



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 18, 2020 – 10:58 AM BST

PDB ID : 5WS5  
Title : Native XFEL structure of photosystem II (preflash dark dataset)  
Authors : Suga, M.; Shen, J.R.  
Deposited on : 2016-12-05  
Resolution : 2.35 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](mailto: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.

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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 : 2.13.1  
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) : 2.13.1

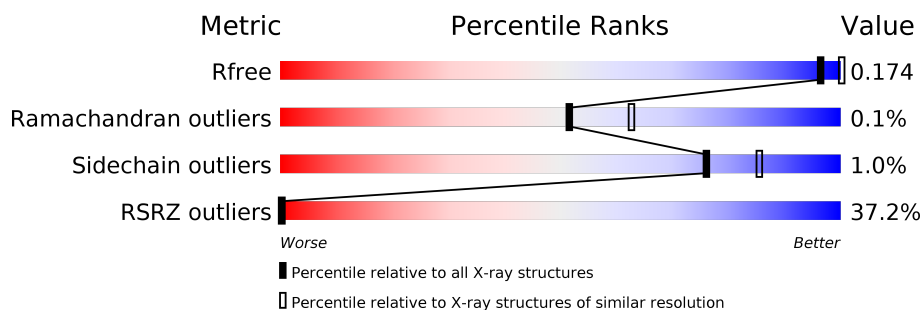
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>25%</div> <div>97%</div> </div>
1	a	344	<div> <div>33%</div> <div>96%</div> </div>
2	B	505	<div> <div>30%</div> <div>99%</div> </div>
2	b	505	<div> <div>35%</div> <div>99%</div> </div>
3	C	455	<div> <div>38%</div> <div>98%</div> </div>
3	c	455	<div> <div>39%</div> <div>99%</div> </div>
4	D	342	<div> <div>27%</div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	
16	v	137	

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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	406	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	608	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	X
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	D	405	X	-	-	-
23	CLA	D	406	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	406	X	-	-	-
23	CLA	a	407	X	-	-	-
23	CLA	a	409	X	-	-	-
23	CLA	b	601	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	514	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-
26	SQD	A	412	-	-	-	X
26	SQD	B	620	-	-	-	X
26	SQD	a	413	-	-	-	X
26	SQD	b	620	-	-	-	X
26	SQD	f	102	-	-	-	X
27	GOL	v	201	-	-	-	X
29	PL9	A	414	-	-	-	X
29	PL9	a	416	-	-	-	X
30	UNL	A	415	-	-	-	X
30	UNL	B	627	-	-	-	X
30	UNL	D	413	-	-	-	X
30	UNL	I	102	-	-	-	X
30	UNL	J	101	-	-	-	X
30	UNL	K	101	-	-	-	X
30	UNL	M	102	-	-	-	X
30	UNL	b	626	-	-	-	X
30	UNL	d	409	-	-	-	X
30	UNL	d	410	-	-	-	X
30	UNL	i	101	-	-	-	X
30	UNL	j	101	-	-	-	X
30	UNL	m	102	-	-	-	X
32	LMT	A	359	-	-	-	X
32	LMT	D	404	-	-	-	X
32	LMT	E	102	-	-	-	X
32	LMT	I	101	-	-	-	X
32	LMT	M	101	-	-	-	X
32	LMT	M	103	-	-	-	X
32	LMT	a	414	-	-	-	X
32	LMT	a	420	-	-	-	X
32	LMT	b	621	-	-	-	X
32	LMT	b	627	-	-	-	X
32	LMT	e	102	-	-	-	X
32	LMT	m	103	-	-	-	X
32	LMT	t	101	-	-	-	X
33	LMG	B	621	-	-	-	X
33	LMG	C	501	-	-	-	X
33	LMG	C	521	-	-	-	X
33	LMG	Z	101	-	-	-	X
33	LMG	a	419	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	LMG	c	521	-	-	-	X
33	LMG	z	101	-	-	-	X
34	HTG	D	414	-	-	-	X
34	HTG	b	623	-	-	-	X
34	HTG	c	522	-	-	-	X
34	HTG	d	411	-	-	-	X
35	DGD	H	102	-	-	-	X
35	DGD	h	102	-	-	-	X
37	LHG	D	409	-	-	-	X
37	LHG	E	101	-	-	-	X
37	LHG	e	101	-	-	-	X

## 2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 52545 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 D1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	3	0
			2634	1728	432	459	15			
1	a	334	Total	C	N	O	S	0	4	0
			2636	1730	431	460	15			

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	8	0
			4007	2630	664	700	13			
2	b	504	Total	C	N	O	S	0	4	0
			3986	2618	661	694	13			

- Molecule 3 is a protein called Photosystem II CP43 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	4	0
			3501	2291	584	613	13			
3	c	455	Total	C	N	O	S	0	4	0
			3536	2316	589	618	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	1	0
			2729	1807	445	465	12			
4	d	341	Total	C	N	O	S	0	1	0
			2720	1802	444	462	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	1	0
			665	434	107	124			
5	e	79	Total	C	N	O	0	0	0
			648	424	105	119			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	1	0
			514	344	84	84	2			
7	h	64	Total	C	N	O	S	0	0	0
			506	339	81	84	2			

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	36	Total	C	N	O	0	1	0
			301	202	47	52			
11	l	36	Total	C	N	O	0	1	0
			301	202	47	52			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			265	178	38	48	1			
12	m	34	Total	C	N	O	S	0	0	0
			269	179	40	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	4	0
			1883	1178	315	385	5			
13	o	243	Total	C	N	O	S	0	2	0
			1873	1171	315	382	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	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
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
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
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
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		

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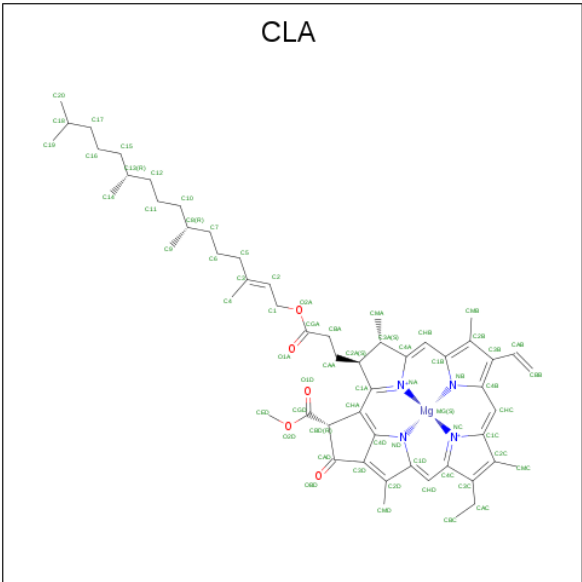
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	a	1	Total	Fe	0	0
			1	1		

- 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: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

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

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

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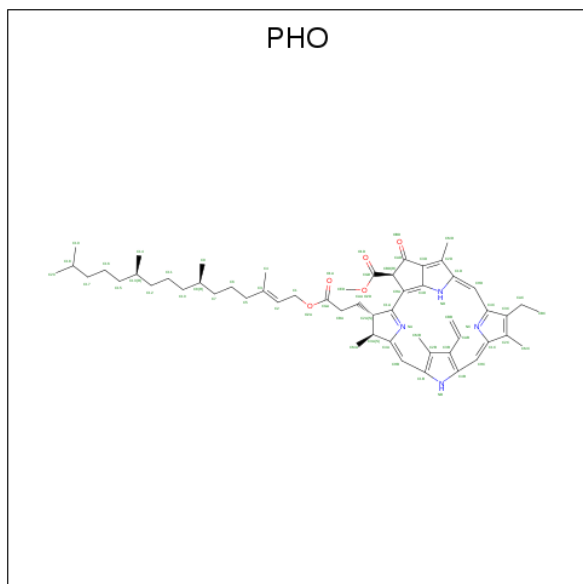
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N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

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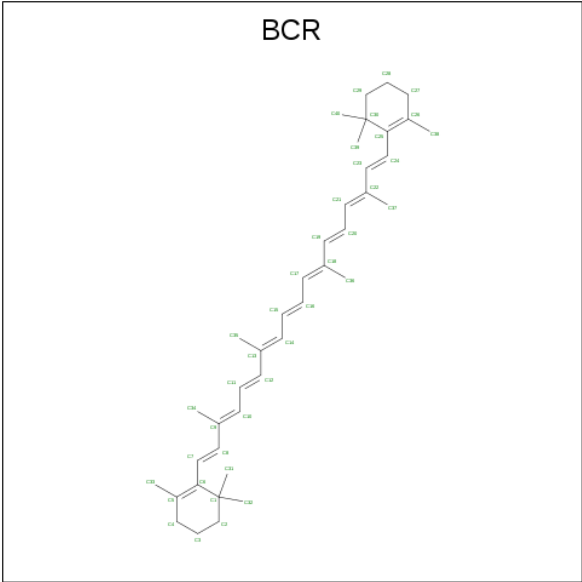
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



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

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



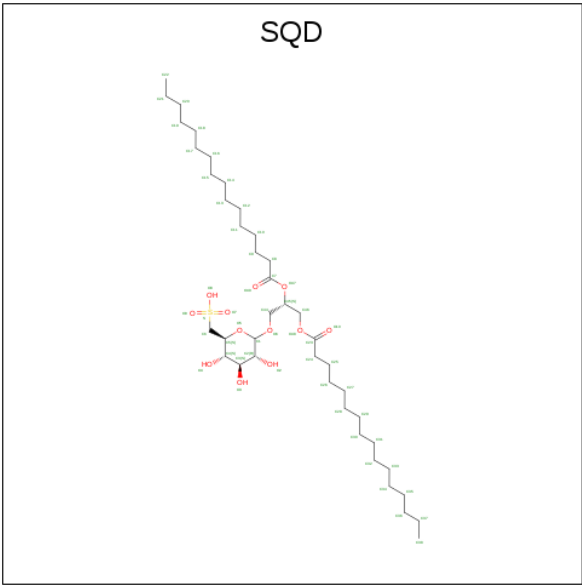
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total C 40 40	0	0
25	a	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	b	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	d	1	Total C 40 40	0	0
25	h	1	Total C 40 40	0	0
25	k	1	Total C 40 40	0	0
25	t	1	Total C 40 40	0	0
25	y	1	Total C 40 40	0	0

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O S 54 41 12 1	0	0
26	A	1	Total C O S 54 41 12 1	0	0
26	B	1	Total C O S 54 41 12 1	0	0

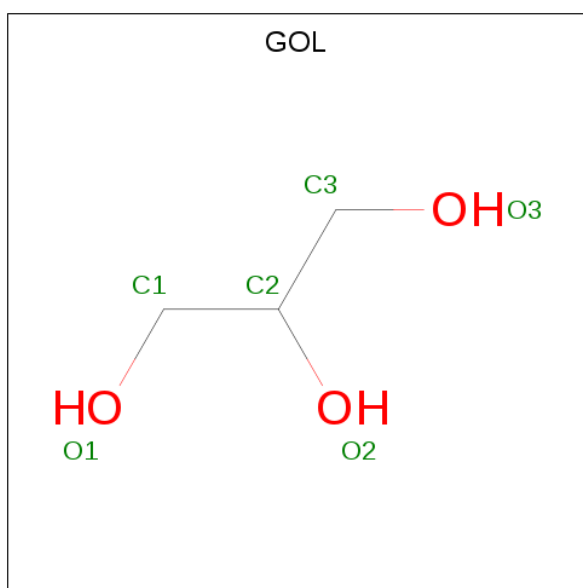
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	F	1	Total	C	O	S	0	0
			43	30	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	b	1	Total	C	O	S	0	0
			54	41	12	1		
26	f	1	Total	C	O	S	0	0
			43	30	12	1		

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



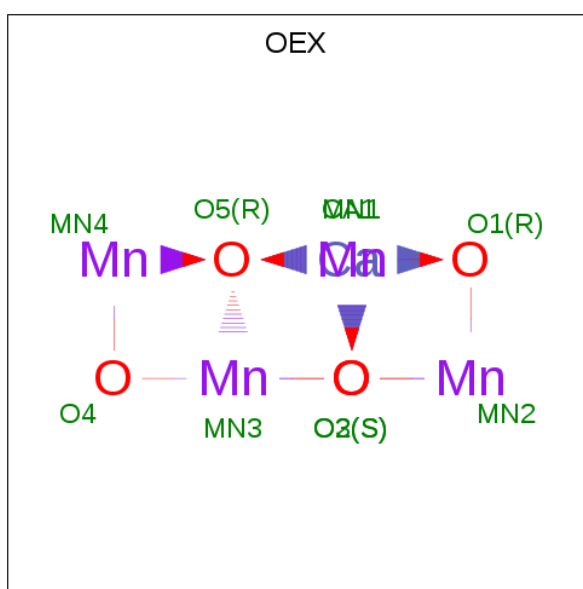
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	0
			6	3	3		
27	V	1	Total	C	O	0	0
			6	3	3		
27	a	1	Total	C	O	0	0
			6	3	3		

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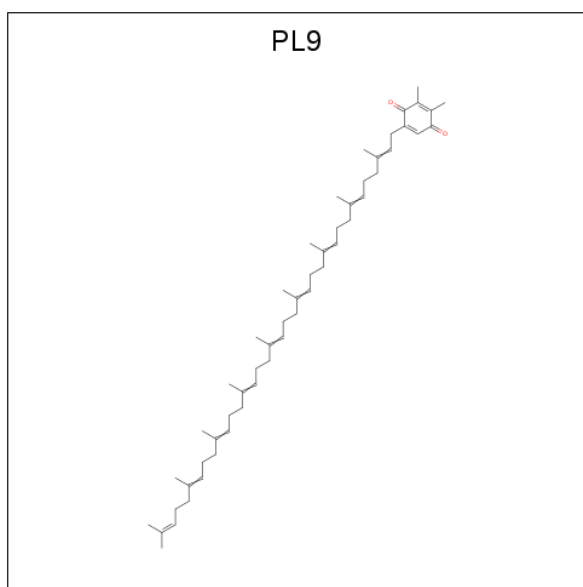
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	a	1	Total	C	O	0	0
			6	3	3		
27	b	1	Total	C	O	0	0
			6	3	3		
27	c	1	Total	C	O	0	0
			6	3	3		
27	v	1	Total	C	O	0	0
			6	3	3		

- Molecule 28 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



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

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:  $\text{C}_{53}\text{H}_{80}\text{O}_2$ ).



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: ).

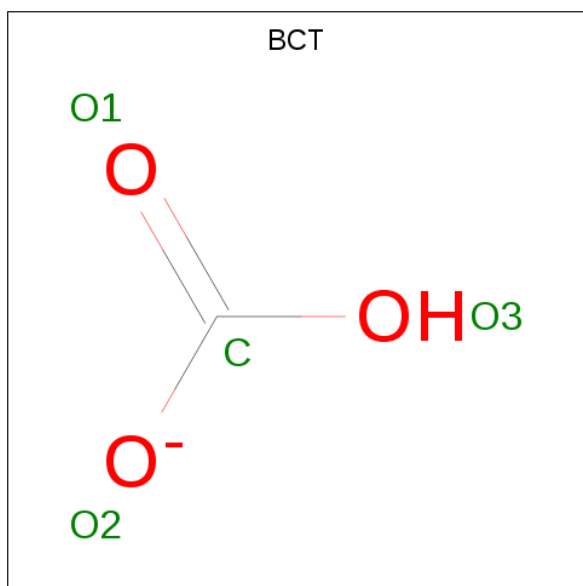
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	J	1	Total	C		0	0
			10	10			
30	i	1	Total	C	O	0	0
			40	35	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	K	1	Total	C	O	0	0
			34	29	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	I	1	Total	C	O	0	0
			40	35	5		
30	c	1	Total	C	O	0	0
			32	27	5		
30	a	1	Total	C	O	0	0
			30	25	5		

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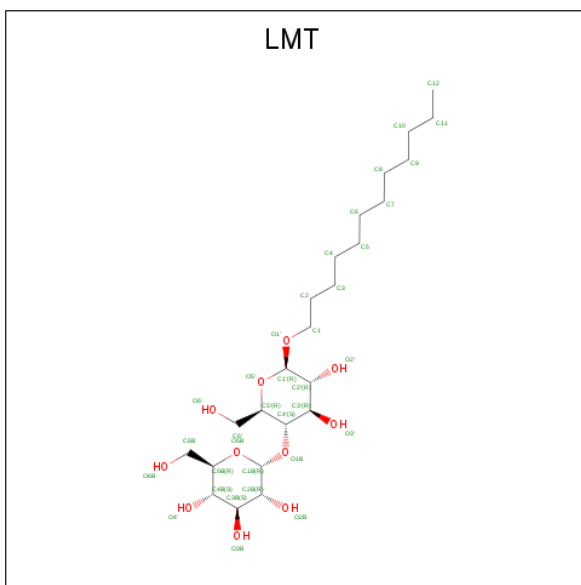
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	x	1	Total C O 18 16 2	0	0
30	A	1	Total C O 28 23 5	0	0
30	j	1	Total C 10 10	0	0
30	X	1	Total C O 18 16 2	0	0
30	d	2	Total C O 53 47 6	0	0
30	m	1	Total C 10 10	0	0
30	b	1	Total C O 33 28 5	0	0
30	M	1	Total C 10 10	0	0

- Molecule 31 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



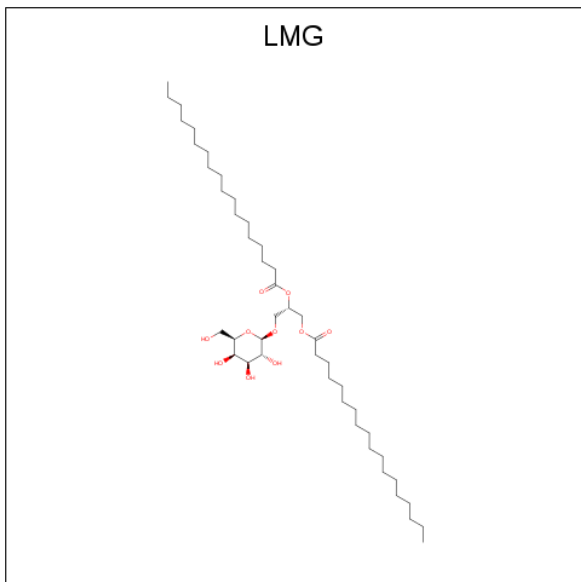
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C O 4 1 3	0	0
31	a	1	Total C O 4 1 3	0	0

- Molecule 32 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula:  $\text{C}_{24}\text{H}_{46}\text{O}_{11}$ ).



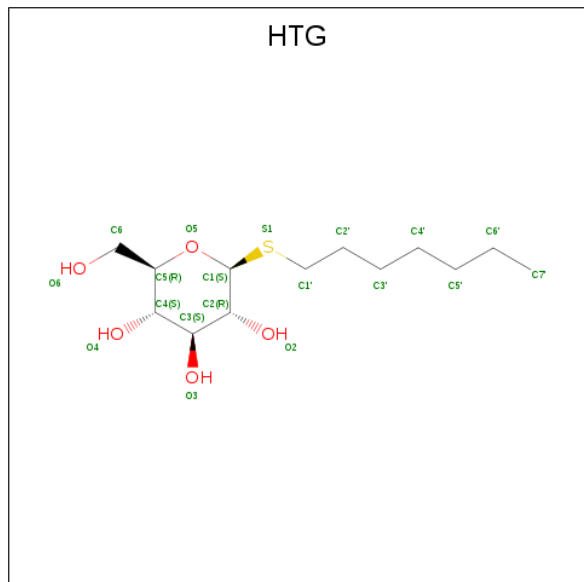
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total 35	C 24	O 11	0	0
32	D	1	Total 35	C 24	O 11	0	0
32	E	1	Total 35	C 24	O 11	0	0
32	I	1	Total 35	C 24	O 11	0	0
32	M	1	Total 35	C 24	O 11	0	0
32	M	1	Total 35	C 24	O 11	0	0
32	a	1	Total 35	C 24	O 11	0	0
32	a	1	Total 35	C 24	O 11	0	0
32	b	1	Total 25	C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

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



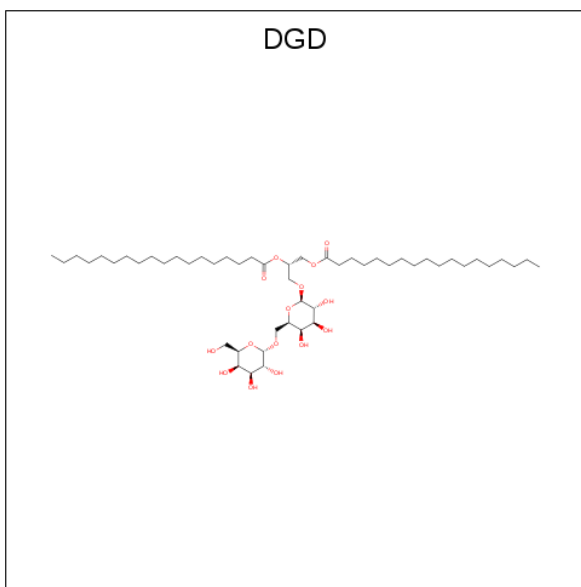
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	B	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	D	1	Total	C	O	0	0
			51	41	10		
33	Z	1	Total	C	O	0	0
			37	27	10		
33	a	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total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

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



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

- 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	c	2	Total	Ca	0	0
			2	2		
36	F	1	Total	Ca	0	0
			1	1		
36	O	1	Total	Ca	0	0
			1	1		

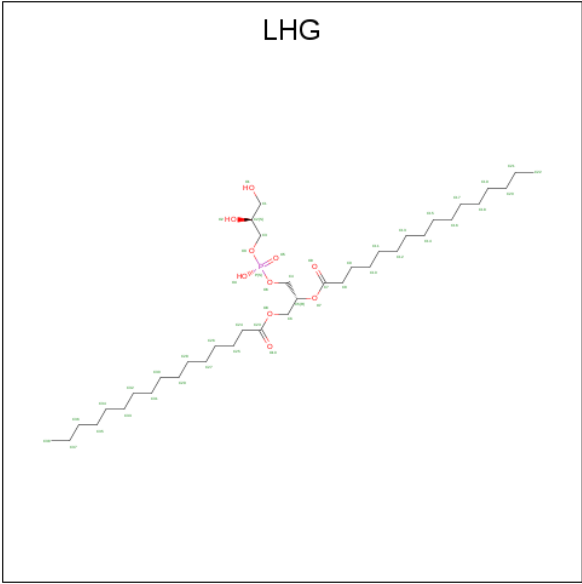
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	o	1	Total	Ca	0	0
			1	1		
36	f	1	Total	Ca	0	0
			1	1		

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



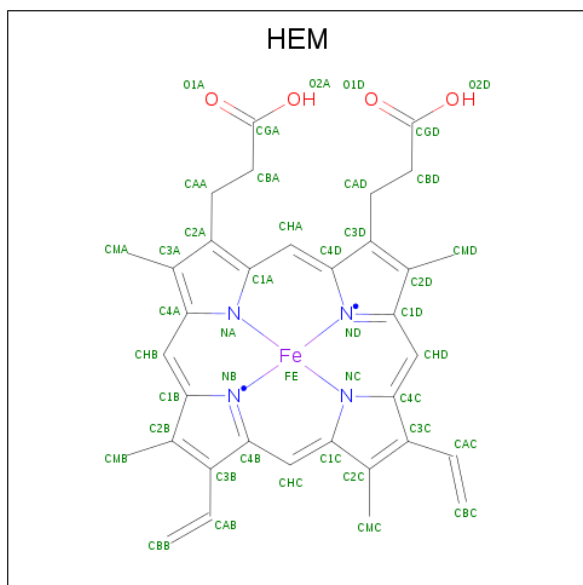
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	E	1	Total	C	O	P	0	0
			42	31	10	1		
37	L	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	1	1	Total	C	O	P	0	0
			49	38	10	1		

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

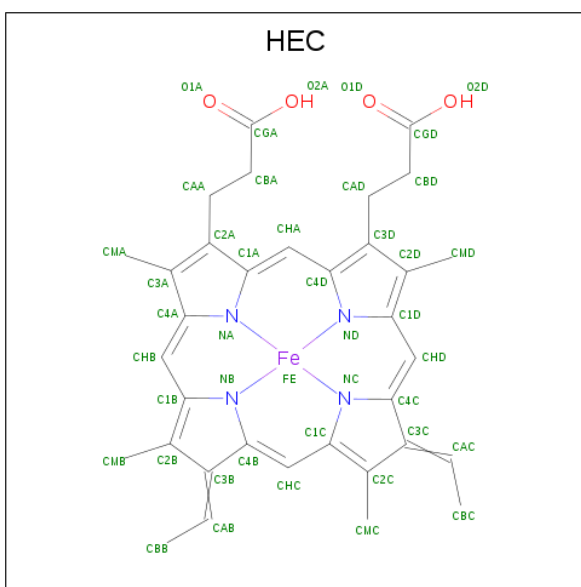


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
38	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	A	130	Total O 130 130	0	0
41	B	167	Total O 167 167	0	0
41	C	144	Total O 144 144	0	0
41	D	122	Total O 122 122	0	0
41	E	15	Total O 15 15	0	0
41	F	4	Total O 4 4	0	0
41	H	19	Total O 19 19	0	0
41	I	6	Total O 6 6	0	0
41	J	5	Total O 5 5	0	0
41	K	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	L	3	Total 3	O 3	0	0
41	M	7	Total 7	O 7	0	0
41	O	71	Total 71	O 71	0	0
41	T	9	Total 9	O 9	0	0
41	U	32	Total 32	O 32	0	0
41	V	67	Total 67	O 67	0	0
41	X	1	Total 1	O 1	0	0
41	Y	1	Total 1	O 1	0	0
41	a	133	Total 133	O 133	0	0
41	b	193	Total 193	O 193	0	0
41	c	142	Total 142	O 142	0	0
41	d	114	Total 114	O 114	0	0
41	e	8	Total 8	O 8	0	0
41	f	4	Total 4	O 4	0	0
41	h	16	Total 16	O 16	0	0
41	i	3	Total 3	O 3	0	0
41	j	2	Total 2	O 2	0	0
41	k	3	Total 3	O 3	0	0
41	l	4	Total 4	O 4	0	0
41	m	15	Total 15	O 15	0	0
41	o	77	Total 77	O 77	0	0

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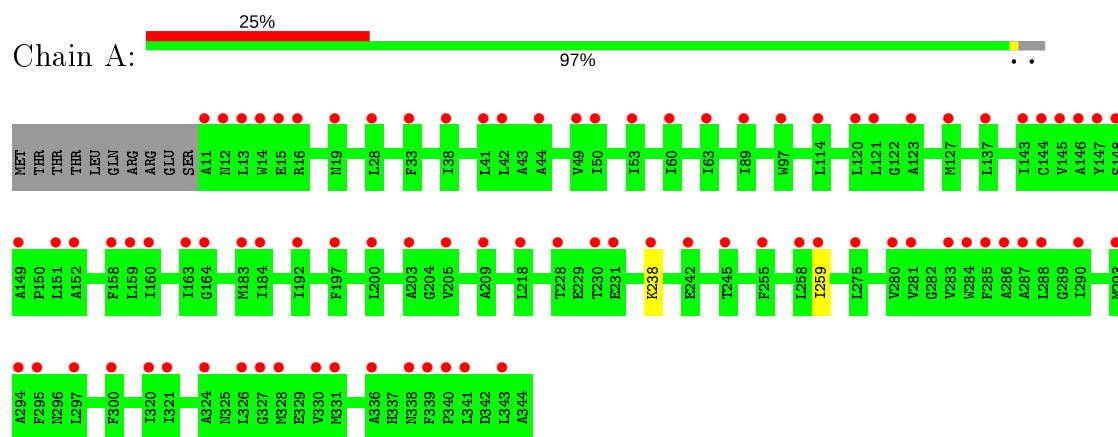
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	t	6	Total 6	O 6	0	0
41	u	47	Total 47	O 47	0	0
41	v	47	Total 47	O 47	0	0
41	x	2	Total 2	O 2	0	0
41	y	1	Total 1	O 1	0	0

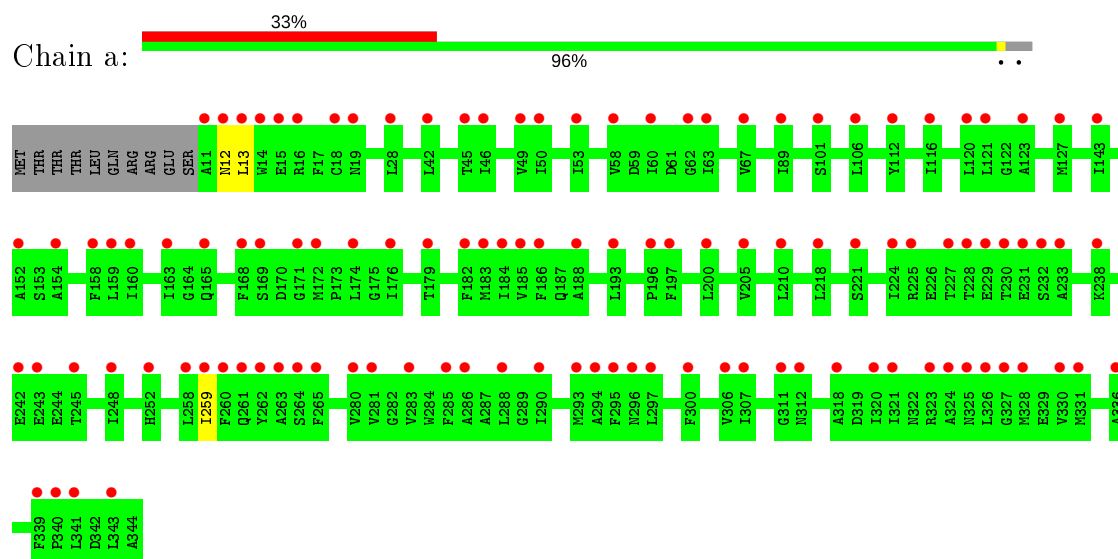
### 3 Residue-property plots [i](#)

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 D1 protein

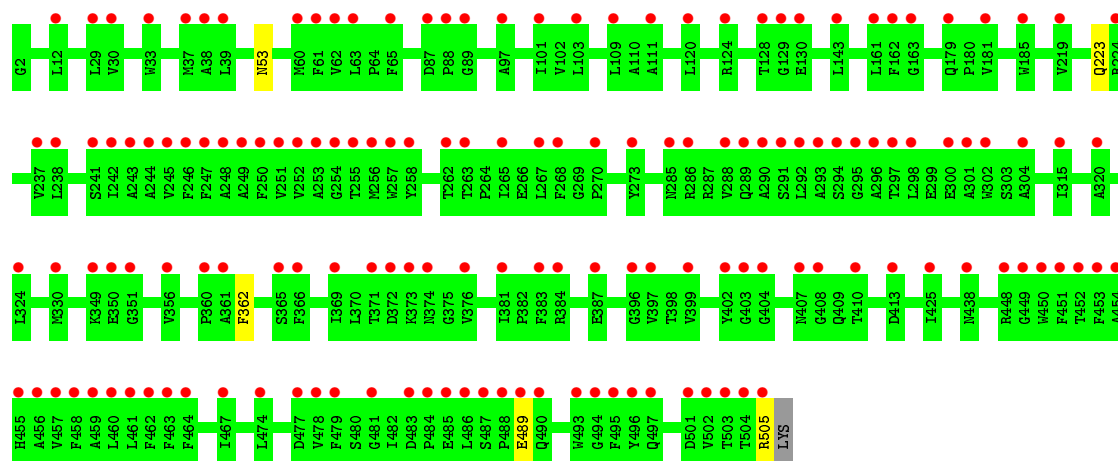


- Molecule 1: Photosystem II D1 protein

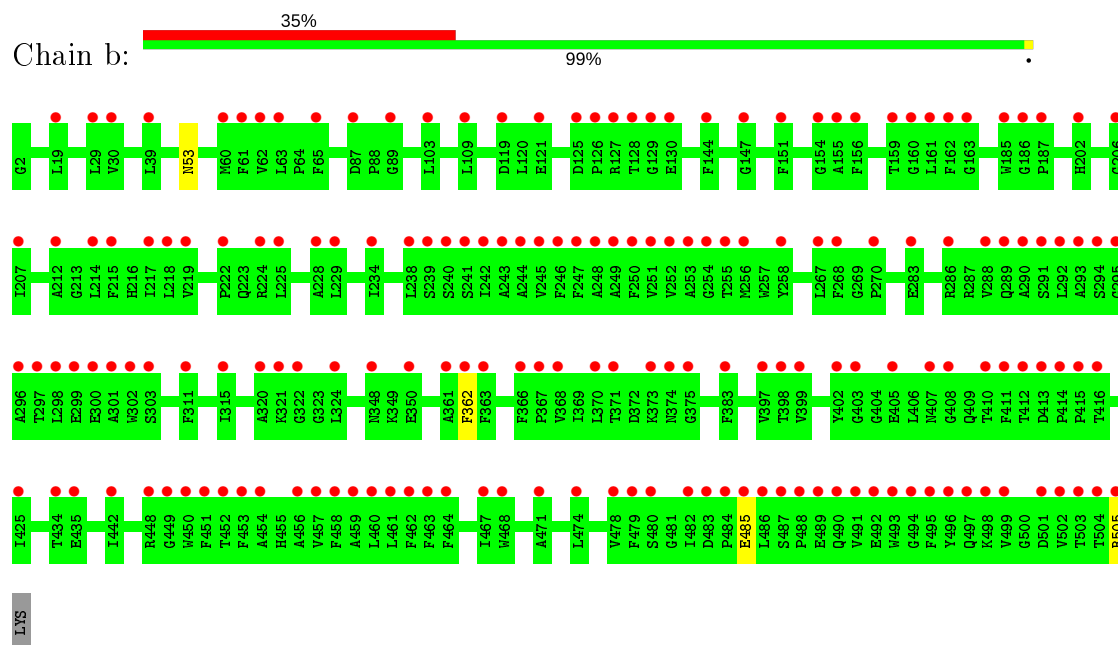


- Molecule 2: Photosystem II CP47 reaction center protein

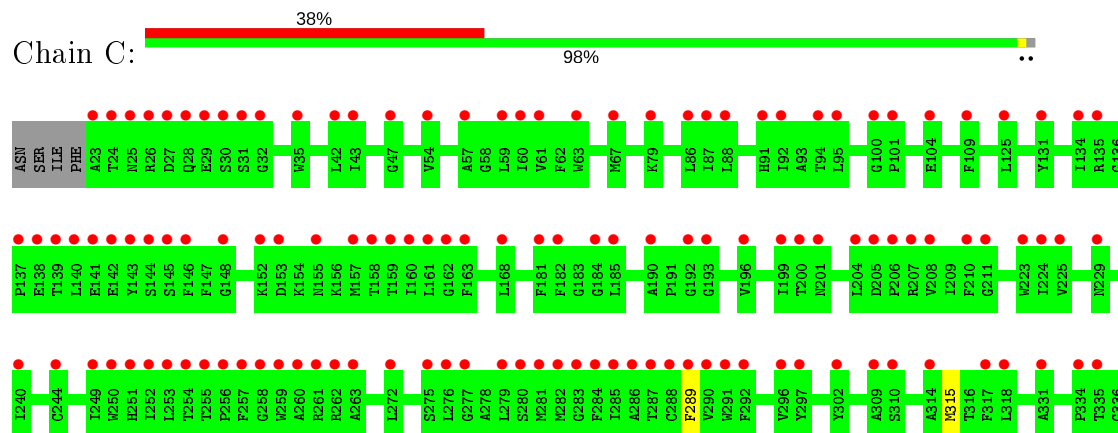


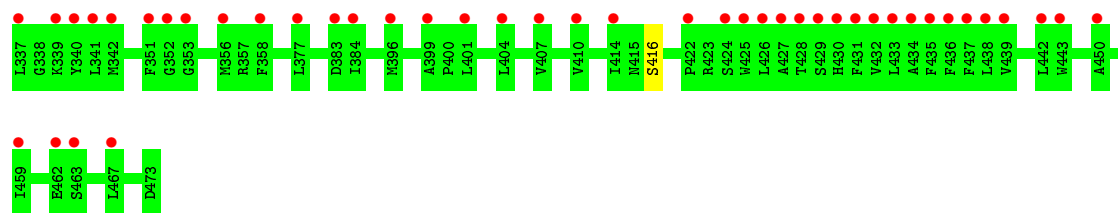


• Molecule 2: Photosystem II CP47 reaction center protein

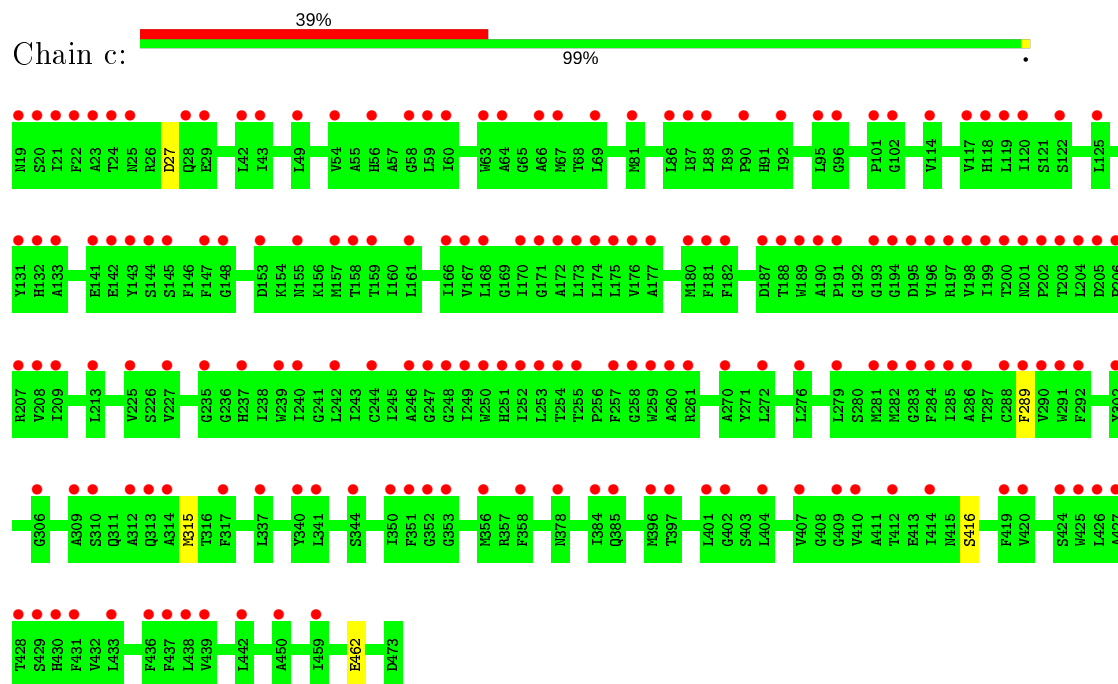


• Molecule 3: Photosystem II CP43 protein

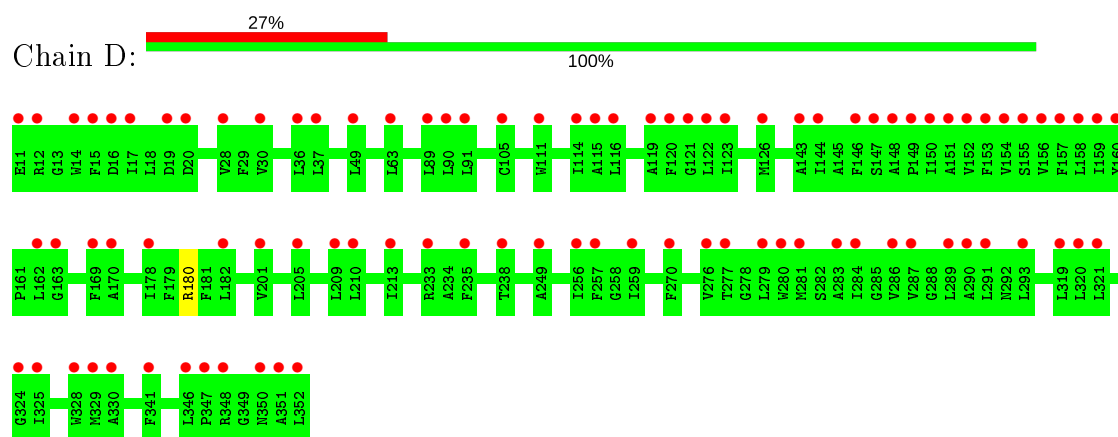




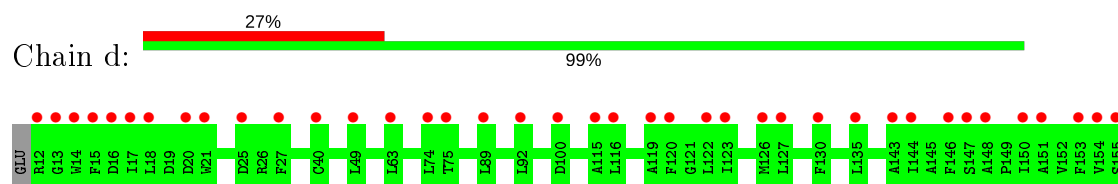
• Molecule 3: Photosystem II CP43 protein



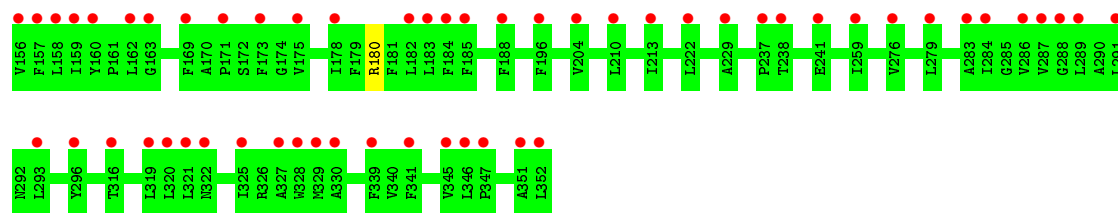
• Molecule 4: Photosystem II D2 protein



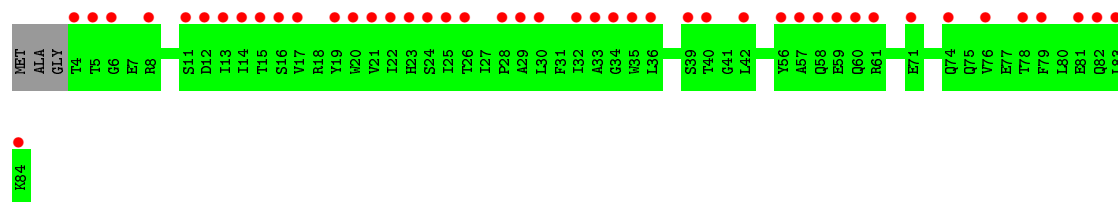
• Molecule 4: Photosystem II D2 protein



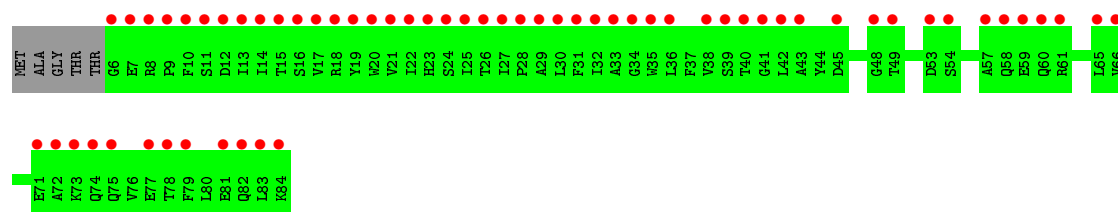
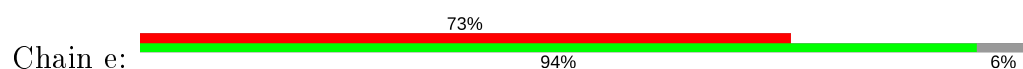




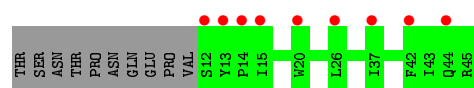
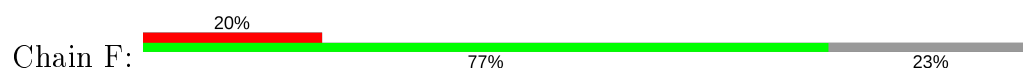
• Molecule 5: Cytochrome b559 subunit alpha



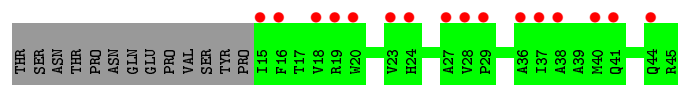
• Molecule 5: Cytochrome b559 subunit alpha



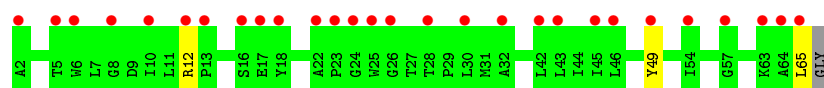
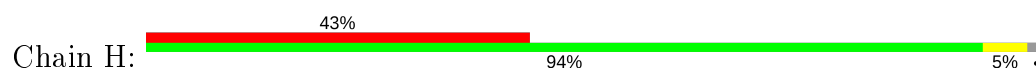
• Molecule 6: Cytochrome b559 subunit beta



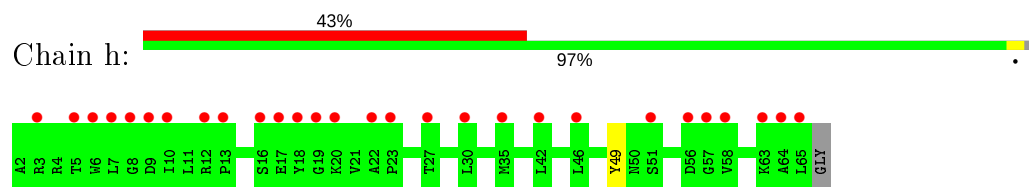
• Molecule 6: Cytochrome b559 subunit beta



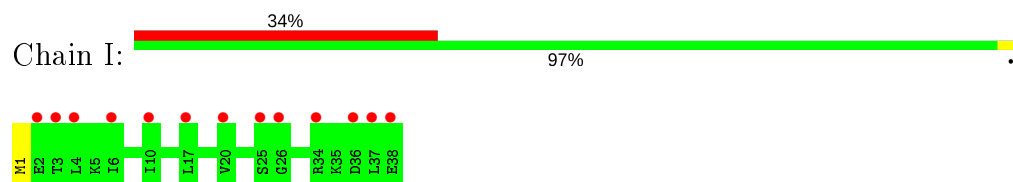
• Molecule 7: Photosystem II reaction center protein H



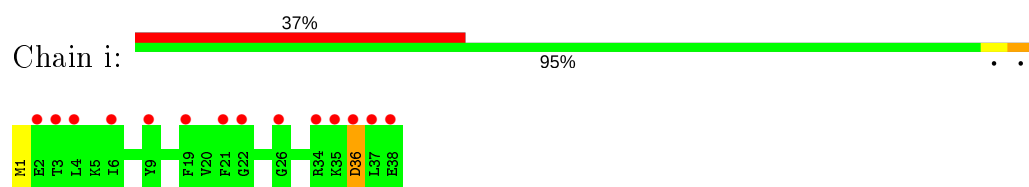
- Molecule 7: Photosystem II reaction center protein H



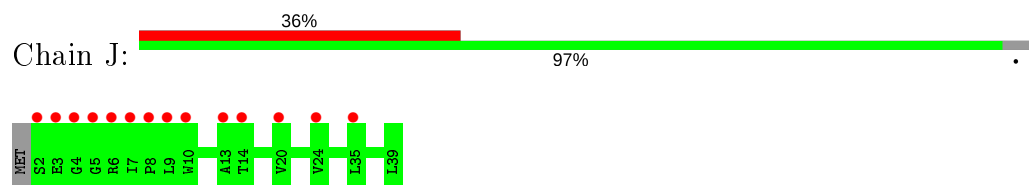
- Molecule 8: Photosystem II reaction center protein I



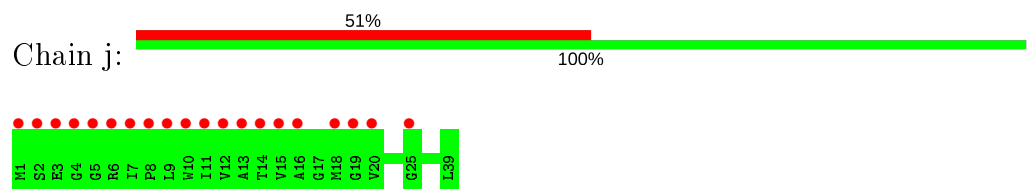
- Molecule 8: Photosystem II reaction center protein I



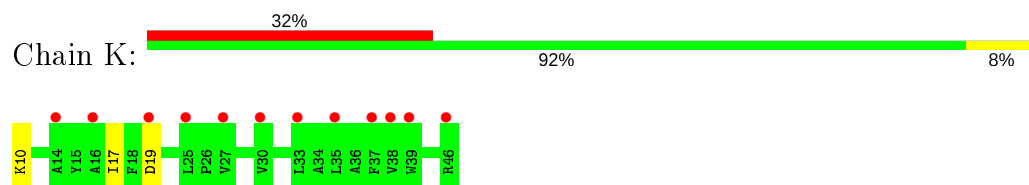
- Molecule 9: Photosystem II reaction center protein J



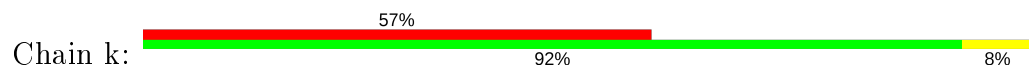
- Molecule 9: Photosystem II reaction center protein J

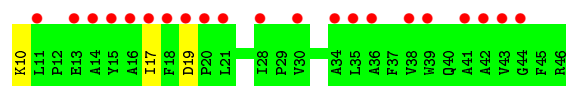


- Molecule 10: Photosystem II protein K

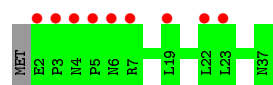


- Molecule 10: Photosystem II protein K

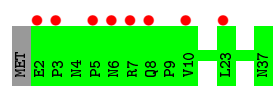




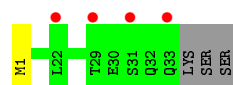
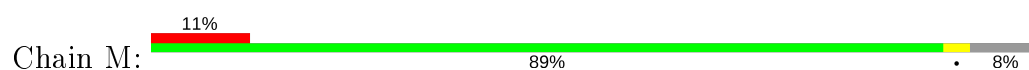
- Molecule 11: Photosystem II reaction center protein L



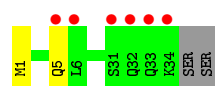
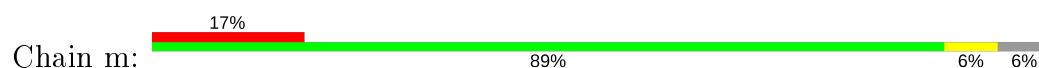
- Molecule 11: Photosystem II reaction center protein L



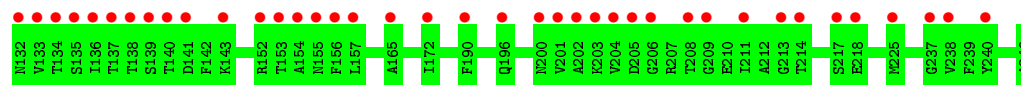
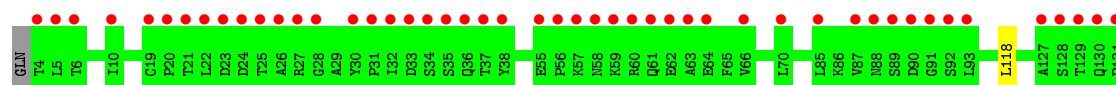
- Molecule 12: Photosystem II protein M



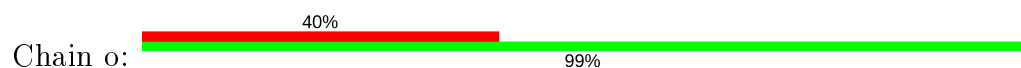
- Molecule 12: Photosystem II protein M

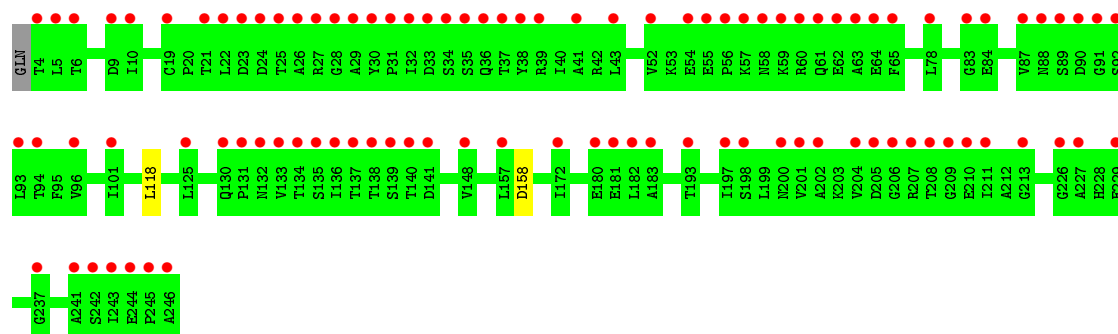


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

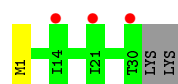


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

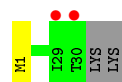
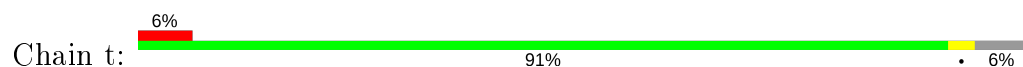




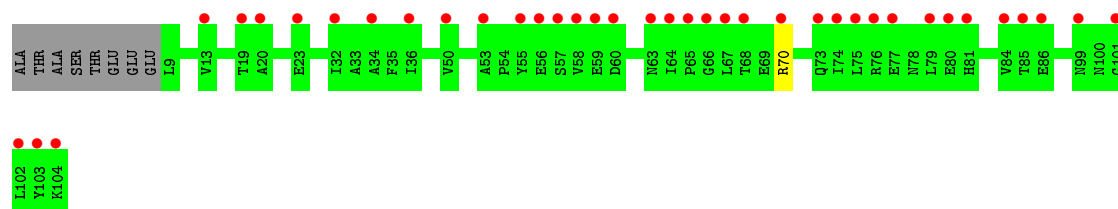
• Molecule 14: Photosystem II reaction center protein T



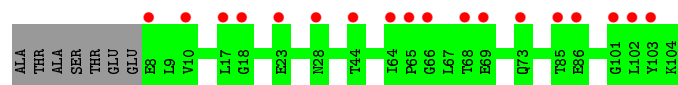
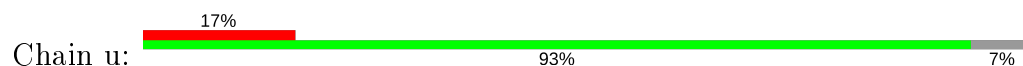
• Molecule 14: Photosystem II reaction center protein T



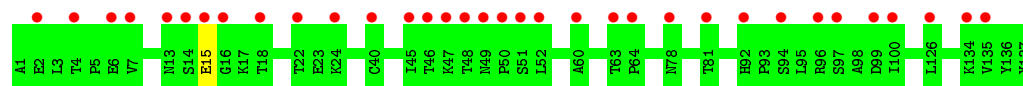
• Molecule 15: Photosystem II 12 kDa extrinsic protein



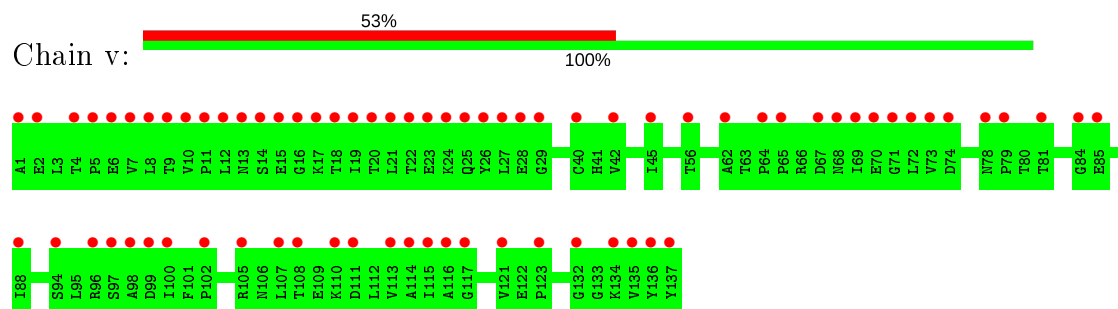
• Molecule 15: Photosystem II 12 kDa extrinsic protein



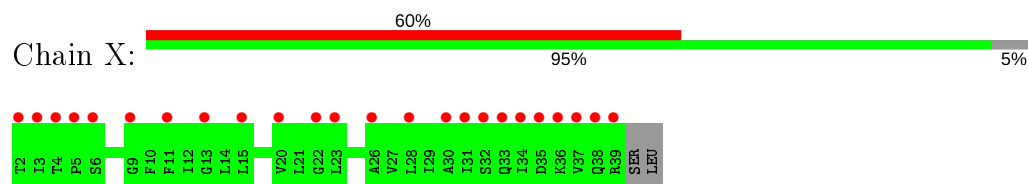
• Molecule 16: Cytochrome c-550



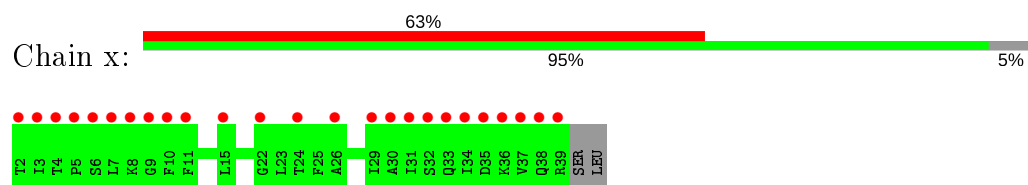
- Molecule 16: Cytochrome c-550



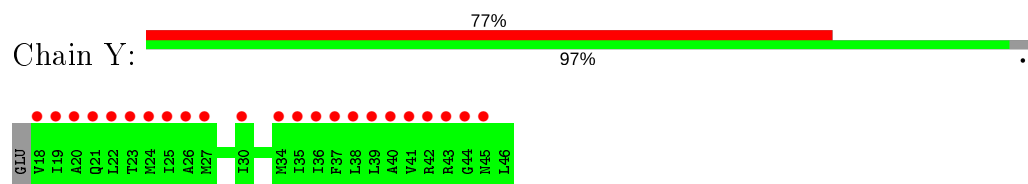
- Molecule 17: Photosystem II reaction center protein X



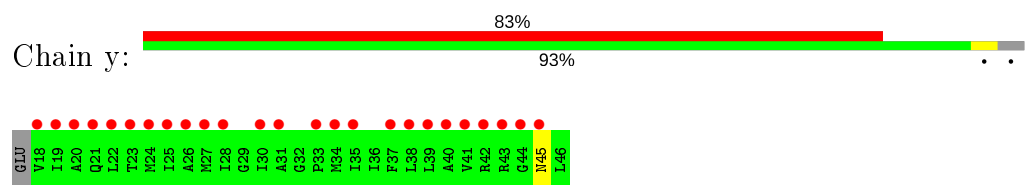
- Molecule 17: Photosystem II reaction center protein X



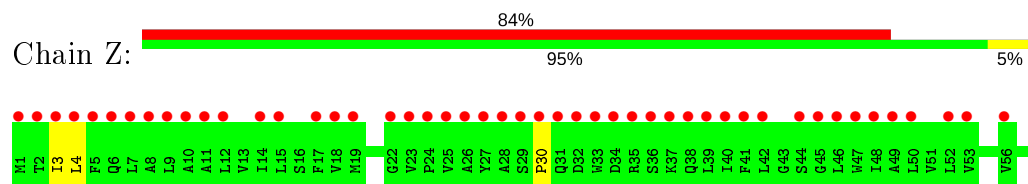
- Molecule 18: Photosystem II reaction center protein Ycf12



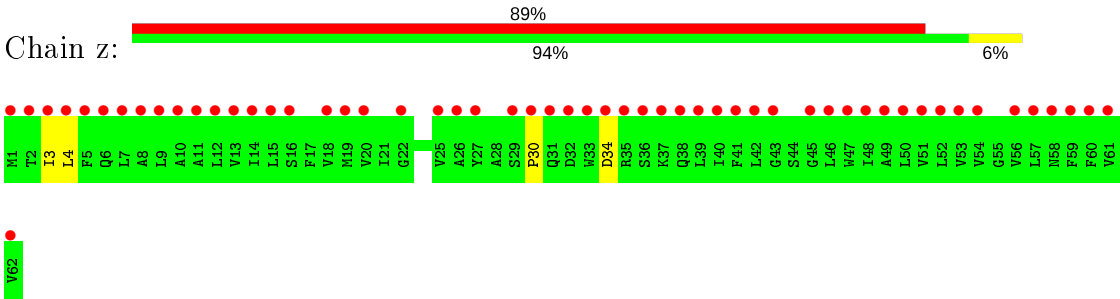
- Molecule 18: Photosystem II reaction center protein Ycf12



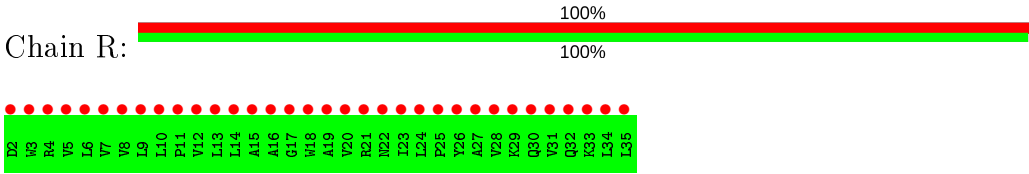
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



● Molecule 20: Photosystem II protein Y



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.70 Å   229.89 Å   285.50 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	20.00 – 2.35 47.31 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.35) 100.0 (47.31-2.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.41 (at 2.34 Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.133   ,   0.171 0.138   ,   0.174	Depositor DCC
$R_{free}$ test set	17041 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.9	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 83.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	52545	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: LHG, GOL, MG, OEX, PHO, DGD, CL, CA, LMT, CLA, PL9, LMG, FE2, HEC, BCT, HEM, FME, UNL, 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	0.48	0/2728	0.58	0/3719
1	a	0.45	0/2733	0.56	0/3727
2	B	0.46	0/4171	0.56	0/5683
2	b	0.44	0/4138	0.54	0/5640
3	C	0.43	0/3626	0.53	0/4936
3	c	0.40	0/3662	0.53	0/4985
4	D	0.48	0/2827	0.56	0/3852
4	d	0.46	0/2818	0.55	0/3840
5	E	0.40	0/687	0.53	0/936
5	e	0.38	0/667	0.52	0/908
6	F	0.41	0/284	0.53	0/387
6	f	0.42	0/257	0.52	0/349
7	H	0.40	0/530	0.56	0/723
7	h	0.36	0/519	0.53	0/708
8	I	0.40	0/311	0.50	0/419
8	i	0.40	0/311	0.50	0/419
9	J	0.36	0/278	0.49	0/376
9	j	0.34	0/283	0.47	0/383
10	K	0.38	0/303	0.54	0/416
10	k	0.36	0/303	0.53	0/416
11	L	0.46	0/311	0.49	0/423
11	l	0.42	0/311	0.47	0/423
12	M	0.48	0/261	0.64	0/357
12	m	0.47	0/262	0.62	0/357
13	O	0.41	0/1926	0.59	0/2611
13	o	0.42	0/1910	0.60	1/2589 (0.0%)
14	T	0.56	0/257	0.56	0/349
14	t	0.49	0/257	0.52	0/349
15	U	0.41	0/776	0.55	0/1052
15	u	0.42	0/785	0.59	0/1064
16	V	0.40	0/1085	0.52	0/1473



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	v	0.38	0/1085	0.50	0/1473
17	X	0.34	0/284	0.49	0/384
17	x	0.32	0/284	0.50	0/384
18	Y	0.31	0/216	0.46	0/289
18	y	0.31	0/216	0.50	0/289
19	Z	0.32	0/490	0.43	0/669
19	z	0.31	0/490	0.43	0/669
20	R	0.28	0/279	0.40	0/383
All	All	0.43	0/42921	0.55	1/58409 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	158	ASP	CB-CG-OD1	5.22	123.00	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/344 (97%)	331 (99%)	3 (1%)	1 (0%)	41	47
1	a	336/344 (98%)	331 (98%)	4 (1%)	1 (0%)	41	47
2	B	510/505 (101%)	505 (99%)	5 (1%)	0	100	100
2	b	506/505 (100%)	500 (99%)	6 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	453/455 (100%)	443 (98%)	8 (2%)	2 (0%)	34	38
3	c	457/455 (100%)	446 (98%)	9 (2%)	2 (0%)	34	38
4	D	341/342 (100%)	333 (98%)	8 (2%)	0	100	100
4	d	340/342 (99%)	333 (98%)	7 (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%)	60 (95%)	3 (5%)	0	100	100
7	h	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	5	2
9	J	36/39 (92%)	36 (100%)	0	0	100	100
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	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%)	32 (100%)	0	0	100	100
13	O	245/244 (100%)	238 (97%)	7 (3%)	0	100	100
13	o	243/244 (100%)	237 (98%)	6 (2%)	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%)	91 (97%)	3 (3%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
16	v	135/137 (98%)	130 (96%)	5 (4%)	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%)	27 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	y	27/30 (90%)	27 (100%)	0	0	100	100
19	Z	60/62 (97%)	59 (98%)	0	1 (2%)	9	7
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	9	7
20	R	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5251/5384 (98%)	5147 (98%)	95 (2%)	9 (0%)	51	56

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	i	36	ASP
3	C	416[A]	SER
3	C	416[B]	SER
1	a	259	ILE
3	c	416[A]	SER
3	c	416[B]	SER
19	Z	30	PRO
19	z	30	PRO
1	A	259	ILE

### 5.3.2 Protein sidechains ⓘ

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	272/279 (98%)	270 (99%)	2 (1%)	84	91
1	a	273/279 (98%)	271 (99%)	2 (1%)	84	91
2	B	410/403 (102%)	405 (99%)	5 (1%)	71	82
2	b	406/403 (101%)	402 (99%)	4 (1%)	76	85
3	C	356/356 (100%)	354 (99%)	2 (1%)	86	93
3	c	360/356 (101%)	355 (99%)	5 (1%)	67	78
4	D	278/277 (100%)	277 (100%)	1 (0%)	91	95
4	d	277/277 (100%)	276 (100%)	1 (0%)	91	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	73/73 (100%)	73 (100%)	0	100	100
5	e	70/73 (96%)	70 (100%)	0	100	100
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	14
7	h	54/54 (100%)	53 (98%)	1 (2%)	57	68
8	I	34/34 (100%)	34 (100%)	0	100	100
8	i	34/34 (100%)	33 (97%)	1 (3%)	42	52
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	6
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	6
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%)	29 (97%)	1 (3%)	38	46
13	O	210/207 (101%)	209 (100%)	1 (0%)	88	94
13	o	208/207 (100%)	207 (100%)	1 (0%)	88	94
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	83/89 (93%)	82 (99%)	1 (1%)	71	82
15	u	84/89 (94%)	84 (100%)	0	100	100
16	V	117/117 (100%)	116 (99%)	1 (1%)	78	87
16	v	117/117 (100%)	117 (100%)	0	100	100
17	X	31/33 (94%)	31 (100%)	0	100	100
17	x	31/33 (94%)	31 (100%)	0	100	100
18	Y	22/23 (96%)	22 (100%)	0	100	100
18	y	22/23 (96%)	21 (96%)	1 (4%)	27	33
19	Z	52/52 (100%)	50 (96%)	2 (4%)	33	41
19	z	52/52 (100%)	49 (94%)	3 (6%)	20	22
20	R	29/29 (100%)	29 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	4357/4403 (99%)	4312 (99%)	45 (1%)	76	85

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	238[A]	LYS
1	A	238[B]	LYS
2	B	53	ASN
2	B	223	GLN
2	B	362	PHE
2	B	489	GLU
2	B	505	ARG
3	C	289	PHE
3	C	315	MET
4	D	180	ARG
7	H	12[A]	ARG
7	H	12[B]	ARG
7	H	49	TYR
7	H	65	LEU
10	K	10	LYS
10	K	17	ILE
10	K	19	ASP
13	O	118	LEU
15	U	70	ARG
16	V	15	GLU
19	Z	3	ILE
19	Z	4	LEU
1	a	12	ASN
1	a	13	LEU
2	b	53	ASN
2	b	362	PHE
2	b	485	GLU
2	b	505	ARG
3	c	27	ASP
3	c	289	PHE
3	c	315	MET
3	c	462[A]	GLU
3	c	462[B]	GLU
4	d	180	ARG
7	h	49	TYR
8	i	36	ASP
10	k	10	LYS

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Mol	Chain	Res	Type
10	k	17	ILE
10	k	19	ASP
12	m	5	GLN
13	o	118	LEU
18	y	45	ASN
19	z	3	ILE
19	z	4	LEU
19	z	34	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	53	ASN
2	B	331	ASN
3	C	201	ASN
4	D	83	ASN
6	F	44	GLN
13	O	61	GLN
13	O	124	ASN
13	O	130	GLN
15	U	73	GLN
19	Z	58	ASN
2	b	53	ASN
2	b	331	ASN
3	c	201	ASN
4	d	83	ASN
5	e	75	GLN
12	m	5	GLN
13	o	124	ASN
13	o	130	GLN
19	z	58	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	FME	m	1	12	8,9,10	0.56	0	7,9,11	1.50	2 (28%)
14	FME	T	1	14	8,9,10	0.60	0	7,9,11	1.53	2 (28%)
12	FME	M	1	12	8,9,10	0.59	0	7,9,11	1.46	2 (28%)
8	FME	I	1	8	8,9,10	0.59	0	7,9,11	1.09	1 (14%)
14	FME	t	1	14	8,9,10	0.61	0	7,9,11	1.66	2 (28%)
8	FME	i	1	8	8,9,10	0.57	0	7,9,11	1.39	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
12	FME	m	1	12	-	2/7/9/11	-
14	FME	T	1	14	-	2/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
14	FME	t	1	14	-	1/7/9/11	-
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	O-C-CA	-2.67	117.79	124.78
14	t	1	FME	CA-N-CN	-2.55	118.89	122.82
12	m	1	FME	CA-N-CN	-2.50	118.98	122.82
14	T	1	FME	CG-CB-CA	2.38	119.57	112.95
12	M	1	FME	O-C-CA	-2.33	118.67	124.78
8	i	1	FME	O-C-CA	-2.29	118.79	124.78
8	I	1	FME	O-C-CA	-2.18	119.07	124.78
12	m	1	FME	O1-CN-N	-2.18	119.53	125.27
12	M	1	FME	CA-N-CN	-2.14	119.53	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	O-C-CA	-2.07	119.36	124.78

There are no chirality outliers.

All (7) torsion outliers are listed below:

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

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 214 ligands modelled in this entry, 18 are unknown and 15 are monoatomic - leaving 181 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$
32	LMT	b	627	-	25,25,36	0.53	1 (4%)	30,30,47	0.76	0
23	CLA	b	610	41	59,73,73	1.96	14 (23%)	67,113,113	2.29	23 (34%)
33	LMG	z	101	-	39,39,55	1.06	2 (5%)	47,47,63	1.10	4 (8%)
28	OEX	a	415	1,3,41	0,15,15	0.00	-	-	-	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	C	512	3	59,73,73	2.05	12 (20%)	67,113,113	2.16	21 (31%)
40	HEC	V	202	16	26,50,50	1.49	4 (15%)	18,82,82	1.64	3 (16%)
32	LMT	E	102	-	36,36,36	0.51	1 (2%)	47,47,47	0.87	0
23	CLA	B	612	2	59,73,73	1.98	13 (22%)	67,113,113	2.40	27 (40%)
34	HTG	V	203	-	11,11,19	0.24	0	15,15,24	1.09	1 (6%)
26	SQD	f	102	-	42,43,54	1.17	3 (7%)	51,54,65	1.46	9 (17%)
23	CLA	C	511	3	59,73,73	1.97	14 (23%)	67,113,113	2.33	24 (35%)
23	CLA	B	610	41	59,73,73	2.01	14 (23%)	67,113,113	2.27	25 (37%)
37	LHG	L	101	-	48,48,48	0.93	3 (6%)	51,54,54	1.08	2 (3%)
25	BCR	H	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.52	13 (23%)
23	CLA	c	508	41	59,73,73	1.97	12 (20%)	67,113,113	2.18	20 (29%)
23	CLA	B	607	41	59,73,73	1.99	14 (23%)	67,113,113	2.23	22 (32%)
35	DGD	C	517	-	63,63,67	0.83	2 (3%)	77,77,81	1.23	6 (7%)
23	CLA	d	402	4	59,73,73	1.95	13 (22%)	67,113,113	2.27	25 (37%)
23	CLA	b	609	2	59,73,73	1.95	13 (22%)	67,113,113	2.27	22 (32%)
33	LMG	C	501	-	51,51,55	0.92	2 (3%)	59,59,63	1.32	5 (8%)
25	BCR	c	515	-	41,41,41	1.07	1 (2%)	56,56,56	1.83	15 (26%)
23	CLA	b	606	2	59,73,73	1.92	12 (20%)	67,113,113	2.26	23 (34%)
32	LMT	t	102	-	26,26,36	0.57	1 (3%)	31,31,47	0.95	2 (6%)
27	GOL	V	201	-	5,5,5	0.41	0	5,5,5	0.49	0
23	CLA	a	405	1	59,73,73	1.99	13 (22%)	67,113,113	2.33	29 (43%)
25	BCR	B	619	-	41,41,41	1.10	2 (4%)	56,56,56	1.51	10 (17%)
34	HTG	b	625	-	19,19,19	0.94	2 (10%)	23,24,24	1.41	3 (13%)
34	HTG	c	522	-	19,19,19	0.98	1 (5%)	23,24,24	1.56	1 (4%)
33	LMG	D	415	39	51,51,55	0.87	2 (3%)	59,59,63	0.89	3 (5%)
34	HTG	b	622	-	19,19,19	1.04	1 (5%)	23,24,24	1.73	5 (21%)
37	LHG	d	406	-	48,48,48	0.88	2 (4%)	51,54,54	1.09	4 (7%)
25	BCR	y	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.77	12 (21%)
23	CLA	b	614	2	59,73,73	1.91	13 (22%)	67,113,113	2.24	22 (32%)
32	LMT	a	420	-	36,36,36	0.49	1 (2%)	47,47,47	0.91	0
25	BCR	A	409	-	41,41,41	1.03	1 (2%)	56,56,56	1.59	12 (21%)
32	LMT	M	101	-	36,36,36	0.49	0	47,47,47	1.06	3 (6%)
23	CLA	a	409	1	59,73,73	1.94	14 (23%)	67,113,113	2.28	26 (38%)
35	DGD	h	102	-	63,63,67	0.84	2 (3%)	77,77,81	0.98	4 (5%)
25	BCR	a	410	-	41,41,41	1.00	1 (2%)	56,56,56	1.61	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	PL9	d	405	-	55,55,55	0.65	1 (1%)	68,69,69	1.82	19 (27%)
35	DGD	c	518	-	63,63,67	0.89	3 (4%)	77,77,81	0.97	3 (3%)
33	LMG	c	520	-	51,51,55	0.93	2 (3%)	59,59,63	1.05	4 (6%)
34	HTG	B	626	-	19,19,19	1.00	2 (10%)	23,24,24	1.54	4 (17%)
26	SQD	F	101	-	42,43,54	1.17	4 (9%)	51,54,65	1.78	11 (21%)
37	LHG	d	408	-	48,48,48	0.93	2 (4%)	51,54,54	1.07	3 (5%)
25	BCR	c	516	-	41,41,41	1.04	1 (2%)	56,56,56	1.62	13 (23%)
23	CLA	C	508	41	59,73,73	1.95	12 (20%)	67,113,113	2.15	20 (29%)
27	GOL	b	624	-	5,5,5	0.29	0	5,5,5	0.54	0
35	DGD	c	517	-	63,63,67	0.82	2 (3%)	77,77,81	1.14	6 (7%)
23	CLA	b	602	2	59,73,73	1.98	13 (22%)	67,113,113	2.31	25 (37%)
25	BCR	C	515	-	41,41,41	1.04	1 (2%)	56,56,56	1.58	9 (16%)
23	CLA	c	504	3	59,73,73	1.94	13 (22%)	67,113,113	2.20	19 (28%)
23	CLA	B	613	2	59,73,73	2.06	15 (25%)	67,113,113	2.28	22 (32%)
24	PHO	A	353	-	67,69,69	2.06	16 (23%)	85,99,99	2.14	25 (29%)
34	HTG	B	623	-	19,19,19	0.91	1 (5%)	23,24,24	1.48	3 (13%)
28	OEX	A	413	1,3,41	0,15,15	0.00	-	-	-	-
27	GOL	c	501	-	5,5,5	0.31	0	5,5,5	0.43	0
23	CLA	A	404	1	59,73,73	2.00	14 (23%)	67,113,113	2.34	25 (37%)
38	HEM	e	87	5,6	27,50,50	0.89	1 (3%)	17,82,82	1.88	4 (23%)
23	CLA	b	605	2	59,73,73	1.94	14 (23%)	67,113,113	2.30	22 (32%)
23	CLA	c	512	3	59,73,73	1.96	12 (20%)	67,113,113	2.25	21 (31%)
33	LMG	B	621	-	51,51,55	0.90	2 (3%)	59,59,63	1.17	4 (6%)
25	BCR	k	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.57	13 (23%)
25	BCR	C	516	-	41,41,41	1.08	1 (2%)	56,56,56	1.64	13 (23%)
32	LMT	D	404	-	36,36,36	0.43	0	47,47,47	1.09	4 (8%)
23	CLA	C	513	3	59,73,73	2.01	13 (22%)	67,113,113	2.28	20 (29%)
34	HTG	b	623	-	19,19,19	1.05	2 (10%)	23,24,24	1.74	3 (13%)
33	LMG	d	412	39	51,51,55	0.88	2 (3%)	59,59,63	1.06	3 (5%)
26	SQD	a	413	-	53,54,54	1.05	3 (5%)	62,65,65	1.21	8 (12%)
23	CLA	B	604	2	59,73,73	1.87	12 (20%)	67,113,113	2.31	23 (34%)
35	DGD	C	518	-	63,63,67	0.85	2 (3%)	77,77,81	1.02	6 (7%)
27	GOL	C	523	-	5,5,5	0.47	0	5,5,5	0.13	0
31	BCT	A	348	21	0,3,3	0.00	-	0,3,3	0.00	-
35	DGD	H	102	-	63,63,67	0.82	3 (4%)	77,77,81	1.00	5 (6%)
23	CLA	b	611	2	59,73,73	1.95	12 (20%)	67,113,113	2.32	23 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	LMT	e	102	-	36,36,36	0.52	1 (2%)	47,47,47	0.91	2 (4%)
26	SQD	B	620	-	53,54,54	1.02	3 (5%)	62,65,65	1.47	9 (14%)
25	BCR	d	404	-	41,41,41	1.08	1 (2%)	56,56,56	1.86	15 (26%)
32	LMT	M	103	-	36,36,36	0.46	0	47,47,47	0.92	2 (4%)
23	CLA	b	601	41	59,73,73	2.06	14 (23%)	67,113,113	2.14	21 (31%)
31	BCT	a	404	21	0,3,3	0.00	-	0,3,3	0.00	-
32	LMT	t	101	-	25,25,36	0.53	1 (4%)	30,30,47	1.03	1 (3%)
25	BCR	T	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.68	13 (23%)
27	GOL	B	625	-	5,5,5	0.60	0	5,5,5	0.76	0
33	LMG	Z	101	-	37,37,55	1.01	3 (8%)	45,45,63	1.48	8 (17%)
23	CLA	B	603	2	59,73,73	1.95	13 (22%)	67,113,113	2.50	26 (38%)
37	LHG	D	410	-	48,48,48	0.86	3 (6%)	51,54,54	0.98	3 (5%)
38	HEM	E	103	5,6	27,50,50	0.86	1 (3%)	17,82,82	2.54	3 (17%)
37	LHG	d	407	-	48,48,48	0.87	3 (6%)	51,54,54	1.00	3 (5%)
23	CLA	B	611	2	59,73,73	1.99	14 (23%)	67,113,113	2.25	23 (34%)
23	CLA	A	406	41	59,73,73	1.95	13 (22%)	67,113,113	2.13	24 (35%)
23	CLA	C	504	3	59,73,73	1.94	13 (22%)	67,113,113	2.17	22 (32%)
27	GOL	a	412	-	5,5,5	0.33	0	5,5,5	0.47	0
24	PHO	a	353	-	67,69,69	2.14	16 (23%)	85,99,99	2.03	22 (25%)
32	LMT	a	414	-	36,36,36	0.55	1 (2%)	47,47,47	1.10	4 (8%)
25	BCR	Y	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.75	15 (26%)
23	CLA	c	509	3	59,73,73	2.05	12 (20%)	67,113,113	2.32	22 (32%)
29	PL9	D	408	-	55,55,55	0.65	1 (1%)	68,69,69	1.77	17 (25%)
37	LHG	D	409	-	48,48,48	0.90	3 (6%)	51,54,54	1.17	6 (11%)
37	LHG	l	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.11	5 (9%)
25	BCR	h	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.37	7 (12%)
24	PHO	a	408	-	67,69,69	2.02	17 (25%)	85,99,99	2.02	24 (28%)
23	CLA	a	406	41	59,73,73	1.99	12 (20%)	67,113,113	2.24	22 (32%)
32	LMT	b	621	-	25,25,36	0.48	0	30,30,47	0.72	0
24	PHO	A	407	-	67,69,69	2.06	17 (25%)	85,99,99	2.02	23 (27%)
27	GOL	a	418	-	5,5,5	0.36	0	5,5,5	0.68	0
25	BCR	K	102	-	41,41,41	1.01	1 (2%)	56,56,56	1.62	12 (21%)
35	DGD	C	519	-	63,63,67	0.82	3 (4%)	77,77,81	1.04	6 (7%)
23	CLA	B	615	2	59,73,73	1.93	11 (18%)	67,113,113	2.21	24 (35%)
25	BCR	b	619	-	41,41,41	1.04	1 (2%)	56,56,56	1.52	13 (23%)
25	BCR	B	617	-	41,41,41	1.01	1 (2%)	56,56,56	1.56	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	B	602	2	59,73,73	2.02	12 (20%)	67,113,113	2.36	27 (40%)
34	HTG	B	622	-	19,19,19	1.03	1 (5%)	23,24,24	1.54	5 (21%)
23	CLA	B	605	2	59,73,73	1.92	12 (20%)	67,113,113	2.40	27 (40%)
23	CLA	c	511	3	59,73,73	1.94	13 (22%)	67,113,113	2.27	25 (37%)
34	HTG	d	411	-	16,16,19	1.16	2 (12%)	20,21,24	1.68	1 (5%)
23	CLA	A	408	1	59,73,73	2.01	14 (23%)	67,113,113	2.24	26 (38%)
32	LMT	I	101	-	36,36,36	0.51	1 (2%)	47,47,47	1.10	3 (6%)
23	CLA	D	405	4	59,73,73	1.91	12 (20%)	67,113,113	2.31	24 (35%)
23	CLA	B	609	2	59,73,73	1.97	13 (22%)	67,113,113	2.15	19 (28%)
23	CLA	b	608	2	59,73,73	2.04	13 (22%)	67,113,113	2.19	26 (38%)
23	CLA	B	606	2	59,73,73	1.88	13 (22%)	67,113,113	2.44	25 (37%)
26	SQD	A	410	-	53,54,54	0.94	3 (5%)	62,65,65	1.94	12 (19%)
23	CLA	C	514	3	59,73,73	2.00	12 (20%)	67,113,113	2.14	23 (34%)
23	CLA	a	407	41	59,73,73	1.95	12 (20%)	67,113,113	2.21	23 (34%)
23	CLA	C	509	3	59,73,73	2.04	13 (22%)	67,113,113	2.30	22 (32%)
23	CLA	C	506	3	59,73,73	1.91	13 (22%)	67,113,113	2.26	22 (32%)
23	CLA	c	505	41	59,73,73	2.01	15 (25%)	67,113,113	2.21	25 (37%)
34	HTG	D	414	-	16,16,19	1.03	2 (12%)	20,21,24	1.60	1 (5%)
34	HTG	C	522	-	19,19,19	0.93	1 (5%)	23,24,24	1.41	2 (8%)
37	LHG	e	101	-	41,41,48	1.04	2 (4%)	44,47,54	0.94	2 (4%)
33	LMG	c	521	-	51,51,55	0.96	2 (3%)	59,59,63	1.16	5 (8%)
23	CLA	b	612	2	59,73,73	1.98	15 (25%)	67,113,113	2.34	20 (29%)
23	CLA	B	601	41	59,73,73	2.05	13 (22%)	67,113,113	2.22	23 (34%)
33	LMG	a	419	-	51,51,55	0.91	2 (3%)	59,59,63	1.13	5 (8%)
23	CLA	c	507	3	59,73,73	2.00	13 (22%)	67,113,113	2.22	22 (32%)
25	BCR	b	618	-	41,41,41	1.01	1 (2%)	56,56,56	1.44	10 (17%)
32	LMT	A	359	-	36,36,36	0.58	1 (2%)	47,47,47	0.87	1 (2%)
35	DGD	c	519	-	63,63,67	0.85	3 (4%)	77,77,81	1.06	6 (7%)
23	CLA	b	615	2	59,73,73	1.95	12 (20%)	67,113,113	2.13	21 (31%)
23	CLA	b	607	41	59,73,73	1.92	13 (22%)	67,113,113	2.16	22 (32%)
25	BCR	b	617	-	41,41,41	1.08	1 (2%)	56,56,56	1.52	6 (10%)
37	LHG	E	101	-	41,41,48	1.03	2 (4%)	44,47,54	1.15	5 (11%)
33	LMG	C	521	-	51,51,55	1.00	3 (5%)	59,59,63	1.26	4 (6%)
23	CLA	B	616	2	59,73,73	1.98	13 (22%)	67,113,113	2.17	20 (29%)
23	CLA	C	503	3	59,73,73	1.95	13 (22%)	67,113,113	2.18	21 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	LMG	C	520	-	51,51,55	0.95	2 (3%)	59,59,63	1.12	5 (8%)
23	CLA	C	502	3	59,73,73	1.92	13 (22%)	67,113,113	2.24	22 (32%)
23	CLA	C	510	3	59,73,73	2.04	15 (25%)	67,113,113	2.17	23 (34%)
23	CLA	b	604	2	59,73,73	1.92	12 (20%)	67,113,113	2.29	21 (31%)
29	PL9	A	414	-	55,55,55	0.63	1 (1%)	68,69,69	2.00	23 (33%)
23	CLA	A	405	41	59,73,73	2.00	12 (20%)	67,113,113	2.29	25 (37%)
27	GOL	B	624	-	5,5,5	0.36	0	5,5,5	0.54	0
29	PL9	a	416	-	55,55,55	0.63	2 (3%)	68,69,69	1.99	21 (30%)
23	CLA	D	406	4	59,73,73	1.99	13 (22%)	67,113,113	2.19	22 (32%)
26	SQD	b	620	-	53,54,54	1.04	3 (5%)	62,65,65	1.56	9 (14%)
25	BCR	B	618	-	41,41,41	0.92	1 (2%)	56,56,56	1.62	16 (28%)
40	HEC	v	202	16	26,50,50	1.58	4 (15%)	18,82,82	1.87	6 (33%)
23	CLA	c	503	3	59,73,73	1.93	13 (22%)	67,113,113	2.20	22 (32%)
23	CLA	c	502	3	59,73,73	1.99	13 (22%)	67,113,113	2.19	24 (35%)
23	CLA	c	510	3	59,73,73	2.04	12 (20%)	67,113,113	2.30	26 (38%)
23	CLA	C	505	41	59,73,73	1.96	13 (22%)	67,113,113	2.25	23 (34%)
37	LHG	D	411	-	48,48,48	0.89	2 (4%)	51,54,54	1.01	3 (5%)
23	CLA	b	603	2	59,73,73	2.02	13 (22%)	67,113,113	2.43	25 (37%)
23	CLA	d	403	4	59,73,73	1.99	13 (22%)	67,113,113	2.18	27 (40%)
32	LMT	m	103	-	36,36,36	0.47	0	47,47,47	0.92	1 (2%)
25	BCR	D	407	-	41,41,41	1.04	1 (2%)	56,56,56	1.92	16 (28%)
23	CLA	c	513	3	59,73,73	1.99	12 (20%)	67,113,113	2.31	24 (35%)
27	GOL	v	201	-	5,5,5	0.40	0	5,5,5	0.36	0
23	CLA	C	507	3	59,73,73	1.97	14 (23%)	67,113,113	2.25	27 (40%)
26	SQD	a	411	-	53,54,54	0.95	3 (5%)	62,65,65	1.70	13 (20%)
26	SQD	A	412	-	53,54,54	1.01	3 (5%)	62,65,65	1.20	9 (14%)
25	BCR	t	103	-	41,41,41	1.00	1 (2%)	56,56,56	1.74	15 (26%)
23	CLA	b	616	2	59,73,73	1.95	12 (20%)	67,113,113	2.28	22 (32%)
23	CLA	B	608	2	59,73,73	1.94	14 (23%)	67,113,113	2.28	24 (35%)
33	LMG	m	101	-	51,51,55	0.87	2 (3%)	59,59,63	1.19	6 (10%)
23	CLA	b	613	2	59,73,73	2.02	15 (25%)	67,113,113	2.31	24 (35%)
23	CLA	c	514	3	59,73,73	1.99	13 (22%)	67,113,113	2.13	23 (34%)
27	GOL	A	411	-	5,5,5	0.39	0	5,5,5	0.22	0
23	CLA	B	614	2	59,73,73	1.94	13 (22%)	67,113,113	2.45	24 (35%)
23	CLA	c	506	3	59,73,73	1.92	12 (20%)	67,113,113	2.20	20 (29%)

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
32	LMT	b	627	-	-	8/17/37/61	0/1/1/2
23	CLA	b	610	41	3/3/20/25	7/37/135/135	-
33	LMG	z	101	-	-	8/34/54/70	0/1/1/1
23	CLA	C	512	3	3/3/20/25	4/37/135/135	-
40	HEC	V	202	16	-	0/6/54/54	-
32	LMT	E	102	-	-	8/21/61/61	0/2/2/2
23	CLA	B	612	2	3/3/20/25	4/37/135/135	-
34	HTG	V	203	-	-	0/2/19/30	0/1/1/1
26	SQD	f	102	-	-	12/38/58/69	0/1/1/1
23	CLA	C	511	3	3/3/20/25	12/37/135/135	-
23	CLA	B	610	41	3/3/20/25	5/37/135/135	-
37	LHG	L	101	-	-	19/53/53/53	-
25	BCR	H	101	-	-	4/29/63/63	0/2/2/2
23	CLA	c	508	41	3/3/20/25	6/37/135/135	-
23	CLA	B	607	41	3/3/20/25	4/37/135/135	-
35	DGD	C	517	-	-	13/51/91/95	0/2/2/2
23	CLA	b	609	2	2/2/20/25	7/37/135/135	-
33	LMG	C	501	-	-	13/46/66/70	0/1/1/1
25	BCR	c	515	-	-	1/29/63/63	0/2/2/2
23	CLA	b	606	2	3/3/20/25	10/37/135/135	-
32	LMT	t	102	-	-	5/17/38/61	0/1/1/2
27	GOL	V	201	-	-	2/4/4/4	-
23	CLA	a	405	1	3/3/20/25	2/37/135/135	-
25	BCR	B	619	-	-	2/29/63/63	0/2/2/2
34	HTG	b	625	-	-	4/10/30/30	0/1/1/1
34	HTG	c	522	-	-	4/10/30/30	0/1/1/1
33	LMG	D	415	39	-	10/46/66/70	0/1/1/1
34	HTG	b	622	-	-	4/10/30/30	0/1/1/1
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
25	BCR	y	101	-	-	6/29/63/63	0/2/2/2
23	CLA	b	614	2	3/3/20/25	13/37/135/135	-
32	LMT	a	420	-	-	4/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	LHG	d	406	-	-	6/53/53/53	-
32	LMT	M	101	-	-	5/21/61/61	0/2/2/2
23	CLA	a	409	1	3/3/20/25	11/37/135/135	-
35	DGD	h	102	-	-	9/51/91/95	0/2/2/2
25	BCR	a	410	-	-	0/29/63/63	0/2/2/2
29	PL9	d	405	-	-	7/53/73/73	0/1/1/1
35	DGD	c	518	-	-	12/51/91/95	0/2/2/2
23	CLA	d	402	4	1/1/20/25	3/37/135/135	-
34	HTG	B	626	-	-	2/10/30/30	0/1/1/1
26	SQD	F	101	-	-	13/38/58/69	0/1/1/1
37	LHG	d	408	-	-	15/53/53/53	-
25	BCR	c	516	-	-	3/29/63/63	0/2/2/2
34	HTG	D	414	-	-	0/7/27/30	0/1/1/1
23	CLA	C	508	41	3/3/20/25	6/37/135/135	-
27	GOL	b	624	-	-	0/4/4/4	-
35	DGD	c	517	-	-	21/51/91/95	0/2/2/2
23	CLA	b	602	2	2/2/20/25	3/37/135/135	-
25	BCR	C	515	-	-	1/29/63/63	0/2/2/2
23	CLA	c	504	3	3/3/20/25	2/37/135/135	-
23	CLA	B	613	2	3/3/20/25	7/37/135/135	-
23	CLA	C	503	3	3/3/20/25	7/37/135/135	-
34	HTG	B	623	-	-	4/10/30/30	0/1/1/1
27	GOL	c	501	-	-	0/4/4/4	-
23	CLA	A	404	1	3/3/20/25	3/37/135/135	-
38	HEM	e	87	5,6	-	1/6/54/54	-
24	PHO	A	407	-	-	3/53/103/103	0/5/6/6
23	CLA	c	512	3	3/3/20/25	5/37/135/135	-
33	LMG	B	621	-	-	15/46/66/70	0/1/1/1
25	BCR	k	101	-	-	2/29/63/63	0/2/2/2
25	BCR	C	516	-	-	1/29/63/63	0/2/2/2
32	LMT	D	404	-	-	7/21/61/61	0/2/2/2
23	CLA	C	513	3	3/3/20/25	11/37/135/135	-
34	HTG	b	623	-	-	4/10/30/30	0/1/1/1
33	LMG	d	412	39	-	7/46/66/70	0/1/1/1
26	SQD	a	413	-	-	18/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	604	2	3/3/20/25	8/37/135/135	-
35	DGD	C	518	-	-	17/51/91/95	0/2/2/2
27	GOL	C	523	-	-	2/4/4/4	-
23	CLA	b	611	2	3/3/20/25	4/37/135/135	-
35	DGD	H	102	-	-	13/51/91/95	0/2/2/2
32	LMT	e	102	-	-	7/21/61/61	0/2/2/2
26	SQD	B	620	-	-	18/49/69/69	0/1/1/1
25	BCR	d	404	-	-	6/29/63/63	0/2/2/2
32	LMT	M	103	-	-	10/21/61/61	0/2/2/2
23	CLA	b	601	41	3/3/20/25	17/37/135/135	-
32	LMT	t	101	-	-	6/17/37/61	0/1/1/2
25	BCR	T	101	-	-	3/29/63/63	0/2/2/2
27	GOL	B	625	-	-	4/4/4/4	-
33	LMG	Z	101	-	-	12/31/51/70	0/1/1/1
23	CLA	B	603	2	2/2/20/25	5/37/135/135	-
25	BCR	D	407	-	-	7/29/63/63	0/2/2/2
38	HEM	E	103	5,6	-	0/6/54/54	-
37	LHG	d	407	-	-	16/53/53/53	-
23	CLA	B	611	2	3/3/20/25	2/37/135/135	-
23	CLA	A	406	41	2/2/20/25	7/37/135/135	-
23	CLA	C	504	3	3/3/20/25	3/37/135/135	-
27	GOL	a	412	-	-	4/4/4/4	-
24	PHO	a	353	-	-	5/53/103/103	0/5/6/6
32	LMT	a	414	-	-	7/21/61/61	0/2/2/2
25	BCR	Y	101	-	-	2/29/63/63	0/2/2/2
23	CLA	c	509	3	3/3/20/25	3/37/135/135	-
29	PL9	D	408	-	-	7/53/73/73	0/1/1/1
37	LHG	D	409	-	-	11/53/53/53	-
37	LHG	l	101	-	-	17/53/53/53	-
25	BCR	h	101	-	-	1/29/63/63	0/2/2/2
24	PHO	a	408	-	-	5/53/103/103	0/5/6/6
23	CLA	a	406	41	2/2/20/25	7/37/135/135	-
32	LMT	b	621	-	-	7/17/37/61	0/1/1/2
23	CLA	b	605	2	3/3/20/25	5/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	GOL	a	418	-	-	2/4/4/4	-
25	BCR	K	102	-	-	1/29/63/63	0/2/2/2
35	DGD	C	519	-	-	13/51/91/95	0/2/2/2
23	CLA	B	615	2	3/3/20/25	8/37/135/135	-
25	BCR	b	619	-	-	4/29/63/63	0/2/2/2
25	BCR	B	617	-	-	2/29/63/63	0/2/2/2
23	CLA	B	602	2	2/2/20/25	7/37/135/135	-
34	HTG	B	622	-	-	5/10/30/30	0/1/1/1
23	CLA	B	605	2	3/3/20/25	7/37/135/135	-
23	CLA	c	511	3	3/3/20/25	10/37/135/135	-
34	HTG	d	411	-	-	0/7/27/30	0/1/1/1
23	CLA	A	408	1	3/3/20/25	11/37/135/135	-
32	LMT	I	101	-	-	9/21/61/61	0/2/2/2
23	CLA	B	609	2	2/2/20/25	4/37/135/135	-
23	CLA	b	608	2	2/2/20/25	4/37/135/135	-
23	CLA	B	606	2	2/2/20/25	8/37/135/135	-
26	SQD	A	410	-	-	15/49/69/69	0/1/1/1
23	CLA	C	514	3	3/3/20/25	5/37/135/135	-
23	CLA	a	407	41	2/2/20/25	5/37/135/135	-
23	CLA	C	509	3	3/3/20/25	4/37/135/135	-
23	CLA	C	506	3	1/1/20/25	7/37/135/135	-
23	CLA	c	505	41	3/3/20/25	6/37/135/135	-
37	LHG	D	410	-	-	14/53/53/53	-
34	HTG	C	522	-	-	1/10/30/30	0/1/1/1
37	LHG	e	101	-	-	12/46/46/53	-
33	LMG	c	521	-	-	8/46/66/70	0/1/1/1
23	CLA	b	612	2	3/3/20/25	4/37/135/135	-
23	CLA	B	601	41	3/3/20/25	13/37/135/135	-
33	LMG	a	419	-	-	12/46/66/70	0/1/1/1
23	CLA	c	507	3	3/3/20/25	10/37/135/135	-
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
32	LMT	A	359	-	-	3/21/61/61	0/2/2/2
35	DGD	c	519	-	-	7/51/91/95	0/2/2/2
23	CLA	b	615	2	3/3/20/25	5/37/135/135	-
23	CLA	b	607	41	3/3/20/25	4/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
37	LHG	E	101	-	-	19/46/46/53	-
33	LMG	C	521	-	-	9/46/66/70	0/1/1/1
23	CLA	B	616	2	3/3/20/25	7/37/135/135	-
24	PHO	A	353	-	-	3/53/103/103	0/5/6/6
33	LMG	C	520	-	-	13/46/66/70	0/1/1/1
33	LMG	c	520	-	-	15/46/66/70	0/1/1/1
23	CLA	C	502	3	3/3/20/25	4/37/135/135	-
23	CLA	C	510	3	3/3/20/25	4/37/135/135	-
23	CLA	b	604	2	3/3/20/25	6/37/135/135	-
29	PL9	A	414	-	-	16/53/73/73	0/1/1/1
23	CLA	A	405	41	3/3/20/25	4/37/135/135	-
27	GOL	B	624	-	-	4/4/4/4	-
29	PL9	a	416	-	-	16/53/73/73	0/1/1/1
23	CLA	D	406	4	3/3/20/25	7/37/135/135	-
26	SQD	b	620	-	-	18/49/69/69	0/1/1/1
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
40	HEC	v	202	16	-	0/6/54/54	-
23	CLA	c	503	3	3/3/20/25	4/37/135/135	-
23	CLA	c	502	3	3/3/20/25	5/37/135/135	-
23	CLA	c	510	3	3/3/20/25	12/37/135/135	-
23	CLA	C	505	41	3/3/20/25	6/37/135/135	-
37	LHG	D	411	-	-	14/53/53/53	-
23	CLA	b	603	2	2/2/20/25	4/37/135/135	-
23	CLA	d	403	4	3/3/20/25	7/37/135/135	-
32	LMT	m	103	-	-	6/21/61/61	0/2/2/2
23	CLA	c	514	3	3/3/20/25	6/37/135/135	-
23	CLA	c	513	3	3/3/20/25	10/37/135/135	-
27	GOL	v	201	-	-	2/4/4/4	-
23	CLA	C	507	3	3/3/20/25	12/37/135/135	-
26	SQD	a	411	-	-	10/49/69/69	0/1/1/1
26	SQD	A	412	-	-	11/49/69/69	0/1/1/1
25	BCR	t	103	-	-	6/29/63/63	0/2/2/2
23	CLA	b	616	2	3/3/20/25	12/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	608	2	2/2/20/25	3/37/135/135	-
33	LMG	m	101	-	-	14/46/66/70	0/1/1/1
23	CLA	b	613	2	3/3/20/25	7/37/135/135	-
23	CLA	D	405	4	1/1/20/25	3/37/135/135	-
27	GOL	A	411	-	-	2/4/4/4	-
23	CLA	B	614	2	3/3/20/25	12/37/135/135	-
23	CLA	c	506	3	1/1/20/25	5/37/135/135	-

All (1132) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	612	CLA	C3B-C2B	6.94	1.50	1.40
23	D	405	CLA	C3B-C2B	6.74	1.49	1.40
23	C	512	CLA	C3B-C2B	6.62	1.49	1.40
23	B	603	CLA	C3B-C2B	6.53	1.49	1.40
23	b	612	CLA	C3B-C2B	6.51	1.49	1.40
23	b	603	CLA	C3B-C2B	6.51	1.49	1.40
23	b	613	CLA	C3B-C2B	6.48	1.49	1.40
23	c	509	CLA	C3B-C2B	6.47	1.49	1.40
23	B	613	CLA	C3B-C2B	6.38	1.49	1.40
23	c	505	CLA	C3B-C2B	6.36	1.49	1.40
23	C	510	CLA	C3B-C2B	6.28	1.49	1.40
23	b	611	CLA	C3B-C2B	6.25	1.49	1.40
23	a	405	CLA	C3B-C2B	6.23	1.49	1.40
23	C	509	CLA	C3B-C2B	6.20	1.49	1.40
23	A	404	CLA	C3B-C2B	6.19	1.49	1.40
23	c	503	CLA	C3B-C2B	6.18	1.48	1.40
23	b	610	CLA	C3B-C2B	6.16	1.48	1.40
23	c	507	CLA	C3D-C2D	6.15	1.50	1.39
23	B	615	CLA	C3D-C2D	6.13	1.50	1.39
23	b	604	CLA	C3B-C2B	6.12	1.48	1.40
23	b	601	CLA	C3D-C2D	6.08	1.50	1.39
23	A	405	CLA	C3D-C2D	6.08	1.50	1.39
23	b	608	CLA	C3B-C2B	6.08	1.48	1.40
23	a	407	CLA	C3D-C2D	6.07	1.50	1.39
23	a	406	CLA	C3D-C2D	6.06	1.50	1.39
23	c	510	CLA	C3B-C2B	6.06	1.48	1.40
23	C	505	CLA	C3B-C2B	6.05	1.48	1.40
23	b	614	CLA	C3B-C2B	6.04	1.48	1.40
23	B	608	CLA	C3B-C2B	6.03	1.48	1.40
23	C	513	CLA	C3D-C2D	6.02	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	353	PHO	C3B-C2B	6.00	1.49	1.37
23	C	509	CLA	C3D-C2D	5.99	1.50	1.39
23	C	512	CLA	C3D-C2D	5.96	1.50	1.39
24	A	353	PHO	C3C-C2C	5.96	1.49	1.36
23	b	613	CLA	C3D-C2D	5.92	1.50	1.39
23	c	502	CLA	C3B-C2B	5.92	1.48	1.40
23	c	509	CLA	C3D-C2D	5.91	1.50	1.39
23	B	602	CLA	C3D-C2D	5.89	1.50	1.39
23	B	614	CLA	C3B-C2B	5.88	1.48	1.40
23	B	611	CLA	C3B-C2B	5.87	1.48	1.40
23	c	511	CLA	C3B-C2B	5.87	1.48	1.40
23	c	512	CLA	C3B-C2B	5.86	1.48	1.40
23	b	615	CLA	C3D-C2D	5.85	1.49	1.39
23	c	512	CLA	C3D-C2D	5.84	1.49	1.39
23	A	408	CLA	C3B-C2B	5.84	1.48	1.40
23	b	601	CLA	C3B-C2B	5.83	1.48	1.40
23	B	610	CLA	C3D-C2D	5.82	1.49	1.39
24	a	408	PHO	C3C-C2C	5.80	1.49	1.36
23	B	610	CLA	C3B-C2B	5.80	1.48	1.40
23	C	502	CLA	C3B-C2B	5.80	1.48	1.40
23	c	508	CLA	C3D-C2D	5.79	1.49	1.39
23	B	616	CLA	C3B-C2B	5.79	1.48	1.40
23	A	406	CLA	C3D-C2D	5.78	1.49	1.39
23	b	611	CLA	C3D-C2D	5.76	1.49	1.39
23	B	611	CLA	C3D-C2D	5.76	1.49	1.39
23	C	511	CLA	C3B-C2B	5.76	1.48	1.40
24	a	408	PHO	C3B-C2B	5.75	1.48	1.37
23	d	403	CLA	C3D-C2D	5.75	1.49	1.39
23	B	609	CLA	C3D-C2D	5.75	1.49	1.39
23	C	514	CLA	C3D-C2D	5.74	1.49	1.39
23	C	513	CLA	C3B-C2B	5.74	1.48	1.40
23	a	409	CLA	C3D-C2D	5.74	1.49	1.39
23	B	606	CLA	C3B-C2B	5.74	1.48	1.40
23	B	613	CLA	C3D-C2D	5.73	1.49	1.39
23	B	604	CLA	C3B-C2B	5.73	1.48	1.40
24	a	353	PHO	C3C-C2C	5.73	1.48	1.36
23	C	507	CLA	C3B-C2B	5.73	1.48	1.40
23	B	608	CLA	C3D-C2D	5.72	1.49	1.39
23	B	601	CLA	C3B-C2B	5.69	1.48	1.40
23	b	606	CLA	C3B-C2B	5.69	1.48	1.40
23	B	605	CLA	C3D-C2D	5.68	1.49	1.39
23	C	510	CLA	C3D-C2D	5.68	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	503	CLA	C3D-C2D	5.67	1.49	1.39
23	B	603	CLA	C3D-C2D	5.67	1.49	1.39
23	c	510	CLA	C3D-C2D	5.66	1.49	1.39
23	d	403	CLA	C3B-C2B	5.65	1.48	1.40
23	c	513	CLA	C3C-C2C	5.64	1.48	1.36
23	B	601	CLA	C3D-C2D	5.64	1.49	1.39
23	c	514	CLA	C3B-C2B	5.63	1.48	1.40
23	c	505	CLA	C3D-C2D	5.63	1.49	1.39
23	C	509	CLA	C3C-C2C	5.62	1.48	1.36
23	C	507	CLA	C3D-C2D	5.62	1.49	1.39
23	c	508	CLA	C3B-C2B	5.61	1.48	1.40
23	d	402	CLA	C3B-C2B	5.61	1.48	1.40
23	c	509	CLA	C3C-C2C	5.61	1.48	1.36
23	C	506	CLA	C3B-C2B	5.60	1.48	1.40
24	A	407	PHO	C3B-C2B	5.60	1.48	1.37
23	A	404	CLA	C3D-C2D	5.60	1.49	1.39
23	b	602	CLA	C3D-C2D	5.60	1.49	1.39
23	B	602	CLA	CHC-C1C	5.59	1.49	1.35
23	c	502	CLA	C3D-C2D	5.59	1.49	1.39
23	B	607	CLA	C3B-C2B	5.58	1.48	1.40
23	c	513	CLA	C3B-C2B	5.58	1.48	1.40
23	c	514	CLA	C3D-C2D	5.57	1.49	1.39
23	D	406	CLA	C3D-C2D	5.57	1.49	1.39
23	a	405	CLA	C3D-C2D	5.57	1.49	1.39
23	b	605	CLA	C3B-C2B	5.56	1.48	1.40
23	C	504	CLA	C3B-C2B	5.56	1.48	1.40
23	B	612	CLA	C3D-C2D	5.56	1.49	1.39
23	A	408	CLA	C3D-C2D	5.56	1.49	1.39
23	C	514	CLA	C3B-C2B	5.55	1.48	1.40
23	b	605	CLA	C3C-C2C	5.55	1.48	1.36
23	C	513	CLA	C3C-C2C	5.54	1.48	1.36
23	b	610	CLA	C3C-C2C	5.53	1.48	1.36
23	B	605	CLA	C3B-C2B	5.52	1.48	1.40
23	B	616	CLA	C3D-C2D	5.51	1.49	1.39
23	B	601	CLA	C3C-C2C	5.49	1.48	1.36
23	b	602	CLA	CHC-C1C	5.48	1.49	1.35
24	a	353	PHO	C3B-C2B	5.48	1.48	1.37
23	b	609	CLA	C3D-C2D	5.48	1.49	1.39
23	b	609	CLA	C3B-C2B	5.48	1.48	1.40
23	b	616	CLA	CHC-C1C	5.47	1.49	1.35
23	C	505	CLA	C3D-C2D	5.47	1.49	1.39
23	C	511	CLA	C3C-C2C	5.46	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	602	CLA	C3C-C2C	5.46	1.48	1.36
23	b	616	CLA	C3D-C2D	5.46	1.49	1.39
23	d	403	CLA	CHC-C1C	5.45	1.49	1.35
23	C	508	CLA	C3D-C2D	5.45	1.49	1.39
23	C	508	CLA	C3C-C2C	5.45	1.48	1.36
23	C	503	CLA	C3B-C2B	5.45	1.47	1.40
23	a	406	CLA	C3C-C2C	5.44	1.48	1.36
23	c	503	CLA	C3D-C2D	5.43	1.49	1.39
23	c	514	CLA	C3C-C2C	5.42	1.48	1.36
23	b	616	CLA	C3B-C2B	5.42	1.47	1.40
23	c	513	CLA	C3D-C2D	5.40	1.49	1.39
23	b	601	CLA	C3C-C2C	5.40	1.48	1.36
23	c	507	CLA	C3B-C2B	5.39	1.47	1.40
23	C	511	CLA	C3D-C2D	5.38	1.49	1.39
23	b	613	CLA	C3C-C2C	5.37	1.48	1.36
23	b	608	CLA	C3D-C2D	5.37	1.49	1.39
23	b	615	CLA	C3C-C2C	5.36	1.48	1.36
23	B	611	CLA	C3C-C2C	5.36	1.48	1.36
23	a	409	CLA	C3B-C2B	5.36	1.47	1.40
23	C	510	CLA	C3C-C2C	5.35	1.48	1.36
23	B	614	CLA	C3C-C2C	5.34	1.48	1.36
23	b	608	CLA	C3C-C2C	5.34	1.48	1.36
23	C	511	CLA	CHC-C1C	5.33	1.48	1.35
23	b	612	CLA	C3D-C2D	5.33	1.49	1.39
23	C	504	CLA	C3D-C2D	5.33	1.49	1.39
23	c	511	CLA	C3D-C2D	5.33	1.49	1.39
23	C	508	CLA	CHC-C1C	5.32	1.48	1.35
23	b	606	CLA	C3C-C2C	5.32	1.48	1.36
23	c	504	CLA	C3D-C2D	5.32	1.49	1.39
23	B	610	CLA	C3C-C2C	5.32	1.48	1.36
23	c	502	CLA	C3C-C2C	5.32	1.48	1.36
23	b	612	CLA	C3C-C2C	5.31	1.48	1.36
23	C	514	CLA	CHC-C1C	5.31	1.48	1.35
23	D	406	CLA	C3B-C2B	5.31	1.47	1.40
23	b	614	CLA	C3D-C2D	5.31	1.48	1.39
23	B	607	CLA	C3C-C2C	5.31	1.48	1.36
23	c	506	CLA	C3B-C2B	5.29	1.47	1.40
23	b	613	CLA	O2D-CGD	5.29	1.46	1.33
23	c	510	CLA	C3C-C2C	5.29	1.48	1.36
23	b	605	CLA	C3D-C2D	5.29	1.48	1.39
23	A	408	CLA	C3C-C2C	5.29	1.48	1.36
23	c	507	CLA	C3C-C2C	5.29	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	604	CLA	C3C-C2C	5.28	1.48	1.36
23	C	513	CLA	CHC-C1C	5.27	1.48	1.35
23	b	607	CLA	C3D-C2D	5.27	1.48	1.39
23	b	604	CLA	C3D-C2D	5.27	1.48	1.39
23	B	606	CLA	C3D-C2D	5.27	1.48	1.39
23	c	509	CLA	CHC-C1C	5.27	1.48	1.35
24	a	353	PHO	CHC-C1C	5.26	1.48	1.38
23	b	606	CLA	C3D-C2D	5.26	1.48	1.39
23	b	607	CLA	C3B-C2B	5.26	1.47	1.40
23	b	602	CLA	C3C-C2C	5.26	1.47	1.36
23	D	406	CLA	C3C-C2C	5.26	1.47	1.36
24	a	353	PHO	CHD-C1D	5.25	1.48	1.38
23	c	513	CLA	CHC-C1C	5.25	1.48	1.35
23	b	603	CLA	C3D-C2D	5.25	1.48	1.39
23	b	604	CLA	C3C-C2C	5.25	1.47	1.36
23	C	514	CLA	C3C-C2C	5.24	1.47	1.36
23	B	608	CLA	C3C-C2C	5.24	1.47	1.36
23	b	603	CLA	C3C-C2C	5.24	1.47	1.36
23	C	508	CLA	C3B-C2B	5.24	1.47	1.40
25	b	617	BCR	C23-C22	-5.24	1.34	1.45
23	d	402	CLA	C3D-C2D	5.24	1.48	1.39
23	C	502	CLA	C3D-C2D	5.23	1.48	1.39
25	B	619	BCR	C23-C22	-5.23	1.34	1.45
23	A	404	CLA	C3C-C2C	5.22	1.47	1.36
23	D	406	CLA	CHC-C1C	5.22	1.48	1.35
23	b	602	CLA	C3B-C2B	5.21	1.47	1.40
23	a	407	CLA	C3B-C2B	5.21	1.47	1.40
23	B	613	CLA	O2D-CGD	5.21	1.45	1.33
23	A	405	CLA	CHC-C1C	5.20	1.48	1.35
23	C	505	CLA	C3C-C2C	5.20	1.47	1.36
23	d	403	CLA	C3C-C2C	5.20	1.47	1.36
23	B	602	CLA	C3B-C2B	5.20	1.47	1.40
23	B	610	CLA	CHC-C1C	5.20	1.48	1.35
23	B	616	CLA	CHC-C1C	5.20	1.48	1.35
23	A	405	CLA	C3C-C2C	5.19	1.47	1.36
23	c	506	CLA	C3D-C2D	5.19	1.48	1.39
23	B	616	CLA	C3C-C2C	5.18	1.47	1.36
23	a	407	CLA	C3C-C2C	5.18	1.47	1.36
23	A	406	CLA	C3C-C2C	5.18	1.47	1.36
25	k	101	BCR	C23-C22	-5.18	1.34	1.45
23	B	601	CLA	CHC-C1C	5.18	1.48	1.35
23	A	408	CLA	CHC-C1C	5.17	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	605	CLA	C3C-C2C	5.17	1.47	1.36
24	A	407	PHO	C3C-C2C	5.17	1.47	1.36
23	c	504	CLA	C3B-C2B	5.17	1.47	1.40
23	b	607	CLA	C3C-C2C	5.17	1.47	1.36
23	C	512	CLA	O2D-CGD	5.16	1.45	1.33
23	C	507	CLA	C3C-C2C	5.16	1.47	1.36
23	C	502	CLA	C3C-C2C	5.16	1.47	1.36
23	c	512	CLA	C3C-C2C	5.15	1.47	1.36
23	B	609	CLA	C3C-C2C	5.15	1.47	1.36
23	b	616	CLA	C3C-C2C	5.14	1.47	1.36
23	A	406	CLA	C3B-C2B	5.14	1.47	1.40
25	C	516	BCR	C23-C22	-5.14	1.34	1.45
23	C	506	CLA	C3C-C2C	5.14	1.47	1.36
23	C	504	CLA	C3C-C2C	5.14	1.47	1.36
23	c	510	CLA	CHC-C1C	5.14	1.48	1.35
23	B	614	CLA	C3D-C2D	5.14	1.48	1.39
23	c	510	CLA	O2D-CGD	5.13	1.45	1.33
25	C	515	BCR	C23-C22	-5.13	1.34	1.45
23	b	615	CLA	C3B-C2B	5.13	1.47	1.40
23	c	514	CLA	CHC-C1C	5.12	1.48	1.35
23	d	402	CLA	C3C-C2C	5.12	1.47	1.36
23	a	409	CLA	C3C-C2C	5.12	1.47	1.36
23	B	605	CLA	CHC-C1C	5.12	1.48	1.35
23	b	606	CLA	CHC-C1C	5.12	1.48	1.35
23	c	502	CLA	CHC-C1C	5.11	1.48	1.35
23	B	609	CLA	CHC-C1C	5.11	1.48	1.35
25	d	404	BCR	C23-C22	-5.10	1.35	1.45
23	b	610	CLA	CHC-C1C	5.10	1.48	1.35
23	B	609	CLA	O2D-CGD	5.10	1.45	1.33
23	c	504	CLA	C3C-C2C	5.09	1.47	1.36
23	C	506	CLA	CHC-C1C	5.09	1.48	1.35
23	a	409	CLA	CHC-C1C	5.08	1.48	1.35
23	b	614	CLA	C3C-C2C	5.08	1.47	1.36
23	D	405	CLA	C3D-C2D	5.08	1.48	1.39
23	c	506	CLA	C3C-C2C	5.07	1.47	1.36
25	c	515	BCR	C23-C22	-5.07	1.35	1.45
23	c	506	CLA	CHC-C1C	5.07	1.48	1.35
24	a	353	PHO	CHB-C1B	5.07	1.48	1.38
23	c	506	CLA	O2D-CGD	5.06	1.45	1.33
23	A	405	CLA	C3B-C2B	5.06	1.47	1.40
23	B	607	CLA	C3D-C2D	5.06	1.48	1.39
23	C	502	CLA	CHC-C1C	5.06	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	406	CLA	CHC-C1C	5.05	1.47	1.35
23	a	406	CLA	O2D-CGD	5.05	1.45	1.33
23	b	615	CLA	CHC-C1C	5.04	1.47	1.35
23	B	614	CLA	CHC-C1C	5.04	1.47	1.35
23	c	509	CLA	O2D-CGD	5.04	1.45	1.33
23	b	616	CLA	O2D-CGD	5.03	1.45	1.33
23	C	512	CLA	CHC-C1C	5.03	1.47	1.35
23	b	611	CLA	C3C-C2C	5.03	1.47	1.36
23	c	508	CLA	OBD-CAD	5.02	1.29	1.22
23	a	405	CLA	C3C-C2C	5.02	1.47	1.36
23	D	406	CLA	O2D-CGD	5.02	1.45	1.33
23	B	607	CLA	OBD-CAD	5.02	1.29	1.22
23	d	402	CLA	CHC-C1C	5.01	1.47	1.35
23	C	503	CLA	CHC-C1C	5.01	1.47	1.35
23	B	609	CLA	C3B-C2B	5.01	1.47	1.40
23	C	504	CLA	CHC-C1C	5.00	1.47	1.35
23	b	608	CLA	O2D-CGD	4.99	1.45	1.33
23	c	507	CLA	O2D-CGD	4.99	1.45	1.33
23	c	503	CLA	C3C-C2C	4.99	1.47	1.36
23	C	503	CLA	C3C-C2C	4.99	1.47	1.36
23	a	405	CLA	O2D-CGD	4.98	1.45	1.33
23	B	606	CLA	C3C-C2C	4.98	1.47	1.36
23	c	504	CLA	CHC-C1C	4.98	1.47	1.35
23	B	615	CLA	OBD-CAD	4.98	1.29	1.22
23	c	505	CLA	C3C-C2C	4.98	1.47	1.36
23	b	611	CLA	CHC-C1C	4.97	1.47	1.35
23	b	610	CLA	C3D-C2D	4.96	1.48	1.39
23	b	601	CLA	O2D-CGD	4.96	1.45	1.33
23	b	603	CLA	O2D-CGD	4.96	1.45	1.33
25	K	102	BCR	C23-C22	-4.96	1.35	1.45
23	B	615	CLA	CHC-C1C	4.95	1.47	1.35
23	b	608	CLA	CHC-C1C	4.95	1.47	1.35
24	a	353	PHO	O2D-CGD	4.95	1.45	1.33
23	c	511	CLA	CHC-C1C	4.95	1.47	1.35
23	C	510	CLA	OBD-CAD	4.95	1.29	1.22
23	b	609	CLA	CHC-C1C	4.95	1.47	1.35
23	B	610	CLA	OBD-CAD	4.94	1.29	1.22
23	c	511	CLA	C3C-C2C	4.94	1.47	1.36
23	B	603	CLA	C3C-C2C	4.94	1.47	1.36
23	a	407	CLA	CHC-C1C	4.93	1.47	1.35
23	B	612	CLA	C3C-C2C	4.93	1.47	1.36
25	c	516	BCR	C23-C22	-4.93	1.35	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	406	CLA	CHC-C1C	4.93	1.47	1.35
23	c	505	CLA	O2D-CGD	4.93	1.45	1.33
23	C	505	CLA	CHC-C1C	4.92	1.47	1.35
23	C	507	CLA	O2D-CGD	4.92	1.45	1.33
25	A	409	BCR	C23-C22	-4.92	1.35	1.45
23	B	601	CLA	O2D-CGD	4.92	1.45	1.33
23	A	405	CLA	O2D-CGD	4.92	1.45	1.33
23	D	405	CLA	C3C-C2C	4.92	1.47	1.36
23	b	608	CLA	OBD-CAD	4.92	1.29	1.22
23	b	609	CLA	O2D-CGD	4.91	1.45	1.33
23	A	404	CLA	CHC-C1C	4.91	1.47	1.35
24	A	353	PHO	O2D-CGD	4.91	1.45	1.33
25	y	101	BCR	C23-C22	-4.89	1.35	1.45
23	c	503	CLA	CHC-C1C	4.88	1.47	1.35
23	B	603	CLA	CHC-C1C	4.88	1.47	1.35
23	b	609	CLA	C3C-C2C	4.88	1.47	1.36
23	C	505	CLA	O2D-CGD	4.88	1.45	1.33
25	b	619	BCR	C23-C22	-4.88	1.35	1.45
24	a	408	PHO	CHD-C1D	4.87	1.48	1.38
24	a	408	PHO	CHB-C1B	4.87	1.48	1.38
23	c	512	CLA	CHC-C1C	4.87	1.47	1.35
23	c	508	CLA	CHC-C1C	4.87	1.47	1.35
23	a	406	CLA	C3B-C2B	4.86	1.47	1.40
23	c	508	CLA	O2D-CGD	4.85	1.45	1.33
23	b	603	CLA	CHC-C1C	4.85	1.47	1.35
23	b	602	CLA	O2D-CGD	4.85	1.45	1.33
25	T	101	BCR	C23-C22	-4.85	1.35	1.45
24	A	407	PHO	CHB-C1B	4.84	1.48	1.38
24	A	407	PHO	O2D-CGD	4.84	1.45	1.33
23	C	509	CLA	CHC-C1C	4.83	1.47	1.35
23	c	511	CLA	O2D-CGD	4.83	1.45	1.33
23	b	614	CLA	O2D-CGD	4.83	1.45	1.33
23	b	605	CLA	O2D-CGD	4.83	1.45	1.33
23	b	601	CLA	CHC-C1C	4.83	1.47	1.35
23	c	513	CLA	OBD-CAD	4.83	1.29	1.22
23	c	508	CLA	C3C-C2C	4.82	1.47	1.36
23	d	402	CLA	O2D-CGD	4.82	1.45	1.33
23	b	607	CLA	CHC-C1C	4.82	1.47	1.35
23	B	604	CLA	CHC-C1C	4.81	1.47	1.35
23	B	614	CLA	O2D-CGD	4.81	1.44	1.33
23	B	604	CLA	C3D-C2D	4.81	1.48	1.39
23	b	613	CLA	CHC-C1C	4.80	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	407	BCR	C23-C22	-4.80	1.35	1.45
23	C	514	CLA	O2D-CGD	4.80	1.44	1.33
25	B	617	BCR	C23-C22	-4.80	1.35	1.45
25	t	103	BCR	C23-C22	-4.80	1.35	1.45
23	D	406	CLA	OBD-CAD	4.79	1.29	1.22
25	b	618	BCR	C23-C22	-4.79	1.35	1.45
23	B	607	CLA	CHC-C1C	4.79	1.47	1.35
23	B	602	CLA	O2D-CGD	4.79	1.44	1.33
23	c	507	CLA	CHC-C1C	4.78	1.47	1.35
23	b	614	CLA	CHC-C1C	4.78	1.47	1.35
23	B	613	CLA	C3C-C2C	4.78	1.46	1.36
23	C	503	CLA	O2D-CGD	4.78	1.44	1.33
23	A	406	CLA	O2D-CGD	4.76	1.44	1.33
23	C	506	CLA	C3D-C2D	4.76	1.48	1.39
23	B	615	CLA	O2D-CGD	4.76	1.44	1.33
23	C	507	CLA	CHC-C1C	4.75	1.47	1.35
23	B	615	CLA	C3C-C2C	4.75	1.46	1.36
23	B	601	CLA	O2A-CGA	4.75	1.47	1.33
23	A	405	CLA	OBD-CAD	4.75	1.28	1.22
23	c	514	CLA	O2D-CGD	4.74	1.44	1.33
23	B	605	CLA	O2D-CGD	4.74	1.44	1.33
24	A	407	PHO	CHD-C1D	4.73	1.47	1.38
23	B	611	CLA	O2D-CGD	4.73	1.44	1.33
23	b	612	CLA	CHC-C1C	4.73	1.47	1.35
23	A	408	CLA	O2D-CGD	4.73	1.44	1.33
23	b	607	CLA	O2D-CGD	4.73	1.44	1.33
23	B	611	CLA	CHC-C1C	4.72	1.47	1.35
23	C	506	CLA	O2D-CGD	4.72	1.44	1.33
23	B	616	CLA	O2D-CGD	4.71	1.44	1.33
23	C	511	CLA	O2D-CGD	4.71	1.44	1.33
23	c	505	CLA	CHC-C1C	4.70	1.47	1.35
23	B	604	CLA	O2D-CGD	4.70	1.44	1.33
23	C	510	CLA	CHC-C1C	4.70	1.47	1.35
23	D	405	CLA	CHC-C1C	4.70	1.47	1.35
25	H	101	BCR	C23-C22	-4.69	1.35	1.45
26	F	101	SQD	O47-C7	4.69	1.47	1.34
23	b	603	CLA	OBD-CAD	4.69	1.28	1.22
23	B	606	CLA	CHC-C1C	4.68	1.47	1.35
23	b	612	CLA	O2D-CGD	4.67	1.44	1.33
23	c	513	CLA	O2D-CGD	4.67	1.44	1.33
23	B	613	CLA	CHC-C1C	4.67	1.46	1.35
23	B	612	CLA	O2D-CGD	4.67	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	612	CLA	CHC-C1C	4.67	1.46	1.35
24	A	407	PHO	CHC-C1C	4.66	1.47	1.38
23	d	403	CLA	OBD-CAD	4.66	1.28	1.22
25	a	410	BCR	C23-C22	-4.65	1.35	1.45
23	c	505	CLA	OBD-CAD	4.64	1.28	1.22
23	C	503	CLA	OBD-CAD	4.64	1.28	1.22
23	C	509	CLA	O2D-CGD	4.64	1.44	1.33
23	b	609	CLA	OBD-CAD	4.64	1.28	1.22
23	c	507	CLA	OBD-CAD	4.63	1.28	1.22
24	A	353	PHO	CHC-C1C	4.63	1.47	1.38
25	h	101	BCR	C23-C22	-4.63	1.36	1.45
23	b	611	CLA	O2D-CGD	4.62	1.44	1.33
23	b	604	CLA	O2D-CGD	4.62	1.44	1.33
23	B	610	CLA	O2D-CGD	4.61	1.44	1.33
23	a	405	CLA	CHC-C1C	4.60	1.46	1.35
23	b	615	CLA	O2D-CGD	4.60	1.44	1.33
23	b	601	CLA	OBD-CAD	4.59	1.28	1.22
23	b	602	CLA	OBD-CAD	4.58	1.28	1.22
23	b	605	CLA	OBD-CAD	4.58	1.28	1.22
23	B	615	CLA	C3B-C2B	4.58	1.46	1.40
23	a	407	CLA	O2D-CGD	4.58	1.44	1.33
23	C	510	CLA	O2D-CGD	4.58	1.44	1.33
23	b	601	CLA	O2A-CGA	4.58	1.46	1.33
23	C	512	CLA	OBD-CAD	4.58	1.28	1.22
23	C	509	CLA	OBD-CAD	4.57	1.28	1.22
23	c	511	CLA	OBD-CAD	4.57	1.28	1.22
23	c	503	CLA	O2D-CGD	4.55	1.44	1.33
23	c	502	CLA	O2D-CGD	4.55	1.44	1.33
23	b	610	CLA	OBD-CAD	4.54	1.28	1.22
25	Y	101	BCR	C23-C22	-4.54	1.36	1.45
23	a	407	CLA	OBD-CAD	4.54	1.28	1.22
23	B	603	CLA	O2D-CGD	4.53	1.44	1.33
23	b	605	CLA	CHC-C1C	4.53	1.46	1.35
33	C	521	LMG	O7-C10	4.53	1.47	1.34
23	c	512	CLA	O2D-CGD	4.52	1.44	1.33
23	a	406	CLA	O2A-CGA	4.52	1.46	1.33
23	b	604	CLA	CHC-C1C	4.51	1.46	1.35
23	C	504	CLA	O2D-CGD	4.50	1.44	1.33
23	B	601	CLA	OBD-CAD	4.50	1.28	1.22
23	B	616	CLA	OBD-CAD	4.50	1.28	1.22
23	A	404	CLA	O2D-CGD	4.49	1.44	1.33
23	B	611	CLA	OBD-CAD	4.48	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	353	PHO	CHB-C1B	4.48	1.47	1.38
23	B	613	CLA	OBD-CAD	4.48	1.28	1.22
23	D	405	CLA	O2D-CGD	4.47	1.44	1.33
26	a	413	SQD	O48-C23	4.47	1.46	1.33
23	B	609	CLA	OBD-CAD	4.45	1.28	1.22
23	c	504	CLA	O2D-CGD	4.45	1.44	1.33
23	C	513	CLA	O2D-CGD	4.45	1.44	1.33
23	C	508	CLA	O2D-CGD	4.45	1.44	1.33
23	a	409	CLA	O2D-CGD	4.45	1.44	1.33
23	C	512	CLA	C3C-C2C	4.44	1.46	1.36
23	C	513	CLA	OBD-CAD	4.44	1.28	1.22
23	c	510	CLA	OBD-CAD	4.43	1.28	1.22
37	E	101	LHG	O8-C23	4.41	1.46	1.33
23	A	404	CLA	OBD-CAD	4.41	1.28	1.22
23	d	402	CLA	OBD-CAD	4.40	1.28	1.22
23	B	615	CLA	O2A-CGA	4.40	1.46	1.33
26	f	102	SQD	O47-C7	4.39	1.46	1.34
23	A	406	CLA	OBD-CAD	4.39	1.28	1.22
24	a	408	PHO	O2D-CGD	4.38	1.43	1.33
23	C	504	CLA	OBD-CAD	4.37	1.28	1.22
23	c	509	CLA	OBD-CAD	4.36	1.28	1.22
23	B	602	CLA	OBD-CAD	4.36	1.28	1.22
23	a	405	CLA	OBD-CAD	4.35	1.28	1.22
33	Z	101	LMG	O7-C10	4.35	1.46	1.34
23	B	607	CLA	O2D-CGD	4.34	1.43	1.33
33	C	521	LMG	O8-C28	4.34	1.46	1.33
26	A	412	SQD	O48-C23	4.34	1.46	1.33
37	e	101	LHG	O8-C23	4.34	1.46	1.33
23	B	608	CLA	O2D-CGD	4.33	1.43	1.33
23	B	608	CLA	CHC-C1C	4.33	1.46	1.35
33	z	101	LMG	O8-C28	4.33	1.46	1.33
23	A	408	CLA	OBD-CAD	4.33	1.28	1.22
23	C	514	CLA	OBD-CAD	4.33	1.28	1.22
33	c	520	LMG	O8-C28	4.31	1.45	1.33
33	B	621	LMG	O8-C28	4.31	1.45	1.33
23	C	511	CLA	OBD-CAD	4.31	1.28	1.22
23	a	406	CLA	OBD-CAD	4.31	1.28	1.22
23	b	615	CLA	OBD-CAD	4.30	1.28	1.22
33	c	521	LMG	O8-C28	4.30	1.45	1.33
23	C	513	CLA	O2A-CGA	4.29	1.45	1.33
23	c	504	CLA	OBD-CAD	4.29	1.28	1.22
37	l	101	LHG	O8-C23	4.29	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	c	518	DGD	O1G-C1A	4.29	1.45	1.33
26	b	620	SQD	O47-C7	4.29	1.46	1.34
33	C	520	LMG	O8-C28	4.28	1.45	1.33
23	b	606	CLA	O2D-CGD	4.28	1.43	1.33
23	C	512	CLA	O2A-CGA	4.28	1.45	1.33
23	c	513	CLA	O2A-CGA	4.27	1.45	1.33
23	B	606	CLA	O2D-CGD	4.27	1.43	1.33
23	b	615	CLA	O2A-CGA	4.27	1.45	1.33
23	C	502	CLA	O2D-CGD	4.27	1.43	1.33
33	c	521	LMG	O7-C10	4.26	1.46	1.34
23	c	503	CLA	OBD-CAD	4.26	1.28	1.22
40	v	202	HEC	CBC-CAC	-4.25	1.33	1.49
26	B	620	SQD	O47-C7	4.25	1.46	1.34
37	e	101	LHG	O7-C7	4.25	1.46	1.34
23	c	512	CLA	OBD-CAD	4.23	1.28	1.22
26	f	102	SQD	O48-C23	4.22	1.45	1.33
23	C	502	CLA	OBD-CAD	4.22	1.28	1.22
33	C	501	LMG	O8-C28	4.21	1.45	1.33
23	B	609	CLA	O2A-CGA	4.21	1.45	1.33
23	a	409	CLA	O2A-CGA	4.20	1.45	1.33
23	C	514	CLA	O2A-CGA	4.19	1.45	1.33
23	B	606	CLA	O2A-CGA	4.18	1.45	1.33
26	B	620	SQD	O48-C23	4.18	1.45	1.33
23	c	508	CLA	O2A-CGA	4.18	1.45	1.33
23	c	514	CLA	O2A-CGA	4.18	1.45	1.33
23	C	508	CLA	OBD-CAD	4.18	1.28	1.22
23	c	502	CLA	OBD-CAD	4.18	1.28	1.22
23	c	514	CLA	OBD-CAD	4.18	1.28	1.22
23	b	608	CLA	O2A-CGA	4.18	1.45	1.33
23	C	507	CLA	O2A-CGA	4.17	1.45	1.33
23	A	408	CLA	O2A-CGA	4.16	1.45	1.33
26	a	413	SQD	O47-C7	4.16	1.46	1.34
23	b	604	CLA	OBD-CAD	4.16	1.28	1.22
33	C	520	LMG	O7-C10	4.15	1.46	1.34
26	b	620	SQD	O48-C23	4.15	1.45	1.33
23	b	610	CLA	O2D-CGD	4.15	1.43	1.33
23	d	403	CLA	O2A-CGA	4.15	1.45	1.33
24	A	407	PHO	O2A-CGA	4.14	1.45	1.33
23	c	512	CLA	O2A-CGA	4.14	1.45	1.33
37	L	101	LHG	O8-C23	4.13	1.45	1.33
23	d	403	CLA	O2D-CGD	4.13	1.43	1.33
23	C	508	CLA	O2A-CGA	4.13	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	606	CLA	OBD-CAD	4.13	1.28	1.22
24	A	353	PHO	CHD-C1D	4.13	1.46	1.38
23	B	613	CLA	O2A-CGA	4.13	1.45	1.33
37	d	408	LHG	O8-C23	4.13	1.45	1.33
33	m	101	LMG	O8-C28	4.12	1.45	1.33
23	C	502	CLA	O2A-CGA	4.12	1.45	1.33
23	c	510	CLA	O2A-CGA	4.12	1.45	1.33
35	c	519	DGD	O1G-C1A	4.12	1.45	1.33
33	C	501	LMG	O7-C10	4.11	1.45	1.34
23	c	509	CLA	O2A-CGA	4.11	1.45	1.33
26	A	410	SQD	O48-C23	4.11	1.45	1.33
40	V	202	HEC	CBC-CAC	-4.11	1.34	1.49
40	V	202	HEC	CBB-CAB	-4.11	1.34	1.49
37	d	408	LHG	O7-C7	4.10	1.45	1.34
26	A	412	SQD	O47-C7	4.08	1.45	1.34
23	c	506	CLA	OBD-CAD	4.08	1.28	1.22
40	v	202	HEC	CBB-CAB	-4.08	1.34	1.49
23	C	503	CLA	O2A-CGA	4.07	1.45	1.33
23	b	612	CLA	O2A-CGA	4.07	1.45	1.33
25	B	618	BCR	C23-C22	-4.07	1.37	1.45
33	a	419	LMG	O8-C28	4.07	1.45	1.33
35	h	102	DGD	O1G-C1A	4.06	1.45	1.33
23	b	616	CLA	O2A-CGA	4.06	1.45	1.33
26	a	411	SQD	O48-C23	4.06	1.45	1.33
37	E	101	LHG	O7-C7	4.05	1.45	1.34
23	c	504	CLA	O2A-CGA	4.05	1.45	1.33
24	a	353	PHO	O2A-CGA	4.05	1.45	1.33
35	C	518	DGD	O1G-C1A	4.04	1.45	1.33
24	a	408	PHO	CHC-C1C	4.03	1.46	1.38
23	b	602	CLA	O2A-CGA	4.02	1.45	1.33
23	C	505	CLA	OBD-CAD	4.02	1.27	1.22
23	b	613	CLA	O2A-CGA	4.00	1.45	1.33
23	D	405	CLA	O2A-CGA	4.00	1.45	1.33
23	c	502	CLA	O2A-CGA	4.00	1.45	1.33
33	a	419	LMG	O7-C10	3.99	1.45	1.34
23	d	402	CLA	O2A-CGA	3.99	1.45	1.33
26	F	101	SQD	O48-C23	3.99	1.45	1.33
23	b	616	CLA	OBD-CAD	3.98	1.27	1.22
33	c	520	LMG	O7-C10	3.98	1.45	1.34
33	z	101	LMG	O7-C10	3.97	1.45	1.34
23	b	606	CLA	O2A-CGA	3.97	1.44	1.33
23	b	612	CLA	OBD-CAD	3.97	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	511	CLA	O2A-CGA	3.96	1.44	1.33
23	c	507	CLA	O2A-CGA	3.95	1.44	1.33
23	B	616	CLA	O2A-CGA	3.94	1.44	1.33
24	A	353	PHO	OBD-CAD	3.94	1.29	1.22
23	B	607	CLA	O2A-CGA	3.94	1.44	1.33
35	c	517	DGD	O1G-C1A	3.94	1.44	1.33
33	d	412	LMG	O8-C28	3.93	1.44	1.33
34	B	622	HTG	C1'-S1	-3.93	1.76	1.81
37	D	411	LHG	O7-C7	3.93	1.45	1.34
23	C	510	CLA	O2A-CGA	3.93	1.44	1.33
23	b	611	CLA	O2A-CGA	3.92	1.44	1.33
23	b	604	CLA	O2A-CGA	3.92	1.44	1.33
23	b	611	CLA	OBD-CAD	3.91	1.27	1.22
23	b	614	CLA	O2A-CGA	3.91	1.44	1.33
23	b	607	CLA	OBD-CAD	3.91	1.27	1.22
23	A	405	CLA	O2A-CGA	3.91	1.44	1.33
23	C	509	CLA	O2A-CGA	3.90	1.44	1.33
33	d	412	LMG	O7-C10	3.90	1.45	1.34
23	a	407	CLA	O2A-CGA	3.90	1.44	1.33
23	B	612	CLA	OBD-CAD	3.89	1.27	1.22
35	C	519	DGD	O1G-C1A	3.89	1.44	1.33
23	C	506	CLA	O2A-CGA	3.89	1.44	1.33
35	C	517	DGD	O2G-C1B	3.88	1.45	1.34
23	C	507	CLA	OBD-CAD	3.87	1.27	1.22
23	B	602	CLA	O2A-CGA	3.86	1.44	1.33
24	a	353	PHO	OBD-CAD	3.86	1.29	1.22
35	H	102	DGD	O1G-C1A	3.85	1.44	1.33
23	B	606	CLA	OBD-CAD	3.83	1.27	1.22
23	B	608	CLA	OBD-CAD	3.83	1.27	1.22
26	a	411	SQD	O47-C7	3.83	1.45	1.34
23	A	406	CLA	O2A-CGA	3.82	1.44	1.33
23	C	506	CLA	OBD-CAD	3.82	1.27	1.22
23	c	506	CLA	O2A-CGA	3.82	1.44	1.33
23	B	604	CLA	O2A-CGA	3.81	1.44	1.33
34	b	622	HTG	C1'-S1	-3.81	1.76	1.81
34	d	411	HTG	C1'-S1	-3.81	1.76	1.81
35	c	518	DGD	O2G-C1B	3.80	1.45	1.34
23	C	504	CLA	O2A-CGA	3.78	1.44	1.33
33	D	415	LMG	O8-C28	3.78	1.44	1.33
37	d	406	LHG	O8-C23	3.78	1.44	1.33
35	C	518	DGD	O2G-C1B	3.78	1.45	1.34
24	a	353	PHO	C3D-C2D	3.77	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	B	621	LMG	O7-C10	3.77	1.44	1.34
23	b	614	CLA	OBD-CAD	3.77	1.27	1.22
37	D	409	LHG	O8-C23	3.76	1.44	1.33
35	h	102	DGD	O2G-C1B	3.76	1.44	1.34
23	b	609	CLA	O2A-CGA	3.75	1.44	1.33
34	b	623	HTG	C1'-S1	-3.75	1.76	1.81
35	C	517	DGD	O1G-C1A	3.75	1.44	1.33
23	C	505	CLA	O2A-CGA	3.75	1.44	1.33
37	L	101	LHG	O7-C7	3.73	1.44	1.34
23	B	614	CLA	OBD-CAD	3.71	1.27	1.22
24	A	407	PHO	C4A-NA	-3.71	1.26	1.35
23	B	608	CLA	O2A-CGA	3.71	1.44	1.33
23	B	603	CLA	OBD-CAD	3.71	1.27	1.22
37	D	411	LHG	O8-C23	3.68	1.44	1.33
35	c	517	DGD	O2G-C1B	3.67	1.44	1.34
35	c	519	DGD	O2G-C1B	3.67	1.44	1.34
24	a	408	PHO	C3D-C2D	3.67	1.49	1.39
23	B	603	CLA	O2A-CGA	3.64	1.44	1.33
23	a	409	CLA	OBD-CAD	3.64	1.27	1.22
23	b	603	CLA	O2A-CGA	3.64	1.44	1.33
26	A	410	SQD	O47-C7	3.63	1.44	1.34
33	m	101	LMG	O7-C10	3.63	1.44	1.34
23	B	605	CLA	OBD-CAD	3.63	1.27	1.22
24	A	353	PHO	C3D-C2D	3.61	1.49	1.39
23	c	503	CLA	O2A-CGA	3.60	1.43	1.33
37	d	407	LHG	O7-C7	3.60	1.44	1.34
23	B	611	CLA	O2A-CGA	3.60	1.43	1.33
23	B	614	CLA	O2A-CGA	3.59	1.43	1.33
33	D	415	LMG	O7-C10	3.59	1.44	1.34
24	A	353	PHO	C4A-NA	-3.55	1.26	1.35
23	B	610	CLA	O2A-CGA	3.55	1.43	1.33
23	D	405	CLA	OBD-CAD	3.55	1.27	1.22
35	H	102	DGD	O2G-C1B	3.55	1.44	1.34
23	b	613	CLA	OBD-CAD	3.53	1.27	1.22
23	b	607	CLA	O2A-CGA	3.53	1.43	1.33
37	D	409	LHG	O7-C7	3.53	1.44	1.34
37	d	407	LHG	O8-C23	3.52	1.43	1.33
23	B	605	CLA	O2A-CGA	3.52	1.43	1.33
23	b	605	CLA	O2A-CGA	3.51	1.43	1.33
24	A	407	PHO	C3D-C2D	3.51	1.48	1.39
23	D	406	CLA	O2A-CGA	3.49	1.43	1.33
35	C	519	DGD	O2G-C1B	3.49	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	511	CLA	O2A-CGA	3.49	1.43	1.33
23	B	604	CLA	OBD-CAD	3.49	1.27	1.22
23	c	505	CLA	O2A-CGA	3.49	1.43	1.33
37	l	101	LHG	O7-C7	3.47	1.44	1.34
24	a	353	PHO	CHC-C4B	3.45	1.48	1.40
37	D	410	LHG	O7-C7	3.43	1.44	1.34
23	b	610	CLA	O2A-CGA	3.43	1.43	1.33
37	d	406	LHG	O7-C7	3.42	1.44	1.34
23	a	405	CLA	O2A-CGA	3.40	1.43	1.33
24	A	353	PHO	O2A-CGA	3.39	1.43	1.33
34	c	522	HTG	C1'-S1	-3.38	1.77	1.81
24	A	407	PHO	CHD-C4C	3.37	1.48	1.40
37	D	410	LHG	O8-C23	3.36	1.43	1.33
23	B	612	CLA	O2A-CGA	3.34	1.43	1.33
24	a	408	PHO	C4A-NA	-3.30	1.27	1.35
24	A	407	PHO	OBD-CAD	3.29	1.28	1.22
24	a	408	PHO	CHD-C4C	3.26	1.48	1.40
34	B	626	HTG	C1'-S1	-3.24	1.77	1.81
24	A	353	PHO	CHC-C4B	3.23	1.48	1.40
24	a	408	PHO	O2A-CGA	3.21	1.42	1.33
23	B	612	CLA	C1B-NB	-3.21	1.32	1.35
34	B	623	HTG	C1'-S1	-3.21	1.77	1.81
23	A	404	CLA	O2A-CGA	3.20	1.42	1.33
34	b	625	HTG	C1'-S1	-3.17	1.77	1.81
34	D	414	HTG	C1'-S1	-3.17	1.77	1.81
34	C	522	HTG	C1'-S1	-3.13	1.77	1.81
24	a	353	PHO	C4A-NA	-3.13	1.27	1.35
23	b	601	CLA	C1D-C2D	3.13	1.49	1.42
23	d	403	CLA	C1D-C2D	3.10	1.49	1.42
40	v	202	HEC	C3B-C2B	-3.08	1.37	1.40
23	B	602	CLA	C1C-C2C	3.06	1.50	1.44
24	a	408	PHO	OBD-CAD	3.05	1.27	1.22
38	e	87	HEM	C3B-C2B	-3.04	1.36	1.40
23	b	603	CLA	C1C-C2C	3.02	1.50	1.44
23	b	605	CLA	C1D-C2D	3.02	1.49	1.42
23	C	514	CLA	C1D-C2D	3.00	1.49	1.42
23	c	514	CLA	C1D-C2D	3.00	1.49	1.42
40	V	202	HEC	C3B-C2B	-2.98	1.37	1.40
23	C	507	CLA	C1D-C2D	2.95	1.49	1.42
24	a	408	PHO	C3B-C4B	2.94	1.49	1.43
24	a	353	PHO	CHD-C4C	2.93	1.47	1.40
23	C	502	CLA	C1D-C2D	2.90	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407	PHO	CHC-C4B	2.90	1.47	1.40
23	c	508	CLA	C1D-C2D	2.90	1.49	1.42
23	c	502	CLA	C1D-C2D	2.90	1.49	1.42
23	D	406	CLA	C1C-C2C	2.90	1.50	1.44
23	b	607	CLA	C1B-NB	-2.90	1.32	1.35
23	a	407	CLA	C1D-C2D	2.89	1.49	1.42
24	A	353	PHO	CHD-C4C	2.88	1.47	1.40
23	b	615	CLA	C1D-C2D	2.87	1.49	1.42
24	a	408	PHO	CHB-C4A	2.87	1.47	1.40
23	C	508	CLA	C1C-C2C	2.86	1.50	1.44
23	C	512	CLA	C1C-C2C	2.85	1.50	1.44
23	A	405	CLA	C1C-C2C	2.85	1.50	1.44
23	B	601	CLA	C1D-C2D	2.85	1.49	1.42
23	c	505	CLA	C1C-C2C	2.83	1.50	1.44
23	C	510	CLA	C1D-C2D	2.83	1.49	1.42
23	a	406	CLA	C1D-C2D	2.83	1.49	1.42
23	b	611	CLA	C1D-C2D	2.83	1.49	1.42
23	c	504	CLA	C4C-C3C	2.82	1.49	1.45
23	a	409	CLA	C1B-NB	-2.82	1.32	1.35
24	a	353	PHO	CHB-C4A	2.82	1.47	1.40
23	A	405	CLA	C4B-CHC	2.80	1.48	1.41
23	B	613	CLA	C1B-NB	-2.79	1.32	1.35
26	f	102	SQD	C6-S	-2.79	1.67	1.77
23	c	505	CLA	C1D-C2D	2.79	1.48	1.42
23	b	602	CLA	C1D-C2D	2.79	1.48	1.42
23	b	610	CLA	C4B-CHC	2.77	1.48	1.41
23	b	609	CLA	C1D-C2D	2.77	1.48	1.42
23	B	602	CLA	C1D-C2D	2.77	1.48	1.42
26	A	410	SQD	C6-S	-2.77	1.67	1.77
24	a	408	PHO	CHC-C4B	2.76	1.46	1.40
23	C	514	CLA	C1C-C2C	2.76	1.49	1.44
23	b	602	CLA	C1C-C2C	2.76	1.49	1.44
26	A	412	SQD	C6-S	-2.75	1.67	1.77
23	B	609	CLA	C1D-C2D	2.74	1.48	1.42
23	b	607	CLA	C1D-C2D	2.74	1.48	1.42
29	a	416	PL9	C6-C5	2.74	1.49	1.35
40	V	202	HEC	C3B-C4B	2.74	1.48	1.43
23	c	506	CLA	C1C-C2C	2.74	1.49	1.44
23	C	508	CLA	C4B-CHC	2.73	1.48	1.41
23	b	602	CLA	C4B-CHC	2.73	1.48	1.41
24	A	407	PHO	C4C-C3C	2.73	1.50	1.45
24	A	353	PHO	C3B-C4B	2.72	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	353	PHO	C3B-C4B	2.72	1.48	1.43
23	A	408	CLA	C1D-C2D	2.72	1.48	1.42
23	c	511	CLA	C1B-CHB	2.72	1.48	1.41
34	B	626	HTG	C1-S1	-2.72	1.76	1.80
23	D	406	CLA	C4B-CHC	2.71	1.48	1.41
23	C	502	CLA	C1C-C2C	2.71	1.49	1.44
29	A	414	PL9	C6-C5	2.71	1.49	1.35
23	b	606	CLA	C1D-C2D	2.71	1.48	1.42
26	a	411	SQD	C6-S	-2.71	1.67	1.77
23	C	506	CLA	C1C-C2C	2.71	1.49	1.44
23	d	403	CLA	C4B-CHC	2.71	1.48	1.41
23	c	512	CLA	C1B-CHB	2.70	1.48	1.41
23	D	405	CLA	C1C-C2C	2.70	1.49	1.44
23	c	514	CLA	C1C-C2C	2.70	1.49	1.44
26	F	101	SQD	C6-S	-2.70	1.67	1.77
23	C	505	CLA	C1D-C2D	2.70	1.48	1.42
23	c	509	CLA	C1C-C2C	2.69	1.49	1.44
23	C	504	CLA	C4C-C3C	2.69	1.49	1.45
23	b	601	CLA	CHD-C4C	2.69	1.48	1.41
23	c	508	CLA	CHD-C4C	2.69	1.48	1.41
40	v	202	HEC	C3B-C4B	2.68	1.47	1.43
23	C	504	CLA	C1D-C2D	2.68	1.48	1.42
26	b	620	SQD	C6-S	-2.68	1.67	1.77
23	c	506	CLA	C4B-CHC	2.68	1.48	1.41
23	d	402	CLA	C4B-CHC	2.67	1.48	1.41
26	a	413	SQD	C6-S	-2.67	1.67	1.77
23	D	406	CLA	C1D-C2D	2.66	1.48	1.42
23	c	507	CLA	C1D-C2D	2.66	1.48	1.42
23	B	613	CLA	C4C-C3C	2.66	1.49	1.45
23	b	608	CLA	C1D-C2D	2.65	1.48	1.42
23	B	602	CLA	C4B-CHC	2.65	1.48	1.41
23	B	614	CLA	C1C-C2C	2.65	1.49	1.44
23	B	611	CLA	C1D-C2D	2.65	1.48	1.42
23	B	605	CLA	C1B-CHB	2.64	1.48	1.41
23	A	404	CLA	C1B-NB	-2.64	1.32	1.35
23	B	601	CLA	C4B-CHC	2.64	1.48	1.41
23	c	504	CLA	C1D-C2D	2.64	1.48	1.42
23	B	607	CLA	C1C-C2C	2.64	1.49	1.44
23	C	508	CLA	C1D-C2D	2.63	1.48	1.42
23	B	607	CLA	C1D-C2D	2.63	1.48	1.42
23	C	513	CLA	C1C-C2C	2.63	1.49	1.44
23	b	610	CLA	C1D-C2D	2.63	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	612	CLA	C1B-CHB	2.62	1.48	1.41
23	c	514	CLA	CHD-C4C	2.62	1.48	1.41
23	B	605	CLA	C4B-CHC	2.61	1.48	1.41
38	E	103	HEM	C3B-C2B	-2.61	1.36	1.40
24	A	407	PHO	C1A-NA	-2.61	1.32	1.37
23	B	613	CLA	C1C-C2C	2.61	1.49	1.44
23	c	502	CLA	CHD-C4C	2.60	1.48	1.41
23	c	510	CLA	C1D-C2D	2.60	1.48	1.42
23	b	616	CLA	C4B-CHC	2.60	1.48	1.41
23	B	603	CLA	C1C-C2C	2.60	1.49	1.44
23	B	615	CLA	C1C-C2C	2.60	1.49	1.44
23	c	509	CLA	C4B-CHC	2.59	1.48	1.41
23	b	611	CLA	C1B-CHB	2.59	1.48	1.41
23	A	406	CLA	C1D-C2D	2.59	1.48	1.42
23	B	604	CLA	C1B-CHB	2.58	1.48	1.41
23	C	509	CLA	C1B-CHB	2.58	1.48	1.41
23	C	514	CLA	CHD-C4C	2.58	1.48	1.41
23	B	605	CLA	C1C-C2C	2.58	1.49	1.44
23	c	510	CLA	C1C-C2C	2.58	1.49	1.44
23	B	614	CLA	C4B-CHC	2.57	1.48	1.41
23	C	506	CLA	C1B-CHB	2.57	1.48	1.41
23	B	612	CLA	C1C-C2C	2.57	1.49	1.44
23	b	607	CLA	C1C-C2C	2.57	1.49	1.44
23	b	603	CLA	C4C-C3C	2.56	1.49	1.45
33	Z	101	LMG	O8-C28	2.56	1.46	1.33
23	B	614	CLA	C1D-C2D	2.56	1.48	1.42
23	B	610	CLA	C1D-C2D	2.56	1.48	1.42
23	c	504	CLA	C1C-C2C	2.56	1.49	1.44
23	C	507	CLA	C4C-C3C	2.56	1.49	1.45
23	C	513	CLA	C4B-CHC	2.56	1.48	1.41
23	A	405	CLA	C1B-CHB	2.55	1.48	1.41
23	B	610	CLA	C4B-CHC	2.55	1.48	1.41
23	c	511	CLA	C1D-C2D	2.55	1.48	1.42
23	A	404	CLA	C1D-C2D	2.55	1.48	1.42
23	c	502	CLA	C4C-C3C	2.55	1.49	1.45
32	A	359	LMT	O1'-C1'	2.55	1.44	1.40
23	c	502	CLA	C1B-CHB	2.55	1.48	1.41
23	C	502	CLA	C4B-CHC	2.55	1.48	1.41
23	A	404	CLA	C4B-CHC	2.54	1.48	1.41
23	C	505	CLA	C4C-C3C	2.54	1.49	1.45
23	d	402	CLA	C1C-C2C	2.54	1.49	1.44
23	c	513	CLA	C1C-C2C	2.54	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	353	PHO	CHB-C4A	2.54	1.46	1.40
23	D	406	CLA	C1B-CHB	2.54	1.48	1.41
23	B	609	CLA	C1B-NB	-2.53	1.32	1.35
23	c	506	CLA	C1B-CHB	2.53	1.48	1.41
23	C	512	CLA	C1D-C2D	2.53	1.48	1.42
23	B	616	CLA	C1D-C2D	2.53	1.48	1.42
23	c	505	CLA	C4C-C3C	2.52	1.49	1.45
23	B	616	CLA	C1C-NC	-2.52	1.34	1.37
23	A	404	CLA	C4C-C3C	2.52	1.49	1.45
23	B	610	CLA	C1B-CHB	2.52	1.48	1.41
23	c	502	CLA	C4B-CHC	2.52	1.48	1.41
23	d	403	CLA	CHD-C4C	2.51	1.48	1.41
23	b	611	CLA	C4B-CHC	2.51	1.48	1.41
23	b	607	CLA	C4C-C3C	2.51	1.49	1.45
23	a	409	CLA	C1C-C2C	2.51	1.49	1.44
23	c	510	CLA	C1B-CHB	2.51	1.48	1.41
23	c	511	CLA	CHD-C4C	2.51	1.48	1.41
23	b	606	CLA	C1C-C2C	2.51	1.49	1.44
23	C	511	CLA	CHD-C4C	2.51	1.48	1.41
23	B	605	CLA	C1D-C2D	2.51	1.48	1.42
23	c	511	CLA	C1C-C2C	2.51	1.49	1.44
23	B	607	CLA	C4C-C3C	2.50	1.49	1.45
23	b	616	CLA	C1D-C2D	2.50	1.48	1.42
23	c	503	CLA	C1C-C2C	2.50	1.49	1.44
23	C	510	CLA	CHD-C4C	2.50	1.48	1.41
23	b	609	CLA	C1C-C2C	2.50	1.49	1.44
23	C	505	CLA	C1C-C2C	2.50	1.49	1.44
23	B	613	CLA	C1D-C2D	2.50	1.48	1.42
23	C	510	CLA	C4C-C3C	2.50	1.49	1.45
26	B	620	SQD	C6-S	-2.50	1.68	1.77
23	B	608	CLA	C1C-NC	-2.49	1.34	1.37
23	A	406	CLA	C4C-C3C	2.49	1.49	1.45
23	c	508	CLA	C1C-C2C	2.49	1.49	1.44
23	c	504	CLA	CHD-C4C	2.49	1.48	1.41
23	b	615	CLA	C1B-NB	-2.48	1.33	1.35
23	B	604	CLA	C1C-C2C	2.48	1.49	1.44
24	A	407	PHO	CHB-C4A	2.48	1.46	1.40
23	b	608	CLA	C1C-C2C	2.48	1.49	1.44
23	c	507	CLA	CHD-C4C	2.48	1.48	1.41
23	b	609	CLA	C1B-CHB	2.48	1.47	1.41
23	b	616	CLA	C1C-C2C	2.47	1.49	1.44
23	B	616	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	503	CLA	C1D-C2D	2.47	1.48	1.42
23	B	615	CLA	C1D-C2D	2.47	1.48	1.42
23	a	405	CLA	C1B-CHB	2.47	1.47	1.41
23	B	609	CLA	C4B-CHC	2.47	1.47	1.41
23	C	504	CLA	C1C-C2C	2.46	1.49	1.44
23	B	609	CLA	C1C-C2C	2.46	1.49	1.44
23	C	511	CLA	C1D-C2D	2.46	1.48	1.42
23	b	602	CLA	CHD-C4C	2.45	1.48	1.41
23	C	510	CLA	C1C-C2C	2.45	1.49	1.44
23	C	509	CLA	C4C-C3C	2.45	1.49	1.45
23	B	608	CLA	C1B-CHB	2.45	1.47	1.41
23	C	512	CLA	C1B-CHB	2.45	1.47	1.41
23	C	512	CLA	C4C-C3C	2.45	1.49	1.45
23	c	512	CLA	C1D-C2D	2.45	1.48	1.42
29	D	408	PL9	C6-C5	2.45	1.48	1.35
23	A	405	CLA	C1D-C2D	2.45	1.48	1.42
23	B	607	CLA	C1B-NB	-2.45	1.33	1.35
23	A	408	CLA	CHD-C4C	2.44	1.48	1.41
23	B	601	CLA	C1C-C2C	2.44	1.49	1.44
29	d	405	PL9	C6-C5	2.44	1.48	1.35
23	a	405	CLA	CHD-C4C	2.44	1.48	1.41
24	a	408	PHO	C4C-C3C	2.44	1.49	1.45
23	c	503	CLA	C1B-CHB	2.44	1.47	1.41
23	a	405	CLA	C4C-C3C	2.43	1.49	1.45
23	b	615	CLA	C4C-C3C	2.43	1.49	1.45
23	A	406	CLA	C1C-C2C	2.43	1.49	1.44
23	C	513	CLA	CHD-C4C	2.43	1.48	1.41
23	c	513	CLA	C4B-CHC	2.43	1.47	1.41
23	C	514	CLA	C1B-CHB	2.43	1.47	1.41
23	c	510	CLA	CHD-C4C	2.42	1.48	1.41
23	c	505	CLA	C1B-CHB	2.42	1.47	1.41
23	b	613	CLA	C1B-CHB	2.42	1.47	1.41
23	b	610	CLA	C1C-C2C	2.42	1.49	1.44
23	a	407	CLA	CHD-C4C	2.42	1.48	1.41
23	a	405	CLA	C1D-C2D	2.42	1.48	1.42
23	C	510	CLA	C1B-CHB	2.42	1.47	1.41
23	b	608	CLA	CHD-C4C	2.41	1.48	1.41
23	b	613	CLA	C4B-CHC	2.41	1.47	1.41
23	C	509	CLA	C1C-C2C	2.41	1.49	1.44
23	B	609	CLA	C1B-CHB	2.41	1.47	1.41
23	B	616	CLA	CHD-C4C	2.41	1.48	1.41
23	A	408	CLA	C4B-CHC	2.40	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	606	CLA	CHD-C4C	2.40	1.48	1.41
23	C	511	CLA	C4B-CHC	2.40	1.47	1.41
23	C	507	CLA	CHD-C4C	2.40	1.48	1.41
23	B	602	CLA	CHD-C4C	2.40	1.48	1.41
23	c	507	CLA	C1B-NB	-2.39	1.33	1.35
23	a	409	CLA	C1D-C2D	2.39	1.48	1.42
23	b	603	CLA	C1B-CHB	2.39	1.47	1.41
23	B	611	CLA	CHD-C4C	2.39	1.48	1.41
23	d	402	CLA	C1B-NB	-2.39	1.33	1.35
23	A	408	CLA	C1C-NC	-2.38	1.34	1.37
23	a	406	CLA	C4B-CHC	2.38	1.47	1.41
23	b	601	CLA	C1B-CHB	2.38	1.47	1.41
23	C	505	CLA	CHD-C4C	2.38	1.47	1.41
23	b	606	CLA	C1B-NB	-2.38	1.33	1.35
23	C	503	CLA	CHD-C4C	2.38	1.47	1.41
23	c	504	CLA	C4B-CHC	2.38	1.47	1.41
35	c	519	DGD	O2G-C2G	-2.38	1.40	1.46
23	C	504	CLA	CHD-C4C	2.38	1.47	1.41
23	C	505	CLA	C1B-CHB	2.38	1.47	1.41
23	b	609	CLA	C4C-C3C	2.37	1.49	1.45
23	c	513	CLA	C1D-C2D	2.37	1.47	1.42
23	b	613	CLA	C1C-C2C	2.37	1.49	1.44
23	c	512	CLA	C1C-C2C	2.37	1.49	1.44
23	A	404	CLA	CHD-C4C	2.37	1.47	1.41
23	c	512	CLA	CHD-C4C	2.37	1.47	1.41
23	B	616	CLA	C1B-CHB	2.37	1.47	1.41
24	a	353	PHO	C1B-NB	-2.37	1.33	1.38
23	C	503	CLA	C4B-CHC	2.37	1.47	1.41
23	C	502	CLA	C1B-CHB	2.36	1.47	1.41
23	B	611	CLA	C1C-C2C	2.36	1.49	1.44
23	c	503	CLA	C1D-C2D	2.36	1.47	1.42
23	C	513	CLA	C1D-C2D	2.36	1.47	1.42
23	d	403	CLA	C1C-C2C	2.36	1.49	1.44
23	C	506	CLA	C1B-NB	-2.36	1.33	1.35
23	B	607	CLA	C1B-CHB	2.36	1.47	1.41
23	C	514	CLA	C4B-CHC	2.35	1.47	1.41
23	b	605	CLA	C1B-CHB	2.35	1.47	1.41
23	B	613	CLA	C1B-CHB	2.35	1.47	1.41
23	C	511	CLA	C1B-CHB	2.35	1.47	1.41
23	C	508	CLA	CHD-C4C	2.35	1.47	1.41
23	B	614	CLA	C4B-NB	-2.35	1.33	1.35
23	b	616	CLA	CHD-C4C	2.34	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	406	CLA	CHD-C4C	2.34	1.47	1.41
23	C	502	CLA	CHD-C4C	2.34	1.47	1.41
23	c	504	CLA	C1B-CHB	2.34	1.47	1.41
23	b	609	CLA	CHD-C4C	2.34	1.47	1.41
23	b	612	CLA	C1C-C2C	2.34	1.49	1.44
23	b	614	CLA	C4C-C3C	2.34	1.49	1.45
23	b	607	CLA	C1B-CHB	2.34	1.47	1.41
23	b	608	CLA	C1B-CHB	2.34	1.47	1.41
23	c	510	CLA	C4B-CHC	2.34	1.47	1.41
23	c	502	CLA	C1C-C2C	2.34	1.49	1.44
23	b	614	CLA	C1B-CHB	2.33	1.47	1.41
23	B	613	CLA	C4B-CHC	2.33	1.47	1.41
23	c	506	CLA	CHD-C4C	2.33	1.47	1.41
23	B	608	CLA	C1D-C2D	2.33	1.47	1.42
23	A	408	CLA	C1C-C2C	2.33	1.49	1.44
23	C	510	CLA	C4B-NB	-2.33	1.33	1.35
23	B	610	CLA	CHD-C4C	2.33	1.47	1.41
23	C	509	CLA	C1D-C2D	2.33	1.47	1.42
23	c	505	CLA	C1C-NC	-2.32	1.34	1.37
23	C	505	CLA	C4B-CHC	2.32	1.47	1.41
23	B	611	CLA	C1B-CHB	2.32	1.47	1.41
23	b	614	CLA	C1D-C2D	2.32	1.47	1.42
23	b	611	CLA	CHD-C4C	2.32	1.47	1.41
23	b	610	CLA	CHD-C4C	2.31	1.47	1.41
23	b	615	CLA	CHD-C4C	2.31	1.47	1.41
23	b	604	CLA	C1C-C2C	2.31	1.49	1.44
23	B	610	CLA	C4C-C3C	2.31	1.49	1.45
23	b	606	CLA	C4B-CHC	2.31	1.47	1.41
23	B	602	CLA	C4C-C3C	2.31	1.49	1.45
32	a	414	LMT	O1'-C1'	2.31	1.44	1.40
23	B	603	CLA	C4B-CHC	2.31	1.47	1.41
23	B	607	CLA	CHD-C4C	2.31	1.47	1.41
23	A	408	CLA	C1B-CHB	2.30	1.47	1.41
23	b	603	CLA	C1D-C2D	2.30	1.47	1.42
35	C	519	DGD	O2G-C2G	-2.30	1.40	1.46
23	C	511	CLA	C1C-C2C	2.30	1.49	1.44
23	B	613	CLA	CHD-C4C	2.30	1.47	1.41
23	C	506	CLA	CHD-C4C	2.30	1.47	1.41
23	C	506	CLA	C1D-C2D	2.29	1.47	1.42
23	C	504	CLA	C4B-CHC	2.29	1.47	1.41
23	c	514	CLA	C4B-CHC	2.29	1.47	1.41
23	B	606	CLA	C1C-C2C	2.29	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	353	PHO	C1A-NA	-2.29	1.33	1.37
23	D	405	CLA	C4C-C3C	2.29	1.49	1.45
23	b	604	CLA	C1D-C2D	2.28	1.47	1.42
23	c	508	CLA	C4B-CHC	2.28	1.47	1.41
23	C	502	CLA	C4C-C3C	2.28	1.49	1.45
23	b	602	CLA	C4C-C3C	2.28	1.49	1.45
23	c	507	CLA	C1B-CHB	2.28	1.47	1.41
23	B	614	CLA	C1B-CHB	2.28	1.47	1.41
23	c	509	CLA	C1B-CHB	2.28	1.47	1.41
23	B	606	CLA	C1B-CHB	2.27	1.47	1.41
23	A	404	CLA	C1C-C2C	2.27	1.49	1.44
23	c	514	CLA	C4C-C3C	2.27	1.49	1.45
23	B	608	CLA	C1C-C2C	2.27	1.49	1.44
23	b	604	CLA	C1B-CHB	2.27	1.47	1.41
23	b	610	CLA	C1B-CHB	2.27	1.47	1.41
23	B	613	CLA	C4B-NB	-2.27	1.33	1.35
23	C	512	CLA	CHD-C4C	2.27	1.47	1.41
23	C	509	CLA	C1C-NC	-2.26	1.34	1.37
34	b	625	HTG	C1-S1	-2.26	1.77	1.80
23	B	616	CLA	C4B-CHC	2.26	1.47	1.41
23	B	601	CLA	CHD-C4C	2.26	1.47	1.41
23	a	406	CLA	CHD-C4C	2.26	1.47	1.41
23	c	514	CLA	C1B-CHB	2.26	1.47	1.41
23	B	610	CLA	C1C-C2C	2.26	1.48	1.44
24	a	408	PHO	C4D-CHA	2.26	1.49	1.43
23	B	606	CLA	C1D-C2D	2.26	1.47	1.42
23	a	406	CLA	C1B-CHB	2.26	1.47	1.41
23	d	402	CLA	C1B-CHB	2.26	1.47	1.41
23	b	605	CLA	CHD-C4C	2.25	1.47	1.41
23	C	507	CLA	C4B-CHC	2.25	1.47	1.41
23	D	405	CLA	C1D-C2D	2.25	1.47	1.42
23	c	513	CLA	CHD-C4C	2.25	1.47	1.41
23	b	615	CLA	C4B-CHC	2.25	1.47	1.41
34	D	414	HTG	C1-S1	-2.25	1.77	1.80
23	c	511	CLA	C4B-CHC	2.25	1.47	1.41
23	C	507	CLA	C1B-CHB	2.25	1.47	1.41
23	b	605	CLA	C1B-NB	-2.25	1.33	1.35
37	D	410	LHG	O7-C5	-2.24	1.41	1.46
23	b	608	CLA	C4B-CHC	2.24	1.47	1.41
23	B	603	CLA	C1D-C2D	2.24	1.47	1.42
23	b	613	CLA	C4B-NB	-2.24	1.33	1.35
23	b	608	CLA	C4C-C3C	2.24	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	507	CLA	C4C-C3C	2.24	1.48	1.45
34	d	411	HTG	C1-S1	-2.23	1.77	1.80
23	B	608	CLA	C1B-NB	-2.23	1.33	1.35
23	a	409	CLA	CHD-C4C	2.22	1.47	1.41
23	C	510	CLA	C1C-NC	-2.22	1.34	1.37
24	A	353	PHO	C1A-NA	-2.22	1.33	1.37
24	A	407	PHO	C4D-CHA	2.22	1.49	1.43
23	a	409	CLA	C4B-CHC	2.22	1.47	1.41
23	C	503	CLA	C1B-CHB	2.21	1.47	1.41
23	d	402	CLA	C4C-C3C	2.21	1.48	1.45
23	B	608	CLA	CHD-C4C	2.21	1.47	1.41
23	c	507	CLA	C4B-CHC	2.21	1.47	1.41
23	a	407	CLA	C4C-C3C	2.21	1.48	1.45
23	D	406	CLA	C1B-NB	-2.21	1.33	1.35
23	B	612	CLA	C4B-CHC	2.20	1.47	1.41
23	B	611	CLA	C1B-NB	-2.20	1.33	1.35
23	b	614	CLA	C1C-C2C	2.20	1.48	1.44
23	b	612	CLA	CHD-C4C	2.20	1.47	1.41
37	d	407	LHG	O7-C5	-2.20	1.41	1.46
23	c	503	CLA	CHD-C4C	2.20	1.47	1.41
23	b	612	CLA	C4B-NB	-2.20	1.33	1.35
23	A	406	CLA	C1B-CHB	2.19	1.47	1.41
23	A	408	CLA	C4B-NB	-2.19	1.33	1.35
23	a	409	CLA	C1B-CHB	2.19	1.47	1.41
23	B	605	CLA	CHD-C4C	2.19	1.47	1.41
23	B	604	CLA	C4B-CHC	2.19	1.47	1.41
23	b	612	CLA	C4B-CHC	2.18	1.47	1.41
37	L	101	LHG	O7-C5	-2.18	1.41	1.46
23	D	406	CLA	CHD-C4C	2.18	1.47	1.41
23	C	504	CLA	C1B-CHB	2.18	1.47	1.41
23	b	613	CLA	CHD-C4C	2.18	1.47	1.41
23	A	406	CLA	C4B-CHC	2.18	1.47	1.41
23	b	604	CLA	C4B-CHC	2.18	1.47	1.41
23	B	612	CLA	C4C-C3C	2.18	1.48	1.45
23	C	506	CLA	C4B-CHC	2.18	1.47	1.41
23	d	403	CLA	C1B-CHB	2.18	1.47	1.41
32	t	102	LMT	O1'-C1'	2.17	1.43	1.40
25	B	619	BCR	C30-C25	-2.17	1.50	1.53
23	c	505	CLA	C4B-CHC	2.17	1.47	1.41
23	d	402	CLA	C1D-C2D	2.17	1.47	1.42
23	b	605	CLA	C1C-C2C	2.17	1.48	1.44
23	b	605	CLA	C4B-CHC	2.17	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	D	409	LHG	O7-C5	-2.17	1.41	1.46
23	c	512	CLA	C4B-CHC	2.17	1.47	1.41
23	b	612	CLA	C4C-C3C	2.17	1.48	1.45
23	a	405	CLA	C1C-C2C	2.16	1.48	1.44
23	b	603	CLA	C4B-CHC	2.16	1.47	1.41
23	D	405	CLA	CHD-C4C	2.16	1.47	1.41
23	B	604	CLA	C1B-NB	-2.16	1.33	1.35
23	B	610	CLA	C1C-NC	-2.16	1.34	1.37
24	A	407	PHO	C3B-C4B	2.16	1.47	1.43
23	a	406	CLA	C1C-C2C	2.15	1.48	1.44
23	b	612	CLA	C1D-C2D	2.15	1.47	1.42
23	b	612	CLA	C1B-CHB	2.15	1.47	1.41
23	A	405	CLA	C1B-NB	-2.15	1.33	1.35
23	c	503	CLA	C4B-CHC	2.15	1.47	1.41
23	b	601	CLA	C4C-C3C	2.14	1.48	1.45
23	b	614	CLA	CHD-C4C	2.14	1.47	1.41
23	B	607	CLA	C4B-CHC	2.14	1.46	1.41
23	c	506	CLA	C4C-C3C	2.14	1.48	1.45
23	B	611	CLA	C4B-NB	-2.14	1.33	1.35
23	B	606	CLA	C4B-NB	-2.14	1.33	1.35
23	B	615	CLA	C1B-CHB	2.14	1.46	1.41
23	b	609	CLA	C4B-CHC	2.14	1.46	1.41
23	B	601	CLA	C1C-NC	-2.14	1.34	1.37
23	b	601	CLA	C1C-C2C	2.14	1.48	1.44
23	b	601	CLA	C4B-CHC	2.14	1.46	1.41
23	b	610	CLA	C4C-C3C	2.13	1.48	1.45
23	b	614	CLA	C4B-CHC	2.13	1.46	1.41
23	c	509	CLA	CHD-C4C	2.13	1.47	1.41
23	C	507	CLA	C1B-NB	-2.13	1.33	1.35
23	b	611	CLA	C1C-C2C	2.13	1.48	1.44
23	B	603	CLA	CHD-C4C	2.13	1.47	1.41
23	b	604	CLA	CHD-C4C	2.12	1.47	1.41
23	B	601	CLA	C1B-CHB	2.12	1.46	1.41
23	c	503	CLA	C4C-C3C	2.12	1.48	1.45
23	B	606	CLA	C4B-CHC	2.12	1.46	1.41
23	b	601	CLA	C1C-NC	-2.11	1.34	1.37
23	C	513	CLA	C1B-CHB	2.11	1.46	1.41
32	t	101	LMT	O1'-C1'	2.11	1.43	1.40
23	c	505	CLA	CHD-C4C	2.11	1.47	1.41
23	B	614	CLA	CHD-C4C	2.11	1.47	1.41
23	a	407	CLA	C1C-C2C	2.11	1.48	1.44
35	H	102	DGD	O5D-C1E	2.10	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	503	CLA	C1C-C2C	2.10	1.48	1.44
23	a	407	CLA	C1B-CHB	2.10	1.46	1.41
23	B	609	CLA	CHD-C4C	2.10	1.47	1.41
23	b	616	CLA	C1B-CHB	2.10	1.46	1.41
32	I	101	LMT	O1'-C1'	2.09	1.43	1.40
23	b	602	CLA	C1B-CHB	2.09	1.46	1.41
23	B	603	CLA	C1B-CHB	2.09	1.46	1.41
23	B	608	CLA	C4C-C3C	2.08	1.48	1.45
33	Z	101	LMG	O1-C1	2.08	1.43	1.40
23	C	503	CLA	C4C-C3C	2.08	1.48	1.45
23	C	507	CLA	C1C-C2C	2.08	1.48	1.44
23	C	508	CLA	C1B-CHB	2.08	1.46	1.41
23	C	510	CLA	C4B-CHC	2.08	1.46	1.41
23	b	610	CLA	C1B-NB	-2.07	1.33	1.35
32	e	102	LMT	O1'-C1'	2.07	1.43	1.40
23	c	509	CLA	C1D-C2D	2.07	1.47	1.42
23	C	509	CLA	CHD-C4C	2.07	1.47	1.41
23	a	409	CLA	C4C-C3C	2.07	1.48	1.45
23	C	513	CLA	C4C-C3C	2.07	1.48	1.45
34	b	623	HTG	C1-S1	-2.06	1.77	1.80
23	b	613	CLA	C1D-C2D	2.06	1.47	1.42
23	B	615	CLA	C4B-CHC	2.06	1.46	1.41
32	a	420	LMT	O1'-C1'	2.06	1.43	1.40
23	b	607	CLA	CHD-C4C	2.05	1.47	1.41
23	C	511	CLA	C1B-NB	-2.05	1.33	1.35
29	a	416	PL9	C2-C3	2.05	1.40	1.34
23	D	405	CLA	C1B-CHB	2.04	1.46	1.41
23	a	405	CLA	C1B-NB	-2.04	1.33	1.35
23	B	606	CLA	CHD-C4C	2.04	1.46	1.41
23	B	612	CLA	C1D-C2D	2.04	1.47	1.42
23	b	612	CLA	C1B-NB	-2.04	1.33	1.35
23	c	513	CLA	C1B-CHB	2.04	1.46	1.41
23	A	404	CLA	C1B-CHB	2.04	1.46	1.41
33	C	521	LMG	O1-C1	2.04	1.43	1.40
23	B	603	CLA	C1B-NB	-2.03	1.33	1.35
23	B	604	CLA	CHD-C4C	2.03	1.46	1.41
32	b	627	LMT	O1'-C1'	2.03	1.43	1.40
23	C	511	CLA	C4C-C3C	2.02	1.48	1.45
24	a	408	PHO	C1A-NA	-2.02	1.33	1.37
23	c	508	CLA	C1B-CHB	2.02	1.46	1.41
23	d	403	CLA	C1C-NC	-2.02	1.34	1.37
35	c	518	DGD	O3G-C1D	2.01	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	613	CLA	C4C-C3C	2.01	1.48	1.45
23	b	605	CLA	C1C-NC	-2.01	1.34	1.37
32	E	102	LMT	O1'-C1'	2.01	1.43	1.40
23	c	505	CLA	C4B-NB	-2.01	1.33	1.35
23	b	613	CLA	C1B-NB	-2.01	1.33	1.35
23	c	511	CLA	C4C-C3C	2.01	1.48	1.45
23	B	611	CLA	C1C-NC	-2.01	1.34	1.37
23	b	603	CLA	CHD-C4C	2.00	1.46	1.41
26	F	101	SQD	O6-C1	2.00	1.43	1.40
24	A	353	PHO	C4D-CHA	2.00	1.49	1.43

