



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 04:55 AM BST

PDB ID : 5WS6
Title : Native XFEL structure of Photosystem II (preflash two-flash 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

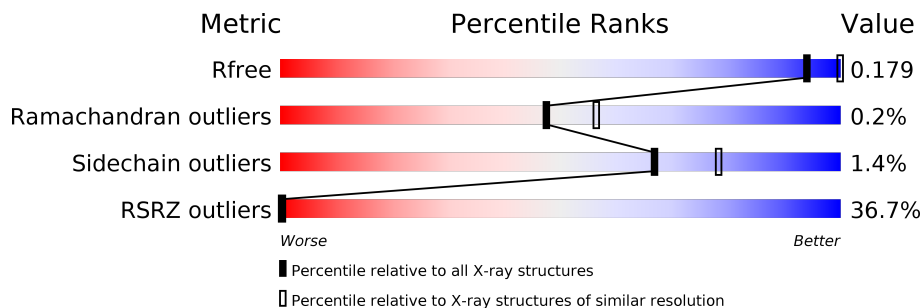
1 Overall quality at a glance

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 ≥ 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	
1	a	344	
2	B	505	
2	b	505	
3	C	455	
3	c	455	
4	D	342	

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Mol	Chain	Length	Quality of chain
4	d	342	30% 99%
5	E	84	48% 96%
5	e	84	73% 94% 6%
6	F	44	23% 77% 23%
6	f	44	34% 68% 30%
7	H	65	37% 94% 5%
7	h	65	43% 95%
8	I	38	32% 95% 5%
8	i	38	39% 92% 5%
9	J	39	41% 97%
9	j	39	62% 97%
10	K	37	35% 95% 5%
10	k	37	68% 92% 8%
11	L	37	27% 97%
11	l	37	19% 95%
12	M	36	17% 89% 8%
12	m	36	11% 92% 6%
13	O	244	33% 97%
13	o	244	39% 99%
14	T	32	9% 94% 6%
14	t	32	6% 88% 6% 6%
15	U	104	35% 90% 8%
15	u	104	19% 91% 7%
16	V	137	24% 99%
16	v	137	54% 99%

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Mol	Chain	Length	Quality of chain
17	X	40	
17	x	40	
18	Y	30	
18	y	30	
19	Z	62	
19	z	62	
20	R	34	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	A	404	X	-	-	-
24	CLA	A	405	X	-	-	-
24	CLA	A	406	X	-	-	-
24	CLA	A	409	X	-	-	-
24	CLA	B	601	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	C	514	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	a	350	X	-	-	-
24	CLA	a	403	X	-	-	-
24	CLA	a	404	X	-	-	-
24	CLA	a	407	X	-	-	-
24	CLA	b	601	X	-	-	-
24	CLA	b	602	X	-	-	-
24	CLA	b	603	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	X
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	c	514	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	c	515	X	-	-	-
24	CLA	d	402	X	-	-	-
24	CLA	d	403	X	-	-	-
27	SQD	A	411	-	-	-	X
27	SQD	A	413	-	-	-	X
27	SQD	B	620	-	-	-	X
27	SQD	a	411	-	-	-	X
27	SQD	b	620	-	-	-	X
27	SQD	f	101	-	-	-	X
28	GOL	V	202	-	-	-	X
28	GOL	v	202	-	-	-	X
31	PL9	a	414[A]	-	-	-	X
31	PL9	a	414[B]	-	-	-	X
32	UNL	A	417	-	-	-	X
32	UNL	B	629	-	-	-	X
32	UNL	D	409	-	-	-	X
32	UNL	K	101	-	-	-	X
32	UNL	a	415	-	-	-	X
32	UNL	d	409	-	-	-	X
32	UNL	d	410	-	-	-	X
32	UNL	i	101	-	-	-	X
32	UNL	j	102	-	-	-	X
32	UNL	m	101	-	-	-	X
33	LMG	A	418	-	-	-	X
33	LMG	B	621	-	-	-	X
33	LMG	C	520	-	-	-	X
33	LMG	C	521	-	-	-	X
33	LMG	Z	101	-	-	-	X
33	LMG	a	417	-	-	-	X
33	LMG	c	522	-	-	-	X
33	LMG	z	101	-	-	-	X
34	LMT	A	359	-	-	-	X
34	LMT	B	622	-	-	-	X
34	LMT	B	630	-	-	-	X
34	LMT	E	102	-	-	-	X
34	LMT	I	101	-	-	-	X
34	LMT	M	101	-	-	-	X
34	LMT	a	359	-	-	-	X
34	LMT	a	418	-	-	-	X
34	LMT	b	622	-	-	-	X
34	LMT	b	630	-	-	-	X
34	LMT	e	101	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	LMT	m	102	-	-	-	X
35	HTG	C	523	-	-	-	X
35	HTG	D	410	-	-	-	X
35	HTG	b	623	-	-	-	X
35	HTG	b	624	-	-	-	X
35	HTG	b	625	-	-	-	X
35	HTG	c	523	-	-	-	X
35	HTG	c	526	-	-	-	X
35	HTG	h	101	-	-	-	X
36	DGD	H	102	-	-	-	X
36	DGD	h	103	-	-	-	X
38	LHG	D	357	-	-	-	X
38	LHG	D	407	-	-	-	X
38	LHG	E	101	-	-	-	X
38	LHG	a	419	-	-	-	X

2 Entry composition i

There are 42 unique types of molecules in this entry. The entry contains 53280 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
			Total	C	N	O	S			
1	A	334	Total 2850	C 1865	N 467	O 502	S 16	0	29	0
1	a	334	Total 2852	C 1867	N 466	O 503	S 16	0	29	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	451	Total 3542	C 2315	N 590	O 624	S 13	0	10	0
3	c	455	Total 3577	C 2340	N 595	O 629	S 13	0	10	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	342	Total 2748	C 1819	N 450	O 467	S 12	0	3	0
4	d	341	Total 2739	C 1814	N 449	O 464	S 12	0	3	0

- 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 reaction center protein K.

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

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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 reaction center 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	5	0
			1889	1182	315	387	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	1
			2	2		

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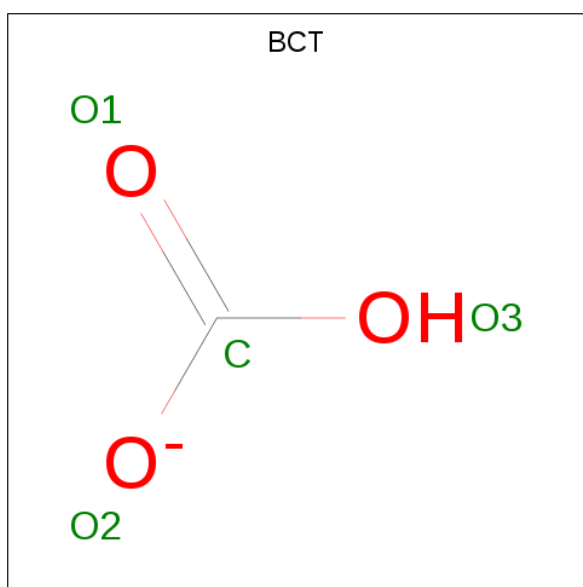
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	a	1	Total Fe 2 2	0	1

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

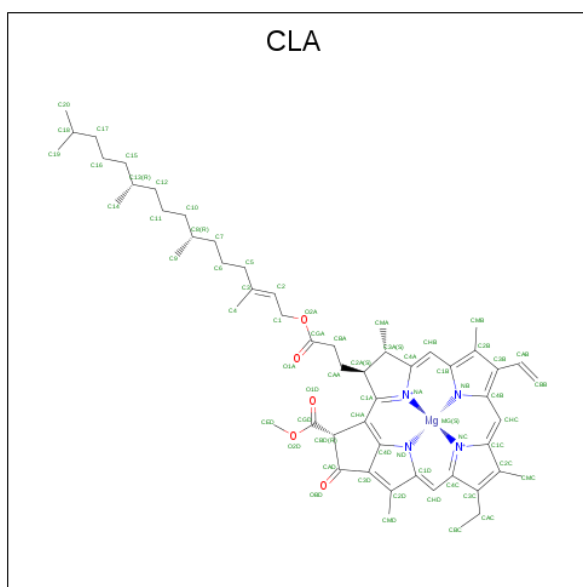
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	2	Total Cl 2 2	0	0
22	a	2	Total Cl 2 2	0	0

- Molecule 23 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O 8 2 6	0	1
23	a	1	Total C O 8 2 6	0	1

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$).



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

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

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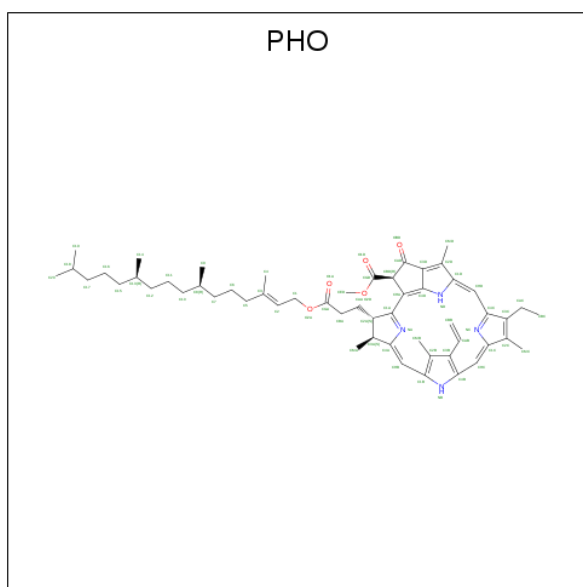
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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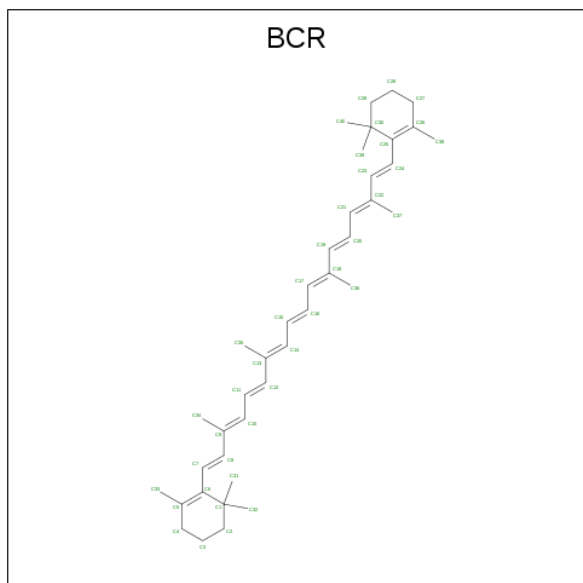
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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



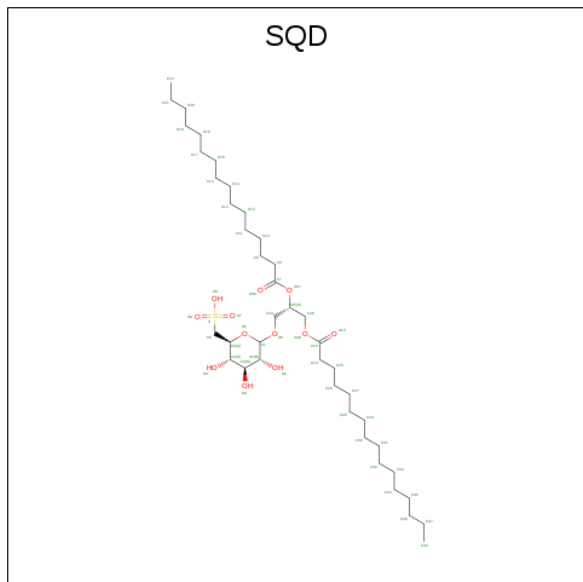
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
25	A	1	64	55	4	5	0	0
25	A	1	64	55	4	5	0	0
25	a	1	64	55	4	5	0	0
25	a	1	64	55	4	5	0	0

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



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

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



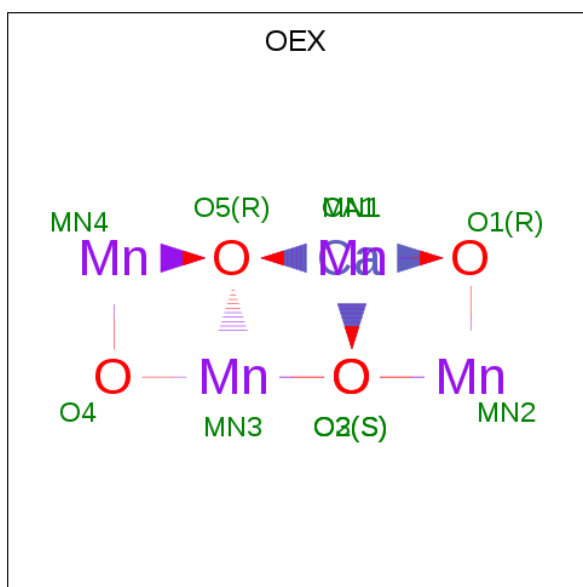
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
27	A	1	Total 54	C 41	O 12	S 1	0	0
27	A	1	Total 54	C 41	O 12	S 1	0	0
27	B	1	Total 54	C 41	O 12	S 1	0	0
27	F	1	Total 43	C 30	O 12	S 1	0	0
27	a	1	Total 54	C 41	O 12	S 1	0	0
27	a	1	Total 54	C 41	O 12	S 1	0	0
27	b	1	Total 54	C 41	O 12	S 1	0	0
27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

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



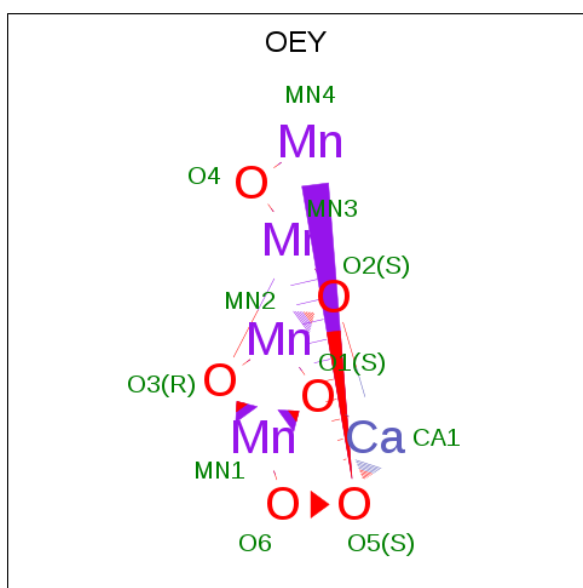
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	C	1	Total C O 6 3 3	0	0
28	V	1	Total C O 6 3 3	0	0
28	a	1	Total C O 6 3 3	0	0
28	a	1	Total C O 6 3 3	0	0
28	b	1	Total C O 6 3 3	0	0
28	c	1	Total C O 6 3 3	0	0
28	v	1	Total C O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

- Molecule 29 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



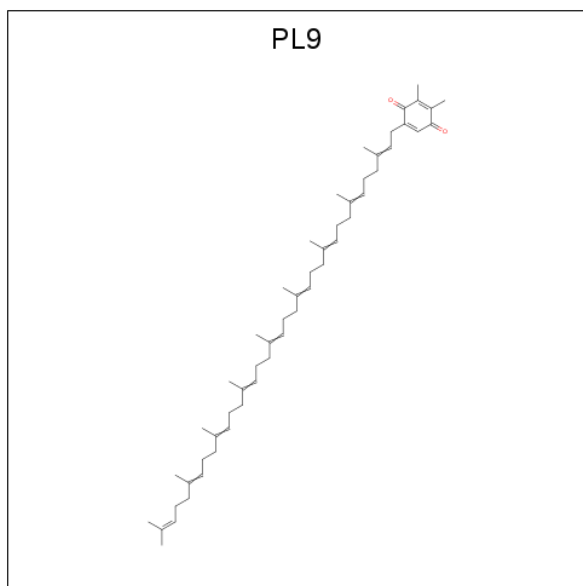
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Ca	Mn	O		
29	A	1	10	1	4	5	0	1
29	a	1	10	1	4	5	0	1

- Molecule 30 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula: CaMn_4O_6).



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

- Molecule 31 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	1
			110	106	4		
31	D	1	Total	C	O	0	0
			55	53	2		
31	a	1	Total	C	O	0	1
			110	106	4		
31	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 32 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

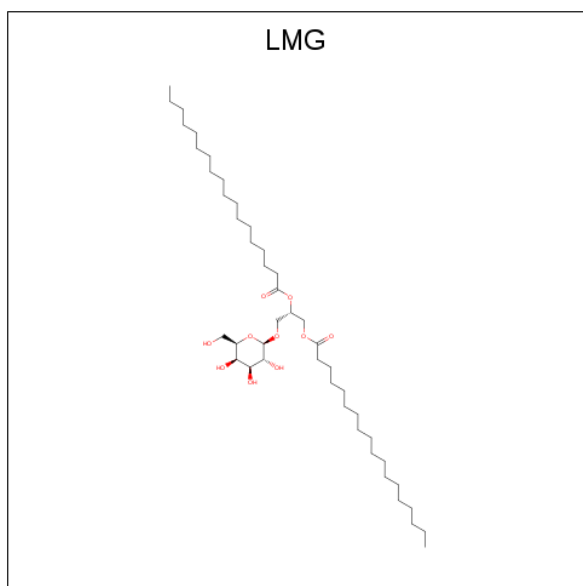
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	J	1	Total	C		0	0
			10	10			
32	i	1	Total	C	O	0	0
			40	35	5		
32	D	2	Total	C	O	0	0
			57	51	6		
32	K	1	Total	C	O	0	0
			34	29	5		
32	B	1	Total	C	O	0	0
			33	28	5		

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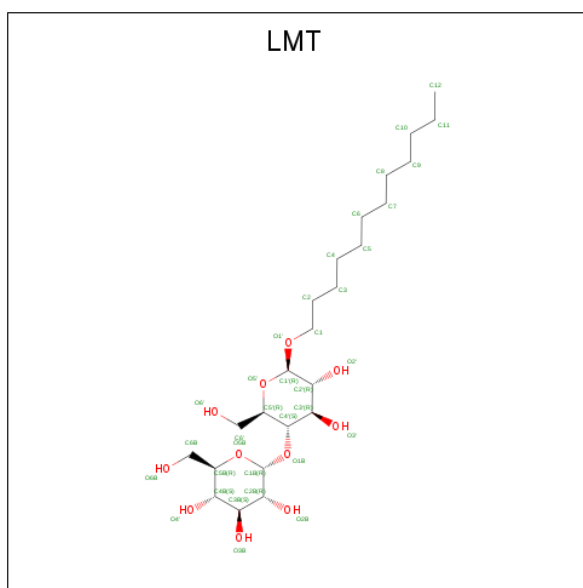
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	I	1	Total C O 40 35 5	0	0
32	c	1	Total C O 32 27 5	0	0
32	a	1	Total C O 30 25 5	0	0
32	x	1	Total C O 18 16 2	0	0
32	A	1	Total C O 28 23 5	0	0
32	j	1	Total C 10 10	0	0
32	X	1	Total C O 18 16 2	0	0
32	d	2	Total C O 53 47 6	0	0
32	m	1	Total C 10 10	0	0
32	b	1	Total C O 33 28 5	0	0
32	M	1	Total C 10 10	0	0

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



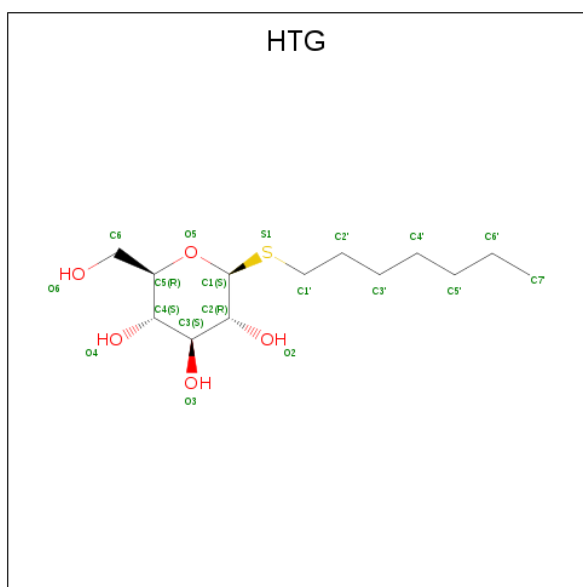
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	A	1	Total	C	O	0	0
			51	41	10		
33	B	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	J	1	Total	C	O	0	0
			51	41	10		
33	Z	1	Total	C	O	0	0
			37	27	10		
33	a	1	Total	C	O	0	0
			51	41	10		
33	b	1	Total	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	j	1	Total	C	O	0	0
			51	41	10		
33	z	1	Total	C	O	0	0
			39	29	10		

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



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

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



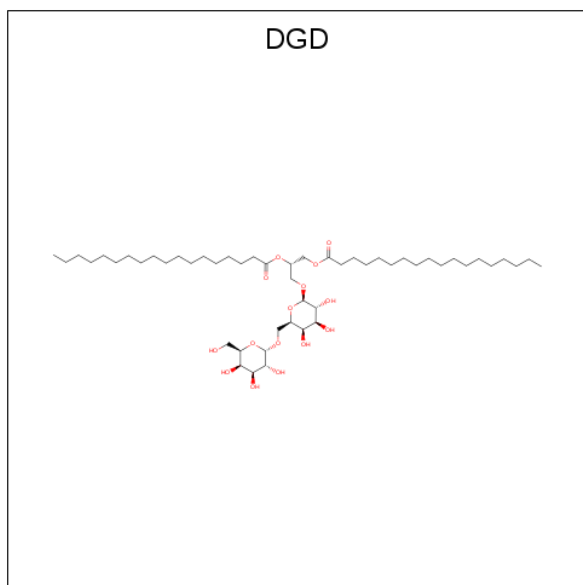
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
35	B	1	19	13	5	1	0	0
35	B	1	19	13	5	1	0	0
35	B	1	19	13	5	1	0	0
35	B	1	19	13	5	1	0	0
35	C	1	19	13	5	1	0	0
35	C	1	19	13	5	1	0	0
35	D	1	16	10	5	1	0	0
35	V	1	11	6	5		0	0
35	b	1	19	13	5	1	0	0
35	b	1	19	13	5	1	0	0
35	b	1	19	13	5	1	0	0
35	b	1	19	13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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
35	h	1	16	10	5	1	0	0

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

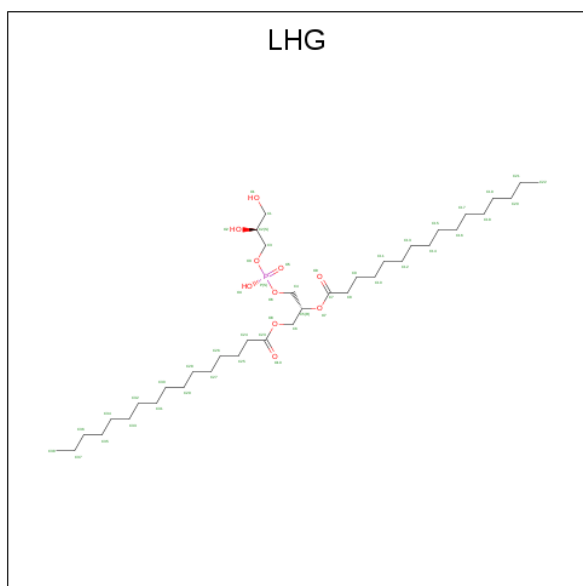


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
36	C	1	62	47	15	0	0
36	C	1	62	47	15	0	0
36	C	1	62	47	15	0	0
36	H	1	62	47	15	0	0
36	c	1	62	47	15	0	0
36	c	1	62	47	15	0	0
36	c	1	62	47	15	0	0
36	h	1	62	47	15	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	b	1	Total Ca 1 1	0	0
37	C	1	Total Ca 1 1	0	0
37	V	1	Total Ca 1 1	0	0
37	c	2	Total Ca 2 2	0	0
37	v	1	Total Ca 1 1	0	0
37	O	1	Total Ca 1 1	0	0
37	o	1	Total Ca 1 1	0	0

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



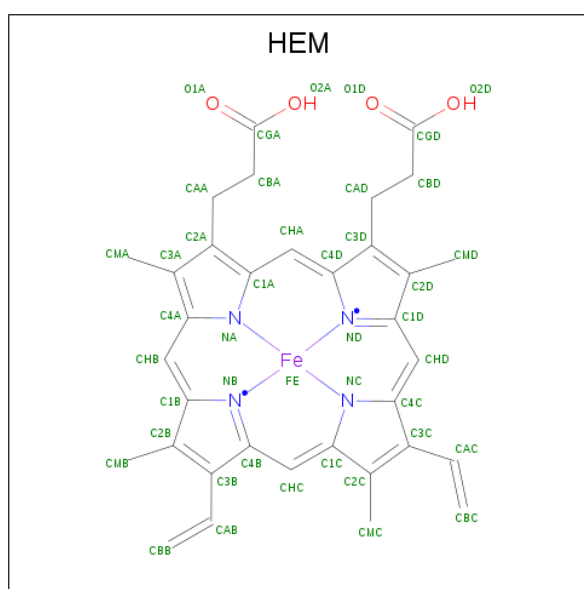
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	D	1	Total C O P 49 38 10 1	0	0
38	D	1	Total C O P 49 38 10 1	0	0
38	D	1	Total C O P 49 38 10 1	0	0
38	E	1	Total C O P 42 31 10 1	0	0

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

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



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

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

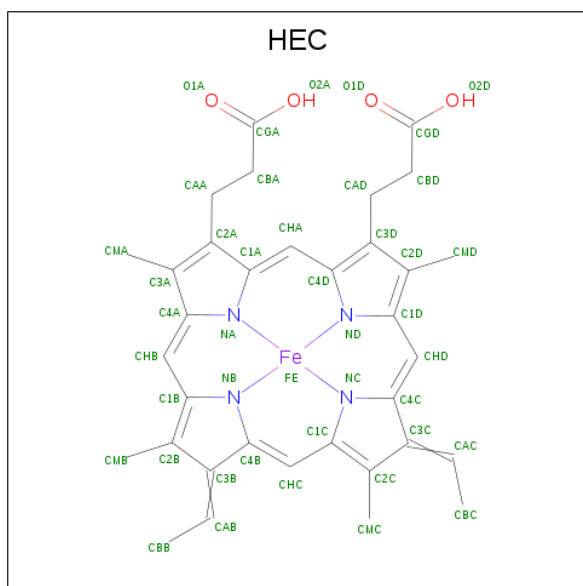
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	J	1	Total	Mg	0	0
			1	1		

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

- Molecule 41 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 42 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
42	A	125	Total O 130 130	0	5
42	B	164	Total O 164 164	0	0
42	C	147	Total O 147 147	0	0
42	D	112	Total O 112 112	0	0
42	E	14	Total O 14 14	0	0
42	F	4	Total O 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
42	H	20	Total O 20 20	0	0
42	I	6	Total O 6 6	0	0
42	J	4	Total O 4 4	0	0
42	K	7	Total O 7 7	0	0
42	L	4	Total O 4 4	0	0
42	M	7	Total O 7 7	0	0
42	O	74	Total O 74 74	0	0
42	T	8	Total O 8 8	0	0
42	U	33	Total O 33 33	0	0
42	V	65	Total O 65 65	0	0
42	X	2	Total O 2 2	0	0
42	Y	1	Total O 1 1	0	0
42	a	128	Total O 133 133	0	5
42	b	185	Total O 185 185	0	0
42	c	122	Total O 122 122	0	0
42	d	109	Total O 109 109	0	0
42	e	7	Total O 7 7	0	0
42	f	3	Total O 3 3	0	0
42	h	14	Total O 14 14	0	0
42	i	3	Total O 3 3	0	0
42	j	2	Total O 2 2	0	0

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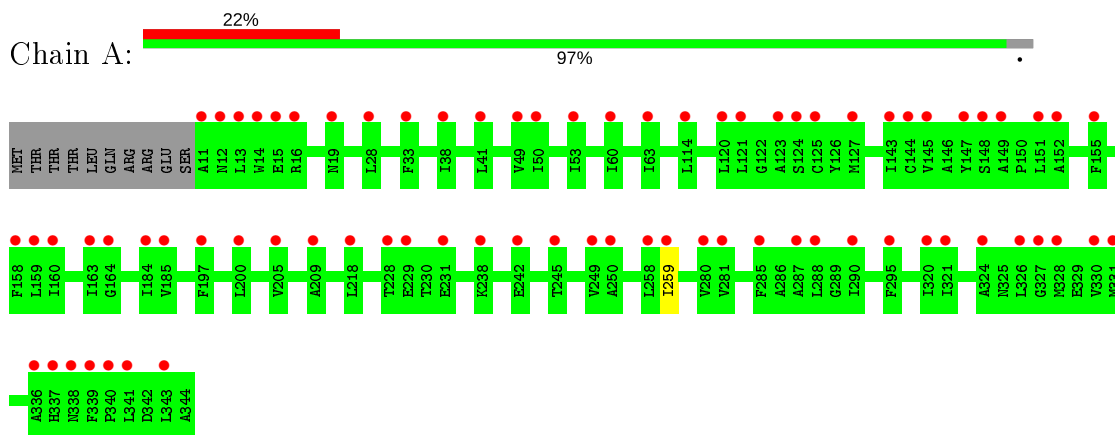
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
42	k	3	Total O 3 3	0	0
42	l	6	Total O 6 6	0	0
42	m	11	Total O 11 11	0	0
42	o	78	Total O 78 78	0	0
42	t	5	Total O 5 5	0	0
42	u	47	Total O 47 47	0	0
42	v	49	Total O 49 49	0	0
42	x	4	Total O 4 4	0	0
42	y	1	Total O 1 1	0	0

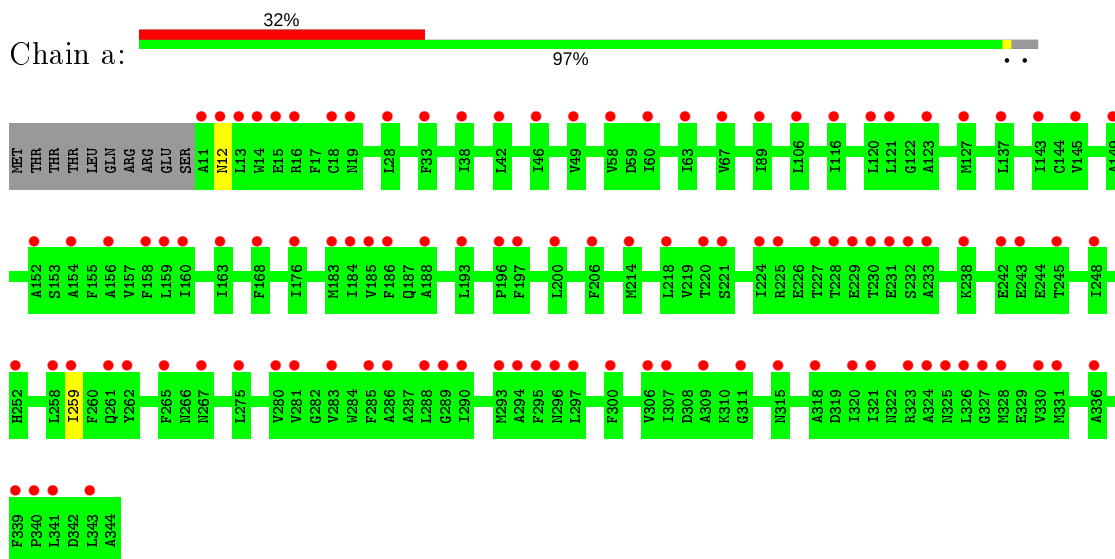
3 Residue-property plots [i](#)

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

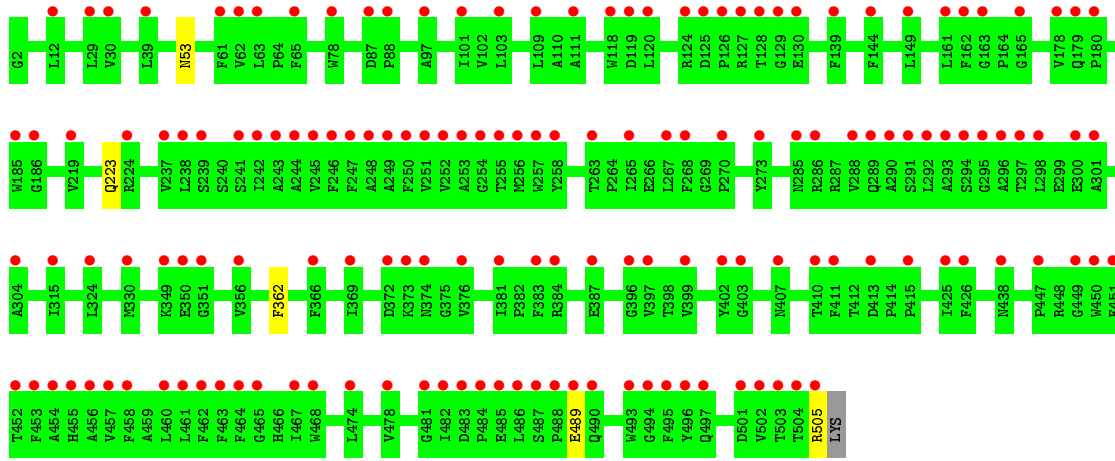


- Molecule 1: Photosystem II D1 protein

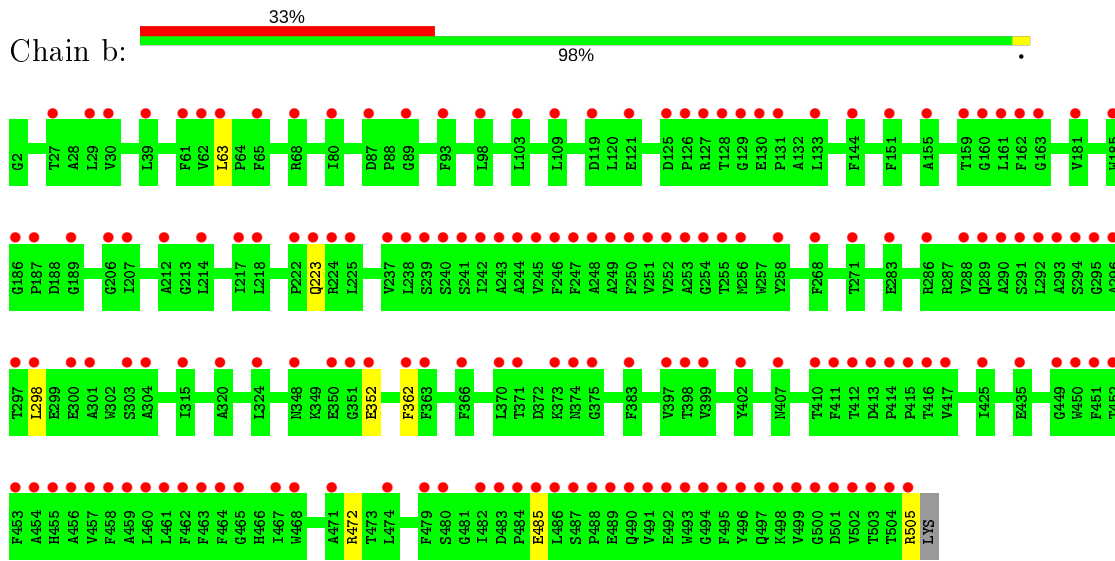


- Molecule 2: Photosystem II CP47 reaction center protein

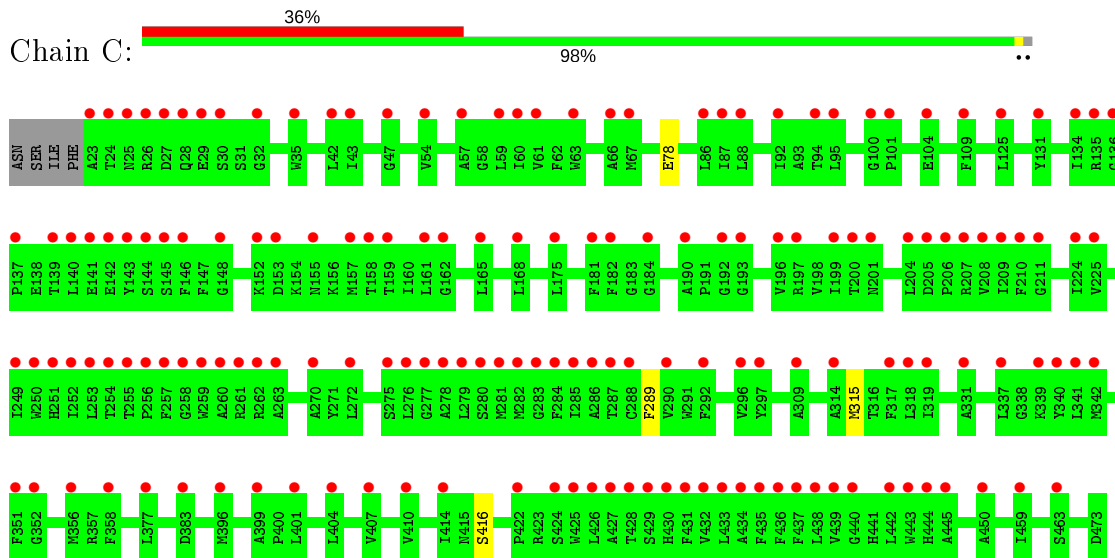




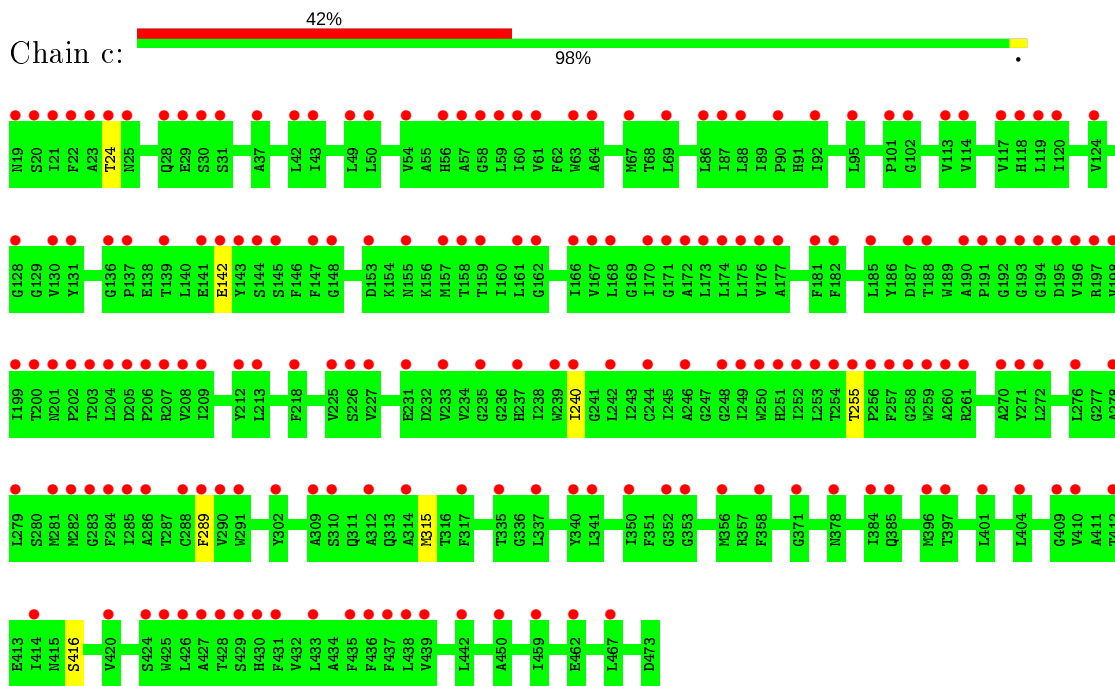
• Molecule 2: Photosystem II CP47 reaction center protein



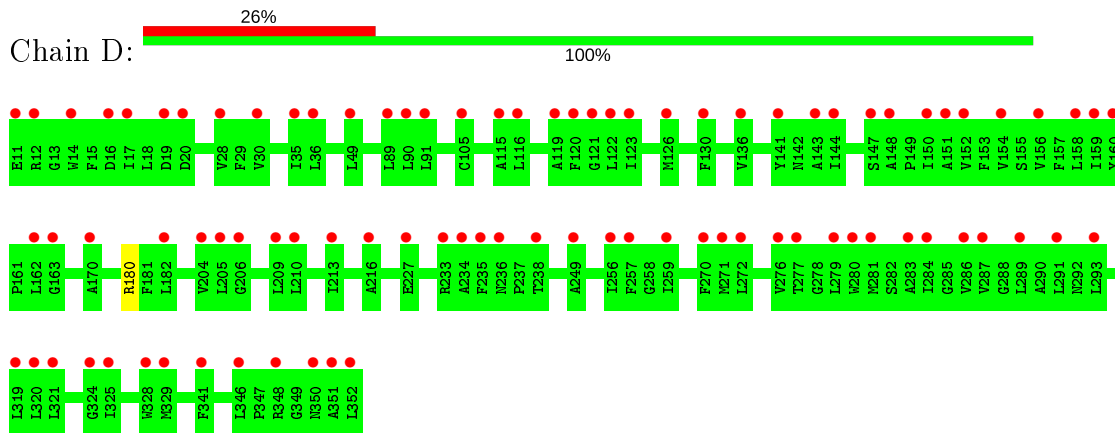
• Molecule 3: Photosystem II CP43 chlorophyll protein



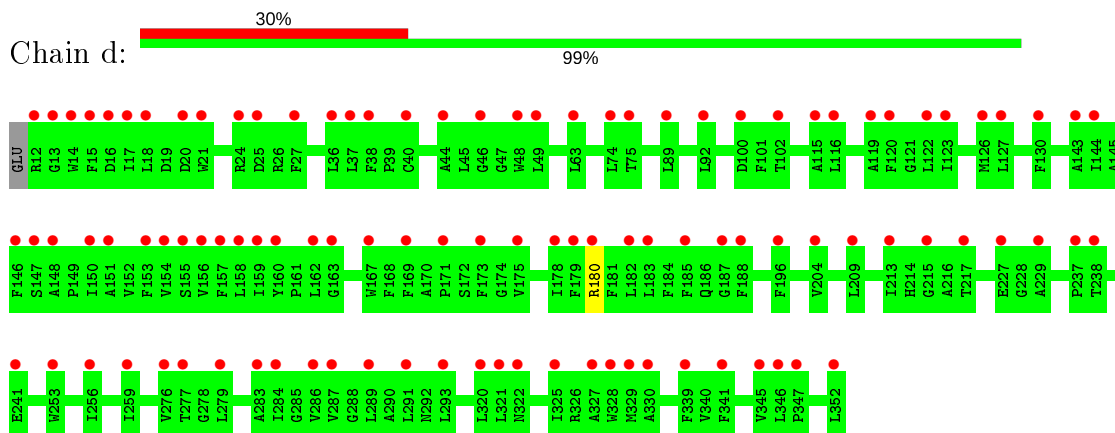
- Molecule 3: Photosystem II CP43 chlorophyll protein



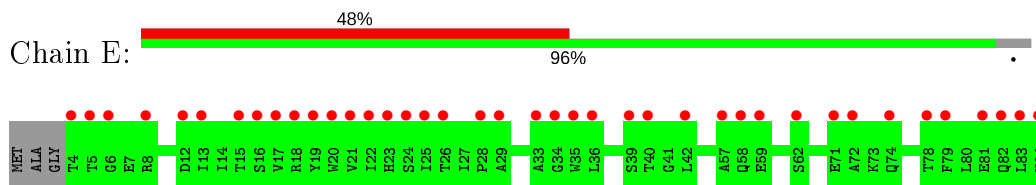
- Molecule 4: Photosystem II D2 protein



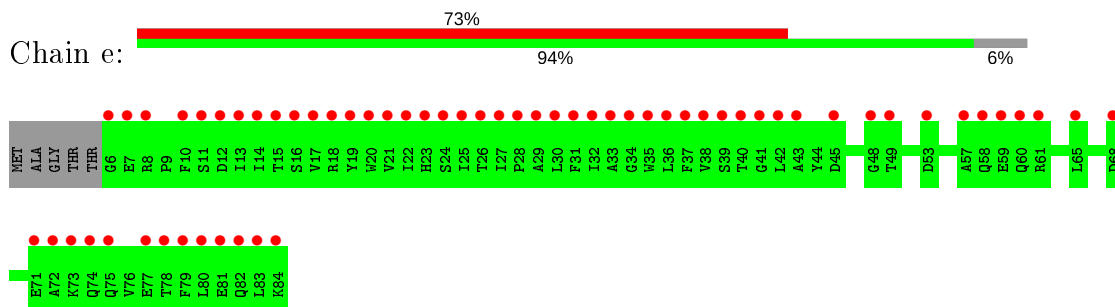
- Molecule 4: Photosystem II D2 protein



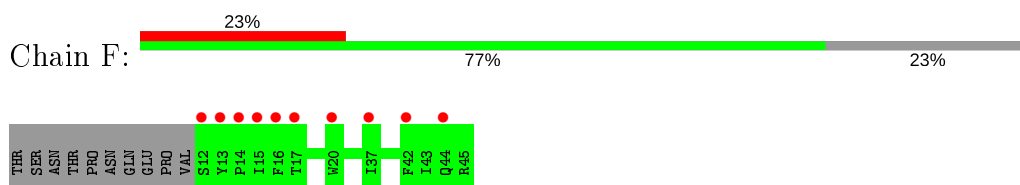
- Molecule 5: Cytochrome b559 subunit alpha



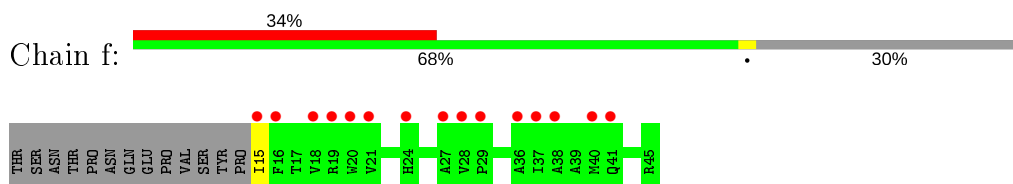
- Molecule 5: Cytochrome b559 subunit alpha



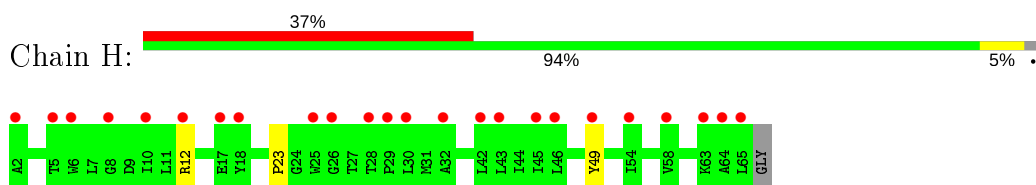
- Molecule 6: Cytochrome b559 subunit beta



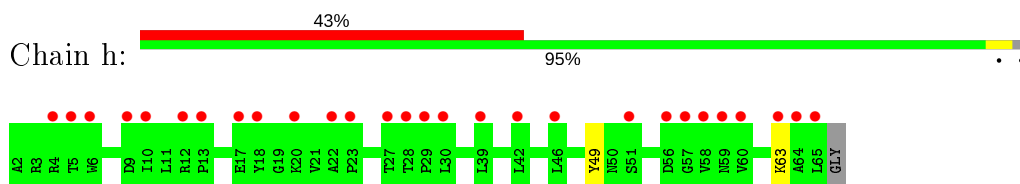
- Molecule 6: Cytochrome b559 subunit beta



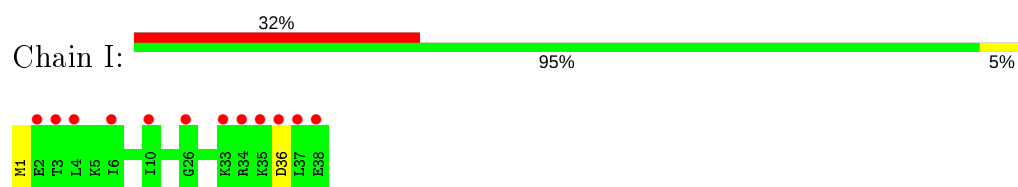
- Molecule 7: Photosystem II reaction center protein H



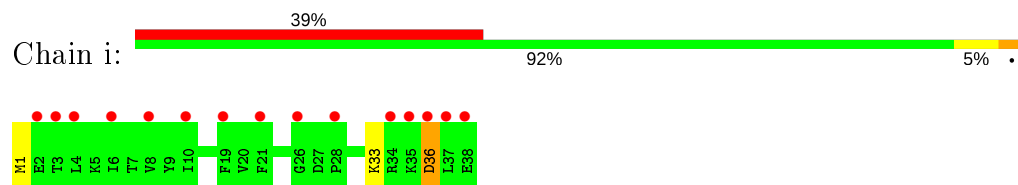
- Molecule 7: Photosystem II reaction center protein H



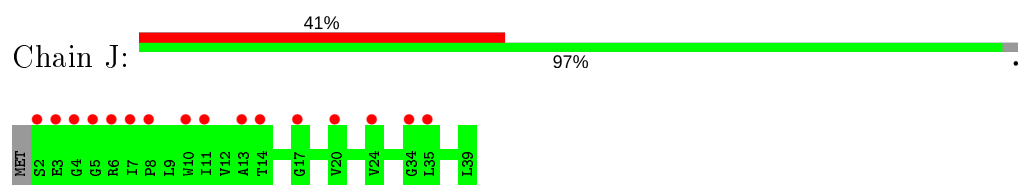
- Molecule 8: Photosystem II reaction center protein I



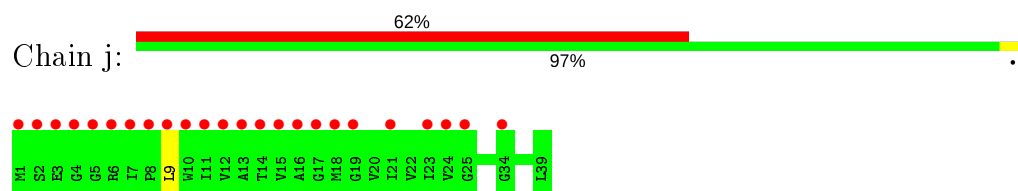
- Molecule 8: Photosystem II reaction center protein I



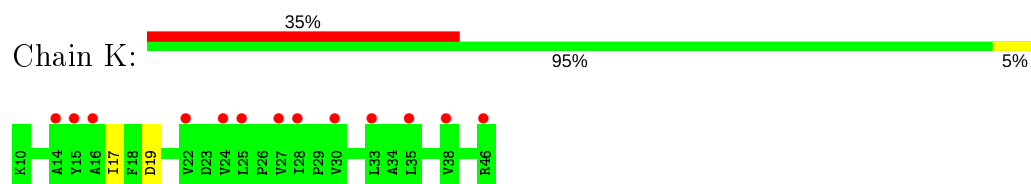
- Molecule 9: Photosystem II reaction center protein J



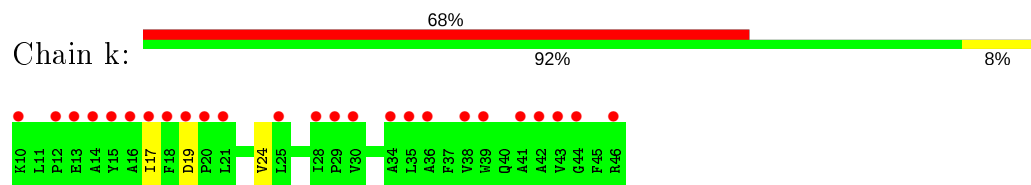
- Molecule 9: Photosystem II reaction center protein J



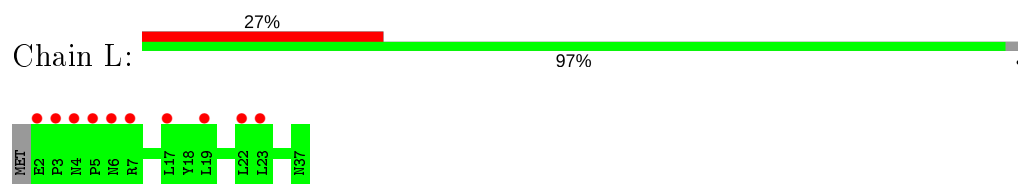
- Molecule 10: Photosystem II reaction center protein K



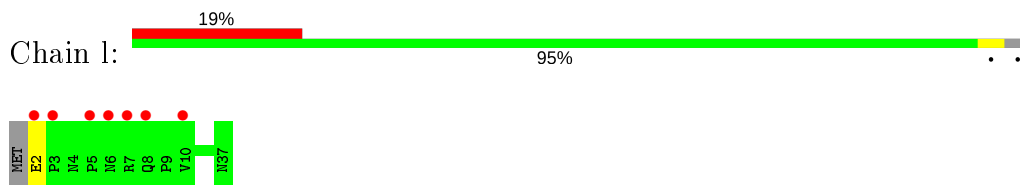
- Molecule 10: Photosystem II reaction center protein K



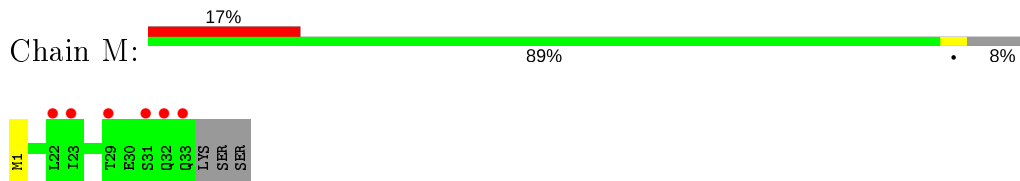
- Molecule 11: Photosystem II reaction center protein L



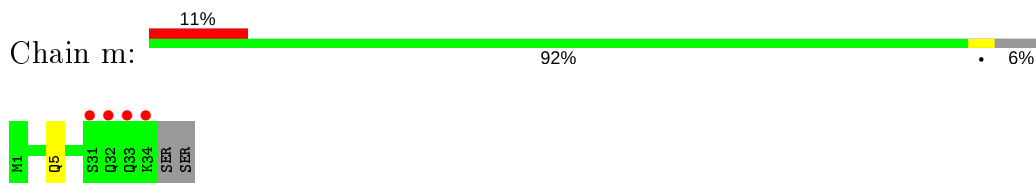
- Molecule 11: Photosystem II reaction center protein L



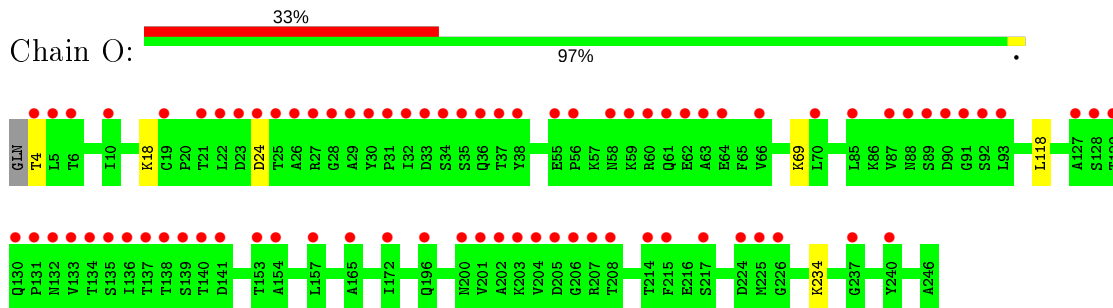
- Molecule 12: Photosystem II reaction center protein M



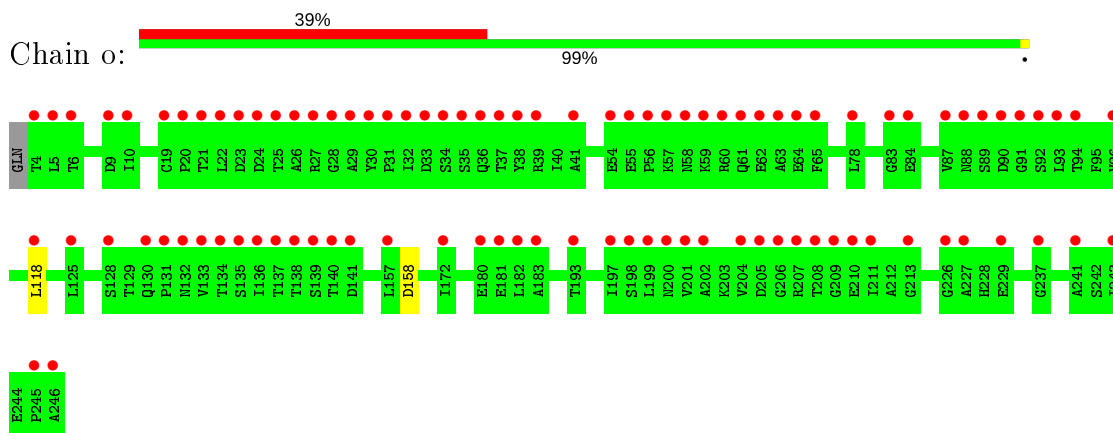
- Molecule 12: Photosystem II reaction center protein M



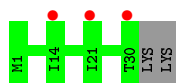
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



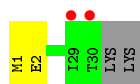
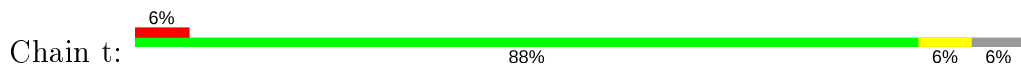
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



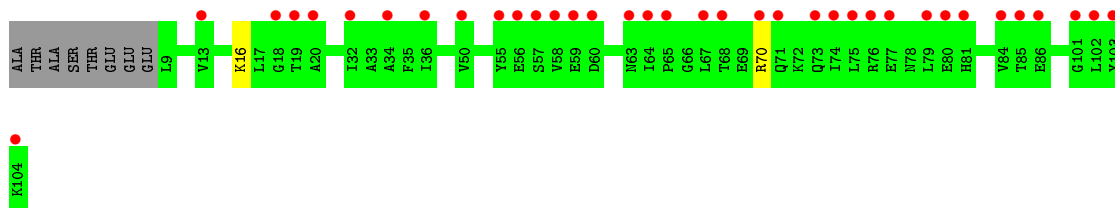
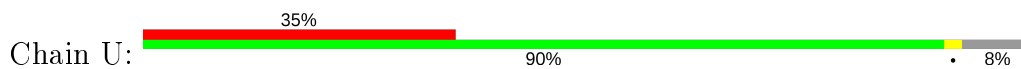
- Molecule 14: Photosystem II reaction center protein T



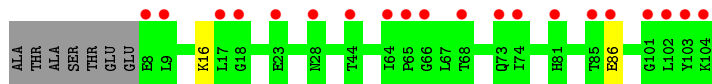
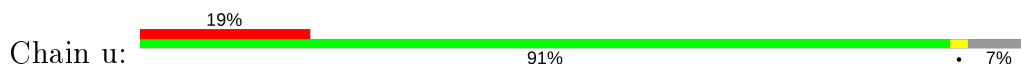
• Molecule 14: Photosystem II reaction center protein T



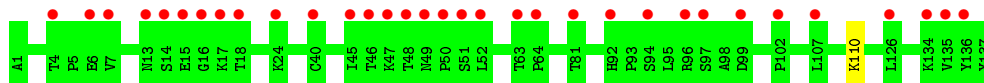
• Molecule 15: Photosystem II 12 kDa extrinsic protein



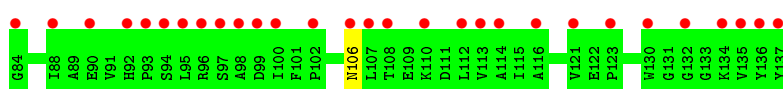
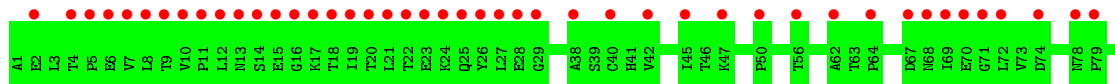
• Molecule 15: Photosystem II 12 kDa extrinsic protein



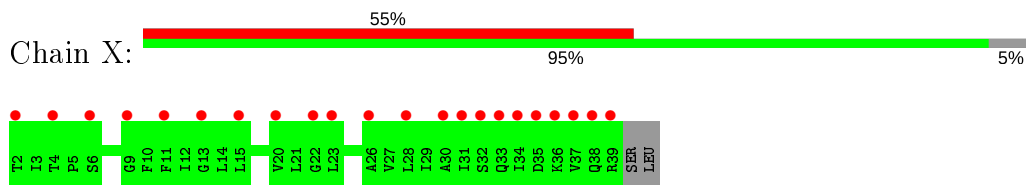
• Molecule 16: Cytochrome c-550



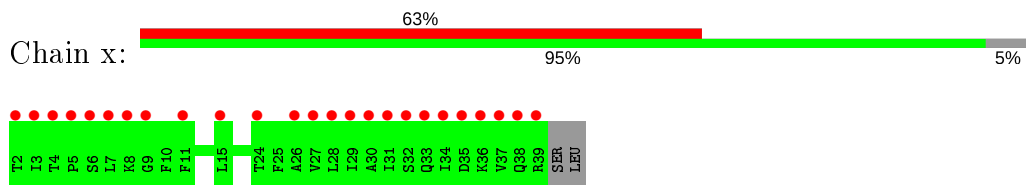
• Molecule 16: Cytochrome c-550



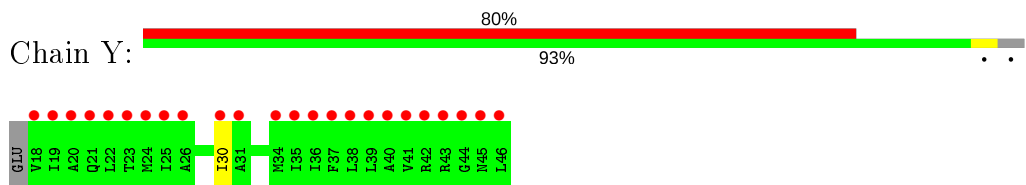
- Molecule 17: Photosystem II reaction center protein X



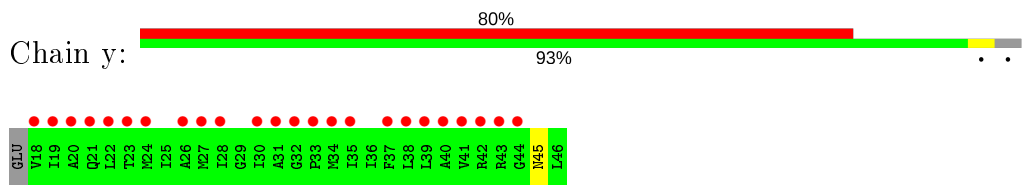
- Molecule 17: Photosystem II reaction center protein X



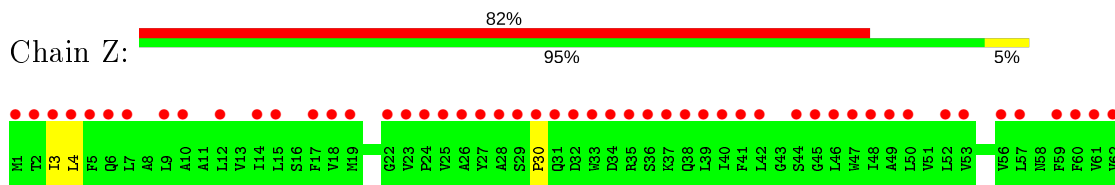
- Molecule 18: Photosystem II reaction center protein Ycf12



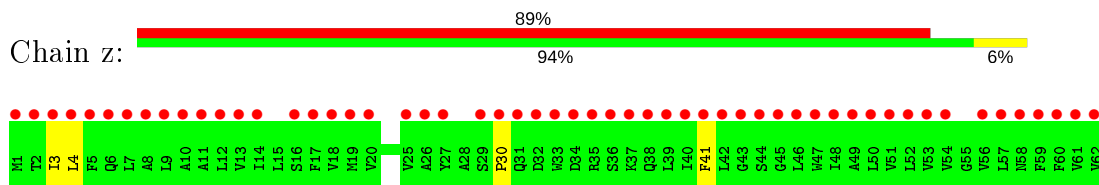
- Molecule 18: Photosystem II reaction center protein Ycf12



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



D2
W3
R4
V5
L6
V7
V8
L9
L10
P11
V12
L13
L14
A15
A16
G17
W18
A19
V20
R21
N22
Y23
L24
P25
Y26
A27
V28
K29
Q30
V31
Q32
K33
L34
L35

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	124.96Å 230.22Å 286.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35 47.05 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.35) 100.0 (47.05-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.34Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.129 , 0.175 0.136 , 0.179	Depositor DCC
R_{free} test set	17119 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	58.3	Xtrriage
Anisotropy	0.387	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 80.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	53280	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PL9, BCT, BCR, DGD, FE2, LHG, GOL, CL, CA, CLA, HEC, HEM, FME, UNL, HTG, MG, OEX, PHO, LMT, OEY, LMG, 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	0.50	0/2952	0.59	0/4019
1	a	0.43	0/2957	0.55	0/4027
2	B	0.43	0/4171	0.54	0/5683
2	b	0.41	0/4138	0.53	0/5640
3	C	0.42	0/3667	0.53	0/4992
3	c	0.38	0/3703	0.50	0/5041
4	D	0.46	0/2847	0.56	0/3878
4	d	0.43	0/2838	0.53	0/3866
5	E	0.36	0/687	0.50	0/936
5	e	0.35	0/667	0.47	0/908
6	F	0.42	0/284	0.50	0/387
6	f	0.38	0/257	0.53	0/349
7	H	0.37	0/530	0.57	0/723
7	h	0.33	0/519	0.50	0/708
8	I	0.37	0/311	0.48	0/419
8	i	0.34	0/311	0.49	0/419
9	J	0.34	0/278	0.46	0/376
9	j	0.32	0/283	0.46	0/383
10	K	0.37	0/303	0.51	0/416
10	k	0.34	0/303	0.49	0/416
11	L	0.43	0/311	0.47	0/423
11	l	0.41	0/311	0.49	0/423
12	M	0.45	0/261	0.61	0/357
12	m	0.42	0/262	0.59	0/357
13	O	0.39	0/1935	0.56	0/2623
13	o	0.39	0/1910	0.57	1/2589 (0.0%)
14	T	0.49	0/257	0.55	0/349
14	t	0.47	0/257	0.51	0/349
15	U	0.38	0/776	0.54	0/1052
15	u	0.37	0/785	0.54	0/1064
16	V	0.38	0/1085	0.49	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.34	0/1085	0.48	0/1473
17	X	0.33	0/284	0.46	0/384
17	x	0.31	0/284	0.45	0/384
18	Y	0.29	0/216	0.44	0/289
18	y	0.30	0/216	0.47	0/289
19	Z	0.31	0/490	0.44	0/669
19	z	0.29	0/490	0.39	0/669
20	R	0.28	0/279	0.39	0/383
All	All	0.41	0/43500	0.53	1/59185 (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	5.06	122.86	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	359/344 (104%)	355 (99%)	3 (1%)	1 (0%)	41	47
1	a	360/344 (105%)	355 (99%)	4 (1%)	1 (0%)	41	47
2	B	510/505 (101%)	506 (99%)	4 (1%)	0	100	100
2	b	506/505 (100%)	497 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	459/455 (101%)	447 (97%)	10 (2%)	2 (0%)	34	38
3	c	463/455 (102%)	449 (97%)	12 (3%)	2 (0%)	34	38
4	D	343/342 (100%)	333 (97%)	10 (3%)	0	100	100
4	d	342/342 (100%)	336 (98%)	6 (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%)	59 (95%)	2 (3%)	1 (2%)	9	8
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	5	2
9	J	36/39 (92%)	35 (97%)	1 (3%)	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%)	30 (94%)	2 (6%)	0	100	100
13	O	246/244 (101%)	237 (96%)	9 (4%)	0	100	100
13	o	243/244 (100%)	238 (98%)	5 (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%)	92 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
17	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
17	x	36/40 (90%)	36 (100%)	0	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%)	58 (97%)	1 (2%)	1 (2%)	9	7
19	z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9	7
20	R	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5316/5384 (99%)	5202 (98%)	104 (2%)	10 (0%)	47	56

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	i	36	ASP
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
19	z	30	PRO
1	a	259	ILE
7	h	63	LYS
19	Z	30	PRO
1	A	259	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	295/279 (106%)	295 (100%)	0	100	100
1	a	296/279 (106%)	295 (100%)	1 (0%)	92	96
2	B	410/403 (102%)	405 (99%)	5 (1%)	71	82
2	b	406/403 (101%)	398 (98%)	8 (2%)	55	66
3	C	360/356 (101%)	357 (99%)	3 (1%)	81	89
3	c	364/356 (102%)	358 (98%)	6 (2%)	62	75
4	D	280/277 (101%)	279 (100%)	1 (0%)	91	95
4	d	279/277 (101%)	278 (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%)	24 (96%)	1 (4%)	31	39
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%)	33 (97%)	1 (3%)	42	52
8	i	34/34 (100%)	32 (94%)	2 (6%)	19	22
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	26/27 (96%)	25 (96%)	1 (4%)	33	41
10	K	30/30 (100%)	28 (93%)	2 (7%)	16	17
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%)	34 (97%)	1 (3%)	42	52
12	M	30/32 (94%)	30 (100%)	0	100	100
12	m	30/32 (94%)	29 (97%)	1 (3%)	38	46
13	O	211/207 (102%)	205 (97%)	6 (3%)	43	53
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%)	25 (96%)	1 (4%)	33	41
15	U	83/89 (93%)	81 (98%)	2 (2%)	49	59
15	u	84/89 (94%)	82 (98%)	2 (2%)	49	59
16	V	117/117 (100%)	116 (99%)	1 (1%)	78	87
16	v	117/117 (100%)	116 (99%)	1 (1%)	78	87
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%)	21 (96%)	1 (4%)	27	33
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	4416/4403 (100%)	4353 (99%)	63 (1%)	67 78

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	53	ASN
2	B	223	GLN
2	B	362	PHE
2	B	489	GLU
2	B	505	ARG
3	C	78	GLU
3	C	289	PHE
3	C	315	MET
4	D	180	ARG
7	H	12[A]	ARG
7	H	12[B]	ARG
7	H	23	PRO
7	H	49	TYR
8	I	36	ASP
10	K	17	ILE
10	K	19	ASP
13	O	4	THR
13	O	18	LYS
13	O	24	ASP
13	O	69	LYS
13	O	118	LEU
13	O	234	LYS
15	U	16	LYS
15	U	70	ARG
16	V	110	LYS
18	Y	30	ILE
19	Z	3	ILE
19	Z	4	LEU
1	a	12	ASN
2	b	63	LEU
2	b	223	GLN
2	b	298	LEU
2	b	352	GLU
2	b	362	PHE
2	b	472	ARG
2	b	485	GLU
2	b	505	ARG

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Mol	Chain	Res	Type
3	c	24	THR
3	c	142	GLU
3	c	240	ILE
3	c	255	THR
3	c	289	PHE
3	c	315	MET
4	d	180	ARG
6	f	15	ILE
7	h	49	TYR
8	i	33	LYS
8	i	36	ASP
9	j	9	LEU
10	k	17	ILE
10	k	19	ASP
10	k	24	VAL
11	l	2	GLU
12	m	5	GLN
13	o	118	LEU
14	t	2	GLU
15	u	16	LYS
15	u	86	GLU
16	v	106	ASN
18	y	45	ASN
19	z	3	ILE
19	z	4	LEU
19	z	41	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	75	ASN
2	B	53	ASN
2	B	331	ASN
4	D	61	HIS
4	D	83	ASN
4	D	142	ASN
5	E	60	GLN
13	O	124	ASN
15	U	73	GLN
15	U	78	ASN
15	U	81	HIS

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Mol	Chain	Res	Type
19	Z	58	ASN
2	b	53	ASN
2	b	223	GLN
2	b	289	GLN
2	b	331	ASN
3	c	201	ASN
4	d	83	ASN
5	e	60	GLN
5	e	75	GLN
6	f	44	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	0.64	0	7,9,11	1.21	1 (14%)
12	FME	m	1	12	8,9,10	0.56	0	7,9,11	1.30	0
8	FME	I	1	8	8,9,10	0.62	0	7,9,11	1.06	1 (14%)
14	FME	t	1	14	8,9,10	0.66	0	7,9,11	1.57	2 (28%)
8	FME	i	1	8	8,9,10	0.65	0	7,9,11	1.22	1 (14%)
14	FME	T	1	14	8,9,10	0.63	0	7,9,11	1.37	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	O-C-CA	-2.72	117.64	124.78
14	t	1	FME	C-CA-N	2.26	113.81	109.73
12	M	1	FME	O-C-CA	-2.09	119.30	124.78
8	I	1	FME	O-C-CA	-2.05	119.39	124.78
8	i	1	FME	O-C-CA	-2.03	119.46	124.78

