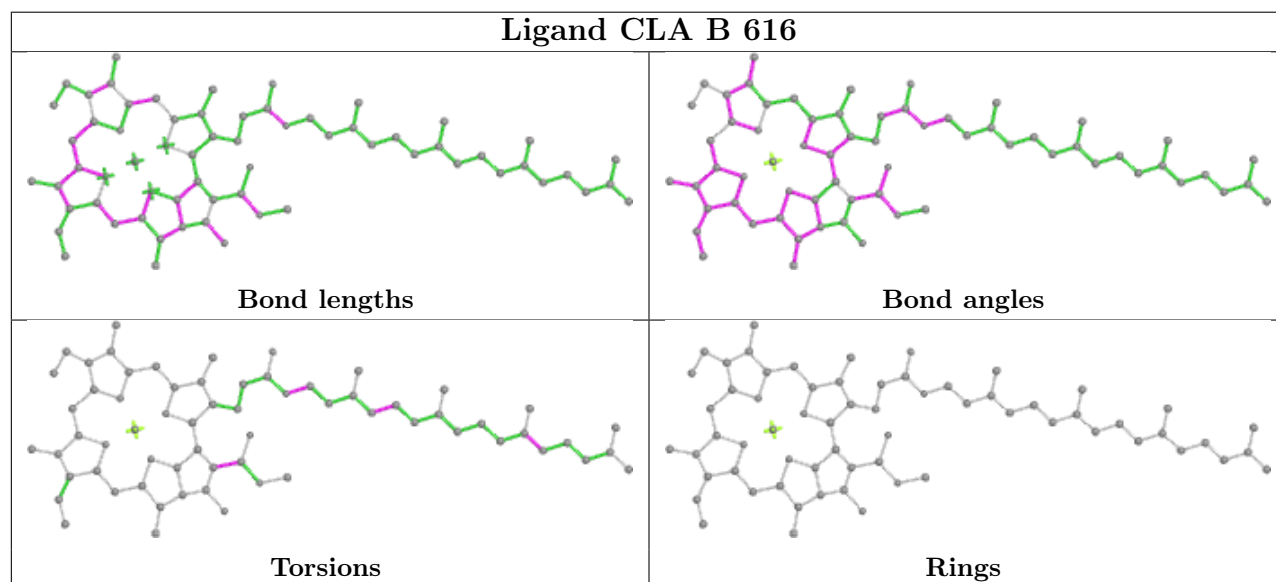
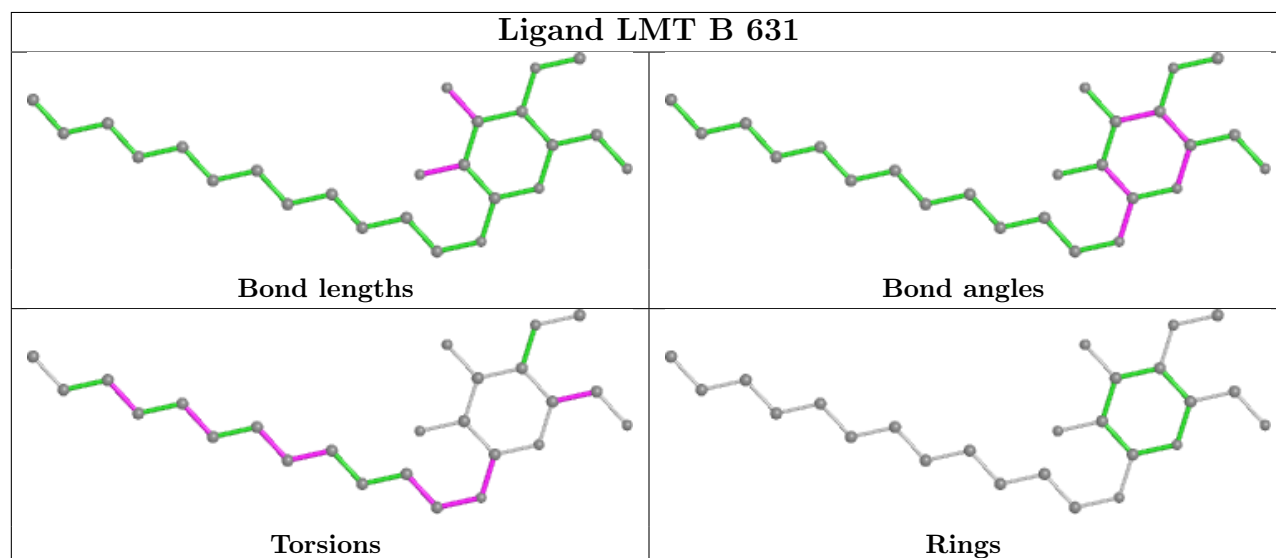
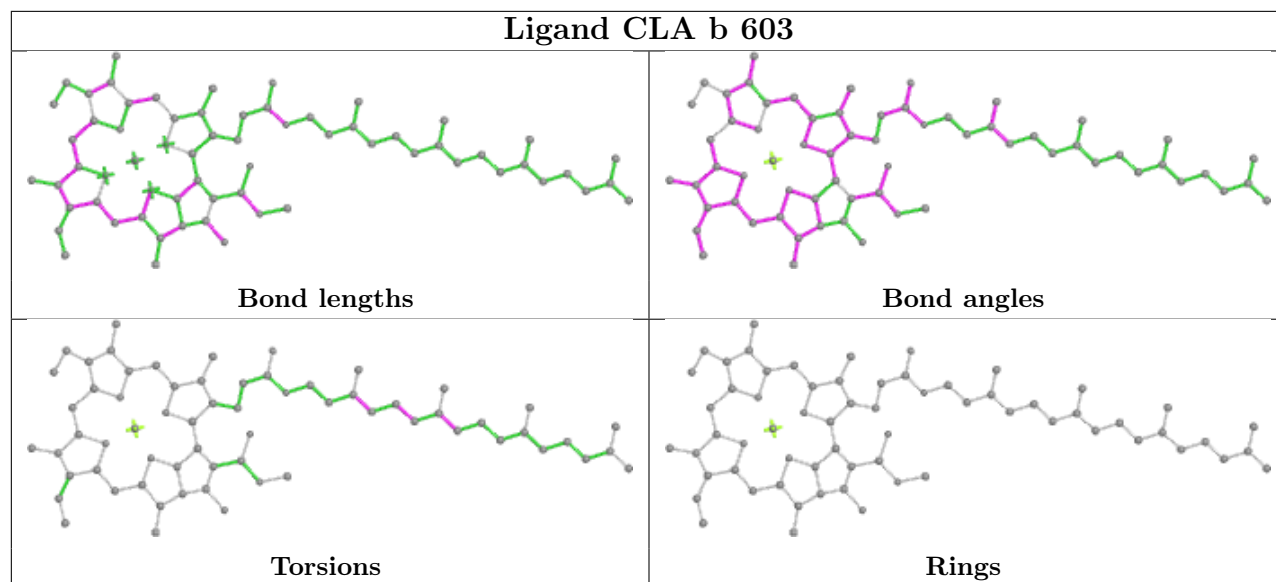


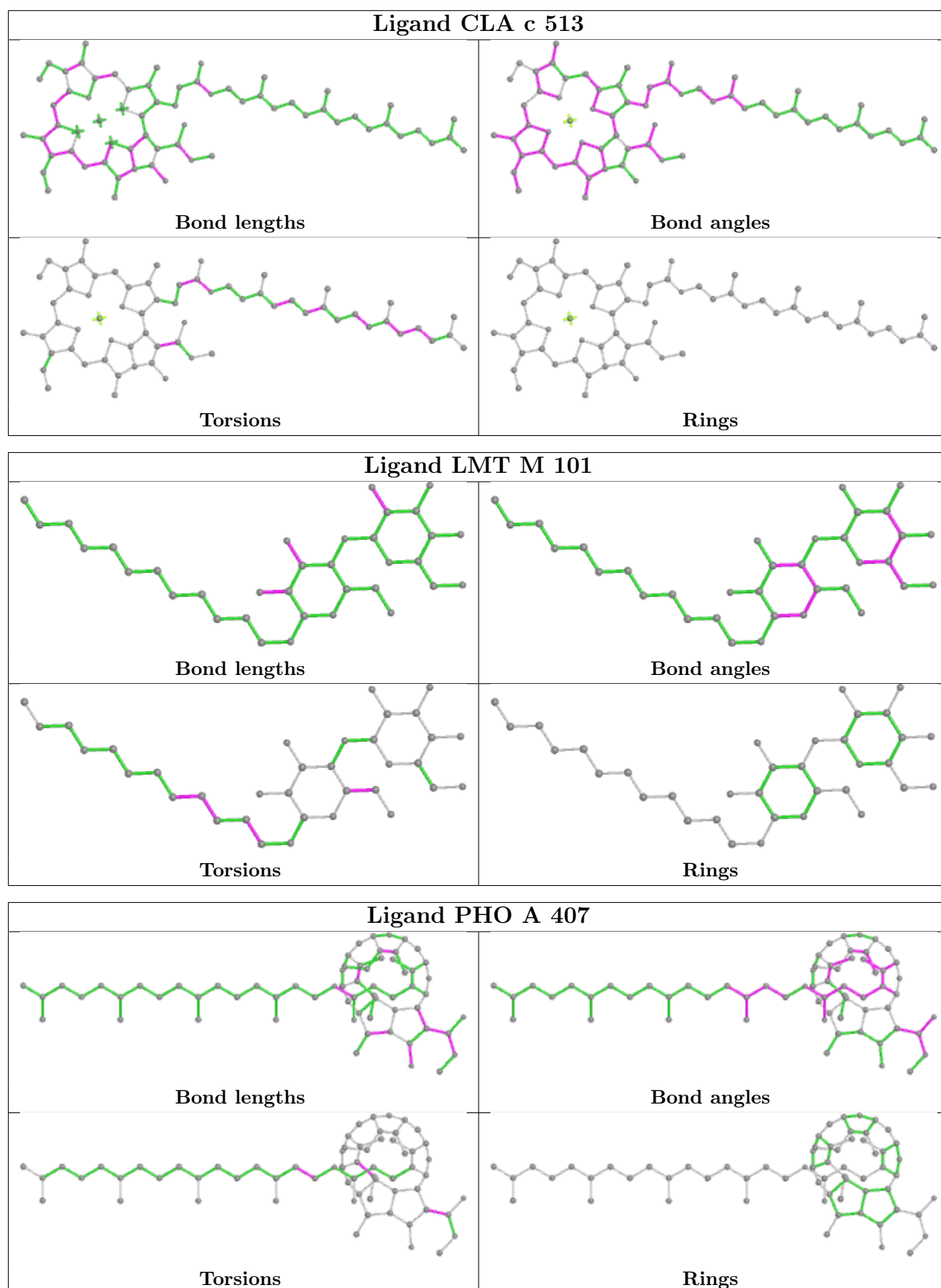


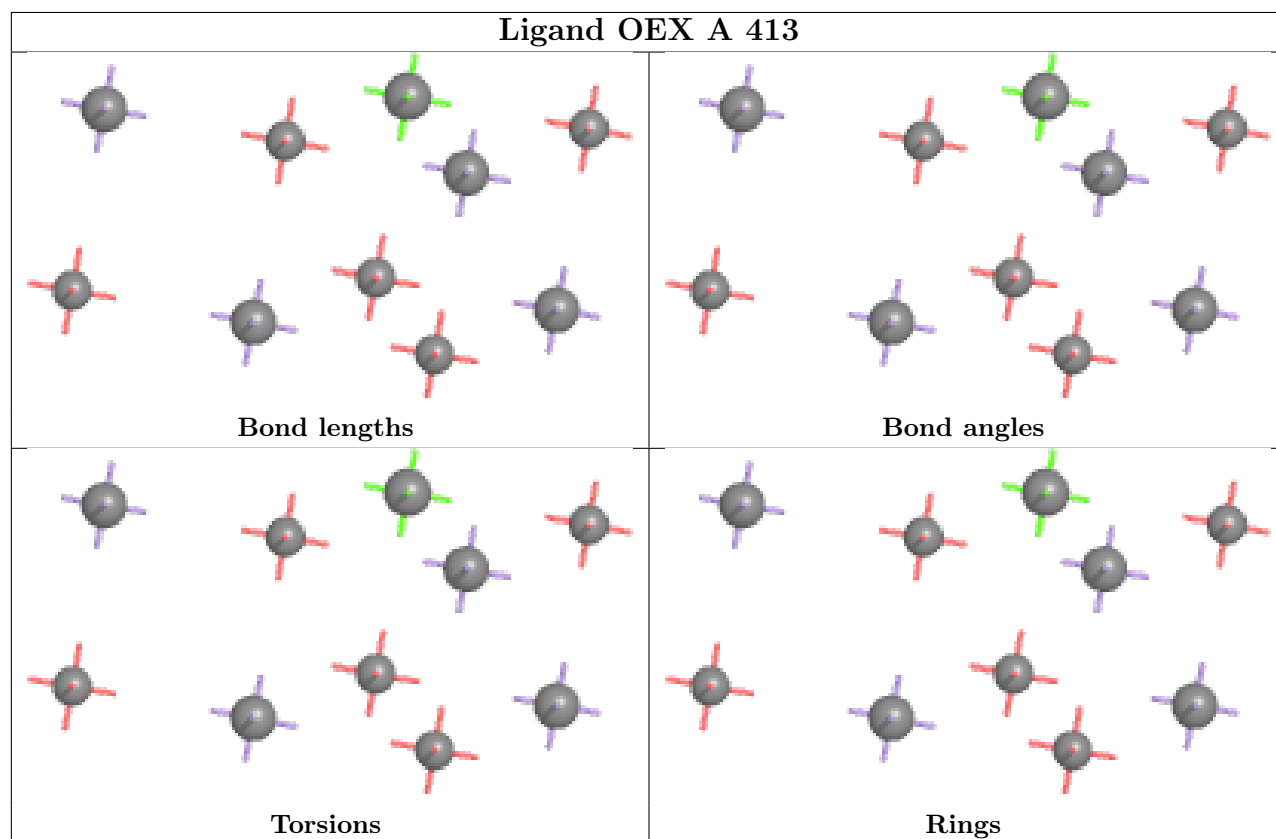
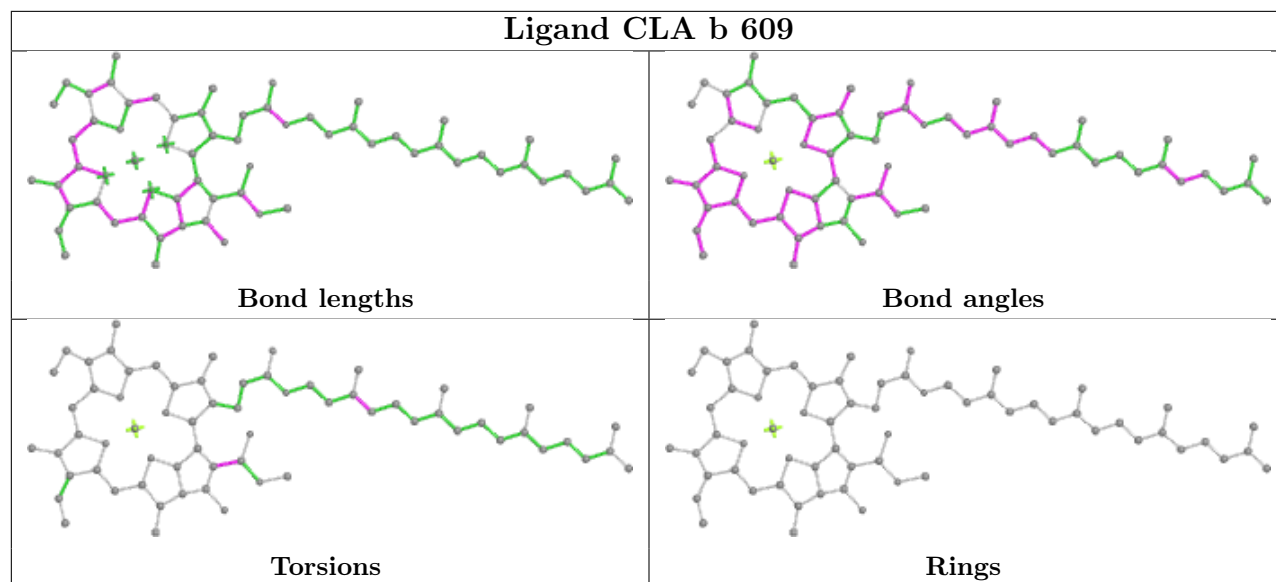


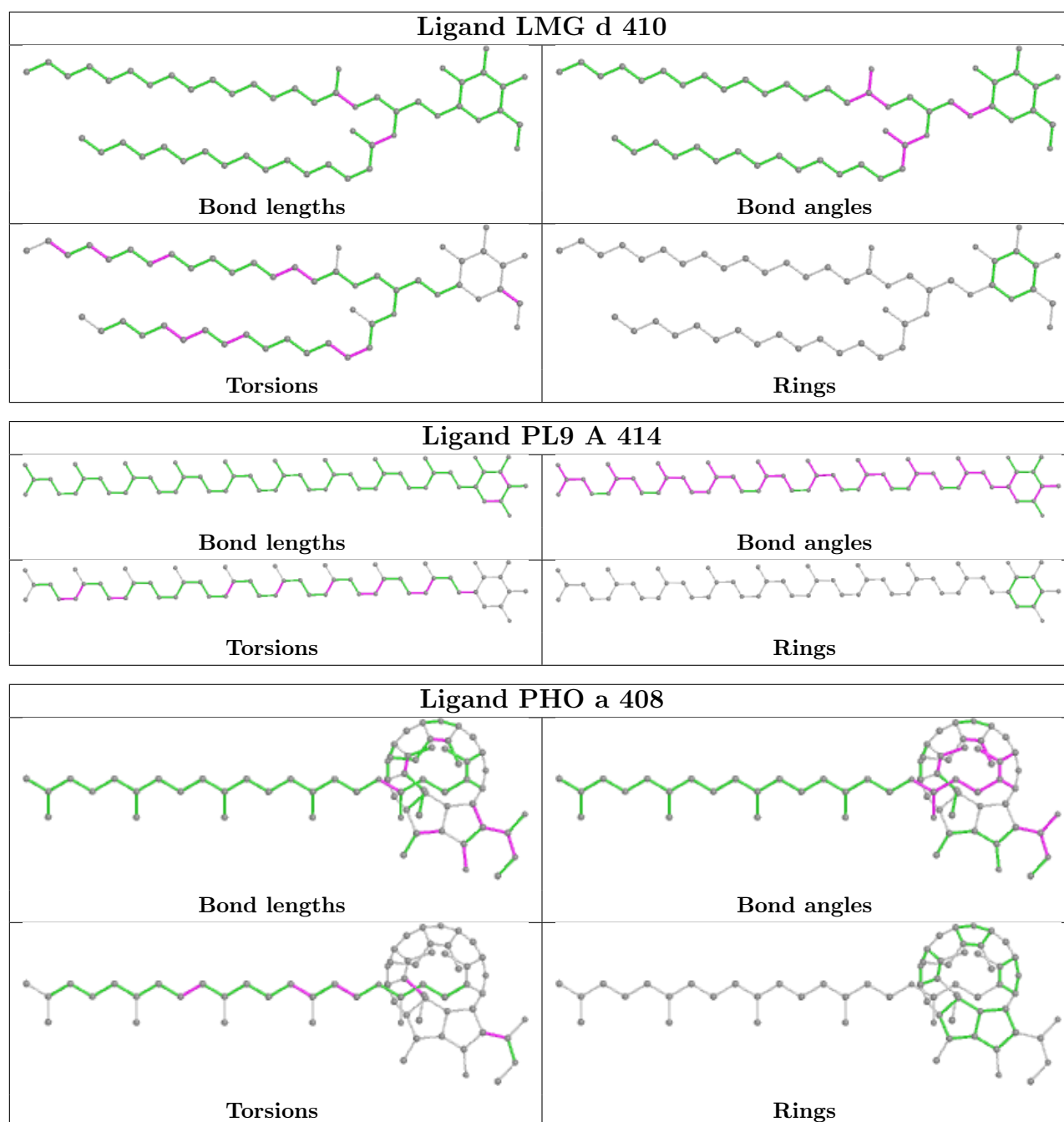


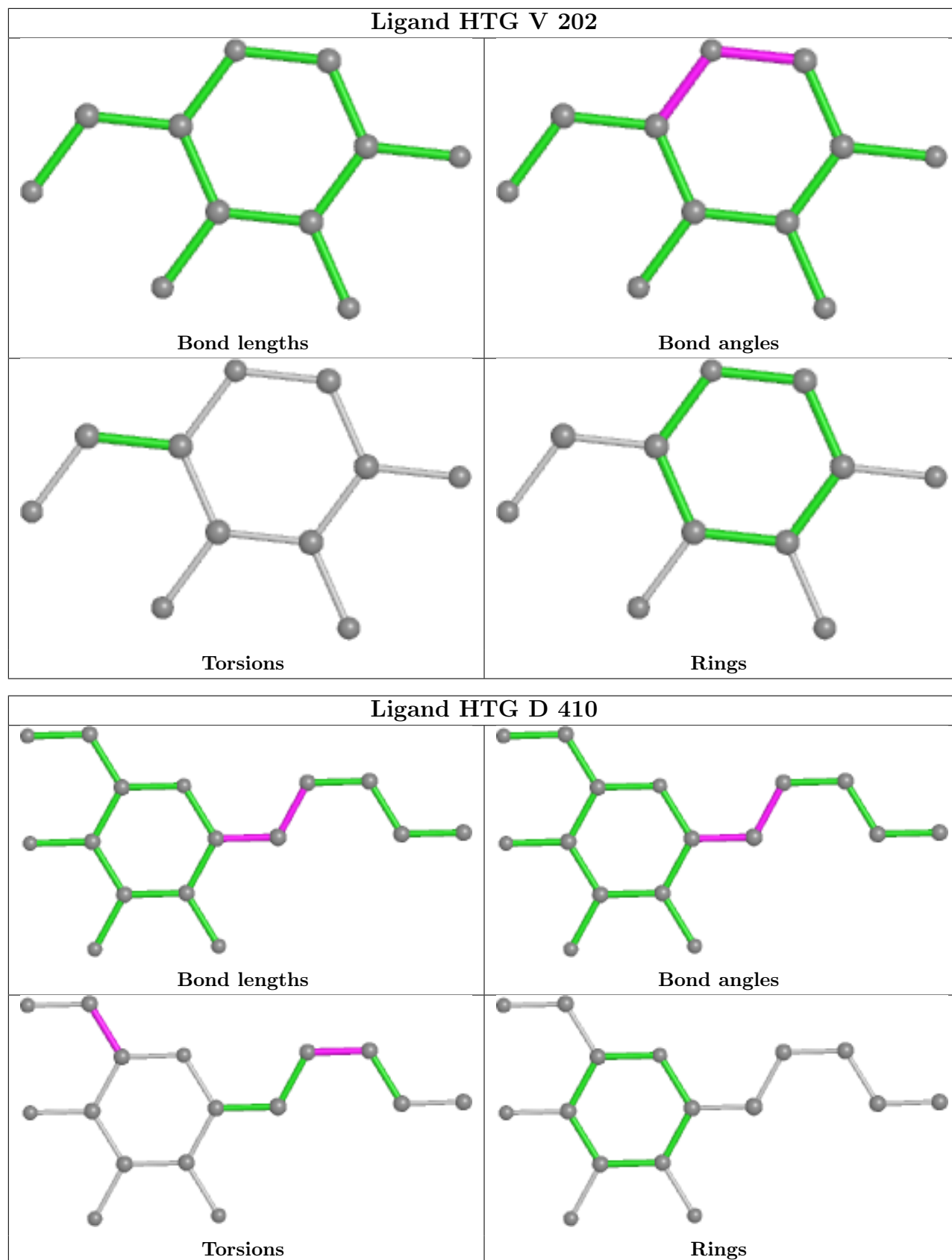


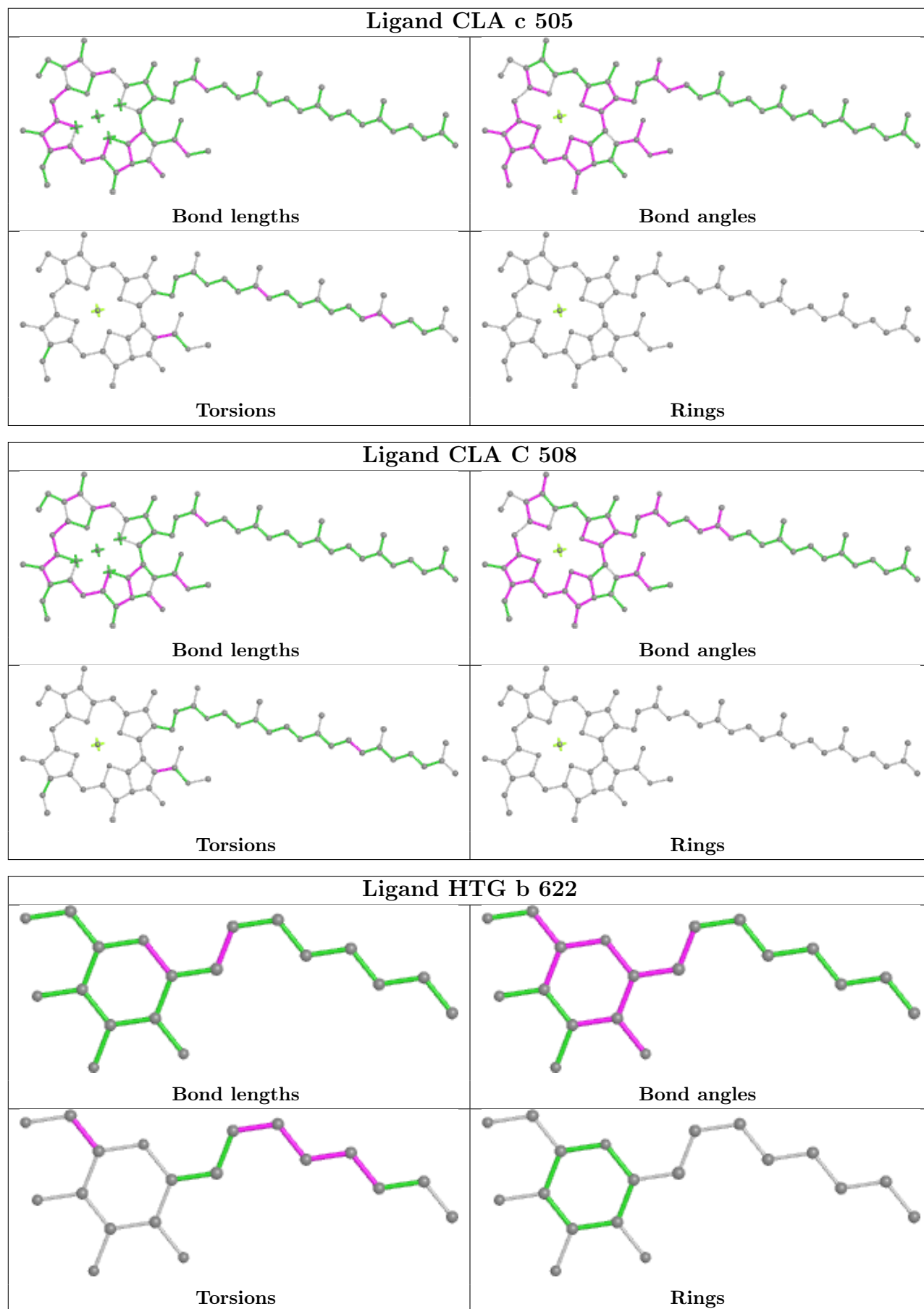


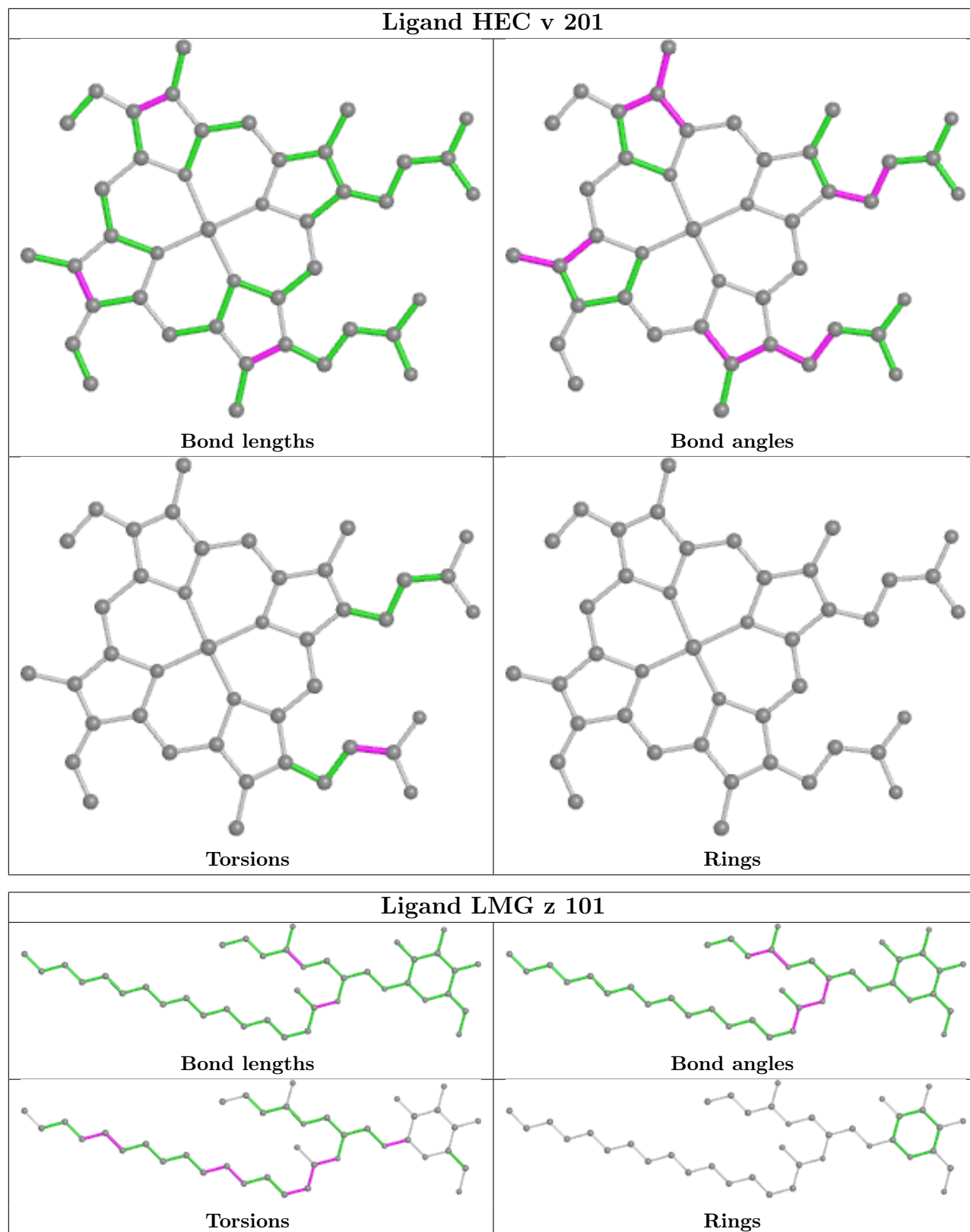


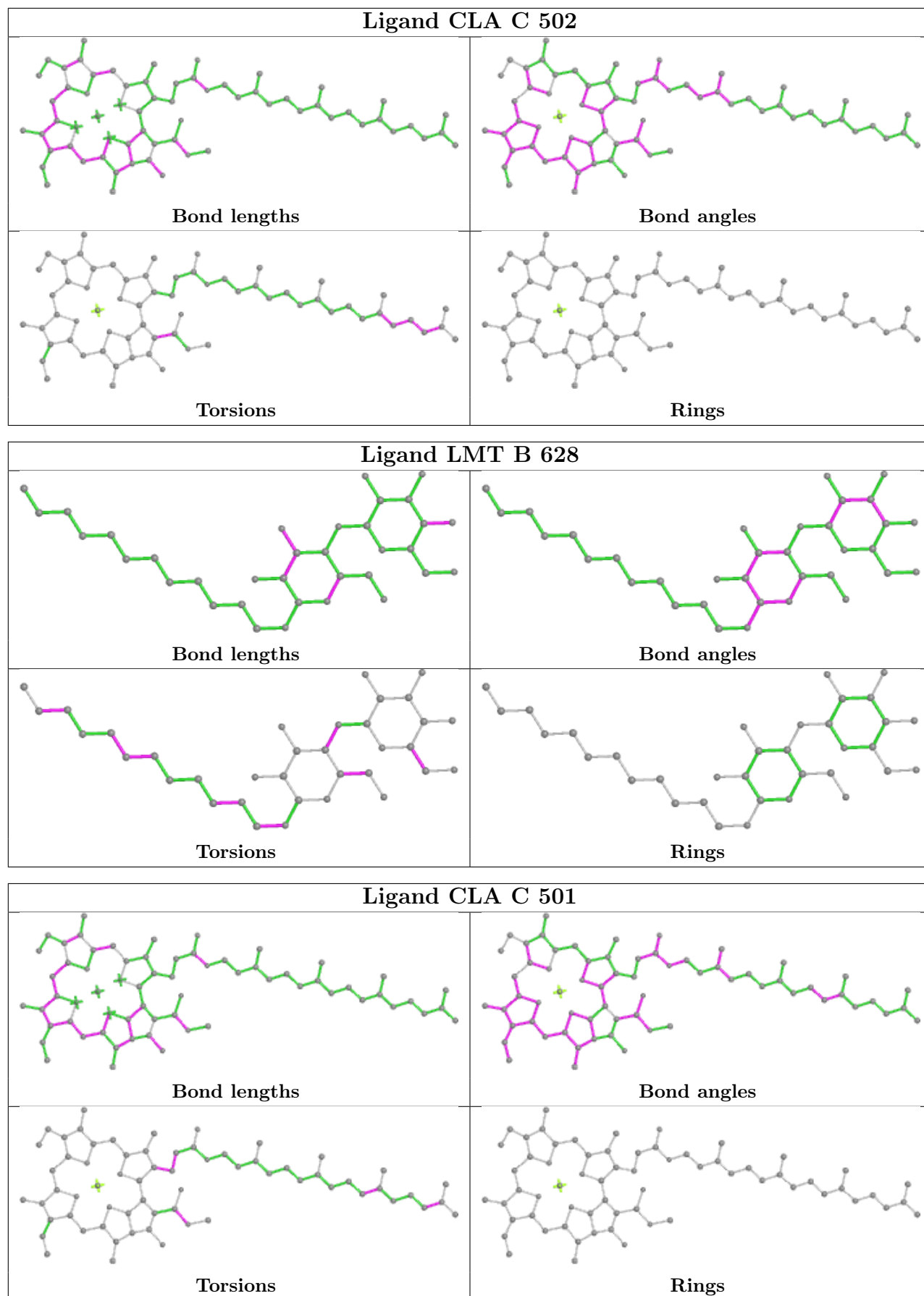


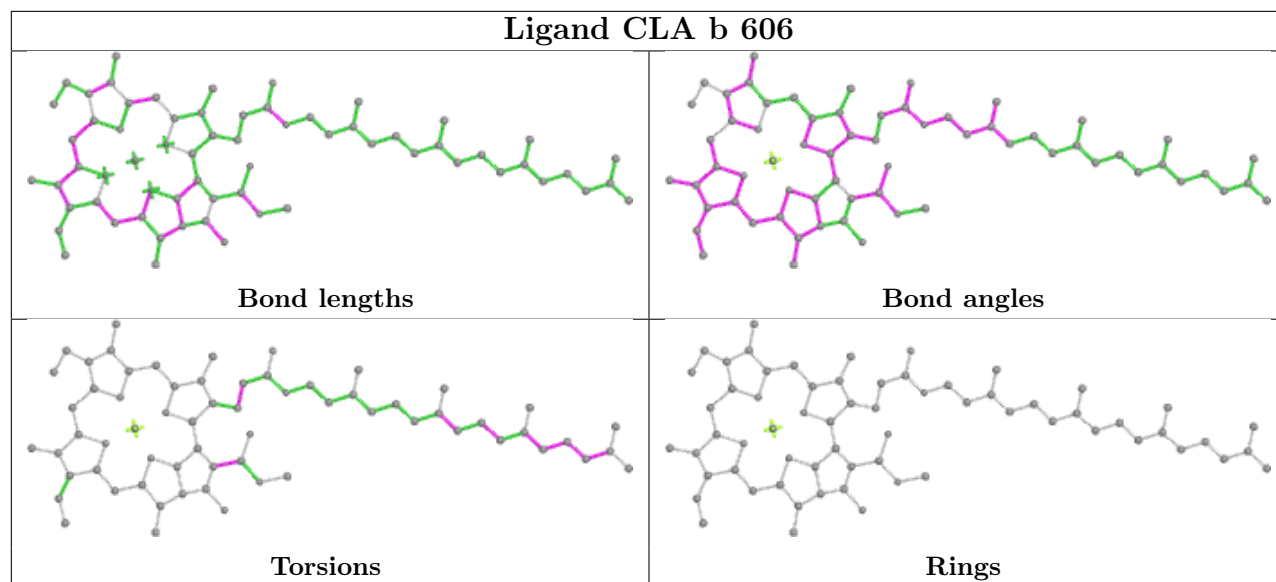












5.7 Other polymers [i](#)

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%)	-0.60	6 (1%) 68 75	41, 48, 69, 119	0
1	a	334/344 (97%)	-0.48	7 (2%) 63 71	43, 52, 79, 125	1 (0%)
2	B	504/505 (99%)	-0.33	15 (2%) 50 59	43, 54, 79, 111	0
2	b	504/505 (99%)	-0.15	39 (7%) 13 18	46, 58, 95, 164	1 (0%)
3	C	451/455 (99%)	-0.41	10 (2%) 62 69	45, 59, 79, 159	0
3	c	455/455 (100%)	-0.31	15 (3%) 46 55	49, 66, 85, 128	2 (0%)
4	D	342/342 (100%)	-0.51	4 (1%) 79 83	41, 50, 67, 137	0
4	d	341/342 (99%)	-0.51	5 (1%) 73 79	43, 54, 75, 131	0
5	E	81/84 (96%)	0.06	9 (11%) 5 7	53, 68, 94, 167	0
5	e	79/84 (94%)	0.42	9 (11%) 5 7	62, 75, 110, 146	0
6	F	34/44 (77%)	-0.28	2 (5%) 22 30	54, 62, 83, 114	0
6	f	31/44 (70%)	-0.11	2 (6%) 18 25	61, 68, 95, 155	0
7	H	64/65 (98%)	-0.11	2 (3%) 49 58	52, 61, 78, 106	0
7	h	64/65 (98%)	-0.15	4 (6%) 20 27	57, 69, 88, 110	0
8	I	37/38 (97%)	0.18	3 (8%) 12 16	55, 63, 122, 168	0
8	i	37/38 (97%)	0.18	5 (13%) 3 3	56, 64, 116, 142	0
9	J	38/39 (97%)	-0.10	3 (7%) 12 17	52, 70, 117, 179	0
9	j	39/39 (100%)	0.39	7 (17%) 1 1	59, 77, 125, 170	0
10	K	37/37 (100%)	-0.40	2 (5%) 25 34	60, 68, 88, 102	0
10	k	37/37 (100%)	-0.27	0 100 100	65, 74, 95, 105	0
11	L	36/37 (97%)	-0.16	4 (11%) 5 7	42, 47, 90, 145	0
11	l	36/37 (97%)	-0.20	3 (8%) 11 15	43, 49, 99, 122	0
12	M	32/36 (88%)	-0.44	1 (3%) 49 58	45, 50, 70, 139	0
12	m	33/36 (91%)	-0.19	2 (6%) 21 28	44, 50, 70, 151	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	0.10	18 (7%) 14 20	42, 65, 113, 181	0
13	o	243/244 (99%)	0.20	26 (10%) 6 8	45, 66, 117, 166	0
14	T	29/32 (90%)	-0.37	3 (10%) 6 9	44, 49, 75, 116	0
14	t	29/32 (90%)	-0.49	1 (3%) 45 53	45, 51, 77, 126	0
15	U	96/104 (92%)	-0.25	2 (2%) 63 71	49, 59, 85, 91	0
15	u	97/104 (93%)	-0.19	3 (3%) 49 58	53, 63, 79, 135	0
16	V	137/137 (100%)	-0.43	3 (2%) 62 69	47, 58, 77, 101	0
16	v	137/137 (100%)	-0.08	4 (2%) 51 61	54, 71, 98, 133	0
17	X	38/40 (95%)	-0.11	4 (10%) 6 9	60, 71, 89, 113	0
17	x	38/40 (95%)	0.26	5 (13%) 3 4	63, 77, 117, 164	0
18	Y	29/30 (96%)	1.23	7 (24%) 0 0	68, 84, 120, 129	0
18	y	29/30 (96%)	0.60	5 (17%) 1 1	74, 90, 107, 113	0
19	Z	62/62 (100%)	0.29	9 (14%) 2 3	67, 80, 136, 162	0
19	z	62/62 (100%)	0.65	13 (20%) 1 1	80, 92, 140, 192	0
20	R	34/34 (100%)	2.41	20 (58%) 0 0	79, 101, 126, 136	0
All	All	5283/5384 (98%)	-0.22	282 (5%) 26 35	41, 59, 97, 192	4 (0%)

All (282) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	23	ALA	9.2
1	a	11	ALA	8.3
5	E	84	LYS	7.7
2	b	495	PHE	7.4
2	b	494	GLY	7.2
13	O	60	ARG	7.2
18	Y	19	ILE	6.8
3	c	20	SER	6.8
13	o	4	THR	6.6
13	O	56	PRO	6.5
18	Y	18	VAL	6.4
19	Z	31	GLN	6.3
20	R	35	LEU	6.1
19	Z	32	ASP	6.1
1	A	11	ALA	5.9
13	O	62	GLU	5.9
19	Z	3	ILE	5.7

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Mol	Chain	Res	Type	RSRZ
19	z	32	ASP	5.7
2	b	502	VAL	5.7
13	O	5	LEU	5.6
6	F	12	SER	5.6
13	o	59	LYS	5.6
17	x	38	GLN	5.5
13	o	57	LYS	5.4
13	o	56	PRO	5.4
12	m	34	LYS	5.4
13	O	4	THR	5.4
3	C	143	TYR	5.3
17	x	2	THR	5.3
3	c	143	TYR	5.3
2	b	504	THR	5.2
20	R	32	GLN	5.2
6	f	15	ILE	5.1
14	T	30	THR	5.1
12	M	33	GLN	5.1
8	I	36	ASP	4.9
13	O	63	ALA	4.9
5	e	84	LYS	4.9
1	a	262	TYR	4.8
2	b	127	ARG	4.8
9	j	3	GLU	4.8
11	L	3	PRO	4.8
20	R	33	LYS	4.8
13	o	62	GLU	4.8
3	c	19	ASN	4.7
19	z	38	GLN	4.7
2	b	503	THR	4.7
13	o	63	ALA	4.6
4	D	11	GLU	4.6
18	y	18	VAL	4.6
19	z	31	GLN	4.6
2	b	493	TRP	4.6
2	b	484	PRO	4.5
3	c	21	ILE	4.5
13	O	59	LYS	4.5
13	o	60	ARG	4.5
8	i	37	LEU	4.4
13	o	207	ARG	4.4
9	j	1	MET	4.4