All (2350) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	602	CLA	C4A-NA-C1A	-8.66	102.81	106.71
23	b	602	CLA	C4A-NA-C1A	-7.71	103.24	106.71
23	c	504	CLA	C4A-NA-C1A	-7.67	103.26	106.71
23	C	504	CLA	C4A-NA-C1A	-7.54	103.31	106.71
38	E	103	HEM	CAD-CBD-CGD	7.42	125.12	112.67
24	A	353	PHO	CMD-C2D-C1D	7.16	136.08	125.06
23	B	605	CLA	CHD-C4C-C3C	-7.11	114.38	124.84
24	A	407	PHO	CMD-C2D-C1D	7.11	136.01	125.06
23	b	616	CLA	C4A-NA-C1A	-7.01	103.56	106.71
23	c	509	CLA	CHD-C4C-C3C	-6.97	114.59	124.84
34	b	623	HTG	C1'-S1-C1	6.96	113.10	100.09
23	B	614	CLA	O2D-CGD-CBD	6.91	123.54	111.27
23	b	606	CLA	C4A-NA-C1A	-6.86	103.62	106.71
23	c	508	CLA	O2D-CGD-CBD	6.83	123.41	111.27
23	B	606	CLA	C4A-NA-C1A	-6.80	103.65	106.71
23	B	612	CLA	CHD-C4C-C3C	-6.78	114.87	124.84
24	a	408	PHO	CMD-C2D-C1D	6.77	135.49	125.06
23	b	611	CLA	C4A-NA-C1A	-6.76	103.67	106.71
23	B	601	CLA	O2D-CGD-CBD	6.74	123.25	111.27
23	b	605	CLA	CHD-C4C-C3C	-6.72	114.95	124.84
23	A	405	CLA	CHD-C4C-C3C	-6.71	114.98	124.84
23	B	615	CLA	CHD-C4C-C3C	-6.69	115.00	124.84
23	B	606	CLA	CHD-C4C-C3C	-6.67	115.03	124.84
23	B	604	CLA	CHD-C4C-C3C	-6.65	115.07	124.84
34	D	414	HTG	C1'-S1-C1	6.52	112.29	100.09
23	B	609	CLA	CHD-C4C-C3C	-6.48	115.31	124.84
23	B	616	CLA	O2D-CGD-CBD	6.48	122.78	111.27
23	b	616	CLA	CHD-C4C-C3C	-6.47	115.32	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	508	CLA	CHD-C4C-C3C	-6.47	115.32	124.84
23	a	405	CLA	C2C-C1C-NC	6.47	116.03	109.97
23	B	616	CLA	CHD-C4C-C3C	-6.45	115.36	124.84
23	c	512	CLA	CHD-C4C-C3C	-6.44	115.38	124.84
23	b	611	CLA	CHD-C4C-C3C	-6.43	115.38	124.84
23	a	406	CLA	CHD-C4C-C3C	-6.41	115.41	124.84
23	B	614	CLA	CHD-C4C-C3C	-6.41	115.41	124.84
23	B	603	CLA	CHD-C4C-C3C	-6.40	115.43	124.84
23	A	408	CLA	CHD-C4C-C3C	-6.38	115.46	124.84
23	b	613	CLA	CHD-C4C-C3C	-6.37	115.48	124.84
26	A	410	SQD	O6-C1-C2	6.36	118.23	108.30
25	D	407	BCR	C7-C8-C9	-6.34	116.65	126.23
23	B	606	CLA	O2D-CGD-CBD	6.34	122.54	111.27
23	D	405	CLA	C4A-NA-C1A	-6.34	103.86	106.71
23	C	506	CLA	CHD-C4C-C3C	-6.34	115.52	124.84
23	b	604	CLA	C2C-C1C-NC	6.33	115.90	109.97
23	c	513	CLA	O2D-CGD-CBD	6.32	122.51	111.27
23	D	406	CLA	CHD-C4C-C3C	-6.31	115.57	124.84
23	B	603	CLA	C4A-NA-C1A	-6.29	103.88	106.71
23	c	513	CLA	CHD-C4C-C3C	-6.28	115.61	124.84
34	d	411	HTG	C1'-S1-C1	6.27	111.82	100.09
23	C	513	CLA	CHD-C4C-C3C	-6.26	115.63	124.84
23	B	601	CLA	CHD-C4C-C3C	-6.26	115.63	124.84
23	B	611	CLA	CHD-C4C-C3C	-6.23	115.69	124.84
23	c	503	CLA	CHD-C4C-C3C	-6.22	115.70	124.84
23	c	506	CLA	CHD-C4C-C3C	-6.22	115.70	124.84
34	c	522	HTG	C1'-S1-C1	6.21	111.70	100.09
23	b	604	CLA	CHD-C4C-C3C	-6.20	115.72	124.84
23	B	603	CLA	O2D-CGD-CBD	6.20	122.28	111.27
23	b	603	CLA	CHD-C4C-C3C	-6.20	115.73	124.84
23	b	603	CLA	C4A-NA-C1A	-6.19	103.92	106.71
26	F	101	SQD	O6-C1-C2	6.14	117.89	108.30
23	D	405	CLA	C2C-C1C-NC	6.12	115.71	109.97
23	b	610	CLA	CHD-C4C-C3C	-6.11	115.86	124.84
23	c	505	CLA	CHD-C4C-C3C	-6.11	115.86	124.84
23	C	508	CLA	O2D-CGD-CBD	6.10	122.11	111.27
23	C	511	CLA	CHD-C4C-C3C	-6.09	115.88	124.84
23	d	402	CLA	CHD-C4C-C3C	-6.09	115.89	124.84
23	c	507	CLA	C2C-C1C-NC	6.08	115.67	109.97
23	b	609	CLA	C4A-NA-C1A	-6.07	103.97	106.71
23	b	606	CLA	CHD-C4C-C3C	-6.07	115.91	124.84
23	C	506	CLA	C4A-NA-C1A	-6.06	103.98	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	616	CLA	O2D-CGD-CBD	6.05	122.01	111.27
24	a	408	PHO	O2D-CGD-CBD	6.04	122.01	111.27
23	B	607	CLA	C2C-C1C-NC	6.04	115.63	109.97
23	C	509	CLA	C2C-C1C-NC	6.02	115.61	109.97
23	c	510	CLA	C1-C2-C3	-6.01	115.64	126.04
23	C	511	CLA	C4A-NA-C1A	-6.01	104.00	106.71
23	b	612	CLA	CHD-C4C-C3C	-5.99	116.04	124.84
23	c	511	CLA	CHD-C4C-C3C	-5.99	116.04	124.84
23	d	403	CLA	C4A-NA-C1A	-5.99	104.02	106.71
23	C	507	CLA	C2C-C1C-NC	5.98	115.58	109.97
23	C	509	CLA	CHD-C4C-C3C	-5.98	116.05	124.84
23	c	508	CLA	CHD-C4C-C3C	-5.97	116.06	124.84
23	B	610	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
23	c	513	CLA	C4A-NA-C1A	-5.95	104.03	106.71
23	B	613	CLA	C2C-C1C-NC	5.94	115.54	109.97
23	c	506	CLA	O2D-CGD-CBD	5.93	121.81	111.27
23	C	514	CLA	CHD-C4C-C3C	-5.93	116.12	124.84
23	B	608	CLA	CHD-C4C-C3C	-5.93	116.12	124.84
23	B	609	CLA	C4A-NA-C1A	-5.92	104.04	106.71
23	c	502	CLA	C4A-NA-C1A	-5.92	104.05	106.71
23	b	603	CLA	O2D-CGD-CBD	5.92	121.78	111.27
23	b	613	CLA	C2C-C1C-NC	5.91	115.50	109.97
23	C	511	CLA	O2D-CGD-CBD	5.90	121.76	111.27
23	C	513	CLA	O2D-CGD-CBD	5.89	121.73	111.27
23	b	602	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
23	C	513	CLA	C4A-NA-C1A	-5.88	104.06	106.71
23	b	612	CLA	C2C-C1C-NC	5.87	115.47	109.97
23	b	610	CLA	O2D-CGD-CBD	5.87	121.70	111.27
23	C	503	CLA	CHD-C4C-C3C	-5.86	116.22	124.84
23	C	512	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
23	C	505	CLA	C2C-C1C-NC	5.83	115.44	109.97
23	B	608	CLA	C2C-C1C-NC	5.83	115.44	109.97
23	c	510	CLA	CHD-C4C-C3C	-5.82	116.28	124.84
23	B	602	CLA	CHD-C4C-C3C	-5.80	116.31	124.84
23	b	601	CLA	O2D-CGD-CBD	5.80	121.58	111.27
23	b	612	CLA	C4A-NA-C1A	-5.79	104.10	106.71
23	a	409	CLA	CHD-C4C-C3C	-5.79	116.32	124.84
23	C	502	CLA	O2D-CGD-CBD	5.79	121.55	111.27
23	C	502	CLA	CHD-C4C-C3C	-5.78	116.34	124.84
23	b	607	CLA	C2C-C1C-NC	5.78	115.39	109.97
23	b	613	CLA	C4A-NA-C1A	-5.78	104.11	106.71
23	B	604	CLA	O2D-CGD-CBD	5.77	121.52	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	612	CLA	O2D-CGD-CBD	5.76	121.51	111.27
23	b	608	CLA	CHD-C4C-C3C	-5.76	116.37	124.84
23	b	609	CLA	CHD-C4C-C3C	-5.76	116.38	124.84
23	c	514	CLA	C4A-NA-C1A	-5.75	104.12	106.71
23	c	505	CLA	C2C-C1C-NC	5.75	115.36	109.97
23	A	404	CLA	C2C-C1C-NC	5.74	115.35	109.97
23	B	605	CLA	O2D-CGD-CBD	5.74	121.46	111.27
23	b	604	CLA	O2D-CGD-CBD	5.73	121.46	111.27
23	a	407	CLA	CHD-C4C-C3C	-5.73	116.42	124.84
23	B	613	CLA	C1-C2-C3	-5.73	116.14	126.04
23	c	502	CLA	O2D-CGD-CBD	5.70	121.41	111.27
23	b	601	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
23	c	504	CLA	C2C-C1C-NC	5.70	115.31	109.97
23	b	603	CLA	C2C-C1C-NC	5.70	115.31	109.97
24	A	353	PHO	C3D-C2D-C1D	-5.69	97.58	105.87
23	d	403	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
23	C	510	CLA	C2C-C1C-NC	5.67	115.29	109.97
23	b	607	CLA	CHD-C4C-C3C	-5.67	116.50	124.84
23	B	607	CLA	CHD-C4C-C3C	-5.67	116.50	124.84
23	D	406	CLA	C4A-NA-C1A	-5.67	104.16	106.71
23	b	614	CLA	O2D-CGD-CBD	5.67	121.33	111.27
23	B	610	CLA	O2D-CGD-CBD	5.66	121.32	111.27
23	B	616	CLA	C4A-NA-C1A	-5.66	104.16	106.71
23	b	606	CLA	O2D-CGD-CBD	5.65	121.32	111.27
23	A	404	CLA	CHD-C4C-C3C	-5.65	116.53	124.84
23	c	509	CLA	O2D-CGD-CBD	5.65	121.31	111.27
24	a	353	PHO	CMD-C2D-C1D	5.62	133.72	125.06
26	b	620	SQD	O6-C1-C2	5.60	117.05	108.30
23	b	615	CLA	C2C-C1C-NC	5.60	115.22	109.97
23	C	505	CLA	O2D-CGD-CBD	5.60	121.22	111.27
23	D	405	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
23	C	504	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
23	C	503	CLA	C4A-NA-C1A	-5.59	104.19	106.71
23	b	615	CLA	C4A-NA-C1A	-5.59	104.19	106.71
24	A	407	PHO	C3D-C2D-C1D	-5.58	97.74	105.87
23	d	402	CLA	C2C-C1C-NC	5.58	115.20	109.97
23	b	611	CLA	O2D-CGD-CBD	5.57	121.17	111.27
23	b	614	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
23	B	612	CLA	C3C-C4C-NC	5.57	116.82	110.57
38	E	103	HEM	CBD-CAD-C3D	-5.56	102.23	112.48
24	A	353	PHO	O2D-CGD-CBD	5.56	121.14	111.27
24	A	353	PHO	C2D-C1D-ND	5.55	118.17	109.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	612	CLA	C2C-C1C-NC	5.55	115.17	109.97
23	b	605	CLA	C4A-NA-C1A	-5.55	104.21	106.71
23	B	606	CLA	C2C-C1C-NC	5.54	115.16	109.97
23	a	407	CLA	C4A-NA-C1A	-5.53	104.22	106.71
23	c	514	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
23	B	602	CLA	O2D-CGD-CBD	5.52	121.08	111.27
23	C	512	CLA	C2C-C1C-NC	5.52	115.14	109.97
23	C	507	CLA	C4A-NA-C1A	-5.50	104.23	106.71
26	F	101	SQD	O47-C7-C8	5.50	123.35	111.50
23	b	615	CLA	CHD-C4C-C3C	-5.50	116.76	124.84
23	c	507	CLA	CHD-C4C-C3C	-5.49	116.76	124.84
23	A	406	CLA	CHD-C4C-C3C	-5.48	116.78	124.84
23	b	614	CLA	C2C-C1C-NC	5.48	115.10	109.97
23	B	611	CLA	C2C-C1C-NC	5.48	115.10	109.97
38	e	87	HEM	CAD-CBD-CGD	5.47	121.86	112.67
23	C	506	CLA	O2D-CGD-CBD	5.47	120.99	111.27
23	a	406	CLA	C4A-NA-C1A	-5.47	104.25	106.71
23	c	503	CLA	C2C-C1C-NC	5.46	115.08	109.97
23	c	503	CLA	O2D-CGD-CBD	5.42	120.91	111.27
23	C	509	CLA	O2D-CGD-CBD	5.42	120.91	111.27
23	B	615	CLA	C4A-NA-C1A	-5.42	104.27	106.71
23	C	510	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
23	B	604	CLA	C2C-C1C-NC	5.40	115.03	109.97
24	a	353	PHO	C1-C2-C3	-5.40	116.70	126.04
23	c	509	CLA	C4A-NA-C1A	-5.38	104.29	106.71
24	a	353	PHO	O2D-CGD-CBD	5.35	120.78	111.27
23	c	508	CLA	C2C-C1C-NC	5.35	114.98	109.97
23	c	506	CLA	C4A-NA-C1A	-5.34	104.30	106.71
23	b	612	CLA	O2D-CGD-CBD	5.33	120.75	111.27
23	a	409	CLA	C2C-C1C-NC	5.33	114.96	109.97
23	b	605	CLA	O2D-CGD-CBD	5.32	120.73	111.27
23	c	512	CLA	O2D-CGD-CBD	5.32	120.72	111.27
23	c	512	CLA	C2C-C1C-NC	5.32	114.95	109.97
23	C	504	CLA	C2C-C1C-NC	5.31	114.94	109.97
23	A	408	CLA	C4A-NA-C1A	-5.30	104.32	106.71
34	B	623	HTG	C1'-S1-C1	5.30	110.00	100.09
23	D	406	CLA	O2D-CGD-CBD	5.30	120.68	111.27
23	C	507	CLA	CHD-C4C-C3C	-5.29	117.06	124.84
26	A	410	SQD	C1-O5-C5	-5.29	103.30	113.69
23	b	602	CLA	O2D-CGD-CBD	5.29	120.66	111.27
23	b	610	CLA	C4A-NA-C1A	-5.28	104.33	106.71
23	b	609	CLA	C2C-C1C-NC	5.28	114.92	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	505	CLA	C4A-NA-C1A	-5.28	104.33	106.71
34	C	522	HTG	C1'-S1-C1	5.28	109.96	100.09
23	C	502	CLA	C2C-C1C-NC	5.26	114.90	109.97
29	A	414	PL9	C7-C8-C9	-5.26	118.03	126.79
23	C	506	CLA	C2C-C1C-NC	5.26	114.90	109.97
23	B	614	CLA	C2C-C1C-NC	5.25	114.89	109.97
23	B	611	CLA	C4A-NA-C1A	-5.25	104.35	106.71
23	c	502	CLA	CHD-C4C-C3C	-5.25	117.12	124.84
23	b	601	CLA	C2C-C1C-NC	5.24	114.88	109.97
23	d	403	CLA	O2D-CGD-CBD	5.23	120.56	111.27
24	A	407	PHO	C2D-C1D-ND	5.22	117.66	109.79
23	A	404	CLA	C4A-NA-C1A	-5.21	104.36	106.71
23	a	407	CLA	C2C-C1C-NC	5.21	114.85	109.97
23	c	511	CLA	C2C-C1C-NC	5.19	114.83	109.97
26	A	410	SQD	O47-C7-C8	5.19	122.68	111.50
23	B	613	CLA	CHD-C4C-C3C	-5.17	117.23	124.84
23	c	506	CLA	C3C-C4C-NC	5.17	116.37	110.57
23	c	510	CLA	C4A-NA-C1A	-5.17	104.38	106.71
24	a	408	PHO	C3D-C2D-C1D	-5.16	98.35	105.87
23	B	603	CLA	C2C-C1C-NC	5.16	114.81	109.97
23	C	503	CLA	O2D-CGD-CBD	5.15	120.42	111.27
23	C	502	CLA	C4A-NA-C1A	-5.15	104.39	106.71
26	f	102	SQD	O47-C7-C8	5.15	122.60	111.50
23	b	605	CLA	C2C-C1C-NC	5.15	114.79	109.97
23	c	502	CLA	C2C-C1C-NC	5.15	114.79	109.97
23	B	610	CLA	C4A-NA-C1A	-5.14	104.39	106.71
23	b	608	CLA	C2C-C1C-NC	5.14	114.79	109.97
23	B	613	CLA	C4A-NA-C1A	-5.13	104.40	106.71
23	c	506	CLA	C2C-C1C-NC	5.13	114.78	109.97
23	C	514	CLA	C4A-NA-C1A	-5.12	104.40	106.71
23	a	409	CLA	O2D-CGD-CBD	5.12	120.37	111.27
23	b	609	CLA	O2D-CGD-CBD	5.11	120.35	111.27
25	y	101	BCR	C33-C5-C6	-5.11	118.79	124.53
26	a	411	SQD	O47-C7-C8	5.10	122.50	111.50
23	B	606	CLA	C3C-C4C-NC	5.10	116.29	110.57
23	B	614	CLA	C4A-NA-C1A	-5.08	104.42	106.71
23	c	509	CLA	C2C-C1C-NC	5.08	114.73	109.97
24	a	353	PHO	C3D-C2D-C1D	-5.07	98.48	105.87
23	B	615	CLA	C2C-C1C-NC	5.06	114.71	109.97
25	Y	101	BCR	C33-C5-C6	-5.04	118.87	124.53
23	B	609	CLA	C2C-C1C-NC	5.04	114.69	109.97
23	a	406	CLA	C2C-C1C-NC	5.03	114.69	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	608	CLA	C4A-NA-C1A	-5.02	104.45	106.71
23	c	510	CLA	O2D-CGD-CBD	5.02	120.18	111.27
23	b	601	CLA	C4A-NA-C1A	-5.01	104.45	106.71
23	B	611	CLA	O2D-CGD-CBD	5.00	120.15	111.27
23	C	505	CLA	CHD-C4C-C3C	-5.00	117.49	124.84
23	d	402	CLA	C3C-C4C-NC	5.00	116.17	110.57
23	A	406	CLA	C4A-NA-C1A	-4.98	104.47	106.71
23	c	504	CLA	CHD-C4C-C3C	-4.98	117.51	124.84
23	c	514	CLA	C2C-C1C-NC	4.98	114.64	109.97
23	b	604	CLA	C1C-C2C-C3C	-4.97	101.73	106.96
23	C	511	CLA	C2C-C1C-NC	4.96	114.62	109.97
26	b	620	SQD	O47-C7-C8	4.96	122.19	111.50
23	C	503	CLA	C2C-C1C-NC	4.96	114.61	109.97
23	b	611	CLA	C2C-C1C-NC	4.95	114.61	109.97
23	B	607	CLA	C4A-NA-C1A	-4.95	104.48	106.71
23	C	509	CLA	C3C-C4C-NC	4.95	116.12	110.57
23	B	610	CLA	C2C-C1C-NC	4.95	114.61	109.97
23	a	409	CLA	C4A-NA-C1A	-4.95	104.48	106.71
25	b	617	BCR	C7-C8-C9	-4.94	118.77	126.23
26	a	411	SQD	O6-C1-C2	4.93	116.00	108.30
24	a	408	PHO	C2D-C1D-ND	4.93	117.22	109.79
23	c	511	CLA	C4A-NA-C1A	-4.92	104.49	106.71
25	d	404	BCR	C38-C26-C25	-4.92	119.00	124.53
23	A	406	CLA	C2C-C1C-NC	4.92	114.58	109.97
23	B	609	CLA	C3C-C4C-NC	4.92	116.09	110.57
23	B	604	CLA	C1-C2-C3	-4.91	117.55	126.04
23	B	607	CLA	C1C-C2C-C3C	-4.91	101.79	106.96
23	C	507	CLA	O2D-CGD-CBD	4.91	119.99	111.27
23	b	603	CLA	C3C-C4C-NC	4.88	116.04	110.57
23	b	603	CLA	C1D-CHD-C4C	-4.87	116.13	122.56
23	A	408	CLA	C2C-C1C-NC	4.87	114.53	109.97
25	C	515	BCR	C7-C8-C9	-4.86	118.88	126.23
23	c	510	CLA	C2C-C1C-NC	4.86	114.53	109.97
23	b	610	CLA	C2C-C1C-NC	4.86	114.53	109.97
23	c	513	CLA	C2C-C1C-NC	4.86	114.53	109.97
23	b	614	CLA	C4A-NA-C1A	-4.85	104.53	106.71
23	b	604	CLA	C4A-NA-C1A	-4.84	104.53	106.71
23	C	511	CLA	C1-C2-C3	-4.84	117.67	126.04
33	C	501	LMG	O7-C10-C11	4.84	121.93	111.50
23	B	604	CLA	C3C-C4C-NC	4.83	115.98	110.57
23	a	405	CLA	C4A-NA-C1A	-4.83	104.54	106.71
23	C	508	CLA	C4A-NA-C1A	-4.82	104.54	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	620	SQD	O6-C1-C2	4.82	115.82	108.30
24	a	353	PHO	C2D-C1D-ND	4.81	117.06	109.79
23	B	614	CLA	O2D-CGD-O1D	-4.80	114.45	123.84
23	B	601	CLA	C2C-C1C-NC	4.80	114.47	109.97
23	B	604	CLA	C4A-NA-C1A	-4.79	104.55	106.71
23	B	605	CLA	C3C-C4C-NC	4.78	115.94	110.57
23	B	605	CLA	C2C-C1C-NC	4.77	114.44	109.97
23	B	608	CLA	O2D-CGD-CBD	4.77	119.74	111.27
23	d	402	CLA	C4A-NA-C1A	-4.76	104.56	106.71
23	B	608	CLA	C4A-NA-C1A	-4.76	104.57	106.71
25	d	404	BCR	C7-C8-C9	-4.75	119.05	126.23
25	c	515	BCR	C11-C10-C9	-4.75	120.53	127.31
23	B	615	CLA	C3C-C4C-NC	4.75	115.90	110.57
23	b	607	CLA	C3C-C4C-NC	4.75	115.89	110.57
23	C	510	CLA	O2D-CGD-CBD	4.74	119.70	111.27
23	a	405	CLA	CHD-C4C-C3C	-4.74	117.87	124.84
23	B	605	CLA	C1D-CHD-C4C	-4.74	116.30	122.56
23	a	405	CLA	C1C-C2C-C3C	-4.73	101.98	106.96
24	A	353	PHO	C1-C2-C3	-4.73	117.86	126.04
23	b	612	CLA	C3C-C4C-NC	4.73	115.88	110.57
23	A	404	CLA	CAA-C2A-C3A	-4.73	99.84	112.78
23	b	608	CLA	O2D-CGD-CBD	4.72	119.66	111.27
23	C	506	CLA	C3C-C4C-NC	4.72	115.87	110.57
23	c	504	CLA	O2D-CGD-CBD	4.72	119.65	111.27
23	c	505	CLA	O2D-CGD-CBD	4.71	119.64	111.27
34	B	626	HTG	C1'-S1-C1	4.71	108.90	100.09
25	b	617	BCR	C33-C5-C6	-4.70	119.25	124.53
23	B	614	CLA	C1-C2-C3	-4.69	117.94	126.04
29	D	408	PL9	C42-C43-C44	-4.69	116.37	127.66
24	A	407	PHO	O2D-CGD-CBD	4.68	119.58	111.27
23	c	511	CLA	O2D-CGD-CBD	4.68	119.58	111.27
23	c	511	CLA	C1-C2-C3	-4.68	117.95	126.04
23	c	509	CLA	C3C-C4C-NC	4.68	115.81	110.57
33	C	520	LMG	O7-C10-C11	4.67	121.57	111.50
23	B	607	CLA	O2D-CGD-CBD	4.67	119.57	111.27
23	D	405	CLA	C1C-C2C-C3C	-4.66	102.06	106.96
23	b	607	CLA	C4A-NA-C1A	-4.66	104.61	106.71
23	b	613	CLA	C3C-C4C-NC	4.66	115.79	110.57
23	C	513	CLA	C2C-C1C-NC	4.65	114.32	109.97
25	c	516	BCR	C7-C8-C9	-4.64	119.22	126.23
37	E	101	LHG	O7-C7-C8	4.64	121.49	111.50
23	B	603	CLA	C3C-C4C-NC	4.63	115.77	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	605	CLA	C4A-NA-C1A	-4.61	104.63	106.71
23	C	508	CLA	C3C-C4C-NC	4.61	115.74	110.57
23	C	508	CLA	C2C-C1C-NC	4.61	114.29	109.97
23	b	611	CLA	C1-C2-C3	-4.61	118.07	126.04
26	B	620	SQD	O7-S-C6	4.58	112.39	106.94
23	A	405	CLA	O2D-CGD-CBD	4.58	119.40	111.27
23	b	604	CLA	C3C-C4C-NC	4.57	115.69	110.57
29	a	416	PL9	C7-C3-C4	4.57	120.59	116.88
34	b	625	HTG	C1'-S1-C1	4.56	108.61	100.09
33	Z	101	LMG	O7-C10-C11	4.55	121.31	111.50
23	B	616	CLA	C3C-C4C-NC	4.55	115.67	110.57
23	b	614	CLA	C1-C2-C3	-4.54	118.19	126.04
23	B	610	CLA	C3C-C4C-NC	4.54	115.66	110.57
25	B	617	BCR	C33-C5-C6	-4.53	119.44	124.53
23	b	610	CLA	C1-C2-C3	-4.53	118.21	126.04
23	b	607	CLA	O2D-CGD-CBD	4.53	119.31	111.27
23	a	407	CLA	O2D-CGD-CBD	4.52	119.31	111.27
23	b	611	CLA	C3C-C4C-NC	4.52	115.64	110.57
23	A	405	CLA	CBC-CAC-C3C	-4.52	99.97	112.43
23	d	402	CLA	C1-C2-C3	-4.52	118.23	126.04
23	C	512	CLA	C3C-C4C-NC	4.51	115.63	110.57
23	B	613	CLA	C3C-C4C-NC	4.50	115.62	110.57
23	c	507	CLA	C4A-NA-C1A	-4.50	104.68	106.71
23	c	513	CLA	C3C-C4C-NC	4.48	115.59	110.57
23	c	508	CLA	C1C-C2C-C3C	-4.47	102.25	106.96
23	c	505	CLA	C3C-C4C-NC	4.47	115.58	110.57
23	b	602	CLA	C2C-C1C-NC	4.47	114.16	109.97
23	C	513	CLA	C3C-C4C-NC	4.47	115.58	110.57
23	B	601	CLA	C4A-NA-C1A	-4.46	104.70	106.71
25	t	103	BCR	C33-C5-C6	-4.46	119.52	124.53
23	a	405	CLA	C3B-C4B-NB	4.46	114.98	109.21
23	C	514	CLA	O2D-CGD-CBD	4.46	119.19	111.27
23	b	606	CLA	C2C-C1C-NC	4.45	114.14	109.97
23	A	405	CLA	C2C-C1C-NC	4.44	114.13	109.97
26	A	410	SQD	C1-C2-C3	-4.44	100.75	110.00
23	B	602	CLA	CAA-C2A-C3A	-4.43	100.64	112.78
23	C	514	CLA	C2C-C1C-NC	4.43	114.12	109.97
24	A	353	PHO	C4C-C3C-C2C	-4.43	101.88	106.78
23	B	609	CLA	O2D-CGD-CBD	4.42	119.12	111.27
23	B	611	CLA	C3C-C4C-NC	4.42	115.52	110.57
23	B	614	CLA	C3C-C4C-NC	4.41	115.52	110.57
23	B	604	CLA	C1D-CHD-C4C	-4.41	116.74	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	406	CLA	C3C-C4C-NC	4.40	115.50	110.57
23	a	409	CLA	C3C-C4C-NC	4.40	115.50	110.57
23	D	405	CLA	C3C-C4C-NC	4.40	115.50	110.57
23	B	616	CLA	C2C-C1C-NC	4.38	114.08	109.97
25	b	619	BCR	C7-C8-C9	-4.38	119.62	126.23
23	B	603	CLA	C1D-CHD-C4C	-4.37	116.80	122.56
23	a	406	CLA	C1C-C2C-C3C	-4.36	102.38	106.96
23	c	508	CLA	C4A-NA-C1A	-4.35	104.75	106.71
23	c	503	CLA	C3C-C4C-NC	4.33	115.42	110.57
34	b	622	HTG	C1-O5-C5	4.32	120.55	112.58
23	b	613	CLA	C1-C2-C3	-4.31	118.58	126.04
33	C	521	LMG	O7-C10-C11	4.31	120.79	111.50
23	C	510	CLA	C4A-NA-C1A	-4.31	104.77	106.71
23	C	509	CLA	C4A-NA-C1A	-4.30	104.77	106.71
23	c	503	CLA	C4A-NA-C1A	-4.30	104.77	106.71
23	b	606	CLA	C3C-C4C-NC	4.30	115.39	110.57
23	C	509	CLA	C1-C2-C3	-4.29	118.61	126.04
23	B	602	CLA	C2C-C1C-NC	4.29	114.00	109.97
23	B	601	CLA	C3C-C4C-NC	4.29	115.38	110.57
29	d	405	PL9	C42-C43-C44	-4.29	117.34	127.66
23	b	613	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
23	D	406	CLA	C2C-C1C-NC	4.28	113.98	109.97
23	A	404	CLA	O2A-CGA-CBA	4.28	125.33	111.91
23	C	503	CLA	C1-C2-C3	-4.27	118.66	126.04
23	b	616	CLA	C3C-C4C-NC	4.27	115.36	110.57
23	c	514	CLA	O2D-CGD-CBD	4.26	118.84	111.27
23	c	507	CLA	C1C-C2C-C3C	-4.26	102.48	106.96
25	D	407	BCR	C38-C26-C25	-4.26	119.75	124.53
23	B	605	CLA	C4-C3-C5	4.25	122.42	115.27
23	C	505	CLA	C1C-C2C-C3C	-4.25	102.49	106.96
25	H	101	BCR	C16-C17-C18	-4.25	121.24	127.31
23	C	505	CLA	C1-C2-C3	-4.25	118.69	126.04
23	D	405	CLA	O2D-CGD-CBD	4.24	118.81	111.27
23	C	502	CLA	C1-C2-C3	-4.24	118.71	126.04
23	B	606	CLA	C1D-CHD-C4C	-4.24	116.96	122.56
23	B	613	CLA	CAC-C3C-C4C	4.23	130.30	124.81
23	c	504	CLA	C3C-C4C-NC	4.23	115.31	110.57
23	B	602	CLA	C3C-C4C-NC	4.23	115.31	110.57
23	b	614	CLA	C3C-C4C-NC	4.23	115.31	110.57
23	B	608	CLA	C3C-C4C-NC	4.23	115.31	110.57
26	B	620	SQD	O47-C7-C8	4.22	120.61	111.50
23	b	616	CLA	C1D-CHD-C4C	-4.22	116.99	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	617	BCR	C7-C8-C9	-4.22	119.86	126.23
32	I	101	LMT	C1'-O5'-C5'	4.22	121.97	113.69
23	A	406	CLA	O2D-CGD-CBD	4.21	118.75	111.27
23	D	405	CLA	C1-C2-C3	-4.20	118.77	126.04
23	C	514	CLA	C3C-C4C-NC	4.20	115.28	110.57
23	A	405	CLA	C4A-NA-C1A	-4.20	104.82	106.71
23	B	614	CLA	C1C-C2C-C3C	-4.20	102.55	106.96
23	A	408	CLA	C3C-C4C-NC	4.19	115.27	110.57
40	v	202	HEC	CBA-CAA-C2A	-4.18	104.78	112.48
23	b	609	CLA	C3C-C4C-NC	4.17	115.25	110.57
23	a	405	CLA	CAA-C2A-C3A	-4.17	101.35	112.78
23	B	605	CLA	O2D-CGD-O1D	-4.17	115.68	123.84
23	C	512	CLA	O2D-CGD-CBD	4.15	118.65	111.27
23	c	512	CLA	C3C-C4C-NC	4.15	115.23	110.57
25	d	404	BCR	C24-C23-C22	-4.15	119.97	126.23
23	A	408	CLA	C1-C2-C3	-4.14	118.88	126.04
23	A	404	CLA	C3C-C4C-NC	4.14	115.21	110.57
23	b	608	CLA	C1-C2-C3	-4.13	118.90	126.04
24	a	353	PHO	C4C-C3C-C2C	-4.12	102.22	106.78
23	A	405	CLA	C1C-C2C-C3C	-4.11	102.64	106.96
23	B	604	CLA	C1C-C2C-C3C	-4.10	102.64	106.96
23	B	615	CLA	C1D-CHD-C4C	-4.09	117.16	122.56
23	C	507	CLA	C1C-C2C-C3C	-4.09	102.66	106.96
23	a	407	CLA	C1-C2-C3	-4.09	118.98	126.04
23	B	612	CLA	C1-C2-C3	-4.08	118.99	126.04
23	c	509	CLA	C1C-C2C-C3C	-4.08	102.67	106.96
23	C	503	CLA	C3C-C4C-NC	4.08	115.14	110.57
23	C	502	CLA	C1C-C2C-C3C	-4.07	102.67	106.96
25	Y	101	BCR	C16-C17-C18	-4.07	121.50	127.31
23	c	502	CLA	O2D-CGD-O1D	-4.07	115.88	123.84
25	C	516	BCR	C7-C8-C9	-4.07	120.09	126.23
23	C	502	CLA	O2D-CGD-O1D	-4.07	115.88	123.84
23	c	512	CLA	C4A-NA-C1A	-4.07	104.88	106.71
23	b	612	CLA	C1-C2-C3	-4.06	119.01	126.04
23	c	512	CLA	O2D-CGD-O1D	-4.06	115.90	123.84
23	d	402	CLA	O2D-CGD-CBD	4.06	118.48	111.27
29	a	416	PL9	C32-C33-C34	-4.05	117.90	127.66
26	a	411	SQD	O8-S-C6	4.05	112.19	105.74
23	b	609	CLA	C1-C2-C3	-4.05	119.05	126.04
23	b	615	CLA	O2D-CGD-CBD	4.04	118.45	111.27
29	a	416	PL9	C7-C8-C9	-4.04	120.07	126.79
23	C	504	CLA	C3C-C4C-NC	4.03	115.09	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	502	CLA	C3C-C4C-NC	4.03	115.09	110.57
34	b	622	HTG	C1'-S1-C1	4.03	107.62	100.09
23	d	403	CLA	C2C-C1C-NC	4.02	113.74	109.97
23	a	406	CLA	O2D-CGD-CBD	4.02	118.40	111.27
33	C	501	LMG	C7-O1-C1	-4.01	105.90	113.74
23	c	514	CLA	C3C-C4C-NC	4.01	115.07	110.57
23	c	504	CLA	C1D-CHD-C4C	-4.01	117.27	122.56
23	C	509	CLA	C3B-C4B-NB	4.00	114.39	109.21
23	c	504	CLA	CAC-C3C-C4C	4.00	130.00	124.81
23	B	612	CLA	C4A-NA-C1A	-4.00	104.91	106.71
29	d	405	PL9	C10-C9-C11	4.00	122.00	115.27
25	c	515	BCR	C20-C21-C22	-3.99	121.61	127.31
23	C	504	CLA	C4-C3-C5	3.99	121.98	115.27
23	b	610	CLA	C3C-C4C-NC	3.99	115.04	110.57
23	C	510	CLA	C1-C2-C3	-3.98	119.16	126.04
23	b	607	CLA	C3B-C4B-NB	3.98	114.35	109.21
23	c	505	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
23	b	602	CLA	C3C-C4C-NC	3.97	115.02	110.57
23	b	612	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
23	C	511	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
23	B	601	CLA	O2D-CGD-O1D	-3.96	116.09	123.84
23	c	513	CLA	C1-C2-C3	-3.96	119.19	126.04
23	c	510	CLA	C1D-CHD-C4C	-3.96	117.33	122.56
23	C	513	CLA	C1D-CHD-C4C	-3.96	117.34	122.56
23	c	506	CLA	C1D-CHD-C4C	-3.96	117.34	122.56
23	C	506	CLA	C1D-CHD-C4C	-3.96	117.34	122.56
23	A	406	CLA	C3C-C4C-NC	3.95	115.00	110.57
23	B	608	CLA	C3B-C4B-NB	3.95	114.32	109.21
23	C	512	CLA	CAC-C3C-C4C	3.95	129.93	124.81
23	C	504	CLA	C1D-CHD-C4C	-3.95	117.35	122.56
25	C	515	BCR	C15-C14-C13	-3.94	121.68	127.31
23	B	608	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
23	C	504	CLA	C1-C2-C3	-3.94	119.23	126.04
23	B	613	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
35	c	517	DGD	O2G-C1B-C2B	3.94	119.99	111.50
26	A	410	SQD	O7-S-C6	3.94	111.62	106.94
23	b	612	CLA	C1D-CHD-C4C	-3.93	117.37	122.56
23	c	507	CLA	O2D-CGD-CBD	3.93	118.25	111.27
25	H	101	BCR	C11-C10-C9	-3.93	121.70	127.31
23	a	406	CLA	CBC-CAC-C3C	-3.93	101.60	112.43
25	T	101	BCR	C11-C10-C9	-3.93	121.71	127.31
24	a	408	PHO	O2D-CGD-O1D	-3.92	116.17	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	602	CLA	O2D-CGD-O1D	-3.92	116.17	123.84
25	c	515	BCR	C15-C14-C13	-3.92	121.71	127.31
23	c	512	CLA	C1D-CHD-C4C	-3.92	117.38	122.56
23	b	607	CLA	C1C-C2C-C3C	-3.92	102.84	106.96
25	K	102	BCR	C7-C8-C9	-3.91	120.32	126.23
23	C	510	CLA	C3C-C4C-NC	3.91	114.96	110.57
23	B	610	CLA	O2A-CGA-CBA	3.91	124.19	111.91
23	b	608	CLA	C1C-C2C-C3C	-3.91	102.85	106.96
25	C	515	BCR	C33-C5-C6	-3.90	120.15	124.53
25	K	102	BCR	C3-C4-C5	-3.89	107.12	114.08
23	B	605	CLA	O2A-CGA-O1A	-3.89	113.77	123.59
35	C	517	DGD	O2G-C1B-C2B	3.89	119.88	111.50
33	B	621	LMG	O7-C10-C11	3.89	119.88	111.50
23	A	404	CLA	C1C-C2C-C3C	-3.88	102.87	106.96
23	c	503	CLA	C1C-C2C-C3C	-3.88	102.87	106.96
23	c	511	CLA	C3C-C4C-NC	3.88	114.92	110.57
23	B	611	CLA	C1-C2-C3	-3.88	119.33	126.04
33	c	520	LMG	O7-C10-C11	3.88	119.86	111.50
25	D	407	BCR	C15-C14-C13	-3.88	121.78	127.31
23	B	603	CLA	O2A-CGA-O1A	-3.88	113.81	123.59
33	C	521	LMG	O6-C5-C4	3.88	116.73	109.69
23	b	608	CLA	C3C-C4C-NC	3.87	114.91	110.57
23	b	613	CLA	O2D-CGD-CBD	3.87	118.15	111.27
26	A	410	SQD	C45-O47-C7	-3.87	108.26	117.79
23	a	406	CLA	C1D-CHD-C4C	-3.87	117.45	122.56
25	y	101	BCR	C38-C26-C25	-3.87	120.18	124.53
23	b	605	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
25	k	101	BCR	C24-C23-C22	-3.85	120.41	126.23
23	C	511	CLA	C1D-CHD-C4C	-3.85	117.47	122.56
23	c	505	CLA	C3B-C4B-NB	3.85	114.19	109.21
23	B	603	CLA	O2D-CGD-O1D	-3.84	116.32	123.84
33	C	521	LMG	C3-C4-C5	3.84	117.09	110.24
23	A	405	CLA	C3C-C4C-NC	3.84	114.88	110.57
23	c	511	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
23	c	507	CLA	C3B-C4B-NB	3.84	114.17	109.21
23	a	407	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
23	b	605	CLA	C3C-C4C-NC	3.83	114.87	110.57
23	c	509	CLA	C1D-CHD-C4C	-3.82	117.51	122.56
23	B	612	CLA	O2D-CGD-O1D	-3.82	116.37	123.84
23	C	509	CLA	O2D-CGD-O1D	-3.82	116.38	123.84
23	C	510	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
26	a	411	SQD	C45-O47-C7	-3.81	108.40	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	404	CLA	O2A-CGA-O1A	-3.81	113.97	123.59
23	b	603	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
23	B	601	CLA	C1D-CHD-C4C	-3.81	117.53	122.56
23	b	610	CLA	O2A-CGA-CBA	3.80	123.84	111.91
23	C	507	CLA	O2D-CGD-O1D	-3.80	116.41	123.84
33	d	412	LMG	O7-C10-C11	3.80	119.69	111.50
26	a	411	SQD	C1-O5-C5	-3.80	106.23	113.69
23	C	505	CLA	C3C-C4C-NC	3.80	114.83	110.57
23	c	511	CLA	C1D-CHD-C4C	-3.79	117.55	122.56
23	b	605	CLA	O2D-CGD-O1D	-3.79	116.42	123.84
23	B	613	CLA	CMC-C2C-C1C	3.79	130.81	125.04
23	b	615	CLA	C3C-C4C-NC	3.79	114.82	110.57
23	b	605	CLA	CHD-C4C-NC	3.79	130.17	124.20
23	B	607	CLA	C3C-C4C-NC	3.79	114.82	110.57
23	a	406	CLA	CAA-C2A-C3A	-3.79	102.41	112.78
23	a	409	CLA	C3B-C4B-NB	3.79	114.10	109.21
23	C	510	CLA	C3B-C4B-NB	3.78	114.10	109.21
23	c	507	CLA	C1-C2-C3	-3.78	119.50	126.04
23	C	507	CLA	C3C-C4C-NC	3.78	114.81	110.57
23	a	409	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
26	f	102	SQD	C1-O5-C5	3.77	121.10	113.69
24	a	353	PHO	O2D-CGD-O1D	-3.77	116.47	123.84
23	B	606	CLA	C1C-C2C-C3C	-3.77	103.00	106.96
23	d	403	CLA	O2D-CGD-O1D	-3.76	116.48	123.84
23	A	405	CLA	CHD-C4C-NC	3.76	130.13	124.20
23	c	513	CLA	C1D-CHD-C4C	-3.75	117.60	122.56
23	B	608	CLA	C1D-CHD-C4C	-3.75	117.61	122.56
23	c	512	CLA	C1C-C2C-C3C	-3.75	103.01	106.96
23	c	508	CLA	C3C-C4C-NC	3.75	114.78	110.57
23	c	507	CLA	C3C-C4C-NC	3.75	114.78	110.57
29	A	414	PL9	C37-C38-C39	-3.75	118.63	127.66
23	c	502	CLA	C1C-C2C-C3C	-3.75	103.02	106.96
23	C	512	CLA	C1-C2-C3	-3.75	119.56	126.04
23	B	611	CLA	C3B-C4B-NB	3.74	114.05	109.21
23	b	609	CLA	O2D-CGD-O1D	-3.74	116.52	123.84
23	c	503	CLA	C1D-CHD-C4C	-3.74	117.62	122.56
23	C	511	CLA	C3C-C4C-NC	3.74	114.76	110.57
23	b	615	CLA	C1D-CHD-C4C	-3.74	117.62	122.56
23	a	405	CLA	O2D-CGD-CBD	3.74	117.91	111.27
24	A	353	PHO	O2D-CGD-O1D	-3.73	116.55	123.84
29	A	414	PL9	C10-C9-C11	3.73	121.54	115.27
23	B	614	CLA	O2A-CGA-O1A	-3.72	114.21	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	612	CLA	C1D-CHD-C4C	-3.72	117.65	122.56
23	b	615	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
23	B	612	CLA	C4C-C3C-C2C	-3.71	101.49	106.90
33	c	521	LMG	O7-C10-C11	3.71	119.50	111.50
23	c	510	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
23	B	612	CLA	CMB-C2B-C3B	3.71	131.61	124.68
23	C	509	CLA	C4C-C3C-C2C	-3.70	101.50	106.90
23	c	510	CLA	C3C-C4C-NC	3.70	114.72	110.57
23	C	512	CLA	C3B-C4B-NB	3.70	113.99	109.21
33	a	419	LMG	O7-C10-C11	3.70	119.47	111.50
23	D	405	CLA	C4D-C3D-CAD	-3.70	106.41	108.47
23	b	604	CLA	C1-C2-C3	-3.70	119.65	126.04
23	b	602	CLA	O2D-CGD-O1D	-3.70	116.61	123.84
23	B	616	CLA	C4C-C3C-C2C	-3.70	101.51	106.90
25	b	618	BCR	C15-C14-C13	-3.69	122.05	127.31
23	a	409	CLA	CAA-C2A-C3A	-3.69	102.68	112.78
23	B	611	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
23	b	606	CLA	C1D-CHD-C4C	-3.68	117.69	122.56
23	C	504	CLA	O2D-CGD-CBD	3.68	117.81	111.27
23	b	601	CLA	C3C-C4C-NC	3.68	114.70	110.57
23	B	611	CLA	C1D-CHD-C4C	-3.68	117.70	122.56
23	B	603	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
23	c	511	CLA	C3B-C4B-NB	3.68	113.97	109.21
23	B	613	CLA	O2D-CGD-CBD	3.67	117.79	111.27
23	b	613	CLA	C3B-C4B-NB	3.67	113.96	109.21
23	A	404	CLA	C3B-C4B-NB	3.67	113.95	109.21
23	a	406	CLA	C3C-C4C-NC	3.67	114.68	110.57
23	a	407	CLA	CAA-C2A-C3A	-3.67	102.74	112.78
23	C	509	CLA	C1D-CHD-C4C	-3.67	117.72	122.56
23	A	405	CLA	C1D-CHD-C4C	-3.67	117.72	122.56
23	c	512	CLA	C1-C2-C3	-3.67	119.70	126.04
23	b	612	CLA	C3B-C4B-NB	3.66	113.95	109.21
25	a	410	BCR	C20-C21-C22	-3.66	122.09	127.31
23	c	502	CLA	C3C-C4C-NC	3.66	114.67	110.57
37	d	408	LHG	O7-C7-C8	3.65	119.38	111.50
29	a	416	PL9	C22-C23-C24	-3.65	118.86	127.66
23	c	503	CLA	O2D-CGD-O1D	-3.65	116.70	123.84
25	K	102	BCR	C24-C23-C22	-3.65	120.72	126.23
23	b	610	CLA	O2D-CGD-O1D	-3.65	116.71	123.84
23	C	505	CLA	CAC-C3C-C4C	3.65	129.54	124.81
23	B	610	CLA	CAA-C2A-C3A	-3.64	102.80	112.78
23	c	514	CLA	C1D-CHD-C4C	-3.64	117.75	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	L	101	LHG	O7-C7-C8	3.64	119.35	111.50
23	b	610	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
23	B	615	CLA	CMC-C2C-C1C	3.64	130.58	125.04
23	c	509	CLA	CMB-C2B-C3B	3.64	131.48	124.68
23	b	601	CLA	C1D-CHD-C4C	-3.64	117.76	122.56
24	a	408	PHO	C2C-C1C-NC	3.63	115.27	109.79
23	b	614	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
23	a	407	CLA	C3C-C4C-NC	3.63	114.64	110.57
23	B	610	CLA	C4C-C3C-C2C	-3.62	101.62	106.90
23	B	608	CLA	O2D-CGD-O1D	-3.62	116.76	123.84
23	d	403	CLA	C1-C2-C3	-3.62	119.78	126.04
23	C	512	CLA	C4A-NA-C1A	-3.62	105.08	106.71
23	a	406	CLA	CHD-C4C-NC	3.62	129.91	124.20
29	a	416	PL9	C37-C38-C39	-3.62	118.95	127.66
23	d	402	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
29	A	414	PL9	C15-C14-C16	3.61	121.34	115.27
23	a	405	CLA	C1D-CHD-C4C	-3.61	117.80	122.56
23	c	512	CLA	C4-C3-C5	3.61	121.34	115.27
25	Y	101	BCR	C15-C14-C13	-3.60	122.17	127.31
25	c	515	BCR	C16-C17-C18	-3.60	122.17	127.31
23	b	608	CLA	C3B-C4B-NB	3.60	113.86	109.21
23	b	604	CLA	C3B-C4B-NB	3.60	113.86	109.21
23	c	507	CLA	C1D-CHD-C4C	-3.60	117.81	122.56
23	b	601	CLA	O2D-CGD-O1D	-3.60	116.81	123.84
33	m	101	LMG	O7-C10-C11	3.60	119.25	111.50
26	a	413	SQD	O47-C7-C8	3.60	119.25	111.50
25	B	618	BCR	C15-C14-C13	-3.60	122.18	127.31
26	A	410	SQD	C44-O6-C1	-3.60	106.71	113.74
24	a	408	PHO	CHC-C1C-C2C	-3.59	116.69	125.73
23	B	613	CLA	C3B-C4B-NB	3.59	113.86	109.21
23	C	514	CLA	C1-C2-C3	-3.59	119.83	126.04
23	c	514	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
29	d	405	PL9	C36-C37-C38	-3.59	100.09	111.88
23	B	603	CLA	C4-C3-C5	3.59	121.30	115.27
23	A	406	CLA	C1-C2-C3	-3.58	119.84	126.04
23	B	613	CLA	CMB-C2B-C3B	3.58	131.38	124.68
29	a	416	PL9	C15-C14-C16	3.58	121.30	115.27
23	b	616	CLA	C2C-C1C-NC	3.58	113.33	109.97
29	A	414	PL9	C32-C33-C34	-3.58	119.05	127.66
24	a	353	PHO	CAC-C3C-C4C	3.58	129.12	125.22
23	b	609	CLA	C1D-CHD-C4C	-3.58	117.84	122.56
23	C	503	CLA	O2D-CGD-O1D	-3.57	116.85	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	612	CLA	CMB-C2B-C3B	3.57	131.36	124.68
23	b	606	CLA	C4-C3-C5	3.57	121.28	115.27
23	C	508	CLA	O2D-CGD-O1D	-3.57	116.86	123.84
23	A	408	CLA	O2D-CGD-CBD	3.56	117.60	111.27
23	B	615	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
25	A	409	BCR	C24-C23-C22	-3.56	120.86	126.23
23	C	503	CLA	C1D-CHD-C4C	-3.56	117.86	122.56
23	a	409	CLA	C1D-CHD-C4C	-3.56	117.86	122.56
23	b	609	CLA	CAC-C3C-C4C	3.55	129.42	124.81
23	C	508	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
23	A	408	CLA	C1D-CHD-C4C	-3.55	117.88	122.56
23	C	506	CLA	C1C-C2C-C3C	-3.55	103.23	106.96
23	b	614	CLA	CAC-C3C-C4C	3.54	129.41	124.81
23	C	512	CLA	C1D-CHD-C4C	-3.54	117.88	122.56
24	a	408	PHO	C1C-C2C-C3C	-3.54	102.44	106.51
23	B	614	CLA	C1D-CHD-C4C	-3.54	117.89	122.56
23	b	605	CLA	C1D-CHD-C4C	-3.54	117.89	122.56
23	A	408	CLA	C1C-C2C-C3C	-3.53	103.24	106.96
23	b	616	CLA	C4C-C3C-C2C	-3.53	101.75	106.90
23	D	406	CLA	C1D-CHD-C4C	-3.53	117.90	122.56
35	c	518	DGD	O2G-C1B-C2B	3.53	119.11	111.50
23	a	407	CLA	C1D-CHD-C4C	-3.53	117.90	122.56
23	d	403	CLA	C3C-C4C-NC	3.53	114.53	110.57
23	C	512	CLA	CMC-C2C-C1C	3.53	130.41	125.04
23	A	405	CLA	C4D-C3D-CAD	-3.52	106.50	108.47
23	B	616	CLA	O2D-CGD-O1D	-3.52	116.95	123.84
23	b	611	CLA	O2D-CGD-O1D	-3.52	116.95	123.84
23	c	510	CLA	C3B-C4B-NB	3.52	113.76	109.21
23	c	513	CLA	C1C-C2C-C3C	-3.52	103.26	106.96
23	A	406	CLA	C1C-C2C-C3C	-3.51	103.26	106.96
23	A	405	CLA	CAA-C2A-C3A	-3.51	103.16	112.78
35	C	517	DGD	C3G-C2G-C1G	-3.51	103.48	111.79
23	b	603	CLA	C3B-C4B-NB	3.51	113.75	109.21
23	c	505	CLA	C4A-NA-C1A	-3.51	105.13	106.71
23	c	508	CLA	O2D-CGD-O1D	-3.51	116.97	123.84
24	a	353	PHO	C4D-CHA-C1A	-3.51	117.47	125.37
40	V	202	HEC	CBA-CAA-C2A	-3.51	106.01	112.48
33	Z	101	LMG	C1-C2-C3	3.51	117.31	110.00
24	a	408	PHO	CAC-C3C-C4C	3.51	129.05	125.22
23	C	505	CLA	C3B-C4B-NB	3.51	113.74	109.21
23	c	506	CLA	C4C-C3C-C2C	-3.51	101.79	106.90
23	b	606	CLA	O2D-CGD-O1D	-3.50	116.99	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	512	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
23	B	615	CLA	O2D-CGD-CBD	3.50	117.48	111.27
23	B	612	CLA	C3B-C4B-NB	3.50	113.73	109.21
23	b	601	CLA	C1C-C2C-C3C	-3.49	103.28	106.96
23	C	509	CLA	C1C-C2C-C3C	-3.49	103.28	106.96
23	a	409	CLA	O2D-CGD-O1D	-3.49	117.01	123.84
29	a	416	PL9	C7-C3-C2	-3.49	118.71	123.30
23	D	405	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
23	A	404	CLA	C1D-CHD-C4C	-3.48	117.96	122.56
40	V	202	HEC	CBD-CAD-C3D	-3.48	106.06	112.49
23	a	405	CLA	C3C-C4C-NC	3.48	114.47	110.57
23	b	611	CLA	C1D-CHD-C4C	-3.48	117.97	122.56
37	d	406	LHG	O7-C7-C8	3.48	119.00	111.50
23	C	511	CLA	C4-C3-C5	3.48	121.12	115.27
23	B	605	CLA	CHD-C4C-NC	3.48	129.68	124.20
33	z	101	LMG	O7-C10-C11	3.47	118.99	111.50
23	b	603	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
29	a	416	PL9	C30-C29-C31	3.47	121.11	115.27
24	A	407	PHO	C4C-C3C-C2C	-3.47	102.94	106.78
23	b	603	CLA	O2A-CGA-O1A	-3.47	114.84	123.59
23	a	405	CLA	O2A-CGA-CBA	3.47	122.78	111.91
23	b	615	CLA	C3B-C4B-NB	3.46	113.69	109.21
23	B	614	CLA	C4-C3-C5	3.46	121.09	115.27
24	A	353	PHO	C2B-C1B-NB	3.46	115.01	109.79
23	B	615	CLA	C11-C10-C8	-3.46	104.75	115.92
24	A	407	PHO	CAC-C3C-C4C	3.46	128.99	125.22
37	l	101	LHG	O7-C7-C8	3.46	118.95	111.50
23	b	609	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
23	C	508	CLA	C1D-CHD-C4C	-3.44	118.01	122.56
23	c	507	CLA	C4D-C3D-CAD	-3.44	106.55	108.47
25	B	618	BCR	C29-C30-C25	3.44	115.78	110.48
23	b	601	CLA	C4-C3-C5	3.44	121.06	115.27
23	b	612	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
23	b	602	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
23	C	513	CLA	C1-C2-C3	-3.44	120.10	126.04
40	v	202	HEC	CBD-CAD-C3D	-3.44	106.15	112.49
23	b	614	CLA	C1D-CHD-C4C	-3.43	118.03	122.56
23	C	502	CLA	C1D-CHD-C4C	-3.43	118.03	122.56
24	a	353	PHO	C4-C3-C5	3.43	121.04	115.27
23	c	502	CLA	C1-C2-C3	-3.43	120.12	126.04
33	c	521	LMG	O6-C5-C4	3.43	115.92	109.69
23	C	503	CLA	C1C-C2C-C3C	-3.43	103.36	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	616	CLA	C1D-CHD-C4C	-3.42	118.04	122.56
23	B	603	CLA	CMB-C2B-C3B	3.42	131.08	124.68
23	C	511	CLA	O2D-CGD-O1D	-3.42	117.15	123.84
33	C	501	LMG	O1-C1-C2	3.42	113.65	108.30
23	c	511	CLA	C4-C3-C5	3.42	121.03	115.27
23	c	509	CLA	CHD-C4C-NC	3.42	129.59	124.20
23	a	405	CLA	CHC-C1C-C2C	-3.41	117.28	126.72
23	b	603	CLA	CAA-C2A-C3A	-3.41	103.44	112.78
23	b	601	CLA	C3B-C4B-NB	3.41	113.62	109.21
29	d	405	PL9	C32-C33-C34	-3.41	119.45	127.66
29	D	408	PL9	C37-C38-C39	-3.41	119.46	127.66
26	A	410	SQD	O9-S-C6	3.41	110.99	106.94
29	A	414	PL9	C7-C3-C2	-3.40	118.82	123.30
23	C	506	CLA	C3B-C4B-NB	3.40	113.61	109.21
23	B	609	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
23	c	504	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
23	B	616	CLA	C3B-C4B-NB	3.40	113.60	109.21
29	A	414	PL9	C27-C28-C29	-3.40	119.48	127.66
23	B	603	CLA	CBC-CAC-C3C	-3.39	103.08	112.43
23	D	406	CLA	CMC-C2C-C1C	3.39	130.20	125.04
23	C	504	CLA	C1C-C2C-C3C	-3.39	103.40	106.96
23	b	613	CLA	C1D-CHD-C4C	-3.38	118.09	122.56
23	B	606	CLA	O2D-CGD-O1D	-3.38	117.23	123.84
25	t	103	BCR	C7-C8-C9	-3.38	121.13	126.23
23	C	511	CLA	C3B-C4B-NB	3.38	113.58	109.21
37	l	101	LHG	O8-C23-C24	3.37	122.50	111.91
23	B	607	CLA	C4-C3-C5	3.37	120.94	115.27
25	A	409	BCR	C33-C5-C6	-3.37	120.74	124.53
23	B	604	CLA	C3B-C4B-NB	3.37	113.56	109.21
34	V	203	HTG	C1-O5-C5	3.37	116.75	112.19
23	b	610	CLA	O2A-CGA-O1A	-3.37	115.09	123.59
23	B	605	CLA	C4C-C3C-C2C	-3.36	101.99	106.90
25	d	404	BCR	C15-C14-C13	-3.36	122.51	127.31
23	B	612	CLA	C1C-C2C-C3C	-3.36	103.42	106.96
25	A	409	BCR	C16-C17-C18	-3.36	122.52	127.31
23	A	405	CLA	CMC-C2C-C1C	3.35	130.15	125.04
23	b	612	CLA	C4-C3-C5	3.35	120.91	115.27
23	c	509	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
24	a	408	PHO	C4C-C3C-C2C	-3.35	103.07	106.78
23	B	607	CLA	C1D-CHD-C4C	-3.35	118.14	122.56
25	k	101	BCR	C29-C30-C25	3.35	115.63	110.48
23	d	402	CLA	CAA-C2A-C3A	-3.34	103.62	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	614	CLA	C3B-C4B-NB	3.34	113.53	109.21
23	B	606	CLA	C3B-C4B-NB	3.34	113.53	109.21
26	A	412	SQD	O47-C7-C8	3.33	118.69	111.50
25	C	516	BCR	C16-C17-C18	-3.33	122.55	127.31
23	d	403	CLA	C1C-C2C-C3C	-3.33	103.46	106.96
29	A	414	PL9	C17-C18-C19	-3.33	119.65	127.66
23	B	601	CLA	C1C-C2C-C3C	-3.32	103.46	106.96
23	b	604	CLA	C11-C12-C13	-3.32	105.18	115.92
23	B	610	CLA	C1-C2-C3	-3.32	120.30	126.04
23	B	601	CLA	C4C-C3C-C2C	-3.32	102.06	106.90
23	b	606	CLA	C1C-C2C-C3C	-3.32	103.47	106.96
25	C	516	BCR	C33-C5-C6	-3.32	120.80	124.53
23	C	513	CLA	C4C-C3C-C2C	-3.32	102.06	106.90
23	c	507	CLA	CHC-C1C-C2C	-3.32	117.54	126.72
23	b	614	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
25	D	407	BCR	C37-C22-C23	3.32	123.30	118.08
29	a	416	PL9	C27-C28-C29	-3.32	119.68	127.66
23	C	514	CLA	C1C-C2C-C3C	-3.32	103.47	106.96
29	D	408	PL9	C40-C39-C41	3.31	120.85	115.27
23	C	508	CLA	C1-C2-C3	-3.31	120.32	126.04
23	b	602	CLA	CAA-C2A-C3A	-3.31	103.72	112.78
23	a	409	CLA	C4-C3-C5	3.31	120.83	115.27
23	A	404	CLA	CMB-C2B-C3B	3.31	130.86	124.68
23	c	503	CLA	C3B-C4B-NB	3.31	113.48	109.21
37	D	409	LHG	O8-C23-O10	-3.30	115.25	123.59
23	C	505	CLA	C1D-CHD-C4C	-3.30	118.20	122.56
34	B	622	HTG	C1-O5-C5	3.30	118.67	112.58
32	M	103	LMT	O5'-C5'-C4'	3.30	116.71	109.75
24	a	408	PHO	C2B-C1B-NB	3.30	114.77	109.79
25	T	101	BCR	C15-C16-C17	-3.30	116.72	123.47
25	h	101	BCR	C16-C17-C18	-3.30	122.61	127.31
23	B	610	CLA	CAC-C3C-C4C	3.29	129.09	124.81
23	A	408	CLA	CAA-C2A-C3A	-3.29	103.76	112.78
23	c	512	CLA	CHD-C4C-NC	3.29	129.39	124.20
23	a	407	CLA	C3B-C4B-NB	3.29	113.47	109.21
23	B	614	CLA	CMC-C2C-C1C	3.29	130.05	125.04
23	b	611	CLA	C1C-C2C-C3C	-3.29	103.50	106.96
23	c	504	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
25	y	101	BCR	C15-C14-C13	-3.29	122.62	127.31
25	T	101	BCR	C12-C13-C14	-3.29	113.90	118.94
23	b	616	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
23	b	610	CLA	C1D-CHD-C4C	-3.29	118.22	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	620	SQD	O8-S-C6	3.28	110.97	105.74
23	B	603	CLA	O2A-CGA-CBA	3.28	122.21	111.91
23	b	605	CLA	CED-O2D-CGD	3.28	123.35	115.94
23	c	509	CLA	C4D-C3D-CAD	-3.28	106.64	108.47
29	d	405	PL9	C40-C39-C41	3.28	120.78	115.27
23	b	613	CLA	C4-C3-C5	3.28	120.78	115.27
24	A	407	PHO	C2C-C1C-NC	3.28	114.73	109.79
23	A	406	CLA	C3B-C4B-NB	3.28	113.44	109.21
23	c	505	CLA	C1D-CHD-C4C	-3.28	118.23	122.56
23	c	512	CLA	C3B-C4B-NB	3.27	113.44	109.21
23	b	605	CLA	C4-C3-C5	3.27	120.78	115.27
23	C	510	CLA	C1D-CHD-C4C	-3.27	118.24	122.56
23	b	616	CLA	OBD-CAD-C3D	-3.27	122.55	127.98
23	C	511	CLA	CHD-C4C-NC	3.27	129.35	124.20
23	C	507	CLA	CAC-C3C-C4C	3.27	129.05	124.81
23	c	506	CLA	C1-C2-C3	-3.27	120.39	126.04
26	a	413	SQD	O7-S-C6	3.26	110.82	106.94
25	D	407	BCR	C24-C23-C22	-3.26	121.30	126.23
25	D	407	BCR	C33-C5-C6	-3.26	120.86	124.53
24	A	407	PHO	CHC-C1C-C2C	-3.26	117.52	125.73
37	d	406	LHG	O8-C23-O10	-3.26	115.36	123.59
23	C	514	CLA	C2A-C1A-CHA	-3.26	118.16	123.86
34	B	622	HTG	O5-C1-C2	3.26	114.41	110.31
25	t	103	BCR	C3-C4-C5	-3.26	108.26	114.08
29	a	416	PL9	C42-C43-C44	-3.26	119.81	127.66
23	B	606	CLA	C4C-C3C-C2C	-3.26	102.15	106.90
23	B	609	CLA	C4C-C3C-C2C	-3.26	102.15	106.90
23	c	508	CLA	CMC-C2C-C1C	3.25	130.00	125.04
23	C	505	CLA	CMC-C2C-C1C	3.25	130.00	125.04
23	d	402	CLA	C4C-C3C-C2C	-3.25	102.16	106.90
23	c	508	CLA	C4-C3-C5	3.25	120.74	115.27
23	d	402	CLA	O2A-CGA-CBA	3.25	122.11	111.91
23	C	506	CLA	C4-C3-C5	3.25	120.73	115.27
23	b	616	CLA	CHD-C4C-NC	3.25	129.32	124.20
25	B	619	BCR	C38-C26-C25	-3.25	120.88	124.53
23	b	605	CLA	O2A-CGA-O1A	-3.25	115.40	123.59
23	d	402	CLA	C1D-CHD-C4C	-3.24	118.28	122.56
23	c	504	CLA	C3B-C4B-NB	3.24	113.40	109.21
37	D	411	LHG	O8-C23-O10	-3.24	115.41	123.59
25	b	618	BCR	C7-C8-C9	-3.24	121.34	126.23
23	B	603	CLA	CAA-C2A-C3A	-3.24	103.91	112.78
23	B	608	CLA	O2A-CGA-O1A	-3.24	115.42	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	407	PHO	C2B-C1B-NB	3.24	114.68	109.79
23	b	607	CLA	C4C-C3C-C2C	-3.24	102.18	106.90
23	b	603	CLA	O2A-CGA-CBA	3.24	122.06	111.91
24	A	407	PHO	C2A-C1A-NA	3.24	115.58	111.86
23	c	503	CLA	C1-C2-C3	-3.23	120.45	126.04
23	A	406	CLA	CAA-C2A-C3A	-3.23	103.93	112.78
23	C	507	CLA	C3B-C4B-NB	3.23	113.38	109.21
23	C	514	CLA	C1D-CHD-C4C	-3.23	118.30	122.56
23	D	405	CLA	C3B-C4B-NB	3.22	113.38	109.21
23	C	507	CLA	CHC-C1C-C2C	-3.22	117.81	126.72
25	C	516	BCR	C11-C10-C9	-3.22	122.71	127.31
23	C	514	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
26	a	411	SQD	C1-C2-C3	-3.22	103.29	110.00
37	D	409	LHG	O7-C7-C8	3.21	118.43	111.50
23	A	408	CLA	CHD-C4C-NC	3.21	129.27	124.20
23	b	615	CLA	CHC-C1C-C2C	-3.21	117.83	126.72
23	c	507	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
23	c	507	CLA	C4-C3-C5	3.21	120.67	115.27
25	c	516	BCR	C38-C26-C25	-3.21	120.92	124.53
23	B	607	CLA	C3B-C4B-NB	3.21	113.36	109.21
23	d	402	CLA	C4-C3-C5	3.21	120.67	115.27
23	b	612	CLA	C4C-C3C-C2C	-3.20	102.23	106.90
25	B	617	BCR	C16-C17-C18	-3.20	122.74	127.31
23	b	603	CLA	C4C-C3C-C2C	-3.20	102.23	106.90
29	d	405	PL9	C20-C19-C21	3.20	120.65	115.27
23	c	513	CLA	C4-C3-C5	3.20	120.65	115.27
25	t	103	BCR	C11-C10-C9	-3.20	122.75	127.31
23	C	506	CLA	C4C-C3C-C2C	-3.20	102.24	106.90
23	A	408	CLA	C3B-C4B-NB	3.20	113.34	109.21
23	C	502	CLA	CMC-C2C-C1C	3.19	129.90	125.04
29	A	414	PL9	C35-C34-C36	3.19	120.64	115.27
23	B	602	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
26	F	101	SQD	O8-S-C6	3.19	110.82	105.74
23	D	406	CLA	C1C-C2C-C3C	-3.19	103.61	106.96
25	A	409	BCR	C15-C14-C13	-3.19	122.76	127.31
25	k	101	BCR	C11-C10-C9	-3.18	122.77	127.31
23	c	513	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
23	B	608	CLA	C1-C2-C3	-3.18	120.54	126.04
23	b	613	CLA	CMB-C2B-C3B	3.18	130.63	124.68
23	b	611	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
23	D	406	CLA	C4-C3-C5	3.18	120.62	115.27
33	C	520	LMG	O8-C28-C29	3.18	121.89	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	607	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
23	c	507	CLA	CBC-CAC-C3C	-3.18	103.67	112.43
23	B	601	CLA	C3B-C4B-NB	3.18	113.32	109.21
23	B	605	CLA	C1C-C2C-C3C	-3.18	103.62	106.96
23	C	510	CLA	CAC-C3C-C4C	3.17	128.93	124.81
25	a	410	BCR	C11-C10-C9	-3.17	122.78	127.31
23	B	610	CLA	C1D-CHD-C4C	-3.17	118.37	122.56
37	D	411	LHG	O7-C7-C8	3.17	118.33	111.50
23	C	507	CLA	C1-C2-C3	-3.17	120.56	126.04
23	c	514	CLA	C3B-C4B-NB	3.16	113.30	109.21
23	B	603	CLA	C3B-C4B-NB	3.16	113.30	109.21
23	B	609	CLA	C1D-CHD-C4C	-3.16	118.38	122.56
23	B	614	CLA	CMB-C2B-C3B	3.16	130.59	124.68
23	a	409	CLA	CBC-CAC-C3C	-3.16	103.71	112.43
23	A	408	CLA	C4C-C3C-C2C	-3.16	102.29	106.90
25	c	515	BCR	C33-C5-C6	-3.16	120.98	124.53
23	c	510	CLA	C1-O2A-CGA	3.16	124.73	116.44
23	b	616	CLA	O2A-CGA-CBA	3.16	121.81	111.91
23	c	512	CLA	CBC-CAC-C3C	-3.16	103.73	112.43
23	B	610	CLA	O2A-CGA-O1A	-3.15	115.64	123.59
23	B	611	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
29	a	416	PL9	C17-C18-C19	-3.15	120.08	127.66
23	B	614	CLA	C3B-C4B-NB	3.15	113.28	109.21
24	A	407	PHO	C1C-C2C-C3C	-3.15	102.90	106.51
23	b	602	CLA	C1D-CHD-C4C	-3.15	118.41	122.56
23	b	609	CLA	C3B-C4B-NB	3.15	113.28	109.21
23	c	513	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
26	B	620	SQD	O48-C23-C24	3.14	121.76	111.91
23	a	405	CLA	O2A-CGA-O1A	-3.14	115.67	123.59
23	c	508	CLA	CHD-C4C-NC	3.14	129.15	124.20
23	A	405	CLA	O2A-CGA-O1A	-3.14	115.67	123.59
23	c	505	CLA	CAC-C3C-C4C	3.13	128.87	124.81
37	e	101	LHG	O7-C7-C8	3.13	118.25	111.50
37	D	409	LHG	O8-C23-C24	3.13	121.73	111.91
26	F	101	SQD	C44-O6-C1	-3.13	107.63	113.74
23	b	604	CLA	C1D-CHD-C4C	-3.13	118.43	122.56
23	a	405	CLA	CMB-C2B-C3B	3.13	130.53	124.68
25	c	515	BCR	C24-C23-C22	-3.12	121.52	126.23
23	b	611	CLA	C3B-C4B-NB	3.12	113.25	109.21
23	C	508	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
23	C	506	CLA	CMC-C2C-C1C	3.12	129.79	125.04
23	d	403	CLA	CMC-C2C-C1C	3.12	129.79	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	615	CLA	C3B-C4B-NB	3.11	113.24	109.21
32	M	101	LMT	O1'-C1'-C2'	3.11	113.16	108.30
23	b	603	CLA	C2A-C1A-CHA	-3.11	118.42	123.86
23	c	506	CLA	C1C-C2C-C3C	-3.11	103.68	106.96
23	B	613	CLA	O2A-CGA-CBA	3.11	121.67	111.91
23	B	615	CLA	CHD-C4C-NC	3.11	129.10	124.20
29	D	408	PL9	C27-C28-C29	-3.11	120.17	127.66
23	b	610	CLA	CHD-C4C-NC	3.11	129.10	124.20
38	E	103	HEM	CBA-CAA-C2A	-3.11	106.75	112.49
26	a	413	SQD	O48-C23-C24	3.11	121.66	111.91
23	b	607	CLA	CAC-C3C-C4C	3.11	128.84	124.81
23	C	514	CLA	CMC-C2C-C1C	3.11	129.77	125.04
23	B	602	CLA	C1C-C2C-C3C	-3.11	103.69	106.96
23	c	505	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
23	c	511	CLA	CBC-CAC-C3C	-3.11	103.87	112.43
23	b	606	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
23	c	508	CLA	CBC-CAC-C3C	-3.11	103.87	112.43
23	C	510	CLA	O2A-CGA-CBA	3.10	121.65	111.91
23	A	406	CLA	CAC-C3C-C4C	3.10	128.84	124.81
23	B	608	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
23	b	612	CLA	O2A-CGA-CBA	3.10	121.63	111.91
23	b	615	CLA	C11-C10-C8	-3.10	105.91	115.92
25	t	103	BCR	C35-C13-C12	3.09	122.95	118.08
23	C	513	CLA	C1C-C2C-C3C	-3.09	103.70	106.96
25	D	407	BCR	C16-C17-C18	-3.09	122.89	127.31
23	c	504	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
23	B	614	CLA	C2A-C1A-CHA	-3.09	118.45	123.86
23	A	406	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
29	a	416	PL9	C10-C9-C11	3.09	120.47	115.27
23	b	616	CLA	CAC-C3C-C4C	3.09	128.82	124.81
23	c	502	CLA	CAC-C3C-C4C	3.09	128.82	124.81
23	c	506	CLA	CAC-C3C-C4C	3.09	128.82	124.81
29	d	405	PL9	C7-C8-C9	-3.09	121.66	126.79
23	B	614	CLA	CHD-C4C-NC	3.08	129.06	124.20
23	b	605	CLA	C2A-C1A-CHA	-3.08	118.47	123.86
23	b	608	CLA	C1D-CHD-C4C	-3.08	118.49	122.56
38	e	87	HEM	CBD-CAD-C3D	-3.08	106.80	112.48
23	C	503	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
23	C	513	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
23	A	404	CLA	CMC-C2C-C1C	3.08	129.72	125.04
23	b	611	CLA	O2A-CGA-O1A	-3.08	115.83	123.59
23	b	604	CLA	O2A-CGA-CBA	3.07	121.56	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	514	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
29	d	405	PL9	C37-C38-C39	-3.07	120.27	127.66
23	c	511	CLA	CHD-C4C-NC	3.07	129.04	124.20
23	a	409	CLA	O2A-CGA-CBA	3.07	121.53	111.91
23	c	506	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
23	c	510	CLA	CAC-C3C-C4C	3.06	128.78	124.81
23	b	603	CLA	CMC-C2C-C1C	3.06	129.70	125.04
25	a	410	BCR	C29-C30-C25	3.06	115.18	110.48
23	B	606	CLA	CMB-C2B-C3B	3.05	130.39	124.68
23	a	407	CLA	CHC-C1C-C2C	-3.05	118.27	126.72
23	C	506	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
25	a	410	BCR	C7-C8-C9	-3.05	121.62	126.23
23	B	612	CLA	C4-C3-C5	3.05	120.40	115.27
25	B	619	BCR	C24-C23-C22	-3.05	121.63	126.23
29	D	408	PL9	C10-C9-C11	3.05	120.40	115.27
35	C	518	DGD	O2G-C1B-C2B	3.05	118.07	111.50
23	A	404	CLA	CAC-C3C-C4C	3.05	128.77	124.81
23	D	406	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
24	A	353	PHO	C4A-NA-C1A	-3.04	105.68	108.14
23	C	504	CLA	CAC-C3C-C4C	3.04	128.76	124.81
23	b	606	CLA	C3B-C4B-NB	3.04	113.14	109.21
23	c	510	CLA	CHD-C4C-NC	3.04	129.00	124.20
23	B	607	CLA	CBC-CAC-C3C	-3.04	104.05	112.43
25	T	101	BCR	C33-C5-C6	-3.04	121.12	124.53
23	B	610	CLA	C1C-C2C-C3C	-3.04	103.76	106.96
23	C	512	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
23	B	604	CLA	O2A-CGA-O1A	-3.04	115.93	123.59
23	D	406	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
23	B	601	CLA	CHD-C4C-NC	3.04	128.99	124.20
23	C	511	CLA	O2A-CGA-CBA	3.03	121.43	111.91
23	d	403	CLA	CHD-C4C-NC	3.03	128.98	124.20
25	C	516	BCR	C15-C14-C13	-3.03	122.98	127.31
23	b	611	CLA	CHD-C4C-NC	3.03	128.98	124.20
23	c	514	CLA	CMC-C2C-C1C	3.03	129.65	125.04
23	B	615	CLA	C4C-C3C-C2C	-3.02	102.49	106.90
26	A	412	SQD	O48-C23-C24	3.02	121.40	111.91
23	C	502	CLA	CBC-CAC-C3C	-3.02	104.09	112.43
26	b	620	SQD	C3-C4-C5	3.02	115.63	110.24
23	a	405	CLA	C4-C3-C5	3.02	120.36	115.27
23	C	510	CLA	C4C-C3C-C2C	-3.02	102.49	106.90
23	a	407	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
23	C	504	CLA	C4C-C3C-C2C	-3.02	102.49	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	602	CLA	C1D-CHD-C4C	-3.02	118.57	122.56
29	A	414	PL9	C42-C43-C44	-3.02	120.39	127.66
23	B	616	CLA	CHD-C4C-NC	3.02	128.96	124.20
26	F	101	SQD	O7-S-C6	3.02	110.53	106.94
23	b	614	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
29	D	408	PL9	C36-C37-C38	-3.02	101.96	111.88
23	C	511	CLA	CMB-C2B-C3B	3.01	130.32	124.68
23	b	609	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
23	C	511	CLA	CBC-CAC-C3C	-3.01	104.13	112.43
23	B	604	CLA	CHD-C4C-NC	3.01	128.95	124.20
23	B	614	CLA	CBC-CAC-C3C	-3.01	104.13	112.43
25	y	101	BCR	C16-C17-C18	-3.01	123.02	127.31
23	C	509	CLA	CHC-C1C-C2C	-3.01	118.40	126.72
23	c	514	CLA	CAC-C3C-C4C	3.01	128.71	124.81
23	a	407	CLA	CHD-C4C-NC	3.01	128.94	124.20
23	D	406	CLA	CAC-C3C-C4C	3.01	128.71	124.81
23	b	608	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
23	c	502	CLA	C1D-CHD-C4C	-3.01	118.59	122.56
23	B	610	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
23	B	603	CLA	C4C-C3C-C2C	-3.00	102.52	106.90
23	C	508	CLA	CHD-C4C-NC	3.00	128.93	124.20
23	c	502	CLA	C3B-C4B-NB	3.00	113.09	109.21
25	h	101	BCR	C38-C26-C25	-3.00	121.16	124.53
23	c	514	CLA	C4C-C3C-C2C	-2.99	102.53	106.90
25	b	619	BCR	C38-C26-C25	-2.99	121.17	124.53
23	b	601	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
25	B	618	BCR	C28-C27-C26	-2.99	108.74	114.08
23	D	406	CLA	CHD-C4C-NC	2.99	128.91	124.20
23	b	603	CLA	C7-C6-C5	-2.99	105.24	113.36
25	B	618	BCR	C11-C10-C9	-2.99	123.04	127.31
23	B	609	CLA	C3B-C4B-NB	2.99	113.08	109.21
23	a	405	CLA	CAA-C2A-C1A	-2.99	102.18	111.97
23	C	502	CLA	C4-C3-C5	2.99	120.30	115.27
23	b	613	CLA	C4D-C3D-CAD	-2.99	106.80	108.47
23	d	402	CLA	C3B-C4B-NB	2.99	113.07	109.21
23	b	610	CLA	CAA-C2A-C3A	-2.98	104.61	112.78
25	C	515	BCR	C16-C17-C18	-2.98	123.05	127.31
23	a	409	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
24	A	353	PHO	C4-C3-C5	2.98	120.29	115.27
23	C	510	CLA	CHC-C1C-C2C	-2.98	118.48	126.72
23	b	613	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
33	Z	101	LMG	O6-C1-C2	2.98	116.65	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	504	CLA	CHC-C1C-C2C	-2.98	118.48	126.72
23	c	509	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
23	C	507	CLA	CAA-C2A-C3A	-2.98	104.63	112.78
23	b	614	CLA	CMC-C2C-C1C	2.98	129.57	125.04
23	b	601	CLA	CHC-C1C-C2C	-2.97	118.49	126.72
37	d	406	LHG	O8-C23-C24	2.97	121.24	111.91
23	a	409	CLA	CMA-C3A-C2A	-2.97	101.84	113.83
23	A	404	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
25	d	404	BCR	C33-C5-C6	-2.97	121.19	124.53
25	h	101	BCR	C7-C8-C9	-2.97	121.75	126.23
25	Y	101	BCR	C28-C27-C26	-2.97	108.78	114.08
23	B	608	CLA	CMB-C2B-C3B	2.97	130.23	124.68
23	b	604	CLA	CHC-C1C-C2C	-2.97	118.51	126.72
25	K	102	BCR	C15-C14-C13	-2.97	123.08	127.31
25	a	410	BCR	C38-C26-C25	-2.97	121.20	124.53
23	c	503	CLA	CHD-C4C-NC	2.97	128.88	124.20
23	c	507	CLA	CAA-C2A-C3A	-2.97	104.66	112.78
23	c	509	CLA	C1-C2-C3	-2.96	120.92	126.04
23	b	610	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
23	A	404	CLA	CAA-CBA-CGA	-2.96	104.59	113.25
33	c	521	LMG	O8-C28-C29	2.96	121.20	111.91
23	A	406	CLA	C2A-C1A-CHA	-2.96	118.68	123.86
23	C	512	CLA	C4-C3-C5	2.96	120.25	115.27
23	c	503	CLA	CMC-C2C-C1C	2.96	129.55	125.04
26	b	620	SQD	C1-O5-C5	-2.96	107.88	113.69
25	B	618	BCR	C37-C22-C21	-2.96	118.78	122.92
23	c	510	CLA	CMC-C2C-C1C	2.96	129.54	125.04
23	A	405	CLA	CMA-C3A-C2A	-2.96	101.90	113.83
23	A	408	CLA	CMA-C3A-C4A	-2.96	103.83	111.77
23	c	505	CLA	CMC-C2C-C1C	2.96	129.54	125.04
26	a	411	SQD	O47-C7-O49	-2.95	116.56	123.70
23	a	405	CLA	C1-C2-C3	-2.95	120.94	126.04
23	a	406	CLA	C3B-C4B-NB	2.95	113.03	109.21
35	C	518	DGD	O1G-C1A-C2A	2.95	121.17	111.91
24	a	408	PHO	C4D-CHA-C1A	-2.95	118.73	125.37
23	d	402	CLA	O2A-CGA-O1A	-2.95	116.15	123.59
23	A	406	CLA	O2A-CGA-O1A	-2.95	116.16	123.59
23	b	604	CLA	CMC-C2C-C1C	2.95	129.52	125.04
25	c	516	BCR	C21-C20-C19	-2.94	114.03	123.22
23	C	509	CLA	C4D-C3D-CAD	-2.94	106.83	108.47
29	D	408	PL9	C7-C8-C9	-2.94	121.89	126.79
23	b	601	CLA	CHD-C4C-NC	2.94	128.84	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	608	CLA	CHC-C1C-C2C	-2.94	118.58	126.72
23	c	511	CLA	CHC-C1C-C2C	-2.94	118.59	126.72
24	a	353	PHO	C2B-C1B-NB	2.94	114.23	109.79
37	E	101	LHG	O8-C23-C24	2.94	121.13	111.91
33	B	621	LMG	O8-C28-C29	2.93	121.12	111.91
23	B	608	CLA	CMA-C3A-C4A	-2.93	103.89	111.77
24	A	353	PHO	C3C-C4C-NC	2.93	114.83	110.28
29	A	414	PL9	C22-C23-C24	-2.93	120.60	127.66
23	b	614	CLA	CHC-C1C-C2C	-2.93	118.61	126.72
23	C	513	CLA	O2A-CGA-CBA	2.93	121.10	111.91
24	a	353	PHO	CHD-C1D-C2D	-2.93	118.37	125.73
23	b	603	CLA	C4-C3-C5	2.92	120.19	115.27
23	b	612	CLA	CHC-C1C-C2C	-2.92	118.63	126.72
23	B	607	CLA	CAA-C2A-C3A	-2.92	104.77	112.78
23	c	512	CLA	CHC-C1C-C2C	-2.92	118.64	126.72
23	b	609	CLA	C4-C3-C5	2.92	120.18	115.27
24	A	353	PHO	CAC-C3C-C4C	2.92	128.41	125.22
23	b	616	CLA	C1-C2-C3	-2.92	120.99	126.04
26	A	412	SQD	O8-S-C6	2.92	110.39	105.74
23	B	612	CLA	O2A-CGA-O1A	-2.92	116.23	123.59
23	B	603	CLA	CHD-C4C-NC	2.92	128.80	124.20
25	K	102	BCR	C10-C11-C12	-2.92	114.12	123.22
37	D	411	LHG	O8-C23-C24	2.92	121.06	111.91
37	D	410	LHG	O8-C23-O10	-2.91	116.24	123.59
23	c	513	CLA	C3B-C4B-NB	2.91	112.98	109.21
23	c	513	CLA	CHD-C4C-NC	2.91	128.79	124.20
25	D	407	BCR	C10-C11-C12	-2.91	114.13	123.22
23	b	602	CLA	CHD-C4C-NC	2.91	128.79	124.20
23	C	513	CLA	CHD-C4C-NC	2.91	128.79	124.20
23	C	504	CLA	C3B-C4B-NB	2.91	112.97	109.21
33	a	419	LMG	O6-C5-C4	2.91	114.98	109.69
23	B	614	CLA	O2A-CGA-CBA	2.91	121.04	111.91
23	B	601	CLA	O2A-CGA-CBA	2.91	121.04	111.91
23	B	611	CLA	CHD-C4C-NC	2.91	128.78	124.20
33	m	101	LMG	O8-C28-C29	2.91	121.03	111.91
25	b	618	BCR	C38-C26-C25	-2.91	121.26	124.53
24	A	407	PHO	C4D-CHA-C1A	-2.91	118.83	125.37
23	b	609	CLA	CMC-C2C-C1C	2.91	129.47	125.04
23	C	510	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
23	B	613	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
25	H	101	BCR	C38-C26-C25	-2.90	121.27	124.53
29	A	414	PL9	C20-C19-C21	2.90	120.15	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	406	CLA	CHC-C1C-C2C	-2.90	118.70	126.72
23	B	611	CLA	CHC-C1C-C2C	-2.90	118.70	126.72
23	B	607	CLA	C1-C2-C3	-2.90	121.03	126.04
29	a	416	PL9	C35-C34-C36	2.90	120.14	115.27
23	b	602	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
23	B	611	CLA	OBD-CAD-C3D	-2.90	123.17	127.98
24	A	353	PHO	C4D-ND-C1D	-2.89	101.56	106.76
23	a	405	CLA	C2A-C1A-CHA	-2.89	118.80	123.86
23	C	513	CLA	C4D-C3D-CAD	-2.89	106.86	108.47
23	b	608	CLA	OBD-CAD-C3D	-2.89	123.18	127.98
23	C	502	CLA	C3B-C4B-NB	2.89	112.95	109.21
23	b	615	CLA	C4-C3-C5	2.89	120.13	115.27
25	c	516	BCR	C33-C5-C6	-2.89	121.28	124.53
23	B	603	CLA	C5-C3-C2	-2.89	115.27	121.12
23	C	512	CLA	CMB-C2B-C3B	2.89	130.08	124.68
24	A	353	PHO	C2A-C1A-NA	2.89	115.18	111.86
23	c	503	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
35	c	519	DGD	O2G-C1B-C2B	2.89	117.72	111.50
23	C	513	CLA	C4-C3-C5	2.89	120.13	115.27
23	c	505	CLA	CED-O2D-CGD	2.89	122.47	115.94
29	a	416	PL9	C25-C24-C26	2.89	120.13	115.27
23	c	509	CLA	C3B-C4B-NB	2.88	112.94	109.21
23	b	605	CLA	C4C-C3C-C2C	-2.88	102.69	106.90
23	B	604	CLA	C4C-C3C-C2C	-2.88	102.69	106.90
23	C	507	CLA	O2A-CGA-CBA	2.88	120.95	111.91
23	C	503	CLA	C3B-C4B-NB	2.88	112.94	109.21
23	A	408	CLA	C4-C3-C5	2.88	120.12	115.27
23	c	510	CLA	O2A-CGA-CBA	2.88	120.95	111.91
23	a	409	CLA	CHC-C1C-C2C	-2.88	118.76	126.72
23	c	512	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
23	b	608	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
25	b	618	BCR	C28-C27-C26	-2.88	108.94	114.08
29	d	405	PL9	C12-C13-C14	-2.88	120.73	127.66
23	b	615	CLA	C4C-C3C-C2C	-2.88	102.71	106.90
23	d	403	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
23	d	403	CLA	C1D-CHD-C4C	-2.87	118.77	122.56
23	c	514	CLA	C2A-C1A-CHA	-2.87	118.83	123.86
23	B	615	CLA	CAC-C3C-C4C	2.87	128.54	124.81
23	c	505	CLA	CHC-C1C-C2C	-2.87	118.78	126.72
23	D	406	CLA	C3B-C4B-NB	2.87	112.92	109.21
23	b	609	CLA	CBC-CAC-C3C	-2.87	104.52	112.43
25	T	101	BCR	C3-C4-C5	-2.87	108.95	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	502	CLA	CHC-C1C-C2C	-2.87	118.78	126.72
23	C	505	CLA	CHC-C1C-C2C	-2.87	118.78	126.72
23	B	604	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
23	A	405	CLA	C4-C3-C5	2.87	120.09	115.27
23	b	613	CLA	CHD-C4C-NC	2.87	128.72	124.20
23	B	607	CLA	OBD-CAD-C3D	-2.87	123.22	127.98
23	B	603	CLA	CMC-C2C-C1C	2.86	129.40	125.04
25	t	103	BCR	C21-C20-C19	-2.86	114.28	123.22
29	A	414	PL9	C7-C3-C4	2.86	119.20	116.88
23	C	505	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
23	B	607	CLA	CHC-C1C-C2C	-2.86	118.81	126.72
35	H	102	DGD	O2G-C1B-C2B	2.86	117.67	111.50
23	a	406	CLA	O2A-CGA-CBA	2.86	120.88	111.91
23	c	511	CLA	O2A-CGA-O1A	-2.86	116.38	123.59
23	b	602	CLA	CMC-C2C-C1C	2.86	129.39	125.04
23	b	608	CLA	CHD-C4C-NC	2.86	128.71	124.20
25	B	619	BCR	C3-C4-C5	-2.86	108.98	114.08
23	c	508	CLA	C1D-CHD-C4C	-2.86	118.79	122.56
23	C	513	CLA	C3B-C4B-NB	2.86	112.90	109.21
23	C	511	CLA	O2A-CGA-O1A	-2.85	116.39	123.59
25	T	101	BCR	C35-C13-C12	2.85	122.57	118.08
23	b	607	CLA	CHC-C1C-C2C	-2.85	118.83	126.72
23	A	408	CLA	O2A-CGA-CBA	2.85	120.86	111.91
23	C	507	CLA	CBC-CAC-C3C	-2.85	104.57	112.43
23	C	507	CLA	OBD-CAD-C3D	-2.85	123.25	127.98
23	c	504	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
23	b	610	CLA	CMB-C2B-C3B	2.85	130.01	124.68
23	b	605	CLA	C3B-C4B-NB	2.85	112.89	109.21
23	b	606	CLA	CHD-C4C-NC	2.85	128.69	124.20
23	c	514	CLA	C4-C3-C5	2.85	120.06	115.27
25	B	618	BCR	C24-C23-C22	-2.84	121.94	126.23
23	A	408	CLA	CMA-C3A-C2A	-2.84	102.36	113.83
29	D	408	PL9	C25-C24-C26	2.84	120.06	115.27
23	C	502	CLA	CAC-C3C-C4C	2.84	128.50	124.81
25	y	101	BCR	C37-C22-C23	2.84	122.55	118.08
26	a	411	SQD	O48-C23-C24	2.84	120.82	111.91
23	b	613	CLA	O2A-CGA-CBA	2.84	120.82	111.91
23	B	606	CLA	C4-C3-C5	2.84	120.05	115.27
23	B	606	CLA	CHD-C4C-NC	2.84	128.67	124.20
23	D	405	CLA	CHC-C1C-C2C	-2.84	118.88	126.72
25	C	515	BCR	C24-C23-C22	-2.83	121.96	126.23
23	d	403	CLA	CAA-C2A-C3A	-2.83	105.03	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	502	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
25	C	516	BCR	C38-C26-C25	-2.83	121.35	124.53
23	a	405	CLA	CAC-C3C-C4C	2.83	128.48	124.81
23	b	608	CLA	CHC-C1C-C2C	-2.83	118.90	126.72
23	B	606	CLA	O2A-CGA-CBA	2.83	120.78	111.91
23	b	611	CLA	C2A-C1A-CHA	-2.83	118.92	123.86
25	B	617	BCR	C31-C1-C6	-2.83	105.72	110.30
23	b	608	CLA	CMB-C2B-C3B	2.83	129.96	124.68
25	Y	101	BCR	C37-C22-C23	2.82	122.53	118.08
23	d	403	CLA	CBC-CAC-C3C	-2.82	104.65	112.43
23	b	602	CLA	C2A-C1A-CHA	-2.82	118.92	123.86
25	A	409	BCR	C11-C10-C9	-2.82	123.28	127.31
23	c	503	CLA	CHC-C1C-C2C	-2.82	118.92	126.72
29	A	414	PL9	C30-C29-C31	2.82	120.01	115.27
23	B	604	CLA	C6-C7-C8	-2.82	106.81	115.92
23	B	607	CLA	CHD-C4C-NC	2.82	128.64	124.20
23	B	608	CLA	O2A-CGA-CBA	2.81	120.73	111.91
23	C	507	CLA	C4-C3-C5	2.81	120.00	115.27
23	a	406	CLA	C4D-C3D-CAD	-2.81	106.90	108.47
23	C	503	CLA	C4-C3-C5	2.81	120.00	115.27
23	C	511	CLA	CHC-C1C-C2C	-2.81	118.95	126.72
23	d	403	CLA	CAC-C3C-C4C	2.81	128.45	124.81
23	B	613	CLA	C4-C3-C5	2.81	119.99	115.27
23	C	507	CLA	C1D-CHD-C4C	-2.81	118.85	122.56
23	C	503	CLA	CHD-C4C-NC	2.81	128.63	124.20
23	c	513	CLA	O2A-CGA-CBA	2.81	120.71	111.91
25	T	101	BCR	C2-C1-C6	2.80	114.80	110.48
23	B	613	CLA	O2D-CGD-O1D	-2.80	118.35	123.84
23	A	405	CLA	C3B-C4B-NB	2.80	112.83	109.21
23	b	602	CLA	C1-C2-C3	-2.80	121.20	126.04
29	a	416	PL9	C40-C39-C41	2.80	119.98	115.27
23	a	407	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
32	I	101	LMT	O1B-C4'-C3'	2.80	114.73	107.28
24	A	353	PHO	C6-C5-C3	-2.80	106.12	113.45
23	C	506	CLA	CHD-C4C-NC	2.80	128.61	124.20
35	C	517	DGD	O6D-C1D-O3G	-2.80	103.35	109.97
23	B	604	CLA	O2A-CGA-CBA	2.80	120.68	111.91
25	T	101	BCR	C36-C18-C19	2.79	122.48	118.08
23	C	510	CLA	O2A-CGA-O1A	-2.79	116.54	123.59
23	B	610	CLA	CHC-C1C-C2C	-2.79	119.00	126.72
23	D	406	CLA	CAA-C2A-C3A	-2.79	105.14	112.78
25	K	102	BCR	C20-C21-C22	-2.79	123.33	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	515	BCR	C28-C27-C26	-2.79	109.10	114.08
24	a	353	PHO	CBD-CHA-C1A	2.79	132.87	126.40
23	B	604	CLA	CMC-C2C-C1C	2.79	129.29	125.04
37	d	408	LHG	O8-C23-C24	2.79	120.66	111.91
35	c	519	DGD	O1G-C1A-C2A	2.79	120.66	111.91
23	b	605	CLA	CHC-C1C-C2C	-2.79	119.01	126.72
23	C	514	CLA	CHD-C4C-NC	2.79	128.60	124.20
23	A	404	CLA	CHC-C1C-C2C	-2.79	119.01	126.72
25	K	102	BCR	C11-C10-C9	-2.79	123.33	127.31
24	A	407	PHO	C1-C2-C3	-2.79	121.22	126.04
23	b	614	CLA	O2A-CGA-O1A	-2.79	116.56	123.59
23	C	514	CLA	CAC-C3C-C4C	2.79	128.42	124.81
23	B	606	CLA	OBD-CAD-C3D	-2.78	123.36	127.98
23	b	613	CLA	CHC-C1C-C2C	-2.78	119.02	126.72
32	a	414	LMT	C1B-O5B-C5B	2.78	119.15	113.69
23	B	614	CLA	C4C-C3C-C2C	-2.78	102.85	106.90
29	d	405	PL9	C27-C28-C29	-2.78	120.97	127.66
23	C	507	CLA	C4C-C3C-C2C	-2.78	102.85	106.90
23	b	604	CLA	CHD-C4C-NC	2.78	128.58	124.20
23	b	607	CLA	C4-C3-C5	2.78	119.94	115.27
23	c	511	CLA	CMC-C2C-C1C	2.78	129.27	125.04
23	C	508	CLA	C4-C3-C5	2.78	119.94	115.27
23	C	503	CLA	CHC-C1C-C2C	-2.78	119.04	126.72
23	d	402	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
23	B	606	CLA	CHC-C1C-C2C	-2.78	119.04	126.72
23	b	606	CLA	CMC-C2C-C1C	2.78	129.27	125.04
26	A	410	SQD	O48-C23-C24	2.78	120.62	111.91
23	B	609	CLA	CHD-C4C-NC	2.78	128.58	124.20
23	c	503	CLA	O2A-CGA-O1A	-2.78	116.59	123.59
23	a	407	CLA	C4D-C3D-CAD	-2.77	106.92	108.47
35	C	519	DGD	O3G-C3G-C2G	-2.77	104.21	110.90
29	D	408	PL9	C53-C6-C1	2.77	120.65	114.99
23	c	503	CLA	CBC-CAC-C3C	-2.77	104.80	112.43
23	a	409	CLA	CAC-C3C-C4C	2.77	128.40	124.81
35	h	102	DGD	O2G-C1B-C2B	2.77	117.47	111.50
23	C	502	CLA	CHD-C4C-NC	2.77	128.56	124.20
23	c	510	CLA	CBC-CAC-C3C	-2.76	104.81	112.43
23	B	608	CLA	CHD-C4C-NC	2.76	128.56	124.20
23	A	406	CLA	O2A-CGA-CBA	2.76	120.58	111.91
23	B	603	CLA	CHC-C1C-C2C	-2.76	119.08	126.72
23	b	609	CLA	CHC-C1C-C2C	-2.76	119.08	126.72
34	B	626	HTG	C3-C4-C5	2.76	115.16	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	505	CLA	CHD-C4C-NC	2.76	128.55	124.20
23	B	612	CLA	C4D-C3D-CAD	-2.76	106.93	108.47
25	K	102	BCR	C2-C1-C6	2.76	114.73	110.48
25	t	103	BCR	C1-C6-C7	2.76	123.58	115.78
23	b	614	CLA	O2A-CGA-CBA	2.76	120.57	111.91
23	B	610	CLA	C3B-C4B-NB	2.76	112.78	109.21
23	B	615	CLA	CMB-C2B-C1B	2.76	132.70	128.46
23	c	508	CLA	CHC-C1C-C2C	-2.76	119.10	126.72
23	b	602	CLA	CMA-C3A-C4A	-2.76	104.36	111.77
35	c	519	DGD	O3G-C3G-C2G	-2.76	104.25	110.90
23	c	503	CLA	C4D-C3D-CAD	-2.75	106.93	108.47
23	c	511	CLA	O2A-CGA-CBA	2.75	120.55	111.91
23	B	605	CLA	C3B-C4B-NB	2.75	112.77	109.21
25	y	101	BCR	C10-C11-C12	-2.75	114.63	123.22
23	a	406	CLA	CMA-C3A-C2A	-2.75	102.73	113.83
33	c	521	LMG	C3-C4-C5	2.75	115.15	110.24
23	c	503	CLA	CAC-C3C-C4C	2.75	128.38	124.81
23	b	615	CLA	CAC-C3C-C4C	2.75	128.38	124.81
23	C	514	CLA	C3B-C4B-NB	2.75	112.76	109.21
23	b	611	CLA	CMC-C2C-C1C	2.75	129.22	125.04
23	C	502	CLA	CHC-C1C-C2C	-2.75	119.12	126.72
26	b	620	SQD	C44-O6-C1	-2.75	108.38	113.74
23	A	404	CLA	CAA-C2A-C1A	-2.75	102.98	111.97
34	b	622	HTG	O5-C5-C4	2.75	114.68	109.69
23	D	406	CLA	CBC-CAC-C3C	-2.74	104.86	112.43
25	B	619	BCR	C34-C9-C8	2.74	122.40	118.08
23	c	506	CLA	CMC-C2C-C1C	2.74	129.22	125.04
23	c	503	CLA	O2A-CGA-CBA	2.74	120.51	111.91
24	a	353	PHO	C4D-ND-C1D	-2.74	101.83	106.76
23	c	514	CLA	CAA-C2A-C3A	-2.74	105.28	112.78
33	z	101	LMG	O8-C28-C29	2.74	120.50	111.91
33	D	415	LMG	O7-C10-C11	2.74	117.40	111.50
26	F	101	SQD	C1-O5-C5	-2.74	108.32	113.69
33	c	520	LMG	O8-C28-C29	2.74	120.49	111.91
23	c	510	CLA	CHC-C1C-C2C	-2.74	119.16	126.72
23	b	614	CLA	C2A-C1A-CHA	-2.73	119.08	123.86
25	y	101	BCR	C11-C10-C9	-2.73	123.41	127.31
29	D	408	PL9	C51-C49-C50	2.73	120.64	114.60
25	c	516	BCR	C15-C14-C13	-2.73	123.41	127.31
23	A	408	CLA	O2A-CGA-O1A	-2.73	116.70	123.59
23	D	405	CLA	OBD-CAD-C3D	-2.73	123.45	127.98
23	c	505	CLA	C2A-C1A-CHA	-2.73	119.09	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	404	BCR	C3-C4-C5	-2.73	109.21	114.08
23	a	409	CLA	O2A-CGA-O1A	-2.72	116.72	123.59
23	d	403	CLA	C2A-C1A-CHA	-2.72	119.10	123.86
23	b	611	CLA	CHC-C1C-C2C	-2.72	119.19	126.72
23	a	407	CLA	O2A-CGA-CBA	2.72	120.44	111.91
23	B	603	CLA	C2A-C1A-CHA	-2.72	119.11	123.86
24	A	353	PHO	CHC-C1C-C2C	-2.72	118.90	125.73
25	Y	101	BCR	C10-C11-C12	-2.72	114.74	123.22
25	b	619	BCR	C2-C1-C6	2.71	114.66	110.48
23	A	405	CLA	CMA-C3A-C4A	-2.71	104.48	111.77
24	A	407	PHO	C4D-ND-C1D	-2.71	101.88	106.76
35	c	517	DGD	C2G-O2G-C1B	-2.71	111.11	117.79
23	A	404	CLA	C2A-C1A-CHA	-2.71	119.12	123.86
25	c	515	BCR	C38-C26-C25	-2.71	121.48	124.53
23	B	616	CLA	CHC-C1C-C2C	-2.71	119.23	126.72
23	A	405	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
23	b	610	CLA	C4-C3-C5	2.71	119.83	115.27
23	A	408	CLA	C2A-C1A-CHA	-2.71	119.13	123.86
23	D	405	CLA	CMC-C2C-C1C	2.70	129.16	125.04
23	c	508	CLA	C3B-C4B-NB	2.70	112.71	109.21
23	C	512	CLA	CHC-C1C-C2C	-2.70	119.24	126.72
33	m	101	LMG	C8-O7-C10	-2.70	111.14	117.79
25	a	410	BCR	C37-C22-C21	-2.70	119.14	122.92
25	t	103	BCR	C37-C22-C23	2.70	122.33	118.08
23	c	502	CLA	C4-C3-C5	2.70	119.81	115.27
23	c	507	CLA	CHD-C4C-NC	2.70	128.46	124.20
23	c	505	CLA	OBD-CAD-C3D	-2.70	123.50	127.98
23	b	606	CLA	O2A-CGA-O1A	-2.70	116.78	123.59
23	b	615	CLA	CBC-CAC-C3C	-2.70	104.99	112.43
23	B	605	CLA	C2A-C1A-CHA	-2.70	119.14	123.86
35	C	519	DGD	O1G-C1A-C2A	2.70	120.38	111.91
23	C	508	CLA	CMC-C2C-C1C	2.70	129.15	125.04
23	B	610	CLA	CAA-CBA-CGA	-2.70	105.37	113.25
23	c	506	CLA	C4-C3-C5	2.70	119.81	115.27
23	c	510	CLA	C4C-C3C-C2C	-2.70	102.97	106.90
23	c	513	CLA	CHC-C1C-C2C	-2.70	119.27	126.72
23	B	613	CLA	CHC-C1C-C2C	-2.69	119.27	126.72
23	a	409	CLA	C4D-C3D-CAD	-2.69	106.97	108.47
23	B	615	CLA	C4D-C3D-CAD	-2.69	106.97	108.47
25	c	515	BCR	C37-C22-C21	-2.69	119.16	122.92
24	A	353	PHO	O2A-CGA-O1A	-2.69	116.81	123.59
23	b	605	CLA	CBC-CAC-C3C	-2.69	105.02	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	406	CLA	C2A-C1A-CHA	-2.69	119.16	123.86
23	C	509	CLA	O2A-CGA-O1A	-2.68	116.82	123.59
23	c	510	CLA	C4-C3-C5	2.68	119.78	115.27
25	B	619	BCR	C2-C1-C6	2.68	114.61	110.48
23	B	612	CLA	CHC-C1C-C2C	-2.68	119.31	126.72
23	B	601	CLA	CHC-C1C-C2C	-2.68	119.31	126.72
23	b	615	CLA	CHD-C4C-NC	2.68	128.42	124.20
23	c	513	CLA	CMA-C3A-C4A	-2.68	104.58	111.77
23	a	406	CLA	C2A-C1A-CHA	-2.68	119.18	123.86
23	B	614	CLA	CHC-C1C-C2C	-2.68	119.32	126.72
24	A	353	PHO	CHD-C1D-C2D	-2.68	119.00	125.73
23	B	612	CLA	O2A-CGA-CBA	2.67	120.30	111.91
25	k	101	BCR	C20-C21-C22	-2.67	123.50	127.31
25	B	617	BCR	C15-C14-C13	-2.67	123.50	127.31
23	B	609	CLA	CHC-C1C-C2C	-2.67	119.33	126.72
23	B	605	CLA	C4D-C3D-CAD	-2.67	106.98	108.47
23	B	611	CLA	O2A-CGA-O1A	-2.67	116.86	123.59
23	C	509	CLA	CAC-C3C-C4C	2.67	128.27	124.81
23	B	606	CLA	CBC-CAC-C3C	-2.67	105.08	112.43
23	c	505	CLA	C4-C3-C5	2.67	119.75	115.27
23	C	513	CLA	CHC-C1C-C2C	-2.66	119.35	126.72
25	b	618	BCR	C11-C10-C9	-2.66	123.51	127.31
37	d	407	LHG	O7-C7-C8	2.66	117.24	111.50
23	c	509	CLA	C2A-C1A-CHA	-2.66	119.20	123.86
23	A	406	CLA	CHC-C1C-C2C	-2.66	119.36	126.72
24	A	353	PHO	C4D-CHA-C1A	-2.66	119.38	125.37
23	A	404	CLA	O2D-CGD-CBD	2.66	116.00	111.27
25	d	404	BCR	C40-C30-C25	-2.66	105.98	110.30
23	b	602	CLA	C1-O2A-CGA	2.66	123.42	116.44
35	H	102	DGD	O1G-C1A-C2A	2.66	120.25	111.91
34	B	622	HTG	C1'-S1-C1	2.66	105.06	100.09
23	C	503	CLA	CBC-CAC-C3C	-2.66	105.11	112.43
23	B	604	CLA	CHC-C1C-C2C	-2.66	119.37	126.72
23	b	606	CLA	CHC-C1C-C2C	-2.66	119.37	126.72
23	b	601	CLA	C2A-C1A-CHA	-2.66	119.22	123.86
23	B	614	CLA	CAC-C3C-C4C	2.65	128.25	124.81
23	D	405	CLA	CBC-CAC-C3C	-2.65	105.12	112.43
23	A	408	CLA	CMB-C2B-C3B	2.65	129.64	124.68
25	c	515	BCR	C34-C9-C10	-2.65	119.21	122.92
23	B	602	CLA	CHD-C4C-NC	2.65	128.38	124.20
25	b	619	BCR	C15-C14-C13	-2.65	123.53	127.31
33	m	101	LMG	C7-O1-C1	-2.65	108.56	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	616	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
23	b	605	CLA	C1-C2-C3	-2.65	121.47	126.04
33	d	412	LMG	O8-C28-O10	-2.65	116.91	123.59
23	C	504	CLA	O2A-CGA-O1A	-2.65	116.92	123.59
23	C	506	CLA	O2A-CGA-O1A	-2.64	116.92	123.59
25	b	618	BCR	C16-C17-C18	-2.64	123.54	127.31
29	D	408	PL9	C17-C18-C19	-2.64	121.30	127.66
25	k	101	BCR	C16-C17-C18	-2.64	123.54	127.31
23	b	610	CLA	CHC-C1C-C2C	-2.64	119.42	126.72
23	b	609	CLA	CHD-C4C-NC	2.64	128.36	124.20
23	C	505	CLA	CBC-CAC-C3C	-2.64	105.15	112.43
23	A	406	CLA	CMC-C2C-C1C	2.64	129.06	125.04
23	a	407	CLA	CAC-C3C-C4C	2.64	128.24	124.81
23	D	405	CLA	C2A-C1A-CHA	-2.64	119.25	123.86
26	f	102	SQD	O5-C1-C2	2.64	115.93	110.35
32	a	414	LMT	O5'-C5'-C4'	2.64	115.31	109.75
23	d	403	CLA	C3B-C4B-NB	2.64	112.62	109.21
25	D	407	BCR	C3-C4-C5	-2.63	109.37	114.08
23	b	607	CLA	C2A-C1A-CHA	-2.63	119.25	123.86
23	c	514	CLA	CMB-C2B-C3B	2.63	129.60	124.68
23	B	615	CLA	CHC-C1C-C2C	-2.63	119.44	126.72
23	B	613	CLA	C7-C6-C5	-2.63	106.21	113.36
23	d	403	CLA	CMB-C2B-C3B	2.63	129.60	124.68
23	c	507	CLA	C4C-C3C-C2C	-2.63	103.06	106.90
23	b	613	CLA	O2A-CGA-O1A	-2.63	116.95	123.59
23	C	511	CLA	C4C-C3C-C2C	-2.63	103.06	106.90
37	l	101	LHG	O8-C23-O10	-2.63	116.96	123.59
23	b	615	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
29	d	405	PL9	C22-C23-C24	-2.63	121.34	127.66
23	c	511	CLA	C4C-C3C-C2C	-2.62	103.07	106.90
29	d	405	PL9	C51-C49-C50	2.62	120.40	114.60
23	b	616	CLA	C3B-C4B-NB	2.62	112.60	109.21
23	B	603	CLA	C6-C7-C8	-2.62	107.44	115.92
25	k	101	BCR	C10-C11-C12	-2.62	115.03	123.22
23	B	606	CLA	CAA-C2A-C3A	-2.62	105.60	112.78
23	B	609	CLA	C1-O2A-CGA	2.62	123.32	116.44
23	b	612	CLA	OBD-CAD-C3D	-2.62	123.63	127.98
23	C	510	CLA	CBC-CAC-C3C	-2.62	105.21	112.43
24	A	353	PHO	C2C-C1C-NC	2.62	113.74	109.79
23	B	605	CLA	O2A-CGA-CBA	2.62	120.12	111.91
23	b	604	CLA	O1D-CGD-CBD	-2.62	119.13	124.48
23	B	606	CLA	CMC-C2C-C1C	2.61	129.02	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402	CLA	CBC-CAC-C3C	-2.61	105.22	112.43
37	d	407	LHG	O8-C23-O10	-2.61	117.00	123.59
23	b	604	CLA	C4C-C3C-C2C	-2.61	103.09	106.90
33	C	521	LMG	O8-C28-C29	2.61	120.09	111.91
24	a	353	PHO	CHC-C1C-C2C	-2.61	119.17	125.73
25	A	409	BCR	C38-C26-C25	-2.61	121.60	124.53
33	z	101	LMG	C8-O7-C10	-2.61	111.37	117.79
23	c	502	CLA	CMC-C2C-C1C	2.61	129.01	125.04
26	f	102	SQD	O8-S-C6	2.61	109.89	105.74
23	C	502	CLA	O2A-CGA-CBA	2.61	120.09	111.91
23	b	608	CLA	CMA-C3A-C4A	-2.61	104.77	111.77
23	b	616	CLA	O2A-CGA-O1A	-2.61	117.02	123.59
23	B	609	CLA	O2A-CGA-CBA	2.61	120.08	111.91
23	B	612	CLA	CHD-C4C-NC	2.60	128.31	124.20
23	B	603	CLA	C16-C15-C13	-2.60	107.51	115.92
23	C	509	CLA	C2A-C1A-CHA	-2.60	119.31	123.86
23	d	402	CLA	CAC-C3C-C4C	2.60	128.19	124.81
40	v	202	HEC	CMB-C2B-C1B	-2.60	124.47	128.46
23	b	606	CLA	O2A-CGA-CBA	2.60	120.06	111.91
25	b	617	BCR	C20-C21-C22	-2.60	123.60	127.31
23	A	406	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
23	D	405	CLA	O2A-CGA-CBA	2.60	120.06	111.91
24	a	408	PHO	CMB-C2B-C1B	2.60	129.06	125.06
23	c	502	CLA	O2A-CGA-O1A	-2.60	117.04	123.59
24	A	407	PHO	C3C-C4C-NC	2.60	114.30	110.28
25	D	407	BCR	C30-C25-C24	2.60	123.12	115.78
23	C	504	CLA	CHD-C4C-NC	2.59	128.29	124.20
23	c	514	CLA	O2A-CGA-CBA	2.59	120.05	111.91
26	A	410	SQD	O47-C7-O49	-2.59	117.44	123.70
33	Z	101	LMG	C9-C8-C7	-2.59	105.66	111.79
23	c	511	CLA	CAC-C3C-C4C	2.59	128.17	124.81
35	c	519	DGD	O5D-C6D-C5D	-2.59	104.26	109.05
23	c	510	CLA	CMB-C2B-C3B	2.59	129.52	124.68
29	D	408	PL9	C12-C13-C14	-2.59	121.43	127.66
24	a	353	PHO	C4A-NA-C1A	-2.59	106.05	108.14
23	C	502	CLA	C4C-C3C-C2C	-2.59	103.13	106.90
23	B	601	CLA	C1-C2-C3	-2.59	121.57	126.04
40	v	202	HEC	C1D-C2D-C3D	-2.58	105.20	107.00
23	b	607	CLA	C1D-CHD-C4C	-2.58	119.15	122.56
23	b	603	CLA	CHC-C1C-C2C	-2.58	119.59	126.72
25	y	101	BCR	C21-C20-C19	-2.58	115.17	123.22
37	D	409	LHG	C5-O7-C7	-2.58	111.44	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	404	BCR	C28-C27-C26	-2.58	109.47	114.08
23	B	612	CLA	CAC-C3C-C4C	2.58	128.16	124.81
23	d	402	CLA	CMC-C2C-C1C	2.58	128.96	125.04
23	c	512	CLA	CMC-C2C-C1C	2.58	128.96	125.04
23	D	405	CLA	CMB-C2B-C3B	2.58	129.50	124.68
23	D	405	CLA	CAA-C2A-C3A	-2.58	105.72	112.78
37	e	101	LHG	O8-C23-C24	2.58	119.99	111.91
29	A	414	PL9	C45-C44-C46	2.58	119.60	115.27
23	b	602	CLA	CAC-C3C-C4C	2.57	128.15	124.81
23	B	610	CLA	CHD-C4C-NC	2.57	128.26	124.20
23	C	512	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
23	A	408	CLA	CHC-C1C-C2C	-2.57	119.61	126.72
25	t	103	BCR	C7-C6-C5	-2.57	115.23	121.46
24	a	353	PHO	CBA-CAA-C2A	-2.57	106.28	113.86
25	B	619	BCR	C15-C14-C13	-2.57	123.64	127.31
24	a	408	PHO	C3C-C4C-NC	2.57	114.26	110.28
23	C	514	CLA	C4-C3-C5	2.57	119.59	115.27
23	b	611	CLA	O2A-CGA-CBA	2.57	119.97	111.91
29	A	414	PL9	C53-C6-C1	2.57	120.24	114.99
25	h	101	BCR	C37-C22-C21	-2.57	119.33	122.92
23	C	509	CLA	C4-C3-C5	2.57	119.59	115.27
23	b	609	CLA	O2A-CGA-CBA	2.56	119.96	111.91
23	b	612	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
25	c	515	BCR	C8-C7-C6	-2.56	120.01	127.20
23	A	404	CLA	CHD-C4C-NC	2.56	128.24	124.20
23	b	611	CLA	CMB-C2B-C3B	2.56	129.47	124.68
25	k	101	BCR	C15-C14-C13	-2.56	123.66	127.31
23	C	502	CLA	C2A-C1A-CHA	-2.56	119.39	123.86
23	B	613	CLA	O2A-CGA-O1A	-2.56	117.14	123.59
23	B	605	CLA	CMC-C2C-C1C	2.56	128.93	125.04
23	a	409	CLA	CMC-C2C-C1C	2.55	128.93	125.04
23	B	608	CLA	C4D-C3D-CAD	-2.55	107.05	108.47
23	A	406	CLA	C1D-CHD-C4C	-2.55	119.19	122.56
32	M	103	LMT	C1'-O5'-C5'	2.55	118.70	113.69
23	a	409	CLA	OBD-CAD-C3D	-2.55	123.74	127.98
29	A	414	PL9	C25-C24-C26	2.55	119.56	115.27
23	b	603	CLA	CHD-C4C-NC	2.55	128.22	124.20
35	C	517	DGD	O3G-C3G-C2G	-2.55	104.74	110.90
23	b	615	CLA	C11-C12-C13	-2.55	107.67	115.92
23	d	403	CLA	C4-C3-C5	2.55	119.56	115.27
25	a	410	BCR	C33-C5-C6	-2.55	121.67	124.53
23	c	514	CLA	CHD-C4C-NC	2.55	128.22	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	605	CLA	OBD-CAD-C3D	-2.55	123.75	127.98
23	a	405	CLA	CMA-C3A-C2A	-2.55	103.56	113.83
23	C	506	CLA	C1-C2-C3	-2.55	121.64	126.04
33	z	101	LMG	C7-O1-C1	-2.54	108.77	113.74
23	B	613	CLA	C1D-CHD-C4C	-2.54	119.20	122.56
32	t	101	LMT	C1'-O5'-C5'	2.54	118.68	113.69
25	T	101	BCR	C21-C20-C19	-2.54	115.28	123.22
37	L	101	LHG	O8-C23-C24	2.54	119.89	111.91
24	a	408	PHO	CBD-CHA-C1A	2.54	132.30	126.40
23	A	406	CLA	CHD-C4C-NC	2.54	128.21	124.20
23	b	607	CLA	CMC-C2C-C1C	2.54	128.91	125.04
23	B	614	CLA	C4-C3-C2	-2.54	117.16	123.68
23	B	610	CLA	C6-C7-C8	-2.54	107.71	115.92
23	C	506	CLA	CHC-C1C-C2C	-2.54	119.69	126.72
25	B	618	BCR	C33-C5-C6	-2.54	121.68	124.53
23	D	405	CLA	C4-C3-C5	2.54	119.54	115.27
23	C	507	CLA	C4D-C3D-CAD	-2.54	107.06	108.47
23	C	505	CLA	C4C-C3C-C2C	-2.54	103.20	106.90
24	A	407	PHO	CHD-C1D-C2D	-2.54	119.35	125.73
23	D	405	CLA	C4C-C3C-C2C	-2.53	103.20	106.90
23	c	502	CLA	CHD-C4C-NC	2.53	128.20	124.20
24	a	408	PHO	O2A-CGA-O1A	-2.53	117.20	123.59
23	B	609	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
23	B	616	CLA	O2A-CGA-CBA	2.53	119.85	111.91
23	b	602	CLA	CHC-C1C-C2C	-2.53	119.72	126.72
23	c	509	CLA	CAC-C3C-C2C	2.53	131.86	127.53
23	d	402	CLA	CHC-C1C-C2C	-2.53	119.72	126.72
25	A	409	BCR	C8-C7-C6	-2.53	120.10	127.20
23	c	504	CLA	C4-C3-C5	2.53	119.52	115.27
25	D	407	BCR	C28-C27-C26	-2.53	109.56	114.08
23	a	407	CLA	C4-C3-C5	2.53	119.52	115.27
23	C	506	CLA	O2A-CGA-CBA	2.53	119.84	111.91
29	d	405	PL9	C17-C18-C19	-2.53	121.58	127.66
25	C	516	BCR	C15-C16-C17	-2.52	118.30	123.47
23	B	605	CLA	C7-C6-C5	-2.52	106.50	113.36
37	D	410	LHG	O7-C7-C8	2.52	116.94	111.50
25	c	515	BCR	C21-C20-C19	-2.52	115.34	123.22
23	b	611	CLA	CBC-CAC-C3C	-2.52	105.48	112.43
23	B	607	CLA	C1-O2A-CGA	2.52	123.06	116.44
23	A	404	CLA	CED-O2D-CGD	2.52	121.63	115.94
23	a	409	CLA	CHD-C4C-NC	2.52	128.17	124.20
23	B	603	CLA	CAC-C3C-C4C	2.52	128.08	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	506	CLA	CAC-C3C-C4C	2.52	128.08	124.81
23	A	408	CLA	CMC-C2C-C1C	2.52	128.87	125.04
25	c	516	BCR	C37-C22-C23	2.51	122.04	118.08
23	C	507	CLA	CMC-C2C-C1C	2.51	128.87	125.04
23	C	513	CLA	CMB-C2B-C3B	2.51	129.38	124.68
23	b	606	CLA	C2A-C1A-CHA	-2.51	119.46	123.86
23	B	611	CLA	CBC-CAC-C3C	-2.51	105.50	112.43
23	C	505	CLA	C4-C3-C5	2.51	119.50	115.27
23	c	502	CLA	CBC-CAC-C3C	-2.51	105.50	112.43
26	f	102	SQD	O5-C5-C4	2.51	114.25	109.69
23	d	402	CLA	C4D-C3D-CAD	-2.51	107.07	108.47
29	a	416	PL9	C20-C19-C21	2.51	119.49	115.27
35	h	102	DGD	O1G-C1A-C2A	2.51	119.78	111.91
23	c	513	CLA	CMB-C2B-C3B	2.51	129.37	124.68
23	B	608	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	c	506	CLA	O2A-CGA-CBA	2.51	119.77	111.91
23	b	606	CLA	CAA-C2A-C3A	-2.50	105.92	112.78
24	a	353	PHO	C7-C6-C5	-2.50	106.56	113.36
23	C	510	CLA	CHD-C4C-NC	2.50	128.15	124.20
23	C	507	CLA	C2A-C1A-CHA	-2.50	119.48	123.86
23	c	508	CLA	O2A-CGA-CBA	2.50	119.75	111.91
23	B	615	CLA	CBC-CAC-C3C	-2.50	105.54	112.43
23	B	607	CLA	C2A-C1A-CHA	-2.50	119.49	123.86
23	A	404	CLA	C4D-C3D-CAD	-2.50	107.08	108.47
23	b	607	CLA	C4D-C3D-CAD	-2.50	107.08	108.47
26	b	620	SQD	O48-C23-C24	2.50	119.74	111.91
26	f	102	SQD	O7-S-C6	2.49	109.90	106.94
29	A	414	PL9	C40-C39-C41	2.49	119.47	115.27
23	C	510	CLA	CMC-C2C-C1C	2.49	128.84	125.04
25	H	101	BCR	C2-C3-C4	-2.49	105.81	111.38
23	B	611	CLA	CMB-C2B-C3B	2.49	129.34	124.68
23	c	514	CLA	CHC-C1C-C2C	-2.49	119.83	126.72
23	C	513	CLA	CMA-C3A-C4A	-2.49	105.07	111.77
23	c	512	CLA	O2A-CGA-CBA	2.49	119.73	111.91
23	C	505	CLA	CMB-C2B-C3B	2.49	129.34	124.68
23	C	512	CLA	CHD-C4C-NC	2.49	128.13	124.20
23	C	507	CLA	CHD-C4C-NC	2.49	128.13	124.20
23	C	507	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
23	A	404	CLA	C1-C2-C3	-2.49	121.74	126.04
23	c	507	CLA	CGD-CBD-CAD	-2.49	102.68	110.73
25	c	516	BCR	C11-C10-C9	-2.49	123.76	127.31
23	c	504	CLA	CMC-C2C-C1C	2.49	128.83	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	610	CLA	C3B-C4B-NB	2.49	112.42	109.21
23	b	612	CLA	O2A-CGA-O1A	-2.49	117.32	123.59
23	b	611	CLA	CAC-C3C-C4C	2.48	128.03	124.81
23	c	510	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
33	Z	101	LMG	C4-C3-C2	2.48	115.16	110.82
23	b	607	CLA	C1-C2-C3	-2.48	121.75	126.04
23	b	607	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
23	b	616	CLA	C4-C3-C5	2.48	119.44	115.27
33	D	415	LMG	O8-C28-O10	-2.48	117.33	123.59
23	c	504	CLA	C1-C2-C3	-2.48	121.75	126.04
25	t	103	BCR	C36-C18-C19	2.48	121.98	118.08
23	B	616	CLA	CAC-C3C-C4C	2.48	128.03	124.81
23	c	504	CLA	O2A-CGA-CBA	2.48	119.69	111.91
23	A	408	CLA	C4D-C3D-CAD	-2.48	107.09	108.47
23	c	502	CLA	O2A-CGA-CBA	2.48	119.68	111.91
23	b	603	CLA	CAC-C3C-C4C	2.48	128.02	124.81
24	a	408	PHO	O2A-CGA-CBA	2.48	119.67	111.91
23	B	602	CLA	C1-C2-C3	-2.47	121.76	126.04
25	a	410	BCR	C10-C11-C12	-2.47	115.50	123.22
23	c	509	CLA	CAA-C2A-C3A	-2.47	106.01	112.78
23	b	603	CLA	C5-C3-C2	-2.47	116.11	121.12
23	b	613	CLA	CED-O2D-CGD	2.47	121.53	115.94
38	e	87	HEM	CMA-C3A-C4A	-2.47	124.67	128.46
34	C	522	HTG	C1-O5-C5	2.47	117.14	112.58
29	a	416	PL9	C45-C44-C46	2.47	119.42	115.27
35	C	517	DGD	C2G-O2G-C1B	-2.47	111.71	117.79
23	C	503	CLA	C2A-C1A-CHA	-2.47	119.54	123.86
35	c	518	DGD	O1G-C1A-C2A	2.47	119.65	111.91
23	b	607	CLA	CAA-C2A-C3A	-2.47	106.02	112.78
23	B	616	CLA	C2A-C1A-CHA	-2.47	119.55	123.86
23	b	612	CLA	CHD-C4C-NC	2.47	128.09	124.20
23	B	612	CLA	OBD-CAD-C3D	-2.47	123.89	127.98
23	b	608	CLA	CMC-C2C-C1C	2.47	128.79	125.04
34	B	626	HTG	O5-C5-C4	2.47	114.17	109.69
26	f	102	SQD	O47-C7-O49	-2.46	117.75	123.70
26	a	411	SQD	C44-O6-C1	-2.46	108.92	113.74
23	c	509	CLA	O2A-CGA-CBA	2.46	119.63	111.91
32	I	101	LMT	O5'-C5'-C4'	2.46	114.94	109.75
23	A	405	CLA	C4C-C3C-C2C	-2.46	103.31	106.90
23	B	611	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
23	b	603	CLA	CMB-C2B-C3B	2.46	129.28	124.68
33	c	521	LMG	O8-C28-O10	-2.46	117.39	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	405	CLA	O2A-CGA-CBA	2.46	119.62	111.91
26	b	620	SQD	C1-C2-C3	-2.46	104.88	110.00
23	C	512	CLA	O2A-CGA-CBA	2.46	119.62	111.91
23	B	601	CLA	CAC-C3C-C4C	2.46	128.00	124.81
25	b	619	BCR	C31-C1-C6	-2.45	106.32	110.30
23	b	616	CLA	CHC-C1C-C2C	-2.45	119.93	126.72
23	a	405	CLA	OBD-CAD-C3D	-2.45	123.91	127.98
23	C	506	CLA	C11-C10-C8	-2.45	107.99	115.92
25	b	619	BCR	C39-C30-C25	-2.45	106.32	110.30
25	Y	101	BCR	C16-C15-C14	-2.45	118.45	123.47
23	B	605	CLA	O2A-C1-C2	-2.45	102.20	108.64
37	d	407	LHG	O8-C23-C24	2.45	119.59	111.91
23	b	604	CLA	O2A-CGA-O1A	-2.45	117.42	123.59
29	d	405	PL9	C53-C6-C1	2.45	119.99	114.99
23	C	512	CLA	C4D-C3D-CAD	-2.45	107.11	108.47
23	C	505	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
23	B	607	CLA	O2A-CGA-O1A	-2.44	117.42	123.59
23	c	506	CLA	C3B-C4B-NB	2.44	112.37	109.21
37	d	408	LHG	O8-C23-O10	-2.44	117.43	123.59
23	b	608	CLA	CBC-CAC-C3C	-2.44	105.70	112.43
23	c	506	CLA	CHC-C1C-C2C	-2.44	119.97	126.72
23	B	610	CLA	OBD-CAD-C3D	-2.44	123.93	127.98
26	f	102	SQD	C4-C3-C2	-2.44	106.56	110.82
29	D	408	PL9	C22-C23-C24	-2.44	121.79	127.66
23	B	607	CLA	C4C-C3C-C2C	-2.44	103.34	106.90
33	d	412	LMG	O8-C28-C29	2.44	119.56	111.91
23	B	602	CLA	CHC-C1C-C2C	-2.44	119.98	126.72
23	B	602	CLA	C2A-C1A-CHA	-2.44	119.60	123.86
26	f	102	SQD	O48-C23-C24	2.44	119.55	111.91
26	F	101	SQD	O48-C23-C24	2.44	119.55	111.91
25	d	404	BCR	C16-C17-C18	-2.43	123.83	127.31
23	A	408	CLA	CHB-C4A-NA	2.43	127.88	124.51
23	A	405	CLA	CHC-C1C-C2C	-2.43	119.99	126.72
24	a	353	PHO	C3A-C4A-CHB	-2.43	117.62	121.83
25	k	101	BCR	C36-C18-C19	2.43	121.91	118.08
23	b	614	CLA	CHD-C4C-NC	2.43	128.04	124.20
23	c	505	CLA	CMB-C2B-C3B	2.43	129.23	124.68
23	c	509	CLA	CHC-C1C-C2C	-2.43	119.99	126.72
23	B	612	CLA	C6-C5-C3	-2.43	107.08	113.45
35	c	517	DGD	O6D-C1D-O3G	-2.43	104.22	109.97
23	b	606	CLA	CAC-C3C-C4C	2.43	127.96	124.81
23	B	609	CLA	CBC-CAC-C3C	-2.43	105.73	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	509	CLA	CMC-C2C-C1C	2.43	128.74	125.04
23	c	505	CLA	CBC-CAC-C3C	-2.43	105.74	112.43
23	b	605	CLA	CAC-C3C-C2C	2.43	131.68	127.53
23	B	608	CLA	CAC-C3C-C4C	2.43	127.96	124.81
23	b	601	CLA	CBC-CAC-C3C	-2.43	105.74	112.43
25	H	101	BCR	C15-C14-C13	-2.42	123.85	127.31
23	A	408	CLA	CAC-C3C-C4C	2.42	127.95	124.81
23	a	406	CLA	C4C-C3C-C2C	-2.42	103.37	106.90
26	a	411	SQD	C3-C4-C5	2.42	114.56	110.24
25	d	404	BCR	C37-C22-C23	2.42	121.89	118.08
25	b	618	BCR	C8-C7-C6	-2.42	120.41	127.20
26	a	411	SQD	O4-C4-C3	-2.42	104.76	110.35
24	a	408	PHO	CBA-CAA-C2A	-2.42	106.73	113.86
23	C	510	CLA	CMB-C2B-C3B	2.42	129.20	124.68
25	d	404	BCR	C21-C20-C19	-2.42	115.68	123.22
34	b	622	HTG	C6-C5-C4	-2.41	107.35	113.00
25	y	101	BCR	C40-C30-C25	-2.41	106.38	110.30
23	a	407	CLA	CBC-CAC-C3C	-2.41	105.78	112.43
33	a	419	LMG	C7-O1-C1	-2.41	109.02	113.74
23	c	509	CLA	C4-C3-C5	2.41	119.33	115.27
26	B	620	SQD	C3-C4-C5	2.41	114.54	110.24
25	H	101	BCR	C16-C15-C14	-2.41	118.53	123.47
23	B	602	CLA	OBD-CAD-C3D	-2.41	123.98	127.98
25	k	101	BCR	C33-C5-C6	-2.41	121.82	124.53
23	C	511	CLA	OBD-CAD-C3D	-2.41	123.98	127.98
29	d	405	PL9	C30-C29-C31	2.41	119.32	115.27
25	Y	101	BCR	C34-C9-C8	2.41	121.87	118.08
23	b	612	CLA	C11-C10-C8	-2.41	108.14	115.92
23	B	607	CLA	CMC-C2C-C1C	2.40	128.70	125.04
29	d	405	PL9	C15-C14-C16	2.40	119.32	115.27
23	B	606	CLA	O2A-CGA-O1A	-2.40	117.52	123.59
23	d	403	CLA	CHC-C1C-C2C	-2.40	120.08	126.72
34	B	623	HTG	O5-C1-C2	2.40	113.33	110.31
23	B	612	CLA	C2A-C1A-CHA	-2.40	119.66	123.86
23	D	405	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
34	B	622	HTG	O2-C2-C3	-2.40	104.80	110.35
23	c	509	CLA	OBD-CAD-C3D	-2.40	124.00	127.98
23	B	612	CLA	C11-C12-C13	-2.40	108.16	115.92
23	B	605	CLA	CAC-C3C-C2C	2.40	131.63	127.53
23	B	602	CLA	C11-C12-C13	-2.40	108.17	115.92
35	H	102	DGD	C2G-O2G-C1B	-2.40	111.89	117.79
26	a	413	SQD	C1-O5-C5	2.40	118.39	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	414	PL9	C51-C49-C50	2.40	119.89	114.60
23	d	402	CLA	C2A-C1A-CHA	-2.39	119.67	123.86
25	B	619	BCR	C21-C20-C19	-2.39	115.75	123.22
25	T	101	BCR	C1-C6-C7	2.39	122.54	115.78
23	B	602	CLA	CAC-C3C-C4C	2.39	127.91	124.81
29	a	416	PL9	C53-C6-C1	2.39	119.87	114.99
23	C	513	CLA	CBA-CAA-C2A	-2.39	106.81	113.86
23	c	505	CLA	CHB-C4A-NA	2.39	127.81	124.51
32	M	101	LMT	C1-O1'-C1'	-2.39	109.88	113.84
24	A	407	PHO	O2A-CGA-CBA	2.39	119.40	111.91
25	d	404	BCR	C38-C26-C27	2.38	118.20	113.62
23	b	608	CLA	C11-C10-C8	-2.38	108.22	115.92
25	b	618	BCR	C24-C23-C22	-2.38	122.64	126.23
23	c	508	CLA	O1D-CGD-CBD	-2.38	119.61	124.48
35	C	518	DGD	O1G-C1A-O1A	-2.38	117.59	123.59
23	C	503	CLA	O2A-CGA-CBA	2.38	119.37	111.91
26	A	410	SQD	O48-C23-O10	-2.38	117.59	123.59
23	C	503	CLA	OBD-CAD-C3D	-2.38	124.04	127.98
23	D	405	CLA	CMA-C3A-C4A	-2.38	105.39	111.77
23	b	610	CLA	CAA-CBA-CGA	-2.38	106.31	113.25
35	c	517	DGD	O1G-C1A-C2A	2.37	119.35	111.91
23	b	607	CLA	CBC-CAC-C3C	-2.37	105.89	112.43
25	c	516	BCR	C20-C21-C22	-2.37	123.92	127.31
23	b	610	CLA	C2A-C1A-CHA	-2.37	119.71	123.86
23	d	402	CLA	CHD-C4C-NC	2.37	127.94	124.20
34	b	625	HTG	C1-O5-C5	2.37	116.95	112.58
35	c	517	DGD	O3G-C3G-C2G	-2.37	105.18	110.90
23	B	610	CLA	CMA-C3A-C4A	-2.37	105.40	111.77
25	B	617	BCR	C29-C30-C25	2.37	114.13	110.48
26	a	413	SQD	O5-C5-C4	2.37	114.00	109.69
23	c	511	CLA	CMB-C2B-C3B	2.37	129.11	124.68
23	a	406	CLA	OBD-CAD-C3D	-2.37	124.05	127.98
35	H	102	DGD	O1G-C1A-O1A	-2.37	117.61	123.59
23	C	510	CLA	C4-C3-C5	2.37	119.25	115.27
23	B	604	CLA	C11-C12-C13	-2.37	108.27	115.92
23	B	615	CLA	C6-C7-C8	-2.37	108.27	115.92
23	c	506	CLA	CHD-C4C-NC	2.36	127.93	124.20
26	a	411	SQD	O9-S-C6	2.36	109.75	106.94
23	C	503	CLA	CAC-C3C-C4C	2.36	127.88	124.81
26	F	101	SQD	C1-C2-C3	-2.36	105.08	110.00
23	B	615	CLA	O2A-CGA-CBA	2.36	119.32	111.91
24	A	353	PHO	CMB-C2B-C1B	2.36	128.70	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	404	CLA	C4-C3-C5	2.36	119.24	115.27
25	B	618	BCR	C37-C22-C23	2.36	121.80	118.08
23	B	605	CLA	CBC-CAC-C3C	-2.36	105.93	112.43
34	b	625	HTG	O5-C5-C4	2.36	113.98	109.69
29	a	416	PL9	C47-C48-C49	-2.36	119.69	127.75
23	c	512	CLA	C11-C10-C8	-2.36	108.30	115.92
23	B	612	CLA	CMC-C2C-C1C	2.36	128.63	125.04
26	B	620	SQD	O48-C23-O10	-2.36	117.65	123.59
23	C	506	CLA	CBC-CAC-C3C	-2.36	105.94	112.43
23	B	611	CLA	C2A-C1A-CHA	-2.36	119.74	123.86
25	H	101	BCR	C24-C23-C22	-2.36	122.68	126.23
23	A	408	CLA	CBC-CAC-C3C	-2.35	105.94	112.43
23	b	605	CLA	O2A-CGA-CBA	2.35	119.29	111.91
25	a	410	BCR	C8-C7-C6	-2.35	120.60	127.20
25	Y	101	BCR	C32-C1-C6	-2.35	106.49	110.30
23	C	509	CLA	O2A-CGA-CBA	2.35	119.28	111.91
29	a	416	PL9	C51-C49-C50	2.35	119.79	114.60
23	A	406	CLA	CBC-CAC-C3C	-2.35	105.95	112.43
23	b	606	CLA	CMB-C2B-C3B	2.35	129.07	124.68
23	c	504	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
23	b	608	CLA	O2A-CGA-CBA	2.35	119.28	111.91
23	b	613	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
23	B	601	CLA	C2A-C1A-CHA	-2.35	119.75	123.86
23	D	406	CLA	CMA-C3A-C2A	-2.35	104.37	113.83
25	A	409	BCR	C31-C1-C6	-2.34	106.50	110.30
23	C	511	CLA	C4-C3-C2	-2.34	117.67	123.68
23	C	514	CLA	O2A-CGA-CBA	2.34	119.26	111.91
23	a	406	CLA	C1-C2-C3	-2.34	121.99	126.04
23	B	610	CLA	CMB-C2B-C3B	2.34	129.06	124.68
23	b	609	CLA	C2A-C1A-CHA	-2.34	119.77	123.86
23	D	406	CLA	CHC-C1C-C2C	-2.34	120.25	126.72
23	B	605	CLA	CHC-C1C-C2C	-2.34	120.25	126.72
35	h	102	DGD	O1G-C1A-O1A	-2.34	117.69	123.59
23	b	616	CLA	CMC-C2C-C1C	2.34	128.60	125.04
23	C	514	CLA	CHC-C1C-C2C	-2.34	120.26	126.72
25	Y	101	BCR	C36-C18-C17	-2.34	119.65	122.92
24	a	408	PHO	C4D-ND-C1D	-2.33	102.56	106.76
33	D	415	LMG	O8-C28-C29	2.33	119.23	111.91
35	c	519	DGD	O6E-C1E-O5D	-2.33	104.45	109.97
24	a	353	PHO	C2A-C1A-NA	2.33	114.54	111.86
23	D	405	CLA	CHD-C4C-NC	2.33	127.88	124.20
23	B	602	CLA	O2A-CGA-CBA	2.33	119.22	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	353	PHO	C1C-C2C-C3C	-2.33	103.83	106.51
23	B	615	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
35	C	519	DGD	O2G-C1B-C2B	2.33	116.52	111.50
34	B	623	HTG	C1-C2-C3	2.33	115.18	110.59
25	Y	101	BCR	C21-C20-C19	-2.33	115.96	123.22
26	a	411	SQD	O48-C23-O10	-2.32	117.73	123.59
32	D	404	LMT	O1B-C4'-C5'	-2.32	103.08	109.45
25	t	103	BCR	C33-C5-C4	2.32	118.08	113.62
33	Z	101	LMG	C3-C4-C5	2.32	114.38	110.24
23	C	510	CLA	C16-C15-C13	-2.32	108.41	115.92
23	c	512	CLA	C4D-C3D-CAD	-2.32	107.18	108.47
23	a	405	CLA	C4C-C3C-C2C	-2.32	103.52	106.90
23	c	507	CLA	CAC-C3C-C4C	2.32	127.82	124.81
23	B	601	CLA	C4-C3-C5	2.32	119.17	115.27
25	t	103	BCR	C12-C13-C14	-2.32	115.39	118.94
25	K	102	BCR	C38-C26-C25	-2.32	121.93	124.53
23	C	502	CLA	O2A-CGA-O1A	-2.31	117.75	123.59
25	c	516	BCR	C23-C24-C25	-2.31	120.70	127.20
23	c	513	CLA	CHB-C4A-NA	2.31	127.71	124.51
23	B	608	CLA	CMC-C2C-C1C	2.31	128.56	125.04
24	a	408	PHO	C4-C3-C5	2.31	119.16	115.27
23	c	513	CLA	CBC-CAC-C3C	-2.31	106.06	112.43
23	b	615	CLA	O2A-CGA-CBA	2.31	119.16	111.91
25	h	101	BCR	C10-C11-C12	-2.31	116.01	123.22
25	c	516	BCR	C15-C16-C17	-2.31	118.74	123.47
23	B	609	CLA	C4D-C3D-CAD	-2.31	107.18	108.47
23	C	512	CLA	CBC-CAC-C3C	-2.31	106.06	112.43
23	b	603	CLA	CMA-C3A-C2A	-2.31	104.52	113.83
23	c	505	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
23	b	602	CLA	C11-C10-C8	-2.31	108.46	115.92
23	b	604	CLA	C11-C10-C8	-2.31	108.46	115.92
40	v	202	HEC	CAD-CBD-CGD	2.31	116.54	112.67
33	B	621	LMG	O1-C1-C2	-2.31	104.70	108.30
25	K	102	BCR	C33-C5-C6	-2.31	121.94	124.53
23	c	510	CLA	O2A-C1-C2	2.31	114.69	108.64
23	C	508	CLA	CHC-C1C-C2C	-2.31	120.34	126.72
26	F	101	SQD	C3-C4-C5	2.31	114.35	110.24
23	a	407	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
24	a	353	PHO	C3C-C4C-NC	2.30	113.85	110.28
32	e	102	LMT	O5'-C5'-C4'	2.30	114.61	109.75
26	A	412	SQD	O7-S-C6	2.30	109.68	106.94
23	B	601	CLA	CMB-C2B-C3B	2.30	128.99	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	C	520	LMG	O6-C5-C6	2.30	112.16	106.44
29	A	414	PL9	C2-C3-C4	2.30	121.97	118.80
23	B	605	CLA	C1-C2-C3	-2.30	122.06	126.04
23	C	509	CLA	CHD-C4C-NC	2.30	127.83	124.20
23	B	613	CLA	C2A-C1A-CHA	-2.30	119.84	123.86
23	c	502	CLA	CMB-C2B-C3B	2.30	128.98	124.68
23	a	409	CLA	CMA-C3A-C4A	-2.30	105.60	111.77
25	b	619	BCR	C3-C4-C5	-2.30	109.97	114.08
23	c	505	CLA	C1-C2-C3	-2.30	122.07	126.04
23	b	604	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
25	K	102	BCR	C36-C18-C19	2.30	121.70	118.08
25	y	101	BCR	C35-C13-C12	2.30	121.69	118.08
37	d	406	LHG	O7-C7-O9	-2.30	118.16	123.70
35	c	518	DGD	O1G-C1A-O1A	-2.29	117.80	123.59
29	D	408	PL9	C42-C41-C39	-2.29	105.43	112.98
23	b	602	CLA	C11-C12-C13	-2.29	108.50	115.92
25	Y	101	BCR	C38-C26-C25	-2.29	121.95	124.53
25	C	516	BCR	C3-C4-C5	-2.29	109.98	114.08
24	a	408	PHO	C2A-C1A-NA	2.29	114.49	111.86
23	b	615	CLA	C4D-C3D-CAD	-2.29	107.19	108.47
34	B	626	HTG	C1-O5-C5	2.29	116.80	112.58
25	B	618	BCR	C2-C1-C6	2.29	114.00	110.48
33	C	501	LMG	O8-C28-C29	2.29	119.08	111.91
23	D	405	CLA	C3D-CAD-CBD	2.29	110.61	107.61
26	A	412	SQD	O48-C23-O10	-2.28	117.83	123.59
26	A	410	SQD	O9-S-O7	-2.28	106.05	113.95
23	c	503	CLA	OBD-CAD-C3D	-2.28	124.19	127.98
23	b	613	CLA	CBC-CAC-C3C	-2.28	106.14	112.43
23	b	609	CLA	C16-C15-C13	-2.28	108.55	115.92
23	c	514	CLA	C1-C2-C3	-2.28	122.10	126.04
23	C	514	CLA	CBC-CAC-C3C	-2.28	106.14	112.43
26	F	101	SQD	O47-C7-O49	-2.28	118.19	123.70
23	c	502	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
23	C	513	CLA	CHB-C4A-NA	2.28	127.66	124.51
25	T	101	BCR	C7-C6-C5	-2.28	115.94	121.46
25	C	516	BCR	C21-C20-C19	-2.28	116.11	123.22
25	T	101	BCR	C29-C28-C27	-2.28	106.29	111.38
23	B	605	CLA	CMB-C2B-C1B	2.28	131.96	128.46
23	c	505	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
35	C	519	DGD	O1G-C1A-O1A	-2.27	117.85	123.59
25	C	515	BCR	C11-C10-C9	-2.27	124.06	127.31
23	B	602	CLA	O2A-CGA-O1A	-2.27	117.86	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	506	CLA	OBD-CAD-C3D	-2.27	124.21	127.98
29	d	405	PL9	C42-C41-C39	-2.27	105.51	112.98
23	B	604	CLA	C11-C10-C8	-2.27	108.58	115.92
32	a	414	LMT	O5B-C5B-C4B	2.27	113.81	109.69
24	A	407	PHO	CBA-CAA-C2A	-2.27	107.17	113.86
38	e	87	HEM	C3C-C4C-NC	-2.27	106.66	110.94
23	c	510	CLA	OBD-CAD-C3D	-2.27	124.22	127.98
23	C	502	CLA	C4D-C3D-CAD	-2.27	107.21	108.47
23	C	509	CLA	C7-C6-C5	-2.26	107.21	113.36
25	C	515	BCR	C10-C11-C12	-2.26	116.16	123.22
29	D	408	PL9	C15-C14-C16	2.26	119.08	115.27
23	b	613	CLA	CMA-C3A-C4A	-2.26	105.70	111.77
25	d	404	BCR	C16-C15-C14	-2.26	118.85	123.47
23	B	614	CLA	CMA-C3A-C2A	-2.26	104.73	113.83
32	D	404	LMT	C3B-C4B-C5B	2.25	114.25	110.24
23	b	608	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
25	B	617	BCR	C37-C22-C23	2.25	121.62	118.08
23	c	513	CLA	O1D-CGD-CBD	-2.25	119.88	124.48
23	C	508	CLA	O2A-CGA-CBA	2.25	118.97	111.91
23	D	406	CLA	C4D-C3D-CAD	-2.25	107.22	108.47
23	B	613	CLA	CAA-C2A-C3A	-2.25	106.62	112.78
23	b	609	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
25	k	101	BCR	C7-C8-C9	-2.25	122.84	126.23
23	B	606	CLA	C2A-C1A-CHA	-2.25	119.93	123.86
23	d	402	CLA	CMB-C2B-C3B	2.25	128.88	124.68
23	b	601	CLA	C1-O2A-CGA	2.25	122.34	116.44
25	y	101	BCR	C15-C16-C17	-2.25	118.87	123.47
23	c	510	CLA	CED-O2D-CGD	2.24	121.01	115.94
23	a	405	CLA	CMC-C2C-C1C	2.24	128.45	125.04
23	c	503	CLA	C4-C3-C5	2.24	119.04	115.27
23	b	601	CLA	C4D-C3D-CAD	-2.24	107.22	108.47
23	B	602	CLA	C3B-C4B-NB	2.24	112.11	109.21
23	C	511	CLA	C6-C7-C8	-2.24	108.68	115.92
23	c	506	CLA	C2A-C1A-CHA	-2.24	119.94	123.86
23	b	602	CLA	C3B-C4B-NB	2.24	112.11	109.21
23	B	611	CLA	CMC-C2C-C1C	2.24	128.45	125.04
35	C	519	DGD	O2G-C1B-O1B	-2.24	118.29	123.70
24	A	353	PHO	O2A-CGA-CBA	2.24	118.93	111.91
23	A	406	CLA	CMB-C2B-C1B	2.24	131.90	128.46
23	C	514	CLA	C11-C10-C8	-2.24	108.69	115.92
23	b	611	CLA	C4-C3-C5	2.24	119.03	115.27
23	b	615	CLA	O2A-CGA-O1A	-2.24	117.95	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	618	BCR	C15-C16-C17	-2.23	118.90	123.47
32	M	101	LMT	O1B-C1B-C2B	2.23	113.89	108.10
25	Y	101	BCR	C29-C28-C27	-2.23	106.39	111.38
29	D	408	PL9	C47-C48-C49	-2.23	120.12	127.75
23	c	514	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
23	c	504	CLA	CBC-CAC-C3C	-2.23	106.28	112.43
23	a	405	CLA	CHB-C4A-NA	2.23	127.60	124.51
23	B	609	CLA	CMC-C2C-C1C	2.23	128.44	125.04
33	m	101	LMG	O7-C10-O9	-2.23	118.31	123.70
23	B	601	CLA	C11-C12-C13	-2.23	108.72	115.92
25	b	617	BCR	C29-C30-C25	2.23	113.91	110.48
25	c	515	BCR	C34-C9-C8	2.23	121.59	118.08
25	C	516	BCR	C36-C18-C19	2.23	121.59	118.08
24	A	407	PHO	CMB-C2B-C1B	2.23	128.49	125.06
23	B	614	CLA	OBD-CAD-C3D	-2.23	124.28	127.98
25	B	619	BCR	C2-C3-C4	-2.23	106.40	111.38
23	b	613	CLA	C2A-C1A-CHA	-2.23	119.97	123.86
23	B	611	CLA	C4-C3-C5	2.23	119.02	115.27
23	b	608	CLA	CAC-C3C-C4C	2.23	127.70	124.81
25	D	407	BCR	C24-C25-C26	-2.23	116.07	121.46
23	A	405	CLA	C2A-C1A-CHA	-2.23	119.97	123.86
23	B	608	CLA	C2A-C1A-CHA	-2.23	119.97	123.86
23	c	502	CLA	C4D-C3D-CAD	-2.23	107.23	108.47
25	c	515	BCR	C16-C15-C14	-2.23	118.92	123.47
23	a	405	CLA	CMA-C3A-C4A	-2.22	105.80	111.77
23	b	608	CLA	C2A-C1A-CHA	-2.22	119.97	123.86
23	b	604	CLA	C6-C7-C8	-2.22	108.73	115.92
23	c	507	CLA	O2A-CGA-CBA	2.22	118.88	111.91
25	B	618	BCR	C10-C11-C12	-2.22	116.28	123.22
23	C	504	CLA	C4-C3-C2	-2.22	117.98	123.68
23	b	601	CLA	CAC-C3C-C4C	2.22	127.69	124.81
25	Y	101	BCR	C40-C30-C25	-2.22	106.70	110.30
33	C	501	LMG	C8-O7-C10	-2.22	112.33	117.79
23	B	608	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
23	a	407	CLA	C2A-C1A-CHA	-2.22	119.98	123.86
37	D	410	LHG	O8-C23-C24	2.22	118.86	111.91
32	t	102	LMT	O1'-C1'-C2'	2.21	111.76	108.30
23	C	507	CLA	C3D-CAD-CBD	2.21	110.52	107.61
23	b	616	CLA	C4D-C3D-CAD	-2.21	107.24	108.47
29	A	414	PL9	C37-C36-C34	-2.21	105.70	112.98
23	b	601	CLA	CMB-C2B-C3B	2.21	128.82	124.68
29	D	408	PL9	C7-C3-C4	2.21	118.67	116.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	D	404	LMT	O5'-C5'-C4'	2.21	114.41	109.75
23	C	505	CLA	C1-O2A-CGA	2.21	122.24	116.44
23	A	405	CLA	CAA-CBA-CGA	2.21	119.70	113.25
23	D	406	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
23	C	505	CLA	CHD-C4C-NC	2.21	127.68	124.20
23	c	508	CLA	C4C-C3C-C2C	-2.21	103.68	106.90
37	E	101	LHG	O7-C7-O9	-2.21	118.37	123.70
33	m	101	LMG	O8-C28-O10	-2.20	118.03	123.59
23	b	614	CLA	CBC-CAC-C3C	-2.20	106.36	112.43
25	H	101	BCR	C2-C1-C6	2.20	113.87	110.48
23	A	406	CLA	CMA-C3A-C2A	-2.20	104.95	113.83
23	C	505	CLA	OBD-CAD-C3D	-2.20	124.33	127.98
25	B	619	BCR	C20-C21-C22	-2.20	124.17	127.31
35	C	517	DGD	CDB-CCB-CBB	-2.20	103.26	114.42
25	h	101	BCR	C20-C21-C22	-2.20	124.17	127.31
25	B	618	BCR	C38-C26-C25	-2.19	122.06	124.53
25	K	102	BCR	C33-C5-C4	2.19	117.83	113.62
25	H	101	BCR	C31-C1-C6	-2.19	106.74	110.30
23	a	406	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
29	A	414	PL9	C47-C48-C49	-2.19	120.26	127.75
23	C	511	CLA	CMC-C2C-C1C	2.19	128.37	125.04
23	a	405	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
25	k	101	BCR	C2-C1-C6	2.19	113.85	110.48
23	b	602	CLA	O2A-CGA-CBA	2.19	118.77	111.91
25	A	409	BCR	C40-C30-C25	-2.18	106.75	110.30
26	A	412	SQD	C44-O6-C1	-2.18	109.47	113.74
23	B	602	CLA	CED-O2D-CGD	2.18	120.88	115.94
25	A	409	BCR	C20-C21-C22	-2.18	124.19	127.31
23	a	405	CLA	CHD-C4C-NC	2.18	127.64	124.20
23	B	606	CLA	C4D-C3D-CAD	-2.18	107.25	108.47
25	y	101	BCR	C23-C24-C25	-2.18	121.07	127.20
23	B	616	CLA	OBD-CAD-C3D	-2.18	124.36	127.98
23	A	404	CLA	CMA-C3A-C2A	-2.18	105.03	113.83
25	t	103	BCR	C2-C1-C6	2.18	113.84	110.48
23	b	610	CLA	CMC-C2C-C1C	2.18	128.36	125.04
23	b	613	CLA	CMC-C2C-C1C	2.18	128.36	125.04
23	C	507	CLA	CMB-C2B-C3B	2.18	128.76	124.68
23	C	510	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
32	m	103	LMT	C1'-C2'-C3'	2.18	114.54	110.00
23	d	403	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
25	a	410	BCR	C15-C16-C17	-2.18	119.01	123.47
25	t	103	BCR	C29-C28-C27	-2.18	106.51	111.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	606	CLA	C11-C10-C8	-2.18	108.88	115.92
23	b	608	CLA	C4-C3-C5	2.18	118.94	115.27
34	b	622	HTG	O5-C1-C2	2.18	113.05	110.31
23	c	503	CLA	C2A-C1A-CHA	-2.18	120.06	123.86
23	a	409	CLA	CMB-C2B-C3B	2.18	128.75	124.68
25	C	515	BCR	C20-C21-C22	-2.17	124.21	127.31
23	B	612	CLA	C7-C6-C5	-2.17	107.45	113.36
23	B	610	CLA	C2A-C1A-CHA	-2.17	120.06	123.86
33	c	520	LMG	O8-C28-O10	-2.17	118.11	123.59
23	b	616	CLA	C1C-C2C-C3C	-2.17	104.67	106.96
23	B	601	CLA	C4D-C3D-CAD	-2.17	107.26	108.47
32	e	102	LMT	O1B-C1B-C2B	2.17	113.73	108.10
23	C	514	CLA	CAA-C2A-C3A	-2.17	106.83	112.78
23	C	512	CLA	C11-C10-C8	-2.17	108.90	115.92
23	d	403	CLA	CHB-C4A-NA	2.17	127.52	124.51
23	C	508	CLA	CAC-C3C-C2C	2.17	131.24	127.53
23	B	602	CLA	CMA-C3A-C2A	-2.17	105.07	113.83
32	t	102	LMT	C1'-O5'-C5'	2.17	117.94	113.69
23	B	615	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
25	b	619	BCR	C24-C23-C22	-2.17	122.96	126.23
23	b	606	CLA	C4D-C3D-CAD	-2.17	107.26	108.47
26	a	413	SQD	O48-C23-O10	-2.17	118.13	123.59
35	c	519	DGD	O6D-C1D-O3G	-2.17	104.84	109.97
23	b	606	CLA	C6-C7-C8	-2.17	108.92	115.92
25	b	619	BCR	C37-C22-C23	2.16	121.49	118.08
23	C	504	CLA	CMC-C2C-C1C	2.16	128.33	125.04
24	a	408	PHO	CHD-C1D-C2D	-2.16	120.29	125.73
23	d	402	CLA	OBD-CAD-C3D	-2.16	124.39	127.98
26	a	413	SQD	C3-C4-C5	2.16	114.10	110.24
23	C	514	CLA	C4D-C3D-CAD	-2.16	107.27	108.47
23	C	503	CLA	CMB-C2B-C1B	2.16	131.78	128.46
23	C	507	CLA	CED-O2D-CGD	2.16	120.82	115.94
24	A	407	PHO	CBD-CHA-C1A	2.16	131.41	126.40
23	a	409	CLA	CHB-C4A-NA	2.16	127.50	124.51
23	B	603	CLA	C4D-C3D-CAD	-2.16	107.27	108.47
25	B	617	BCR	C11-C10-C9	-2.16	124.23	127.31
23	B	615	CLA	C1-C2-C3	-2.16	122.31	126.04
37	l	101	LHG	O7-C7-O9	-2.16	118.49	123.70
23	a	406	CLA	CED-O2D-CGD	2.16	120.81	115.94
23	B	608	CLA	C4-C3-C5	2.16	118.90	115.27
25	H	101	BCR	C7-C6-C5	2.15	126.68	121.46
23	C	505	CLA	C6-C7-C8	-2.15	108.96	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	601	CLA	CAA-C2A-C3A	-2.15	106.88	112.78
23	B	610	CLA	CMC-C2C-C1C	2.15	128.32	125.04
23	C	504	CLA	CMB-C2B-C3B	2.15	128.70	124.68
23	c	510	CLA	C2A-C1A-CHA	-2.15	120.10	123.86
23	c	508	CLA	C1-C2-C3	-2.15	122.33	126.04
23	b	607	CLA	CHD-C4C-NC	2.15	127.59	124.20
23	C	509	CLA	CHB-C4A-NA	2.15	127.48	124.51
23	b	607	CLA	CAA-CBA-CGA	2.14	119.52	113.25
29	d	405	PL9	C25-C24-C26	2.14	118.88	115.27
23	b	616	CLA	C2A-C1A-CHA	-2.14	120.11	123.86
26	b	620	SQD	O47-C7-O49	-2.14	118.52	123.70
25	a	410	BCR	C32-C1-C6	-2.14	106.83	110.30
32	D	404	LMT	O1B-C4'-C3'	2.14	112.97	107.28
23	c	512	CLA	CAC-C3C-C4C	2.14	127.59	124.81
25	b	619	BCR	C7-C6-C5	2.14	126.65	121.46
23	B	611	CLA	C4D-C3D-CAD	-2.14	107.28	108.47
26	B	620	SQD	O9-S-C6	2.14	109.48	106.94
23	B	601	CLA	CHB-C4A-NA	2.14	127.47	124.51
26	B	620	SQD	O47-C7-O49	-2.14	118.54	123.70
37	l	101	LHG	O4-P-O5	2.14	122.81	112.24
33	a	419	LMG	O8-C28-C29	2.14	118.61	111.91
23	C	508	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
25	A	409	BCR	C36-C18-C17	-2.14	119.93	122.92
23	b	614	CLA	CMB-C2B-C3B	2.14	128.67	124.68
25	T	101	BCR	C7-C8-C9	-2.13	123.01	126.23
23	b	602	CLA	C4-C3-C5	2.13	118.86	115.27
34	B	622	HTG	C1-C2-C3	2.13	114.80	110.59
23	c	513	CLA	C1-O2A-CGA	2.13	122.04	116.44
23	b	607	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
23	c	511	CLA	C2A-C1A-CHA	-2.13	120.14	123.86
23	C	507	CLA	CGD-CBD-CAD	-2.13	103.85	110.73
40	v	202	HEC	CMB-C2B-C3B	2.13	128.32	125.82
23	C	504	CLA	CHA-C1A-NA	-2.12	121.53	126.40
23	B	611	CLA	O2A-CGA-CBA	2.12	118.57	111.91
25	k	101	BCR	C21-C20-C19	-2.12	116.60	123.22
23	B	616	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
23	B	613	CLA	CHB-C4A-NA	2.12	127.44	124.51
26	B	620	SQD	C1-C2-C3	-2.12	105.58	110.00
25	b	619	BCR	C16-C15-C14	-2.12	119.14	123.47
33	C	520	LMG	O8-C28-O10	-2.12	118.25	123.59
23	c	513	CLA	CBA-CAA-C2A	-2.12	107.61	113.86
23	d	403	CLA	O2A-CGA-CBA	2.12	118.55	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	511	CLA	O1D-CGD-CBD	-2.12	120.16	124.48
23	A	408	CLA	C1B-CHB-C4A	-2.12	125.93	130.12
25	D	407	BCR	C29-C28-C27	-2.11	106.65	111.38
25	Y	101	BCR	C36-C18-C19	2.11	121.41	118.08
25	D	407	BCR	C37-C22-C21	-2.11	119.96	122.92
37	D	409	LHG	O7-C7-O9	-2.11	118.59	123.70
37	E	101	LHG	O8-C23-O10	-2.11	118.26	123.59
24	a	408	PHO	C3A-C4A-CHB	-2.11	118.18	121.83
25	C	516	BCR	C36-C18-C17	-2.11	119.96	122.92
25	D	407	BCR	C29-C30-C25	2.11	113.73	110.48
23	b	611	CLA	OBD-CAD-C3D	-2.11	124.47	127.98
23	C	511	CLA	CAA-C2A-C3A	-2.11	107.00	112.78
23	b	613	CLA	CAC-C3C-C2C	2.11	131.14	127.53
25	a	410	BCR	C40-C30-C25	-2.11	106.88	110.30
23	b	602	CLA	CMA-C3A-C2A	-2.11	105.32	113.83
23	B	604	CLA	OBD-CAD-C3D	-2.11	124.48	127.98
25	B	618	BCR	C16-C17-C18	-2.11	124.30	127.31
23	a	405	CLA	C17-C16-C15	-2.11	103.56	113.24
23	C	511	CLA	C2A-C1A-CHA	-2.11	120.18	123.86
23	b	605	CLA	OBD-CAD-C3D	-2.11	124.48	127.98
25	A	409	BCR	C36-C18-C19	2.11	121.39	118.08
25	c	516	BCR	C37-C22-C21	-2.11	119.97	122.92
25	d	404	BCR	C30-C25-C24	2.10	121.73	115.78
23	c	512	CLA	OBD-CAD-C3D	-2.10	124.49	127.98
33	a	419	LMG	C3-C4-C5	2.10	113.99	110.24
23	C	506	CLA	CHA-C1A-NA	-2.10	121.58	126.40
24	A	353	PHO	C3A-C4A-NA	2.10	116.64	113.05
25	H	101	BCR	C36-C18-C17	-2.10	119.98	122.92
23	a	407	CLA	CMA-C3A-C2A	-2.10	105.35	113.83
23	b	603	CLA	C11-C10-C8	-2.10	109.13	115.92
23	B	604	CLA	CAC-C3C-C2C	2.10	131.12	127.53
23	B	604	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
35	c	517	DGD	O1G-C1A-O1A	-2.10	118.30	123.59
23	b	603	CLA	CBC-CAC-C3C	-2.10	106.65	112.43
23	B	604	CLA	C4-C3-C5	2.10	118.80	115.27
25	B	617	BCR	C21-C20-C19	-2.10	116.67	123.22
23	c	514	CLA	C11-C10-C8	-2.10	109.15	115.92
23	c	511	CLA	CHB-C4A-NA	2.09	127.41	124.51
23	b	616	CLA	CBC-CAC-C3C	-2.09	106.66	112.43
33	Z	101	LMG	C7-O1-C1	-2.09	109.65	113.74
25	k	101	BCR	C34-C9-C8	2.09	121.37	118.08
23	B	606	CLA	C1-C2-C3	-2.09	122.42	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	509	CLA	CMB-C2B-C3B	2.09	128.59	124.68
33	c	520	LMG	O7-C10-O9	-2.09	118.65	123.70
23	C	503	CLA	CED-O2D-CGD	2.09	120.67	115.94
23	C	502	CLA	C11-C12-C13	-2.09	109.16	115.92
23	d	402	CLA	CED-O2D-CGD	2.09	120.67	115.94
33	B	621	LMG	C12-C11-C10	-2.09	106.02	113.62
23	c	513	CLA	CAC-C3C-C2C	2.09	131.10	127.53
23	B	612	CLA	CMA-C3A-C4A	-2.09	106.16	111.77
23	C	508	CLA	OBD-CAD-C3D	-2.09	124.51	127.98
23	C	508	CLA	C16-C15-C13	-2.09	109.17	115.92
25	b	617	BCR	C33-C5-C4	2.09	117.62	113.62
26	A	412	SQD	C1-C2-C3	-2.09	105.65	110.00
23	c	504	CLA	C2A-C1A-CHA	-2.09	120.21	123.86
37	E	101	LHG	C5-O7-C7	-2.09	112.66	117.79
23	d	403	CLA	CMA-C3A-C2A	-2.09	105.42	113.83
23	C	505	CLA	C4D-C3D-CAD	-2.08	107.31	108.47
32	a	414	LMT	C1'-O5'-C5'	2.08	117.77	113.69
23	B	606	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
23	d	403	CLA	C1-O2A-CGA	2.08	121.90	116.44
25	C	515	BCR	C21-C20-C19	-2.08	116.73	123.22
23	D	406	CLA	O2A-CGA-CBA	2.08	118.43	111.91
23	b	614	CLA	C4-C3-C2	-2.08	118.35	123.68
25	D	407	BCR	C21-C20-C19	-2.08	116.73	123.22
23	B	609	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
23	a	406	CLA	O2D-CGD-O1D	-2.08	119.78	123.84
23	B	602	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
23	C	508	CLA	C6-C7-C8	-2.08	109.21	115.92
25	b	619	BCR	C29-C30-C25	2.08	113.68	110.48
23	A	405	CLA	OBD-CAD-C3D	-2.08	124.53	127.98
35	h	102	DGD	C3B-C2B-C1B	-2.07	106.08	113.62
25	B	618	BCR	C7-C8-C9	-2.07	123.10	126.23
25	c	516	BCR	C3-C4-C5	-2.07	110.38	114.08
23	c	505	CLA	CMA-C3A-C4A	-2.07	106.20	111.77
25	C	516	BCR	C37-C22-C23	2.07	121.34	118.08
23	c	502	CLA	C6-C7-C8	-2.07	109.23	115.92
23	c	505	CLA	O2A-CGA-CBA	2.07	118.40	111.91
23	a	407	CLA	CMC-C2C-C1C	2.07	128.19	125.04
23	B	605	CLA	C5-C3-C2	-2.07	116.93	121.12
26	A	412	SQD	C46-C45-C44	-2.07	106.89	111.79
23	A	406	CLA	CHB-C4A-NA	2.07	127.37	124.51
23	c	502	CLA	OBD-CAD-C3D	-2.07	124.55	127.98
24	A	407	PHO	O2D-CGD-O1D	-2.07	119.80	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	t	103	BCR	C19-C18-C17	-2.07	115.77	118.94
23	c	506	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
23	b	615	CLA	CHA-C1A-NA	-2.07	121.67	126.40
25	b	617	BCR	C15-C16-C17	-2.07	119.24	123.47
23	B	602	CLA	CMC-C2C-C1C	2.07	128.18	125.04
24	A	407	PHO	C4-C3-C5	2.06	118.74	115.27
23	b	609	CLA	C4D-C3D-CAD	-2.06	107.32	108.47
23	c	513	CLA	CHA-C1A-NA	-2.06	121.67	126.40
23	B	601	CLA	CMC-C2C-C1C	2.06	128.18	125.04
23	B	616	CLA	CMC-C2C-C1C	2.06	128.18	125.04
23	c	507	CLA	CHB-C4A-NA	2.06	127.36	124.51
23	B	616	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
25	h	101	BCR	C34-C9-C8	2.06	121.32	118.08
35	H	102	DGD	C3G-O3G-C1D	-2.06	109.72	113.74
23	c	510	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
29	a	416	PL9	C10-C9-C8	-2.06	118.40	123.68
23	B	601	CLA	CAA-C2A-C3A	-2.06	107.15	112.78
23	a	405	CLA	CBC-CAC-C3C	-2.06	106.76	112.43
25	B	618	BCR	C38-C26-C27	2.06	117.57	113.62
23	a	409	CLA	C2A-C1A-CHA	-2.06	120.27	123.86
23	c	508	CLA	C6-C7-C8	-2.06	109.28	115.92
23	C	504	CLA	O2A-CGA-CBA	2.05	118.35	111.91
35	C	519	DGD	C3G-C2G-C1G	-2.05	106.93	111.79
23	b	610	CLA	CMA-C3A-C2A	-2.05	105.55	113.83
23	b	610	CLA	OBD-CAD-C3D	-2.05	124.57	127.98
23	b	608	CLA	C6-C7-C8	-2.05	109.28	115.92
25	b	619	BCR	C21-C20-C19	-2.05	116.81	123.22
23	b	608	CLA	CHB-C4A-NA	2.05	127.35	124.51
23	b	601	CLA	C5-C3-C2	-2.05	116.97	121.12
37	D	409	LHG	O4-P-O5	2.05	122.36	112.24
23	d	403	CLA	C6-C7-C8	-2.05	109.30	115.92
23	c	511	CLA	C4-C3-C2	-2.05	118.43	123.68
23	B	611	CLA	C11-C12-C13	-2.04	109.31	115.92
25	B	618	BCR	C40-C30-C25	-2.04	106.98	110.30
35	C	518	DGD	O5D-C6D-C5D	-2.04	105.27	109.05
25	B	619	BCR	C16-C15-C14	-2.04	119.29	123.47
23	b	602	CLA	CHB-C4A-NA	2.04	127.33	124.51
23	B	602	CLA	C4-C3-C5	2.04	118.70	115.27
23	b	604	CLA	C2A-C1A-CHA	-2.04	120.29	123.86
23	b	606	CLA	CBC-CAC-C3C	-2.04	106.81	112.43
23	C	510	CLA	C11-C12-C13	-2.04	109.33	115.92
23	c	511	CLA	CED-O2D-CGD	2.04	120.55	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	504	CLA	CBC-CAC-C3C	-2.04	106.82	112.43
40	V	202	HEC	C1D-C2D-C3D	-2.04	105.58	107.00
29	d	405	PL9	C40-C39-C38	-2.04	118.46	123.68
23	c	510	CLA	C4-C3-C2	-2.03	118.46	123.68
23	B	609	CLA	OBD-CAD-C3D	-2.03	124.60	127.98
33	Z	101	LMG	C1-O6-C5	2.03	117.68	113.69
25	H	101	BCR	C29-C30-C25	2.03	113.61	110.48
23	C	514	CLA	CMB-C2B-C3B	2.03	128.48	124.68
23	c	506	CLA	O1D-CGD-CBD	-2.03	120.32	124.48
26	a	413	SQD	O8-S-C6	2.03	108.98	105.74
23	B	602	CLA	CMB-C2B-C3B	2.03	128.47	124.68
32	A	359	LMT	O5B-C5B-C4B	2.03	113.38	109.69
33	C	520	LMG	O7-C10-O9	-2.03	118.80	123.70
25	c	516	BCR	C24-C23-C22	-2.03	123.17	126.23
23	C	504	CLA	C2A-C1A-CHA	-2.03	120.31	123.86
23	B	607	CLA	O2A-CGA-CBA	2.02	118.26	111.91
23	A	406	CLA	C11-C10-C8	-2.02	109.38	115.92
29	A	414	PL9	C12-C13-C14	-2.02	122.79	127.66
25	H	101	BCR	C3-C4-C5	-2.02	110.47	114.08
23	c	514	CLA	CED-O2D-CGD	2.02	120.51	115.94
23	B	615	CLA	CED-O2D-CGD	2.02	120.50	115.94
23	b	614	CLA	CMA-C3A-C2A	-2.02	105.69	113.83
24	A	407	PHO	CBC-CAC-C3C	-2.02	106.87	112.43
25	b	618	BCR	C33-C5-C6	-2.02	122.26	124.53
25	d	404	BCR	C29-C30-C25	2.02	113.59	110.48
35	C	518	DGD	C2G-O2G-C1B	-2.02	112.83	117.79
26	F	101	SQD	O48-C23-O10	-2.02	118.50	123.59
24	A	353	PHO	CBD-CHA-C1A	2.02	131.08	126.40
23	c	507	CLA	C2A-C1A-CHA	-2.02	120.33	123.86
23	b	605	CLA	CMB-C2B-C3B	2.02	128.45	124.68
34	b	623	HTG	O5-C1-C2	2.02	112.85	110.31
34	b	623	HTG	C6-C5-C4	-2.01	108.29	113.00
23	d	403	CLA	C11-C10-C8	-2.01	109.41	115.92
23	c	514	CLA	CBC-CAC-C3C	-2.01	106.88	112.43
23	B	612	CLA	CAA-CBA-CGA	-2.01	107.37	113.25
23	c	508	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
25	c	515	BCR	C11-C12-C13	-2.01	120.77	126.42
23	B	616	CLA	C4-C3-C5	2.01	118.65	115.27
23	B	602	CLA	C4D-C3D-CAD	-2.01	107.35	108.47
35	C	518	DGD	O5D-C1E-C2E	2.01	111.44	108.30
25	B	618	BCR	C21-C20-C19	-2.01	116.95	123.22
23	B	610	CLA	CHB-C4A-NA	2.01	127.29	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	603	CLA	C7-C6-C5	-2.01	107.91	113.36
26	A	412	SQD	O6-C44-C45	-2.01	106.06	110.90
23	a	405	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
23	B	605	CLA	CAA-C2A-C3A	-2.01	107.29	112.78
25	B	617	BCR	C28-C27-C26	-2.00	110.50	114.08
24	a	353	PHO	C4-C3-C2	-2.00	118.54	123.68
24	a	408	PHO	CMC-C2C-C1C	2.00	128.15	125.06
23	b	611	CLA	C11-C12-C13	-2.00	109.45	115.92
23	A	405	CLA	C1-C2-C3	-2.00	122.58	126.04
23	c	511	CLA	OBD-CAD-C3D	-2.00	124.66	127.98
23	B	615	CLA	CHA-C1A-NA	-2.00	121.82	126.40
25	C	516	BCR	C2-C1-C6	2.00	113.56	110.48