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 227 ligands modelled in this entry, 18 are unknown and 18 are monoatomic - leaving 191 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	SQD	f	101	-	42,43,54	1.17	3 (7%)	51,54,65	1.43	9 (17%)
24	CLA	C	508	42	59,73,73	1.95	13 (22%)	67,113,113	2.17	23 (34%)
26	BCR	C	515	-	41,41,41	1.03	1 (2%)	56,56,56	1.50	8 (14%)
24	CLA	b	609	2	59,73,73	1.98	13 (22%)	67,113,113	2.25	21 (31%)
35	HTG	C	522	-	19,19,19	1.00	1 (5%)	23,24,24	1.41	2 (8%)
24	CLA	B	615	2	59,73,73	1.92	12 (20%)	67,113,113	2.18	22 (32%)
26	BCR	D	404	-	41,41,41	1.04	1 (2%)	56,56,56	1.84	18 (32%)
24	CLA	C	506	3	59,73,73	1.93	13 (22%)	67,113,113	2.22	21 (31%)
24	CLA	C	509	3	59,73,73	2.06	14 (23%)	67,113,113	2.29	23 (34%)
24	CLA	D	403	4	59,73,73	1.96	12 (20%)	67,113,113	2.16	25 (37%)
26	BCR	B	619	-	41,41,41	1.09	2 (4%)	56,56,56	1.49	14 (25%)
36	DGD	c	518	-	63,63,67	0.83	2 (3%)	77,77,81	1.09	4 (5%)
26	BCR	a	408	-	41,41,41	0.97	1 (2%)	56,56,56	1.56	11 (19%)
35	HTG	h	101	-	16,16,19	1.15	2 (12%)	20,21,24	1.62	2 (10%)
39	HEM	E	103	5,6	27,50,50	0.85	1 (3%)	17,82,82	2.37	3 (17%)
34	LMT	A	359	-	36,36,36	0.55	1 (2%)	47,47,47	0.86	0
24	CLA	b	601	42	59,73,73	2.05	13 (22%)	67,113,113	2.20	22 (32%)
27	SQD	b	620	-	53,54,54	1.03	3 (5%)	62,65,65	1.47	9 (14%)
24	CLA	d	402	4	59,73,73	1.96	14 (23%)	67,113,113	2.23	25 (37%)
24	CLA	d	403	4	59,73,73	1.99	12 (20%)	67,113,113	2.18	24 (35%)
34	LMT	M	103	-	36,36,36	0.42	0	47,47,47	0.95	2 (4%)
25	PHO	a	406	-	67,69,69	2.16	16 (23%)	85,99,99	2.01	24 (28%)
24	CLA	C	514	3	59,73,73	2.00	13 (22%)	67,113,113	2.15	21 (31%)
24	CLA	c	505	3	59,73,73	1.94	13 (22%)	67,113,113	2.13	18 (26%)
36	DGD	c	520	-	63,63,67	0.82	2 (3%)	77,77,81	1.09	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	GOL	c	502	-	5,5,5	0.41	0	5,5,5	0.31	0
35	HTG	b	625	-	19,19,19	1.09	2 (10%)	23,24,24	1.75	3 (13%)
26	BCR	b	618	-	41,41,41	0.99	1 (2%)	56,56,56	1.43	16 (28%)
38	LHG	D	406	-	48,48,48	0.89	3 (6%)	51,54,54	0.99	3 (5%)
33	LMG	C	521	-	51,51,55	1.00	3 (5%)	59,59,63	1.19	4 (6%)
24	CLA	b	613	2	59,73,73	2.05	13 (22%)	67,113,113	2.25	22 (32%)
34	LMT	b	630	-	25,25,36	0.52	1 (4%)	30,30,47	0.85	0
26	BCR	k	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.61	12 (21%)
34	LMT	a	359	-	36,36,36	0.50	1 (2%)	47,47,47	0.90	2 (4%)
24	CLA	a	403	1	59,73,73	2.00	12 (20%)	67,113,113	2.36	28 (41%)
31	PL9	D	405	-	55,55,55	0.67	2 (3%)	68,69,69	1.74	20 (29%)
26	BCR	b	619	-	41,41,41	1.01	1 (2%)	56,56,56	1.63	12 (21%)
35	HTG	b	623	-	19,19,19	1.03	1 (5%)	23,24,24	1.51	3 (13%)
35	HTG	B	628	-	19,19,19	0.97	2 (10%)	23,24,24	1.31	3 (13%)
36	DGD	h	103	-	63,63,67	0.86	3 (4%)	77,77,81	0.96	3 (3%)
24	CLA	a	404	42	59,73,73	1.98	14 (23%)	67,113,113	2.14	23 (34%)
28	GOL	a	416	-	5,5,5	0.35	0	5,5,5	0.65	0
24	CLA	c	512	3	59,73,73	1.96	13 (22%)	67,113,113	2.24	23 (34%)
24	CLA	a	350	42	59,73,73	2.00	13 (22%)	67,113,113	2.24	21 (31%)
24	CLA	b	605	2	59,73,73	1.92	14 (23%)	67,113,113	2.29	20 (29%)
26	BCR	c	517	-	41,41,41	1.04	1 (2%)	56,56,56	1.64	13 (23%)
24	CLA	B	614	2	59,73,73	1.93	14 (23%)	67,113,113	2.32	23 (34%)
35	HTG	B	624	-	19,19,19	0.90	1 (5%)	23,24,24	1.39	1 (4%)
24	CLA	C	502	3	59,73,73	1.96	13 (22%)	67,113,113	2.24	24 (35%)
24	CLA	b	615	2	59,73,73	1.97	12 (20%)	67,113,113	2.12	21 (31%)
24	CLA	C	510	3	59,73,73	2.07	13 (22%)	67,113,113	2.19	22 (32%)
24	CLA	c	508	3	59,73,73	2.03	13 (22%)	67,113,113	2.16	25 (37%)
28	GOL	A	412	-	5,5,5	0.40	0	5,5,5	0.35	0
38	LHG	L	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.08	4 (7%)
39	HEM	e	102	5,6	27,50,50	0.88	1 (3%)	17,82,82	1.86	3 (17%)
34	LMT	B	622	-	36,36,36	0.41	0	47,47,47	1.07	2 (4%)
24	CLA	c	506	42	59,73,73	2.04	13 (22%)	67,113,113	2.10	23 (34%)
35	HTG	b	624	-	19,19,19	1.02	1 (5%)	23,24,24	1.37	1 (4%)
24	CLA	A	405	42	59,73,73	1.99	13 (22%)	67,113,113	2.37	25 (37%)
24	CLA	B	603	2	59,73,73	1.95	13 (22%)	67,113,113	2.45	24 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	LHG	E	101	-	41,41,48	1.01	2 (4%)	44,47,54	1.11	5 (11%)
33	LMG	c	522	-	51,51,55	0.97	2 (3%)	59,59,63	1.13	6 (10%)
31	PL9	a	414[B]	-	55,55,55	0.63	2 (3%)	68,69,69	1.89	21 (30%)
31	PL9	A	416[B]	-	55,55,55	0.64	2 (3%)	68,69,69	1.87	20 (29%)
24	CLA	b	616	2	59,73,73	1.95	14 (23%)	67,113,113	2.36	23 (34%)
36	DGD	C	519	-	63,63,67	0.82	3 (4%)	77,77,81	0.94	4 (5%)
36	DGD	C	518	-	63,63,67	0.86	2 (3%)	77,77,81	1.02	6 (7%)
24	CLA	b	606	2	59,73,73	1.92	12 (20%)	67,113,113	2.30	25 (37%)
33	LMG	A	418	-	51,51,55	0.91	2 (3%)	59,59,63	1.21	5 (8%)
26	BCR	A	410	-	41,41,41	1.02	1 (2%)	56,56,56	1.64	11 (19%)
26	BCR	T	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.75	14 (25%)
26	BCR	t	102	-	41,41,41	1.01	1 (2%)	56,56,56	1.71	15 (26%)
34	LMT	I	101	-	36,36,36	0.48	1 (2%)	47,47,47	1.07	3 (6%)
34	LMT	t	101	-	26,26,36	0.56	1 (3%)	31,31,47	1.14	2 (6%)
24	CLA	B	604	2	59,73,73	1.92	11 (18%)	67,113,113	2.25	22 (32%)
24	CLA	A	404	1	59,73,73	2.01	14 (23%)	67,113,113	2.35	23 (34%)
24	CLA	B	616	2	59,73,73	1.98	13 (22%)	67,113,113	2.24	20 (29%)
24	CLA	a	407	1	59,73,73	1.97	14 (23%)	67,113,113	2.35	25 (37%)
29	OEX	a	412[A]	1,3,42	0,15,15	0.00	-	-	-	-
38	LHG	D	357	-	48,48,48	0.89	2 (4%)	51,54,54	1.20	5 (9%)
24	CLA	A	406	42	59,73,73	1.99	14 (23%)	67,113,113	2.19	27 (40%)
34	LMT	M	101	-	36,36,36	0.50	0	47,47,47	1.08	3 (6%)
24	CLA	c	511	3	59,73,73	2.03	14 (23%)	67,113,113	2.25	23 (34%)
28	GOL	C	525	-	5,5,5	0.42	0	5,5,5	0.12	0
33	LMG	J	101	40	51,51,55	0.88	2 (3%)	59,59,63	0.90	3 (5%)
33	LMG	a	417	-	51,51,55	0.92	2 (3%)	59,59,63	1.18	6 (10%)
23	BCT	a	420[B]	21	0,3,3	0.00	-	0,3,3	0.00	-
35	HTG	c	523	-	19,19,19	0.97	1 (5%)	23,24,24	1.35	1 (4%)
27	SQD	a	409	-	53,54,54	0.96	3 (5%)	62,65,65	1.78	13 (20%)
26	BCR	B	617	-	41,41,41	1.01	2 (4%)	56,56,56	1.54	10 (17%)
26	BCR	K	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.62	12 (21%)
24	CLA	b	610	42	59,73,73	2.02	14 (23%)	67,113,113	2.26	22 (32%)
33	LMG	Z	101	-	37,37,55	0.99	3 (8%)	45,45,63	1.48	7 (15%)
24	CLA	D	402	4	59,73,73	1.93	15 (25%)	67,113,113	2.23	24 (35%)
27	SQD	a	411	-	53,54,54	1.05	3 (5%)	62,65,65	1.25	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PL9	d	405	-	55,55,55	0.61	1 (1%)	68,69,69	1.73	19 (27%)
24	CLA	b	602	2	59,73,73	2.02	13 (22%)	67,113,113	2.27	25 (37%)
24	CLA	C	503	3	59,73,73	1.96	12 (20%)	67,113,113	2.18	20 (29%)
28	GOL	v	202	-	5,5,5	0.37	0	5,5,5	0.29	0
35	HTG	V	204	-	11,11,19	0.23	0	15,15,24	1.05	1 (6%)
34	LMT	a	418	-	36,36,36	0.49	1 (2%)	47,47,47	0.83	0
26	BCR	C	516	-	41,41,41	1.07	1 (2%)	56,56,56	1.62	12 (21%)
24	CLA	B	612	2	59,73,73	1.97	15 (25%)	67,113,113	2.32	22 (32%)
24	CLA	A	409	1	59,73,73	1.98	14 (23%)	67,113,113	2.25	26 (38%)
24	CLA	C	505	42	59,73,73	1.95	13 (22%)	67,113,113	2.20	26 (38%)
38	LHG	D	407	-	48,48,48	0.90	2 (4%)	51,54,54	0.99	3 (5%)
24	CLA	B	605	2	59,73,73	1.93	13 (22%)	67,113,113	2.35	25 (37%)
35	HTG	B	625	-	19,19,19	0.99	1 (5%)	23,24,24	1.60	3 (13%)
24	CLA	B	610	42	59,73,73	2.03	12 (20%)	67,113,113	2.24	25 (37%)
26	BCR	h	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.49	11 (19%)
26	BCR	d	404	-	41,41,41	1.14	1 (2%)	56,56,56	1.83	14 (25%)
33	LMG	z	101	-	39,39,55	1.07	2 (5%)	47,47,63	1.10	4 (8%)
41	HEC	v	203	16	26,50,50	1.57	4 (15%)	18,82,82	1.61	4 (22%)
27	SQD	A	411	-	53,54,54	0.94	3 (5%)	62,65,65	1.81	13 (20%)
24	CLA	B	602	2	59,73,73	2.00	13 (22%)	67,113,113	2.30	26 (38%)
26	BCR	Y	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.75	14 (25%)
28	GOL	V	202	-	5,5,5	0.37	0	5,5,5	0.35	0
24	CLA	b	608	2	59,73,73	2.00	14 (23%)	67,113,113	2.20	25 (37%)
34	LMT	E	102	-	36,36,36	0.47	0	47,47,47	0.82	0
24	CLA	C	507	3	59,73,73	1.96	14 (23%)	67,113,113	2.25	24 (35%)
24	CLA	c	504	3	59,73,73	1.93	14 (23%)	67,113,113	2.19	22 (32%)
28	GOL	b	627	-	5,5,5	0.34	0	5,5,5	0.37	0
27	SQD	A	413	-	53,54,54	1.01	3 (5%)	62,65,65	1.10	6 (9%)
34	LMT	b	622	-	25,25,36	0.46	0	30,30,47	0.70	0
24	CLA	B	601	42	59,73,73	2.03	12 (20%)	67,113,113	2.19	22 (32%)
34	LMT	e	101	-	36,36,36	0.47	0	47,47,47	0.80	1 (2%)
36	DGD	H	102	-	63,63,67	0.82	3 (4%)	77,77,81	0.93	4 (5%)
27	SQD	F	101	-	42,43,54	1.16	3 (7%)	51,54,65	1.66	8 (15%)
33	LMG	c	521	-	51,51,55	0.93	2 (3%)	59,59,63	1.07	5 (8%)
35	HTG	B	623	-	19,19,19	0.97	1 (5%)	23,24,24	1.39	5 (21%)
24	CLA	C	513	3	59,73,73	2.00	13 (22%)	67,113,113	2.30	21 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	HTG	D	410	-	16,16,19	1.08	2 (12%)	20,21,24	1.36	1 (5%)
26	BCR	B	618	-	41,41,41	0.97	1 (2%)	56,56,56	1.57	14 (25%)
28	GOL	B	626	-	5,5,5	0.37	0	5,5,5	0.47	0
24	CLA	B	606	2	59,73,73	1.90	13 (22%)	67,113,113	2.40	23 (34%)
24	CLA	c	515	3	59,73,73	2.02	14 (23%)	67,113,113	2.18	24 (35%)
24	CLA	B	607	42	59,73,73	1.93	13 (22%)	67,113,113	2.19	22 (32%)
33	LMG	B	621	-	51,51,55	0.90	2 (3%)	59,59,63	1.11	3 (5%)
24	CLA	c	507	3	59,73,73	1.94	12 (20%)	67,113,113	2.16	19 (28%)
26	BCR	b	617	-	41,41,41	1.05	1 (2%)	56,56,56	1.56	10 (17%)
38	LHG	l	101	-	48,48,48	0.90	2 (4%)	51,54,54	1.10	3 (5%)
24	CLA	c	513	3	59,73,73	2.00	13 (22%)	67,113,113	2.12	23 (34%)
24	CLA	b	612	2	59,73,73	1.99	14 (23%)	67,113,113	2.28	22 (32%)
25	PHO	a	405	-	67,69,69	2.02	18 (26%)	85,99,99	2.02	23 (27%)
24	CLA	B	611	2	59,73,73	1.92	12 (20%)	67,113,113	2.38	24 (35%)
35	HTG	c	526	-	19,19,19	1.03	2 (10%)	23,24,24	1.49	3 (13%)
27	SQD	B	620	-	53,54,54	1.02	3 (5%)	62,65,65	1.40	8 (12%)
36	DGD	C	517	-	63,63,67	0.81	2 (3%)	77,77,81	1.16	5 (6%)
33	LMG	b	621	-	51,51,55	0.86	2 (3%)	59,59,63	1.27	5 (8%)
26	BCR	y	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.68	11 (19%)
24	CLA	b	603	2	59,73,73	2.01	13 (22%)	67,113,113	2.34	20 (29%)
24	CLA	c	503	3	59,73,73	1.99	13 (22%)	67,113,113	2.14	22 (32%)
33	LMG	j	101	40	51,51,55	0.88	2 (3%)	59,59,63	1.13	5 (8%)
24	CLA	c	509	42	59,73,73	1.97	12 (20%)	67,113,113	2.16	19 (28%)
24	CLA	C	504	3	59,73,73	1.94	13 (22%)	67,113,113	2.11	17 (25%)
41	HEC	V	203	16	26,50,50	1.54	4 (15%)	18,82,82	1.55	4 (22%)
35	HTG	C	523	-	19,19,19	1.06	2 (10%)	23,24,24	1.82	5 (21%)
24	CLA	B	609	2	59,73,73	1.96	13 (22%)	67,113,113	2.19	21 (31%)
36	DGD	c	519	-	63,63,67	0.87	2 (3%)	77,77,81	0.94	4 (5%)
29	OEX	A	414[A]	1,3,42	0,15,15	0.00	-	-		
26	BCR	c	516	-	41,41,41	1.05	1 (2%)	56,56,56	1.77	12 (21%)
24	CLA	c	510	3	59,73,73	2.05	13 (22%)	67,113,113	2.25	22 (32%)
31	PL9	a	414[A]	-	55,55,55	0.63	2 (3%)	68,69,69	1.98	22 (32%)
24	CLA	b	604	2	59,73,73	1.92	12 (20%)	67,113,113	2.25	20 (29%)
34	LMT	B	630	-	25,25,36	0.43	0	30,30,47	0.73	1 (3%)
23	BCT	a	420[A]	21	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	LMT	m	102	-	36,36,36	0.42	0	47,47,47	0.87	1 (2%)
31	PL9	A	416[A]	-	55,55,55	0.63	1 (1%)	68,69,69	2.01	23 (33%)
38	LHG	d	408	-	48,48,48	0.91	2 (4%)	51,54,54	1.11	4 (7%)
24	CLA	C	511	3	59,73,73	1.97	13 (22%)	67,113,113	2.28	24 (35%)
38	LHG	d	406	-	48,48,48	0.89	3 (6%)	51,54,54	1.09	5 (9%)
28	GOL	a	410	-	5,5,5	0.36	0	5,5,5	0.35	0
24	CLA	b	607	42	59,73,73	1.95	14 (23%)	67,113,113	2.16	21 (31%)
23	BCT	A	403[B]	21	0,3,3	0.00	-	0,3,3	0.00	-
35	HTG	b	628	-	19,19,19	0.91	2 (10%)	23,24,24	1.29	3 (13%)
23	BCT	A	403[A]	21	0,3,3	0.00	-	0,3,3	0.00	-
25	PHO	A	407	-	67,69,69	2.05	17 (25%)	85,99,99	1.98	22 (25%)
24	CLA	B	608	2	59,73,73	1.97	12 (20%)	67,113,113	2.24	24 (35%)
25	PHO	A	408	-	67,69,69	2.08	15 (22%)	85,99,99	2.14	23 (27%)
24	CLA	c	514	3	59,73,73	1.98	13 (22%)	67,113,113	2.28	24 (35%)
28	GOL	B	627	-	5,5,5	0.47	0	5,5,5	0.38	0
30	OEY	a	413[B]	1,3,42	0,16,16	0.00	-	-	-	-
24	CLA	C	512	3	59,73,73	2.04	14 (23%)	67,113,113	2.14	21 (31%)
38	LHG	d	407	-	48,48,48	0.89	2 (4%)	51,54,54	0.90	3 (5%)
24	CLA	b	611	2	59,73,73	1.95	13 (22%)	67,113,113	2.26	19 (28%)
26	BCR	H	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.48	11 (19%)
38	LHG	a	419	-	41,41,48	1.03	2 (4%)	44,47,54	0.90	2 (4%)
24	CLA	b	614	2	59,73,73	1.95	13 (22%)	67,113,113	2.25	23 (34%)
33	LMG	C	520	-	51,51,55	0.95	2 (3%)	59,59,63	1.12	4 (6%)
30	OEY	A	415[B]	1,3,42	0,16,16	0.00	-	-	-	-
24	CLA	B	613	2	59,73,73	2.01	13 (22%)	67,113,113	2.24	25 (37%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SQD	f	101	-	-	13/38/58/69	0/1/1/1
24	CLA	C	508	42	3/3/20/25	6/37/135/135	-
26	BCR	C	515	-	-	0/29/63/63	0/2/2/2
24	CLA	b	609	2	2/2/20/25	6/37/135/135	-
35	HTG	C	522	-	-	0/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	615	2	3/3/20/25	10/37/135/135	-
26	BCR	D	404	-	-	5/29/63/63	0/2/2/2
24	CLA	C	506	3	1/1/20/25	7/37/135/135	-
24	CLA	D	403	4	3/3/20/25	10/37/135/135	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
36	DGD	c	518	-	-	21/51/91/95	0/2/2/2
26	BCR	a	408	-	-	0/29/63/63	0/2/2/2
35	HTG	h	101	-	-	0/7/27/30	0/1/1/1
39	HEM	E	103	5,6	-	0/6/54/54	-
34	LMT	A	359	-	-	4/21/61/61	0/2/2/2
24	CLA	b	601	42	3/3/20/25	16/37/135/135	-
27	SQD	b	620	-	-	20/49/69/69	0/1/1/1
24	CLA	d	402	4	1/1/20/25	4/37/135/135	-
24	CLA	d	403	4	3/3/20/25	6/37/135/135	-
25	PHO	a	406	-	-	3/53/103/103	0/5/6/6
24	CLA	C	514	3	3/3/20/25	9/37/135/135	-
24	CLA	c	505	3	3/3/20/25	1/37/135/135	-
28	GOL	c	502	-	-	0/4/4/4	-
35	HTG	b	625	-	-	2/10/30/30	0/1/1/1
26	BCR	b	618	-	-	0/29/63/63	0/2/2/2
38	LHG	D	406	-	-	16/53/53/53	-
33	LMG	C	521	-	-	10/46/66/70	0/1/1/1
34	LMT	M	103	-	-	7/21/61/61	0/2/2/2
34	LMT	b	630	-	-	9/17/37/61	0/1/1/2
26	BCR	k	101	-	-	1/29/63/63	0/2/2/2
34	LMT	a	359	-	-	7/21/61/61	0/2/2/2
24	CLA	a	403	1	2/2/20/25	1/37/135/135	-
31	PL9	D	405	-	-	15/53/73/73	0/1/1/1
36	DGD	c	520	-	-	11/51/91/95	0/2/2/2
35	HTG	b	623	-	-	6/10/30/30	0/1/1/1
24	CLA	C	503	3	3/3/20/25	9/37/135/135	-
36	DGD	h	103	-	-	11/51/91/95	0/2/2/2
24	CLA	a	404	42	2/2/20/25	3/37/135/135	-
28	GOL	a	416	-	-	3/4/4/4	-
24	CLA	c	512	3	3/3/20/25	8/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	a	350	42	3/3/20/25	7/37/135/135	-
24	CLA	b	605	2	3/3/20/25	5/37/135/135	-
26	BCR	c	517	-	-	4/29/63/63	0/2/2/2
24	CLA	B	614	2	3/3/20/25	13/37/135/135	-
35	HTG	B	624	-	-	5/10/30/30	0/1/1/1
24	CLA	C	502	3	3/3/20/25	6/37/135/135	-
24	CLA	C	510	3	3/3/20/25	4/37/135/135	-
24	CLA	c	508	3	3/3/20/25	13/37/135/135	-
28	GOL	A	412	-	-	2/4/4/4	-
38	LHG	L	101	-	-	13/53/53/53	-
39	HEM	e	102	5,6	-	1/6/54/54	-
34	LMT	B	622	-	-	8/21/61/61	0/2/2/2
24	CLA	c	506	42	3/3/20/25	6/37/135/135	-
35	HTG	b	624	-	-	3/10/30/30	0/1/1/1
24	CLA	A	405	42	3/3/20/25	6/37/135/135	-
24	CLA	B	603	2	2/2/20/25	4/37/135/135	-
38	LHG	E	101	-	-	16/46/46/53	-
33	LMG	c	522	-	-	10/46/66/70	0/1/1/1
24	CLA	b	616	2	3/3/20/25	12/37/135/135	-
31	PL9	A	416[B]	-	-	18/53/73/73	0/1/1/1
36	DGD	C	519	-	-	11/51/91/95	0/2/2/2
26	BCR	c	516	-	-	0/29/63/63	0/2/2/2
36	DGD	C	518	-	-	10/51/91/95	0/2/2/2
24	CLA	b	606	2	3/3/20/25	10/37/135/135	-
33	LMG	A	418	-	-	10/46/66/70	0/1/1/1
26	BCR	A	410	-	-	1/29/63/63	0/2/2/2
26	BCR	T	101	-	-	1/29/63/63	0/2/2/2
26	BCR	t	102	-	-	0/29/63/63	0/2/2/2
34	LMT	I	101	-	-	9/21/61/61	0/2/2/2
34	LMT	t	101	-	-	5/17/38/61	0/1/1/2
24	CLA	B	604	2	3/3/20/25	11/37/135/135	-
24	CLA	A	404	1	3/3/20/25	1/37/135/135	-
24	CLA	B	616	2	3/3/20/25	8/37/135/135	-
24	CLA	a	407	1	3/3/20/25	8/37/135/135	-
38	LHG	D	357	-	-	14/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	406	42	3/3/20/25	4/37/135/135	-
34	LMT	M	101	-	-	3/21/61/61	0/2/2/2
24	CLA	c	511	3	3/3/20/25	10/37/135/135	-
26	BCR	b	619	-	-	2/29/63/63	0/2/2/2
28	GOL	C	525	-	-	2/4/4/4	-
33	LMG	J	101	40	-	11/46/66/70	0/1/1/1
24	CLA	C	509	3	3/3/20/25	4/37/135/135	-
35	HTG	c	523	-	-	4/10/30/30	0/1/1/1
27	SQD	a	409	-	-	12/49/69/69	0/1/1/1
26	BCR	B	617	-	-	2/29/63/63	0/2/2/2
26	BCR	K	102	-	-	2/29/63/63	0/2/2/2
24	CLA	b	610	42	3/3/20/25	7/37/135/135	-
33	LMG	Z	101	-	-	12/31/51/70	0/1/1/1
24	CLA	D	402	4	1/1/20/25	0/37/135/135	-
27	SQD	a	411	-	-	15/49/69/69	0/1/1/1
31	PL9	d	405	-	-	9/53/73/73	0/1/1/1
24	CLA	b	602	2	3/3/20/25	4/37/135/135	-
35	HTG	B	628	-	-	3/10/30/30	0/1/1/1
28	GOL	v	202	-	-	2/4/4/4	-
35	HTG	V	204	-	-	0/2/19/30	0/1/1/1
34	LMT	a	418	-	-	4/21/61/61	0/2/2/2
26	BCR	C	516	-	-	1/29/63/63	0/2/2/2
24	CLA	B	612	2	3/3/20/25	5/37/135/135	-
24	CLA	A	409	1	2/2/20/25	10/37/135/135	-
24	CLA	C	505	42	3/3/20/25	6/37/135/135	-
38	LHG	D	407	-	-	10/53/53/53	-
26	BCR	B	618	-	-	0/29/63/63	0/2/2/2
24	CLA	B	605	2	3/3/20/25	7/37/135/135	-
35	HTG	B	625	-	-	4/10/30/30	0/1/1/1
24	CLA	B	610	42	3/3/20/25	8/37/135/135	-
26	BCR	h	102	-	-	2/29/63/63	0/2/2/2
26	BCR	d	404	-	-	6/29/63/63	0/2/2/2
33	LMG	z	101	-	-	6/34/54/70	0/1/1/1
41	HEC	v	203	16	-	0/6/54/54	-
27	SQD	A	411	-	-	15/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	602	2	2/2/20/25	7/37/135/135	-
26	BCR	Y	101	-	-	3/29/63/63	0/2/2/2
28	GOL	V	202	-	-	2/4/4/4	-
24	CLA	b	608	2	2/2/20/25	2/37/135/135	-
34	LMT	E	102	-	-	9/21/61/61	0/2/2/2
25	PHO	A	407	-	-	3/53/103/103	0/5/6/6
24	CLA	c	504	3	3/3/20/25	7/37/135/135	-
28	GOL	b	627	-	-	2/4/4/4	-
27	SQD	A	413	-	-	7/49/69/69	0/1/1/1
24	CLA	b	613	2	3/3/20/25	8/37/135/135	-
34	LMT	b	622	-	-	5/17/37/61	0/1/1/2
24	CLA	B	601	42	3/3/20/25	12/37/135/135	-
34	LMT	e	101	-	-	6/21/61/61	0/2/2/2
36	DGD	H	102	-	-	15/51/91/95	0/2/2/2
27	SQD	F	101	-	-	10/38/58/69	0/1/1/1
33	LMG	c	521	-	-	8/46/66/70	0/1/1/1
35	HTG	B	623	-	-	2/10/30/30	0/1/1/1
24	CLA	C	513	3	3/3/20/25	9/37/135/135	-
35	HTG	D	410	-	-	0/7/27/30	0/1/1/1
24	CLA	b	615	2	3/3/20/25	4/37/135/135	-
28	GOL	B	626	-	-	4/4/4/4	-
24	CLA	B	606	2	3/3/20/25	7/37/135/135	-
24	CLA	c	515	3	3/3/20/25	7/37/135/135	-
24	CLA	B	607	42	3/3/20/25	4/37/135/135	-
33	LMG	B	621	-	-	12/46/66/70	0/1/1/1
24	CLA	c	507	3	1/1/20/25	3/37/135/135	-
26	BCR	b	617	-	-	2/29/63/63	0/2/2/2
38	LHG	l	101	-	-	16/53/53/53	-
24	CLA	c	513	3	3/3/20/25	5/37/135/135	-
24	CLA	b	612	2	3/3/20/25	6/37/135/135	-
25	PHO	a	405	-	-	3/53/103/103	0/5/6/6
24	CLA	B	611	2	3/3/20/25	3/37/135/135	-
35	HTG	c	526	-	-	1/10/30/30	0/1/1/1
27	SQD	B	620	-	-	17/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	DGD	C	517	-	-	15/51/91/95	0/2/2/2
33	LMG	b	621	-	-	10/46/66/70	0/1/1/1
26	BCR	y	101	-	-	6/29/63/63	0/2/2/2
24	CLA	b	603	2	2/2/20/25	5/37/135/135	-
24	CLA	c	503	3	3/3/20/25	4/37/135/135	-
33	LMG	j	101	40	-	9/46/66/70	0/1/1/1
24	CLA	c	509	42	3/3/20/25	9/37/135/135	-
24	CLA	C	504	3	2/2/20/25	3/37/135/135	-
41	HEC	V	203	16	-	0/6/54/54	-
35	HTG	C	523	-	-	1/10/30/30	0/1/1/1
24	CLA	B	609	2	2/2/20/25	6/37/135/135	-
36	DGD	c	519	-	-	11/51/91/95	0/2/2/2
33	LMG	a	417	-	-	13/46/66/70	0/1/1/1
24	CLA	c	510	3	3/3/20/25	4/37/135/135	-
31	PL9	a	414[A]	-	-	16/53/73/73	0/1/1/1
24	CLA	b	604	2	3/3/20/25	7/37/135/135	-
34	LMT	B	630	-	-	11/17/37/61	0/1/1/2
31	PL9	a	414[B]	-	-	21/53/73/73	0/1/1/1
34	LMT	m	102	-	-	5/21/61/61	0/2/2/2
31	PL9	A	416[A]	-	-	15/53/73/73	0/1/1/1
38	LHG	d	408	-	-	12/53/53/53	-
24	CLA	C	511	3	3/3/20/25	10/37/135/135	-
38	LHG	d	406	-	-	8/53/53/53	-
28	GOL	a	410	-	-	4/4/4/4	-
24	CLA	b	607	42	3/3/20/25	2/37/135/135	-
35	HTG	b	628	-	-	4/10/30/30	0/1/1/1
24	CLA	C	507	3	3/3/20/25	11/37/135/135	-
24	CLA	B	608	2	2/2/20/25	4/37/135/135	-
25	PHO	A	408	-	-	3/53/103/103	0/5/6/6
24	CLA	c	514	3	3/3/20/25	9/37/135/135	-
28	GOL	B	627	-	-	3/4/4/4	-
24	CLA	C	512	3	3/3/20/25	5/37/135/135	-
38	LHG	d	407	-	-	15/53/53/53	-
24	CLA	b	611	2	3/3/20/25	3/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	H	101	-	-	3/29/63/63	0/2/2/2
38	LHG	a	419	-	-	9/46/46/53	-
24	CLA	b	614	2	3/3/20/25	13/37/135/135	-
33	LMG	C	520	-	-	14/46/66/70	0/1/1/1
24	CLA	B	613	2	3/3/20/25	6/37/135/135	-

