



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 03:53 PM JST

PDB ID : 7COU
Title : Structure of cyanobacterial photosystem II in the dark S1 state
Authors : Li, H.; Shen, J.-R.; Suga, M.
Deposited on : 2020-08-05
Resolution : 2.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

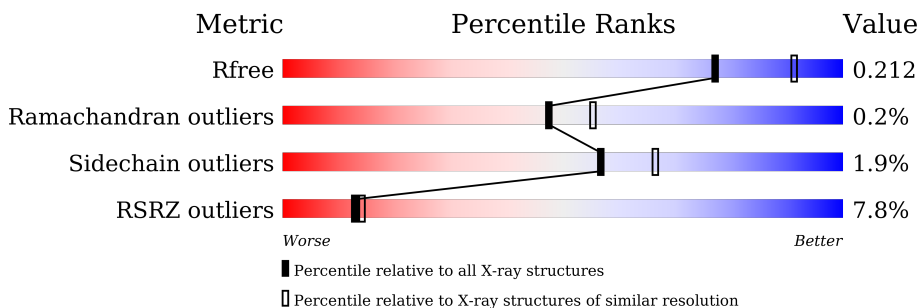
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	344	 4% 97% ..
1	a	344	 6% 97% ..
2	B	505	 5% 99% .
2	b	505	 10% 99% .
3	C	455	 5% 97% ..
3	c	455	 8% 99% .
4	D	342	 3% 99% .

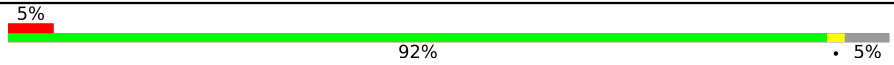
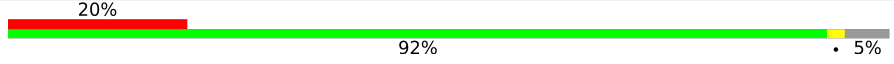
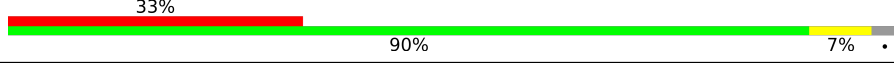
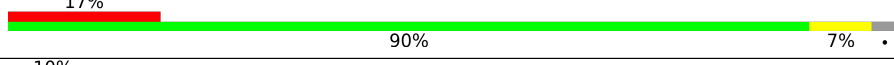
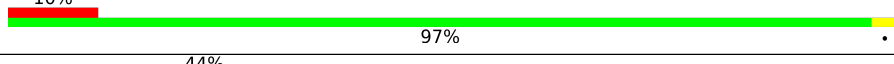
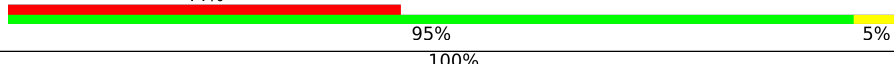

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Mol	Chain	Length	Quality of chain
4	d	342	5% 99%
5	E	84	10% 92% 5%
5	e	84	10% 90% 6%
6	F	44	5% 77% 23%
6	f	44	7% 70% 30%
7	H	65	94% 5%
7	h	65	6% 94% 5%
8	I	38	5% 92% 8%
8	i	38	3% 95% 5%
9	J	39	18% 90% 8%
9	j	39	13% 100%
10	K	37	92% 8%
10	k	37	8% 92% 8%
11	L	37	3% 97%
11	l	37	3% 97%
12	M	36	3% 89% 8%
12	m	36	6% 86% 8% 6%
13	O	244	10% 98%
13	o	244	17% 98%
14	T	32	88% 6% 6%
14	t	32	6% 91% 6%
15	U	104	3% 90% 8%
15	u	104	91% 7%
16	V	137	100%
16	v	137	4% 98%

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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	405	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	503	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	-	-	-

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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	C	514	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	D	404	X	-	-	-
23	CLA	a	404	X	-	-	-
23	CLA	a	405	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	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	c	515	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-
26	GOL	B	629	-	-	-	X
30	UNL	A	414	-	-	-	X
30	UNL	b	626	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	LMG	C	522	-	-	-	X
32	LMG	c	522	-	-	-	X
33	HTG	b	623	-	-	-	X
34	LMT	C	526	-	-	-	X
34	LMT	E	102	-	-	-	X
34	LMT	a	418	-	-	-	X
34	LMT	e	101	-	-	-	X

2 Entry composition [i](#)

There are 40 unique types of molecules in this entry. The entry contains 53138 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	2634	1725	433	461	15	0	2	0
1	a	334	2642	1731	434	462	15	0	3	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	4050	2650	677	710	13	0	10	0
2	b	504	3998	2622	665	698	13	0	4	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	3513	2295	588	617	13	0	4	0
3	c	455	3534	2311	591	619	13	0	2	0

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	342	2726	1805	445	464	12	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	d	341	2717	1800	444	461	12	0	0	0

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	81	668	435	108	125		0	1	0
5	e	79	648	424	105	119		0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	34	275	187	45	42	1	0	0	0
6	f	31	250	170	42	37	1	0	0	0

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

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

- 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	304	203	48	53	0	1	0
11	l	36	304	203	48	53	0	1	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
12	m	34	269	179	40	49	1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	O	243	1886	1177	318	386	5	0	3	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	o	243	Total	C	N	O	S	0	2	0
			1879	1173	317	384	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	T	30	Total	C	N	O	S	0	0	0
			258	181	36	39	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
			Total	C	N	O			
15	U	96	Total	C	N	O	0	0	0
			765	486	128	151			
15	u	97	Total	C	N	O	0	0	0
			774	491	129	154			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	V	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	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
			Total	C	N	O			
17	X	38	Total	C	N	O	0	0	0
			281	188	45	48			
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
			Total	C	N	O	S			
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			

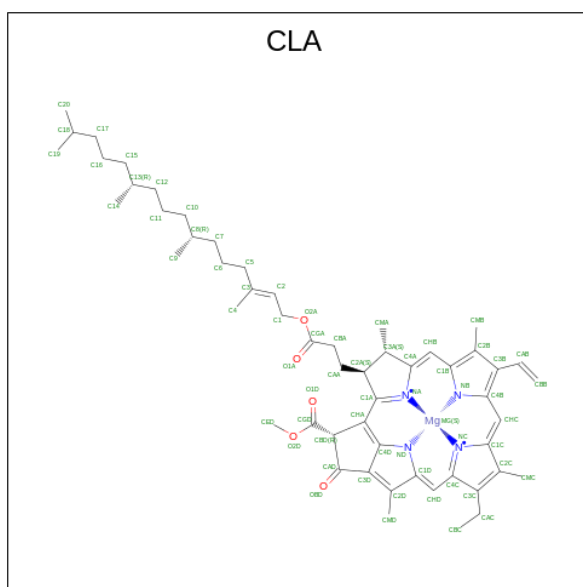
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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).

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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Mg	N			O
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		

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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	C	1	65	55	1	4	5	0	0
23	C	1	65	55	1	4	5	0	0
23	C	1	65	55	1	4	5	0	0
23	C	1	65	55	1	4	5	0	0
23	C	1	65	55	1	4	5	0	0
23	C	1	65	55	1	4	5	0	0
23	C	1	65	55	1	4	5	0	0
23	C	1	65	55	1	4	5	0	0
23	C	1	65	55	1	4	5	0	0
23	C	1	65	55	1	4	5	0	0
23	C	1	65	55	1	4	5	0	0
23	C	1	65	55	1	4	5	0	0
23	D	1	65	55	1	4	5	0	0
23	D	1	65	55	1	4	5	0	0

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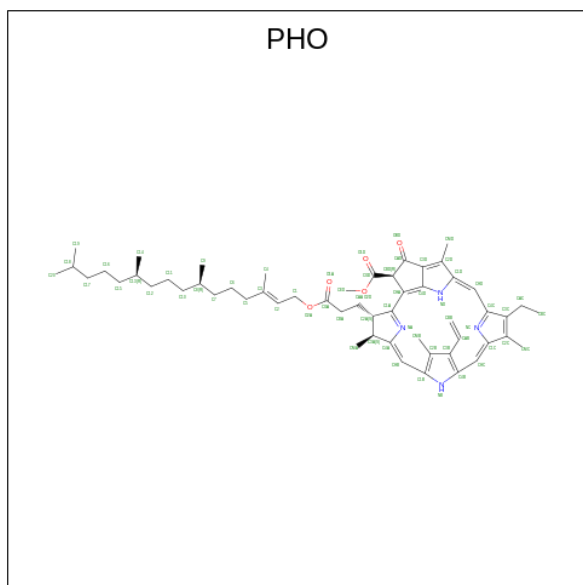
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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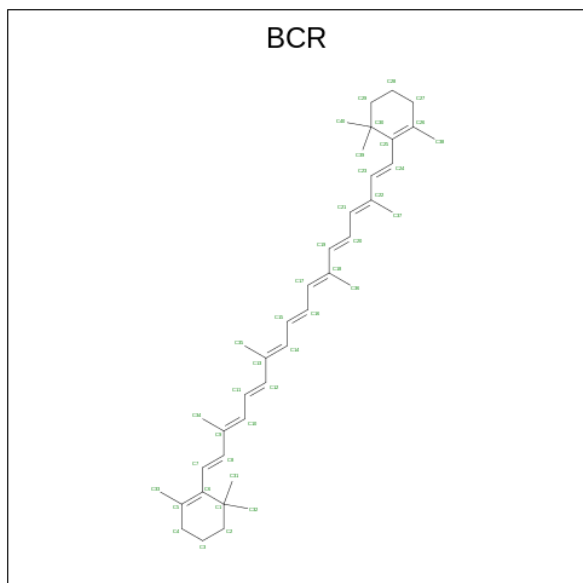
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	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: C₅₅H₇₄N₄O₅).



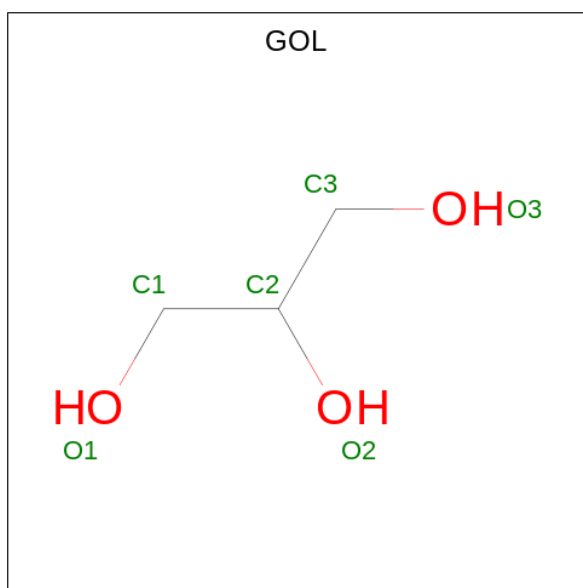
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			
24	A	1	Total	64	55	4	5	0	0
24	A	1	Total	64	55	4	5	0	0
24	a	1	Total	64	55	4	5	0	0
24	a	1	Total	64	55	4	5	0	0

- 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	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total C 40 40	0	0
25	a	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	d	1	Total C 40 40	0	0
25	h	1	Total C 40 40	0	0
25	k	1	Total C 40 40	0	0
25	t	1	Total C 40 40	0	0
25	y	1	Total C 40 40	0	0

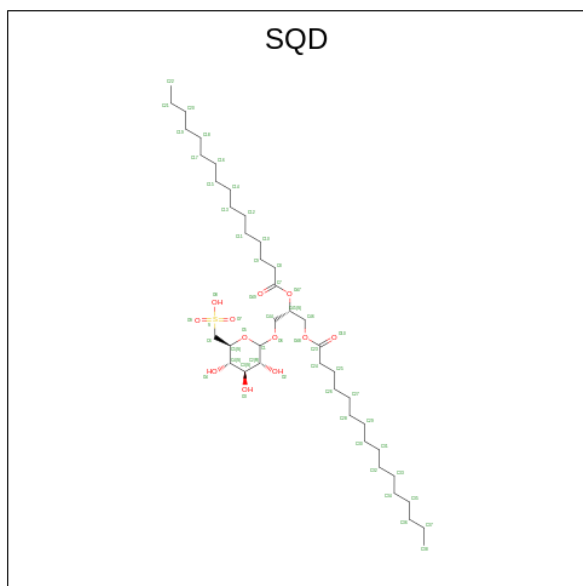
- Molecule 26 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O 6 3 3	0	0
26	B	1	Total C O 6 3 3	0	0
26	B	1	Total C O 6 3 3	0	0
26	B	1	Total C O 6 3 3	0	0
26	C	1	Total C O 6 3 3	0	0
26	O	1	Total C O 6 3 3	0	0
26	a	1	Total C O 6 3 3	0	0
26	b	1	Total C O 6 3 3	0	0
26	b	1	Total C O 6 3 3	0	0
26	c	1	Total C O 6 3 3	0	0
26	o	1	Total C O 6 3 3	0	0
26	v	1	Total C O 6 3 3	0	0

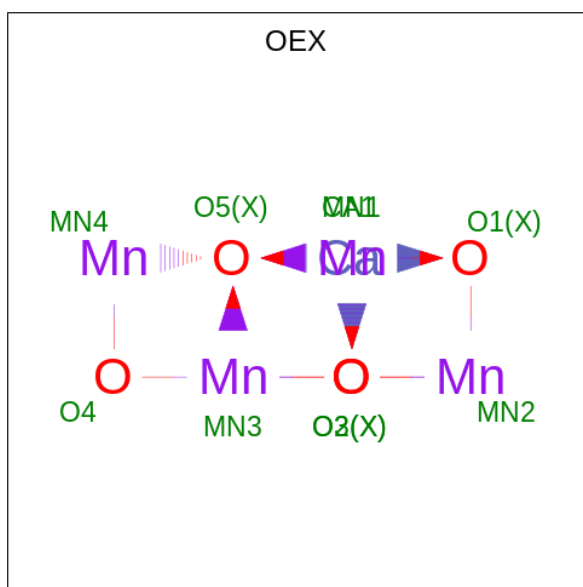
- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



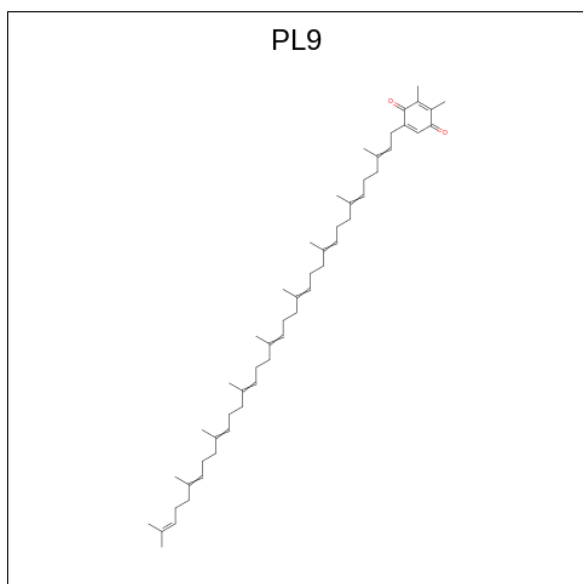
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
27	A	1	Total 54	C 41	O 12	S 1	0	0
27	B	1	Total 54	C 41	O 12	S 1	0	0
27	C	1	Total 54	C 41	O 12	S 1	0	0
27	D	1	Total 43	C 30	O 12	S 1	0	0
27	a	1	Total 54	C 41	O 12	S 1	0	0
27	a	1	Total 54	C 41	O 12	S 1	0	0
27	b	1	Total 54	C 41	O 12	S 1	0	0
27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

- Molecule 28 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).



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

- 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: $C_{53}H_{80}O_2$).



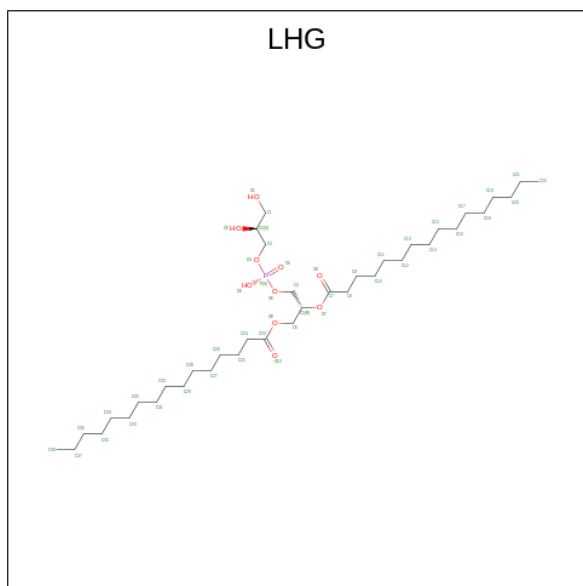
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			55	53	2		
29	D	1	Total	C	O	0	0
			55	53	2		
29	a	1	Total	C	O	0	0
			55	53	2		
29	d	1	Total	C	O	0	0
			55	53	2		

- 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	C	1	Total	C	O	0	0
			34	29	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	M	1	Total	C		0	0
			10	10			
30	X	1	Total	C	O	0	0
			18	16	2		
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	3	Total	C	O	0	0
			71	63	8		
30	i	1	Total	C	O	0	0
			40	35	5		
30	j	1	Total	C		0	0
			10	10			
30	m	1	Total	C		0	0
			10	10			

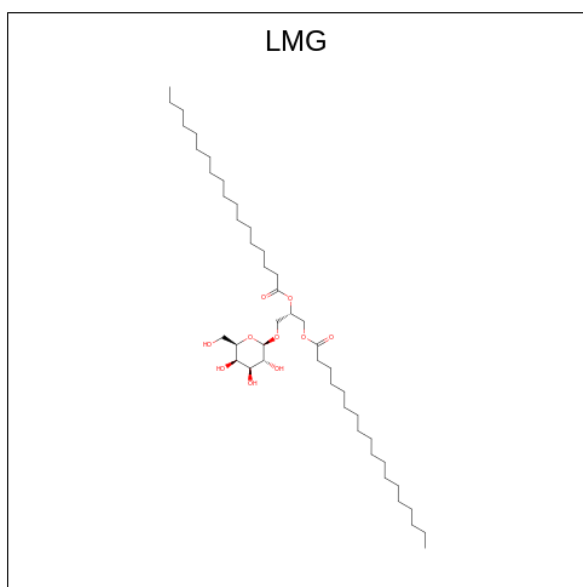
- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code:

LHG) (formula: C₃₈H₇₅O₁₀P).



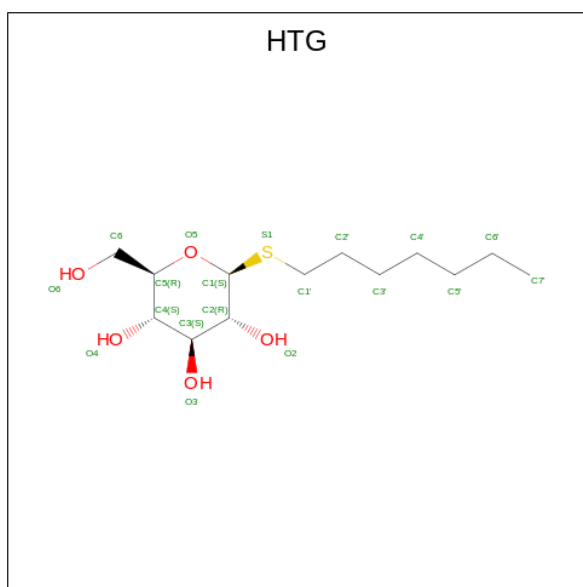
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	E	1	Total	C	O	P	0	0
			42	31	10	1		
31	L	1	Total	C	O	P	0	0
			49	38	10	1		
31	a	1	Total	C	O	P	0	0
			42	31	10	1		
31	b	1	Total	C	O	P	0	0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

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



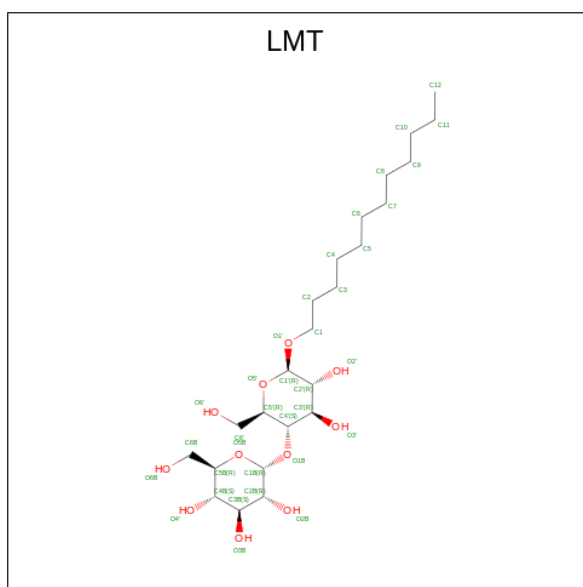
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	B	1	Total	C	O	0	0
			51	41	10		
32	C	1	Total	C	O	0	0
			51	41	10		
32	C	1	Total	C	O	0	0
			51	41	10		
32	C	1	Total	C	O	0	0
			51	41	10		
32	D	1	Total	C	O	0	0
			51	41	10		
32	Z	1	Total	C	O	0	0
			37	27	10		
32	c	1	Total	C	O	0	0
			51	41	10		
32	c	1	Total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

- Molecule 33 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



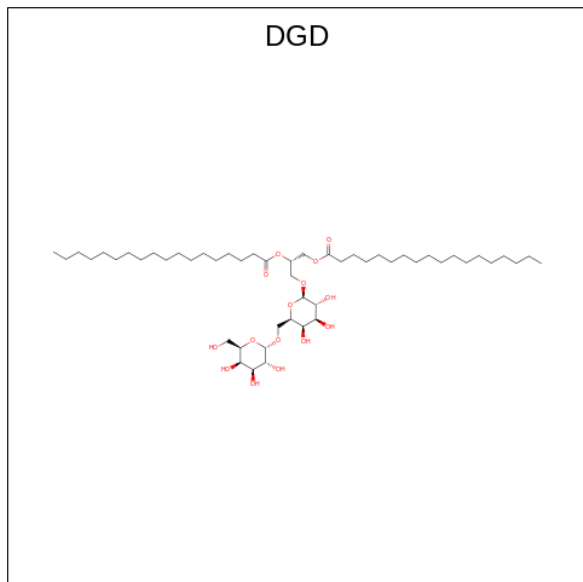
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	C	1	Total	C	O	S	0	0
			19	13	5	1		
33	D	1	Total	C	O	S	0	0
			16	10	5	1		
33	V	1	Total	C	O		0	0
			11	6	5			
33	b	1	Total	C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

- Molecule 34 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



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

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



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

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

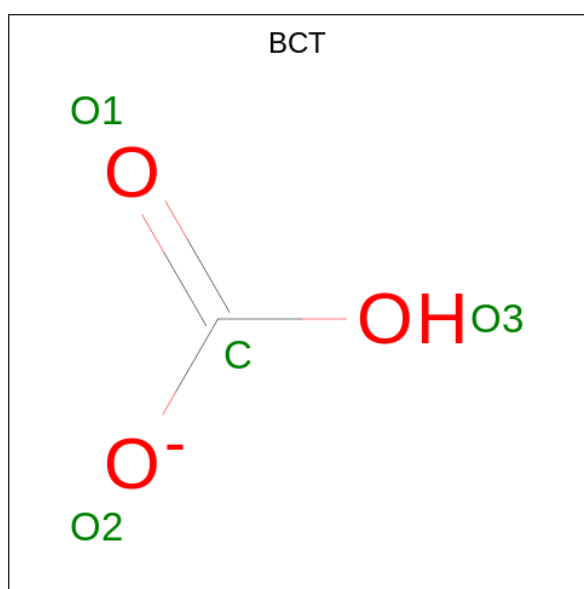
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	C	1	Total	Ca	0	0
			1	1		
36	F	1	Total	Ca	0	0
			1	1		

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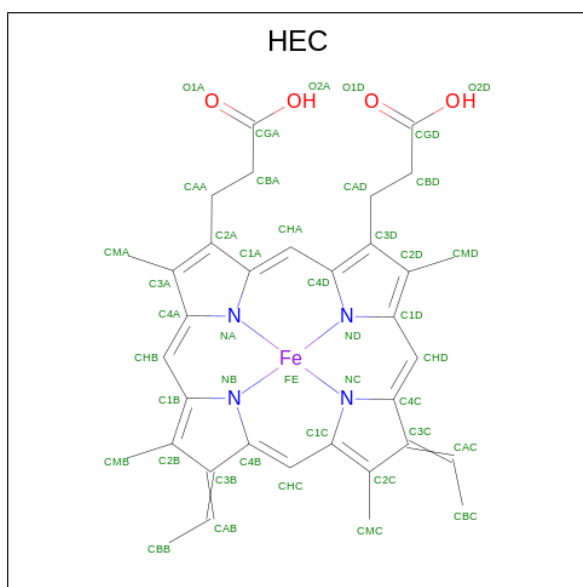
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	O	1	Total Ca 1 1	0	0
36	a	1	Total Ca 1 1	0	0
36	c	2	Total Ca 2 2	0	0
36	o	1	Total Ca 1 1	0	0

- Molecule 37 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



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

- Molecule 38 is HEME C (three-letter code: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



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

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

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

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	A	143	Total	O	0	0
			143	143		
40	B	223	Total	O	0	0
			223	223		
40	C	203	Total	O	0	0
			203	203		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	D	136	Total O 136 136	0	0
40	E	27	Total O 27 27	0	0
40	F	9	Total O 9 9	0	0
40	H	26	Total O 26 26	0	0
40	I	5	Total O 5 5	0	0
40	J	5	Total O 5 5	0	0
40	K	7	Total O 7 7	0	0
40	L	6	Total O 6 6	0	0
40	M	17	Total O 17 17	0	0
40	O	125	Total O 125 125	0	0
40	T	16	Total O 16 16	0	0
40	U	56	Total O 56 56	0	0
40	V	102	Total O 102 102	0	0
40	X	9	Total O 9 9	0	0
40	Y	1	Total O 1 1	0	0
40	R	1	Total O 1 1	0	0
40	a	143	Total O 143 143	0	0
40	b	234	Total O 234 234	0	0
40	c	174	Total O 174 174	0	0
40	d	125	Total O 125 125	0	0
40	e	16	Total O 16 16	0	0

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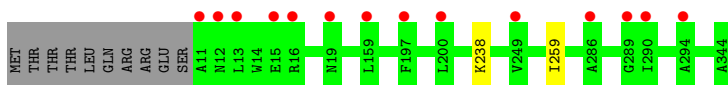
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	f	4	Total 4	O 4	0	0
40	h	23	Total 23	O 23	0	0
40	i	2	Total 2	O 2	0	0
40	j	3	Total 3	O 3	0	0
40	k	5	Total 5	O 5	0	0
40	l	7	Total 7	O 7	0	0
40	m	11	Total 11	O 11	0	0
40	o	99	Total 99	O 99	0	0
40	t	11	Total 11	O 11	0	0
40	u	71	Total 71	O 71	0	0
40	v	60	Total 60	O 60	0	0
40	x	9	Total 9	O 9	0	0
40	y	4	Total 4	O 4	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.

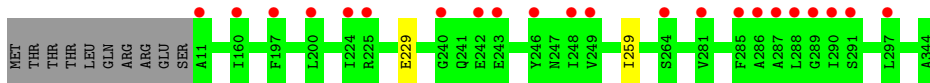
- Molecule 1: Photosystem II protein D1

Chain A: 4% 97%



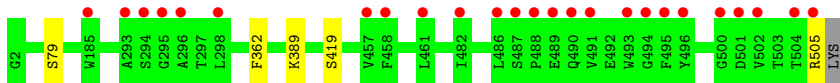
- Molecule 1: Photosystem II protein D1

Chain a: 6% 97%



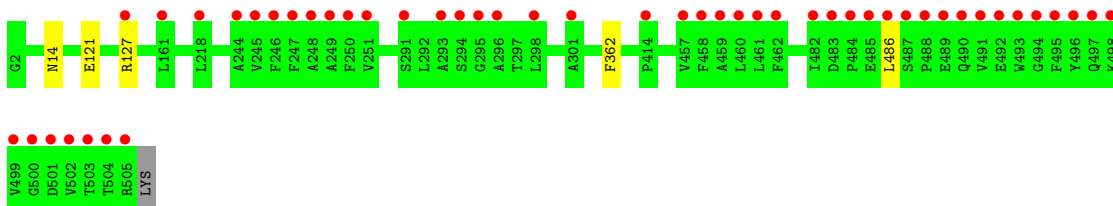
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B: 5% 99%



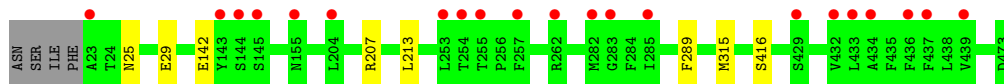
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b: 10% 99%

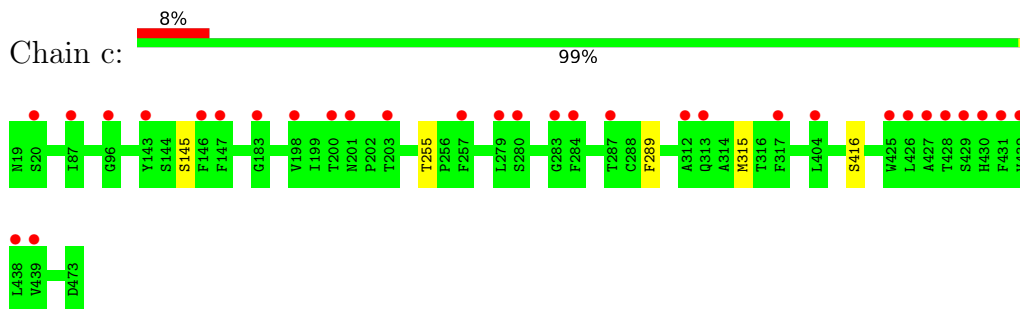


- Molecule 3: Photosystem II CP43 reaction center protein

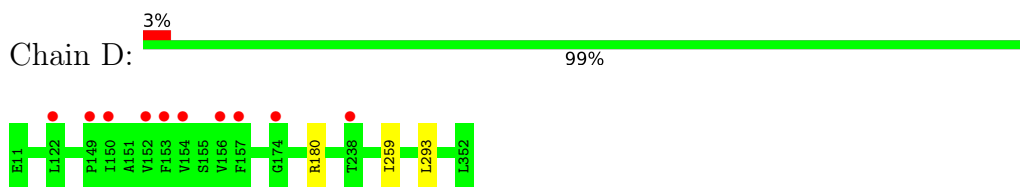
Chain C: 5% 97%



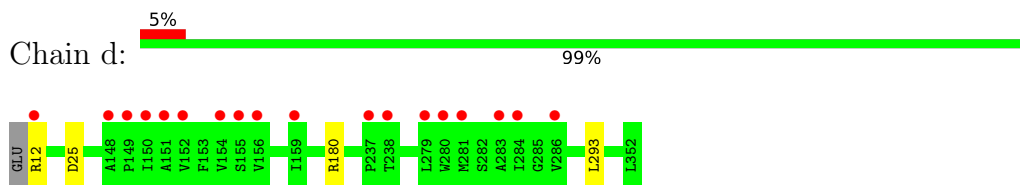
- Molecule 3: Photosystem II CP43 reaction center protein



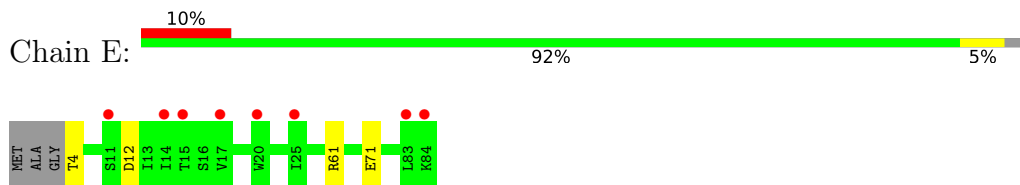
- Molecule 4: Photosystem II D2 protein



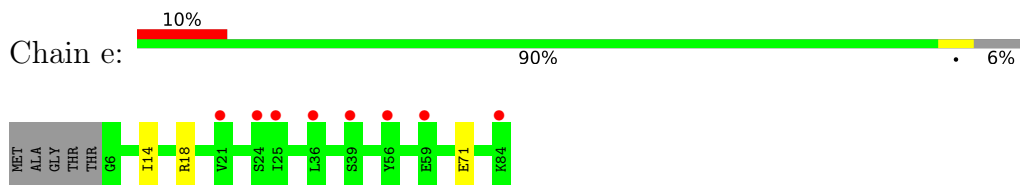
- Molecule 4: Photosystem II D2 protein



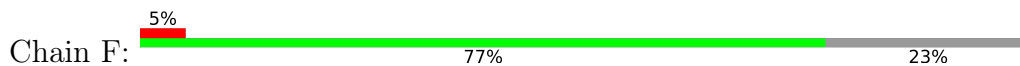
- Molecule 5: Cytochrome b559 subunit alpha

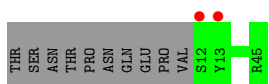


- Molecule 5: Cytochrome b559 subunit alpha

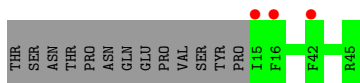


- Molecule 6: Cytochrome b559 subunit beta

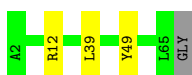




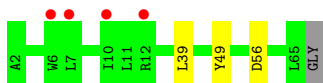
- Molecule 6: Cytochrome b559 subunit beta



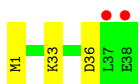
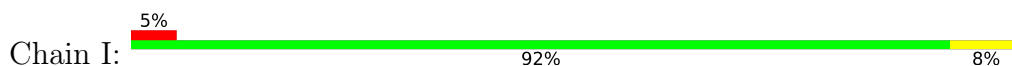
- Molecule 7: Photosystem II reaction center protein H



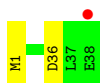
- Molecule 7: Photosystem II reaction center protein H



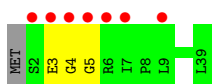
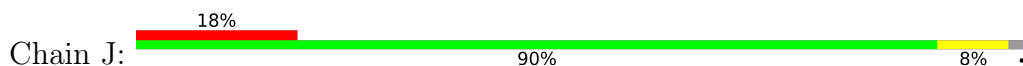
- Molecule 8: Photosystem II reaction center protein I



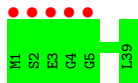
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



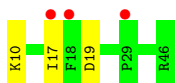
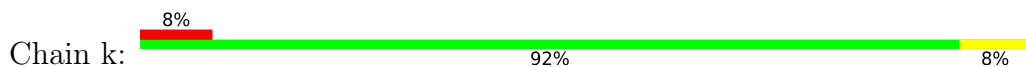
- Molecule 9: Photosystem II reaction center protein J



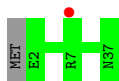
- Molecule 10: Photosystem II reaction center protein K



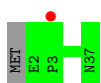
- Molecule 10: Photosystem II reaction center protein K



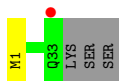
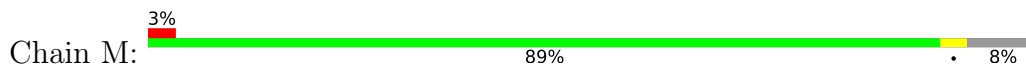
- Molecule 11: Photosystem II reaction center protein L



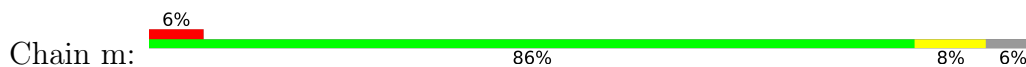
- Molecule 11: Photosystem II reaction center protein L



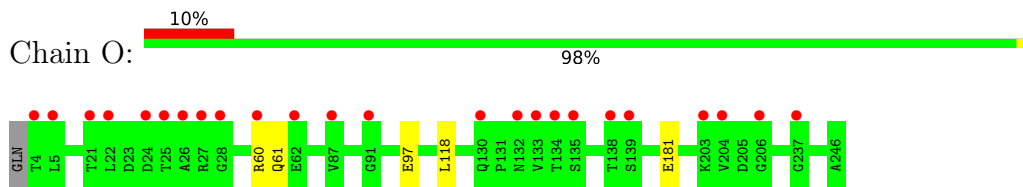
- Molecule 12: Photosystem II reaction center protein M



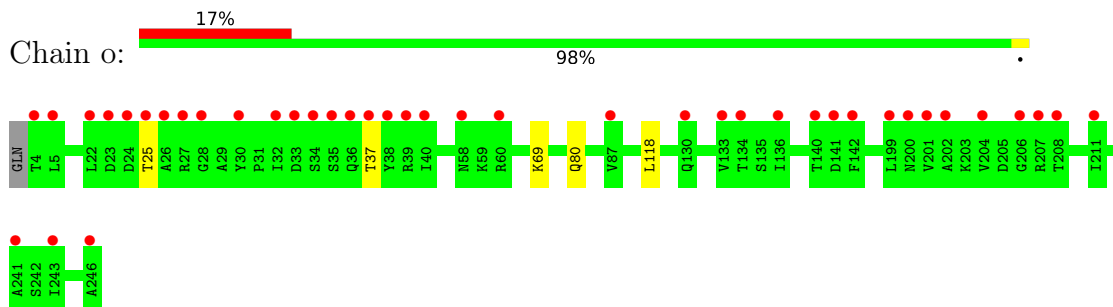
- Molecule 12: Photosystem II reaction center protein M



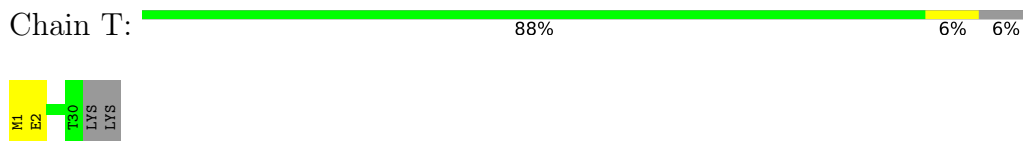
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



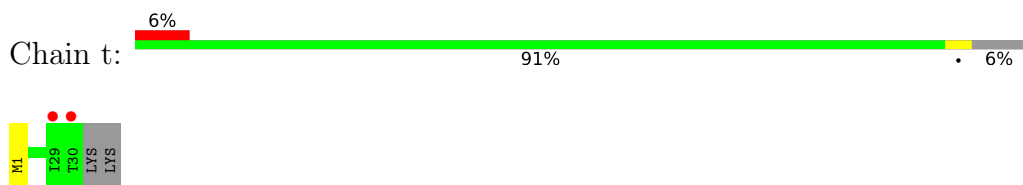
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



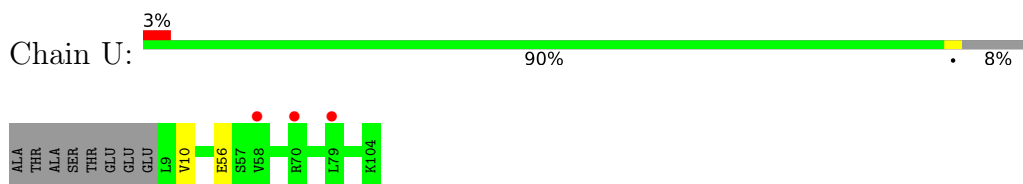
- Molecule 14: Photosystem II reaction center protein T



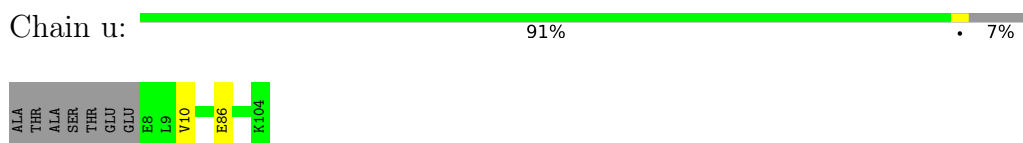
- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein

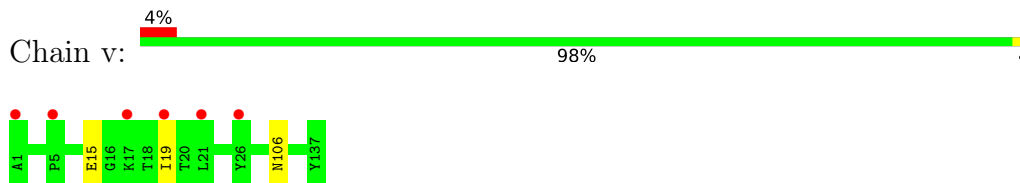


- Molecule 16: Cytochrome c-550

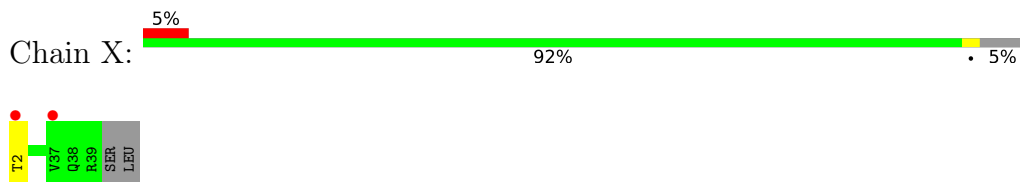


There are no outlier residues recorded for this chain.

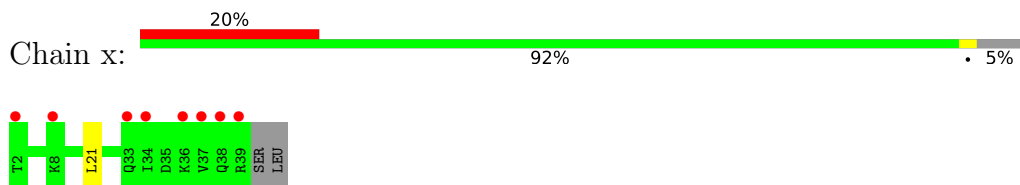
- Molecule 16: Cytochrome c-550



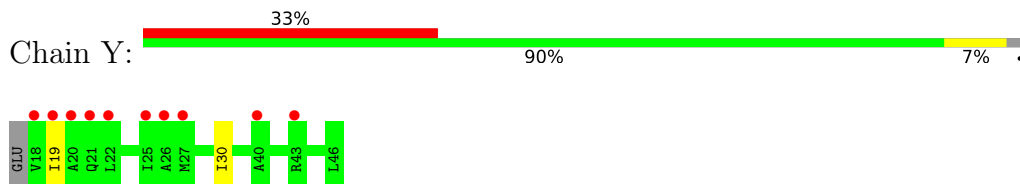
- Molecule 17: Photosystem II reaction center protein X



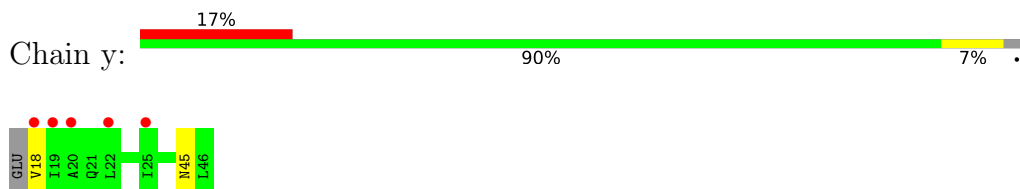
- Molecule 17: Photosystem II reaction center protein X



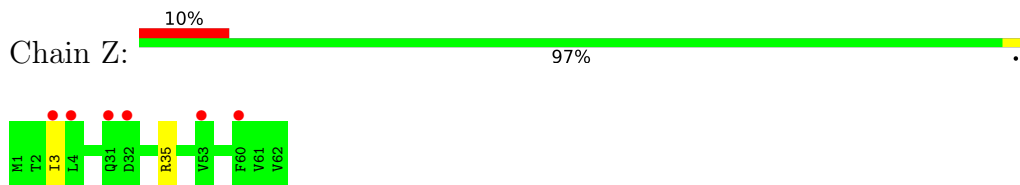
- Molecule 18: Photosystem II reaction center protein Ycf12



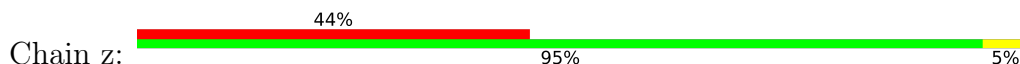
- Molecule 18: Photosystem II reaction center protein Ycf12

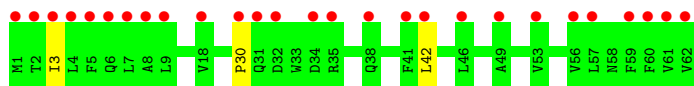


- Molecule 19: Photosystem II reaction center protein Z

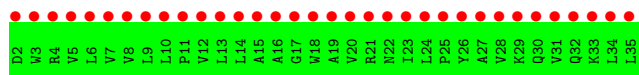


- Molecule 19: Photosystem II reaction center protein Z





- 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	126.15Å 232.70Å 288.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.97 – 2.25 52.83 – 2.25	Depositor EDS
% Data completeness (in resolution range)	96.0 (39.97-2.25) 85.6 (52.83-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.25Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.169 , 0.211 0.170 , 0.212	Depositor DCC
R_{free} test set	20023 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	43.9	Xtrriage
Anisotropy	0.424	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 70.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	53138	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% 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: PL9, LMT, LMG, CLA, LHG, BCT, CA, GOL, FME, FE2, HEC, DGD, UNL, CL, OEX, PHO, MG, HTG, BCR, SQD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.44	0/2719	0.56	0/3708
1	a	0.41	0/2727	0.54	0/3719
2	B	0.42	0/4190	0.55	0/5708
2	b	0.40	0/4138	0.53	0/5640
3	C	0.39	0/3626	0.51	0/4936
3	c	0.36	0/3648	0.49	0/4966
4	D	0.44	0/2821	0.55	0/3844
4	d	0.41	0/2812	0.53	0/3832
5	E	0.35	0/687	0.48	0/936
5	e	0.34	0/667	0.46	0/908
6	F	0.35	0/284	0.44	0/387
6	f	0.30	0/257	0.47	0/349
7	H	0.34	0/530	0.57	0/723
7	h	0.33	0/519	0.53	0/708
8	I	0.35	0/311	0.47	0/419
8	i	0.33	0/311	0.48	0/419
9	J	0.31	0/278	0.49	0/376
9	j	0.33	0/283	0.49	0/383
10	K	0.35	0/303	0.47	0/416
10	k	0.32	0/303	0.51	0/416
11	L	0.45	0/311	0.50	0/423
11	l	0.39	0/311	0.48	0/423
12	M	0.38	0/261	0.53	0/357
12	m	0.41	0/262	0.51	0/357
13	O	0.38	0/1917	0.58	0/2599
13	o	0.36	0/1910	0.57	0/2589
14	T	0.46	0/257	0.49	0/349
14	t	0.43	0/257	0.45	0/349
15	U	0.38	0/776	0.56	0/1052
15	u	0.36	0/785	0.59	0/1064
16	V	0.34	0/1085	0.52	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.33	0/1085	0.50	0/1473
17	X	0.29	0/284	0.47	0/384
17	x	0.28	0/284	0.43	0/384
18	Y	0.29	0/216	0.42	0/289
18	y	0.28	0/216	0.43	0/289
19	Z	0.30	0/490	0.39	0/669
19	z	0.29	0/490	0.41	0/669
20	R	0.26	0/279	0.40	0/383
All	All	0.39	0/42890	0.52	0/58368

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	334/344 (97%)	330 (99%)	3 (1%)	1 (0%)	41	46
1	a	335/344 (97%)	328 (98%)	6 (2%)	1 (0%)	41	46
2	B	512/505 (101%)	505 (99%)	7 (1%)	0	100	100
2	b	506/505 (100%)	497 (98%)	9 (2%)	0	100	100
3	C	453/455 (100%)	443 (98%)	8 (2%)	2 (0%)	34	37
3	c	455/455 (100%)	444 (98%)	10 (2%)	1 (0%)	47	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	340/342 (99%)	329 (97%)	11 (3%)	0	100	100
4	d	339/342 (99%)	331 (98%)	8 (2%)	0	100	100
5	E	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
5	e	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	29/44 (66%)	29 (100%)	0	0	100	100
7	H	63/65 (97%)	61 (97%)	2 (3%)	0	100	100
7	h	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
8	I	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
9	J	36/39 (92%)	33 (92%)	0	3 (8%)	1	0
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	32/36 (89%)	30 (94%)	2 (6%)	0	100	100
13	O	244/244 (100%)	237 (97%)	6 (2%)	1 (0%)	34	37
13	o	243/244 (100%)	236 (97%)	7 (3%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	94/104 (90%)	92 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
16	v	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
17	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
17	x	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
18	Y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
18	y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	9	4
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	5246/5384 (97%)	5129 (98%)	107 (2%)	10 (0%)	47	55

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416	SER
9	J	4	GLY
9	J	5	GLY
13	O	61	GLN
9	J	3	GLU
1	a	259	ILE
19	z	30	PRO
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	271/279 (97%)	270 (100%)	1 (0%)	91	94
1	a	272/279 (98%)	271 (100%)	1 (0%)	91	94
2	B	412/403 (102%)	407 (99%)	5 (1%)	71	80
2	b	406/403 (101%)	401 (99%)	5 (1%)	71	80
3	C	356/356 (100%)	349 (98%)	7 (2%)	55	64
3	c	358/356 (101%)	354 (99%)	4 (1%)	73	82
4	D	277/277 (100%)	274 (99%)	3 (1%)	73	82
4	d	276/277 (100%)	272 (99%)	4 (1%)	67	76
5	E	73/73 (100%)	69 (94%)	4 (6%)	21	21
5	e	70/73 (96%)	67 (96%)	3 (4%)	29	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	25/38 (66%)	25 (100%)	0	100	100
7	H	55/54 (102%)	51 (93%)	4 (7%)	14	12
7	h	54/54 (100%)	51 (94%)	3 (6%)	21	21
8	I	34/34 (100%)	32 (94%)	2 (6%)	19	19
8	i	34/34 (100%)	33 (97%)	1 (3%)	42	51
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	26/27 (96%)	26 (100%)	0	100	100
10	K	30/30 (100%)	27 (90%)	3 (10%)	7	5
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	5
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	30/32 (94%)	30 (100%)	0	100	100
12	m	30/32 (94%)	28 (93%)	2 (7%)	16	15
13	O	209/207 (101%)	205 (98%)	4 (2%)	57	66
13	o	208/207 (100%)	203 (98%)	5 (2%)	49	58
14	T	26/28 (93%)	25 (96%)	1 (4%)	33	39
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	83/89 (93%)	81 (98%)	2 (2%)	49	58
15	u	84/89 (94%)	82 (98%)	2 (2%)	49	58
16	V	117/117 (100%)	117 (100%)	0	100	100
16	v	117/117 (100%)	114 (97%)	3 (3%)	46	55
17	X	31/33 (94%)	30 (97%)	1 (3%)	39	47
17	x	31/33 (94%)	30 (97%)	1 (3%)	39	47
18	Y	22/23 (96%)	20 (91%)	2 (9%)	9	7
18	y	22/23 (96%)	20 (91%)	2 (9%)	9	7
19	Z	52/52 (100%)	50 (96%)	2 (4%)	33	39
19	z	52/52 (100%)	50 (96%)	2 (4%)	33	39
20	R	29/29 (100%)	29 (100%)	0	100	100
All	All	4352/4403 (99%)	4270 (98%)	82 (2%)	57	66

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	238	LYS
2	B	79	SER
2	B	362	PHE
2	B	389	LYS
2	B	419	SER
2	B	505	ARG
3	C	25	ASN
3	C	29	GLU
3	C	142	GLU
3	C	207	ARG
3	C	213	LEU
3	C	289	PHE
3	C	315	MET
4	D	180	ARG
4	D	259	ILE
4	D	293	LEU
5	E	4	THR
5	E	12	ASP
5	E	61	ARG
5	E	71	GLU
7	H	12[A]	ARG
7	H	12[B]	ARG
7	H	39	LEU
7	H	49	TYR
8	I	33	LYS
8	I	36	ASP
10	K	10	LYS
10	K	17	ILE
10	K	19	ASP
13	O	60	ARG
13	O	97	GLU
13	O	118	LEU
13	O	181	GLU
14	T	2	GLU
15	U	10	VAL
15	U	56	GLU
17	X	2	THR
18	Y	19	ILE
18	Y	30	ILE
19	Z	3	ILE
19	Z	35	ARG
1	a	229	GLU
2	b	14	ASN

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Mol	Chain	Res	Type
2	b	121	GLU
2	b	127	ARG
2	b	362	PHE
2	b	486	LEU
3	c	145	SER
3	c	255	THR
3	c	289	PHE
3	c	315	MET
4	d	12	ARG
4	d	25	ASP
4	d	180	ARG
4	d	293	LEU
5	e	14	ILE
5	e	18	ARG
5	e	71	GLU
7	h	39	LEU
7	h	49	TYR
7	h	56	ASP
8	i	36	ASP
10	k	10	LYS
10	k	17	ILE
10	k	19	ASP
12	m	5	GLN
12	m	16	LEU
13	o	25	THR
13	o	37	THR
13	o	69	LYS
13	o	80	GLN
13	o	118	LEU
15	u	10	VAL
15	u	86	GLU
16	v	15	GLU
16	v	19	ILE
16	v	106	ASN
17	x	21	LEU
18	y	18	VAL
18	y	45	ASN
19	z	3	ILE
19	z	42	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	490	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	FME	T	1	14	8,9,10	0.70	0	7,9,11	1.44	2 (28%)
8	FME	i	1	8	8,9,10	0.56	0	7,9,11	1.05	1 (14%)
14	FME	t	1	14	8,9,10	0.62	0	7,9,11	1.74	2 (28%)
12	FME	M	1	12	8,9,10	0.60	0	7,9,11	1.70	2 (28%)
12	FME	m	1	12	8,9,10	0.56	0	7,9,11	1.46	2 (28%)
8	FME	I	1	8	8,9,10	0.66	0	7,9,11	1.15	1 (14%)

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

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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	CA-N-CN	-3.25	117.82	122.82
12	M	1	FME	CA-N-CN	-3.08	118.08	122.82
14	t	1	FME	O-C-CA	-2.60	117.96	124.78
14	T	1	FME	O-C-CA	-2.48	118.29	124.78
12	m	1	FME	C-CA-N	2.39	114.04	109.73
14	T	1	FME	CA-N-CN	-2.36	119.19	122.82
12	m	1	FME	O-C-CA	-2.24	118.90	124.78
8	I	1	FME	O-C-CA	-2.04	119.44	124.78
8	i	1	FME	O-C-CA	-2.04	119.44	124.78
12	M	1	FME	O1-CN-N	-2.03	119.93	125.27

There are no chirality outliers.

All (7) torsion outliers are listed below:

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

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 216 ligands modelled in this entry, 15 are monoatomic and 18 are unknown - leaving 183 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
27	SQD	f	101	-	42,43,54	1.17	3 (7%)	51,54,65	1.30	8 (15%)
23	CLA	b	601	40	65,73,73	2.14	16 (24%)	76,113,113	2.74	26 (34%)
23	CLA	c	510	-	65,73,73	2.14	16 (24%)	76,113,113	2.78	27 (35%)
26	GOL	o	302	-	5,5,5	0.82	0	5,5,5	1.04	0
23	CLA	b	614	-	65,73,73	2.01	16 (24%)	76,113,113	2.85	29 (38%)
23	CLA	b	607	40	65,73,73	2.00	17 (26%)	76,113,113	2.77	27 (35%)
33	HTG	h	101	-	16,16,19	1.14	2 (12%)	20,21,24	2.11	5 (25%)
26	GOL	B	624	-	5,5,5	0.89	0	5,5,5	1.02	0
23	CLA	C	510	-	65,73,73	2.07	17 (26%)	76,113,113	2.80	29 (38%)
23	CLA	C	514	-	65,73,73	2.08	16 (24%)	76,113,113	2.72	29 (38%)
35	DGD	c	519	-	63,63,67	0.85	2 (3%)	77,77,81	1.00	3 (3%)
23	CLA	B	603	-	65,73,73	2.04	16 (24%)	76,113,113	2.89	27 (35%)
25	BCR	B	619	-	41,41,41	1.03	1 (2%)	56,56,56	1.30	9 (16%)
27	SQD	D	412	-	42,43,54	1.15	3 (7%)	51,54,65	1.79	11 (21%)
23	CLA	a	404	-	65,73,73	2.02	16 (24%)	76,113,113	2.82	31 (40%)
34	LMT	e	101	-	36,36,36	0.53	1 (2%)	47,47,47	1.04	2 (4%)
29	PL9	D	406	-	55,55,55	0.67	2 (3%)	68,69,69	1.66	17 (25%)
27	SQD	b	620	-	53,54,54	1.03	3 (5%)	62,65,65	1.55	8 (12%)
23	CLA	b	609	-	65,73,73	2.04	18 (27%)	76,113,113	2.71	29 (38%)
23	CLA	b	613	-	65,73,73	2.05	15 (23%)	76,113,113	2.76	27 (35%)
35	DGD	c	518	-	63,63,67	0.89	2 (3%)	77,77,81	1.05	6 (7%)
26	GOL	b	628	-	5,5,5	0.97	0	5,5,5	1.07	0
23	CLA	B	601	40	65,73,73	2.10	17 (26%)	76,113,113	2.77	27 (35%)
32	LMG	c	501	-	51,51,55	0.92	2 (3%)	59,59,63	1.09	3 (5%)
34	LMT	a	413	-	36,36,36	0.59	1 (2%)	47,47,47	1.14	3 (6%)
26	GOL	B	627	-	5,5,5	0.99	0	5,5,5	1.15	0
31	LHG	D	408	-	48,48,48	0.90	2 (4%)	51,54,54	0.96	3 (5%)
23	CLA	D	403	-	65,73,73	2.00	16 (24%)	76,113,113	2.91	29 (38%)
23	CLA	d	402	-	65,73,73	2.01	16 (24%)	76,113,113	2.71	31 (40%)
23	CLA	b	606	-	65,73,73	1.99	15 (23%)	76,113,113	2.92	29 (38%)
25	BCR	T	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.57	12 (21%)
24	PHO	a	417	-	51,69,69	1.85	8 (15%)	47,99,99	2.07	9 (19%)
25	BCR	H	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.36	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	HEC	V	201	16	32,50,50	2.03	4 (12%)	24,82,82	1.95	6 (25%)
23	CLA	b	611	-	65,73,73	2.00	16 (24%)	76,113,113	2.82	27 (35%)
23	CLA	B	610	40	65,73,73	2.07	17 (26%)	76,113,113	2.79	26 (34%)
23	CLA	b	616	-	65,73,73	2.01	15 (23%)	76,113,113	2.86	30 (39%)
32	LMG	Z	101	-	37,37,55	1.01	3 (8%)	45,45,63	1.53	6 (13%)
23	CLA	B	616	-	65,73,73	1.98	16 (24%)	76,113,113	2.76	28 (36%)
25	BCR	b	618	-	41,41,41	1.03	1 (2%)	56,56,56	1.30	8 (14%)
23	CLA	b	612	-	65,73,73	2.05	17 (26%)	76,113,113	2.83	27 (35%)
25	BCR	a	409	-	41,41,41	1.08	1 (2%)	56,56,56	1.47	10 (17%)
23	CLA	c	503	-	65,73,73	2.01	17 (26%)	76,113,113	2.78	27 (35%)
23	CLA	B	614	-	65,73,73	1.95	17 (26%)	76,113,113	3.02	28 (36%)
35	DGD	c	520	-	63,63,67	0.88	2 (3%)	77,77,81	1.02	5 (6%)
23	CLA	C	507	-	65,73,73	1.98	16 (24%)	76,113,113	2.68	25 (32%)
26	GOL	O	302	-	5,5,5	0.86	0	5,5,5	1.01	0
34	LMT	M	101	-	36,36,36	0.45	0	47,47,47	0.97	3 (6%)
29	PL9	A	413	-	55,55,55	0.66	2 (3%)	68,69,69	1.87	21 (30%)
25	BCR	h	102	-	41,41,41	1.07	1 (2%)	56,56,56	1.31	7 (12%)
32	LMG	d	412	39	51,51,55	0.92	2 (3%)	59,59,63	0.87	2 (3%)
25	BCR	b	617	-	41,41,41	1.10	1 (2%)	56,56,56	1.50	7 (12%)
23	CLA	A	404	-	65,73,73	2.07	18 (27%)	76,113,113	2.80	31 (40%)
23	CLA	B	613	-	65,73,73	1.99	16 (24%)	76,113,113	2.76	27 (35%)
23	CLA	A	406	40	65,73,73	2.01	17 (26%)	76,113,113	2.73	25 (32%)
34	LMT	C	526	-	36,36,36	0.49	1 (2%)	47,47,47	1.04	3 (6%)
33	HTG	D	411	-	16,16,19	1.06	2 (12%)	20,21,24	1.33	1 (5%)
26	GOL	A	410	-	5,5,5	1.12	0	5,5,5	0.81	0
31	LHG	d	408	-	48,48,48	0.90	2 (4%)	51,54,54	1.07	3 (5%)
35	DGD	h	103	-	63,63,67	0.91	3 (4%)	77,77,81	1.01	3 (3%)
25	BCR	c	517	-	41,41,41	1.06	1 (2%)	56,56,56	1.44	11 (19%)
33	HTG	V	202	-	11,11,19	0.21	0	15,15,24	1.25	2 (13%)
23	CLA	C	511	-	65,73,73	2.14	18 (27%)	76,113,113	2.70	28 (36%)
33	HTG	B	623	-	19,19,19	0.81	1 (5%)	23,24,24	1.82	5 (21%)
32	LMG	D	413	39	51,51,55	0.83	2 (3%)	59,59,63	0.96	4 (6%)
25	BCR	B	617	-	41,41,41	1.06	1 (2%)	56,56,56	1.35	7 (12%)
24	PHO	a	407	-	51,69,69	1.85	9 (17%)	47,99,99	1.89	10 (21%)
32	LMG	c	522	-	51,51,55	0.96	2 (3%)	59,59,63	1.11	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LHG	A	416	-	48,48,48	0.89	2 (4%)	51,54,54	1.12	6 (11%)
31	LHG	d	407	-	48,48,48	0.89	2 (4%)	51,54,54	1.01	4 (7%)
27	SQD	B	620	-	53,54,54	1.04	3 (5%)	62,65,65	1.44	11 (17%)
23	CLA	C	506	40	65,73,73	1.99	17 (26%)	76,113,113	2.75	28 (36%)
23	CLA	c	514	-	65,73,73	2.04	16 (24%)	76,113,113	2.76	30 (39%)
23	CLA	B	611	-	65,73,73	2.04	16 (24%)	76,113,113	2.91	30 (39%)
23	CLA	b	610	40	65,73,73	2.04	17 (26%)	76,113,113	2.78	29 (38%)
38	HEC	e	102	5,6	32,50,50	1.57	4 (12%)	24,82,82	1.80	5 (20%)
31	LHG	D	407	-	48,48,48	0.88	2 (4%)	51,54,54	1.00	3 (5%)
25	BCR	k	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.45	11 (19%)
25	BCR	y	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.61	10 (17%)
31	LHG	L	101	-	48,48,48	0.92	3 (6%)	51,54,54	1.11	3 (5%)
23	CLA	D	404	-	65,73,73	2.02	16 (24%)	76,113,113	2.74	25 (32%)
23	CLA	a	405	40	65,73,73	2.08	15 (23%)	76,113,113	2.82	28 (36%)
23	CLA	B	605	-	65,73,73	2.01	15 (23%)	76,113,113	2.73	25 (32%)
23	CLA	B	615	-	65,73,73	1.95	15 (23%)	76,113,113	2.84	27 (35%)
23	CLA	a	406	40	65,73,73	1.93	14 (21%)	76,113,113	2.83	27 (35%)
34	LMT	b	621	-	25,25,36	0.51	0	30,30,47	0.58	0
26	GOL	b	624	-	5,5,5	0.95	0	5,5,5	1.06	0
27	SQD	a	410	-	53,54,54	0.98	3 (5%)	62,65,65	1.68	11 (17%)
23	CLA	B	609	-	65,73,73	1.97	16 (24%)	76,113,113	2.82	26 (34%)
34	LMT	m	103	-	36,36,36	0.46	0	47,47,47	0.99	4 (8%)
23	CLA	d	403	-	65,73,73	2.10	17 (26%)	76,113,113	2.81	30 (39%)
33	HTG	B	625	-	19,19,19	1.04	2 (10%)	23,24,24	1.11	1 (4%)
35	DGD	C	520	-	63,63,67	0.84	2 (3%)	77,77,81	1.04	5 (6%)
34	LMT	D	402	-	36,36,36	0.52	1 (2%)	47,47,47	0.85	1 (2%)
32	LMG	z	101	-	39,39,55	1.08	2 (5%)	47,47,63	1.10	3 (6%)
23	CLA	C	505	-	65,73,73	2.03	16 (24%)	76,113,113	2.84	24 (31%)
25	BCR	D	405	-	41,41,41	1.06	1 (2%)	56,56,56	1.64	12 (21%)
23	CLA	B	612	-	65,73,73	1.97	16 (24%)	76,113,113	2.97	28 (36%)
23	CLA	C	504	-	65,73,73	1.99	16 (24%)	76,113,113	2.69	27 (35%)
34	LMT	t	101	-	26,26,36	0.55	1 (3%)	31,31,47	1.14	4 (12%)
23	CLA	C	513	3	65,73,73	2.07	19 (29%)	76,113,113	2.72	27 (35%)
33	HTG	b	625	-	19,19,19	0.99	2 (10%)	23,24,24	1.30	3 (13%)
26	GOL	a	411	-	5,5,5	0.87	0	5,5,5	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	DGD	H	102	-	63,63,67	0.83	3 (4%)	77,77,81	1.04	5 (6%)
33	HTG	b	623	-	19,19,19	1.00	1 (5%)	23,24,24	1.59	2 (8%)
23	CLA	b	615	-	65,73,73	1.99	15 (23%)	76,113,113	2.74	27 (35%)
23	CLA	c	511	-	65,73,73	2.11	17 (26%)	76,113,113	2.72	26 (34%)
31	LHG	E	101	-	41,41,48	1.04	2 (4%)	44,47,54	1.03	2 (4%)
32	LMG	m	101	-	51,51,55	0.89	2 (3%)	59,59,63	1.12	5 (8%)
37	BCT	d	401	21	2,3,3	0.58	0	2,3,3	1.69	1 (50%)
32	LMG	C	521	-	51,51,55	0.99	2 (3%)	59,59,63	1.03	3 (5%)
26	GOL	v	201	-	5,5,5	1.15	0	5,5,5	0.82	0
29	PL9	d	405	-	55,55,55	0.64	1 (1%)	68,69,69	1.66	16 (23%)
23	CLA	c	513	3	65,73,73	2.05	15 (23%)	76,113,113	2.85	28 (36%)
23	CLA	B	606	-	65,73,73	2.04	16 (24%)	76,113,113	2.85	28 (36%)
23	CLA	b	604	-	65,73,73	2.04	16 (24%)	76,113,113	2.70	29 (38%)
23	CLA	c	505	-	65,73,73	2.04	16 (24%)	76,113,113	2.74	25 (32%)
23	CLA	C	512	-	65,73,73	2.05	16 (24%)	76,113,113	2.76	28 (36%)
33	HTG	B	622	-	19,19,19	1.00	1 (5%)	23,24,24	1.59	5 (21%)
34	LMT	E	102	-	36,36,36	0.52	1 (2%)	47,47,47	0.85	1 (2%)
35	DGD	C	519	-	63,63,67	0.90	2 (3%)	77,77,81	1.10	4 (5%)
23	CLA	C	508	-	65,73,73	2.08	17 (26%)	76,113,113	2.73	30 (39%)
27	SQD	C	501	-	53,54,54	0.95	3 (5%)	62,65,65	1.90	10 (16%)
23	CLA	c	506	40	65,73,73	2.12	17 (26%)	76,113,113	2.83	30 (39%)
38	HEC	E	103	5,6	32,50,50	1.53	4 (12%)	24,82,82	1.93	6 (25%)
25	BCR	C	516	-	41,41,41	1.00	1 (2%)	56,56,56	1.62	10 (17%)
23	CLA	B	607	40	65,73,73	1.99	17 (26%)	76,113,113	2.73	28 (36%)
25	BCR	K	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.41	9 (16%)
32	LMG	C	522	-	51,51,55	1.01	3 (5%)	59,59,63	1.31	5 (8%)
23	CLA	c	515	-	65,73,73	2.07	16 (24%)	76,113,113	2.76	29 (38%)
23	CLA	c	512	-	65,73,73	2.00	16 (24%)	76,113,113	2.69	28 (36%)
34	LMT	B	628	-	36,36,36	0.42	0	47,47,47	1.10	3 (6%)
28	OEX	A	412	3,1,40	0,15,15	-	-	-	-	-
23	CLA	c	508	-	65,73,73	2.06	16 (24%)	76,113,113	2.76	29 (38%)
24	PHO	A	415	-	51,69,69	1.87	7 (13%)	47,99,99	1.86	12 (25%)
23	CLA	A	405	40	65,73,73	2.00	17 (26%)	76,113,113	2.84	28 (36%)
25	BCR	c	516	-	41,41,41	1.03	1 (2%)	56,56,56	1.45	10 (17%)
25	BCR	A	409	-	41,41,41	1.03	1 (2%)	56,56,56	1.48	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	HTG	c	523	-	19,19,19	0.96	2 (10%)	23,24,24	1.48	1 (4%)
23	CLA	b	602	-	65,73,73	2.10	16 (24%)	76,113,113	2.82	30 (39%)
23	CLA	B	608	-	65,73,73	2.02	16 (24%)	76,113,113	2.80	32 (42%)
31	LHG	d	406	-	48,48,48	0.88	2 (4%)	51,54,54	1.12	5 (9%)
34	LMT	a	418	-	36,36,36	0.45	0	47,47,47	0.92	1 (2%)
37	BCT	D	401	21	2,3,3	0.55	0	2,3,3	1.18	0
32	LMG	B	621	-	51,51,55	0.91	2 (3%)	59,59,63	1.16	4 (6%)
23	CLA	A	408	-	65,73,73	2.07	16 (24%)	76,113,113	2.71	30 (39%)
23	CLA	b	603	-	65,73,73	2.08	16 (24%)	76,113,113	2.86	28 (36%)
25	BCR	Y	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.84	17 (30%)
23	CLA	C	509	40	65,73,73	2.03	16 (24%)	76,113,113	2.74	25 (32%)
26	GOL	c	502	-	5,5,5	1.06	0	5,5,5	0.89	0
31	LHG	a	419	-	41,41,48	1.05	2 (4%)	44,47,54	0.97	2 (4%)
27	SQD	a	412	-	53,54,54	1.04	3 (5%)	62,65,65	1.28	6 (9%)
25	BCR	d	404	-	41,41,41	1.12	1 (2%)	56,56,56	1.73	11 (19%)
33	HTG	C	523	-	19,19,19	0.92	1 (5%)	23,24,24	1.41	1 (4%)
32	LMG	C	502	-	51,51,55	0.92	2 (3%)	59,59,63	1.02	2 (3%)
34	LMT	B	630	-	25,25,36	0.44	0	30,30,47	1.02	2 (6%)
23	CLA	c	504	-	65,73,73	2.05	15 (23%)	76,113,113	2.72	24 (31%)
25	BCR	C	517	-	41,41,41	1.01	1 (2%)	56,56,56	1.56	12 (21%)
35	DGD	C	518	-	63,63,67	0.88	2 (3%)	77,77,81	0.99	3 (3%)
23	CLA	B	602	-	65,73,73	2.05	16 (24%)	76,113,113	2.81	30 (39%)
23	CLA	C	503	-	65,73,73	1.99	16 (24%)	76,113,113	2.89	27 (35%)
34	LMT	M	103	-	36,36,36	0.46	0	47,47,47	1.03	2 (4%)
23	CLA	c	509	40	65,73,73	2.08	15 (23%)	76,113,113	2.83	28 (36%)
25	BCR	B	618	-	41,41,41	0.93	1 (2%)	56,56,56	1.41	7 (12%)
23	CLA	b	605	-	65,73,73	1.98	18 (27%)	76,113,113	2.94	24 (31%)
34	LMT	b	627	-	25,25,36	0.45	0	30,30,47	0.90	1 (3%)
23	CLA	B	604	-	65,73,73	2.04	18 (27%)	76,113,113	2.68	29 (38%)
26	GOL	C	524	-	5,5,5	1.08	0	5,5,5	0.94	0
28	OEX	a	414	3,1,40	0,15,15	-	-	-	-	-
23	CLA	b	608	-	65,73,73	2.07	16 (24%)	76,113,113	2.74	29 (38%)
24	PHO	A	407	-	51,69,69	1.80	8 (15%)	47,99,99	1.71	9 (19%)
23	CLA	c	507	-	65,73,73	2.01	16 (24%)	76,113,113	2.66	26 (34%)
32	LMG	c	521	-	51,51,55	0.92	2 (3%)	59,59,63	1.01	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	b	619	-	41,41,41	1.16	2 (4%)	56,56,56	1.50	11 (19%)
23	CLA	a	408	-	65,73,73	1.99	16 (24%)	76,113,113	2.79	28 (36%)
26	GOL	B	629	-	5,5,5	1.01	0	5,5,5	0.87	0
25	BCR	t	102	-	41,41,41	1.06	1 (2%)	56,56,56	1.41	10 (17%)
31	LHG	b	629	-	48,48,48	0.90	2 (4%)	51,54,54	1.04	3 (5%)
23	CLA	C	515	-	65,73,73	2.05	16 (24%)	76,113,113	2.75	26 (34%)
27	SQD	A	411	-	53,54,54	1.04	3 (5%)	62,65,65	1.26	7 (11%)
38	HEC	v	202	16	32,50,50	2.09	4 (12%)	24,82,82	1.87	5 (20%)
29	PL9	a	415	-	55,55,55	0.65	2 (3%)	68,69,69	1.98	22 (32%)
33	HTG	b	622	-	19,19,19	1.10	1 (5%)	23,24,24	1.42	2 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SQD	f	101	-	-	19/38/58/69	0/1/1/1
23	CLA	b	601	40	1/1/15/20	15/37/115/115	-
23	CLA	c	510	-	1/1/15/20	10/37/115/115	-
26	GOL	o	302	-	-	2/4/4/4	-
23	CLA	b	614	-	1/1/15/20	13/37/115/115	-
23	CLA	b	607	40	1/1/15/20	1/37/115/115	-
33	HTG	h	101	-	-	2/7/27/30	0/1/1/1
26	GOL	B	624	-	-	2/4/4/4	-
23	CLA	C	510	-	1/1/15/20	5/37/115/115	-
23	CLA	C	514	-	1/1/15/20	14/37/115/115	-
35	DGD	c	519	-	-	17/51/91/95	0/2/2/2
23	CLA	B	603	-	1/1/15/20	6/37/115/115	-
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
27	SQD	D	412	-	-	15/38/58/69	0/1/1/1
23	CLA	a	404	-	1/1/15/20	6/37/115/115	-
34	LMT	e	101	-	-	9/21/61/61	0/2/2/2
29	PL9	D	406	-	-	8/53/73/73	0/1/1/1
27	SQD	b	620	-	-	24/49/69/69	0/1/1/1
23	CLA	b	609	-	1/1/15/20	6/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	613	-	1/1/15/20	7/37/115/115	-
35	DGD	c	518	-	-	18/51/91/95	0/2/2/2
26	GOL	b	628	-	-	0/4/4/4	-
23	CLA	B	601	40	1/1/15/20	10/37/115/115	-
32	LMG	c	501	-	-	18/46/66/70	0/1/1/1
34	LMT	a	413	-	-	7/21/61/61	0/2/2/2
26	GOL	B	627	-	-	0/4/4/4	-
31	LHG	D	408	-	-	13/53/53/53	-
23	CLA	D	403	-	1/1/15/20	4/37/115/115	-
23	CLA	d	402	-	1/1/15/20	3/37/115/115	-
23	CLA	b	606	-	1/1/15/20	11/37/115/115	-
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
24	PHO	a	417	-	-	3/37/103/103	0/5/6/6
25	BCR	H	101	-	-	1/29/63/63	0/2/2/2
38	HEC	V	201	16	-	2/10/54/54	-
23	CLA	b	611	-	1/1/15/20	5/37/115/115	-
23	CLA	B	610	40	1/1/15/20	8/37/115/115	-
23	CLA	b	616	-	1/1/15/20	7/37/115/115	-
32	LMG	Z	101	-	-	9/31/51/70	0/1/1/1
23	CLA	B	616	-	1/1/15/20	6/37/115/115	-
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
23	CLA	b	612	-	1/1/15/20	4/37/115/115	-
25	BCR	a	409	-	-	2/29/63/63	0/2/2/2
23	CLA	c	503	-	1/1/15/20	5/37/115/115	-
23	CLA	B	614	-	1/1/15/20	14/37/115/115	-
35	DGD	c	520	-	-	10/51/91/95	0/2/2/2
23	CLA	C	507	-	1/1/15/20	7/37/115/115	-
26	GOL	O	302	-	-	4/4/4/4	-
34	LMT	M	101	-	-	6/21/61/61	0/2/2/2
29	PL9	A	413	-	-	16/53/73/73	0/1/1/1
25	BCR	h	102	-	-	0/29/63/63	0/2/2/2
32	LMG	d	412	39	-	9/46/66/70	0/1/1/1
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
23	CLA	A	404	-	1/1/15/20	2/37/115/115	-
23	CLA	B	613	-	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	A	406	40	-	4/37/115/115	-
34	LMT	C	526	-	-	8/21/61/61	0/2/2/2
33	HTG	D	411	-	-	2/7/27/30	0/1/1/1
26	GOL	A	410	-	-	2/4/4/4	-
31	LHG	d	408	-	-	10/53/53/53	-
35	DGD	h	103	-	-	14/51/91/95	0/2/2/2
25	BCR	c	517	-	-	0/29/63/63	0/2/2/2
33	HTG	V	202	-	-	1/2/19/30	0/1/1/1
23	CLA	C	511	-	1/1/15/20	5/37/115/115	-
33	HTG	B	623	-	-	4/10/30/30	0/1/1/1
32	LMG	D	413	39	-	8/46/66/70	0/1/1/1
25	BCR	B	617	-	-	0/29/63/63	0/2/2/2
24	PHO	a	407	-	-	5/37/103/103	0/5/6/6
32	LMG	c	522	-	-	11/46/66/70	0/1/1/1
31	LHG	A	416	-	-	16/53/53/53	-
31	LHG	d	407	-	-	20/53/53/53	-
27	SQD	B	620	-	-	17/49/69/69	0/1/1/1
23	CLA	C	506	40	1/1/15/20	6/37/115/115	-
23	CLA	c	514	-	1/1/15/20	13/37/115/115	-
23	CLA	B	611	-	1/1/15/20	3/37/115/115	-
23	CLA	b	610	40	1/1/15/20	9/37/115/115	-
38	HEC	e	102	5,6	-	3/10/54/54	-
31	LHG	D	407	-	-	12/53/53/53	-
25	BCR	k	101	-	-	2/29/63/63	0/2/2/2
25	BCR	y	101	-	-	6/29/63/63	0/2/2/2
31	LHG	L	101	-	-	14/53/53/53	-
23	CLA	D	404	-	1/1/15/20	10/37/115/115	-
23	CLA	a	405	40	1/1/15/20	11/37/115/115	-
23	CLA	B	605	-	1/1/15/20	4/37/115/115	-
23	CLA	B	615	-	1/1/15/20	7/37/115/115	-
23	CLA	a	406	40	-	6/37/115/115	-
34	LMT	b	621	-	-	7/17/37/61	0/1/1/2
26	GOL	b	624	-	-	3/4/4/4	-
27	SQD	a	410	-	-	14/49/69/69	0/1/1/1
23	CLA	B	609	-	1/1/15/20	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMT	m	103	-	-	7/21/61/61	0/2/2/2
23	CLA	d	403	-	1/1/15/20	8/37/115/115	-
33	HTG	B	625	-	-	3/10/30/30	0/1/1/1
35	DGD	C	520	-	-	10/51/91/95	0/2/2/2
34	LMT	D	402	-	-	8/21/61/61	0/2/2/2
32	LMG	z	101	-	-	8/34/54/70	0/1/1/1
23	CLA	C	505	-	1/1/15/20	4/37/115/115	-
25	BCR	D	405	-	-	8/29/63/63	0/2/2/2
23	CLA	B	612	-	1/1/15/20	3/37/115/115	-
23	CLA	C	504	-	-	8/37/115/115	-
34	LMT	t	101	-	-	6/17/38/61	0/1/1/2
23	CLA	C	513	3	1/1/15/20	2/37/115/115	-
33	HTG	b	625	-	-	4/10/30/30	0/1/1/1
26	GOL	a	411	-	-	4/4/4/4	-
35	DGD	H	102	-	-	11/51/91/95	0/2/2/2
33	HTG	b	623	-	-	2/10/30/30	0/1/1/1
23	CLA	b	615	-	1/1/15/20	8/37/115/115	-
23	CLA	c	511	-	1/1/15/20	14/37/115/115	-
31	LHG	E	101	-	-	15/46/46/53	-
32	LMG	m	101	-	-	10/46/66/70	0/1/1/1
32	LMG	C	521	-	-	10/46/66/70	0/1/1/1
26	GOL	v	201	-	-	2/4/4/4	-
29	PL9	d	405	-	-	7/53/73/73	0/1/1/1
23	CLA	c	513	3	1/1/15/20	8/37/115/115	-
23	CLA	B	606	-	1/1/15/20	11/37/115/115	-
23	CLA	b	604	-	1/1/15/20	11/37/115/115	-
23	CLA	c	505	-	1/1/15/20	1/37/115/115	-
23	CLA	C	512	-	1/1/15/20	10/37/115/115	-
33	HTG	B	622	-	-	5/10/30/30	0/1/1/1
34	LMT	E	102	-	-	7/21/61/61	0/2/2/2
35	DGD	C	519	-	-	16/51/91/95	0/2/2/2
23	CLA	C	508	-	1/1/15/20	11/37/115/115	-
27	SQD	C	501	-	-	12/49/69/69	0/1/1/1
23	CLA	c	506	40	1/1/15/20	6/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	HEC	E	103	5,6	-	4/10/54/54	-
25	BCR	C	516	-	-	3/29/63/63	0/2/2/2
23	CLA	B	607	40	1/1/15/20	2/37/115/115	-
25	BCR	K	101	-	-	1/29/63/63	0/2/2/2
32	LMG	C	522	-	-	12/46/66/70	0/1/1/1
23	CLA	c	515	-	1/1/15/20	7/37/115/115	-
23	CLA	c	512	-	1/1/15/20	7/37/115/115	-
34	LMT	B	628	-	-	10/21/61/61	0/2/2/2
23	CLA	c	508	-	1/1/15/20	10/37/115/115	-
24	PHO	A	415	-	-	3/37/103/103	0/5/6/6
23	CLA	A	405	40	1/1/15/20	5/37/115/115	-
25	BCR	c	516	-	-	0/29/63/63	0/2/2/2
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
33	HTG	c	523	-	-	3/10/30/30	0/1/1/1
23	CLA	b	602	-	1/1/15/20	3/37/115/115	-
23	CLA	B	608	-	-	2/37/115/115	-
31	LHG	d	406	-	-	15/53/53/53	-
34	LMT	a	418	-	-	4/21/61/61	0/2/2/2
32	LMG	B	621	-	-	11/46/66/70	0/1/1/1
23	CLA	A	408	-	1/1/15/20	9/37/115/115	-
23	CLA	b	603	-	1/1/15/20	3/37/115/115	-
25	BCR	Y	101	-	-	6/29/63/63	0/2/2/2
23	CLA	C	509	40	1/1/15/20	5/37/115/115	-
26	GOL	c	502	-	-	0/4/4/4	-
31	LHG	a	419	-	-	18/46/46/53	-
27	SQD	a	412	-	-	17/49/69/69	0/1/1/1
25	BCR	d	404	-	-	4/29/63/63	0/2/2/2
33	HTG	C	523	-	-	1/10/30/30	0/1/1/1
32	LMG	C	502	-	-	25/46/66/70	0/1/1/1
34	LMT	B	630	-	-	5/17/37/61	0/1/1/2
23	CLA	c	504	-	1/1/15/20	5/37/115/115	-
25	BCR	C	517	-	-	2/29/63/63	0/2/2/2
35	DGD	C	518	-	-	14/51/91/95	0/2/2/2
23	CLA	B	602	-	1/1/15/20	5/37/115/115	-
23	CLA	C	503	-	1/1/15/20	4/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMT	M	103	-	-	9/21/61/61	0/2/2/2
23	CLA	c	509	40	1/1/15/20	5/37/115/115	-
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
23	CLA	b	605	-	1/1/15/20	5/37/115/115	-
34	LMT	b	627	-	-	9/17/37/61	0/1/1/2
23	CLA	B	604	-	1/1/15/20	10/37/115/115	-
26	GOL	C	524	-	-	0/4/4/4	-
23	CLA	b	608	-	-	2/37/115/115	-
24	PHO	A	407	-	-	2/37/103/103	0/5/6/6
23	CLA	c	507	-	1/1/15/20	6/37/115/115	-
32	LMG	c	521	-	-	6/46/66/70	0/1/1/1
25	BCR	b	619	-	-	4/29/63/63	0/2/2/2
23	CLA	a	408	-	1/1/15/20	14/37/115/115	-
26	GOL	B	629	-	-	0/4/4/4	-
25	BCR	t	102	-	-	4/29/63/63	0/2/2/2
31	LHG	b	629	-	-	15/53/53/53	-
23	CLA	C	515	-	-	13/37/115/115	-
27	SQD	A	411	-	-	11/49/69/69	0/1/1/1
38	HEC	v	202	16	-	2/10/54/54	-
29	PL9	a	415	-	-	13/53/73/73	0/1/1/1
33	HTG	b	622	-	-	2/10/30/30	0/1/1/1

All (1325) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	506	CLA	C3B-C2B	6.93	1.50	1.40
23	b	612	CLA	C3B-C2B	6.85	1.49	1.40
24	A	415	PHO	C3B-C2B	6.75	1.49	1.40
23	C	510	CLA	C3B-C2B	6.73	1.49	1.40
23	c	510	CLA	C3B-C2B	6.61	1.49	1.40
23	A	404	CLA	C3B-C2B	6.59	1.49	1.40
23	B	612	CLA	C3B-C2B	6.54	1.49	1.40
38	v	202	HEC	C2B-C3B	-6.54	1.33	1.40
23	b	613	CLA	C3B-C2B	6.46	1.49	1.40
23	b	611	CLA	C3B-C2B	6.43	1.49	1.40
23	d	402	CLA	C3B-C2B	6.39	1.49	1.40
23	c	513	CLA	C3B-C2B	6.38	1.49	1.40
23	C	514	CLA	C3B-C2B	6.37	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	603	CLA	C3B-C2B	6.36	1.49	1.40
23	b	609	CLA	C3B-C2B	6.28	1.49	1.40
23	B	608	CLA	C3B-C2B	6.28	1.49	1.40
23	b	616	CLA	C3B-C2B	6.26	1.49	1.40
23	c	511	CLA	C3B-C2B	6.24	1.49	1.40
23	B	616	CLA	C3B-C2B	6.23	1.49	1.40
23	B	613	CLA	C3B-C2B	6.22	1.49	1.40
23	C	513	CLA	C3B-C2B	6.20	1.49	1.40
23	b	614	CLA	C3B-C2B	6.19	1.49	1.40
23	B	603	CLA	C3B-C2B	6.18	1.48	1.40
23	B	610	CLA	C3B-C2B	6.17	1.48	1.40
38	V	201	HEC	C2B-C3B	-6.15	1.34	1.40
23	B	606	CLA	C3B-C2B	6.14	1.48	1.40
23	C	511	CLA	C3B-C2B	6.13	1.48	1.40
23	C	509	CLA	C3B-C2B	6.12	1.48	1.40
24	a	407	PHO	C3B-C2B	6.12	1.48	1.40
23	c	504	CLA	C3B-C2B	6.11	1.48	1.40
24	a	417	PHO	C3B-C2B	6.10	1.48	1.40
23	b	602	CLA	C3B-C2B	6.06	1.48	1.40
23	B	604	CLA	C3B-C2B	6.04	1.48	1.40
23	c	512	CLA	C3B-C2B	6.01	1.48	1.40
23	b	604	CLA	C3B-C2B	5.99	1.48	1.40
23	D	403	CLA	C3B-C2B	5.94	1.48	1.40
23	c	508	CLA	C3B-C2B	5.94	1.48	1.40
23	d	403	CLA	C1D-ND	5.92	1.45	1.37
24	A	407	PHO	C3B-C2B	5.92	1.48	1.40
23	b	601	CLA	C3B-C2B	5.90	1.48	1.40
23	b	606	CLA	C3B-C2B	5.89	1.48	1.40
23	a	404	CLA	C3B-C2B	5.89	1.48	1.40
23	B	601	CLA	C3B-C2B	5.85	1.48	1.40
23	B	611	CLA	C3B-C2B	5.85	1.48	1.40
23	b	608	CLA	C3B-C2B	5.82	1.48	1.40
23	C	510	CLA	C3C-C2C	5.82	1.49	1.36
23	B	610	CLA	C3C-C2C	5.81	1.49	1.36
23	C	506	CLA	C3B-C2B	5.78	1.48	1.40
23	C	515	CLA	C3B-C2B	5.75	1.48	1.40
23	a	405	CLA	C1D-ND	5.75	1.44	1.37
23	A	408	CLA	C3B-C2B	5.75	1.48	1.40
23	C	503	CLA	C3B-C2B	5.73	1.48	1.40
23	a	408	CLA	C3C-C2C	5.71	1.48	1.36
23	a	405	CLA	C3C-C2C	5.71	1.48	1.36
24	a	407	PHO	C3D-C2D	5.71	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	601	CLA	C3C-C2C	5.68	1.48	1.36
23	c	510	CLA	C3C-C2C	5.66	1.48	1.36
23	C	512	CLA	C3B-C2B	5.64	1.48	1.40
23	b	601	CLA	C1D-ND	5.64	1.44	1.37
23	C	509	CLA	C3C-C2C	5.63	1.48	1.36
23	c	515	CLA	C3B-C2B	5.63	1.48	1.40
23	C	515	CLA	C1D-ND	5.62	1.44	1.37
23	D	404	CLA	C1D-ND	5.62	1.44	1.37
23	c	506	CLA	C1D-ND	5.62	1.44	1.37
24	A	415	PHO	C3D-C2D	5.61	1.49	1.39
24	a	417	PHO	C3D-C2D	5.60	1.49	1.39
23	a	404	CLA	C3C-C2C	5.59	1.48	1.36
23	b	610	CLA	C3B-C2B	5.57	1.48	1.40
23	a	408	CLA	C3B-C2B	5.55	1.48	1.40
23	c	509	CLA	C1D-ND	5.55	1.44	1.37
23	B	601	CLA	C3C-C2C	5.54	1.48	1.36
23	C	514	CLA	C3C-C2C	5.54	1.48	1.36
23	c	511	CLA	C1D-ND	5.50	1.44	1.37
23	B	614	CLA	C3C-C2C	5.50	1.48	1.36
23	B	602	CLA	CHC-C1C	5.49	1.49	1.35
23	A	406	CLA	C3C-C2C	5.49	1.48	1.36
23	d	403	CLA	C3C-C2C	5.48	1.48	1.36
23	C	504	CLA	C3B-C2B	5.47	1.48	1.40
23	c	504	CLA	C3C-C2C	5.47	1.48	1.36
23	d	403	CLA	C3B-C2B	5.46	1.47	1.40
23	B	606	CLA	C1D-ND	5.46	1.44	1.37
23	B	611	CLA	C1D-ND	5.45	1.44	1.37
23	b	606	CLA	C3C-C2C	5.44	1.48	1.36
23	C	507	CLA	C3B-C2B	5.44	1.47	1.40
23	C	505	CLA	C3C-C2C	5.44	1.48	1.36
23	A	404	CLA	C1D-ND	5.44	1.44	1.37
23	C	508	CLA	C3B-C2B	5.43	1.47	1.40
23	b	615	CLA	C3C-C2C	5.42	1.48	1.36
23	C	503	CLA	C3C-C2C	5.41	1.48	1.36
23	C	505	CLA	C3B-C2B	5.41	1.47	1.40
23	b	605	CLA	C3C-C2C	5.41	1.48	1.36
23	c	514	CLA	C3B-C2B	5.40	1.47	1.40
23	C	513	CLA	O2D-CGD	5.39	1.46	1.33
23	C	511	CLA	C1D-ND	5.39	1.44	1.37
23	c	513	CLA	C3C-C2C	5.38	1.48	1.36
23	D	403	CLA	C3C-C2C	5.37	1.48	1.36
23	c	514	CLA	CHC-C1C	5.37	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	510	CLA	C1D-ND	5.36	1.44	1.37
23	c	504	CLA	O2D-CGD	5.35	1.46	1.33
25	d	404	BCR	C23-C22	-5.35	1.34	1.45
23	b	610	CLA	C3C-C2C	5.33	1.48	1.36
38	v	202	HEC	C3D-C2D	5.33	1.53	1.37
23	a	405	CLA	C3B-C2B	5.32	1.47	1.40
23	c	509	CLA	CHC-C1C	5.31	1.48	1.35
23	C	504	CLA	CHC-C1C	5.31	1.48	1.35
23	c	507	CLA	C3C-C2C	5.30	1.48	1.36
23	B	605	CLA	CHC-C1C	5.30	1.48	1.35
23	b	603	CLA	C3C-C2C	5.30	1.48	1.36
23	b	604	CLA	C1D-ND	5.29	1.44	1.37
23	c	515	CLA	CHC-C1C	5.28	1.48	1.35
23	c	507	CLA	C3B-C2B	5.28	1.47	1.40
23	c	513	CLA	C1D-ND	5.27	1.44	1.37
23	b	609	CLA	CHC-C1C	5.27	1.48	1.35
23	c	505	CLA	C3C-C2C	5.27	1.47	1.36
23	d	403	CLA	CHC-C1C	5.27	1.48	1.35
23	B	602	CLA	C3C-C2C	5.27	1.47	1.36
23	C	512	CLA	C1D-ND	5.27	1.44	1.37
23	c	514	CLA	C3C-C2C	5.26	1.47	1.36
23	b	613	CLA	C3C-C2C	5.26	1.47	1.36
23	A	404	CLA	C3C-C2C	5.25	1.47	1.36
23	c	515	CLA	C1D-ND	5.25	1.44	1.37
23	a	404	CLA	C1D-ND	5.24	1.44	1.37
23	b	613	CLA	C1D-ND	5.24	1.44	1.37
23	A	405	CLA	C3C-C2C	5.24	1.47	1.36
23	c	508	CLA	C1D-ND	5.24	1.44	1.37
23	A	408	CLA	C3C-C2C	5.23	1.47	1.36
23	B	615	CLA	C3B-C2B	5.23	1.47	1.40
23	D	404	CLA	C3C-C2C	5.22	1.47	1.36
23	B	611	CLA	C3C-C2C	5.22	1.47	1.36
23	c	503	CLA	C1D-ND	5.21	1.44	1.37
23	b	609	CLA	C3C-C2C	5.21	1.47	1.36
23	B	611	CLA	O2D-CGD	5.21	1.45	1.33
23	a	405	CLA	CHC-C1C	5.21	1.48	1.35
23	B	603	CLA	C3C-C2C	5.21	1.47	1.36
23	C	505	CLA	C1D-ND	5.21	1.44	1.37
23	C	515	CLA	C3C-C2C	5.20	1.47	1.36
23	A	408	CLA	CHC-C1C	5.20	1.48	1.35
23	c	508	CLA	C3C-C2C	5.20	1.47	1.36
23	B	614	CLA	C3B-C2B	5.20	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	605	CLA	C1D-ND	5.20	1.44	1.37
23	b	614	CLA	O2D-CGD	5.20	1.45	1.33
23	b	602	CLA	O2D-CGD	5.19	1.45	1.33
23	c	510	CLA	O2D-CGD	5.19	1.45	1.33
23	B	608	CLA	C3C-C2C	5.19	1.47	1.36
23	d	402	CLA	C3C-C2C	5.18	1.47	1.36
23	B	604	CLA	C3C-C2C	5.18	1.47	1.36
23	b	607	CLA	C3C-C2C	5.17	1.47	1.36
23	C	508	CLA	C1D-ND	5.17	1.44	1.37
23	b	613	CLA	O2D-CGD	5.17	1.45	1.33
23	c	515	CLA	O2D-CGD	5.16	1.45	1.33
23	a	406	CLA	CHC-C1C	5.15	1.48	1.35
23	C	511	CLA	C3C-C2C	5.15	1.47	1.36
23	b	602	CLA	C3C-C2C	5.15	1.47	1.36
23	c	509	CLA	C3C-C2C	5.15	1.47	1.36
23	B	605	CLA	C3C-C2C	5.15	1.47	1.36
23	b	615	CLA	C3B-C2B	5.15	1.47	1.40
23	c	505	CLA	C3B-C2B	5.14	1.47	1.40
23	a	408	CLA	CHC-C1C	5.13	1.48	1.35
23	B	601	CLA	O2D-CGD	5.13	1.45	1.33
23	B	602	CLA	C1D-ND	5.13	1.44	1.37
23	c	507	CLA	CHC-C1C	5.13	1.48	1.35
23	b	614	CLA	CHC-C1C	5.13	1.48	1.35
23	C	507	CLA	CHC-C1C	5.13	1.48	1.35
23	A	406	CLA	O2D-CGD	5.12	1.45	1.33
23	A	406	CLA	CHC-C1C	5.12	1.48	1.35
23	b	615	CLA	C1D-ND	5.11	1.44	1.37
23	b	614	CLA	C3C-C2C	5.11	1.47	1.36
23	c	505	CLA	C1D-ND	5.11	1.44	1.37
23	c	511	CLA	O2D-CGD	5.11	1.45	1.33
23	c	515	CLA	C3C-C2C	5.11	1.47	1.36
23	c	509	CLA	C3B-C2B	5.11	1.47	1.40
23	B	601	CLA	CHC-C1C	5.11	1.48	1.35
23	a	406	CLA	C3B-C2B	5.11	1.47	1.40
24	A	407	PHO	OBD-CAD	5.10	1.29	1.22
23	b	612	CLA	C3C-C2C	5.10	1.47	1.36
23	c	503	CLA	C3B-C2B	5.10	1.47	1.40
23	b	601	CLA	CHC-C1C	5.10	1.48	1.35
24	a	417	PHO	O2D-CGD	5.10	1.45	1.33
23	c	503	CLA	C3C-C2C	5.09	1.47	1.36
23	C	507	CLA	C3C-C2C	5.09	1.47	1.36
23	b	603	CLA	O2D-CGD	5.09	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	512	CLA	C3C-C2C	5.09	1.47	1.36
25	b	619	BCR	C23-C22	-5.09	1.35	1.45
23	A	405	CLA	CHC-C1C	5.09	1.48	1.35
23	C	506	CLA	CHC-C1C	5.09	1.48	1.35
23	A	408	CLA	O2D-CGD	5.08	1.45	1.33
23	B	602	CLA	C3B-C2B	5.08	1.47	1.40
23	C	512	CLA	CHC-C1C	5.08	1.48	1.35
23	D	404	CLA	CHC-C1C	5.08	1.48	1.35
23	b	608	CLA	CHC-C1C	5.08	1.48	1.35
23	c	504	CLA	C1D-ND	5.07	1.44	1.37
23	c	508	CLA	O2D-CGD	5.06	1.45	1.33
23	c	509	CLA	O2D-CGD	5.06	1.45	1.33
23	C	514	CLA	CHC-C1C	5.06	1.47	1.35
23	c	510	CLA	CHC-C1C	5.05	1.47	1.35
23	c	503	CLA	CHC-C1C	5.05	1.47	1.35
23	B	604	CLA	CHC-C1C	5.05	1.47	1.35
23	B	612	CLA	CHC-C1C	5.05	1.47	1.35
23	c	506	CLA	O2D-CGD	5.05	1.45	1.33
23	C	504	CLA	O2D-CGD	5.04	1.45	1.33
23	C	512	CLA	C3C-C2C	5.04	1.47	1.36
23	b	609	CLA	O2D-CGD	5.04	1.45	1.33
38	V	201	HEC	C3D-C2D	5.04	1.52	1.37
23	b	606	CLA	C1D-ND	5.03	1.44	1.37
23	c	504	CLA	CHC-C1C	5.03	1.47	1.35
25	t	102	BCR	C23-C22	-5.03	1.35	1.45
23	B	616	CLA	C3C-C2C	5.03	1.47	1.36
23	b	610	CLA	O2D-CGD	5.03	1.45	1.33
23	c	513	CLA	CHC-C1C	5.03	1.47	1.35
23	B	606	CLA	C3C-C2C	5.03	1.47	1.36
23	c	514	CLA	O2D-CGD	5.02	1.45	1.33
23	b	603	CLA	C1D-ND	5.02	1.44	1.37
23	b	604	CLA	O2D-CGD	5.02	1.45	1.33
23	A	404	CLA	CHC-C1C	5.02	1.47	1.35
23	b	608	CLA	O2D-CGD	5.01	1.45	1.33
23	C	504	CLA	C3C-C2C	5.01	1.47	1.36
23	b	608	CLA	C3C-C2C	5.01	1.47	1.36
23	B	607	CLA	CHC-C1C	5.01	1.47	1.35
38	V	201	HEC	C3C-C2C	-5.01	1.35	1.40
23	B	607	CLA	C3C-C2C	5.01	1.47	1.36
23	A	408	CLA	C1D-ND	5.00	1.43	1.37
23	b	616	CLA	C3C-C2C	5.00	1.47	1.36
23	c	506	CLA	C3C-C2C	5.00	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	508	CLA	O2D-CGD	5.00	1.45	1.33
23	c	511	CLA	C3C-C2C	5.00	1.47	1.36
23	B	605	CLA	C3B-C2B	4.99	1.47	1.40
23	D	404	CLA	O2D-CGD	4.99	1.45	1.33
23	b	616	CLA	O2D-CGD	4.99	1.45	1.33
23	b	611	CLA	C3C-C2C	4.99	1.47	1.36
23	b	601	CLA	O2D-CGD	4.99	1.45	1.33
23	c	512	CLA	C1D-ND	4.98	1.43	1.37
23	B	603	CLA	CHC-C1C	4.98	1.47	1.35
23	b	602	CLA	CHC-C1C	4.98	1.47	1.35
23	b	605	CLA	C3B-C2B	4.98	1.47	1.40
23	C	510	CLA	CHC-C1C	4.98	1.47	1.35
23	b	607	CLA	C3B-C2B	4.98	1.47	1.40
23	C	514	CLA	C1D-ND	4.98	1.43	1.37
23	B	607	CLA	C3B-C2B	4.97	1.47	1.40
23	b	603	CLA	CHC-C1C	4.97	1.47	1.35
23	B	601	CLA	C1D-ND	4.97	1.43	1.37
23	B	609	CLA	O2D-CGD	4.97	1.45	1.33
23	b	611	CLA	CHC-C1C	4.97	1.47	1.35
23	b	610	CLA	CHC-C1C	4.96	1.47	1.35
23	B	615	CLA	CHC-C1C	4.96	1.47	1.35
23	c	508	CLA	CHC-C1C	4.96	1.47	1.35
23	C	513	CLA	CHC-C1C	4.96	1.47	1.35
23	C	508	CLA	CHD-C1D	4.96	1.48	1.38
23	B	615	CLA	C3C-C2C	4.95	1.47	1.36
23	B	613	CLA	CHC-C1C	4.95	1.47	1.35
23	C	509	CLA	CHC-C1C	4.95	1.47	1.35
25	k	101	BCR	C23-C22	-4.94	1.35	1.45
23	b	602	CLA	C1D-ND	4.94	1.43	1.37
25	c	517	BCR	C23-C22	-4.94	1.35	1.45
23	B	615	CLA	O2D-CGD	4.94	1.45	1.33
23	B	614	CLA	C1D-ND	4.93	1.43	1.37
23	c	505	CLA	CHC-C1C	4.93	1.47	1.35
23	C	505	CLA	CHC-C1C	4.93	1.47	1.35
23	B	610	CLA	CHC-C1C	4.93	1.47	1.35
23	C	512	CLA	O2D-CGD	4.92	1.45	1.33
23	b	613	CLA	CHC-C1C	4.92	1.47	1.35
23	a	405	CLA	O2D-CGD	4.92	1.45	1.33
25	H	101	BCR	C23-C22	-4.92	1.35	1.45
23	B	615	CLA	C1D-ND	4.91	1.43	1.37
23	C	510	CLA	C1D-ND	4.91	1.43	1.37
23	b	615	CLA	CHC-C1C	4.91	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	606	CLA	CHC-C1C	4.91	1.47	1.35
23	c	511	CLA	CHC-C1C	4.91	1.47	1.35
23	C	506	CLA	C3C-C2C	4.90	1.47	1.36
23	B	603	CLA	O2D-CGD	4.90	1.45	1.33
23	C	508	CLA	C3C-C2C	4.89	1.47	1.36
25	K	101	BCR	C23-C22	-4.88	1.35	1.45
23	B	609	CLA	CHC-C1C	4.87	1.47	1.35
23	B	608	CLA	C1D-ND	4.87	1.43	1.37
23	C	503	CLA	CHC-C1C	4.86	1.47	1.35
23	C	506	CLA	O2D-CGD	4.86	1.45	1.33
24	A	407	PHO	C3D-C2D	4.86	1.48	1.39
23	c	506	CLA	CHC-C1C	4.86	1.47	1.35
25	C	516	BCR	C23-C22	-4.85	1.35	1.45
23	B	608	CLA	CHC-C1C	4.85	1.47	1.35
23	B	604	CLA	O2D-CGD	4.85	1.45	1.33
24	A	415	PHO	O2D-CGD	4.85	1.45	1.33
23	a	404	CLA	CHC-C1C	4.84	1.47	1.35
23	B	616	CLA	O2D-CGD	4.84	1.45	1.33
23	C	508	CLA	CHC-C1C	4.83	1.47	1.35
23	C	503	CLA	C1D-ND	4.83	1.43	1.37
23	D	403	CLA	CHC-C1C	4.82	1.47	1.35
23	a	406	CLA	C3C-C2C	4.82	1.47	1.36
25	c	516	BCR	C23-C22	-4.82	1.35	1.45
25	a	409	BCR	C23-C22	-4.81	1.35	1.45
24	a	407	PHO	O2D-CGD	4.81	1.44	1.33
23	c	514	CLA	C1D-ND	4.81	1.43	1.37
23	B	605	CLA	O2D-CGD	4.81	1.44	1.33
23	b	605	CLA	CHC-C1C	4.81	1.47	1.35
23	c	513	CLA	O2D-CGD	4.80	1.44	1.33
23	c	503	CLA	O2D-CGD	4.80	1.44	1.33
23	C	505	CLA	O2D-CGD	4.80	1.44	1.33
23	b	607	CLA	CHC-C1C	4.79	1.47	1.35
25	b	617	BCR	C23-C22	-4.78	1.35	1.45
23	C	515	CLA	CHC-C1C	4.78	1.47	1.35
23	b	604	CLA	CHC-C1C	4.77	1.47	1.35
23	B	606	CLA	CHC-C1C	4.77	1.47	1.35
25	D	405	BCR	C23-C22	-4.77	1.35	1.45
23	b	615	CLA	O2D-CGD	4.76	1.44	1.33
23	c	507	CLA	O2D-CGD	4.76	1.44	1.33
23	b	605	CLA	O2D-CGD	4.76	1.44	1.33
23	B	616	CLA	CHC-C1C	4.76	1.47	1.35
23	A	405	CLA	C3B-C2B	4.76	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	512	CLA	CHC-C1C	4.76	1.47	1.35
23	B	609	CLA	C3C-C2C	4.75	1.46	1.36
23	B	613	CLA	O2D-CGD	4.75	1.44	1.33
24	a	417	PHO	OBD-CAD	4.75	1.28	1.22
23	C	511	CLA	CHC-C1C	4.74	1.47	1.35
23	C	515	CLA	O2D-CGD	4.74	1.44	1.33
23	B	609	CLA	C3B-C2B	4.74	1.46	1.40
23	B	607	CLA	C1D-ND	4.74	1.43	1.37
23	C	513	CLA	C1D-ND	4.73	1.43	1.37
25	y	101	BCR	C23-C22	-4.73	1.35	1.45
23	C	507	CLA	O2D-CGD	4.73	1.44	1.33
38	v	202	HEC	C3C-C2C	-4.73	1.35	1.40
23	b	601	CLA	O2A-CGA	4.72	1.47	1.33
23	B	611	CLA	CHC-C1C	4.72	1.47	1.35
23	A	405	CLA	O2D-CGD	4.71	1.44	1.33
23	B	614	CLA	CHC-C1C	4.71	1.47	1.35
23	A	406	CLA	C3B-C2B	4.71	1.46	1.40
23	B	606	CLA	O2D-CGD	4.71	1.44	1.33
23	C	513	CLA	C3C-C2C	4.70	1.46	1.36
23	b	608	CLA	C1D-ND	4.70	1.43	1.37
23	d	402	CLA	CHC-C1C	4.70	1.47	1.35
23	C	514	CLA	O2D-CGD	4.70	1.44	1.33
25	b	618	BCR	C23-C22	-4.69	1.35	1.45
23	B	605	CLA	C1D-ND	4.69	1.43	1.37
23	B	612	CLA	O2D-CGD	4.69	1.44	1.33
23	B	604	CLA	C1D-ND	4.69	1.43	1.37
23	b	616	CLA	CHC-C1C	4.69	1.47	1.35
23	b	612	CLA	C1D-ND	4.68	1.43	1.37
23	C	509	CLA	C1D-ND	4.67	1.43	1.37
23	b	614	CLA	C1D-ND	4.67	1.43	1.37
24	A	407	PHO	O2D-CGD	4.67	1.44	1.33
23	B	612	CLA	C3C-C2C	4.67	1.46	1.36
23	B	610	CLA	C1D-ND	4.67	1.43	1.37
24	a	407	PHO	OBD-CAD	4.67	1.28	1.22
23	b	604	CLA	C3C-C2C	4.66	1.46	1.36
23	B	609	CLA	C1D-ND	4.66	1.43	1.37
23	A	405	CLA	C1D-ND	4.65	1.43	1.37
23	b	611	CLA	O2D-CGD	4.65	1.44	1.33
23	C	511	CLA	O2D-CGD	4.64	1.44	1.33
23	c	505	CLA	O2D-CGD	4.63	1.44	1.33
23	D	404	CLA	C3B-C2B	4.63	1.46	1.40
23	b	601	CLA	CHD-C1D	4.63	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	601	CLA	O2A-CGA	4.62	1.46	1.33
23	a	404	CLA	O2D-CGD	4.62	1.44	1.33
23	B	602	CLA	CHD-C1D	4.59	1.47	1.38
23	C	510	CLA	O2D-CGD	4.59	1.44	1.33
23	b	607	CLA	C1D-ND	4.59	1.43	1.37
23	C	509	CLA	O2D-CGD	4.57	1.44	1.33
23	C	511	CLA	CHD-C1D	4.56	1.47	1.38
25	C	517	BCR	C23-C22	-4.56	1.36	1.45
23	b	612	CLA	CHC-C1C	4.56	1.46	1.35
23	A	404	CLA	O2D-CGD	4.56	1.44	1.33
25	h	102	BCR	C23-C22	-4.56	1.36	1.45
25	B	619	BCR	C23-C22	-4.54	1.36	1.45
23	b	610	CLA	C1D-ND	4.54	1.43	1.37
23	b	611	CLA	C1D-ND	4.53	1.43	1.37
23	D	403	CLA	O2D-CGD	4.52	1.44	1.33
27	A	411	SQD	O48-C23	4.52	1.46	1.33
23	B	614	CLA	O2D-CGD	4.52	1.44	1.33
23	B	607	CLA	O2D-CGD	4.52	1.44	1.33
23	A	406	CLA	CHD-C1D	4.51	1.47	1.38
23	a	408	CLA	O2D-CGD	4.51	1.44	1.33
23	B	602	CLA	O2D-CGD	4.50	1.44	1.33
25	A	409	BCR	C23-C22	-4.50	1.36	1.45
23	C	503	CLA	O2D-CGD	4.50	1.44	1.33
23	b	602	CLA	CHD-C1D	4.48	1.47	1.38
23	b	607	CLA	CHD-C1D	4.48	1.47	1.38
23	d	402	CLA	O2D-CGD	4.47	1.44	1.33
23	b	611	CLA	O2A-CGA	4.46	1.46	1.33
23	d	403	CLA	O2D-CGD	4.46	1.44	1.33
23	B	615	CLA	C3D-C2D	4.46	1.51	1.39
23	B	616	CLA	C1D-ND	4.45	1.43	1.37
25	B	617	BCR	C23-C22	-4.45	1.36	1.45
23	c	505	CLA	CHD-C1D	4.45	1.47	1.38
23	c	510	CLA	CHD-C1D	4.44	1.47	1.38
23	c	507	CLA	CHD-C1D	4.43	1.47	1.38
31	a	419	LHG	O7-C7	4.42	1.46	1.34
23	a	406	CLA	O2D-CGD	4.42	1.44	1.33
31	E	101	LHG	O8-C23	4.42	1.46	1.33
23	B	609	CLA	O2A-CGA	4.42	1.46	1.33
23	C	506	CLA	C1D-ND	4.42	1.43	1.37
23	C	514	CLA	CHD-C1D	4.42	1.47	1.38
23	a	405	CLA	O2A-CGA	4.41	1.46	1.33
32	C	522	LMG	O7-C10	4.41	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	601	CLA	CHD-C1D	4.40	1.46	1.38
23	B	606	CLA	CHD-C1D	4.39	1.46	1.38
23	b	616	CLA	C1D-ND	4.39	1.43	1.37
32	C	521	LMG	O8-C28	4.39	1.46	1.33
23	d	402	CLA	O2A-CGA	4.39	1.46	1.33
32	z	101	LMG	O8-C28	4.38	1.46	1.33
23	b	608	CLA	CHD-C1D	4.37	1.46	1.38
23	b	607	CLA	O2D-CGD	4.37	1.43	1.33
24	A	415	PHO	OBD-CAD	4.37	1.28	1.22
32	C	522	LMG	O8-C28	4.36	1.46	1.33
23	C	515	CLA	CHD-C1D	4.36	1.46	1.38
27	a	412	SQD	O47-C7	4.35	1.46	1.34
27	D	412	SQD	O47-C7	4.35	1.46	1.34
25	Y	101	BCR	C23-C22	-4.35	1.36	1.45
31	a	419	LHG	O8-C23	4.35	1.46	1.33
23	c	513	CLA	O2A-CGA	4.35	1.46	1.33
32	c	522	LMG	O7-C10	4.35	1.46	1.34
35	c	520	DGD	O1G-C1A	4.34	1.46	1.33
23	C	507	CLA	C1D-ND	4.34	1.43	1.37
23	c	510	CLA	O2A-CGA	4.34	1.46	1.33
27	f	101	SQD	O47-C7	4.34	1.46	1.34
23	C	504	CLA	C1D-ND	4.34	1.43	1.37
38	e	102	HEC	CBC-CAC	-4.34	1.33	1.49
23	D	403	CLA	O2A-CGA	4.34	1.46	1.33
23	c	512	CLA	O2D-CGD	4.34	1.43	1.33
23	c	507	CLA	C1D-ND	4.33	1.43	1.37
23	b	612	CLA	O2D-CGD	4.33	1.43	1.33
32	C	521	LMG	O7-C10	4.33	1.46	1.34
23	c	515	CLA	CHD-C1D	4.33	1.46	1.38
25	T	101	BCR	C23-C22	-4.32	1.36	1.45
32	c	522	LMG	O8-C28	4.32	1.46	1.33
23	B	613	CLA	C3C-C2C	4.32	1.45	1.36
27	B	620	SQD	O48-C23	4.32	1.46	1.33
23	c	514	CLA	O2A-CGA	4.32	1.46	1.33
32	Z	101	LMG	O7-C10	4.31	1.46	1.34
23	d	403	CLA	C3D-C2D	4.31	1.50	1.39
23	D	404	CLA	CHD-C1D	4.31	1.46	1.38
23	B	603	CLA	C1D-ND	4.31	1.43	1.37
23	a	408	CLA	C1D-ND	4.31	1.43	1.37
27	b	620	SQD	O47-C7	4.31	1.46	1.34
27	a	412	SQD	O48-C23	4.31	1.45	1.33
23	b	609	CLA	CHD-C1D	4.31	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	620	SQD	O47-C7	4.30	1.46	1.34
32	d	412	LMG	O8-C28	4.30	1.45	1.33
23	A	408	CLA	CHD-C1D	4.30	1.46	1.38
38	E	103	HEC	CBC-CAC	-4.29	1.33	1.49
23	B	605	CLA	CHD-C1D	4.29	1.46	1.38
23	b	602	CLA	O2A-CGA	4.29	1.45	1.33
27	b	620	SQD	O48-C23	4.28	1.45	1.33
38	e	102	HEC	CBB-CAB	-4.28	1.33	1.49
23	b	609	CLA	C1D-ND	4.27	1.43	1.37
23	a	405	CLA	C3D-C2D	4.27	1.50	1.39
23	d	403	CLA	CHD-C4C	4.26	1.49	1.39
23	d	403	CLA	O2A-CGA	4.25	1.45	1.33
23	C	508	CLA	CHD-C4C	4.25	1.48	1.39
23	B	610	CLA	CHD-C1D	4.25	1.46	1.38
23	c	509	CLA	CHD-C4C	4.24	1.48	1.39
32	C	502	LMG	O8-C28	4.24	1.45	1.33
23	c	509	CLA	CHD-C1D	4.24	1.46	1.38
23	d	403	CLA	CHD-C1D	4.24	1.46	1.38
23	A	405	CLA	CHD-C1D	4.23	1.46	1.38
32	B	621	LMG	O8-C28	4.23	1.45	1.33
23	B	608	CLA	O2D-CGD	4.23	1.43	1.33
23	c	514	CLA	CHD-C1D	4.23	1.46	1.38
23	c	508	CLA	CHD-C1D	4.23	1.46	1.38
23	C	511	CLA	CHD-C4C	4.23	1.48	1.39
23	b	601	CLA	CHD-C4C	4.23	1.48	1.39
23	c	511	CLA	CHD-C1D	4.22	1.46	1.38
23	C	515	CLA	O2A-CGA	4.22	1.45	1.33
23	C	509	CLA	O2A-CGA	4.22	1.45	1.33
23	B	609	CLA	CHD-C1D	4.22	1.46	1.38
23	D	403	CLA	CHD-C4C	4.22	1.48	1.39
38	E	103	HEC	CBB-CAB	-4.21	1.33	1.49
27	f	101	SQD	O48-C23	4.21	1.45	1.33
23	c	515	CLA	O2A-CGA	4.21	1.45	1.33
23	b	602	CLA	CHD-C4C	4.20	1.48	1.39
23	a	408	CLA	O2A-CGA	4.20	1.45	1.33
23	C	513	CLA	O2A-CGA	4.20	1.45	1.33
23	D	403	CLA	CHD-C1D	4.20	1.46	1.38
32	m	101	LMG	O8-C28	4.19	1.45	1.33
23	b	610	CLA	OBD-CAD	4.19	1.29	1.22
23	C	508	CLA	O2A-CGA	4.19	1.45	1.33
23	B	610	CLA	O2D-CGD	4.19	1.43	1.33
32	c	501	LMG	O8-C28	4.18	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	CHD-C1D	4.18	1.46	1.38
23	c	512	CLA	CHD-C1D	4.18	1.46	1.38
23	C	509	CLA	CHD-C1D	4.18	1.46	1.38
23	B	613	CLA	C1D-ND	4.17	1.42	1.37
32	c	521	LMG	O7-C10	4.17	1.46	1.34
23	c	509	CLA	O2A-CGA	4.17	1.45	1.33
35	h	103	DGD	O1G-C1A	4.16	1.45	1.33
35	c	518	DGD	O1G-C1A	4.16	1.45	1.33
23	C	510	CLA	O2A-CGA	4.16	1.45	1.33
23	b	608	CLA	CHD-C4C	4.16	1.48	1.39
23	b	614	CLA	O2A-CGA	4.15	1.45	1.33
23	A	408	CLA	CHD-C4C	4.15	1.48	1.39
32	c	521	LMG	O8-C28	4.14	1.45	1.33
23	b	608	CLA	O2A-CGA	4.14	1.45	1.33
23	c	504	CLA	CHD-C1D	4.14	1.46	1.38
31	E	101	LHG	O7-C7	4.13	1.46	1.34
23	a	404	CLA	OBD-CAD	4.13	1.29	1.22
23	c	506	CLA	CHD-C1D	4.13	1.46	1.38
23	C	503	CLA	O2A-CGA	4.13	1.45	1.33
23	a	406	CLA	O2A-CGA	4.12	1.45	1.33
27	D	412	SQD	O48-C23	4.12	1.45	1.33
23	B	606	CLA	O2A-CGA	4.12	1.45	1.33
23	b	603	CLA	CHD-C1D	4.12	1.46	1.38
23	c	515	CLA	CHD-C4C	4.12	1.48	1.39
23	C	503	CLA	CHD-C1D	4.12	1.46	1.38
23	A	408	CLA	O2A-CGA	4.12	1.45	1.33
32	z	101	LMG	O7-C10	4.11	1.45	1.34
23	B	602	CLA	CHD-C4C	4.11	1.48	1.39
23	B	610	CLA	OBD-CAD	4.11	1.29	1.22
27	A	411	SQD	O47-C7	4.11	1.45	1.34
27	a	410	SQD	O48-C23	4.11	1.45	1.33
23	C	514	CLA	O2A-CGA	4.11	1.45	1.33
31	L	101	LHG	O8-C23	4.11	1.45	1.33
31	d	408	LHG	O7-C7	4.11	1.45	1.34
23	c	511	CLA	O2A-CGA	4.10	1.45	1.33
31	b	629	LHG	O7-C7	4.09	1.45	1.34
27	a	410	SQD	O47-C7	4.09	1.45	1.34
23	a	406	CLA	C1D-ND	4.09	1.42	1.37
23	C	511	CLA	OBD-CAD	4.09	1.29	1.22
35	C	518	DGD	O2G-C1B	4.09	1.45	1.34
35	C	518	DGD	O1G-C1A	4.09	1.45	1.33
23	b	603	CLA	OBD-CAD	4.08	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	607	CLA	CHD-C1D	4.08	1.46	1.38
35	C	520	DGD	O1G-C1A	4.08	1.45	1.33
24	A	407	PHO	O2A-CGA	4.07	1.45	1.33
23	b	610	CLA	CHD-C1D	4.07	1.46	1.38
23	c	503	CLA	O2A-CGA	4.07	1.45	1.33
23	C	506	CLA	O2A-CGA	4.07	1.45	1.33
23	B	612	CLA	O2A-CGA	4.06	1.45	1.33
23	C	507	CLA	CHD-C4C	4.05	1.48	1.39
23	B	605	CLA	O2A-CGA	4.05	1.45	1.33
23	a	405	CLA	CHD-C1D	4.05	1.46	1.38
23	B	616	CLA	O2A-CGA	4.04	1.45	1.33
23	B	603	CLA	O2A-CGA	4.04	1.45	1.33
23	C	511	CLA	C3D-C2D	4.04	1.50	1.39
23	B	604	CLA	CHD-C4C	4.04	1.48	1.39
23	c	508	CLA	O2A-CGA	4.04	1.45	1.33
23	b	612	CLA	O2A-CGA	4.04	1.45	1.33
35	C	519	DGD	O2G-C1B	4.04	1.45	1.34
23	C	504	CLA	CHD-C1D	4.04	1.46	1.38
23	b	614	CLA	CHD-C1D	4.04	1.46	1.38
23	b	613	CLA	C3D-C2D	4.03	1.50	1.39
23	B	611	CLA	CHD-C1D	4.03	1.46	1.38
23	b	601	CLA	C3D-C2D	4.02	1.50	1.39
23	C	511	CLA	O2A-CGA	4.02	1.45	1.33
23	C	504	CLA	C3D-C2D	4.02	1.50	1.39
35	C	519	DGD	O1G-C1A	4.02	1.45	1.33
23	B	615	CLA	O2A-CGA	4.02	1.45	1.33
23	C	505	CLA	O2A-CGA	4.02	1.45	1.33
23	b	605	CLA	CHD-C1D	4.01	1.46	1.38
27	C	501	SQD	O48-C23	4.01	1.45	1.33
23	B	608	CLA	O2A-CGA	4.01	1.45	1.33
32	c	501	LMG	O7-C10	4.01	1.45	1.34
23	B	615	CLA	OBD-CAD	4.01	1.29	1.22
23	c	503	CLA	CHD-C4C	4.01	1.48	1.39
23	b	602	CLA	C3D-C2D	4.01	1.50	1.39
23	c	511	CLA	CHD-C4C	4.00	1.48	1.39
32	C	502	LMG	O7-C10	4.00	1.45	1.34
23	a	404	CLA	CHD-C4C	4.00	1.48	1.39
35	c	519	DGD	O1G-C1A	4.00	1.45	1.33
23	C	512	CLA	C3D-C2D	4.00	1.50	1.39
35	c	518	DGD	O2G-C1B	4.00	1.45	1.34
23	c	511	CLA	C3D-C2D	4.00	1.50	1.39
23	b	604	CLA	C3D-C2D	4.00	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	h	103	DGD	O2G-C1B	4.00	1.45	1.34
23	a	404	CLA	CHD-C1D	4.00	1.46	1.38
23	c	507	CLA	CHD-C4C	3.99	1.48	1.39
23	B	608	CLA	CHD-C1D	3.99	1.46	1.38
23	B	604	CLA	CHD-C1D	3.99	1.46	1.38
23	c	508	CLA	CHD-C4C	3.99	1.48	1.39
23	B	613	CLA	O2A-CGA	3.99	1.45	1.33
23	C	513	CLA	CHD-C1D	3.98	1.46	1.38
23	c	504	CLA	O2A-CGA	3.98	1.45	1.33
23	b	604	CLA	CHD-C1D	3.98	1.46	1.38
23	b	615	CLA	CHD-C1D	3.98	1.46	1.38
23	b	607	CLA	C3D-C2D	3.97	1.50	1.39
23	A	405	CLA	O2A-CGA	3.97	1.44	1.33
23	c	506	CLA	CHD-C4C	3.97	1.48	1.39
23	C	515	CLA	C3D-C2D	3.97	1.50	1.39
23	C	512	CLA	CHD-C1D	3.97	1.46	1.38
23	c	510	CLA	C3D-C2D	3.97	1.50	1.39
23	c	506	CLA	C3D-C2D	3.97	1.50	1.39
32	m	101	LMG	O7-C10	3.97	1.45	1.34
23	b	616	CLA	CHD-C1D	3.96	1.46	1.38
23	B	607	CLA	CHD-C4C	3.96	1.48	1.39
23	b	615	CLA	O2A-CGA	3.96	1.44	1.33
23	C	506	CLA	C3D-C2D	3.96	1.49	1.39
23	b	606	CLA	O2D-CGD	3.96	1.42	1.33
23	b	612	CLA	CHD-C1D	3.96	1.46	1.38
23	b	609	CLA	O2A-CGA	3.95	1.44	1.33
32	d	412	LMG	O7-C10	3.95	1.45	1.34
23	B	605	CLA	C3D-C2D	3.94	1.49	1.39
23	C	505	CLA	CHD-C4C	3.94	1.48	1.39
23	c	510	CLA	CHD-C4C	3.94	1.48	1.39
23	B	603	CLA	C3D-C2D	3.94	1.49	1.39
23	c	512	CLA	CHD-C4C	3.94	1.48	1.39
23	d	402	CLA	C1D-ND	3.94	1.42	1.37
23	B	601	CLA	CHD-C4C	3.93	1.48	1.39
23	c	509	CLA	OBD-CAD	3.93	1.29	1.22
23	B	610	CLA	CHD-C4C	3.93	1.48	1.39
35	C	520	DGD	O2G-C1B	3.93	1.45	1.34
23	B	604	CLA	O2A-CGA	3.93	1.44	1.33
23	B	605	CLA	OBD-CAD	3.93	1.29	1.22
23	C	505	CLA	C3D-C2D	3.92	1.49	1.39
23	B	613	CLA	C3D-C2D	3.91	1.49	1.39
23	c	510	CLA	OBD-CAD	3.91	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	515	CLA	CHD-C4C	3.91	1.48	1.39
23	C	510	CLA	C3D-C2D	3.91	1.49	1.39
23	c	504	CLA	C3D-C2D	3.91	1.49	1.39
23	c	507	CLA	O2A-CGA	3.90	1.44	1.33
23	C	513	CLA	CHD-C4C	3.90	1.48	1.39
23	D	403	CLA	C1D-ND	3.90	1.42	1.37
23	c	508	CLA	C3D-C2D	3.90	1.49	1.39
23	c	505	CLA	CHD-C4C	3.90	1.48	1.39
23	B	607	CLA	OBD-CAD	3.89	1.29	1.22
23	c	515	CLA	C3D-C2D	3.89	1.49	1.39
23	B	614	CLA	O2A-CGA	3.89	1.44	1.33
23	B	610	CLA	C3D-C2D	3.88	1.49	1.39
23	b	616	CLA	O2A-CGA	3.88	1.44	1.33
23	A	406	CLA	CHD-C4C	3.87	1.48	1.39
23	c	509	CLA	C3D-C2D	3.87	1.49	1.39
31	D	408	LHG	O7-C7	3.87	1.45	1.34
23	c	505	CLA	O2A-CGA	3.87	1.44	1.33
23	b	603	CLA	O2A-CGA	3.87	1.44	1.33
38	e	102	HEC	C2B-C3B	-3.87	1.36	1.40
23	B	613	CLA	CHD-C1D	3.87	1.45	1.38
23	C	512	CLA	CHD-C4C	3.86	1.48	1.39
23	C	513	CLA	C3D-C2D	3.86	1.49	1.39
33	b	622	HTG	C1'-S1	-3.86	1.76	1.81
31	d	406	LHG	O8-C23	3.86	1.44	1.33
23	b	605	CLA	CHD-C4C	3.85	1.48	1.39
23	b	611	CLA	CHD-C4C	3.85	1.48	1.39
23	b	604	CLA	CHD-C4C	3.85	1.48	1.39
23	b	606	CLA	OBD-CAD	3.84	1.29	1.22
23	c	503	CLA	CHD-C1D	3.84	1.45	1.38
23	a	406	CLA	C3D-C2D	3.84	1.49	1.39
23	b	604	CLA	O2A-CGA	3.84	1.44	1.33
23	B	609	CLA	C3D-C2D	3.84	1.49	1.39
23	B	601	CLA	C3D-C2D	3.84	1.49	1.39
23	B	607	CLA	O2A-CGA	3.83	1.44	1.33
23	c	513	CLA	CHD-C1D	3.83	1.45	1.38
23	B	609	CLA	CHD-C4C	3.83	1.48	1.39
23	C	510	CLA	CHD-C1D	3.83	1.45	1.38
31	d	408	LHG	O8-C23	3.82	1.44	1.33
23	C	512	CLA	O2A-CGA	3.82	1.44	1.33
23	b	609	CLA	C3D-C2D	3.82	1.49	1.39
23	B	608	CLA	CHD-C4C	3.82	1.48	1.39
23	B	602	CLA	O2A-CGA	3.82	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	405	CLA	C3D-C2D	3.82	1.49	1.39
35	H	102	DGD	O1G-C1A	3.82	1.44	1.33
24	a	407	PHO	O2A-CGA	3.82	1.44	1.33
23	d	402	CLA	CHD-C1D	3.81	1.45	1.38
31	D	407	LHG	O7-C7	3.81	1.45	1.34
23	a	408	CLA	CHD-C1D	3.81	1.45	1.38
23	b	601	CLA	OBD-CAD	3.80	1.29	1.22
31	d	407	LHG	O8-C23	3.80	1.44	1.33
23	b	606	CLA	CHD-C1D	3.80	1.45	1.38
23	b	613	CLA	O2A-CGA	3.80	1.44	1.33
23	b	615	CLA	CHD-C4C	3.79	1.47	1.39
23	b	616	CLA	OBD-CAD	3.79	1.29	1.22
23	C	504	CLA	O2A-CGA	3.79	1.44	1.33
23	C	508	CLA	C3D-C2D	3.79	1.49	1.39
32	B	621	LMG	O7-C10	3.79	1.45	1.34
35	c	519	DGD	O2G-C1B	3.79	1.45	1.34
35	c	520	DGD	O2G-C1B	3.79	1.45	1.34
23	d	402	CLA	OBD-CAD	3.79	1.29	1.22
23	b	605	CLA	OBD-CAD	3.79	1.29	1.22
23	A	408	CLA	C3D-C2D	3.79	1.49	1.39
23	B	606	CLA	C3D-C2D	3.78	1.49	1.39
23	b	616	CLA	CHD-C4C	3.78	1.47	1.39
24	a	417	PHO	O2A-CGA	3.78	1.44	1.33
23	A	406	CLA	C3D-C2D	3.77	1.49	1.39
23	C	514	CLA	C3D-C2D	3.77	1.49	1.39
23	A	404	CLA	C3D-C2D	3.77	1.49	1.39
23	A	406	CLA	O2A-CGA	3.77	1.44	1.33
23	C	504	CLA	OBD-CAD	3.77	1.29	1.22
23	B	602	CLA	C3D-C2D	3.77	1.49	1.39
31	L	101	LHG	O7-C7	3.77	1.44	1.34
25	B	618	BCR	C23-C22	-3.76	1.37	1.45
23	c	504	CLA	CHD-C4C	3.76	1.47	1.39
23	D	404	CLA	O2A-CGA	3.76	1.44	1.33
23	a	406	CLA	CHD-C1D	3.76	1.45	1.38
23	C	514	CLA	CHD-C4C	3.76	1.47	1.39
23	a	405	CLA	CHD-C4C	3.75	1.47	1.39
23	c	514	CLA	C3D-C2D	3.75	1.49	1.39
23	C	506	CLA	CHD-C1D	3.75	1.45	1.38
23	b	606	CLA	CHD-C4C	3.75	1.47	1.39
23	b	610	CLA	C3D-C2D	3.75	1.49	1.39
23	b	609	CLA	CHD-C4C	3.75	1.47	1.39
23	b	603	CLA	CHD-C4C	3.74	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	508	CLA	OBD-CAD	3.74	1.28	1.22
23	b	615	CLA	C3D-C2D	3.73	1.49	1.39
23	b	610	CLA	CHD-C4C	3.72	1.47	1.39
31	b	629	LHG	O8-C23	3.72	1.44	1.33
23	C	509	CLA	CHD-C4C	3.72	1.47	1.39
23	B	611	CLA	OBD-CAD	3.72	1.28	1.22
23	c	514	CLA	CHD-C4C	3.72	1.47	1.39
23	a	404	CLA	C3D-C2D	3.72	1.49	1.39
31	A	416	LHG	O8-C23	3.72	1.44	1.33
23	c	503	CLA	C3D-C2D	3.71	1.49	1.39
23	c	507	CLA	C3D-C2D	3.71	1.49	1.39
23	D	404	CLA	CHD-C4C	3.71	1.47	1.39
24	a	407	PHO	C3C-C2C	3.71	1.48	1.37
23	c	513	CLA	CHD-C4C	3.71	1.47	1.39
23	B	611	CLA	C3D-C2D	3.71	1.49	1.39
31	A	416	LHG	O7-C7	3.70	1.44	1.34
23	C	503	CLA	CHD-C4C	3.69	1.47	1.39
23	B	616	CLA	CHD-C1D	3.69	1.45	1.38
23	a	406	CLA	OBD-CAD	3.69	1.28	1.22
31	d	407	LHG	O7-C7	3.69	1.44	1.34
23	b	611	CLA	CHD-C1D	3.69	1.45	1.38
24	A	415	PHO	O2A-CGA	3.69	1.44	1.33
23	c	512	CLA	C3D-C2D	3.68	1.49	1.39
23	c	513	CLA	C3D-C2D	3.68	1.49	1.39
23	B	608	CLA	C3D-C2D	3.68	1.49	1.39
23	b	614	CLA	C3D-C2D	3.68	1.49	1.39
23	C	509	CLA	C3D-C2D	3.67	1.49	1.39
23	b	607	CLA	CHD-C4C	3.67	1.47	1.39
23	b	613	CLA	CHD-C4C	3.66	1.47	1.39
23	b	613	CLA	CHD-C1D	3.66	1.45	1.38
23	d	402	CLA	C3D-C2D	3.65	1.49	1.39
33	h	101	HTG	C1'-S1	-3.65	1.76	1.81
23	B	603	CLA	CHD-C4C	3.65	1.47	1.39
23	b	607	CLA	O2A-CGA	3.65	1.44	1.33
23	C	514	CLA	OBD-CAD	3.65	1.28	1.22
23	b	616	CLA	C3D-C2D	3.65	1.49	1.39
23	C	505	CLA	OBD-CAD	3.65	1.28	1.22
23	B	611	CLA	O2A-CGA	3.64	1.44	1.33
27	C	501	SQD	O47-C7	3.64	1.44	1.34
23	D	404	CLA	C3D-C2D	3.64	1.49	1.39
23	A	406	CLA	OBD-CAD	3.64	1.28	1.22
23	B	604	CLA	C3D-C2D	3.64	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	506	CLA	O2A-CGA	3.63	1.44	1.33
23	A	405	CLA	CHD-C4C	3.63	1.47	1.39
23	b	603	CLA	C3D-C2D	3.63	1.49	1.39
23	b	612	CLA	C3D-C2D	3.63	1.49	1.39
31	d	406	LHG	O7-C7	3.63	1.44	1.34
23	B	606	CLA	CHD-C4C	3.63	1.47	1.39
23	d	402	CLA	CHD-C4C	3.63	1.47	1.39
23	a	406	CLA	CHD-C4C	3.62	1.47	1.39
23	A	404	CLA	CHD-C1D	3.62	1.45	1.38
31	D	408	LHG	O8-C23	3.62	1.43	1.33
23	B	616	CLA	OBD-CAD	3.62	1.28	1.22
23	b	608	CLA	C3D-C2D	3.62	1.49	1.39
23	B	601	CLA	OBD-CAD	3.61	1.28	1.22
23	B	616	CLA	C3D-C2D	3.61	1.49	1.39
23	b	606	CLA	O2A-CGA	3.61	1.43	1.33
23	b	605	CLA	O2A-CGA	3.60	1.43	1.33
23	C	508	CLA	OBD-CAD	3.60	1.28	1.22
31	D	407	LHG	O8-C23	3.60	1.43	1.33
24	A	415	PHO	C3C-C2C	3.60	1.48	1.37
23	b	615	CLA	OBD-CAD	3.60	1.28	1.22
23	c	514	CLA	OBD-CAD	3.59	1.28	1.22
23	B	612	CLA	C1D-ND	3.59	1.42	1.37
24	a	417	PHO	C3C-C2C	3.59	1.48	1.37
23	a	408	CLA	C3D-C2D	3.58	1.48	1.39
23	C	503	CLA	OBD-CAD	3.58	1.28	1.22
23	C	507	CLA	C3D-C2D	3.58	1.48	1.39
23	c	512	CLA	OBD-CAD	3.58	1.28	1.22
23	b	614	CLA	CHD-C4C	3.58	1.47	1.39
23	C	505	CLA	CHD-C1D	3.57	1.45	1.38
23	B	612	CLA	C1C-C2C	3.57	1.51	1.44
32	D	413	LMG	O8-C28	3.57	1.43	1.33
23	C	506	CLA	CHD-C4C	3.57	1.47	1.39
23	c	505	CLA	C3D-C2D	3.57	1.48	1.39
23	D	404	CLA	OBD-CAD	3.56	1.28	1.22
23	B	611	CLA	CHD-C4C	3.56	1.47	1.39
23	C	507	CLA	O2A-CGA	3.56	1.43	1.33
23	b	602	CLA	OBD-CAD	3.55	1.28	1.22
23	B	604	CLA	OBD-CAD	3.55	1.28	1.22
33	b	623	HTG	C1'-S1	-3.55	1.76	1.81
23	c	511	CLA	OBD-CAD	3.54	1.28	1.22
23	b	605	CLA	C3D-C2D	3.54	1.48	1.39
23	B	607	CLA	C3D-C2D	3.53	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	612	CLA	C3D-C2D	3.53	1.48	1.39
23	B	608	CLA	OBD-CAD	3.53	1.28	1.22
23	A	408	CLA	OBD-CAD	3.53	1.28	1.22
23	B	603	CLA	CHD-C1D	3.53	1.45	1.38
38	E	103	HEC	C2B-C3B	-3.53	1.37	1.40
23	B	614	CLA	CHD-C4C	3.52	1.47	1.39
33	B	622	HTG	C1'-S1	-3.50	1.76	1.81
23	B	603	CLA	OBD-CAD	3.50	1.28	1.22
23	b	608	CLA	OBD-CAD	3.50	1.28	1.22
23	c	506	CLA	OBD-CAD	3.50	1.28	1.22
23	A	404	CLA	O2A-CGA	3.49	1.43	1.33
23	C	504	CLA	CHD-C4C	3.49	1.47	1.39
24	A	407	PHO	C3C-C2C	3.49	1.48	1.37
23	B	610	CLA	O2A-CGA	3.48	1.43	1.33
23	B	614	CLA	C3D-C2D	3.48	1.48	1.39
23	b	604	CLA	OBD-CAD	3.48	1.28	1.22
23	C	503	CLA	C3D-C2D	3.47	1.48	1.39
23	B	616	CLA	CHD-C4C	3.47	1.47	1.39
23	A	406	CLA	C1D-ND	3.47	1.42	1.37
23	C	510	CLA	CHD-C4C	3.46	1.47	1.39
23	d	403	CLA	OBD-CAD	3.46	1.28	1.22
23	A	404	CLA	CHD-C4C	3.46	1.47	1.39
23	B	605	CLA	CHD-C4C	3.45	1.47	1.39
23	a	408	CLA	CHD-C4C	3.44	1.47	1.39
23	b	612	CLA	OBD-CAD	3.44	1.28	1.22
23	C	515	CLA	OBD-CAD	3.43	1.28	1.22
23	A	406	CLA	C1B-NB	-3.43	1.32	1.35
23	B	613	CLA	OBD-CAD	3.43	1.28	1.22
23	a	405	CLA	OBD-CAD	3.42	1.28	1.22
23	C	512	CLA	OBD-CAD	3.42	1.28	1.22
23	b	607	CLA	OBD-CAD	3.41	1.28	1.22
24	A	415	PHO	CHA-CBD	-3.41	1.48	1.52
23	C	513	CLA	OBD-CAD	3.41	1.28	1.22
23	b	610	CLA	O2A-CGA	3.38	1.43	1.33
23	D	403	CLA	C3D-C2D	3.38	1.48	1.39
23	b	611	CLA	C3D-C2D	3.38	1.48	1.39
32	D	413	LMG	O7-C10	3.36	1.43	1.34
23	c	513	CLA	OBD-CAD	3.35	1.28	1.22
23	c	504	CLA	OBD-CAD	3.35	1.28	1.22
23	B	613	CLA	CHD-C4C	3.35	1.46	1.39
23	B	615	CLA	CHD-C1D	3.33	1.44	1.38
23	b	606	CLA	C3D-C2D	3.33	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	615	CLA	CHD-C4C	3.32	1.46	1.39
23	c	512	CLA	O2A-CGA	3.32	1.43	1.33
23	b	613	CLA	OBD-CAD	3.32	1.28	1.22
23	C	510	CLA	OBD-CAD	3.32	1.28	1.22
23	c	505	CLA	C4C-C3C	3.31	1.50	1.45
23	B	614	CLA	OBD-CAD	3.30	1.28	1.22
23	B	612	CLA	CHD-C1D	3.29	1.44	1.38
23	C	509	CLA	OBD-CAD	3.29	1.28	1.22
23	A	405	CLA	OBD-CAD	3.28	1.28	1.22
23	B	602	CLA	C1C-C2C	3.28	1.50	1.44
33	D	411	HTG	C1'-S1	-3.27	1.77	1.81
23	c	507	CLA	OBD-CAD	3.27	1.28	1.22
23	C	507	CLA	OBD-CAD	3.27	1.28	1.22
35	H	102	DGD	O2G-C1B	3.26	1.43	1.34
23	b	614	CLA	OBD-CAD	3.26	1.28	1.22
38	e	102	HEC	C4B-C3B	3.26	1.49	1.43
23	B	614	CLA	C4B-NB	-3.25	1.32	1.35
23	B	612	CLA	OBD-CAD	3.25	1.28	1.22
33	b	625	HTG	C1'-S1	-3.24	1.77	1.81
23	b	612	CLA	CHD-C4C	3.22	1.46	1.39
33	c	523	HTG	C1'-S1	-3.22	1.77	1.81
33	B	625	HTG	C1'-S1	-3.22	1.77	1.81
23	A	404	CLA	OBD-CAD	3.20	1.28	1.22
23	c	515	CLA	OBD-CAD	3.19	1.28	1.22
23	a	404	CLA	O2A-CGA	3.18	1.42	1.33
23	c	505	CLA	OBD-CAD	3.17	1.27	1.22
23	a	408	CLA	OBD-CAD	3.17	1.27	1.22
23	C	506	CLA	OBD-CAD	3.17	1.27	1.22
23	c	511	CLA	C4C-C3C	3.16	1.50	1.45
33	C	523	HTG	C1'-S1	-3.15	1.77	1.81
38	E	103	HEC	C4B-C3B	3.15	1.48	1.43
23	b	612	CLA	C1B-NB	-3.13	1.32	1.35
23	b	609	CLA	OBD-CAD	3.10	1.27	1.22
23	B	602	CLA	OBD-CAD	3.09	1.27	1.22
23	c	505	CLA	C1C-C2C	3.08	1.50	1.44
23	B	609	CLA	OBD-CAD	3.05	1.27	1.22
23	a	408	CLA	C1C-C2C	3.04	1.50	1.44
23	D	403	CLA	OBD-CAD	3.04	1.27	1.22
23	B	605	CLA	C4B-CHC	3.02	1.49	1.41
23	B	612	CLA	C1B-CHB	3.02	1.49	1.41
23	c	513	CLA	C1B-CHB	3.01	1.49	1.41
23	c	509	CLA	C1C-C2C	3.01	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	611	CLA	OBD-CAD	3.01	1.27	1.22
23	B	612	CLA	CHD-C4C	2.99	1.46	1.39
23	c	503	CLA	OBD-CAD	2.99	1.27	1.22
23	C	508	CLA	C4C-C3C	2.98	1.50	1.45
23	B	604	CLA	C4D-CHA	2.97	1.48	1.38
23	B	606	CLA	OBD-CAD	2.96	1.27	1.22
23	B	603	CLA	C1C-C2C	2.94	1.50	1.44
23	C	506	CLA	C1C-C2C	2.94	1.50	1.44
23	A	405	CLA	C4D-CHA	2.93	1.48	1.38
23	C	512	CLA	C1C-C2C	2.93	1.50	1.44
23	B	602	CLA	C4B-CHC	2.92	1.49	1.41
27	f	101	SQD	C6-S	-2.91	1.66	1.77
23	c	503	CLA	C1B-CHB	2.89	1.49	1.41
23	C	503	CLA	C1C-C2C	2.88	1.50	1.44
23	B	611	CLA	C1C-C2C	2.87	1.50	1.44
23	b	604	CLA	C4D-CHA	2.87	1.48	1.38
23	b	607	CLA	C1B-NB	-2.87	1.32	1.35
23	B	613	CLA	C1C-C2C	2.86	1.50	1.44
23	C	513	CLA	C4D-CHA	2.86	1.48	1.38
23	B	607	CLA	C4D-CHA	2.86	1.48	1.38
23	D	404	CLA	C1B-CHB	2.86	1.48	1.41
23	c	512	CLA	C4D-CHA	2.85	1.48	1.38
23	c	515	CLA	C1C-C2C	2.84	1.50	1.44
23	c	509	CLA	C4B-CHC	2.83	1.48	1.41
23	c	507	CLA	C4C-C3C	2.83	1.49	1.45
23	D	403	CLA	C1B-CHB	2.83	1.48	1.41
23	C	509	CLA	C4D-CHA	2.82	1.48	1.38
23	B	607	CLA	C4C-C3C	2.82	1.49	1.45
23	C	507	CLA	C4C-C3C	2.82	1.49	1.45
23	c	512	CLA	C1B-CHB	2.82	1.48	1.41
23	b	615	CLA	C4C-C3C	2.82	1.49	1.45
27	C	501	SQD	C6-S	-2.81	1.67	1.77
23	C	506	CLA	C4D-CHA	2.81	1.48	1.38
23	D	404	CLA	C1C-C2C	2.80	1.50	1.44
23	b	610	CLA	C1C-C2C	2.79	1.50	1.44
23	b	603	CLA	C1C-C2C	2.79	1.50	1.44
23	B	608	CLA	C4D-CHA	2.79	1.48	1.38
23	B	606	CLA	C4D-CHA	2.79	1.48	1.38
23	c	507	CLA	C1C-C2C	2.78	1.49	1.44
23	C	507	CLA	C1C-C2C	2.78	1.49	1.44
27	a	410	SQD	C6-S	-2.78	1.67	1.77
23	b	616	CLA	C4D-CHA	2.77	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	613	CLA	C4C-C3C	2.77	1.49	1.45
23	b	612	CLA	C1B-CHB	2.76	1.48	1.41
23	c	509	CLA	C4D-CHA	2.76	1.48	1.38
33	B	625	HTG	C1-S1	-2.76	1.76	1.80
23	b	615	CLA	C4D-CHA	2.75	1.48	1.38
23	B	614	CLA	C4D-CHA	2.75	1.48	1.38
23	C	511	CLA	C1C-C2C	2.75	1.49	1.44
23	B	607	CLA	C1B-CHB	2.75	1.48	1.41
23	c	514	CLA	C1C-C2C	2.75	1.49	1.44
23	a	405	CLA	C1C-C2C	2.75	1.49	1.44
23	c	506	CLA	C4C-C3C	2.74	1.49	1.45
23	A	404	CLA	C1C-C2C	2.73	1.49	1.44
23	C	515	CLA	C1C-C2C	2.73	1.49	1.44
23	c	514	CLA	C4B-CHC	2.73	1.48	1.41
23	b	608	CLA	C4D-CHA	2.73	1.48	1.38
23	C	514	CLA	C4D-CHA	2.73	1.48	1.38
23	b	611	CLA	C1B-CHB	2.73	1.48	1.41
23	C	513	CLA	C1C-C2C	2.72	1.49	1.44
23	C	511	CLA	C4C-C3C	2.71	1.49	1.45
23	b	609	CLA	C4D-CHA	2.71	1.48	1.38
23	c	511	CLA	C4D-CHA	2.71	1.48	1.38
23	b	608	CLA	C3D-C4D	-2.71	1.38	1.44
23	D	403	CLA	C4D-CHA	2.70	1.48	1.38
27	a	412	SQD	C6-S	-2.70	1.67	1.77
23	C	508	CLA	C4D-CHA	2.70	1.48	1.38
23	c	505	CLA	C4D-CHA	2.69	1.48	1.38
33	B	623	HTG	C1'-S1	-2.69	1.78	1.81
23	B	605	CLA	C1C-C2C	2.68	1.49	1.44
23	c	507	CLA	C4B-CHC	2.68	1.48	1.41
29	A	413	PL9	C6-C5	2.68	1.49	1.35
23	B	614	CLA	C1B-CHB	2.68	1.48	1.41
27	B	620	SQD	C6-S	-2.68	1.67	1.77
23	d	402	CLA	C4D-CHA	2.67	1.47	1.38
23	C	513	CLA	C4C-C3C	2.67	1.49	1.45
23	C	503	CLA	C4D-CHA	2.67	1.47	1.38
23	c	513	CLA	C4D-CHA	2.67	1.47	1.38
23	B	601	CLA	C4B-CHC	2.67	1.48	1.41
23	C	512	CLA	C4B-CHC	2.66	1.48	1.41
23	b	616	CLA	C3D-C4D	-2.66	1.38	1.44
23	C	511	CLA	C4D-CHA	2.65	1.47	1.38
23	A	405	CLA	C1C-C2C	2.65	1.49	1.44
23	b	614	CLA	C1B-CHB	2.65	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	411	SQD	C6-S	-2.65	1.67	1.77
27	b	620	SQD	C6-S	-2.64	1.67	1.77
23	B	614	CLA	CHD-C1D	2.64	1.43	1.38
23	C	512	CLA	C4D-CHA	2.64	1.47	1.38
23	B	610	CLA	C4D-CHA	2.64	1.47	1.38
23	c	506	CLA	C4D-CHA	2.64	1.47	1.38
23	C	510	CLA	C4D-CHA	2.64	1.47	1.38
23	B	610	CLA	C4B-CHC	2.64	1.48	1.41
23	c	514	CLA	C4D-CHA	2.64	1.47	1.38
23	C	504	CLA	C1C-C2C	2.64	1.49	1.44
23	B	614	CLA	C4C-C3C	2.64	1.49	1.45
23	c	507	CLA	C4D-CHA	2.64	1.47	1.38
23	C	510	CLA	C1B-CHB	2.63	1.48	1.41
23	A	404	CLA	C4C-C3C	2.63	1.49	1.45
23	A	408	CLA	C4D-CHA	2.63	1.47	1.38
23	C	507	CLA	C4D-CHA	2.63	1.47	1.38
23	b	602	CLA	C4C-C3C	2.63	1.49	1.45
29	a	415	PL9	C6-C5	2.62	1.48	1.35
23	b	602	CLA	C1C-C2C	2.61	1.49	1.44
23	b	607	CLA	C1B-CHB	2.61	1.48	1.41
23	C	506	CLA	C1B-CHB	2.61	1.48	1.41
23	b	606	CLA	C1C-C2C	2.61	1.49	1.44
23	a	406	CLA	C1C-C2C	2.61	1.49	1.44
23	c	511	CLA	C1B-CHB	2.60	1.48	1.41
23	b	602	CLA	C4D-CHA	2.60	1.47	1.38
23	A	408	CLA	C4B-CHC	2.60	1.48	1.41
23	C	503	CLA	C4B-CHC	2.60	1.48	1.41
23	c	506	CLA	C1B-CHB	2.60	1.48	1.41
23	b	607	CLA	C4D-CHA	2.60	1.47	1.38
23	d	402	CLA	C4C-C3C	2.60	1.49	1.45
23	b	608	CLA	C4C-C3C	2.59	1.49	1.45
23	B	616	CLA	C1B-CHB	2.59	1.48	1.41
23	A	406	CLA	C4B-CHC	2.59	1.48	1.41
23	B	611	CLA	C4D-CHA	2.59	1.47	1.38
23	b	609	CLA	C1C-C2C	2.58	1.49	1.44
23	b	610	CLA	C4B-CHC	2.58	1.48	1.41
24	a	417	PHO	CHA-CBD	-2.58	1.49	1.52
23	B	604	CLA	C1C-C2C	2.58	1.49	1.44
23	B	603	CLA	C4D-CHA	2.58	1.47	1.38
23	b	603	CLA	C4D-CHA	2.58	1.47	1.38
23	B	602	CLA	C3D-C4D	-2.57	1.38	1.44
23	C	512	CLA	C1B-CHB	2.57	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	604	CLA	C4B-CHC	2.57	1.48	1.41
27	D	412	SQD	C6-S	-2.57	1.67	1.77
23	c	504	CLA	C1B-CHB	2.57	1.48	1.41
23	C	515	CLA	C1B-CHB	2.57	1.48	1.41
23	c	503	CLA	C3D-C4D	-2.57	1.38	1.44
23	B	615	CLA	C4D-CHA	2.56	1.47	1.38
23	b	607	CLA	C1C-C2C	2.56	1.49	1.44
23	b	610	CLA	C4D-CHA	2.56	1.47	1.38
23	B	609	CLA	C4D-CHA	2.56	1.47	1.38
23	C	513	CLA	C1B-CHB	2.56	1.48	1.41
23	b	614	CLA	C4D-CHA	2.56	1.47	1.38
23	c	507	CLA	C1B-CHB	2.56	1.48	1.41
23	c	503	CLA	C4D-CHA	2.56	1.47	1.38
23	c	512	CLA	C1C-C2C	2.56	1.49	1.44
23	a	408	CLA	C4B-CHC	2.56	1.48	1.41
23	b	603	CLA	C4C-C3C	2.55	1.49	1.45
23	C	507	CLA	C1B-CHB	2.55	1.48	1.41
23	B	611	CLA	C1B-CHB	2.55	1.48	1.41
23	B	609	CLA	C1C-C2C	2.55	1.49	1.44
23	A	408	CLA	C1C-C2C	2.55	1.49	1.44
32	Z	101	LMG	O8-C28	2.55	1.46	1.33
23	c	505	CLA	C1B-CHB	2.55	1.48	1.41
23	C	515	CLA	C4D-CHA	2.55	1.47	1.38
23	B	613	CLA	C1B-CHB	2.55	1.48	1.41
23	b	603	CLA	C1B-CHB	2.55	1.48	1.41
23	c	515	CLA	C4D-CHA	2.54	1.47	1.38
23	B	616	CLA	C4D-CHA	2.54	1.47	1.38
23	c	505	CLA	C4B-CHC	2.54	1.48	1.41
23	b	606	CLA	C4D-CHA	2.54	1.47	1.38
23	d	402	CLA	C1C-C2C	2.54	1.49	1.44
23	a	405	CLA	C4D-CHA	2.54	1.47	1.38
23	B	608	CLA	C3D-C4D	-2.54	1.38	1.44
23	B	612	CLA	C4B-CHC	2.54	1.48	1.41
23	A	405	CLA	C1B-CHB	2.53	1.48	1.41
23	A	405	CLA	C4B-CHC	2.53	1.48	1.41
23	B	602	CLA	C4C-C3C	2.53	1.49	1.45
23	C	505	CLA	C4B-CHC	2.53	1.48	1.41
33	b	625	HTG	C1-S1	-2.52	1.76	1.80
23	d	403	CLA	C1C-C2C	2.52	1.49	1.44
23	A	404	CLA	C1B-CHB	2.52	1.48	1.41
23	c	507	CLA	C3D-C4D	-2.52	1.38	1.44
23	b	605	CLA	C4B-CHC	2.52	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	406	CLA	C4D-CHA	2.52	1.47	1.38
23	d	402	CLA	C3D-C4D	-2.52	1.38	1.44
23	c	503	CLA	C1C-C2C	2.52	1.49	1.44
23	B	613	CLA	C4D-CHA	2.52	1.47	1.38
23	c	510	CLA	C1B-CHB	2.52	1.48	1.41
23	B	602	CLA	C4D-CHA	2.52	1.47	1.38
23	B	608	CLA	C1B-CHB	2.52	1.48	1.41
23	C	507	CLA	C4B-CHC	2.51	1.48	1.41
23	D	404	CLA	C4D-CHA	2.51	1.47	1.38
23	a	408	CLA	C4D-CHA	2.50	1.47	1.38
23	b	601	CLA	C4D-CHA	2.50	1.47	1.38
23	c	510	CLA	C4D-CHA	2.50	1.47	1.38
23	B	615	CLA	C1B-CHB	2.50	1.47	1.41
23	b	613	CLA	C1C-C2C	2.49	1.49	1.44
23	d	403	CLA	C4B-CHC	2.49	1.47	1.41
23	B	605	CLA	C4D-CHA	2.49	1.47	1.38
34	a	413	LMT	O1'-C1'	2.49	1.44	1.40
23	b	613	CLA	C4C-C3C	2.49	1.49	1.45
23	c	511	CLA	C1C-C2C	2.49	1.49	1.44
23	B	601	CLA	C1C-C2C	2.49	1.49	1.44
23	B	614	CLA	C4B-CHC	2.49	1.47	1.41
23	c	514	CLA	C4C-C3C	2.49	1.49	1.45
23	b	613	CLA	C4D-CHA	2.49	1.47	1.38
23	b	604	CLA	C1C-C2C	2.49	1.49	1.44
23	C	512	CLA	C4C-C3C	2.49	1.49	1.45
23	a	406	CLA	C4D-CHA	2.49	1.47	1.38
23	b	612	CLA	C1C-C2C	2.48	1.49	1.44
23	c	515	CLA	C3D-C4D	-2.48	1.38	1.44
23	C	511	CLA	C1B-CHB	2.48	1.47	1.41
23	c	512	CLA	C3D-C4D	-2.48	1.38	1.44
23	B	610	CLA	C4C-C3C	2.48	1.49	1.45
23	a	405	CLA	C1B-CHB	2.48	1.47	1.41
23	C	514	CLA	C3D-C4D	-2.48	1.38	1.44
23	A	404	CLA	C4D-CHA	2.48	1.47	1.38
24	a	407	PHO	CHA-CBD	-2.48	1.49	1.52
23	c	506	CLA	C1C-C2C	2.48	1.49	1.44
23	B	609	CLA	C4B-CHC	2.47	1.47	1.41
23	B	601	CLA	C4D-CHA	2.47	1.47	1.38
23	B	609	CLA	C1B-CHB	2.47	1.47	1.41
23	C	509	CLA	C3D-C4D	-2.47	1.38	1.44
23	C	504	CLA	C1B-CHB	2.47	1.47	1.41
23	C	505	CLA	C1C-C2C	2.47	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	504	CLA	C4D-CHA	2.47	1.47	1.38
23	c	508	CLA	C1B-CHB	2.47	1.47	1.41
23	C	511	CLA	C4B-NB	-2.47	1.33	1.35
23	a	408	CLA	C1B-CHB	2.47	1.47	1.41
23	b	616	CLA	C1B-CHB	2.47	1.47	1.41
23	B	606	CLA	C3D-C4D	-2.46	1.38	1.44
23	d	402	CLA	C1B-CHB	2.46	1.47	1.41
23	d	403	CLA	C4D-CHA	2.46	1.47	1.38
23	B	603	CLA	C1B-CHB	2.46	1.47	1.41
23	b	602	CLA	C4B-CHC	2.46	1.47	1.41
23	C	505	CLA	C4D-CHA	2.45	1.47	1.38
23	c	506	CLA	C1D-C2D	2.45	1.50	1.45
23	c	505	CLA	C3D-C4D	-2.45	1.38	1.44
23	C	514	CLA	C1C-C2C	2.45	1.49	1.44
23	c	503	CLA	C4B-CHC	2.45	1.47	1.41
23	c	508	CLA	C4D-CHA	2.45	1.47	1.38
35	h	103	DGD	O5D-C1E	2.44	1.44	1.40
23	B	610	CLA	C1B-CHB	2.44	1.47	1.41
23	C	510	CLA	C3D-C4D	-2.44	1.38	1.44
23	B	609	CLA	C3D-C4D	-2.44	1.38	1.44
23	b	612	CLA	C4D-CHA	2.44	1.47	1.38
23	C	509	CLA	C4C-C3C	2.44	1.49	1.45
23	a	404	CLA	C4D-CHA	2.44	1.47	1.38
23	C	505	CLA	C1B-CHB	2.44	1.47	1.41
23	C	509	CLA	C1C-C2C	2.44	1.49	1.44
23	b	605	CLA	C1B-NB	-2.44	1.33	1.35
23	b	604	CLA	C1B-CHB	2.44	1.47	1.41
23	c	508	CLA	C4B-CHC	2.44	1.47	1.41
23	a	404	CLA	C1B-CHB	2.43	1.47	1.41
23	b	616	CLA	C1C-C2C	2.43	1.49	1.44
23	D	403	CLA	C3D-C4D	-2.43	1.38	1.44
23	b	616	CLA	C4B-CHC	2.43	1.47	1.41
23	A	408	CLA	C4C-C3C	2.43	1.49	1.45
23	B	612	CLA	C4D-CHA	2.43	1.47	1.38
23	b	603	CLA	C3D-C4D	-2.42	1.38	1.44
23	b	610	CLA	C3D-C4D	-2.42	1.38	1.44
23	C	514	CLA	C4B-CHC	2.42	1.47	1.41
23	C	508	CLA	C1D-C2D	2.42	1.50	1.45
23	b	608	CLA	C1B-CHB	2.42	1.47	1.41
23	b	611	CLA	C4D-CHA	2.42	1.47	1.38
23	b	602	CLA	C3D-C4D	-2.41	1.38	1.44
23	C	504	CLA	C4B-CHC	2.41	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	612	CLA	C4C-C3C	2.41	1.49	1.45
23	b	613	CLA	C1B-CHB	2.41	1.47	1.41
29	d	405	PL9	C6-C5	2.40	1.47	1.35
23	D	404	CLA	C4B-CHC	2.40	1.47	1.41
23	c	504	CLA	C4D-CHA	2.40	1.46	1.38
23	c	504	CLA	C1C-C2C	2.40	1.49	1.44
23	c	512	CLA	C4B-CHC	2.39	1.47	1.41
23	C	511	CLA	C4B-CHC	2.39	1.47	1.41
23	b	603	CLA	C4B-CHC	2.39	1.47	1.41
23	B	610	CLA	C3D-C4D	-2.39	1.38	1.44
23	b	614	CLA	C4B-CHC	2.39	1.47	1.41
23	b	611	CLA	C3D-C4D	-2.39	1.38	1.44
23	C	506	CLA	C4B-CHC	2.39	1.47	1.41
23	b	606	CLA	C4B-CHC	2.39	1.47	1.41
23	b	601	CLA	C4B-CHC	2.38	1.47	1.41
23	B	604	CLA	C1B-CHB	2.38	1.47	1.41
23	c	515	CLA	C1B-CHB	2.38	1.47	1.41
23	B	616	CLA	C1C-C2C	2.38	1.49	1.44
23	c	513	CLA	C4B-CHC	2.38	1.47	1.41
23	b	605	CLA	C4D-CHA	2.38	1.46	1.38
23	b	615	CLA	C4B-CHC	2.37	1.47	1.41
23	B	601	CLA	C4C-C3C	2.37	1.49	1.45
23	b	609	CLA	C1B-CHB	2.37	1.47	1.41
23	C	509	CLA	C4B-CHC	2.37	1.47	1.41
23	a	405	CLA	C4B-CHC	2.37	1.47	1.41
23	b	609	CLA	C4B-CHC	2.37	1.47	1.41
23	c	514	CLA	C1B-CHB	2.37	1.47	1.41
23	C	509	CLA	C1B-CHB	2.37	1.47	1.41
23	B	604	CLA	C4B-CHC	2.37	1.47	1.41
23	b	605	CLA	C1B-CHB	2.37	1.47	1.41
23	c	515	CLA	C4C-C3C	2.36	1.49	1.45
23	B	607	CLA	C4B-CHC	2.36	1.47	1.41
23	a	406	CLA	C1B-CHB	2.36	1.47	1.41
23	A	405	CLA	C4C-C3C	2.36	1.49	1.45
23	a	406	CLA	C3D-C4D	-2.36	1.38	1.44
23	b	601	CLA	C1B-CHB	2.36	1.47	1.41
23	b	611	CLA	C1C-C2C	2.36	1.49	1.44
23	C	508	CLA	C1B-CHB	2.35	1.47	1.41
23	b	610	CLA	C1B-CHB	2.35	1.47	1.41
23	A	408	CLA	C3D-C4D	-2.35	1.38	1.44
23	B	607	CLA	C1C-C2C	2.35	1.49	1.44
23	C	507	CLA	C3D-C4D	-2.34	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	508	CLA	C1C-C2C	2.34	1.49	1.44
23	d	403	CLA	C1B-CHB	2.34	1.47	1.41
23	C	504	CLA	C3D-C4D	-2.34	1.38	1.44
23	C	503	CLA	C1B-CHB	2.34	1.47	1.41
24	A	407	PHO	CBD-CGD	-2.33	1.49	1.52
23	C	505	CLA	C4C-C3C	2.33	1.49	1.45
23	d	403	CLA	C3D-C4D	-2.33	1.38	1.44
23	D	403	CLA	C4B-NB	-2.33	1.33	1.35
23	b	611	CLA	C4B-CHC	2.33	1.47	1.41
23	c	513	CLA	C1C-C2C	2.32	1.49	1.44
23	C	515	CLA	C4B-CHC	2.32	1.47	1.41
23	C	514	CLA	C1B-CHB	2.32	1.47	1.41
23	b	615	CLA	C1B-CHB	2.32	1.47	1.41
23	B	615	CLA	C1C-C2C	2.32	1.49	1.44
23	c	508	CLA	C3D-C4D	-2.32	1.38	1.44
23	B	614	CLA	C3D-C4D	-2.32	1.38	1.44
23	B	603	CLA	C1B-NB	-2.31	1.33	1.35
23	C	512	CLA	C3D-C4D	-2.31	1.39	1.44
35	H	102	DGD	O5D-C1E	2.31	1.44	1.40
23	A	406	CLA	C4C-C3C	2.30	1.49	1.45
23	B	604	CLA	C4C-C3C	2.30	1.49	1.45
23	A	405	CLA	C1B-NB	-2.30	1.33	1.35
23	C	503	CLA	C3D-C4D	-2.29	1.39	1.44
23	B	609	CLA	C4C-C3C	2.29	1.49	1.45
23	c	506	CLA	C4B-CHC	2.29	1.47	1.41
23	B	612	CLA	C4C-C3C	2.29	1.49	1.45
33	D	411	HTG	C1-S1	-2.29	1.77	1.80
23	b	612	CLA	C4B-CHC	2.29	1.47	1.41
23	B	603	CLA	C4B-CHC	2.29	1.47	1.41
23	B	606	CLA	C1B-CHB	2.29	1.47	1.41
32	Z	101	LMG	O1-C1	2.28	1.44	1.40
23	c	512	CLA	C4C-C3C	2.28	1.49	1.45
23	c	515	CLA	C4B-CHC	2.28	1.47	1.41
23	b	608	CLA	C1C-C2C	2.28	1.49	1.44
23	b	614	CLA	C1C-C2C	2.28	1.49	1.44
23	B	614	CLA	C1C-C2C	2.27	1.49	1.44
23	B	608	CLA	C4C-C3C	2.27	1.48	1.45
23	d	402	CLA	C4B-CHC	2.27	1.47	1.41
23	c	503	CLA	C4C-C3C	2.27	1.48	1.45
23	a	408	CLA	C1B-NB	-2.27	1.33	1.35
23	c	510	CLA	C4C-C3C	2.26	1.48	1.45
23	b	610	CLA	C4C-C3C	2.26	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	510	CLA	C4B-CHC	2.26	1.47	1.41
23	c	504	CLA	C4B-CHC	2.25	1.47	1.41
23	B	603	CLA	C4C-C3C	2.25	1.48	1.45
23	c	513	CLA	C4C-C3C	2.25	1.48	1.45
23	C	508	CLA	C3D-C4D	-2.25	1.39	1.44
23	C	510	CLA	C1C-C2C	2.25	1.48	1.44
23	b	608	CLA	C4B-CHC	2.25	1.47	1.41
23	D	403	CLA	C1C-C2C	2.24	1.48	1.44
24	A	407	PHO	CHA-CBD	-2.24	1.49	1.52
34	t	101	LMT	O1'-C1'	2.24	1.44	1.40
23	B	616	CLA	C1C-NC	-2.23	1.34	1.37
29	A	413	PL9	C2-C3	2.23	1.40	1.34
23	B	615	CLA	C4B-CHC	2.23	1.47	1.41
23	b	607	CLA	C4C-C3C	2.23	1.48	1.45
23	b	612	CLA	C3D-C4D	-2.23	1.39	1.44
23	b	605	CLA	C3D-C4D	-2.23	1.39	1.44
23	B	610	CLA	C1C-C2C	2.23	1.48	1.44
23	b	606	CLA	C3D-C4D	-2.22	1.39	1.44
23	B	613	CLA	C4B-CHC	2.22	1.47	1.41
23	B	605	CLA	C4C-C3C	2.22	1.48	1.45
23	B	616	CLA	C4B-CHC	2.21	1.47	1.41
23	B	605	CLA	C3D-C4D	-2.21	1.39	1.44
23	a	404	CLA	C1C-C2C	2.21	1.48	1.44
29	D	406	PL9	C6-C5	2.21	1.46	1.35
23	b	604	CLA	C1B-NB	-2.20	1.33	1.35
23	b	614	CLA	C4C-C3C	2.20	1.48	1.45
23	c	514	CLA	C3D-C4D	-2.20	1.39	1.44
23	b	611	CLA	C4C-C3C	2.20	1.48	1.45
23	B	608	CLA	C4B-CHC	2.19	1.47	1.41
23	A	404	CLA	C4B-CHC	2.19	1.47	1.41
24	a	417	PHO	C3A-C2A	-2.19	1.52	1.54
23	B	610	CLA	C1B-NB	-2.19	1.33	1.35
23	C	513	CLA	C4B-CHC	2.19	1.47	1.41
23	B	616	CLA	C3D-C4D	-2.18	1.39	1.44
23	c	511	CLA	C1B-NB	-2.18	1.33	1.35
23	b	602	CLA	C1B-CHB	2.18	1.47	1.41
23	b	607	CLA	C1A-CHA	2.18	1.52	1.43
23	A	406	CLA	C1C-NC	-2.18	1.34	1.37
23	C	510	CLA	C4C-C3C	2.18	1.48	1.45
23	A	405	CLA	C3D-C4D	-2.18	1.39	1.44
23	c	508	CLA	C1C-C2C	2.18	1.48	1.44
23	B	604	CLA	C3D-C4D	-2.17	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	609	CLA	C4C-C3C	2.17	1.48	1.45
23	C	513	CLA	C3D-C4D	-2.17	1.39	1.44
23	b	609	CLA	C3D-C4D	-2.17	1.39	1.44
23	B	602	CLA	C1B-CHB	2.17	1.47	1.41
23	B	601	CLA	C3D-C4D	-2.17	1.39	1.44
23	b	605	CLA	C1C-C2C	2.17	1.48	1.44
23	B	613	CLA	C1B-NB	-2.17	1.33	1.35
23	b	601	CLA	C3D-C4D	-2.17	1.39	1.44
23	d	403	CLA	C1D-C2D	2.16	1.49	1.45
23	C	514	CLA	C4C-C3C	2.16	1.48	1.45
23	b	601	CLA	C1C-C2C	2.16	1.48	1.44
23	C	503	CLA	C4C-C3C	2.16	1.48	1.45
23	b	610	CLA	C1B-NB	-2.15	1.33	1.35
34	D	402	LMT	O1'-C1'	2.15	1.43	1.40
23	c	509	CLA	C1B-CHB	2.15	1.47	1.41
23	C	511	CLA	C1B-NB	-2.15	1.33	1.35
23	b	607	CLA	C4B-CHC	2.15	1.47	1.41
23	C	515	CLA	C4C-C3C	2.14	1.48	1.45
23	C	515	CLA	C3D-C4D	-2.14	1.39	1.44
23	c	510	CLA	C1C-C2C	2.14	1.48	1.44
23	B	606	CLA	C1C-C2C	2.14	1.48	1.44
23	A	406	CLA	C1C-C2C	2.14	1.48	1.44
23	B	611	CLA	C4B-CHC	2.13	1.46	1.41
23	A	408	CLA	C1B-CHB	2.13	1.46	1.41
23	A	404	CLA	C1D-C2D	2.13	1.49	1.45
23	C	513	CLA	C1C-NC	-2.13	1.34	1.37
23	c	510	CLA	C3D-C4D	-2.13	1.39	1.44
23	b	609	CLA	C1D-C2D	2.13	1.49	1.45
23	a	408	CLA	C3D-C4D	-2.13	1.39	1.44
38	V	201	HEC	C3C-C4C	2.13	1.46	1.43
23	C	506	CLA	C3D-C4D	-2.13	1.39	1.44
33	c	523	HTG	C1-S1	-2.13	1.77	1.80
25	b	619	BCR	C30-C25	-2.12	1.50	1.53
23	B	601	CLA	C1D-C2D	2.12	1.49	1.45
34	E	102	LMT	O1'-C1'	2.12	1.43	1.40
23	A	404	CLA	C1B-NB	-2.12	1.33	1.35
32	C	522	LMG	O1-C1	2.11	1.43	1.40
23	b	614	CLA	C3D-C4D	-2.11	1.39	1.44
34	C	526	LMT	O1'-C1'	2.11	1.43	1.40
23	b	605	CLA	C1D-C2D	2.11	1.49	1.45
23	d	403	CLA	C4C-C3C	2.11	1.48	1.45
23	B	611	CLA	C3D-C4D	-2.10	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	511	CLA	C3D-C4D	-2.10	1.39	1.44
23	B	611	CLA	C1B-NB	-2.10	1.33	1.35
23	c	511	CLA	C4B-CHC	2.09	1.46	1.41
23	a	404	CLA	C3D-C4D	-2.09	1.39	1.44
23	C	508	CLA	C4B-CHC	2.08	1.46	1.41
23	C	511	CLA	C3D-C4D	-2.08	1.39	1.44
23	B	608	CLA	C1C-C2C	2.08	1.48	1.44
33	h	101	HTG	C1-S1	-2.08	1.77	1.80
23	c	504	CLA	C3D-C4D	-2.07	1.39	1.44
23	B	604	CLA	C1B-NB	-2.07	1.33	1.35
23	C	504	CLA	C4C-C3C	2.07	1.48	1.45
23	c	510	CLA	C4B-CHC	2.07	1.46	1.41
34	e	101	LMT	O1'-C1'	2.07	1.43	1.40
24	a	407	PHO	C3A-C2A	-2.07	1.52	1.54
23	C	513	CLA	C1A-CHA	2.07	1.51	1.43
23	b	615	CLA	C3D-C4D	-2.06	1.39	1.44
23	B	601	CLA	C1B-CHB	2.06	1.46	1.41
31	L	101	LHG	O7-C5	-2.06	1.41	1.46
29	D	406	PL9	C2-C3	2.06	1.40	1.34
23	A	406	CLA	C3D-C4D	-2.06	1.39	1.44
23	C	513	CLA	C4B-NB	-2.06	1.33	1.35
23	D	403	CLA	C4C-C3C	2.05	1.48	1.45
23	b	604	CLA	C4C-C3C	2.05	1.48	1.45
23	B	607	CLA	C1B-NB	-2.05	1.33	1.35
24	a	407	PHO	CBD-CGD	-2.05	1.49	1.52
23	a	404	CLA	C4B-CHC	2.05	1.46	1.41
23	B	607	CLA	C3D-C4D	-2.04	1.39	1.44
23	c	506	CLA	C3D-C4D	-2.04	1.39	1.44
23	D	404	CLA	C3D-C4D	-2.04	1.39	1.44
23	C	505	CLA	MG-NA	2.04	2.11	2.06
29	a	415	PL9	C2-C3	2.04	1.40	1.34
23	B	606	CLA	MG-NA	2.04	2.11	2.06
23	c	503	CLA	C1C-NC	-2.03	1.34	1.37
23	c	508	CLA	C4C-C3C	2.03	1.48	1.45
23	C	506	CLA	C1A-CHA	2.03	1.51	1.43
23	b	606	CLA	C1D-C2D	2.02	1.49	1.45
23	c	509	CLA	C1D-C2D	2.02	1.49	1.45
23	C	510	CLA	C1C-NC	-2.02	1.34	1.37
23	b	613	CLA	C4B-CHC	2.02	1.46	1.41
23	C	506	CLA	C4C-C3C	2.02	1.48	1.45
38	v	202	HEC	C3C-C4C	2.02	1.46	1.43
23	B	615	CLA	C3D-C4D	-2.02	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	612	CLA	C1B-NB	-2.02	1.33	1.35
23	B	606	CLA	C4B-CHC	2.01	1.46	1.41
23	B	604	CLA	MG-NA	2.01	2.11	2.06
23	b	601	CLA	C1D-C2D	2.01	1.49	1.45
23	b	609	CLA	C1C-NC	-2.01	1.34	1.37
23	b	605	CLA	C4C-C3C	2.01	1.48	1.45
23	D	404	CLA	C1B-NB	-2.01	1.33	1.35
23	a	405	CLA	C3D-C4D	-2.00	1.39	1.44
23	A	404	CLA	C4B-NB	-2.00	1.33	1.35
23	a	404	CLA	C4C-C3C	2.00	1.48	1.45