All (190) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	b	610	CLA	NC
23	b	610	CLA	ND
23	b	610	CLA	NA
23	C	512	CLA	NC
23	C	512	CLA	ND
23	C	512	CLA	NA
23	B	612	CLA	NC
23	B	612	CLA	ND
23	B	612	CLA	NA
23	C	511	CLA	NC
23	C	511	CLA	ND
23	C	511	CLA	NA
23	B	610	CLA	NC
23	B	610	CLA	ND
23	B	610	CLA	NA
23	c	508	CLA	NC
23	c	508	CLA	ND
23	c	508	CLA	NA
23	B	607	CLA	NC
23	B	607	CLA	ND
23	B	607	CLA	NA
23	b	609	CLA	NC
23	b	609	CLA	ND
23	b	606	CLA	NC
23	b	606	CLA	ND
23	b	606	CLA	NA

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Mol	Chain	Res	Type	Atom
23	a	405	CLA	NC
23	a	405	CLA	ND
23	a	405	CLA	NA
23	b	614	CLA	NC
23	b	614	CLA	ND
23	b	614	CLA	NA
23	a	409	CLA	NC
23	a	409	CLA	ND
23	a	409	CLA	NA
23	d	402	CLA	ND
23	C	508	CLA	NC
23	C	508	CLA	ND
23	C	508	CLA	NA
23	b	602	CLA	NC
23	b	602	CLA	ND
23	c	504	CLA	NC
23	c	504	CLA	ND
23	c	504	CLA	NA
23	B	613	CLA	NC
23	B	613	CLA	ND
23	B	613	CLA	NA
23	A	404	CLA	NC
23	A	404	CLA	ND
23	A	404	CLA	NA
23	b	605	CLA	NC
23	b	605	CLA	ND
23	b	605	CLA	NA
23	c	512	CLA	NC
23	c	512	CLA	ND
23	c	512	CLA	NA
23	C	513	CLA	NC
23	C	513	CLA	ND
23	C	513	CLA	NA
23	B	604	CLA	NC
23	B	604	CLA	ND
23	B	604	CLA	NA
23	b	611	CLA	NC
23	b	611	CLA	ND
23	b	611	CLA	NA
23	b	601	CLA	NC
23	b	601	CLA	ND
23	b	601	CLA	NA

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Mol	Chain	Res	Type	Atom
23	B	603	CLA	NC
23	B	603	CLA	ND
23	B	611	CLA	NC
23	B	611	CLA	ND
23	B	611	CLA	NA
23	A	406	CLA	NC
23	A	406	CLA	NA
23	C	504	CLA	NC
23	C	504	CLA	ND
23	C	504	CLA	NA
23	c	509	CLA	NC
23	c	509	CLA	ND
23	c	509	CLA	NA
23	a	406	CLA	NC
23	a	406	CLA	NA
23	B	615	CLA	NA
23	B	615	CLA	NC
23	B	615	CLA	ND
23	B	602	CLA	NC
23	B	602	CLA	ND
23	B	605	CLA	NC
23	B	605	CLA	ND
23	B	605	CLA	NA
23	c	511	CLA	NC
23	c	511	CLA	ND
23	c	511	CLA	NA
23	A	408	CLA	NC
23	A	408	CLA	ND
23	A	408	CLA	NA
23	B	609	CLA	NC
23	B	609	CLA	ND
23	b	608	CLA	NC
23	b	608	CLA	NA
23	B	606	CLA	NC
23	B	606	CLA	ND
23	C	514	CLA	NC
23	C	514	CLA	ND
23	C	514	CLA	NA
23	a	407	CLA	NC
23	a	407	CLA	NA
23	C	509	CLA	NC
23	C	509	CLA	ND

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Mol	Chain	Res	Type	Atom
23	C	509	CLA	NA
23	C	506	CLA	ND
23	c	505	CLA	NC
23	c	505	CLA	ND
23	c	505	CLA	NA
23	b	612	CLA	NC
23	b	612	CLA	ND
23	b	612	CLA	NA
23	B	601	CLA	NC
23	B	601	CLA	ND
23	B	601	CLA	NA
23	c	507	CLA	NC
23	c	507	CLA	ND
23	c	507	CLA	NA
23	b	615	CLA	NC
23	b	615	CLA	ND
23	b	615	CLA	NA
23	b	607	CLA	NC
23	b	607	CLA	ND
23	b	607	CLA	NA
23	B	616	CLA	NA
23	B	616	CLA	NC
23	B	616	CLA	ND
23	C	503	CLA	NC
23	C	503	CLA	ND
23	C	503	CLA	NA
23	C	502	CLA	NC
23	C	502	CLA	ND
23	C	502	CLA	NA
23	C	510	CLA	NC
23	C	510	CLA	ND
23	C	510	CLA	NA
23	b	604	CLA	NC
23	b	604	CLA	ND
23	b	604	CLA	NA
23	A	405	CLA	NC
23	A	405	CLA	ND
23	A	405	CLA	NA
23	D	406	CLA	NC
23	D	406	CLA	ND
23	D	406	CLA	NA
23	c	503	CLA	NC

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Mol	Chain	Res	Type	Atom
23	c	503	CLA	ND
23	c	503	CLA	NA
23	c	502	CLA	NC
23	c	502	CLA	ND
23	c	502	CLA	NA
23	c	510	CLA	NC
23	c	510	CLA	ND
23	c	510	CLA	NA
23	C	505	CLA	NC
23	C	505	CLA	ND
23	C	505	CLA	NA
23	b	603	CLA	NC
23	b	603	CLA	ND
23	d	403	CLA	NC
23	d	403	CLA	ND
23	d	403	CLA	NA
23	D	405	CLA	ND
23	c	513	CLA	NC
23	c	513	CLA	ND
23	c	513	CLA	NA
23	C	507	CLA	NC
23	C	507	CLA	ND
23	C	507	CLA	NA
23	b	616	CLA	NA
23	b	616	CLA	NC
23	b	616	CLA	ND
23	B	608	CLA	NC
23	B	608	CLA	NA
23	b	613	CLA	NC
23	b	613	CLA	ND
23	b	613	CLA	NA
23	c	514	CLA	NC
23	c	514	CLA	ND
23	c	514	CLA	NA
23	B	614	CLA	NC
23	B	614	CLA	ND
23	B	614	CLA	NA
23	c	506	CLA	ND

All (1213) torsion outliers are listed below:

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Mol	Chain	Res	Type	Atoms
32	b	627	LMT	C2'-C1'-O1'-C1
32	b	627	LMT	O5'-C1'-O1'-C1
33	z	101	LMG	O6-C1-O1-C7
33	z	101	LMG	C11-C10-O7-C8
32	E	102	LMT	C2'-C1'-O1'-C1
32	E	102	LMT	O5'-C1'-O1'-C1
26	f	102	SQD	O6-C44-C45-O47
26	f	102	SQD	O49-C7-O47-C45
26	f	102	SQD	C8-C7-O47-C45
37	L	101	LHG	C3-O3-P-O4
37	L	101	LHG	C4-O6-P-O4
33	C	501	LMG	O9-C10-O7-C8
32	t	102	LMT	O5'-C1'-O1'-C1
27	V	201	GOL	O1-C1-C2-O2
27	V	201	GOL	O1-C1-C2-C3
25	y	101	BCR	C1-C6-C7-C8
25	y	101	BCR	C5-C6-C7-C8
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	614	CLA	C4-C3-C5-C6
32	a	420	LMT	C2'-C1'-O1'-C1
32	a	420	LMT	O5'-C1'-O1'-C1
23	a	409	CLA	C2-C3-C5-C6
23	a	409	CLA	C4-C3-C5-C6
26	F	101	SQD	O49-C7-O47-C45
26	F	101	SQD	C8-C7-O47-C45
37	d	408	LHG	C4-O6-P-O4
37	e	101	LHG	C4-O6-P-O4
37	e	101	LHG	C4-O6-P-O5
34	B	623	HTG	C2'-C1'-S1-C1
23	b	605	CLA	C4-C3-C5-C6
26	a	413	SQD	O6-C44-C45-O47
26	a	413	SQD	C5-C6-S-O7
26	a	413	SQD	C5-C6-S-O8
26	a	413	SQD	C5-C6-S-O9
27	C	523	GOL	O1-C1-C2-C3
32	e	102	LMT	C2'-C1'-O1'-C1
32	e	102	LMT	O5'-C1'-O1'-C1
26	B	620	SQD	O49-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
25	d	404	BCR	C7-C8-C9-C10
25	d	404	BCR	C7-C8-C9-C34
25	d	404	BCR	C21-C22-C23-C24
25	d	404	BCR	C37-C22-C23-C24
32	M	103	LMT	C2'-C1'-O1'-C1
32	M	103	LMT	O5'-C1'-O1'-C1
32	t	101	LMT	C2'-C1'-O1'-C1
32	t	101	LMT	O5'-C1'-O1'-C1
25	T	101	BCR	C11-C12-C13-C35
27	B	625	GOL	C1-C2-C3-O3
27	B	625	GOL	O2-C2-C3-O3
33	Z	101	LMG	O9-C10-O7-C8
33	Z	101	LMG	C11-C10-O7-C8
23	B	603	CLA	C2-C3-C5-C6
23	B	603	CLA	C4-C3-C5-C6
25	D	407	BCR	C21-C22-C23-C24
25	D	407	BCR	C37-C22-C23-C24
37	d	407	LHG	O2-C2-C3-O3
37	d	407	LHG	C3-O3-P-O4
37	d	407	LHG	C4-O6-P-O4
27	a	412	GOL	C1-C2-C3-O3
32	a	414	LMT	C2'-C1'-O1'-C1
32	a	414	LMT	O5'-C1'-O1'-C1
25	Y	101	BCR	C1-C6-C7-C8
25	Y	101	BCR	C5-C6-C7-C8
23	c	509	CLA	CHA-CBD-CGD-O1D
37	l	101	LHG	C4-O6-P-O3
37	l	101	LHG	C4-O6-P-O4
37	l	101	LHG	C4-O6-P-O5
32	b	621	LMT	O5'-C1'-O1'-C1
27	a	418	GOL	O1-C1-C2-C3
25	b	619	BCR	C5-C6-C7-C8
34	B	622	HTG	C2'-C1'-S1-C1
32	I	101	LMT	O5'-C1'-O1'-C1
23	B	606	CLA	CHA-CBD-CGD-O1D
23	C	509	CLA	CHA-CBD-CGD-O1D
33	c	521	LMG	O9-C10-O7-C8
33	c	521	LMG	C11-C10-O7-C8
32	A	359	LMT	C2'-C1'-O1'-C1
32	A	359	LMT	O5'-C1'-O1'-C1
25	b	617	BCR	C1-C6-C7-C8
37	E	101	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
37	E	101	LHG	C3-O3-P-O5
37	E	101	LHG	C3-O3-P-O6
33	C	520	LMG	C11-C10-O7-C8
29	A	414	PL9	C9-C11-C12-C13
29	A	414	PL9	C14-C16-C17-C18
29	A	414	PL9	C18-C19-C21-C22
29	A	414	PL9	C20-C19-C21-C22
27	B	624	GOL	C1-C2-C3-O3
29	a	416	PL9	C14-C16-C17-C18
29	a	416	PL9	C28-C29-C31-C32
29	a	416	PL9	C30-C29-C31-C32
26	b	620	SQD	O49-C7-O47-C45
26	b	620	SQD	C8-C7-O47-C45
23	c	510	CLA	C2-C1-O2A-CGA
23	c	510	CLA	C11-C10-C8-C9
23	C	505	CLA	C2-C3-C5-C6
23	C	505	CLA	C4-C3-C5-C6
23	d	403	CLA	C4-C3-C5-C6
27	v	201	GOL	O1-C1-C2-C3
26	A	412	SQD	O6-C44-C45-O47
37	D	410	LHG	O2-C2-C3-O3
37	D	410	LHG	C3-O3-P-O4
37	D	410	LHG	C4-O6-P-O4
25	t	103	BCR	C11-C12-C13-C14
25	t	103	BCR	C11-C12-C13-C35
27	A	411	GOL	O1-C1-C2-C3
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	B	614	CLA	C2-C3-C5-C6
23	B	614	CLA	C4-C3-C5-C6
32	I	101	LMT	C3'-C4'-O1B-C1B
37	e	101	LHG	O10-C23-O8-C6
37	E	101	LHG	O10-C23-O8-C6
37	e	101	LHG	C24-C23-O8-C6
37	E	101	LHG	C24-C23-O8-C6
23	C	504	CLA	CBD-CGD-O2D-CED
23	C	514	CLA	CBD-CGD-O2D-CED
23	C	502	CLA	CBD-CGD-O2D-CED
33	z	101	LMG	O9-C10-O7-C8
33	C	520	LMG	O9-C10-O7-C8
23	B	604	CLA	C3-C5-C6-C7
23	c	507	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
23	b	616	CLA	C3-C5-C6-C7
33	C	501	LMG	C11-C10-O7-C8
26	B	620	SQD	C8-C7-O47-C45
29	a	416	PL9	C25-C24-C26-C27
23	d	403	CLA	C2-C3-C5-C6
23	b	606	CLA	C2A-CAA-CBA-CGA
23	B	606	CLA	C2A-CAA-CBA-CGA
23	A	408	CLA	C3-C5-C6-C7
23	d	403	CLA	C3-C5-C6-C7
23	c	513	CLA	C3-C5-C6-C7
32	E	102	LMT	O5'-C5'-C6'-O6'
32	t	101	LMT	O5'-C5'-C6'-O6'
33	c	521	LMG	O6-C5-C6-O5
32	b	627	LMT	O5'-C5'-C6'-O6'
32	I	101	LMT	O5B-C5B-C6B-O6B
23	B	616	CLA	C3-C5-C6-C7
32	M	103	LMT	O5'-C5'-C6'-O6'
32	D	404	LMT	C3'-C4'-O1B-C1B
32	D	404	LMT	O5B-C5B-C6B-O6B
23	c	508	CLA	C4-C3-C5-C6
23	C	508	CLA	C4-C3-C5-C6
23	B	605	CLA	C4-C3-C5-C6
29	A	414	PL9	C15-C14-C16-C17
29	a	416	PL9	C15-C14-C16-C17
23	b	603	CLA	C4-C3-C5-C6
33	c	521	LMG	C4-C5-C6-O5
23	c	508	CLA	C2-C3-C5-C6
23	b	614	CLA	C2-C3-C5-C6
23	C	508	CLA	C2-C3-C5-C6
23	b	605	CLA	C2-C3-C5-C6
23	B	605	CLA	C2-C3-C5-C6
29	A	414	PL9	C13-C14-C16-C17
29	a	416	PL9	C13-C14-C16-C17
23	b	603	CLA	C2-C3-C5-C6
33	C	521	LMG	O6-C5-C6-O5
26	B	620	SQD	O5-C1-O6-C44
29	d	405	PL9	C39-C41-C42-C43
29	D	408	PL9	C39-C41-C42-C43
29	A	414	PL9	C44-C46-C47-C48
32	D	404	LMT	C4B-C5B-C6B-O6B
23	c	502	CLA	CBD-CGD-O2D-CED
23	C	514	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
34	c	522	HTG	C4-C5-C6-O6
23	B	614	CLA	C3-C5-C6-C7
23	c	510	CLA	CBA-CGA-O2A-C1
35	H	102	DGD	C9B-CAB-CBB-CCB
32	b	627	LMT	C4'-C5'-C6'-O6'
32	t	101	LMT	C4'-C5'-C6'-O6'
32	E	102	LMT	C4'-C5'-C6'-O6'
23	b	606	CLA	C10-C11-C12-C13
23	b	606	CLA	C13-C15-C16-C17
23	B	601	CLA	C5-C6-C7-C8
37	E	101	LHG	O2-C2-C3-O3
32	t	102	LMT	C2'-C1'-O1'-C1
32	I	101	LMT	C2'-C1'-O1'-C1
23	c	505	CLA	C4-C3-C5-C6
23	c	505	CLA	C2-C3-C5-C6
29	a	416	PL9	C23-C24-C26-C27
23	C	513	CLA	C6-C7-C8-C9
23	B	605	CLA	C6-C7-C8-C9
23	B	601	CLA	C11-C10-C8-C9
23	c	507	CLA	C6-C7-C8-C9
23	B	616	CLA	C6-C7-C8-C9
23	C	503	CLA	C14-C13-C15-C16
23	b	616	CLA	C6-C7-C8-C9
23	b	610	CLA	C2A-CAA-CBA-CGA
25	B	619	BCR	C7-C8-C9-C34
25	b	619	BCR	C7-C8-C9-C34
25	b	619	BCR	C7-C8-C9-C10
26	f	102	SQD	C26-C27-C28-C29
26	F	101	SQD	C7-C8-C9-C10
33	B	621	LMG	C32-C33-C34-C35
23	a	409	CLA	CBA-CGA-O2A-C1
23	B	606	CLA	C13-C15-C16-C17
23	C	504	CLA	O1D-CGD-O2D-CED
23	B	613	CLA	C15-C16-C17-C18
23	b	611	CLA	C15-C16-C17-C18
23	c	513	CLA	C10-C11-C12-C13
23	B	614	CLA	C8-C10-C11-C12
23	B	614	CLA	C10-C11-C12-C13
27	a	418	GOL	O1-C1-C2-O2
27	B	624	GOL	O2-C2-C3-O3
27	v	201	GOL	O1-C1-C2-O2
27	A	411	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
37	L	101	LHG	C23-C24-C25-C26
35	C	518	DGD	C1A-C2A-C3A-C4A
33	Z	101	LMG	C10-C11-C12-C13
32	D	404	LMT	O5'-C5'-C6'-O6'
32	D	404	LMT	C5'-C4'-O1B-C1B
23	B	610	CLA	C13-C15-C16-C17
23	b	614	CLA	C13-C15-C16-C17
32	M	103	LMT	O1'-C1-C2-C3
23	b	601	CLA	C2-C1-O2A-CGA
23	B	615	CLA	C10-C11-C12-C13
23	B	608	CLA	C13-C15-C16-C17
23	B	603	CLA	C11-C12-C13-C15
23	A	408	CLA	C11-C10-C8-C7
23	B	609	CLA	C13-C15-C16-C17
23	C	503	CLA	C13-C15-C16-C17
32	I	101	LMT	O1'-C1-C2-C3
23	c	510	CLA	O1A-CGA-O2A-C1
29	a	416	PL9	C9-C11-C12-C13
35	c	518	DGD	C1B-C2B-C3B-C4B
34	c	522	HTG	S1-C1'-C2'-C3'
33	z	101	LMG	O6-C5-C6-O5
33	B	621	LMG	O6-C5-C6-O5
33	z	101	LMG	C4-C5-C6-O5
32	I	101	LMT	C4B-C5B-C6B-O6B
23	C	513	CLA	C3-C5-C6-C7
23	b	602	CLA	C15-C16-C17-C18
23	b	608	CLA	C13-C15-C16-C17
23	c	511	CLA	C10-C11-C12-C13
23	B	616	CLA	C10-C11-C12-C13
23	C	507	CLA	C13-C15-C16-C17
33	C	521	LMG	C4-C5-C6-O5
26	A	410	SQD	C8-C7-O47-C45
23	C	506	CLA	C10-C11-C12-C13
37	L	101	LHG	C3-O3-P-O6
37	L	101	LHG	C4-O6-P-O3
37	e	101	LHG	C4-O6-P-O3
37	d	407	LHG	C3-O3-P-O6
37	D	410	LHG	C3-O3-P-O6
34	B	622	HTG	C1'-C2'-C3'-C4'
23	A	405	CLA	C15-C16-C17-C18
35	c	517	DGD	O6D-C5D-C6D-O5D
37	d	407	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
37	D	410	LHG	C1-C2-C3-O3
26	A	410	SQD	O49-C7-O47-C45
23	C	502	CLA	O1D-CGD-O2D-CED
23	B	610	CLA	C16-C17-C18-C20
23	b	601	CLA	C13-C15-C16-C17
33	D	415	LMG	C19-C20-C21-C22
37	L	101	LHG	C17-C18-C19-C20
34	B	623	HTG	C2'-C3'-C4'-C5'
33	B	621	LMG	C36-C37-C38-C39
26	a	413	SQD	C24-C25-C26-C27
33	C	521	LMG	C35-C36-C37-C38
26	b	620	SQD	C27-C28-C29-C30
23	C	511	CLA	C16-C17-C18-C20
37	L	101	LHG	C25-C26-C27-C28
32	D	404	LMT	C6-C7-C8-C9
33	d	412	LMG	C11-C12-C13-C14
26	A	410	SQD	C9-C10-C11-C12
37	E	101	LHG	C24-C25-C26-C27
37	D	411	LHG	C13-C14-C15-C16
32	m	103	LMT	O5'-C5'-C6'-O6'
23	B	614	CLA	C5-C6-C7-C8
33	B	621	LMG	C17-C18-C19-C20
35	H	102	DGD	CCA-CDA-CEA-CFA
26	a	411	SQD	C30-C31-C32-C33
34	c	522	HTG	O5-C5-C6-O6
35	C	518	DGD	C2E-C1E-O5D-C6D
33	Z	101	LMG	C2-C1-O1-C7
32	b	621	LMT	C2'-C1'-O1'-C1
32	m	103	LMT	C2'-C1'-O1'-C1
23	C	511	CLA	CBA-CGA-O2A-C1
33	d	412	LMG	C38-C39-C40-C41
33	a	419	LMG	C20-C21-C22-C23
33	m	101	LMG	C38-C39-C40-C41
23	a	409	CLA	O1A-CGA-O2A-C1
35	H	102	DGD	CBB-CCB-CDB-CEB
37	l	101	LHG	C14-C15-C16-C17
23	b	610	CLA	C11-C12-C13-C14
23	C	513	CLA	C11-C10-C8-C9
23	B	603	CLA	C11-C12-C13-C14
23	A	408	CLA	C11-C10-C8-C9
23	c	510	CLA	C14-C13-C15-C16
35	C	517	DGD	O6D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
33	C	520	LMG	C10-C11-C12-C13
26	F	101	SQD	C30-C31-C32-C33
26	B	620	SQD	C30-C31-C32-C33
32	t	101	LMT	C3-C4-C5-C6
25	H	101	BCR	C7-C8-C9-C34
33	C	501	LMG	C18-C19-C20-C21
26	b	620	SQD	C12-C13-C14-C15
26	b	620	SQD	C14-C15-C16-C17
27	a	412	GOL	O1-C1-C2-C3
37	D	409	LHG	O1-C1-C2-C3
27	B	624	GOL	O1-C1-C2-C3
25	H	101	BCR	C7-C8-C9-C10
23	b	606	CLA	C15-C16-C17-C18
35	h	102	DGD	C5B-C6B-C7B-C8B
24	a	353	PHO	C2C-C3C-CAC-CBC
33	C	521	LMG	C15-C16-C17-C18
33	C	520	LMG	C19-C20-C21-C22
37	d	408	LHG	C27-C28-C29-C30
35	H	102	DGD	CAB-CBB-CCB-CDB
26	A	410	SQD	C15-C16-C17-C18
32	A	359	LMT	O1'-C1-C2-C3
33	C	521	LMG	C12-C13-C14-C15
26	a	411	SQD	C11-C12-C13-C14
23	B	610	CLA	C16-C17-C18-C19
23	c	503	CLA	C16-C17-C18-C20
23	B	606	CLA	C10-C11-C12-C13
23	c	507	CLA	C10-C11-C12-C13
35	h	102	DGD	C9A-CAA-CBA-CCA
35	c	517	DGD	C9A-CAA-CBA-CCA
35	c	517	DGD	C2B-C3B-C4B-C5B
37	e	101	LHG	C26-C27-C28-C29
33	C	521	LMG	C17-C18-C19-C20
35	c	517	DGD	C4D-C5D-C6D-O5D
35	C	517	DGD	C4B-C5B-C6B-C7B
35	c	517	DGD	C5A-C6A-C7A-C8A
37	D	409	LHG	C32-C33-C34-C35
37	L	101	LHG	C13-C14-C15-C16
33	d	412	LMG	C29-C30-C31-C32
33	C	521	LMG	C18-C19-C20-C21
33	C	521	LMG	C33-C34-C35-C36
32	e	102	LMT	C2B-C1B-O1B-C4'
35	h	102	DGD	CAA-CBA-CCA-CDA

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Mol	Chain	Res	Type	Atoms
33	C	521	LMG	C16-C17-C18-C19
32	I	101	LMT	C1-C2-C3-C4
32	t	102	LMT	C2-C1-O1'-C1'
33	c	520	LMG	C34-C35-C36-C37
35	c	518	DGD	C2B-C3B-C4B-C5B
35	C	519	DGD	CBA-CCA-CDA-CEA
26	A	410	SQD	C12-C13-C14-C15
26	a	411	SQD	C9-C10-C11-C12
33	Z	101	LMG	C15-C16-C17-C18
26	a	411	SQD	C17-C18-C19-C20
23	C	508	CLA	C5-C6-C7-C8
33	B	621	LMG	O9-C10-O7-C8
33	c	520	LMG	C4-C5-C6-O5
35	c	517	DGD	CAA-CBA-CCA-CDA
33	Z	101	LMG	C19-C20-C21-C22
33	z	101	LMG	C10-C11-C12-C13
23	C	511	CLA	C4-C3-C5-C6
29	d	405	PL9	C15-C14-C16-C17
29	A	414	PL9	C12-C11-C9-C10
23	B	601	CLA	CBA-CGA-O2A-C1
29	d	405	PL9	C13-C14-C16-C17
33	B	621	LMG	C11-C10-O7-C8
33	m	101	LMG	C39-C40-C41-C42
32	M	101	LMT	C2-C3-C4-C5
33	c	520	LMG	C31-C32-C33-C34
35	C	517	DGD	C4D-C5D-C6D-O5D
26	F	101	SQD	C32-C33-C34-C35
23	C	511	CLA	O1A-CGA-O2A-C1
34	b	622	HTG	S1-C1'-C2'-C3'
33	c	520	LMG	C28-C29-C30-C31
33	m	101	LMG	C35-C36-C37-C38
23	C	510	CLA	C2-C1-O2A-CGA
37	d	406	LHG	C32-C33-C34-C35
37	L	101	LHG	C12-C13-C14-C15
35	c	518	DGD	C9A-CAA-CBA-CCA
26	a	413	SQD	C25-C26-C27-C28
35	H	102	DGD	C7A-C8A-C9A-CAA
23	a	409	CLA	C16-C17-C18-C20
25	d	404	BCR	C23-C24-C25-C26
25	d	404	BCR	C23-C24-C25-C30
25	D	407	BCR	C23-C24-C25-C26
25	D	407	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
25	H	101	BCR	C1-C6-C7-C8
25	H	101	BCR	C5-C6-C7-C8
25	b	619	BCR	C1-C6-C7-C8
25	b	617	BCR	C5-C6-C7-C8
34	b	625	HTG	O5-C5-C6-O6
33	D	415	LMG	C16-C17-C18-C19
23	d	403	CLA	CBA-CGA-O2A-C1
23	c	513	CLA	C13-C15-C16-C17
23	b	613	CLA	C13-C15-C16-C17
33	d	412	LMG	C19-C20-C21-C22
32	e	102	LMT	C4-C5-C6-C7
32	b	621	LMT	C3-C4-C5-C6
33	d	412	LMG	O6-C5-C6-O5
33	m	101	LMG	C14-C15-C16-C17
23	B	601	CLA	C10-C11-C12-C13
37	E	101	LHG	C11-C10-C9-C8
23	b	609	CLA	C4-C3-C5-C6
29	d	405	PL9	C35-C34-C36-C37
23	C	511	CLA	C2-C3-C5-C6
23	b	609	CLA	C2-C3-C5-C6
23	b	606	CLA	C12-C13-C15-C16
23	b	614	CLA	C6-C7-C8-C10
23	B	613	CLA	C11-C10-C8-C7
23	b	601	CLA	C6-C7-C8-C10
23	c	511	CLA	C2-C3-C5-C6
23	C	503	CLA	C12-C13-C15-C16
29	A	414	PL9	C12-C11-C9-C8
23	c	510	CLA	C12-C13-C15-C16
23	c	506	CLA	C2-C3-C5-C6
23	B	601	CLA	O1A-CGA-O2A-C1
23	d	403	CLA	O1A-CGA-O2A-C1
23	B	601	CLA	C15-C16-C17-C18
35	c	517	DGD	C2A-C1A-O1G-C1G
23	b	601	CLA	CBA-CGA-O2A-C1
26	B	620	SQD	C34-C35-C36-C37
37	D	410	LHG	C13-C14-C15-C16
23	b	614	CLA	C15-C16-C17-C18
23	A	404	CLA	C13-C15-C16-C17
23	A	408	CLA	C10-C11-C12-C13
23	b	616	CLA	C5-C6-C7-C8
33	D	415	LMG	C30-C31-C32-C33
33	D	415	LMG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
37	e	101	LHG	C11-C12-C13-C14
33	a	419	LMG	C30-C31-C32-C33
23	C	510	CLA	C3-C5-C6-C7
26	F	101	SQD	C29-C30-C31-C32
23	C	507	CLA	C16-C17-C18-C20
35	C	518	DGD	O6E-C1E-O5D-C6D
32	m	103	LMT	O5'-C1'-O1'-C1
32	a	414	LMT	C2-C3-C4-C5
26	F	101	SQD	C23-C24-C25-C26
33	a	419	LMG	C11-C10-O7-C8
33	m	101	LMG	C11-C10-O7-C8
37	l	101	LHG	C16-C17-C18-C19
37	L	101	LHG	C24-C25-C26-C27
35	c	518	DGD	C7A-C8A-C9A-CAA
26	b	620	SQD	C33-C34-C35-C36
33	m	101	LMG	O9-C10-O7-C8
23	C	503	CLA	C3-C5-C6-C7
35	c	518	DGD	C7B-C8B-C9B-CAB
26	A	410	SQD	O6-C44-C45-O47
33	Z	101	LMG	O6-C5-C6-O5
32	I	101	LMT	O5'-C5'-C6'-O6'
23	C	513	CLA	CBA-CGA-O2A-C1
23	C	512	CLA	CBD-CGD-O2D-CED
26	f	102	SQD	C29-C30-C31-C32
35	C	517	DGD	C5B-C6B-C7B-C8B
34	b	623	HTG	O5-C5-C6-O6
23	b	605	CLA	C8-C10-C11-C12
23	B	615	CLA	C5-C6-C7-C8
23	c	511	CLA	C4-C3-C5-C6
23	c	506	CLA	C4-C3-C5-C6
29	a	416	PL9	C4-C3-C7-C8
23	C	511	CLA	C14-C13-C15-C16
23	b	614	CLA	C6-C7-C8-C9
23	b	601	CLA	C6-C7-C8-C9
23	D	406	CLA	C11-C10-C8-C9
26	F	101	SQD	C24-C25-C26-C27
32	b	621	LMT	C4-C5-C6-C7
33	m	101	LMG	C30-C31-C32-C33
33	C	520	LMG	C36-C37-C38-C39
25	y	101	BCR	C37-C22-C23-C24
35	C	518	DGD	C7B-C8B-C9B-CAB
24	A	353	PHO	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
35	C	519	DGD	CAB-CBB-CCB-CDB
23	a	406	CLA	C1A-C2A-CAA-CBA
23	a	409	CLA	C16-C17-C18-C19
23	c	503	CLA	C16-C17-C18-C19
33	a	419	LMG	O9-C10-O7-C8
35	c	519	DGD	C9A-CAA-CBA-CCA
23	b	613	CLA	C8-C10-C11-C12
23	c	514	CLA	C10-C11-C12-C13
37	D	410	LHG	C4-O6-P-O3
33	B	621	LMG	C34-C35-C36-C37
23	b	601	CLA	O1A-CGA-O2A-C1
33	D	415	LMG	O6-C5-C6-O5
37	d	408	LHG	C33-C34-C35-C36
26	a	413	SQD	C12-C13-C14-C15
35	c	517	DGD	C1A-C2A-C3A-C4A
32	I	101	LMT	C4-C5-C6-C7
37	d	406	LHG	C24-C25-C26-C27
37	l	101	LHG	C12-C13-C14-C15
23	c	512	CLA	CBD-CGD-O2D-CED
32	E	102	LMT	C2B-C1B-O1B-C4'
26	A	410	SQD	C11-C10-C9-C8
26	a	411	SQD	C27-C28-C29-C30
26	a	411	SQD	C34-C35-C36-C37
33	C	501	LMG	C36-C37-C38-C39
26	B	620	SQD	C16-C17-C18-C19
37	d	407	LHG	C31-C32-C33-C34
33	a	419	LMG	C29-C30-C31-C32
34	b	625	HTG	C3'-C4'-C5'-C6'
35	C	518	DGD	C8B-C9B-CAB-CBB
23	C	511	CLA	C16-C17-C18-C19
35	c	517	DGD	O6E-C5E-C6E-O5E
23	b	601	CLA	C3-C5-C6-C7
32	E	102	LMT	O1'-C1-C2-C3
34	B	626	HTG	C4'-C5'-C6'-C7'
37	e	101	LHG	C4-C5-C6-O8
26	B	620	SQD	C44-C45-C46-O48
26	A	410	SQD	O6-C44-C45-C46
37	E	101	LHG	C4-C5-C6-O8
26	b	620	SQD	C44-C45-C46-O48
26	A	412	SQD	O6-C44-C45-C46
35	C	518	DGD	C2G-C3G-O3G-C1D
35	c	518	DGD	C5D-C6D-O5D-C1E

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Mol	Chain	Res	Type	Atoms
26	B	620	SQD	C11-C12-C13-C14
34	B	622	HTG	C2'-C3'-C4'-C5'
23	c	507	CLA	C15-C16-C17-C18
26	A	410	SQD	C18-C19-C20-C21
33	m	101	LMG	C37-C38-C39-C40
35	h	102	DGD	O2G-C1B-C2B-C3B
23	b	601	CLA	CAA-CBA-CGA-O2A
35	C	517	DGD	O6E-C5E-C6E-O5E
23	C	513	CLA	O1A-CGA-O2A-C1
26	F	101	SQD	C11-C10-C9-C8
33	C	501	LMG	C29-C30-C31-C32
26	b	620	SQD	C13-C14-C15-C16
37	D	411	LHG	C27-C28-C29-C30
27	a	412	GOL	O2-C2-C3-O3
32	E	102	LMT	O5B-C1B-O1B-C4'
35	c	517	DGD	CDB-CEB-CFB-CGB
37	l	101	LHG	C13-C14-C15-C16
34	B	626	HTG	O5-C5-C6-O6
29	d	405	PL9	C33-C34-C36-C37
23	c	512	CLA	CBA-CGA-O2A-C1
33	c	520	LMG	C33-C34-C35-C36
37	D	409	LHG	C16-C17-C18-C19
23	A	408	CLA	CBD-CGD-O2D-CED
23	B	602	CLA	C15-C16-C17-C18
35	c	519	DGD	CAA-CBA-CCA-CDA
34	b	625	HTG	C4'-C5'-C6'-C7'
33	D	415	LMG	C36-C37-C38-C39
26	B	620	SQD	C26-C27-C28-C29
23	B	604	CLA	C13-C15-C16-C17
33	B	621	LMG	C14-C15-C16-C17
37	E	101	LHG	C14-C15-C16-C17
23	C	507	CLA	C16-C17-C18-C19
23	b	611	CLA	C8-C10-C11-C12
32	M	101	LMT	O1'-C1-C2-C3
35	c	517	DGD	O1A-C1A-O1G-C1G
34	B	623	HTG	C1'-C2'-C3'-C4'
23	c	508	CLA	C5-C6-C7-C8
35	C	517	DGD	C2E-C1E-O5D-C6D
26	A	412	SQD	C2-C1-O6-C44
32	E	102	LMT	C3-C4-C5-C6
37	D	410	LHG	C28-C29-C30-C31
23	c	512	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
37	D	409	LHG	C25-C26-C27-C28
23	C	511	CLA	C12-C13-C15-C16
23	b	614	CLA	C12-C13-C15-C16
23	B	615	CLA	C11-C12-C13-C15
23	B	605	CLA	C6-C7-C8-C10
23	B	606	CLA	C11-C10-C8-C7
23	a	407	CLA	C11-C12-C13-C15
23	B	616	CLA	C12-C13-C15-C16
23	D	406	CLA	C11-C10-C8-C7
23	C	505	CLA	C12-C13-C15-C16
23	d	403	CLA	C12-C13-C15-C16
26	f	102	SQD	C25-C26-C27-C28
23	B	606	CLA	C11-C10-C8-C9
23	a	407	CLA	C11-C12-C13-C14
23	B	616	CLA	C14-C13-C15-C16
23	C	505	CLA	C14-C13-C15-C16
23	d	403	CLA	C14-C13-C15-C16
23	B	614	CLA	C14-C13-C15-C16
26	A	410	SQD	C16-C17-C18-C19
26	b	620	SQD	C24-C23-O48-C46
23	B	605	CLA	C13-C15-C16-C17
23	b	604	CLA	C13-C15-C16-C17
23	c	502	CLA	O1D-CGD-O2D-CED
25	t	103	BCR	C7-C8-C9-C34
33	C	520	LMG	C37-C38-C39-C40
38	e	87	HEM	C2A-CAA-CBA-CGA
26	b	620	SQD	C18-C19-C20-C21
37	l	101	LHG	O6-C4-C5-C6
35	c	517	DGD	C7B-C8B-C9B-CAB
33	B	621	LMG	C28-C29-C30-C31
32	M	103	LMT	O5B-C1B-O1B-C4'
32	M	101	LMT	C9-C10-C11-C12
35	C	518	DGD	CCB-CDB-CEB-CFB
23	A	408	CLA	CBA-CGA-O2A-C1
37	D	411	LHG	C24-C23-O8-C6
23	B	606	CLA	C15-C16-C17-C18
23	C	509	CLA	C10-C11-C12-C13
37	E	101	LHG	C25-C26-C27-C28
29	d	405	PL9	C45-C44-C46-C47
23	b	601	CLA	C4-C3-C5-C6
29	A	414	PL9	C25-C24-C26-C27
29	A	414	PL9	C45-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
29	A	414	PL9	C43-C44-C46-C47
33	d	412	LMG	C28-C29-C30-C31
37	E	101	LHG	C7-C8-C9-C10
32	M	103	LMT	C11-C10-C9-C8
23	a	406	CLA	C15-C16-C17-C18
37	d	406	LHG	C25-C26-C27-C28
37	d	407	LHG	C30-C31-C32-C33
26	a	413	SQD	C24-C23-O48-C46
23	b	609	CLA	C3A-C2A-CAA-CBA
23	B	609	CLA	C3A-C2A-CAA-CBA
23	b	616	CLA	C15-C16-C17-C18
37	D	410	LHG	C26-C27-C28-C29
33	Z	101	LMG	C17-C18-C19-C20
35	c	518	DGD	CBA-CCA-CDA-CEA
26	f	102	SQD	O6-C44-C45-C46
26	f	102	SQD	C44-C45-C46-O48
35	H	102	DGD	O1G-C1G-C2G-C3G
33	c	521	LMG	C7-C8-C9-O8
32	D	404	LMT	C4'-C5'-C6'-O6'
33	C	501	LMG	C37-C38-C39-C40
33	c	521	LMG	C29-C30-C31-C32
26	a	411	SQD	C10-C11-C12-C13
24	a	408	PHO	O2A-C1-C2-C3
23	c	509	CLA	C5-C6-C7-C8
23	C	506	CLA	C4-C3-C5-C6
32	e	102	LMT	O5B-C1B-O1B-C4'
23	b	601	CLA	C2-C3-C5-C6
23	C	506	CLA	C2-C3-C5-C6
33	c	520	LMG	C32-C33-C34-C35
35	c	518	DGD	CAA-CBA-CCA-CDA
37	D	409	LHG	O1-C1-C2-O2
27	B	624	GOL	O1-C1-C2-O2
32	a	420	LMT	C6-C7-C8-C9
37	D	411	LHG	C24-C25-C26-C27
35	C	518	DGD	CDA-CEA-CFA-CGA
33	a	419	LMG	C35-C36-C37-C38
26	b	620	SQD	O47-C45-C46-O48
23	c	511	CLA	CBA-CGA-O2A-C1
26	a	413	SQD	C31-C32-C33-C34
35	C	517	DGD	C1B-C2B-C3B-C4B
35	c	517	DGD	O6E-C1E-O5D-C6D
26	A	412	SQD	O5-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
33	a	419	LMG	O6-C5-C6-O5
33	z	101	LMG	C12-C13-C14-C15
37	L	101	LHG	C14-C15-C16-C17
23	C	513	CLA	C2-C1-O2A-CGA
23	b	608	CLA	C2-C1-O2A-CGA
23	B	608	CLA	C2-C1-O2A-CGA
29	d	405	PL9	C43-C44-C46-C47
35	C	517	DGD	C6A-C7A-C8A-C9A
34	c	522	HTG	C2'-C3'-C4'-C5'
33	D	415	LMG	C35-C36-C37-C38
32	M	103	LMT	C2B-C1B-O1B-C4'
23	b	606	CLA	C11-C10-C8-C9
23	c	506	CLA	C11-C12-C13-C14
33	C	520	LMG	C18-C19-C20-C21
35	H	102	DGD	C5B-C6B-C7B-C8B
37	D	410	LHG	C17-C18-C19-C20
37	d	408	LHG	C2-C3-O3-P
37	D	411	LHG	C2-C3-O3-P
35	C	517	DGD	C3B-C4B-C5B-C6B
32	a	414	LMT	C6-C7-C8-C9
25	B	617	BCR	C1-C6-C7-C8
25	B	617	BCR	C5-C6-C7-C8
23	B	607	CLA	C10-C11-C12-C13
32	b	627	LMT	C1-C2-C3-C4
35	c	517	DGD	C2A-C3A-C4A-C5A
25	B	619	BCR	C7-C8-C9-C10
25	y	101	BCR	C21-C22-C23-C24
25	T	101	BCR	C11-C12-C13-C14
33	m	101	LMG	C22-C23-C24-C25
33	C	520	LMG	C16-C17-C18-C19
23	B	615	CLA	C16-C17-C18-C20
26	A	412	SQD	C15-C16-C17-C18
23	A	408	CLA	O1D-CGD-O2D-CED
35	C	518	DGD	CBB-CCB-CDB-CEB
37	d	408	LHG	C25-C26-C27-C28
23	C	512	CLA	O1D-CGD-O2D-CED
32	t	102	LMT	O1'-C1-C2-C3
37	E	101	LHG	C10-C11-C12-C13
23	a	409	CLA	C11-C10-C8-C7
23	A	406	CLA	C12-C13-C15-C16
23	a	406	CLA	C11-C12-C13-C15
23	B	602	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
23	C	514	CLA	C11-C10-C8-C7
23	C	507	CLA	C11-C12-C13-C15
23	B	614	CLA	C12-C13-C15-C16
23	c	506	CLA	C11-C12-C13-C15
33	B	621	LMG	C18-C19-C20-C21
23	b	611	CLA	C13-C15-C16-C17
23	D	406	CLA	C8-C10-C11-C12
23	B	615	CLA	C16-C17-C18-C19
33	a	419	LMG	C33-C34-C35-C36
26	A	412	SQD	C29-C30-C31-C32
23	C	511	CLA	C8-C10-C11-C12
23	A	408	CLA	O1A-CGA-O2A-C1
35	H	102	DGD	CBA-CCA-CDA-CEA
32	b	627	LMT	C11-C10-C9-C8
35	h	102	DGD	CBA-CCA-CDA-CEA
35	C	519	DGD	C2A-C1A-O1G-C1G
35	c	519	DGD	C2A-C1A-O1G-C1G
23	c	513	CLA	CBA-CGA-O2A-C1
37	d	406	LHG	C33-C34-C35-C36
35	C	519	DGD	C6B-C7B-C8B-C9B
23	C	507	CLA	C5-C6-C7-C8
26	b	620	SQD	O10-C23-O48-C46
23	b	610	CLA	CAD-CBD-CGD-O2D
23	B	610	CLA	CAD-CBD-CGD-O2D
23	c	504	CLA	CAD-CBD-CGD-O2D
24	A	353	PHO	CAD-CBD-CGD-O2D
23	C	513	CLA	CAD-CBD-CGD-O2D
23	c	511	CLA	CAD-CBD-CGD-O2D
23	D	406	CLA	CAD-CBD-CGD-O2D
26	b	620	SQD	C46-C45-O47-C7
23	c	502	CLA	CAD-CBD-CGD-O2D
23	b	616	CLA	CAD-CBD-CGD-O2D
23	b	610	CLA	C15-C16-C17-C18
23	b	615	CLA	C10-C11-C12-C13
32	M	103	LMT	O5B-C5B-C6B-O6B
35	C	517	DGD	O6E-C1E-O5D-C6D
23	B	602	CLA	C13-C15-C16-C17
26	a	413	SQD	O6-C44-C45-C46
23	c	513	CLA	O1A-CGA-O2A-C1
34	b	622	HTG	O5-C5-C6-O6
35	C	517	DGD	C7A-C8A-C9A-CAA
23	c	508	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	B	607	CLA	CHA-CBD-CGD-O1D
23	b	606	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O1D
23	b	601	CLA	CHA-CBD-CGD-O1D
23	b	601	CLA	CHA-CBD-CGD-O2D
23	c	509	CLA	CHA-CBD-CGD-O2D
23	B	606	CLA	CHA-CBD-CGD-O2D
23	C	509	CLA	CHA-CBD-CGD-O2D
23	B	601	CLA	CHA-CBD-CGD-O1D
23	B	601	CLA	CHA-CBD-CGD-O2D
23	C	503	CLA	CHA-CBD-CGD-O1D
23	C	503	CLA	CHA-CBD-CGD-O2D
37	d	407	LHG	C26-C27-C28-C29
26	a	413	SQD	O10-C23-O48-C46
37	D	411	LHG	O10-C23-O8-C6
35	c	517	DGD	C2E-C1E-O5D-C6D
33	C	501	LMG	O1-C7-C8-O7
37	e	101	LHG	O7-C5-C6-O8
35	H	102	DGD	O1G-C1G-C2G-O2G
26	B	620	SQD	O47-C45-C46-O48
37	E	101	LHG	O7-C5-C6-O8
26	b	620	SQD	C9-C10-C11-C12
35	h	102	DGD	C4E-C5E-C6E-O5E
35	c	519	DGD	O1A-C1A-O1G-C1G
37	l	101	LHG	C27-C28-C29-C30
27	C	523	GOL	O1-C1-C2-O2
27	B	625	GOL	O1-C1-C2-O2
29	D	408	PL9	C45-C44-C46-C47
23	B	615	CLA	C4-C3-C5-C6
29	a	416	PL9	C12-C11-C9-C10
33	c	520	LMG	C29-C30-C31-C32
35	C	519	DGD	O1A-C1A-O1G-C1G
23	c	511	CLA	O1A-CGA-O2A-C1
29	A	414	PL9	C4-C3-C7-C8
23	a	409	CLA	C11-C10-C8-C9
23	a	406	CLA	C11-C12-C13-C14
23	B	602	CLA	C11-C12-C13-C14
23	C	514	CLA	C11-C10-C8-C9
23	c	510	CLA	C11-C12-C13-C14
32	t	101	LMT	C4-C5-C6-C7
23	b	604	CLA	C2C-C3C-CAC-CBC
23	B	601	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
35	C	518	DGD	CCA-CDA-CEA-CFA
33	c	520	LMG	C35-C36-C37-C38
37	L	101	LHG	C35-C36-C37-C38
37	e	101	LHG	C24-C25-C26-C27
23	b	615	CLA	C5-C6-C7-C8
37	e	101	LHG	C3-O3-P-O6
35	h	102	DGD	C6A-C7A-C8A-C9A
23	b	607	CLA	C3-C5-C6-C7
23	B	615	CLA	C2-C3-C5-C6
37	d	407	LHG	C13-C14-C15-C16
37	L	101	LHG	C3-O3-P-O5
37	L	101	LHG	C4-O6-P-O5
37	D	410	LHG	C4-O6-P-O5
35	c	517	DGD	C5B-C6B-C7B-C8B
37	D	409	LHG	C24-C25-C26-C27
37	E	101	LHG	C15-C16-C17-C18
35	C	517	DGD	CAA-CBA-CCA-CDA
37	D	411	LHG	C17-C18-C19-C20
23	B	607	CLA	CAD-CBD-CGD-O1D
23	b	609	CLA	CAD-CBD-CGD-O1D
26	B	620	SQD	C5-C6-S-O7
23	b	601	CLA	CAD-CBD-CGD-O1D
23	c	505	CLA	CAD-CBD-CGD-O1D
23	B	601	CLA	CAD-CBD-CGD-O1D
23	c	507	CLA	CAD-CBD-CGD-O1D
23	C	503	CLA	CAD-CBD-CGD-O1D
23	c	503	CLA	CAD-CBD-CGD-O1D
33	C	501	LMG	O8-C28-C29-C30
23	D	405	CLA	C8-C10-C11-C12
35	C	519	DGD	O6D-C5D-C6D-O5D
34	B	622	HTG	C4'-C5'-C6'-C7'
23	b	606	CLA	C11-C10-C8-C7
23	d	402	CLA	C11-C12-C13-C15
23	C	513	CLA	C6-C7-C8-C10
23	B	604	CLA	C11-C12-C13-C15
37	l	101	LHG	O6-C4-C5-O7
23	b	608	CLA	C12-C13-C15-C16
23	B	601	CLA	C11-C10-C8-C7
23	c	507	CLA	C6-C7-C8-C10
23	b	615	CLA	C12-C13-C15-C16
23	c	510	CLA	C6-C7-C8-C10
23	c	510	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
23	C	507	CLA	C6-C7-C8-C10
23	b	616	CLA	C6-C7-C8-C10
23	B	612	CLA	C10-C11-C12-C13
35	H	102	DGD	O2G-C1B-C2B-C3B
37	d	408	LHG	C9-C10-C11-C12
23	B	611	CLA	C8-C10-C11-C12
33	c	520	LMG	C30-C31-C32-C33
35	H	102	DGD	CDA-CEA-CFA-CGA
23	B	608	CLA	C3-C5-C6-C7
37	d	406	LHG	C7-C8-C9-C10
33	a	419	LMG	C10-C11-C12-C13
33	C	501	LMG	O1-C7-C8-C9
26	f	102	SQD	O47-C45-C46-O48
33	c	520	LMG	C21-C22-C23-C24
37	E	101	LHG	C26-C27-C28-C29
35	C	518	DGD	C5D-C6D-O5D-C1E
35	c	518	DGD	C2G-C3G-O3G-C1D
23	A	405	CLA	C13-C15-C16-C17
35	h	102	DGD	C9B-CAB-CBB-CCB
24	a	353	PHO	C8-C10-C11-C12
23	b	615	CLA	C13-C15-C16-C17
23	B	604	CLA	C11-C12-C13-C14
23	A	406	CLA	C14-C13-C15-C16
23	C	506	CLA	C14-C13-C15-C16
23	c	505	CLA	C14-C13-C15-C16
23	C	507	CLA	C11-C12-C13-C14
37	d	408	LHG	O10-C23-O8-C6
35	C	518	DGD	C9B-CAB-CBB-CCB
32	m	103	LMT	C7-C8-C9-C10
23	C	509	CLA	C13-C15-C16-C17
33	B	621	LMG	C33-C34-C35-C36
23	a	409	CLA	C3-C5-C6-C7
23	c	511	CLA	C13-C15-C16-C17
23	B	613	CLA	C13-C15-C16-C17
23	c	512	CLA	O1D-CGD-O2D-CED
37	D	411	LHG	C25-C26-C27-C28
26	B	620	SQD	C46-C45-O47-C7
37	E	101	LHG	C1-C2-C3-O3
23	b	609	CLA	O1A-CGA-O2A-C1
23	A	408	CLA	C2-C1-O2A-CGA
23	c	514	CLA	C2-C1-O2A-CGA
26	f	102	SQD	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
32	b	627	LMT	C4-C5-C6-C7
37	d	408	LHG	C30-C31-C32-C33
26	A	410	SQD	C14-C15-C16-C17
23	D	406	CLA	C4-C3-C5-C6
25	y	101	BCR	C23-C24-C25-C26
25	y	101	BCR	C23-C24-C25-C30
23	c	507	CLA	C13-C15-C16-C17
23	c	508	CLA	C2A-CAA-CBA-CGA
26	F	101	SQD	C2-C1-O6-C44
23	B	604	CLA	C2C-C3C-CAC-CBC
32	m	103	LMT	C4'-C5'-C6'-O6'
26	A	412	SQD	C32-C33-C34-C35
37	d	408	LHG	C24-C23-O8-C6
37	d	406	LHG	C3-O3-P-O6
37	d	407	LHG	C4-O6-P-O3
37	E	101	LHG	C4-O6-P-O3
37	D	409	LHG	C12-C13-C14-C15
35	C	518	DGD	CAB-CBB-CCB-CDB
26	a	413	SQD	C27-C28-C29-C30
23	C	513	CLA	C11-C10-C8-C7
29	D	408	PL9	C13-C14-C16-C17
29	D	408	PL9	C43-C44-C46-C47
23	C	506	CLA	C12-C13-C15-C16
23	c	505	CLA	C12-C13-C15-C16
23	b	604	CLA	C12-C13-C15-C16
29	a	416	PL9	C12-C11-C9-C8
23	c	514	CLA	C12-C13-C15-C16
33	C	520	LMG	C31-C32-C33-C34
33	C	520	LMG	O7-C10-C11-C12
24	a	353	PHO	C4C-C3C-CAC-CBC
32	M	103	LMT	C4B-C5B-C6B-O6B
23	d	402	CLA	C11-C12-C13-C14
23	b	608	CLA	C14-C13-C15-C16
23	b	615	CLA	C14-C13-C15-C16
23	b	613	CLA	C14-C13-C15-C16
25	T	101	BCR	C13-C14-C15-C16
23	D	405	CLA	C16-C17-C18-C20
35	C	519	DGD	C1B-C2B-C3B-C4B
35	c	519	DGD	C7B-C8B-C9B-CAB
35	c	517	DGD	CCB-CDB-CEB-CFB
32	M	103	LMT	C4'-C5'-C6'-O6'
26	a	413	SQD	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
37	l	101	LHG	C28-C29-C30-C31
33	a	419	LMG	C34-C35-C36-C37
37	d	408	LHG	C32-C33-C34-C35
26	A	410	SQD	C13-C14-C15-C16
37	D	411	LHG	C29-C30-C31-C32
37	D	411	LHG	O1-C1-C2-C3
34	b	625	HTG	C1'-C2'-C3'-C4'
37	D	411	LHG	C33-C34-C35-C36
33	m	101	LMG	C13-C14-C15-C16
32	b	621	LMT	C3'-C4'-O1B-C1B
26	a	413	SQD	C10-C11-C12-C13
26	A	412	SQD	C30-C31-C32-C33
37	e	101	LHG	C23-C24-C25-C26
23	b	610	CLA	C16-C17-C18-C19
23	b	609	CLA	CBA-CGA-O2A-C1
37	L	101	LHG	C11-C12-C13-C14
34	b	622	HTG	C2'-C3'-C4'-C5'
33	C	501	LMG	C30-C31-C32-C33
23	C	512	CLA	O1A-CGA-O2A-C1
37	d	407	LHG	C24-C23-O8-C6
35	h	102	DGD	O1B-C1B-C2B-C3B
32	M	101	LMT	O5'-C1'-O1'-C1
35	c	518	DGD	O6E-C1E-O5D-C6D
33	Z	101	LMG	O6-C1-O1-C7
23	C	508	CLA	C13-C15-C16-C17
37	l	101	LHG	C35-C36-C37-C38
23	A	408	CLA	C5-C6-C7-C8
35	C	517	DGD	C3A-C4A-C5A-C6A
37	D	410	LHG	C9-C10-C11-C12
37	d	407	LHG	C9-C10-C11-C12
33	c	520	LMG	O6-C5-C6-O5
29	D	408	PL9	C15-C14-C16-C17
23	b	603	CLA	C13-C15-C16-C17
24	a	408	PHO	C2-C3-C5-C6
23	b	601	CLA	C10-C11-C12-C13
23	c	513	CLA	C2-C1-O2A-CGA
26	A	410	SQD	C32-C33-C34-C35
35	c	518	DGD	C2E-C1E-O5D-C6D
37	d	407	LHG	O10-C23-O8-C6
32	m	103	LMT	C11-C10-C9-C8
23	b	601	CLA	CAA-CBA-CGA-O1A
23	C	507	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
35	H	102	DGD	CDB-CEB-CFB-CGB
35	C	519	DGD	C7B-C8B-C9B-CAB
26	B	620	SQD	C31-C32-C33-C34
23	c	514	CLA	O1D-CGD-O2D-CED
35	c	519	DGD	C3B-C4B-C5B-C6B
37	D	410	LHG	C33-C34-C35-C36
23	b	601	CLA	C11-C10-C8-C9
23	a	407	CLA	C14-C13-C15-C16
33	B	621	LMG	C15-C16-C17-C18
24	a	353	PHO	NC-C1C-CHC-C4B
35	C	518	DGD	C9A-CAA-CBA-CCA
23	a	405	CLA	C2A-CAA-CBA-CGA
37	D	411	LHG	C15-C16-C17-C18
24	A	407	PHO	O2A-C1-C2-C3
26	F	101	SQD	O5-C1-O6-C44
25	D	407	BCR	C7-C8-C9-C34
29	a	416	PL9	C2-C3-C7-C8
34	b	623	HTG	C3'-C4'-C5'-C6'
24	a	408	PHO	C4-C3-C5-C6
29	a	416	PL9	C20-C19-C21-C22
23	b	609	CLA	C1A-C2A-CAA-CBA
23	c	512	CLA	C1A-C2A-CAA-CBA
23	a	407	CLA	C1A-C2A-CAA-CBA
23	C	502	CLA	C1A-C2A-CAA-CBA
26	a	413	SQD	C13-C14-C15-C16
23	B	616	CLA	C6-C7-C8-C10
26	F	101	SQD	C27-C28-C29-C30
33	C	520	LMG	C30-C31-C32-C33
33	d	412	LMG	C10-C11-C12-C13
33	D	415	LMG	C37-C38-C39-C40
23	A	404	CLA	C2A-CAA-CBA-CGA
23	C	502	CLA	C2A-CAA-CBA-CGA
33	C	501	LMG	C28-C29-C30-C31
26	A	412	SQD	C19-C20-C21-C22
33	c	520	LMG	C10-C11-C12-C13
23	b	601	CLA	C8-C10-C11-C12
32	e	102	LMT	C4'-C5'-C6'-O6'
37	D	409	LHG	C26-C27-C28-C29
33	Z	101	LMG	C29-C28-O8-C9
33	c	521	LMG	O7-C8-C9-O8
26	a	411	SQD	O6-C44-C45-O47
23	C	512	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	k	101	BCR	C9-C10-C11-C12
24	a	408	PHO	C8-C10-C11-C12
26	b	620	SQD	C35-C36-C37-C38
35	H	102	DGD	C7B-C8B-C9B-CAB
37	l	101	LHG	C34-C35-C36-C37
23	C	506	CLA	C15-C16-C17-C18
23	A	408	CLA	C4-C3-C5-C6
29	a	416	PL9	C45-C44-C46-C47
23	B	613	CLA	C2-C1-O2A-CGA
23	C	514	CLA	C2-C1-O2A-CGA
23	c	507	CLA	C2-C1-O2A-CGA
23	b	613	CLA	C2-C1-O2A-CGA
23	a	407	CLA	C10-C11-C12-C13
35	C	519	DGD	O6E-C5E-C6E-O5E
23	c	514	CLA	CBD-CGD-O2D-CED
23	B	601	CLA	C3-C5-C6-C7
33	C	520	LMG	C21-C22-C23-C24
35	C	519	DGD	C3B-C4B-C5B-C6B
23	D	405	CLA	C16-C17-C18-C19
35	c	519	DGD	C8A-C9A-CAA-CBA
23	b	604	CLA	C4C-C3C-CAC-CBC
25	c	515	BCR	C1-C6-C7-C8
25	C	515	BCR	C1-C6-C7-C8
25	c	516	BCR	C1-C6-C7-C8
25	c	516	BCR	C23-C24-C25-C30
25	C	516	BCR	C1-C6-C7-C8
25	D	407	BCR	C1-C6-C7-C8
25	h	101	BCR	C23-C24-C25-C30
26	a	411	SQD	O6-C44-C45-C46
27	B	625	GOL	O1-C1-C2-C3
32	b	627	LMT	C5-C6-C7-C8
32	a	414	LMT	C3-C4-C5-C6
26	A	412	SQD	C25-C26-C27-C28
25	k	101	BCR	C19-C20-C21-C22
29	A	414	PL9	C23-C24-C26-C27
23	b	605	CLA	C13-C15-C16-C17
35	c	517	DGD	C5D-C6D-O5D-C1E
37	l	101	LHG	C25-C26-C27-C28
23	a	406	CLA	C2C-C3C-CAC-CBC
37	D	409	LHG	C17-C18-C19-C20
37	D	411	LHG	C26-C27-C28-C29
23	B	604	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
23	B	601	CLA	C2A-CAA-CBA-CGA
34	B	623	HTG	C4-C5-C6-O6
33	a	419	LMG	C31-C32-C33-C34
33	B	621	LMG	O8-C28-C29-C30
23	B	604	CLA	C4-C3-C5-C6
23	C	511	CLA	C11-C12-C13-C15
29	a	416	PL9	C18-C19-C21-C22
23	b	613	CLA	C11-C12-C13-C15
32	a	414	LMT	C4-C5-C6-C7
34	b	623	HTG	S1-C1'-C2'-C3'
26	A	410	SQD	O47-C7-C8-C9
23	b	612	CLA	C13-C15-C16-C17
23	b	610	CLA	C16-C17-C18-C20
23	C	511	CLA	CAA-CBA-CGA-O2A
29	D	408	PL9	C35-C34-C36-C37
29	A	414	PL9	C30-C29-C31-C32
26	a	413	SQD	C30-C31-C32-C33
32	a	414	LMT	O5B-C5B-C6B-O6B
23	B	613	CLA	CAA-CBA-CGA-O2A
37	l	101	LHG	O7-C7-C8-C9
23	b	614	CLA	C14-C13-C15-C16
23	c	507	CLA	C11-C12-C13-C14
23	c	510	CLA	C6-C7-C8-C9
23	C	507	CLA	C6-C7-C8-C9
23	c	514	CLA	C14-C13-C15-C16
34	b	622	HTG	C3'-C4'-C5'-C6'
37	d	407	LHG	C28-C29-C30-C31
26	b	620	SQD	C11-C10-C9-C8
23	b	613	CLA	CAA-CBA-CGA-O2A
23	B	612	CLA	CAD-CBD-CGD-O2D
23	B	604	CLA	CAD-CBD-CGD-O2D
23	B	603	CLA	CAD-CBD-CGD-O2D
24	a	408	PHO	CAD-CBD-CGD-O2D
24	A	407	PHO	CAD-CBD-CGD-O2D
23	b	612	CLA	CAD-CBD-CGD-O2D
23	C	510	CLA	CAD-CBD-CGD-O2D
23	b	604	CLA	CAD-CBD-CGD-O2D
32	a	420	LMT	C4-C5-C6-C7
23	d	402	CLA	C2-C1-O2A-CGA
23	C	505	CLA	C2-C1-O2A-CGA
23	b	616	CLA	C4-C3-C5-C6
23	c	513	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
23	b	614	CLA	C3-C5-C6-C7
29	a	416	PL9	C43-C44-C46-C47
23	b	616	CLA	C2-C3-C5-C6
33	c	520	LMG	O7-C10-C11-C12
35	c	517	DGD	CCA-CDA-CEA-CFA
33	B	621	LMG	C35-C36-C37-C38
32	e	102	LMT	C3-C4-C5-C6
25	D	407	BCR	C7-C8-C9-C10
37	d	407	LHG	C32-C33-C34-C35
33	m	101	LMG	C21-C22-C23-C24
33	m	101	LMG	C16-C17-C18-C19
23	B	605	CLA	C8-C10-C11-C12
23	B	602	CLA	O2A-C1-C2-C3
37	D	409	LHG	C33-C34-C35-C36
26	f	102	SQD	O47-C7-C8-C9
23	A	406	CLA	C3-C5-C6-C7
33	C	501	LMG	C21-C22-C23-C24
23	c	508	CLA	CHA-CBD-CGD-O2D
23	B	607	CLA	CHA-CBD-CGD-O2D
23	b	606	CLA	CHA-CBD-CGD-O2D
23	C	508	CLA	CHA-CBD-CGD-O2D
23	C	513	CLA	CHA-CBD-CGD-O2D
23	A	406	CLA	CHA-CBD-CGD-O1D
23	A	406	CLA	CHA-CBD-CGD-O2D
24	a	353	PHO	CHA-CBD-CGD-O2D
23	a	406	CLA	CHA-CBD-CGD-O1D
23	a	406	CLA	CHA-CBD-CGD-O2D
23	c	505	CLA	CHA-CBD-CGD-O1D
23	A	405	CLA	CHA-CBD-CGD-O1D
23	A	405	CLA	CHA-CBD-CGD-O2D
23	c	503	CLA	CHA-CBD-CGD-O1D
23	c	510	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O2D
23	a	405	CLA	C15-C16-C17-C18
37	d	408	LHG	C26-C27-C28-C29
32	M	101	LMT	C2'-C1'-O1'-C1
23	C	504	CLA	C15-C16-C17-C18
23	b	612	CLA	CAA-CBA-CGA-O2A
23	b	602	CLA	C10-C11-C12-C13
23	D	406	CLA	C10-C11-C12-C13
33	D	415	LMG	O7-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
23	c	513	CLA	CAA-CBA-CGA-O2A
24	A	353	PHO	C4C-C3C-CAC-CBC
33	Z	101	LMG	O7-C10-C11-C12
32	t	102	LMT	C5-C6-C7-C8
23	c	507	CLA	C11-C12-C13-C15
23	b	607	CLA	C12-C13-C15-C16
35	c	517	DGD	O2G-C1B-C2B-C3B
23	c	511	CLA	CAA-CBA-CGA-O2A
26	b	620	SQD	O48-C23-C24-C25
37	l	101	LHG	C32-C33-C34-C35
23	B	613	CLA	C11-C10-C8-C9
23	b	604	CLA	C14-C13-C15-C16
23	b	616	CLA	C11-C12-C13-C14
26	B	620	SQD	C5-C6-S-O8
23	B	611	CLA	C16-C17-C18-C20
34	C	522	HTG	C4-C5-C6-O6
26	A	412	SQD	C26-C27-C28-C29
23	B	610	CLA	C2A-CAA-CBA-CGA
29	D	408	PL9	C36-C37-C38-C39
26	f	102	SQD	O49-C7-C8-C9
35	C	518	DGD	C8A-C9A-CAA-CBA
25	K	102	BCR	C7-C8-C9-C10
23	B	609	CLA	C1A-C2A-CAA-CBA
32	b	621	LMT	C11-C10-C9-C8
23	B	602	CLA	C16-C17-C18-C20
23	C	511	CLA	CAA-CBA-CGA-O1A
26	B	620	SQD	C24-C23-O48-C46
33	c	520	LMG	O9-C10-C11-C12
23	B	613	CLA	CAA-CBA-CGA-O1A
37	l	101	LHG	O9-C7-C8-C9
26	A	410	SQD	O49-C7-C8-C9
33	m	101	LMG	O1-C7-C8-C9
23	B	602	CLA	C2A-CAA-CBA-CGA
35	C	519	DGD	C9B-CAB-CBB-CCB
23	c	511	CLA	CAA-CBA-CGA-O1A
26	F	101	SQD	C31-C32-C33-C34
23	B	612	CLA	C13-C15-C16-C17
23	a	409	CLA	C8-C10-C11-C12
33	a	419	LMG	C21-C22-C23-C24
26	b	620	SQD	O10-C23-C24-C25
23	D	406	CLA	C2-C3-C5-C6
26	B	620	SQD	O10-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
37	d	408	LHG	C4-O6-P-O5
37	d	407	LHG	C4-O6-P-O5
37	E	101	LHG	C4-O6-P-O5
37	L	101	LHG	C16-C17-C18-C19
23	b	613	CLA	CAA-CBA-CGA-O1A
33	B	621	LMG	C4-C5-C6-O5
34	B	622	HTG	S1-C1'-C2'-C3'
25	c	516	BCR	C5-C6-C7-C8
25	t	103	BCR	C1-C6-C7-C8
25	t	103	BCR	C5-C6-C7-C8
23	C	513	CLA	C10-C11-C12-C13
35	c	517	DGD	O1B-C1B-C2B-C3B
37	D	410	LHG	C32-C33-C34-C35
35	C	519	DGD	CAA-CBA-CCA-CDA
33	C	501	LMG	C17-C18-C19-C20
26	a	411	SQD	C26-C27-C28-C29
26	B	620	SQD	C11-C10-C9-C8
33	m	101	LMG	C19-C20-C21-C22
23	B	615	CLA	C8-C10-C11-C12
23	b	605	CLA	CAD-CBD-CGD-O1D
23	A	406	CLA	CAD-CBD-CGD-O1D
23	B	605	CLA	CAD-CBD-CGD-O1D
23	B	609	CLA	CAD-CBD-CGD-O1D
23	b	607	CLA	CAD-CBD-CGD-O1D
23	C	505	CLA	CAD-CBD-CGD-O1D
23	b	603	CLA	CAD-CBD-CGD-O1D
23	C	507	CLA	CAD-CBD-CGD-O1D
23	c	513	CLA	CAA-CBA-CGA-O1A
37	L	101	LHG	C11-C10-C9-C8
33	z	101	LMG	O7-C10-C11-C12
23	b	606	CLA	C14-C13-C15-C16
23	b	607	CLA	C14-C13-C15-C16
23	C	510	CLA	C6-C7-C8-C9
23	c	502	CLA	C11-C10-C8-C9
23	C	507	CLA	C14-C13-C15-C16
23	b	616	CLA	C14-C13-C15-C16
27	a	412	GOL	O1-C1-C2-O2
24	A	407	PHO	C10-C11-C12-C13
33	D	415	LMG	O9-C10-C11-C12
35	C	518	DGD	O2G-C1B-C2B-C3B
37	d	408	LHG	O8-C23-C24-C25
23	a	409	CLA	C15-C16-C17-C18

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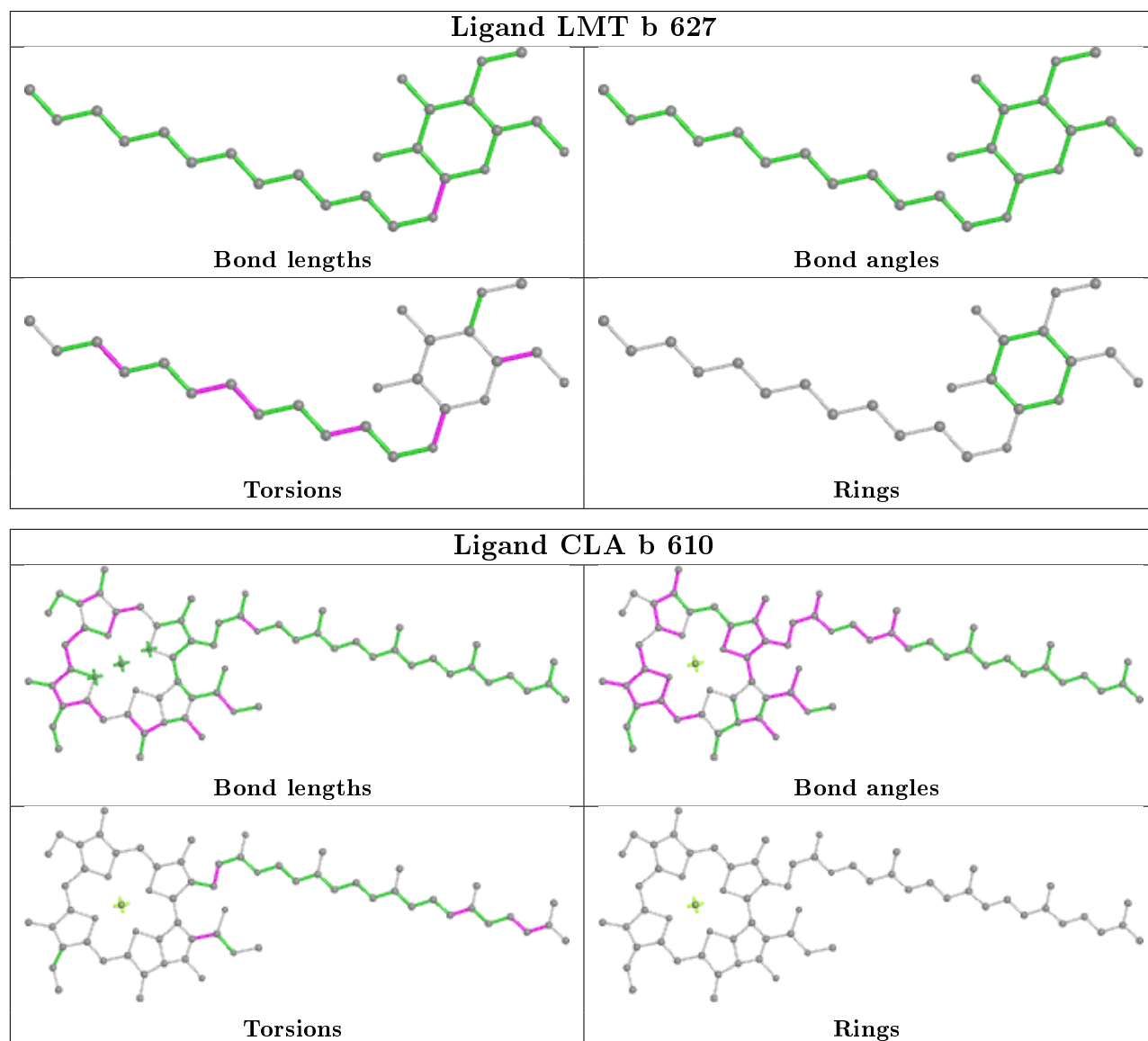
Mol	Chain	Res	Type	Atoms
33	c	520	LMG	O10-C28-O8-C9
23	A	404	CLA	C15-C16-C17-C18
23	c	502	CLA	C2A-CAA-CBA-CGA
37	d	408	LHG	C28-C29-C30-C31
35	c	518	DGD	C5A-C6A-C7A-C8A
35	C	519	DGD	CDA-CEA-CFA-CGA
37	D	409	LHG	C1-C2-C3-O3
26	B	620	SQD	C35-C36-C37-C38
32	b	621	LMT	C6-C7-C8-C9
29	A	414	PL9	C35-C34-C36-C37
23	C	507	CLA	C8-C10-C11-C12
37	D	411	LHG	C12-C13-C14-C15
23	b	610	CLA	C11-C12-C13-C15
23	b	611	CLA	C12-C13-C15-C16
23	A	406	CLA	C11-C10-C8-C7
23	c	511	CLA	C6-C7-C8-C10
23	C	506	CLA	C11-C12-C13-C15
23	B	616	CLA	C11-C12-C13-C15
23	b	616	CLA	C11-C12-C13-C15
37	L	101	LHG	O7-C7-C8-C9
33	C	520	LMG	C28-C29-C30-C31
25	t	103	BCR	C7-C8-C9-C10
23	c	506	CLA	CAA-CBA-CGA-O2A
23	b	602	CLA	C13-C15-C16-C17
23	c	513	CLA	C8-C10-C11-C12
35	C	518	DGD	O1B-C1B-C2B-C3B
23	b	612	CLA	CAA-CBA-CGA-O1A
23	b	616	CLA	C10-C11-C12-C13
26	a	413	SQD	O48-C23-C24-C25
33	c	521	LMG	O7-C10-C11-C12
34	b	623	HTG	C4'-C5'-C6'-C7'
23	c	504	CLA	C15-C16-C17-C18
23	B	612	CLA	C8-C10-C11-C12
23	c	510	CLA	C13-C15-C16-C17
37	L	101	LHG	O9-C7-C8-C9
37	d	408	LHG	O10-C23-C24-C25
33	Z	101	LMG	O9-C10-C11-C12
26	a	413	SQD	C19-C20-C21-C22

There are no ring outliers.

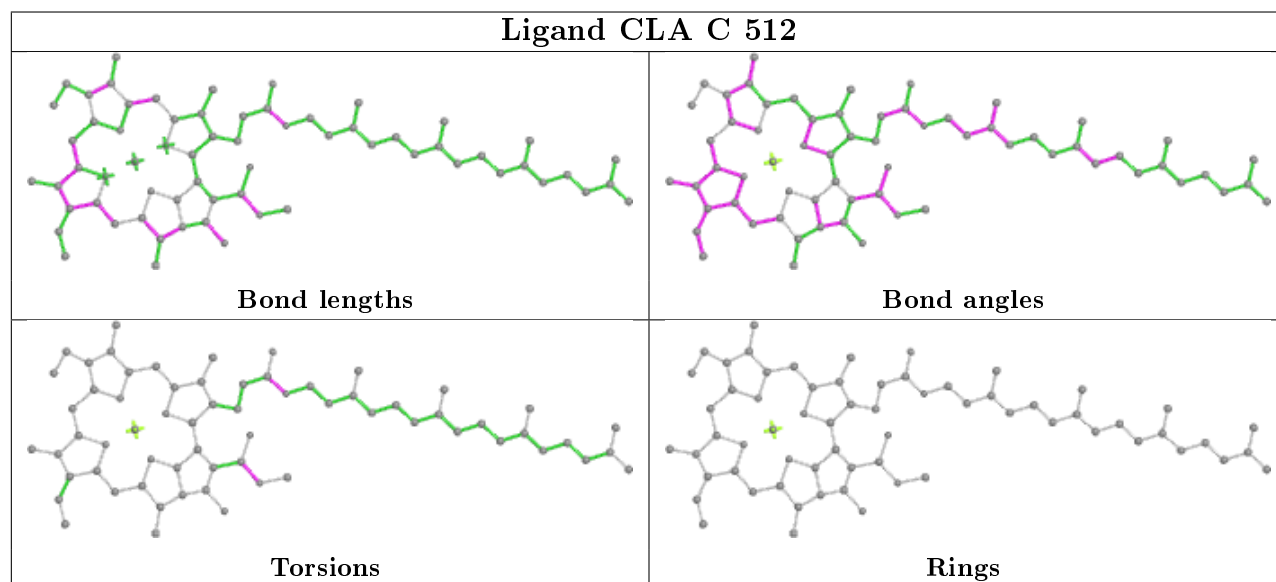
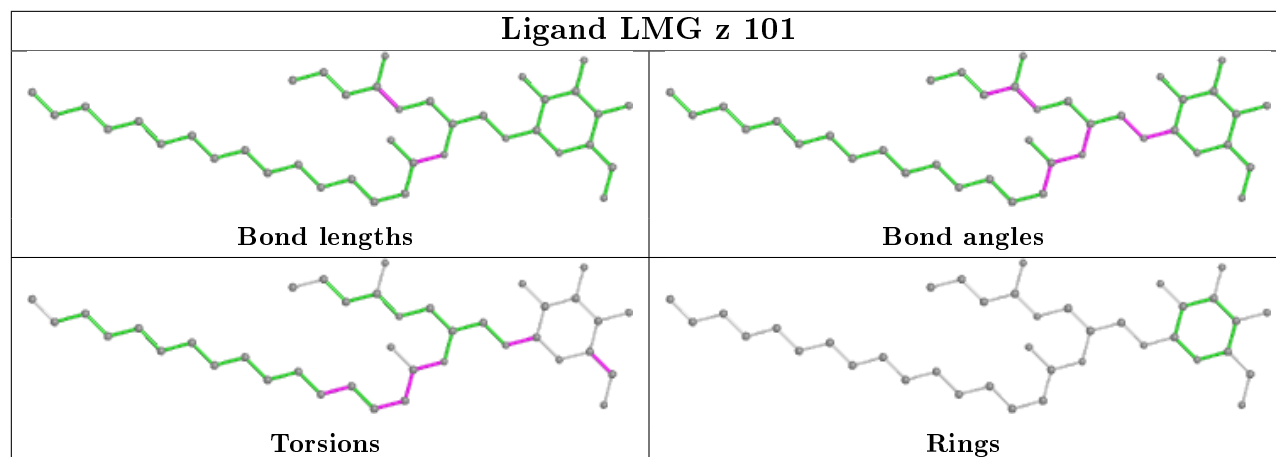
No monomer is involved in short contacts.