All (1145) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	510	CLA	C3B-C2B	6.97	1.50	1.40
24	B	613	CLA	C3B-C2B	6.61	1.49	1.40
24	B	612	CLA	C3B-C2B	6.52	1.49	1.40
24	A	404	CLA	C3B-C2B	6.46	1.49	1.40
24	C	509	CLA	C3B-C2B	6.46	1.49	1.40
24	C	512	CLA	C3B-C2B	6.41	1.49	1.40
24	b	610	CLA	C3B-C2B	6.39	1.49	1.40
24	a	403	CLA	C3B-C2B	6.25	1.49	1.40
24	b	612	CLA	C3B-C2B	6.24	1.49	1.40
24	B	603	CLA	C3B-C2B	6.24	1.49	1.40
24	c	506	CLA	C3B-C2B	6.23	1.49	1.40
24	b	613	CLA	C3B-C2B	6.18	1.48	1.40
24	D	402	CLA	C3B-C2B	6.10	1.48	1.40
24	B	608	CLA	C3B-C2B	6.09	1.48	1.40
24	c	510	CLA	C3B-C2B	6.08	1.48	1.40
24	C	512	CLA	C3D-C2D	6.06	1.50	1.39
24	C	505	CLA	C3B-C2B	6.05	1.48	1.40
24	b	613	CLA	C3D-C2D	6.05	1.50	1.39
24	A	405	CLA	C3D-C2D	6.03	1.50	1.39
25	a	406	PHO	C3C-C2C	6.02	1.49	1.36
24	B	614	CLA	C3B-C2B	6.02	1.48	1.40
24	b	601	CLA	C3D-C2D	6.02	1.50	1.39
24	c	508	CLA	C3D-C2D	6.01	1.50	1.39
24	C	503	CLA	C3B-C2B	5.99	1.48	1.40
25	A	408	PHO	C3C-C2C	5.98	1.49	1.36
24	b	601	CLA	C3B-C2B	5.98	1.48	1.40
24	C	509	CLA	C3D-C2D	5.96	1.50	1.39
25	A	408	PHO	C3B-C2B	5.96	1.49	1.37
24	a	350	CLA	C3D-C2D	5.95	1.50	1.39
24	B	610	CLA	C3D-C2D	5.90	1.50	1.39
24	c	512	CLA	C3B-C2B	5.89	1.48	1.40
24	C	502	CLA	C3B-C2B	5.87	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	402	CLA	C3B-C2B	5.86	1.48	1.40
24	A	406	CLA	C3D-C2D	5.86	1.49	1.39
24	c	511	CLA	C3B-C2B	5.86	1.48	1.40
24	c	510	CLA	C3D-C2D	5.85	1.49	1.39
24	c	514	CLA	C3D-C2D	5.84	1.49	1.39
24	c	515	CLA	C3D-C2D	5.84	1.49	1.39
24	a	404	CLA	C3D-C2D	5.83	1.49	1.39
24	c	513	CLA	C3B-C2B	5.83	1.48	1.40
24	b	614	CLA	C3B-C2B	5.83	1.48	1.40
24	C	514	CLA	C3D-C2D	5.83	1.49	1.39
25	a	405	PHO	C3B-C2B	5.82	1.49	1.37
24	B	609	CLA	C3D-C2D	5.80	1.49	1.39
24	B	602	CLA	C3D-C2D	5.80	1.49	1.39
24	C	508	CLA	C3D-C2D	5.78	1.49	1.39
25	A	407	PHO	C3B-C2B	5.78	1.49	1.37
24	B	610	CLA	C3C-C2C	5.77	1.49	1.36
24	a	407	CLA	C3D-C2D	5.77	1.49	1.39
24	A	405	CLA	C3B-C2B	5.77	1.48	1.40
24	b	606	CLA	C3B-C2B	5.77	1.48	1.40
24	B	611	CLA	C3B-C2B	5.76	1.48	1.40
24	C	511	CLA	C3B-C2B	5.76	1.48	1.40
24	c	511	CLA	C3D-C2D	5.75	1.49	1.39
24	B	604	CLA	C3B-C2B	5.75	1.48	1.40
24	A	409	CLA	C3B-C2B	5.75	1.48	1.40
24	B	616	CLA	C3B-C2B	5.74	1.48	1.40
24	b	603	CLA	C3B-C2B	5.73	1.48	1.40
24	b	602	CLA	C3B-C2B	5.73	1.48	1.40
24	B	616	CLA	C3D-C2D	5.72	1.49	1.39
24	B	601	CLA	C3B-C2B	5.71	1.48	1.40
24	B	601	CLA	C3D-C2D	5.71	1.49	1.39
24	b	608	CLA	C3B-C2B	5.70	1.48	1.40
24	C	513	CLA	C3D-C2D	5.69	1.49	1.39
24	c	503	CLA	C3D-C2D	5.69	1.49	1.39
24	B	605	CLA	C3D-C2D	5.68	1.49	1.39
24	b	608	CLA	C3D-C2D	5.68	1.49	1.39
24	d	403	CLA	C3D-C2D	5.68	1.49	1.39
24	B	615	CLA	C3D-C2D	5.68	1.49	1.39
24	c	506	CLA	C3D-C2D	5.66	1.49	1.39
24	C	506	CLA	C3B-C2B	5.66	1.48	1.40
24	B	611	CLA	C3D-C2D	5.66	1.49	1.39
24	c	504	CLA	C3B-C2B	5.66	1.48	1.40
25	a	406	PHO	C3B-C2B	5.66	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	514	CLA	C3B-C2B	5.65	1.48	1.40
25	a	405	PHO	C3C-C2C	5.64	1.48	1.36
24	C	503	CLA	C3D-C2D	5.63	1.49	1.39
24	c	503	CLA	C3B-C2B	5.62	1.48	1.40
24	c	509	CLA	C3D-C2D	5.61	1.49	1.39
24	b	609	CLA	C3B-C2B	5.60	1.48	1.40
24	b	614	CLA	C3D-C2D	5.60	1.49	1.39
24	b	616	CLA	C3D-C2D	5.59	1.49	1.39
24	B	610	CLA	C3B-C2B	5.59	1.48	1.40
24	B	608	CLA	C3D-C2D	5.58	1.49	1.39
24	b	602	CLA	CHC-C1C	5.58	1.49	1.35
24	B	613	CLA	C3D-C2D	5.58	1.49	1.39
24	C	513	CLA	C3C-C2C	5.57	1.48	1.36
24	b	602	CLA	C3D-C2D	5.56	1.49	1.39
24	b	613	CLA	C3C-C2C	5.56	1.48	1.36
24	C	508	CLA	C3B-C2B	5.56	1.48	1.40
24	d	402	CLA	C3D-C2D	5.56	1.49	1.39
24	b	615	CLA	C3D-C2D	5.55	1.49	1.39
24	C	507	CLA	C3B-C2B	5.55	1.48	1.40
24	a	407	CLA	C3B-C2B	5.55	1.48	1.40
24	b	615	CLA	C3C-C2C	5.54	1.48	1.36
24	c	507	CLA	C3B-C2B	5.53	1.48	1.40
24	B	602	CLA	CHC-C1C	5.53	1.49	1.35
24	c	508	CLA	C3B-C2B	5.52	1.48	1.40
24	b	612	CLA	C3D-C2D	5.52	1.49	1.39
24	A	409	CLA	C3D-C2D	5.52	1.49	1.39
24	b	610	CLA	C3C-C2C	5.51	1.48	1.36
24	a	350	CLA	C3C-C2C	5.50	1.48	1.36
24	a	403	CLA	C3D-C2D	5.50	1.49	1.39
24	b	603	CLA	C3C-C2C	5.50	1.48	1.36
24	b	611	CLA	C3D-C2D	5.50	1.49	1.39
24	c	514	CLA	C3C-C2C	5.50	1.48	1.36
24	B	606	CLA	C3B-C2B	5.49	1.48	1.40
24	C	513	CLA	C3B-C2B	5.49	1.48	1.40
24	C	509	CLA	C3C-C2C	5.49	1.48	1.36
24	b	603	CLA	C3D-C2D	5.49	1.49	1.39
24	c	515	CLA	C3B-C2B	5.48	1.48	1.40
24	B	606	CLA	C3D-C2D	5.48	1.49	1.39
24	c	503	CLA	C3C-C2C	5.47	1.48	1.36
24	c	510	CLA	C3C-C2C	5.47	1.48	1.36
24	c	513	CLA	C3D-C2D	5.46	1.49	1.39
24	b	607	CLA	C3B-C2B	5.45	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	404	CLA	C3D-C2D	5.45	1.49	1.39
24	B	601	CLA	C3C-C2C	5.45	1.48	1.36
24	b	606	CLA	C3D-C2D	5.45	1.49	1.39
24	a	404	CLA	C3B-C2B	5.45	1.47	1.40
24	d	403	CLA	CHC-C1C	5.44	1.48	1.35
24	b	605	CLA	C3C-C2C	5.44	1.48	1.36
24	c	505	CLA	C3D-C2D	5.44	1.49	1.39
24	b	606	CLA	C3C-C2C	5.42	1.48	1.36
24	D	403	CLA	C3D-C2D	5.42	1.49	1.39
24	C	510	CLA	C3D-C2D	5.41	1.49	1.39
24	D	403	CLA	C3B-C2B	5.41	1.47	1.40
24	B	605	CLA	CHC-C1C	5.40	1.48	1.35
24	b	616	CLA	C3B-C2B	5.40	1.47	1.40
24	B	616	CLA	C3C-C2C	5.40	1.48	1.36
24	c	510	CLA	O2D-CGD	5.40	1.46	1.33
24	C	502	CLA	C3D-C2D	5.40	1.49	1.39
24	b	602	CLA	C3C-C2C	5.40	1.48	1.36
24	c	509	CLA	C3B-C2B	5.40	1.47	1.40
24	C	502	CLA	C3C-C2C	5.39	1.48	1.36
24	d	403	CLA	C3B-C2B	5.39	1.47	1.40
24	B	612	CLA	C3D-C2D	5.38	1.49	1.39
24	a	350	CLA	C3B-C2B	5.38	1.47	1.40
24	b	611	CLA	C3C-C2C	5.37	1.48	1.36
24	b	605	CLA	C3D-C2D	5.37	1.49	1.39
24	c	508	CLA	C3C-C2C	5.37	1.48	1.36
24	b	609	CLA	C3D-C2D	5.37	1.49	1.39
24	C	510	CLA	C3C-C2C	5.37	1.48	1.36
26	d	404	BCR	C23-C22	-5.37	1.34	1.45
24	b	605	CLA	C3B-C2B	5.37	1.47	1.40
24	b	604	CLA	C3D-C2D	5.36	1.49	1.39
24	b	612	CLA	C3C-C2C	5.36	1.48	1.36
24	A	406	CLA	C3C-C2C	5.36	1.48	1.36
24	C	505	CLA	C3D-C2D	5.35	1.49	1.39
24	C	508	CLA	C3C-C2C	5.35	1.48	1.36
24	c	512	CLA	C3D-C2D	5.35	1.49	1.39
24	B	608	CLA	C3C-C2C	5.35	1.48	1.36
24	B	616	CLA	CHC-C1C	5.35	1.48	1.35
24	b	601	CLA	C3C-C2C	5.35	1.48	1.36
24	C	511	CLA	C3C-C2C	5.35	1.48	1.36
25	a	406	PHO	CHC-C1C	5.35	1.49	1.38
24	A	409	CLA	C3C-C2C	5.34	1.48	1.36
25	A	407	PHO	C3C-C2C	5.34	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	511	CLA	CHC-C1C	5.34	1.48	1.35
24	c	505	CLA	C3B-C2B	5.34	1.47	1.40
24	b	604	CLA	C3B-C2B	5.33	1.47	1.40
24	b	608	CLA	C3C-C2C	5.32	1.48	1.36
24	b	615	CLA	C3B-C2B	5.31	1.47	1.40
24	c	513	CLA	C3C-C2C	5.29	1.48	1.36
26	K	102	BCR	C23-C22	-5.29	1.34	1.45
24	C	504	CLA	C3D-C2D	5.29	1.48	1.39
24	b	607	CLA	C3D-C2D	5.29	1.48	1.39
24	C	507	CLA	C3D-C2D	5.28	1.48	1.39
24	B	602	CLA	C3C-C2C	5.28	1.48	1.36
24	c	515	CLA	C3C-C2C	5.28	1.48	1.36
24	c	511	CLA	C3C-C2C	5.28	1.47	1.36
24	b	607	CLA	C3C-C2C	5.28	1.47	1.36
24	B	602	CLA	C3B-C2B	5.27	1.47	1.40
24	c	509	CLA	C3C-C2C	5.27	1.47	1.36
24	D	403	CLA	CHC-C1C	5.26	1.48	1.35
24	c	504	CLA	C3D-C2D	5.26	1.48	1.39
24	B	603	CLA	C3C-C2C	5.24	1.47	1.36
26	B	619	BCR	C23-C22	-5.24	1.34	1.45
24	C	514	CLA	C3C-C2C	5.24	1.47	1.36
24	c	512	CLA	C3C-C2C	5.24	1.47	1.36
24	C	513	CLA	CHC-C1C	5.24	1.48	1.35
24	a	404	CLA	C3C-C2C	5.23	1.47	1.36
24	B	603	CLA	C3D-C2D	5.23	1.48	1.39
24	B	609	CLA	C3B-C2B	5.23	1.47	1.40
24	b	611	CLA	C3B-C2B	5.22	1.47	1.40
24	B	601	CLA	CHC-C1C	5.22	1.48	1.35
24	B	615	CLA	C3C-C2C	5.21	1.47	1.36
24	B	605	CLA	C3C-C2C	5.21	1.47	1.36
24	B	611	CLA	C3C-C2C	5.20	1.47	1.36
24	C	506	CLA	CHC-C1C	5.20	1.48	1.35
24	b	616	CLA	CHC-C1C	5.19	1.48	1.35
24	B	607	CLA	C3D-C2D	5.19	1.48	1.39
24	c	505	CLA	C3C-C2C	5.19	1.47	1.36
24	c	514	CLA	C3B-C2B	5.19	1.47	1.40
24	b	616	CLA	C3C-C2C	5.18	1.47	1.36
24	c	507	CLA	C3C-C2C	5.18	1.47	1.36
24	A	406	CLA	CHC-C1C	5.18	1.48	1.35
24	b	610	CLA	CHC-C1C	5.17	1.48	1.35
24	D	403	CLA	C3C-C2C	5.16	1.47	1.36
24	B	614	CLA	C3D-C2D	5.16	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	406	PHO	O2D-CGD	5.16	1.45	1.33
24	B	604	CLA	C3C-C2C	5.16	1.47	1.36
24	b	613	CLA	O2D-CGD	5.15	1.45	1.33
24	a	407	CLA	C3C-C2C	5.15	1.47	1.36
24	c	514	CLA	CHC-C1C	5.15	1.48	1.35
24	c	511	CLA	O2D-CGD	5.14	1.45	1.33
24	B	601	CLA	O2D-CGD	5.14	1.45	1.33
24	c	507	CLA	O2D-CGD	5.14	1.45	1.33
24	b	616	CLA	O2D-CGD	5.14	1.45	1.33
24	C	511	CLA	C3D-C2D	5.14	1.48	1.39
24	C	503	CLA	CHC-C1C	5.14	1.48	1.35
24	b	604	CLA	CHC-C1C	5.14	1.48	1.35
24	B	610	CLA	CHC-C1C	5.14	1.48	1.35
24	C	504	CLA	C3B-C2B	5.14	1.47	1.40
26	k	101	BCR	C23-C22	-5.13	1.34	1.45
24	D	402	CLA	C3C-C2C	5.13	1.47	1.36
26	C	516	BCR	C23-C22	-5.13	1.34	1.45
24	a	404	CLA	CHC-C1C	5.13	1.48	1.35
24	A	405	CLA	C3C-C2C	5.13	1.47	1.36
24	C	514	CLA	CHC-C1C	5.13	1.48	1.35
24	B	609	CLA	O2D-CGD	5.13	1.45	1.33
24	A	405	CLA	CHC-C1C	5.12	1.48	1.35
24	c	504	CLA	C3C-C2C	5.12	1.47	1.36
24	B	607	CLA	C3C-C2C	5.12	1.47	1.36
24	C	504	CLA	C3C-C2C	5.11	1.47	1.36
24	C	502	CLA	CHC-C1C	5.11	1.48	1.35
24	C	505	CLA	C3C-C2C	5.10	1.47	1.36
24	c	505	CLA	CHC-C1C	5.10	1.48	1.35
24	d	403	CLA	C3C-C2C	5.09	1.47	1.36
24	B	604	CLA	CHC-C1C	5.09	1.48	1.35
24	c	503	CLA	CHC-C1C	5.08	1.48	1.35
24	c	508	CLA	O2D-CGD	5.08	1.45	1.33
24	b	604	CLA	C3C-C2C	5.08	1.47	1.36
24	D	402	CLA	C3D-C2D	5.08	1.48	1.39
24	C	507	CLA	O2D-CGD	5.08	1.45	1.33
24	A	406	CLA	C3B-C2B	5.08	1.47	1.40
24	B	605	CLA	C3B-C2B	5.08	1.47	1.40
24	B	607	CLA	C3B-C2B	5.08	1.47	1.40
24	C	512	CLA	O2D-CGD	5.08	1.45	1.33
24	B	610	CLA	OBD-CAD	5.07	1.29	1.22
24	C	507	CLA	C3C-C2C	5.07	1.47	1.36
24	c	510	CLA	CHC-C1C	5.07	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	406	PHO	CHB-C1B	5.07	1.48	1.38
24	a	350	CLA	CHC-C1C	5.06	1.48	1.35
24	B	609	CLA	C3C-C2C	5.06	1.47	1.36
24	A	404	CLA	C3C-C2C	5.06	1.47	1.36
24	b	601	CLA	O2D-CGD	5.05	1.45	1.33
24	B	606	CLA	CHC-C1C	5.05	1.47	1.35
24	a	403	CLA	O2D-CGD	5.05	1.45	1.33
24	c	513	CLA	CHC-C1C	5.05	1.47	1.35
24	B	609	CLA	CHC-C1C	5.05	1.47	1.35
24	B	614	CLA	C3C-C2C	5.05	1.47	1.36
25	a	406	PHO	CHD-C1D	5.04	1.48	1.38
24	c	506	CLA	O2D-CGD	5.04	1.45	1.33
24	B	613	CLA	O2D-CGD	5.03	1.45	1.33
24	c	506	CLA	OBD-CAD	5.03	1.29	1.22
24	a	350	CLA	O2D-CGD	5.03	1.45	1.33
24	b	615	CLA	CHC-C1C	5.02	1.47	1.35
26	C	515	BCR	C23-C22	-5.02	1.35	1.45
24	b	609	CLA	O2D-CGD	5.02	1.45	1.33
24	c	507	CLA	C3D-C2D	5.02	1.48	1.39
24	C	503	CLA	C3C-C2C	5.02	1.47	1.36
26	c	517	BCR	C23-C22	-5.01	1.35	1.45
24	A	406	CLA	O2D-CGD	5.01	1.45	1.33
24	C	512	CLA	CHC-C1C	5.01	1.47	1.35
24	c	506	CLA	C3C-C2C	5.00	1.47	1.36
24	b	611	CLA	CHC-C1C	5.00	1.47	1.35
24	C	504	CLA	CHC-C1C	5.00	1.47	1.35
24	C	506	CLA	C3C-C2C	5.00	1.47	1.36
26	c	516	BCR	C23-C22	-4.99	1.35	1.45
24	A	409	CLA	O2D-CGD	4.99	1.45	1.33
24	A	404	CLA	CHC-C1C	4.98	1.47	1.35
24	a	407	CLA	CHC-C1C	4.98	1.47	1.35
24	b	603	CLA	CHC-C1C	4.98	1.47	1.35
24	b	603	CLA	OBD-CAD	4.98	1.29	1.22
24	a	403	CLA	C3C-C2C	4.98	1.47	1.36
24	d	402	CLA	CHC-C1C	4.98	1.47	1.35
24	C	511	CLA	O2D-CGD	4.98	1.45	1.33
24	c	508	CLA	CHC-C1C	4.98	1.47	1.35
24	C	509	CLA	CHC-C1C	4.97	1.47	1.35
24	c	511	CLA	CHC-C1C	4.97	1.47	1.35
24	c	509	CLA	CHC-C1C	4.97	1.47	1.35
24	C	510	CLA	CHC-C1C	4.96	1.47	1.35
24	b	609	CLA	CHC-C1C	4.96	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	604	CLA	C3D-C2D	4.95	1.48	1.39
24	B	605	CLA	O2D-CGD	4.95	1.45	1.33
26	t	102	BCR	C23-C22	-4.95	1.35	1.45
26	y	101	BCR	C23-C22	-4.94	1.35	1.45
24	c	515	CLA	CHC-C1C	4.93	1.47	1.35
24	c	504	CLA	O2D-CGD	4.93	1.45	1.33
24	b	614	CLA	CHC-C1C	4.93	1.47	1.35
24	b	613	CLA	CHC-C1C	4.93	1.47	1.35
24	b	614	CLA	C3C-C2C	4.92	1.47	1.36
24	B	615	CLA	CHC-C1C	4.92	1.47	1.35
24	c	507	CLA	CHC-C1C	4.92	1.47	1.35
24	b	610	CLA	C3D-C2D	4.91	1.48	1.39
24	C	510	CLA	OBD-CAD	4.91	1.29	1.22
24	B	606	CLA	C3C-C2C	4.90	1.47	1.36
24	c	512	CLA	CHC-C1C	4.90	1.47	1.35
24	C	505	CLA	O2D-CGD	4.90	1.45	1.33
24	b	606	CLA	CHC-C1C	4.89	1.47	1.35
26	T	101	BCR	C23-C22	-4.89	1.35	1.45
24	D	403	CLA	O2D-CGD	4.89	1.45	1.33
24	c	504	CLA	CHC-C1C	4.89	1.47	1.35
24	b	605	CLA	O2D-CGD	4.89	1.45	1.33
24	C	503	CLA	O2D-CGD	4.89	1.45	1.33
24	d	402	CLA	C3C-C2C	4.88	1.47	1.36
24	c	508	CLA	OBD-CAD	4.88	1.29	1.22
24	c	515	CLA	O2D-CGD	4.88	1.45	1.33
24	B	611	CLA	CHC-C1C	4.88	1.47	1.35
24	B	602	CLA	O2D-CGD	4.88	1.45	1.33
24	b	608	CLA	CHC-C1C	4.88	1.47	1.35
24	b	602	CLA	O2D-CGD	4.88	1.45	1.33
25	A	408	PHO	CHC-C1C	4.88	1.48	1.38
26	b	617	BCR	C23-C22	-4.88	1.35	1.45
24	C	505	CLA	CHC-C1C	4.87	1.47	1.35
24	b	603	CLA	O2D-CGD	4.86	1.45	1.33
24	B	608	CLA	O2D-CGD	4.86	1.45	1.33
24	b	609	CLA	C3C-C2C	4.85	1.47	1.36
24	B	612	CLA	C3C-C2C	4.85	1.47	1.36
24	B	614	CLA	CHC-C1C	4.85	1.47	1.35
26	A	410	BCR	C23-C22	-4.84	1.35	1.45
24	c	509	CLA	O2D-CGD	4.84	1.45	1.33
26	D	404	BCR	C23-C22	-4.84	1.35	1.45
24	A	409	CLA	CHC-C1C	4.83	1.47	1.35
24	c	512	CLA	O2D-CGD	4.83	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	513	CLA	OBD-CAD	4.82	1.29	1.22
25	A	407	PHO	O2D-CGD	4.82	1.45	1.33
24	b	608	CLA	O2D-CGD	4.81	1.44	1.33
24	a	403	CLA	CHC-C1C	4.81	1.47	1.35
24	B	613	CLA	C3C-C2C	4.80	1.46	1.36
24	C	506	CLA	O2D-CGD	4.80	1.44	1.33
24	B	603	CLA	CHC-C1C	4.80	1.47	1.35
24	B	615	CLA	O2D-CGD	4.80	1.44	1.33
24	B	613	CLA	CHC-C1C	4.80	1.47	1.35
24	B	607	CLA	CHC-C1C	4.79	1.47	1.35
24	b	601	CLA	CHC-C1C	4.79	1.47	1.35
24	B	608	CLA	CHC-C1C	4.79	1.47	1.35
25	A	407	PHO	CHB-C1B	4.78	1.48	1.38
26	b	619	BCR	C23-C22	-4.78	1.35	1.45
24	c	514	CLA	O2D-CGD	4.77	1.44	1.33
24	C	508	CLA	CHC-C1C	4.77	1.47	1.35
24	C	514	CLA	O2D-CGD	4.77	1.44	1.33
24	B	612	CLA	CHC-C1C	4.76	1.47	1.35
24	c	506	CLA	CHC-C1C	4.76	1.47	1.35
24	B	615	CLA	C3B-C2B	4.76	1.47	1.40
24	A	405	CLA	O2D-CGD	4.76	1.44	1.33
26	h	102	BCR	C23-C22	-4.76	1.35	1.45
25	A	408	PHO	O2D-CGD	4.75	1.44	1.33
24	b	614	CLA	O2D-CGD	4.75	1.44	1.33
24	C	512	CLA	C3C-C2C	4.74	1.46	1.36
24	b	609	CLA	OBD-CAD	4.74	1.28	1.22
24	b	612	CLA	O2D-CGD	4.74	1.44	1.33
25	A	407	PHO	CHD-C1D	4.74	1.47	1.38
26	b	618	BCR	C23-C22	-4.74	1.35	1.45
24	b	611	CLA	O2D-CGD	4.74	1.44	1.33
24	C	509	CLA	O2D-CGD	4.74	1.44	1.33
24	a	404	CLA	O2D-CGD	4.71	1.44	1.33
24	C	506	CLA	C3D-C2D	4.70	1.47	1.39
24	c	503	CLA	O2D-CGD	4.70	1.44	1.33
24	c	509	CLA	OBD-CAD	4.70	1.28	1.22
24	a	407	CLA	O2D-CGD	4.70	1.44	1.33
24	b	615	CLA	OBD-CAD	4.69	1.28	1.22
24	c	505	CLA	O2D-CGD	4.69	1.44	1.33
24	d	402	CLA	O2D-CGD	4.69	1.44	1.33
24	D	402	CLA	O2D-CGD	4.69	1.44	1.33
24	C	513	CLA	O2D-CGD	4.69	1.44	1.33
24	B	607	CLA	OBD-CAD	4.69	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	608	CLA	OBD-CAD	4.69	1.28	1.22
24	C	510	CLA	O2D-CGD	4.68	1.44	1.33
26	H	101	BCR	C23-C22	-4.67	1.35	1.45
24	c	513	CLA	O2D-CGD	4.67	1.44	1.33
25	a	405	PHO	CHB-C1B	4.66	1.47	1.38
24	b	607	CLA	CHC-C1C	4.65	1.46	1.35
25	A	407	PHO	CHC-C1C	4.65	1.47	1.38
24	b	607	CLA	O2D-CGD	4.65	1.44	1.33
24	a	404	CLA	OBD-CAD	4.64	1.28	1.22
24	c	510	CLA	OBD-CAD	4.64	1.28	1.22
26	a	408	BCR	C23-C22	-4.63	1.36	1.45
24	B	604	CLA	O2D-CGD	4.63	1.44	1.33
24	d	403	CLA	OBD-CAD	4.63	1.28	1.22
24	B	615	CLA	OBD-CAD	4.63	1.28	1.22
24	C	513	CLA	OBD-CAD	4.62	1.28	1.22
24	B	612	CLA	O2D-CGD	4.62	1.44	1.33
24	b	615	CLA	O2D-CGD	4.62	1.44	1.33
24	b	601	CLA	O2A-CGA	4.62	1.46	1.33
24	C	503	CLA	OBD-CAD	4.60	1.28	1.22
24	C	504	CLA	O2D-CGD	4.60	1.44	1.33
24	D	402	CLA	CHC-C1C	4.60	1.46	1.35
27	F	101	SQD	O47-C7	4.60	1.47	1.34
26	Y	101	BCR	C23-C22	-4.59	1.36	1.45
24	b	601	CLA	OBD-CAD	4.58	1.28	1.22
24	C	507	CLA	CHC-C1C	4.58	1.46	1.35
24	B	616	CLA	O2D-CGD	4.58	1.44	1.33
26	B	617	BCR	C23-C22	-4.56	1.36	1.45
24	B	610	CLA	O2D-CGD	4.56	1.44	1.33
24	A	404	CLA	O2D-CGD	4.55	1.44	1.33
24	c	514	CLA	OBD-CAD	4.55	1.28	1.22
24	B	601	CLA	O2A-CGA	4.54	1.46	1.33
24	C	514	CLA	OBD-CAD	4.54	1.28	1.22
24	A	406	CLA	OBD-CAD	4.54	1.28	1.22
24	C	509	CLA	OBD-CAD	4.54	1.28	1.22
24	b	610	CLA	OBD-CAD	4.53	1.28	1.22
24	b	605	CLA	CHC-C1C	4.53	1.46	1.35
24	B	616	CLA	OBD-CAD	4.52	1.28	1.22
24	B	611	CLA	OBD-CAD	4.52	1.28	1.22
24	B	603	CLA	O2D-CGD	4.52	1.44	1.33
24	C	508	CLA	O2D-CGD	4.51	1.44	1.33
24	B	604	CLA	OBD-CAD	4.50	1.28	1.22
24	C	512	CLA	OBD-CAD	4.50	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	405	PHO	O2D-CGD	4.49	1.44	1.33
24	B	611	CLA	O2D-CGD	4.48	1.44	1.33
24	b	612	CLA	CHC-C1C	4.48	1.46	1.35
33	z	101	LMG	O8-C28	4.48	1.46	1.33
24	B	601	CLA	OBD-CAD	4.47	1.28	1.22
24	D	403	CLA	OBD-CAD	4.47	1.28	1.22
24	A	404	CLA	OBD-CAD	4.47	1.28	1.22
24	B	614	CLA	O2D-CGD	4.46	1.44	1.33
33	C	521	LMG	O8-C28	4.45	1.46	1.33
24	b	615	CLA	O2A-CGA	4.45	1.46	1.33
25	A	408	PHO	CHB-C1B	4.44	1.47	1.38
24	b	610	CLA	O2D-CGD	4.43	1.44	1.33
26	B	618	BCR	C23-C22	-4.42	1.36	1.45
25	a	405	PHO	CHC-C1C	4.41	1.47	1.38
24	c	512	CLA	OBD-CAD	4.41	1.28	1.22
27	a	411	SQD	O48-C23	4.41	1.46	1.33
27	f	101	SQD	O47-C7	4.41	1.46	1.34
24	C	508	CLA	OBD-CAD	4.40	1.28	1.22
24	B	606	CLA	O2D-CGD	4.40	1.43	1.33
33	C	521	LMG	O7-C10	4.40	1.46	1.34
24	c	515	CLA	OBD-CAD	4.39	1.28	1.22
25	a	405	PHO	CHD-C1D	4.39	1.47	1.38
24	b	614	CLA	OBD-CAD	4.39	1.28	1.22
24	b	604	CLA	O2D-CGD	4.38	1.43	1.33
24	b	606	CLA	O2D-CGD	4.38	1.43	1.33
24	C	504	CLA	OBD-CAD	4.37	1.28	1.22
24	B	602	CLA	OBD-CAD	4.36	1.28	1.22
25	A	408	PHO	CHD-C1D	4.35	1.47	1.38
24	c	503	CLA	OBD-CAD	4.35	1.28	1.22
33	c	522	LMG	O7-C10	4.35	1.46	1.34
24	a	350	CLA	OBD-CAD	4.34	1.28	1.22
24	b	602	CLA	OBD-CAD	4.34	1.28	1.22
24	C	502	CLA	OBD-CAD	4.33	1.28	1.22
24	c	511	CLA	OBD-CAD	4.32	1.28	1.22
24	C	511	CLA	OBD-CAD	4.32	1.28	1.22
38	E	101	LHG	O8-C23	4.31	1.45	1.33
24	B	607	CLA	O2D-CGD	4.31	1.43	1.33
38	a	419	LHG	O8-C23	4.31	1.45	1.33
24	B	609	CLA	O2A-CGA	4.31	1.45	1.33
24	b	604	CLA	OBD-CAD	4.30	1.28	1.22
33	c	521	LMG	O8-C28	4.30	1.45	1.33
33	c	522	LMG	O8-C28	4.30	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	413	SQD	O48-C23	4.29	1.45	1.33
33	C	520	LMG	O8-C28	4.29	1.45	1.33
33	Z	101	LMG	O7-C10	4.29	1.46	1.34
24	a	403	CLA	OBD-CAD	4.27	1.28	1.22
24	C	513	CLA	O2A-CGA	4.26	1.45	1.33
24	C	514	CLA	O2A-CGA	4.26	1.45	1.33
24	B	612	CLA	OBD-CAD	4.26	1.28	1.22
24	d	403	CLA	O2A-CGA	4.26	1.45	1.33
33	B	621	LMG	O8-C28	4.25	1.45	1.33
24	d	403	CLA	O2D-CGD	4.25	1.43	1.33
24	c	515	CLA	O2A-CGA	4.24	1.45	1.33
41	v	203	HEC	CBC-CAC	-4.24	1.33	1.49
24	C	502	CLA	O2D-CGD	4.24	1.43	1.33
24	c	514	CLA	O2A-CGA	4.24	1.45	1.33
24	a	350	CLA	O2A-CGA	4.24	1.45	1.33
24	B	613	CLA	OBD-CAD	4.23	1.28	1.22
24	C	512	CLA	O2A-CGA	4.22	1.45	1.33
24	c	511	CLA	O2A-CGA	4.22	1.45	1.33
24	c	513	CLA	O2A-CGA	4.21	1.45	1.33
38	a	419	LHG	O7-C7	4.20	1.46	1.34
27	b	620	SQD	O47-C7	4.20	1.46	1.34
24	b	614	CLA	O2A-CGA	4.19	1.45	1.33
24	c	505	CLA	OBD-CAD	4.19	1.28	1.22
24	a	407	CLA	O2A-CGA	4.19	1.45	1.33
24	b	607	CLA	OBD-CAD	4.19	1.28	1.22
27	B	620	SQD	O48-C23	4.19	1.45	1.33
24	c	509	CLA	O2A-CGA	4.18	1.45	1.33
24	d	402	CLA	OBD-CAD	4.18	1.28	1.22
24	A	405	CLA	O2A-CGA	4.18	1.45	1.33
27	f	101	SQD	O48-C23	4.18	1.45	1.33
24	C	502	CLA	O2A-CGA	4.17	1.45	1.33
41	v	203	HEC	CBB-CAB	-4.16	1.33	1.49
24	c	503	CLA	O2A-CGA	4.16	1.45	1.33
24	C	506	CLA	OBD-CAD	4.16	1.28	1.22
24	c	510	CLA	O2A-CGA	4.16	1.45	1.33
27	B	620	SQD	O47-C7	4.16	1.46	1.34
38	d	408	LHG	O7-C7	4.16	1.46	1.34
27	A	411	SQD	O48-C23	4.16	1.45	1.33
33	a	417	LMG	O8-C28	4.15	1.45	1.33
36	h	103	DGD	O1G-C1A	4.15	1.45	1.33
36	c	519	DGD	O1G-C1A	4.15	1.45	1.33
27	A	413	SQD	O47-C7	4.15	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	507	CLA	OBD-CAD	4.15	1.28	1.22
33	b	621	LMG	O8-C28	4.14	1.45	1.33
24	C	508	CLA	O2A-CGA	4.14	1.45	1.33
24	c	507	CLA	OBD-CAD	4.14	1.28	1.22
24	b	602	CLA	O2A-CGA	4.14	1.45	1.33
24	A	409	CLA	OBD-CAD	4.13	1.28	1.22
27	b	620	SQD	O48-C23	4.13	1.45	1.33
24	b	605	CLA	OBD-CAD	4.13	1.28	1.22
24	C	509	CLA	O2A-CGA	4.12	1.45	1.33
33	A	418	LMG	O8-C28	4.12	1.45	1.33
24	B	615	CLA	O2A-CGA	4.11	1.45	1.33
38	l	101	LHG	O8-C23	4.11	1.45	1.33
24	b	616	CLA	OBD-CAD	4.11	1.28	1.22
24	c	504	CLA	OBD-CAD	4.11	1.28	1.22
33	C	520	LMG	O7-C10	4.10	1.45	1.34
24	b	608	CLA	O2A-CGA	4.10	1.45	1.33
24	C	507	CLA	O2A-CGA	4.10	1.45	1.33
24	b	611	CLA	O2A-CGA	4.10	1.45	1.33
24	b	606	CLA	O2A-CGA	4.09	1.45	1.33
38	L	101	LHG	O8-C23	4.08	1.45	1.33
36	c	518	DGD	O1G-C1A	4.07	1.45	1.33
24	B	607	CLA	O2A-CGA	4.07	1.45	1.33
24	b	616	CLA	O2A-CGA	4.07	1.45	1.33
24	B	603	CLA	OBD-CAD	4.07	1.28	1.22
41	V	203	HEC	CBC-CAC	-4.06	1.34	1.49
24	C	503	CLA	O2A-CGA	4.06	1.45	1.33
27	a	411	SQD	O47-C7	4.06	1.45	1.34
24	C	505	CLA	OBD-CAD	4.06	1.28	1.22
24	A	405	CLA	OBD-CAD	4.05	1.28	1.22
24	B	608	CLA	OBD-CAD	4.05	1.28	1.22
24	A	409	CLA	O2A-CGA	4.05	1.45	1.33
24	c	506	CLA	O2A-CGA	4.05	1.45	1.33
25	a	406	PHO	O2A-CGA	4.04	1.45	1.33
36	c	520	DGD	O1G-C1A	4.03	1.45	1.33
41	V	203	HEC	CBB-CAB	-4.03	1.34	1.49
33	a	417	LMG	O7-C10	4.03	1.45	1.34
24	b	613	CLA	O2A-CGA	4.03	1.45	1.33
33	A	418	LMG	O7-C10	4.02	1.45	1.34
36	C	518	DGD	O1G-C1A	4.02	1.45	1.33
24	B	606	CLA	O2A-CGA	4.02	1.45	1.33
24	b	609	CLA	O2A-CGA	4.02	1.45	1.33
27	F	101	SQD	O48-C23	4.02	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	z	101	LMG	O7-C10	4.02	1.45	1.34
27	a	409	SQD	O48-C23	4.00	1.45	1.33
24	c	507	CLA	O2A-CGA	4.00	1.45	1.33
36	C	519	DGD	O1G-C1A	3.99	1.45	1.33
33	c	521	LMG	O7-C10	3.99	1.45	1.34
35	b	623	HTG	C1'-S1	-3.97	1.76	1.81
38	E	101	LHG	O7-C7	3.97	1.45	1.34
24	d	402	CLA	O2A-CGA	3.97	1.44	1.33
24	B	616	CLA	O2A-CGA	3.97	1.44	1.33
24	b	607	CLA	O2A-CGA	3.96	1.44	1.33
24	b	613	CLA	OBD-CAD	3.96	1.27	1.22
24	B	613	CLA	O2A-CGA	3.96	1.44	1.33
24	c	508	CLA	O2A-CGA	3.96	1.44	1.33
33	j	101	LMG	O8-C28	3.95	1.44	1.33
24	B	603	CLA	O2A-CGA	3.95	1.44	1.33
24	B	614	CLA	OBD-CAD	3.95	1.27	1.22
33	j	101	LMG	O7-C10	3.94	1.45	1.34
27	a	409	SQD	O47-C7	3.94	1.45	1.34
24	c	505	CLA	O2A-CGA	3.94	1.44	1.33
24	a	404	CLA	O2A-CGA	3.93	1.44	1.33
24	b	612	CLA	O2A-CGA	3.93	1.44	1.33
24	C	511	CLA	O2A-CGA	3.93	1.44	1.33
38	D	407	LHG	O8-C23	3.92	1.44	1.33
24	c	504	CLA	O2A-CGA	3.92	1.44	1.33
24	b	611	CLA	OBD-CAD	3.91	1.27	1.22
36	h	103	DGD	O2G-C1B	3.91	1.45	1.34
36	H	102	DGD	O1G-C1A	3.91	1.44	1.33
35	b	625	HTG	C1'-S1	-3.90	1.76	1.81
24	b	604	CLA	O2A-CGA	3.89	1.44	1.33
24	B	608	CLA	O2A-CGA	3.88	1.44	1.33
33	B	621	LMG	O7-C10	3.88	1.45	1.34
24	D	402	CLA	O2A-CGA	3.87	1.44	1.33
24	C	510	CLA	O2A-CGA	3.87	1.44	1.33
33	J	101	LMG	O8-C28	3.86	1.44	1.33
36	C	517	DGD	O2G-C1B	3.86	1.45	1.34
38	d	408	LHG	O8-C23	3.86	1.44	1.33
38	D	357	LHG	O8-C23	3.85	1.44	1.33
24	C	506	CLA	O2A-CGA	3.84	1.44	1.33
25	A	407	PHO	O2A-CGA	3.84	1.44	1.33
36	C	518	DGD	O2G-C1B	3.82	1.45	1.34
24	a	407	CLA	OBD-CAD	3.82	1.27	1.22
38	d	406	LHG	O8-C23	3.81	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	603	CLA	O2A-CGA	3.81	1.44	1.33
24	B	609	CLA	OBD-CAD	3.81	1.27	1.22
24	c	512	CLA	O2A-CGA	3.80	1.44	1.33
36	c	518	DGD	O2G-C1B	3.80	1.45	1.34
25	A	408	PHO	OBD-CAD	3.80	1.29	1.22
38	l	101	LHG	O7-C7	3.80	1.45	1.34
24	D	403	CLA	O2A-CGA	3.79	1.44	1.33
24	B	614	CLA	O2A-CGA	3.78	1.44	1.33
24	C	505	CLA	O2A-CGA	3.78	1.44	1.33
35	B	623	HTG	C1'-S1	-3.78	1.76	1.81
38	D	407	LHG	O7-C7	3.78	1.45	1.34
25	a	406	PHO	OBD-CAD	3.77	1.29	1.22
24	C	504	CLA	O2A-CGA	3.77	1.44	1.33
24	D	402	CLA	OBD-CAD	3.77	1.27	1.22
24	B	606	CLA	OBD-CAD	3.76	1.27	1.22
38	d	407	LHG	O8-C23	3.74	1.44	1.33
24	b	612	CLA	OBD-CAD	3.74	1.27	1.22
24	A	406	CLA	O2A-CGA	3.73	1.44	1.33
24	B	605	CLA	O2A-CGA	3.73	1.44	1.33
35	h	101	HTG	C1'-S1	-3.73	1.76	1.81
25	a	406	PHO	C3D-C2D	3.72	1.49	1.39
33	J	101	LMG	O7-C10	3.72	1.44	1.34
36	c	519	DGD	O2G-C1B	3.72	1.44	1.34
24	B	612	CLA	O2A-CGA	3.72	1.44	1.33
24	b	605	CLA	O2A-CGA	3.71	1.44	1.33
24	B	602	CLA	O2A-CGA	3.71	1.44	1.33
38	L	101	LHG	O7-C7	3.71	1.44	1.34
36	c	520	DGD	O2G-C1B	3.68	1.44	1.34
38	D	406	LHG	O7-C7	3.68	1.44	1.34
24	B	604	CLA	O2A-CGA	3.67	1.44	1.33
36	C	517	DGD	O1G-C1A	3.66	1.44	1.33
35	C	523	HTG	C1'-S1	-3.66	1.76	1.81
25	A	407	PHO	C4A-NA	-3.65	1.26	1.35
24	B	610	CLA	O2A-CGA	3.65	1.44	1.33
24	b	606	CLA	OBD-CAD	3.65	1.27	1.22
38	D	357	LHG	O7-C7	3.64	1.44	1.34
35	c	526	HTG	C1'-S1	-3.63	1.76	1.81
35	b	624	HTG	C1'-S1	-3.62	1.76	1.81
38	D	406	LHG	O8-C23	3.61	1.43	1.33
24	a	403	CLA	O2A-CGA	3.60	1.43	1.33
36	C	519	DGD	O2G-C1B	3.60	1.44	1.34
38	d	406	LHG	O7-C7	3.59	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	408	PHO	C3D-C2D	3.59	1.48	1.39
24	b	610	CLA	O2A-CGA	3.57	1.43	1.33
24	B	605	CLA	OBD-CAD	3.57	1.27	1.22
38	d	407	LHG	O7-C7	3.56	1.44	1.34
25	A	408	PHO	C4A-NA	-3.53	1.26	1.35
27	A	411	SQD	O47-C7	3.53	1.44	1.34
25	A	407	PHO	C3D-C2D	3.52	1.48	1.39
33	b	621	LMG	O7-C10	3.49	1.44	1.34
24	B	611	CLA	O2A-CGA	3.49	1.43	1.33
35	B	625	HTG	C1'-S1	-3.49	1.77	1.81
36	H	102	DGD	O2G-C1B	3.47	1.44	1.34
35	C	522	HTG	C1'-S1	-3.47	1.77	1.81
24	A	404	CLA	O2A-CGA	3.46	1.43	1.33
25	a	406	PHO	CHC-C4B	3.44	1.48	1.40
25	A	408	PHO	O2A-CGA	3.42	1.43	1.33
25	a	405	PHO	O2A-CGA	3.41	1.43	1.33
35	c	523	HTG	C1'-S1	-3.41	1.77	1.81
25	a	405	PHO	C3D-C2D	3.40	1.48	1.39
25	a	405	PHO	C4A-NA	-3.37	1.27	1.35
25	A	408	PHO	CHC-C4B	3.37	1.48	1.40
41	V	203	HEC	C3B-C2B	-3.32	1.37	1.40
35	D	410	HTG	C1'-S1	-3.26	1.77	1.81
35	B	628	HTG	C1'-S1	-3.26	1.77	1.81
25	A	407	PHO	CHD-C4C	3.23	1.48	1.40
25	a	405	PHO	OBD-CAD	3.22	1.28	1.22
25	a	406	PHO	C4A-NA	-3.22	1.27	1.35
24	C	506	CLA	C1C-C2C	3.17	1.50	1.44
24	C	507	CLA	C1D-C2D	3.13	1.49	1.42
25	a	405	PHO	CHC-C4B	3.12	1.47	1.40
35	B	624	HTG	C1'-S1	-3.12	1.77	1.81
24	c	515	CLA	C1D-C2D	3.12	1.49	1.42
24	c	509	CLA	C1D-C2D	3.11	1.49	1.42
24	b	615	CLA	C1D-C2D	3.09	1.49	1.42
25	A	408	PHO	C3B-C4B	3.08	1.49	1.43
24	d	403	CLA	C1D-C2D	3.05	1.49	1.42
24	b	605	CLA	C1D-C2D	3.05	1.49	1.42
24	C	502	CLA	C1D-C2D	3.04	1.49	1.42
35	b	628	HTG	C1'-S1	-3.02	1.77	1.81
24	c	507	CLA	C1C-C2C	2.98	1.50	1.44
24	C	510	CLA	C1D-C2D	2.98	1.49	1.42
24	c	506	CLA	C1D-C2D	2.98	1.49	1.42
41	v	203	HEC	C3B-C2B	-2.97	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	609	CLA	C1D-C2D	2.97	1.49	1.42
24	c	503	CLA	C1D-C2D	2.94	1.49	1.42
24	b	611	CLA	C1D-C2D	2.94	1.49	1.42
24	b	610	CLA	C4B-CHC	2.94	1.49	1.41
25	A	407	PHO	CHC-C4B	2.93	1.47	1.40
25	a	406	PHO	C3B-C4B	2.93	1.49	1.43
24	B	602	CLA	C1C-C2C	2.91	1.50	1.44
24	a	404	CLA	C1D-C2D	2.89	1.49	1.42
24	b	602	CLA	C1C-C2C	2.89	1.50	1.44
25	a	406	PHO	CHB-C4A	2.89	1.47	1.40
25	A	407	PHO	OBD-CAD	2.89	1.27	1.22
24	C	504	CLA	C1D-C2D	2.88	1.49	1.42
39	e	102	HEM	C3B-C2B	-2.88	1.36	1.40
41	v	203	HEC	C3B-C4B	2.88	1.48	1.43
24	C	514	CLA	C1D-C2D	2.87	1.49	1.42
25	a	406	PHO	CHD-C4C	2.86	1.47	1.40
27	A	413	SQD	C6-S	-2.86	1.66	1.77
24	c	513	CLA	C1D-C2D	2.86	1.49	1.42
24	B	602	CLA	C1D-C2D	2.86	1.49	1.42
24	A	405	CLA	C1C-C2C	2.86	1.50	1.44
24	b	603	CLA	C1C-C2C	2.86	1.50	1.44
24	b	602	CLA	C1D-C2D	2.85	1.49	1.42
25	a	405	PHO	C3B-C4B	2.84	1.49	1.43
27	f	101	SQD	C6-S	-2.83	1.66	1.77
25	A	408	PHO	CHD-C4C	2.83	1.47	1.40
24	b	601	CLA	C1D-C2D	2.83	1.49	1.42
24	B	614	CLA	C1D-C2D	2.83	1.49	1.42
24	C	512	CLA	C1D-C2D	2.80	1.48	1.42
24	b	607	CLA	C1B-NB	-2.80	1.32	1.35
25	A	407	PHO	C1A-NA	-2.80	1.32	1.37
24	C	513	CLA	C1C-C2C	2.80	1.50	1.44
27	a	409	SQD	C6-S	-2.80	1.67	1.77
25	A	408	PHO	CHB-C4A	2.80	1.47	1.40
24	b	606	CLA	C1B-NB	-2.80	1.32	1.35
24	A	404	CLA	C1C-C2C	2.79	1.50	1.44
24	d	403	CLA	C4B-CHC	2.79	1.48	1.41
24	b	613	CLA	C1C-C2C	2.78	1.50	1.44
24	B	606	CLA	C1C-C2C	2.78	1.49	1.44
24	c	508	CLA	C1D-C2D	2.77	1.48	1.42
25	a	405	PHO	CHB-C4A	2.77	1.46	1.40
24	C	510	CLA	C1C-C2C	2.76	1.49	1.44
24	B	605	CLA	C1C-C2C	2.76	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	411	SQD	C6-S	-2.76	1.67	1.77
24	c	505	CLA	C1D-C2D	2.76	1.48	1.42
24	B	607	CLA	C1C-C2C	2.75	1.49	1.44
27	b	620	SQD	C6-S	-2.75	1.67	1.77
24	B	613	CLA	C1C-C2C	2.75	1.49	1.44
24	b	610	CLA	C1D-C2D	2.74	1.48	1.42
24	a	350	CLA	C1D-C2D	2.74	1.48	1.42
24	a	407	CLA	C1B-NB	-2.74	1.32	1.35
24	B	604	CLA	C1B-CHB	2.74	1.48	1.41
24	B	601	CLA	C1C-C2C	2.73	1.49	1.44
24	B	609	CLA	C1D-C2D	2.73	1.48	1.42
24	A	406	CLA	C1D-C2D	2.73	1.48	1.42
31	a	414[A]	PL9	C6-C5	2.73	1.49	1.35
25	A	407	PHO	C3B-C4B	2.72	1.48	1.43
24	C	514	CLA	C1C-C2C	2.72	1.49	1.44
24	D	403	CLA	C1D-C2D	2.72	1.48	1.42
41	V	203	HEC	C3B-C4B	2.71	1.48	1.43
27	F	101	SQD	C6-S	-2.71	1.67	1.77
24	c	511	CLA	C1D-C2D	2.71	1.48	1.42
24	C	507	CLA	C4C-C3C	2.71	1.49	1.45
31	A	416[A]	PL9	C6-C5	2.71	1.49	1.35
24	B	613	CLA	C4C-C3C	2.70	1.49	1.45
24	b	607	CLA	C1D-C2D	2.70	1.48	1.42
27	B	620	SQD	C6-S	-2.70	1.67	1.77
24	b	602	CLA	C4B-CHC	2.69	1.48	1.41
24	c	509	CLA	CHD-C4C	2.69	1.48	1.41
24	b	604	CLA	C1C-C2C	2.68	1.49	1.44
24	A	405	CLA	C4B-CHC	2.68	1.48	1.41
24	B	603	CLA	C1C-C2C	2.68	1.49	1.44
24	C	504	CLA	C4C-C3C	2.68	1.49	1.45
24	d	402	CLA	C1B-NB	-2.67	1.32	1.35
24	A	404	CLA	C1D-C2D	2.67	1.48	1.42
24	c	511	CLA	C4C-C3C	2.67	1.49	1.45
24	c	513	CLA	C1B-CHB	2.67	1.48	1.41
27	A	411	SQD	C6-S	-2.66	1.67	1.77
31	a	414[B]	PL9	C6-C5	2.66	1.49	1.35
24	A	406	CLA	CHD-C4C	2.65	1.48	1.41
24	c	512	CLA	C1B-CHB	2.64	1.48	1.41
24	D	403	CLA	C1C-C2C	2.64	1.49	1.44
24	b	612	CLA	C1B-CHB	2.64	1.48	1.41
24	C	502	CLA	C4B-CHC	2.63	1.48	1.41
24	C	511	CLA	C1C-C2C	2.63	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	612	CLA	C1B-CHB	2.63	1.48	1.41
24	B	607	CLA	C1D-C2D	2.63	1.48	1.42
31	A	416[B]	PL9	C6-C5	2.63	1.49	1.35
24	C	511	CLA	C1D-C2D	2.63	1.48	1.42
24	c	515	CLA	C1C-C2C	2.63	1.49	1.44
24	B	615	CLA	C1D-C2D	2.63	1.48	1.42
24	B	601	CLA	C1D-C2D	2.62	1.48	1.42
24	B	615	CLA	C1C-C2C	2.62	1.49	1.44
24	C	513	CLA	C1D-C2D	2.62	1.48	1.42
24	D	402	CLA	C4C-C3C	2.62	1.49	1.45
24	D	403	CLA	C4B-CHC	2.62	1.48	1.41
24	B	613	CLA	C1D-C2D	2.62	1.48	1.42
25	a	405	PHO	CHD-C4C	2.62	1.46	1.40
24	B	609	CLA	C1C-C2C	2.61	1.49	1.44
24	B	602	CLA	C4B-CHC	2.61	1.48	1.41
24	c	508	CLA	CHD-C4C	2.61	1.48	1.41
24	C	512	CLA	C1C-C2C	2.61	1.49	1.44
24	c	514	CLA	C1D-C2D	2.61	1.48	1.42
24	B	604	CLA	C1C-C2C	2.61	1.49	1.44
24	C	505	CLA	C1D-C2D	2.60	1.48	1.42
24	B	610	CLA	C4B-CHC	2.60	1.48	1.41
24	b	608	CLA	C1D-C2D	2.60	1.48	1.42
24	C	510	CLA	CHD-C4C	2.60	1.48	1.41
24	a	407	CLA	C1C-C2C	2.59	1.49	1.44
24	B	601	CLA	C4B-CHC	2.59	1.48	1.41
24	C	508	CLA	C1C-C2C	2.59	1.49	1.44
24	b	609	CLA	C1B-CHB	2.59	1.48	1.41
24	d	403	CLA	C1C-C2C	2.58	1.49	1.44
24	b	610	CLA	C1C-C2C	2.58	1.49	1.44
24	a	403	CLA	CHD-C4C	2.58	1.48	1.41
24	A	404	CLA	C4B-CHC	2.57	1.48	1.41
24	c	510	CLA	C1C-C2C	2.57	1.49	1.44
24	d	402	CLA	C4B-CHC	2.57	1.48	1.41
24	C	509	CLA	C1B-CHB	2.57	1.48	1.41
31	D	405	PL9	C6-C5	2.57	1.48	1.35
24	B	610	CLA	C1B-CHB	2.57	1.48	1.41
24	d	403	CLA	CHD-C4C	2.57	1.48	1.41
24	B	616	CLA	C1D-C2D	2.57	1.48	1.42
24	B	614	CLA	C1C-C2C	2.57	1.49	1.44
24	c	515	CLA	CHD-C4C	2.57	1.48	1.41
24	c	507	CLA	C4B-CHC	2.57	1.48	1.41
24	C	505	CLA	C1C-C2C	2.57	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	Z	101	LMG	O8-C28	2.57	1.46	1.33
24	b	614	CLA	C1C-C2C	2.57	1.49	1.44
24	A	409	CLA	C1D-C2D	2.56	1.48	1.42
24	c	506	CLA	C1C-C2C	2.56	1.49	1.44
24	b	614	CLA	C1D-C2D	2.56	1.48	1.42
24	C	511	CLA	C1B-CHB	2.56	1.48	1.41
24	b	612	CLA	C1B-NB	-2.56	1.32	1.35
24	A	404	CLA	C4C-C3C	2.56	1.49	1.45
24	B	602	CLA	CHD-C4C	2.56	1.48	1.41
24	b	602	CLA	CHD-C4C	2.56	1.48	1.41
24	C	509	CLA	C1D-C2D	2.55	1.48	1.42
24	C	502	CLA	C1C-C2C	2.55	1.49	1.44
24	c	511	CLA	C1B-CHB	2.55	1.48	1.41
24	B	614	CLA	C4C-C3C	2.55	1.49	1.45
24	c	515	CLA	C4C-C3C	2.55	1.49	1.45
24	B	607	CLA	C4C-C3C	2.55	1.49	1.45
31	d	405	PL9	C6-C5	2.54	1.48	1.35
24	c	507	CLA	C1B-CHB	2.54	1.48	1.41
24	C	510	CLA	C4C-C3C	2.54	1.49	1.45
24	C	506	CLA	C1B-CHB	2.54	1.48	1.41
24	B	602	CLA	C4C-C3C	2.54	1.49	1.45
24	C	514	CLA	CHD-C4C	2.54	1.48	1.41
25	a	406	PHO	C1A-NA	-2.54	1.32	1.37
24	b	610	CLA	C4C-C3C	2.54	1.49	1.45
24	b	611	CLA	C4B-CHC	2.54	1.48	1.41
24	c	512	CLA	CHD-C4C	2.53	1.48	1.41
24	B	610	CLA	C1D-C2D	2.53	1.48	1.42
24	c	514	CLA	C4B-CHC	2.53	1.48	1.41
24	A	406	CLA	C1C-C2C	2.53	1.49	1.44
24	b	613	CLA	C4B-CHC	2.53	1.48	1.41
24	C	507	CLA	CHD-C4C	2.53	1.48	1.41
25	A	407	PHO	CHB-C4A	2.53	1.46	1.40
24	c	513	CLA	C1C-C2C	2.53	1.49	1.44
24	a	403	CLA	C1D-C2D	2.53	1.48	1.42
24	B	605	CLA	C4B-CHC	2.52	1.48	1.41
24	B	605	CLA	C1B-CHB	2.52	1.48	1.41
24	C	508	CLA	C1D-C2D	2.51	1.48	1.42
24	C	504	CLA	CHD-C4C	2.51	1.48	1.41
24	C	509	CLA	C1C-C2C	2.51	1.49	1.44
24	b	606	CLA	C1D-C2D	2.51	1.48	1.42
25	A	408	PHO	C1A-NA	-2.50	1.32	1.37
24	C	505	CLA	C1B-CHB	2.50	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	504	CLA	C1D-C2D	2.50	1.48	1.42
24	B	615	CLA	C4B-CHC	2.50	1.47	1.41
24	C	510	CLA	C1B-CHB	2.50	1.47	1.41
24	b	601	CLA	CHD-C4C	2.50	1.48	1.41
24	a	404	CLA	CHD-C4C	2.50	1.48	1.41
24	D	402	CLA	C1D-C2D	2.50	1.48	1.42
24	c	503	CLA	CHD-C4C	2.49	1.48	1.41
24	c	512	CLA	C1D-C2D	2.49	1.48	1.42
24	b	608	CLA	C1C-C2C	2.48	1.49	1.44
24	b	607	CLA	C1C-C2C	2.48	1.49	1.44
24	C	513	CLA	C4B-CHC	2.48	1.47	1.41
24	a	350	CLA	C4B-CHC	2.48	1.47	1.41
24	B	609	CLA	C1B-NB	-2.48	1.33	1.35
24	B	607	CLA	CHD-C4C	2.48	1.48	1.41
35	D	410	HTG	C1-S1	-2.48	1.76	1.80
24	B	605	CLA	C1D-C2D	2.48	1.48	1.42
34	A	359	LMT	O1'-C1'	2.48	1.44	1.40
24	A	405	CLA	C1D-C2D	2.47	1.48	1.42
24	B	603	CLA	C4B-CHC	2.47	1.47	1.41
24	C	511	CLA	CHD-C4C	2.47	1.48	1.41
24	D	402	CLA	C1C-C2C	2.47	1.49	1.44
24	b	612	CLA	C4C-C3C	2.47	1.49	1.45
24	c	505	CLA	C4C-C3C	2.46	1.49	1.45
24	B	608	CLA	C1B-CHB	2.46	1.47	1.41
24	b	611	CLA	C1C-C2C	2.46	1.49	1.44
24	b	612	CLA	C1C-C2C	2.46	1.49	1.44
24	B	606	CLA	C1D-C2D	2.45	1.48	1.42
24	b	607	CLA	C1B-CHB	2.45	1.47	1.41
24	c	505	CLA	CHD-C4C	2.45	1.48	1.41
24	b	605	CLA	C1B-CHB	2.45	1.47	1.41
24	b	615	CLA	CHD-C4C	2.45	1.48	1.41
24	d	402	CLA	C1B-CHB	2.45	1.47	1.41
24	c	508	CLA	C1B-CHB	2.44	1.47	1.41
24	c	505	CLA	C4B-CHC	2.44	1.47	1.41
24	b	609	CLA	C4C-C3C	2.44	1.49	1.45
24	b	606	CLA	C1C-C2C	2.44	1.49	1.44
24	b	611	CLA	C1B-CHB	2.43	1.47	1.41
24	c	511	CLA	C1B-NB	-2.43	1.33	1.35
24	A	409	CLA	C1C-NC	-2.43	1.34	1.37
24	C	512	CLA	CHD-C4C	2.43	1.48	1.41
24	b	603	CLA	C4C-C3C	2.42	1.49	1.45
24	D	403	CLA	C1B-CHB	2.42	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	511	CLA	CHD-C4C	2.42	1.48	1.41
24	b	604	CLA	CHD-C4C	2.42	1.48	1.41
24	b	610	CLA	CHD-C4C	2.42	1.48	1.41
24	B	610	CLA	C1C-C2C	2.42	1.49	1.44
24	c	505	CLA	C1C-C2C	2.42	1.49	1.44
24	b	610	CLA	C1B-CHB	2.42	1.47	1.41
24	c	503	CLA	C4B-CHC	2.42	1.47	1.41
24	c	513	CLA	CHD-C4C	2.42	1.48	1.41
24	b	603	CLA	C1D-C2D	2.42	1.48	1.42
35	B	628	HTG	C1-S1	-2.41	1.77	1.80
24	b	612	CLA	C4B-CHC	2.41	1.47	1.41
24	C	511	CLA	C4B-CHC	2.41	1.47	1.41
24	c	514	CLA	CHD-C4C	2.41	1.48	1.41
24	c	510	CLA	C4B-CHC	2.41	1.47	1.41
24	c	504	CLA	C1B-CHB	2.41	1.47	1.41
25	a	405	PHO	C1A-NA	-2.41	1.32	1.37
24	C	506	CLA	CHD-C4C	2.40	1.48	1.41
24	b	609	CLA	CHD-C4C	2.40	1.48	1.41
24	C	502	CLA	CHD-C4C	2.40	1.48	1.41
24	b	614	CLA	C1B-CHB	2.40	1.47	1.41
24	C	514	CLA	C1B-CHB	2.40	1.47	1.41
24	B	612	CLA	C1D-C2D	2.40	1.48	1.42
24	b	609	CLA	C1C-C2C	2.40	1.49	1.44
24	c	509	CLA	C4B-CHC	2.40	1.47	1.41
24	B	611	CLA	C1B-CHB	2.39	1.47	1.41
24	C	508	CLA	C4B-CHC	2.39	1.47	1.41
24	B	616	CLA	C1C-C2C	2.39	1.49	1.44
24	A	409	CLA	CHD-C4C	2.39	1.48	1.41
24	B	614	CLA	C4B-NB	-2.39	1.33	1.35
24	c	503	CLA	C1C-C2C	2.39	1.49	1.44
24	b	615	CLA	C4C-C3C	2.38	1.49	1.45
24	C	512	CLA	C1B-CHB	2.38	1.47	1.41
24	C	513	CLA	CHD-C4C	2.38	1.47	1.41
24	b	610	CLA	C1B-NB	-2.38	1.33	1.35
24	b	604	CLA	C1D-C2D	2.38	1.48	1.42
24	c	512	CLA	C1C-C2C	2.38	1.49	1.44
24	C	503	CLA	CHD-C4C	2.38	1.47	1.41
24	b	607	CLA	C4C-C3C	2.38	1.49	1.45
24	B	607	CLA	C1B-CHB	2.37	1.47	1.41
24	b	616	CLA	C1D-C2D	2.37	1.47	1.42
24	c	506	CLA	C4C-C3C	2.37	1.49	1.45
24	c	509	CLA	C1C-C2C	2.37	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	508	CLA	C4B-CHC	2.37	1.47	1.41
24	B	608	CLA	C1D-C2D	2.37	1.47	1.42
24	C	502	CLA	C1B-CHB	2.37	1.47	1.41
24	c	510	CLA	C4C-C3C	2.37	1.49	1.45
24	b	604	CLA	C1B-CHB	2.37	1.47	1.41
24	c	504	CLA	C1C-C2C	2.36	1.49	1.44
24	b	612	CLA	C1D-C2D	2.36	1.47	1.42
24	c	503	CLA	C1B-CHB	2.36	1.47	1.41
24	b	608	CLA	CHD-C4C	2.36	1.47	1.41
24	B	614	CLA	C4B-CHC	2.36	1.47	1.41
24	C	509	CLA	C4C-C3C	2.36	1.49	1.45
24	B	603	CLA	CHD-C4C	2.36	1.47	1.41
24	B	613	CLA	C1B-CHB	2.36	1.47	1.41
24	A	406	CLA	C4B-CHC	2.36	1.47	1.41
24	a	404	CLA	C1B-CHB	2.35	1.47	1.41
24	a	407	CLA	C1D-C2D	2.35	1.47	1.42
24	b	613	CLA	C4B-NB	-2.35	1.33	1.35
24	B	612	CLA	C1C-C2C	2.35	1.49	1.44
24	B	614	CLA	CHD-C4C	2.35	1.47	1.41
24	C	503	CLA	C4B-CHC	2.34	1.47	1.41
24	A	409	CLA	C1B-CHB	2.34	1.47	1.41
24	C	505	CLA	C4C-C3C	2.34	1.49	1.45
24	b	604	CLA	C4B-CHC	2.34	1.47	1.41
24	b	613	CLA	C1D-C2D	2.34	1.47	1.42
24	C	512	CLA	C4C-C3C	2.34	1.49	1.45
24	B	616	CLA	C4B-CHC	2.34	1.47	1.41
24	c	513	CLA	C4B-CHC	2.34	1.47	1.41
24	C	506	CLA	C4C-C3C	2.34	1.49	1.45
24	c	508	CLA	C4C-C3C	2.34	1.49	1.45
24	d	402	CLA	C1C-C2C	2.34	1.49	1.44
24	C	506	CLA	C1D-C2D	2.34	1.47	1.42
24	c	506	CLA	C1B-CHB	2.33	1.47	1.41
24	b	601	CLA	C1B-CHB	2.33	1.47	1.41
24	A	405	CLA	C1B-CHB	2.33	1.47	1.41
24	B	612	CLA	C1C-NC	-2.33	1.34	1.37
24	b	608	CLA	C1B-CHB	2.33	1.47	1.41
24	c	503	CLA	C4C-C3C	2.33	1.49	1.45
24	C	504	CLA	C1C-C2C	2.33	1.49	1.44
24	C	504	CLA	C4B-CHC	2.33	1.47	1.41
24	c	514	CLA	C1C-C2C	2.32	1.49	1.44
24	b	613	CLA	C1B-CHB	2.32	1.47	1.41
24	c	510	CLA	C1B-CHB	2.32	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	350	CLA	CHD-C4C	2.32	1.47	1.41
24	B	610	CLA	CHD-C4C	2.32	1.47	1.41
24	C	510	CLA	C4B-CHC	2.32	1.47	1.41
24	D	403	CLA	CHD-C4C	2.32	1.47	1.41
24	d	402	CLA	C1D-C2D	2.32	1.47	1.42
24	C	508	CLA	CHD-C4C	2.31	1.47	1.41
24	D	402	CLA	CHD-C4C	2.31	1.47	1.41
24	D	402	CLA	C1B-CHB	2.31	1.47	1.41
24	a	404	CLA	C1C-C2C	2.31	1.49	1.44
24	A	409	CLA	C1C-C2C	2.31	1.49	1.44
24	B	608	CLA	C1C-C2C	2.31	1.49	1.44
24	b	603	CLA	C4B-CHC	2.30	1.47	1.41
24	a	403	CLA	C1B-CHB	2.30	1.47	1.41
24	B	612	CLA	C1B-NB	-2.30	1.33	1.35
24	B	609	CLA	C4B-CHC	2.30	1.47	1.41
24	C	506	CLA	C4B-CHC	2.30	1.47	1.41
24	c	505	CLA	C1B-CHB	2.30	1.47	1.41
35	h	101	HTG	C1-S1	-2.30	1.77	1.80
24	b	608	CLA	C4B-CHC	2.29	1.47	1.41
24	C	503	CLA	C1D-C2D	2.29	1.47	1.42
24	B	606	CLA	C4B-CHC	2.29	1.47	1.41
24	C	505	CLA	CHD-C4C	2.29	1.47	1.41
24	c	512	CLA	C4C-C3C	2.29	1.49	1.45
24	c	506	CLA	CHD-C4C	2.29	1.47	1.41
24	b	614	CLA	CHD-C4C	2.29	1.47	1.41
24	B	611	CLA	C1D-C2D	2.29	1.47	1.42
24	b	611	CLA	CHD-C4C	2.29	1.47	1.41
24	c	510	CLA	C1D-C2D	2.29	1.47	1.42
24	a	407	CLA	CHD-C4C	2.28	1.47	1.41
24	b	613	CLA	CHD-C4C	2.28	1.47	1.41
24	c	515	CLA	C4B-CHC	2.28	1.47	1.41
24	b	606	CLA	C4B-CHC	2.28	1.47	1.41
24	B	603	CLA	C1D-C2D	2.28	1.47	1.42
24	b	606	CLA	CHD-C4C	2.28	1.47	1.41
24	b	614	CLA	C4B-CHC	2.28	1.47	1.41
24	d	403	CLA	C1B-CHB	2.28	1.47	1.41
24	a	403	CLA	C4C-C3C	2.28	1.49	1.45
24	A	404	CLA	C1B-NB	-2.28	1.33	1.35
24	b	612	CLA	CHD-C4C	2.27	1.47	1.41
24	b	605	CLA	C4C-C3C	2.27	1.49	1.45
24	b	601	CLA	C4B-CHC	2.27	1.47	1.41
24	B	609	CLA	C1B-CHB	2.27	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	601	CLA	C1C-NC	-2.27	1.34	1.37
24	B	616	CLA	C1B-CHB	2.27	1.47	1.41
24	C	503	CLA	C1B-CHB	2.27	1.47	1.41
24	c	511	CLA	C1C-C2C	2.26	1.48	1.44
24	A	404	CLA	CHD-C4C	2.26	1.47	1.41
24	c	504	CLA	CHD-C4C	2.26	1.47	1.41
24	C	508	CLA	C1B-CHB	2.26	1.47	1.41
24	a	350	CLA	C1B-NB	-2.26	1.33	1.35
24	c	515	CLA	C1B-CHB	2.26	1.47	1.41
24	b	605	CLA	CHD-C4C	2.26	1.47	1.41
24	b	615	CLA	C4B-CHC	2.26	1.47	1.41
24	B	604	CLA	C4B-CHC	2.26	1.47	1.41
24	a	407	CLA	C4C-C3C	2.25	1.48	1.45
31	D	405	PL9	C2-C3	2.25	1.40	1.34
24	a	403	CLA	C1C-C2C	2.24	1.48	1.44
24	B	612	CLA	C4B-CHC	2.24	1.47	1.41
24	a	350	CLA	C1C-C2C	2.24	1.48	1.44
24	B	604	CLA	CHD-C4C	2.24	1.47	1.41
25	a	405	PHO	C4D-CHA	2.24	1.49	1.43
24	b	616	CLA	C4B-CHC	2.23	1.47	1.41
24	b	602	CLA	C1B-CHB	2.23	1.47	1.41
24	B	607	CLA	C4B-CHC	2.23	1.47	1.41
35	b	625	HTG	C1-S1	-2.23	1.77	1.80
24	B	614	CLA	C1B-CHB	2.23	1.47	1.41
24	B	601	CLA	CHD-C4C	2.23	1.47	1.41
24	C	502	CLA	C4C-C3C	2.23	1.48	1.45
24	B	609	CLA	CHD-C4C	2.22	1.47	1.41
24	C	514	CLA	C4B-CHC	2.22	1.47	1.41
24	B	616	CLA	CHD-C4C	2.22	1.47	1.41
24	C	509	CLA	CHD-C4C	2.22	1.47	1.41
24	c	510	CLA	CHD-C4C	2.22	1.47	1.41
24	B	611	CLA	CHD-C4C	2.22	1.47	1.41
24	c	512	CLA	C4B-CHC	2.22	1.47	1.41
35	c	526	HTG	C1-S1	-2.22	1.77	1.80
24	b	616	CLA	C1C-C2C	2.22	1.48	1.44
25	A	407	PHO	C4C-C3C	2.22	1.49	1.45
24	A	405	CLA	C1B-NB	-2.21	1.33	1.35
24	b	601	CLA	C1C-C2C	2.21	1.48	1.44
24	B	613	CLA	CHD-C4C	2.21	1.47	1.41
24	b	616	CLA	C1B-NB	-2.21	1.33	1.35
24	C	507	CLA	C4B-CHC	2.21	1.47	1.41
24	C	512	CLA	C4B-CHC	2.21	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	603	CLA	C4C-C3C	2.21	1.48	1.45
24	c	509	CLA	C1B-CHB	2.20	1.47	1.41
24	d	402	CLA	C4C-C3C	2.20	1.48	1.45
24	C	504	CLA	C1B-CHB	2.20	1.47	1.41
24	c	507	CLA	C4C-C3C	2.20	1.48	1.45
24	C	507	CLA	C1B-CHB	2.20	1.47	1.41
25	A	407	PHO	C4D-CHA	2.20	1.49	1.43
24	a	407	CLA	C4B-CHC	2.20	1.47	1.41
24	c	511	CLA	C4B-CHC	2.20	1.47	1.41
24	B	612	CLA	C4C-C3C	2.20	1.48	1.45
24	a	407	CLA	C1B-CHB	2.19	1.47	1.41
24	B	601	CLA	C1B-CHB	2.19	1.47	1.41
24	b	605	CLA	C4B-CHC	2.19	1.47	1.41
24	C	509	CLA	C4B-CHC	2.19	1.47	1.41
24	b	608	CLA	C4C-C3C	2.19	1.48	1.45
24	B	613	CLA	C4B-CHC	2.19	1.47	1.41
24	A	406	CLA	C1B-NB	-2.19	1.33	1.35
26	B	619	BCR	C30-C25	-2.19	1.50	1.53
39	E	103	HEM	C3B-C2B	-2.19	1.37	1.40
35	b	628	HTG	C1-S1	-2.18	1.77	1.80
24	b	603	CLA	CHD-C4C	2.18	1.47	1.41
24	B	611	CLA	C1C-C2C	2.18	1.48	1.44
38	d	406	LHG	O7-C5	-2.18	1.41	1.46
24	B	615	CLA	C1B-CHB	2.17	1.47	1.41
24	C	505	CLA	C4B-CHC	2.17	1.47	1.41
24	B	606	CLA	C1B-NB	-2.17	1.33	1.35
24	c	514	CLA	C4C-C3C	2.17	1.48	1.45
36	C	519	DGD	O2G-C2G	-2.17	1.41	1.46
24	c	513	CLA	C4C-C3C	2.17	1.48	1.45
24	b	614	CLA	C4C-C3C	2.17	1.48	1.45
24	b	616	CLA	CHD-C4C	2.17	1.47	1.41
26	B	617	BCR	C1-C6	-2.17	1.50	1.53
24	C	511	CLA	C4C-C3C	2.16	1.48	1.45
24	c	506	CLA	C4B-CHC	2.16	1.47	1.41
24	A	406	CLA	C1B-CHB	2.16	1.47	1.41
24	c	507	CLA	CHD-C4C	2.16	1.47	1.41
24	d	402	CLA	CHD-C4C	2.15	1.47	1.41
24	B	605	CLA	CHD-C4C	2.15	1.47	1.41
24	A	406	CLA	C4C-C3C	2.15	1.48	1.45
24	b	611	CLA	C4C-C3C	2.15	1.48	1.45
24	B	606	CLA	C1B-CHB	2.15	1.47	1.41
38	D	406	LHG	O7-C5	-2.15	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	t	101	LMT	O1'-C1'	2.15	1.43	1.40
34	a	359	LMT	O1'-C1'	2.15	1.43	1.40
24	C	503	CLA	C1C-C2C	2.15	1.48	1.44
24	c	514	CLA	C1B-CHB	2.15	1.47	1.41
25	a	405	PHO	C4C-C3C	2.15	1.49	1.45
24	B	611	CLA	C1C-NC	-2.14	1.34	1.37
24	C	507	CLA	C1B-NB	-2.14	1.33	1.35
24	b	616	CLA	C1C-NC	-2.14	1.34	1.37
24	c	508	CLA	C1B-NB	-2.14	1.33	1.35
24	b	616	CLA	C1B-CHB	2.13	1.46	1.41
24	a	404	CLA	C4C-C3C	2.13	1.48	1.45
24	D	402	CLA	C1C-NC	-2.13	1.34	1.37
36	H	102	DGD	O5D-C1E	2.13	1.43	1.40
24	b	609	CLA	C4B-CHC	2.13	1.46	1.41
24	b	602	CLA	C4C-C3C	2.13	1.48	1.45
24	b	603	CLA	C1B-CHB	2.12	1.46	1.41
24	C	513	CLA	C4C-C3C	2.12	1.48	1.45
24	C	507	CLA	C1C-C2C	2.11	1.48	1.44
33	C	521	LMG	O1-C1	2.11	1.43	1.40
24	C	513	CLA	C1B-CHB	2.11	1.46	1.41
24	A	404	CLA	C1B-CHB	2.11	1.46	1.41
24	c	515	CLA	C4B-NB	-2.11	1.33	1.35
24	B	608	CLA	C4B-CHC	2.10	1.46	1.41
24	B	608	CLA	CHD-C4C	2.10	1.47	1.41
24	B	616	CLA	C1C-NC	-2.10	1.34	1.37
24	C	512	CLA	C1C-NC	-2.10	1.34	1.37
34	a	418	LMT	O1'-C1'	2.10	1.43	1.40
25	a	405	PHO	C1D-ND	-2.09	1.34	1.38
33	Z	101	LMG	O1-C1	2.09	1.43	1.40
24	B	602	CLA	C1B-CHB	2.09	1.46	1.41
24	D	402	CLA	C1B-NB	-2.09	1.33	1.35
24	a	350	CLA	C1B-CHB	2.09	1.46	1.41
24	B	603	CLA	C1B-CHB	2.09	1.46	1.41
24	a	404	CLA	C4B-CHC	2.08	1.46	1.41
24	b	607	CLA	CHD-C4C	2.08	1.47	1.41
24	B	606	CLA	CHD-C4C	2.08	1.47	1.41
35	C	523	HTG	C1-S1	-2.08	1.77	1.80
24	b	608	CLA	C4B-NB	-2.08	1.33	1.35
24	C	509	CLA	C1C-NC	-2.08	1.34	1.37
24	b	607	CLA	C1C-NC	-2.08	1.34	1.37
24	b	605	CLA	C1C-C2C	2.07	1.48	1.44
24	C	514	CLA	C4C-C3C	2.07	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	508	CLA	C4C-C3C	2.07	1.48	1.45
24	b	615	CLA	C1B-CHB	2.07	1.46	1.41
36	h	103	DGD	O5D-C1E	2.07	1.43	1.40
24	B	615	CLA	CHD-C4C	2.07	1.47	1.41
24	A	405	CLA	CHD-C4C	2.07	1.47	1.41
24	D	402	CLA	C4B-NB	-2.07	1.33	1.35
34	b	630	LMT	O1'-C1'	2.06	1.43	1.40
24	B	612	CLA	CHD-C4C	2.06	1.47	1.41
24	a	404	CLA	C1C-NC	-2.05	1.34	1.37
24	c	504	CLA	C4B-CHC	2.04	1.46	1.41
25	a	406	PHO	C1B-NB	-2.04	1.34	1.38
24	A	409	CLA	C4B-CHC	2.04	1.46	1.41
31	a	414[A]	PL9	C2-C3	2.04	1.40	1.34
31	a	414[B]	PL9	C2-C3	2.04	1.40	1.34
31	A	416[B]	PL9	C2-C3	2.03	1.40	1.34
24	A	409	CLA	C4C-C3C	2.03	1.48	1.45
24	c	504	CLA	C1C-NC	-2.03	1.34	1.37
24	B	605	CLA	C4C-C3C	2.02	1.48	1.45
34	I	101	LMT	O1'-C1'	2.02	1.43	1.40
24	b	605	CLA	C1C-NC	-2.01	1.34	1.37
24	c	504	CLA	C4C-C3C	2.01	1.48	1.45