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Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	4.4
20	R	3	TRP	4.4
19	z	3	ILE	4.4
2	b	293	ALA	4.3
7	h	6	TRP	4.3
19	z	60	PHE	4.3
2	b	505	ARG	4.3
11	l	3	PRO	4.3
18	y	41	VAL	4.3
19	Z	30	PRO	4.1
9	j	4	GLY	4.1
5	e	81	GLU	4.1
3	c	22	PHE	4.1
18	y	43	ARG	4.0
2	b	489	GLU	4.0
20	R	20	VAL	4.0
2	B	494	GLY	4.0
11	L	7	ARG	4.0
19	z	42	LEU	4.0
6	f	16[A]	PHE	4.0
8	I	37	LEU	4.0
3	C	207	ARG	4.0
4	D	12	ARG	3.9
7	H	6	TRP	3.9
20	R	34	LEU	3.9
20	R	24	LEU	3.8
18	Y	43	ARG	3.8
8	I	34	ARG	3.8
13	o	24	ASP	3.7
1	A	13	LEU	3.7
17	X	2	THR	3.7
9	j	5	GLY	3.7
13	o	5	LEU	3.6
20	R	18	TRP	3.6
18	Y	20	ALA	3.6
1	a	235	TYR	3.6
20	R	29	LYS	3.6
2	B	485	GLU	3.6
16	v	15	GLU	3.6
13	O	61	GLN	3.6
2	b	373	LYS	3.5
2	b	485	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
8	i	34	ARG	3.5
6	F	13	TYR	3.5
13	o	64	GLU	3.5
14	T	29	ILE	3.5
2	b	486	LEU	3.5
8	i	38	GLU	3.5
9	j	2	SER	3.5
19	z	30	PRO	3.4
13	o	61	GLN	3.4
20	R	16	ALA	3.4
12	m	33	GLN	3.4
20	R	21	ARG	3.4
3	c	23	ALA	3.4
19	z	35	ARG	3.4
13	o	55	GLU	3.3
2	b	479[A]	PHE	3.3
17	x	3	ILE	3.3
18	y	19	ILE	3.3
19	z	34	ASP	3.3
13	o	35	SER	3.2
2	b	496	TYR	3.2
2	B	295	GLY	3.2
2	B	487	SER	3.2
2	b	86	ILE	3.2
19	z	61	VAL	3.2
9	J	3	GLU	3.2
17	X	38	GLN	3.2
20	R	19	ALA	3.2
20	R	6	LEU	3.1
3	C	24	THR	3.1
9	j	6	ARG	3.1
3	C	142	GLU	3.1
18	Y	22	LEU	3.1
19	z	62	VAL	3.1
3	c	207	ARG	3.0
13	o	27	ARG	3.0
5	E	6	GLY	3.0
13	O	89	SER	3.0
13	o	25	THR	3.0
1	a	13	LEU	3.0
2	b	85	GLY	3.0
16	v	17	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
11	l	2	GLU	3.0
2	B	495	PHE	3.0
1	A	262	TYR	3.0
19	Z	35	ARG	3.0
20	R	28	VAL	2.9
2	b	295	GLY	2.9
20	R	31	VAL	2.9
4	d	12	ARG	2.9
5	E	59	GLU	2.9
13	O	207	ARG	2.9
17	x	39	ARG	2.9
3	c	192	GLY	2.9
13	O	55	GLU	2.9
13	O	27	ARG	2.9
13	o	246	ALA	2.9
1	a	221[A]	SER	2.9
5	E	61	ARG	2.8
5	e	59	GLU	2.8
9	J	6	ARG	2.8
20	R	5	VAL	2.8
5	e	25	ILE	2.8
2	b	375	GLY	2.8
7	h	3[A]	ARG	2.8
19	Z	34	ASP	2.7
18	Y	21	GLN	2.7
2	b	376	VAL	2.7
2	b	20	ILE	2.7
2	b	294	SER	2.7
2	B	293	ALA	2.7
2	b	488	PRO	2.7
2	b	497	GLN	2.7
9	J	5	GLY	2.7
5	e	6	GLY	2.7
2	B	162	PHE	2.6
13	o	22	LEU	2.6
13	O	25	THR	2.6
10	K	10	LYS	2.6
15	U	27	LEU	2.6
2	b	499	VAL	2.6
2	b	374	ASN	2.6
2	b	161	LEU	2.6
20	R	4	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
4	d	237	PRO	2.5
19	Z	38	GLN	2.5
13	o	130	GLN	2.5
2	B	373	LYS	2.5
2	b	501	ASP	2.5
13	O	35	SER	2.5
13	o	23	ASP	2.5
13	o	211	ILE	2.5
5	E	82	GLN	2.5
15	u	75	LEU	2.5
13	o	134	THR	2.5
13	O	132	ASN	2.5
8	i	36	ASP	2.5
3	c	462[A]	GLU	2.5
10	K	13	GLU	2.5
16	v	16	GLY	2.4
8	i	35	LYS	2.4
4	d	227	GLU	2.4
2	b	126	PRO	2.4
1	a	228	THR	2.4
4	D	107	LEU	2.4
3	C	181	PHE	2.4
7	H	65	LEU	2.4
11	L	2	GLU	2.4
16	V	16	GLY	2.4
17	x	37	VAL	2.4
2	b	435	GLU	2.4
5	E	60	GLN	2.4
11	L	5	PRO	2.4
18	y	20	ALA	2.4
19	z	59	PHE	2.3
3	c	233	VAL	2.3
13	O	57	LYS	2.3
5	e	24	SER	2.3
20	R	17	GLY	2.3
1	a	242	GLU	2.3
2	b	130	GLU	2.3
2	b	492	GLU	2.3
7	h	65	LEU	2.3
2	B	489	GLU	2.3
3	C	263	ALA	2.3
2	b	162	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
3	c	142	GLU	2.3
5	e	79[A]	PHE	2.3
16	v	128	ASP	2.3
14	t	30	THR	2.3
5	e	82	GLN	2.3
15	u	23	GLU	2.3
19	Z	60	PHE	2.2
15	U	10	VAL	2.2
5	e	61	ARG	2.2
17	X	3	ILE	2.2
13	o	33	ASP	2.2
3	c	190	ALA	2.2
1	A	243	GLU	2.2
3	C	182	PHE	2.2
2	B	374	ASN	2.2
2	b	487	SER	2.2
13	O	211	ILE	2.2
7	h	23	PRO	2.2
14	T	28	ARG	2.2
4	d	238	THR	2.2
9	j	7	ILE	2.2
2	B	122	LEU	2.2
5	E	57	ALA	2.2
1	A	242	GLU	2.2
2	B	503	THR	2.2
19	z	33	TRP	2.2
5	E	17	VAL	2.2
16	V	5	PRO	2.2
3	c	234	VAL	2.1
13	o	98	GLU	2.1
20	R	14	LEU	2.1
2	b	17	GLY	2.1
3	C	192	GLY	2.1
2	B	435[A]	GLU	2.1
2	b	223	GLN	2.1
16	V	15	GLU	2.1
13	o	89	SER	2.1
2	B	128	THR	2.1
1	A	16	ARG	2.1
4	d	228	GLY	2.1
5	E	83	LEU	2.1
18	Y	38	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
13	O	24	ASP	2.1
4	D	238	THR	2.1
11	l	5	PRO	2.0
19	Z	2	THR	2.0
20	R	25	PRO	2.0
3	c	253	LEU	2.0
17	X	37	VAL	2.0
3	C	264	PHE	2.0
2	B	504	THR	2.0
2	b	128	THR	2.0
2	b	87	ASP	2.0
3	c	106	VAL	2.0
15	u	61	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	FME	i	1	10/11	0.91	0.16	59,69,77,78	0
14	FME	t	1	10/11	0.94	0.08	47,51,60,72	0
12	FME	M	1	10/11	0.95	0.14	48,62,84,86	0
14	FME	T	1	10/11	0.95	0.09	47,54,66,71	0
12	FME	m	1	10/11	0.97	0.13	54,64,82,94	0
8	FME	I	1	10/11	0.97	0.07	61,69,78,79	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(\AA^2)	Q<0.9
30	UNL	b	626	33/-	0.27	0.36	72,99,138,140	0
30	UNL	B	626	33/-	0.30	0.40	67,102,124,131	0
30	UNL	I	101	40/-	0.34	0.35	85,110,133,135	0
31	LMT	b	621	25/35	0.41	0.35	94,115,138,141	0
32	LMG	C	519	51/55	0.41	0.34	69,116,136,139	0
31	LMT	T	101	35/35	0.42	0.35	85,118,145,149	0
30	UNL	i	101	40/-	0.45	0.32	82,104,130,136	0
27	GOL	a	419	6/6	0.48	0.58	80,92,94,96	0
31	LMT	b	627	25/35	0.53	0.29	69,89,123,125	0
31	LMT	B	630	35/35	0.53	0.40	82,106,122,128	0
30	UNL	x	101	18/-	0.55	0.27	75,83,119,121	0
31	LMT	B	631	25/35	0.55	0.29	70,91,121,130	0
32	LMG	Z	101	37/55	0.56	0.32	77,118,134,143	0
31	LMT	M	101	35/35	0.58	0.29	67,90,98,103	0
30	UNL	j	101	10/-	0.58	0.34	86,95,100,102	0
30	UNL	K	102	34/-	0.59	0.33	94,112,126,126	0
32	LMG	c	521	51/55	0.60	0.31	80,125,148,151	0
31	LMT	F	101	35/35	0.60	0.52	115,135,160,163	0
34	HTG	b	623	19/19	0.60	0.46	93,129,136,139	0
36	CA	f	103	1/1	0.60	0.09	125,125,125,125	0
31	LMT	m	103	35/35	0.61	0.28	69,89,99,104	0
30	UNL	A	415	28/-	0.62	0.33	103,117,125,134	0
30	UNL	d	408	36/-	0.63	0.23	73,97,115,119	0
31	LMT	t	101	26/35	0.64	0.24	89,110,127,136	0
30	UNL	c	525	32/-	0.65	0.37	100,115,126,133	0
31	LMT	e	101	35/35	0.65	0.54	124,145,169,174	0
31	LMT	A	417	35/35	0.65	0.35	86,110,122,126	0
31	LMT	B	628	35/35	0.66	0.28	79,103,120,123	0
31	LMT	A	421	35/35	0.67	0.35	121,134,154,156	0
34	HTG	D	410	16/19	0.67	0.29	94,109,119,129	0
30	UNL	D	409	40/-	0.68	0.21	74,93,114,120	0
33	LHG	a	421	42/49	0.69	0.37	99,144,155,158	0
30	UNL	m	102	10/-	0.69	0.31	80,83,89,95	0
36	CA	F	104	1/1	0.70	0.25	126,126,126,126	0
30	UNL	a	416	30/-	0.70	0.30	107,122,136,137	0
26	SQD	f	102	43/54	0.72	0.34	115,129,152,155	0
27	GOL	a	420	6/6	0.72	0.47	64,71,78,79	0
27	GOL	b	624	6/6	0.73	0.20	93,95,96,107	0
27	GOL	o	303	6/6	0.73	0.23	86,90,93,96	0
34	HTG	d	409	16/19	0.74	0.30	99,117,124,135	0
32	LMG	z	101	39/55	0.74	0.27	81,123,136,146	0
30	UNL	X	101	18/-	0.74	0.21	66,74,99,102	0
31	LMT	c	501	35/35	0.75	0.39	122,132,145,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
27	GOL	l	102	6/6	0.75	0.79	71,97,99,101	0
27	GOL	A	418	6/6	0.76	0.47	57,75,75,77	0
26	SQD	A	412	54/54	0.77	0.20	73,92,117,124	0
26	SQD	b	620	54/54	0.78	0.20	69,92,107,117	0
34	HTG	b	622	19/19	0.78	0.20	70,80,87,96	0
30	UNL	J	101	10/-	0.78	0.18	80,86,89,96	0
32	LMG	A	419	51/55	0.78	0.18	79,91,102,109	0
27	GOL	B	627	6/6	0.78	0.26	73,76,85,102	0
34	HTG	B	623	19/19	0.78	0.25	71,85,102,104	0
27	GOL	A	411	6/6	0.79	0.20	69,77,81,82	0
27	GOL	O	302	6/6	0.79	0.22	86,95,97,100	0
30	UNL	l	101	10/-	0.79	0.26	73,79,91,91	0
26	SQD	B	620	54/54	0.79	0.18	75,96,117,127	0
29	PL9	A	414	55/55	0.80	0.21	76,100,113,116	0
32	LMG	a	418	51/55	0.81	0.17	74,92,100,113	0
26	SQD	a	413	54/54	0.81	0.19	76,95,120,124	0
29	PL9	a	415	55/55	0.81	0.21	88,111,123,129	0
36	CA	o	301	1/1	0.81	0.06	102,102,102,102	0
27	GOL	o	302	6/6	0.82	0.28	88,101,106,109	0
27	GOL	b	629	6/6	0.82	0.29	58,69,75,76	0
33	LHG	E	101	42/49	0.82	0.23	79,104,117,122	0
34	HTG	C	520	19/19	0.84	0.31	121,127,141,144	0
32	LMG	D	411	51/55	0.84	0.18	51,67,103,106	0
34	HTG	B	622	19/19	0.84	0.18	66,83,92,93	0
27	GOL	V	203	6/6	0.84	0.14	60,68,74,76	0
32	LMG	d	410	51/55	0.85	0.18	58,71,102,107	0
34	HTG	c	522	19/19	0.85	0.27	123,132,138,140	0
27	GOL	c	527	6/6	0.85	0.24	107,114,117,121	0
23	CLA	b	616	65/65	0.86	0.17	54,62,117,125	0
27	GOL	O	303	6/6	0.86	0.20	86,95,97,100	0
23	CLA	B	616	65/65	0.86	0.18	49,59,106,115	0
27	GOL	a	412	6/6	0.86	0.25	75,79,87,88	0
23	CLA	b	601	65/65	0.86	0.16	66,85,114,125	0
27	GOL	v	202	6/6	0.87	0.12	66,78,83,85	0
23	CLA	B	601	65/65	0.87	0.14	57,77,100,115	0
23	CLA	d	402	65/65	0.87	0.14	55,65,113,123	0
30	UNL	D	408	17/-	0.88	0.13	66,75,99,104	0
23	CLA	C	513	65/65	0.88	0.14	65,83,103,109	0
25	BCR	K	101	40/40	0.88	0.14	62,76,85,89	0
25	BCR	K	103	40/40	0.88	0.17	57,64,72,74	0
23	CLA	c	514	65/65	0.88	0.17	71,89,112,120	0
23	CLA	c	513	65/65	0.89	0.17	66,80,114,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	LMG	C	518	51/55	0.89	0.17	58,84,102,108	0
32	LMG	c	520	51/55	0.89	0.19	63,91,116,123	0
30	UNL	d	407	17/-	0.89	0.13	74,83,97,98	0
25	BCR	d	403	40/40	0.90	0.11	53,67,92,95	0
25	BCR	h	101	40/40	0.90	0.13	57,68,87,93	0
34	HTG	b	625	19/19	0.90	0.11	71,82,88,96	0
23	CLA	B	606	65/65	0.90	0.14	44,57,97,104	0
32	LMG	B	621	51/55	0.90	0.13	61,74,87,95	0
23	CLA	C	506	65/65	0.90	0.14	59,69,103,104	0
32	LMG	m	101	51/55	0.90	0.13	62,77,90,99	0
23	CLA	b	606	65/65	0.90	0.14	48,60,97,106	0
25	BCR	Y	101	40/40	0.91	0.13	57,65,78,80	0
27	GOL	B	629	6/6	0.91	0.23	53,63,68,74	0
23	CLA	c	507	65/65	0.91	0.14	58,69,100,105	0
26	SQD	F	103	43/54	0.91	0.18	70,95,116,122	0
23	CLA	C	512	65/65	0.91	0.14	63,72,101,106	0
35	DGD	H	102	62/66	0.92	0.12	51,62,72,74	0
35	DGD	c	519	62/66	0.92	0.12	53,67,100,116	0
34	HTG	V	202	11/19	0.92	0.41	92,107,115,116	0
25	BCR	b	618	40/40	0.92	0.10	49,59,74,77	0
23	CLA	a	409	65/65	0.92	0.17	47,55,113,119	0
34	HTG	B	625	19/19	0.93	0.09	77,81,92,95	0
23	CLA	B	609	65/65	0.93	0.15	49,59,69,74	0
35	DGD	C	516	62/66	0.93	0.12	51,64,102,106	0
35	DGD	C	517	62/66	0.93	0.11	48,61,89,100	0
23	CLA	D	403	65/65	0.93	0.14	51,59,104,108	0
35	DGD	c	518	62/66	0.93	0.12	54,68,111,123	0
25	BCR	D	404	40/40	0.93	0.10	50,60,92,98	0
35	DGD	h	102	62/66	0.93	0.11	57,65,74,79	0
23	CLA	C	508	65/65	0.93	0.10	48,56,105,113	0
25	BCR	k	101	40/40	0.93	0.14	60,74,81,82	0
23	CLA	A	408	65/65	0.93	0.14	45,53,110,114	0
23	CLA	b	609	65/65	0.94	0.14	51,64,72,80	0
33	LHG	d	406	49/49	0.94	0.15	55,65,109,123	0
23	CLA	a	407	65/65	0.94	0.11	43,54,120,125	0
27	GOL	C	521	6/6	0.94	0.10	57,60,65,66	0
23	CLA	c	505	65/65	0.94	0.10	56,63,97,100	0
25	BCR	c	515	40/40	0.94	0.10	73,83,89,90	0
25	BCR	B	618	40/40	0.94	0.08	47,56,69,74	0
23	CLA	C	504	65/65	0.94	0.10	47,56,89,99	0
23	CLA	c	509	65/65	0.94	0.12	51,62,115,121	0
33	LHG	D	407	49/49	0.94	0.15	52,61,99,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
26	SQD	A	410	54/54	0.94	0.14	59,81,104,109	0
25	BCR	H	101	40/40	0.95	0.09	53,65,85,87	0
33	LHG	A	420	49/49	0.95	0.12	52,65,81,84	0
23	CLA	B	614	65/65	0.95	0.10	43,51,85,92	0
25	BCR	t	102	40/40	0.95	0.08	48,57,75,79	0
27	GOL	b	628	6/6	0.95	0.19	79,84,94,95	0
33	LHG	b	630	49/49	0.95	0.12	54,59,69,83	0
25	BCR	y	101	40/40	0.95	0.08	62,71,80,86	0
33	LHG	d	411	49/49	0.95	0.14	57,68,77,81	0
35	DGD	c	517	62/66	0.95	0.10	48,62,97,101	0
23	CLA	b	612	65/65	0.95	0.09	43,52,61,66	0
25	BCR	T	102	40/40	0.95	0.07	47,58,68,69	0
25	BCR	A	409	40/40	0.95	0.09	42,53,65,66	0
23	CLA	b	614	65/65	0.95	0.10	45,52,84,88	0
25	BCR	C	514	40/40	0.95	0.12	55,64,71,80	0
23	CLA	B	611	65/65	0.95	0.10	41,47,64,67	0
38	HEM	f	101	43/43	0.95	0.15	67,81,101,109	0
23	CLA	b	615	65/65	0.96	0.10	51,59,77,78	0
26	SQD	a	411	54/54	0.96	0.12	64,84,111,117	0
27	GOL	c	526	6/6	0.96	0.23	65,65,71,74	0
23	CLA	C	507	65/65	0.96	0.11	52,62,78,87	0
23	CLA	c	502	65/65	0.96	0.10	59,66,75,78	0
23	CLA	C	501	65/65	0.96	0.08	52,61,70,76	0
23	CLA	C	509	65/65	0.96	0.10	52,58,77,80	0
23	CLA	c	508	65/65	0.96	0.10	56,68,79,83	0
27	GOL	B	624	6/6	0.96	0.20	73,77,85,86	0
29	PL9	D	405	55/55	0.96	0.10	39,51,57,66	0
25	BCR	b	619	40/40	0.96	0.07	52,62,82,86	0
29	PL9	d	404	55/55	0.96	0.11	43,52,60,65	0
23	CLA	b	602	65/65	0.96	0.12	52,60,72,76	0
23	CLA	c	512	65/65	0.96	0.10	59,67,83,93	0
23	CLA	b	604	65/65	0.96	0.10	42,52,87,99	0
23	CLA	b	605	65/65	0.96	0.11	43,51,71,77	0
23	CLA	C	511	65/65	0.96	0.12	52,64,77,80	0
23	CLA	b	607	65/65	0.96	0.09	40,49,72,77	0
23	CLA	C	503	65/65	0.96	0.09	49,61,68,77	0
36	CA	O	301	1/1	0.96	0.09	100,100,100,100	0
33	LHG	d	405	49/49	0.96	0.15	49,58,72,76	0
23	CLA	B	610	65/65	0.96	0.12	46,56,61,75	0
23	CLA	A	406	65/65	0.96	0.10	40,49,109,115	0
23	CLA	c	511	65/65	0.97	0.09	53,63,74,89	0
23	CLA	B	613	65/65	0.97	0.08	41,47,84,90	0

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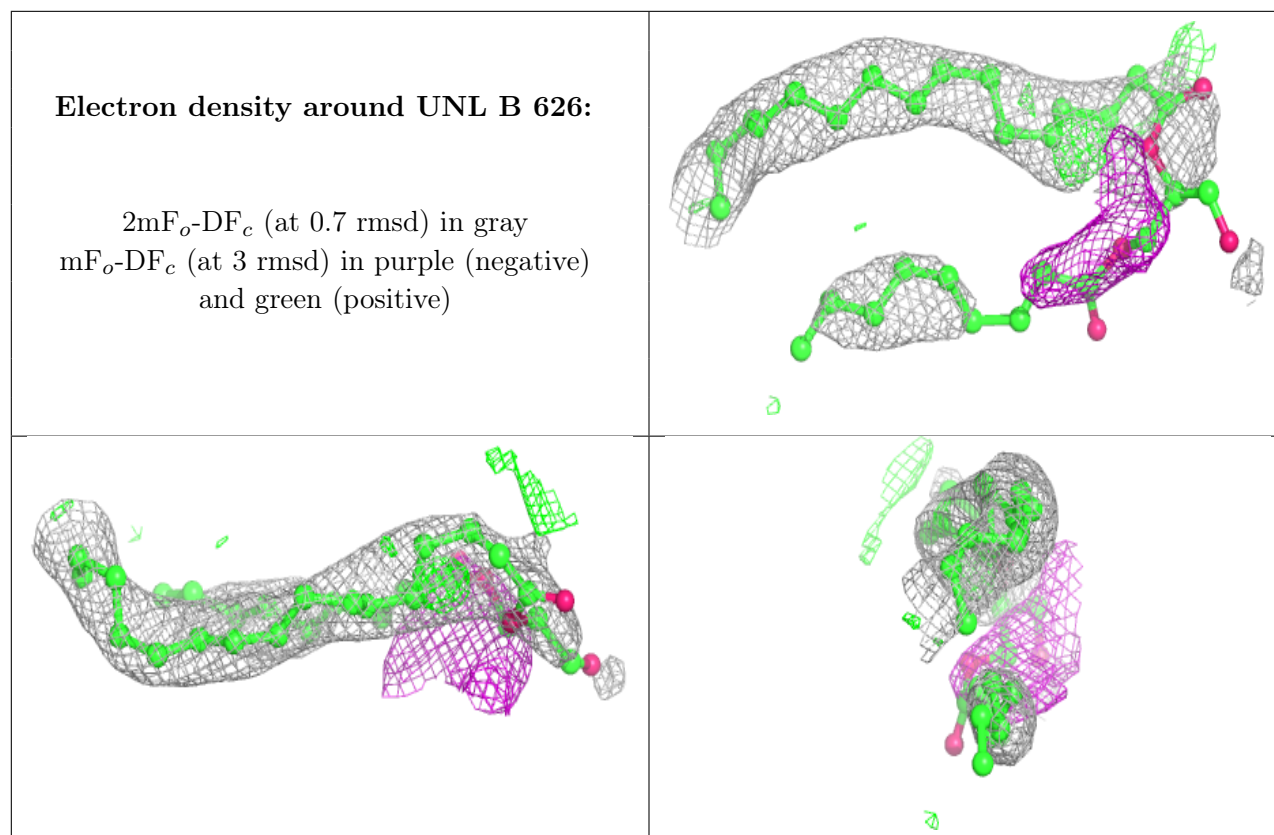
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	B	605	65/65	0.97	0.11	43,49,66,73	0
23	CLA	C	510	65/65	0.97	0.07	52,60,75,76	0
23	CLA	B	615	65/65	0.97	0.10	46,54,74,80	0
24	PHO	A	416	64/64	0.97	0.09	39,51,58,64	0
24	PHO	a	417	64/64	0.97	0.11	46,54,62,68	0
23	CLA	A	404	65/65	0.97	0.12	38,45,62,66	0
25	BCR	B	617	40/40	0.97	0.08	45,53,61,64	0
23	CLA	b	610	65/65	0.97	0.08	51,58,64,69	0
25	BCR	B	619	40/40	0.97	0.07	51,60,83,88	0
23	CLA	b	611	65/65	0.97	0.08	43,51,66,70	0
23	CLA	B	607	65/65	0.97	0.09	40,47,68,73	0
23	CLA	b	613	65/65	0.97	0.07	43,50,81,87	0
23	CLA	D	402	65/65	0.97	0.11	36,44,69,76	0
23	CLA	B	602	65/65	0.97	0.11	48,56,67,77	0
35	DGD	C	515	62/66	0.97	0.09	48,56,95,100	0
23	CLA	a	405	65/65	0.97	0.12	42,48,63,74	0
23	CLA	B	603	65/65	0.97	0.09	44,52,70,74	0
25	BCR	a	410	40/40	0.97	0.07	46,55,62,64	0
23	CLA	c	504	65/65	0.97	0.09	53,69,78,88	0
23	CLA	C	505	65/65	0.97	0.08	51,59,83,90	0
23	CLA	c	506	65/65	0.97	0.09	52,63,84,92	0
25	BCR	c	516	40/40	0.97	0.10	60,66,73,78	0
36	CA	C	522	1/1	0.97	0.06	73,73,73,73	0
23	CLA	B	604	65/65	0.97	0.09	41,47,97,103	0
23	CLA	B	612	65/65	0.97	0.07	39,49,59,63	0
36	CA	c	524	1/1	0.97	0.07	76,76,76,76	0
23	CLA	b	603	65/65	0.97	0.08	47,58,78,84	0
23	CLA	c	510	65/65	0.97	0.08	49,64,83,85	0
33	LHG	L	101	49/49	0.97	0.11	52,58,70,87	0
39	MG	J	102	1/1	0.97	0.04	59,59,59,59	0
40	HEC	v	201	43/43	0.97	0.11	55,61,67,69	0
23	CLA	d	401	65/65	0.98	0.11	41,47,77,91	0
23	CLA	c	503	65/65	0.98	0.08	49,60,89,107	0
24	PHO	A	407	64/64	0.98	0.08	37,46,54,59	0
23	CLA	b	608	65/65	0.98	0.07	46,56,78,86	0
24	PHO	a	408	64/64	0.98	0.08	43,49,54,56	0
36	CA	c	523	1/1	0.98	0.06	75,75,75,75	0
23	CLA	B	608	65/65	0.98	0.07	44,51,69,77	0
23	CLA	A	405	65/65	0.98	0.09	37,44,58,70	0
33	LHG	D	406	49/49	0.98	0.13	48,56,68,73	0
37	BCT	a	404	4/4	0.98	0.07	58,60,68,77	0
38	HEM	F	102	43/43	0.98	0.10	60,68,75,85	0

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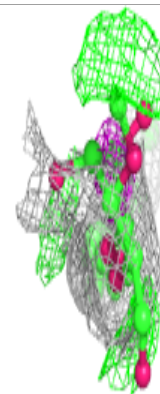
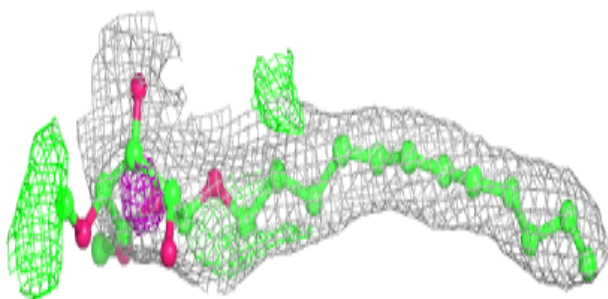
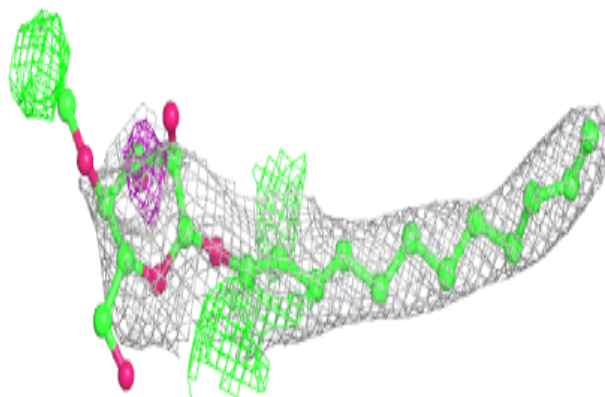
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	a	406	65/65	0.98	0.08	41,46,63,69	0
23	CLA	C	502	65/65	0.98	0.08	48,56,78,85	0
40	HEC	V	201	43/43	0.98	0.11	44,51,56,57	0
25	BCR	b	617	40/40	0.98	0.07	48,54,61,61	0
28	OEX	a	414	10/10	0.99	0.06	47,50,51,55	0
22	CL	A	403	1/1	0.99	0.03	47,47,47,47	0
21	FE2	a	401	1/1	0.99	0.04	55,55,55,55	0
22	CL	A	402	1/1	0.99	0.03	43,43,43,43	0
39	MG	j	102	1/1	0.99	0.05	63,63,63,63	0
28	OEX	A	413	10/10	0.99	0.05	41,44,48,50	0
37	BCT	D	401	4/4	0.99	0.11	54,58,61,66	0
21	FE2	A	401	1/1	1.00	0.04	52,52,52,52	0
22	CL	a	402	1/1	1.00	0.03	50,50,50,50	0
22	CL	a	403	1/1	1.00	0.03	52,52,52,52	0

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.

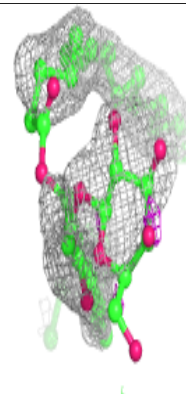
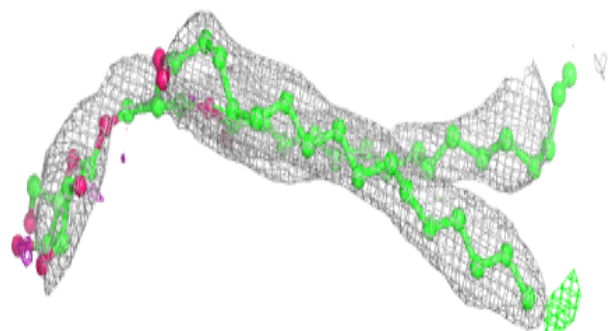
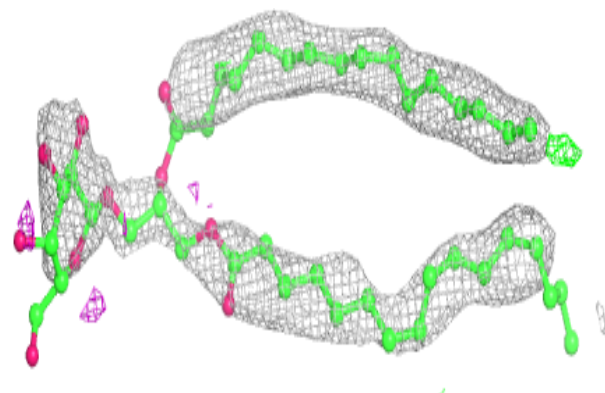


Electron density around LMT b 621:

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

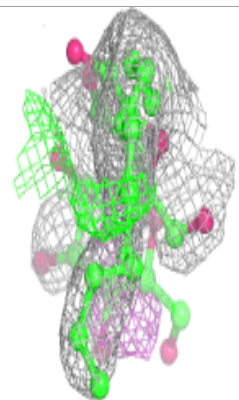
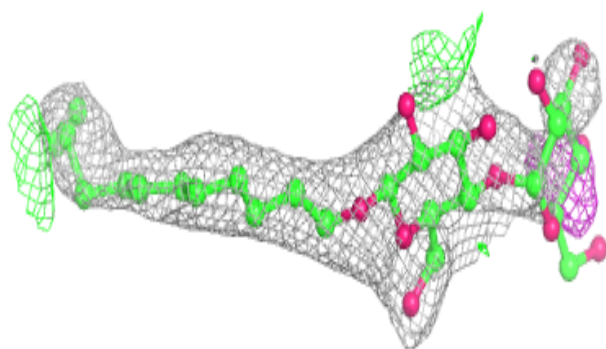
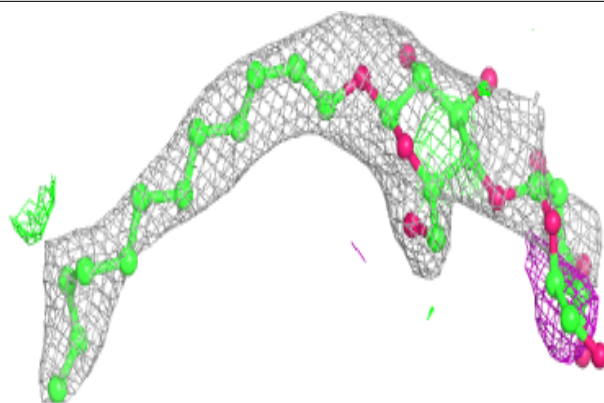
**Electron density around LMG C 519:**

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

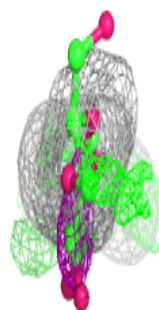
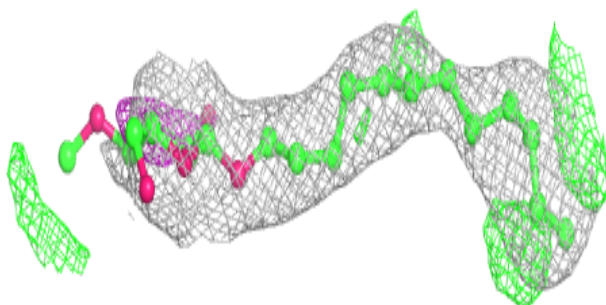
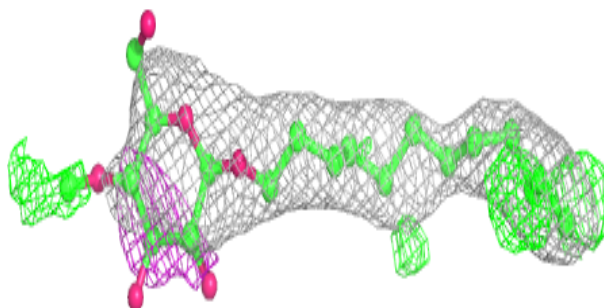


Electron density around LMT T 101:

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

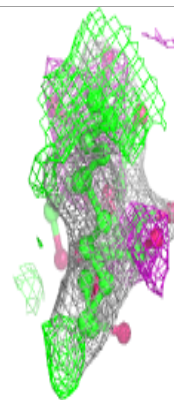
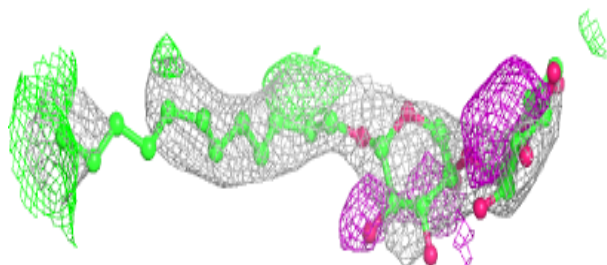
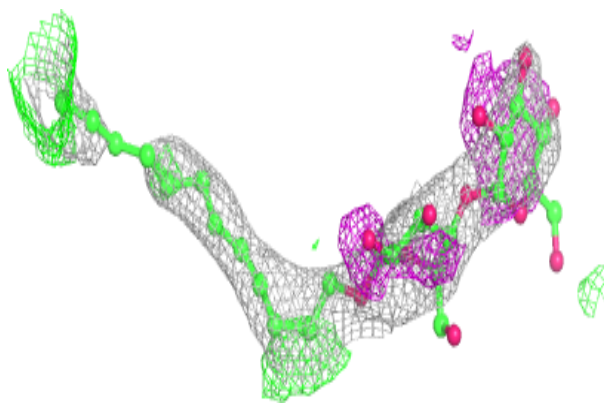
**Electron density around LMT b 627:**

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

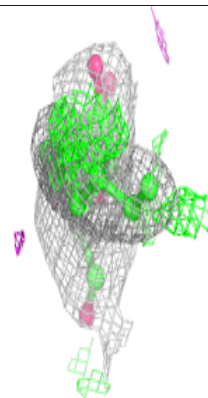
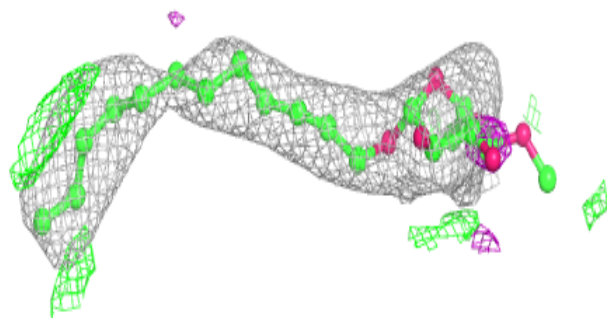
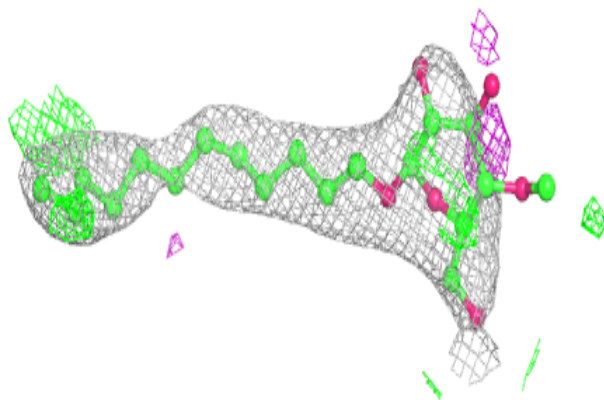


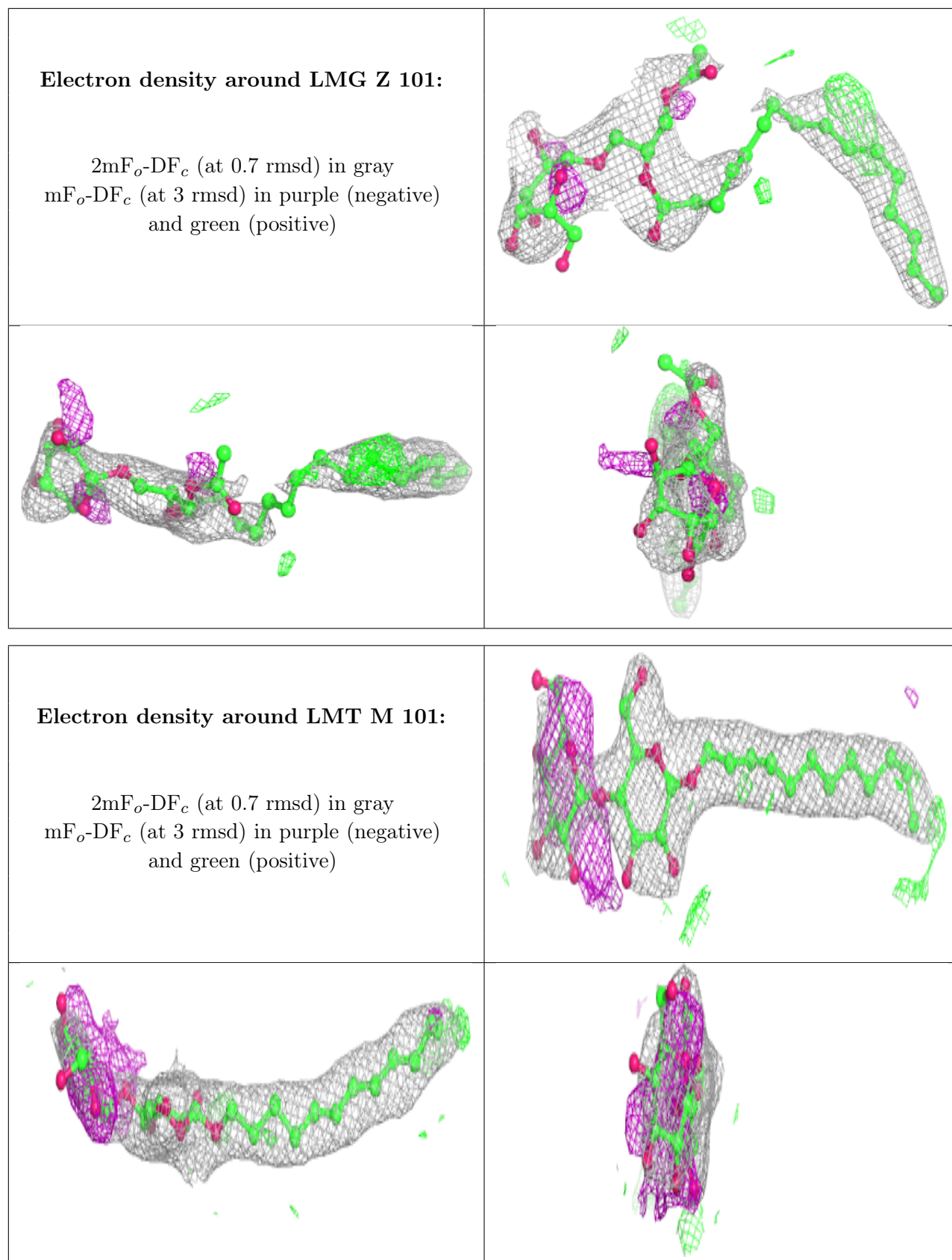
Electron density around LMT B 630:

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

**Electron density around LMT B 631:**

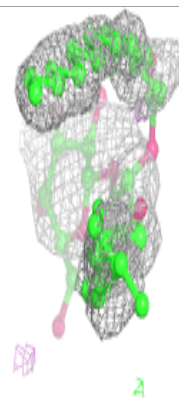
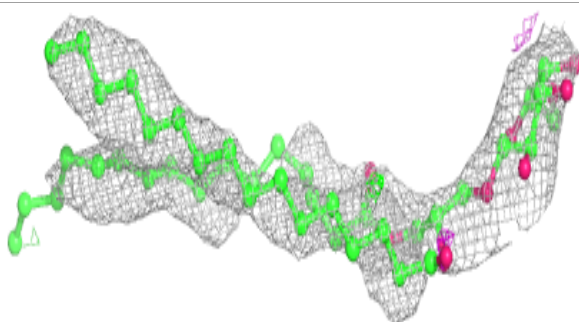
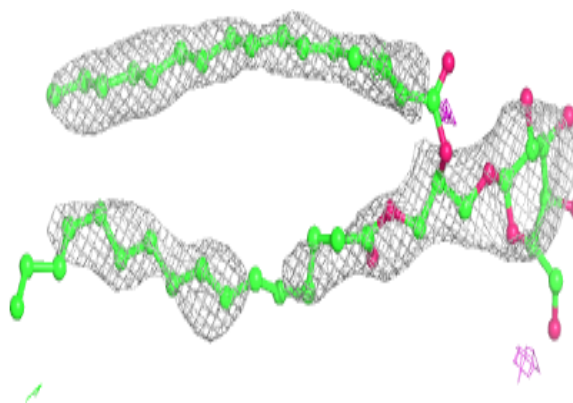
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



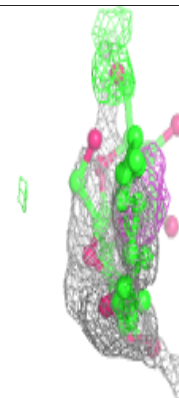
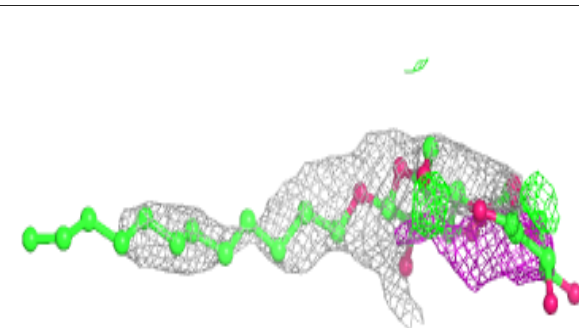
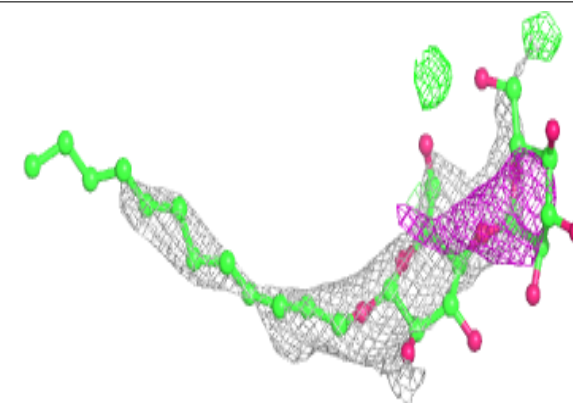


Electron density around LMG c 521:

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

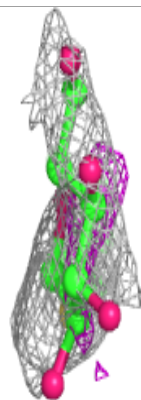
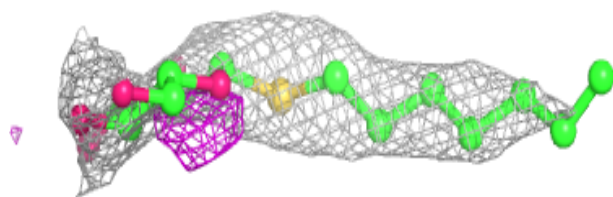
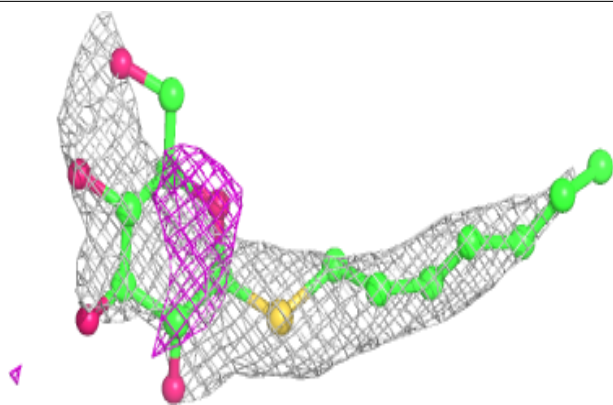
**Electron density around LMT F 101:**

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

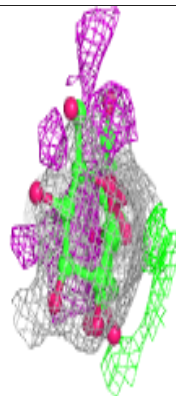
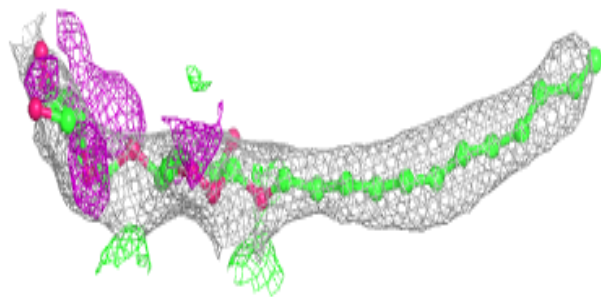
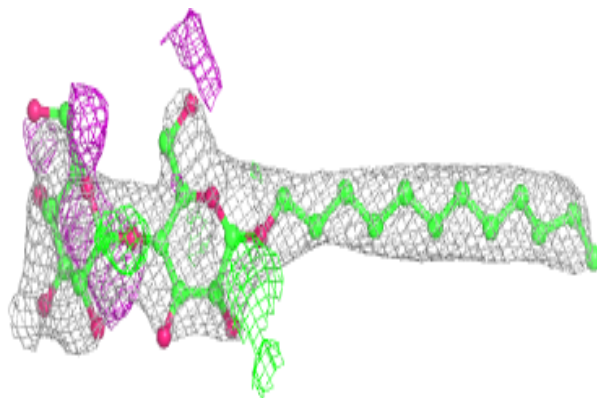


Electron density around HTG b 623:

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

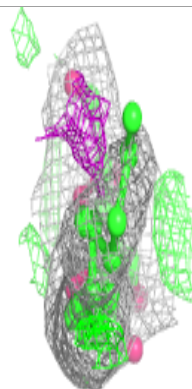
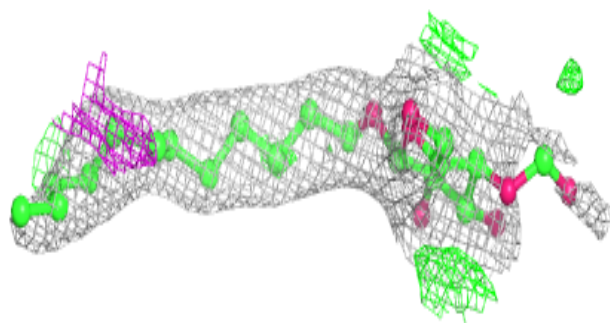
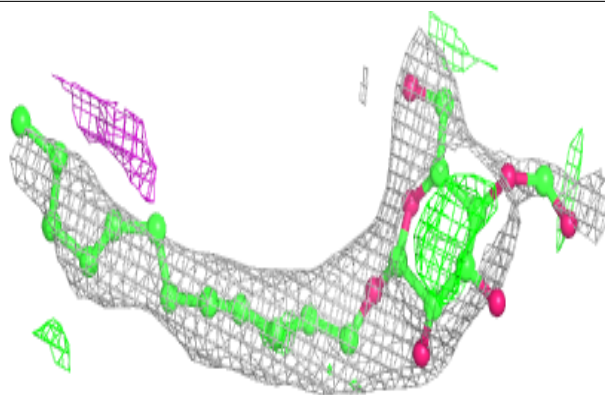
**Electron density around LMT m 103:**

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

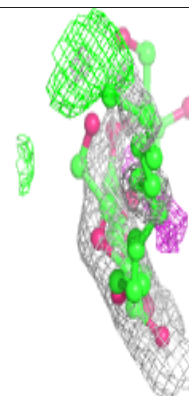
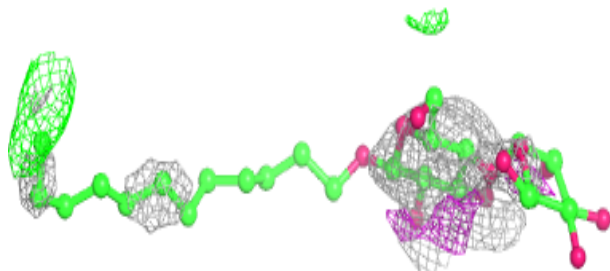
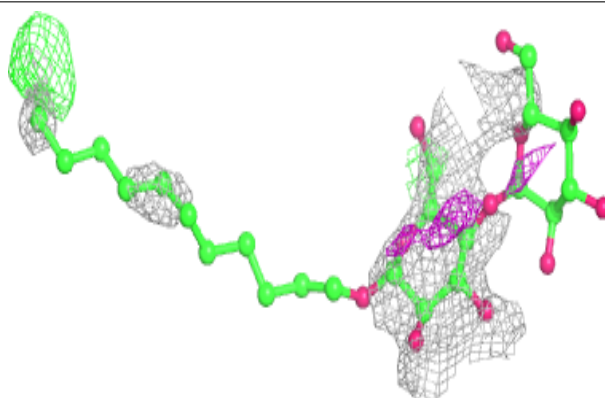


Electron density around LMT t 101:

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

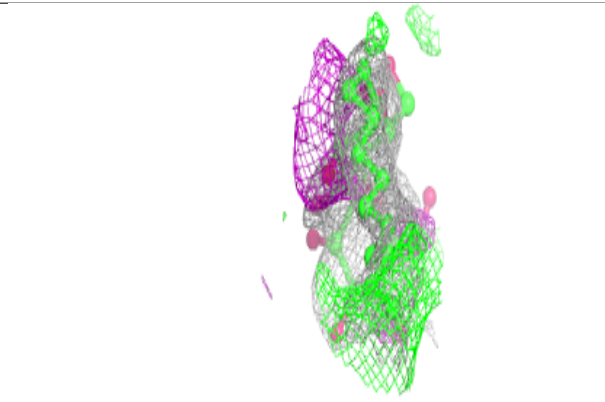
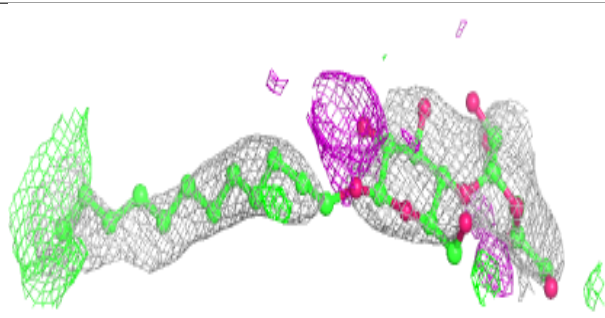
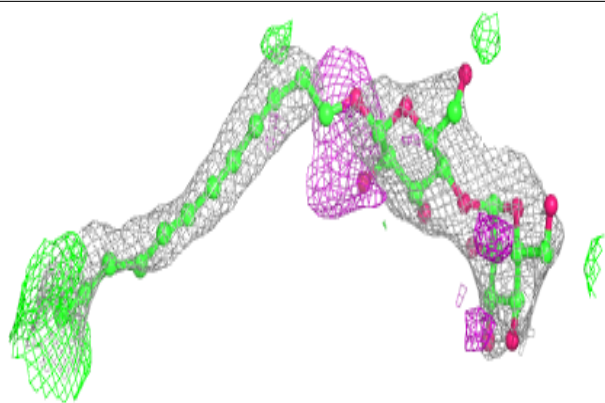
**Electron density around LMT e 101:**

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

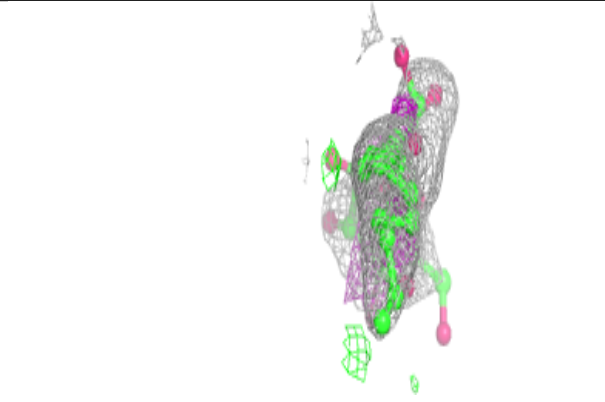
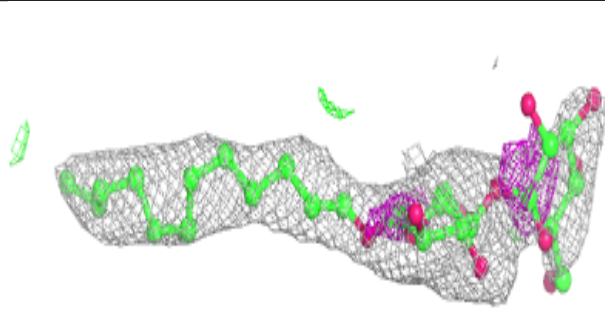
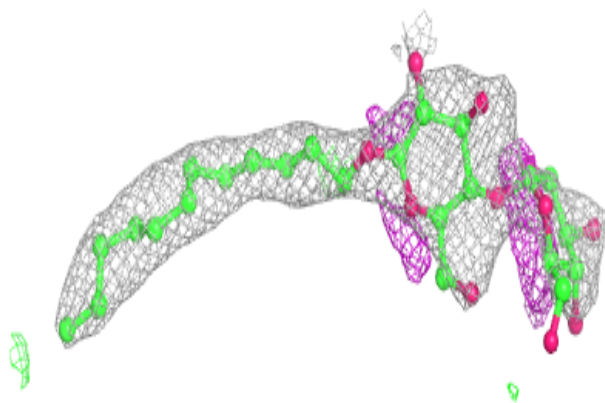


Electron density around LMT A 417:

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

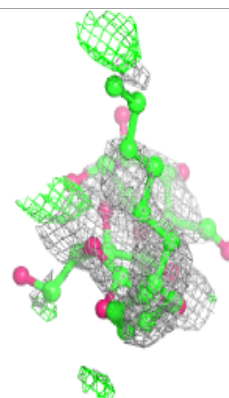
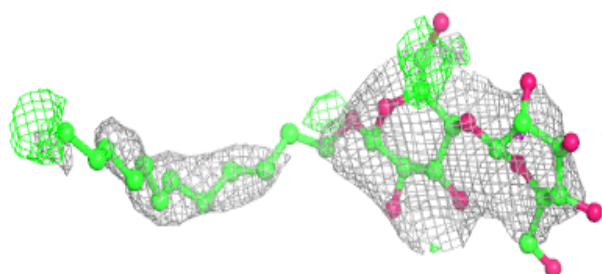
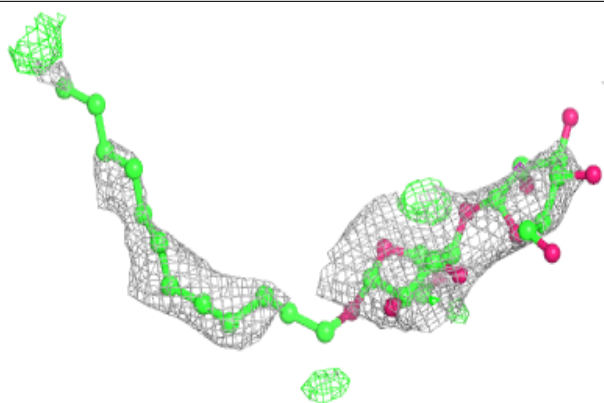
**Electron density around LMT B 628:**

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

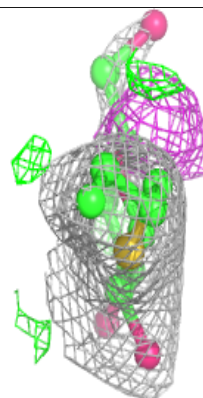
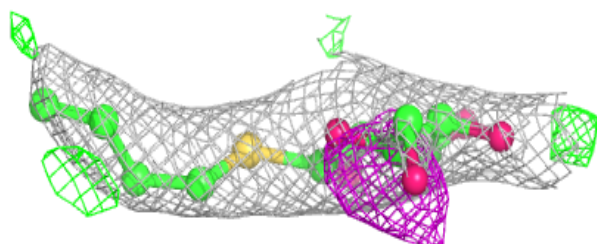
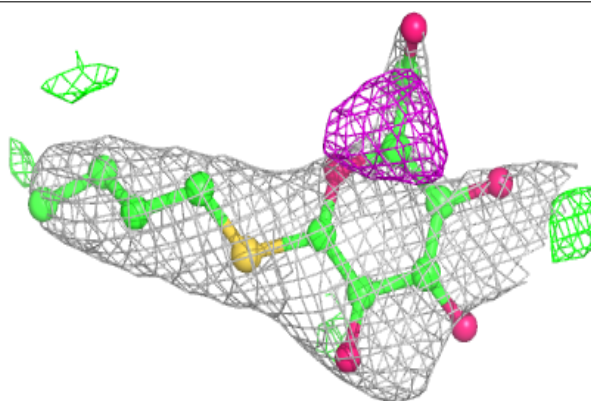


Electron density around LMT A 421:

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

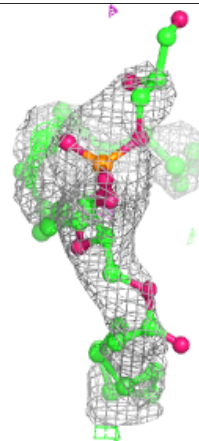
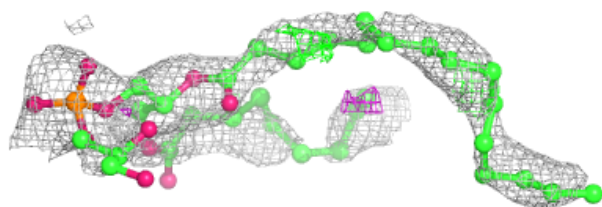
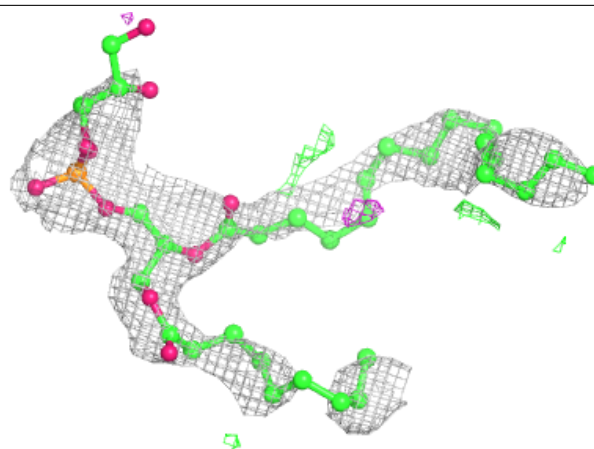
**Electron density around HTG D 410:**

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

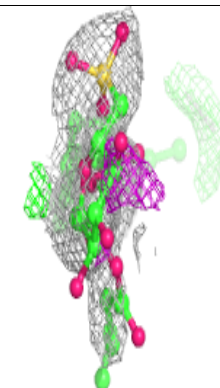
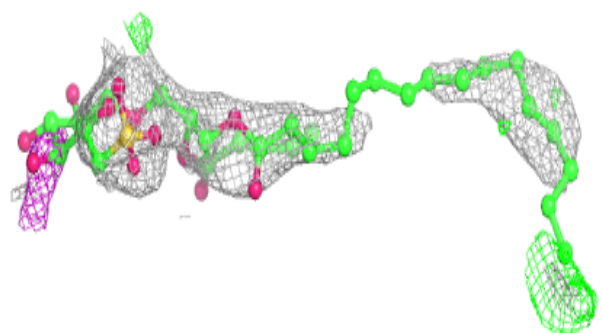
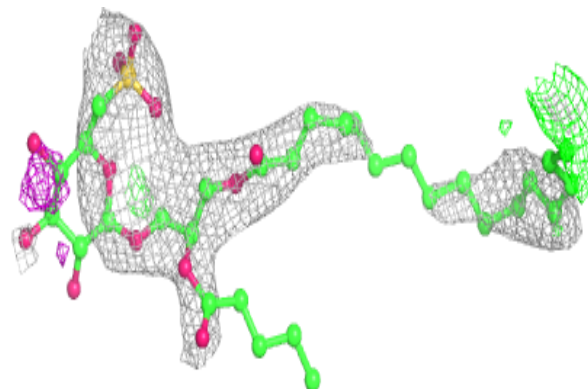


Electron density around LHG a 421:

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

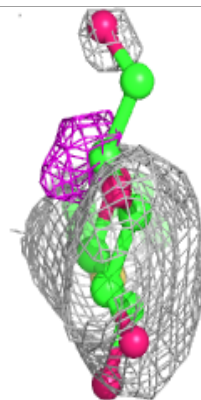
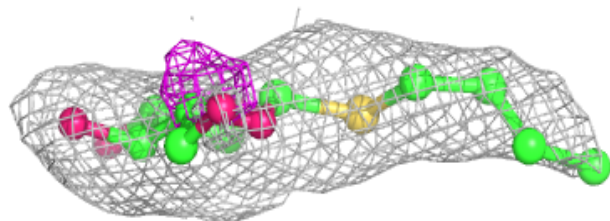
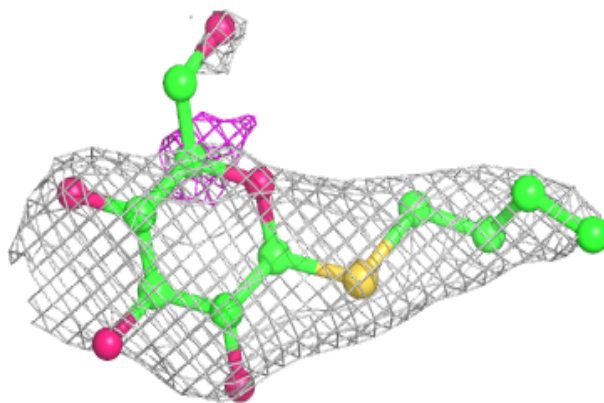
**Electron density around SQD f 102:**

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

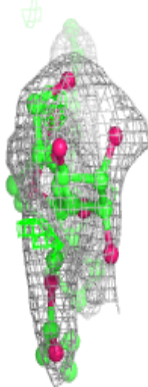
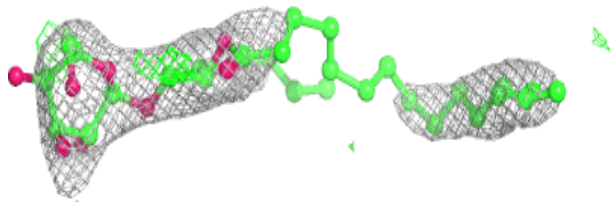
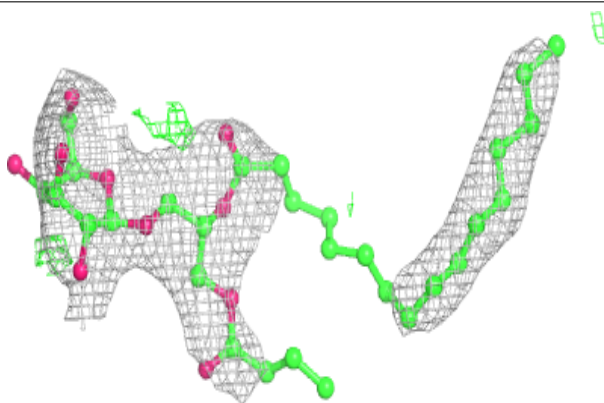


Electron density around HTG d 409:

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

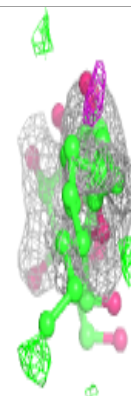
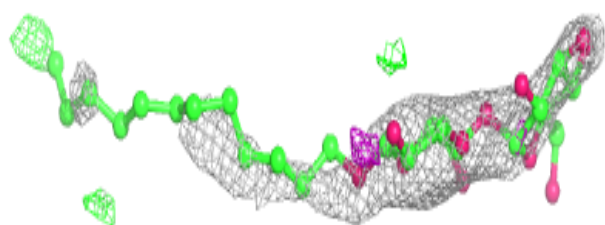
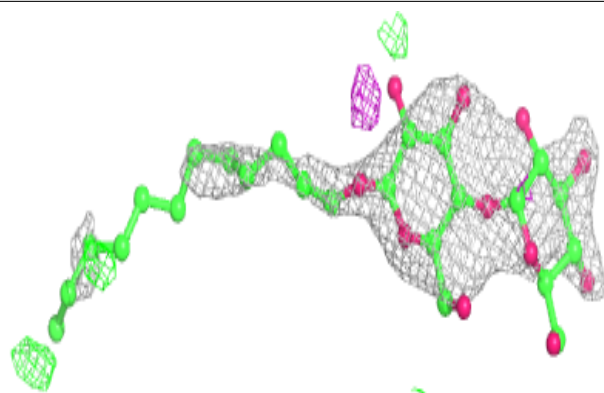
**Electron density around LMG z 101:**

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

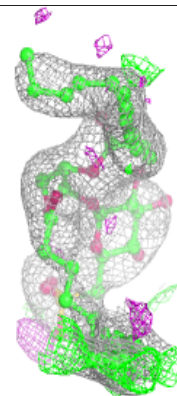
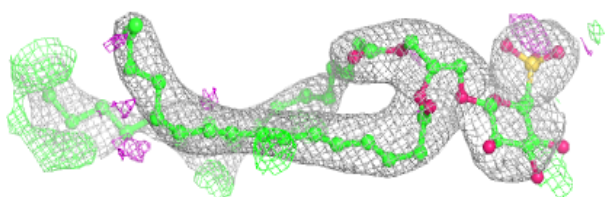
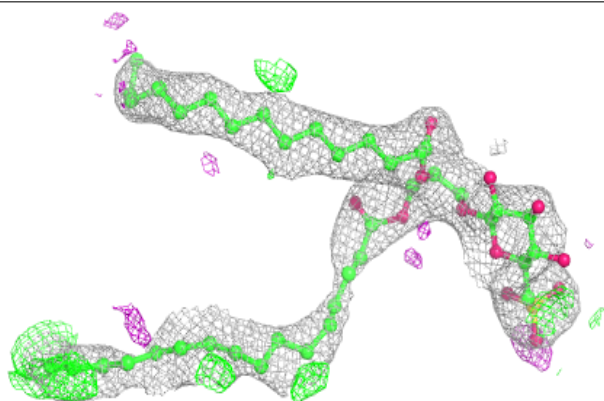


Electron density around LMT c 501:

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

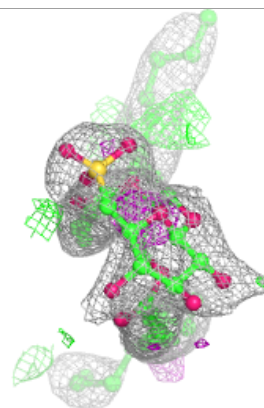
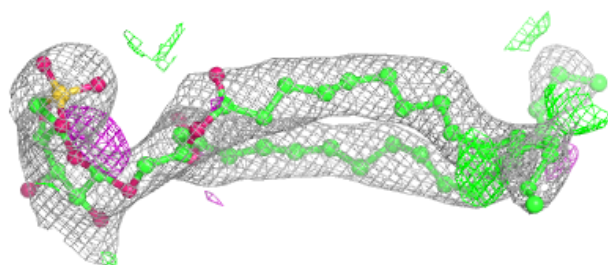
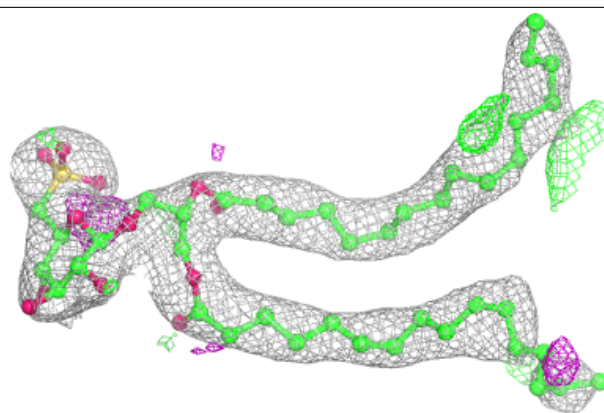
**Electron density around SQD A 412:**

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

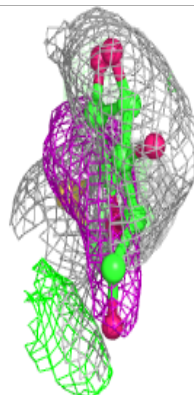
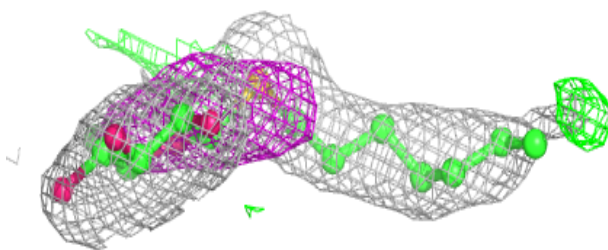
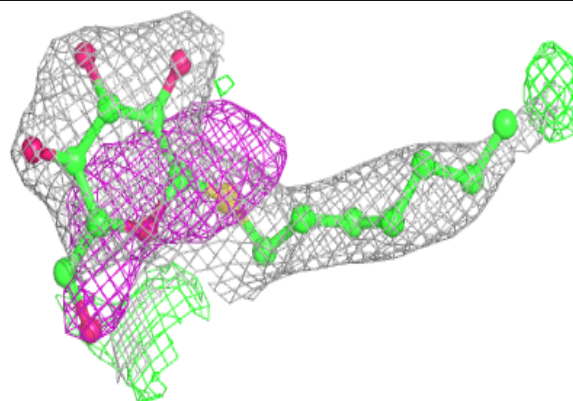


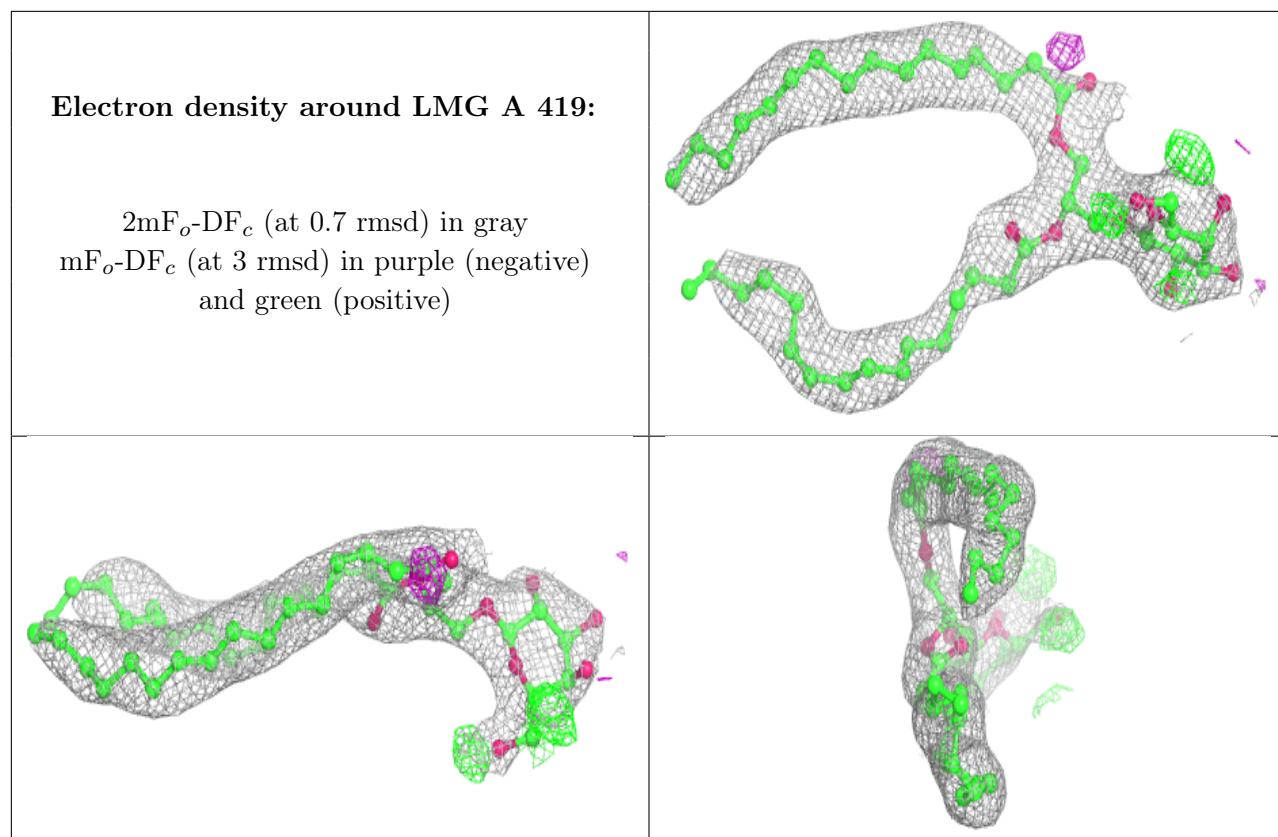
Electron density around SQD b 620:

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

**Electron density around HTG b 622:**

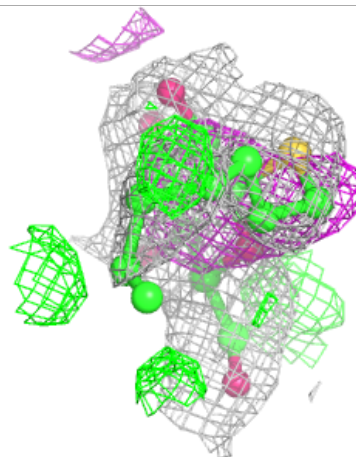
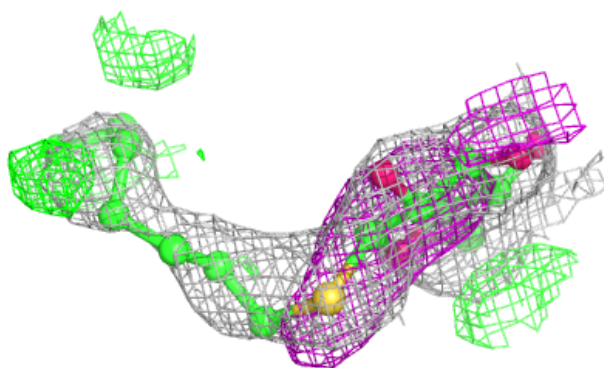
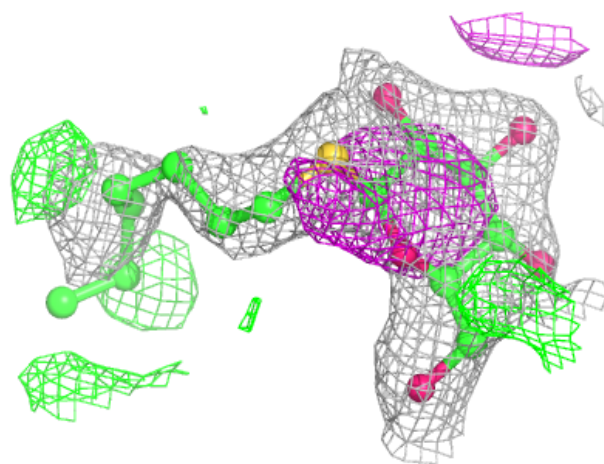
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





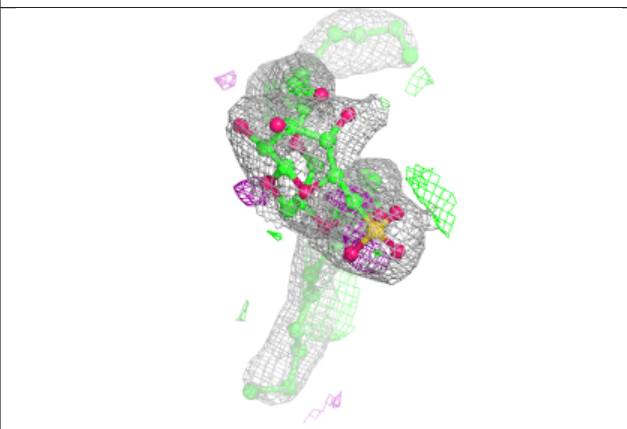
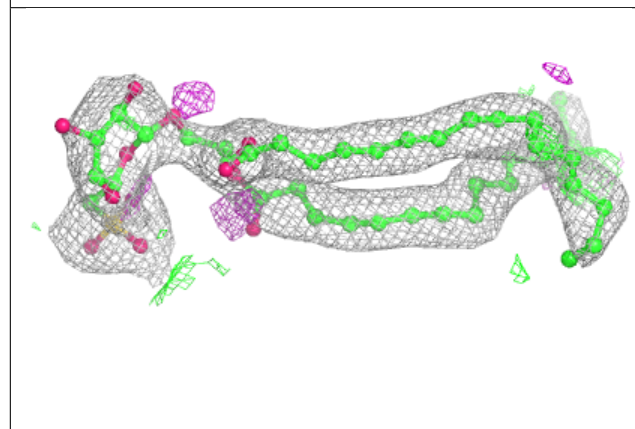
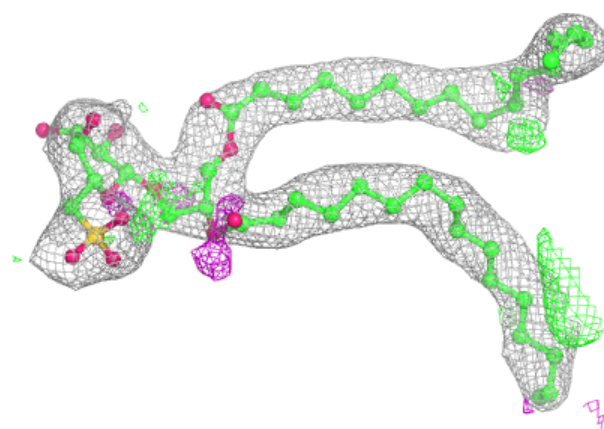
Electron density around HTG B 623:

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

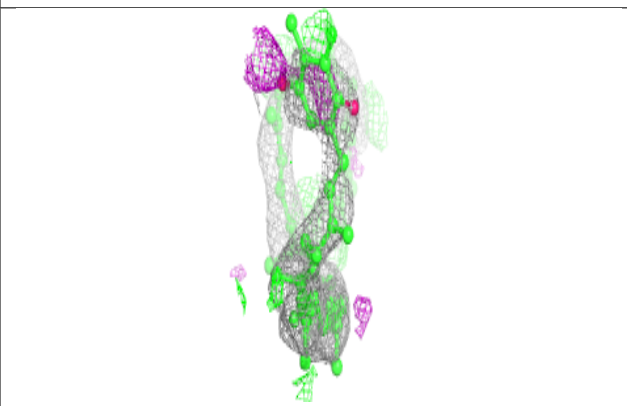
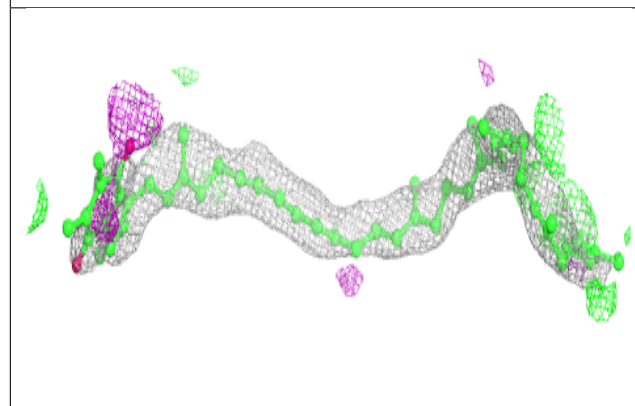
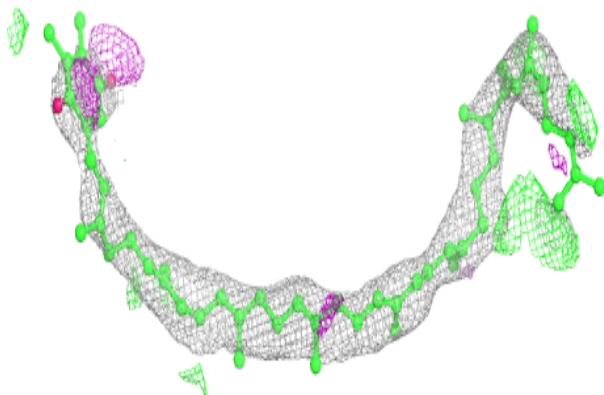


Electron density around SQD B 620:

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

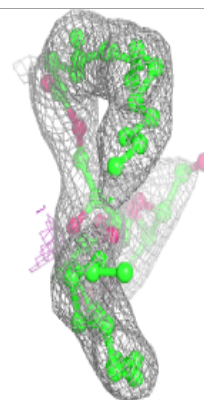
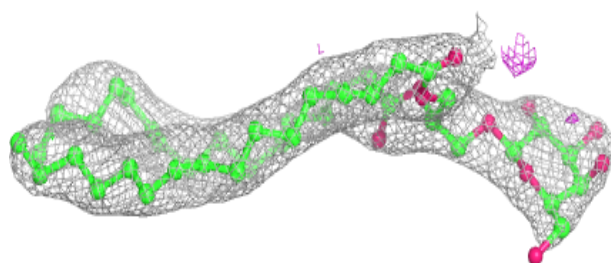
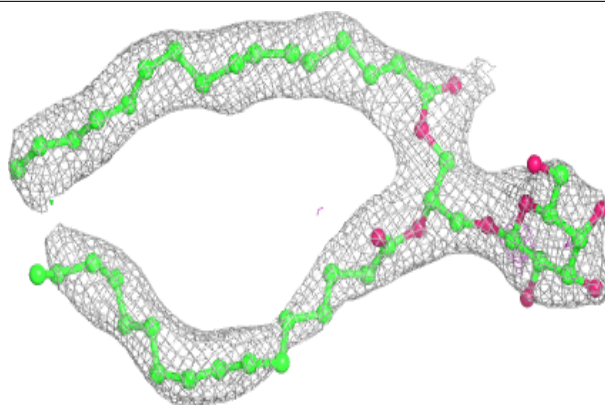
**Electron density around PL9 A 414:**

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

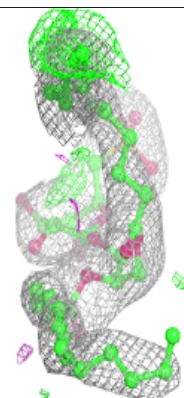
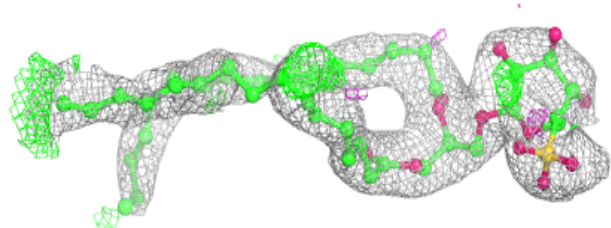
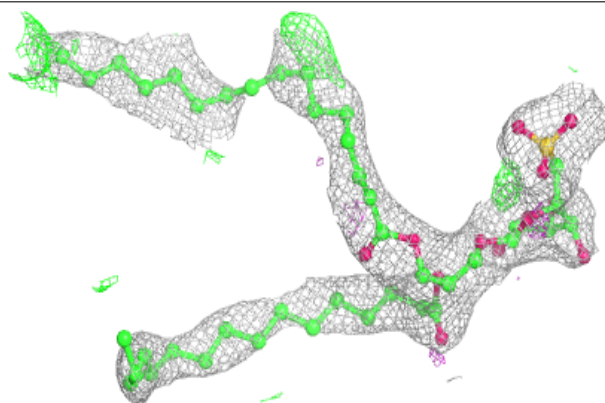


Electron density around LMG a 418:

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

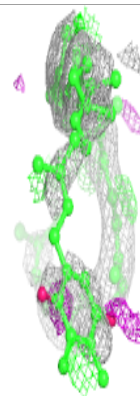
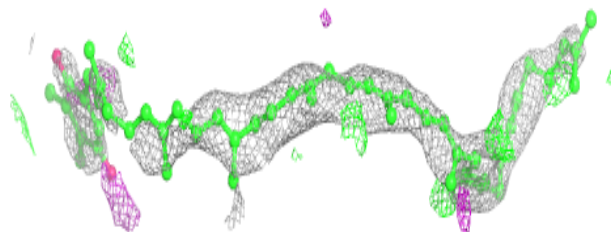
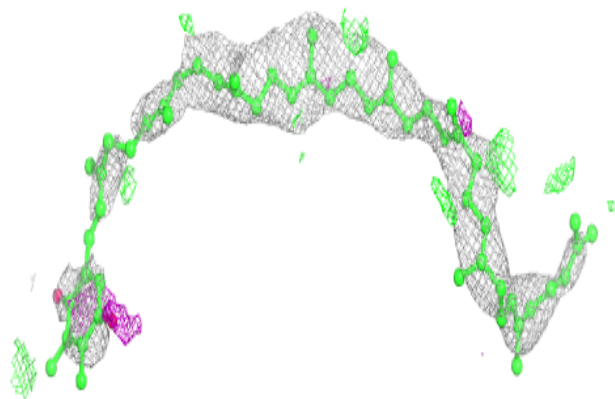
**Electron density around SQD a 413:**

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

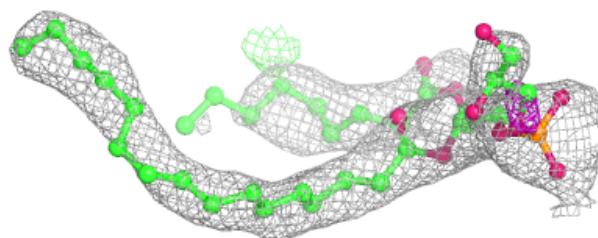
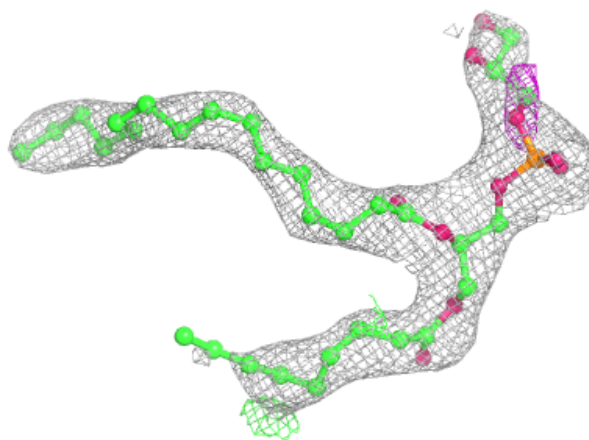


Electron density around PL9 a 415:

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

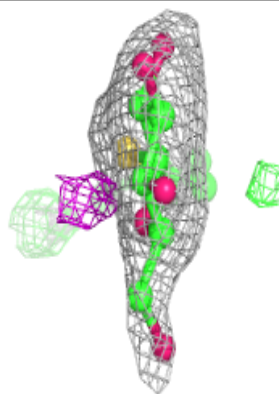
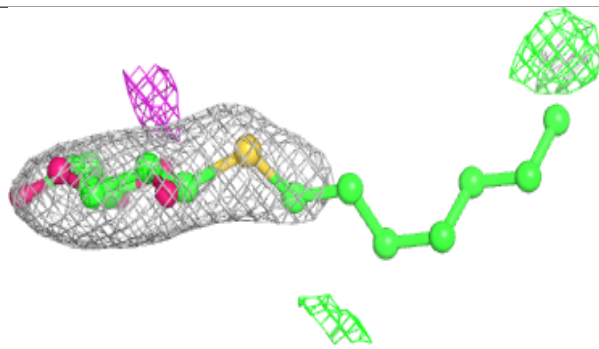
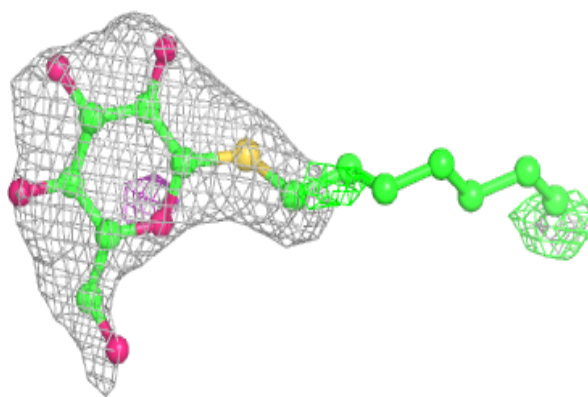
**Electron density around LHG E 101:**

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

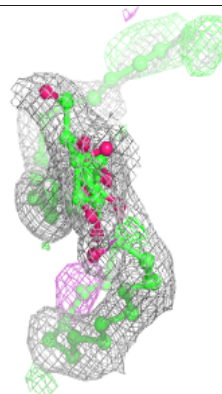
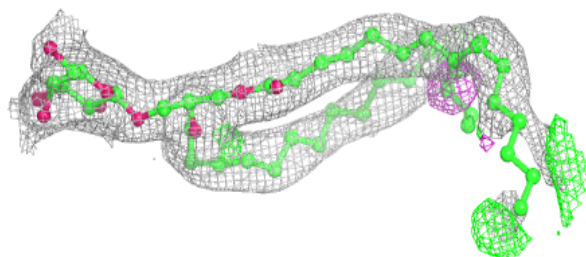
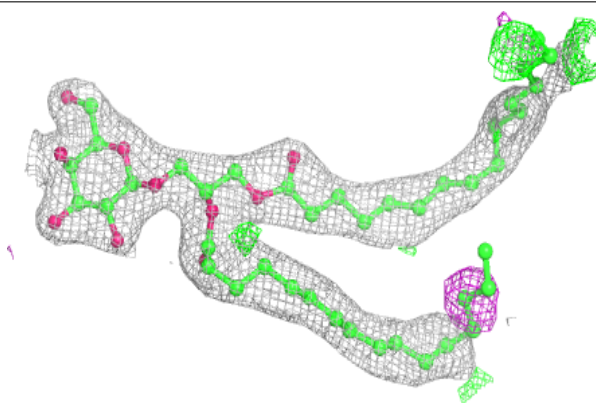


Electron density around HTG C 520:

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

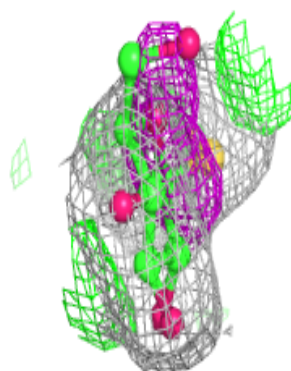
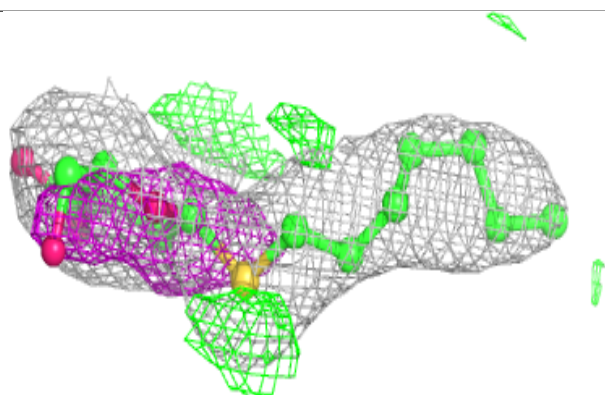
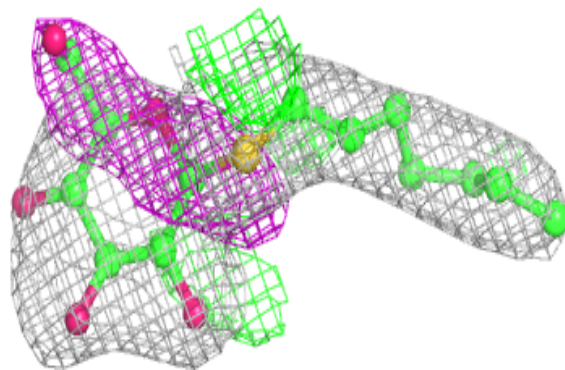
**Electron density around LMG D 411:**

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

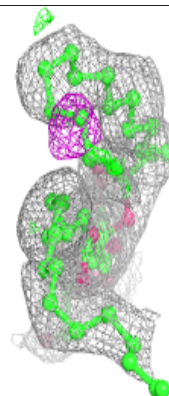
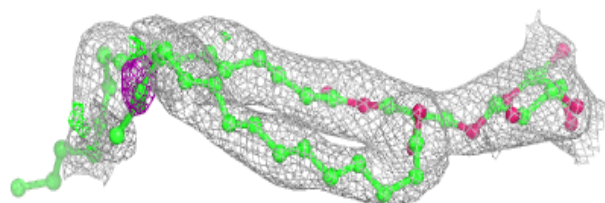
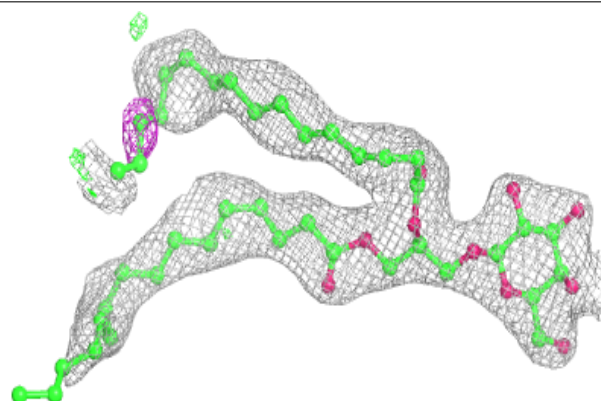


Electron density around HTG B 622:

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

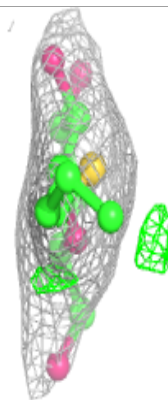
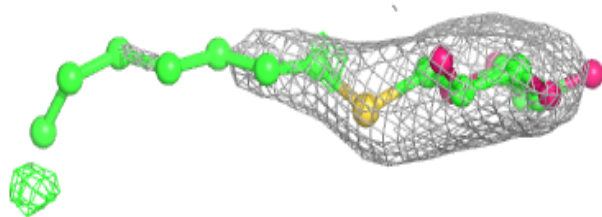
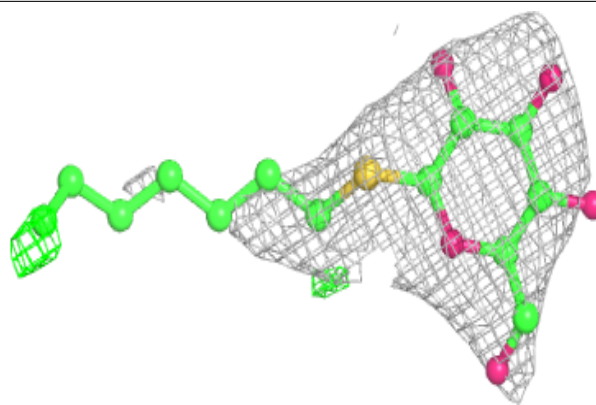
**Electron density around LMG d 410:**

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



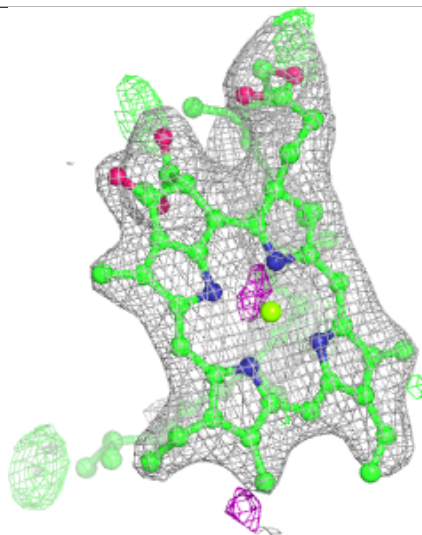
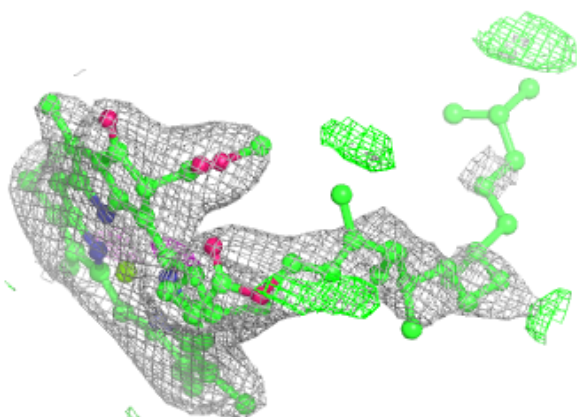
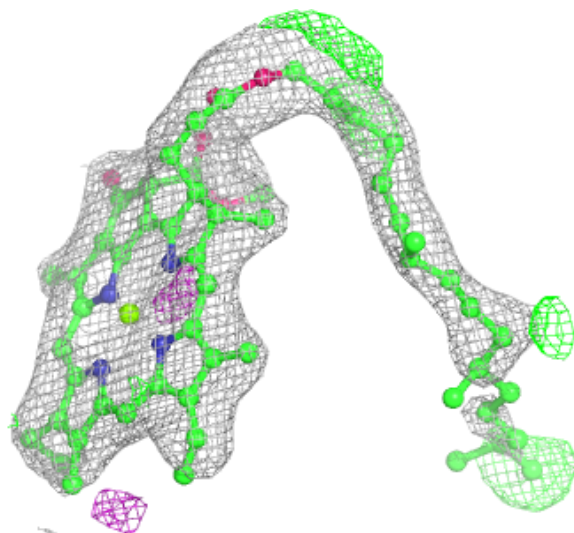
Electron density around HTG c 522:

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



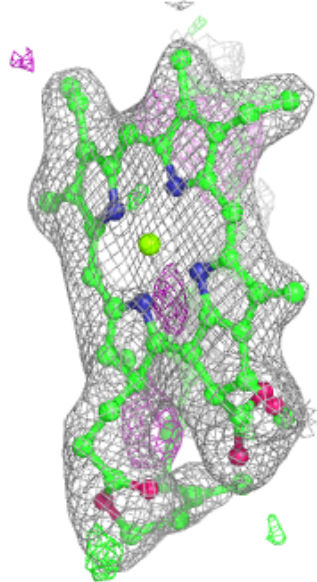
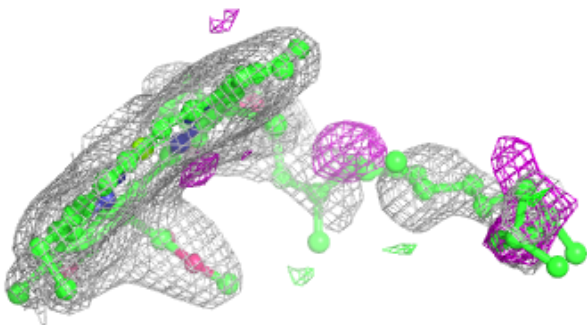
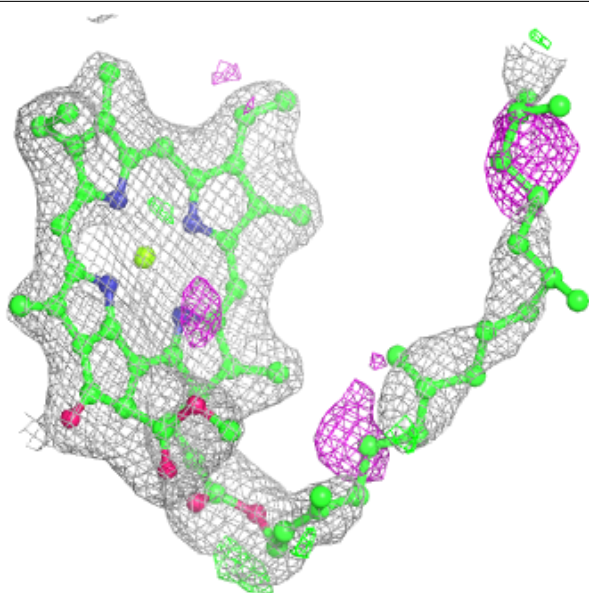
Electron density around CLA b 616:

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



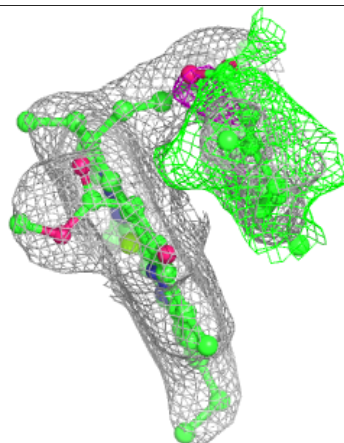
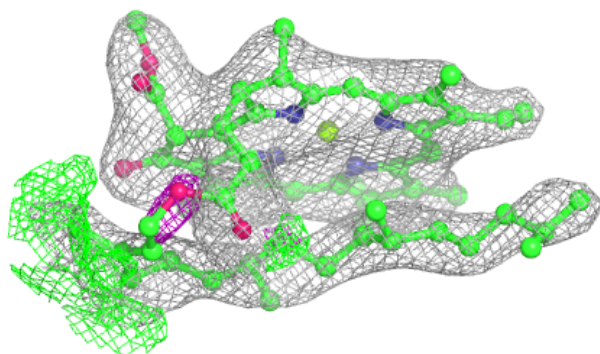
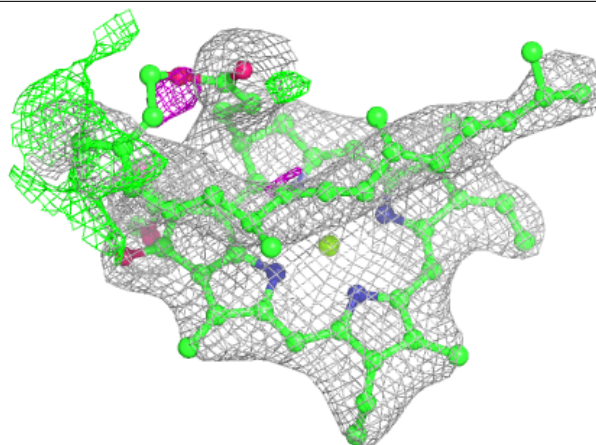
Electron density around CLA B 616:

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



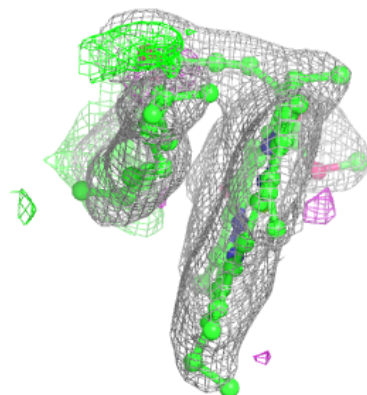
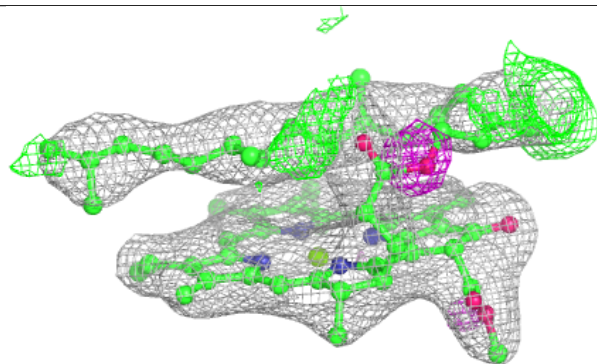
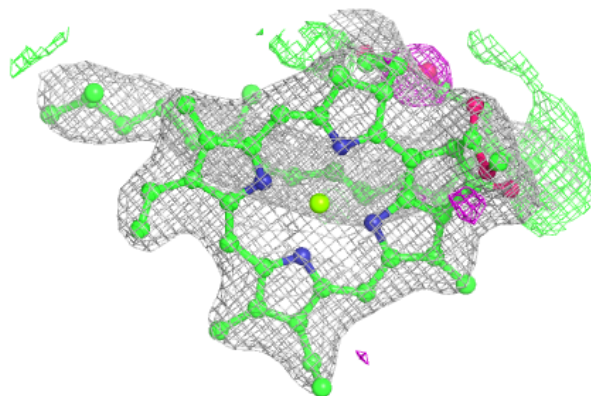
Electron density around CLA b 601:

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

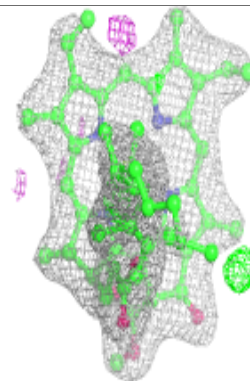
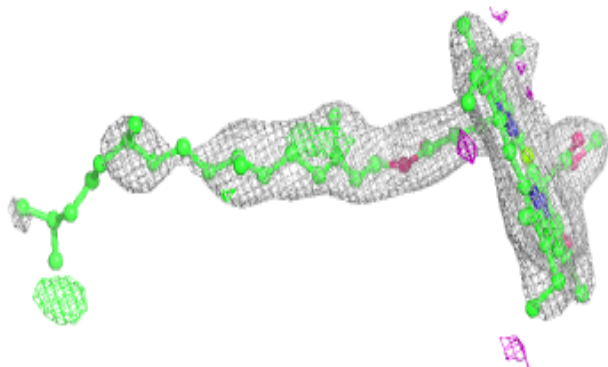
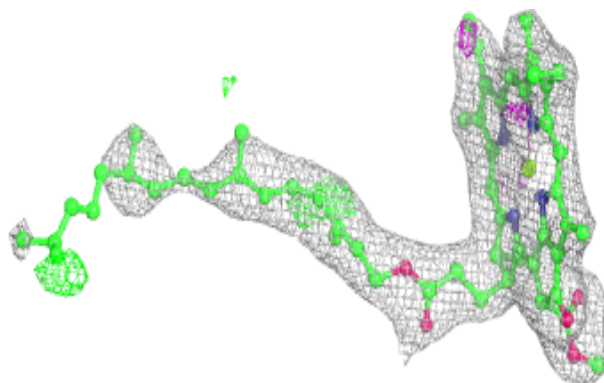


Electron density around CLA B 601:

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

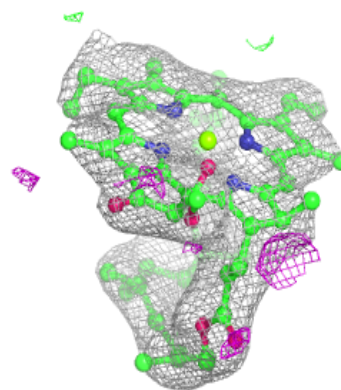
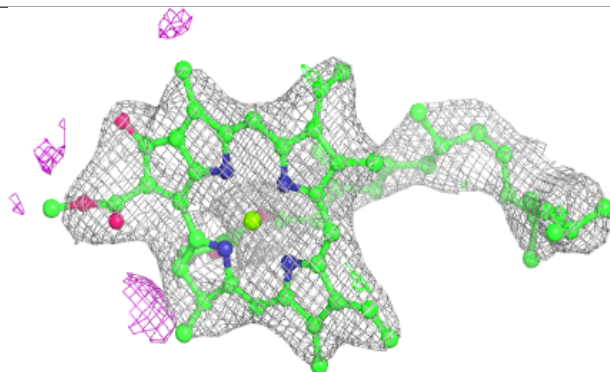
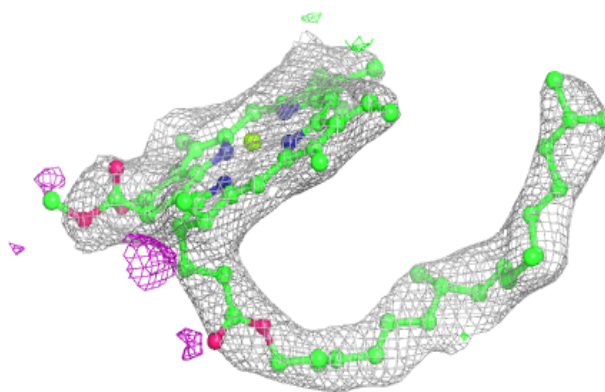
**Electron density around CLA d 402:**

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

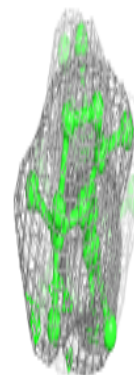
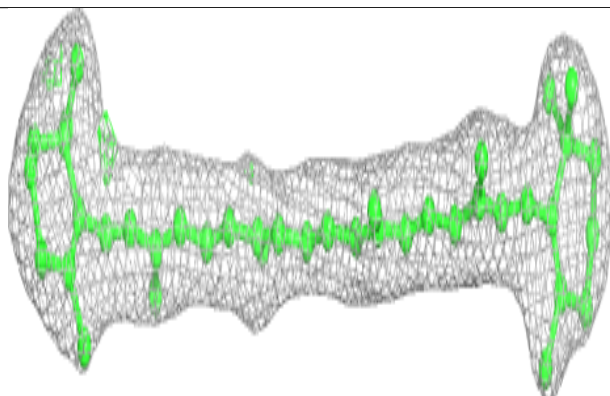
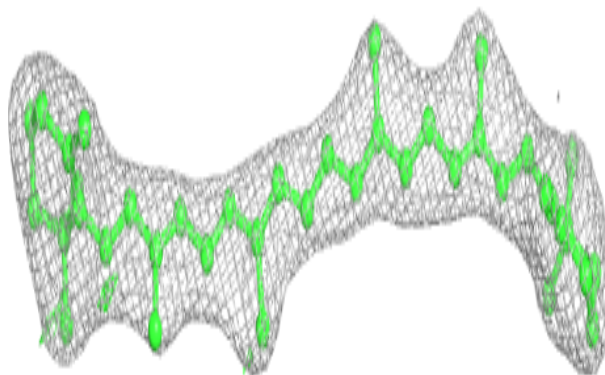