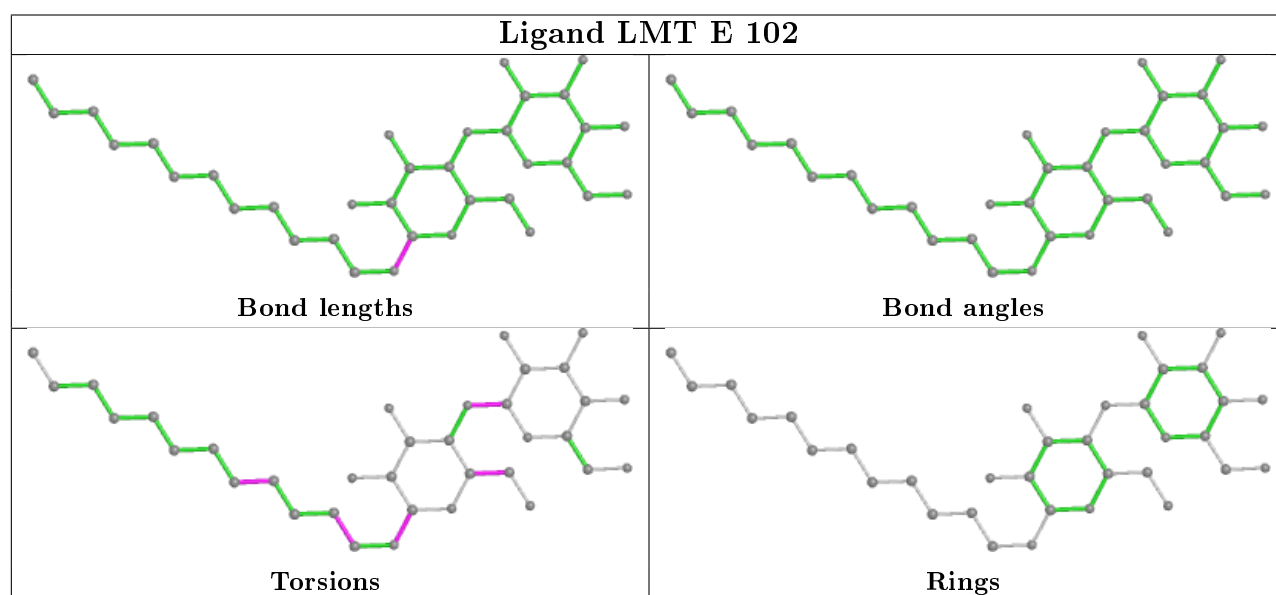
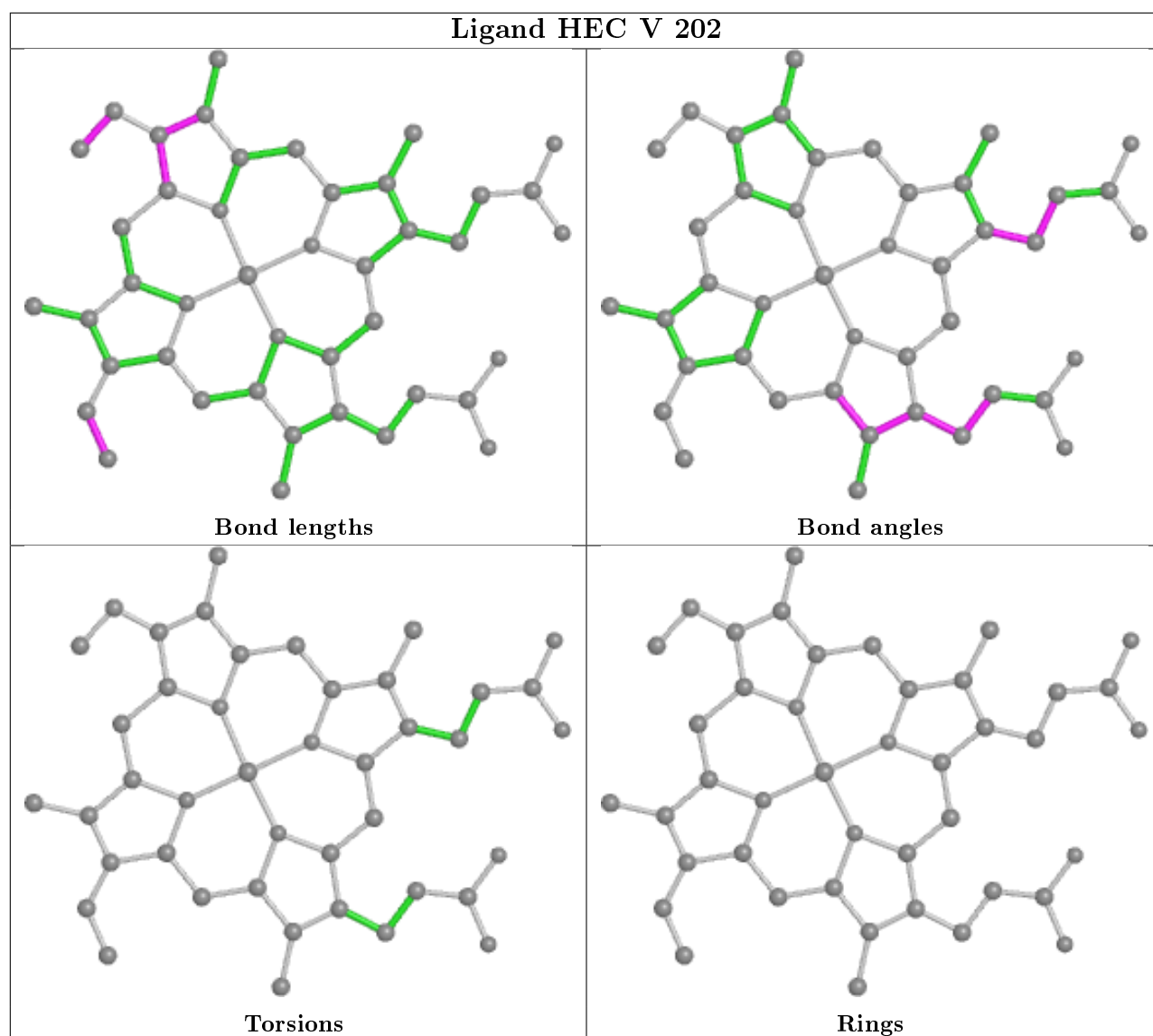
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

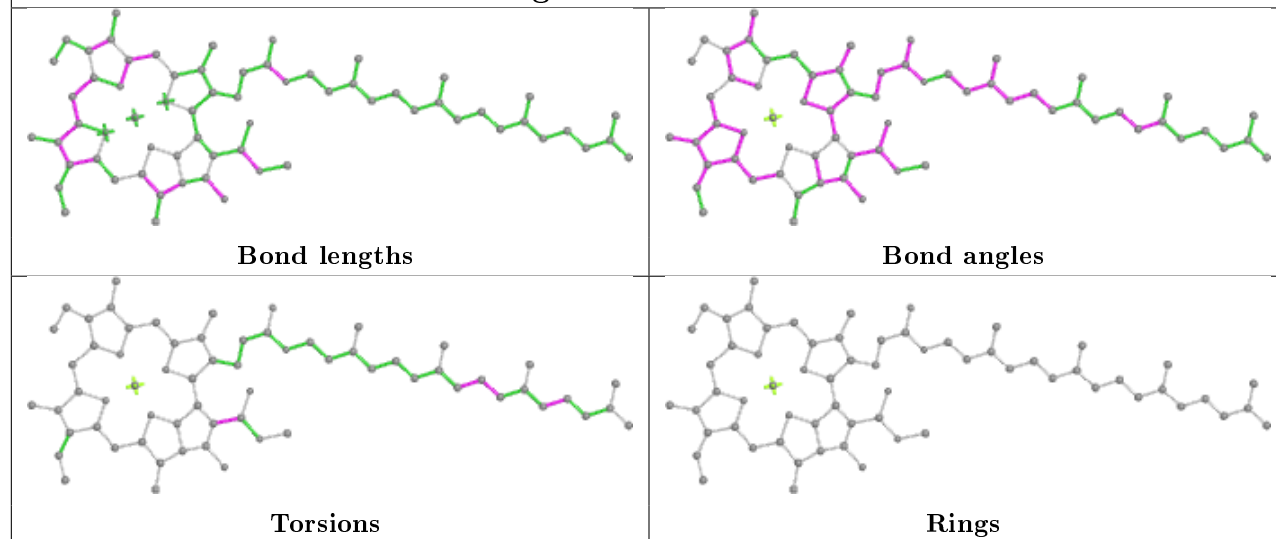




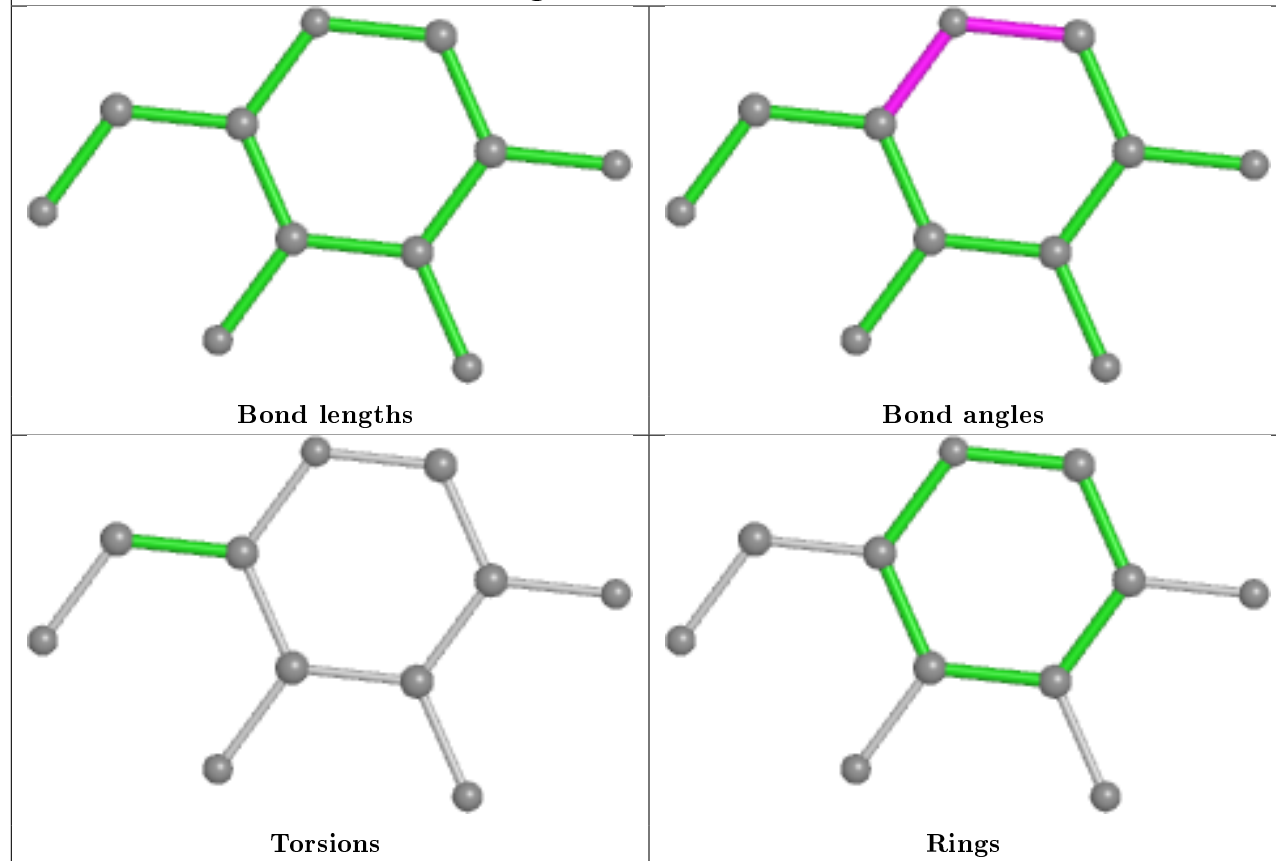


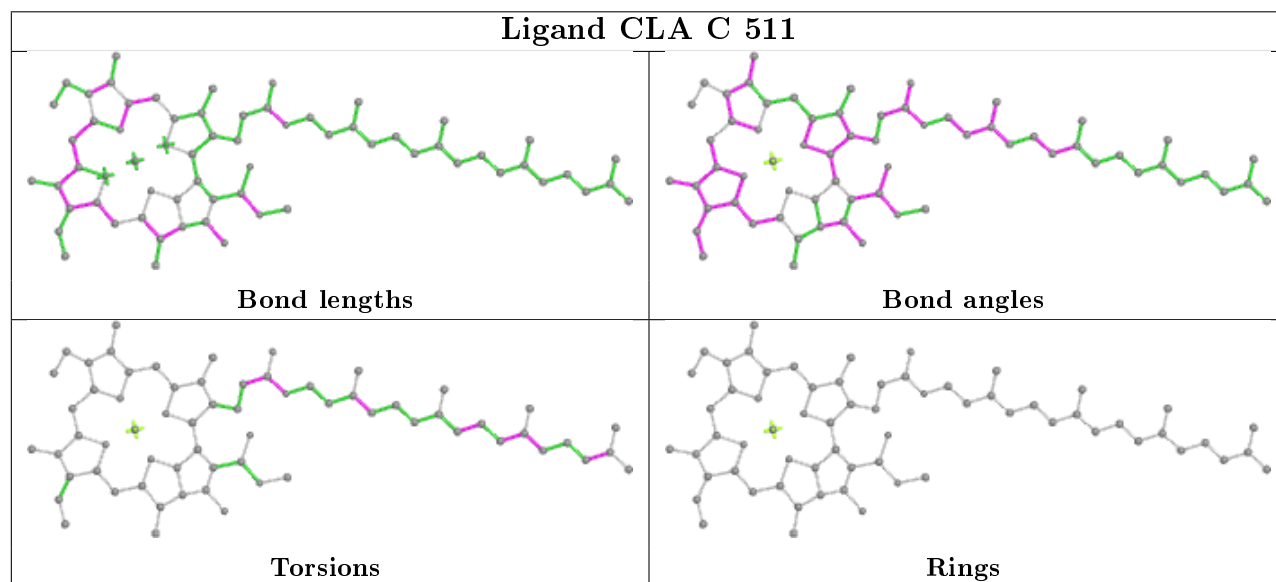
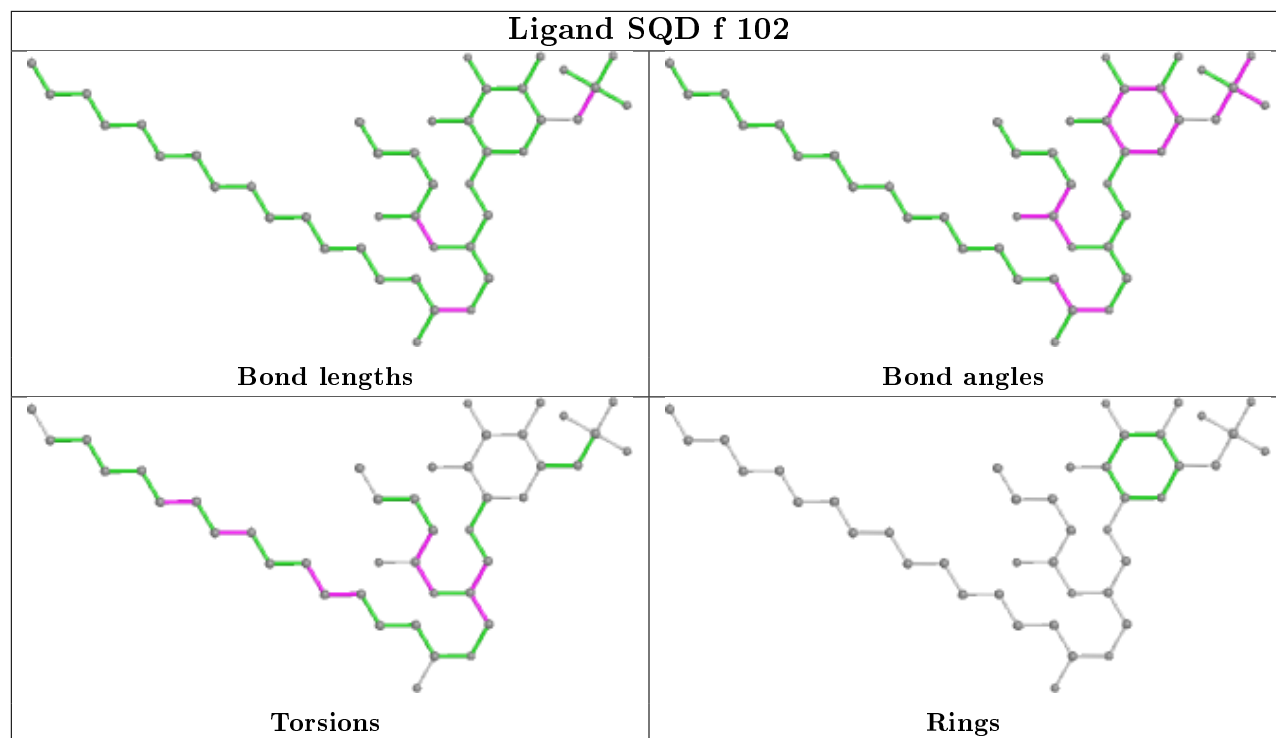


## Ligand CLA B 612

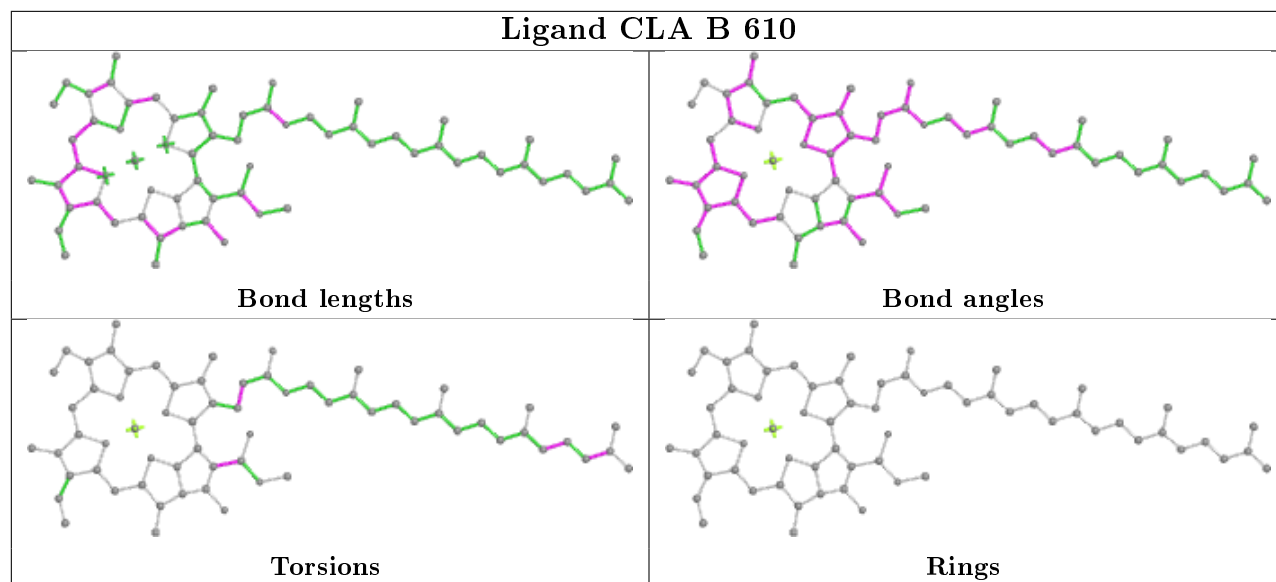


## Ligand HTG V 203

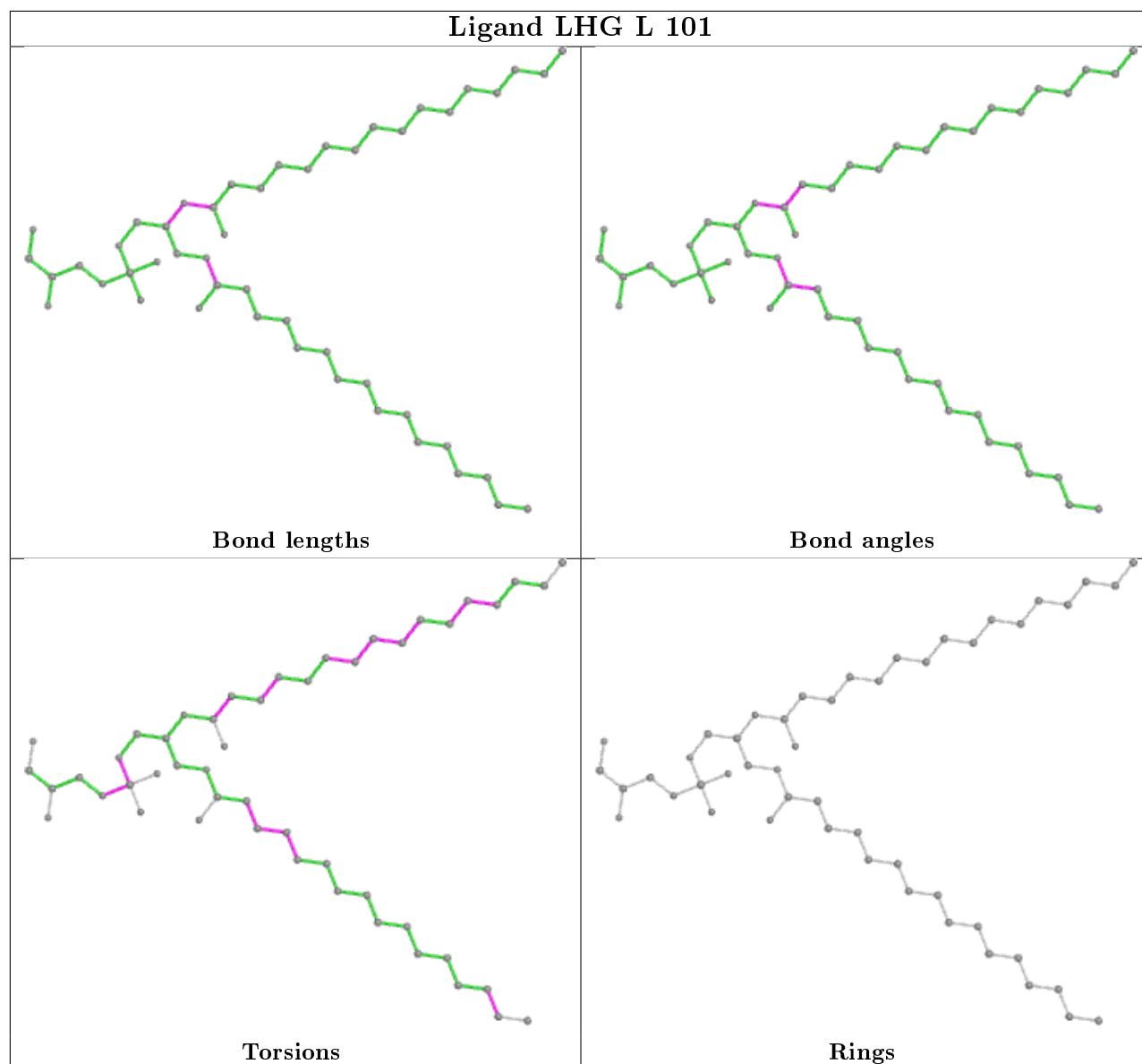


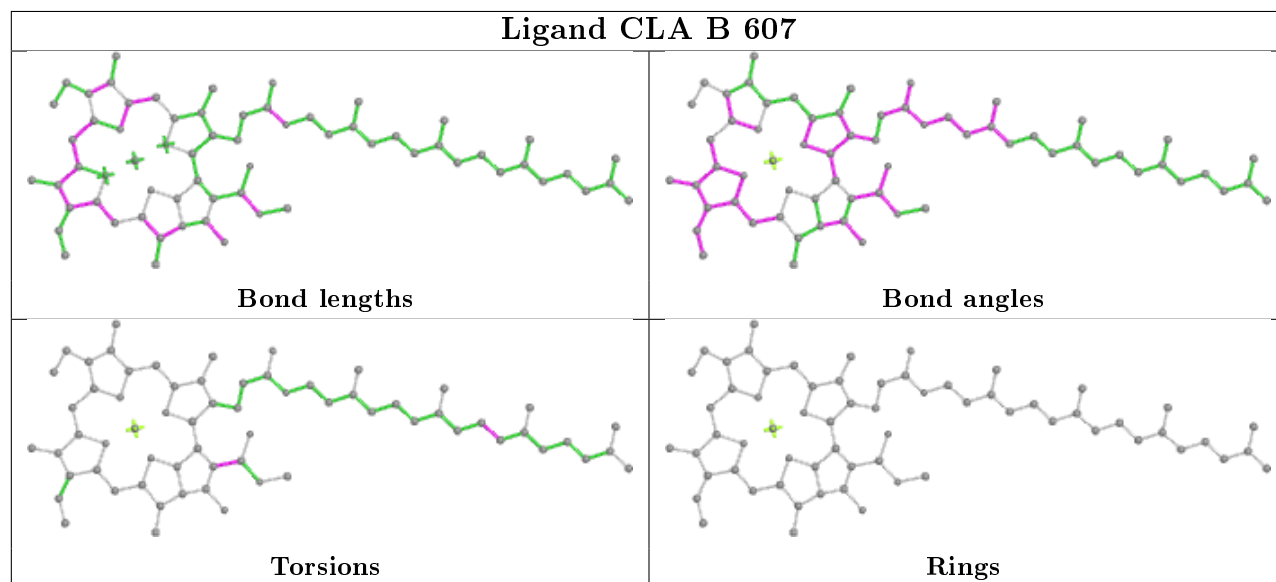
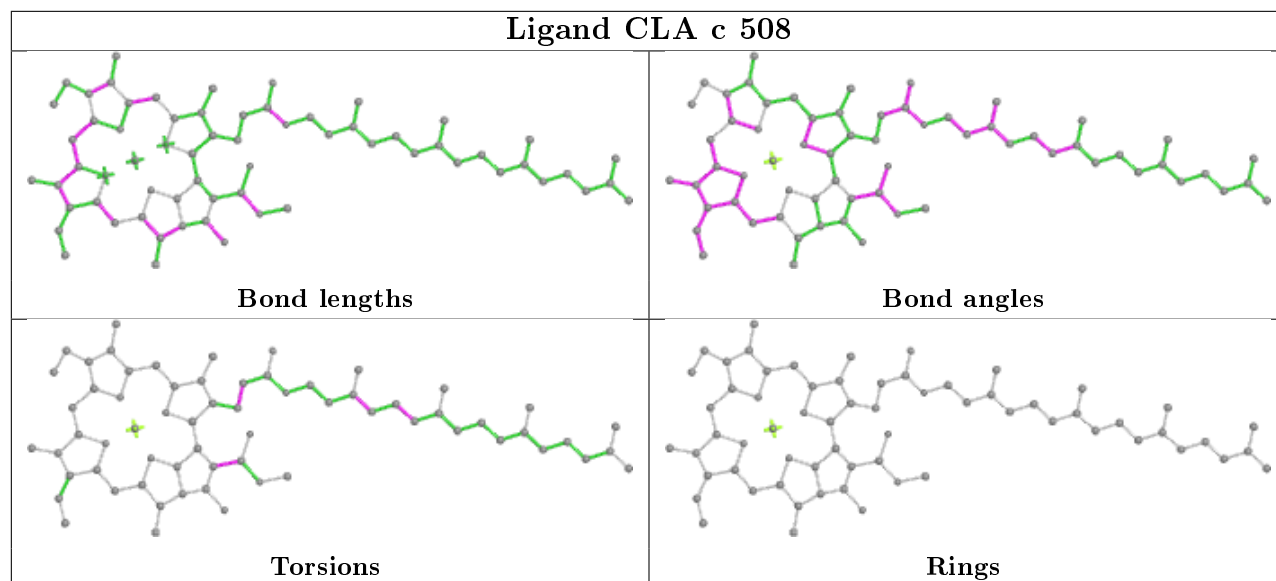
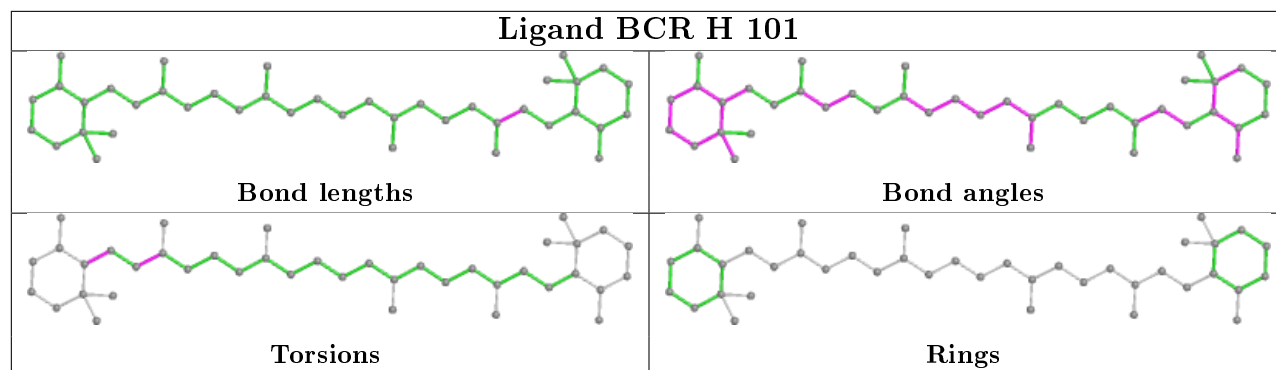


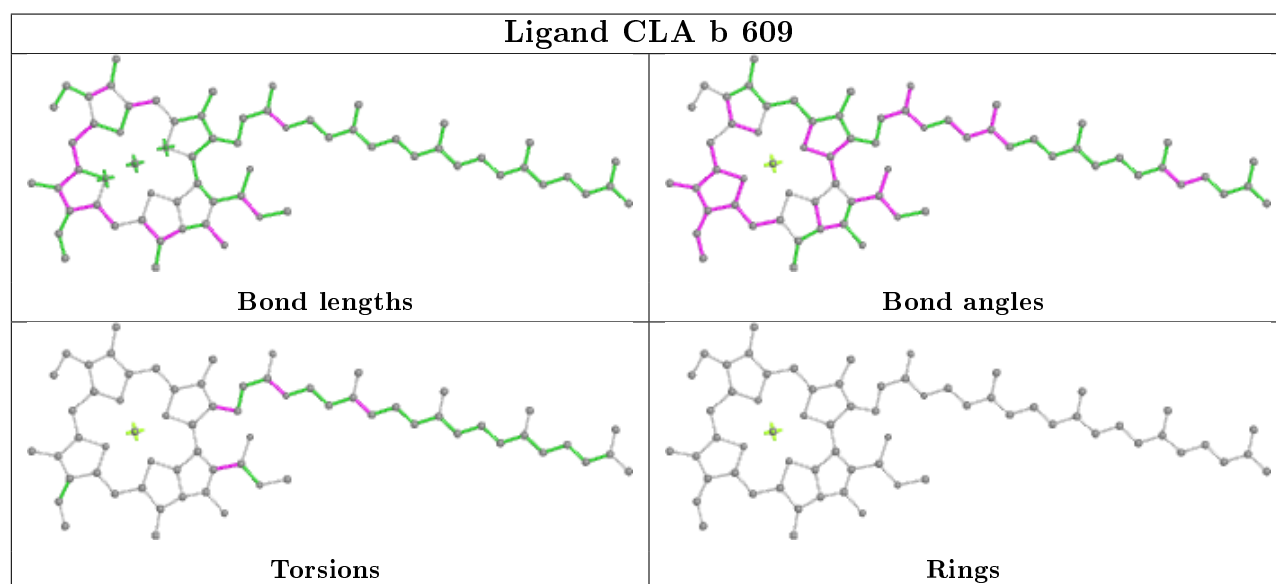
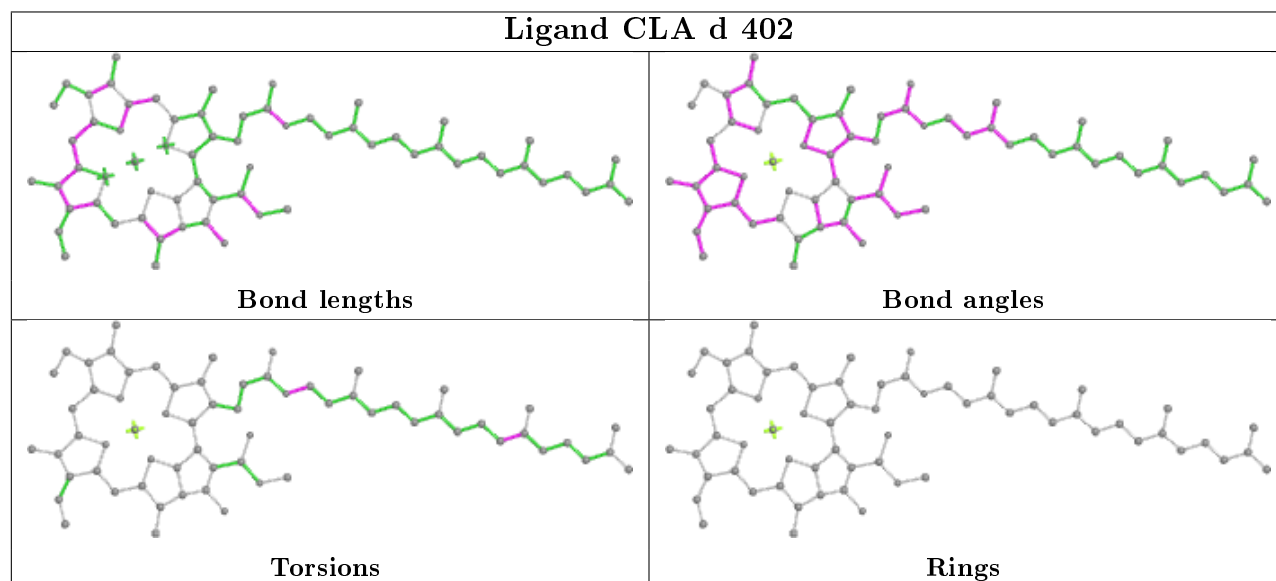
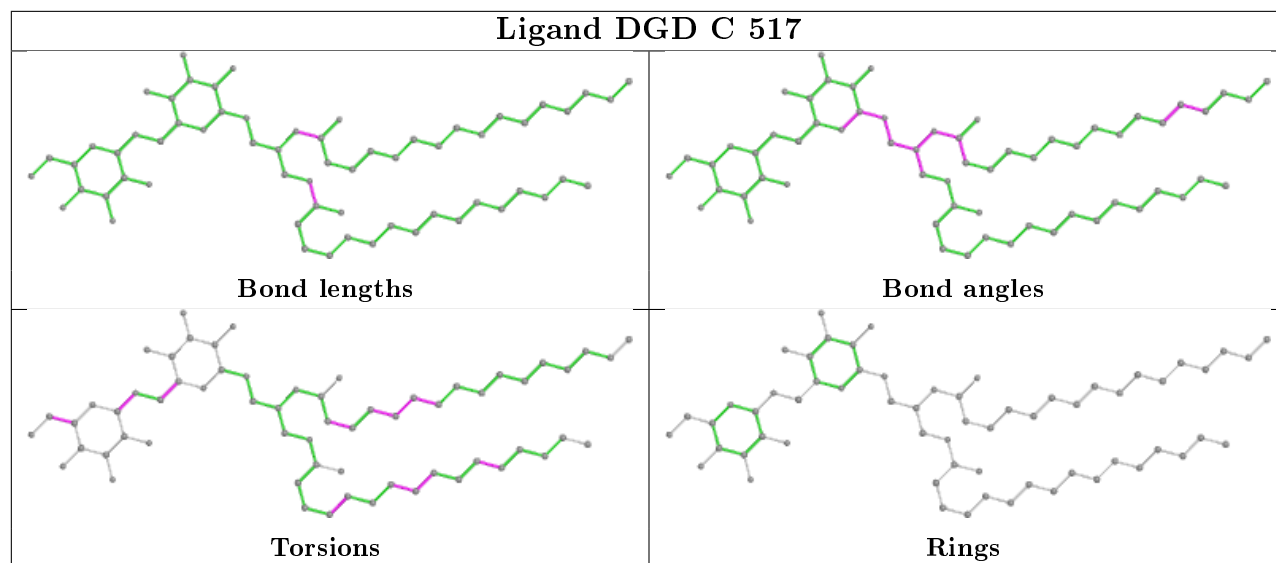
## Ligand CLA B 610

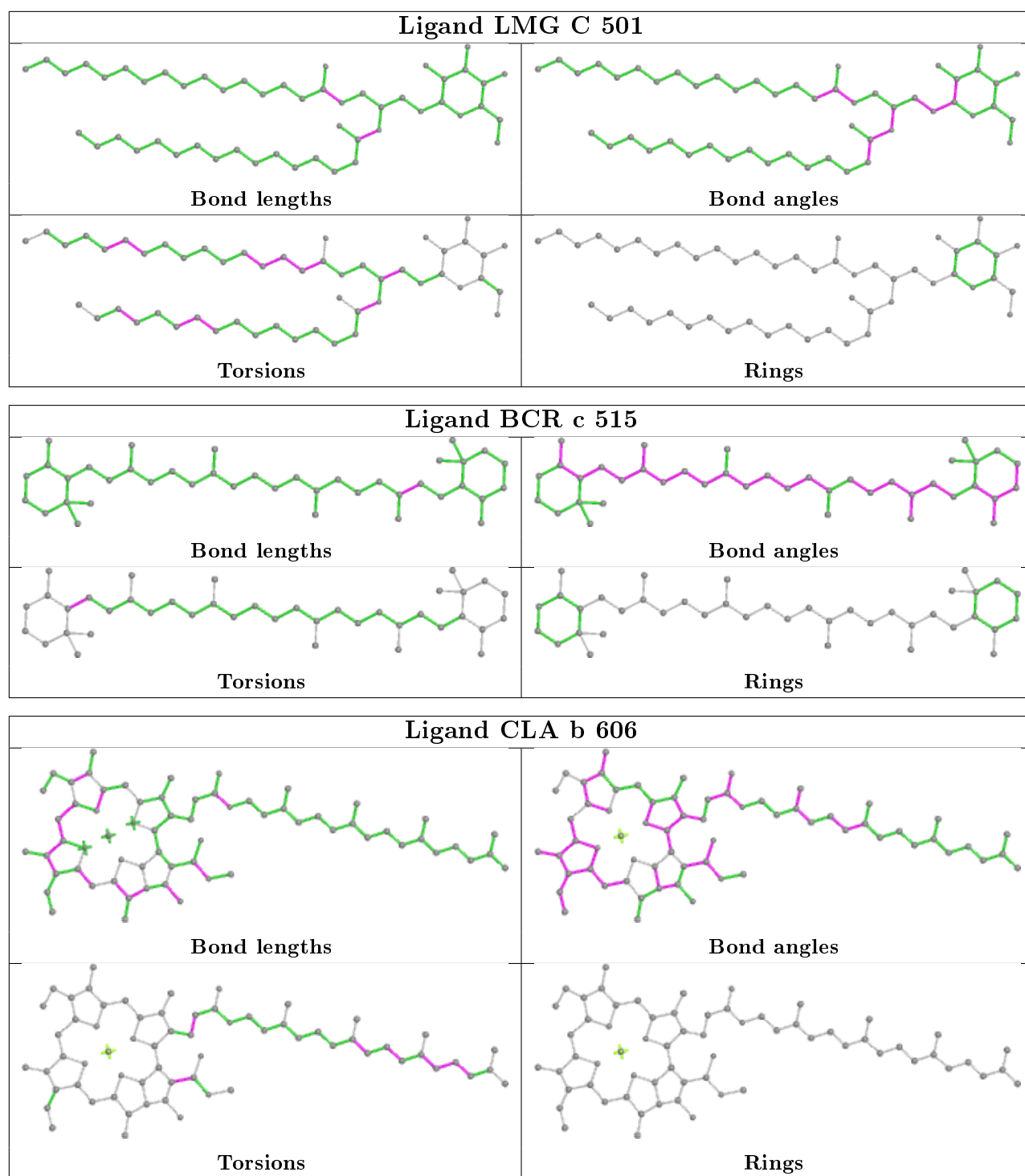


## Ligand LHG L 101



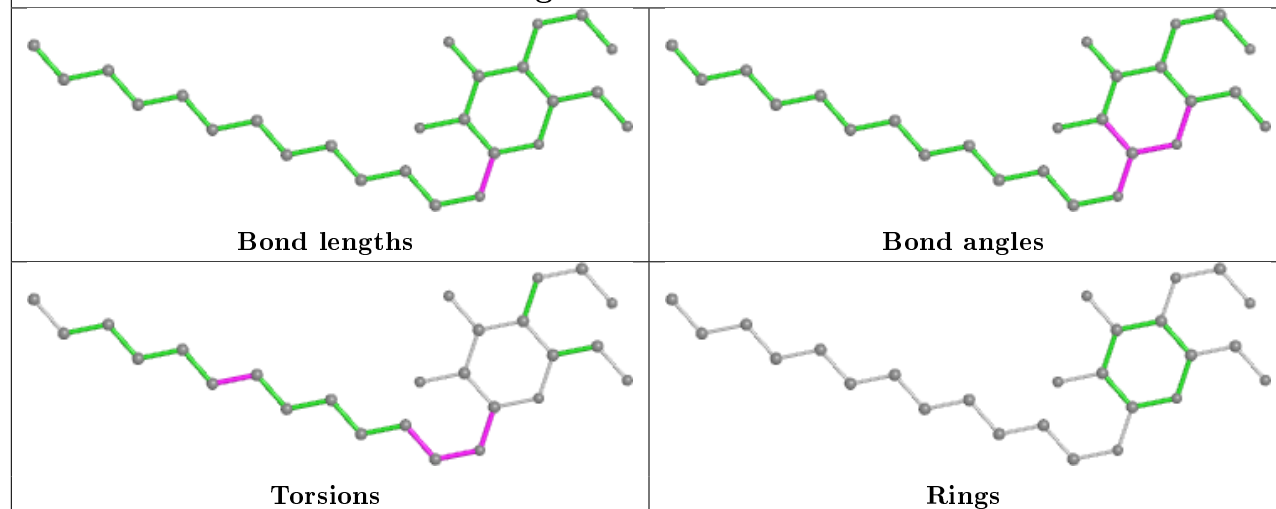




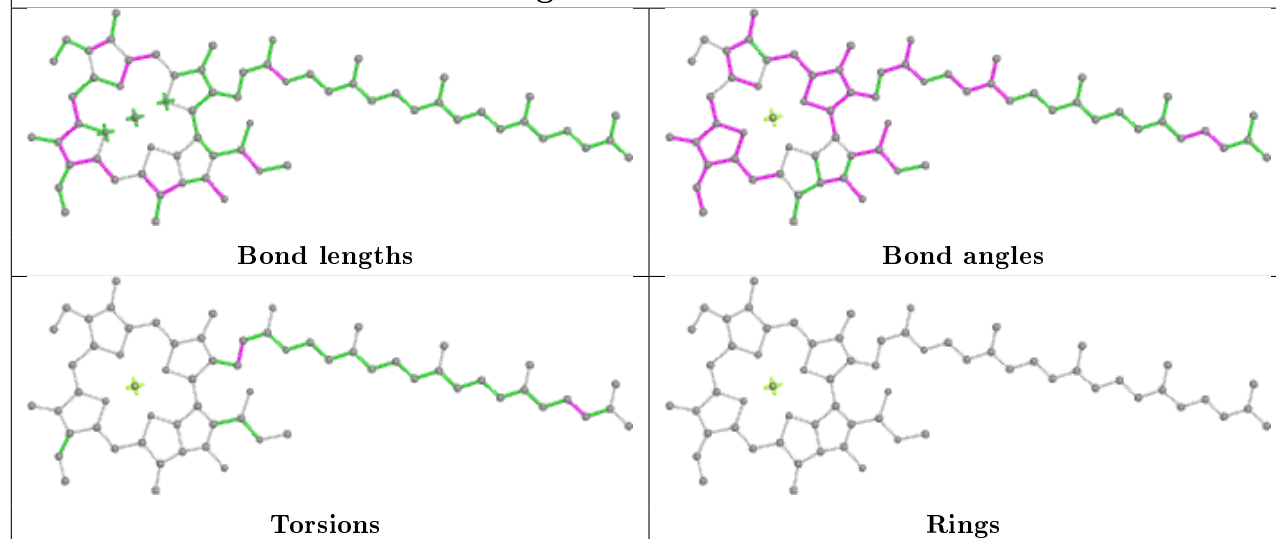




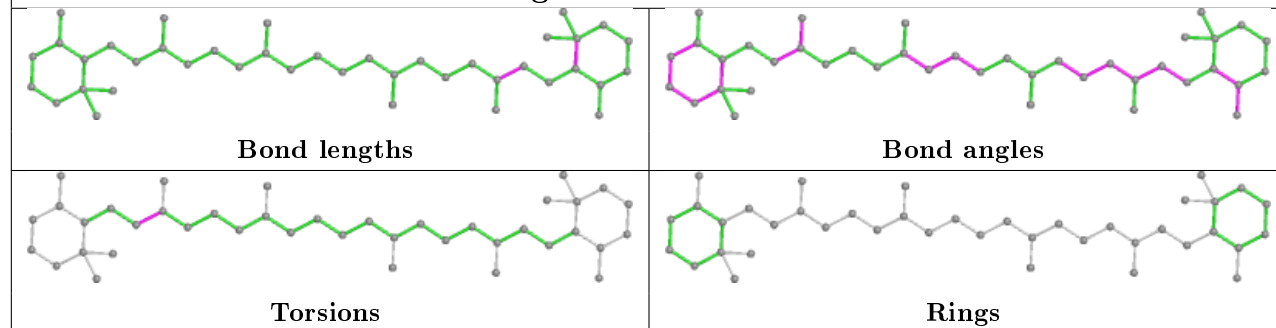
## Ligand LMT t 102

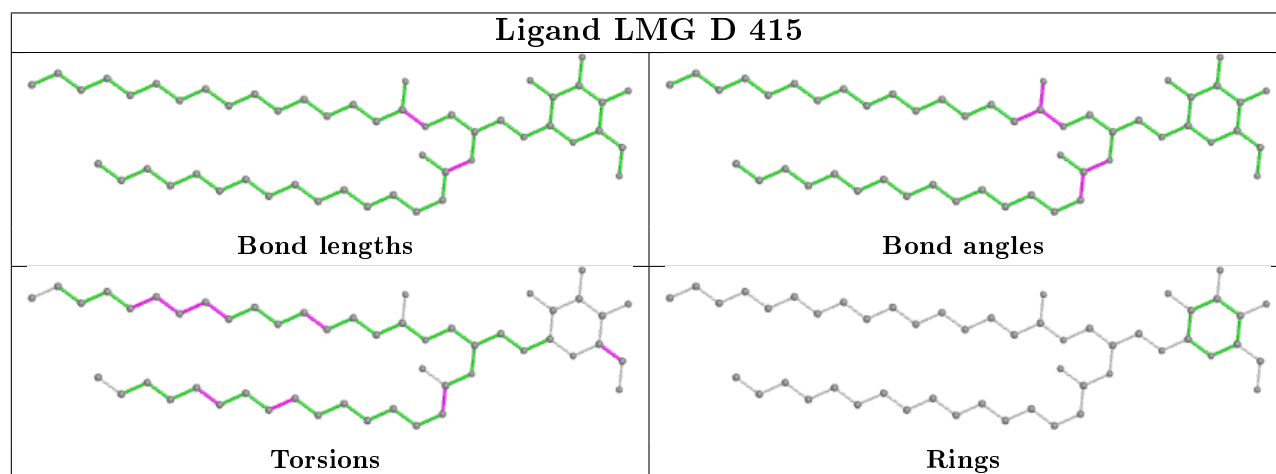
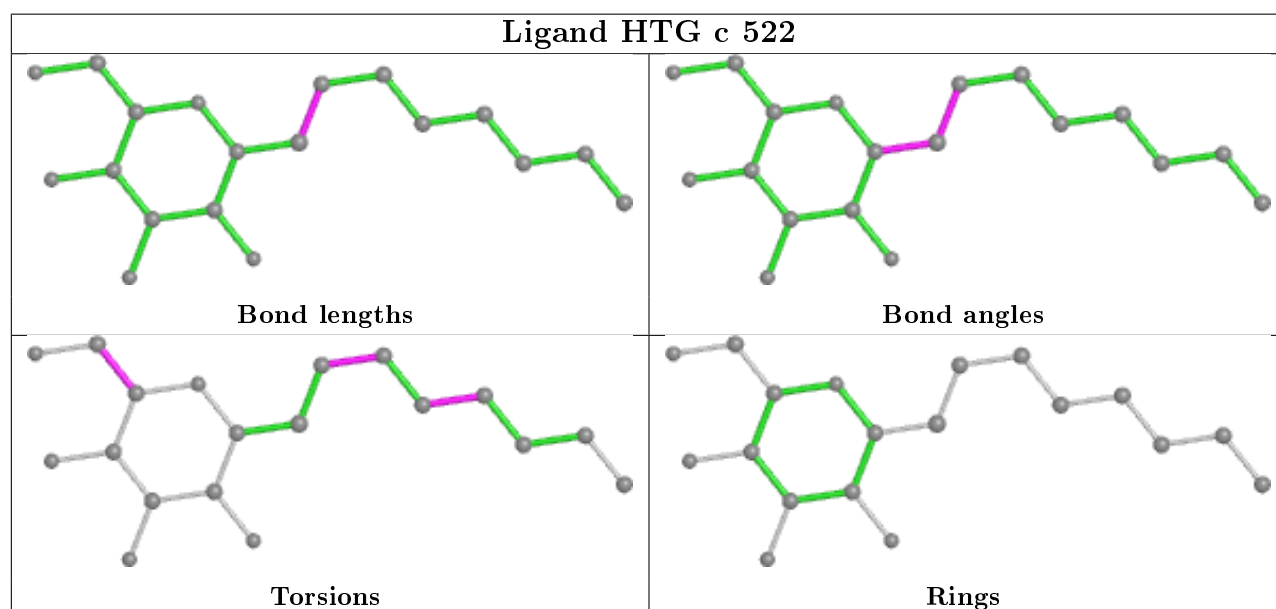
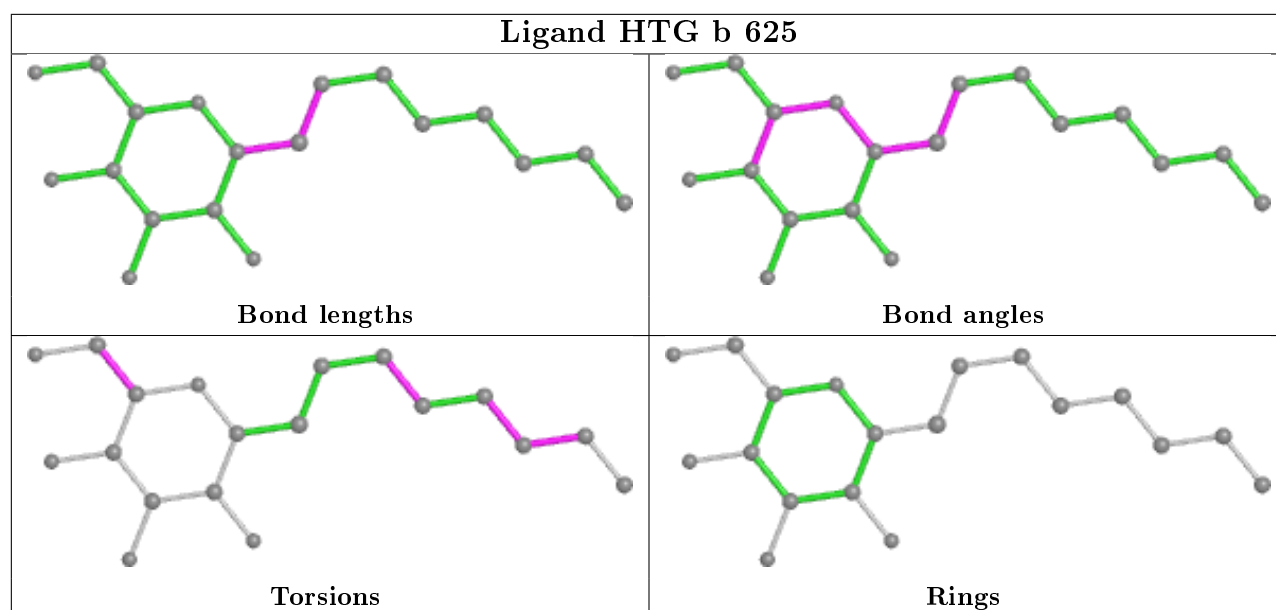


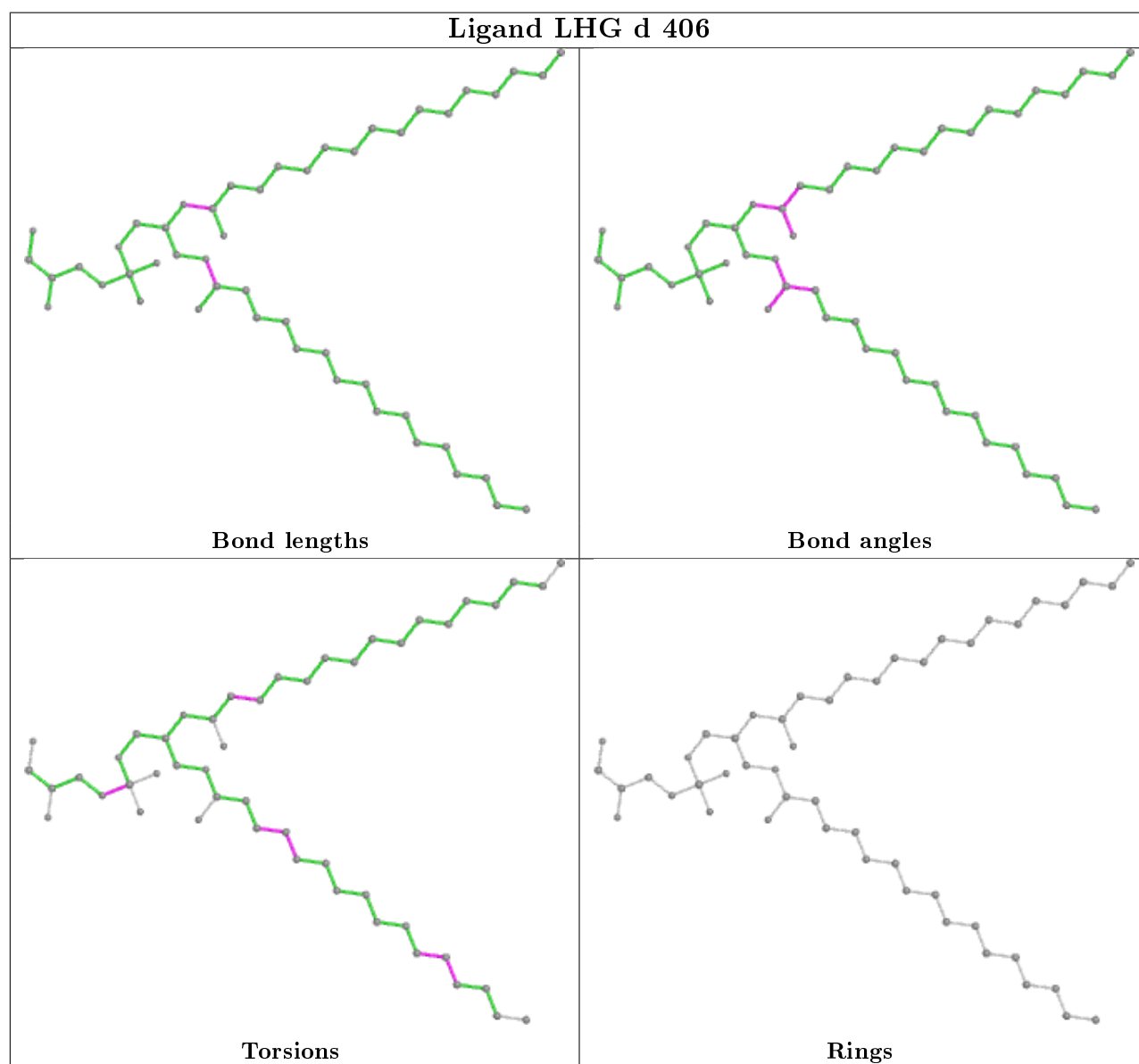
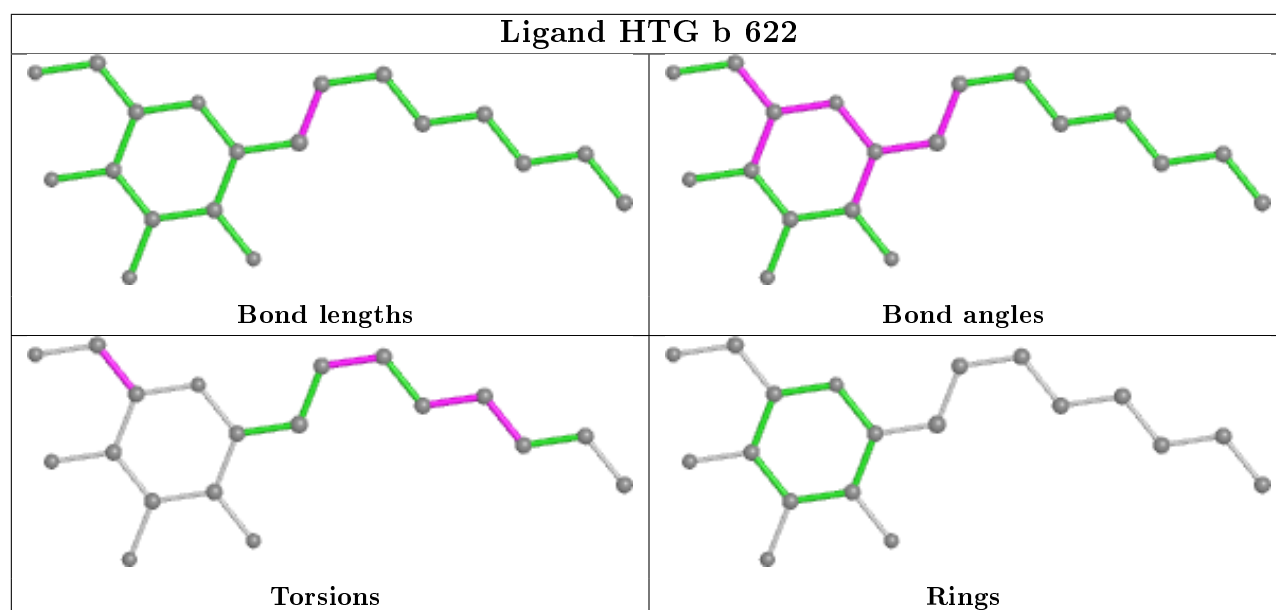
## Ligand CLA a 405



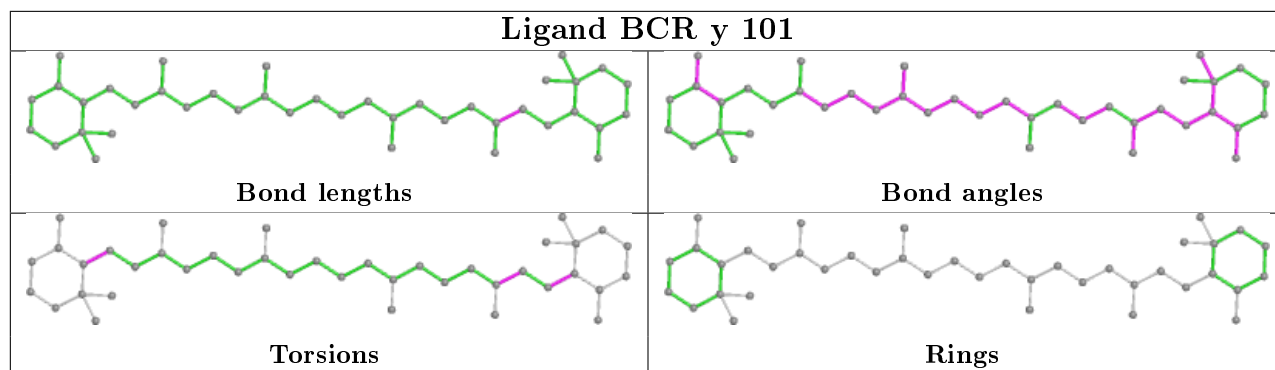
## Ligand BCR B 619



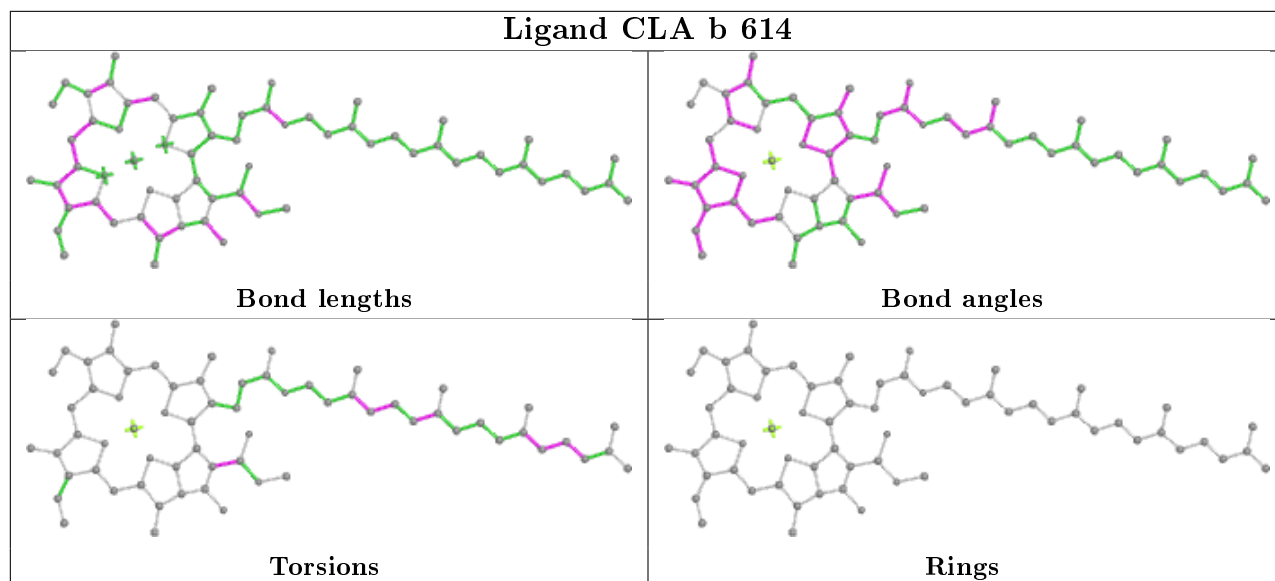




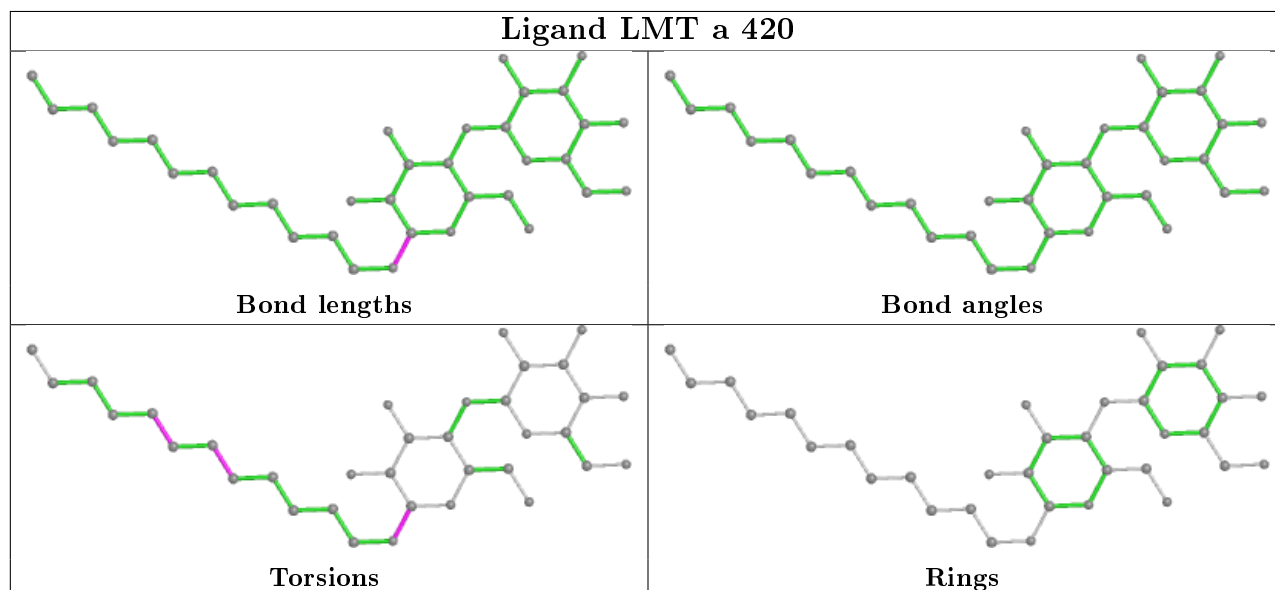
## Ligand BCR y 101

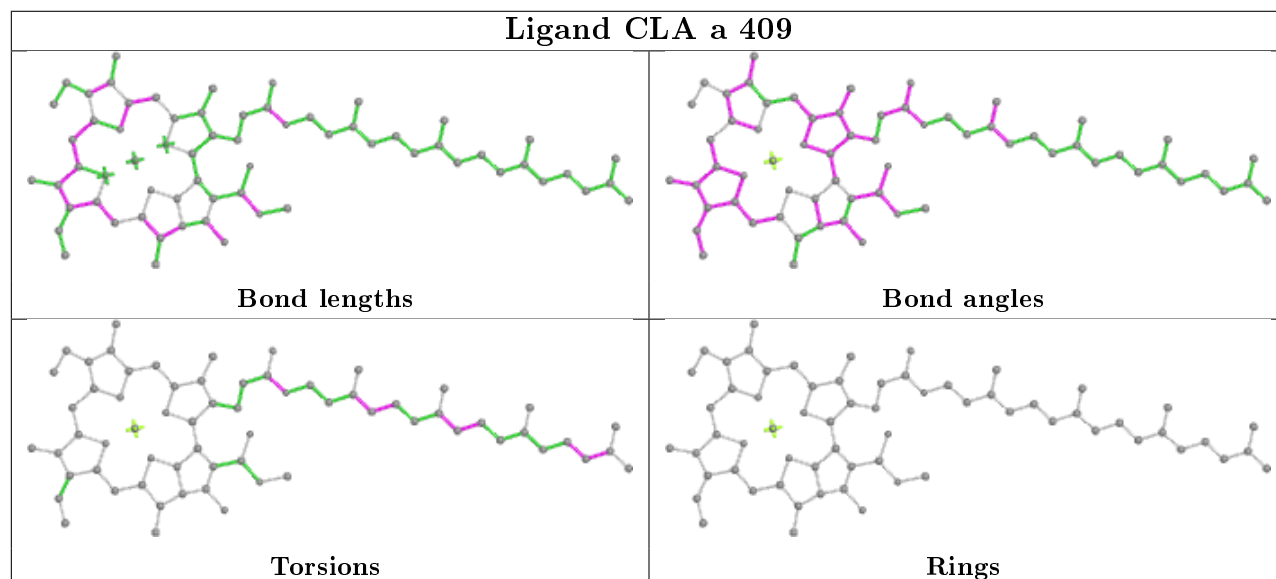
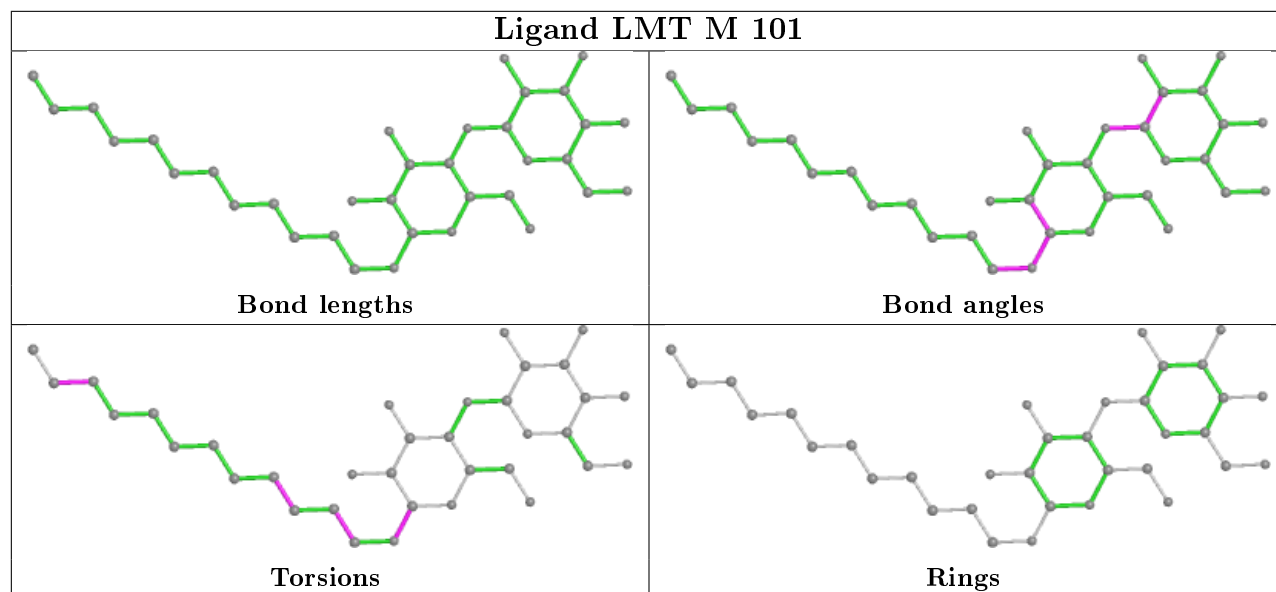
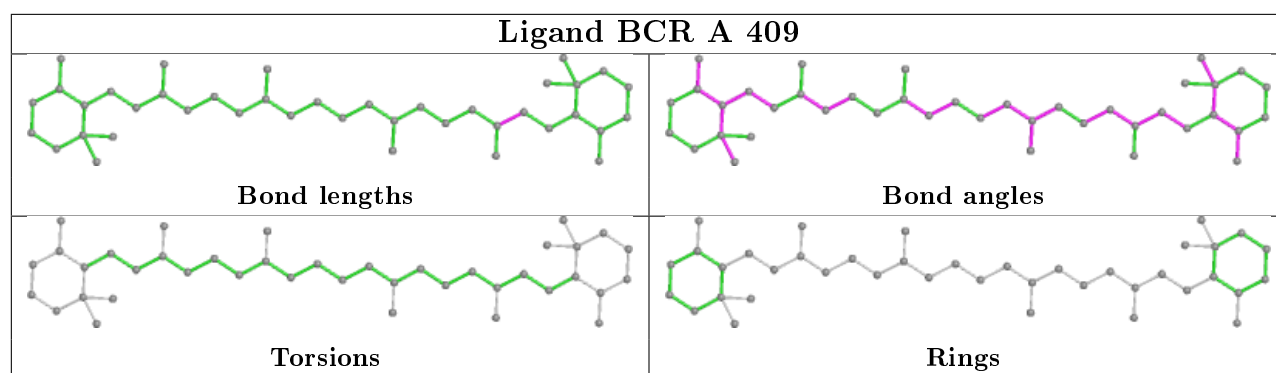


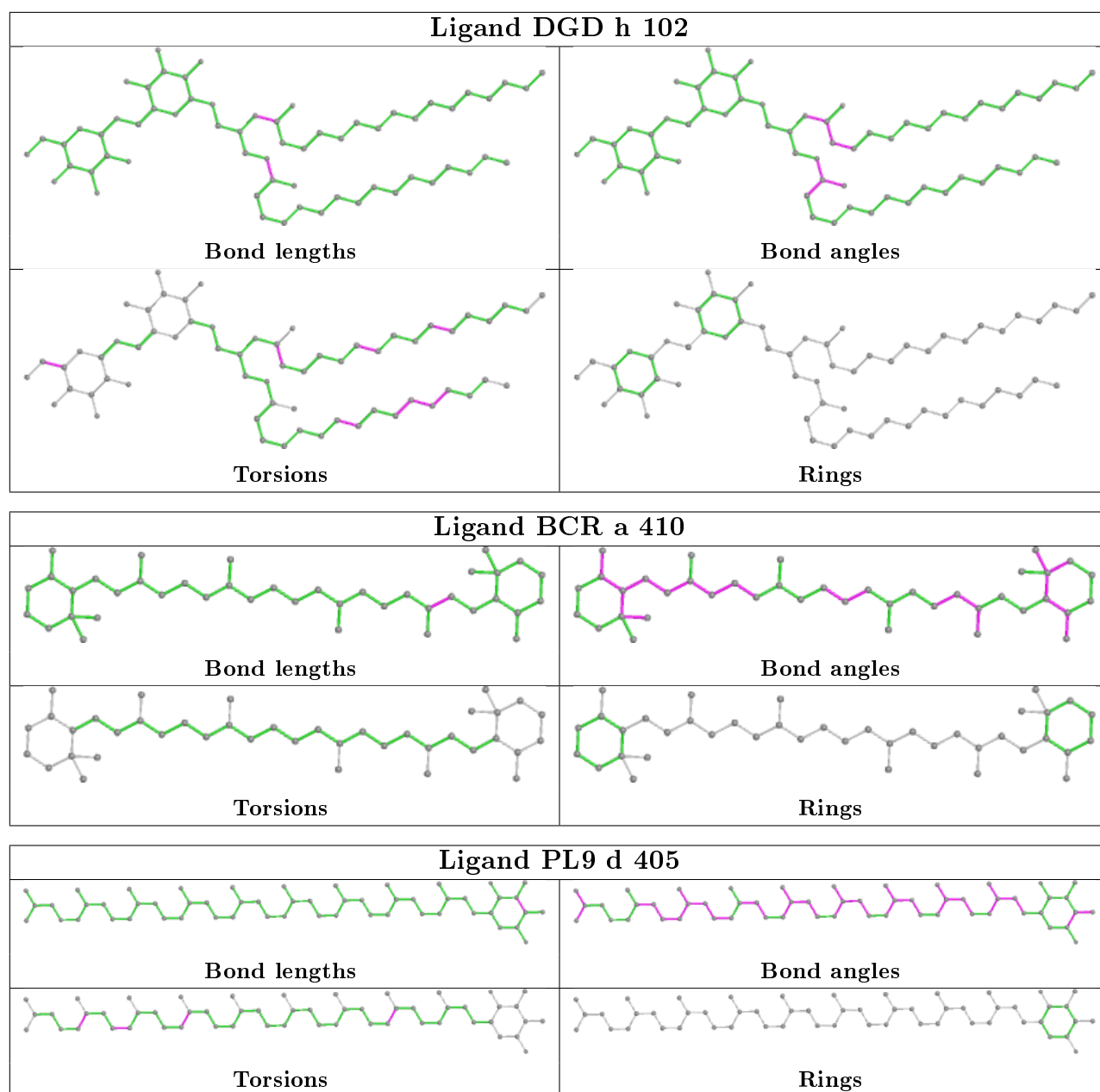
## Ligand CLA b 614



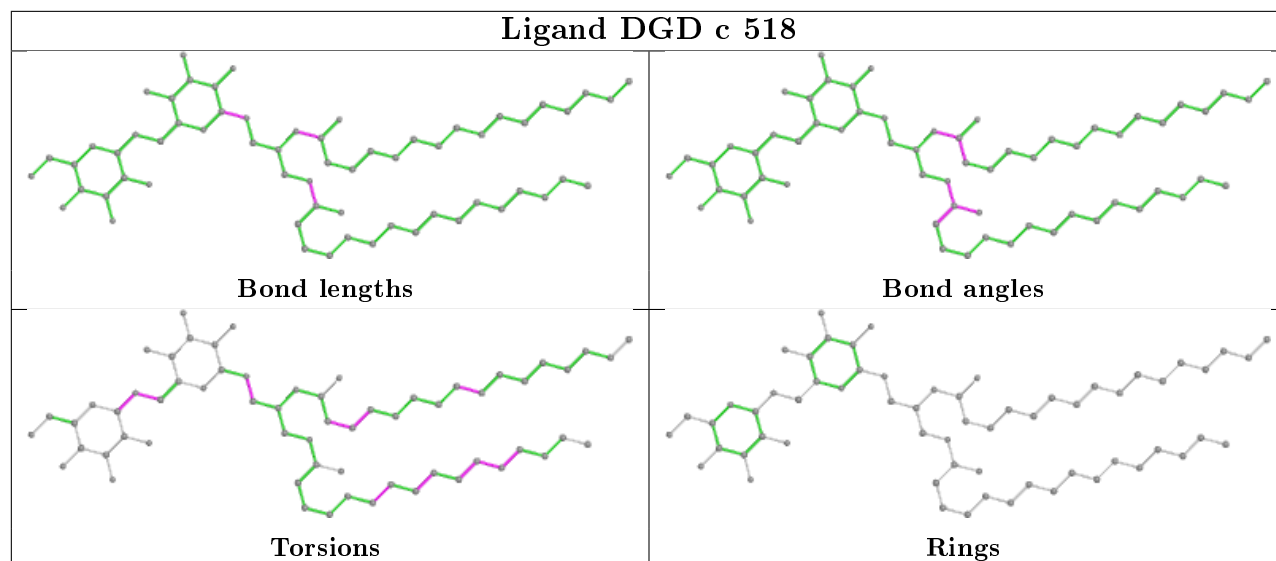
## Ligand LMT a 420



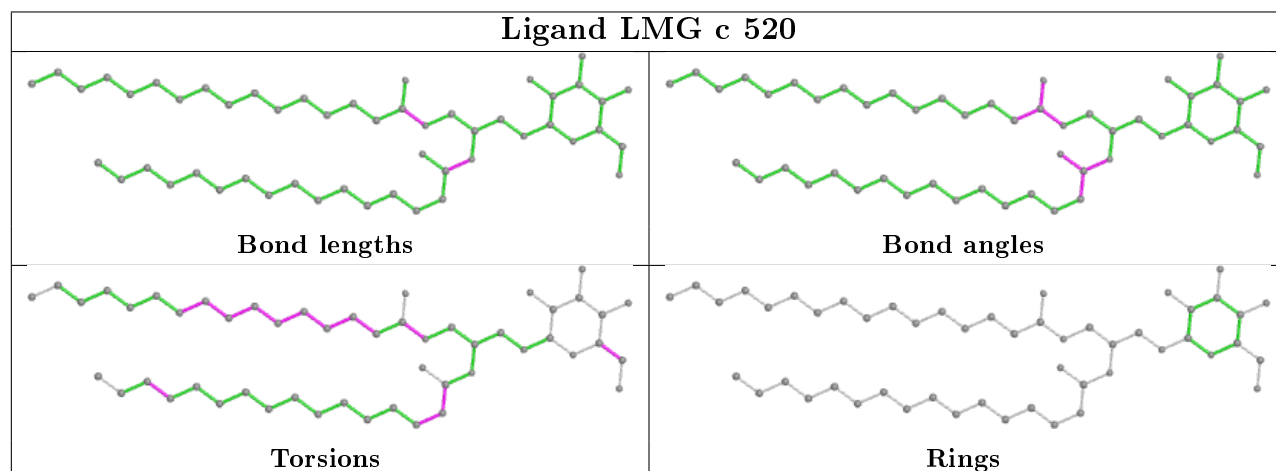




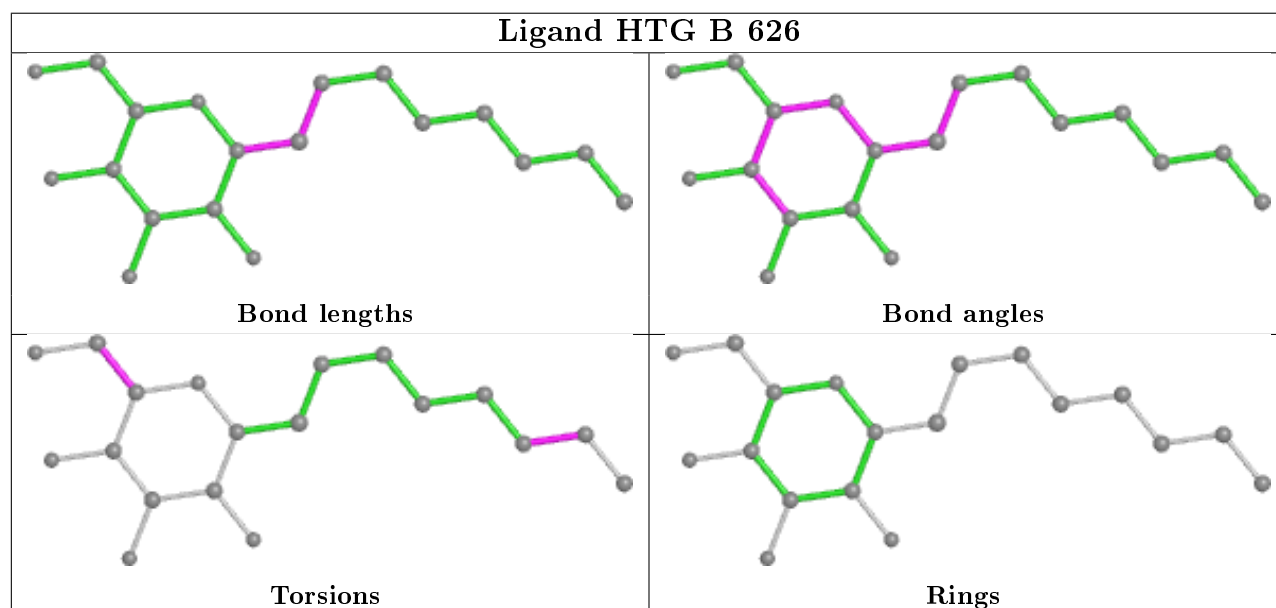
## Ligand DGD c 518

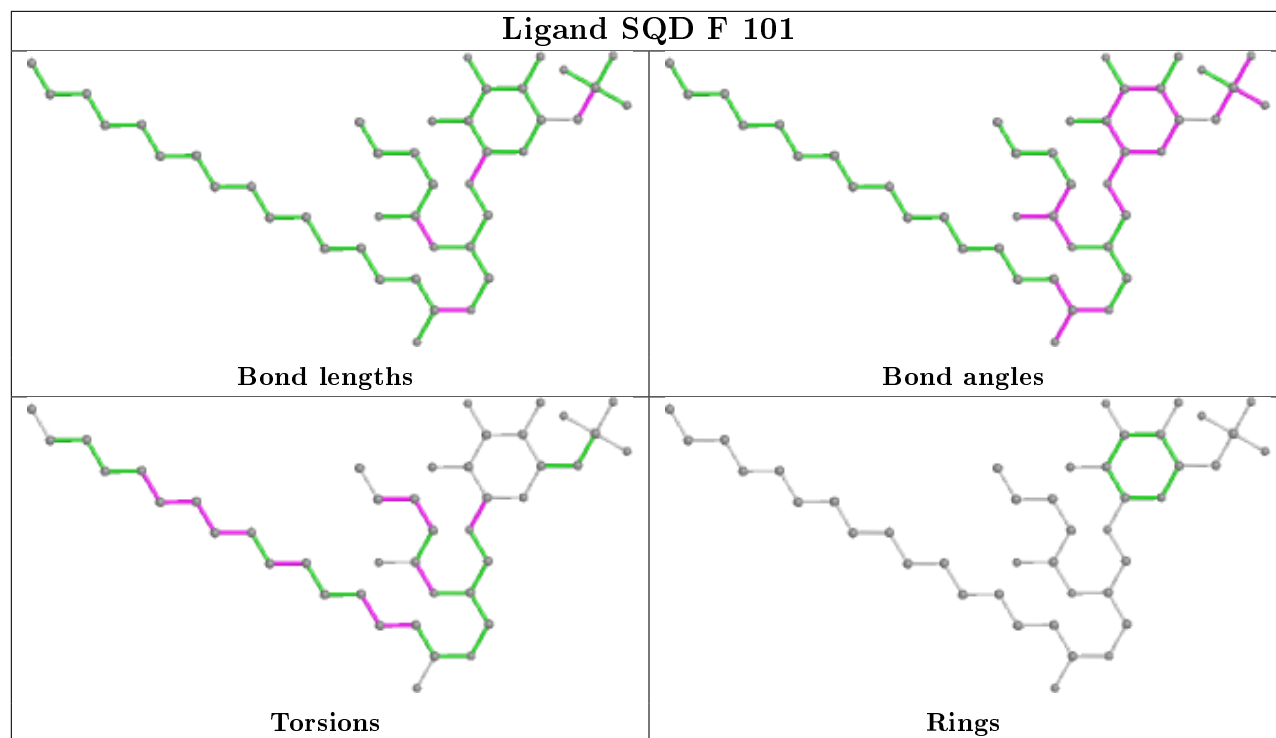


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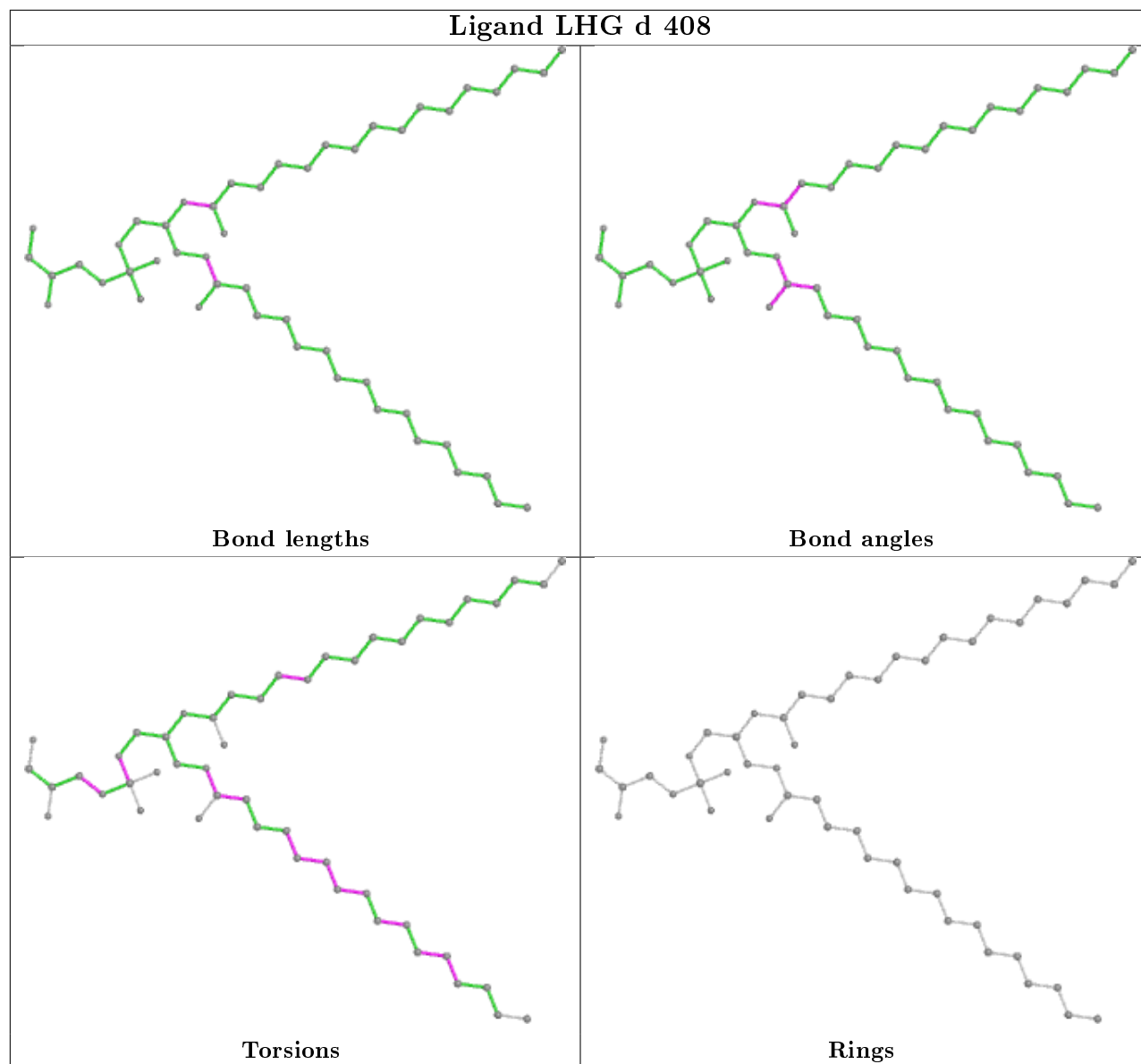
## Ligand HTG B 626



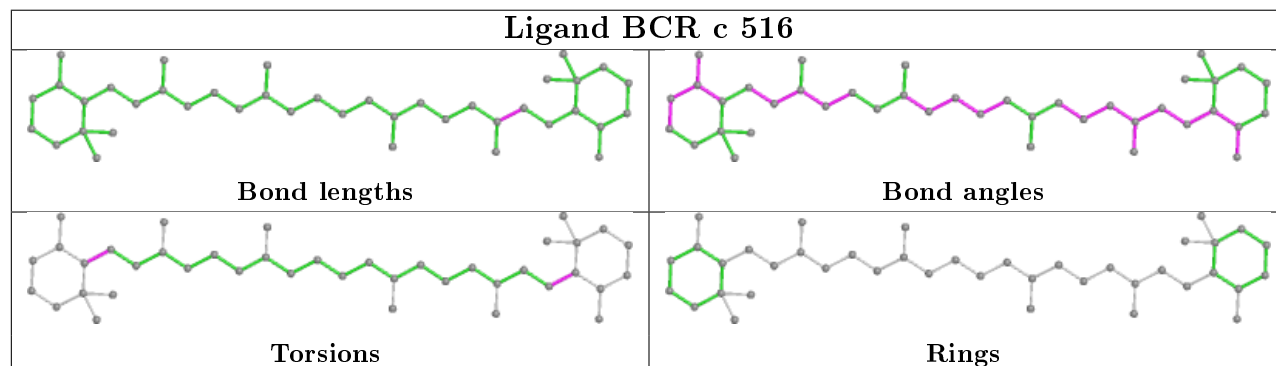




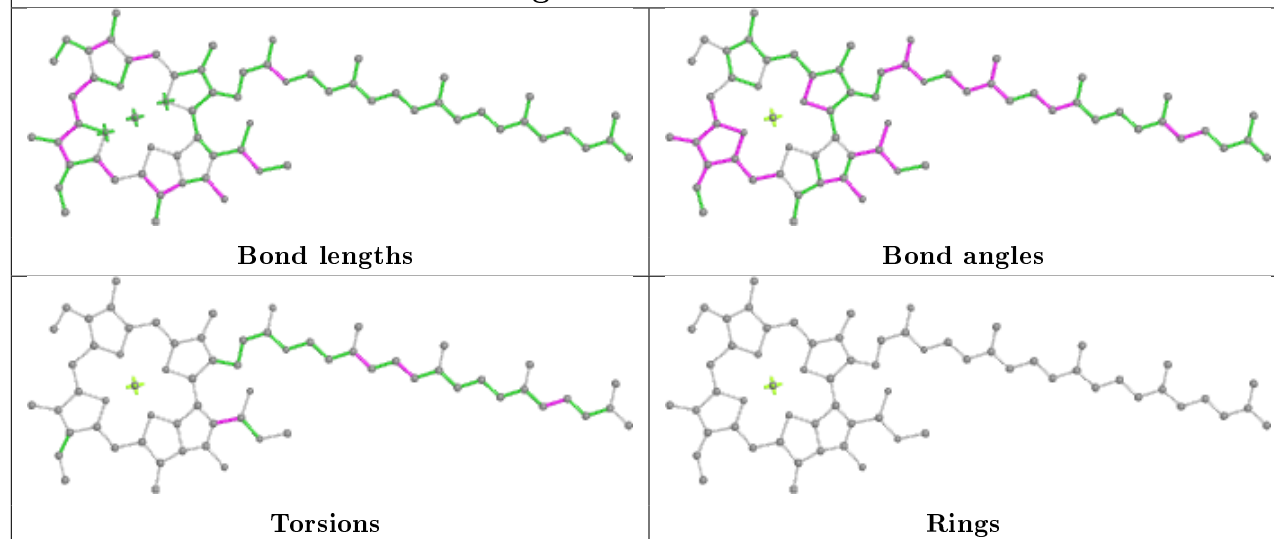
## Ligand LHG d 408



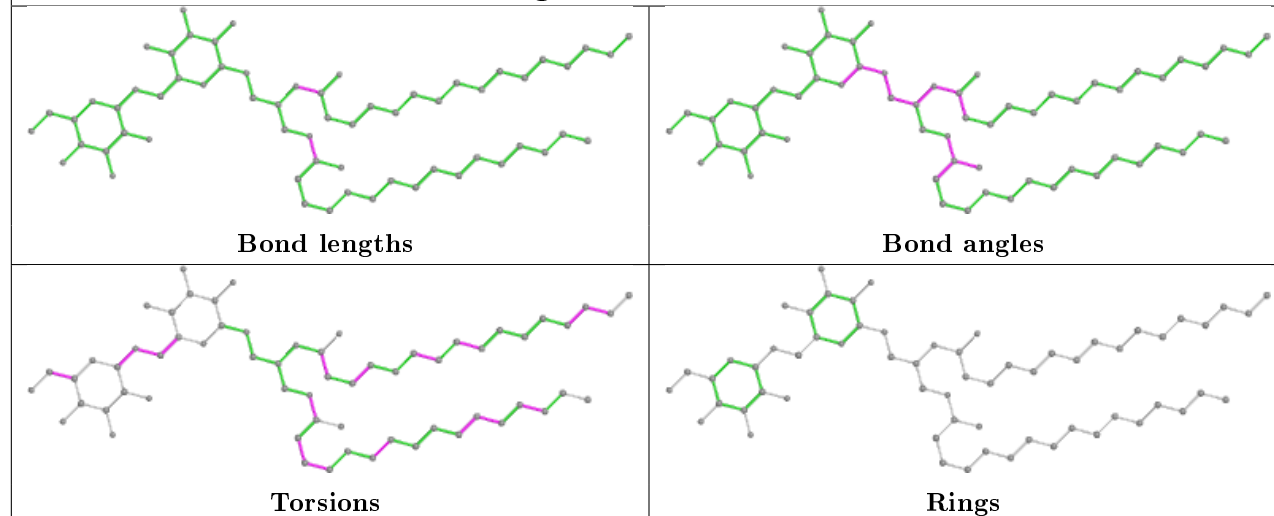
## Ligand BCR c 516



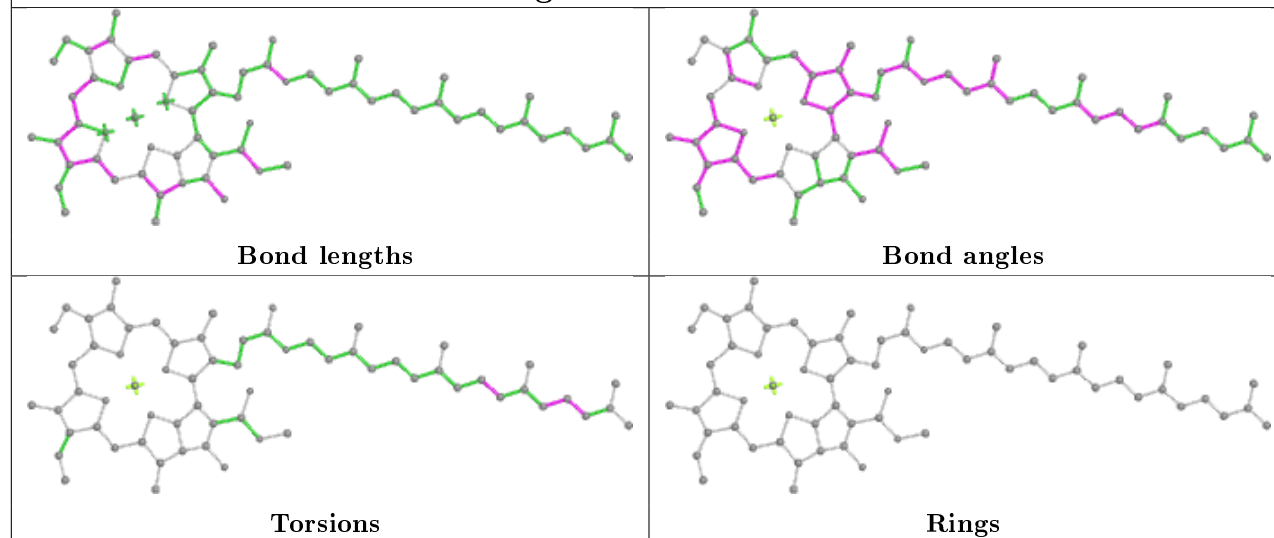
## Ligand CLA C 508

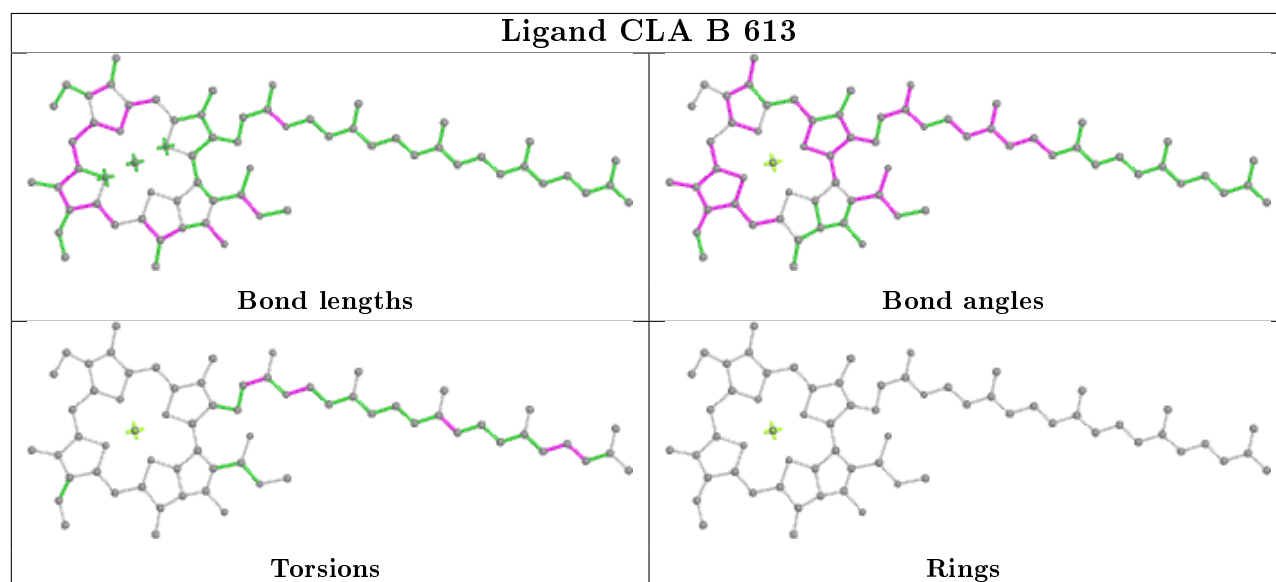
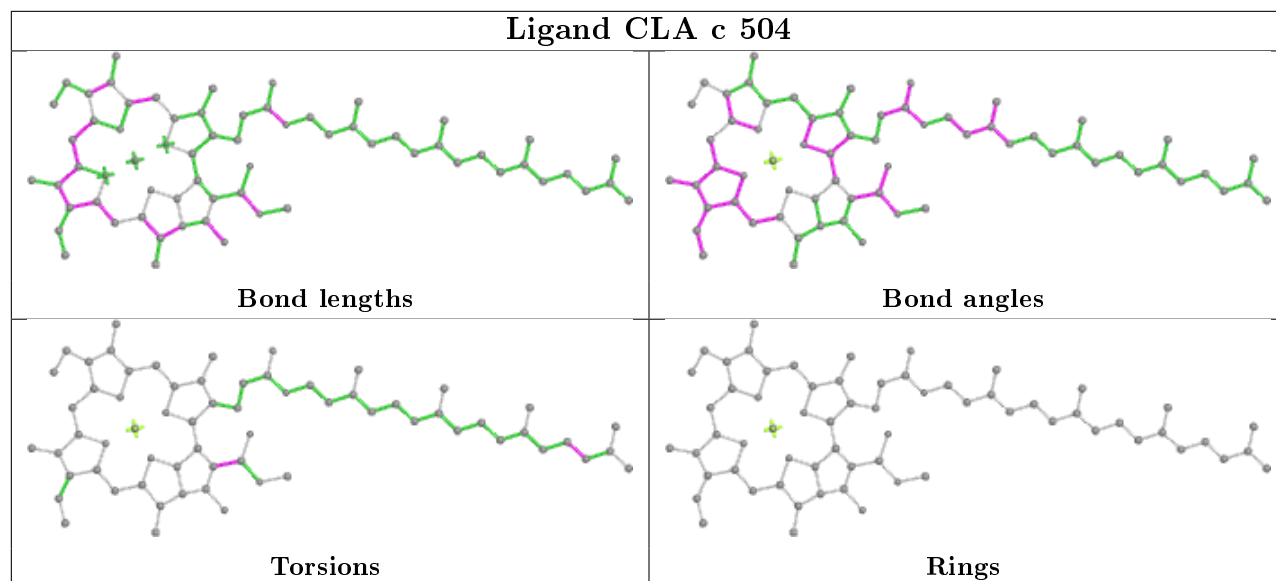
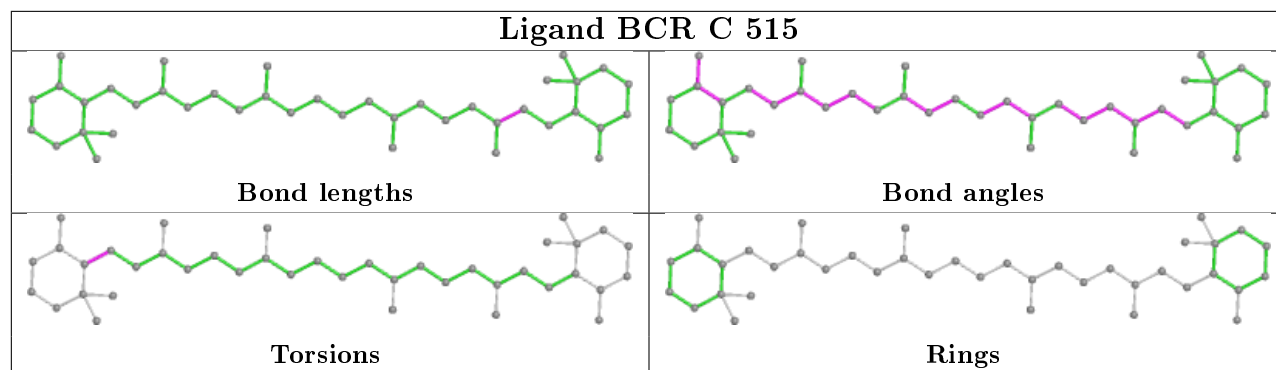


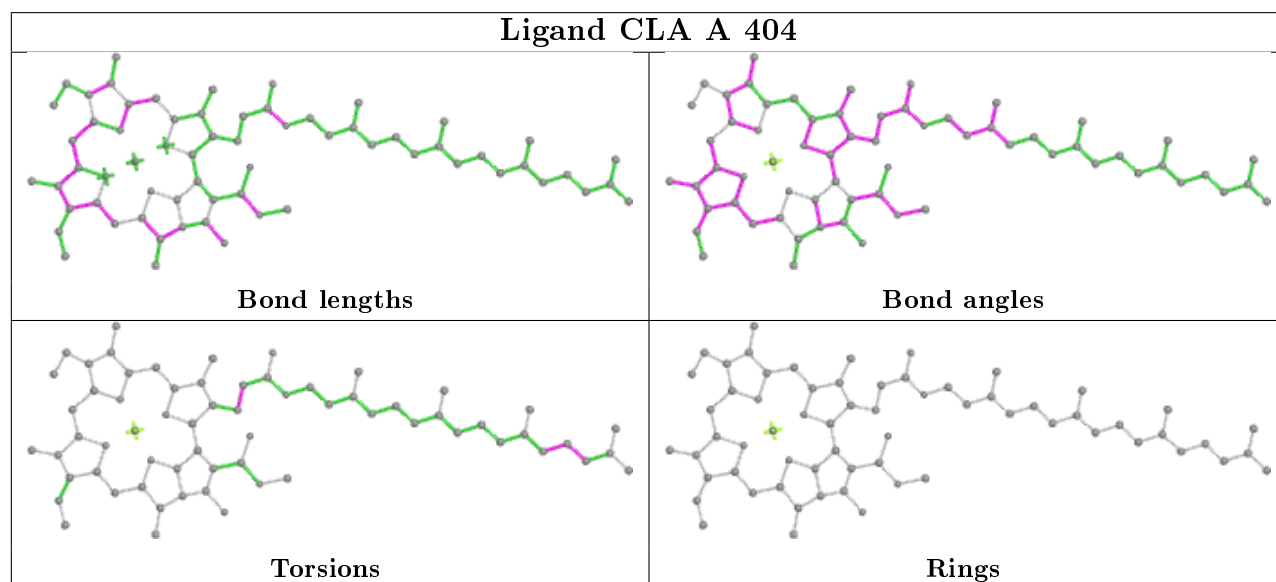
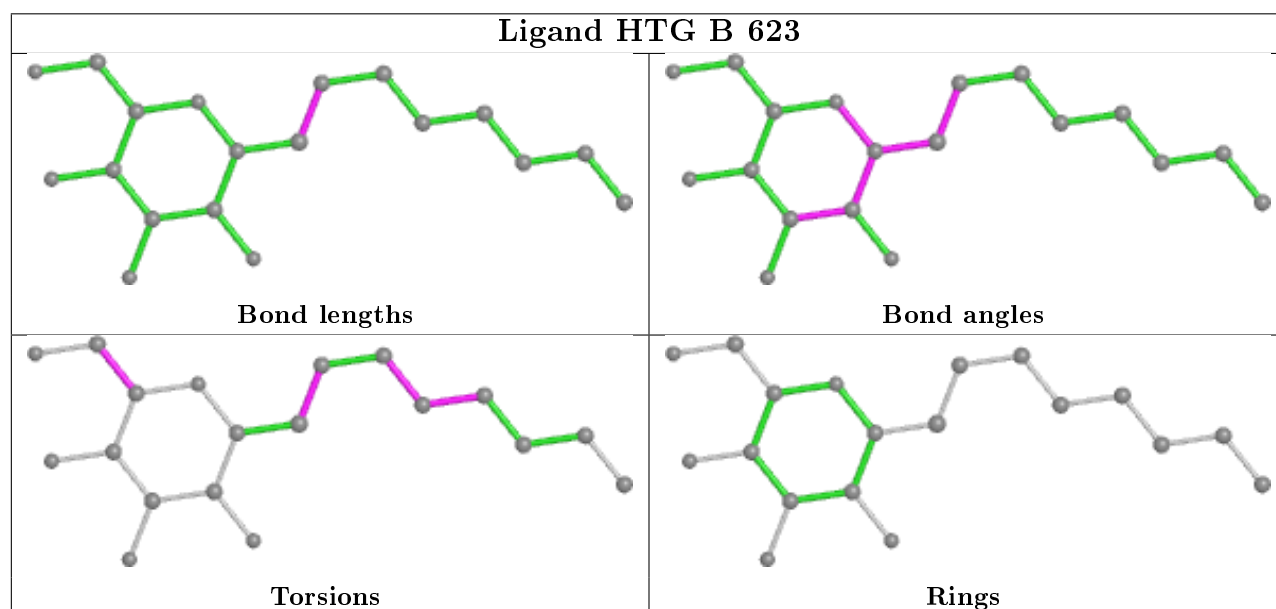
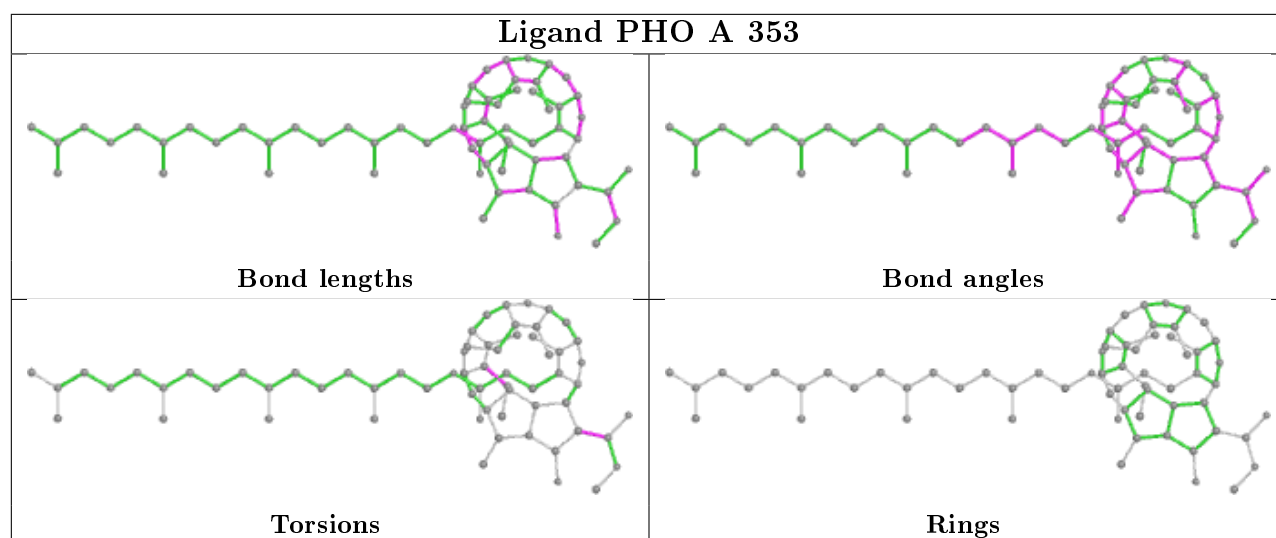
## Ligand DGD c 517



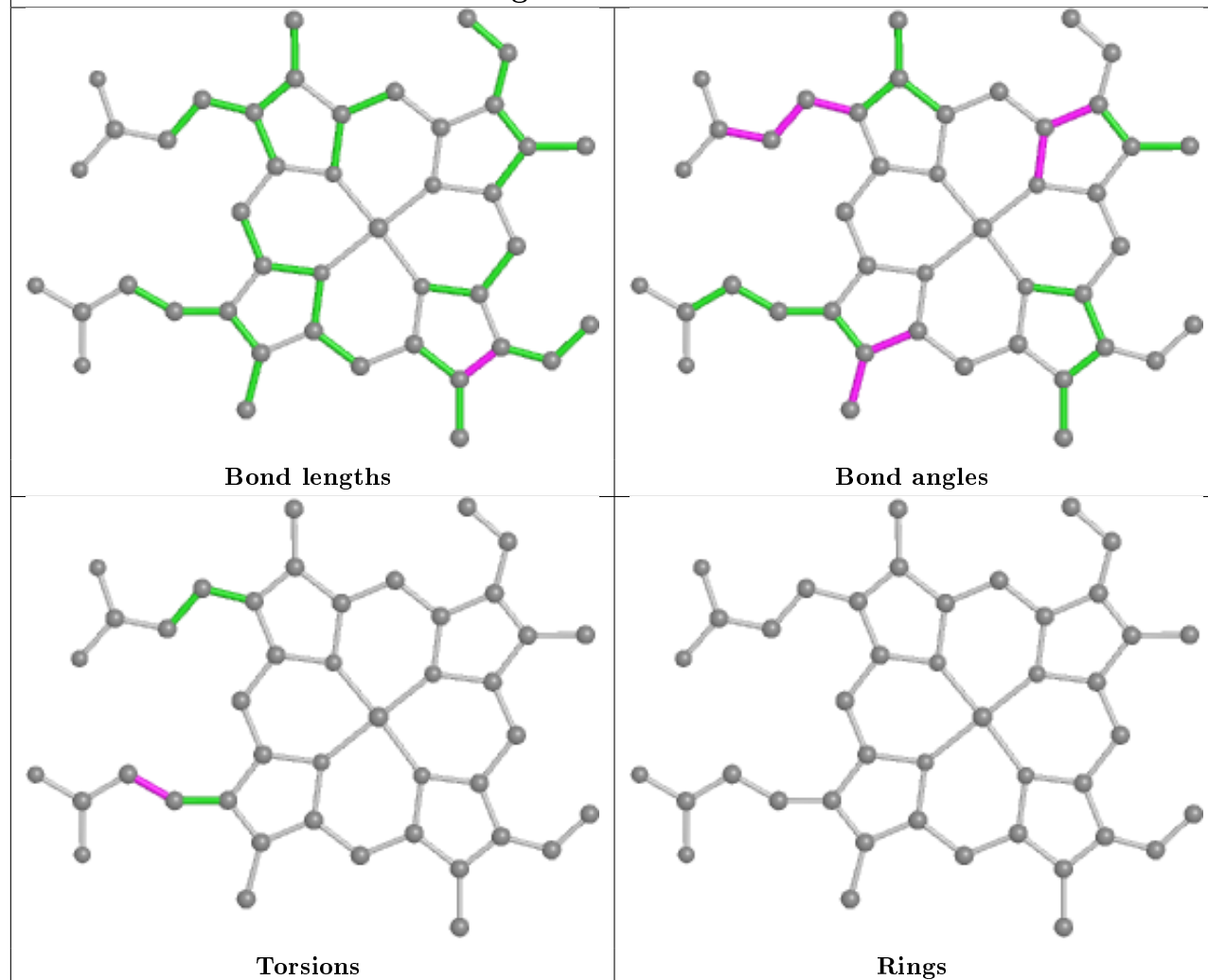
## Ligand CLA b 602



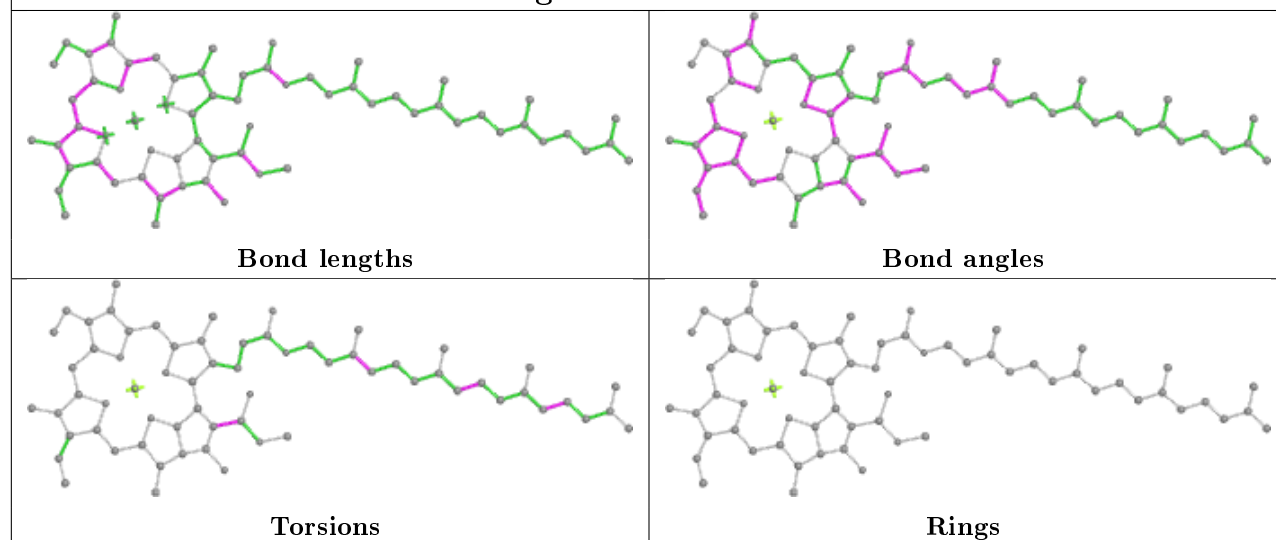




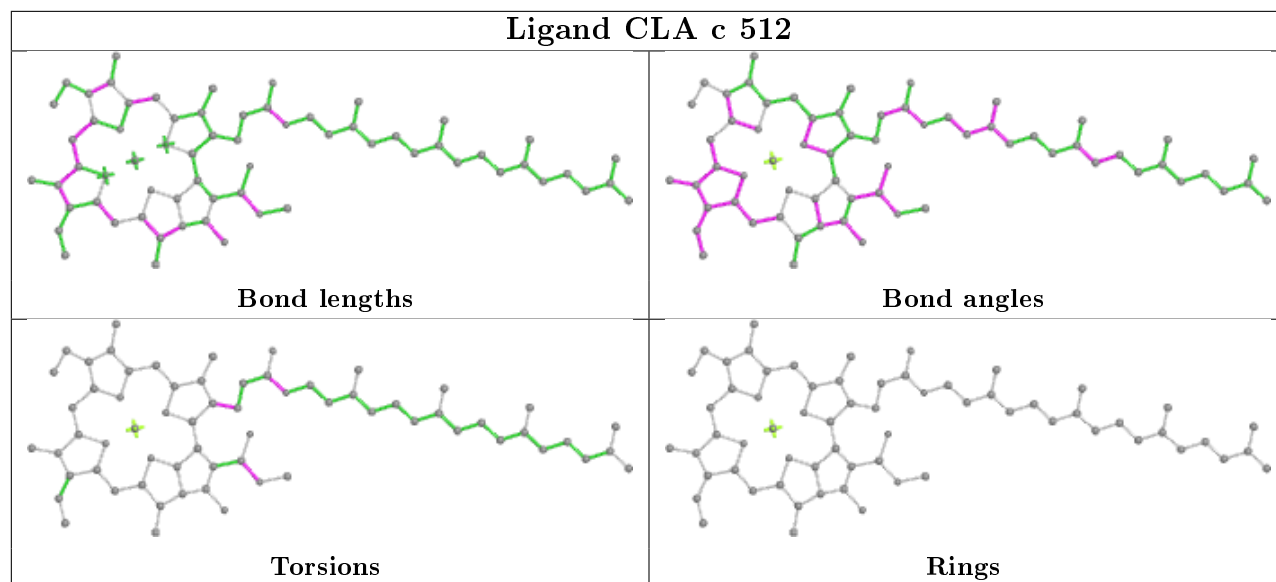
## Ligand HEM e 87



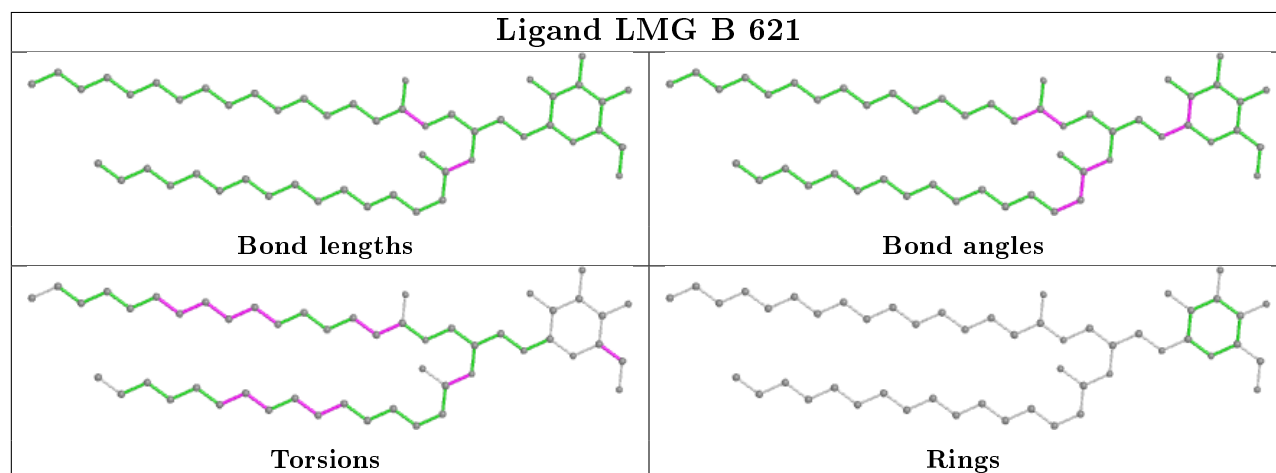
## Ligand CLA b 605



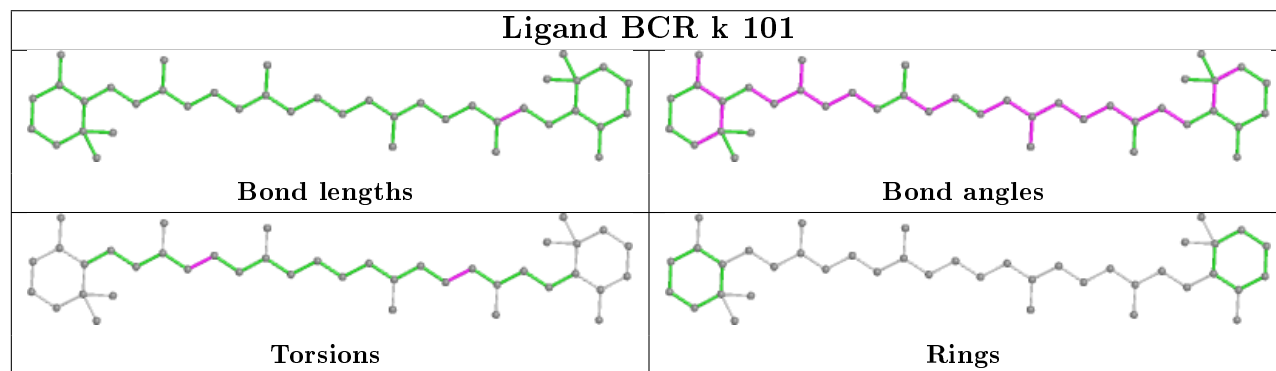
## Ligand CLA c 512

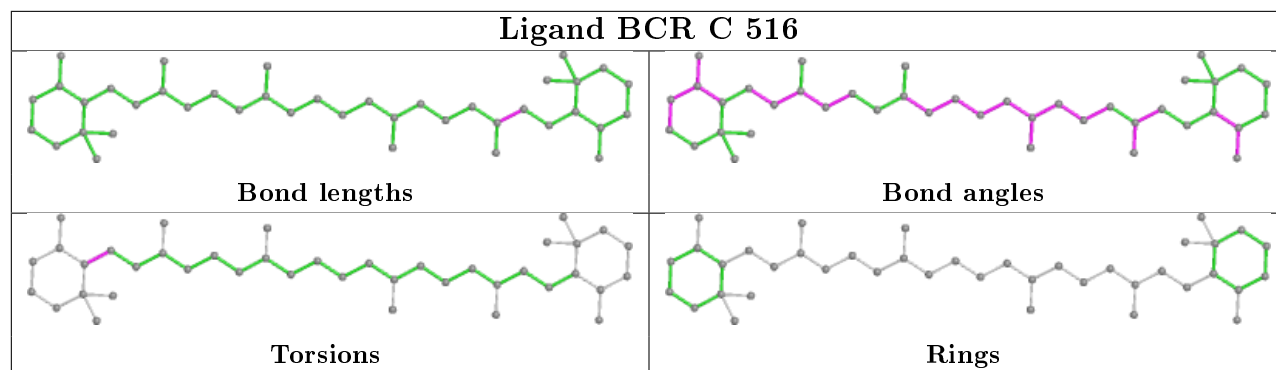
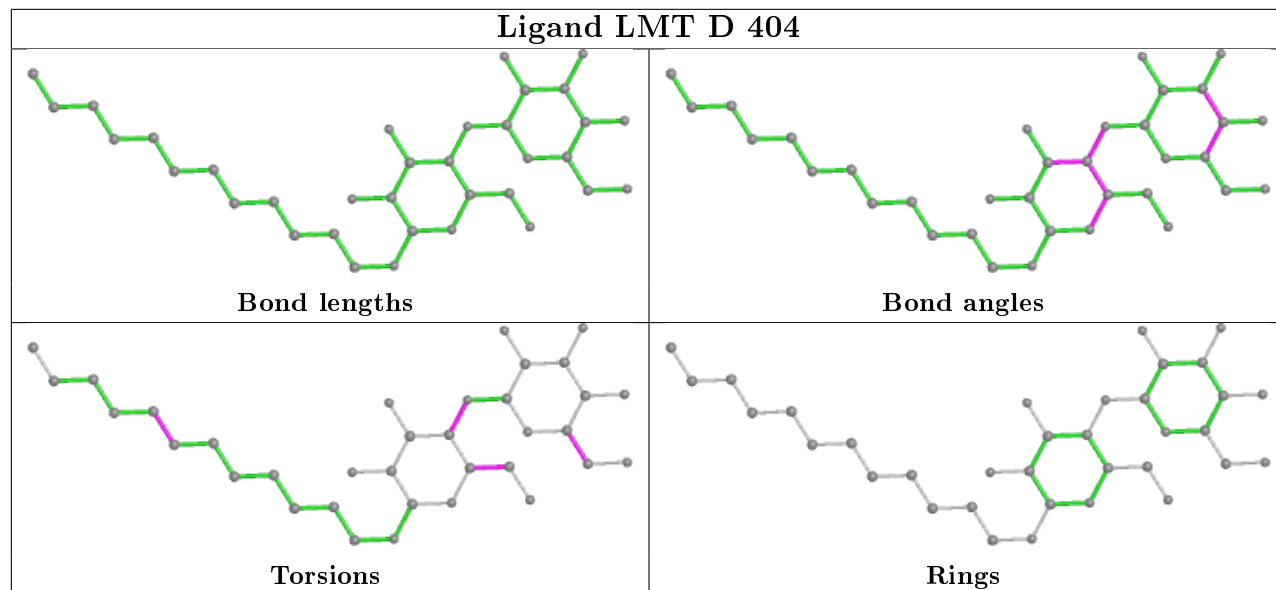
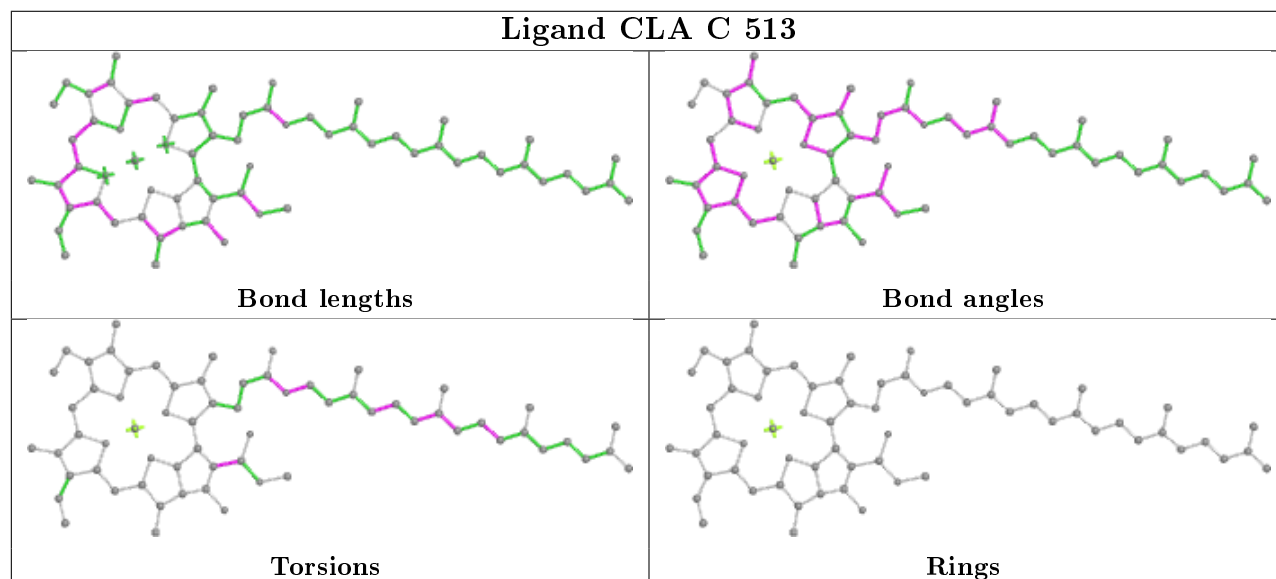


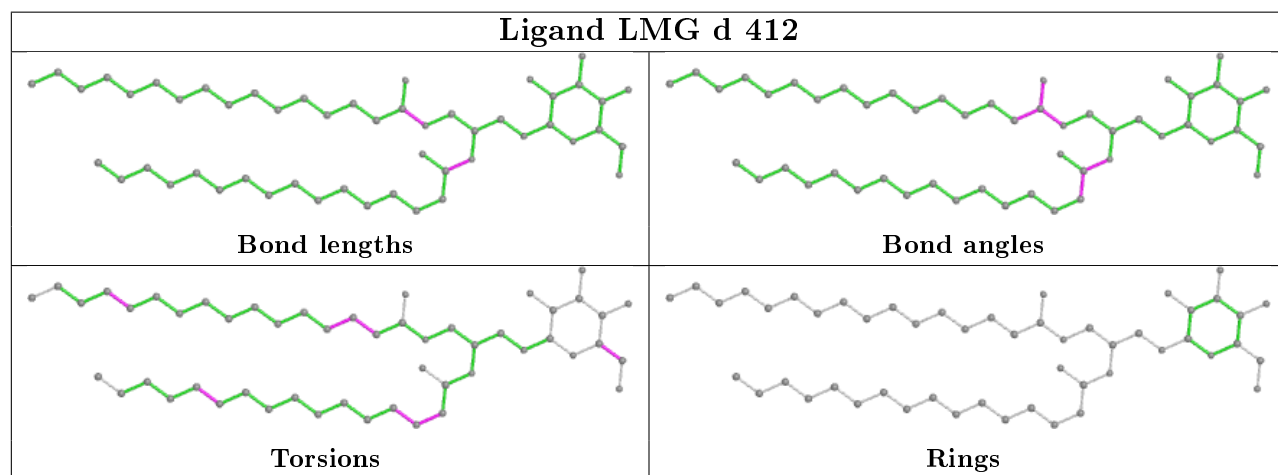
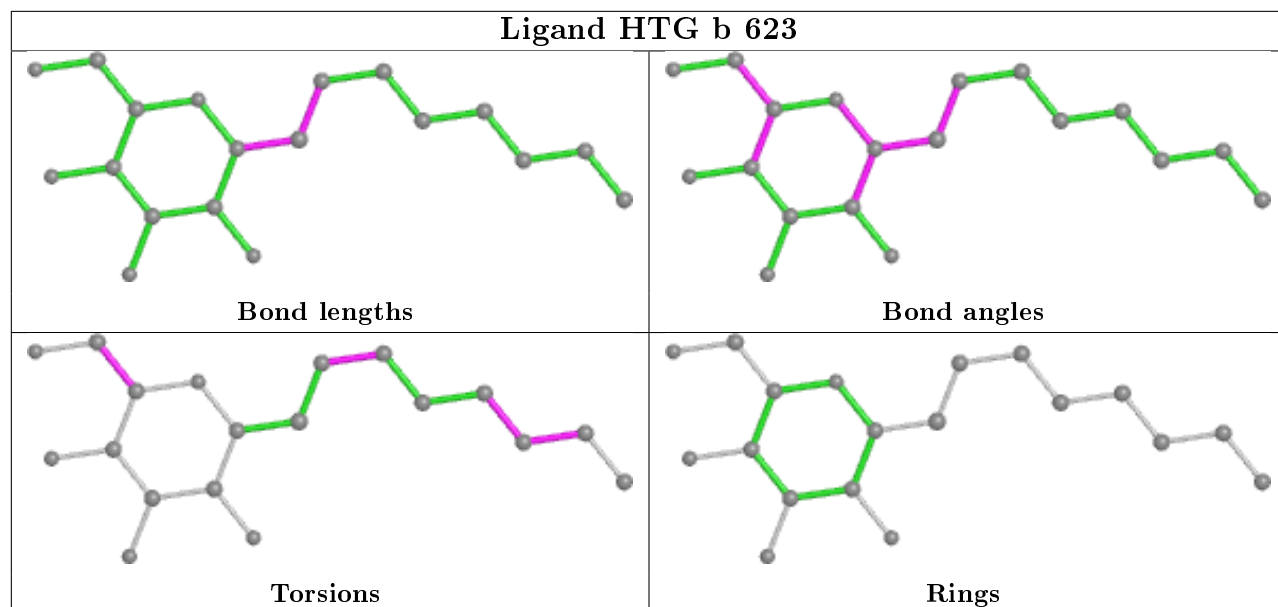
## Ligand LMG B 621



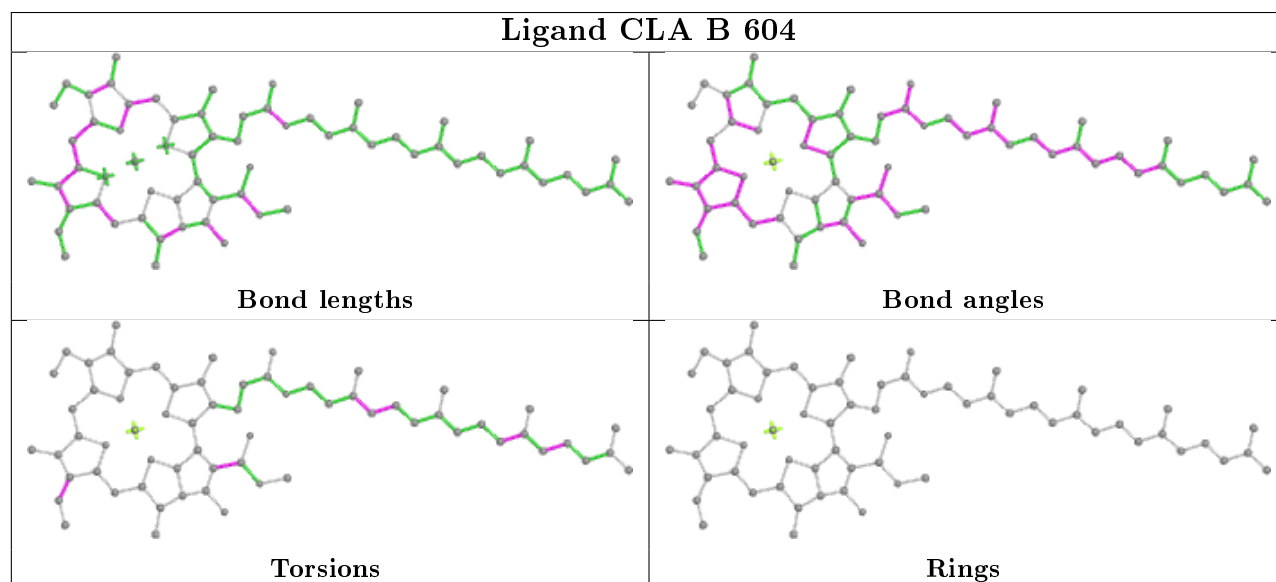
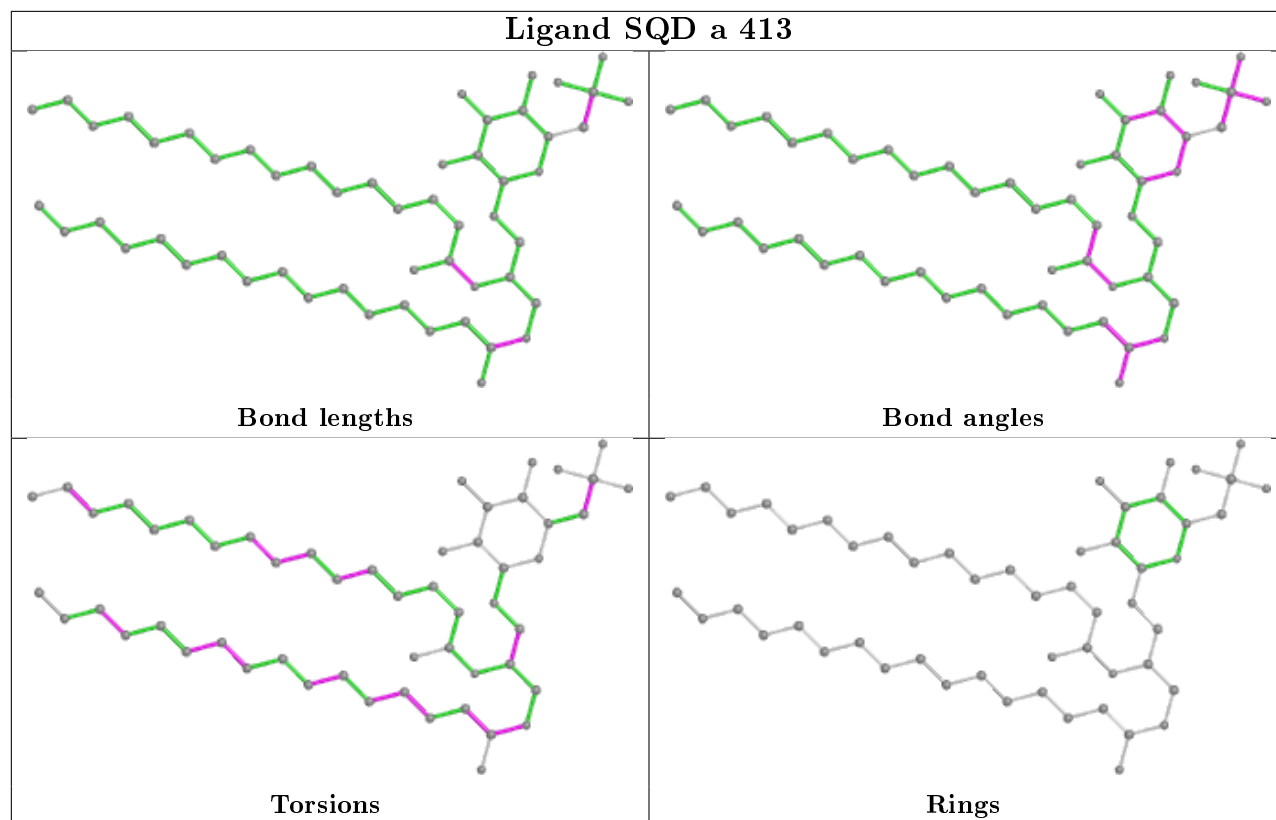
## Ligand BCR k 101

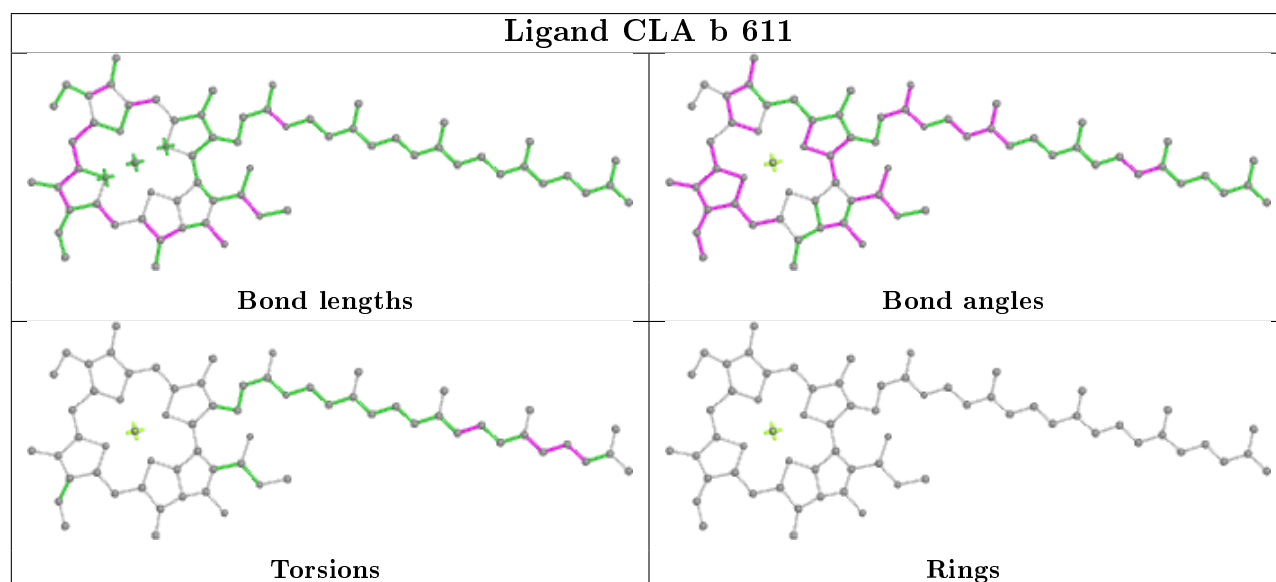
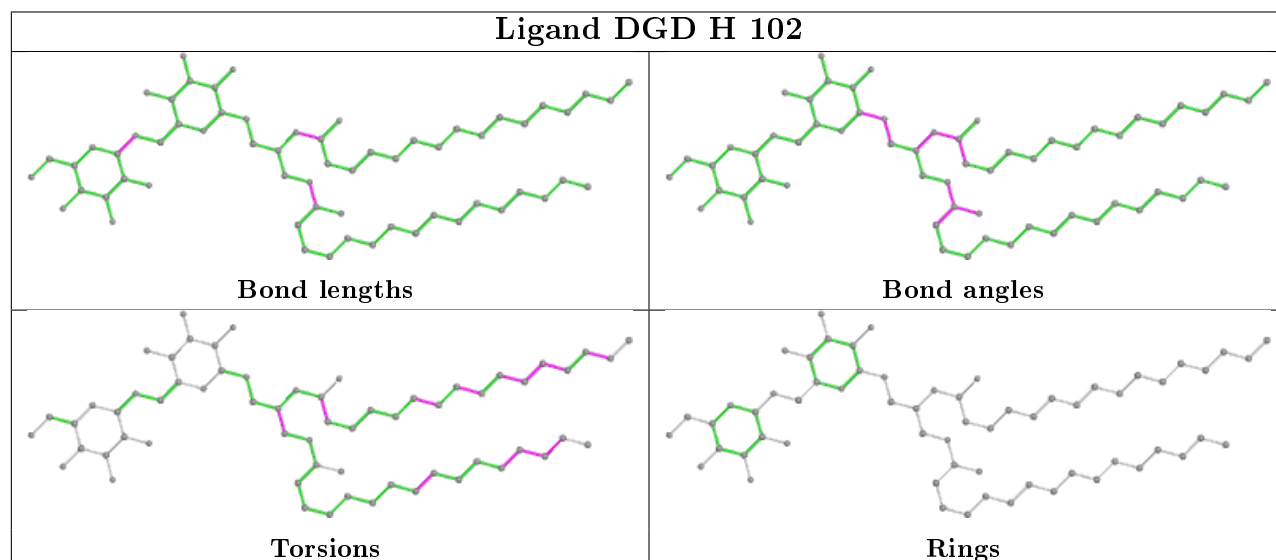
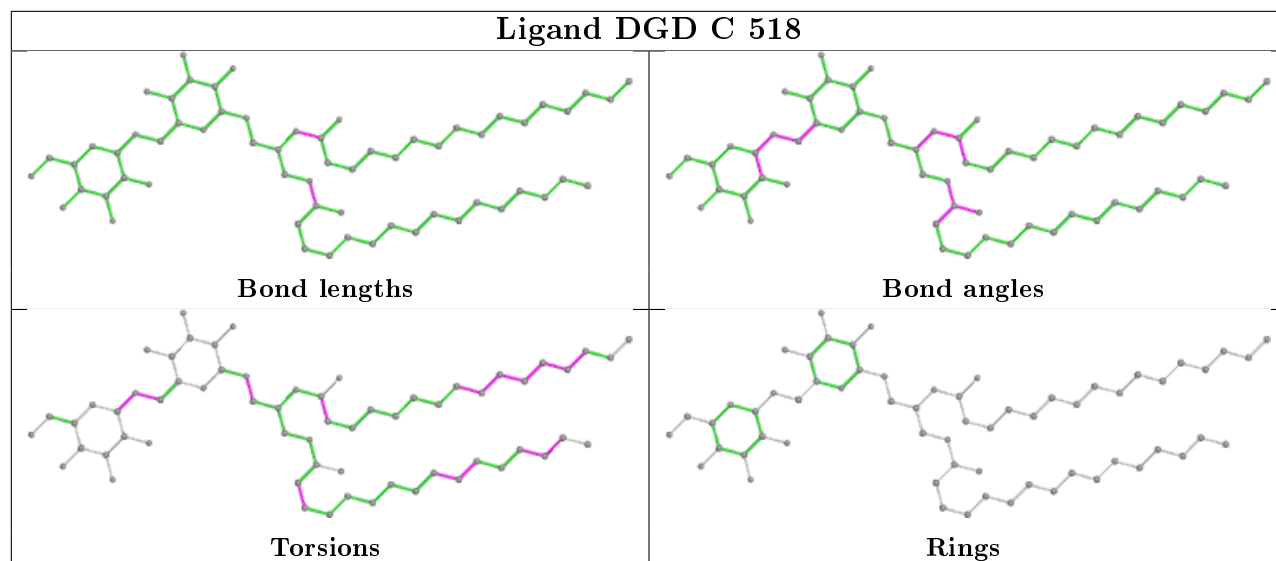


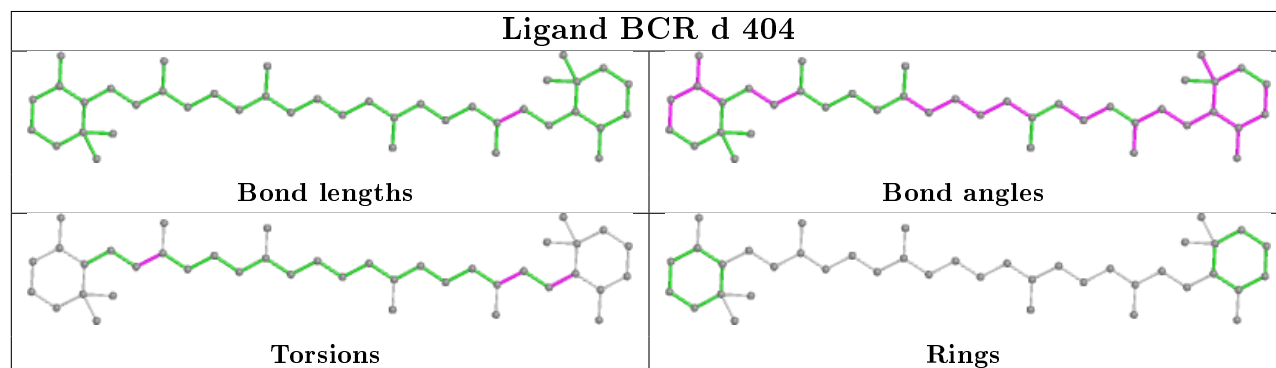
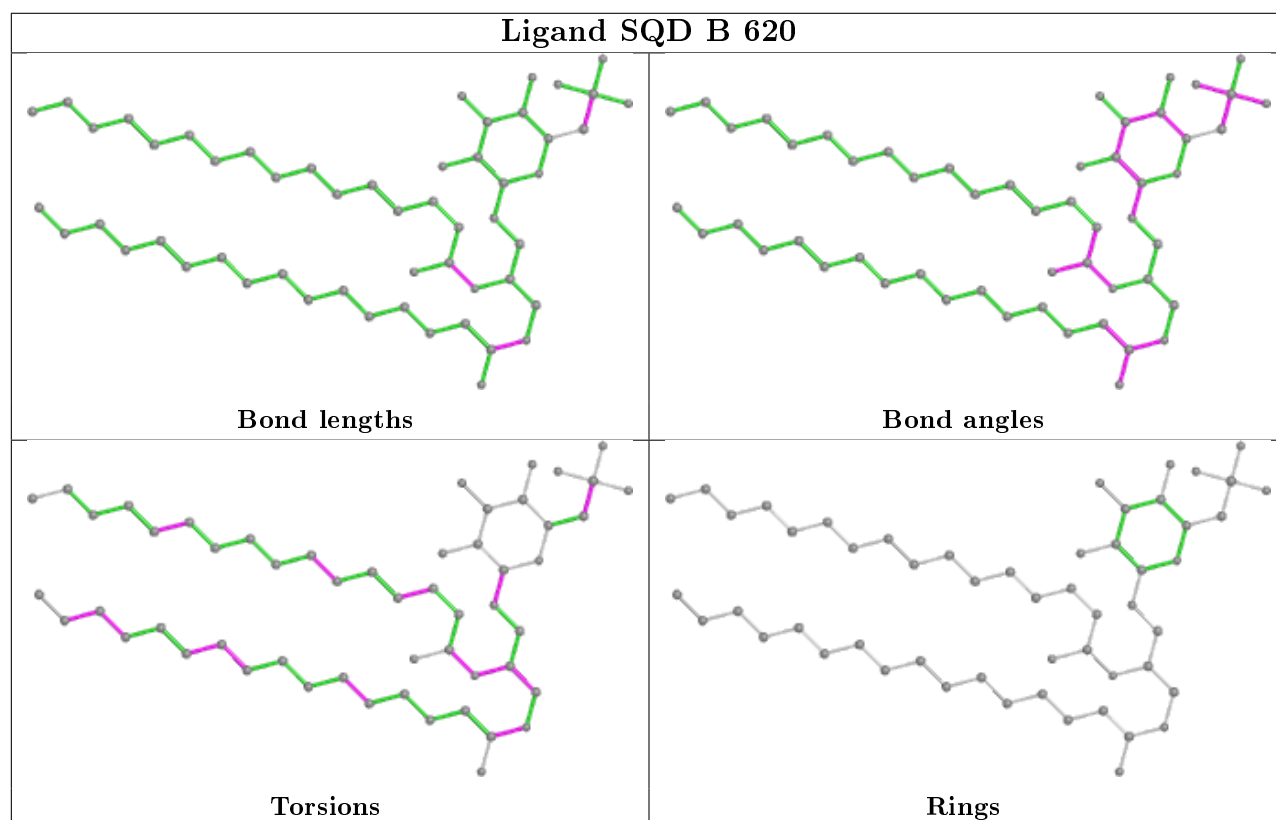
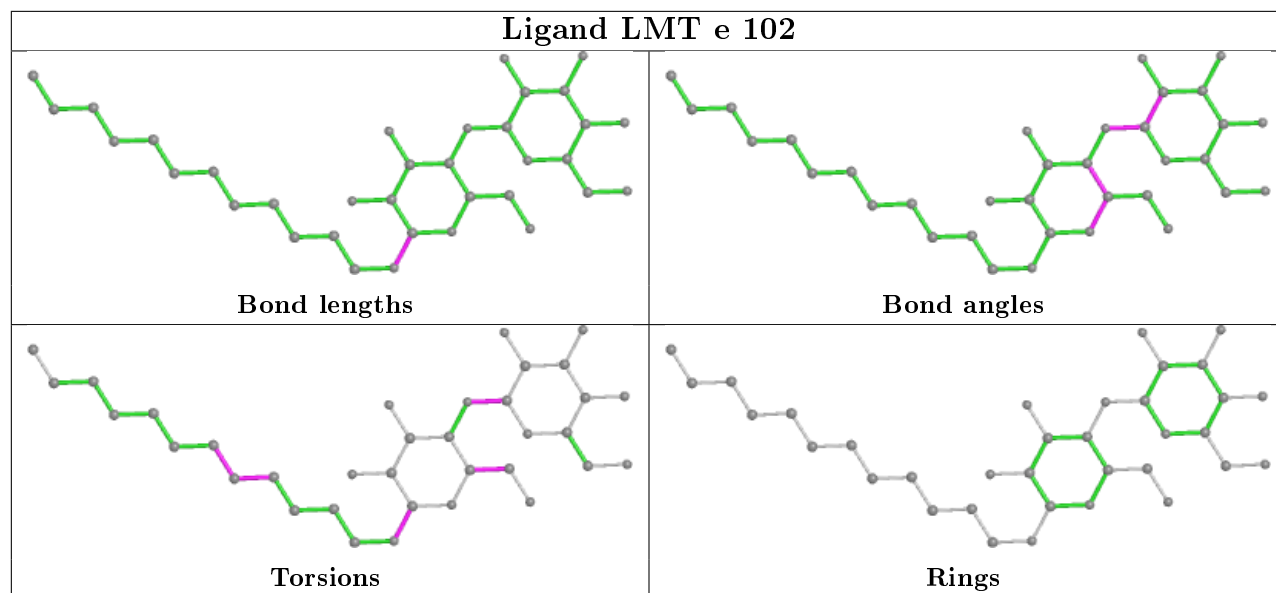
**Ligand BCR C 516****Ligand LMT D 404****Ligand CLA C 513**

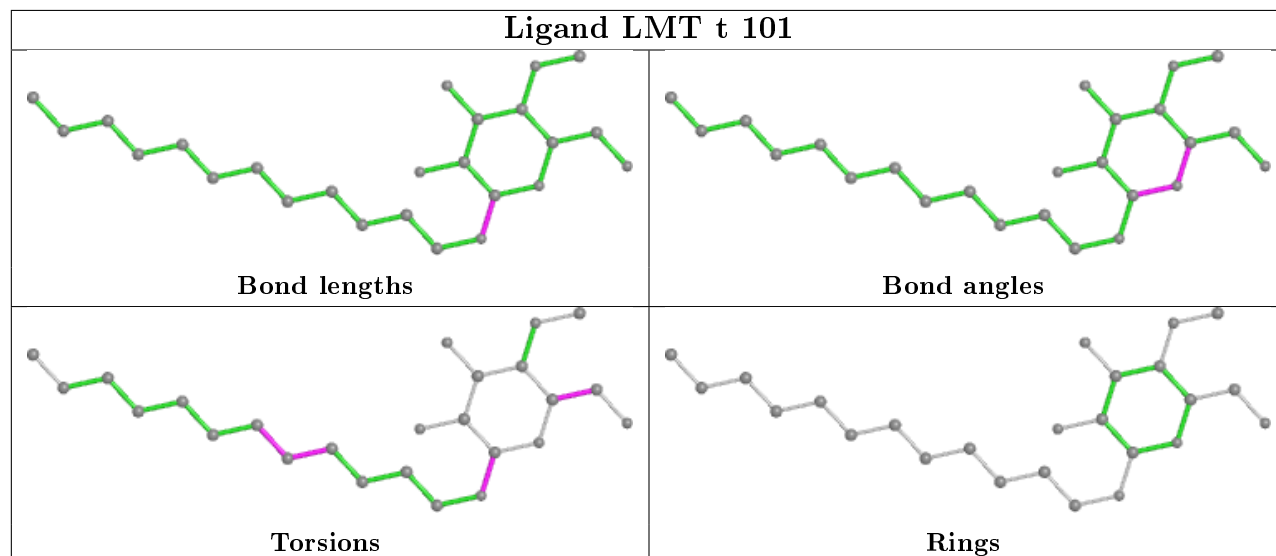
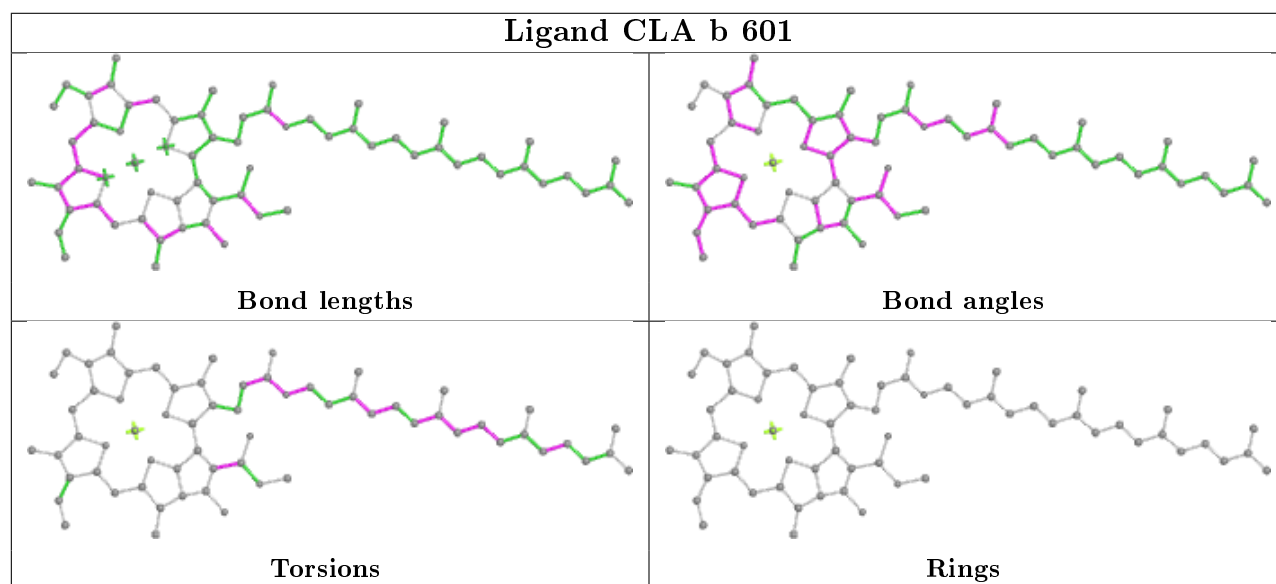
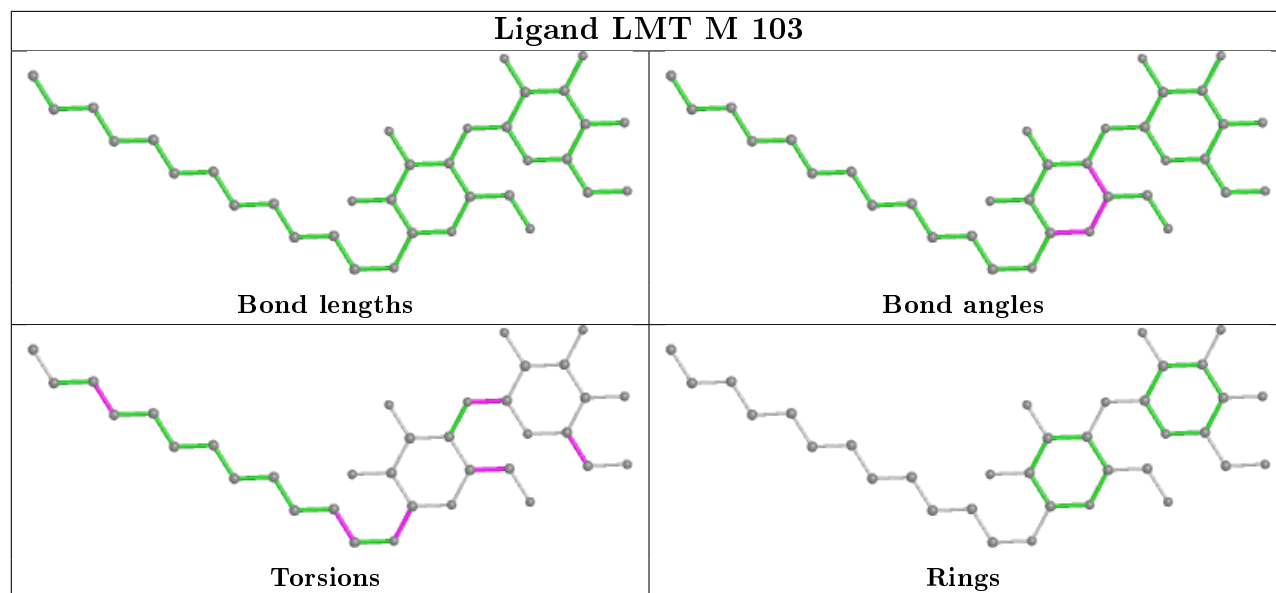


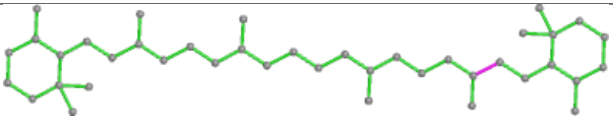
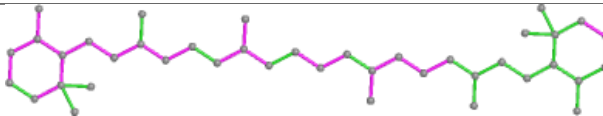
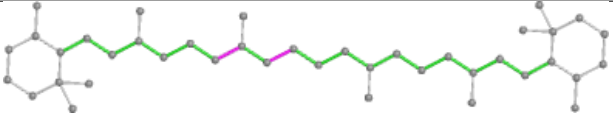
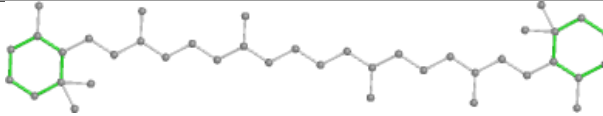


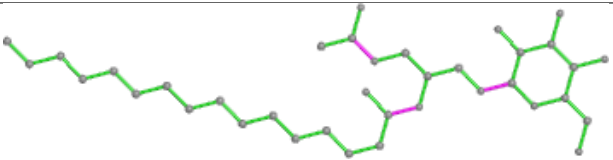
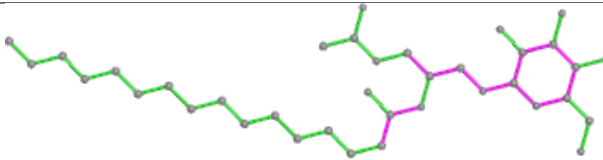
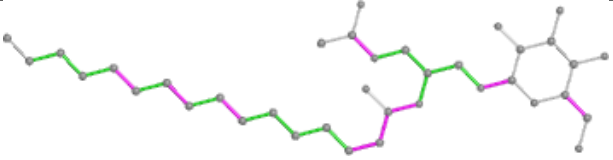
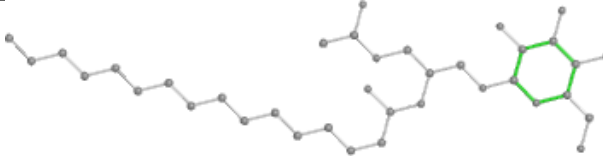


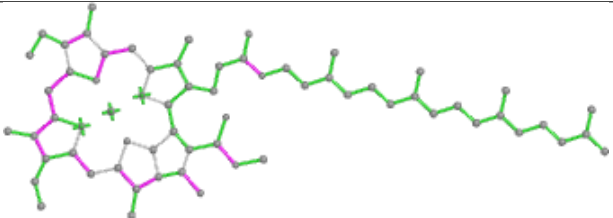
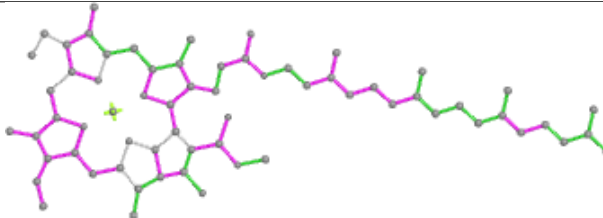
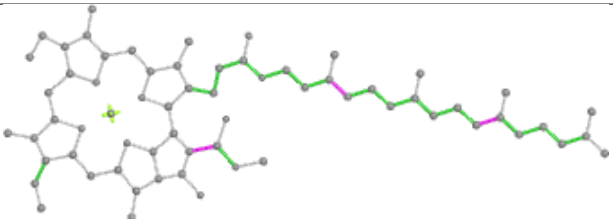
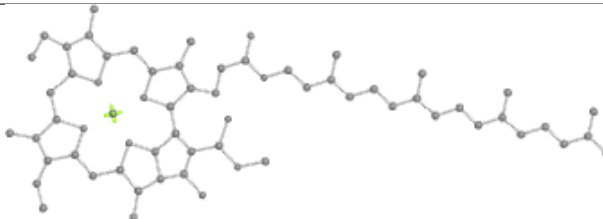


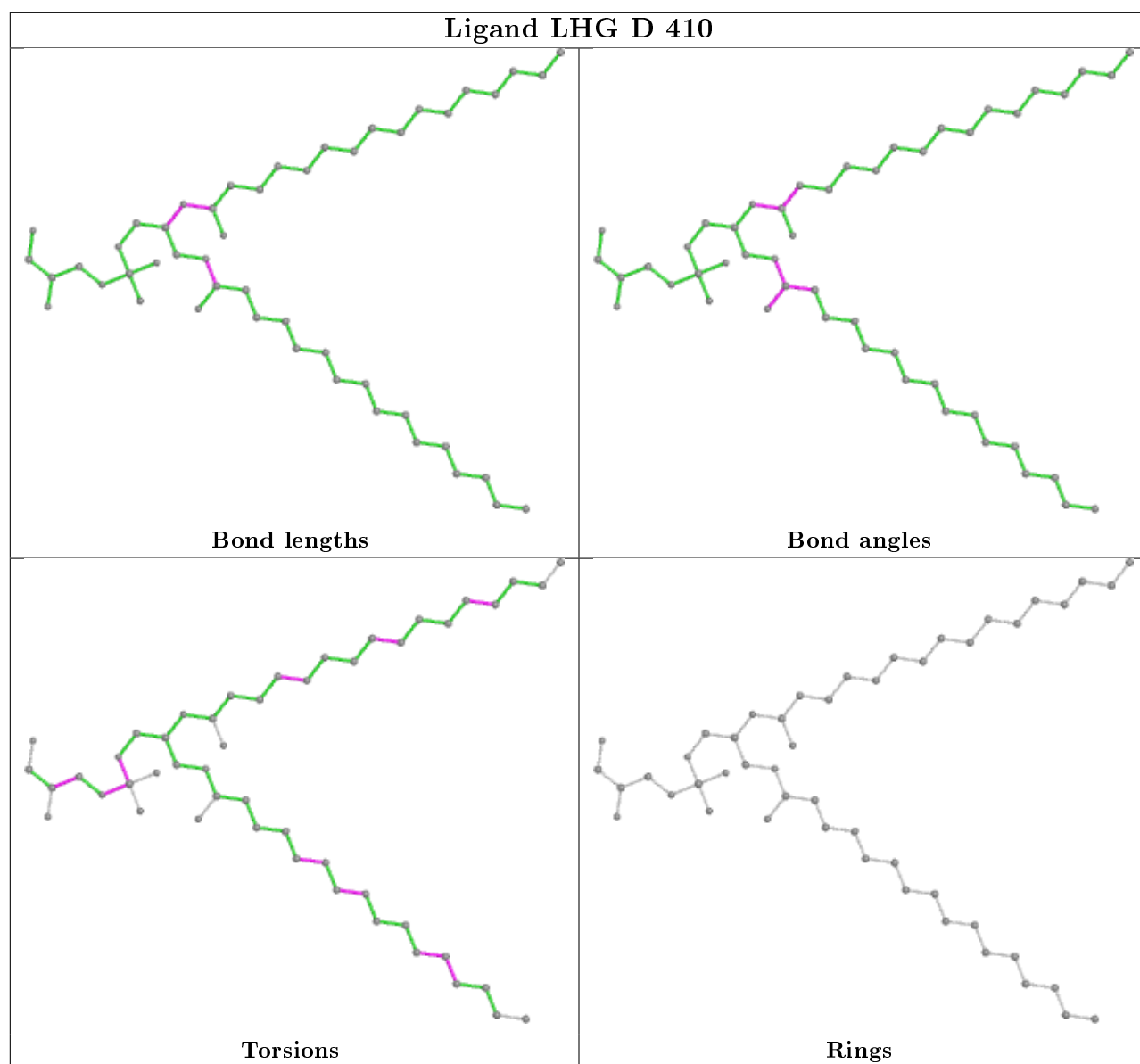


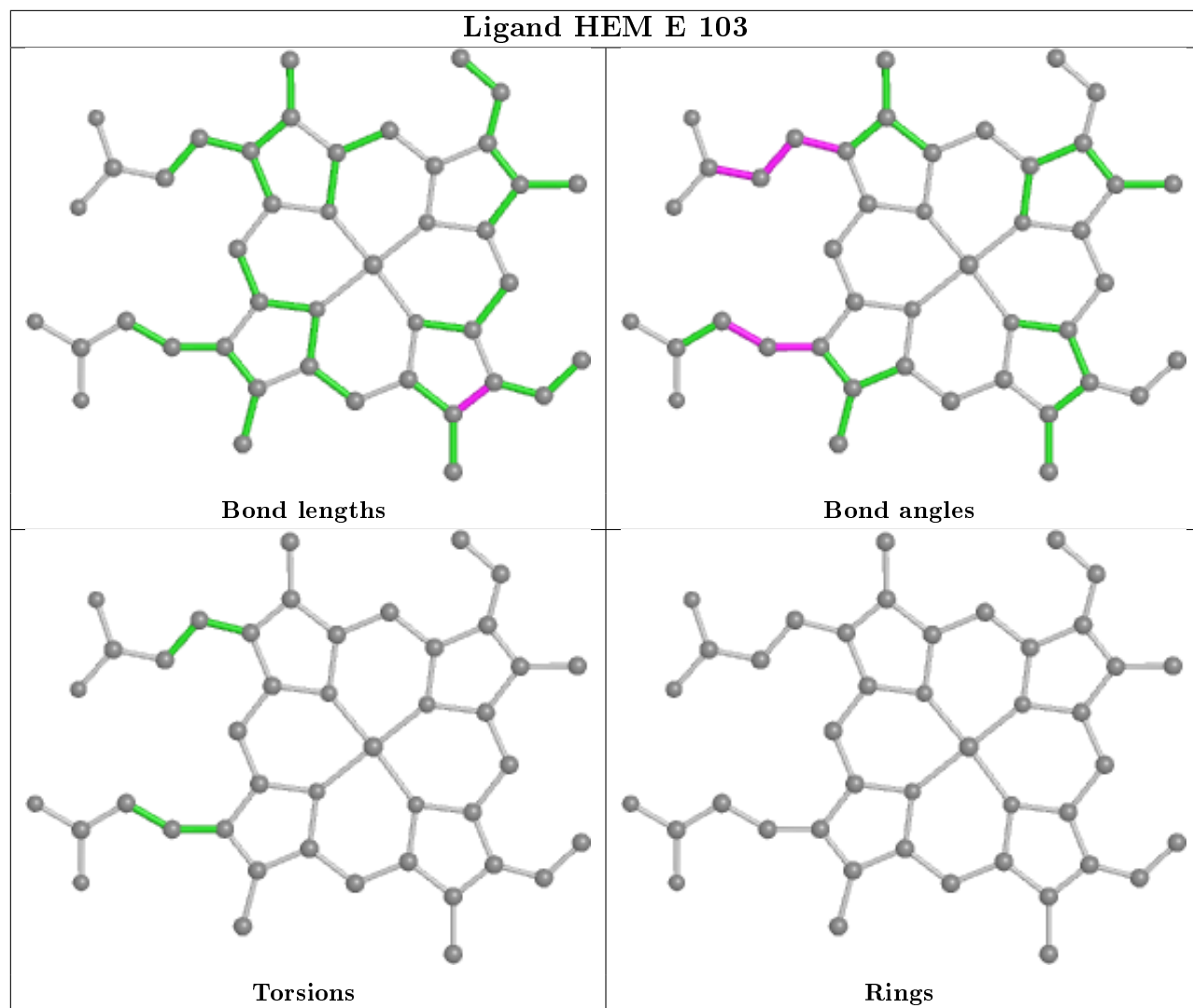


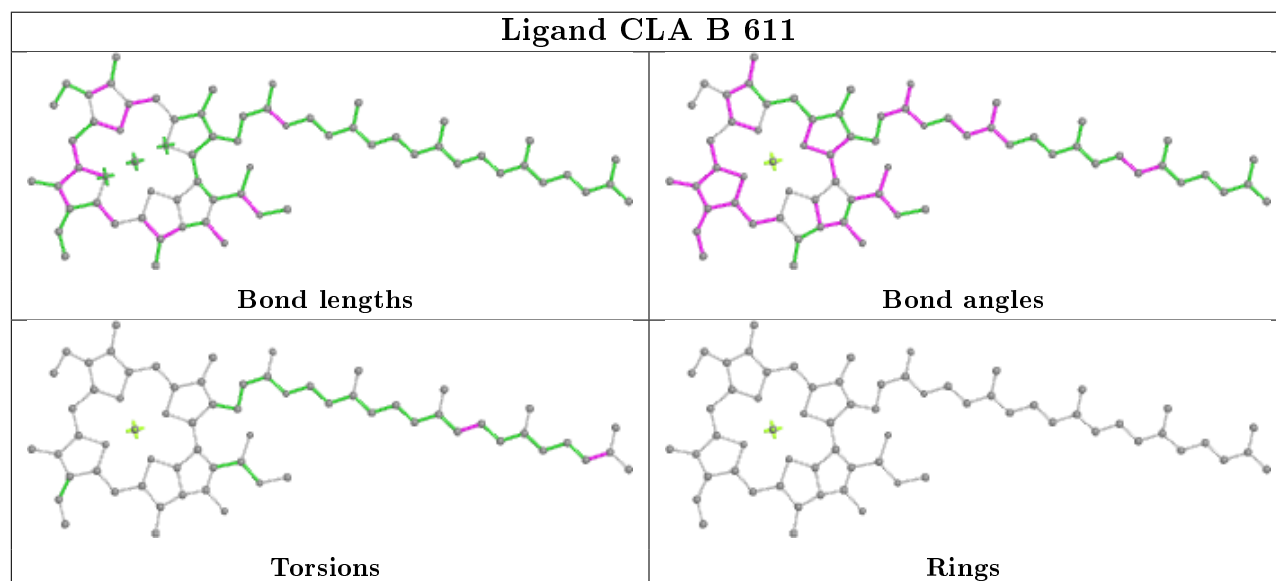
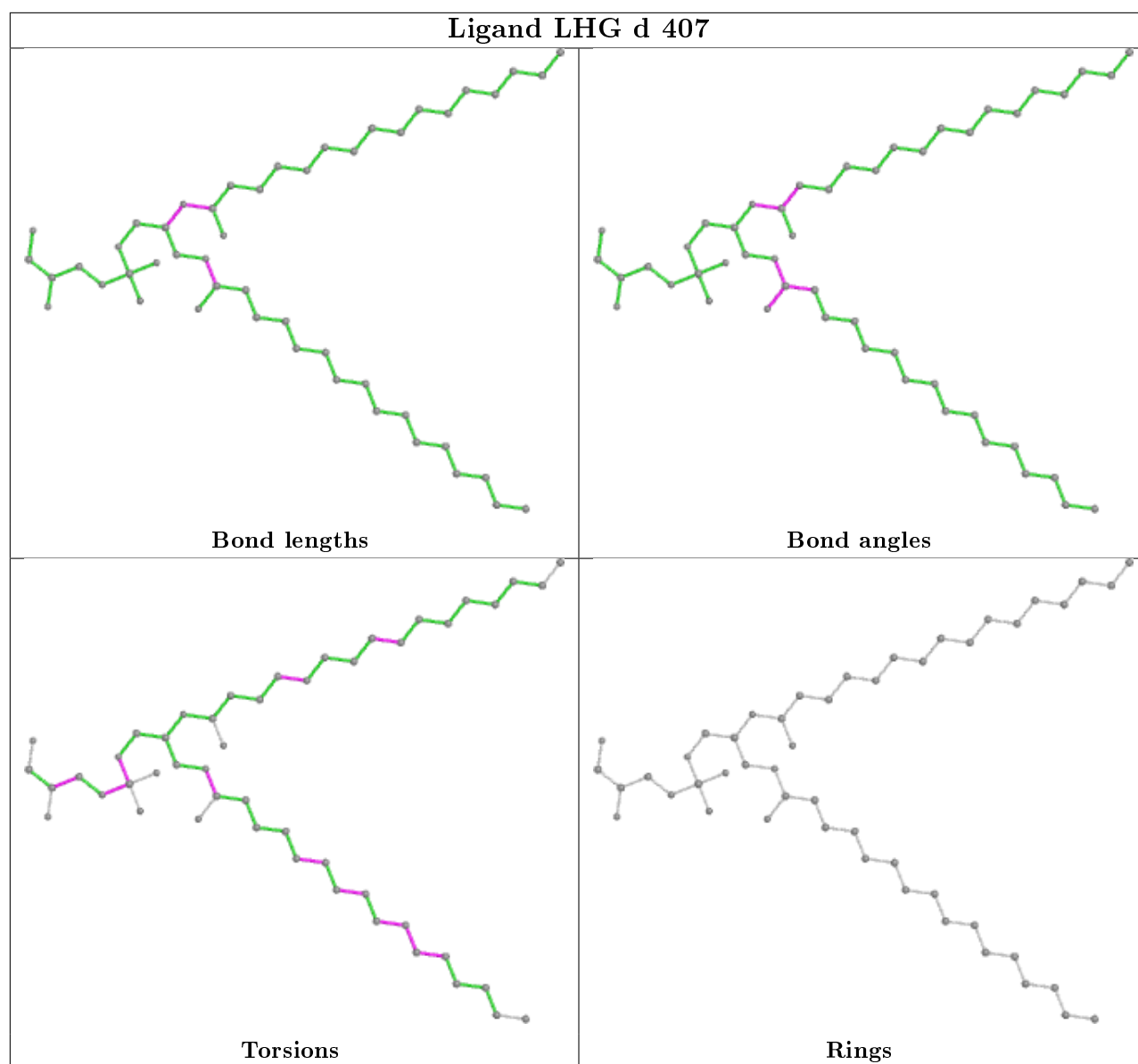
Ligand BCR T 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG Z 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