All (2351) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	602	CLA	C4A-NA-C1A	-8.32	102.97	106.71
24	b	616	CLA	C4A-NA-C1A	-7.38	103.39	106.71
25	A	408	PHO	CMD-C2D-C1D	7.38	136.43	125.06
24	C	504	CLA	C4A-NA-C1A	-7.37	103.39	106.71
24	B	606	CLA	C4A-NA-C1A	-7.36	103.40	106.71
24	b	611	CLA	C4A-NA-C1A	-7.33	103.41	106.71
24	B	616	CLA	C4A-NA-C1A	-7.13	103.50	106.71
24	b	602	CLA	C4A-NA-C1A	-7.13	103.50	106.71
24	A	405	CLA	CHD-C4C-C3C	-7.07	114.44	124.84
24	A	404	CLA	C4A-NA-C1A	-7.07	103.53	106.71
39	E	103	HEM	CAD-CBD-CGD	7.04	124.48	112.67
24	B	615	CLA	CHD-C4C-C3C	-7.03	114.51	124.84
24	b	606	CLA	C4A-NA-C1A	-7.02	103.55	106.71
24	B	605	CLA	CHD-C4C-C3C	-6.95	114.62	124.84
24	B	606	CLA	CHD-C4C-C3C	-6.85	114.77	124.84
25	a	405	PHO	CMD-C2D-C1D	6.70	135.38	125.06
24	B	604	CLA	CHD-C4C-C3C	-6.67	115.04	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	b	625	HTG	C1'-S1-C1	6.67	112.56	100.09
24	B	616	CLA	CHD-C4C-C3C	-6.62	115.11	124.84
24	B	606	CLA	O2D-CGD-CBD	6.56	122.93	111.27
24	b	613	CLA	CHD-C4C-C3C	-6.55	115.21	124.84
24	a	407	CLA	C4A-NA-C1A	-6.55	103.76	106.71
25	A	407	PHO	CMD-C2D-C1D	6.54	135.13	125.06
24	B	601	CLA	CHD-C4C-C3C	-6.52	115.25	124.84
24	b	616	CLA	CHD-C4C-C3C	-6.51	115.27	124.84
24	B	609	CLA	CHD-C4C-C3C	-6.50	115.28	124.84
24	B	611	CLA	CHD-C4C-C3C	-6.50	115.29	124.84
24	b	603	CLA	C4A-NA-C1A	-6.49	103.79	106.71
24	a	350	CLA	CHD-C4C-C3C	-6.48	115.31	124.84
24	c	507	CLA	CHD-C4C-C3C	-6.45	115.36	124.84
24	C	513	CLA	CHD-C4C-C3C	-6.44	115.38	124.84
24	b	609	CLA	C4A-NA-C1A	-6.43	103.81	106.71
24	b	604	CLA	C4A-NA-C1A	-6.42	103.82	106.71
25	a	406	PHO	CMD-C2D-C1D	6.41	134.94	125.06
24	B	616	CLA	O2D-CGD-CBD	6.40	122.64	111.27
24	c	513	CLA	CHD-C4C-C3C	-6.40	115.43	124.84
27	A	411	SQD	O6-C1-C2	6.40	118.29	108.30
24	B	611	CLA	C4A-NA-C1A	-6.39	103.83	106.71
24	D	402	CLA	C2C-C1C-NC	6.38	115.95	109.97
24	C	506	CLA	CHD-C4C-C3C	-6.35	115.50	124.84
24	D	403	CLA	CHD-C4C-C3C	-6.35	115.51	124.84
24	B	612	CLA	O2D-CGD-CBD	6.33	122.52	111.27
24	B	608	CLA	CHD-C4C-C3C	-6.33	115.54	124.84
24	a	403	CLA	C2C-C1C-NC	6.32	115.89	109.97
24	C	507	CLA	C2C-C1C-NC	6.32	115.89	109.97
24	B	603	CLA	C4A-NA-C1A	-6.30	103.87	106.71
24	C	511	CLA	CHD-C4C-C3C	-6.30	115.58	124.84
25	a	405	PHO	O2D-CGD-CBD	6.28	122.43	111.27
24	B	607	CLA	C2C-C1C-NC	6.28	115.86	109.97
24	b	605	CLA	CHD-C4C-C3C	-6.28	115.61	124.84
24	c	504	CLA	CHD-C4C-C3C	-6.28	115.61	124.84
24	B	603	CLA	O2D-CGD-CBD	6.27	122.42	111.27
24	b	601	CLA	CHD-C4C-C3C	-6.27	115.62	124.84
24	D	402	CLA	C4A-NA-C1A	-6.27	103.89	106.71
24	c	514	CLA	O2D-CGD-CBD	6.26	122.40	111.27
24	b	612	CLA	C4A-NA-C1A	-6.24	103.90	106.71
24	C	503	CLA	CHD-C4C-C3C	-6.23	115.68	124.84
24	C	513	CLA	C4A-NA-C1A	-6.23	103.91	106.71
24	B	610	CLA	CHD-C4C-C3C	-6.22	115.69	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	603	CLA	CHD-C4C-C3C	-6.22	115.70	124.84
24	d	403	CLA	C4A-NA-C1A	-6.21	103.91	106.71
24	c	509	CLA	O2D-CGD-CBD	6.20	122.29	111.27
24	b	606	CLA	CHD-C4C-C3C	-6.20	115.73	124.84
24	b	611	CLA	CHD-C4C-C3C	-6.20	115.73	124.84
24	c	510	CLA	CHD-C4C-C3C	-6.19	115.73	124.84
24	b	604	CLA	CHD-C4C-C3C	-6.15	115.80	124.84
24	b	614	CLA	O2D-CGD-CBD	6.14	122.19	111.27
24	a	404	CLA	CHD-C4C-C3C	-6.14	115.81	124.84
24	C	513	CLA	O2D-CGD-CBD	6.13	122.17	111.27
24	B	612	CLA	CHD-C4C-C3C	-6.11	115.86	124.84
24	b	602	CLA	CHD-C4C-C3C	-6.10	115.86	124.84
35	B	625	HTG	C1'-S1-C1	6.10	111.51	100.09
24	c	505	CLA	C4A-NA-C1A	-6.10	103.96	106.71
24	C	506	CLA	C4A-NA-C1A	-6.07	103.98	106.71
24	b	613	CLA	C4A-NA-C1A	-6.07	103.98	106.71
24	B	614	CLA	O2D-CGD-CBD	6.04	121.99	111.27
24	b	603	CLA	CHD-C4C-C3C	-6.03	115.98	124.84
24	b	608	CLA	CHD-C4C-C3C	-6.02	115.98	124.84
24	C	509	CLA	CHD-C4C-C3C	-6.02	115.99	124.84
24	C	508	CLA	O2D-CGD-CBD	6.01	121.95	111.27
24	C	502	CLA	C4A-NA-C1A	-5.98	104.02	106.71
24	c	515	CLA	C4A-NA-C1A	-5.97	104.02	106.71
24	c	514	CLA	C4A-NA-C1A	-5.96	104.03	106.71
24	b	605	CLA	C4A-NA-C1A	-5.96	104.03	106.71
24	C	502	CLA	CHD-C4C-C3C	-5.95	116.09	124.84
24	C	511	CLA	C4A-NA-C1A	-5.95	104.03	106.71
24	A	409	CLA	CHD-C4C-C3C	-5.91	116.14	124.84
24	b	607	CLA	CHD-C4C-C3C	-5.91	116.15	124.84
24	B	614	CLA	CHD-C4C-C3C	-5.91	116.16	124.84
24	A	406	CLA	CHD-C4C-C3C	-5.89	116.17	124.84
24	b	616	CLA	O2D-CGD-CBD	5.89	121.73	111.27
24	C	505	CLA	C2C-C1C-NC	5.89	115.49	109.97
24	b	614	CLA	CHD-C4C-C3C	-5.88	116.19	124.84
24	b	601	CLA	O2D-CGD-CBD	5.86	121.68	111.27
24	C	509	CLA	C2C-C1C-NC	5.86	115.46	109.97
24	A	404	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
24	c	510	CLA	C2C-C1C-NC	5.85	115.45	109.97
24	C	508	CLA	CHD-C4C-C3C	-5.84	116.25	124.84
24	C	514	CLA	CHD-C4C-C3C	-5.84	116.26	124.84
24	b	603	CLA	O2D-CGD-CBD	5.83	121.64	111.27
24	c	505	CLA	CHD-C4C-C3C	-5.83	116.27	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	h	101	HTG	C1'-S1-C1	5.83	110.99	100.09
24	B	601	CLA	O2D-CGD-CBD	5.82	121.61	111.27
24	c	509	CLA	CHD-C4C-C3C	-5.82	116.28	124.84
24	c	508	CLA	C2C-C1C-NC	5.81	115.42	109.97
24	c	514	CLA	CHD-C4C-C3C	-5.81	116.30	124.84
24	d	402	CLA	CHD-C4C-C3C	-5.80	116.31	124.84
24	B	613	CLA	C2C-C1C-NC	5.80	115.41	109.97
24	c	510	CLA	O2D-CGD-CBD	5.79	121.56	111.27
24	b	615	CLA	C4A-NA-C1A	-5.79	104.10	106.71
24	B	614	CLA	C2C-C1C-NC	5.78	115.39	109.97
24	c	503	CLA	O2D-CGD-CBD	5.78	121.54	111.27
24	b	604	CLA	O2D-CGD-CBD	5.78	121.53	111.27
24	C	512	CLA	CHD-C4C-C3C	-5.78	116.35	124.84
24	A	409	CLA	C4A-NA-C1A	-5.77	104.11	106.71
24	d	403	CLA	CHD-C4C-C3C	-5.77	116.35	124.84
24	C	507	CLA	C4A-NA-C1A	-5.77	104.11	106.71
24	b	612	CLA	C2C-C1C-NC	5.76	115.37	109.97
24	a	403	CLA	C4A-NA-C1A	-5.75	104.12	106.71
24	B	602	CLA	CHD-C4C-C3C	-5.73	116.41	124.84
24	C	510	CLA	CHD-C4C-C3C	-5.71	116.44	124.84
24	C	502	CLA	O2D-CGD-CBD	5.69	121.38	111.27
25	a	406	PHO	O2D-CGD-CBD	5.69	121.37	111.27
25	A	407	PHO	C3D-C2D-C1D	-5.68	97.59	105.87
24	b	612	CLA	CHD-C4C-C3C	-5.67	116.51	124.84
24	B	609	CLA	C4A-NA-C1A	-5.66	104.16	106.71
24	b	602	CLA	O2D-CGD-CBD	5.66	121.32	111.27
24	b	609	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
24	b	610	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
24	b	605	CLA	C2C-C1C-NC	5.65	115.27	109.97
24	b	607	CLA	C2C-C1C-NC	5.65	115.26	109.97
24	b	609	CLA	C2C-C1C-NC	5.65	115.26	109.97
35	b	624	HTG	C1'-S1-C1	5.64	110.65	100.09
24	c	512	CLA	CHD-C4C-C3C	-5.63	116.57	124.84
26	D	404	BCR	C7-C8-C9	-5.62	117.74	126.23
27	F	101	SQD	O47-C7-C8	5.62	123.61	111.50
24	b	611	CLA	O2D-CGD-CBD	5.62	121.25	111.27
24	B	607	CLA	CHD-C4C-C3C	-5.61	116.59	124.84
24	c	505	CLA	C2C-C1C-NC	5.61	115.23	109.97
25	A	408	PHO	C3D-C2D-C1D	-5.61	97.70	105.87
27	a	409	SQD	O6-C1-C2	5.60	117.04	108.30
24	a	407	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
24	b	615	CLA	C2C-C1C-NC	5.60	115.22	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	506	CLA	CHD-C4C-C3C	-5.59	116.63	124.84
24	d	402	CLA	C2C-C1C-NC	5.58	115.20	109.97
24	b	614	CLA	C4A-NA-C1A	-5.57	104.20	106.71
24	C	511	CLA	O2D-CGD-CBD	5.57	121.16	111.27
24	C	506	CLA	O2D-CGD-CBD	5.56	121.15	111.27
24	b	610	CLA	O2D-CGD-CBD	5.54	121.11	111.27
35	D	410	HTG	C1'-S1-C1	5.54	110.44	100.09
24	C	509	CLA	O2D-CGD-CBD	5.53	121.10	111.27
24	c	512	CLA	C2C-C1C-NC	5.53	115.15	109.97
24	b	615	CLA	CHD-C4C-C3C	-5.52	116.73	124.84
24	c	507	CLA	O2D-CGD-CBD	5.51	121.05	111.27
25	A	408	PHO	O2D-CGD-CBD	5.50	121.05	111.27
25	a	405	PHO	C2D-C1D-ND	5.50	118.09	109.79
24	B	615	CLA	C4A-NA-C1A	-5.50	104.23	106.71
39	e	102	HEM	CAD-CBD-CGD	5.50	121.89	112.67
24	B	603	CLA	C2C-C1C-NC	5.50	115.12	109.97
24	B	604	CLA	O2D-CGD-CBD	5.49	121.03	111.27
24	C	505	CLA	O2D-CGD-CBD	5.49	121.02	111.27
24	c	504	CLA	C2C-C1C-NC	5.49	115.11	109.97
24	C	504	CLA	C2C-C1C-NC	5.48	115.10	109.97
24	A	404	CLA	C2C-C1C-NC	5.48	115.10	109.97
25	a	405	PHO	C3D-C2D-C1D	-5.47	97.89	105.87
24	B	612	CLA	C2C-C1C-NC	5.47	115.10	109.97
24	A	406	CLA	C4A-NA-C1A	-5.47	104.25	106.71
24	b	613	CLA	C2C-C1C-NC	5.46	115.09	109.97
25	A	407	PHO	C2D-C1D-ND	5.46	118.02	109.79
24	C	508	CLA	C2C-C1C-NC	5.45	115.08	109.97
24	b	606	CLA	O2D-CGD-CBD	5.44	120.93	111.27
24	c	503	CLA	CHD-C4C-C3C	-5.43	116.86	124.84
24	B	608	CLA	C2C-C1C-NC	5.43	115.06	109.97
25	A	408	PHO	C2D-C1D-ND	5.41	117.96	109.79
31	A	416[A]	PL9	C7-C8-C9	-5.41	117.78	126.79
24	C	504	CLA	CHD-C4C-C3C	-5.39	116.91	124.84
24	B	613	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
24	A	409	CLA	C2C-C1C-NC	5.39	115.02	109.97
24	c	511	CLA	C4A-NA-C1A	-5.39	104.28	106.71
24	b	604	CLA	C2C-C1C-NC	5.38	115.01	109.97
24	c	507	CLA	C3C-C4C-NC	5.38	116.61	110.57
24	c	515	CLA	C2C-C1C-NC	5.38	115.01	109.97
24	c	506	CLA	C2C-C1C-NC	5.37	115.00	109.97
24	a	350	CLA	C4A-NA-C1A	-5.36	104.30	106.71
27	a	409	SQD	O47-C7-C8	5.35	123.03	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	510	CLA	O2D-CGD-CBD	5.35	120.77	111.27
24	B	610	CLA	O2D-CGD-CBD	5.34	120.76	111.27
24	B	605	CLA	C4A-NA-C1A	-5.33	104.31	106.71
35	B	624	HTG	C1'-S1-C1	5.33	110.05	100.09
26	Y	101	BCR	C33-C5-C6	-5.33	118.55	124.53
24	c	511	CLA	C2C-C1C-NC	5.32	114.96	109.97
24	C	510	CLA	C2C-C1C-NC	5.31	114.95	109.97
24	b	603	CLA	C2C-C1C-NC	5.30	114.94	109.97
24	c	515	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
24	B	611	CLA	C2C-C1C-NC	5.30	114.93	109.97
27	b	620	SQD	O6-C1-C2	5.30	116.57	108.30
24	c	512	CLA	C4A-NA-C1A	-5.29	104.33	106.71
24	b	605	CLA	O2D-CGD-CBD	5.29	120.66	111.27
24	B	604	CLA	C2C-C1C-NC	5.28	114.92	109.97
24	c	507	CLA	C2C-C1C-NC	5.28	114.92	109.97
24	c	509	CLA	C4A-NA-C1A	-5.27	104.34	106.71
24	b	608	CLA	C2C-C1C-NC	5.25	114.89	109.97
24	C	512	CLA	C2C-C1C-NC	5.25	114.89	109.97
24	b	607	CLA	C4A-NA-C1A	-5.25	104.35	106.71
24	C	505	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
24	c	508	CLA	CHD-C4C-C3C	-5.23	117.15	124.84
25	A	408	PHO	C1-C2-C3	-5.23	117.00	126.04
24	d	403	CLA	O2D-CGD-CBD	5.23	120.55	111.27
24	B	609	CLA	C2C-C1C-NC	5.23	114.87	109.97
24	C	503	CLA	C4A-NA-C1A	-5.22	104.36	106.71
24	B	605	CLA	O2D-CGD-CBD	5.22	120.54	111.27
27	f	101	SQD	O47-C7-C8	5.21	122.73	111.50
24	B	604	CLA	C1-C2-C3	-5.21	117.03	126.04
35	c	523	HTG	C1'-S1-C1	5.19	109.80	100.09
24	c	509	CLA	C2C-C1C-NC	5.18	114.83	109.97
24	c	504	CLA	O2D-CGD-CBD	5.18	120.48	111.27
24	D	402	CLA	CHD-C4C-C3C	-5.17	117.23	124.84
24	b	614	CLA	C2C-C1C-NC	5.17	114.81	109.97
24	a	407	CLA	C2C-C1C-NC	5.16	114.81	109.97
24	C	503	CLA	C2C-C1C-NC	5.15	114.80	109.97
24	A	405	CLA	C4A-NA-C1A	-5.15	104.39	106.71
24	c	503	CLA	C4A-NA-C1A	-5.15	104.39	106.71
24	b	610	CLA	C2C-C1C-NC	5.14	114.79	109.97
25	a	406	PHO	C3D-C2D-C1D	-5.14	98.38	105.87
24	b	601	CLA	C4A-NA-C1A	-5.13	104.40	106.71
39	E	103	HEM	CBD-CAD-C3D	-5.12	103.04	112.48
24	B	604	CLA	C3C-C4C-NC	5.12	116.31	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	c	526	HTG	C1'-S1-C1	5.12	109.66	100.09
24	B	607	CLA	O2D-CGD-CBD	5.11	120.36	111.27
24	B	612	CLA	C3C-C4C-NC	5.10	116.29	110.57
24	c	511	CLA	CHD-C4C-C3C	-5.10	117.34	124.84
24	b	601	CLA	C2C-C1C-NC	5.09	114.74	109.97
25	a	406	PHO	C1-C2-C3	-5.09	117.23	126.04
35	C	522	HTG	C1'-S1-C1	5.09	109.60	100.09
24	D	403	CLA	C4A-NA-C1A	-5.08	104.42	106.71
24	a	407	CLA	O2D-CGD-CBD	5.06	120.26	111.27
24	a	404	CLA	C4A-NA-C1A	-5.06	104.43	106.71
26	b	617	BCR	C7-C8-C9	-5.06	118.60	126.23
27	F	101	SQD	O6-C1-C2	5.05	116.19	108.30
31	a	414[B]	PL9	C7-C3-C4	5.05	120.98	116.88
24	C	502	CLA	C2C-C1C-NC	5.04	114.69	109.97
24	A	405	CLA	O2D-CGD-CBD	5.04	120.22	111.27
24	B	613	CLA	C1-C2-C3	-5.03	117.35	126.04
24	c	511	CLA	O2D-CGD-CBD	5.02	120.19	111.27
24	C	506	CLA	C2C-C1C-NC	5.02	114.67	109.97
24	c	514	CLA	C2C-C1C-NC	5.01	114.67	109.97
24	C	503	CLA	O2D-CGD-CBD	4.99	120.14	111.27
24	b	606	CLA	C2C-C1C-NC	4.98	114.64	109.97
35	C	523	HTG	C1-O5-C5	4.98	121.76	112.58
24	c	503	CLA	C2C-C1C-NC	4.98	114.63	109.97
24	c	507	CLA	C4A-NA-C1A	-4.97	104.47	106.71
24	a	404	CLA	C2C-C1C-NC	4.97	114.62	109.97
24	a	403	CLA	CHD-C4C-C3C	-4.97	117.54	124.84
24	c	511	CLA	C1-C2-C3	-4.96	117.46	126.04
24	B	610	CLA	C2C-C1C-NC	4.95	114.61	109.97
24	c	504	CLA	C4A-NA-C1A	-4.95	104.48	106.71
24	B	611	CLA	O2D-CGD-CBD	4.94	120.04	111.27
24	C	506	CLA	C3C-C4C-NC	4.92	116.09	110.57
26	y	101	BCR	C33-C5-C6	-4.91	119.01	124.53
24	b	610	CLA	C4A-NA-C1A	-4.90	104.50	106.71
24	b	608	CLA	C4A-NA-C1A	-4.90	104.50	106.71
24	C	511	CLA	C2C-C1C-NC	4.90	114.56	109.97
24	C	509	CLA	C3C-C4C-NC	4.89	116.06	110.57
24	c	513	CLA	O2D-CGD-CBD	4.89	119.96	111.27
24	B	601	CLA	C4A-NA-C1A	-4.88	104.51	106.71
25	A	407	PHO	O2D-CGD-CBD	4.87	119.92	111.27
24	C	507	CLA	CHD-C4C-C3C	-4.87	117.68	124.84
24	B	607	CLA	C1C-C2C-C3C	-4.87	101.84	106.96
24	B	609	CLA	C3C-C4C-NC	4.86	116.02	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	508	CLA	C4A-NA-C1A	-4.86	104.52	106.71
24	A	406	CLA	O2D-CGD-CBD	4.81	119.81	111.27
24	b	608	CLA	O2D-CGD-CBD	4.81	119.81	111.27
24	b	610	CLA	C1-C2-C3	-4.80	117.73	126.04
24	B	606	CLA	C3C-C4C-NC	4.80	115.95	110.57
24	B	605	CLA	C3C-C4C-NC	4.79	115.94	110.57
24	b	609	CLA	O2D-CGD-CBD	4.79	119.77	111.27
25	a	406	PHO	C2D-C1D-ND	4.78	117.00	109.79
27	b	620	SQD	O47-C7-C8	4.77	121.79	111.50
24	C	509	CLA	C4A-NA-C1A	-4.77	104.56	106.71
24	B	610	CLA	C4A-NA-C1A	-4.77	104.56	106.71
24	C	510	CLA	C4A-NA-C1A	-4.77	104.56	106.71
24	d	402	CLA	C3C-C4C-NC	4.77	115.92	110.57
24	b	604	CLA	C3C-C4C-NC	4.76	115.91	110.57
24	C	514	CLA	C2C-C1C-NC	4.76	114.43	109.97
26	t	102	BCR	C33-C5-C6	-4.76	119.18	124.53
24	B	615	CLA	C3C-C4C-NC	4.76	115.90	110.57
24	C	507	CLA	O2D-CGD-CBD	4.75	119.71	111.27
24	A	404	CLA	CAA-C2A-C3A	-4.75	99.77	112.78
24	c	506	CLA	O2D-CGD-CBD	4.75	119.70	111.27
35	C	523	HTG	C1'-S1-C1	4.73	108.94	100.09
24	d	402	CLA	C4A-NA-C1A	-4.71	104.59	106.71
33	j	101	LMG	O7-C10-C11	4.71	121.65	111.50
24	c	505	CLA	C1D-CHD-C4C	-4.71	116.34	122.56
24	b	612	CLA	O2D-CGD-CBD	4.71	119.64	111.27
26	H	101	BCR	C11-C10-C9	-4.71	120.59	127.31
24	b	611	CLA	C2C-C1C-NC	4.71	114.38	109.97
24	b	613	CLA	C3C-C4C-NC	4.69	115.83	110.57
24	B	605	CLA	C2C-C1C-NC	4.69	114.37	109.97
24	D	403	CLA	O2D-CGD-CBD	4.69	119.60	111.27
24	a	350	CLA	C2C-C1C-NC	4.68	114.36	109.97
26	d	404	BCR	C15-C14-C13	-4.67	120.64	127.31
24	c	513	CLA	C2C-C1C-NC	4.67	114.35	109.97
24	B	613	CLA	CAC-C3C-C4C	4.67	130.86	124.81
24	a	403	CLA	C1C-C2C-C3C	-4.67	102.05	106.96
24	B	612	CLA	C1-C2-C3	-4.63	118.03	126.04
24	C	513	CLA	C2C-C1C-NC	4.63	114.31	109.97
31	a	414[A]	PL9	C7-C3-C4	4.62	120.63	116.88
26	c	517	BCR	C7-C8-C9	-4.61	119.26	126.23
24	B	608	CLA	O2D-CGD-CBD	4.60	119.45	111.27
24	C	514	CLA	O2D-CGD-CBD	4.60	119.44	111.27
33	Z	101	LMG	O7-C10-C11	4.60	121.41	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	607	CLA	C3C-C4C-NC	4.60	115.73	110.57
24	B	615	CLA	C2C-C1C-NC	4.59	114.27	109.97
33	A	418	LMG	O7-C10-C11	4.59	121.39	111.50
24	a	403	CLA	CAA-C2A-C3A	-4.57	100.26	112.78
24	A	405	CLA	C2C-C1C-NC	4.56	114.24	109.97
24	C	514	CLA	C4A-NA-C1A	-4.56	104.66	106.71
24	B	602	CLA	C2C-C1C-NC	4.55	114.23	109.97
24	b	603	CLA	C3C-C4C-NC	4.54	115.66	110.57
24	b	614	CLA	C3C-C4C-NC	4.54	115.66	110.57
24	A	406	CLA	C2C-C1C-NC	4.53	114.21	109.97
24	d	402	CLA	O2D-CGD-CBD	4.52	119.31	111.27
24	B	614	CLA	C4A-NA-C1A	-4.52	104.67	106.71
24	A	409	CLA	O2D-CGD-CBD	4.50	119.27	111.27
24	B	605	CLA	C1D-CHD-C4C	-4.50	116.61	122.56
24	b	616	CLA	C3C-C4C-NC	4.48	115.60	110.57
24	C	512	CLA	O2D-CGD-CBD	4.48	119.23	111.27
31	A	416[B]	PL9	C7-C3-C4	4.48	120.52	116.88
24	B	602	CLA	O2D-CGD-CBD	4.48	119.22	111.27
27	a	409	SQD	C1-O5-C5	-4.47	104.91	113.69
24	B	616	CLA	C3C-C4C-NC	4.46	115.58	110.57
24	D	403	CLA	C3C-C4C-NC	4.46	115.57	110.57
24	C	513	CLA	C3C-C4C-NC	4.45	115.56	110.57
24	B	615	CLA	O2D-CGD-CBD	4.45	119.18	111.27
24	C	508	CLA	C3C-C4C-NC	4.45	115.56	110.57
24	C	507	CLA	C1C-C2C-C3C	-4.45	102.28	106.96
24	D	402	CLA	C1C-C2C-C3C	-4.44	102.29	106.96
26	T	101	BCR	C15-C16-C17	-4.44	114.38	123.47
24	b	603	CLA	C1D-CHD-C4C	-4.44	116.70	122.56
24	b	612	CLA	C3C-C4C-NC	4.43	115.54	110.57
24	B	615	CLA	C1D-CHD-C4C	-4.43	116.71	122.56
24	a	403	CLA	C1D-CHD-C4C	-4.42	116.72	122.56
24	c	510	CLA	C3C-C4C-NC	4.40	115.51	110.57
24	B	611	CLA	C3C-C4C-NC	4.40	115.50	110.57
24	B	608	CLA	C3C-C4C-NC	4.40	115.50	110.57
27	A	411	SQD	O47-C7-C8	4.40	120.98	111.50
24	c	510	CLA	C1C-C2C-C3C	-4.39	102.34	106.96
33	C	520	LMG	O7-C10-C11	4.39	120.97	111.50
24	B	613	CLA	C4A-NA-C1A	-4.39	104.73	106.71
24	B	611	CLA	C1D-CHD-C4C	-4.39	116.77	122.56
24	c	515	CLA	O2D-CGD-CBD	4.38	119.06	111.27
24	B	607	CLA	C4A-NA-C1A	-4.38	104.73	106.71
31	D	405	PL9	C37-C38-C39	-4.38	117.12	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	513	CLA	C1D-CHD-C4C	-4.37	116.79	122.56
24	C	514	CLA	C3C-C4C-NC	4.37	115.47	110.57
27	B	620	SQD	O47-C7-C8	4.37	120.92	111.50
27	A	411	SQD	C1-O5-C5	-4.37	105.11	113.69
24	b	606	CLA	C3C-C4C-NC	4.36	115.46	110.57
25	A	408	PHO	C4C-C3C-C2C	-4.35	101.96	106.78
24	B	606	CLA	C2C-C1C-NC	4.34	114.04	109.97
24	B	614	CLA	C1C-C2C-C3C	-4.34	102.40	106.96
24	B	605	CLA	C4-C3-C5	4.33	122.55	115.27
24	A	404	CLA	C3C-C4C-NC	4.33	115.42	110.57
24	B	613	CLA	C3C-C4C-NC	4.33	115.42	110.57
26	b	617	BCR	C33-C5-C6	-4.32	119.68	124.53
24	B	614	CLA	O2D-CGD-O1D	-4.31	115.41	123.84
24	a	403	CLA	C3B-C4B-NB	4.31	114.78	109.21
24	c	505	CLA	C3C-C4C-NC	4.31	115.40	110.57
26	d	404	BCR	C38-C26-C25	-4.30	119.69	124.53
38	E	101	LHG	O7-C7-C8	4.30	120.76	111.50
24	c	512	CLA	O2D-CGD-CBD	4.29	118.88	111.27
24	a	407	CLA	C3C-C4C-NC	4.28	115.38	110.57
24	B	610	CLA	C3C-C4C-NC	4.28	115.37	110.57
24	b	616	CLA	C2C-C1C-NC	4.28	113.98	109.97
24	B	601	CLA	C2C-C1C-NC	4.28	113.98	109.97
24	B	603	CLA	C3C-C4C-NC	4.28	115.37	110.57
24	b	616	CLA	C1D-CHD-C4C	-4.28	116.92	122.56
24	B	611	CLA	C1-C2-C3	-4.28	118.65	126.04
24	A	405	CLA	C3C-C4C-NC	4.27	115.36	110.57
24	C	503	CLA	C3C-C4C-NC	4.27	115.36	110.57
35	B	628	HTG	C1'-S1-C1	4.27	108.07	100.09
27	B	620	SQD	O6-C1-C2	4.26	114.96	108.30
24	B	601	CLA	C3C-C4C-NC	4.26	115.35	110.57
24	B	609	CLA	O2D-CGD-CBD	4.26	118.83	111.27
24	A	409	CLA	C3C-C4C-NC	4.24	115.33	110.57
24	C	511	CLA	C1-C2-C3	-4.24	118.71	126.04
24	b	610	CLA	C3C-C4C-NC	4.23	115.31	110.57
24	b	611	CLA	C3C-C4C-NC	4.23	115.31	110.57
24	B	603	CLA	C4-C3-C5	4.23	122.38	115.27
24	c	509	CLA	C1C-C2C-C3C	-4.23	102.51	106.96
24	C	505	CLA	C1C-C2C-C3C	-4.22	102.52	106.96
26	K	102	BCR	C24-C23-C22	-4.22	119.85	126.23
24	C	512	CLA	C3C-C4C-NC	4.22	115.31	110.57
27	A	411	SQD	C1-C2-C3	-4.22	101.20	110.00
26	B	617	BCR	C7-C8-C9	-4.22	119.86	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	601	CLA	C1D-CHD-C4C	-4.21	117.00	122.56
24	c	506	CLA	C4A-NA-C1A	-4.21	104.81	106.71
24	C	512	CLA	C4A-NA-C1A	-4.20	104.82	106.71
24	c	505	CLA	O2D-CGD-CBD	4.20	118.73	111.27
24	C	512	CLA	CAC-C3C-C4C	4.19	130.24	124.81
26	c	516	BCR	C15-C14-C13	-4.19	121.33	127.31
24	B	612	CLA	C4A-NA-C1A	-4.18	104.83	106.71
24	D	402	CLA	C1-C2-C3	-4.18	118.81	126.04
24	B	602	CLA	C3C-C4C-NC	4.18	115.26	110.57
24	C	503	CLA	C1-C2-C3	-4.18	118.81	126.04
24	b	602	CLA	C3C-C4C-NC	4.18	115.25	110.57
24	D	403	CLA	C2C-C1C-NC	4.17	113.88	109.97
24	b	607	CLA	O2D-CGD-CBD	4.17	118.68	111.27
24	C	510	CLA	C3C-C4C-NC	4.17	115.25	110.57
24	C	510	CLA	C1-C2-C3	-4.17	118.83	126.04
24	C	502	CLA	O2D-CGD-O1D	-4.16	115.70	123.84
24	D	402	CLA	C3C-C4C-NC	4.15	115.22	110.57
33	C	521	LMG	O7-C10-C11	4.15	120.44	111.50
24	b	609	CLA	C3C-C4C-NC	4.15	115.22	110.57
24	c	504	CLA	C3C-C4C-NC	4.14	115.22	110.57
24	B	603	CLA	C1C-C2C-C3C	-4.14	102.60	106.96
24	A	405	CLA	C1D-CHD-C4C	-4.14	117.09	122.56
24	c	512	CLA	C1-C2-C3	-4.14	118.88	126.04
24	c	512	CLA	C1C-C2C-C3C	-4.14	102.60	106.96
24	B	616	CLA	C2C-C1C-NC	4.14	113.85	109.97
24	b	608	CLA	C3C-C4C-NC	4.14	115.21	110.57
24	b	604	CLA	C1-C2-C3	-4.14	118.89	126.04
24	b	611	CLA	C1-C2-C3	-4.14	118.89	126.04
24	b	602	CLA	C2C-C1C-NC	4.13	113.84	109.97
24	c	510	CLA	C4A-NA-C1A	-4.10	104.86	106.71
24	a	350	CLA	O2D-CGD-CBD	4.09	118.54	111.27
24	C	511	CLA	C1D-CHD-C4C	-4.09	117.16	122.56
27	A	411	SQD	O9-S-C6	4.09	111.80	106.94
24	c	506	CLA	C1C-C2C-C3C	-4.08	102.66	106.96
31	A	416[B]	PL9	C7-C8-C9	-4.08	120.01	126.79
24	B	601	CLA	C1D-CHD-C4C	-4.07	117.19	122.56
24	c	513	CLA	C4A-NA-C1A	-4.07	104.88	106.71
24	B	604	CLA	C1D-CHD-C4C	-4.07	117.19	122.56
26	B	617	BCR	C33-C5-C6	-4.07	119.96	124.53
26	K	102	BCR	C3-C4-C5	-4.07	106.82	114.08
24	a	404	CLA	O2D-CGD-CBD	4.06	118.49	111.27
24	c	513	CLA	C3C-C4C-NC	4.06	115.12	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	405	CLA	C4D-C3D-CAD	-4.05	106.21	108.47
24	C	505	CLA	C3C-C4C-NC	4.05	115.11	110.57
24	a	350	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
26	c	516	BCR	C11-C10-C9	-4.03	121.56	127.31
24	b	612	CLA	C1D-CHD-C4C	-4.03	117.24	122.56
24	B	608	CLA	C4A-NA-C1A	-4.02	104.90	106.71
24	b	613	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
24	A	405	CLA	CMC-C2C-C1C	4.01	131.15	125.04
24	c	503	CLA	O2D-CGD-O1D	-4.01	116.00	123.84
26	C	515	BCR	C7-C8-C9	-4.01	120.18	126.23
24	B	614	CLA	C3C-C4C-NC	4.00	115.06	110.57
25	a	405	PHO	C4C-C3C-C2C	-4.00	102.36	106.78
38	D	357	LHG	O7-C7-C8	3.99	120.11	111.50
24	C	502	CLA	C3C-C4C-NC	3.99	115.05	110.57
27	a	409	SQD	O8-S-C6	3.98	112.09	105.74
24	B	611	CLA	C3B-C4B-NB	3.98	114.36	109.21
24	B	606	CLA	O2D-CGD-O1D	-3.98	116.05	123.84
26	D	404	BCR	C24-C23-C22	-3.98	120.22	126.23
24	c	508	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
24	b	605	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
24	b	607	CLA	C3B-C4B-NB	3.97	114.35	109.21
24	C	504	CLA	C3C-C4C-NC	3.97	115.02	110.57
24	A	404	CLA	C1D-CHD-C4C	-3.97	117.32	122.56
38	d	408	LHG	O7-C7-C8	3.96	120.05	111.50
24	c	504	CLA	C1C-C2C-C3C	-3.96	102.79	106.96
24	C	508	CLA	C4A-NA-C1A	-3.96	104.93	106.71
24	C	509	CLA	C1D-CHD-C4C	-3.96	117.34	122.56
26	c	516	BCR	C20-C21-C22	-3.95	121.67	127.31
26	k	101	BCR	C29-C30-C25	3.95	116.56	110.48
26	D	404	BCR	C38-C26-C25	-3.95	120.09	124.53
34	I	101	LMT	C1'-O5'-C5'	3.95	121.44	113.69
24	a	404	CLA	C3C-C4C-NC	3.95	115.00	110.57
31	a	414[A]	PL9	C7-C8-C9	-3.94	120.23	126.79
24	c	511	CLA	CAC-C3C-C4C	3.94	129.92	124.81
24	B	607	CLA	C3C-C4C-NC	3.94	114.99	110.57
24	b	601	CLA	C3C-C4C-NC	3.94	114.99	110.57
33	c	522	LMG	O7-C10-C11	3.93	119.98	111.50
33	c	521	LMG	O7-C10-C11	3.93	119.97	111.50
24	b	615	CLA	C3C-C4C-NC	3.93	114.98	110.57
24	B	613	CLA	CMC-C2C-C1C	3.93	131.02	125.04
24	A	404	CLA	O2A-CGA-CBA	3.93	124.24	111.91
24	A	405	CLA	C1C-C2C-C3C	-3.92	102.83	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	608	CLA	C1-C2-C3	-3.92	119.27	126.04
24	B	606	CLA	C1D-CHD-C4C	-3.92	117.39	122.56
24	B	608	CLA	C1C-C2C-C3C	-3.91	102.85	106.96
24	B	612	CLA	O2D-CGD-O1D	-3.91	116.20	123.84
31	a	414[A]	PL9	C32-C33-C34	-3.90	118.26	127.66
24	c	512	CLA	C3B-C4B-NB	3.90	114.26	109.21
24	c	508	CLA	O2D-CGD-CBD	3.90	118.20	111.27
24	C	511	CLA	C3C-C4C-NC	3.90	114.94	110.57
24	B	613	CLA	C1C-C2C-C3C	-3.90	102.86	106.96
24	c	515	CLA	C3C-C4C-NC	3.89	114.94	110.57
33	a	417	LMG	O7-C10-C11	3.89	119.88	111.50
25	a	406	PHO	C4C-C3C-C2C	-3.89	102.48	106.78
24	b	610	CLA	O2A-CGA-CBA	3.89	124.11	111.91
24	b	612	CLA	C3B-C4B-NB	3.88	114.23	109.21
24	B	611	CLA	O2D-CGD-O1D	-3.88	116.26	123.84
24	a	407	CLA	C4-C3-C5	3.87	121.79	115.27
24	C	505	CLA	C3B-C4B-NB	3.87	114.21	109.21
24	a	350	CLA	CBC-CAC-C3C	-3.87	101.76	112.43
24	b	605	CLA	O2D-CGD-O1D	-3.86	116.29	123.84
24	b	615	CLA	O2D-CGD-CBD	3.86	118.12	111.27
24	b	608	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
31	A	416[A]	PL9	C37-C38-C39	-3.85	118.38	127.66
24	C	508	CLA	C1D-CHD-C4C	-3.85	117.47	122.56
26	T	101	BCR	C11-C10-C9	-3.84	121.83	127.31
24	D	402	CLA	O2D-CGD-CBD	3.84	118.09	111.27
24	a	350	CLA	C1D-CHD-C4C	-3.84	117.49	122.56
26	b	619	BCR	C15-C14-C13	-3.83	121.84	127.31
24	b	614	CLA	O2D-CGD-O1D	-3.83	116.35	123.84
24	B	604	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
36	C	517	DGD	O2G-C1B-C2B	3.82	119.73	111.50
27	B	620	SQD	O7-S-C6	3.82	111.48	106.94
24	d	403	CLA	C2C-C1C-NC	3.82	113.55	109.97
24	A	406	CLA	C1-C2-C3	-3.81	119.45	126.04
26	C	515	BCR	C15-C14-C13	-3.81	121.87	127.31
24	b	604	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
24	C	508	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
24	c	508	CLA	C3B-C4B-NB	3.81	114.13	109.21
24	B	604	CLA	C4A-NA-C1A	-3.81	105.00	106.71
24	b	605	CLA	C3C-C4C-NC	3.81	114.84	110.57
24	B	603	CLA	C1D-CHD-C4C	-3.81	117.54	122.56
24	A	409	CLA	C3B-C4B-NB	3.80	114.12	109.21
27	a	409	SQD	C1-C2-C3	-3.80	102.08	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	609	CLA	C1-C2-C3	-3.80	119.47	126.04
24	c	514	CLA	C3C-C4C-NC	3.80	114.83	110.57
24	c	511	CLA	C3B-C4B-NB	3.79	114.11	109.21
24	b	606	CLA	C1D-CHD-C4C	-3.79	117.55	122.56
24	C	503	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
33	B	621	LMG	O7-C10-C11	3.79	119.67	111.50
24	a	407	CLA	C1D-CHD-C4C	-3.79	117.56	122.56
24	B	612	CLA	C3B-C4B-NB	3.79	114.11	109.21
24	A	405	CLA	CHD-C4C-NC	3.79	130.17	124.20
24	A	409	CLA	C1-C2-C3	-3.79	119.50	126.04
35	b	623	HTG	C1-O5-C5	3.78	119.54	112.58
31	a	414[A]	PL9	C22-C23-C24	-3.78	118.57	127.66
24	C	502	CLA	C1D-CHD-C4C	-3.77	117.58	122.56
26	t	102	BCR	C11-C10-C9	-3.77	121.92	127.31
36	c	518	DGD	O2G-C1B-C2B	3.77	119.62	111.50
26	A	410	BCR	C15-C14-C13	-3.76	121.94	127.31
24	c	503	CLA	C3C-C4C-NC	3.76	114.79	110.57
26	K	102	BCR	C7-C8-C9	-3.76	120.55	126.23
26	y	101	BCR	C38-C26-C25	-3.76	120.31	124.53
27	a	409	SQD	C45-O47-C7	-3.76	108.54	117.79
24	B	616	CLA	C1D-CHD-C4C	-3.75	117.60	122.56
24	B	611	CLA	C1C-C2C-C3C	-3.75	103.02	106.96
33	b	621	LMG	O7-C10-C11	3.74	119.57	111.50
24	b	603	CLA	C1C-C2C-C3C	-3.74	103.02	106.96
24	D	402	CLA	C3B-C4B-NB	3.74	114.05	109.21
24	B	608	CLA	C3B-C4B-NB	3.74	114.05	109.21
24	B	605	CLA	O2D-CGD-O1D	-3.74	116.53	123.84
24	C	503	CLA	C1D-CHD-C4C	-3.73	117.63	122.56
33	A	418	LMG	C7-O1-C1	-3.73	106.45	113.74
24	C	504	CLA	C1D-CHD-C4C	-3.73	117.64	122.56
27	a	411	SQD	O47-C7-C8	3.73	119.53	111.50
24	A	405	CLA	CBC-CAC-C3C	-3.72	102.18	112.43
26	C	516	BCR	C11-C10-C9	-3.72	122.01	127.31
24	C	509	CLA	O2D-CGD-O1D	-3.72	116.57	123.84
24	B	612	CLA	C4C-C3C-C2C	-3.72	101.48	106.90
24	C	509	CLA	C1-C2-C3	-3.72	119.62	126.04
24	b	609	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
24	C	508	CLA	O2D-CGD-O1D	-3.71	116.58	123.84
24	C	506	CLA	C1D-CHD-C4C	-3.71	117.66	122.56
24	c	507	CLA	C1D-CHD-C4C	-3.71	117.66	122.56
24	c	514	CLA	C1D-CHD-C4C	-3.71	117.66	122.56
24	b	609	CLA	CAC-C3C-C4C	3.71	129.62	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	350	CLA	C3C-C4C-NC	3.70	114.73	110.57
24	b	612	CLA	C1-C2-C3	-3.70	119.64	126.04
24	c	512	CLA	C1D-CHD-C4C	-3.70	117.67	122.56
31	D	405	PL9	C42-C43-C44	-3.70	118.76	127.66
24	c	514	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
24	b	614	CLA	CAC-C3C-C4C	3.69	129.60	124.81
24	c	503	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
24	C	502	CLA	C1C-C2C-C3C	-3.68	103.08	106.96
24	c	506	CLA	C3B-C4B-NB	3.68	113.97	109.21
24	B	613	CLA	C3B-C4B-NB	3.68	113.96	109.21
25	a	406	PHO	C4-C3-C5	3.67	121.45	115.27
24	a	407	CLA	CAA-C2A-C3A	-3.67	102.74	112.78
24	d	403	CLA	O2D-CGD-O1D	-3.66	116.68	123.84
24	C	512	CLA	CMC-C2C-C1C	3.66	130.61	125.04
26	k	101	BCR	C20-C21-C22	-3.66	122.09	127.31
24	a	350	CLA	CHD-C4C-NC	3.66	129.97	124.20
24	c	508	CLA	C1-C2-C3	-3.66	119.72	126.04
24	B	608	CLA	C1D-CHD-C4C	-3.66	117.73	122.56
24	c	515	CLA	C1D-CHD-C4C	-3.65	117.74	122.56
26	h	102	BCR	C7-C8-C9	-3.65	120.72	126.23
26	Y	101	BCR	C16-C17-C18	-3.65	122.10	127.31
31	a	414[B]	PL9	C7-C3-C2	-3.65	118.50	123.30
26	C	516	BCR	C7-C8-C9	-3.65	120.72	126.23
31	A	416[A]	PL9	C10-C9-C11	3.65	121.41	115.27
24	c	507	CLA	C4C-C3C-C2C	-3.65	101.58	106.90
24	A	409	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
24	C	511	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
24	c	515	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
24	A	406	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
27	f	101	SQD	C1-O5-C5	3.64	120.84	113.69
24	c	506	CLA	C3C-C4C-NC	3.64	114.66	110.57
24	c	511	CLA	C3C-C4C-NC	3.64	114.65	110.57
24	A	406	CLA	C3C-C4C-NC	3.64	114.65	110.57
31	a	414[A]	PL9	C15-C14-C16	3.64	121.39	115.27
24	d	402	CLA	C1-C2-C3	-3.64	119.75	126.04
24	C	514	CLA	C1-C2-C3	-3.64	119.75	126.04
24	a	407	CLA	C3B-C4B-NB	3.63	113.91	109.21
26	b	619	BCR	C7-C8-C9	-3.63	120.75	126.23
24	B	603	CLA	O2D-CGD-O1D	-3.63	116.74	123.84
25	A	408	PHO	O2D-CGD-O1D	-3.63	116.74	123.84
24	b	606	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
24	B	605	CLA	O2A-CGA-O1A	-3.62	114.45	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	416[A]	PL9	C32-C33-C34	-3.62	118.94	127.66
24	B	606	CLA	CMC-C2C-C1C	3.62	130.55	125.04
24	A	404	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
24	C	504	CLA	C4-C3-C5	3.61	121.34	115.27
24	a	404	CLA	C1D-CHD-C4C	-3.61	117.80	122.56
31	A	416[B]	PL9	C7-C3-C2	-3.61	118.56	123.30
24	d	403	CLA	C3C-C4C-NC	3.60	114.61	110.57
26	a	408	BCR	C7-C8-C9	-3.60	120.79	126.23
27	a	411	SQD	O7-S-C6	3.60	111.22	106.94
24	b	607	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
38	l	101	LHG	O7-C7-C8	3.60	119.25	111.50
24	c	508	CLA	C1D-CHD-C4C	-3.59	117.82	122.56
26	h	102	BCR	C16-C17-C18	-3.59	122.19	127.31
24	C	511	CLA	C4-C3-C5	3.59	121.31	115.27
24	b	614	CLA	CMC-C2C-C1C	3.59	130.50	125.04
24	B	607	CLA	C3B-C4B-NB	3.59	113.85	109.21
24	B	612	CLA	CAC-C3C-C4C	3.59	129.47	124.81
24	a	407	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
24	B	610	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
38	L	101	LHG	O7-C7-C8	3.58	119.22	111.50
24	B	616	CLA	C4C-C3C-C2C	-3.58	101.68	106.90
24	b	615	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
24	c	511	CLA	C1D-CHD-C4C	-3.58	117.84	122.56
24	b	613	CLA	C1D-CHD-C4C	-3.58	117.84	122.56
24	a	407	CLA	O2D-CGD-O1D	-3.57	116.86	123.84
24	c	508	CLA	C3C-C4C-NC	3.55	114.56	110.57
24	B	609	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
24	C	505	CLA	C4A-NA-C1A	-3.55	105.11	106.71
24	A	404	CLA	CAC-C3C-C4C	3.55	129.41	124.81
24	C	507	CLA	C3B-C4B-NB	3.55	113.80	109.21
24	C	509	CLA	C4C-C3C-C2C	-3.55	101.73	106.90
24	C	512	CLA	C3B-C4B-NB	3.55	113.80	109.21
24	b	606	CLA	O2D-CGD-O1D	-3.54	116.91	123.84
24	C	510	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
24	b	616	CLA	C4C-C3C-C2C	-3.53	101.75	106.90
24	a	404	CLA	C1C-C2C-C3C	-3.53	103.24	106.96
27	A	411	SQD	C44-O6-C1	-3.53	106.84	113.74
31	a	414[A]	PL9	C37-C38-C39	-3.53	119.15	127.66
35	b	623	HTG	C1'-S1-C1	3.53	106.70	100.09
24	C	509	CLA	C3B-C4B-NB	3.53	113.78	109.21
24	c	504	CLA	C1D-CHD-C4C	-3.53	117.90	122.56
31	a	414[B]	PL9	C27-C28-C29	-3.53	119.16	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	404	BCR	C24-C23-C22	-3.53	120.91	126.23
24	c	515	CLA	CAC-C3C-C4C	3.53	129.38	124.81
31	A	416[A]	PL9	C7-C3-C2	-3.52	118.67	123.30
24	b	612	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
24	B	614	CLA	C1D-CHD-C4C	-3.52	117.91	122.56
26	B	617	BCR	C16-C17-C18	-3.52	122.29	127.31
31	a	414[A]	PL9	C7-C3-C2	-3.52	118.67	123.30
24	a	403	CLA	O2D-CGD-CBD	3.52	117.52	111.27
24	B	604	CLA	O2A-CGA-O1A	-3.52	114.72	123.59
24	c	512	CLA	C3C-C4C-NC	3.51	114.51	110.57
26	D	404	BCR	C15-C14-C13	-3.51	122.29	127.31
31	a	414[B]	PL9	C32-C33-C34	-3.51	119.20	127.66
24	b	613	CLA	O2D-CGD-CBD	3.51	117.51	111.27
24	c	514	CLA	C1-C2-C3	-3.51	119.97	126.04
24	C	513	CLA	C1-C2-C3	-3.51	119.97	126.04
24	C	509	CLA	C1C-C2C-C3C	-3.51	103.27	106.96
24	b	603	CLA	CAA-C2A-C3A	-3.51	103.17	112.78
24	A	405	CLA	CAA-C2A-C3A	-3.51	103.18	112.78
24	B	602	CLA	CAA-C2A-C3A	-3.50	103.18	112.78
24	b	605	CLA	C1D-CHD-C4C	-3.50	117.93	122.56
24	B	612	CLA	C1D-CHD-C4C	-3.50	117.94	122.56
31	d	405	PL9	C42-C43-C44	-3.50	119.23	127.66
24	B	616	CLA	O2D-CGD-O1D	-3.50	117.00	123.84
35	C	523	HTG	O5-C5-C4	3.50	116.04	109.69
24	B	613	CLA	O2D-CGD-CBD	3.49	117.47	111.27
24	b	611	CLA	C1D-CHD-C4C	-3.49	117.95	122.56
24	C	504	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
24	A	404	CLA	CMC-C2C-C1C	3.48	130.34	125.04
24	B	607	CLA	O2D-CGD-O1D	-3.48	117.04	123.84
24	c	509	CLA	C3C-C4C-NC	3.48	114.47	110.57
24	c	513	CLA	O2D-CGD-O1D	-3.47	117.04	123.84
24	b	601	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
24	d	403	CLA	CMC-C2C-C1C	3.47	130.32	125.04
25	A	407	PHO	C4C-C3C-C2C	-3.47	102.94	106.78
24	d	402	CLA	C4-C3-C5	3.47	121.11	115.27
24	A	404	CLA	O2A-CGA-O1A	-3.47	114.84	123.59
24	c	511	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
24	A	409	CLA	C1D-CHD-C4C	-3.47	117.98	122.56
24	c	510	CLA	C1D-CHD-C4C	-3.47	117.98	122.56
24	c	513	CLA	C1-C2-C3	-3.46	120.05	126.04
31	a	414[A]	PL9	C30-C29-C31	3.46	121.10	115.27
24	D	403	CLA	CAC-C3C-C4C	3.46	129.30	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	402	CLA	C3B-C4B-NB	3.46	113.68	109.21
24	C	512	CLA	C1D-CHD-C4C	-3.46	118.00	122.56
24	b	615	CLA	C1D-CHD-C4C	-3.45	118.00	122.56
24	b	601	CLA	C4-C3-C5	3.45	121.08	115.27
26	B	618	BCR	C29-C30-C25	3.45	115.80	110.48
24	d	402	CLA	CAC-C3C-C4C	3.45	129.29	124.81
38	D	407	LHG	O7-C7-C8	3.45	118.94	111.50
24	B	610	CLA	CMA-C3A-C4A	-3.45	102.50	111.77
24	b	616	CLA	OBD-CAD-C3D	-3.45	122.25	127.98
25	A	408	PHO	CAC-C3C-C4C	3.45	128.98	125.22
24	c	505	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
24	b	615	CLA	C3B-C4B-NB	3.45	113.67	109.21
24	B	610	CLA	O2A-CGA-CBA	3.45	122.72	111.91
31	A	416[A]	PL9	C17-C18-C19	-3.44	119.36	127.66
24	C	507	CLA	CAC-C3C-C4C	3.44	129.28	124.81
24	b	613	CLA	C1-C2-C3	-3.44	120.09	126.04
24	b	613	CLA	C3B-C4B-NB	3.44	113.66	109.21
24	a	407	CLA	CMA-C3A-C2A	-3.44	99.95	113.83
31	d	405	PL9	C10-C9-C11	3.44	121.06	115.27
24	b	603	CLA	C3B-C4B-NB	3.44	113.65	109.21
24	b	610	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
24	C	514	CLA	C1D-CHD-C4C	-3.43	118.03	122.56
24	a	404	CLA	C1-C2-C3	-3.43	120.11	126.04
24	B	605	CLA	C4C-C3C-C2C	-3.43	101.90	106.90
24	a	403	CLA	C3C-C4C-NC	3.43	114.41	110.57
24	d	402	CLA	C1C-C2C-C3C	-3.43	103.36	106.96
24	b	611	CLA	O2D-CGD-O1D	-3.43	117.14	123.84
24	C	505	CLA	C1D-CHD-C4C	-3.42	118.04	122.56
26	A	410	BCR	C16-C17-C18	-3.42	122.42	127.31
26	b	618	BCR	C15-C14-C13	-3.42	122.43	127.31
26	c	516	BCR	C16-C17-C18	-3.42	122.43	127.31
24	a	407	CLA	CAC-C3C-C4C	3.42	129.24	124.81
31	a	414[B]	PL9	C42-C43-C44	-3.42	119.43	127.66
33	Z	101	LMG	C1-C2-C3	3.41	117.11	110.00
24	B	615	CLA	CHD-C4C-NC	3.41	129.58	124.20
24	b	610	CLA	C1D-CHD-C4C	-3.41	118.05	122.56
24	B	614	CLA	C3B-C4B-NB	3.41	113.62	109.21
24	c	514	CLA	C4-C3-C5	3.41	121.01	115.27
24	b	601	CLA	C1C-C2C-C3C	-3.41	103.37	106.96
26	A	410	BCR	C33-C5-C6	-3.41	120.70	124.53
31	d	405	PL9	C37-C38-C39	-3.41	119.46	127.66
24	c	504	CLA	C1-C2-C3	-3.40	120.16	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	618	BCR	C15-C14-C13	-3.40	122.45	127.31
24	B	614	CLA	CMB-C2B-C3B	3.40	131.04	124.68
24	c	510	CLA	C3B-C4B-NB	3.40	113.60	109.21
24	b	605	CLA	C4-C3-C5	3.39	120.98	115.27
24	D	403	CLA	CMC-C2C-C1C	3.39	130.21	125.04
24	B	606	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
24	b	612	CLA	C4-C3-C5	3.39	120.98	115.27
24	b	605	CLA	CHD-C4C-NC	3.39	129.55	124.20
24	d	402	CLA	C1D-CHD-C4C	-3.39	118.08	122.56
24	A	406	CLA	CAA-C2A-C3A	-3.39	103.50	112.78
26	a	408	BCR	C20-C21-C22	-3.39	122.47	127.31
24	B	611	CLA	OBD-CAD-C3D	-3.39	122.36	127.98
24	B	610	CLA	CAA-C2A-C3A	-3.39	103.50	112.78
24	A	404	CLA	C3B-C4B-NB	3.39	113.59	109.21
31	a	414[B]	PL9	C37-C38-C39	-3.39	119.51	127.66
24	b	605	CLA	C3B-C4B-NB	3.38	113.58	109.21
31	A	416[A]	PL9	C27-C28-C29	-3.38	119.52	127.66
34	M	101	LMT	O1'-C1'-C2'	3.38	113.58	108.30
24	B	614	CLA	C4-C3-C5	3.38	120.95	115.27
24	B	610	CLA	C1D-CHD-C4C	-3.38	118.10	122.56
24	b	614	CLA	C1C-C2C-C3C	-3.38	103.41	106.96
24	b	608	CLA	C3B-C4B-NB	3.37	113.57	109.21
24	C	507	CLA	C3C-C4C-NC	3.37	114.35	110.57
24	B	614	CLA	CMC-C2C-C1C	3.37	130.17	125.04
24	a	404	CLA	CAA-C2A-C3A	-3.37	103.55	112.78
31	a	414[A]	PL9	C42-C43-C44	-3.37	119.55	127.66
26	t	102	BCR	C7-C8-C9	-3.37	121.15	126.23
24	C	506	CLA	C4C-C3C-C2C	-3.37	101.99	106.90
24	C	505	CLA	CAC-C3C-C4C	3.37	129.18	124.81
24	b	604	CLA	C1D-CHD-C4C	-3.36	118.12	122.56
36	c	520	DGD	O2G-C1B-C2B	3.36	118.74	111.50
33	b	621	LMG	O8-C28-C29	3.35	122.44	111.91
24	b	614	CLA	C1D-CHD-C4C	-3.35	118.13	122.56
24	B	603	CLA	C5-C3-C2	-3.35	114.33	121.12
24	c	504	CLA	C3B-C4B-NB	3.35	113.55	109.21
24	b	601	CLA	C3B-C4B-NB	3.35	113.54	109.21
24	C	511	CLA	CHD-C4C-NC	3.35	129.47	124.20
33	z	101	LMG	O7-C10-C11	3.35	118.71	111.50
24	d	403	CLA	CAC-C3C-C4C	3.34	129.15	124.81
31	A	416[B]	PL9	C17-C18-C19	-3.34	119.61	127.66
24	b	607	CLA	C4C-C3C-C2C	-3.34	102.03	106.90
24	c	512	CLA	C4-C3-C5	3.34	120.89	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	513	CLA	C1D-CHD-C4C	-3.34	118.15	122.56
24	a	404	CLA	C3B-C4B-NB	3.34	113.53	109.21
26	C	515	BCR	C33-C5-C6	-3.34	120.78	124.53
24	C	505	CLA	C1-C2-C3	-3.33	120.28	126.04
24	C	512	CLA	C1C-C2C-C3C	-3.33	103.45	106.96
24	b	616	CLA	O2A-CGA-CBA	3.33	122.36	111.91
36	c	519	DGD	O2G-C1B-C2B	3.33	118.68	111.50
36	C	518	DGD	O2G-C1B-C2B	3.33	118.68	111.50
24	B	603	CLA	O2A-CGA-O1A	-3.33	115.19	123.59
24	c	513	CLA	CHD-C4C-NC	3.33	129.45	124.20
24	b	602	CLA	CAA-C2A-C3A	-3.33	103.67	112.78
26	C	516	BCR	C33-C5-C6	-3.32	120.80	124.53
24	a	403	CLA	CHC-C1C-C2C	-3.32	117.53	126.72
35	b	628	HTG	C1'-S1-C1	3.32	106.30	100.09
26	k	101	BCR	C24-C23-C22	-3.32	121.22	126.23
24	B	605	CLA	CHD-C4C-NC	3.32	129.44	124.20
24	C	507	CLA	CBC-CAC-C3C	-3.32	103.28	112.43
24	C	510	CLA	C3B-C4B-NB	3.32	113.50	109.21
24	B	604	CLA	C3B-C4B-NB	3.32	113.50	109.21
24	C	507	CLA	CHC-C1C-C2C	-3.31	117.55	126.72
26	Y	101	BCR	C15-C14-C13	-3.31	122.58	127.31
24	B	602	CLA	C1D-CHD-C4C	-3.31	118.19	122.56
24	B	615	CLA	C1C-C2C-C3C	-3.31	103.48	106.96
24	c	513	CLA	C4-C3-C5	3.31	120.84	115.27
38	d	406	LHG	O7-C7-C8	3.31	118.63	111.50
31	A	416[A]	PL9	C15-C14-C16	3.31	120.83	115.27
24	D	403	CLA	C1D-CHD-C4C	-3.31	118.19	122.56
24	B	602	CLA	CAC-C3C-C4C	3.30	129.09	124.81
24	B	601	CLA	CHD-C4C-NC	3.30	129.40	124.20
31	a	414[B]	PL9	C22-C23-C24	-3.30	119.72	127.66
24	d	402	CLA	C4C-C3C-C2C	-3.30	102.09	106.90
24	c	512	CLA	CBC-CAC-C3C	-3.30	103.34	112.43
24	c	513	CLA	C3B-C4B-NB	3.29	113.47	109.21
24	C	511	CLA	C3B-C4B-NB	3.29	113.47	109.21
24	b	601	CLA	CHD-C4C-NC	3.29	129.39	124.20
35	c	526	HTG	C1-O5-C5	3.29	118.64	112.58
26	y	101	BCR	C15-C14-C13	-3.29	122.62	127.31
26	T	101	BCR	C33-C5-C6	-3.29	120.84	124.53
33	C	520	LMG	O8-C28-C29	3.29	122.22	111.91
26	h	102	BCR	C38-C26-C25	-3.29	120.84	124.53
24	d	403	CLA	C1-C2-C3	-3.28	120.37	126.04
24	b	610	CLA	O2A-CGA-O1A	-3.28	115.31	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	515	CLA	C3B-C4B-NB	3.28	113.45	109.21
24	C	504	CLA	C1-C2-C3	-3.28	120.37	126.04
31	A	416[B]	PL9	C42-C43-C44	-3.28	119.76	127.66
24	a	403	CLA	CMB-C2B-C3B	3.28	130.81	124.68
24	B	612	CLA	C4-C3-C5	3.27	120.77	115.27
24	b	612	CLA	CAC-C3C-C4C	3.27	129.05	124.81
26	A	410	BCR	C11-C10-C9	-3.27	122.65	127.31
26	T	101	BCR	C7-C8-C9	-3.27	121.30	126.23
26	a	408	BCR	C11-C10-C9	-3.27	122.65	127.31
24	B	609	CLA	C3B-C4B-NB	3.26	113.43	109.21
24	c	506	CLA	CMC-C2C-C1C	3.26	130.01	125.04
24	c	510	CLA	C1-C2-C3	-3.26	120.40	126.04
31	d	405	PL9	C45-C44-C46	3.26	120.76	115.27
24	C	507	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
24	C	514	CLA	C4C-C3C-C2C	-3.26	102.15	106.90
24	B	608	CLA	C1-C2-C3	-3.26	120.41	126.04
24	c	513	CLA	C1C-C2C-C3C	-3.26	103.53	106.96
24	c	508	CLA	CHC-C1C-C2C	-3.26	117.71	126.72
31	a	414[A]	PL9	C27-C28-C29	-3.25	119.83	127.66
25	a	406	PHO	O2D-CGD-O1D	-3.25	117.48	123.84
24	c	514	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
24	a	350	CLA	C1-C2-C3	-3.25	120.42	126.04
25	A	407	PHO	C2B-C1B-NB	3.25	114.70	109.79
24	b	609	CLA	C1D-CHD-C4C	-3.25	118.27	122.56
31	a	414[B]	PL9	C17-C18-C19	-3.25	119.83	127.66
24	C	514	CLA	CAC-C3C-C4C	3.25	129.03	124.81
24	D	403	CLA	C4C-C3C-C2C	-3.25	102.17	106.90
24	B	606	CLA	CMB-C2B-C3B	3.25	130.75	124.68
24	C	506	CLA	C1C-C2C-C3C	-3.25	103.54	106.96
24	b	612	CLA	C4C-C3C-C2C	-3.24	102.17	106.90
24	B	616	CLA	CHD-C4C-NC	3.24	129.31	124.20
24	C	513	CLA	C4C-C3C-C2C	-3.24	102.17	106.90
24	b	602	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
24	c	505	CLA	C3B-C4B-NB	3.24	113.40	109.21
24	c	509	CLA	C4-C3-C5	3.24	120.71	115.27
24	c	507	CLA	CAC-C3C-C4C	3.24	129.01	124.81
24	C	513	CLA	C1C-C2C-C3C	-3.24	103.56	106.96
24	b	614	CLA	C3B-C4B-NB	3.23	113.39	109.21
24	b	611	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
24	a	403	CLA	CAC-C3C-C4C	3.23	129.00	124.81
34	I	101	LMT	O1B-C4'-C3'	3.23	115.87	107.28
31	A	416[B]	PL9	C37-C38-C39	-3.23	119.89	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	615	CLA	CMC-C2C-C1C	3.23	129.96	125.04
24	b	614	CLA	C1-C2-C3	-3.23	120.46	126.04
25	A	408	PHO	C2B-C1B-NB	3.22	114.66	109.79
33	C	521	LMG	C3-C4-C5	3.22	115.99	110.24
24	B	606	CLA	CHD-C4C-NC	3.22	129.28	124.20
38	l	101	LHG	O8-C23-C24	3.22	122.03	111.91
24	b	615	CLA	CHC-C1C-C2C	-3.22	117.81	126.72
24	b	613	CLA	CMB-C2B-C3B	3.22	130.71	124.68
24	A	409	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
24	B	610	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
27	A	413	SQD	O47-C7-C8	3.22	118.44	111.50
27	F	101	SQD	O8-S-C6	3.22	110.87	105.74
24	d	403	CLA	C1D-CHD-C4C	-3.22	118.31	122.56
24	A	405	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
26	T	101	BCR	C12-C13-C14	-3.21	114.01	118.94
26	D	404	BCR	C28-C27-C26	-3.21	108.34	114.08
31	A	416[B]	PL9	C32-C33-C34	-3.21	119.92	127.66
24	b	605	CLA	O2A-CGA-O1A	-3.21	115.48	123.59
38	D	357	LHG	O8-C23-C24	3.21	121.97	111.91
24	C	514	CLA	C3B-C4B-NB	3.20	113.35	109.21
24	C	514	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
33	B	621	LMG	O8-C28-C29	3.20	121.96	111.91
25	A	407	PHO	C1C-C2C-C3C	-3.20	102.84	106.51
24	B	602	CLA	C4C-C3C-C2C	-3.20	102.24	106.90
24	c	508	CLA	C4-C3-C5	3.20	120.65	115.27
24	b	611	CLA	C1C-C2C-C3C	-3.19	103.60	106.96
24	B	609	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
24	c	509	CLA	CHD-C4C-NC	3.19	129.23	124.20
24	b	609	CLA	C3B-C4B-NB	3.19	113.33	109.21
25	a	405	PHO	CHC-C1C-C2C	-3.19	117.71	125.73
24	C	504	CLA	C3B-C4B-NB	3.19	113.33	109.21
26	k	101	BCR	C15-C14-C13	-3.19	122.76	127.31
25	A	407	PHO	C2A-C1A-NA	3.18	115.52	111.86
24	B	601	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
24	C	514	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
24	c	507	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
24	b	610	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
24	B	603	CLA	CBC-CAC-C3C	-3.18	103.67	112.43
34	t	101	LMT	C1'-O5'-C5'	3.18	119.92	113.69
24	B	615	CLA	C4C-C3C-C2C	-3.17	102.27	106.90
24	B	611	CLA	CHD-C4C-NC	3.17	129.20	124.20
24	c	509	CLA	C1D-CHD-C4C	-3.17	118.37	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	405	PHO	C2B-C1B-NB	3.17	114.57	109.79
24	c	510	CLA	C4D-C3D-CAD	-3.17	106.70	108.47
26	b	619	BCR	C38-C26-C25	-3.17	120.97	124.53
24	c	507	CLA	CMC-C2C-C1C	3.17	129.86	125.04
24	c	515	CLA	C1-C2-C3	-3.16	120.58	126.04
38	d	406	LHG	O8-C23-O10	-3.16	115.61	123.59
24	a	404	CLA	CHD-C4C-NC	3.16	129.18	124.20
41	v	203	HEC	CBA-CAA-C2A	-3.16	106.66	112.48
24	d	402	CLA	O2A-CGA-CBA	3.16	121.81	111.91
26	d	404	BCR	C7-C8-C9	-3.16	121.47	126.23
25	A	407	PHO	CHC-C1C-C2C	-3.15	117.80	125.73
24	b	602	CLA	C1C-C2C-C3C	-3.15	103.64	106.96
24	b	615	CLA	C4C-C3C-C2C	-3.15	102.30	106.90
25	a	405	PHO	C2C-C1C-NC	3.15	114.55	109.79
24	b	608	CLA	C1D-CHD-C4C	-3.15	118.40	122.56
24	B	613	CLA	C4-C3-C5	3.15	120.57	115.27
24	B	608	CLA	CMA-C3A-C4A	-3.15	103.30	111.77
24	a	350	CLA	CAA-C2A-C3A	-3.15	104.15	112.78
24	C	510	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
24	c	504	CLA	CHD-C4C-NC	3.15	129.17	124.20
36	C	517	DGD	C3G-C2G-C1G	-3.15	104.34	111.79
24	b	604	CLA	O2A-CGA-CBA	3.15	121.79	111.91
26	B	619	BCR	C24-C23-C22	-3.15	121.48	126.23
24	B	604	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
24	c	505	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
24	B	601	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
24	c	503	CLA	C1D-CHD-C4C	-3.14	118.41	122.56
24	b	607	CLA	C1D-CHD-C4C	-3.14	118.41	122.56
24	B	601	CLA	C1C-C2C-C3C	-3.14	103.66	106.96
24	b	616	CLA	C3B-C4B-NB	3.14	113.27	109.21
24	B	607	CLA	CMC-C2C-C1C	3.14	129.82	125.04
25	A	408	PHO	C2A-C1A-NA	3.14	115.46	111.86
25	a	405	PHO	O2D-CGD-O1D	-3.14	117.70	123.84
24	C	510	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
24	b	603	CLA	O2A-CGA-O1A	-3.13	115.68	123.59
24	A	409	CLA	CAA-C2A-C3A	-3.13	104.19	112.78
39	e	102	HEM	CBD-CAD-C3D	-3.13	106.70	112.48
24	A	406	CLA	CHD-C4C-NC	3.13	129.14	124.20
24	b	616	CLA	CHD-C4C-NC	3.13	129.14	124.20
38	D	357	LHG	O8-C23-O10	-3.13	115.69	123.59
24	B	605	CLA	C4D-C3D-CAD	-3.13	106.73	108.47
31	A	416[A]	PL9	C35-C34-C36	3.13	120.53	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	614	CLA	C4C-C3C-C2C	-3.13	102.34	106.90
24	B	602	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
36	h	103	DGD	O1G-C1A-C2A	3.12	121.71	111.91
26	c	517	BCR	C33-C5-C6	-3.12	121.02	124.53
33	c	522	LMG	O6-C5-C4	3.12	115.36	109.69
24	B	608	CLA	CMB-C2B-C3B	3.12	130.51	124.68
24	b	603	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
24	b	613	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
24	C	506	CLA	CMC-C2C-C1C	3.12	129.79	125.04
24	B	609	CLA	C1-O2A-CGA	3.12	124.62	116.44
24	B	606	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
24	b	603	CLA	O2A-CGA-CBA	3.12	121.69	111.91
24	D	403	CLA	O2D-CGD-O1D	-3.12	117.75	123.84
24	b	602	CLA	C4C-C3C-C2C	-3.12	102.36	106.90
24	D	403	CLA	C3B-C4B-NB	3.11	113.23	109.21
33	C	521	LMG	O6-C5-C4	3.11	115.35	109.69
24	B	603	CLA	O2A-CGA-CBA	3.11	121.67	111.91
24	B	605	CLA	C3B-C4B-NB	3.11	113.23	109.21
31	A	416[A]	PL9	C7-C3-C4	3.11	119.40	116.88
24	b	601	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
24	b	604	CLA	C3B-C4B-NB	3.11	113.23	109.21
25	A	407	PHO	C2C-C1C-NC	3.11	114.48	109.79
25	A	408	PHO	C4-C3-C5	3.11	120.50	115.27
24	d	402	CLA	O2D-CGD-O1D	-3.11	117.77	123.84
24	a	350	CLA	C3B-C4B-NB	3.10	113.22	109.21
24	C	510	CLA	CAC-C3C-C4C	3.10	128.84	124.81
24	C	508	CLA	C4-C3-C5	3.10	120.49	115.27
41	V	203	HEC	CBD-CAD-C3D	-3.10	106.76	112.49
24	C	504	CLA	CHC-C1C-C2C	-3.10	118.14	126.72
24	B	612	CLA	C1C-C2C-C3C	-3.10	103.70	106.96
24	C	510	CLA	CMB-C2B-C3B	3.10	130.48	124.68
24	C	512	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
24	C	507	CLA	C1-C2-C3	-3.10	120.69	126.04
24	B	605	CLA	C1C-C2C-C3C	-3.10	103.70	106.96
24	a	403	CLA	CAA-C2A-C1A	-3.10	101.83	111.97
24	C	504	CLA	O2D-CGD-CBD	3.10	116.77	111.27
24	D	402	CLA	CHC-C1C-C2C	-3.10	118.16	126.72
24	c	506	CLA	C1D-CHD-C4C	-3.09	118.48	122.56
24	b	605	CLA	CHC-C1C-C2C	-3.09	118.17	126.72
25	a	405	PHO	C3C-C4C-NC	3.09	115.07	110.28
24	b	615	CLA	C4-C3-C5	3.09	120.47	115.27
24	C	506	CLA	C3B-C4B-NB	3.09	113.20	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	606	CLA	C3B-C4B-NB	3.09	113.20	109.21
24	b	610	CLA	CMB-C2B-C3B	3.09	130.45	124.68
24	B	614	CLA	O2A-CGA-O1A	-3.09	115.80	123.59
26	b	619	BCR	C2-C1-C6	3.09	115.23	110.48
31	a	414[A]	PL9	C10-C9-C11	3.09	120.46	115.27
24	c	503	CLA	C1-C2-C3	-3.08	120.71	126.04
24	b	612	CLA	CHC-C1C-C2C	-3.08	118.19	126.72
38	D	357	LHG	C5-O7-C7	-3.08	110.20	117.79
24	C	513	CLA	CHD-C4C-NC	3.08	129.06	124.20
31	A	416[B]	PL9	C10-C9-C8	-3.08	115.78	123.68
24	C	510	CLA	C1D-CHD-C4C	-3.08	118.49	122.56
26	c	517	BCR	C21-C20-C19	-3.08	113.61	123.22
24	C	503	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
36	c	518	DGD	C2G-O2G-C1B	-3.08	110.22	117.79
24	c	511	CLA	CHC-C1C-C2C	-3.08	118.21	126.72
26	A	410	BCR	C38-C26-C25	-3.08	121.07	124.53
33	c	521	LMG	O8-C28-C29	3.07	121.55	111.91
33	a	417	LMG	O6-C5-C4	3.07	115.27	109.69
24	a	403	CLA	O2A-CGA-CBA	3.07	121.53	111.91
24	d	403	CLA	CHD-C4C-NC	3.07	129.03	124.20
24	B	602	CLA	C1-C2-C3	-3.07	120.74	126.04
24	b	604	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
24	A	409	CLA	C4-C3-C5	3.06	120.42	115.27
31	d	405	PL9	C40-C39-C41	3.06	120.42	115.27
24	c	504	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
38	d	406	LHG	O8-C23-C24	3.06	121.50	111.91
24	b	611	CLA	C3B-C4B-NB	3.06	113.16	109.21
24	b	606	CLA	C4C-C3C-C2C	-3.05	102.44	106.90
24	c	513	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
24	b	603	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
24	C	504	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
24	b	609	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
24	A	404	CLA	CMB-C2B-C3B	3.05	130.38	124.68
36	C	517	DGD	O3G-C3G-C2G	-3.05	103.54	110.90
24	B	601	CLA	O2A-CGA-CBA	3.05	121.47	111.91
24	B	614	CLA	CHC-C1C-C2C	-3.05	118.29	126.72
24	a	407	CLA	C4C-C3C-C2C	-3.05	102.46	106.90
24	c	504	CLA	CBC-CAC-C3C	-3.04	104.04	112.43
24	a	404	CLA	C4C-C3C-C2C	-3.04	102.46	106.90
26	c	517	BCR	C38-C26-C25	-3.04	121.11	124.53
26	K	102	BCR	C20-C21-C22	-3.04	122.97	127.31
24	b	606	CLA	C4-C3-C5	3.04	120.38	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	620	SQD	O48-C23-C24	3.04	121.43	111.91
24	C	508	CLA	C4C-C3C-C2C	-3.03	102.47	106.90
31	a	414[A]	PL9	C17-C18-C19	-3.03	120.35	127.66
24	B	611	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
24	B	604	CLA	O2A-CGA-CBA	3.03	121.41	111.91
33	J	101	LMG	O7-C10-C11	3.02	118.02	111.50
24	b	610	CLA	CAC-C3C-C4C	3.02	128.73	124.81
24	c	512	CLA	CHC-C1C-C2C	-3.02	118.36	126.72
24	c	506	CLA	CAC-C3C-C4C	3.02	128.73	124.81
24	B	608	CLA	CHD-C4C-NC	3.02	128.96	124.20
24	b	613	CLA	CHD-C4C-NC	3.02	128.96	124.20
24	D	403	CLA	C1C-C2C-C3C	-3.02	103.78	106.96
24	B	610	CLA	C3B-C4B-NB	3.02	113.11	109.21
24	b	611	CLA	CHD-C4C-NC	3.02	128.96	124.20
24	b	615	CLA	C11-C10-C8	-3.01	106.18	115.92
26	Y	101	BCR	C28-C27-C26	-3.01	108.70	114.08
24	B	602	CLA	C1C-C2C-C3C	-3.01	103.79	106.96
24	c	509	CLA	CMC-C2C-C1C	3.01	129.62	125.04
24	c	505	CLA	C4-C3-C5	3.01	120.33	115.27
24	C	503	CLA	CHD-C4C-NC	3.01	128.94	124.20
24	B	606	CLA	C4-C3-C5	3.01	120.33	115.27
25	A	408	PHO	C3C-C4C-NC	3.01	114.94	110.28
24	B	610	CLA	CHD-C4C-NC	3.01	128.94	124.20
24	B	608	CLA	C4C-C3C-C2C	-3.01	102.52	106.90
31	D	405	PL9	C40-C39-C41	3.00	120.33	115.27
24	b	610	CLA	C4-C3-C5	3.00	120.33	115.27
36	C	518	DGD	O1G-C1A-C2A	3.00	121.33	111.91
34	M	103	LMT	O5'-C5'-C4'	3.00	116.08	109.75
24	B	603	CLA	CHD-C4C-NC	3.00	128.93	124.20
24	b	605	CLA	C2A-C1A-CHA	-3.00	118.62	123.86
24	C	512	CLA	C4-C3-C5	3.00	120.31	115.27
24	b	613	CLA	C4-C3-C5	3.00	120.31	115.27
24	A	406	CLA	O2A-CGA-CBA	2.99	121.30	111.91
24	B	603	CLA	CAA-C2A-C3A	-2.99	104.58	112.78
26	D	404	BCR	C37-C22-C23	2.99	122.79	118.08
24	A	406	CLA	O2A-CGA-O1A	-2.99	116.04	123.59
24	c	503	CLA	C3B-C4B-NB	2.99	113.08	109.21
24	b	609	CLA	CBC-CAC-C3C	-2.99	104.18	112.43
24	B	608	CLA	O2A-CGA-O1A	-2.99	116.04	123.59
24	A	406	CLA	CMC-C2C-C1C	2.99	129.59	125.04
24	C	510	CLA	CMC-C2C-C1C	2.99	129.59	125.04
24	c	512	CLA	CHD-C4C-NC	2.99	128.92	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	503	CLA	CAC-C3C-C4C	2.99	128.69	124.81
24	A	404	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
24	c	515	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
36	c	520	DGD	O3G-C3G-C2G	-2.99	103.69	110.90
24	C	506	CLA	C4-C3-C5	2.99	120.29	115.27
24	b	608	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
24	B	607	CLA	CBC-CAC-C3C	-2.98	104.21	112.43
24	b	602	CLA	C1D-CHD-C4C	-2.98	118.62	122.56
24	D	403	CLA	CHD-C4C-NC	2.98	128.90	124.20
24	B	613	CLA	CMB-C2B-C3B	2.98	130.25	124.68
24	B	614	CLA	CAC-C3C-C4C	2.98	128.67	124.81
24	a	403	CLA	C1-C2-C3	-2.97	120.90	126.04
24	b	602	CLA	C2A-C1A-CHA	-2.97	118.66	123.86
27	a	409	SQD	O47-C7-O49	-2.97	116.52	123.70
24	b	613	CLA	O2A-CGA-CBA	2.97	121.24	111.91
24	c	505	CLA	CAC-C3C-C4C	2.97	128.67	124.81
25	A	408	PHO	C4D-CHA-C1A	-2.97	118.68	125.37
26	D	404	BCR	C10-C11-C12	-2.97	113.95	123.22
24	c	509	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
24	B	616	CLA	C3B-C4B-NB	2.97	113.05	109.21
26	b	619	BCR	C10-C11-C12	-2.97	113.95	123.22
24	c	508	CLA	CAA-C2A-C3A	-2.97	104.65	112.78
24	b	602	CLA	CHD-C4C-NC	2.97	128.88	124.20
24	c	514	CLA	C3B-C4B-NB	2.97	113.05	109.21
38	D	407	LHG	O8-C23-O10	-2.97	116.10	123.59
24	a	404	CLA	C4-C3-C5	2.97	120.26	115.27
24	b	607	CLA	C4-C3-C5	2.97	120.26	115.27
24	C	504	CLA	CAC-C3C-C4C	2.97	128.66	124.81
31	A	416[A]	PL9	C20-C19-C21	2.97	120.26	115.27
24	b	609	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
24	A	406	CLA	C2A-C1A-CHA	-2.96	118.67	123.86
24	b	612	CLA	CMB-C2B-C3B	2.96	130.22	124.68
27	A	413	SQD	O48-C23-C24	2.96	121.20	111.91
24	c	512	CLA	O2A-CGA-CBA	2.96	121.20	111.91
24	c	514	CLA	CHD-C4C-NC	2.96	128.87	124.20
24	B	603	CLA	CMC-C2C-C1C	2.96	129.55	125.04
24	c	509	CLA	C3B-C4B-NB	2.96	113.04	109.21
31	A	416[B]	PL9	C27-C28-C29	-2.96	120.54	127.66
24	C	502	CLA	CHD-C4C-NC	2.96	128.87	124.20
31	A	416[B]	PL9	C53-C6-C1	2.96	121.03	114.99
24	b	612	CLA	O2A-CGA-CBA	2.96	121.19	111.91
31	A	416[A]	PL9	C42-C43-C44	-2.95	120.56	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	609	CLA	C1D-CHD-C4C	-2.95	118.67	122.56
24	C	503	CLA	CBC-CAC-C3C	-2.95	104.30	112.43
24	A	406	CLA	C1D-CHD-C4C	-2.95	118.67	122.56
24	d	403	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
24	c	510	CLA	CMB-C2B-C3B	2.94	130.19	124.68
24	c	515	CLA	CMC-C2C-C1C	2.94	129.52	125.04
27	A	411	SQD	O48-C23-C24	2.94	121.14	111.91
31	A	416[A]	PL9	C22-C23-C24	-2.94	120.58	127.66
24	B	603	CLA	C3B-C4B-NB	2.94	113.01	109.21
24	b	616	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
24	C	502	CLA	C4-C3-C5	2.94	120.22	115.27
24	C	512	CLA	C1-C2-C3	-2.94	120.96	126.04
24	c	511	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
24	b	606	CLA	CMB-C2B-C3B	2.94	130.18	124.68
26	B	619	BCR	C38-C26-C25	-2.94	121.23	124.53
24	b	610	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
31	D	405	PL9	C53-C6-C1	2.94	121.00	114.99
24	b	611	CLA	CHC-C1C-C2C	-2.94	118.60	126.72
24	a	407	CLA	CMC-C2C-C1C	2.94	129.51	125.04
24	b	609	CLA	CMC-C2C-C1C	2.94	129.51	125.04
26	H	101	BCR	C38-C26-C25	-2.93	121.23	124.53
31	d	405	PL9	C12-C13-C14	-2.93	120.60	127.66
24	B	613	CLA	C1D-CHD-C4C	-2.93	118.69	122.56
31	D	405	PL9	C45-C44-C46	2.93	120.20	115.27
26	C	516	BCR	C38-C26-C25	-2.93	121.23	124.53
24	c	510	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
24	C	503	CLA	C3B-C4B-NB	2.93	113.00	109.21
24	d	403	CLA	C1C-C2C-C3C	-2.93	103.88	106.96
24	b	604	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
24	C	505	CLA	CHC-C1C-C2C	-2.93	118.62	126.72
24	d	402	CLA	CMC-C2C-C1C	2.93	129.49	125.04
24	B	608	CLA	CHC-C1C-C2C	-2.92	118.63	126.72
24	b	606	CLA	CHD-C4C-NC	2.92	128.81	124.20
25	A	407	PHO	CAC-C3C-C4C	2.92	128.41	125.22
24	b	608	CLA	CHD-C4C-NC	2.92	128.81	124.20
24	A	406	CLA	CMA-C3A-C2A	-2.92	102.05	113.83
24	c	515	CLA	CAA-C2A-C3A	-2.92	104.78	112.78
26	t	102	BCR	C37-C22-C23	2.92	122.68	118.08
31	a	414[B]	PL9	C35-C34-C36	2.92	120.18	115.27
24	A	404	CLA	CAA-C2A-C1A	-2.92	102.41	111.97
25	a	406	PHO	CHC-C1C-C2C	-2.92	118.39	125.73
24	C	505	CLA	CMC-C2C-C1C	2.92	129.48	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	404	BCR	C33-C5-C6	-2.91	121.26	124.53
25	A	408	PHO	C4D-ND-C1D	-2.91	101.52	106.76
24	b	605	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
24	b	607	CLA	CHC-C1C-C2C	-2.91	118.67	126.72
24	c	510	CLA	CHC-C1C-C2C	-2.91	118.67	126.72
24	C	502	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
35	b	628	HTG	C1-O5-C5	2.91	117.94	112.58
24	B	612	CLA	CMB-C2B-C3B	2.91	130.12	124.68
24	C	514	CLA	CMC-C2C-C1C	2.90	129.46	125.04
24	B	615	CLA	C3B-C4B-NB	2.90	112.96	109.21
24	b	608	CLA	O2A-CGA-CBA	2.90	121.02	111.91
35	b	625	HTG	O5-C1-C2	2.90	113.96	110.31
24	B	613	CLA	C7-C6-C5	-2.90	105.49	113.36
24	C	511	CLA	O2A-CGA-CBA	2.90	121.00	111.91
24	B	614	CLA	CHD-C4C-NC	2.90	128.77	124.20
24	c	503	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
38	a	419	LHG	O7-C7-C8	2.89	117.74	111.50
25	a	406	PHO	C2B-C1B-NB	2.89	114.15	109.79
24	c	510	CLA	CHD-C4C-NC	2.89	128.76	124.20
24	B	601	CLA	CMC-C2C-C1C	2.89	129.44	125.04
24	C	507	CLA	C1D-CHD-C4C	-2.89	118.75	122.56
24	C	513	CLA	O2A-CGA-CBA	2.89	120.97	111.91
24	B	601	CLA	C3B-C4B-NB	2.89	112.94	109.21
38	D	407	LHG	O8-C23-C24	2.88	120.95	111.91