Electron density around CLA C 513:

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

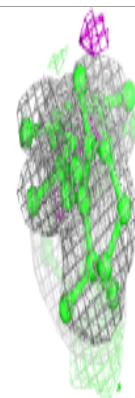
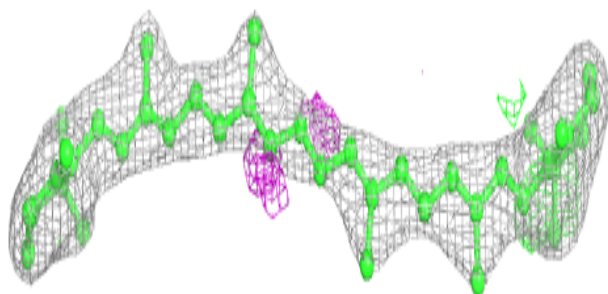
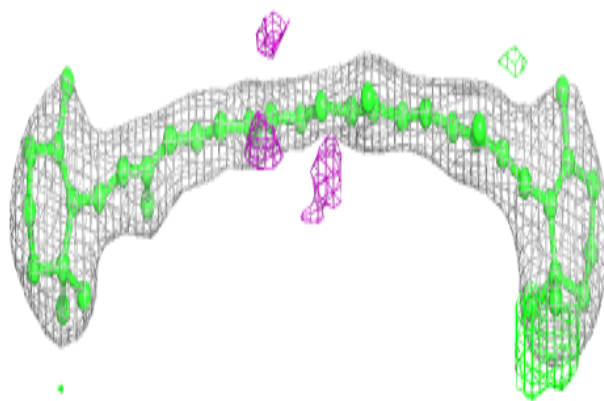
**Electron density around BCR K 101:**

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

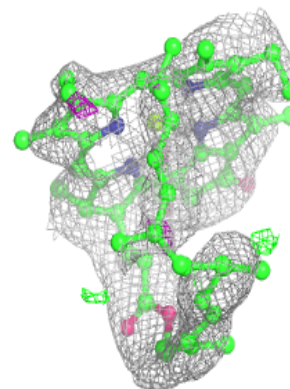
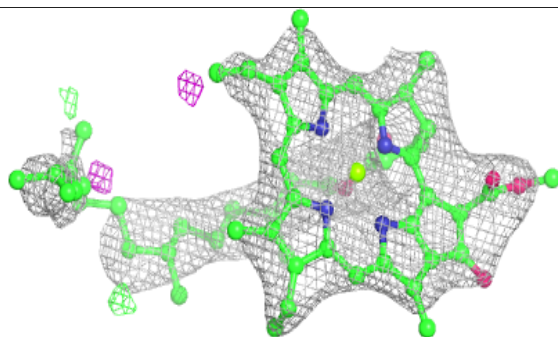
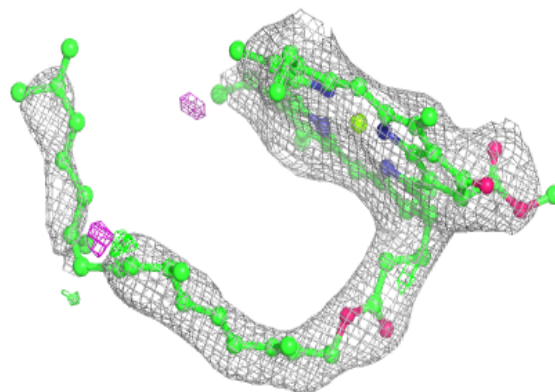


Electron density around BCR K 103:

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

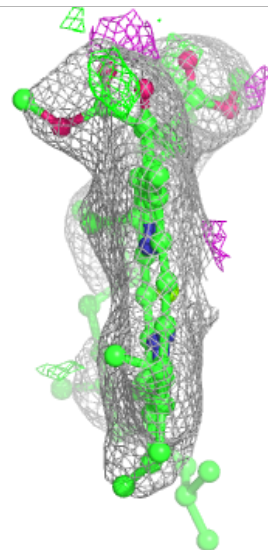
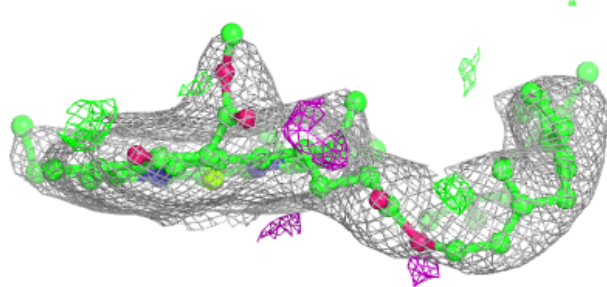
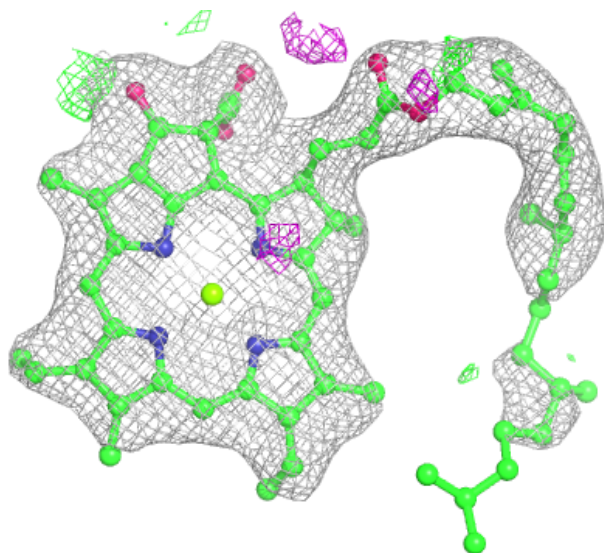
**Electron density around CLA c 514:**

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



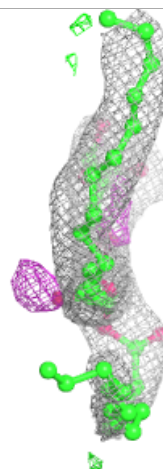
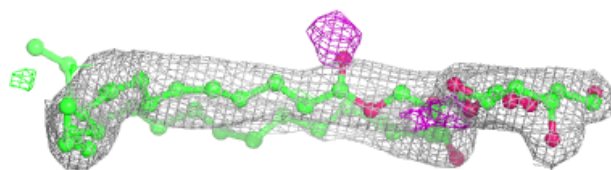
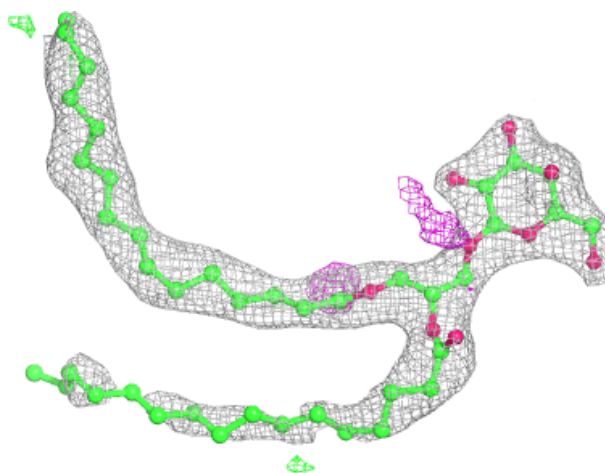
Electron density around CLA c 513:

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



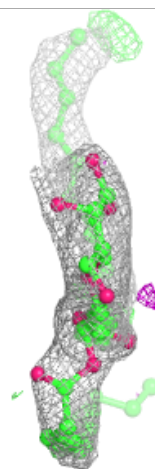
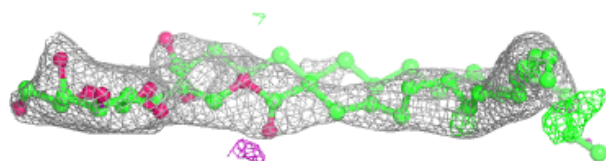
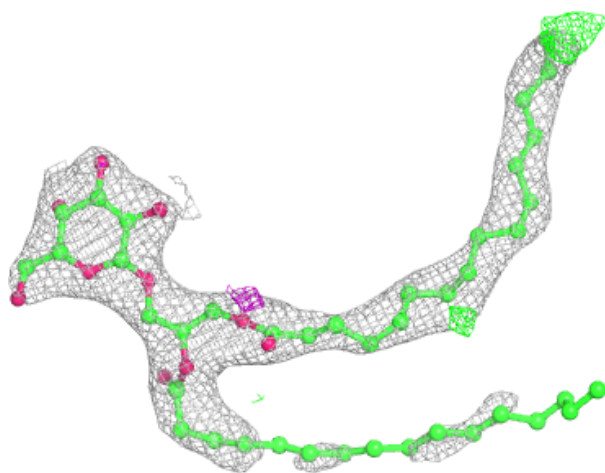
Electron density around LMG C 518:

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



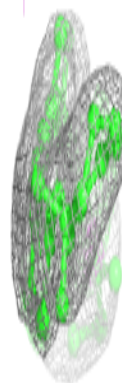
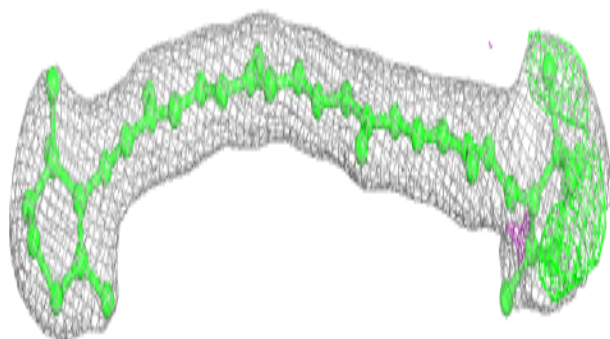
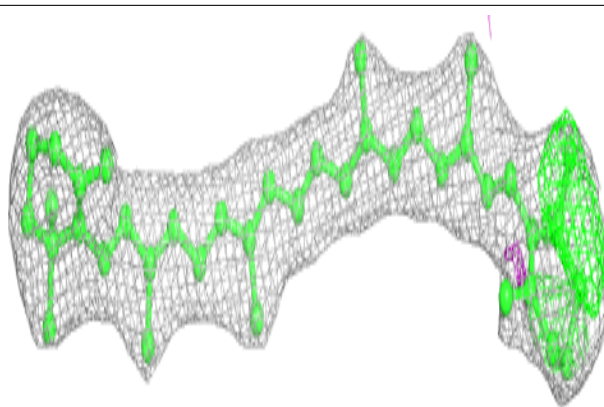
Electron density around LMG c 520:

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

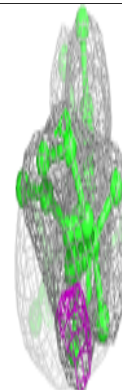
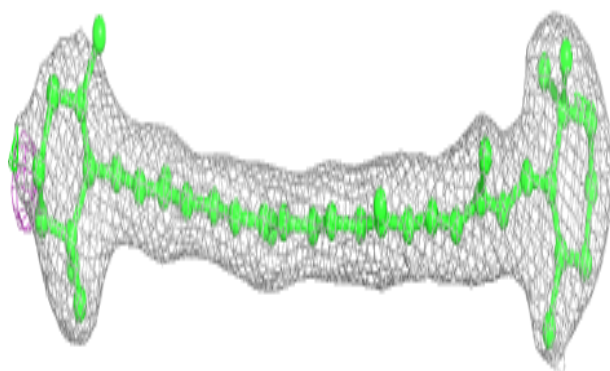
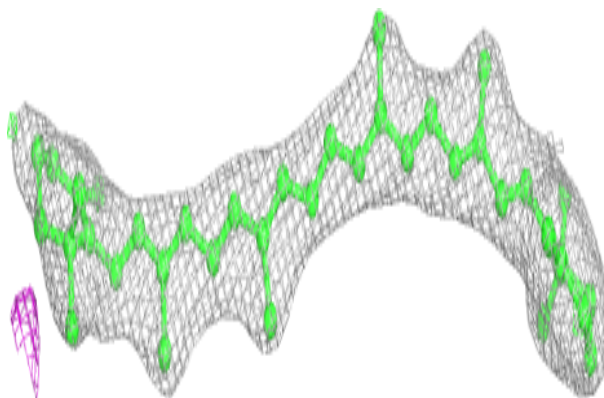


Electron density around BCR d 403:

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

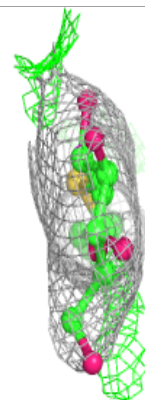
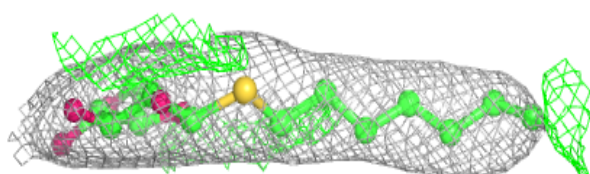
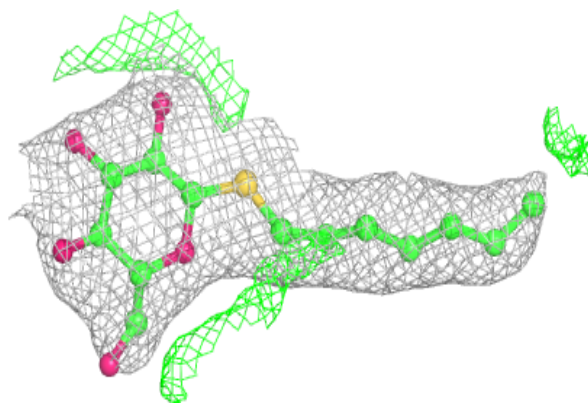
**Electron density around BCR h 101:**

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

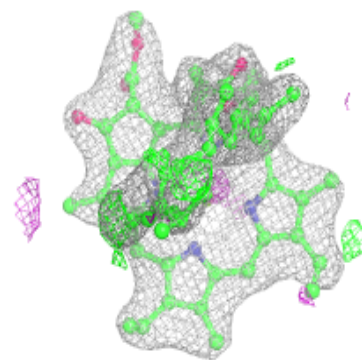
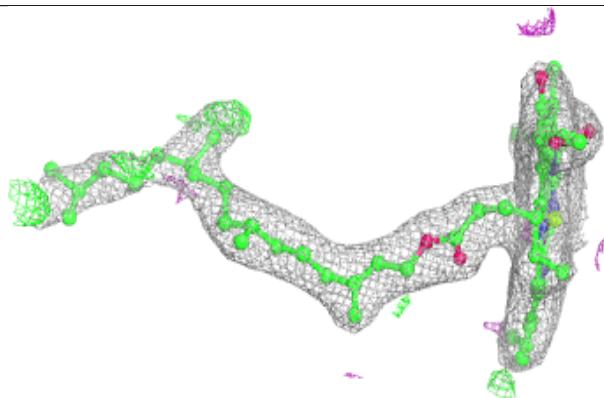
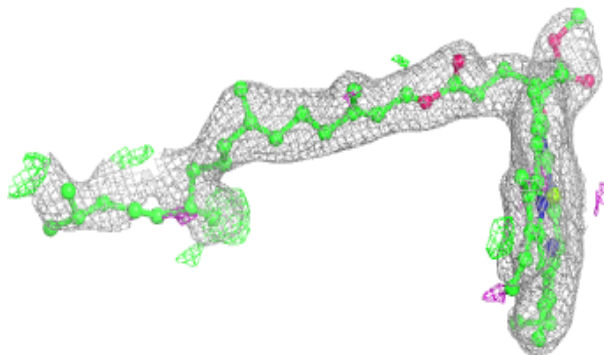


Electron density around HTG b 625:

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

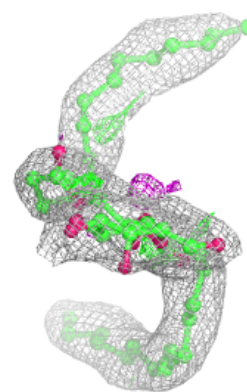
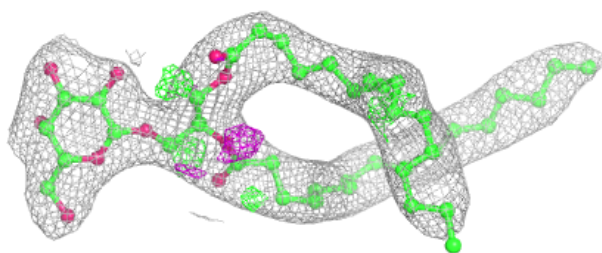
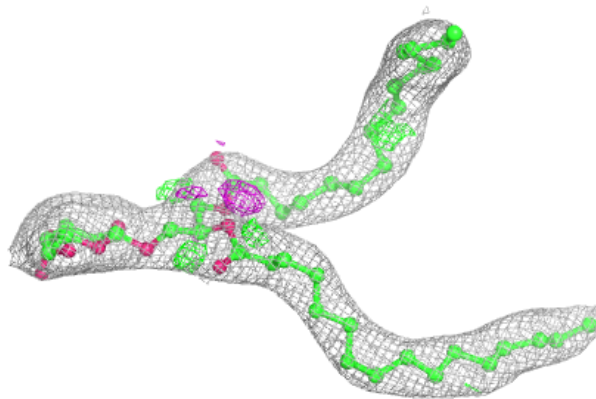
**Electron density around CLA B 606:**

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

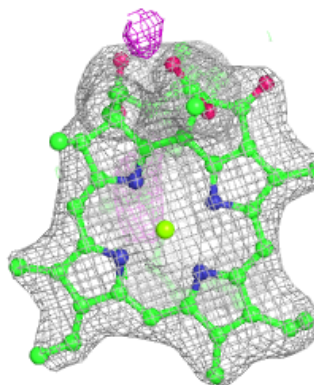
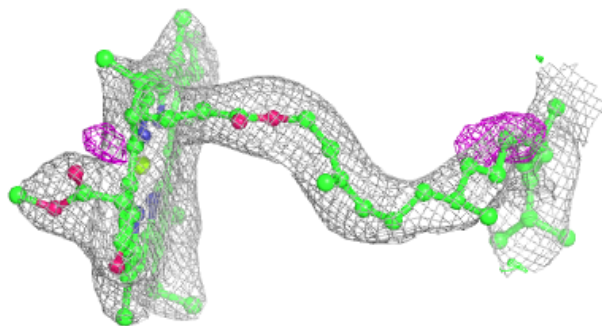
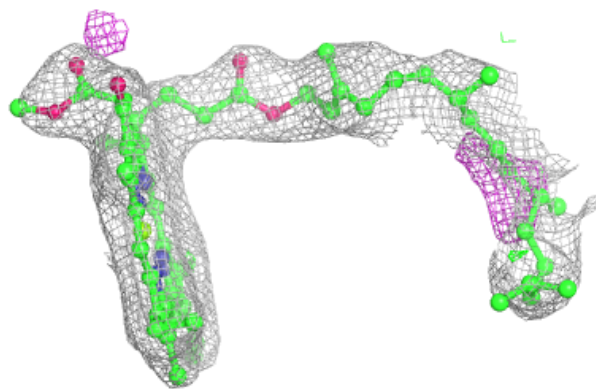


Electron density around LMG B 621:

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

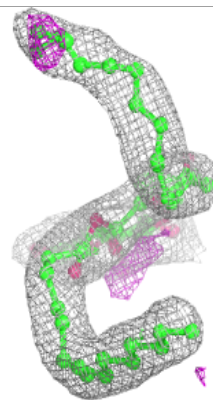
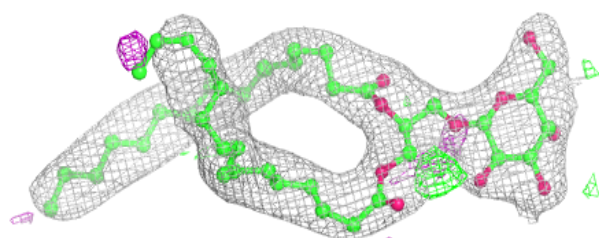
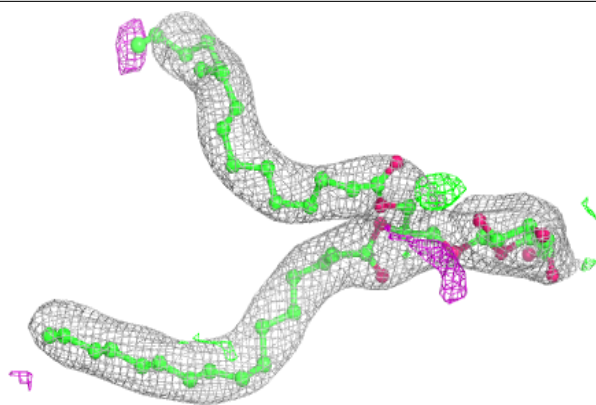
**Electron density around CLA C 506:**

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

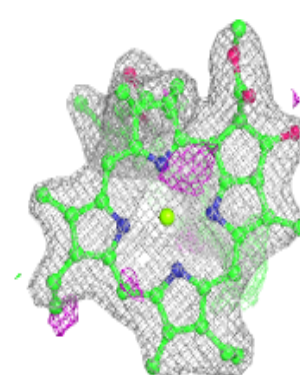
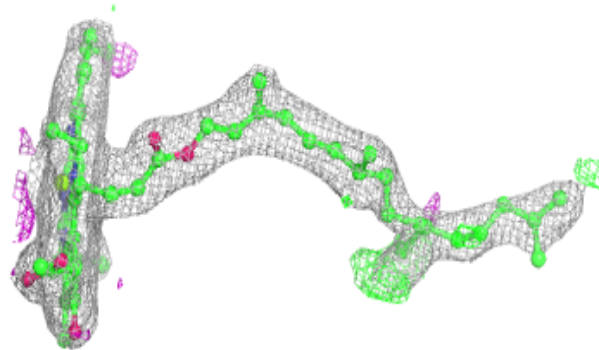
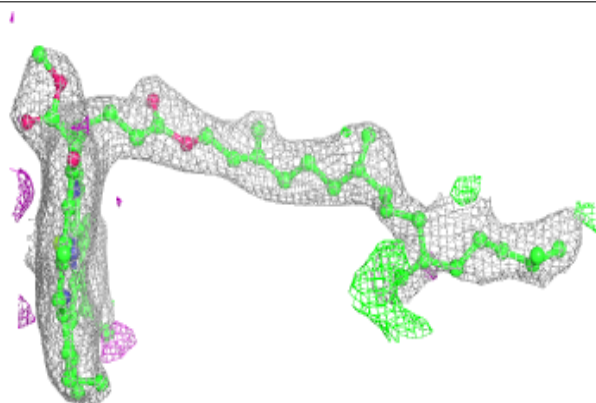


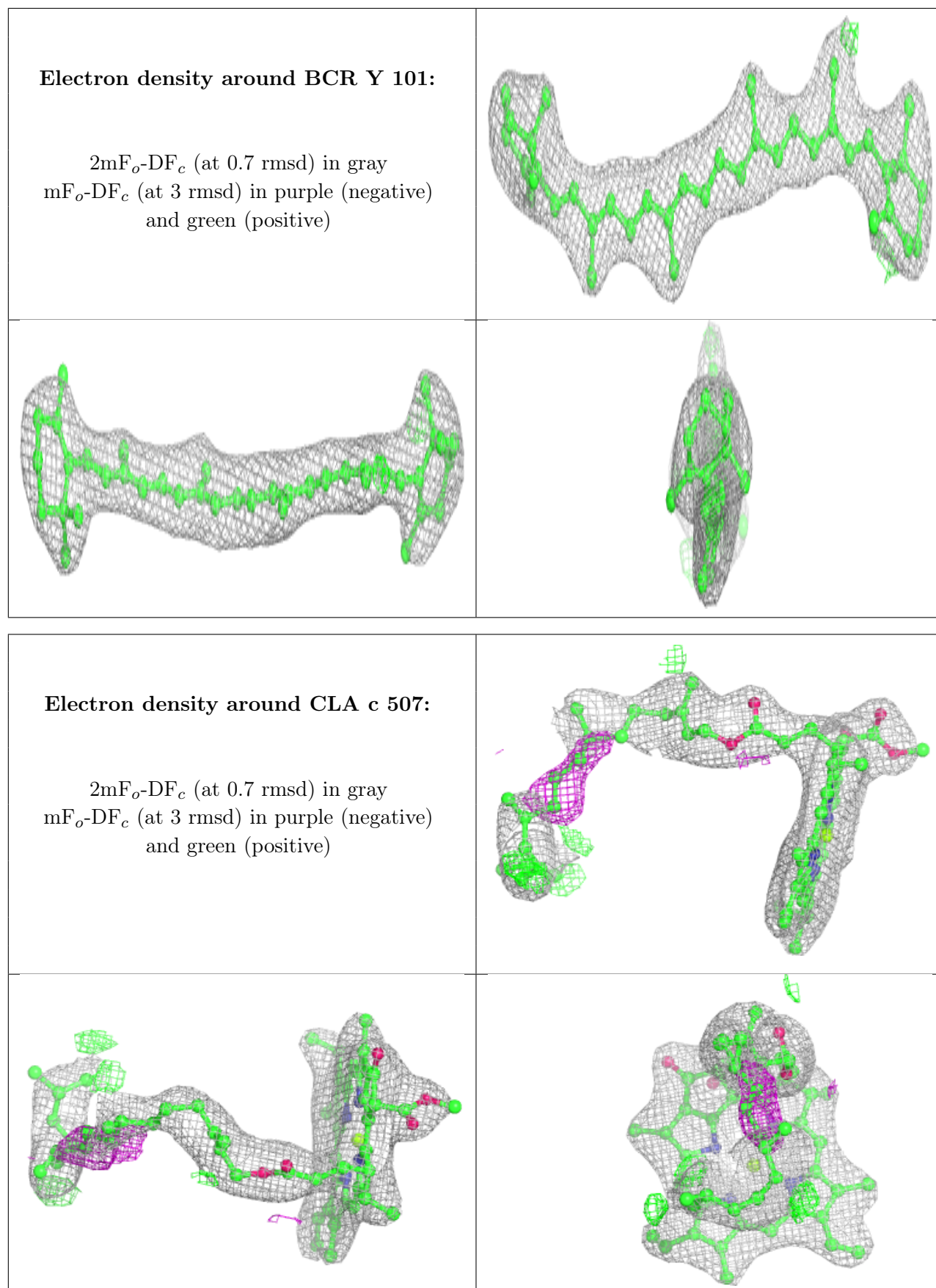
Electron density around LMG m 101:

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

**Electron density around CLA b 606:**

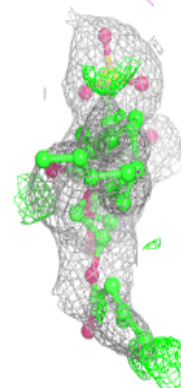
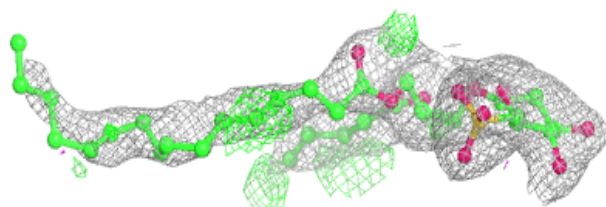
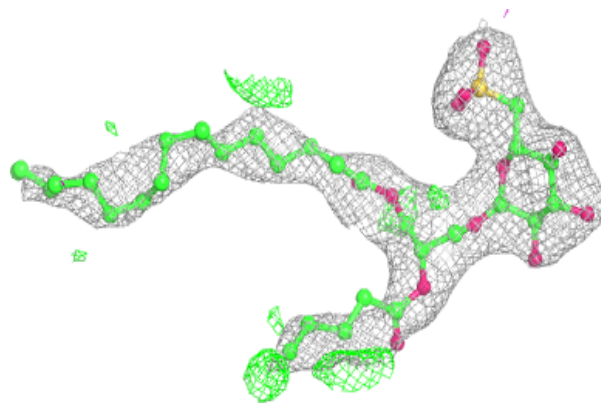
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





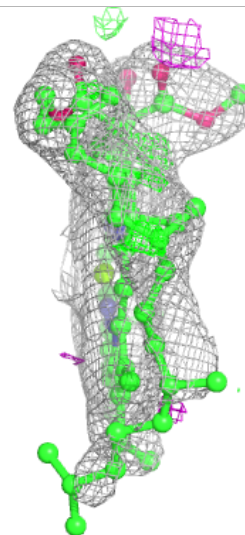
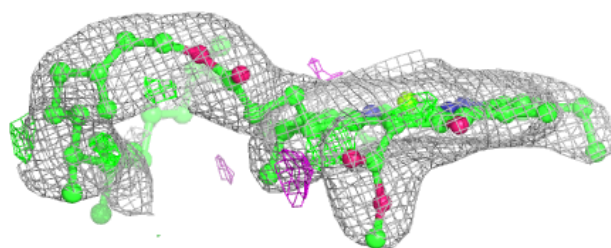
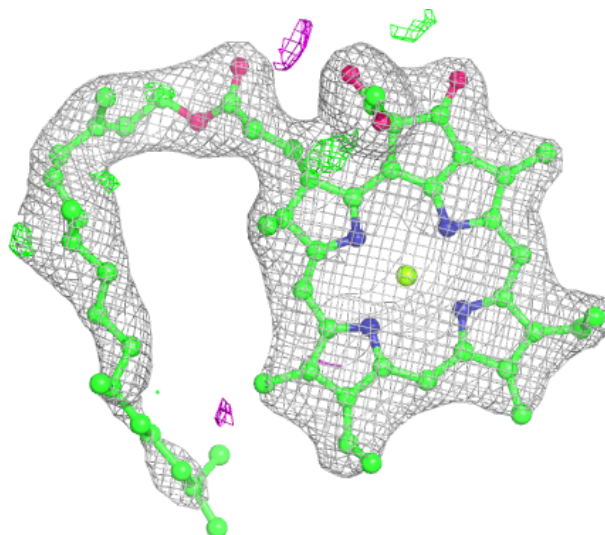
Electron density around SQD F 103:

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



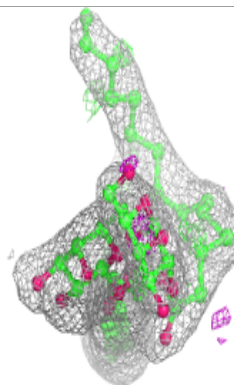
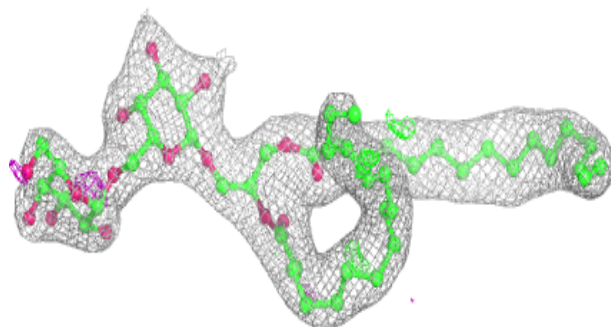
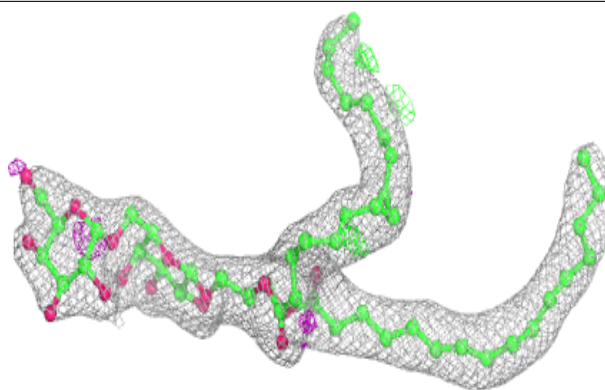
Electron density around CLA C 512:

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

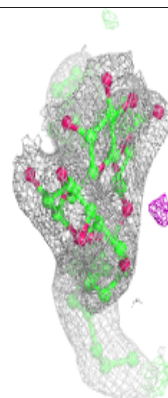
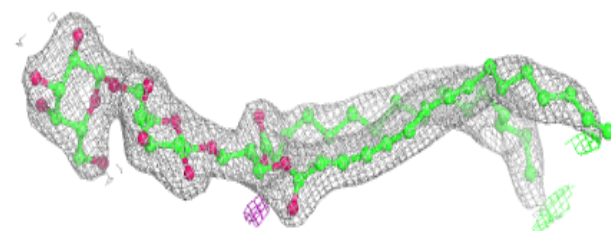
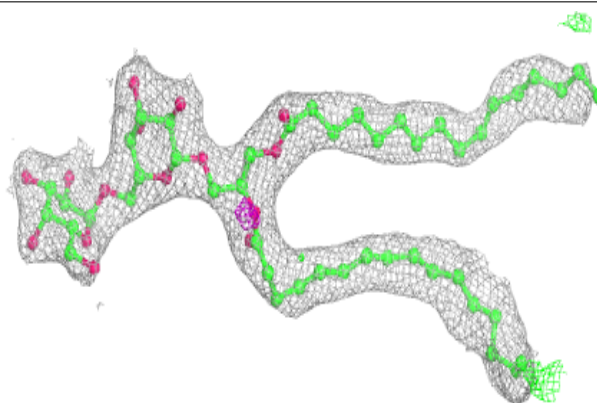


Electron density around DGD H 102:

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

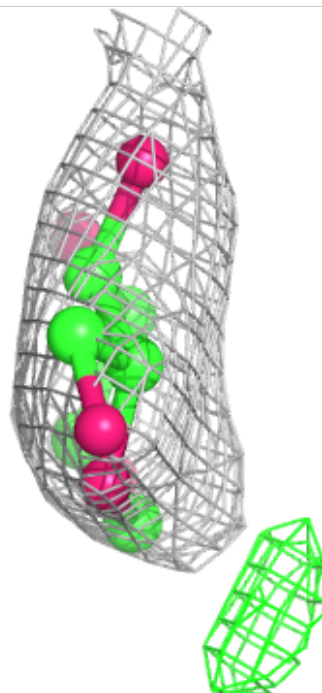
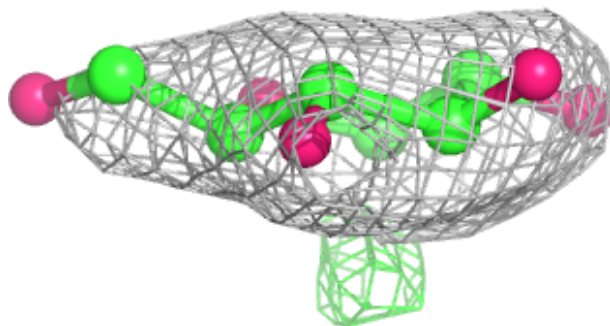
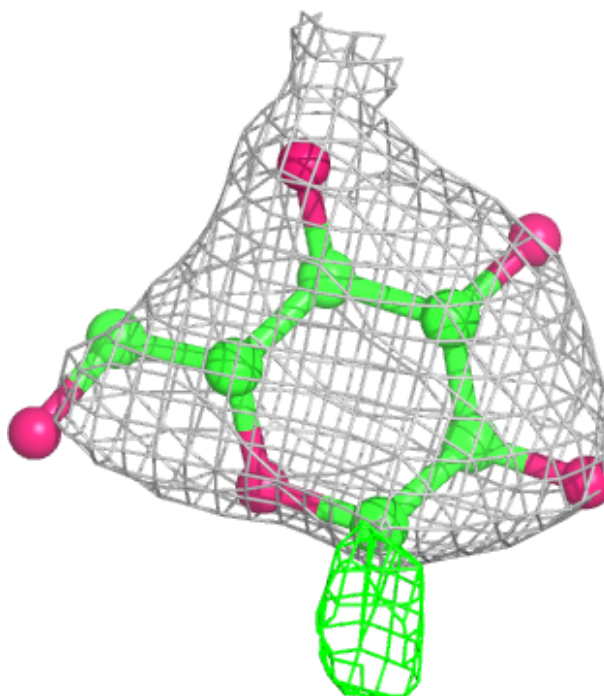
**Electron density around DGD c 519:**

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



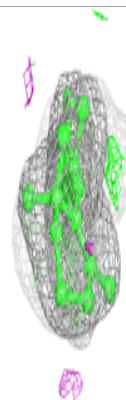
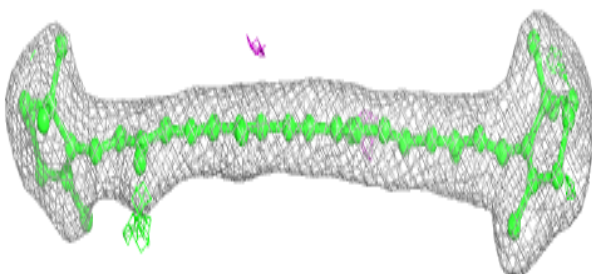
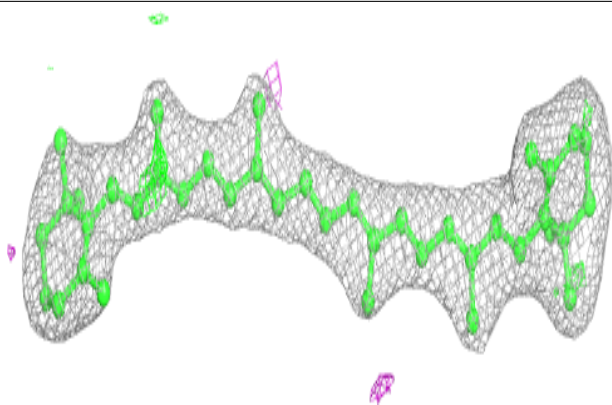
Electron density around HTG V 202:

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

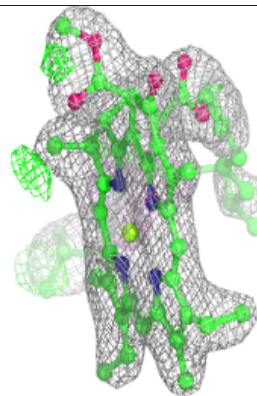
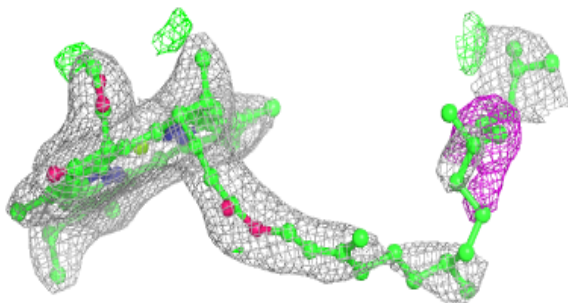
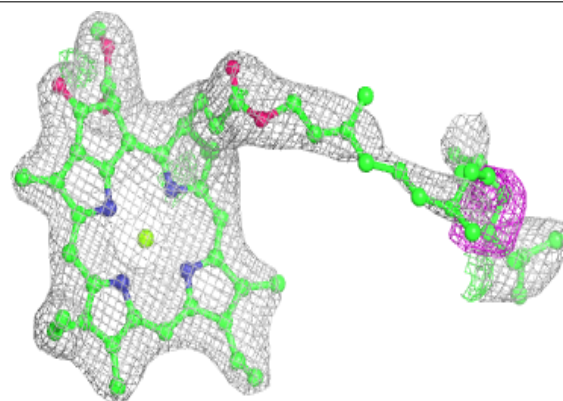


Electron density around BCR b 618:

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

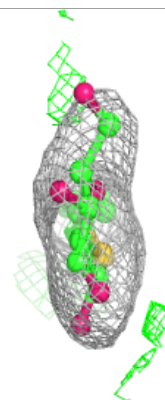
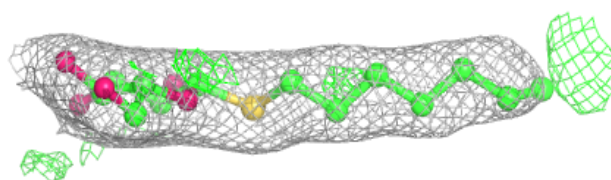
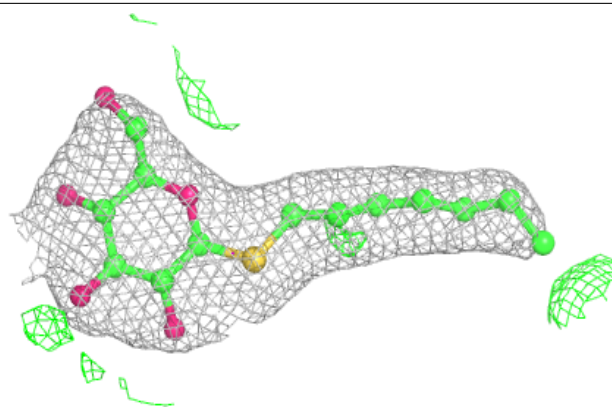
**Electron density around CLA a 409:**

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

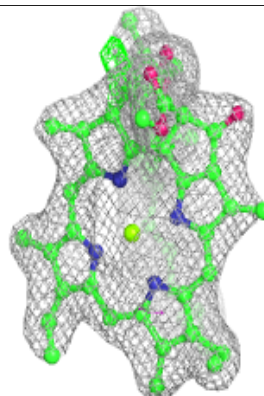
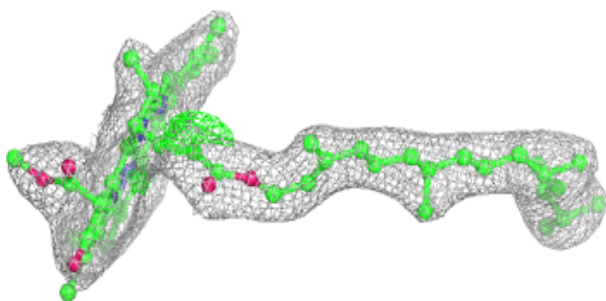
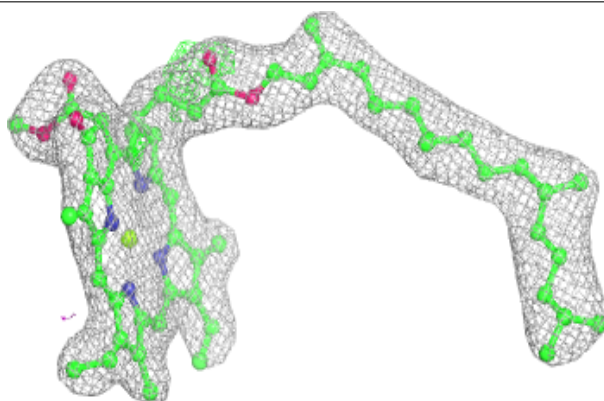


Electron density around HTG B 625:

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

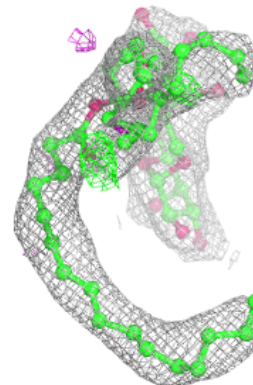
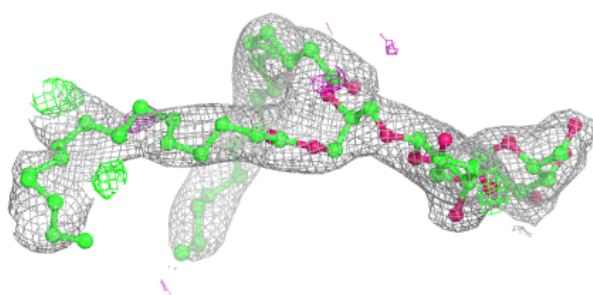
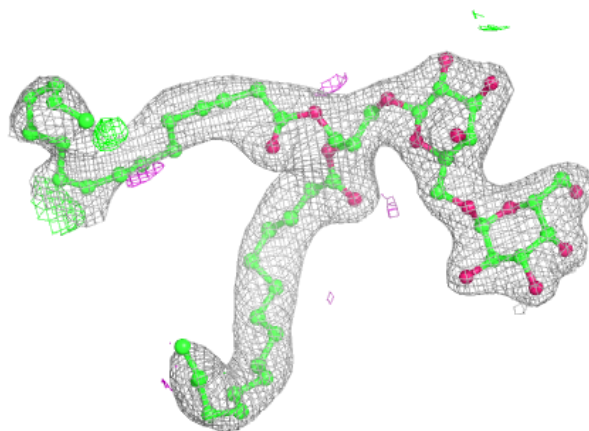
**Electron density around CLA B 609:**

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

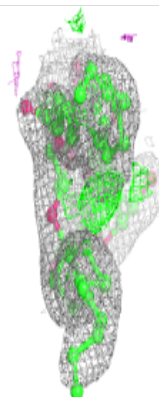
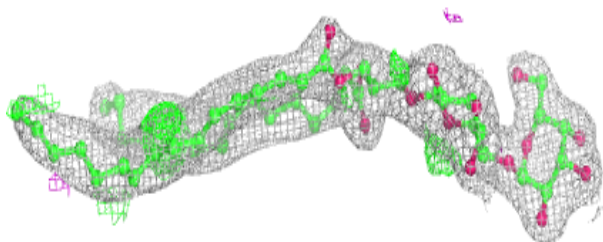
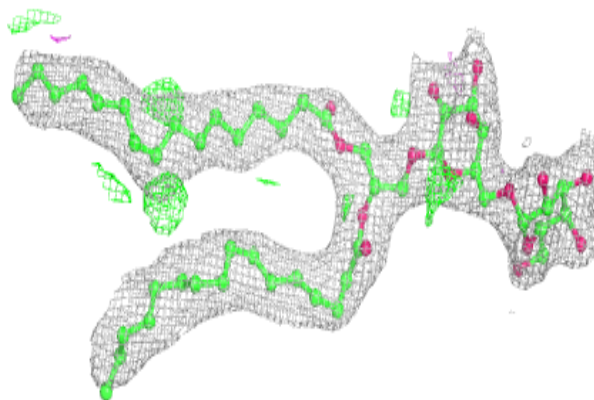


Electron density around DGD C 516:

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

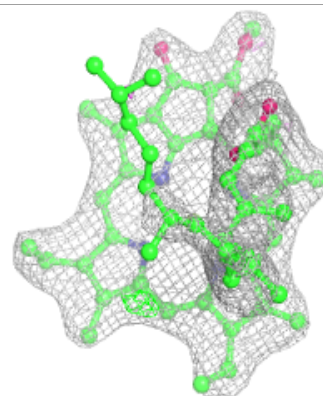
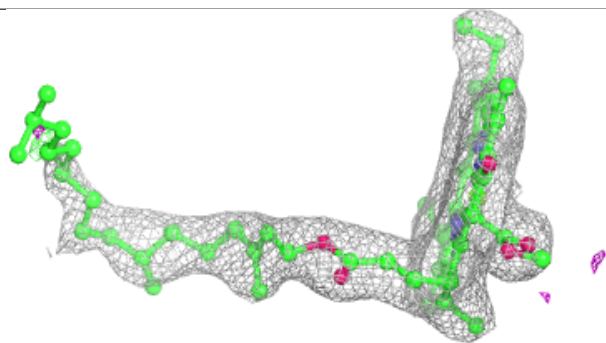
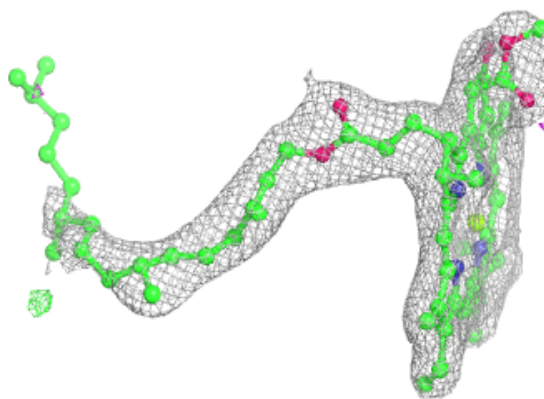
**Electron density around DGD C 517:**

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

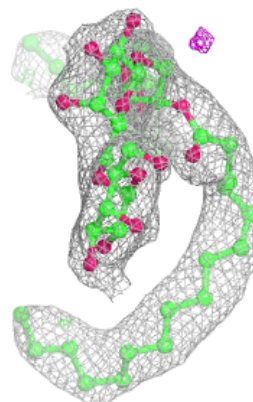
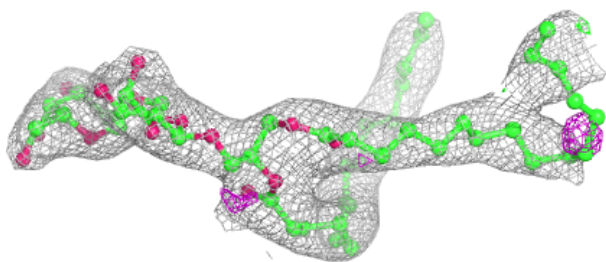
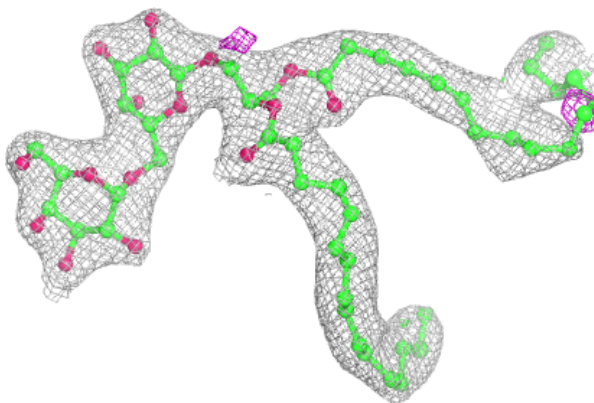