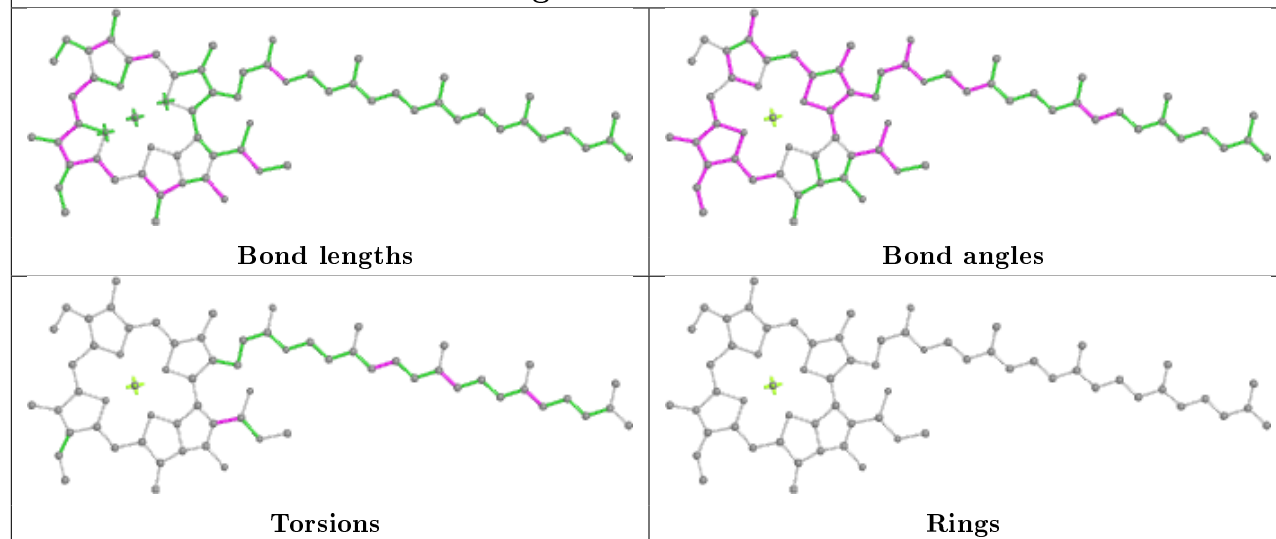




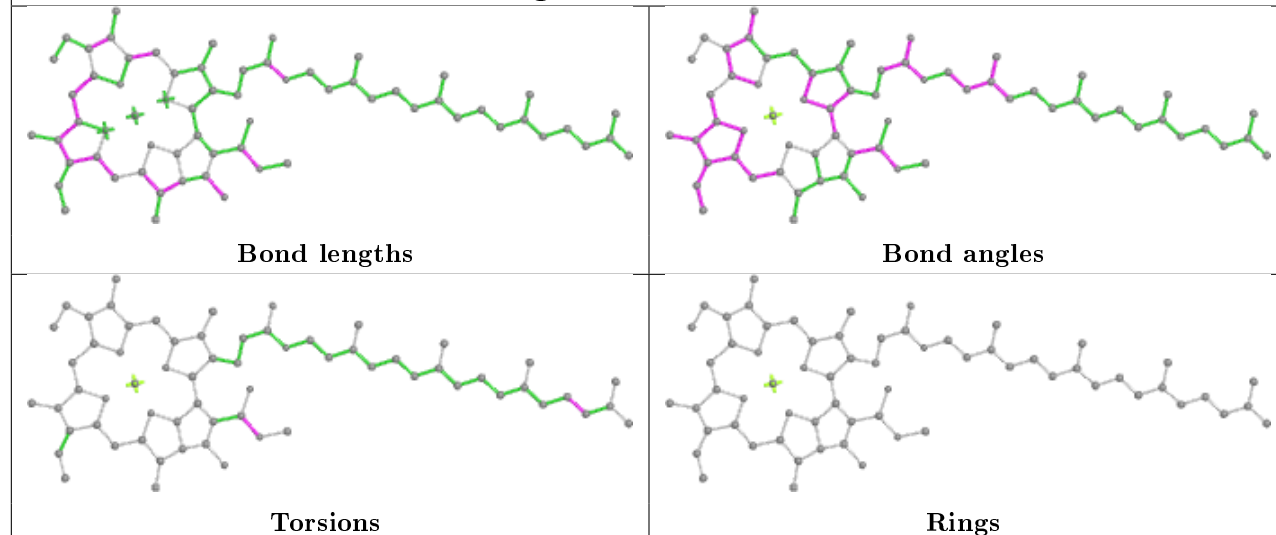




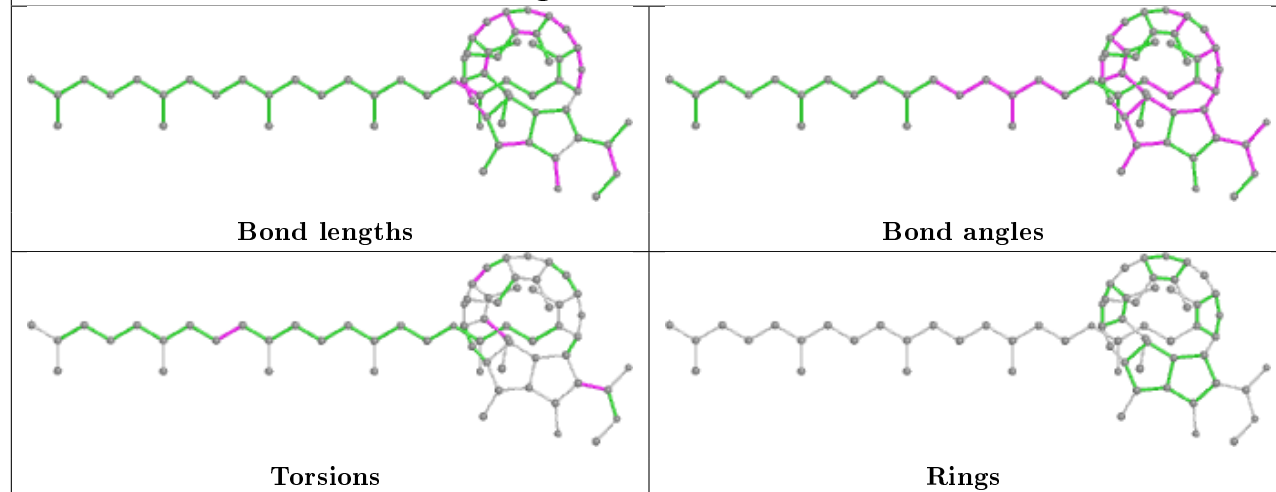
## Ligand CLA A 406

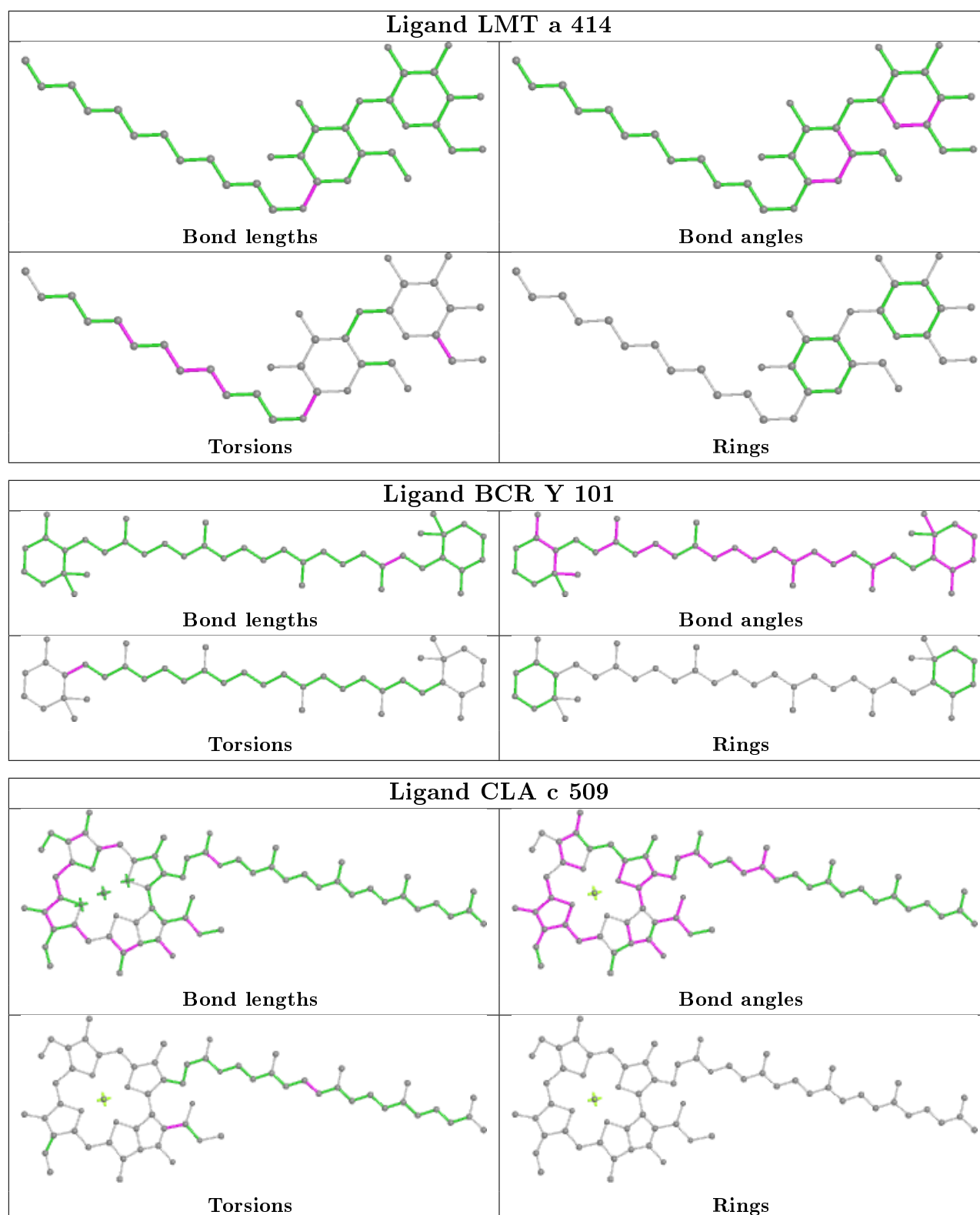


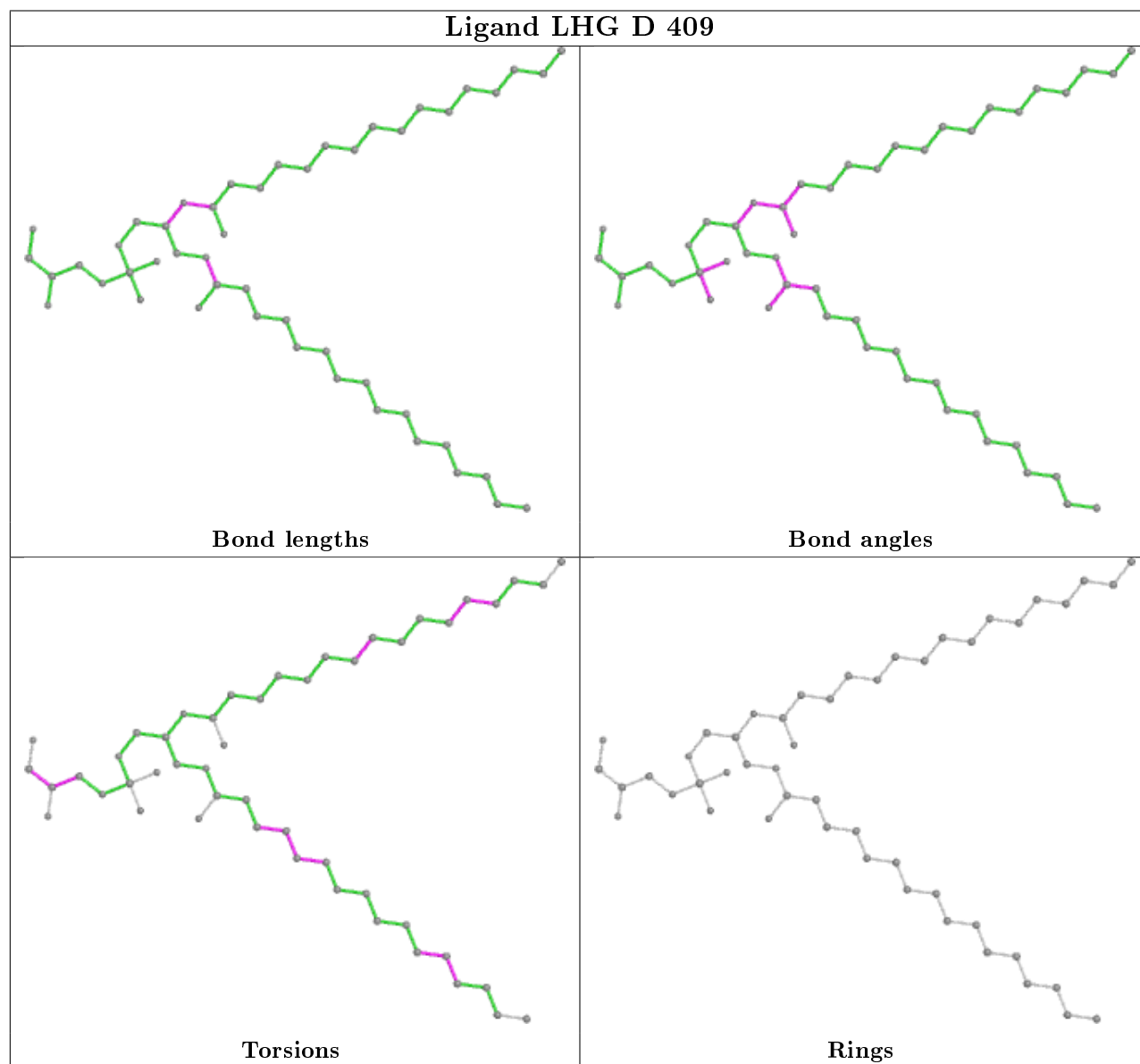
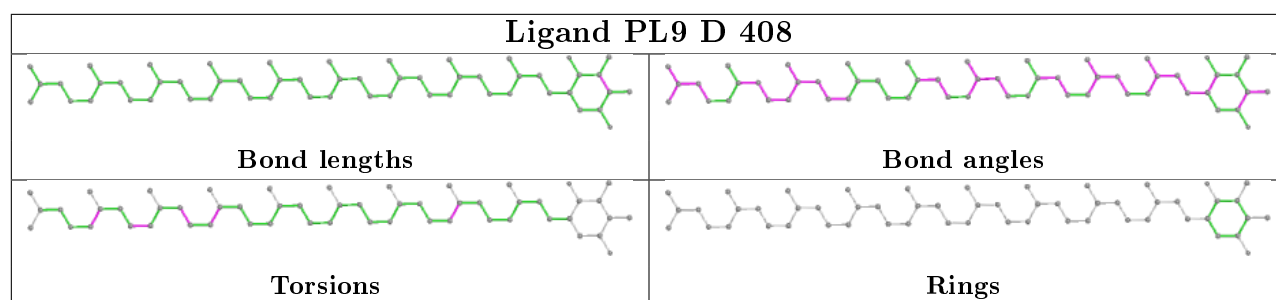
## Ligand CLA C 504



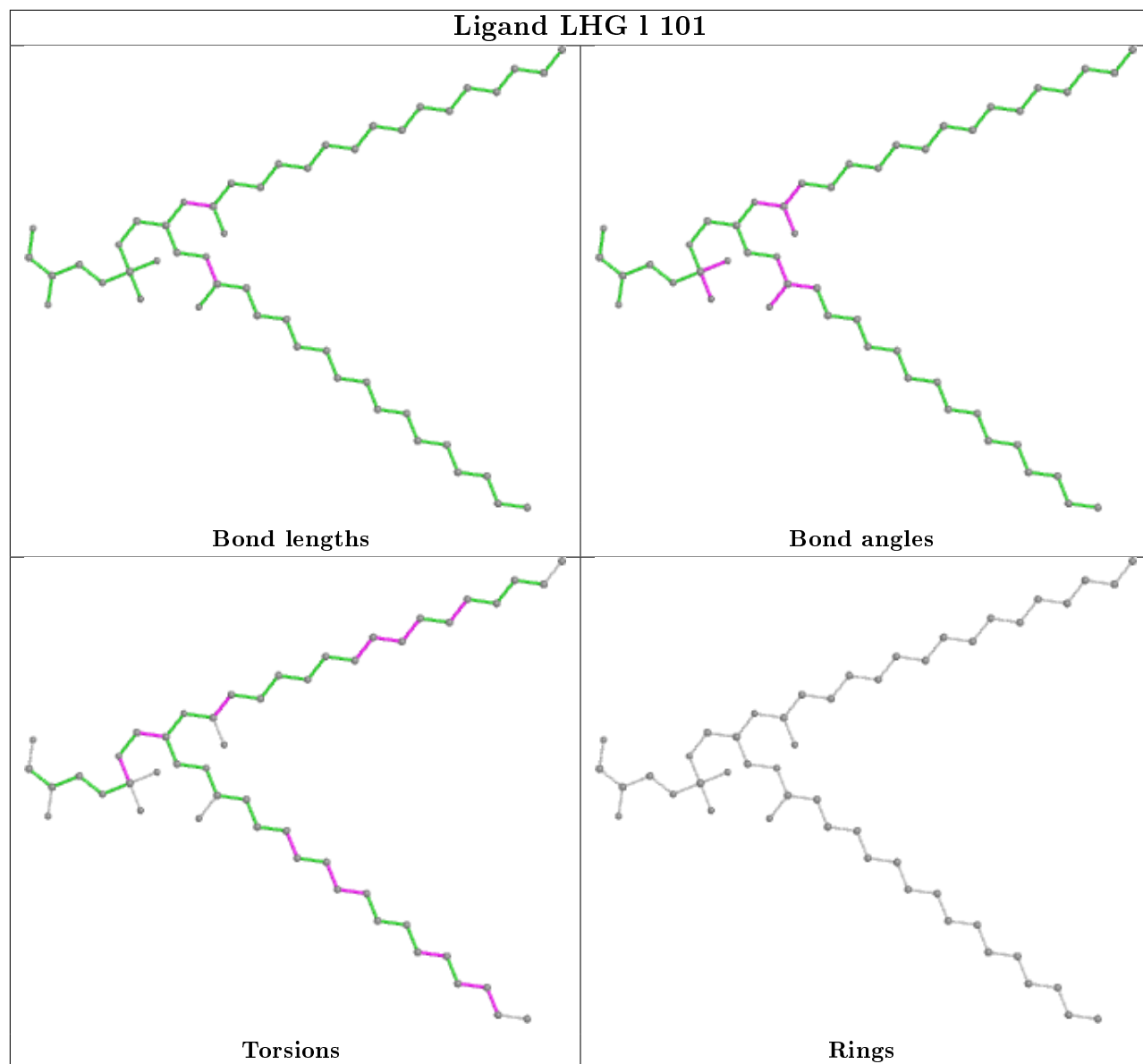
## Ligand PHO a 353



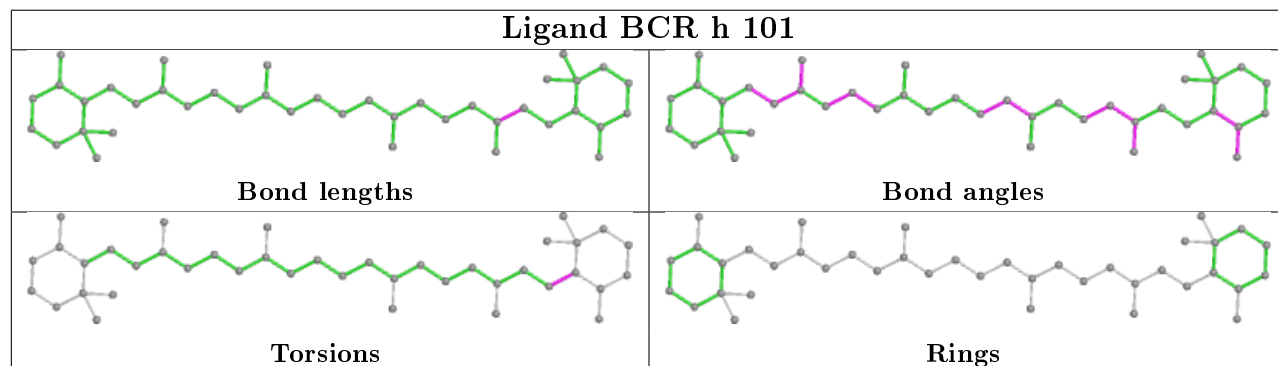


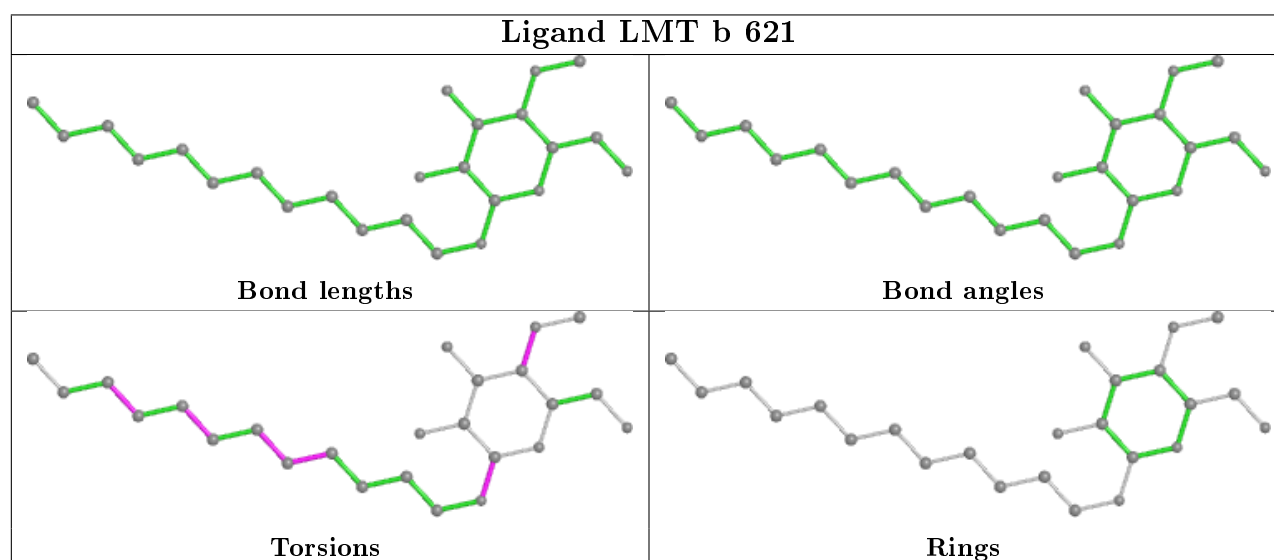
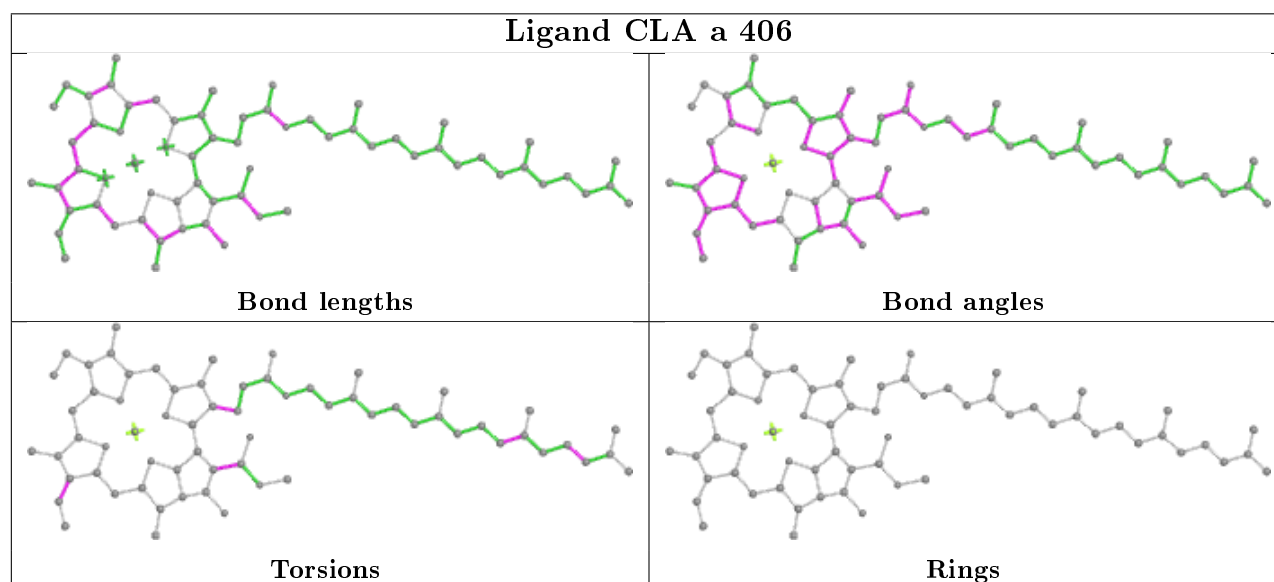
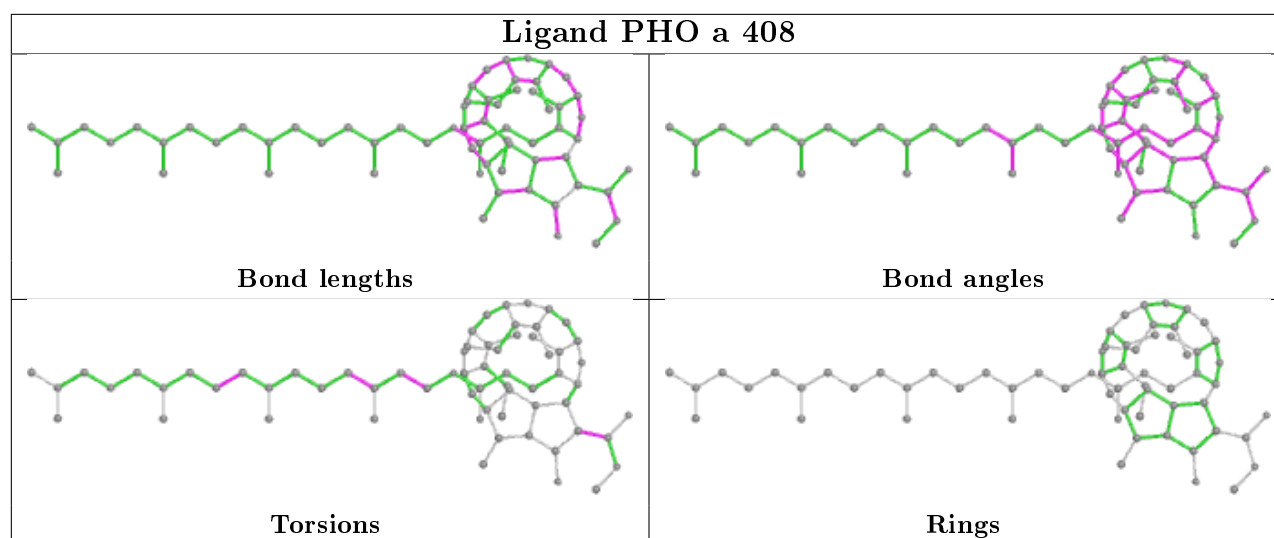


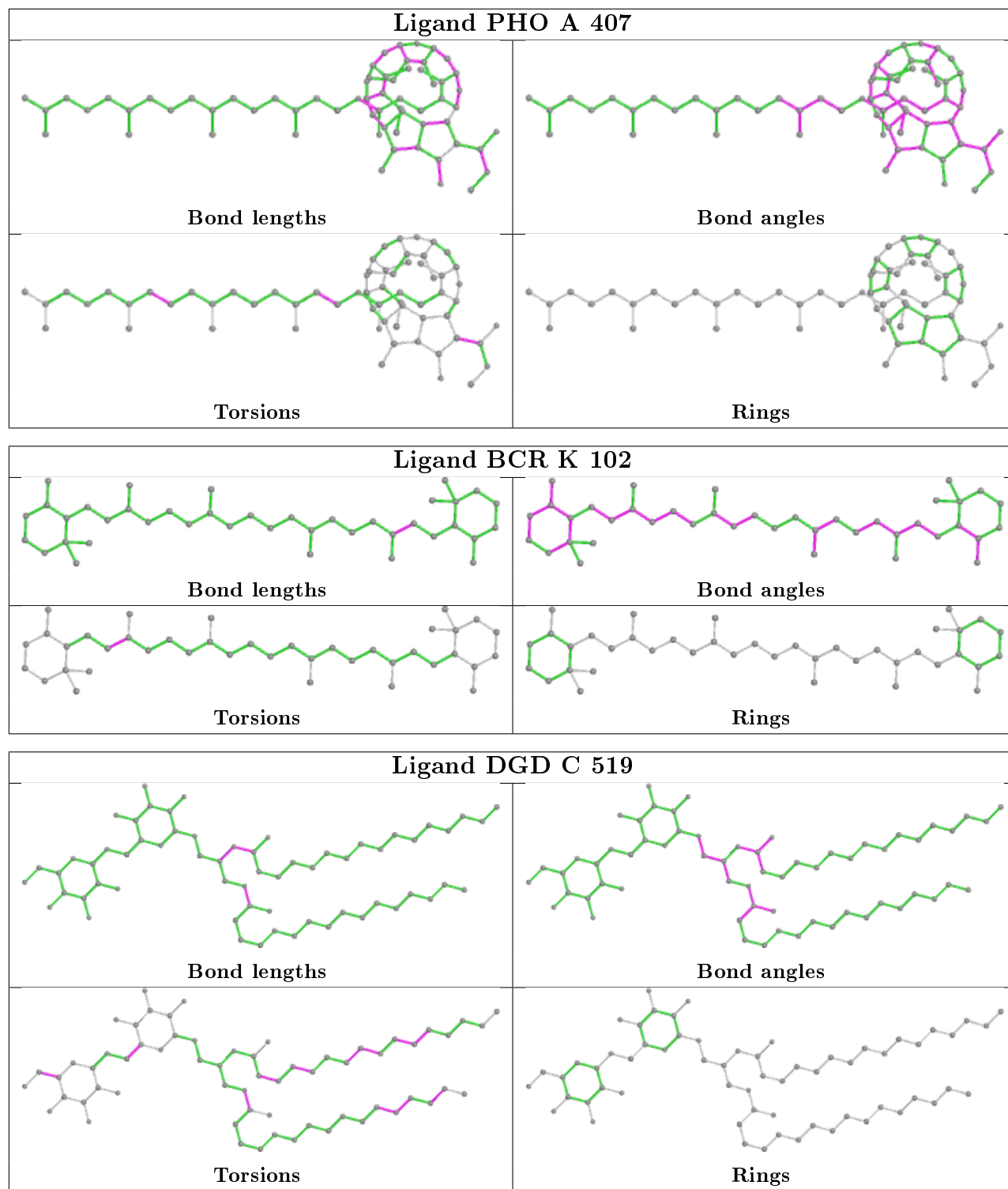
## Ligand LHG 1 101

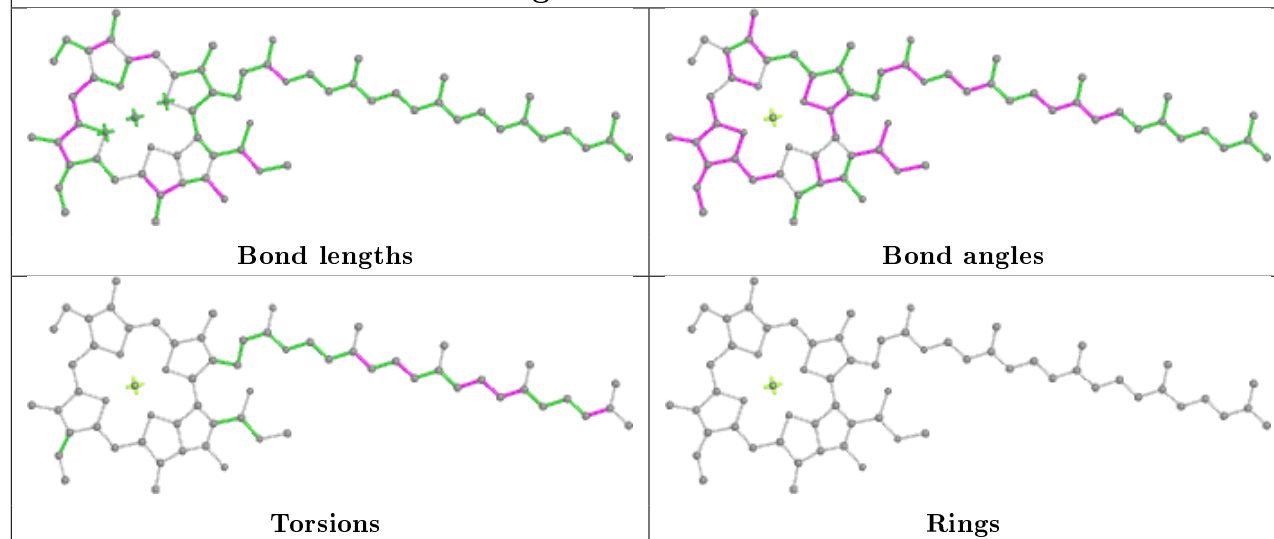
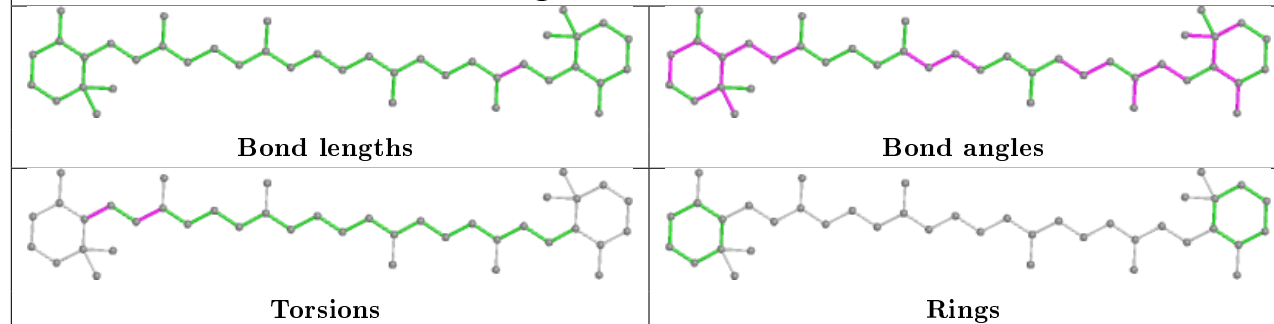
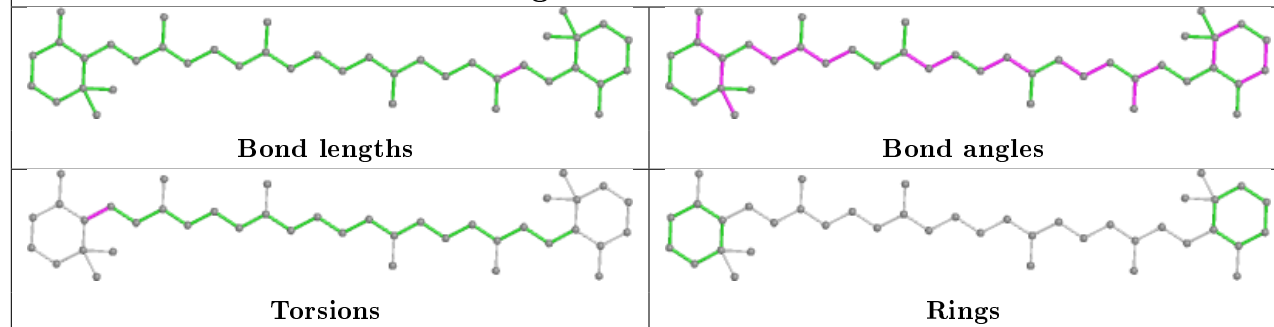


## Ligand BCR h 101

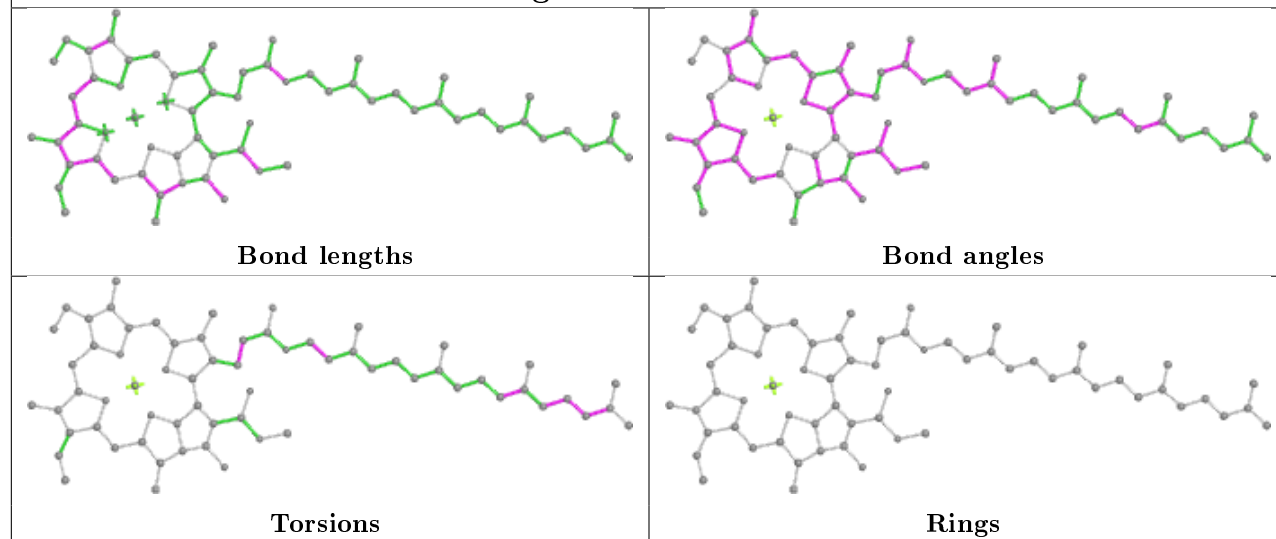




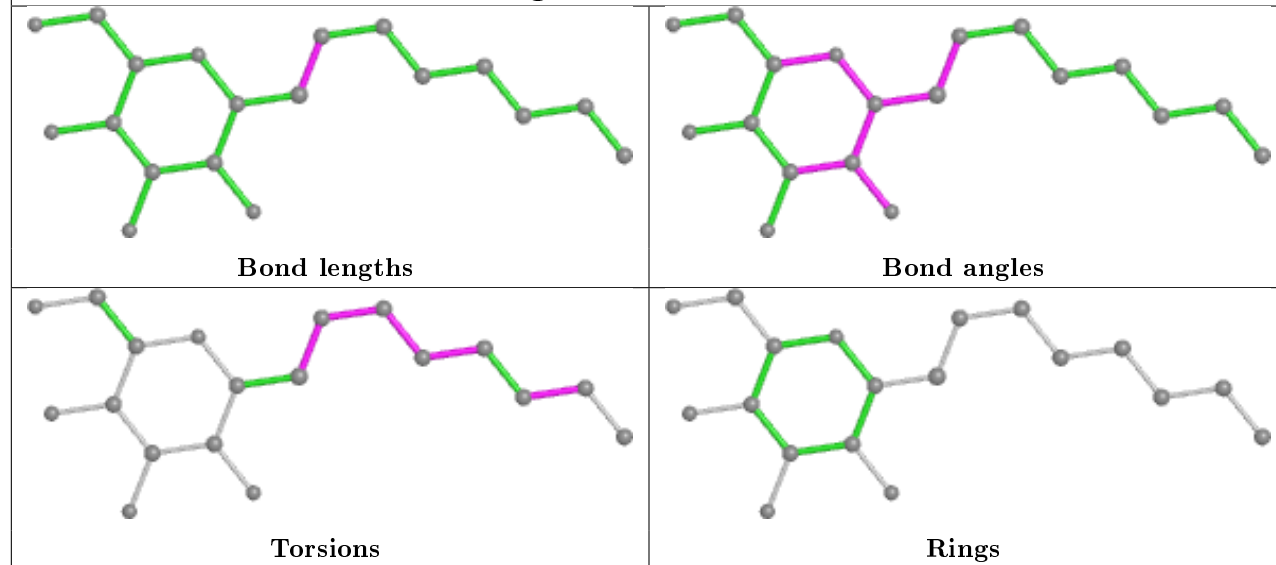


**Ligand CLA B 615****Ligand BCR b 619****Ligand BCR B 617**

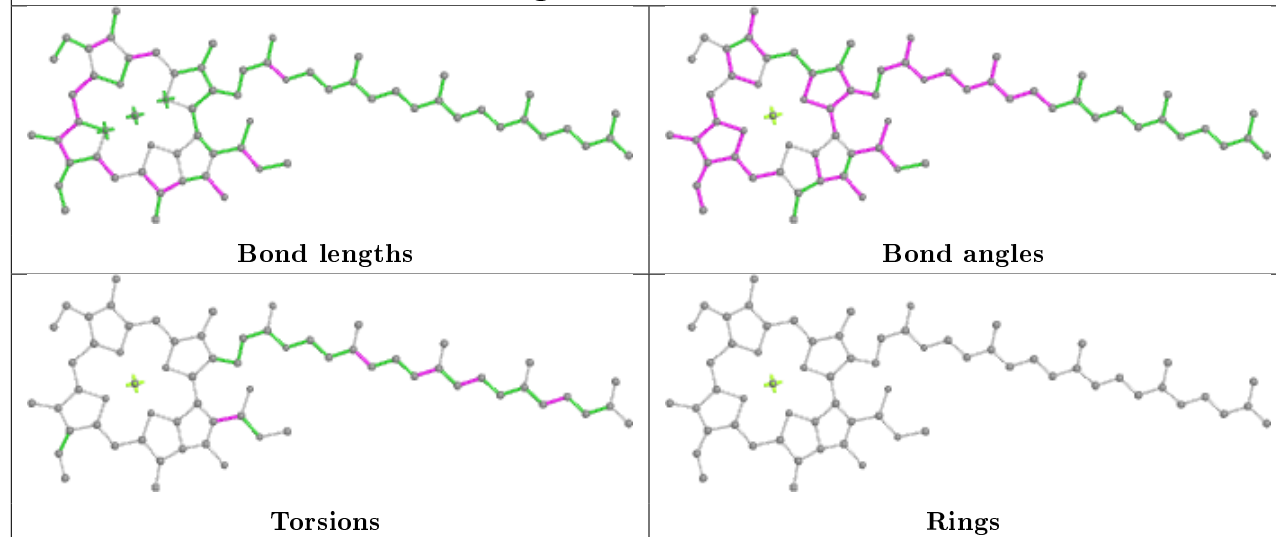
## Ligand CLA B 602



## Ligand HTG B 622

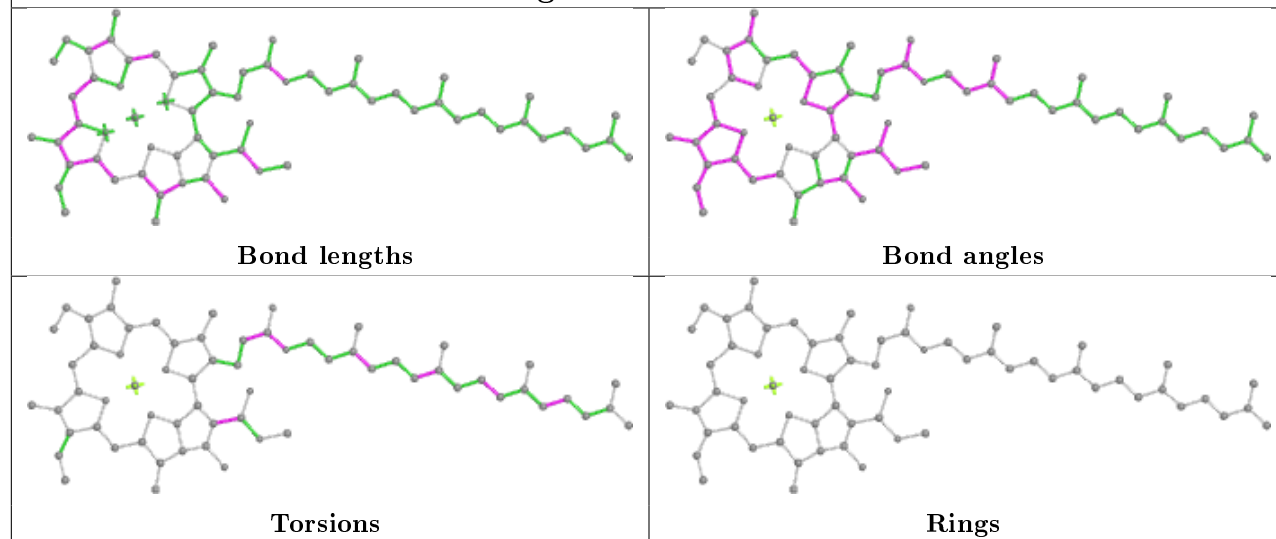


## Ligand CLA B 605

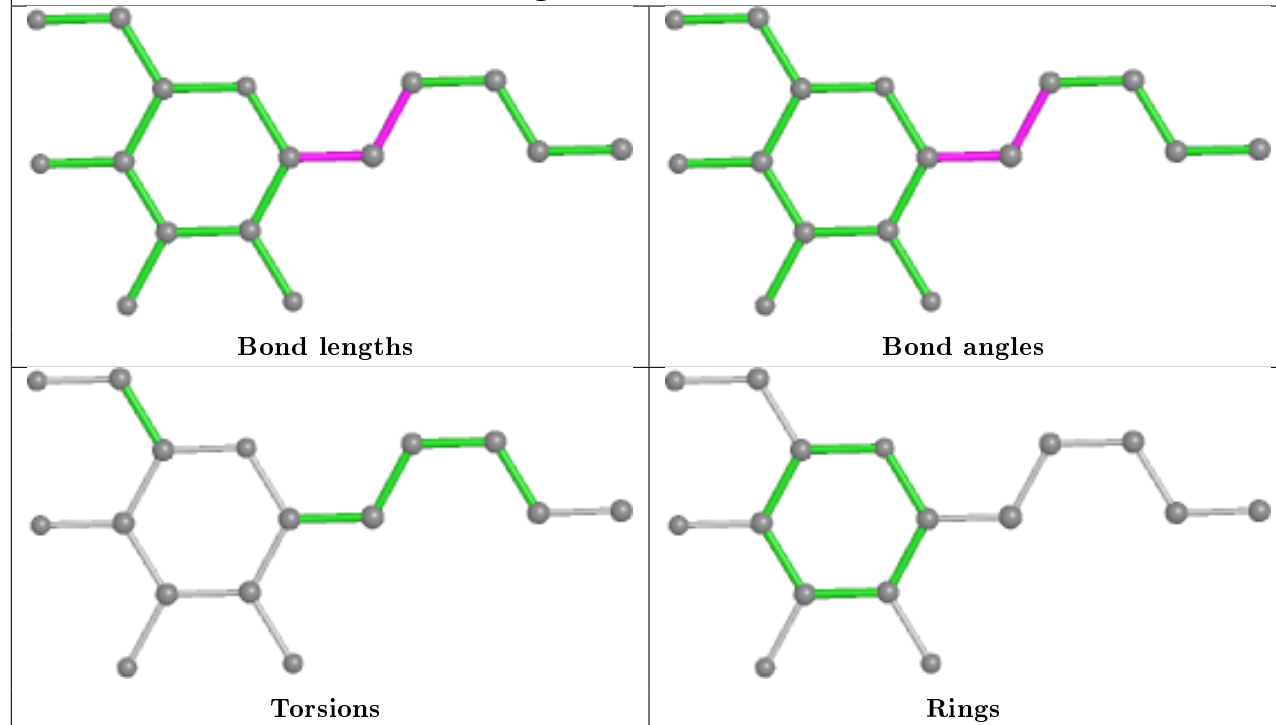




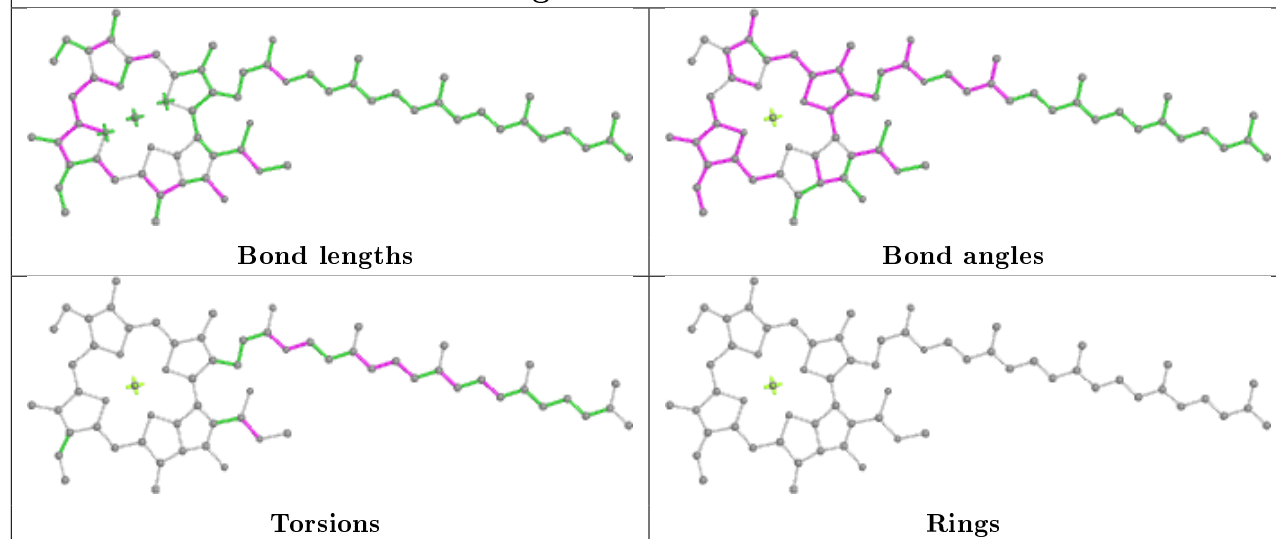
## Ligand CLA c 511



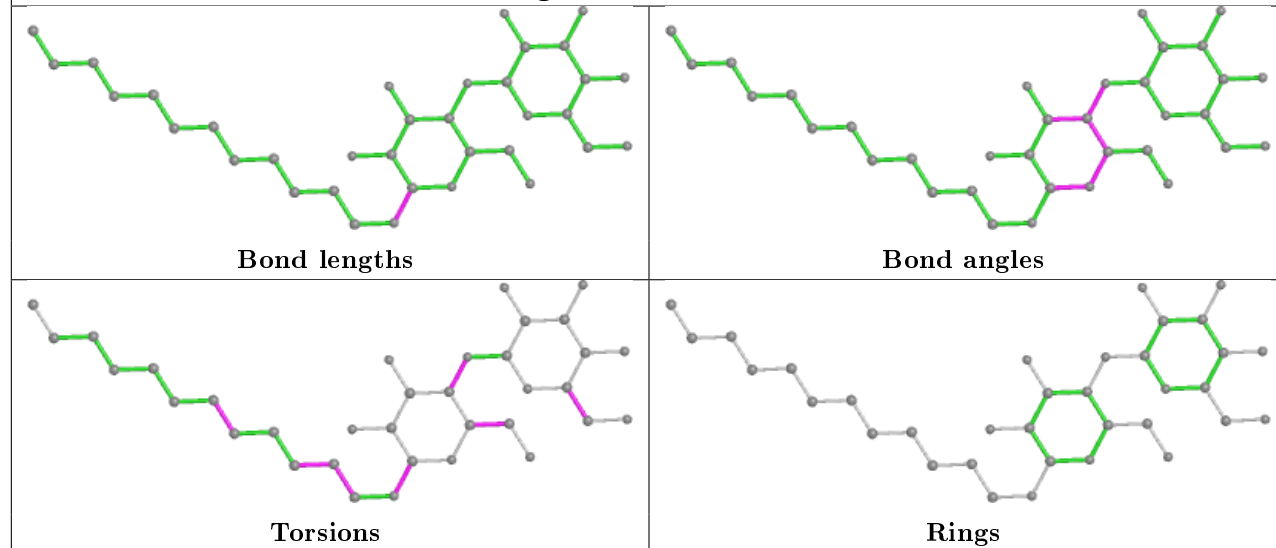
## Ligand HTG d 411



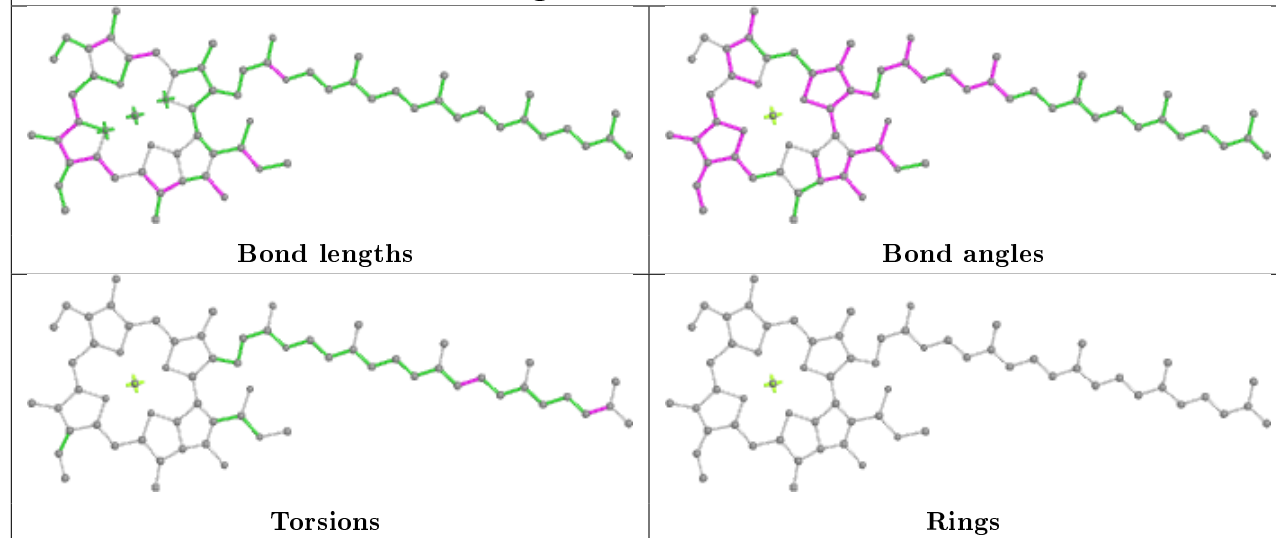
## Ligand CLA A 408



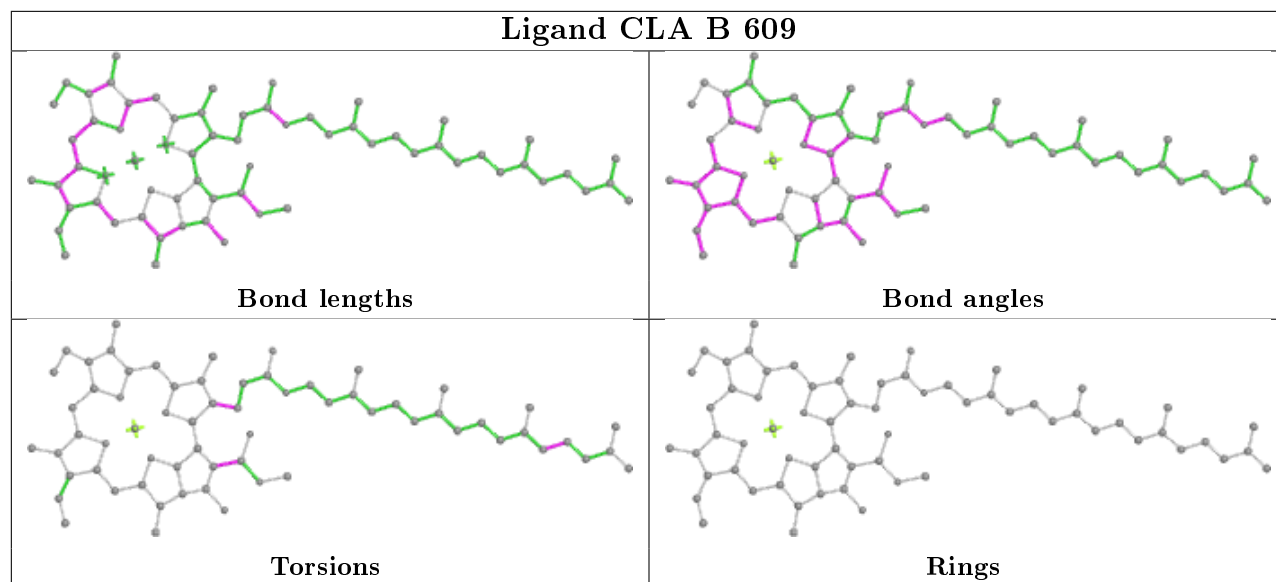
## Ligand LMT I 101



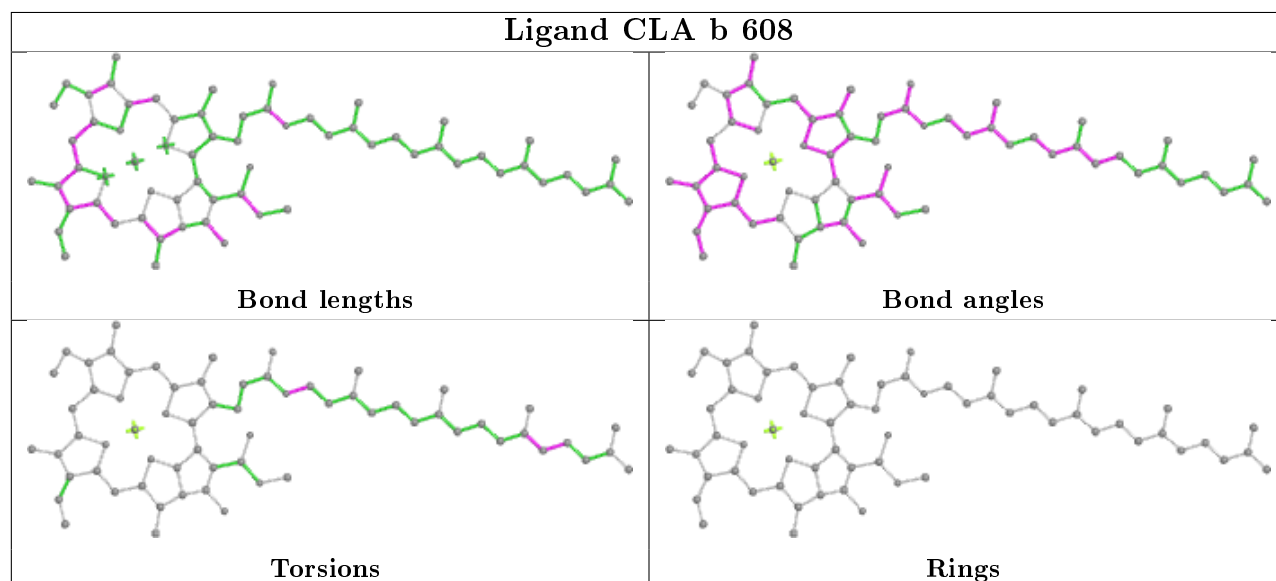
## Ligand CLA D 405



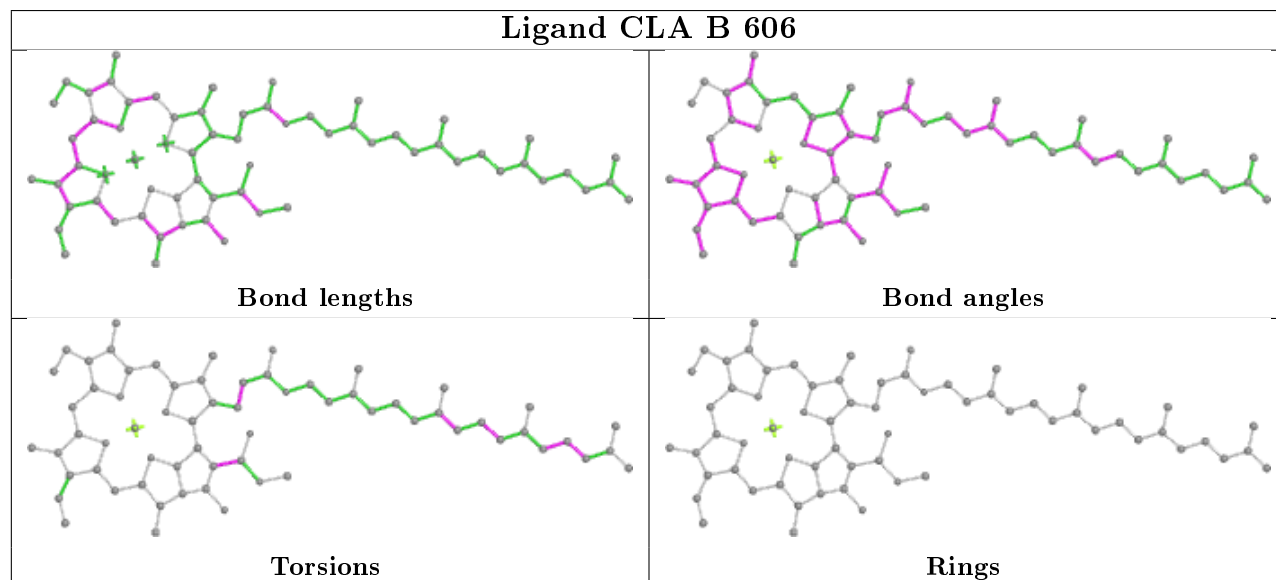
## Ligand CLA B 609

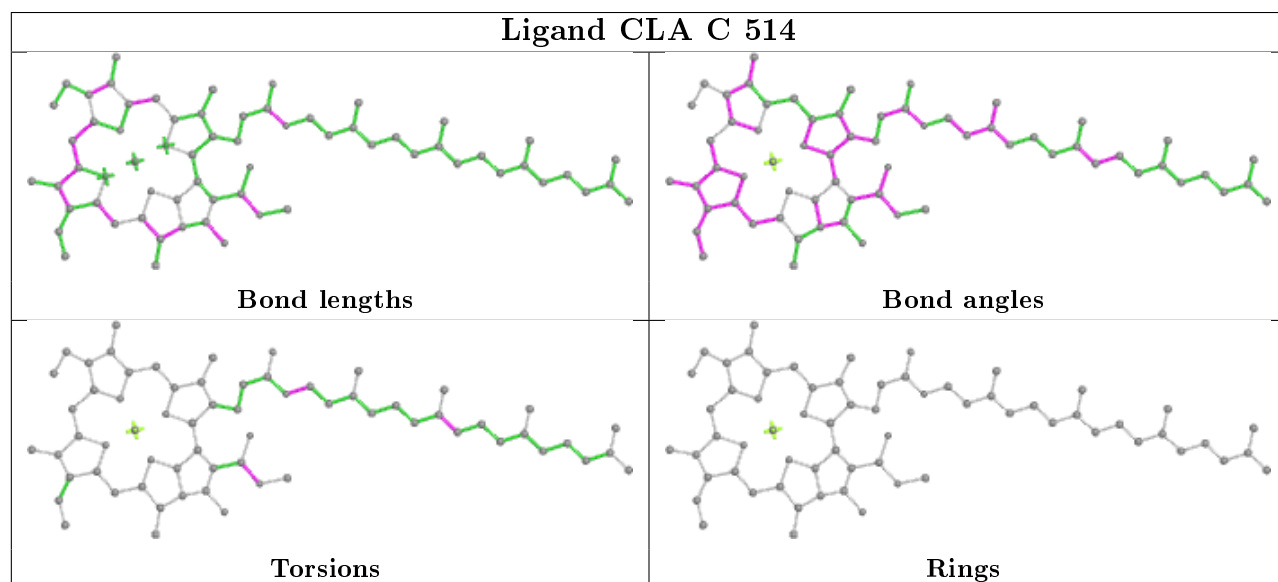
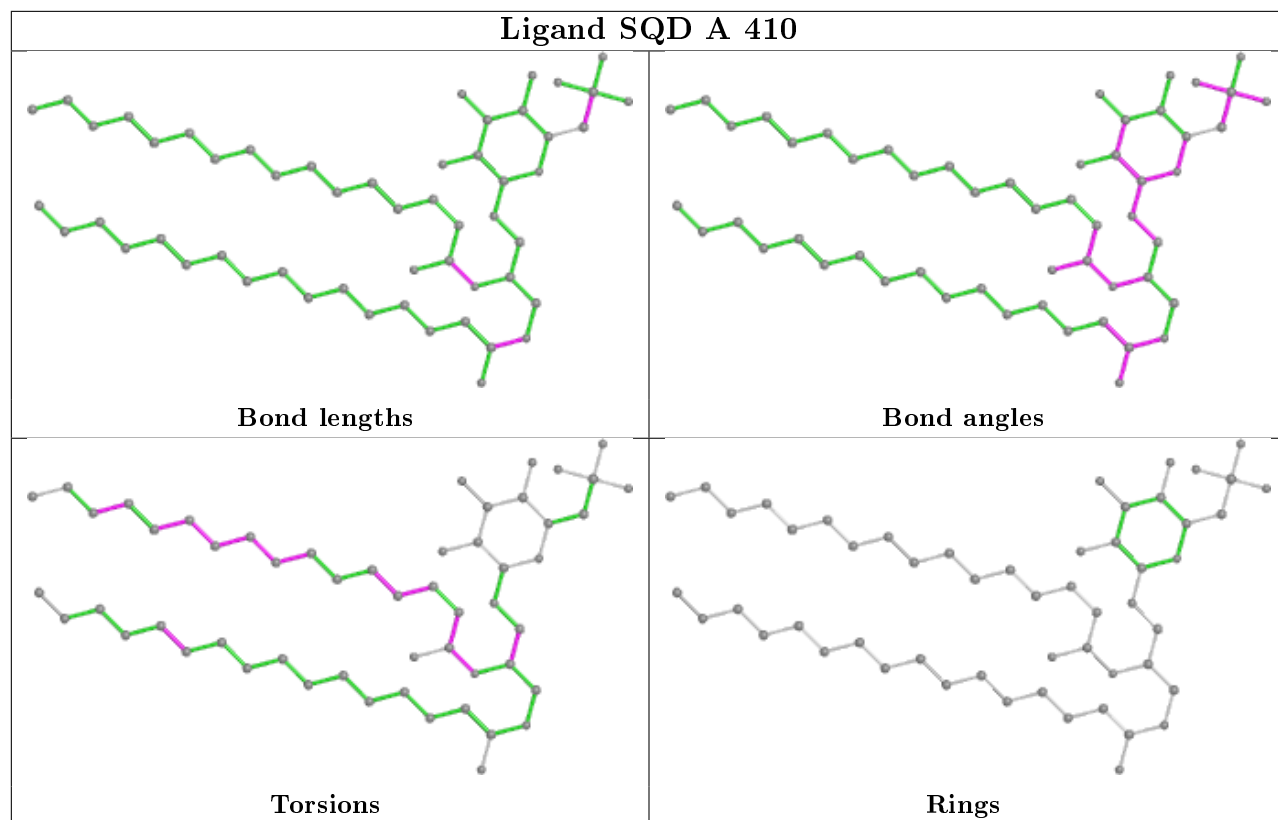


## Ligand CLA b 608

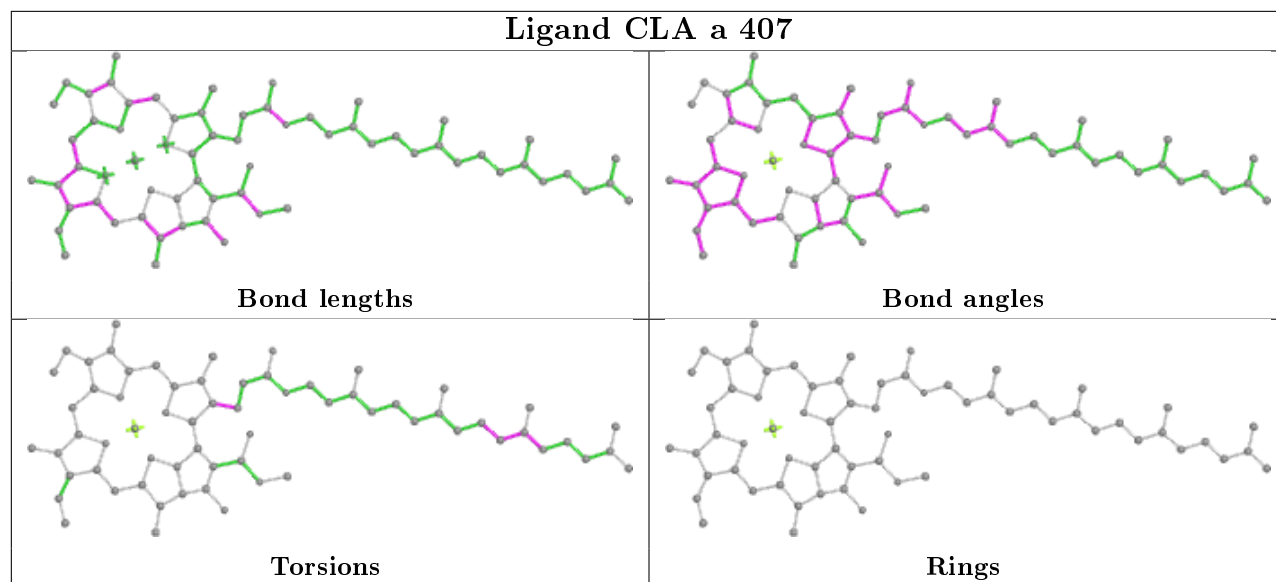


## Ligand CLA B 606

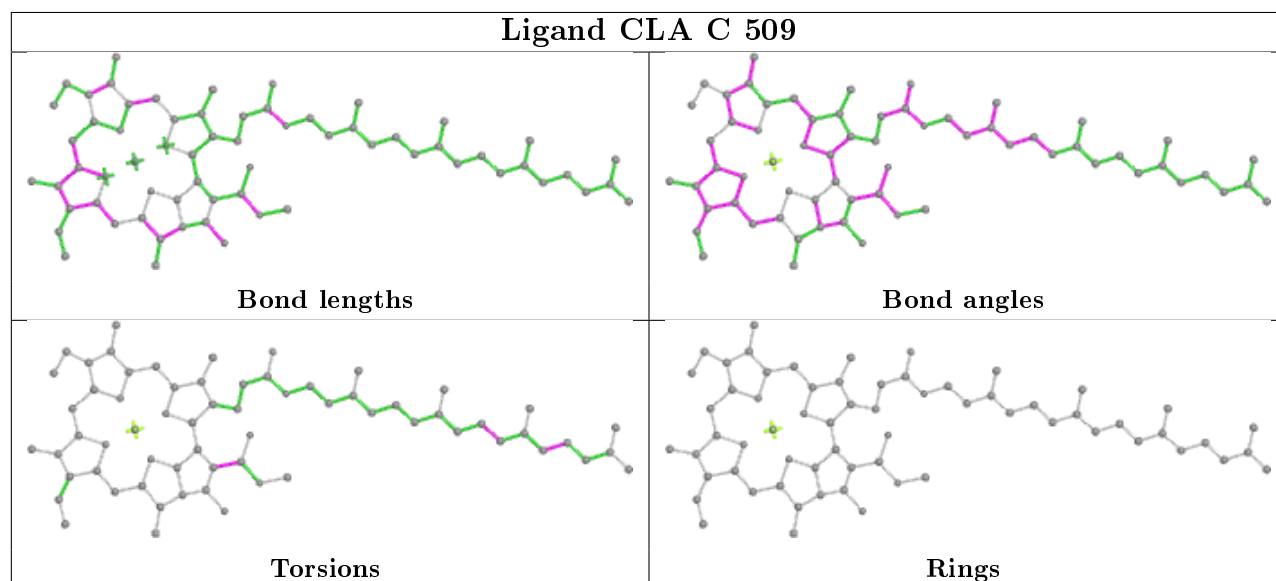




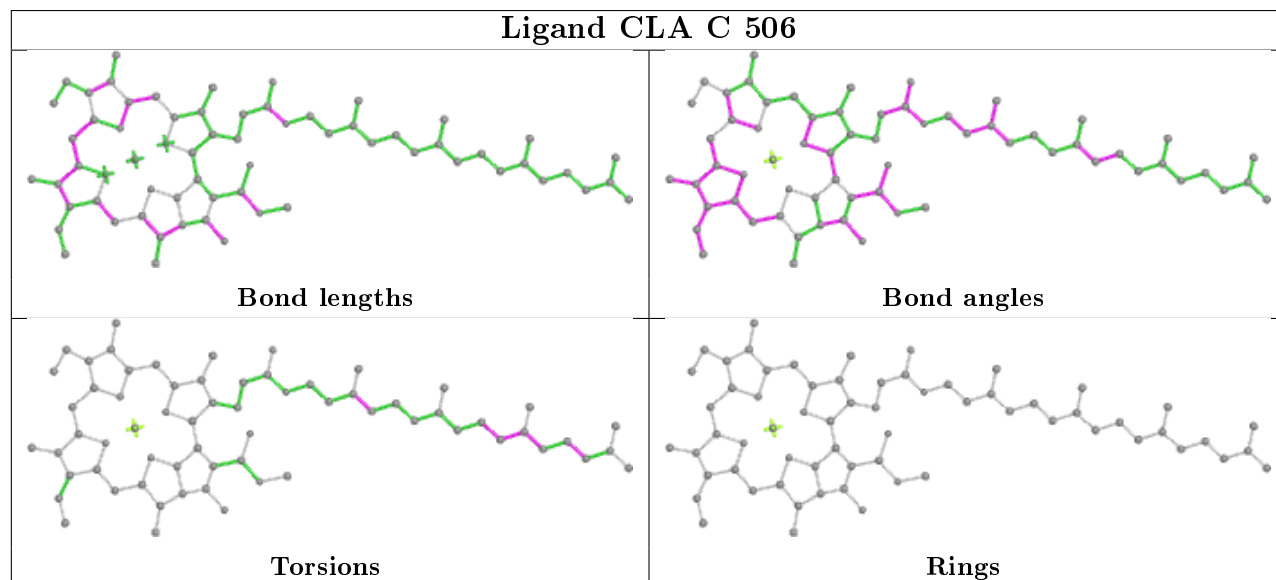
## Ligand CLA a 407



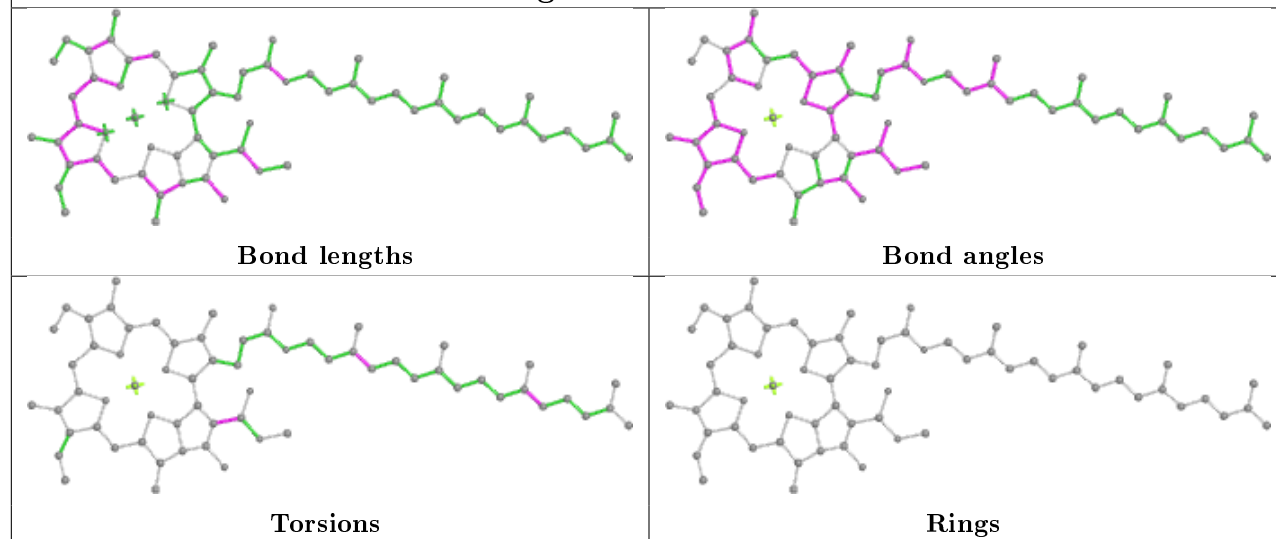
## Ligand CLA C 509



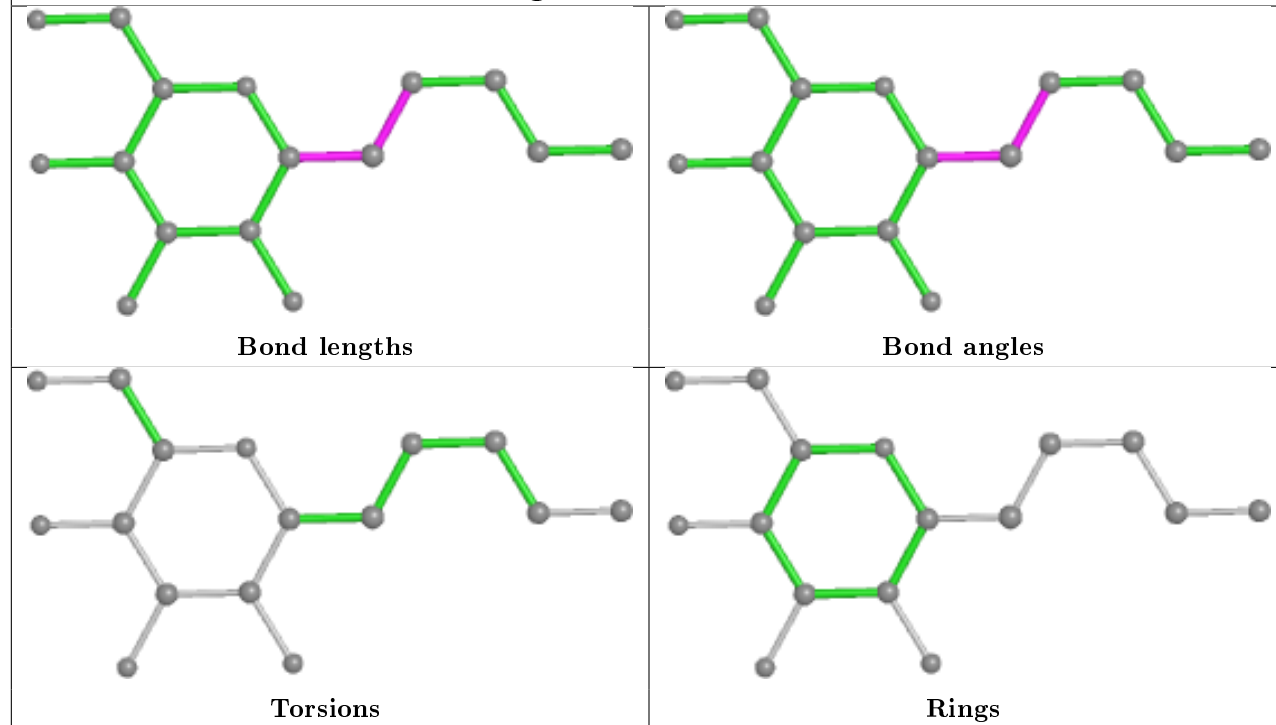
## Ligand CLA C 506

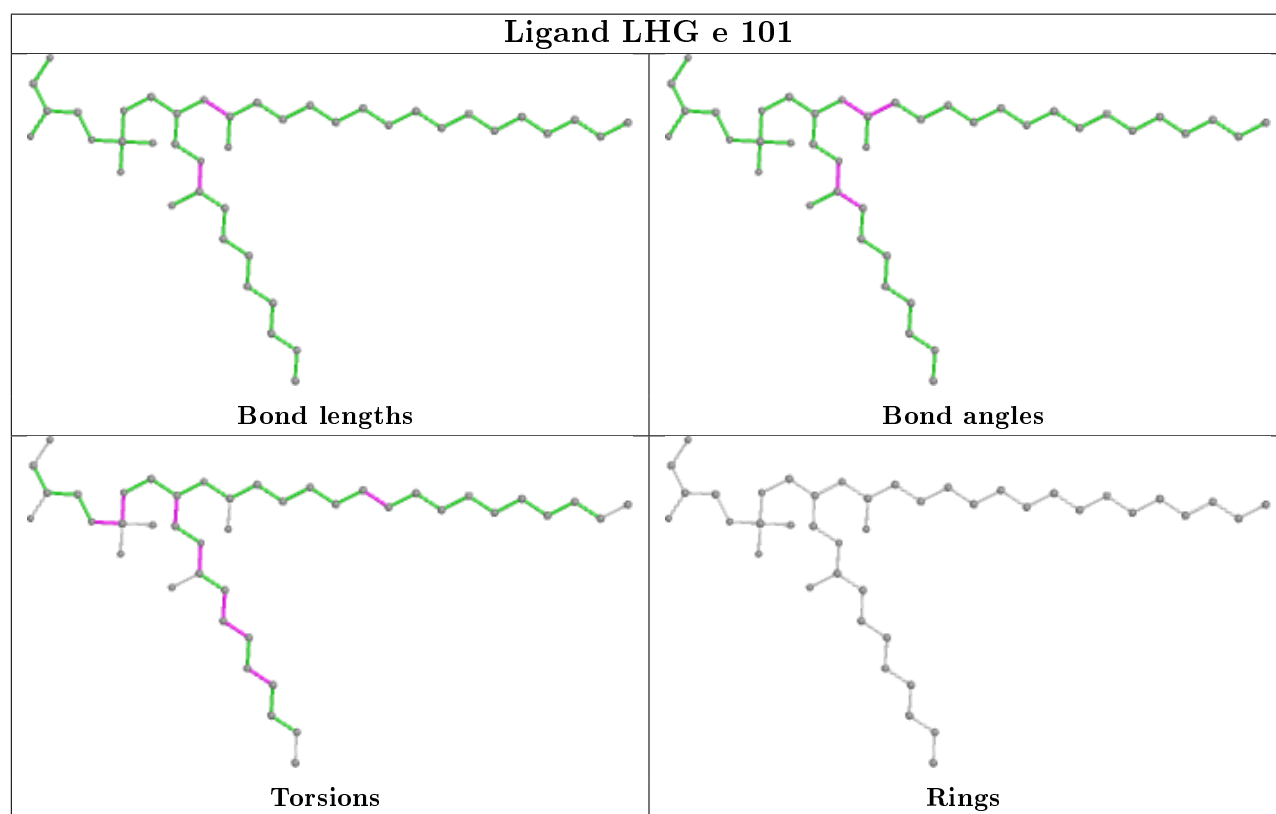
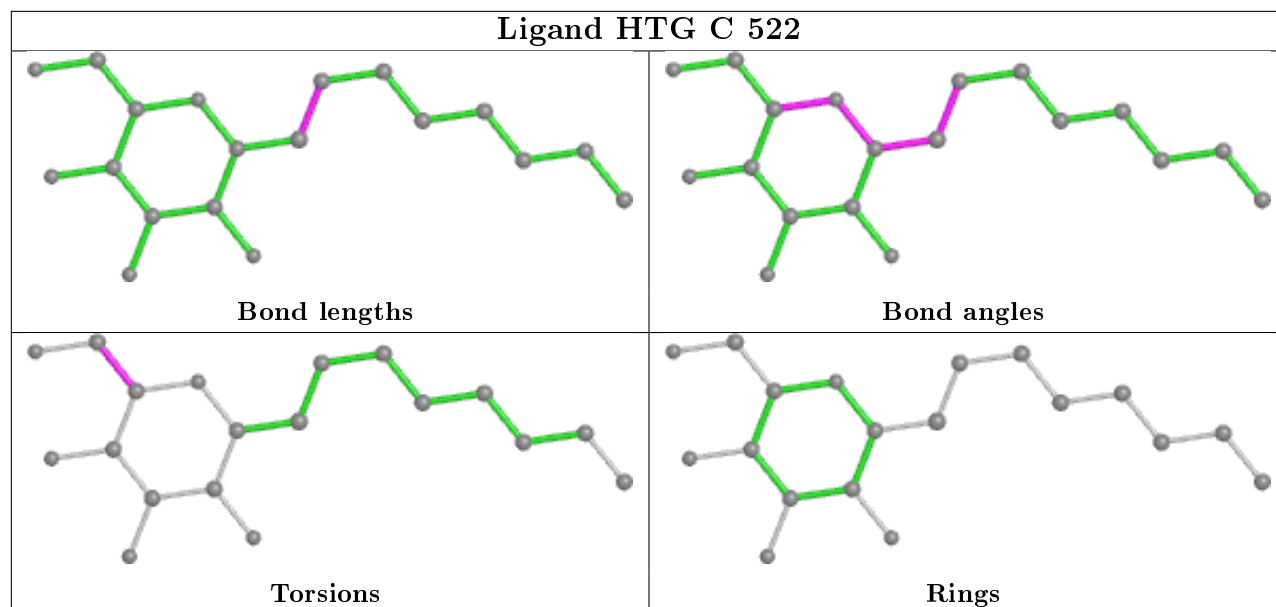


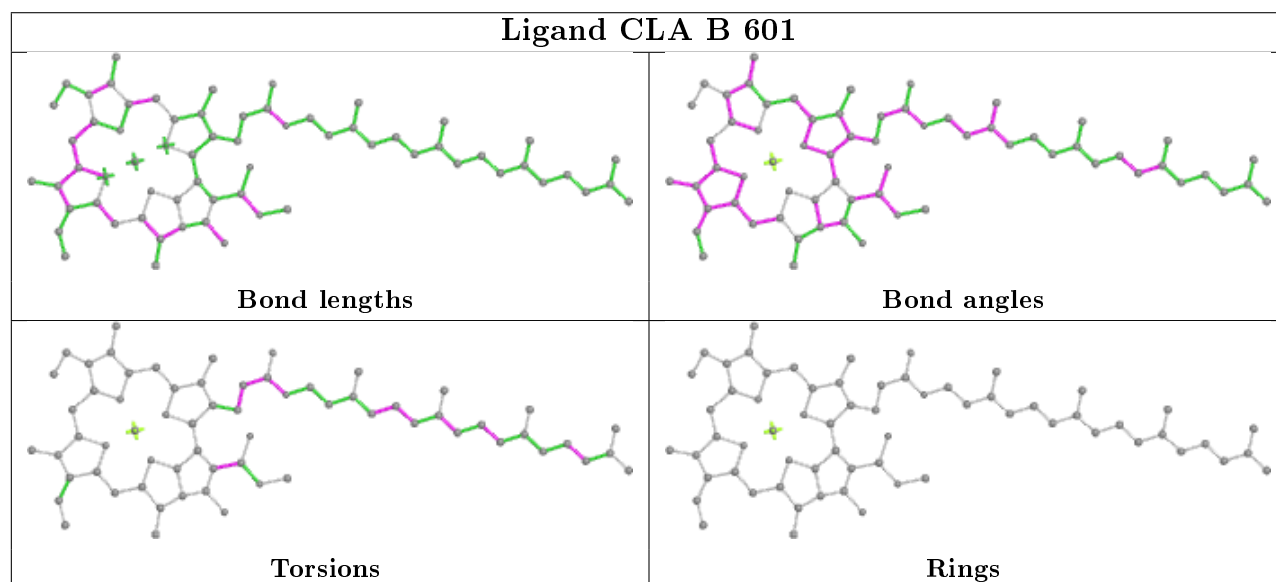
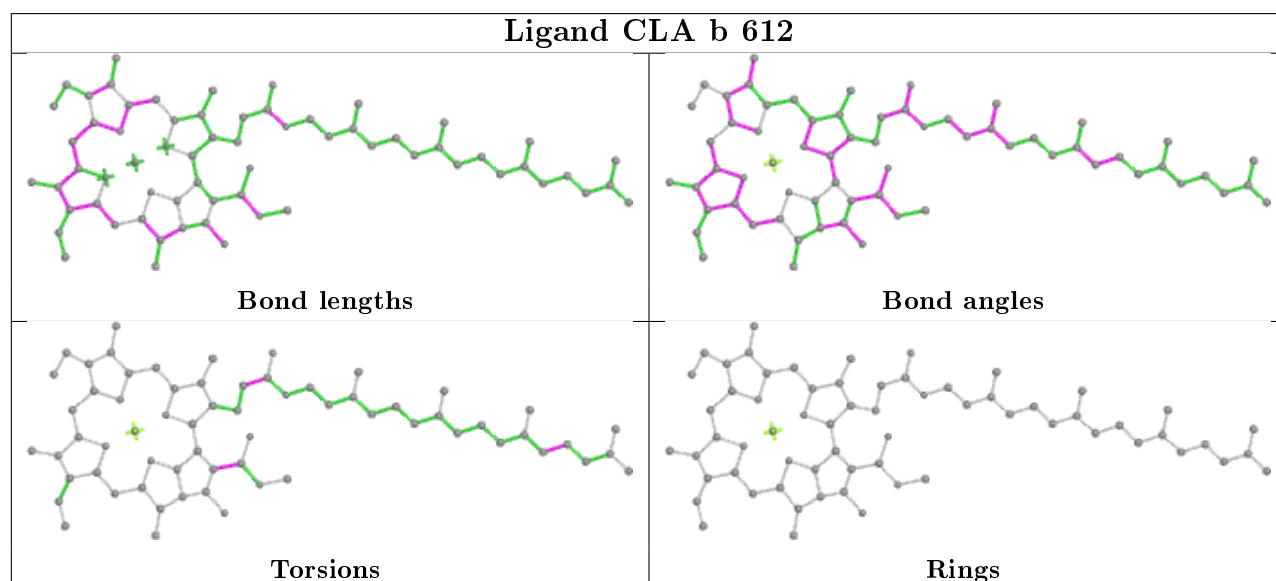
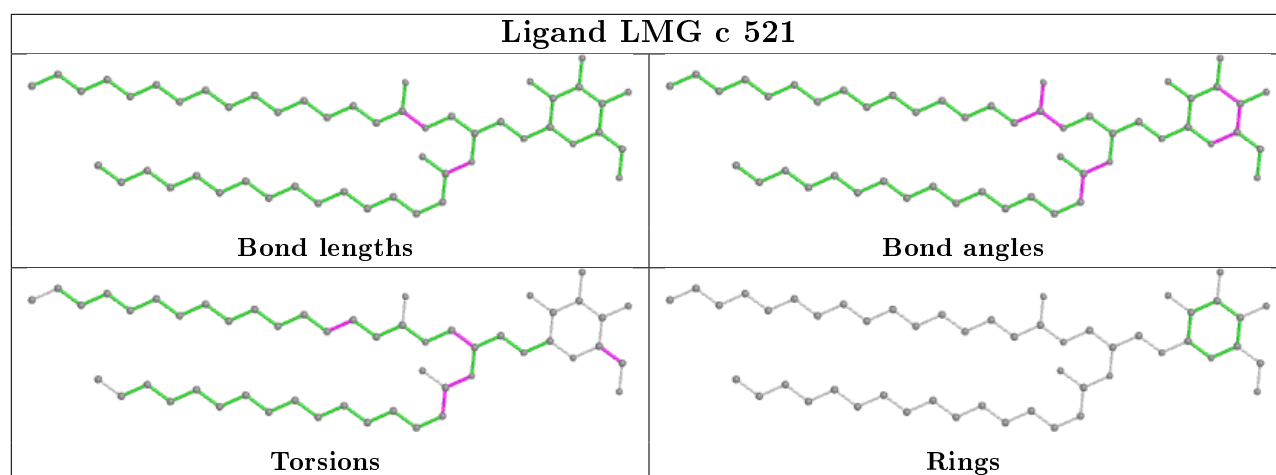
## Ligand CLA c 505



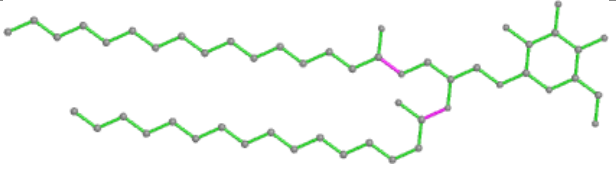
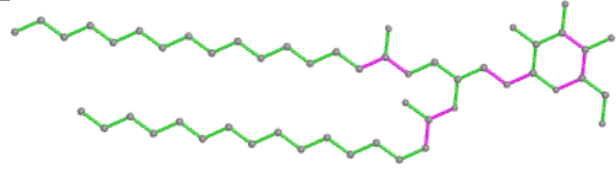
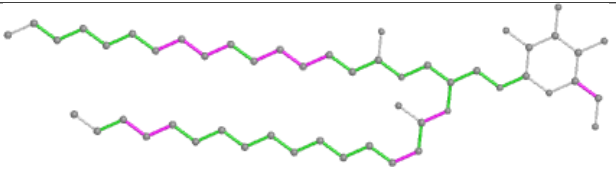
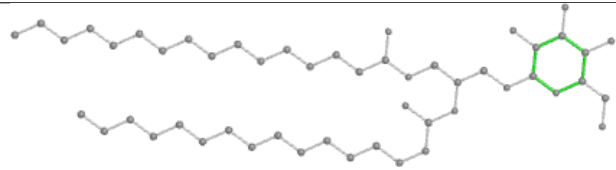
## Ligand HTG D 414

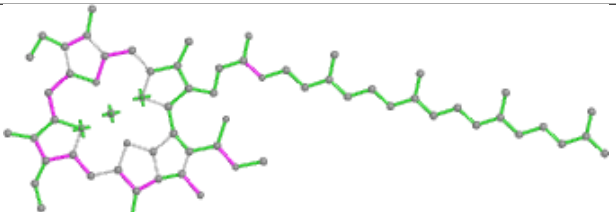
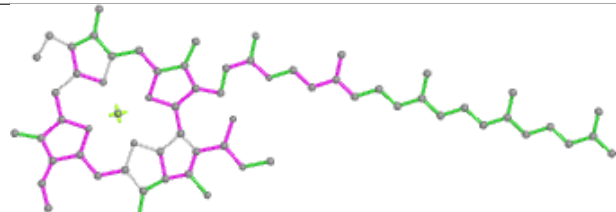
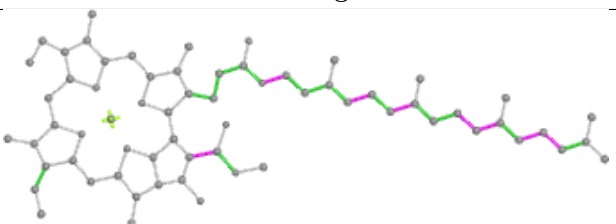
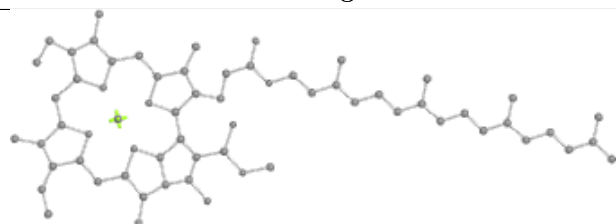



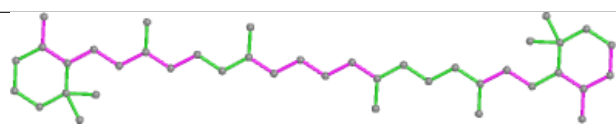
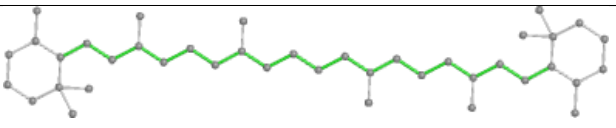
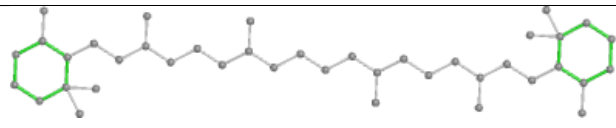


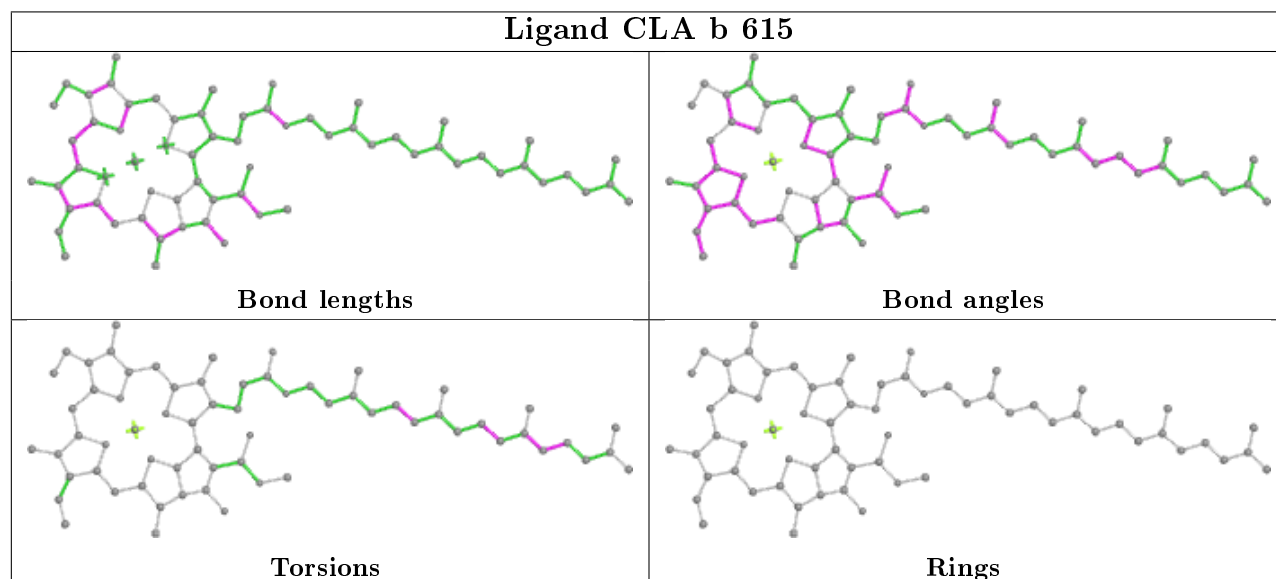
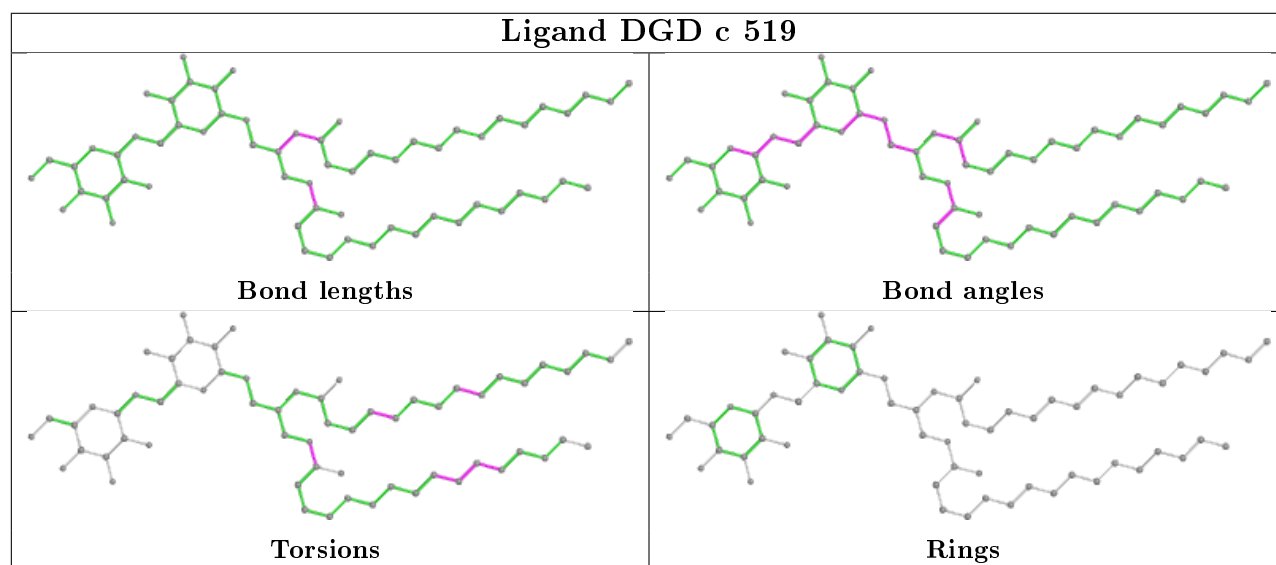
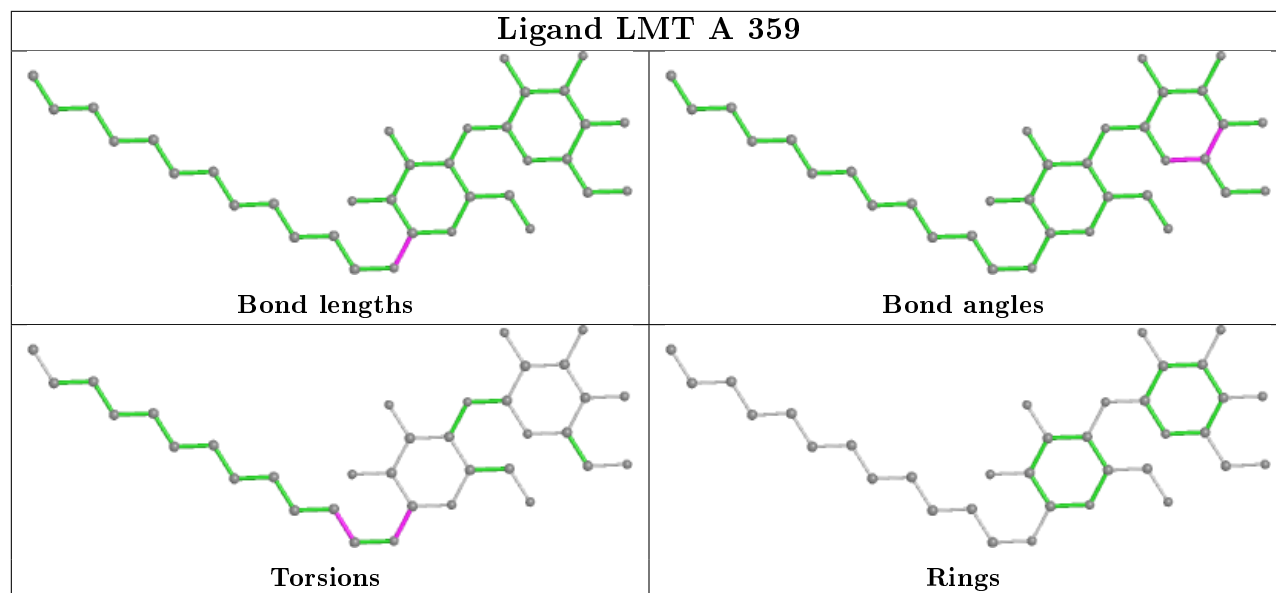




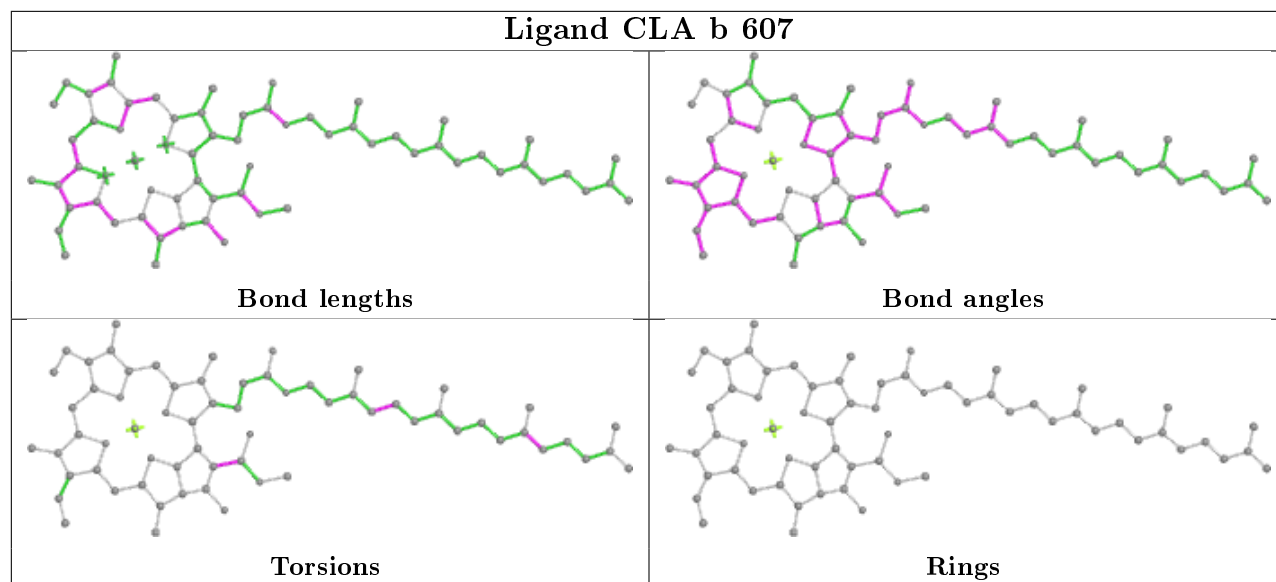
Ligand LMG a 419	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

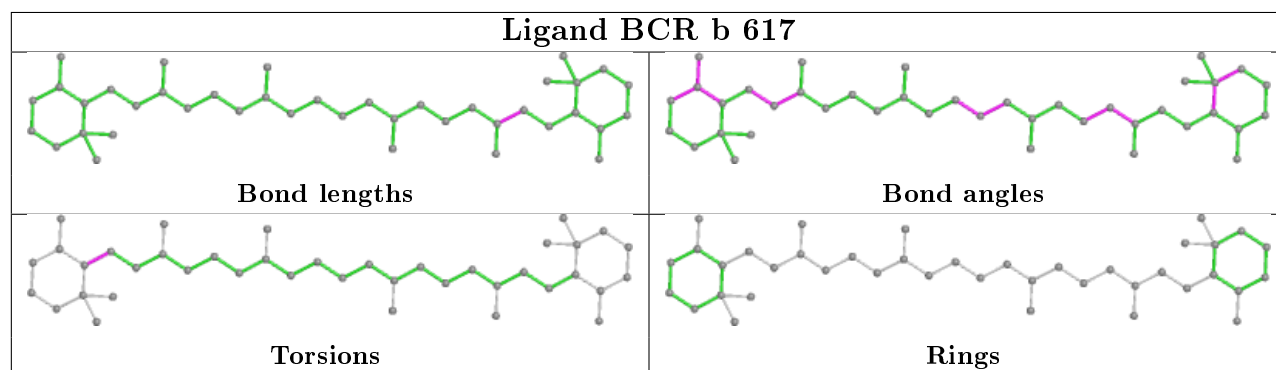
Ligand BCR b 618	
	
Bond lengths	Bond angles
	
Torsions	Rings



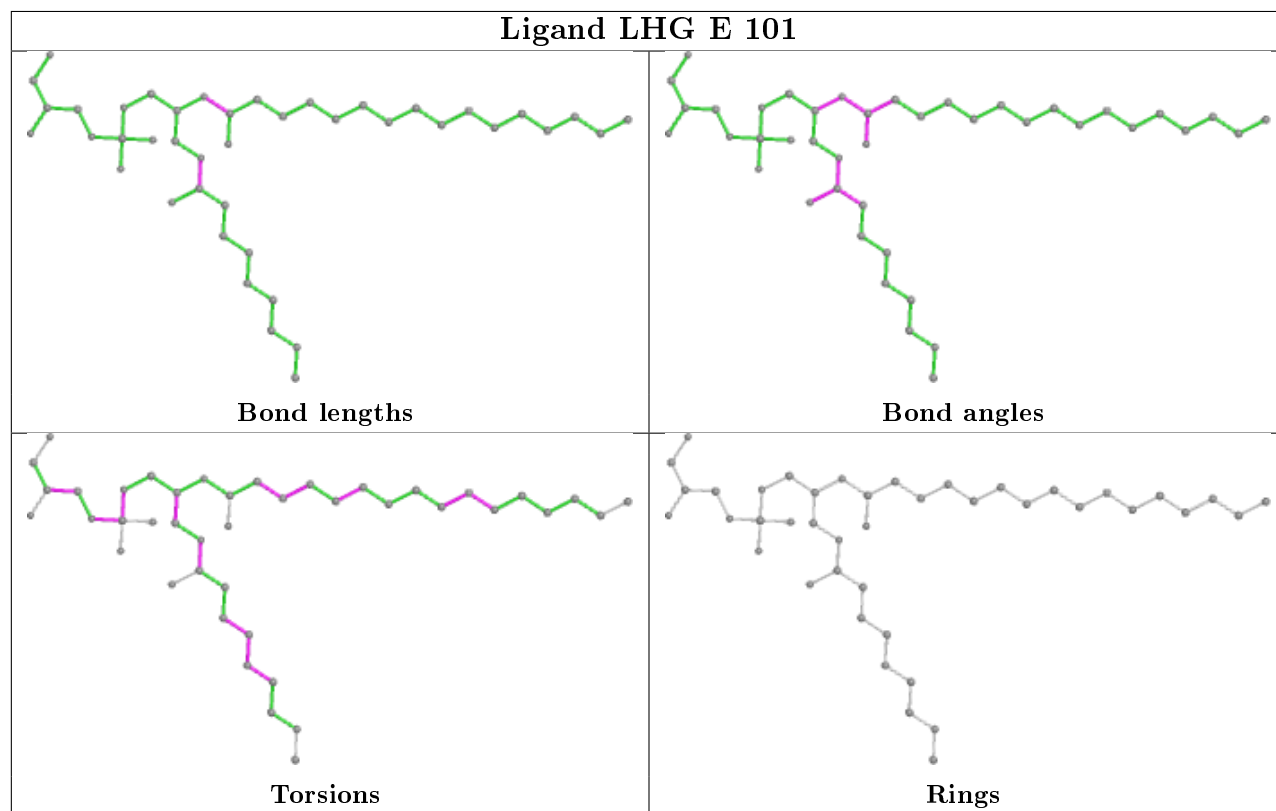
## Ligand CLA b 607

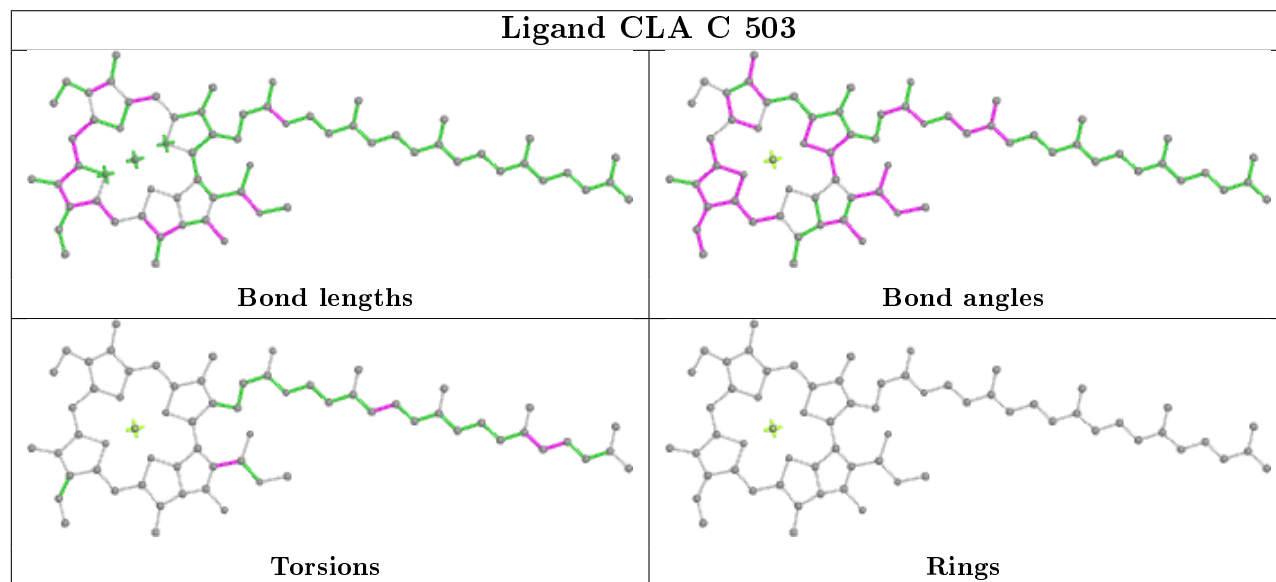
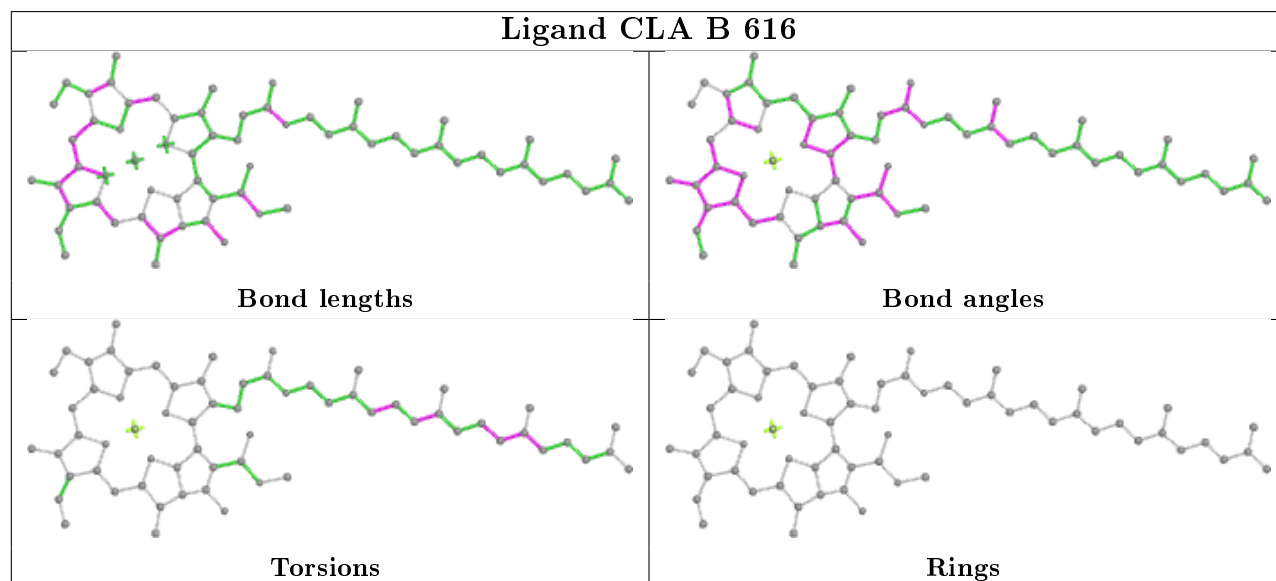
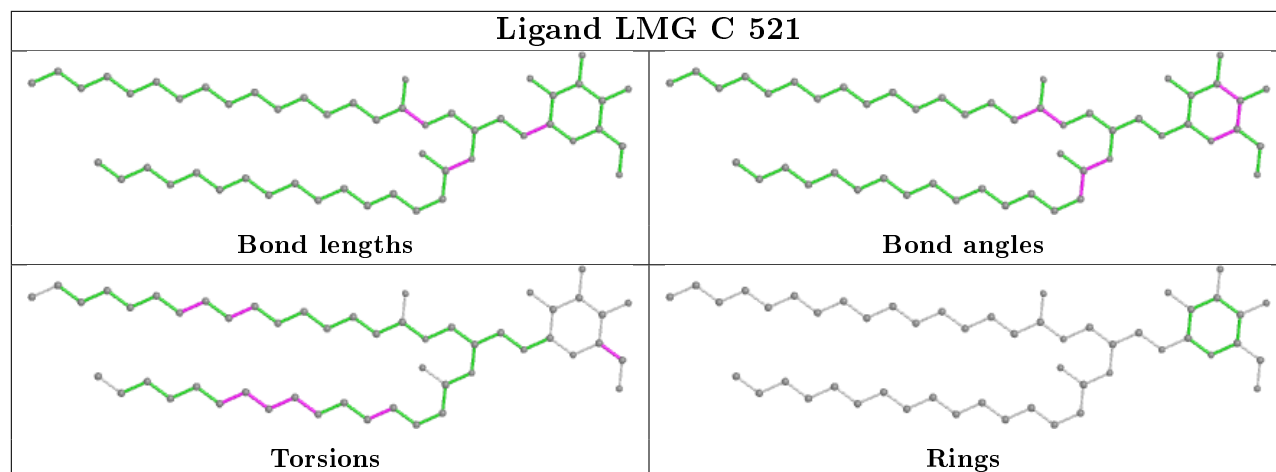


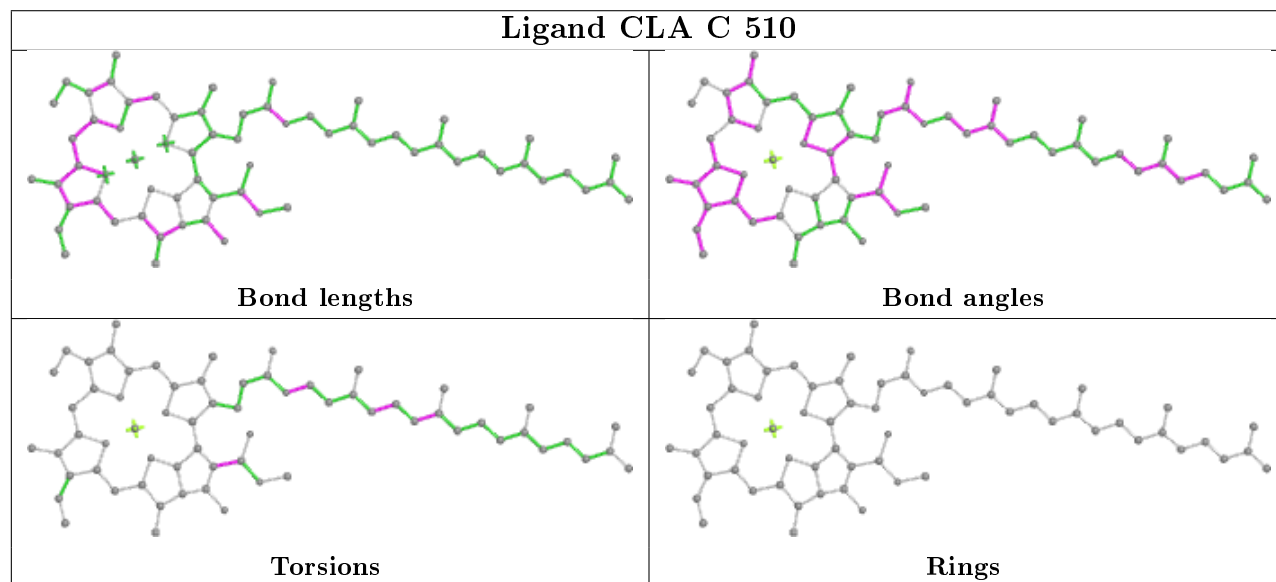
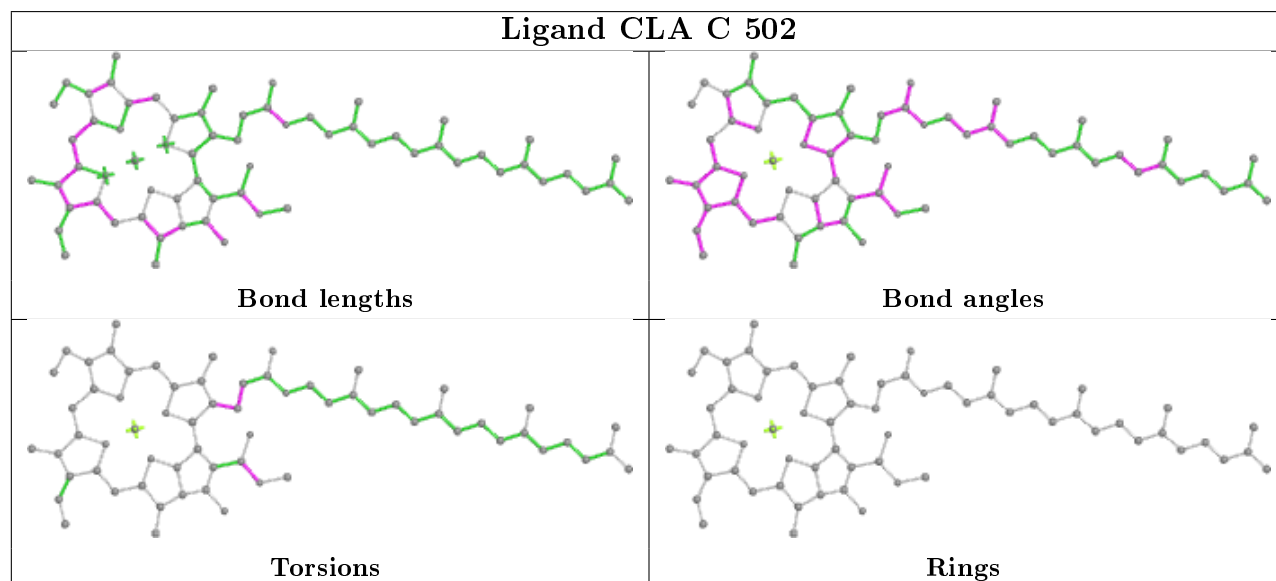
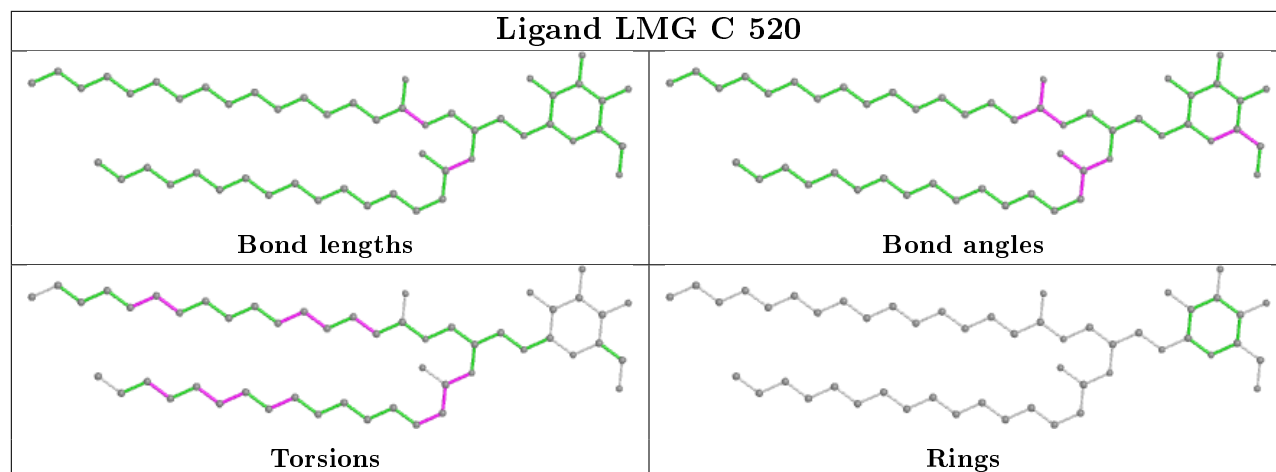
## Ligand BCR b 617



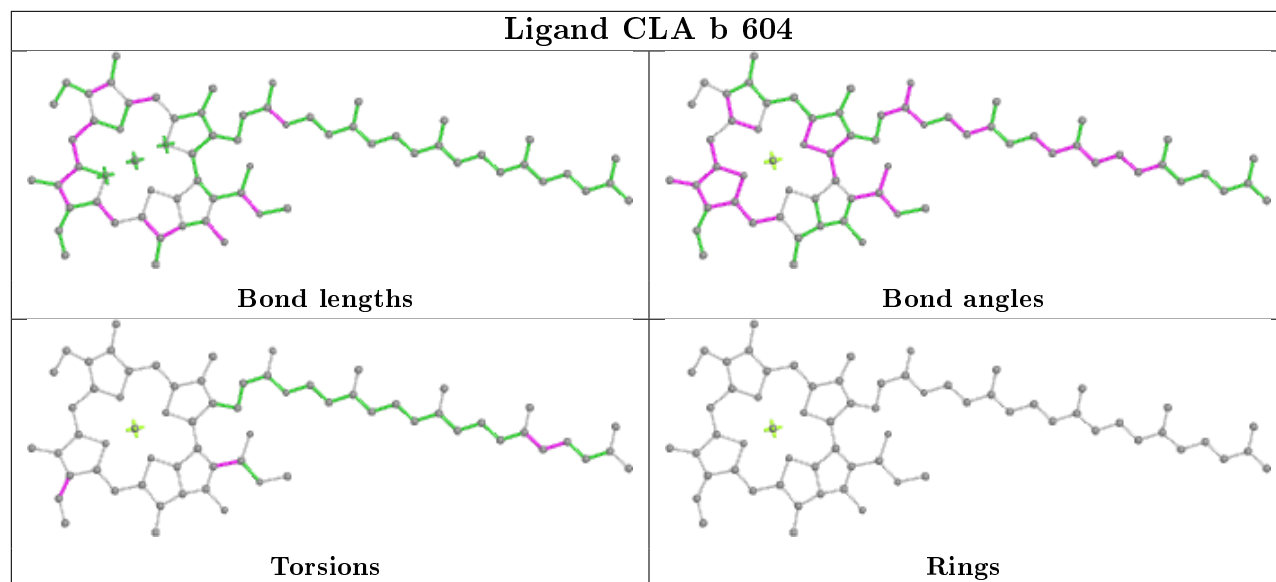
## Ligand LHG E 101



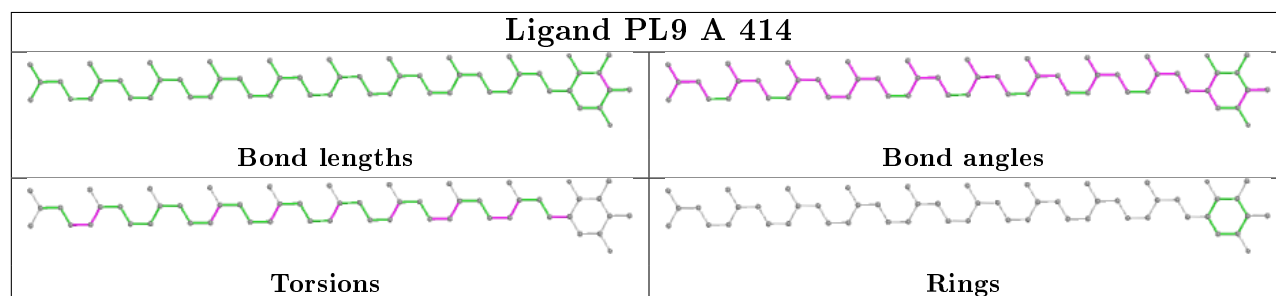




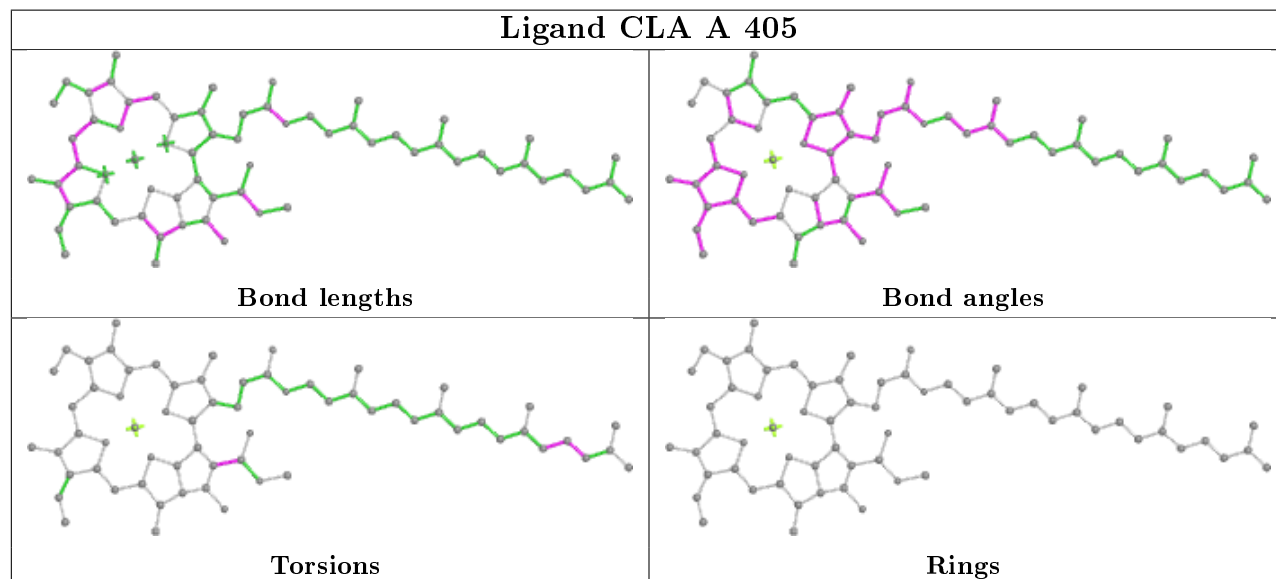
## Ligand CLA b 604



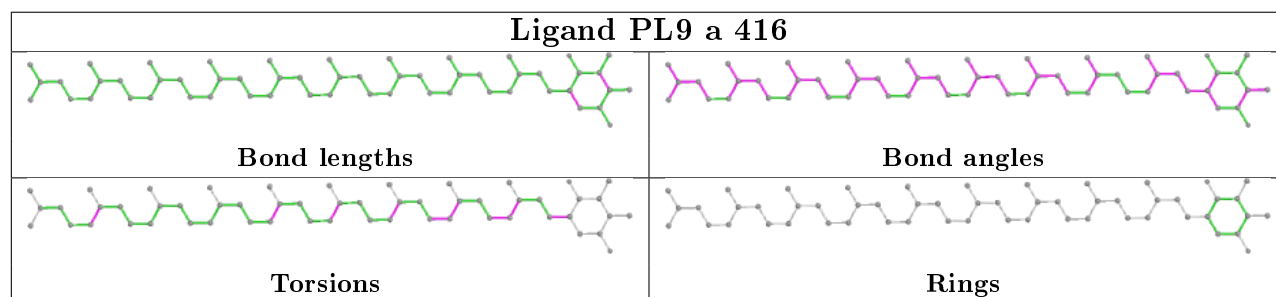
## Ligand PL9 A 414



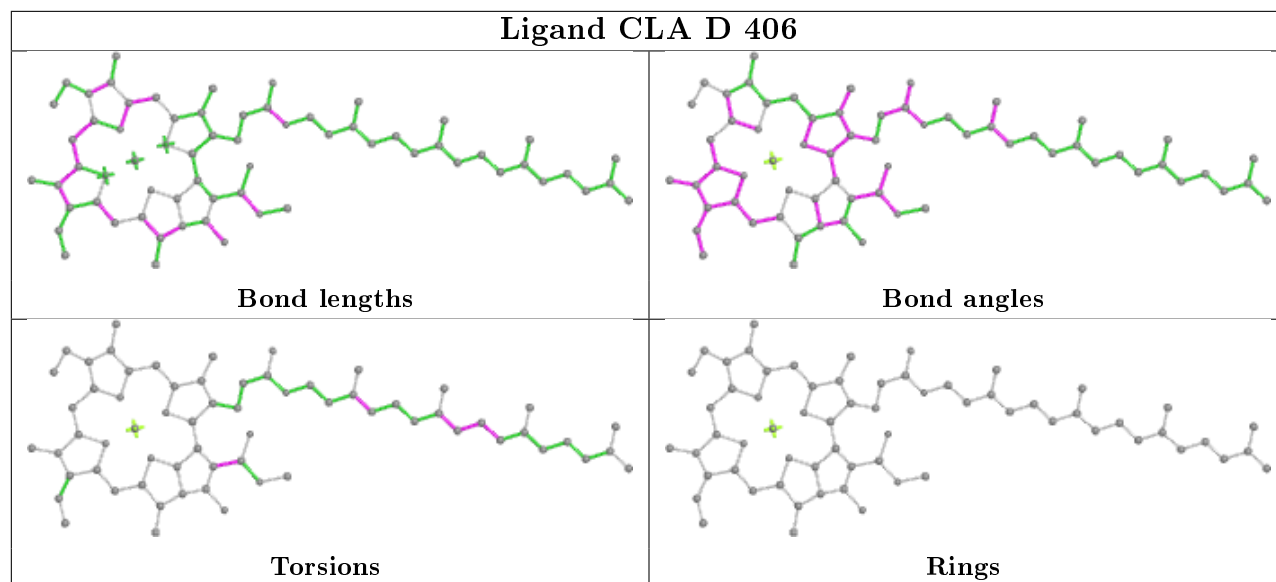
## Ligand CLA A 405



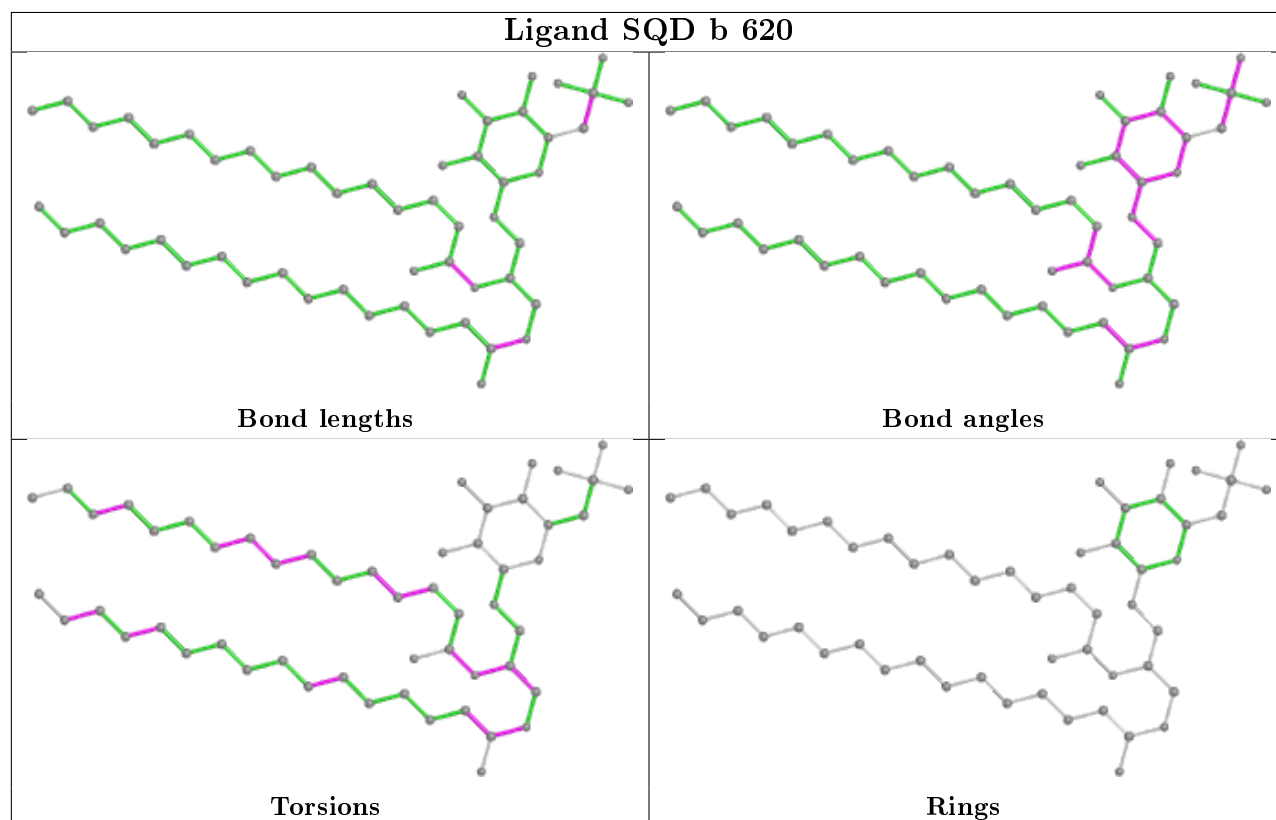
## Ligand PL9 a 416



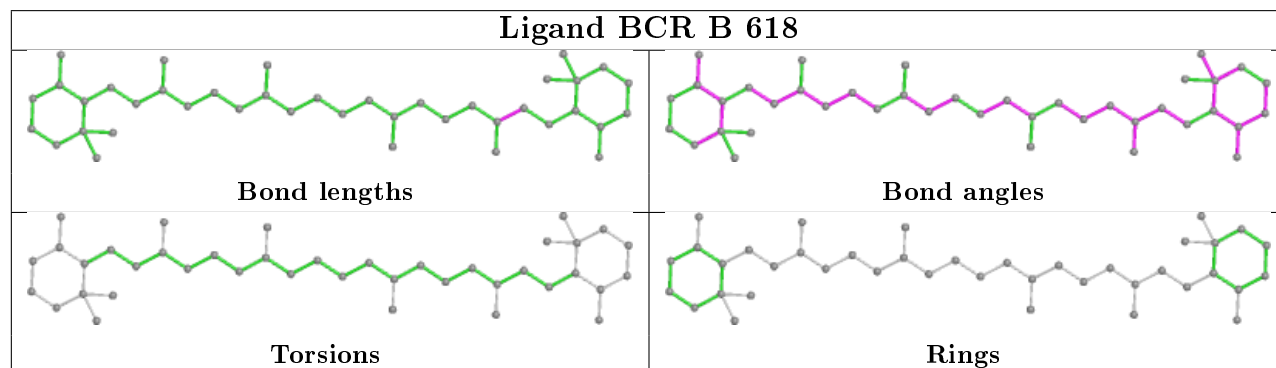
## Ligand CLA D 406



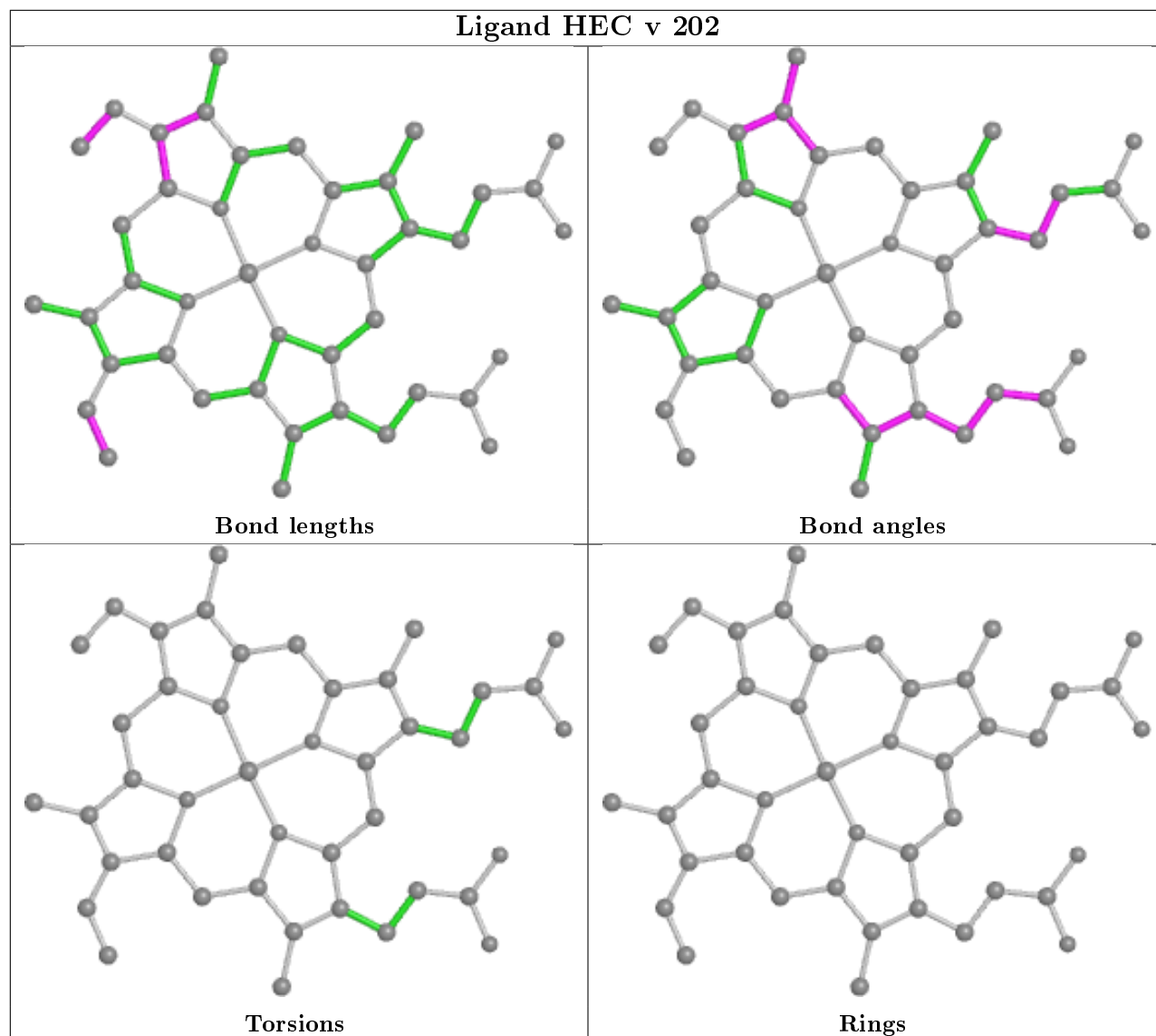
## Ligand SQD b 620



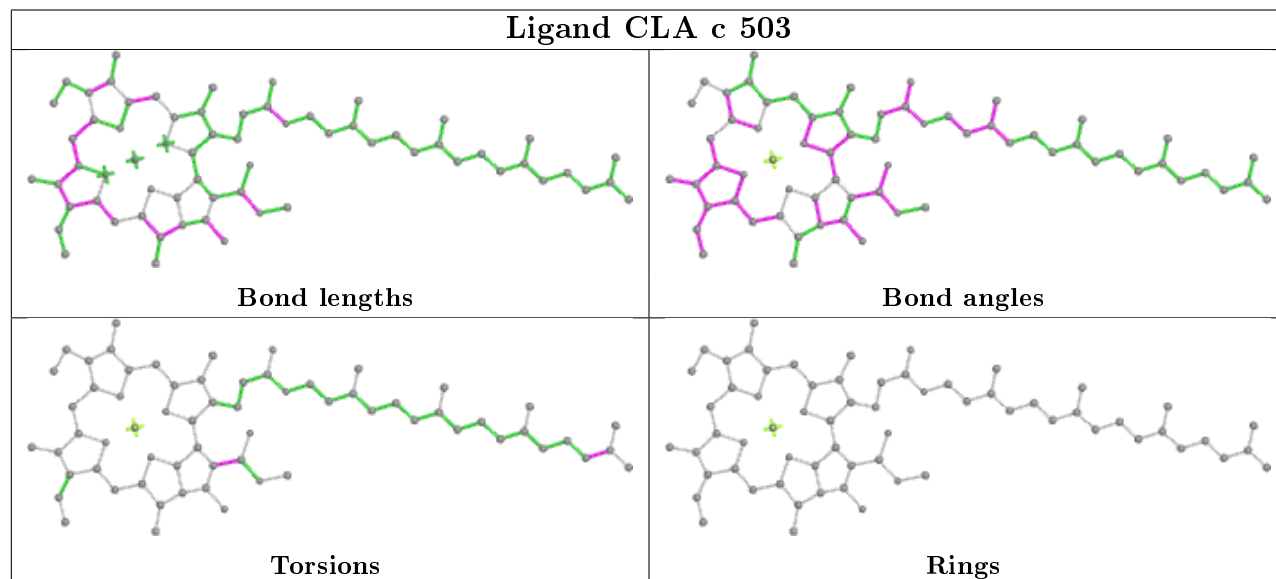
## Ligand BCR B 618



## Ligand HEC v 202

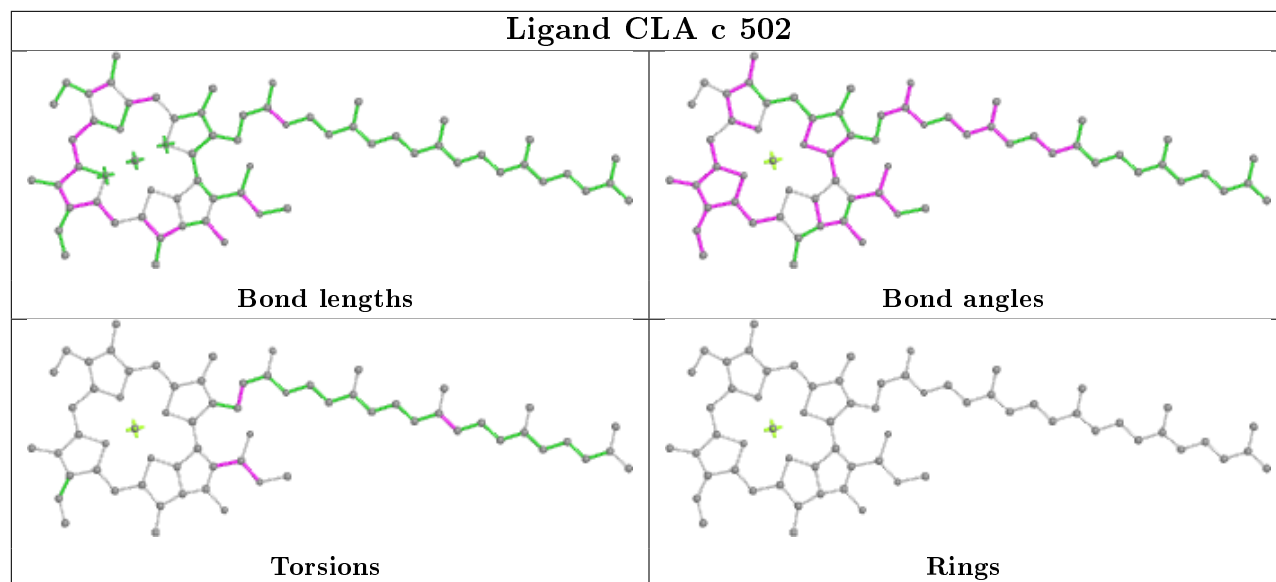


## Ligand CLA c 503

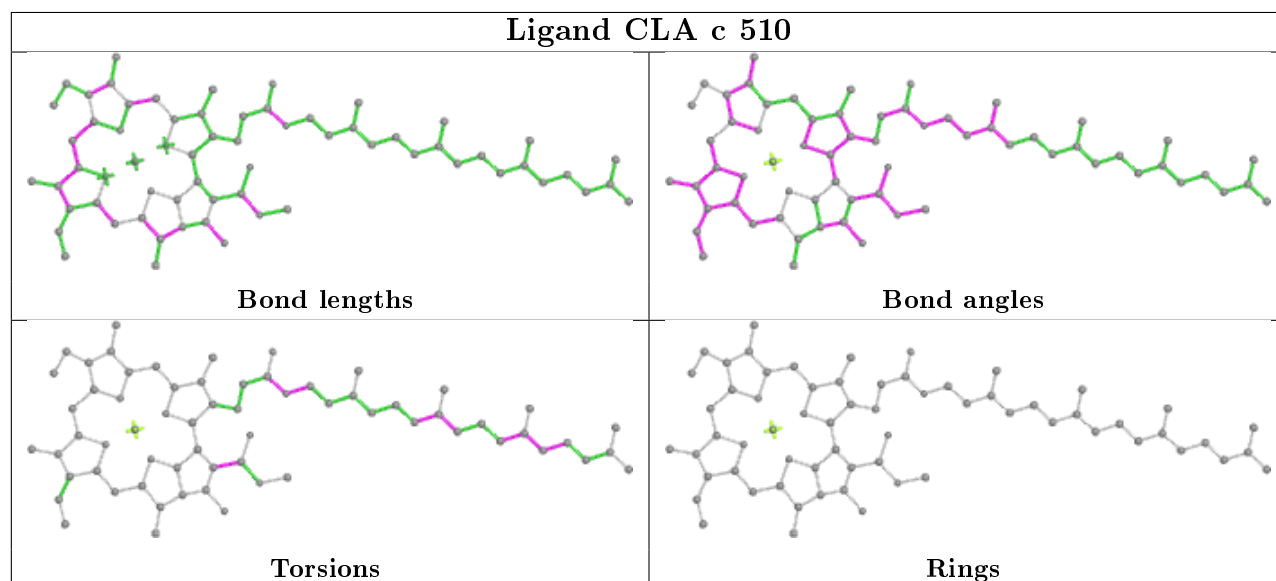




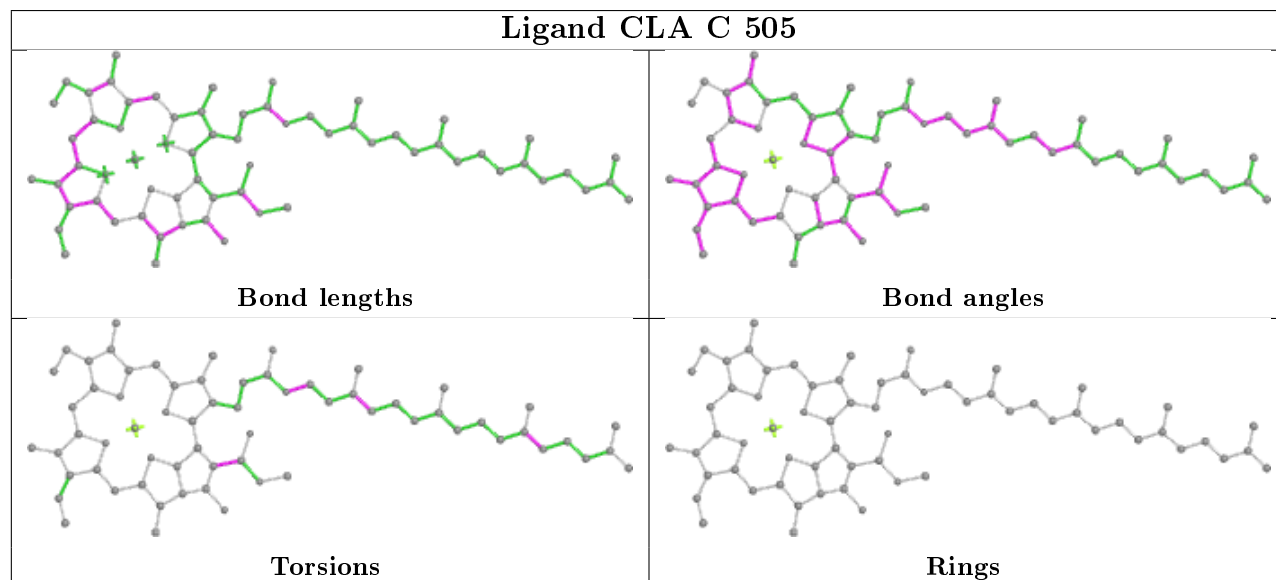
## Ligand CLA c 502

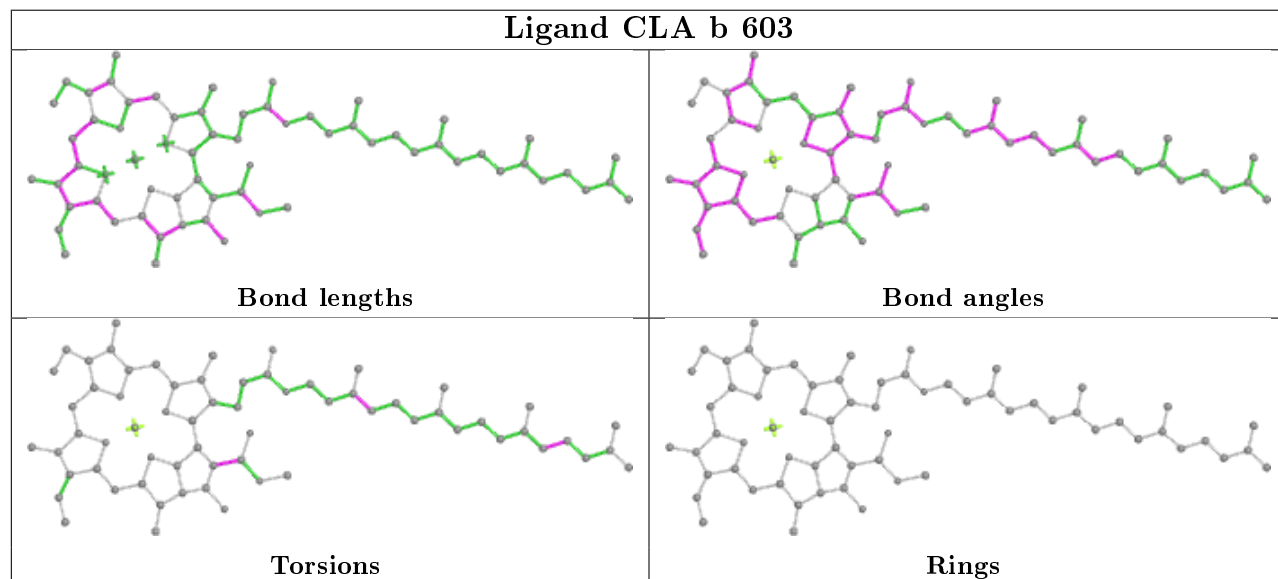
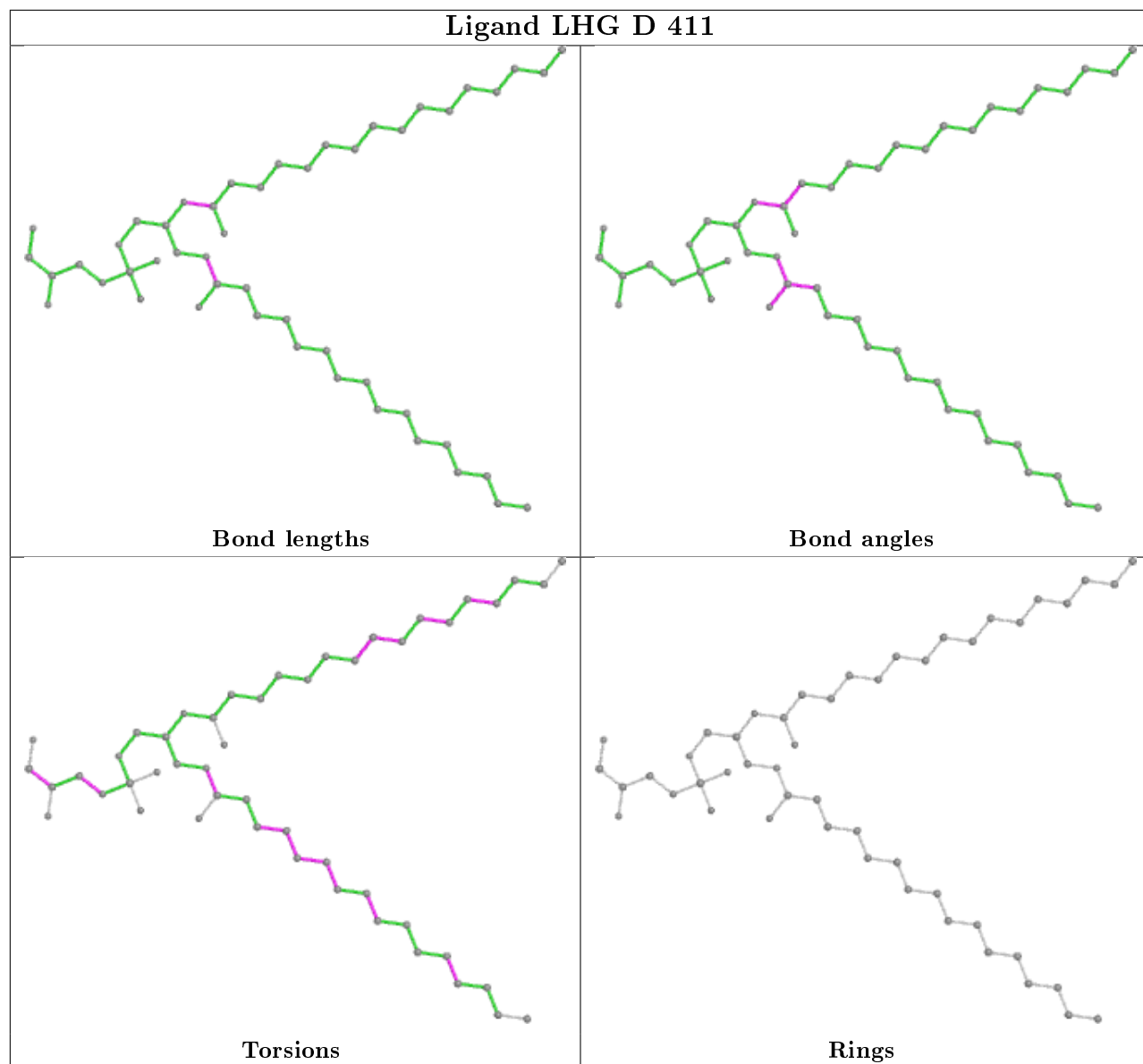