All (2548) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	614	CLA	C2D-C1D-ND	10.44	117.80	110.10
23	c	513	CLA	C1D-ND-C4D	-10.37	98.97	106.33
23	b	605	CLA	C1D-ND-C4D	-10.34	98.99	106.33
23	B	614	CLA	C1D-ND-C4D	-10.29	99.02	106.33
23	B	612	CLA	C2D-C1D-ND	10.19	117.61	110.10
23	B	612	CLA	C1D-ND-C4D	-10.12	99.14	106.33
23	C	505	CLA	C1D-ND-C4D	-10.11	99.15	106.33
23	a	406	CLA	C1D-ND-C4D	-10.07	99.18	106.33
23	c	504	CLA	C1D-ND-C4D	-9.87	99.32	106.33
23	C	503	CLA	C1D-ND-C4D	-9.86	99.33	106.33
23	D	403	CLA	C1D-ND-C4D	-9.84	99.35	106.33
23	B	611	CLA	C1D-ND-C4D	-9.77	99.40	106.33
23	B	601	CLA	C1D-ND-C4D	-9.67	99.47	106.33
23	b	603	CLA	C1D-ND-C4D	-9.58	99.53	106.33
23	A	405	CLA	C1D-ND-C4D	-9.57	99.53	106.33
23	b	614	CLA	C1D-ND-C4D	-9.54	99.56	106.33
23	b	606	CLA	C1D-ND-C4D	-9.53	99.56	106.33
23	c	506	CLA	C1D-ND-C4D	-9.52	99.57	106.33
23	B	607	CLA	C1D-ND-C4D	-9.47	99.61	106.33
23	B	603	CLA	C1D-ND-C4D	-9.47	99.61	106.33
23	d	403	CLA	C1D-ND-C4D	-9.47	99.61	106.33
23	c	503	CLA	C1D-ND-C4D	-9.46	99.61	106.33
23	a	408	CLA	C1D-ND-C4D	-9.46	99.62	106.33
23	C	505	CLA	C2D-C1D-ND	9.42	117.04	110.10
23	b	615	CLA	C1D-ND-C4D	-9.42	99.65	106.33
23	C	515	CLA	C1D-ND-C4D	-9.38	99.67	106.33
23	a	406	CLA	C2D-C1D-ND	9.37	117.01	110.10
23	D	404	CLA	C1D-ND-C4D	-9.33	99.71	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	605	CLA	C1D-ND-C4D	-9.32	99.71	106.33
23	b	611	CLA	C1D-ND-C4D	-9.31	99.72	106.33
23	B	609	CLA	C1D-ND-C4D	-9.31	99.72	106.33
23	c	513	CLA	C2D-C1D-ND	9.29	116.95	110.10
23	B	615	CLA	C2D-C1D-ND	9.25	116.92	110.10
23	B	608	CLA	C1D-ND-C4D	-9.24	99.77	106.33
23	A	406	CLA	C1D-ND-C4D	-9.23	99.78	106.33
23	A	404	CLA	C1D-ND-C4D	-9.22	99.78	106.33
23	b	601	CLA	C1D-ND-C4D	-9.18	99.81	106.33
23	c	505	CLA	C1D-ND-C4D	-9.18	99.82	106.33
23	A	405	CLA	C2D-C1D-ND	9.17	116.86	110.10
23	c	508	CLA	C1D-ND-C4D	-9.16	99.83	106.33
23	B	615	CLA	C1D-ND-C4D	-9.14	99.84	106.33
23	B	616	CLA	C1D-ND-C4D	-9.14	99.85	106.33
23	c	515	CLA	C1D-ND-C4D	-9.12	99.86	106.33
23	B	603	CLA	C2D-C1D-ND	9.10	116.81	110.10
23	a	405	CLA	C1D-ND-C4D	-9.08	99.88	106.33
23	C	513	CLA	C1D-ND-C4D	-9.07	99.89	106.33
23	c	509	CLA	C1D-ND-C4D	-9.02	99.92	106.33
23	C	506	CLA	C1D-ND-C4D	-9.02	99.93	106.33
23	C	507	CLA	C1D-ND-C4D	-8.99	99.95	106.33
23	C	504	CLA	C1D-ND-C4D	-8.94	99.99	106.33
23	C	510	CLA	C1D-ND-C4D	-8.94	99.99	106.33
23	B	611	CLA	C2D-C1D-ND	8.93	116.69	110.10
23	B	613	CLA	C2D-C1D-ND	8.93	116.69	110.10
23	a	404	CLA	C1D-ND-C4D	-8.93	99.99	106.33
23	c	514	CLA	C1D-ND-C4D	-8.91	100.00	106.33
23	b	614	CLA	C2D-C1D-ND	8.91	116.67	110.10
23	b	610	CLA	C1D-ND-C4D	-8.89	100.02	106.33
23	b	607	CLA	C2D-C1D-ND	8.87	116.64	110.10
23	B	613	CLA	C1D-ND-C4D	-8.84	100.06	106.33
23	b	607	CLA	C1D-ND-C4D	-8.82	100.07	106.33
23	b	609	CLA	C1D-ND-C4D	-8.82	100.07	106.33
23	C	511	CLA	C1D-ND-C4D	-8.80	100.08	106.33
23	C	506	CLA	C2D-C1D-ND	8.77	116.57	110.10
23	B	616	CLA	C2D-C1D-ND	8.74	116.55	110.10
23	C	512	CLA	C1D-ND-C4D	-8.74	100.13	106.33
23	b	613	CLA	C2D-C1D-ND	8.73	116.54	110.10
23	c	510	CLA	C1D-ND-C4D	-8.72	100.14	106.33
23	a	405	CLA	C2D-C1D-ND	8.71	116.52	110.10
23	a	408	CLA	C2D-C1D-ND	8.71	116.52	110.10
23	c	504	CLA	C2D-C1D-ND	8.69	116.51	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	507	CLA	C1D-ND-C4D	-8.68	100.17	106.33
23	c	511	CLA	C1D-ND-C4D	-8.67	100.17	106.33
23	C	503	CLA	C2D-C1D-ND	8.67	116.49	110.10
23	C	509	CLA	C1D-ND-C4D	-8.66	100.18	106.33
23	b	615	CLA	C2D-C1D-ND	8.66	116.49	110.10
23	A	408	CLA	C1D-ND-C4D	-8.65	100.19	106.33
23	b	608	CLA	C1D-ND-C4D	-8.63	100.21	106.33
23	b	616	CLA	C1D-ND-C4D	-8.59	100.23	106.33
23	b	613	CLA	C1D-ND-C4D	-8.58	100.24	106.33
23	b	602	CLA	C1D-ND-C4D	-8.57	100.25	106.33
23	c	512	CLA	C1D-ND-C4D	-8.53	100.28	106.33
23	B	607	CLA	C2D-C1D-ND	8.51	116.38	110.10
23	C	508	CLA	C1D-ND-C4D	-8.51	100.29	106.33
23	C	510	CLA	C2D-C1D-ND	8.50	116.37	110.10
23	b	605	CLA	C2D-C1D-ND	8.50	116.37	110.10
23	b	611	CLA	C2D-C1D-ND	8.48	116.35	110.10
23	D	403	CLA	C2D-C1D-ND	8.48	116.35	110.10
23	c	503	CLA	C2D-C1D-ND	8.42	116.31	110.10
23	C	504	CLA	C2D-C1D-ND	8.41	116.30	110.10
23	B	610	CLA	C1D-ND-C4D	-8.37	100.39	106.33
23	d	402	CLA	C1D-ND-C4D	-8.35	100.41	106.33
23	c	510	CLA	C2D-C1D-ND	8.34	116.25	110.10
23	C	509	CLA	C2D-C1D-ND	8.29	116.21	110.10
23	c	509	CLA	C2D-C1D-ND	8.28	116.20	110.10
23	B	602	CLA	C4A-NA-C1A	-8.21	103.01	106.71
23	C	514	CLA	C1D-ND-C4D	-8.20	100.51	106.33
23	B	608	CLA	C2D-C1D-ND	8.16	116.12	110.10
23	B	606	CLA	C1D-ND-C4D	-8.16	100.54	106.33
24	a	407	PHO	O2D-CGD-CBD	8.16	121.33	111.00
23	C	513	CLA	C2D-C1D-ND	8.15	116.11	110.10
23	B	609	CLA	C2D-C1D-ND	8.13	116.09	110.10
23	C	515	CLA	C2D-C1D-ND	8.13	116.09	110.10
23	b	604	CLA	C1D-ND-C4D	-8.12	100.57	106.33
24	a	417	PHO	O2D-CGD-CBD	8.11	121.27	111.00
23	b	612	CLA	C1D-ND-C4D	-8.07	100.61	106.33
23	d	403	CLA	C2D-C1D-ND	8.06	116.04	110.10
23	B	602	CLA	C1D-ND-C4D	-8.05	100.61	106.33
23	c	515	CLA	C2D-C1D-ND	8.05	116.04	110.10
23	b	616	CLA	C2D-C1D-ND	8.03	116.02	110.10
23	b	609	CLA	C2D-C1D-ND	8.00	116.00	110.10
23	c	506	CLA	C2D-C1D-ND	7.99	115.99	110.10
23	c	508	CLA	C2D-C1D-ND	7.99	115.99	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	514	CLA	C2D-C1D-ND	7.98	115.99	110.10
23	b	604	CLA	C2D-C1D-ND	7.98	115.98	110.10
23	D	404	CLA	C2D-C1D-ND	7.98	115.98	110.10
23	B	605	CLA	C2D-C1D-ND	7.97	115.98	110.10
23	b	603	CLA	C2D-C1D-ND	7.95	115.97	110.10
23	A	406	CLA	C2D-C1D-ND	7.92	115.94	110.10
23	b	606	CLA	C2D-C1D-ND	7.92	115.94	110.10
23	B	604	CLA	C1D-ND-C4D	-7.91	100.71	106.33
23	A	408	CLA	C2D-C1D-ND	7.86	115.90	110.10
23	b	610	CLA	C2D-C1D-ND	7.85	115.89	110.10
23	B	610	CLA	C2D-C1D-ND	7.80	115.86	110.10
23	B	601	CLA	C2D-C1D-ND	7.78	115.84	110.10
23	B	606	CLA	C2D-C1D-ND	7.78	115.84	110.10
23	c	505	CLA	C2D-C1D-ND	7.75	115.81	110.10
23	b	612	CLA	C2D-C1D-ND	7.66	115.75	110.10
23	b	601	CLA	C2D-C1D-ND	7.59	115.69	110.10
23	c	511	CLA	C2D-C1D-ND	7.57	115.69	110.10
23	b	602	CLA	C4A-NA-C1A	-7.56	103.31	106.71
23	B	604	CLA	C2D-C1D-ND	7.55	115.67	110.10
23	C	512	CLA	C2D-C1D-ND	7.53	115.65	110.10
23	B	609	CLA	C4A-NA-C1A	-7.45	103.36	106.71
23	C	511	CLA	C2D-C1D-ND	7.43	115.58	110.10
23	A	404	CLA	C2D-C1D-ND	7.39	115.55	110.10
23	d	402	CLA	C2D-C1D-ND	7.37	115.53	110.10
23	D	403	CLA	C4A-NA-C1A	-7.35	103.40	106.71
24	A	415	PHO	O2D-CGD-CBD	7.28	120.22	111.00
23	b	606	CLA	C4A-NA-C1A	-7.25	103.44	106.71
23	C	514	CLA	C2D-C1D-ND	7.24	115.44	110.10
23	B	615	CLA	CHD-C4C-C3C	-7.22	114.22	124.84
23	b	611	CLA	CMD-C2D-C1D	7.17	137.35	124.71
23	B	606	CLA	CMD-C2D-C1D	7.16	137.34	124.71
23	C	507	CLA	C2D-C1D-ND	7.16	115.38	110.10
23	a	404	CLA	C2D-C1D-ND	7.14	115.36	110.10
23	c	512	CLA	C2D-C1D-ND	7.10	115.34	110.10
23	C	508	CLA	CMD-C2D-C1D	7.06	137.16	124.71
23	b	606	CLA	CMD-C2D-C1D	7.00	137.04	124.71
23	b	602	CLA	C2D-C1D-ND	6.95	115.23	110.10
23	B	611	CLA	CHD-C4C-C3C	-6.95	114.63	124.84
23	b	605	CLA	CMD-C2D-C1D	6.91	136.89	124.71
23	c	507	CLA	C2D-C1D-ND	6.88	115.17	110.10
23	B	610	CLA	CMD-C2D-C1D	6.86	136.80	124.71
23	b	608	CLA	C2D-C1D-ND	6.83	115.14	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	403	CLA	CHD-C1D-ND	-6.81	118.19	124.45
23	c	509	CLA	CMD-C2D-C1D	6.81	136.71	124.71
23	b	605	CLA	CHD-C4C-C3C	-6.80	114.84	124.84
23	c	506	CLA	CMD-C2D-C1D	6.77	136.64	124.71
23	b	616	CLA	C4A-NA-C1A	-6.74	103.68	106.71
27	C	501	SQD	O6-C1-C2	6.74	118.82	108.30
23	B	602	CLA	C2D-C1D-ND	6.72	115.06	110.10
23	D	403	CLA	CHD-C1D-ND	-6.72	118.28	124.45
23	c	509	CLA	CHD-C1D-ND	-6.71	118.28	124.45
23	c	503	CLA	CMD-C2D-C1D	6.70	136.52	124.71
23	b	616	CLA	O2D-CGD-CBD	6.70	123.17	111.27
23	b	608	CLA	CMD-C2D-C1D	6.69	136.50	124.71
23	C	509	CLA	CMD-C2D-C1D	6.68	136.49	124.71
23	B	612	CLA	CHD-C4C-C3C	-6.68	115.02	124.84
23	a	408	CLA	CHD-C4C-C3C	-6.67	115.03	124.84
23	a	405	CLA	CHD-C4C-C3C	-6.67	115.03	124.84
23	c	506	CLA	CHD-C1D-ND	-6.67	118.33	124.45
23	B	614	CLA	CHD-C1D-ND	-6.66	118.33	124.45
23	B	606	CLA	C4A-NA-C1A	-6.62	103.73	106.71
23	C	508	CLA	CHD-C1D-ND	-6.58	118.40	124.45
23	C	508	CLA	C2D-C1D-ND	6.57	114.94	110.10
23	B	612	CLA	O2D-CGD-CBD	6.56	122.93	111.27
23	B	614	CLA	CMD-C2D-C1D	6.56	136.27	124.71
23	b	601	CLA	CMD-C2D-C1D	6.55	136.26	124.71
23	B	611	CLA	CMD-C2D-C1D	6.55	136.26	124.71
23	b	605	CLA	CHD-C1D-ND	-6.55	118.44	124.45
23	B	604	CLA	O2D-CGD-CBD	6.54	122.90	111.27
23	a	406	CLA	CHD-C4C-C3C	-6.53	115.24	124.84
23	B	608	CLA	CMD-C2D-C1D	6.51	136.18	124.71
23	B	606	CLA	CHD-C1D-ND	-6.50	118.48	124.45
23	b	608	CLA	C4A-NA-C1A	-6.48	103.79	106.71
23	C	503	CLA	CMD-C2D-C1D	6.48	136.14	124.71
23	C	505	CLA	C4A-NA-C1A	-6.47	103.80	106.71
23	b	606	CLA	CHD-C1D-ND	-6.46	118.52	124.45
23	b	616	CLA	CHD-C4C-C3C	-6.46	115.35	124.84
23	b	612	CLA	C2C-C1C-NC	6.45	116.02	109.97
23	C	515	CLA	CHD-C4C-C3C	-6.45	115.35	124.84
23	d	402	CLA	C2C-C1C-NC	6.45	116.02	109.97
23	B	614	CLA	CHD-C4C-C3C	-6.45	115.36	124.84
23	B	602	CLA	CMD-C2D-C1D	6.44	136.06	124.71
23	B	603	CLA	C4A-NA-C1A	-6.44	103.81	106.71
23	c	515	CLA	CMD-C2D-C1D	6.44	136.06	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	611	CLA	CHD-C1D-ND	-6.42	118.56	124.45
23	B	603	CLA	CHD-C4C-C3C	-6.42	115.41	124.84
23	C	507	CLA	O2D-CGD-CBD	6.42	122.67	111.27
23	a	404	CLA	CMD-C2D-C1D	6.40	136.00	124.71
23	c	503	CLA	CHD-C1D-ND	-6.40	118.57	124.45
23	B	616	CLA	CHD-C4C-C3C	-6.39	115.45	124.84
23	c	504	CLA	CHD-C4C-C3C	-6.39	115.45	124.84
23	b	610	CLA	CHD-C4C-C3C	-6.38	115.46	124.84
23	C	510	CLA	CHD-C4C-C3C	-6.37	115.48	124.84
23	c	509	CLA	O2D-CGD-CBD	6.36	122.57	111.27
23	c	510	CLA	C2C-C1C-NC	6.36	115.93	109.97
23	B	605	CLA	CHD-C4C-C3C	-6.36	115.49	124.84
23	C	505	CLA	CHD-C4C-C3C	-6.35	115.51	124.84
23	c	513	CLA	CHD-C4C-C3C	-6.34	115.51	124.84
23	c	515	CLA	CHD-C1D-ND	-6.34	118.63	124.45
23	B	609	CLA	CMD-C2D-C1D	6.34	135.88	124.71
23	C	514	CLA	CHD-C4C-C3C	-6.33	115.53	124.84
23	C	503	CLA	CHD-C4C-C3C	-6.33	115.54	124.84
23	d	403	CLA	CMD-C2D-C1D	6.32	135.85	124.71
23	C	505	CLA	CHD-C1D-ND	-6.32	118.65	124.45
23	b	604	CLA	O2D-CGD-CBD	6.31	122.49	111.27
23	b	616	CLA	CMD-C2D-C1D	6.31	135.84	124.71
23	C	505	CLA	CMD-C2D-C1D	6.31	135.83	124.71
23	b	605	CLA	C4A-NA-C1A	-6.30	103.87	106.71
23	C	512	CLA	CMD-C2D-C1D	6.30	135.82	124.71
23	c	505	CLA	CMD-C2D-C1D	6.30	135.82	124.71
23	b	610	CLA	O2D-CGD-CBD	6.28	122.42	111.27
33	b	623	HTG	C1'-S1-C1	6.27	111.81	100.09
23	C	511	CLA	C2C-C1C-NC	6.27	115.84	109.97
23	C	513	CLA	CMD-C2D-C1D	6.24	135.72	124.71
23	A	404	CLA	CHD-C1D-ND	-6.23	118.73	124.45
23	b	603	CLA	CMD-C2D-C1D	6.23	135.69	124.71
23	b	609	CLA	CHD-C1D-ND	-6.23	118.73	124.45
23	B	601	CLA	O2D-CGD-CBD	6.22	122.32	111.27
23	B	614	CLA	C2C-C1C-NC	6.22	115.80	109.97
23	b	614	CLA	CMD-C2D-C1D	6.21	135.66	124.71
23	D	404	CLA	CMD-C2D-C1D	6.21	135.65	124.71
23	B	610	CLA	O2D-CGD-CBD	6.20	122.29	111.27
23	B	601	CLA	CMD-C2D-C1D	6.20	135.64	124.71
23	B	601	CLA	CHD-C1D-ND	-6.19	118.77	124.45
23	c	505	CLA	C4A-NA-C1A	-6.18	103.93	106.71
23	A	406	CLA	CHD-C1D-ND	-6.18	118.78	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	601	CLA	CHD-C1D-ND	-6.17	118.78	124.45
23	b	613	CLA	C2C-C1C-NC	6.17	115.75	109.97
23	D	404	CLA	CHD-C4C-C3C	-6.17	115.77	124.84
23	c	514	CLA	O2D-CGD-CBD	6.17	122.23	111.27
23	B	614	CLA	C3D-C2D-C1D	-6.16	97.42	105.83
23	b	604	CLA	C2C-C1C-NC	6.16	115.74	109.97
23	c	509	CLA	CHD-C4C-C3C	-6.16	115.79	124.84
23	c	512	CLA	CMD-C2D-C1D	6.16	135.56	124.71
23	b	612	CLA	CHD-C4C-C3C	-6.16	115.79	124.84
23	B	606	CLA	O2D-CGD-CBD	6.15	122.19	111.27
23	B	613	CLA	C2C-C1C-NC	6.14	115.73	109.97
23	B	608	CLA	CHD-C1D-ND	-6.14	118.81	124.45
23	a	406	CLA	CHD-C1D-ND	-6.12	118.83	124.45
23	D	403	CLA	C2C-C1C-NC	6.09	115.68	109.97
23	b	612	CLA	CMD-C2D-C1D	6.08	135.43	124.71
23	b	602	CLA	O2D-CGD-CBD	6.08	122.06	111.27
23	C	514	CLA	CMD-C2D-C1D	6.07	135.41	124.71
23	D	403	CLA	CMD-C2D-C1D	6.06	135.40	124.71
23	b	608	CLA	CHD-C1D-ND	-6.06	118.89	124.45
23	C	504	CLA	CHD-C4C-C3C	-6.06	115.94	124.84
23	b	614	CLA	O2D-CGD-CBD	6.06	122.03	111.27
23	b	614	CLA	CHD-C1D-ND	-6.05	118.89	124.45
23	A	404	CLA	CMD-C2D-C1D	6.05	135.37	124.71
23	B	604	CLA	CHD-C4C-C3C	-6.04	115.96	124.84
23	C	503	CLA	O2D-CGD-CBD	6.04	121.99	111.27
33	B	623	HTG	C1'-S1-C1	6.03	111.37	100.09
23	A	405	CLA	CHD-C1D-ND	-6.03	118.91	124.45
23	b	606	CLA	O2D-CGD-CBD	6.02	121.97	111.27
23	B	609	CLA	CHD-C1D-ND	-6.02	118.92	124.45
23	c	508	CLA	CMD-C2D-C1D	6.02	135.32	124.71
23	b	606	CLA	CHD-C4C-C3C	-6.02	115.99	124.84
23	b	614	CLA	CHD-C4C-C3C	-6.01	116.00	124.84
27	C	501	SQD	C1-O5-C5	-6.01	101.88	113.69
23	c	507	CLA	O2D-CGD-CBD	6.01	121.95	111.27
23	c	513	CLA	CHD-C1D-ND	-6.01	118.93	124.45
33	c	523	HTG	C1'-S1-C1	6.00	111.32	100.09
23	C	506	CLA	C2C-C1C-NC	6.00	115.59	109.97
23	b	615	CLA	C2C-C1C-NC	5.99	115.59	109.97
23	b	611	CLA	CHD-C4C-C3C	-5.99	116.04	124.84
23	C	509	CLA	O2D-CGD-CBD	5.99	121.90	111.27
23	b	615	CLA	CMD-C2D-C1D	5.98	135.26	124.71
23	C	513	CLA	CHD-C1D-ND	-5.98	118.96	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	601	CLA	CHD-C4C-C3C	-5.98	116.06	124.84
23	A	408	CLA	CMD-C2D-C1D	5.96	135.22	124.71
23	c	508	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
23	c	510	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
23	A	406	CLA	C4A-NA-C1A	-5.96	104.03	106.71
23	C	506	CLA	CHD-C4C-C3C	-5.95	116.09	124.84
23	c	508	CLA	CHD-C1D-ND	-5.95	118.99	124.45
23	c	512	CLA	CHD-C4C-C3C	-5.95	116.10	124.84
23	a	404	CLA	C2C-C1C-NC	5.95	115.54	109.97
23	C	509	CLA	CHD-C4C-C3C	-5.95	116.10	124.84
23	b	613	CLA	CMD-C2D-C1D	5.94	135.19	124.71
24	A	407	PHO	O2D-CGD-CBD	5.94	118.53	111.00
23	B	610	CLA	CHD-C1D-ND	-5.94	118.99	124.45
23	B	607	CLA	C2C-C1C-NC	5.94	115.54	109.97
23	b	603	CLA	CHD-C4C-C3C	-5.93	116.12	124.84
23	c	507	CLA	C4A-NA-C1A	-5.92	104.04	106.71
23	c	512	CLA	C2C-C1C-NC	5.91	115.51	109.97
23	C	510	CLA	C2C-C1C-NC	5.90	115.50	109.97
23	B	609	CLA	CHD-C4C-C3C	-5.90	116.17	124.84
23	c	510	CLA	O2D-CGD-CBD	5.89	121.73	111.27
23	C	508	CLA	C2C-C1C-NC	5.89	115.49	109.97
23	b	609	CLA	CHD-C4C-C3C	-5.89	116.19	124.84
23	B	612	CLA	C3C-C4C-NC	5.88	117.17	110.57
33	C	523	HTG	C1'-S1-C1	5.88	111.09	100.09
23	A	405	CLA	C2C-C1C-NC	5.87	115.47	109.97
23	C	514	CLA	O2D-CGD-CBD	5.87	121.70	111.27
23	b	602	CLA	CMD-C2D-C1D	5.86	135.05	124.71
23	c	513	CLA	CMD-C2D-C1D	5.86	135.04	124.71
23	B	602	CLA	CHD-C4C-C3C	-5.86	116.23	124.84
23	c	505	CLA	C2C-C1C-NC	5.85	115.46	109.97
23	C	515	CLA	CMD-C2D-C1D	5.85	135.03	124.71
23	b	609	CLA	CMD-C2D-C1D	5.85	135.03	124.71
23	B	616	CLA	O2D-CGD-CBD	5.85	121.67	111.27
23	c	514	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
23	B	607	CLA	CHD-C1D-ND	-5.84	119.08	124.45
23	C	512	CLA	CHD-C4C-C3C	-5.84	116.25	124.84
23	B	606	CLA	C2C-C1C-NC	5.84	115.45	109.97
23	B	608	CLA	CHD-C4C-C3C	-5.84	116.26	124.84
23	B	603	CLA	CHD-C1D-ND	-5.84	119.09	124.45
23	C	503	CLA	CHD-C1D-ND	-5.83	119.09	124.45
23	b	612	CLA	O2D-CGD-CBD	5.82	121.61	111.27
23	a	404	CLA	CHD-C1D-ND	-5.82	119.11	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	603	CLA	O2D-CGD-CBD	5.80	121.58	111.27
23	C	507	CLA	CMD-C2D-C1D	5.79	134.92	124.71
23	b	613	CLA	CHD-C4C-C3C	-5.79	116.33	124.84
23	C	509	CLA	CHD-C1D-ND	-5.78	119.14	124.45
23	A	406	CLA	CHD-C4C-C3C	-5.78	116.35	124.84
23	c	507	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
23	B	605	CLA	C4A-NA-C1A	-5.76	104.12	106.71
23	c	511	CLA	C2C-C1C-NC	5.76	115.36	109.97
23	C	508	CLA	C4A-NA-C1A	-5.75	104.12	106.71
23	c	508	CLA	C2C-C1C-NC	5.75	115.36	109.97
23	B	602	CLA	CHD-C1D-ND	-5.74	119.18	124.45
23	b	604	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
23	b	603	CLA	O2D-CGD-CBD	5.74	121.47	111.27
23	C	507	CLA	CHD-C4C-C3C	-5.74	116.41	124.84
23	A	408	CLA	C4A-NA-C1A	-5.73	104.13	106.71
23	B	615	CLA	CMD-C2D-C1D	5.72	134.80	124.71
23	c	509	CLA	C4A-NA-C1A	-5.72	104.13	106.71
23	a	405	CLA	C2C-C1C-NC	5.72	115.33	109.97
23	B	614	CLA	O2D-CGD-CBD	5.72	121.43	111.27
23	c	504	CLA	CHD-C1D-ND	-5.72	119.20	124.45
23	A	408	CLA	CHD-C1D-ND	-5.72	119.20	124.45
23	B	606	CLA	CHD-C4C-C3C	-5.71	116.44	124.84
23	A	405	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
23	c	503	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
23	c	515	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
23	B	613	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
23	C	512	CLA	C2C-C1C-NC	5.70	115.31	109.97
23	b	612	CLA	C4A-NA-C1A	-5.70	104.14	106.71
23	C	504	CLA	CHD-C1D-ND	-5.70	119.22	124.45
23	c	511	CLA	CMD-C2D-C1D	5.70	134.75	124.71
23	c	514	CLA	C4A-NA-C1A	-5.69	104.15	106.71
23	b	607	CLA	CHD-C1D-ND	-5.68	119.23	124.45
23	B	601	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
23	C	513	CLA	CHD-C4C-C3C	-5.68	116.50	124.84
23	b	603	CLA	C2C-C1C-NC	5.67	115.28	109.97
23	d	403	CLA	CHD-C4C-C3C	-5.67	116.51	124.84
23	c	507	CLA	C2C-C1C-NC	5.66	115.28	109.97
23	a	404	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
23	C	511	CLA	CMD-C2D-C1D	5.66	134.68	124.71
23	b	601	CLA	O2D-CGD-CBD	5.66	121.32	111.27
23	C	504	CLA	CMD-C2D-C1D	5.64	134.66	124.71
23	c	506	CLA	O2D-CGD-CBD	5.62	121.25	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	507	CLA	CMD-C2D-C1D	5.61	134.61	124.71
23	b	607	CLA	CMD-C2D-C1D	5.61	134.60	124.71
24	a	417	PHO	C1-C2-C3	-5.61	116.34	126.04
23	A	405	CLA	CMD-C2D-C1D	5.61	134.60	124.71
23	A	404	CLA	C2C-C1C-NC	5.61	115.23	109.97
23	d	403	CLA	C4A-NA-C1A	-5.61	104.19	106.71
23	b	615	CLA	CHD-C1D-ND	-5.60	119.30	124.45
23	a	408	CLA	C4A-NA-C1A	-5.60	104.19	106.71
23	b	607	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
23	b	602	CLA	CHD-C1D-ND	-5.59	119.31	124.45
23	B	604	CLA	C2C-C1C-NC	5.59	115.21	109.97
23	C	506	CLA	CHD-C1D-ND	-5.59	119.32	124.45
23	C	510	CLA	O2D-CGD-CBD	5.58	121.19	111.27
23	B	616	CLA	C4A-NA-C1A	-5.58	104.20	106.71
23	B	603	CLA	C2C-C1C-NC	5.58	115.20	109.97
23	b	607	CLA	C2C-C1C-NC	5.57	115.19	109.97
23	a	405	CLA	CMD-C2D-C1D	5.57	134.53	124.71
23	d	402	CLA	CMD-C2D-C1D	5.57	134.53	124.71
23	A	408	CLA	CHD-C4C-C3C	-5.57	116.66	124.84
25	Y	101	BCR	C33-C5-C6	-5.55	118.29	124.53
23	B	607	CLA	CMD-C2D-C1D	5.55	134.49	124.71
23	c	506	CLA	C2C-C1C-NC	5.54	115.16	109.97
23	b	610	CLA	C2C-C1C-NC	5.53	115.16	109.97
23	C	507	CLA	C2C-C1C-NC	5.53	115.16	109.97
23	B	611	CLA	CHD-C1D-ND	-5.52	119.38	124.45
23	A	406	CLA	CMD-C2D-C1D	5.51	134.43	124.71
23	B	615	CLA	C2C-C1C-NC	5.51	115.13	109.97
23	c	514	CLA	CMD-C2D-C1D	5.51	134.42	124.71
23	C	515	CLA	C2C-C1C-NC	5.50	115.13	109.97
27	D	412	SQD	O6-C1-C2	5.50	116.89	108.30
23	C	510	CLA	CMD-C2D-C1D	5.50	134.40	124.71
23	A	405	CLA	C3D-C2D-C1D	-5.49	98.33	105.83
23	d	402	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
23	B	609	CLA	C2C-C1C-NC	5.49	115.11	109.97
23	B	608	CLA	C2C-C1C-NC	5.47	115.10	109.97
23	b	611	CLA	C4A-NA-C1A	-5.47	104.25	106.71
23	C	511	CLA	CHD-C4C-C3C	-5.46	116.82	124.84
23	b	610	CLA	CMD-C2D-C1D	5.46	134.33	124.71
23	B	613	CLA	CHD-C1D-ND	-5.46	119.44	124.45
23	C	503	CLA	C2C-C1C-NC	5.45	115.07	109.97
23	b	609	CLA	C4A-NA-C1A	-5.45	104.26	106.71
23	C	514	CLA	C4A-NA-C1A	-5.44	104.26	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	512	CLA	CHD-C1D-ND	-5.44	119.46	124.45
23	C	513	CLA	C2C-C1C-NC	5.43	115.06	109.97
23	b	615	CLA	C4A-NA-C1A	-5.43	104.26	106.71
23	C	505	CLA	C2C-C1C-NC	5.43	115.06	109.97
23	b	615	CLA	CHD-C4C-C3C	-5.42	116.87	124.84
23	b	611	CLA	C2C-C1C-NC	5.40	115.03	109.97
23	c	505	CLA	CHD-C4C-C3C	-5.40	116.90	124.84
23	B	613	CLA	CMD-C2D-C1D	5.40	134.22	124.71
23	A	408	CLA	C2C-C1C-NC	5.39	115.02	109.97
23	B	610	CLA	C4A-NA-C1A	-5.39	104.28	106.71
33	h	101	HTG	C1'-S1-C1	5.39	110.17	100.09
23	c	506	CLA	CHD-C4C-C3C	-5.38	116.93	124.84
23	b	614	CLA	C2C-C1C-NC	5.38	115.01	109.97
23	b	601	CLA	C4A-NA-C1A	-5.38	104.29	106.71
23	C	507	CLA	CHD-C1D-ND	-5.37	119.52	124.45
23	C	512	CLA	O2D-CGD-CBD	5.37	120.81	111.27
23	B	616	CLA	CMD-C2D-C1D	5.37	134.18	124.71
33	D	411	HTG	C1'-S1-C1	5.36	110.12	100.09
27	b	620	SQD	O6-C1-C2	5.36	116.68	108.30
23	b	602	CLA	C2C-C1C-NC	5.36	114.99	109.97
38	e	102	HEC	CBD-CAD-C3D	-5.36	103.48	112.62
23	C	515	CLA	CHD-C1D-ND	-5.35	119.54	124.45
23	C	509	CLA	C2C-C1C-NC	5.34	114.98	109.97
23	B	615	CLA	CHD-C1D-ND	-5.33	119.55	124.45
23	B	611	CLA	C2C-C1C-NC	5.33	114.96	109.97
23	B	605	CLA	CHD-C1D-ND	-5.33	119.56	124.45
23	b	604	CLA	CMD-C2D-C1D	5.32	134.09	124.71
23	C	503	CLA	C4A-NA-C1A	-5.31	104.32	106.71
23	c	504	CLA	C2C-C1C-NC	5.31	114.94	109.97
23	C	504	CLA	C4A-NA-C1A	-5.28	104.33	106.71
23	C	507	CLA	C4A-NA-C1A	-5.28	104.33	106.71
23	B	616	CLA	C2C-C1C-NC	5.27	114.91	109.97
23	b	608	CLA	C2C-C1C-NC	5.27	114.91	109.97
23	D	404	CLA	CHD-C1D-ND	-5.27	119.61	124.45
23	c	513	CLA	C2C-C1C-NC	5.26	114.90	109.97
23	a	405	CLA	O2D-CGD-CBD	5.25	120.60	111.27
23	b	602	CLA	CHD-C4C-C3C	-5.25	117.12	124.84
23	C	511	CLA	CHD-C1D-ND	-5.24	119.64	124.45
23	B	606	CLA	C3D-C2D-C1D	-5.23	98.70	105.83
23	c	508	CLA	C4A-NA-C1A	-5.22	104.36	106.71
27	b	620	SQD	O47-C7-C8	5.22	122.75	111.50
38	E	103	HEC	CBD-CAD-C3D	-5.22	103.72	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	503	CLA	C2C-C1C-NC	5.22	114.86	109.97
23	B	611	CLA	C3D-C2D-C1D	-5.22	98.71	105.83
23	b	613	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
23	b	611	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
23	B	612	CLA	CHD-C1D-ND	-5.21	119.67	124.45
23	b	613	CLA	CHD-C1D-ND	-5.19	119.68	124.45
23	d	403	CLA	O2D-CGD-CBD	5.19	120.50	111.27
23	c	510	CLA	CMD-C2D-C1D	5.19	133.86	124.71
23	A	404	CLA	CHD-C4C-C3C	-5.19	117.21	124.84
23	D	403	CLA	CHD-C4C-C3C	-5.18	117.22	124.84
23	B	616	CLA	C3C-C4C-NC	5.18	116.38	110.57
27	C	501	SQD	C1-C2-C3	-5.18	99.21	110.00
38	V	201	HEC	CBD-CAD-C3D	-5.17	103.80	112.62
23	d	402	CLA	CHD-C1D-ND	-5.17	119.70	124.45
23	B	615	CLA	C3C-C4C-NC	5.17	116.37	110.57
23	c	507	CLA	CHD-C1D-ND	-5.16	119.72	124.45
23	B	610	CLA	CHD-C4C-C3C	-5.15	117.27	124.84
23	A	406	CLA	C2C-C1C-NC	5.15	114.80	109.97
23	B	604	CLA	C4A-NA-C1A	-5.15	104.39	106.71
23	B	604	CLA	CMD-C2D-C1D	5.14	133.76	124.71
25	D	405	BCR	C7-C8-C9	-5.13	118.48	126.23
23	C	506	CLA	CMD-C2D-C1D	5.13	133.75	124.71
23	C	505	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
25	y	101	BCR	C33-C5-C6	-5.13	118.77	124.53
23	c	505	CLA	CHD-C1D-ND	-5.13	119.74	124.45
23	C	514	CLA	C2C-C1C-NC	5.12	114.77	109.97
23	B	603	CLA	C3C-C4C-NC	5.12	116.31	110.57
23	B	603	CLA	CMD-C2D-C1D	5.12	133.74	124.71
27	a	410	SQD	O6-C1-C2	5.11	116.28	108.30
23	a	405	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
23	B	612	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
23	a	406	CLA	CMD-C2D-C1D	5.10	133.71	124.71
25	d	404	BCR	C7-C8-C9	-5.10	118.53	126.23
23	B	610	CLA	C2C-C1C-NC	5.10	114.75	109.97
23	C	506	CLA	O2D-CGD-CBD	5.10	120.33	111.27
23	a	406	CLA	C3D-C2D-C1D	-5.09	98.88	105.83
23	b	612	CLA	C3C-C4C-NC	5.09	116.28	110.57
23	c	503	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
23	c	510	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
23	a	405	CLA	CHD-C1D-ND	-5.08	119.78	124.45
23	b	616	CLA	CHD-C1D-ND	-5.08	119.78	124.45
38	v	202	HEC	CBD-CAD-C3D	-5.08	103.95	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	515	CLA	C2C-C1C-NC	5.06	114.72	109.97
23	a	408	CLA	C3C-C4C-NC	5.06	116.24	110.57
23	b	607	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
23	B	607	CLA	CHD-C4C-C3C	-5.05	117.41	124.84
29	a	415	PL9	C7-C3-C4	5.05	120.98	116.88
23	B	616	CLA	CHD-C1D-ND	-5.05	119.81	124.45
23	B	613	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
23	C	512	CLA	C4A-NA-C1A	-5.05	104.44	106.71
23	A	404	CLA	C4A-NA-C1A	-5.05	104.44	106.71
23	B	601	CLA	C4A-NA-C1A	-5.04	104.44	106.71
23	c	511	CLA	CHD-C1D-ND	-5.03	119.83	124.45
23	c	503	CLA	O2D-CGD-CBD	5.03	120.21	111.27
23	C	509	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
23	a	408	CLA	CMD-C2D-C1D	5.03	133.57	124.71
23	b	614	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
23	b	615	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
23	b	608	CLA	CHD-C4C-C3C	-5.02	117.46	124.84
23	c	511	CLA	CHD-C4C-C3C	-5.02	117.46	124.84
23	C	513	CLA	O2D-CGD-CBD	5.02	120.18	111.27
23	c	514	CLA	C2C-C1C-NC	5.02	114.67	109.97
23	B	613	CLA	C1-C2-C3	-5.01	117.38	126.04
23	c	511	CLA	C4A-NA-C1A	-5.01	104.45	106.71
23	c	515	CLA	C4A-NA-C1A	-5.00	104.46	106.71
27	f	101	SQD	O47-C7-C8	4.99	122.26	111.50
23	C	506	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
23	B	613	CLA	C3C-C4C-NC	4.98	116.16	110.57
23	b	601	CLA	C2C-C1C-NC	4.98	114.64	109.97
23	c	504	CLA	O2D-CGD-CBD	4.97	120.10	111.27
23	d	403	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
23	b	603	CLA	CHD-C1D-ND	-4.97	119.89	124.45
23	B	605	CLA	CMD-C2D-C1D	4.96	133.46	124.71
23	C	510	CLA	C3C-C4C-NC	4.96	116.14	110.57
23	B	615	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
23	C	504	CLA	C2C-C1C-NC	4.95	114.61	109.97
23	c	509	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
23	d	402	CLA	C4A-NA-C1A	-4.95	104.48	106.71
23	B	605	CLA	C3C-C4C-NC	4.95	116.12	110.57
23	B	601	CLA	C2C-C1C-NC	4.94	114.60	109.97
23	A	406	CLA	C3D-C4D-ND	4.94	118.23	110.24
23	c	511	CLA	O2D-CGD-CBD	4.94	120.04	111.27
23	B	609	CLA	C3C-C4C-NC	4.93	116.10	110.57
23	B	612	CLA	CMD-C2D-C1D	4.93	133.41	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	510	CLA	C3D-C2D-C1D	-4.93	99.11	105.83
23	c	513	CLA	C3D-C2D-C1D	-4.93	99.11	105.83
23	B	608	CLA	C4A-NA-C1A	-4.92	104.49	106.71
23	B	602	CLA	O2D-CGD-CBD	4.92	120.01	111.27
27	D	412	SQD	O47-C7-C8	4.92	122.10	111.50
23	B	616	CLA	C3D-C2D-C1D	-4.91	99.12	105.83
23	D	404	CLA	C2C-C1C-NC	4.91	114.57	109.97
23	B	610	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
23	b	613	CLA	C3C-C4C-NC	4.90	116.06	110.57
23	c	511	CLA	CAC-C3C-C4C	4.90	131.16	124.81
23	b	608	CLA	O2D-CGD-CBD	4.90	119.97	111.27
23	c	504	CLA	CMD-C2D-C1D	4.89	133.34	124.71
23	B	612	CLA	C2C-C1C-NC	4.89	114.55	109.97
23	C	506	CLA	C3C-C4C-NC	4.89	116.05	110.57
23	C	510	CLA	CHD-C1D-ND	-4.88	119.97	124.45
23	c	505	CLA	C3C-C4C-NC	4.88	116.04	110.57
23	b	605	CLA	C3D-C2D-C1D	-4.88	99.18	105.83
23	C	503	CLA	C3D-C2D-C1D	-4.88	99.18	105.83
23	b	616	CLA	C2C-C1C-NC	4.87	114.54	109.97
29	a	415	PL9	C15-C14-C16	4.87	123.46	115.27
23	B	603	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
23	a	406	CLA	C2C-C1C-NC	4.86	114.53	109.97
23	b	605	CLA	O2D-CGD-CBD	4.86	119.91	111.27
23	C	509	CLA	C4A-NA-C1A	-4.86	104.52	106.71
23	a	406	CLA	C4A-NA-C1A	-4.86	104.52	106.71
23	B	605	CLA	O2D-CGD-CBD	4.86	119.90	111.27
23	A	408	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
23	b	605	CLA	C2C-C1C-NC	4.85	114.52	109.97
23	c	507	CLA	C3C-C4C-NC	4.85	116.01	110.57
23	b	603	CLA	C4A-NA-C1A	-4.85	104.53	106.71
23	b	616	CLA	C3D-C2D-C1D	-4.85	99.22	105.83
23	C	514	CLA	CHD-C1D-ND	-4.84	120.01	124.45
23	C	511	CLA	O2D-CGD-CBD	4.84	119.86	111.27
23	C	515	CLA	O2D-CGD-CBD	4.83	119.84	111.27
23	b	607	CLA	C4A-NA-C1A	-4.82	104.54	106.71
23	a	404	CLA	C4A-NA-C1A	-4.82	104.54	106.71
23	c	512	CLA	CHD-C1D-ND	-4.80	120.04	124.45
23	b	605	CLA	C3D-C4D-ND	4.80	118.01	110.24
23	c	515	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
23	c	514	CLA	CHD-C1D-ND	-4.80	120.04	124.45
23	D	404	CLA	O2D-CGD-CBD	4.80	119.80	111.27
23	B	608	CLA	C3D-C2D-C1D	-4.79	99.29	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	513	CLA	O2D-CGD-CBD	4.79	119.78	111.27
23	c	505	CLA	O2D-CGD-CBD	4.79	119.78	111.27
23	a	408	CLA	O2D-CGD-CBD	4.78	119.77	111.27
23	A	406	CLA	O2D-CGD-CBD	4.78	119.77	111.27
23	c	510	CLA	CHD-C1D-ND	-4.78	120.06	124.45
25	b	617	BCR	C7-C8-C9	-4.78	119.01	126.23
23	C	504	CLA	C3C-C4C-NC	4.78	115.93	110.57
23	c	506	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
23	B	601	CLA	C3D-C4D-ND	4.77	117.95	110.24
23	B	605	CLA	C3D-C4D-ND	4.77	117.95	110.24
23	a	408	CLA	C2C-C1C-NC	4.77	114.44	109.97
23	b	609	CLA	C2C-C1C-NC	4.75	114.42	109.97
23	B	609	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
23	a	408	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
23	D	403	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
23	C	511	CLA	C4A-NA-C1A	-4.74	104.58	106.71
23	d	403	CLA	C2C-C1C-NC	4.73	114.41	109.97
23	b	609	CLA	C3D-C2D-C1D	-4.73	99.37	105.83
23	D	404	CLA	C4A-NA-C1A	-4.73	104.58	106.71
23	D	404	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
23	c	508	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
23	a	408	CLA	CHD-C1D-ND	-4.72	120.11	124.45
23	C	504	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
23	A	405	CLA	O2D-CGD-CBD	4.72	119.65	111.27
23	B	615	CLA	C4A-NA-C1A	-4.70	104.59	106.71
23	C	513	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
23	c	504	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
23	c	509	CLA	C2C-C1C-NC	4.69	114.36	109.97
23	B	607	CLA	C3D-C2D-C1D	-4.69	99.44	105.83
23	A	404	CLA	CAA-C2A-C3A	-4.69	99.95	112.78
23	A	405	CLA	C1C-C2C-C3C	-4.68	102.03	106.96
23	C	515	CLA	C3C-C4C-NC	4.68	115.82	110.57
23	b	606	CLA	C2C-C1C-NC	4.68	114.36	109.97
23	B	611	CLA	O2D-CGD-CBD	4.68	119.58	111.27
23	c	512	CLA	C4A-NA-C1A	-4.68	104.60	106.71
23	B	604	CLA	C3C-C4C-NC	4.68	115.81	110.57
23	c	512	CLA	O2D-CGD-CBD	4.67	119.57	111.27
23	B	607	CLA	O2D-CGD-CBD	4.67	119.57	111.27
23	b	604	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
23	b	610	CLA	C3C-C4C-NC	4.64	115.78	110.57
23	b	612	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
23	C	504	CLA	O2D-CGD-CBD	4.64	119.51	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	612	CLA	O2D-CGD-O1D	-4.63	114.78	123.84
23	b	606	CLA	O2D-CGD-O1D	-4.63	114.78	123.84
23	B	608	CLA	O2D-CGD-CBD	4.62	119.49	111.27
33	h	101	HTG	O5-C5-C4	4.62	118.09	109.69
23	b	609	CLA	O2D-CGD-CBD	4.62	119.48	111.27
23	C	515	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
23	c	505	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
23	B	611	CLA	C3C-C4C-NC	4.61	115.74	110.57
23	C	508	CLA	O2D-CGD-CBD	4.61	119.46	111.27
23	b	604	CLA	C3C-C4C-NC	4.61	115.74	110.57
25	Y	101	BCR	C16-C17-C18	-4.61	120.73	127.31
23	b	612	CLA	CHD-C1D-ND	-4.61	120.22	124.45
23	c	504	CLA	C3D-C4D-ND	4.61	117.69	110.24
32	Z	101	LMG	O7-C10-C11	4.61	121.43	111.50
23	b	606	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
23	a	405	CLA	C4A-NA-C1A	-4.60	104.64	106.71
27	B	620	SQD	O6-C1-C2	4.59	115.48	108.30
23	A	404	CLA	C3D-C4D-ND	4.59	117.67	110.24
23	a	404	CLA	C1D-CHD-C4C	-4.59	116.15	126.06
23	D	403	CLA	C3D-C4D-ND	4.59	117.67	110.24
23	a	406	CLA	C3D-C4D-ND	4.59	117.67	110.24
23	d	403	CLA	C3D-C4D-ND	4.59	117.67	110.24
23	b	603	CLA	C1D-CHD-C4C	-4.57	116.19	126.06
23	C	508	CLA	CHD-C4C-C3C	-4.56	118.13	124.84
23	a	405	CLA	C1C-C2C-C3C	-4.56	102.16	106.96
25	C	516	BCR	C7-C8-C9	-4.56	119.35	126.23
23	C	512	CLA	C1-C2-C3	-4.55	118.18	126.04
23	c	514	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
23	b	601	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
23	D	404	CLA	C3C-C4C-NC	4.53	115.65	110.57
23	b	604	CLA	CHD-C1D-ND	-4.52	120.30	124.45
23	D	403	CLA	C1C-C2C-C3C	-4.52	102.21	106.96
23	B	605	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
23	B	605	CLA	C2C-C1C-NC	4.51	114.20	109.97
23	b	610	CLA	CHD-C1D-ND	-4.51	120.31	124.45
23	b	603	CLA	C3C-C4C-NC	4.51	115.63	110.57
29	a	415	PL9	C37-C38-C39	-4.51	116.80	127.66
27	B	620	SQD	O47-C7-C8	4.51	121.22	111.50
23	b	610	CLA	C4A-NA-C1A	-4.51	104.68	106.71
23	C	514	CLA	C3D-C2D-C1D	-4.50	99.68	105.83
23	b	601	CLA	C3D-C4D-ND	4.50	117.53	110.24
23	B	610	CLA	CAC-C3C-C4C	4.50	130.65	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	614	CLA	C1C-C2C-C3C	-4.50	102.22	106.96
23	c	506	CLA	C3D-C4D-ND	4.50	117.51	110.24
23	b	603	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
23	C	514	CLA	C3C-C4C-NC	4.49	115.61	110.57
23	c	505	CLA	CAC-C3C-C4C	4.48	130.63	124.81
23	a	406	CLA	C3C-C4C-NC	4.48	115.59	110.57
23	c	513	CLA	C3D-C4D-ND	4.48	117.48	110.24
23	c	511	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
23	c	511	CLA	C1-C2-C3	-4.48	118.30	126.04
23	b	610	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
23	C	512	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
23	B	602	CLA	CMC-C2C-C1C	4.48	131.85	125.04
25	C	517	BCR	C7-C8-C9	-4.47	119.49	126.23
23	B	602	CLA	C2C-C1C-NC	4.47	114.16	109.97
23	C	510	CLA	C4A-NA-C1A	-4.46	104.70	106.71
23	d	402	CLA	C1C-C2C-C3C	-4.46	102.26	106.96
23	b	611	CLA	O2D-CGD-CBD	4.46	119.19	111.27
23	B	604	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
23	B	602	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
23	b	602	CLA	C3D-C4D-ND	4.44	117.42	110.24
23	C	506	CLA	C1C-C2C-C3C	-4.43	102.30	106.96
25	b	619	BCR	C38-C26-C25	-4.43	119.55	124.53
23	b	607	CLA	O2D-CGD-CBD	4.43	119.14	111.27
23	C	508	CLA	C3D-C4D-ND	4.43	117.40	110.24
23	a	405	CLA	C1D-CHD-C4C	-4.42	116.52	126.06
23	a	404	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
23	b	611	CLA	C3C-C4C-NC	4.40	115.51	110.57
23	B	614	CLA	C3C-C4C-NC	4.40	115.50	110.57
24	a	417	PHO	C4-C3-C5	4.40	122.67	115.27
23	b	609	CLA	C3C-C4C-NC	4.40	115.50	110.57
23	C	507	CLA	C3D-C4D-ND	4.39	117.34	110.24
23	C	509	CLA	C3C-C4C-NC	4.38	115.48	110.57
33	B	622	HTG	O5-C1-C2	4.38	115.82	110.31
23	b	616	CLA	C3C-C4C-NC	4.37	115.48	110.57
23	b	603	CLA	C3D-C4D-ND	4.37	117.31	110.24
23	b	616	CLA	C1D-CHD-C4C	-4.37	116.62	126.06
23	c	507	CLA	C3D-C4D-ND	4.36	117.29	110.24
23	B	607	CLA	C4A-NA-C1A	-4.36	104.75	106.71
23	B	604	CLA	C1D-CHD-C4C	-4.36	116.66	126.06
23	B	609	CLA	C3D-C4D-ND	4.36	117.28	110.24
23	C	503	CLA	C3C-C4C-NC	4.35	115.45	110.57
23	C	507	CLA	C3C-C4C-NC	4.35	115.45	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	513	CLA	C3C-C4C-NC	4.35	115.45	110.57
23	a	404	CLA	C3D-C4D-ND	4.35	117.27	110.24
27	a	410	SQD	O47-C7-C8	4.34	120.86	111.50
25	t	102	BCR	C33-C5-C6	-4.34	119.65	124.53
23	C	512	CLA	C1C-C2C-C3C	-4.34	102.39	106.96
23	c	510	CLA	C1C-C2C-C3C	-4.34	102.39	106.96
33	h	101	HTG	C1-O5-C5	4.34	120.58	112.58
23	b	607	CLA	C3C-C4C-NC	4.33	115.43	110.57
24	A	415	PHO	C1-C2-C3	-4.33	118.56	126.04
23	C	515	CLA	C3D-C4D-ND	4.32	117.22	110.24
32	c	501	LMG	O7-C10-C11	4.32	120.81	111.50
32	C	522	LMG	O6-C5-C4	4.31	117.53	109.69
23	B	601	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
23	c	508	CLA	C3D-C4D-ND	4.31	117.21	110.24
23	b	612	CLA	C3B-C4B-NB	4.31	114.78	109.21
23	a	406	CLA	O2D-CGD-CBD	4.30	118.91	111.27
23	B	609	CLA	O2D-CGD-CBD	4.29	118.90	111.27
23	C	511	CLA	C3C-C4C-NC	4.29	115.39	110.57
23	b	614	CLA	C3D-C4D-ND	4.29	117.17	110.24
23	A	408	CLA	C1-C2-C3	-4.28	118.64	126.04
23	b	606	CLA	C3C-C4C-NC	4.28	115.37	110.57
23	c	515	CLA	C3C-C4C-NC	4.28	115.37	110.57
23	a	404	CLA	CAA-C2A-C3A	-4.28	101.07	112.78
23	C	505	CLA	C3D-C4D-ND	4.27	117.15	110.24
23	B	612	CLA	CMC-C2C-C1C	4.27	131.54	125.04
23	B	602	CLA	C3C-C4C-NC	4.27	115.36	110.57
23	d	402	CLA	C3C-C4C-NC	4.27	115.36	110.57
23	b	604	CLA	C1C-C2C-C3C	-4.27	102.47	106.96
23	C	511	CLA	C3D-C4D-ND	4.26	117.13	110.24
23	b	609	CLA	C3D-C4D-ND	4.25	117.12	110.24
23	B	607	CLA	C3D-C4D-ND	4.25	117.12	110.24
23	B	613	CLA	O2D-CGD-CBD	4.25	118.83	111.27
23	A	405	CLA	C3D-C4D-ND	4.25	117.11	110.24
23	c	509	CLA	CMC-C2C-C1C	4.25	131.51	125.04
23	C	503	CLA	C3D-C4D-ND	4.23	117.08	110.24
23	B	603	CLA	C3D-C4D-ND	4.23	117.08	110.24
23	C	504	CLA	C3D-C4D-ND	4.23	117.08	110.24
23	C	505	CLA	C3C-C4C-NC	4.23	115.31	110.57
25	C	516	BCR	C33-C5-C6	-4.23	119.78	124.53
27	C	501	SQD	O9-S-C6	4.22	111.96	106.94
23	a	404	CLA	C3B-C4B-NB	4.22	114.67	109.21
23	b	612	CLA	C1-C2-C3	-4.22	118.75	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	413	PL9	C15-C14-C16	4.22	122.36	115.27
23	B	606	CLA	C3C-C4C-NC	4.21	115.30	110.57
23	A	404	CLA	C3D-C2D-C1D	-4.21	100.08	105.83
23	C	514	CLA	C1D-CHD-C4C	-4.21	116.98	126.06
23	c	503	CLA	C3D-C4D-ND	4.21	117.04	110.24
23	B	615	CLA	C1D-CHD-C4C	-4.21	116.98	126.06
23	A	406	CLA	C3D-C2D-C1D	-4.21	100.09	105.83
23	c	510	CLA	C3C-C4C-NC	4.20	115.28	110.57
23	c	503	CLA	O2D-CGD-O1D	-4.20	115.62	123.84
23	a	408	CLA	C3D-C4D-ND	4.20	117.03	110.24
23	C	511	CLA	C3D-C2D-C1D	-4.20	100.10	105.83
23	c	512	CLA	C1C-C2C-C3C	-4.20	102.54	106.96
23	a	405	CLA	C3C-C4C-NC	4.20	115.28	110.57
23	C	512	CLA	C3D-C4D-ND	4.19	117.02	110.24
23	C	503	CLA	C1D-CHD-C4C	-4.19	117.02	126.06
23	C	513	CLA	C3D-C4D-ND	4.19	117.02	110.24
23	c	508	CLA	C1C-C2C-C3C	-4.18	102.56	106.96
23	c	515	CLA	O2D-CGD-CBD	4.18	118.69	111.27
29	d	405	PL9	C42-C43-C44	-4.18	117.61	127.66
23	b	610	CLA	C3D-C4D-ND	4.18	116.99	110.24
23	C	510	CLA	C1D-CHD-C4C	-4.18	117.05	126.06
23	D	404	CLA	CAC-C3C-C4C	4.17	130.22	124.81
23	b	602	CLA	C3D-C2D-C1D	-4.17	100.14	105.83
23	b	605	CLA	C3C-C4C-NC	4.17	115.25	110.57
23	c	514	CLA	C3C-C4C-NC	4.17	115.25	110.57
32	C	522	LMG	O7-C10-C11	4.17	120.48	111.50
23	C	513	CLA	C3C-C4C-NC	4.17	115.24	110.57
23	c	505	CLA	C3D-C4D-ND	4.17	116.98	110.24
23	B	607	CLA	C1C-C2C-C3C	-4.16	102.58	106.96
32	B	621	LMG	O7-C10-C11	4.16	120.47	111.50
23	b	606	CLA	C3D-C4D-ND	4.16	116.96	110.24
23	b	608	CLA	C3D-C4D-ND	4.16	116.96	110.24
23	c	512	CLA	C3D-C2D-C1D	-4.16	100.16	105.83
27	D	412	SQD	C44-O6-C1	-4.16	105.62	113.74
23	d	402	CLA	C3D-C2D-C1D	-4.15	100.16	105.83
23	C	508	CLA	C3D-C2D-C1D	-4.15	100.16	105.83
23	A	404	CLA	O2D-CGD-CBD	4.15	118.65	111.27
27	a	412	SQD	O47-C7-C8	4.15	120.44	111.50
23	b	608	CLA	C3D-C2D-C1D	-4.15	100.17	105.83
23	c	504	CLA	C1C-C2C-C3C	-4.14	102.60	106.96
23	B	611	CLA	C4A-NA-C1A	-4.14	104.84	106.71
23	c	514	CLA	C3D-C4D-ND	4.14	116.93	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	613	CLA	C1C-C2C-C3C	-4.14	102.61	106.96
23	a	404	CLA	O2D-CGD-CBD	4.13	118.61	111.27
23	c	515	CLA	C3D-C4D-ND	4.13	116.92	110.24
23	c	505	CLA	C1D-CHD-C4C	-4.13	117.14	126.06
23	c	504	CLA	C3C-C4C-NC	4.13	115.20	110.57
23	B	613	CLA	CAC-C3C-C4C	4.13	130.17	124.81
23	b	614	CLA	C3C-C4C-NC	4.13	115.20	110.57
23	B	611	CLA	C3D-C4D-ND	4.13	116.92	110.24
23	D	404	CLA	C3D-C4D-ND	4.13	116.91	110.24
23	b	615	CLA	C3D-C4D-ND	4.13	116.91	110.24
23	B	611	CLA	C1D-CHD-C4C	-4.12	117.16	126.06
23	C	508	CLA	CAC-C3C-C4C	4.12	130.15	124.81
23	B	611	CLA	CMC-C2C-C1C	4.11	131.31	125.04
23	b	611	CLA	C3D-C4D-ND	4.11	116.89	110.24
29	A	413	PL9	C7-C3-C4	4.11	120.22	116.88
23	b	614	CLA	C4A-NA-C1A	-4.10	104.86	106.71
23	b	607	CLA	C3B-C4B-NB	4.10	114.51	109.21
23	d	402	CLA	C3D-C4D-ND	4.09	116.86	110.24
23	C	505	CLA	C1D-CHD-C4C	-4.09	117.23	126.06
23	c	510	CLA	C1D-CHD-C4C	-4.09	117.23	126.06
23	b	610	CLA	C1D-CHD-C4C	-4.09	117.23	126.06
23	A	408	CLA	O2D-CGD-CBD	4.08	118.52	111.27
23	b	607	CLA	O2D-CGD-O1D	-4.08	115.86	123.84
23	c	511	CLA	C3D-C4D-ND	4.08	116.83	110.24
23	C	515	CLA	C1D-CHD-C4C	-4.08	117.27	126.06
23	B	610	CLA	C3C-C4C-NC	4.07	115.14	110.57
23	B	608	CLA	C3C-C4C-NC	4.07	115.14	110.57
23	B	612	CLA	C3D-C4D-ND	4.06	116.81	110.24
23	a	405	CLA	C3D-C4D-ND	4.06	116.81	110.24
23	c	512	CLA	C3D-C4D-ND	4.06	116.80	110.24
23	c	512	CLA	C3C-C4C-NC	4.06	115.12	110.57
23	B	602	CLA	CAC-C3C-C4C	4.05	130.07	124.81
23	C	508	CLA	C1C-C2C-C3C	-4.05	102.69	106.96
34	C	526	LMT	C1'-O5'-C5'	4.05	121.64	113.69
23	c	510	CLA	C3B-C4B-NB	4.05	114.45	109.21
23	C	506	CLA	C3D-C4D-ND	4.05	116.79	110.24
23	B	608	CLA	C3D-C4D-ND	4.05	116.79	110.24
23	C	503	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
23	B	610	CLA	C3D-C4D-ND	4.05	116.78	110.24
23	A	406	CLA	C3C-C4C-NC	4.04	115.11	110.57
23	b	612	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
23	c	512	CLA	C1D-CHD-C4C	-4.03	117.36	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	613	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
27	a	410	SQD	O9-S-C6	4.03	111.73	106.94
23	c	508	CLA	O2D-CGD-CBD	4.03	118.43	111.27
23	c	506	CLA	C4A-NA-C1A	-4.03	104.89	106.71
23	C	513	CLA	C3B-C4B-NB	4.03	114.42	109.21
27	a	410	SQD	O8-S-C6	4.03	112.16	105.74
25	b	617	BCR	C33-C5-C6	-4.03	120.01	124.53
23	a	404	CLA	C3D-C2D-C1D	-4.02	100.34	105.83
23	c	509	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
35	C	519	DGD	O2G-C1B-C2B	4.02	120.16	111.50
23	C	512	CLA	C3C-C4C-NC	4.01	115.07	110.57
23	c	510	CLA	C3D-C4D-ND	4.01	116.73	110.24
23	A	408	CLA	C3D-C4D-ND	4.01	116.73	110.24
23	c	511	CLA	C3B-C4B-NB	4.01	114.39	109.21
23	C	511	CLA	C1-C2-C3	-4.01	119.11	126.04
35	C	520	DGD	O2G-C1B-C2B	4.00	120.13	111.50
23	B	615	CLA	C3D-C4D-ND	4.00	116.72	110.24
32	C	521	LMG	O7-C10-C11	4.00	120.13	111.50
23	b	605	CLA	C1D-CHD-C4C	-4.00	117.42	126.06
23	B	602	CLA	C3D-C4D-ND	4.00	116.71	110.24
23	B	615	CLA	CED-O2D-CGD	4.00	124.98	115.94
23	c	503	CLA	C4A-NA-C1A	-4.00	104.91	106.71
23	B	613	CLA	C3B-C4B-NB	3.99	114.37	109.21
23	a	408	CLA	C1D-CHD-C4C	-3.99	117.45	126.06
34	M	103	LMT	O5'-C5'-C4'	3.99	118.16	109.75
23	B	613	CLA	CMC-C2C-C1C	3.98	131.11	125.04
23	B	606	CLA	C1D-CHD-C4C	-3.98	117.47	126.06
31	E	101	LHG	O7-C7-C8	3.98	120.08	111.50
23	C	510	CLA	C3D-C4D-ND	3.98	116.68	110.24
23	D	403	CLA	C1-C2-C3	-3.98	119.16	126.04
23	A	404	CLA	C3B-C4B-NB	3.98	114.35	109.21
23	D	404	CLA	C1D-CHD-C4C	-3.98	117.48	126.06
23	A	405	CLA	CBC-CAC-C3C	-3.97	101.49	112.43
23	b	601	CLA	C1D-CHD-C4C	-3.97	117.50	126.06
27	a	410	SQD	C1-C2-C3	-3.96	101.75	110.00
23	C	511	CLA	C1C-C2C-C3C	-3.96	102.80	106.96
27	a	410	SQD	C44-O6-C1	-3.96	106.01	113.74
23	B	606	CLA	C1C-C2C-C3C	-3.95	102.80	106.96
29	a	415	PL9	C27-C28-C29	-3.95	118.14	127.66
23	b	613	CLA	C3B-C4B-NB	3.95	114.32	109.21
23	b	606	CLA	C4-C3-C5	3.95	121.91	115.27
23	B	613	CLA	C3D-C4D-ND	3.95	116.62	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	T	101	BCR	C15-C16-C17	-3.95	115.39	123.47
23	c	503	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
23	b	615	CLA	C3C-C4C-NC	3.94	114.99	110.57
23	b	613	CLA	C1-C2-C3	-3.94	119.23	126.04
23	b	607	CLA	C1C-C2C-C3C	-3.94	102.82	106.96
23	B	614	CLA	C3D-C4D-ND	3.94	116.61	110.24
23	b	616	CLA	O2D-CGD-O1D	-3.93	116.15	123.84
32	Z	101	LMG	C1-C2-C3	3.93	118.18	110.00
23	D	403	CLA	O2D-CGD-CBD	3.93	118.25	111.27
23	B	611	CLA	C3B-C4B-NB	3.93	114.29	109.21
23	A	408	CLA	C3C-C4C-NC	3.92	114.97	110.57
32	c	522	LMG	O7-C10-C11	3.92	119.95	111.50
23	c	509	CLA	C3D-C4D-ND	3.92	116.58	110.24
23	b	607	CLA	C3D-C4D-ND	3.92	116.58	110.24
23	c	503	CLA	C3C-C4C-NC	3.92	114.96	110.57
23	B	612	CLA	CAC-C3C-C4C	3.92	129.89	124.81
23	c	509	CLA	C3C-C4C-NC	3.91	114.96	110.57
23	b	604	CLA	C3B-C4B-NB	3.91	114.27	109.21
23	B	606	CLA	C3B-C4B-NB	3.91	114.26	109.21
23	B	616	CLA	C3D-C4D-ND	3.91	116.56	110.24
23	c	508	CLA	C1D-CHD-C4C	-3.91	117.63	126.06
23	b	612	CLA	O2D-CGD-O1D	-3.90	116.20	123.84
23	C	509	CLA	C1D-CHD-C4C	-3.90	117.64	126.06
31	d	408	LHG	O7-C7-C8	3.90	119.91	111.50
23	c	511	CLA	C3C-C4C-NC	3.90	114.94	110.57
23	b	606	CLA	C1D-CHD-C4C	-3.90	117.65	126.06
23	b	607	CLA	CAA-C2A-C3A	-3.89	102.11	112.78
23	c	514	CLA	C1D-CHD-C4C	-3.89	117.66	126.06
23	b	612	CLA	C1D-CHD-C4C	-3.89	117.66	126.06
23	B	611	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
23	B	615	CLA	O2D-CGD-CBD	3.89	118.17	111.27
23	A	405	CLA	C3C-C4C-NC	3.88	114.92	110.57
23	C	510	CLA	O2D-CGD-O1D	-3.88	116.26	123.84
23	C	513	CLA	CAC-C3C-C4C	3.87	129.84	124.81
23	b	605	CLA	C4-C3-C5	3.87	121.78	115.27
23	c	513	CLA	C3B-C4B-NB	3.87	114.22	109.21
23	C	514	CLA	C3D-C4D-ND	3.87	116.50	110.24
23	C	510	CLA	C3B-C4B-NB	3.86	114.20	109.21
32	C	502	LMG	O7-C10-C11	3.86	119.82	111.50
23	d	402	CLA	C3B-C4B-NB	3.86	114.19	109.21
23	B	601	CLA	C3C-C4C-NC	3.85	114.89	110.57
23	B	602	CLA	CAA-C2A-C3A	-3.85	102.23	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	607	CLA	C3C-C4C-NC	3.85	114.89	110.57
23	c	510	CLA	C1-C2-C3	-3.85	119.39	126.04
25	y	101	BCR	C15-C14-C13	-3.85	121.82	127.31
23	c	506	CLA	CAC-C3C-C4C	3.85	129.80	124.81
23	B	610	CLA	O2D-CGD-O1D	-3.84	116.32	123.84
27	C	501	SQD	C44-O6-C1	-3.84	106.24	113.74
23	b	603	CLA	CAA-C2A-C3A	-3.84	102.27	112.78
27	C	501	SQD	O47-C7-C8	3.83	119.75	111.50
23	c	508	CLA	C3C-C4C-NC	3.82	114.86	110.57
23	A	404	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
23	b	608	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
23	B	615	CLA	CMC-C2C-C1C	3.82	130.86	125.04
23	b	614	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
38	E	103	HEC	CBA-CAA-C2A	-3.82	106.17	112.60
23	A	408	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
23	c	515	CLA	C1D-CHD-C4C	-3.81	117.83	126.06
27	D	412	SQD	O8-S-C6	3.81	111.82	105.74
23	d	402	CLA	O2D-CGD-CBD	3.80	118.03	111.27
23	b	615	CLA	C1D-CHD-C4C	-3.80	117.85	126.06
23	C	515	CLA	C4A-NA-C1A	-3.80	105.00	106.71
23	b	616	CLA	C3D-C4D-ND	3.80	116.39	110.24
23	B	604	CLA	CHD-C1D-ND	-3.80	120.96	124.45
23	C	507	CLA	C3D-C2D-C1D	-3.80	100.65	105.83
23	A	404	CLA	C3C-C4C-NC	3.79	114.83	110.57
23	B	604	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
23	b	615	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
23	c	511	CLA	C1D-CHD-C4C	-3.79	117.89	126.06
33	b	622	HTG	C1-O5-C5	3.79	119.56	112.58
23	D	403	CLA	C3C-C4C-NC	3.78	114.81	110.57
23	B	603	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
23	c	510	CLA	O2D-CGD-O1D	-3.77	116.46	123.84
25	D	405	BCR	C38-C26-C25	-3.77	120.30	124.53
23	b	610	CLA	O2A-CGA-CBA	3.77	123.73	111.91
23	c	510	CLA	C4A-NA-C1A	-3.77	105.01	106.71
23	D	403	CLA	C3B-C4B-NB	3.77	114.08	109.21
25	Y	101	BCR	C15-C14-C13	-3.76	121.94	127.31
23	C	506	CLA	O2D-CGD-O1D	-3.76	116.49	123.84
23	C	503	CLA	O2D-CGD-O1D	-3.75	116.50	123.84
23	c	507	CLA	C3D-C2D-C1D	-3.75	100.71	105.83
23	c	512	CLA	C3B-C4B-NB	3.75	114.06	109.21
23	b	602	CLA	CAA-C2A-C3A	-3.75	102.51	112.78
23	b	611	CLA	C3B-C4B-NB	3.75	114.05	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	404	CLA	CMC-C2C-C1C	3.75	130.74	125.04
23	b	613	CLA	C3D-C4D-ND	3.74	116.29	110.24
23	b	610	CLA	C1C-C2C-C3C	-3.74	103.02	106.96
23	c	506	CLA	C3C-C4C-NC	3.74	114.77	110.57
23	B	605	CLA	C1D-CHD-C4C	-3.74	117.99	126.06
27	D	412	SQD	C1-C2-C3	-3.74	102.22	110.00
23	C	506	CLA	C3B-C4B-NB	3.73	114.04	109.21
23	C	515	CLA	C3B-C4B-NB	3.73	114.04	109.21
23	b	602	CLA	C3C-C4C-NC	3.73	114.76	110.57
23	c	506	CLA	C3B-C4B-NB	3.73	114.03	109.21
32	C	522	LMG	C3-C4-C5	3.73	116.89	110.24
23	b	601	CLA	C3C-C4C-NC	3.72	114.75	110.57
35	c	519	DGD	O2G-C1B-C2B	3.72	119.52	111.50
23	C	511	CLA	C3B-C4B-NB	3.72	114.02	109.21
23	B	608	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
23	b	613	CLA	O2A-CGA-O1A	-3.72	114.21	123.59
23	A	404	CLA	CMB-C2B-C3B	3.71	131.62	124.68
23	b	611	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
23	C	508	CLA	C3B-C4B-NB	3.71	114.01	109.21
23	c	506	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
25	d	404	BCR	C33-C5-C6	-3.70	120.37	124.53
23	d	402	CLA	C1D-CHD-C4C	-3.70	118.07	126.06
23	b	603	CLA	C1C-C2C-C3C	-3.70	103.06	106.96
23	d	403	CLA	C1C-C2C-C3C	-3.70	103.06	106.96
23	B	614	CLA	C3B-C4B-NB	3.70	113.99	109.21
23	B	615	CLA	C1C-C2C-C3C	-3.69	103.07	106.96
23	B	612	CLA	C4C-C3C-C2C	-3.69	101.51	106.90
23	B	601	CLA	C1D-CHD-C4C	-3.69	118.09	126.06
27	a	410	SQD	C1-O5-C5	-3.69	106.44	113.69
23	B	607	CLA	C3B-C4B-NB	3.69	113.98	109.21
25	h	102	BCR	C7-C8-C9	-3.69	120.66	126.23
23	C	507	CLA	O2D-CGD-O1D	-3.69	116.63	123.84
23	B	612	CLA	C1-C2-C3	-3.68	119.67	126.04
23	b	610	CLA	CAA-C2A-C3A	-3.68	102.69	112.78
23	C	510	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
23	C	512	CLA	C1D-CHD-C4C	-3.68	118.13	126.06
27	A	411	SQD	O47-C7-C8	3.67	119.42	111.50
32	c	521	LMG	O7-C10-C11	3.67	119.41	111.50
23	C	513	CLA	C1D-CHD-C4C	-3.67	118.14	126.06
23	B	616	CLA	C3B-C4B-NB	3.67	113.95	109.21
24	A	407	PHO	CMA-C3A-C4A	-3.67	106.34	114.38
27	a	412	SQD	O48-C23-C24	3.67	123.42	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	403	CLA	O2D-CGD-O1D	-3.67	116.67	123.84
29	D	406	PL9	C53-C6-C1	3.66	122.48	114.99
23	b	604	CLA	C4A-NA-C1A	-3.66	105.06	106.71
25	C	517	BCR	C33-C5-C6	-3.66	120.42	124.53
23	A	408	CLA	C1D-CHD-C4C	-3.66	118.16	126.06
32	z	101	LMG	O7-C10-C11	3.66	119.39	111.50
23	b	614	CLA	C1D-CHD-C4C	-3.66	118.16	126.06
23	b	604	CLA	C3D-C4D-ND	3.66	116.16	110.24
23	b	613	CLA	C4A-NA-C1A	-3.66	105.06	106.71
23	B	604	CLA	O2D-CGD-O1D	-3.66	116.69	123.84
23	B	606	CLA	O2D-CGD-O1D	-3.65	116.69	123.84
23	C	505	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
23	a	406	CLA	CMC-C2C-C1C	3.65	130.60	125.04
23	C	509	CLA	C3D-C4D-ND	3.65	116.14	110.24
35	c	518	DGD	O2G-C1B-C2B	3.64	119.35	111.50
23	b	613	CLA	O2A-CGA-CBA	3.64	123.32	111.91
23	A	405	CLA	C1D-CHD-C4C	-3.63	118.22	126.06
23	B	605	CLA	C4C-C3C-C2C	-3.63	101.61	106.90
25	d	404	BCR	C15-C14-C13	-3.62	122.14	127.31
23	b	608	CLA	C3B-C4B-NB	3.62	113.89	109.21
23	b	604	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
23	b	608	CLA	O2D-CGD-O1D	-3.62	116.77	123.84
23	B	602	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
23	b	605	CLA	CHD-C4C-NC	3.62	129.90	124.20
23	b	603	CLA	C3B-C4B-NB	3.62	113.89	109.21
23	A	404	CLA	O2A-CGA-CBA	3.62	123.25	111.91
23	a	406	CLA	C1D-CHD-C4C	-3.61	118.26	126.06
33	V	202	HTG	C1-O5-C5	3.61	117.09	112.19
23	b	602	CLA	C1D-CHD-C4C	-3.61	118.26	126.06
23	B	613	CLA	C4A-NA-C1A	-3.61	105.08	106.71
23	a	406	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
23	B	614	CLA	O2D-CGD-O1D	-3.61	116.78	123.84
23	C	507	CLA	C1D-CHD-C4C	-3.61	118.28	126.06
25	B	618	BCR	C29-C30-C25	3.61	116.03	110.48
23	a	405	CLA	O2D-CGD-O1D	-3.60	116.79	123.84
23	C	510	CLA	C4C-C3C-C2C	-3.60	101.65	106.90
23	c	508	CLA	C3B-C4B-NB	3.60	113.87	109.21
23	C	507	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
23	a	404	CLA	C3C-C4C-NC	3.60	114.61	110.57
23	C	509	CLA	O2D-CGD-O1D	-3.60	116.80	123.84
23	B	615	CLA	C3B-C4B-NB	3.60	113.86	109.21
23	C	511	CLA	CAC-C3C-C4C	3.60	129.48	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	513	CLA	C1-C2-C3	-3.60	119.82	126.04
23	b	602	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
23	C	511	CLA	C1D-CHD-C4C	-3.59	118.31	126.06
23	C	512	CLA	CMC-C2C-C1C	3.58	130.50	125.04
23	b	608	CLA	C1-C2-C3	-3.58	119.84	126.04
38	V	201	HEC	CMC-C2C-C1C	-3.58	122.96	128.46
23	b	602	CLA	CAC-C3C-C4C	3.58	129.45	124.81
23	c	514	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
23	b	602	CLA	C1-C2-C3	-3.58	119.86	126.04
23	a	408	CLA	O2D-CGD-O1D	-3.58	116.84	123.84
23	b	607	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
29	A	413	PL9	C27-C28-C29	-3.58	119.05	127.66
23	c	504	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
23	B	616	CLA	C4C-C3C-C2C	-3.57	101.69	106.90
23	b	605	CLA	O2D-CGD-O1D	-3.57	116.85	123.84
23	B	616	CLA	C1D-CHD-C4C	-3.57	118.35	126.06
23	c	515	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
23	a	405	CLA	C3B-C4B-NB	3.57	113.82	109.21
23	b	609	CLA	O2D-CGD-O1D	-3.57	116.86	123.84
23	A	406	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
31	d	406	LHG	O7-C7-C8	3.56	119.17	111.50
23	b	601	CLA	C3B-C4B-NB	3.56	113.81	109.21
23	B	604	CLA	C3D-C4D-ND	3.56	116.00	110.24
23	B	603	CLA	C1D-CHD-C4C	-3.56	118.38	126.06
23	b	602	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
23	c	505	CLA	C4C-C3C-C2C	-3.56	101.71	106.90
29	a	415	PL9	C7-C3-C2	-3.55	118.63	123.30
23	B	608	CLA	C1D-CHD-C4C	-3.55	118.40	126.06
23	C	514	CLA	C3B-C4B-NB	3.55	113.80	109.21
23	B	603	CLA	O2D-CGD-O1D	-3.55	116.90	123.84
23	A	406	CLA	CAA-C2A-C3A	-3.55	103.06	112.78
25	d	404	BCR	C38-C26-C25	-3.54	120.56	124.53
32	m	101	LMG	O7-C10-C11	3.54	119.12	111.50
23	B	607	CLA	CAA-C2A-C3A	-3.53	103.11	112.78
27	B	620	SQD	C3-C4-C5	3.53	116.54	110.24
23	B	602	CLA	O2D-CGD-O1D	-3.53	116.94	123.84
23	b	603	CLA	O2D-CGD-O1D	-3.53	116.94	123.84
23	b	603	CLA	O2A-CGA-O1A	-3.53	114.69	123.59
23	C	509	CLA	C1C-C2C-C3C	-3.53	103.25	106.96
31	a	419	LHG	O7-C7-C8	3.53	119.10	111.50
25	a	409	BCR	C24-C23-C22	-3.52	120.91	126.23
23	c	504	CLA	C4A-NA-C1A	-3.52	105.12	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	D	408	LHG	O7-C7-C8	3.52	119.09	111.50
23	c	512	CLA	C4-C3-C5	3.52	121.19	115.27
23	b	607	CLA	CBC-CAC-C3C	-3.52	102.74	112.43
25	c	516	BCR	C11-C10-C9	-3.52	122.29	127.31
23	c	513	CLA	C1D-CHD-C4C	-3.51	118.48	126.06
23	b	614	CLA	C3B-C4B-NB	3.51	113.75	109.21
23	B	605	CLA	CAC-C3C-C4C	3.51	129.36	124.81
23	B	614	CLA	C1D-CHD-C4C	-3.51	118.49	126.06
24	A	407	PHO	C1A-C2A-C3A	-3.51	99.50	102.84
38	v	202	HEC	CMC-C2C-C1C	-3.51	123.08	128.46
23	d	403	CLA	C3C-C4C-NC	3.50	114.50	110.57
23	C	515	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
38	V	201	HEC	C1D-C2D-C3D	-3.50	104.56	107.00
23	C	504	CLA	C1-C2-C3	-3.49	120.00	126.04
23	B	612	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
25	K	101	BCR	C7-C8-C9	-3.49	120.97	126.23
29	D	406	PL9	C42-C43-C44	-3.49	119.26	127.66
23	A	408	CLA	CAA-C2A-C3A	-3.49	103.23	112.78
23	B	605	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
23	a	408	CLA	C4C-C3C-C2C	-3.49	101.82	106.90
23	B	601	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
23	B	606	CLA	C3D-C4D-ND	3.49	115.88	110.24
23	B	605	CLA	O2A-CGA-O1A	-3.49	114.79	123.59
23	B	612	CLA	C4A-NA-C1A	-3.49	105.14	106.71
23	C	506	CLA	C1D-CHD-C4C	-3.48	118.55	126.06
23	B	610	CLA	O2A-CGA-CBA	3.48	122.83	111.91
23	A	404	CLA	C1D-CHD-C4C	-3.48	118.55	126.06
23	c	507	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
23	c	513	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
23	a	405	CLA	CHD-C4C-NC	3.48	129.68	124.20
23	B	608	CLA	O2D-CGD-O1D	-3.48	117.04	123.84
23	c	514	CLA	C1-C2-C3	-3.47	120.04	126.04
23	b	612	CLA	C3D-C4D-ND	3.47	115.85	110.24
38	E	103	HEC	CAD-CBD-CGD	3.47	123.48	113.76
23	c	509	CLA	C1D-CHD-C4C	-3.46	118.58	126.06
23	d	402	CLA	C1-C2-C3	-3.46	120.06	126.04
29	A	413	PL9	C25-C24-C26	3.46	121.09	115.27
23	b	614	CLA	O2D-CGD-O1D	-3.46	117.08	123.84
23	B	608	CLA	C3B-C4B-NB	3.45	113.68	109.21
23	c	511	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
27	a	412	SQD	O7-S-C6	3.45	111.04	106.94
23	a	408	CLA	C3B-C4B-NB	3.45	113.67	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	503	CLA	CMC-C2C-C1C	3.45	130.30	125.04
31	A	416	LHG	O8-C23-O10	-3.45	114.89	123.59
23	C	512	CLA	C3B-C4B-NB	3.45	113.67	109.21
25	c	517	BCR	C7-C8-C9	-3.44	121.03	126.23
23	C	504	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
23	A	405	CLA	C3B-C4B-NB	3.44	113.66	109.21
23	B	611	CLA	CHD-C4C-NC	3.44	129.62	124.20
23	b	608	CLA	C1D-CHD-C4C	-3.44	118.64	126.06
24	a	417	PHO	CMB-C2B-C3B	3.44	131.11	124.68
38	v	202	HEC	CBA-CAA-C2A	-3.44	106.81	112.60
23	b	612	CLA	CMB-C2B-C3B	3.44	131.11	124.68
23	C	506	CLA	CMC-C2C-C1C	3.44	130.27	125.04
23	c	513	CLA	C4A-NA-C1A	-3.43	105.16	106.71
23	C	503	CLA	C1-C2-C3	-3.43	120.11	126.04
33	b	625	HTG	C1'-S1-C1	3.42	106.49	100.09
23	b	613	CLA	O2D-CGD-CBD	3.42	117.34	111.27
23	B	610	CLA	CAA-C2A-C3A	-3.42	103.41	112.78
25	d	404	BCR	C28-C27-C26	-3.42	107.97	114.08
23	B	611	CLA	C1-C2-C3	-3.42	120.13	126.04
23	b	615	CLA	CAC-C3C-C4C	3.42	129.24	124.81
23	C	513	CLA	C4A-NA-C1A	-3.42	105.17	106.71
29	A	413	PL9	C10-C9-C11	3.42	121.02	115.27
23	B	614	CLA	CHC-C1C-C2C	-3.41	117.28	126.72
23	b	615	CLA	C3B-C4B-NB	3.41	113.62	109.21
25	k	101	BCR	C29-C30-C25	3.41	115.73	110.48
23	c	512	CLA	CMC-C2C-C1C	3.41	130.23	125.04
23	B	607	CLA	O2D-CGD-O1D	-3.40	117.18	123.84
23	c	507	CLA	O2D-CGD-O1D	-3.40	117.18	123.84
23	B	603	CLA	C3B-C4B-NB	3.40	113.61	109.21
23	b	604	CLA	CMC-C2C-C1C	3.40	130.22	125.04
23	b	601	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
23	d	402	CLA	CAA-C2A-C3A	-3.40	103.47	112.78
24	A	415	PHO	O2D-CGD-O1D	-3.40	117.19	123.84
25	c	517	BCR	C33-C5-C6	-3.40	120.71	124.53
23	c	515	CLA	CAC-C3C-C4C	3.40	129.22	124.81
27	A	411	SQD	C3-C4-C5	3.39	116.29	110.24
23	b	610	CLA	C1-C2-C3	-3.39	120.18	126.04
23	b	615	CLA	CHC-C1C-C2C	-3.39	117.35	126.72
25	K	101	BCR	C24-C23-C22	-3.39	121.11	126.23
23	c	515	CLA	C3B-C4B-NB	3.39	113.59	109.21
23	B	604	CLA	O2A-CGA-O1A	-3.39	115.05	123.59
23	B	612	CLA	C3B-C4B-NB	3.39	113.59	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	614	CLA	CMC-C2C-C1C	3.38	130.19	125.04
23	b	616	CLA	C3B-C4B-NB	3.38	113.58	109.21
23	B	609	CLA	C1C-C2C-C3C	-3.38	103.40	106.96
23	C	513	CLA	C1C-C2C-C3C	-3.38	103.40	106.96
23	b	606	CLA	C1C-C2C-C3C	-3.38	103.40	106.96
23	b	612	CLA	O2A-CGA-CBA	3.38	122.51	111.91
25	C	516	BCR	C15-C14-C13	-3.38	122.49	127.31
31	L	101	LHG	O7-C7-C8	3.38	118.78	111.50
23	B	603	CLA	C4C-C3C-C2C	-3.37	101.98	106.90
23	A	404	CLA	C2A-C1A-CHA	-3.37	117.96	123.86
25	B	618	BCR	C15-C14-C13	-3.37	122.50	127.31
23	C	505	CLA	O2D-CGD-CBD	3.37	117.25	111.27
23	D	404	CLA	C1C-C2C-C3C	-3.37	103.42	106.96
24	A	415	PHO	C1A-C2A-C3A	-3.36	99.64	102.84
34	a	413	LMT	O5'-C5'-C4'	3.36	116.84	109.75
23	b	601	CLA	C4-C3-C5	3.36	120.93	115.27
24	a	407	PHO	C1-C2-C3	-3.36	120.23	126.04
23	C	508	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
23	c	505	CLA	C3B-C4B-NB	3.36	113.55	109.21
23	b	613	CLA	CAC-C3C-C4C	3.35	129.16	124.81
23	c	507	CLA	C4C-C3C-C2C	-3.35	102.01	106.90
23	B	604	CLA	C1-C2-C3	-3.35	120.25	126.04
23	d	403	CLA	C1D-CHD-C4C	-3.35	118.84	126.06
23	C	504	CLA	C1D-CHD-C4C	-3.35	118.84	126.06
23	c	503	CLA	C3B-C4B-NB	3.35	113.54	109.21
23	D	404	CLA	C3B-C4B-NB	3.35	113.53	109.21
23	C	508	CLA	C1D-CHD-C4C	-3.34	118.85	126.06
23	a	404	CLA	CMB-C2B-C3B	3.34	130.93	124.68
23	c	513	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
23	c	506	CLA	C1D-CHD-C4C	-3.34	118.85	126.06
23	C	507	CLA	C3B-C4B-NB	3.34	113.53	109.21
23	A	406	CLA	C1D-CHD-C4C	-3.34	118.86	126.06
23	B	616	CLA	C1C-C2C-C3C	-3.34	103.45	106.96
23	a	408	CLA	C1C-C2C-C3C	-3.34	103.45	106.96
23	b	610	CLA	O2D-CGD-O1D	-3.33	117.32	123.84
35	c	520	DGD	O2G-C1B-C2B	3.33	118.68	111.50
23	B	606	CLA	CHC-C1C-C2C	-3.33	117.51	126.72
29	A	413	PL9	C37-C38-C39	-3.33	119.65	127.66
33	B	625	HTG	C1'-S1-C1	3.33	106.32	100.09
23	c	511	CLA	CMC-C2C-C1C	3.33	130.11	125.04
23	C	515	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
25	a	409	BCR	C38-C26-C25	-3.32	120.80	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	d	405	PL9	C40-C39-C41	3.32	120.86	115.27
23	C	514	CLA	C1C-C2C-C3C	-3.32	103.46	106.96
23	A	405	CLA	C4A-NA-C1A	-3.32	105.21	106.71
23	c	503	CLA	C1D-CHD-C4C	-3.32	118.89	126.06
23	b	609	CLA	C4C-C3C-C2C	-3.32	102.06	106.90
33	b	622	HTG	C1'-S1-C1	3.32	106.30	100.09
23	b	612	CLA	CAC-C3C-C4C	3.32	129.12	124.81
23	b	608	CLA	C3C-C4C-NC	3.31	114.29	110.57
23	A	404	CLA	O2A-CGA-O1A	-3.31	115.23	123.59
23	b	604	CLA	CAC-C3C-C4C	3.31	129.11	124.81
23	c	507	CLA	C1D-CHD-C4C	-3.31	118.92	126.06
29	A	413	PL9	C7-C8-C9	-3.31	121.29	126.79
23	B	603	CLA	CMC-C2C-C1C	3.31	130.07	125.04
34	e	101	LMT	C4B-C3B-C2B	3.31	116.59	110.82
23	B	615	CLA	CHD-C4C-NC	3.31	129.41	124.20
23	C	513	CLA	C4-C3-C5	3.30	120.83	115.27
29	d	405	PL9	C53-C6-C1	3.30	121.74	114.99
23	B	608	CLA	CMB-C2B-C3B	3.30	130.86	124.68
23	b	608	CLA	CAC-C3C-C4C	3.30	129.09	124.81
25	b	619	BCR	C24-C23-C22	-3.30	121.25	126.23
23	B	607	CLA	C4-C3-C5	3.30	120.82	115.27
23	c	512	CLA	CBC-CAC-C3C	-3.30	103.34	112.43
31	d	406	LHG	O8-C23-O10	-3.30	115.27	123.59
25	B	617	BCR	C7-C8-C9	-3.29	121.27	126.23
23	c	511	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
23	B	610	CLA	C1C-C2C-C3C	-3.28	103.50	106.96
23	a	404	CLA	CHC-C1C-C2C	-3.28	117.64	126.72
23	b	614	CLA	C1-C2-C3	-3.28	120.37	126.04
23	b	612	CLA	C4C-C3C-C2C	-3.28	102.12	106.90
23	b	615	CLA	O2D-CGD-CBD	3.28	117.09	111.27
23	B	609	CLA	C1D-CHD-C4C	-3.28	118.99	126.06
25	a	409	BCR	C11-C10-C9	-3.27	122.64	127.31
29	d	405	PL9	C10-C9-C11	3.27	120.78	115.27
23	b	604	CLA	C1-C2-C3	-3.27	120.39	126.04
23	C	503	CLA	C3B-C4B-NB	3.27	113.44	109.21
23	A	405	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
23	c	504	CLA	CMC-C2C-C1C	3.26	130.01	125.04
23	B	610	CLA	C4C-C3C-C2C	-3.26	102.14	106.90
23	C	509	CLA	C4C-C3C-C2C	-3.26	102.14	106.90
23	b	603	CLA	O2A-CGA-CBA	3.26	122.15	111.91
23	C	511	CLA	CMC-C2C-C1C	3.26	130.01	125.04
23	A	406	CLA	C4C-C3C-C2C	-3.26	102.14	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	605	CLA	C4C-C3C-C2C	-3.26	102.14	106.90
23	c	504	CLA	CHD-C4C-NC	3.26	129.34	124.20
23	b	602	CLA	C3B-C4B-NB	3.26	113.43	109.21
23	C	514	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
23	B	604	CLA	C3B-C4B-NB	3.26	113.42	109.21
25	b	617	BCR	C29-C30-C25	3.26	115.50	110.48
23	b	614	CLA	CHC-C1C-C2C	-3.25	117.72	126.72
29	a	415	PL9	C25-C24-C26	3.25	120.74	115.27
25	D	405	BCR	C24-C23-C22	-3.25	121.33	126.23
25	H	101	BCR	C16-C17-C18	-3.25	122.67	127.31
23	C	514	CLA	C4C-C3C-C2C	-3.25	102.16	106.90
23	B	609	CLA	C4C-C3C-C2C	-3.25	102.17	106.90
38	e	102	HEC	CAD-CBD-CGD	3.24	122.85	113.76
23	b	611	CLA	C1D-CHD-C4C	-3.24	119.06	126.06
23	C	515	CLA	C4C-C3C-C2C	-3.24	102.17	106.90
31	A	416	LHG	O7-C7-C8	3.24	118.49	111.50
23	b	616	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
23	B	601	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
23	A	404	CLA	CAC-C3C-C4C	3.24	129.01	124.81
24	A	415	PHO	C4-C3-C5	3.24	120.72	115.27
29	D	406	PL9	C42-C41-C39	-3.24	102.33	112.98
23	b	609	CLA	C1C-C2C-C3C	-3.23	103.56	106.96
25	H	101	BCR	C38-C26-C25	-3.23	120.90	124.53
23	c	514	CLA	CMC-C2C-C1C	3.23	129.96	125.04
25	h	102	BCR	C38-C26-C25	-3.23	120.90	124.53
23	b	613	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
23	C	508	CLA	CHC-C1C-C2C	-3.22	117.81	126.72
23	d	402	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
29	a	415	PL9	C20-C19-C21	3.22	120.68	115.27
23	B	601	CLA	C3B-C4B-NB	3.22	113.37	109.21
23	b	610	CLA	C4C-C3C-C2C	-3.22	102.21	106.90
27	b	620	SQD	C1-C2-C3	-3.22	103.30	110.00
24	a	417	PHO	O2D-CGD-O1D	-3.22	117.55	123.84
23	d	403	CLA	CMC-C2C-C1C	3.21	129.93	125.04
23	C	512	CLA	C4-C3-C5	3.21	120.67	115.27
23	A	405	CLA	CAA-C2A-C3A	-3.21	103.99	112.78
23	b	606	CLA	C3B-C4B-NB	3.21	113.36	109.21
23	B	607	CLA	C1D-CHD-C4C	-3.21	119.14	126.06
25	k	101	BCR	C15-C14-C13	-3.21	122.73	127.31
23	c	509	CLA	CHD-C4C-NC	3.20	129.25	124.20
23	c	515	CLA	CMC-C2C-C1C	3.20	129.92	125.04
23	b	609	CLA	C1-C2-C3	-3.20	120.50	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	612	CLA	CMC-C2C-C1C	3.20	129.92	125.04
29	A	413	PL9	C20-C19-C21	3.20	120.66	115.27
29	a	415	PL9	C37-C36-C34	-3.20	102.44	112.98
23	b	616	CLA	C1-C2-C3	-3.20	120.51	126.04
25	K	101	BCR	C38-C26-C25	-3.20	120.93	124.53
23	b	606	CLA	CMB-C2B-C3B	3.20	130.66	124.68
29	D	406	PL9	C45-C44-C46	3.20	120.65	115.27
23	C	508	CLA	CBC-CAC-C3C	-3.20	103.62	112.43
38	v	202	HEC	C1D-C2D-C3D	-3.20	104.77	107.00
23	C	514	CLA	CMB-C2B-C3B	3.20	130.66	124.68
27	C	501	SQD	O48-C23-C24	3.20	121.94	111.91
25	b	618	BCR	C15-C14-C13	-3.20	122.75	127.31
23	c	514	CLA	C4-C3-C5	3.19	120.63	115.27
25	H	101	BCR	C7-C8-C9	-3.19	121.42	126.23
23	B	602	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
25	T	101	BCR	C33-C5-C6	-3.18	120.95	124.53
29	D	406	PL9	C10-C9-C11	3.18	120.62	115.27
23	B	607	CLA	CBC-CAC-C3C	-3.18	103.67	112.43
31	b	629	LHG	O7-C7-C8	3.18	118.34	111.50
23	C	504	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
25	y	101	BCR	C38-C26-C25	-3.17	120.97	124.53
23	b	613	CLA	C4-C3-C5	3.17	120.60	115.27
23	b	613	CLA	C1D-CHD-C4C	-3.17	119.22	126.06
23	d	402	CLA	C4-C3-C5	3.17	120.60	115.27
23	b	601	CLA	CHD-C4C-NC	3.17	129.20	124.20
23	c	513	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
23	C	512	CLA	CBC-CAC-C3C	-3.16	103.71	112.43
23	a	404	CLA	C4-C3-C5	3.16	120.59	115.27
23	b	609	CLA	C1D-CHD-C4C	-3.16	119.24	126.06
23	C	505	CLA	CHD-C4C-NC	3.16	129.18	124.20
23	A	406	CLA	O2A-CGA-O1A	-3.16	115.62	123.59
23	b	616	CLA	CHD-C4C-NC	3.16	129.18	124.20
23	b	616	CLA	C4C-C3C-C2C	-3.15	102.30	106.90
23	a	405	CLA	CAA-C2A-C3A	-3.15	104.14	112.78
23	b	605	CLA	C2A-C1A-CHA	-3.15	118.35	123.86
23	B	604	CLA	C4-C3-C5	3.15	120.57	115.27
23	B	606	CLA	CMB-C2B-C3B	3.15	130.57	124.68
25	K	101	BCR	C33-C5-C6	-3.15	121.00	124.53
23	a	406	CLA	CHD-C4C-NC	3.15	129.16	124.20
23	b	610	CLA	C3B-C4B-NB	3.14	113.27	109.21
23	d	403	CLA	C3B-C4B-NB	3.14	113.27	109.21
32	C	522	LMG	O8-C28-C29	3.14	121.77	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	C	518	DGD	O2G-C1B-C2B	3.14	118.27	111.50
23	A	408	CLA	C3B-C4B-NB	3.14	113.27	109.21
23	C	508	CLA	C1-C2-C3	-3.14	120.62	126.04
23	C	505	CLA	C1-C2-C3	-3.13	120.62	126.04
23	D	403	CLA	C1D-CHD-C4C	-3.13	119.30	126.06
23	b	612	CLA	O2A-CGA-O1A	-3.13	115.69	123.59
23	c	505	CLA	CMC-C2C-C1C	3.13	129.80	125.04
29	d	405	PL9	C51-C49-C50	3.13	121.51	114.60
23	C	506	CLA	C1-C2-C3	-3.13	120.64	126.04
32	B	621	LMG	O8-C28-C29	3.13	121.72	111.91
23	B	614	CLA	CHD-C4C-NC	3.12	129.12	124.20
23	B	605	CLA	C4-C3-C5	3.12	120.52	115.27
23	b	612	CLA	C4-C3-C5	3.12	120.51	115.27
23	B	601	CLA	O2A-CGA-CBA	3.12	121.69	111.91
23	c	515	CLA	C1-C2-C3	-3.11	120.66	126.04
23	B	612	CLA	C1C-C2C-C3C	-3.11	103.69	106.96
23	d	403	CLA	CAA-C2A-C3A	-3.11	104.26	112.78
23	c	510	CLA	CHC-C1C-C2C	-3.11	118.12	126.72
23	C	513	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
23	b	611	CLA	O2A-CGA-CBA	3.11	121.66	111.91
23	B	615	CLA	C4-C3-C5	3.11	120.50	115.27
23	c	514	CLA	CAC-C3C-C4C	3.10	128.84	124.81
23	a	408	CLA	C4-C3-C5	3.10	120.49	115.27
23	a	406	CLA	CAA-C2A-C3A	-3.10	104.29	112.78
23	c	508	CLA	CBC-CAC-C3C	-3.10	103.89	112.43
23	a	408	CLA	CAA-C2A-C3A	-3.10	104.29	112.78
23	C	508	CLA	C3C-C4C-NC	3.10	114.05	110.57
27	A	411	SQD	O48-C23-C24	3.09	121.62	111.91
23	C	506	CLA	C4A-NA-C1A	-3.09	105.32	106.71
25	B	618	BCR	C37-C22-C21	-3.09	118.60	122.92
23	b	604	CLA	CHC-C1C-C2C	-3.09	118.18	126.72
23	b	603	CLA	C4C-C3C-C2C	-3.09	102.40	106.90
23	c	508	CLA	CHD-C4C-NC	3.08	129.06	124.20
23	b	605	CLA	C1C-C2C-C3C	-3.08	103.72	106.96
29	a	415	PL9	C42-C43-C44	-3.08	120.24	127.66
23	c	503	CLA	O2A-CGA-O1A	-3.08	115.82	123.59
23	b	603	CLA	C4-C3-C5	3.08	120.45	115.27
23	D	403	CLA	CBC-CAC-C3C	-3.08	103.95	112.43
23	B	611	CLA	CAC-C3C-C4C	3.07	128.79	124.81
25	c	516	BCR	C15-C14-C13	-3.07	122.93	127.31
23	B	603	CLA	C4-C3-C5	3.07	120.43	115.27
23	A	405	CLA	C4-C3-C5	3.07	120.43	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	511	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
23	C	510	CLA	CMB-C2B-C3B	3.07	130.42	124.68
23	B	604	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
25	a	409	BCR	C33-C5-C6	-3.07	121.08	124.53
23	C	505	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
23	c	513	CLA	CHD-C4C-NC	3.07	129.03	124.20
23	B	611	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
23	d	402	CLA	O2A-CGA-CBA	3.06	121.52	111.91
23	B	601	CLA	C4C-C3C-C2C	-3.06	102.43	106.90
23	C	504	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
25	Y	101	BCR	C37-C22-C23	3.06	122.90	118.08
23	b	610	CLA	O2A-CGA-O1A	-3.06	115.87	123.59
23	C	507	CLA	CAC-C3C-C4C	3.06	128.78	124.81
23	b	604	CLA	O2A-CGA-O1A	-3.06	115.88	123.59
23	c	505	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
23	B	607	CLA	CHC-C1C-C2C	-3.05	118.27	126.72
34	e	101	LMT	C1B-C2B-C3B	3.05	116.35	110.00
23	C	503	CLA	CHD-C4C-NC	3.05	129.01	124.20
23	B	612	CLA	C4-C3-C5	3.05	120.40	115.27
23	b	613	CLA	CHC-C1C-C2C	-3.05	118.29	126.72
23	c	505	CLA	C4-C3-C5	3.05	120.40	115.27
23	b	607	CLA	CHC-C1C-C2C	-3.05	118.29	126.72
23	a	404	CLA	C1-C2-C3	-3.05	120.78	126.04
35	C	519	DGD	O1G-C1A-C2A	3.05	121.46	111.91
23	c	506	CLA	C1-O2A-CGA	3.04	124.43	116.44
25	b	619	BCR	C7-C8-C9	-3.04	121.64	126.23
23	D	404	CLA	C4C-C3C-C2C	-3.04	102.46	106.90
25	b	619	BCR	C11-C10-C9	-3.04	122.97	127.31
23	c	505	CLA	C1C-C2C-C3C	-3.04	103.76	106.96
23	b	601	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
23	A	406	CLA	C3B-C4B-NB	3.04	113.14	109.21
23	c	508	CLA	CAA-C2A-C3A	-3.04	104.46	112.78
23	B	614	CLA	O2A-CGA-O1A	-3.04	115.92	123.59
23	d	403	CLA	CHD-C4C-NC	3.04	128.99	124.20
23	b	601	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
23	C	514	CLA	C4-C3-C5	3.04	120.38	115.27
23	b	606	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
23	a	404	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
32	C	521	LMG	O8-C28-C29	3.03	121.42	111.91
23	c	506	CLA	CMC-C2C-C1C	3.03	129.65	125.04
23	c	511	CLA	O2A-CGA-CBA	3.03	121.41	111.91
23	C	511	CLA	O2D-CGD-O1D	-3.03	117.92	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	510	CLA	CHC-C1C-C2C	-3.03	118.35	126.72
35	h	103	DGD	O2G-C1B-C2B	3.03	118.02	111.50
23	B	609	CLA	C3B-C4B-NB	3.03	113.12	109.21
32	m	101	LMG	O8-C28-C29	3.02	121.40	111.91
23	D	404	CLA	CAA-C2A-C3A	-3.02	104.50	112.78
29	D	406	PL9	C40-C39-C41	3.02	120.35	115.27
23	B	610	CLA	C1D-CHD-C4C	-3.02	119.55	126.06
23	B	609	CLA	CAC-C3C-C4C	3.02	128.73	124.81
23	B	614	CLA	O2A-CGA-CBA	3.02	121.38	111.91
23	B	606	CLA	C4-C3-C5	3.02	120.34	115.27
23	B	615	CLA	C4C-C3C-C2C	-3.01	102.50	106.90
25	B	617	BCR	C11-C10-C9	-3.01	123.01	127.31
23	c	507	CLA	CAC-C3C-C4C	3.01	128.72	124.81
23	B	613	CLA	C4-C3-C5	3.01	120.33	115.27
23	C	513	CLA	CHC-C1C-C2C	-3.01	118.40	126.72
23	c	515	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
31	d	406	LHG	O8-C23-C24	3.01	121.35	111.91
23	B	609	CLA	CMB-C2B-C1B	3.00	133.08	128.46
23	b	609	CLA	CMB-C2B-C3B	3.00	130.30	124.68
23	C	514	CLA	C1-C2-C3	-3.00	120.85	126.04
23	D	403	CLA	CHC-C1C-C2C	-3.00	118.42	126.72
23	a	406	CLA	C4C-C3C-C2C	-3.00	102.52	106.90
23	B	601	CLA	CAC-C3C-C4C	3.00	128.70	124.81
23	c	514	CLA	CMA-C3A-C4A	-3.00	103.72	111.77
23	a	408	CLA	O2A-CGA-CBA	2.99	121.31	111.91
27	b	620	SQD	O8-S-C6	2.99	110.51	105.74
25	d	404	BCR	C40-C30-C25	-2.99	105.45	110.30
23	b	611	CLA	CHC-C1C-C2C	-2.99	118.45	126.72
32	Z	101	LMG	O6-C1-C2	2.99	116.68	110.35
23	b	604	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
23	A	408	CLA	C4-C3-C5	2.99	120.30	115.27
23	C	511	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
24	a	407	PHO	O2A-CGA-CBA	2.99	121.28	111.91
23	d	403	CLA	O2A-CGA-CBA	2.99	121.28	111.91
23	B	611	CLA	CBC-CAC-C3C	-2.99	104.20	112.43
25	T	101	BCR	C11-C10-C9	-2.99	123.05	127.31
23	D	403	CLA	CMB-C2B-C3B	2.99	130.26	124.68
23	b	616	CLA	OBD-CAD-C3D	-2.99	121.34	128.52
25	b	618	BCR	C29-C30-C25	2.98	115.08	110.48
29	a	415	PL9	C22-C23-C24	-2.98	120.48	127.66
32	Z	101	LMG	C4-C3-C2	2.98	116.02	110.82
23	C	505	CLA	C3B-C4B-NB	2.98	113.06	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	515	CLA	C1-C2-C3	-2.98	120.90	126.04
23	c	513	CLA	CHC-C1C-C2C	-2.97	118.50	126.72
23	C	507	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
23	C	515	CLA	CMC-C2C-C1C	2.97	129.56	125.04
23	a	406	CLA	C3B-C4B-NB	2.97	113.05	109.21
23	b	601	CLA	CHC-C1C-C2C	-2.97	118.51	126.72
23	B	609	CLA	CHC-C1C-C2C	-2.97	118.51	126.72
35	H	102	DGD	O1G-C1A-C2A	2.97	121.22	111.91
29	A	413	PL9	C53-C6-C1	2.97	121.06	114.99
23	d	402	CLA	CHC-C1C-C2C	-2.97	118.52	126.72
33	B	622	HTG	C1-C2-C3	2.97	116.44	110.59
23	B	610	CLA	C3B-C4B-NB	2.96	113.04	109.21
23	c	510	CLA	O2A-CGA-CBA	2.96	121.20	111.91
25	A	409	BCR	C24-C23-C22	-2.96	121.76	126.23
23	B	608	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
23	B	602	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
23	D	403	CLA	O2A-CGA-CBA	2.96	121.19	111.91
31	D	408	LHG	O8-C23-O10	-2.96	116.13	123.59
23	c	506	CLA	CHC-C1C-C2C	-2.96	118.55	126.72
32	d	412	LMG	O7-C10-C11	2.95	117.87	111.50
23	C	506	CLA	CBC-CAC-C3C	-2.95	104.29	112.43
27	B	620	SQD	O48-C23-C24	2.95	121.17	111.91
23	b	614	CLA	CBC-CAC-C3C	-2.95	104.29	112.43
23	b	611	CLA	CMC-C2C-C1C	2.95	129.53	125.04
23	C	514	CLA	CHD-C4C-NC	2.95	128.85	124.20
23	b	611	CLA	CAC-C3C-C4C	2.95	128.64	124.81
34	C	526	LMT	O1B-C4'-C3'	2.95	115.13	107.28
23	b	616	CLA	O2A-CGA-CBA	2.95	121.16	111.91
23	C	510	CLA	C4-C3-C5	2.95	120.23	115.27
23	A	404	CLA	CMC-C2C-C1C	2.95	129.53	125.04
23	D	403	CLA	CAA-C2A-C3A	-2.94	104.71	112.78
23	c	510	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
35	H	102	DGD	O1G-C1A-O1A	-2.94	116.17	123.59
23	b	611	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
23	A	405	CLA	CHC-C1C-C2C	-2.94	118.59	126.72
23	c	511	CLA	CHC-C1C-C2C	-2.94	118.60	126.72
31	b	629	LHG	O8-C23-C24	2.94	121.12	111.91
23	c	512	CLA	CHC-C1C-C2C	-2.94	118.60	126.72
25	B	617	BCR	C33-C5-C6	-2.94	121.23	124.53
23	B	610	CLA	CHC-C1C-C2C	-2.93	118.60	126.72
23	C	515	CLA	CHD-C4C-NC	2.93	128.83	124.20
23	B	612	CLA	O2A-CGA-CBA	2.93	121.11	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	608	CLA	CMB-C2B-C3B	2.93	130.16	124.68
23	c	513	CLA	C4-C3-C5	2.93	120.20	115.27
23	c	504	CLA	C3B-C4B-NB	2.93	113.00	109.21
31	d	407	LHG	O7-C7-C8	2.93	117.81	111.50
23	b	602	CLA	CMC-C2C-C1C	2.93	129.50	125.04
23	a	404	CLA	CHD-C4C-NC	2.93	128.82	124.20
29	D	406	PL9	C51-C49-C50	2.93	121.07	114.60
25	B	619	BCR	C38-C26-C25	-2.93	121.24	124.53
23	c	508	CLA	CHC-C1C-C2C	-2.92	118.63	126.72
38	V	201	HEC	CMB-C2B-C1B	-2.92	123.97	128.46
23	c	509	CLA	O2A-CGA-CBA	2.92	121.08	111.91
27	A	411	SQD	O7-S-C6	2.92	110.41	106.94
23	c	503	CLA	CMC-C2C-C1C	2.92	129.49	125.04
29	D	406	PL9	C22-C23-C24	-2.92	120.63	127.66
23	C	507	CLA	CHC-C1C-C2C	-2.92	118.64	126.72
23	B	604	CLA	CHC-C1C-C2C	-2.92	118.65	126.72
32	c	521	LMG	O8-C28-C29	2.92	121.06	111.91
23	b	612	CLA	OBD-CAD-C3D	-2.91	121.51	128.52
23	b	608	CLA	CMC-C2C-C1C	2.91	129.47	125.04
23	C	514	CLA	CHC-C1C-C2C	-2.91	118.67	126.72
23	b	614	CLA	CHD-C4C-NC	2.91	128.79	124.20
24	a	417	PHO	C4A-C3A-C2A	-2.91	100.07	102.84
23	c	512	CLA	CHD-C4C-NC	2.91	128.78	124.20
24	a	407	PHO	C1A-C2A-C3A	-2.90	100.08	102.84
31	d	407	LHG	C6-C5-C4	-2.90	104.92	111.79
23	b	605	CLA	C3B-C4B-NB	2.90	112.96	109.21
25	k	101	BCR	C24-C23-C22	-2.90	121.85	126.23
23	b	611	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
29	D	406	PL9	C37-C38-C39	-2.89	120.70	127.66
23	b	610	CLA	CHD-C4C-NC	2.89	128.76	124.20
23	B	613	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
23	b	612	CLA	CHC-C1C-C2C	-2.89	118.73	126.72
23	C	508	CLA	CMC-C2C-C1C	2.89	129.44	125.04
23	C	512	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
23	C	504	CLA	C3B-C4B-NB	2.89	112.94	109.21
23	B	612	CLA	CMB-C2B-C3B	2.89	130.08	124.68
23	a	406	CLA	O2A-CGA-O1A	-2.89	116.31	123.59
32	c	522	LMG	O8-C28-C29	2.89	120.96	111.91
23	b	615	CLA	C4C-C3C-C2C	-2.88	102.69	106.90
25	C	516	BCR	C16-C17-C18	-2.88	123.19	127.31
34	a	413	LMT	C1B-O5B-C5B	2.88	119.35	113.69
32	D	413	LMG	O8-C28-O10	-2.88	116.32	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402	CLA	CMB-C2B-C3B	2.88	130.07	124.68
31	A	416	LHG	O8-C23-C24	2.88	120.94	111.91
23	b	607	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
29	d	405	PL9	C31-C32-C33	-2.88	102.43	111.88
29	A	413	PL9	C22-C23-C24	-2.87	120.74	127.66
23	c	506	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
25	h	102	BCR	C36-C18-C17	-2.87	118.91	122.92
23	a	408	CLA	CHD-C4C-NC	2.87	128.72	124.20
23	d	403	CLA	CAC-C3C-C4C	2.87	128.53	124.81
23	B	606	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
23	b	614	CLA	C4-C3-C5	2.86	120.09	115.27
27	a	412	SQD	O48-C23-O10	-2.86	116.37	123.59
25	A	409	BCR	C31-C1-C6	-2.86	105.66	110.30
23	B	605	CLA	CMC-C2C-C1C	2.86	129.39	125.04
25	A	409	BCR	C15-C14-C13	-2.86	123.23	127.31
23	c	503	CLA	CBC-CAC-C3C	-2.86	104.56	112.43
29	A	413	PL9	C17-C18-C19	-2.86	120.78	127.66
24	a	417	PHO	CBA-CAA-C2A	-2.86	105.46	113.81
34	B	628	LMT	C1-O1'-C1'	-2.86	109.11	113.84
23	B	601	CLA	C2A-C1A-CHA	-2.85	118.87	123.86
23	c	515	CLA	O2A-CGA-CBA	2.85	120.86	111.91
23	C	505	CLA	C4-C3-C5	2.85	120.07	115.27
23	c	512	CLA	O2A-CGA-O1A	-2.85	116.39	123.59
23	C	505	CLA	CHC-C1C-C2C	-2.85	118.83	126.72
23	C	511	CLA	O2A-CGA-O1A	-2.85	116.40	123.59
27	f	101	SQD	O8-S-C6	2.85	110.28	105.74
25	b	619	BCR	C39-C30-C25	-2.85	105.68	110.30
23	A	404	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
23	b	604	CLA	O2A-CGA-CBA	2.85	120.85	111.91
23	c	508	CLA	CMC-C2C-C1C	2.85	129.38	125.04
23	B	615	CLA	CHC-C1C-C2C	-2.84	118.85	126.72
23	b	605	CLA	CED-O2D-CGD	2.84	122.37	115.94
23	b	616	CLA	CBC-CAC-C3C	-2.84	104.60	112.43
25	T	101	BCR	C15-C14-C13	2.84	131.37	127.31
23	b	616	CLA	CMB-C2B-C3B	2.84	129.99	124.68
23	d	403	CLA	O2A-CGA-O1A	-2.84	116.43	123.59
23	C	512	CLA	CAC-C3C-C4C	2.84	128.49	124.81
23	C	512	CLA	CHD-C4C-NC	2.84	128.68	124.20
31	E	101	LHG	O8-C23-C24	2.84	120.81	111.91
23	c	507	CLA	C3B-C4B-NB	2.84	112.88	109.21
23	B	616	CLA	O2A-CGA-CBA	2.84	120.81	111.91
23	b	602	CLA	C4C-C3C-C2C	-2.84	102.77	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	610	CLA	CAA-CBA-CGA	-2.83	104.97	113.25
23	C	503	CLA	C4-C3-C5	2.83	120.03	115.27
31	D	407	LHG	O8-C23-O10	-2.83	116.45	123.59
24	A	407	PHO	C1-C2-C3	-2.83	121.15	126.04
23	B	616	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
23	b	603	CLA	CHC-C1C-C2C	-2.83	118.90	126.72
32	z	101	LMG	O8-C28-C29	2.83	120.78	111.91
23	c	503	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
23	B	611	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
25	k	101	BCR	C3-C4-C5	-2.83	109.03	114.08
23	C	507	CLA	CMC-C2C-C1C	2.82	129.34	125.04
23	b	608	CLA	CHC-C1C-C2C	-2.82	118.92	126.72
35	c	520	DGD	O1G-C1A-C2A	2.82	120.75	111.91
23	a	405	CLA	CHC-C1C-C2C	-2.82	118.92	126.72
23	b	614	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
23	a	406	CLA	C1-C2-C3	-2.82	121.17	126.04
23	C	511	CLA	CHC-C1C-C2C	-2.82	118.93	126.72
23	b	606	CLA	CHD-C4C-NC	2.81	128.64	124.20
24	a	407	PHO	CMA-C3A-C4A	-2.81	108.21	114.38
23	D	403	CLA	C2A-C1A-CHA	-2.81	118.94	123.86
23	A	408	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
23	c	510	CLA	CHD-C4C-NC	2.81	128.64	124.20
27	b	620	SQD	O7-S-C6	2.81	110.28	106.94
23	D	404	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
23	C	514	CLA	O2A-CGA-CBA	2.81	120.72	111.91
23	A	405	CLA	CHD-C4C-NC	2.81	128.63	124.20
23	B	603	CLA	CAA-C2A-C3A	-2.81	105.09	112.78
23	c	508	CLA	C1-C2-C3	-2.81	121.19	126.04
23	c	503	CLA	CHC-C1C-C2C	-2.81	118.96	126.72
23	A	406	CLA	CHC-C1C-C2C	-2.81	118.96	126.72
23	B	608	CLA	CHC-C1C-C2C	-2.81	118.96	126.72
23	C	503	CLA	CBC-CAC-C3C	-2.80	104.70	112.43
23	b	610	CLA	CAA-CBA-CGA	-2.80	105.06	113.25
23	b	606	CLA	O2A-CGA-O1A	-2.80	116.52	123.59
23	C	509	CLA	C3B-C4B-NB	2.80	112.83	109.21
23	c	509	CLA	O1D-CGD-CBD	-2.80	118.75	124.48
23	a	404	CLA	O2A-CGA-O1A	-2.80	116.52	123.59
34	b	627	LMT	C1'-O5'-C5'	2.80	119.19	113.69
23	b	603	CLA	C2A-C1A-CHA	-2.80	118.96	123.86
33	h	101	HTG	C3-C4-C5	2.80	115.23	110.24
23	b	605	CLA	O2A-CGA-O1A	-2.80	116.53	123.59
23	B	601	CLA	CHD-C4C-NC	2.80	128.61	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	514	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
23	C	509	CLA	CHC-C1C-C2C	-2.80	118.99	126.72
35	C	520	DGD	O1G-C1A-C2A	2.79	120.68	111.91
23	B	610	CLA	CMC-C2C-C1C	2.79	129.29	125.04
23	B	608	CLA	CHD-C4C-NC	2.79	128.60	124.20
23	c	509	CLA	CBC-CAC-C3C	-2.79	104.74	112.43
23	b	605	CLA	CHC-C1C-C2C	-2.79	119.00	126.72
23	a	408	CLA	O2A-CGA-O1A	-2.79	116.56	123.59
23	A	406	CLA	C1-C2-C3	-2.79	121.22	126.04
23	b	606	CLA	CHC-C1C-C2C	-2.79	119.01	126.72
23	B	605	CLA	C2A-C1A-CHA	-2.79	118.99	123.86
23	C	512	CLA	O2A-CGA-CBA	2.78	120.64	111.91
23	b	608	CLA	CBC-CAC-C3C	-2.78	104.76	112.43
29	a	415	PL9	C53-C6-C1	2.78	120.68	114.99
23	c	503	CLA	CHD-C4C-NC	2.78	128.59	124.20
25	D	405	BCR	C37-C22-C23	2.78	122.46	118.08
23	c	503	CLA	CAC-C3C-C4C	2.78	128.42	124.81
23	c	503	CLA	O2A-CGA-CBA	2.78	120.63	111.91
29	a	415	PL9	C10-C9-C11	2.78	119.95	115.27
23	B	609	CLA	O2A-CGA-CBA	2.78	120.63	111.91
23	B	604	CLA	CMB-C2B-C3B	2.78	129.88	124.68
23	a	404	CLA	C1B-CHB-C4A	-2.78	124.62	130.12
25	B	618	BCR	C37-C22-C23	2.78	122.45	118.08
25	d	404	BCR	C29-C30-C25	2.78	114.75	110.48
29	A	413	PL9	C42-C43-C44	-2.77	120.98	127.66
23	D	404	CLA	CHD-C4C-NC	2.77	128.57	124.20
23	B	613	CLA	C1D-CHD-C4C	-2.77	120.07	126.06
29	d	405	PL9	C37-C38-C39	-2.77	120.98	127.66
23	c	507	CLA	CMC-C2C-C1C	2.77	129.26	125.04
27	f	101	SQD	O48-C23-C24	2.77	120.59	111.91
23	b	616	CLA	O2A-CGA-O1A	-2.77	116.61	123.59
29	D	406	PL9	C25-C24-C26	2.77	119.93	115.27
23	C	511	CLA	O2A-CGA-CBA	2.76	120.58	111.91
23	B	608	CLA	C1-C2-C3	-2.76	121.27	126.04
23	c	506	CLA	C4-C3-C5	2.76	119.92	115.27
23	C	503	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
23	a	406	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
23	A	408	CLA	CHC-C1C-C2C	-2.76	119.10	126.72
23	a	404	CLA	O2A-CGA-CBA	2.76	120.56	111.91
23	B	611	CLA	CED-O2D-CGD	2.75	122.16	115.94
24	a	407	PHO	O1D-CGD-CBD	-2.75	120.16	124.74
31	D	408	LHG	O8-C23-C24	2.75	120.54	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406	CLA	CHD-C4C-NC	2.75	128.53	124.20
32	D	413	LMG	O8-C28-C29	2.75	120.53	111.91
23	B	601	CLA	CHC-C1C-C2C	-2.75	119.12	126.72
23	c	509	CLA	C4-C3-C5	2.75	119.89	115.27
23	C	508	CLA	C2A-C1A-CHA	-2.74	119.06	123.86
23	a	408	CLA	C2A-C1A-CHA	-2.74	119.06	123.86
27	C	501	SQD	O48-C23-O10	-2.74	116.68	123.59
25	c	516	BCR	C38-C26-C25	-2.74	121.45	124.53
29	a	415	PL9	C45-C44-C46	2.74	119.88	115.27
23	c	504	CLA	C1-C2-C3	-2.74	121.31	126.04
23	B	616	CLA	CHC-C1C-C2C	-2.73	119.16	126.72
23	B	614	CLA	CAC-C3C-C4C	2.73	128.36	124.81
23	c	506	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
29	A	413	PL9	C30-C29-C31	2.73	119.87	115.27
23	c	514	CLA	CHD-C4C-NC	2.73	128.51	124.20
32	D	413	LMG	O7-C10-C11	2.73	117.39	111.50
23	c	507	CLA	CHC-C1C-C2C	-2.73	119.16	126.72
23	B	614	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
23	b	611	CLA	O2A-CGA-O1A	-2.73	116.70	123.59
23	b	616	CLA	CMC-C2C-C1C	2.73	129.20	125.04
23	b	602	CLA	C11-C12-C13	-2.73	107.09	115.92
24	a	407	PHO	O2D-CGD-O1D	-2.73	118.50	123.84
23	B	613	CLA	CHC-C1C-C2C	-2.73	119.17	126.72
25	D	405	BCR	C10-C11-C12	-2.73	114.71	123.22
23	c	508	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
23	B	606	CLA	CAC-C3C-C4C	2.72	128.34	124.81
25	b	619	BCR	C34-C9-C10	-2.72	119.11	122.92
23	b	607	CLA	C4-C3-C5	2.72	119.85	115.27
35	C	519	DGD	O1G-C1A-O1A	-2.72	116.72	123.59
23	C	513	CLA	CMC-C2C-C1C	2.72	129.18	125.04
23	B	615	CLA	CAC-C3C-C4C	2.72	128.34	124.81
33	B	623	HTG	O5-C1-C2	2.72	113.73	110.31
23	c	514	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
29	A	413	PL9	C32-C33-C34	-2.72	121.11	127.66
23	b	613	CLA	CMC-C2C-C1C	2.72	129.18	125.04
23	C	512	CLA	CHC-C1C-C2C	-2.72	119.20	126.72
23	a	405	CLA	CMA-C3A-C2A	-2.72	102.87	113.83
33	b	625	HTG	O5-C5-C4	2.72	114.63	109.69
23	C	504	CLA	C4-C3-C5	2.72	119.84	115.27
31	d	407	LHG	O8-C23-O10	-2.72	116.74	123.59
31	d	408	LHG	O8-C23-C24	2.72	120.43	111.91
23	C	513	CLA	O2D-CGD-O1D	-2.71	118.53	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	415	PHO	CMB-C2B-C3B	2.71	129.75	124.68
25	b	617	BCR	C16-C17-C18	-2.71	123.44	127.31
29	A	413	PL9	C7-C3-C2	-2.71	119.74	123.30
23	c	507	CLA	O2A-CGA-CBA	2.70	120.39	111.91
23	c	511	CLA	C1-O2A-CGA	2.70	123.54	116.44
31	D	407	LHG	O7-C7-C8	2.70	117.33	111.50
23	b	603	CLA	CAC-C3C-C4C	2.70	128.31	124.81
24	A	407	PHO	C4-C3-C5	2.70	119.81	115.27
23	a	408	CLA	CMA-C3A-C2A	-2.70	102.94	113.83
23	b	602	CLA	CHC-C1C-C2C	-2.70	119.25	126.72
23	D	404	CLA	O2A-CGA-CBA	2.70	120.38	111.91
23	c	504	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
23	A	406	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
23	C	506	CLA	C4C-C3C-C2C	-2.70	102.97	106.90
25	B	619	BCR	C37-C22-C21	-2.70	119.15	122.92
23	b	607	CLA	C1-O2A-CGA	2.70	123.52	116.44
27	A	411	SQD	O5-C5-C4	2.70	114.59	109.69
25	K	101	BCR	C15-C14-C13	-2.69	123.46	127.31
23	c	510	CLA	CMB-C2B-C3B	2.69	129.72	124.68
27	a	412	SQD	C3-C4-C5	2.69	115.04	110.24
25	t	102	BCR	C2-C1-C6	2.69	114.62	110.48
23	c	514	CLA	O2A-CGA-CBA	2.69	120.36	111.91
23	B	608	CLA	CMA-C3A-C4A	-2.69	104.54	111.77
29	d	405	PL9	C25-C24-C26	2.69	119.80	115.27
33	B	623	HTG	C1-O5-C5	2.69	117.54	112.58
23	b	616	CLA	CHC-C1C-C2C	-2.69	119.28	126.72
24	A	407	PHO	CBA-CAA-C2A	-2.69	105.95	113.81
23	B	609	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
25	C	517	BCR	C38-C26-C25	-2.69	121.51	124.53
32	c	522	LMG	O6-C5-C4	2.68	114.57	109.69
23	C	511	CLA	CMB-C2B-C3B	2.68	129.70	124.68
23	b	611	CLA	CHD-C4C-NC	2.68	128.43	124.20
23	B	610	CLA	CMA-C3A-C4A	-2.68	104.56	111.77
27	b	620	SQD	C3-C4-C5	2.68	115.02	110.24
23	c	505	CLA	C1-C2-C3	-2.68	121.41	126.04
35	c	520	DGD	O3G-C3G-C2G	-2.68	104.43	110.90
23	B	616	CLA	CAC-C3C-C4C	2.68	128.29	124.81
23	C	515	CLA	CHC-C1C-C2C	-2.68	119.31	126.72
23	B	614	CLA	C4-C3-C5	2.68	119.78	115.27
23	a	404	CLA	CHB-C4A-NA	2.68	128.21	124.51
23	d	402	CLA	C4C-C3C-C2C	-2.68	103.00	106.90
23	c	512	CLA	CAC-C3C-C4C	2.68	128.28	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	409	BCR	C38-C26-C25	-2.67	121.53	124.53
23	A	404	CLA	CHC-C1C-C2C	-2.67	119.33	126.72
23	C	509	CLA	CHD-C4C-NC	2.67	128.41	124.20
23	C	515	CLA	CAC-C3C-C4C	2.67	128.28	124.81
23	b	602	CLA	C2A-C1A-CHA	-2.67	119.19	123.86
32	Z	101	LMG	C9-C8-C7	-2.67	105.47	111.79
23	a	405	CLA	C4C-C3C-C2C	-2.67	103.01	106.90
23	b	611	CLA	CBC-CAC-C3C	-2.67	105.08	112.43
25	K	101	BCR	C10-C11-C12	-2.67	114.89	123.22
23	B	602	CLA	CHD-C4C-NC	2.67	128.41	124.20
23	A	404	CLA	CAA-C2A-C1A	-2.67	103.24	111.97
23	b	608	CLA	C4C-C3C-C2C	-2.66	103.01	106.90
23	c	508	CLA	CMB-C2B-C3B	2.66	129.66	124.68
23	c	508	CLA	O2A-CGA-O1A	-2.66	116.88	123.59
23	c	515	CLA	CHC-C1C-C2C	-2.66	119.36	126.72
23	b	607	CLA	CAC-C3C-C4C	2.66	128.26	124.81
23	b	604	CLA	C11-C12-C13	-2.66	107.32	115.92
25	C	516	BCR	C11-C10-C9	-2.66	123.52	127.31
35	h	103	DGD	O1G-C1A-C2A	2.66	120.25	111.91
29	D	406	PL9	C30-C29-C31	2.66	119.74	115.27
23	c	515	CLA	CAA-C2A-C3A	-2.66	105.50	112.78
23	d	403	CLA	CHC-C1C-C2C	-2.66	119.37	126.72
23	B	605	CLA	O2A-CGA-CBA	2.66	120.25	111.91
23	b	610	CLA	C4-C3-C5	2.66	119.74	115.27
23	c	509	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
23	c	514	CLA	C3B-C4B-NB	2.66	112.64	109.21
23	c	512	CLA	O2D-CGD-O1D	-2.66	118.65	123.84
23	C	509	CLA	O2A-CGA-CBA	2.65	120.23	111.91
23	B	605	CLA	CHD-C4C-NC	2.65	128.38	124.20
23	C	510	CLA	CHD-C4C-NC	2.65	128.38	124.20
25	C	516	BCR	C37-C22-C23	2.65	122.25	118.08
23	B	605	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
23	c	514	CLA	CHC-C1C-C2C	-2.65	119.40	126.72
23	A	408	CLA	CHD-C4C-NC	2.64	128.37	124.20
23	b	601	CLA	O2A-CGA-CBA	2.64	120.20	111.91
23	B	602	CLA	O2A-CGA-O1A	-2.64	116.92	123.59
23	c	514	CLA	CBA-CAA-C2A	-2.64	106.06	113.86
25	c	516	BCR	C16-C17-C18	-2.64	123.54	127.31
23	B	604	CLA	O2A-CGA-CBA	2.64	120.20	111.91
23	c	513	CLA	O2A-CGA-CBA	2.64	120.19	111.91
23	b	609	CLA	CBC-CAC-C3C	-2.64	105.15	112.43
24	a	407	PHO	CBA-CAA-C2A	-2.64	106.10	113.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	CHC-C1C-C2C	-2.64	119.43	126.72
23	b	608	CLA	C2A-C1A-CHA	-2.64	119.25	123.86
23	a	405	CLA	C2A-C1A-CHA	-2.64	119.25	123.86
23	B	603	CLA	O2A-CGA-O1A	-2.63	116.95	123.59
23	B	607	CLA	C4C-C3C-C2C	-2.63	103.06	106.90
25	Y	101	BCR	C34-C9-C8	2.63	122.22	118.08
23	B	607	CLA	O2A-CGA-O1A	-2.63	116.95	123.59
23	B	606	CLA	CBC-CAC-C3C	-2.63	105.18	112.43
23	b	614	CLA	CMB-C2B-C3B	2.63	129.60	124.68
27	b	620	SQD	O48-C23-C24	2.63	120.16	111.91
25	H	101	BCR	C11-C10-C9	-2.63	123.56	127.31
25	y	101	BCR	C24-C23-C22	-2.63	122.26	126.23
23	c	509	CLA	O2A-CGA-O1A	-2.63	116.96	123.59
24	A	407	PHO	CMB-C2B-C3B	2.63	129.59	124.68
23	c	504	CLA	CHC-C1C-C2C	-2.63	119.45	126.72
23	B	614	CLA	C2A-C1A-CHA	-2.63	119.27	123.86
23	A	404	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
23	B	603	CLA	O2A-CGA-CBA	2.62	120.14	111.91
23	C	506	CLA	CHC-C1C-C2C	-2.62	119.47	126.72
23	B	605	CLA	C3B-C4B-NB	2.62	112.59	109.21
23	C	504	CLA	CMB-C2B-C1B	2.62	132.48	128.46
25	b	618	BCR	C37-C22-C21	-2.61	119.26	122.92
23	B	613	CLA	CMB-C2B-C3B	2.61	129.57	124.68
23	A	408	CLA	CMC-C2C-C1C	2.61	129.02	125.04
23	A	408	CLA	CBC-CAC-C3C	-2.61	105.23	112.43
25	B	619	BCR	C24-C23-C22	-2.61	122.29	126.23
23	c	508	CLA	C4-C3-C5	2.61	119.66	115.27
25	H	101	BCR	C24-C23-C22	-2.61	122.30	126.23
25	t	102	BCR	C1-C6-C7	2.61	123.15	115.78
23	C	504	CLA	CHC-C1C-C2C	-2.61	119.51	126.72
31	b	629	LHG	O8-C23-O10	-2.61	117.01	123.59
23	b	615	CLA	C7-C6-C5	-2.60	106.28	113.36
23	B	614	CLA	CMB-C2B-C3B	2.60	129.55	124.68
23	b	602	CLA	CMB-C2B-C3B	2.60	129.55	124.68
25	C	517	BCR	C36-C18-C19	2.60	122.18	118.08
23	b	604	CLA	C4C-C3C-C2C	-2.60	103.10	106.90
23	B	602	CLA	O2A-CGA-CBA	2.60	120.08	111.91
23	c	506	CLA	CHD-C4C-NC	2.60	128.31	124.20
25	b	619	BCR	C8-C9-C10	2.60	122.94	118.94
25	A	409	BCR	C33-C5-C6	-2.60	121.61	124.53
25	B	617	BCR	C34-C9-C10	-2.60	119.28	122.92
23	c	506	CLA	CMB-C2B-C3B	2.60	129.55	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	L	101	LHG	O8-C23-C24	2.60	120.07	111.91
23	c	506	CLA	C2A-C1A-CHA	-2.60	119.31	123.86
23	d	403	CLA	C4C-C3C-C2C	-2.60	103.11	106.90
23	b	610	CLA	CHC-C1C-C2C	-2.60	119.53	126.72
23	b	609	CLA	CHD-C4C-NC	2.60	128.30	124.20
23	A	406	CLA	O2A-CGA-CBA	2.60	120.06	111.91
23	D	403	CLA	CMC-C2C-C1C	2.60	128.99	125.04
23	D	404	CLA	CHC-C1C-C2C	-2.60	119.54	126.72
29	a	415	PL9	C32-C33-C34	-2.60	121.41	127.66
23	C	508	CLA	CGD-CBD-CAD	-2.60	102.33	110.73
23	C	504	CLA	O2A-CGA-CBA	2.59	120.05	111.91
23	b	614	CLA	O2A-CGA-CBA	2.59	120.05	111.91
23	C	515	CLA	C4-C3-C5	2.59	119.63	115.27
23	b	609	CLA	C3B-C4B-NB	2.59	112.56	109.21
33	b	625	HTG	C1-O5-C5	2.59	117.36	112.58
31	d	408	LHG	O8-C23-O10	-2.59	117.05	123.59
23	c	505	CLA	O2A-CGA-O1A	-2.59	117.05	123.59
23	B	608	CLA	O2A-CGA-CBA	2.59	120.04	111.91
23	c	504	CLA	CBC-CAC-C3C	-2.59	105.29	112.43
23	c	510	CLA	CAA-C2A-C3A	-2.59	105.69	112.78
23	C	515	CLA	C2A-C1A-CHA	-2.59	119.34	123.86
23	B	603	CLA	CHD-C4C-NC	2.59	128.28	124.20
27	f	101	SQD	O7-S-C6	2.58	110.01	106.94
23	C	508	CLA	O2A-CGA-CBA	2.58	120.02	111.91
23	B	611	CLA	C2A-C1A-CHA	-2.58	119.34	123.86
29	A	413	PL9	C40-C39-C41	2.58	119.62	115.27
23	C	513	CLA	CMB-C2B-C3B	2.58	129.51	124.68
27	A	411	SQD	O8-S-C6	2.58	109.86	105.74
27	a	410	SQD	O48-C23-C24	2.58	120.01	111.91
29	d	405	PL9	C27-C28-C29	-2.58	121.45	127.66
23	a	406	CLA	O2A-CGA-CBA	2.58	119.99	111.91
31	d	406	LHG	C5-O7-C7	-2.58	111.45	117.79
23	B	611	CLA	O2A-CGA-O1A	-2.58	117.09	123.59
23	C	513	CLA	CHD-C4C-NC	2.57	128.26	124.20
23	B	606	CLA	CHD-C4C-NC	2.57	128.26	124.20
23	B	609	CLA	C4-C3-C5	2.57	119.60	115.27
23	A	406	CLA	C2A-C1A-CHA	-2.57	119.36	123.86
23	c	507	CLA	C1-C2-C3	-2.57	121.60	126.04
29	d	405	PL9	C20-C19-C21	2.57	119.60	115.27
23	c	508	CLA	O2A-CGA-CBA	2.57	119.97	111.91
23	b	608	CLA	CHD-C4C-NC	2.57	128.25	124.20
23	d	403	CLA	C2A-C1A-CHA	-2.57	119.37	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	603	CLA	CHD-C4C-NC	2.57	128.25	124.20
33	B	622	HTG	C1-O5-C5	2.57	117.31	112.58
23	C	506	CLA	C1-O2A-CGA	2.57	123.18	116.44
23	C	503	CLA	CHC-C1C-C2C	-2.57	119.62	126.72
25	C	517	BCR	C15-C16-C17	-2.56	118.22	123.47
23	B	610	CLA	O2A-CGA-O1A	-2.56	117.12	123.59
23	b	613	CLA	CED-O2D-CGD	2.56	121.74	115.94
23	c	503	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
23	b	609	CLA	CHC-C1C-C2C	-2.56	119.64	126.72
23	b	615	CLA	O2A-CGA-CBA	2.56	119.94	111.91
23	c	511	CLA	CMB-C2B-C3B	2.56	129.46	124.68
23	c	514	CLA	O1D-CGD-CBD	-2.56	119.25	124.48
23	a	405	CLA	C1-O2A-CGA	2.56	123.15	116.44
29	a	415	PL9	C17-C18-C19	-2.56	121.51	127.66
23	b	609	CLA	CAC-C3C-C4C	2.55	128.12	124.81
23	A	408	CLA	CAC-C3C-C4C	2.55	128.12	124.81
23	B	604	CLA	CHD-C4C-NC	2.55	128.22	124.20
23	b	606	CLA	C1-O2A-CGA	2.55	123.14	116.44
23	b	608	CLA	C4-C3-C5	2.55	119.56	115.27
23	B	613	CLA	O2A-CGA-CBA	2.55	119.91	111.91
31	a	419	LHG	O8-C23-C24	2.55	119.91	111.91
25	t	102	BCR	C21-C20-C19	-2.55	115.27	123.22
25	Y	101	BCR	C28-C27-C26	-2.55	109.53	114.08
23	c	512	CLA	C11-C10-C8	-2.55	107.69	115.92
29	a	415	PL9	C7-C8-C9	-2.55	122.55	126.79
23	b	602	CLA	C4-C3-C5	2.55	119.55	115.27
33	B	622	HTG	O2-C2-C3	-2.55	104.47	110.35
23	B	603	CLA	CHC-C1C-C2C	-2.54	119.68	126.72
25	B	619	BCR	C7-C8-C9	-2.54	122.39	126.23
33	B	623	HTG	C1-C2-C3	2.54	115.61	110.59
25	t	102	BCR	C37-C22-C23	2.54	122.08	118.08
23	c	508	CLA	C4C-C3C-C2C	-2.54	103.20	106.90
23	d	403	CLA	C1-C2-C3	-2.54	121.66	126.04
23	a	404	CLA	CAA-CBA-CGA	-2.54	105.84	113.25
23	c	510	CLA	C6-C7-C8	-2.53	107.73	115.92
23	B	608	CLA	CMC-C2C-C1C	2.53	128.89	125.04
23	B	616	CLA	CMB-C2B-C3B	2.53	129.41	124.68
23	C	504	CLA	CAC-C3C-C4C	2.52	128.09	124.81
35	H	102	DGD	C3G-O3G-C1D	-2.52	108.81	113.74
23	C	508	CLA	CAA-C2A-C3A	-2.52	105.87	112.78
23	b	610	CLA	CBC-CAC-C3C	-2.52	105.48	112.43
23	a	404	CLA	C2A-C1A-CHA	-2.52	119.45	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	515	CLA	CHD-C4C-NC	2.52	128.17	124.20
23	B	616	CLA	CHD-C4C-NC	2.52	128.17	124.20
27	D	412	SQD	O48-C23-C24	2.51	119.80	111.91
23	C	512	CLA	CMB-C2B-C3B	2.51	129.38	124.68
23	a	405	CLA	CBC-CAC-C3C	-2.51	105.50	112.43
23	C	512	CLA	O2A-CGA-O1A	-2.51	117.25	123.59
25	B	618	BCR	C28-C27-C26	-2.51	109.59	114.08
25	b	617	BCR	C24-C23-C22	-2.51	122.44	126.23
23	b	611	CLA	CMB-C2B-C3B	2.51	129.37	124.68
25	y	101	BCR	C10-C11-C12	-2.50	115.40	123.22
25	A	409	BCR	C16-C17-C18	-2.50	123.74	127.31
23	c	505	CLA	CHC-C1C-C2C	-2.50	119.80	126.72
25	C	516	BCR	C20-C21-C22	-2.50	123.74	127.31
35	H	102	DGD	O2G-C1B-C2B	2.50	116.90	111.50
29	d	405	PL9	C35-C34-C36	2.50	119.48	115.27
23	A	408	CLA	O2A-CGA-CBA	2.50	119.76	111.91
24	a	417	PHO	C4-C3-C2	-2.50	117.26	123.68
25	d	404	BCR	C21-C20-C19	-2.50	115.42	123.22
23	b	616	CLA	CAC-C3C-C4C	2.50	128.05	124.81
23	b	609	CLA	CMC-C2C-C1C	2.50	128.84	125.04
23	B	613	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
23	C	513	CLA	C1-C2-C3	-2.50	121.72	126.04
23	b	615	CLA	CHD-C4C-NC	2.50	128.14	124.20
25	k	101	BCR	C34-C9-C8	2.50	122.01	118.08
31	D	407	LHG	O8-C23-C24	2.50	119.74	111.91
23	c	514	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	c	517	BCR	C38-C26-C25	-2.50	121.72	124.53
23	C	504	CLA	CHD-C4C-NC	2.50	128.14	124.20
23	C	507	CLA	CHD-C4C-NC	2.50	128.14	124.20
23	B	616	CLA	CMC-C2C-C1C	2.50	128.84	125.04
25	B	619	BCR	C29-C30-C25	2.50	114.32	110.48
23	c	512	CLA	C4C-C3C-C2C	-2.49	103.26	106.90
23	b	608	CLA	O2A-CGA-CBA	2.49	119.74	111.91
23	c	513	CLA	C2A-C1A-CHA	-2.49	119.50	123.86
23	A	405	CLA	CMA-C3A-C4A	-2.49	105.07	111.77
25	C	517	BCR	C3-C4-C5	-2.49	109.63	114.08
23	b	603	CLA	CMA-C3A-C2A	-2.49	103.78	113.83
23	c	510	CLA	C4-C3-C5	2.49	119.46	115.27
23	B	608	CLA	CBC-CAC-C3C	-2.49	105.57	112.43
25	b	618	BCR	C3-C4-C5	-2.49	109.64	114.08
23	b	608	CLA	C11-C10-C8	-2.49	107.88	115.92
23	b	602	CLA	CHD-C4C-NC	2.48	128.12	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	504	CLA	O2A-CGA-O1A	-2.48	117.32	123.59
23	D	403	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
23	c	504	CLA	C2A-C1A-CHA	-2.48	119.52	123.86
23	b	603	CLA	CMC-C2C-C1C	2.48	128.82	125.04
25	h	102	BCR	C16-C17-C18	-2.48	123.77	127.31
25	k	101	BCR	C11-C10-C9	-2.48	123.77	127.31
27	D	412	SQD	C1-O5-C5	-2.48	108.82	113.69
23	B	603	CLA	C2A-C1A-CHA	-2.48	119.52	123.86
25	D	405	BCR	C37-C22-C21	-2.48	119.45	122.92
27	A	411	SQD	O48-C23-O10	-2.48	117.34	123.59
35	c	520	DGD	C2G-O2G-C1B	-2.48	111.69	117.79
23	a	406	CLA	CHC-C1C-C2C	-2.48	119.87	126.72
23	a	404	CLA	C4C-C3C-C2C	-2.47	103.29	106.90
23	b	615	CLA	C1-C2-C3	-2.47	121.76	126.04
27	a	410	SQD	C45-O47-C7	-2.47	111.70	117.79
23	D	403	CLA	C4C-C3C-C2C	-2.47	103.29	106.90
23	b	615	CLA	CBC-CAC-C3C	-2.47	105.62	112.43
33	h	101	HTG	C1-C2-C3	-2.47	105.71	110.59
23	B	608	CLA	CAC-C3C-C4C	2.47	128.01	124.81
25	Y	101	BCR	C36-C18-C17	-2.47	119.46	122.92
23	c	505	CLA	C2A-C1A-CHA	-2.47	119.54	123.86
23	a	405	CLA	O2A-CGA-CBA	2.47	119.65	111.91
34	M	103	LMT	C1'-O5'-C5'	2.46	118.52	113.69
25	y	101	BCR	C16-C17-C18	-2.46	123.80	127.31
23	C	515	CLA	C1-O2A-CGA	2.46	122.90	116.44
23	B	611	CLA	OBD-CAD-C3D	-2.46	122.60	128.52
23	c	513	CLA	CAC-C3C-C4C	2.46	128.00	124.81
23	C	509	CLA	O2A-CGA-O1A	-2.46	117.39	123.59
24	A	407	PHO	O2A-CGA-CBA	2.46	119.62	111.91
23	c	510	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
25	B	617	BCR	C16-C17-C18	-2.45	123.81	127.31
23	b	614	CLA	C2A-C1A-CHA	-2.45	119.57	123.86
25	D	405	BCR	C33-C5-C6	-2.45	121.78	124.53
23	D	404	CLA	C4-C3-C5	2.45	119.39	115.27
23	b	611	CLA	C1-C2-C3	-2.45	121.80	126.04
23	b	607	CLA	CMC-C2C-C1C	2.45	128.77	125.04
25	T	101	BCR	C16-C17-C18	-2.45	123.81	127.31
25	T	101	BCR	C21-C20-C19	-2.45	115.58	123.22
23	b	601	CLA	C2A-C1A-CHA	-2.45	119.58	123.86
25	D	405	BCR	C40-C30-C25	-2.45	106.33	110.30
23	b	615	CLA	O2A-CGA-O1A	-2.45	117.42	123.59
23	b	604	CLA	O1D-CGD-CBD	-2.44	119.49	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	t	102	BCR	C7-C8-C9	-2.44	122.55	126.23
23	b	616	CLA	C4-C3-C5	2.44	119.38	115.27
27	a	412	SQD	O8-S-C6	2.44	109.63	105.74
23	B	611	CLA	C4-C3-C5	2.44	119.38	115.27
23	C	515	CLA	O2A-CGA-CBA	2.44	119.57	111.91
23	c	512	CLA	O2A-CGA-CBA	2.44	119.57	111.91
25	C	517	BCR	C37-C22-C23	2.44	121.92	118.08
25	Y	101	BCR	C36-C18-C19	2.44	121.92	118.08
23	C	505	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
23	c	509	CLA	C4C-C3C-C2C	-2.44	103.35	106.90
23	b	611	CLA	C2A-C1A-CHA	-2.43	119.60	123.86
25	t	102	BCR	C7-C6-C5	-2.43	115.57	121.46
23	A	405	CLA	C4C-C3C-C2C	-2.43	103.35	106.90
23	B	608	CLA	CHB-C4A-NA	2.43	127.88	124.51
23	C	504	CLA	CMC-C2C-C1C	2.43	128.74	125.04
29	A	413	PL9	C45-C44-C46	2.43	119.35	115.27
23	b	606	CLA	CAA-C2A-C3A	-2.42	106.14	112.78
23	A	405	CLA	C2A-C1A-CHA	-2.42	119.62	123.86
31	d	407	LHG	O8-C23-C24	2.42	119.49	111.91
23	b	609	CLA	C4-C3-C5	2.42	119.34	115.27
23	C	510	CLA	CHB-C4A-NA	2.42	127.85	124.51
25	Y	101	BCR	C38-C26-C25	-2.42	121.82	124.53
23	b	614	CLA	O2A-CGA-O1A	-2.42	117.50	123.59
25	T	101	BCR	C12-C13-C14	-2.41	115.24	118.94
25	k	101	BCR	C36-C18-C19	2.41	121.88	118.08
23	c	509	CLA	CAC-C3C-C4C	2.41	127.94	124.81
23	C	507	CLA	C4-C3-C5	2.41	119.33	115.27
35	C	518	DGD	O1G-C1A-O1A	-2.41	117.50	123.59
23	B	601	CLA	CMC-C2C-C1C	2.41	128.71	125.04
23	C	512	CLA	C4C-C3C-C2C	-2.41	103.39	106.90
23	c	515	CLA	C2A-C1A-CHA	-2.41	119.65	123.86
25	C	516	BCR	C23-C24-C25	-2.40	120.45	127.20
27	C	501	SQD	O8-S-C6	2.40	109.57	105.74
23	B	609	CLA	CMC-C2C-C1C	2.40	128.69	125.04
23	b	607	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
25	C	517	BCR	C29-C30-C25	2.40	114.17	110.48
23	C	510	CLA	C2A-C1A-CHA	-2.40	119.66	123.86
23	b	609	CLA	O2A-CGA-CBA	2.40	119.43	111.91
23	C	503	CLA	OBD-CAD-C3D	-2.39	122.76	128.52
29	d	405	PL9	C36-C34-C33	-2.39	116.27	121.12
25	T	101	BCR	C3-C4-C5	-2.39	109.80	114.08
23	A	406	CLA	CMA-C3A-C2A	-2.39	104.18	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	408	CLA	CMC-C2C-C1C	2.39	128.68	125.04
32	C	521	LMG	O8-C28-O10	-2.39	117.56	123.59
23	D	403	CLA	CHD-C4C-NC	2.39	127.97	124.20
23	d	403	CLA	C4-C3-C5	2.39	119.29	115.27
23	A	405	CLA	OBD-CAD-C3D	-2.39	122.78	128.52
23	B	610	CLA	C1-C2-C3	-2.39	121.92	126.04
23	B	605	CLA	CHC-C1C-C2C	-2.39	120.12	126.72
23	C	508	CLA	C4C-C3C-C2C	-2.39	103.42	106.90
23	B	615	CLA	C11-C10-C8	-2.39	108.21	115.92
23	b	607	CLA	CHD-C4C-NC	2.39	127.96	124.20
25	c	516	BCR	C33-C5-C6	-2.38	121.85	124.53
23	c	503	CLA	C1-C2-C3	-2.38	121.92	126.04
27	B	620	SQD	O7-S-C6	2.38	109.77	106.94
35	c	519	DGD	O1G-C1A-C2A	2.38	119.38	111.91
34	M	101	LMT	O1'-C1'-C2'	2.38	112.02	108.30
25	b	619	BCR	C15-C14-C13	-2.38	123.91	127.31
25	b	617	BCR	C40-C30-C25	-2.38	106.44	110.30
23	b	603	CLA	CBC-CAC-C3C	-2.38	105.87	112.43
23	c	507	CLA	CBC-CAC-C3C	-2.38	105.87	112.43
25	B	619	BCR	C21-C20-C19	-2.38	115.79	123.22
23	B	615	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
23	b	606	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
23	A	404	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
23	b	613	CLA	CMB-C2B-C3B	2.38	129.12	124.68
27	B	620	SQD	O8-S-C6	2.38	109.53	105.74
23	B	609	CLA	C2A-C1A-CHA	-2.38	119.71	123.86
23	C	510	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
23	c	515	CLA	CED-O2D-CGD	2.37	121.31	115.94
23	A	404	CLA	CHD-C4C-NC	2.37	127.94	124.20
25	T	101	BCR	C1-C6-C7	2.37	122.49	115.78
25	d	404	BCR	C10-C11-C12	-2.37	115.82	123.22
23	c	513	CLA	CMC-C2C-C1C	2.37	128.65	125.04
23	c	509	CLA	C1-C2-C3	-2.37	121.95	126.04
23	C	508	CLA	C4-C3-C5	2.37	119.25	115.27
38	E	103	HEC	O2D-CGD-CBD	2.37	121.64	114.03
25	b	619	BCR	C21-C20-C19	-2.37	115.83	123.22
29	d	405	PL9	C36-C37-C38	-2.36	104.11	111.88
23	b	612	CLA	CHD-C4C-NC	2.36	127.93	124.20
23	C	512	CLA	C4-C3-C2	-2.36	117.62	123.68
24	a	407	PHO	CMC-C2C-C3C	2.36	129.40	124.94
23	B	614	CLA	CAA-C2A-C3A	-2.36	106.31	112.78
23	C	509	CLA	CBC-CAC-C3C	-2.36	105.93	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	508	CLA	CGD-CBD-CAD	-2.36	103.09	110.73
23	B	612	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
25	C	517	BCR	C11-C10-C9	-2.36	123.95	127.31
31	d	406	LHG	O7-C7-O9	-2.36	118.01	123.70
23	a	404	CLA	CAA-C2A-C1A	-2.36	104.26	111.97
23	B	608	CLA	O2A-CGA-O1A	-2.36	117.65	123.59
23	C	503	CLA	CAC-C3C-C4C	2.35	127.86	124.81
35	c	518	DGD	O3G-C3G-C2G	-2.35	105.22	110.90
23	c	511	CLA	CAA-C2A-C3A	-2.35	106.34	112.78
24	a	407	PHO	O2A-CGA-O1A	-2.35	117.66	123.59
23	b	604	CLA	CMB-C2B-C3B	2.35	129.08	124.68
25	T	101	BCR	C29-C30-C25	2.35	114.10	110.48
38	e	102	HEC	CMC-C2C-C1C	-2.35	124.85	128.46
23	c	506	CLA	CAA-C2A-C3A	-2.35	106.35	112.78
23	B	607	CLA	CAC-C3C-C4C	2.35	127.86	124.81
23	B	604	CLA	CMC-C2C-C1C	2.35	128.61	125.04
25	D	405	BCR	C21-C20-C19	-2.34	115.91	123.22
23	c	506	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
23	b	602	CLA	CMA-C3A-C2A	-2.34	104.39	113.83
23	b	608	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
23	C	506	CLA	OBD-CAD-C3D	-2.34	122.89	128.52
23	a	405	CLA	CAC-C3C-C2C	2.34	131.53	127.53
23	B	606	CLA	OBD-CAD-C3D	-2.34	122.89	128.52
29	D	406	PL9	C27-C28-C29	-2.34	122.03	127.66
23	a	404	CLA	CMA-C3A-C2A	-2.34	104.40	113.83
23	a	405	CLA	CAA-CBA-CGA	2.34	120.08	113.25
25	a	409	BCR	C7-C8-C9	-2.33	122.71	126.23
25	c	517	BCR	C15-C16-C17	-2.33	118.69	123.47
23	B	612	CLA	C2A-C1A-CHA	-2.33	119.78	123.86
23	B	609	CLA	C1-O2A-CGA	2.33	122.56	116.44
23	C	504	CLA	C2A-C1A-CHA	-2.33	119.78	123.86
23	a	408	CLA	CHC-C1C-C2C	-2.33	120.28	126.72
23	B	603	CLA	CAC-C3C-C4C	2.33	127.83	124.81
23	B	615	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
27	f	101	SQD	C46-C45-C44	-2.33	106.28	111.79
25	b	618	BCR	C11-C10-C9	-2.33	123.99	127.31
25	D	405	BCR	C29-C30-C25	2.33	114.06	110.48
23	C	507	CLA	C1-C2-C3	-2.33	122.02	126.04
38	V	201	HEC	CAD-CBD-CGD	-2.33	107.24	113.76
23	c	513	CLA	CBC-CAC-C3C	-2.33	106.02	112.43
23	b	606	CLA	CMC-C2C-C1C	2.32	128.58	125.04
23	c	504	CLA	O2A-CGA-CBA	2.32	119.20	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	616	CLA	C2A-C1A-CHA	-2.32	119.80	123.86
32	c	522	LMG	O8-C28-O10	-2.32	117.73	123.59
23	a	408	CLA	OBD-CAD-C3D	-2.32	122.93	128.52
25	c	516	BCR	C20-C21-C22	-2.32	124.00	127.31
23	C	506	CLA	CHD-C4C-NC	2.32	127.86	124.20
23	C	506	CLA	C2A-C1A-CHA	-2.32	119.80	123.86
23	b	604	CLA	CHD-C4C-NC	2.32	127.86	124.20
23	c	509	CLA	CHC-C1C-C2C	-2.32	120.31	126.72
25	a	409	BCR	C3-C4-C5	-2.32	109.94	114.08
38	E	103	HEC	O2A-CGA-CBA	2.31	121.47	114.03
35	c	518	DGD	C2G-O2G-C1B	-2.31	112.09	117.79
27	f	101	SQD	O47-C7-O49	-2.31	118.11	123.70
23	d	402	CLA	C2A-C1A-CHA	-2.31	119.82	123.86
23	B	602	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
23	B	607	CLA	C2A-C1A-CHA	-2.31	119.82	123.86
34	t	101	LMT	O1'-C1'-C2'	2.31	111.91	108.30
23	A	406	CLA	CAC-C3C-C4C	2.31	127.81	124.81
23	d	402	CLA	C4-C3-C2	-2.31	117.75	123.68
23	d	402	CLA	CHD-C4C-NC	2.31	127.84	124.20
23	B	608	CLA	C2A-C1A-CHA	-2.31	119.83	123.86
35	c	519	DGD	O6E-C5E-C6E	2.30	112.16	106.44
23	C	506	CLA	C4-C3-C5	2.30	119.14	115.27
29	a	415	PL9	C35-C34-C36	2.30	119.14	115.27
29	A	413	PL9	C16-C14-C13	-2.30	116.46	121.12
31	L	101	LHG	O4-P-O5	2.30	123.61	112.24
24	A	415	PHO	C4A-C3A-C2A	-2.30	100.65	102.84
23	C	508	CLA	CHD-C4C-NC	2.30	127.83	124.20
23	b	615	CLA	C11-C12-C13	-2.30	108.49	115.92
27	D	412	SQD	O47-C7-O49	-2.30	118.15	123.70
29	D	406	PL9	C36-C37-C38	-2.30	104.34	111.88
35	h	103	DGD	O4D-C4D-C3D	-2.29	105.04	110.35
32	m	101	LMG	O8-C28-O10	-2.29	117.80	123.59
23	b	606	CLA	CAC-C3C-C4C	2.29	127.78	124.81
25	b	617	BCR	C39-C30-C25	-2.29	106.58	110.30
23	c	506	CLA	CBC-CAC-C3C	-2.29	106.11	112.43
23	A	404	CLA	CHB-C4A-NA	2.29	127.68	124.51
23	B	608	CLA	C11-C12-C13	-2.29	108.52	115.92
23	A	405	CLA	CAA-CBA-CGA	2.29	119.94	113.25
23	B	602	CLA	CHC-C1C-C2C	-2.28	120.41	126.72
23	B	612	CLA	CHD-C4C-NC	2.28	127.80	124.20
23	C	511	CLA	CHD-C4C-NC	2.28	127.80	124.20
23	d	403	CLA	CMA-C3A-C2A	-2.28	104.64	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B	630	LMT	C1'-O5'-C5'	2.28	118.16	113.69
23	C	505	CLA	CMC-C2C-C1C	2.28	128.50	125.04
23	B	606	CLA	CAA-C2A-C3A	-2.27	106.55	112.78
23	C	504	CLA	CBC-CAC-C3C	-2.27	106.16	112.43
25	a	409	BCR	C34-C9-C10	-2.27	119.74	122.92
35	c	518	DGD	O1G-C1A-O1A	-2.27	117.86	123.59
25	B	619	BCR	C10-C11-C12	-2.27	116.13	123.22
23	c	507	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
23	B	614	CLA	OBD-CAD-C3D	-2.27	123.06	128.52
23	B	604	CLA	C6-C7-C8	-2.27	108.58	115.92
25	t	102	BCR	C20-C21-C22	-2.27	124.07	127.31
23	b	606	CLA	CBC-CAC-C3C	-2.27	106.18	112.43
25	y	101	BCR	C21-C20-C19	-2.27	116.14	123.22
29	A	413	PL9	C35-C34-C36	2.27	119.08	115.27
23	b	607	CLA	CAA-CBA-CGA	2.27	119.87	113.25
23	C	510	CLA	CAC-C3C-C4C	2.27	127.75	124.81
23	C	514	CLA	OBD-CAD-C3D	-2.27	123.07	128.52
38	e	102	HEC	O2D-CGD-CBD	2.26	121.30	114.03
23	C	506	CLA	CAC-C3C-C4C	2.26	127.75	124.81
27	B	620	SQD	O9-S-C6	2.26	109.63	106.94
23	a	405	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
25	h	102	BCR	C34-C9-C8	2.26	121.64	118.08
34	t	101	LMT	O5'-C5'-C4'	2.26	114.52	109.75
23	c	515	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
23	c	508	CLA	CAC-C3C-C4C	2.26	127.74	124.81
23	B	616	CLA	C1-O2A-CGA	2.26	122.36	116.44
23	D	403	CLA	C4-C3-C5	2.26	119.07	115.27
32	Z	101	LMG	C1-O6-C5	2.25	118.11	113.69
23	C	513	CLA	C1-O2A-CGA	2.25	122.35	116.44
23	C	514	CLA	CHB-C4A-NA	2.25	127.62	124.51
23	A	408	CLA	C2A-C1A-CHA	-2.25	119.93	123.86
23	c	504	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
23	C	506	CLA	CAA-C2A-C3A	-2.25	106.62	112.78
23	C	514	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
25	k	101	BCR	C2-C1-C6	2.25	113.94	110.48
23	c	515	CLA	CMB-C2B-C3B	2.24	128.88	124.68
25	y	101	BCR	C1-C6-C7	2.24	122.13	115.78
23	B	602	CLA	CMB-C2B-C3B	2.24	128.88	124.68
23	b	606	CLA	C1-C2-C3	-2.24	122.16	126.04
27	f	101	SQD	O5-C1-C2	2.24	115.10	110.35
23	C	512	CLA	C2A-C1A-CHA	-2.24	119.94	123.86
25	c	517	BCR	C32-C1-C6	-2.24	106.66	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	619	BCR	C16-C17-C18	-2.24	124.11	127.31
23	C	507	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
23	b	611	CLA	OBD-CAD-C3D	-2.24	123.13	128.52
23	b	613	CLA	CHB-C4A-NA	2.24	127.61	124.51
23	B	601	CLA	CAA-C2A-C3A	-2.23	106.66	112.78
23	c	505	CLA	O2A-CGA-CBA	2.23	118.92	111.91
23	B	609	CLA	CHD-C4C-NC	2.23	127.72	124.20
23	b	601	CLA	C1-O2A-CGA	2.23	122.30	116.44
23	b	602	CLA	O2A-CGA-CBA	2.23	118.90	111.91
29	a	415	PL9	C30-C29-C31	2.23	119.02	115.27
23	B	607	CLA	O2A-CGA-CBA	2.23	118.90	111.91
29	D	406	PL9	C25-C24-C23	-2.23	117.97	123.68
23	C	505	CLA	O2A-CGA-CBA	2.23	118.89	111.91
34	a	418	LMT	C1B-O1B-C4'	-2.23	112.46	117.96
25	y	101	BCR	C37-C22-C23	2.23	121.58	118.08
23	B	602	CLA	C11-C12-C13	-2.22	108.73	115.92
23	c	515	CLA	CBC-CAC-C3C	-2.22	106.30	112.43
31	A	416	LHG	C5-O7-C7	-2.22	112.32	117.79
27	a	410	SQD	O47-C7-O49	-2.22	118.33	123.70
23	B	607	CLA	CHD-C4C-NC	2.22	127.70	124.20
25	A	409	BCR	C36-C18-C19	2.22	121.57	118.08
23	C	513	CLA	O2A-CGA-CBA	2.22	118.86	111.91
35	c	518	DGD	O6D-C1D-O3G	-2.22	104.73	109.97
23	C	510	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
25	h	102	BCR	C24-C23-C22	-2.21	122.89	126.23
23	C	514	CLA	CBC-CAC-C3C	-2.21	106.33	112.43
23	c	515	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
23	B	601	CLA	C4-C3-C5	2.21	118.99	115.27
23	a	406	CLA	CAC-C3C-C4C	2.21	127.68	124.81
34	B	628	LMT	O1B-C4'-C3'	2.21	113.17	107.28
23	d	402	CLA	CBC-CAC-C3C	-2.21	106.33	112.43
23	A	405	CLA	CHB-C4A-NA	2.21	127.57	124.51
32	m	101	LMG	C9-C8-C7	-2.21	106.56	111.79
25	C	517	BCR	C21-C20-C19	-2.21	116.32	123.22
27	B	620	SQD	O48-C23-O10	-2.21	118.02	123.59
25	b	619	BCR	C29-C30-C25	2.21	113.88	110.48
25	H	101	BCR	C10-C11-C12	-2.21	116.33	123.22
29	a	415	PL9	C51-C49-C50	2.20	119.47	114.60
34	m	103	LMT	O6'-C6'-C5'	-2.20	103.73	111.29
23	b	612	CLA	C2A-C1A-CHA	-2.20	120.01	123.86
23	A	408	CLA	CMA-C3A-C2A	-2.20	104.94	113.83
23	d	402	CLA	O2A-CGA-O1A	-2.20	118.04	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B	621	LMG	O8-C28-O10	-2.20	118.04	123.59
23	c	509	CLA	C3B-C4B-NB	2.20	112.05	109.21
35	C	519	DGD	O5D-C6D-C5D	-2.20	104.98	109.05
25	C	516	BCR	C38-C26-C25	-2.20	122.06	124.53
23	c	503	CLA	OBD-CAD-C3D	-2.20	123.23	128.52
25	Y	101	BCR	C10-C11-C12	-2.20	116.36	123.22
25	D	405	BCR	C3-C4-C5	-2.20	110.16	114.08
25	b	618	BCR	C15-C16-C17	-2.20	118.97	123.47
32	c	501	LMG	C30-C29-C28	-2.20	105.64	113.62
35	C	518	DGD	O1G-C1A-C2A	2.19	118.80	111.91
27	b	620	SQD	C44-O6-C1	-2.19	109.46	113.74
23	A	408	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
23	b	614	CLA	CMC-C2C-C1C	2.19	128.38	125.04
32	c	521	LMG	O8-C28-O10	-2.19	118.06	123.59
23	B	613	CLA	CBC-CAC-C3C	-2.19	106.39	112.43
37	d	401	BCT	O2-C-O1	2.19	125.22	119.55
25	T	101	BCR	C7-C6-C5	-2.19	116.16	121.46
23	c	507	CLA	C2A-C1A-CHA	-2.19	120.03	123.86
38	E	103	HEC	CMC-C2C-C1C	-2.19	125.10	128.46
23	C	511	CLA	C11-C12-C13	-2.19	108.85	115.92
29	D	406	PL9	O2-C1-C6	-2.19	116.81	120.59
23	c	503	CLA	CMB-C2B-C3B	2.19	128.77	124.68
23	A	405	CLA	O2A-CGA-O1A	-2.19	118.08	123.59
23	b	608	CLA	C11-C12-C13	-2.19	108.85	115.92
23	b	615	CLA	CMC-C2C-C1C	2.18	128.36	125.04
23	a	405	CLA	CMC-C2C-C1C	2.18	128.36	125.04
23	C	511	CLA	C16-C15-C13	-2.18	108.87	115.92
25	c	516	BCR	C28-C27-C26	-2.18	110.19	114.08
23	B	616	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
32	C	502	LMG	O8-C28-C29	2.18	118.74	111.91
23	B	602	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
27	D	412	SQD	O7-S-C6	2.18	109.53	106.94
23	C	511	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
23	c	513	CLA	C1-O2A-CGA	2.18	122.16	116.44
23	B	607	CLA	CMC-C2C-C1C	2.18	128.35	125.04
25	h	102	BCR	C10-C11-C12	-2.18	116.42	123.22
25	c	517	BCR	C21-C20-C19	-2.17	116.43	123.22
23	c	507	CLA	CHD-C4C-NC	2.17	127.63	124.20
23	a	406	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
23	b	613	CLA	CMA-C3A-C4A	-2.17	105.95	111.77
23	a	406	CLA	CBC-CAC-C3C	-2.17	106.46	112.43
25	K	101	BCR	C36-C18-C19	2.17	121.49	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	408	CLA	CBC-CAC-C3C	-2.17	106.46	112.43
25	B	619	BCR	C37-C22-C23	2.16	121.49	118.08
25	Y	101	BCR	C35-C13-C12	2.16	121.49	118.08
25	D	405	BCR	C28-C27-C26	-2.16	110.22	114.08
23	B	615	CLA	CBC-CAC-C3C	-2.16	106.47	112.43
23	b	601	CLA	CMB-C2B-C3B	2.16	128.72	124.68
23	b	604	CLA	C6-C7-C8	-2.16	108.94	115.92
35	C	520	DGD	O1G-C1A-O1A	-2.16	118.14	123.59
25	Y	101	BCR	C11-C10-C9	-2.16	124.23	127.31
23	b	613	CLA	CHD-C4C-NC	2.16	127.61	124.20
24	A	407	PHO	CMC-C2C-C3C	2.16	129.01	124.94
35	C	520	DGD	O6E-C1E-O5D	-2.16	104.86	109.97
23	B	607	CLA	C1-O2A-CGA	2.16	122.10	116.44
23	D	404	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
23	B	604	CLA	CHA-C1A-NA	-2.16	121.46	126.40
32	z	101	LMG	C8-O7-C10	-2.15	112.49	117.79
23	B	611	CLA	CHB-C4A-NA	2.15	127.49	124.51
23	c	511	CLA	CHD-C4C-NC	2.15	127.60	124.20
25	H	101	BCR	C29-C30-C25	2.15	113.79	110.48
27	B	620	SQD	O5-C5-C4	2.15	113.60	109.69
25	B	618	BCR	C35-C13-C14	-2.15	119.91	122.92
23	b	601	CLA	CBC-CAC-C3C	-2.15	106.50	112.43
23	B	610	CLA	CHD-C4C-NC	2.15	127.59	124.20
25	c	517	BCR	C24-C23-C22	-2.15	122.99	126.23
23	B	602	CLA	C1-C2-C3	-2.15	122.33	126.04
23	B	615	CLA	C1-C2-C3	-2.15	122.33	126.04
25	A	409	BCR	C36-C18-C17	-2.15	119.91	122.92
23	c	506	CLA	O2A-CGA-CBA	2.15	118.65	111.91
23	b	602	CLA	C1-O2A-CGA	2.15	122.08	116.44
23	C	508	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
23	B	611	CLA	O2A-CGA-CBA	2.15	118.64	111.91
23	B	606	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
23	B	614	CLA	C4A-NA-C1A	-2.14	105.74	106.71
32	c	501	LMG	O6-C5-C4	2.14	113.59	109.69
23	B	601	CLA	CMB-C2B-C3B	2.14	128.69	124.68
24	a	417	PHO	O1D-CGD-CBD	-2.14	121.17	124.74
23	b	607	CLA	CMA-C3A-C2A	-2.14	105.19	113.83
38	e	102	HEC	C3C-C4C-NC	-2.14	106.90	110.94
23	B	612	CLA	OBD-CAD-C3D	-2.14	123.37	128.52
23	B	603	CLA	CMB-C2B-C3B	2.14	128.68	124.68
27	B	620	SQD	C44-O6-C1	-2.14	109.56	113.74
23	c	512	CLA	CMB-C2B-C3B	2.14	128.68	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	415	PL9	C47-C48-C49	-2.14	120.44	127.75
29	A	413	PL9	C51-C49-C50	2.14	119.33	114.60
23	B	613	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
23	c	512	CLA	C2A-C1A-CHA	-2.14	120.12	123.86
25	A	409	BCR	C28-C27-C26	-2.14	110.26	114.08
23	C	515	CLA	CBC-CAC-C3C	-2.14	106.54	112.43
25	C	516	BCR	C33-C5-C4	2.14	117.72	113.62
23	b	614	CLA	CAC-C3C-C4C	2.14	127.58	124.81
31	A	416	LHG	O7-C7-O9	-2.14	118.54	123.70
23	A	408	CLA	CHB-C4A-NA	2.13	127.46	124.51
23	a	406	CLA	C4-C3-C5	2.13	118.86	115.27
23	C	503	CLA	C2A-C1A-CHA	-2.13	120.13	123.86
29	D	406	PL9	C32-C33-C34	-2.13	122.52	127.66
23	B	612	CLA	CHB-C4A-NA	2.13	127.46	124.51
23	A	405	CLA	CMA-C3A-C2A	-2.13	105.23	113.83
23	c	504	CLA	C4-C3-C5	2.13	118.86	115.27
23	A	408	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
23	D	404	CLA	C1-O2A-CGA	2.13	122.03	116.44
25	Y	101	BCR	C29-C30-C25	2.13	113.76	110.48
23	C	506	CLA	O2A-CGA-CBA	2.13	118.58	111.91
25	c	516	BCR	C8-C7-C6	-2.13	121.23	127.20
23	c	507	CLA	C4-C3-C5	2.13	118.85	115.27
23	B	608	CLA	C1B-CHB-C4A	-2.13	125.91	130.12
23	B	606	CLA	CHA-C1A-NA	-2.13	121.53	126.40
23	C	509	CLA	OBD-CAD-C3D	-2.13	123.41	128.52
23	c	508	CLA	C2A-C1A-CHA	-2.12	120.14	123.86
34	m	103	LMT	C1'-C2'-C3'	2.12	114.42	110.00
23	B	602	CLA	CED-O2D-CGD	2.12	120.74	115.94
25	Y	101	BCR	C1-C6-C7	2.12	121.78	115.78
23	b	605	CLA	C1-C2-C3	-2.12	122.37	126.04
24	A	415	PHO	O2A-CGA-O1A	-2.12	118.24	123.59
34	t	101	LMT	C2'-C3'-C4'	2.12	114.52	109.68
23	B	603	CLA	CMA-C3A-C2A	-2.12	105.28	113.83
23	b	610	CLA	CHB-C4A-NA	2.12	127.44	124.51
32	C	522	LMG	O8-C28-O10	-2.12	118.25	123.59
23	B	612	CLA	C11-C12-C13	-2.11	109.09	115.92
23	D	403	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
25	K	101	BCR	C29-C30-C25	2.11	113.73	110.48
33	B	622	HTG	C1'-S1-C1	2.11	104.04	100.09
25	Y	101	BCR	C21-C20-C19	-2.11	116.63	123.22
27	C	501	SQD	O9-S-O7	-2.11	106.64	113.95
25	B	617	BCR	C29-C30-C25	2.11	113.73	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	616	CLA	C4-C3-C5	2.11	118.82	115.27
23	a	404	CLA	CMA-C3A-C4A	-2.11	106.10	111.77
25	C	517	BCR	C36-C18-C17	-2.11	119.97	122.92
34	M	101	LMT	O1B-C1B-C2B	2.11	113.56	108.10
27	D	412	SQD	O5-C1-C2	-2.11	105.89	110.35
32	d	412	LMG	O8-C28-C29	2.11	118.52	111.91
23	B	601	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
23	C	513	CLA	C11-C10-C8	-2.11	109.11	115.92
23	b	601	CLA	CAA-C2A-C3A	-2.11	107.01	112.78
23	c	514	CLA	CMB-C2B-C3B	2.11	128.62	124.68
23	B	604	CLA	CAC-C3C-C4C	2.11	127.54	124.81
29	d	405	PL9	C22-C23-C24	-2.11	122.59	127.66
23	A	404	CLA	CMA-C3A-C2A	-2.11	105.34	113.83
25	Y	101	BCR	C15-C16-C17	-2.10	119.16	123.47
25	b	618	BCR	C38-C26-C25	-2.10	122.17	124.53
25	c	516	BCR	C34-C9-C10	-2.10	119.98	122.92
23	C	510	CLA	OBD-CAD-C3D	-2.10	123.46	128.52
23	d	402	CLA	C1B-CHB-C4A	-2.10	125.95	130.12
34	M	101	LMT	C1B-C2B-C3B	2.10	114.37	110.00
33	V	202	HTG	C6-C5-C4	-2.10	108.08	113.00
25	C	517	BCR	C37-C22-C21	-2.10	119.98	122.92
34	B	630	LMT	O5'-C1'-C2'	2.10	114.79	110.35
23	b	604	CLA	CHA-C1A-NA	-2.10	121.59	126.40
38	V	201	HEC	CBA-CAA-C2A	-2.10	109.06	112.60
34	m	103	LMT	O5B-C5B-C6B	2.10	111.65	106.44
23	d	403	CLA	CBC-CAC-C3C	-2.10	106.65	112.43
25	c	516	BCR	C35-C13-C14	-2.09	119.99	122.92
23	C	508	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
34	C	526	LMT	O5'-C5'-C4'	2.09	114.16	109.75
34	B	628	LMT	O1B-C4'-C5'	-2.09	103.72	109.45
23	B	613	CLA	CHB-C4A-NA	2.09	127.40	124.51
25	k	101	BCR	C16-C17-C18	-2.09	124.33	127.31
23	b	604	CLA	C11-C10-C8	-2.09	109.17	115.92
23	B	602	CLA	C11-C10-C8	-2.09	109.17	115.92
23	b	609	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
23	C	505	CLA	C2A-C1A-CHA	-2.09	120.21	123.86
23	b	609	CLA	C2A-C1A-CHA	-2.09	120.21	123.86
35	c	518	DGD	O1G-C1A-C2A	2.08	118.45	111.91
23	b	603	CLA	C1B-CHB-C4A	-2.08	125.99	130.12
23	c	509	CLA	CMB-C2B-C3B	2.08	128.57	124.68
23	b	609	CLA	C7-C6-C5	-2.08	107.70	113.36
23	B	606	CLA	CMC-C2C-C1C	2.08	128.21	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	605	CLA	CAA-C2A-C3A	-2.08	107.08	112.78
25	k	101	BCR	C7-C8-C9	-2.08	123.09	126.23
25	k	101	BCR	C36-C18-C17	-2.08	120.01	122.92
33	B	623	HTG	C6-C5-C4	-2.08	108.13	113.00
23	C	509	CLA	C4-C3-C5	2.08	118.77	115.27
23	B	606	CLA	O2A-CGA-CBA	2.08	118.43	111.91
25	a	409	BCR	C10-C11-C12	-2.08	116.73	123.22
23	d	402	CLA	CMC-C2C-C1C	2.08	128.20	125.04
23	A	404	CLA	C7-C6-C5	-2.08	107.72	113.36
32	m	101	LMG	O1-C7-C8	-2.08	105.89	110.90
23	c	506	CLA	O1D-CGD-CBD	-2.08	120.24	124.48
23	b	616	CLA	C2A-C1A-CHA	-2.08	120.23	123.86
25	y	101	BCR	C29-C28-C27	-2.07	106.74	111.38
23	c	505	CLA	OBD-CAD-C3D	-2.07	123.53	128.52
29	a	415	PL9	C16-C14-C13	-2.07	116.92	121.12
35	H	102	DGD	O6E-C5E-C6E	2.07	111.59	106.44
25	T	101	BCR	C2-C1-C6	2.07	113.67	110.48
23	B	608	CLA	CAA-C2A-C3A	-2.07	107.10	112.78
23	b	610	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
25	b	618	BCR	C8-C7-C6	-2.07	121.39	127.20
23	C	505	CLA	CBC-CAC-C3C	-2.07	106.72	112.43
23	C	503	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
23	B	614	CLA	C1-C2-C3	-2.07	122.46	126.04
34	t	101	LMT	O2'-C2'-C3'	-2.07	105.57	110.35
25	t	102	BCR	C3-C4-C5	-2.07	110.38	114.08
23	C	514	CLA	CBA-CAA-C2A	-2.07	107.76	113.86
27	a	410	SQD	O48-C23-O10	-2.07	118.37	123.59
23	C	507	CLA	O2A-CGA-CBA	2.07	118.40	111.91
23	B	609	CLA	CHA-C1A-NA	-2.07	121.66	126.40
23	C	514	CLA	CAC-C3C-C4C	2.07	127.49	124.81
23	c	514	CLA	CHA-C1A-NA	-2.07	121.67	126.40
23	B	615	CLA	CMB-C2B-C1B	2.07	131.64	128.46
23	C	514	CLA	C2A-C1A-CHA	-2.07	120.25	123.86
27	f	101	SQD	O48-C23-O10	-2.07	118.38	123.59
25	c	517	BCR	C37-C22-C23	2.06	121.33	118.08
25	A	409	BCR	C15-C16-C17	-2.06	119.25	123.47
25	Y	101	BCR	C37-C22-C21	-2.06	120.03	122.92
23	b	610	CLA	CAC-C3C-C2C	2.06	131.06	127.53
23	D	403	CLA	C11-C12-C13	-2.06	109.26	115.92
34	m	103	LMT	C1-O1'-C1'	-2.06	110.42	113.84
23	b	609	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
23	b	610	CLA	OBD-CAD-C3D	-2.06	123.56	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402	CLA	CHB-C4A-NA	2.06	127.36	124.51
25	c	517	BCR	C36-C18-C19	2.06	121.32	118.08
23	b	615	CLA	CHA-C1A-NA	-2.06	121.69	126.40
23	b	602	CLA	CAA-CBA-CGA	-2.06	107.24	113.25
25	K	101	BCR	C3-C4-C5	-2.06	110.41	114.08
23	B	616	CLA	CBC-CAC-C3C	-2.06	106.76	112.43
25	d	404	BCR	C24-C23-C22	-2.06	123.13	126.23
23	b	606	CLA	O2A-CGA-CBA	2.05	118.36	111.91
23	C	503	CLA	O2A-CGA-CBA	2.05	118.35	111.91
23	C	511	CLA	CED-O2D-CGD	2.05	120.58	115.94
27	B	620	SQD	C1-C2-C3	-2.05	105.72	110.00
23	C	507	CLA	C2A-C1A-CHA	-2.05	120.27	123.86
23	c	511	CLA	C2A-C1A-CHA	-2.05	120.27	123.86
23	c	512	CLA	C11-C12-C13	-2.05	109.29	115.92
23	B	604	CLA	C11-C12-C13	-2.05	109.30	115.92
23	c	513	CLA	C11-C10-C8	-2.05	109.30	115.92
23	c	515	CLA	C4-C3-C5	2.05	118.72	115.27
33	b	623	HTG	C1-O5-C5	2.05	116.36	112.58
23	b	601	CLA	CHB-C4A-NA	2.05	127.34	124.51
23	c	513	CLA	CMB-C2B-C3B	2.05	128.50	124.68
25	t	102	BCR	C33-C5-C4	2.04	117.54	113.62
25	A	409	BCR	C34-C9-C10	-2.04	120.06	122.92
23	b	614	CLA	CED-O2D-CGD	2.04	120.56	115.94
38	v	202	HEC	CMB-C2B-C1B	-2.04	125.33	128.46
23	C	509	CLA	CMB-C2B-C3B	2.04	128.50	124.68
29	D	406	PL9	C12-C13-C14	-2.04	122.75	127.66
31	A	416	LHG	O4-P-O5	2.04	122.32	112.24
23	C	509	CLA	CAC-C3C-C2C	2.04	131.02	127.53
35	C	520	DGD	O2G-C1B-O1B	-2.04	118.78	123.70
25	a	409	BCR	C15-C16-C17	-2.03	119.31	123.47
25	B	618	BCR	C33-C5-C6	-2.03	122.24	124.53
23	c	509	CLA	CHA-C1A-NA	-2.03	121.74	126.40
23	d	402	CLA	CMA-C3A-C4A	-2.03	106.31	111.77
23	B	601	CLA	CHB-C4A-NA	2.03	127.32	124.51
23	c	514	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
23	d	403	CLA	CMB-C2B-C3B	2.03	128.48	124.68
25	c	517	BCR	C20-C21-C22	-2.03	124.41	127.31
23	C	510	CLA	C1-O2A-CGA	2.03	121.77	116.44
23	b	616	CLA	CMA-C3A-C4A	-2.03	106.33	111.77
24	A	415	PHO	CMC-C2C-C3C	2.03	128.76	124.94
29	d	405	PL9	C30-C29-C31	2.03	118.68	115.27
23	B	611	CLA	C1-O2A-CGA	2.02	121.76	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	415	PHO	O2A-CGA-CBA	2.02	118.26	111.91
23	c	506	CLA	C11-C10-C8	-2.02	109.38	115.92
23	c	510	CLA	CHB-C4A-NA	2.02	127.31	124.51
34	D	402	LMT	O5'-C5'-C4'	2.02	114.02	109.75
29	d	405	PL9	C47-C48-C49	-2.02	120.83	127.75
23	A	408	CLA	CMB-C2B-C3B	2.02	128.46	124.68
25	B	617	BCR	C24-C23-C22	-2.02	123.18	126.23
25	c	517	BCR	C15-C14-C13	-2.02	124.42	127.31
35	c	520	DGD	O6E-C5E-C4E	2.02	113.36	109.69
24	A	415	PHO	C6-C5-C3	-2.02	108.16	113.45
32	c	522	LMG	C9-C8-C7	-2.02	107.01	111.79
23	b	614	CLA	CHC-C1C-NC	2.02	127.27	124.20
32	D	413	LMG	C7-O1-C1	-2.02	109.80	113.74
23	C	508	CLA	CMB-C2B-C3B	2.02	128.45	124.68
29	A	413	PL9	C47-C48-C49	-2.02	120.85	127.75
25	d	404	BCR	C23-C24-C25	-2.02	121.54	127.20
23	C	513	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
23	B	613	CLA	CHD-C4C-NC	2.02	127.38	124.20
23	A	404	CLA	CAA-CBA-CGA	-2.02	107.36	113.25
23	B	604	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
23	b	616	CLA	CHA-C1A-NA	-2.01	121.79	126.40
34	a	413	LMT	C1'-O5'-C5'	2.01	117.63	113.69
25	a	409	BCR	C8-C7-C6	-2.01	121.56	127.20
23	B	608	CLA	C4-C3-C5	2.01	118.65	115.27
23	B	602	CLA	CAA-CBA-CGA	-2.01	107.38	113.25
24	A	415	PHO	C7-C6-C5	-2.01	107.91	113.36
23	b	605	CLA	CMC-C2C-C1C	2.01	128.09	125.04
25	B	619	BCR	C2-C3-C4	-2.01	106.89	111.38
23	a	408	CLA	CAC-C3C-C2C	2.01	130.96	127.53
32	B	621	LMG	C4-C3-C2	-2.01	107.32	110.82
27	D	412	SQD	O48-C23-O10	-2.00	118.53	123.59
34	E	102	LMT	O5'-C5'-C4'	2.00	113.98	109.75
23	C	510	CLA	C1-C2-C3	-2.00	122.58	126.04
23	c	510	CLA	C2A-C1A-CHA	-2.00	120.36	123.86
29	a	415	PL9	C40-C39-C41	2.00	118.64	115.27
23	B	607	CLA	CMA-C3A-C2A	-2.00	105.75	113.83
23	b	615	CLA	C1-O2A-CGA	2.00	121.70	116.44
25	A	409	BCR	C34-C9-C8	2.00	121.23	118.08
23	C	510	CLA	O2A-CGA-CBA	2.00	118.19	111.91
23	B	616	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
23	D	403	CLA	C1B-CHB-C4A	-2.00	126.15	130.12
23	d	403	CLA	C6-C7-C8	-2.00	109.45	115.92