24	c	504	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
38	E	101	LHG	O8-C23-C24	2.88	120.94	111.91
33	z	101	LMG	O8-C28-C29	2.88	120.93	111.91
27	a	411	SQD	O48-C23-C24	2.87	120.93	111.91
24	B	607	CLA	CHC-C1C-C2C	-2.87	118.77	126.72
41	v	203	HEC	CAD-CBD-CGD	2.87	117.49	112.67
24	C	503	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
31	A	416[B]	PL9	C22-C23-C24	-2.87	120.75	127.66
27	a	409	SQD	O48-C23-C24	2.87	120.92	111.91
26	d	404	BCR	C28-C27-C26	-2.87	108.95	114.08
26	b	619	BCR	C3-C4-C5	-2.87	108.95	114.08
24	c	514	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
24	B	604	CLA	CMC-C2C-C1C	2.87	129.41	125.04
24	C	507	CLA	C4-C3-C5	2.87	120.09	115.27
24	B	603	CLA	C2A-C1A-CHA	-2.87	118.85	123.86
25	A	408	PHO	CHD-C1D-C2D	-2.87	118.52	125.73
24	c	503	CLA	CHC-C1C-C2C	-2.87	118.79	126.72
25	a	405	PHO	C4D-ND-C1D	-2.86	101.61	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	513	CLA	C4-C3-C5	2.86	120.09	115.27
24	c	506	CLA	CHD-C4C-NC	2.86	128.71	124.20
25	a	406	PHO	C4D-CHA-C1A	-2.86	118.94	125.37
24	C	508	CLA	C3B-C4B-NB	2.86	112.91	109.21
24	C	509	CLA	C4D-C3D-CAD	-2.85	106.88	108.47
24	B	607	CLA	C4-C3-C5	2.85	120.07	115.27
26	T	101	BCR	C21-C20-C19	-2.85	114.31	123.22
26	T	101	BCR	C16-C17-C18	-2.85	123.24	127.31
31	a	414[B]	PL9	C7-C8-C9	-2.85	122.05	126.79
24	a	404	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
24	B	611	CLA	CMC-C2C-C1C	2.85	129.38	125.04
26	K	102	BCR	C11-C10-C9	-2.85	123.25	127.31
24	C	502	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
24	b	612	CLA	C2A-C1A-CHA	-2.85	118.88	123.86
24	c	504	CLA	O2A-CGA-O1A	-2.85	116.41	123.59
26	A	410	BCR	C24-C23-C22	-2.85	121.94	126.23
24	B	609	CLA	CHD-C4C-NC	2.84	128.69	124.20
35	B	625	HTG	O5-C1-C2	2.84	113.89	110.31
25	a	405	PHO	C1C-C2C-C3C	-2.84	103.24	106.51
24	D	402	CLA	C4C-C3C-C2C	-2.84	102.75	106.90
24	a	407	CLA	O2A-CGA-CBA	2.84	120.83	111.91
24	b	609	CLA	CHC-C1C-C2C	-2.84	118.86	126.72
24	B	607	CLA	C1D-CHD-C4C	-2.84	118.81	122.56
24	B	611	CLA	CHC-C1C-C2C	-2.84	118.87	126.72
24	C	509	CLA	C2A-C1A-CHA	-2.84	118.90	123.86
24	C	509	CLA	CAC-C3C-C4C	2.83	128.49	124.81
24	C	514	CLA	C2A-C1A-CHA	-2.83	118.90	123.86
31	D	405	PL9	C32-C33-C34	-2.83	120.84	127.66
31	a	414[A]	PL9	C35-C34-C36	2.83	120.04	115.27
26	t	102	BCR	C1-C6-C7	2.83	123.79	115.78
24	b	606	CLA	CHC-C1C-C2C	-2.83	118.89	126.72
24	c	506	CLA	CHC-C1C-C2C	-2.83	118.89	126.72
24	c	513	CLA	O2A-CGA-CBA	2.83	120.78	111.91
31	A	416[B]	PL9	C25-C24-C26	2.83	120.03	115.27
38	d	408	LHG	O8-C23-C24	2.83	120.78	111.91
24	B	606	CLA	C3B-C4B-NB	2.83	112.86	109.21
24	a	350	CLA	CHC-C1C-C2C	-2.83	118.91	126.72
24	c	504	CLA	CHC-C1C-C2C	-2.83	118.91	126.72
24	C	505	CLA	CBC-CAC-C3C	-2.82	104.65	112.43
24	B	604	CLA	CHD-C4C-NC	2.82	128.65	124.20
24	B	613	CLA	C4C-C3C-C2C	-2.82	102.78	106.90
24	C	502	CLA	C3B-C4B-NB	2.82	112.86	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	514	CLA	CHC-C1C-C2C	-2.82	118.91	126.72
24	A	409	CLA	CHC-C1C-C2C	-2.82	118.92	126.72
26	k	101	BCR	C10-C11-C12	-2.82	114.41	123.22
24	D	403	CLA	C4-C3-C5	2.82	120.02	115.27
24	c	509	CLA	CHC-C1C-C2C	-2.82	118.92	126.72
24	B	614	CLA	CBC-CAC-C3C	-2.82	104.66	112.43
26	c	516	BCR	C37-C22-C21	-2.82	118.97	122.92
24	a	403	CLA	C2A-C1A-CHA	-2.82	118.93	123.86
24	c	505	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
24	c	514	CLA	O2A-CGA-CBA	2.82	120.75	111.91
24	c	504	CLA	CMC-C2C-C1C	2.82	129.33	125.04
24	B	615	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
24	b	604	CLA	CMC-C2C-C1C	2.82	129.33	125.04
24	b	601	CLA	CHC-C1C-C2C	-2.81	118.94	126.72
24	C	510	CLA	O2A-CGA-CBA	2.81	120.74	111.91
24	a	407	CLA	C1-C2-C3	-2.81	121.18	126.04
24	c	511	CLA	C4-C3-C5	2.81	120.00	115.27
24	C	507	CLA	O2A-CGA-CBA	2.81	120.73	111.91
39	E	103	HEM	CBA-CAA-C2A	-2.81	107.30	112.49
24	B	603	CLA	CHC-C1C-C2C	-2.81	118.94	126.72
24	C	513	CLA	C3B-C4B-NB	2.81	112.84	109.21
24	C	502	CLA	C1-C2-C3	-2.81	121.18	126.04
24	C	509	CLA	CHC-C1C-C2C	-2.81	118.95	126.72
31	a	414[A]	PL9	C25-C24-C26	2.81	120.00	115.27
26	c	516	BCR	C28-C27-C26	-2.81	109.06	114.08
31	D	405	PL9	C12-C13-C14	-2.81	120.90	127.66
24	a	403	CLA	C4-C3-C5	2.81	119.99	115.27
26	B	617	BCR	C15-C14-C13	-2.81	123.30	127.31
24	C	507	CLA	O2A-CGA-O1A	-2.81	116.51	123.59
26	b	618	BCR	C29-C30-C25	2.81	114.80	110.48
24	b	608	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
24	C	508	CLA	CHC-C1C-C2C	-2.81	118.96	126.72
24	d	403	CLA	CAA-C2A-C3A	-2.80	105.10	112.78
24	B	614	CLA	O2A-CGA-CBA	2.80	120.70	111.91
36	C	517	DGD	C2G-O2G-C1B	-2.80	110.89	117.79
24	C	512	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
31	A	416[A]	PL9	C30-C29-C31	2.80	119.98	115.27
35	V	204	HTG	C1-O5-C5	2.80	115.99	112.19
24	c	510	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
24	a	404	CLA	C4D-C3D-CAD	-2.80	106.91	108.47
24	C	506	CLA	CAC-C3C-C4C	2.80	128.44	124.81
24	C	503	CLA	O2A-CGA-CBA	2.80	120.69	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	413	SQD	O8-S-C6	2.80	110.20	105.74
25	A	407	PHO	C3C-C4C-NC	2.80	114.62	110.28
24	B	601	CLA	C1-C2-C3	-2.80	121.20	126.04
33	c	522	LMG	O8-C28-C29	2.80	120.68	111.91
24	A	405	CLA	C4-C3-C5	2.79	119.97	115.27
24	C	507	CLA	CAA-C2A-C3A	-2.79	105.13	112.78
24	A	406	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
24	b	610	CLA	CMC-C2C-C1C	2.79	129.29	125.04
24	B	613	CLA	O2A-CGA-CBA	2.79	120.67	111.91
24	b	607	CLA	CAC-C3C-C4C	2.79	128.43	124.81
24	B	603	CLA	CMB-C2B-C3B	2.79	129.90	124.68
24	B	610	CLA	CHC-C1C-C2C	-2.79	119.01	126.72
24	D	403	CLA	CAA-C2A-C3A	-2.79	105.15	112.78
24	c	508	CLA	C4D-C3D-CAD	-2.79	106.92	108.47
26	B	618	BCR	C28-C27-C26	-2.79	109.10	114.08
24	c	510	CLA	C4-C3-C5	2.79	119.96	115.27
24	c	506	CLA	C2A-C1A-CHA	-2.78	118.99	123.86
24	c	505	CLA	CHC-C1C-C2C	-2.78	119.02	126.72
25	A	407	PHO	CHD-C1D-C2D	-2.78	118.73	125.73
24	A	406	CLA	C3B-C4B-NB	2.78	112.81	109.21
26	c	516	BCR	C38-C26-C25	-2.78	121.40	124.53
24	b	612	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
24	C	505	CLA	C4-C3-C5	2.78	119.94	115.27
24	c	512	CLA	CMC-C2C-C1C	2.77	129.26	125.04
24	c	514	CLA	CMA-C3A-C4A	-2.77	104.32	111.77
24	b	614	CLA	C2A-C1A-CHA	-2.77	119.01	123.86
26	B	618	BCR	C37-C22-C23	2.77	122.45	118.08
26	h	102	BCR	C37-C22-C21	-2.77	119.04	122.92
24	a	350	CLA	C2A-C1A-CHA	-2.77	119.02	123.86
24	B	610	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
31	A	416[B]	PL9	C12-C13-C14	-2.77	121.00	127.66
24	b	614	CLA	CHC-C1C-C2C	-2.77	119.07	126.72
24	b	610	CLA	CAA-C2A-C3A	-2.77	105.20	112.78
24	b	606	CLA	OBD-CAD-C3D	-2.76	123.40	127.98
24	C	511	CLA	CBC-CAC-C3C	-2.76	104.82	112.43
24	C	506	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
27	B	620	SQD	C3-C4-C5	2.76	115.15	110.24
24	c	513	CLA	CHC-C1C-C2C	-2.76	119.10	126.72
26	C	516	BCR	C15-C14-C13	-2.75	123.38	127.31
26	a	408	BCR	C38-C26-C25	-2.75	121.44	124.53
24	B	609	CLA	CHC-C1C-C2C	-2.75	119.11	126.72
31	a	414[A]	PL9	C40-C39-C41	2.75	119.90	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	510	CLA	O2A-CGA-O1A	-2.75	116.65	123.59
26	b	618	BCR	C28-C27-C26	-2.75	109.17	114.08
24	b	605	CLA	CED-O2D-CGD	2.75	122.16	115.94
24	B	612	CLA	C2A-C1A-CHA	-2.75	119.05	123.86
24	b	613	CLA	O2A-CGA-O1A	-2.75	116.65	123.59
26	t	102	BCR	C7-C6-C5	-2.75	114.80	121.46
24	b	614	CLA	O2A-CGA-CBA	2.75	120.54	111.91
24	c	504	CLA	C4D-C3D-CAD	-2.75	106.94	108.47
27	b	620	SQD	C3-C4-C5	2.75	115.14	110.24
24	D	402	CLA	CAC-C3C-C4C	2.75	128.38	124.81
24	c	511	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
26	a	408	BCR	C37-C22-C21	-2.75	119.08	122.92
24	a	407	CLA	CHC-C1C-C2C	-2.75	119.13	126.72
24	A	409	CLA	CHD-C4C-NC	2.75	128.53	124.20
36	c	520	DGD	O1G-C1A-C2A	2.75	120.52	111.91
38	d	408	LHG	O8-C23-O10	-2.75	116.66	123.59
24	C	511	CLA	C4C-C3C-C2C	-2.75	102.90	106.90
24	C	512	CLA	CHC-C1C-C2C	-2.74	119.13	126.72
24	b	602	CLA	CMC-C2C-C1C	2.74	129.22	125.04
24	D	403	CLA	CBC-CAC-C3C	-2.74	104.86	112.43
24	B	611	CLA	CBC-CAC-C3C	-2.74	104.87	112.43
24	D	402	CLA	C4-C3-C5	2.74	119.88	115.27
24	C	514	CLA	C4-C3-C5	2.74	119.88	115.27
31	A	416[A]	PL9	C25-C24-C26	2.74	119.88	115.27
26	y	101	BCR	C37-C22-C23	2.74	122.39	118.08
24	B	606	CLA	CBC-CAC-C3C	-2.74	104.89	112.43
26	C	515	BCR	C16-C17-C18	-2.74	123.41	127.31
25	A	407	PHO	C4D-ND-C1D	-2.73	101.85	106.76
27	F	101	SQD	C3-C4-C5	2.73	115.11	110.24
24	b	608	CLA	CHC-C1C-C2C	-2.73	119.17	126.72
24	b	615	CLA	CAC-C3C-C4C	2.73	128.35	124.81
24	B	612	CLA	CHC-C1C-C2C	-2.73	119.18	126.72
25	A	408	PHO	C6-C5-C3	-2.73	106.31	113.45
24	D	402	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
24	d	403	CLA	C1-O2A-CGA	2.72	123.59	116.44
33	j	101	LMG	O8-C28-O10	-2.72	116.72	123.59
24	b	616	CLA	C4D-C3D-CAD	-2.72	106.95	108.47
24	b	603	CLA	C4-C3-C5	2.72	119.85	115.27
24	B	608	CLA	O2A-CGA-CBA	2.72	120.45	111.91
24	C	507	CLA	OBD-CAD-C3D	-2.72	123.46	127.98
24	B	609	CLA	C4D-C3D-CAD	-2.72	106.95	108.47
25	a	405	PHO	C4D-CHA-C1A	-2.72	119.25	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	405	PHO	C2A-C1A-NA	2.72	114.98	111.86
24	C	511	CLA	CHC-C1C-C2C	-2.72	119.20	126.72
33	b	621	LMG	C8-O7-C10	-2.72	111.11	117.79
26	k	101	BCR	C11-C10-C9	-2.71	123.44	127.31
24	c	515	CLA	C2A-C1A-CHA	-2.71	119.11	123.86
24	C	505	CLA	OBD-CAD-C3D	-2.71	123.48	127.98
24	B	610	CLA	O2A-CGA-O1A	-2.71	116.75	123.59
24	d	403	CLA	C2A-C1A-CHA	-2.71	119.12	123.86
24	c	508	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
24	D	402	CLA	O2A-CGA-O1A	-2.71	116.77	123.59
24	c	508	CLA	CBC-CAC-C3C	-2.70	104.98	112.43
26	b	619	BCR	C37-C22-C23	2.70	122.33	118.08
24	b	601	CLA	CBC-CAC-C3C	-2.70	104.99	112.43
26	Y	101	BCR	C38-C26-C25	-2.70	121.50	124.53
24	B	613	CLA	CHC-C1C-C2C	-2.70	119.25	126.72
41	V	203	HEC	CBA-CAA-C2A	-2.70	107.50	112.48
24	b	603	CLA	C2A-C1A-CHA	-2.70	119.14	123.86
24	B	607	CLA	C1-C2-C3	-2.70	121.38	126.04
24	b	616	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
24	b	610	CLA	CHC-C1C-C2C	-2.70	119.26	126.72
24	b	603	CLA	CHC-C1C-C2C	-2.70	119.26	126.72
26	D	404	BCR	C33-C5-C6	-2.70	121.50	124.53
26	t	102	BCR	C35-C13-C12	2.69	122.32	118.08
24	C	512	CLA	CMB-C2B-C3B	2.69	129.72	124.68
24	A	409	CLA	CMA-C3A-C2A	-2.69	102.97	113.83
26	A	410	BCR	C8-C7-C6	-2.69	119.64	127.20
24	b	613	CLA	C4D-C3D-CAD	-2.69	106.97	108.47
33	z	101	LMG	C8-O7-C10	-2.69	111.17	117.79
24	b	605	CLA	C1-C2-C3	-2.69	121.39	126.04
24	c	515	CLA	CHC-C1C-C2C	-2.69	119.28	126.72
24	C	505	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
36	H	102	DGD	O2G-C1B-C2B	2.69	117.30	111.50
24	c	504	CLA	O2A-CGA-CBA	2.69	120.34	111.91
24	b	608	CLA	OBD-CAD-C3D	-2.69	123.52	127.98
26	d	404	BCR	C40-C30-C25	-2.68	105.94	110.30
26	H	101	BCR	C16-C17-C18	-2.68	123.48	127.31
24	C	513	CLA	CBA-CAA-C2A	-2.68	105.95	113.86
24	B	610	CLA	CAA-CBA-CGA	-2.68	105.42	113.25
31	a	414[B]	PL9	C40-C39-C41	2.68	119.78	115.27
24	C	503	CLA	CHC-C1C-C2C	-2.68	119.31	126.72
24	A	406	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
24	A	405	CLA	CMA-C3A-C2A	-2.68	103.03	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	405	CLA	C1-C2-C3	-2.68	121.41	126.04
27	a	411	SQD	C1-O5-C5	2.68	118.94	113.69
24	B	607	CLA	CHD-C4C-NC	2.68	128.42	124.20
24	B	611	CLA	O2A-CGA-O1A	-2.67	116.84	123.59
26	b	617	BCR	C29-C30-C25	2.67	114.60	110.48
24	A	405	CLA	C4C-C3C-C2C	-2.67	103.00	106.90
24	B	614	CLA	C2A-C1A-CHA	-2.67	119.19	123.86
24	c	511	CLA	CMB-C2B-C3B	2.67	129.67	124.68
33	C	521	LMG	O8-C28-C29	2.67	120.29	111.91
24	b	608	CLA	CMA-C3A-C4A	-2.67	104.60	111.77
24	B	603	CLA	C4C-C3C-C2C	-2.67	103.01	106.90
24	b	603	CLA	CMC-C2C-C1C	2.67	129.10	125.04
33	j	101	LMG	C8-O7-C10	-2.67	111.22	117.79
24	B	613	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
36	C	518	DGD	O1G-C1A-O1A	-2.67	116.86	123.59
27	F	101	SQD	O7-S-C6	2.67	110.11	106.94
24	C	506	CLA	CHD-C4C-NC	2.67	128.40	124.20
24	C	513	CLA	CHC-C1C-C2C	-2.66	119.36	126.72
26	T	101	BCR	C3-C4-C5	-2.66	109.33	114.08
26	T	101	BCR	C35-C13-C12	2.66	122.26	118.08
26	c	517	BCR	C11-C10-C9	-2.65	123.52	127.31
24	b	611	CLA	C2A-C1A-CHA	-2.65	119.22	123.86
24	c	511	CLA	O2A-CGA-CBA	2.65	120.23	111.91
31	D	405	PL9	C25-C24-C26	2.65	119.73	115.27
24	C	510	CLA	CHC-C1C-C2C	-2.65	119.38	126.72
24	D	403	CLA	C2A-C1A-CHA	-2.65	119.22	123.86
24	D	402	CLA	O2A-CGA-CBA	2.65	120.23	111.91
24	B	616	CLA	CHC-C1C-C2C	-2.65	119.39	126.72
33	c	522	LMG	C3-C4-C5	2.65	114.97	110.24
24	c	511	CLA	C1-O2A-CGA	2.65	123.40	116.44
24	A	404	CLA	C2A-C1A-CHA	-2.65	119.23	123.86
25	A	408	PHO	CHC-C1C-C2C	-2.65	119.07	125.73
24	c	507	CLA	C4-C3-C5	2.65	119.72	115.27
31	a	414[B]	PL9	C53-C6-C1	2.65	120.40	114.99
24	B	609	CLA	O2A-CGA-CBA	2.64	120.21	111.91
24	b	616	CLA	CBC-CAC-C3C	-2.64	105.14	112.43
24	C	514	CLA	C4D-C3D-CAD	-2.64	107.00	108.47
24	b	616	CLA	CHC-C1C-C2C	-2.64	119.42	126.72
24	b	604	CLA	CHC-C1C-C2C	-2.64	119.42	126.72
24	b	616	CLA	C4-C3-C5	2.64	119.71	115.27
26	c	517	BCR	C20-C21-C22	-2.64	123.54	127.31
26	B	617	BCR	C29-C30-C25	2.64	114.54	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	b	621	LMG	O8-C28-O10	-2.64	116.93	123.59
27	a	409	SQD	O9-S-C6	2.64	110.07	106.94
26	D	404	BCR	C16-C17-C18	-2.64	123.55	127.31
24	B	613	CLA	CHB-C4A-NA	2.64	128.16	124.51
24	A	409	CLA	C2A-C1A-CHA	-2.64	119.25	123.86
24	c	503	CLA	CHD-C4C-NC	2.64	128.36	124.20
26	C	516	BCR	C15-C16-C17	-2.63	118.08	123.47
24	B	608	CLA	CHB-C4A-NA	2.63	128.16	124.51
24	b	603	CLA	CHD-C4C-NC	2.63	128.35	124.20
24	c	515	CLA	C4-C3-C5	2.63	119.70	115.27
26	B	618	BCR	C7-C8-C9	-2.63	122.26	126.23
26	b	619	BCR	C16-C17-C18	-2.63	123.55	127.31
27	F	101	SQD	C44-O6-C1	-2.63	108.60	113.74
24	C	513	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
24	d	402	CLA	CHC-C1C-C2C	-2.63	119.45	126.72
24	c	508	CLA	CAC-C3C-C4C	2.63	128.22	124.81
24	c	508	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
24	C	512	CLA	CHD-C4C-NC	2.63	128.34	124.20
24	A	405	CLA	C3B-C4B-NB	2.63	112.61	109.21
31	d	405	PL9	C22-C23-C24	-2.63	121.34	127.66
33	Z	101	LMG	C3-C4-C5	2.63	114.92	110.24
24	b	607	CLA	CAA-C2A-C3A	-2.63	105.59	112.78
24	C	509	CLA	C4-C3-C5	2.62	119.68	115.27
26	b	619	BCR	C31-C1-C6	-2.62	106.05	110.30
24	c	512	CLA	O2A-CGA-O1A	-2.62	116.97	123.59
24	b	608	CLA	CMC-C2C-C1C	2.62	129.03	125.04
31	D	405	PL9	C27-C28-C29	-2.62	121.35	127.66
24	c	503	CLA	CBC-CAC-C3C	-2.62	105.21	112.43
24	B	602	CLA	CHD-C4C-NC	2.62	128.33	124.20
24	B	612	CLA	CMC-C2C-C1C	2.62	129.03	125.04
24	c	515	CLA	CMB-C2B-C3B	2.62	129.57	124.68
24	B	616	CLA	C1C-C2C-C3C	-2.62	104.21	106.96
24	B	603	CLA	C7-C6-C5	-2.61	106.26	113.36
24	b	604	CLA	O2A-CGA-O1A	-2.61	117.00	123.59
24	c	505	CLA	CHD-C4C-NC	2.61	128.32	124.20
36	c	518	DGD	O3G-C3G-C2G	-2.61	104.59	110.90
24	B	616	CLA	O2A-CGA-CBA	2.61	120.11	111.91
24	C	513	CLA	O1D-CGD-CBD	-2.61	119.14	124.48
31	A	416[A]	PL9	C53-C6-C1	2.61	120.33	114.99
36	H	102	DGD	O1G-C1A-C2A	2.61	120.10	111.91
24	C	511	CLA	CMC-C2C-C1C	2.61	129.02	125.04
25	a	405	PHO	CMB-C2B-C1B	2.61	129.08	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	506	CLA	C4C-C3C-C2C	-2.61	103.09	106.90
36	C	519	DGD	O2G-C1B-C2B	2.61	117.12	111.50
24	C	510	CLA	CHD-C4C-NC	2.61	128.31	124.20
24	b	611	CLA	O2A-CGA-O1A	-2.61	117.01	123.59
24	d	402	CLA	O2A-CGA-O1A	-2.61	117.01	123.59
24	a	403	CLA	CMC-C2C-C1C	2.61	129.01	125.04
24	c	507	CLA	C3B-C4B-NB	2.61	112.58	109.21
41	v	203	HEC	CMB-C2B-C1B	-2.61	124.46	128.46
24	b	606	CLA	CMC-C2C-C1C	2.60	129.00	125.04
24	A	404	CLA	CHD-C4C-NC	2.60	128.31	124.20
26	B	619	BCR	C3-C4-C5	-2.60	109.43	114.08
36	C	519	DGD	O1G-C1A-C2A	2.60	120.07	111.91
31	D	405	PL9	C17-C18-C19	-2.60	121.40	127.66
24	a	350	CLA	C4C-C3C-C2C	-2.60	103.11	106.90
24	C	502	CLA	CBC-CAC-C3C	-2.60	105.26	112.43
24	c	514	CLA	CBC-CAC-C3C	-2.60	105.27	112.43
26	y	101	BCR	C10-C11-C12	-2.60	115.11	123.22
24	b	615	CLA	CHD-C4C-NC	2.60	128.29	124.20
24	C	502	CLA	C2A-C1A-CHA	-2.60	119.32	123.86
24	C	509	CLA	CMB-C2B-C3B	2.60	129.53	124.68
24	A	404	CLA	CHC-C1C-C2C	-2.60	119.54	126.72
24	c	508	CLA	CHD-C4C-NC	2.59	128.29	124.20
35	B	628	HTG	C1-O5-C5	2.59	117.36	112.58
24	c	512	CLA	CMB-C2B-C3B	2.59	129.53	124.68
24	B	606	CLA	O2A-CGA-CBA	2.59	120.04	111.91
24	b	613	CLA	CHC-C1C-C2C	-2.59	119.56	126.72
24	b	604	CLA	CHD-C4C-NC	2.59	128.28	124.20
24	B	602	CLA	CHC-C1C-C2C	-2.59	119.56	126.72
24	B	605	CLA	CHC-C1C-C2C	-2.59	119.57	126.72
38	D	406	LHG	O8-C23-O10	-2.59	117.06	123.59
24	C	514	CLA	CHC-C1C-C2C	-2.59	119.57	126.72
26	k	101	BCR	C7-C8-C9	-2.58	122.33	126.23
24	b	612	CLA	O2A-CGA-O1A	-2.58	117.07	123.59
33	c	521	LMG	C8-O7-C10	-2.58	111.43	117.79
24	a	407	CLA	OBD-CAD-C3D	-2.58	123.69	127.98
24	b	606	CLA	CAA-C2A-C3A	-2.58	105.71	112.78
24	C	505	CLA	C2A-C1A-CHA	-2.58	119.34	123.86
24	C	505	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
26	B	618	BCR	C24-C23-C22	-2.58	122.33	126.23
27	b	620	SQD	C44-O6-C1	-2.58	108.70	113.74
24	C	507	CLA	C2A-C1A-CHA	-2.58	119.35	123.86
24	C	514	CLA	CHD-C4C-NC	2.58	128.27	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	406	PHO	CHD-C1D-C2D	-2.58	119.25	125.73
24	b	607	CLA	CBC-CAC-C3C	-2.58	105.33	112.43
24	b	611	CLA	O2A-CGA-CBA	2.57	119.99	111.91
31	d	405	PL9	C25-C24-C26	2.57	119.60	115.27
24	c	508	CLA	O2A-CGA-O1A	-2.57	117.10	123.59
26	H	101	BCR	C3-C4-C5	-2.57	109.48	114.08
24	c	503	CLA	O2A-CGA-CBA	2.57	119.97	111.91
24	b	609	CLA	CHD-C4C-NC	2.57	128.25	124.20
27	f	101	SQD	O48-C23-C24	2.57	119.97	111.91
24	c	514	CLA	CHB-C4A-NA	2.57	128.06	124.51
31	D	405	PL9	C10-C9-C11	2.57	119.59	115.27
24	a	407	CLA	C4D-C3D-CAD	-2.57	107.04	108.47
24	b	616	CLA	C1-C2-C3	-2.57	121.61	126.04
26	d	404	BCR	C29-C30-C25	2.57	114.43	110.48
26	c	516	BCR	C33-C5-C6	-2.57	121.65	124.53
24	B	614	CLA	C4C-C3C-C2C	-2.56	103.16	106.90
26	B	618	BCR	C37-C22-C21	-2.56	119.34	122.92
27	b	620	SQD	O8-S-C6	2.56	109.82	105.74
24	C	511	CLA	CMB-C2B-C3B	2.55	129.46	124.68
38	D	406	LHG	O7-C7-C8	2.55	117.01	111.50
24	C	508	CLA	CMC-C2C-C1C	2.55	128.93	125.04
24	A	409	CLA	O2A-CGA-CBA	2.55	119.92	111.91
33	a	417	LMG	C3-C4-C5	2.55	114.79	110.24
24	a	350	CLA	C4D-C3D-CAD	-2.55	107.05	108.47
24	b	602	CLA	C11-C10-C8	-2.55	107.67	115.92
25	a	406	PHO	C4D-ND-C1D	-2.55	102.18	106.76
24	B	601	CLA	C4-C3-C5	2.55	119.56	115.27
26	h	102	BCR	C10-C11-C12	-2.55	115.26	123.22
25	a	405	PHO	CAC-C3C-C4C	2.55	128.00	125.22
33	Z	101	LMG	C4-C3-C2	2.55	115.27	110.82
24	b	616	CLA	CAC-C3C-C4C	2.55	128.12	124.81
24	B	611	CLA	C2A-C1A-CHA	-2.55	119.41	123.86
33	Z	101	LMG	O6-C1-C2	2.55	115.74	110.35
24	c	508	CLA	O2A-CGA-CBA	2.55	119.90	111.91
31	A	416[A]	PL9	C45-C44-C46	2.55	119.55	115.27
26	Y	101	BCR	C37-C22-C23	2.54	122.09	118.08
38	l	101	LHG	O8-C23-O10	-2.54	117.17	123.59
24	b	607	CLA	O2A-CGA-O1A	-2.54	117.18	123.59
35	C	523	HTG	O5-C1-C2	2.54	113.51	110.31
24	C	506	CLA	C1-C2-C3	-2.54	121.65	126.04
24	A	404	CLA	CAA-CBA-CGA	-2.54	105.83	113.25
25	a	405	PHO	CHD-C1D-C2D	-2.54	119.35	125.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	404	BCR	C16-C17-C18	-2.54	123.69	127.31
26	Y	101	BCR	C10-C11-C12	-2.54	115.30	123.22
24	a	403	CLA	C17-C16-C15	-2.54	101.59	113.24
24	c	507	CLA	O2A-CGA-CBA	2.53	119.85	111.91
24	B	606	CLA	OBD-CAD-C3D	-2.53	123.78	127.98
24	b	607	CLA	C2A-C1A-CHA	-2.53	119.44	123.86
35	B	623	HTG	O2-C2-C3	-2.53	104.51	110.35
24	C	508	CLA	CHD-C4C-NC	2.53	128.18	124.20
24	B	607	CLA	CAA-C2A-C3A	-2.53	105.86	112.78
24	C	507	CLA	CMC-C2C-C1C	2.52	128.88	125.04
35	B	623	HTG	C1-O5-C5	2.52	117.23	112.58
26	B	618	BCR	C33-C5-C6	-2.52	121.70	124.53
26	b	618	BCR	C24-C23-C22	-2.52	122.43	126.23
24	d	403	CLA	C3B-C4B-NB	2.52	112.47	109.21
24	A	409	CLA	CMA-C3A-C4A	-2.52	105.00	111.77
31	a	414[B]	PL9	C15-C14-C16	2.52	119.51	115.27
25	a	406	PHO	CAC-C3C-C4C	2.52	127.97	125.22
35	B	623	HTG	O5-C1-C2	2.52	113.48	110.31
24	A	404	CLA	OBD-CAD-C3D	-2.52	123.80	127.98
26	C	515	BCR	C11-C10-C9	-2.52	123.72	127.31
33	j	101	LMG	O8-C28-C29	2.51	119.80	111.91
24	b	610	CLA	CHD-C4C-NC	2.51	128.16	124.20
24	B	613	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
26	d	404	BCR	C21-C20-C19	-2.51	115.38	123.22
24	B	614	CLA	C1-C2-C3	-2.51	121.70	126.04
24	C	502	CLA	CAC-C3C-C4C	2.51	128.07	124.81
26	D	404	BCR	C29-C30-C25	2.51	114.34	110.48
26	B	619	BCR	C7-C8-C9	-2.51	122.44	126.23
24	d	402	CLA	CMB-C2B-C3B	2.51	129.37	124.68
24	B	604	CLA	C4-C3-C5	2.51	119.49	115.27
24	C	511	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
24	c	515	CLA	O2A-CGA-CBA	2.50	119.77	111.91
24	A	409	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
27	F	101	SQD	O48-C23-C24	2.50	119.77	111.91
26	c	517	BCR	C24-C23-C22	-2.50	122.45	126.23
24	b	614	CLA	CHD-C4C-NC	2.50	128.15	124.20
33	Z	101	LMG	C9-C8-C7	-2.50	105.87	111.79
24	C	509	CLA	O2A-CGA-CBA	2.50	119.75	111.91
25	A	408	PHO	C2C-C1C-NC	2.50	113.56	109.79
35	C	522	HTG	C1-O5-C5	2.50	117.19	112.58
25	a	406	PHO	C2A-C1A-NA	2.50	114.73	111.86
24	a	350	CLA	O2A-CGA-CBA	2.50	119.75	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	y	101	BCR	C21-C20-C19	-2.50	115.42	123.22
24	c	507	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
26	C	516	BCR	C3-C4-C5	-2.50	109.62	114.08
24	C	503	CLA	CMC-C2C-C1C	2.50	128.84	125.04
24	a	404	CLA	O2A-CGA-CBA	2.50	119.74	111.91
24	b	602	CLA	C4-C3-C5	2.49	119.47	115.27
26	a	408	BCR	C33-C5-C6	-2.49	121.73	124.53
24	B	604	CLA	CHC-C1C-C2C	-2.49	119.83	126.72
24	B	605	CLA	OBD-CAD-C3D	-2.49	123.85	127.98
24	b	607	CLA	CHD-C4C-NC	2.49	128.12	124.20
26	B	617	BCR	C31-C1-C6	-2.49	106.27	110.30
24	C	502	CLA	O2A-CGA-CBA	2.49	119.71	111.91
24	b	616	CLA	O2A-CGA-O1A	-2.49	117.32	123.59
26	C	516	BCR	C37-C22-C23	2.49	121.99	118.08
27	f	101	SQD	O47-C7-O49	-2.48	117.70	123.70
24	a	403	CLA	O2A-CGA-O1A	-2.48	117.32	123.59
24	C	502	CLA	CMC-C2C-C1C	2.48	128.82	125.04
26	c	516	BCR	C24-C23-C22	-2.48	122.48	126.23
34	M	101	LMT	C1-O1'-C1'	-2.48	109.72	113.84
24	A	405	CLA	OBD-CAD-C3D	-2.48	123.86	127.98
36	h	103	DGD	O2G-C1B-C2B	2.48	116.85	111.50
24	B	602	CLA	CED-O2D-CGD	2.48	121.55	115.94
24	B	601	CLA	CAC-C3C-C4C	2.48	128.03	124.81
31	a	414[A]	PL9	C45-C44-C46	2.48	119.44	115.27
26	b	618	BCR	C16-C17-C18	-2.48	123.77	127.31
27	f	101	SQD	O8-S-C6	2.48	109.69	105.74
24	B	604	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
26	y	101	BCR	C40-C30-C25	-2.48	106.28	110.30
24	A	405	CLA	O2A-CGA-O1A	-2.48	117.34	123.59
24	D	403	CLA	CHC-C1C-C2C	-2.48	119.87	126.72
24	b	605	CLA	CBC-CAC-C3C	-2.48	105.60	112.43
26	H	101	BCR	C2-C1-C6	2.48	114.29	110.48
24	C	507	CLA	C4C-C3C-C2C	-2.47	103.29	106.90
24	d	402	CLA	CAA-C2A-C3A	-2.47	106.00	112.78
36	c	519	DGD	O1G-C1A-C2A	2.47	119.66	111.91
24	c	513	CLA	CBC-CAC-C3C	-2.47	105.62	112.43
27	b	620	SQD	C1-O5-C5	-2.47	108.84	113.69
24	B	601	CLA	CHC-C1C-C2C	-2.47	119.89	126.72
27	f	101	SQD	O5-C1-C2	2.47	115.57	110.35
26	c	517	BCR	C15-C14-C13	-2.47	123.79	127.31
24	c	512	CLA	CAC-C3C-C4C	2.47	128.01	124.81
24	B	605	CLA	C2A-C1A-CHA	-2.47	119.55	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	F	101	SQD	O47-C7-O49	-2.46	117.75	123.70
24	B	611	CLA	CMB-C2B-C3B	2.46	129.29	124.68
24	A	406	CLA	CHC-C1C-C2C	-2.46	119.91	126.72
24	C	512	CLA	O2A-CGA-CBA	2.46	119.64	111.91
24	A	409	CLA	CMB-C2B-C3B	2.46	129.28	124.68
24	B	609	CLA	CMC-C2C-C1C	2.46	128.79	125.04
34	B	630	LMT	C1-O1'-C1'	-2.46	109.76	113.84
31	a	414[A]	PL9	C20-C19-C21	2.46	119.41	115.27
25	A	407	PHO	C4D-CHA-C1A	-2.46	119.84	125.37
38	a	419	LHG	O8-C23-C24	2.46	119.62	111.91
25	A	407	PHO	O1D-CGD-CBD	-2.46	119.45	124.48
24	B	615	CLA	O2A-CGA-CBA	2.46	119.62	111.91
24	B	602	CLA	CMC-C2C-C1C	2.46	128.78	125.04
24	b	606	CLA	O2A-CGA-O1A	-2.46	117.40	123.59
24	C	506	CLA	CHC-C1C-C2C	-2.45	119.93	126.72
35	b	628	HTG	O5-C5-C4	2.45	114.15	109.69
26	y	101	BCR	C35-C13-C12	2.45	121.94	118.08
24	b	615	CLA	O2A-CGA-CBA	2.45	119.60	111.91
31	a	414[A]	PL9	C53-C6-C1	2.45	120.00	114.99
24	A	409	CLA	CBC-CAC-C3C	-2.45	105.67	112.43
31	D	405	PL9	C22-C23-C24	-2.45	121.76	127.66
33	A	418	LMG	O1-C1-C2	2.45	112.13	108.30
24	C	504	CLA	CHD-C4C-NC	2.45	128.07	124.20
26	T	101	BCR	C2-C1-C6	2.45	114.25	110.48
31	A	416[B]	PL9	C47-C48-C49	-2.45	119.38	127.75
25	a	406	PHO	CMB-C2B-C1B	2.45	128.84	125.06
24	c	513	CLA	CMC-C2C-C1C	2.45	128.77	125.04
24	d	402	CLA	C2A-C1A-CHA	-2.45	119.58	123.86
24	C	514	CLA	O2A-CGA-CBA	2.45	119.58	111.91
27	a	411	SQD	O5-C5-C4	2.45	114.14	109.69
24	C	503	CLA	C4-C3-C5	2.44	119.38	115.27
24	c	511	CLA	CBC-CAC-C3C	-2.44	105.69	112.43
24	d	403	CLA	O2A-CGA-CBA	2.44	119.57	111.91
25	a	405	PHO	CBD-CHA-C1A	2.44	132.07	126.40
24	D	402	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
27	A	411	SQD	O48-C23-O10	-2.44	117.43	123.59
26	a	408	BCR	C29-C30-C25	2.44	114.24	110.48
31	a	414[B]	PL9	C30-C29-C31	2.44	119.38	115.27
24	B	608	CLA	CMC-C2C-C1C	2.44	128.75	125.04
24	B	614	CLA	OBD-CAD-C3D	-2.44	123.93	127.98
26	B	619	BCR	C21-C20-C19	-2.44	115.61	123.22
24	c	512	CLA	C4C-C3C-C2C	-2.44	103.34	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	602	CLA	CAC-C3C-C4C	2.44	127.97	124.81
26	C	516	BCR	C16-C17-C18	-2.44	123.83	127.31
24	C	502	CLA	C1-O2A-CGA	2.44	122.83	116.44
38	d	407	LHG	O7-C7-C8	2.44	116.75	111.50
24	D	403	CLA	C1-C2-C3	-2.43	121.84	126.04
24	B	609	CLA	CBC-CAC-C3C	-2.43	105.73	112.43
34	m	102	LMT	C1-O1'-C1'	-2.43	109.81	113.84
36	h	103	DGD	O1G-C1A-O1A	-2.43	117.45	123.59
24	c	506	CLA	CBC-CAC-C3C	-2.43	105.73	112.43
31	d	405	PL9	C17-C18-C19	-2.43	121.81	127.66
24	c	507	CLA	CHD-C4C-NC	2.43	128.03	124.20
31	A	416[B]	PL9	C20-C19-C21	2.43	119.36	115.27
31	d	405	PL9	C36-C37-C38	-2.43	103.89	111.88
24	a	407	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
24	c	510	CLA	C2A-C1A-CHA	-2.43	119.61	123.86
38	L	101	LHG	O8-C23-C24	2.43	119.53	111.91
24	a	403	CLA	CHD-C4C-NC	2.43	128.03	124.20
33	A	418	LMG	O8-C28-C29	2.43	119.52	111.91
38	d	406	LHG	C5-O7-C7	-2.43	111.82	117.79
26	B	619	BCR	C16-C15-C14	-2.43	118.50	123.47
24	B	612	CLA	C11-C12-C13	-2.43	108.08	115.92
24	B	607	CLA	C4C-C3C-C2C	-2.43	103.36	106.90
25	A	408	PHO	C4A-NA-C1A	-2.42	106.18	108.14
27	b	620	SQD	O48-C23-C24	2.42	119.51	111.91
24	B	602	CLA	C2A-C1A-CHA	-2.42	119.62	123.86
24	b	602	CLA	CHC-C1C-C2C	-2.42	120.02	126.72
24	c	509	CLA	CBC-CAC-C3C	-2.42	105.76	112.43
31	A	416[A]	PL9	C40-C39-C41	2.42	119.34	115.27
26	y	101	BCR	C16-C15-C14	-2.42	118.52	123.47
24	a	404	CLA	CMB-C2B-C3B	2.42	129.20	124.68
24	a	407	CLA	CHD-C4C-NC	2.42	128.01	124.20
24	c	515	CLA	CHD-C4C-NC	2.42	128.01	124.20
26	H	101	BCR	C16-C15-C14	-2.42	118.52	123.47
24	b	608	CLA	CMB-C2B-C3B	2.42	129.20	124.68
24	c	503	CLA	CMC-C2C-C1C	2.42	128.72	125.04
31	A	416[B]	PL9	C40-C39-C41	2.41	119.33	115.27
24	c	506	CLA	CMB-C2B-C3B	2.41	129.19	124.68
26	b	617	BCR	C24-C23-C22	-2.41	122.59	126.23
24	b	615	CLA	C11-C12-C13	-2.41	108.13	115.92
24	D	402	CLA	CMC-C2C-C1C	2.41	128.71	125.04
24	C	508	CLA	C6-C7-C8	-2.41	108.13	115.92
24	a	403	CLA	CMA-C3A-C2A	-2.41	104.11	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	511	CLA	CHD-C4C-NC	2.41	128.00	124.20
26	d	404	BCR	C37-C22-C23	2.41	121.87	118.08
27	b	620	SQD	O7-S-C6	2.41	109.80	106.94
26	K	102	BCR	C10-C11-C12	-2.41	115.71	123.22
24	C	504	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
24	C	511	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
25	a	405	PHO	O2A-CGA-CBA	2.40	119.45	111.91
24	B	610	CLA	C1-C2-C3	-2.40	121.89	126.04
26	H	101	BCR	C7-C8-C9	-2.40	122.61	126.23
38	d	407	LHG	O8-C23-O10	-2.40	117.54	123.59
24	B	601	CLA	CMB-C2B-C3B	2.40	129.17	124.68
24	c	506	CLA	C4-C3-C5	2.40	119.31	115.27
25	a	405	PHO	CBA-CAA-C2A	-2.40	106.79	113.86
24	C	508	CLA	C1-C2-C3	-2.40	121.90	126.04
24	C	508	CLA	O2A-CGA-CBA	2.39	119.42	111.91
24	c	506	CLA	O2A-CGA-CBA	2.39	119.42	111.91
24	b	602	CLA	C1-O2A-CGA	2.39	122.72	116.44
24	A	406	CLA	C4-C3-C5	2.39	119.29	115.27
26	Y	101	BCR	C29-C30-C25	2.39	114.16	110.48
24	C	507	CLA	CHD-C4C-NC	2.39	127.97	124.20
24	c	504	CLA	C2A-C1A-CHA	-2.39	119.68	123.86
24	B	615	CLA	C4-C3-C5	2.39	119.29	115.27
24	B	615	CLA	O2A-CGA-O1A	-2.39	117.57	123.59
24	b	615	CLA	CBC-CAC-C3C	-2.39	105.85	112.43
26	b	617	BCR	C15-C16-C17	-2.39	118.59	123.47
26	b	619	BCR	C24-C23-C22	-2.39	122.63	126.23
27	B	620	SQD	O48-C23-O10	-2.38	117.57	123.59
35	b	623	HTG	O5-C5-C4	2.38	114.02	109.69
24	B	616	CLA	CAC-C3C-C4C	2.38	127.90	124.81
24	B	609	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
26	H	101	BCR	C34-C9-C10	-2.38	119.59	122.92
27	f	101	SQD	O5-C5-C4	2.38	114.02	109.69
26	B	617	BCR	C11-C10-C9	-2.38	123.92	127.31
24	A	404	CLA	O2D-CGD-CBD	2.38	115.50	111.27
24	c	508	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
27	f	101	SQD	O7-S-C6	2.38	109.76	106.94
26	c	516	BCR	C34-C9-C10	-2.37	119.60	122.92
24	b	605	CLA	C4D-C3D-CAD	-2.37	107.15	108.47
24	b	612	CLA	CHD-C4C-NC	2.37	127.94	124.20
24	B	605	CLA	O2A-CGA-CBA	2.37	119.36	111.91
31	d	405	PL9	C32-C33-C34	-2.37	121.95	127.66
24	C	514	CLA	CAA-C2A-C3A	-2.37	106.28	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	403	CLA	CMB-C2B-C3B	2.37	129.12	124.68
31	D	405	PL9	C40-C39-C38	-2.37	117.59	123.68
26	T	101	BCR	C1-C6-C7	2.37	122.49	115.78
24	A	405	CLA	CMB-C2B-C3B	2.37	129.12	124.68
27	A	413	SQD	O48-C23-O10	-2.37	117.61	123.59
24	B	605	CLA	C7-C6-C5	-2.37	106.92	113.36
24	c	507	CLA	C1-C2-C3	-2.37	121.94	126.04
24	B	615	CLA	CHC-C1C-C2C	-2.37	120.16	126.72
24	C	509	CLA	CHD-C4C-NC	2.37	127.94	124.20
31	D	405	PL9	C20-C19-C21	2.37	119.26	115.27
31	d	405	PL9	C27-C28-C29	-2.37	121.96	127.66
31	D	405	PL9	C7-C8-C9	-2.37	122.85	126.79
33	a	417	LMG	C8-O7-C10	-2.37	111.96	117.79
24	B	615	CLA	CBC-CAC-C3C	-2.37	105.90	112.43
26	b	617	BCR	C36-C18-C19	2.37	121.81	118.08
26	k	101	BCR	C16-C17-C18	-2.37	123.93	127.31
24	a	407	CLA	CBC-CAC-C3C	-2.37	105.91	112.43
24	b	608	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
24	B	607	CLA	C2A-C1A-CHA	-2.37	119.72	123.86
24	c	514	CLA	CBA-CAA-C2A	-2.37	106.88	113.86
24	b	613	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
24	C	503	CLA	C2A-C1A-CHA	-2.37	119.72	123.86
26	H	101	BCR	C24-C23-C22	-2.36	122.66	126.23
24	c	510	CLA	O2A-CGA-CBA	2.36	119.33	111.91
24	B	606	CLA	C4D-C3D-CAD	-2.36	107.15	108.47
26	K	102	BCR	C15-C14-C13	-2.36	123.94	127.31
24	B	615	CLA	CED-O2D-CGD	2.36	121.28	115.94
24	B	610	CLA	CHB-C4A-NA	2.36	127.78	124.51
24	b	601	CLA	O2A-CGA-CBA	2.36	119.32	111.91
26	A	410	BCR	C20-C21-C22	-2.36	123.94	127.31
34	M	103	LMT	C1'-O5'-C5'	2.36	118.32	113.69
36	C	518	DGD	C3G-O3G-C1D	-2.36	109.13	113.74
38	d	406	LHG	O7-C7-O9	-2.36	118.01	123.70
26	t	102	BCR	C21-C20-C19	-2.36	115.87	123.22
33	C	520	LMG	O6-C5-C6	2.35	112.29	106.44
24	b	601	CLA	C2A-C1A-CHA	-2.35	119.74	123.86
24	C	511	CLA	C2A-C1A-CHA	-2.35	119.74	123.86
24	c	507	CLA	CHC-C1C-C2C	-2.35	120.21	126.72
24	B	606	CLA	C2A-C1A-CHA	-2.35	119.74	123.86
24	c	509	CLA	O1D-CGD-CBD	-2.35	119.67	124.48
24	A	409	CLA	CAC-C3C-C4C	2.35	127.86	124.81
24	B	616	CLA	C4-C3-C5	2.35	119.23	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	C	520	LMG	O8-C28-O10	-2.35	117.66	123.59
26	B	619	BCR	C34-C9-C8	2.35	121.78	118.08
24	A	406	CLA	CBC-CAC-C3C	-2.35	105.95	112.43
26	b	618	BCR	C38-C26-C25	-2.35	121.89	124.53
24	b	606	CLA	C6-C7-C8	-2.35	108.33	115.92
24	b	614	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
24	b	602	CLA	CMA-C3A-C2A	-2.35	104.37	113.83
24	c	511	CLA	CMC-C2C-C1C	2.34	128.61	125.04
26	B	619	BCR	C20-C21-C22	-2.34	123.97	127.31
34	B	622	LMT	C1-O1'-C1'	-2.34	109.96	113.84
24	C	508	CLA	CAC-C3C-C4C	2.34	127.85	124.81
24	B	611	CLA	CAC-C3C-C4C	2.34	127.85	124.81
24	c	504	CLA	CAC-C3C-C4C	2.34	127.84	124.81
26	C	516	BCR	C21-C20-C19	-2.34	115.92	123.22
26	d	404	BCR	C16-C15-C14	-2.34	118.69	123.47
26	b	619	BCR	C21-C20-C19	-2.34	115.92	123.22
26	a	408	BCR	C15-C16-C17	-2.34	118.69	123.47
34	I	101	LMT	O5'-C5'-C4'	2.33	114.67	109.75
24	c	503	CLA	C4-C3-C5	2.33	119.20	115.27
24	A	405	CLA	O2A-CGA-CBA	2.33	119.23	111.91
24	a	407	CLA	CMB-C2B-C3B	2.33	129.04	124.68
26	t	102	BCR	C15-C16-C17	-2.33	118.70	123.47
24	B	612	CLA	O2A-CGA-CBA	2.33	119.22	111.91
24	a	404	CLA	CBC-CAC-C3C	-2.33	106.01	112.43
26	h	102	BCR	C36-C18-C17	-2.33	119.66	122.92
24	C	510	CLA	C4-C3-C5	2.33	119.19	115.27
24	b	604	CLA	C4-C3-C5	2.33	119.19	115.27
36	c	519	DGD	C2G-O2G-C1B	-2.33	112.06	117.79
26	a	408	BCR	C37-C22-C23	2.33	121.74	118.08
24	b	609	CLA	O2A-CGA-CBA	2.33	119.21	111.91
24	b	606	CLA	C4D-C3D-CAD	-2.33	107.17	108.47
24	b	606	CLA	O2A-CGA-CBA	2.33	119.21	111.91
31	d	405	PL9	C35-C34-C36	2.33	119.18	115.27
24	B	601	CLA	C2A-C1A-CHA	-2.32	119.80	123.86
24	d	403	CLA	CBC-CAC-C3C	-2.32	106.02	112.43
24	B	610	CLA	C2A-C1A-CHA	-2.32	119.80	123.86
31	A	416[A]	PL9	C51-C49-C50	2.32	119.73	114.60
24	c	515	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
24	B	603	CLA	OBD-CAD-C3D	-2.32	124.12	127.98
24	B	605	CLA	CMC-C2C-C1C	2.32	128.57	125.04
31	A	416[A]	PL9	C37-C36-C34	-2.32	105.34	112.98
24	B	615	CLA	CAC-C3C-C4C	2.32	127.82	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	505	CLA	CMC-C2C-C1C	2.32	128.57	125.04
24	a	404	CLA	O2A-CGA-O1A	-2.32	117.75	123.59
24	b	609	CLA	C4-C3-C5	2.32	119.17	115.27
24	b	610	CLA	C2A-C1A-CHA	-2.32	119.81	123.86
24	B	612	CLA	CHD-C4C-NC	2.31	127.85	124.20
24	c	510	CLA	CAA-C2A-C3A	-2.31	106.45	112.78
24	b	601	CLA	CMB-C2B-C3B	2.31	129.00	124.68
25	A	408	PHO	C1C-C2C-C3C	-2.31	103.85	106.51
24	a	404	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
24	C	509	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
24	b	601	CLA	CAA-C2A-C3A	-2.31	106.45	112.78
24	b	612	CLA	OBD-CAD-C3D	-2.31	124.15	127.98
24	a	350	CLA	CMA-C3A-C2A	-2.31	104.52	113.83
24	B	616	CLA	C1-O2A-CGA	2.31	122.50	116.44
26	K	102	BCR	C2-C1-C6	2.31	114.03	110.48
38	D	357	LHG	O7-C7-O9	-2.30	118.13	123.70
25	A	407	PHO	CBA-CAA-C2A	-2.30	107.06	113.86
24	b	604	CLA	C2A-C1A-CHA	-2.30	119.83	123.86
26	K	102	BCR	C36-C18-C19	2.30	121.71	118.08
24	B	610	CLA	CMB-C2B-C3B	2.30	128.99	124.68
31	a	414[A]	PL9	C51-C49-C50	2.30	119.69	114.60
24	a	350	CLA	CED-O2D-CGD	2.30	121.14	115.94
33	J	101	LMG	O8-C28-C29	2.30	119.13	111.91
24	C	511	CLA	C4-C3-C2	-2.30	117.78	123.68
24	B	608	CLA	C4-C3-C5	2.30	119.14	115.27
38	D	406	LHG	O8-C23-C24	2.30	119.12	111.91
24	C	509	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
31	a	414[B]	PL9	C12-C13-C14	-2.30	122.13	127.66
35	h	101	HTG	C1-O5-C5	2.30	116.82	112.58
33	z	101	LMG	C7-O1-C1	-2.30	109.25	113.74
24	d	402	CLA	CHB-C4A-NA	2.30	127.69	124.51
24	D	403	CLA	O2A-CGA-CBA	2.30	119.11	111.91
24	b	605	CLA	O2A-CGA-CBA	2.30	119.11	111.91
24	c	503	CLA	CMB-C2B-C3B	2.30	128.97	124.68
24	c	510	CLA	CMC-C2C-C1C	2.29	128.53	125.04
36	C	519	DGD	O3G-C3G-C2G	-2.29	105.36	110.90
24	B	608	CLA	C4D-C3D-CAD	-2.29	107.19	108.47
27	a	409	SQD	O48-C23-O10	-2.29	117.81	123.59
24	A	405	CLA	CHC-C1C-C2C	-2.29	120.38	126.72
24	a	350	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
31	d	405	PL9	C20-C19-C18	-2.29	117.80	123.68
24	b	602	CLA	C3B-C4B-NB	2.29	112.17	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	517	BCR	C15-C16-C17	-2.29	118.79	123.47
24	b	608	CLA	C6-C7-C8	-2.29	108.53	115.92
24	B	613	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
24	b	604	CLA	C6-C7-C8	-2.28	108.54	115.92
24	d	403	CLA	CHC-C1C-C2C	-2.28	120.41	126.72
24	b	602	CLA	C11-C12-C13	-2.28	108.54	115.92
26	d	404	BCR	C38-C26-C27	2.28	118.00	113.62
24	a	404	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
24	c	504	CLA	OBD-CAD-C3D	-2.28	124.19	127.98
24	c	503	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
26	k	101	BCR	C15-C16-C17	-2.28	118.81	123.47
26	b	619	BCR	C16-C15-C14	-2.28	118.81	123.47
24	b	612	CLA	CMC-C2C-C1C	2.28	128.51	125.04
24	d	403	CLA	C4-C3-C5	2.28	119.11	115.27
25	a	406	PHO	CBD-CHA-C1A	2.28	131.69	126.40
24	d	402	CLA	CBC-CAC-C3C	-2.28	106.15	112.43
24	c	512	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
26	Y	101	BCR	C40-C30-C25	-2.28	106.60	110.30
26	D	404	BCR	C30-C25-C24	2.28	122.22	115.78
31	a	414[A]	PL9	C47-C48-C49	-2.28	119.97	127.75
33	j	101	LMG	O7-C10-O9	-2.28	118.20	123.70
24	B	606	CLA	CHC-C1C-C2C	-2.27	120.43	126.72
25	a	406	PHO	C3C-C4C-NC	2.27	113.81	110.28
24	c	509	CLA	C4C-C3C-C2C	-2.27	103.58	106.90
24	b	613	CLA	CAC-C3C-C2C	2.27	131.42	127.53
31	d	405	PL9	C7-C8-C9	-2.27	123.01	126.79
24	B	610	CLA	C6-C7-C8	-2.27	108.57	115.92
24	b	601	CLA	C4D-C3D-CAD	-2.27	107.20	108.47
26	y	101	BCR	C11-C10-C9	-2.27	124.07	127.31
24	a	407	CLA	C2A-C1A-CHA	-2.27	119.89	123.86
25	A	408	PHO	O2A-CGA-O1A	-2.27	117.86	123.59
27	b	620	SQD	C1-C2-C3	-2.27	105.27	110.00
24	C	510	CLA	C16-C15-C13	-2.27	108.58	115.92
31	A	416[A]	PL9	C2-C3-C4	2.27	121.92	118.80
26	h	102	BCR	C20-C21-C22	-2.27	124.07	127.31
24	D	402	CLA	CMA-C3A-C4A	-2.27	105.68	111.77
36	C	518	DGD	C2G-O2G-C1B	-2.27	112.21	117.79
24	B	608	CLA	O2D-CGD-O1D	-2.27	119.41	123.84
24	B	611	CLA	C4-C3-C5	2.26	119.08	115.27
24	d	402	CLA	CHD-C4C-NC	2.26	127.77	124.20
24	B	602	CLA	C11-C12-C13	-2.26	108.60	115.92
26	h	102	BCR	C16-C15-C14	-2.26	118.84	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	513	CLA	CAC-C3C-C4C	2.26	127.74	124.81
24	B	606	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
25	A	407	PHO	CMB-C2B-C1B	2.26	128.54	125.06
26	Y	101	BCR	C36-C18-C17	-2.26	119.76	122.92
31	a	414[B]	PL9	C10-C9-C11	2.26	119.07	115.27
25	a	405	PHO	O1D-CGD-CBD	-2.26	119.87	124.48
36	H	102	DGD	O1G-C1A-O1A	-2.25	117.90	123.59
24	c	514	CLA	CMC-C2C-C1C	2.25	128.47	125.04
24	c	509	CLA	O2A-CGA-CBA	2.25	118.98	111.91
24	c	513	CLA	CAA-CBA-CGA	-2.25	106.67	113.25
24	b	607	CLA	C6-C7-C8	-2.25	108.64	115.92
27	A	411	SQD	O8-S-C6	2.25	109.33	105.74
24	C	510	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
24	B	604	CLA	C6-C7-C8	-2.25	108.64	115.92
25	a	405	PHO	O2A-CGA-O1A	-2.25	117.91	123.59
26	C	515	BCR	C37-C22-C23	2.25	121.62	118.08
27	A	413	SQD	O7-S-C6	2.25	109.61	106.94
24	A	404	CLA	CMA-C3A-C2A	-2.25	104.75	113.83
26	b	618	BCR	C37-C22-C21	-2.25	119.78	122.92
24	D	403	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
26	c	516	BCR	C7-C8-C9	-2.25	122.84	126.23
24	C	505	CLA	CHD-C4C-NC	2.24	127.74	124.20
24	B	611	CLA	O2A-CGA-CBA	2.24	118.95	111.91
24	B	601	CLA	CBC-CAC-C3C	-2.24	106.25	112.43
25	a	406	PHO	CBA-CAA-C2A	-2.24	107.24	113.86
24	b	603	CLA	CAC-C3C-C4C	2.24	127.72	124.81
26	c	516	BCR	C21-C20-C19	-2.24	116.22	123.22
36	c	519	DGD	O1G-C1A-O1A	-2.24	117.94	123.59
24	C	511	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
24	b	614	CLA	C4-C3-C5	2.24	119.04	115.27
26	y	101	BCR	C23-C24-C25	-2.24	120.91	127.20
34	B	622	LMT	O5'-C5'-C4'	2.24	114.47	109.75
38	d	407	LHG	O8-C23-C24	2.24	118.93	111.91
26	Y	101	BCR	C21-C20-C19	-2.24	116.23	123.22
25	A	407	PHO	C1-C2-C3	-2.24	122.17	126.04
26	T	101	BCR	C7-C6-C5	-2.24	116.04	121.46
24	C	512	CLA	C4D-C3D-CAD	-2.23	107.22	108.47
39	e	102	HEM	C3C-C4C-NC	-2.23	106.73	110.94
24	b	615	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
24	b	606	CLA	C2A-C1A-CHA	-2.23	119.95	123.86
24	C	506	CLA	O2A-CGA-CBA	2.23	118.91	111.91
24	a	403	CLA	C4C-C3C-C2C	-2.23	103.64	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	504	CLA	O2A-CGA-CBA	2.23	118.91	111.91
26	h	102	BCR	C35-C13-C12	2.23	121.59	118.08
24	B	609	CLA	OBD-CAD-C3D	-2.23	124.28	127.98
24	b	616	CLA	C2A-C1A-CHA	-2.23	119.96	123.86
26	c	517	BCR	C3-C4-C5	-2.23	110.10	114.08
26	t	102	BCR	C3-C4-C5	-2.23	110.10	114.08
36	H	102	DGD	C2G-O2G-C1B	-2.23	112.31	117.79
26	C	515	BCR	C20-C21-C22	-2.23	124.13	127.31
25	A	407	PHO	C4A-NA-C1A	-2.23	106.34	108.14
26	H	101	BCR	C31-C1-C6	-2.23	106.69	110.30
24	c	514	CLA	CMB-C2B-C3B	2.23	128.84	124.68
25	A	408	PHO	CBD-CHA-C1A	2.23	131.56	126.40
26	B	618	BCR	C3-C4-C5	-2.23	110.10	114.08
24	b	610	CLA	C3B-C4B-NB	2.23	112.09	109.21
35	c	526	HTG	O5-C5-C4	2.23	113.73	109.69
26	B	619	BCR	C39-C30-C25	-2.23	106.69	110.30
24	C	505	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
24	A	406	CLA	C4D-C3D-CAD	-2.22	107.23	108.47
33	Z	101	LMG	C1-O6-C5	2.22	118.05	113.69
33	c	522	LMG	O8-C28-O10	-2.22	117.99	123.59
33	J	101	LMG	O8-C28-O10	-2.22	117.99	123.59
27	A	411	SQD	O47-C7-O49	-2.22	118.33	123.70
24	B	608	CLA	OBD-CAD-C3D	-2.22	124.29	127.98
24	B	604	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
24	d	402	CLA	C4D-C3D-CAD	-2.22	107.23	108.47
24	c	513	CLA	CMB-C2B-C3B	2.22	128.83	124.68
31	d	405	PL9	C40-C39-C38	-2.22	117.99	123.68
24	c	506	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
24	A	405	CLA	C2A-C1A-CHA	-2.22	119.98	123.86
34	M	101	LMT	O1B-C1B-C2B	2.22	113.84	108.10
26	b	617	BCR	C16-C17-C18	-2.21	124.15	127.31
24	c	503	CLA	C2A-C1A-CHA	-2.21	119.99	123.86
24	D	402	CLA	OBD-CAD-C3D	-2.21	124.31	127.98
31	a	414[B]	PL9	C25-C24-C26	2.21	118.99	115.27
26	B	618	BCR	C38-C26-C25	-2.21	122.05	124.53
24	b	602	CLA	C1-C2-C3	-2.21	122.22	126.04
27	A	413	SQD	O6-C44-C45	-2.21	105.57	110.90
35	B	623	HTG	C1'-S1-C1	2.21	104.22	100.09
27	f	101	SQD	C4-C3-C2	-2.21	106.97	110.82
26	D	404	BCR	C3-C4-C5	-2.21	110.14	114.08
26	t	102	BCR	C36-C18-C19	2.20	121.55	118.08
27	B	620	SQD	O47-C7-O49	-2.20	118.38	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	616	CLA	C2A-C1A-CHA	-2.20	120.01	123.86
24	B	608	CLA	C2A-C1A-CHA	-2.20	120.01	123.86
24	C	511	CLA	OBD-CAD-C3D	-2.20	124.32	127.98
24	c	506	CLA	C1-O2A-CGA	2.20	122.22	116.44
24	c	507	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
31	A	416[A]	PL9	C47-C48-C49	-2.20	120.22	127.75
24	C	505	CLA	CMB-C2B-C3B	2.20	128.80	124.68
24	b	602	CLA	O2A-CGA-CBA	2.20	118.81	111.91
26	T	101	BCR	C15-C14-C13	2.20	130.45	127.31
24	B	607	CLA	C1-O2A-CGA	2.20	122.21	116.44
26	B	619	BCR	C10-C11-C12	-2.20	116.36	123.22
24	C	508	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
26	A	410	BCR	C31-C1-C6	-2.20	106.74	110.30
25	A	407	PHO	O2A-CGA-CBA	2.20	118.80	111.91
24	B	601	CLA	OBD-CAD-C3D	-2.20	124.33	127.98
27	A	411	SQD	O9-S-O7	-2.20	106.35	113.95
24	c	512	CLA	CMA-C3A-C4A	-2.19	105.87	111.77
26	Y	101	BCR	C34-C9-C8	2.19	121.53	118.08
31	a	414[B]	PL9	C47-C48-C49	-2.19	120.25	127.75
24	B	607	CLA	CMB-C2B-C1B	2.19	131.84	128.46
24	B	609	CLA	C1-C2-C3	-2.19	122.25	126.04
26	K	102	BCR	C38-C26-C25	-2.19	122.07	124.53
27	a	409	SQD	C44-O6-C1	-2.19	109.46	113.74
27	a	409	SQD	O4-C4-C3	-2.19	105.28	110.35
24	B	613	CLA	CMA-C3A-C4A	-2.19	105.88	111.77
26	B	618	BCR	C10-C11-C12	-2.19	116.38	123.22
24	c	508	CLA	CHB-C4A-NA	2.19	127.54	124.51
26	K	102	BCR	C16-C17-C18	-2.19	124.18	127.31
24	C	513	CLA	CMB-C2B-C3B	2.19	128.78	124.68
24	B	613	CLA	CHD-C4C-NC	2.19	127.66	124.20
27	A	411	SQD	C45-O47-C7	-2.19	112.40	117.79
26	D	404	BCR	C40-C30-C25	-2.19	106.75	110.30
24	D	403	CLA	CMA-C3A-C2A	-2.19	105.00	113.83
24	B	603	CLA	C16-C15-C13	-2.19	108.84	115.92
24	c	511	CLA	C2A-C1A-CHA	-2.19	120.03	123.86
26	B	619	BCR	C11-C10-C9	-2.19	124.19	127.31
24	b	608	CLA	C2A-C1A-CHA	-2.19	120.04	123.86
24	c	504	CLA	C4-C3-C5	2.18	118.95	115.27
24	d	403	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
34	a	359	LMT	O5'-C5'-C4'	2.18	114.36	109.75
24	C	502	CLA	C11-C12-C13	-2.18	108.86	115.92
24	A	405	CLA	C3D-CAD-CBD	2.18	110.48	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	601	CLA	CMC-C2C-C1C	2.18	128.36	125.04
24	b	608	CLA	CBC-CAC-C3C	-2.18	106.42	112.43
24	c	515	CLA	CED-O2D-CGD	2.18	120.87	115.94
26	k	101	BCR	C39-C30-C25	-2.18	106.76	110.30
24	C	506	CLA	OBD-CAD-C3D	-2.18	124.36	127.98
26	B	619	BCR	C2-C3-C4	-2.18	106.50	111.38
25	A	408	PHO	O2A-CGA-CBA	2.18	118.75	111.91
24	C	508	CLA	OBD-CAD-C3D	-2.18	124.36	127.98
24	D	402	CLA	CBC-CAC-C3C	-2.18	106.42	112.43
25	a	406	PHO	C1C-C2C-C3C	-2.18	104.01	106.51
31	a	414[B]	PL9	C51-C49-C50	2.18	119.41	114.60
41	V	203	HEC	C3B-C4B-NB	-2.17	106.84	110.94
26	D	404	BCR	C15-C16-C17	-2.17	119.02	123.47
31	D	405	PL9	C45-C44-C43	-2.17	118.10	123.68
24	a	403	CLA	CAA-CBA-CGA	-2.17	106.90	113.25
26	B	618	BCR	C15-C16-C17	-2.17	119.02	123.47
24	c	508	CLA	CMB-C2B-C3B	2.17	128.74	124.68
24	c	508	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
26	t	102	BCR	C10-C11-C12	-2.17	116.44	123.22
24	c	515	CLA	C4D-C3D-CAD	-2.17	107.26	108.47
24	C	505	CLA	CED-O2D-CGD	2.17	120.84	115.94
26	b	618	BCR	C2-C1-C6	2.17	113.82	110.48
24	b	602	CLA	C4D-C3D-CAD	-2.17	107.26	108.47
33	c	521	LMG	O7-C10-O9	-2.17	118.47	123.70
26	b	618	BCR	C11-C10-C9	-2.17	124.22	127.31
24	c	509	CLA	C1-C2-C3	-2.16	122.30	126.04
24	A	406	CLA	CMA-C3A-C4A	-2.16	105.97	111.77
26	B	618	BCR	C2-C1-C6	2.16	113.81	110.48
24	b	601	CLA	C1-O2A-CGA	2.16	122.11	116.44
24	c	505	CLA	O2A-CGA-CBA	2.16	118.68	111.91
24	B	611	CLA	C4D-C3D-CAD	-2.16	107.27	108.47
26	t	102	BCR	C23-C22-C21	-2.16	115.63	118.94
25	a	406	PHO	O2A-CGA-CBA	2.16	118.67	111.91
38	E	101	LHG	O8-C23-O10	-2.16	118.15	123.59
25	a	405	PHO	C3A-C4A-CHB	-2.15	118.11	121.83
24	c	514	CLA	CAA-C2A-C3A	-2.15	106.88	112.78
24	D	403	CLA	CMA-C3A-C4A	-2.15	105.99	111.77
24	b	613	CLA	C2A-C1A-CHA	-2.15	120.10	123.86
24	B	610	CLA	CMA-C3A-C2A	-2.15	105.15	113.83
36	C	517	DGD	O1G-C1A-O1A	-2.15	118.16	123.59
24	C	506	CLA	C11-C10-C8	-2.15	108.97	115.92
24	C	507	CLA	CMB-C2B-C3B	2.15	128.70	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	406	CLA	CAC-C3C-C4C	2.15	127.60	124.81
31	D	405	PL9	C42-C41-C39	-2.15	105.91	112.98
24	B	602	CLA	O2A-CGA-CBA	2.15	118.64	111.91
24	D	402	CLA	CMB-C2B-C3B	2.15	128.69	124.68
24	b	613	CLA	CMC-C2C-C1C	2.15	128.31	125.04
26	Y	101	BCR	C16-C15-C14	-2.14	119.08	123.47
24	b	608	CLA	C11-C10-C8	-2.14	108.99	115.92
24	c	505	CLA	C4D-C3D-CAD	-2.14	107.28	108.47
24	B	602	CLA	C3B-C4B-NB	2.14	111.98	109.21
24	b	609	CLA	CMA-C3A-C4A	-2.14	106.02	111.77
31	d	405	PL9	C31-C29-C28	-2.14	116.78	121.12
38	d	408	LHG	C6-C5-C4	-2.14	106.72	111.79
36	C	518	DGD	O6E-C5E-C6E	2.14	111.76	106.44
31	A	416[B]	PL9	C35-C34-C33	-2.14	118.18	123.68
24	B	608	CLA	CBC-CAC-C3C	-2.14	106.53	112.43
26	A	410	BCR	C40-C30-C25	-2.14	106.83	110.30
27	a	411	SQD	O8-S-C6	2.14	109.15	105.74
24	B	602	CLA	CMA-C3A-C4A	-2.14	106.03	111.77
31	A	416[A]	PL9	C12-C13-C14	-2.14	122.51	127.66
26	b	618	BCR	C37-C22-C23	2.14	121.44	118.08
24	a	403	CLA	CBC-CAC-C3C	-2.14	106.54	112.43
34	a	359	LMT	C1B-O5B-C5B	2.14	117.88	113.69
24	d	403	CLA	C11-C10-C8	-2.14	109.01	115.92
35	B	625	HTG	C1-C2-C3	2.13	114.80	110.59
34	e	101	LMT	O5'-C5'-C4'	2.13	114.25	109.75
26	b	617	BCR	C20-C21-C22	-2.13	124.27	127.31
24	c	514	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
24	B	607	CLA	CAC-C3C-C4C	2.13	127.58	124.81
24	B	610	CLA	C4D-C3D-CAD	-2.13	107.28	108.47
26	K	102	BCR	C29-C30-C25	2.13	113.76	110.48
26	a	408	BCR	C10-C11-C12	-2.13	116.57	123.22
24	b	606	CLA	CBC-CAC-C3C	-2.13	106.56	112.43
24	B	602	CLA	OBD-CAD-C3D	-2.13	124.45	127.98
24	c	512	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
24	b	603	CLA	CMB-C2B-C3B	2.13	128.66	124.68
26	t	102	BCR	C12-C13-C14	-2.13	115.68	118.94
24	B	609	CLA	C7-C6-C5	-2.13	107.58	113.36
24	B	605	CLA	CAA-C2A-C3A	-2.12	106.96	112.78
24	c	503	CLA	OBD-CAD-C3D	-2.12	124.45	127.98
24	b	612	CLA	C11-C12-C13	-2.12	109.06	115.92
24	C	503	CLA	OBD-CAD-C3D	-2.12	124.46	127.98
24	B	605	CLA	CAC-C3C-C2C	2.12	131.16	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	409	CLA	C4D-C3D-CAD	-2.12	107.29	108.47
38	E	101	LHG	C5-O7-C7	-2.12	112.57	117.79
27	a	411	SQD	C3-C4-C5	2.12	114.02	110.24
24	b	606	CLA	C1-C2-C3	-2.12	122.38	126.04
41	v	203	HEC	CMB-C2B-C3B	2.12	128.31	125.82
24	D	402	CLA	CAA-C2A-C3A	-2.12	106.97	112.78
33	B	621	LMG	O8-C28-O10	-2.12	118.25	123.59
26	c	517	BCR	C37-C22-C21	-2.12	119.96	122.92
24	D	402	CLA	CHD-C4C-NC	2.12	127.54	124.20
24	a	403	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
31	A	416[B]	PL9	C35-C34-C36	2.11	118.83	115.27
24	B	602	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
24	c	506	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
24	B	612	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
25	a	406	PHO	C4A-NA-C1A	-2.11	106.43	108.14
24	b	602	CLA	CMB-C2B-C3B	2.11	128.63	124.68
41	V	203	HEC	C1D-C2D-C3D	-2.11	105.53	107.00
24	c	506	CLA	CHB-C4A-NA	2.11	127.43	124.51
24	C	502	CLA	OBD-CAD-C3D	-2.11	124.48	127.98
24	c	511	CLA	OBD-CAD-C3D	-2.11	124.48	127.98
24	A	409	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
24	c	511	CLA	CAA-C2A-C3A	-2.11	107.01	112.78
25	a	406	PHO	C3A-C4A-CHB	-2.11	118.19	121.83
24	C	508	CLA	C1-O2A-CGA	2.10	121.97	116.44
24	a	404	CLA	CMC-C2C-C1C	2.10	128.24	125.04
26	b	618	BCR	C39-C30-C25	-2.10	106.89	110.30
35	C	523	HTG	C3-C4-C5	2.10	113.99	110.24
24	D	403	CLA	OBD-CAD-C3D	-2.10	124.49	127.98
24	b	616	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
24	b	607	CLA	O2A-CGA-CBA	2.10	118.50	111.91
24	C	513	CLA	CMC-C2C-C1C	2.10	128.24	125.04
24	C	505	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
26	D	404	BCR	C38-C26-C27	2.10	117.65	113.62
26	B	618	BCR	C21-C20-C19	-2.10	116.67	123.22
33	a	417	LMG	C30-C29-C28	-2.10	105.99	113.62
24	b	614	CLA	CMB-C2B-C3B	2.10	128.60	124.68
33	b	621	LMG	O1-C1-C2	-2.10	105.03	108.30
24	b	614	CLA	C4D-C3D-CAD	-2.10	107.30	108.47
24	c	505	CLA	C2A-C1A-CHA	-2.09	120.20	123.86
26	b	617	BCR	C36-C18-C17	-2.09	119.99	122.92
24	A	406	CLA	OBD-CAD-C3D	-2.09	124.51	127.98
24	B	612	CLA	C6-C5-C3	-2.09	107.97	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	513	CLA	CHB-C4A-NA	2.09	127.41	124.51
26	A	410	BCR	C10-C11-C12	-2.09	116.69	123.22
24	C	513	CLA	CBC-CAC-C3C	-2.09	106.67	112.43
26	d	404	BCR	C35-C13-C14	-2.09	120.00	122.92
24	b	615	CLA	C2A-C1A-CHA	-2.09	120.21	123.86
24	B	604	CLA	C11-C12-C13	-2.09	109.17	115.92
36	c	518	DGD	O1G-C1A-C2A	2.09	118.46	111.91
24	B	602	CLA	CMA-C3A-C2A	-2.09	105.41	113.83
24	c	515	CLA	C11-C10-C8	-2.09	109.18	115.92
31	D	405	PL9	C15-C14-C16	2.09	118.78	115.27
27	A	411	SQD	C3-C4-C5	2.08	113.96	110.24
24	B	614	CLA	CHB-C4A-NA	2.08	127.39	124.51
35	B	628	HTG	O5-C5-C4	2.08	113.48	109.69
24	C	507	CLA	CGD-CBD-CAD	-2.08	103.98	110.73
24	b	611	CLA	OBD-CAD-C3D	-2.08	124.52	127.98
33	c	521	LMG	O8-C28-O10	-2.08	118.34	123.59
24	B	616	CLA	CMC-C2C-C1C	2.08	128.21	125.04
24	C	502	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
24	a	404	CLA	CAC-C3C-C4C	2.08	127.51	124.81
24	A	406	CLA	CHB-C4A-NA	2.08	127.39	124.51
26	Y	101	BCR	C36-C18-C19	2.08	121.35	118.08
24	B	606	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
24	D	403	CLA	C4D-C3D-CAD	-2.08	107.31	108.47
24	d	402	CLA	CMA-C3A-C4A	-2.08	106.19	111.77
24	B	606	CLA	CAC-C3C-C4C	2.08	127.51	124.81
26	b	618	BCR	C8-C7-C6	-2.08	121.37	127.20
24	c	508	CLA	CGD-CBD-CAD	-2.08	104.01	110.73
24	c	513	CLA	OBD-CAD-C3D	-2.08	124.53	127.98
26	B	617	BCR	C38-C26-C25	-2.07	122.20	124.53
33	a	417	LMG	O8-C28-C29	2.07	118.41	111.91
24	c	513	CLA	C11-C10-C8	-2.07	109.22	115.92
24	b	611	CLA	CAC-C3C-C4C	2.07	127.50	124.81
26	C	516	BCR	C34-C9-C10	-2.07	120.02	122.92
26	H	101	BCR	C2-C3-C4	-2.07	106.75	111.38
38	L	101	LHG	C6-C5-C4	-2.07	106.89	111.79
24	B	602	CLA	C4-C3-C5	2.07	118.75	115.27
24	B	609	CLA	C2A-C1A-CHA	-2.07	120.24	123.86
33	A	418	LMG	C8-O7-C10	-2.07	112.70	117.79
24	B	616	CLA	CHA-C1A-NA	-2.07	121.66	126.40
26	h	102	BCR	C36-C18-C19	2.07	121.33	118.08
24	C	512	CLA	C2A-C1A-CHA	-2.07	120.25	123.86
24	b	613	CLA	CED-O2D-CGD	2.07	120.61	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	506	CLA	CAA-C2A-C3A	-2.07	107.12	112.78
26	b	618	BCR	C21-C20-C19	-2.06	116.78	123.22
24	B	613	CLA	CED-O2D-CGD	2.06	120.60	115.94
25	A	407	PHO	CMC-C2C-C1C	2.06	128.24	125.06
31	A	416[B]	PL9	C15-C14-C16	2.06	118.74	115.27
26	T	101	BCR	C16-C15-C14	2.06	127.69	123.47
26	B	617	BCR	C21-C20-C19	-2.06	116.79	123.22
24	B	613	CLA	C1B-CHB-C4A	-2.06	126.04	130.12
35	b	625	HTG	C1-O5-C5	2.06	116.38	112.58
24	C	506	CLA	CHA-C1A-NA	-2.06	121.69	126.40
38	E	101	LHG	O7-C7-O9	-2.05	118.74	123.70
24	b	611	CLA	CAA-C2A-C3A	-2.05	107.15	112.78
26	D	404	BCR	C21-C20-C19	-2.05	116.81	123.22
24	B	607	CLA	OBD-CAD-C3D	-2.05	124.57	127.98
26	B	619	BCR	C37-C22-C21	-2.05	120.05	122.92
24	B	601	CLA	CHB-C4A-NA	2.05	127.35	124.51
24	C	514	CLA	CBC-CAC-C3C	-2.05	106.78	112.43
24	A	409	CLA	OBD-CAD-C3D	-2.05	124.58	127.98
34	t	101	LMT	C3'-C4'-C5'	-2.05	106.22	110.93
24	b	604	CLA	O1D-CGD-CBD	-2.05	120.30	124.48
24	C	504	CLA	CMB-C2B-C3B	2.05	128.51	124.68
24	b	606	CLA	CAC-C3C-C4C	2.05	127.47	124.81
24	B	602	CLA	CMB-C2B-C3B	2.05	128.51	124.68
25	a	406	PHO	C4-C3-C2	-2.05	118.43	123.68
24	b	614	CLA	CAA-C2A-C3A	-2.05	107.18	112.78
26	D	404	BCR	C24-C25-C26	-2.05	116.51	121.46
26	b	618	BCR	C33-C5-C6	-2.04	122.23	124.53
24	C	509	CLA	CAA-C2A-C3A	-2.04	107.18	112.78
24	B	615	CLA	C2A-C1A-CHA	-2.04	120.28	123.86
24	b	608	CLA	C11-C12-C13	-2.04	109.31	115.92
24	B	611	CLA	C11-C12-C13	-2.04	109.31	115.92
31	D	405	PL9	C30-C29-C28	-2.04	118.44	123.68
26	B	617	BCR	C37-C22-C23	2.04	121.30	118.08
36	C	519	DGD	O1G-C1A-O1A	-2.04	118.44	123.59
24	a	403	CLA	O2D-CGD-O1D	-2.04	119.84	123.84
24	B	615	CLA	CMB-C2B-C1B	2.04	131.60	128.46
31	a	414[B]	PL9	C25-C24-C23	-2.04	118.44	123.68
24	A	409	CLA	CHB-C4A-NA	2.04	127.33	124.51
24	c	513	CLA	C2A-C1A-CHA	-2.04	120.29	123.86
31	d	405	PL9	C15-C14-C16	2.04	118.70	115.27
24	B	604	CLA	C2A-C1A-CHA	-2.04	120.29	123.86
31	a	414[A]	PL9	C10-C9-C8	-2.04	118.45	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	508	CLA	CBC-CAC-C3C	-2.04	106.81	112.43
24	c	507	CLA	CMB-C2B-C1B	2.04	131.60	128.46
24	B	605	CLA	C1-C2-C3	-2.04	122.52	126.04
26	C	516	BCR	C36-C18-C19	2.04	121.29	118.08
31	d	405	PL9	C47-C48-C49	-2.04	120.79	127.75
24	C	512	CLA	CBC-CAC-C3C	-2.04	106.82	112.43
26	b	617	BCR	C11-C10-C9	-2.04	124.41	127.31
26	D	404	BCR	C37-C22-C21	-2.04	120.07	122.92
24	c	514	CLA	CHA-C1A-NA	-2.04	121.74	126.40
24	C	508	CLA	C16-C15-C13	-2.04	109.34	115.92
24	b	610	CLA	C4-C3-C2	-2.03	118.46	123.68
26	k	101	BCR	C36-C18-C19	2.03	121.28	118.08
33	c	522	LMG	C9-C8-C7	-2.03	106.98	111.79
24	b	615	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
24	b	614	CLA	CBC-CAC-C3C	-2.03	106.83	112.43
24	B	610	CLA	OBD-CAD-C3D	-2.03	124.61	127.98
24	c	510	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
26	h	102	BCR	C24-C23-C22	-2.03	123.17	126.23
26	b	618	BCR	C10-C11-C12	-2.03	116.88	123.22
35	B	623	HTG	C1-C2-C3	2.03	114.60	110.59
24	C	503	CLA	CAC-C3C-C4C	2.03	127.44	124.81
31	a	414[A]	PL9	C12-C13-C14	-2.03	122.78	127.66
38	L	101	LHG	O8-C23-O10	-2.03	118.47	123.59
24	A	406	CLA	CMB-C2B-C1B	2.03	131.58	128.46
26	a	408	BCR	C3-C4-C5	-2.03	110.46	114.08
24	C	509	CLA	CHB-C4A-NA	2.03	127.32	124.51
24	b	601	CLA	OBD-CAD-C3D	-2.03	124.61	127.98
31	D	405	PL9	C25-C24-C23	-2.03	118.48	123.68
26	C	515	BCR	C21-C20-C19	-2.03	116.89	123.22
24	B	605	CLA	C5-C3-C2	-2.03	117.02	121.12
26	c	517	BCR	C37-C22-C23	2.03	121.27	118.08
31	a	414[B]	PL9	C30-C29-C28	-2.03	118.48	123.68
24	a	350	CLA	CAA-CBA-CGA	2.02	119.17	113.25
26	t	102	BCR	C34-C9-C10	-2.02	120.09	122.92
26	B	619	BCR	C15-C14-C13	-2.02	124.43	127.31
24	C	505	CLA	CHB-C4A-NA	2.02	127.31	124.51
24	c	509	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
26	k	101	BCR	C2-C1-C6	2.02	113.59	110.48
26	c	517	BCR	C29-C30-C25	2.02	113.59	110.48
24	c	510	CLA	OBD-CAD-C3D	-2.02	124.63	127.98
24	D	402	CLA	C4D-C3D-CAD	-2.02	107.34	108.47
24	A	404	CLA	CBC-CAC-C3C	-2.02	106.87	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	403	CLA	OBD-CAD-C3D	-2.02	124.63	127.98
24	c	512	CLA	C4-C3-C2	-2.02	118.50	123.68
24	b	609	CLA	C16-C15-C13	-2.02	109.40	115.92
24	C	505	CLA	C1-O2A-CGA	2.02	121.73	116.44
24	B	616	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
24	B	615	CLA	CHB-C4A-NA	2.01	127.30	124.51
24	C	505	CLA	O2A-CGA-CBA	2.01	118.23	111.91
24	C	511	CLA	CAC-C3C-C4C	2.01	127.42	124.81
24	C	502	CLA	CMB-C2B-C3B	2.01	128.44	124.68
24	c	515	CLA	CBC-CAC-C3C	-2.01	106.89	112.43
24	B	605	CLA	C3D-CAD-CBD	2.01	110.25	107.61
26	b	618	BCR	C7-C8-C9	-2.01	123.20	126.23
24	b	608	CLA	CAC-C3C-C4C	2.01	127.42	124.81
24	C	506	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
24	b	609	CLA	C2A-C1A-CHA	-2.01	120.35	123.86
24	C	510	CLA	CBC-CAC-C3C	-2.01	106.90	112.43
24	B	604	CLA	CAC-C3C-C2C	2.00	130.96	127.53
24	b	616	CLA	CMC-C2C-C1C	2.00	128.09	125.04
27	B	620	SQD	C1-C2-C3	-2.00	105.82	110.00
27	a	409	SQD	C3-C4-C5	2.00	113.81	110.24
24	b	607	CLA	CMC-C2C-C1C	2.00	128.09	125.04
31	A	416[B]	PL9	C51-C49-C50	2.00	119.03	114.60
24	b	607	CLA	C1-C2-C3	-2.00	122.58	126.04
24	b	615	CLA	C1-O2A-CGA	2.00	121.69	116.44