## Ligand CLA c 510

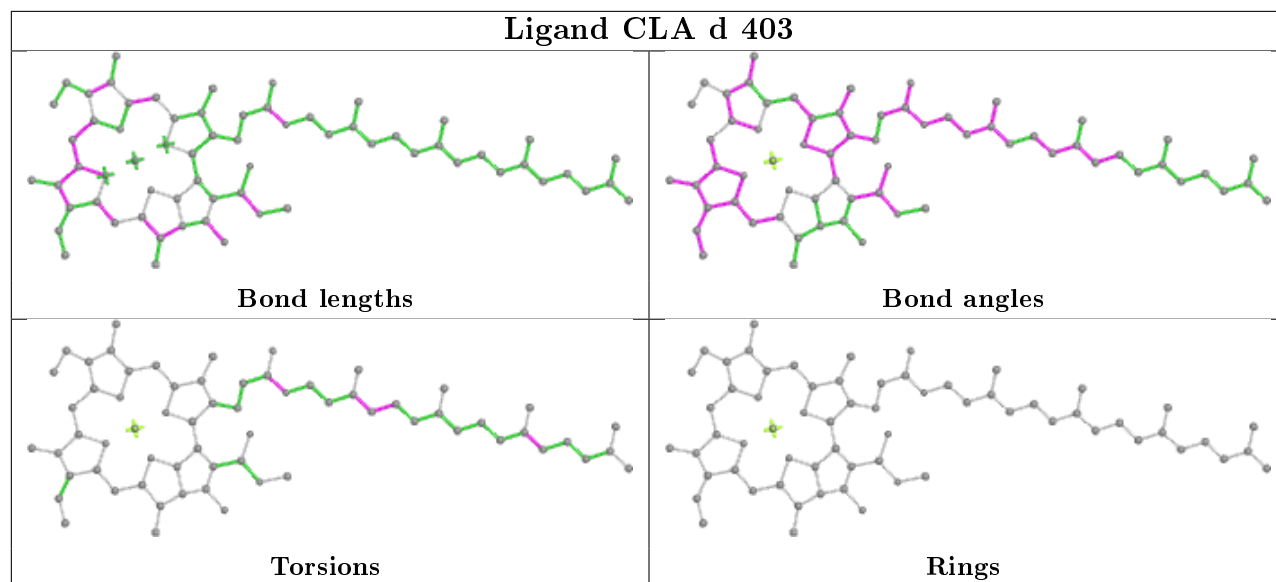


## Ligand CLA C 505

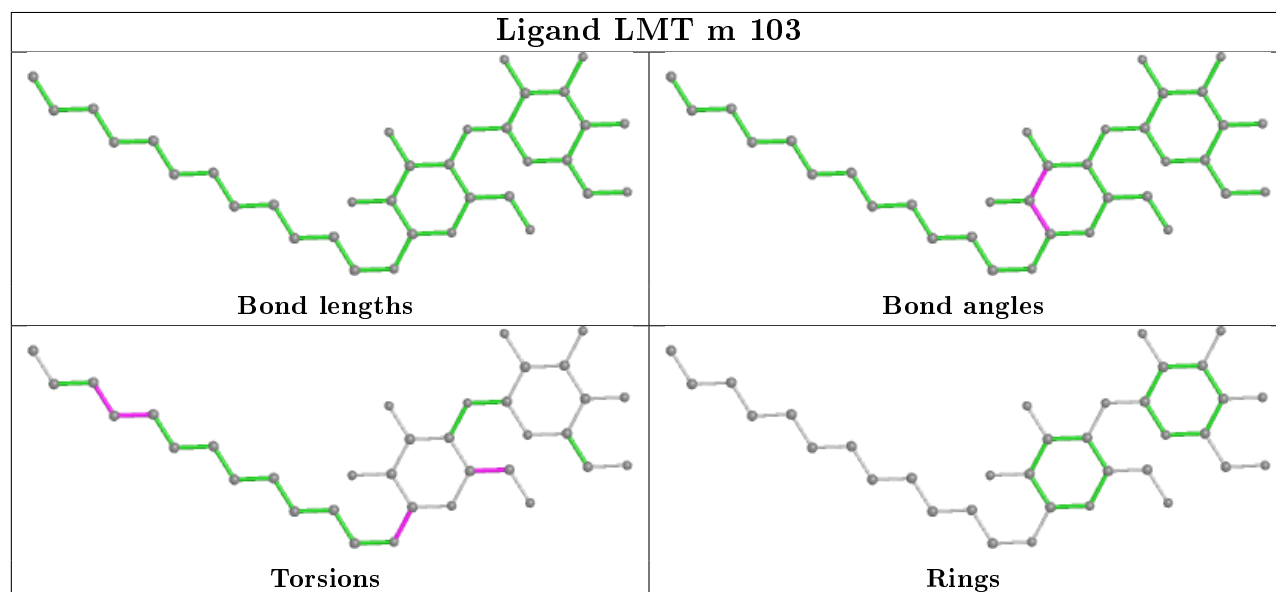




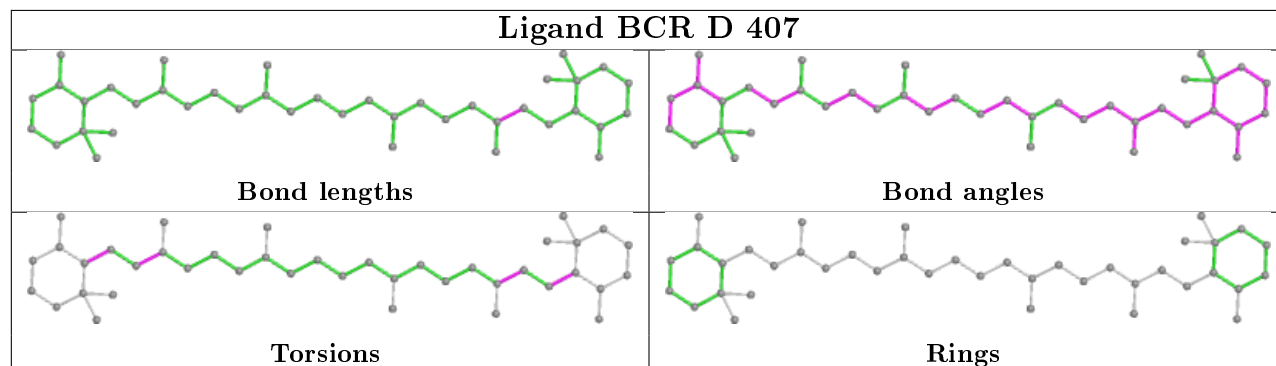
## Ligand CLA d 403



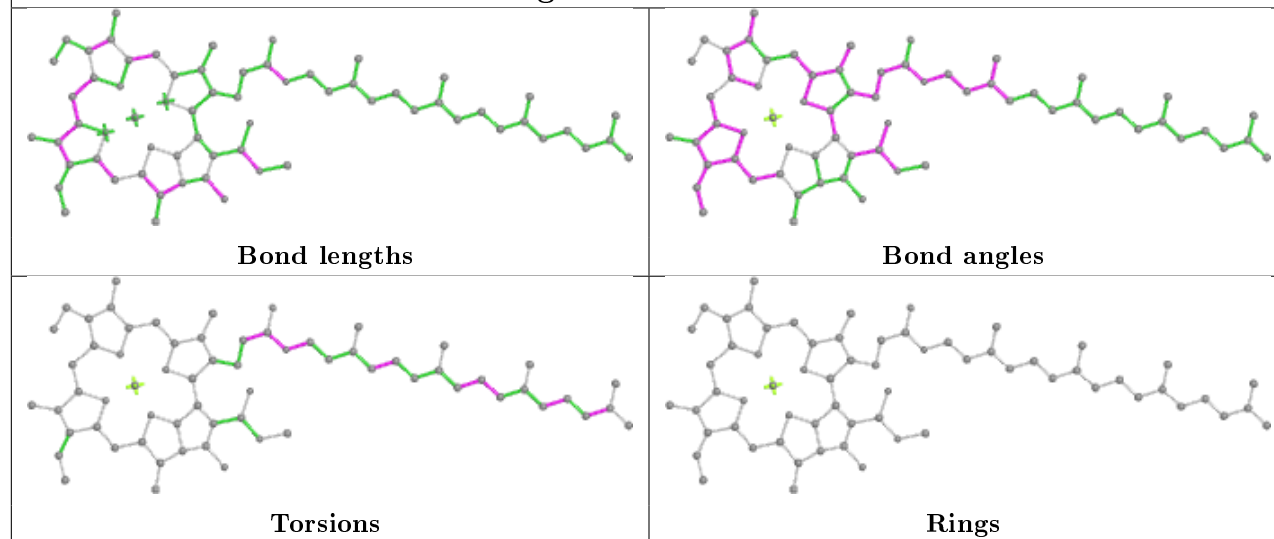
## Ligand LMT m 103



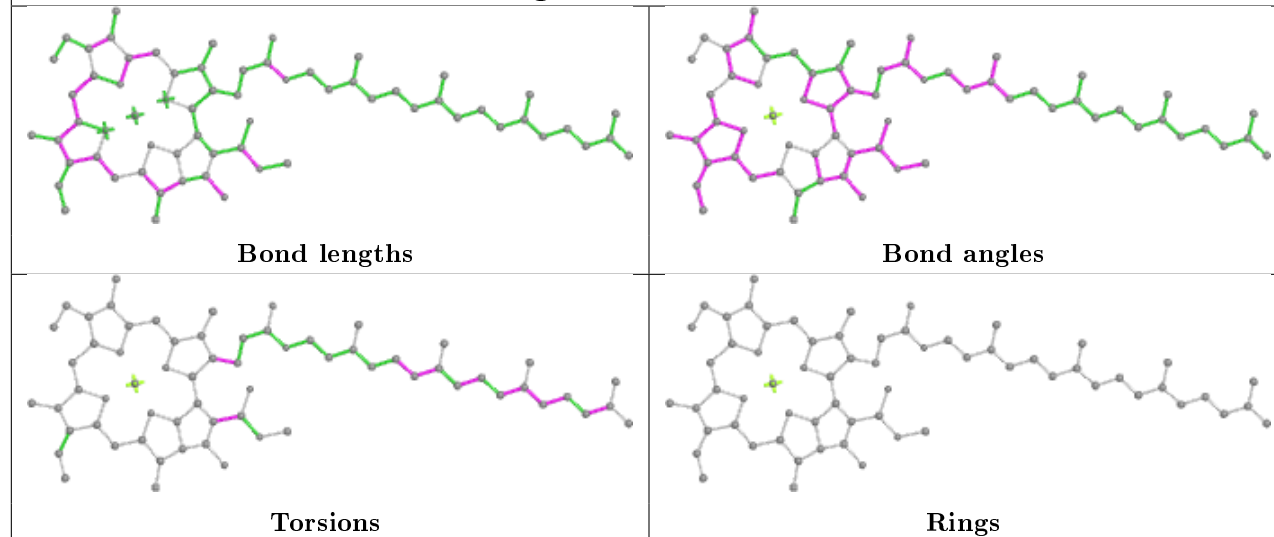
## Ligand BCR D 407

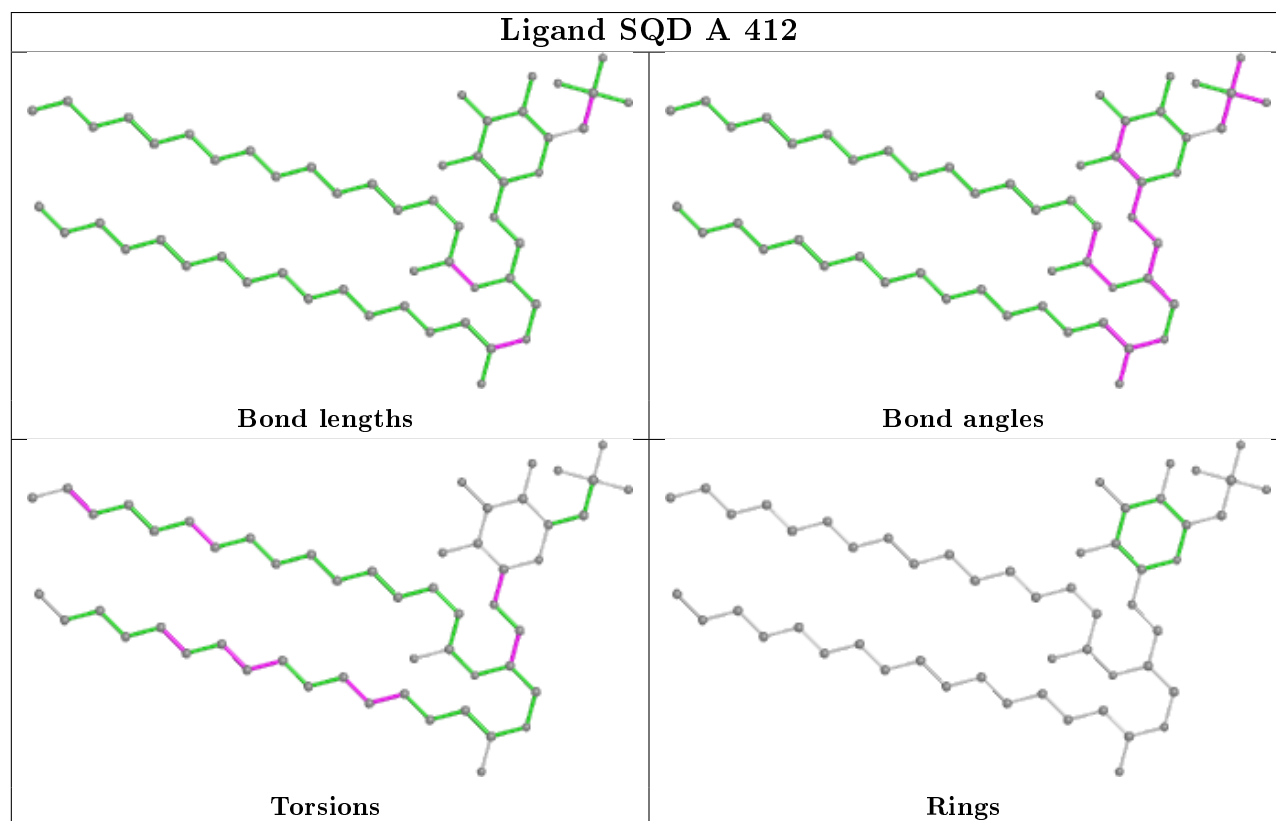
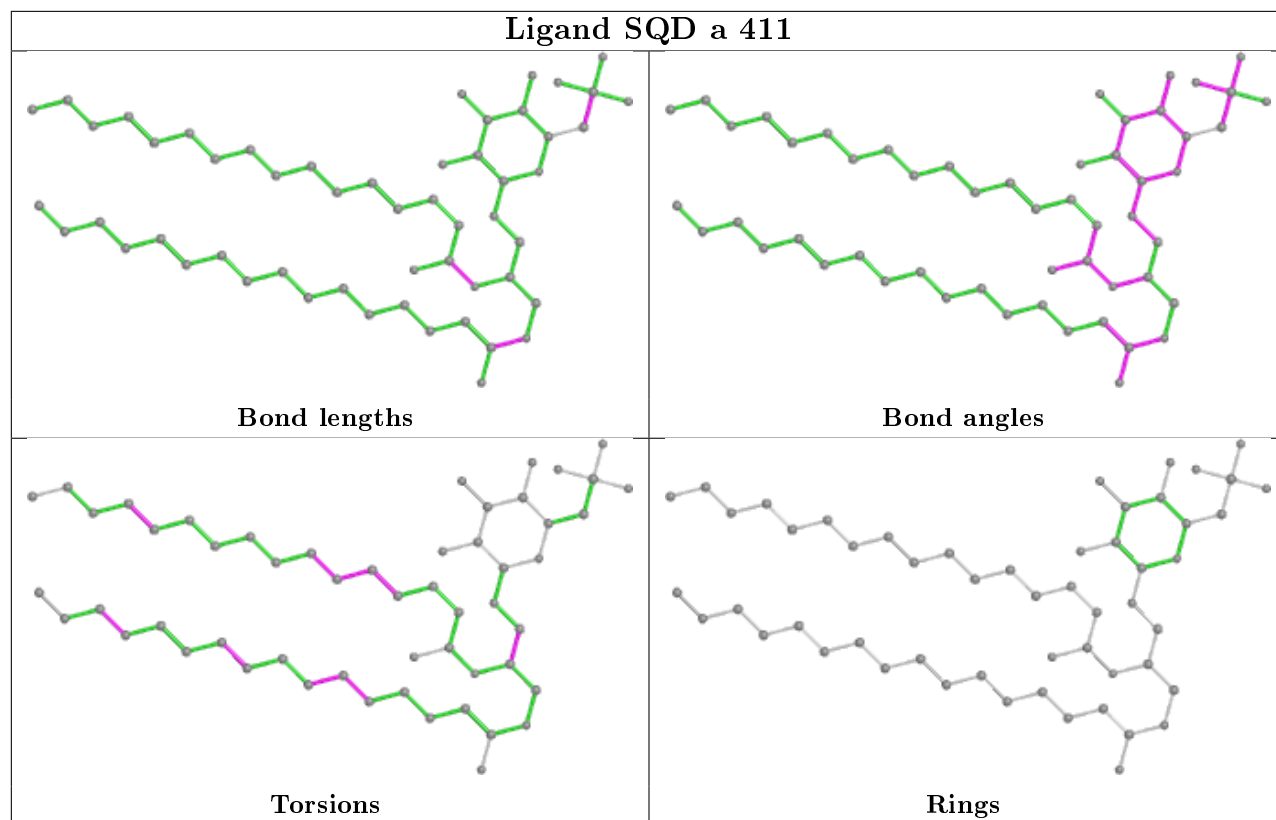


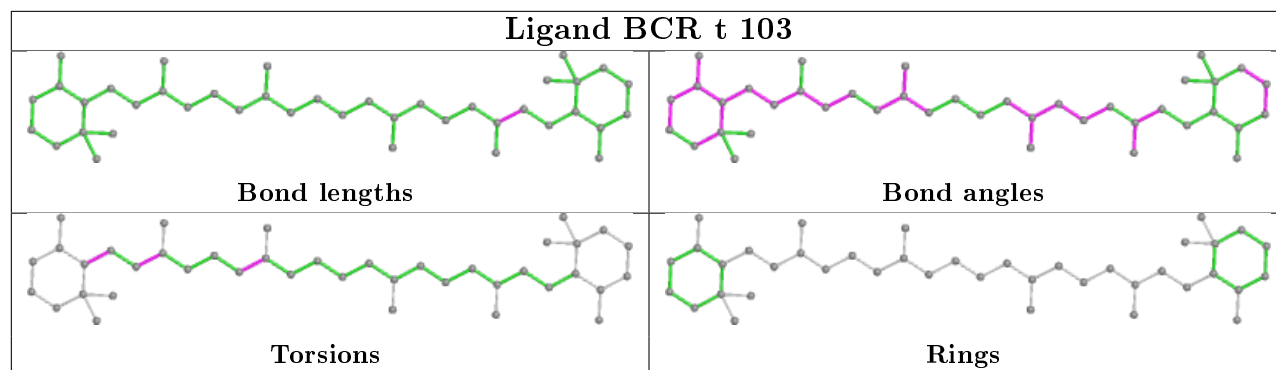
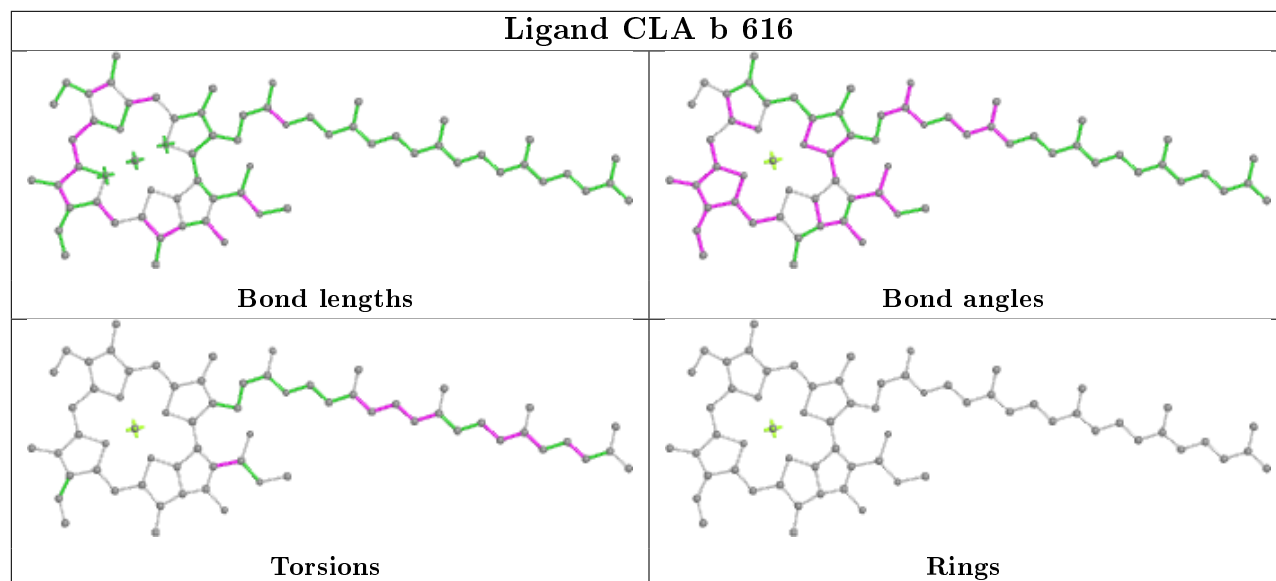
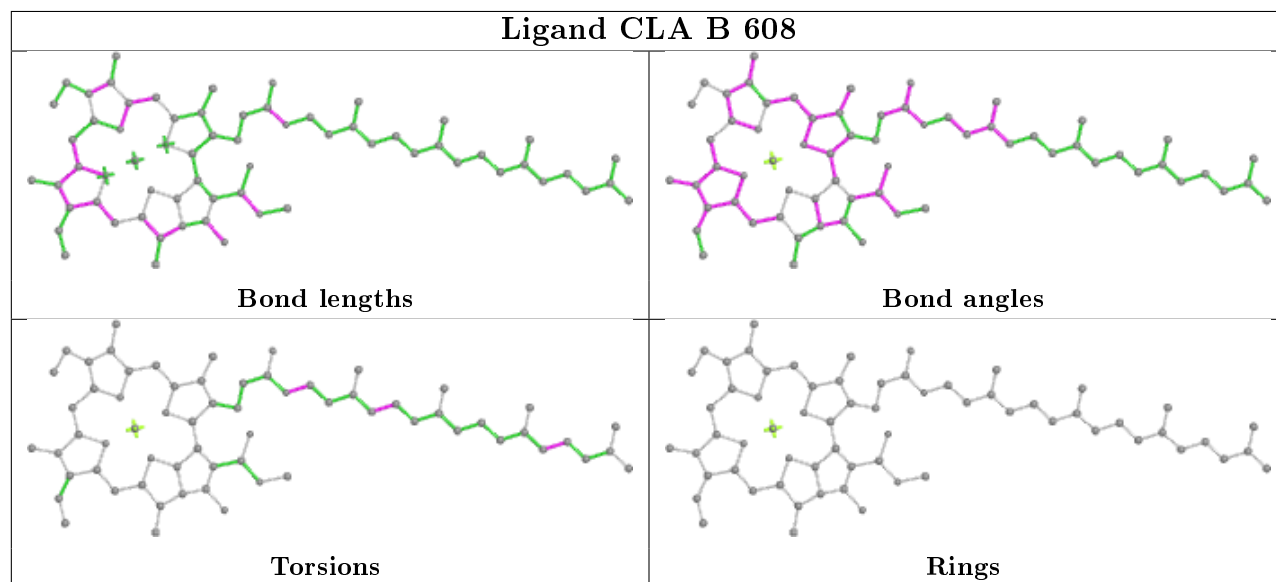
## Ligand CLA c 513

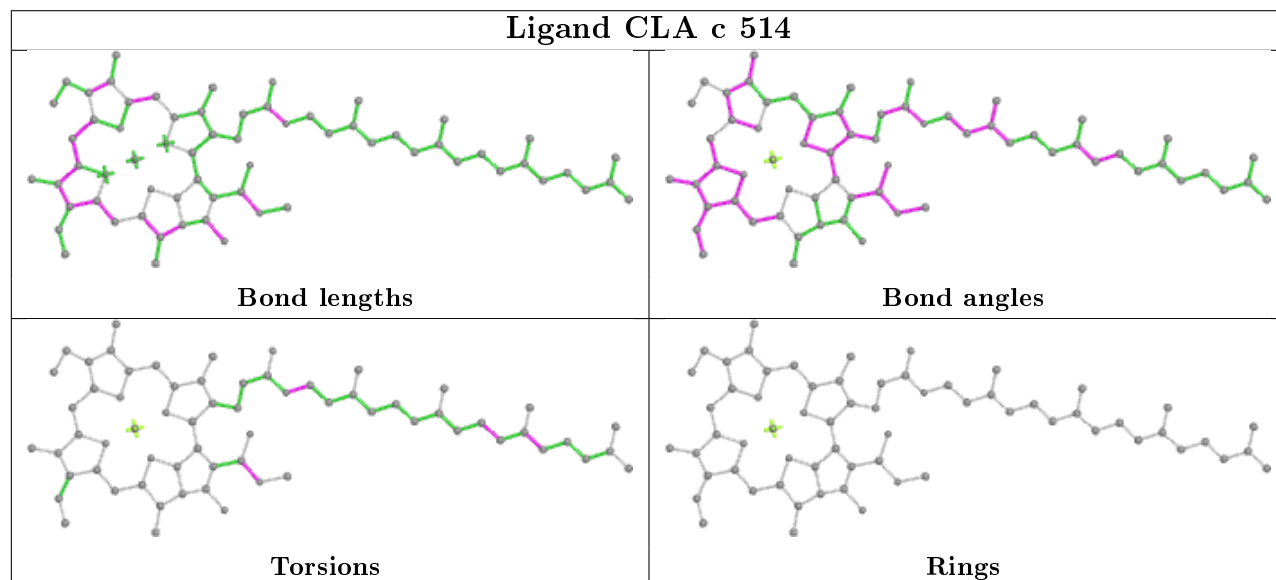
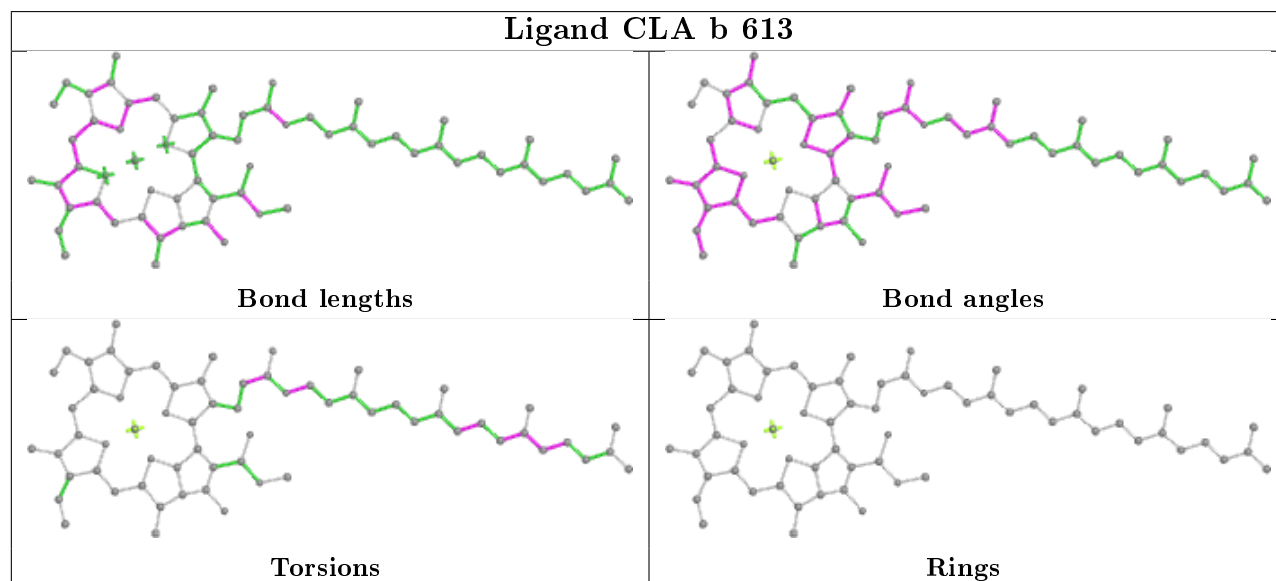
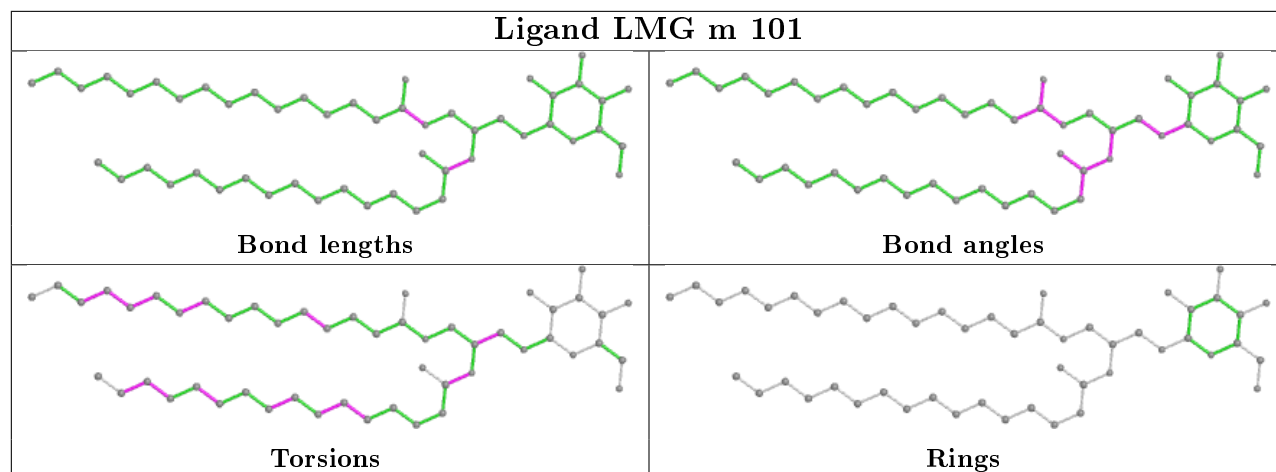


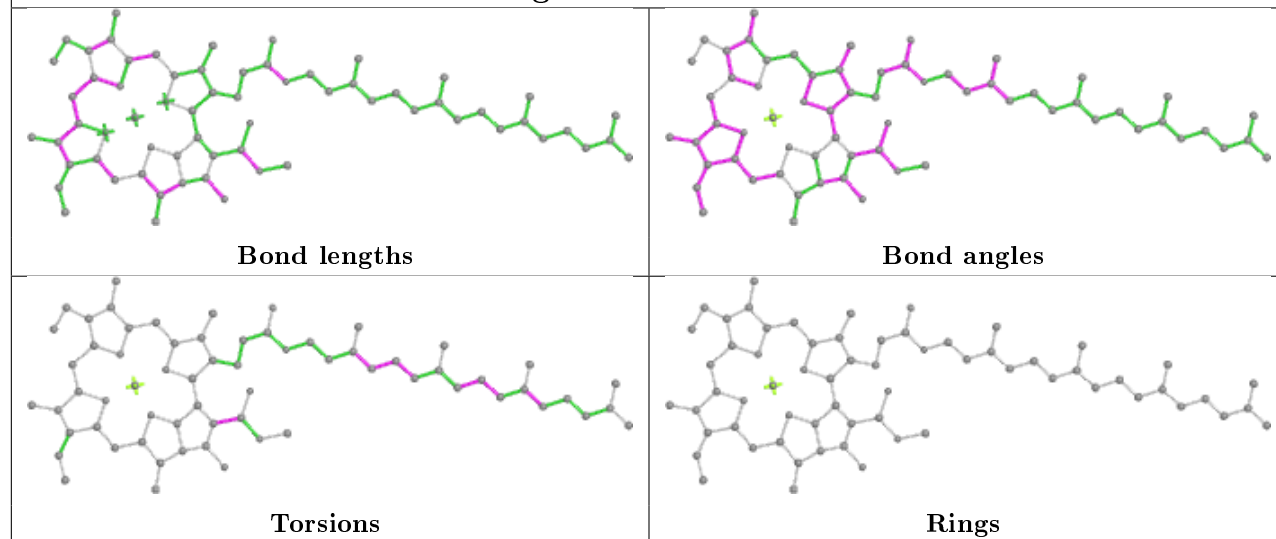
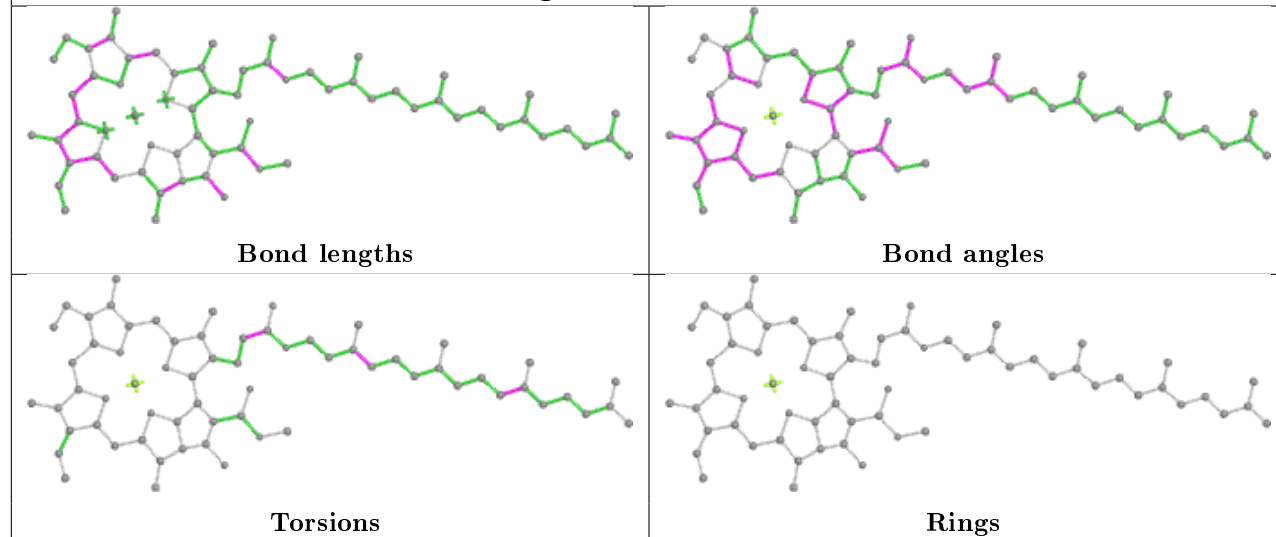
## Ligand CLA C 507



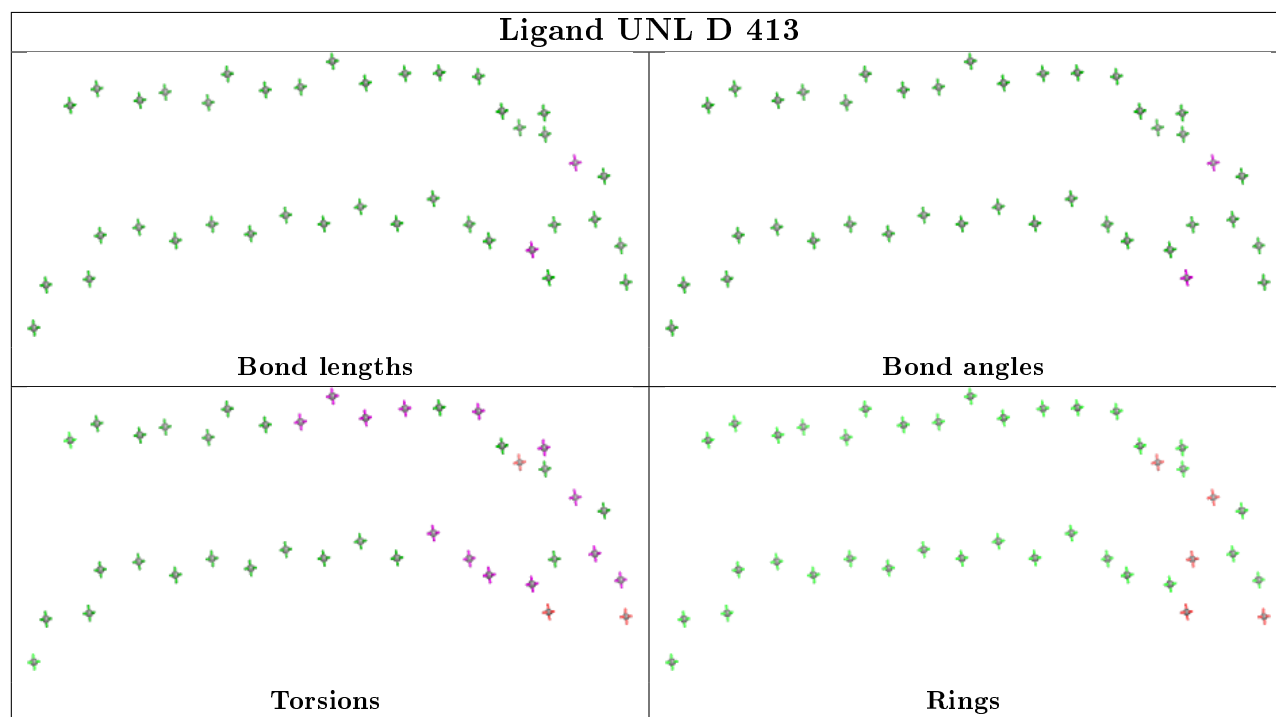
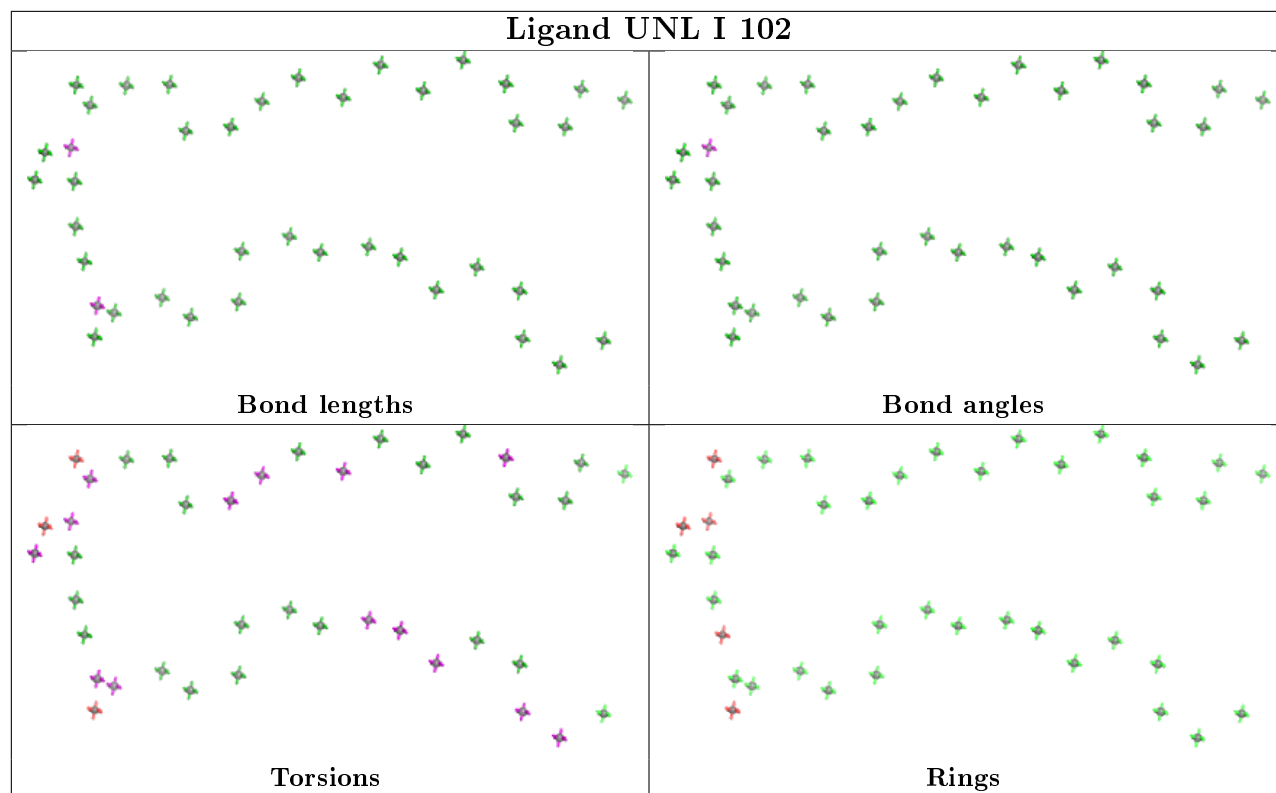


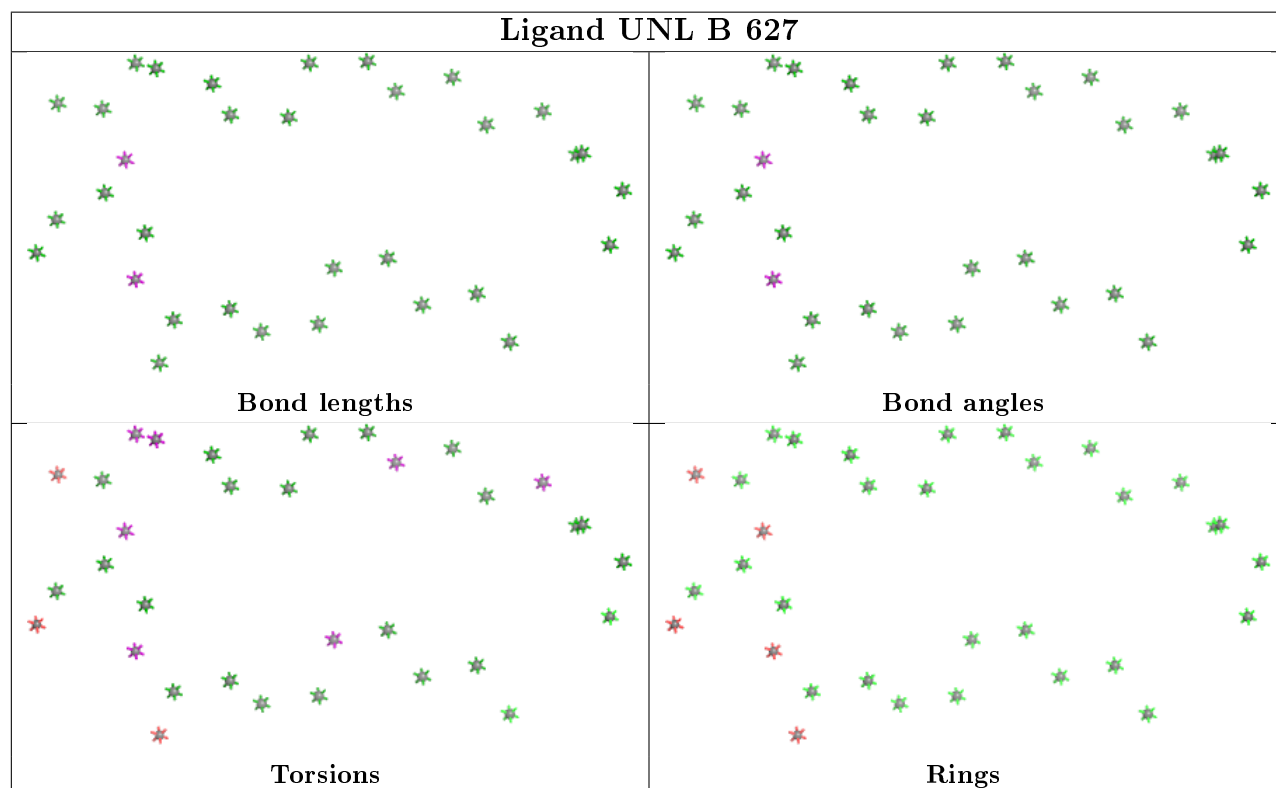
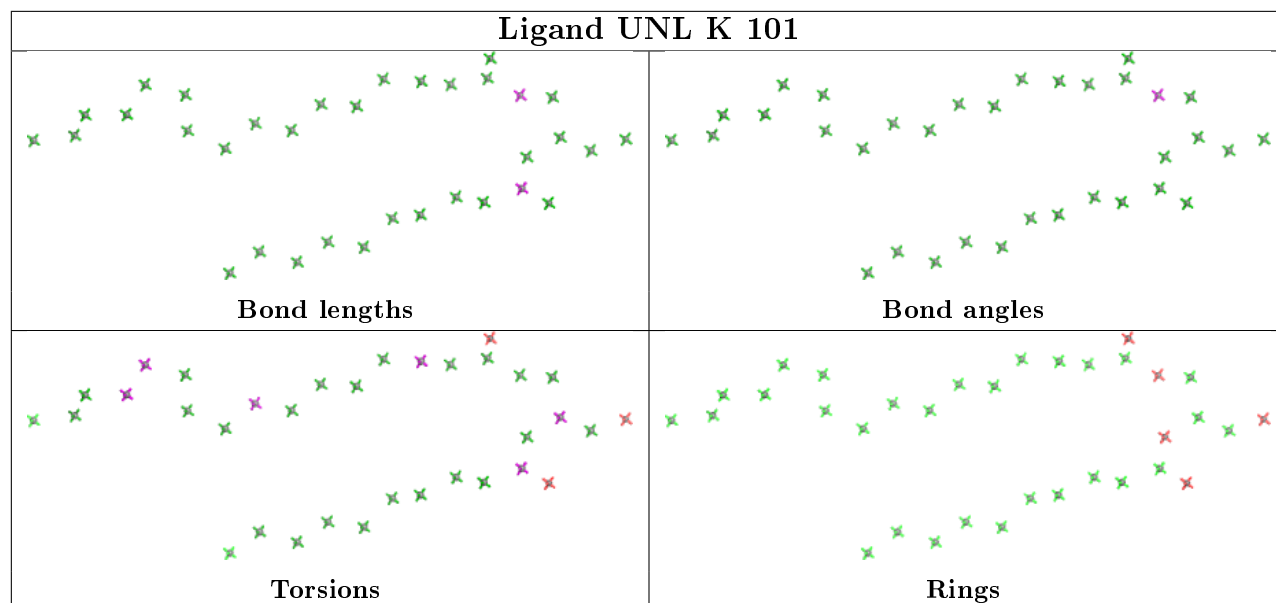
**Ligand BCR t 103****Ligand CLA b 616****Ligand CLA B 608**

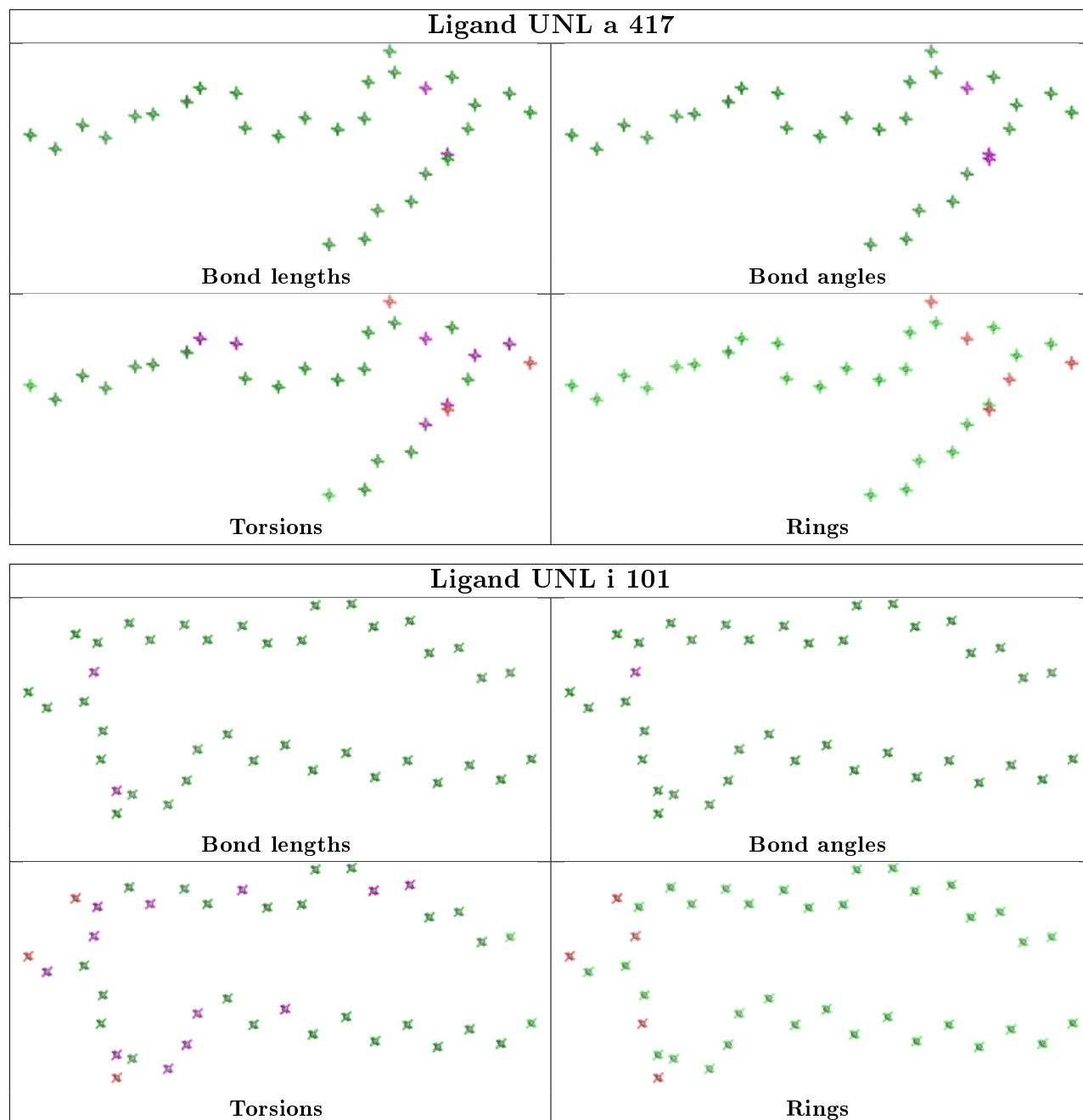


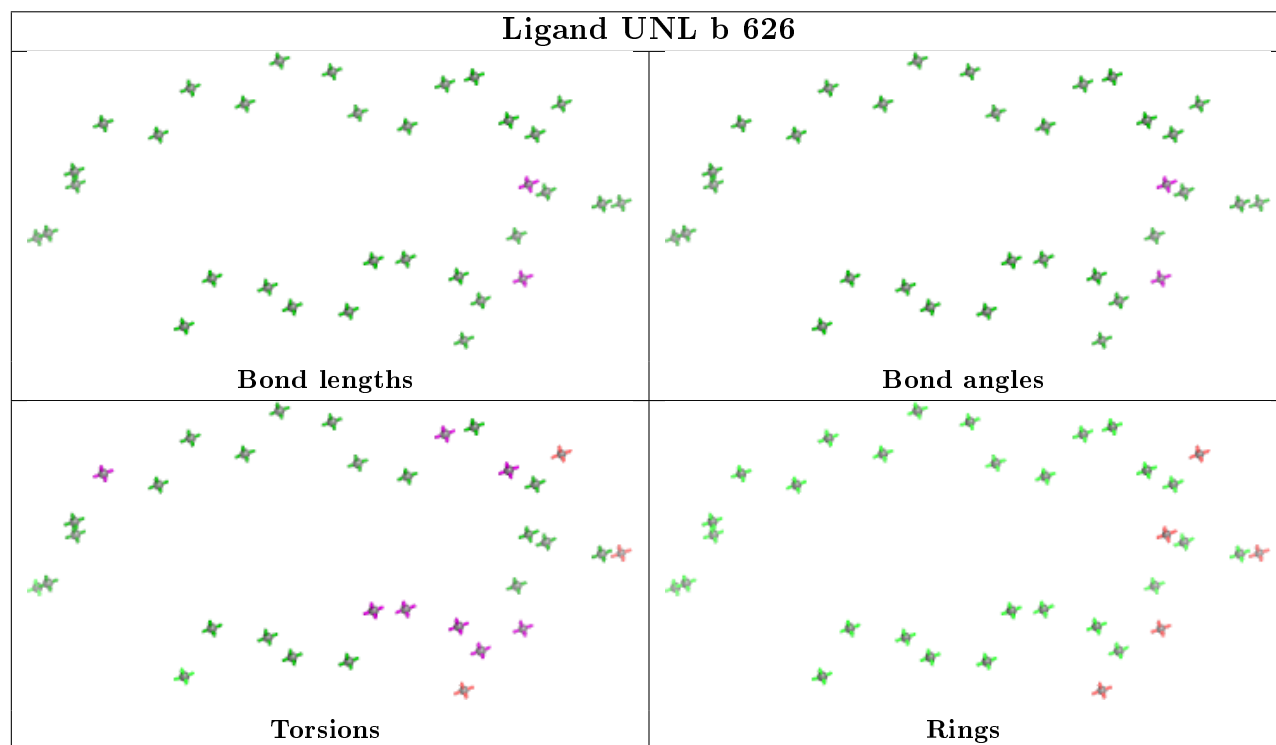
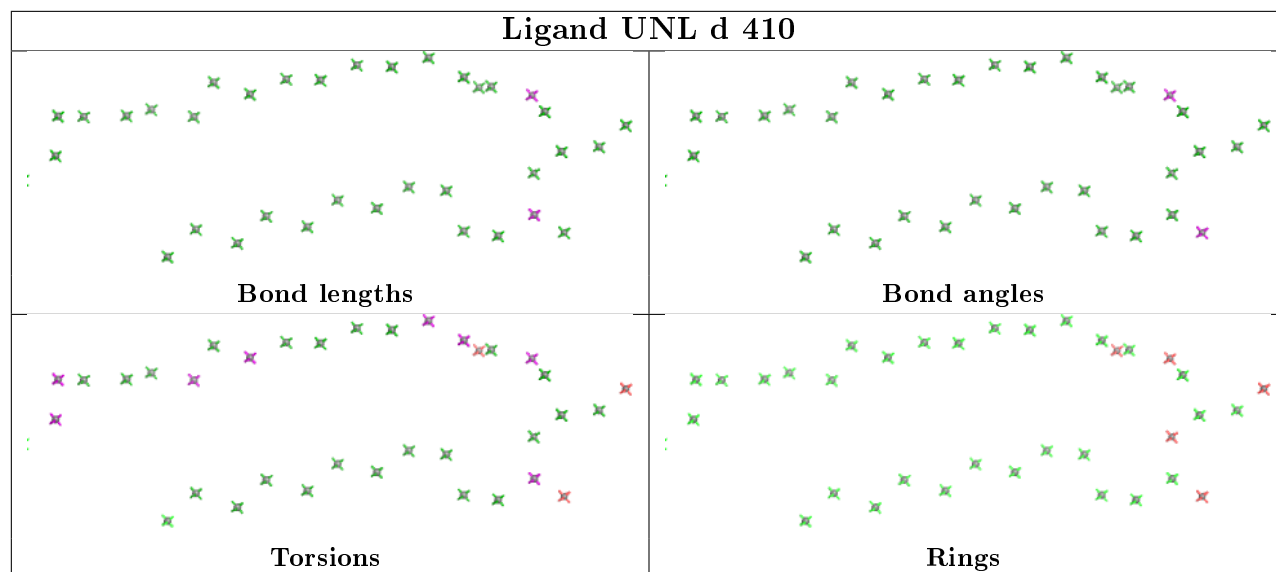
**Ligand CLA B 614****Ligand CLA c 506**

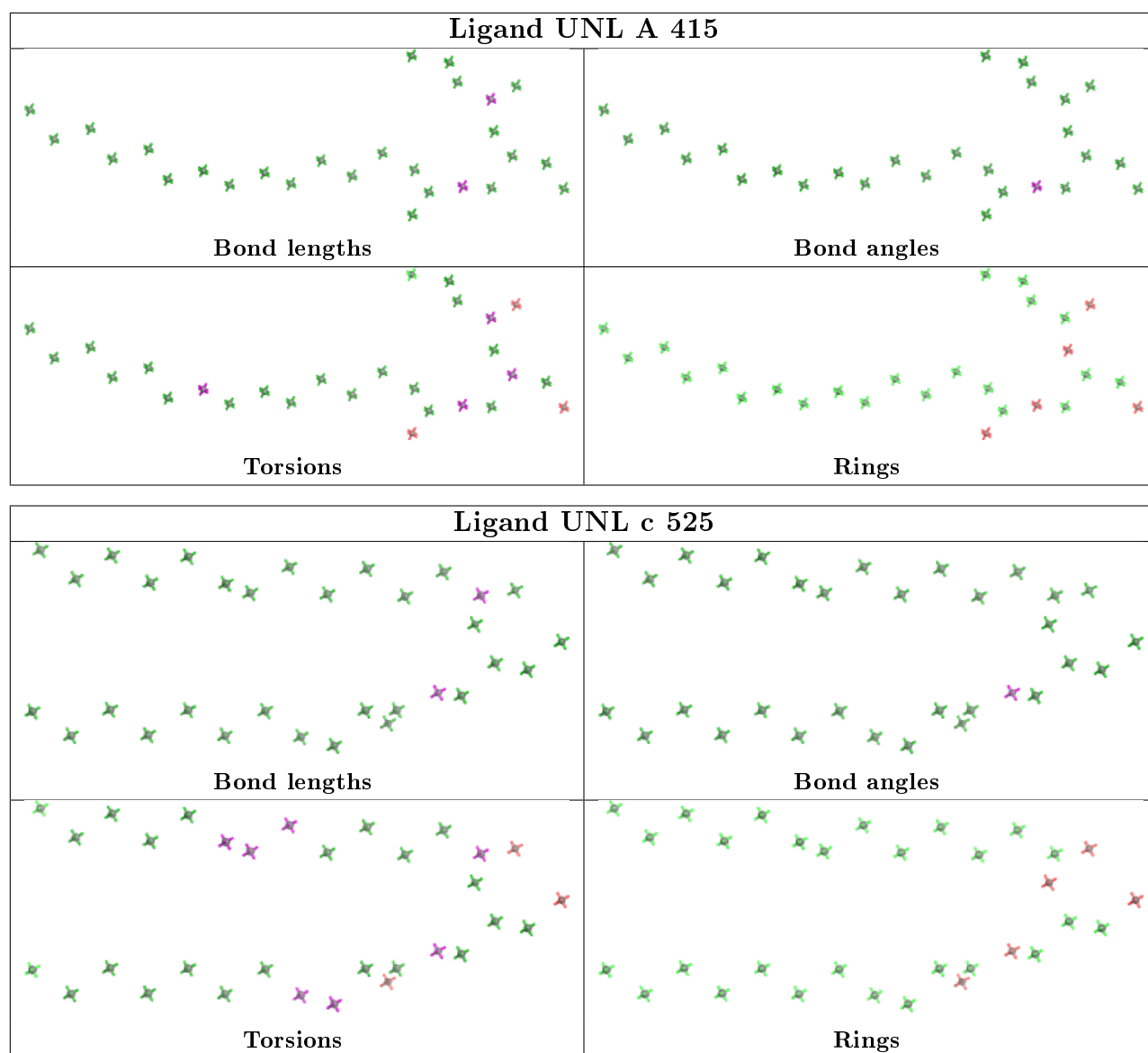












## 5.7 Other polymers [i](#)

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	334/344 (97%)	1.54	87 (26%) 0 0	46, 54, 76, 123	0
1	a	334/344 (97%)	1.82	114 (34%) 0 0	48, 58, 88, 134	0
2	B	504/505 (99%)	1.68	153 (30%) 0 0	47, 60, 88, 130	0
2	b	504/505 (99%)	1.85	176 (34%) 0 0	49, 63, 102, 155	0
3	C	451/455 (99%)	1.81	171 (37%) 0 0	49, 65, 86, 146	0
3	c	455/455 (100%)	1.91	179 (39%) 0 0	54, 73, 95, 133	0
4	D	342/342 (100%)	1.51	92 (26%) 0 0	46, 55, 75, 139	0
4	d	341/342 (99%)	1.56	94 (27%) 0 0	48, 60, 83, 160	0
5	E	81/84 (96%)	2.51	45 (55%) 0 0	59, 76, 104, 157	0
5	e	79/84 (94%)	3.49	61 (77%) 0 0	68, 85, 123, 148	0
6	F	34/44 (77%)	1.46	9 (26%) 0 0	62, 69, 95, 128	0
6	f	31/44 (70%)	2.58	16 (51%) 0 0	68, 75, 106, 142	0
7	H	64/65 (98%)	1.97	28 (43%) 0 0	55, 68, 84, 128	0
7	h	64/65 (98%)	2.24	28 (43%) 0 0	61, 75, 93, 140	0
8	I	37/38 (97%)	2.03	13 (35%) 0 0	59, 68, 122, 144	0
8	i	37/38 (97%)	2.08	14 (37%) 0 0	59, 70, 130, 139	0
9	J	38/39 (97%)	2.12	14 (36%) 0 0	59, 78, 130, 185	0
9	j	39/39 (100%)	2.68	20 (51%) 0 0	67, 85, 134, 172	0
10	K	37/37 (100%)	1.65	12 (32%) 0 0	68, 75, 93, 103	0
10	k	37/37 (100%)	2.27	21 (56%) 0 0	72, 82, 101, 111	0
11	L	36/37 (97%)	1.70	9 (25%) 0 1	47, 52, 103, 152	0
11	l	36/37 (97%)	1.55	8 (22%) 0 1	50, 54, 106, 151	0
12	M	32/36 (88%)	1.40	4 (12%) 3 6	48, 55, 76, 144	0
12	m	33/36 (91%)	1.54	6 (18%) 1 2	49, 55, 83, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/244 (99%)	1.94	87 (35%) 0 0	45, 70, 117, 175	0
13	o	243/244 (99%)	2.10	98 (40%) 0 0	49, 71, 121, 168	0
14	T	29/32 (90%)	0.97	3 (10%) 6 10	49, 54, 84, 117	0
14	t	29/32 (90%)	1.21	2 (6%) 16 24	49, 56, 86, 150	0
15	U	96/104 (92%)	1.80	38 (39%) 0 0	52, 66, 90, 101	0
15	u	97/104 (93%)	1.27	18 (18%) 1 2	58, 68, 86, 131	0
16	V	137/137 (100%)	1.51	34 (24%) 0 1	52, 64, 88, 113	0
16	v	137/137 (100%)	2.40	73 (53%) 0 0	59, 76, 106, 153	0
17	X	38/40 (95%)	2.55	24 (63%) 0 0	65, 79, 102, 123	0
17	x	38/40 (95%)	3.15	25 (65%) 0 0	70, 86, 123, 162	0
18	Y	29/30 (96%)	4.39	23 (79%) 0 0	76, 92, 127, 141	0
18	y	29/30 (96%)	3.95	25 (86%) 0 0	85, 103, 127, 133	0
19	Z	62/62 (100%)	3.96	52 (83%) 0 0	75, 90, 138, 173	0
19	z	62/62 (100%)	5.00	55 (88%) 0 0	89, 104, 148, 194	0
20	R	34/34 (100%)	7.15	34 (100%) 0 0	103, 130, 154, 159	0
All	All	5283/5384 (98%)	1.96	1965 (37%) 0 0	45, 65, 107, 194	0

All (1965) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	Y	19	ILE	13.2
2	b	494	GLY	13.1
19	z	3	ILE	13.1
20	R	18	TRP	11.5
2	b	504	THR	11.4
20	R	28	VAL	11.2
18	Y	20	ALA	11.0
2	b	487	SER	10.7
19	z	33	TRP	10.6
11	L	2	GLU	10.6
17	x	2	THR	10.5
2	B	494	GLY	10.5
20	R	6	LEU	10.1
2	b	503	THR	10.0
17	x	38	GLN	9.9
6	f	15	ILE	9.8
19	z	32	ASP	9.6

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Mol	Chain	Res	Type	RSRZ
20	R	27	ALA	9.4
19	Z	42	LEU	9.4
20	R	24	LEU	9.4
13	O	61	GLN	9.3
1	a	11	ALA	9.3
19	Z	3	ILE	9.2
18	y	41	VAL	9.2
19	z	34	ASP	9.0
17	x	37	VAL	9.0
7	h	65	LEU	9.0
20	R	7	VAL	8.9
19	z	30	PRO	8.9
20	R	23	ILE	8.9
2	b	502	VAL	8.8
19	z	7	LEU	8.8
3	c	200	THR	8.5
20	R	3	TRP	8.5
18	Y	18	VAL	8.4
19	Z	31	GLN	8.4
2	b	496	TYR	8.3
12	M	33	GLN	8.3
20	R	32	GLN	8.3
8	i	36	ASP	8.3
2	b	493	TRP	8.3
20	R	26	TYR	8.2
20	R	11	PRO	8.2
2	b	293	ALA	8.1
5	E	84	LYS	8.1
13	o	246	ALA	8.1
19	Z	33	TRP	8.0
19	z	2	THR	8.0
20	R	25	PRO	8.0
2	b	295	GLY	8.0
13	O	133	VAL	8.0
19	z	39	LEU	8.0
20	R	31	VAL	8.0
20	R	22	ASN	7.9
8	i	37	LEU	7.8
19	z	31	GLN	7.8
20	R	21	ARG	7.8
16	v	14	SER	7.7
2	B	496	TYR	7.7

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Mol	Chain	Res	Type	RSRZ
2	b	495	PHE	7.6
9	J	3	GLU	7.6
1	A	13	LEU	7.6
13	O	27	ARG	7.6
3	C	155	ASN	7.6
2	B	495	PHE	7.6
13	O	25	THR	7.5
19	Z	34	ASP	7.5
11	l	3	PRO	7.5
19	Z	35	ARG	7.5
19	z	5	PHE	7.4
20	R	13	LEU	7.4
13	o	208	THR	7.4
2	B	293	ALA	7.4
9	j	6	ARG	7.4
16	v	16	GLY	7.3
19	Z	38	GLN	7.3
4	D	11	GLU	7.3
13	o	134	THR	7.2
13	O	139	SER	7.2
13	o	33	ASP	7.2
13	o	58	ASN	7.1
18	y	37	PHE	7.1
13	O	91	GLY	7.1
19	z	61	VAL	7.1
20	R	33	LYS	7.1
13	o	37	THR	7.1
2	b	488	PRO	7.1
19	Z	30	PRO	7.1
19	Z	41	PHE	7.1
2	B	295	GLY	7.1
5	E	25	ILE	7.0
19	z	50	LEU	7.0
13	o	140	THR	7.0
18	Y	23	THR	7.0
5	e	84	LYS	7.0
9	j	9	LEU	7.0
2	B	290	ALA	7.0
19	z	42	LEU	7.0
2	b	294	SER	7.0
3	c	203	THR	6.9
12	m	34	LYS	6.9

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Mol	Chain	Res	Type	RSRZ
19	z	29	SER	6.9
13	o	63	ALA	6.9
19	z	41	PHE	6.9
19	z	60	PHE	6.9
7	h	64	ALA	6.9
8	I	36	ASP	6.8
3	c	143	TYR	6.8
13	O	59	LYS	6.8
5	e	34	GLY	6.8
2	b	497	GLN	6.8
20	R	14	LEU	6.8
19	z	38	GLN	6.8
18	y	19	ILE	6.8
8	I	38	GLU	6.7
19	z	35	ARG	6.7
5	e	19	TYR	6.7
20	R	15	ALA	6.7
5	e	20	TRP	6.7
20	R	35	LEU	6.7
13	O	23	ASP	6.7
2	b	482	ILE	6.7
7	h	6	TRP	6.7
7	H	65	LEU	6.7
13	o	209	GLY	6.7
13	o	4	THR	6.6
5	e	6	GLY	6.6
12	m	33	GLN	6.6
13	o	207	ARG	6.6
13	O	130	GLN	6.6
19	Z	32	ASP	6.6
13	o	35	SER	6.5
2	b	296	ALA	6.5
13	o	133	VAL	6.5
13	o	36	GLN	6.5
19	z	46	LEU	6.5
13	o	27	ARG	6.5
5	e	39	SER	6.4
5	e	79	PHE	6.4
19	z	10	ALA	6.4
20	R	10	LEU	6.4
13	o	139	SER	6.4
13	O	28	GLY	6.4

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Mol	Chain	Res	Type	RSRZ
18	y	20	ALA	6.4
9	J	4	GLY	6.4
3	c	201	ASN	6.4
2	B	294	SER	6.4
5	E	4	THR	6.3
7	H	64	ALA	6.3
9	J	2	SER	6.3
3	c	426	LEU	6.2
3	C	30	SER	6.2
2	b	491	VAL	6.2
3	C	257	PHE	6.2
19	z	36	SER	6.2
20	R	2	ASP	6.2
9	j	3	GLU	6.2
20	R	12	VAL	6.2
19	z	59	PHE	6.2
20	R	34	LEU	6.2
5	E	17	VAL	6.2
19	Z	61	VAL	6.2
7	H	6	TRP	6.1
1	A	12	ASN	6.1
19	z	4	LEU	6.1
3	c	166	ILE	6.1
3	C	23	ALA	6.1
2	B	487	SER	6.1
17	X	2	THR	6.0
5	e	21	VAL	6.0
5	e	57	ALA	6.0
19	z	25	VAL	6.0
19	z	1	MET	6.0
5	E	83	LEU	6.0
13	o	91	GLY	6.0
1	a	12	ASN	6.0
13	O	137	THR	6.0
5	e	24	SER	6.0
2	b	290	ALA	6.0
16	v	15	GLU	5.9
20	R	5	VAL	5.9
18	Y	26	ALA	5.9
3	C	145[A]	SER	5.9
19	Z	26	ALA	5.9
4	d	17	ILE	5.9

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Mol	Chain	Res	Type	RSRZ
16	v	19	ILE	5.9
3	c	24	THR	5.9
16	v	5	PRO	5.9
3	C	433	LEU	5.8
4	D	238	THR	5.8
3	c	235	GLY	5.8
19	Z	1	MET	5.8
16	v	17	LYS	5.8
13	o	25	THR	5.8
13	o	31	PRO	5.8
2	B	504	THR	5.8
5	e	17	VAL	5.8
10	k	14	ALA	5.8
13	o	21	THR	5.7
5	E	22	ILE	5.7
1	A	11	ALA	5.7
20	R	30	GLN	5.7
3	c	181	PHE	5.7
3	c	257	PHE	5.7
4	d	14	TRP	5.7
13	O	208	THR	5.7
3	C	207	ARG	5.7
13	O	21	THR	5.7
13	o	137	THR	5.7
15	U	102	LEU	5.7
16	v	22	THR	5.7
20	R	29	LYS	5.7
19	Z	4	LEU	5.7
5	e	16	SER	5.7
13	o	24	ASP	5.6
19	Z	36	SER	5.6
13	o	132	ASN	5.6
5	e	29	ALA	5.6
3	c	250	TRP	5.6
4	d	12	ARG	5.6
16	v	4	THR	5.6
2	B	245	VAL	5.6
20	R	4	ARG	5.6
13	O	131	PRO	5.6
17	x	9	GLY	5.6
17	x	3	ILE	5.6
6	f	20	TRP	5.6

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Mol	Chain	Res	Type	RSRZ
1	a	341	LEU	5.6
3	c	202	PRO	5.6
2	B	297	THR	5.6
13	o	59	LYS	5.6
13	O	58	ASN	5.5
19	Z	25	VAL	5.5
16	V	16	GLY	5.5
9	j	4	GLY	5.5
18	y	22	LEU	5.5
2	b	501	ASP	5.5
3	c	260	ALA	5.5
5	e	15	THR	5.5
4	D	17	ILE	5.5
13	o	204	VAL	5.5
3	C	143	TYR	5.4
18	y	23	THR	5.4
17	X	38	GLN	5.4
19	z	8	ALA	5.4
4	d	159	ILE	5.4
16	v	9	THR	5.4
2	b	505	ARG	5.4
18	y	40	ALA	5.4
2	B	502	VAL	5.4
18	Y	42	ARG	5.4
17	X	15	LEU	5.3
11	L	7	ARG	5.3
1	A	339	PHE	5.3
7	h	23	PRO	5.3
3	c	193	GLY	5.3
5	e	74	GLN	5.3
19	Z	45	GLY	5.3
5	e	33	ALA	5.3
3	c	182	PHE	5.3
2	B	497	GLN	5.3
2	b	486	LEU	5.3
4	D	352	LEU	5.3
16	v	13	ASN	5.3
19	z	43	GLY	5.3
1	a	15	GLU	5.2
5	e	71	GLU	5.2
19	Z	15	LEU	5.3
5	e	25	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
2	B	296	ALA	5.2
4	D	14	TRP	5.2
3	C	181	PHE	5.2
3	C	438	LEU	5.2
2	b	129	GLY	5.2
20	R	19	ALA	5.2
13	o	245	PRO	5.2
20	R	8	VAL	5.2
3	c	101	PRO	5.2
19	z	11	ALA	5.2
3	c	205	ASP	5.2
13	O	90	ASP	5.2
9	J	7	ILE	5.2
6	f	16	PHE	5.1
1	a	297	LEU	5.1
3	C	258	GLY	5.1
2	b	301	ALA	5.1
2	b	485	GLU	5.1
3	C	437	PHE	5.1
13	O	60	ARG	5.1
19	z	49	ALA	5.1
15	U	80	GLU	5.1
1	a	326	LEU	5.1
19	Z	37	LYS	5.1
18	y	21	GLN	5.1
4	D	159	ILE	5.1
16	v	78	ASN	5.1
3	c	159	THR	5.1
13	o	29	ALA	5.1
19	z	40	ILE	5.1
1	a	14	TRP	5.1
18	Y	22	LEU	5.0
5	E	5	THR	5.0
13	O	63	ALA	5.0
3	c	142	GLU	5.0
3	C	25	ASN	5.0
13	O	24	ASP	5.0
13	O	200	ASN	5.0
2	B	247	PHE	5.0
9	j	2	SER	5.0
4	D	346	LEU	5.0
2	b	297	THR	5.0

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Mol	Chain	Res	Type	RSRZ
9	J	6	ARG	5.0
13	O	26	ALA	5.0
3	c	144	SER	5.0
13	O	138	THR	5.0
16	v	6	GLU	5.0
2	b	292	LEU	5.0
2	b	463	PHE	5.0
10	K	16	ALA	5.0
3	C	285	ILE	4.9
13	O	22	LEU	4.9
18	Y	38	LEU	4.9
2	b	291	SER	4.9
2	B	292	LEU	4.9
19	z	57	LEU	4.9
6	F	14	PRO	4.9
19	z	6	GLN	4.9
3	c	60	ILE	4.9
1	A	341	LEU	4.9
3	c	279	LEU	4.9
13	o	56	PRO	4.9
16	v	135	VAL	4.9
18	Y	41	VAL	4.9
13	o	205	ASP	4.9
8	I	37	LEU	4.9
19	Z	7	LEU	4.9
1	a	13	LEU	4.8
3	C	131	TYR	4.8
5	E	81	GLU	4.8
8	i	38	GLU	4.8
3	C	439	VAL	4.8
9	j	7	ILE	4.8
3	C	317	PHE	4.8
13	O	140	THR	4.8
18	y	18	VAL	4.8
20	R	17	GLY	4.8
1	A	326	LEU	4.8
3	c	438	LEU	4.8
18	Y	36	ILE	4.8
19	z	27	TYR	4.8
15	U	101	GLY	4.8
18	Y	43	ARG	4.8
6	f	24	HIS	4.8

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Mol	Chain	Res	Type	RSRZ
4	d	13	GLY	4.8
16	v	20	THR	4.8
1	A	343	LEU	4.8
19	Z	60	PHE	4.7
2	b	128	THR	4.7
2	B	289	GLN	4.7
3	c	433	LEU	4.7
5	E	12	ASP	4.7
9	j	5	GLY	4.7
13	O	62	GLU	4.7
2	B	458	PHE	4.7
17	x	4	THR	4.7
13	O	56	PRO	4.7
3	c	23	ALA	4.7
2	B	251	VAL	4.7
2	b	461	LEU	4.7
5	E	16	SER	4.7
3	c	255	THR	4.7
2	b	489	GLU	4.7
1	a	343	LEU	4.7
3	c	401	LEU	4.7
13	o	34	SER	4.7
13	o	32	ILE	4.7
2	B	488	PRO	4.7
13	O	89	SER	4.7
17	x	15	LEU	4.7
3	C	139	THR	4.7
18	y	34	MET	4.7
1	a	330	VAL	4.7
3	c	20	SER	4.7
2	b	460	LEU	4.7
19	Z	2	THR	4.7
3	c	190	ALA	4.7
4	d	20	ASP	4.6
2	b	298	LEU	4.6
8	I	6	ILE	4.6
3	c	258	GLY	4.6
5	e	81	GLU	4.6
3	c	251	HIS	4.6
16	v	113	VAL	4.6
3	C	201	ASN	4.6
2	B	350	GLU	4.6

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Mol	Chain	Res	Type	RSRZ
18	y	24	MET	4.6
2	b	186	GLY	4.6
2	b	484	PRO	4.6
3	C	100	GLY	4.6
3	C	426	LEU	4.6
19	z	14	ILE	4.6
1	a	295	PHE	4.6
5	e	10	PHE	4.6
3	C	251	HIS	4.6
18	Y	34	MET	4.6
13	o	206	GLY	4.6
3	C	253	LEU	4.6
9	j	10	TRP	4.6
9	J	8	PRO	4.6
3	C	28	GLN	4.5
18	Y	21	GLN	4.5
2	b	249	ALA	4.5
3	c	21	ILE	4.5
4	d	16	ASP	4.5
11	L	3	PRO	4.5
4	d	352	LEU	4.5
4	d	325	ILE	4.5
2	b	250	PHE	4.5
16	V	7	VAL	4.5
3	C	279	LEU	4.5
4	d	158	LEU	4.5
19	Z	46	LEU	4.5
16	V	99	ASP	4.5
16	V	6	GLU	4.5
16	v	69	ILE	4.5
2	B	250	PHE	4.5
9	j	14	THR	4.5
13	O	132	ASN	4.5
13	o	23	ASP	4.5
1	a	262	TYR	4.5
10	k	16	ALA	4.5
3	c	87	ILE	4.5
5	e	22	ILE	4.5
2	B	161	LEU	4.5
2	B	486	LEU	4.5
3	C	341	LEU	4.5
4	d	287	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
5	E	21	VAL	4.5
16	v	107	LEU	4.5
13	o	41	ALA	4.5
11	L	5	PRO	4.5
12	m	31	SER	4.4
13	o	60	ARG	4.4
6	F	13	TYR	4.4
5	e	40	THR	4.4
2	B	301	ALA	4.4
16	v	79	PRO	4.4
17	x	33	GLN	4.4
2	B	505	ARG	4.4
3	C	254	THR	4.4
2	b	483	ASP	4.4
2	B	288	VAL	4.4
5	e	23	HIS	4.4
15	u	68	THR	4.4
16	v	108	THR	4.4
7	h	13	PRO	4.4
2	b	252	VAL	4.4
15	u	66	GLY	4.4
17	x	34	ILE	4.4
1	A	15	GLU	4.4
13	O	134	THR	4.4
2	B	383	PHE	4.4
5	E	79	PHE	4.4
13	O	4	THR	4.4
13	O	202	ALA	4.4
20	R	20	VAL	4.3
13	o	200	ASN	4.3
2	b	300	GLU	4.3
13	o	64	GLU	4.3
13	O	30	TYR	4.3
3	C	162	GLY	4.3
4	d	321	LEU	4.3
19	Z	39	LEU	4.3
9	j	15	VAL	4.3
19	z	18	VAL	4.3
17	X	4	THR	4.3
3	C	435	PHE	4.3
13	o	61	GLN	4.3
2	b	251	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
3	c	254	THR	4.3
2	b	243	ALA	4.3
4	d	119	ALA	4.3
17	x	39	ARG	4.3
1	a	160	ILE	4.3
1	a	163	ILE	4.3
1	a	184	ILE	4.3
8	i	26	GLY	4.3
4	D	116	LEU	4.3
13	O	205	ASP	4.3
3	c	424	SER	4.3
5	e	11	SER	4.3
3	c	207	ARG	4.2
4	d	346	LEU	4.2
5	e	28	PRO	4.2
11	l	5	PRO	4.2
15	U	73	GLN	4.2
2	B	248	ALA	4.2
5	E	57	ALA	4.2
3	C	159	THR	4.2
13	O	141	ASP	4.2
3	C	193	GLY	4.2
3	c	145	SER	4.2
5	e	82	GLN	4.2
13	O	36	GLN	4.2
5	e	36	LEU	4.2
17	X	28	LEU	4.2
17	X	37	VAL	4.2
3	c	261	ARG	4.2
2	B	298	LEU	4.2
4	d	162	LEU	4.2
5	e	78	THR	4.2
1	a	188	ALA	4.2
2	b	247	PHE	4.2
5	e	83	LEU	4.2
2	b	467	ILE	4.2
3	C	60	ILE	4.2
19	Z	52	LEU	4.1
16	v	68	ASN	4.1
16	v	23	GLU	4.1
17	x	36	LYS	4.1
6	f	37	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
2	b	245	VAL	4.1
5	e	26	THR	4.1
13	O	5	LEU	4.1
2	B	485	GLU	4.1
3	C	158	THR	4.1
5	E	15	THR	4.1
13	O	88	ASN	4.1
5	E	26	THR	4.1
3	c	259	TRP	4.1
17	X	26	ALA	4.1
8	I	3	THR	4.1
2	b	498	LYS	4.1
19	Z	23	VAL	4.0
4	d	284	ILE	4.0
3	C	32	GLY	4.0
3	C	282	MET	4.0
18	Y	24	MET	4.0
1	a	120	LEU	4.0
16	v	11	PRO	4.0
19	Z	62	VAL	4.0
3	C	255	THR	4.0
13	o	10	ILE	4.0
14	t	29	ILE	4.0
18	Y	44	GLY	4.0
17	X	32	SER	4.0
17	x	5	PRO	4.0
1	A	330	VAL	4.0
1	A	151	LEU	4.0
3	c	95	LEU	4.0
4	D	89	LEU	4.0
2	B	300	GLU	4.0
2	B	453	PHE	4.0
2	b	244	ALA	4.0
7	h	57	GLY	4.0
2	b	288	VAL	4.0
3	c	249	ILE	4.0
8	i	2	GLU	4.0
5	E	78	THR	4.0
5	e	8	ARG	4.0
1	a	63	ILE	4.0
5	E	23	HIS	4.0
5	e	27	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
3	c	282	MET	4.0
19	z	37	LYS	4.0
13	o	28	GLY	4.0
5	e	12	ASP	4.0
1	A	295	PHE	4.0
2	b	458	PHE	4.0
19	Z	17	PHE	4.0
4	d	154	VAL	4.0
13	o	38	TYR	3.9
2	B	490	GLN	3.9
3	C	442	LEU	3.9
18	Y	45	ASN	3.9
2	b	462	PHE	3.9
13	o	6	THR	3.9
5	e	14	ILE	3.9
13	o	243	ILE	3.9
2	B	256	MET	3.9
3	C	276	LEU	3.9
3	c	442	LEU	3.9
16	V	52	LEU	3.9
2	B	249	ALA	3.9
18	y	31	ALA	3.9
3	c	22	PHE	3.9
2	b	256	MET	3.9
1	a	242	GLU	3.9
13	o	55	GLU	3.9
3	C	153	ASP	3.9
19	z	45	GLY	3.9
1	A	63	ILE	3.9
2	B	242	ILE	3.9
2	B	252	VAL	3.9
4	D	287	VAL	3.9
16	V	50	PRO	3.9
2	b	127	ARG	3.9
13	o	22	LEU	3.9
16	v	114	ALA	3.9
2	B	258	TYR	3.9
2	b	246	PHE	3.9
3	C	436	PHE	3.9
3	c	248	GLY	3.9
18	Y	37	PHE	3.9
5	e	59	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
3	c	54	VAL	3.9
16	v	7	VAL	3.9
4	D	351	ALA	3.9
20	R	16	ALA	3.9
3	c	404	LEU	3.9
18	y	38	LEU	3.9
1	A	14	TRP	3.8
10	k	20	PRO	3.8
1	A	163	ILE	3.8
7	h	10	ILE	3.8
4	D	151	ALA	3.8
3	C	401	LEU	3.8
1	a	16	ARG	3.8
18	y	43	ARG	3.8
13	o	201	VAL	3.8
3	C	286	ALA	3.8
3	c	246	ALA	3.8
3	c	427	ALA	3.8
19	z	58	ASN	3.8
8	I	34	ARG	3.8
4	d	27	PHE	3.8
8	i	6	ILE	3.8
13	O	32	ILE	3.8
17	X	34	ILE	3.8
3	C	288	CYS	3.8
5	e	42	LEU	3.8
15	U	68	THR	3.8
2	B	162	PHE	3.8
11	L	6	ASN	3.8
3	C	432	VAL	3.8
18	Y	35	ILE	3.8
1	A	331	MET	3.8
17	X	23	LEU	3.8
6	f	28	VAL	3.8
15	U	64	ILE	3.8
1	A	159	LEU	3.8
2	B	460	LEU	3.8
4	D	162	LEU	3.8
7	h	42	LEU	3.8
16	v	8	LEU	3.8
2	b	130[A]	GLU	3.8
2	b	373	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
4	d	169	PHE	3.7
4	d	188	PHE	3.7
17	x	11	PHE	3.7
3	C	200	THR	3.7
19	Z	18	VAL	3.7
18	y	27	MET	3.7
4	d	127	LEU	3.7
4	d	320	LEU	3.7
3	c	431	PHE	3.7
3	c	117	VAL	3.7
3	C	318	LEU	3.7
3	c	206	PRO	3.7
14	t	30	THR	3.7
1	A	160	ILE	3.7
2	b	242	ILE	3.7
13	O	92	SER	3.7
5	e	65	LEU	3.7
7	h	46	LEU	3.7
15	U	79	LEU	3.7
3	c	194	GLY	3.7
3	C	135	ARG	3.7
2	B	65	PHE	3.7
2	B	456	ALA	3.7
5	e	7	GLU	3.7
6	F	15	ILE	3.7
15	U	59	GLU	3.7
1	a	238	LYS	3.7
2	B	461	LEU	3.7
7	H	46	LEU	3.7
13	o	90	ASP	3.7
18	y	26	ALA	3.7
1	a	228	THR	3.7
19	Z	27	TYR	3.7
3	C	262	ARG	3.7
5	E	13	ILE	3.7
10	k	38	VAL	3.7
13	o	202	ALA	3.7
3	C	431	PHE	3.7
5	E	20	TRP	3.7
1	a	248	ILE	3.7
3	c	198	VAL	3.7
4	D	210	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
3	C	24	THR	3.6
16	v	18	THR	3.6
2	b	449	GLY	3.6
3	C	284	PHE	3.6
2	b	248	ALA	3.6
1	a	89	ILE	3.6
1	a	331	MET	3.6
4	d	21	TRP	3.6
8	I	10	ILE	3.6
18	Y	30	ILE	3.6
4	d	286	VAL	3.6
1	a	28	LEU	3.6
11	l	7	ARG	3.6
19	z	52	LEU	3.6
5	e	58	GLN	3.6
15	U	86	GLU	3.6
2	b	456	ALA	3.6
13	o	237	GLY	3.6
7	H	5	THR	3.6
2	b	126	PRO	3.6
2	B	483	ASP	3.6
3	c	284	PHE	3.6
4	d	123	ILE	3.6
3	c	88	LEU	3.6
13	O	240	TYR	3.6
1	a	263	ALA	3.6
8	i	3	THR	3.6
9	J	14	THR	3.6
13	O	129	THR	3.6
15	u	64	ILE	3.6
2	b	238	LEU	3.6
3	c	119	LEU	3.6
4	D	154	VAL	3.6
16	v	10	VAL	3.6
15	u	8	GLU	3.6
4	d	151	ALA	3.6
15	u	73	GLN	3.6
16	v	25	GLN	3.6
3	c	285	ILE	3.6
5	e	18	ARG	3.6
7	h	56	ASP	3.6
16	v	27	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
17	x	26	ALA	3.5
16	V	97	SER	3.5
17	x	35	ASP	3.5
3	C	59	LEU	3.5
3	c	253	LEU	3.5
4	D	158	LEU	3.5
15	U	58	VAL	3.5
5	E	40	THR	3.5
13	o	241	ALA	3.5
3	C	192	GLY	3.5
13	o	89	SER	3.5
3	c	208	VAL	3.5
16	v	121	VAL	3.5
13	o	62	GLU	3.5
1	a	230	THR	3.5
2	B	503	THR	3.5
19	z	47	TRP	3.5
3	C	283	GLY	3.5
19	z	16	SER	3.5
4	d	122	LEU	3.5
9	j	12	VAL	3.5
3	C	427	ALA	3.5
7	H	2	ALA	3.5
15	U	103	TYR	3.5
16	V	13	ASN	3.5
3	c	425	TRP	3.5
1	a	328	MET	3.5
2	B	366	PHE	3.5
2	b	411	PHE	3.5
3	C	146	PHE	3.5
13	O	203	LYS	3.5
1	a	321	ILE	3.5
13	O	157	LEU	3.5
2	b	452	THR	3.5
2	b	402	TYR	3.5
3	c	141	GLU	3.5
2	b	163	GLY	3.5
4	d	25	ASP	3.5
18	y	33	PRO	3.5
5	e	72	ALA	3.5
16	v	98	ALA	3.5
19	Z	29	SER	3.5

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Mol	Chain	Res	Type	RSRZ
4	D	12	ARG	3.5
4	D	321	LEU	3.4
7	H	30	LEU	3.4
13	o	138	THR	3.4
2	B	454	ALA	3.4
13	O	204	VAL	3.4
16	V	135	VAL	3.4
1	a	232	SER	3.4
7	H	12[A]	ARG	3.4
3	C	27	ASP	3.4
16	v	64	PRO	3.4
3	C	337	LEU	3.4
3	c	199	ILE	3.4
18	y	30	ILE	3.4
1	A	145	VAL	3.4
1	a	67	VAL	3.4
2	B	253	ALA	3.4
3	C	142	GLU	3.4
3	c	429	SER	3.4
2	B	413	ASP	3.4
13	O	64	GLU	3.4
1	a	261	GLN	3.4
19	z	54	VAL	3.4
3	C	152	LYS	3.4
17	X	36	LYS	3.4
15	U	56	GLU	3.4
3	C	352	GLY	3.4
9	j	19	GLY	3.4
2	b	289	GLN	3.4
1	A	288	LEU	3.4
1	A	336	ALA	3.4
1	a	116	ILE	3.4
1	a	259	ILE	3.4
6	f	36	ALA	3.4
10	k	21	LEU	3.4
2	B	457	VAL	3.4
2	B	493	TRP	3.4
3	C	250	TRP	3.4
13	O	55	GLU	3.4
1	a	340	PRO	3.4
1	a	252	HIS	3.4
15	U	104	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
7	h	16	SER	3.4
1	A	60	ILE	3.4
2	b	383	PHE	3.4
4	D	120	PHE	3.4
13	O	93	LEU	3.4
16	v	70	GLU	3.4
19	z	13	VAL	3.4
19	z	62	VAL	3.4
13	o	130	GLN	3.4
2	B	452	THR	3.4
1	A	120	LEU	3.4
16	v	116	ALA	3.4
3	c	240	ILE	3.4
3	c	153	ASP	3.3
15	u	101	GLY	3.3
2	B	410	THR	3.3
13	o	39	ARG	3.3
16	V	63	THR	3.3
3	C	281	MET	3.3
1	a	159	LEU	3.3
10	K	33	LEU	3.3
3	c	384	ILE	3.3
4	D	325	ILE	3.3
15	U	74	ILE	3.3
1	A	281	VAL	3.3
1	a	306	VAL	3.3
16	v	26	TYR	3.3
4	d	229	ALA	3.3
13	o	26	ALA	3.3
2	B	267	LEU	3.3
2	b	324	LEU	3.3
1	a	224	ILE	3.3
3	c	92	ILE	3.3
2	b	206	GLY	3.3
13	o	213	GLY	3.3
6	f	19	ARG	3.3
16	v	110	LYS	3.3
1	a	324	ALA	3.3
2	b	268	PHE	3.3
3	C	224	ILE	3.3
3	C	101	PRO	3.3
9	j	8	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
16	v	28	GLU	3.3
2	b	413	ASP	3.3
15	U	60	ASP	3.3
13	o	57	LYS	3.3
13	o	30	TYR	3.3
3	c	414	ILE	3.3
15	U	65	PRO	3.3
17	X	33	GLN	3.3
13	o	135	SER	3.3
2	B	62	VAL	3.3
19	z	53	VAL	3.3
16	V	81	THR	3.3
7	h	12	ARG	3.3
18	y	44	GLY	3.3
3	c	86	LEU	3.3
2	b	464	PHE	3.3
3	c	437	PHE	3.3
2	B	219	VAL	3.3
3	C	225	VAL	3.3
13	O	66	VAL	3.3
19	Z	56	VAL	3.3
11	l	2	GLU	3.3
3	c	148	GLY	3.2
1	a	286	ALA	3.2
4	d	115	ALA	3.2
9	j	13	ALA	3.2
1	a	200	LEU	3.2
4	D	90	LEU	3.2
3	c	170	ILE	3.2
5	E	82	GLN	3.2
3	c	286	ALA	3.2
5	E	71	GLU	3.2
5	e	45	ASP	3.2
15	u	65	PRO	3.2
3	C	261	ARG	3.2
3	c	63	TRP	3.2
4	D	233	ARG	3.2
19	Z	12	LEU	3.2
16	V	24	LYS	3.2
11	l	6	ASN	3.2
2	B	489	GLU	3.2
15	U	77	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
13	O	135	SER	3.2
16	v	97	SER	3.2
2	b	214	LEU	3.2
16	v	72	LEU	3.2
4	d	178	ILE	3.2
5	E	35	TRP	3.2
5	e	13	ILE	3.2
2	b	65	PHE	3.2
4	D	16	ASP	3.2
1	A	16	ARG	3.2
1	A	340	PRO	3.2
3	c	191	PRO	3.2
13	O	35	SER	3.2
5	E	74	GLN	3.2
5	E	42	LEU	3.2
1	a	231	GLU	3.2
3	C	43	ILE	3.2
3	C	87	ILE	3.2
3	C	92	ILE	3.2
7	h	19	GLY	3.2
13	o	226	GLY	3.2
2	b	398	THR	3.2
4	D	119	ALA	3.2
2	b	299	GLU	3.2
2	B	39	LEU	3.2
3	C	95	LEU	3.2
1	A	338	ASN	3.2
15	U	63	ASN	3.2
2	B	265	ILE	3.2
3	c	350	ILE	3.2
4	d	144	ILE	3.2
4	d	339	PHE	3.2
3	c	439	VAL	3.2
2	B	291	SER	3.2
16	V	15	GLU	3.2
2	B	163	GLY	3.2
19	Z	50	LEU	3.2
15	U	57	SER	3.1
15	u	103	TYR	3.1
5	e	41	GLY	3.1
5	E	59	GLU	3.1
2	b	39	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
4	d	183	LEU	3.1
1	A	285	PHE	3.1
2	B	464	PHE	3.1
2	b	162	PHE	3.1
2	b	457	VAL	3.1
17	X	20	VAL	3.1
2	b	454	ALA	3.1
3	c	64	ALA	3.1
2	B	185	TRP	3.1
3	c	29	GLU	3.1
2	b	29	LEU	3.1
16	v	12	LEU	3.1
1	a	320	ILE	3.1
2	b	241	SER	3.1
4	D	144	ILE	3.1
4	D	284	ILE	3.1
4	d	153	PHE	3.1
15	u	86	GLU	3.1
1	a	336	ALA	3.1
13	O	237	GLY	3.1
1	A	121[A]	LEU	3.1
2	b	286	ARG	3.1
7	h	51	SER	3.1
18	Y	25	ILE	3.1
19	Z	14	ILE	3.1
2	b	363	PHE	3.1
3	C	358	PHE	3.1
4	d	120	PHE	3.1
4	d	146	PHE	3.1
17	x	30	ALA	3.1
9	J	10	TRP	3.1
1	A	328	MET	3.1
3	c	356	MET	3.1
5	e	53	ASP	3.1
18	Y	39	LEU	3.1
19	Z	6	GLN	3.1
1	A	143	ILE	3.1
1	A	324	ALA	3.1
2	b	459	ALA	3.1
10	k	41	ALA	3.1
9	J	24	VAL	3.1
16	v	2	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
16	v	136	TYR	3.1
5	e	30	LEU	3.1
1	a	243	GLU	3.1
2	B	254	GLY	3.1
2	b	121	GLU	3.1
4	D	123	ILE	3.1
1	a	294	ALA	3.1
1	a	185	VAL	3.0
2	B	30	VAL	3.0
4	D	276	VAL	3.0
3	c	25	ASN	3.0
1	A	245	THR	3.0
3	C	140	LEU	3.0
3	C	404	LEU	3.0
3	c	272	LEU	3.0
4	d	182	LEU	3.0
8	I	4	LEU	3.0
2	B	129	GLY	3.0
2	B	124	ARG	3.0
2	B	463	PHE	3.0
1	A	205	VAL	3.0
3	c	227	VAL	3.0
3	C	42	LEU	3.0
3	c	158	THR	3.0
13	o	141	ASP	3.0
10	k	42	ALA	3.0
14	T	14	ILE	3.0
2	B	268	PHE	3.0
3	C	210	PHE	3.0
18	y	45	ASN	3.0
3	C	208	VAL	3.0
3	C	296	VAL	3.0
2	B	402	TYR	3.0
5	e	48	GLY	3.0
16	v	99	ASP	3.0
1	a	60	ILE	3.0
15	U	32	ILE	3.0
4	d	157	PHE	3.0
16	v	94	SER	3.0
2	B	372	ASP	3.0
6	f	44	GLN	3.0
3	C	168	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
4	d	116	LEU	3.0
13	o	92	SER	3.0
3	c	358	PHE	3.0
2	b	499	VAL	3.0
3	c	385	GLN	3.0
3	c	410	VAL	3.0
4	d	238	THR	3.0
19	Z	24	PRO	3.0
10	k	15	TYR	3.0
1	a	288	LEU	3.0
2	B	63	LEU	3.0
2	b	63	LEU	3.0
20	R	9	LEU	3.0
4	D	115	ALA	3.0
13	O	34	SER	3.0
9	J	5	GLY	3.0
16	v	71	GLY	3.0
7	h	58	VAL	3.0
13	O	31	PRO	3.0
4	d	74	LEU	2.9
13	o	93	LEU	2.9
17	X	35	ASP	2.9
4	d	163	GLY	2.9
7	H	10	ILE	2.9
7	H	26	GLY	2.9
8	i	22	GLY	2.9
1	A	158	PHE	2.9
1	a	300	PHE	2.9
6	F	42	PHE	2.9
3	C	35	TRP	2.9
3	c	378	ASN	2.9
16	v	96	ARG	2.9
19	Z	47	TRP	2.9
1	A	297	LEU	2.9
1	a	258	LEU	2.9
5	E	58	GLN	2.9
1	a	46	ILE	2.9
1	a	290	ILE	2.9
3	C	252	ILE	2.9
19	Z	40	ILE	2.9
2	b	348	ASN	2.9
1	a	168	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	462	PHE	2.9
2	B	478	VAL	2.9
13	O	87	VAL	2.9
4	D	19	ASP	2.9
4	d	18	LEU	2.9
9	j	18	MET	2.9
2	b	89	GLY	2.9
3	c	340	TYR	2.9
10	k	34	ALA	2.9
13	o	229	GLU	2.9
3	c	288	CYS	2.9
16	V	45	ILE	2.9
3	C	256	PRO	2.9
3	C	428	THR	2.9
7	H	28	THR	2.9
3	C	383	ASP	2.9
4	D	156	VAL	2.9
7	h	9	ASP	2.9
12	M	31	SER	2.9
19	z	12	LEU	2.9
4	d	143	ALA	2.9
1	a	19	ASN	2.9
2	B	285	ASN	2.9
11	l	8	GLN	2.9
2	B	467	ILE	2.9
14	T	21	ILE	2.9
3	c	428	THR	2.9
13	O	6	THR	2.9
1	a	158	PHE	2.9
1	a	225	ARG	2.9
3	C	429	SER	2.9
13	O	213	GLY	2.9
3	c	291	TRP	2.9
1	A	123	ALA	2.9
1	A	228	THR	2.9
13	O	128	SER	2.9
1	a	49	VAL	2.9
2	b	397	VAL	2.9
4	D	28	VAL	2.9
13	O	201	VAL	2.9
4	D	122	LEU	2.9
4	d	279	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
5	e	77	GLU	2.9
10	K	14	ALA	2.9
2	B	501	ASP	2.9
4	D	20	ASP	2.9
1	A	321	ILE	2.8
1	a	176	ILE	2.8
13	o	94	THR	2.8
1	a	327	GLY	2.8
1	a	186	PHE	2.8
2	b	435	GLU	2.8
2	b	479	PHE	2.8
13	o	96	VAL	2.8
1	A	287	ALA	2.8
3	C	125	LEU	2.8
3	c	195	ASP	2.8
4	d	293	LEU	2.8
5	E	29	ALA	2.8
13	o	183	ALA	2.8
2	B	484	PRO	2.8
2	b	350	GLU	2.8
5	e	32	ILE	2.8
3	c	353	GLY	2.8
4	d	130	PHE	2.8
19	z	51	VAL	2.8
1	a	174	LEU	2.8
2	B	109	LEU	2.8
3	c	314	ALA	2.8
7	H	42	LEU	2.8
13	o	182	LEU	2.8
2	B	396	GLY	2.8
3	c	171	GLY	2.8
7	h	5	THR	2.8
13	O	38	TYR	2.8
5	E	61	ARG	2.8
16	V	96	ARG	2.8
1	A	197	PHE	2.8
3	c	317	PHE	2.8
10	k	18	PHE	2.8
3	c	196	VAL	2.8
4	D	152	VAL	2.8
2	b	187	PRO	2.8
3	c	175	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
5	E	36	LEU	2.8
3	C	211	GLY	2.8
4	D	150	ILE	2.8
7	H	54	ILE	2.8
10	k	28	ILE	2.8
1	a	265	PHE	2.8
17	X	30	ALA	2.8
18	Y	40	ALA	2.8
3	c	276	LEU	2.8
4	D	293	LEU	2.8
7	H	23	PRO	2.8
19	z	9	LEU	2.8
3	C	280	SER	2.8
5	E	39	SER	2.8
2	b	492	GLU	2.8
8	I	2	GLU	2.8
2	b	185	TRP	2.8
2	b	450	TRP	2.8
3	c	28	GLN	2.8
7	H	25	TRP	2.8
2	b	215	PHE	2.8
4	D	257	PHE	2.8
2	B	88	PRO	2.8
3	C	137	PRO	2.8
3	C	331	ALA	2.8
3	c	176	VAL	2.8
3	c	420	VAL	2.8
11	L	4	ASN	2.8
3	C	29	GLU	2.8
3	c	396	MET	2.8
4	D	36	LEU	2.8
4	d	147	SER	2.8
17	X	22	GLY	2.8
16	V	4	THR	2.8
4	d	150	ILE	2.8
7	H	45	ILE	2.8
17	x	29	ILE	2.8
4	d	328	TRP	2.8
2	B	286	ARG	2.8
3	C	292	PHE	2.7
3	C	410	VAL	2.7
6	f	38	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
13	o	227	ALA	2.7
19	Z	10	ALA	2.7
4	D	209	LEU	2.7
16	V	18	THR	2.7
2	B	369	ILE	2.7
13	o	180	GLU	2.7
16	v	45	ILE	2.7
16	v	134	LYS	2.7
17	x	8	LYS	2.7
10	K	46	ARG	2.7
16	v	137	TYR	2.7
16	v	84	GLY	2.7
1	a	283	VAL	2.7
2	B	246	PHE	2.7
2	b	366	PHE	2.7
3	c	147	PHE	2.7
4	D	270	PHE	2.7
3	C	88	LEU	2.7
3	C	272	LEU	2.7
15	u	102	LEU	2.7
2	B	449	GLY	2.7
5	E	19	TYR	2.7
13	o	83	GLY	2.7
2	b	155	ALA	2.7
16	V	94	SER	2.7
2	b	30	VAL	2.7
4	D	328	TRP	2.7
15	U	84	VAL	2.7
16	V	2	GLU	2.7
1	A	200	LEU	2.7
1	a	106	LEU	2.7
2	B	481	GLY	2.7
4	d	327	ALA	2.7
5	E	56	TYR	2.7
19	z	26	ALA	2.7
1	a	197	PHE	2.7
3	c	197	ARG	2.7
2	B	474	LEU	2.7
13	O	19	CYS	2.7
2	B	255	THR	2.7
16	v	74	ASP	2.7
3	C	339	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
13	o	54	GLU	2.7
3	c	252	ILE	2.7
3	C	309	ALA	2.7
17	X	39	ARG	2.7
2	B	451	PHE	2.7
4	d	15	PHE	2.7
4	d	185	PHE	2.7
2	B	12	LEU	2.7
2	B	262	THR	2.7
3	C	204	LEU	2.7
10	K	25	LEU	2.7
10	k	43	VAL	2.7
3	c	412	THR	2.7
2	B	373	LYS	2.7
3	C	63	TRP	2.7
3	c	244	CYS	2.7
2	b	375	GLY	2.7
17	X	13	GLY	2.7
3	C	414	ILE	2.7
10	k	17	ILE	2.7
1	a	339	PHE	2.7
2	b	399	VAL	2.7
2	b	453	PHE	2.7
3	c	292	PHE	2.7
11	L	22	LEU	2.7
3	C	342	MET	2.7
2	b	239[A]	SER	2.6
5	E	28	PRO	2.6
2	B	349	LYS	2.6
6	F	37	ILE	2.6
13	o	211	ILE	2.6
2	B	179	GLN	2.6
4	D	283	ALA	2.6
4	d	283	ALA	2.6
7	h	22	ALA	2.6
13	O	127	ALA	2.6
1	A	280	VAL	2.6
2	B	61	PHE	2.6
2	B	238	LEU	2.6
2	B	403	GLY	2.6
3	C	351	PHE	2.6
3	c	59	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
3	c	213[A]	LEU	2.6
8	i	21	PHE	2.6
19	Z	19	MET	2.6
19	Z	22	GLY	2.6
2	B	425	ILE	2.6
16	v	115	ILE	2.6
19	Z	28	ALA	2.6
2	b	144	PHE	2.6
3	c	114	VAL	2.6
3	c	168	LEU	2.6
3	c	337	LEU	2.6
6	f	18	VAL	2.6
16	v	24	LYS	2.6
18	y	39	LEU	2.6
4	d	347	PRO	2.6
4	D	324	GLY	2.6
5	E	34	GLY	2.6
1	a	58	VAL	2.6
3	C	61	VAL	2.6
3	C	144	SER	2.6
3	C	297	TYR	2.6
3	c	49	LEU	2.6
3	c	289	PHE	2.6
4	D	153	PHE	2.6
11	L	23	LEU	2.6
13	o	65	PHE	2.6
15	U	67	LEU	2.6
17	X	11	PHE	2.6
3	C	396	MET	2.6
2	B	130[A]	GLU	2.6
1	A	290	ILE	2.6
2	B	257	TRP	2.6
4	D	213	ILE	2.6
16	v	29	GLY	2.6
13	o	19	CYS	2.6
5	e	49	THR	2.6
3	C	463	SER	2.6
8	I	25	SER	2.6
2	b	156	PHE	2.6
3	C	334	PRO	2.6
7	H	43	LEU	2.6
2	b	258	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
4	D	160	TYR	2.6
19	z	19	MET	2.6
3	C	190	ALA	2.6
3	C	450	ALA	2.6
3	c	102	GLY	2.6
3	c	450	ALA	2.6
16	v	62	ALA	2.6
19	z	22	GLY	2.6
1	A	38	ILE	2.6
3	C	287	THR	2.6
4	D	350	ASN	2.6
3	C	141	GLU	2.6
13	o	242	SER	2.6
8	i	35	LYS	2.6
2	b	370	LEU	2.6
2	b	414	PRO	2.6
8	i	4	LEU	2.6
1	A	127	MET	2.6
4	d	329	MET	2.6
1	a	112	TYR	2.6
3	c	302	TYR	2.6
3	c	270	ALA	2.6
3	c	312	ALA	2.6
15	u	23	GLU	2.6
18	y	35	ILE	2.6
2	B	371	THR	2.5
2	B	384	ARG	2.5
4	d	155	SER	2.5
17	X	6	SER	2.5
4	d	289	LEU	2.5
1	A	33	PHE	2.5
3	C	109	PHE	2.5
4	d	126	MET	2.5
15	U	13	VAL	2.5
3	c	118	HIS	2.5
1	A	242	GLU	2.5
4	d	241	GLU	2.5
13	o	244	GLU	2.5
15	U	55	TYR	2.5
1	A	50	ILE	2.5
1	A	53	ILE	2.5
2	B	101	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
2	b	412	THR	2.5
2	b	425	ILE	2.5
13	O	37	THR	2.5
18	y	28	ILE	2.5
6	f	29	PRO	2.5
1	A	231	GLU	2.5
1	a	42	LEU	2.5
2	b	405	GLU	2.5
3	C	86	LEU	2.5
4	D	289	LEU	2.5
4	d	92	LEU	2.5
7	h	30	LEU	2.5
10	k	39	TRP	2.5
13	o	84	GLU	2.5
3	C	290	VAL	2.5
1	A	144	CYS	2.5
2	b	407	ASN	2.5
4	d	160	TYR	2.5
15	U	76	ARG	2.5
18	y	42	ARG	2.5
16	V	14	SER	2.5
2	b	159	THR	2.5
2	b	315	ILE	2.5
1	a	196	PRO	2.5
12	m	32	GLN	2.5
2	b	109	LEU	2.5
3	C	430	HIS	2.5
7	h	7	LEU	2.5
10	K	35	LEU	2.5
15	u	17	LEU	2.5
16	v	105	ARG	2.5
16	v	132	GLY	2.5
2	b	61	PHE	2.5
3	C	182	PHE	2.5
4	D	169	PHE	2.5
9	J	20	VAL	2.5
3	C	260	ALA	2.5
3	C	424	SER	2.5
4	D	155	SER	2.5
7	H	18	TYR	2.5
13	o	210	GLU	2.5
7	h	63	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
15	U	85	THR	2.5
5	E	32	ILE	2.5
4	D	121	GLY	2.5
13	o	88	ASN	2.5
11	L	19	LEU	2.5
3	c	189	TRP	2.5
4	d	156	VAL	2.5
1	a	264	SER	2.5
2	b	253	ALA	2.5
2	b	303	SER	2.5
3	c	309	ALA	2.5
2	B	273	TYR	2.5
2	b	125	ASP	2.5
13	O	214	THR	2.5
3	C	148	GLY	2.5
3	c	409	GLY	2.5
1	A	218	LEU	2.5
4	D	205	LEU	2.5
4	D	320	LEU	2.5
1	A	300	PHE	2.5
4	d	100	ASP	2.5
4	D	290	ALA	2.5
19	Z	11	ALA	2.5
3	C	104	GLU	2.5
4	D	178	ILE	2.5
3	C	185	LEU	2.5
3	c	242	LEU	2.5
4	D	63	LEU	2.5
4	D	182	LEU	2.5
3	C	356	MET	2.4
3	c	180	MET	2.4
1	a	233	ALA	2.4
3	C	57	ALA	2.4
4	D	249	ALA	2.4
13	O	154	ALA	2.4
19	Z	5	PHE	2.4
1	A	19	ASN	2.4
3	C	259	TRP	2.4
6	F	20	TRP	2.4
13	o	131	PRO	2.4
2	B	404	GLY	2.4
3	C	340	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
3	c	352	GLY	2.4
7	h	8	GLY	2.4
2	b	490	GLN	2.4
1	a	218	LEU	2.4
4	D	291	LEU	2.4
18	Y	27	MET	2.4
2	B	361	ALA	2.4
2	b	362	PHE	2.4
2	b	471	ALA	2.4
3	C	263	ALA	2.4
4	d	196	PHE	2.4
1	A	164	GLY	2.4
2	B	351	GLY	2.4
2	b	403	GLY	2.4
3	c	397	THR	2.4
15	U	19	THR	2.4
16	v	81	THR	2.4
13	o	9	ASP	2.4
4	D	256	ILE	2.4
17	x	31	ILE	2.4
1	A	258	LEU	2.4
2	b	161	LEU	2.4
3	c	69	LEU	2.4
12	M	22	LEU	2.4
16	v	21	LEU	2.4
19	z	15	LEU	2.4
1	a	325	ASN	2.4
2	b	320	ALA	2.4
1	A	49	VAL	2.4
1	a	281	VAL	2.4
2	b	451	PHE	2.4
3	c	290	VAL	2.4
3	c	436	PHE	2.4
7	H	57	GLY	2.4
13	O	209	GLY	2.4
16	V	92	HIS	2.4
3	C	425	TRP	2.4
1	A	259	ILE	2.4
2	b	234	ILE	2.4
9	j	11	ILE	2.4
1	a	221[A]	SER	2.4
2	B	438	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
3	c	161	LEU	2.4
13	O	196	GLN	2.4
17	x	7	LEU	2.4
1	A	152	ALA	2.4
1	a	152	ALA	2.4
2	b	212	ALA	2.4
3	C	462[A]	GLU	2.4
3	C	289	PHE	2.4
4	D	15	PHE	2.4
4	D	341	PHE	2.4
15	u	85	THR	2.4
19	Z	53	VAL	2.4
16	V	47	LYS	2.4
2	B	241	SER	2.4
1	A	97	TRP	2.4
1	a	165	GLN	2.4
3	c	459	ILE	2.4
1	a	121[A]	LEU	2.4
5	E	30	LEU	2.4
1	a	323	ARG	2.4
2	B	87	ASP	2.4
2	B	477	ASP	2.4
3	c	237	HIS	2.4
9	j	1	MET	2.4
16	v	67	ASP	2.4
17	X	5	PRO	2.4
1	a	18	CYS	2.4
2	b	62	VAL	2.4
2	b	410	THR	2.4
3	C	407	VAL	2.4
3	C	31	SER	2.4
5	e	54	SER	2.4
16	v	85	GLU	2.4
1	A	284	TRP	2.4
1	A	41	LEU	2.4
10	k	35	LEU	2.4
3	c	177	ALA	2.4
16	v	65	PRO	2.4
19	Z	49	ALA	2.4
6	F	44	GLN	2.4
15	u	10	VAL	2.4
2	b	374	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	448	ARG	2.3
3	C	199	ILE	2.3
4	D	259	ILE	2.3
4	d	259	ILE	2.3
19	Z	48	ILE	2.3
1	A	147	TYR	2.3
2	b	254	GLY	2.3
3	c	283	GLY	2.3
7	H	24	GLY	2.3
2	B	450	TRP	2.3
4	D	279	LEU	2.3
4	D	319	LEU	2.3
7	H	22	ALA	2.3
13	O	70	LEU	2.3
5	E	60	GLN	2.3
13	O	57	LYS	2.3
4	d	204	VAL	2.3
13	O	155	ASN	2.3
13	o	198	SER	2.3
2	b	87	ASP	2.3
3	c	187	ASP	2.3
13	O	33	ASP	2.3
4	D	105	CYS	2.3
3	c	43	ILE	2.3
7	h	17	GLU	2.3
13	o	172	ILE	2.3
16	v	100	ILE	2.3
16	V	64	PRO	2.3
1	a	318	ALA	2.3
3	C	377	LEU	2.3
9	J	9	LEU	2.3
15	U	20	ALA	2.3
16	V	126	LEU	2.3
19	Z	8	ALA	2.3
1	A	230	THR	2.3
1	a	245	THR	2.3
3	c	281	MET	2.3
5	e	35	TRP	2.3
12	M	29	THR	2.3
2	B	356	VAL	2.3
4	d	173	PHE	2.3
11	l	10	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	327	GLY	2.3
3	C	184	GLY	2.3
9	j	25	GLY	2.3
2	B	38	ALA	2.3
2	b	361	ALA	2.3
3	c	204	LEU	2.3
4	D	148	ALA	2.3
7	H	49	TYR	2.3
9	J	13	ALA	2.3
13	o	5	LEU	2.3
15	U	70	ARG	2.3
2	b	119	ASP	2.3
6	F	12	SER	2.3
2	b	219	VAL	2.3
4	d	175	VAL	2.3
10	K	30	VAL	2.3
13	O	156	PHE	2.3
13	o	87	VAL	2.3
1	a	171	GLY	2.3
16	V	134	LYS	2.3
2	B	455	HIS	2.3
5	e	60	GLN	2.3
2	b	207	ILE	2.3
3	C	422	PRO	2.3
13	O	10	ILE	2.3
16	v	88	ILE	2.3
2	B	111	ALA	2.3
4	d	330	ALA	2.3
7	H	32	ALA	2.3
13	o	181	GLU	2.3
2	b	225	LEU	2.3
4	D	49	LEU	2.3
4	d	222	LEU	2.3
3	C	310	SER	2.3
3	c	310	SER	2.3
3	C	67	MET	2.3
3	C	291	TRP	2.3
4	D	163	GLY	2.3
10	k	44	GLY	2.3
16	v	117	GLY	2.3
2	B	237	VAL	2.3
6	f	23	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
19	z	20	VAL	2.3
4	D	348	ARG	2.3
1	a	312	ASN	2.3
15	U	23	GLU	2.3
2	B	360	PRO	2.3
13	o	136	ILE	2.3
2	B	304	ALA	2.3
2	B	459	ALA	2.3
2	b	416	THR	2.3
4	D	277	THR	2.3
13	o	193	THR	2.3
5	e	75	GLN	2.3
7	h	18	TYR	2.3
3	C	157	MET	2.3
3	c	81	MET	2.3
8	I	26	GLY	2.3
13	O	206	GLY	2.3
1	a	229	GLU	2.3
2	b	448	ARG	2.3
5	e	61	ARG	2.3
4	D	280	TRP	2.3
4	d	345	VAL	2.3
10	K	37	PHE	2.3
10	K	38	VAL	2.3
1	A	238[A]	LYS	2.3
2	B	270	PRO	2.3
1	A	146	ALA	2.3
1	A	209	ALA	2.3
2	B	381	ILE	2.3
3	c	120	ILE	2.3
16	V	51	SER	2.3
17	x	32	SER	2.3
19	Z	44	SER	2.3
1	A	28	LEU	2.2
2	B	143	LEU	2.2
2	B	324	LEU	2.2
3	c	174	LEU	2.2
3	c	341	LEU	2.2
4	D	37	LEU	2.2
4	d	49	LEU	2.2
13	o	78	LEU	2.2
19	Z	9	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
5	E	6	GLY	2.2
1	a	127	MET	2.2
16	v	111	ASP	2.2
1	a	205	VAL	2.2
1	a	260	PHE	2.2
3	c	351	PHE	2.2
10	K	27	VAL	2.2
2	b	270	PRO	2.2
2	b	415	PRO	2.2
7	H	13	PRO	2.2
16	v	123	PRO	2.2
3	c	209	ILE	2.2
10	k	13	GLU	2.2
9	j	16	ALA	2.2
13	O	211	ILE	2.2
15	U	36	ILE	2.2
19	z	48	ILE	2.2
2	B	128	THR	2.2
2	b	229	LEU	2.2
3	C	47	GLY	2.2
3	C	277	GLY	2.2
15	u	44	THR	2.2
3	c	125	LEU	2.2
3	c	173	LEU	2.2
13	o	43	LEU	2.2
17	x	22	GLY	2.2
4	D	281	MET	2.2
1	A	283	VAL	2.2
2	B	399	VAL	2.2
3	c	90	PRO	2.2
19	z	56	VAL	2.2
1	A	148	SER	2.2
2	b	240	SER	2.2
2	b	302	TRP	2.2
1	a	311	GLY	2.2
2	B	97	ALA	2.2
4	D	330	ALA	2.2
4	d	75	THR	2.2
7	H	8	GLY	2.2
13	O	165	ALA	2.2
13	o	197	ILE	2.2
17	x	24	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	b	202	HIS	2.2
6	f	41	GLN	2.2
4	D	149	PRO	2.2
13	O	20	PRO	2.2
4	d	276	VAL	2.2
5	e	38	VAL	2.2
10	k	30	VAL	2.2
16	V	40	CYS	2.2
2	b	147	GLY	2.2
1	A	44	ALA	2.2
1	a	123	ALA	2.2
2	B	33	TRP	2.2
2	b	371	THR	2.2
3	C	249	ILE	2.2
3	C	335	THR	2.2
5	E	33	ALA	2.2
15	U	53	ALA	2.2
13	o	101	ILE	2.2
17	X	31	ILE	2.2
2	b	283	GLU	2.2
10	k	11	LEU	2.2
15	U	75	LEU	2.2
2	b	224	ARG	2.2
3	c	67	MET	2.2
3	C	206	PRO	2.2
3	c	131	TYR	2.2
1	a	280	VAL	2.2
3	c	407	VAL	2.2
16	v	73	VAL	2.2
1	a	182	PHE	2.2
2	B	479	PHE	2.2
2	b	151	PHE	2.2
4	D	235	PHE	2.2
2	B	244	ALA	2.2
2	B	263	THR	2.2
3	c	66	ALA	2.2
16	v	1	ALA	2.2
2	B	302	TRP	2.2
2	b	468	TRP	2.2
13	O	172	ILE	2.2
2	B	29	LEU	2.2
2	B	120	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
7	h	3	ARG	2.2
11	l	23	LEU	2.2
4	D	347	PRO	2.2
3	C	275	SER	2.2
3	c	122	SER	2.2
2	b	368	VAL	2.2
3	c	402	GLY	2.2
3	c	155	ASN	2.2
3	c	225	VAL	2.2
3	c	419	PHE	2.2
12	m	5	GLN	2.2
3	c	188	THR	2.2
4	d	351	ALA	2.2
6	f	27	ALA	2.2
7	h	27	THR	2.2
2	B	315	ILE	2.2
1	a	193	LEU	2.2
4	D	111	TRP	2.2
13	o	125	LEU	2.2
15	u	69	GLU	2.2
1	a	183	MET	2.2
2	b	367	PRO	2.2
4	D	329	MET	2.2
2	b	480	SER	2.2
5	E	24	SER	2.2
10	K	19	ASP	2.2
1	a	296	ASN	2.1
2	b	408	GLY	2.2
3	C	229	ASN	2.1
4	d	322	ASN	2.1
5	e	66	VAL	2.1
1	A	255	PHE	2.1
4	D	157	PHE	2.1
8	i	19	PHE	2.1
19	Z	59	PHE	2.1
3	C	314	ALA	2.1
4	D	170	ALA	2.1
4	d	316	THR	2.1
13	O	153	THR	2.1
1	a	53	ILE	2.1
13	O	136	ILE	2.1
18	y	25	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	137	LEU	2.1
1	a	210	LEU	2.1
3	C	161	LEU	2.1
4	d	319	LEU	2.1
5	e	9	PRO	2.1
1	a	172	MET	2.1
2	B	407	ASN	2.1
15	u	18	GLY	2.1
3	c	430	HIS	2.1
7	H	17	GLU	2.1
8	i	9	TYR	2.1
2	B	397	VAL	2.1
4	D	286	VAL	2.1
15	U	50	VAL	2.1
16	v	42	VAL	2.1
1	A	149	ALA	2.1
1	A	286	ALA	2.1
1	A	294	ALA	2.1
1	a	285	PHE	2.1
2	B	320	ALA	2.1
3	C	94	THR	2.1
4	d	184	PHE	2.1
4	d	341	PHE	2.1
5	e	31	PHE	2.1
15	U	34	ALA	2.1
13	O	143	LYS	2.1
3	C	134	ILE	2.1
3	C	240	ILE	2.1
2	b	474	LEU	2.1
4	d	291	LEU	2.1
5	E	11	SER	2.1
7	H	16	SER	2.1
9	J	35	LEU	2.1
16	v	102	PRO	2.1
2	B	408	GLY	2.1
3	c	306	GLY	2.1
2	b	60	MET	2.1
3	c	239	TRP	2.1
3	C	91	HIS	2.1
1	a	227	THR	2.1
2	b	255	THR	2.1
4	D	143	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
5	e	43	ALA	2.1
16	V	48	THR	2.1
16	v	56	THR	2.1
1	A	192	ILE	2.1
1	A	320	ILE	2.1
1	a	307[A]	ILE	2.1
2	b	217	ILE	2.1
2	B	103	LEU	2.1
2	b	218	LEU	2.1
3	C	138	GLU	2.1
3	C	160	ILE	2.1
5	E	8	ARG	2.1
15	u	28	ASN	2.1
17	X	3	ILE	2.1
12	m	6	LEU	2.1
13	O	85	LEU	2.1
3	c	157	MET	2.1
2	b	321	LYS	2.1
10	K	39	TRP	2.1
1	a	45	THR	2.1
3	C	302	TYR	2.1
3	C	399	ALA	2.1
3	c	172	ALA	2.1
4	d	148	ALA	2.1
8	I	20	VAL	2.1
10	k	36	ALA	2.1
16	V	46	THR	2.1
3	C	163	PHE	2.1
3	c	19	ASN	2.1
1	a	101	SER	2.1
2	B	365	SER	2.1
2	b	222	PRO	2.1
3	c	96	GLY	2.1
4	d	288	GLY	2.1
1	a	143	ILE	2.1
2	B	60	MET	2.1
4	D	126	MET	2.1
6	f	40	MET	2.1
15	U	81	HIS	2.1
1	a	179	THR	2.1
8	i	34	ARG	2.1
3	C	434	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
16	V	22	THR	2.1
16	V	49	ASN	2.1
4	D	30	VAL	2.1
1	a	62	GLY	2.1
2	b	311	PHE	2.1
3	c	58	GLY	2.1
13	O	190	PHE	2.1
17	x	6	SER	2.1
17	x	10	PHE	2.1
1	A	275	LEU	2.1
3	c	56	HIS	2.1
3	c	132	HIS	2.1
3	c	313	GLN	2.1
4	d	63	LEU	2.1
4	d	135	LEU	2.1
4	d	213	ILE	2.1
5	E	14	ILE	2.1
6	F	26	LEU	2.1
1	a	293	MET	2.1
2	b	228	ALA	2.1
7	H	63	LYS	2.1
16	V	60	ALA	2.1
2	B	89	GLY	2.1
3	C	196	VAL	2.1
3	C	443	TRP	2.1
3	c	247	GLY	2.1
4	D	147	SER	2.1
4	D	201	VAL	2.1
4	d	40	CYS	2.1
5	E	76	VAL	2.1
9	j	20	VAL	2.1
13	O	238	VAL	2.1
4	D	146	PHE	2.1
4	d	171	PRO	2.1
4	d	237	PRO	2.1
3	C	205	ASP	2.0
2	b	103	LEU	2.0
2	b	267	LEU	2.0
3	C	459	ILE	2.0
3	c	42	LEU	2.0
4	d	210	LEU	2.0
8	I	17	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
13	O	152	ARG	2.0
1	A	293	MET	2.0
2	B	330	MET	2.0
3	C	79	LYS	2.0
2	B	374	ASN	2.0
7	h	35	MET	2.0
15	U	99	ASN	2.0
16	V	78	ASN	2.0
2	B	243	ALA	2.0
2	b	154	GLY	2.0
2	b	160	GLY	2.0
3	C	353	GLY	2.0
2	b	478	VAL	2.0
3	C	54	VAL	2.0
3	c	167	VAL	2.0
3	C	26	ARG	2.0
1	A	42	LEU	2.0
1	A	89	ILE	2.0
1	a	50	ILE	2.0
4	D	91	LEU	2.0
4	D	114	ILE	2.0
4	d	89	LEU	2.0
13	o	157	LEU	2.0
16	V	100	ILE	2.0
1	A	183	MET	2.0
2	B	37	MET	2.0
2	b	322	GLY	2.0
15	U	66	GLY	2.0
17	X	9	GLY	2.0
1	a	154	ALA	2.0
1	a	169	SER	2.0
3	c	133	ALA	2.0
3	c	344	SER	2.0
13	O	217[A]	SER	2.0
2	B	224	ARG	2.0
10	k	19	ASP	2.0
2	B	181	VAL	2.0
2	B	376	VAL	2.0
7	h	20	LYS	2.0
13	o	52	VAL	2.0
13	o	148	VAL	2.0
3	C	223	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
4	d	296	TYR	2.0
3	C	244	CYS	2.0
16	v	40	CYS	2.0
1	A	114	LEU	2.0
1	A	184	ILE	2.0
2	B	387	GLU	2.0
2	b	19	LEU	2.0
2	b	442	ILE	2.0
3	C	384	ILE	2.0
3	C	467	LEU	2.0
13	O	218	GLU	2.0
13	O	225	MET	2.0
2	b	434	THR	2.0
5	e	73	LYS	2.0
14	T	30	THR	2.0
1	A	203	ALA	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
8	FME	I	1	10/11	0.81	0.23	60,72,75,79	0
8	FME	i	1	10/11	0.83	0.26	60,70,79,79	0
12	FME	M	1	10/11	0.85	0.21	54,65,84,92	0
12	FME	m	1	10/11	0.89	0.18	59,67,83,96	0
14	FME	t	1	10/11	0.91	0.16	49,57,68,72	0
14	FME	T	1	10/11	0.94	0.17	53,59,69,70	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
34	HTG	c	522	19/19	-0.14	0.64	122,143,151,152	0
32	LMT	b	621	25/35	-0.09	0.65	105,119,144,144	0
34	HTG	b	623	19/19	0.08	0.52	103,124,138,158	0
30	UNL	i	101	40/-	0.08	0.46	91,109,147,151	0
33	LMG	C	521	51/55	0.15	0.50	91,116,139,141	0
33	LMG	c	521	51/55	0.17	0.57	103,127,143,146	0
30	UNL	b	626	33/-	0.18	0.41	88,107,143,146	0
34	HTG	d	411	16/19	0.18	0.52	112,133,141,153	0
30	UNL	A	415	28/-	0.19	0.45	101,116,129,137	0
30	UNL	B	627	33/-	0.20	0.43	76,108,140,145	0
32	LMT	M	103	35/35	0.21	0.47	93,135,153,154	0
36	CA	F	102	1/1	0.21	0.15	147,147,147,147	0
26	SQD	f	102	43/54	0.21	0.56	121,146,161,163	0
32	LMT	m	103	35/35	0.21	0.46	73,95,108,111	0
32	LMT	a	414	35/35	0.22	0.57	77,121,131,134	0
32	LMT	A	359	35/35	0.22	0.56	85,123,132,134	0
32	LMT	D	404	35/35	0.23	0.47	87,111,134,136	0
32	LMT	M	101	35/35	0.25	0.43	69,95,111,113	0
32	LMT	e	102	35/35	0.26	0.65	132,156,166,171	0
37	LHG	e	101	42/49	0.26	0.56	108,140,159,166	0
30	UNL	K	101	34/-	0.29	0.59	98,118,130,146	0
32	LMT	t	101	25/35	0.29	0.57	80,99,127,128	0
30	UNL	a	417	30/-	0.29	0.39	105,118,135,144	0
30	UNL	I	102	40/-	0.33	0.44	83,112,137,141	0
34	HTG	D	414	16/19	0.33	0.50	93,117,129,133	0
33	LMG	Z	101	37/55	0.34	0.46	94,122,137,139	0
32	LMT	a	420	35/35	0.34	0.49	124,142,152,152	0
32	LMT	I	101	35/35	0.35	0.48	112,139,150,154	0
33	LMG	z	101	39/55	0.35	0.44	102,127,141,143	0
26	SQD	B	620	54/54	0.36	0.48	81,100,120,129	0
37	LHG	E	101	42/49	0.37	0.48	95,119,132,134	0
34	HTG	C	522	19/19	0.38	0.39	112,128,136,139	0
26	SQD	b	620	54/54	0.38	0.46	78,97,128,130	0
30	UNL	d	410	36/-	0.38	0.65	84,104,130,135	0
33	LMG	a	419	51/55	0.42	0.50	85,100,111,117	0
32	LMT	b	627	25/35	0.42	0.42	68,90,129,132	0
26	SQD	a	413	54/54	0.43	0.43	82,98,124,129	0
34	HTG	b	622	19/19	0.46	0.39	71,90,118,119	0
36	CA	f	103	1/1	0.47	0.14	136,136,136,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
30	UNL	D	413	40/-	0.48	0.43	77,100,127,131	0
33	LMG	C	501	51/55	0.49	0.49	79,98,110,117	0
34	HTG	b	625	19/19	0.50	0.33	79,86,107,111	0
34	HTG	B	622	19/19	0.51	0.40	81,91,122,125	0
32	LMT	E	102	35/35	0.51	0.53	118,142,160,165	0
26	SQD	A	412	54/54	0.53	0.41	72,92,109,117	0
35	DGD	h	102	62/66	0.54	0.49	62,72,79,84	0
30	UNL	c	525	32/-	0.55	0.34	99,116,133,137	0
33	LMG	B	621	51/55	0.56	0.41	69,78,97,108	0
29	PL9	A	414	55/55	0.59	0.50	90,112,121,124	0
29	PL9	a	416	55/55	0.59	0.44	104,118,129,130	0
27	GOL	v	201	6/6	0.60	0.84	77,89,97,99	0
34	HTG	B	623	19/19	0.60	0.37	81,103,114,114	0
33	LMG	m	101	51/55	0.60	0.36	65,77,96,113	0
35	DGD	H	102	62/66	0.62	0.51	59,68,77,78	0
32	LMT	t	102	26/35	0.63	0.28	85,105,128,129	0
33	LMG	C	520	51/55	0.63	0.40	74,94,110,120	0
23	CLA	C	514	65/65	0.63	0.32	72,85,107,112	0
30	UNL	x	101	18/-	0.63	0.27	82,91,108,111	0
23	CLA	b	602	65/65	0.63	0.35	59,66,79,89	0
30	UNL	j	101	10/-	0.63	0.57	92,102,116,117	0
33	LMG	c	520	51/55	0.64	0.38	85,101,121,129	0
27	GOL	a	418	6/6	0.64	0.34	65,79,86,90	0
26	SQD	A	410	54/54	0.65	0.40	70,87,106,114	0
35	DGD	C	518	62/66	0.65	0.34	60,71,105,112	0
23	CLA	B	609	65/65	0.65	0.29	58,64,70,74	0
36	CA	O	301	1/1	0.66	0.32	121,121,121,121	0
30	UNL	m	102	10/-	0.66	0.57	70,81,92,93	0
26	SQD	F	101	43/54	0.66	0.32	91,107,124,129	0
23	CLA	c	514	65/65	0.67	0.32	83,97,115,122	0
25	BCR	h	101	40/40	0.67	0.24	65,75,84,85	0
27	GOL	a	412	6/6	0.68	0.37	82,88,94,97	0
30	UNL	X	101	18/-	0.69	0.31	72,79,98,98	0
23	CLA	c	504	65/65	0.70	0.40	65,72,82,97	0
23	CLA	B	602	65/65	0.70	0.36	55,60,76,82	0
30	UNL	J	101	10/-	0.70	0.52	85,93,100,106	0
23	CLA	b	609	65/65	0.71	0.30	61,68,82,98	0
23	CLA	c	506	65/65	0.71	0.28	58,69,85,91	0
23	CLA	C	504	65/65	0.72	0.40	58,65,74,84	0
37	LHG	l	101	49/49	0.72	0.31	55,65,77,87	0
34	HTG	B	626	19/19	0.72	0.25	78,85,96,102	0
30	UNL	M	102	10/-	0.73	0.55	72,78,87,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	C	505	65/65	0.73	0.36	55,63,88,103	0
23	CLA	b	601	65/65	0.73	0.32	76,88,109,125	0
26	SQD	a	411	54/54	0.74	0.30	79,90,116,119	0
23	CLA	C	512	65/65	0.74	0.22	60,73,82,88	0
35	DGD	c	517	62/66	0.74	0.37	62,69,85,94	0
23	CLA	B	606	65/65	0.75	0.25	51,59,90,98	0
33	LMG	D	415	51/55	0.75	0.29	62,75,104,108	0
23	CLA	B	611	65/65	0.75	0.32	46,52,63,68	0
35	DGD	c	518	62/66	0.76	0.34	64,76,106,114	0
23	CLA	c	513	65/65	0.76	0.27	71,87,107,113	0
23	CLA	B	601	65/65	0.76	0.29	69,81,102,119	0
23	CLA	a	406	65/65	0.76	0.27	48,52,63,71	0
37	LHG	L	101	49/49	0.76	0.35	55,63,69,84	0
23	CLA	c	511	65/65	0.77	0.36	62,71,80,84	0
37	LHG	D	409	49/49	0.77	0.45	58,69,84,96	0
23	CLA	b	603	65/65	0.77	0.35	52,62,78,88	0
23	CLA	b	606	65/65	0.77	0.24	55,65,89,102	0
23	CLA	C	513	65/65	0.77	0.25	71,80,101,108	0
23	CLA	c	507	65/65	0.77	0.25	71,81,103,112	0
23	CLA	C	507	65/65	0.77	0.26	61,75,112,117	0
23	CLA	c	512	65/65	0.78	0.23	67,78,91,94	0
23	CLA	B	605	65/65	0.78	0.33	47,54,63,69	0
23	CLA	c	509	65/65	0.78	0.26	57,69,106,115	0
36	CA	o	301	1/1	0.78	0.24	107,107,107,107	0
23	CLA	C	509	65/65	0.78	0.33	54,63,97,106	0
35	DGD	C	519	62/66	0.78	0.27	57,66,90,97	0
23	CLA	B	608	65/65	0.78	0.34	51,59,69,72	0
35	DGD	C	517	62/66	0.78	0.37	55,65,89,93	0
23	CLA	b	615	65/65	0.78	0.20	56,64,74,80	0
38	HEM	E	103	43/43	0.78	0.25	65,73,87,116	0
30	UNL	d	409	17/-	0.78	0.71	78,88,109,111	0
23	CLA	B	613	65/65	0.79	0.34	47,54,80,87	0
37	LHG	d	406	49/49	0.79	0.38	60,71,88,100	0
23	CLA	C	508	65/65	0.79	0.27	59,66,77,79	0
23	CLA	B	612	65/65	0.79	0.31	47,54,61,67	0
25	BCR	H	101	40/40	0.79	0.19	58,69,79,80	0
33	LMG	d	412	51/55	0.79	0.24	69,77,107,115	0
23	CLA	C	506	65/65	0.79	0.32	55,63,81,93	0
23	CLA	A	405	65/65	0.80	0.24	44,51,59,60	0
27	GOL	b	624	6/6	0.80	0.28	93,100,106,108	0
23	CLA	b	612	65/65	0.80	0.33	53,60,66,77	0
23	CLA	D	406	65/65	0.80	0.22	55,65,105,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	B	615	65/65	0.80	0.20	48,58,74,77	0
23	CLA	b	608	65/65	0.80	0.40	57,64,79,88	0
23	CLA	b	610	65/65	0.80	0.32	57,64,73,78	0
23	CLA	C	502	65/65	0.80	0.32	56,65,71,76	0
37	LHG	d	407	49/49	0.80	0.34	55,62,72,80	0
23	CLA	b	614	65/65	0.80	0.23	49,58,92,99	0
23	CLA	b	607	65/65	0.81	0.29	47,55,76,83	0
37	LHG	D	411	49/49	0.81	0.40	60,67,105,110	0
23	CLA	c	508	65/65	0.81	0.23	64,75,83,90	0
23	CLA	C	511	65/65	0.81	0.41	58,67,77,87	0
23	CLA	B	604	65/65	0.81	0.37	44,53,90,103	0
37	LHG	d	408	49/49	0.81	0.30	64,72,102,105	0
23	CLA	a	407	65/65	0.81	0.25	52,59,102,109	0
23	CLA	c	503	65/65	0.81	0.34	59,69,79,81	0
23	CLA	c	510	65/65	0.82	0.29	61,73,84,92	0
23	CLA	b	616	65/65	0.82	0.21	58,67,97,103	0
23	CLA	A	404	65/65	0.82	0.27	43,50,60,70	0
23	CLA	B	610	65/65	0.82	0.29	52,59,69,75	0
25	BCR	c	515	40/40	0.82	0.22	86,93,98,101	0
27	GOL	V	201	6/6	0.82	0.55	64,71,83,87	0
23	CLA	B	614	65/65	0.82	0.24	48,54,87,95	0
23	CLA	d	403	65/65	0.82	0.19	58,71,98,106	0
23	CLA	B	607	65/65	0.83	0.29	44,52,69,76	0
25	BCR	B	618	40/40	0.83	0.35	53,61,74,81	0
23	CLA	a	405	65/65	0.83	0.29	48,54,64,81	0
23	CLA	b	605	65/65	0.83	0.30	51,57,70,72	0
23	CLA	b	604	65/65	0.83	0.32	49,56,91,101	0
37	LHG	D	410	49/49	0.83	0.38	55,61,74,84	0
23	CLA	c	505	65/65	0.83	0.32	63,71,94,111	0
23	CLA	A	406	65/65	0.83	0.23	47,54,92,96	0
25	BCR	y	101	40/40	0.83	0.16	72,79,88,91	0
30	UNL	D	412	17/-	0.83	0.46	70,84,100,106	0
24	PHO	a	353	64/64	0.83	0.27	53,60,65,67	0
23	CLA	D	405	65/65	0.83	0.26	43,50,66,81	0
24	PHO	A	353	64/64	0.83	0.30	47,56,61,64	0
34	HTG	V	203	11/19	0.84	0.50	103,119,123,128	0
23	CLA	B	603	65/65	0.84	0.34	50,58,69,75	0
23	CLA	d	402	65/65	0.84	0.27	48,55,66,78	0
23	CLA	b	611	65/65	0.84	0.28	52,58,68,75	0
25	BCR	b	618	40/40	0.84	0.33	53,62,71,76	0
23	CLA	c	502	65/65	0.84	0.29	64,72,80,84	0
25	BCR	d	404	40/40	0.84	0.20	67,78,91,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	BCR	T	101	40/40	0.85	0.31	52,62,69,72	0
38	HEM	e	87	43/43	0.85	0.39	80,94,117,126	0
23	CLA	C	503	65/65	0.85	0.38	54,62,73,86	0
39	MG	J	102	1/1	0.85	0.18	64,64,64,64	0
25	BCR	k	101	40/40	0.85	0.26	71,80,90,95	0
25	BCR	B	619	40/40	0.85	0.19	56,64,78,81	0
40	HEC	V	202	43/43	0.85	0.18	50,60,63,64	0
25	BCR	b	619	40/40	0.86	0.20	56,67,80,82	0
40	HEC	v	202	43/43	0.86	0.17	61,70,75,79	0
25	BCR	a	410	40/40	0.86	0.23	51,59,65,67	0
27	GOL	C	523	6/6	0.86	0.31	63,67,73,76	0
23	CLA	B	616	65/65	0.86	0.20	53,63,108,111	0
23	CLA	b	613	65/65	0.86	0.32	48,55,84,89	0
23	CLA	A	408	65/65	0.86	0.20	51,59,101,112	0
27	GOL	A	411	6/6	0.86	0.21	79,87,89,100	0
35	DGD	c	519	62/66	0.86	0.26	64,74,94,102	0
25	BCR	C	516	40/40	0.86	0.30	59,69,76,80	0
23	CLA	C	510	65/65	0.86	0.31	57,67,80,86	0
25	BCR	t	103	40/40	0.87	0.33	54,64,79,80	0
25	BCR	C	515	40/40	0.87	0.16	74,79,87,92	0
24	PHO	A	407	64/64	0.87	0.30	46,51,56,59	0
27	GOL	B	625	6/6	0.87	0.32	65,82,86,93	0
25	BCR	D	407	40/40	0.87	0.24	59,68,91,92	0
29	PL9	d	405	55/55	0.88	0.32	51,58,66,90	0
25	BCR	c	516	40/40	0.88	0.20	66,74,81,85	0
24	PHO	a	408	64/64	0.88	0.29	49,55,60,66	0
25	BCR	K	102	40/40	0.89	0.21	64,72,81,83	0
23	CLA	a	409	65/65	0.89	0.18	53,62,108,115	0
25	BCR	b	617	40/40	0.89	0.26	51,58,65,67	0
25	BCR	B	617	40/40	0.89	0.31	51,56,63,64	0
25	BCR	Y	101	40/40	0.90	0.18	67,75,80,82	0
36	CA	c	524	1/1	0.90	0.19	93,93,93,93	0
31	BCT	A	348	4/4	0.90	0.20	60,62,64,69	0
29	PL9	D	408	55/55	0.91	0.32	47,55,61,73	0
25	BCR	A	409	40/40	0.91	0.21	48,55,62,65	0
27	GOL	B	624	6/6	0.91	0.29	85,88,93,95	0
31	BCT	a	404	4/4	0.92	0.19	59,65,66,76	0
28	OEX	a	415	10/10	0.92	0.20	58,62,66,67	0
27	GOL	c	501	6/6	0.92	0.54	73,74,77,78	0
28	OEX	A	413	10/10	0.93	0.21	56,57,57,57	0
39	MG	j	102	1/1	0.94	0.17	70,70,70,70	0
36	CA	c	523	1/1	0.95	0.27	84,84,84,84	0

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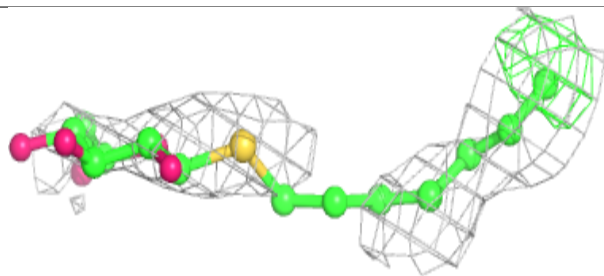
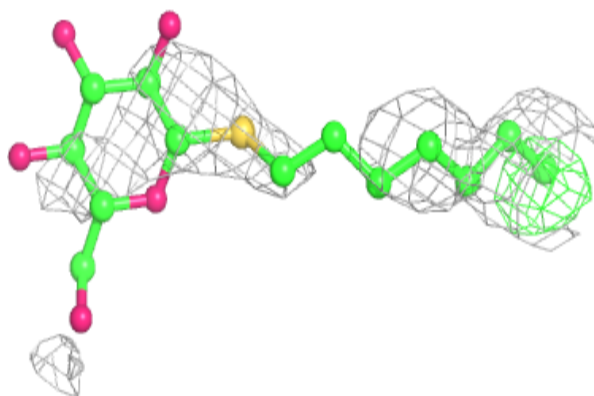
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	CL	a	403	1/1	0.97	0.33	58,58,58,58	0
22	CL	A	403	1/1	0.98	0.39	52,52,52,52	0
36	CA	C	524	1/1	0.99	0.24	81,81,81,81	0
21	FE2	A	401	1/1	0.99	0.05	64,64,64,64	0
21	FE2	a	401	1/1	0.99	0.08	67,67,67,67	0
22	CL	a	402	1/1	0.99	0.39	56,56,56,56	0
22	CL	A	402	1/1	0.99	0.37	51,51,51,51	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.