All (64) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404	CLA	ND
23	A	405	CLA	ND
23	A	408	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND
23	B	604	CLA	ND
23	B	605	CLA	ND
23	B	606	CLA	ND
23	B	607	CLA	ND
23	B	609	CLA	ND
23	B	610	CLA	ND
23	B	611	CLA	ND
23	B	612	CLA	ND
23	B	613	CLA	ND
23	B	614	CLA	ND
23	B	615	CLA	ND
23	B	616	CLA	ND
23	C	503	CLA	ND
23	C	505	CLA	ND
23	C	506	CLA	ND
23	C	507	CLA	ND
23	C	508	CLA	ND
23	C	509	CLA	ND
23	C	510	CLA	ND
23	C	511	CLA	ND
23	C	512	CLA	ND
23	C	513	CLA	ND
23	C	514	CLA	ND
23	D	403	CLA	ND
23	D	404	CLA	ND
23	a	404	CLA	ND
23	a	405	CLA	ND
23	a	408	CLA	ND
23	b	601	CLA	ND
23	b	602	CLA	ND
23	b	603	CLA	ND
23	b	604	CLA	ND
23	b	605	CLA	ND
23	b	606	CLA	ND
23	b	607	CLA	ND
23	b	609	CLA	ND

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Mol	Chain	Res	Type	Atom
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	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	c	515	CLA	ND
23	d	402	CLA	ND
23	d	403	CLA	ND

All (1275) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	605	CLA	C2-C3-C5-C6
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	B	616	CLA	C4-C3-C5-C6
23	C	504	CLA	C14-C13-C15-C16
23	C	506	CLA	C2-C3-C5-C6
23	C	506	CLA	C4-C3-C5-C6
23	C	510	CLA	CHA-CBD-CGD-O1D
23	C	510	CLA	CHA-CBD-CGD-O2D
23	D	404	CLA	C2-C3-C5-C6
23	D	404	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	b	603	CLA	C2-C3-C5-C6
23	b	603	CLA	C4-C3-C5-C6
23	b	605	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	c	506	CLA	C4-C3-C5-C6
23	c	509	CLA	C2-C3-C5-C6
23	c	509	CLA	C4-C3-C5-C6
23	c	510	CLA	CHA-CBD-CGD-O1D
23	c	510	CLA	CHA-CBD-CGD-O2D
23	c	515	CLA	C2-C3-C5-C6
23	c	515	CLA	C4-C3-C5-C6
23	d	403	CLA	C2-C3-C5-C6
23	d	403	CLA	C4-C3-C5-C6
25	D	405	BCR	C21-C22-C23-C24
25	D	405	BCR	C37-C22-C23-C24
25	D	405	BCR	C23-C24-C25-C30
25	Y	101	BCR	C1-C6-C7-C8
25	Y	101	BCR	C5-C6-C7-C8
25	b	619	BCR	C7-C8-C9-C10
25	b	619	BCR	C7-C8-C9-C34
25	y	101	BCR	C1-C6-C7-C8
25	y	101	BCR	C5-C6-C7-C8
26	B	624	GOL	C1-C2-C3-O3
26	O	302	GOL	O1-C1-C2-C3
26	O	302	GOL	C1-C2-C3-O3
26	O	302	GOL	O2-C2-C3-O3
26	a	411	GOL	O1-C1-C2-C3
26	b	624	GOL	C1-C2-C3-O3
26	o	302	GOL	C1-C2-C3-O3
26	v	201	GOL	O1-C1-C2-C3
27	A	411	SQD	O6-C44-C45-O47
27	B	620	SQD	O49-C7-O47-C45
27	D	412	SQD	O49-C7-O47-C45
27	D	412	SQD	C8-C7-O47-C45
27	a	412	SQD	C5-C6-S-O7
27	a	412	SQD	C5-C6-S-O8
27	a	412	SQD	C5-C6-S-O9
27	b	620	SQD	O49-C7-O47-C45
27	b	620	SQD	C8-C7-O47-C45
27	f	101	SQD	C2-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
27	f	101	SQD	O5-C1-O6-C44
27	f	101	SQD	C8-C7-O47-C45
27	f	101	SQD	C5-C6-S-O7
27	f	101	SQD	C5-C6-S-O8
27	f	101	SQD	C5-C6-S-O9
29	A	413	PL9	C15-C14-C16-C17
29	A	413	PL9	C14-C16-C17-C18
29	A	413	PL9	C19-C21-C22-C23
29	A	413	PL9	C25-C24-C26-C27
29	a	415	PL9	C19-C21-C22-C23
31	D	407	LHG	C3-O3-P-O6
31	E	101	LHG	C3-O3-P-O4
31	E	101	LHG	C3-O3-P-O5
31	E	101	LHG	C3-O3-P-O6
31	E	101	LHG	C4-O6-P-O5
31	E	101	LHG	O10-C23-O8-C6
31	E	101	LHG	C24-C23-O8-C6
31	L	101	LHG	C4-O6-P-O4
31	L	101	LHG	C4-O6-P-O5
31	a	419	LHG	C3-O3-P-O4
31	a	419	LHG	C3-O3-P-O5
31	a	419	LHG	C3-O3-P-O6
31	a	419	LHG	C4-O6-P-O3
31	a	419	LHG	O10-C23-O8-C6
31	a	419	LHG	C24-C23-O8-C6
31	b	629	LHG	C4-O6-P-O5
31	d	406	LHG	C4-O6-P-O5
31	d	407	LHG	O2-C2-C3-O3
31	d	407	LHG	C3-O3-P-O4
31	d	407	LHG	C4-O6-P-O4
32	C	522	LMG	C11-C10-O7-C8
32	Z	101	LMG	O9-C10-O7-C8
32	Z	101	LMG	C11-C10-O7-C8
32	c	501	LMG	C2-C1-O1-C7
32	c	522	LMG	C11-C10-O7-C8
32	z	101	LMG	O6-C1-O1-C7
32	z	101	LMG	C11-C10-O7-C8
33	B	622	HTG	C2'-C1'-S1-C1
33	b	622	HTG	C2'-C1'-S1-C1
34	B	630	LMT	C2'-C1'-O1'-C1
34	B	630	LMT	O5'-C1'-O1'-C1
34	C	526	LMT	C3'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
34	C	526	LMT	C2'-C1'-O1'-C1
34	C	526	LMT	O5'-C1'-O1'-C1
34	D	402	LMT	C2'-C1'-O1'-C1
34	D	402	LMT	O5'-C1'-O1'-C1
34	E	102	LMT	C2'-C1'-O1'-C1
34	E	102	LMT	O5'-C1'-O1'-C1
34	M	103	LMT	C2'-C1'-O1'-C1
34	M	103	LMT	O5'-C1'-O1'-C1
34	a	413	LMT	C2'-C1'-O1'-C1
34	a	413	LMT	O5'-C1'-O1'-C1
34	a	418	LMT	C2'-C1'-O1'-C1
34	a	418	LMT	O5'-C1'-O1'-C1
34	b	621	LMT	O5'-C1'-O1'-C1
34	b	627	LMT	C2'-C1'-O1'-C1
34	b	627	LMT	O5'-C1'-O1'-C1
34	e	101	LMT	C2'-C1'-O1'-C1
34	e	101	LMT	O5'-C1'-O1'-C1
34	t	101	LMT	O5'-C1'-O1'-C1
34	B	628	LMT	C4'-C5'-C6'-O6'
23	C	505	CLA	CBD-CGD-O2D-CED
27	f	101	SQD	O49-C7-O47-C45
32	C	522	LMG	O9-C10-O7-C8
32	z	101	LMG	O9-C10-O7-C8
23	A	408	CLA	C3-C5-C6-C7
23	B	614	CLA	C3-C5-C6-C7
23	a	408	CLA	C3-C5-C6-C7
23	c	508	CLA	C3-C5-C6-C7
27	B	620	SQD	C8-C7-O47-C45
23	B	603	CLA	C4-C3-C5-C6
23	C	509	CLA	C4-C3-C5-C6
23	a	408	CLA	C4-C3-C5-C6
29	A	413	PL9	C12-C11-C9-C10
23	b	605	CLA	C2-C3-C5-C6
29	A	413	PL9	C13-C14-C16-C17
23	B	606	CLA	C2A-CAA-CBA-CGA
23	b	606	CLA	C2A-CAA-CBA-CGA
23	B	616	CLA	C3-C5-C6-C7
27	f	101	SQD	C24-C23-O48-C46
34	e	101	LMT	O5'-C5'-C6'-O6'
23	C	503	CLA	CBD-CGD-O2D-CED
32	c	522	LMG	O9-C10-O7-C8
34	B	628	LMT	C3'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
23	c	513	CLA	CBD-CGD-O2D-CED
34	E	102	LMT	C4'-C5'-C6'-O6'
32	C	502	LMG	O6-C5-C6-O5
32	c	522	LMG	O6-C5-C6-O5
33	b	625	HTG	O5-C5-C6-O6
34	M	103	LMT	C4'-C5'-C6'-O6'
27	f	101	SQD	O10-C23-O48-C46
32	C	522	LMG	O6-C5-C6-O5
34	B	628	LMT	O5'-C5'-C6'-O6'
23	c	514	CLA	C3-C5-C6-C7
23	b	615	CLA	C13-C15-C16-C17
34	B	628	LMT	O5B-C5B-C6B-O6B
23	A	408	CLA	C4-C3-C5-C6
23	b	614	CLA	C4-C3-C5-C6
29	a	415	PL9	C15-C14-C16-C17
29	a	415	PL9	C25-C24-C26-C27
23	A	408	CLA	C2-C3-C5-C6
23	B	616	CLA	C2-C3-C5-C6
23	b	614	CLA	C2-C3-C5-C6
23	c	506	CLA	C2-C3-C5-C6
29	A	413	PL9	C23-C24-C26-C27
29	a	415	PL9	C13-C14-C16-C17
29	a	415	PL9	C23-C24-C26-C27
34	C	526	LMT	O5B-C5B-C6B-O6B
27	B	620	SQD	O5-C1-O6-C44
32	c	501	LMG	O6-C1-O1-C7
29	D	406	PL9	C39-C41-C42-C43
29	d	405	PL9	C39-C41-C42-C43
33	c	523	HTG	C4-C5-C6-O6
33	D	411	HTG	C4-C5-C6-O6
23	C	505	CLA	O1D-CGD-O2D-CED
23	B	615	CLA	C13-C15-C16-C17
31	d	407	LHG	C1-C2-C3-O3
23	C	514	CLA	C3-C5-C6-C7
23	d	403	CLA	C3-C5-C6-C7
23	B	601	CLA	CBA-CGA-O2A-C1
23	C	514	CLA	CBA-CGA-O2A-C1
23	c	511	CLA	CBA-CGA-O2A-C1
23	b	613	CLA	CBD-CGD-O2D-CED
34	C	526	LMT	C4B-C5B-C6B-O6B
23	A	408	CLA	C5-C6-C7-C8
32	C	502	LMG	C4-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
34	e	101	LMT	C4'-C5'-C6'-O6'
23	B	604	CLA	C8-C10-C11-C12
23	B	606	CLA	C10-C11-C12-C13
23	B	614	CLA	C10-C11-C12-C13
32	Z	101	LMG	C10-C11-C12-C13
34	b	621	LMT	C2'-C1'-O1'-C1
34	t	101	LMT	C2'-C1'-O1'-C1
27	a	412	SQD	O6-C44-C45-O47
34	E	102	LMT	O5'-C5'-C6'-O6'
23	C	509	CLA	C2-C3-C5-C6
23	a	408	CLA	C2-C3-C5-C6
23	B	610	CLA	C11-C12-C13-C14
23	B	611	CLA	C11-C12-C13-C14
23	C	514	CLA	C6-C7-C8-C9
23	C	515	CLA	C14-C13-C15-C16
23	c	508	CLA	C6-C7-C8-C9
23	c	511	CLA	C11-C10-C8-C9
23	c	514	CLA	C6-C7-C8-C9
25	D	405	BCR	C7-C8-C9-C34
25	d	404	BCR	C7-C8-C9-C34
25	k	101	BCR	C7-C8-C9-C34
25	t	102	BCR	C11-C12-C13-C35
25	y	101	BCR	C37-C22-C23-C24
32	c	501	LMG	O6-C5-C6-O5
32	B	621	LMG	O9-C10-O7-C8
32	B	621	LMG	C11-C10-O7-C8
35	c	518	DGD	C1A-C2A-C3A-C4A
23	c	511	CLA	O1A-CGA-O2A-C1
23	C	510	CLA	C5-C6-C7-C8
23	b	601	CLA	C10-C11-C12-C13
34	B	628	LMT	C4B-C5B-C6B-O6B
23	B	613	CLA	C15-C16-C17-C18
33	B	623	HTG	C1'-C2'-C3'-C4'
23	C	507	CLA	C8-C10-C11-C12
23	C	512	CLA	C5-C6-C7-C8
23	a	406	CLA	C10-C11-C12-C13
23	b	616	CLA	C13-C15-C16-C17
23	c	506	CLA	C5-C6-C7-C8
27	A	411	SQD	C7-C8-C9-C10
32	c	501	LMG	C10-C11-C12-C13
35	c	519	DGD	C1B-C2B-C3B-C4B
34	C	526	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
23	C	507	CLA	C15-C16-C17-C18
23	C	514	CLA	C13-C15-C16-C17
23	c	511	CLA	C2-C1-O2A-CGA
23	B	614	CLA	C8-C10-C11-C12
27	D	412	SQD	C23-C24-C25-C26
23	c	503	CLA	CBD-CGD-O2D-CED
31	E	101	LHG	C11-C10-C9-C8
23	C	514	CLA	C15-C16-C17-C18
23	C	514	CLA	C12-C13-C15-C16
23	a	408	CLA	C6-C7-C8-C10
23	b	606	CLA	C11-C10-C8-C7
23	B	610	CLA	C2A-CAA-CBA-CGA
23	B	608	CLA	C13-C15-C16-C17
23	B	615	CLA	C10-C11-C12-C13
23	C	504	CLA	C13-C15-C16-C17
23	a	406	CLA	C8-C10-C11-C12
23	b	605	CLA	C8-C10-C11-C12
33	D	411	HTG	O5-C5-C6-O6
33	c	523	HTG	O5-C5-C6-O6
34	M	103	LMT	O5'-C5'-C6'-O6'
23	C	514	CLA	O1A-CGA-O2A-C1
34	M	101	LMT	O5'-C1'-O1'-C1
35	C	519	DGD	O6E-C1E-O5D-C6D
29	A	413	PL9	C24-C26-C27-C28
29	a	415	PL9	C24-C26-C27-C28
29	a	415	PL9	C29-C31-C32-C33
35	c	518	DGD	C2A-C3A-C4A-C5A
27	C	501	SQD	C7-C8-C9-C10
23	C	508	CLA	C3-C5-C6-C7
23	A	405	CLA	C15-C16-C17-C18
23	B	603	CLA	C8-C10-C11-C12
23	B	614	CLA	C5-C6-C7-C8
23	C	506	CLA	C8-C10-C11-C12
23	C	508	CLA	C10-C11-C12-C13
23	a	408	CLA	C5-C6-C7-C8
23	b	606	CLA	C13-C15-C16-C17
23	b	611	CLA	C15-C16-C17-C18
23	C	515	CLA	CBD-CGD-O2D-CED
23	B	601	CLA	O1A-CGA-O2A-C1
34	M	101	LMT	C4B-C5B-C6B-O6B
27	C	501	SQD	C11-C10-C9-C8
23	B	606	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	B	615	CLA	C5-C6-C7-C8
23	C	510	CLA	C10-C11-C12-C13
23	c	508	CLA	C15-C16-C17-C18
23	c	510	CLA	C10-C11-C12-C13
35	C	519	DGD	CBB-CCB-CDB-CEB
23	B	601	CLA	C5-C6-C7-C8
23	B	602	CLA	C8-C10-C11-C12
23	B	602	CLA	C15-C16-C17-C18
23	C	508	CLA	C8-C10-C11-C12
23	D	404	CLA	C10-C11-C12-C13
23	c	514	CLA	C10-C11-C12-C13
31	L	101	LHG	C4-O6-P-O3
31	b	629	LHG	C4-O6-P-O3
31	d	406	LHG	C3-O3-P-O6
31	d	407	LHG	C3-O3-P-O6
35	C	519	DGD	C1A-C2A-C3A-C4A
23	b	604	CLA	CBD-CGD-O2D-CED
34	M	101	LMT	O5B-C5B-C6B-O6B
27	D	412	SQD	C7-C8-C9-C10
23	C	508	CLA	C13-C15-C16-C17
23	C	504	CLA	C15-C16-C17-C18
23	c	512	CLA	C10-C11-C12-C13
25	T	101	BCR	C13-C14-C15-C16
31	D	408	LHG	C29-C30-C31-C32
35	c	519	DGD	C9A-CAA-CBA-CCA
27	a	412	SQD	C16-C17-C18-C19
31	L	101	LHG	C25-C26-C27-C28
31	a	419	LHG	C13-C14-C15-C16
32	c	521	LMG	C32-C33-C34-C35
32	c	521	LMG	C36-C37-C38-C39
23	b	615	CLA	C16-C17-C18-C20
27	B	620	SQD	C30-C31-C32-C33
27	C	501	SQD	C15-C16-C17-C18
31	D	407	LHG	C32-C33-C34-C35
32	C	522	LMG	C36-C37-C38-C39
32	D	413	LMG	C19-C20-C21-C22
32	d	412	LMG	C21-C22-C23-C24
32	m	101	LMG	C32-C33-C34-C35
35	C	520	DGD	C6B-C7B-C8B-C9B
35	H	102	DGD	C5B-C6B-C7B-C8B
35	c	519	DGD	C7A-C8A-C9A-CAA
23	A	408	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	a	405	CLA	C15-C16-C17-C18
31	D	408	LHG	C32-C33-C34-C35
31	a	419	LHG	C17-C18-C19-C20
31	a	419	LHG	C25-C26-C27-C28
32	C	502	LMG	C34-C35-C36-C37
35	h	103	DGD	CAA-CBA-CCA-CDA
32	C	502	LMG	C14-C15-C16-C17
32	D	413	LMG	C35-C36-C37-C38
32	Z	101	LMG	C16-C17-C18-C19
35	C	518	DGD	C3A-C4A-C5A-C6A
35	H	102	DGD	C9B-CAB-CBB-CCB
35	c	518	DGD	CAB-CBB-CCB-CDB
23	B	611	CLA	C8-C10-C11-C12
31	D	408	LHG	C33-C34-C35-C36
23	B	604	CLA	C3-C5-C6-C7
27	D	412	SQD	C2-C1-O6-C44
32	C	502	LMG	C2-C1-O1-C7
34	M	101	LMT	C2'-C1'-O1'-C1
35	C	519	DGD	C2E-C1E-O5D-C6D
27	D	412	SQD	C30-C31-C32-C33
31	d	407	LHG	C33-C34-C35-C36
31	d	408	LHG	C28-C29-C30-C31
32	C	521	LMG	C37-C38-C39-C40
34	b	621	LMT	C5-C6-C7-C8
23	c	504	CLA	C16-C17-C18-C19
23	C	503	CLA	O1D-CGD-O2D-CED
24	a	407	PHO	C4-C3-C5-C6
29	a	415	PL9	C30-C29-C31-C32
34	B	628	LMT	C5'-C4'-O1B-C1B
35	C	518	DGD	C4B-C5B-C6B-C7B
23	B	603	CLA	C2-C3-C5-C6
23	B	606	CLA	C11-C10-C8-C9
23	C	514	CLA	C14-C13-C15-C16
23	d	403	CLA	C14-C13-C15-C16
31	E	101	LHG	C23-C24-C25-C26
32	d	412	LMG	C28-C29-C30-C31
27	a	410	SQD	C9-C10-C11-C12
32	C	502	LMG	C12-C13-C14-C15
23	B	613	CLA	C10-C11-C12-C13
26	A	410	GOL	C1-C2-C3-O3
26	a	411	GOL	C1-C2-C3-O3
31	A	416	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
31	D	408	LHG	O1-C1-C2-C3
31	d	406	LHG	O1-C1-C2-C3
27	B	620	SQD	C14-C15-C16-C17
32	B	621	LMG	C32-C33-C34-C35
32	C	502	LMG	C18-C19-C20-C21
35	C	519	DGD	C8A-C9A-CAA-CBA
27	a	410	SQD	C34-C35-C36-C37
31	a	419	LHG	C18-C19-C20-C21
31	d	408	LHG	C29-C30-C31-C32
32	C	502	LMG	C37-C38-C39-C40
32	C	521	LMG	C30-C31-C32-C33
32	D	413	LMG	C12-C13-C14-C15
32	c	501	LMG	C30-C31-C32-C33
32	m	101	LMG	C38-C39-C40-C41
35	h	103	DGD	C9A-CAA-CBA-CCA
34	m	103	LMT	O5'-C5'-C6'-O6'
23	a	408	CLA	C16-C17-C18-C19
23	b	610	CLA	C16-C17-C18-C19
23	b	615	CLA	C16-C17-C18-C19
23	c	511	CLA	C16-C17-C18-C20
32	C	502	LMG	O6-C1-O1-C7
27	D	412	SQD	C29-C30-C31-C32
27	a	412	SQD	C25-C26-C27-C28
27	b	620	SQD	C28-C29-C30-C31
31	E	101	LHG	C27-C28-C29-C30
31	b	629	LHG	C14-C15-C16-C17
35	C	518	DGD	C5A-C6A-C7A-C8A
23	b	604	CLA	C13-C15-C16-C17
32	C	521	LMG	C21-C22-C23-C24
34	B	630	LMT	C4-C5-C6-C7
34	e	101	LMT	C5-C6-C7-C8
35	c	519	DGD	C7B-C8B-C9B-CAB
35	h	103	DGD	CCB-CDB-CEB-CFB
31	d	407	LHG	C28-C29-C30-C31
23	B	602	CLA	C13-C15-C16-C17
23	c	515	CLA	C10-C11-C12-C13
27	D	412	SQD	C24-C25-C26-C27
31	D	408	LHG	C12-C13-C14-C15
32	C	502	LMG	C17-C18-C19-C20
35	h	103	DGD	CAB-CBB-CCB-CDB
23	a	408	CLA	C16-C17-C18-C20
23	c	504	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
31	b	629	LHG	C16-C17-C18-C19
27	C	501	SQD	O6-C44-C45-C46
31	a	419	LHG	C4-C5-C6-O8
32	z	101	LMG	C4-C5-C6-O5
23	b	604	CLA	C3-C5-C6-C7
31	E	101	LHG	C7-C8-C9-C10
32	C	522	LMG	C18-C19-C20-C21
23	c	512	CLA	C4-C3-C5-C6
29	D	406	PL9	C30-C29-C31-C32
29	d	405	PL9	C15-C14-C16-C17
27	b	620	SQD	C24-C23-O48-C46
23	c	512	CLA	C2-C3-C5-C6
24	a	407	PHO	C2-C3-C5-C6
29	D	406	PL9	C13-C14-C16-C17
27	C	501	SQD	C8-C7-O47-C45
32	C	502	LMG	C11-C10-O7-C8
32	C	521	LMG	C29-C30-C31-C32
26	B	624	GOL	O2-C2-C3-O3
26	v	201	GOL	O1-C1-C2-O2
31	A	416	LHG	C34-C35-C36-C37
32	C	521	LMG	C31-C32-C33-C34
32	m	101	LMG	C39-C40-C41-C42
34	D	402	LMT	C5-C6-C7-C8
35	C	519	DGD	CAB-CBB-CCB-CDB
23	c	513	CLA	O1D-CGD-O2D-CED
31	d	406	LHG	C23-C24-C25-C26
33	V	202	HTG	O5-C5-C6-O6
27	b	620	SQD	C10-C11-C12-C13
27	D	412	SQD	C34-C35-C36-C37
31	A	416	LHG	C26-C27-C28-C29
31	D	407	LHG	C12-C13-C14-C15
31	d	407	LHG	C32-C33-C34-C35
31	L	101	LHG	C17-C18-C19-C20
34	D	402	LMT	C3-C4-C5-C6
35	C	518	DGD	C5B-C6B-C7B-C8B
35	c	519	DGD	C6A-C7A-C8A-C9A
27	C	501	SQD	O49-C7-O47-C45
32	C	502	LMG	O9-C10-O7-C8
23	B	616	CLA	C2-C1-O2A-CGA
32	m	101	LMG	C14-C15-C16-C17
35	C	519	DGD	C9B-CAB-CBB-CCB
23	b	604	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	a	410	SQD	C30-C31-C32-C33
33	B	623	HTG	C2'-C3'-C4'-C5'
34	a	418	LMT	C4-C5-C6-C7
35	c	519	DGD	CBB-CCB-CDB-CEB
23	C	504	CLA	C3-C5-C6-C7
25	D	405	BCR	C23-C24-C25-C26
25	d	404	BCR	C23-C24-C25-C30
27	C	501	SQD	C18-C19-C20-C21
27	D	412	SQD	C24-C23-O48-C46
23	C	507	CLA	C5-C6-C7-C8
31	D	407	LHG	C16-C17-C18-C19
32	C	521	LMG	C17-C18-C19-C20
23	B	604	CLA	C4-C3-C5-C6
23	b	601	CLA	C4-C3-C5-C6
23	c	507	CLA	C4-C3-C5-C6
29	D	406	PL9	C15-C14-C16-C17
23	B	606	CLA	C11-C10-C8-C7
23	b	601	CLA	C2-C3-C5-C6
23	b	606	CLA	C12-C13-C15-C16
23	c	507	CLA	C2-C3-C5-C6
23	d	403	CLA	C12-C13-C15-C16
29	D	406	PL9	C28-C29-C31-C32
29	a	415	PL9	C28-C29-C31-C32
29	d	405	PL9	C13-C14-C16-C17
27	b	620	SQD	O10-C23-O48-C46
23	C	512	CLA	CBA-CGA-O2A-C1
23	d	403	CLA	CBA-CGA-O2A-C1
27	b	620	SQD	C14-C15-C16-C17
34	M	103	LMT	O1'-C1-C2-C3
34	B	630	LMT	O1'-C1-C2-C3
32	B	621	LMG	C28-C29-C30-C31
27	A	411	SQD	C29-C30-C31-C32
31	E	101	LHG	C24-C25-C26-C27
31	d	407	LHG	C30-C31-C32-C33
34	b	627	LMT	C11-C10-C9-C8
31	b	629	LHG	C27-C28-C29-C30
35	c	519	DGD	O6E-C1E-O5D-C6D
23	b	606	CLA	C10-C11-C12-C13
23	b	616	CLA	C10-C11-C12-C13
31	D	408	LHG	C28-C29-C30-C31
34	b	627	LMT	C5-C6-C7-C8
34	t	101	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
35	h	103	DGD	CCA-CDA-CEA-CFA
27	a	410	SQD	C7-C8-C9-C10
32	d	412	LMG	C10-C11-C12-C13
35	C	518	DGD	O6D-C5D-C6D-O5D
34	a	413	LMT	C1-C2-C3-C4
34	M	103	LMT	C2B-C1B-O1B-C4'
23	B	601	CLA	C3-C5-C6-C7
23	c	511	CLA	C3-C5-C6-C7
34	B	628	LMT	C11-C10-C9-C8
34	b	621	LMT	C3-C4-C5-C6
27	C	501	SQD	O6-C44-C45-O47
27	D	412	SQD	O10-C23-O48-C46
27	a	410	SQD	C26-C27-C28-C29
31	d	407	LHG	C34-C35-C36-C37
32	c	522	LMG	C30-C31-C32-C33
23	B	609	CLA	C4-C3-C5-C6
23	B	609	CLA	C2-C3-C5-C6
29	A	413	PL9	C4-C3-C7-C8
29	a	415	PL9	C4-C3-C7-C8
32	C	522	LMG	C17-C18-C19-C20
23	D	404	CLA	C14-C13-C15-C16
23	a	408	CLA	C6-C7-C8-C9
23	b	606	CLA	C6-C7-C8-C9
23	b	606	CLA	C11-C10-C8-C9
23	c	507	CLA	C11-C12-C13-C14
34	t	101	LMT	C2-C3-C4-C5
23	a	404	CLA	C2A-CAA-CBA-CGA
23	b	610	CLA	C2A-CAA-CBA-CGA
35	h	103	DGD	C5B-C6B-C7B-C8B
33	h	101	HTG	O5-C5-C6-O6
23	B	604	CLA	C13-C15-C16-C17
23	b	601	CLA	CBD-CGD-O2D-CED
35	c	520	DGD	C8B-C9B-CAB-CBB
25	y	101	BCR	C21-C22-C23-C24
23	C	512	CLA	O1A-CGA-O2A-C1
23	d	403	CLA	O1A-CGA-O2A-C1
23	C	503	CLA	C1A-C2A-CAA-CBA
23	c	511	CLA	C16-C17-C18-C19
32	c	501	LMG	C16-C17-C18-C19
31	b	629	LHG	C13-C14-C15-C16
23	D	404	CLA	C3-C5-C6-C7
34	B	630	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
23	c	511	CLA	C15-C16-C17-C18
31	a	419	LHG	O6-C4-C5-C6
32	C	502	LMG	C28-C29-C30-C31
33	b	623	HTG	O5-C5-C6-O6
32	D	413	LMG	O6-C5-C6-O5
31	E	101	LHG	C10-C11-C12-C13
35	c	519	DGD	CCA-CDA-CEA-CFA
23	B	615	CLA	C8-C10-C11-C12
23	b	608	CLA	C13-C15-C16-C17
33	b	625	HTG	S1-C1'-C2'-C3'
32	c	501	LMG	C17-C18-C19-C20
23	b	610	CLA	C13-C15-C16-C17
35	c	518	DGD	CAA-CBA-CCA-CDA
32	C	502	LMG	C11-C12-C13-C14
34	D	402	LMT	C4-C5-C6-C7
35	h	103	DGD	CDB-CEB-CFB-CGB
23	B	604	CLA	C16-C17-C18-C20
23	b	610	CLA	C16-C17-C18-C20
27	B	620	SQD	C44-C45-C46-O48
27	a	410	SQD	O6-C44-C45-C46
27	a	412	SQD	O6-C44-C45-C46
32	Z	101	LMG	C7-C8-C9-O8
35	c	518	DGD	O6E-C5E-C6E-O5E
23	B	609	CLA	C13-C15-C16-C17
31	L	101	LHG	C24-C25-C26-C27
31	A	416	LHG	C23-C24-C25-C26
35	c	519	DGD	C2G-C3G-O3G-C1D
35	c	519	DGD	C5D-C6D-O5D-C1E
27	f	101	SQD	C25-C26-C27-C28
32	c	522	LMG	C29-C30-C31-C32
35	C	519	DGD	C2A-C3A-C4A-C5A
35	C	519	DGD	CDA-CEA-CFA-CGA
35	C	519	DGD	C6B-C7B-C8B-C9B
32	d	412	LMG	O6-C5-C6-O5
32	c	522	LMG	O6-C1-O1-C7
29	A	413	PL9	C9-C11-C12-C13
27	A	411	SQD	C17-C18-C19-C20
31	L	101	LHG	C12-C13-C14-C15
34	m	103	LMT	C7-C8-C9-C10
35	c	518	DGD	C5A-C6A-C7A-C8A
26	a	411	GOL	O1-C1-C2-O2
26	a	411	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
31	d	406	LHG	O1-C1-C2-O2
27	b	620	SQD	C31-C32-C33-C34
31	d	406	LHG	C16-C17-C18-C19
32	C	502	LMG	C35-C36-C37-C38
34	B	628	LMT	C4-C5-C6-C7
33	B	625	HTG	O5-C5-C6-O6
35	C	518	DGD	O6E-C5E-C6E-O5E
23	C	507	CLA	C4-C3-C5-C6
23	b	615	CLA	C4-C3-C5-C6
23	C	511	CLA	C13-C15-C16-C17
23	b	611	CLA	C8-C10-C11-C12
31	d	406	LHG	C29-C30-C31-C32
33	B	623	HTG	C4'-C5'-C6'-C7'
23	D	403	CLA	C15-C16-C17-C18
23	b	601	CLA	C2-C1-O2A-CGA
34	M	103	LMT	O5B-C1B-O1B-C4'
35	C	520	DGD	O6E-C5E-C6E-O5E
27	a	410	SQD	C33-C34-C35-C36
23	b	613	CLA	O1D-CGD-O2D-CED
27	a	412	SQD	C19-C20-C21-C22
23	a	408	CLA	CBA-CGA-O2A-C1
23	c	513	CLA	CBA-CGA-O2A-C1
23	c	514	CLA	CBA-CGA-O2A-C1
31	b	629	LHG	O6-C4-C5-O7
35	C	519	DGD	C3A-C4A-C5A-C6A
35	C	520	DGD	C4B-C5B-C6B-C7B
35	c	518	DGD	O6D-C5D-C6D-O5D
23	c	514	CLA	C15-C16-C17-C18
27	b	620	SQD	C13-C14-C15-C16
23	c	513	CLA	O1A-CGA-O2A-C1
32	C	521	LMG	C12-C13-C14-C15
34	M	101	LMT	C7-C8-C9-C10
23	a	405	CLA	C13-C15-C16-C17
23	c	510	CLA	C8-C10-C11-C12
27	a	410	SQD	O6-C44-C45-O47
27	b	620	SQD	O47-C45-C46-O48
27	A	411	SQD	C30-C31-C32-C33
27	b	620	SQD	C25-C26-C27-C28
33	B	625	HTG	C4'-C5'-C6'-C7'
23	a	408	CLA	O1A-CGA-O2A-C1
27	A	411	SQD	C16-C17-C18-C19
31	A	416	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
32	c	521	LMG	C31-C32-C33-C34
23	A	406	CLA	C12-C13-C15-C16
23	C	504	CLA	C12-C13-C15-C16
23	C	512	CLA	C12-C13-C15-C16
23	C	515	CLA	C12-C13-C15-C16
23	D	403	CLA	C12-C13-C15-C16
23	D	404	CLA	C12-C13-C15-C16
23	b	614	CLA	C6-C7-C8-C10
23	c	507	CLA	C11-C12-C13-C15
23	d	402	CLA	C11-C12-C13-C15
35	h	103	DGD	O2G-C1B-C2B-C3B
32	D	413	LMG	C30-C31-C32-C33
23	A	406	CLA	C14-C13-C15-C16
23	B	614	CLA	C14-C13-C15-C16
23	C	512	CLA	C14-C13-C15-C16
23	D	404	CLA	C11-C10-C8-C9
23	a	408	CLA	C11-C10-C8-C9
23	a	405	CLA	CBD-CGD-O2D-CED
23	b	601	CLA	CBA-CGA-O2A-C1
32	c	522	LMG	C29-C28-O8-C9
23	D	403	CLA	C10-C11-C12-C13
35	c	519	DGD	CBA-CCA-CDA-CEA
35	c	520	DGD	CBA-CCA-CDA-CEA
34	b	621	LMT	C3'-C4'-O1B-C1B
23	B	604	CLA	C16-C17-C18-C19
33	b	622	HTG	S1-C1'-C2'-C3'
23	b	601	CLA	C3-C5-C6-C7
32	c	501	LMG	C29-C30-C31-C32
27	a	412	SQD	C24-C23-O48-C46
32	C	502	LMG	C13-C14-C15-C16
35	C	518	DGD	C6B-C7B-C8B-C9B
29	a	415	PL9	C2-C3-C7-C8
34	b	627	LMT	C4'-C5'-C6'-O6'
32	z	101	LMG	C19-C20-C21-C22
34	C	526	LMT	C3-C4-C5-C6
23	b	606	CLA	C15-C16-C17-C18
23	b	611	CLA	C10-C11-C12-C13
31	b	629	LHG	O6-C4-C5-C6
23	C	507	CLA	C2-C3-C5-C6
23	b	615	CLA	C2-C3-C5-C6
29	A	413	PL9	C12-C11-C9-C8
23	c	503	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
35	C	519	DGD	C5A-C6A-C7A-C8A
35	c	518	DGD	C2A-C1A-O1G-C1G
35	c	520	DGD	C2A-C1A-O1G-C1G
23	C	508	CLA	C3A-C2A-CAA-CBA
23	b	612	CLA	C8-C10-C11-C12
34	b	627	LMT	C2-C1-O1'-C1'
34	e	101	LMT	C2-C1-O1'-C1'
34	t	101	LMT	C2-C1-O1'-C1'
35	H	102	DGD	CCA-CDA-CEA-CFA
23	c	511	CLA	C10-C11-C12-C13
34	b	621	LMT	C6-C7-C8-C9
32	Z	101	LMG	O6-C5-C6-O5
27	a	412	SQD	C18-C19-C20-C21
27	A	411	SQD	O6-C44-C45-C46
27	f	101	SQD	O6-C44-C45-C46
31	E	101	LHG	C4-C5-C6-O8
32	C	522	LMG	C7-C8-C9-O8
23	c	513	CLA	C8-C10-C11-C12
23	C	515	CLA	C4-C3-C5-C6
23	a	404	CLA	C16-C17-C18-C19
31	D	407	LHG	C11-C12-C13-C14
32	C	521	LMG	C36-C37-C38-C39
32	d	412	LMG	C38-C39-C40-C41
27	B	620	SQD	C24-C25-C26-C27
23	b	615	CLA	C15-C16-C17-C18
32	z	101	LMG	O6-C5-C6-O5
35	C	520	DGD	C2A-C3A-C4A-C5A
33	b	625	HTG	C4-C5-C6-O6
26	O	302	GOL	O1-C1-C2-O2
26	b	624	GOL	O2-C2-C3-O3
31	a	419	LHG	O6-C4-C5-O7
35	C	518	DGD	C4D-C5D-C6D-O5D
23	b	601	CLA	O1A-CGA-O2A-C1
27	a	412	SQD	C26-C27-C28-C29
23	C	509	CLA	C5-C6-C7-C8
32	c	522	LMG	O10-C28-O8-C9
32	B	621	LMG	C34-C35-C36-C37
33	b	625	HTG	C4'-C5'-C6'-C7'
31	D	408	LHG	C9-C10-C11-C12
31	E	101	LHG	O7-C5-C6-O8
32	C	502	LMG	O1-C7-C8-O7
23	a	404	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
23	b	614	CLA	C16-C17-C18-C19
27	D	412	SQD	O5-C1-O6-C44
27	B	620	SQD	C19-C20-C21-C22
23	C	508	CLA	C2-C1-O2A-CGA
23	b	613	CLA	C2-C1-O2A-CGA
35	H	102	DGD	C9A-CAA-CBA-CCA
23	C	506	CLA	C14-C13-C15-C16
23	C	508	CLA	C11-C10-C8-C9
23	C	515	CLA	C11-C10-C8-C9
23	b	614	CLA	C6-C7-C8-C9
23	b	616	CLA	C11-C12-C13-C14
31	d	408	LHG	C11-C10-C9-C8
32	C	522	LMG	C32-C33-C34-C35
23	A	408	CLA	C13-C15-C16-C17
31	D	408	LHG	C2-C3-O3-P
32	C	521	LMG	C13-C14-C15-C16
32	m	101	LMG	C33-C34-C35-C36
23	B	614	CLA	C16-C17-C18-C20
25	b	617	BCR	C1-C6-C7-C8
25	b	617	BCR	C5-C6-C7-C8
25	d	404	BCR	C23-C24-C25-C26
35	C	519	DGD	C9A-CAA-CBA-CCA
32	C	522	LMG	C33-C34-C35-C36
25	D	405	BCR	C7-C8-C9-C10
25	d	404	BCR	C7-C8-C9-C10
25	k	101	BCR	C7-C8-C9-C10
25	t	102	BCR	C11-C12-C13-C14
23	b	613	CLA	C15-C16-C17-C18
32	c	501	LMG	C32-C33-C34-C35
32	c	501	LMG	O9-C10-O7-C8
32	m	101	LMG	C11-C10-O7-C8
31	a	419	LHG	C26-C27-C28-C29
27	b	620	SQD	C18-C19-C20-C21
23	c	514	CLA	O1A-CGA-O2A-C1
23	C	515	CLA	O1D-CGD-O2D-CED
23	b	602	CLA	C10-C11-C12-C13
32	m	101	LMG	C29-C30-C31-C32
23	B	614	CLA	C12-C13-C15-C16
23	C	506	CLA	C12-C13-C15-C16
23	C	515	CLA	C11-C10-C8-C7
23	D	404	CLA	C11-C10-C8-C7
23	a	406	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
23	a	408	CLA	C11-C10-C8-C7
23	c	506	CLA	C12-C13-C15-C16
23	c	511	CLA	C11-C10-C8-C7
31	d	407	LHG	C13-C14-C15-C16
34	m	103	LMT	C6-C7-C8-C9
35	c	518	DGD	C4D-C5D-C6D-O5D
31	b	629	LHG	C9-C10-C11-C12
31	d	407	LHG	C31-C32-C33-C34
27	C	501	SQD	C14-C15-C16-C17
23	B	606	CLA	C8-C10-C11-C12
23	C	507	CLA	C10-C11-C12-C13
23	b	601	CLA	C8-C10-C11-C12
35	H	102	DGD	C7A-C8A-C9A-CAA
23	B	610	CLA	CAD-CBD-CGD-O2D
23	C	511	CLA	CAD-CBD-CGD-O2D
23	b	610	CLA	CAD-CBD-CGD-O2D
23	b	614	CLA	CAD-CBD-CGD-O2D
23	c	503	CLA	CAD-CBD-CGD-O2D
23	d	403	CLA	CAD-CBD-CGD-O2D
24	A	407	PHO	CAD-CBD-CGD-O2D
24	A	415	PHO	CAD-CBD-CGD-O2D
24	a	407	PHO	CAD-CBD-CGD-O2D
27	B	620	SQD	C46-C45-O47-C7
27	b	620	SQD	C46-C45-O47-C7
27	A	411	SQD	O49-C7-O47-C45
35	H	102	DGD	CBB-CCB-CDB-CEB
35	h	103	DGD	C7B-C8B-C9B-CAB
23	c	514	CLA	C16-C17-C18-C20
27	b	620	SQD	O5-C1-O6-C44
31	d	408	LHG	C2-C3-O3-P
32	C	502	LMG	O1-C7-C8-C9
23	A	408	CLA	C8-C10-C11-C12
23	b	601	CLA	CAA-CBA-CGA-O2A
35	H	102	DGD	O2G-C1B-C2B-C3B
23	a	405	CLA	C2C-C3C-CAC-CBC
33	B	622	HTG	C2'-C3'-C4'-C5'
35	c	519	DGD	CDA-CEA-CFA-CGA
27	a	410	SQD	C11-C12-C13-C14
32	z	101	LMG	C10-C11-C12-C13
35	C	519	DGD	C6A-C7A-C8A-C9A
32	m	101	LMG	O9-C10-O7-C8
23	B	601	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	B	601	CLA	CHA-CBD-CGD-O2D
23	C	504	CLA	CHA-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O1D
32	c	522	LMG	C4-C5-C6-O5
23	C	511	CLA	C3-C5-C6-C7
27	a	412	SQD	O10-C23-O48-C46
35	c	520	DGD	O1A-C1A-O1G-C1G
35	c	519	DGD	C2E-C1E-O5D-C6D
29	A	413	PL9	C2-C3-C7-C8
32	Z	101	LMG	O7-C8-C9-O8
32	c	501	LMG	O1-C7-C8-O7
32	D	413	LMG	C38-C39-C40-C41
35	C	518	DGD	C7A-C8A-C9A-CAA
35	C	520	DGD	C9A-CAA-CBA-CCA
23	C	515	CLA	C16-C17-C18-C19
31	A	416	LHG	O1-C1-C2-O2
34	B	628	LMT	C6-C7-C8-C9
32	c	501	LMG	C11-C10-O7-C8
33	B	625	HTG	C2'-C3'-C4'-C5'
35	C	518	DGD	CDB-CEB-CFB-CGB
23	c	506	CLA	C14-C13-C15-C16
35	c	518	DGD	O1A-C1A-O1G-C1G
33	b	623	HTG	C3'-C4'-C5'-C6'
34	b	627	LMT	C7-C8-C9-C10
23	b	603	CLA	C13-C15-C16-C17
31	b	629	LHG	C12-C13-C14-C15
32	C	502	LMG	O8-C28-C29-C30
32	C	502	LMG	C36-C37-C38-C39
25	Y	101	BCR	C37-C22-C23-C24
25	b	619	BCR	C37-C22-C23-C24
23	a	406	CLA	C1A-C2A-CAA-CBA
23	c	508	CLA	C1A-C2A-CAA-CBA
23	A	408	CLA	C16-C17-C18-C19
27	A	411	SQD	C8-C7-O47-C45
35	H	102	DGD	CBA-CCA-CDA-CEA
23	a	404	CLA	C15-C16-C17-C18
31	E	101	LHG	C4-O6-P-O3
32	B	621	LMG	C20-C21-C22-C23
23	b	604	CLA	O1D-CGD-O2D-CED
27	B	620	SQD	C11-C12-C13-C14
31	a	419	LHG	C19-C20-C21-C22
23	b	616	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	d	408	LHG	C9-C10-C11-C12
29	A	413	PL9	C3-C7-C8-C9
31	D	407	LHG	C3-O3-P-O4
31	a	419	LHG	C4-O6-P-O4
31	d	406	LHG	C3-O3-P-O4
31	d	406	LHG	C3-O3-P-O5
23	B	603	CLA	C16-C17-C18-C20
23	B	615	CLA	C16-C17-C18-C20
23	c	513	CLA	C16-C17-C18-C19
23	B	604	CLA	C2C-C3C-CAC-CBC
32	c	501	LMG	C4-C5-C6-O5
31	d	407	LHG	C24-C23-O8-C6
32	C	522	LMG	C37-C38-C39-C40
27	a	412	SQD	C31-C32-C33-C34
23	B	601	CLA	CAD-CBD-CGD-O1D
23	C	504	CLA	CAD-CBD-CGD-O1D
23	C	508	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	504	CLA	CAD-CBD-CGD-O1D
23	c	508	CLA	CAD-CBD-CGD-O1D
27	B	620	SQD	C5-C6-S-O7
31	d	407	LHG	C29-C30-C31-C32
31	A	416	LHG	C1-C2-C3-O3
23	B	616	CLA	C12-C13-C15-C16
23	b	601	CLA	C6-C7-C8-C10
23	b	610	CLA	C12-C13-C15-C16
23	b	615	CLA	C12-C13-C15-C16
23	c	508	CLA	C6-C7-C8-C10
23	c	510	CLA	C6-C7-C8-C10
23	c	510	CLA	C11-C12-C13-C15
31	L	101	LHG	C23-C24-C25-C26
33	B	622	HTG	C2-C1-S1-C1'
31	D	407	LHG	C28-C29-C30-C31
23	B	610	CLA	C15-C16-C17-C18
35	h	103	DGD	CDA-CEA-CFA-CGA
23	D	403	CLA	C13-C15-C16-C17
35	c	520	DGD	C2B-C3B-C4B-C5B
32	B	621	LMG	C15-C16-C17-C18
34	b	627	LMT	O5'-C5'-C6'-O6'
27	b	620	SQD	C44-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
32	c	501	LMG	O1-C7-C8-C9
27	B	620	SQD	O47-C45-C46-O48
27	f	101	SQD	O6-C44-C45-O47
31	a	419	LHG	O7-C5-C6-O8
32	C	522	LMG	O7-C8-C9-O8
27	a	412	SQD	C34-C35-C36-C37
31	d	408	LHG	C24-C23-O8-C6
27	b	620	SQD	C15-C16-C17-C18
34	a	413	LMT	C6-C7-C8-C9
35	c	520	DGD	CDB-CEB-CFB-CGB
35	C	519	DGD	C2G-C3G-O3G-C1D
23	B	606	CLA	C16-C17-C18-C20
23	B	614	CLA	C16-C17-C18-C19
23	b	614	CLA	C16-C17-C18-C20
23	B	607	CLA	C3-C5-C6-C7
31	d	407	LHG	O10-C23-O8-C6
31	d	408	LHG	O10-C23-O8-C6
32	C	502	LMG	C21-C22-C23-C24
35	C	520	DGD	C8A-C9A-CAA-CBA
29	D	406	PL9	C43-C44-C46-C47
23	B	601	CLA	CAA-CBA-CGA-O2A
23	A	405	CLA	C2C-C3C-CAC-CBC
27	f	101	SQD	C29-C30-C31-C32
23	D	404	CLA	C8-C10-C11-C12
31	D	408	LHG	C30-C31-C32-C33
23	C	515	CLA	C16-C17-C18-C20
23	b	604	CLA	C16-C17-C18-C20
35	C	520	DGD	C5B-C6B-C7B-C8B
27	a	412	SQD	C24-C25-C26-C27
31	d	408	LHG	C10-C11-C12-C13
23	C	513	CLA	O1A-CGA-O2A-C1
31	A	416	LHG	O10-C23-O8-C6
25	H	101	BCR	C9-C10-C11-C12
25	Y	101	BCR	C21-C22-C23-C24
25	b	619	BCR	C21-C22-C23-C24
31	d	408	LHG	C31-C32-C33-C34
34	a	418	LMT	C6-C7-C8-C9
27	a	410	SQD	C19-C20-C21-C22
29	D	406	PL9	C45-C44-C46-C47
31	b	629	LHG	C10-C11-C12-C13
34	D	402	LMT	C7-C8-C9-C10
31	d	407	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
27	a	410	SQD	C11-C10-C9-C8
23	B	605	CLA	C10-C11-C12-C13
23	B	613	CLA	C2-C1-O2A-CGA
23	C	514	CLA	C2-C1-O2A-CGA
23	C	515	CLA	C2-C1-O2A-CGA
23	b	608	CLA	C2-C1-O2A-CGA
31	A	416	LHG	C24-C23-O8-C6
35	c	519	DGD	C1A-C2A-C3A-C4A
27	B	620	SQD	C9-C10-C11-C12
25	C	516	BCR	C1-C6-C7-C8
25	a	409	BCR	C1-C6-C7-C8
25	y	101	BCR	C23-C24-C25-C26
25	y	101	BCR	C23-C24-C25-C30
23	B	604	CLA	C2-C3-C5-C6
29	a	415	PL9	C43-C44-C46-C47
23	A	406	CLA	C16-C17-C18-C19
34	m	103	LMT	O5'-C1'-O1'-C1
35	C	520	DGD	C1B-C2B-C3B-C4B
34	m	103	LMT	C2'-C1'-O1'-C1
35	C	518	DGD	C3B-C4B-C5B-C6B
31	d	406	LHG	C4-O6-P-O3
27	B	620	SQD	C11-C10-C9-C8
27	C	501	SQD	C12-C13-C14-C15
34	m	103	LMT	C4'-C5'-C6'-O6'
35	c	520	DGD	O6D-C5D-C6D-O5D
34	b	621	LMT	C4-C5-C6-C7
23	b	614	CLA	C12-C13-C15-C16
23	b	616	CLA	C2-C3-C5-C6
23	b	616	CLA	C11-C12-C13-C15
23	c	515	CLA	C12-C13-C15-C16
23	B	616	CLA	C14-C13-C15-C16
23	a	406	CLA	C11-C12-C13-C14
23	b	610	CLA	C14-C13-C15-C16
23	b	615	CLA	C14-C13-C15-C16
23	c	510	CLA	C11-C12-C13-C14
23	d	402	CLA	C11-C12-C13-C14
27	b	620	SQD	C35-C36-C37-C38
27	a	412	SQD	C27-C28-C29-C30
23	c	513	CLA	C16-C17-C18-C20
23	c	514	CLA	C16-C17-C18-C19
35	C	518	DGD	CCB-CDB-CEB-CFB
23	a	405	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
23	A	404	CLA	C13-C15-C16-C17
33	B	622	HTG	C3'-C4'-C5'-C6'
31	D	407	LHG	C10-C11-C12-C13
32	C	522	LMG	C4-C5-C6-O5
23	B	603	CLA	C16-C17-C18-C19
27	b	620	SQD	C17-C18-C19-C20
23	b	601	CLA	O1D-CGD-O2D-CED
31	d	408	LHG	C35-C36-C37-C38
23	C	513	CLA	CBA-CGA-O2A-C1
23	B	614	CLA	C2A-CAA-CBA-CGA
23	c	509	CLA	C5-C6-C7-C8
32	C	521	LMG	C32-C33-C34-C35
23	b	612	CLA	C10-C11-C12-C13
24	a	407	PHO	C8-C10-C11-C12
31	L	101	LHG	C11-C12-C13-C14
32	C	502	LMG	C32-C33-C34-C35
35	C	518	DGD	C2A-C3A-C4A-C5A
23	C	512	CLA	C4-C3-C5-C6
23	a	404	CLA	C2C-C3C-CAC-CBC
32	m	101	LMG	C30-C31-C32-C33
23	C	512	CLA	C2-C3-C5-C6
33	B	622	HTG	C1'-C2'-C3'-C4'
27	a	410	SQD	C31-C32-C33-C34
23	B	610	CLA	C13-C15-C16-C17
23	a	408	CLA	C2-C1-O2A-CGA
23	b	614	CLA	C2-C1-O2A-CGA
23	c	513	CLA	C2-C1-O2A-CGA
23	d	402	CLA	C2-C1-O2A-CGA
23	c	510	CLA	C13-C15-C16-C17
23	B	615	CLA	C16-C17-C18-C19
27	b	620	SQD	C26-C27-C28-C29
31	d	407	LHG	C9-C10-C11-C12
31	d	407	LHG	C26-C27-C28-C29
35	c	518	DGD	CCA-CDA-CEA-CFA
23	C	503	CLA	C2A-CAA-CBA-CGA
27	D	412	SQD	O47-C45-C46-O48
35	h	103	DGD	C8B-C9B-CAB-CBB
38	E	103	HEC	CAD-CBD-CGD-O1D
31	L	101	LHG	C32-C33-C34-C35
35	C	519	DGD	C5B-C6B-C7B-C8B
29	d	405	PL9	C45-C44-C46-C47
35	c	518	DGD	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
23	B	613	CLA	C11-C12-C13-C14
23	B	614	CLA	C6-C7-C8-C9
23	C	514	CLA	C11-C10-C8-C9
23	a	406	CLA	C14-C13-C15-C16
23	b	609	CLA	C6-C7-C8-C9
23	c	510	CLA	C6-C7-C8-C9
23	c	515	CLA	C6-C7-C8-C9
35	C	520	DGD	CBA-CCA-CDA-CEA
23	A	406	CLA	C16-C17-C18-C20
23	b	606	CLA	C16-C17-C18-C19
23	B	602	CLA	O2A-C1-C2-C3
27	A	411	SQD	C15-C16-C17-C18
31	d	406	LHG	C27-C28-C29-C30
27	a	412	SQD	C30-C31-C32-C33
32	c	501	LMG	C18-C19-C20-C21
34	t	101	LMT	C4-C5-C6-C7
23	B	611	CLA	C11-C12-C13-C15
23	B	613	CLA	C12-C13-C15-C16
23	B	615	CLA	C11-C12-C13-C15
23	C	508	CLA	C11-C10-C8-C7
23	b	604	CLA	C12-C13-C15-C16
23	c	510	CLA	C12-C13-C15-C16
23	c	511	CLA	C6-C7-C8-C10
23	c	512	CLA	C12-C13-C15-C16
31	D	407	LHG	C4-O6-P-O3
34	E	102	LMT	O1'-C1-C2-C3
34	a	413	LMT	C4'-C5'-C6'-O6'
23	A	404	CLA	C2A-CAA-CBA-CGA
23	B	603	CLA	C13-C15-C16-C17
23	C	510	CLA	C13-C15-C16-C17
23	C	512	CLA	C8-C10-C11-C12
38	v	202	HEC	CAD-CBD-CGD-O1D
34	e	101	LMT	C4-C5-C6-C7
27	D	412	SQD	C33-C34-C35-C36
27	f	101	SQD	C28-C29-C30-C31
29	D	406	PL9	C35-C34-C36-C37
29	a	415	PL9	C45-C44-C46-C47
23	b	609	CLA	C2-C3-C5-C6
38	E	103	HEC	CAD-CBD-CGD-O2D
23	C	515	CLA	C10-C11-C12-C13
23	B	604	CLA	C4C-C3C-CAC-CBC
31	b	629	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
35	c	518	DGD	C5B-C6B-C7B-C8B
23	c	508	CLA	C16-C17-C18-C19
23	a	405	CLA	O1D-CGD-O2D-CED
23	C	511	CLA	C2-C1-O2A-CGA
23	c	514	CLA	C2-C1-O2A-CGA
23	c	515	CLA	C2-C1-O2A-CGA
32	C	502	LMG	C16-C17-C18-C19
24	A	415	PHO	C6-C7-C8-C9
38	v	202	HEC	CAD-CBD-CGD-O2D
35	c	519	DGD	CCB-CDB-CEB-CFB
27	B	620	SQD	C7-C8-C9-C10
31	D	407	LHG	C34-C35-C36-C37
25	C	516	BCR	C5-C6-C7-C8
25	C	517	BCR	C1-C6-C7-C8
25	C	517	BCR	C5-C6-C7-C8
25	D	405	BCR	C1-C6-C7-C8
25	K	101	BCR	C1-C6-C7-C8
25	Y	101	BCR	C23-C24-C25-C26
25	Y	101	BCR	C23-C24-C25-C30
25	a	409	BCR	C5-C6-C7-C8
32	B	621	LMG	C37-C38-C39-C40
34	b	627	LMT	C1-C2-C3-C4
34	e	101	LMT	C2B-C1B-O1B-C4'
23	C	508	CLA	C4-C3-C5-C6
23	b	604	CLA	C4-C3-C5-C6
29	A	413	PL9	C45-C44-C46-C47
27	a	410	SQD	C27-C28-C29-C30
34	M	101	LMT	C2-C3-C4-C5
32	c	501	LMG	C19-C20-C21-C22
31	A	416	LHG	C30-C31-C32-C33
35	c	520	DGD	O6E-C5E-C6E-O5E
35	c	518	DGD	O6E-C1E-O5D-C6D
35	c	520	DGD	CCB-CDB-CEB-CFB
23	C	514	CLA	C11-C10-C8-C7
23	C	515	CLA	C2-C3-C5-C6
38	V	201	HEC	CAD-CBD-CGD-O1D
35	H	102	DGD	CAA-CBA-CCA-CDA
33	c	523	HTG	S1-C1'-C2'-C3'
26	A	410	GOL	O2-C2-C3-O3
26	o	302	GOL	O2-C2-C3-O3
38	V	201	HEC	CAD-CBD-CGD-O2D
27	f	101	SQD	O47-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
23	B	613	CLA	CAA-CBA-CGA-O2A
23	B	612	CLA	C10-C11-C12-C13
23	B	606	CLA	C16-C17-C18-C19
27	C	501	SQD	C10-C11-C12-C13
32	d	412	LMG	C29-C30-C31-C32
33	B	623	HTG	C2'-C1'-S1-C1
23	C	512	CLA	CAA-CBA-CGA-O2A
32	c	521	LMG	C10-C11-C12-C13
32	d	412	LMG	C12-C13-C14-C15
34	E	102	LMT	C6-C7-C8-C9
23	b	604	CLA	C16-C17-C18-C19
33	C	523	HTG	C4-C5-C6-O6
23	b	601	CLA	C6-C7-C8-C9
23	b	604	CLA	C14-C13-C15-C16
23	b	610	CLA	C11-C12-C13-C14
23	c	511	CLA	C6-C7-C8-C9
27	b	620	SQD	C12-C13-C14-C15
31	L	101	LHG	C29-C30-C31-C32
23	B	609	CLA	C3A-C2A-CAA-CBA
38	e	102	HEC	C2A-CAA-CBA-CGA
32	Z	101	LMG	O7-C10-C11-C12
34	E	102	LMT	C7-C8-C9-C10
23	B	604	CLA	CAD-CBD-CGD-O2D
23	B	612	CLA	CAD-CBD-CGD-O2D
23	C	507	CLA	CAD-CBD-CGD-O2D
23	C	514	CLA	CAD-CBD-CGD-O2D
23	b	604	CLA	CAD-CBD-CGD-O2D
23	b	607	CLA	CAD-CBD-CGD-O2D
23	b	616	CLA	CAD-CBD-CGD-O2D
23	c	507	CLA	CAD-CBD-CGD-O2D
23	c	514	CLA	CAD-CBD-CGD-O2D
24	a	417	PHO	CAD-CBD-CGD-O2D
23	a	405	CLA	C16-C17-C18-C20
34	M	103	LMT	C6-C7-C8-C9
23	B	608	CLA	C2-C1-O2A-CGA
23	C	514	CLA	CAA-CBA-CGA-O2A
27	f	101	SQD	O48-C23-C24-C25
31	b	629	LHG	O7-C7-C8-C9
31	d	406	LHG	O8-C23-C24-C25
35	c	518	DGD	O2G-C1B-C2B-C3B
32	z	101	LMG	C15-C16-C17-C18
35	h	103	DGD	C6A-C7A-C8A-C9A