All (191) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	C	508	CLA	NC
24	C	508	CLA	ND
24	C	508	CLA	NA
24	b	609	CLA	NC
24	b	609	CLA	ND
24	B	615	CLA	NA
24	B	615	CLA	NC
24	B	615	CLA	ND
24	C	506	CLA	ND
24	D	403	CLA	NC
24	D	403	CLA	ND
24	D	403	CLA	NA
24	B	610	CLA	NC
24	B	610	CLA	ND

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Mol	Chain	Res	Type	Atom
24	B	610	CLA	NA
24	b	601	CLA	NC
24	b	601	CLA	ND
24	b	601	CLA	NA
24	d	402	CLA	ND
24	d	403	CLA	NC
24	d	403	CLA	ND
24	d	403	CLA	NA
24	C	514	CLA	NC
24	C	514	CLA	ND
24	C	514	CLA	NA
24	c	505	CLA	NC
24	c	505	CLA	ND
24	c	505	CLA	NA
24	b	613	CLA	NC
24	b	613	CLA	ND
24	b	613	CLA	NA
24	a	403	CLA	NC
24	a	403	CLA	ND
24	C	503	CLA	NC
24	C	503	CLA	ND
24	C	503	CLA	NA
24	a	404	CLA	NC
24	a	404	CLA	NA
24	c	512	CLA	NC
24	c	512	CLA	ND
24	c	512	CLA	NA
24	a	350	CLA	NC
24	a	350	CLA	ND
24	a	350	CLA	NA
24	B	614	CLA	NC
24	B	614	CLA	ND
24	B	614	CLA	NA
24	C	502	CLA	NC
24	C	502	CLA	ND
24	C	502	CLA	NA
24	C	510	CLA	NC
24	C	510	CLA	ND
24	C	510	CLA	NA
24	c	508	CLA	NC
24	c	508	CLA	ND
24	c	508	CLA	NA

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Mol	Chain	Res	Type	Atom
24	c	506	CLA	NC
24	c	506	CLA	ND
24	c	506	CLA	NA
24	A	405	CLA	NC
24	A	405	CLA	ND
24	A	405	CLA	NA
24	B	603	CLA	NC
24	B	603	CLA	ND
24	b	616	CLA	NA
24	b	616	CLA	NC
24	b	616	CLA	ND
24	b	606	CLA	NC
24	b	606	CLA	ND
24	b	606	CLA	NA
24	B	604	CLA	NC
24	B	604	CLA	ND
24	B	604	CLA	NA
24	A	404	CLA	NC
24	A	404	CLA	ND
24	A	404	CLA	NA
24	B	616	CLA	NA
24	B	616	CLA	NC
24	B	616	CLA	ND
24	a	407	CLA	NC
24	a	407	CLA	ND
24	a	407	CLA	NA
24	A	406	CLA	NC
24	A	406	CLA	ND
24	A	406	CLA	NA
24	c	511	CLA	NC
24	c	511	CLA	ND
24	c	511	CLA	NA
24	C	509	CLA	NC
24	C	509	CLA	ND
24	C	509	CLA	NA
24	b	610	CLA	NC
24	b	610	CLA	ND
24	b	610	CLA	NA
24	D	402	CLA	ND
24	b	602	CLA	NC
24	b	602	CLA	ND
24	b	602	CLA	NA

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Mol	Chain	Res	Type	Atom
24	B	612	CLA	NC
24	B	612	CLA	ND
24	B	612	CLA	NA
24	A	409	CLA	NC
24	A	409	CLA	NA
24	C	505	CLA	NC
24	C	505	CLA	ND
24	C	505	CLA	NA
24	B	605	CLA	NC
24	B	605	CLA	ND
24	B	605	CLA	NA
24	B	602	CLA	NC
24	B	602	CLA	ND
24	b	608	CLA	NC
24	b	608	CLA	NA
24	C	507	CLA	NC
24	C	507	CLA	ND
24	C	507	CLA	NA
24	c	504	CLA	NC
24	c	504	CLA	ND
24	c	504	CLA	NA
24	B	601	CLA	NC
24	B	601	CLA	ND
24	B	601	CLA	NA
24	b	605	CLA	NC
24	b	605	CLA	ND
24	b	605	CLA	NA
24	C	513	CLA	NC
24	C	513	CLA	ND
24	C	513	CLA	NA
24	b	615	CLA	NA
24	b	615	CLA	NC
24	b	615	CLA	ND
24	B	606	CLA	NC
24	B	606	CLA	ND
24	B	606	CLA	NA
24	c	515	CLA	NC
24	c	515	CLA	ND
24	c	515	CLA	NA
24	B	607	CLA	NC
24	B	607	CLA	ND
24	B	607	CLA	NA

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Mol	Chain	Res	Type	Atom
24	c	507	CLA	ND
24	c	513	CLA	NC
24	c	513	CLA	ND
24	c	513	CLA	NA
24	b	612	CLA	NC
24	b	612	CLA	ND
24	b	612	CLA	NA
24	B	611	CLA	NC
24	B	611	CLA	ND
24	B	611	CLA	NA
24	b	603	CLA	NC
24	b	603	CLA	ND
24	c	503	CLA	NC
24	c	503	CLA	ND
24	c	503	CLA	NA
24	c	509	CLA	NC
24	c	509	CLA	ND
24	c	509	CLA	NA
24	C	504	CLA	NC
24	C	504	CLA	NA
24	B	609	CLA	NC
24	B	609	CLA	ND
24	c	510	CLA	NC
24	c	510	CLA	ND
24	c	510	CLA	NA
24	b	604	CLA	NC
24	b	604	CLA	ND
24	b	604	CLA	NA
24	C	511	CLA	NC
24	C	511	CLA	ND
24	C	511	CLA	NA
24	b	607	CLA	NC
24	b	607	CLA	ND
24	b	607	CLA	NA
24	B	608	CLA	NC
24	B	608	CLA	NA
24	c	514	CLA	NC
24	c	514	CLA	ND
24	c	514	CLA	NA
24	C	512	CLA	NC
24	C	512	CLA	ND
24	C	512	CLA	NA

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Mol	Chain	Res	Type	Atom
24	b	611	CLA	NC
24	b	611	CLA	ND
24	b	611	CLA	NA
24	b	614	CLA	NC
24	b	614	CLA	ND
24	b	614	CLA	NA
24	B	613	CLA	NC
24	B	613	CLA	ND
24	B	613	CLA	NA

All (1227) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	f	101	SQD	O6-C44-C45-O47
27	f	101	SQD	O49-C7-O47-C45
27	f	101	SQD	C8-C7-O47-C45
26	D	404	BCR	C21-C22-C23-C24
26	D	404	BCR	C37-C22-C23-C24
38	D	406	LHG	O2-C2-C3-O3
38	D	406	LHG	C3-O3-P-O4
38	D	406	LHG	C4-O6-P-O4
27	b	620	SQD	O49-C7-O47-C45
34	M	103	LMT	C2'-C1'-O1'-C1
34	M	103	LMT	O5'-C1'-O1'-C1
35	b	624	HTG	O5-C1-S1-C1'
34	b	630	LMT	O5'-C1'-O1'-C1
34	b	630	LMT	C2-C1-O1'-C1'
34	a	359	LMT	C2'-C1'-O1'-C1
34	a	359	LMT	O5'-C1'-O1'-C1
31	D	405	PL9	C32-C33-C34-C36
31	D	405	PL9	C38-C39-C41-C42
31	D	405	PL9	C42-C43-C44-C45
28	a	416	GOL	O1-C1-C2-O2
28	a	416	GOL	O1-C1-C2-C3
24	B	614	CLA	CAD-CBD-CGD-O1D
24	B	614	CLA	CAD-CBD-CGD-O2D
24	B	614	CLA	C2-C3-C5-C6
24	B	614	CLA	C4-C3-C5-C6
35	B	624	HTG	C2'-C1'-S1-C1
28	A	412	GOL	O1-C1-C2-C3
38	L	101	LHG	C4-O6-P-O4
39	e	102	HEM	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
31	a	414[A]	PL9	C14-C16-C17-C18
34	B	630	LMT	O5'-C1'-O1'-C1
24	c	506	CLA	C2-C3-C5-C6
24	c	506	CLA	C4-C3-C5-C6
24	B	603	CLA	C2-C3-C5-C6
24	B	603	CLA	C4-C3-C5-C6
38	E	101	LHG	C3-O3-P-O4
38	E	101	LHG	C3-O3-P-O5
38	E	101	LHG	C3-O3-P-O6
38	E	101	LHG	O10-C23-O8-C6
38	E	101	LHG	C24-C23-O8-C6
33	c	522	LMG	C11-C10-O7-C8
31	a	414[B]	PL9	C7-C8-C9-C10
31	a	414[B]	PL9	C7-C8-C9-C11
31	a	414[B]	PL9	C15-C14-C16-C17
31	a	414[B]	PL9	C17-C18-C19-C20
31	a	414[B]	PL9	C22-C23-C24-C25
31	a	414[B]	PL9	C25-C24-C26-C27
31	A	416[B]	PL9	C7-C8-C9-C11
31	A	416[B]	PL9	C15-C14-C16-C17
31	A	416[B]	PL9	C20-C19-C21-C22
31	A	416[B]	PL9	C25-C24-C26-C27
26	T	101	BCR	C13-C14-C15-C16
34	I	101	LMT	O5'-C1'-O1'-C1
34	t	101	LMT	O5'-C1'-O1'-C1
24	c	511	CLA	C2-C1-O2A-CGA
28	C	525	GOL	O1-C1-C2-C3
24	C	509	CLA	CHA-CBD-CGD-O1D
33	Z	101	LMG	O9-C10-O7-C8
33	Z	101	LMG	C11-C10-O7-C8
27	a	411	SQD	O6-C44-C45-O47
27	a	411	SQD	C5-C6-S-O7
27	a	411	SQD	C5-C6-S-O8
27	a	411	SQD	C5-C6-S-O9
28	v	202	GOL	O1-C1-C2-C3
34	a	418	LMT	C2'-C1'-O1'-C1
34	a	418	LMT	O5'-C1'-O1'-C1
24	C	505	CLA	C2-C3-C5-C6
24	C	505	CLA	C4-C3-C5-C6
35	B	625	HTG	O5-C1-S1-C1'
34	A	359	LMT	C2'-C1'-O1'-C1
34	A	359	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
26	d	404	BCR	C7-C8-C9-C10
26	d	404	BCR	C7-C8-C9-C34
26	d	404	BCR	C21-C22-C23-C24
26	d	404	BCR	C37-C22-C23-C24
26	d	404	BCR	C23-C24-C25-C30
33	z	101	LMG	C11-C10-O7-C8
26	Y	101	BCR	C1-C6-C7-C8
26	Y	101	BCR	C5-C6-C7-C8
28	V	202	GOL	O1-C1-C2-O2
28	V	202	GOL	O1-C1-C2-C3
34	E	102	LMT	C2'-C1'-O1'-C1
34	E	102	LMT	O5'-C1'-O1'-C1
27	A	413	SQD	O6-C44-C45-O47
34	b	622	LMT	O5'-C1'-O1'-C1
24	B	601	CLA	CHA-CBD-CGD-O1D
34	e	101	LMT	C2'-C1'-O1'-C1
34	e	101	LMT	O5'-C1'-O1'-C1
27	F	101	SQD	O49-C7-O47-C45
27	F	101	SQD	C8-C7-O47-C45
28	B	626	GOL	O1-C1-C2-C3
38	l	101	LHG	C4-O6-P-O4
38	l	101	LHG	C4-O6-P-O5
27	B	620	SQD	O49-C7-O47-C45
26	y	101	BCR	C1-C6-C7-C8
26	y	101	BCR	C5-C6-C7-C8
26	y	101	BCR	C21-C22-C23-C24
26	y	101	BCR	C37-C22-C23-C24
24	b	603	CLA	C2-C3-C5-C6
24	b	603	CLA	C4-C3-C5-C6
24	c	510	CLA	CHA-CBD-CGD-O1D
24	c	510	CLA	CHA-CBD-CGD-O2D
31	A	416[A]	PL9	C9-C11-C12-C13
31	A	416[A]	PL9	C14-C16-C17-C18
31	A	416[A]	PL9	C20-C19-C21-C22
28	a	410	GOL	O1-C1-C2-C3
28	a	410	GOL	C1-C2-C3-O3
28	B	627	GOL	C1-C2-C3-O3
28	B	627	GOL	O2-C2-C3-O3
38	d	407	LHG	C3-O3-P-O4
38	d	407	LHG	C4-O6-P-O4
38	d	407	LHG	C4-O6-P-O5
26	H	101	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
26	H	101	BCR	C7-C8-C9-C34
38	a	419	LHG	C4-O6-P-O5
24	b	614	CLA	CHA-CBD-CGD-O1D
24	b	614	CLA	CHA-CBD-CGD-O2D
24	b	614	CLA	CAD-CBD-CGD-O1D
24	b	614	CLA	CAD-CBD-CGD-O2D
34	I	101	LMT	C3'-C4'-O1B-C1B
38	a	419	LHG	O10-C23-O8-C6
38	a	419	LHG	C24-C23-O8-C6
24	C	514	CLA	CBD-CGD-O2D-CED
24	c	513	CLA	CBD-CGD-O2D-CED
24	C	502	CLA	CBD-CGD-O2D-CED
33	c	522	LMG	O9-C10-O7-C8
33	A	418	LMG	O9-C10-O7-C8
33	z	101	LMG	O9-C10-O7-C8
24	d	403	CLA	C3-C5-C6-C7
24	c	508	CLA	C3-C5-C6-C7
24	B	604	CLA	C3-C5-C6-C7
24	c	514	CLA	C3-C5-C6-C7
27	b	620	SQD	C8-C7-O47-C45
27	B	620	SQD	C8-C7-O47-C45
31	D	405	PL9	C40-C39-C41-C42
31	a	414[A]	PL9	C25-C24-C26-C27
31	a	414[A]	PL9	C30-C29-C31-C32
31	A	416[A]	PL9	C18-C19-C21-C22
24	b	606	CLA	C2A-CAA-CBA-CGA
24	b	616	CLA	C3-C5-C6-C7
24	A	409	CLA	C3-C5-C6-C7
34	E	102	LMT	O5'-C5'-C6'-O6'
31	A	416[B]	PL9	C27-C28-C29-C30
24	C	504	CLA	CBD-CGD-O2D-CED
31	D	405	PL9	C42-C43-C44-C46
35	c	523	HTG	O5-C5-C6-O6
24	c	503	CLA	CBD-CGD-O2D-CED
38	d	407	LHG	O2-C2-C3-O3
24	B	614	CLA	C3-C5-C6-C7
34	I	101	LMT	O5B-C5B-C6B-O6B
33	A	418	LMG	C11-C10-O7-C8
27	A	411	SQD	C8-C7-O47-C45
35	c	523	HTG	C4-C5-C6-O6
33	C	521	LMG	O6-C5-C6-O5
33	c	522	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
24	B	616	CLA	C3-C5-C6-C7
35	B	625	HTG	O5-C5-C6-O6
33	z	101	LMG	O6-C5-C6-O5
34	E	102	LMT	C4'-C5'-C6'-O6'
24	C	508	CLA	C4-C3-C5-C6
24	d	403	CLA	C4-C3-C5-C6
31	a	414[A]	PL9	C15-C14-C16-C17
24	B	605	CLA	C4-C3-C5-C6
24	b	605	CLA	C4-C3-C5-C6
24	c	509	CLA	C4-C3-C5-C6
31	A	416[A]	PL9	C15-C14-C16-C17
24	b	614	CLA	C4-C3-C5-C6
24	C	508	CLA	C2-C3-C5-C6
24	d	403	CLA	C2-C3-C5-C6
31	a	414[A]	PL9	C13-C14-C16-C17
31	a	414[B]	PL9	C13-C14-C16-C17
31	A	416[B]	PL9	C13-C14-C16-C17
31	A	416[B]	PL9	C18-C19-C21-C22
24	B	605	CLA	C2-C3-C5-C6
24	b	605	CLA	C2-C3-C5-C6
24	c	509	CLA	C2-C3-C5-C6
31	A	416[A]	PL9	C13-C14-C16-C17
24	b	614	CLA	C2-C3-C5-C6
24	B	606	CLA	C2A-CAA-CBA-CGA
34	B	622	LMT	O5B-C5B-C6B-O6B
27	B	620	SQD	O5-C1-O6-C44
33	a	417	LMG	O6-C5-C6-O5
31	D	405	PL9	C47-C48-C49-C51
31	a	414[B]	PL9	C27-C28-C29-C30
24	C	514	CLA	O1D-CGD-O2D-CED
24	a	407	CLA	CBA-CGA-O2A-C1
24	c	511	CLA	CBA-CGA-O2A-C1
33	C	521	LMG	C4-C5-C6-O5
34	B	622	LMT	C4B-C5B-C6B-O6B
24	B	614	CLA	C10-C11-C12-C13
24	B	601	CLA	C5-C6-C7-C8
24	B	601	CLA	C10-C11-C12-C13
24	b	611	CLA	C15-C16-C17-C18
34	b	630	LMT	C2'-C1'-O1'-C1
34	B	630	LMT	C2'-C1'-O1'-C1
34	I	101	LMT	C2'-C1'-O1'-C1
34	t	101	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
34	b	622	LMT	C2'-C1'-O1'-C1
33	b	621	LMG	C30-C31-C32-C33
31	a	414[A]	PL9	C23-C24-C26-C27
31	a	414[A]	PL9	C28-C29-C31-C32
24	C	503	CLA	C14-C13-C15-C16
24	c	508	CLA	C6-C7-C8-C9
24	B	616	CLA	C6-C7-C8-C9
24	b	610	CLA	C11-C12-C13-C14
24	B	605	CLA	C6-C7-C8-C9
24	c	504	CLA	C14-C13-C15-C16
27	A	411	SQD	O49-C7-O47-C45
24	c	511	CLA	O1A-CGA-O2A-C1
24	b	608	CLA	C13-C15-C16-C17
24	b	614	CLA	C3-C5-C6-C7
24	B	601	CLA	CBA-CGA-O2A-C1
24	C	508	CLA	C5-C6-C7-C8
24	B	615	CLA	C8-C10-C11-C12
24	B	614	CLA	C5-C6-C7-C8
24	A	409	CLA	C5-C6-C7-C8
36	C	518	DGD	C1A-C2A-C3A-C4A
24	B	603	CLA	CBD-CGD-O2D-CED
24	b	606	CLA	C10-C11-C12-C13
24	B	601	CLA	C15-C16-C17-C18
24	b	605	CLA	C8-C10-C11-C12
24	C	511	CLA	C5-C6-C7-C8
24	b	614	CLA	C13-C15-C16-C17
24	B	613	CLA	C15-C16-C17-C18
28	v	202	GOL	O1-C1-C2-O2
24	b	616	CLA	C5-C6-C7-C8
24	B	606	CLA	C13-C15-C16-C17
24	C	511	CLA	CBA-CGA-O2A-C1
24	c	513	CLA	O1D-CGD-O2D-CED
33	Z	101	LMG	O6-C5-C6-O5
24	b	601	CLA	C2-C1-O2A-CGA
34	I	101	LMT	O1'-C1-C2-C3
24	A	409	CLA	C6-C7-C8-C10
24	c	504	CLA	C12-C13-C15-C16
24	b	614	CLA	C6-C7-C8-C10
24	a	407	CLA	O1A-CGA-O2A-C1
24	C	502	CLA	C15-C16-C17-C18
24	B	604	CLA	C13-C15-C16-C17
24	b	602	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
24	B	615	CLA	C5-C6-C7-C8
31	a	414[A]	PL9	C9-C11-C12-C13
31	a	414[B]	PL9	C24-C26-C27-C28
31	d	405	PL9	C39-C41-C42-C43
31	A	416[A]	PL9	C44-C46-C47-C48
34	M	103	LMT	O1'-C1-C2-C3
35	b	623	HTG	S1-C1'-C2'-C3'
35	b	623	HTG	O5-C5-C6-O6
34	b	630	LMT	O5'-C5'-C6'-O6'
24	B	614	CLA	C8-C10-C11-C12
24	C	507	CLA	C13-C15-C16-C17
24	c	509	CLA	C8-C10-C11-C12
34	B	622	LMT	C5'-C4'-O1B-C1B
24	C	511	CLA	O1A-CGA-O2A-C1
24	B	602	CLA	C13-C15-C16-C17
38	E	101	LHG	C11-C10-C9-C8
34	b	630	LMT	C4'-C5'-C6'-O6'
34	I	101	LMT	C4B-C5B-C6B-O6B
24	B	601	CLA	O1A-CGA-O2A-C1
27	A	411	SQD	C11-C10-C9-C8
24	c	512	CLA	C10-C11-C12-C13
24	C	507	CLA	C8-C10-C11-C12
38	D	406	LHG	C3-O3-P-O6
38	L	101	LHG	C4-O6-P-O3
38	l	101	LHG	C4-O6-P-O3
38	d	407	LHG	C3-O3-P-O6
38	d	407	LHG	C4-O6-P-O3
38	L	101	LHG	C23-C24-C25-C26
34	B	630	LMT	C4'-C5'-C6'-O6'
33	z	101	LMG	C4-C5-C6-O5
31	D	405	PL9	C37-C38-C39-C40
24	B	616	CLA	C10-C11-C12-C13
38	D	406	LHG	C1-C2-C3-O3
34	M	103	LMT	O5'-C5'-C6'-O6'
38	d	407	LHG	C1-C2-C3-O3
24	B	606	CLA	C10-C11-C12-C13
24	b	610	CLA	C2A-CAA-CBA-CGA
34	B	630	LMT	O5'-C5'-C6'-O6'
34	B	622	LMT	O5'-C5'-C6'-O6'
24	C	513	CLA	C3-C5-C6-C7
24	d	403	CLA	CBA-CGA-O2A-C1
36	c	520	DGD	C8A-C9A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
33	C	520	LMG	C11-C10-O7-C8
35	B	624	HTG	C2'-C3'-C4'-C5'
38	L	101	LHG	C12-C13-C14-C15
38	E	101	LHG	C24-C25-C26-C27
33	J	101	LMG	C19-C20-C21-C22
34	B	622	LMT	C3'-C4'-O1B-C1B
36	H	102	DGD	CBB-CCB-CDB-CEB
36	C	517	DGD	CAA-CBA-CCA-CDA
24	C	502	CLA	O1D-CGD-O2D-CED
24	C	514	CLA	C16-C17-C18-C20
33	C	521	LMG	C16-C17-C18-C19
38	D	357	LHG	C32-C33-C34-C35
33	B	621	LMG	C36-C37-C38-C39
33	C	520	LMG	O9-C10-O7-C8
36	c	519	DGD	C7A-C8A-C9A-CAA
27	b	620	SQD	C14-C15-C16-C17
33	c	522	LMG	C32-C33-C34-C35
38	d	408	LHG	C27-C28-C29-C30
27	a	409	SQD	C11-C12-C13-C14
33	A	418	LMG	C37-C38-C39-C40
27	b	620	SQD	C27-C28-C29-C30
27	A	411	SQD	C9-C10-C11-C12
33	Z	101	LMG	C10-C11-C12-C13
36	C	518	DGD	C2E-C1E-O5D-C6D
33	Z	101	LMG	C2-C1-O1-C7
34	m	102	LMT	C2'-C1'-O1'-C1
34	a	359	LMT	C3-C4-C5-C6
34	B	630	LMT	C5-C6-C7-C8
33	A	418	LMG	C29-C30-C31-C32
24	B	615	CLA	C16-C17-C18-C20
24	B	610	CLA	C16-C17-C18-C19
24	a	407	CLA	C16-C17-C18-C20
24	c	504	CLA	C16-C17-C18-C20
24	b	615	CLA	C16-C17-C18-C19
33	C	521	LMG	C15-C16-C17-C18
33	j	101	LMG	C21-C22-C23-C24
33	A	418	LMG	C18-C19-C20-C21
24	b	616	CLA	C6-C7-C8-C9
24	b	606	CLA	C11-C10-C8-C9
24	C	513	CLA	C6-C7-C8-C9
35	b	623	HTG	C2'-C3'-C4'-C5'
33	C	521	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
38	L	101	LHG	C25-C26-C27-C28
34	M	101	LMT	C3-C4-C5-C6
27	F	101	SQD	C32-C33-C34-C35
24	B	610	CLA	C13-C15-C16-C17
24	d	403	CLA	O1A-CGA-O2A-C1
26	b	619	BCR	C37-C22-C23-C24
26	K	102	BCR	C7-C8-C9-C34
36	h	103	DGD	C9A-CAA-CBA-CCA
36	H	102	DGD	CAB-CBB-CCB-CDB
38	D	357	LHG	O1-C1-C2-C3
28	b	627	GOL	O1-C1-C2-C3
28	B	626	GOL	C1-C2-C3-O3
24	A	405	CLA	C15-C16-C17-C18
33	b	621	LMG	C11-C10-O7-C8
38	D	406	LHG	C13-C14-C15-C16
36	h	103	DGD	C5B-C6B-C7B-C8B
27	a	409	SQD	C13-C14-C15-C16
27	a	411	SQD	C24-C25-C26-C27
38	l	101	LHG	C27-C28-C29-C30
33	b	621	LMG	C38-C39-C40-C41
36	c	519	DGD	C1B-C2B-C3B-C4B
24	C	504	CLA	O1D-CGD-O2D-CED
31	A	416[B]	PL9	C47-C48-C49-C51
36	c	518	DGD	CBB-CCB-CDB-CEB
33	c	521	LMG	C33-C34-C35-C36
35	B	625	HTG	C4-C5-C6-O6
24	c	508	CLA	C10-C11-C12-C13
24	c	515	CLA	C10-C11-C12-C13
31	A	416[B]	PL9	C29-C31-C32-C33
31	d	405	PL9	C34-C36-C37-C38
34	a	359	LMT	C6-C7-C8-C9
33	j	101	LMG	C29-C30-C31-C32
34	a	418	LMT	C6-C7-C8-C9
38	d	407	LHG	C30-C31-C32-C33
38	a	419	LHG	C26-C27-C28-C29
24	c	503	CLA	O1D-CGD-O2D-CED
36	c	519	DGD	CAA-CBA-CCA-CDA
27	A	411	SQD	C15-C16-C17-C18
36	C	517	DGD	C5B-C6B-C7B-C8B
27	A	413	SQD	C26-C27-C28-C29
38	l	101	LHG	C14-C15-C16-C17
24	b	606	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
34	t	101	LMT	C2-C1-O1'-C1'
38	L	101	LHG	C13-C14-C15-C16
36	C	518	DGD	C7B-C8B-C9B-CAB
27	B	620	SQD	C11-C12-C13-C14
27	B	620	SQD	C26-C27-C28-C29
27	B	620	SQD	C31-C32-C33-C34
24	C	514	CLA	C16-C17-C18-C19
35	c	523	HTG	S1-C1'-C2'-C3'
36	H	102	DGD	CBA-CCA-CDA-CEA
36	C	517	DGD	C4B-C5B-C6B-C7B
38	a	419	LHG	C4-C5-C6-O8
27	b	620	SQD	C18-C19-C20-C21
33	Z	101	LMG	C19-C20-C21-C22
36	c	518	DGD	O6D-C5D-C6D-O5D
24	a	407	CLA	C3-C5-C6-C7
36	c	518	DGD	C9A-CAA-CBA-CCA
34	A	359	LMT	O1'-C1-C2-C3
27	F	101	SQD	C30-C31-C32-C33
24	D	403	CLA	C4-C3-C5-C6
31	d	405	PL9	C15-C14-C16-C17
31	A	416[A]	PL9	C12-C11-C9-C10
24	C	511	CLA	C4-C3-C5-C6
31	D	405	PL9	C43-C44-C46-C47
31	A	416[B]	PL9	C23-C24-C26-C27
24	c	507	CLA	C2-C3-C5-C6
24	B	609	CLA	C2-C3-C5-C6
31	A	416[A]	PL9	C12-C11-C9-C8
24	C	511	CLA	C2-C3-C5-C6
28	A	412	GOL	O1-C1-C2-O2
38	D	357	LHG	O1-C1-C2-O2
28	C	525	GOL	O1-C1-C2-O2
28	B	626	GOL	O1-C1-C2-O2
28	a	410	GOL	O1-C1-C2-O2
28	a	410	GOL	O2-C2-C3-O3
34	a	359	LMT	C2-C3-C4-C5
38	L	101	LHG	C14-C15-C16-C17
27	a	409	SQD	C9-C10-C11-C12
27	a	411	SQD	C25-C26-C27-C28
33	C	520	LMG	C30-C31-C32-C33
36	C	517	DGD	C3B-C4B-C5B-C6B
27	F	101	SQD	C24-C25-C26-C27
24	b	611	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
33	b	621	LMG	O9-C10-O7-C8
31	d	405	PL9	C32-C33-C34-C36
36	C	517	DGD	O6D-C5D-C6D-O5D
38	L	101	LHG	C17-C18-C19-C20
33	J	101	LMG	C35-C36-C37-C38
24	c	514	CLA	C10-C11-C12-C13
33	b	621	LMG	C39-C40-C41-C42
27	F	101	SQD	C23-C24-C25-C26
26	D	404	BCR	C23-C24-C25-C26
26	D	404	BCR	C23-C24-C25-C30
26	d	404	BCR	C23-C24-C25-C26
26	b	617	BCR	C1-C6-C7-C8
26	b	617	BCR	C5-C6-C7-C8
38	D	406	LHG	C28-C29-C30-C31
36	h	103	DGD	CAA-CBA-CCA-CDA
33	C	520	LMG	C17-C18-C19-C20
38	d	408	LHG	C24-C23-O8-C6
24	c	514	CLA	CBA-CGA-O2A-C1
24	c	509	CLA	C5-C6-C7-C8
34	I	101	LMT	C1-C2-C3-C4
33	a	417	LMG	C34-C35-C36-C37
27	a	409	SQD	C30-C31-C32-C33
33	b	621	LMG	C35-C36-C37-C38
24	c	504	CLA	C15-C16-C17-C18
31	D	405	PL9	C13-C14-C16-C17
24	C	503	CLA	C12-C13-C15-C16
24	c	506	CLA	C12-C13-C15-C16
24	b	606	CLA	C11-C10-C8-C7
24	c	511	CLA	C12-C13-C15-C16
31	d	405	PL9	C28-C29-C31-C32
24	A	409	CLA	C12-C13-C15-C16
24	c	515	CLA	C3-C5-C6-C7
38	d	408	LHG	O10-C23-O8-C6
24	B	610	CLA	C16-C17-C18-C20
24	C	513	CLA	CBA-CGA-O2A-C1
36	H	102	DGD	CCA-CDA-CEA-CFA
34	B	630	LMT	C3'-C4'-O1B-C1B
34	m	102	LMT	O5'-C5'-C6'-O6'
24	b	601	CLA	C13-C15-C16-C17
38	D	406	LHG	C16-C17-C18-C19
27	a	411	SQD	C10-C11-C12-C13
33	B	621	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
31	a	414[B]	PL9	C37-C38-C39-C40
24	C	510	CLA	C3-C5-C6-C7
27	f	101	SQD	C26-C27-C28-C29
27	b	620	SQD	C12-C13-C14-C15
27	a	409	SQD	C27-C28-C29-C30
24	b	601	CLA	CBA-CGA-O2A-C1
36	c	518	DGD	O6E-C1E-O5D-C6D
36	c	519	DGD	O6E-C1E-O5D-C6D
36	C	518	DGD	O6E-C1E-O5D-C6D
34	m	102	LMT	O5'-C1'-O1'-C1
24	C	509	CLA	C10-C11-C12-C13
27	B	620	SQD	C34-C35-C36-C37
33	a	417	LMG	C11-C10-O7-C8
33	B	621	LMG	C11-C10-O7-C8
34	B	630	LMT	C11-C10-C9-C8
38	d	407	LHG	C16-C17-C18-C19
24	b	613	CLA	CBD-CGD-O2D-CED
24	C	512	CLA	CBD-CGD-O2D-CED
38	D	357	LHG	C25-C26-C27-C28
27	A	411	SQD	C18-C19-C20-C21
33	B	621	LMG	O9-C10-O7-C8
36	c	519	DGD	C2E-C1E-O5D-C6D
33	B	621	LMG	C17-C18-C19-C20
35	B	624	HTG	C1'-C2'-C3'-C4'
33	C	521	LMG	C33-C34-C35-C36
38	l	101	LHG	C34-C35-C36-C37
35	C	523	HTG	O5-C5-C6-O6
24	B	604	CLA	C4-C3-C5-C6
24	c	507	CLA	C4-C3-C5-C6
24	B	609	CLA	C4-C3-C5-C6
31	A	416[A]	PL9	C25-C24-C26-C27
24	D	403	CLA	C2-C3-C5-C6
31	A	416[B]	PL9	C12-C11-C9-C8
31	a	414[A]	PL9	C4-C3-C7-C8
36	C	519	DGD	CCB-CDB-CEB-CFB
35	B	623	HTG	C3'-C4'-C5'-C6'
24	D	403	CLA	C11-C10-C8-C9
24	b	601	CLA	C6-C7-C8-C9
24	a	404	CLA	C11-C12-C13-C14
24	c	506	CLA	C14-C13-C15-C16
24	c	511	CLA	C14-C13-C15-C16
24	A	409	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	b	614	CLA	C6-C7-C8-C9
35	b	628	HTG	O5-C5-C6-O6
27	b	620	SQD	C13-C14-C15-C16
24	c	508	CLA	C15-C16-C17-C18
38	D	407	LHG	C29-C30-C31-C32
33	J	101	LMG	O6-C5-C6-O5
24	B	615	CLA	C16-C17-C18-C19
24	b	615	CLA	C16-C17-C18-C20
27	F	101	SQD	C29-C30-C31-C32
38	d	407	LHG	C13-C14-C15-C16
24	b	606	CLA	C15-C16-C17-C18
38	D	406	LHG	C4-O6-P-O3
36	c	519	DGD	C2B-C3B-C4B-C5B
36	c	518	DGD	C4D-C5D-C6D-O5D
33	C	520	LMG	C37-C38-C39-C40
24	a	407	CLA	C16-C17-C18-C19
24	c	504	CLA	C16-C17-C18-C19
33	B	621	LMG	C33-C34-C35-C36
24	C	503	CLA	C3-C5-C6-C7
24	c	513	CLA	CBA-CGA-O2A-C1
33	a	417	LMG	O9-C10-O7-C8
33	C	521	LMG	C17-C18-C19-C20
34	t	101	LMT	O1'-C1-C2-C3
27	f	101	SQD	C25-C26-C27-C28
24	C	513	CLA	O1A-CGA-O2A-C1
24	c	514	CLA	O1A-CGA-O2A-C1
34	b	630	LMT	C3-C4-C5-C6
34	I	101	LMT	O5'-C5'-C6'-O6'
24	b	601	CLA	C3-C5-C6-C7
36	C	517	DGD	C4D-C5D-C6D-O5D
27	f	101	SQD	O6-C44-C45-C46
27	b	620	SQD	C44-C45-C46-O48
38	E	101	LHG	C4-C5-C6-O8
27	B	620	SQD	C44-C45-C46-O48
24	c	513	CLA	O1A-CGA-O2A-C1
33	a	417	LMG	C4-C5-C6-O5
36	c	519	DGD	C5D-C6D-O5D-C1E
36	C	518	DGD	C5D-C6D-O5D-C1E
34	b	630	LMT	C4-C5-C6-C7
38	D	357	LHG	C16-C17-C18-C19
36	C	518	DGD	CDA-CEA-CFA-CGA
35	b	625	HTG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
36	c	520	DGD	CBA-CCA-CDA-CEA
36	C	518	DGD	CCB-CDB-CEB-CFB
36	C	517	DGD	O6E-C5E-C6E-O5E
36	c	518	DGD	CAA-CBA-CCA-CDA
36	c	518	DGD	C7B-C8B-C9B-CAB
27	b	620	SQD	C24-C25-C26-C27
34	E	102	LMT	O1'-C1-C2-C3
24	b	601	CLA	O1A-CGA-O2A-C1
36	c	518	DGD	O6E-C5E-C6E-O5E
35	B	628	HTG	O5-C5-C6-O6
24	C	506	CLA	C4-C3-C5-C6
31	D	405	PL9	C45-C44-C46-C47
35	b	628	HTG	C4'-C5'-C6'-C7'
31	d	405	PL9	C13-C14-C16-C17
38	D	357	LHG	C23-C24-C25-C26
35	c	526	HTG	O5-C5-C6-O6
35	B	628	HTG	C2'-C3'-C4'-C5'
27	A	411	SQD	C16-C17-C18-C19
33	c	521	LMG	C35-C36-C37-C38
38	d	406	LHG	C25-C26-C27-C28
33	j	101	LMG	O6-C5-C6-O5
38	D	357	LHG	C24-C25-C26-C27
34	M	103	LMT	O5B-C1B-O1B-C4'
36	c	519	DGD	C7B-C8B-C9B-CAB
36	c	518	DGD	C5A-C6A-C7A-C8A
34	e	101	LMT	C4-C5-C6-C7
36	c	518	DGD	C2A-C1A-O1G-C1G
36	C	519	DGD	C2A-C1A-O1G-C1G
24	A	409	CLA	CBA-CGA-O2A-C1
38	l	101	LHG	C12-C13-C14-C15
35	B	628	HTG	C4'-C5'-C6'-C7'
38	a	419	LHG	C11-C12-C13-C14
36	c	518	DGD	C2E-C1E-O5D-C6D
27	A	411	SQD	O6-C44-C45-O47
27	b	620	SQD	C26-C27-C28-C29
31	d	405	PL9	C45-C44-C46-C47
34	M	101	LMT	C4-C5-C6-C7
24	B	615	CLA	C11-C12-C13-C15
24	D	403	CLA	C11-C10-C8-C7
24	b	601	CLA	C6-C7-C8-C10
24	a	404	CLA	C11-C12-C13-C15
24	a	407	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
24	A	406	CLA	C12-C13-C15-C16
24	c	515	CLA	C12-C13-C15-C16
24	b	603	CLA	C11-C10-C8-C7
24	b	601	CLA	CAA-CBA-CGA-O2A
24	C	506	CLA	C14-C13-C15-C16
24	B	616	CLA	C14-C13-C15-C16
24	C	505	CLA	C14-C13-C15-C16
24	B	606	CLA	C11-C10-C8-C9
34	M	101	LMT	C2-C3-C4-C5
25	A	408	PHO	C2C-C3C-CAC-CBC
38	D	357	LHG	C11-C12-C13-C14
36	H	102	DGD	C7B-C8B-C9B-CAB
28	a	416	GOL	C1-C2-C3-O3
24	a	350	CLA	C13-C15-C16-C17
33	J	101	LMG	C36-C37-C38-C39
36	c	520	DGD	C2A-C1A-O1G-C1G
34	e	101	LMT	C2B-C1B-O1B-C4'
36	C	519	DGD	C8B-C9B-CAB-CBB
24	a	350	CLA	C15-C16-C17-C18
33	B	621	LMG	O8-C28-C29-C30
34	B	630	LMT	C3-C4-C5-C6
38	l	101	LHG	O6-C4-C5-C6
31	a	414[B]	PL9	C14-C16-C17-C18
31	A	416[B]	PL9	C9-C11-C12-C13
36	c	518	DGD	C4B-C5B-C6B-C7B
36	c	520	DGD	C2B-C3B-C4B-C5B
34	E	102	LMT	C3-C4-C5-C6
24	c	512	CLA	C4-C3-C5-C6
31	a	414[B]	PL9	C20-C19-C21-C22
24	C	506	CLA	C2-C3-C5-C6
31	D	405	PL9	C28-C29-C31-C32
31	d	405	PL9	C43-C44-C46-C47
34	M	103	LMT	C2B-C1B-O1B-C4'
36	C	519	DGD	O1A-C1A-O1G-C1G
33	j	101	LMG	C38-C39-C40-C41
31	a	414[B]	PL9	C32-C33-C34-C35
24	b	610	CLA	C15-C16-C17-C18
36	H	102	DGD	O2G-C1B-C2B-C3B
38	L	101	LHG	C16-C17-C18-C19
24	A	409	CLA	O1A-CGA-O2A-C1
24	b	609	CLA	C3A-C2A-CAA-CBA
24	B	609	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
33	J	101	LMG	C16-C17-C18-C19
38	l	101	LHG	C13-C14-C15-C16
33	J	101	LMG	C34-C35-C36-C37
38	d	408	LHG	C25-C26-C27-C28
38	d	406	LHG	C24-C25-C26-C27
38	L	101	LHG	C24-C25-C26-C27
25	a	406	PHO	NC-C1C-CHC-C4B
27	a	411	SQD	O6-C44-C45-C46
27	A	411	SQD	O6-C44-C45-C46
27	A	413	SQD	O6-C44-C45-C46
36	H	102	DGD	O1G-C1G-C2G-C3G
35	b	623	HTG	C1'-C2'-C3'-C4'
25	a	405	PHO	O2A-C1-C2-C3
24	B	601	CLA	CAA-CBA-CGA-O2A
33	j	101	LMG	C19-C20-C21-C22
24	b	607	CLA	C3-C5-C6-C7
31	A	416[A]	PL9	C45-C44-C46-C47
31	A	416[A]	PL9	C43-C44-C46-C47
27	A	411	SQD	C12-C13-C14-C15
27	f	101	SQD	C35-C36-C37-C38
33	b	621	LMG	C37-C38-C39-C40
28	B	626	GOL	O2-C2-C3-O3
36	c	518	DGD	CDB-CEB-CFB-CGB
36	c	518	DGD	O1A-C1A-O1G-C1G
36	h	103	DGD	O2G-C1B-C2B-C3B
38	D	406	LHG	C9-C10-C11-C12
34	e	101	LMT	C3-C4-C5-C6
36	c	520	DGD	O1A-C1A-O1G-C1G
27	f	101	SQD	C29-C30-C31-C32
27	f	101	SQD	O47-C45-C46-O48
33	a	417	LMG	O7-C8-C9-O8
33	A	418	LMG	O1-C7-C8-O7
38	d	406	LHG	C33-C34-C35-C36
33	z	101	LMG	O6-C1-O1-C7
24	b	601	CLA	C8-C10-C11-C12
24	b	602	CLA	C13-C15-C16-C17
34	B	622	LMT	C6-C7-C8-C9
33	b	621	LMG	C14-C15-C16-C17
24	B	608	CLA	C2-C1-O2A-CGA
31	a	414[B]	PL9	C47-C48-C49-C51
24	c	512	CLA	C2-C3-C5-C6
38	E	101	LHG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	C	514	CLA	C11-C10-C8-C9
24	C	506	CLA	C10-C11-C12-C13
26	h	102	BCR	C23-C24-C25-C26
26	h	102	BCR	C23-C24-C25-C30
26	y	101	BCR	C23-C24-C25-C26
26	y	101	BCR	C23-C24-C25-C30
38	D	406	LHG	C26-C27-C28-C29
36	c	518	DGD	CAB-CBB-CCB-CDB
33	c	522	LMG	C30-C31-C32-C33
36	C	517	DGD	C8A-C9A-CAA-CBA
24	b	613	CLA	C5-C6-C7-C8
24	A	404	CLA	C13-C15-C16-C17
24	B	612	CLA	C10-C11-C12-C13
36	H	102	DGD	CDB-CEB-CFB-CGB
36	c	519	DGD	C9A-CAA-CBA-CCA
36	C	519	DGD	O6E-C5E-C6E-O5E
35	B	624	HTG	C4-C5-C6-O6
27	f	101	SQD	C31-C32-C33-C34
38	E	101	LHG	C25-C26-C27-C28
33	c	522	LMG	C4-C5-C6-O5
24	B	615	CLA	C12-C13-C15-C16
24	C	506	CLA	C12-C13-C15-C16
24	C	514	CLA	C11-C10-C8-C7
24	B	614	CLA	C12-C13-C15-C16
31	A	416[B]	PL9	C43-C44-C46-C47
24	B	604	CLA	C6-C7-C8-C10
24	B	616	CLA	C12-C13-C15-C16
24	C	505	CLA	C12-C13-C15-C16
24	C	507	CLA	C6-C7-C8-C10
24	b	615	CLA	C12-C13-C15-C16
24	B	606	CLA	C11-C10-C8-C7
33	c	521	LMG	C31-C32-C33-C34
24	B	605	CLA	C13-C15-C16-C17
24	C	511	CLA	C16-C17-C18-C19
36	c	518	DGD	CCB-CDB-CEB-CFB
24	B	603	CLA	O1D-CGD-O2D-CED
24	b	612	CLA	C10-C11-C12-C13
24	c	511	CLA	C3-C5-C6-C7
33	Z	101	LMG	C29-C28-O8-C9
33	a	417	LMG	O8-C28-C29-C30
27	a	411	SQD	C27-C28-C29-C30
33	C	520	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
24	B	605	CLA	C8-C10-C11-C12
24	B	610	CLA	CAD-CBD-CGD-O2D
24	b	616	CLA	CAD-CBD-CGD-O2D
24	b	610	CLA	CAD-CBD-CGD-O2D
24	b	612	CLA	CAD-CBD-CGD-O2D
27	B	620	SQD	C46-C45-O47-C7
24	b	604	CLA	CAD-CBD-CGD-O2D
25	A	408	PHO	CAD-CBD-CGD-O2D
24	c	508	CLA	C13-C15-C16-C17
24	c	514	CLA	C15-C16-C17-C18
34	b	630	LMT	C6-C7-C8-C9
24	b	616	CLA	CBA-CGA-O2A-C1
27	b	620	SQD	O5-C1-O6-C44
24	B	602	CLA	C15-C16-C17-C18
24	C	511	CLA	C8-C10-C11-C12
38	D	406	LHG	C14-C15-C16-C17
27	f	101	SQD	C44-C45-C46-O48
33	a	417	LMG	C7-C8-C9-O8
38	D	407	LHG	C2-C3-O3-P
38	d	408	LHG	C2-C3-O3-P
34	e	101	LMT	O5B-C1B-O1B-C4'
38	l	101	LHG	O6-C4-C5-O7
36	h	103	DGD	CBA-CCA-CDA-CEA
33	C	521	LMG	C38-C39-C40-C41
36	C	519	DGD	CBA-CCA-CDA-CEA
24	C	508	CLA	CHA-CBD-CGD-O1D
24	C	508	CLA	CHA-CBD-CGD-O2D
24	b	601	CLA	CHA-CBD-CGD-O1D
24	b	601	CLA	CHA-CBD-CGD-O2D
24	C	503	CLA	CHA-CBD-CGD-O1D
24	C	503	CLA	CHA-CBD-CGD-O2D
24	B	614	CLA	CHA-CBD-CGD-O1D
24	b	606	CLA	CHA-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O2D
24	B	601	CLA	CHA-CBD-CGD-O2D
24	B	606	CLA	CHA-CBD-CGD-O1D
24	B	607	CLA	CHA-CBD-CGD-O1D
24	b	612	CLA	CHA-CBD-CGD-O1D
33	C	520	LMG	O7-C10-C11-C12
38	l	101	LHG	C16-C17-C18-C19
24	c	512	CLA	CBA-CGA-O2A-C1
38	E	101	LHG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
38	D	357	LHG	C12-C13-C14-C15
24	b	601	CLA	C4-C3-C5-C6
31	a	414[A]	PL9	C12-C11-C9-C10
33	B	621	LMG	C14-C15-C16-C17
24	b	601	CLA	C2-C3-C5-C6
31	A	416[A]	PL9	C4-C3-C7-C8
24	C	508	CLA	C13-C15-C16-C17
24	B	615	CLA	C14-C13-C15-C16
24	d	402	CLA	C11-C12-C13-C14
24	B	614	CLA	C14-C13-C15-C16
24	B	602	CLA	C11-C12-C13-C14
24	c	512	CLA	O1A-CGA-O2A-C1
24	b	616	CLA	O1A-CGA-O2A-C1
33	a	417	LMG	C20-C21-C22-C23
26	c	517	BCR	C7-C8-C9-C34
27	A	413	SQD	C15-C16-C17-C18
26	K	102	BCR	C7-C8-C9-C10
34	b	622	LMT	C3'-C4'-O1B-C1B
27	B	620	SQD	C11-C10-C9-C8
24	C	502	CLA	C1A-C2A-CAA-CBA
36	C	519	DGD	O6D-C5D-C6D-O5D
24	B	616	CLA	C2-C1-O2A-CGA
36	C	519	DGD	CDA-CEA-CFA-CGA
24	C	512	CLA	O1D-CGD-O2D-CED
34	E	102	LMT	C2B-C1B-O1B-C4'
27	B	620	SQD	C30-C31-C32-C33
24	D	403	CLA	C3-C5-C6-C7
38	d	408	LHG	C28-C29-C30-C31
38	D	406	LHG	C4-O6-P-O5
38	L	101	LHG	C4-O6-P-O5
24	C	507	CLA	C16-C17-C18-C20
24	D	403	CLA	C8-C10-C11-C12
27	b	620	SQD	C24-C23-O48-C46
27	a	411	SQD	C24-C23-O48-C46
31	A	416[B]	PL9	C14-C16-C17-C18
33	C	520	LMG	C14-C15-C16-C17
24	B	609	CLA	C13-C15-C16-C17
24	c	510	CLA	C5-C6-C7-C8
34	E	102	LMT	O5B-C1B-O1B-C4'
38	d	408	LHG	C33-C34-C35-C36
24	b	609	CLA	CAD-CBD-CGD-O1D
24	b	601	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	C	503	CLA	CAD-CBD-CGD-O1D
24	B	605	CLA	CAD-CBD-CGD-O1D
24	c	504	CLA	CAD-CBD-CGD-O1D
24	B	601	CLA	CAD-CBD-CGD-O1D
24	b	605	CLA	CAD-CBD-CGD-O1D
24	B	607	CLA	CAD-CBD-CGD-O1D
27	B	620	SQD	C5-C6-S-O7
36	H	102	DGD	C7A-C8A-C9A-CAA
27	a	411	SQD	O10-C23-O48-C46
27	F	101	SQD	C27-C28-C29-C30
24	A	405	CLA	C13-C15-C16-C17
24	B	608	CLA	C13-C15-C16-C17
27	a	411	SQD	C31-C32-C33-C34
38	d	406	LHG	C32-C33-C34-C35
38	a	419	LHG	C24-C25-C26-C27
31	D	405	PL9	C30-C29-C31-C32
24	B	610	CLA	C12-C13-C15-C16
24	d	402	CLA	C11-C12-C13-C15
33	j	101	LMG	C28-C29-C30-C31
24	B	604	CLA	C11-C12-C13-C15
24	B	616	CLA	C6-C7-C8-C10
35	c	523	HTG	C2-C1-S1-C1'
35	B	625	HTG	C2-C1-S1-C1'
35	B	623	HTG	C2'-C3'-C4'-C5'
36	c	520	DGD	C3B-C4B-C5B-C6B
27	B	620	SQD	C7-C8-C9-C10
27	a	411	SQD	C12-C13-C14-C15
33	A	418	LMG	O1-C7-C8-C9
38	E	101	LHG	O7-C5-C6-O8
36	H	102	DGD	O1G-C1G-C2G-O2G
27	B	620	SQD	O47-C45-C46-O48
38	a	419	LHG	O7-C5-C6-O8
36	C	519	DGD	C9A-CAA-CBA-CCA
33	C	521	LMG	C35-C36-C37-C38
33	c	521	LMG	C29-C30-C31-C32
36	c	519	DGD	C2G-C3G-O3G-C1D
24	C	511	CLA	C16-C17-C18-C20
24	d	403	CLA	C10-C11-C12-C13
34	b	622	LMT	C4-C5-C6-C7
27	B	620	SQD	C16-C17-C18-C19
24	b	613	CLA	O1D-CGD-O2D-CED
31	D	405	PL9	C15-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
38	D	407	LHG	C24-C23-O8-C6
34	m	102	LMT	C7-C8-C9-C10
24	c	508	CLA	C11-C10-C8-C9
24	B	604	CLA	C6-C7-C8-C9
24	C	507	CLA	C6-C7-C8-C9
24	b	615	CLA	C14-C13-C15-C16
27	b	620	SQD	O10-C23-O48-C46
38	D	407	LHG	O10-C23-O8-C6
27	b	620	SQD	C11-C10-C9-C8
36	C	517	DGD	CAB-CBB-CCB-CDB
35	b	628	HTG	C3'-C4'-C5'-C6'
36	C	517	DGD	C2A-C3A-C4A-C5A
36	H	102	DGD	C9B-CAB-CBB-CCB
27	a	409	SQD	C16-C17-C18-C19
36	C	517	DGD	C7A-C8A-C9A-CAA
24	B	611	CLA	C8-C10-C11-C12
33	c	521	LMG	C21-C22-C23-C24
36	h	103	DGD	C7B-C8B-C9B-CAB
36	C	517	DGD	CBB-CCB-CDB-CEB
27	b	620	SQD	C46-C45-O47-C7
24	C	502	CLA	C2A-CAA-CBA-CGA
24	c	509	CLA	C2A-CAA-CBA-CGA
33	c	522	LMG	C29-C30-C31-C32
33	B	621	LMG	C29-C30-C31-C32
38	d	406	LHG	C13-C14-C15-C16
24	b	613	CLA	C2-C1-O2A-CGA
24	C	510	CLA	C2-C1-O2A-CGA
24	A	409	CLA	C2-C1-O2A-CGA
24	b	608	CLA	C2-C1-O2A-CGA
24	b	614	CLA	C2-C1-O2A-CGA
24	B	613	CLA	C2-C1-O2A-CGA
33	a	417	LMG	C10-C11-C12-C13
33	Z	101	LMG	C4-C5-C6-O5
24	C	512	CLA	O1A-CGA-O2A-C1
38	D	407	LHG	C27-C28-C29-C30
33	C	520	LMG	C34-C35-C36-C37
24	B	615	CLA	C4-C3-C5-C6
38	D	407	LHG	C13-C14-C15-C16
31	a	414[A]	PL9	C12-C11-C9-C8
31	A	416[A]	PL9	C23-C24-C26-C27
36	H	102	DGD	C5B-C6B-C7B-C8B
35	b	625	HTG	C1'-C2'-C3'-C4'

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Mol	Chain	Res	Type	Atoms
35	b	628	HTG	C1'-C2'-C3'-C4'
24	b	610	CLA	C16-C17-C18-C19
33	C	521	LMG	C18-C19-C20-C21
34	a	359	LMT	C5-C6-C7-C8
36	C	517	DGD	C2E-C1E-O5D-C6D
27	b	620	SQD	O47-C45-C46-O48
38	E	101	LHG	C4-O6-P-O3
38	d	406	LHG	C3-O3-P-O6
38	a	419	LHG	C3-O3-P-O6
38	E	101	LHG	C7-C8-C9-C10
33	J	101	LMG	C30-C31-C32-C33
36	h	103	DGD	CDB-CEB-CFB-CGB
33	A	418	LMG	C30-C31-C32-C33
24	c	508	CLA	C6-C7-C8-C10
24	b	606	CLA	C12-C13-C15-C16
24	B	610	CLA	C14-C13-C15-C16
24	a	407	CLA	C11-C10-C8-C9
24	A	406	CLA	C14-C13-C15-C16
24	c	515	CLA	C14-C13-C15-C16
24	b	603	CLA	C11-C10-C8-C9
26	c	517	BCR	C19-C20-C21-C22
24	c	512	CLA	C15-C16-C17-C18
35	b	624	HTG	C4-C5-C6-O6
36	c	520	DGD	C1A-C2A-C3A-C4A
38	d	408	LHG	C9-C10-C11-C12
38	E	101	LHG	C15-C16-C17-C18
24	C	512	CLA	CBA-CGA-O2A-C1
38	d	407	LHG	C26-C27-C28-C29
38	l	101	LHG	C35-C36-C37-C38
24	C	503	CLA	O1D-CGD-O2D-CED
28	b	627	GOL	O1-C1-C2-O2
33	A	418	LMG	O8-C28-C29-C30
34	A	359	LMT	O5B-C5B-C6B-O6B
24	c	511	CLA	C13-C15-C16-C17
36	c	519	DGD	CCA-CDA-CEA-CFA
34	t	101	LMT	C5-C6-C7-C8
36	H	102	DGD	C4E-C5E-C6E-O5E
36	C	517	DGD	O6E-C1E-O5D-C6D
24	C	509	CLA	C13-C15-C16-C17
34	a	418	LMT	C5-C6-C7-C8
34	B	630	LMT	C4-C5-C6-C7
24	B	608	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
24	B	607	CLA	C3-C5-C6-C7
34	I	101	LMT	C4-C5-C6-C7
24	D	403	CLA	C10-C11-C12-C13
33	j	101	LMG	C11-C12-C13-C14
38	D	357	LHG	C17-C18-C19-C20
24	d	402	CLA	C2-C1-O2A-CGA
24	C	513	CLA	C2-C1-O2A-CGA
24	c	513	CLA	C2-C1-O2A-CGA
36	h	103	DGD	O1G-C1G-C2G-O2G
27	a	409	SQD	O6-C44-C45-O47
27	A	411	SQD	C30-C31-C32-C33
33	z	101	LMG	C10-C11-C12-C13
34	b	630	LMT	C11-C10-C9-C8
24	C	503	CLA	CBD-CGD-O2D-CED
27	a	409	SQD	C35-C36-C37-C38
33	c	522	LMG	C12-C13-C14-C15
27	a	409	SQD	C10-C11-C12-C13
27	a	409	SQD	C26-C27-C28-C29
24	b	609	CLA	C6-C7-C8-C9
24	B	610	CLA	C11-C12-C13-C14
24	b	602	CLA	C6-C7-C8-C9
24	c	510	CLA	C6-C7-C8-C9
33	j	101	LMG	C16-C17-C18-C19
38	D	406	LHG	C33-C34-C35-C36
36	H	102	DGD	O1B-C1B-C2B-C3B
24	b	610	CLA	C16-C17-C18-C20
25	A	407	PHO	O2A-C1-C2-C3
33	Z	101	LMG	O6-C1-O1-C7
27	F	101	SQD	O5-C1-O6-C44
31	a	414[A]	PL9	C2-C3-C7-C8
38	d	407	LHG	C9-C10-C11-C12
24	A	406	CLA	C1A-C2A-CAA-CBA
24	C	506	CLA	C11-C12-C13-C15
24	b	616	CLA	C11-C12-C13-C15
24	B	602	CLA	C11-C12-C13-C15
24	c	509	CLA	C12-C13-C15-C16
38	d	408	LHG	C32-C33-C34-C35
24	C	507	CLA	C5-C6-C7-C8
24	C	514	CLA	C3-C5-C6-C7
24	C	512	CLA	C3-C5-C6-C7
35	B	624	HTG	C4'-C5'-C6'-C7'
34	B	622	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
36	c	520	DGD	C7B-C8B-C9B-CAB
24	a	404	CLA	C16-C17-C18-C20
33	c	521	LMG	C4-C5-C6-O5
24	a	403	CLA	C2A-CAA-CBA-CGA
24	B	602	CLA	C2A-CAA-CBA-CGA
35	b	624	HTG	C3'-C4'-C5'-C6'
34	B	630	LMT	C7-C8-C9-C10
24	C	507	CLA	C16-C17-C18-C19
31	a	414[A]	PL9	C45-C44-C46-C47
24	b	609	CLA	C2-C3-C5-C6
36	c	520	DGD	CAB-CBB-CCB-CDB
38	D	407	LHG	C12-C13-C14-C15
24	B	611	CLA	C16-C17-C18-C20
25	a	406	PHO	C8-C10-C11-C12
24	b	614	CLA	C15-C16-C17-C18
27	b	620	SQD	C9-C10-C11-C12
27	A	413	SQD	C32-C33-C34-C35
36	C	517	DGD	C9A-CAA-CBA-CCA
31	D	405	PL9	C32-C33-C34-C35
24	C	514	CLA	C2-C1-O2A-CGA
24	c	514	CLA	C2-C1-O2A-CGA
24	B	615	CLA	C2-C3-C5-C6
31	a	414[B]	PL9	C43-C44-C46-C47
24	B	604	CLA	C2C-C3C-CAC-CBC
36	C	519	DGD	C9B-CAB-CBB-CCB
36	c	518	DGD	C2A-C3A-C4A-C5A
36	h	103	DGD	C6A-C7A-C8A-C9A
38	d	407	LHG	C25-C26-C27-C28
24	C	503	CLA	C10-C11-C12-C13
24	b	613	CLA	C8-C10-C11-C12
26	c	517	BCR	C1-C6-C7-C8
26	A	410	BCR	C1-C6-C7-C8
26	B	617	BCR	C1-C6-C7-C8
26	C	516	BCR	C1-C6-C7-C8
36	h	103	DGD	O1G-C1G-C2G-C3G
38	D	357	LHG	C29-C30-C31-C32
24	b	602	CLA	C10-C11-C12-C13
24	b	601	CLA	CAA-CBA-CGA-O1A
33	B	621	LMG	O10-C28-C29-C30
31	a	414[A]	PL9	C20-C19-C21-C22
24	b	616	CLA	C4-C3-C5-C6
26	b	619	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
31	a	414[A]	PL9	C43-C44-C46-C47
24	B	604	CLA	C2-C3-C5-C6
38	l	101	LHG	C32-C33-C34-C35
36	c	518	DGD	C5D-C6D-O5D-C1E
36	C	518	DGD	C2G-C3G-O3G-C1D
33	A	418	LMG	C12-C13-C14-C15
34	B	630	LMT	C2-C3-C4-C5
35	b	623	HTG	C3'-C4'-C5'-C6'
24	B	601	CLA	C2A-CAA-CBA-CGA
33	Z	101	LMG	O10-C28-O8-C9
24	B	613	CLA	C16-C17-C18-C19
38	D	357	LHG	C9-C10-C11-C12
34	b	622	LMT	C6-C7-C8-C9
24	C	502	CLA	C12-C13-C15-C16
24	c	508	CLA	C11-C10-C8-C7
24	c	508	CLA	C12-C13-C15-C16
24	b	614	CLA	C12-C13-C15-C16
36	c	520	DGD	CCB-CDB-CEB-CFB
27	F	101	SQD	C2-C1-O6-C44
27	b	620	SQD	O48-C23-C24-C25
24	C	511	CLA	CAA-CBA-CGA-O2A
24	B	613	CLA	CAA-CBA-CGA-O2A
38	d	407	LHG	C28-C29-C30-C31
24	C	513	CLA	C10-C11-C12-C13
24	C	504	CLA	C8-C10-C11-C12
24	b	611	CLA	C13-C15-C16-C17
34	m	102	LMT	C4'-C5'-C6'-O6'
31	a	414[B]	PL9	C35-C34-C36-C37
31	A	416[B]	PL9	C40-C39-C41-C42
31	A	416[B]	PL9	C45-C44-C46-C47
24	c	515	CLA	C4-C3-C5-C6
31	A	416[A]	PL9	C30-C29-C31-C32
24	b	606	CLA	C8-C10-C11-C12
24	b	603	CLA	C13-C15-C16-C17
31	D	405	PL9	C18-C19-C21-C22
31	a	414[B]	PL9	C18-C19-C21-C22
24	b	604	CLA	C2C-C3C-CAC-CBC
24	b	613	CLA	CAA-CBA-CGA-O2A
24	b	616	CLA	C11-C12-C13-C14
24	B	604	CLA	C11-C12-C13-C14
24	c	511	CLA	C11-C10-C8-C9
24	c	509	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	D	403	CLA	O1A-CGA-O2A-C1
24	C	507	CLA	C3A-C2A-CAA-CBA
24	B	601	CLA	C3A-C2A-CAA-CBA
38	d	408	LHG	C30-C31-C32-C33
33	B	621	LMG	C15-C16-C17-C18
24	B	604	CLA	CAD-CBD-CGD-O2D
24	B	616	CLA	CAD-CBD-CGD-O2D
24	B	612	CLA	CAD-CBD-CGD-O2D
24	C	513	CLA	CAD-CBD-CGD-O2D
24	c	503	CLA	CAD-CBD-CGD-O2D
25	A	407	PHO	CAD-CBD-CGD-O2D
38	D	407	LHG	C33-C34-C35-C36
26	H	101	BCR	C9-C10-C11-C12
33	C	520	LMG	C29-C30-C31-C32
33	B	621	LMG	C32-C33-C34-C35
24	A	409	CLA	C4-C3-C5-C6
33	j	101	LMG	C36-C37-C38-C39
33	J	101	LMG	C37-C38-C39-C40
31	a	414[A]	PL9	C18-C19-C21-C22
38	L	101	LHG	O7-C7-C8-C9
38	l	101	LHG	O7-C7-C8-C9
26	D	404	BCR	C7-C8-C9-C10
33	c	522	LMG	O10-C28-O8-C9
24	b	613	CLA	O2A-C1-C2-C3
24	B	602	CLA	O2A-C1-C2-C3
27	A	413	SQD	C17-C18-C19-C20
25	a	405	PHO	C4B-C3B-CAB-CBB
24	c	503	CLA	C2A-CAA-CBA-CGA
24	A	405	CLA	C2C-C3C-CAC-CBC
27	A	411	SQD	O47-C7-C8-C9
24	C	510	CLA	C8-C10-C11-C12
34	B	622	LMT	C5-C6-C7-C8
24	c	505	CLA	CHA-CBD-CGD-O2D
24	a	350	CLA	CHA-CBD-CGD-O2D
24	B	614	CLA	CHA-CBD-CGD-O2D
24	c	506	CLA	CHA-CBD-CGD-O1D
24	A	405	CLA	CHA-CBD-CGD-O1D
24	A	405	CLA	CHA-CBD-CGD-O2D
24	b	606	CLA	CHA-CBD-CGD-O2D
24	c	511	CLA	CHA-CBD-CGD-O1D
24	c	511	CLA	CHA-CBD-CGD-O2D
24	c	504	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	B	606	CLA	CHA-CBD-CGD-O2D
24	B	607	CLA	CHA-CBD-CGD-O2D
24	c	509	CLA	CHA-CBD-CGD-O1D
24	c	509	CLA	CHA-CBD-CGD-O2D
24	c	514	CLA	CHA-CBD-CGD-O2D
24	c	512	CLA	CAA-CBA-CGA-O2A
24	B	604	CLA	C4C-C3C-CAC-CBC
27	f	101	SQD	O47-C7-C8-C9
33	c	521	LMG	O7-C10-C11-C12
27	a	411	SQD	C34-C35-C36-C37
24	B	601	CLA	CAA-CBA-CGA-O1A
36	C	519	DGD	C7B-C8B-C9B-CAB
24	A	406	CLA	C13-C15-C16-C17
24	b	604	CLA	C13-C15-C16-C17
33	J	101	LMG	O7-C10-C11-C12
36	C	518	DGD	C8A-C9A-CAA-CBA
25	a	406	PHO	C2C-C3C-CAC-CBC
33	a	417	LMG	C37-C38-C39-C40
24	b	616	CLA	C2-C3-C5-C6
24	b	616	CLA	C12-C13-C15-C16
24	b	610	CLA	C11-C12-C13-C15
24	A	409	CLA	C2-C3-C5-C6
31	a	414[B]	PL9	C4-C3-C7-C8
24	a	350	CLA	C2C-C3C-CAC-CBC
33	J	101	LMG	C12-C13-C14-C15
24	b	612	CLA	CAA-CBA-CGA-O2A
27	a	411	SQD	C13-C14-C15-C16
24	C	506	CLA	C11-C12-C13-C14
26	k	101	BCR	C9-C10-C11-C12
33	C	520	LMG	C36-C37-C38-C39
33	c	522	LMG	C29-C28-O8-C9
27	B	620	SQD	C5-C6-S-O8
24	B	611	CLA	C16-C17-C18-C19
33	b	621	LMG	C21-C22-C23-C24
31	a	414[B]	PL9	C26-C27-C28-C29
31	a	414[B]	PL9	C36-C37-C38-C39
35	b	623	HTG	C4-C5-C6-O6
38	L	101	LHG	O9-C7-C8-C9
24	b	604	CLA	C4C-C3C-CAC-CBC
28	B	627	GOL	O1-C1-C2-C3
38	d	406	LHG	C27-C28-C29-C30
24	b	613	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
26	c	517	BCR	C7-C8-C9-C10
34	E	102	LMT	C5-C6-C7-C8
24	D	403	CLA	CBA-CGA-O2A-C1
38	d	406	LHG	O10-C23-O8-C6
24	b	609	CLA	C1A-C2A-CAA-CBA
24	c	515	CLA	C1A-C2A-CAA-CBA
24	B	609	CLA	C1A-C2A-CAA-CBA
38	d	407	LHG	C14-C15-C16-C17
24	B	608	CLA	C16-C17-C18-C19
27	b	620	SQD	O10-C23-C24-C25
36	H	102	DGD	CDA-CEA-CFA-CGA
24	C	505	CLA	C2-C1-O2A-CGA
24	c	515	CLA	C2-C1-O2A-CGA
38	l	101	LHG	O9-C7-C8-C9
38	D	406	LHG	C25-C26-C27-C28
34	M	103	LMT	C11-C10-C9-C8
34	a	359	LMT	C7-C8-C9-C10
38	D	357	LHG	C33-C34-C35-C36
27	a	409	SQD	O6-C44-C45-C46
33	C	520	LMG	O1-C7-C8-C9
24	B	610	CLA	C2A-CAA-CBA-CGA
24	B	614	CLA	C2A-CAA-CBA-CGA
36	h	103	DGD	O1B-C1B-C2B-C3B
36	c	520	DGD	C8B-C9B-CAB-CBB
24	a	407	CLA	C15-C16-C17-C18
27	A	411	SQD	O49-C7-C8-C9
24	C	511	CLA	CAA-CBA-CGA-O1A
24	B	613	CLA	CAA-CBA-CGA-O1A
27	A	411	SQD	C34-C35-C36-C37
38	E	101	LHG	C4-O6-P-O5
24	c	512	CLA	CAA-CBA-CGA-O1A
38	D	406	LHG	C34-C35-C36-C37
26	B	617	BCR	C5-C6-C7-C8
27	f	101	SQD	O49-C7-C8-C9
24	C	507	CLA	C3-C5-C6-C7
27	B	620	SQD	O10-C23-O48-C46
31	A	416[B]	PL9	C12-C13-C14-C16
24	b	605	CLA	C13-C15-C16-C17
36	c	518	DGD	C6A-C7A-C8A-C9A
27	A	413	SQD	C25-C26-C27-C28
33	c	521	LMG	O9-C10-C11-C12
33	C	520	LMG	O9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	b	609	CLA	C4-C3-C5-C6
24	c	508	CLA	C4-C3-C5-C6
31	d	405	PL9	C11-C12-C13-C14
31	a	414[B]	PL9	C12-C11-C9-C8
27	a	409	SQD	C15-C16-C17-C18
24	c	508	CLA	CAD-CBD-CGD-O1D
24	c	506	CLA	CAD-CBD-CGD-O1D
24	A	405	CLA	CAD-CBD-CGD-O1D
24	C	505	CLA	CAD-CBD-CGD-O1D
24	C	507	CLA	CAD-CBD-CGD-O1D
24	B	609	CLA	CAD-CBD-CGD-O1D
24	b	607	CLA	CAD-CBD-CGD-O1D
38	l	101	LHG	C17-C18-C19-C20
38	d	408	LHG	O8-C23-C24-C25
24	B	615	CLA	C11-C12-C13-C14
24	a	350	CLA	C11-C12-C13-C14
24	c	508	CLA	C11-C12-C13-C14
24	b	616	CLA	C14-C13-C15-C16
24	C	513	CLA	C11-C10-C8-C9
24	b	604	CLA	C14-C13-C15-C16
33	Z	101	LMG	C15-C16-C17-C18
25	a	405	PHO	C8-C10-C11-C12
24	C	514	CLA	O1A-CGA-O2A-C1
33	a	417	LMG	O10-C28-C29-C30
24	B	612	CLA	CAA-CBA-CGA-O2A
24	c	514	CLA	CAA-CBA-CGA-O2A
33	a	417	LMG	C30-C31-C32-C33
24	C	510	CLA	C10-C11-C12-C13
24	b	612	CLA	C13-C15-C16-C17
33	b	621	LMG	C22-C23-C24-C25
24	d	402	CLA	CAA-CBA-CGA-O2A
36	C	518	DGD	O2G-C1B-C2B-C3B
33	Z	101	LMG	O7-C10-C11-C12
24	B	605	CLA	C5-C6-C7-C8
33	C	520	LMG	C16-C17-C18-C19
24	B	602	CLA	C4-C3-C5-C6
24	D	403	CLA	C12-C13-C15-C16
24	a	350	CLA	C6-C7-C8-C10
24	a	350	CLA	C11-C12-C13-C15
24	c	508	CLA	C11-C12-C13-C15
24	C	507	CLA	C12-C13-C15-C16
24	b	604	CLA	C11-C12-C13-C15