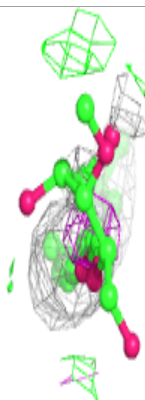
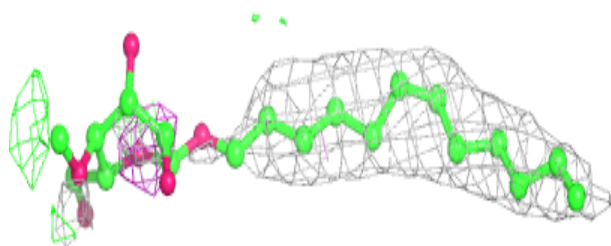
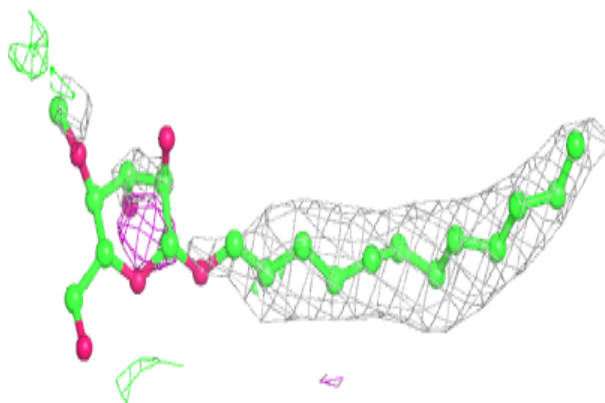
**Electron density around HTG c 522:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

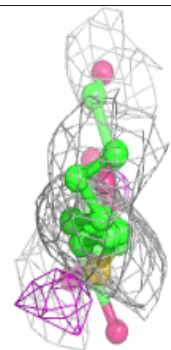
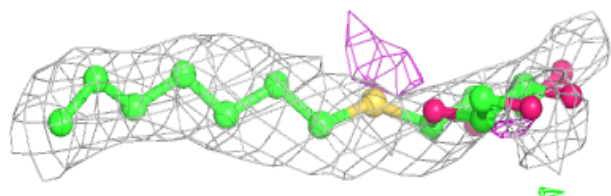
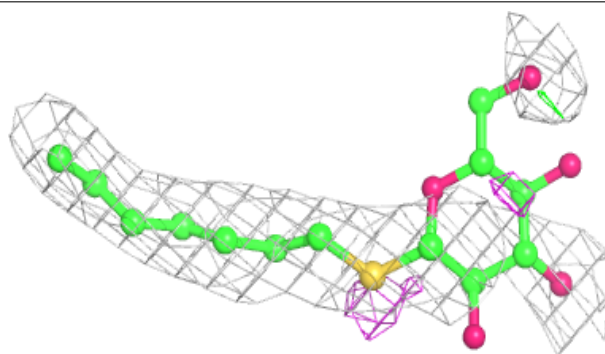


**Electron density around LMT b 621:**

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

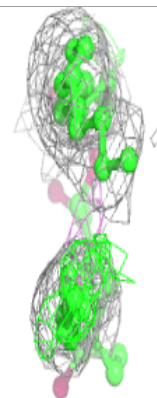
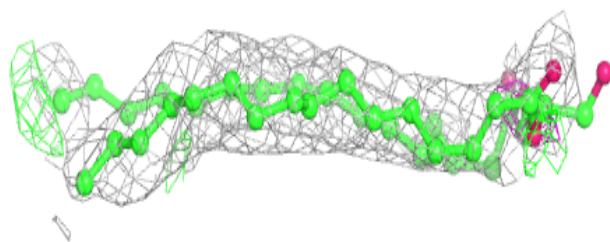
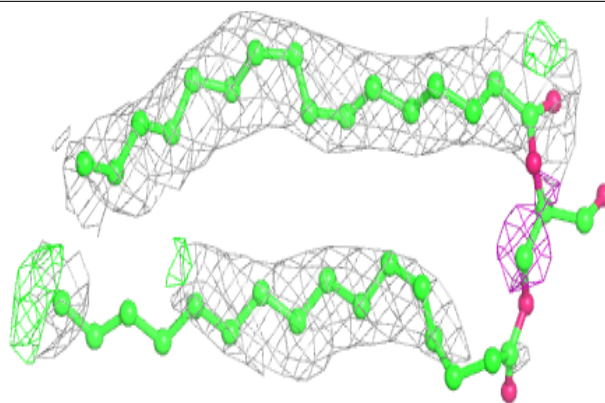
**Electron density around HTG b 623:**

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

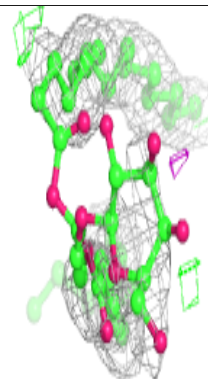
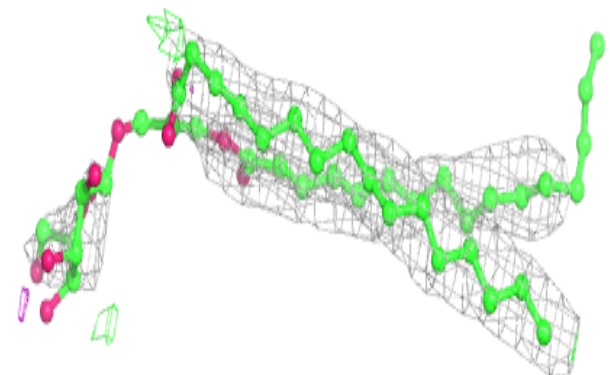
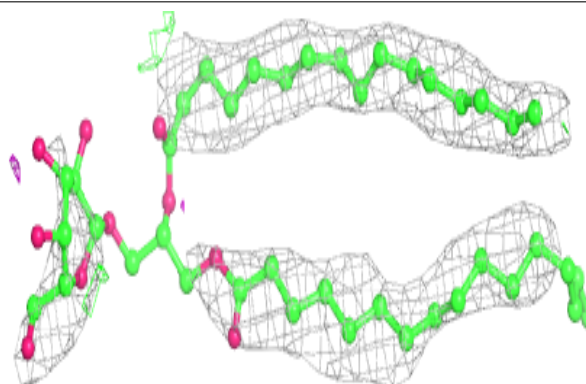


**Electron density around UNL i 101:**

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

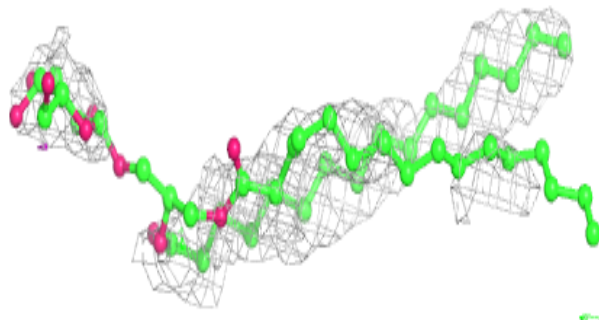
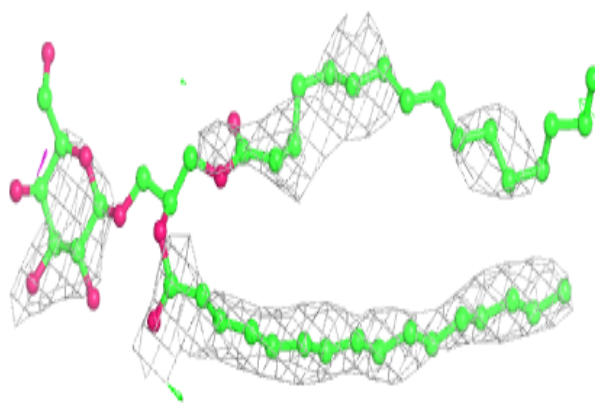
**Electron density around LMG C 521:**

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

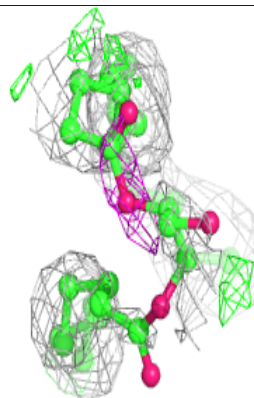
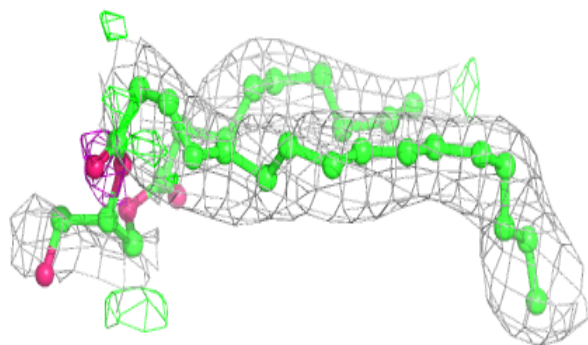
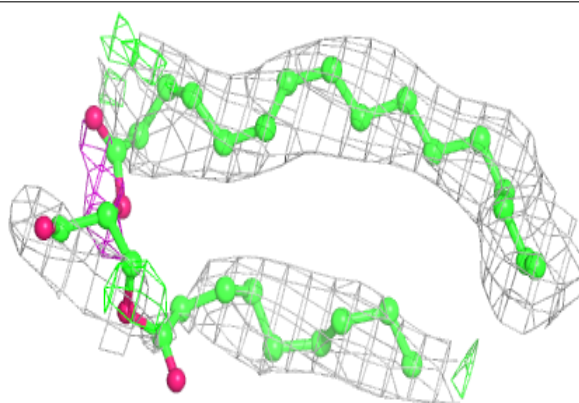


**Electron density around LMG c 521:**

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

**Electron density around UNL b 626:**

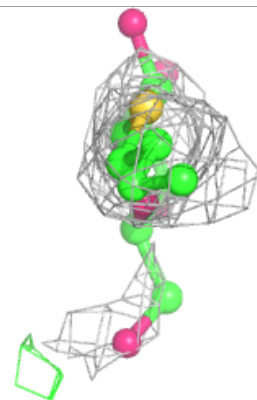
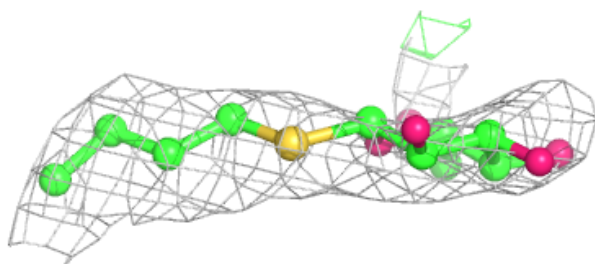
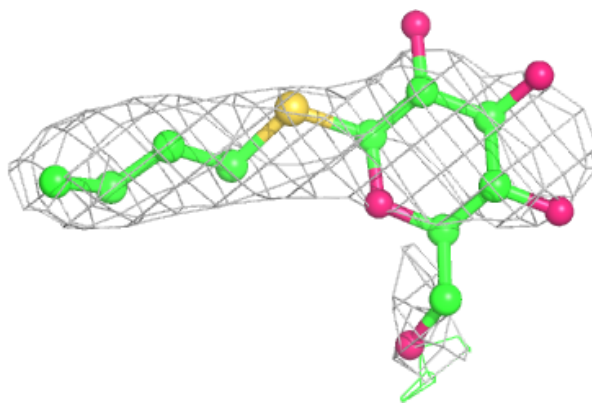
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



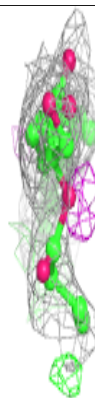
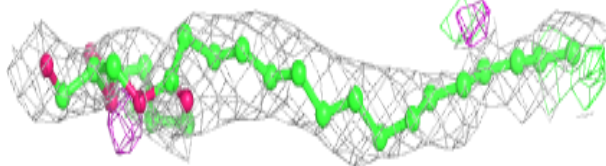
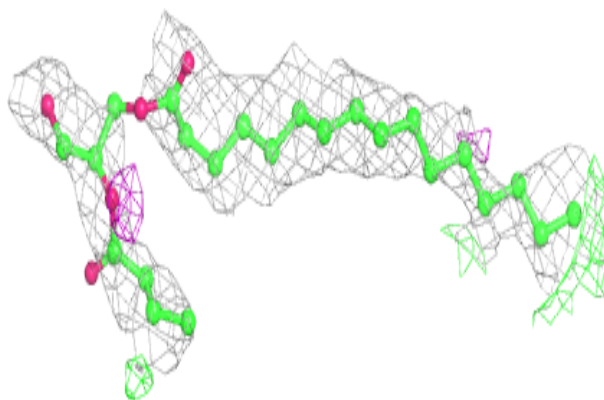


**Electron density around HTG d 411:**

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

**Electron density around UNL A 415:**

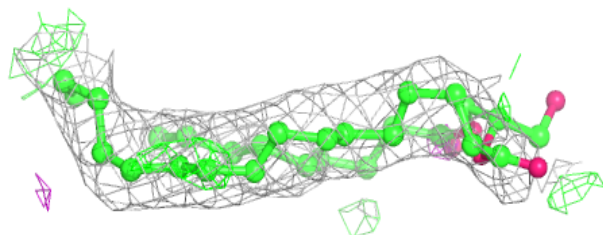
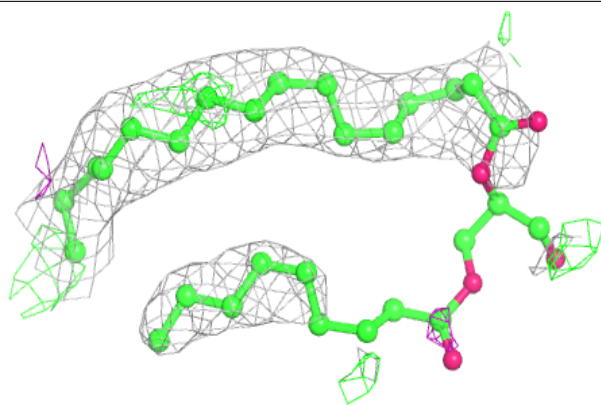
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



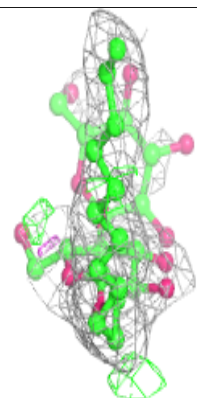
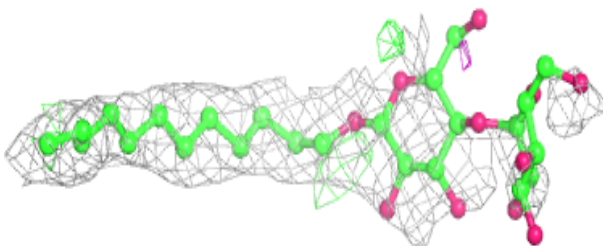
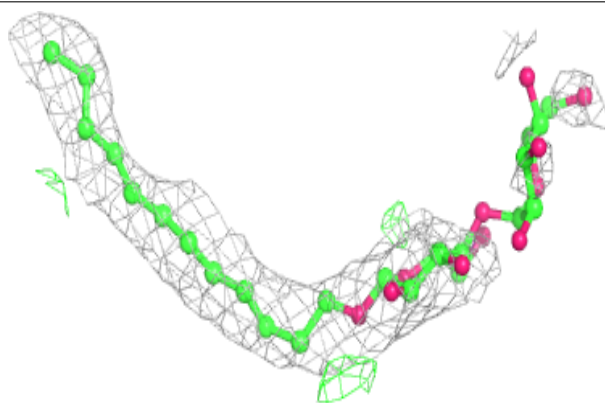


**Electron density around UNL B 627:**

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

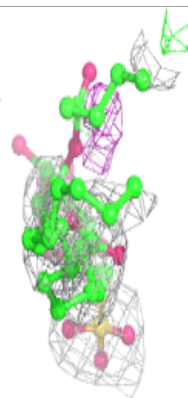
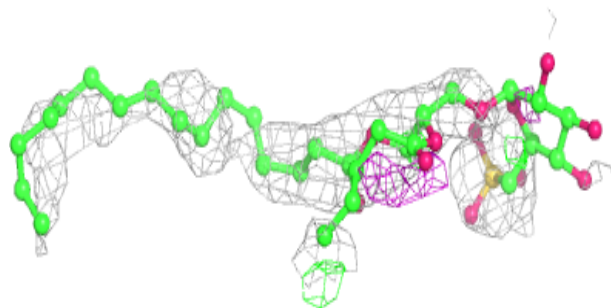
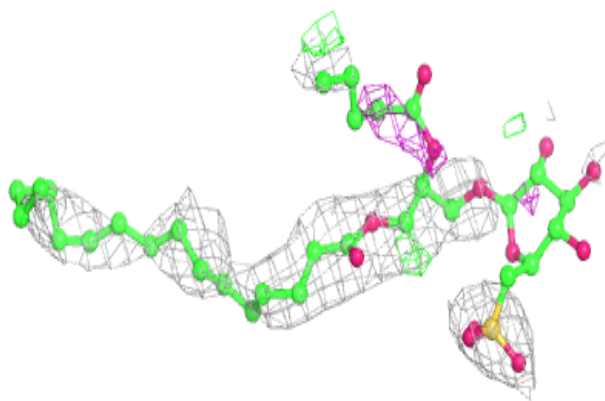
**Electron density around LMT M 103:**

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

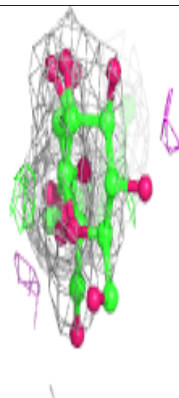
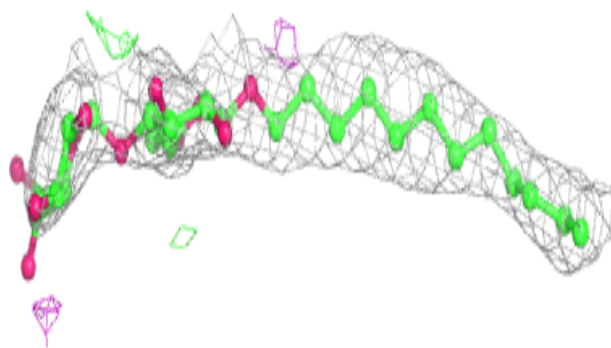
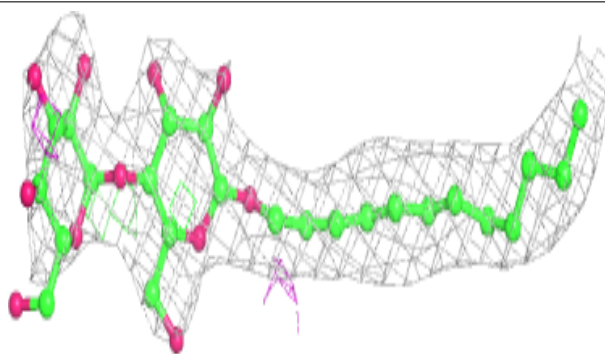


**Electron density around SQD f 102:**

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

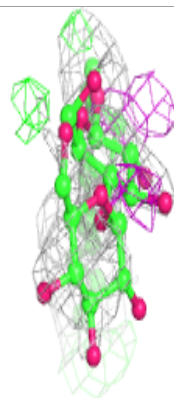
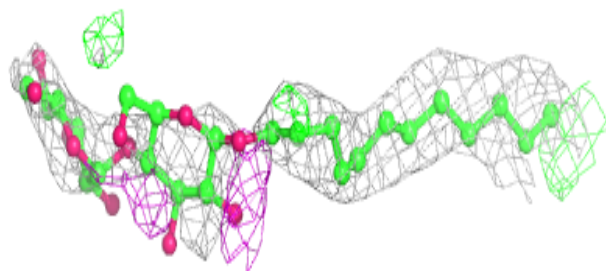
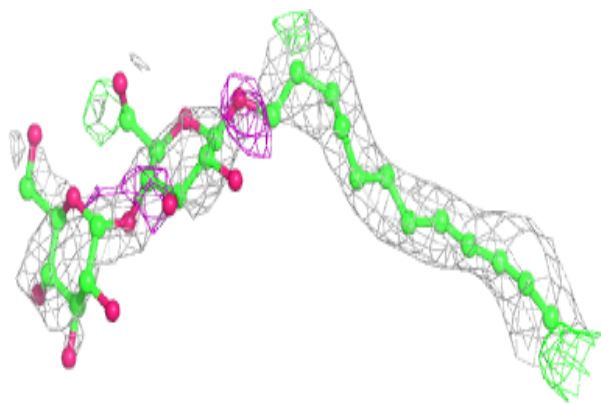
**Electron density around LMT m 103:**

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

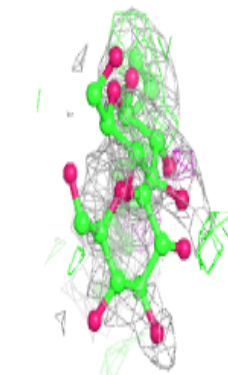
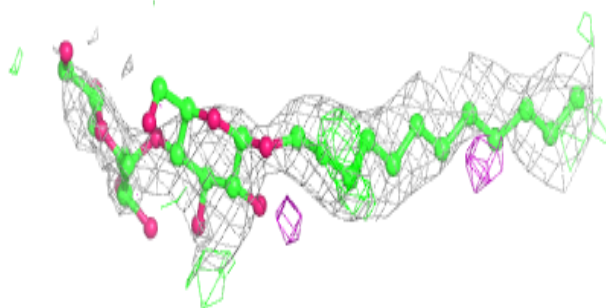
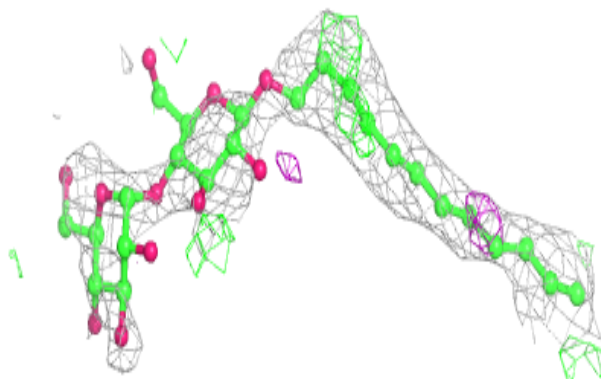


**Electron density around LMT a 414:**

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

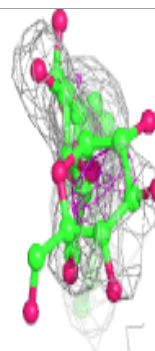
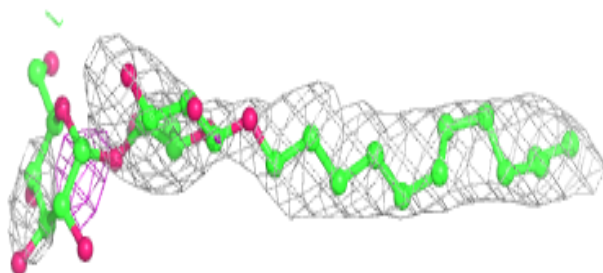
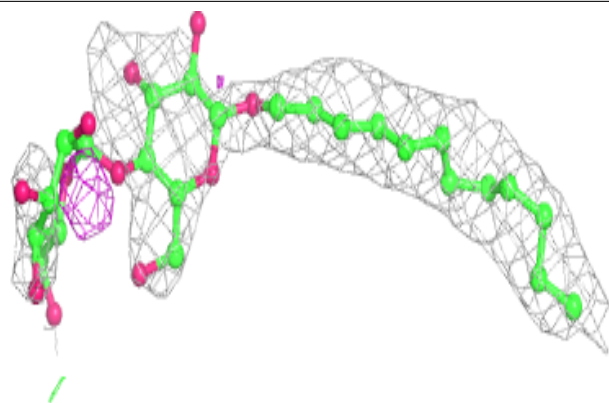
**Electron density around LMT A 359:**

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

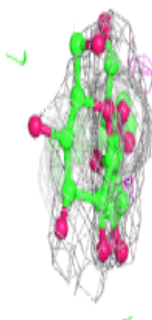
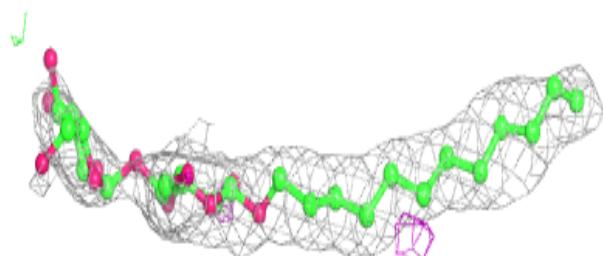
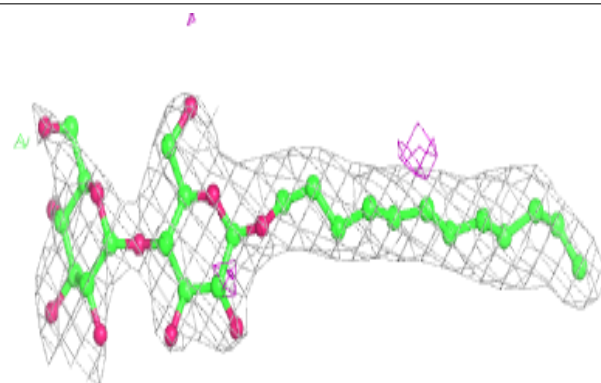


**Electron density around LMT D 404:**

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

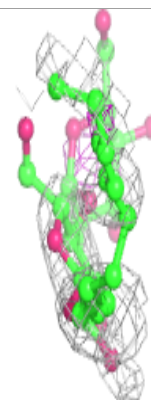
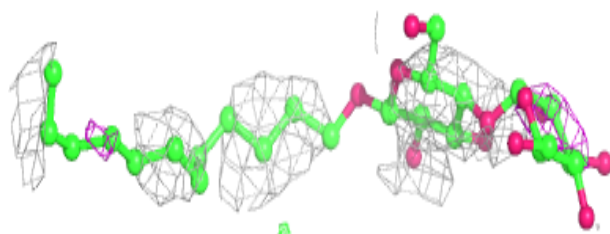
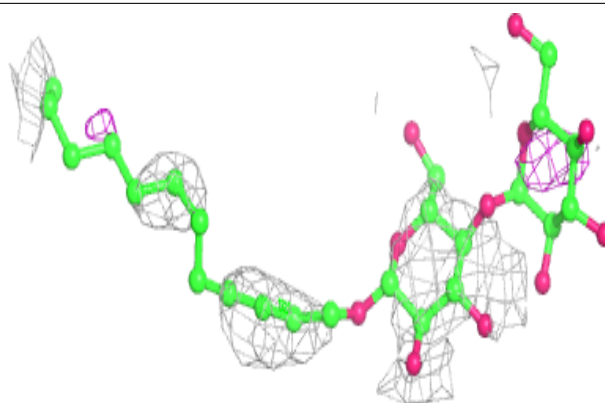
**Electron density around LMT M 101:**

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

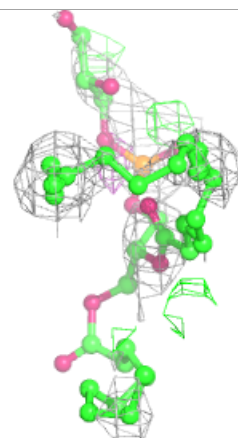
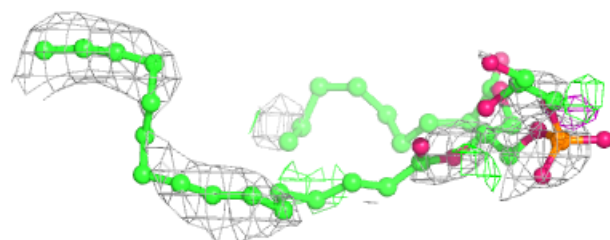
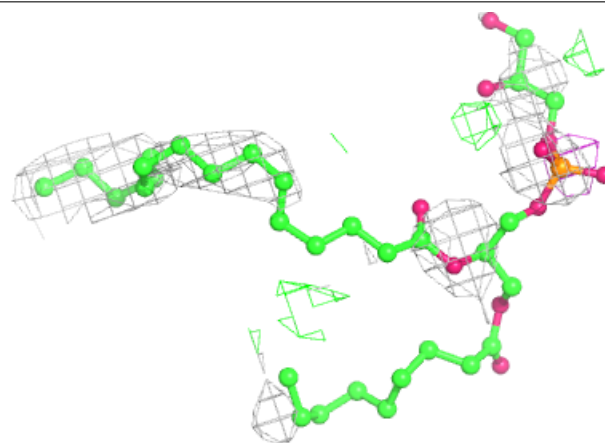


**Electron density around LMT e 102:**

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

**Electron density around LHG e 101:**

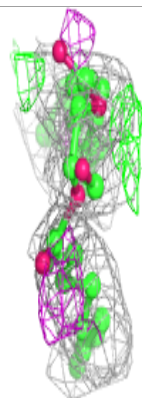
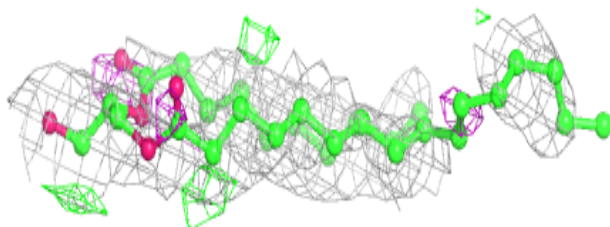
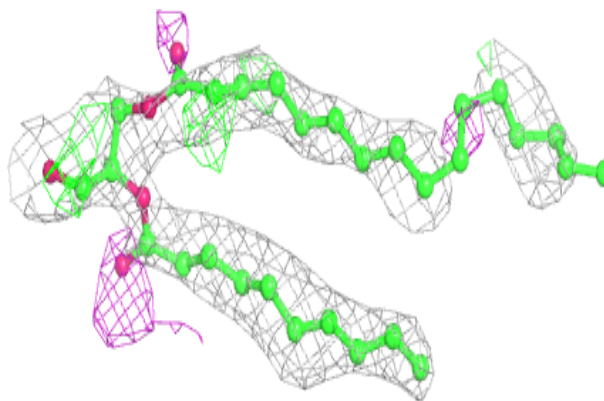
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



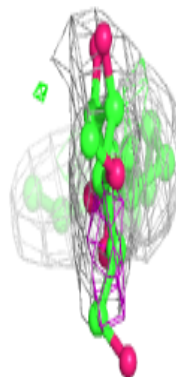
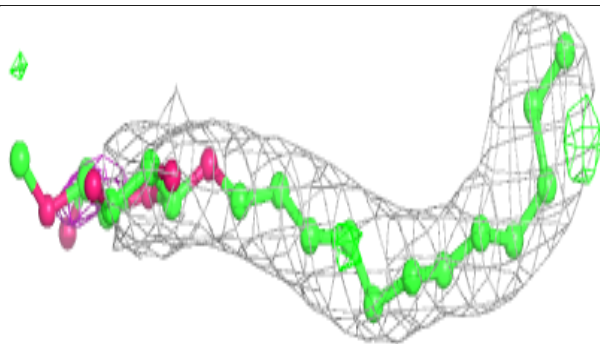
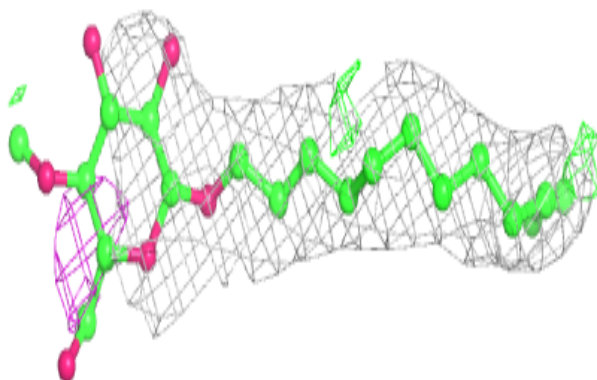


**Electron density around UNL K 101:**

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

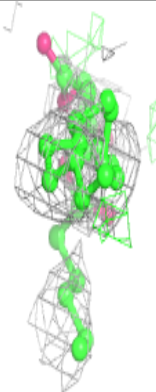
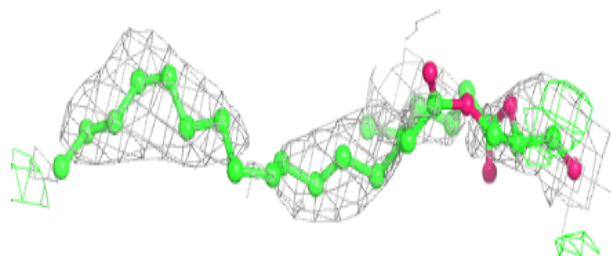
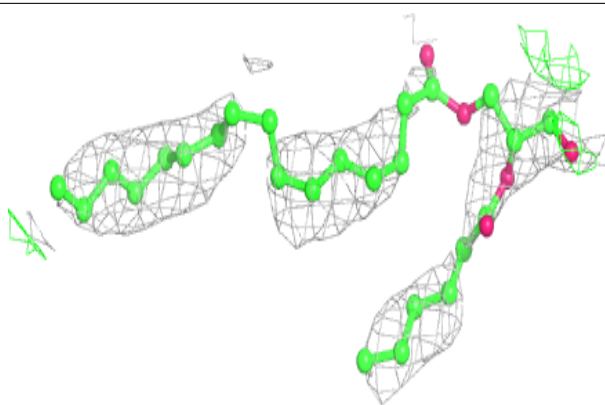
**Electron density around LMT t 101:**

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

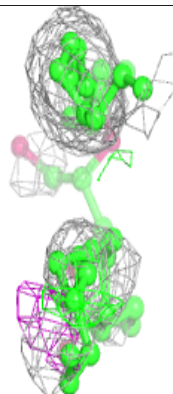
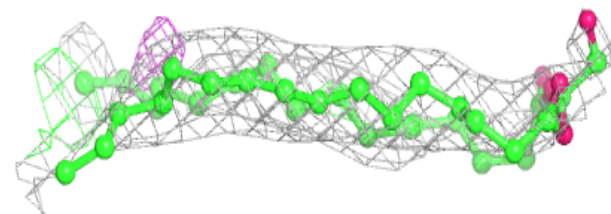
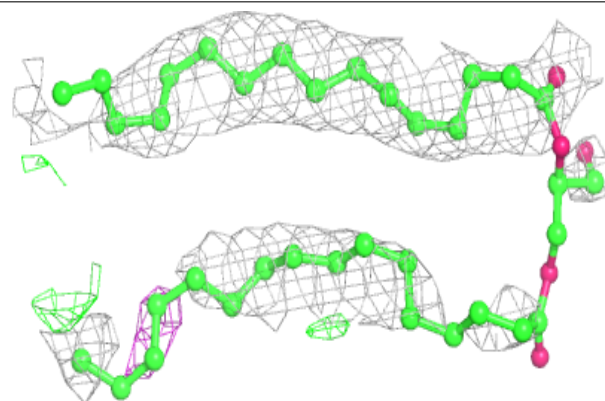


**Electron density around UNL a 417:**

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

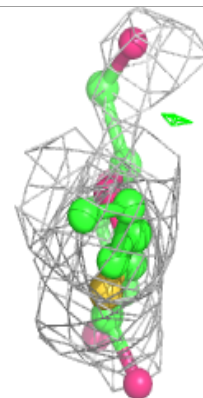
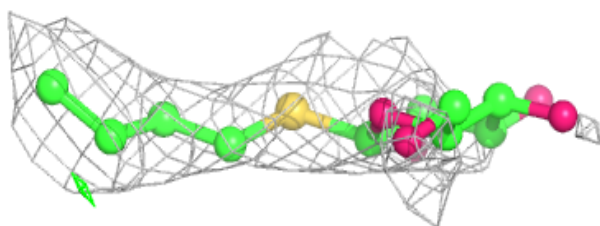
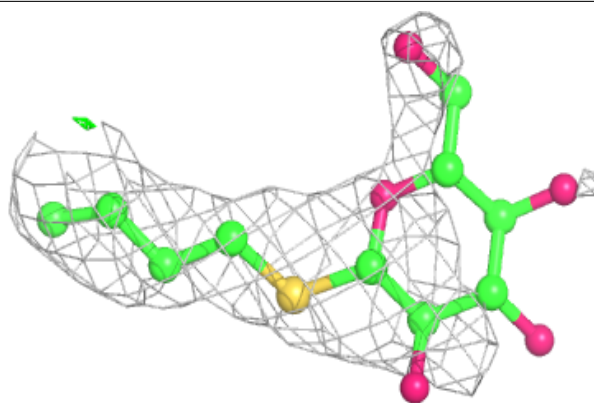
**Electron density around UNL I 102:**

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

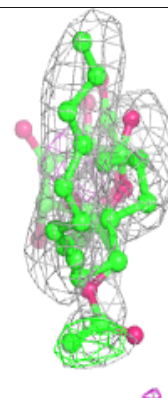
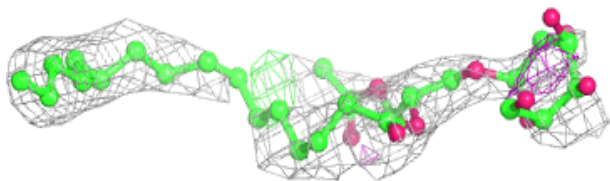
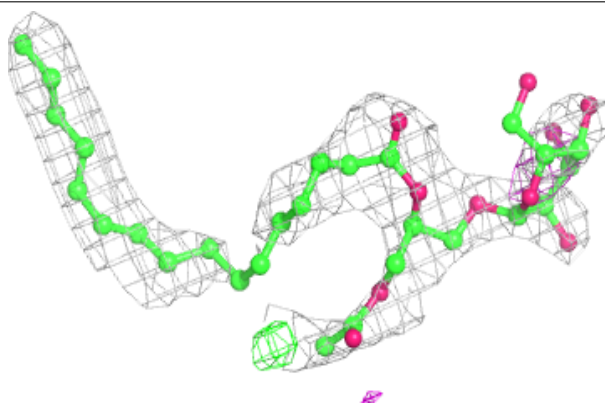


**Electron density around HTG D 414:**

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

**Electron density around LMG Z 101:**

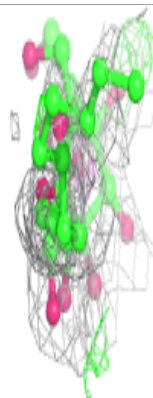
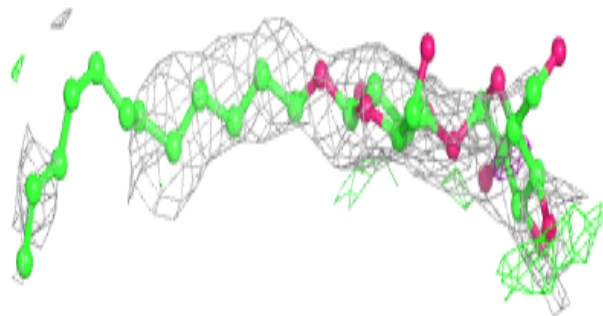
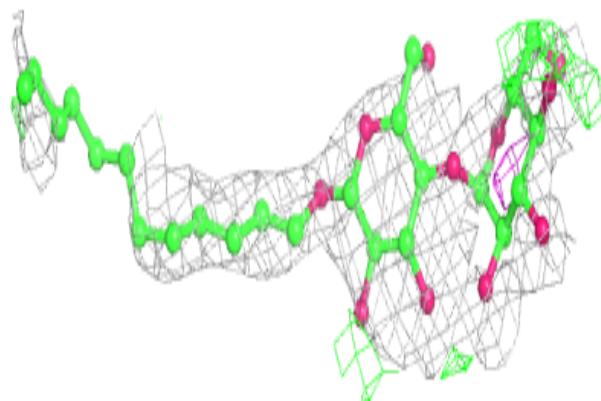
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



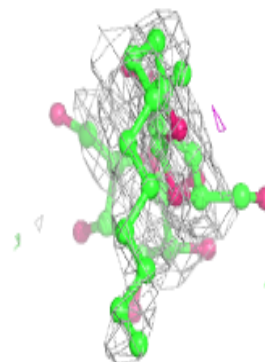
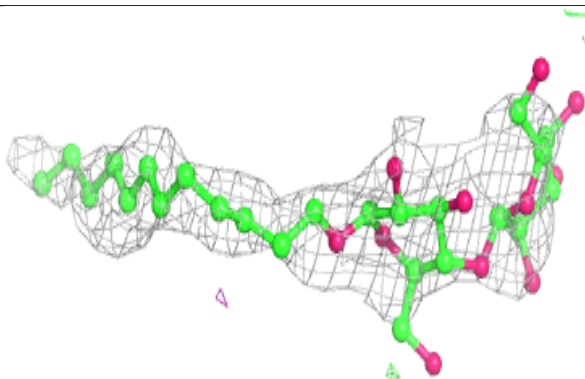
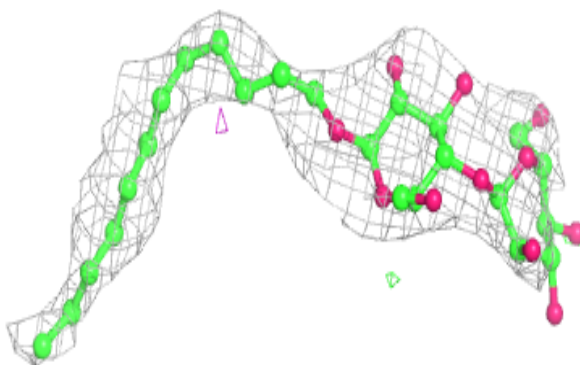


**Electron density around LMT a 420:**

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

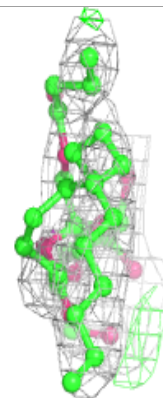
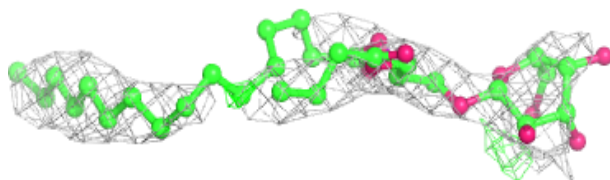
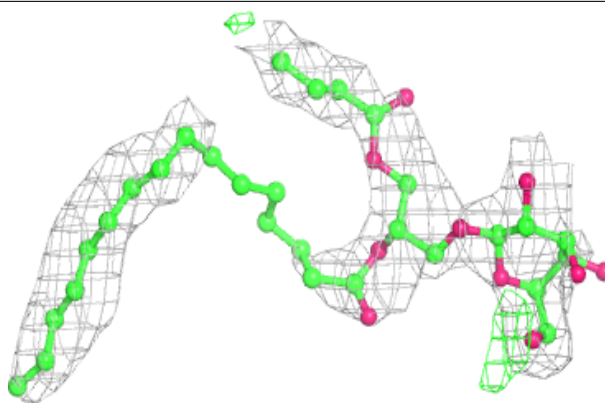
**Electron density around LMT I 101:**

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

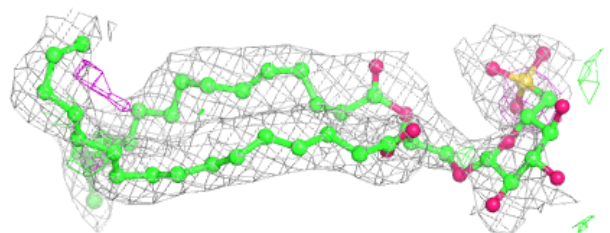
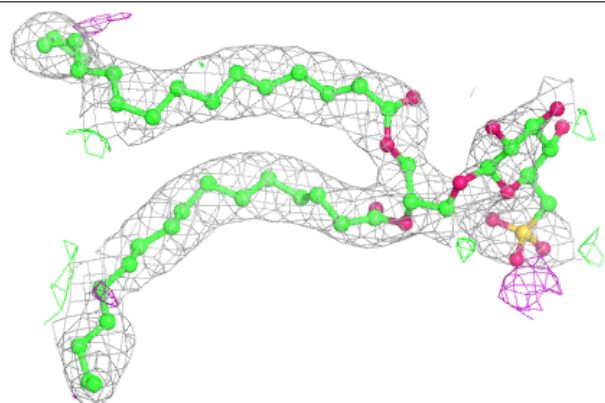


**Electron density around LMG z 101:**

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

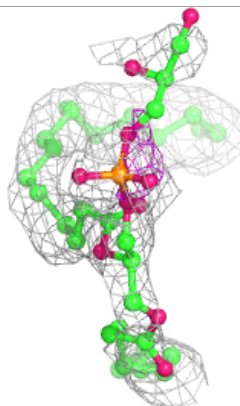
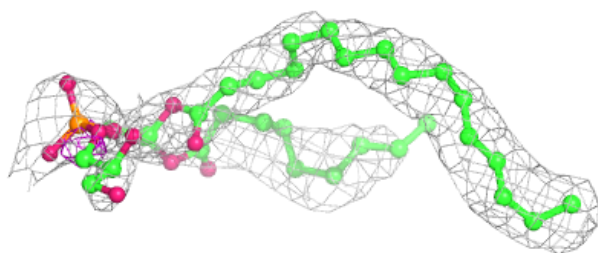
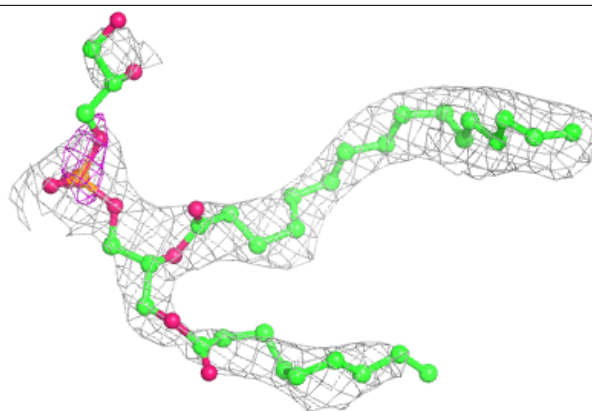
**Electron density around SQD B 620:**

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

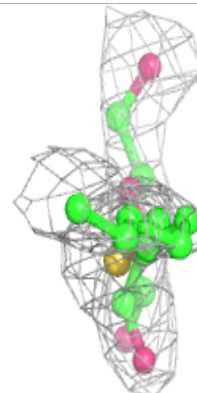
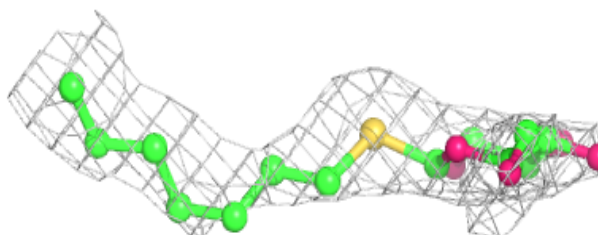
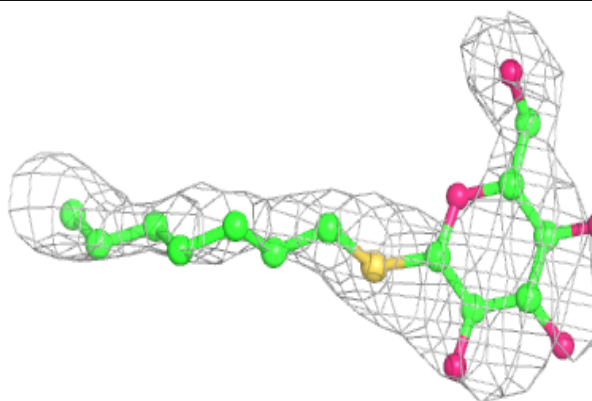


**Electron density around LHG E 101:**

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

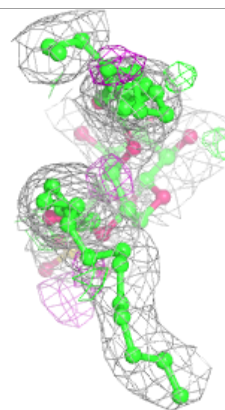
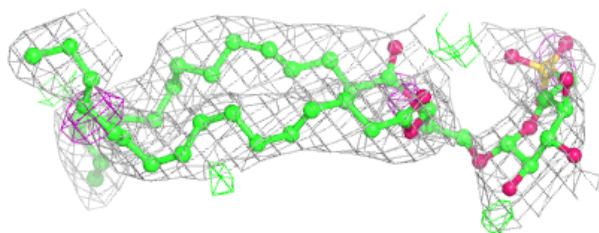
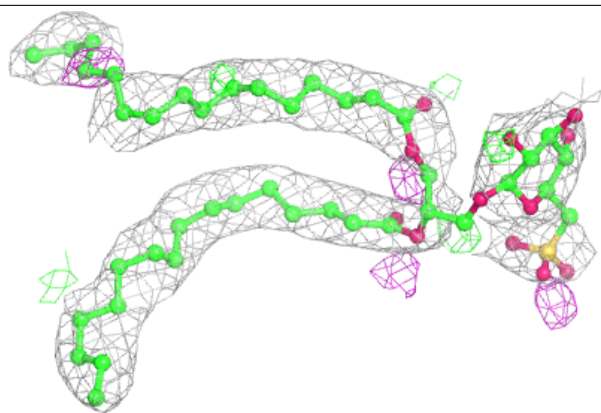
**Electron density around HTG C 522:**

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

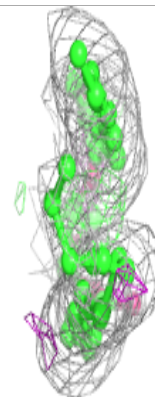
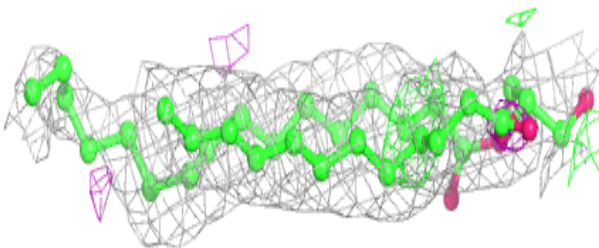
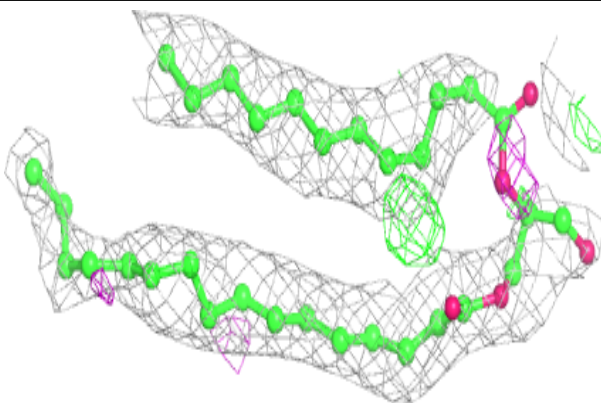


**Electron density around SQD b 620:**

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

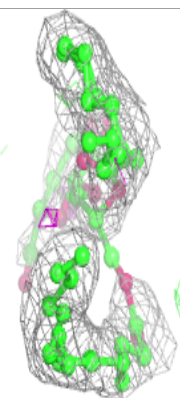
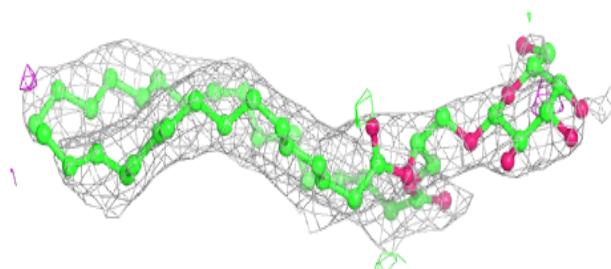
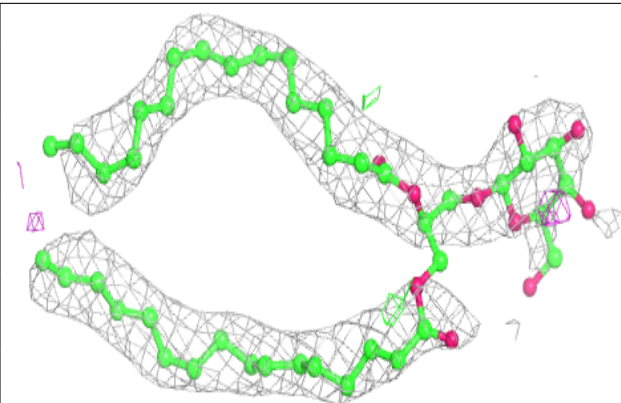
**Electron density around UNL d 410:**

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

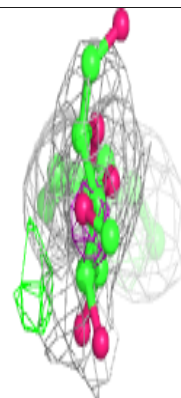
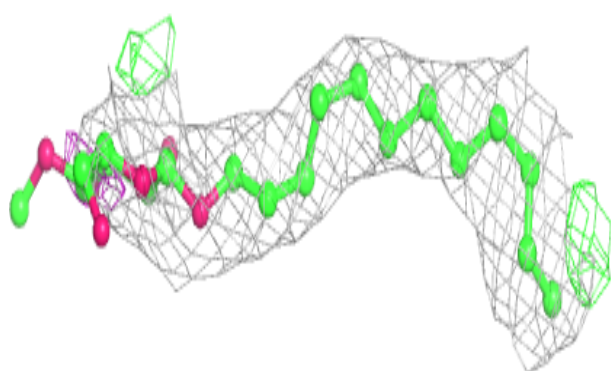
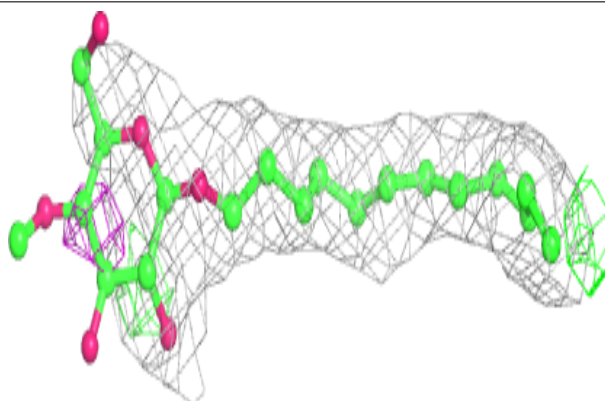


**Electron density around LMG a 419:**

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

**Electron density around LMT b 627:**

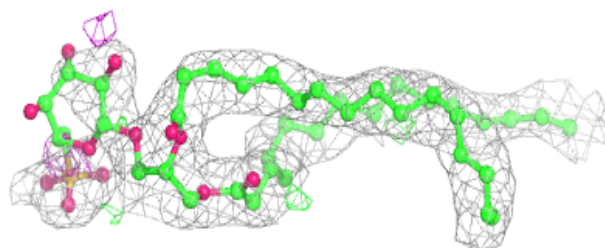
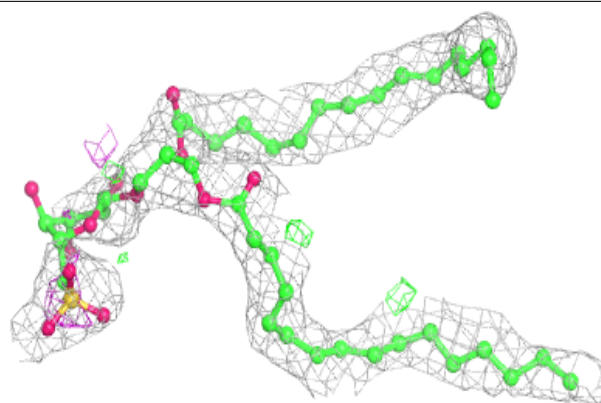
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



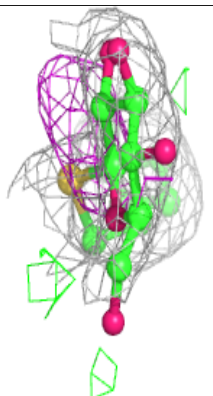
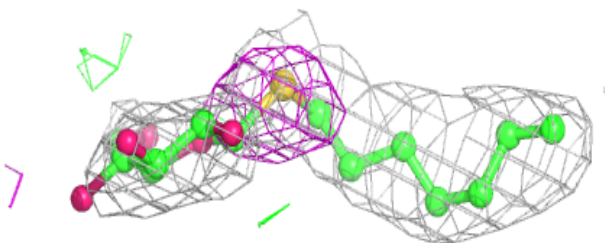
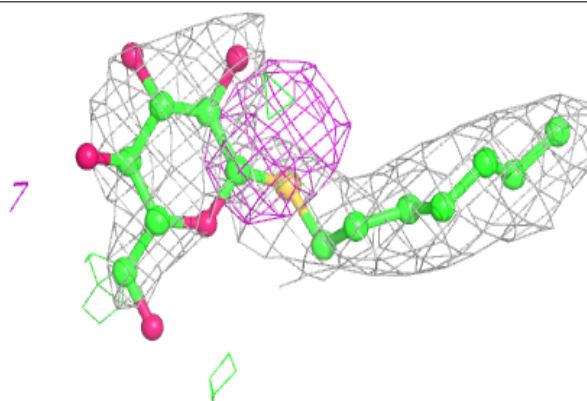


**Electron density around SQD a 413:**

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

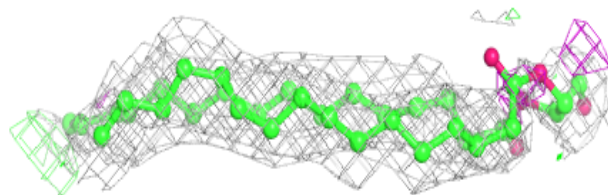
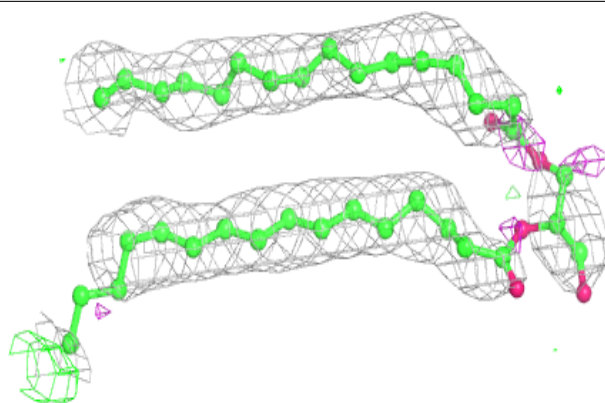
**Electron density around HTG b 622:**

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

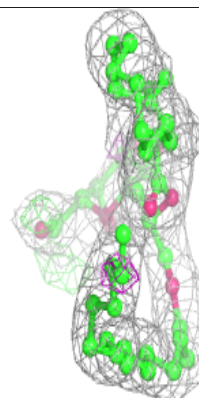
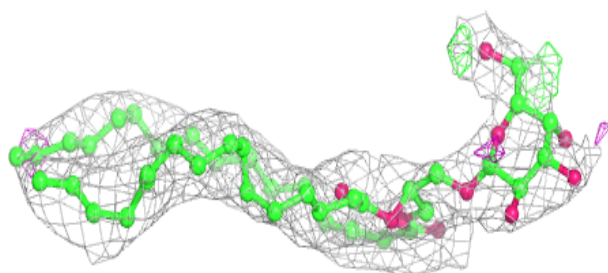
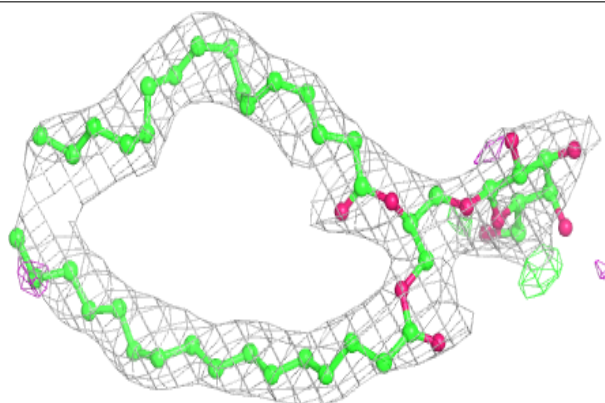


**Electron density around UNL D 413:**

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

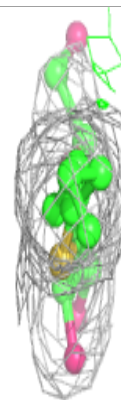
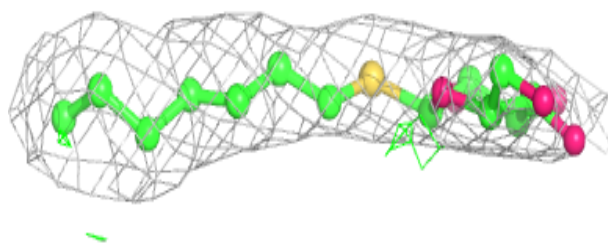
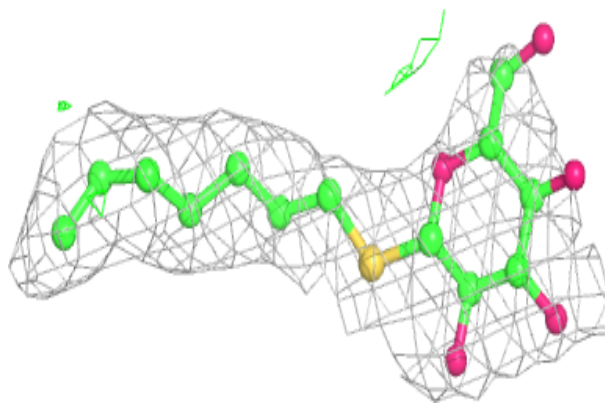
**Electron density around LMG C 501:**

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

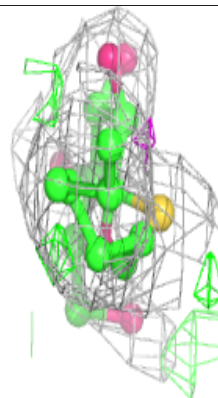
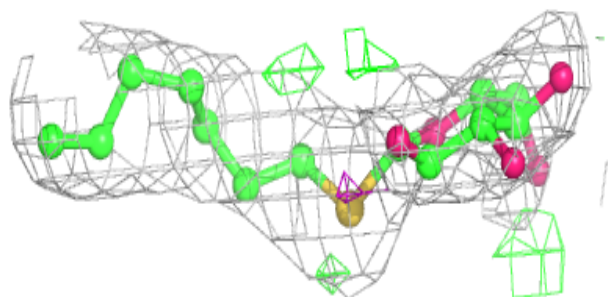
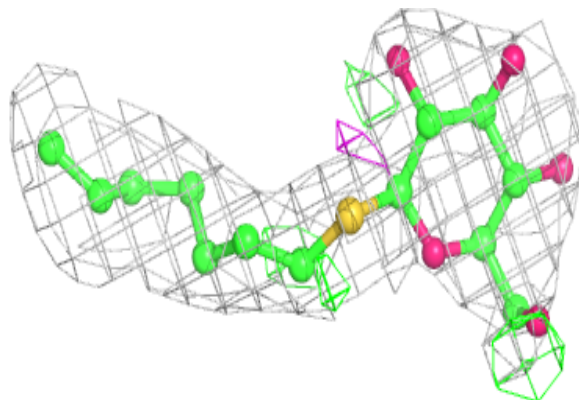


**Electron density around HTG b 625:**

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

**Electron density around HTG B 622:**

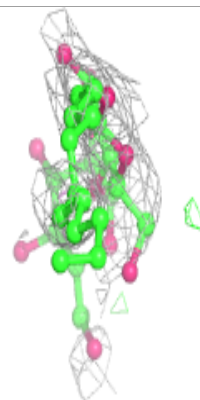
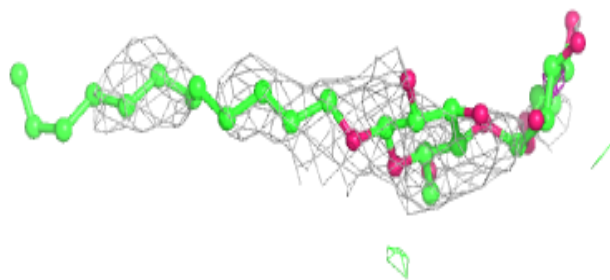
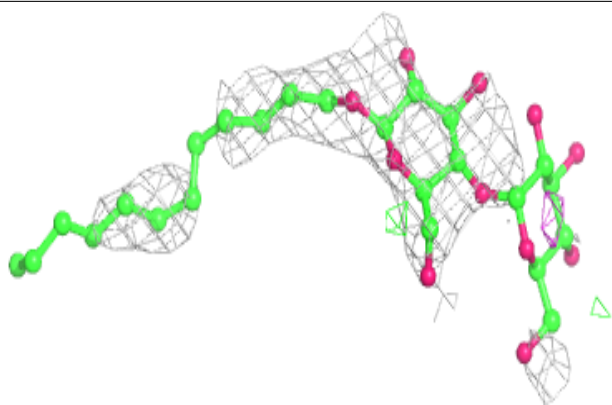
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



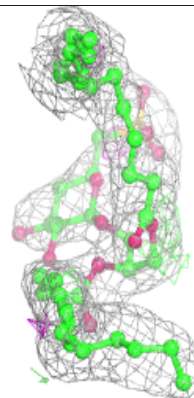
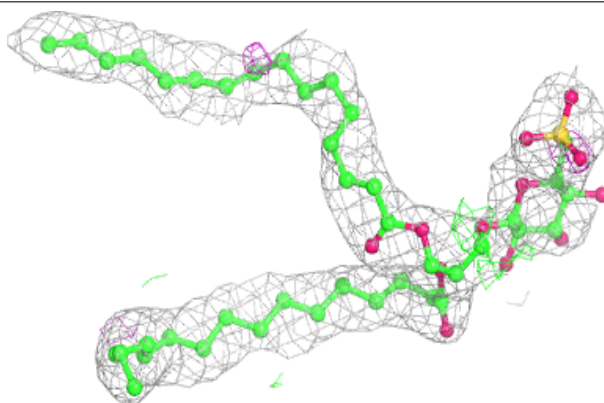


**Electron density around LMT E 102:**

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

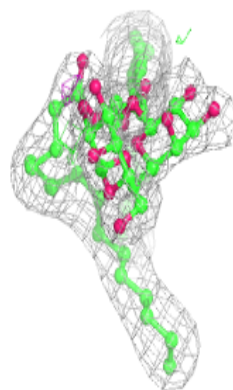
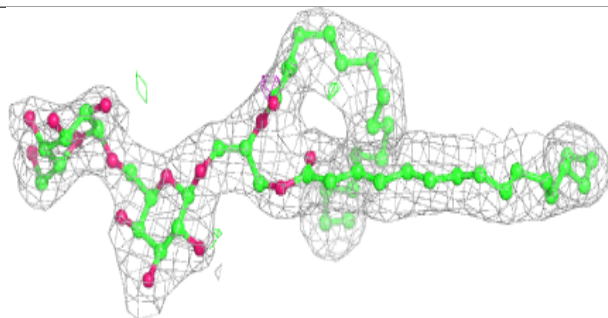
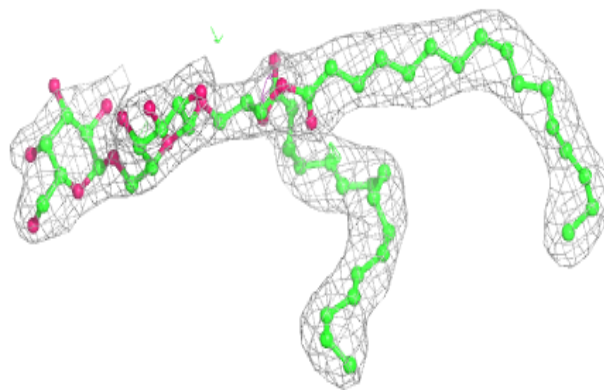
**Electron density around SQD A 412:**

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

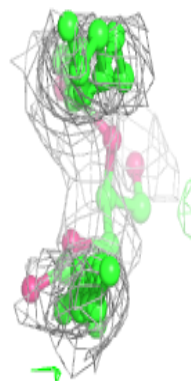
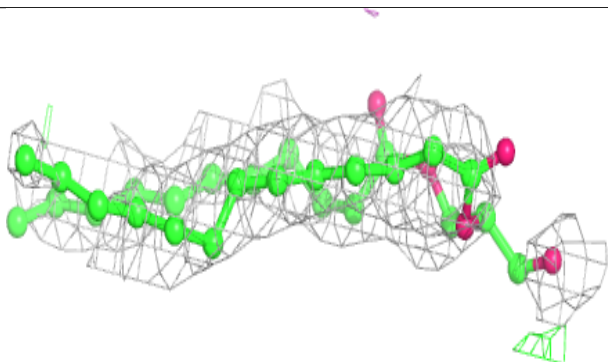
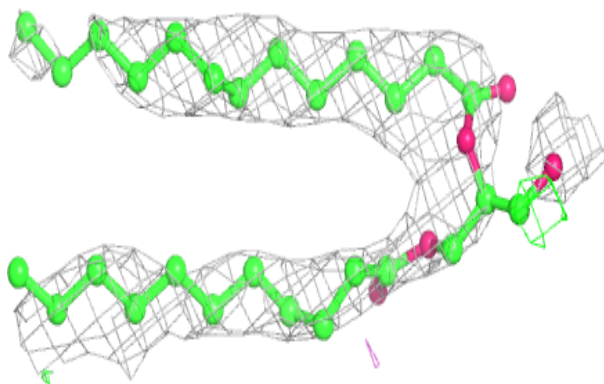


**Electron density around DGD h 102:**

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

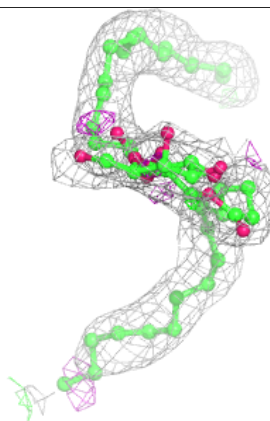
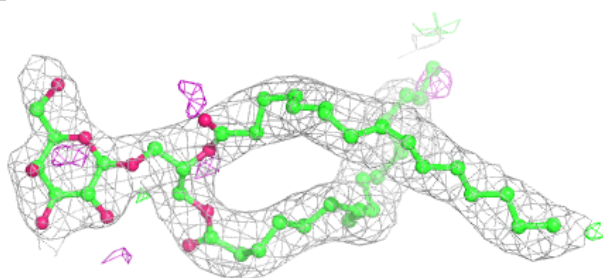
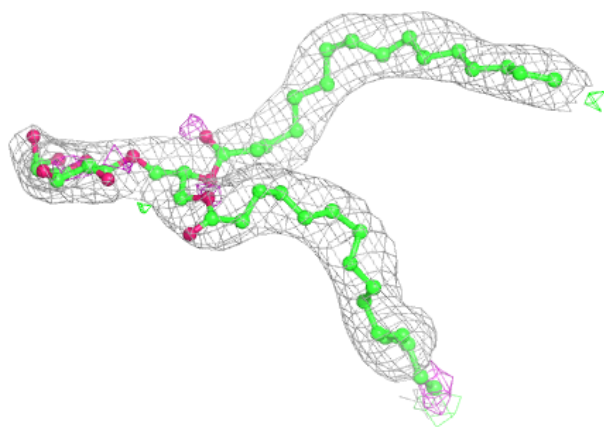
**Electron density around UNL c 525:**

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

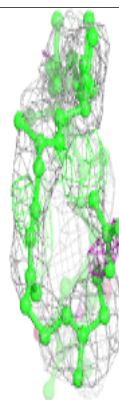
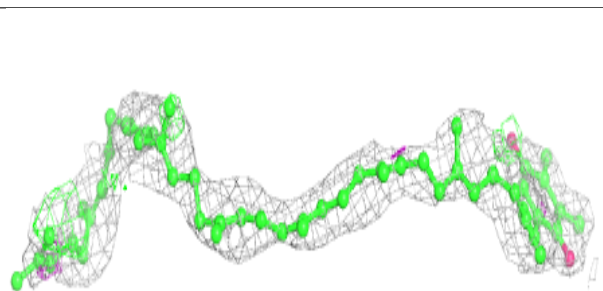
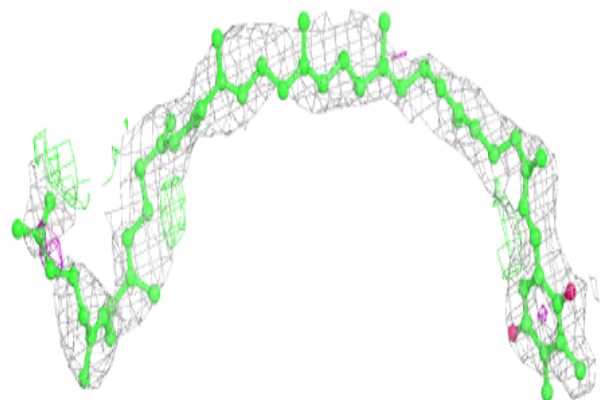


**Electron density around LMG B 621:**

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

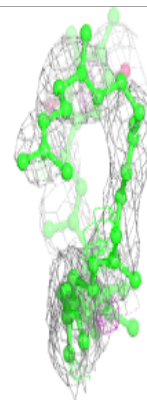
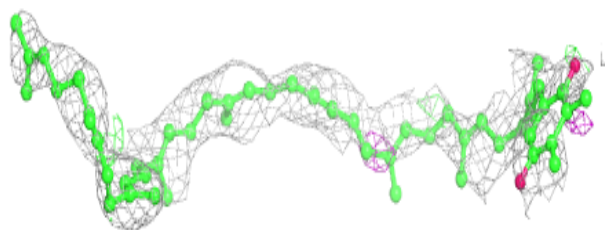
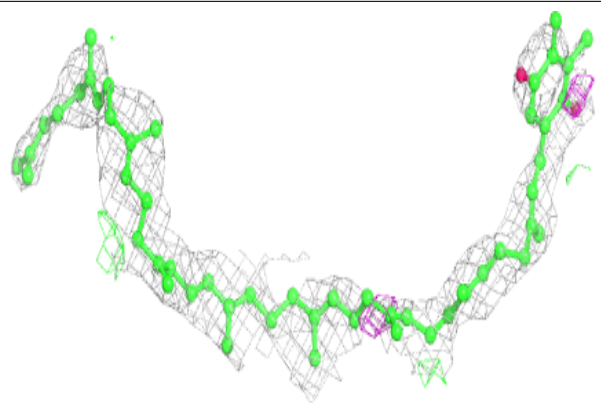
**Electron density around PL9 A 414:**

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

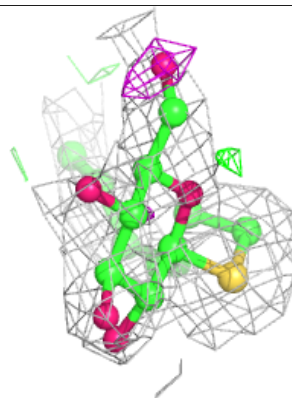
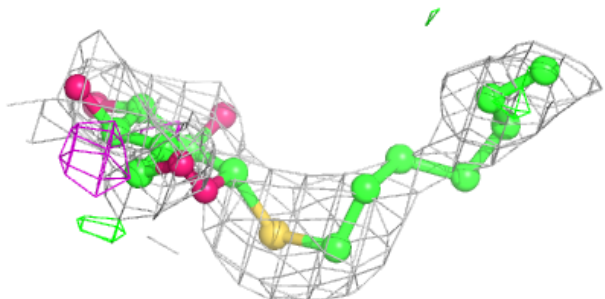
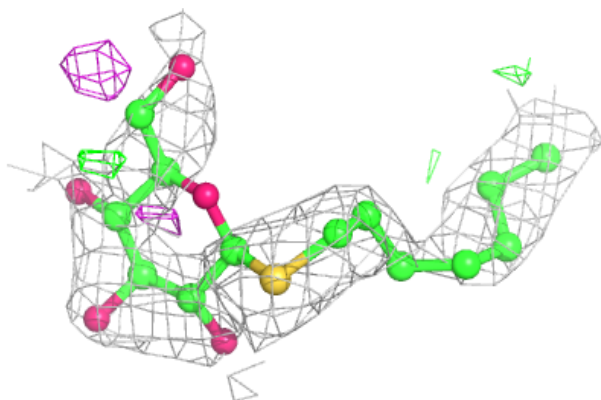


**Electron density around PL9 a 416:**

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

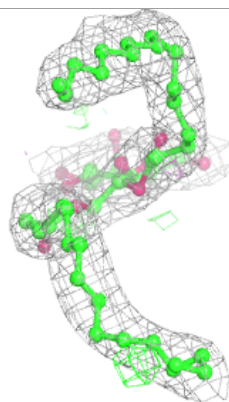
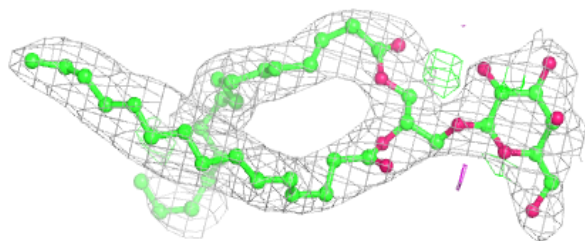
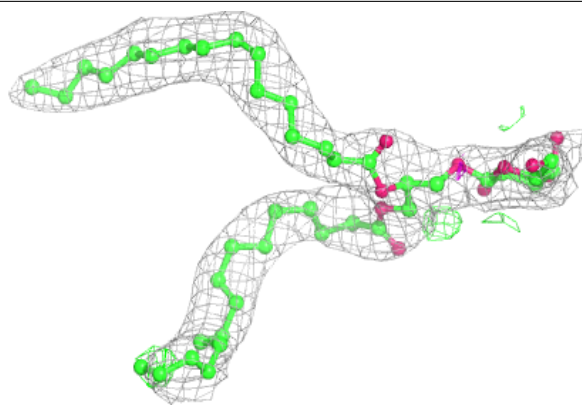
**Electron density around HTG B 623:**

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

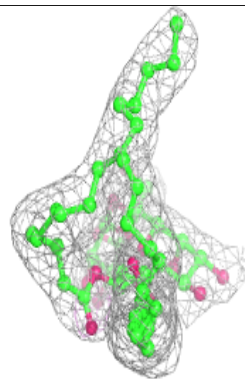
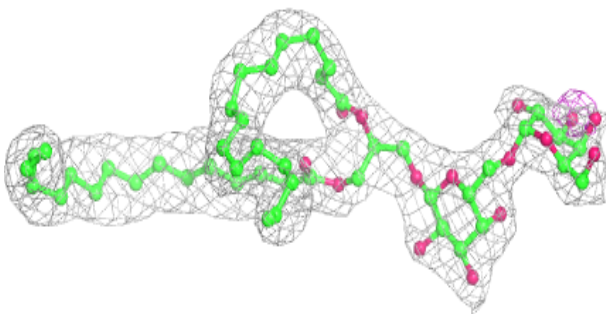
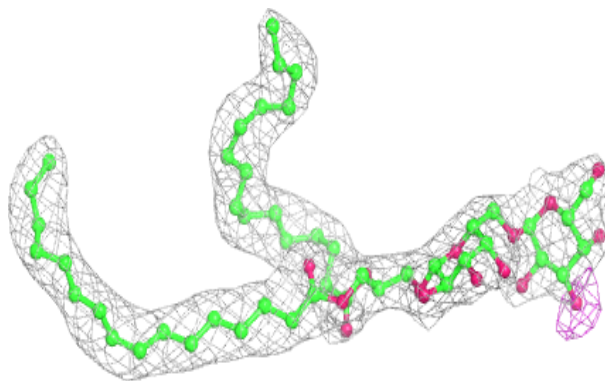


**Electron density around LMG m 101:**

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

**Electron density around DGD H 102:**

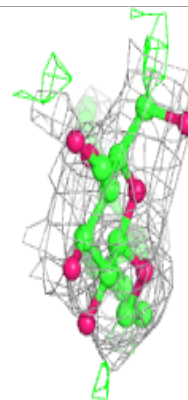
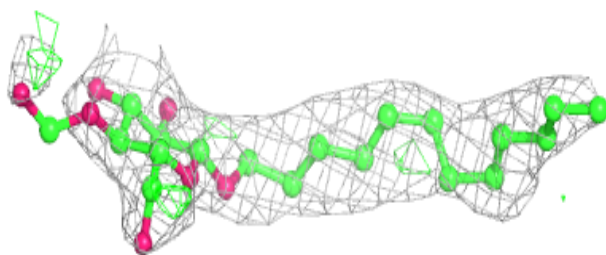
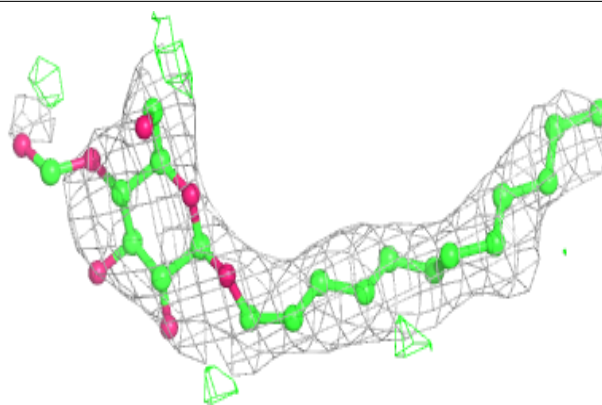
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





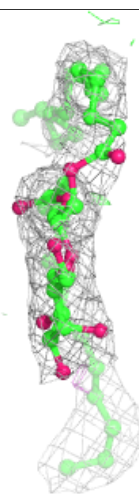
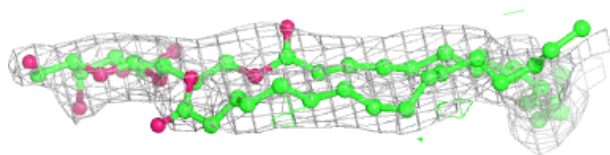
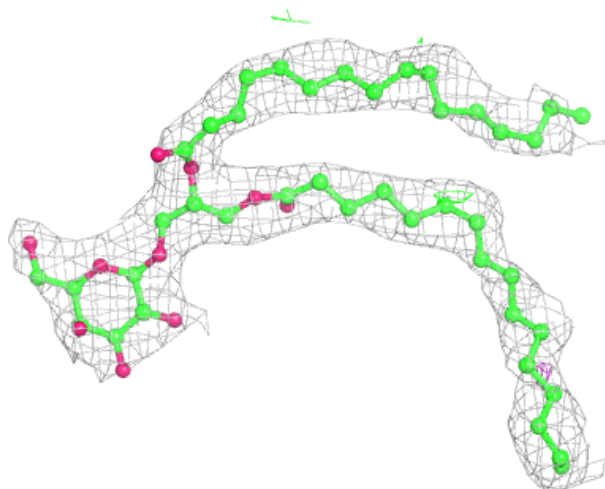
**Electron density around LMT t 102:**

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



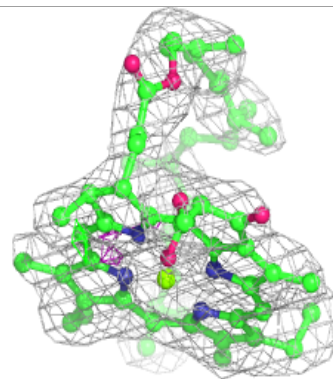
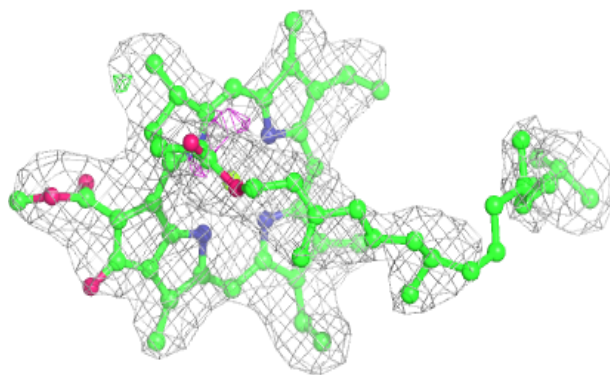
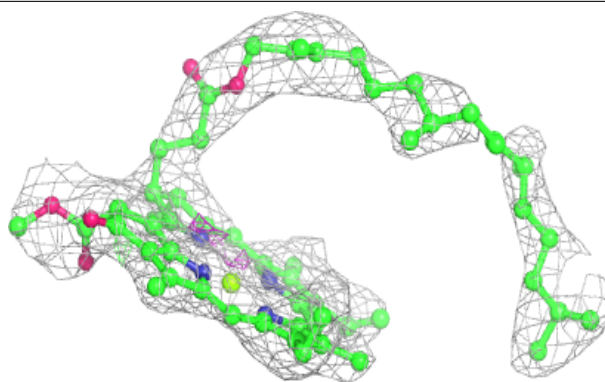
**Electron density around LMG C 520:**

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

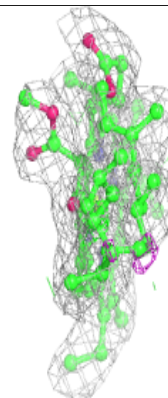
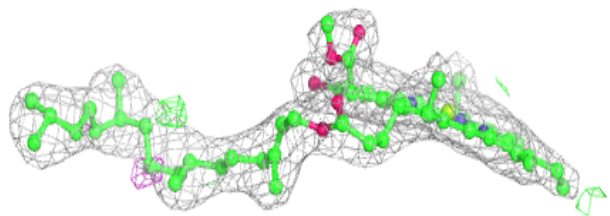
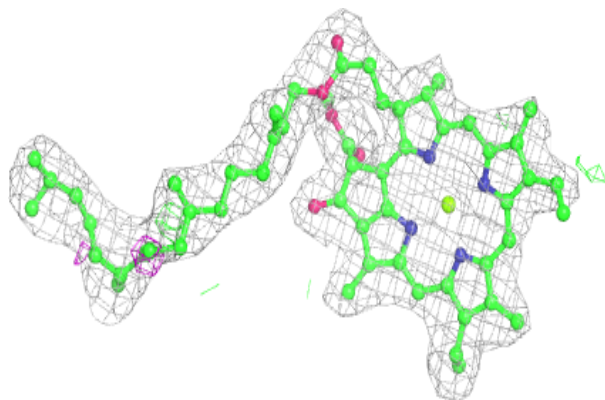


**Electron density around CLA C 514:**

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

**Electron density around CLA b 602:**

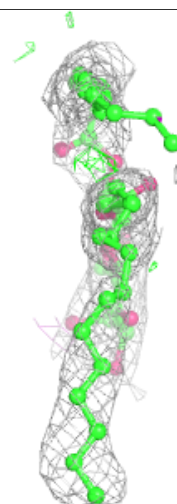
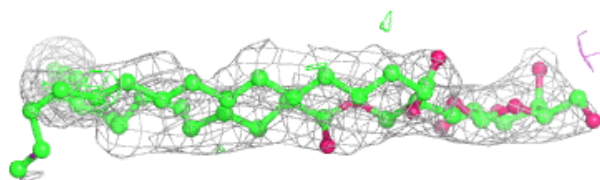
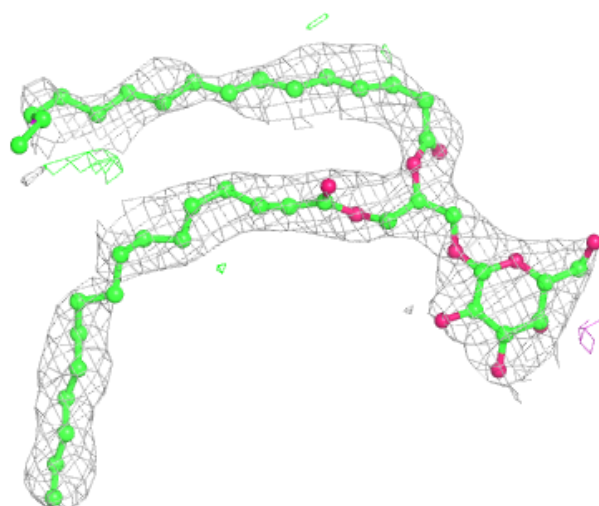
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





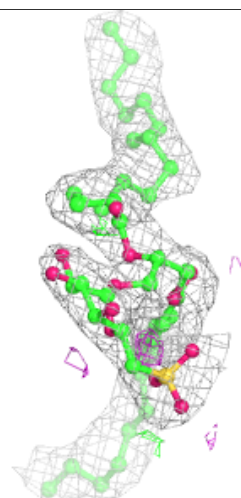
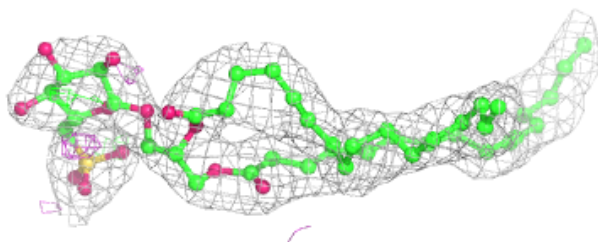
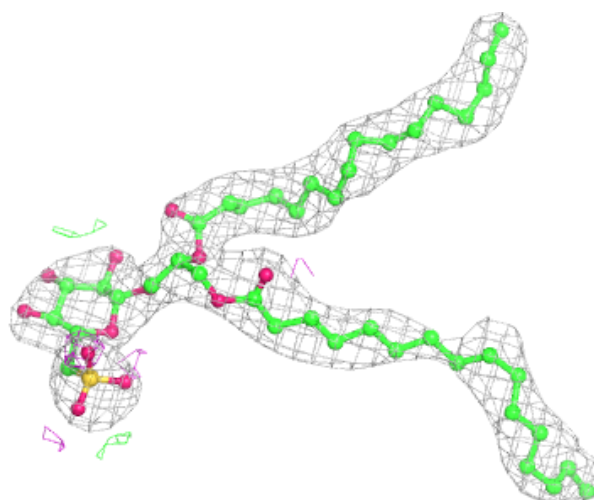
**Electron density around LMG c 520:**

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



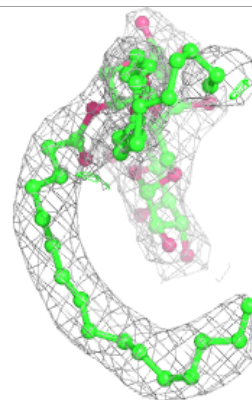
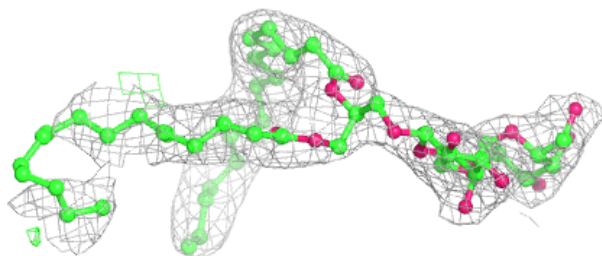
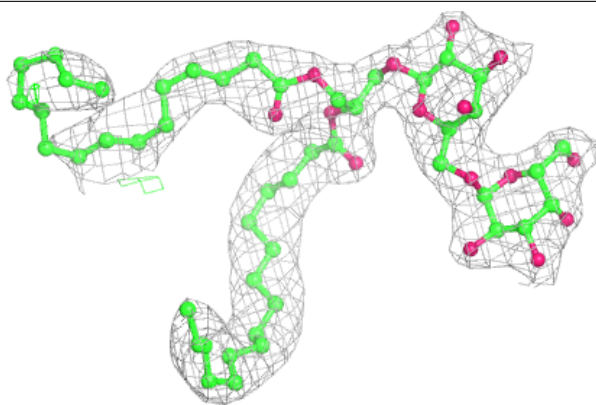
**Electron density around SQD A 410:**

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

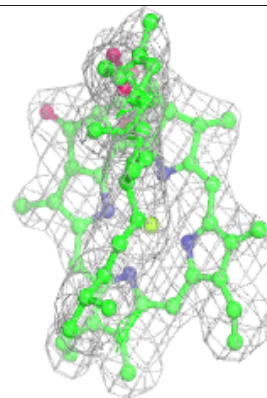
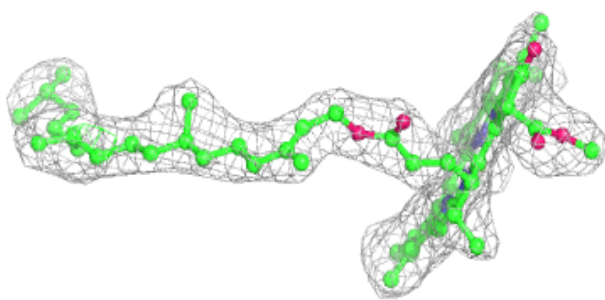
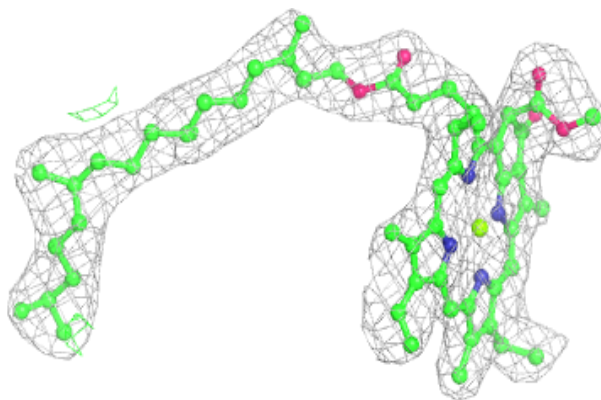


**Electron density around DGD C 518:**

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

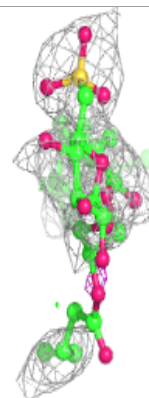
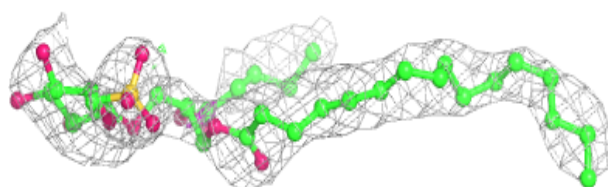
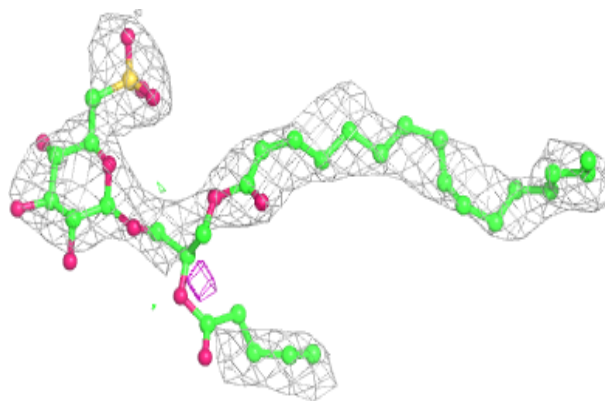
**Electron density around CLA B 609:**

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

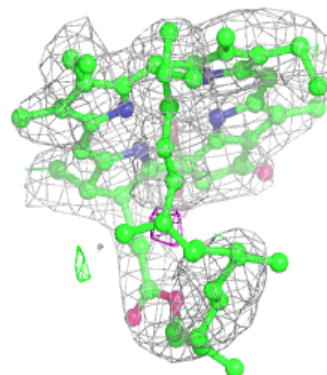
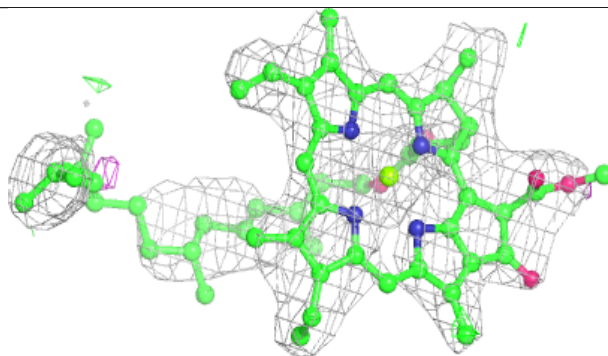
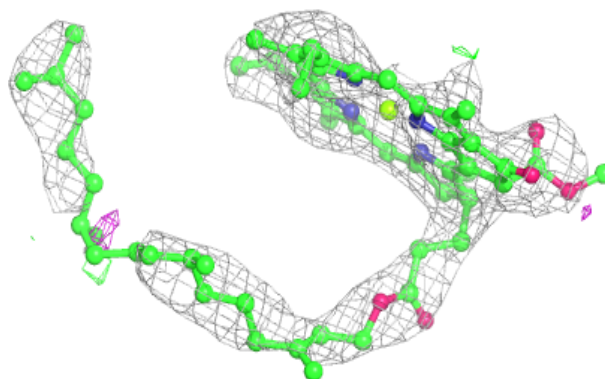


**Electron density around SQD F 101:**

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

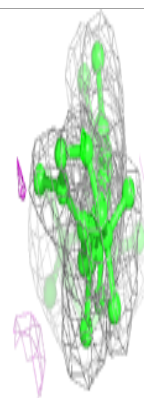
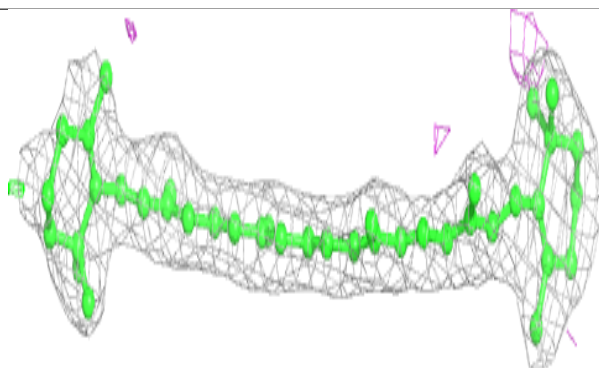
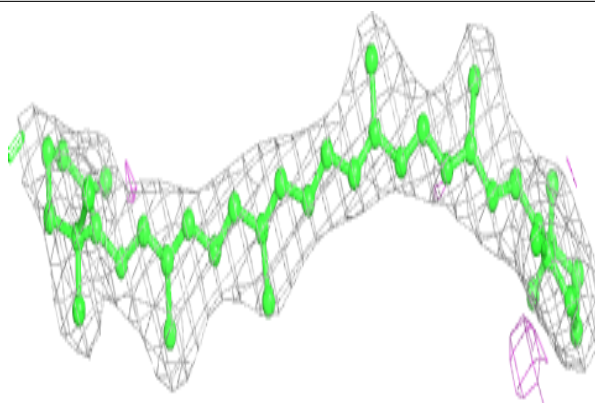
**Electron density around CLA c 514:**

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

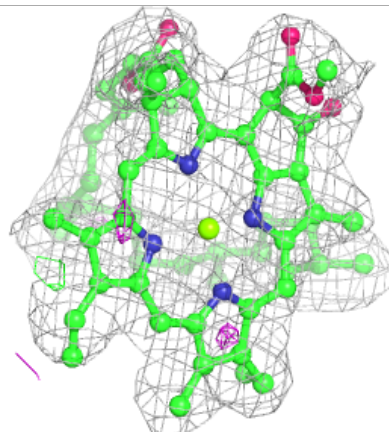
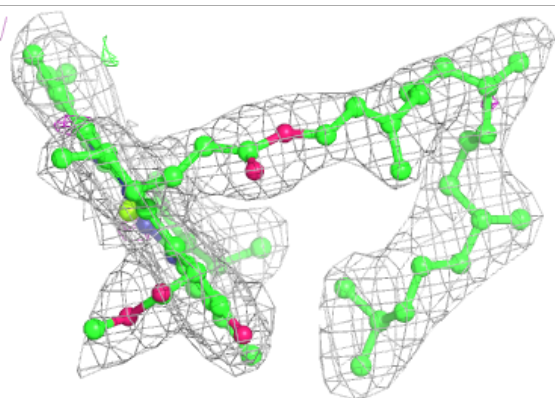
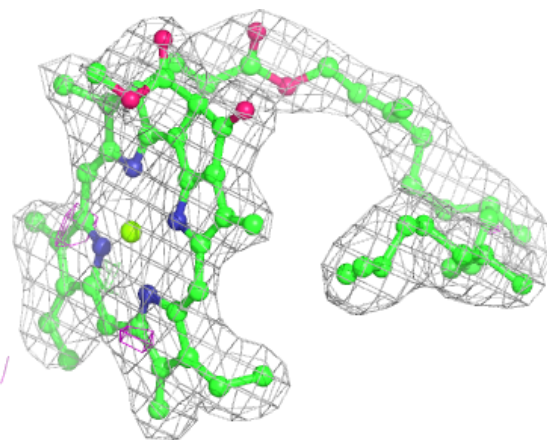


**Electron density around BCR h 101:**

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

**Electron density around CLA c 504:**

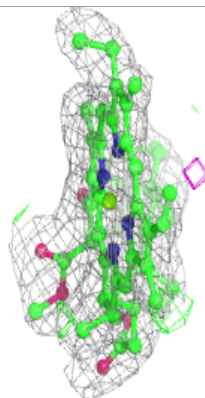
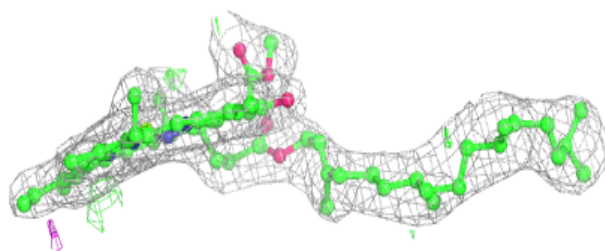
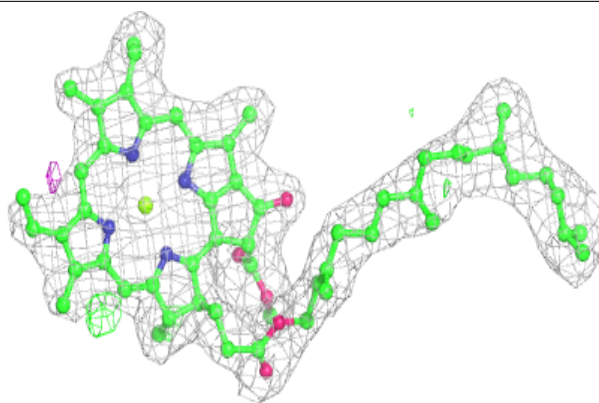
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



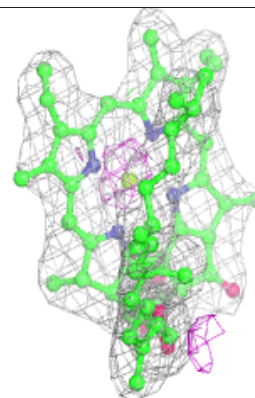
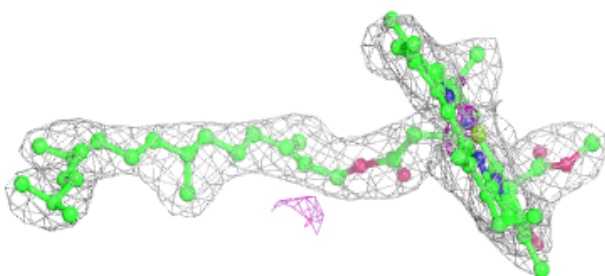
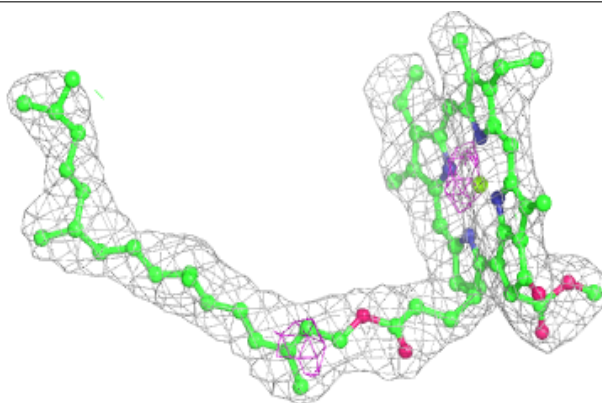


**Electron density around CLA B 602:**

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

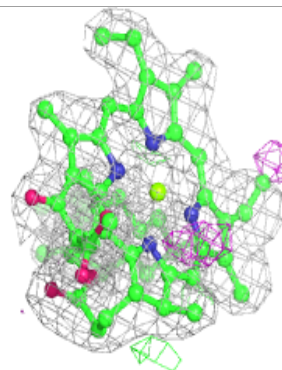
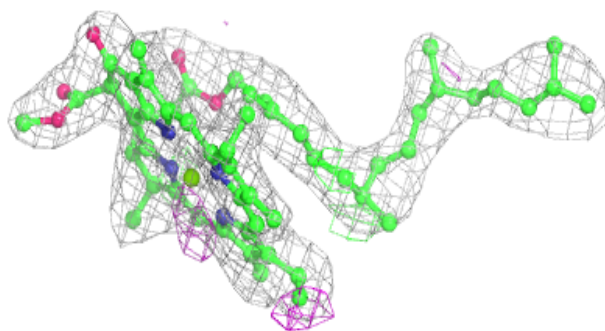
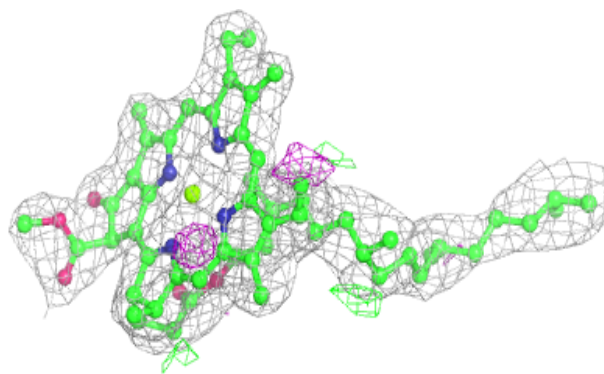
**Electron density around CLA b 609:**

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



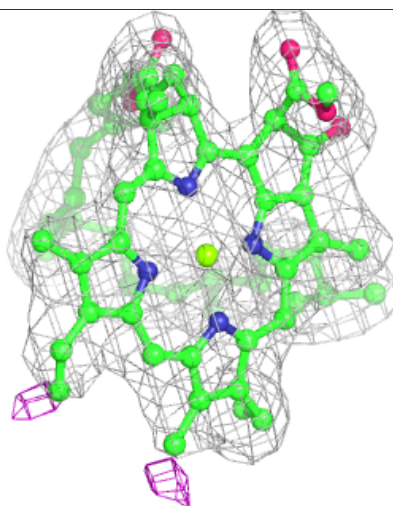
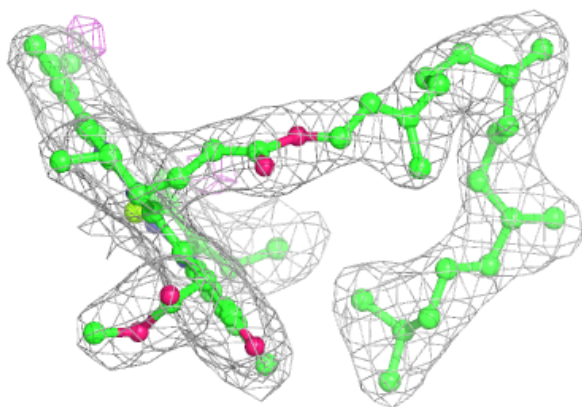
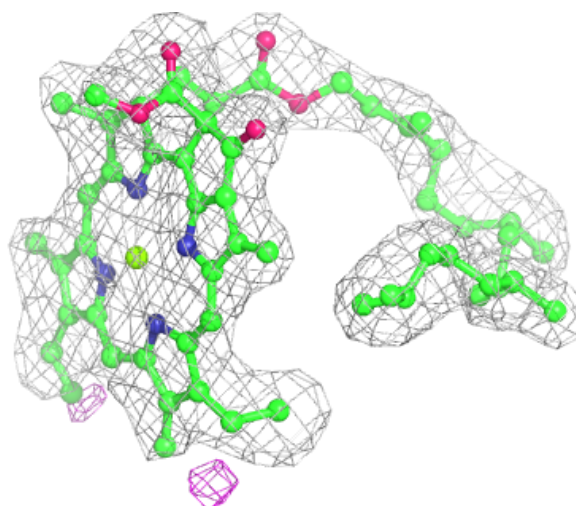
**Electron density around CLA c 506:**

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



**Electron density around CLA C 504:**

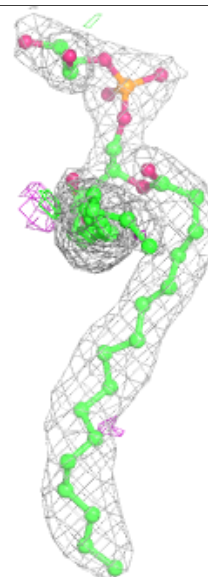
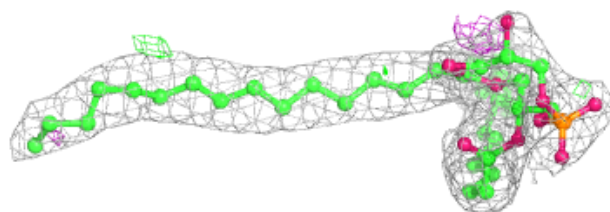
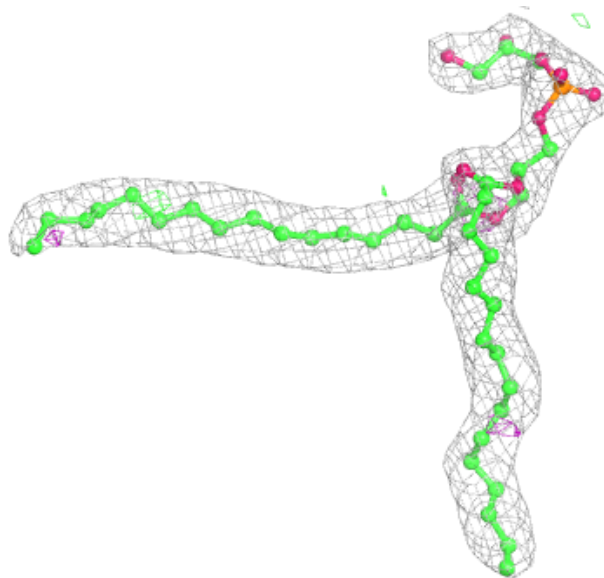
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





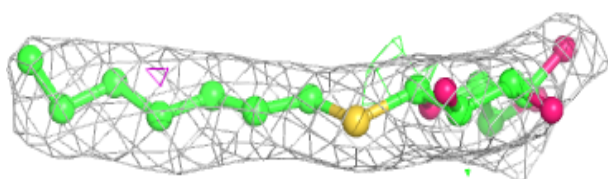
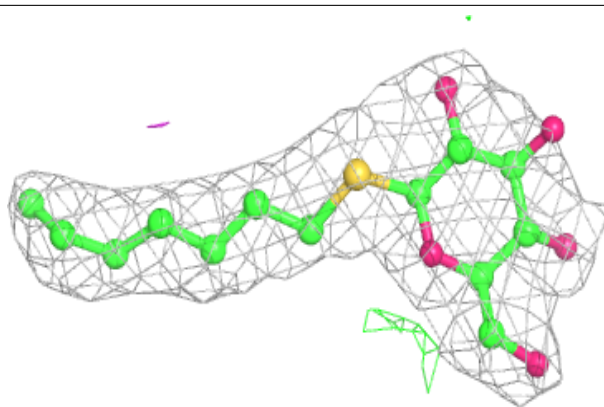
**Electron density around LHG 1 101:**

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

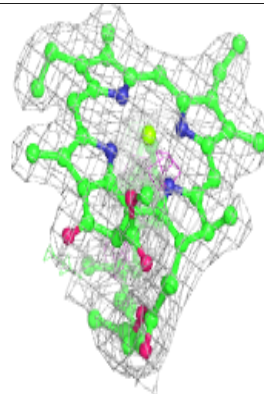
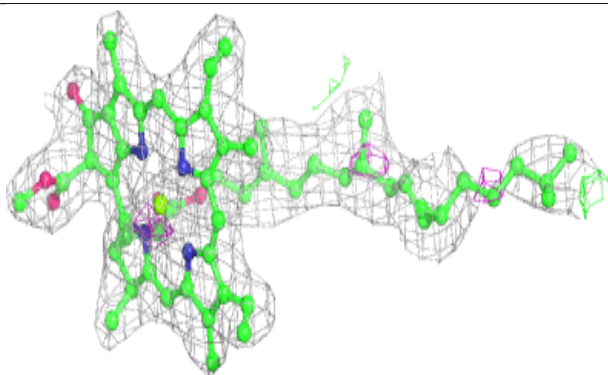
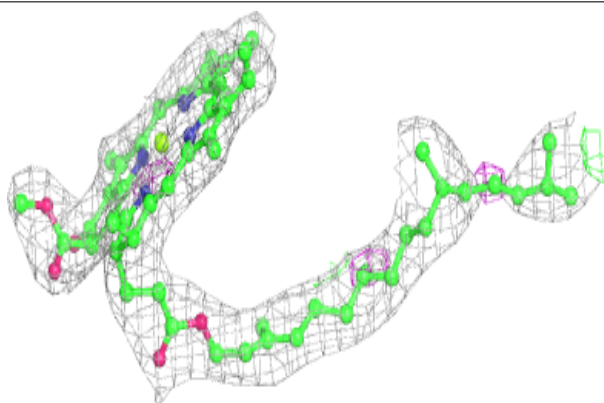


**Electron density around HTG B 626:**

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

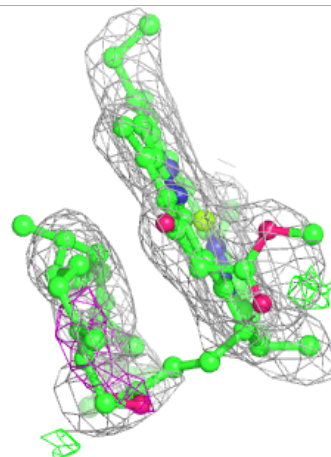
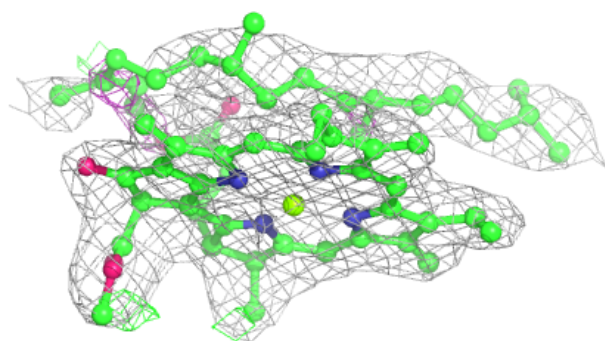
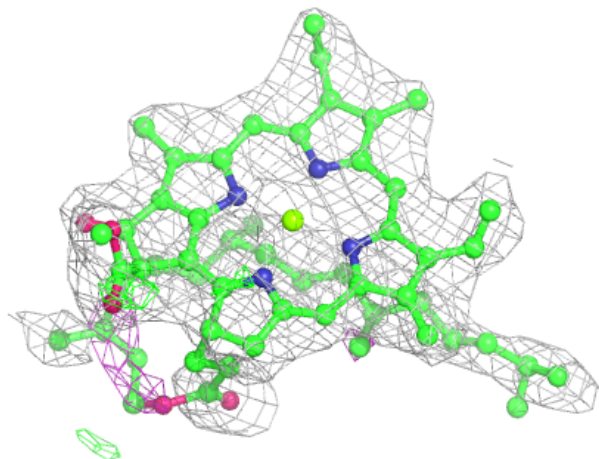
**Electron density around CLA C 505:**

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



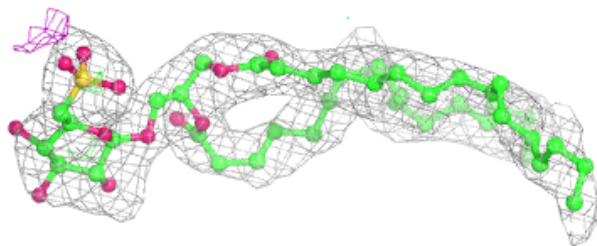
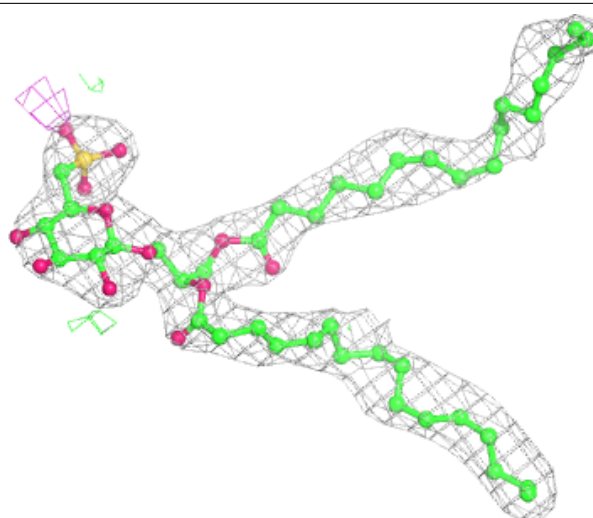
**Electron density around CLA b 601:**

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



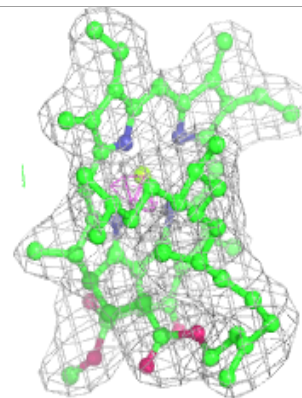
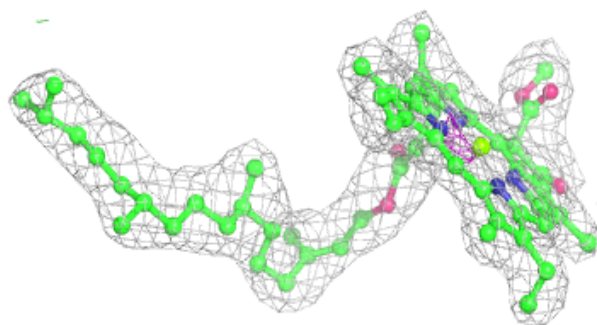
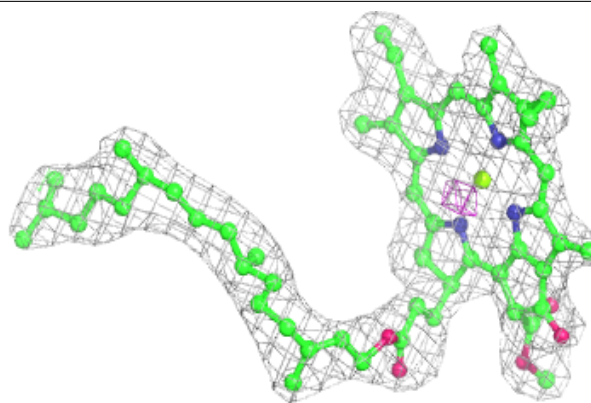
**Electron density around SQD a 411:**

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

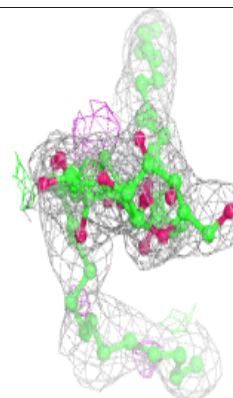
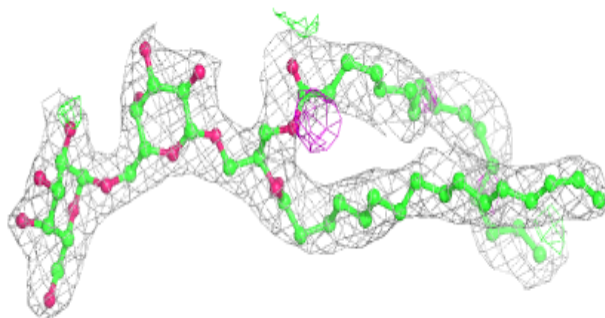
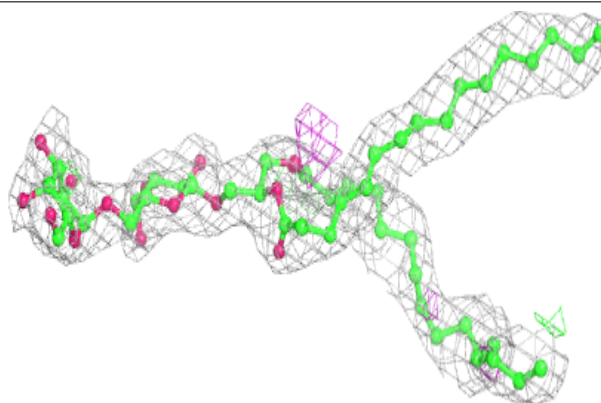


**Electron density around CLA C 512:**

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

**Electron density around DGD c 517:**

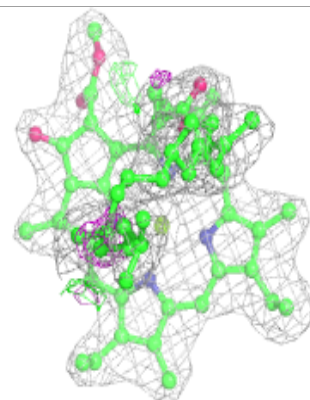
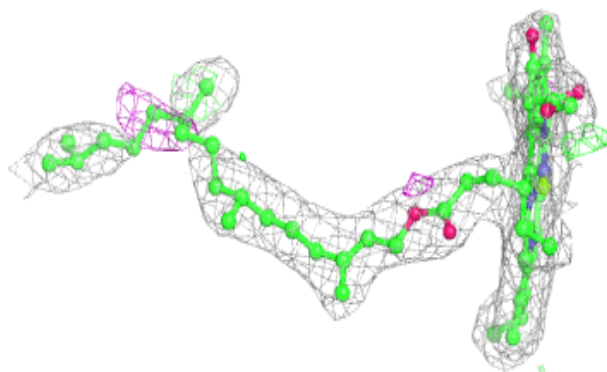
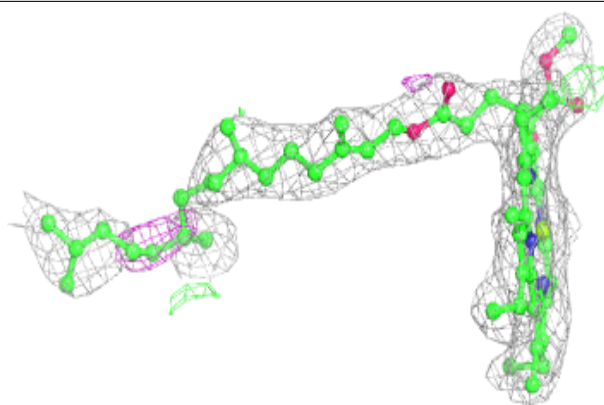
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



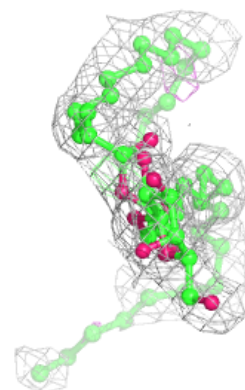
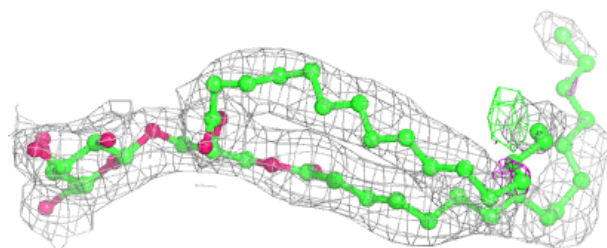
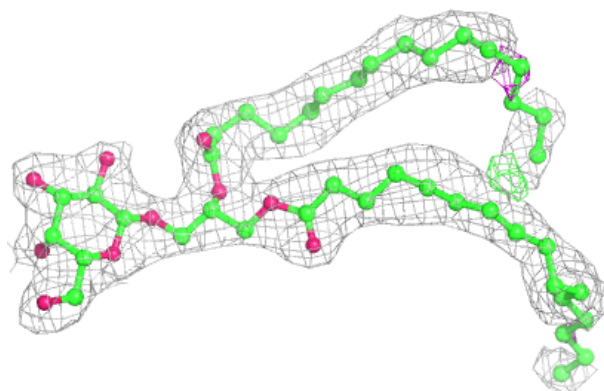


**Electron density around CLA B 606:**

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

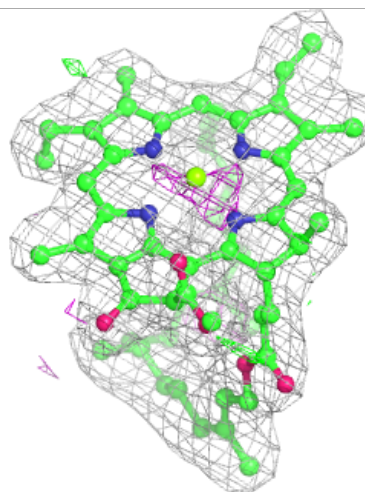
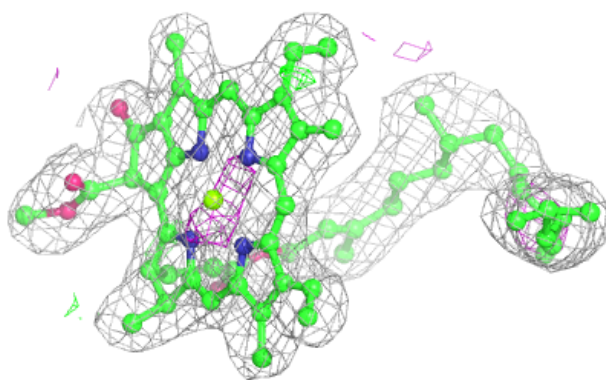
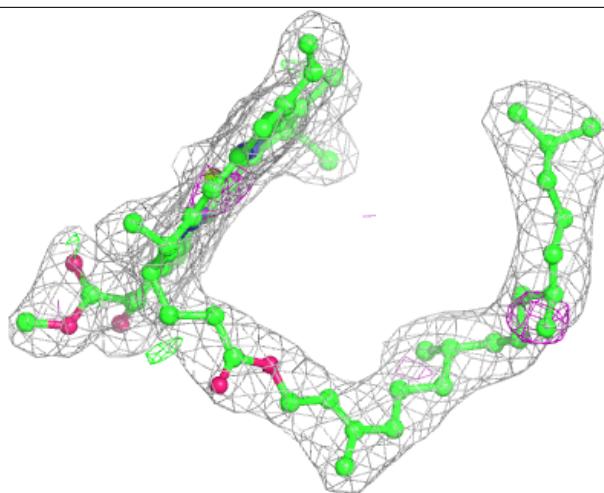
**Electron density around LMG D 415:**

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



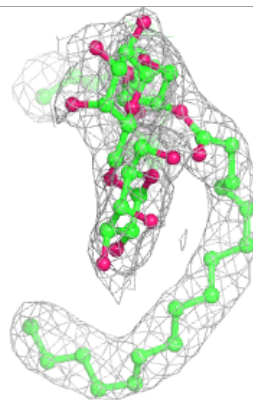
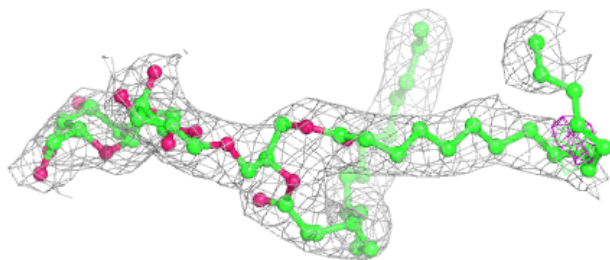
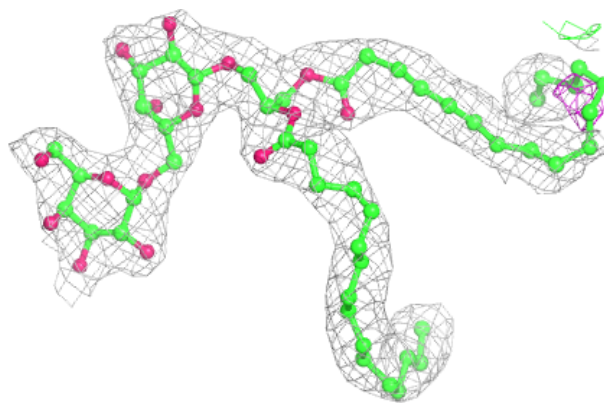
**Electron density around CLA B 611:**

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



**Electron density around DGD c 518:**

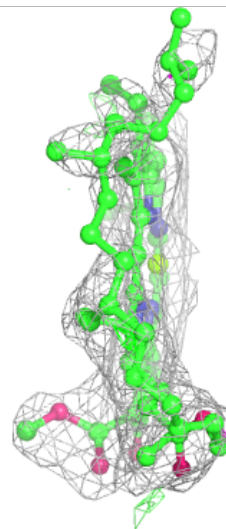
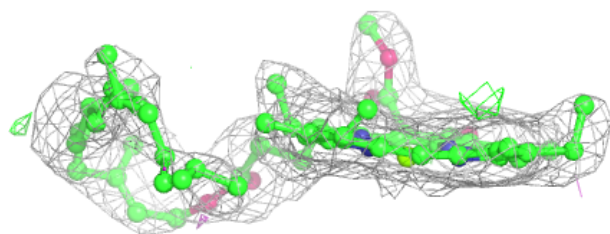
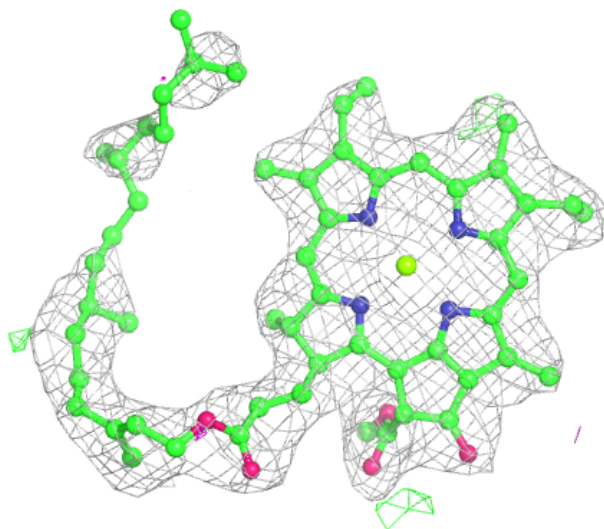
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





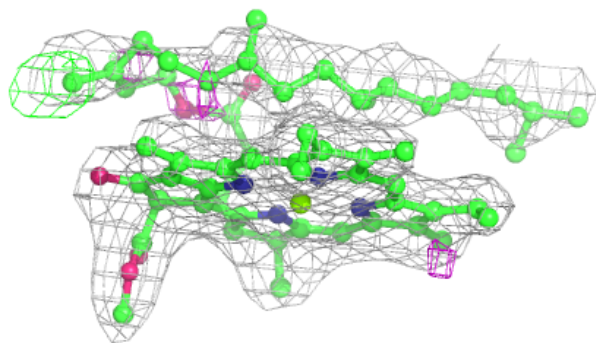
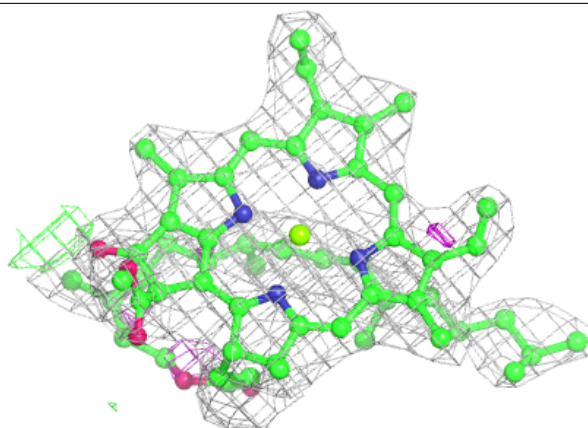
**Electron density around CLA c 513:**

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

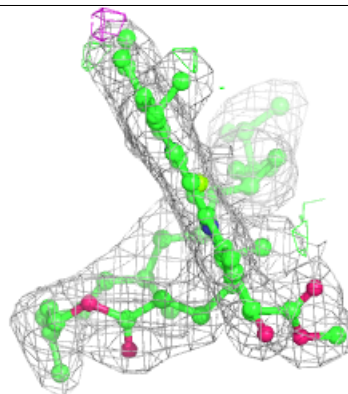
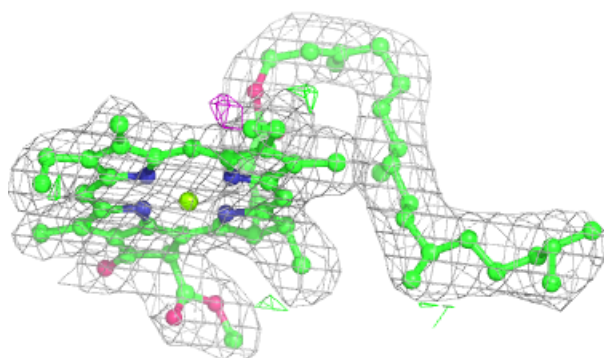
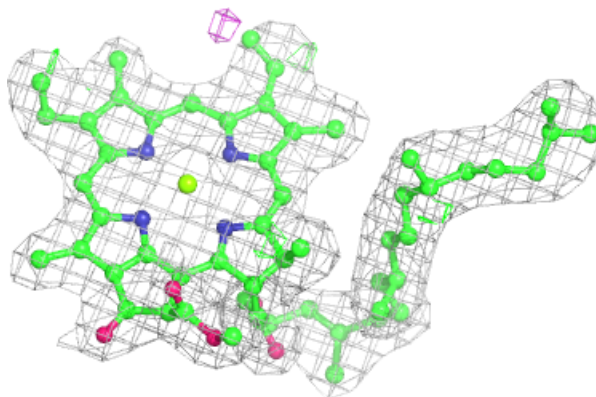


**Electron density around CLA B 601:**

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

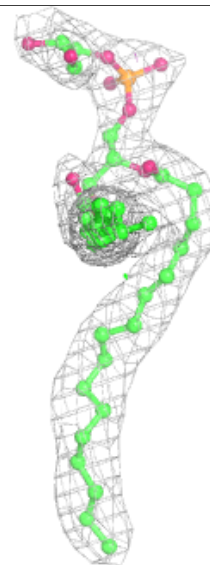
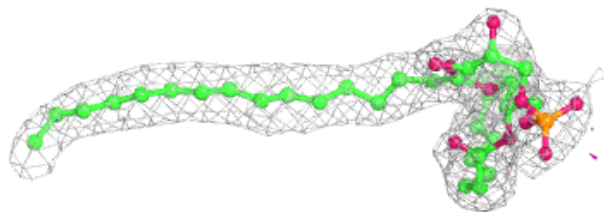
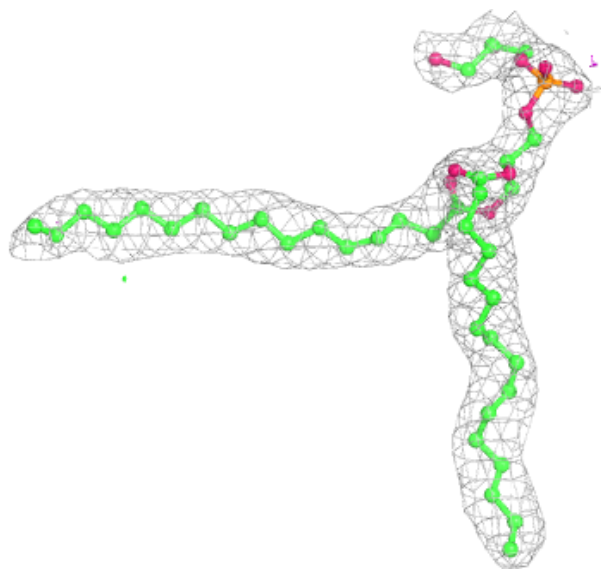
**Electron density around CLA a 406:**

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



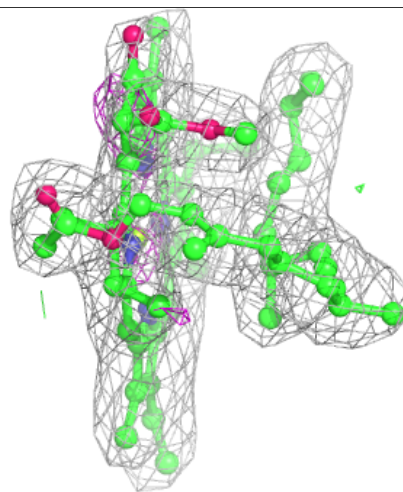
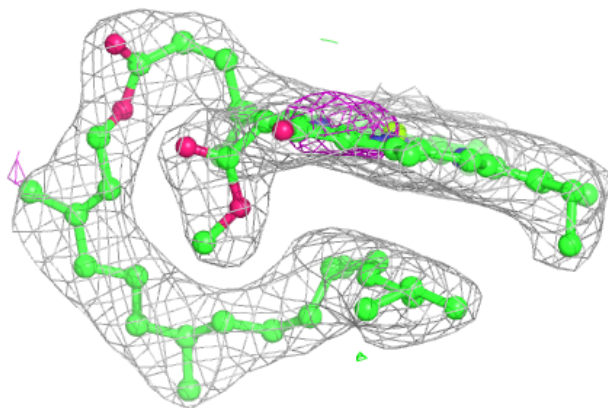
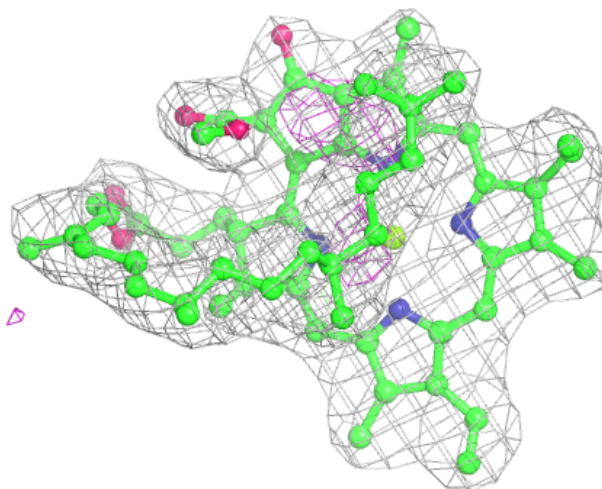
**Electron density around LHG L 101:**

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



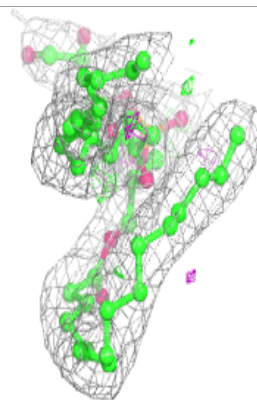
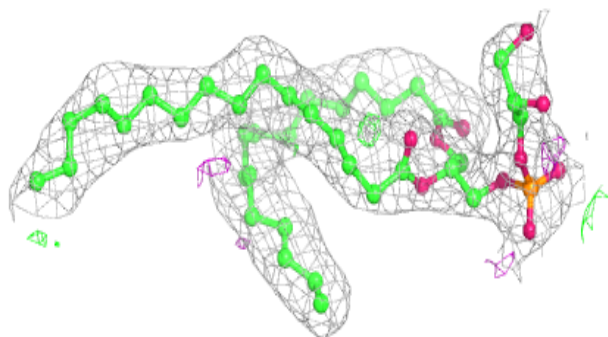
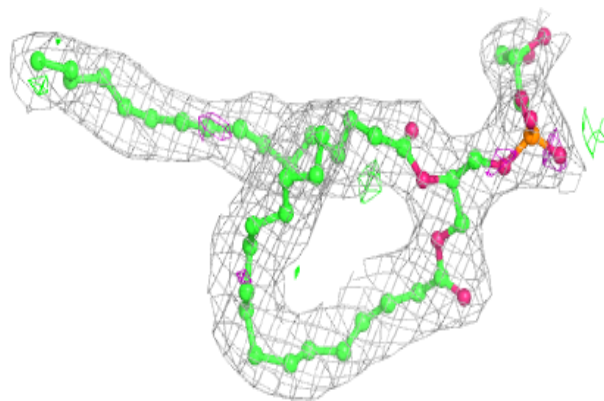
**Electron density around CLA c 511:**

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

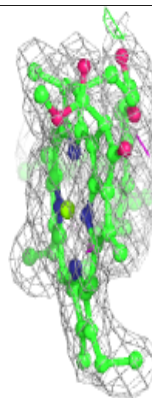
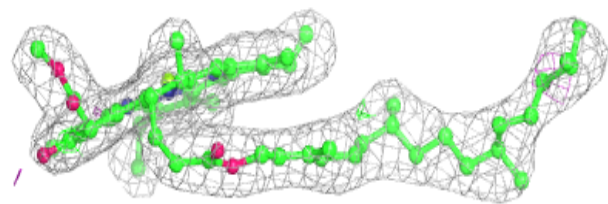
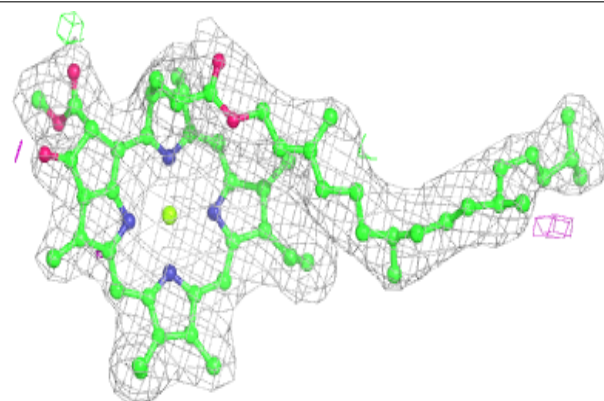


**Electron density around LHG D 409:**

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

**Electron density around CLA b 603:**

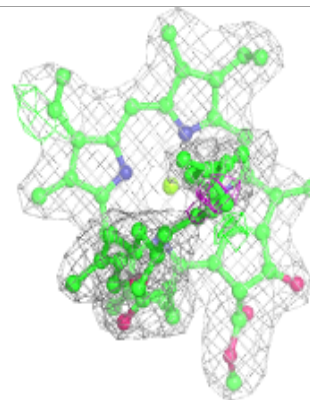
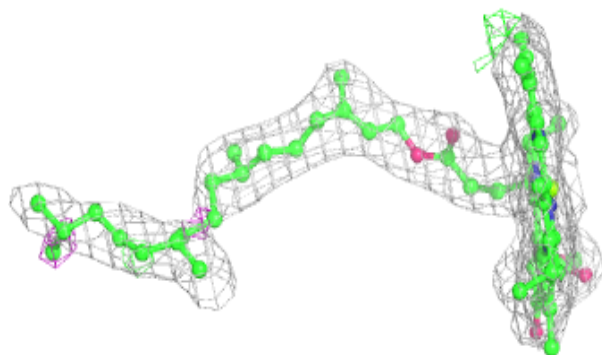
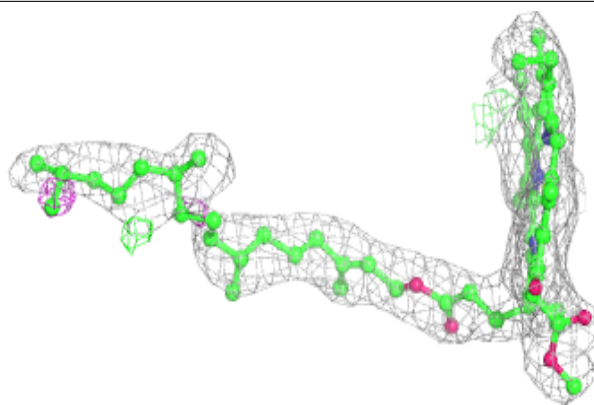
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





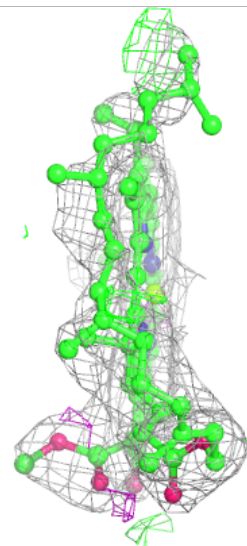
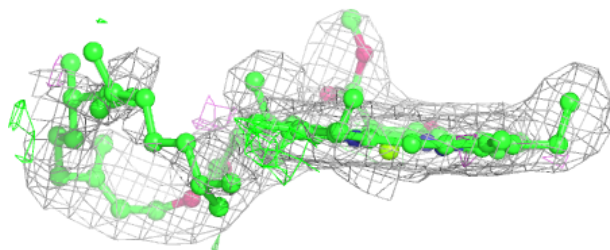
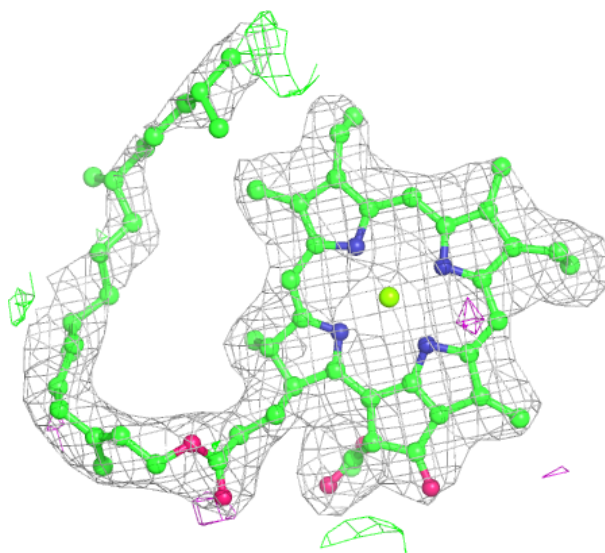
**Electron density around CLA b 606:**

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



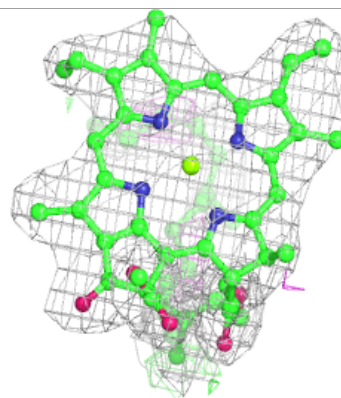
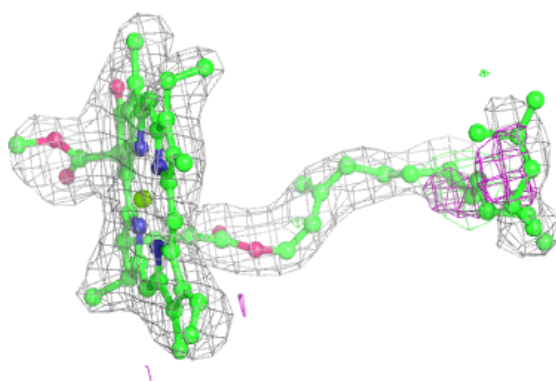
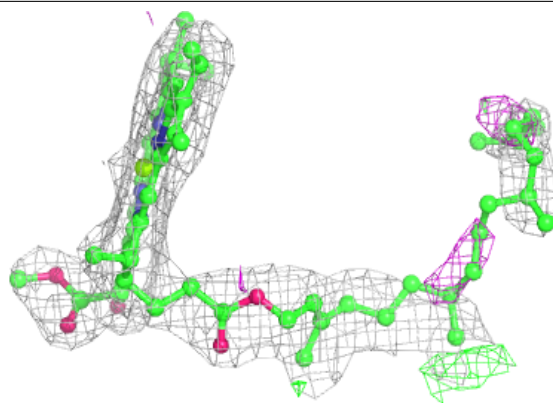
**Electron density around CLA C 513:**

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

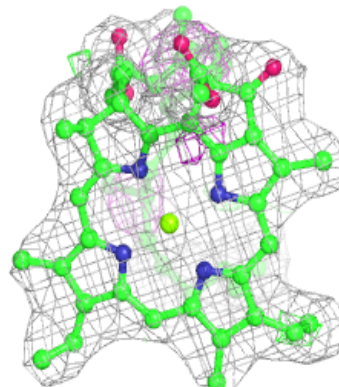
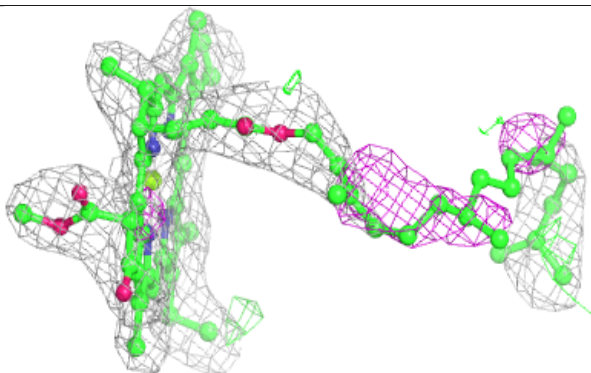
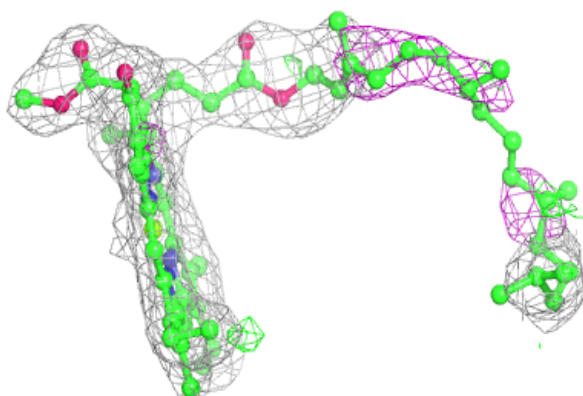


**Electron density around CLA c 507:**

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

**Electron density around CLA C 507:**

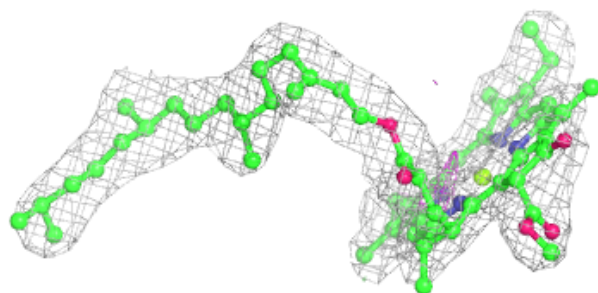
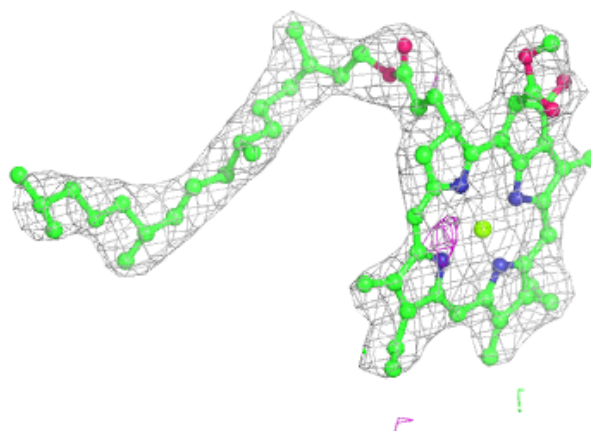
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



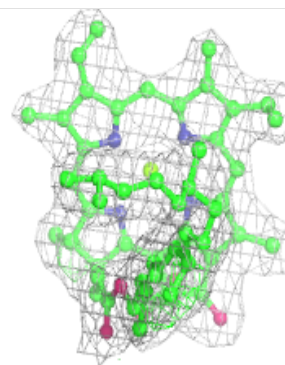
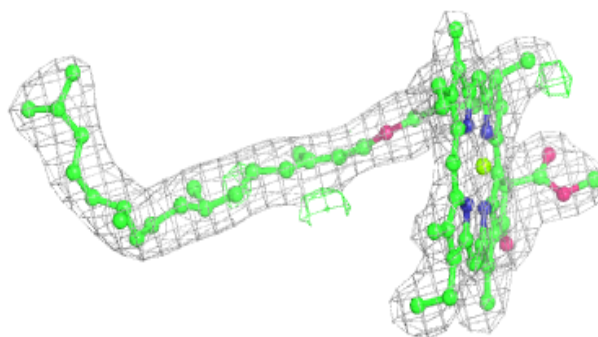
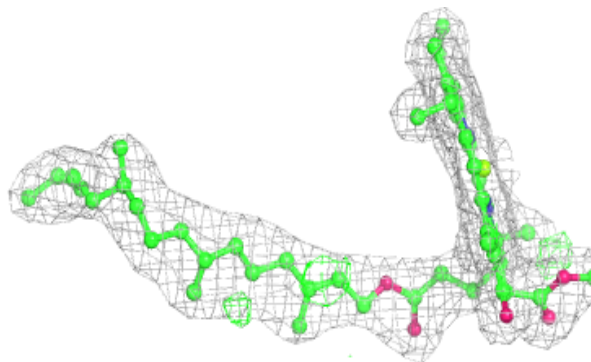


**Electron density around CLA c 512:**

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

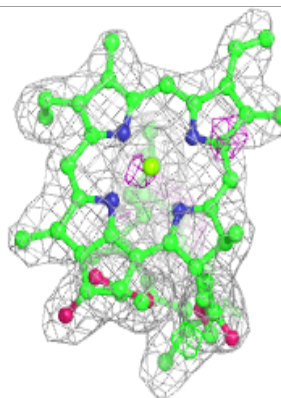
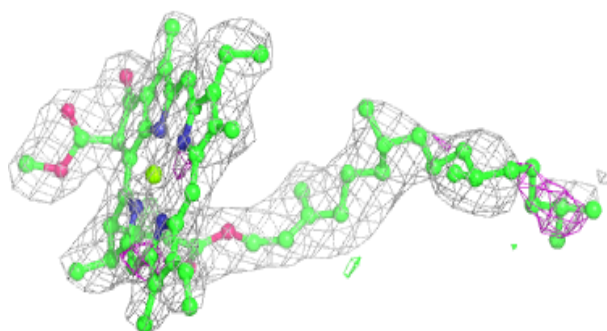
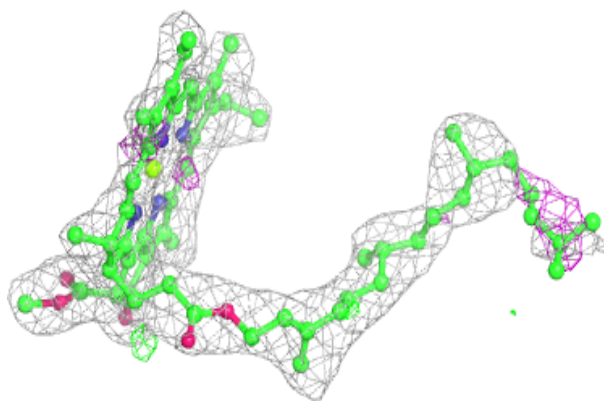
**Electron density around CLA B 605:**

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

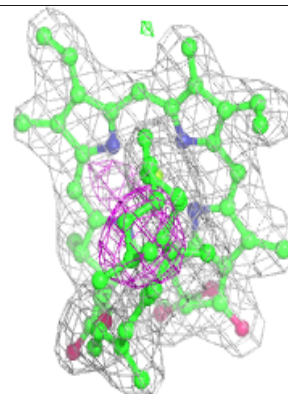
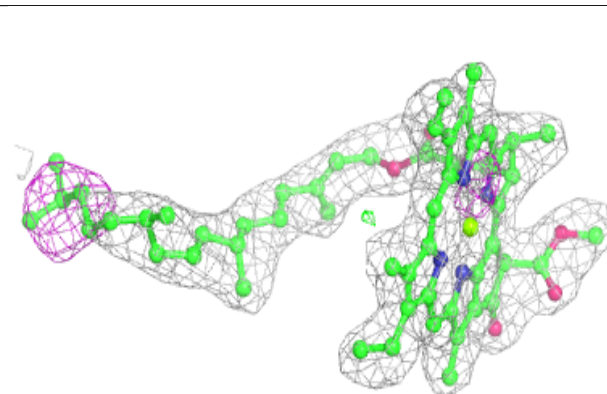
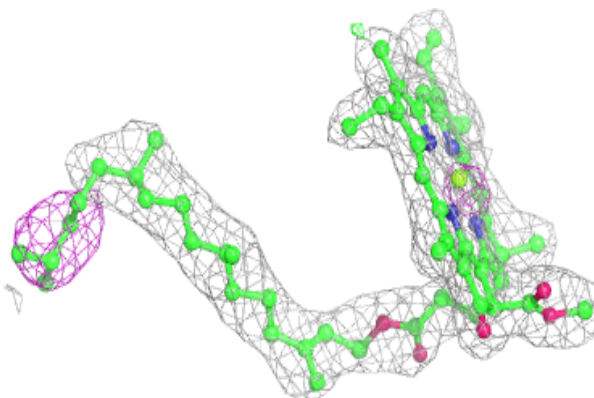