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Mol	Chain	Res	Type	Atoms
23	c	508	CLA	C4-C3-C5-C6
29	A	413	PL9	C43-C44-C46-C47
32	B	621	LMG	C17-C18-C19-C20
35	c	519	DGD	C5B-C6B-C7B-C8B
29	d	405	PL9	C34-C36-C37-C38
23	b	610	CLA	C15-C16-C17-C18
24	A	415	PHO	C2C-C3C-CAC-CBC
24	a	417	PHO	C2C-C3C-CAC-CBC
35	h	103	DGD	O1B-C1B-C2B-C3B
27	A	411	SQD	C24-C25-C26-C27
32	D	413	LMG	O7-C10-C11-C12
23	b	605	CLA	C13-C15-C16-C17
23	C	511	CLA	O2A-C1-C2-C3
23	C	515	CLA	O2A-C1-C2-C3
23	b	613	CLA	O2A-C1-C2-C3
24	A	407	PHO	O2A-C1-C2-C3
24	a	407	PHO	O2A-C1-C2-C3
32	m	101	LMG	C37-C38-C39-C40
27	b	620	SQD	C11-C10-C9-C8
31	d	406	LHG	C26-C27-C28-C29
34	a	413	LMT	C9-C10-C11-C12
31	A	416	LHG	O2-C2-C3-O3
23	A	405	CLA	CHA-CBD-CGD-O1D
23	A	405	CLA	CHA-CBD-CGD-O2D
23	C	504	CLA	CHA-CBD-CGD-O2D
23	C	509	CLA	CHA-CBD-CGD-O1D
23	C	509	CLA	CHA-CBD-CGD-O2D
23	a	405	CLA	CHA-CBD-CGD-O2D
23	b	601	CLA	CHA-CBD-CGD-O1D
23	b	606	CLA	CHA-CBD-CGD-O1D
23	b	606	CLA	CHA-CBD-CGD-O2D
23	c	504	CLA	CHA-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O2D
23	c	511	CLA	CHA-CBD-CGD-O1D
23	c	512	CLA	CHA-CBD-CGD-O2D
23	c	504	CLA	C3-C5-C6-C7
23	c	514	CLA	CAA-CBA-CGA-O2A
27	b	620	SQD	O48-C23-C24-C25
31	A	416	LHG	O8-C23-C24-C25
31	D	407	LHG	C17-C18-C19-C20
38	e	102	HEC	CAD-CBD-CGD-O1D
23	b	613	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
31	D	408	LHG	O8-C23-C24-C25
31	L	101	LHG	O7-C7-C8-C9
32	C	502	LMG	O7-C10-C11-C12
38	E	103	HEC	CAA-CBA-CGA-O1A
34	a	413	LMT	C2-C3-C4-C5
35	c	518	DGD	O1G-C1A-C2A-C3A
27	b	620	SQD	C27-C28-C29-C30
32	c	501	LMG	C37-C38-C39-C40
38	e	102	HEC	CAD-CBD-CGD-O2D
32	B	621	LMG	C29-C30-C31-C32
23	B	601	CLA	C6-C7-C8-C10
23	b	611	CLA	C6-C7-C8-C10
34	D	402	LMT	C1-C2-C3-C4
32	c	521	LMG	O7-C10-C11-C12
27	f	101	SQD	C33-C34-C35-C36
31	A	416	LHG	C29-C30-C31-C32
23	B	601	CLA	C6-C7-C8-C9
23	B	610	CLA	C14-C13-C15-C16
23	c	515	CLA	C14-C13-C15-C16
27	B	620	SQD	C33-C34-C35-C36
35	h	103	DGD	C6B-C7B-C8B-C9B
23	B	613	CLA	C13-C15-C16-C17
27	B	620	SQD	C5-C6-S-O8
23	a	405	CLA	C16-C17-C18-C19
35	c	519	DGD	C2B-C3B-C4B-C5B
34	M	103	LMT	C3-C4-C5-C6
27	f	101	SQD	O10-C23-C24-C25
23	b	612	CLA	CAA-CBA-CGA-O2A
23	c	512	CLA	CAA-CBA-CGA-O2A
23	C	505	CLA	C5-C6-C7-C8
23	b	602	CLA	C13-C15-C16-C17
26	b	624	GOL	O1-C1-C2-C3
29	d	405	PL9	C43-C44-C46-C47
34	C	526	LMT	C4-C5-C6-C7
35	c	518	DGD	O1B-C1B-C2B-C3B
31	A	416	LHG	C11-C10-C9-C8
31	L	101	LHG	C18-C19-C20-C21
32	B	621	LMG	C14-C15-C16-C17
23	C	508	CLA	C1A-C2A-CAA-CBA
23	a	405	CLA	C1A-C2A-CAA-CBA
31	A	416	LHG	C33-C34-C35-C36
31	a	419	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
23	C	514	CLA	CAA-CBA-CGA-O1A
23	a	408	CLA	C15-C16-C17-C18
23	C	512	CLA	CAA-CBA-CGA-O1A
31	d	407	LHG	C14-C15-C16-C17
27	D	412	SQD	C44-C45-C46-O48
35	H	102	DGD	O1G-C1G-C2G-C3G
23	c	505	CLA	C15-C16-C17-C18
31	b	629	LHG	O9-C7-C8-C9
23	c	508	CLA	C13-C15-C16-C17
27	f	101	SQD	C23-C24-C25-C26
23	B	613	CLA	CAA-CBA-CGA-O1A
31	d	406	LHG	O10-C23-C24-C25
23	b	602	CLA	C8-C10-C11-C12
32	c	501	LMG	C36-C37-C38-C39
34	m	103	LMT	O1'-C1-C2-C3
31	D	407	LHG	C4-O6-P-O5
31	b	629	LHG	C4-O6-P-O4
31	d	406	LHG	C4-O6-P-O4
31	d	407	LHG	C4-O6-P-O5
23	c	508	CLA	C16-C17-C18-C20
23	c	514	CLA	CAA-CBA-CGA-O1A
31	A	416	LHG	O10-C23-C24-C25
32	D	413	LMG	O9-C10-C11-C12
32	c	521	LMG	O9-C10-C11-C12
38	E	103	HEC	CAA-CBA-CGA-O2A
25	D	405	BCR	C5-C6-C7-C8
25	t	102	BCR	C1-C6-C7-C8
25	t	102	BCR	C5-C6-C7-C8
23	A	405	CLA	C4C-C3C-CAC-CBC
35	C	518	DGD	C2B-C3B-C4B-C5B
23	a	404	CLA	C4C-C3C-CAC-CBC
32	Z	101	LMG	O9-C10-C11-C12
35	c	518	DGD	O1A-C1A-C2A-C3A
35	H	102	DGD	O1B-C1B-C2B-C3B
23	b	609	CLA	C4-C3-C5-C6
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	C	506	CLA	CAD-CBD-CGD-O1D
23	a	405	CLA	CAD-CBD-CGD-O1D
23	c	506	CLA	CAD-CBD-CGD-O1D
31	D	408	LHG	O10-C23-C24-C25

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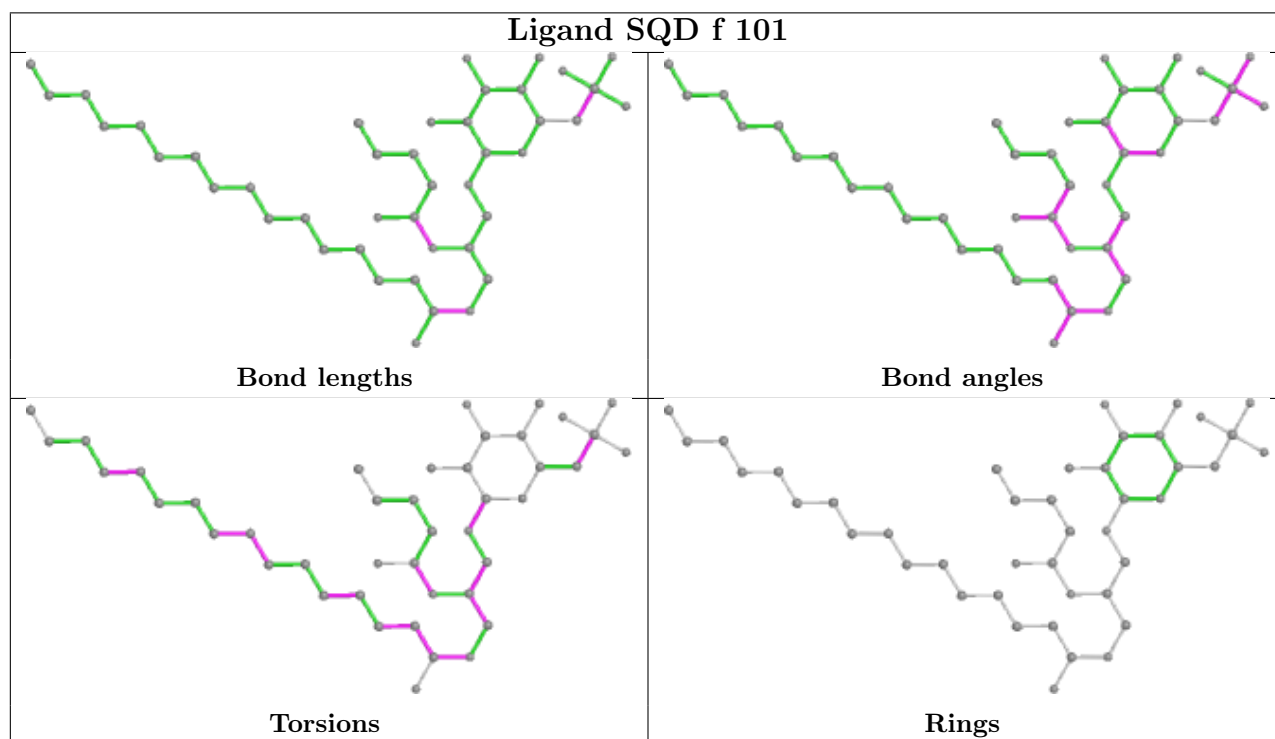
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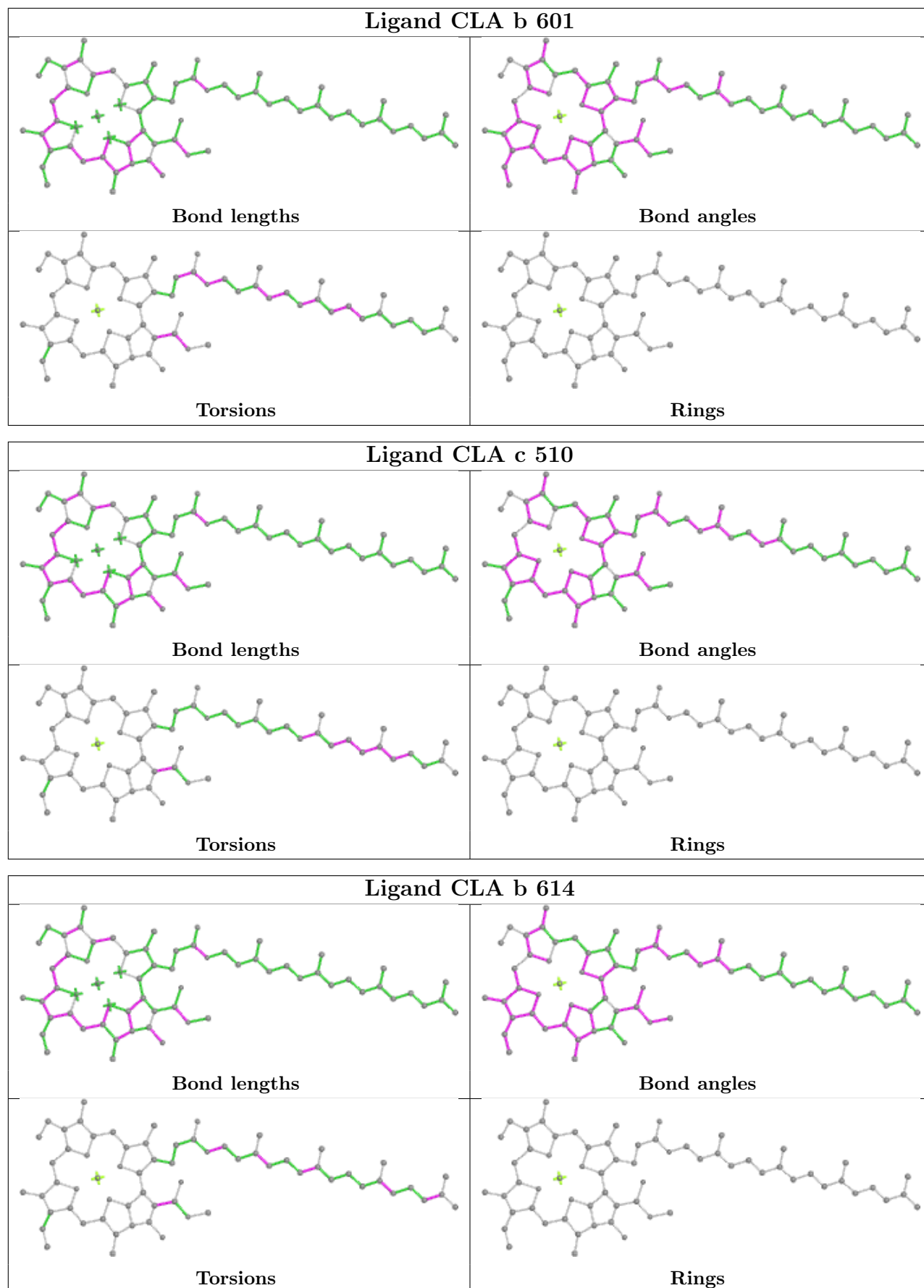
Mol	Chain	Res	Type	Atoms
23	b	609	CLA	C14-C13-C15-C16
23	b	611	CLA	C6-C7-C8-C9
23	b	614	CLA	C14-C13-C15-C16
31	D	408	LHG	O1-C1-C2-O2
24	a	417	PHO	CBD-CGD-O2D-CED
23	C	505	CLA	C15-C16-C17-C18
32	d	412	LMG	C19-C20-C21-C22
23	B	612	CLA	CAA-CBA-CGA-O2A
27	b	620	SQD	O10-C23-C24-C25
27	C	501	SQD	C28-C29-C30-C31
23	B	602	CLA	C2A-CAA-CBA-CGA
23	c	507	CLA	CAA-CBA-CGA-O2A
29	A	413	PL9	C46-C47-C48-C49
23	c	512	CLA	CAA-CBA-CGA-O1A
32	C	502	LMG	O9-C10-C11-C12
25	C	516	BCR	C11-C12-C13-C35
23	A	408	CLA	C12-C13-C15-C16
23	B	606	CLA	C12-C13-C15-C16
23	B	610	CLA	C11-C12-C13-C15
23	B	610	CLA	C12-C13-C15-C16
23	b	609	CLA	C12-C13-C15-C16
23	c	514	CLA	C6-C7-C8-C10
33	h	101	HTG	C2-C1-S1-C1'
32	c	522	LMG	O7-C10-C11-C12
35	C	520	DGD	C9B-CAB-CBB-CCB
23	c	503	CLA	CAA-CBA-CGA-O1A
31	L	101	LHG	O9-C7-C8-C9
27	a	410	SQD	C25-C26-C27-C28
23	c	503	CLA	CAA-CBA-CGA-O2A
32	d	412	LMG	O7-C10-C11-C12
35	c	520	DGD	O1G-C1A-C2A-C3A
31	D	408	LHG	C25-C26-C27-C28
34	B	628	LMT	O5'-C1'-O1'-C1
23	c	511	CLA	C8-C10-C11-C12
23	b	613	CLA	CAA-CBA-CGA-O1A
32	c	522	LMG	O9-C10-C11-C12
29	d	405	PL9	C9-C11-C12-C13
34	D	402	LMT	C4'-C5'-C6'-O6'
23	D	404	CLA	C5-C6-C7-C8
23	b	612	CLA	CAA-CBA-CGA-O1A
34	e	101	LMT	O5B-C1B-O1B-C4'

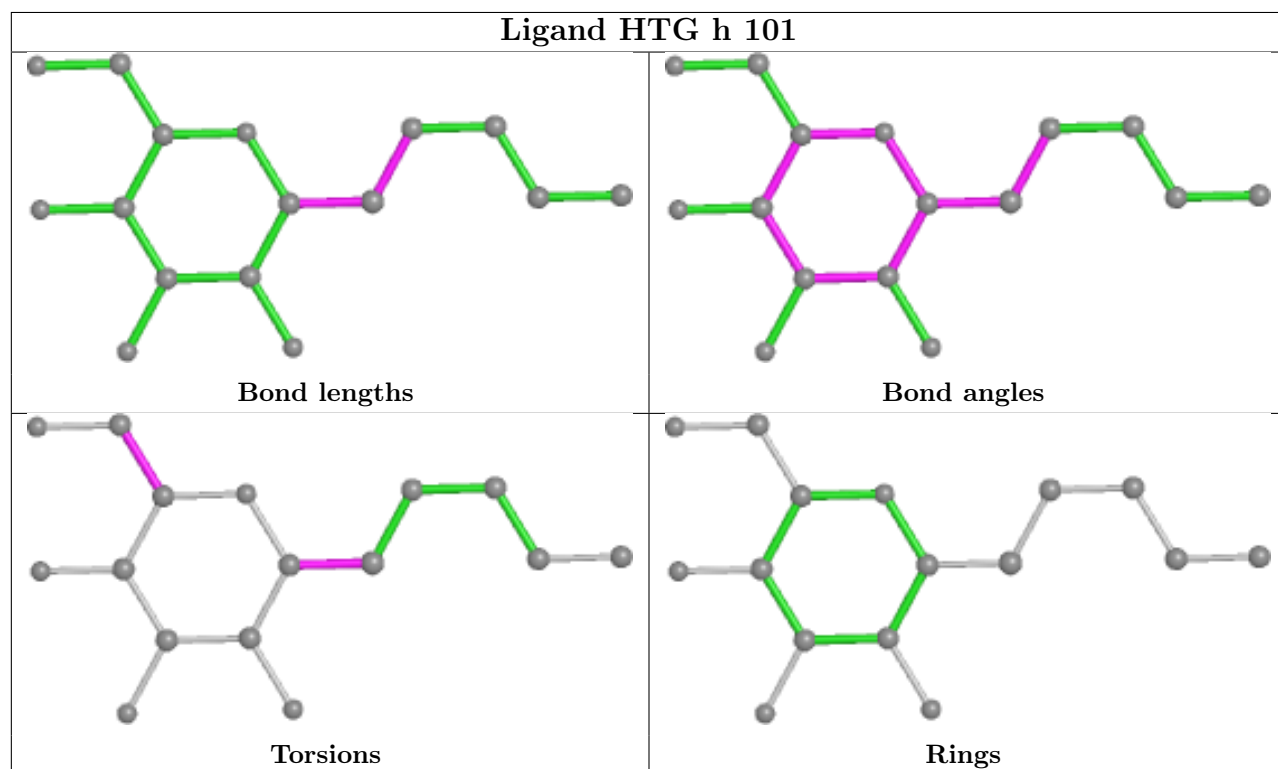
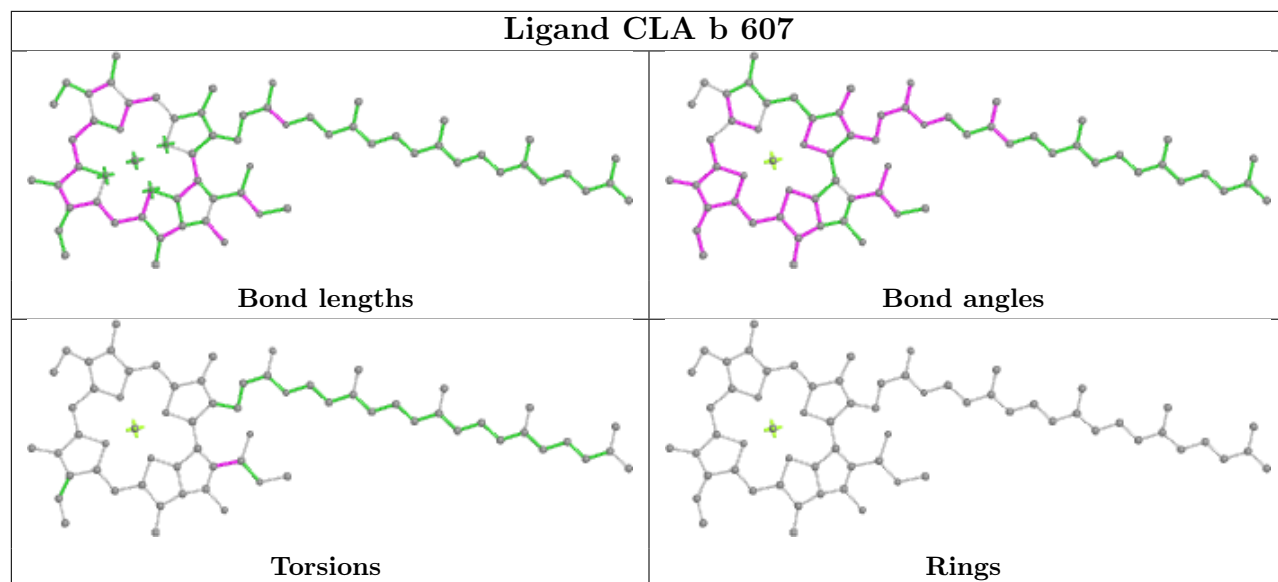
There are no ring outliers.

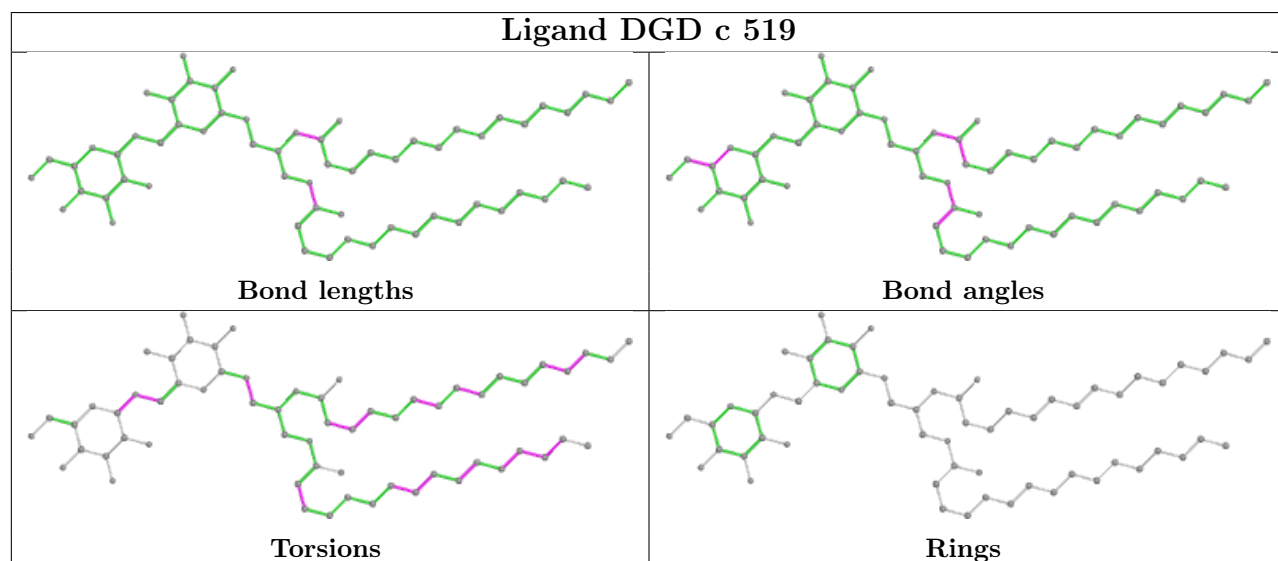
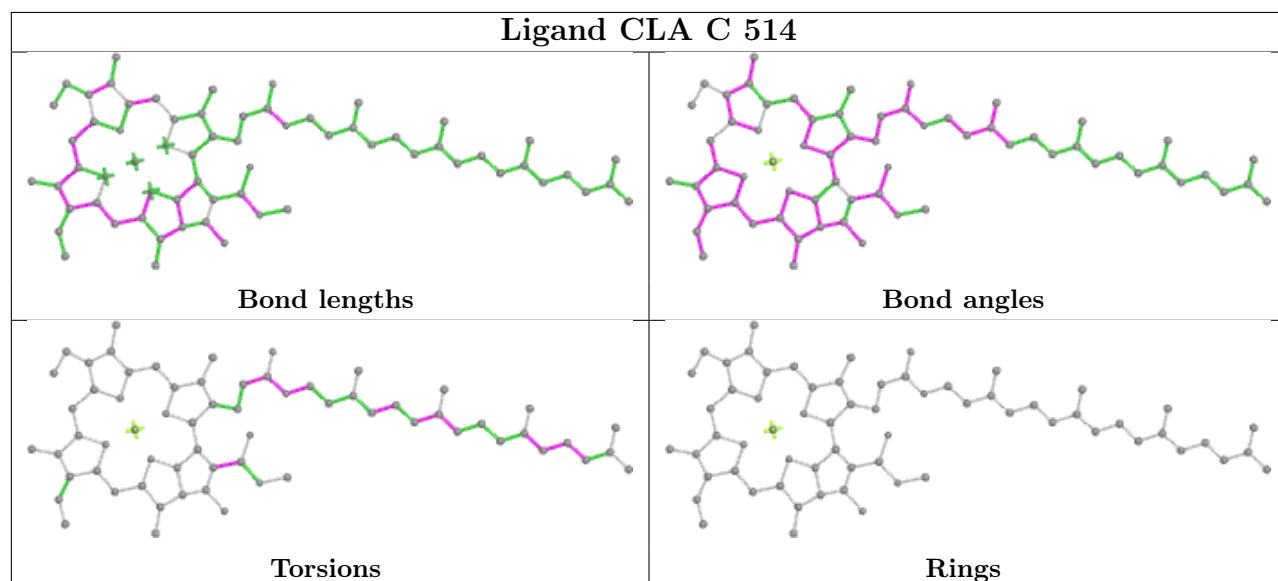
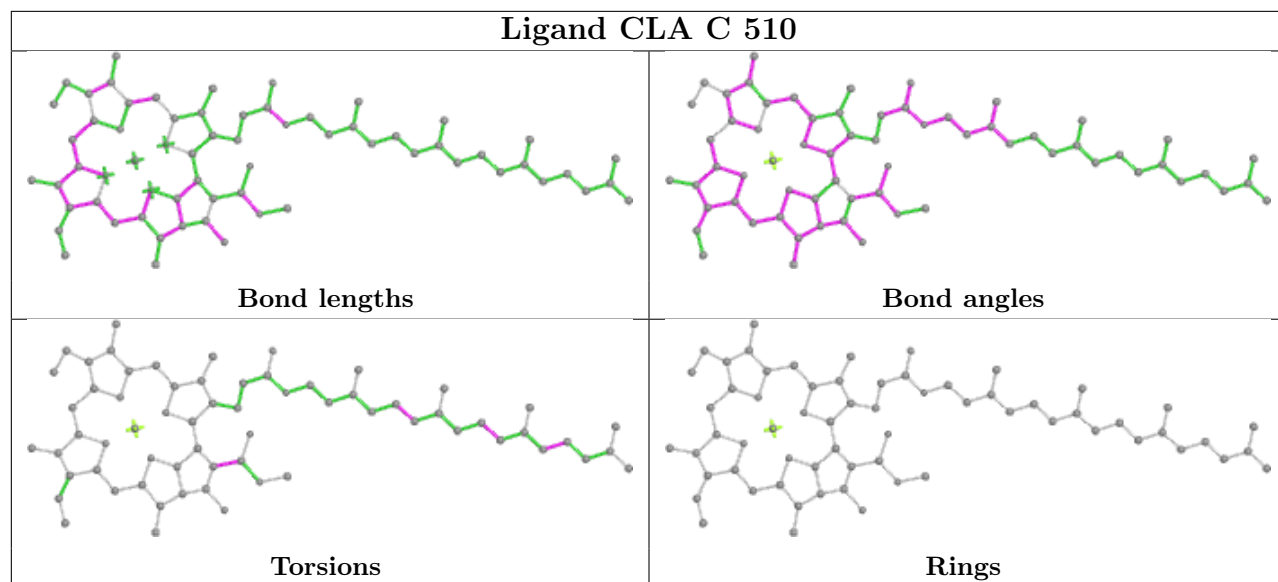
No monomer is involved in short contacts.

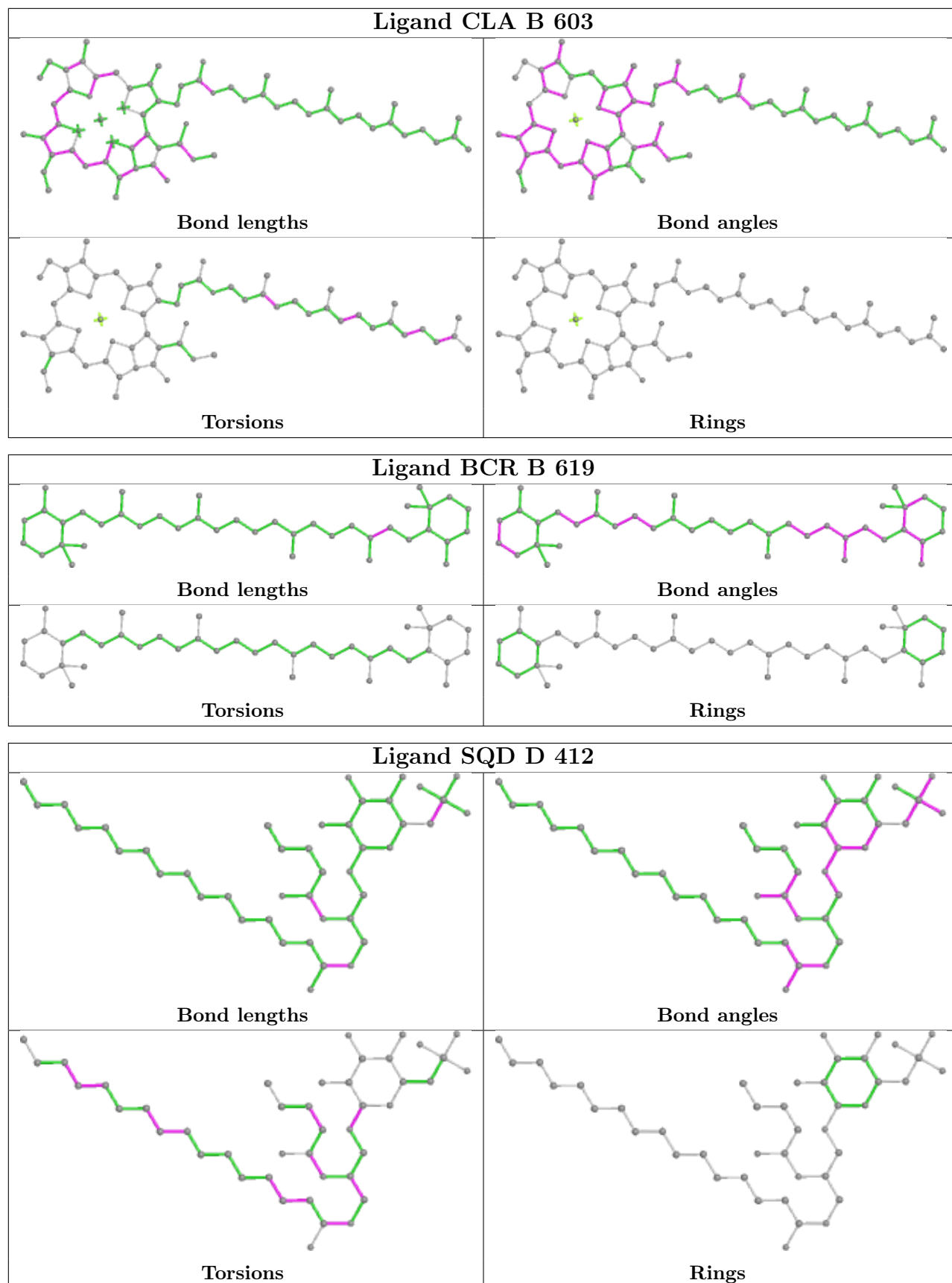
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

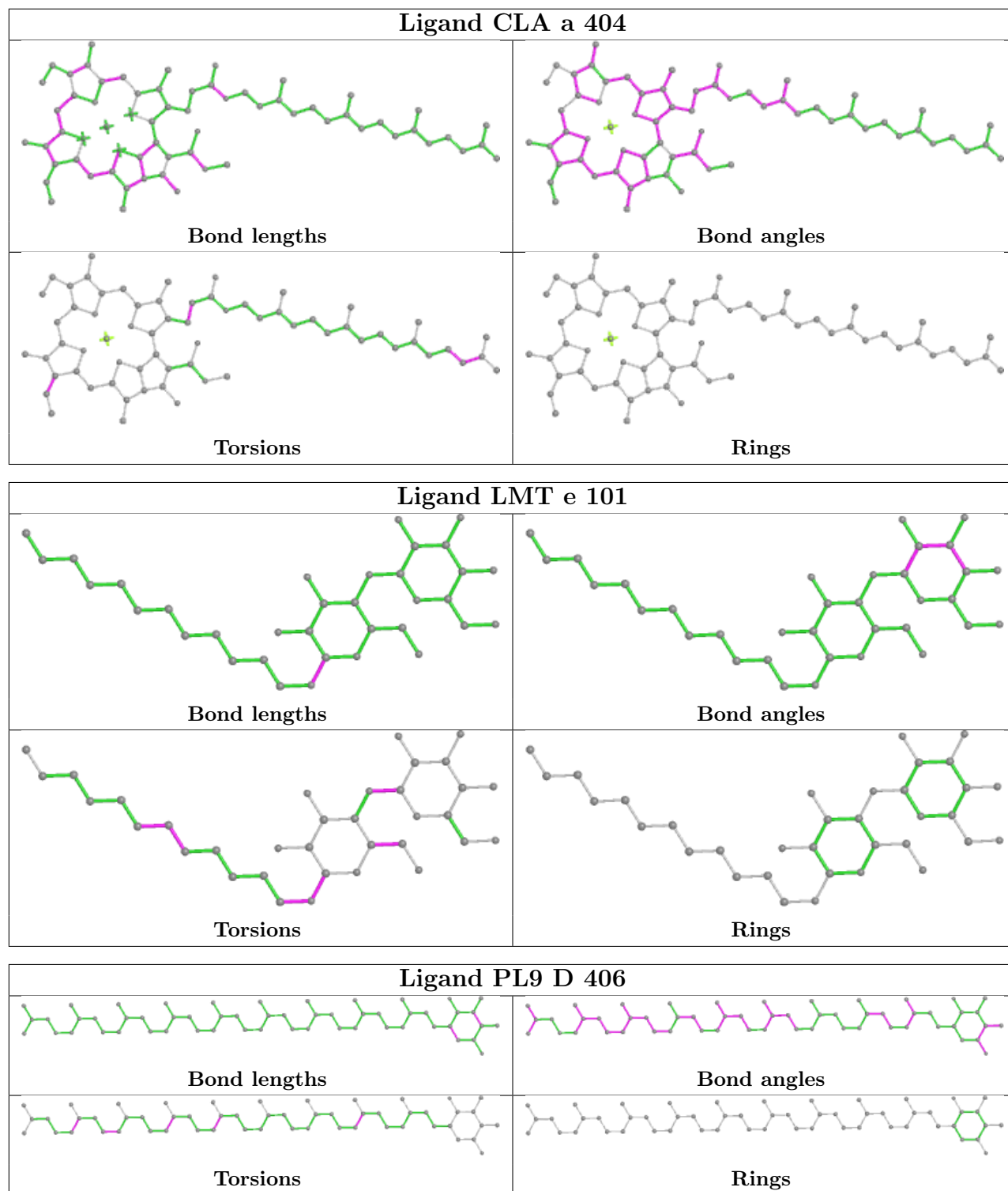


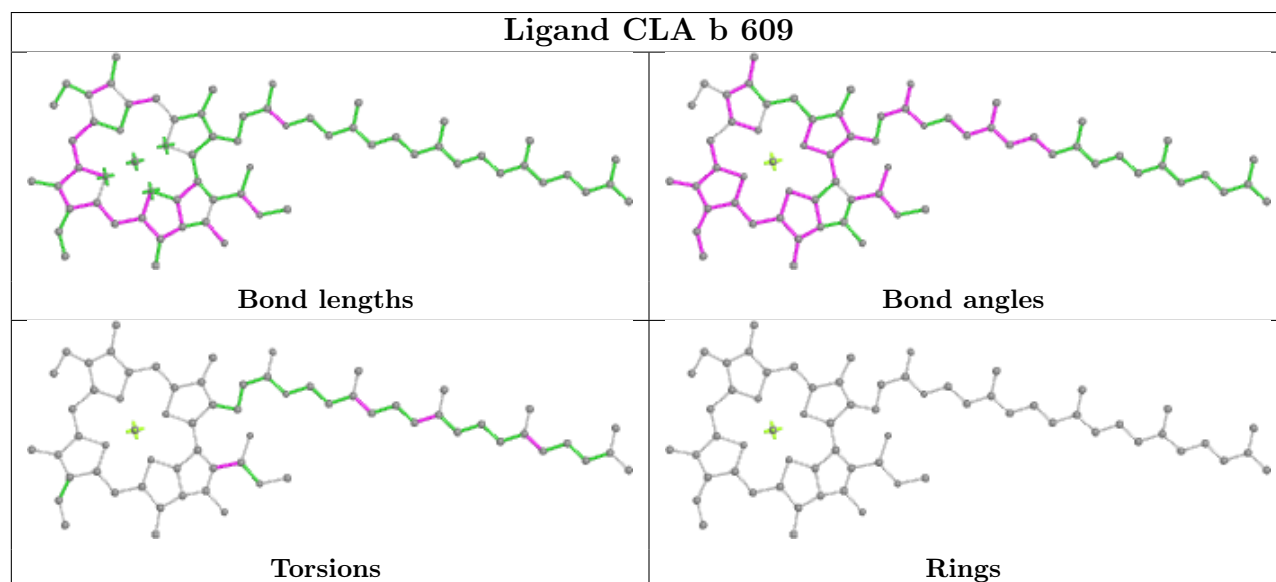
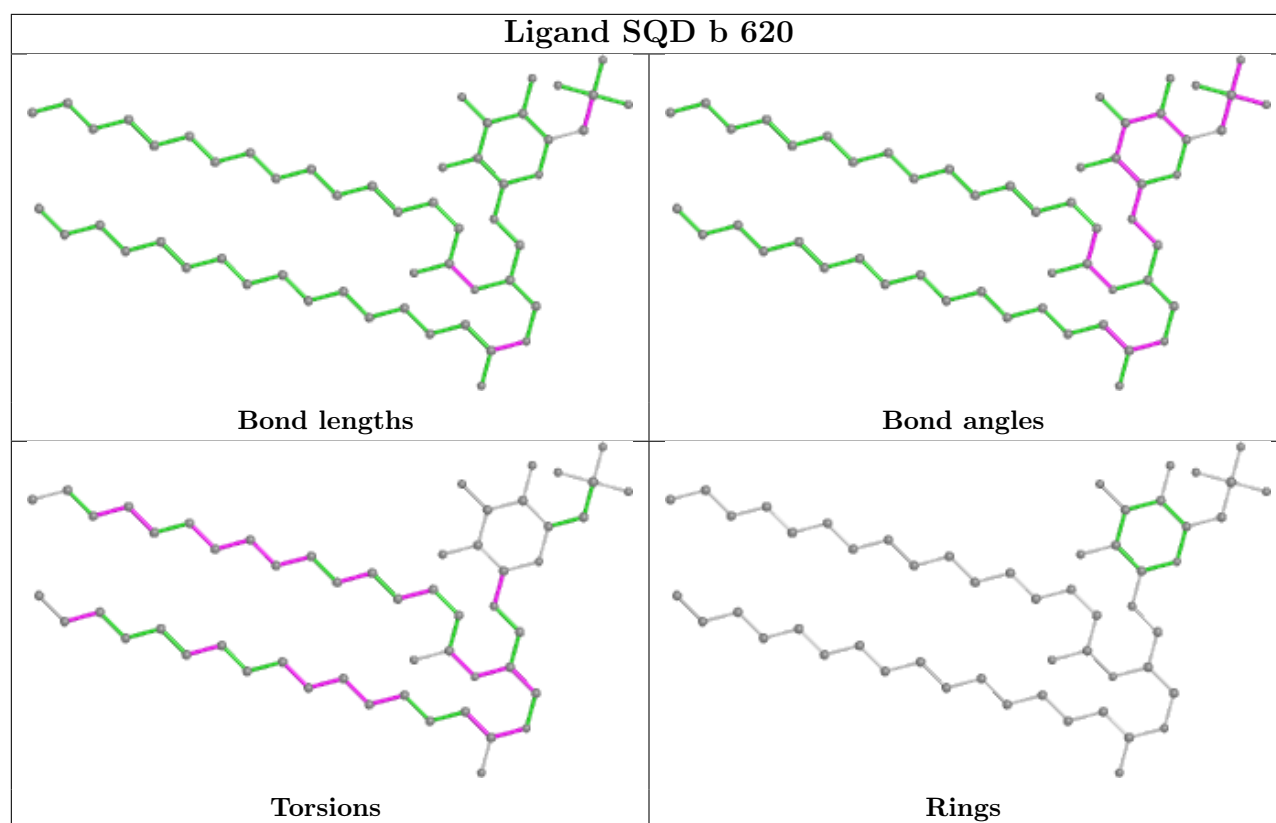


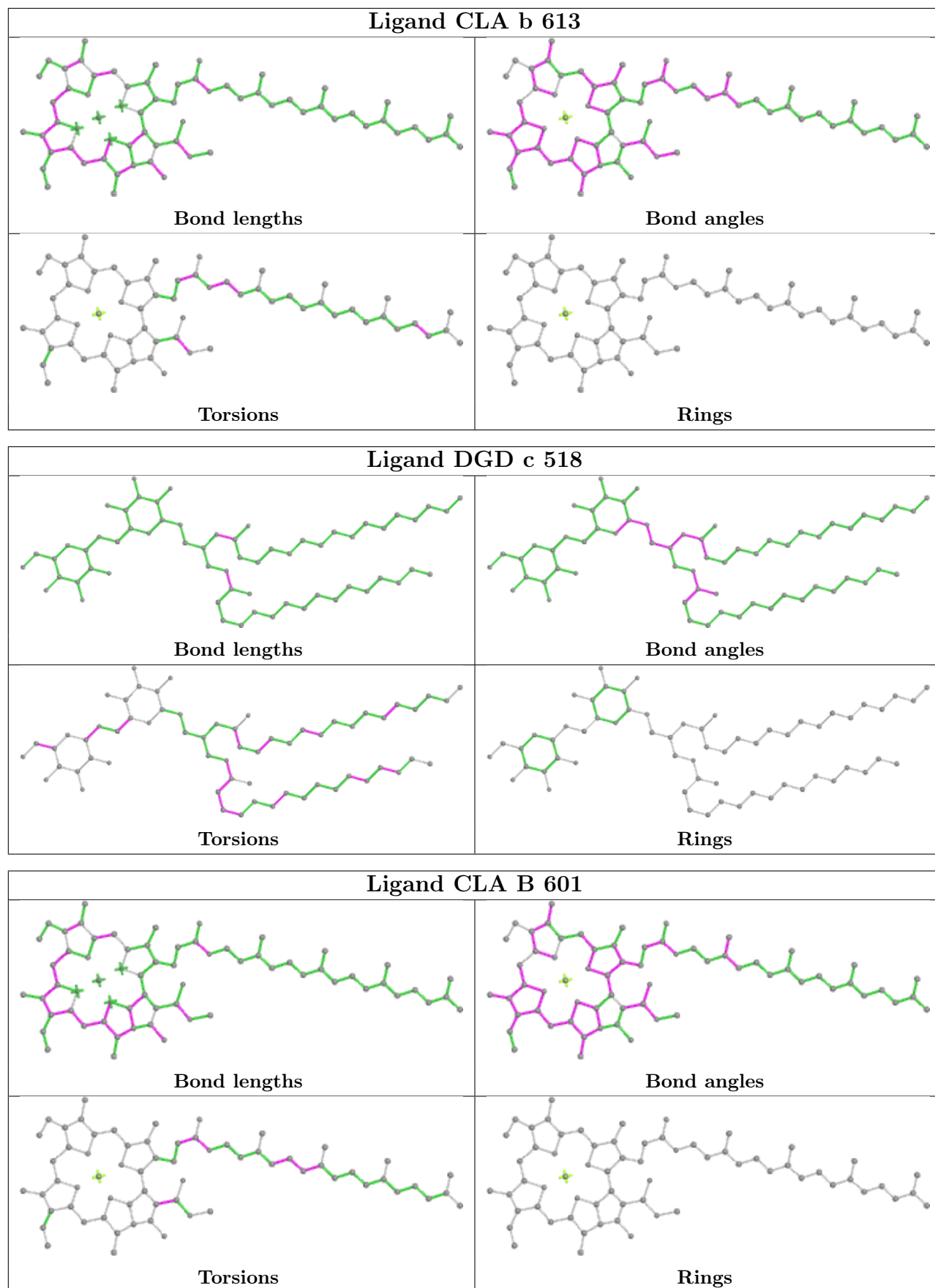


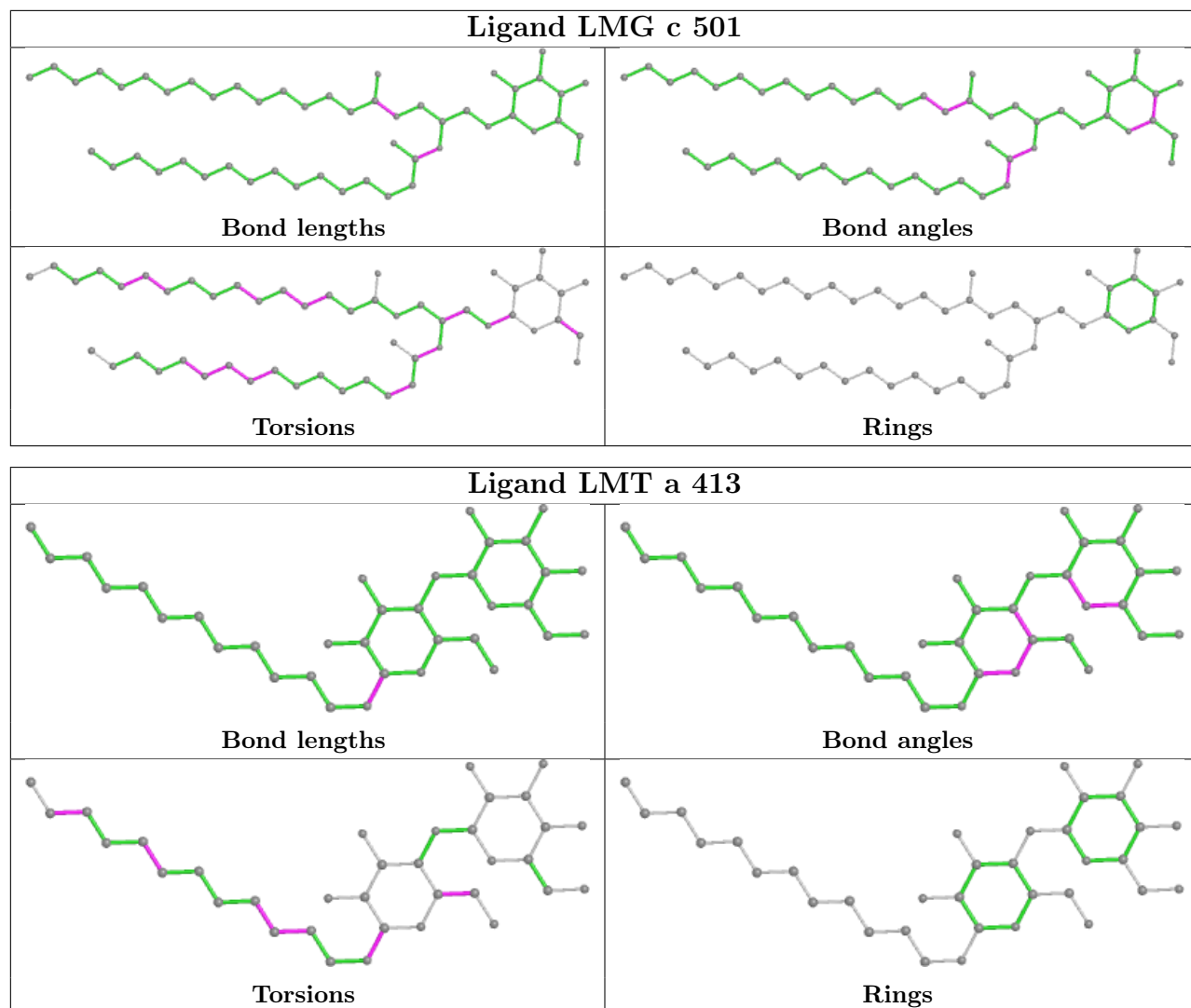


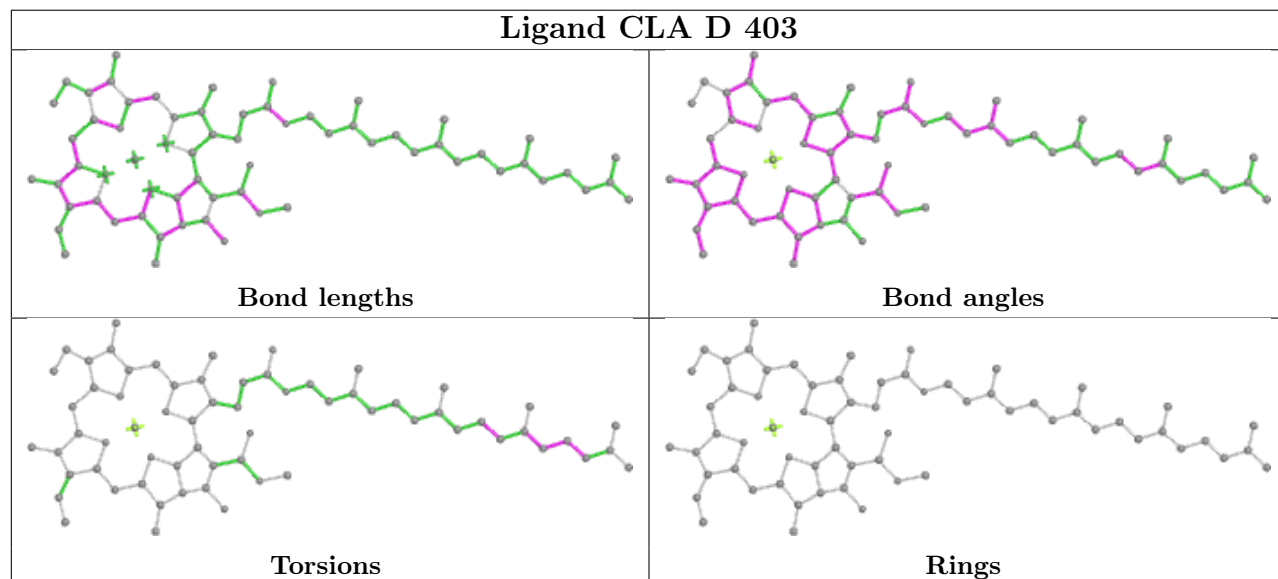
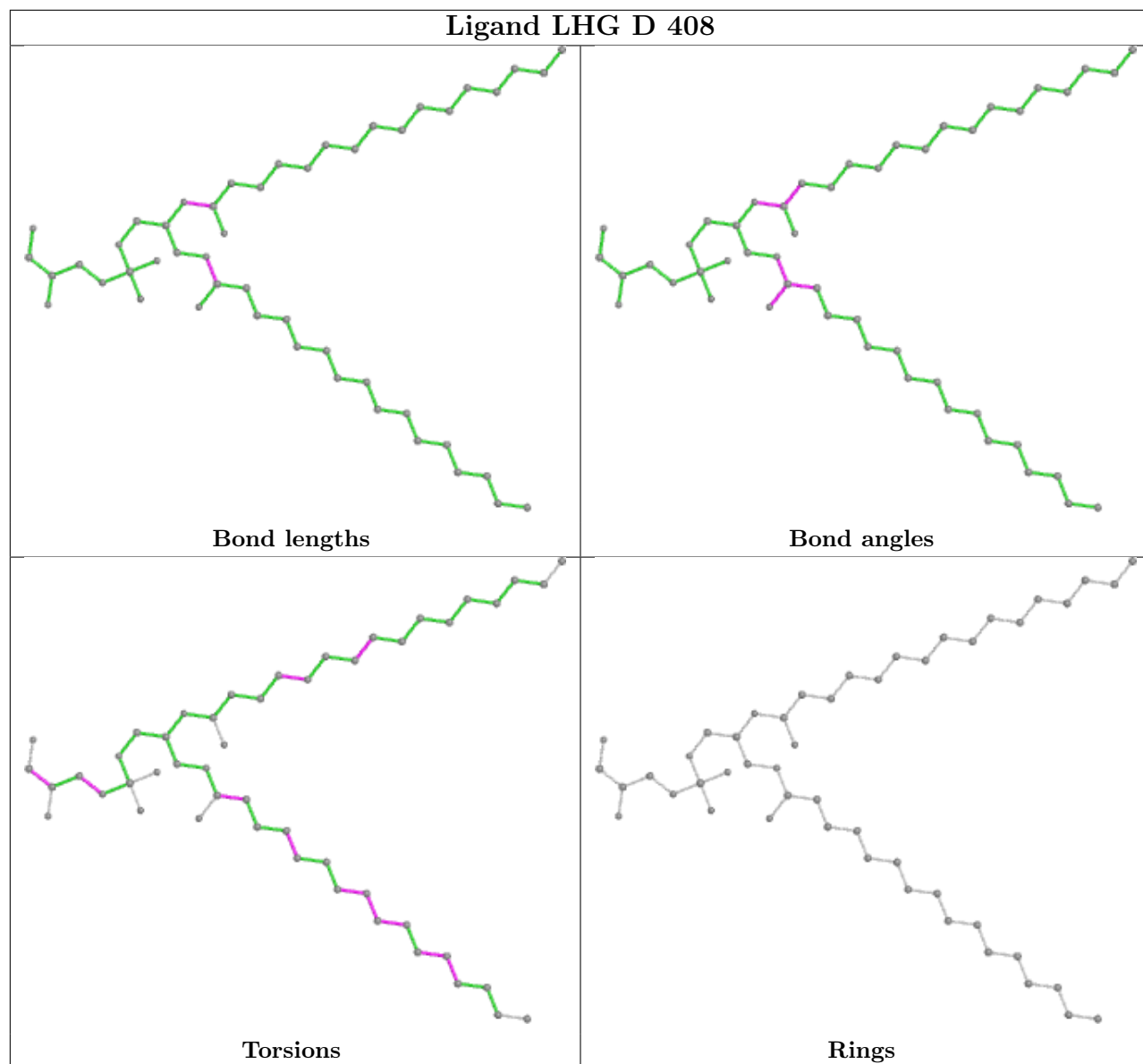


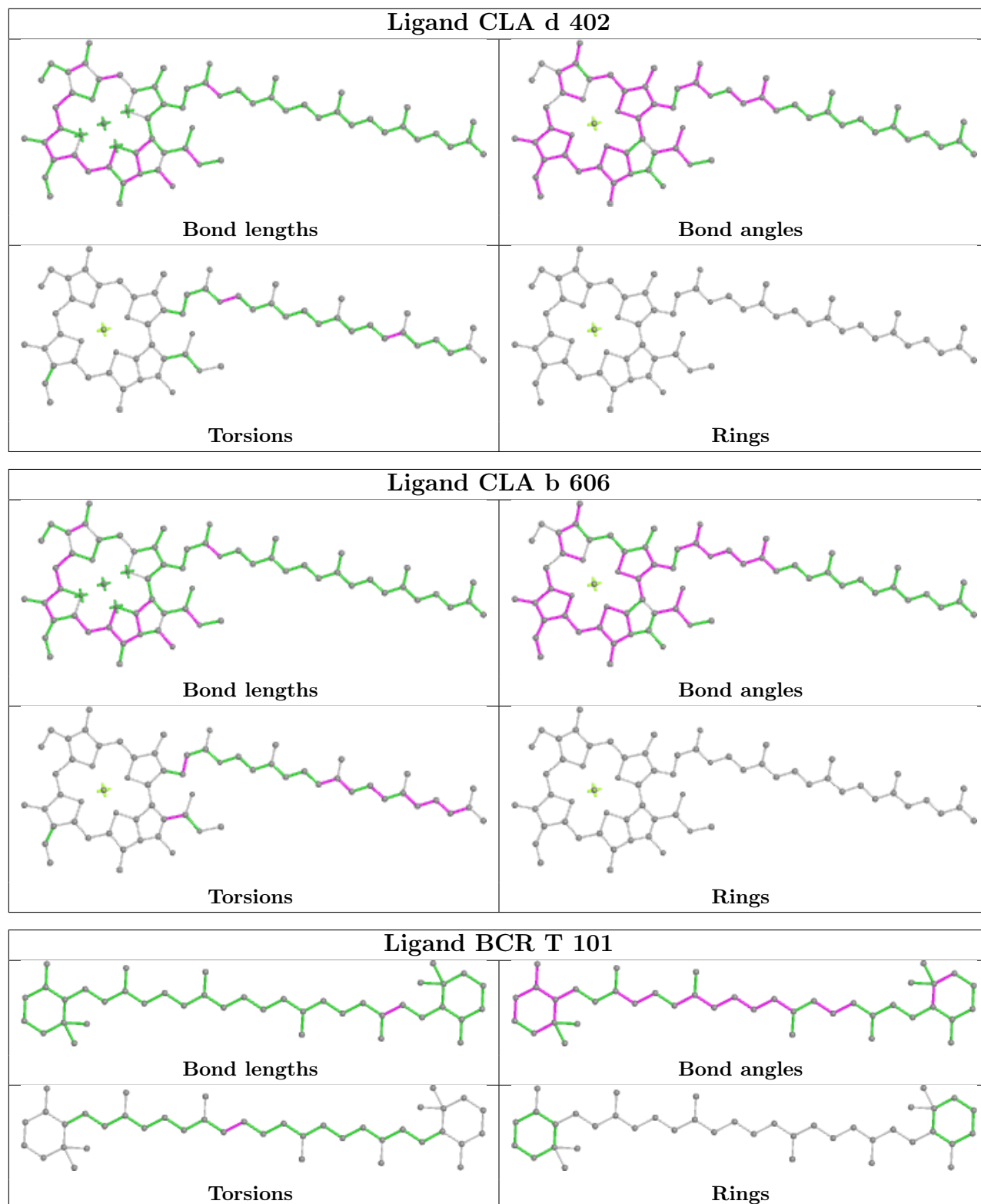


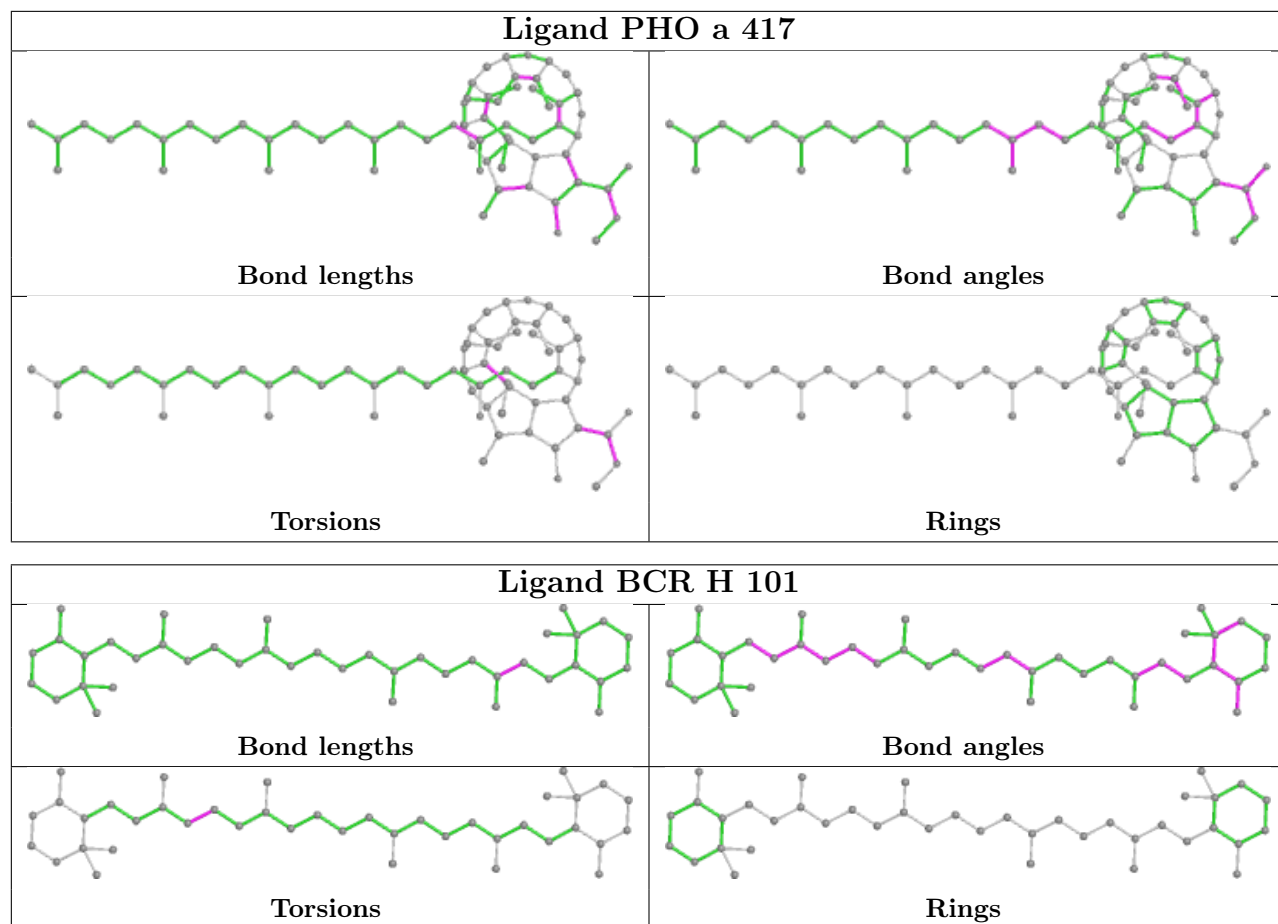


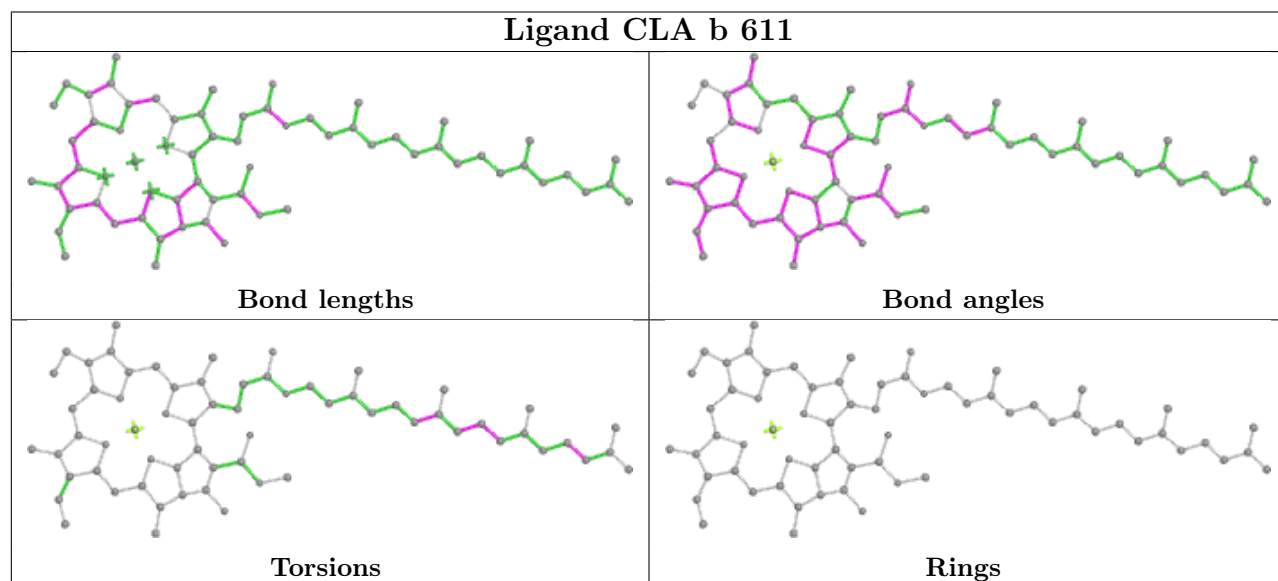
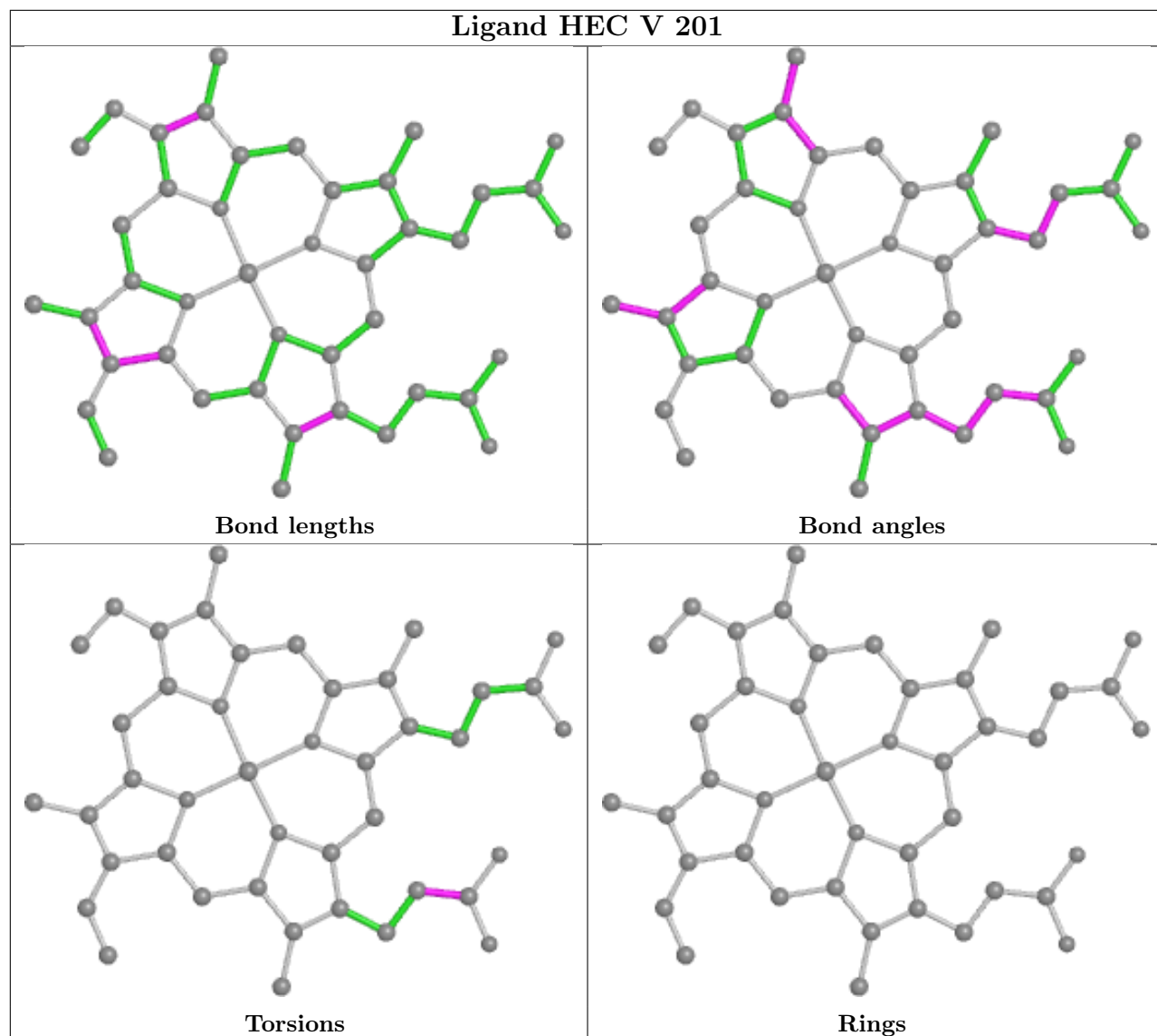


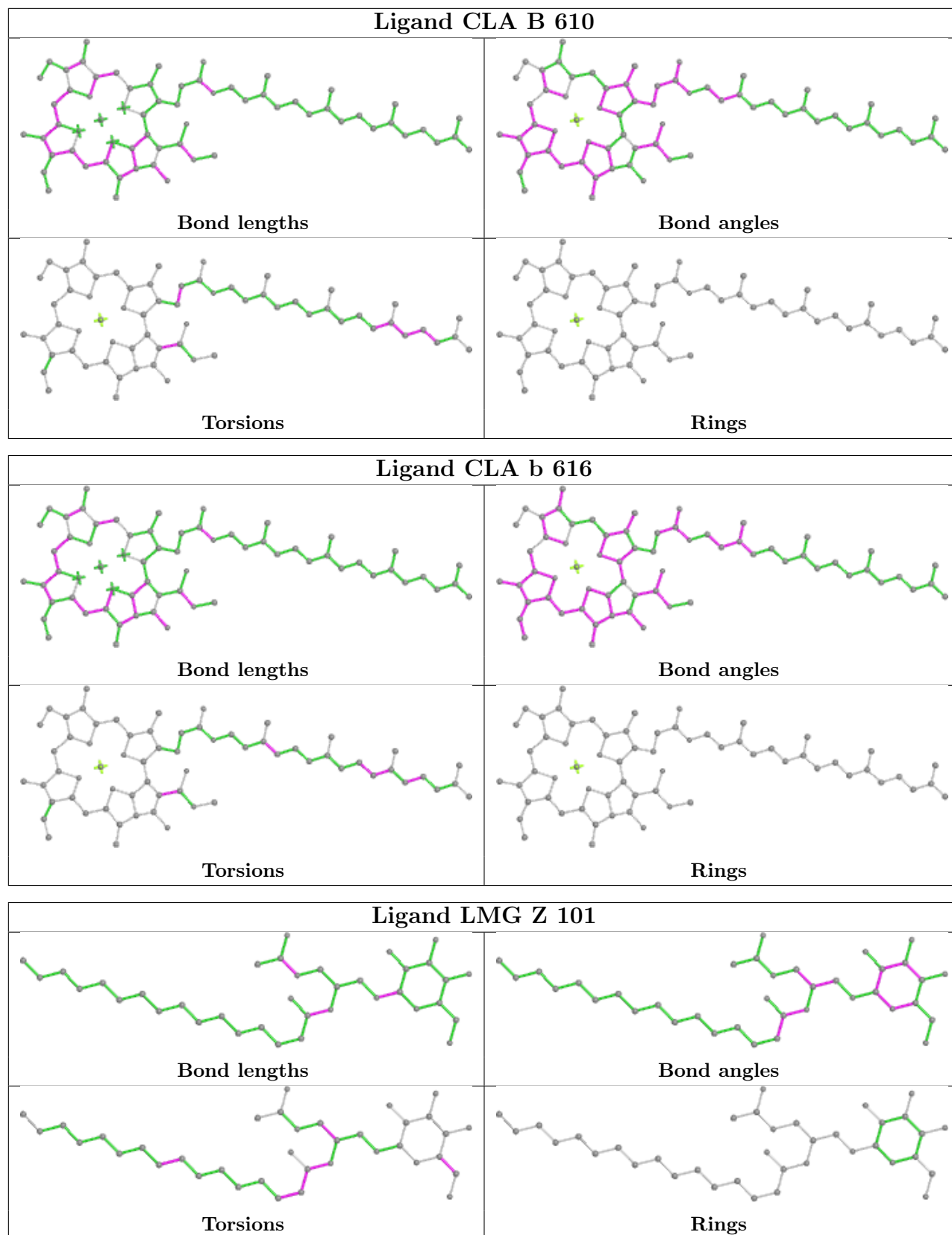


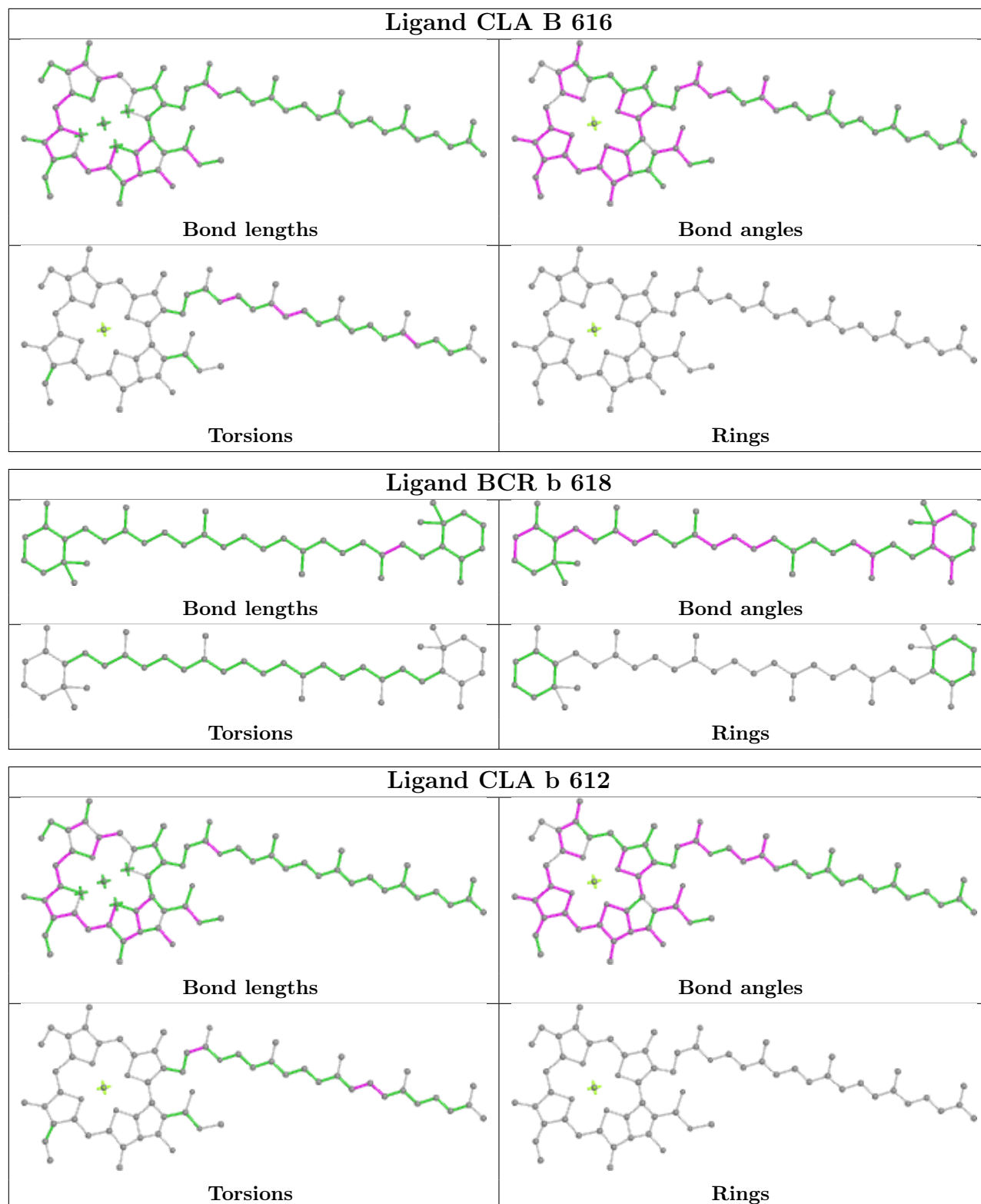


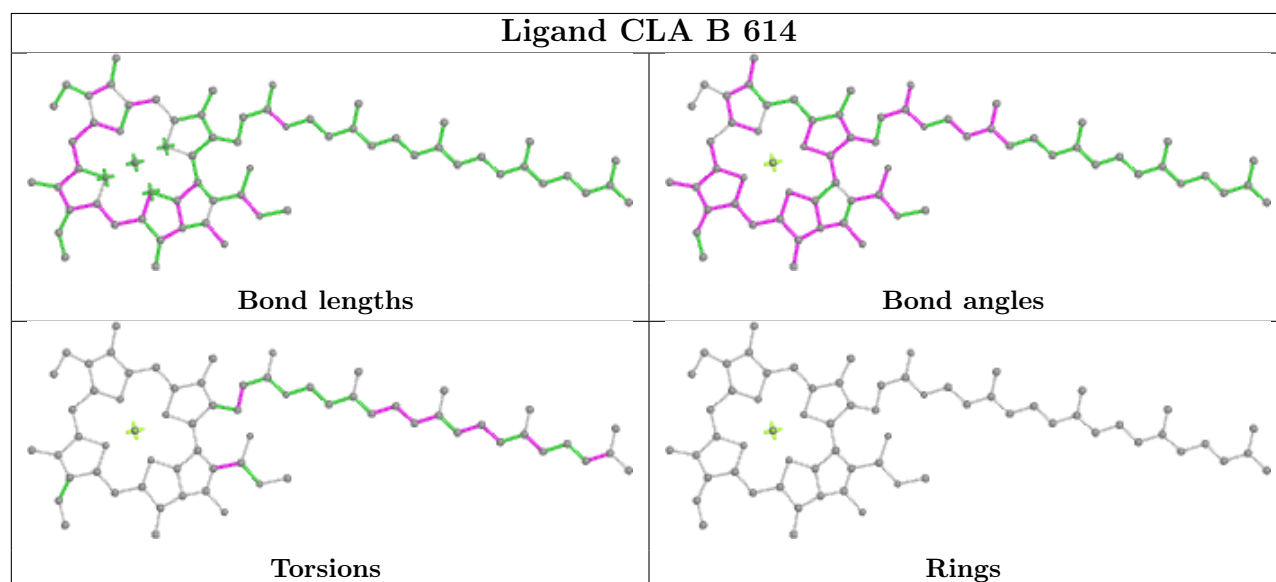
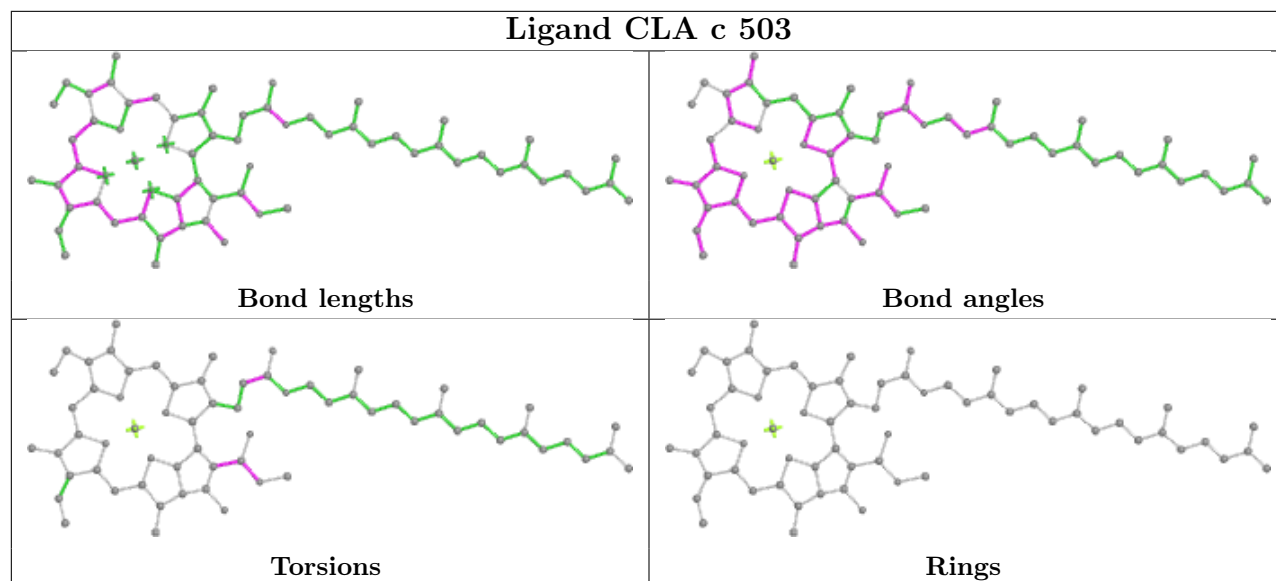
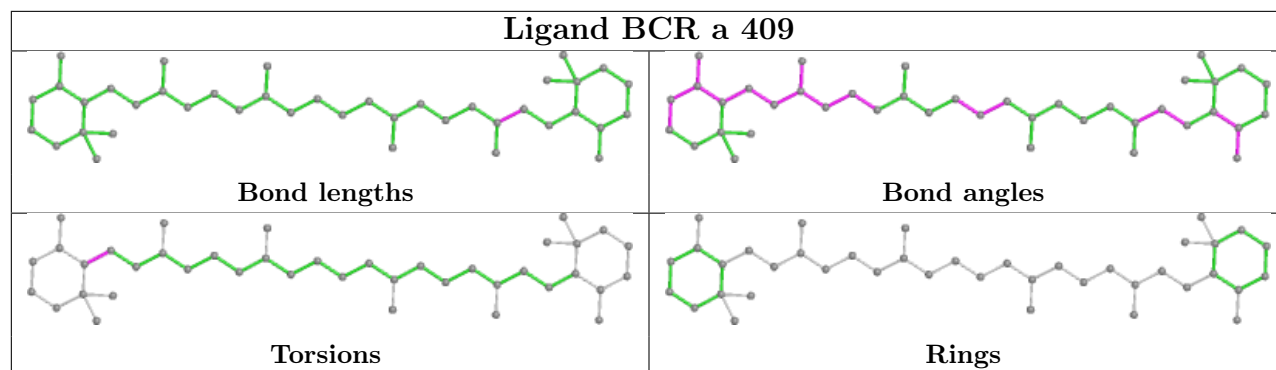


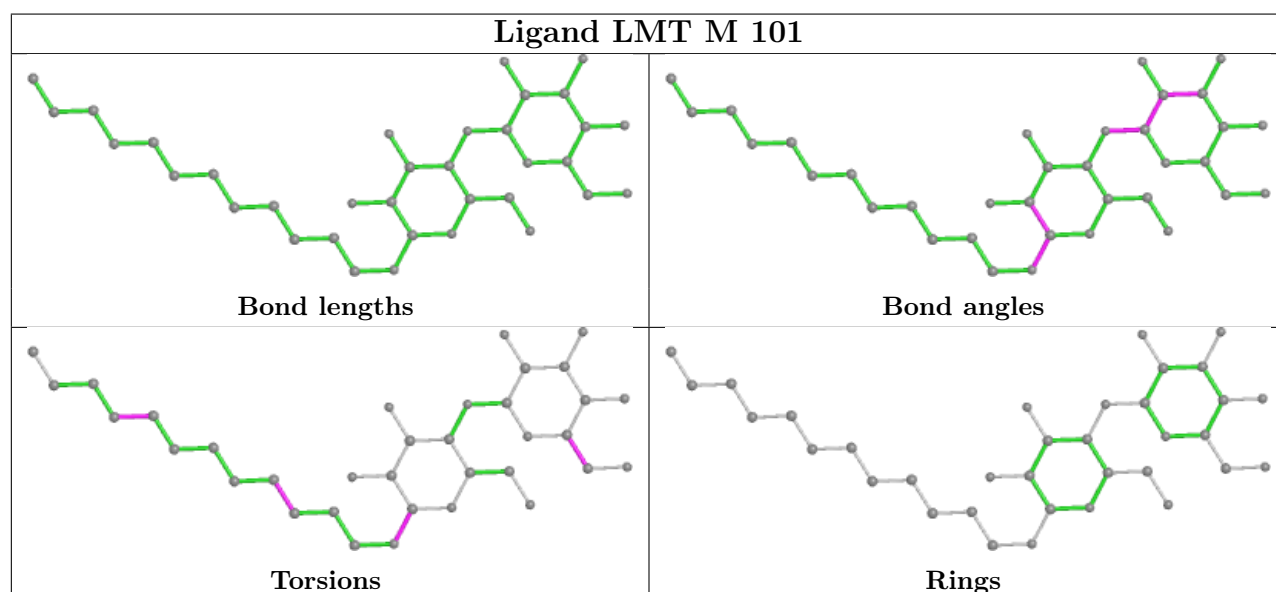
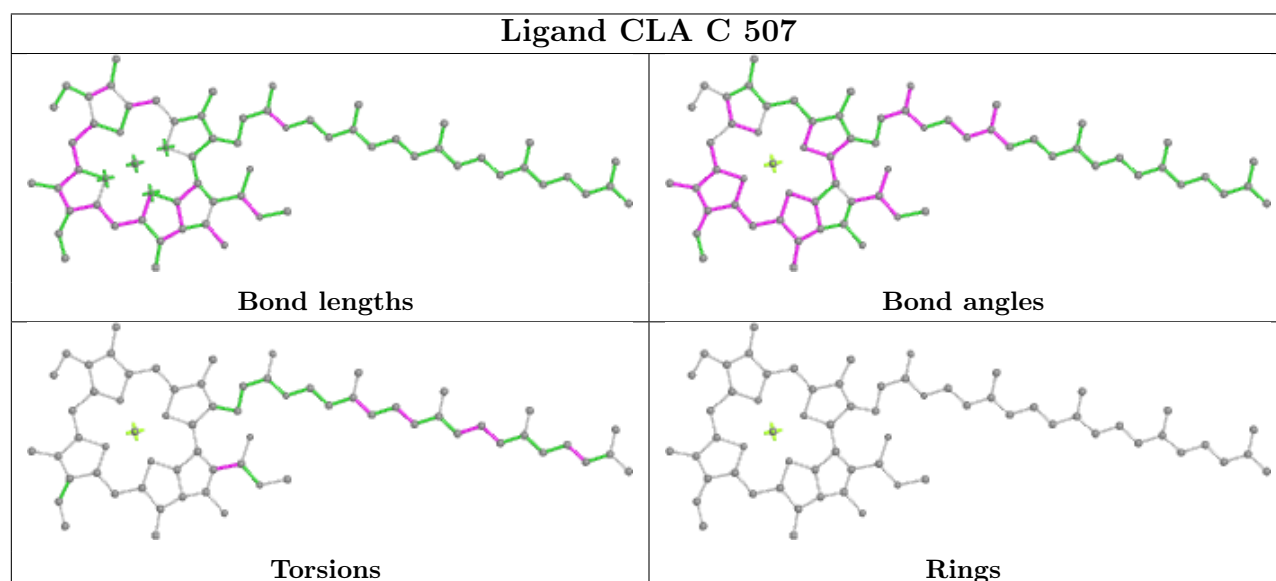
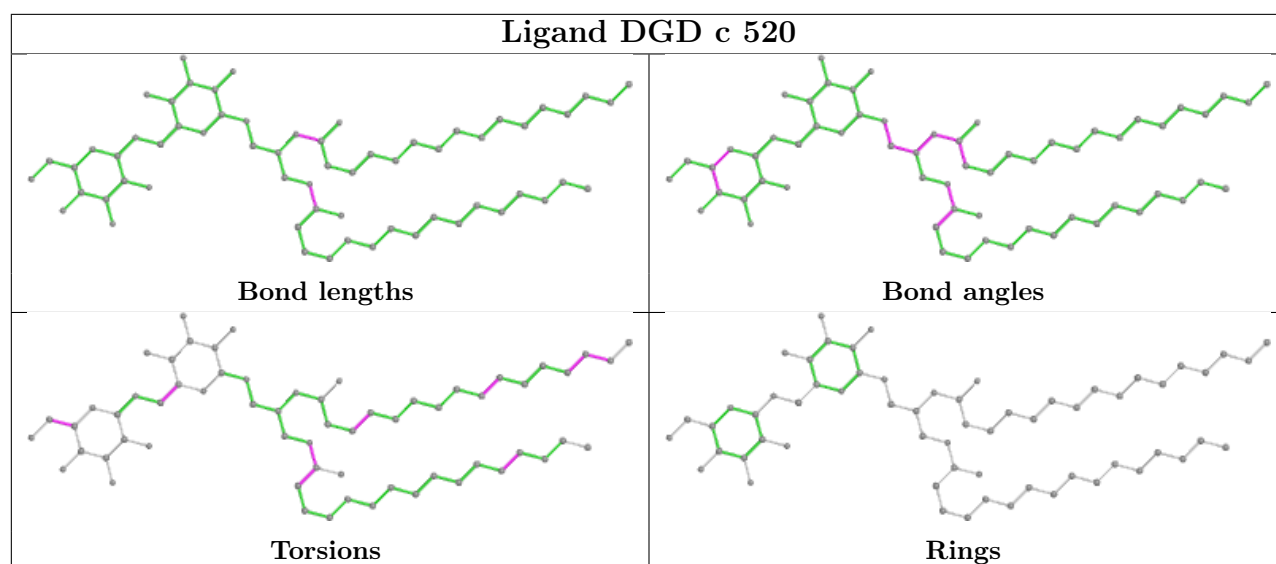


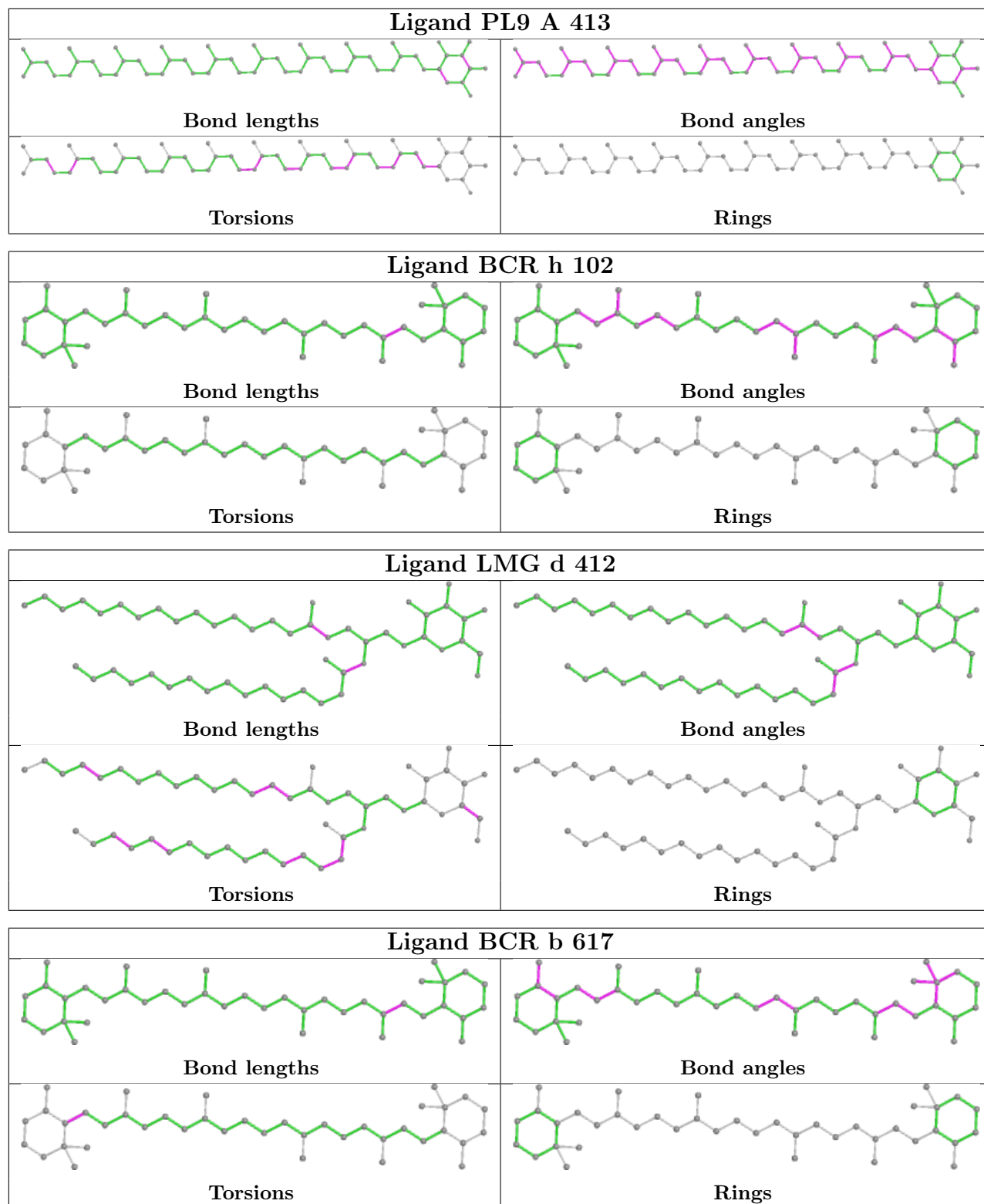


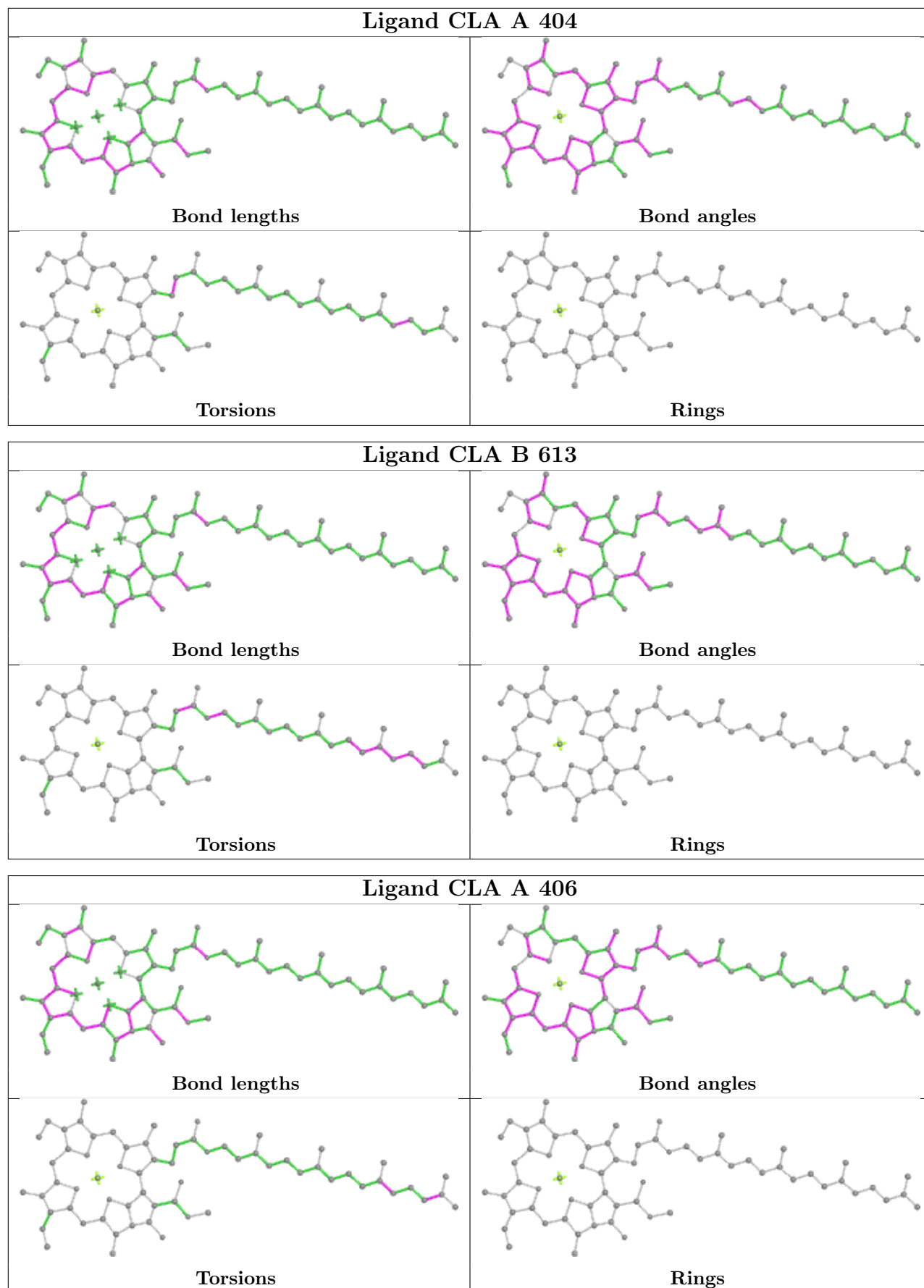


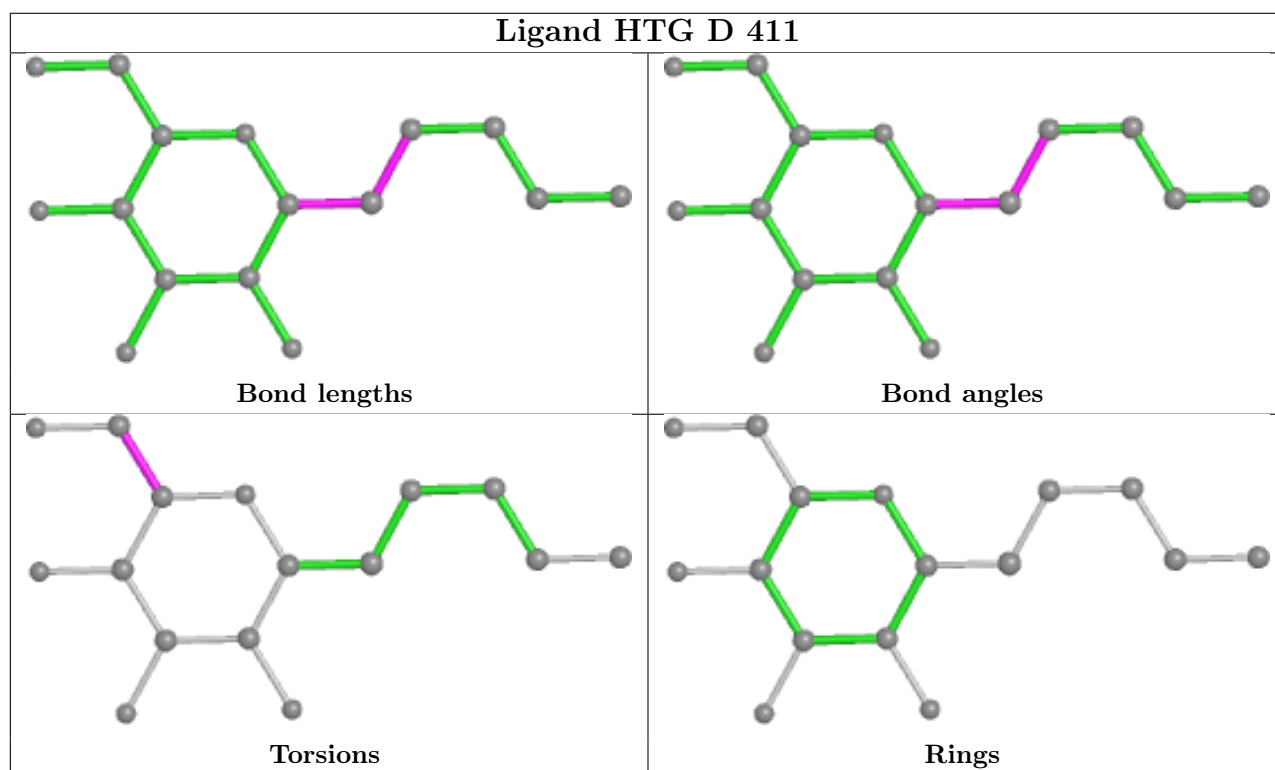
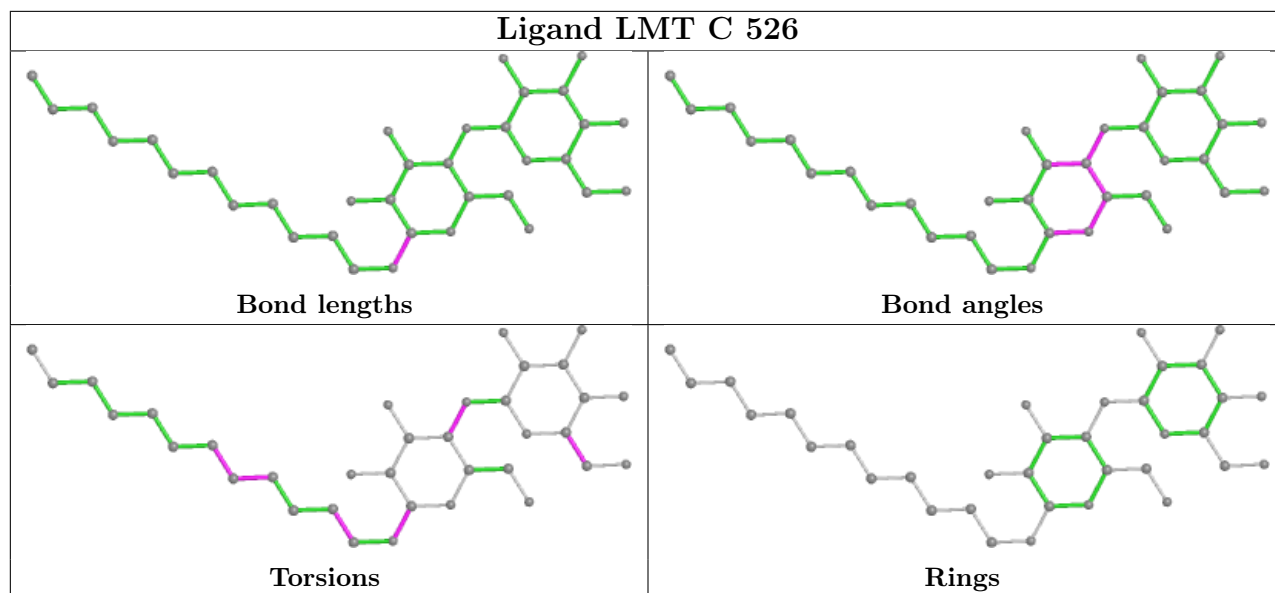


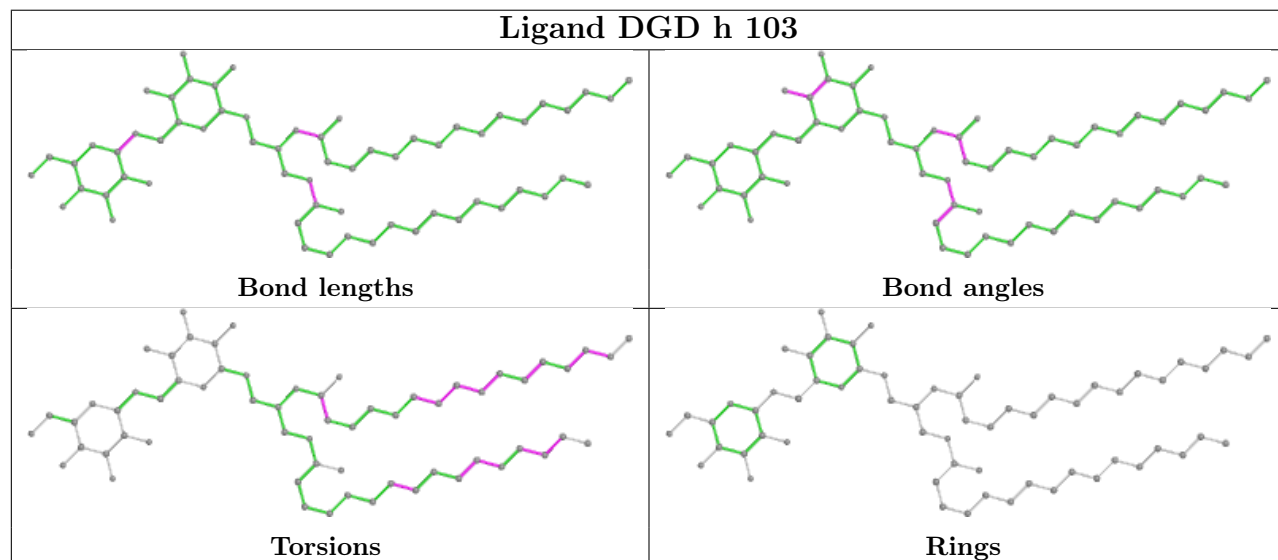
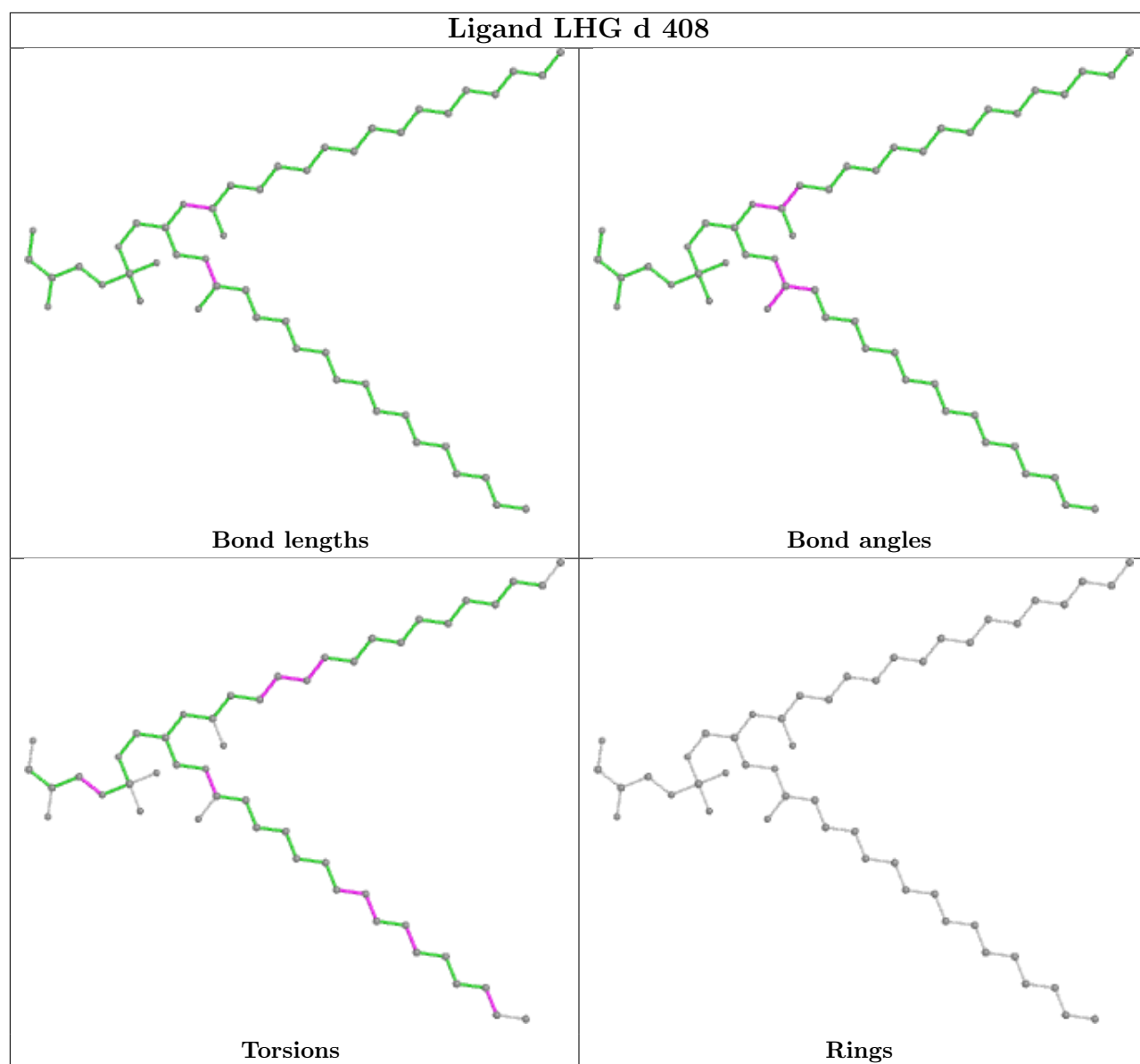


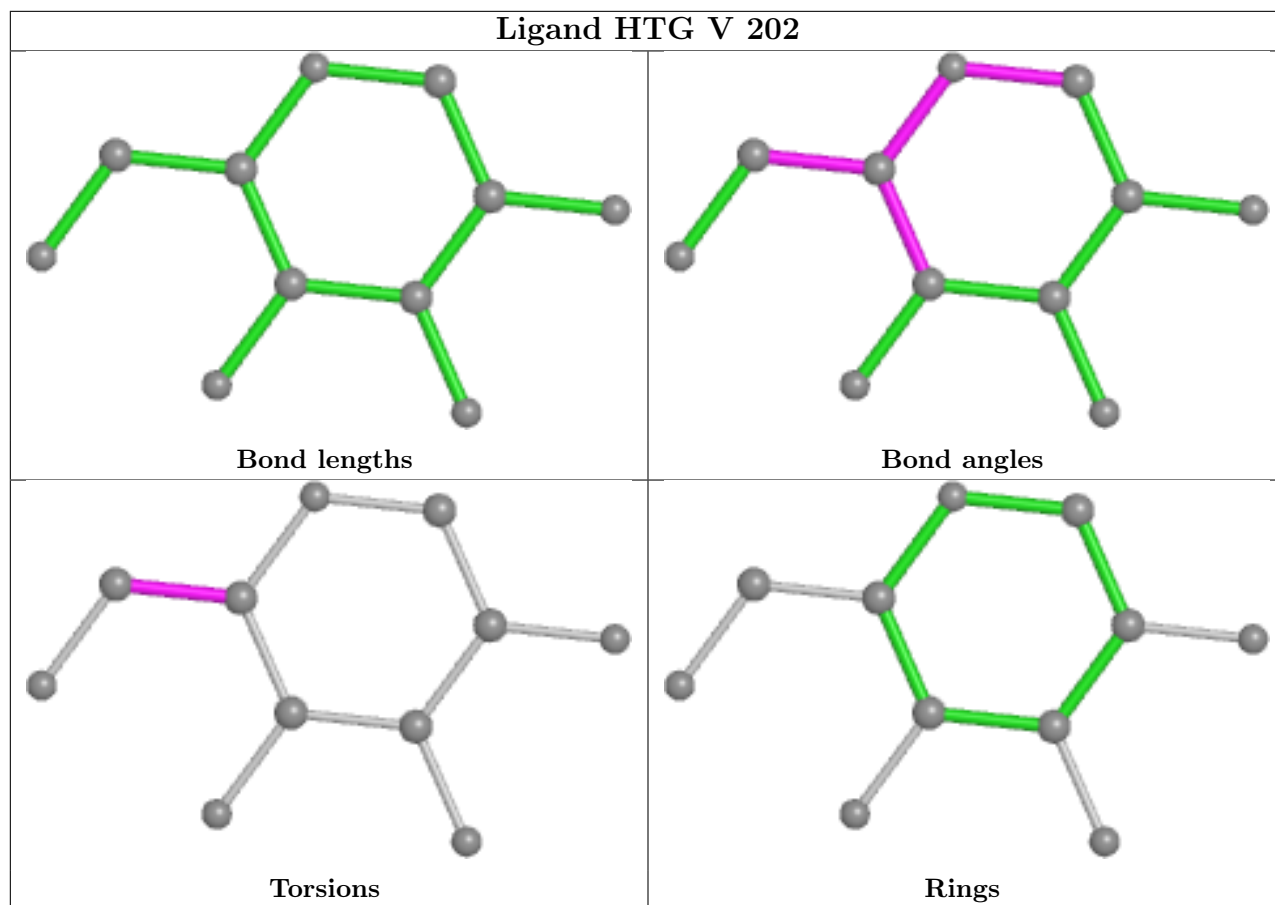
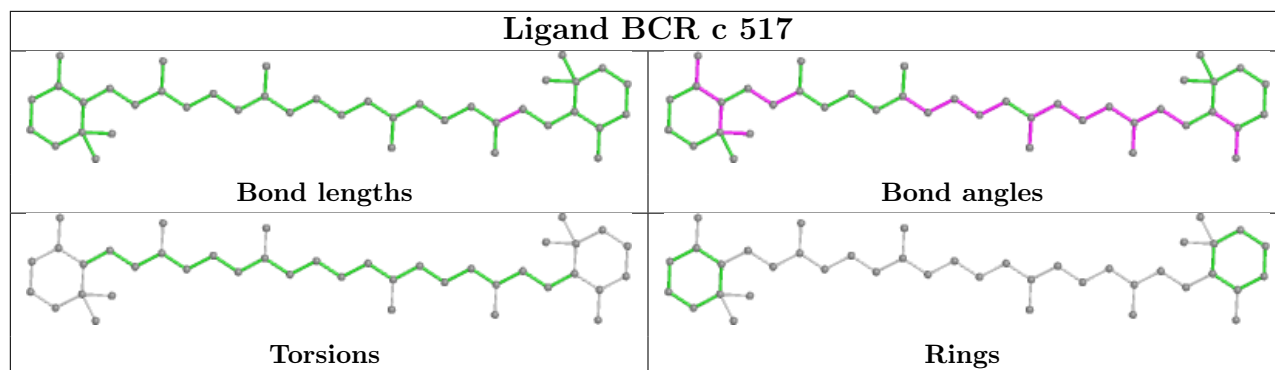


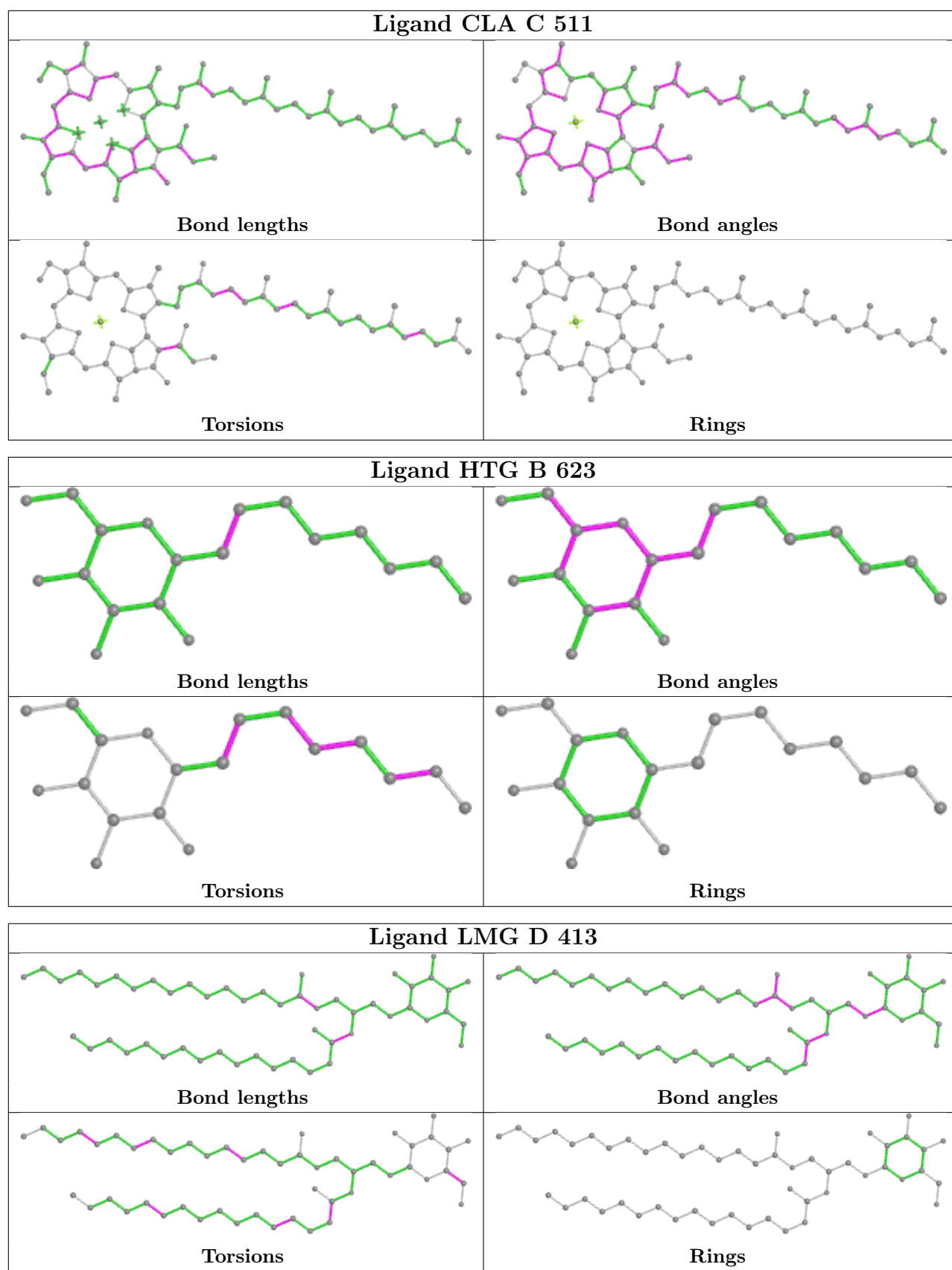


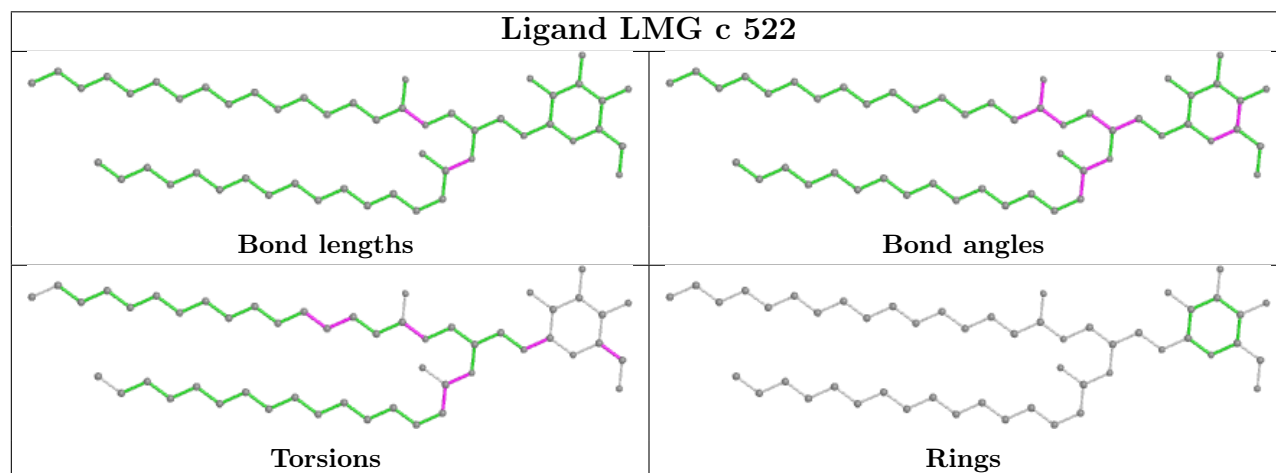
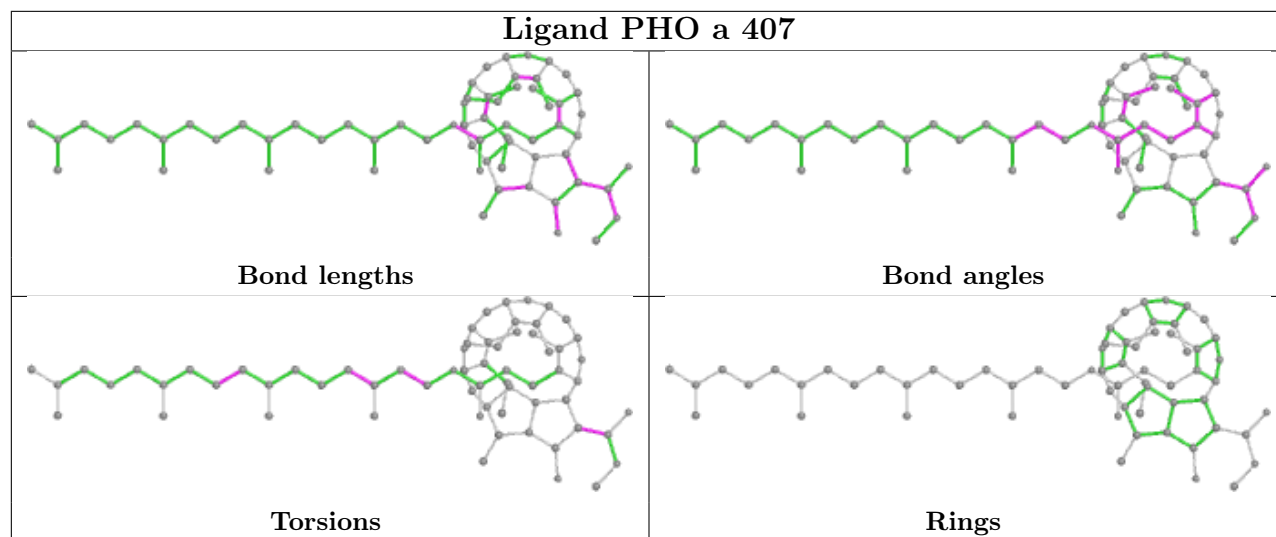
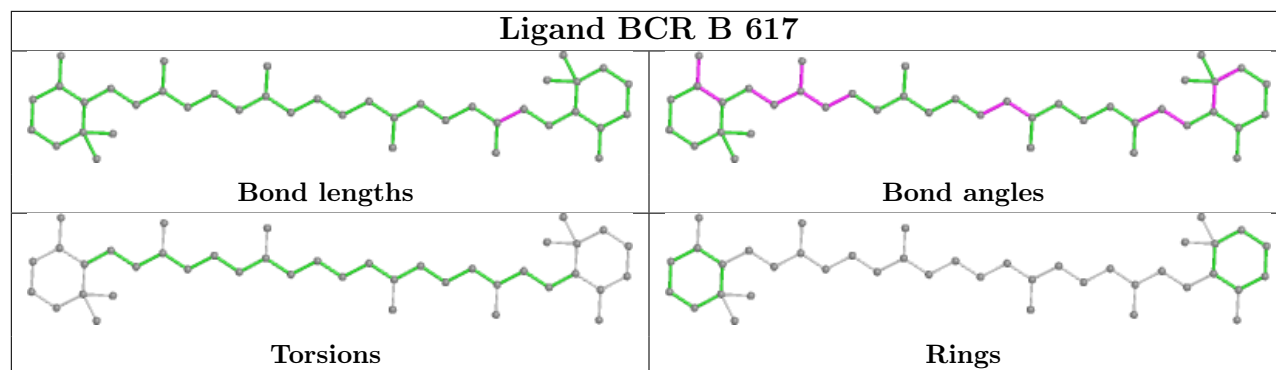