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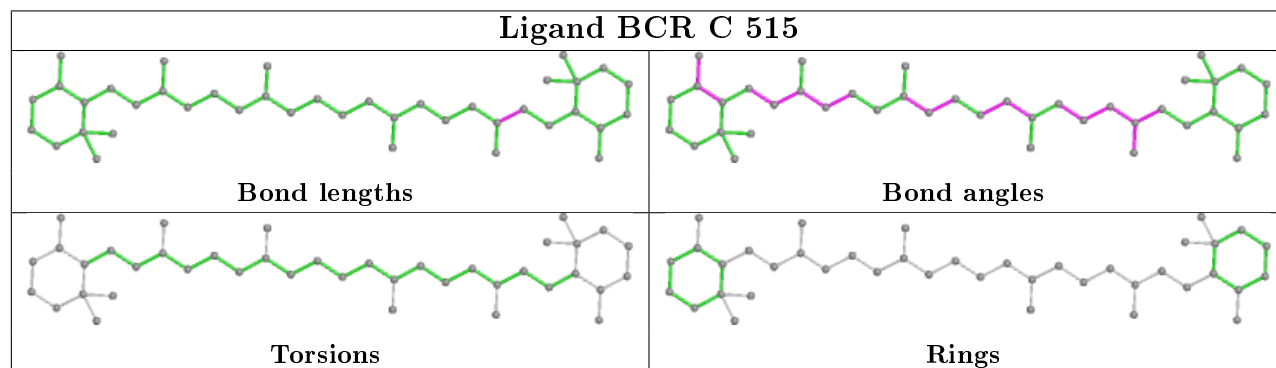
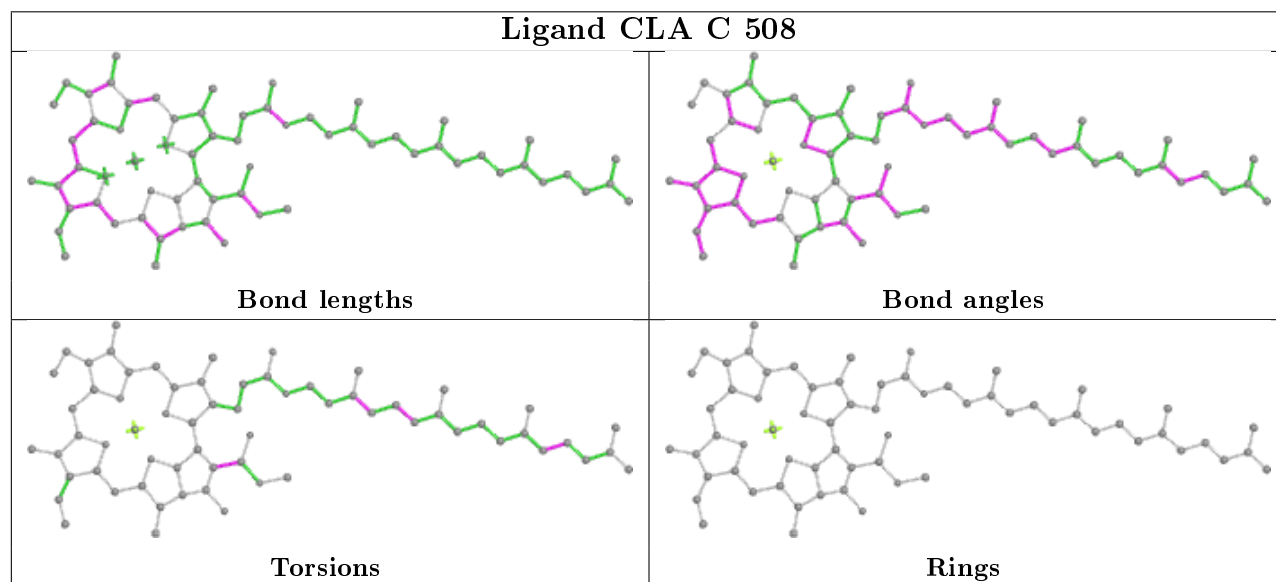
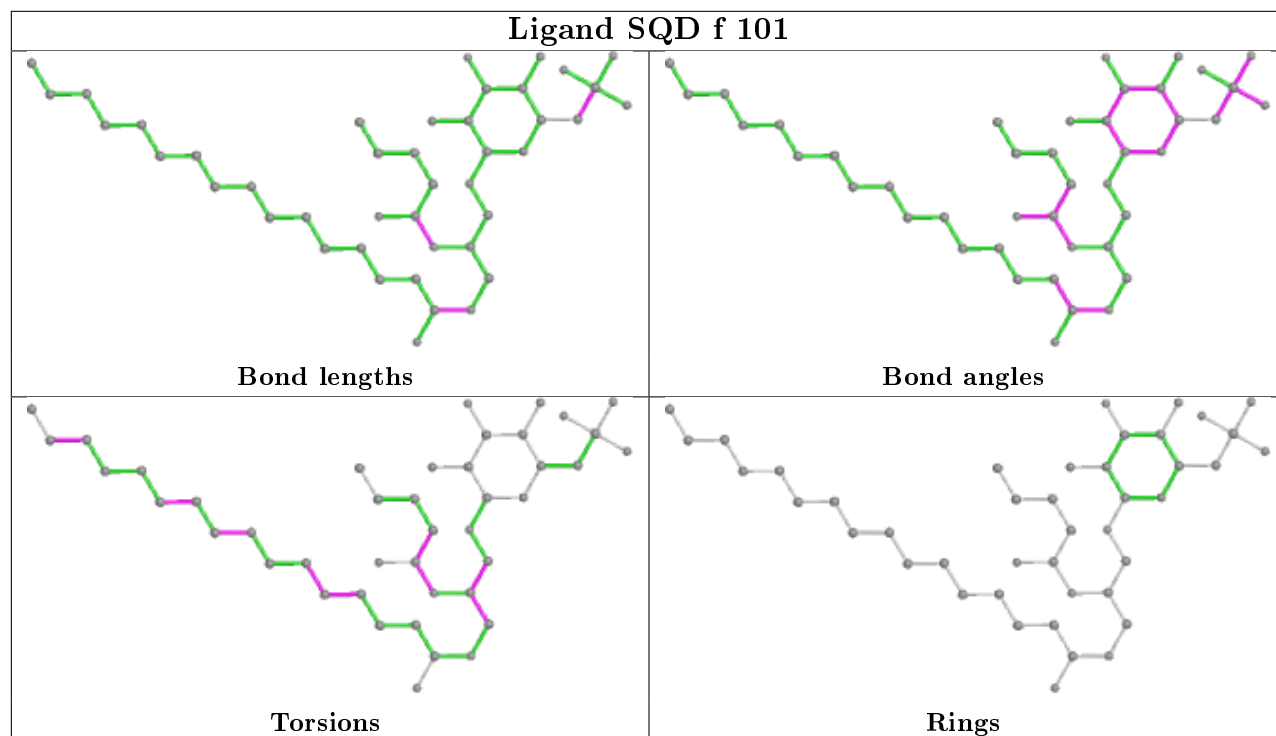
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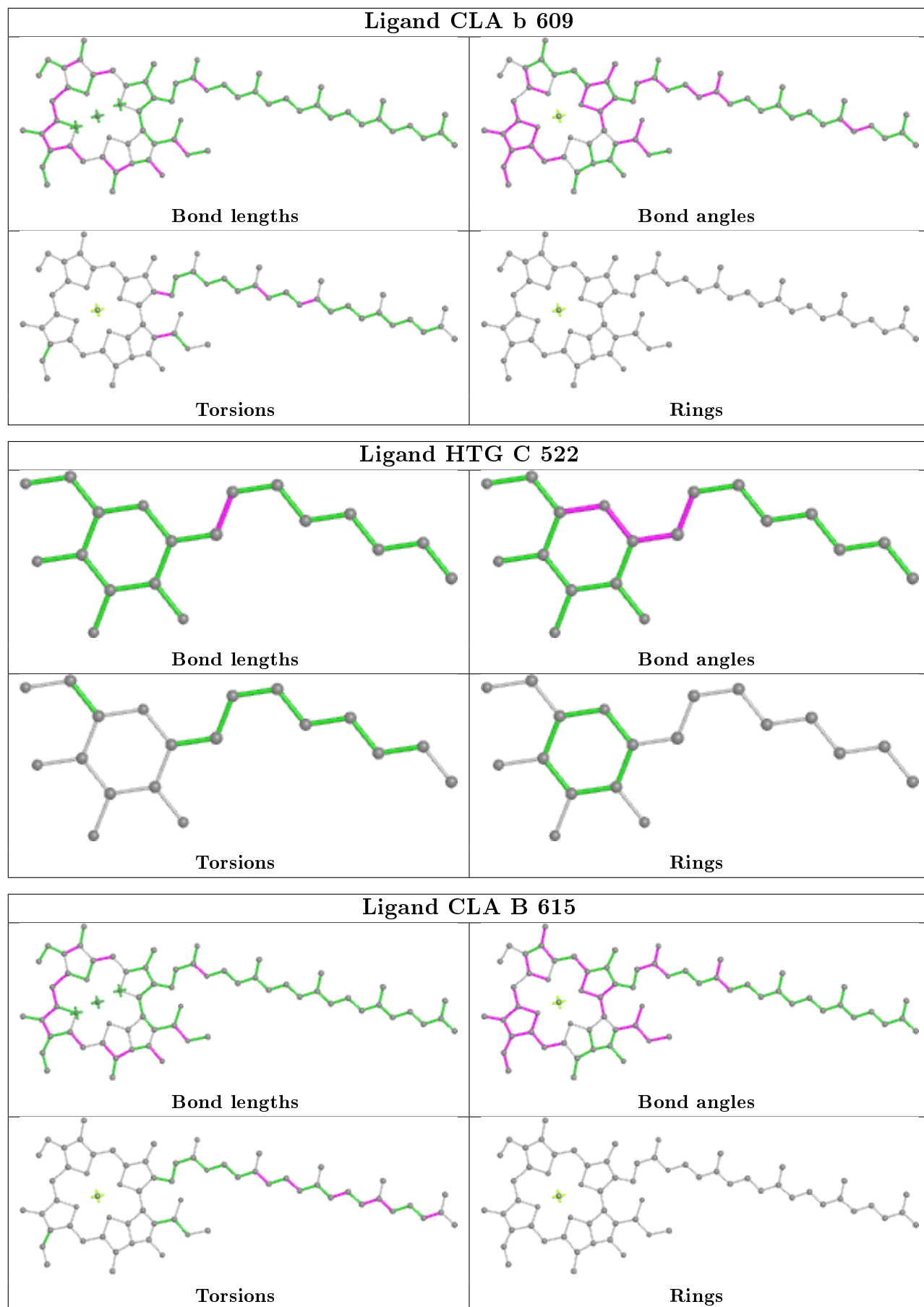
Mol	Chain	Res	Type	Atoms
24	b	604	CLA	C12-C13-C15-C16
24	B	613	CLA	C11-C10-C8-C7
33	J	101	LMG	O9-C10-C11-C12
36	c	518	DGD	O2G-C1B-C2B-C3B
27	b	620	SQD	C19-C20-C21-C22
38	D	407	LHG	C9-C10-C11-C12
25	A	407	PHO	C10-C11-C12-C13
26	Y	101	BCR	C21-C22-C23-C24
25	A	408	PHO	C4C-C3C-CAC-CBC
38	D	357	LHG	C30-C31-C32-C33
24	b	612	CLA	CAA-CBA-CGA-O1A
38	d	408	LHG	O10-C23-C24-C25
31	A	416[B]	PL9	C44-C46-C47-C48
24	c	507	CLA	CAA-CBA-CGA-O2A
38	D	407	LHG	C26-C27-C28-C29
24	B	612	CLA	C13-C15-C16-C17
24	B	612	CLA	CAA-CBA-CGA-O1A
27	A	411	SQD	C14-C15-C16-C17
24	b	601	CLA	C10-C11-C12-C13
36	c	518	DGD	O1B-C1B-C2B-C3B
24	c	514	CLA	CAA-CBA-CGA-O1A
24	C	513	CLA	CAA-CBA-CGA-O2A

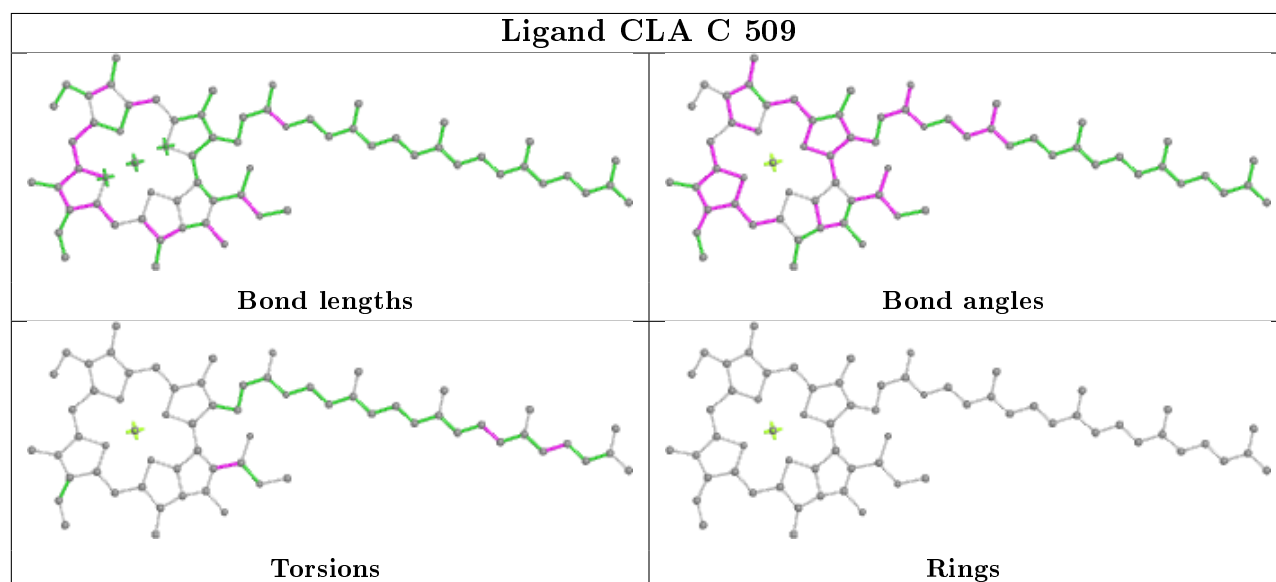
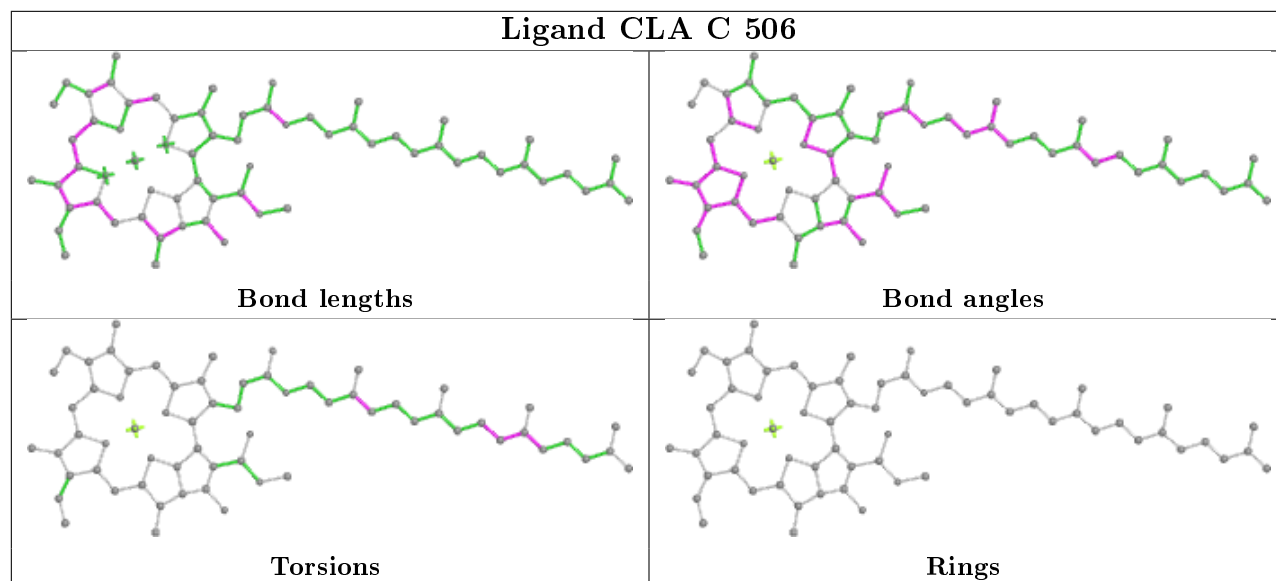
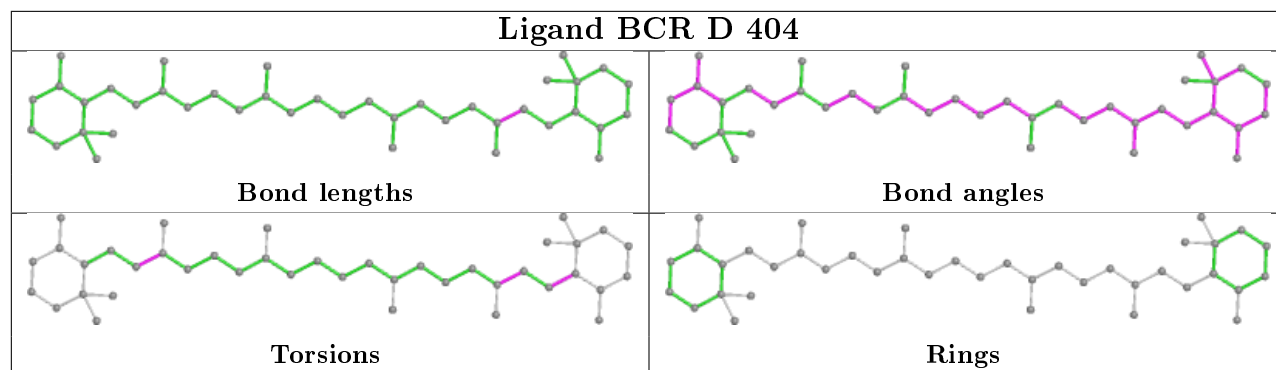
There are no ring outliers.

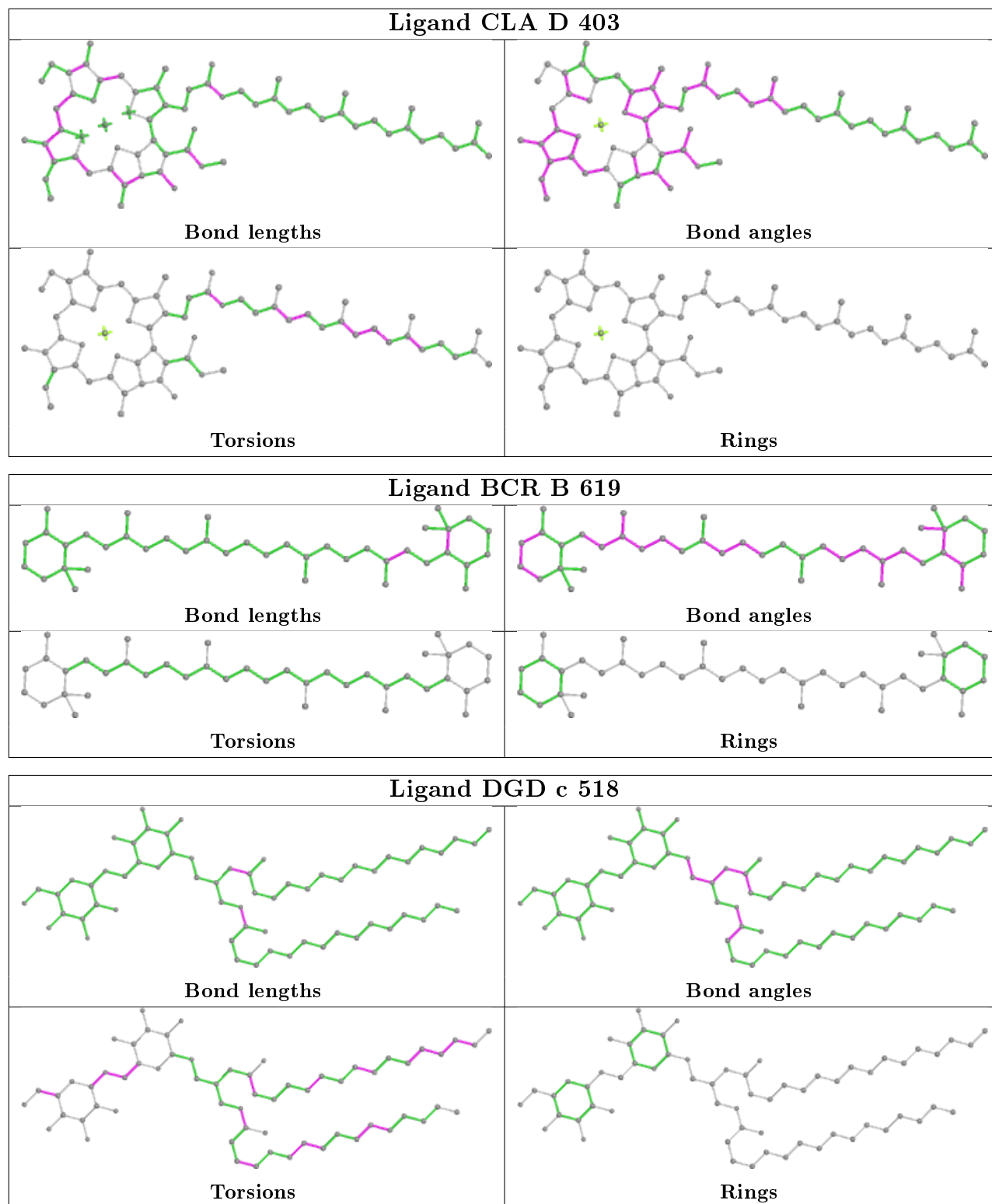
No monomer is involved in short contacts.

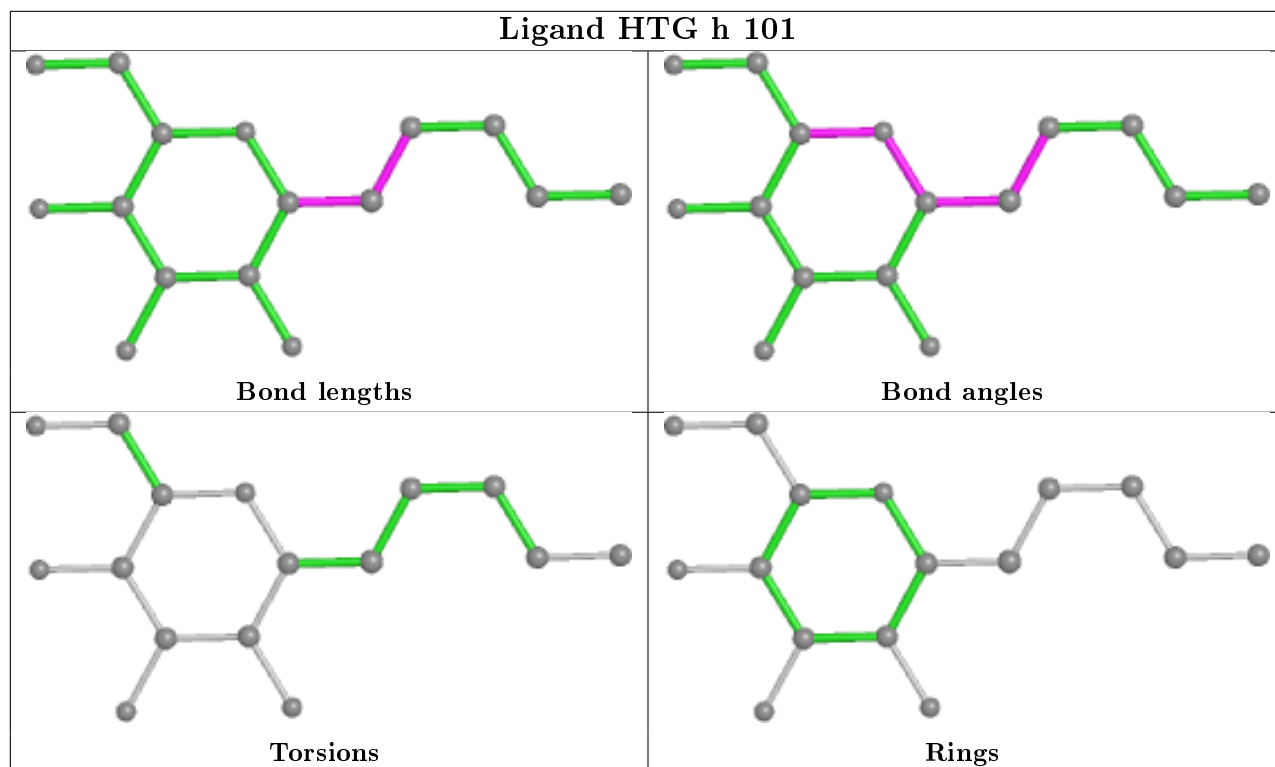
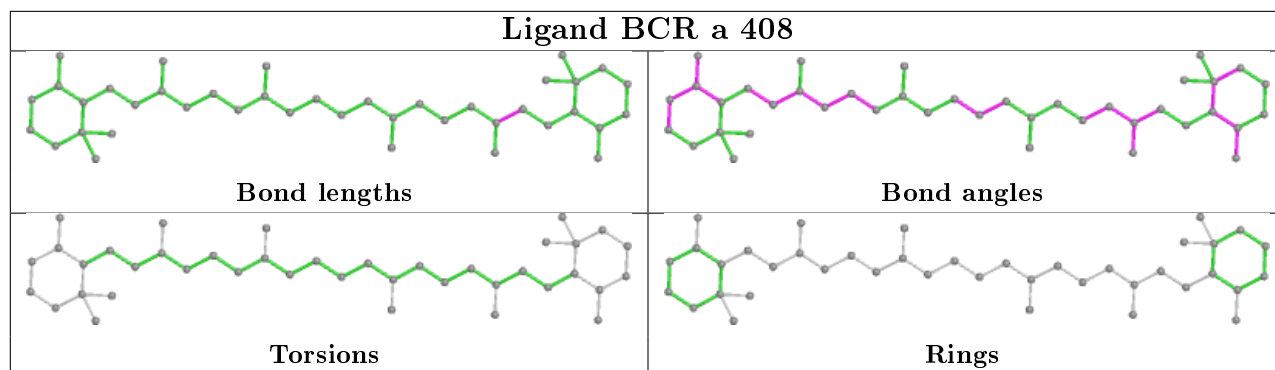
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

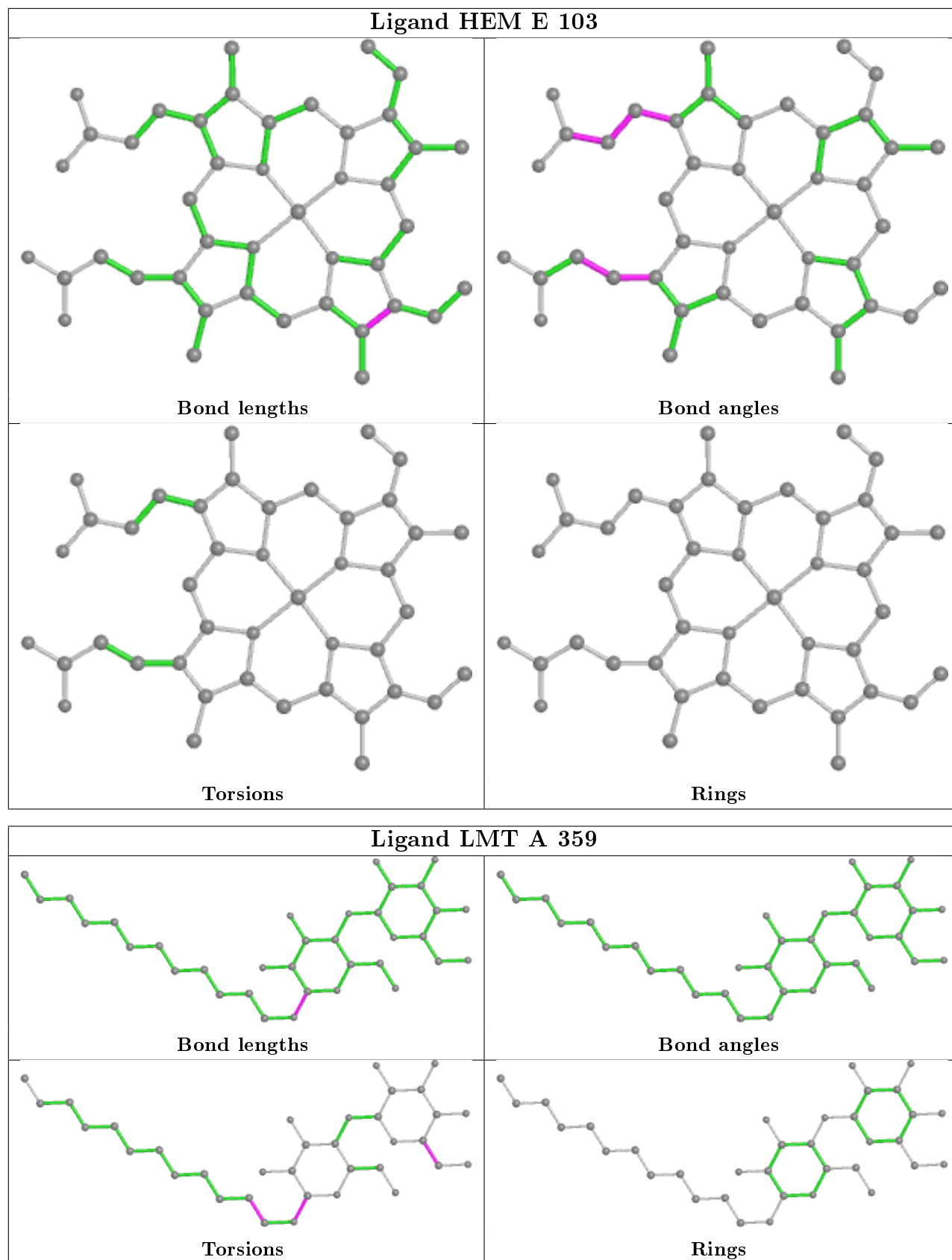


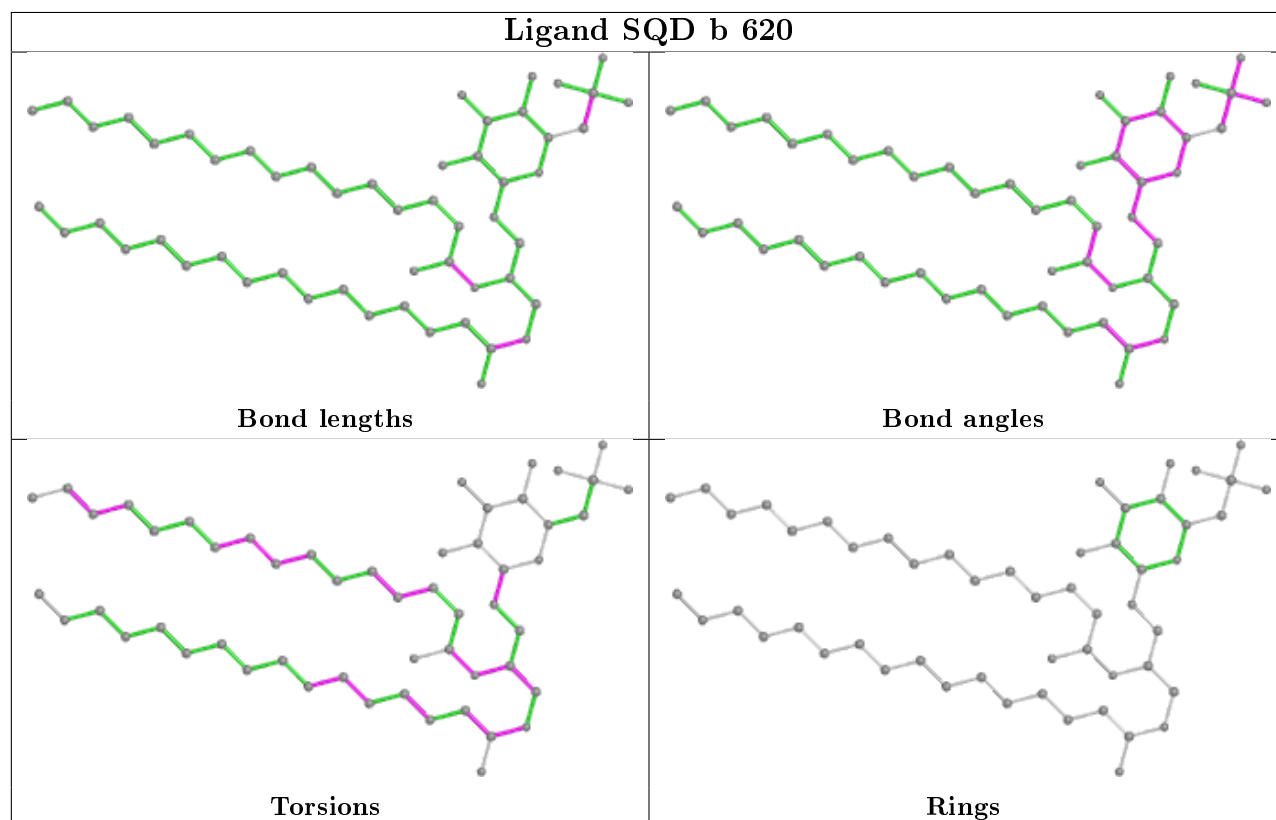
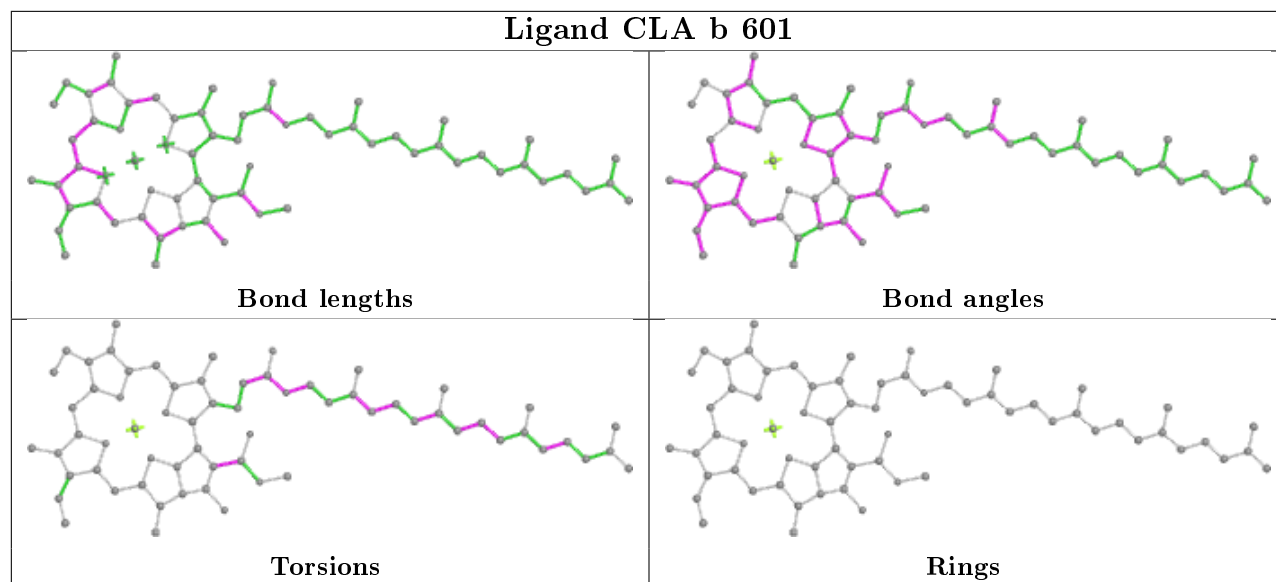


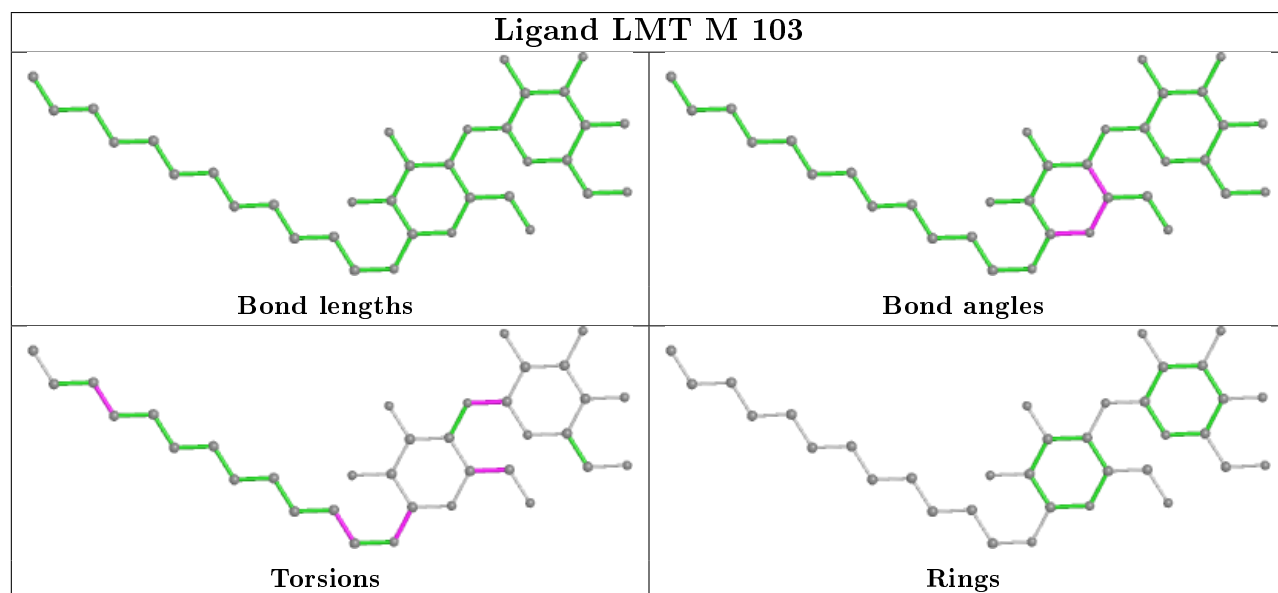
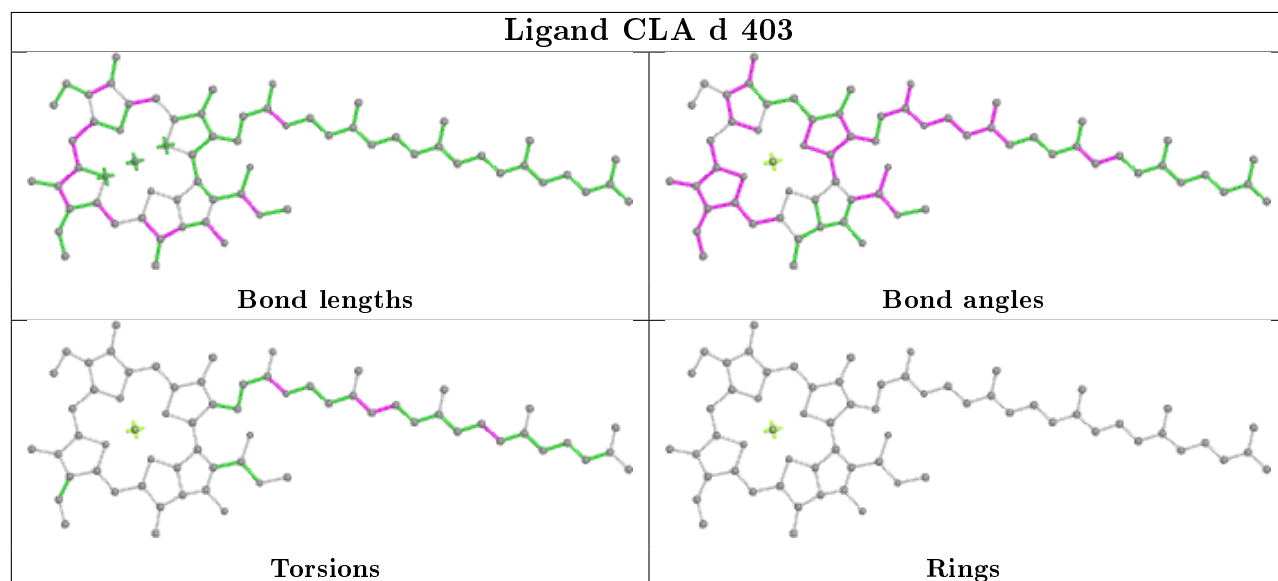
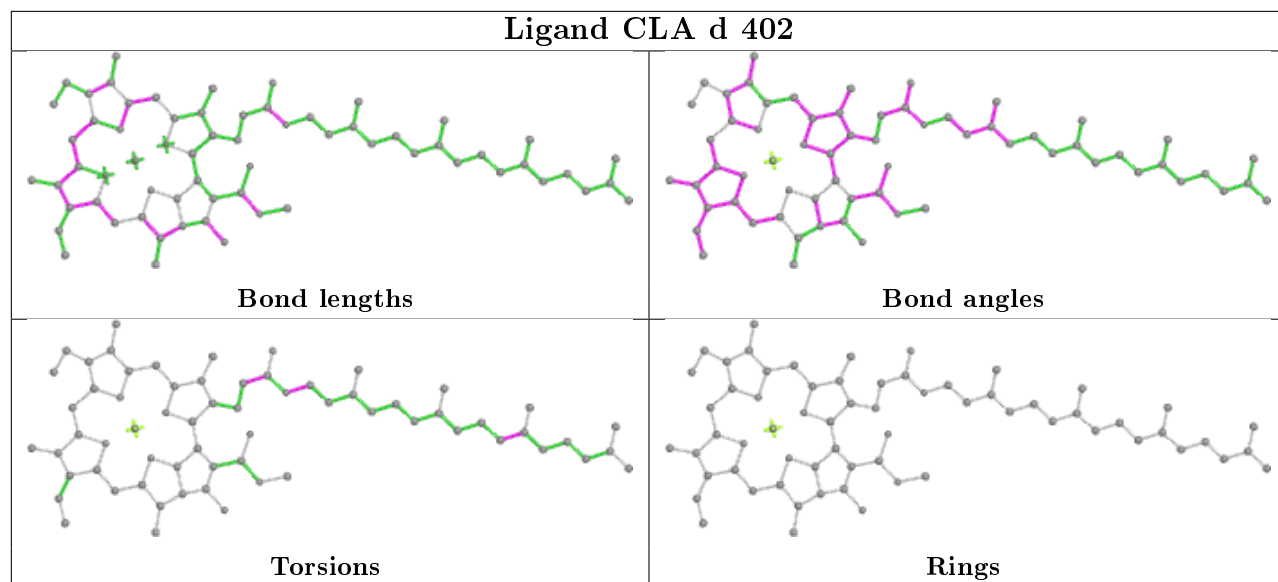


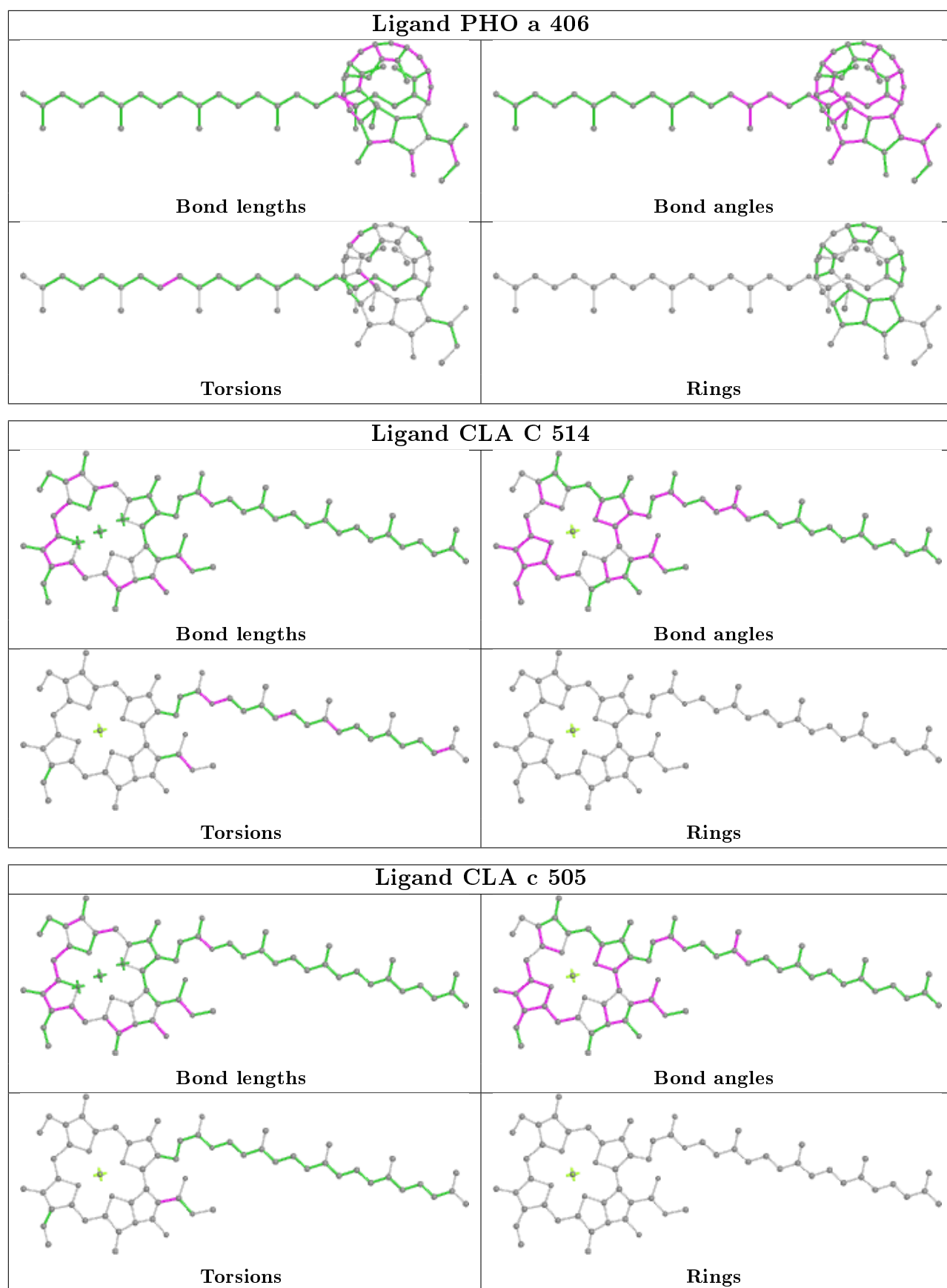


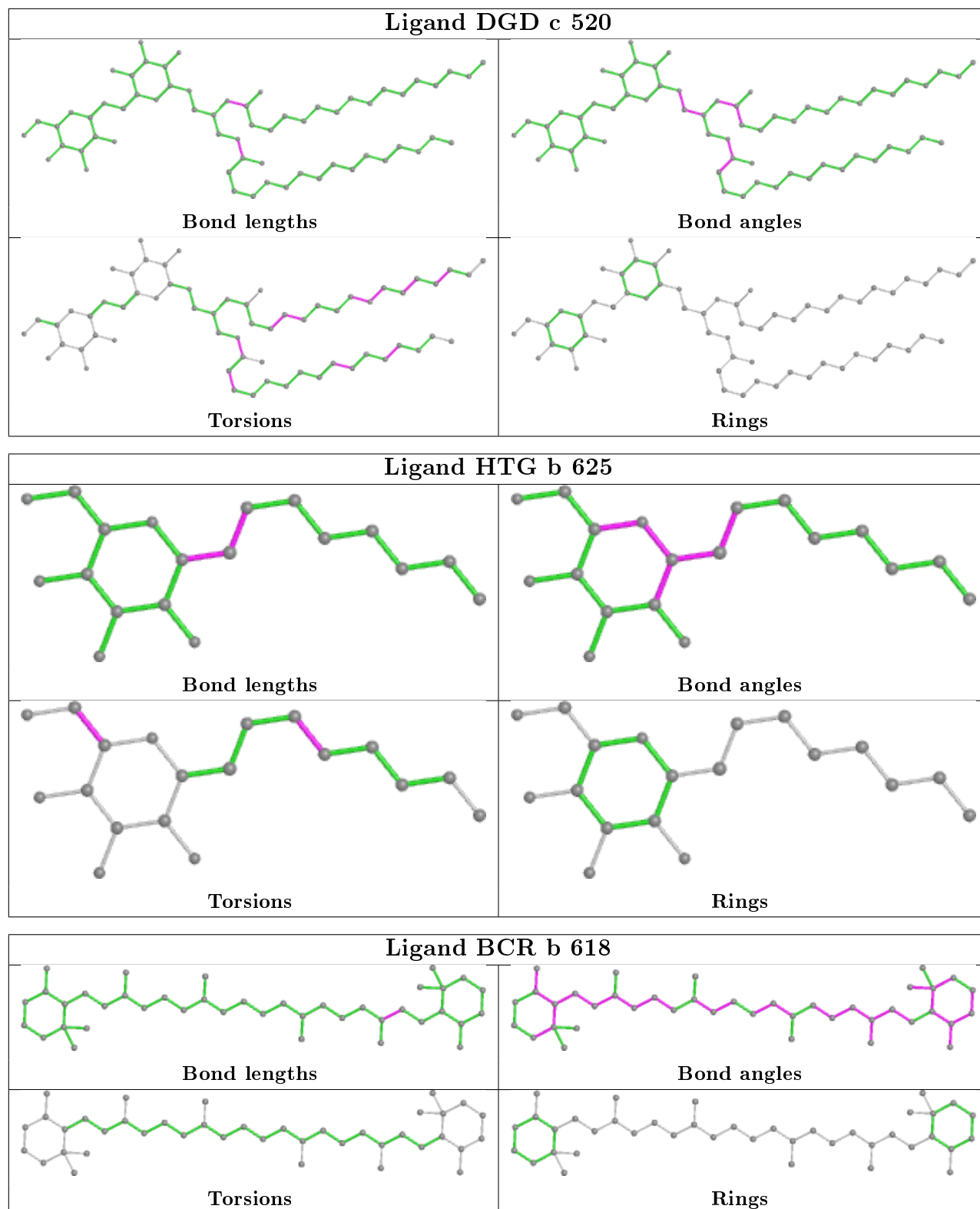


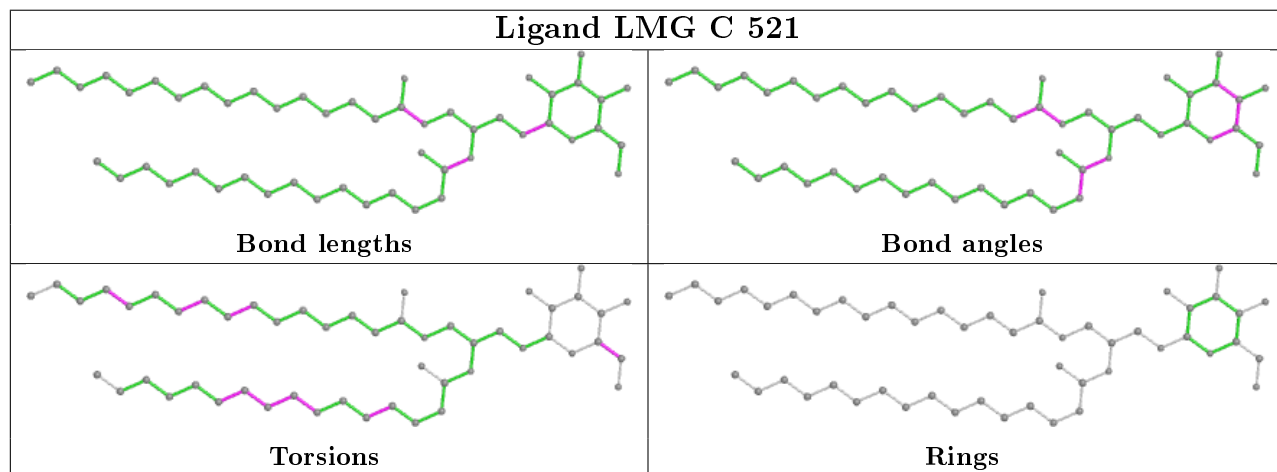
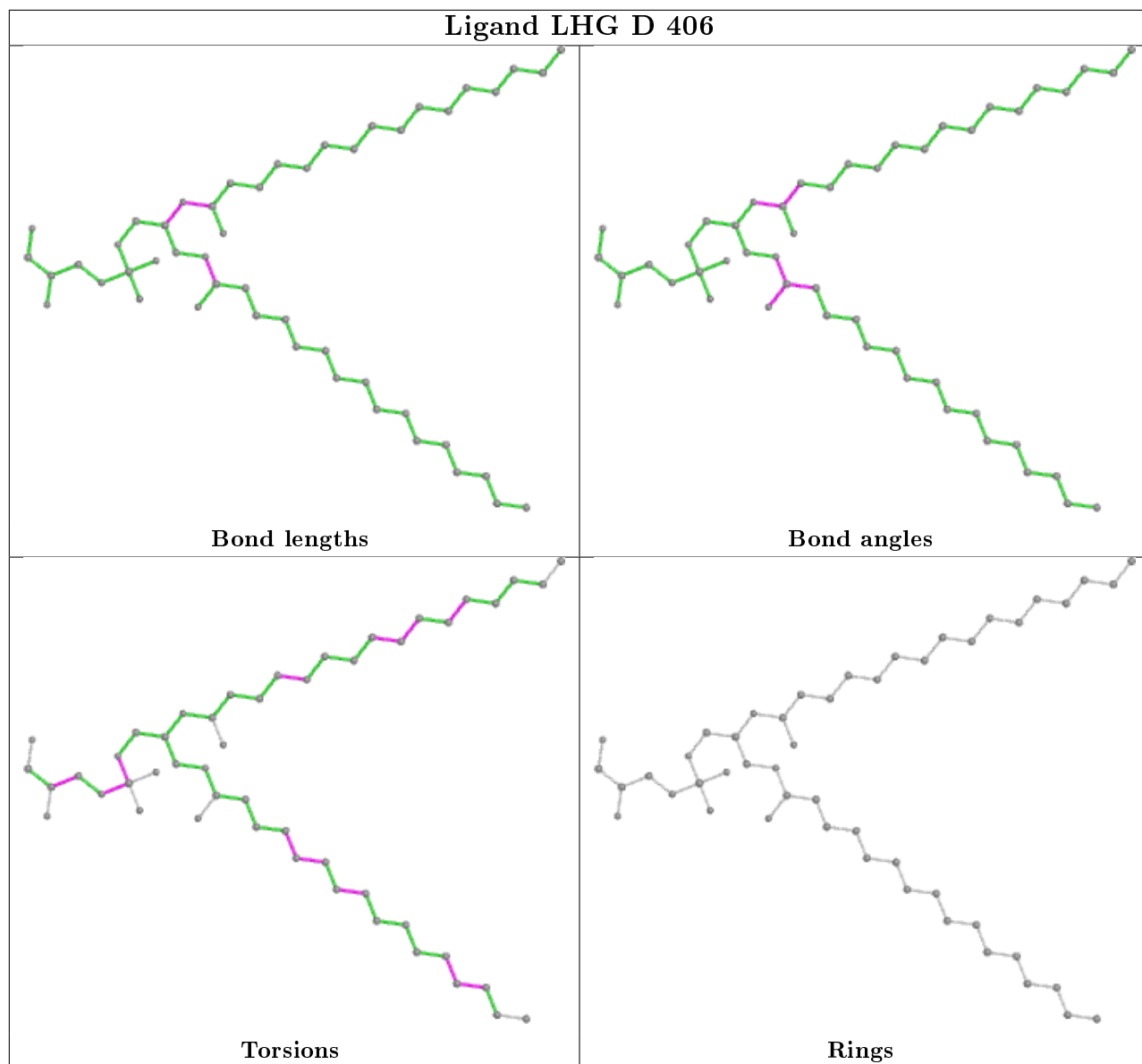


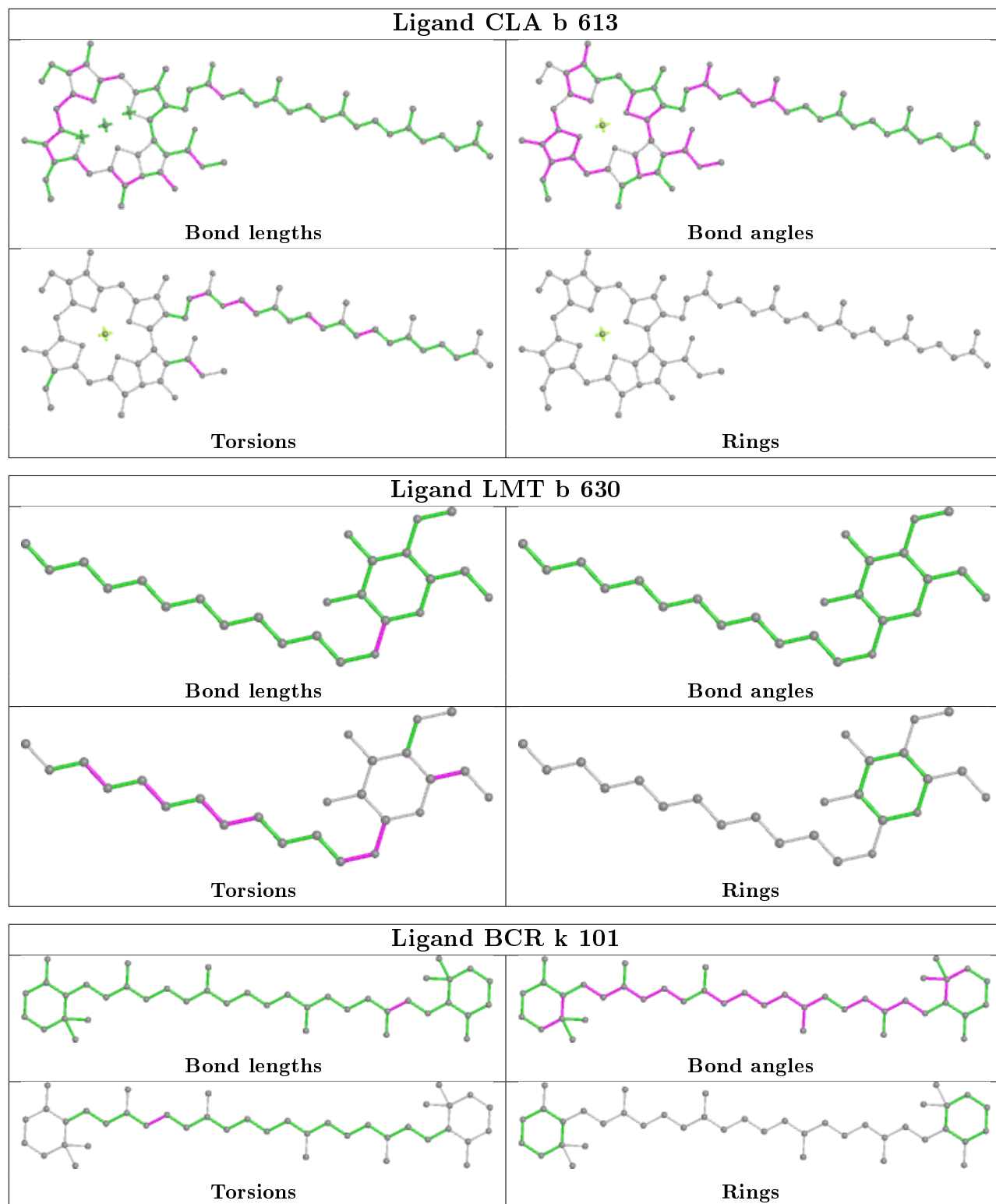


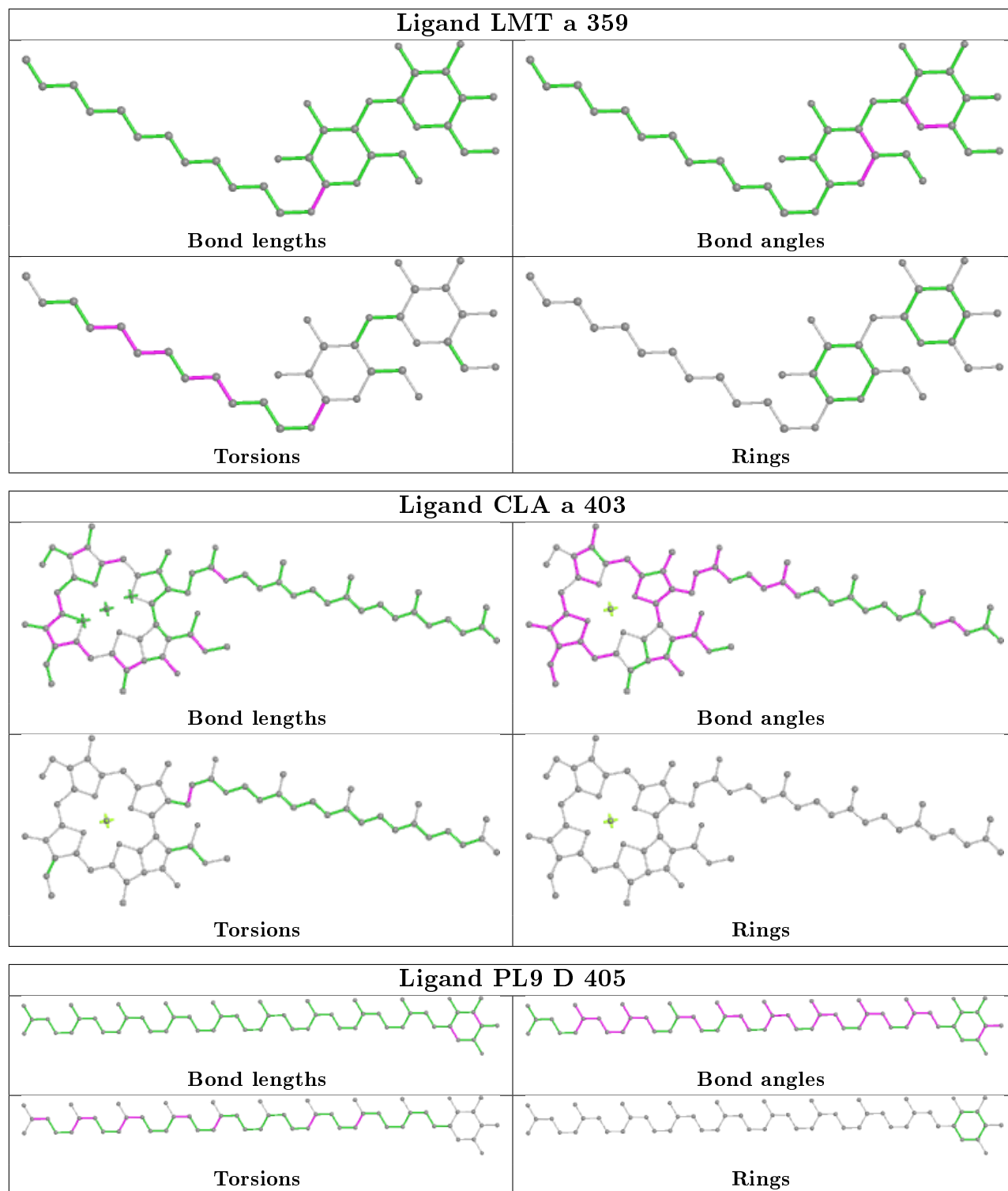


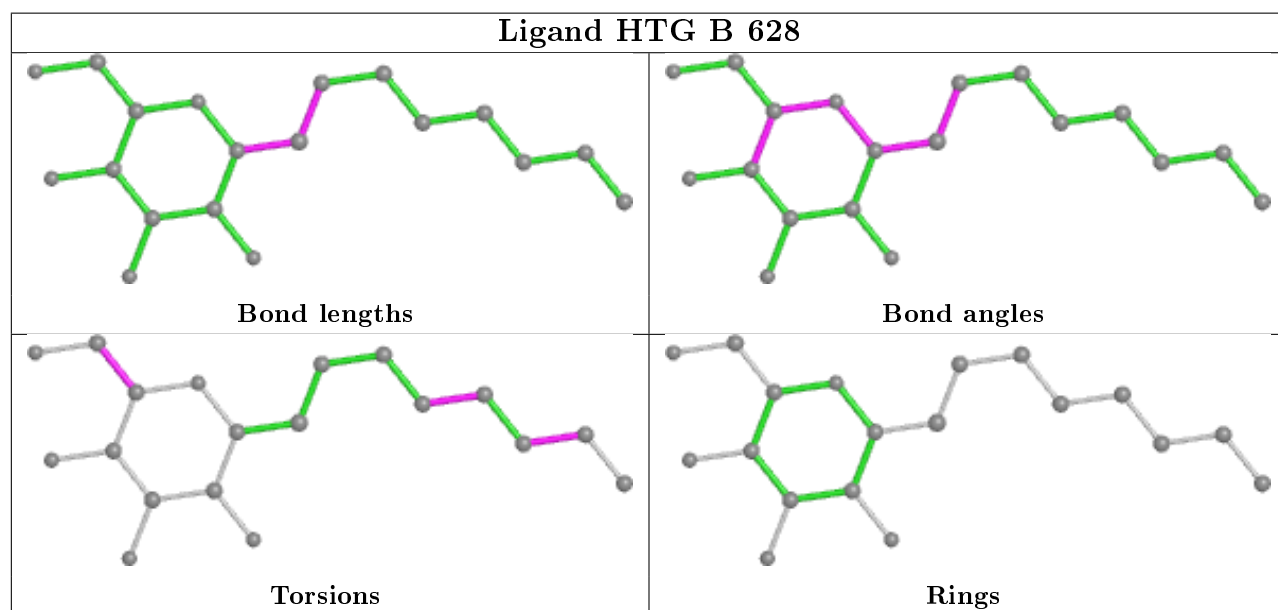
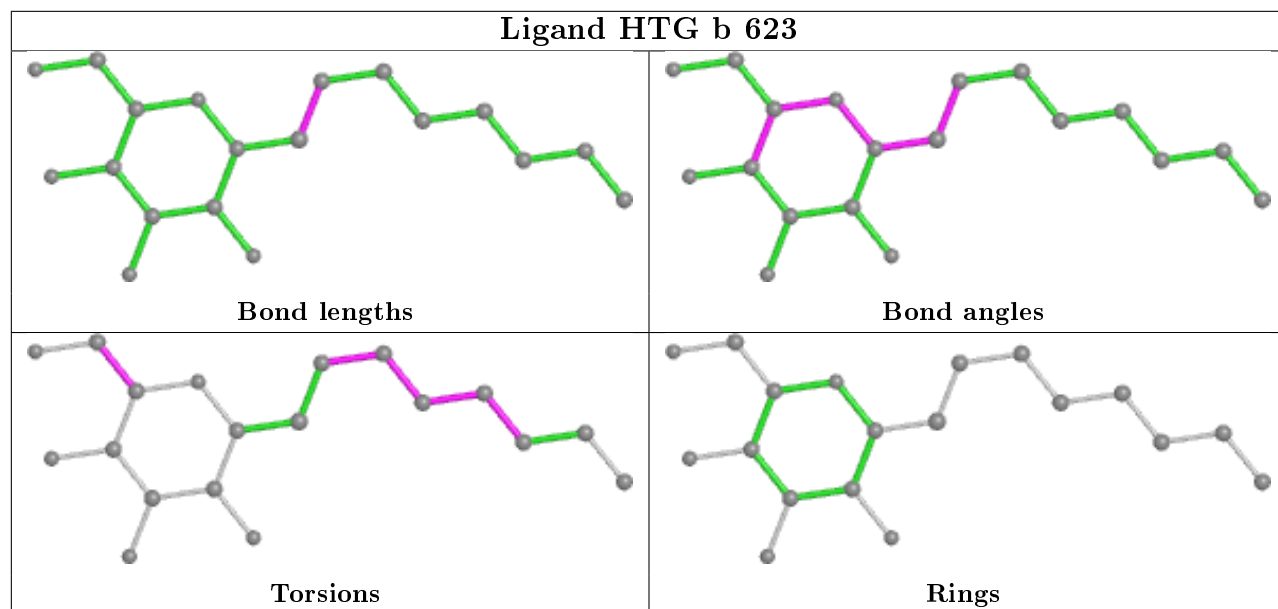
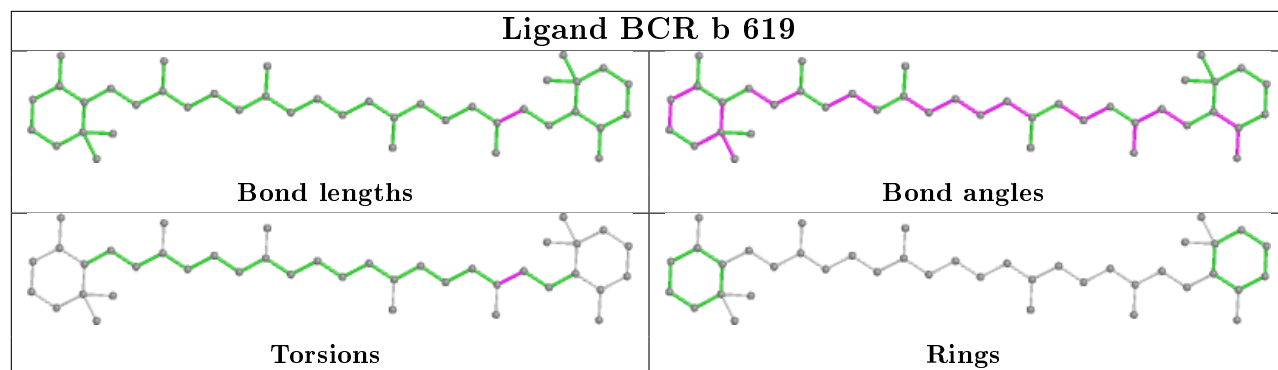