**Electron density around CLA c 509:**

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

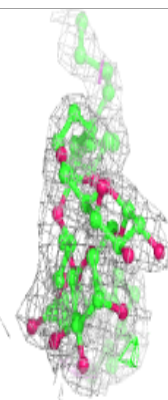
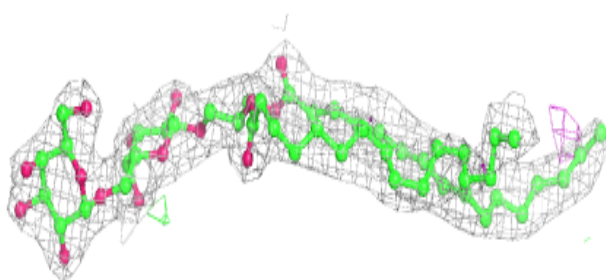
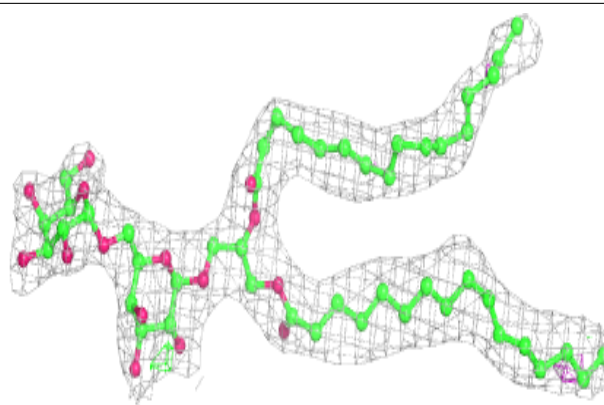
**Electron density around CLA C 509:**

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

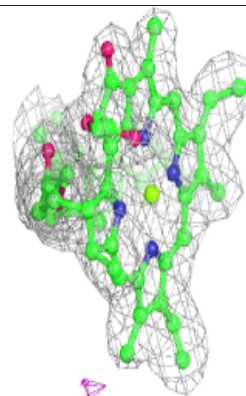
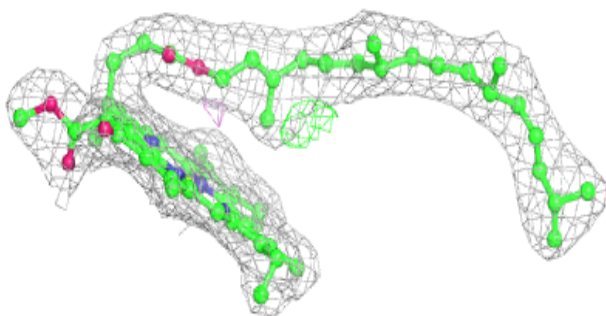
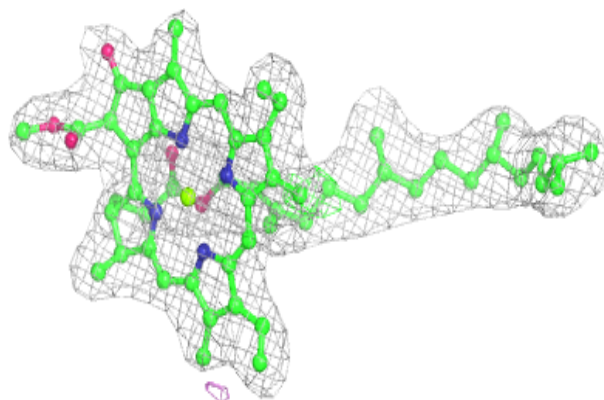


**Electron density around DGD C 519:**

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

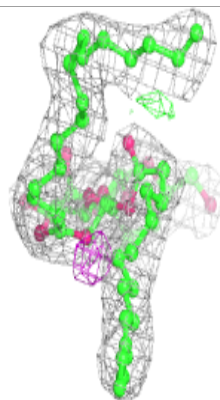
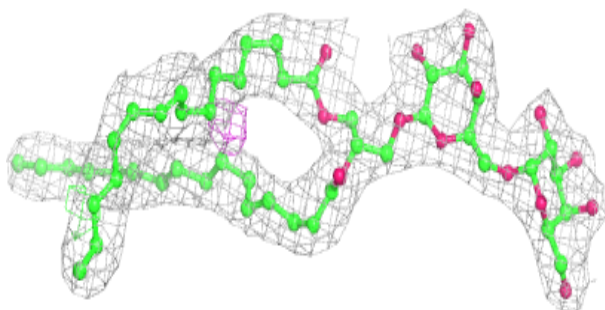
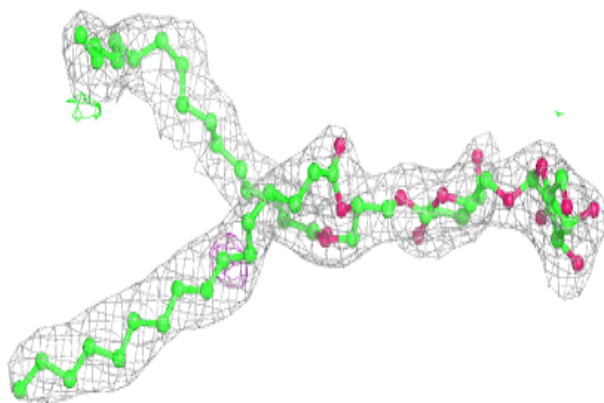
**Electron density around CLA B 608:**

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



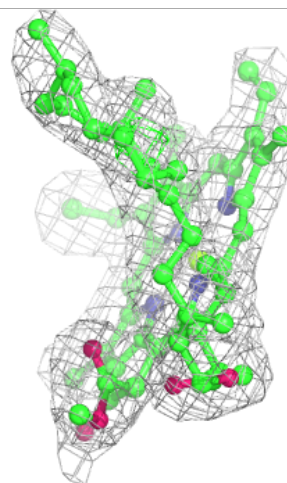
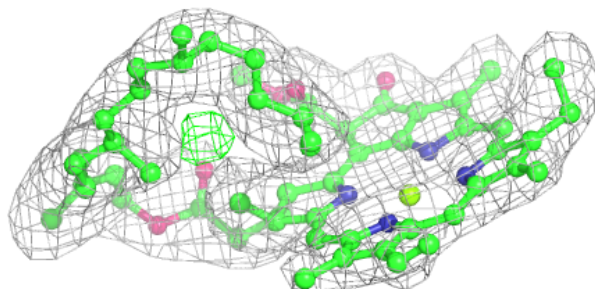
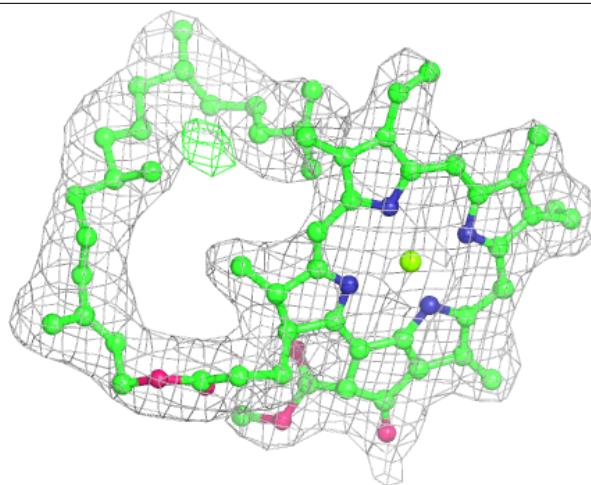
**Electron density around DGD C 517:**

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



**Electron density around CLA b 615:**

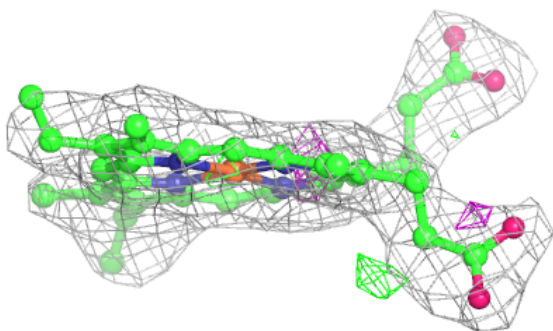
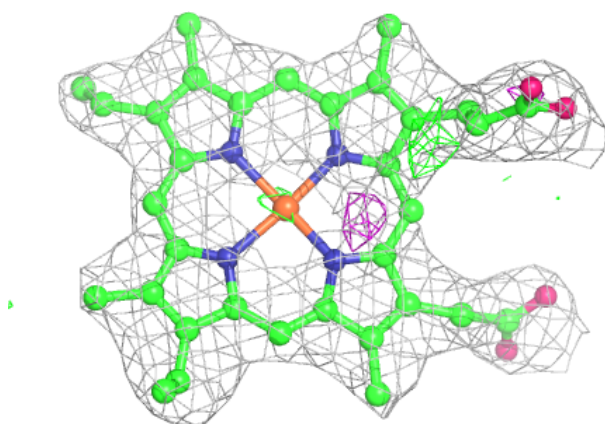
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





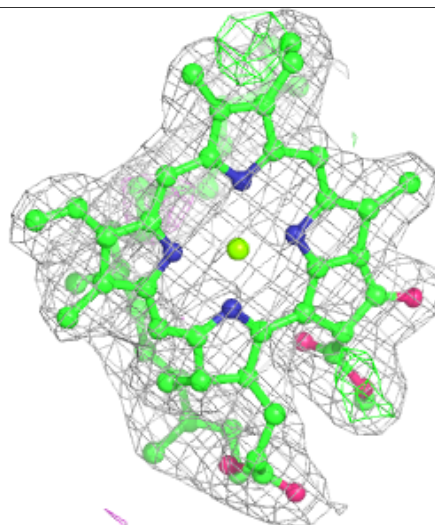
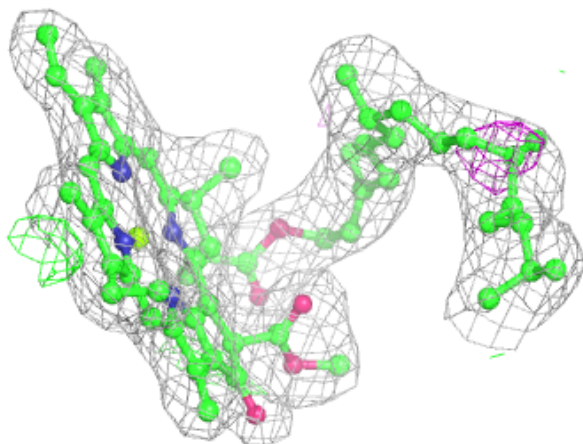
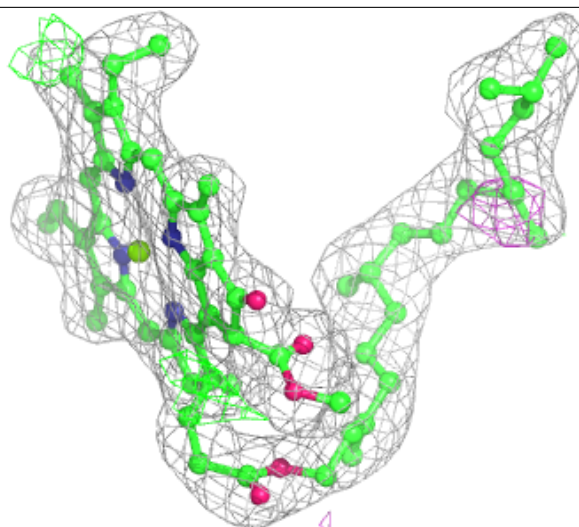
**Electron density around HEM E 103:**

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



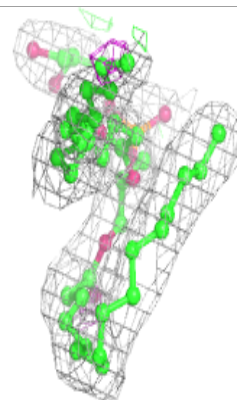
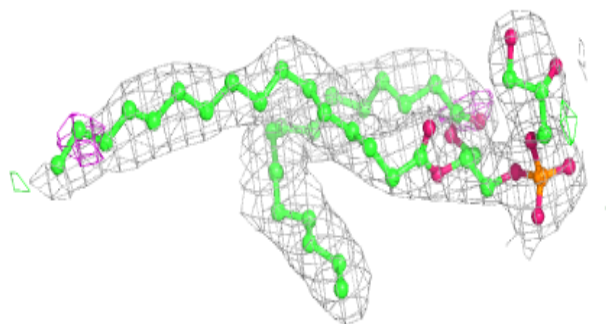
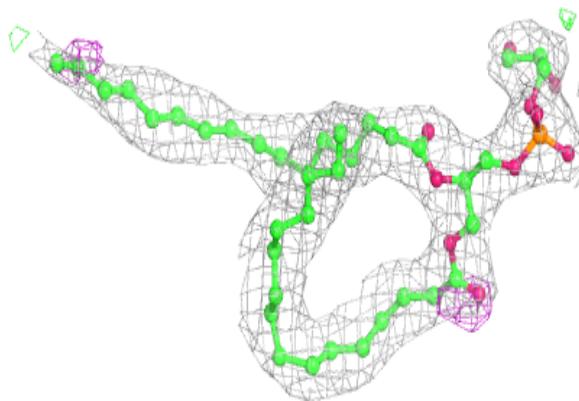
**Electron density around CLA B 613:**

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



**Electron density around LHG d 406:**

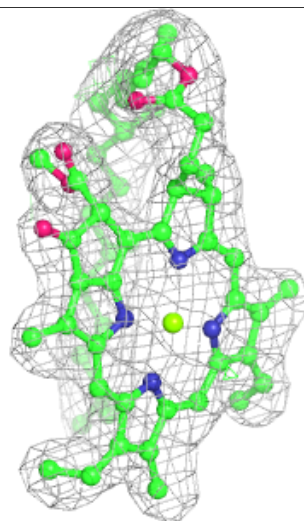
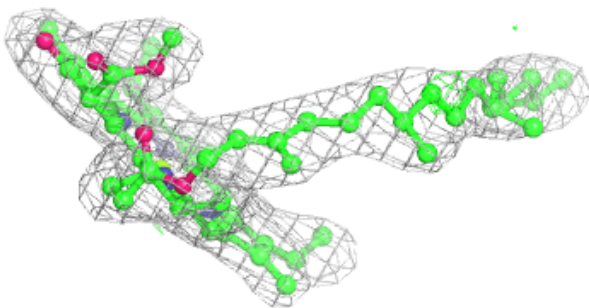
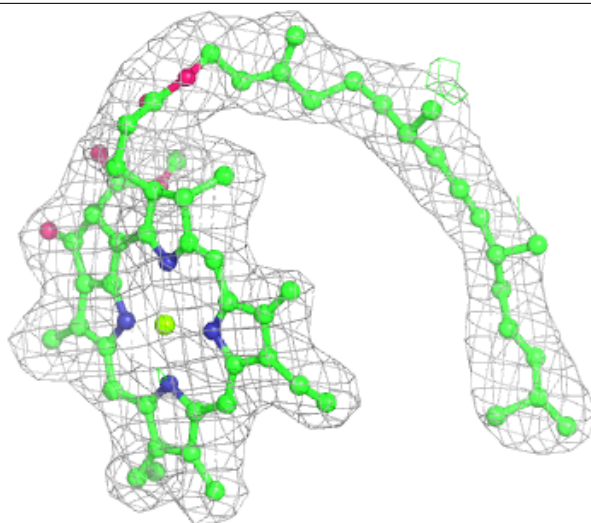
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





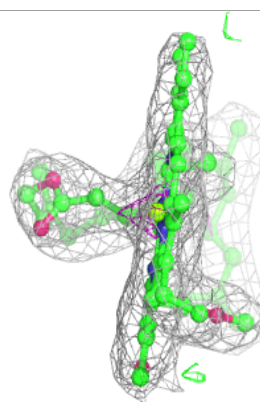
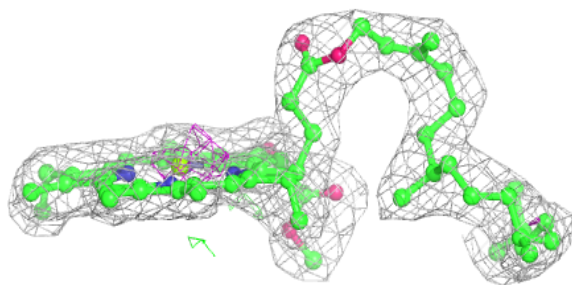
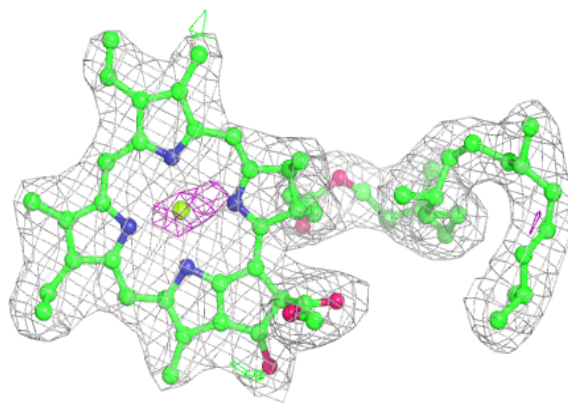
**Electron density around CLA C 508:**

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

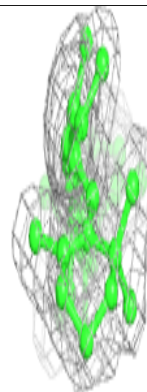
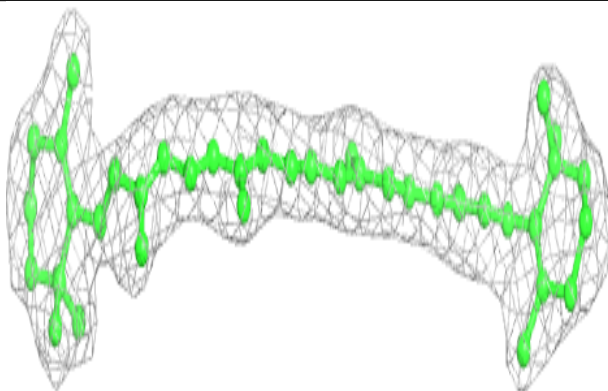
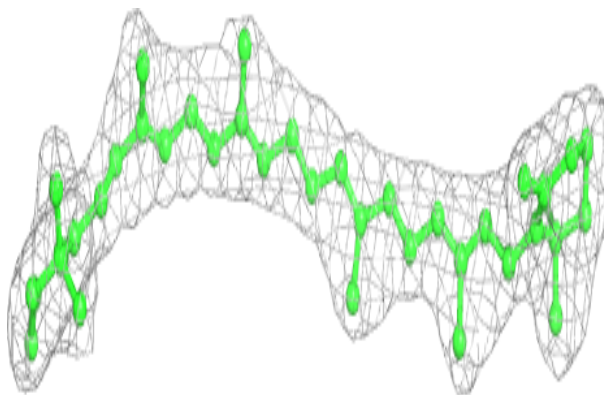


**Electron density around CLA B 612:**

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

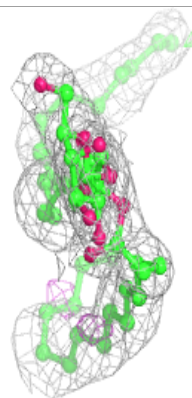
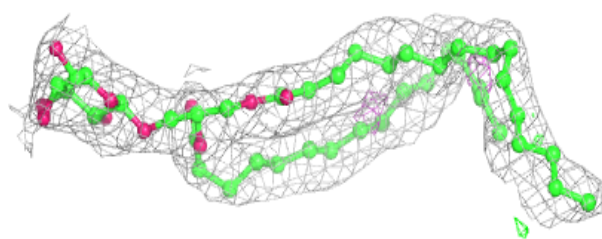
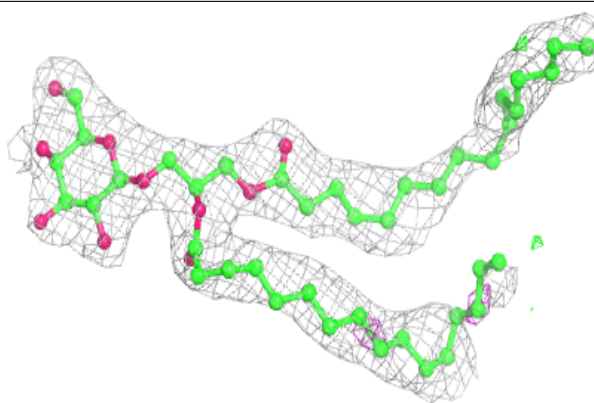
**Electron density around BCR H 101:**

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

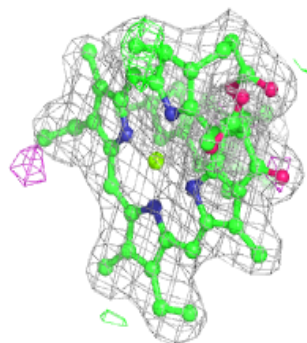
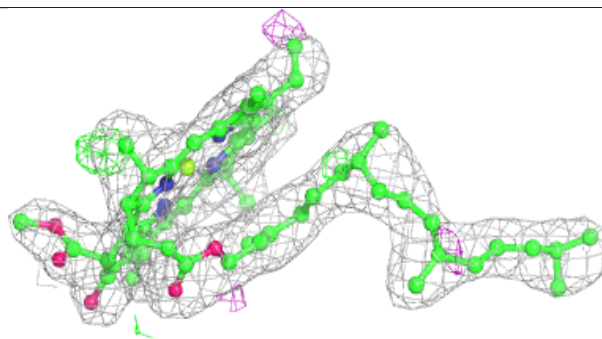
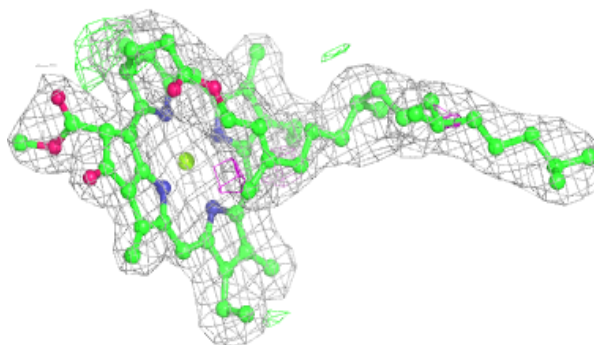


**Electron density around LMG d 412:**

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

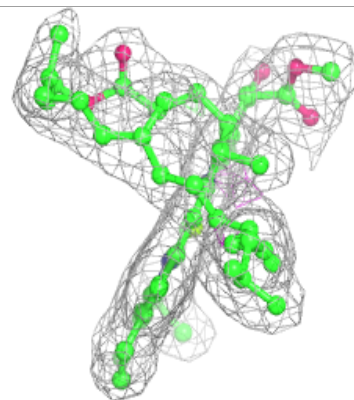
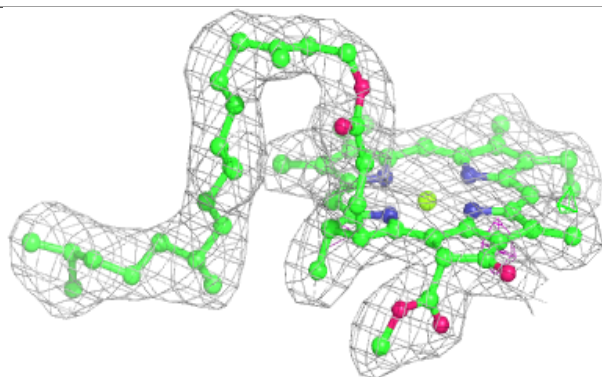
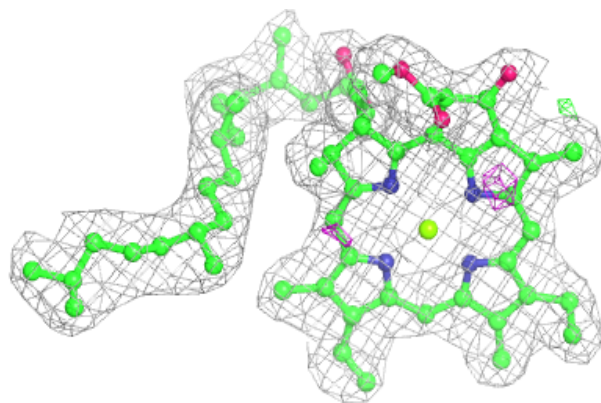
**Electron density around CLA C 506:**

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

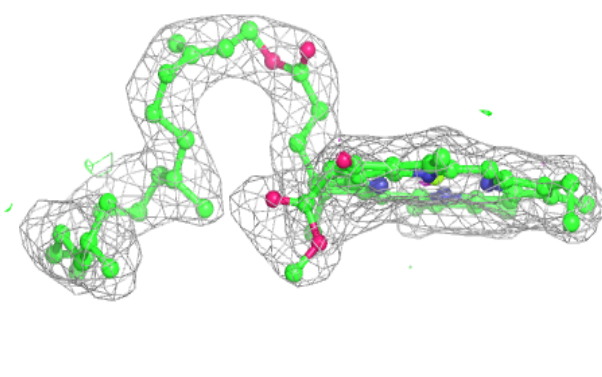
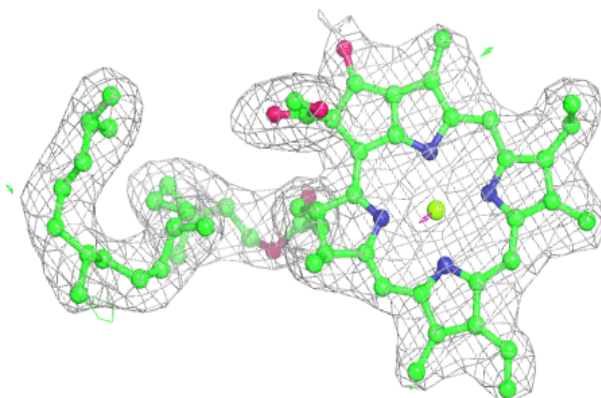


**Electron density around CLA A 405:**

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

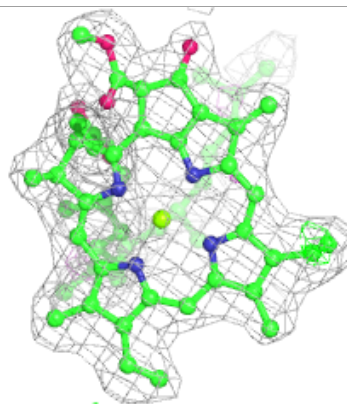
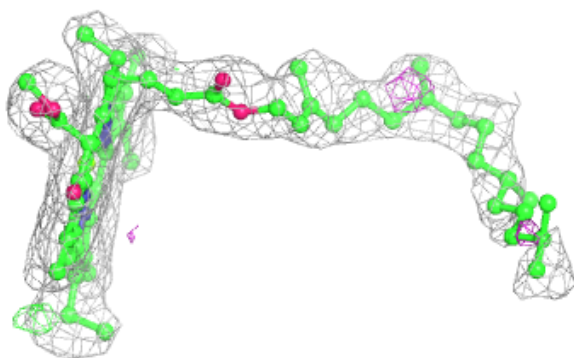
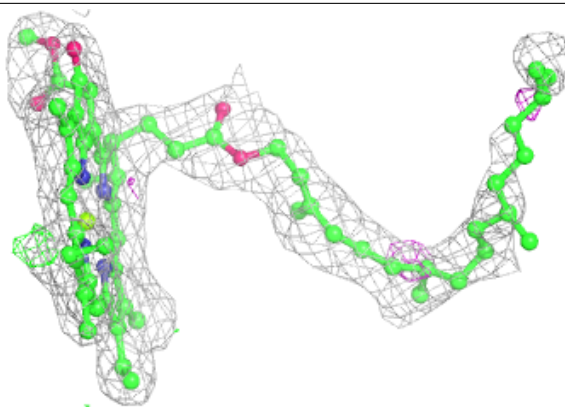
**Electron density around CLA b 612:**

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



**Electron density around CLA D 406:**

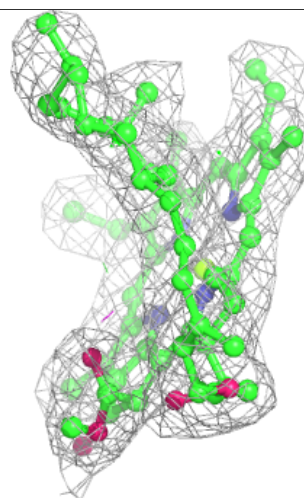
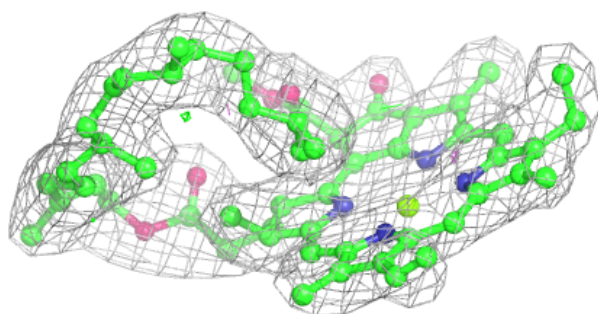
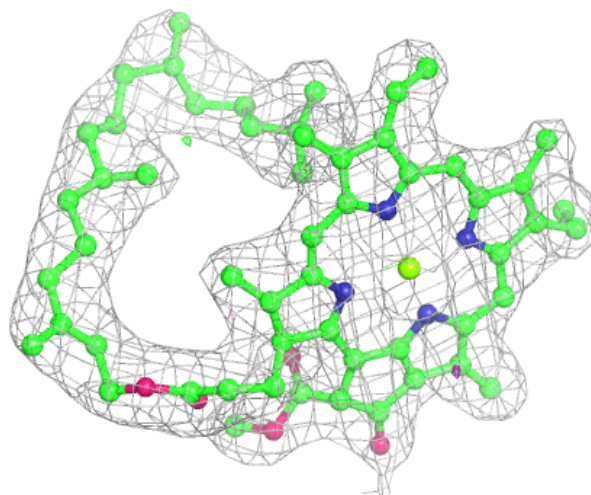
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





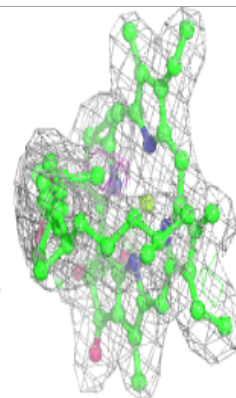
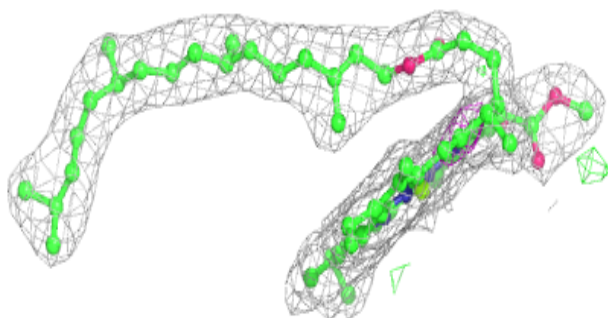
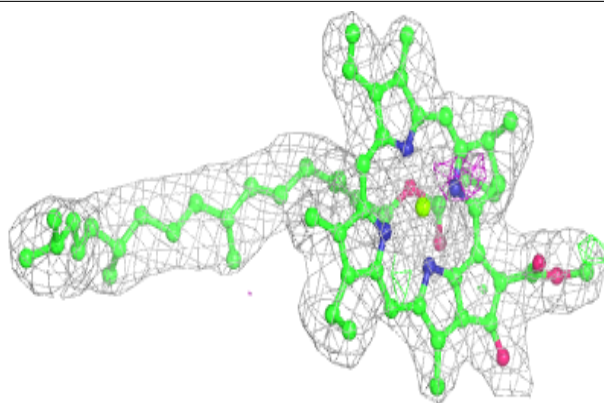
**Electron density around CLA B 615:**

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



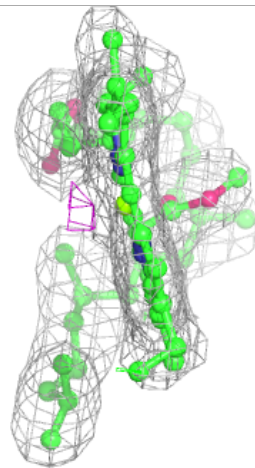
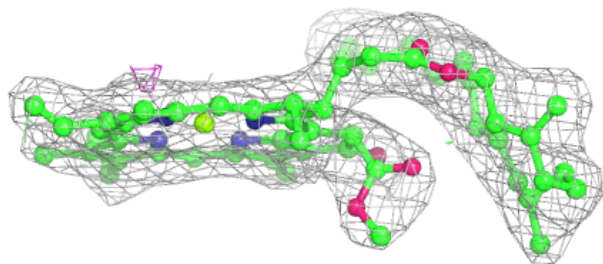
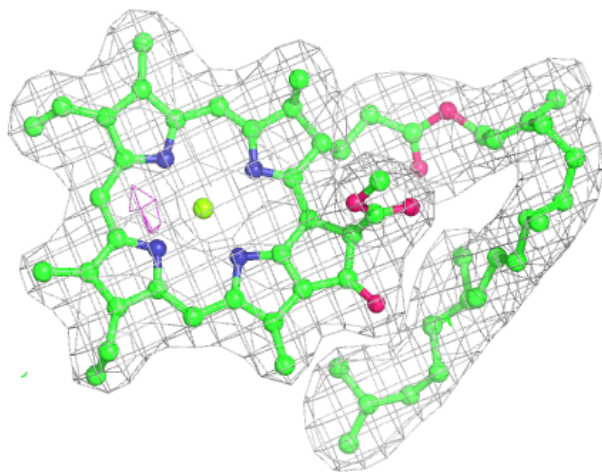
**Electron density around CLA b 608:**

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



**Electron density around CLA b 610:**

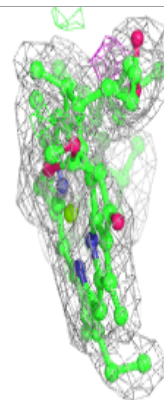
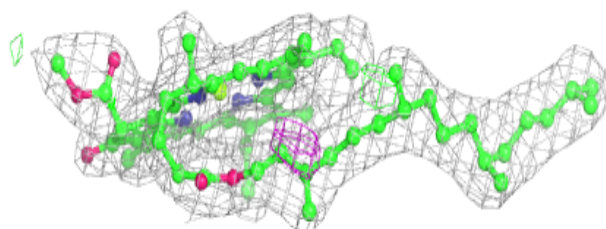
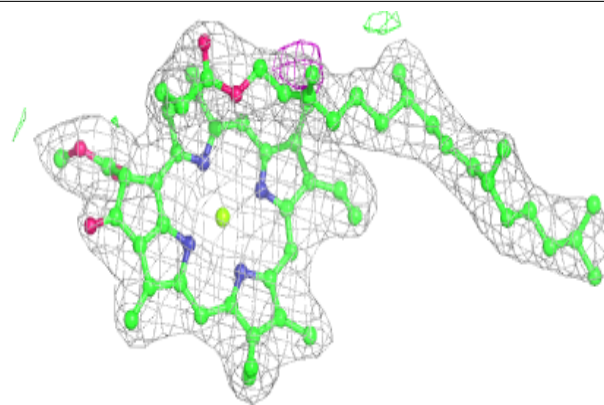
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





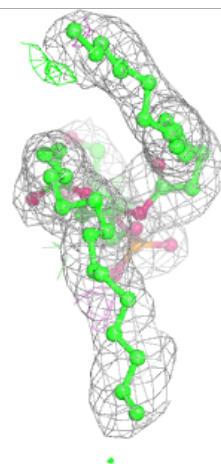
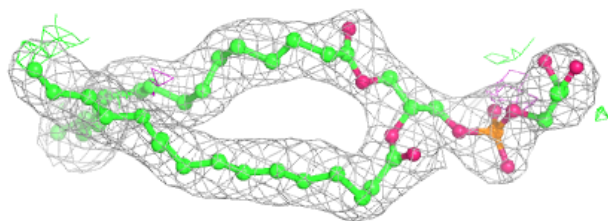
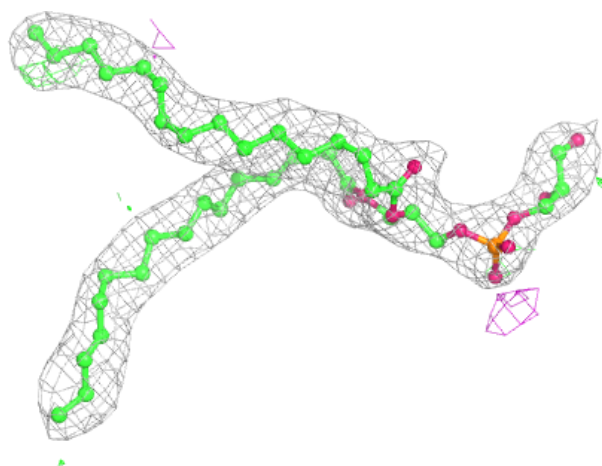
**Electron density around CLA C 502:**

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



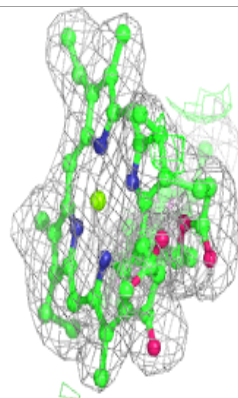
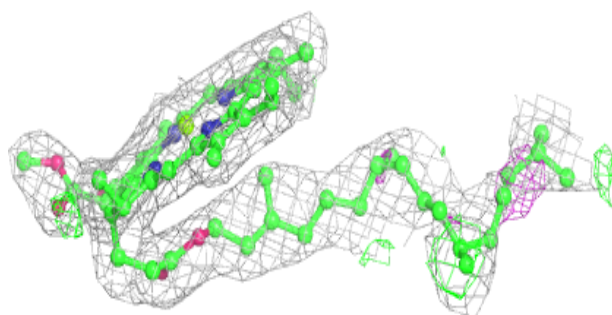
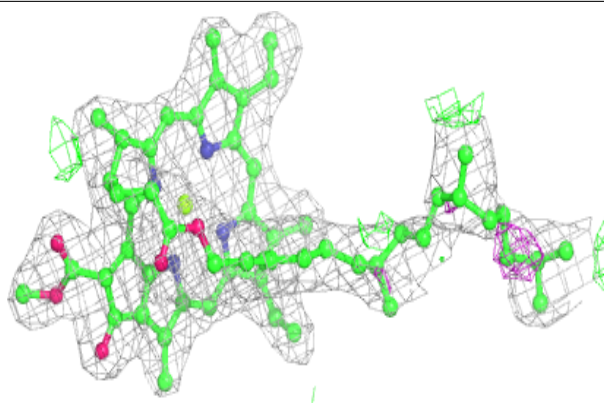
**Electron density around LHG d 407:**

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

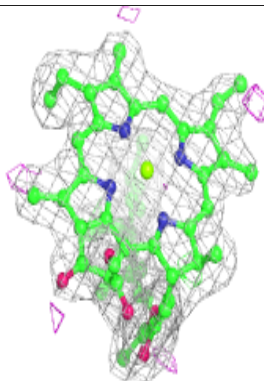
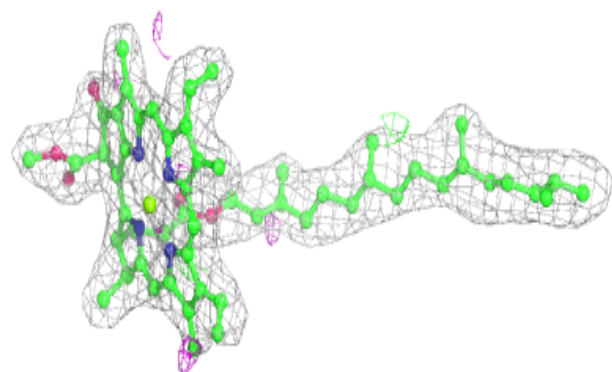
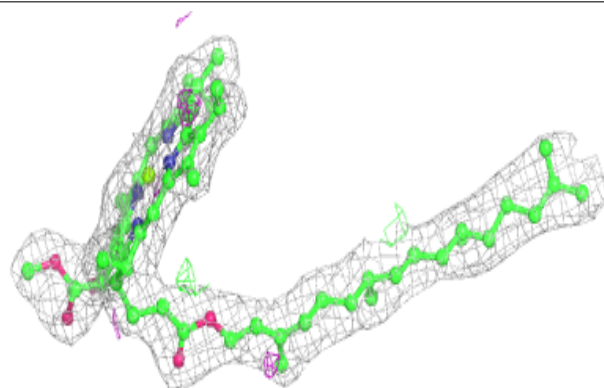


**Electron density around CLA b 614:**

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

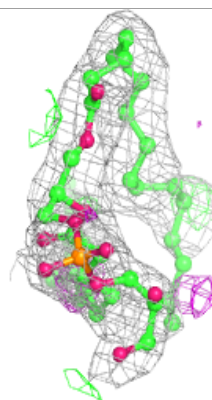
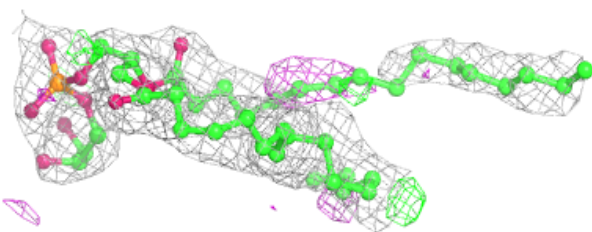
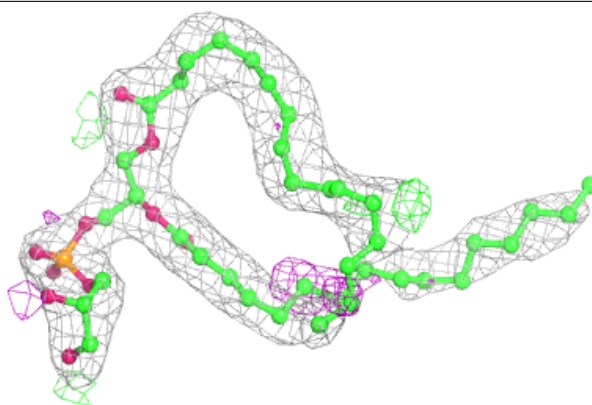
**Electron density around CLA b 607:**

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



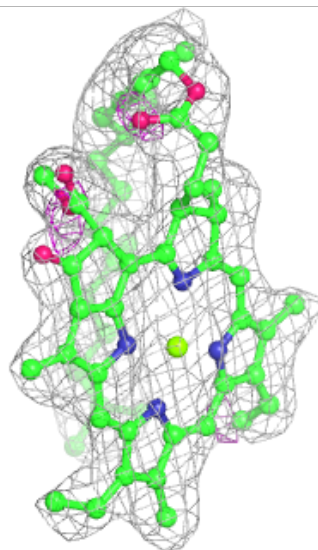
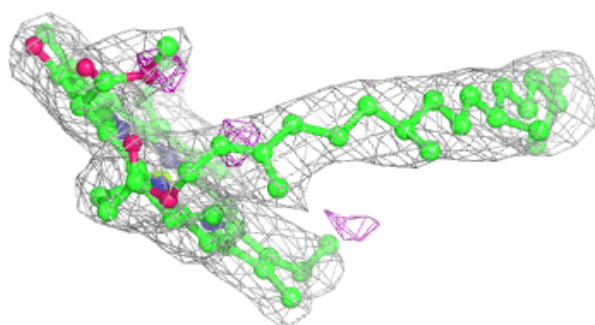
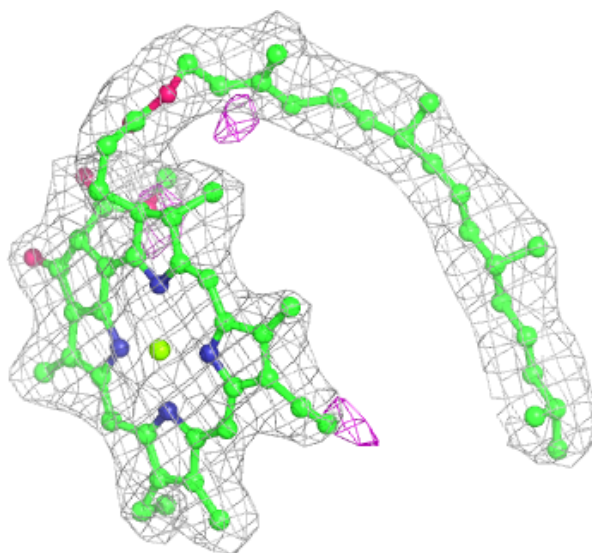
**Electron density around LHG D 411:**

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



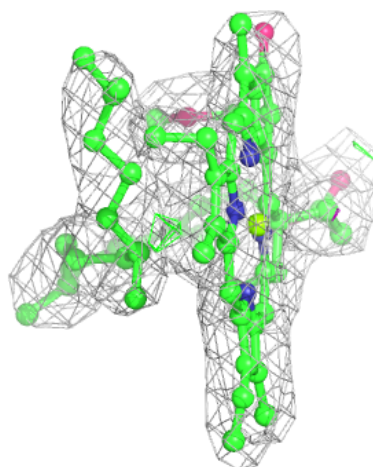
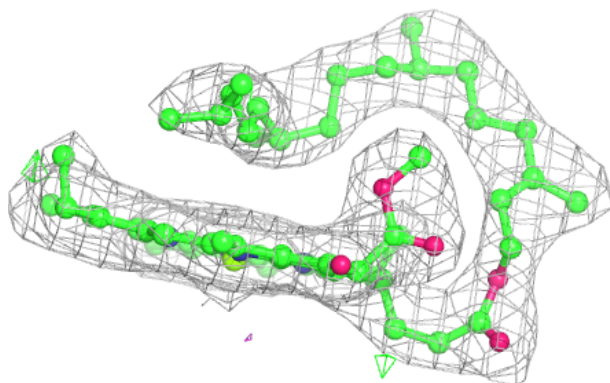
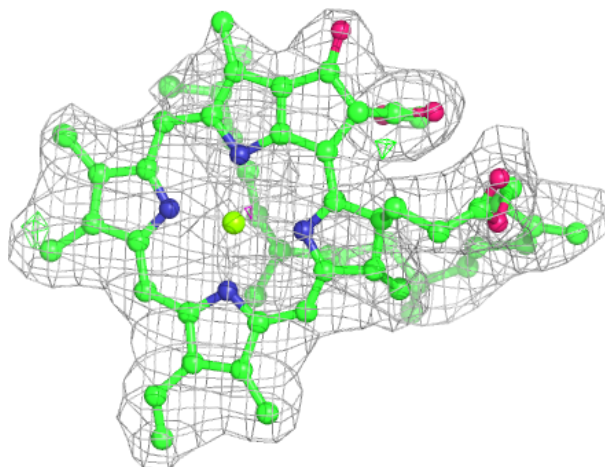
**Electron density around CLA c 508:**

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



**Electron density around CLA C 511:**

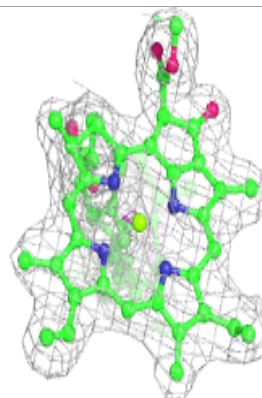
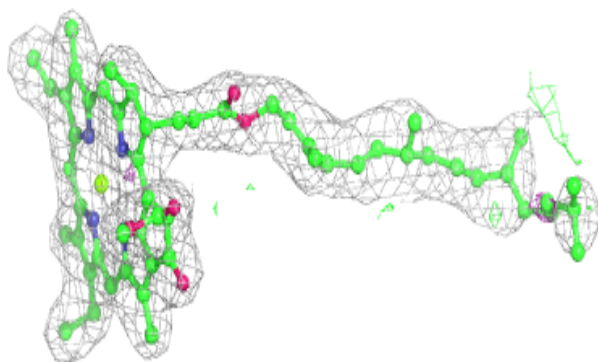
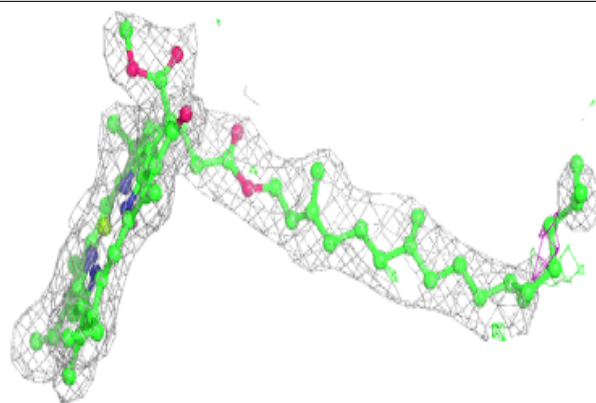
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



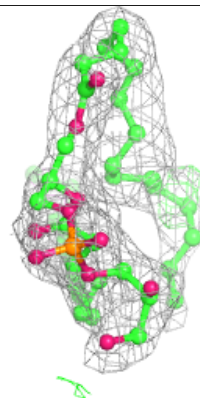
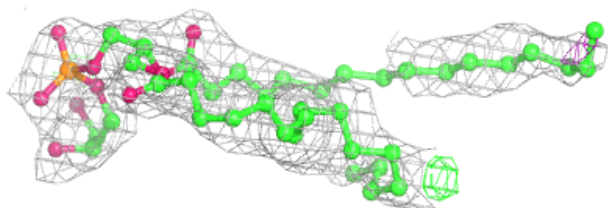


**Electron density around CLA B 604:**

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

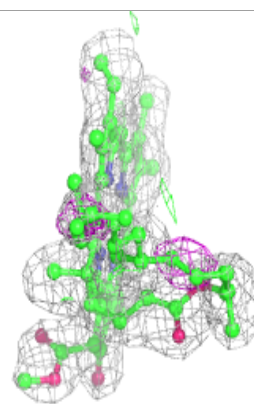
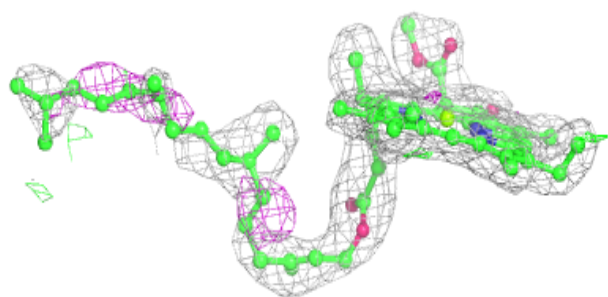
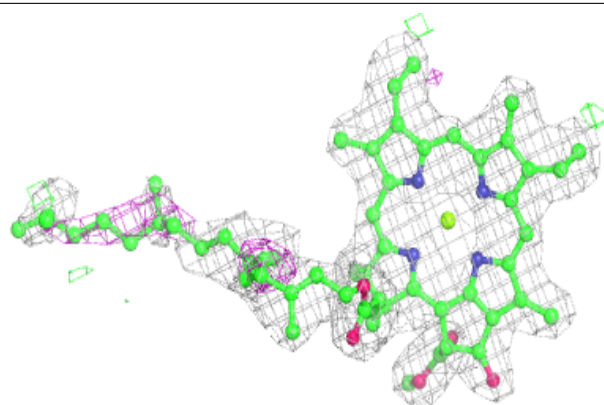
**Electron density around LHG d 408:**

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

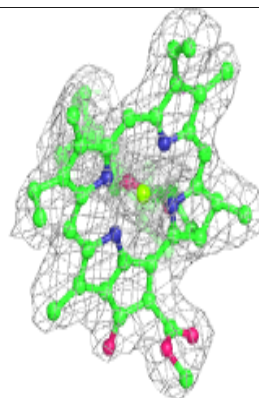
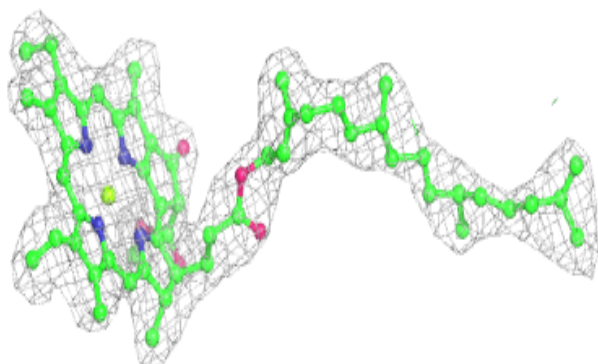
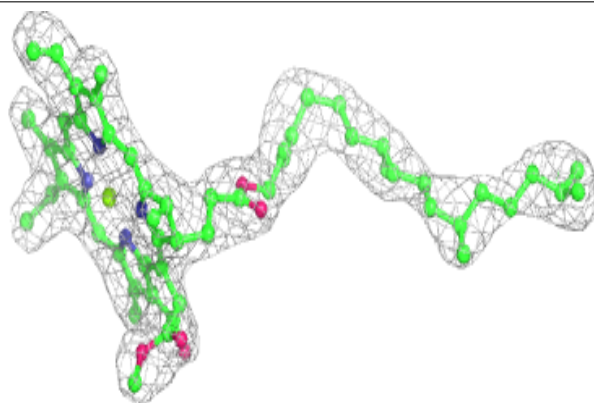


**Electron density around CLA a 407:**

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

**Electron density around CLA c 503:**

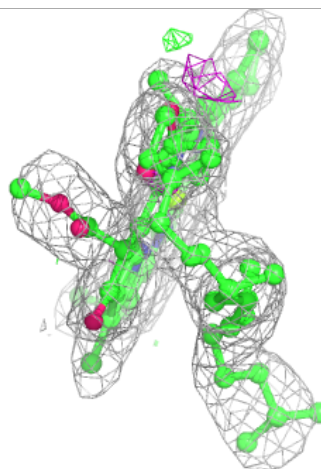
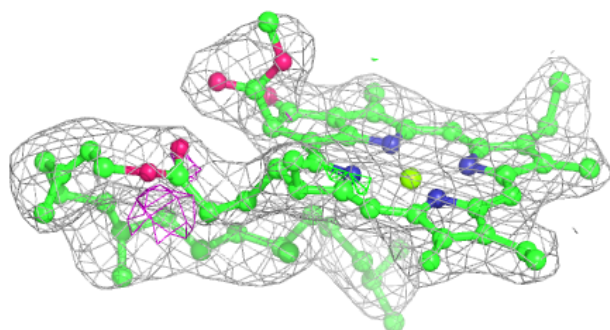
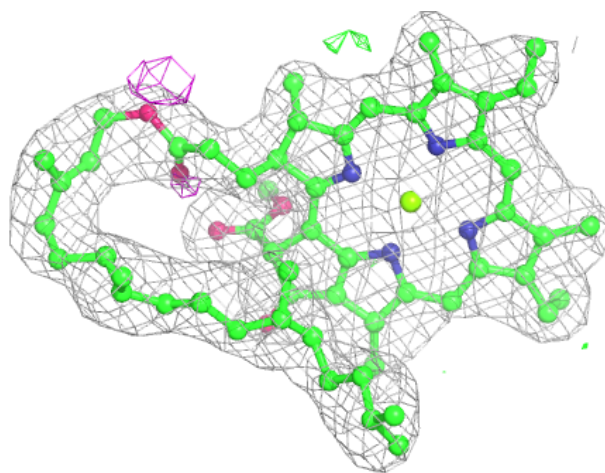
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





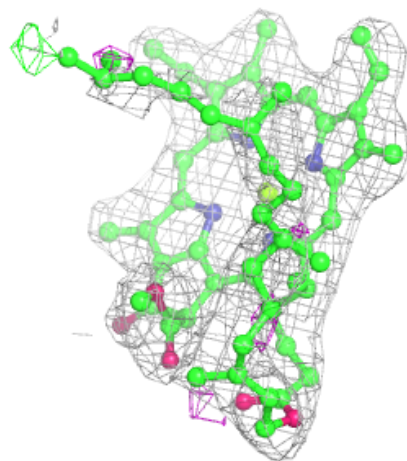
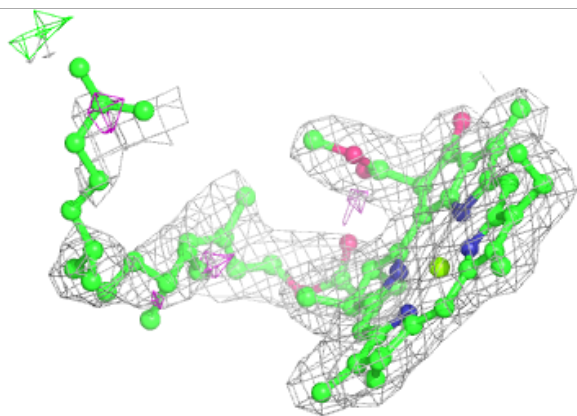
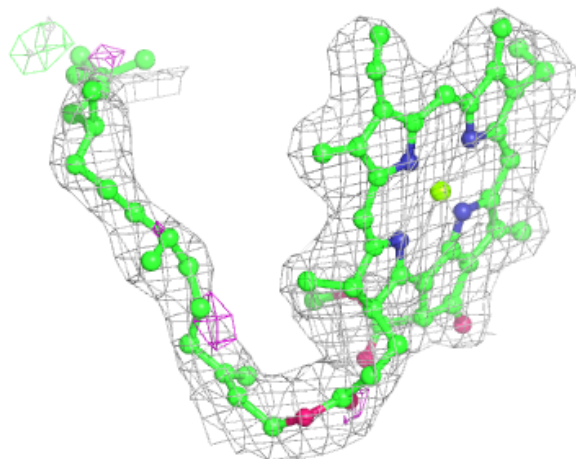
**Electron density around CLA c 510:**

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



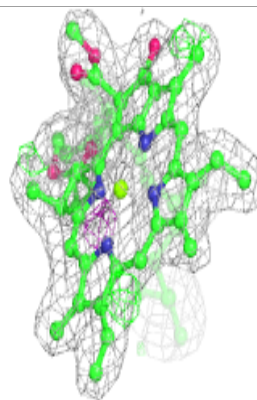
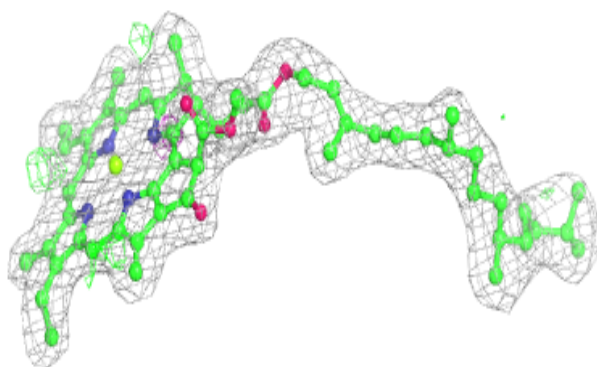
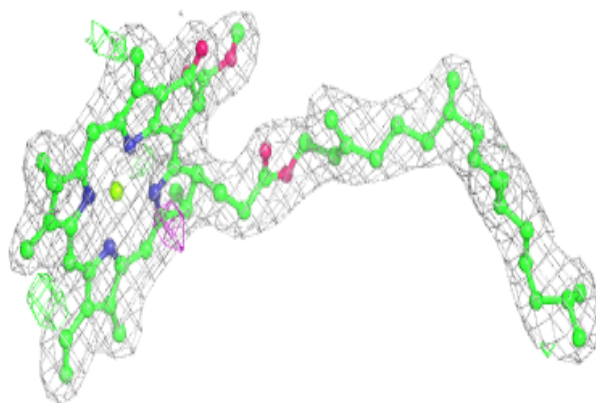
**Electron density around CLA b 616:**

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

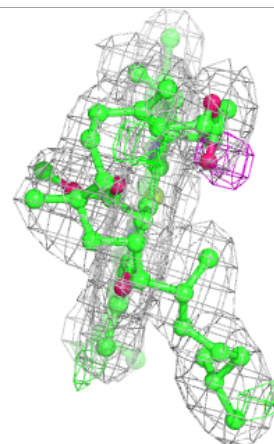
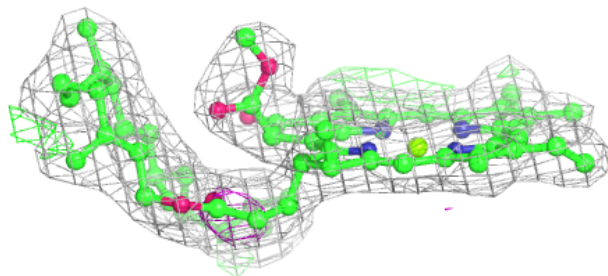
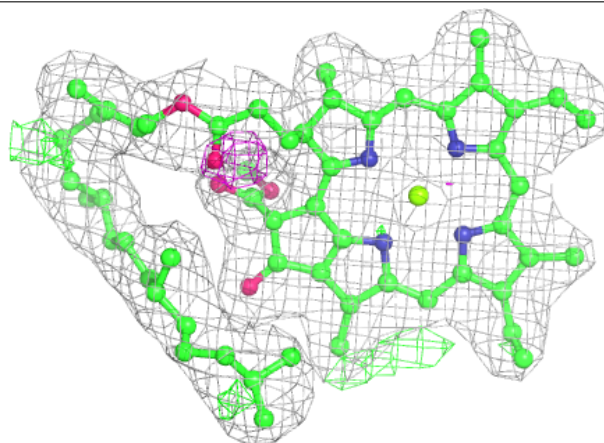


**Electron density around CLA A 404:**

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

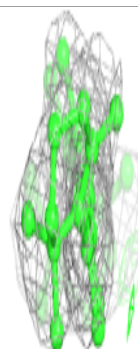
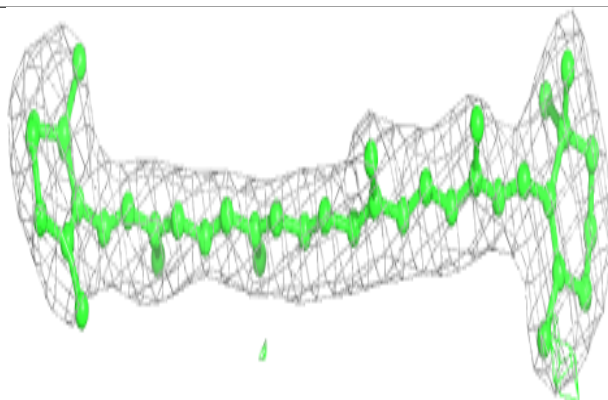
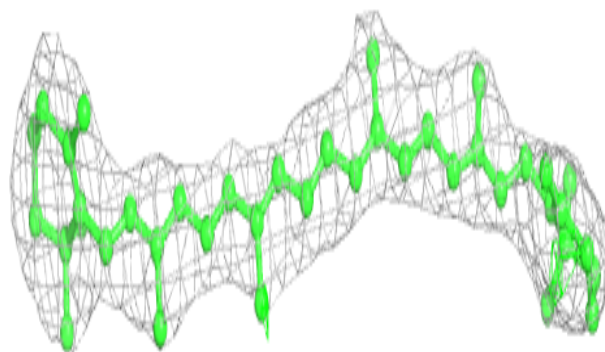
**Electron density around CLA B 610:**

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

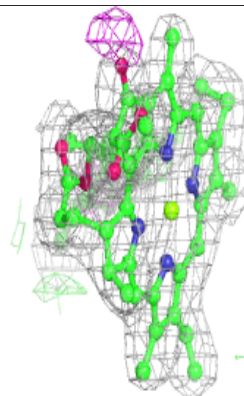
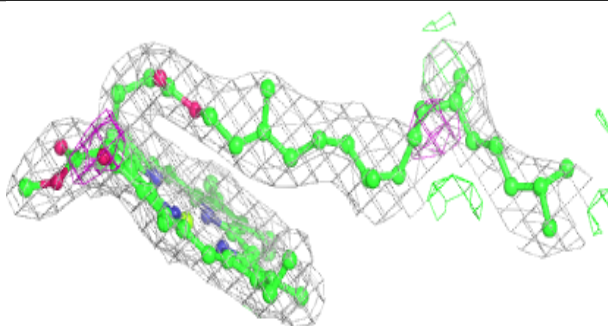
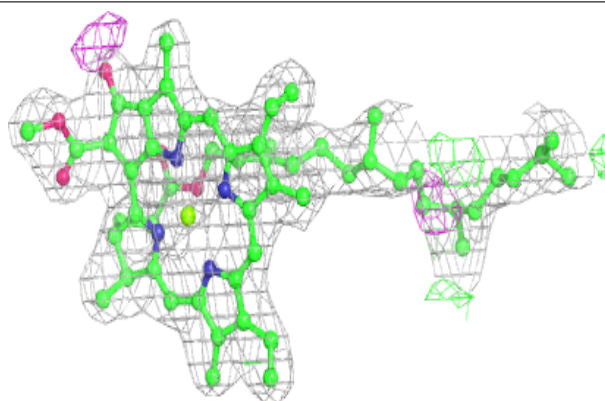


**Electron density around BCR c 515:**

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

**Electron density around CLA B 614:**

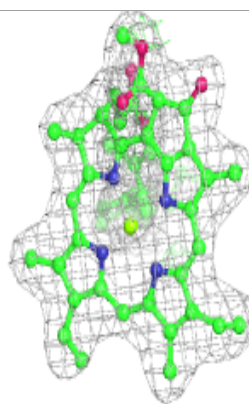
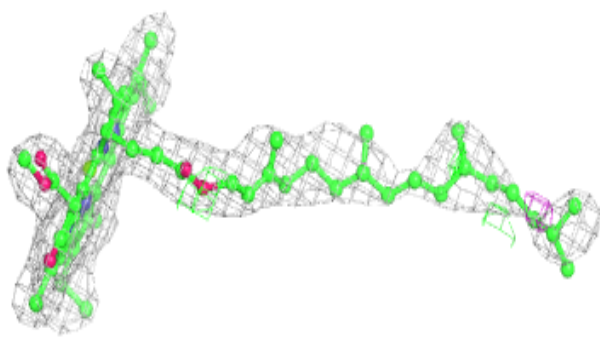
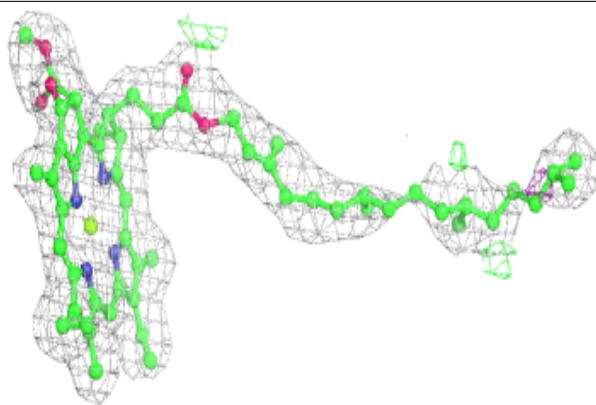
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



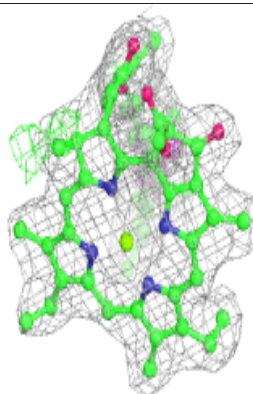
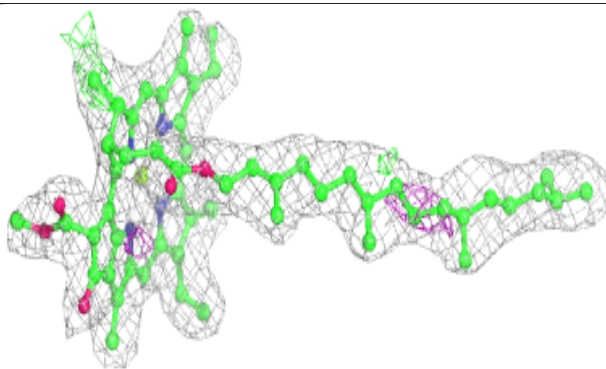
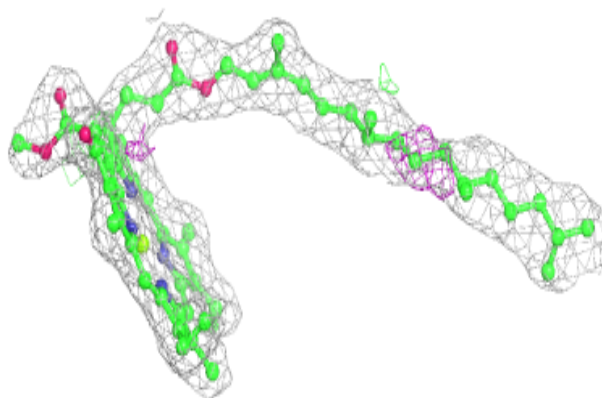


**Electron density around CLA d 403:**

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

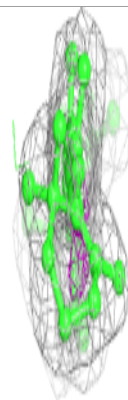
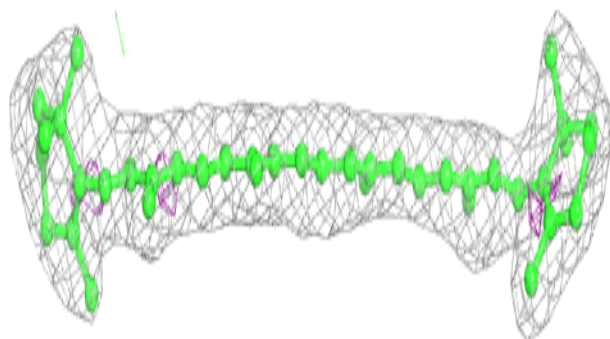
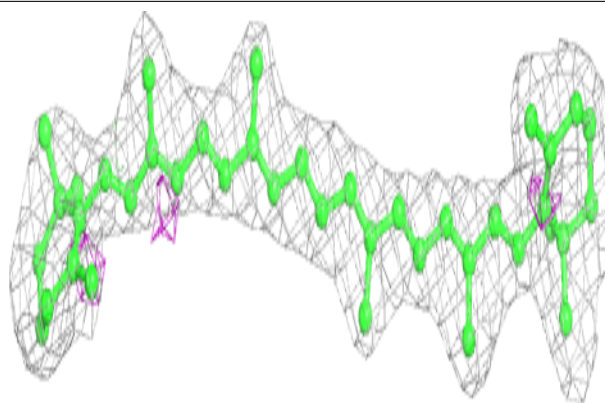
**Electron density around CLA B 607:**

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

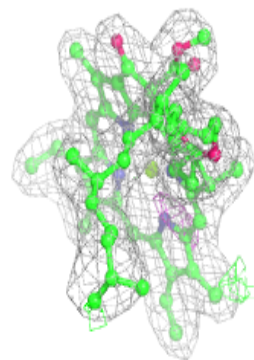
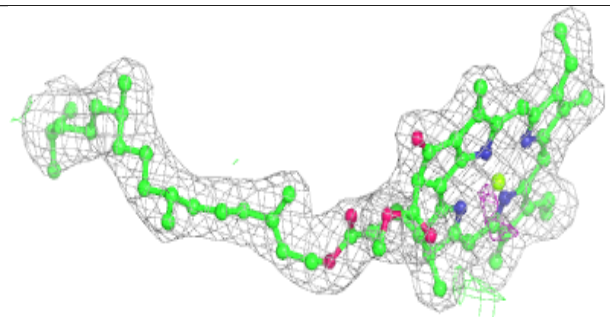
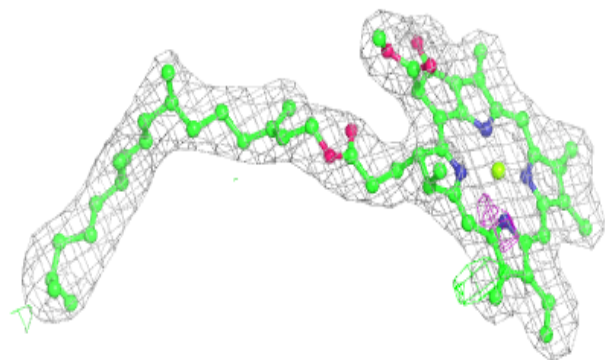


**Electron density around BCR B 618:**

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

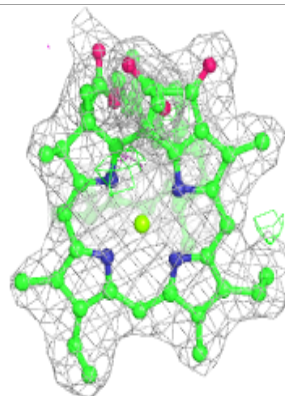
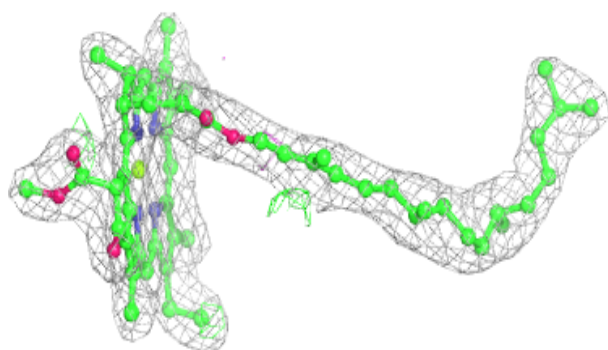
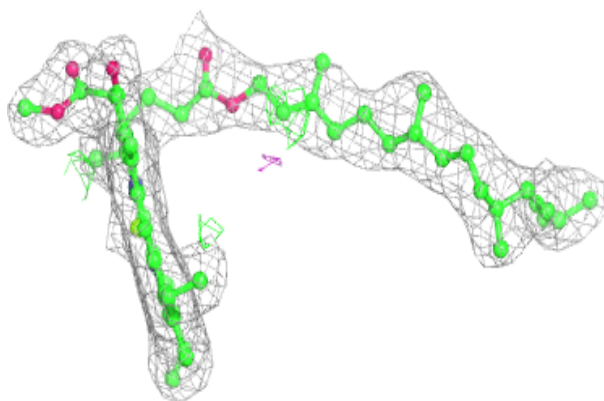
**Electron density around CLA a 405:**

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

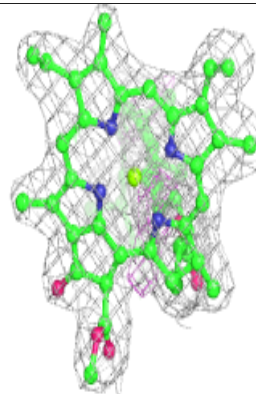
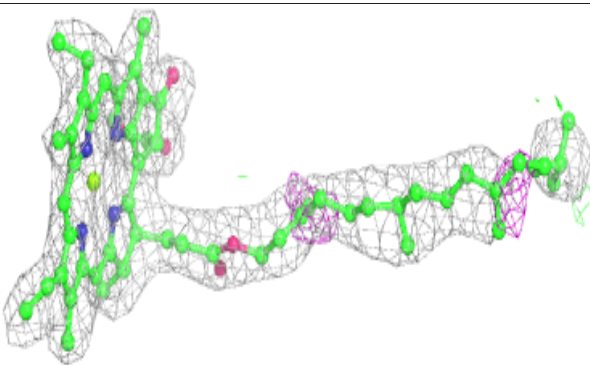
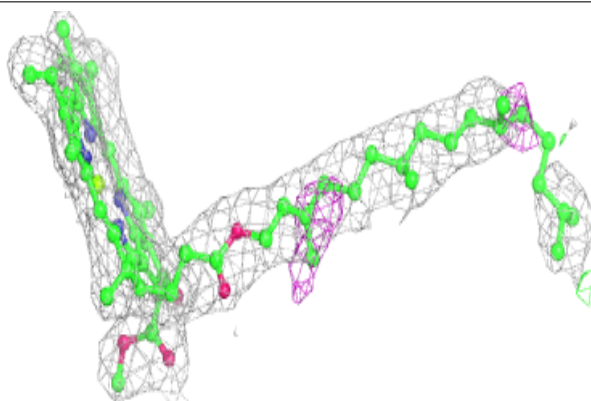


**Electron density around CLA b 605:**

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

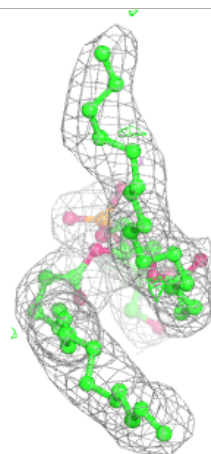
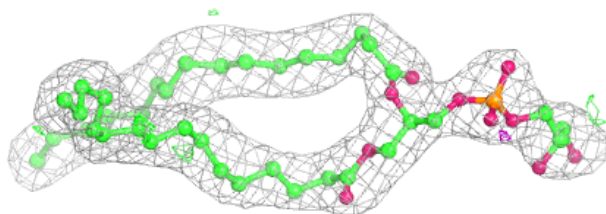
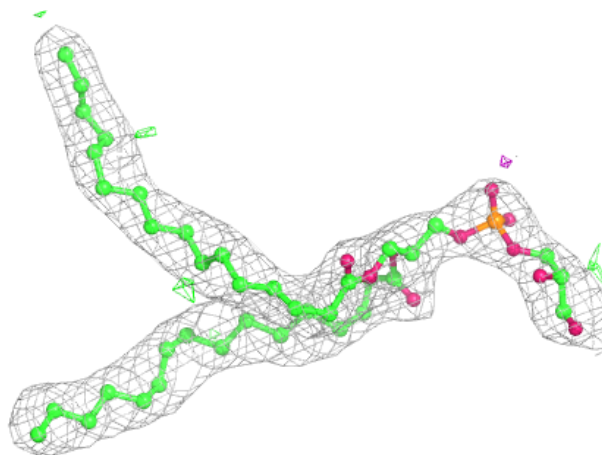
**Electron density around CLA b 604:**

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



**Electron density around LHG D 410:**

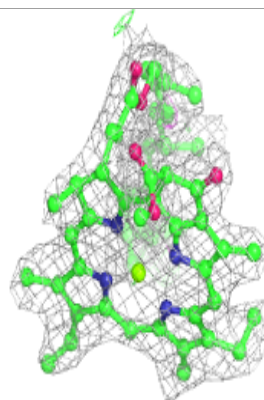
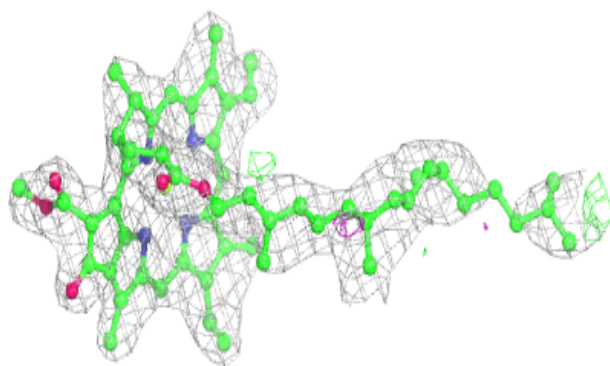
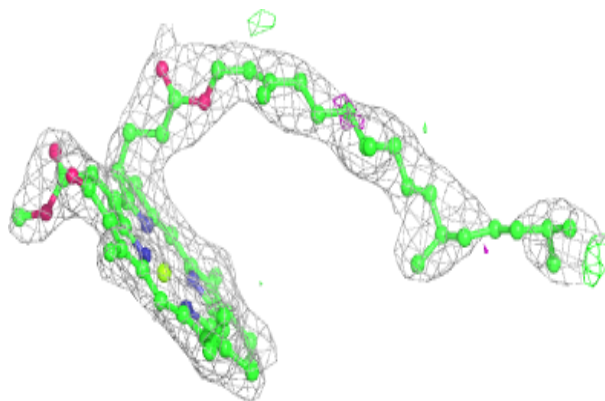
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



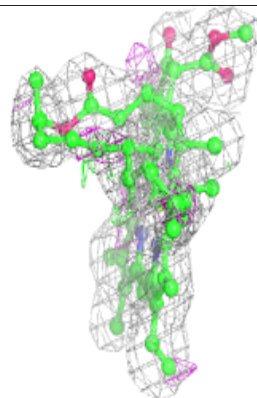
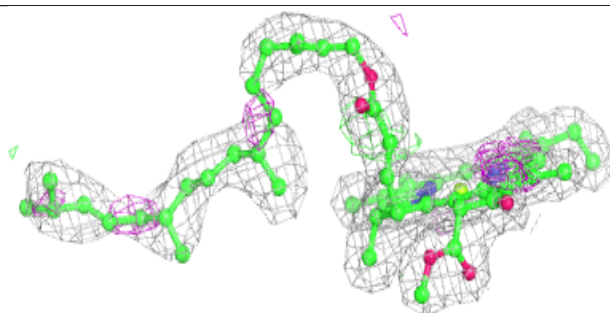
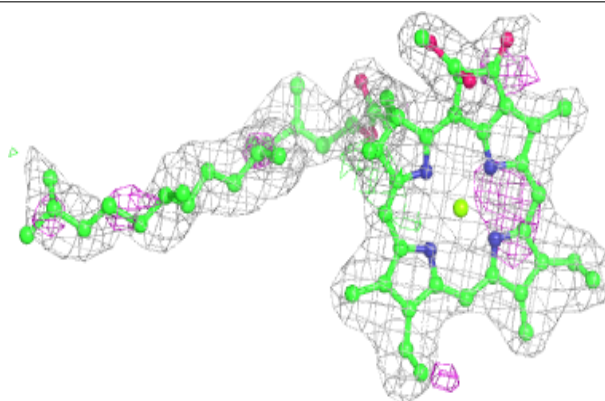


**Electron density around CLA c 505:**

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

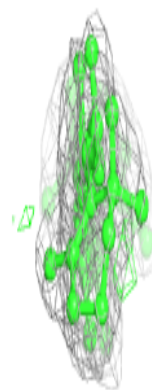
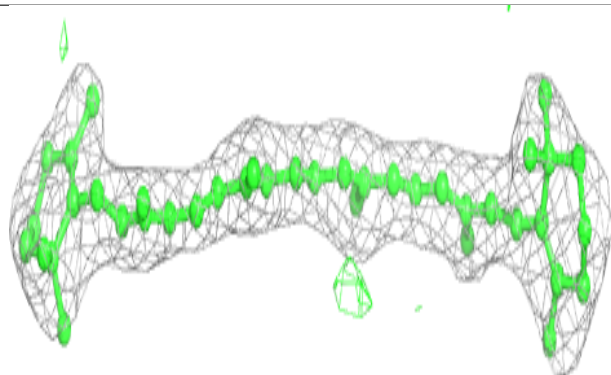
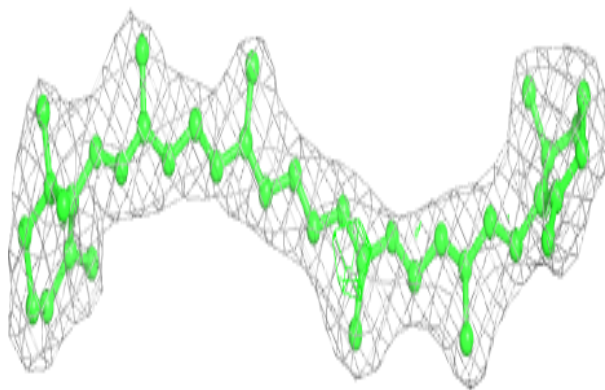
**Electron density around CLA A 406:**

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

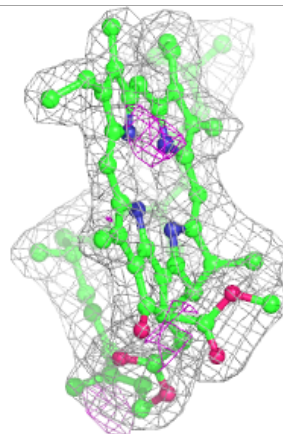
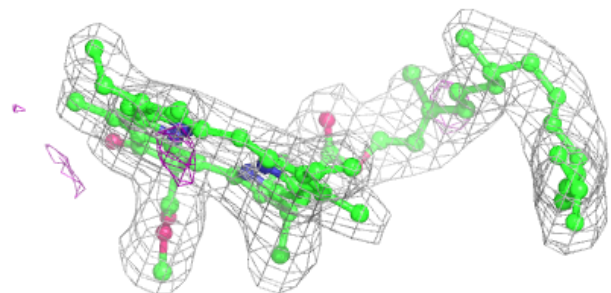
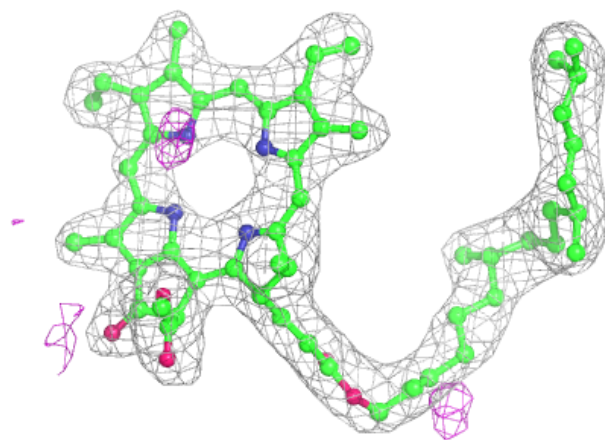


**Electron density around BCR y 101:**

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

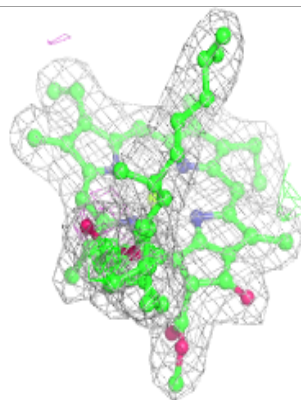
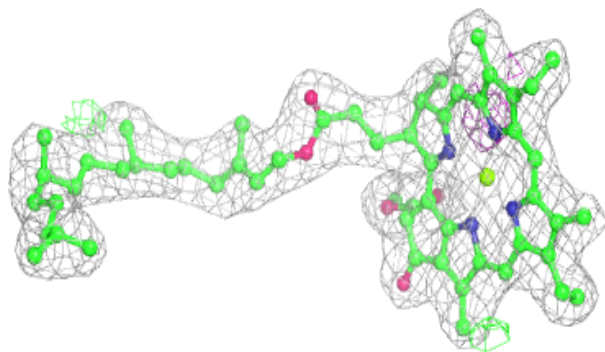
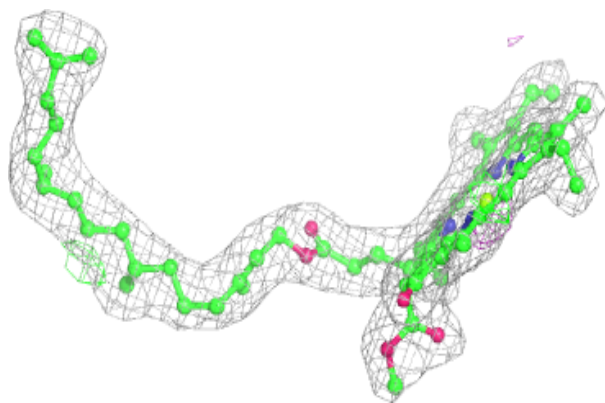
**Electron density around PHO a 353:**

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



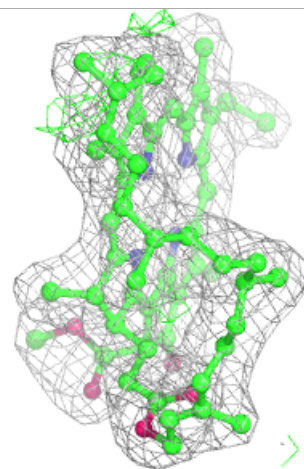
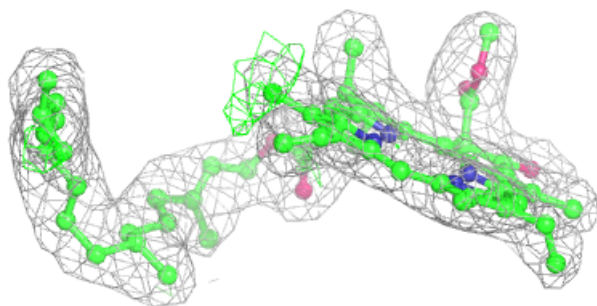
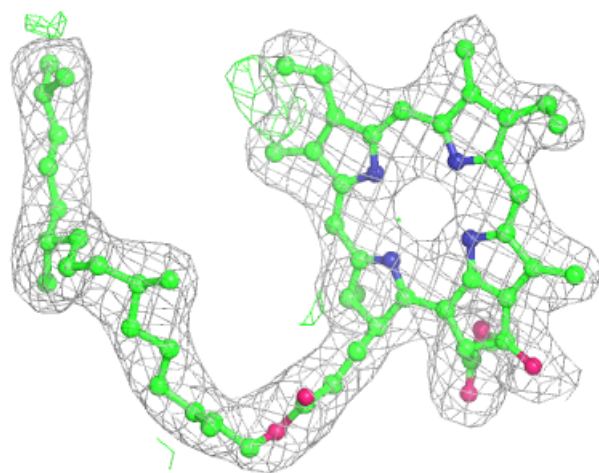
**Electron density around CLA D 405:**

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



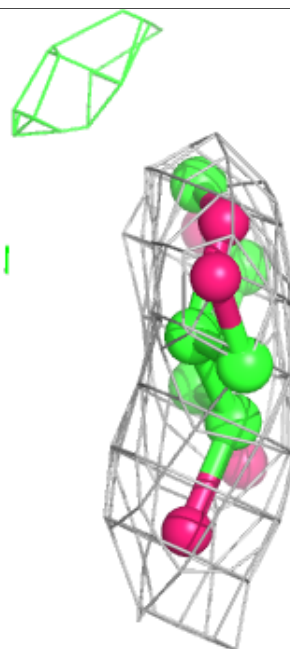
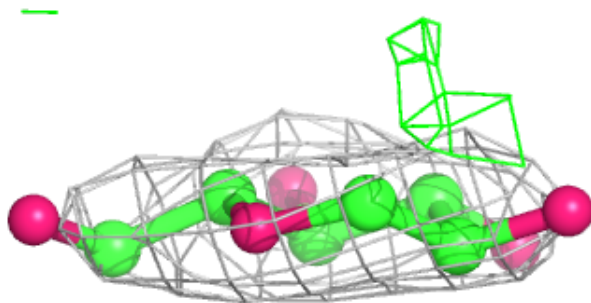
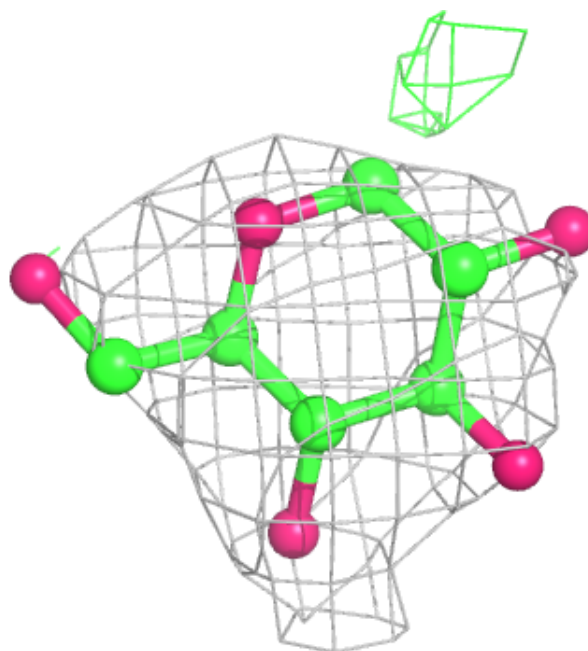
**Electron density around PHO A 353:**

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



**Electron density around HTG V 203:**

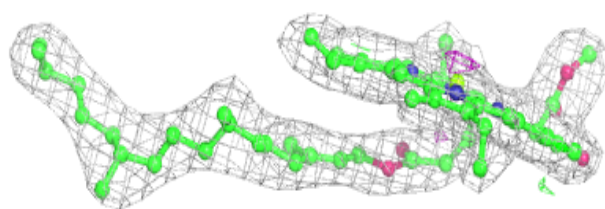
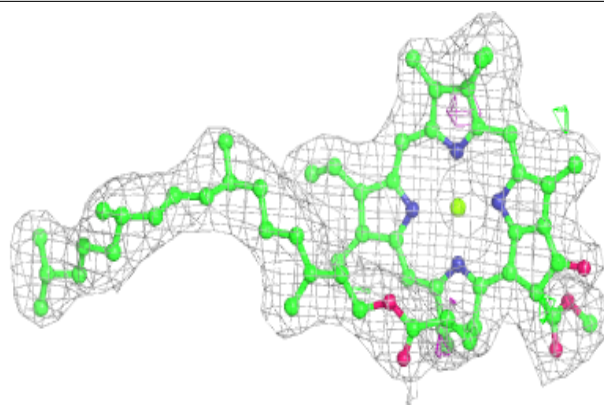
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



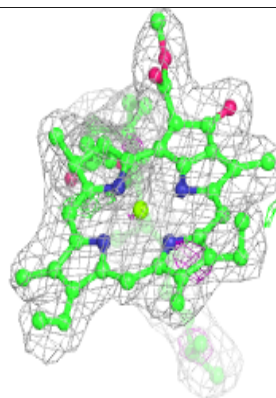
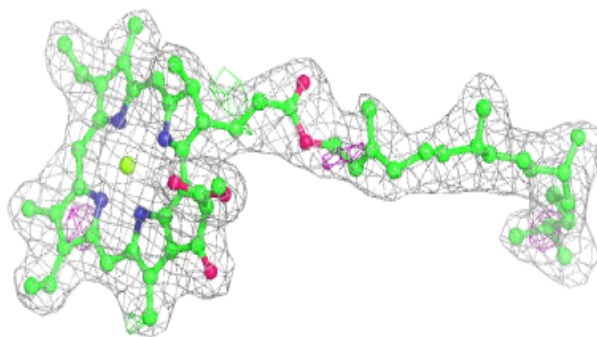
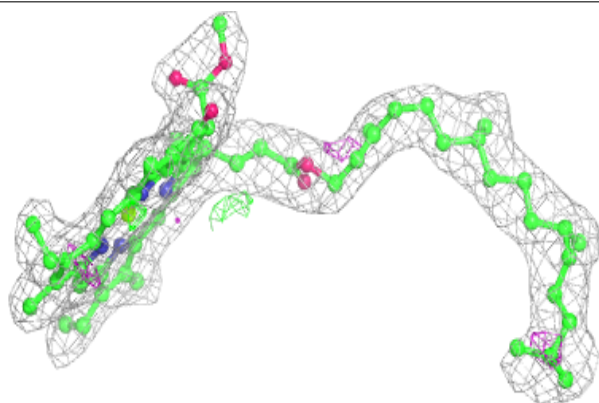


**Electron density around CLA B 603:**

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

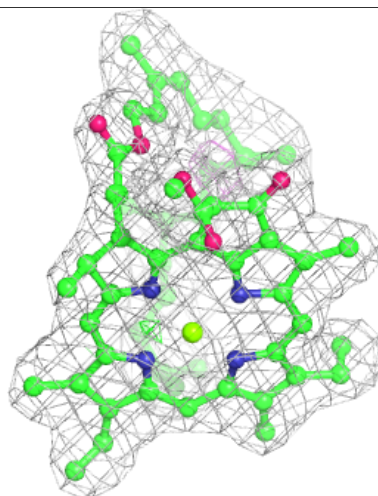
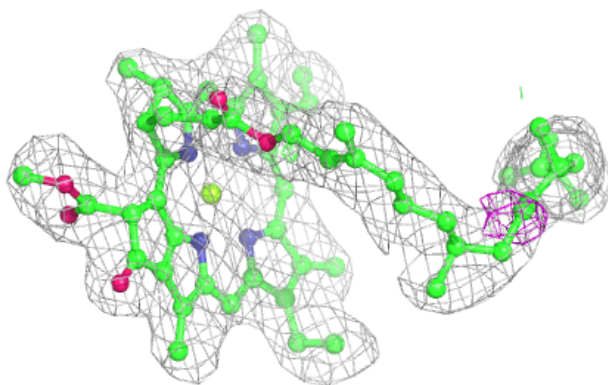
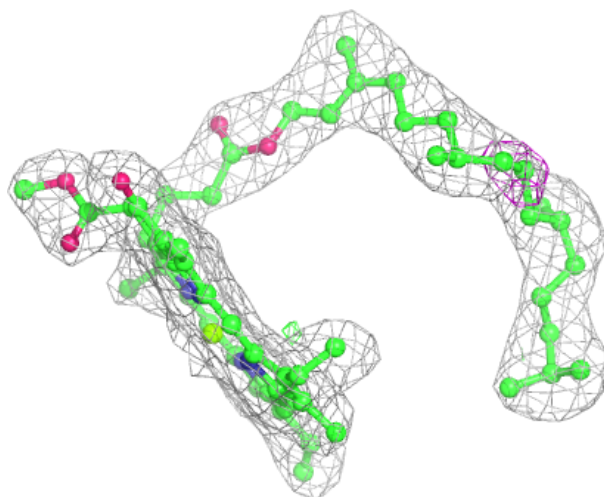
**Electron density around CLA d 402:**

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



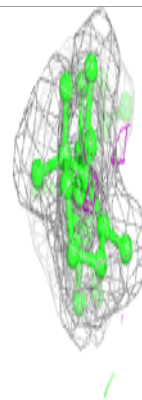
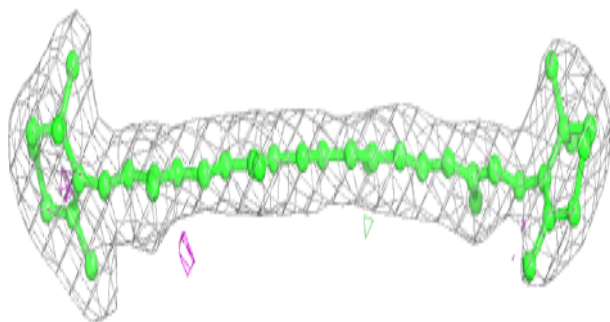
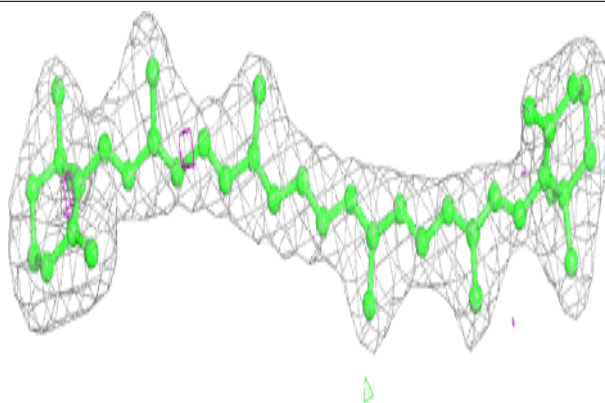
**Electron density around CLA b 611:**

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

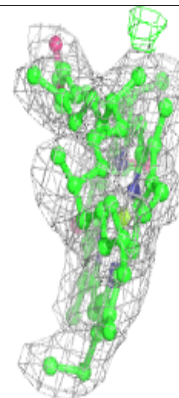
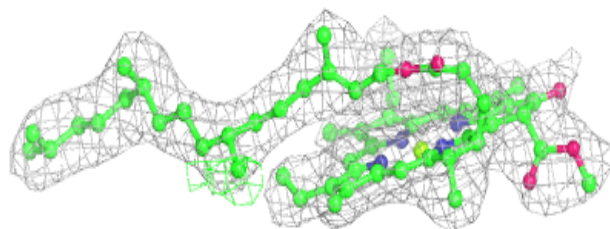
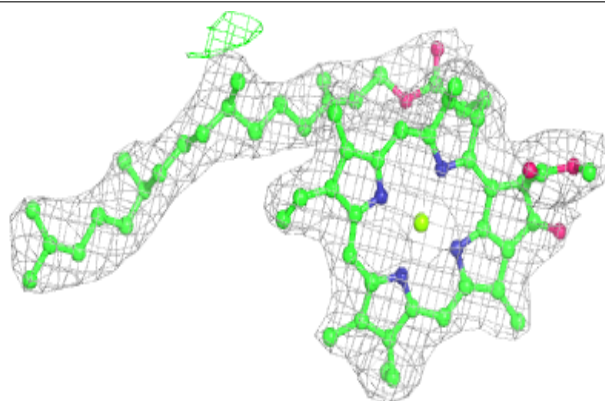


**Electron density around BCR b 618:**

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

**Electron density around CLA c 502:**

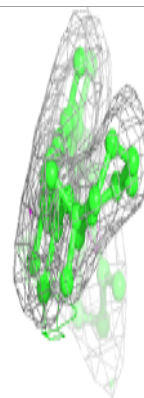
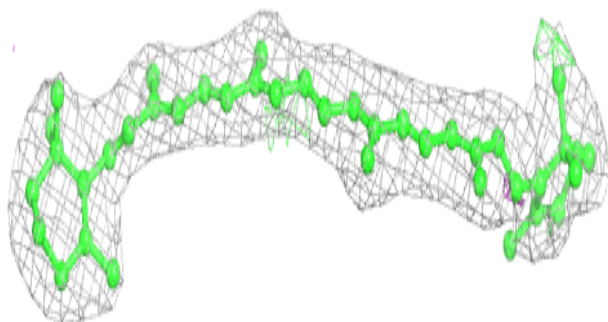
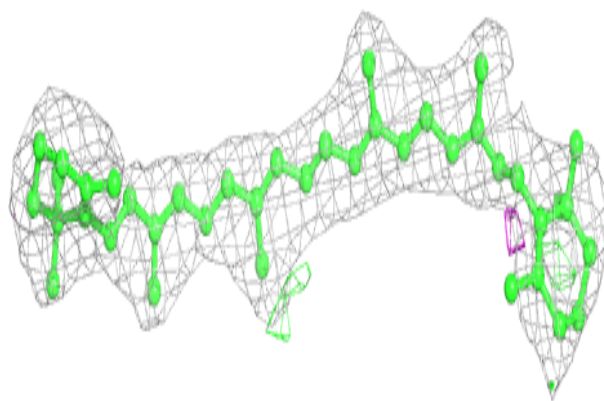
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



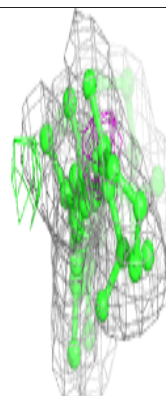
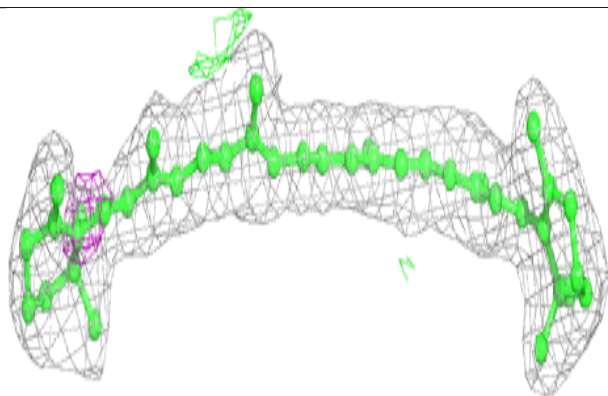
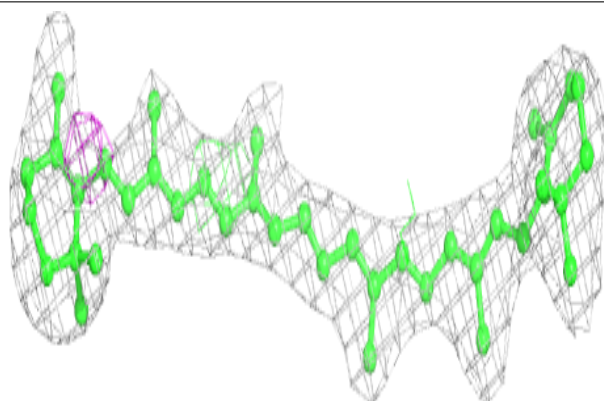


**Electron density around BCR d 404:**

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

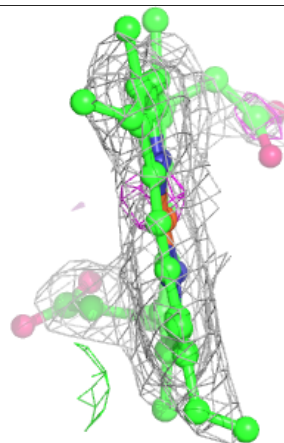
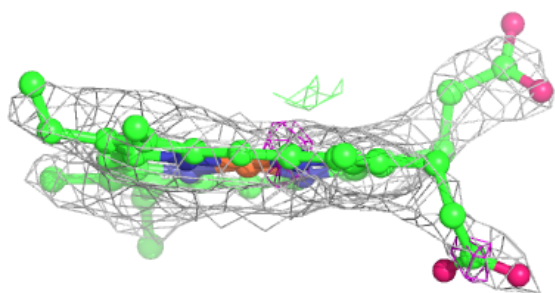
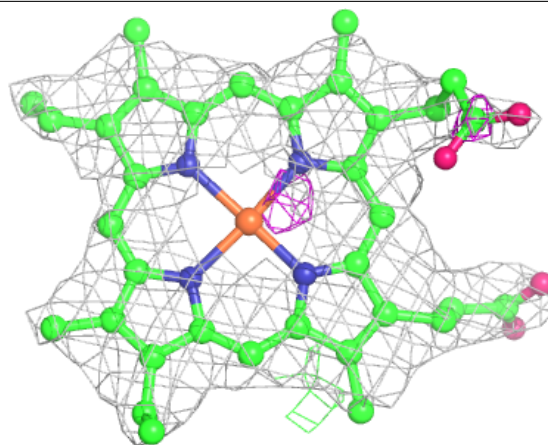
**Electron density around BCR T 101:**

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

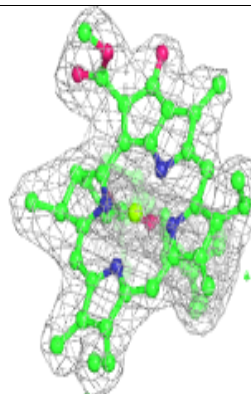
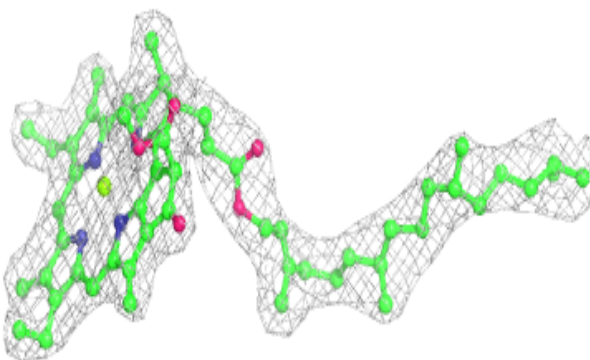
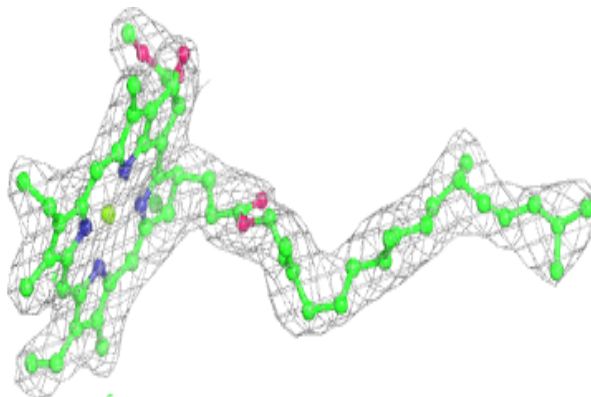


**Electron density around HEM e 87:**

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

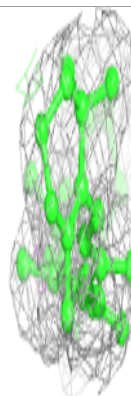
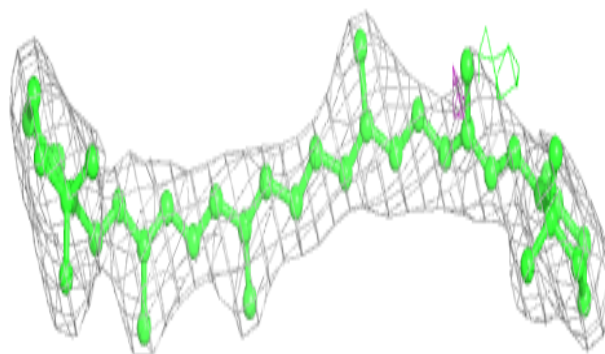
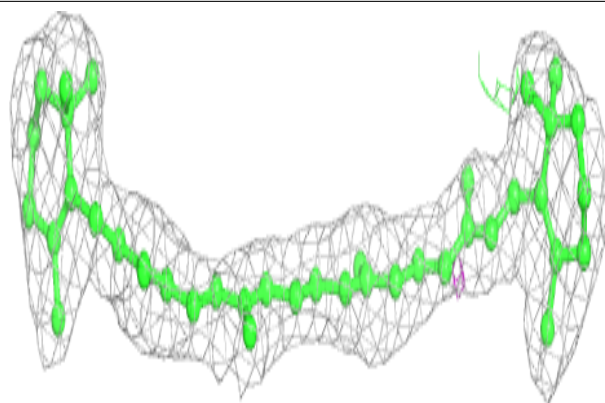
**Electron density around CLA C 503:**

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

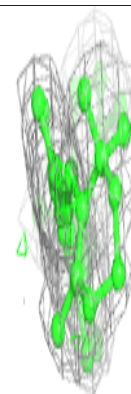
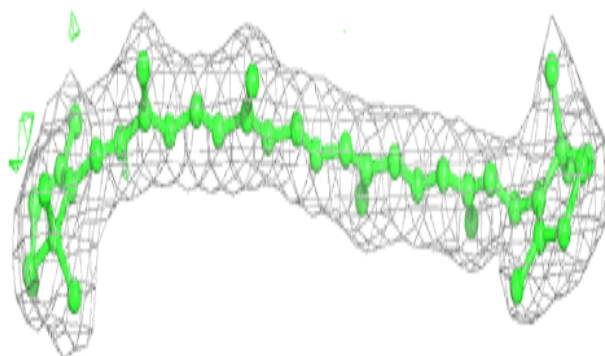
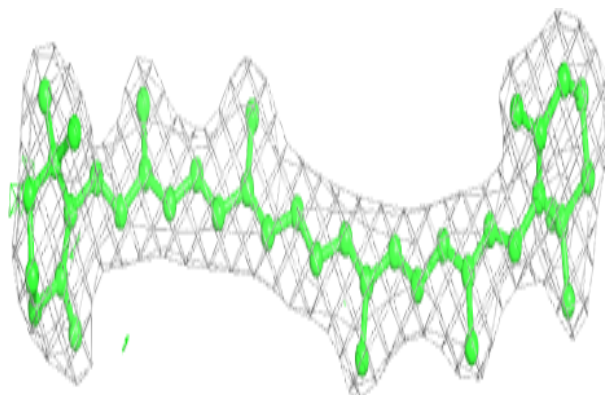


**Electron density around BCR k 101:**

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

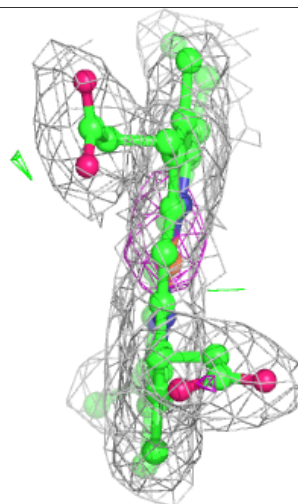
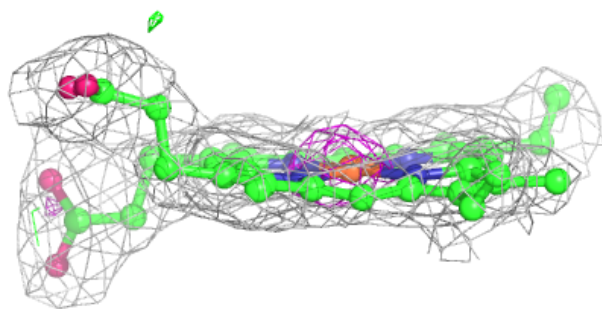
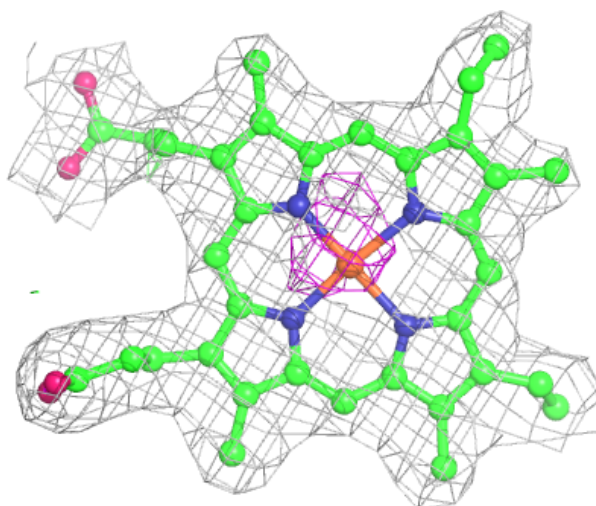
**Electron density around BCR B 619:**

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



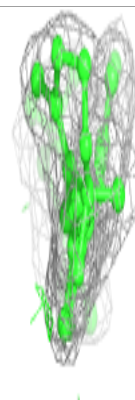
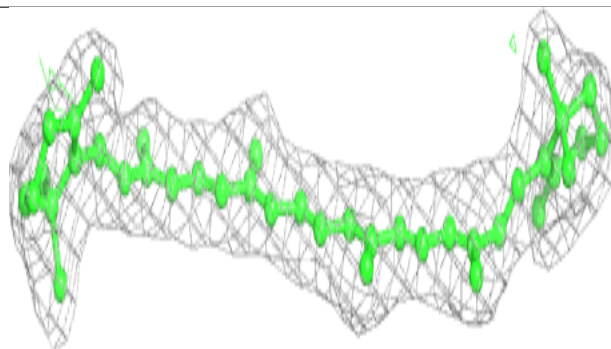
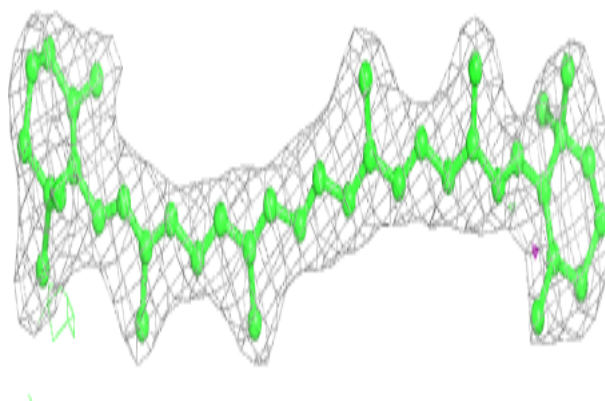
**Electron density around HEC V 202:**

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



**Electron density around BCR b 619:**

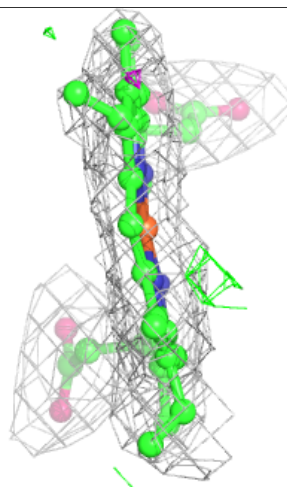
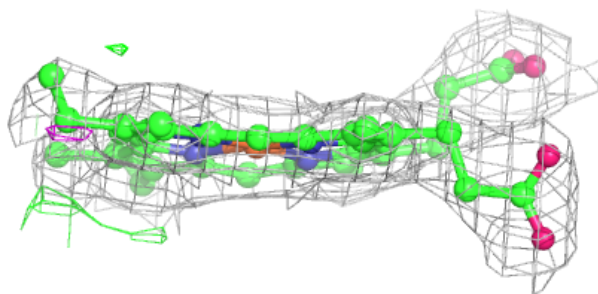
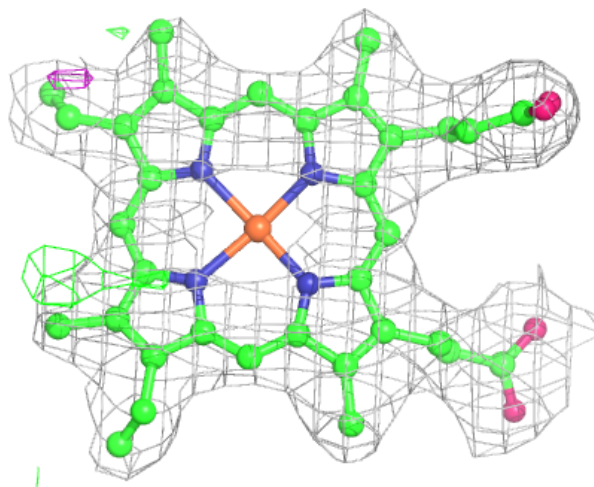
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





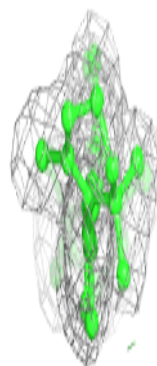
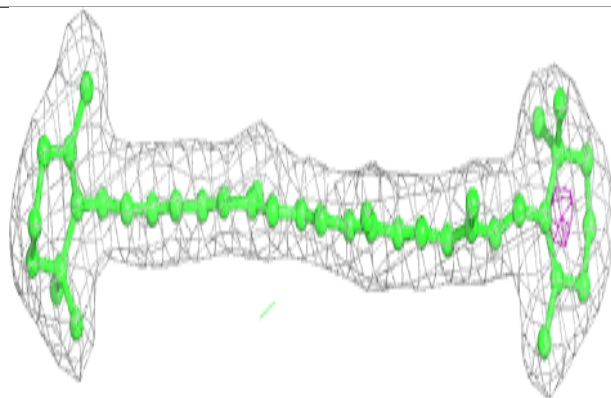
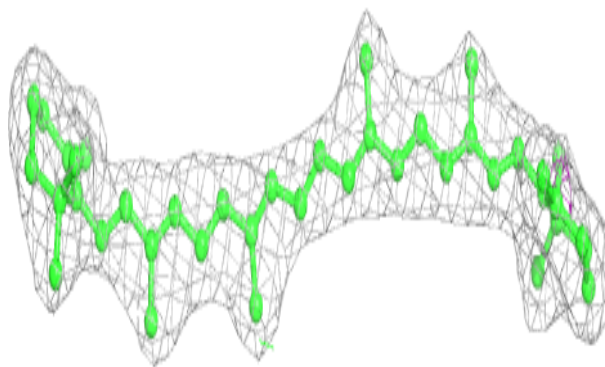
**Electron density around HEC v 202:**

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



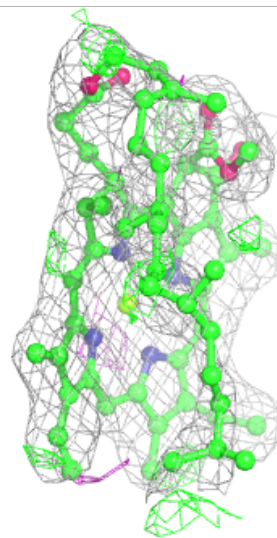
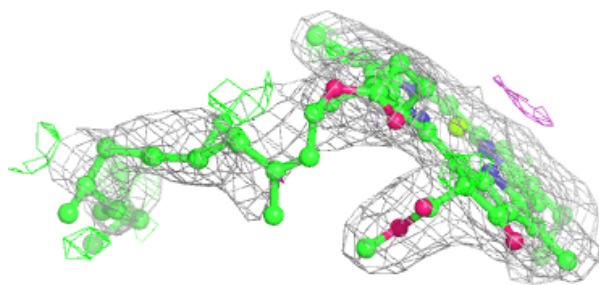
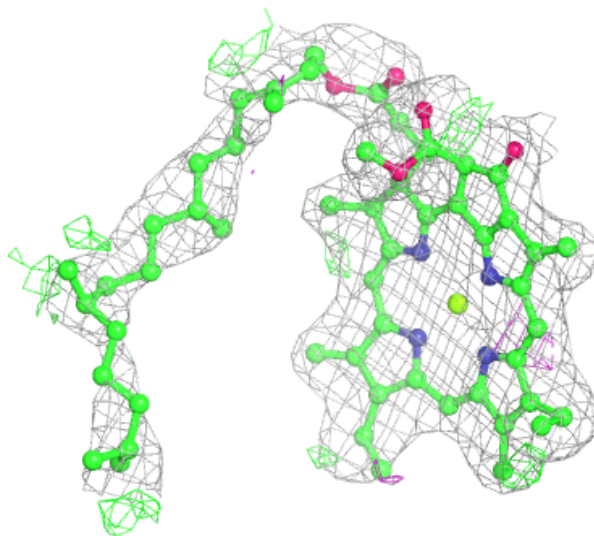
**Electron density around BCR a 410:**

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



**Electron density around CLA B 616:**

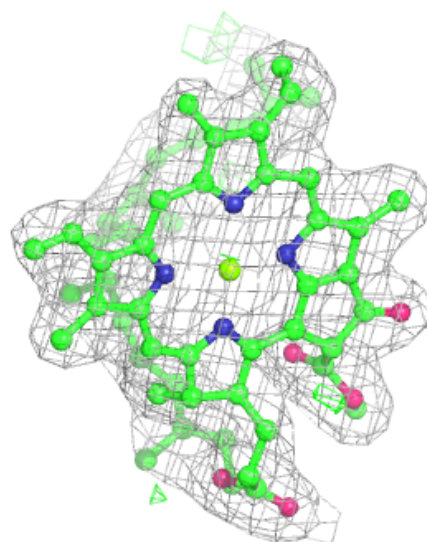
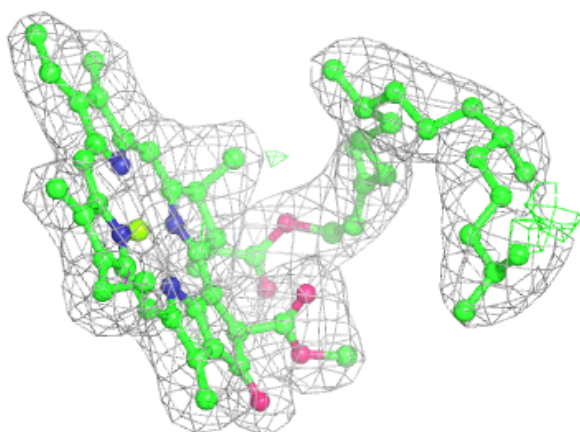
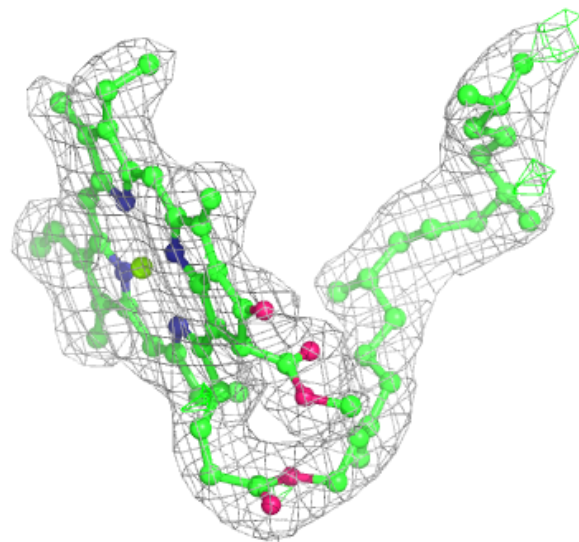
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





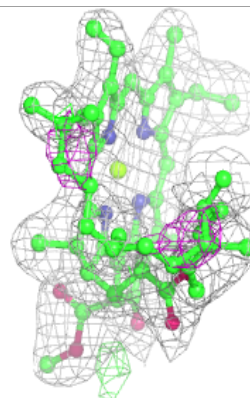
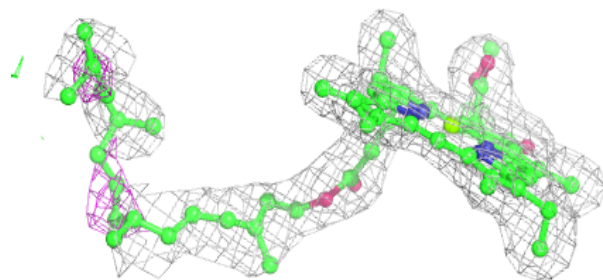
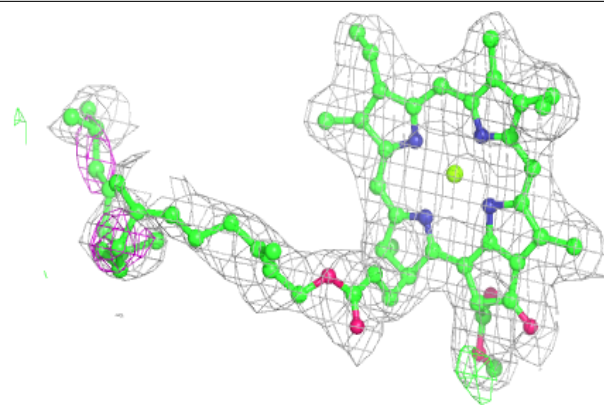
**Electron density around CLA b 613:**

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

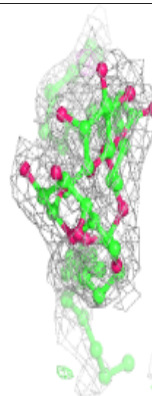
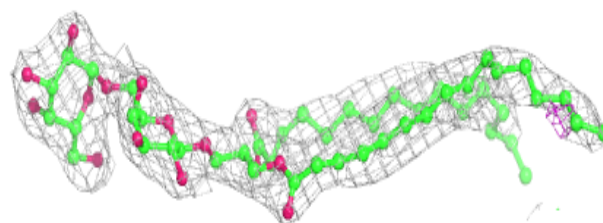
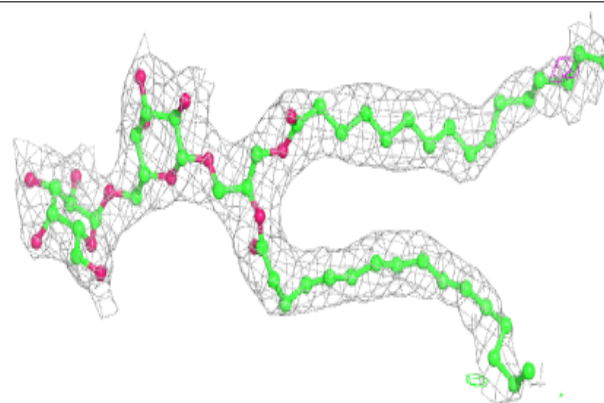


**Electron density around CLA A 408:**

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

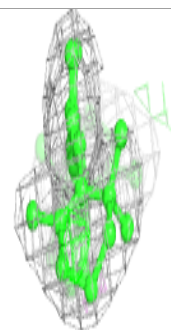
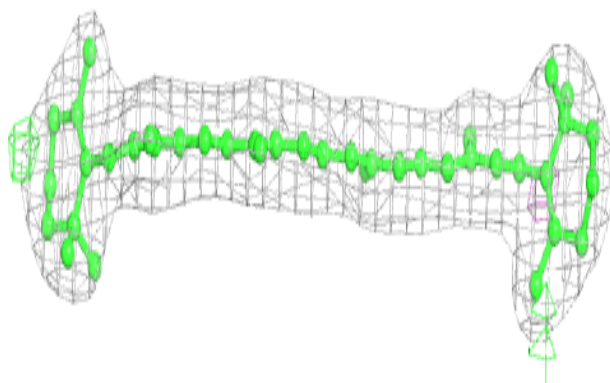
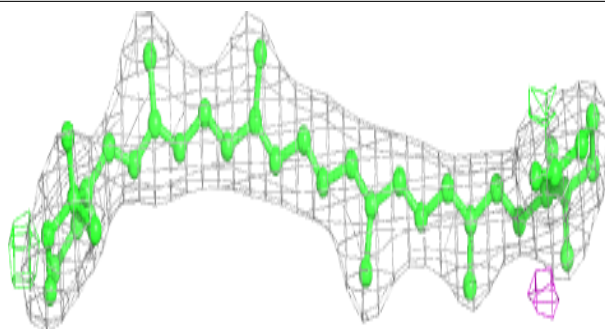
**Electron density around DGD c 519:**

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



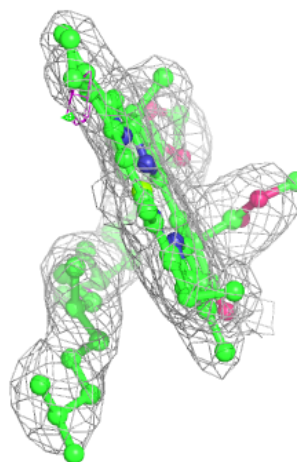
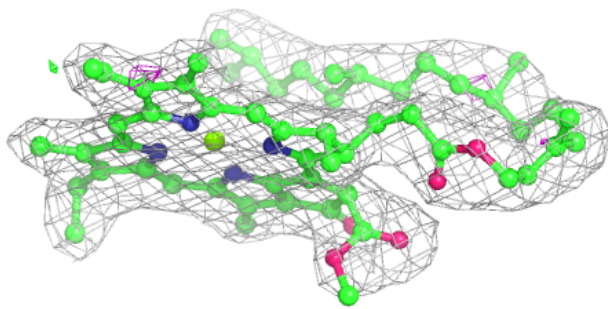
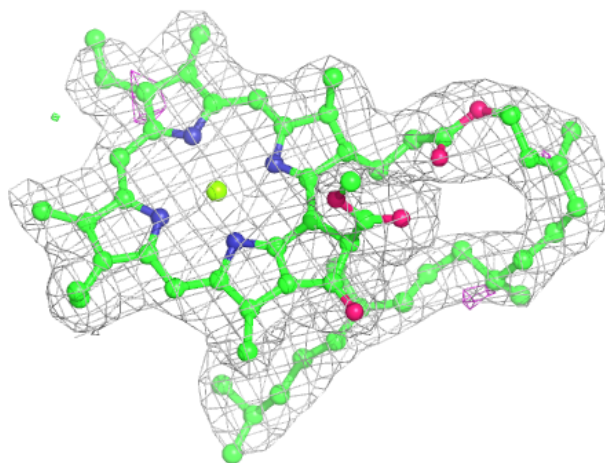
**Electron density around BCR C 516:**

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



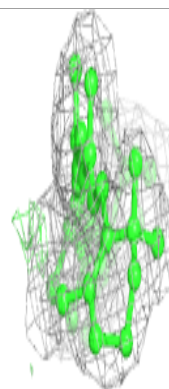
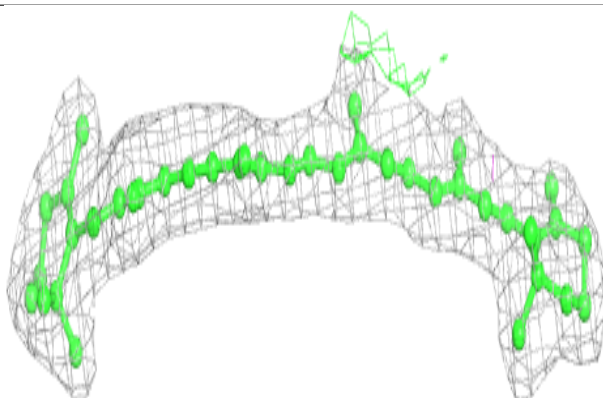
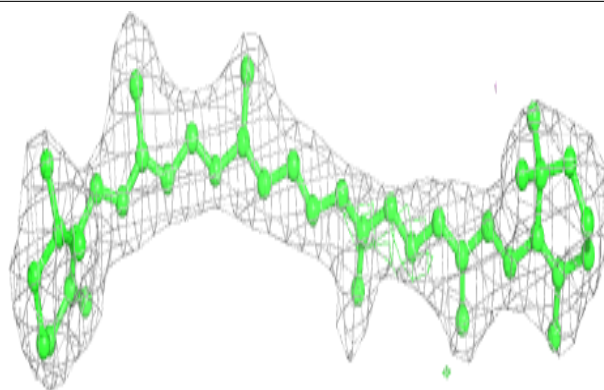
**Electron density around CLA C 510:**

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

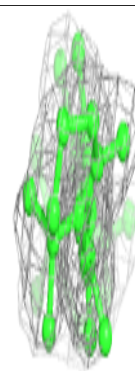
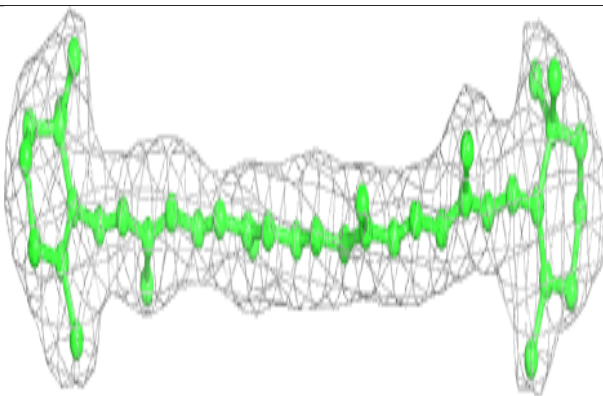
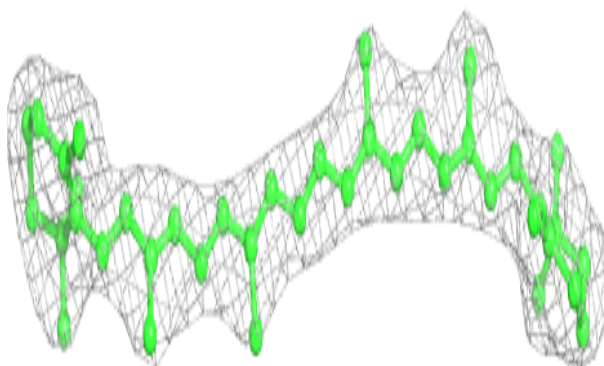


**Electron density around BCR t 103:**

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

**Electron density around BCR C 515:**

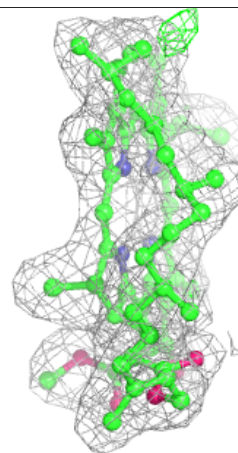
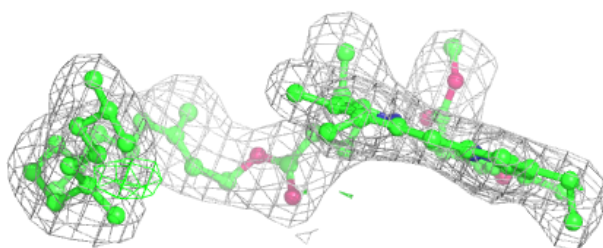
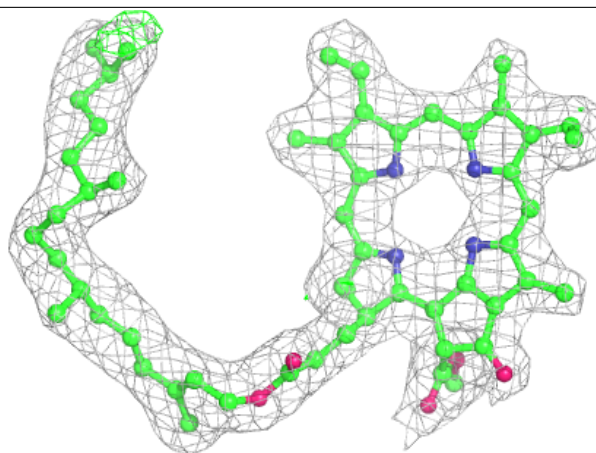
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



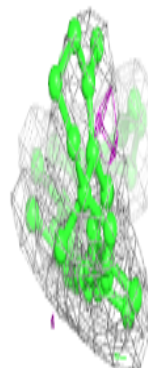
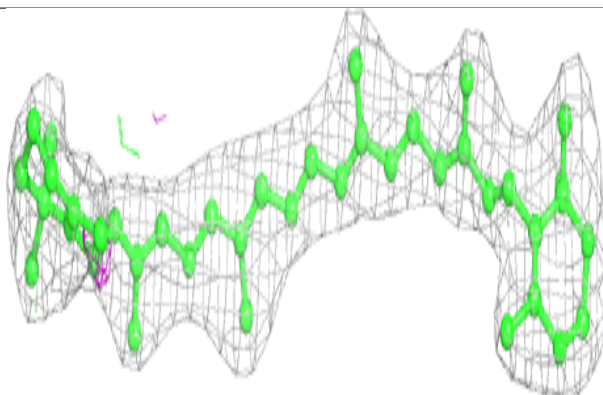
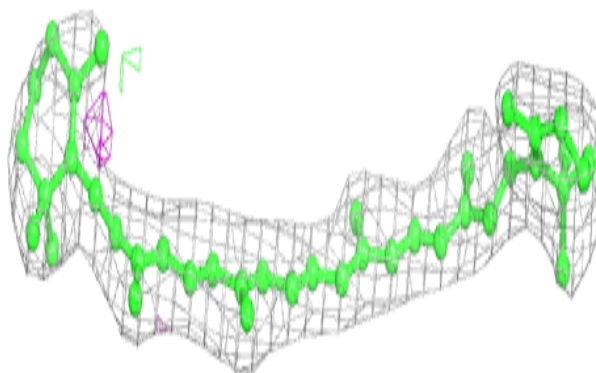


**Electron density around PHO A 407:**

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

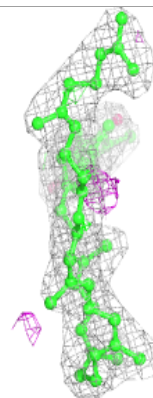
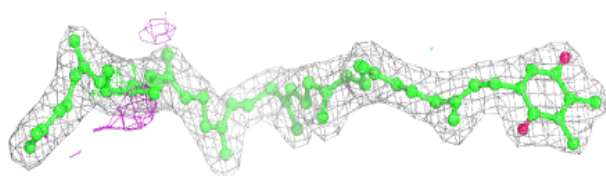
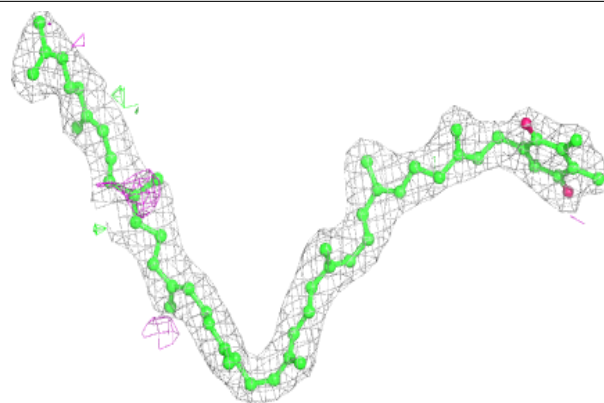
**Electron density around BCR D 407:**

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

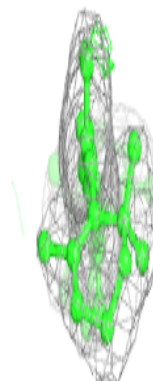
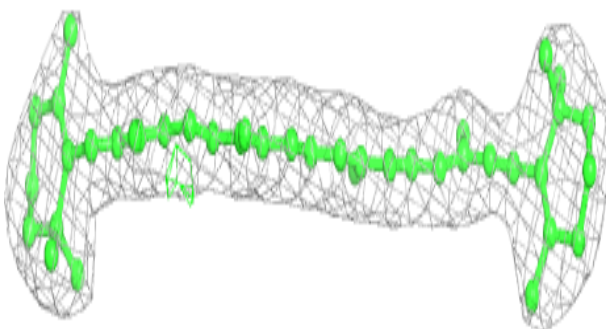
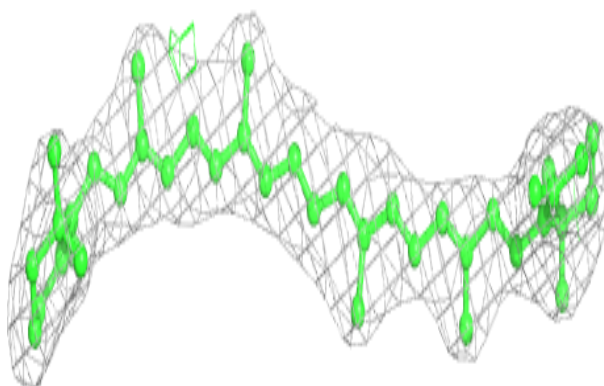


**Electron density around PL9 d 405:**

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

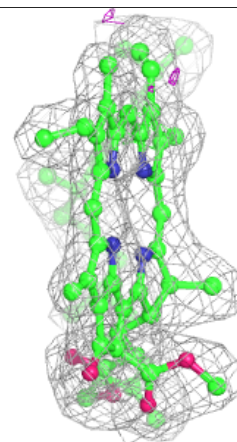
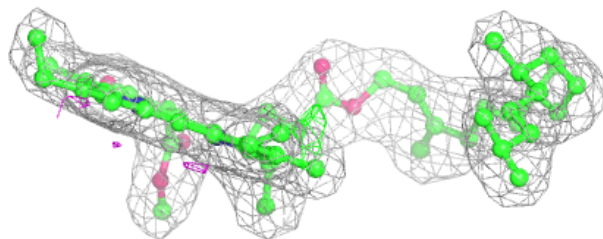
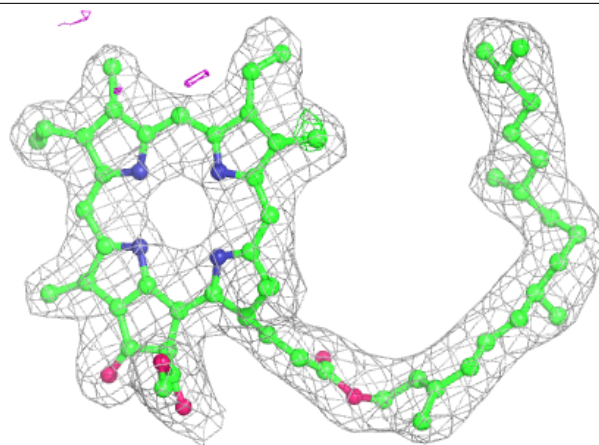
**Electron density around BCR c 516:**

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

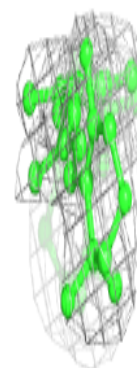
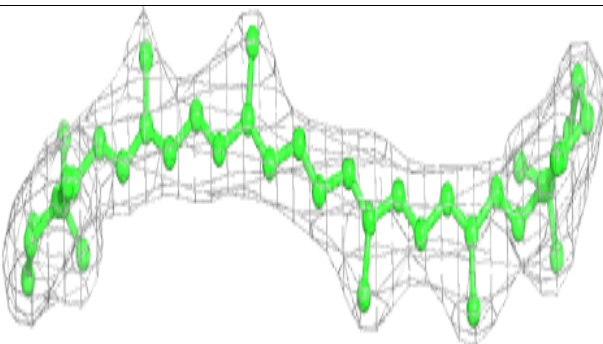
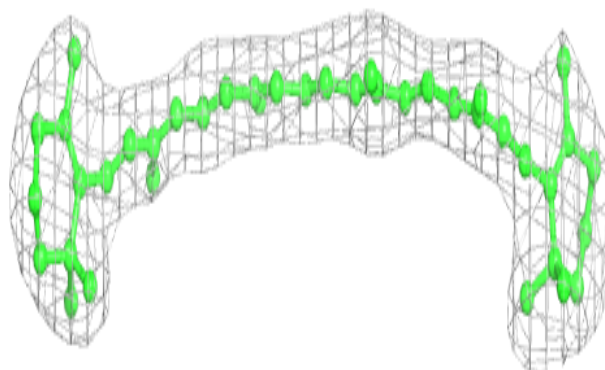


**Electron density around PHO a 408:**

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

**Electron density around BCR K 102:**

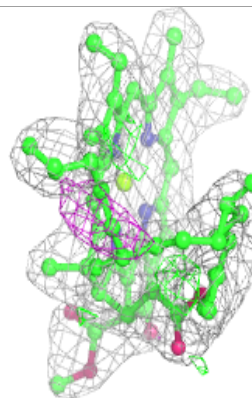
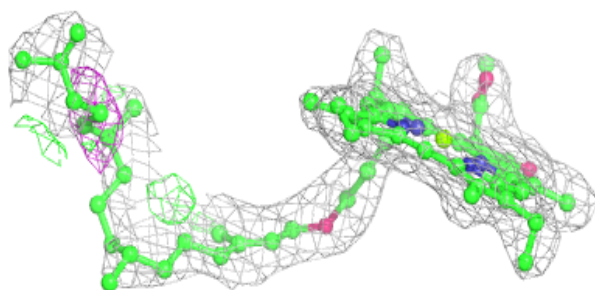
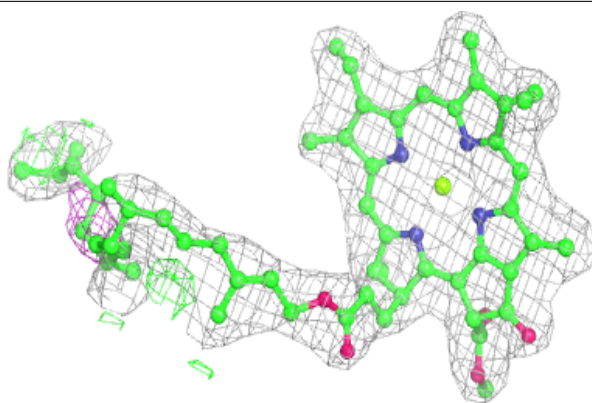
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



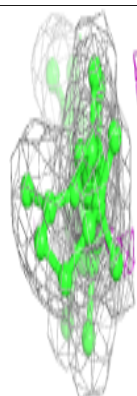
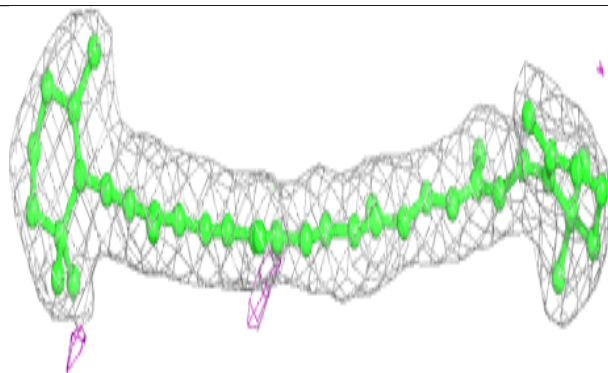
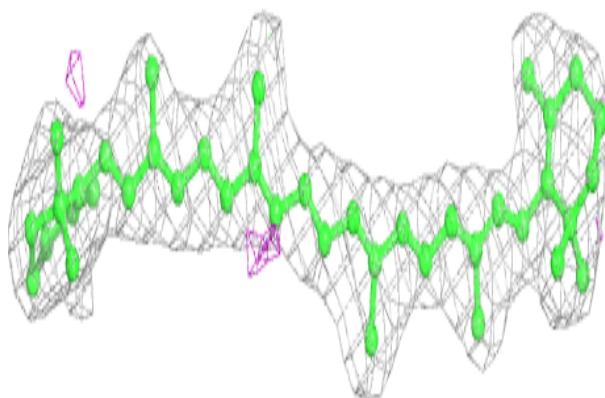


**Electron density around CLA a 409:**

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

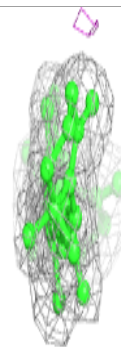
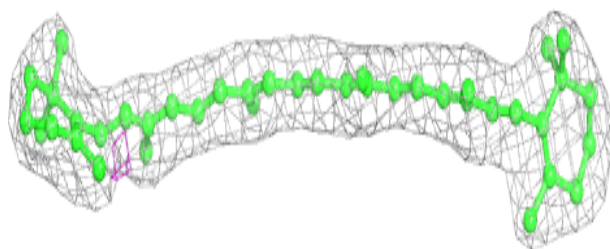
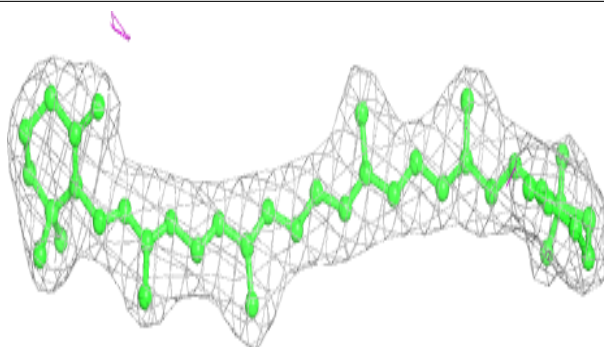
**Electron density around BCR b 617:**

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

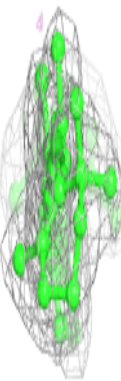
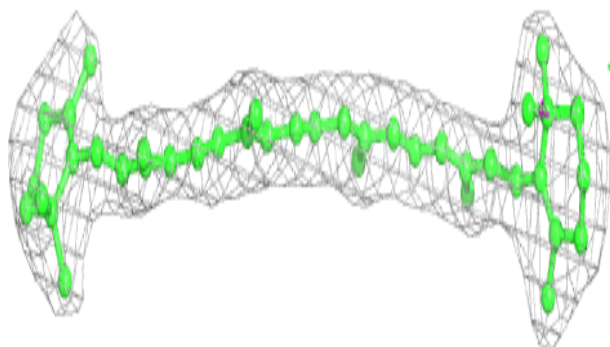
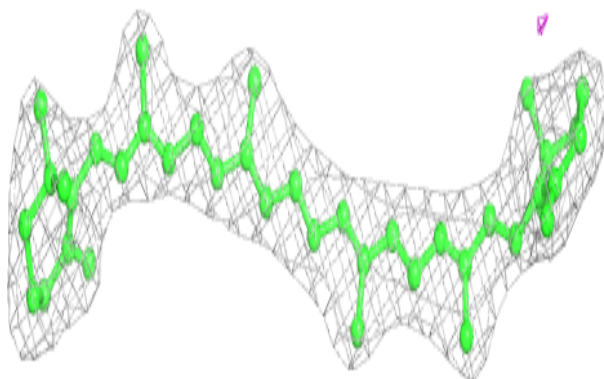


**Electron density around BCR B 617:**

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

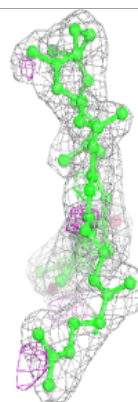
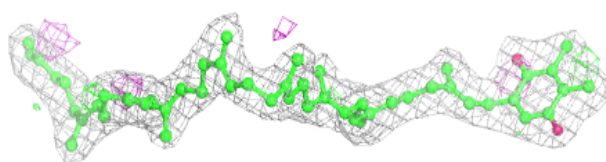
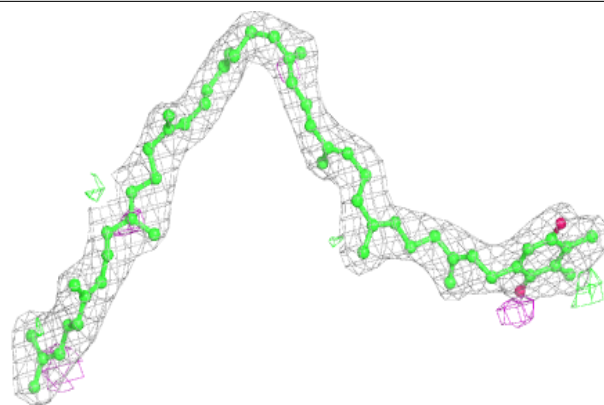
**Electron density around BCR Y 101:**

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

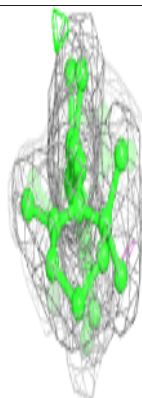
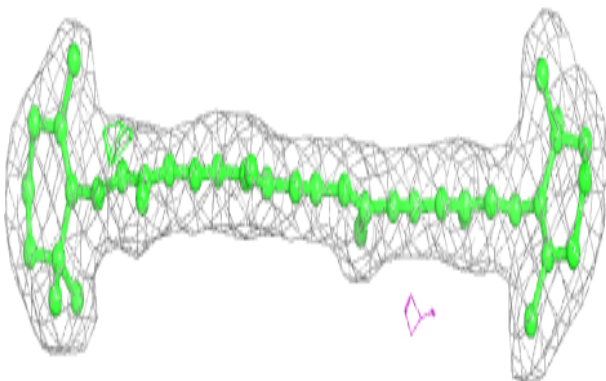
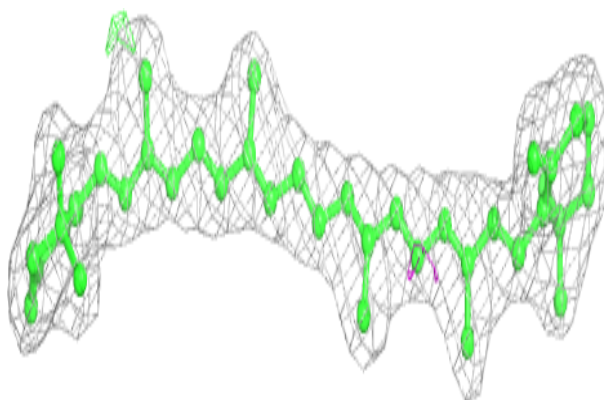


**Electron density around PL9 D 408:**

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

**Electron density around 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)



## 6.5 Other polymers

There are no such residues in this entry.