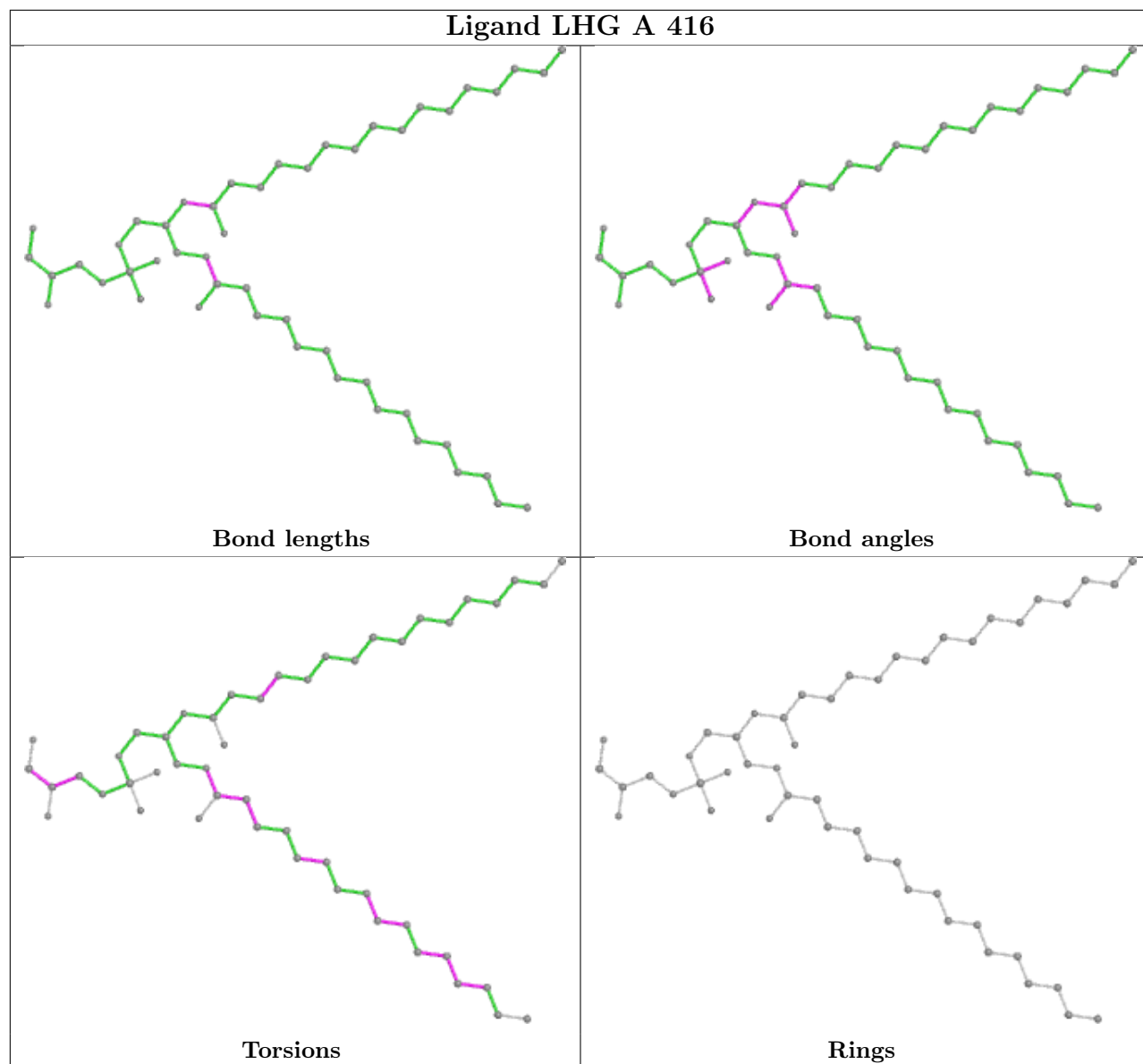


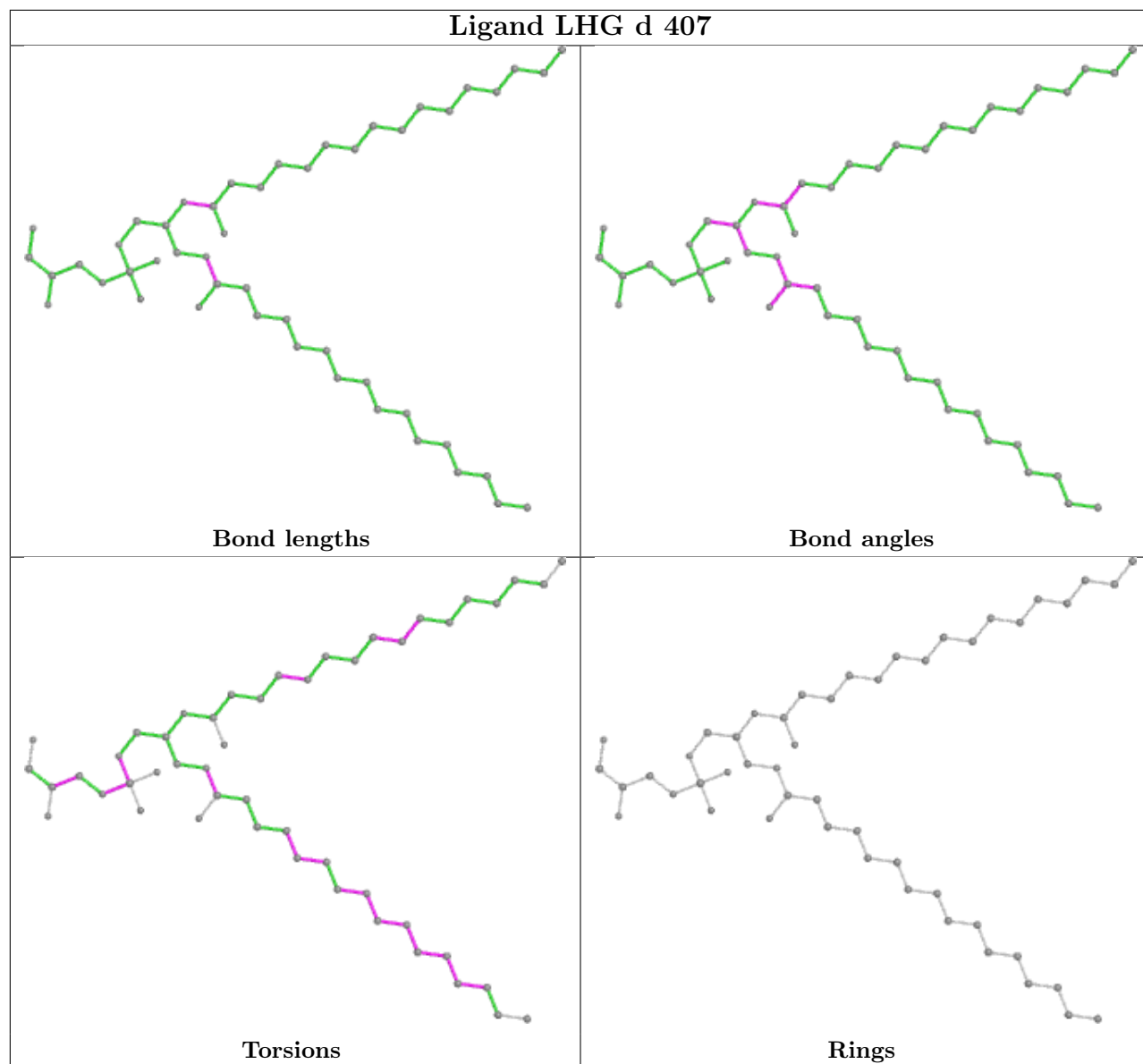


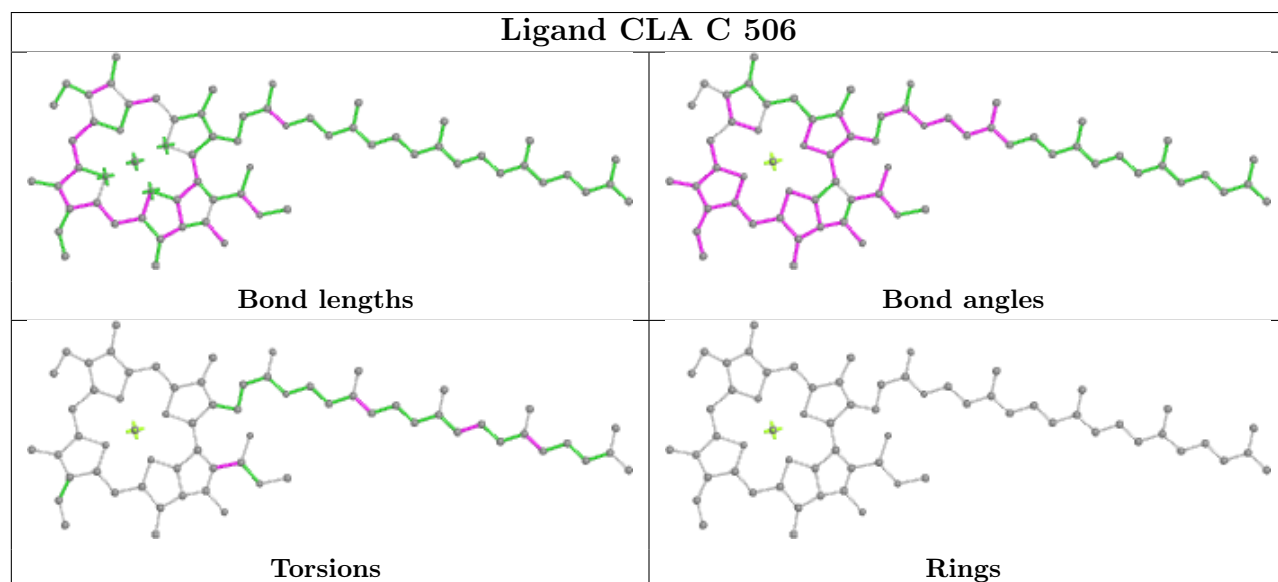
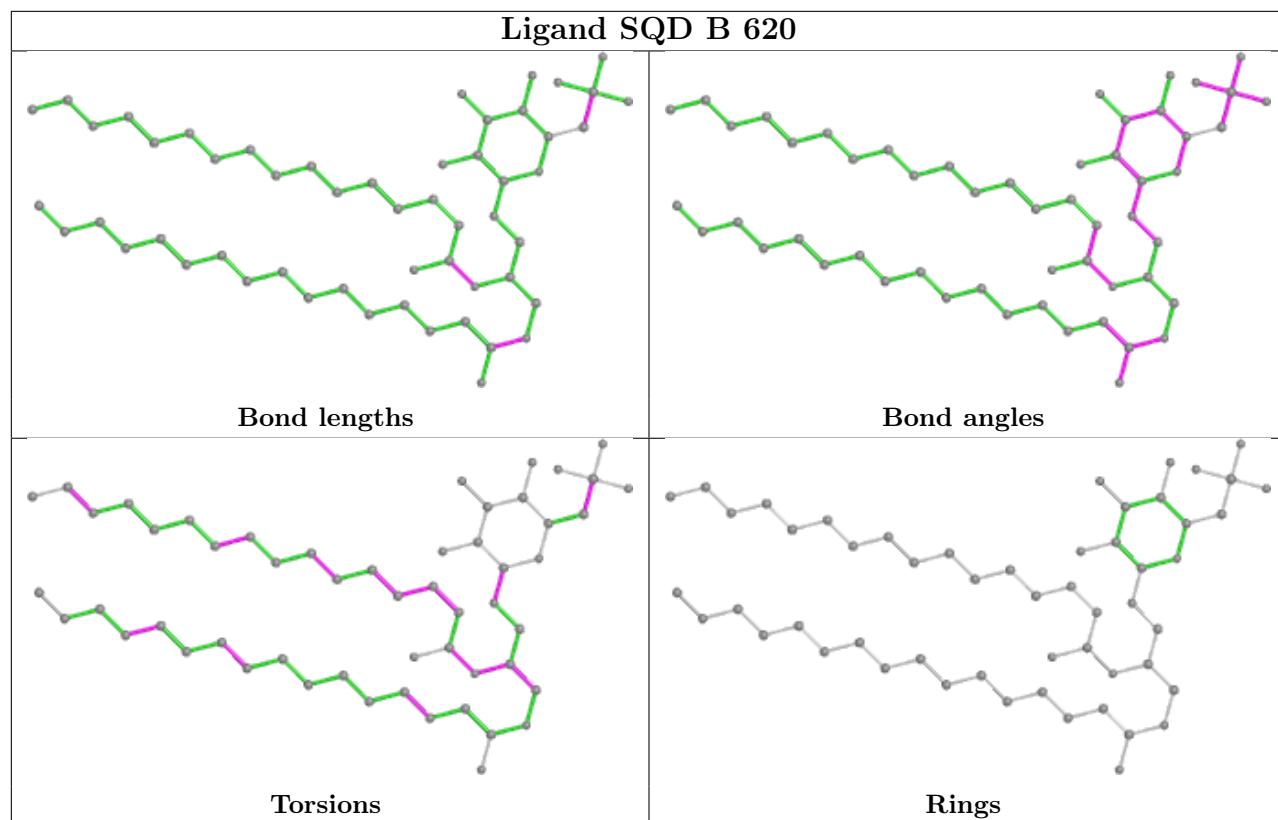


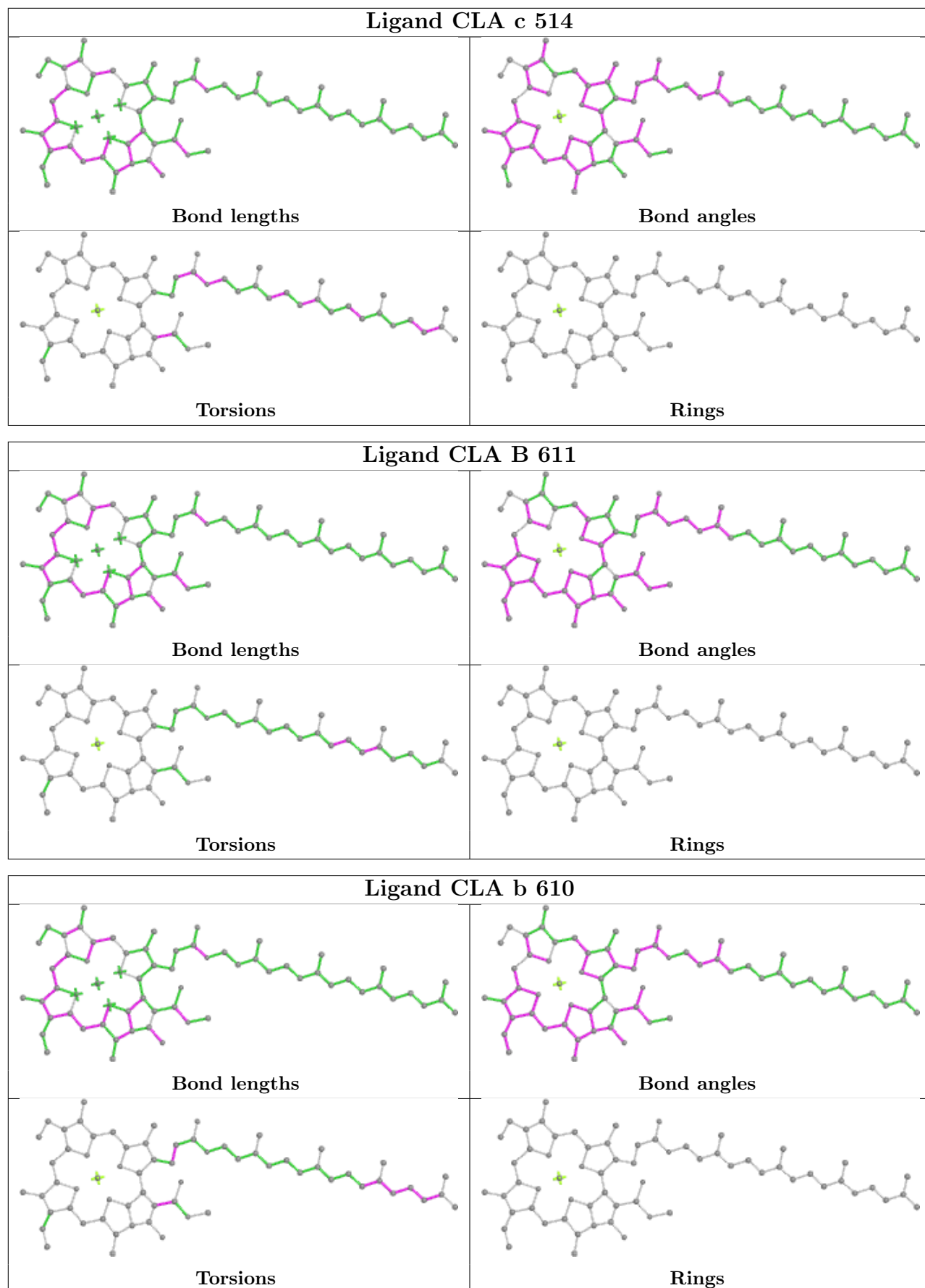


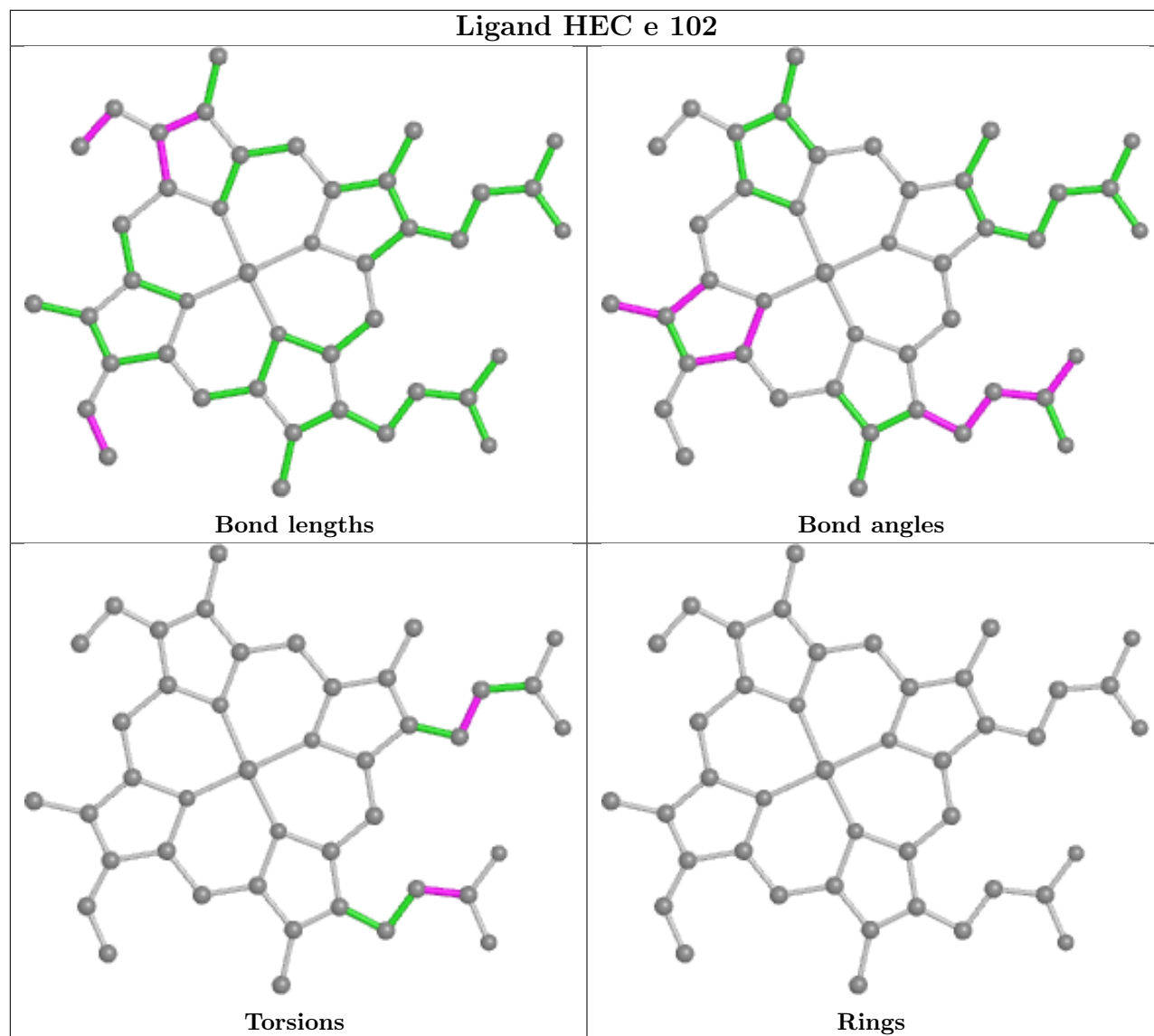


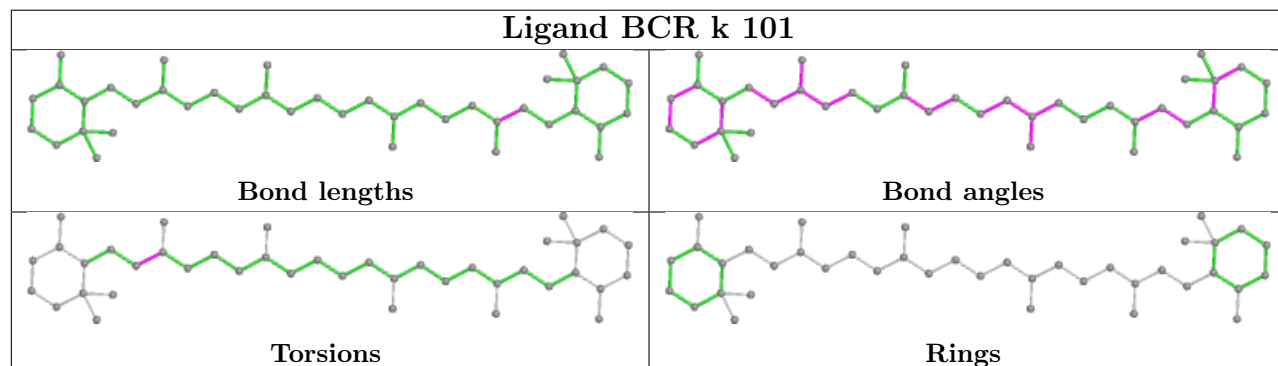
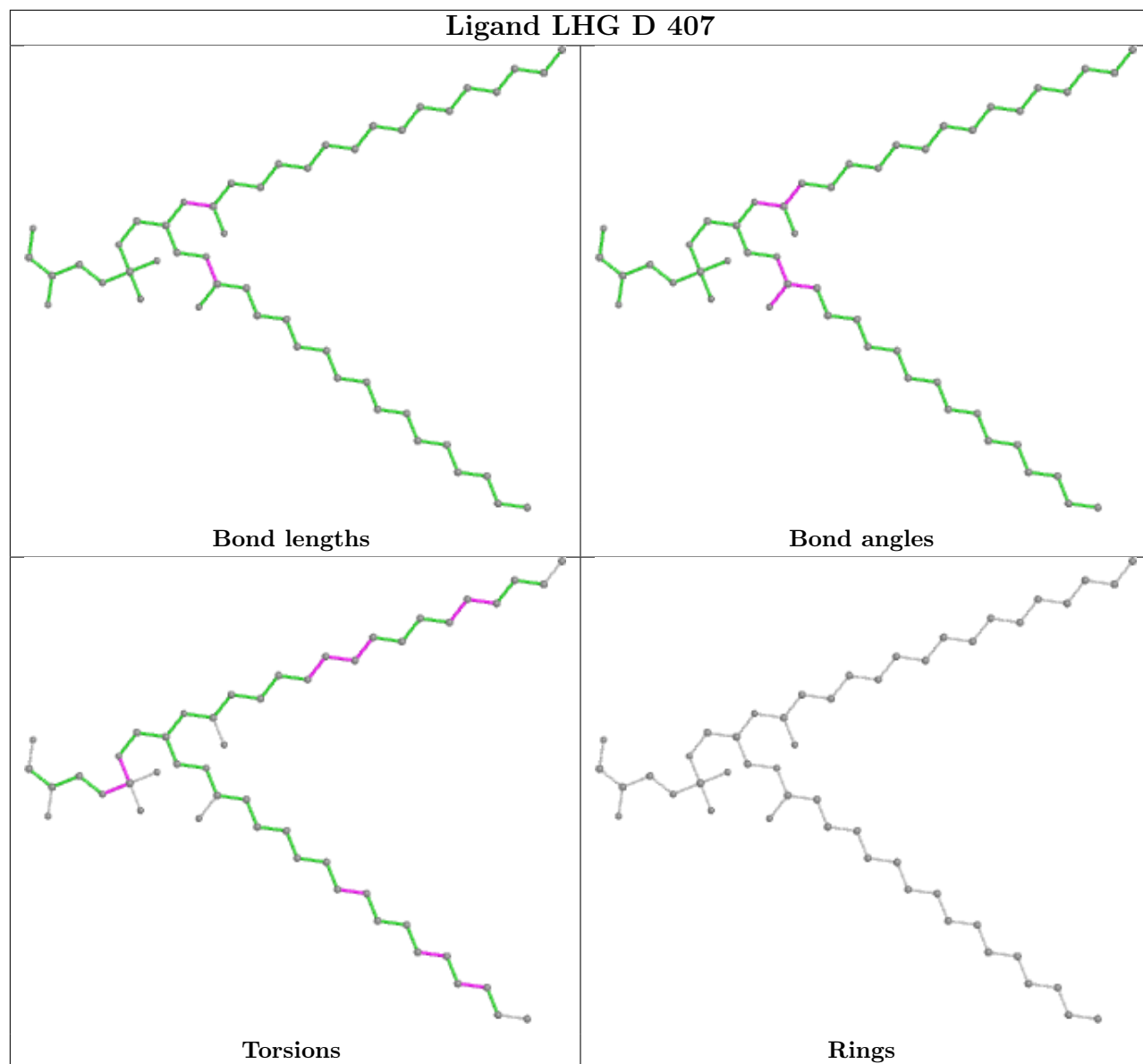


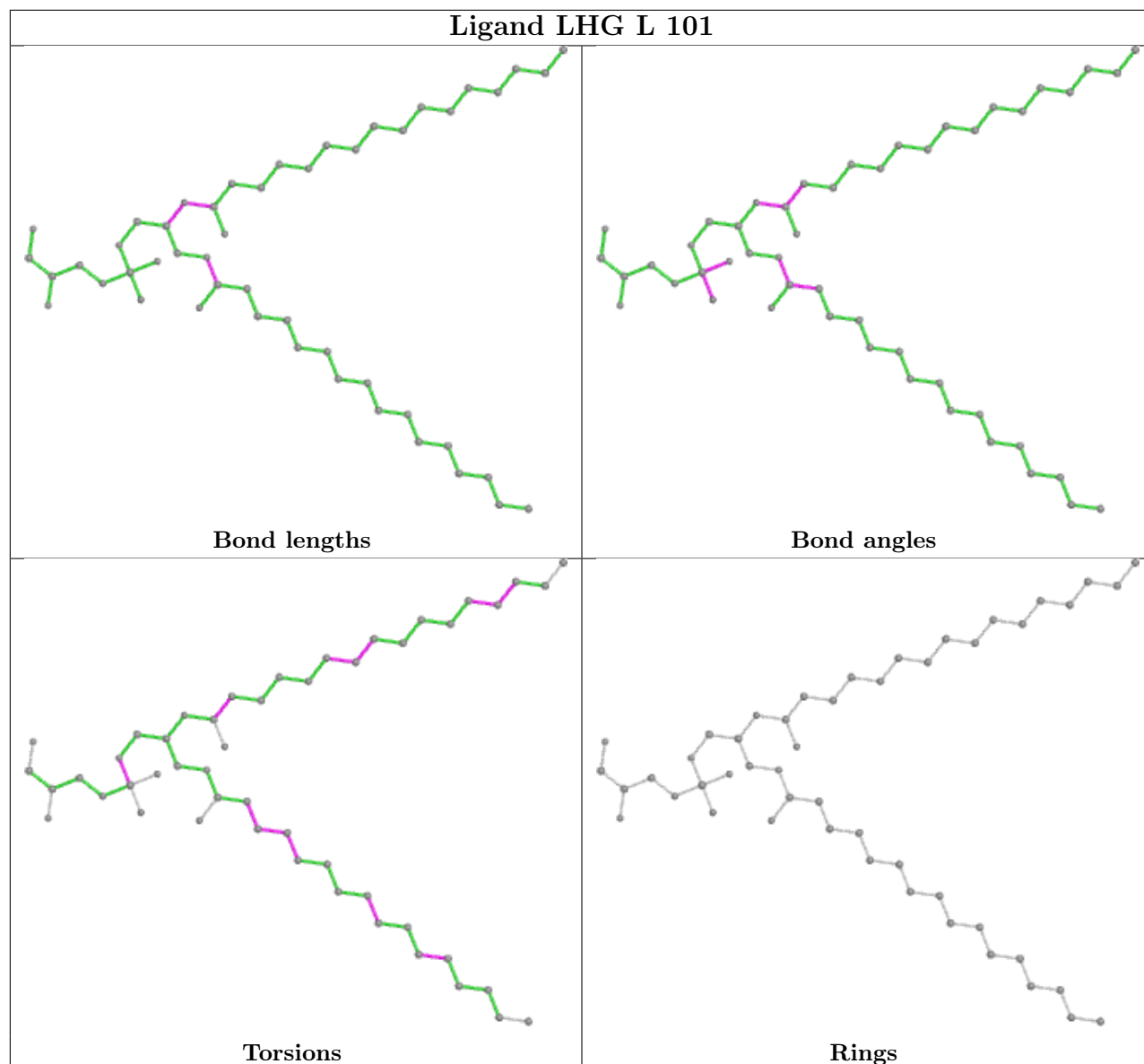
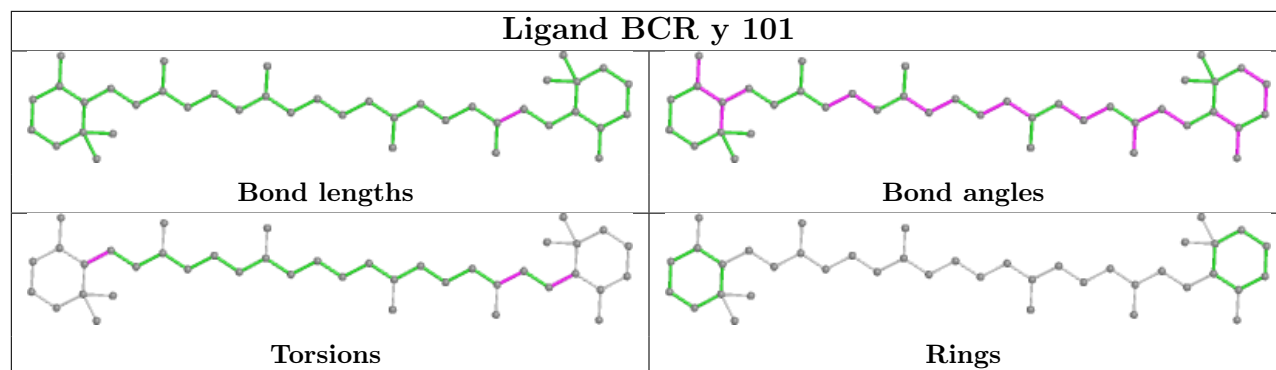


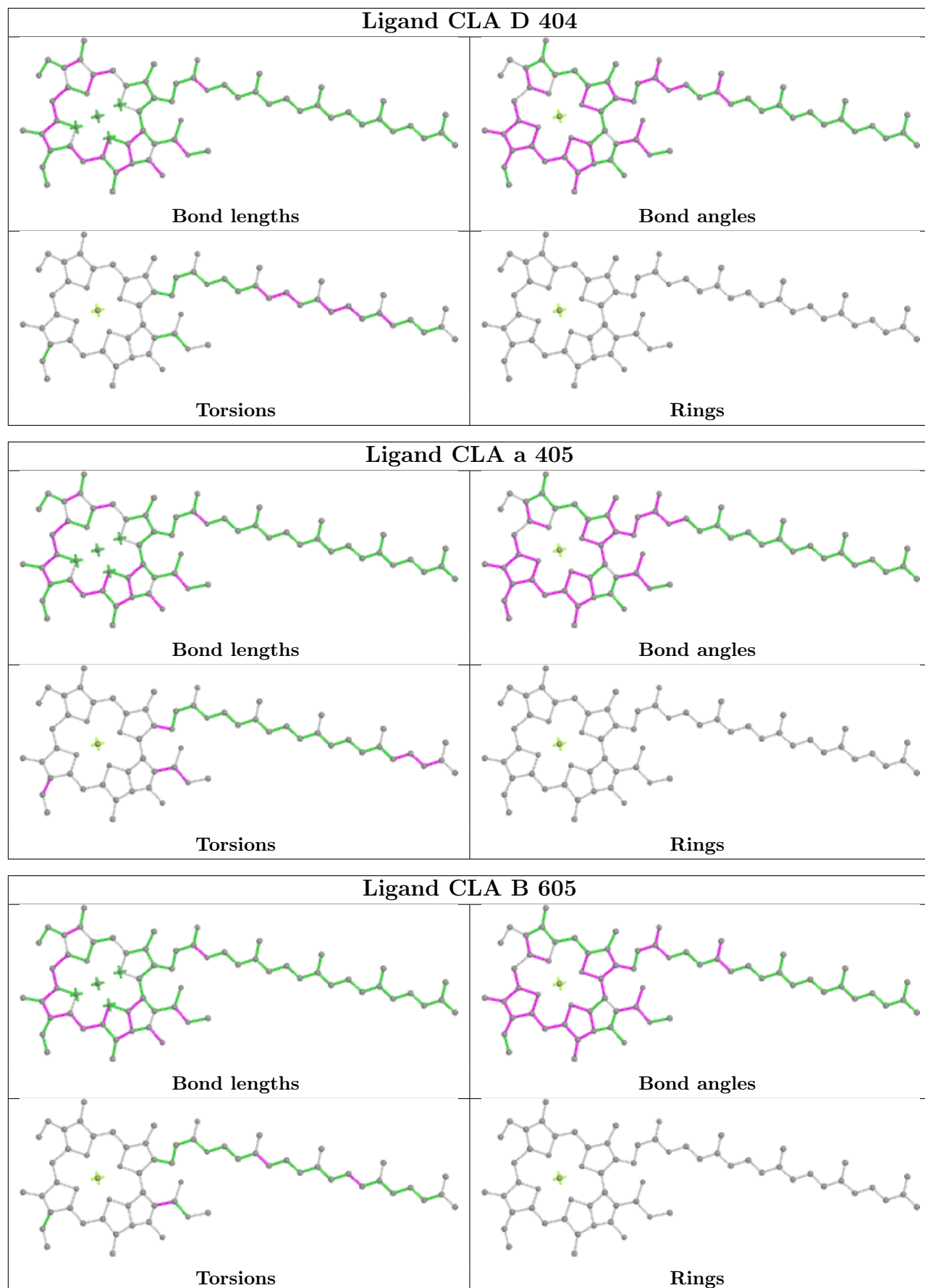


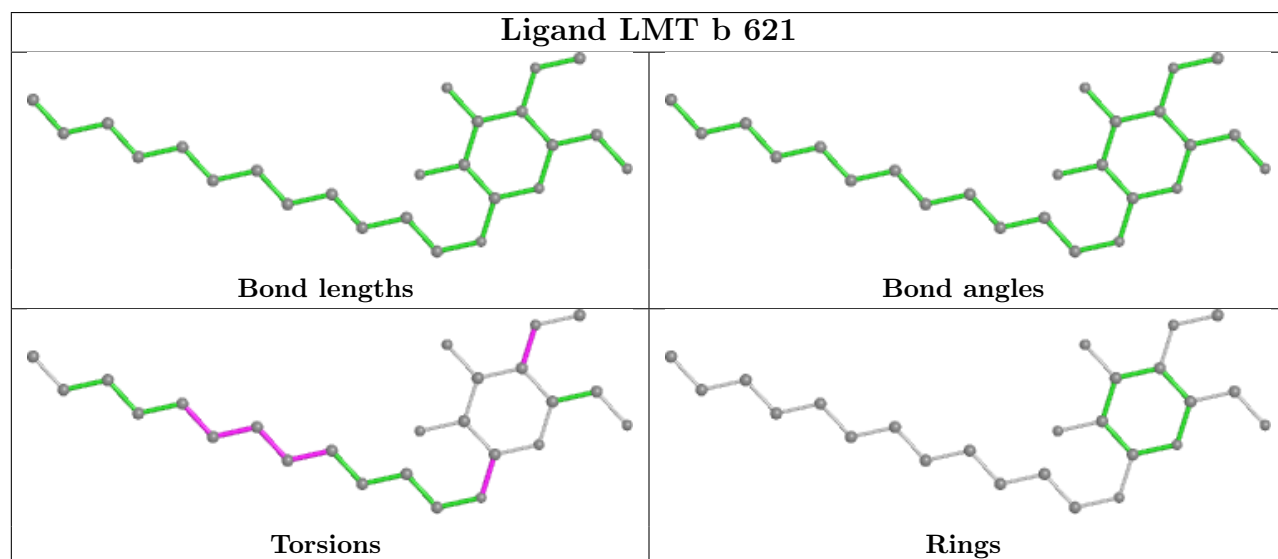
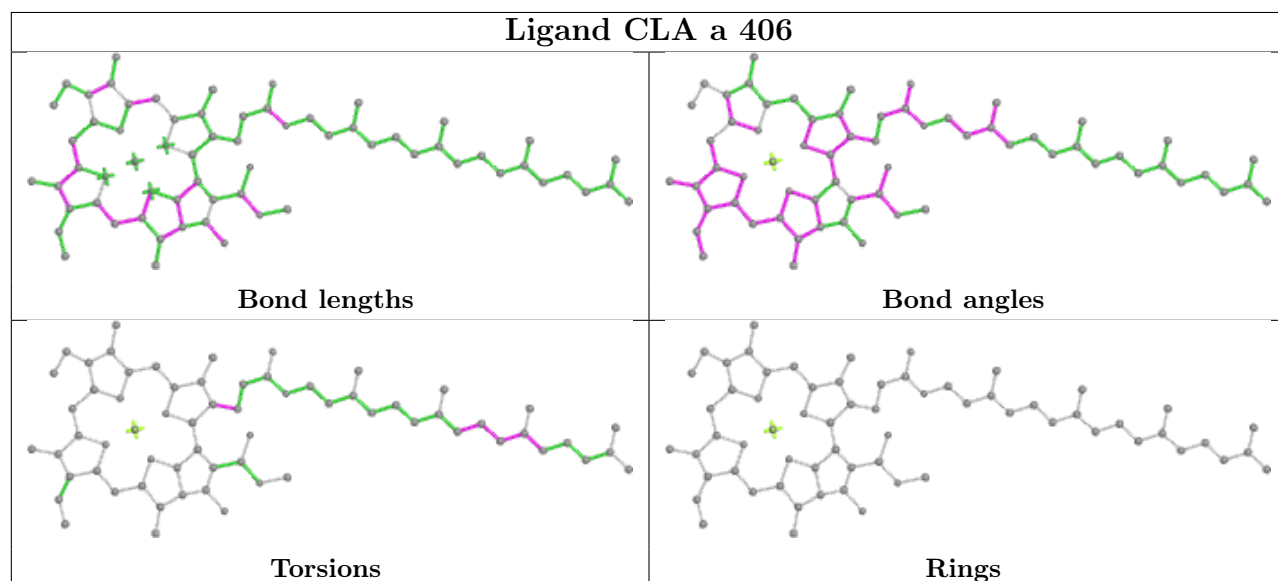
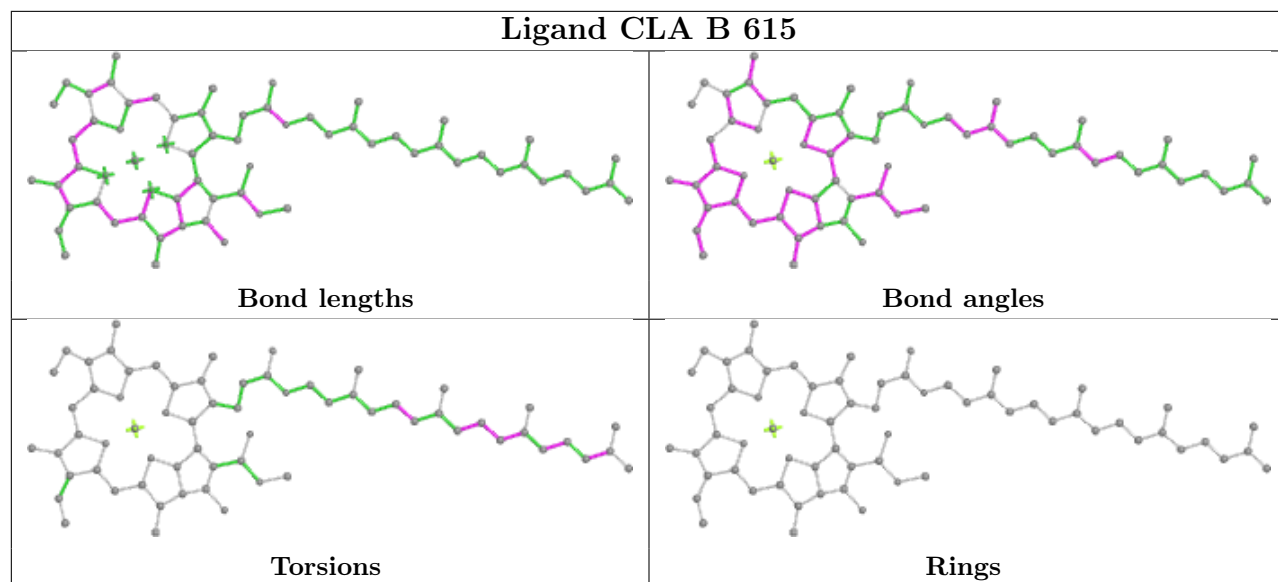


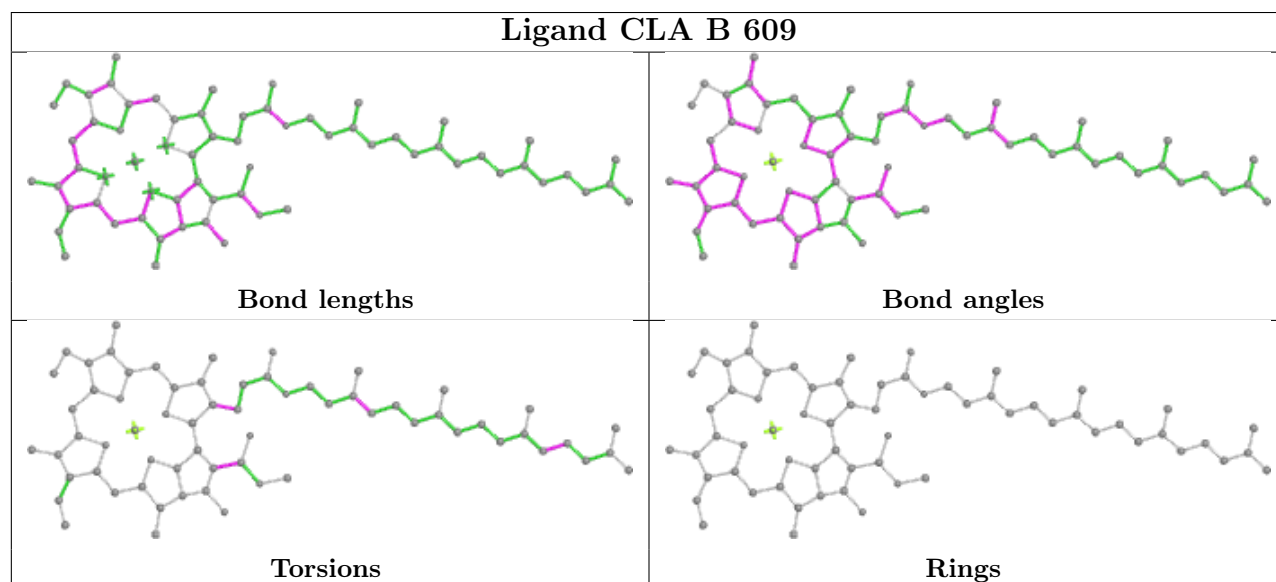
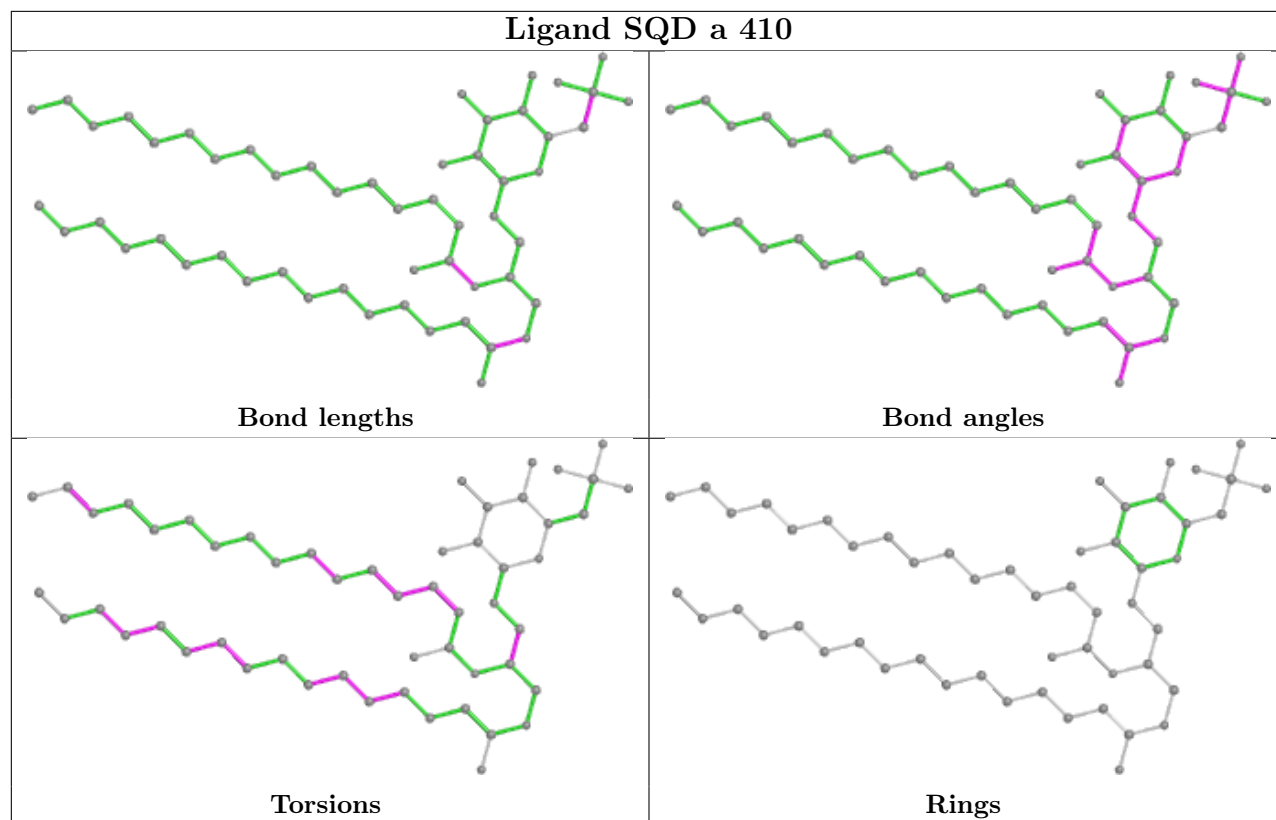


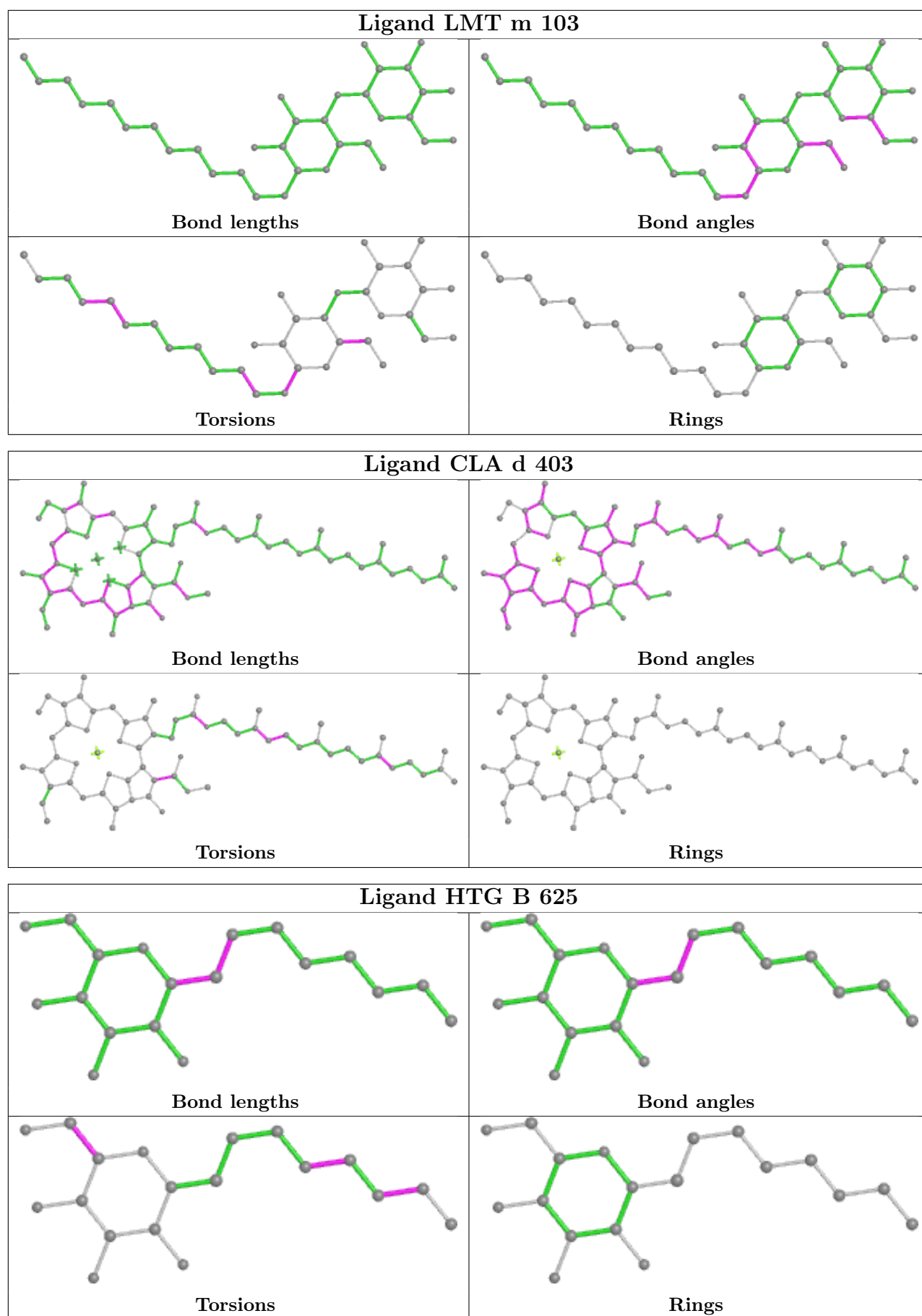


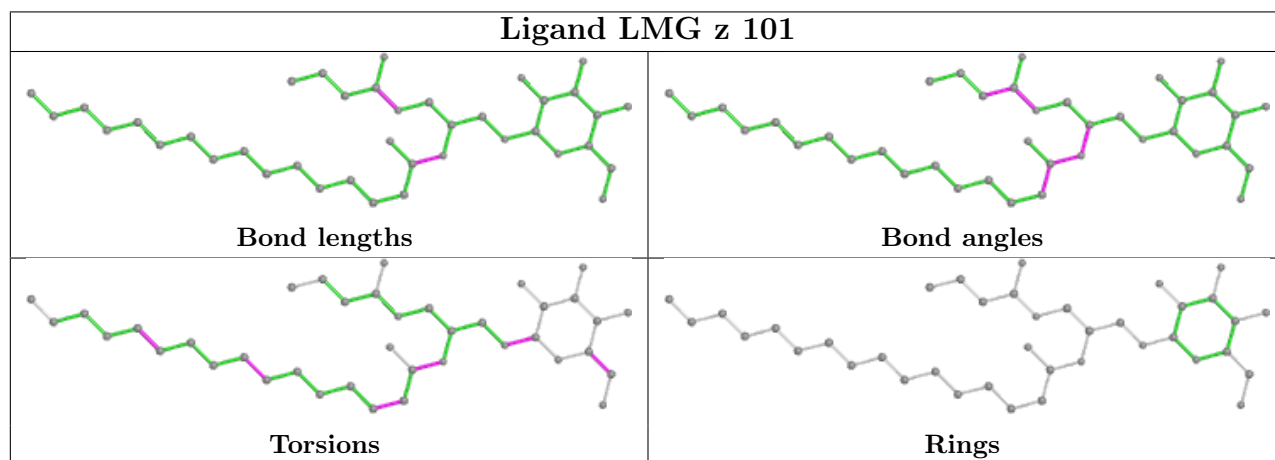
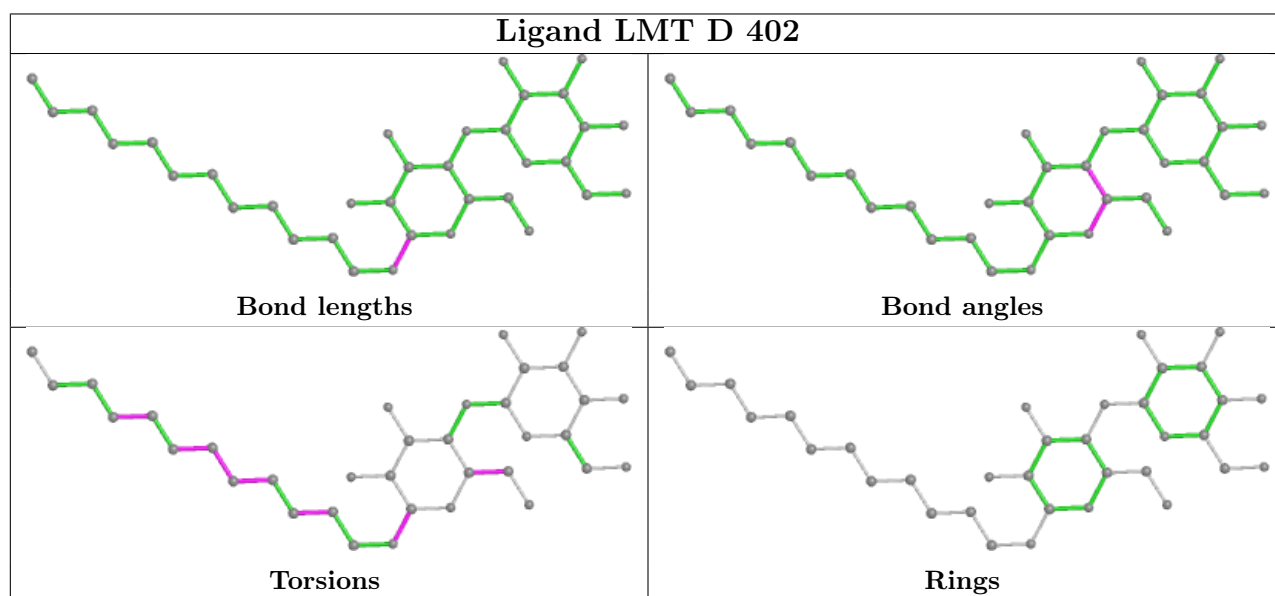
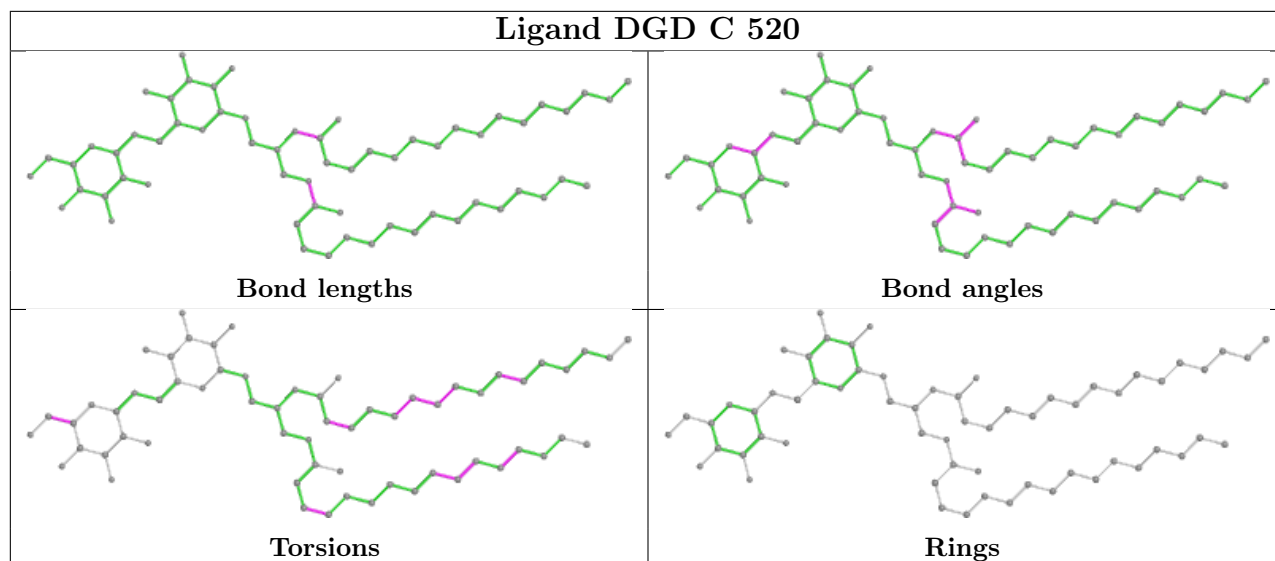


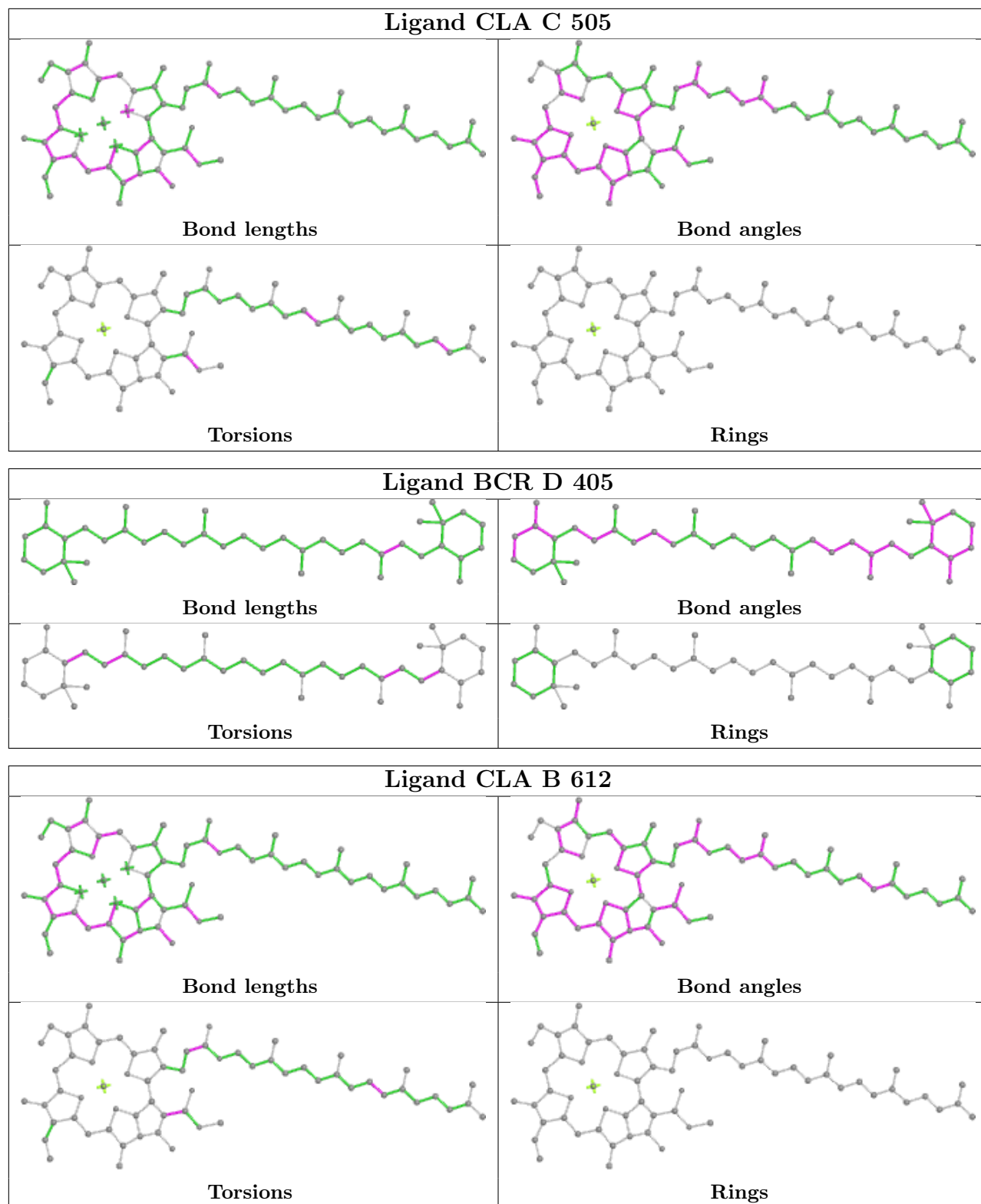


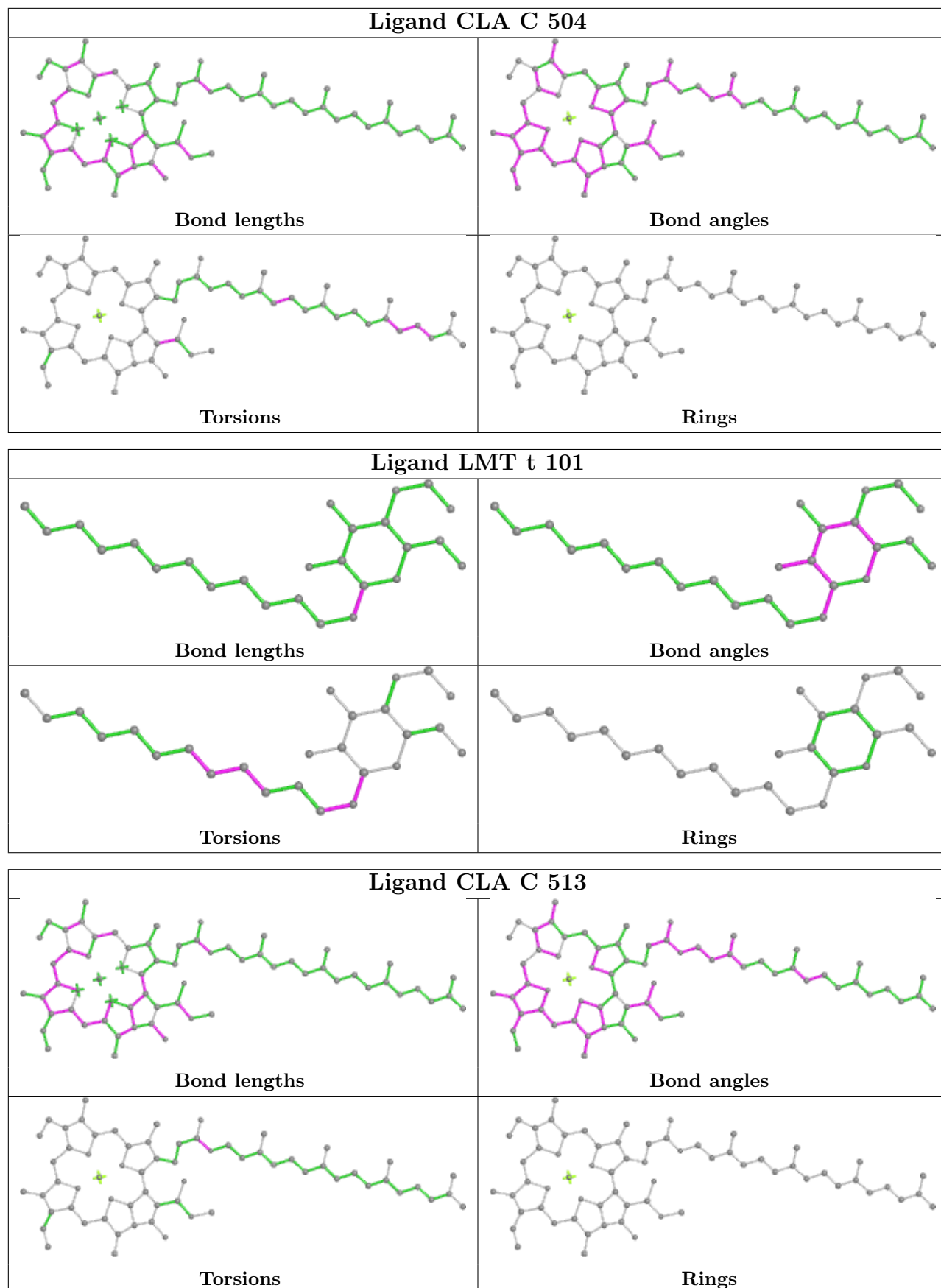


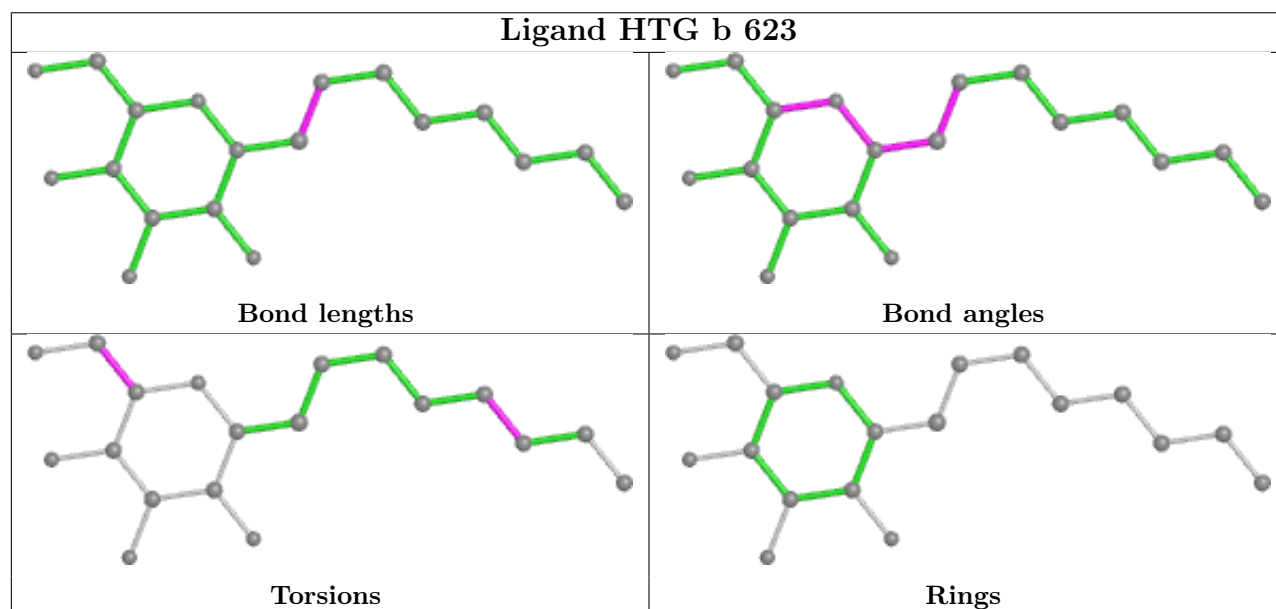
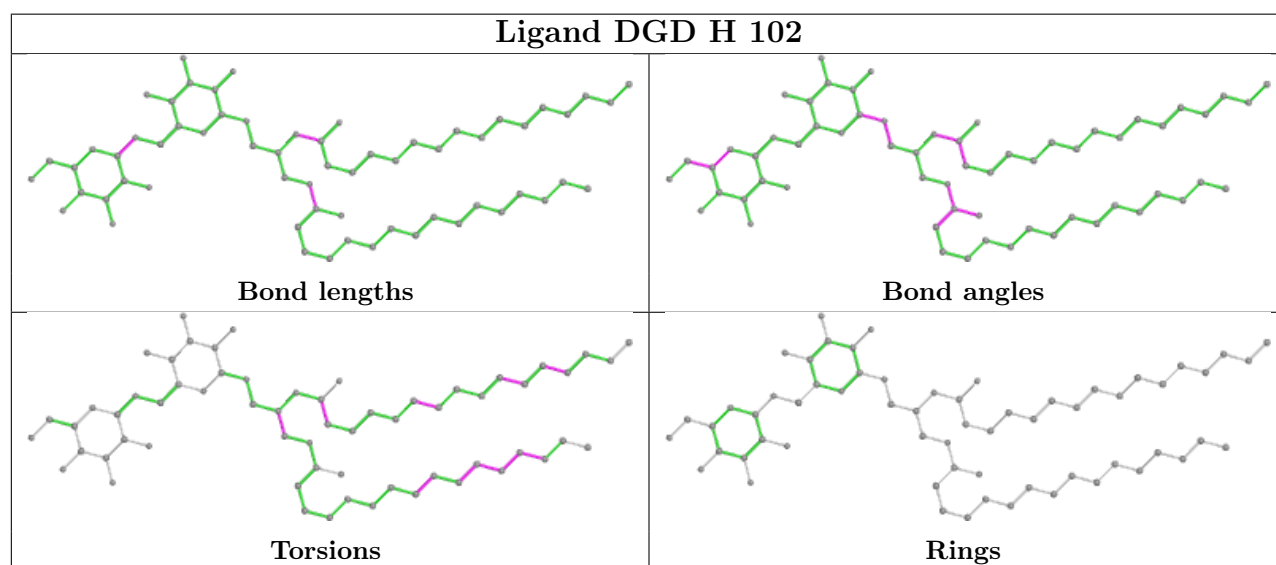
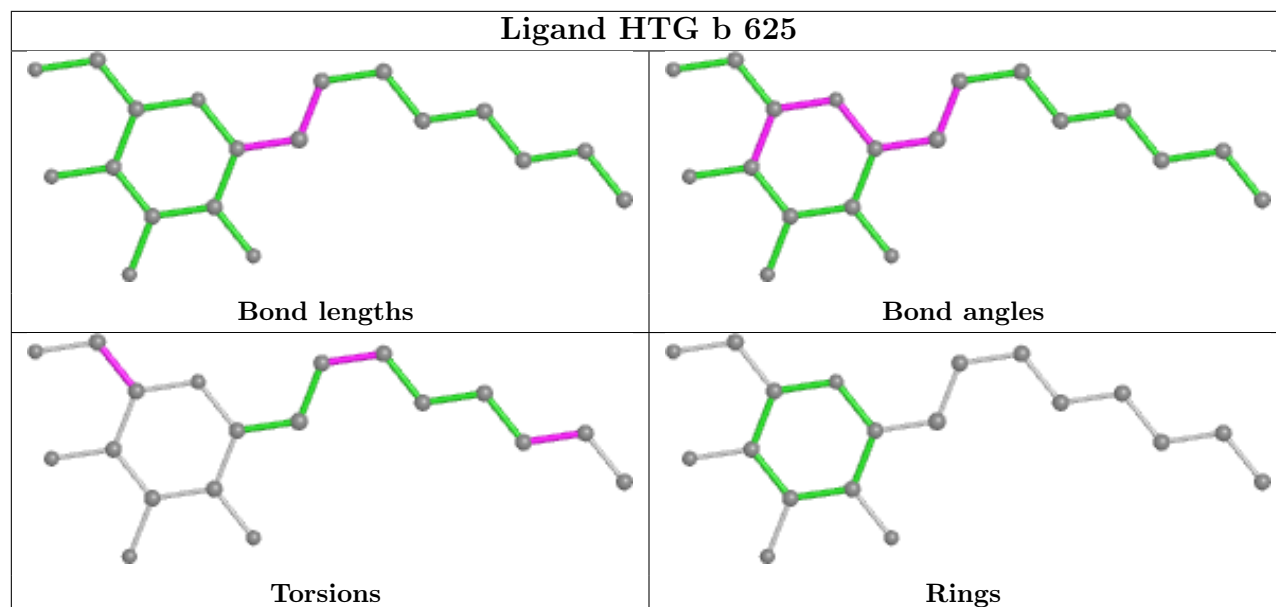


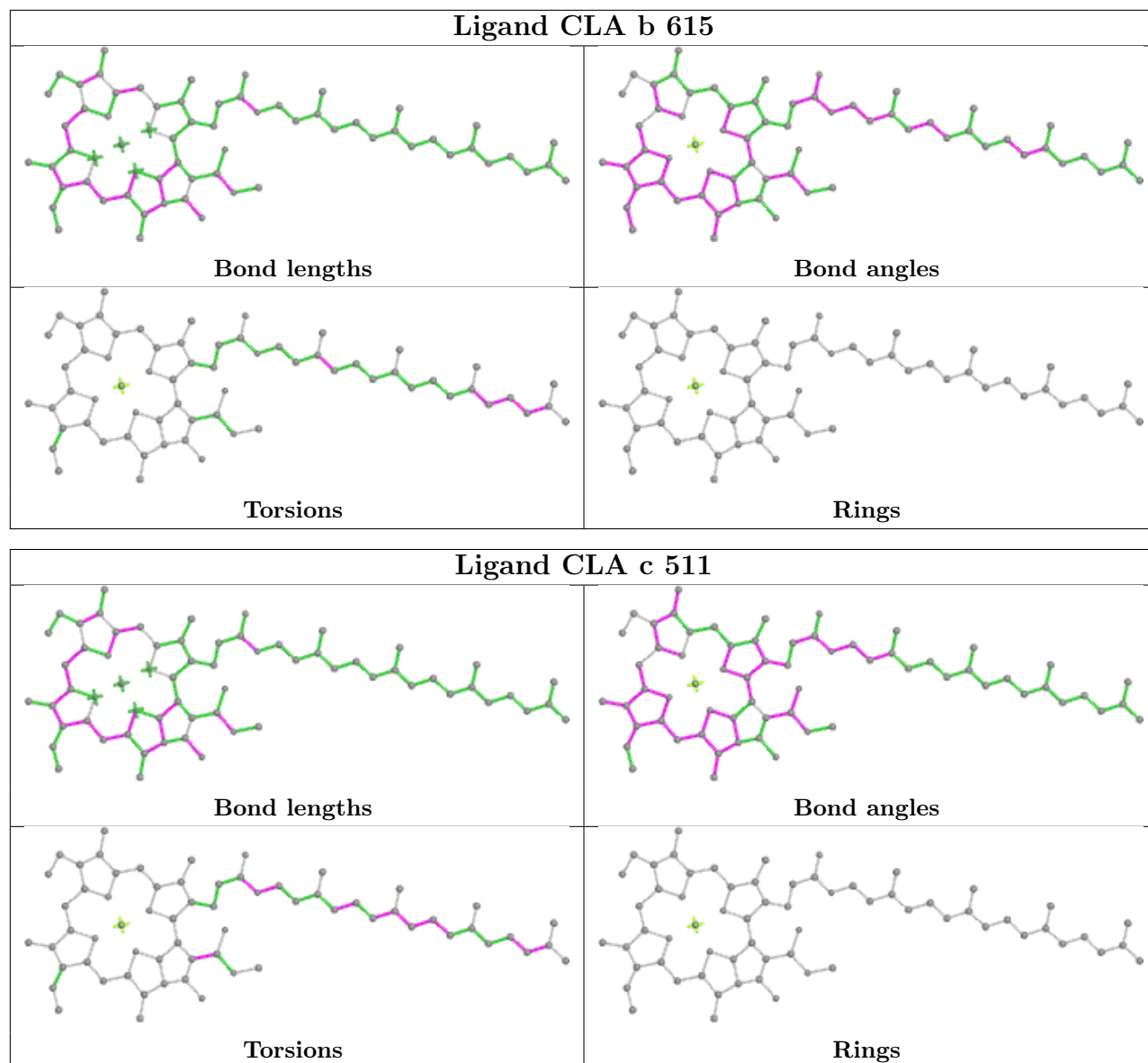


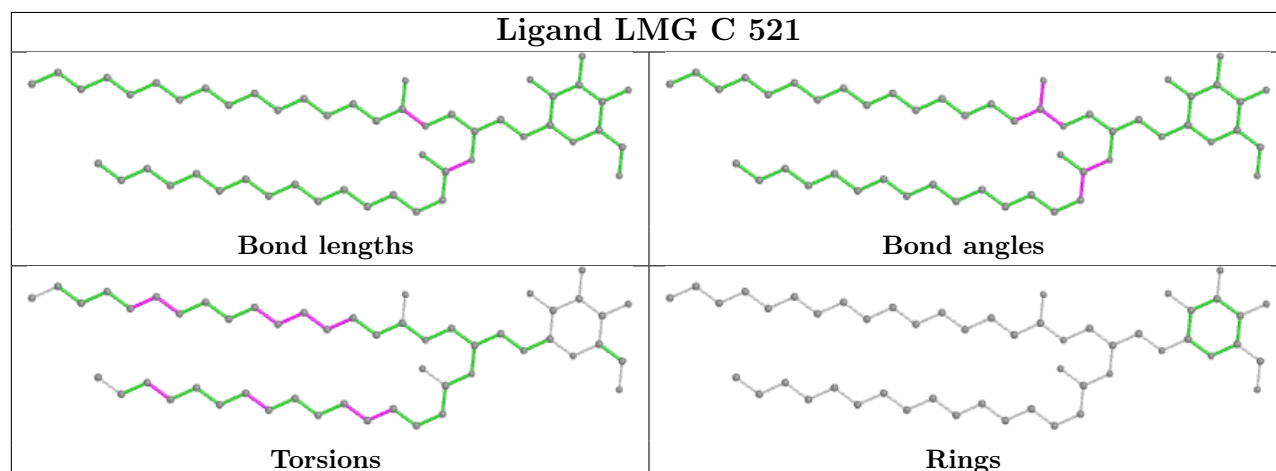
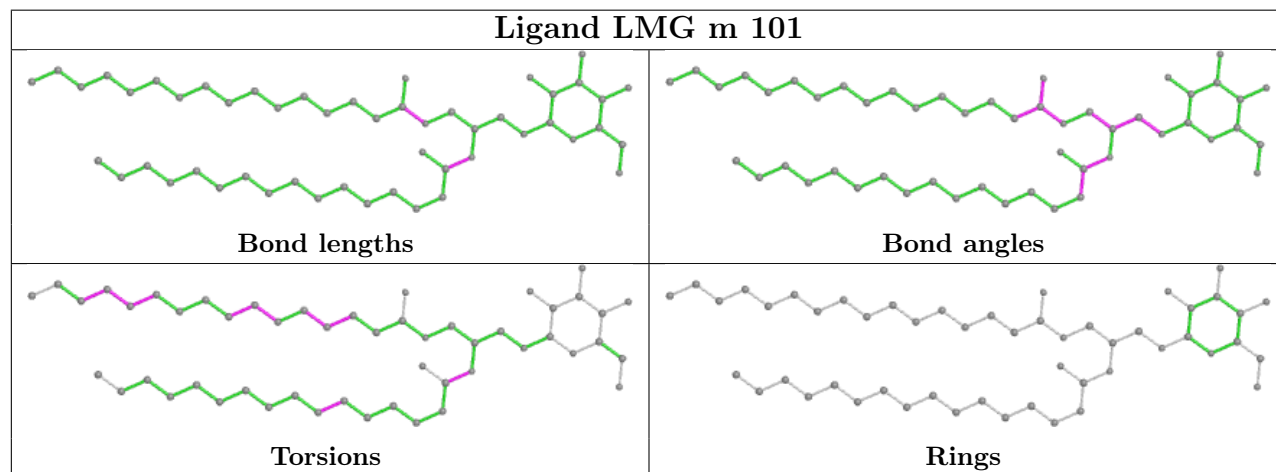
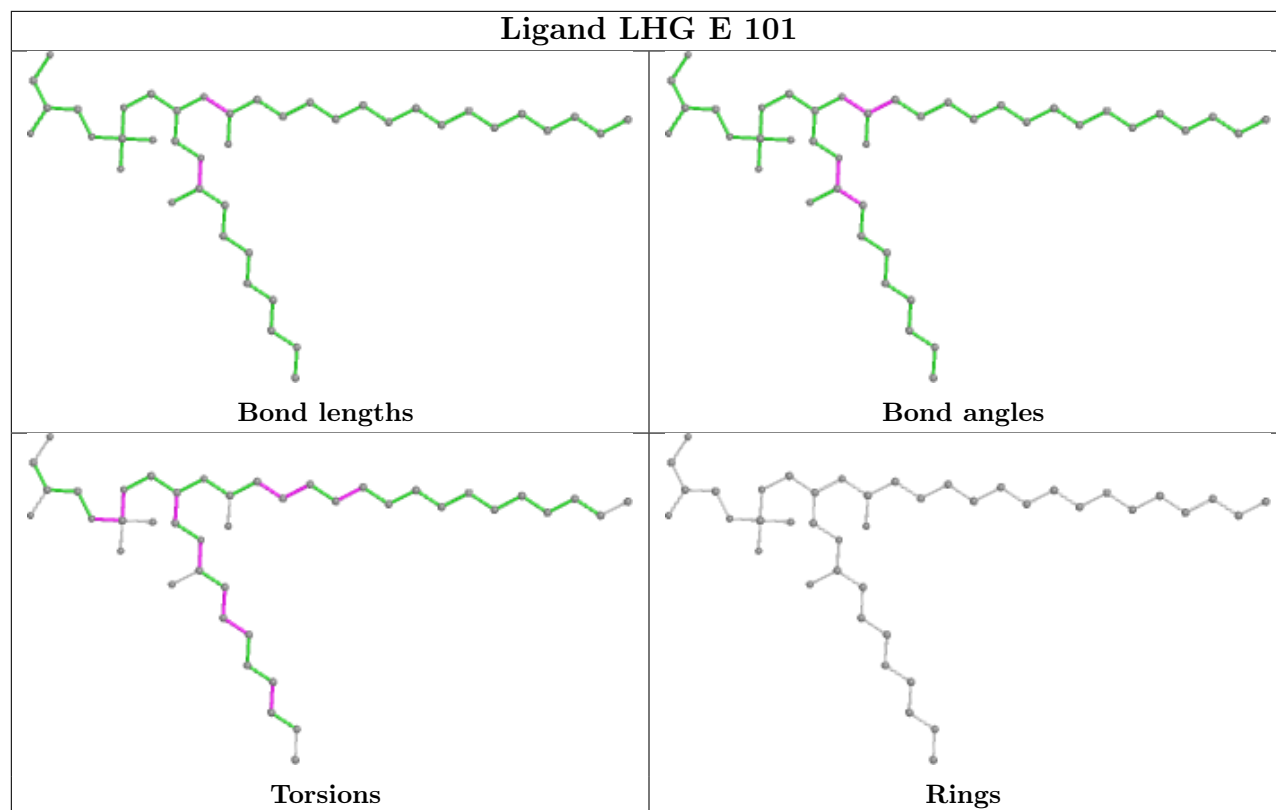


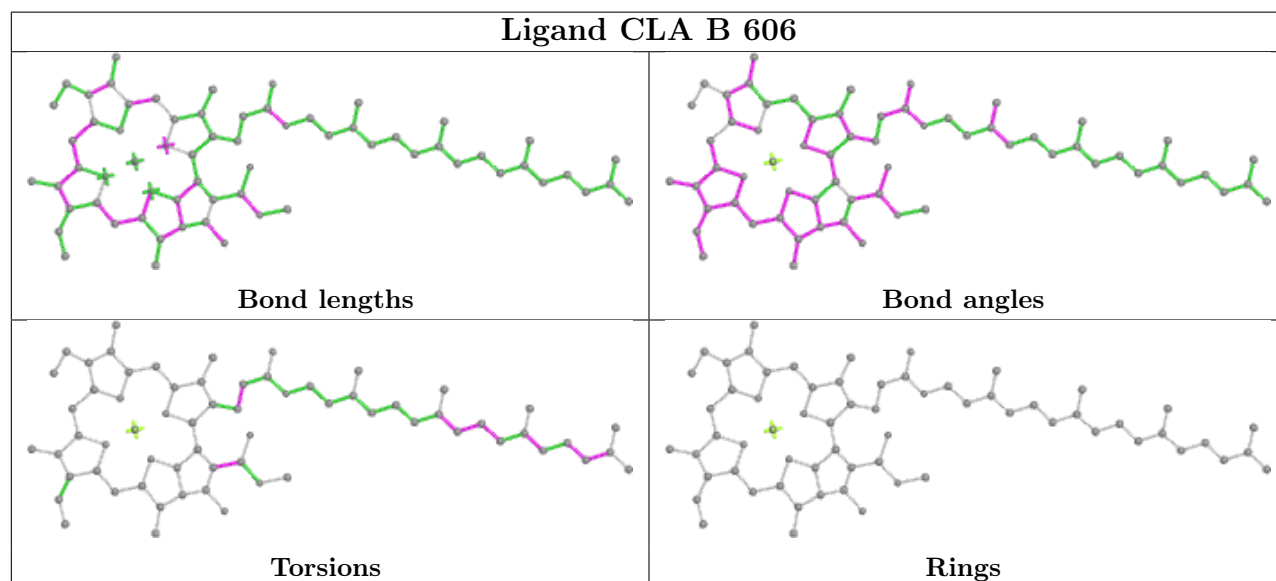
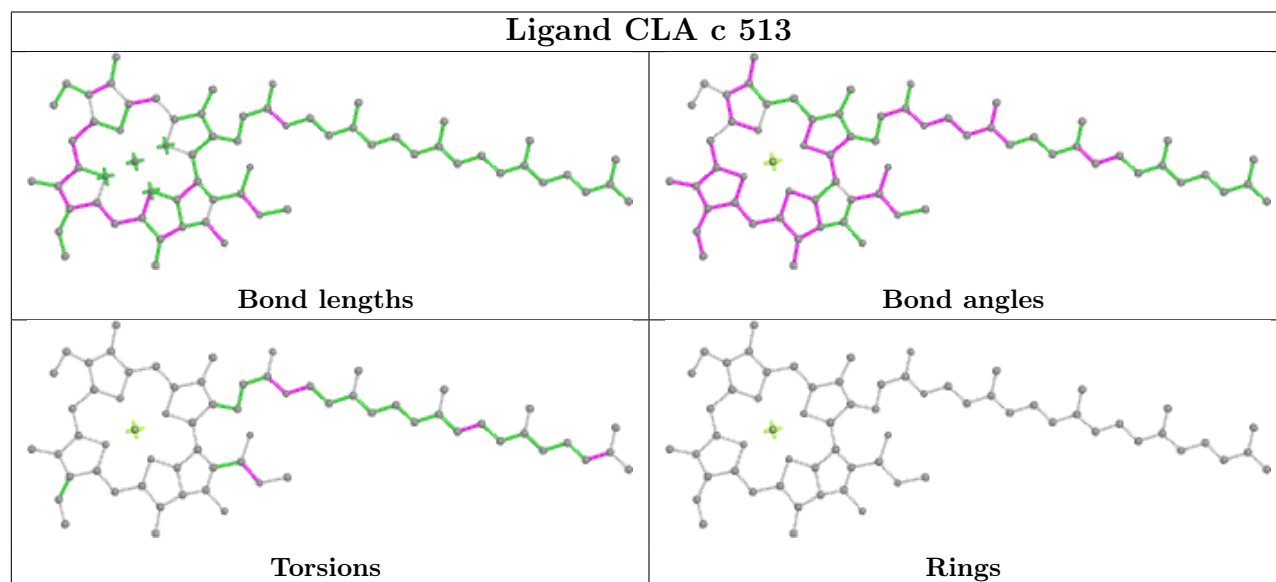
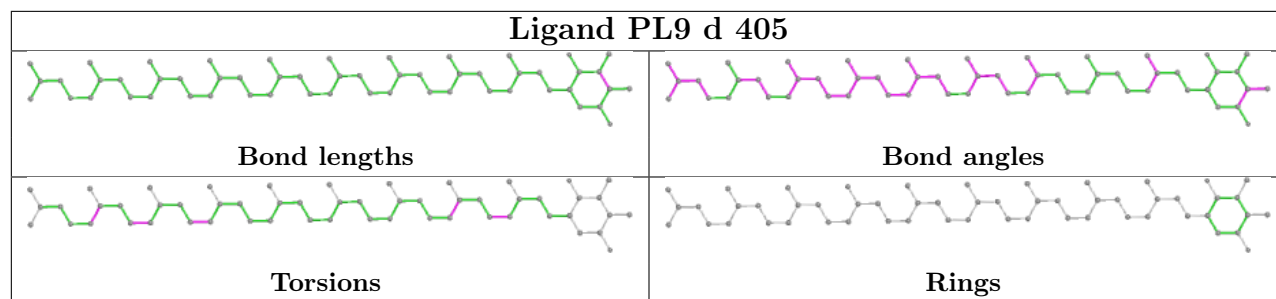


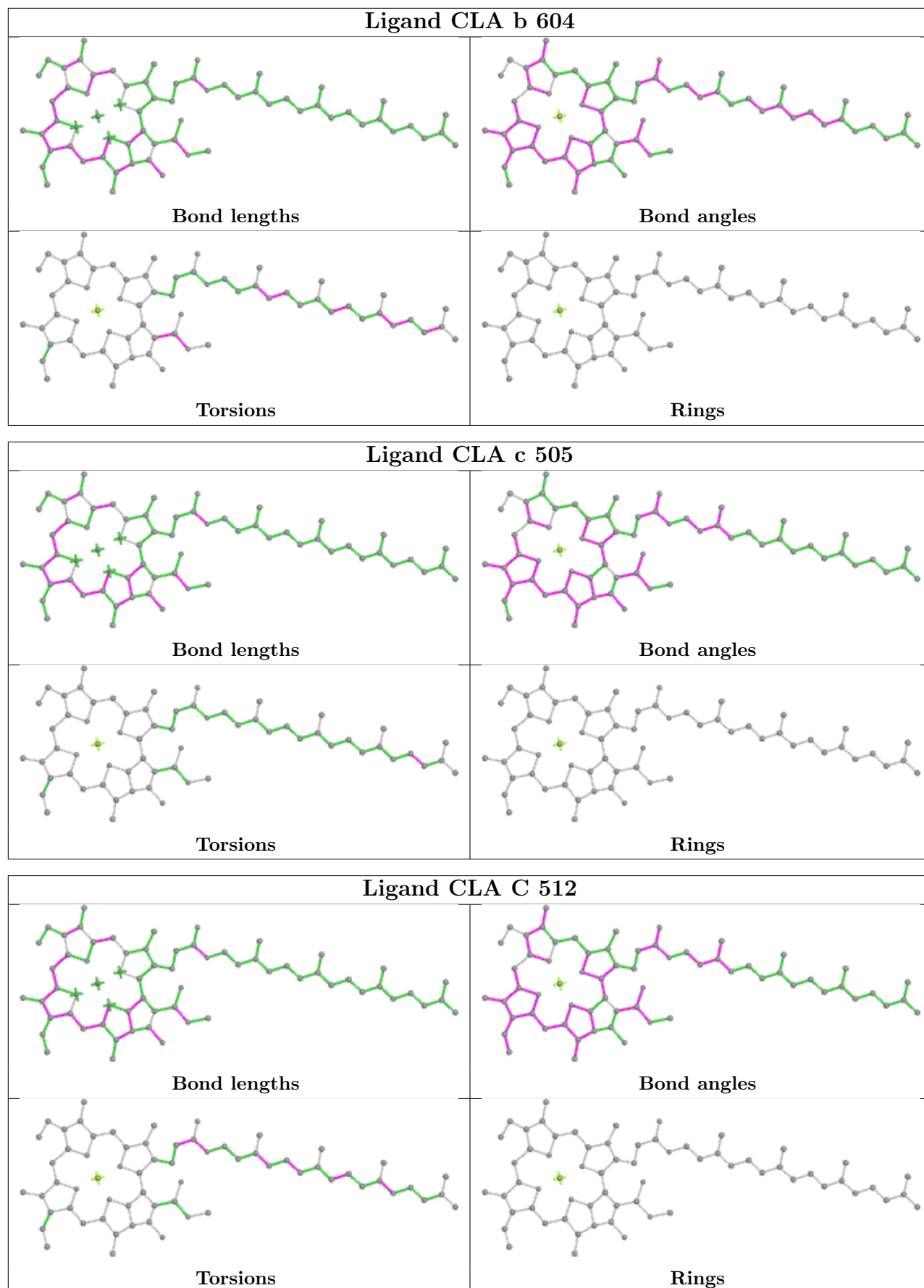


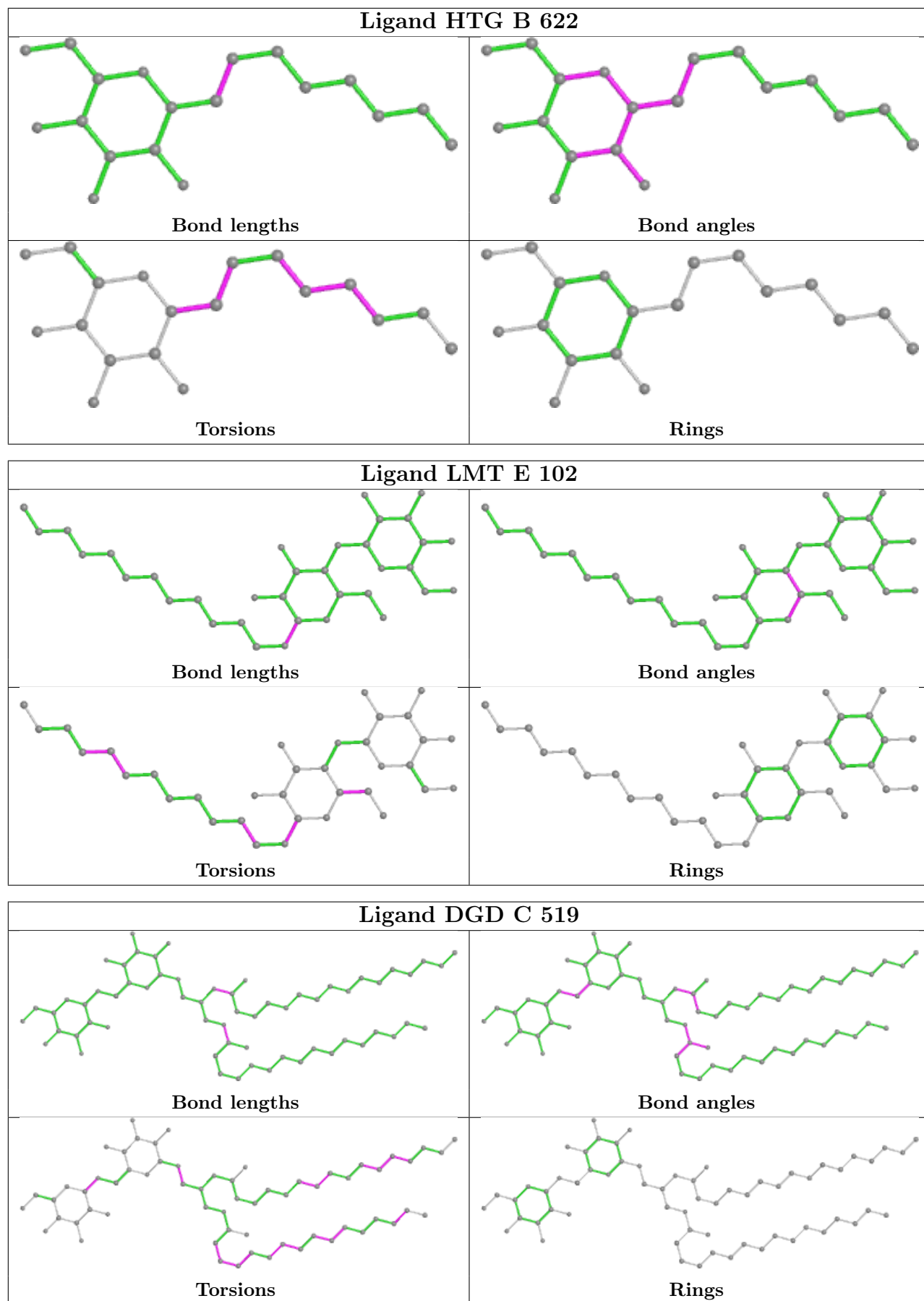


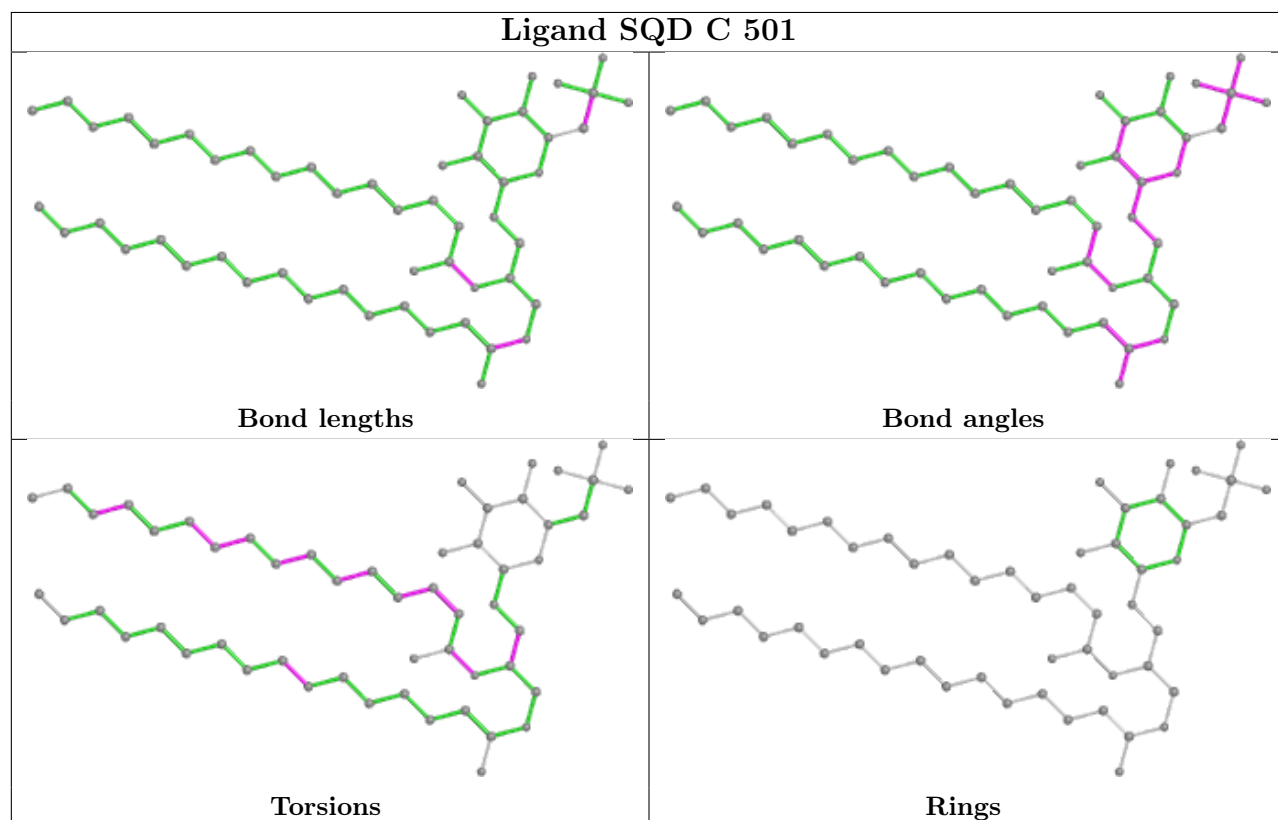
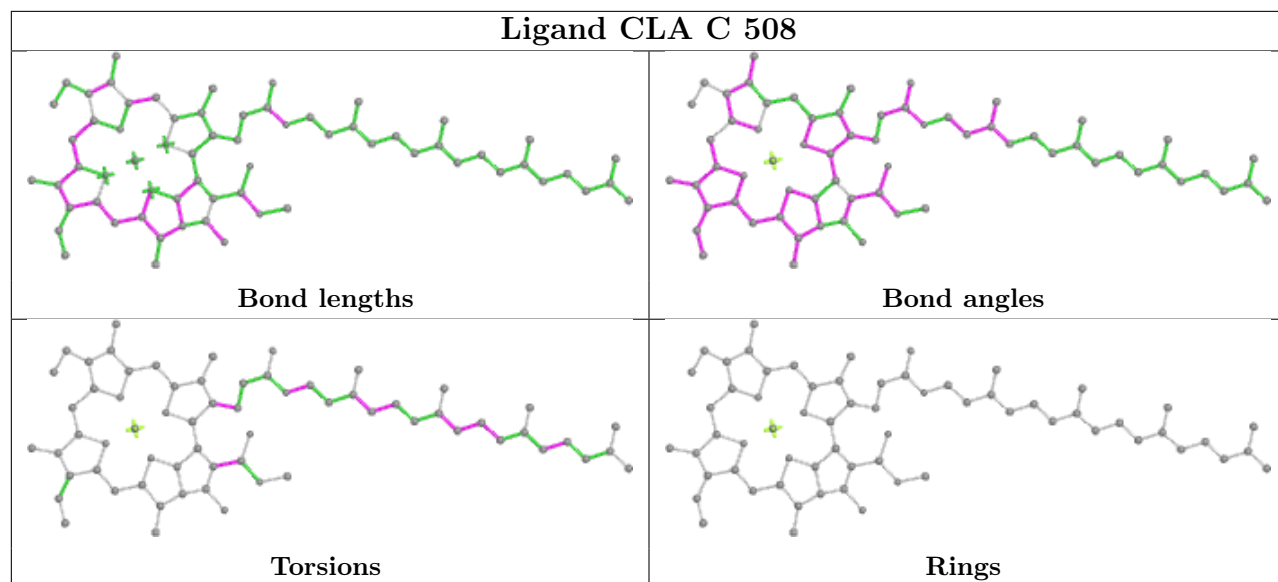


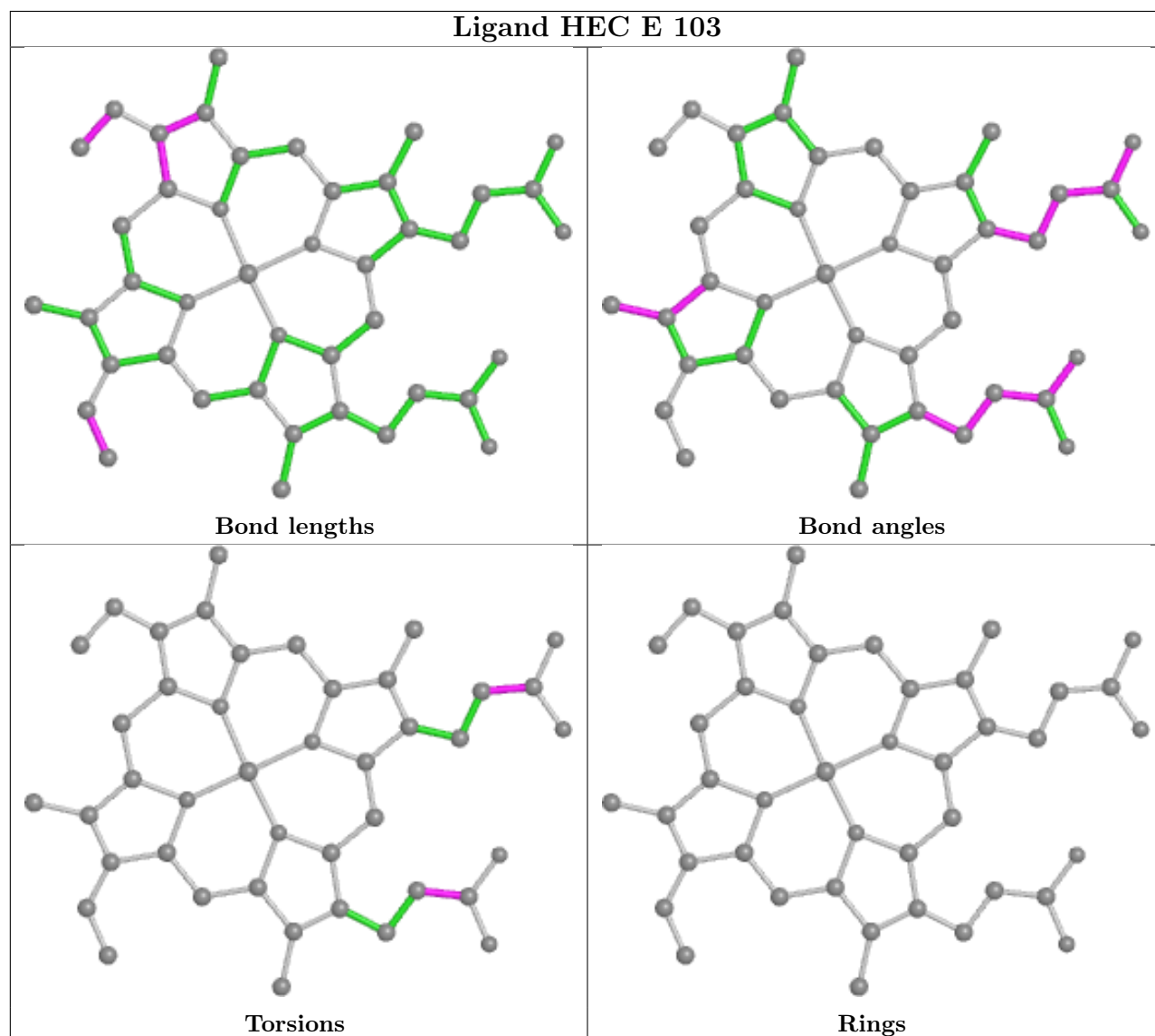
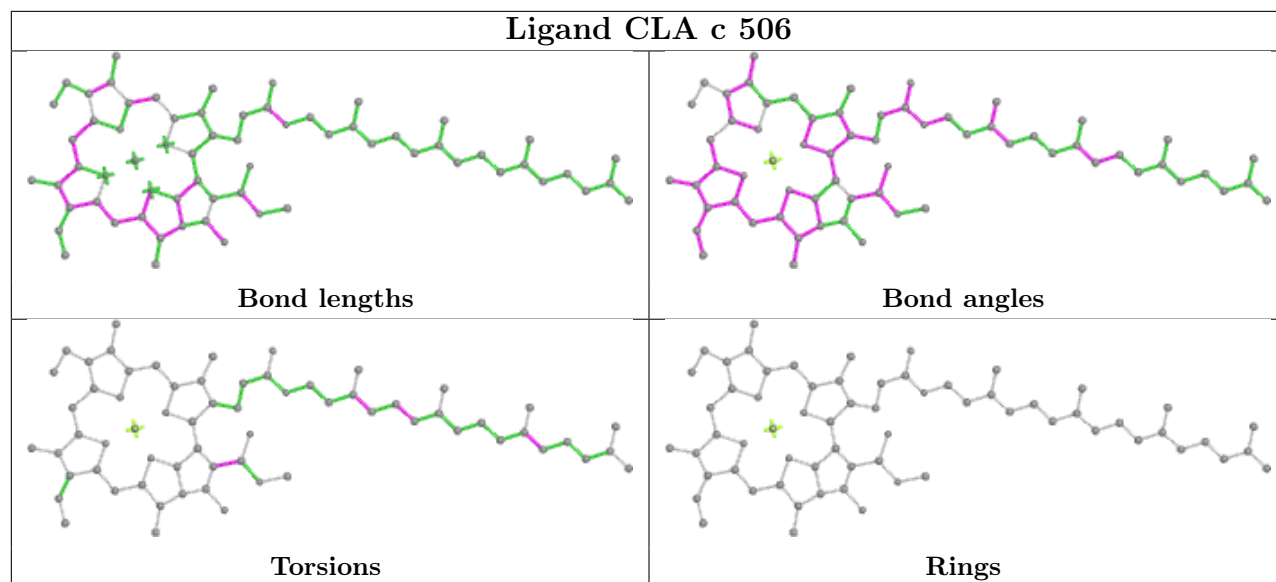


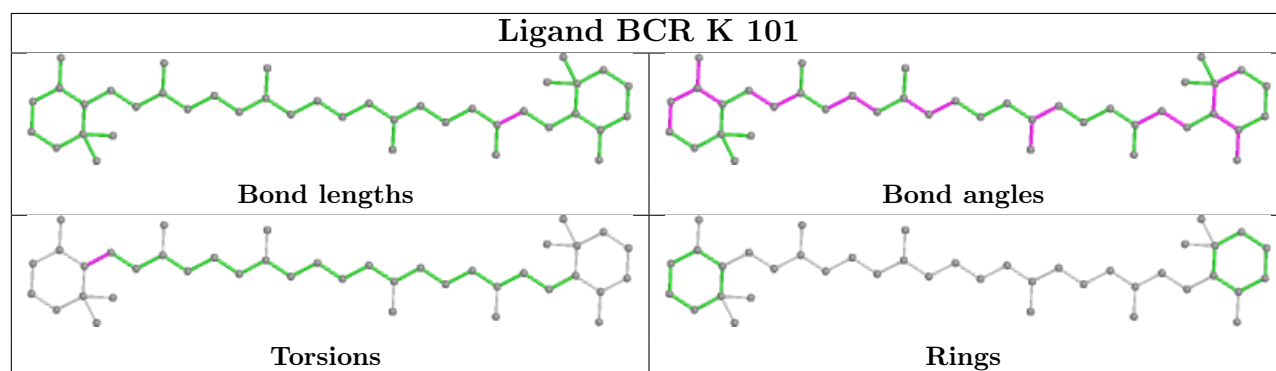
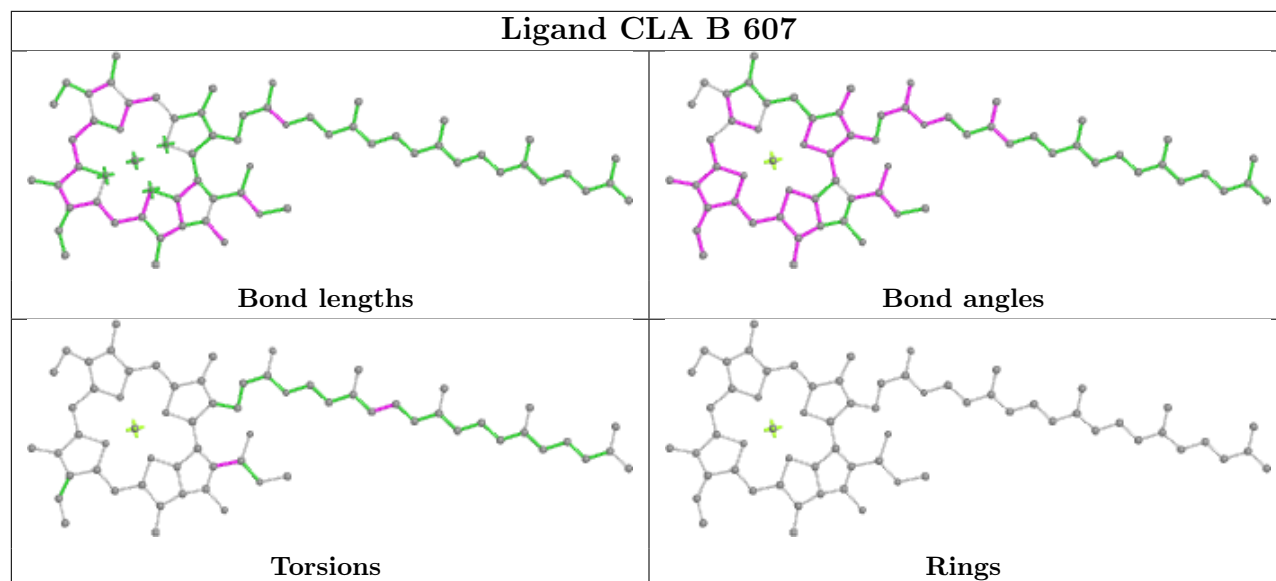
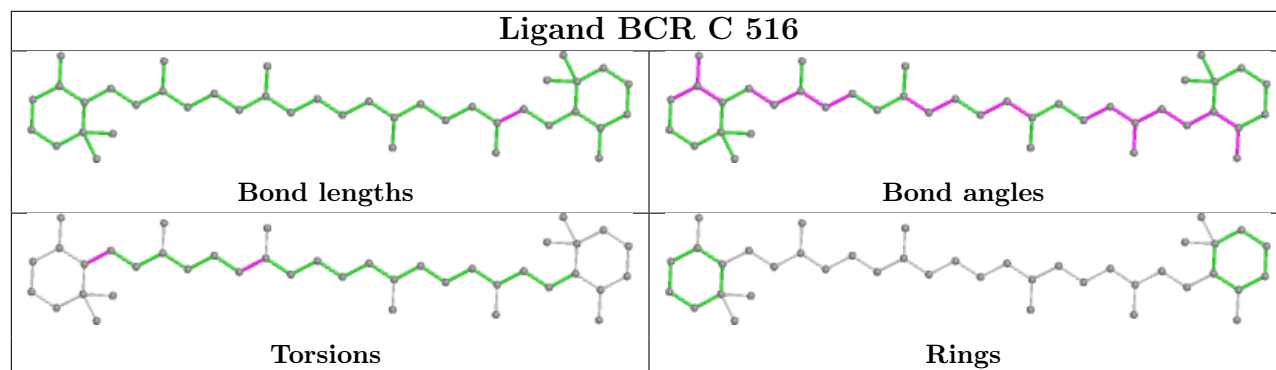


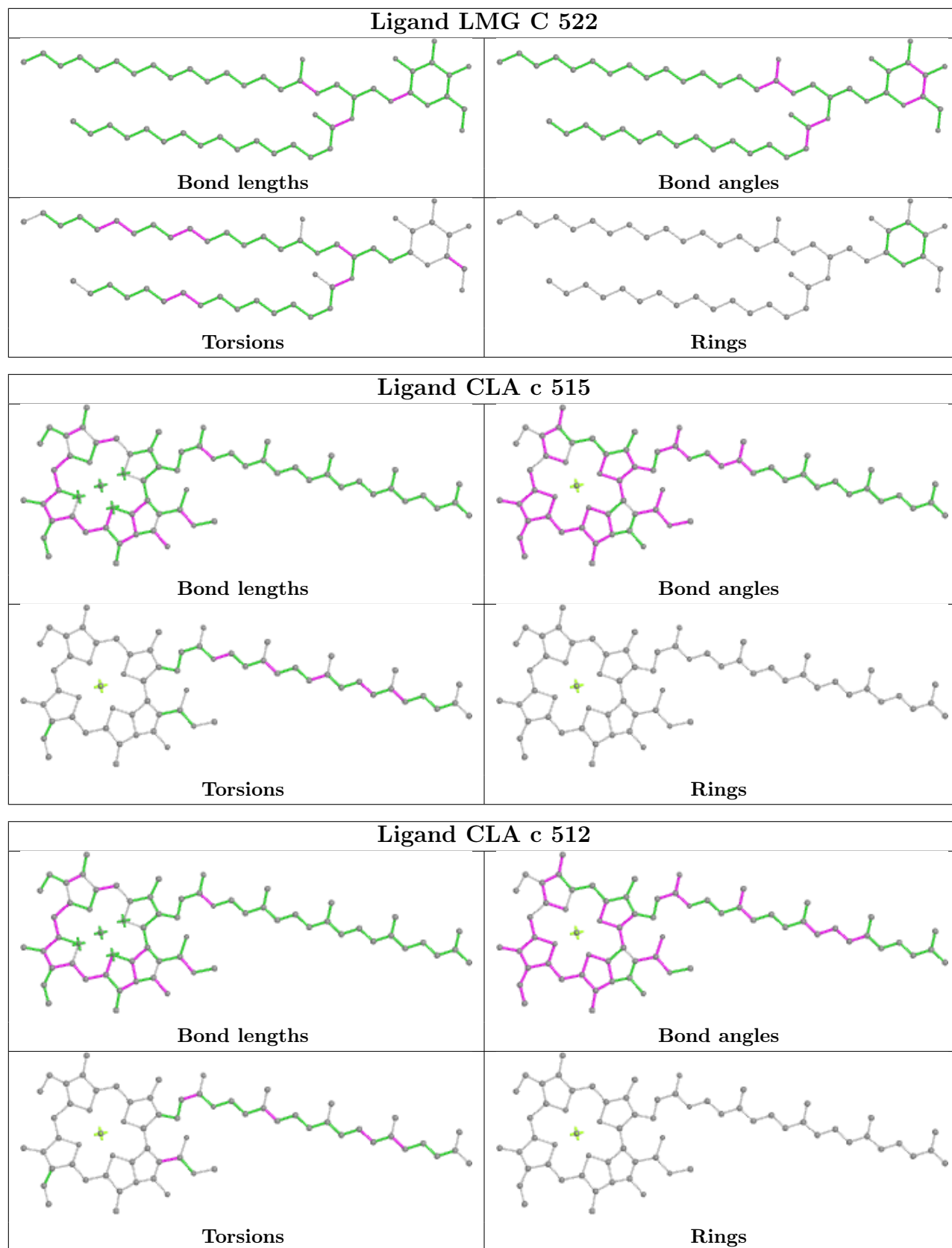


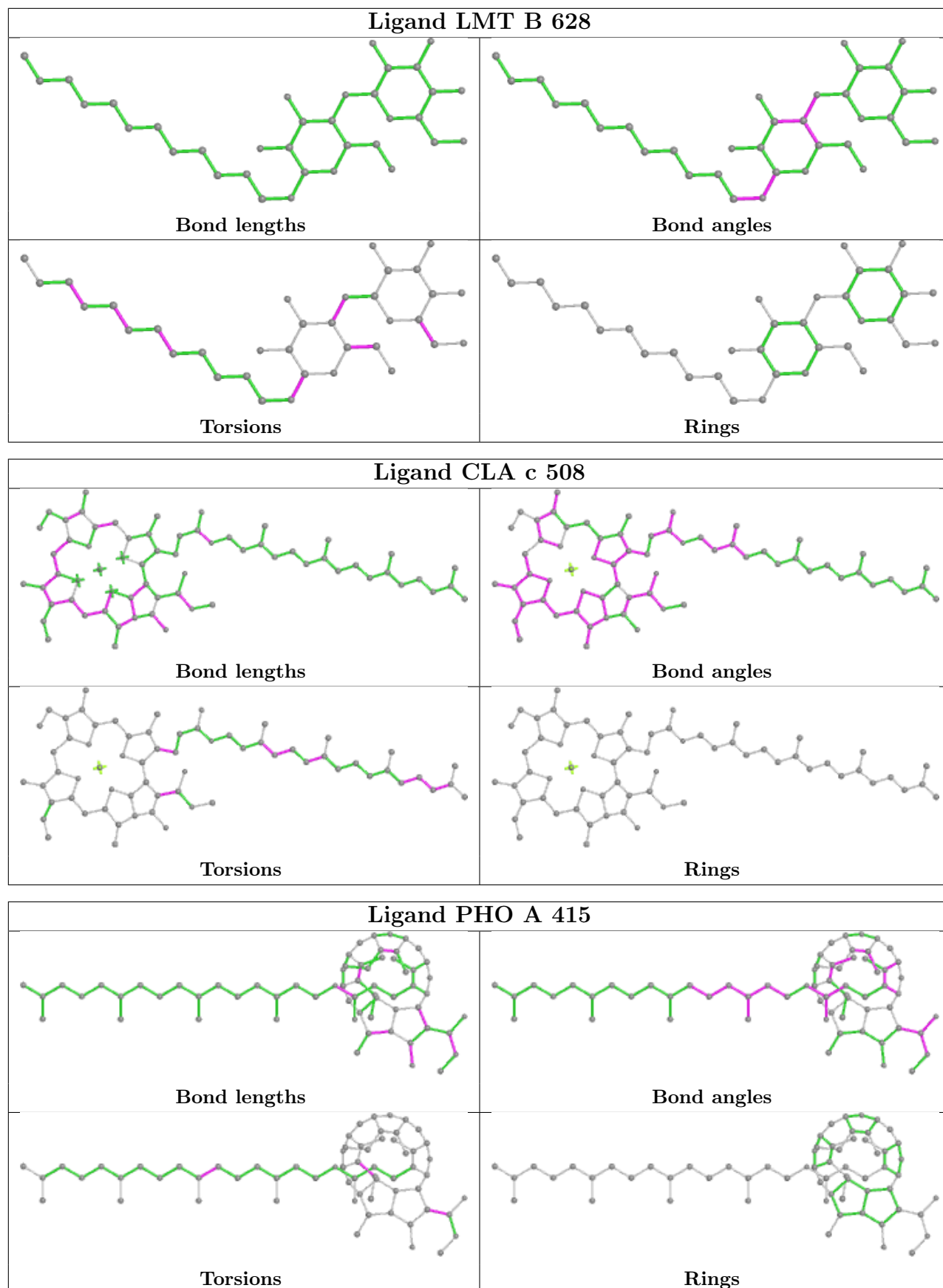


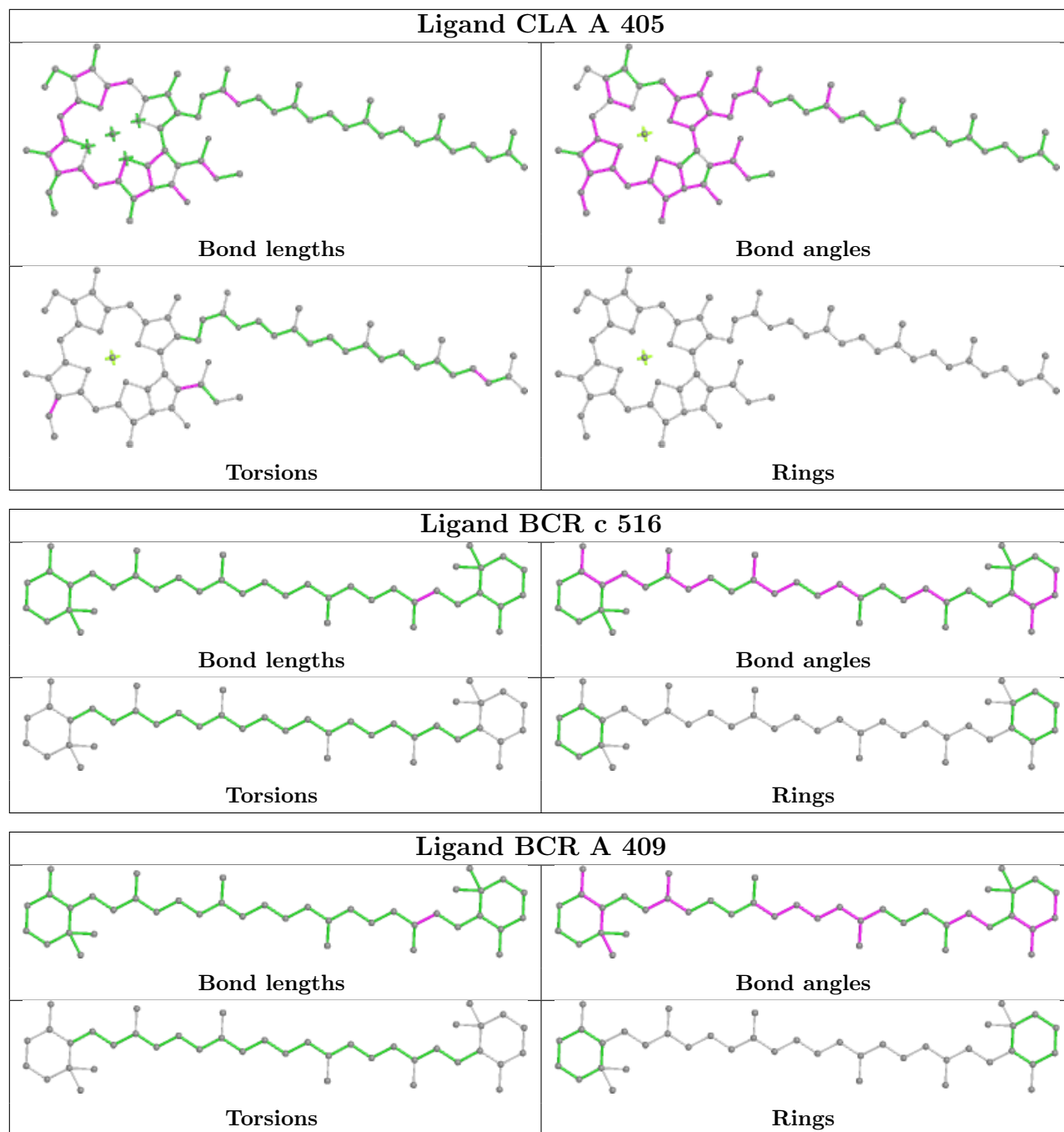


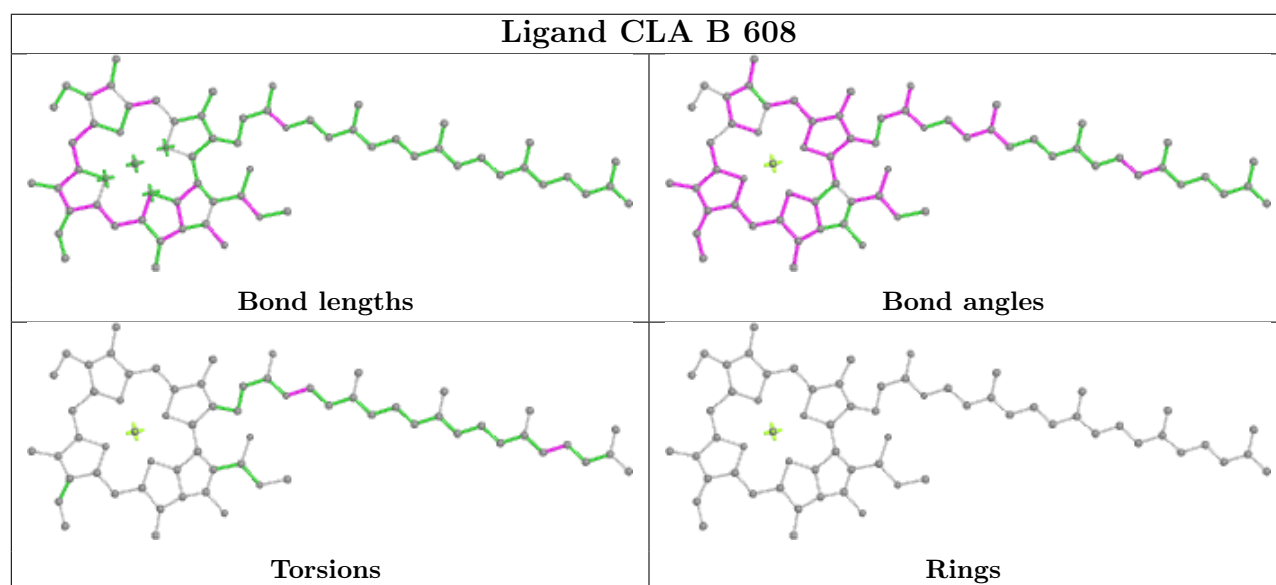
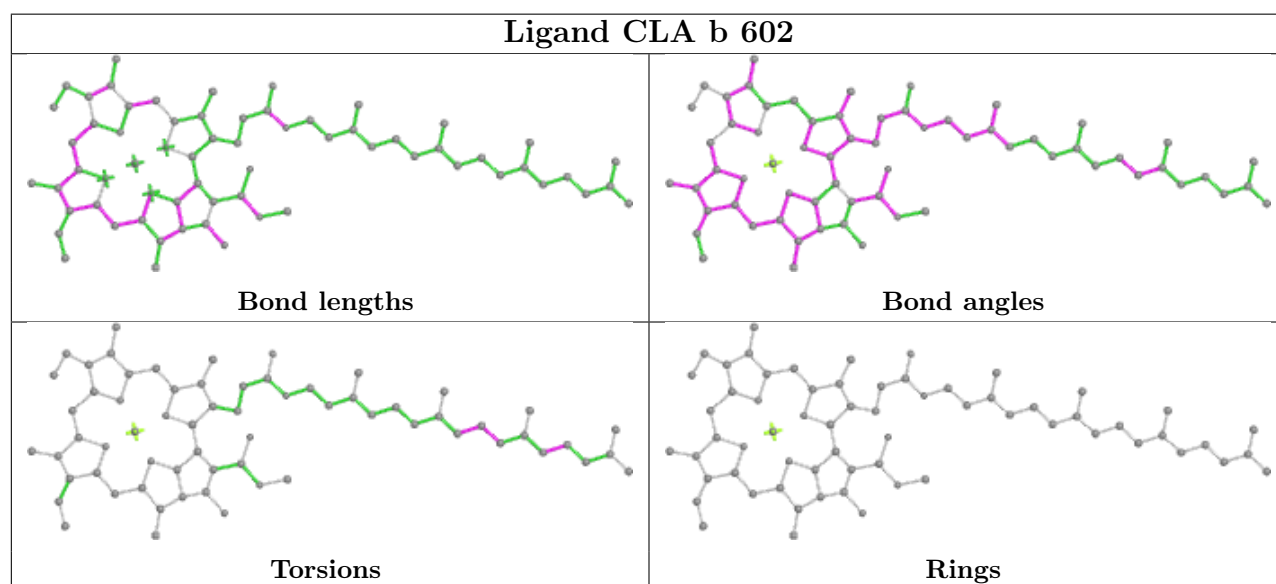
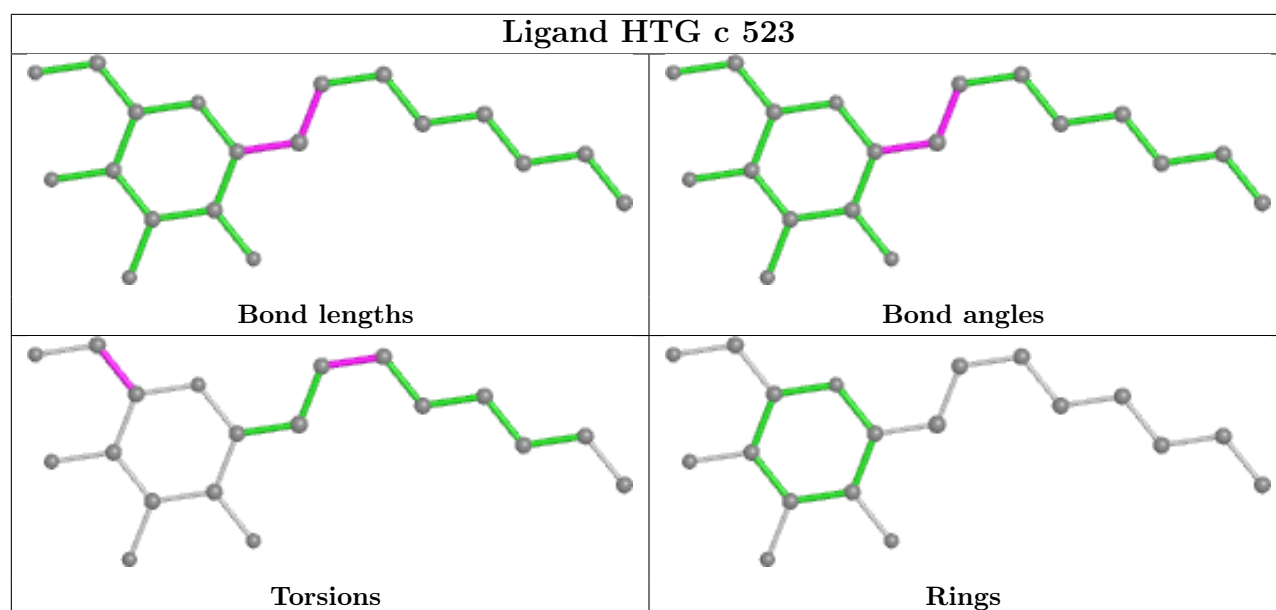


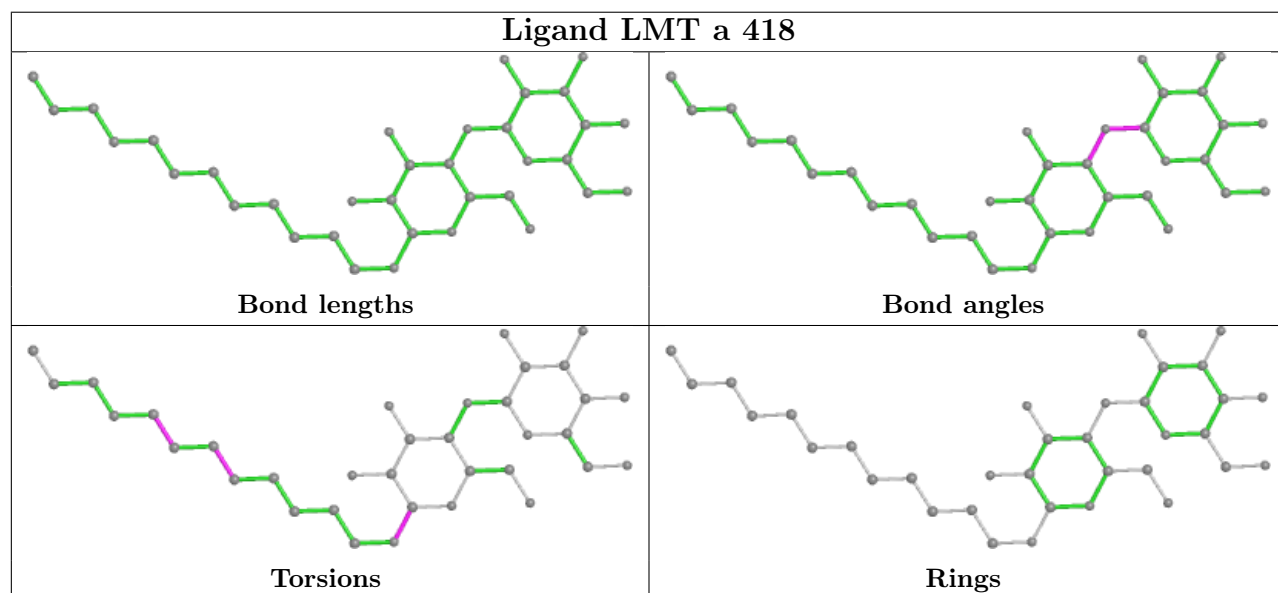
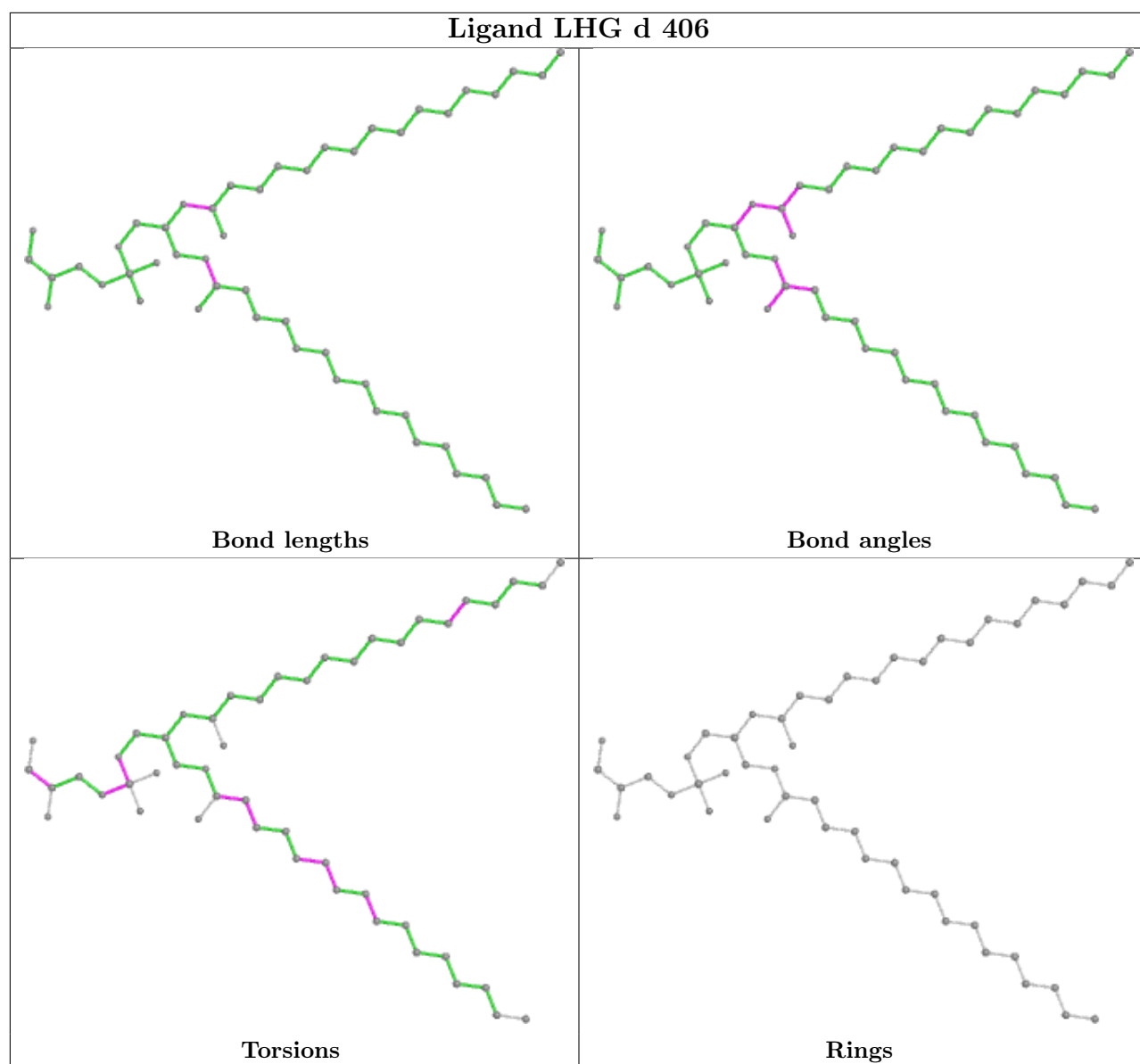