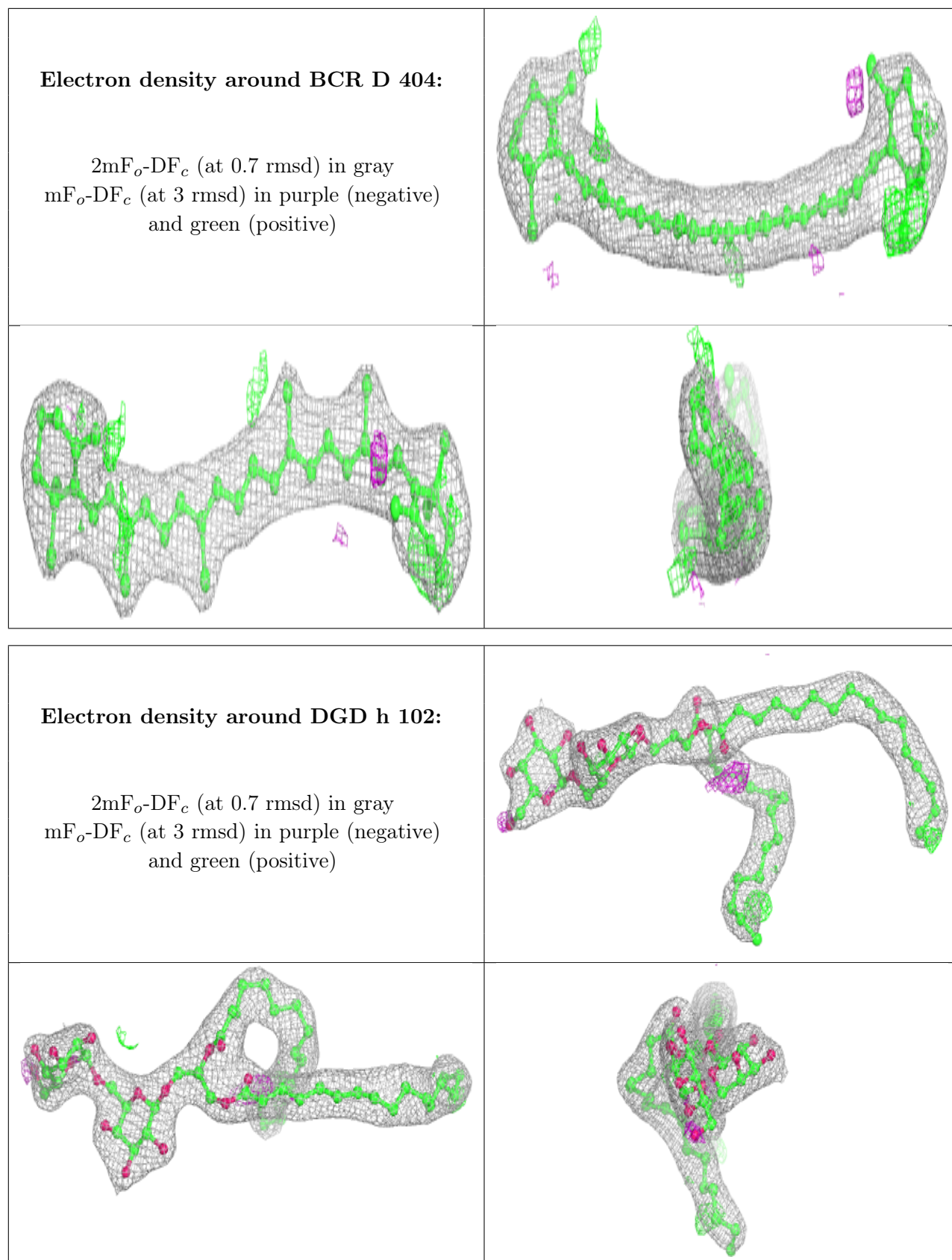
Electron density around CLA D 403:

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

**Electron density around DGD c 518:**

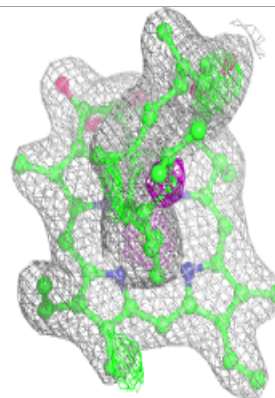
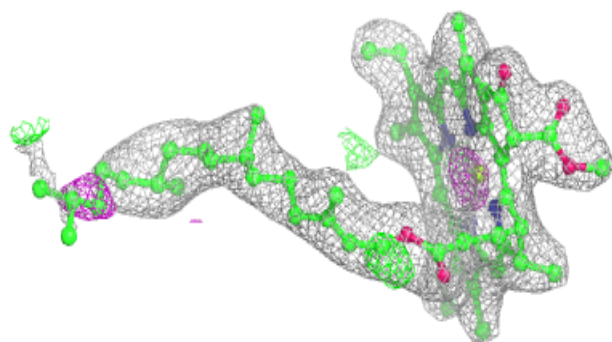
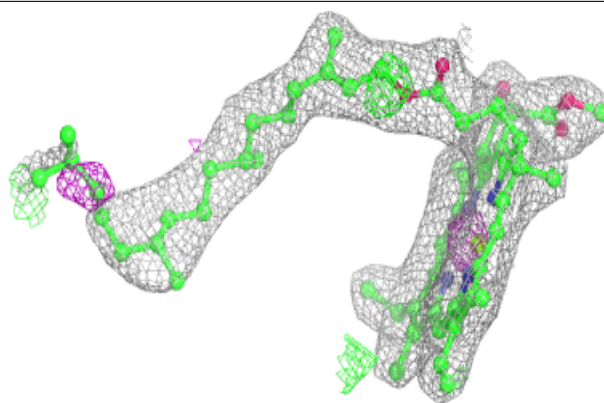
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



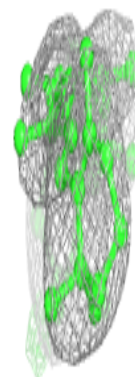
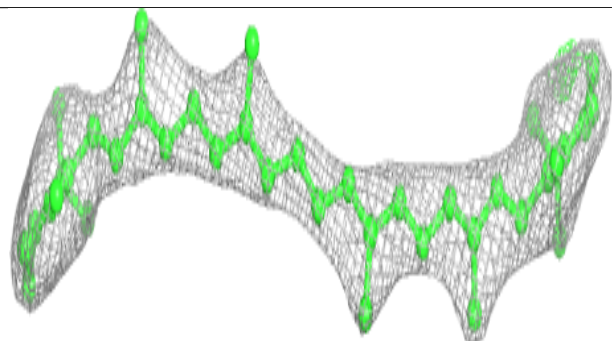
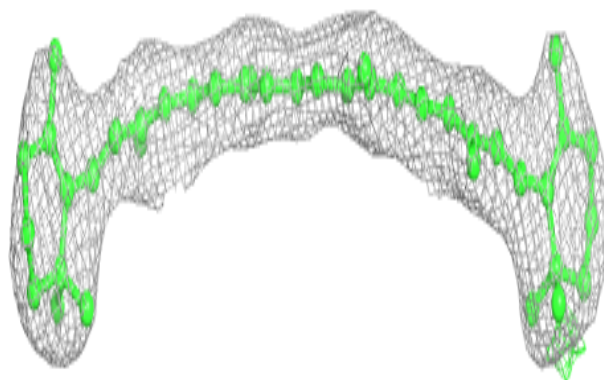


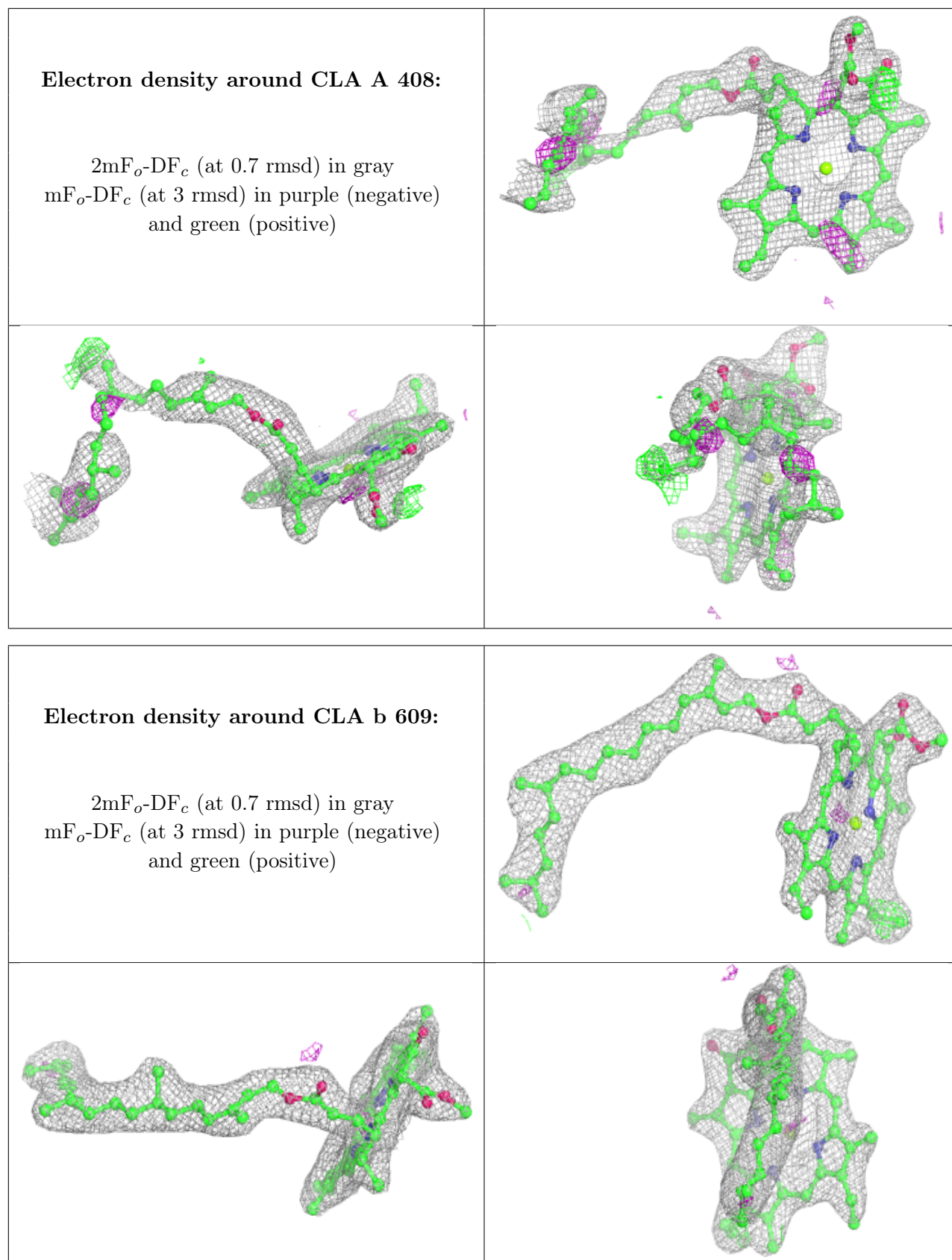
Electron density around CLA C 508:

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

**Electron density around BCR k 101:**

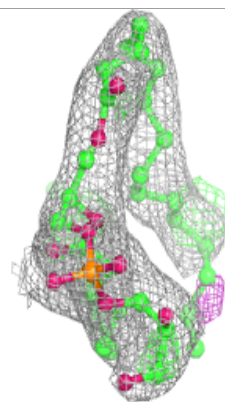
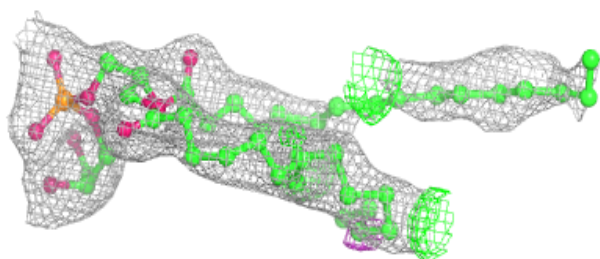
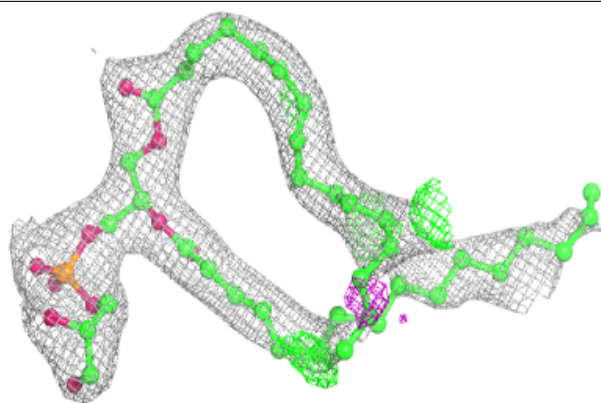
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



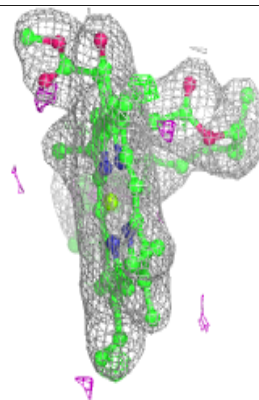
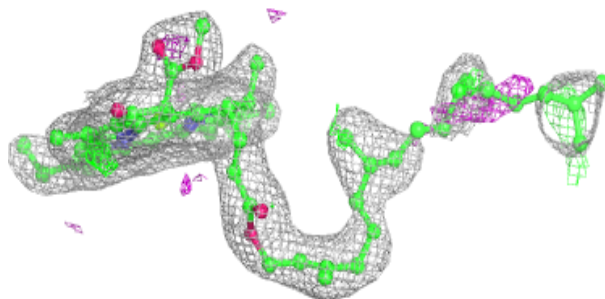
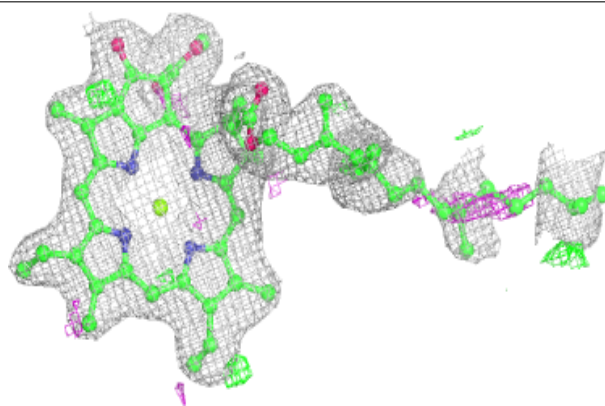


Electron density around LHG d 406:

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

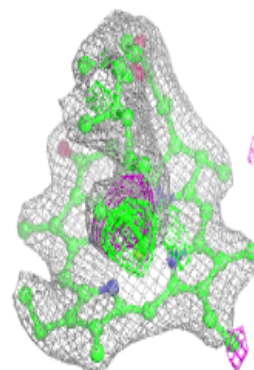
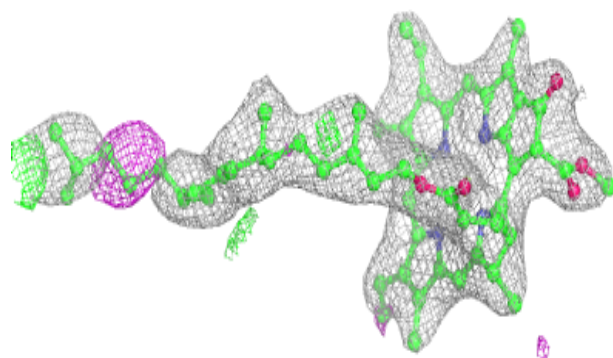
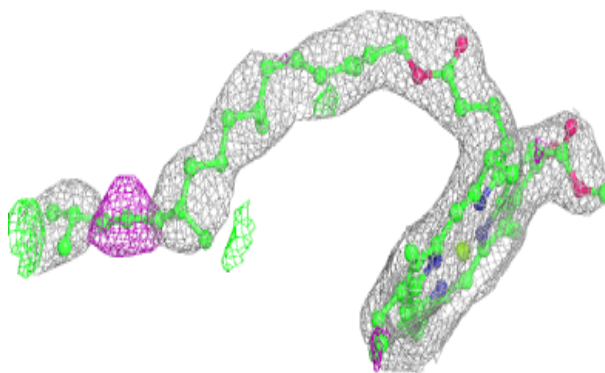
**Electron density around CLA a 407:**

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

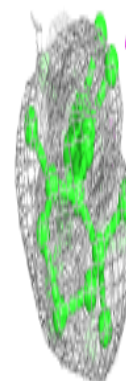
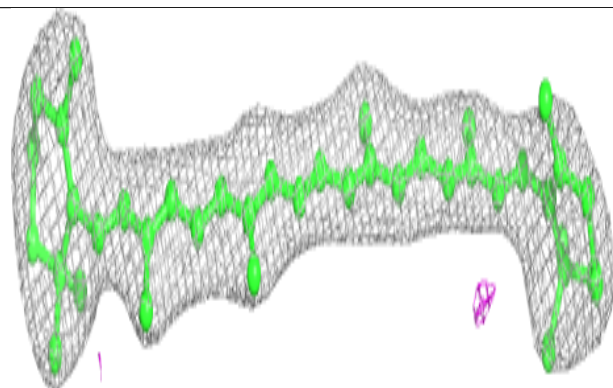
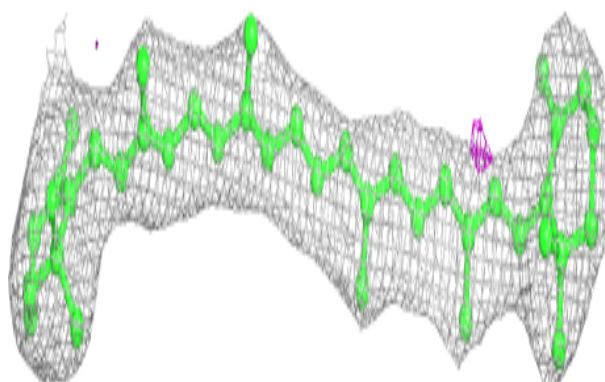


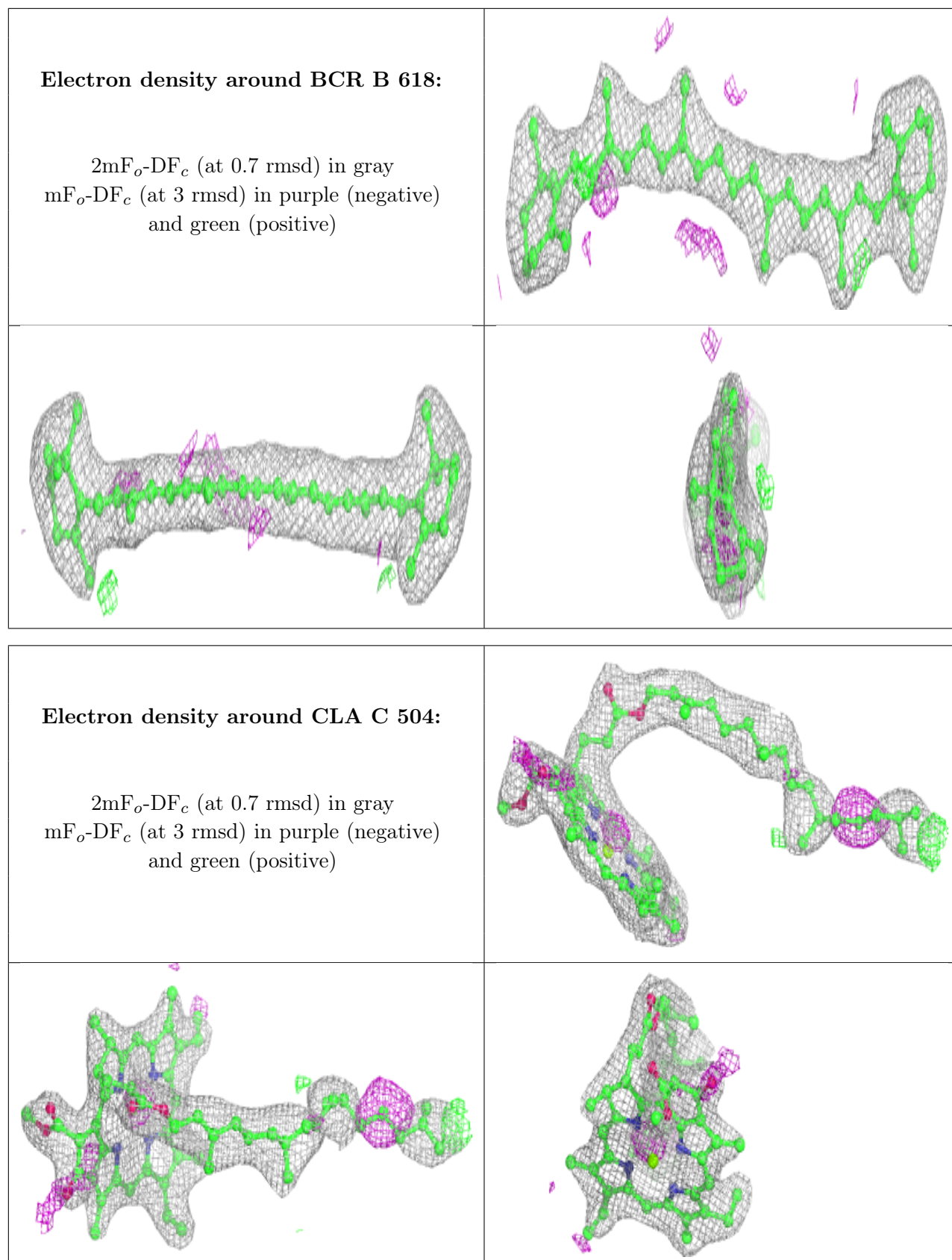
Electron density around CLA c 505:

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

**Electron density around BCR c 515:**

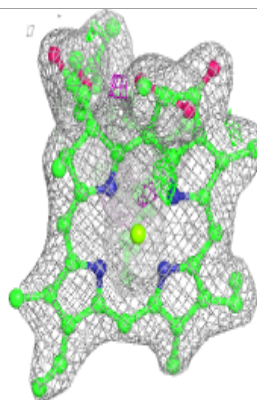
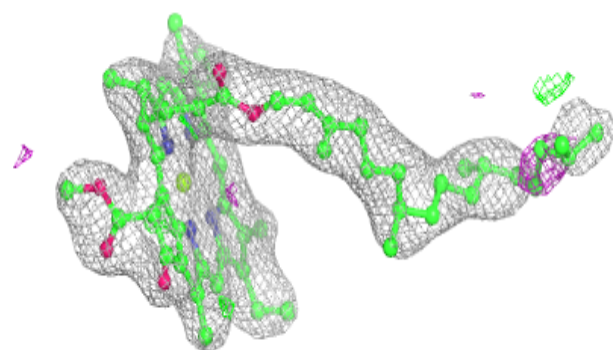
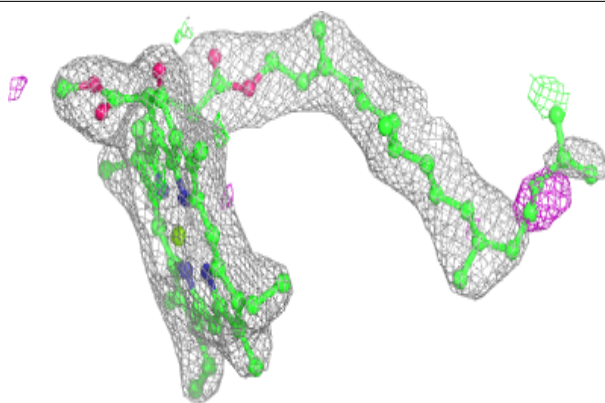
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



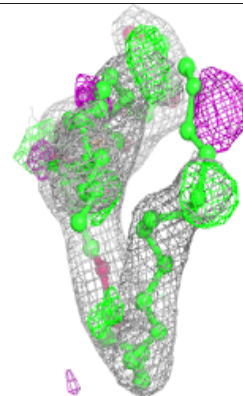
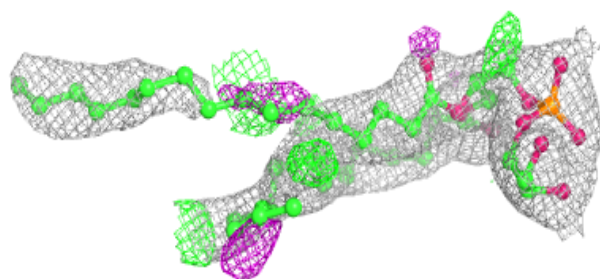
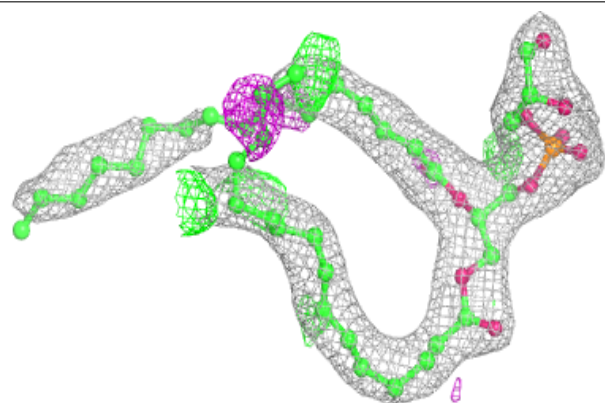


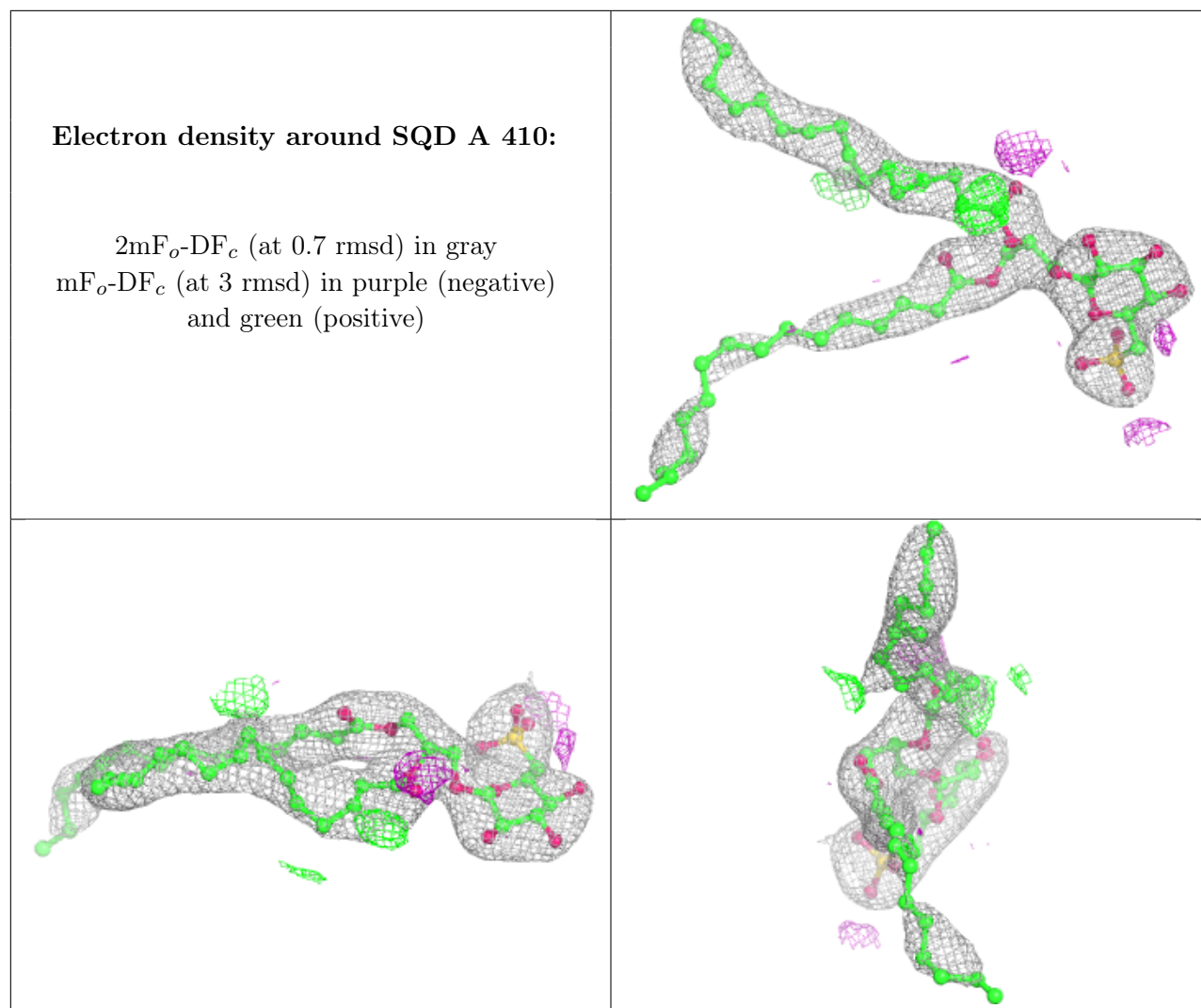
Electron density around CLA c 509:

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

**Electron density around LHG D 407:**

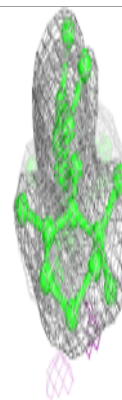
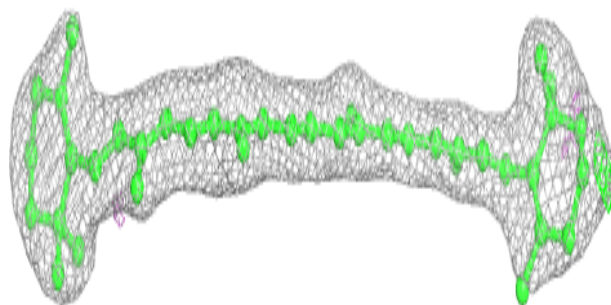
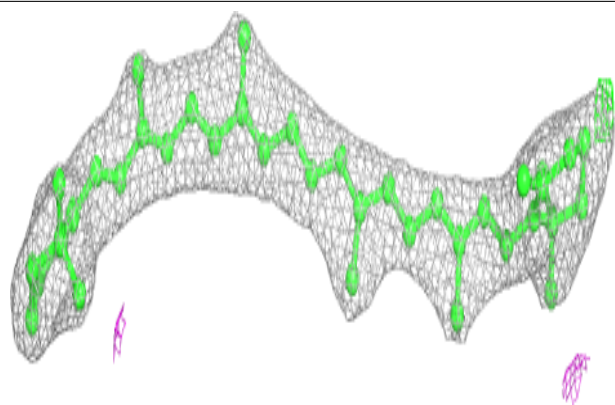
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



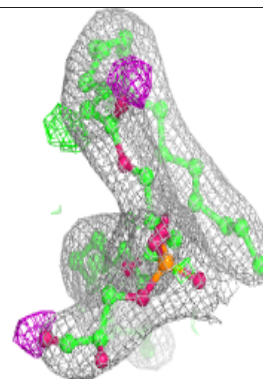
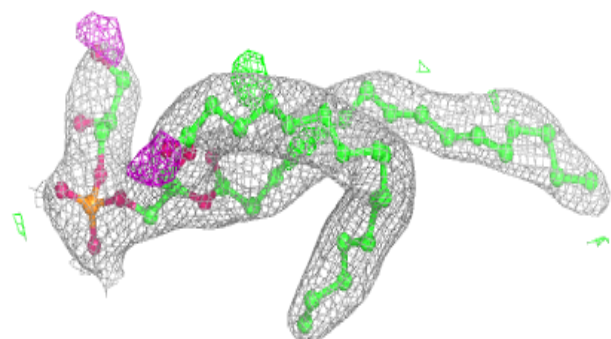
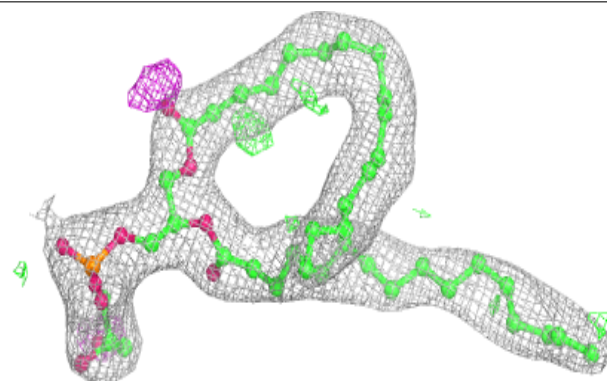


Electron density around BCR H 101:

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

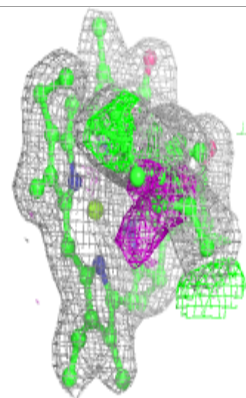
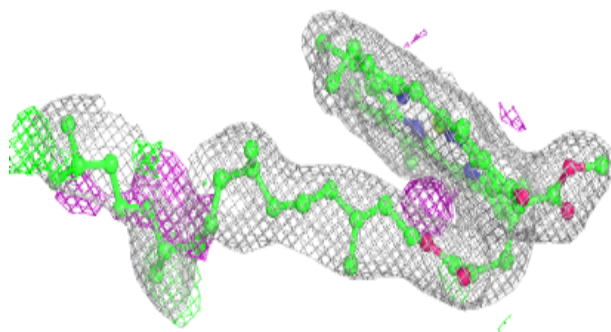
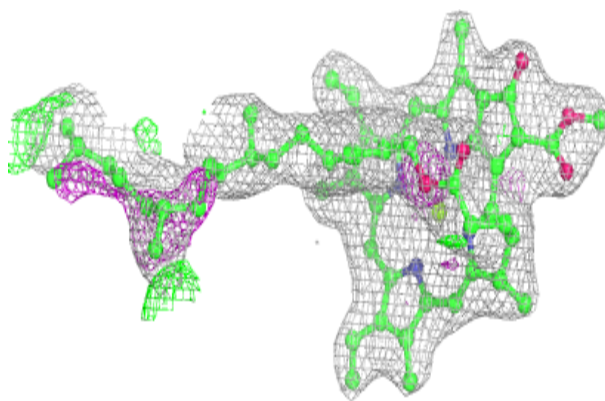
**Electron density around LHG A 420:**

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

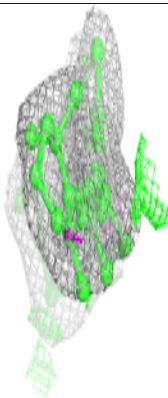
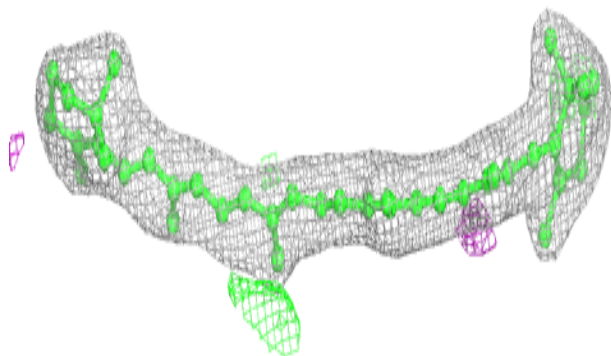
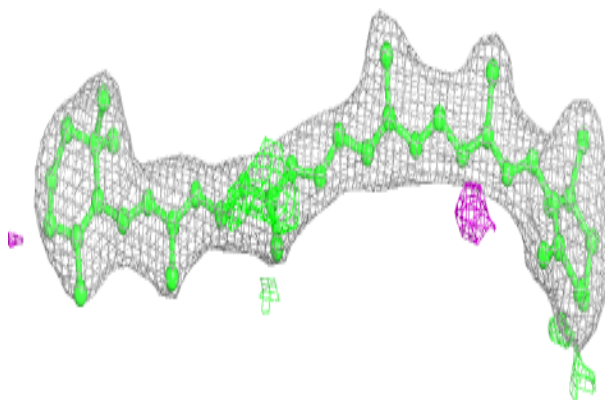


Electron density around CLA B 614:

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

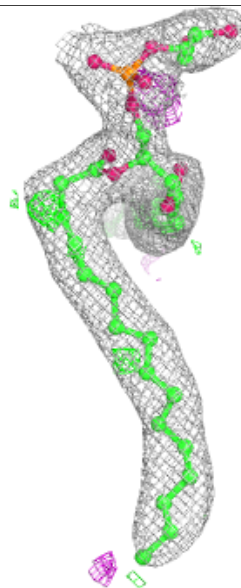
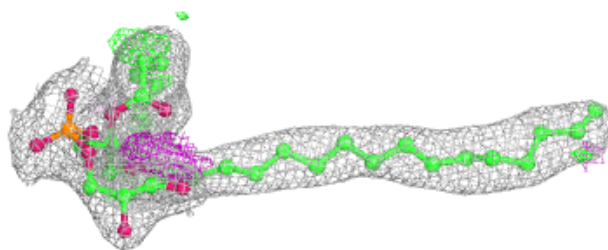
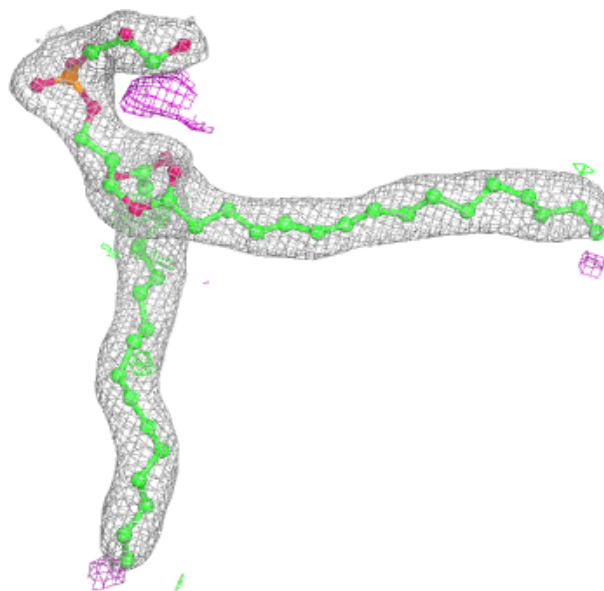
**Electron density around BCR t 102:**

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



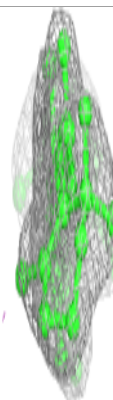
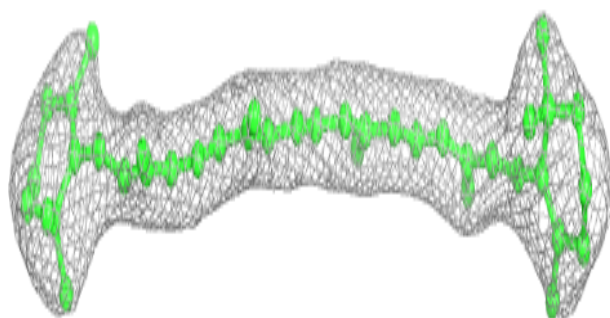
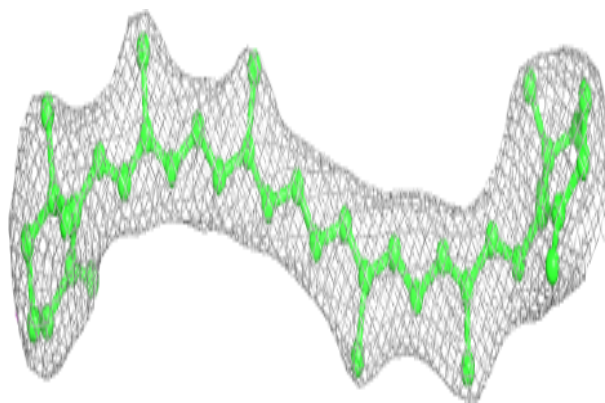
Electron density around LHG b 630:

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

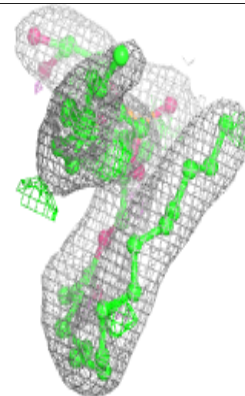
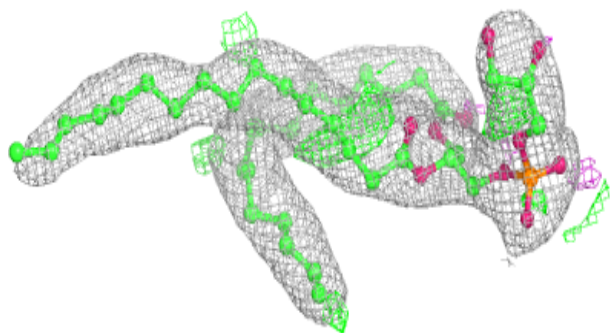
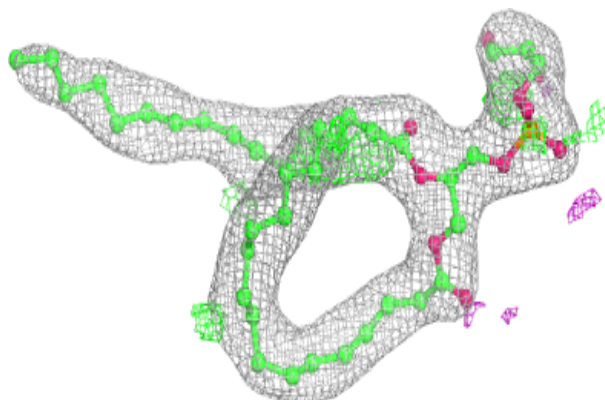


Electron density around BCR y 101:

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

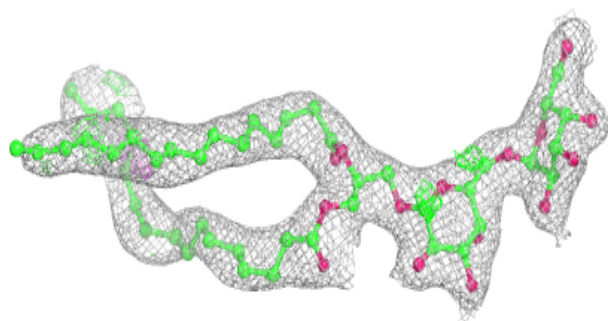
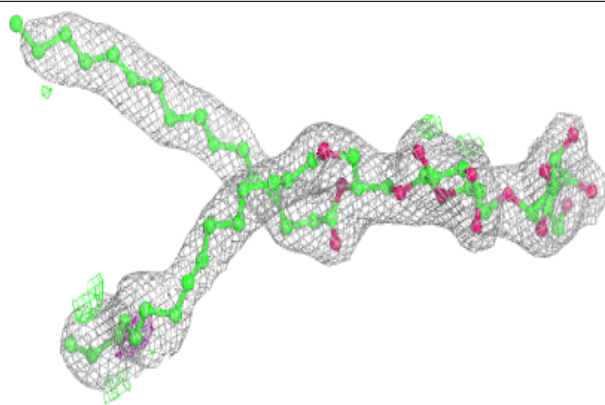
**Electron density around LHG d 411:**

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

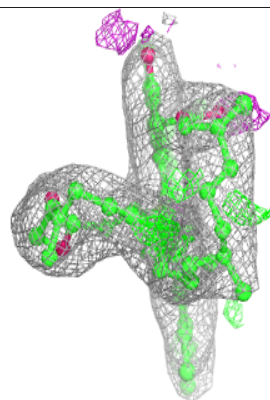
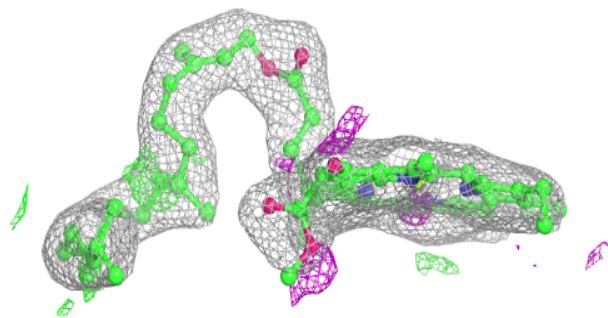
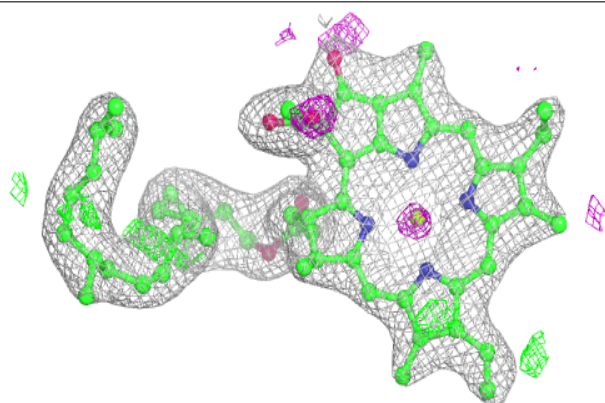


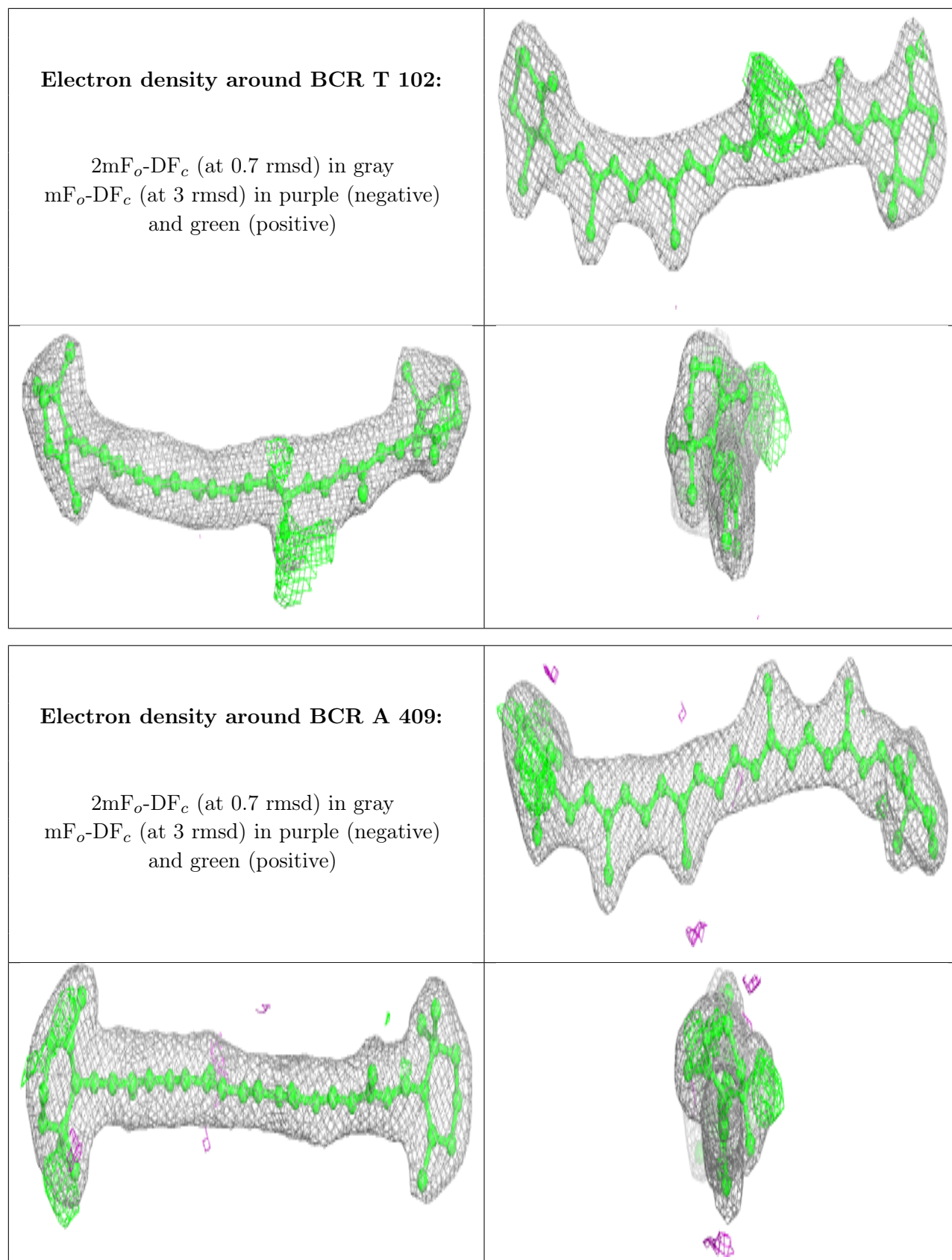
Electron density around DGD c 517:

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

**Electron density around CLA b 612:**

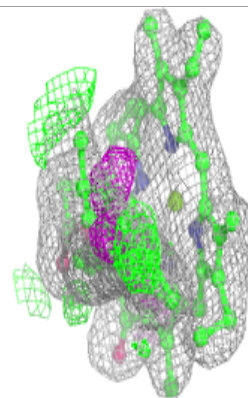
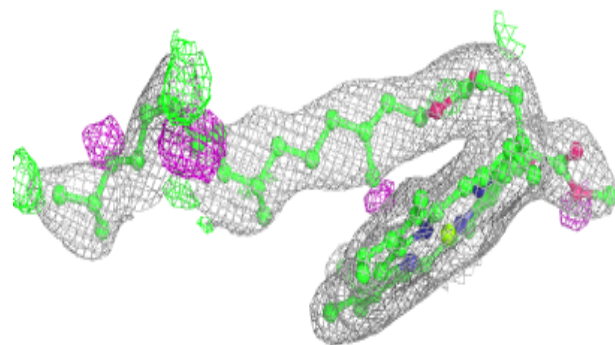
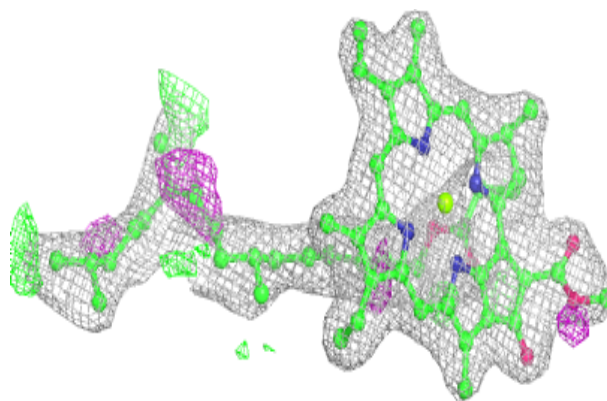
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



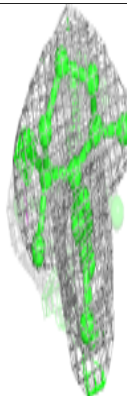
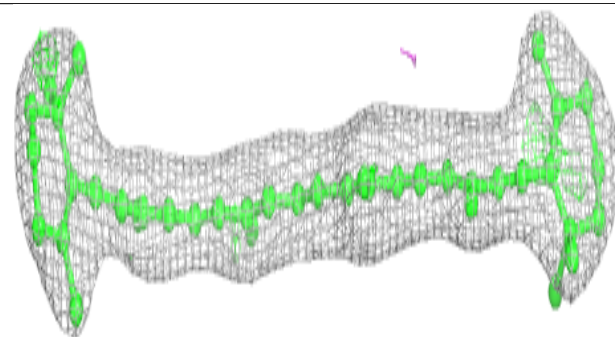
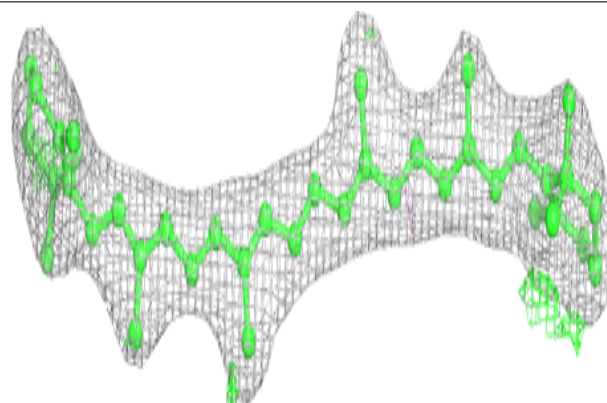


Electron density around CLA b 614:

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

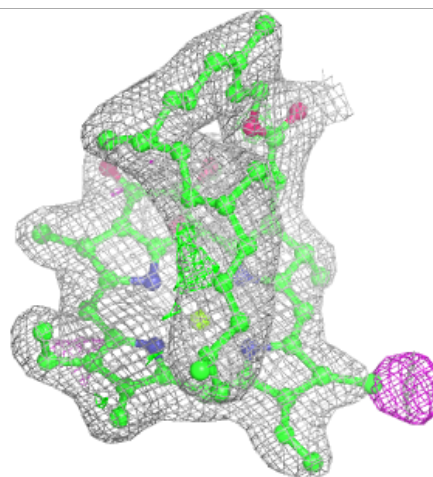
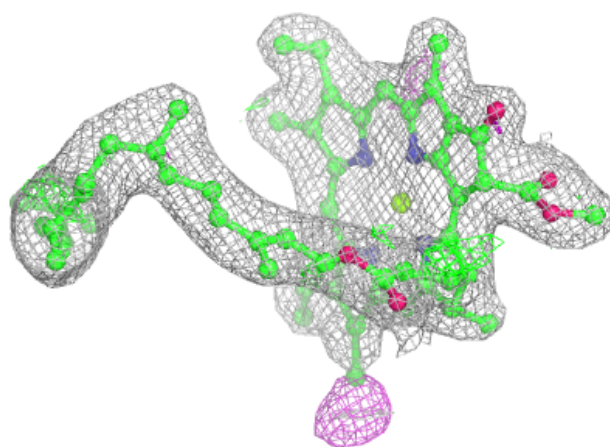
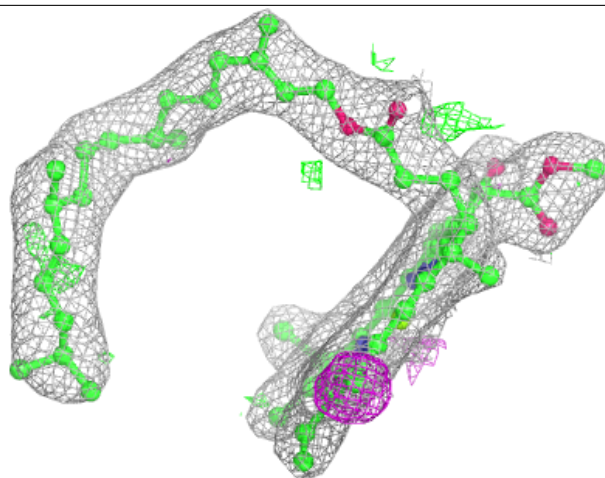
**Electron density around BCR C 514:**

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



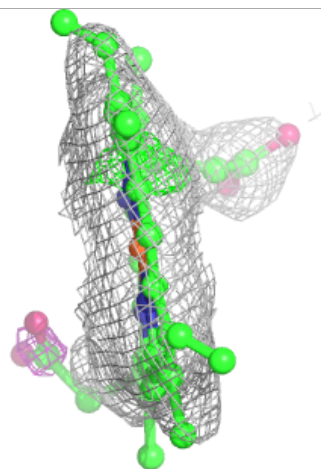
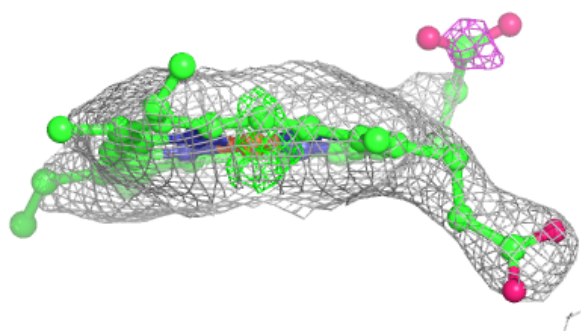
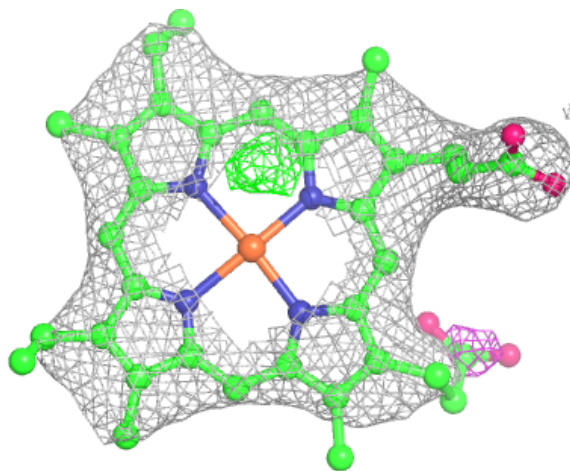
Electron density around CLA B 611:

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



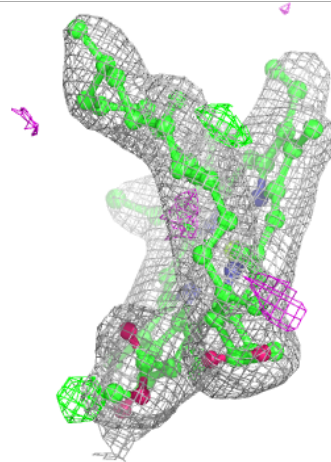
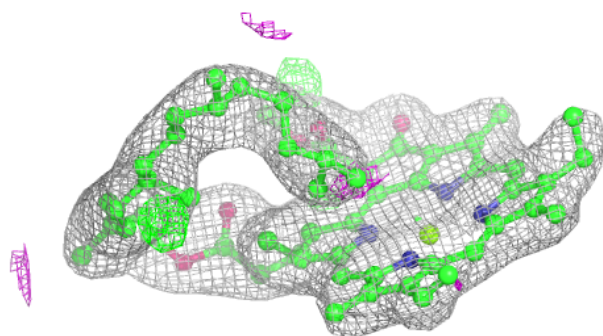
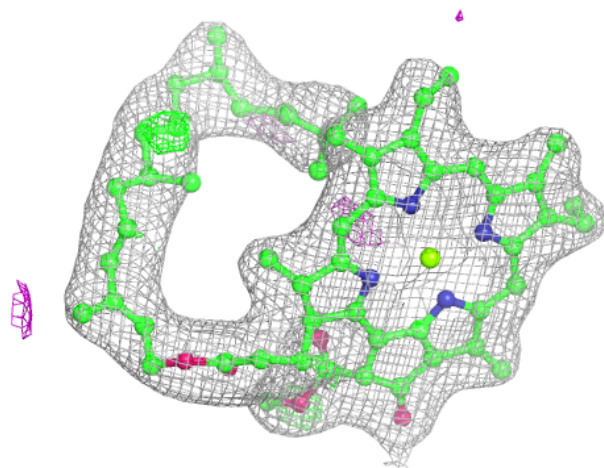
Electron density around HEM f 101:

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



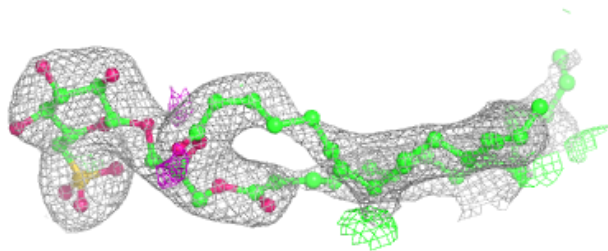
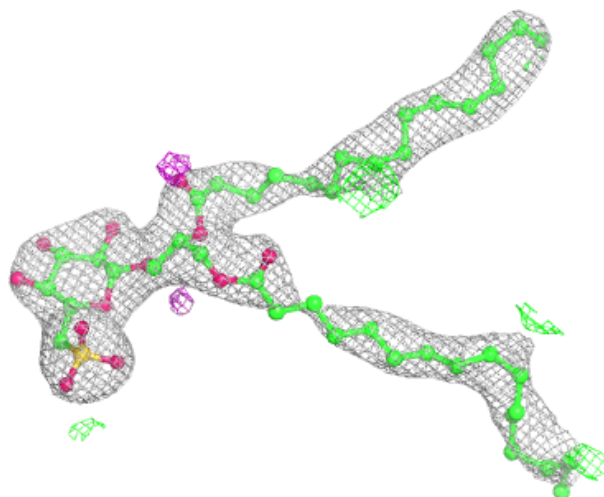
Electron density around CLA b 615:

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



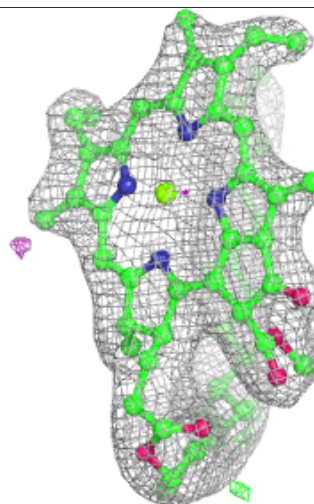
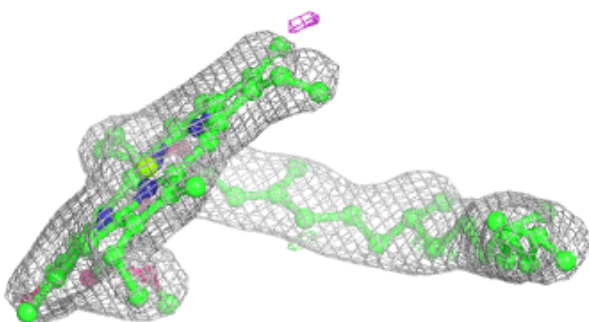
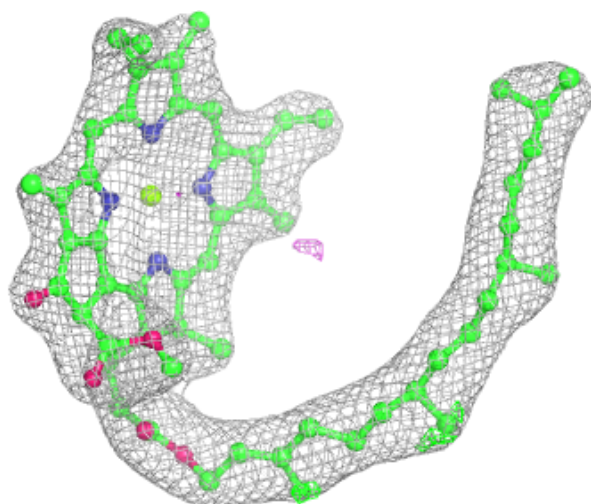
Electron density around SQD a 411:

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



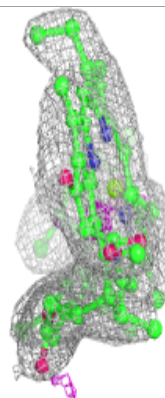
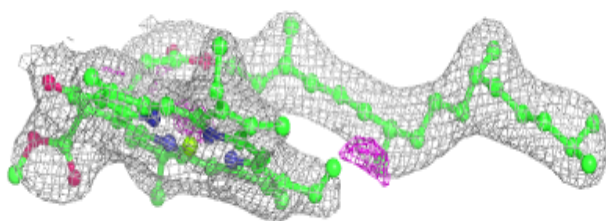
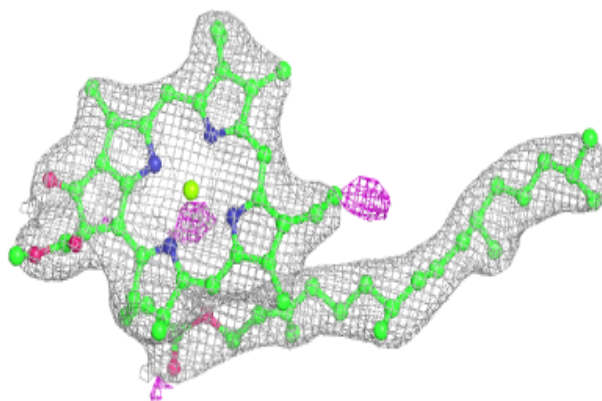
Electron density around CLA C 507:

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

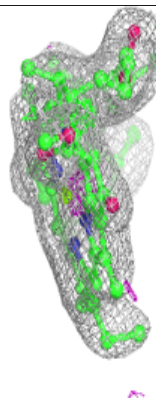
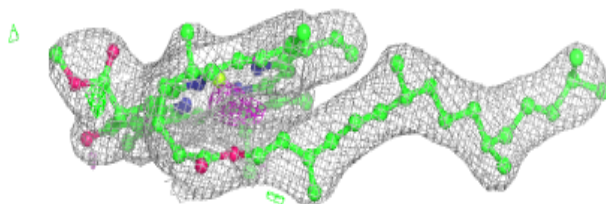
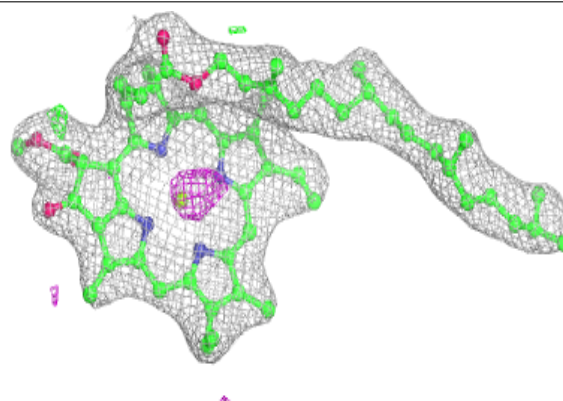


Electron density around CLA c 502:

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

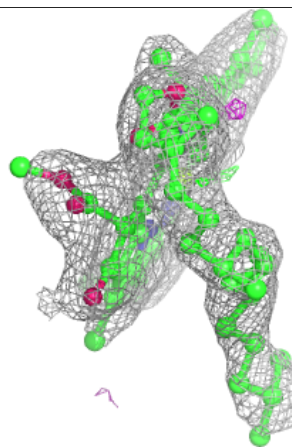
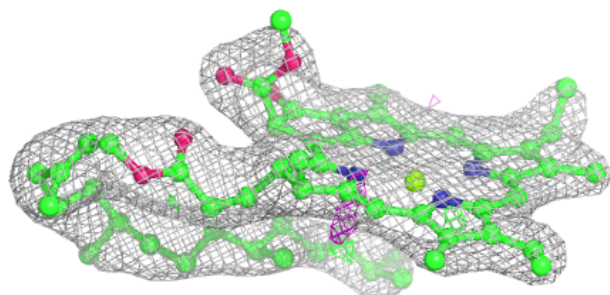
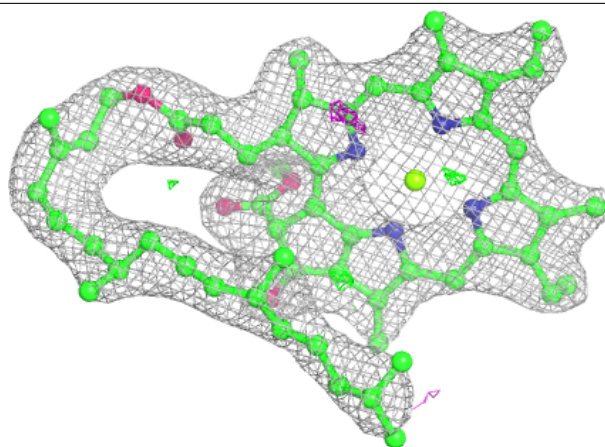
**Electron density around CLA C 501:**

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



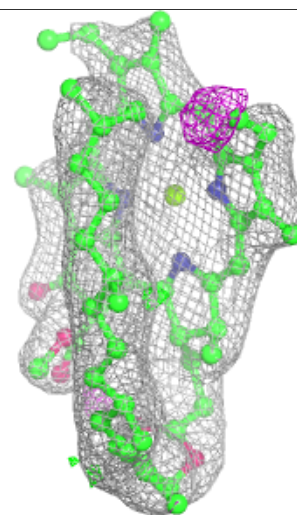
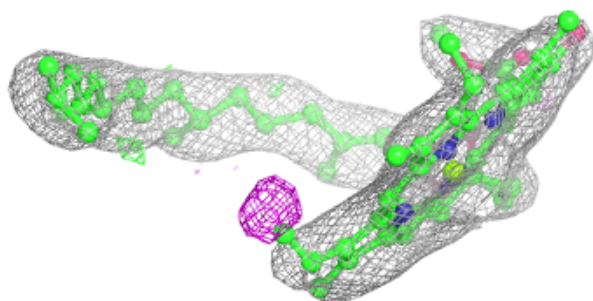
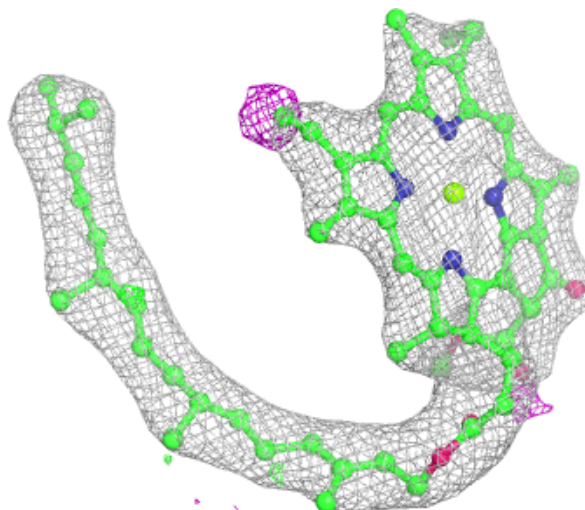
Electron density around CLA C 509:

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



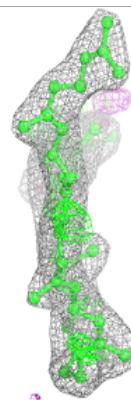
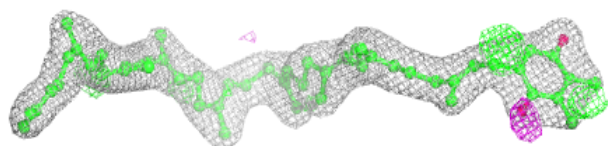
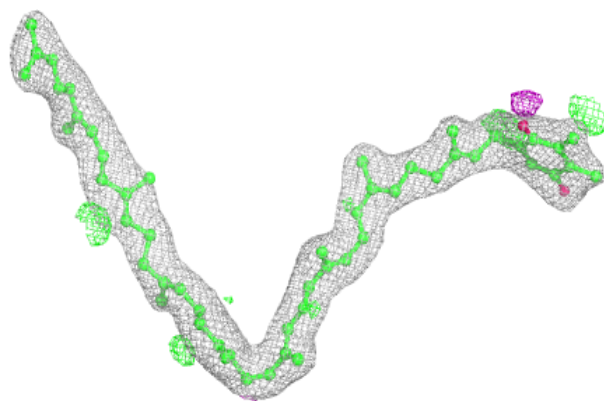
Electron density around CLA c 508:

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

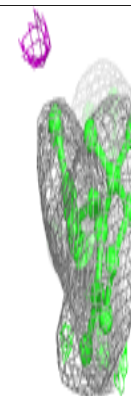
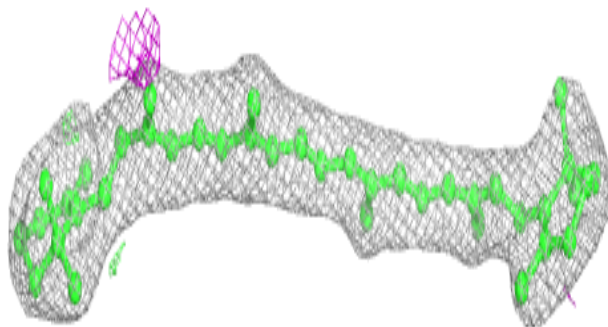
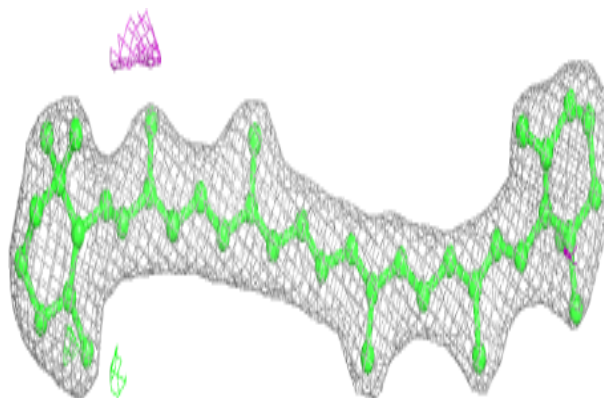


Electron density around PL9 D 405:

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

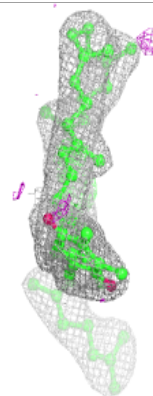
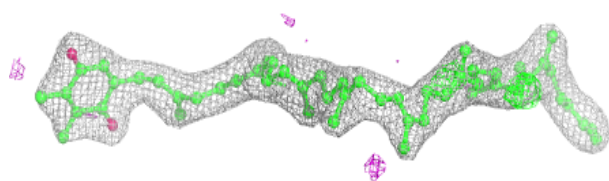
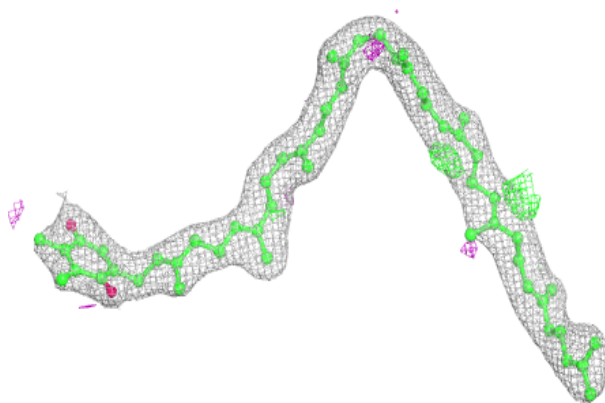
**Electron density around BCR b 619:**

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

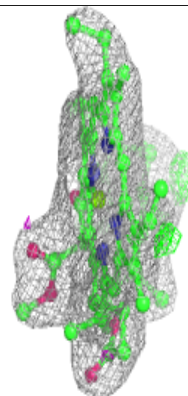
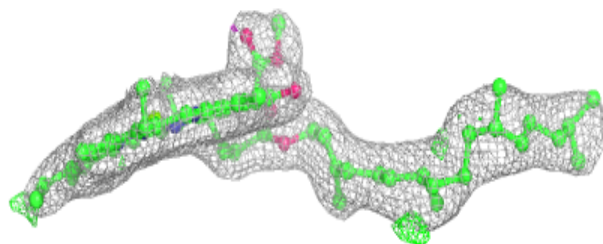
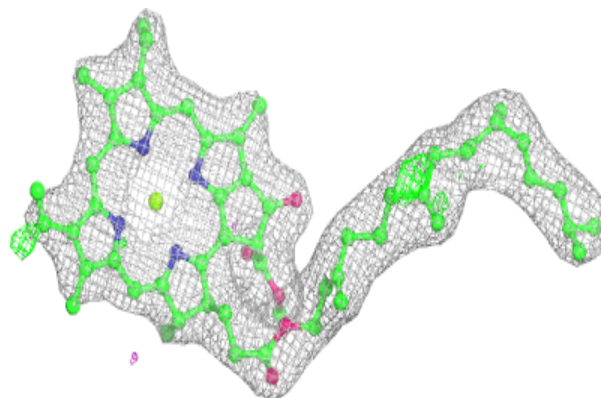


Electron density around PL9 d 404:

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

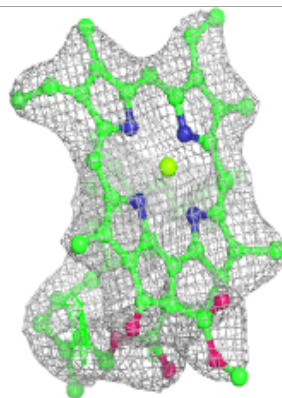
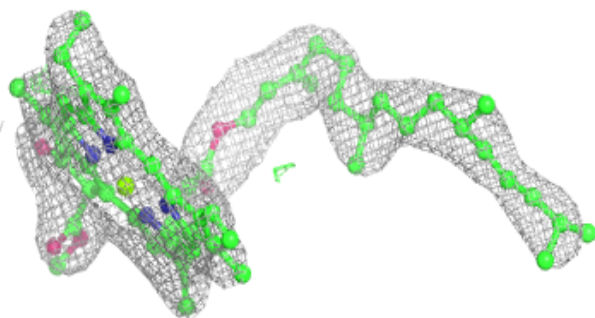
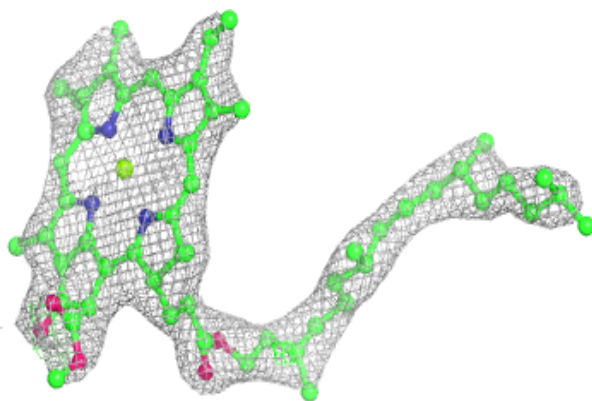
**Electron density around CLA b 602:**

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

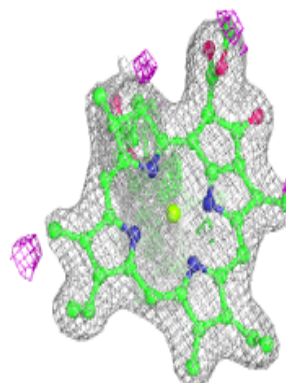
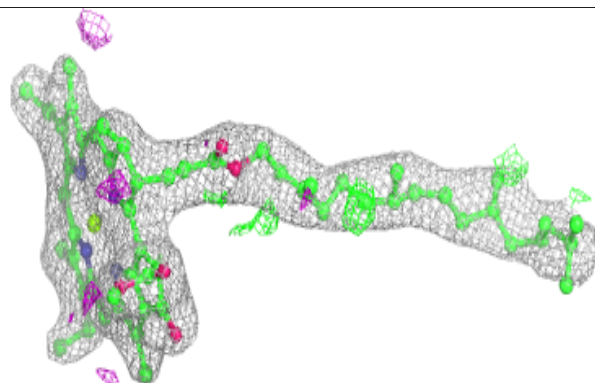
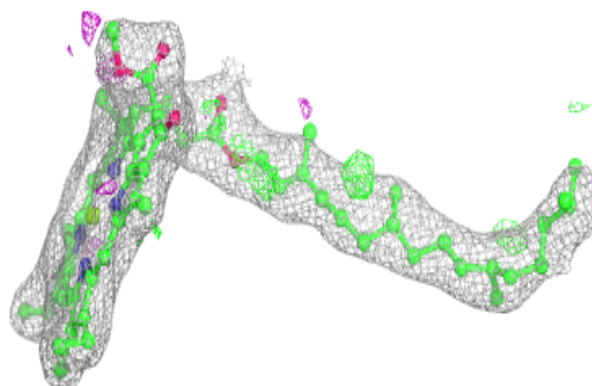


Electron density around CLA c 512:

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

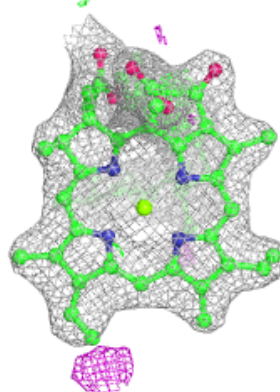
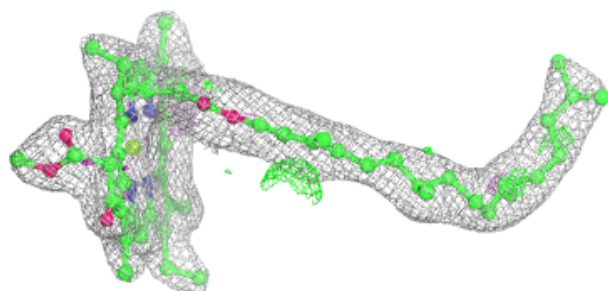
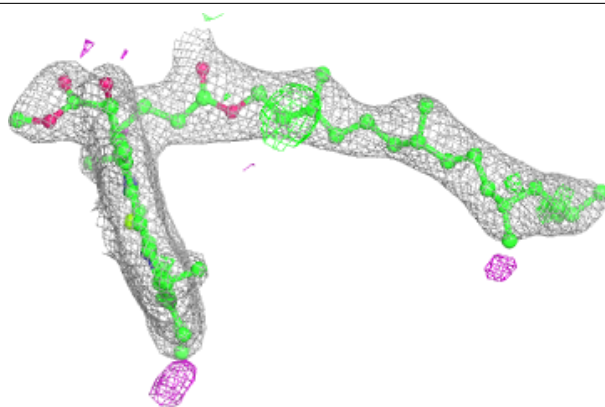
**Electron density around CLA b 604:**

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

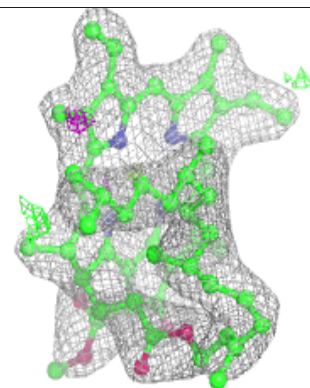
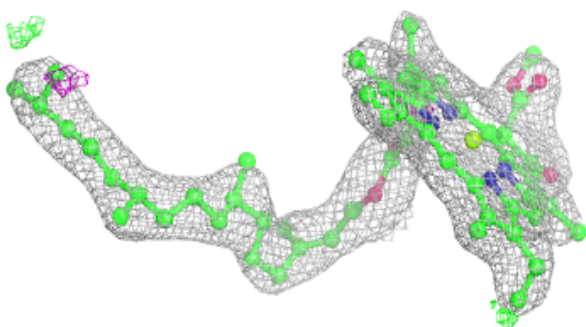
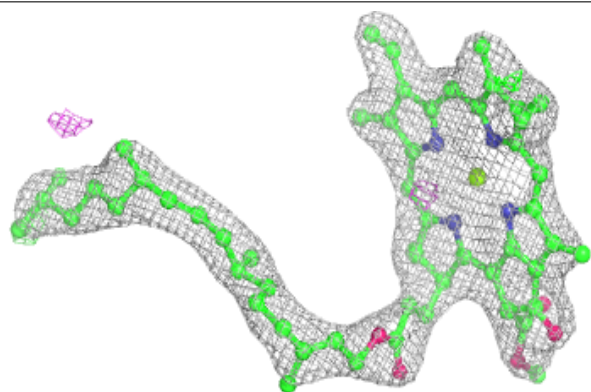


Electron density around CLA b 605:

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

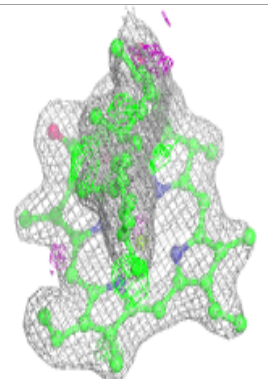
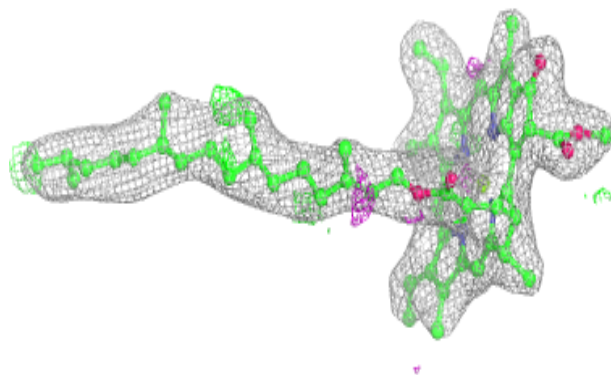
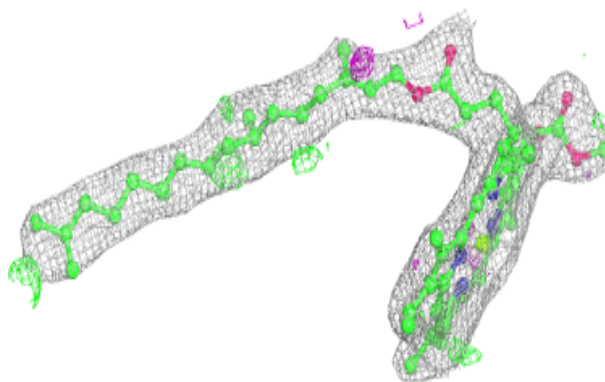
**Electron density around CLA C 511:**

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



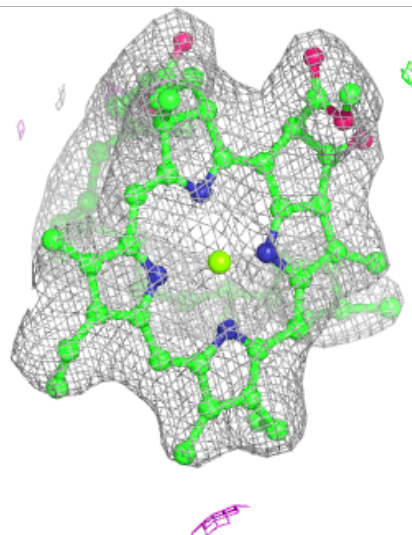
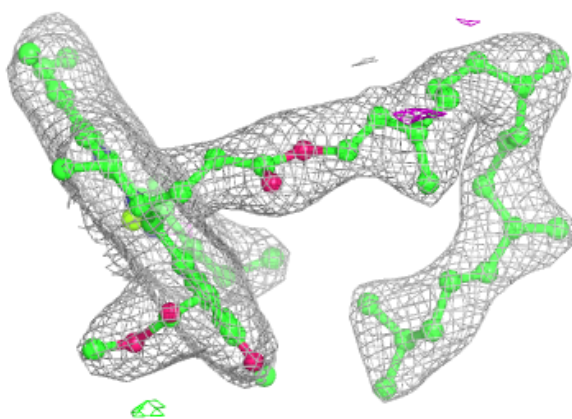
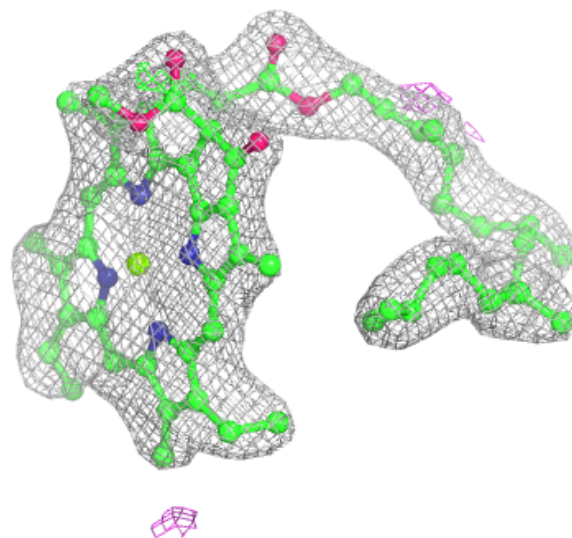
Electron density around CLA b 607:

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



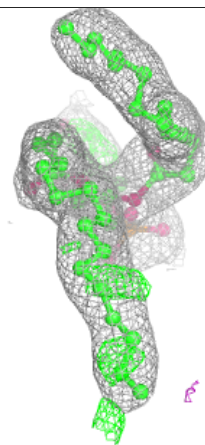
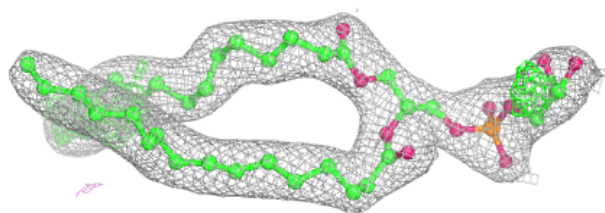
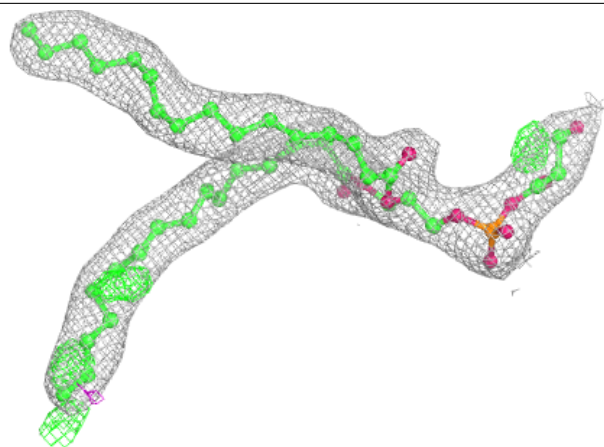
Electron density around CLA C 503:

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



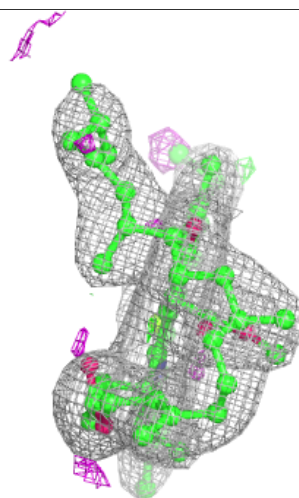
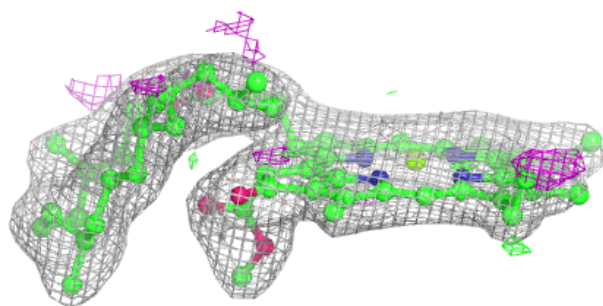
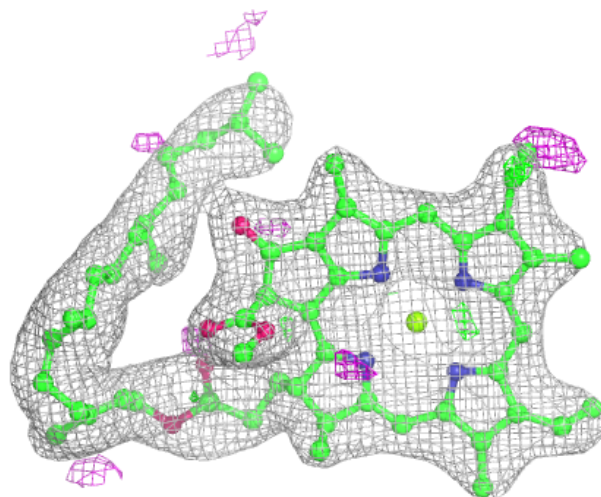
Electron density around LHG d 405:

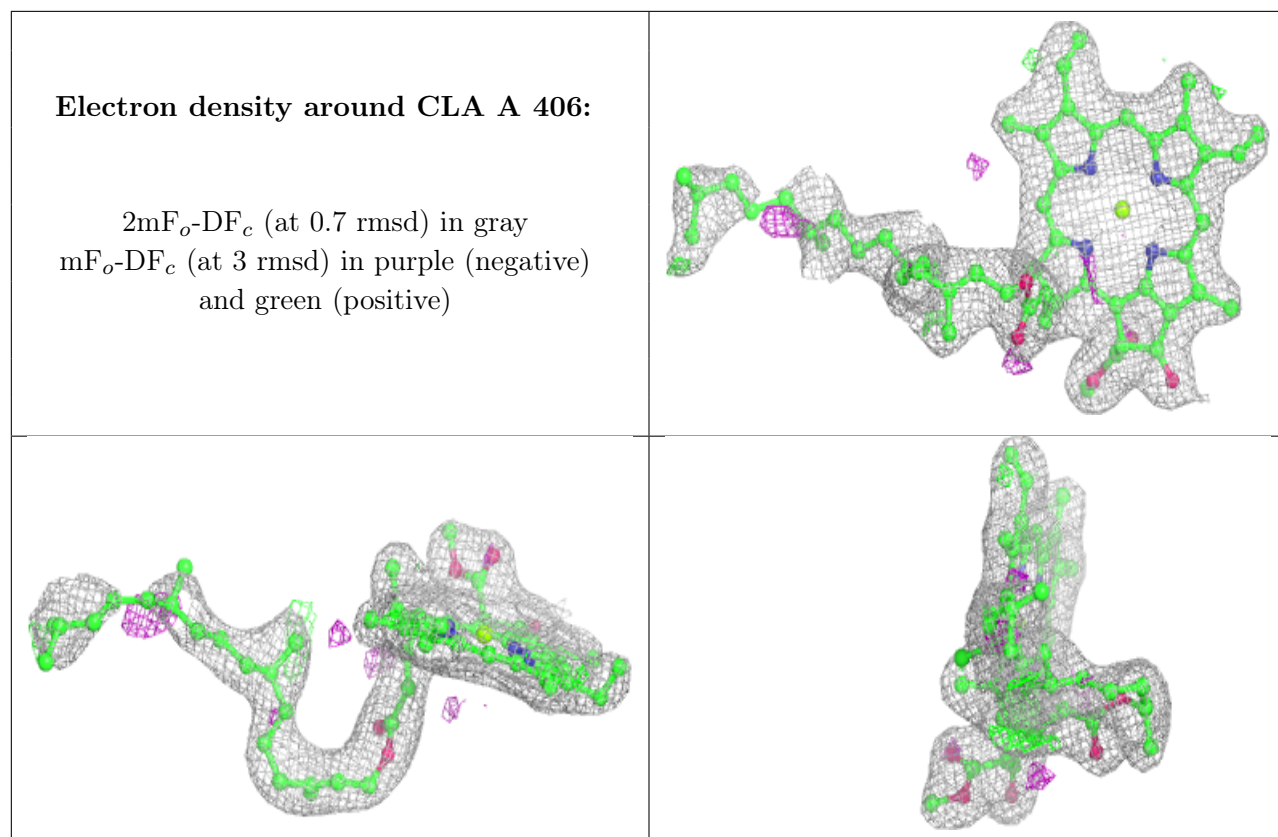
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 610:

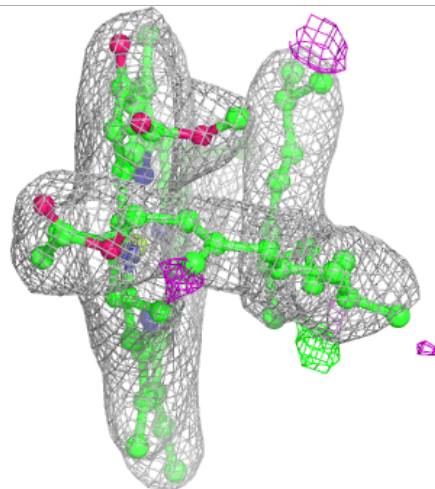
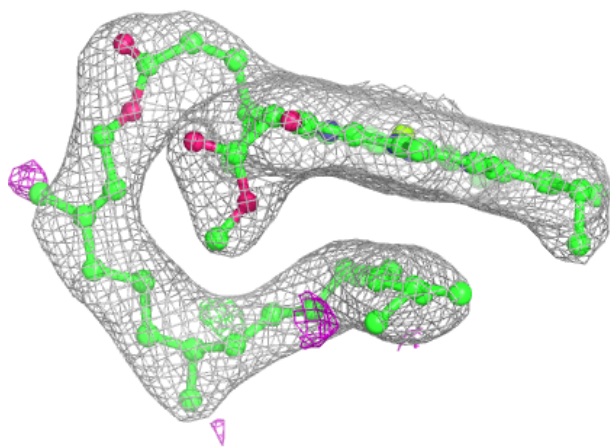
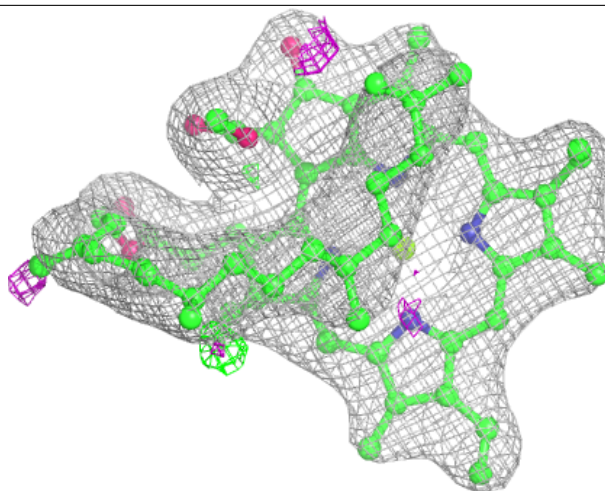
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





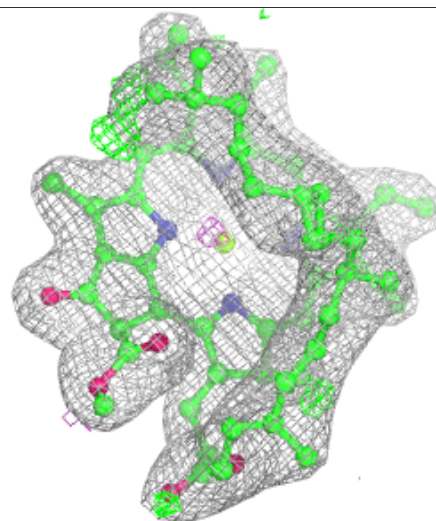
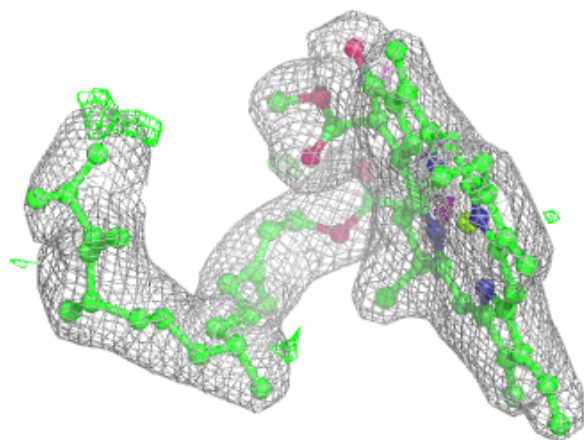
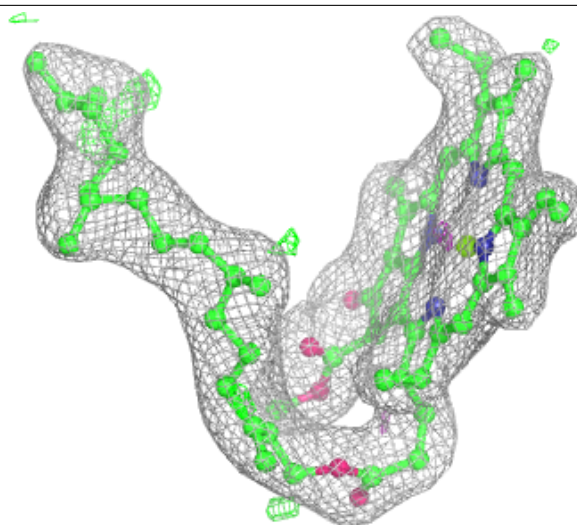
Electron density around CLA c 511:

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



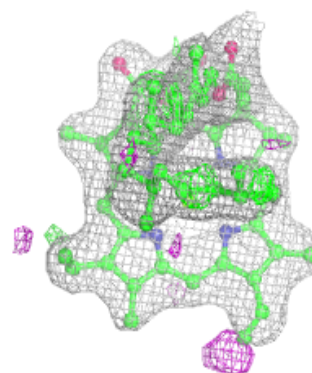
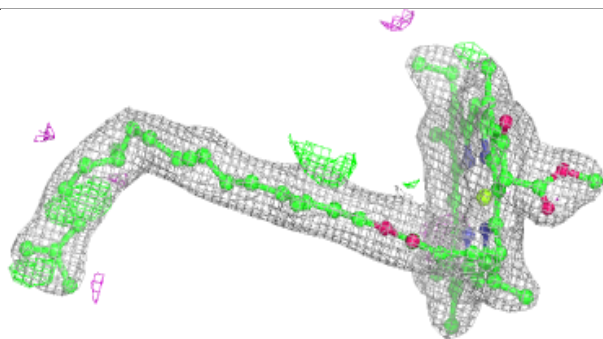
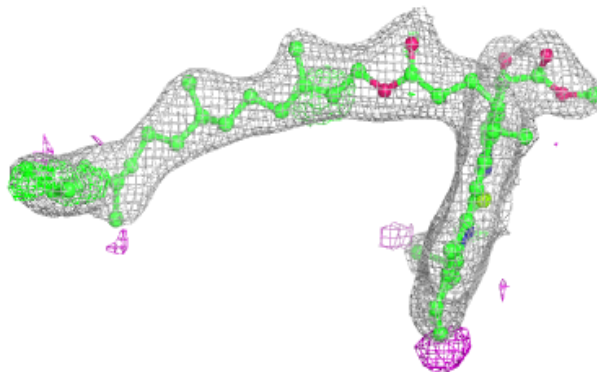
Electron density around CLA B 613:

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

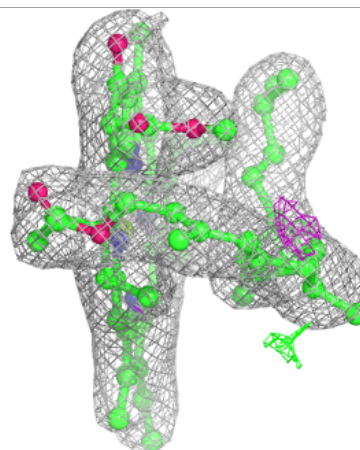
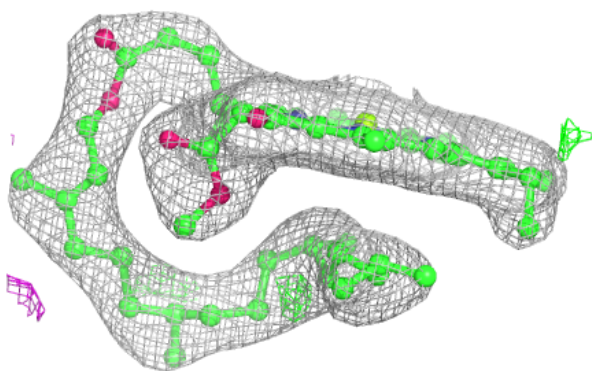
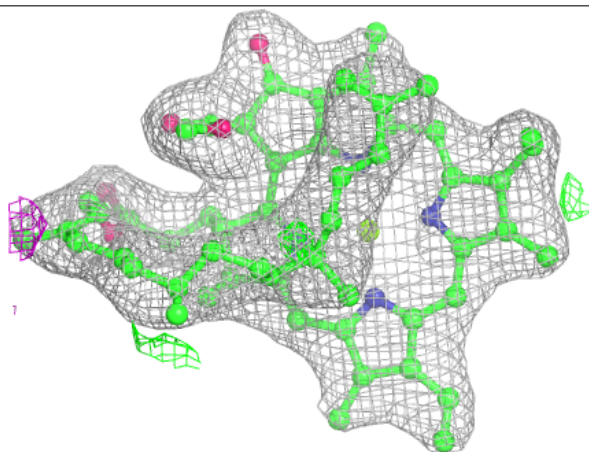


Electron density around CLA B 605:

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

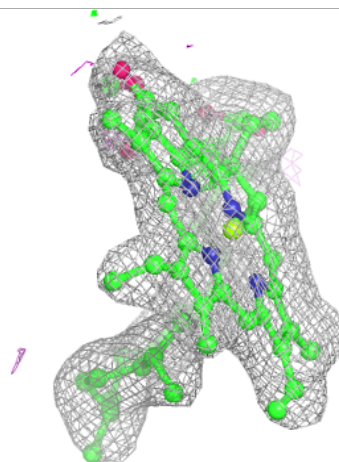
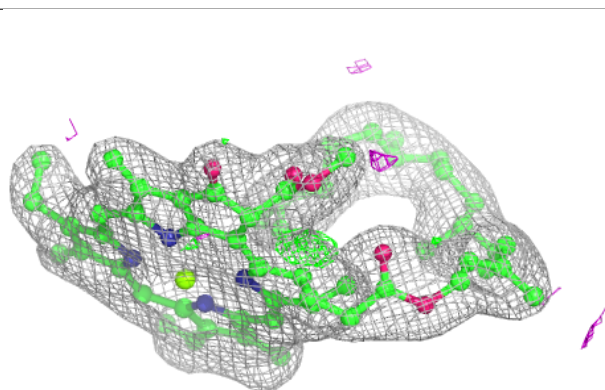
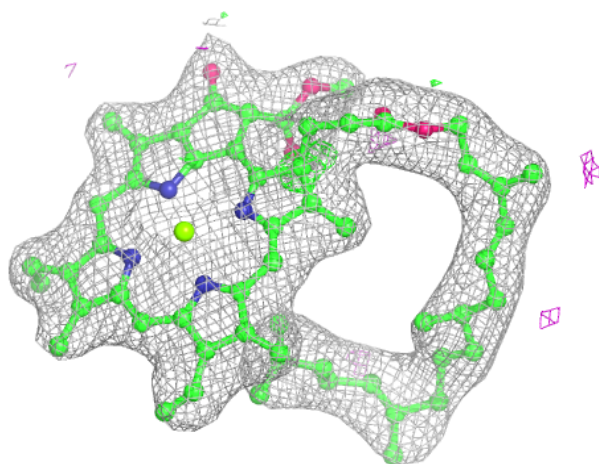
**Electron density around CLA C 510:**