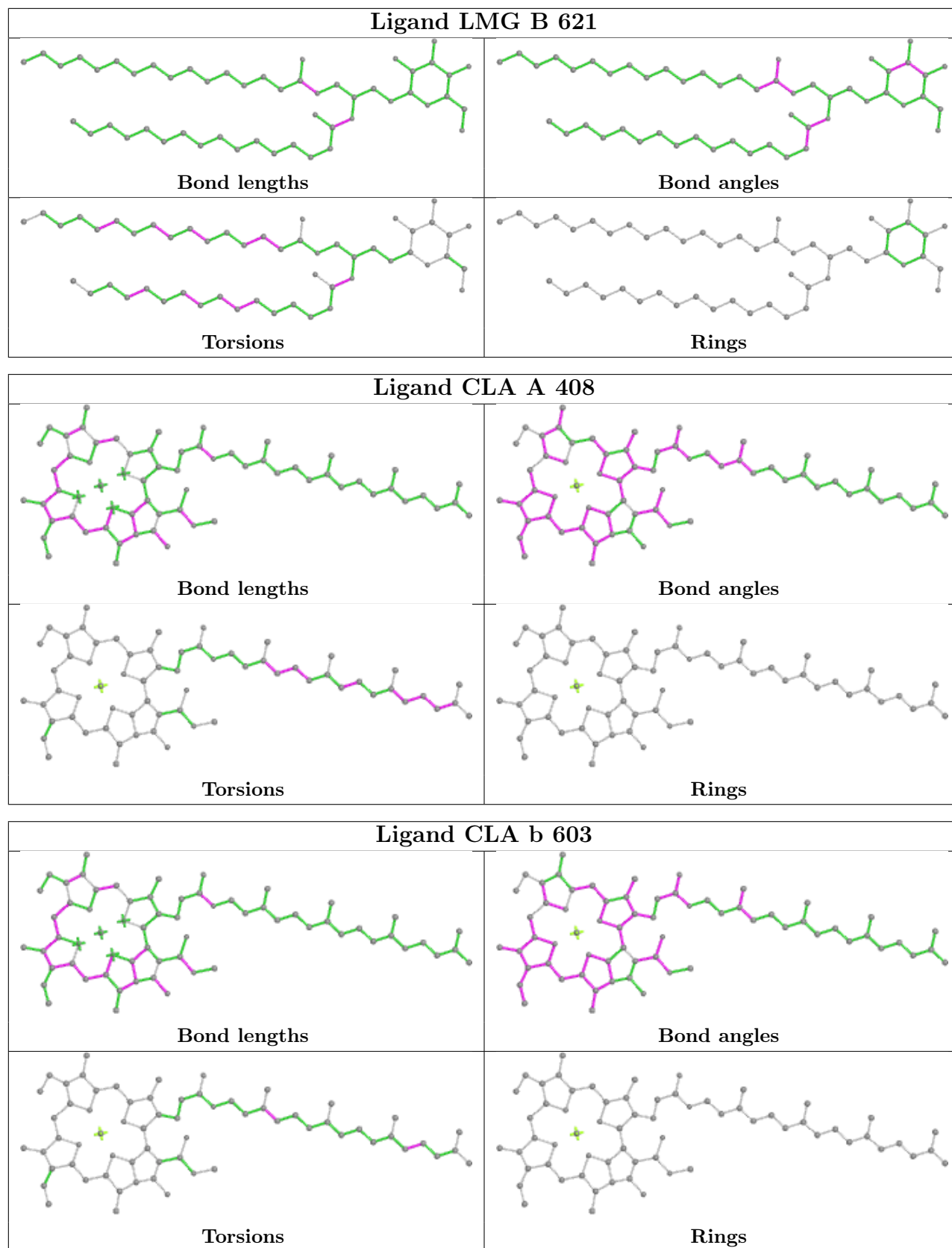


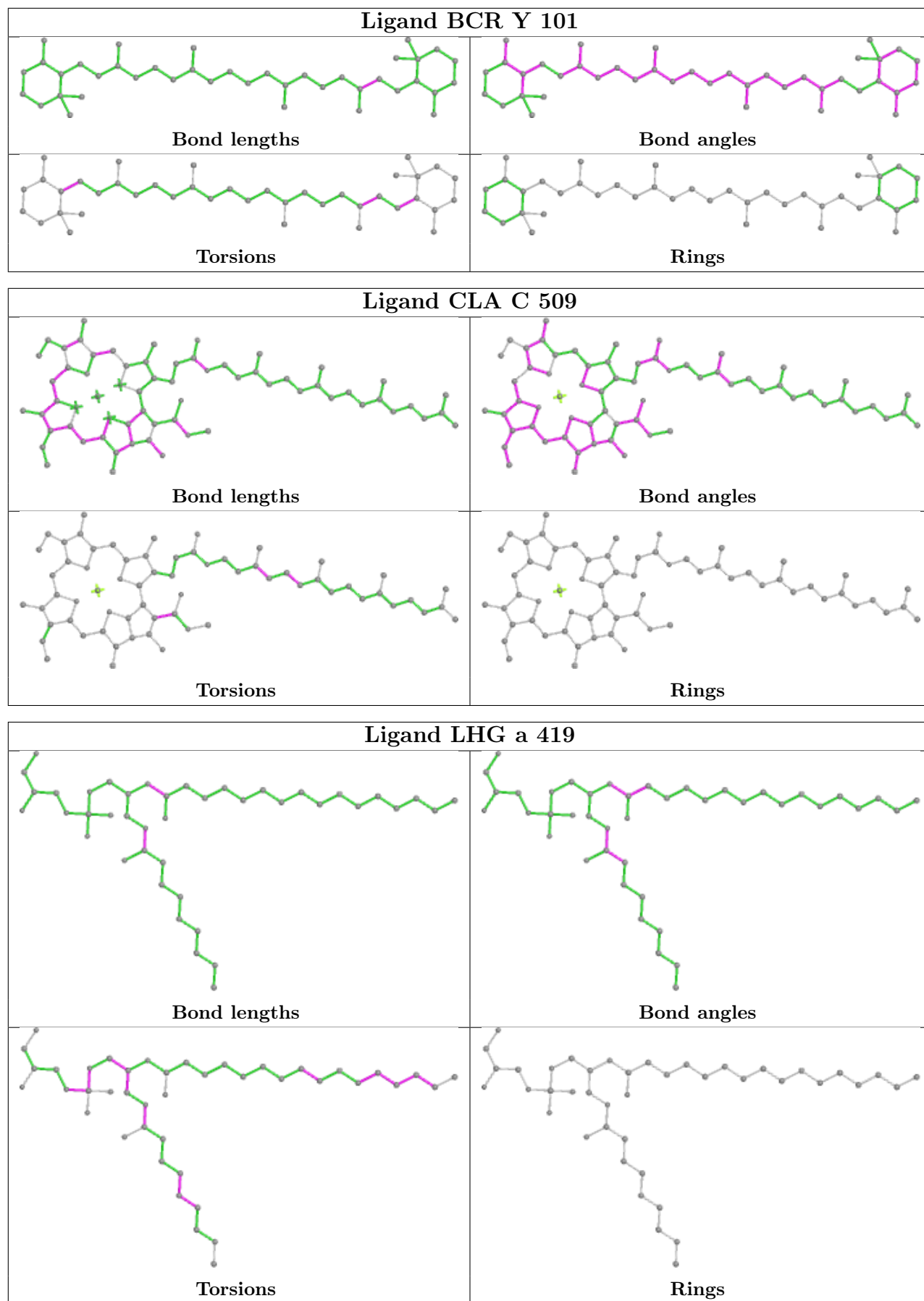


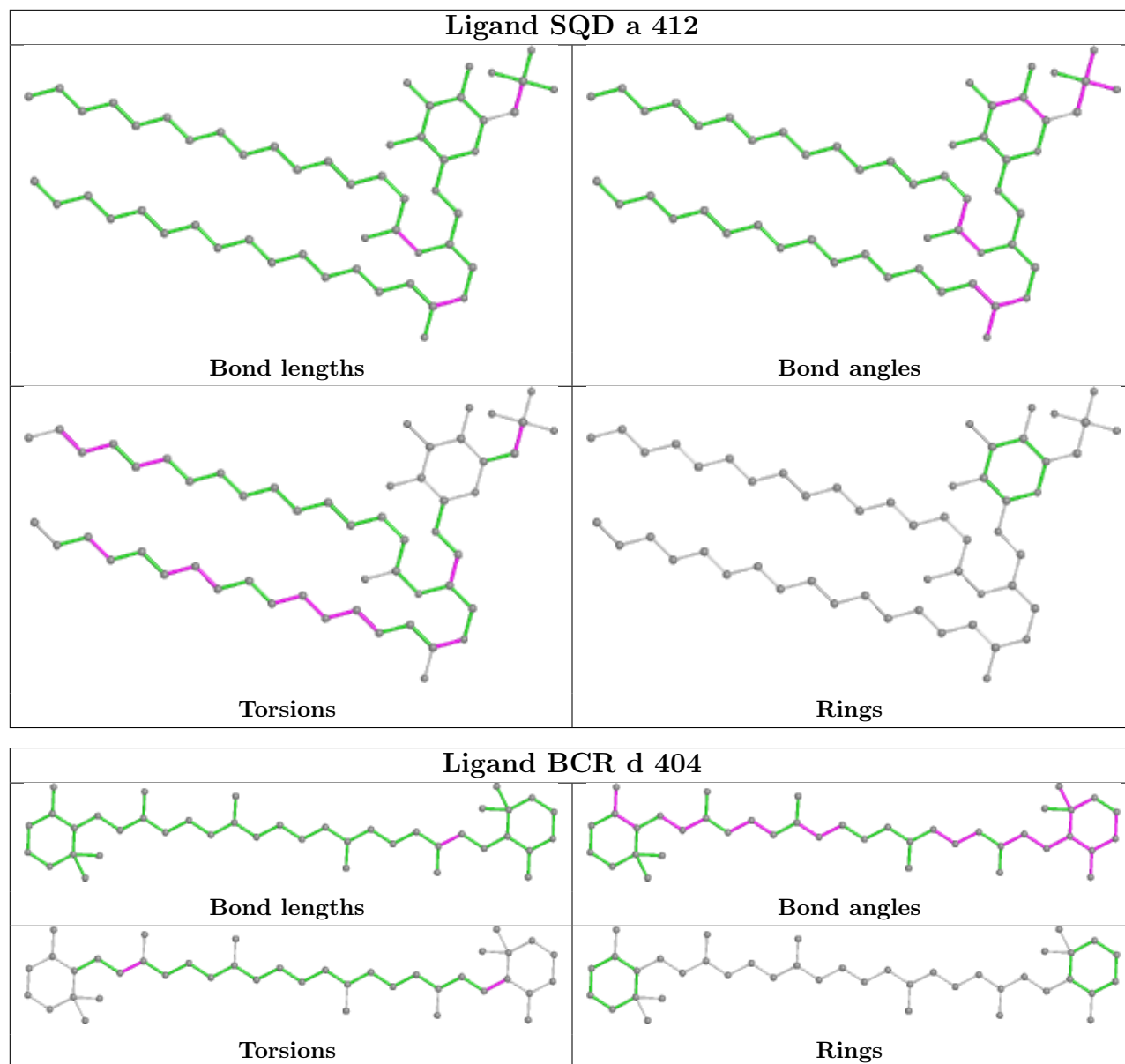


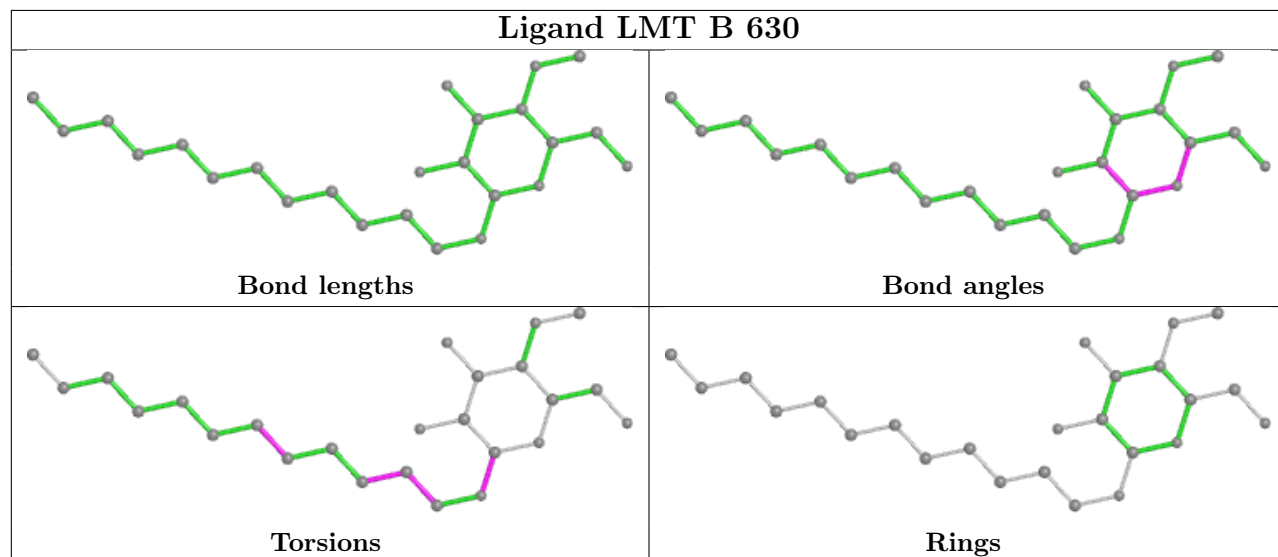
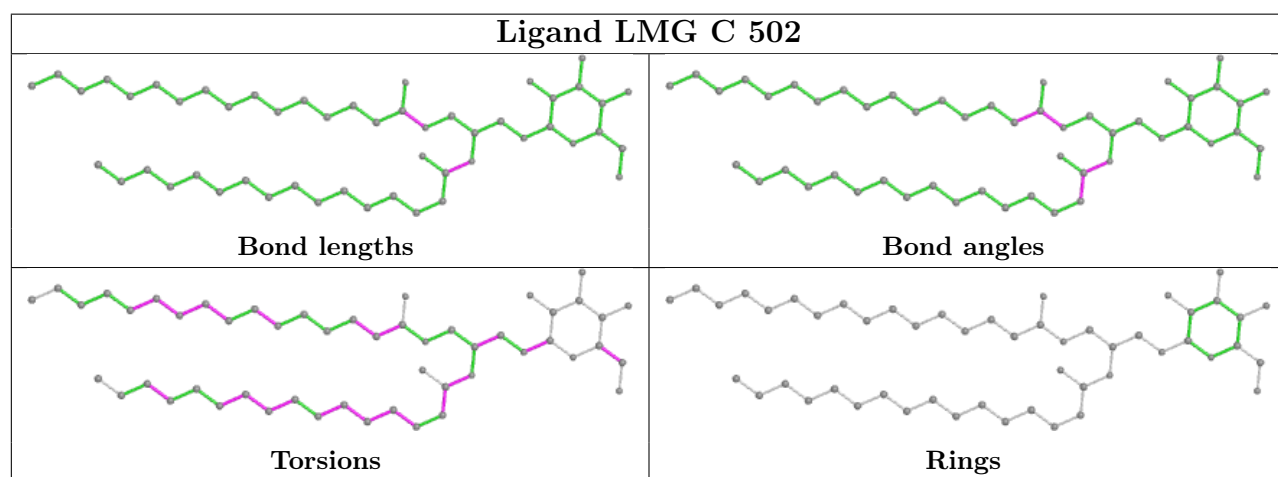
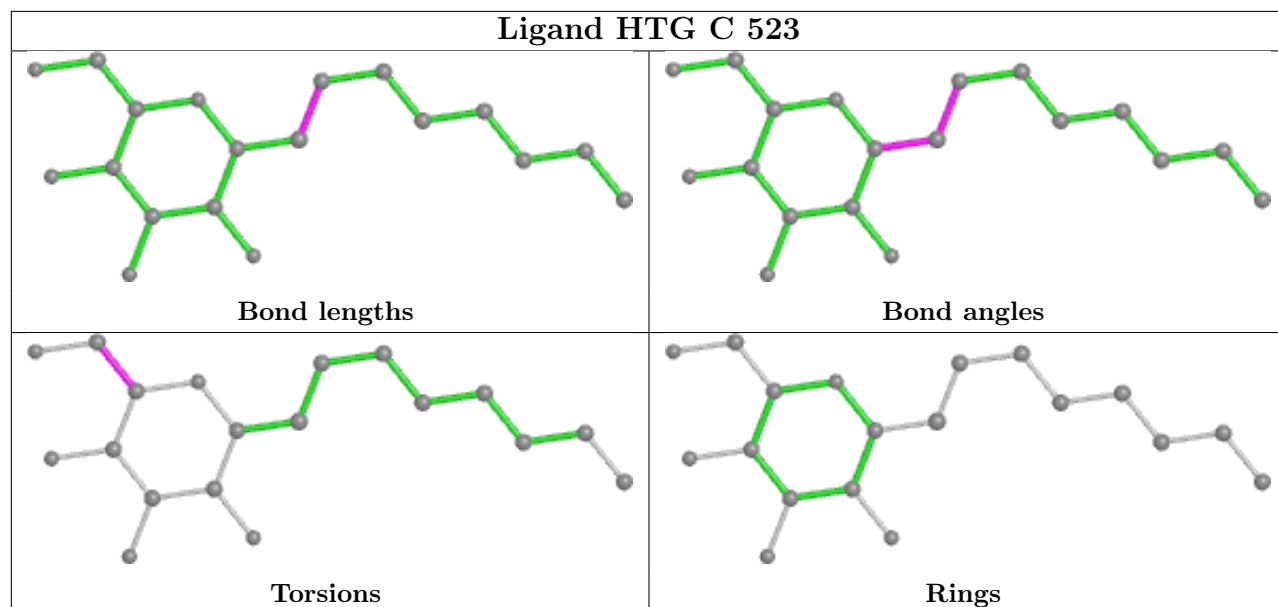


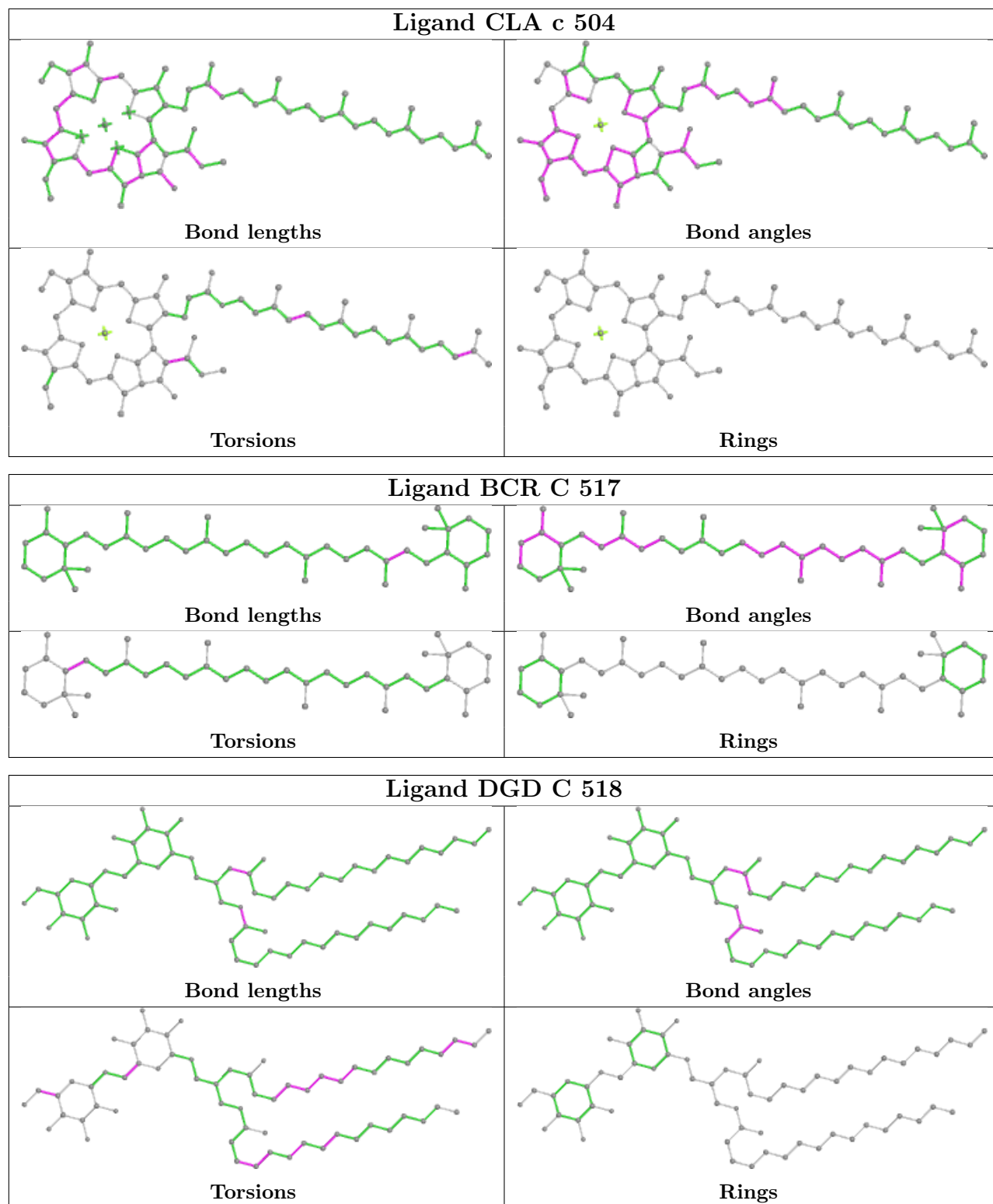


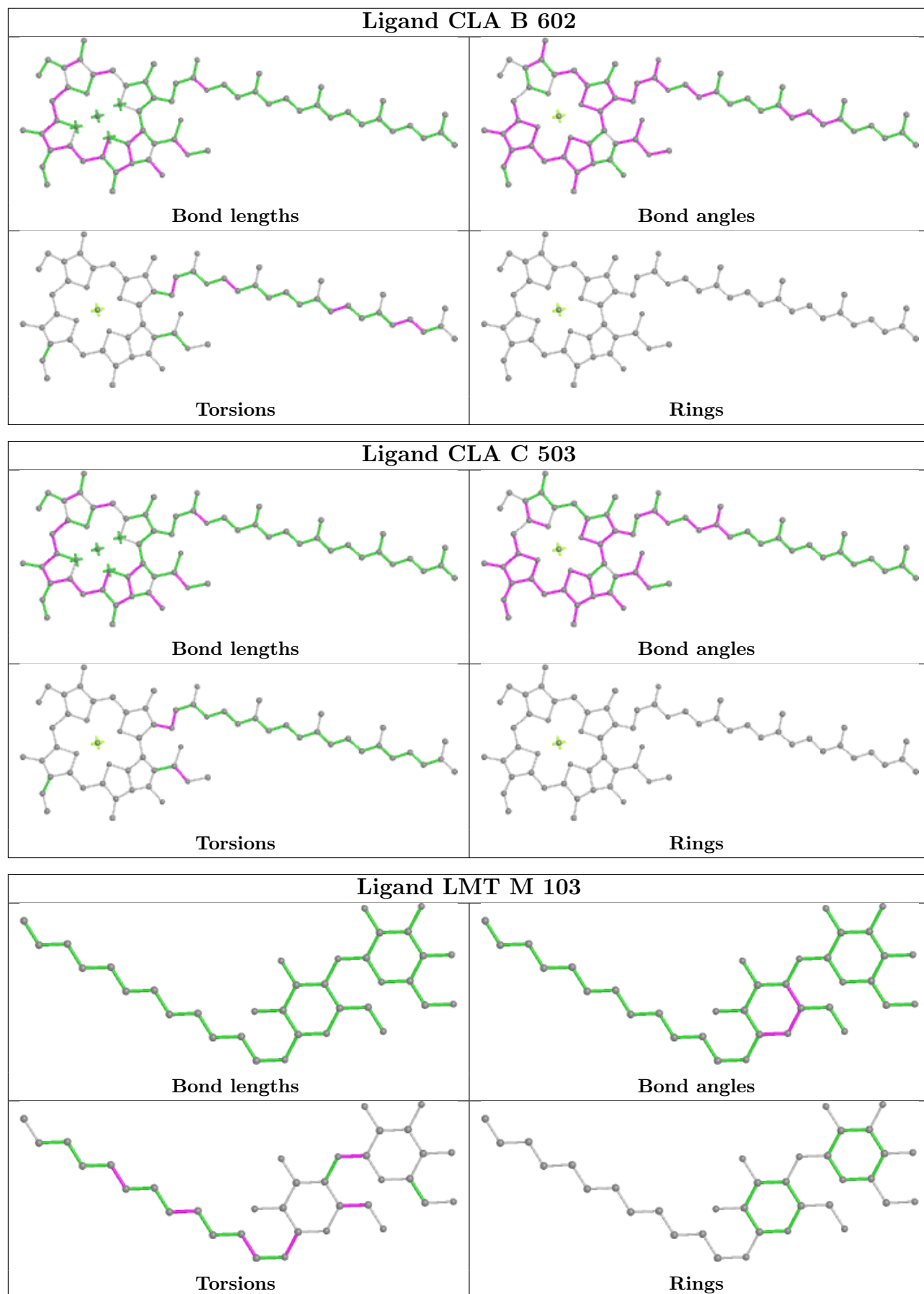


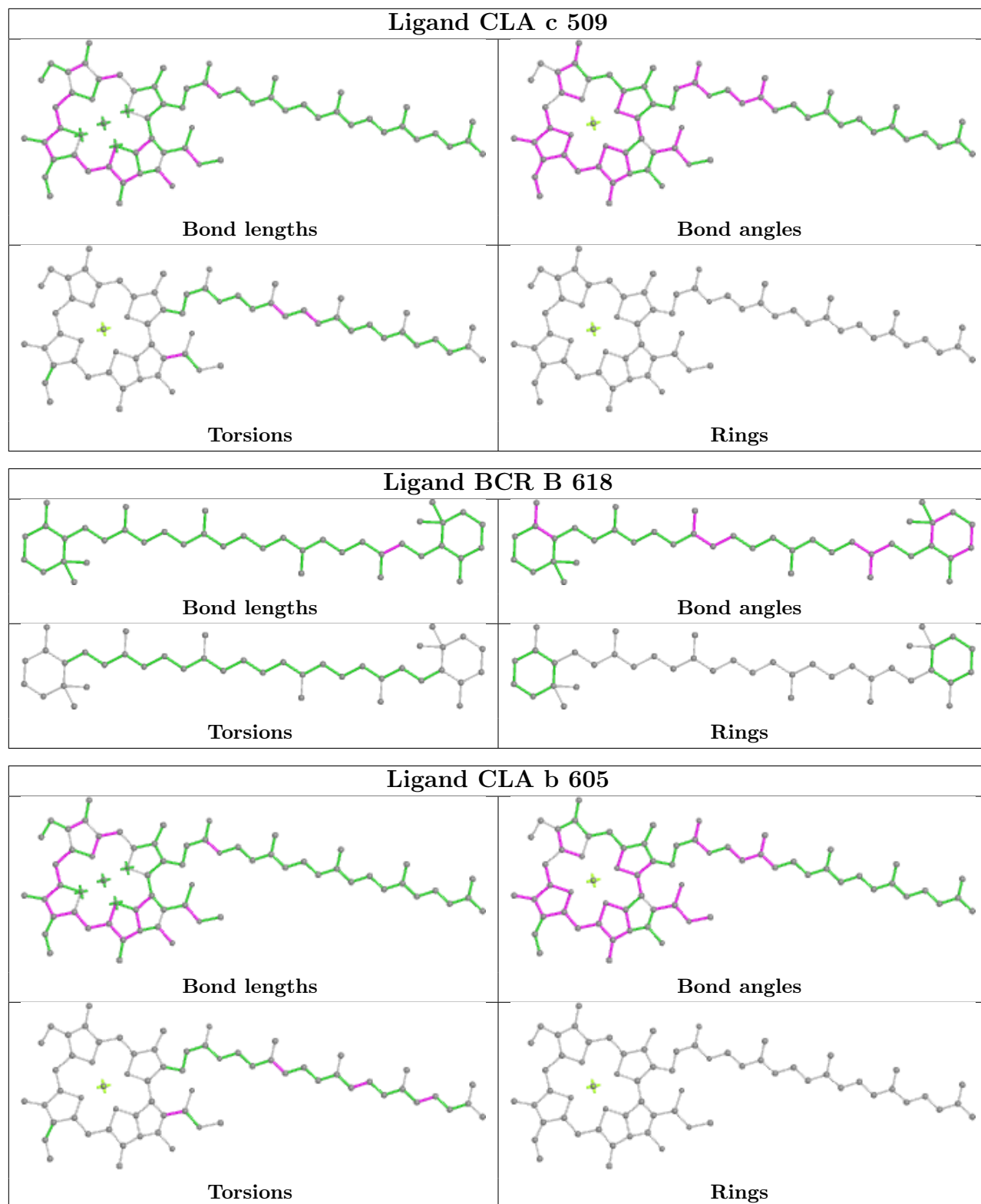


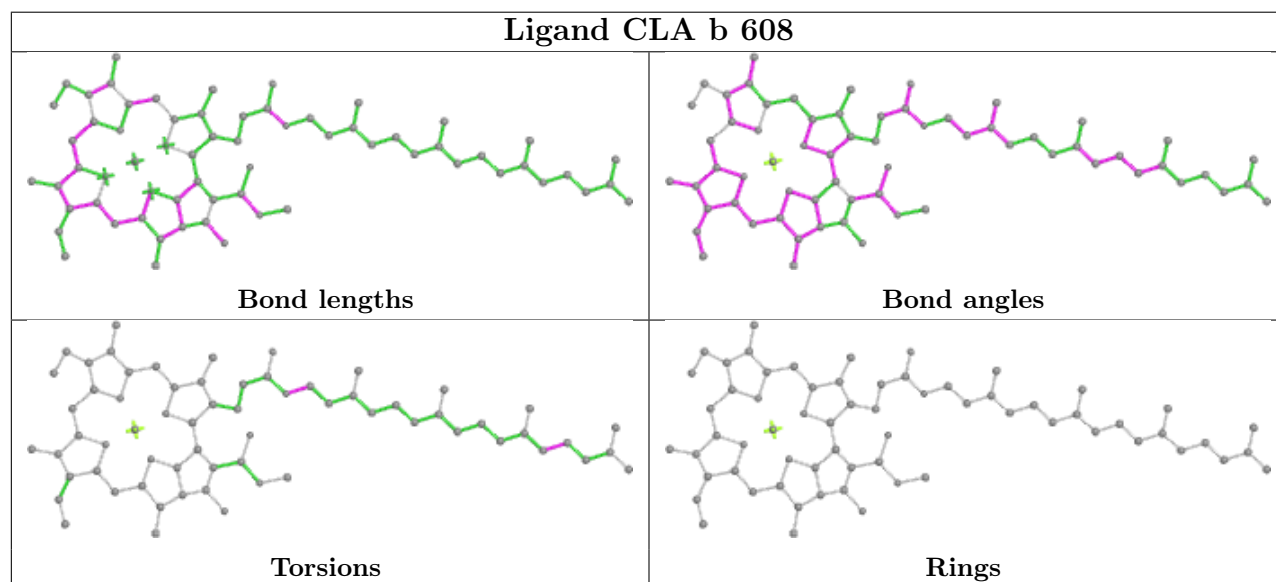
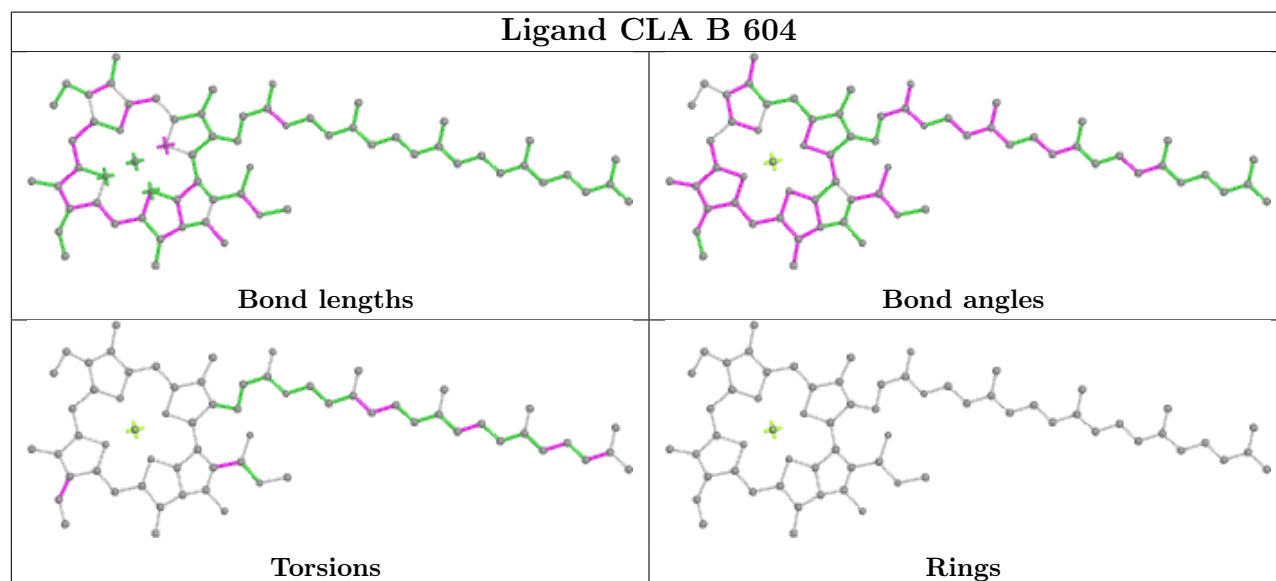
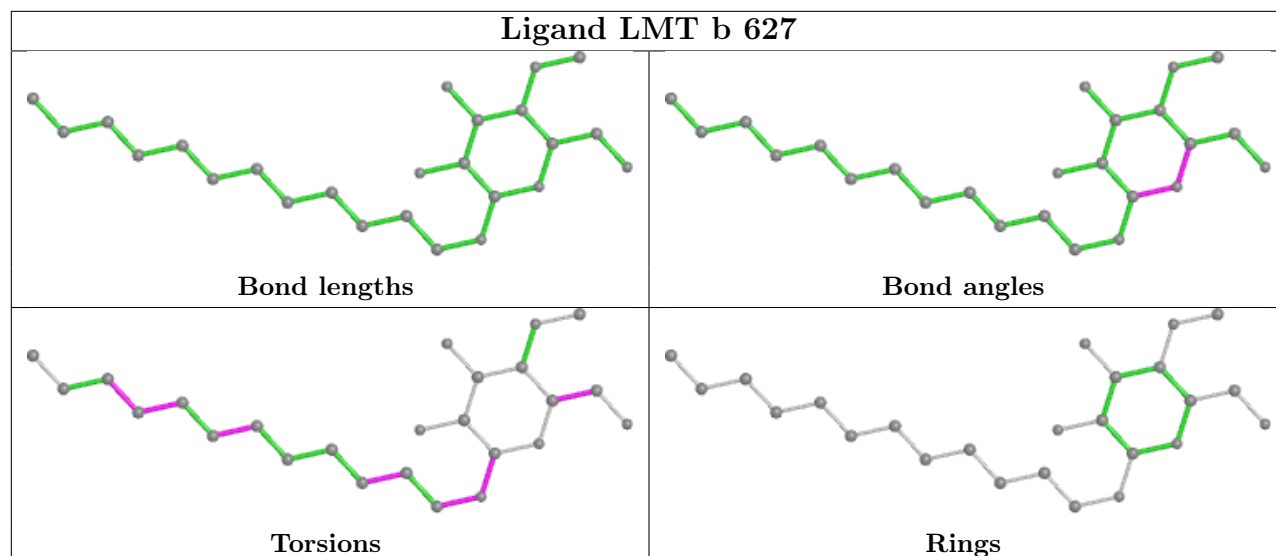


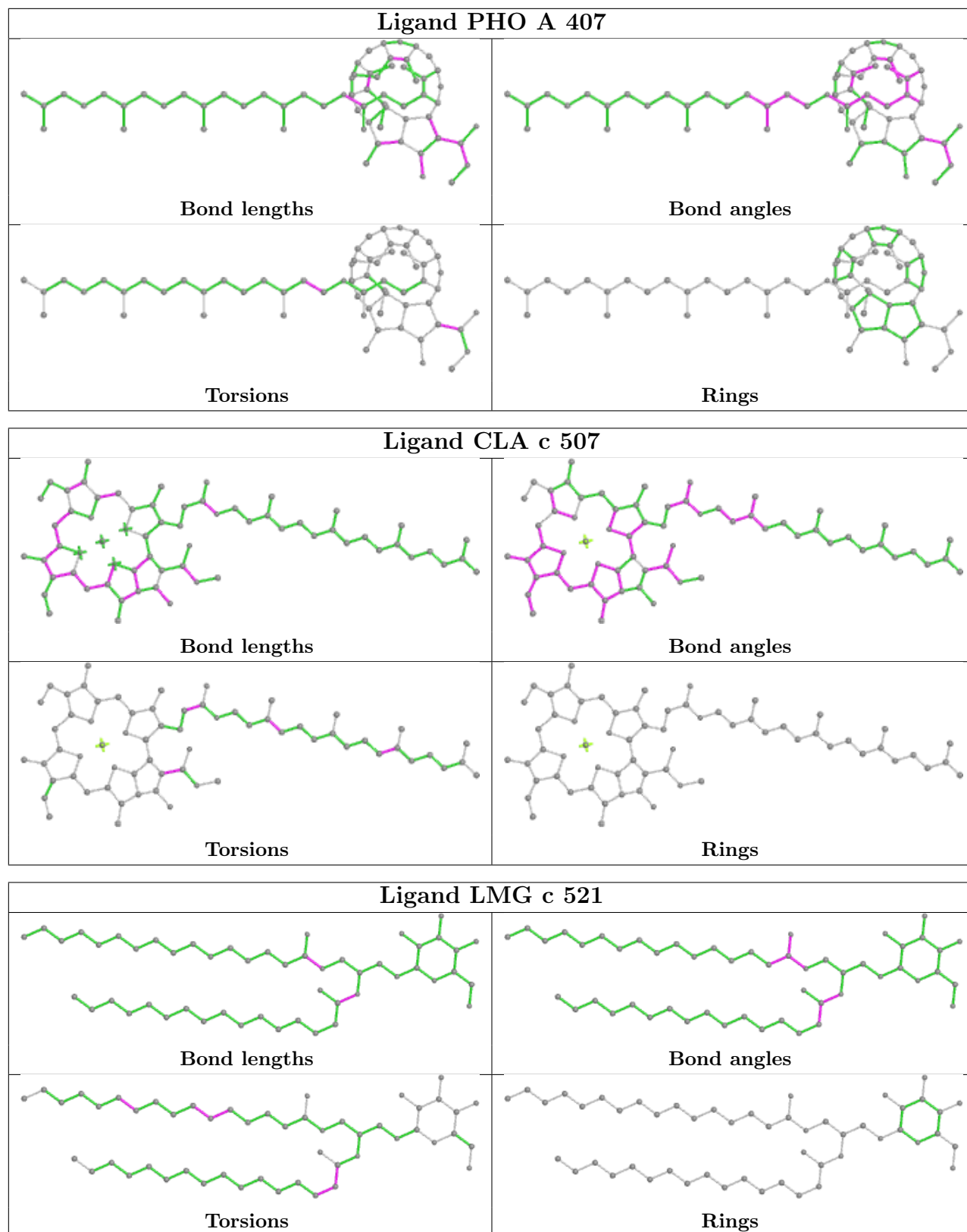


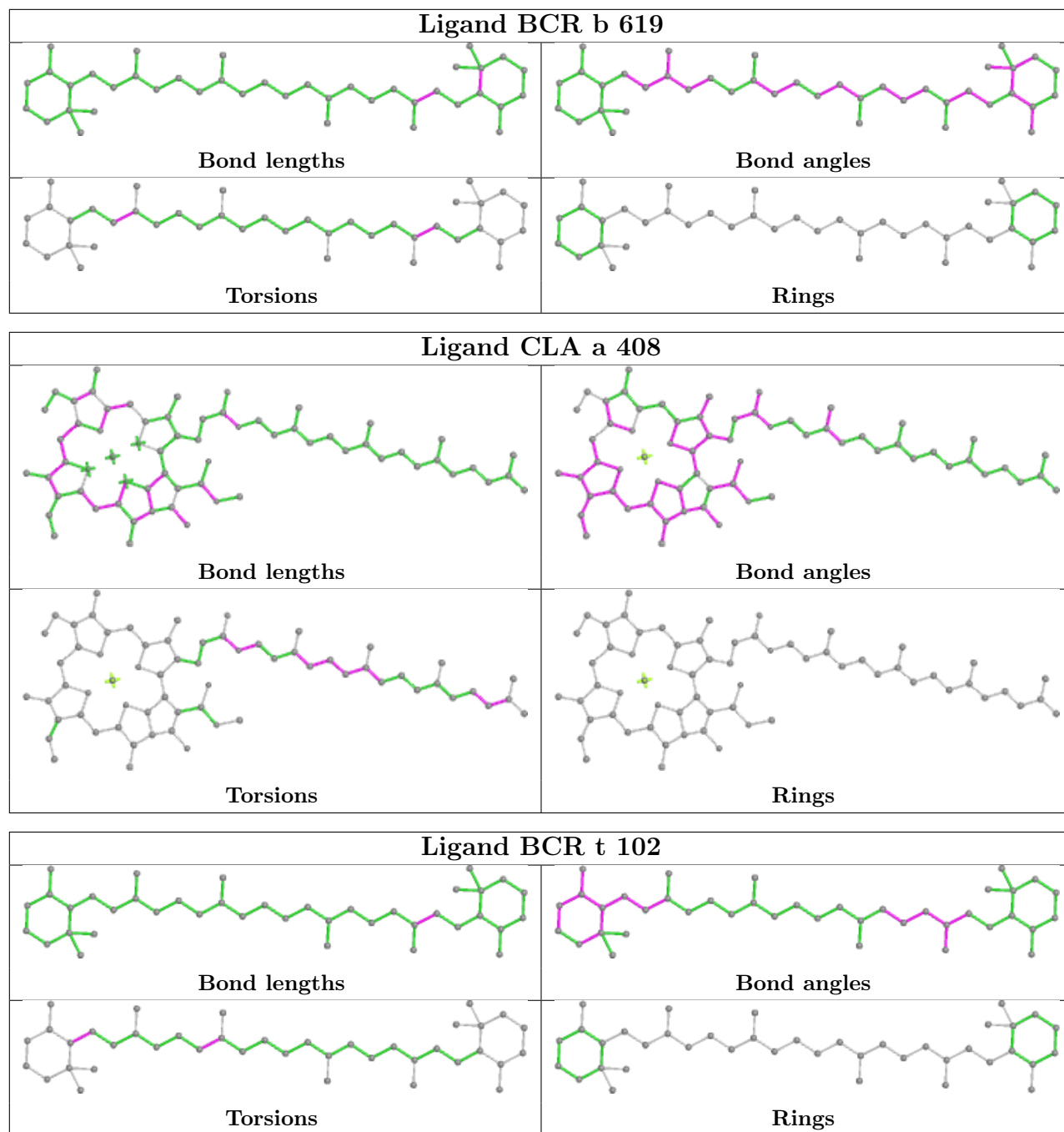


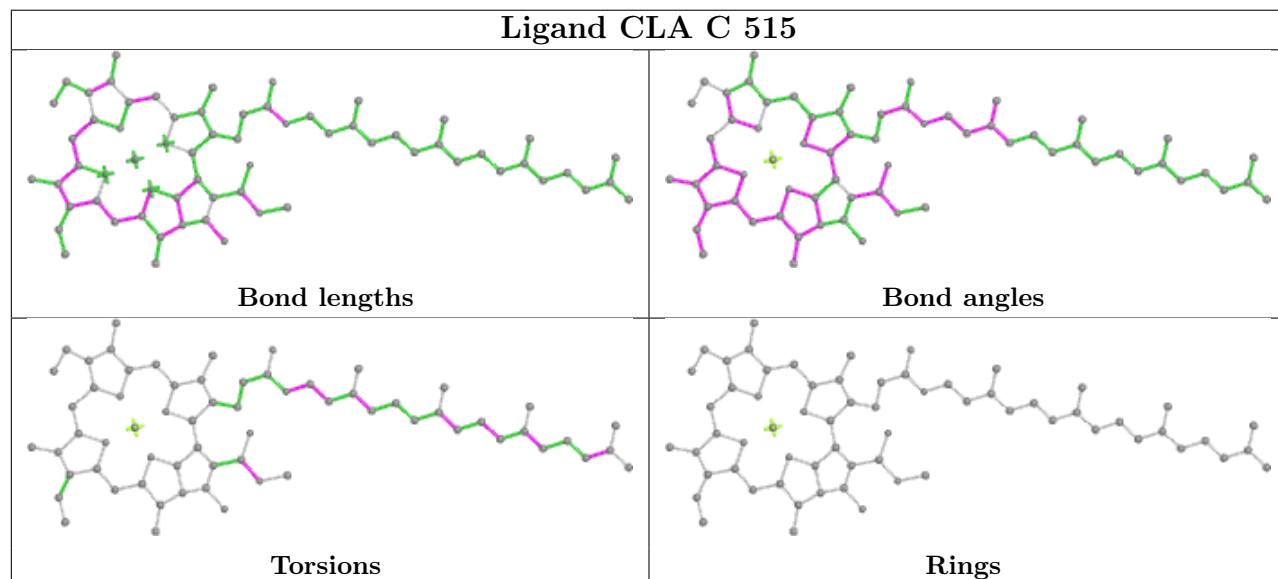
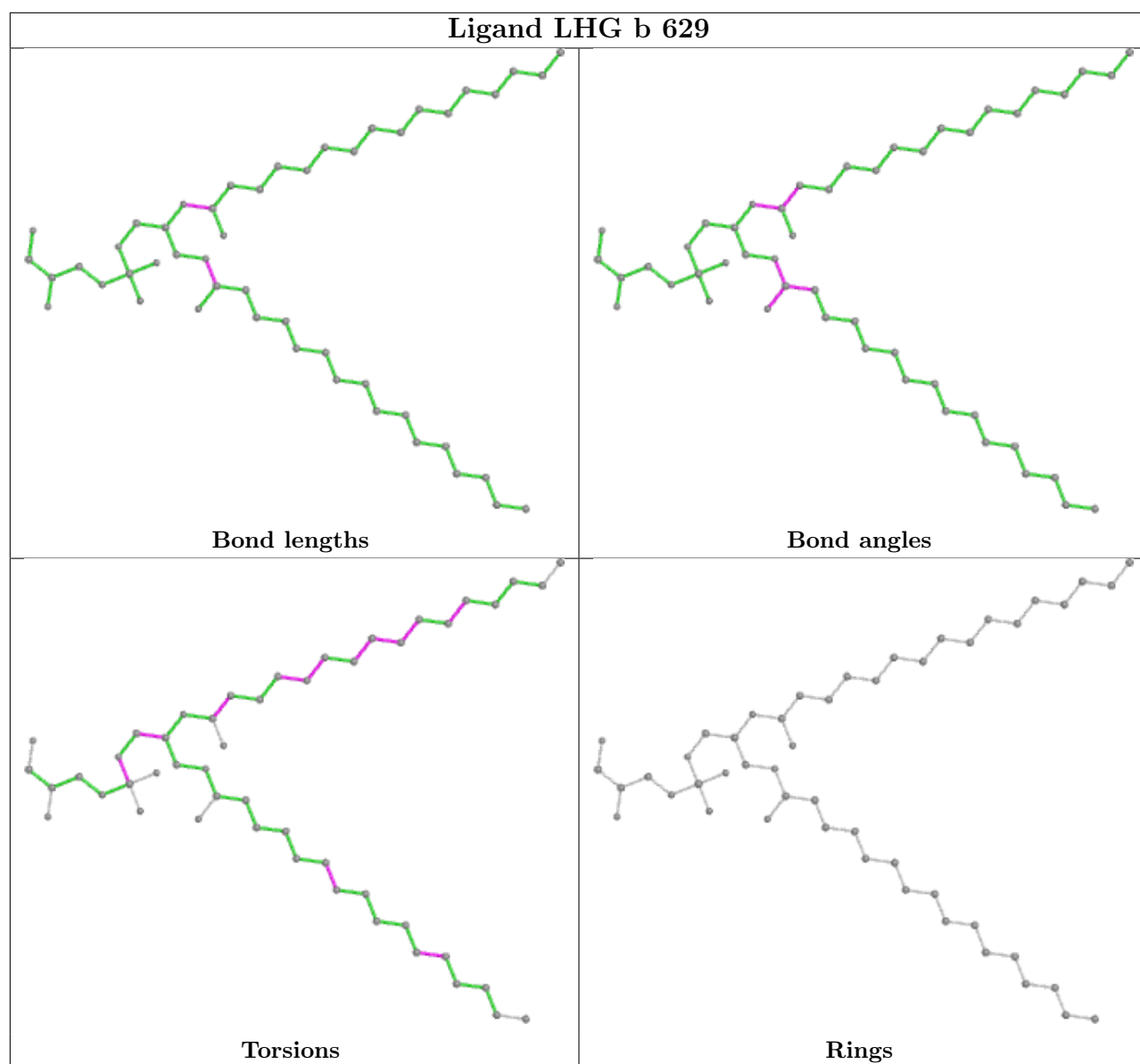


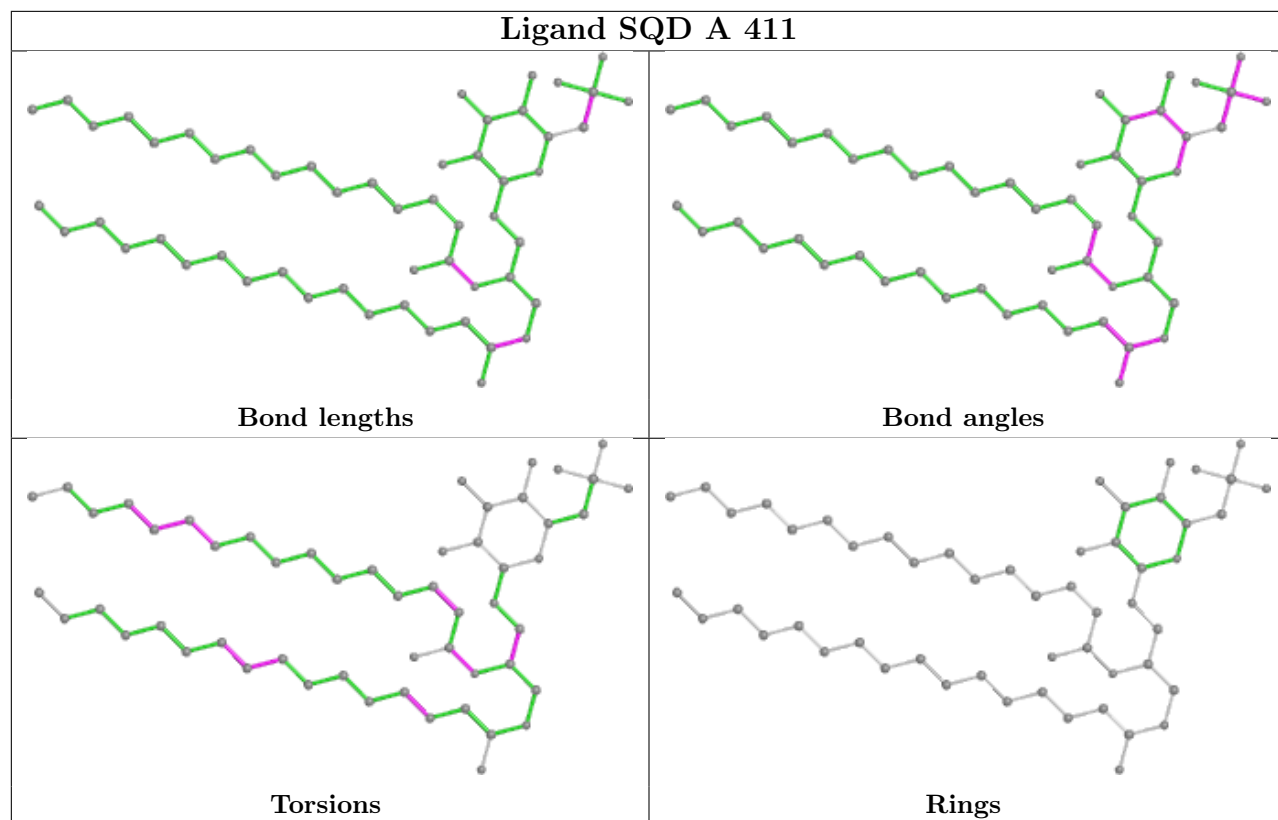


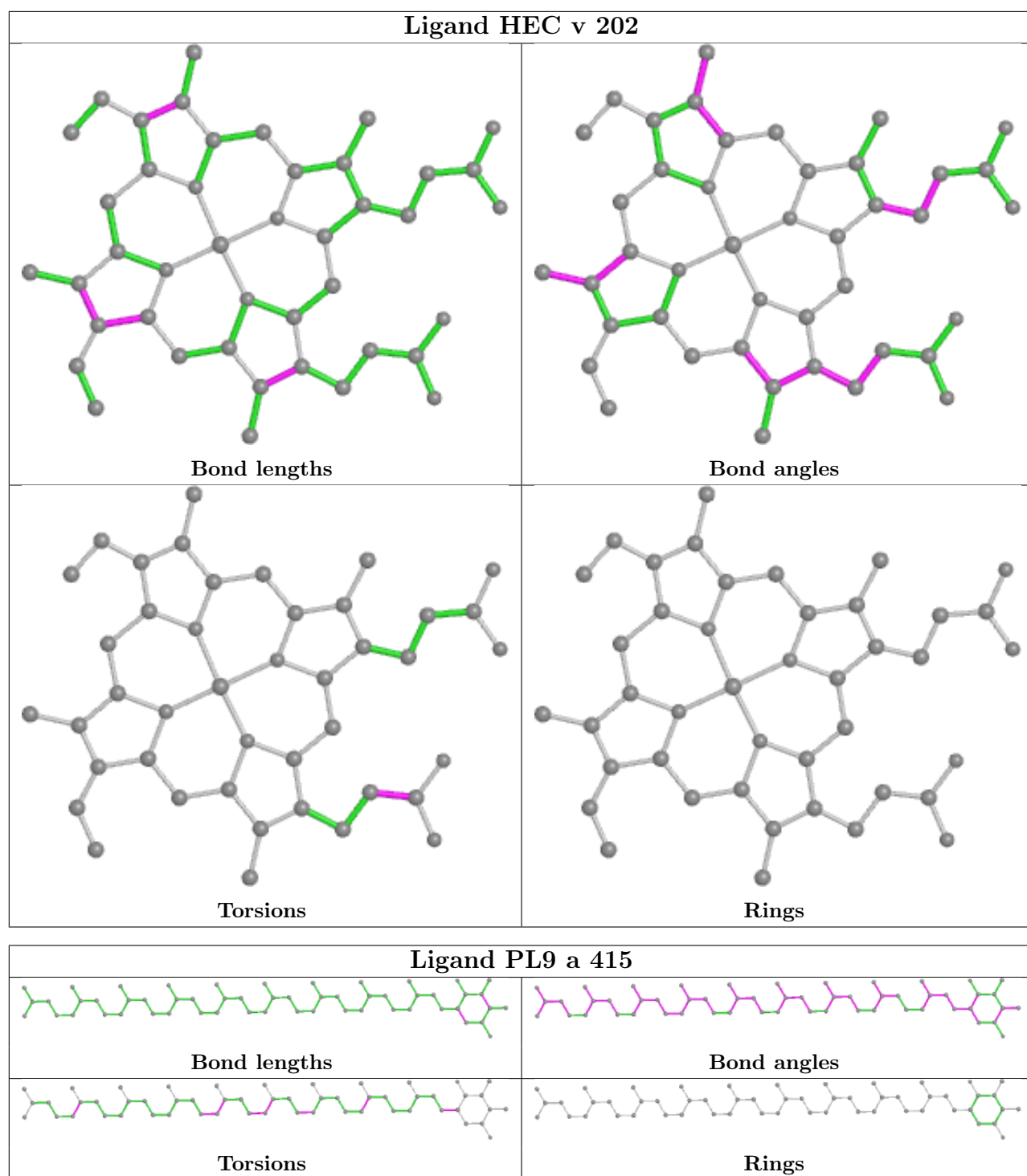


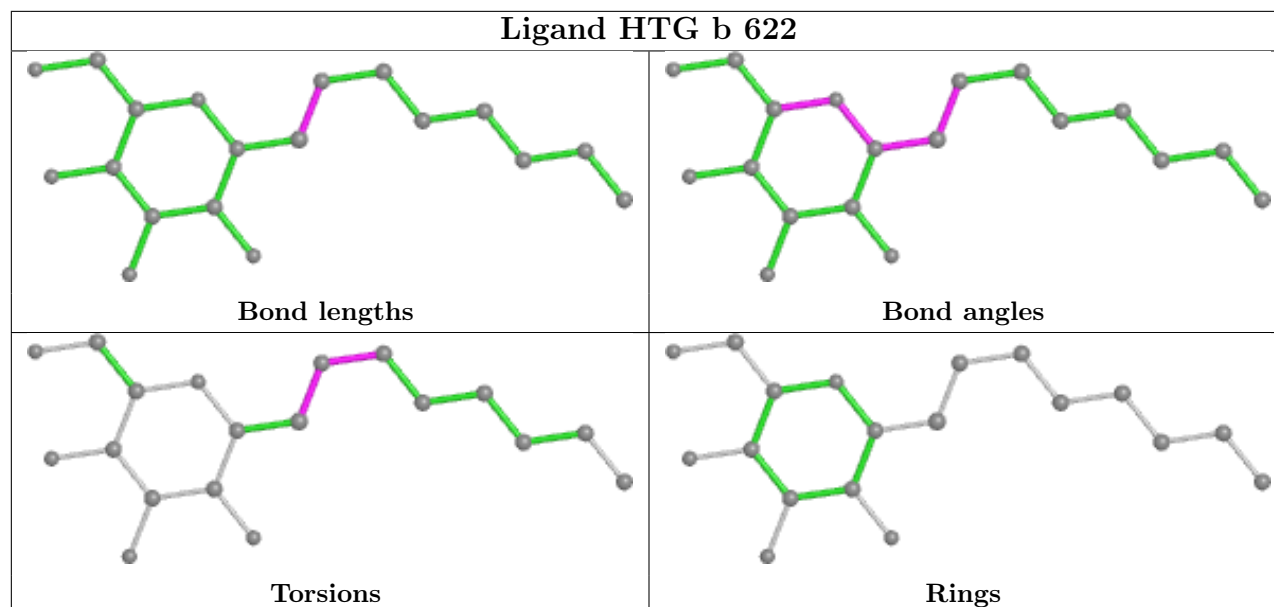












5.7 Other polymers [i](#)

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%)	0.09	14 (4%) 36 38	33, 41, 67, 126	0
1	a	334/344 (97%)	0.17	22 (6%) 18 20	33, 46, 80, 122	0
2	B	504/505 (99%)	-0.18	25 (4%) 28 31	34, 47, 79, 129	0
2	b	504/505 (99%)	0.08	49 (9%) 7 8	35, 51, 92, 164	0
3	C	451/455 (99%)	-0.09	21 (4%) 31 34	38, 54, 77, 144	0
3	c	455/455 (100%)	0.16	36 (7%) 12 14	43, 62, 84, 127	0
4	D	342/342 (100%)	-0.00	10 (2%) 51 55	33, 43, 65, 134	0
4	d	341/342 (99%)	0.02	18 (5%) 26 29	35, 49, 74, 136	0
5	E	81/84 (96%)	0.31	8 (9%) 7 7	48, 66, 95, 140	0
5	e	79/84 (94%)	0.40	8 (10%) 7 7	57, 74, 117, 150	0
6	F	34/44 (77%)	-0.20	2 (5%) 22 24	48, 58, 92, 113	0
6	f	31/44 (70%)	-0.15	3 (9%) 7 8	57, 66, 93, 154	0
7	H	64/65 (98%)	-0.45	0 100 100	43, 58, 77, 105	0
7	h	64/65 (98%)	0.16	4 (6%) 20 22	51, 63, 85, 108	0
8	I	37/38 (97%)	-0.11	2 (5%) 25 28	47, 58, 120, 144	0
8	i	37/38 (97%)	-0.29	1 (2%) 54 57	49, 59, 117, 145	0
9	J	38/39 (97%)	0.27	7 (18%) 1 1	47, 66, 127, 181	0
9	j	39/39 (100%)	0.32	5 (12%) 3 3	55, 74, 135, 179	0
10	K	37/37 (100%)	-0.61	0 100 100	53, 65, 88, 102	0
10	k	37/37 (100%)	0.21	3 (8%) 12 13	66, 72, 94, 109	0
11	L	36/37 (97%)	-0.10	1 (2%) 53 55	34, 39, 95, 137	0
11	l	36/37 (97%)	0.12	1 (2%) 53 55	36, 40, 96, 132	0
12	M	32/36 (88%)	-0.12	1 (3%) 49 52	37, 42, 66, 135	0
12	m	33/36 (91%)	-0.09	2 (6%) 21 23	36, 43, 78, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	0.12	24 (9%) 7 7	34, 57, 110, 186	0
13	o	243/244 (99%)	0.49	41 (16%) 1 1	38, 59, 124, 166	0
14	T	29/32 (90%)	-0.21	0 100 100	36, 40, 78, 109	0
14	t	29/32 (90%)	-0.03	2 (6%) 16 18	36, 43, 70, 137	0
15	U	96/104 (92%)	-0.30	3 (3%) 49 52	41, 53, 85, 90	0
15	u	97/104 (93%)	-0.53	0 100 100	46, 58, 80, 132	0
16	V	137/137 (100%)	-0.41	0 100 100	40, 53, 79, 115	0
16	v	137/137 (100%)	0.01	6 (4%) 34 37	47, 68, 96, 138	0
17	X	38/40 (95%)	-0.04	2 (5%) 26 29	56, 68, 93, 110	0
17	x	38/40 (95%)	0.64	8 (21%) 1 1	60, 74, 114, 163	0
18	Y	29/30 (96%)	1.62	10 (34%) 0 0	66, 82, 139, 159	0
18	y	29/30 (96%)	0.63	5 (17%) 1 1	77, 89, 119, 120	0
19	Z	62/62 (100%)	0.66	6 (9%) 7 8	66, 80, 132, 180	0
19	z	62/62 (100%)	1.92	27 (43%) 0 0	77, 94, 135, 178	0
20	R	34/34 (100%)	6.90	34 (100%) 0 0	102, 124, 154, 164	0
All	All	5283/5384 (98%)	0.11	411 (7%) 13 14	33, 54, 98, 186	0

All (411) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	6	LEU	11.3
20	R	14	LEU	10.7
20	R	18	TRP	10.5
20	R	5	VAL	9.6
20	R	35	LEU	9.5
20	R	8	VAL	8.9
20	R	20	VAL	8.9
17	x	38	GLN	8.7
20	R	7	VAL	8.6
20	R	15	ALA	8.6
20	R	3	TRP	8.5
1	A	11	ALA	8.4
20	R	19	ALA	8.0
20	R	10	LEU	7.8
2	b	486	LEU	7.6
20	R	34	LEU	7.6
2	b	499	VAL	7.6

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Mol	Chain	Res	Type	RSRZ
20	R	16	ALA	7.3
20	R	12	VAL	7.3
17	x	37	VAL	7.2
18	Y	19	ILE	6.8
20	R	2	ASP	6.8
2	b	495	PHE	6.8
20	R	9	LEU	6.7
20	R	21	ARG	6.6
13	O	27	ARG	6.5
20	R	4	ARG	6.4
20	R	23	ILE	6.3
20	R	13	LEU	6.2
20	R	31	VAL	6.2
2	b	488	PRO	6.1
20	R	17	GLY	5.7
2	b	493	TRP	5.7
19	z	3	ILE	5.7
20	R	24	LEU	5.6
13	o	27	ARG	5.6
9	j	3	GLU	5.6
20	R	25	PRO	5.6
20	R	27	ALA	5.5
2	b	484	PRO	5.4
5	E	84	LYS	5.4
19	z	60	PHE	5.3
13	o	22	LEU	5.3
2	b	489	GLU	5.3
18	Y	18	VAL	5.2
2	b	487	SER	5.2
2	b	491	VAL	5.1
9	j	1	MET	5.1
13	o	4	THR	5.1
10	k	18	PHE	5.1
18	y	18	VAL	5.0
19	z	9	LEU	5.0
1	A	13	LEU	5.0
19	z	2	THR	4.9
19	z	42	LEU	4.9
18	Y	25	ILE	4.8
13	o	32	ILE	4.8
20	R	32	GLN	4.8
3	c	143	TYR	4.7

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Mol	Chain	Res	Type	RSRZ
2	b	500	GLY	4.7
19	z	46	LEU	4.7
19	z	5	PHE	4.7
2	b	504	THR	4.7
3	C	143	TYR	4.7
20	R	26	TYR	4.7
2	b	498	LYS	4.7
18	y	19	ILE	4.6
13	o	25	THR	4.6
8	I	38	GLU	4.6
2	B	489	GLU	4.6
13	o	30	TYR	4.5
13	o	134	THR	4.5
13	o	26	ALA	4.5
19	Z	3	ILE	4.5
2	b	505	ARG	4.4
13	o	133	VAL	4.4
19	z	7	LEU	4.4
1	a	11	ALA	4.4
20	R	11	PRO	4.4
3	c	426	LEU	4.3
20	R	28	VAL	4.3
4	d	12	ARG	4.3
17	x	39	ARG	4.3
20	R	33	LYS	4.3
4	D	238	THR	4.3
3	c	433	LEU	4.3
16	v	21	LEU	4.3
2	b	496	TYR	4.3
9	j	2	SER	4.3
3	C	23	ALA	4.2
20	R	22	ASN	4.2
13	O	5	LEU	4.2
9	J	4	GLY	4.1
2	b	502	VAL	4.1
18	Y	21	GLN	4.1
9	J	7	ILE	4.1
19	z	62	VAL	4.1
13	o	243	ILE	4.1
1	a	224	ILE	4.0
2	B	504	THR	4.0
9	J	2	SER	4.0

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Mol	Chain	Res	Type	RSRZ
9	J	3	GLU	3.9
3	c	427	ALA	3.9
13	O	4	THR	3.9
9	j	4	GLY	3.9
2	b	494	GLY	3.8
2	B	496	TYR	3.8
18	y	20	ALA	3.8
19	Z	60	PHE	3.8
2	b	457	VAL	3.8
13	o	204	VAL	3.8
2	b	492	GLU	3.8
10	k	17	ILE	3.8
13	O	25	THR	3.8
19	Z	32	ASP	3.7
1	A	249	VAL	3.7
13	o	5	LEU	3.7
4	d	152	VAL	3.7
3	C	257	PHE	3.7
2	b	459	ALA	3.7
11	l	3	PRO	3.7
7	h	6	TRP	3.7
2	B	293	ALA	3.7
2	B	495	PHE	3.7
3	c	428	THR	3.7
13	O	60	ARG	3.7
19	Z	31	GLN	3.7
2	b	497	GLN	3.7
13	O	28	GLY	3.6
2	b	460	LEU	3.6
20	R	30	GLN	3.6
2	B	487	SER	3.6
8	I	37	LEU	3.5
2	B	494	GLY	3.5
3	C	432	VAL	3.5
2	b	249	ALA	3.5
14	t	30	THR	3.5
13	o	24	ASP	3.5
3	c	436	PHE	3.5
19	z	4	LEU	3.5
18	Y	22	LEU	3.5
13	O	204	VAL	3.5
13	o	206	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
19	z	1	MET	3.4
5	E	17	VAL	3.4
1	a	285	PHE	3.4
19	z	41	PHE	3.4
1	a	288	LEU	3.4
13	o	136	ILE	3.4
2	b	485	GLU	3.4
4	d	283	ALA	3.4
9	J	6	ARG	3.4
4	d	154	VAL	3.3
1	a	242	GLU	3.3
17	X	37	VAL	3.3
2	b	248	ALA	3.3
2	b	461	LEU	3.3
2	B	491	VAL	3.3
3	c	430	HIS	3.3
13	o	58	ASN	3.3
16	v	17	LYS	3.3
20	R	29	LYS	3.3
3	c	429	SER	3.3
13	O	26	ALA	3.2
2	B	486	LEU	3.2
13	o	34	SER	3.2
13	O	139	SER	3.2
13	O	24	ASP	3.2
2	b	501	ASP	3.2
3	c	198	VAL	3.2
3	c	434	ALA	3.2
2	b	482	ILE	3.2
13	o	37	THR	3.2
19	z	30	PRO	3.2
2	B	490	GLN	3.1
3	C	155	ASN	3.1
19	z	61	VAL	3.1
5	e	36	LEU	3.1
2	b	503	THR	3.1
5	E	15	THR	3.1
12	m	34	LYS	3.1
2	b	458	PHE	3.1
3	C	253	LEU	3.1
3	c	87	ILE	3.1
13	o	246	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
18	Y	20	ALA	3.0
3	c	432	VAL	3.0
2	b	298	LEU	3.0
13	o	35	SER	3.0
4	d	148	ALA	3.0
18	Y	43	ARG	3.0
3	c	280	SER	3.0
13	O	206	GLY	3.0
2	B	461	LEU	2.9
2	b	301	ALA	2.9
13	o	36	GLN	2.9
13	o	202	ALA	2.9
4	d	156	VAL	2.9
13	o	38	TYR	2.9
4	D	150	ILE	2.9
2	B	296	ALA	2.9
13	O	130	GLN	2.9
3	c	284	PHE	2.9
19	Z	53	VAL	2.9
3	c	283	GLY	2.9
6	f	15	ILE	2.9
13	o	39	ARG	2.9
2	b	293	ALA	2.9
5	e	59	GLU	2.9
3	C	145[A]	SER	2.8
2	b	251	VAL	2.8
13	o	207	ARG	2.8
2	b	291	SER	2.8
3	c	200	THR	2.8
18	Y	40	ALA	2.8
13	o	40	ILE	2.8
19	z	8	ALA	2.8
2	b	246	PHE	2.8
2	B	501	ASP	2.8
17	x	2	THR	2.8
6	F	13	TYR	2.8
17	x	34	ILE	2.8
1	A	16	ARG	2.8
1	A	200	LEU	2.8
13	O	62	GLU	2.8
19	z	56	VAL	2.7
4	D	122	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
13	O	22	LEU	2.7
18	y	22	LEU	2.7
1	a	225	ARG	2.7
4	D	153	PHE	2.7
4	D	156	VAL	2.7
13	O	87	VAL	2.7
13	o	199	LEU	2.7
3	C	254	THR	2.7
2	b	127	ARG	2.7
13	o	33	ASP	2.7
2	B	295	GLY	2.7
2	b	295	GLY	2.7
3	C	283	GLY	2.7
2	b	294	SER	2.7
2	B	502	VAL	2.7
2	b	462	PHE	2.7
3	c	439	VAL	2.7
12	M	33	GLN	2.7
1	a	286	ALA	2.7
2	b	218	LEU	2.7
19	z	49	ALA	2.7
3	C	433	LEU	2.7
5	e	21	VAL	2.7
19	z	57	LEU	2.7
4	d	281	MET	2.7
3	C	255	THR	2.6
3	c	203	THR	2.6
6	f	42	PHE	2.6
13	o	60	ARG	2.6
1	a	240	GLY	2.6
8	i	38	GLU	2.6
19	z	18	VAL	2.6
4	d	279	LEU	2.6
4	d	159	ILE	2.6
3	c	435	PHE	2.6
1	a	246	TYR	2.6
1	a	287	ALA	2.6
4	d	150	ILE	2.6
13	o	211	ILE	2.6
19	z	6	GLN	2.6
4	d	280	TRP	2.6
13	o	142	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
14	t	29	ILE	2.6
4	D	152	VAL	2.5
18	Y	27	MET	2.5
4	d	151	ALA	2.5
1	A	15	GLU	2.5
6	f	16	PHE	2.5
13	o	208	THR	2.5
10	k	29	PRO	2.5
3	c	438	LEU	2.5
2	B	457	VAL	2.5
3	c	146	PHE	2.5
3	c	317	PHE	2.5
13	O	133	VAL	2.5
1	A	286	ALA	2.5
1	a	200	LEU	2.5
3	c	312	ALA	2.5
19	z	31	GLN	2.5
1	a	281	VAL	2.4
16	v	1	ALA	2.4
3	c	425	TRP	2.4
19	z	35	ARG	2.4
7	h	7	LEU	2.4
3	c	201	ASN	2.4
2	B	505	ARG	2.4
4	d	284	ILE	2.4
5	E	14	ILE	2.4
2	b	245	VAL	2.4
1	a	243	GLU	2.4
2	B	500	GLY	2.4
15	U	70	ARG	2.4
19	z	59	PHE	2.4
7	h	10	ILE	2.4
13	O	132	ASN	2.4
19	Z	4	LEU	2.4
16	v	5	PRO	2.4
4	D	154	VAL	2.4
13	O	134	THR	2.4
15	U	58	VAL	2.4
9	J	5	GLY	2.4
17	X	2	THR	2.4
13	o	23	ASP	2.3
9	j	5	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
16	v	26	TYR	2.3
13	o	130	GLN	2.3
1	a	249	VAL	2.3
13	o	87	VAL	2.3
4	D	149	PRO	2.3
4	d	237	PRO	2.3
2	B	298	LEU	2.3
2	b	250	PHE	2.3
13	o	28	GLY	2.3
2	b	161	LEU	2.3
1	a	197	PHE	2.3
3	C	262	ARG	2.3
1	a	248	ILE	2.3
2	B	482	ILE	2.3
2	B	488	PRO	2.3
1	a	289	GLY	2.3
2	B	493	TRP	2.3
17	x	36	LYS	2.3
3	C	204	LEU	2.3
13	O	138	THR	2.3
13	o	140	THR	2.3
3	C	282	MET	2.3
2	B	185	TRP	2.3
1	a	264	SER	2.3
13	O	91	GLY	2.2
1	A	12	ASN	2.2
3	c	257	PHE	2.2
4	D	157	PHE	2.2
6	F	12	SER	2.2
4	D	174	GLY	2.2
1	A	197	PHE	2.2
2	B	294	SER	2.2
5	E	11	SER	2.2
5	E	20	TRP	2.2
5	e	24	SER	2.2
7	h	12	ARG	2.2
13	O	135	SER	2.2
4	d	238	THR	2.2
3	c	147	PHE	2.2
1	A	294	ALA	2.2
13	o	141	ASP	2.2
1	A	19	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	b	490	GLN	2.2
2	b	414	PRO	2.2
3	c	431	PHE	2.2
3	c	437	PHE	2.2
19	z	34	ASP	2.2
13	o	200	ASN	2.2
12	m	33	GLN	2.2
1	a	290	ILE	2.2
1	a	297	LEU	2.2
3	c	279	LEU	2.2
5	e	39	SER	2.2
3	C	439	VAL	2.2
19	z	53	VAL	2.2
3	C	436	PHE	2.2
2	b	296	ALA	2.2
11	L	7	ARG	2.2
1	a	291	SER	2.2
3	c	96	GLY	2.2
17	x	33	GLN	2.2
13	O	21	THR	2.1
1	a	160	ILE	2.1
3	C	285	ILE	2.1
16	v	19	ILE	2.1
9	J	9	LEU	2.1
3	C	144	SER	2.1
4	d	155	SER	2.1
13	O	237	GLY	2.1
5	e	56	TYR	2.1
13	o	241	ALA	2.1
18	Y	26	ALA	2.1
5	e	84	LYS	2.1
1	A	290	ILE	2.1
19	z	38	GLN	2.1
3	c	183	GLY	2.1
3	C	437	PHE	2.1
18	y	25	ILE	2.1
1	A	159	LEU	2.1
2	b	244	ALA	2.1
3	C	434	ALA	2.1
5	e	25	ILE	2.1
5	E	83	LEU	2.1
3	c	313	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
4	d	286	VAL	2.1
19	z	32	ASP	2.0
3	c	404	LEU	2.0
5	E	25	ILE	2.0
15	U	79	LEU	2.0
13	O	203	LYS	2.0
13	o	201	VAL	2.0
2	b	247	PHE	2.0
3	C	429	SER	2.0
3	c	20	SER	2.0
2	b	483	ASP	2.0
4	d	149	PRO	2.0
17	x	8	LYS	2.0
2	B	458	PHE	2.0
1	A	289	GLY	2.0
3	c	287	THR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	T	1	10/11	0.96	0.08	40,46,63,64	0
8	FME	I	1	10/11	0.97	0.11	44,65,72,73	0
12	FME	M	1	10/11	0.98	0.10	37,50,80,87	0
8	FME	i	1	10/11	0.98	0.10	49,58,67,73	0
12	FME	m	1	10/11	0.98	0.07	41,53,62,76	0
14	FME	t	1	10/11	0.98	0.08	36,43,68,73	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
32	LMG	C	522	51/55	0.51	0.41	69,127,161,165	0
34	LMT	a	413	35/35	0.51	0.39	66,131,140,142	0
34	LMT	E	102	35/35	0.52	0.48	102,145,164,166	0
30	UNL	j	101	10/-	0.52	0.38	78,87,93,94	0
33	HTG	b	623	19/19	0.54	0.52	83,144,150,150	0
30	UNL	A	414	28/-	0.56	0.45	83,97,113,115	0
34	LMT	e	101	35/35	0.59	0.64	122,163,170,171	0
34	LMT	M	103	35/35	0.62	0.30	78,152,175,176	0
34	LMT	m	103	35/35	0.62	0.35	52,93,109,110	0
34	LMT	C	526	35/35	0.63	0.55	88,140,155,158	0
30	UNL	a	416	30/-	0.65	0.35	96,111,134,138	0
33	HTG	D	411	16/19	0.65	0.30	91,113,123,129	0
29	PL9	A	413	55/55	0.65	0.36	72,102,112,115	0
30	UNL	i	101	40/-	0.66	0.27	69,98,148,152	0
32	LMG	c	522	51/55	0.66	0.41	72,129,152,157	0
34	LMT	D	402	35/35	0.69	0.31	69,124,137,143	0
34	LMT	M	101	35/35	0.69	0.28	53,98,131,139	0
30	UNL	b	626	33/-	0.70	0.40	63,90,146,148	0
30	UNL	J	101	10/-	0.71	0.23	75,79,91,92	0
30	UNL	I	101	40/-	0.72	0.25	68,107,149,150	0
30	UNL	C	527	34/-	0.72	0.30	83,110,123,126	0
31	LHG	a	419	42/49	0.72	0.31	100,147,177,181	0
36	CA	F	101	1/1	0.72	0.06	115,115,115,115	0
32	LMG	Z	101	37/55	0.73	0.27	72,123,156,161	0
34	LMT	b	621	25/35	0.75	0.23	89,129,154,154	0
26	GOL	b	624	6/6	0.75	0.23	86,95,99,105	0
30	UNL	M	102	10/-	0.76	0.22	63,73,84,84	0
32	LMG	c	501	51/55	0.76	0.24	60,88,109,117	0
30	UNL	c	526	32/-	0.76	0.37	94,113,130,132	0
30	UNL	B	626	33/-	0.77	0.24	52,108,152,156	0
26	GOL	B	629	6/6	0.77	0.45	103,111,114,116	0
31	LHG	E	101	42/49	0.77	0.23	72,126,138,141	0
29	PL9	a	415	55/55	0.77	0.29	87,111,124,126	0
26	GOL	B	627	6/6	0.77	0.25	63,92,96,97	0
30	UNL	m	102	10/-	0.78	0.24	59,68,91,92	0
34	LMT	a	418	35/35	0.78	0.51	118,150,157,158	0
30	UNL	d	410	36/-	0.79	0.23	70,94,127,130	0
27	SQD	f	101	43/54	0.80	0.42	111,132,160,166	0
33	HTG	b	622	19/19	0.80	0.20	64,71,105,109	0
26	GOL	O	302	6/6	0.80	0.28	78,85,86,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
34	LMT	B	630	25/35	0.80	0.21	55,84,135,139	0
33	HTG	B	623	19/19	0.80	0.40	61,86,94,95	0
33	HTG	B	622	19/19	0.81	0.22	61,83,110,111	0
33	HTG	V	202	11/19	0.81	0.44	110,119,121,121	0
34	LMT	B	628	35/35	0.81	0.25	63,110,126,130	0
36	CA	a	420	1/1	0.81	0.29	105,105,105,105	0
27	SQD	B	620	54/54	0.82	0.19	54,88,124,129	0
33	HTG	h	101	16/19	0.82	0.29	103,133,139,143	0
27	SQD	b	620	54/54	0.83	0.19	59,88,112,115	0
30	UNL	d	411	18/-	0.83	0.25	74,78,109,112	0
32	LMG	z	101	39/55	0.83	0.32	80,128,136,139	0
30	UNL	D	410	40/-	0.83	0.23	56,85,125,129	0
30	UNL	X	101	18/-	0.84	0.18	60,68,98,99	0
34	LMT	t	101	26/35	0.84	0.20	77,117,136,140	0
34	LMT	b	627	25/35	0.85	0.22	50,75,135,136	0
26	GOL	o	302	6/6	0.85	0.49	110,113,118,120	0
25	BCR	h	102	40/40	0.85	0.17	50,61,74,75	0
27	SQD	A	411	54/54	0.86	0.16	60,82,123,130	0
26	GOL	A	410	6/6	0.86	0.19	68,68,74,81	0
33	HTG	c	523	19/19	0.86	0.27	119,138,143,144	0
32	LMG	B	621	51/55	0.86	0.18	49,65,92,114	0
25	BCR	H	101	40/40	0.87	0.17	44,61,71,74	0
32	LMG	C	521	51/55	0.87	0.20	52,87,119,120	0
32	LMG	c	521	51/55	0.87	0.26	68,92,125,127	0
26	GOL	v	201	6/6	0.87	0.24	51,70,78,80	0
32	LMG	m	101	51/55	0.87	0.20	51,68,96,98	0
35	DGD	h	103	62/66	0.88	0.22	50,59,68,71	0
26	GOL	a	411	6/6	0.88	0.20	57,68,80,81	0
33	HTG	C	523	19/19	0.88	0.31	106,118,127,127	0
32	LMG	C	502	51/55	0.89	0.18	57,84,104,106	0
31	LHG	A	416	49/49	0.89	0.22	41,57,80,87	0
35	DGD	H	102	62/66	0.89	0.20	40,55,67,69	0
27	SQD	a	412	54/54	0.89	0.16	59,85,125,127	0
29	PL9	d	405	55/55	0.89	0.19	35,46,56,61	0
25	BCR	k	101	40/40	0.89	0.17	58,70,81,81	0
23	CLA	C	515	65/65	0.90	0.16	59,70,111,114	0
25	BCR	y	101	40/40	0.90	0.12	57,70,83,86	0
26	GOL	b	628	6/6	0.90	0.25	94,100,102,103	0
23	CLA	c	504	65/65	0.91	0.28	48,56,73,83	0
26	GOL	c	502	6/6	0.91	0.23	61,75,77,81	0
35	DGD	C	519	62/66	0.91	0.17	42,62,116,121	0
30	UNL	d	409	17/-	0.91	0.21	67,82,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	c	505	65/65	0.91	0.22	53,63,73,77	0
30	UNL	D	409	17/-	0.91	0.29	56,77,114,114	0
23	CLA	B	602	65/65	0.91	0.14	39,48,72,77	0
23	CLA	C	514	65/65	0.92	0.15	55,65,114,119	0
23	CLA	C	508	65/65	0.92	0.13	51,63,123,130	0
35	DGD	c	519	62/66	0.92	0.19	50,70,107,118	0
23	CLA	c	509	65/65	0.92	0.14	53,63,73,83	0
23	CLA	c	514	65/65	0.92	0.18	64,77,112,122	0
23	CLA	b	609	65/65	0.92	0.13	49,57,78,100	0
23	CLA	b	602	65/65	0.93	0.19	43,54,70,80	0
31	LHG	b	629	49/49	0.93	0.17	40,55,71,78	0
33	HTG	B	625	19/19	0.93	0.11	65,75,82,87	0
31	LHG	d	407	49/49	0.93	0.14	41,51,68,78	0
23	CLA	c	515	65/65	0.93	0.27	64,83,117,119	0
23	CLA	d	403	65/65	0.93	0.15	48,58,115,123	0
23	CLA	C	509	65/65	0.93	0.12	50,57,76,80	0
27	SQD	C	501	54/54	0.93	0.17	59,79,105,107	0
32	LMG	D	413	51/55	0.93	0.17	44,64,111,123	0
27	SQD	D	412	43/54	0.93	0.21	74,111,131,138	0
35	DGD	C	520	62/66	0.93	0.16	40,53,95,108	0
27	SQD	a	410	54/54	0.93	0.19	64,83,117,118	0
25	BCR	b	618	40/40	0.93	0.20	37,50,67,72	0
23	CLA	C	506	65/65	0.93	0.16	42,51,85,95	0
23	CLA	B	609	65/65	0.93	0.12	43,51,74,81	0
23	CLA	D	404	65/65	0.93	0.16	44,54,126,133	0
25	BCR	b	617	40/40	0.94	0.15	35,43,56,58	0
23	CLA	C	513	65/65	0.94	0.12	49,62,77,78	0
25	BCR	c	516	40/40	0.94	0.17	68,83,90,94	0
25	BCR	d	404	40/40	0.94	0.11	52,63,87,92	0
23	CLA	b	601	65/65	0.94	0.20	58,80,120,129	0
23	CLA	c	506	65/65	0.94	0.24	49,58,103,110	0
23	CLA	B	611	65/65	0.94	0.16	34,39,61,68	0
23	CLA	c	510	65/65	0.94	0.24	47,57,127,132	0
26	GOL	B	624	6/6	0.94	0.14	76,87,95,97	0
32	LMG	d	412	51/55	0.94	0.13	53,67,111,119	0
23	CLA	c	513	65/65	0.94	0.14	55,65,81,85	0
29	PL9	D	406	55/55	0.94	0.16	32,42,54,60	0
23	CLA	b	604	65/65	0.94	0.23	34,43,111,119	0
23	CLA	B	601	65/65	0.94	0.21	52,72,115,121	0
23	CLA	b	610	65/65	0.94	0.15	43,50,62,73	0
25	BCR	C	516	40/40	0.94	0.11	59,74,81,83	0
23	CLA	b	612	65/65	0.94	0.17	38,46,61,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	BCR	K	101	40/40	0.94	0.13	54,63,69,71	0
35	DGD	c	518	62/66	0.94	0.20	45,58,90,95	0
31	LHG	d	406	49/49	0.94	0.25	50,61,76,81	0
35	DGD	c	520	62/66	0.94	0.15	48,60,98,111	0
25	BCR	Y	101	40/40	0.94	0.11	53,64,73,77	0
33	HTG	b	625	19/19	0.94	0.10	66,72,92,98	0
36	CA	O	301	1/1	0.94	0.18	103,103,103,103	0
31	LHG	d	408	49/49	0.94	0.20	53,65,117,122	0
36	CA	o	301	1/1	0.94	0.10	100,100,100,100	0
23	CLA	b	611	65/65	0.95	0.22	36,44,70,76	0
25	BCR	T	101	40/40	0.95	0.13	37,48,57,61	0
23	CLA	B	610	65/65	0.95	0.15	41,48,59,77	0
23	CLA	b	614	65/65	0.95	0.15	35,44,102,105	0
23	CLA	b	616	65/65	0.95	0.17	43,55,114,116	0
23	CLA	c	503	65/65	0.95	0.13	53,61,74,82	0
23	CLA	B	603	65/65	0.95	0.13	38,46,62,66	0
23	CLA	a	408	65/65	0.95	0.15	40,48,128,132	0
23	CLA	B	614	65/65	0.95	0.15	33,43,93,97	0
23	CLA	c	507	65/65	0.95	0.13	43,56,83,86	0
23	CLA	C	510	65/65	0.95	0.18	43,51,117,130	0
23	CLA	b	603	65/65	0.95	0.15	41,50,70,88	0
35	DGD	C	518	62/66	0.95	0.21	40,54,93,96	0
31	LHG	D	407	49/49	0.95	0.13	40,48,64,76	0
31	LHG	D	408	49/49	0.95	0.18	45,57,124,134	0
23	CLA	C	512	65/65	0.95	0.21	46,56,78,87	0
31	LHG	L	101	49/49	0.95	0.14	39,51,65,84	0
23	CLA	b	605	65/65	0.95	0.15	35,43,66,75	0
23	CLA	b	606	65/65	0.95	0.12	38,49,110,115	0
23	CLA	b	607	65/65	0.95	0.16	32,40,73,80	0
25	BCR	A	409	40/40	0.95	0.11	33,42,54,58	0
23	CLA	C	503	65/65	0.95	0.13	45,53,68,78	0
25	BCR	C	517	40/40	0.95	0.11	49,56,64,73	0
36	CA	c	525	1/1	0.95	0.02	80,80,80,80	0
23	CLA	C	505	65/65	0.95	0.14	47,55,67,72	0
23	CLA	c	508	65/65	0.96	0.12	56,69,121,126	0
23	CLA	B	607	65/65	0.96	0.15	31,40,64,69	0
25	BCR	a	409	40/40	0.96	0.09	36,45,56,59	0
23	CLA	A	408	65/65	0.96	0.12	38,45,111,119	0
23	CLA	c	511	65/65	0.96	0.20	54,62,86,88	0
25	BCR	b	619	40/40	0.96	0.10	46,53,74,84	0
23	CLA	c	512	65/65	0.96	0.31	52,59,73,76	0
25	BCR	c	517	40/40	0.96	0.10	53,65,71,71	0

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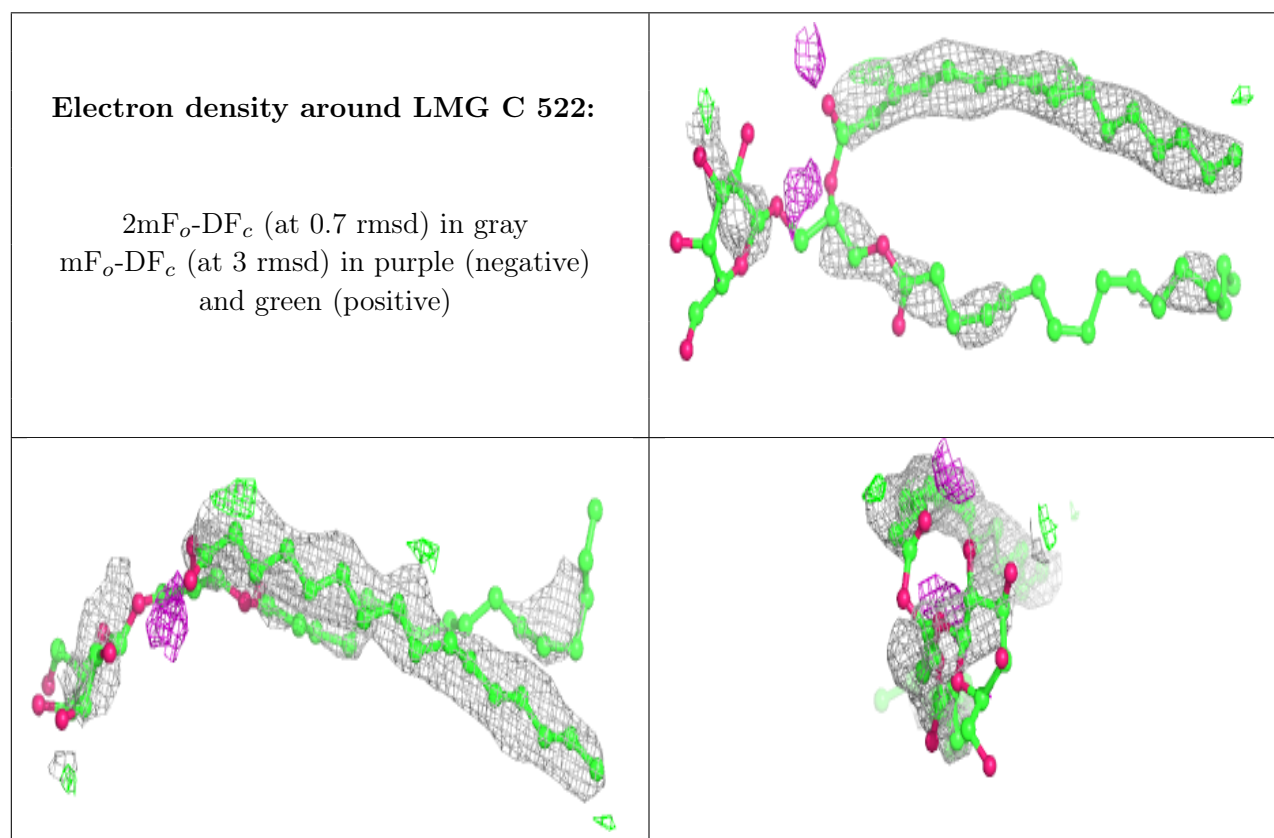
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	b	613	65/65	0.96	0.26	33,42,84,88	0
23	CLA	C	507	65/65	0.96	0.15	43,52,86,93	0
23	CLA	b	615	65/65	0.96	0.11	42,50,74,79	0
25	BCR	t	102	40/40	0.96	0.13	37,51,66,70	0
23	CLA	B	616	65/65	0.96	0.17	41,52,136,137	0
24	PHO	A	407	64/64	0.96	0.14	32,37,47,52	0
24	PHO	A	415	64/64	0.96	0.22	35,43,52,54	0
23	CLA	B	606	65/65	0.96	0.11	38,46,101,108	0
25	BCR	B	619	40/40	0.96	0.10	43,53,72,75	0
26	GOL	C	524	6/6	0.96	0.13	53,56,60,61	0
23	CLA	a	406	65/65	0.96	0.21	39,49,114,118	0
23	CLA	b	608	65/65	0.96	0.19	45,52,69,76	0
25	BCR	D	405	40/40	0.96	0.17	45,58,95,103	0
36	CA	c	524	1/1	0.96	0.06	73,73,73,73	0
23	CLA	C	504	65/65	0.96	0.17	43,50,71,82	0
23	CLA	C	511	65/65	0.96	0.14	48,56,77,79	0
39	MG	j	102	1/1	0.96	0.11	60,60,60,60	0
24	PHO	a	407	64/64	0.97	0.14	35,42,47,50	0
24	PHO	a	417	64/64	0.97	0.19	39,47,55,60	0
23	CLA	a	404	65/65	0.97	0.19	37,41,64,73	0
25	BCR	B	617	40/40	0.97	0.14	34,45,55,58	0
25	BCR	B	618	40/40	0.97	0.15	35,50,63,72	0
23	CLA	a	405	65/65	0.97	0.14	34,40,57,62	0
23	CLA	B	613	65/65	0.97	0.20	34,41,89,94	0
23	CLA	A	405	65/65	0.97	0.17	31,37,52,56	0
23	CLA	B	615	65/65	0.97	0.12	40,46,77,83	0
36	CA	C	525	1/1	0.97	0.20	66,66,66,66	0
23	CLA	A	406	65/65	0.97	0.20	34,42,114,117	0
23	CLA	B	608	65/65	0.97	0.17	39,47,62,65	0
23	CLA	A	404	65/65	0.97	0.22	33,36,61,75	0
23	CLA	B	604	65/65	0.97	0.19	32,39,110,116	0
23	CLA	B	605	65/65	0.97	0.12	35,41,61,73	0
23	CLA	D	403	65/65	0.97	0.24	32,37,53,62	0
38	HEC	E	103	43/43	0.97	0.11	57,65,80,93	0
38	HEC	e	102	43/43	0.97	0.17	64,78,119,130	0
38	HEC	v	202	43/43	0.97	0.11	52,58,63,64	0
23	CLA	B	612	65/65	0.97	0.15	35,44,54,59	0
38	HEC	V	201	43/43	0.98	0.09	43,46,51,54	0
28	OEX	A	412	10/10	0.98	0.11	35,38,45,46	0
37	BCT	D	401	4/4	0.98	0.06	51,57,61,62	0
39	MG	J	102	1/1	0.98	0.07	50,50,50,50	0
23	CLA	d	402	65/65	0.98	0.23	36,40,68,77	0

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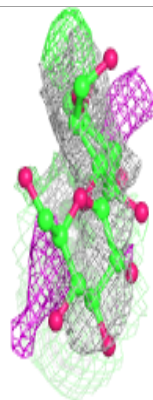
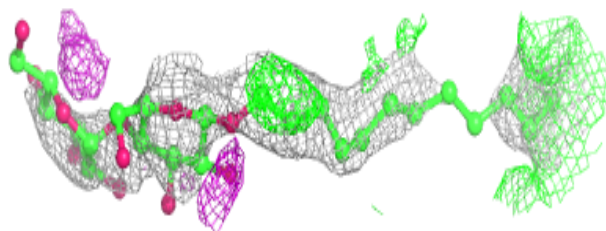
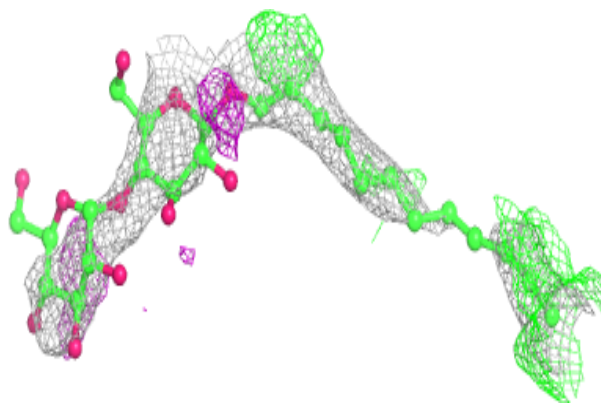
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CL	A	403	1/1	0.99	0.11	40,40,40,40	0
37	BCT	d	401	4/4	0.99	0.07	52,54,62,64	0
22	CL	a	402	1/1	0.99	0.06	42,42,42,42	0
22	CL	a	403	1/1	0.99	0.09	44,44,44,44	0
21	FE2	A	401	1/1	0.99	0.03	53,53,53,53	0
21	FE2	a	401	1/1	0.99	0.03	57,57,57,57	0
22	CL	A	402	1/1	0.99	0.05	35,35,35,35	0
28	OEX	a	414	10/10	0.99	0.11	39,45,49,49	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.

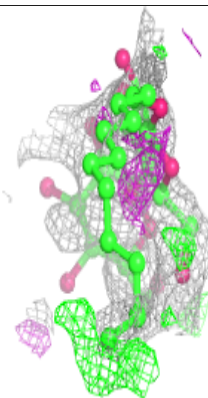
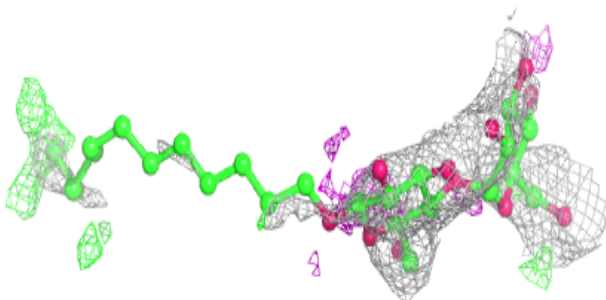
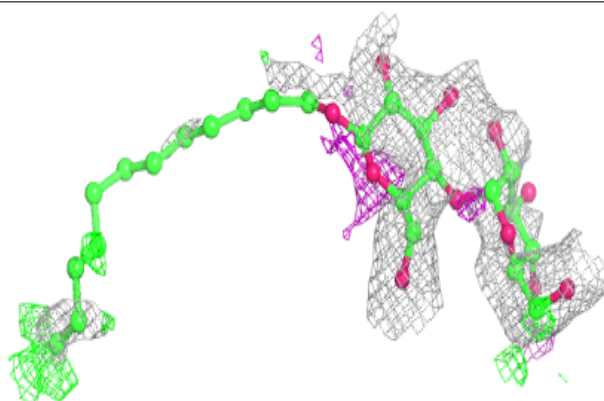


Electron density around LMT a 413:

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

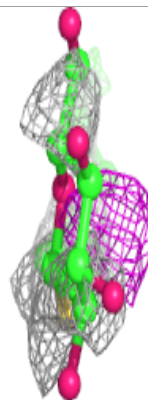
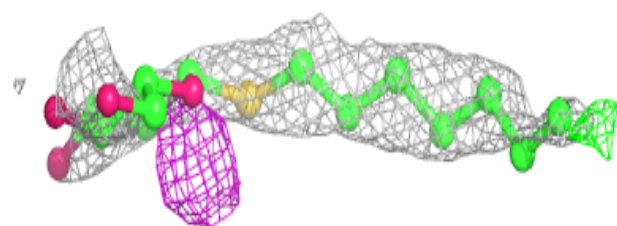
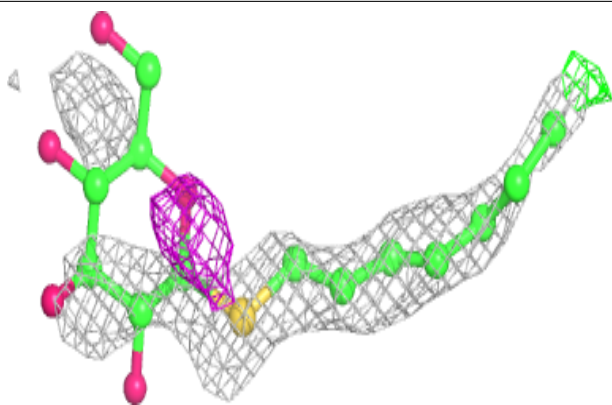
**Electron density around LMT E 102:**

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

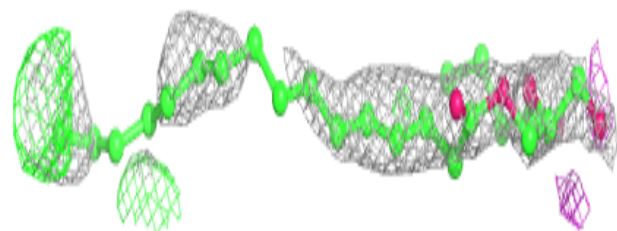
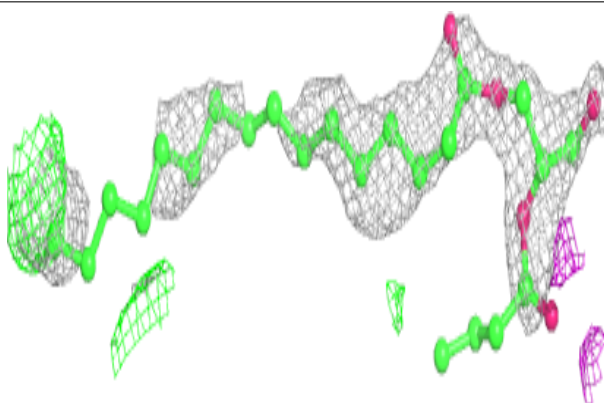


Electron density around HTG b 623:

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

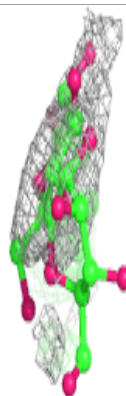
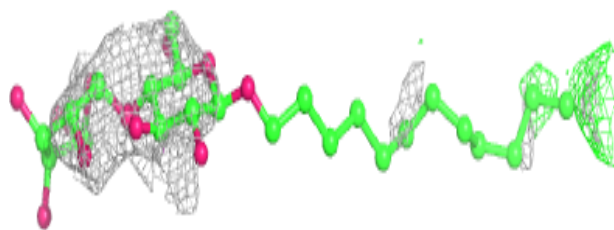
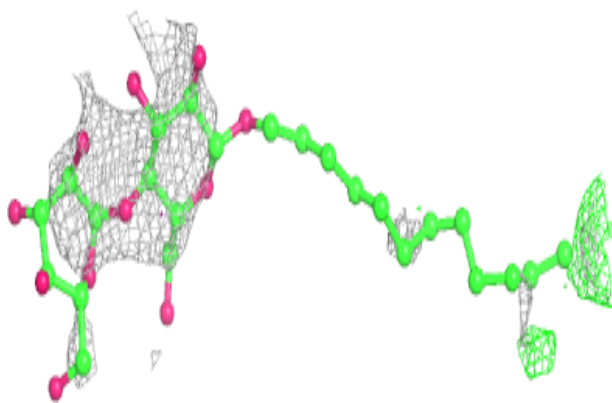
**Electron density around UNL A 414:**

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

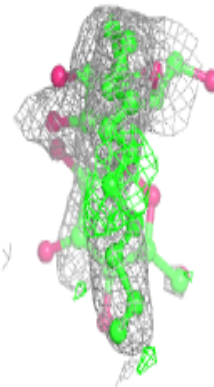
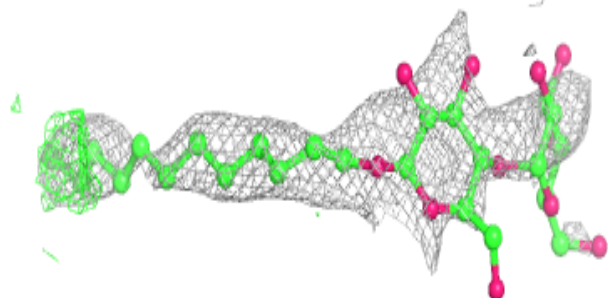
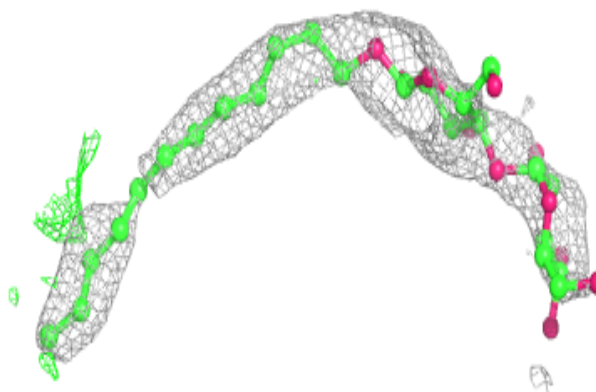


Electron density around LMT e 101:

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

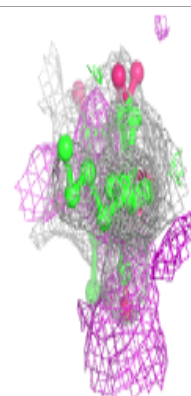
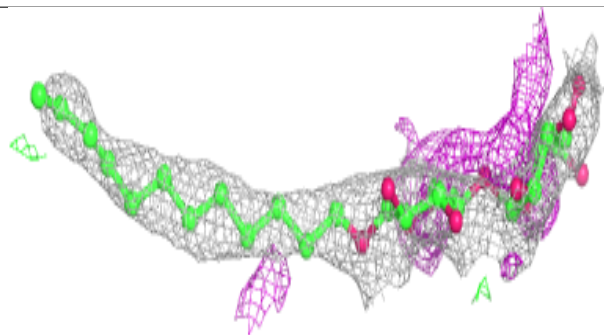
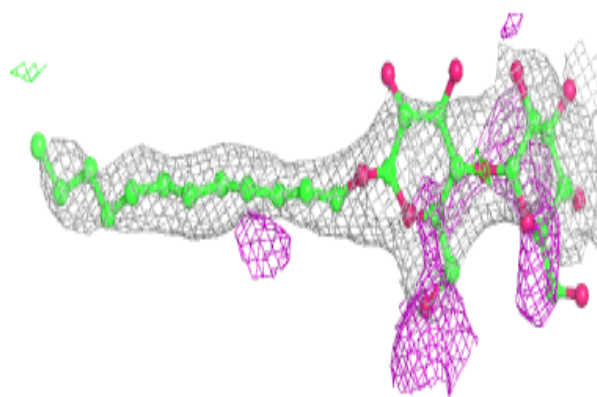
**Electron density around LMT M 103:**

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

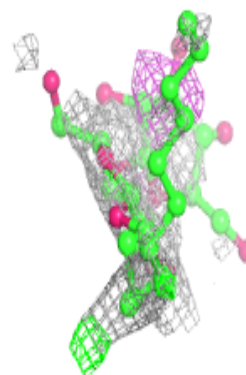
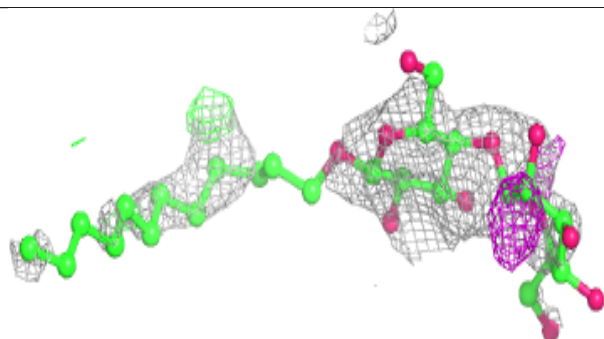
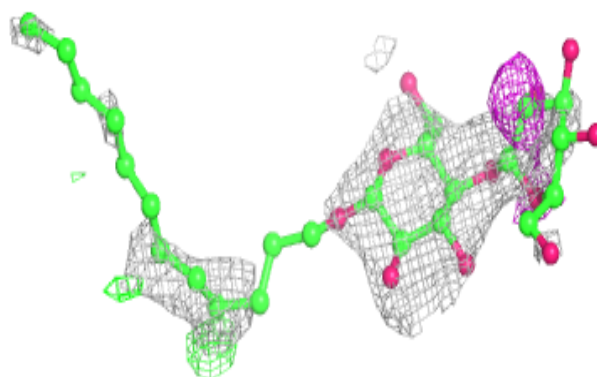


Electron density around LMT m 103:

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

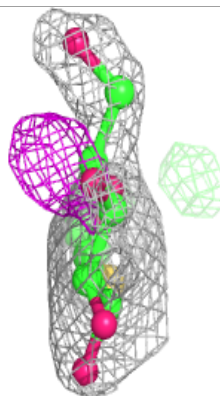
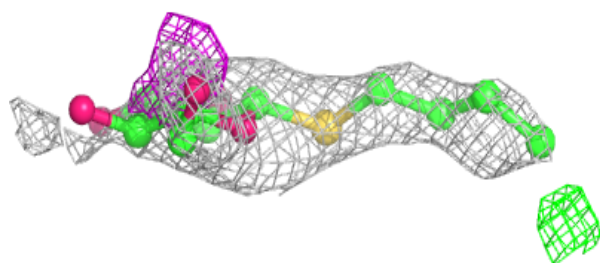
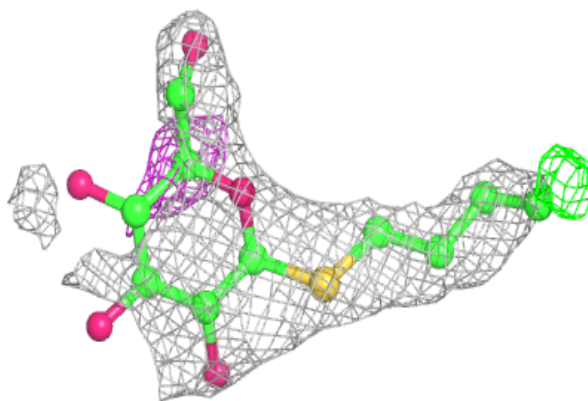
**Electron density around LMT C 526:**

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

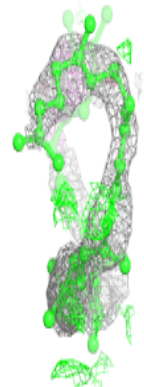
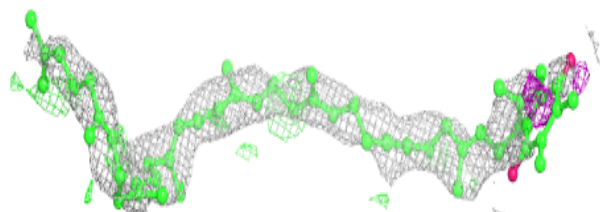
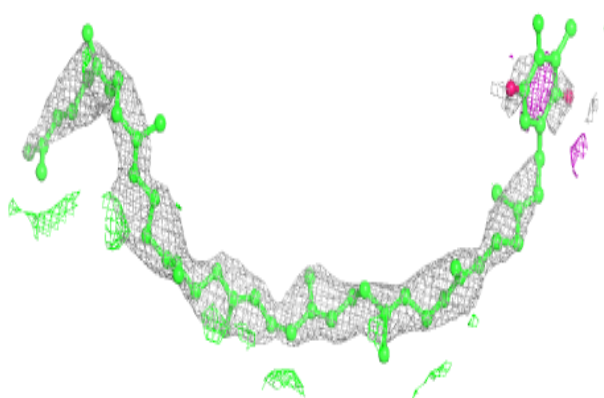


Electron density around HTG D 411:

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

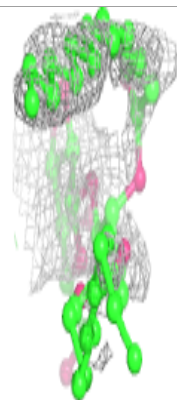
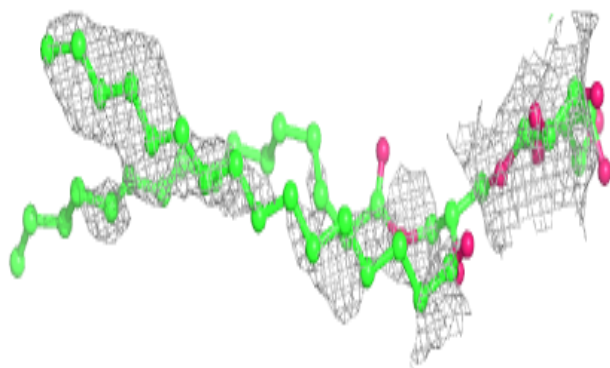
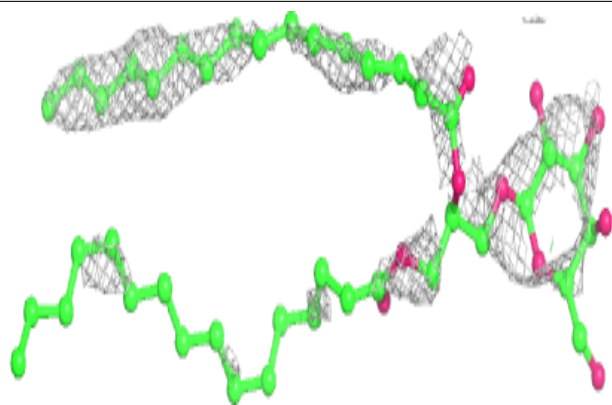
**Electron density around PL9 A 413:**

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

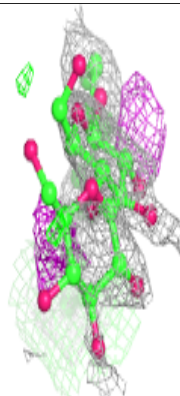
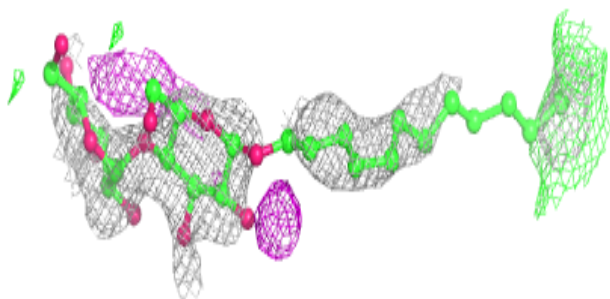
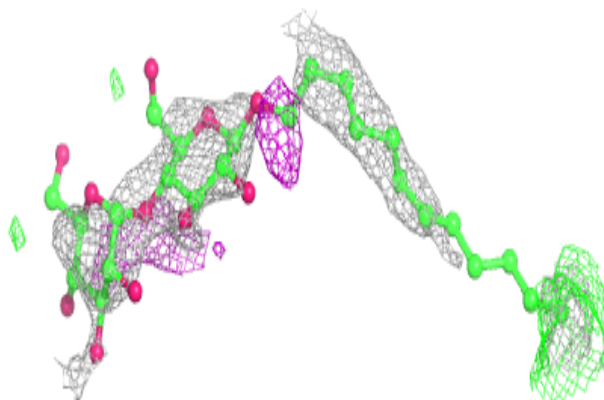


Electron density around LMG c 522:

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

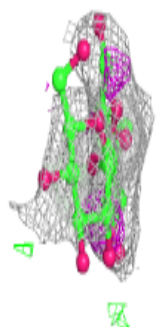
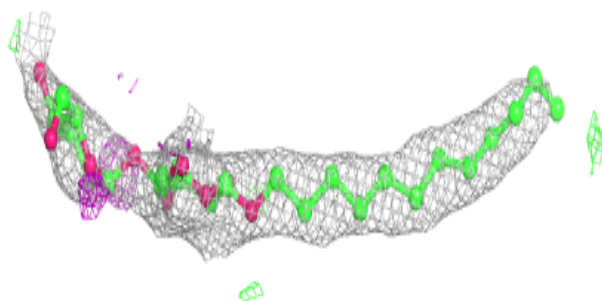
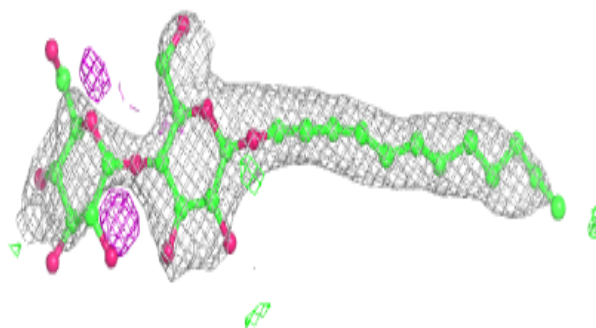
**Electron density around LMT D 402:**

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

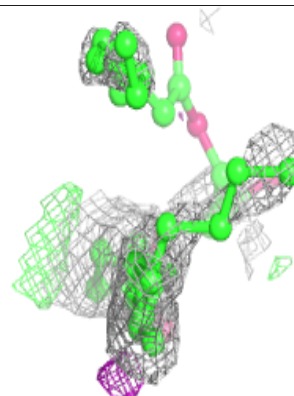
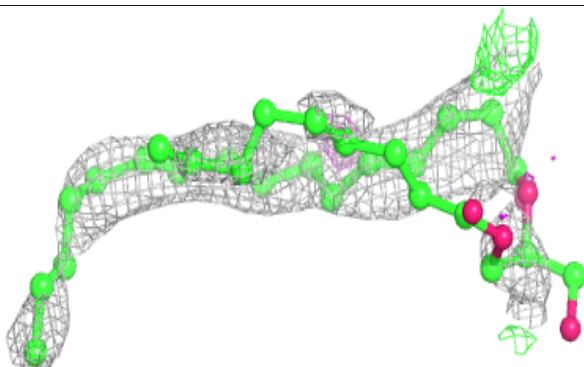
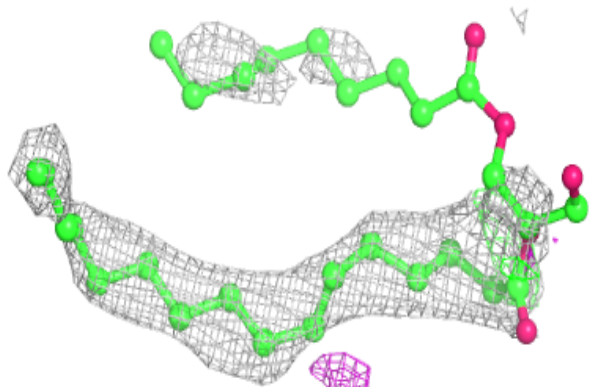


Electron density around LMT M 101:

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

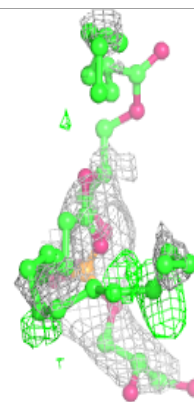
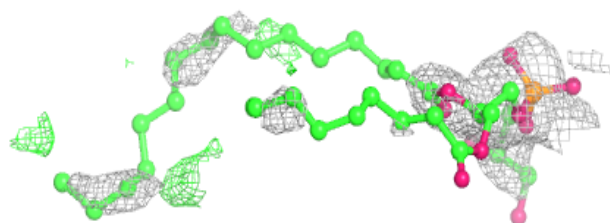
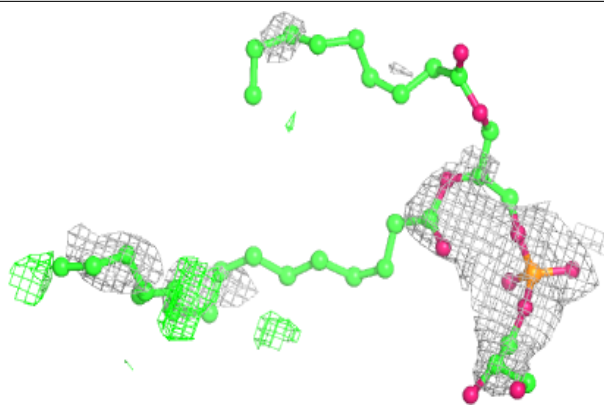
**Electron density around UNL b 626:**

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

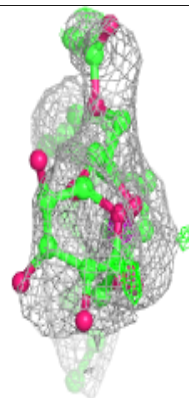
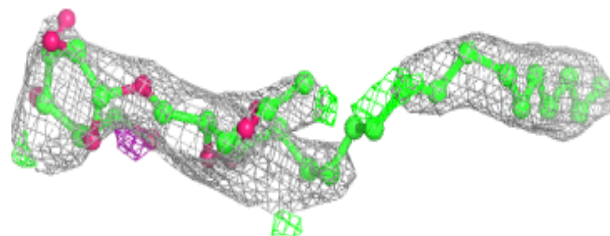
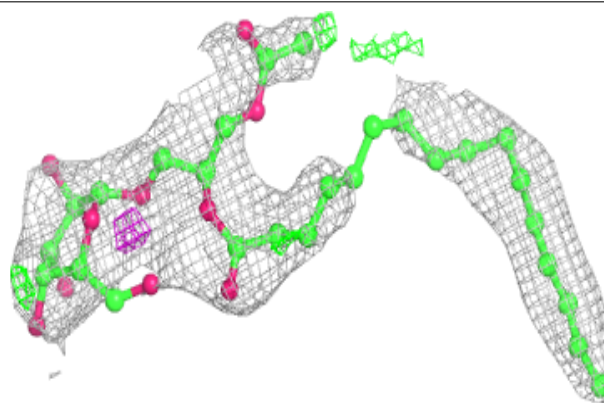


Electron density around LHG a 419:

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

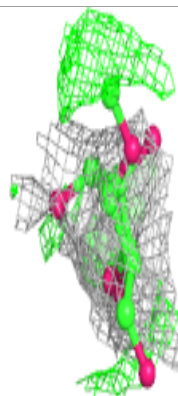
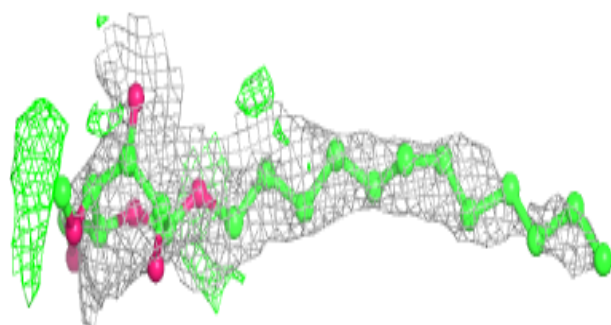
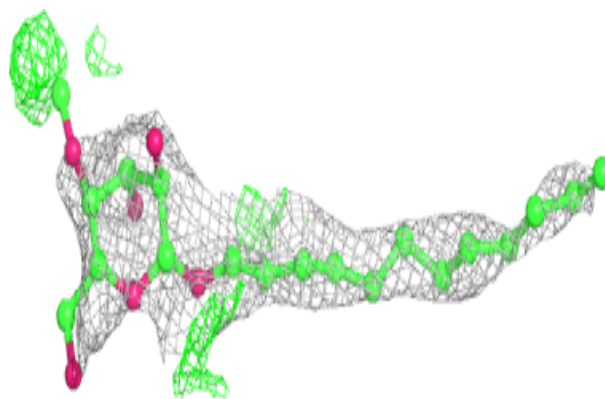
**Electron density around LMG Z 101:**

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

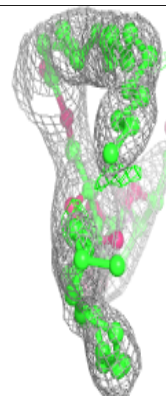
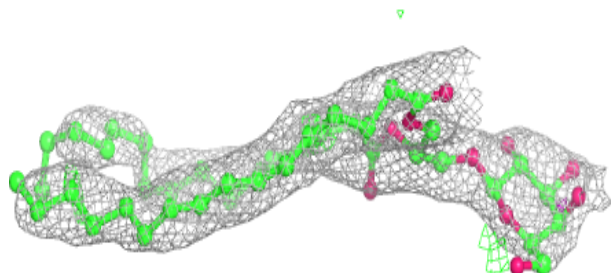
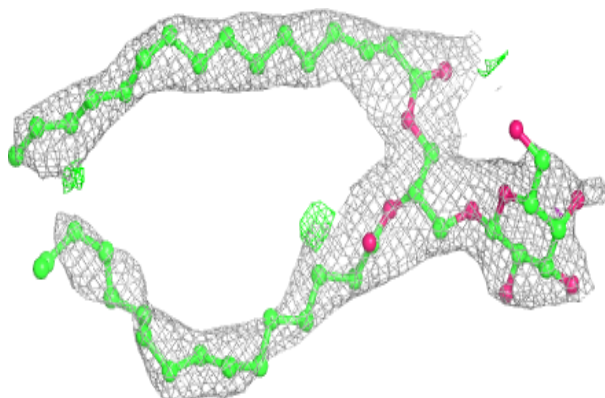


Electron density around LMT b 621:

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

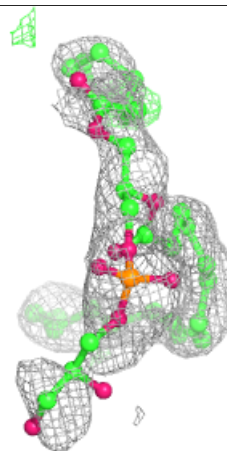
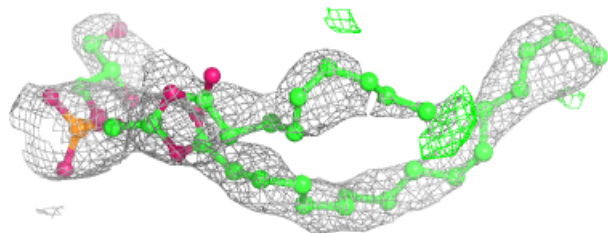
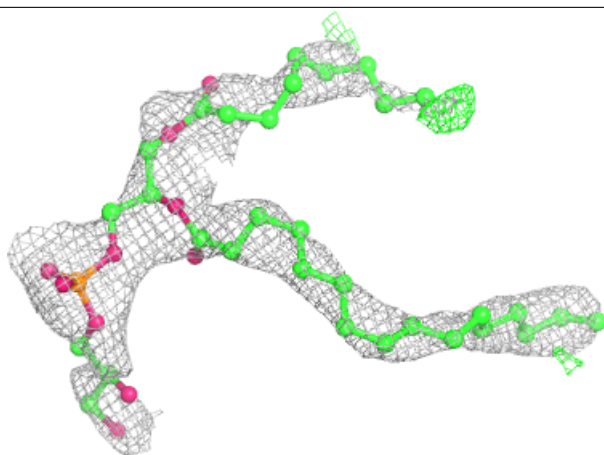
**Electron density around LMG c 501:**

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

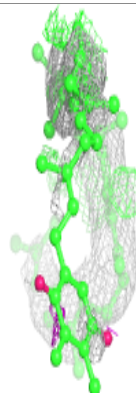
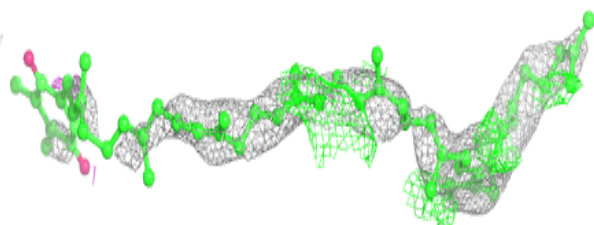
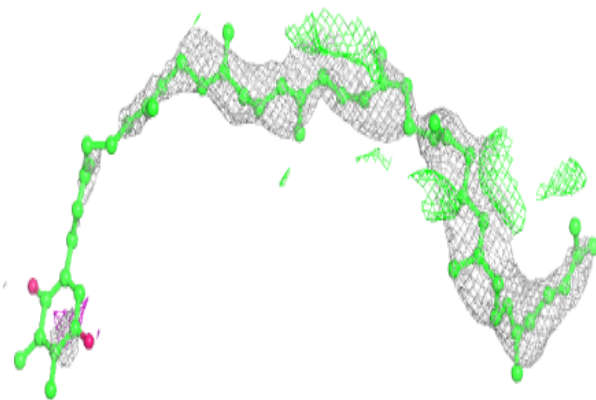


Electron density around LHG E 101:

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

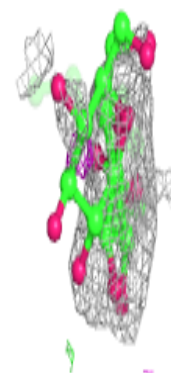
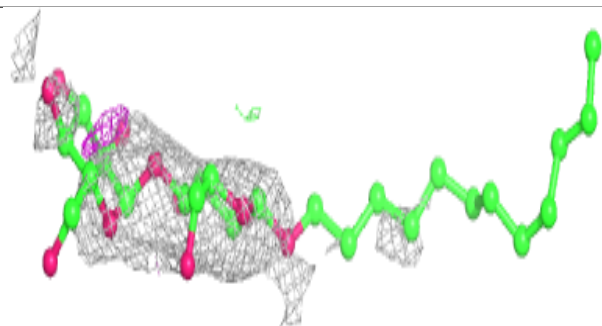
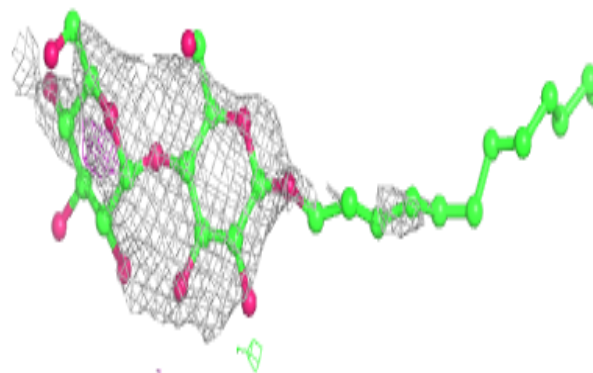
**Electron density around PL9 a 415:**

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

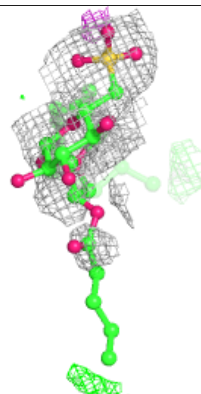
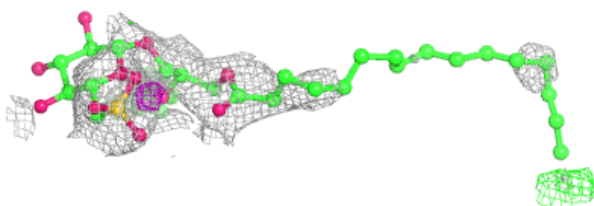
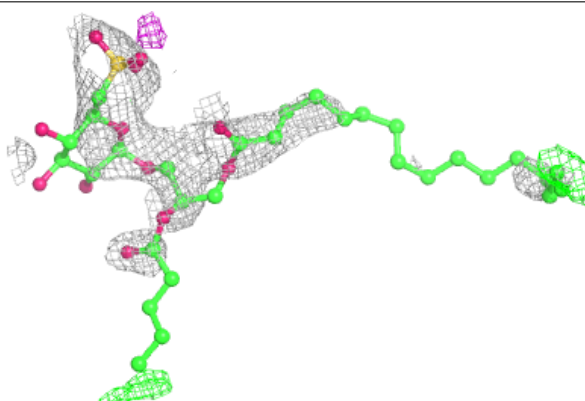


Electron density around LMT a 418:

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

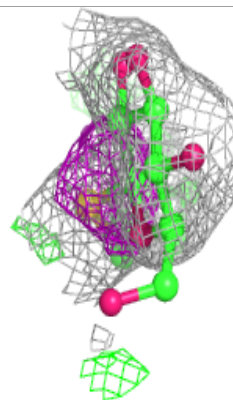
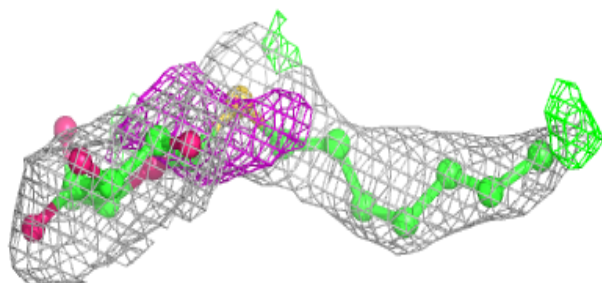
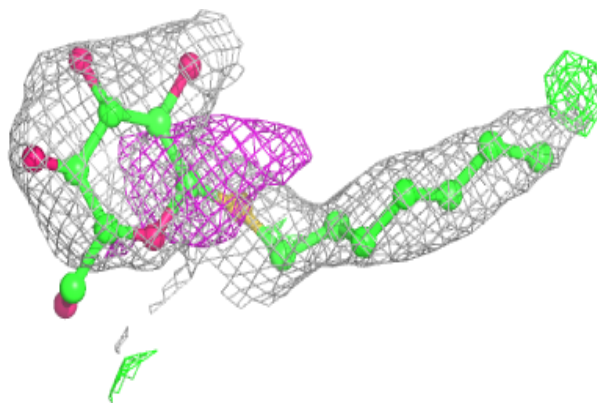
**Electron density around SQD f 101:**

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

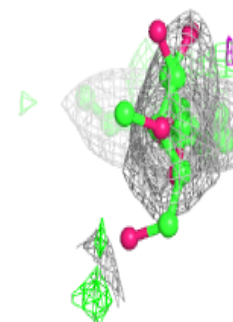
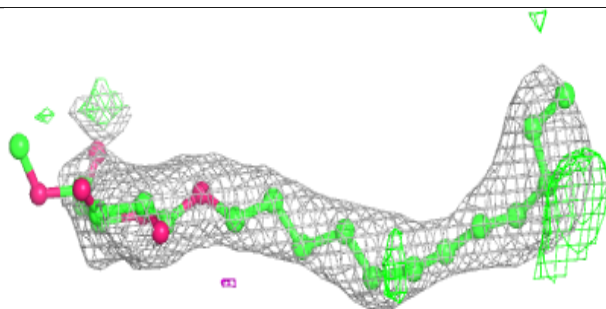
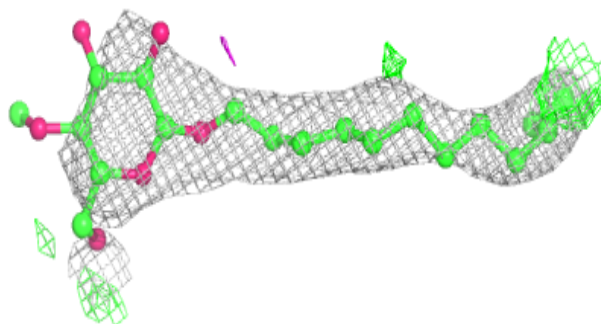


Electron density around HTG b 622:

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

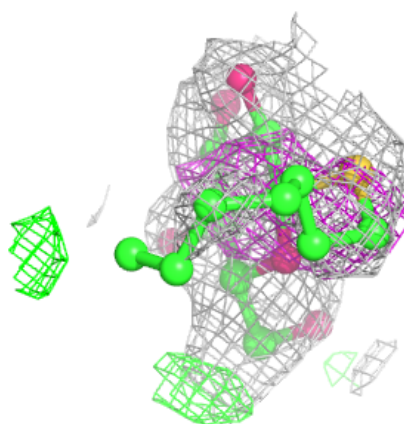
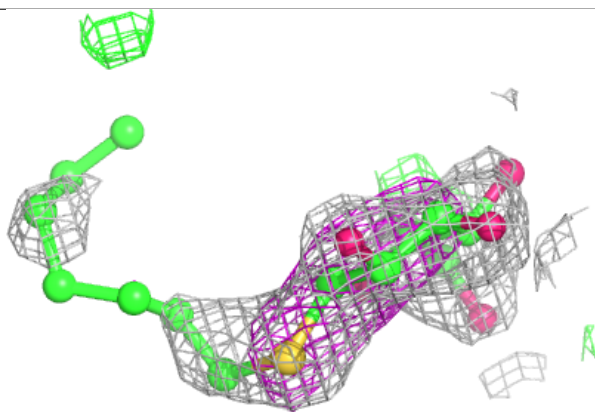
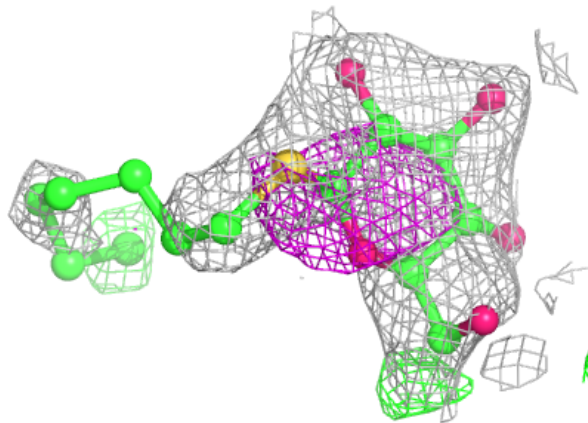
**Electron density around LMT B 630:**

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



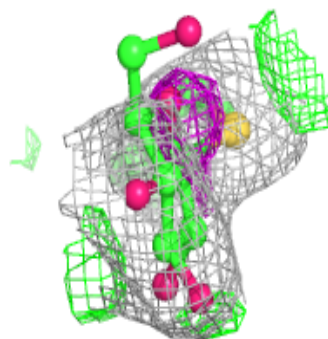
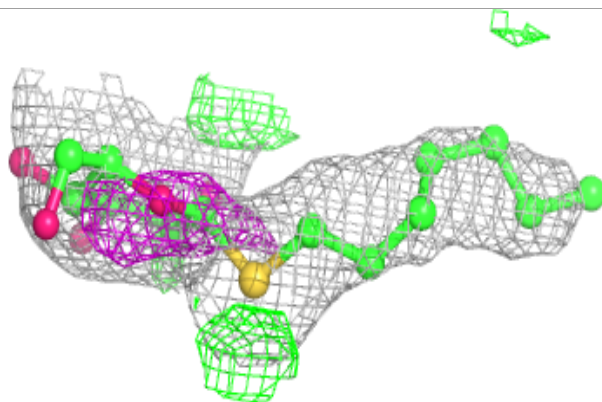
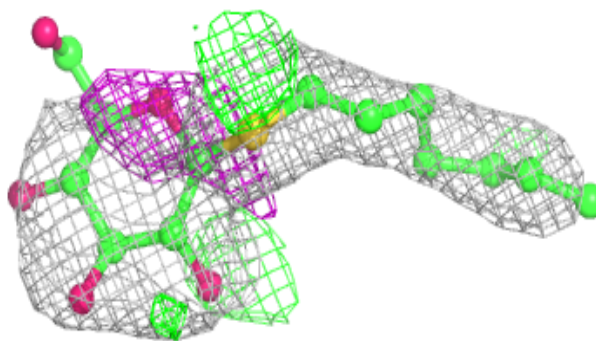
Electron density around HTG B 623:

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



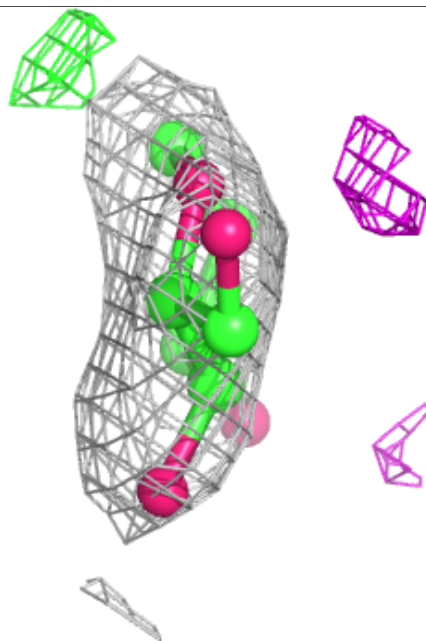
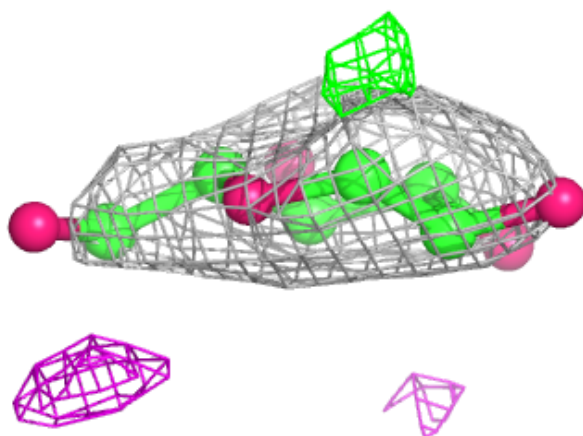
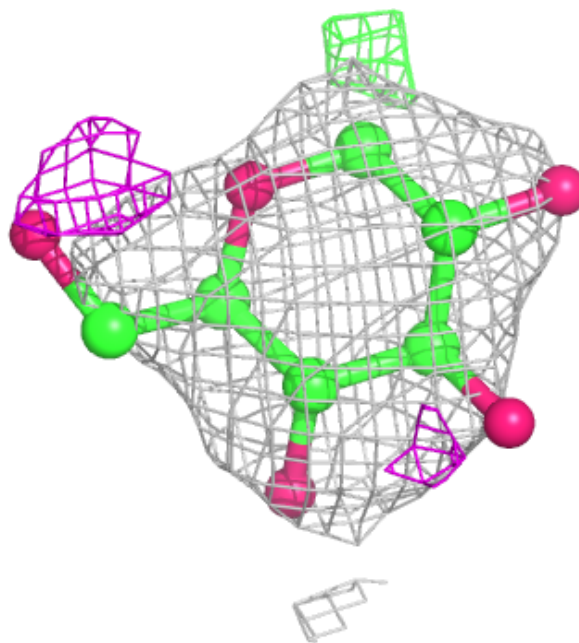
Electron density around HTG B 622:

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



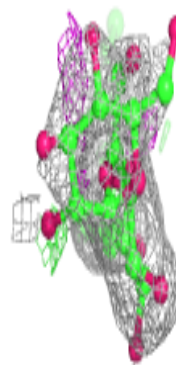
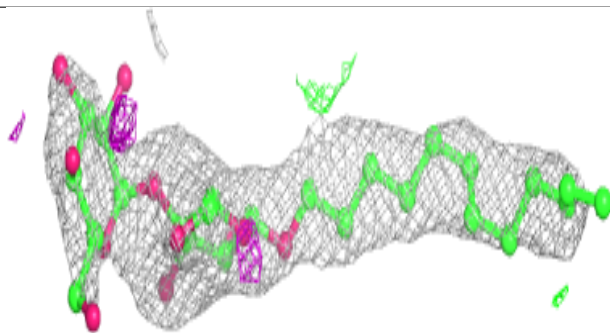
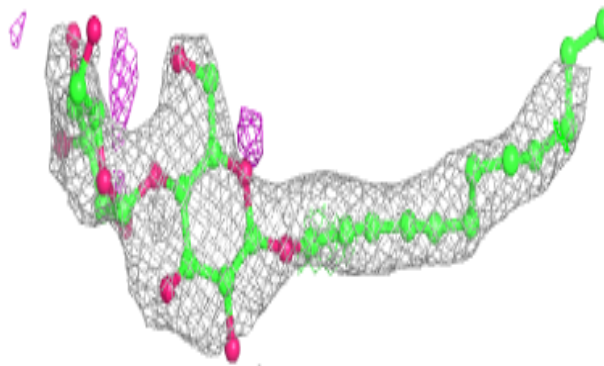
Electron density around HTG V 202:

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

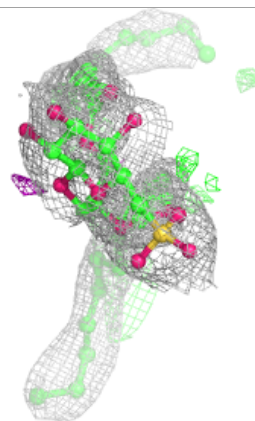
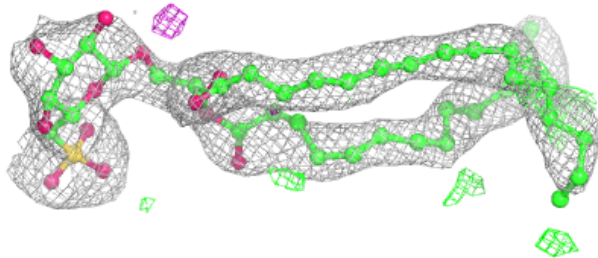
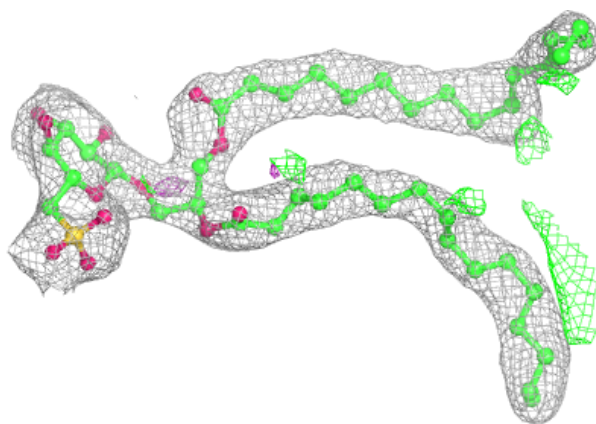


Electron density around LMT B 628:

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

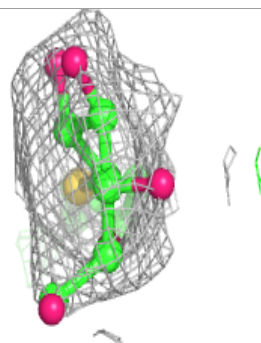
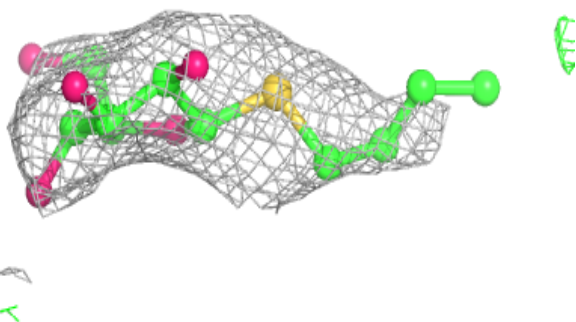
**Electron density around SQD B 620:**

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

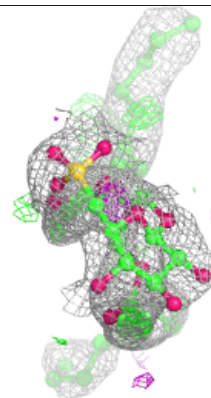
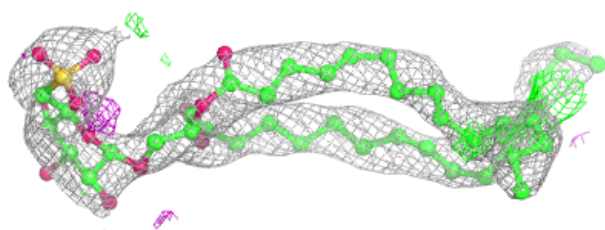
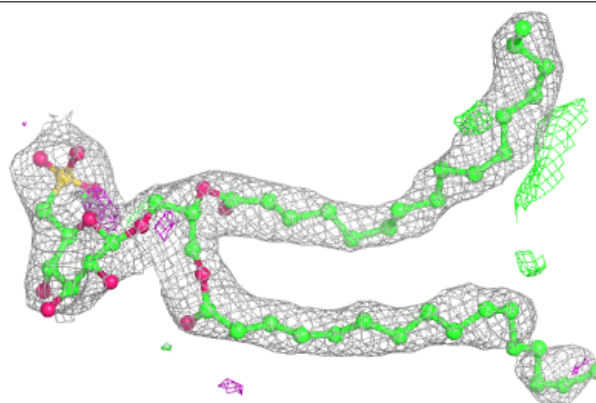


Electron density around HTG h 101:

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

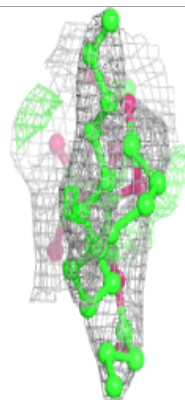
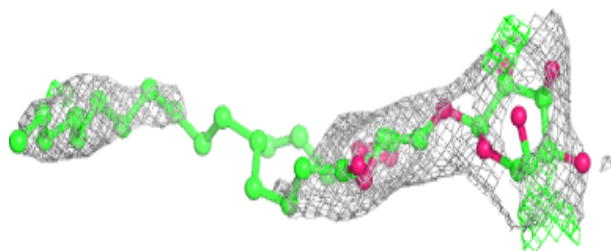
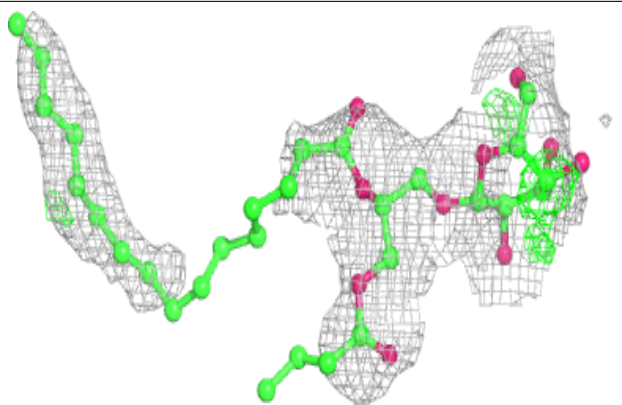
**Electron density around SQD b 620:**

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

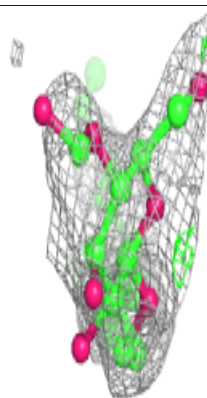
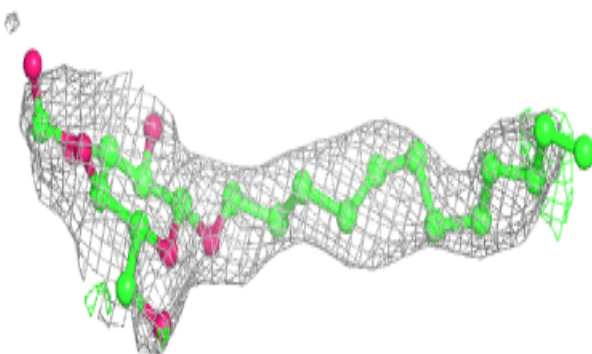
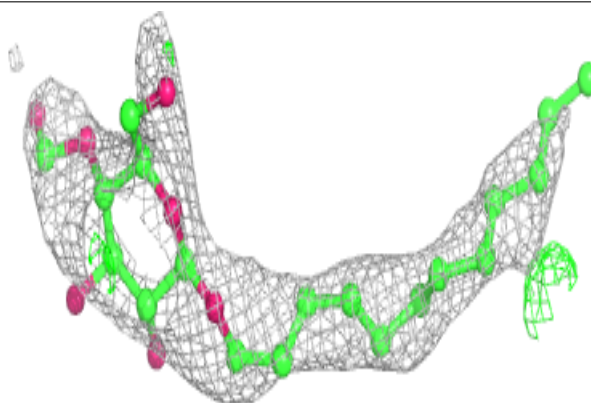


Electron density around LMG z 101:

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

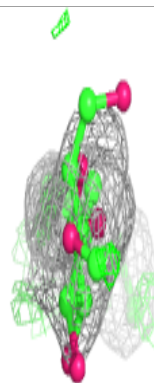
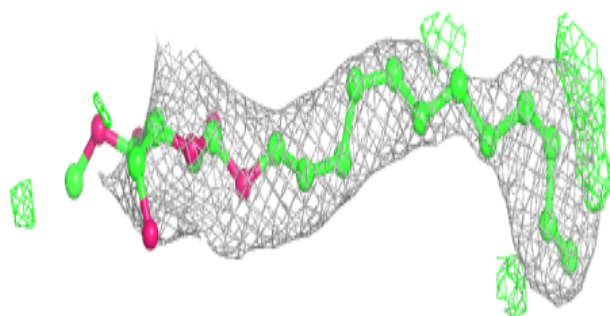
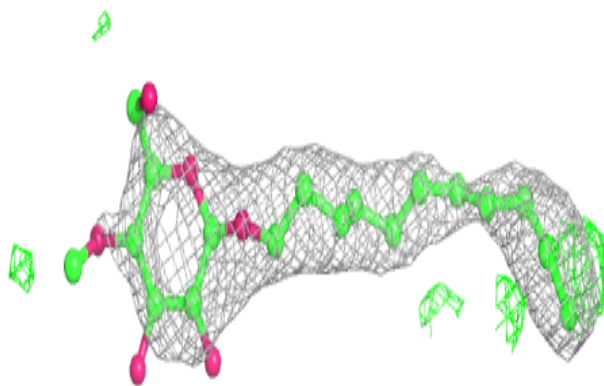
**Electron density around LMT t 101:**

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

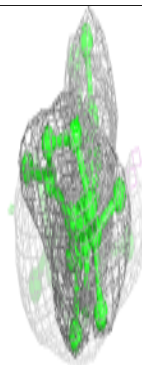
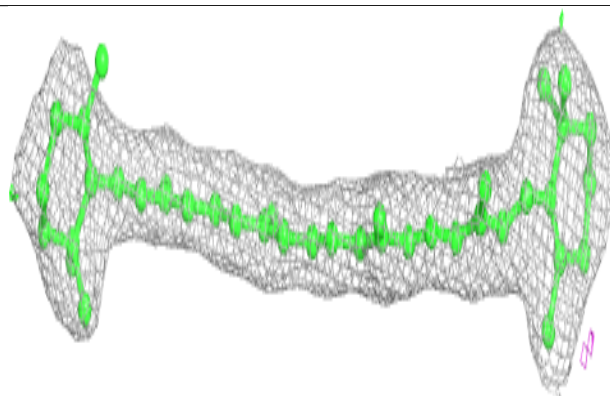
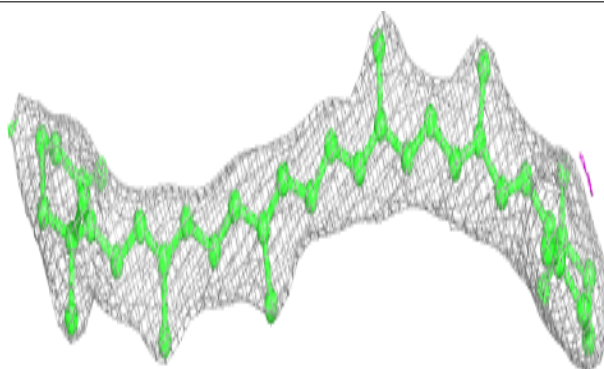


Electron density around LMT b 627:

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

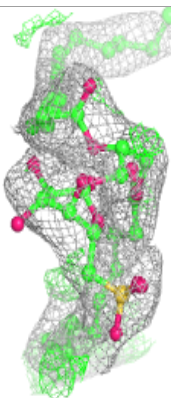
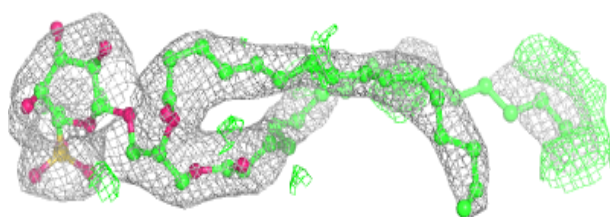
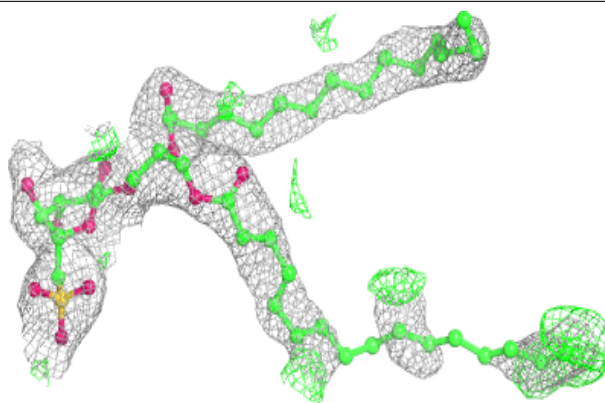
**Electron density around BCR h 102:**

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

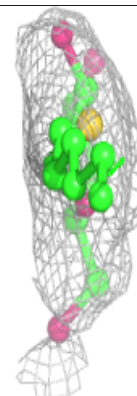
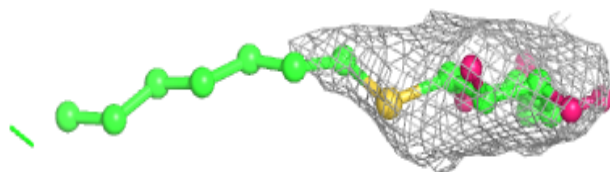
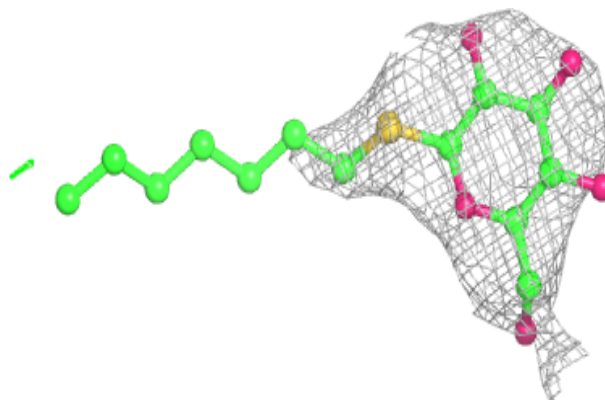


Electron density around SQD A 411:

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

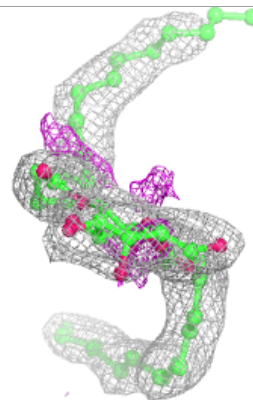
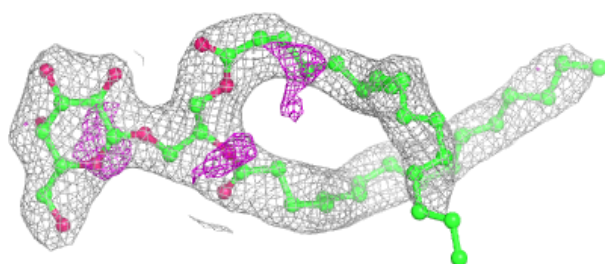
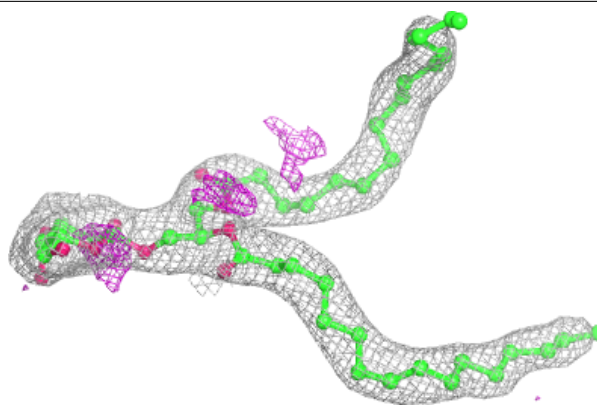
**Electron density around HTG c 523:**

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

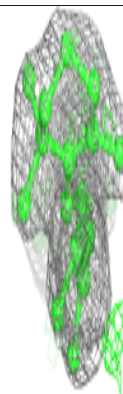
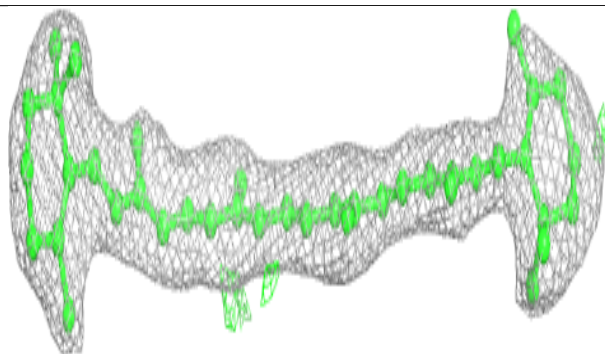
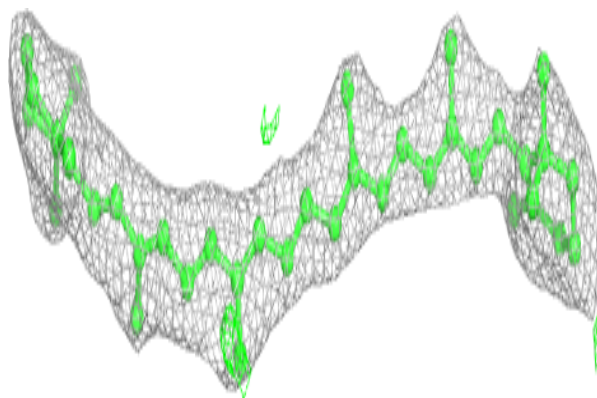


Electron density around LMG B 621:

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

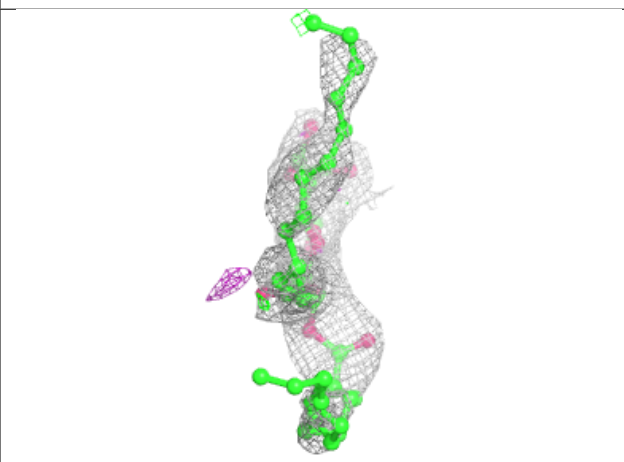
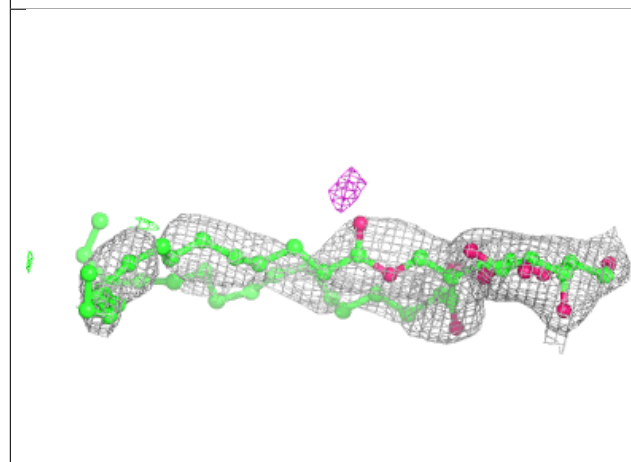
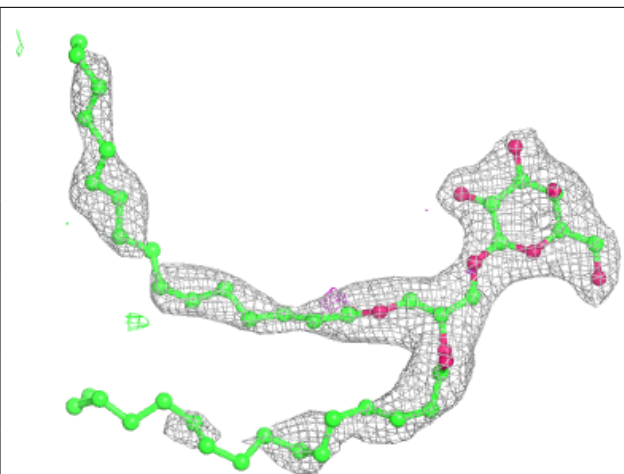
**Electron density around BCR H 101:**

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



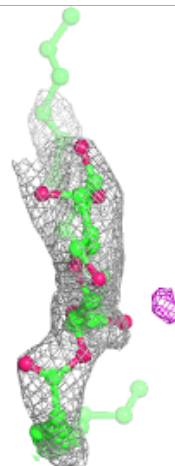
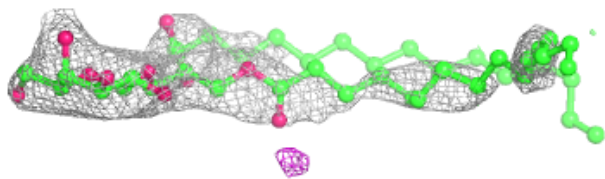
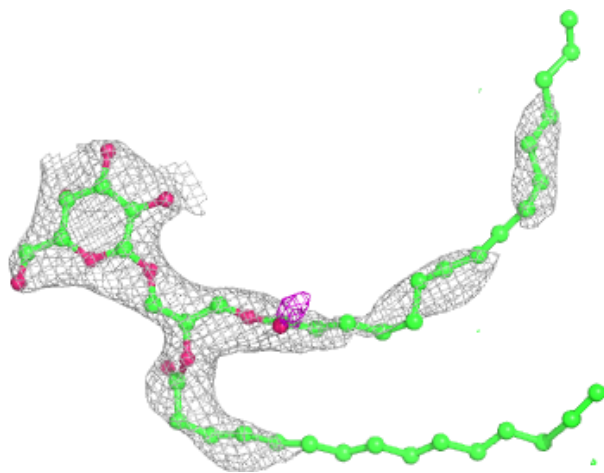
Electron density around LMG C 521:

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



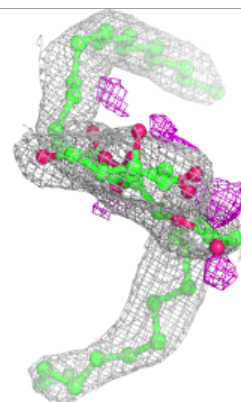
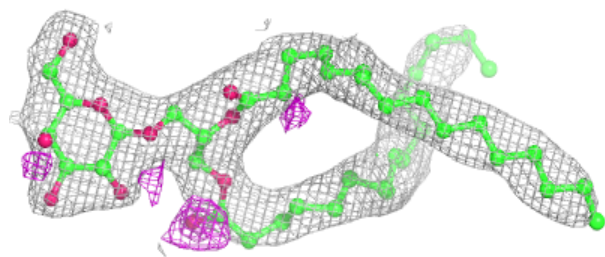
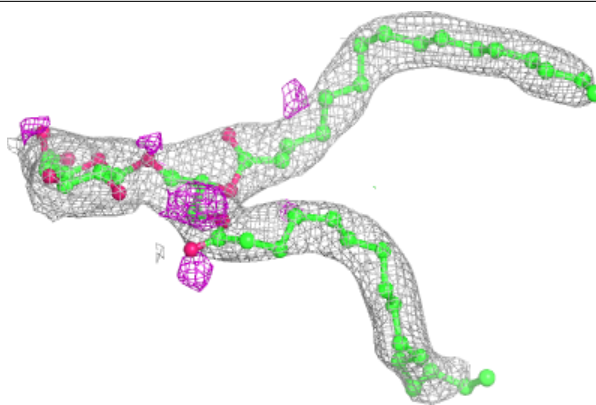
Electron density around LMG c 521:

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

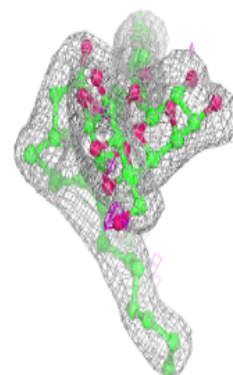
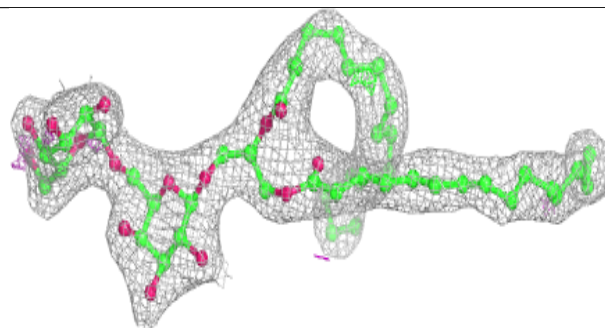
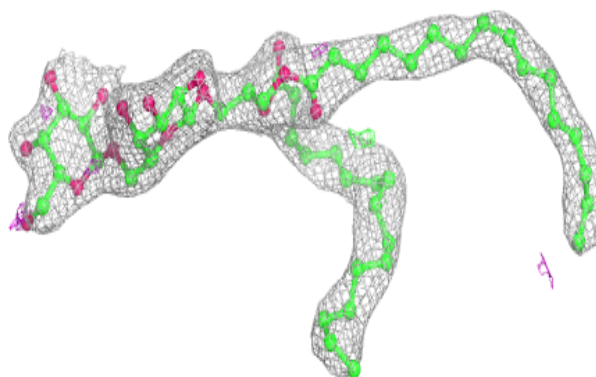


Electron density around LMG m 101:

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

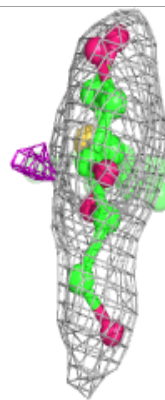
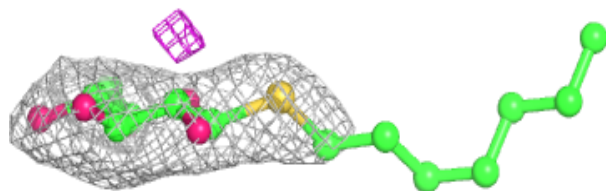
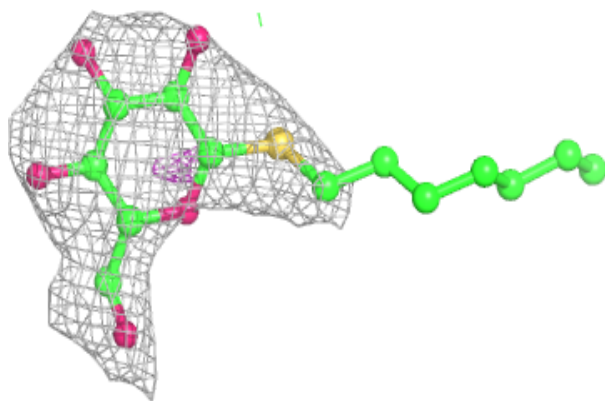
**Electron density around DGD h 103:**

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

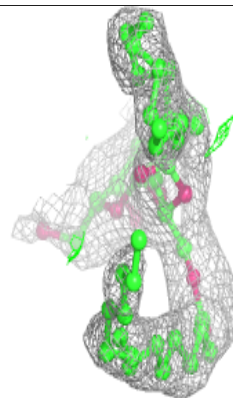
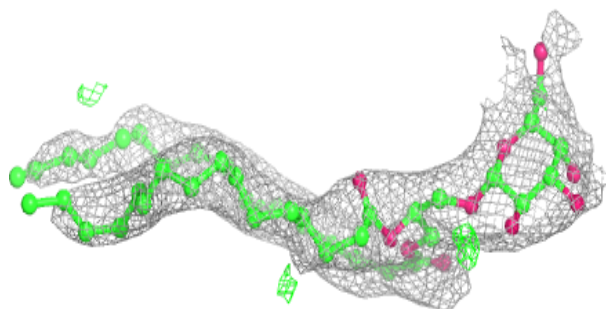
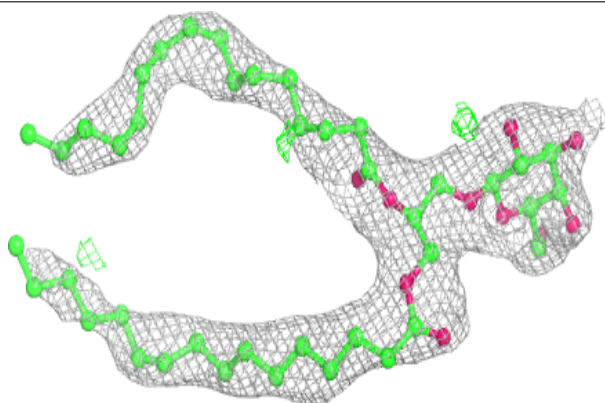


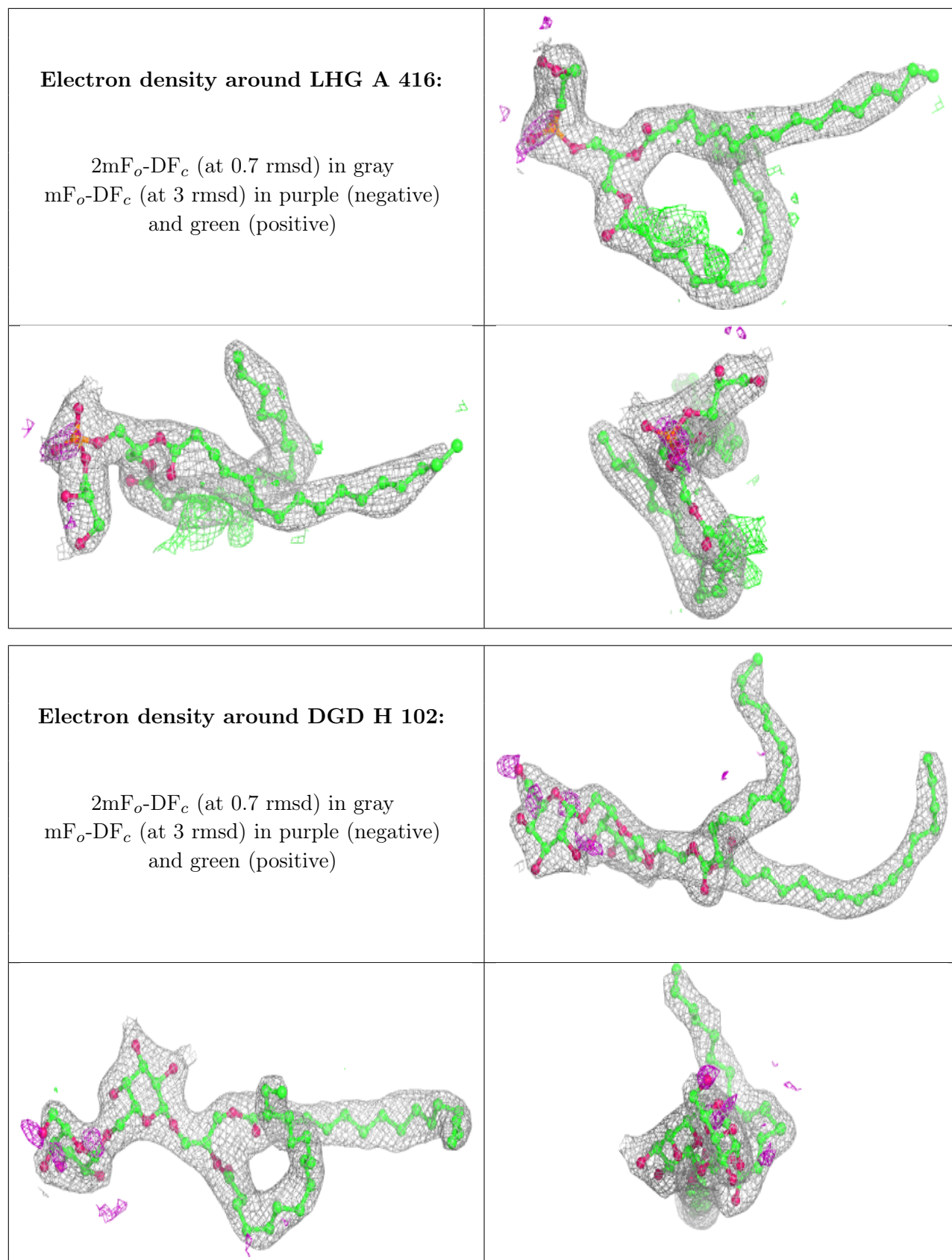
Electron density around HTG C 523:

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

**Electron density around LMG C 502:**

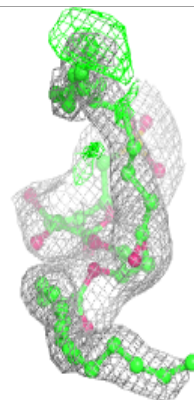
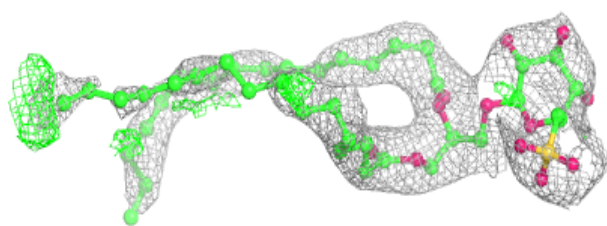
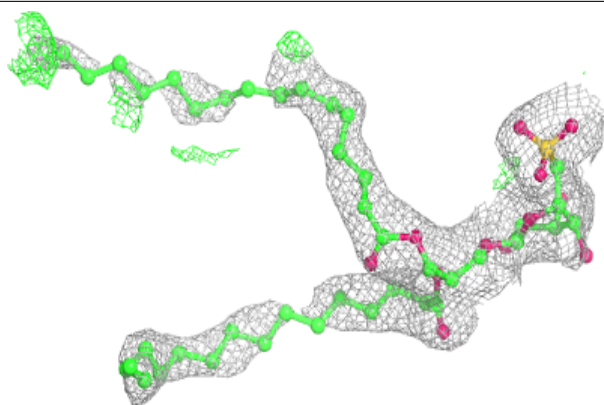
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



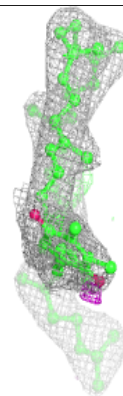
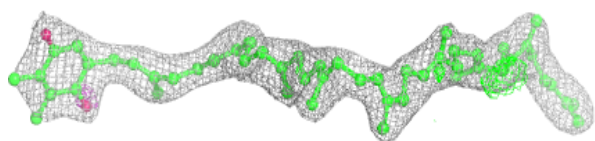
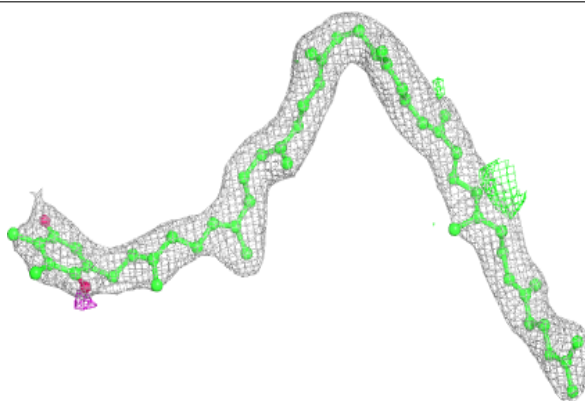


Electron density around SQD a 412:

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

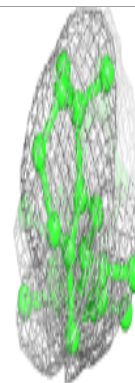
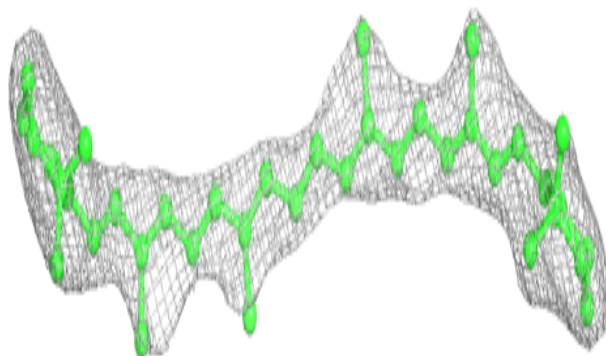
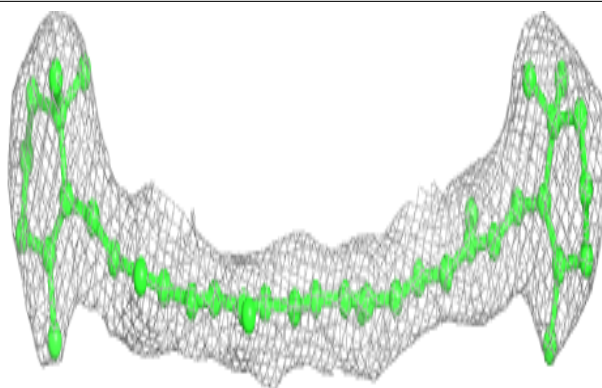
**Electron density around PL9 d 405:**

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

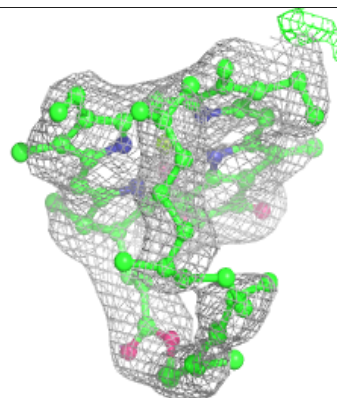
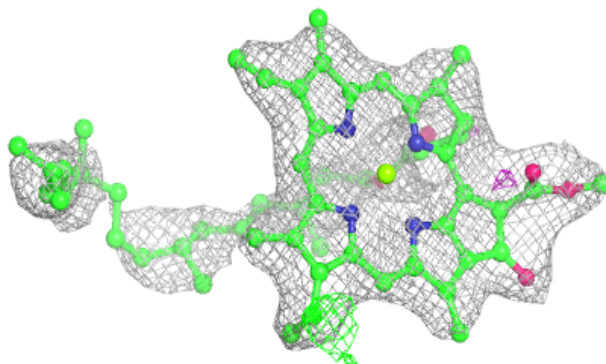
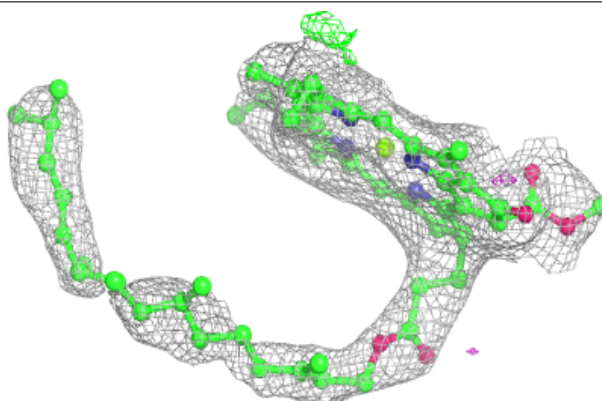


Electron density around BCR k 101:

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

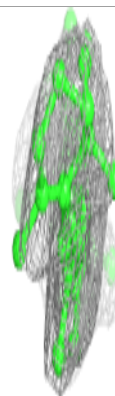
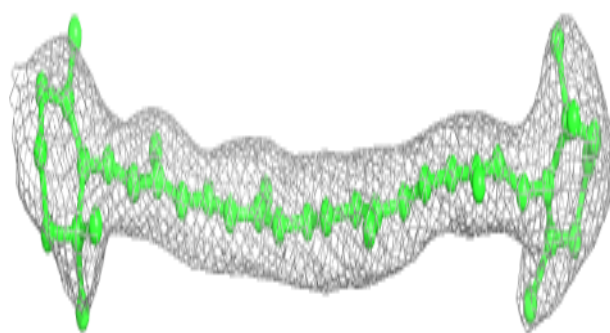
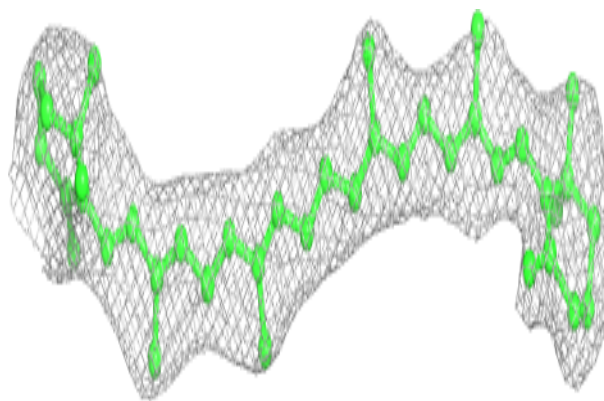
**Electron density around CLA C 515:**

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

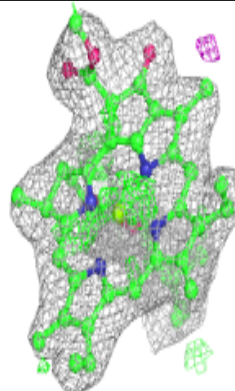
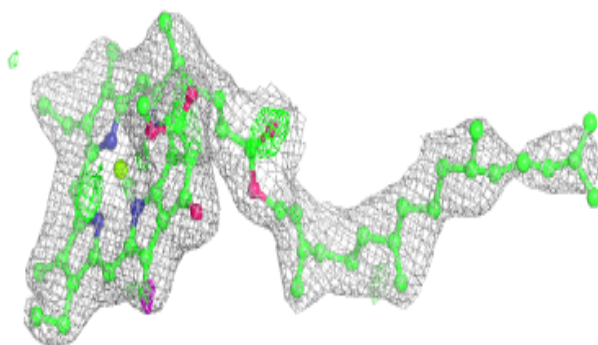
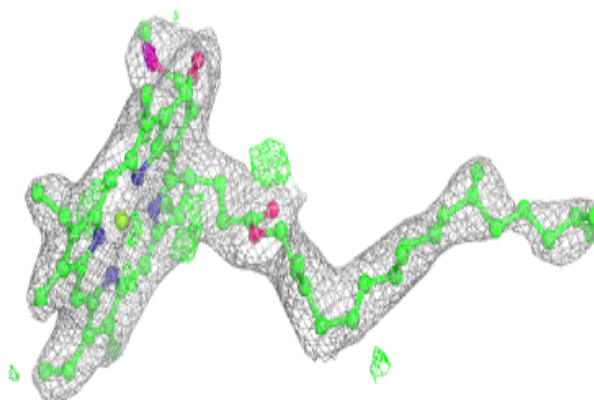


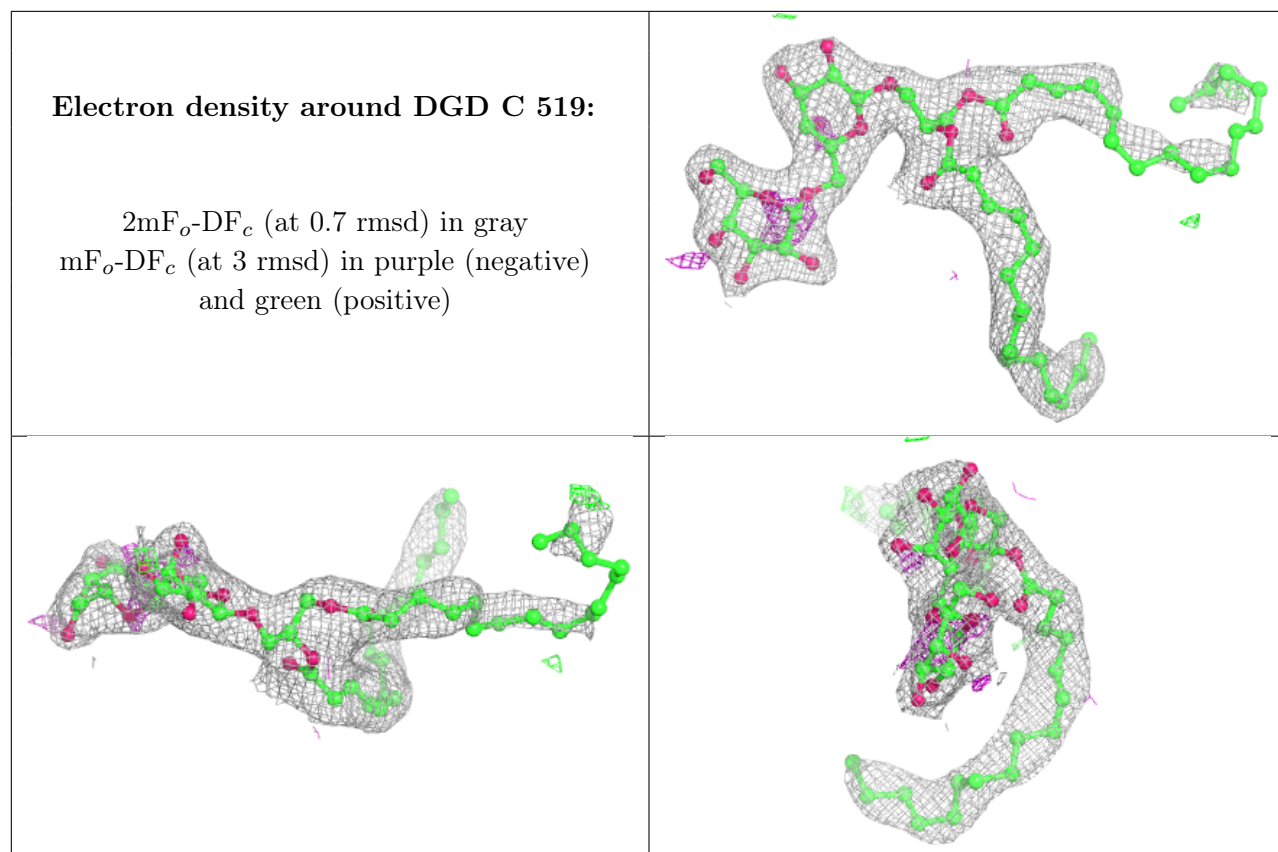
Electron density around BCR y 101:

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

**Electron density around CLA c 504:**

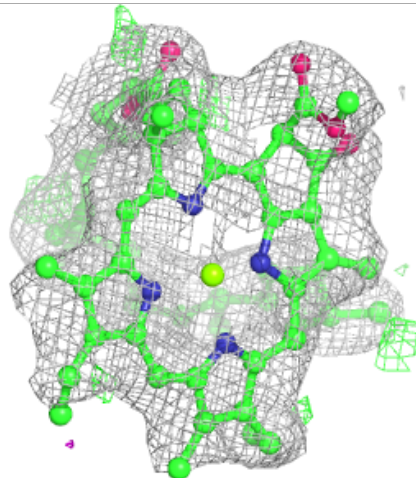
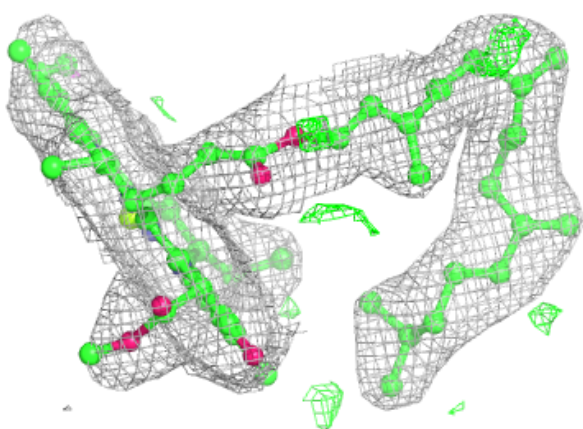
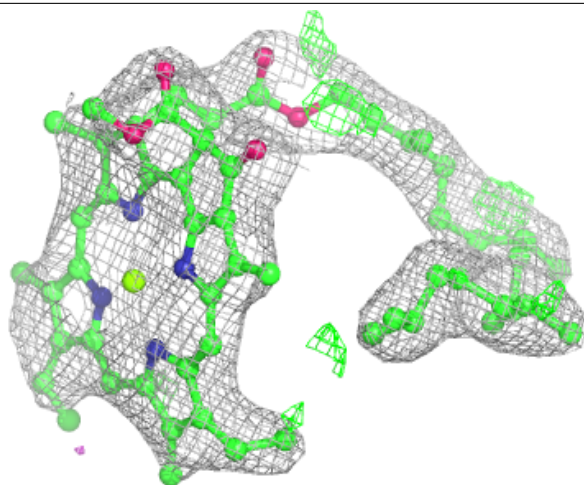
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

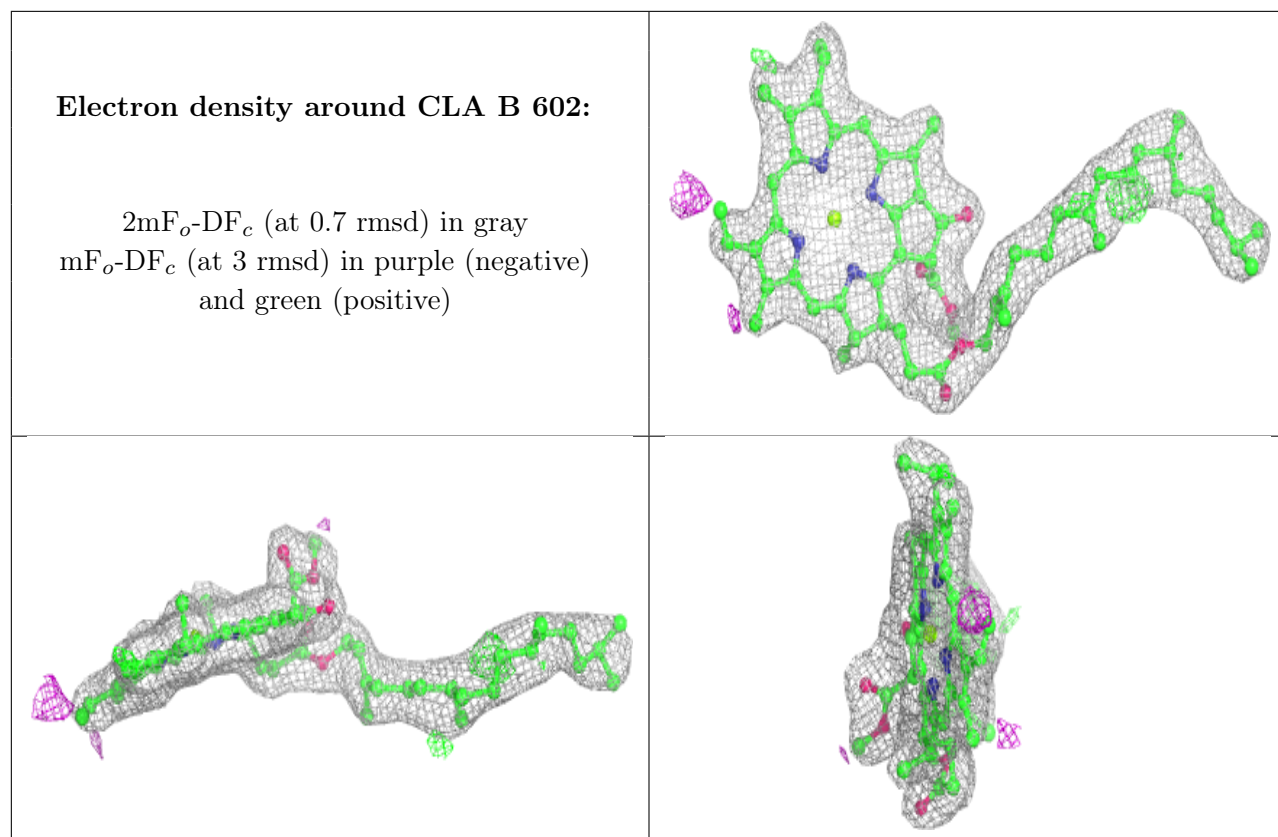




Electron density around CLA c 505:

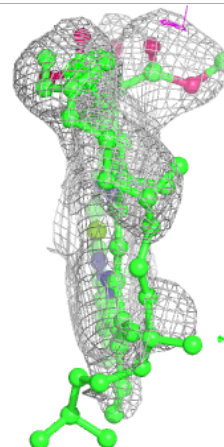
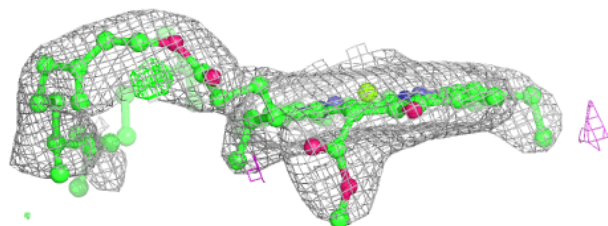
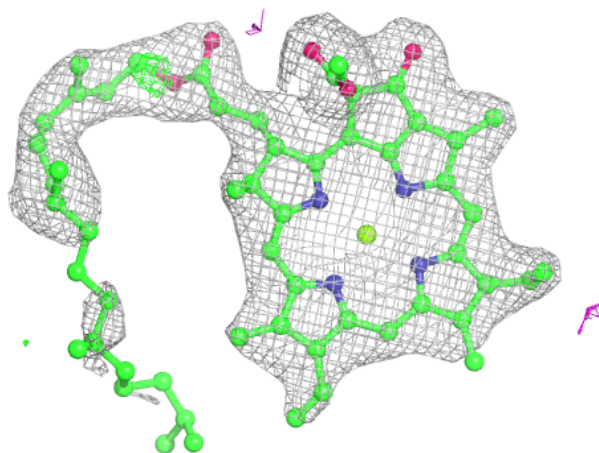
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





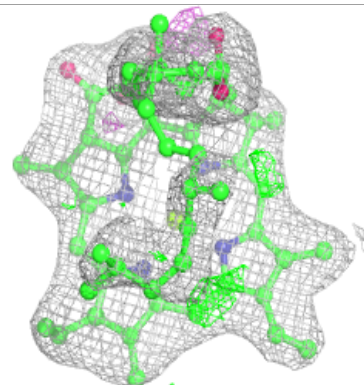
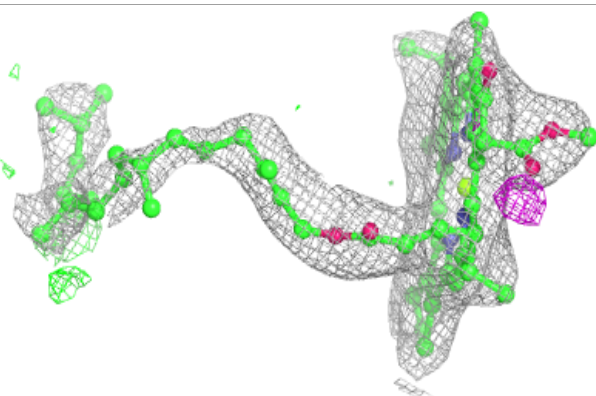
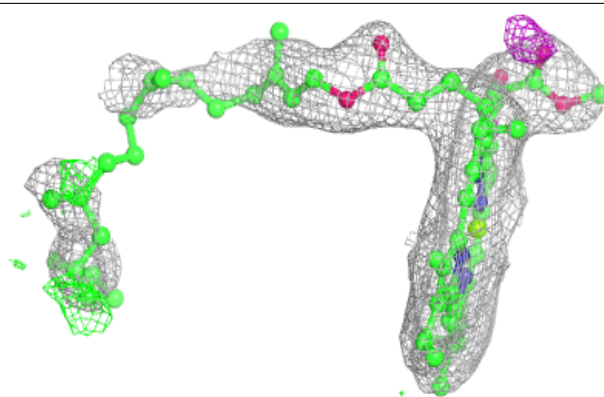
Electron density around CLA C 514:

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

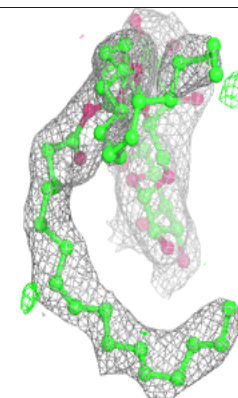
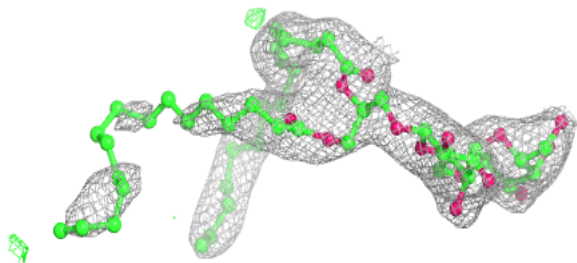
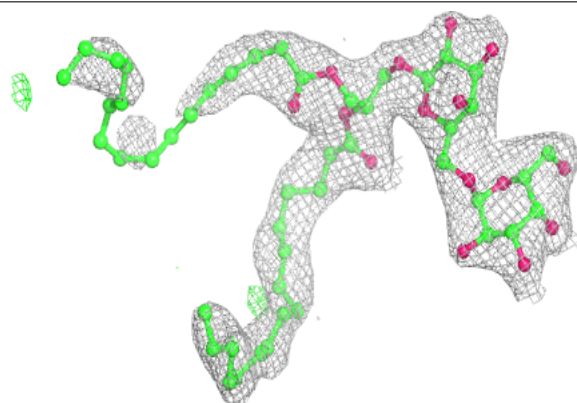


Electron density around CLA C 508:

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

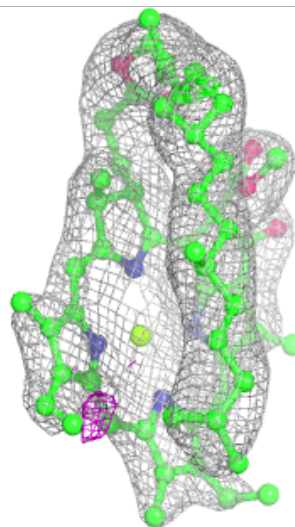
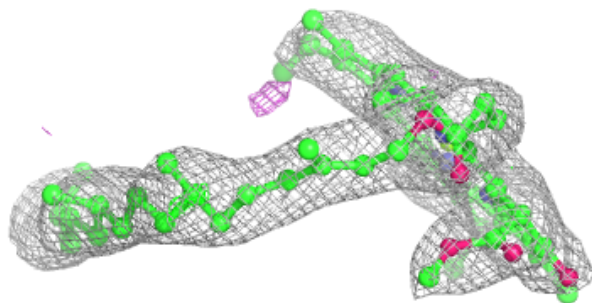
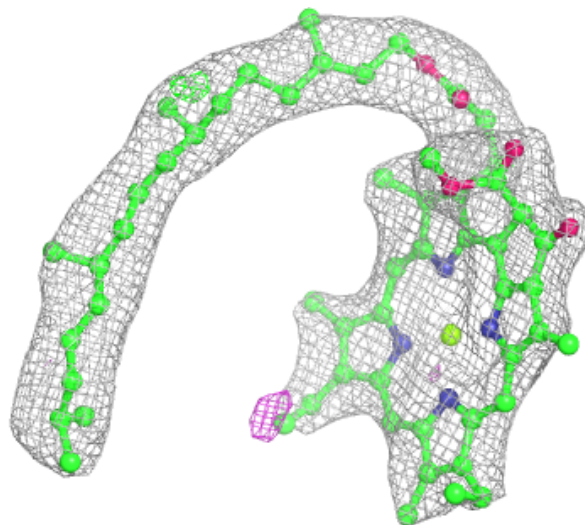
**Electron density around DGD c 519:**

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



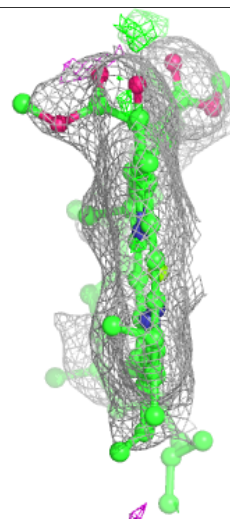
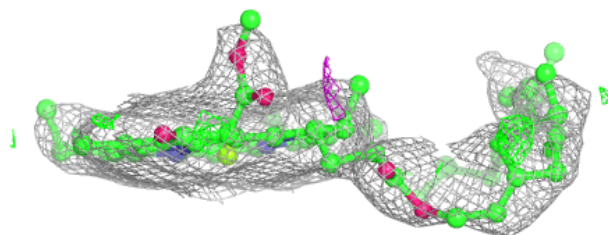
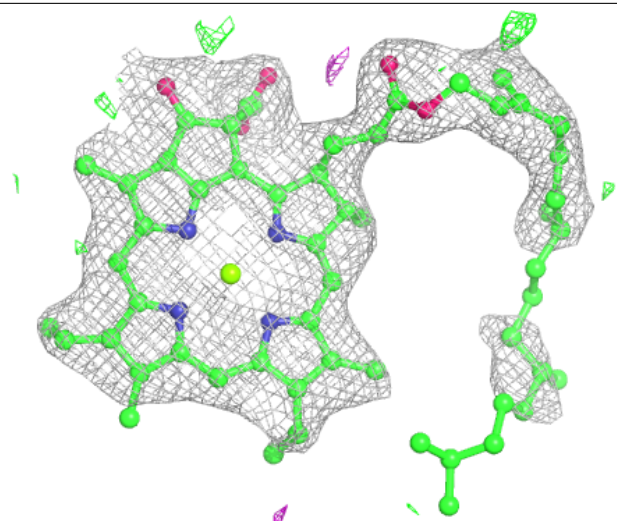
Electron density around CLA c 509:

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



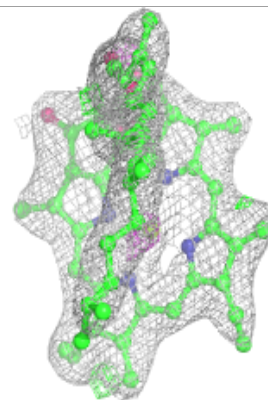
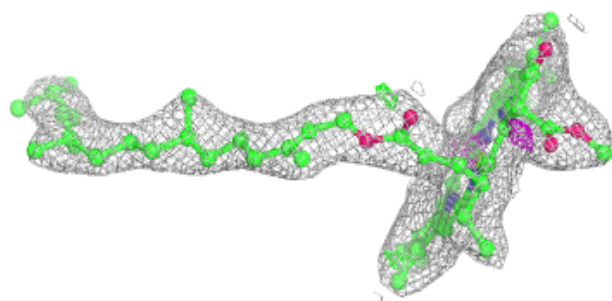
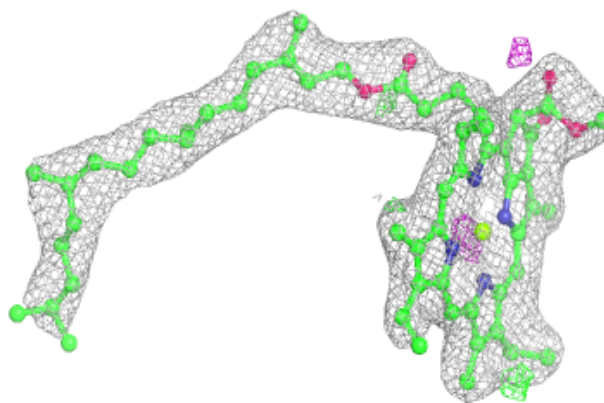
Electron density around CLA c 514:

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

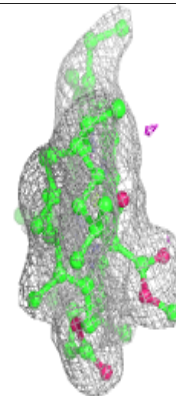
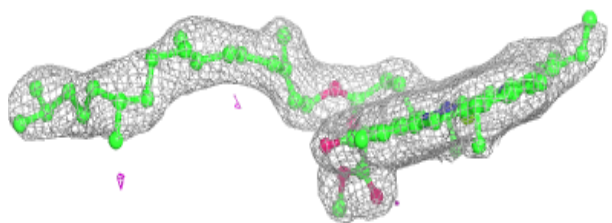
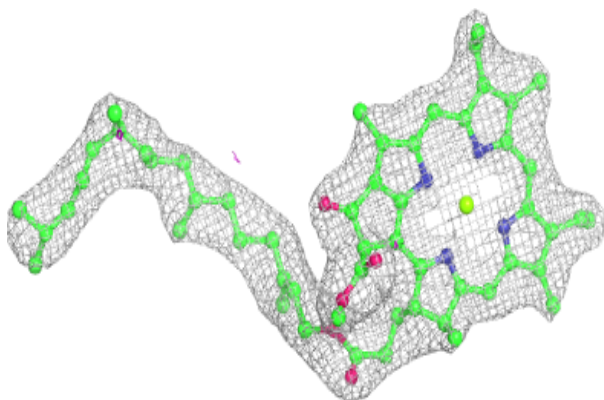


Electron density around CLA b 609:

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

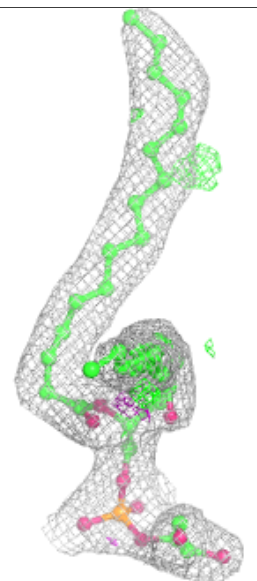
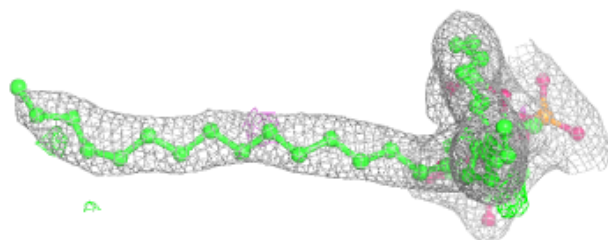
**Electron density around CLA b 602:**

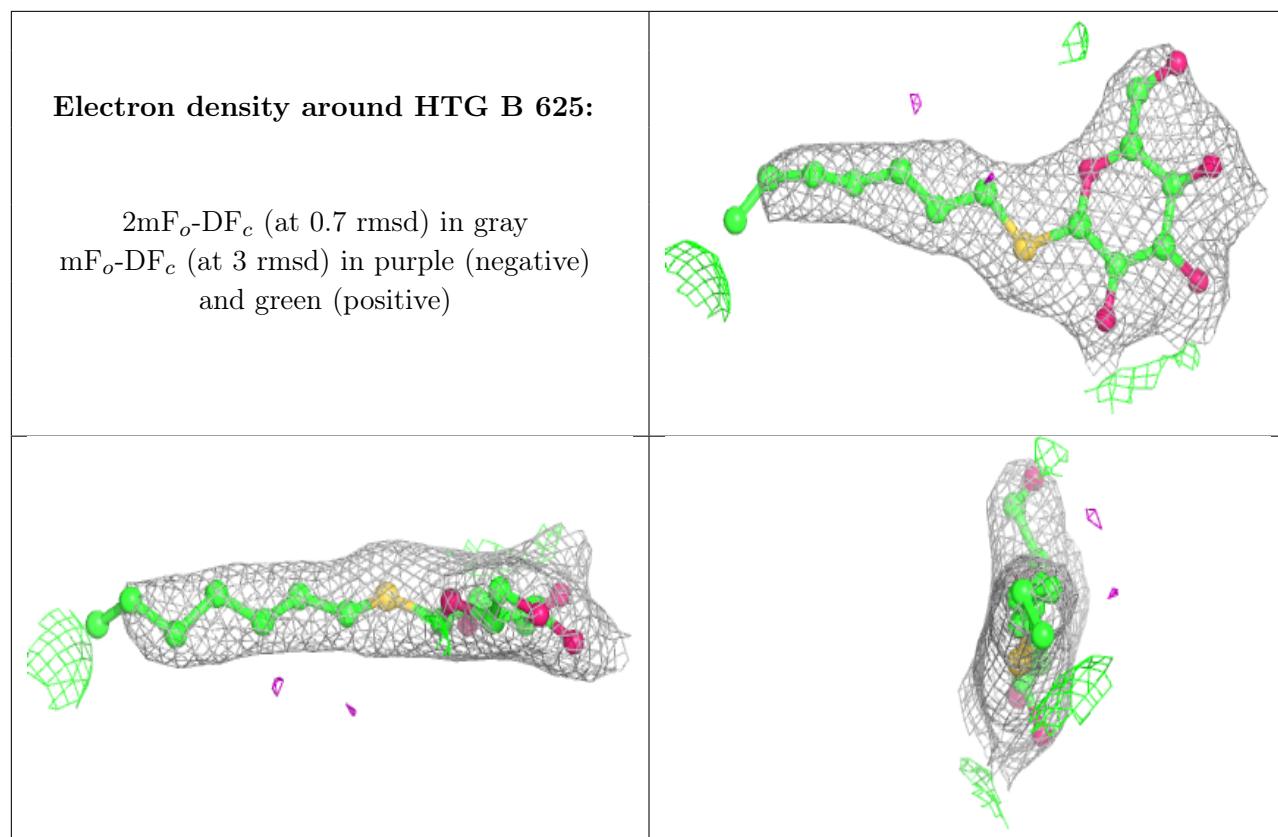
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LHG b 629:

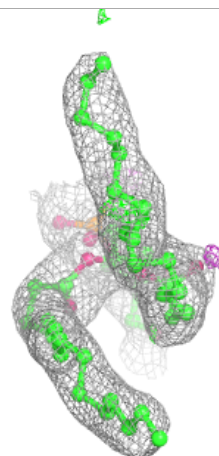
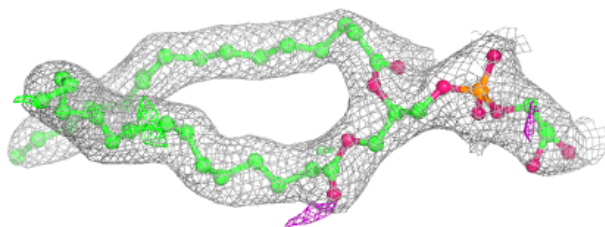
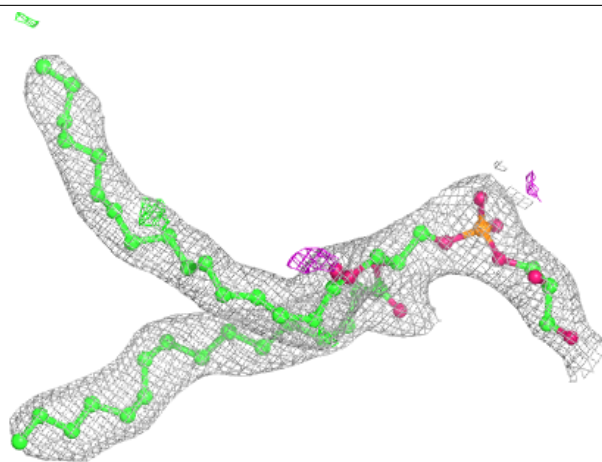
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





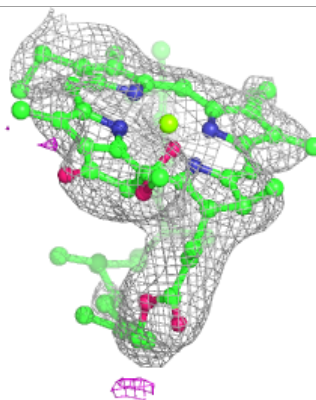
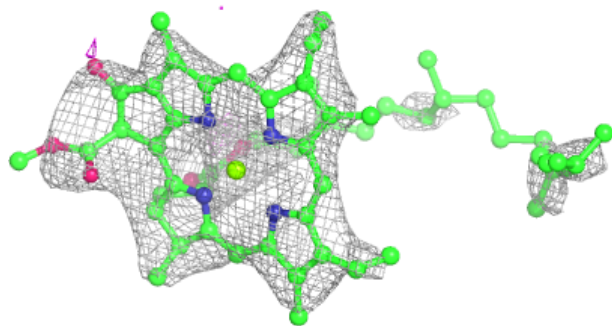
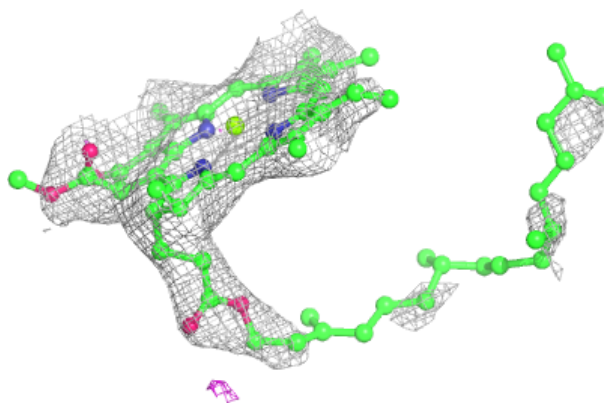
Electron density around LHG d 407:

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

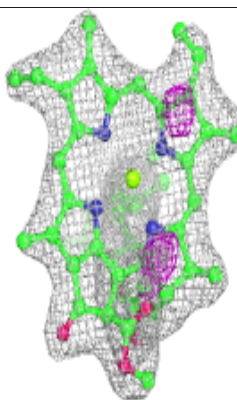
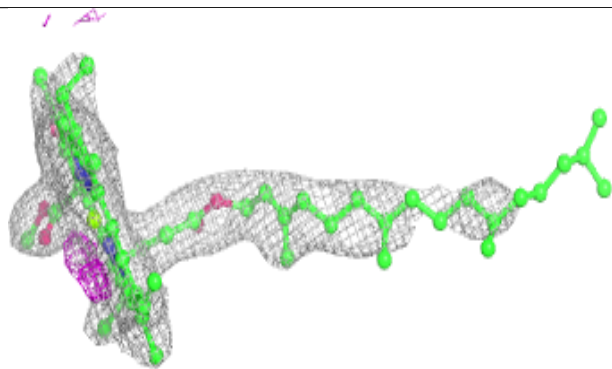
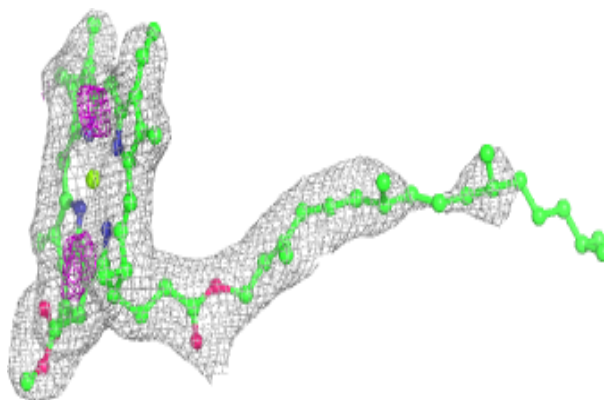


Electron density around CLA c 515:

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

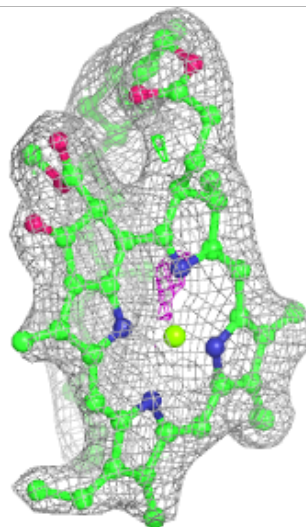
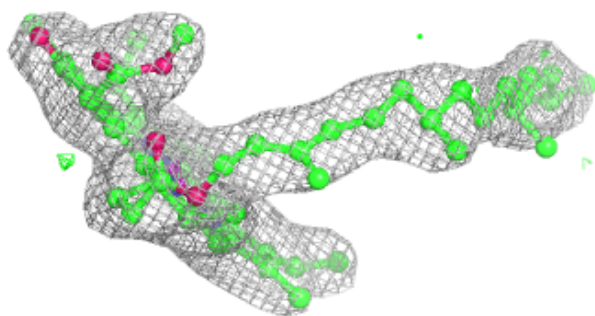
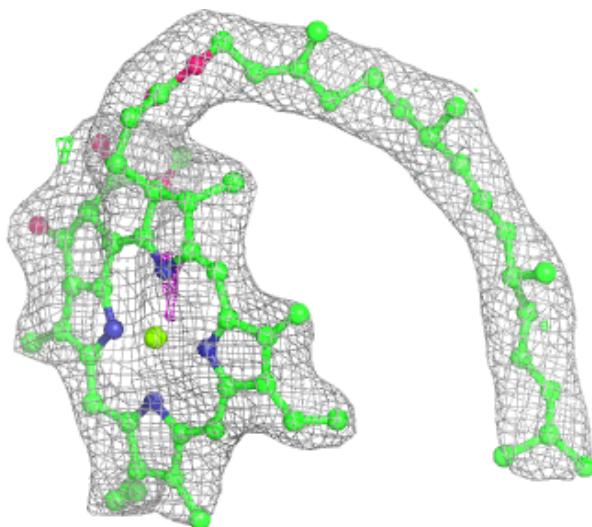
**Electron density around CLA d 403:**

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



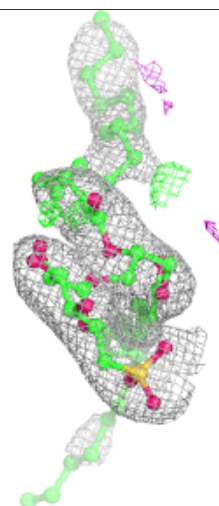
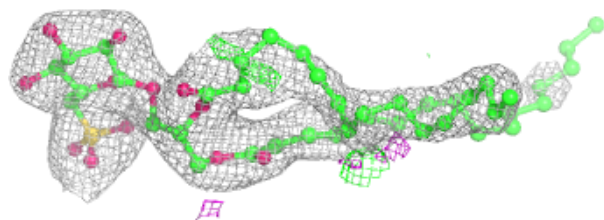
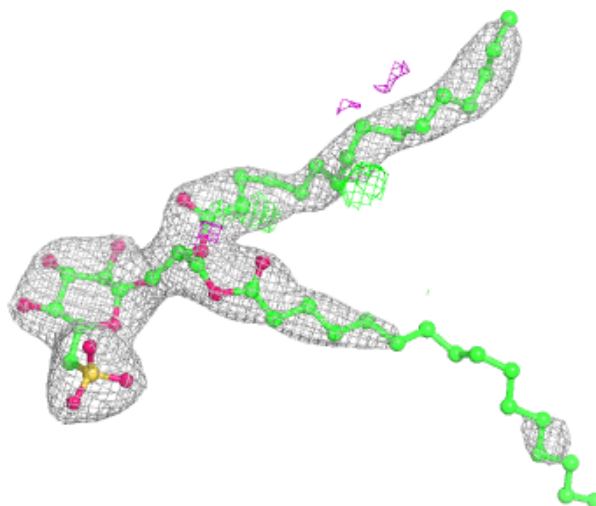
Electron density around CLA C 509:

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



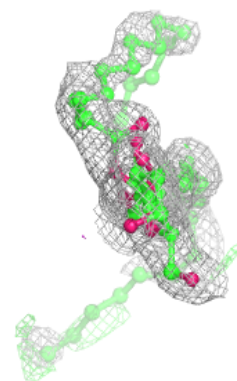
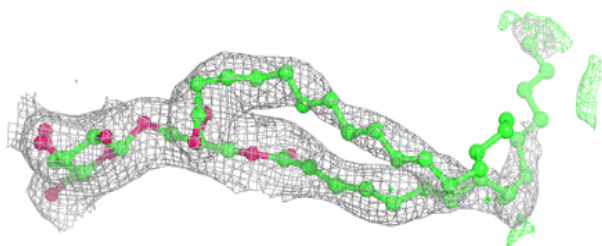
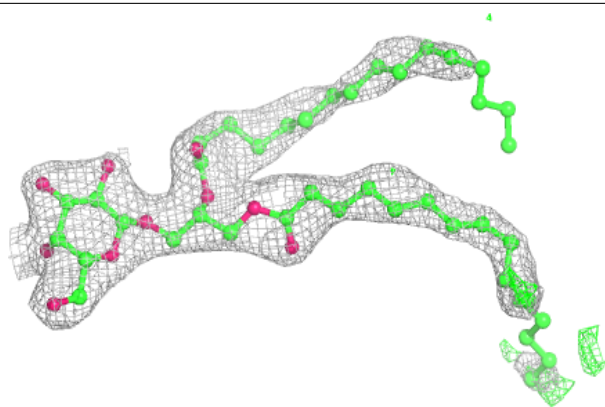
Electron density around SQD C 501:

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

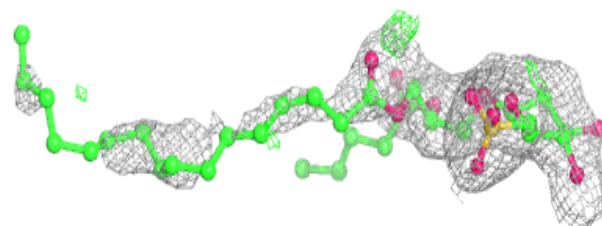
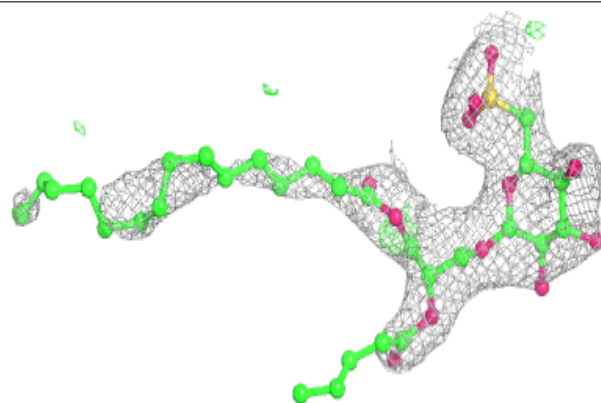


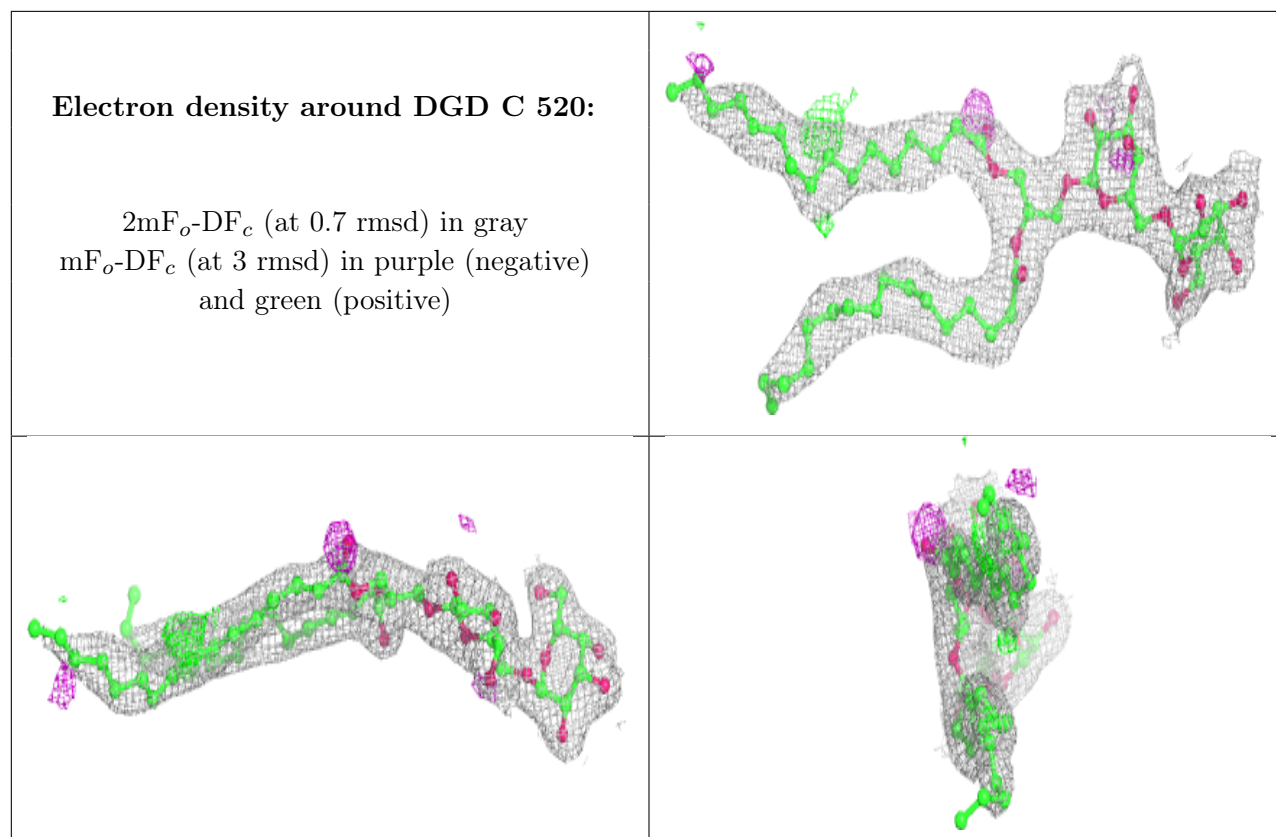
Electron density around LMG D 413:

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

**Electron density around SQD D 412:**

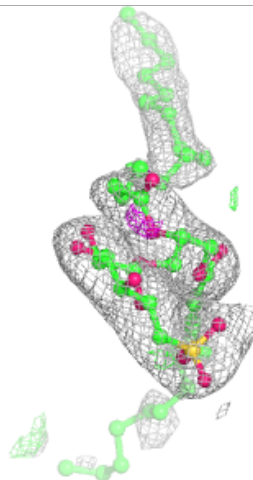
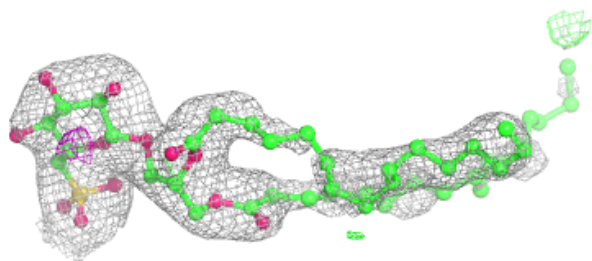
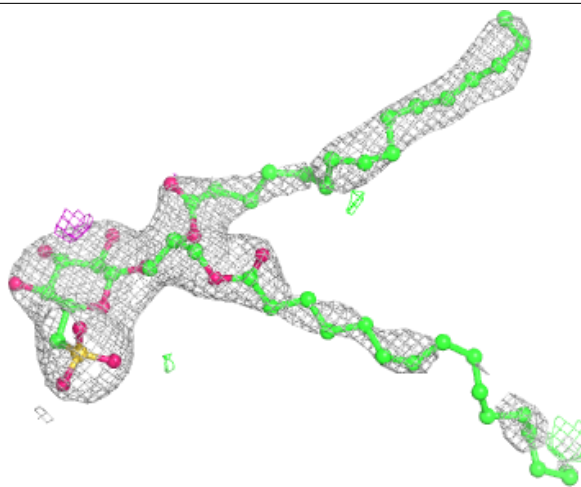
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





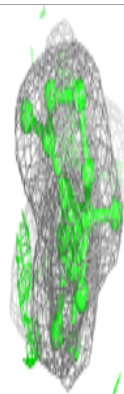
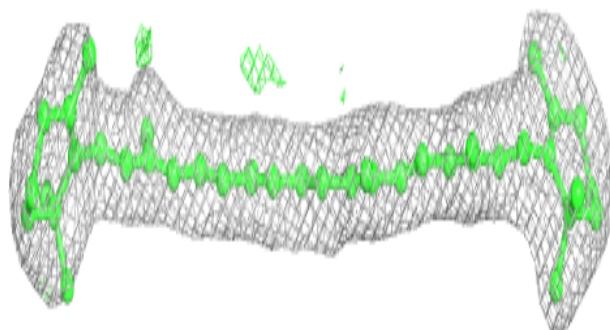
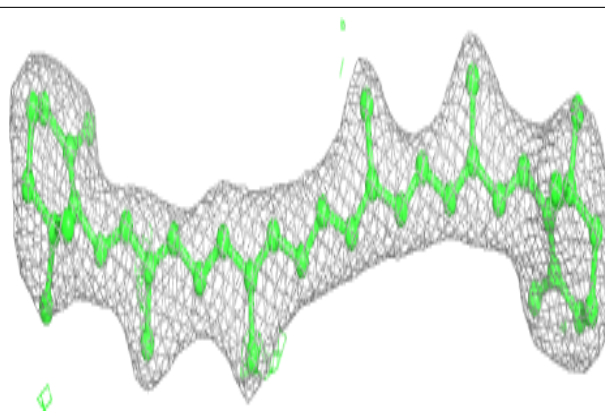
Electron density around SQD a 410:

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

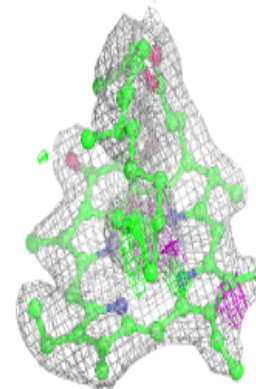
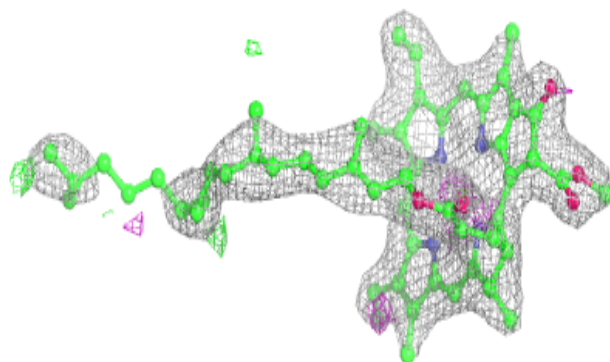
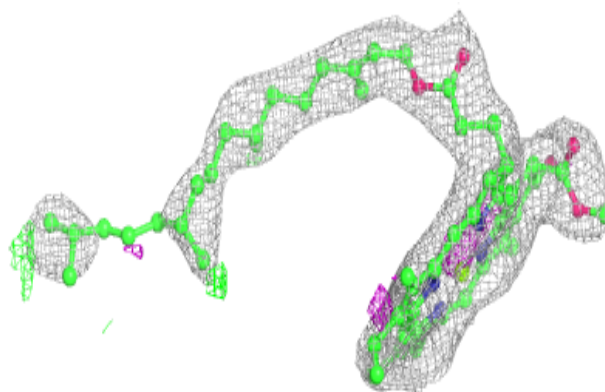


Electron density around BCR b 618:

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

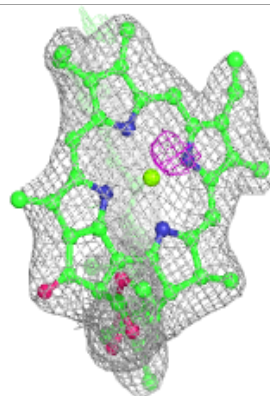
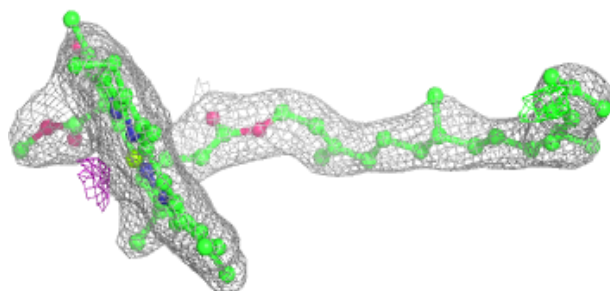
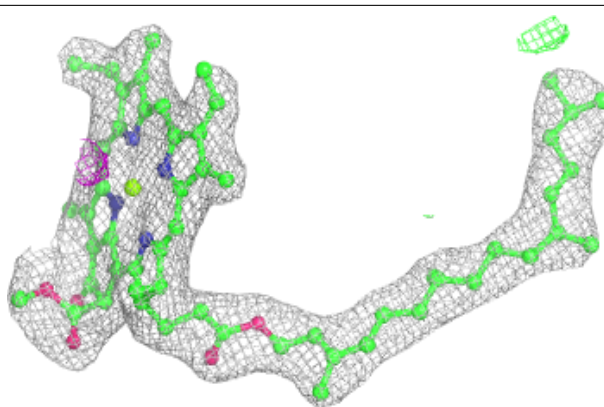
**Electron density around CLA C 506:**

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

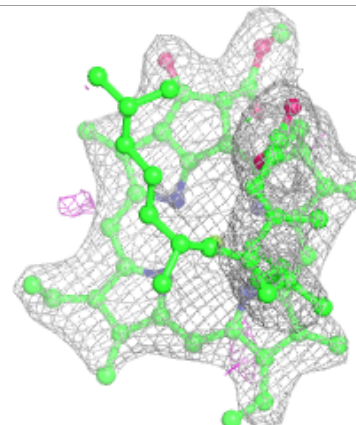
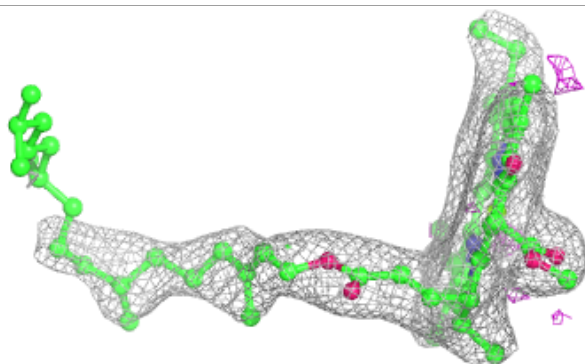
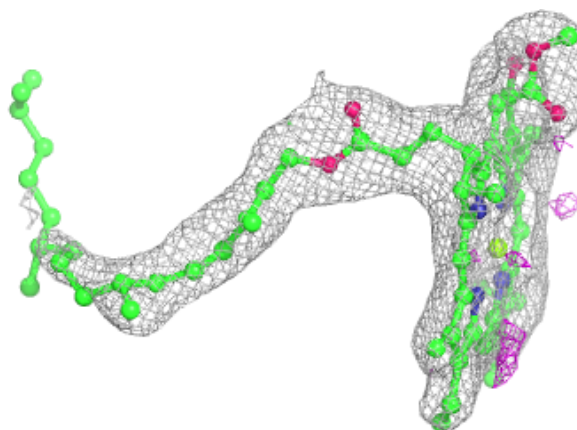


Electron density around CLA B 609:

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

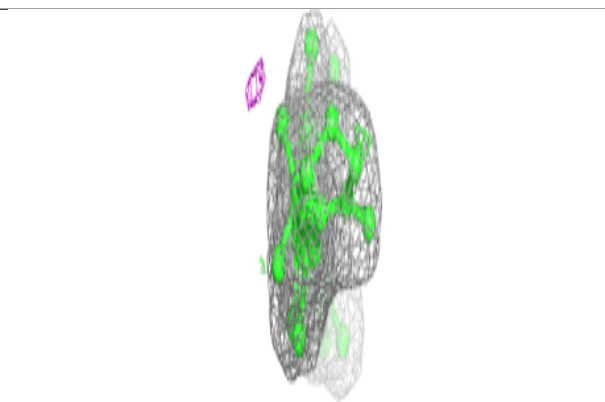
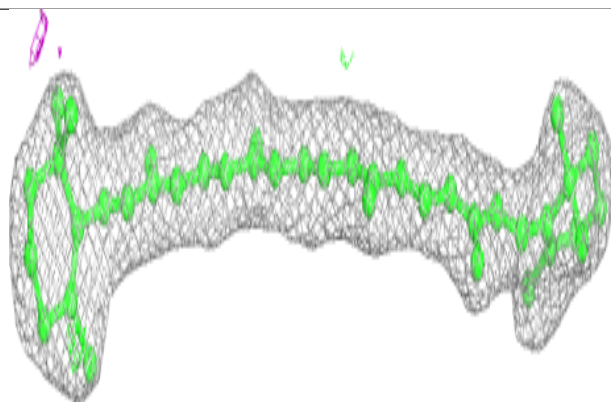
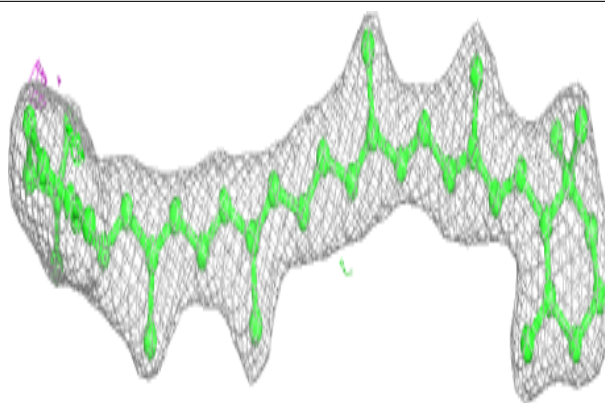
**Electron density around CLA D 404:**

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

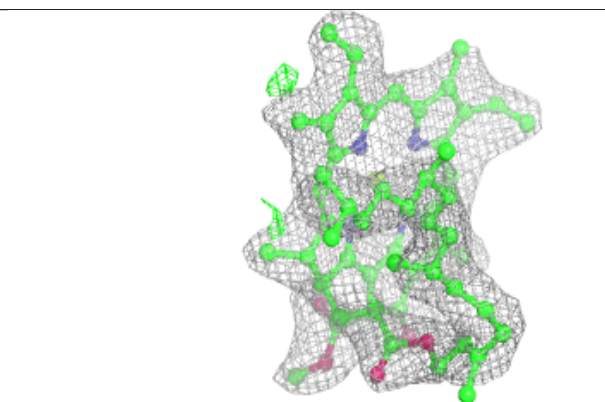
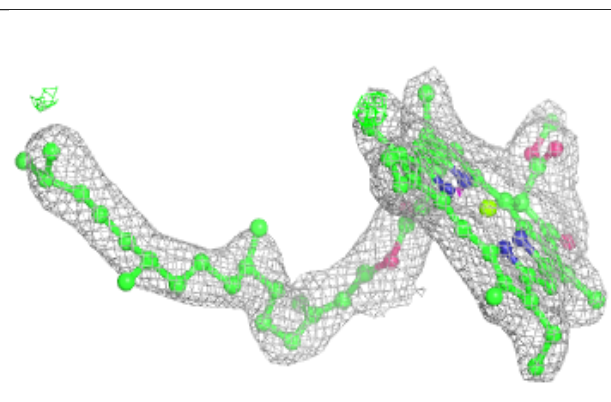
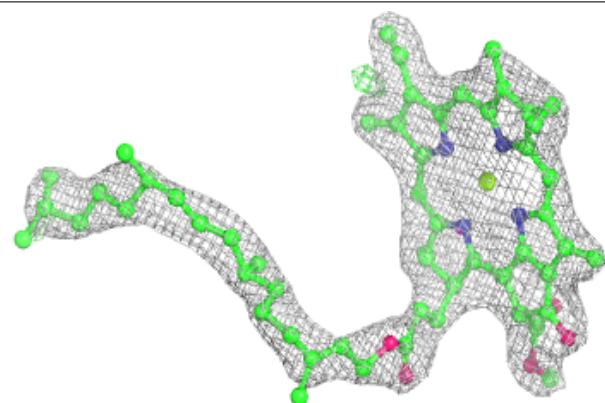


Electron density around BCR b 617:

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

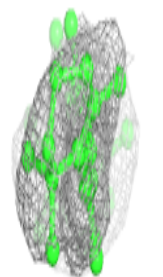
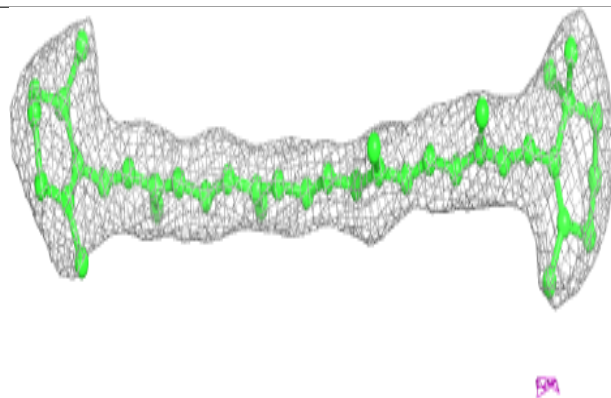
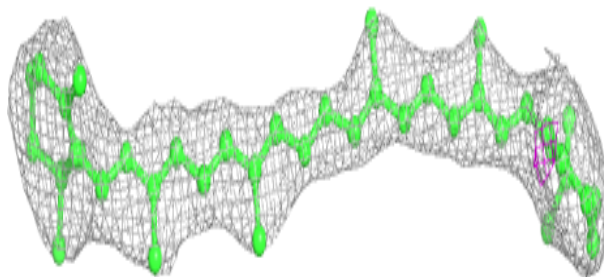
**Electron density around CLA C 513:**

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

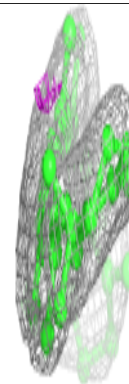
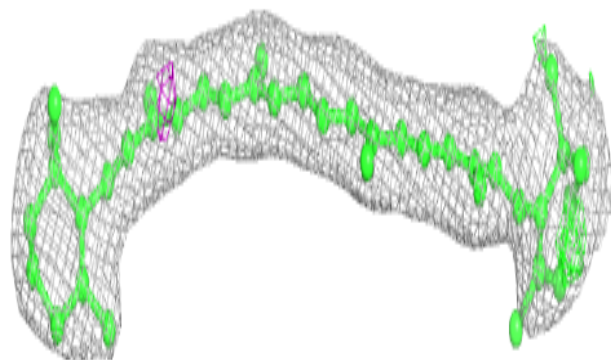
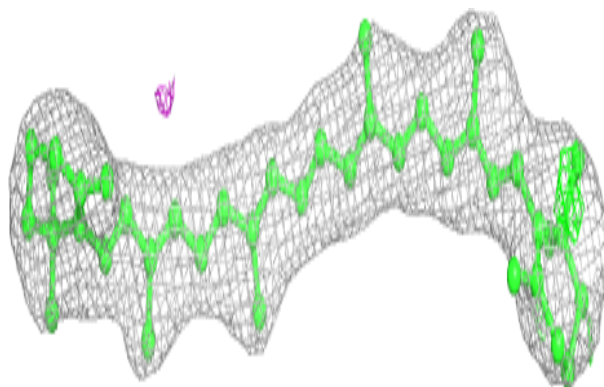


Electron density around BCR c 516:

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

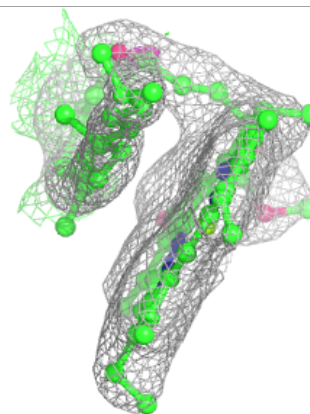
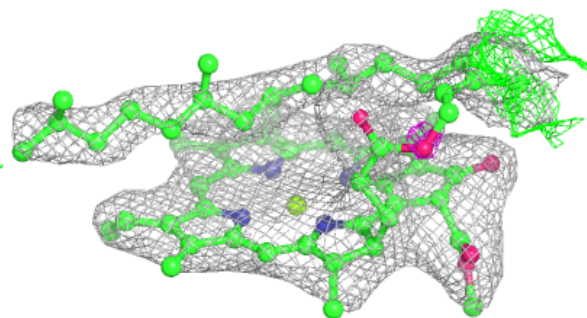
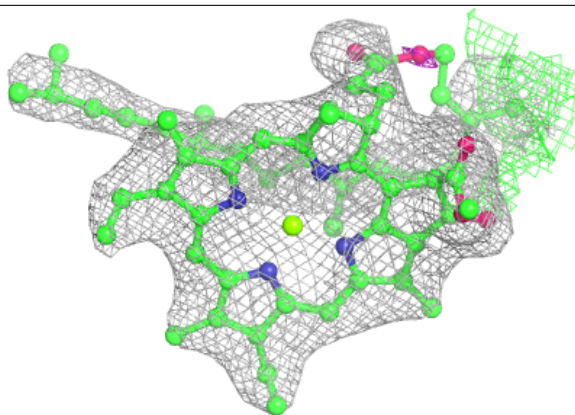
**Electron density around BCR d 404:**

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

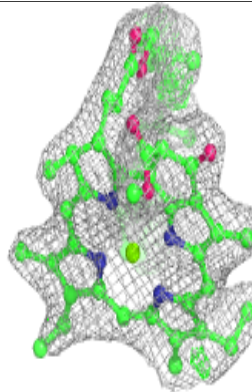
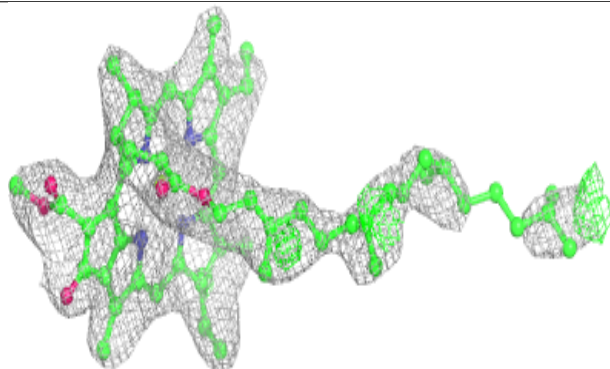
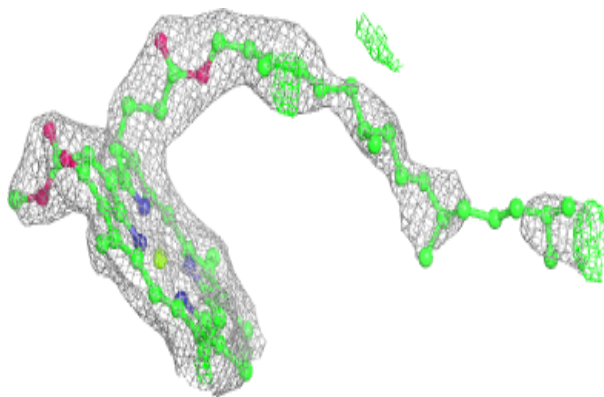


Electron density around CLA b 601:

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

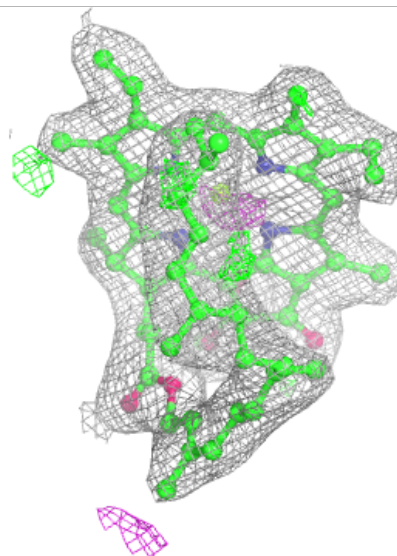
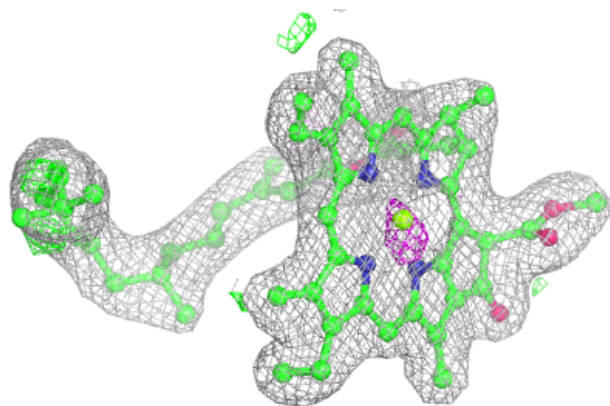
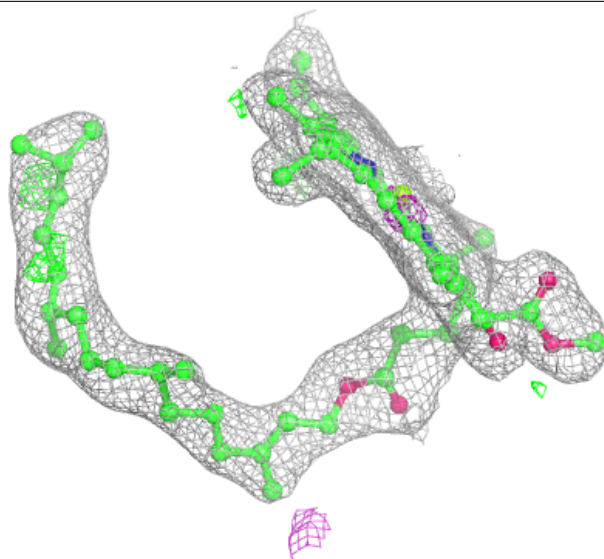
**Electron density around CLA c 506:**

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



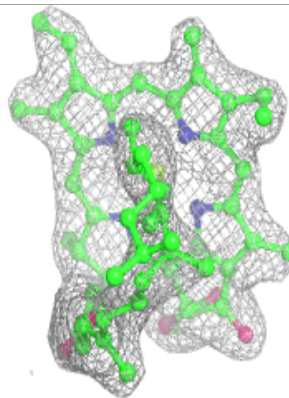
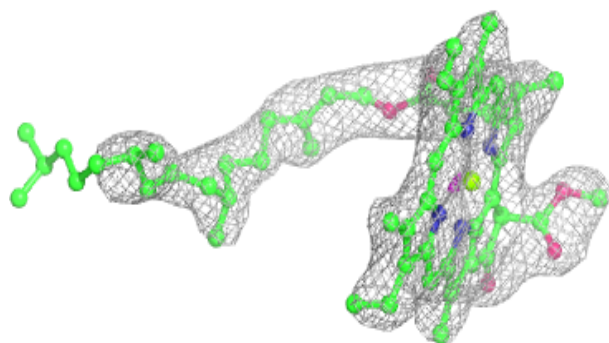
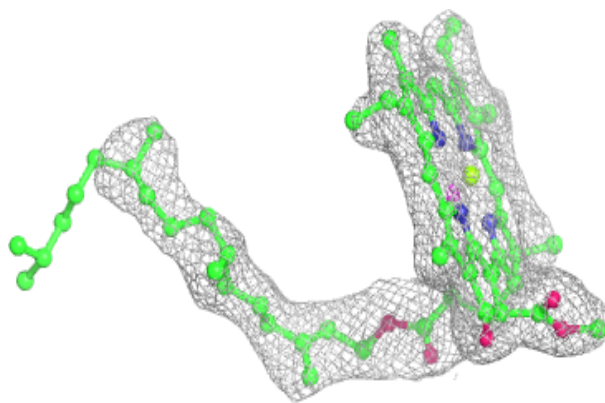
Electron density around CLA B 611:

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

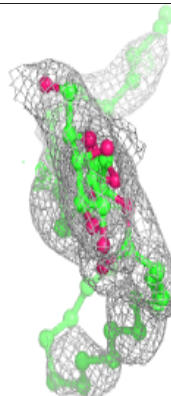
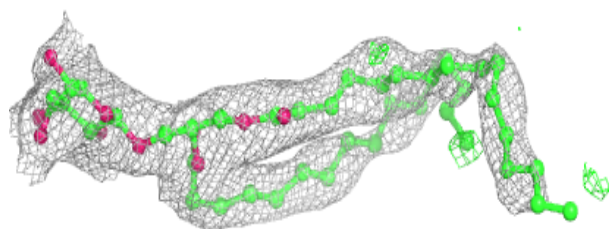
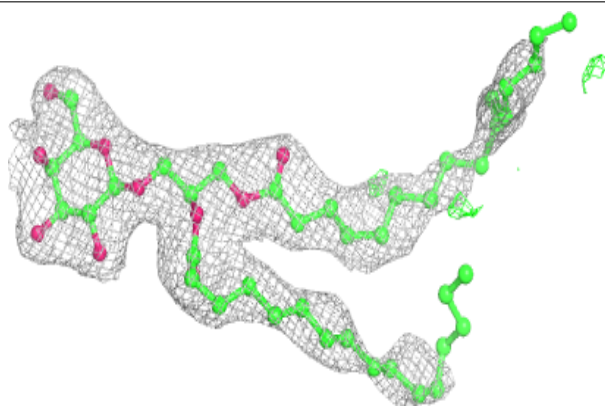


Electron density around CLA c 510:

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

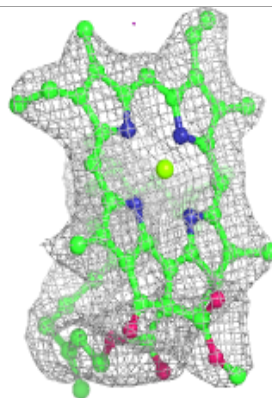
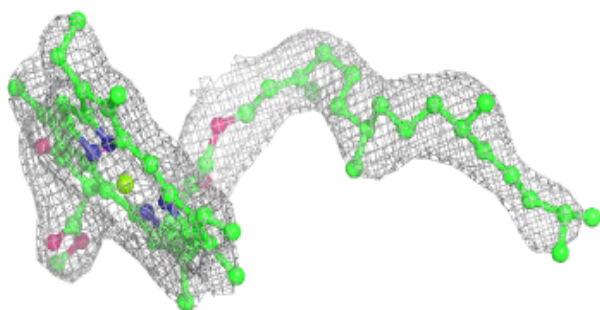
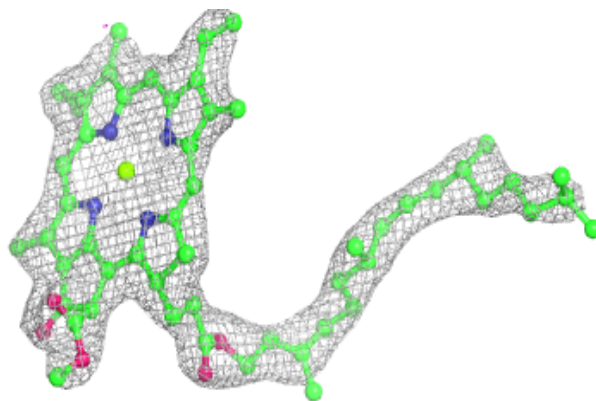
**Electron density around LMG d 412:**

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

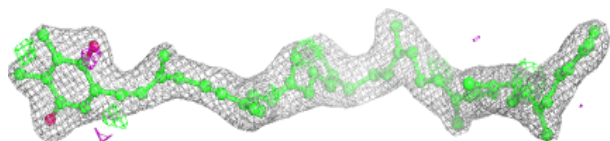
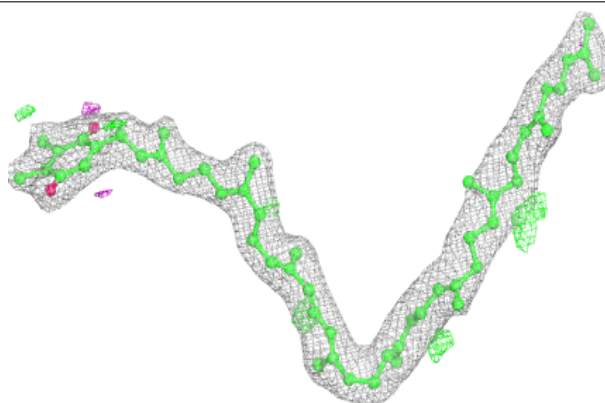


Electron density around CLA c 513:

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

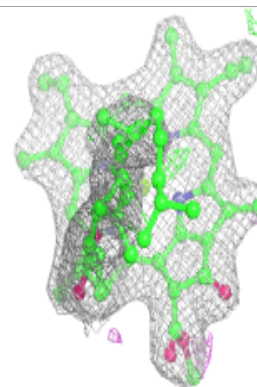
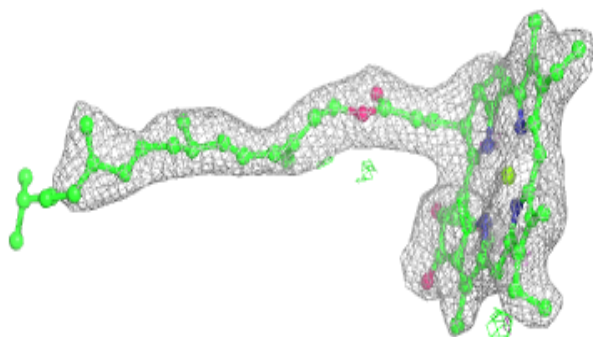
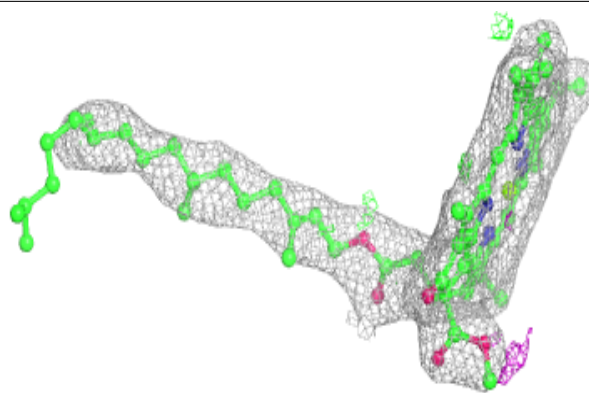
**Electron density around PL9 D 406:**

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

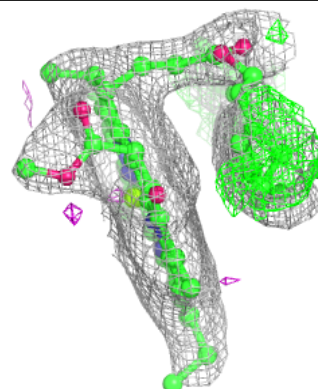
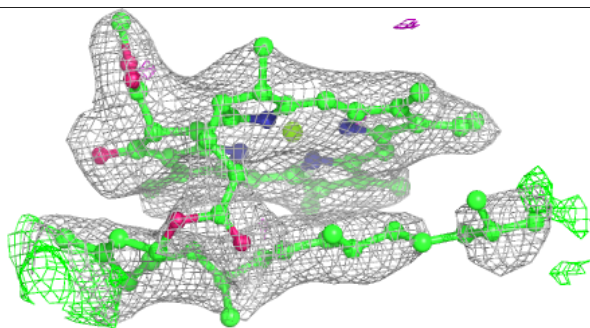
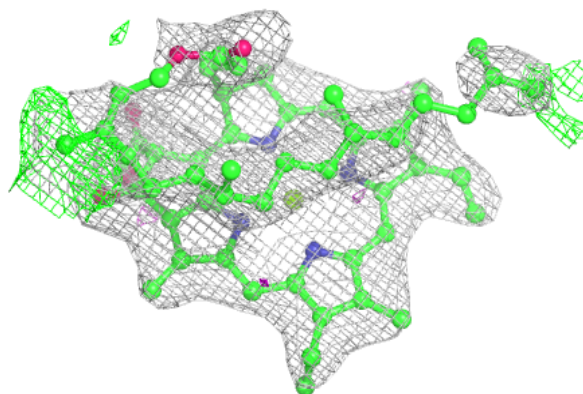


Electron density around CLA b 604:

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

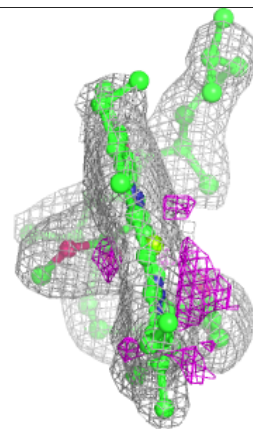
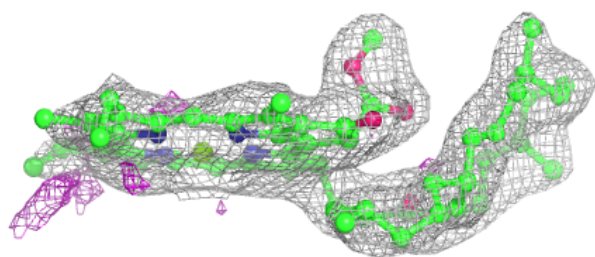
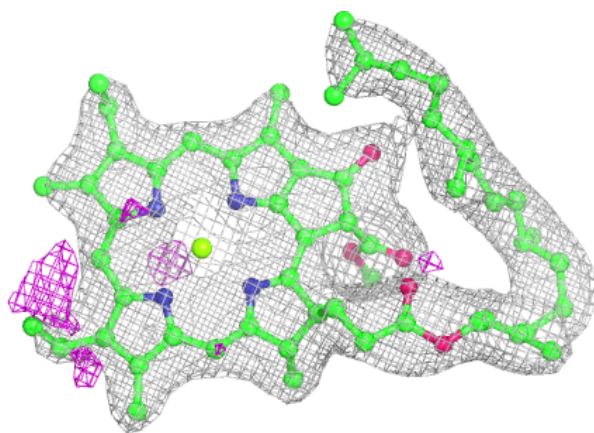
**Electron density around CLA B 601:**

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

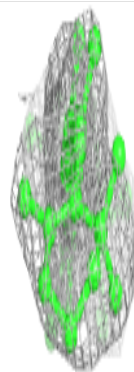
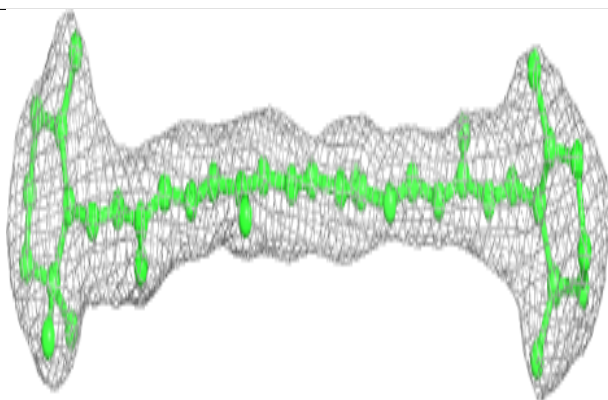
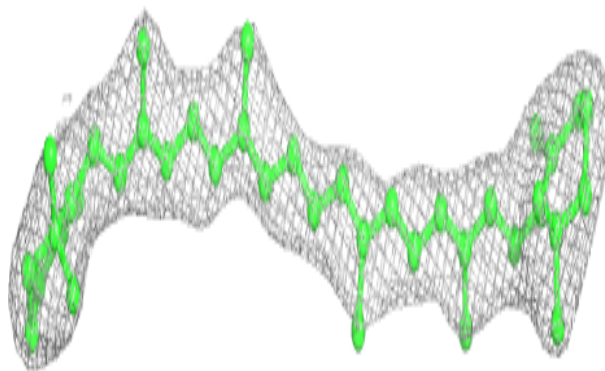


Electron density around CLA b 610:

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

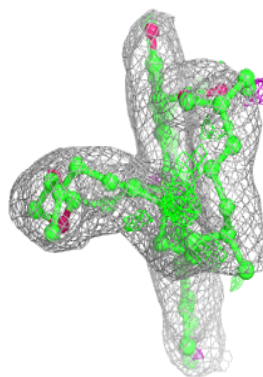
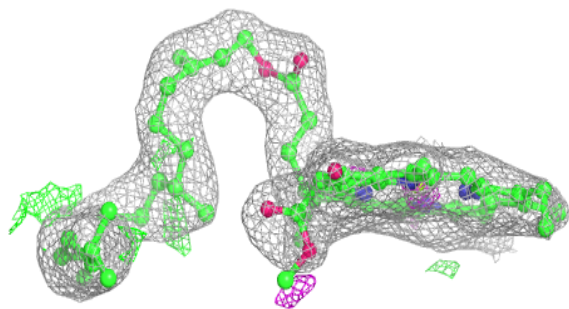
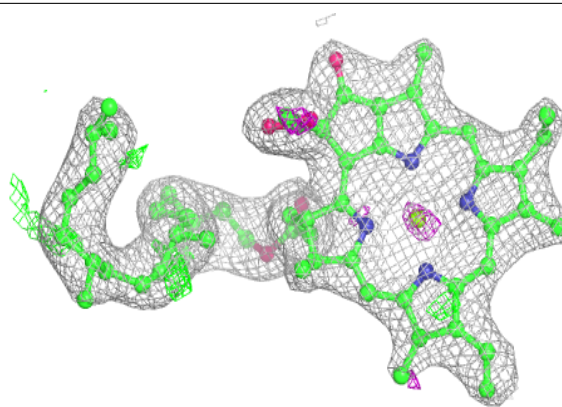
**Electron density around BCR C 516:**

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

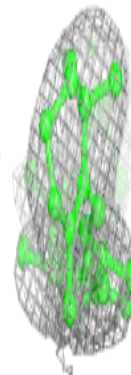
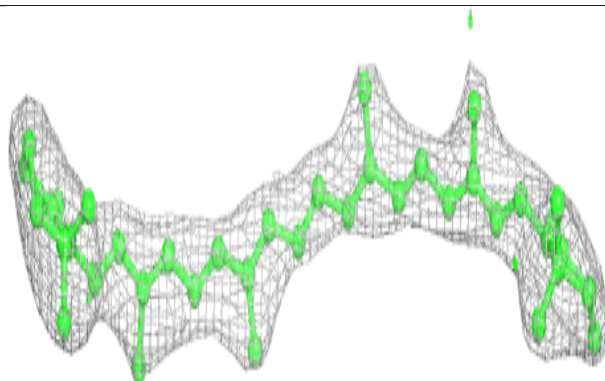
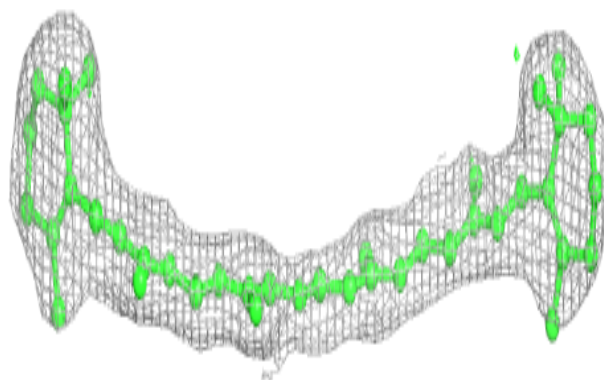


Electron density around CLA b 612:

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

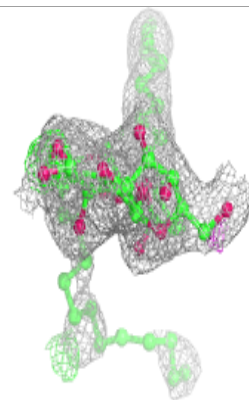
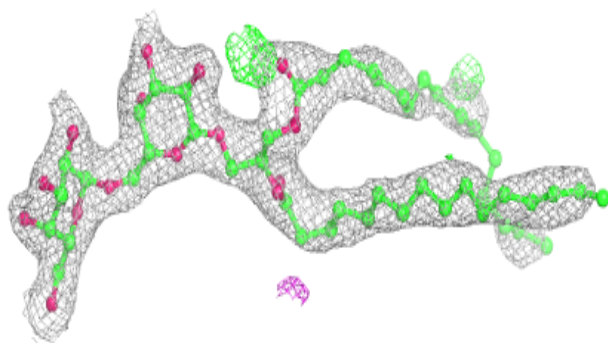
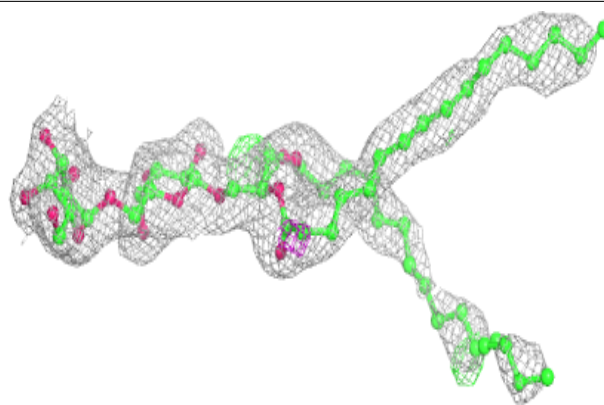
**Electron density around BCR K 101:**

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

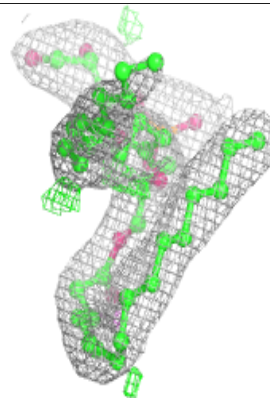
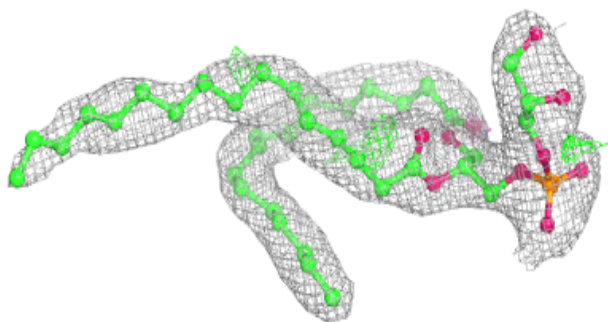
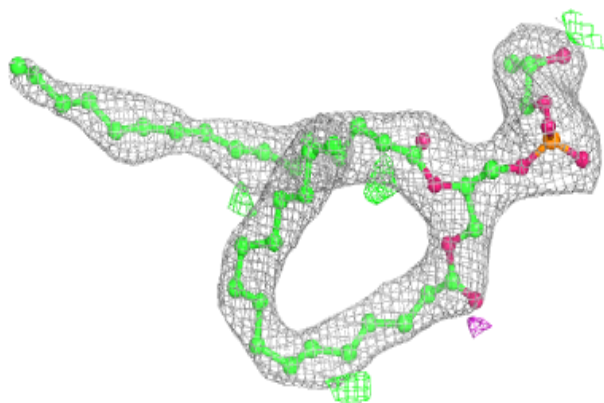


Electron density around DGD c 518:

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

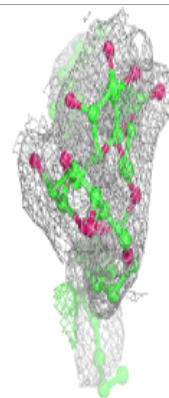
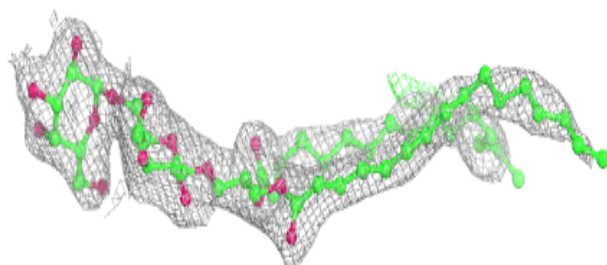
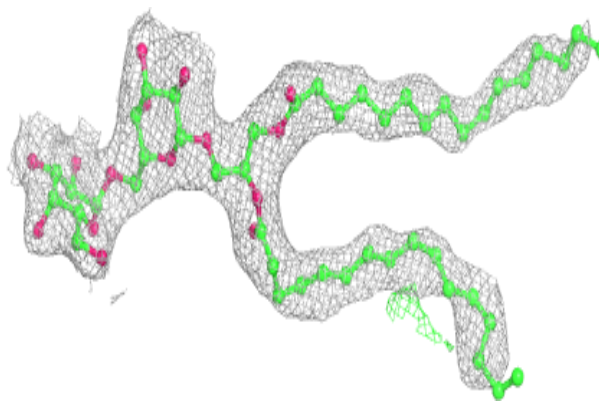
**Electron density around LHG d 406:**

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

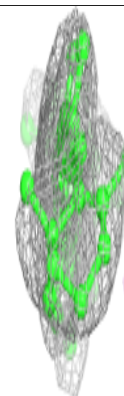
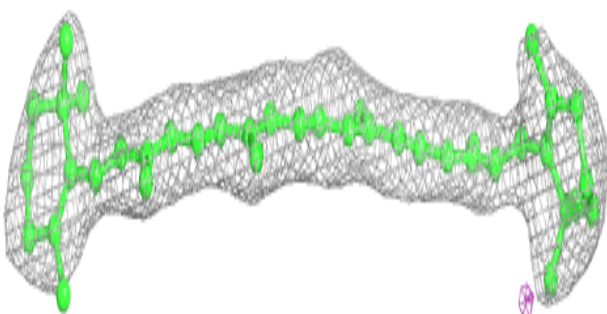
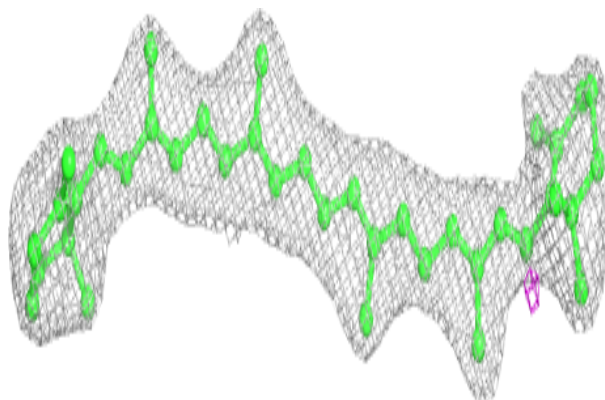