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



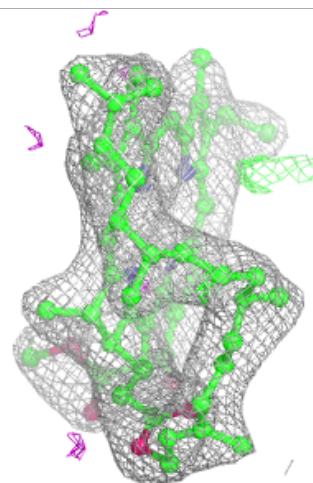
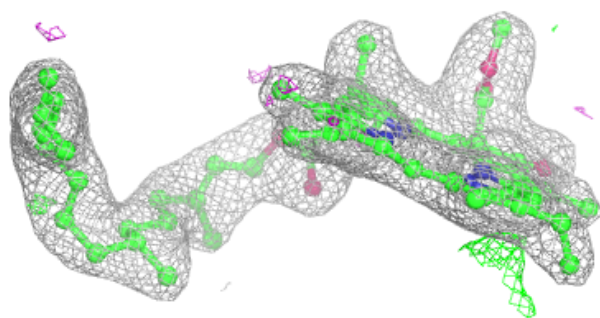
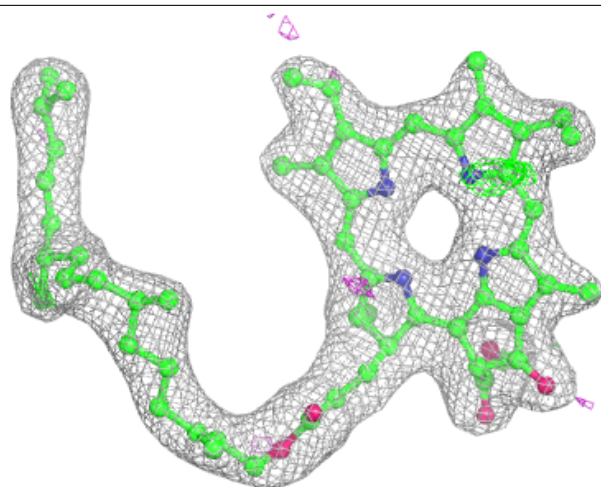
Electron density around CLA B 615:

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



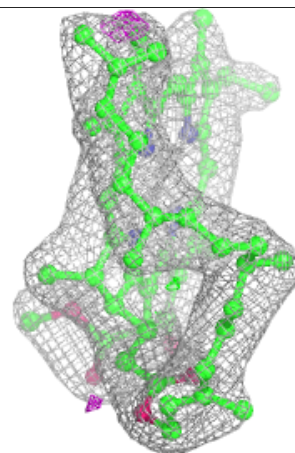
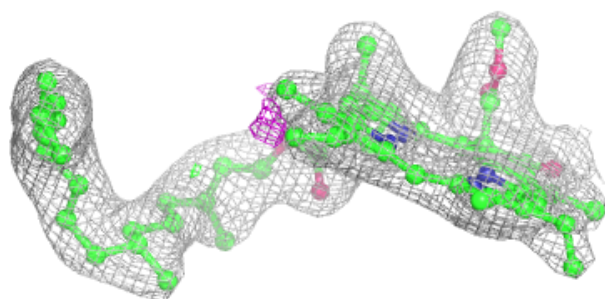
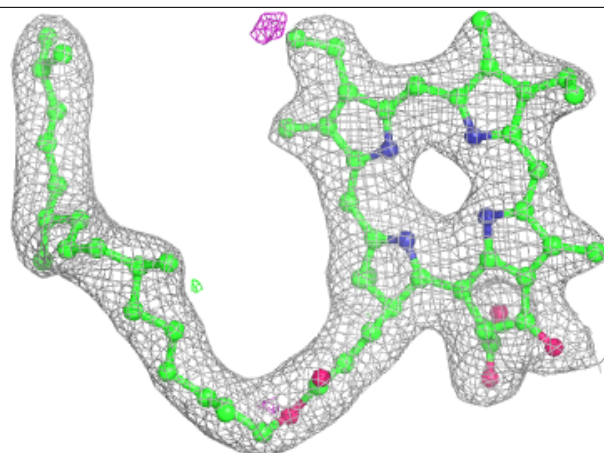
Electron density around PHO A 416:

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

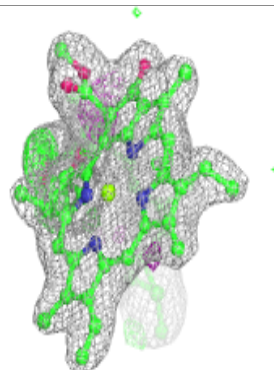
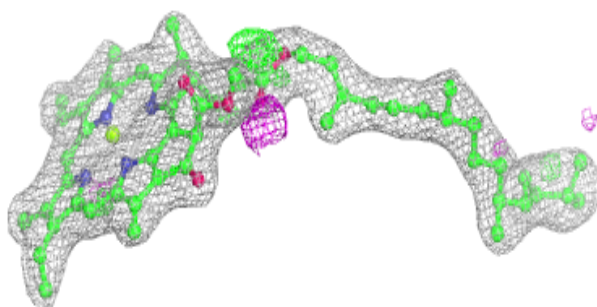
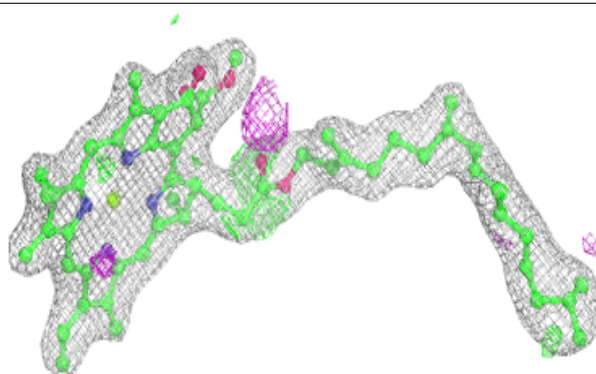


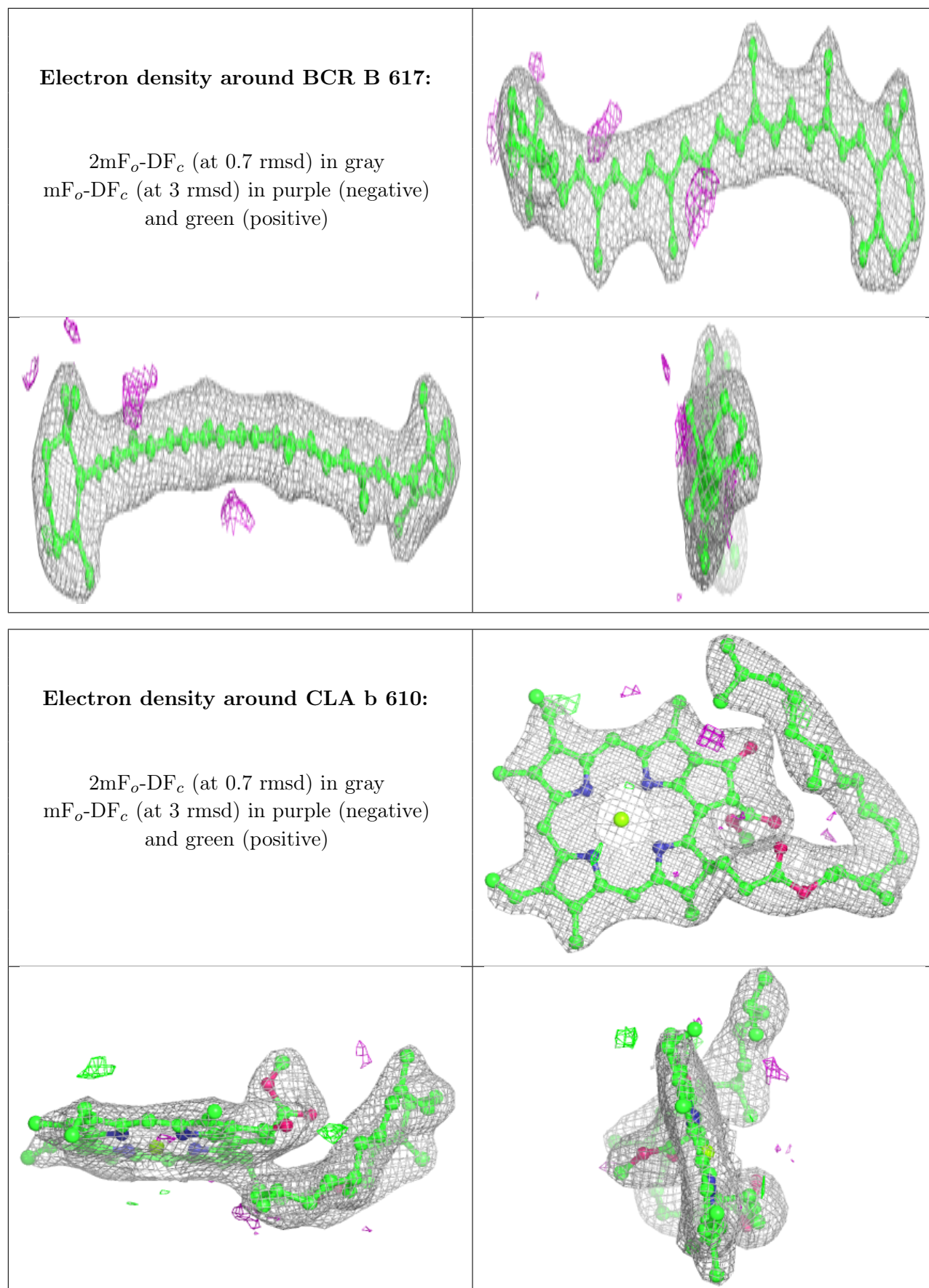
Electron density around PHO a 417:

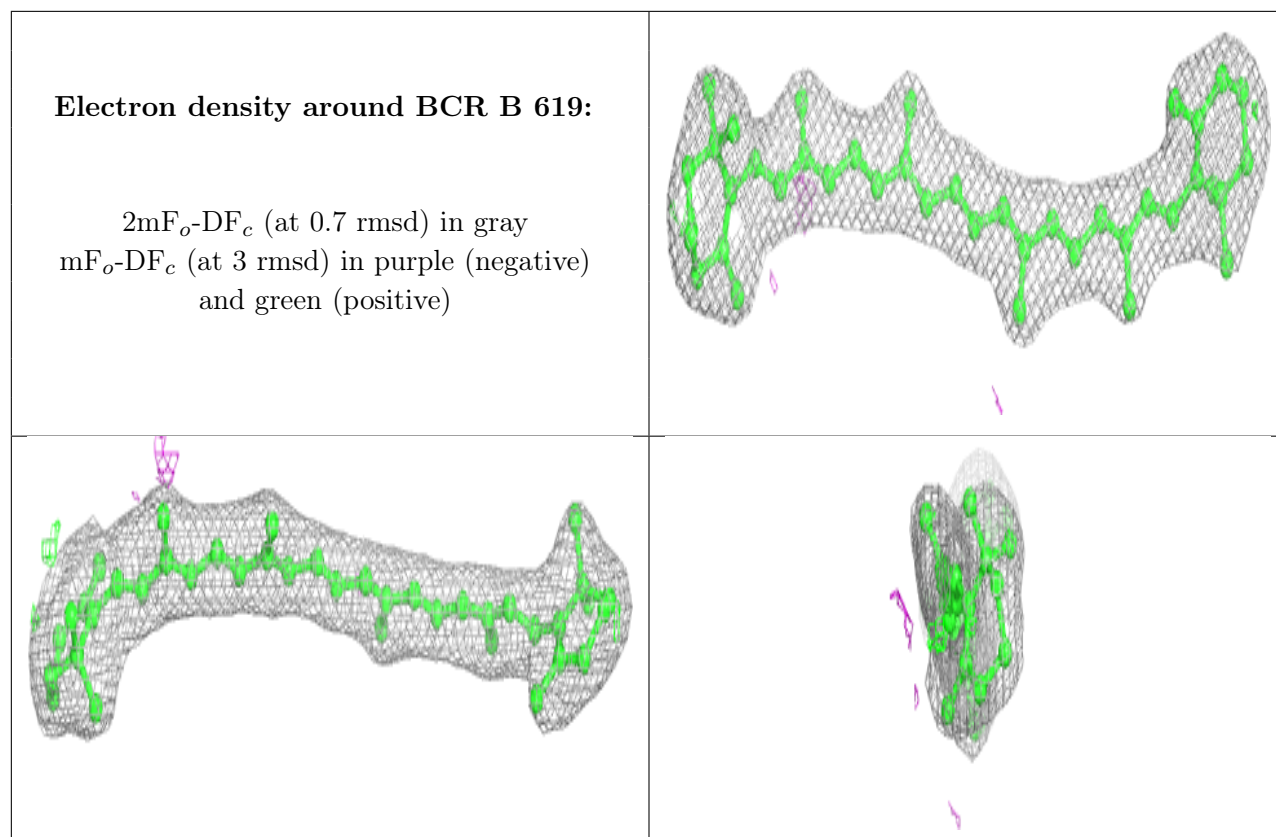
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around CLA A 404:**

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

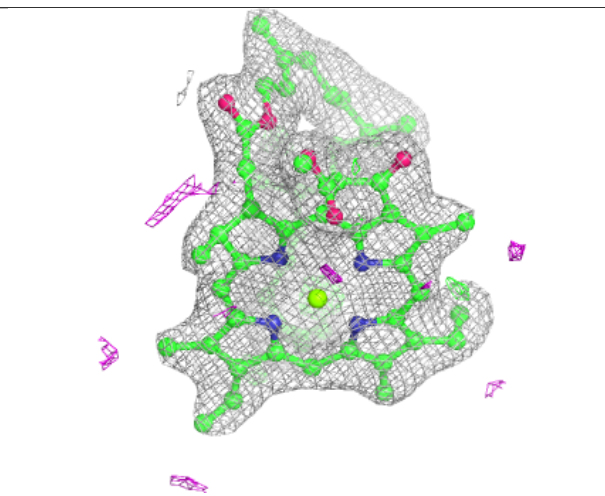
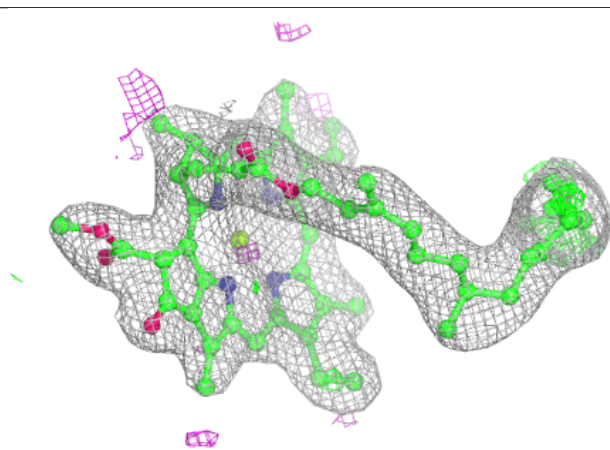
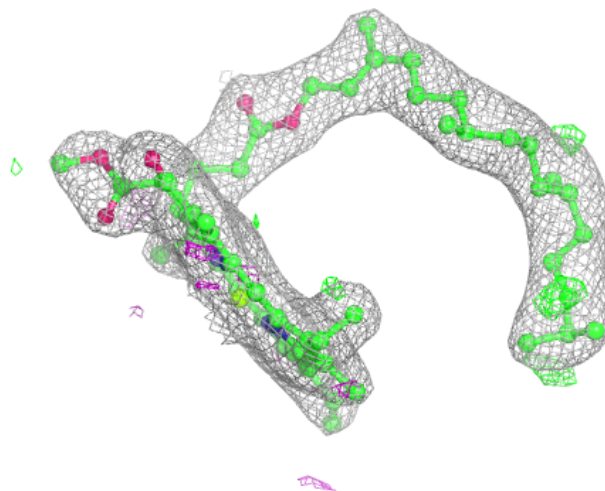


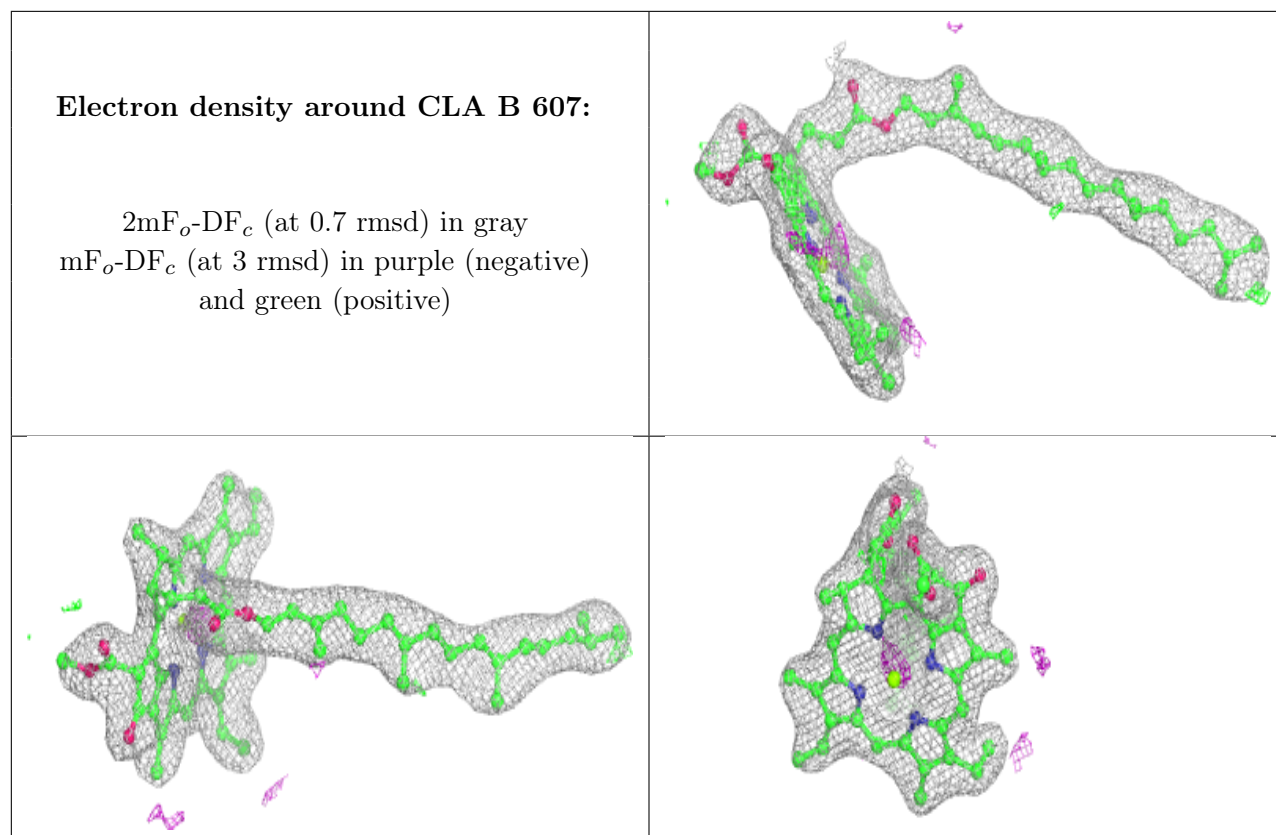




Electron density around CLA b 611:

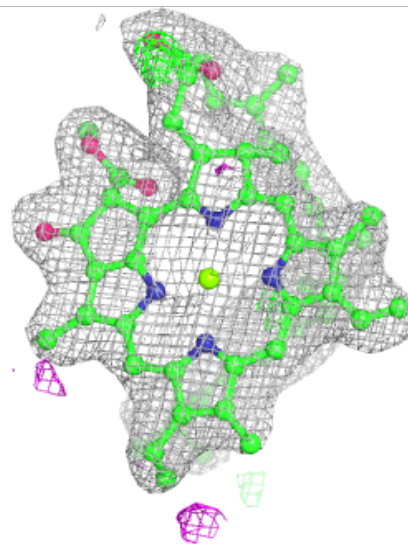
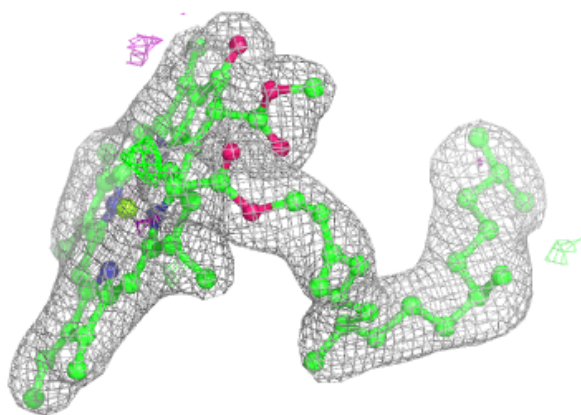
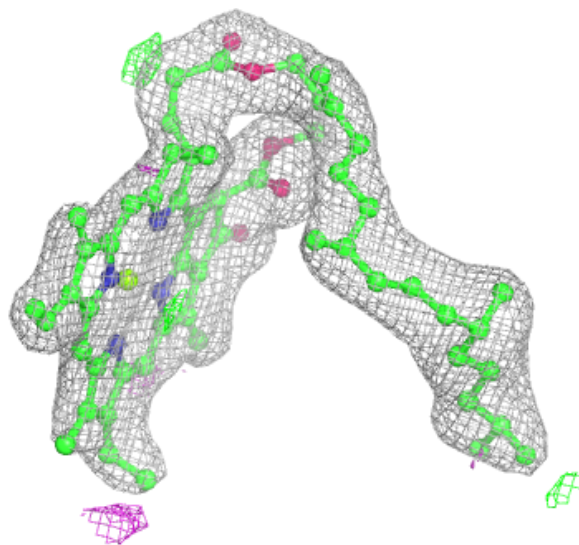
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





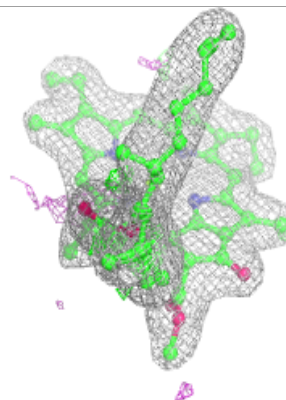
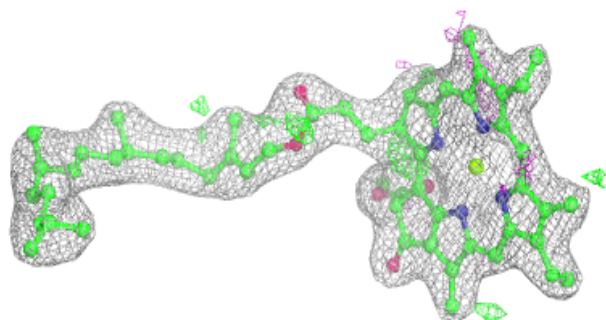
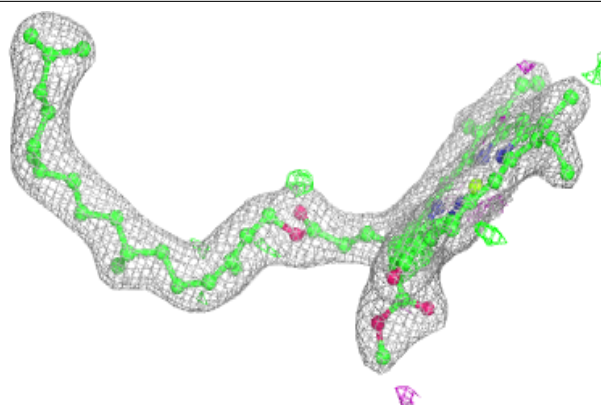
Electron density around CLA b 613:

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

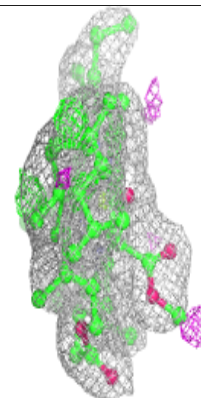
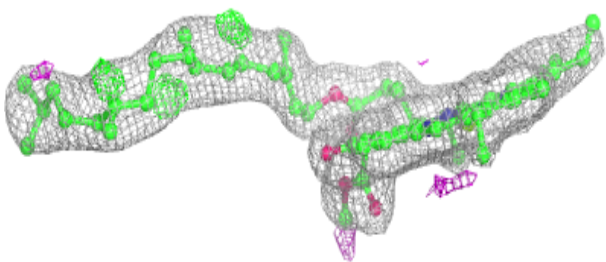
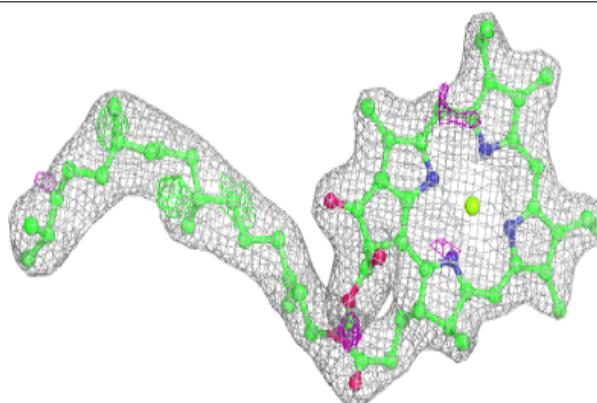


Electron density around CLA D 402:

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

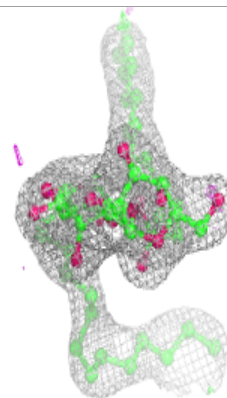
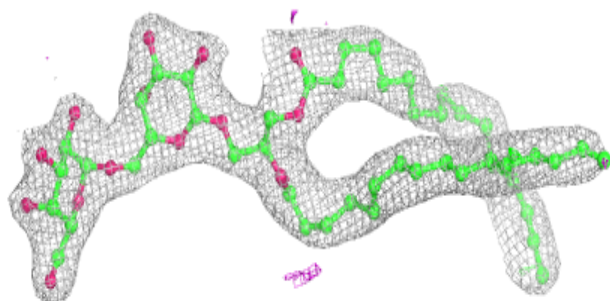
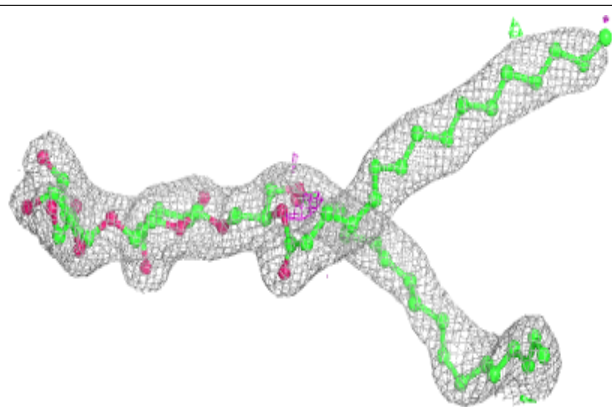
**Electron density around CLA B 602:**

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

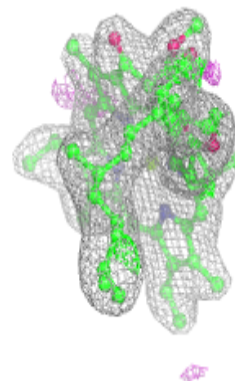
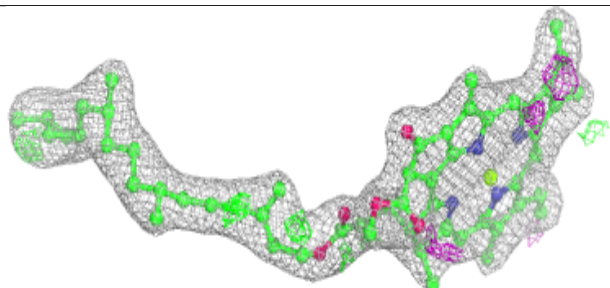
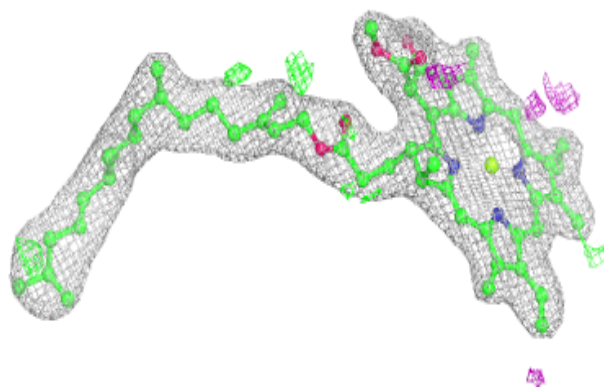


Electron density around DGD C 515:

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

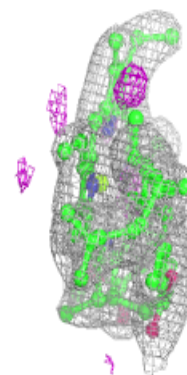
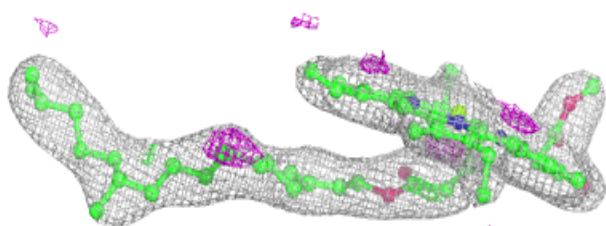
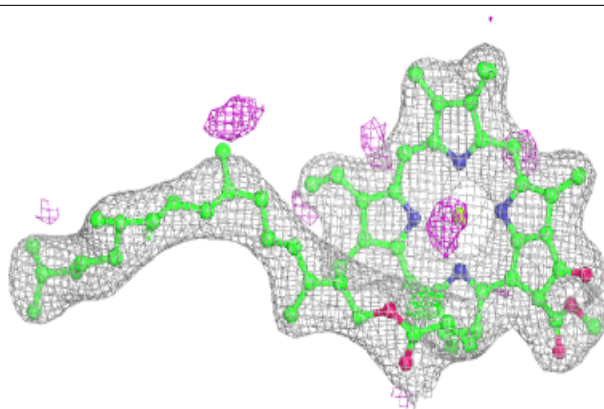
**Electron density around CLA a 405:**

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

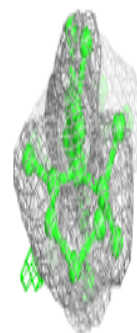
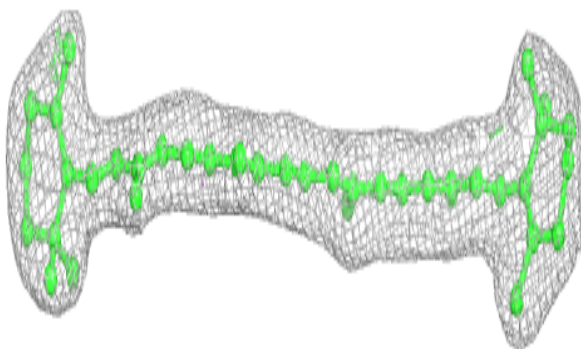
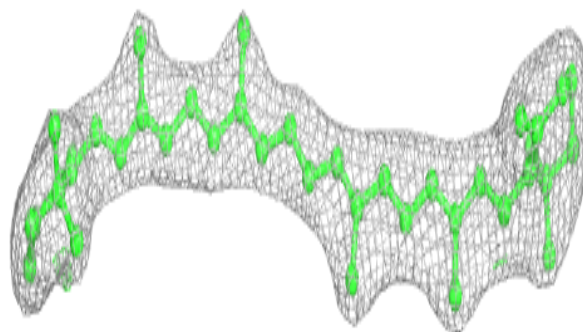


Electron density around CLA B 603:

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

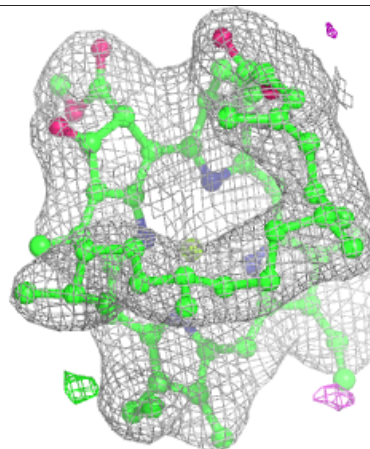
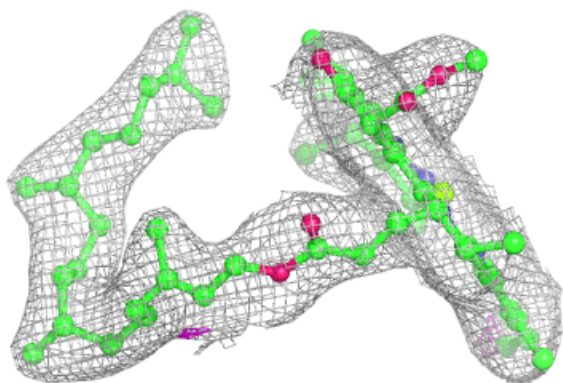
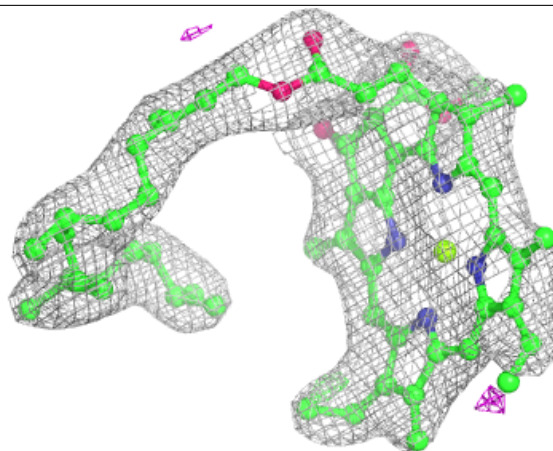
**Electron density around BCR a 410:**

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

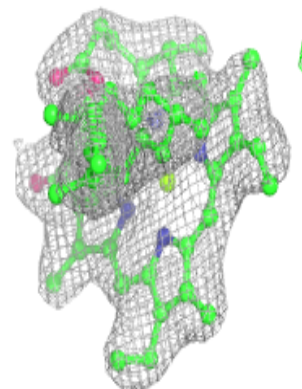
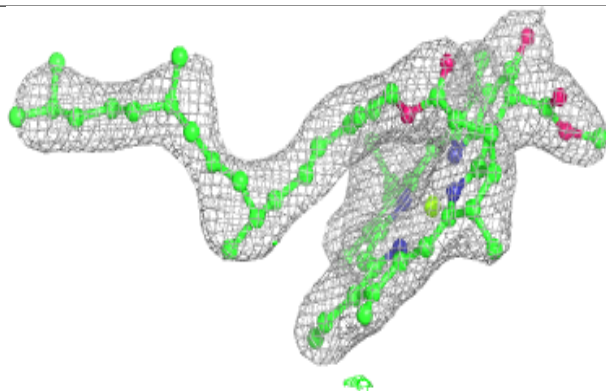
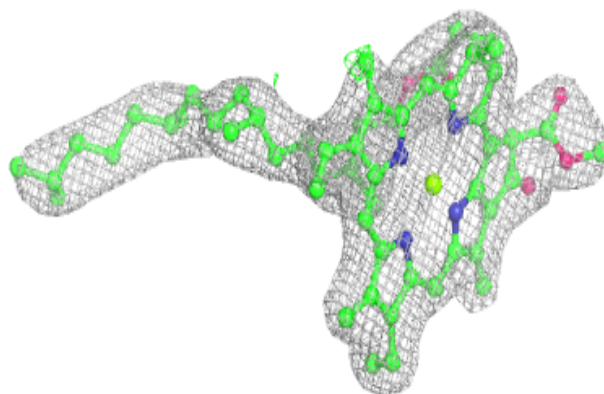


Electron density around CLA c 504:

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

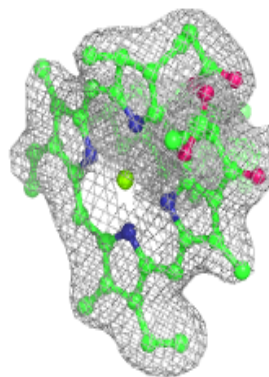
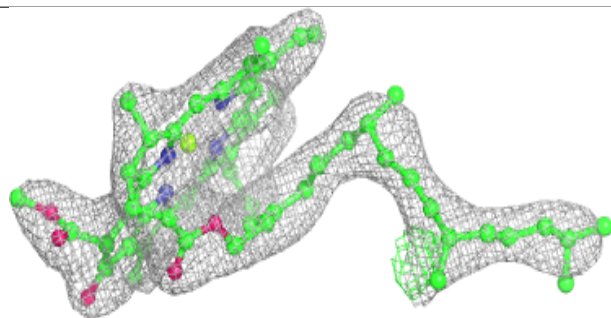
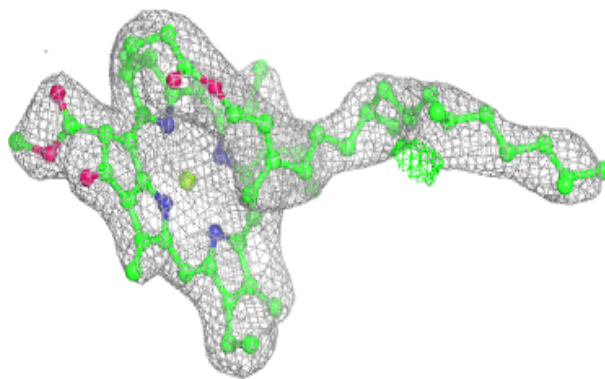
**Electron density around CLA C 505:**

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

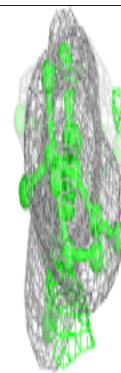
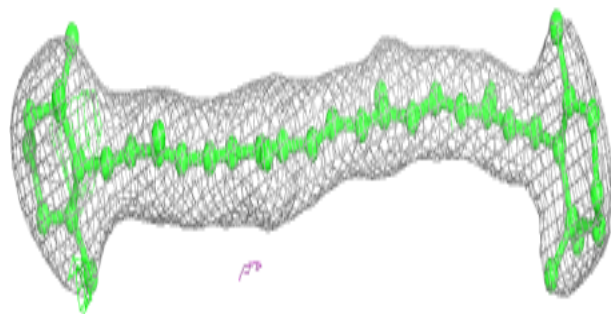
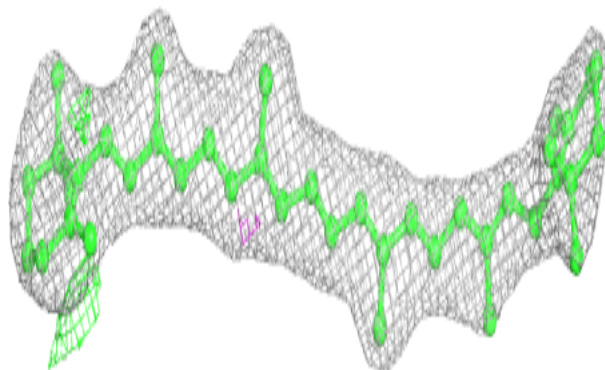


Electron density around CLA c 506:

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

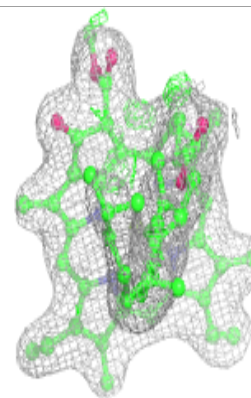
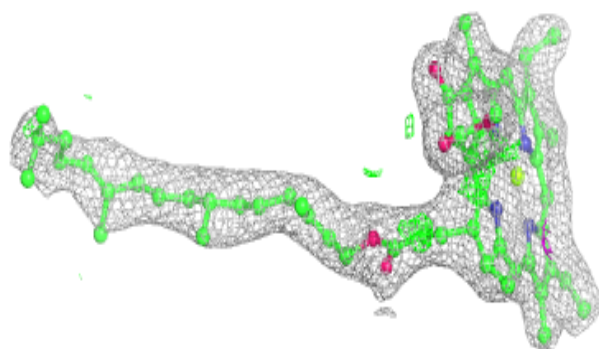
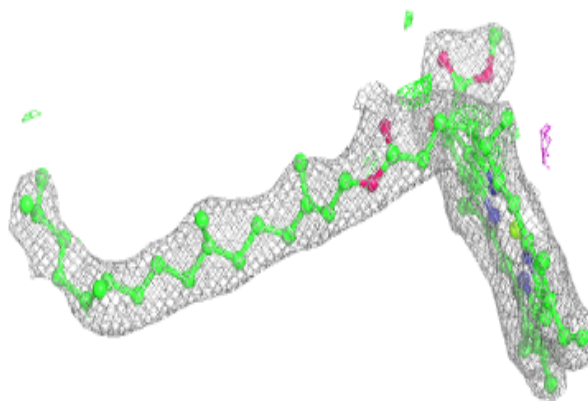
**Electron density around BCR c 516:**

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

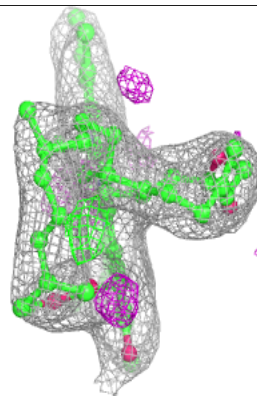
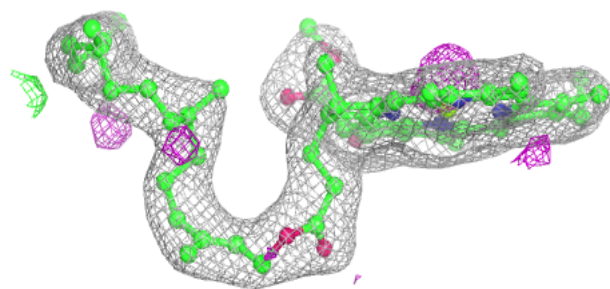
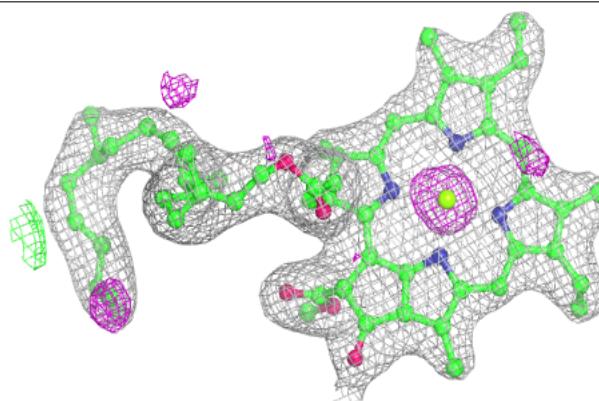


Electron density around CLA B 604:

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

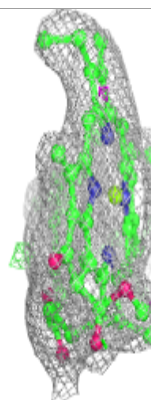
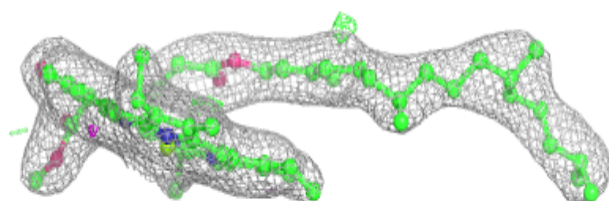
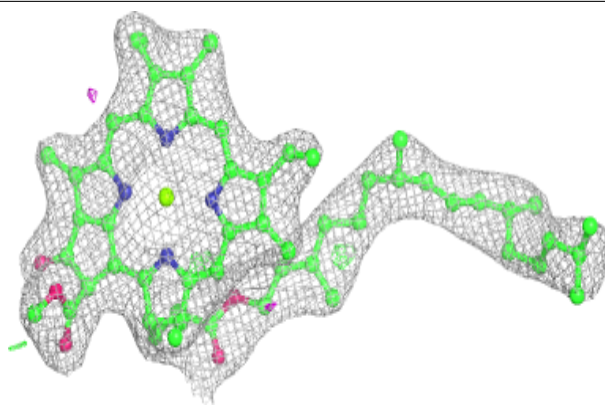
**Electron density around CLA B 612:**

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

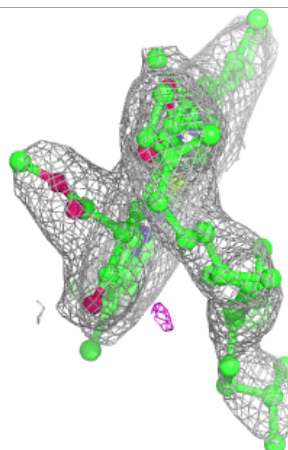
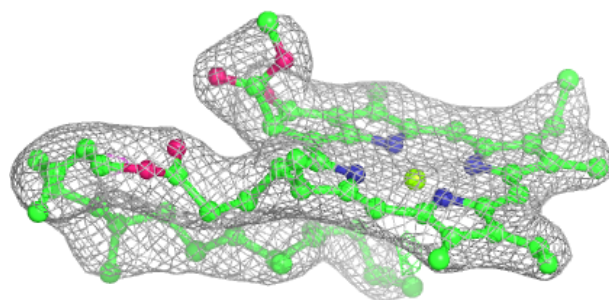
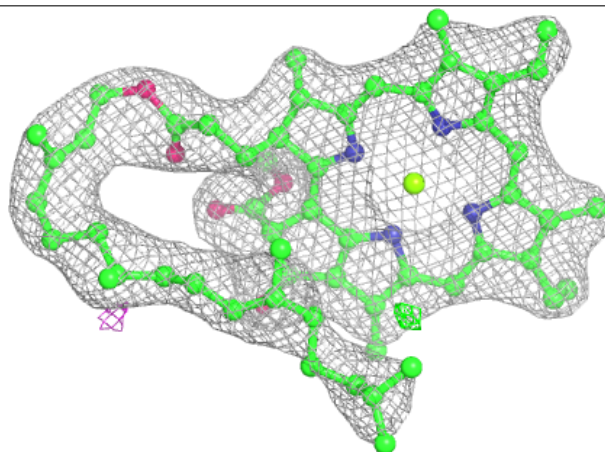


Electron density around CLA b 603:

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

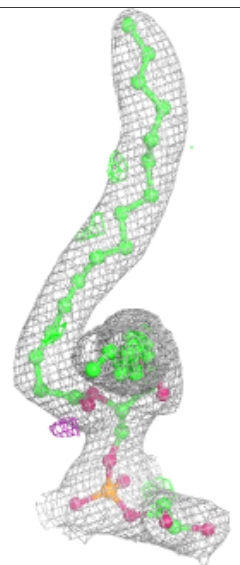
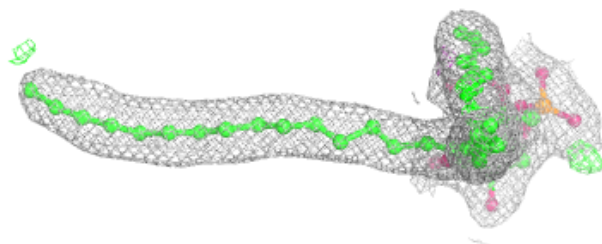
**Electron density around CLA c 510:**

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



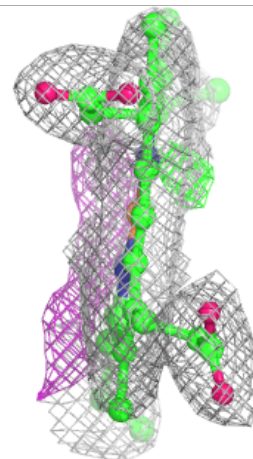
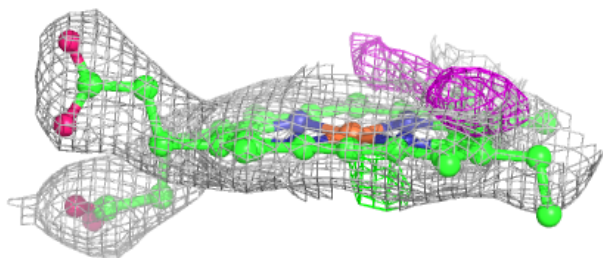
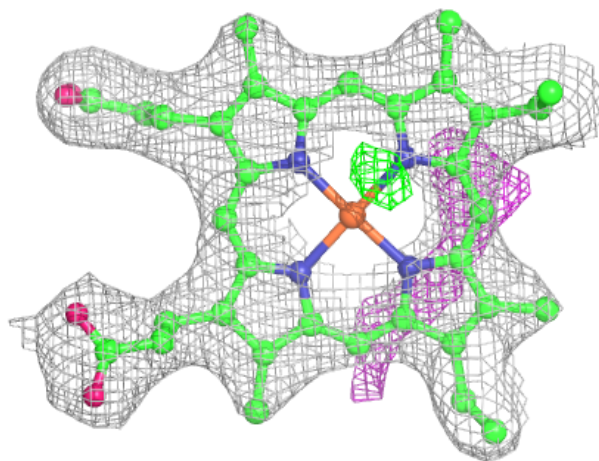
Electron density around LHG L 101:

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



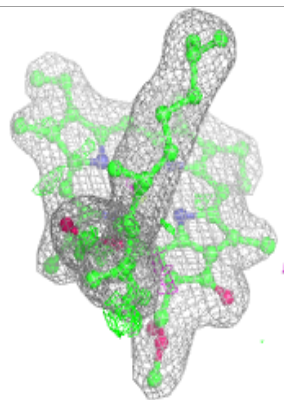
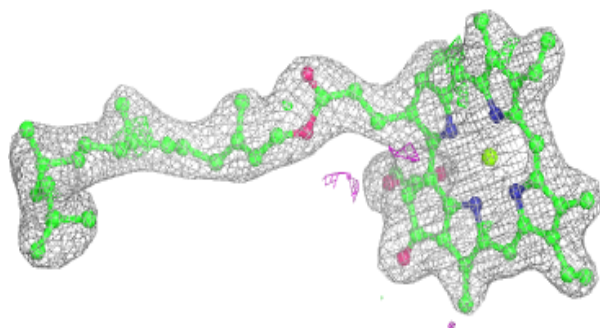
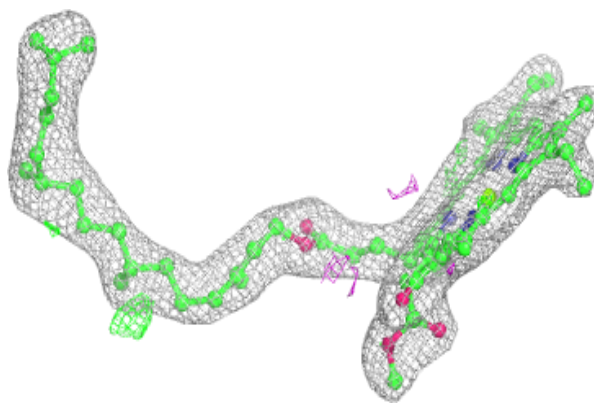
Electron density around HEC v 201:

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

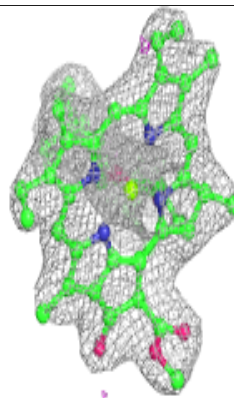
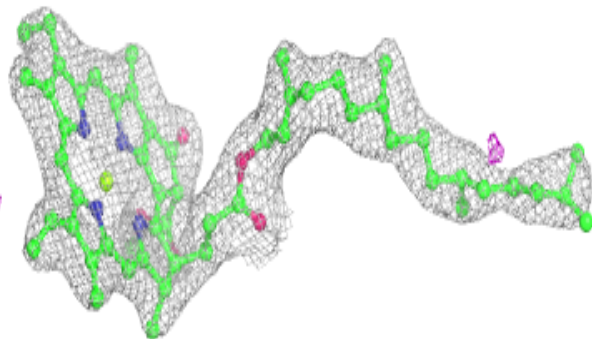
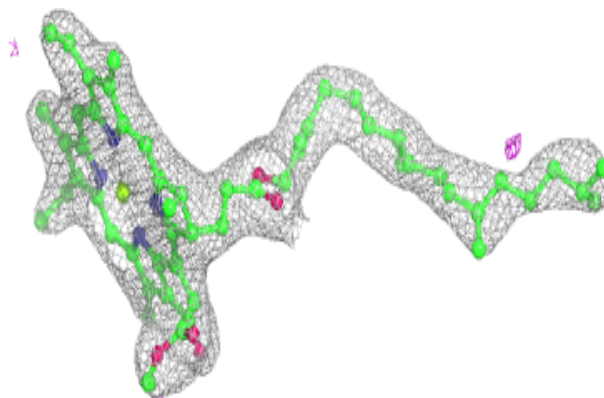


Electron density around CLA d 401:

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

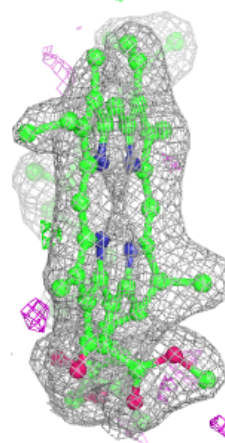
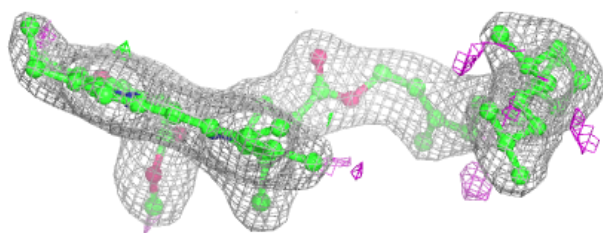
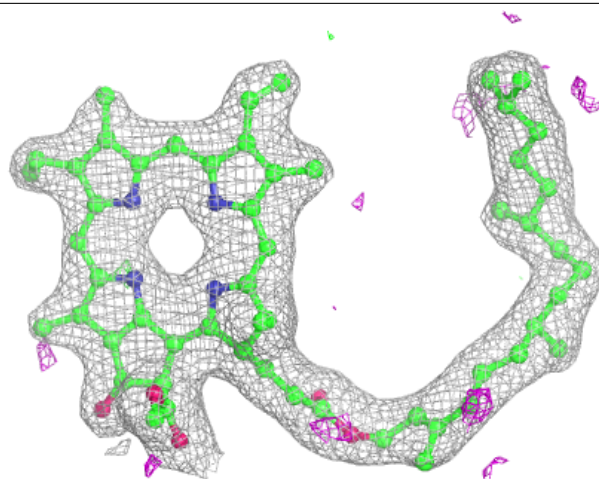
**Electron density around CLA c 503:**

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



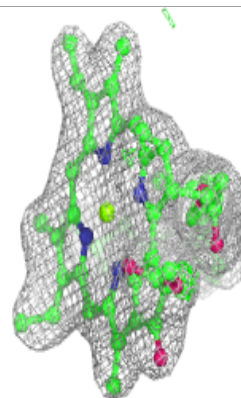
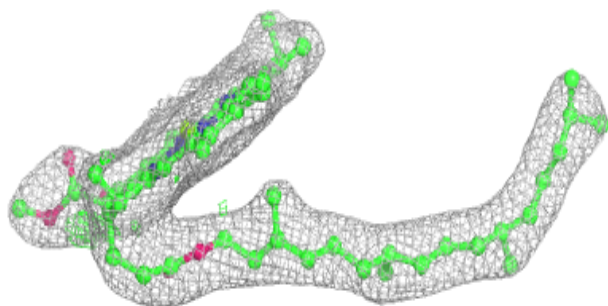
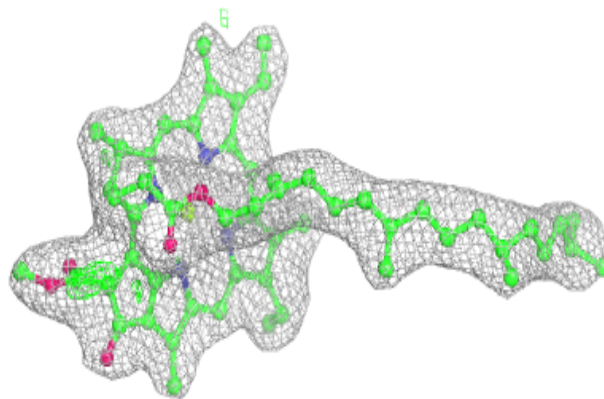
Electron density around PHO A 407:

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

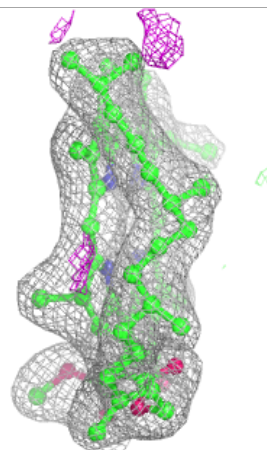
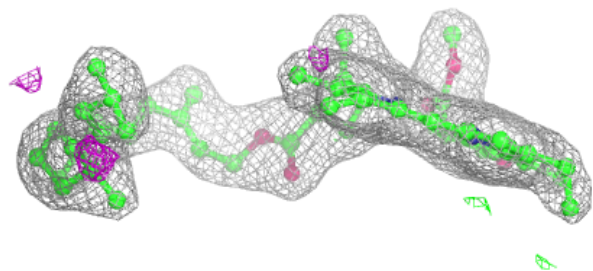
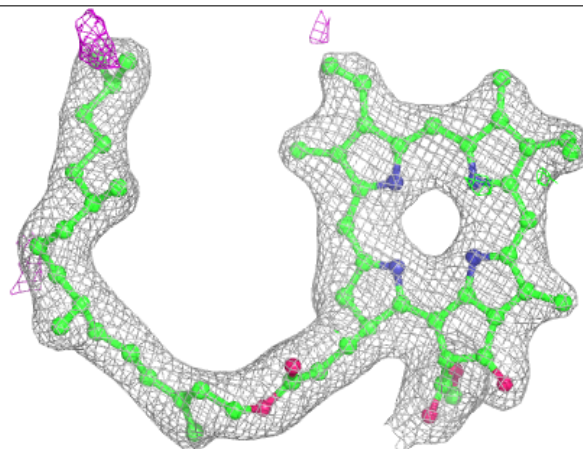


Electron density around CLA b 608:

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

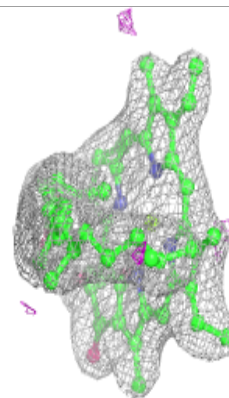
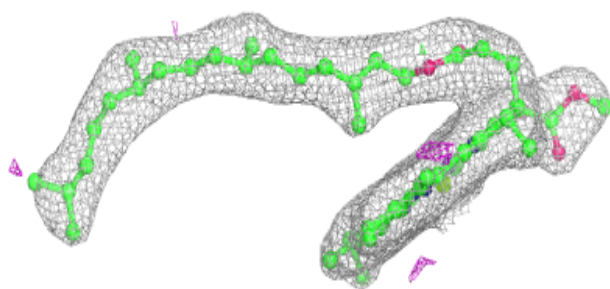
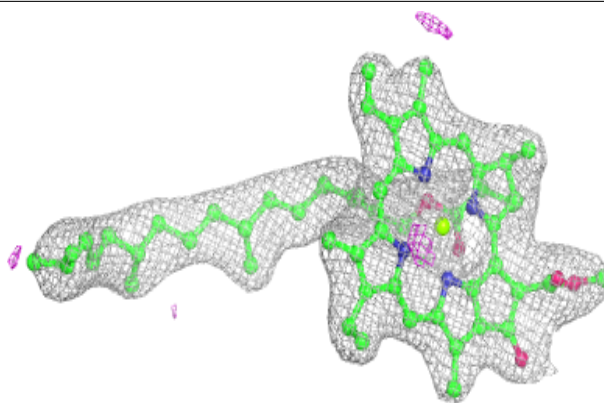
**Electron density around PHO a 408:**

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

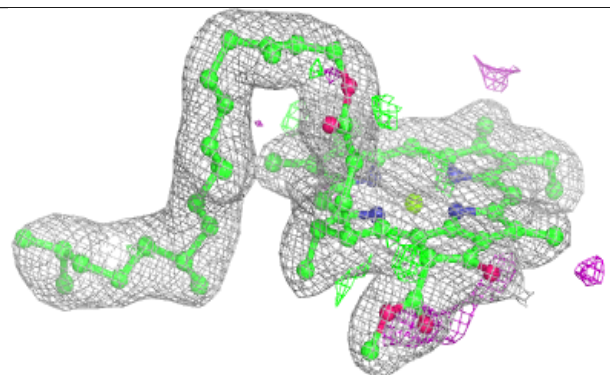
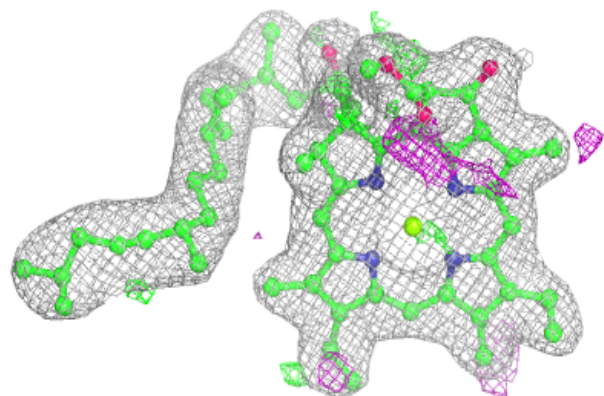


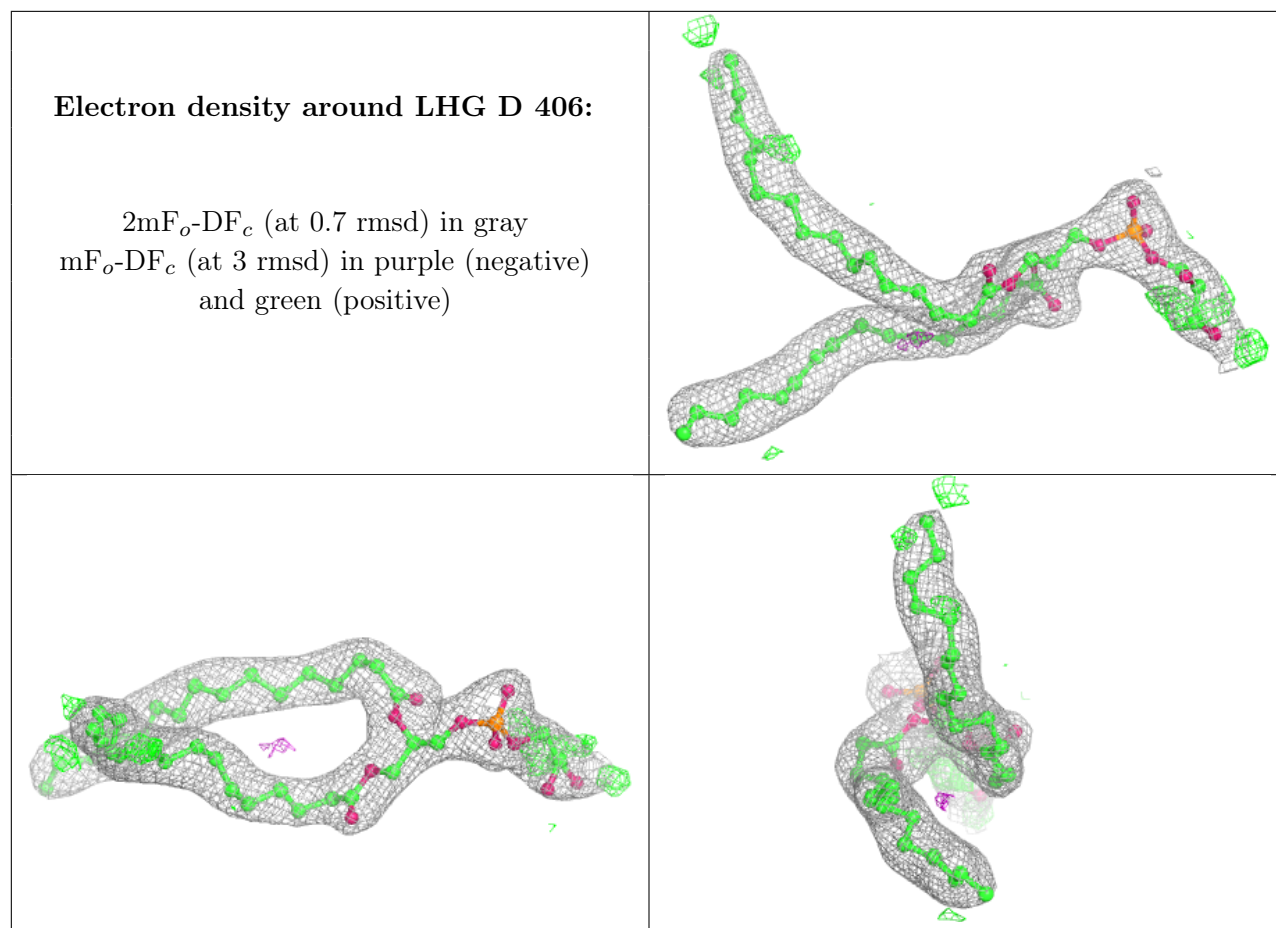
Electron density around CLA B 608:

$2mF_o-DF_c$ (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:**

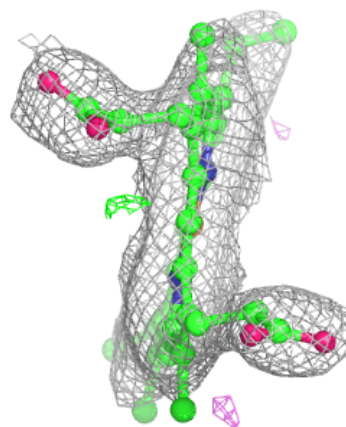
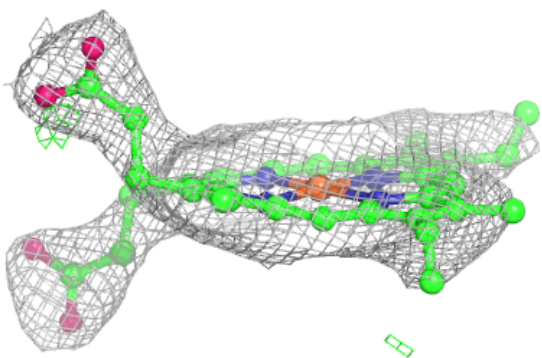
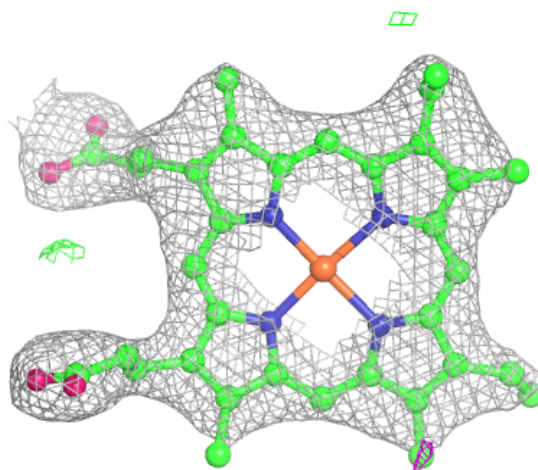
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





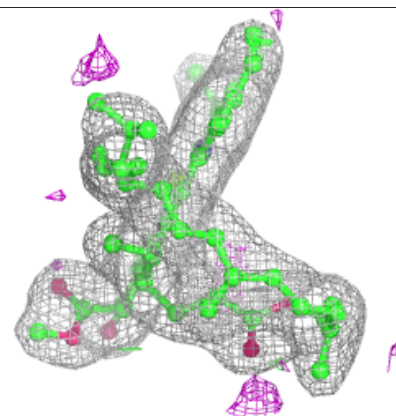
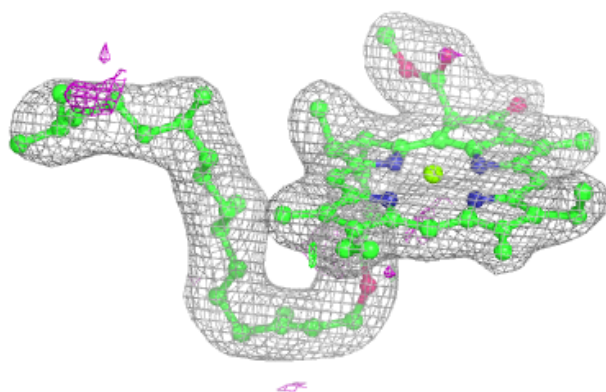
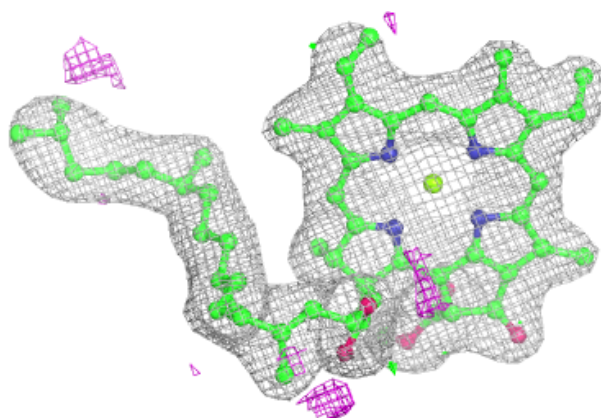
Electron density around HEM F 102:

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

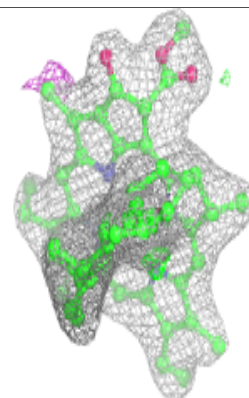
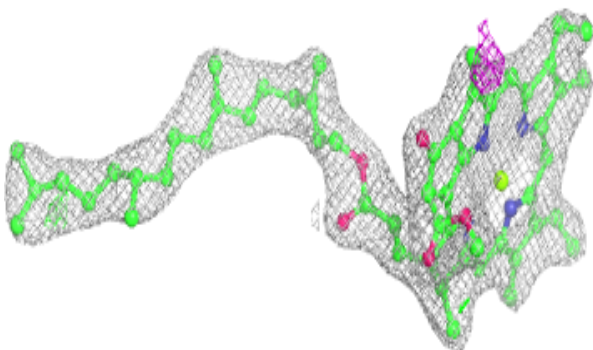
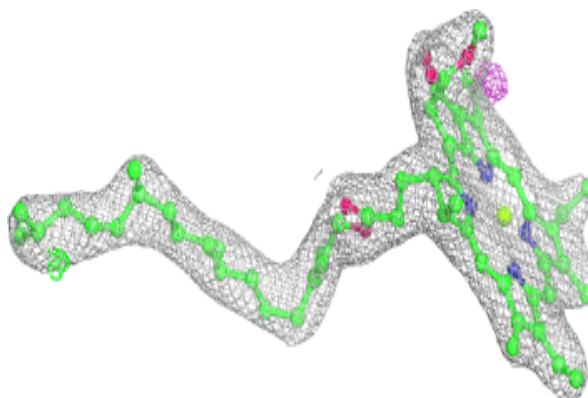


Electron density around CLA a 406:

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

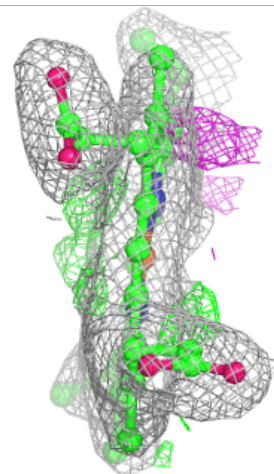
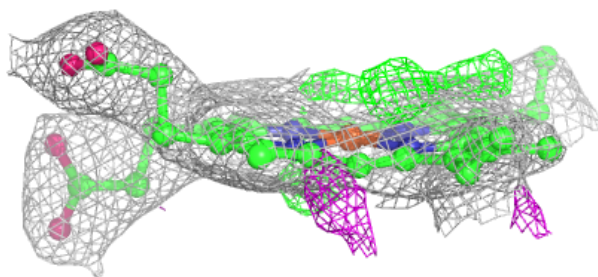
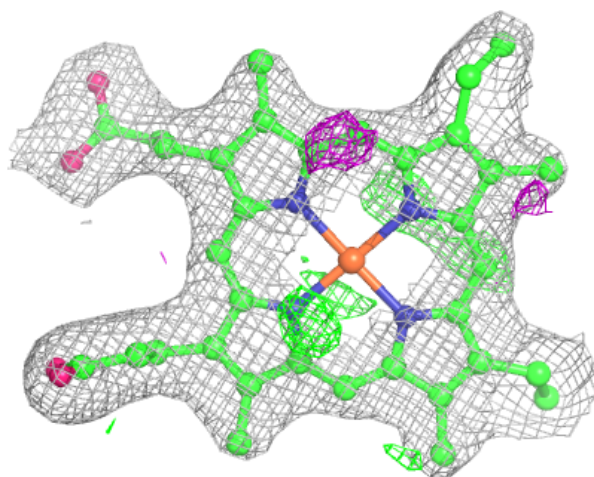
**Electron density around CLA C 502:**

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



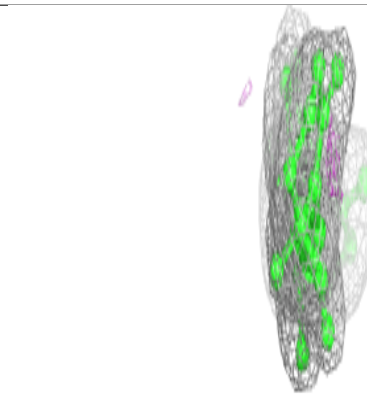
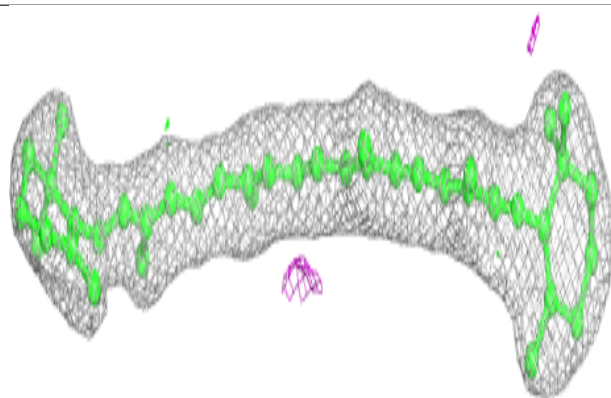
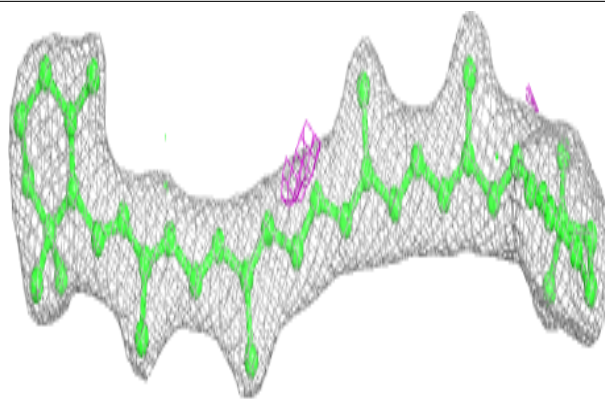
Electron density around HEC V 201:

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

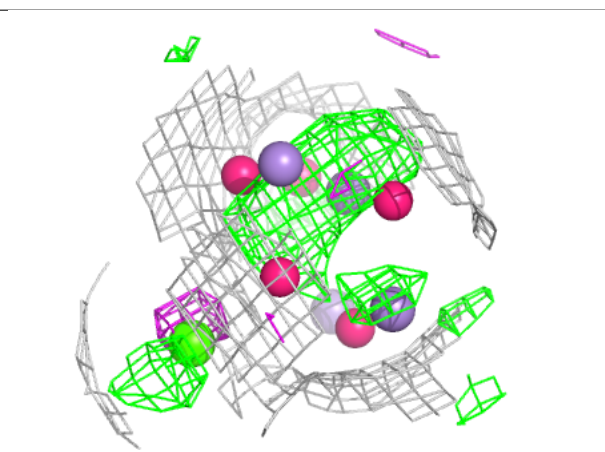
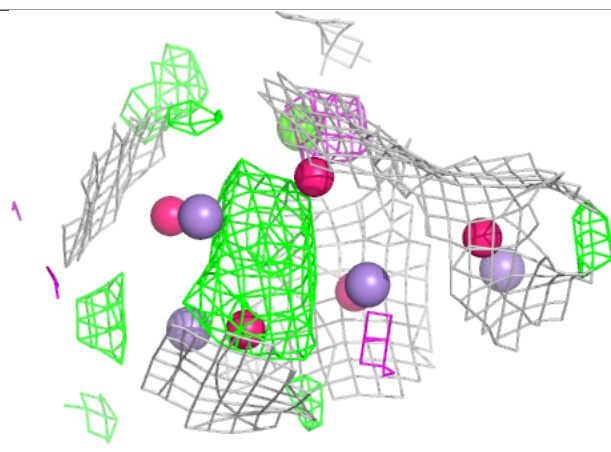
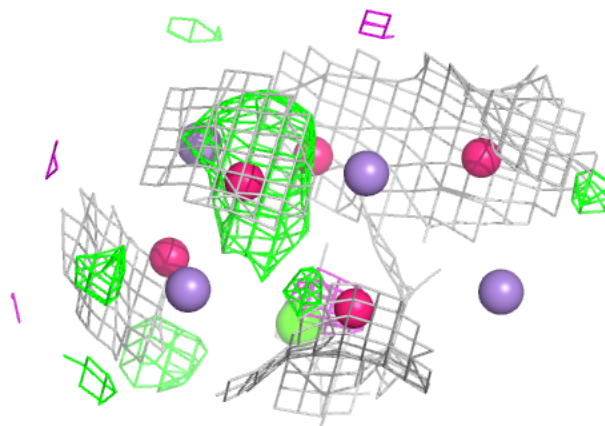


Electron density around BCR b 617:

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

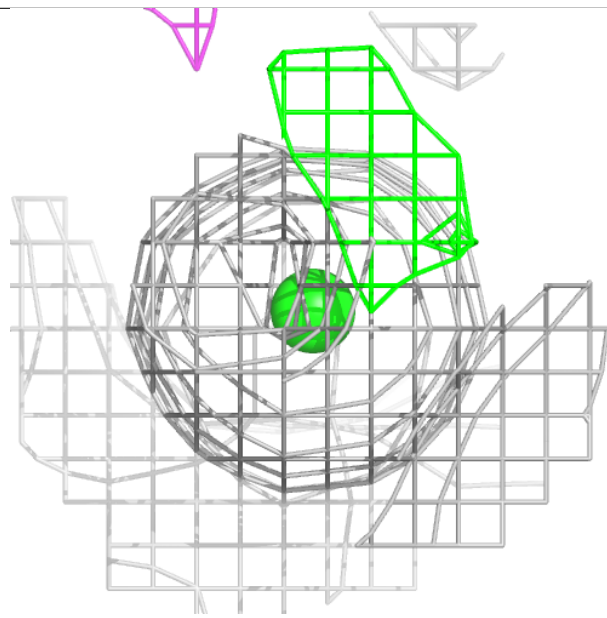
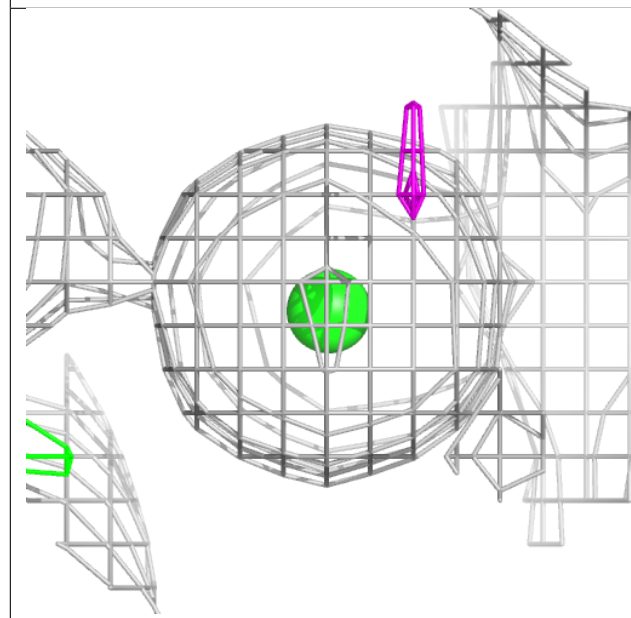
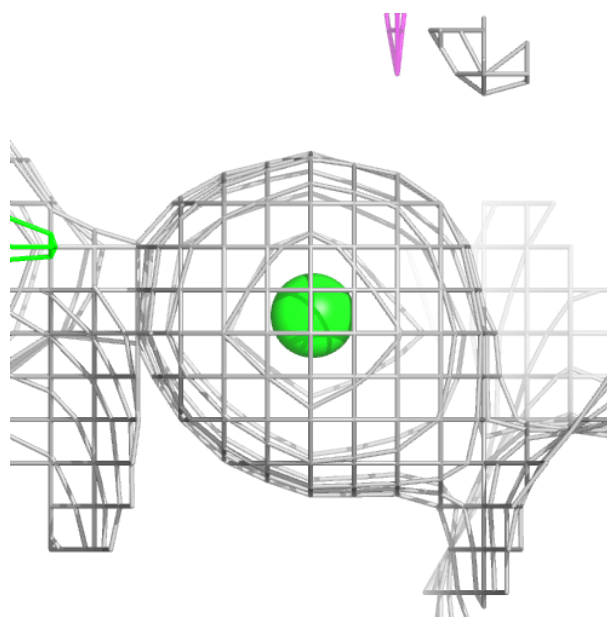
**Electron density around OEX a 414:**

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



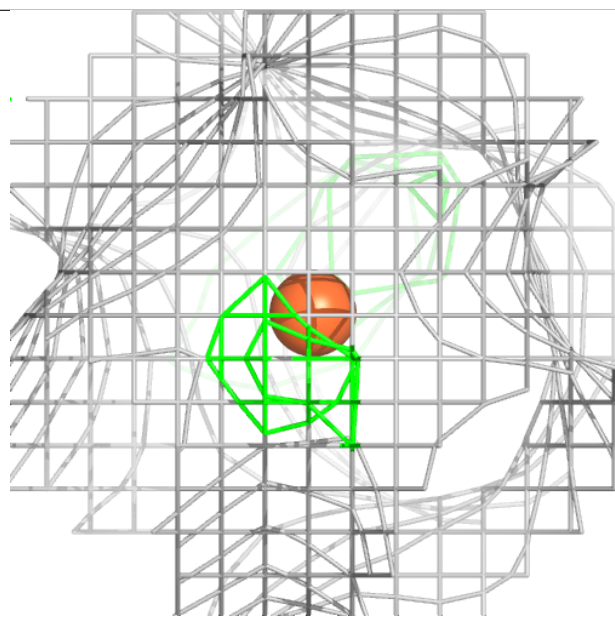
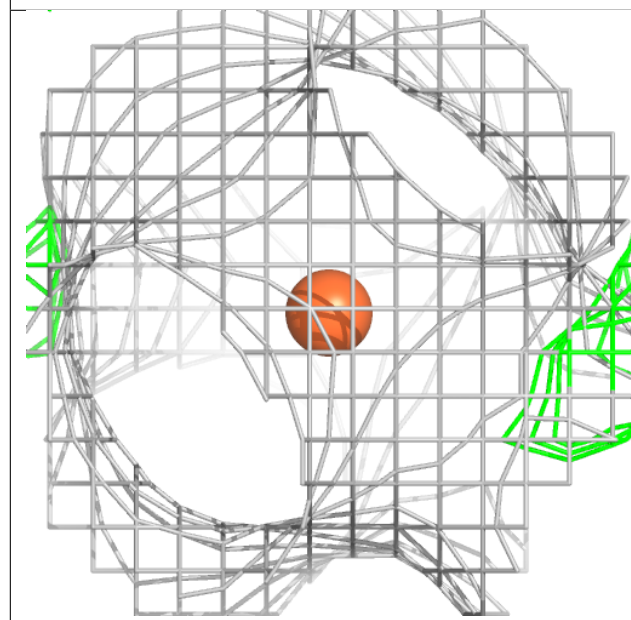
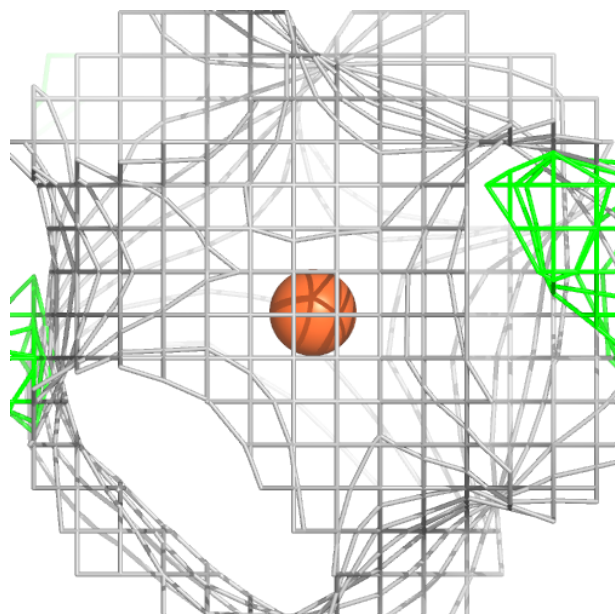
Electron density around CL A 403:

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



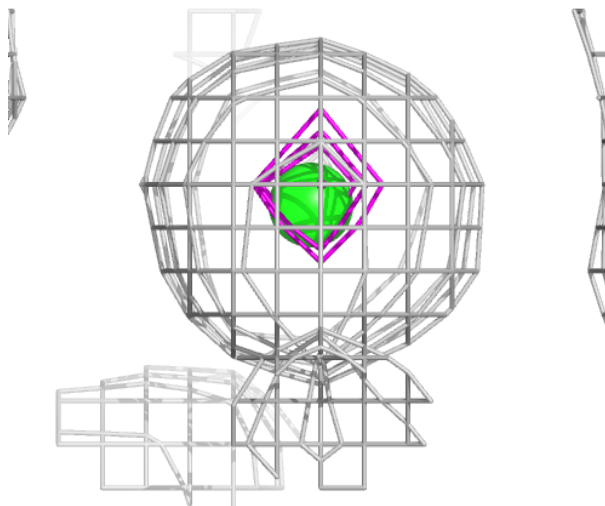
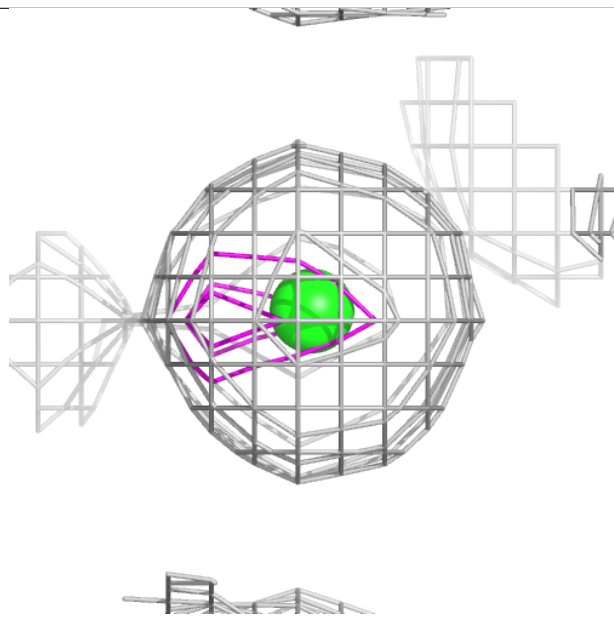
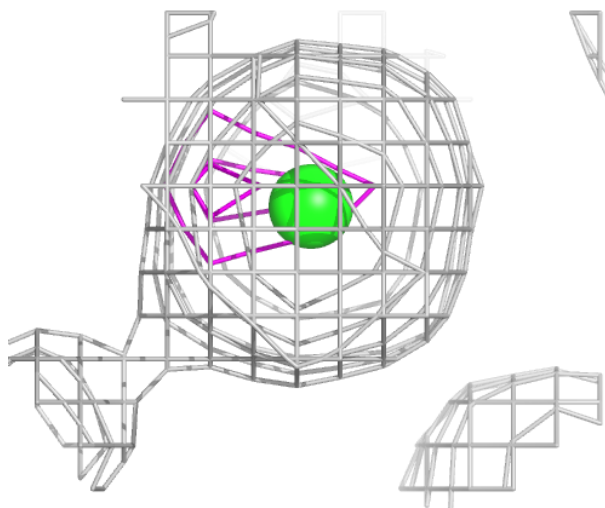
Electron density around FE2 a 401:

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



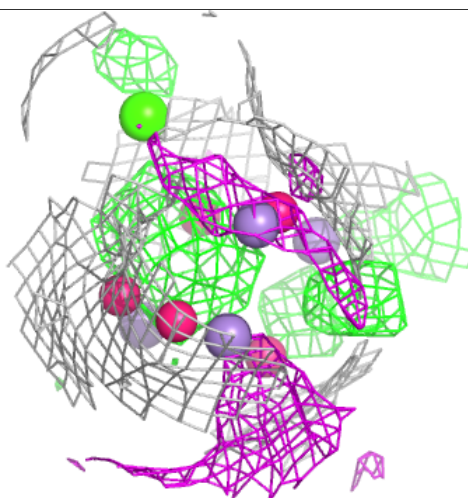
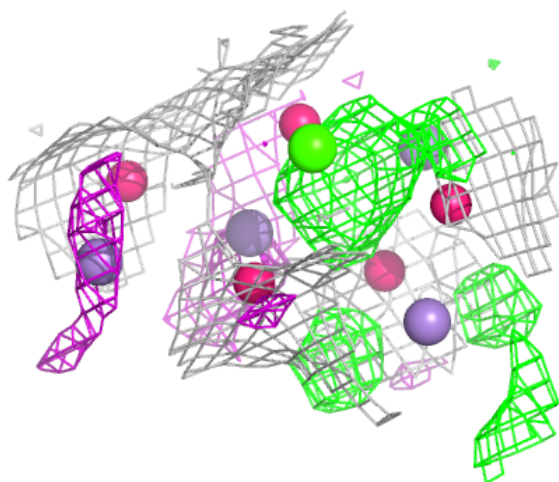
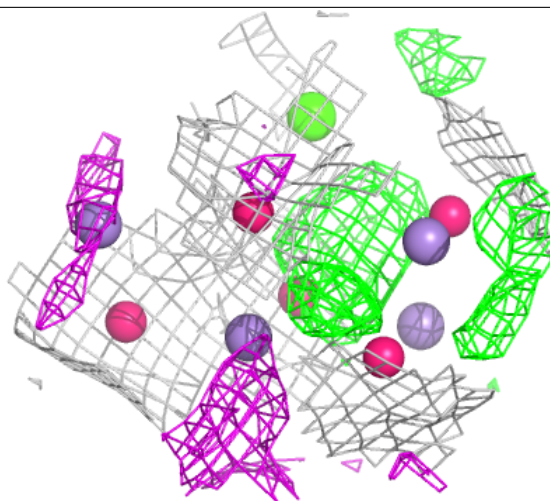
Electron density around CL A 402:

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



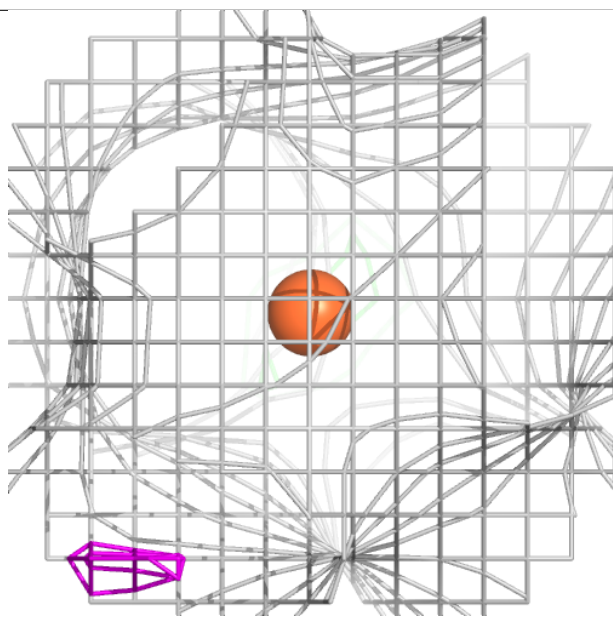
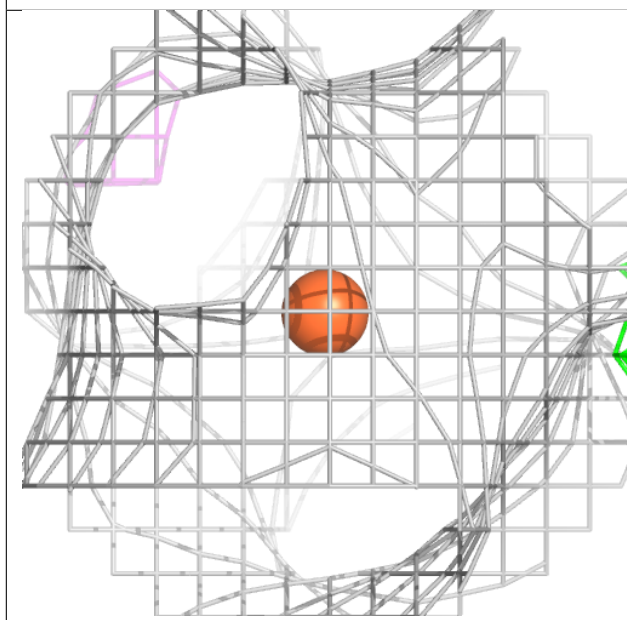
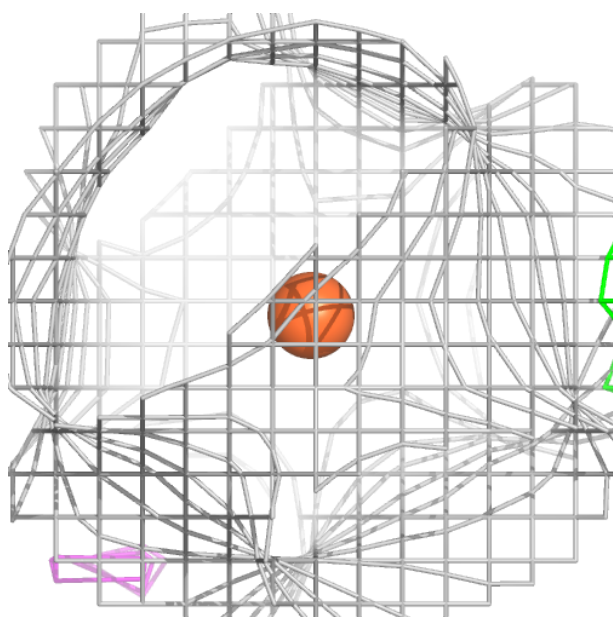
Electron density around OEX A 413:

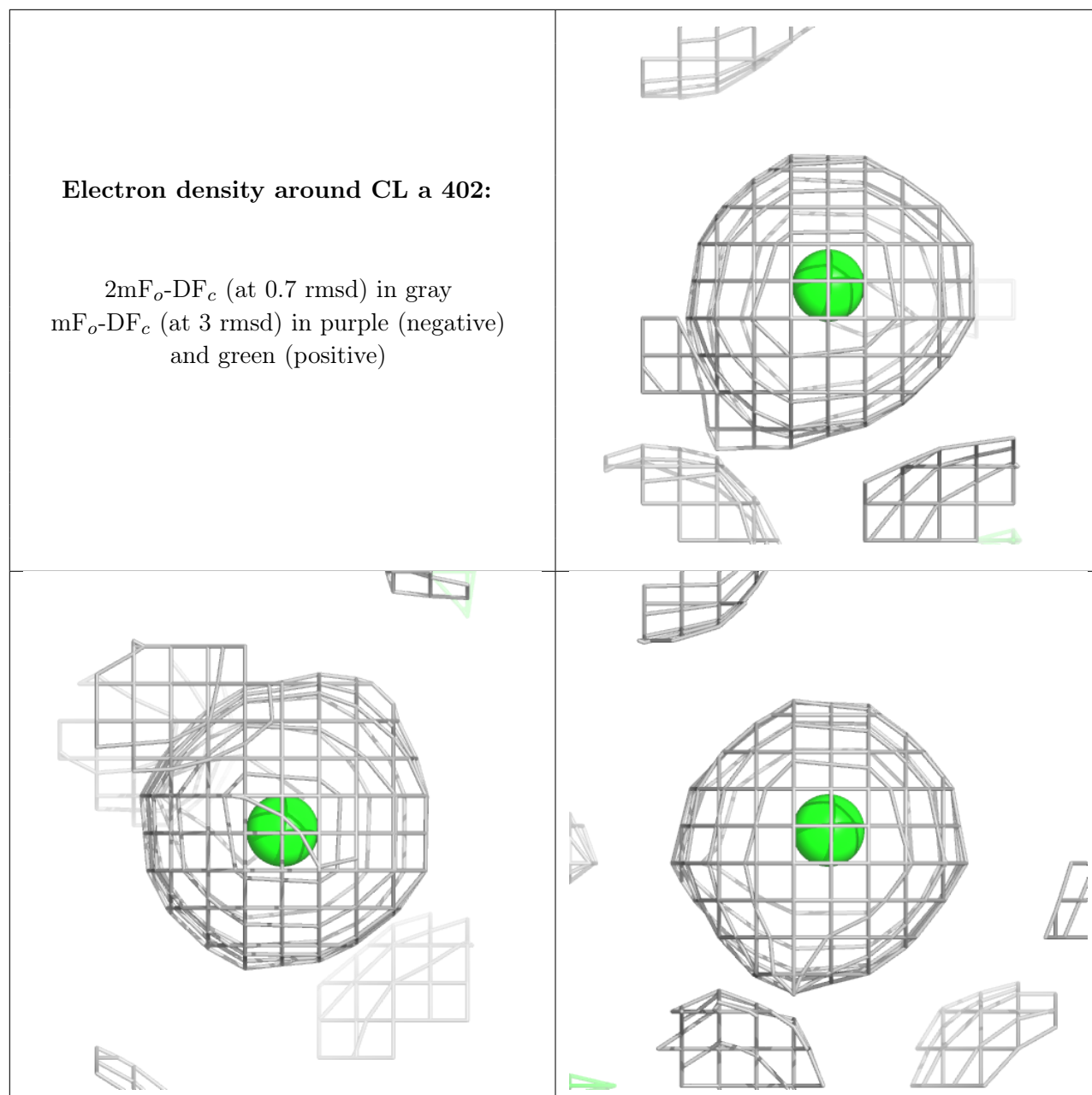
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

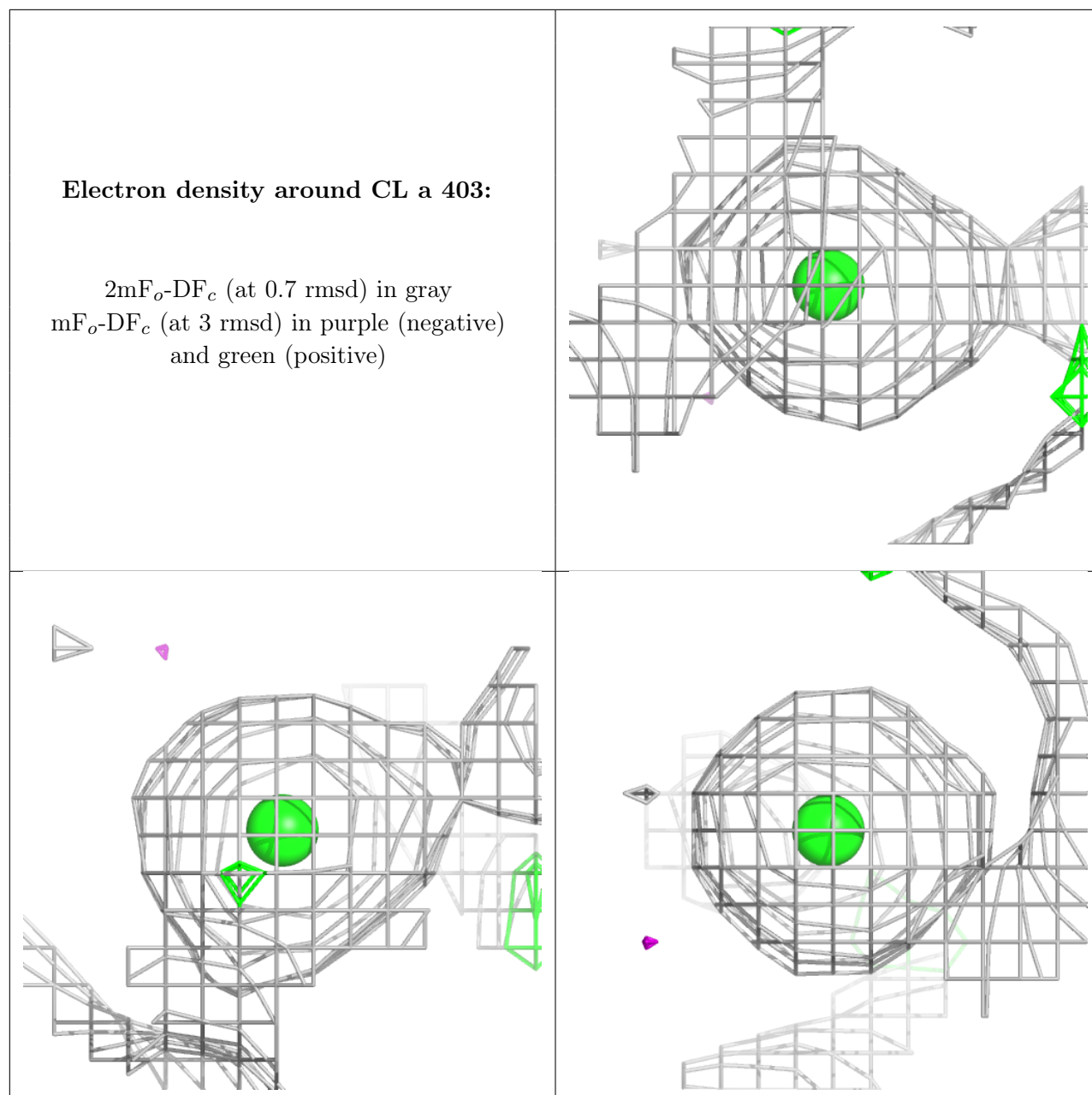


Electron density around FE2 A 401:

$2mF_o-DF_c$ (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.