Electron density around DGD c 520:

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

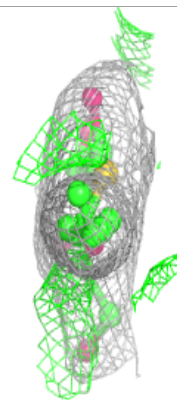
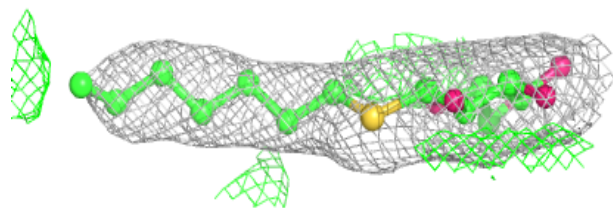
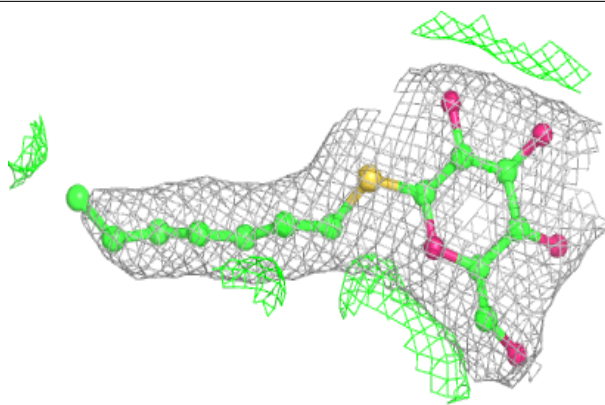
**Electron density around BCR Y 101:**

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

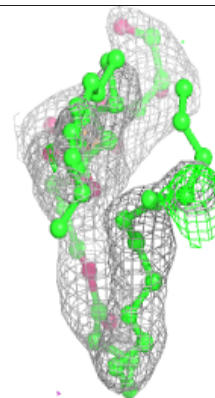
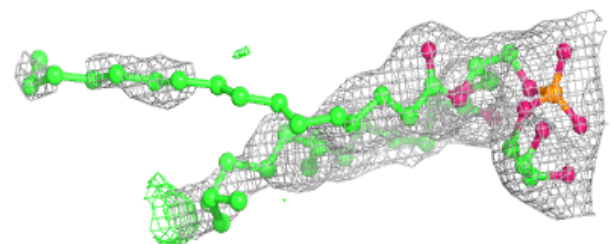
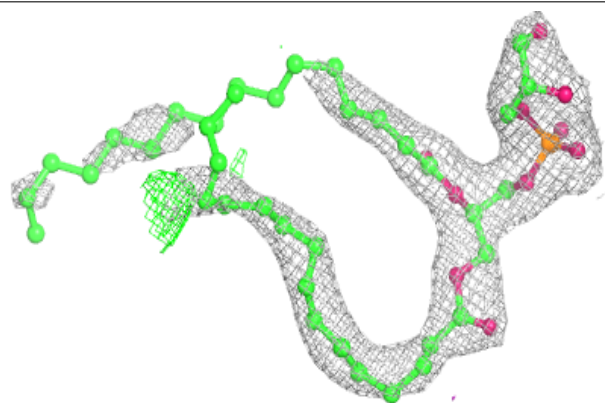


Electron density around HTG b 625:

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

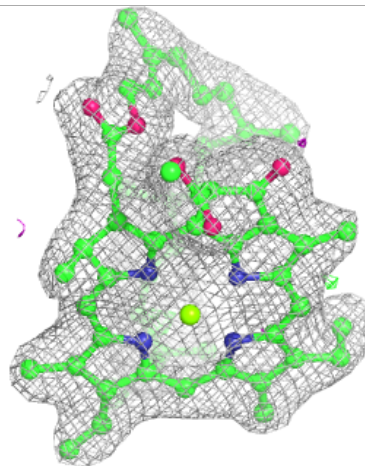
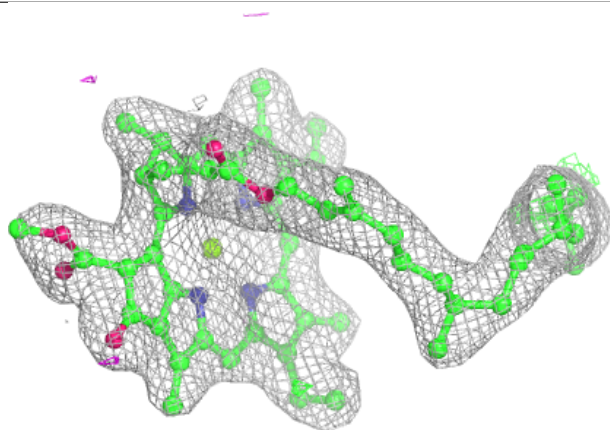
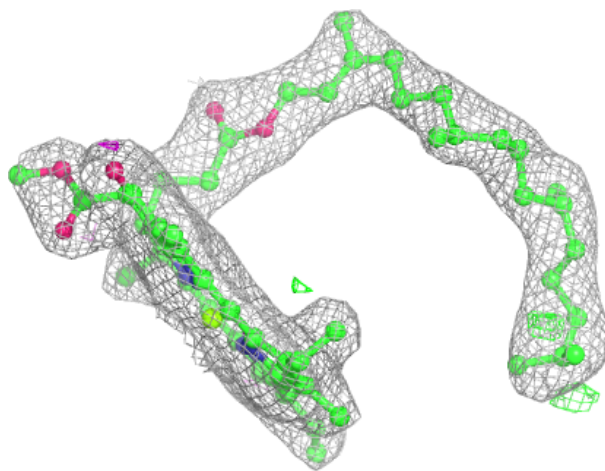
**Electron density around LHG d 408:**

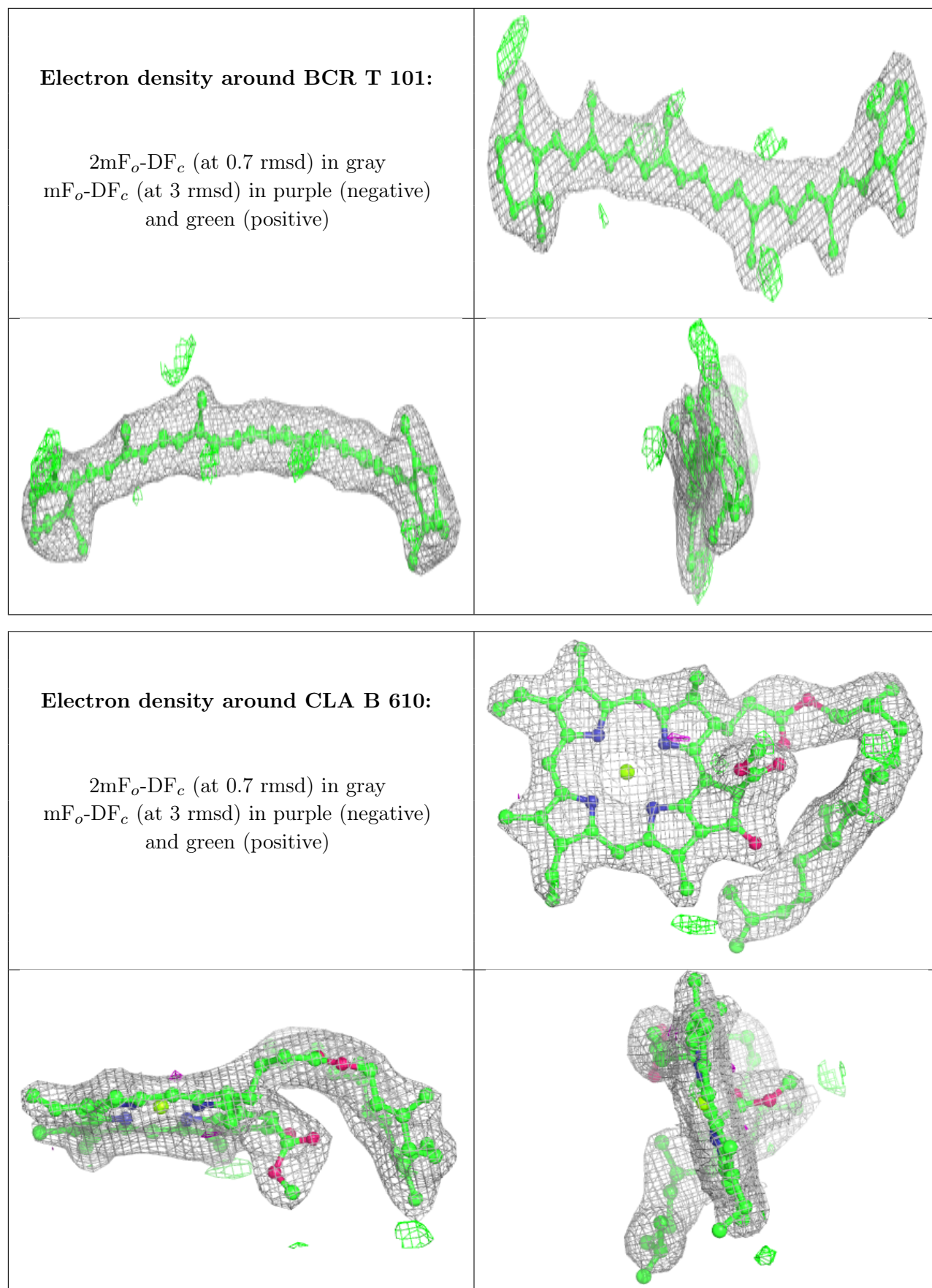
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA b 611:

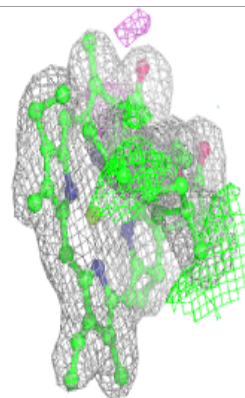
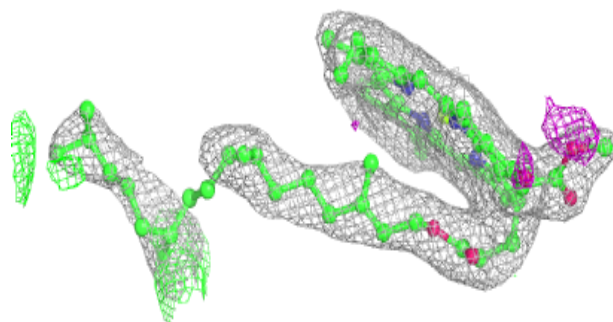
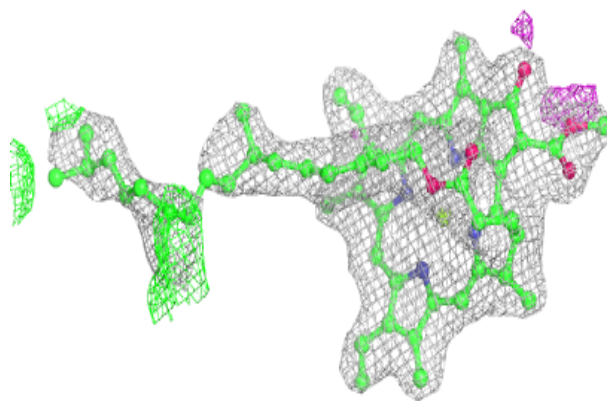
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





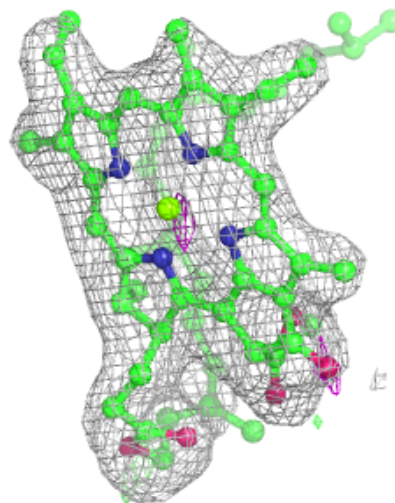
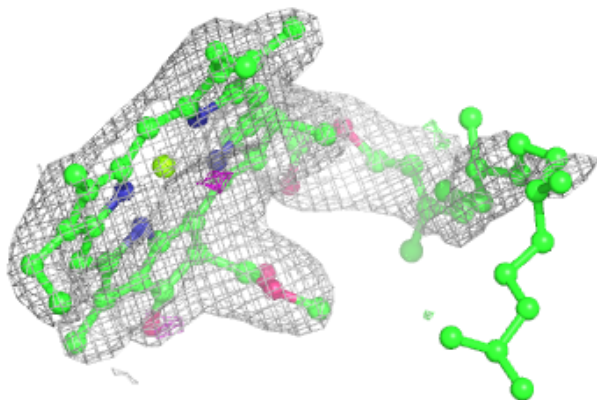
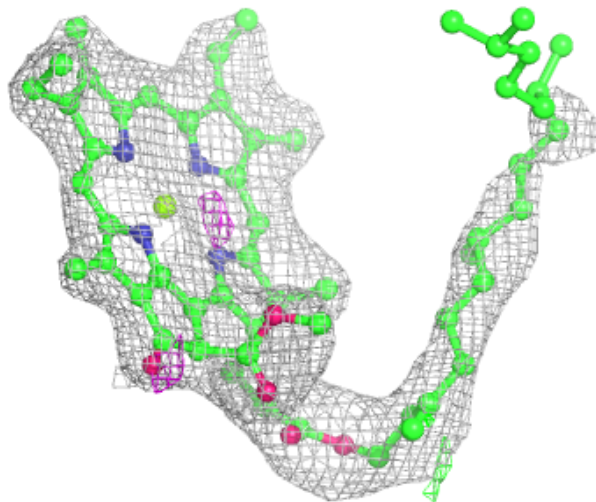
Electron density around CLA b 614:

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



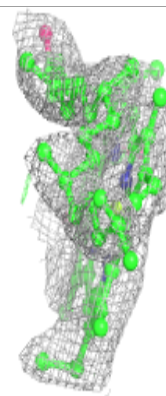
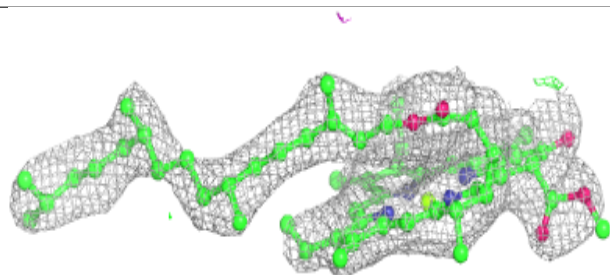
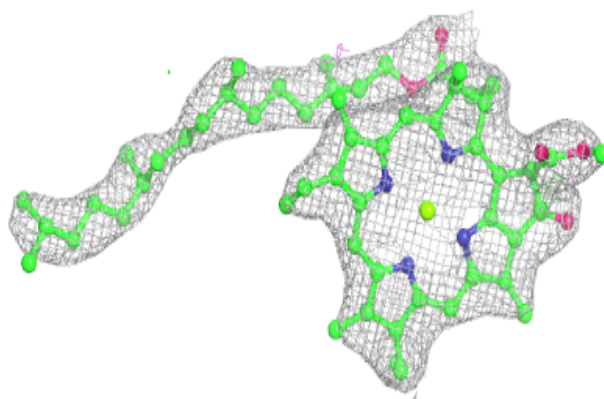
Electron density around CLA b 616:

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

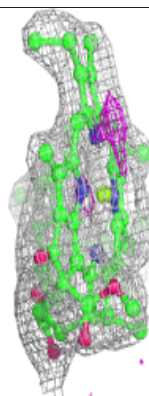
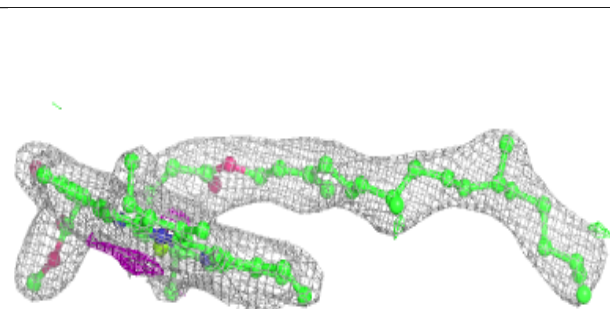
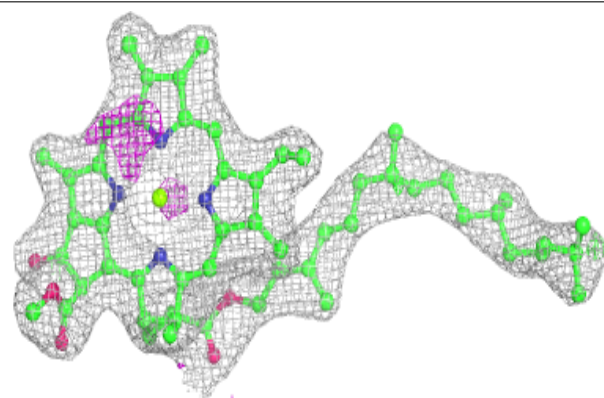


Electron density around CLA c 503:

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

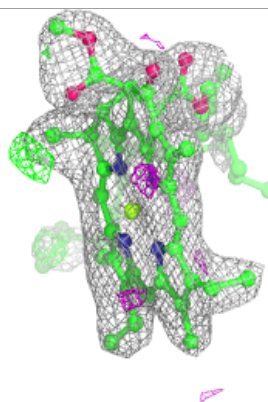
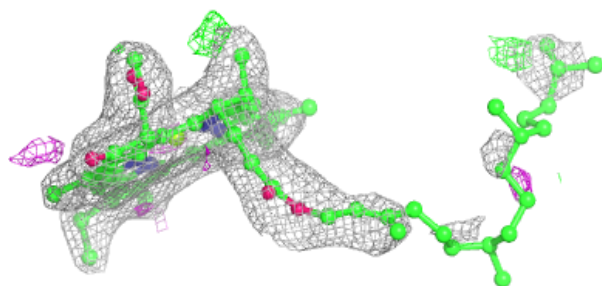
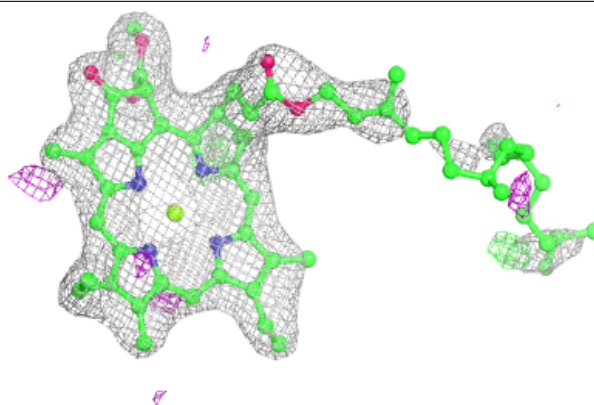
**Electron density around CLA B 603:**

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

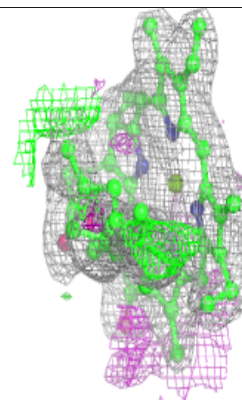
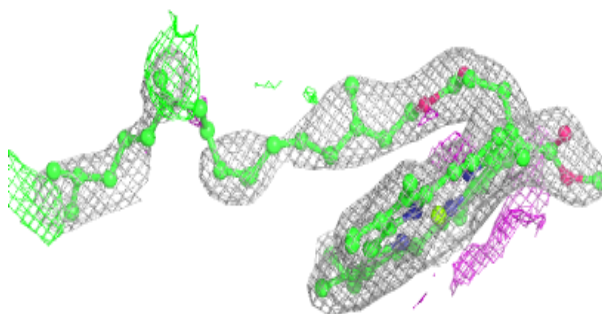
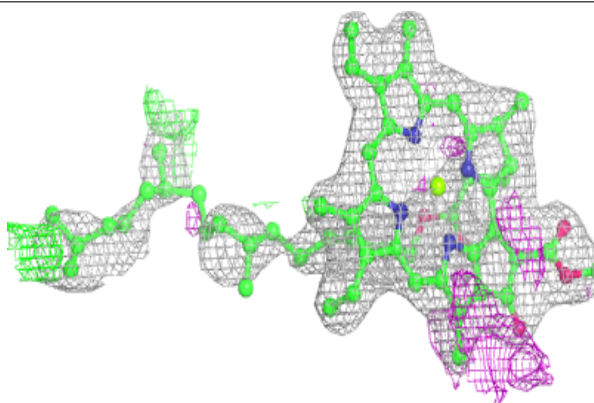


Electron density around CLA a 408:

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

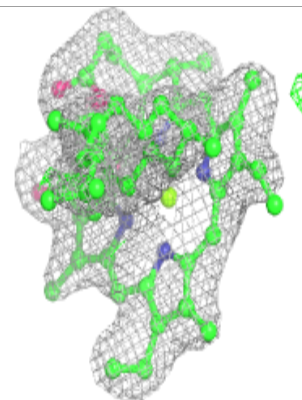
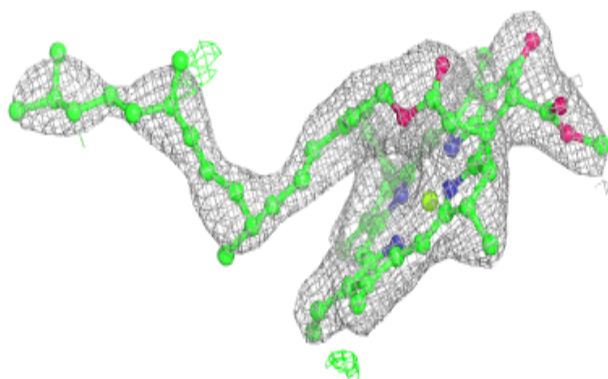
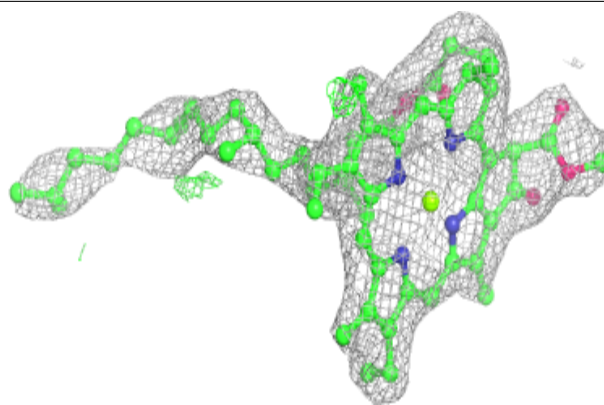
**Electron density around CLA B 614:**

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

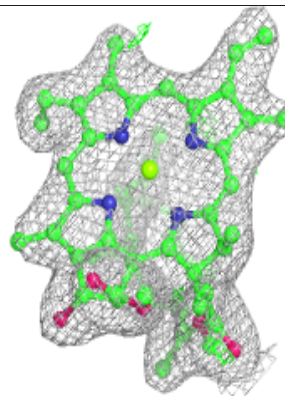
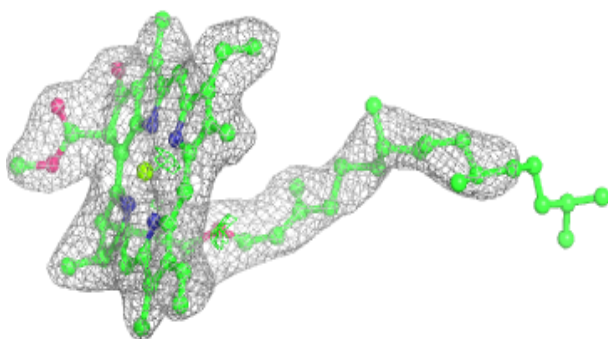
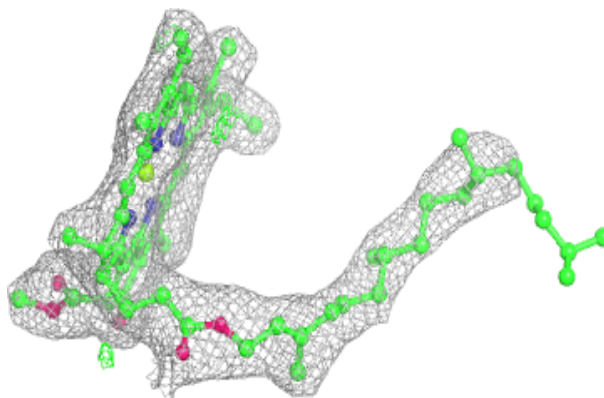


Electron density around CLA c 507:

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

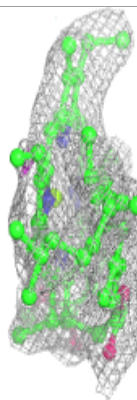
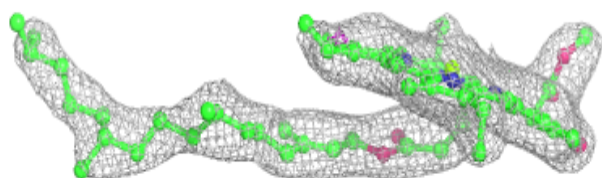
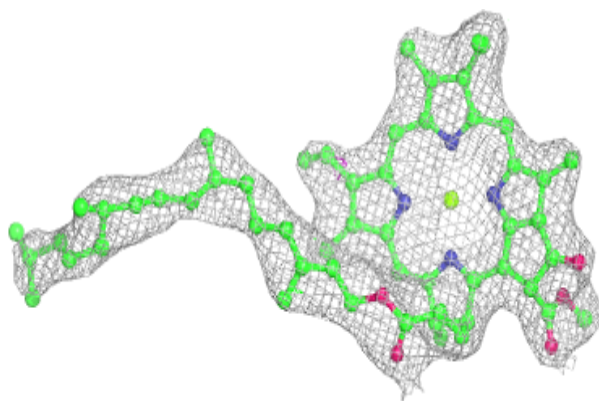
**Electron density around CLA C 510:**

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

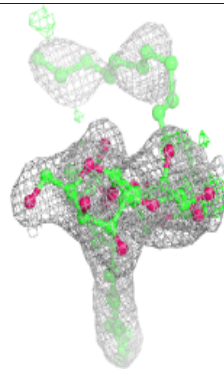
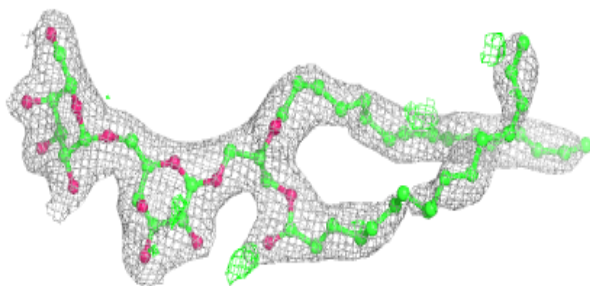
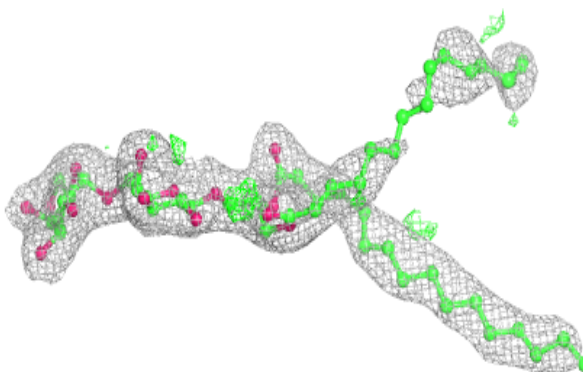


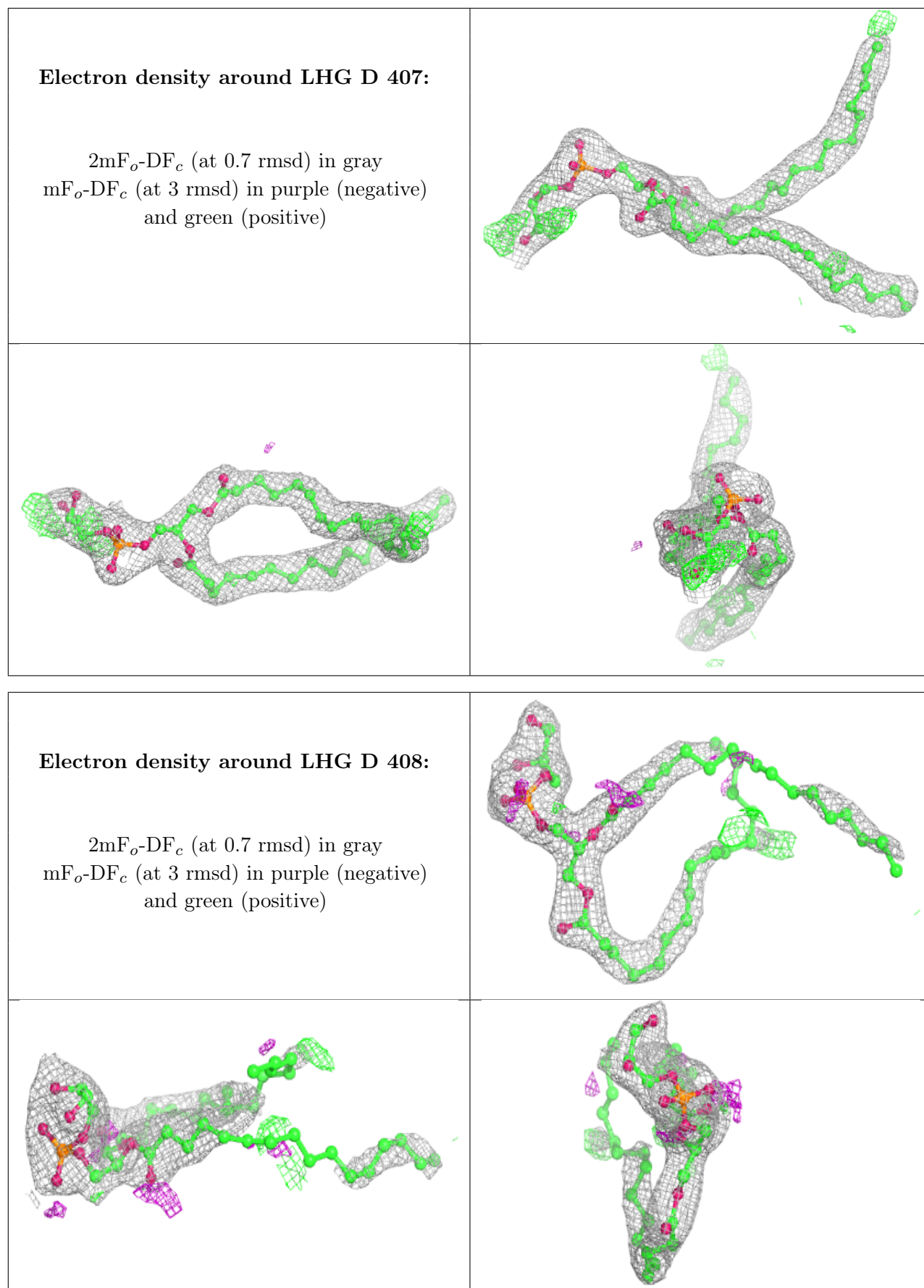
Electron density around CLA b 603:

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

**Electron density around DGD C 518:**

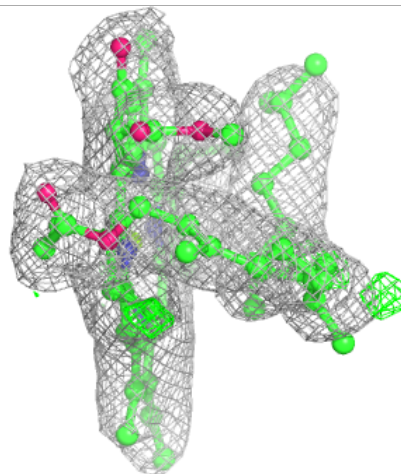
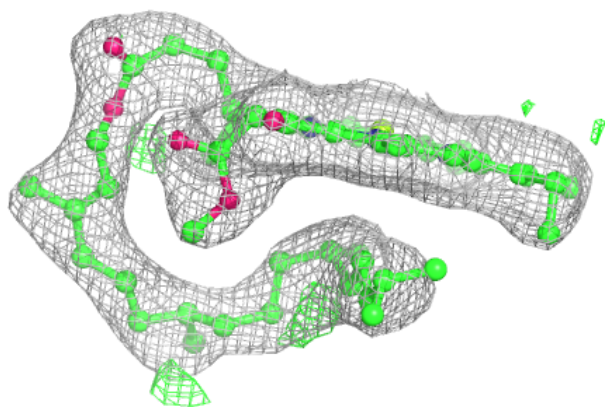
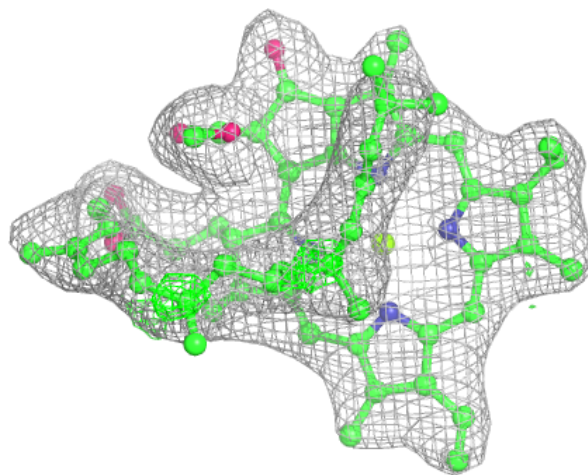
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





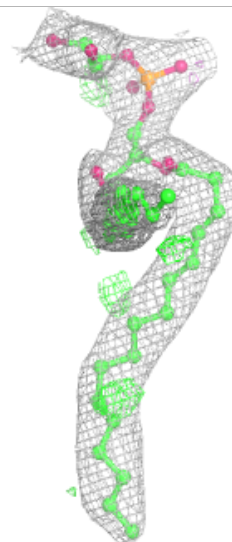
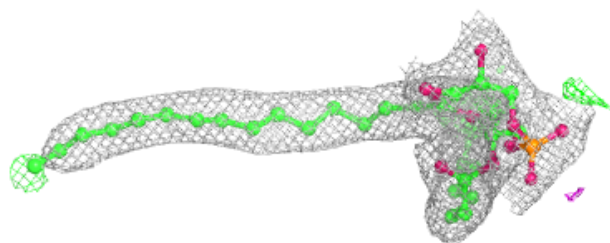
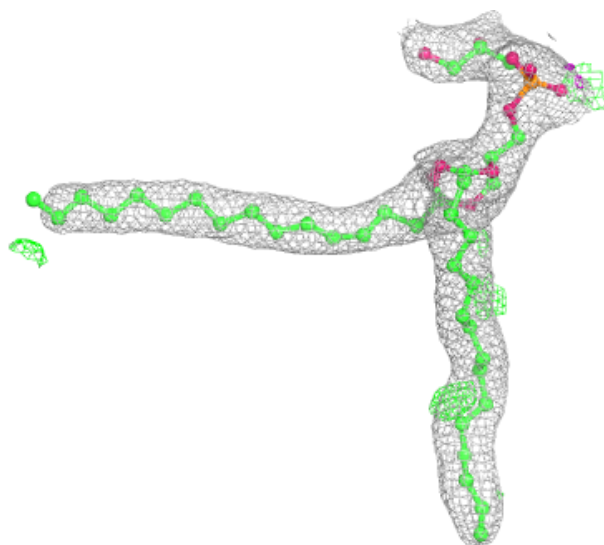
Electron density around CLA C 512:

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



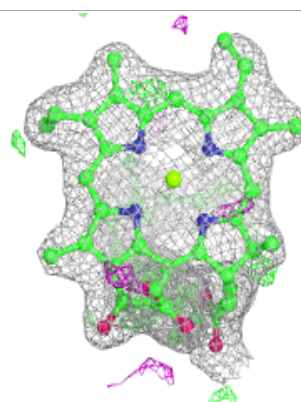
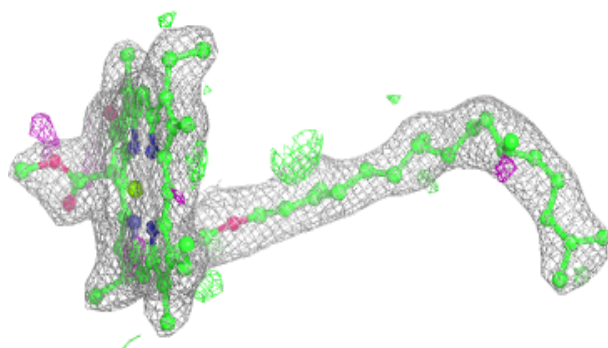
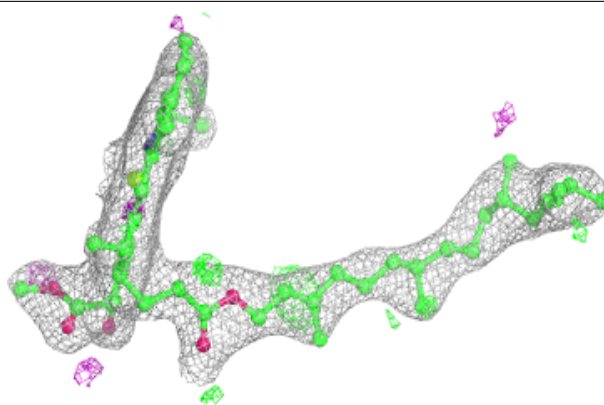
Electron density around LHG L 101:

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

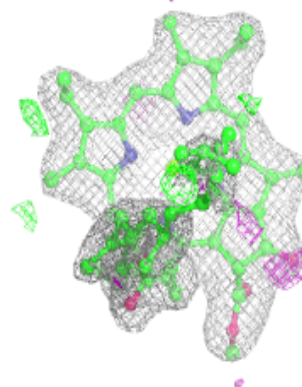
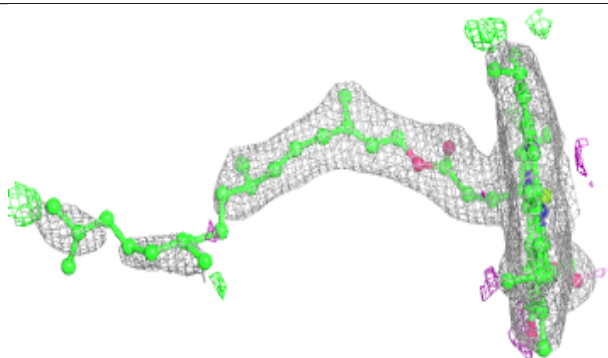
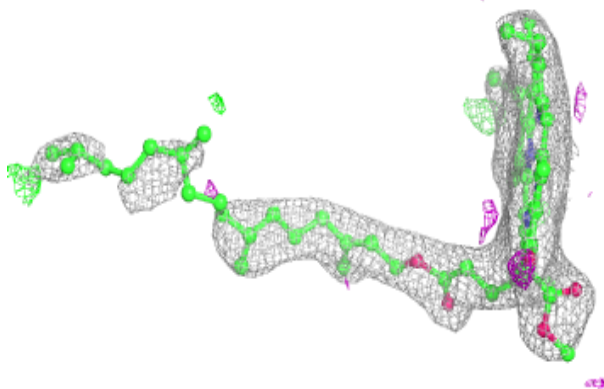


Electron density around CLA b 605:

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

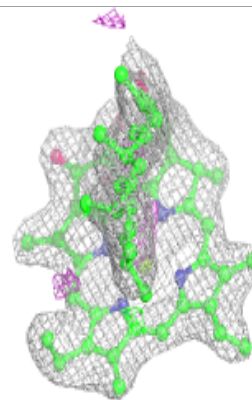
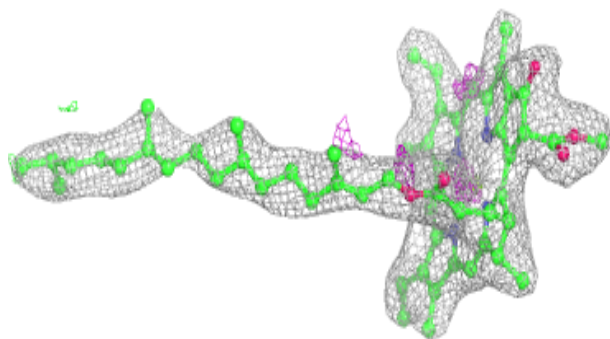
**Electron density around CLA b 606:**

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

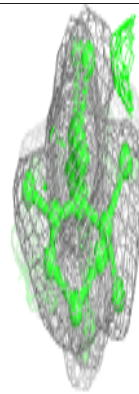
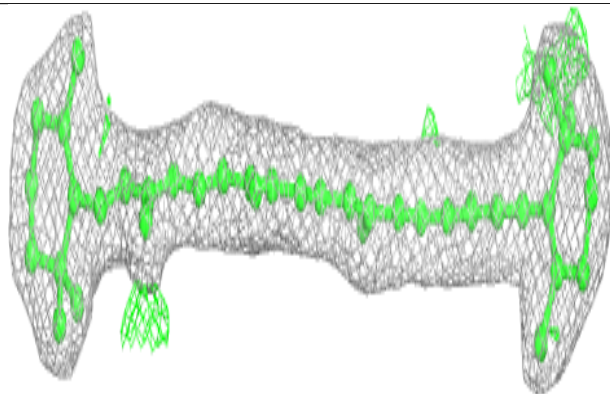
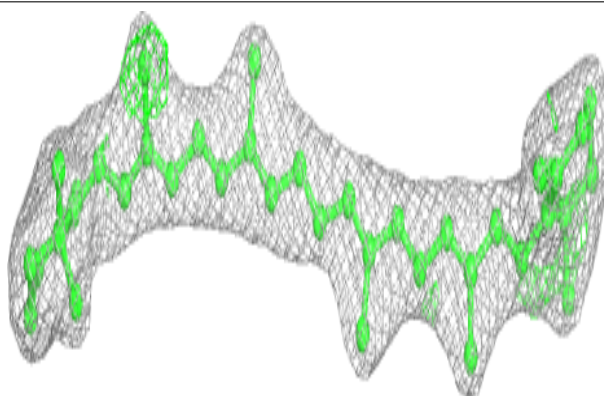


Electron density around CLA b 607:

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

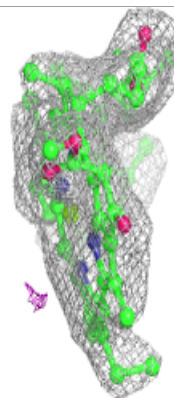
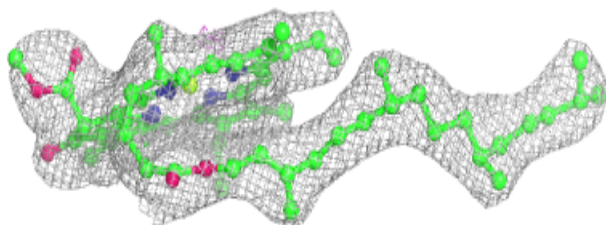
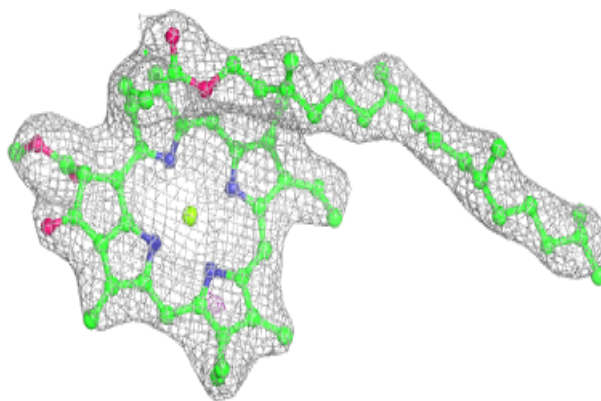
**Electron density around BCR A 409:**

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

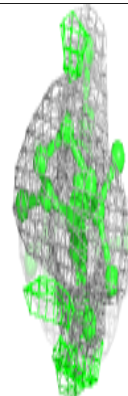
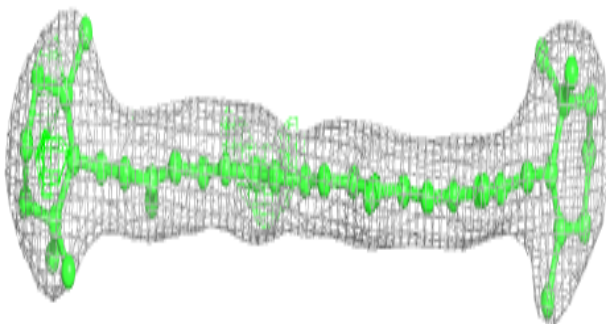
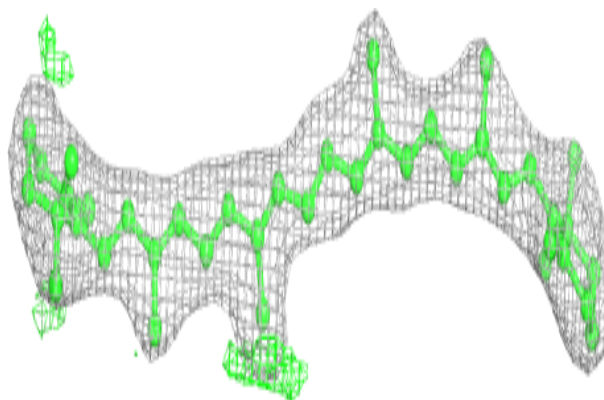


Electron density around CLA C 503:

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

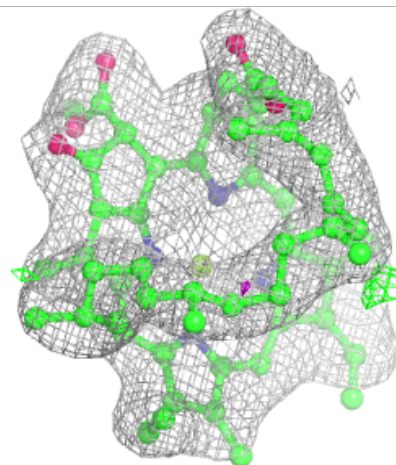
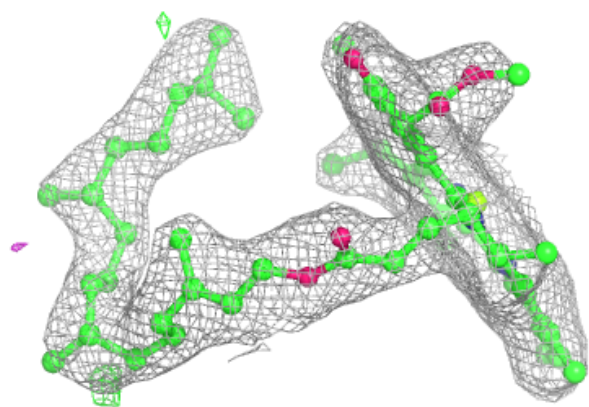
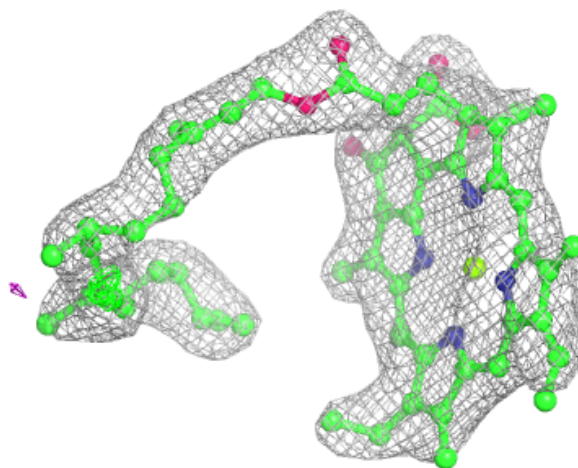
**Electron density around BCR C 517:**

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



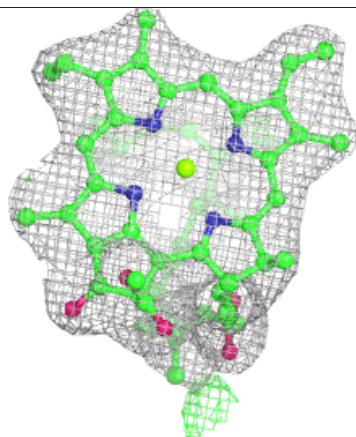
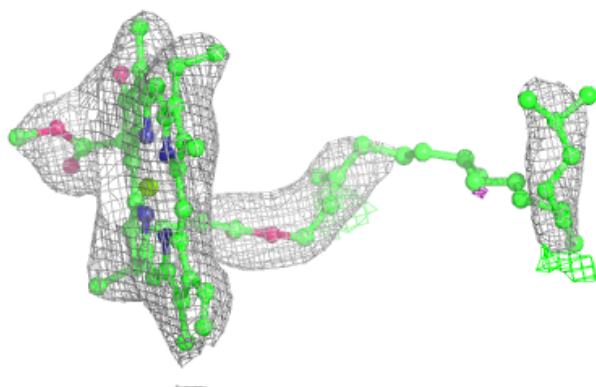
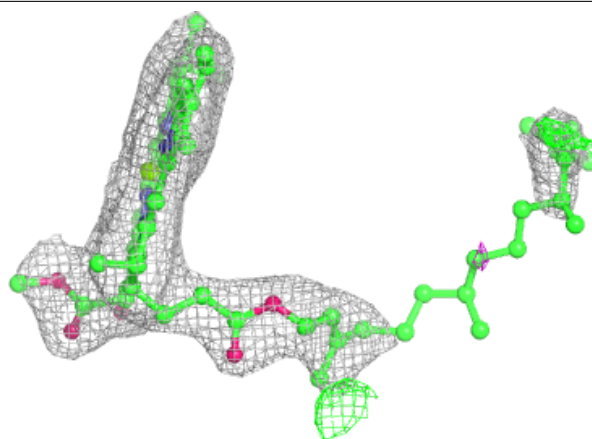
Electron density around CLA C 505:

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

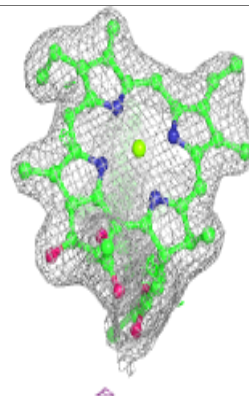
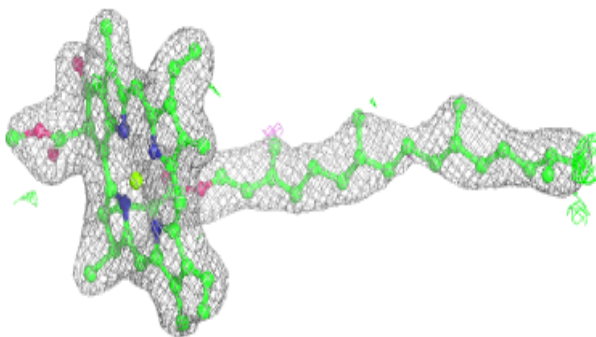
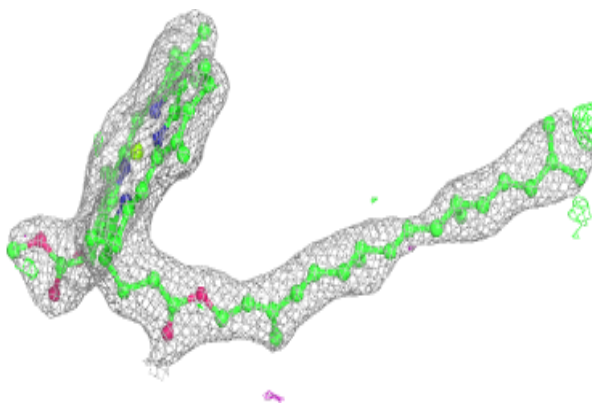


Electron density around CLA c 508:

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

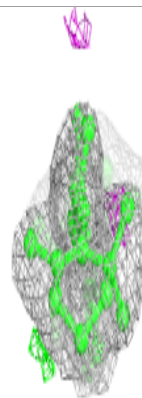
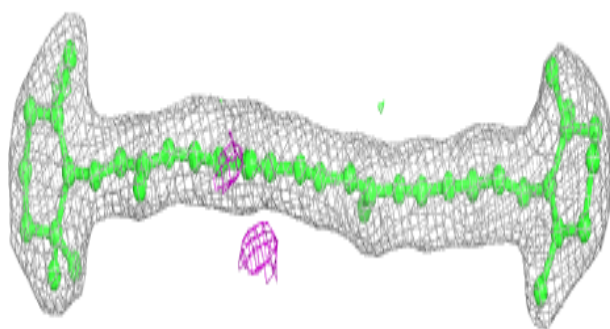
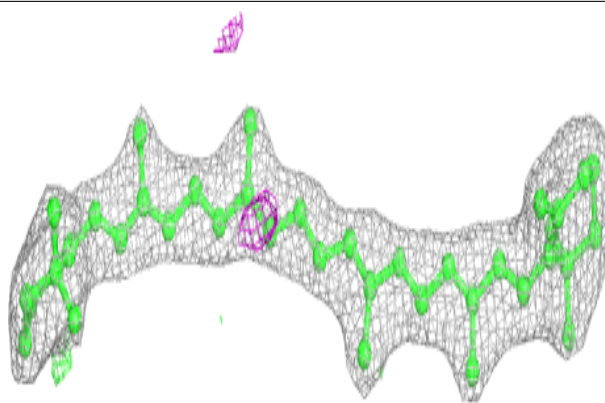
**Electron density around CLA B 607:**

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

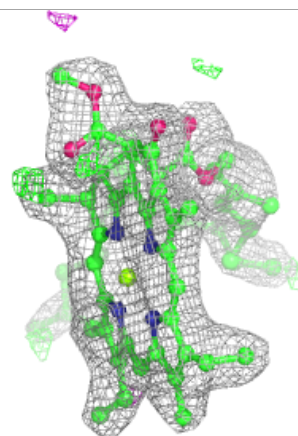
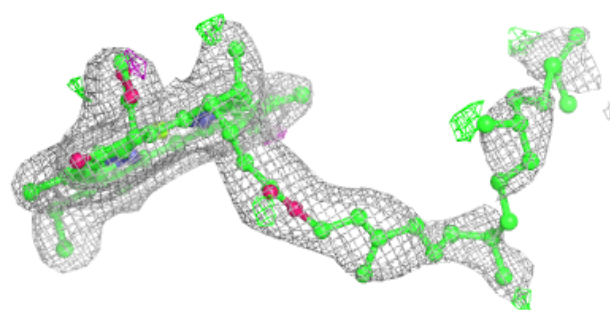
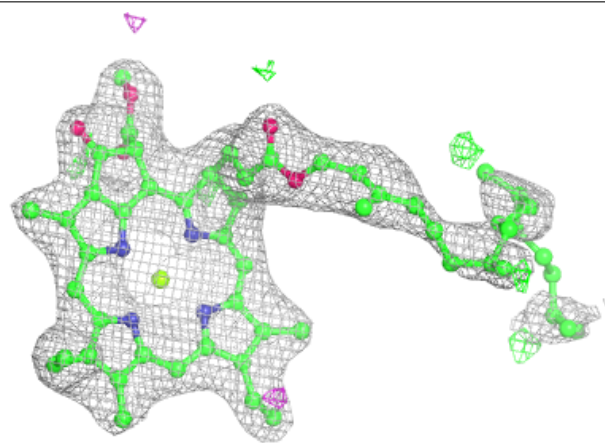


Electron density around BCR a 409:

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

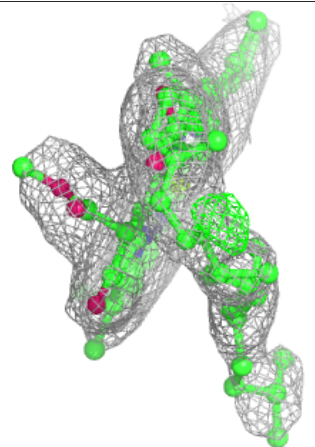
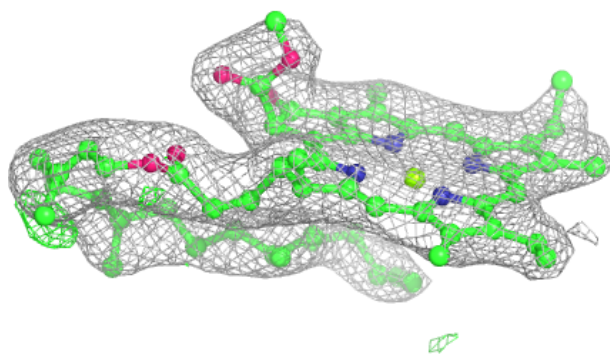
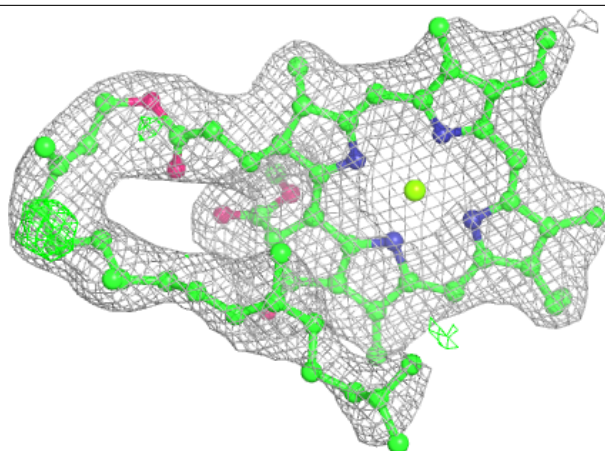
**Electron density around CLA A 408:**

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

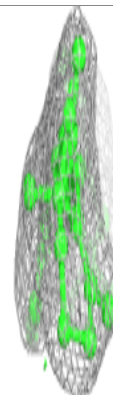
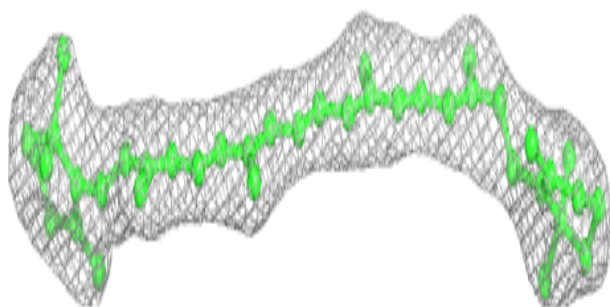
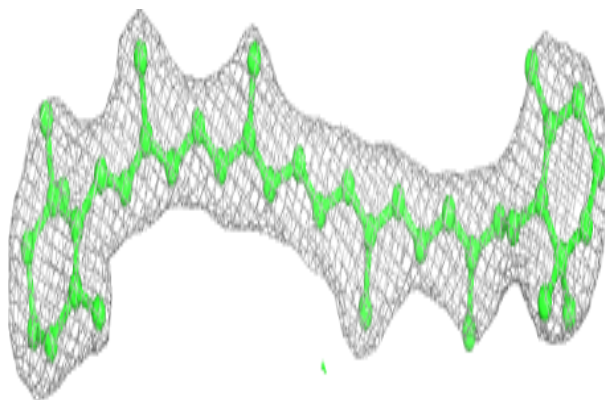


Electron density around CLA c 511:

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

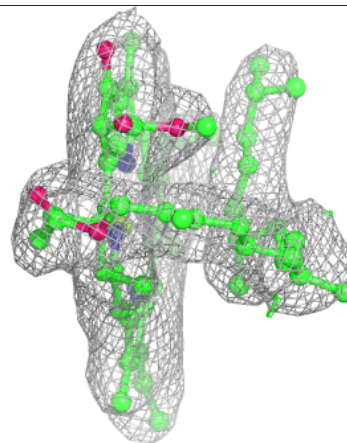
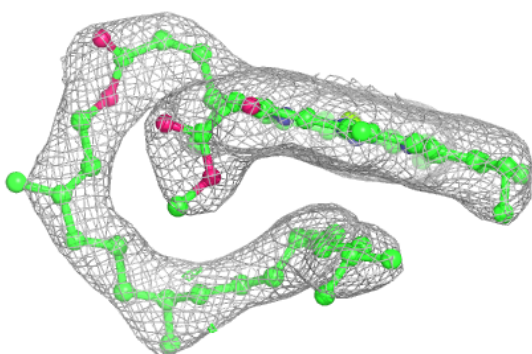
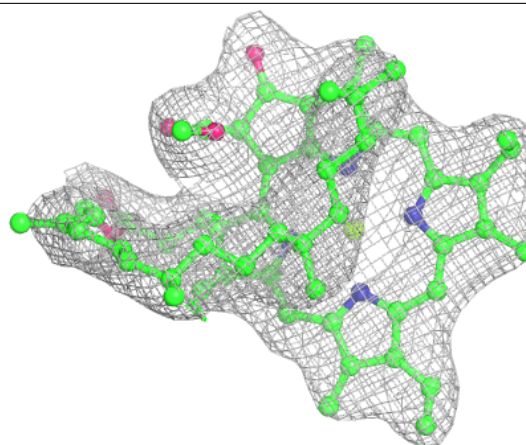
**Electron density around BCR b 619:**

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

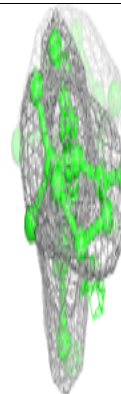
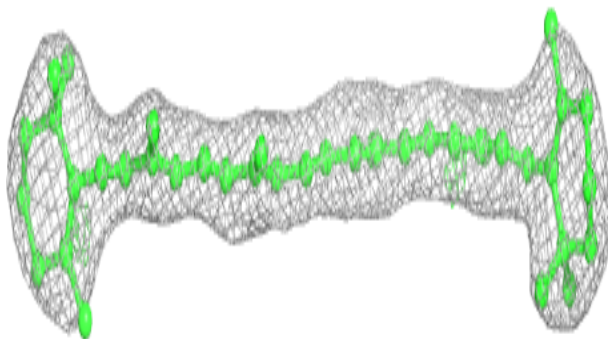
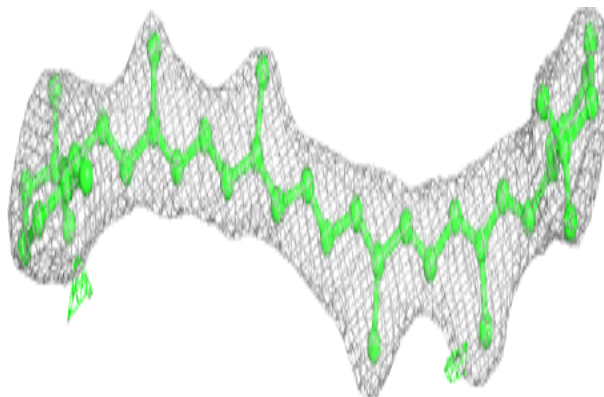


Electron density around CLA c 512:

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

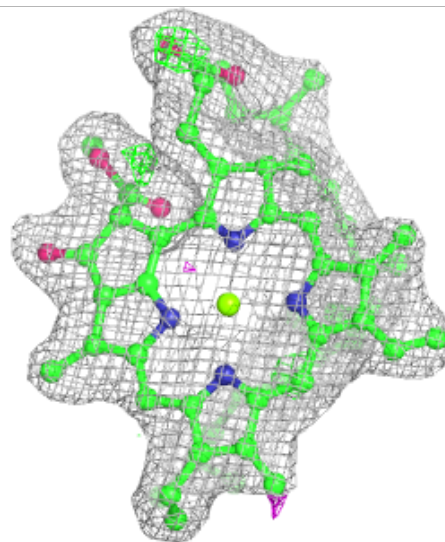
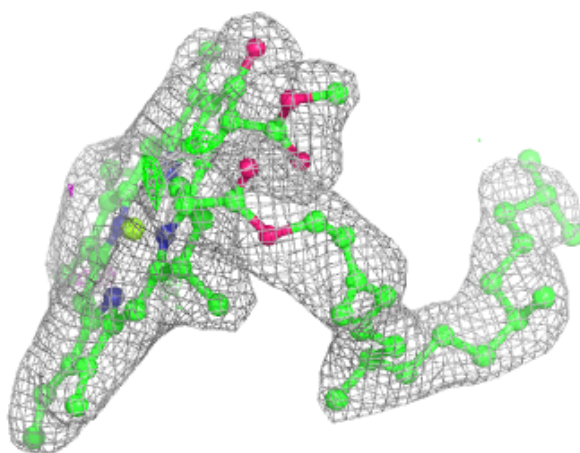
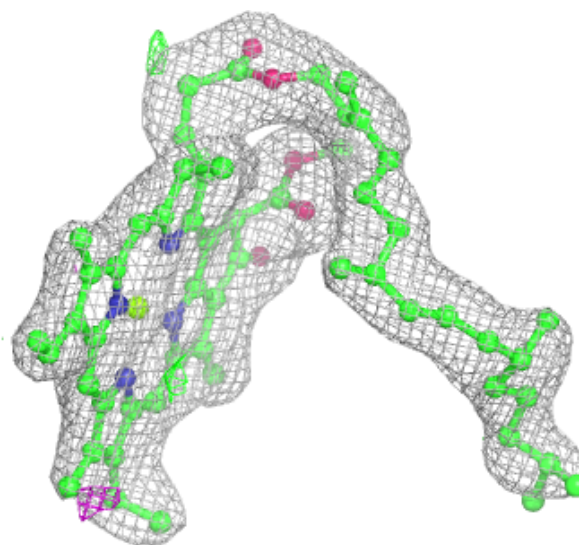
**Electron density around BCR c 517:**

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



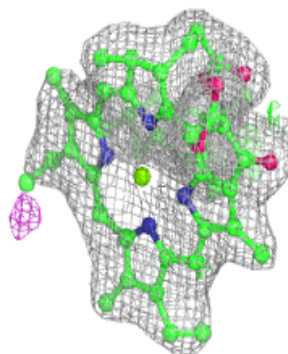
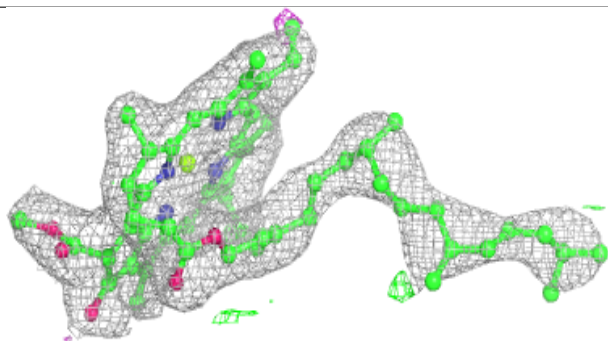
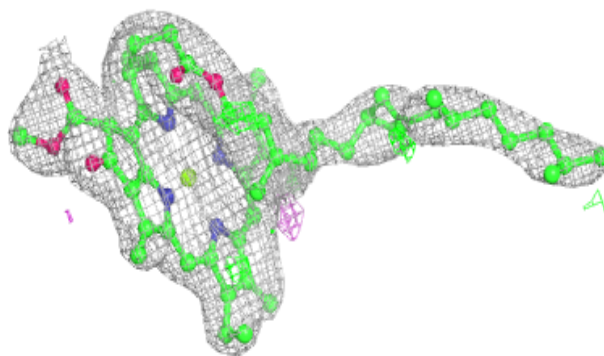
Electron density around CLA b 613:

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

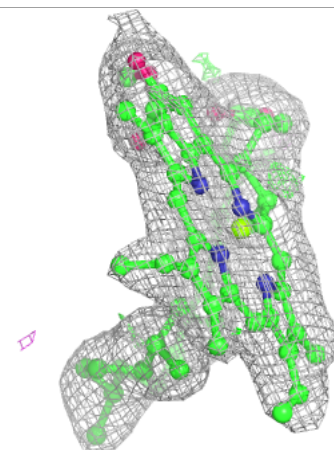
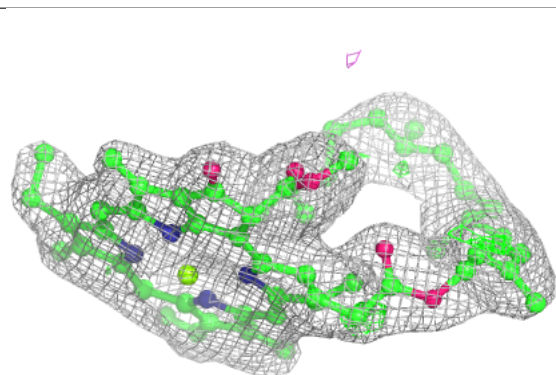
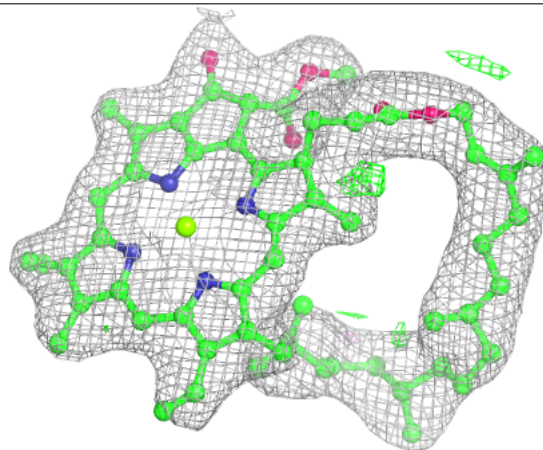


Electron density around CLA C 507:

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

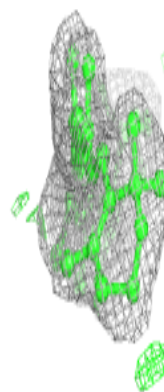
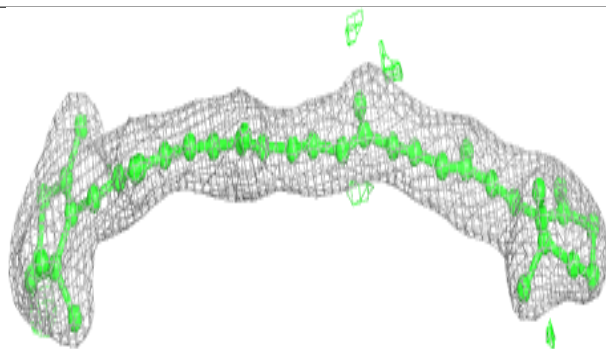
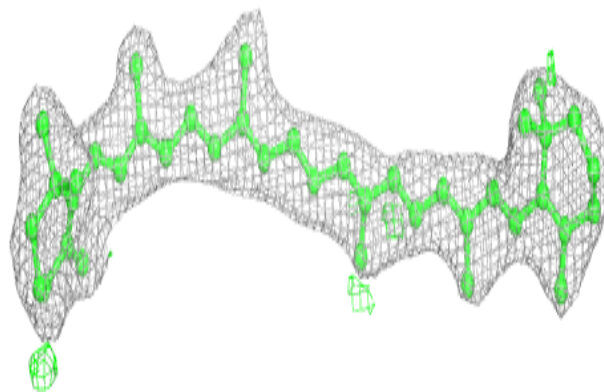
**Electron density around CLA b 615:**

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



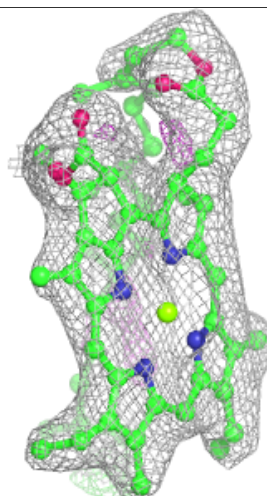
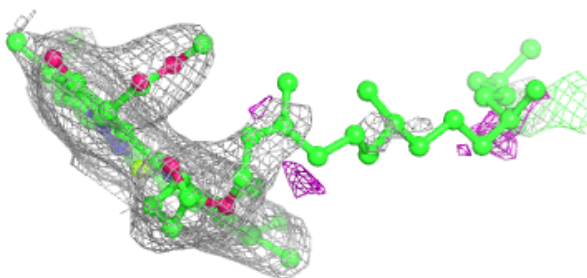
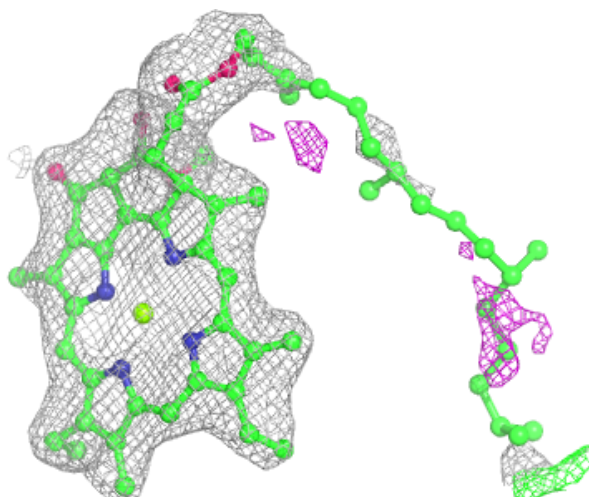
Electron density around BCR t 102:

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



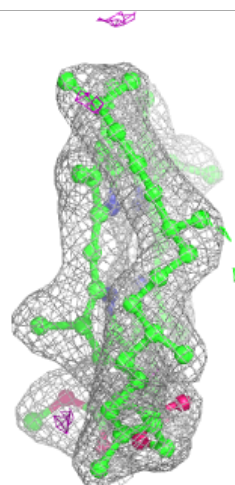
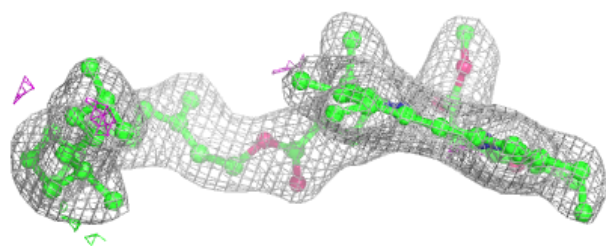
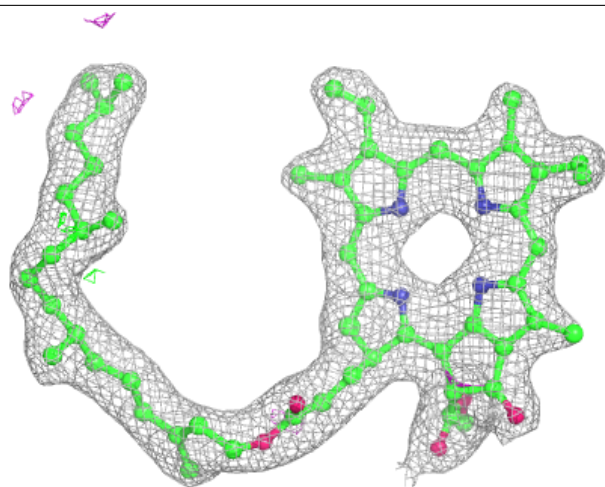
Electron density around CLA B 616:

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



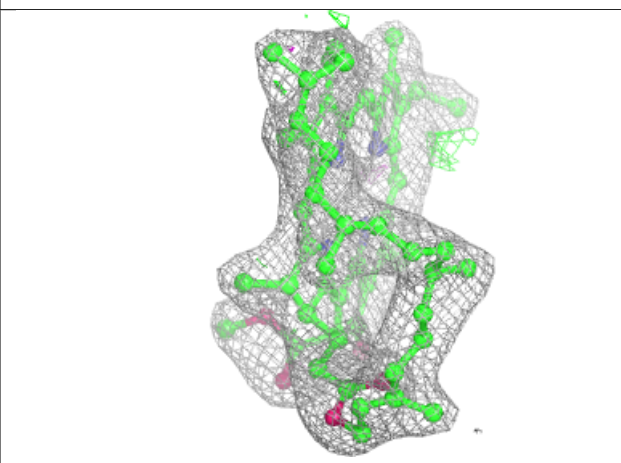
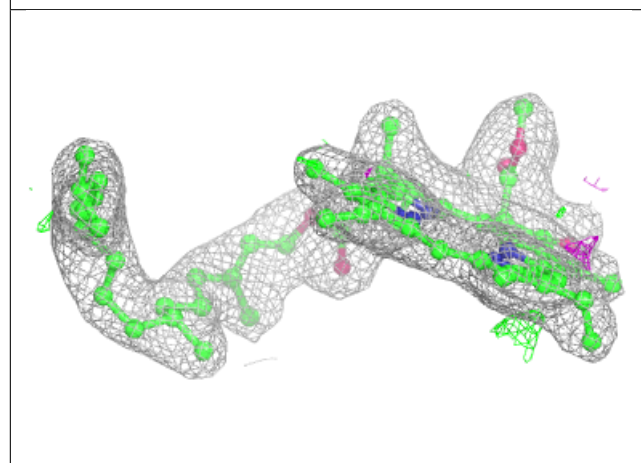
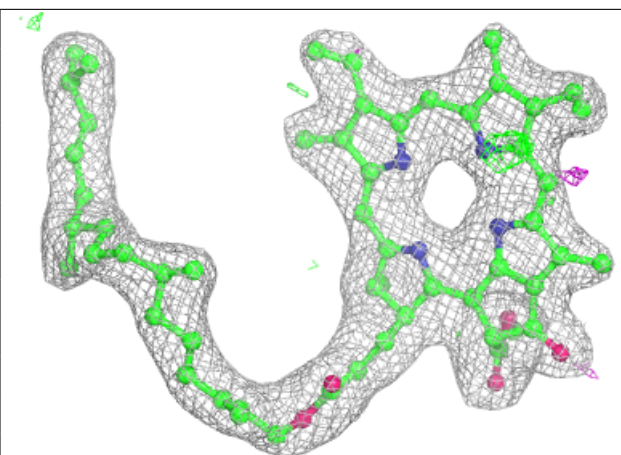
Electron density around PHO A 407:

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

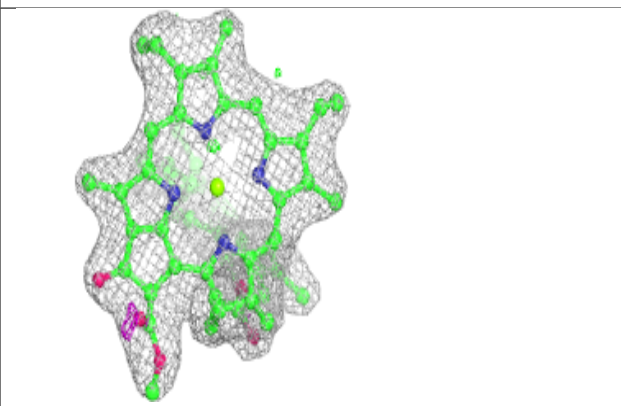
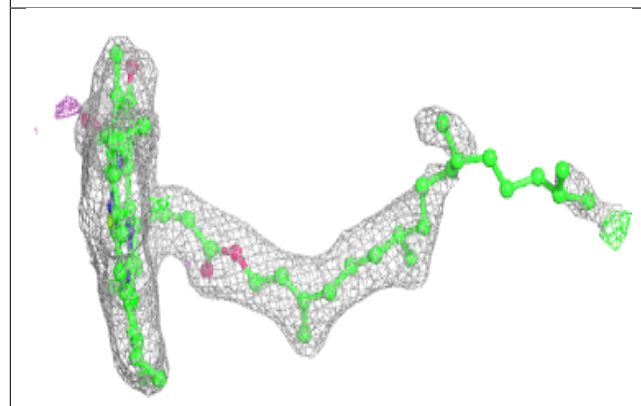
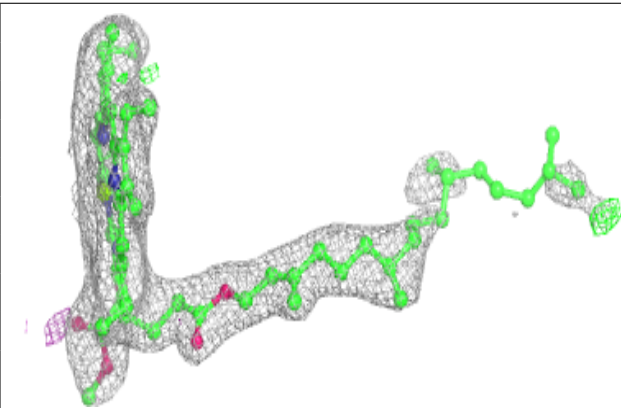


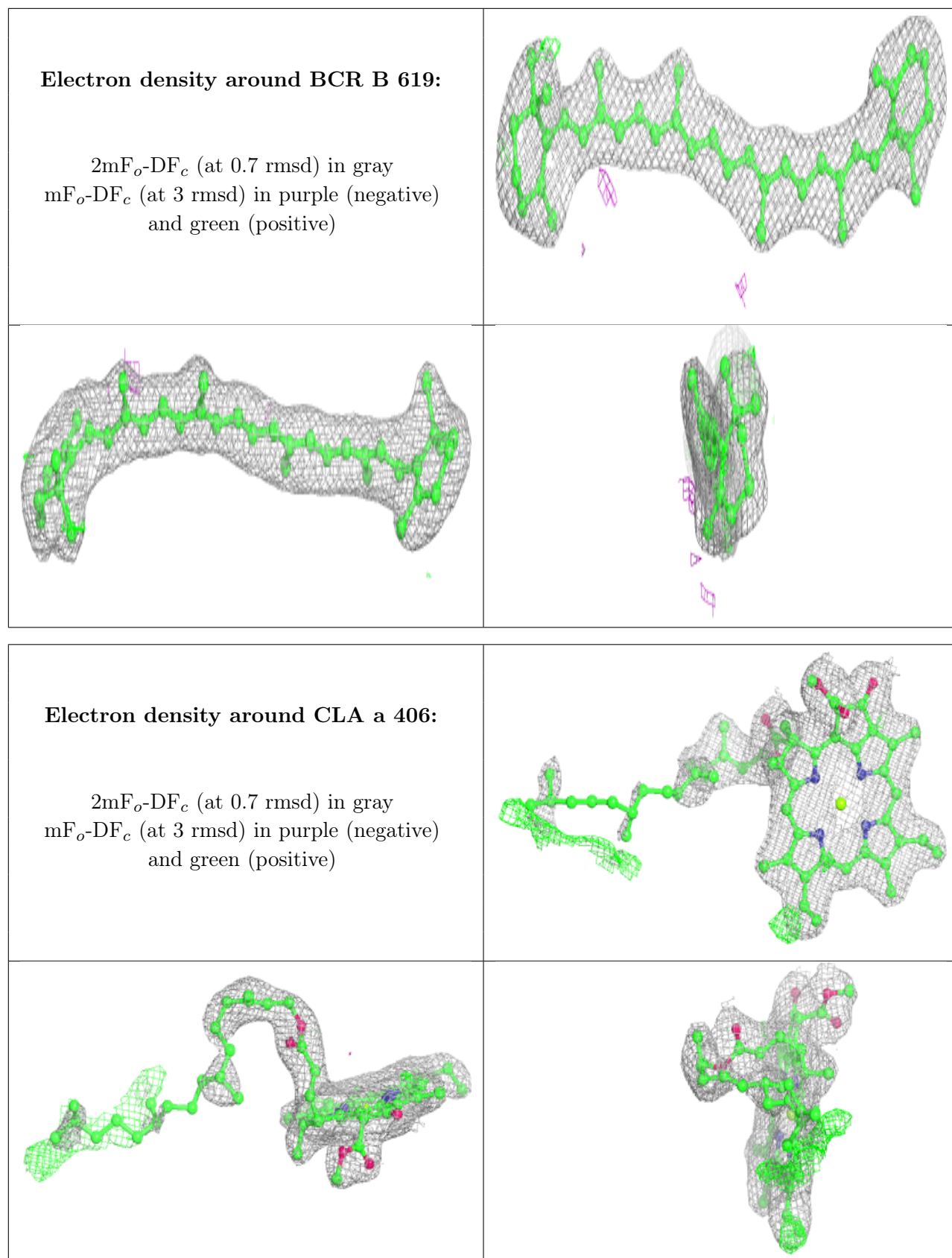
Electron density around PHO A 415:

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

**Electron density around CLA B 606:**

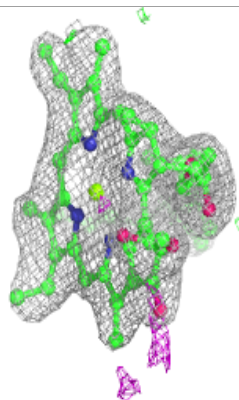
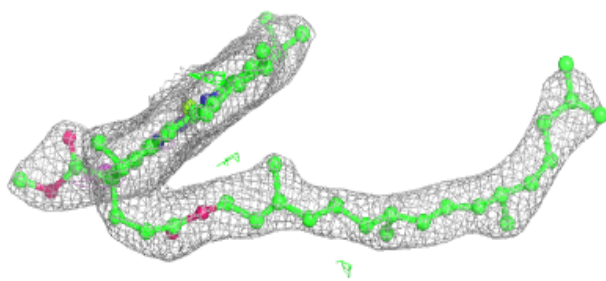
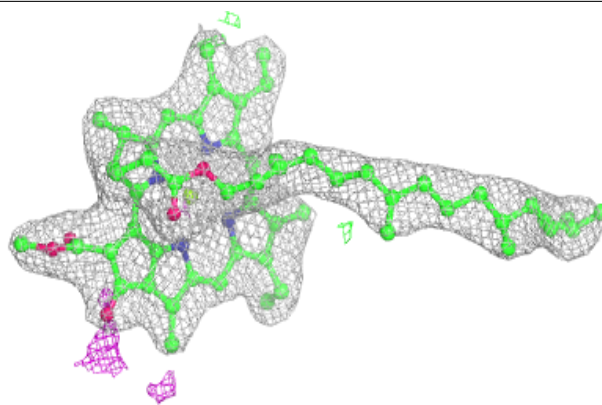
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



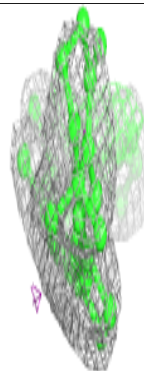
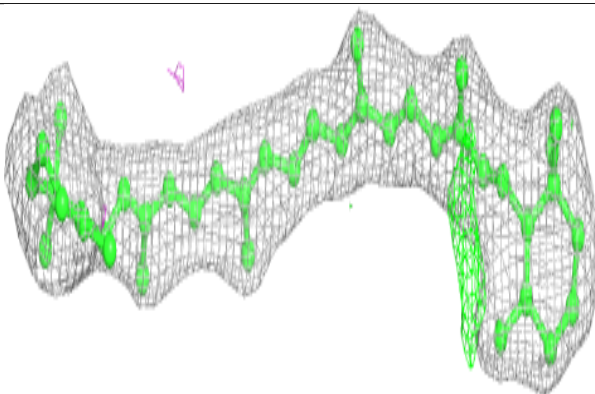
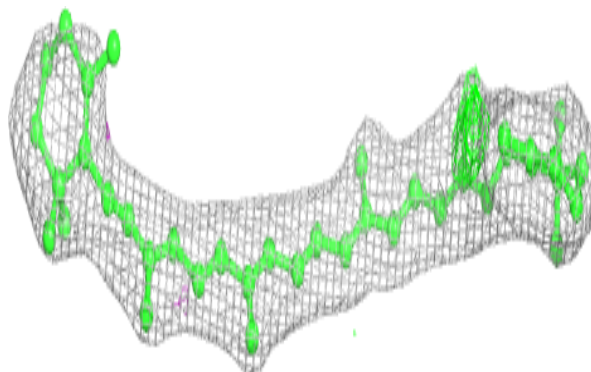


Electron density around CLA b 608:

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

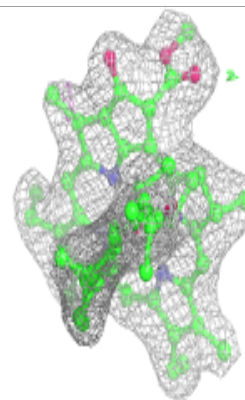
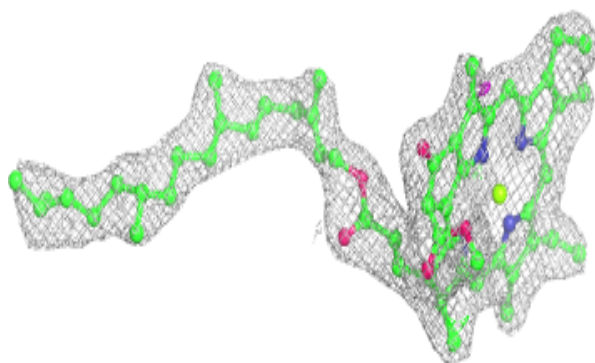
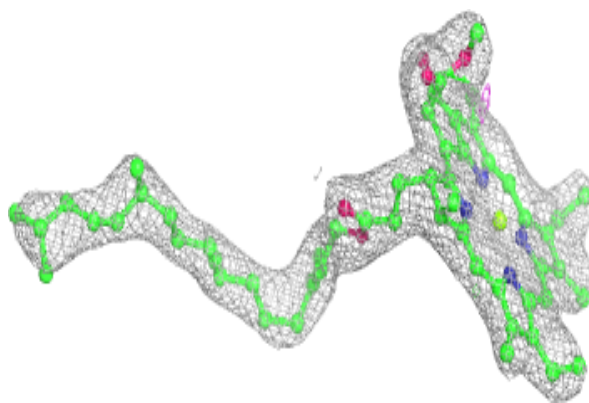
**Electron density around BCR D 405:**

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

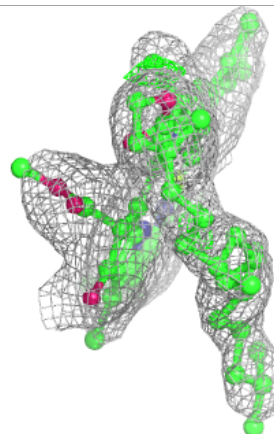
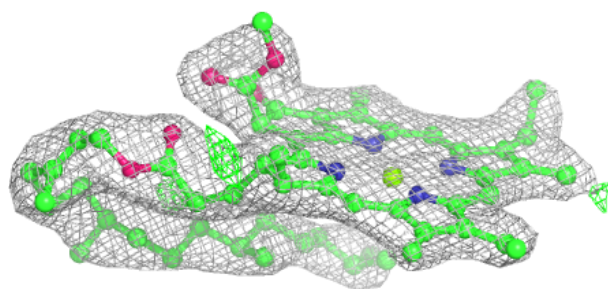
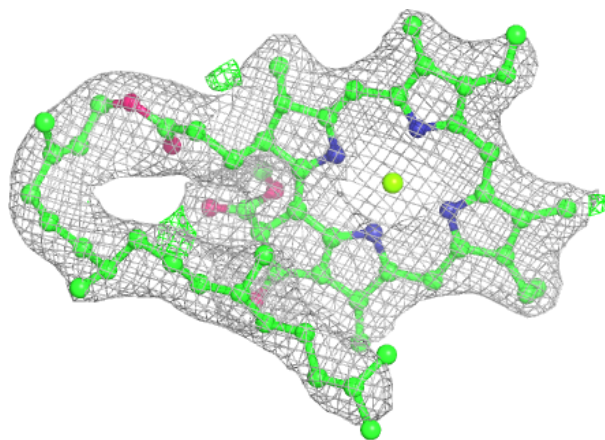


Electron density around CLA C 504:

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

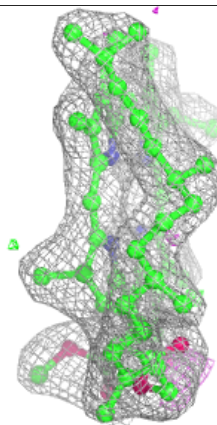
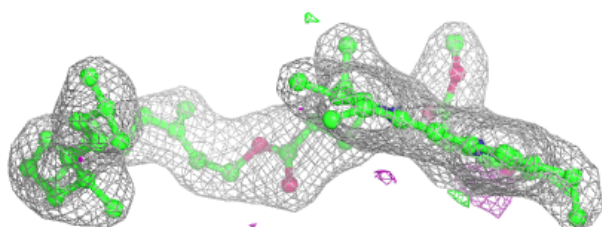
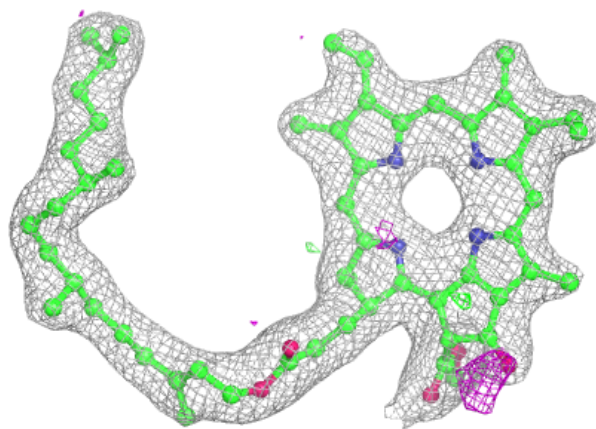
**Electron density around CLA C 511:**

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



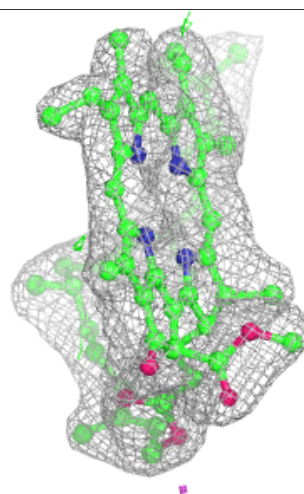
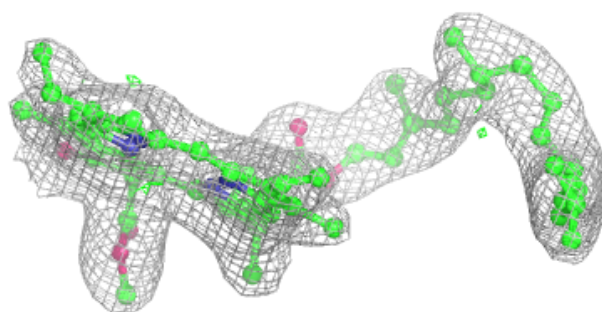
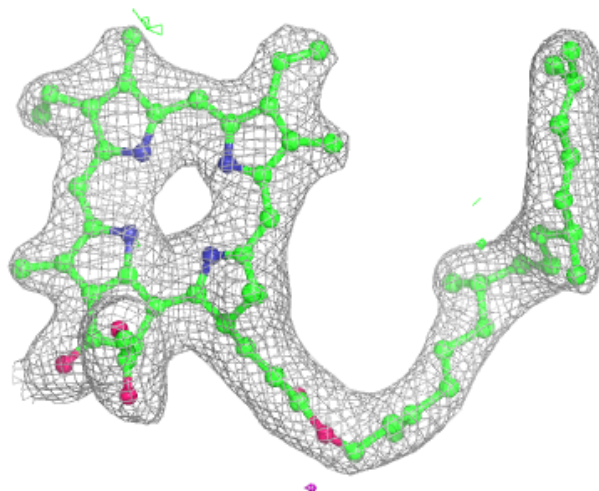
Electron density around PHO a 407:

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



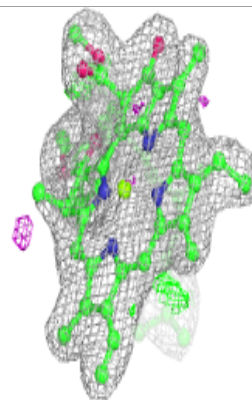
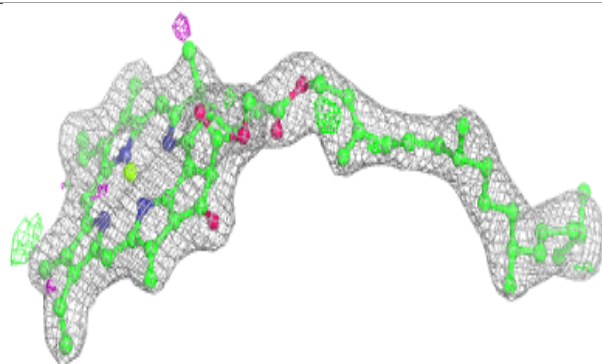
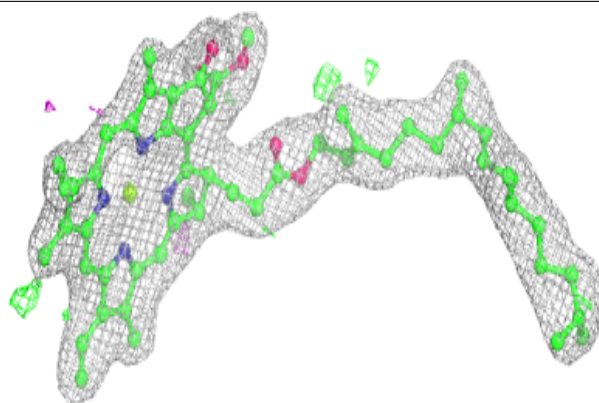
Electron density around PHO a 417:

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

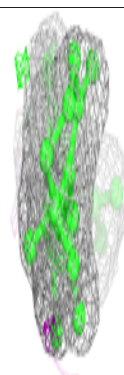
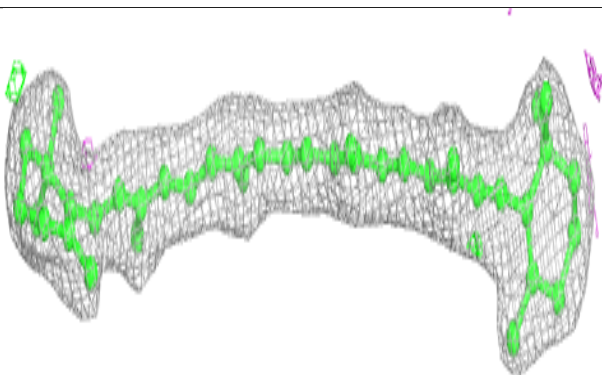
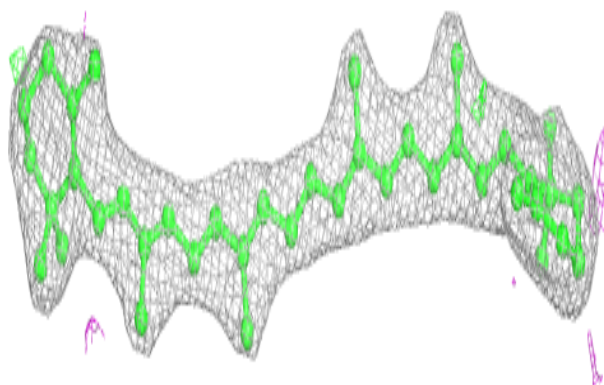


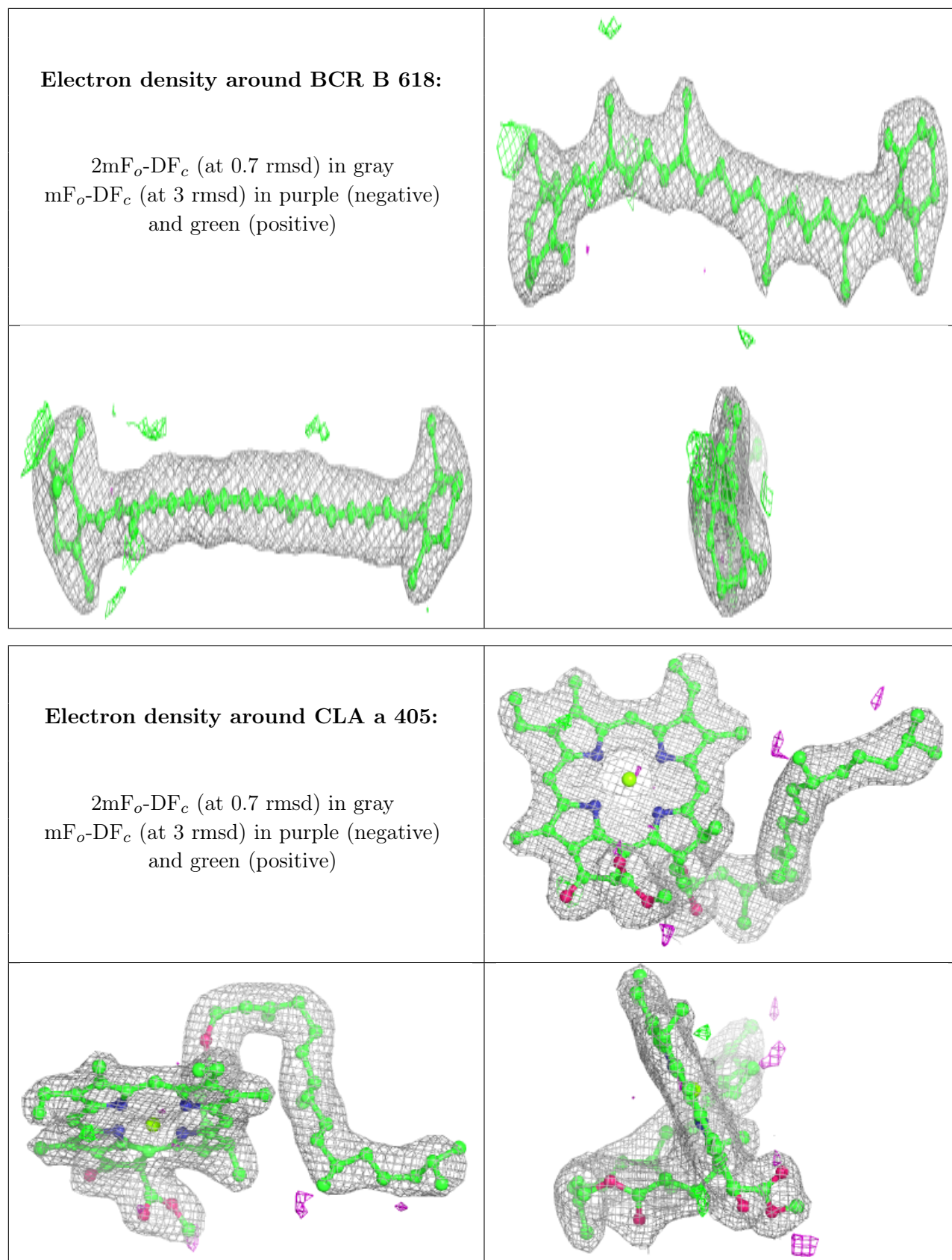
Electron density around CLA a 404:

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

**Electron density around BCR B 617:**

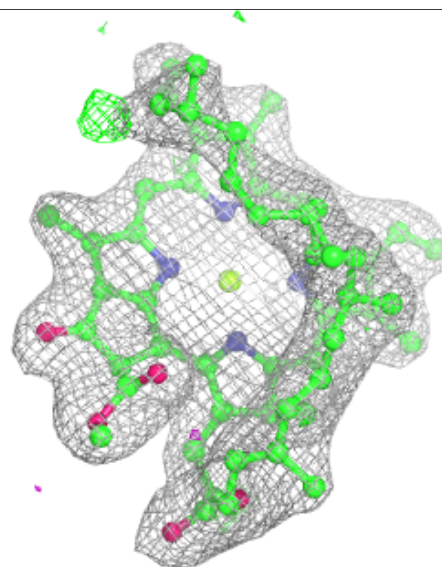
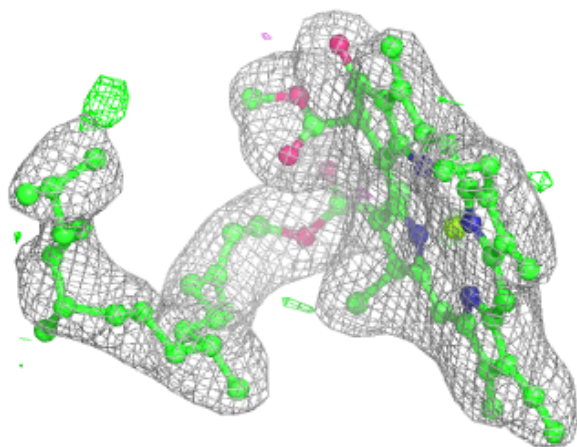
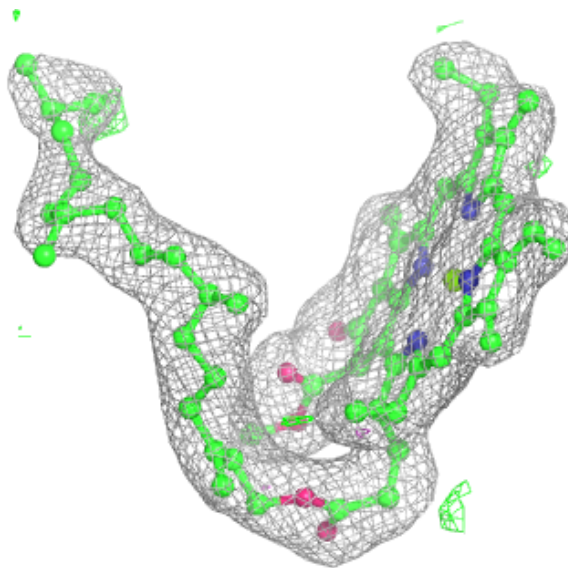
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

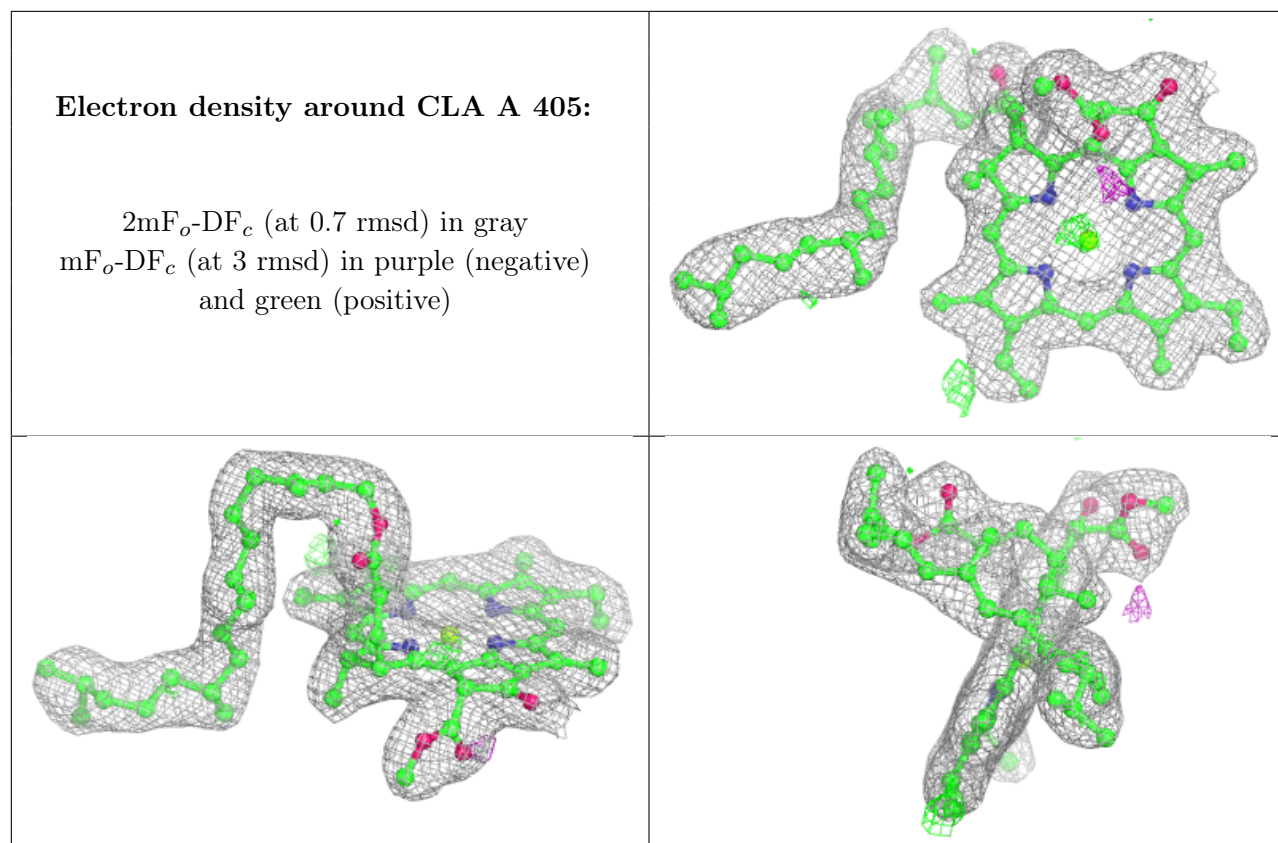




Electron density around CLA B 613:

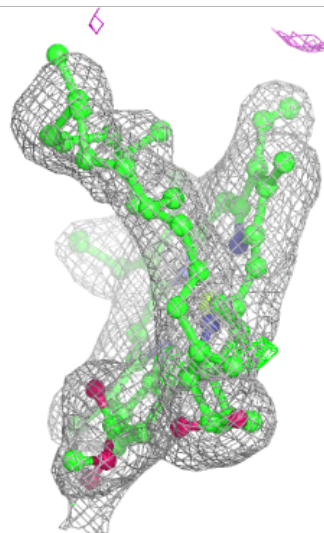
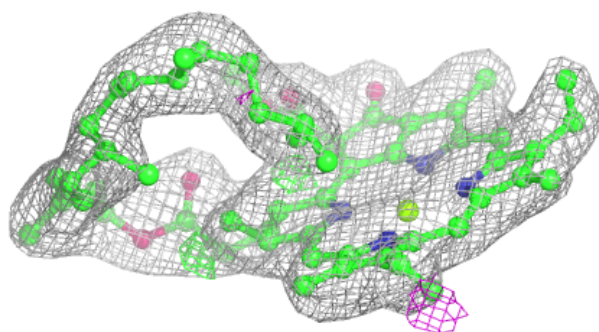
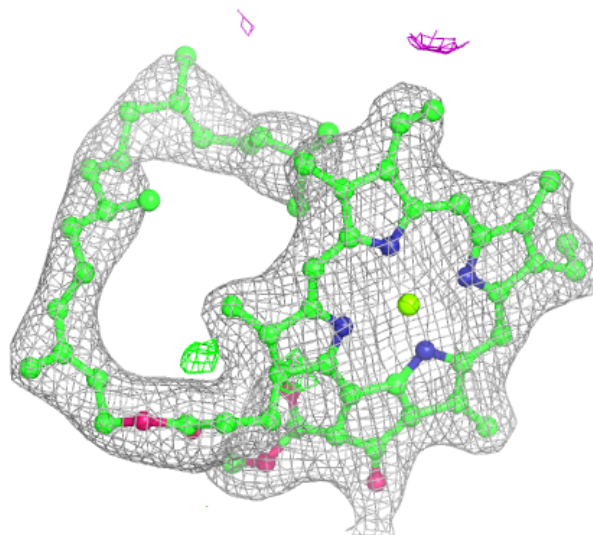
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





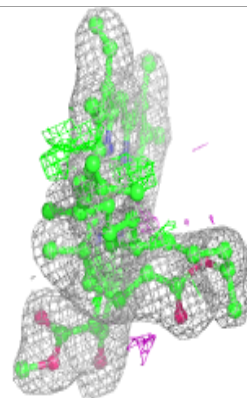
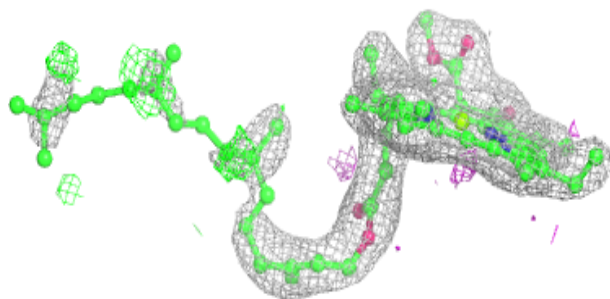
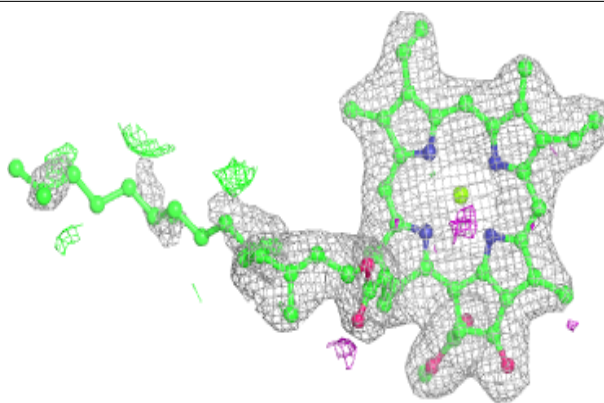
Electron density around CLA B 615:

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

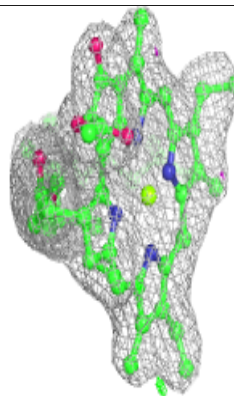
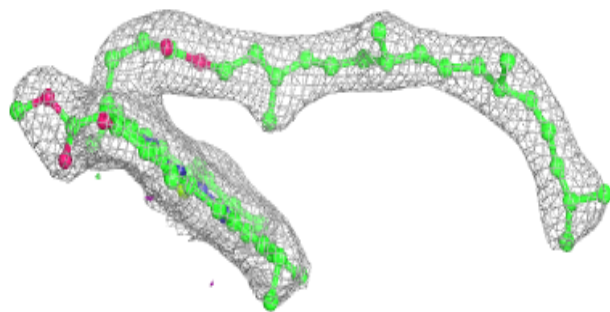
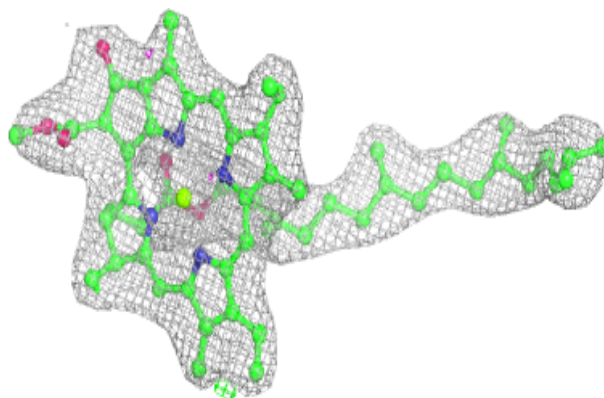


Electron density around CLA A 406:

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

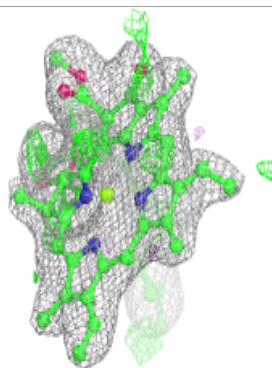
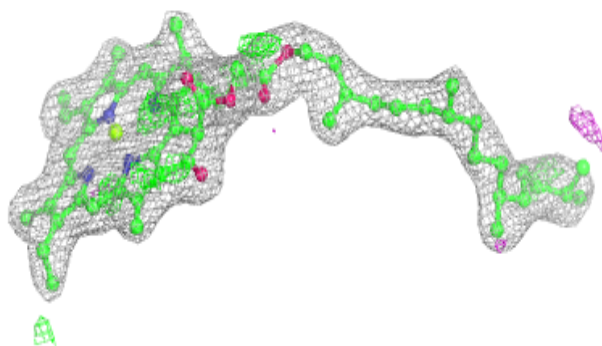
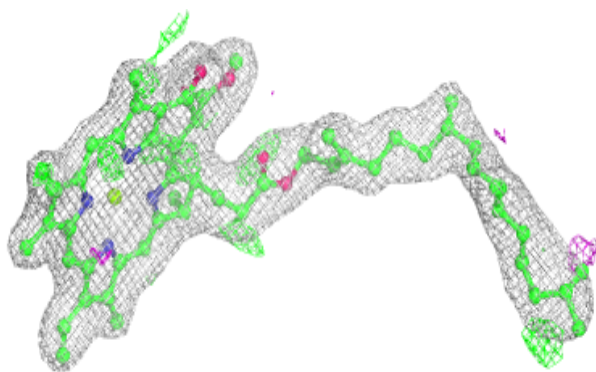
**Electron density around CLA B 608:**

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

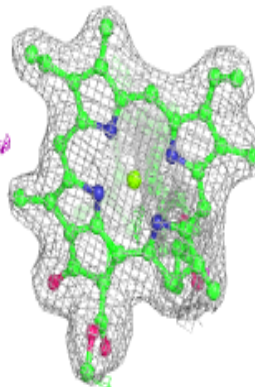
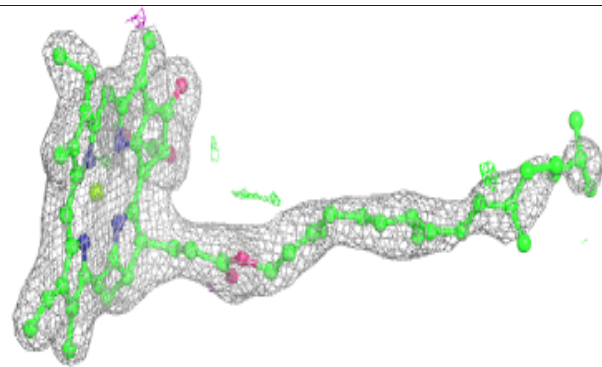
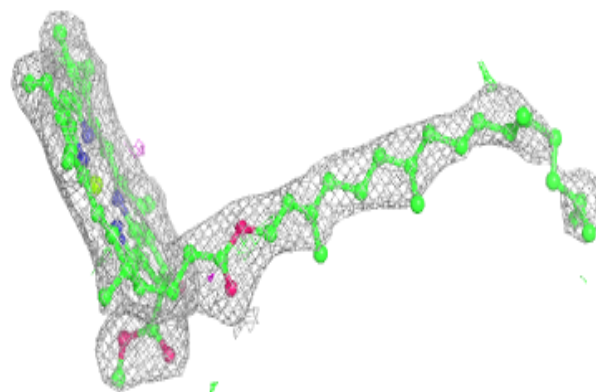


Electron density around CLA A 404:

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

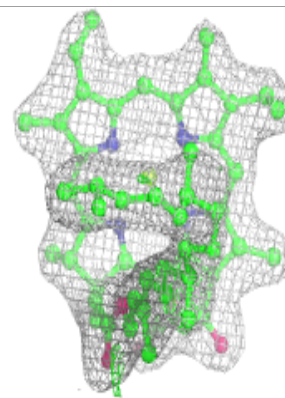
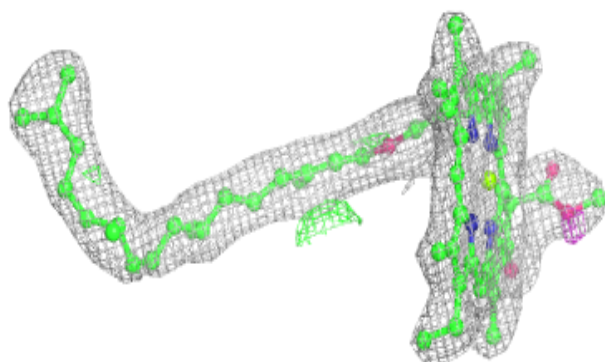
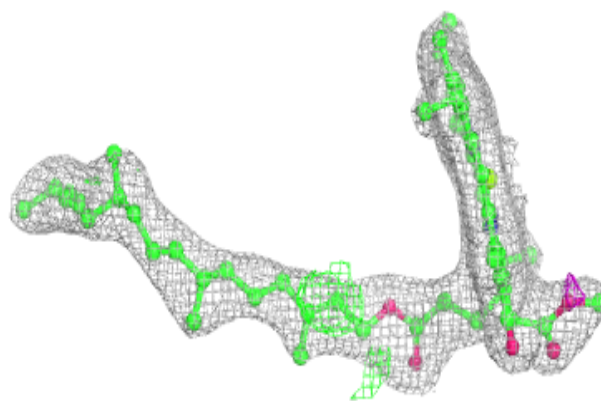
**Electron density around CLA B 604:**

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

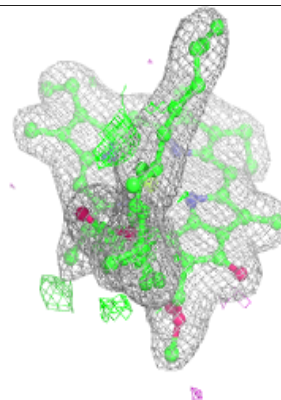
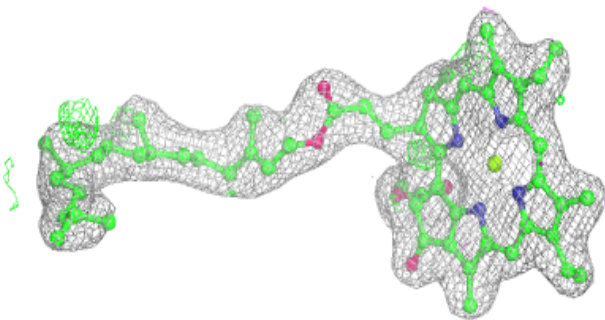
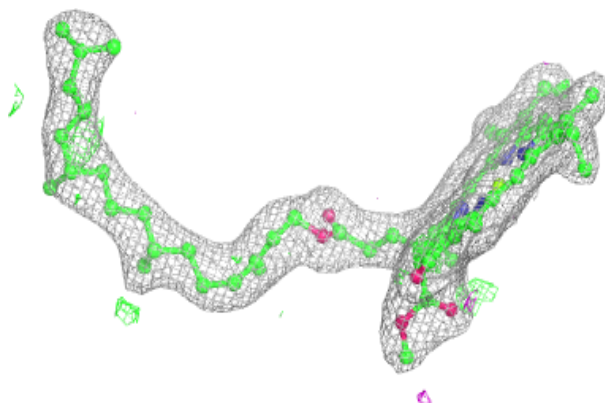


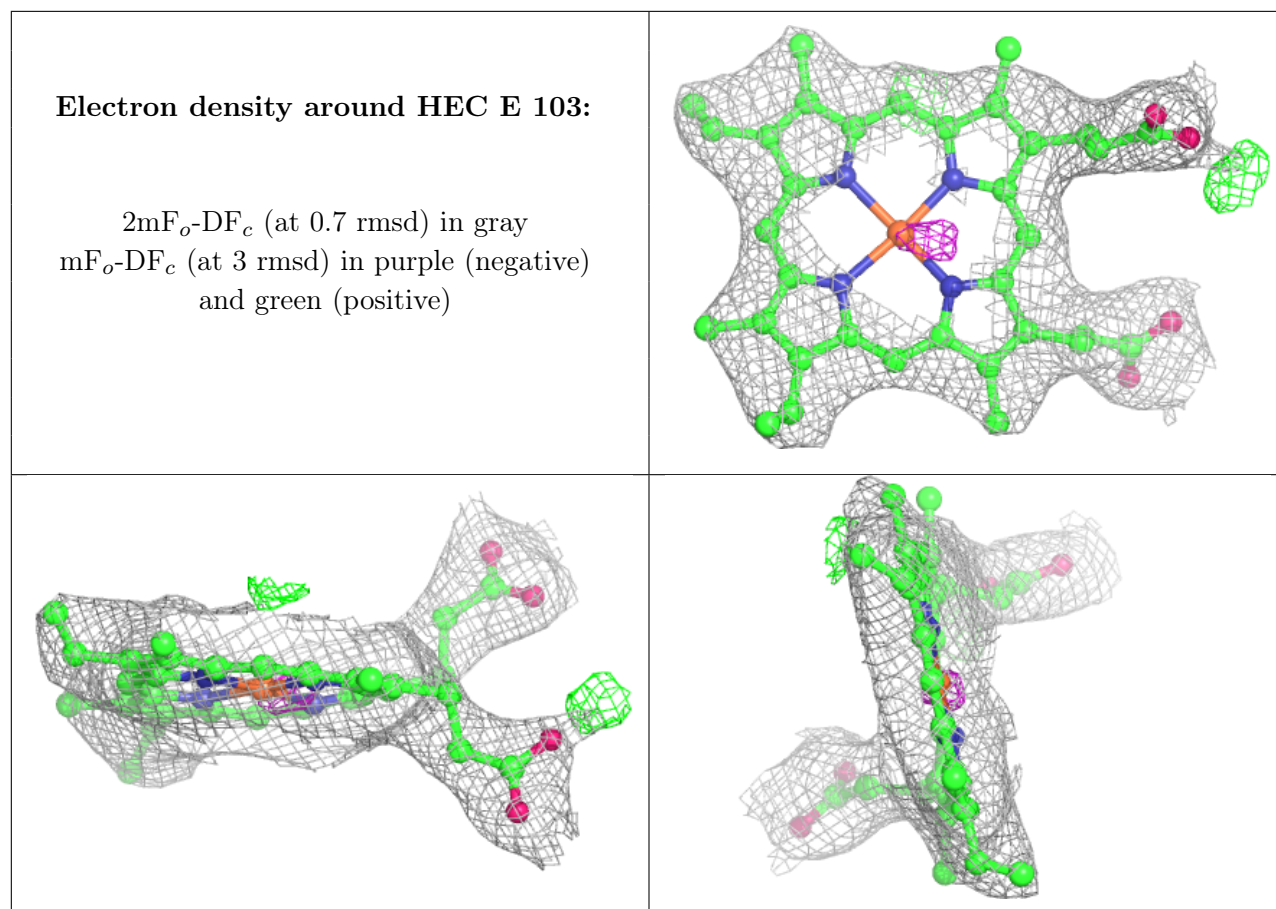
Electron density around CLA B 605:

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

**Electron density around CLA D 403:**

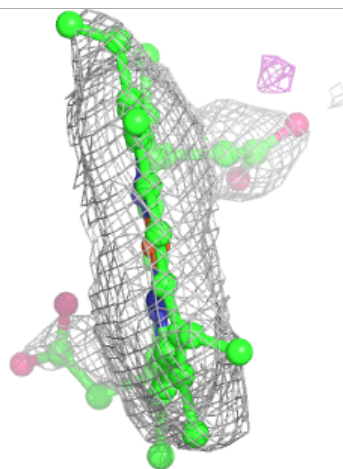
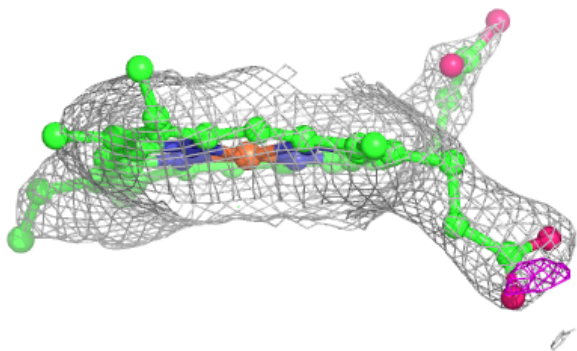
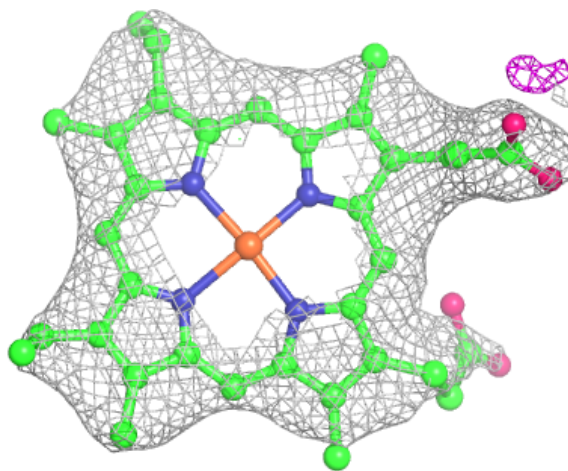
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





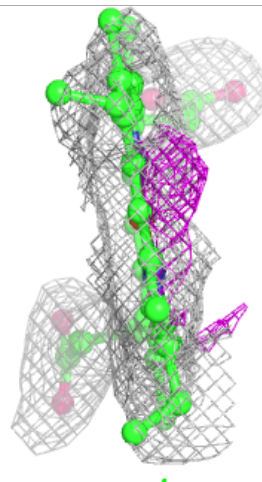
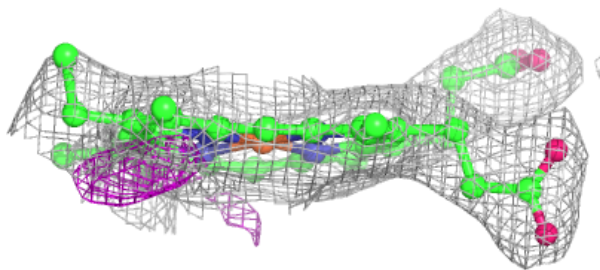
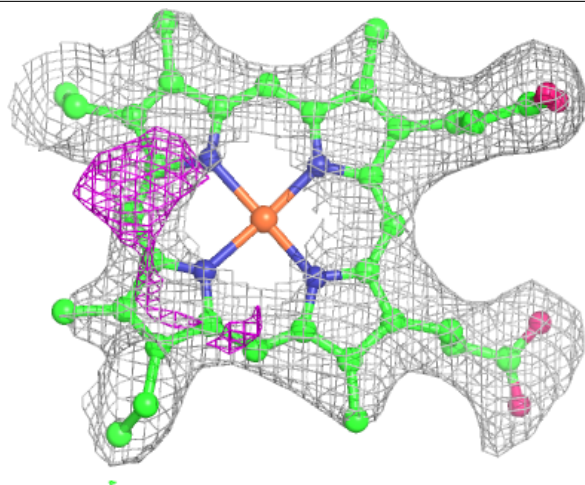
Electron density around HEC e 102:

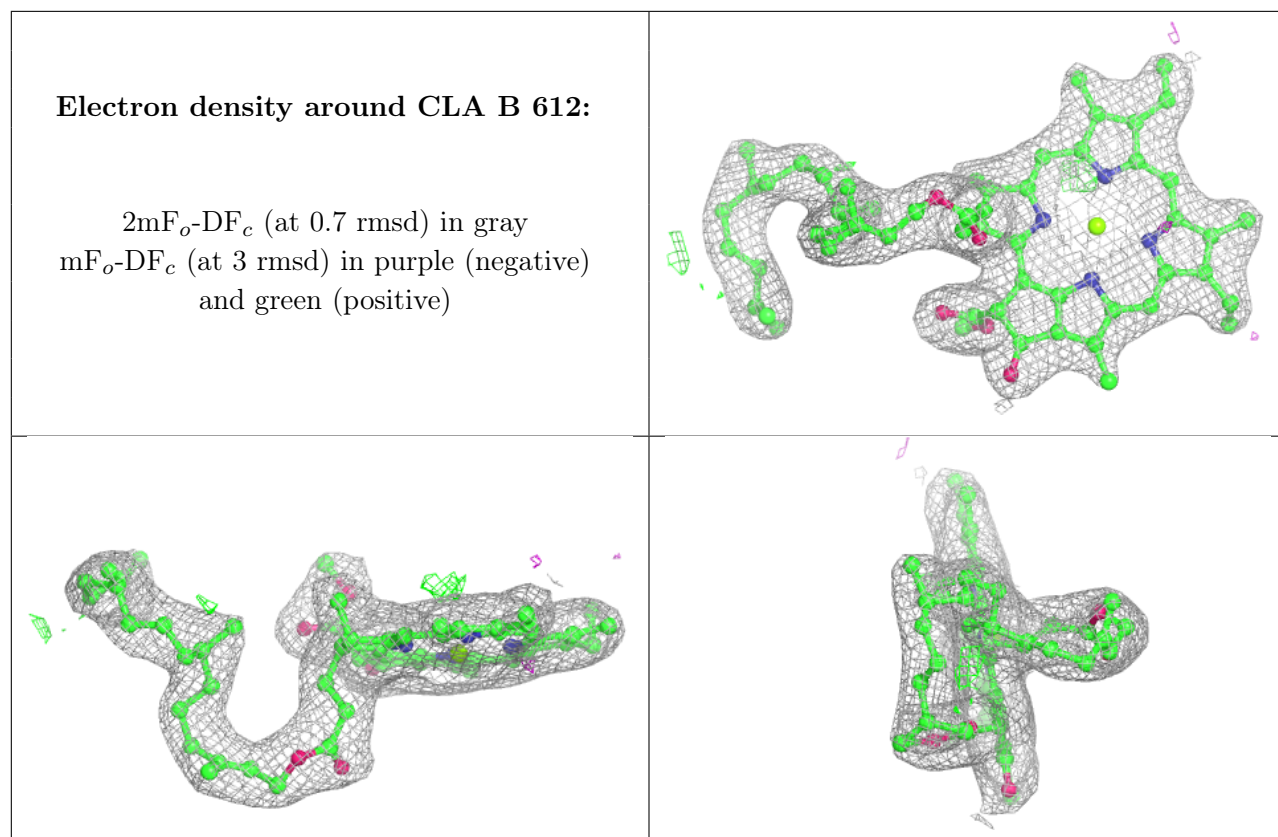
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC v 202:

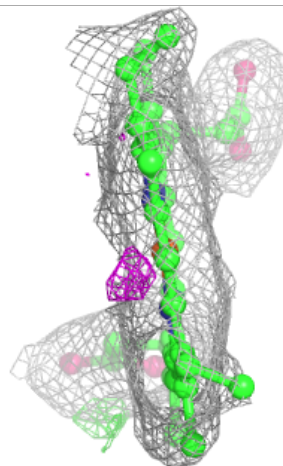
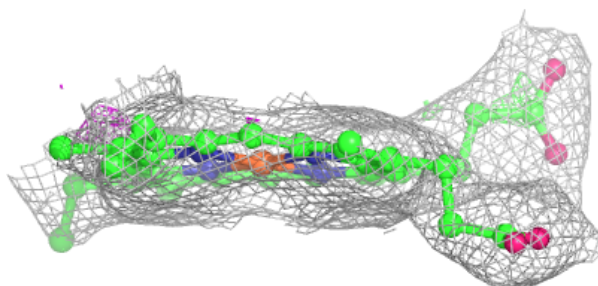
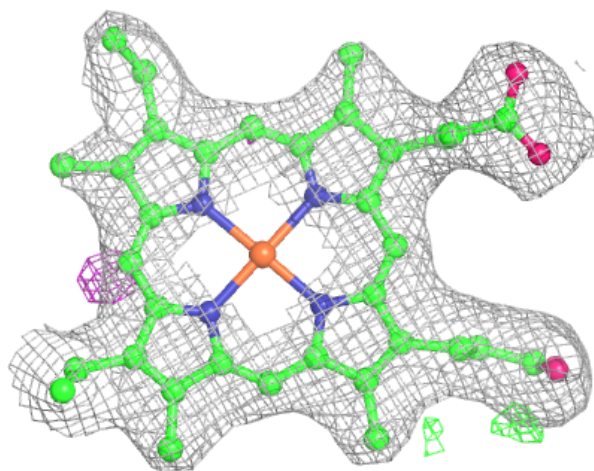
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

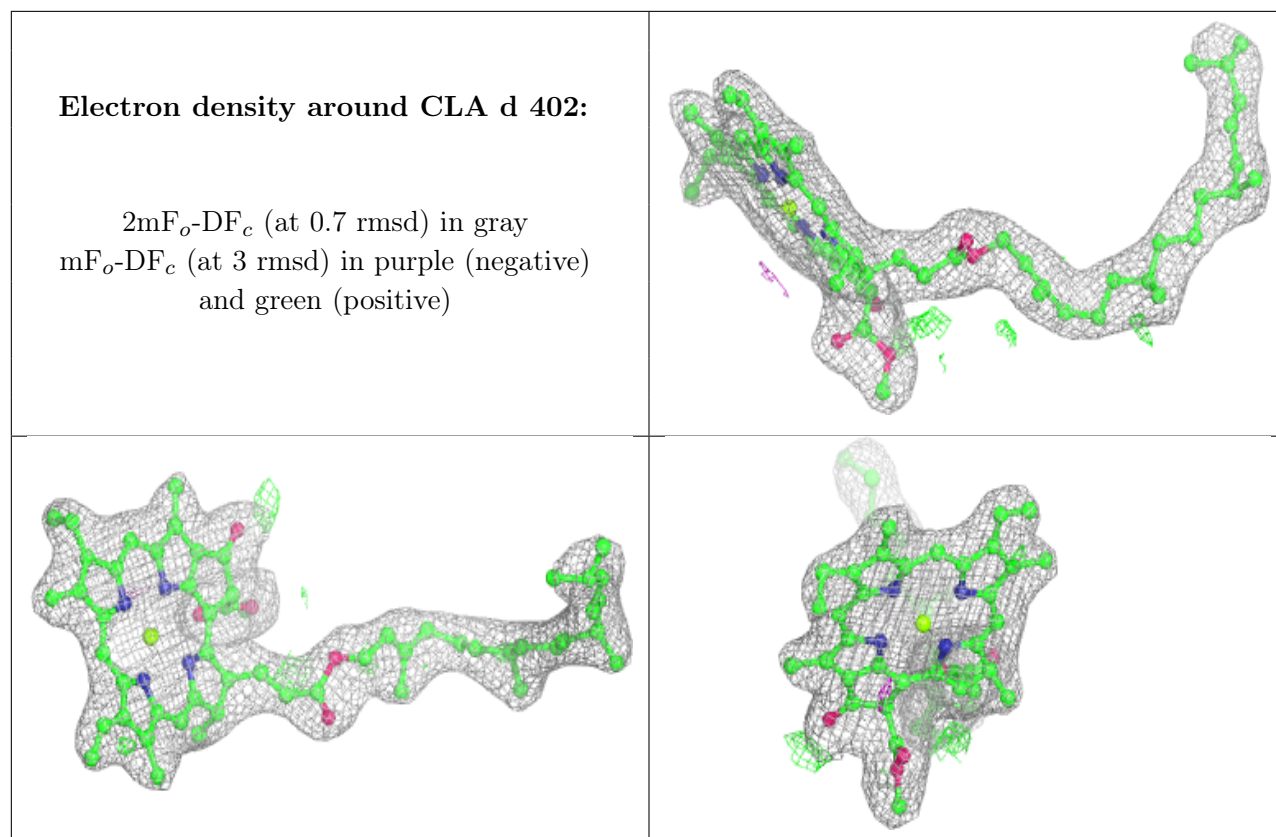




Electron density around HEC V 201:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.