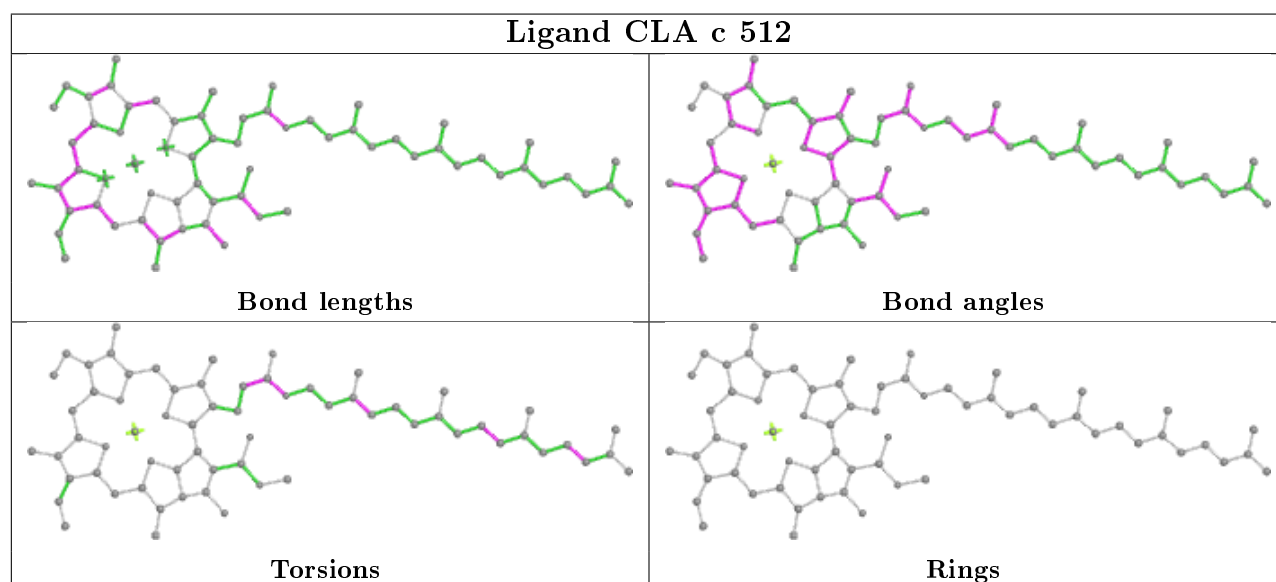
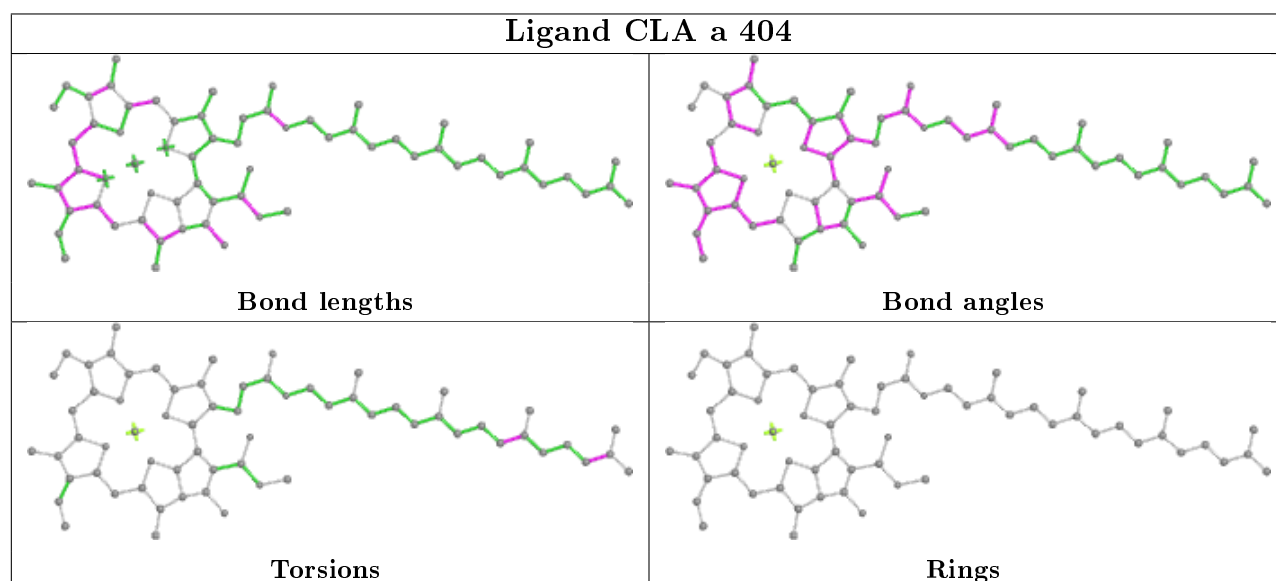
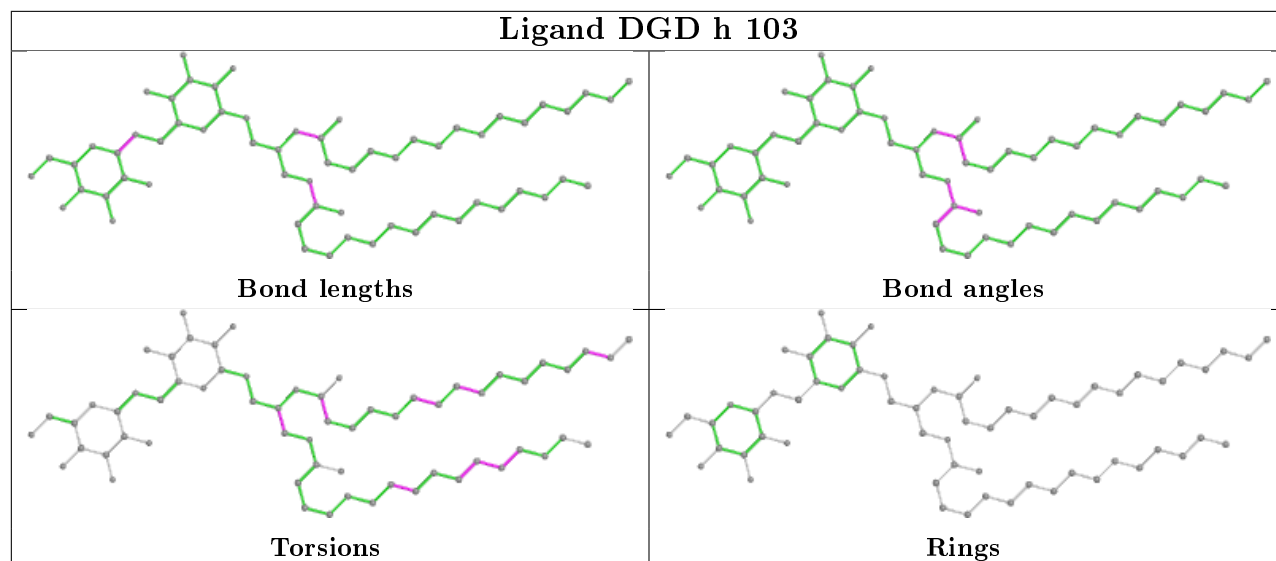


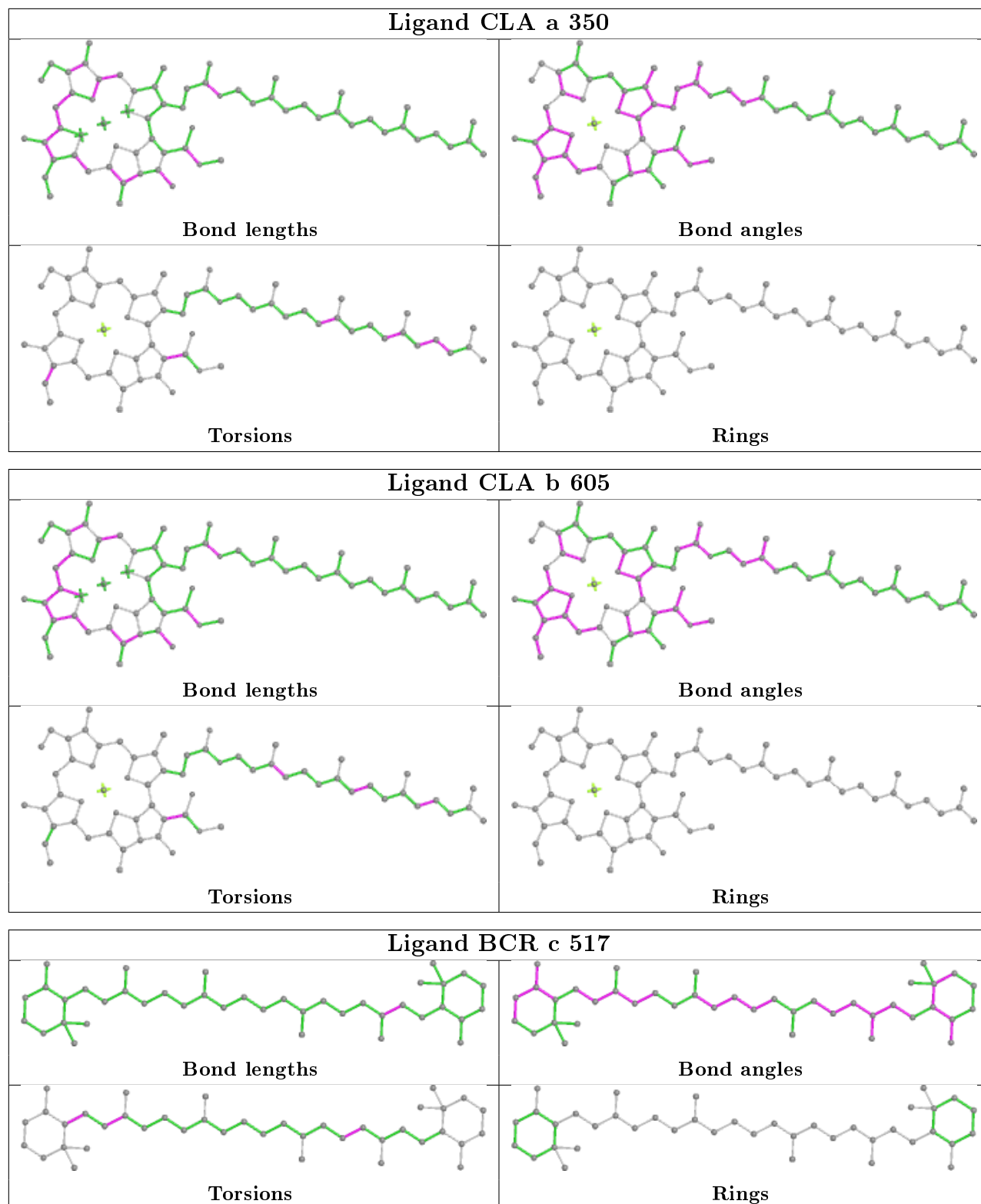


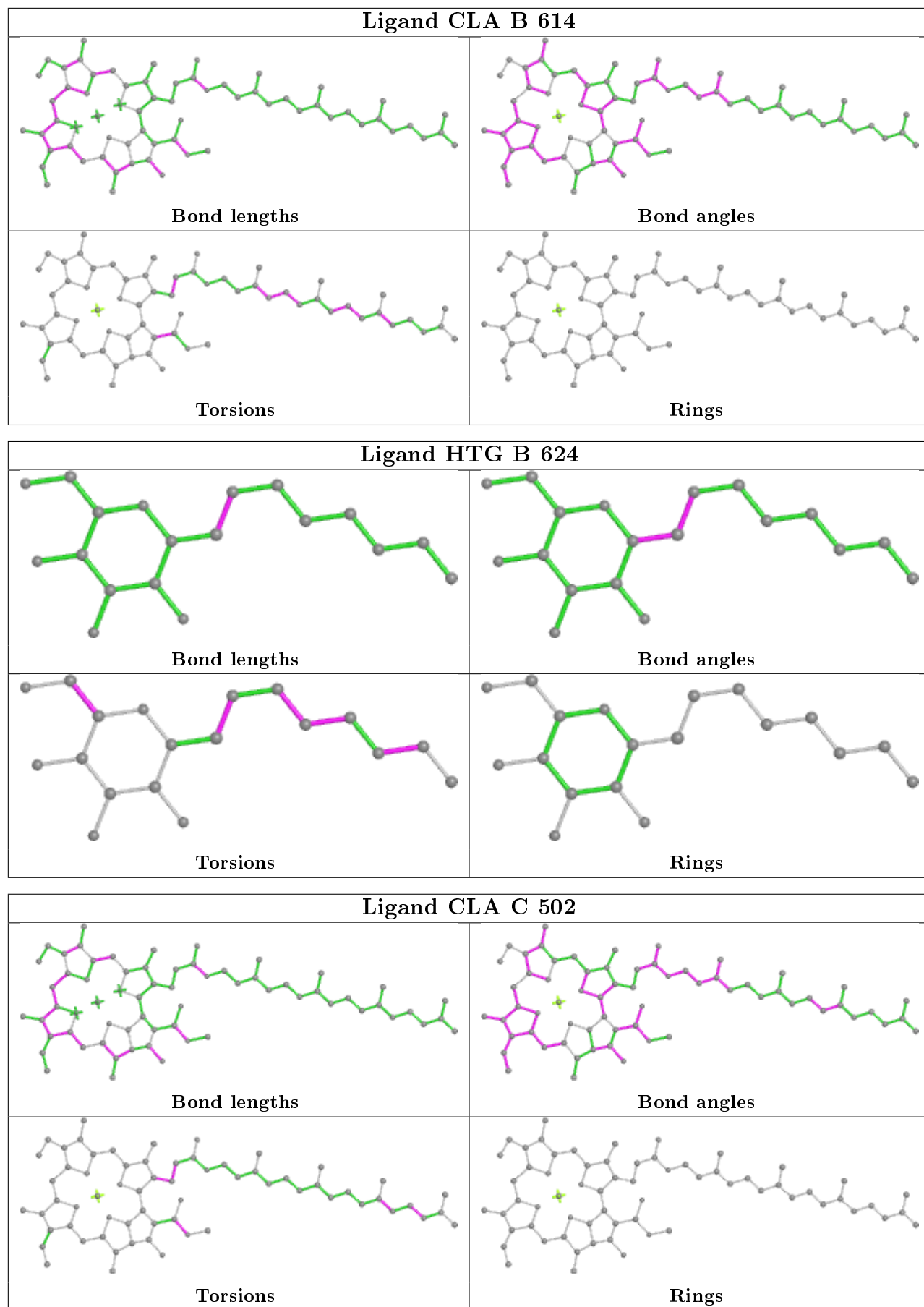


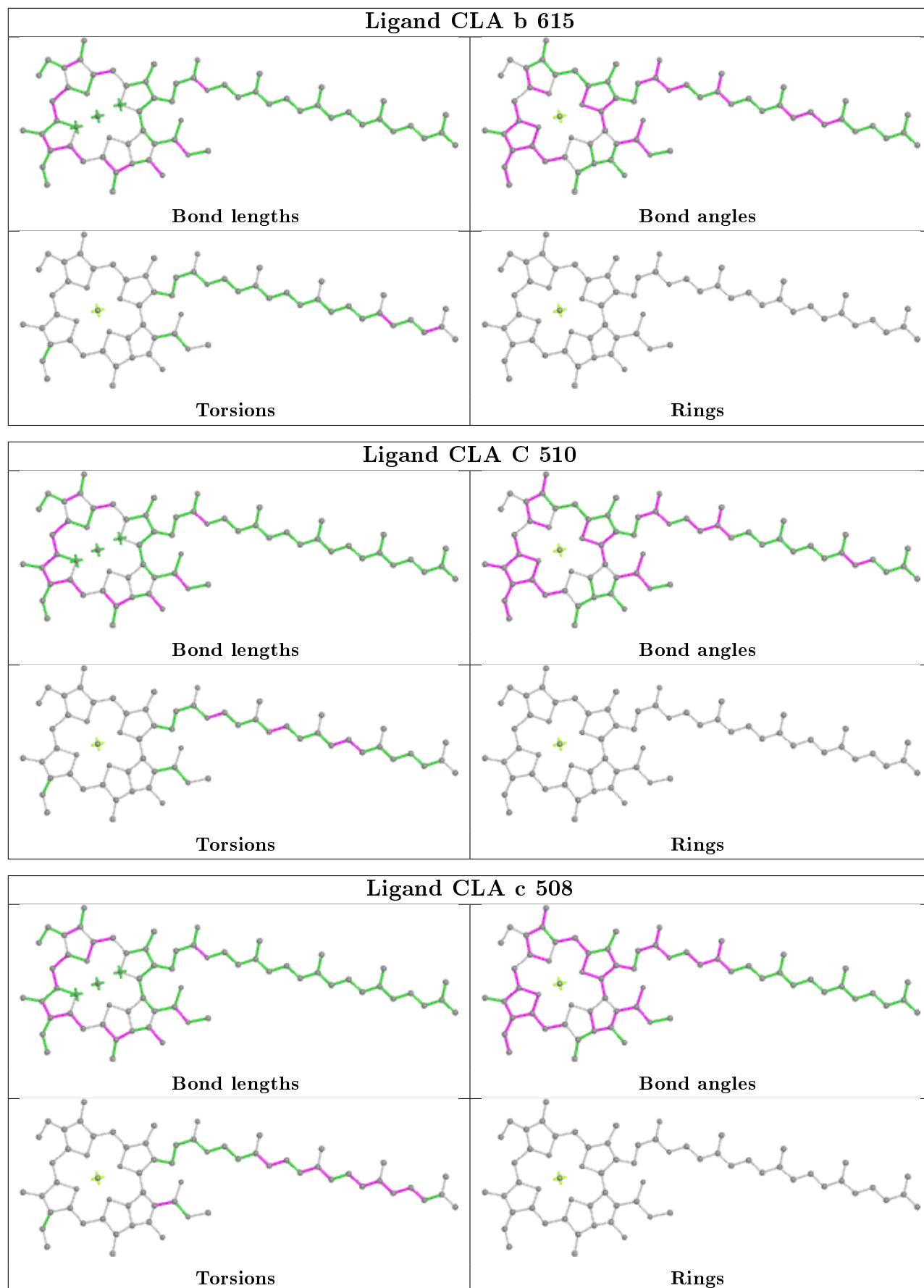


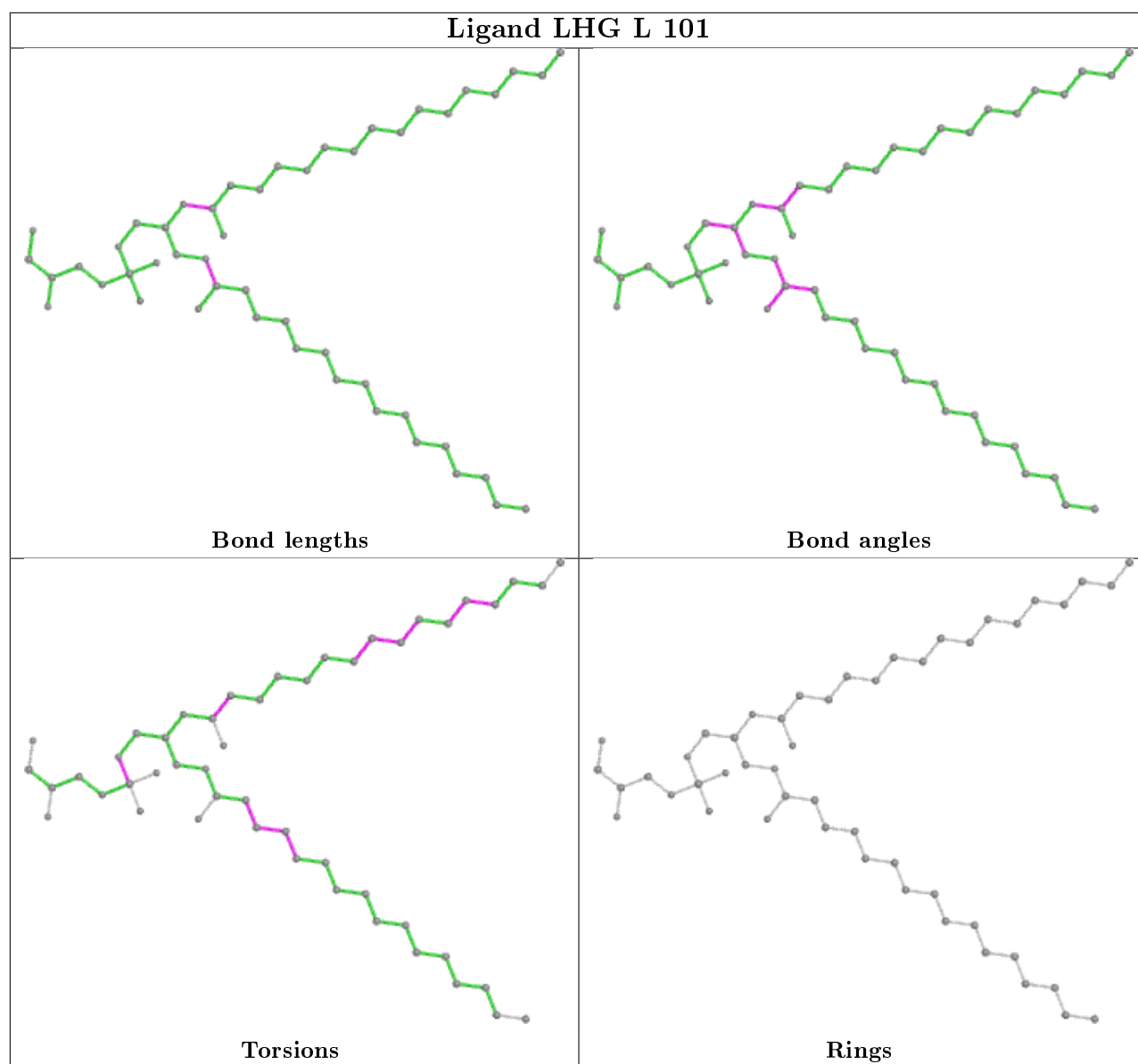


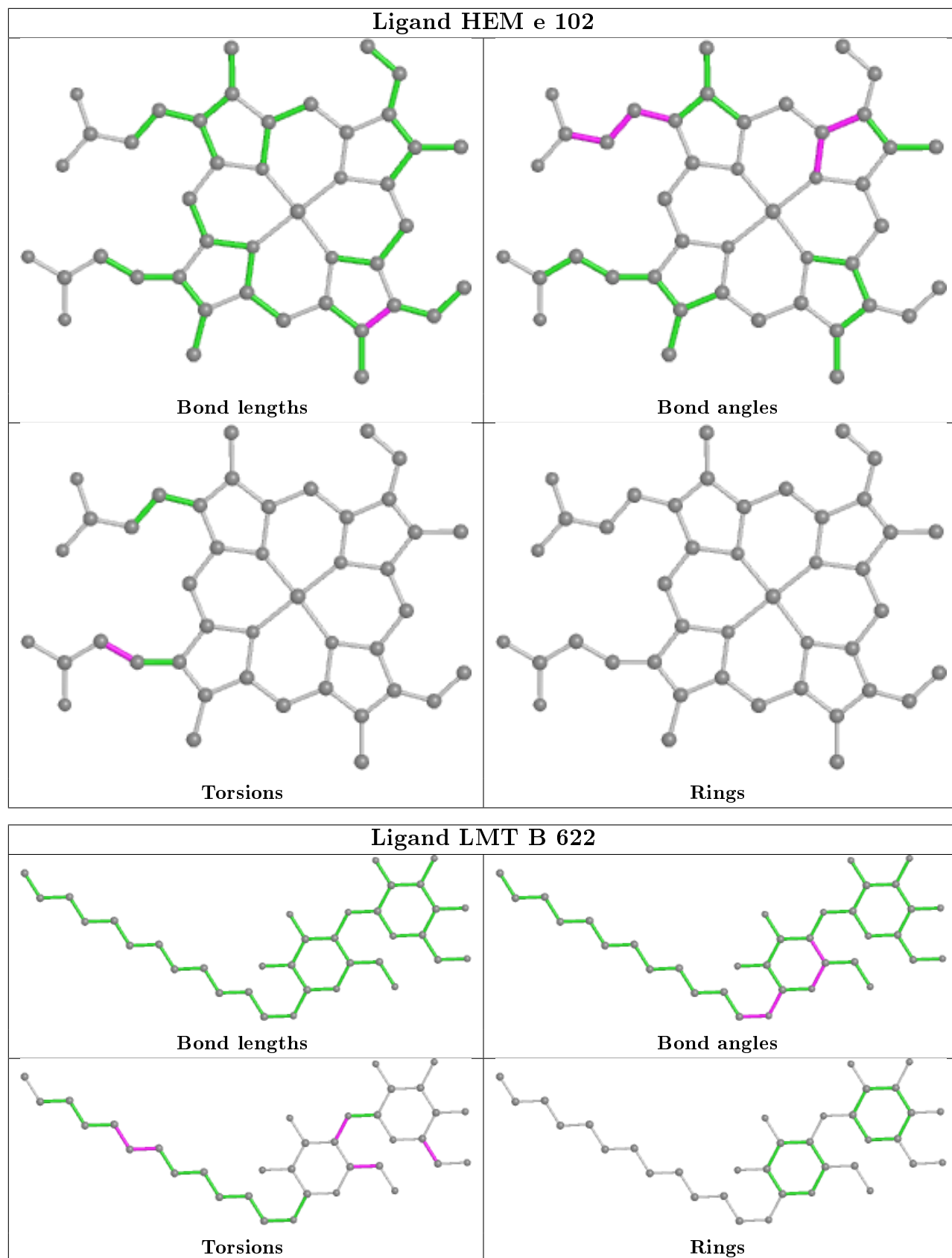


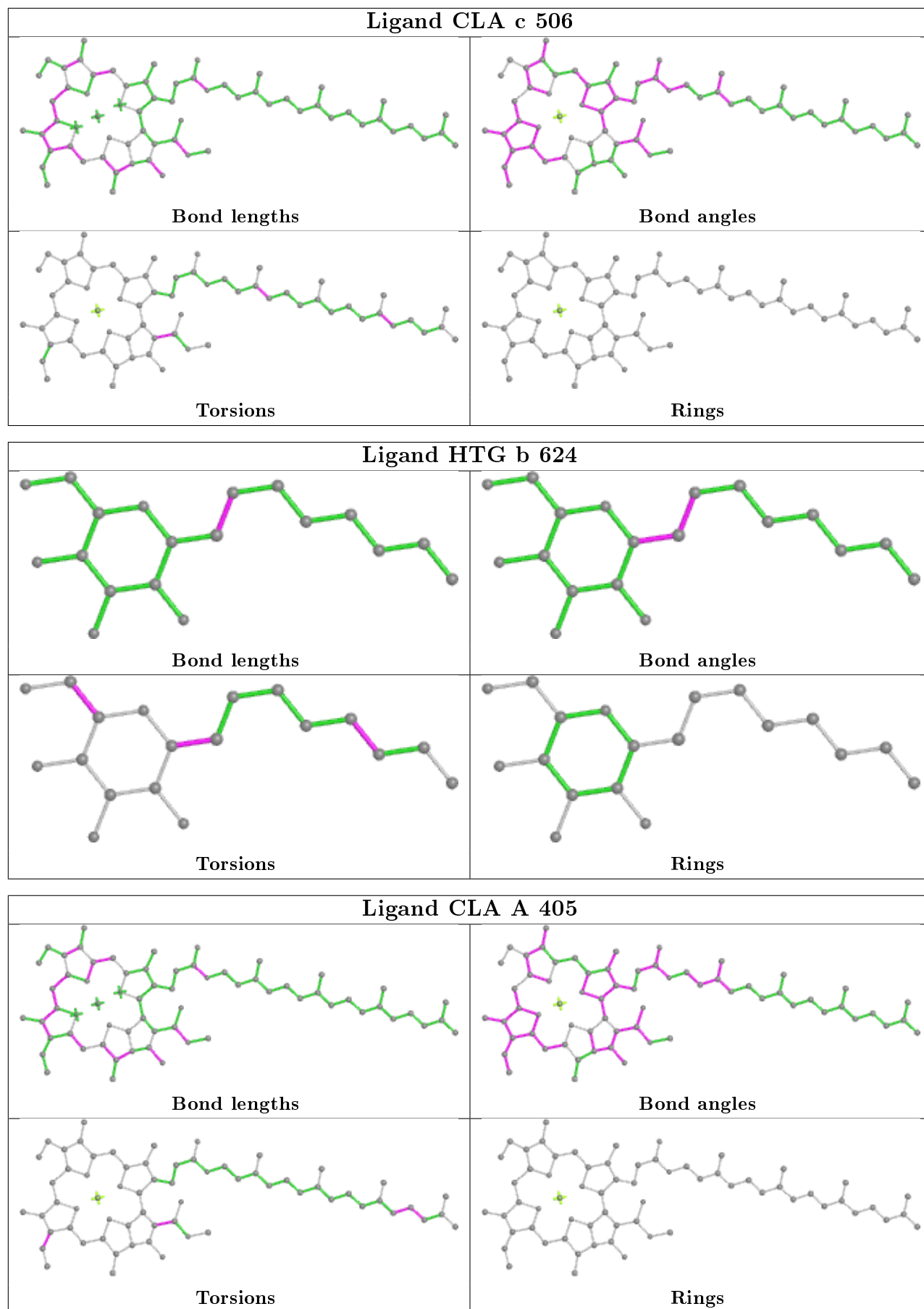


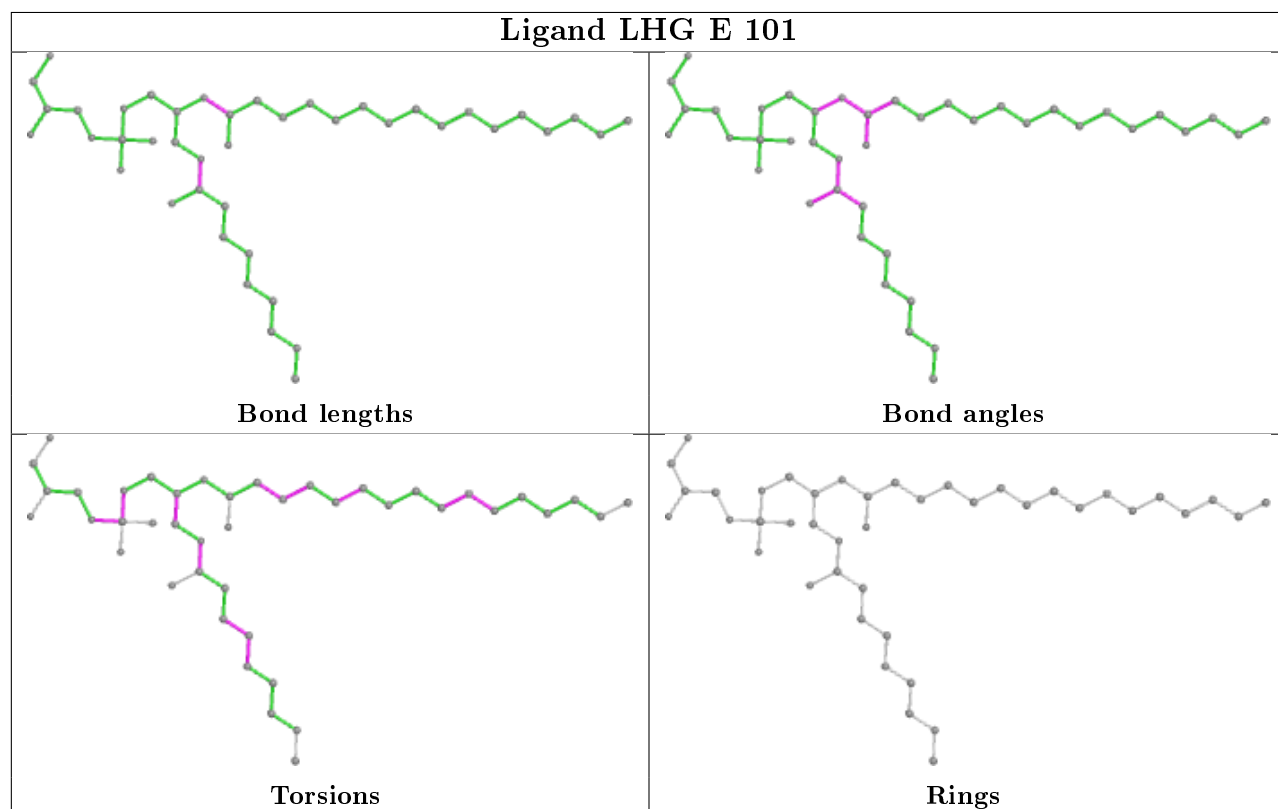
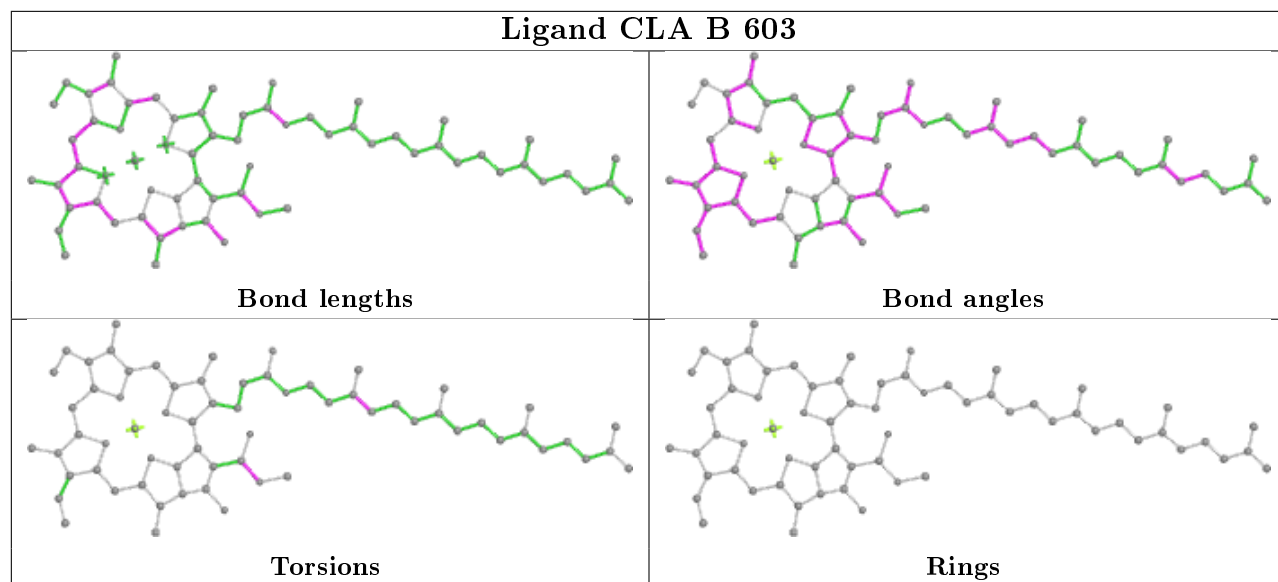


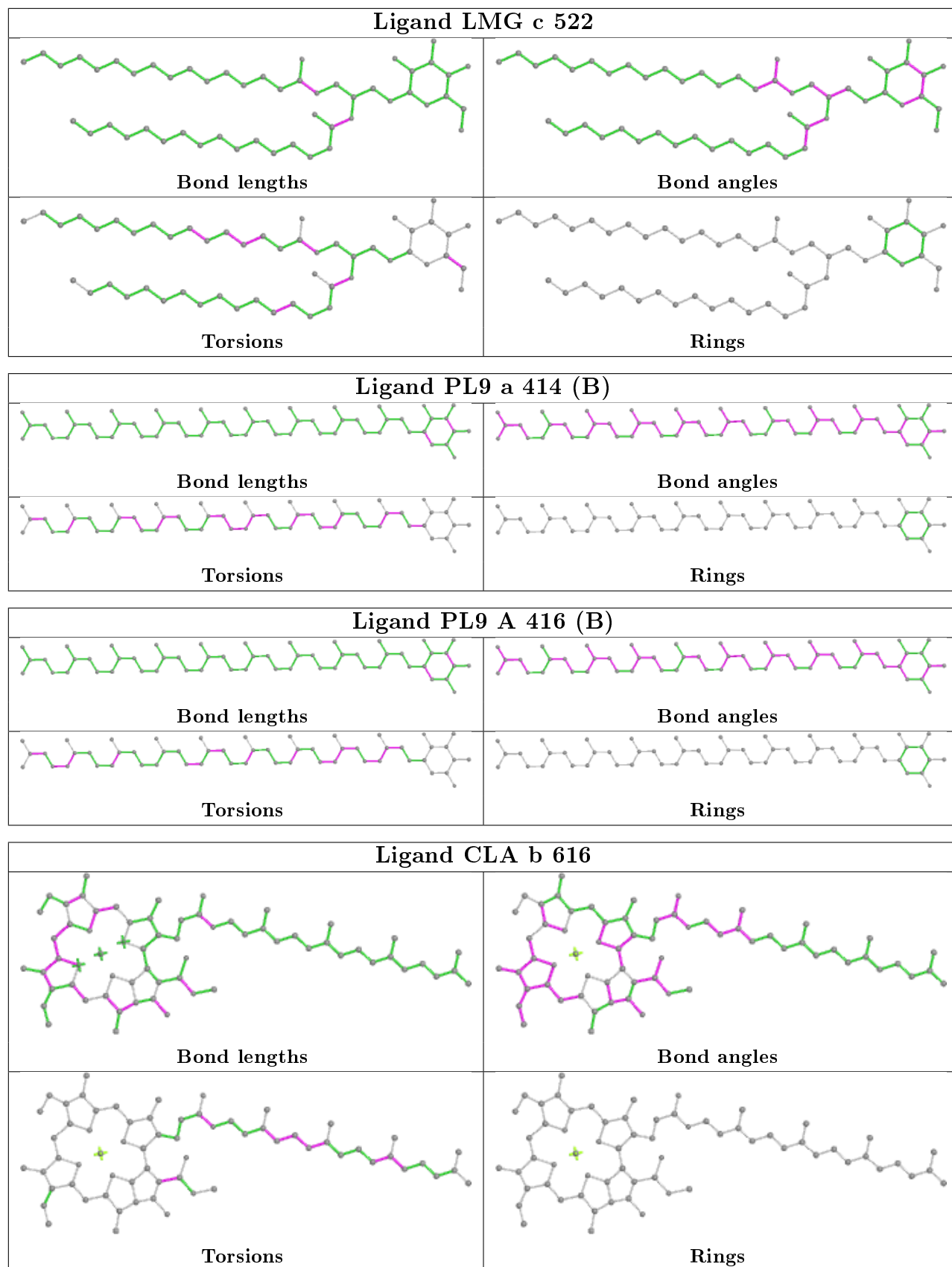


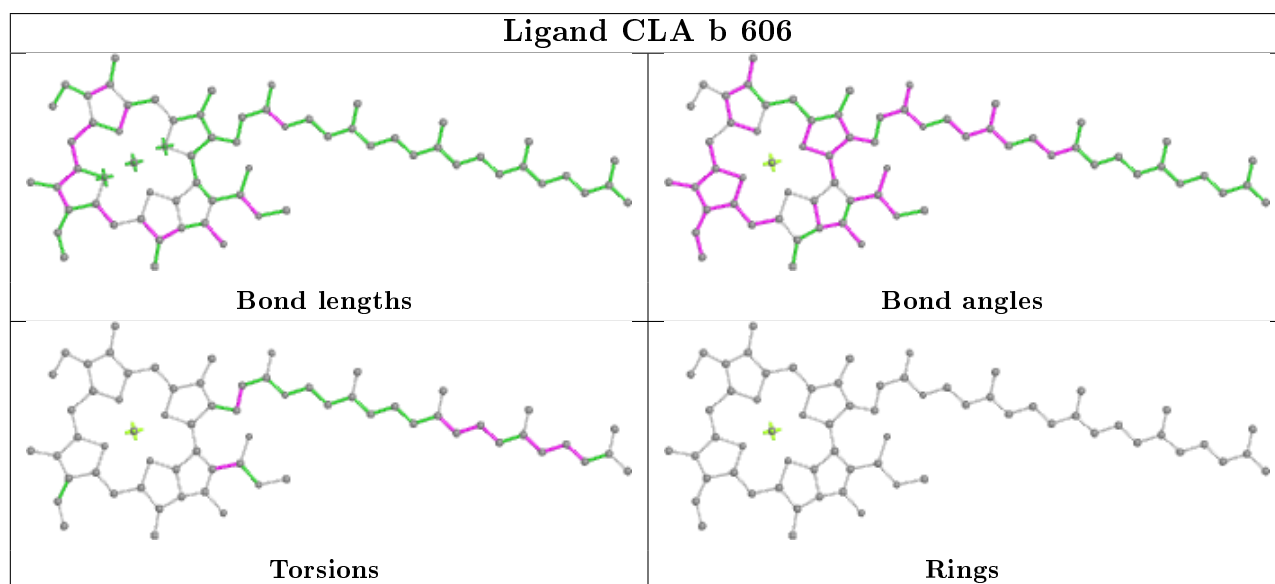
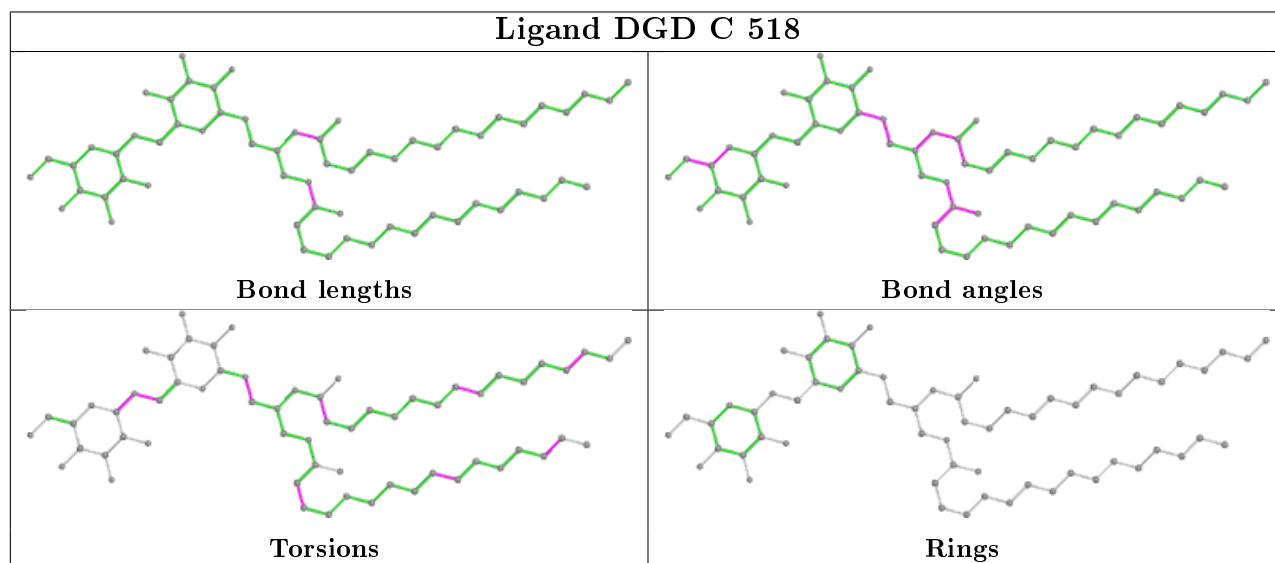
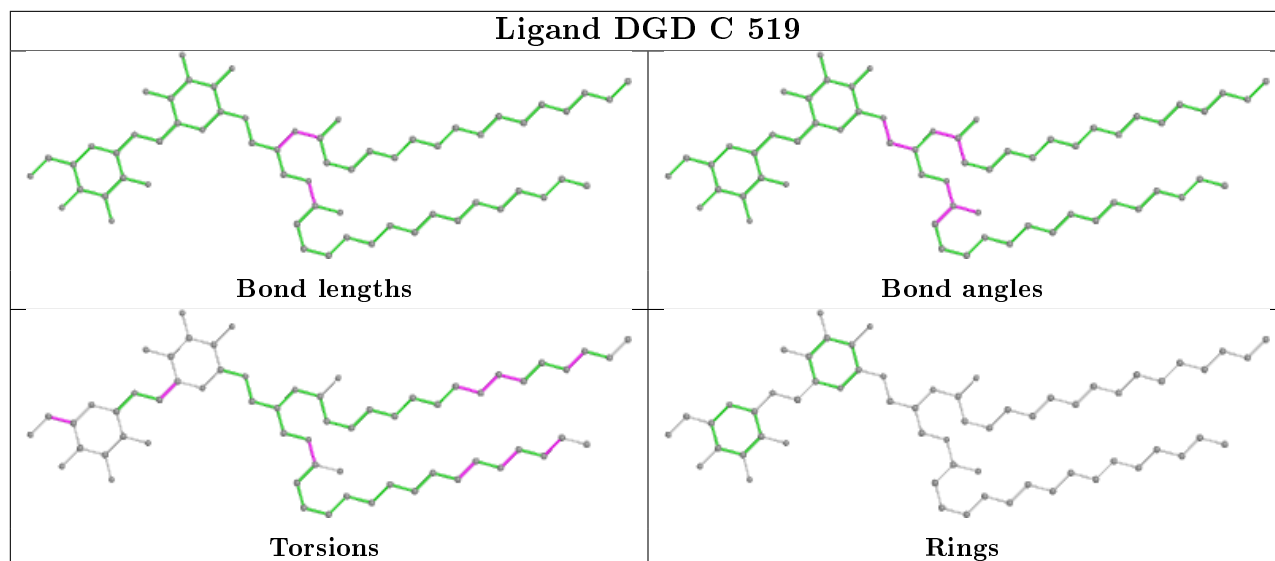


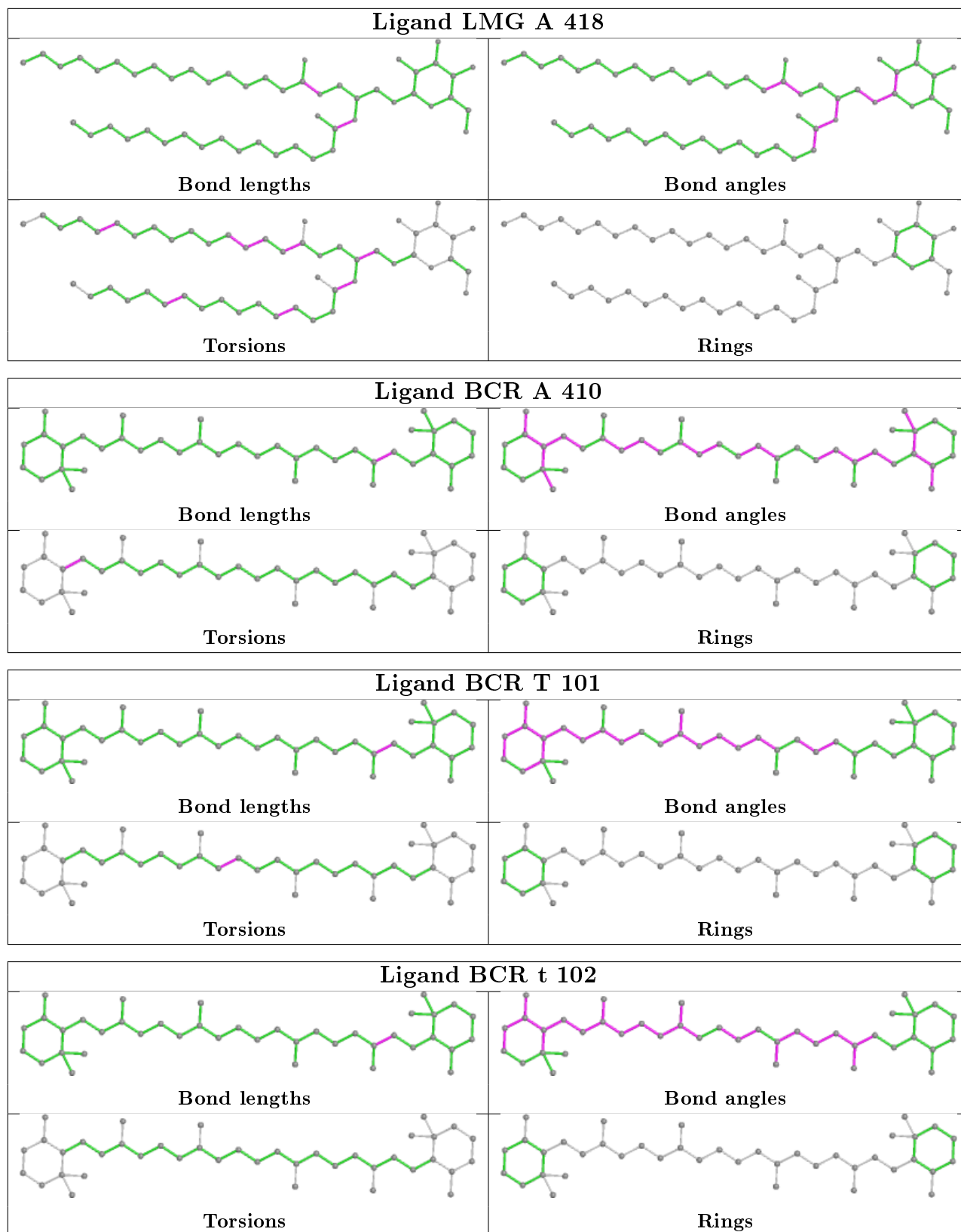


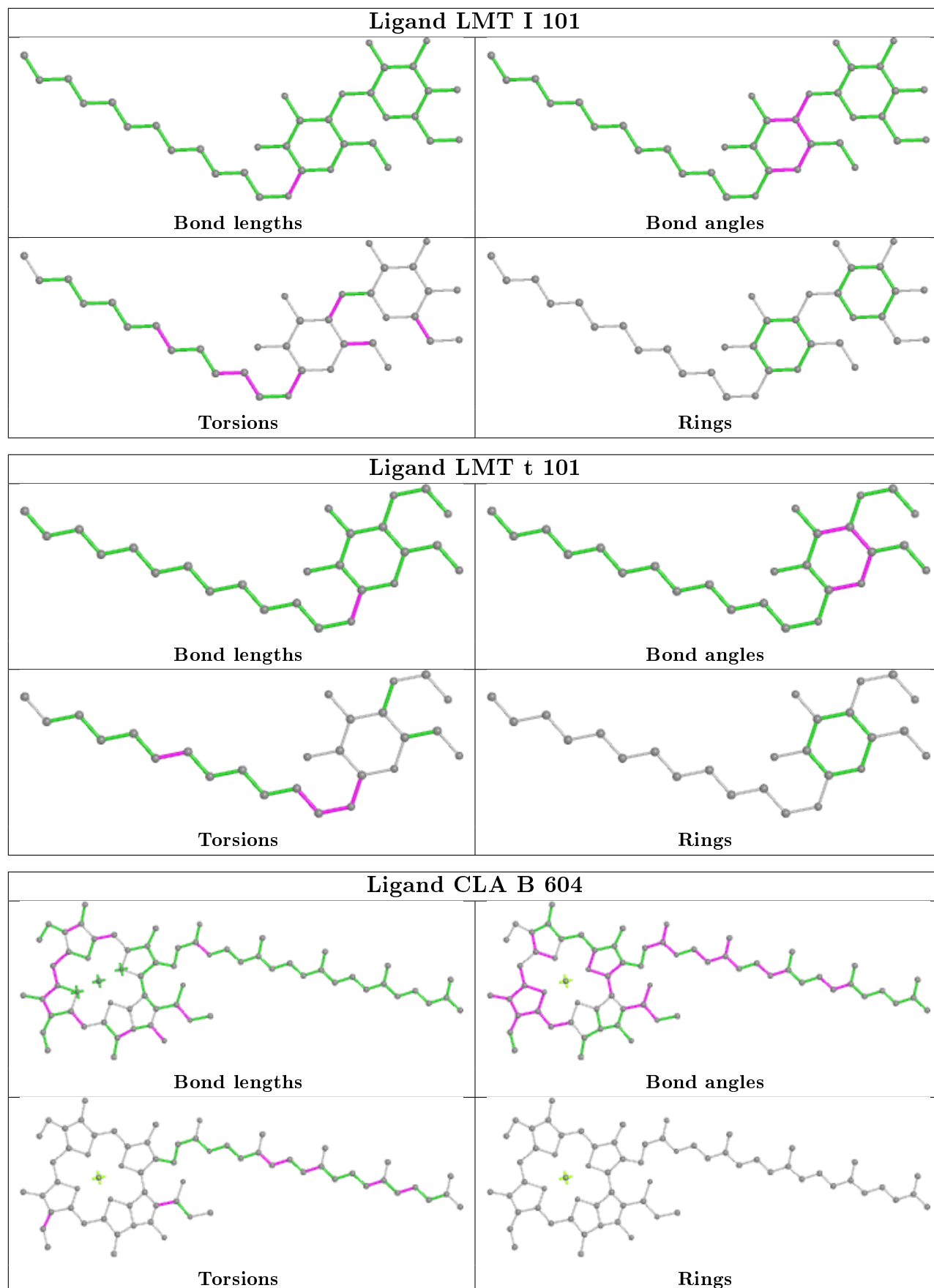


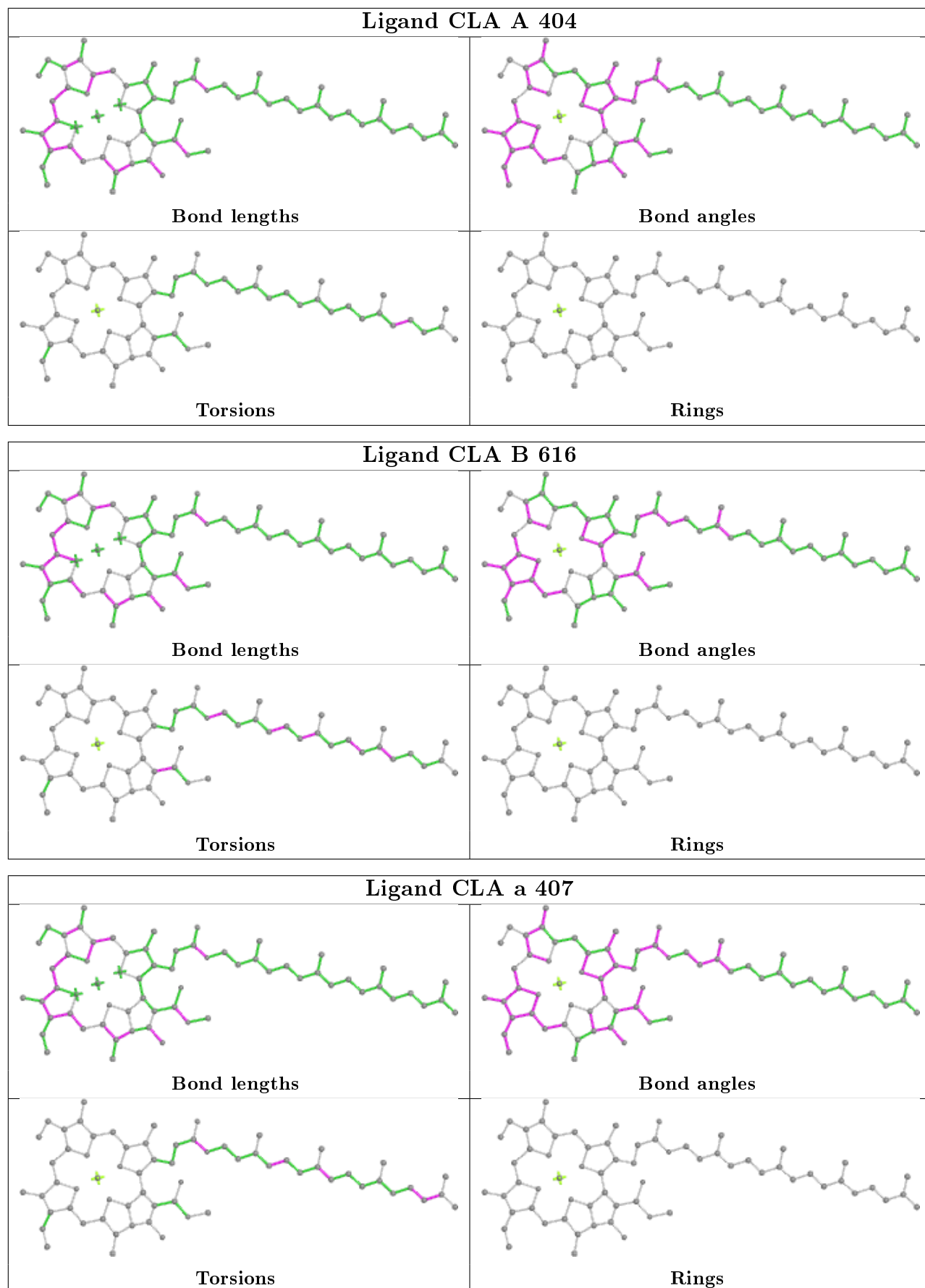


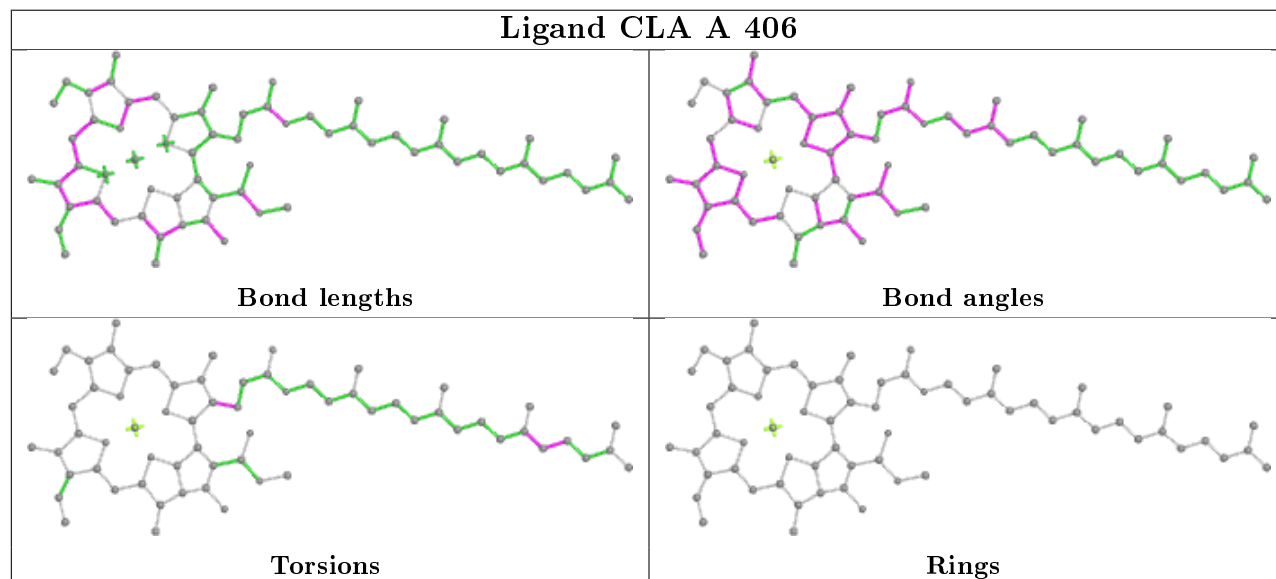
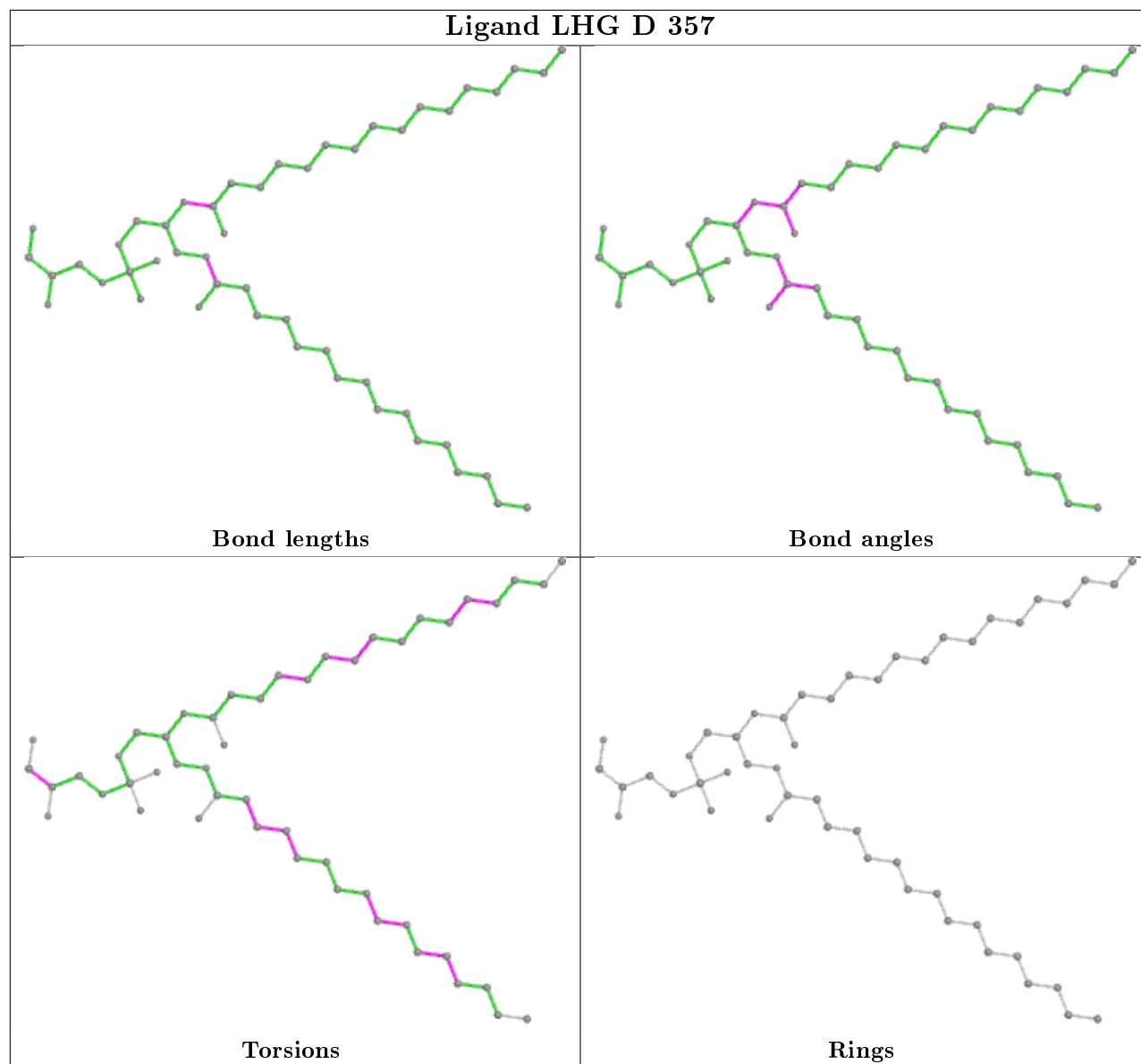


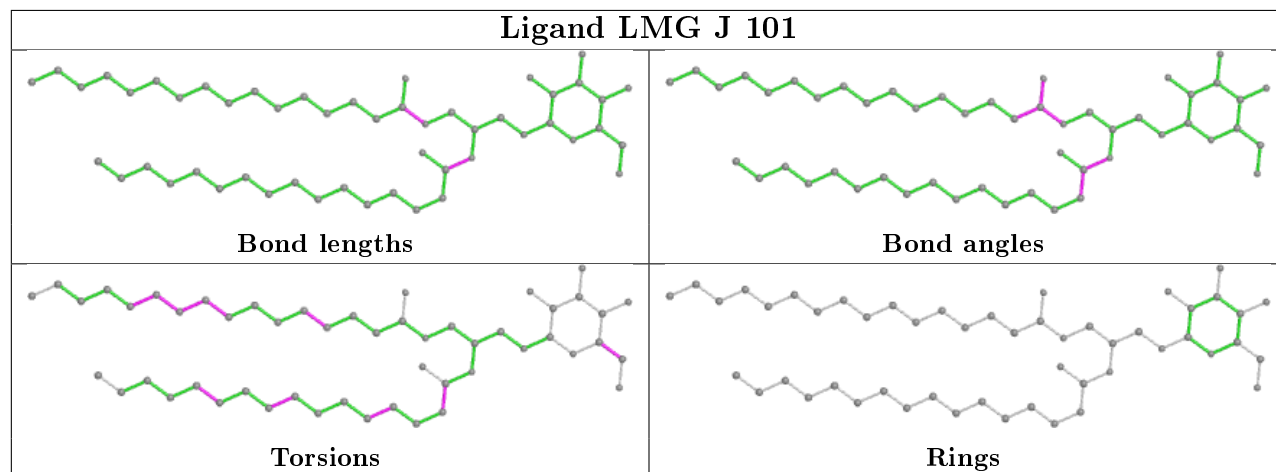
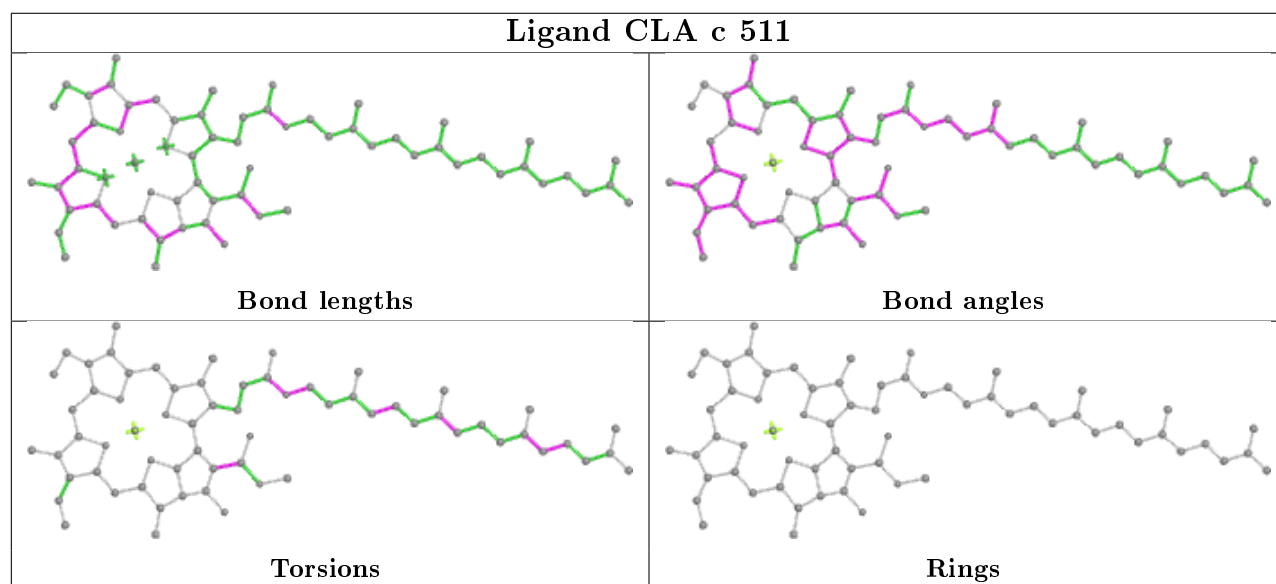
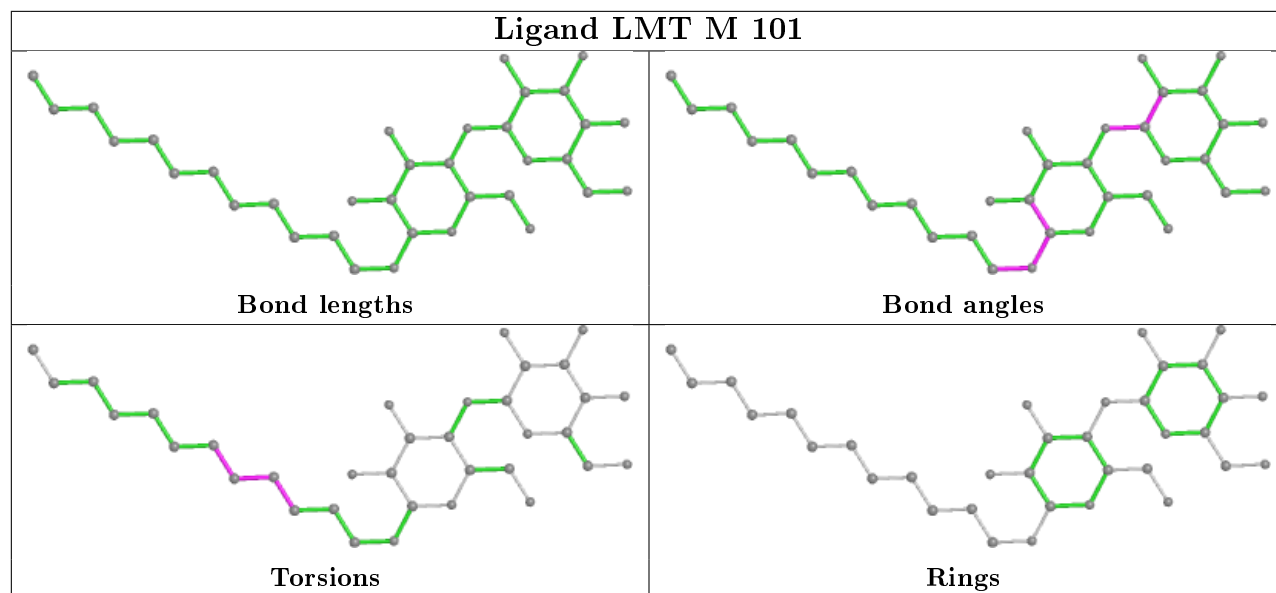


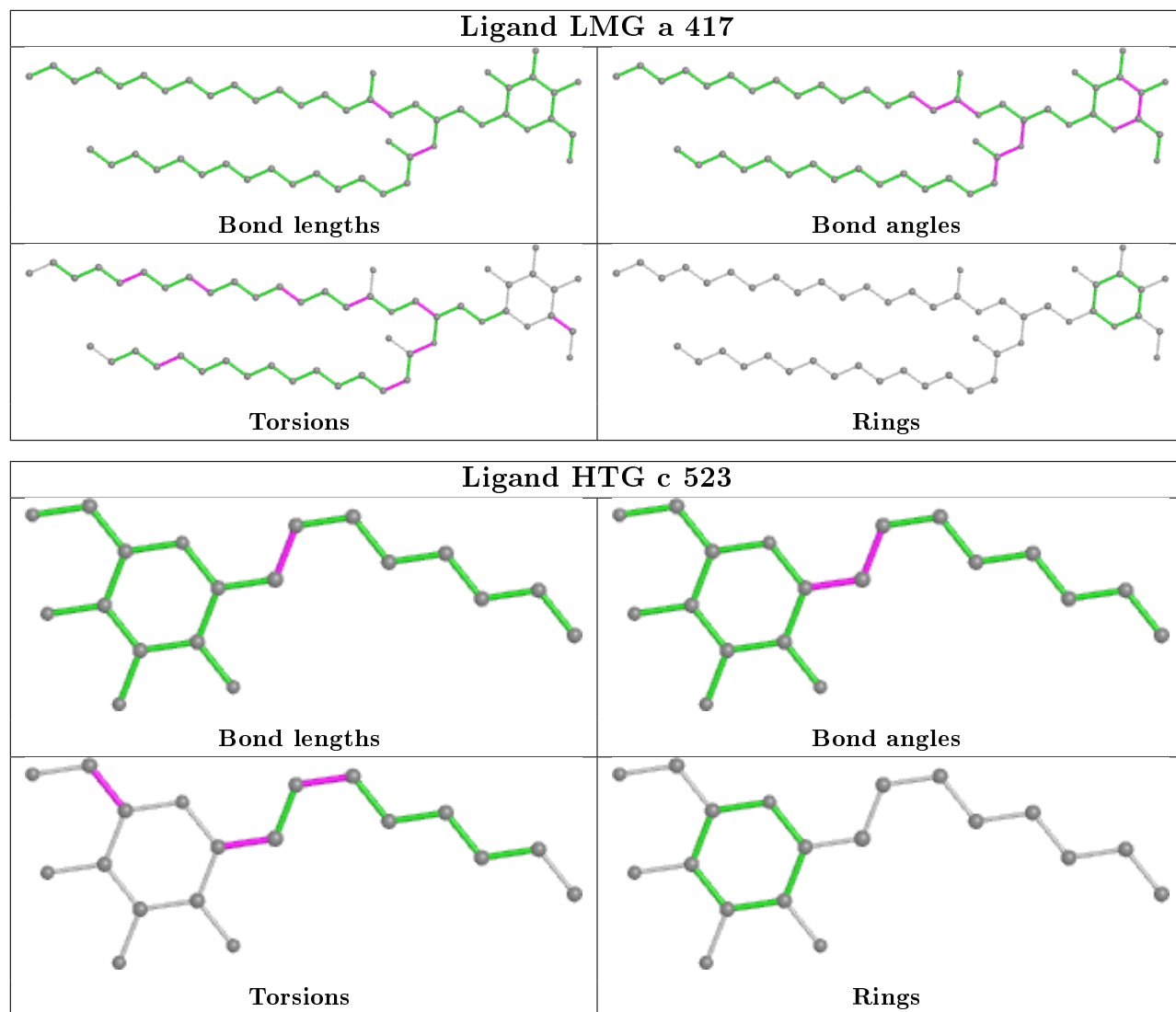


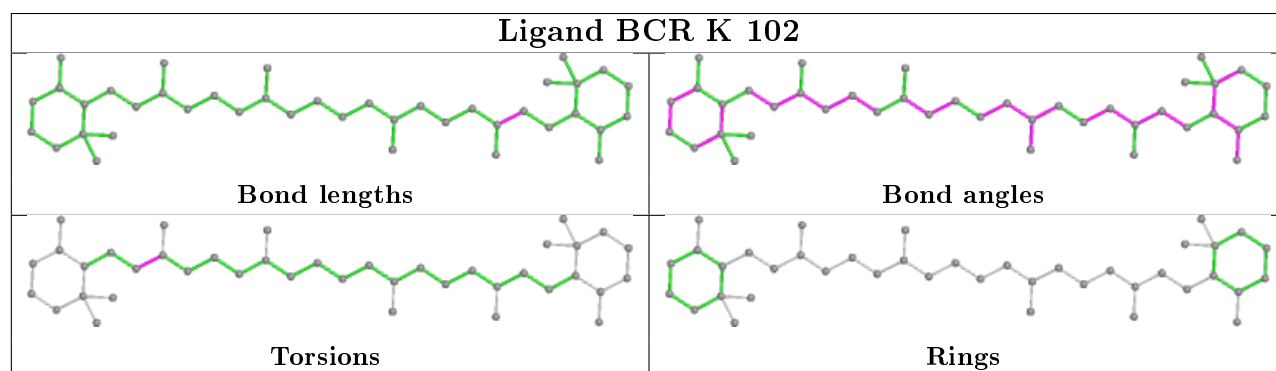
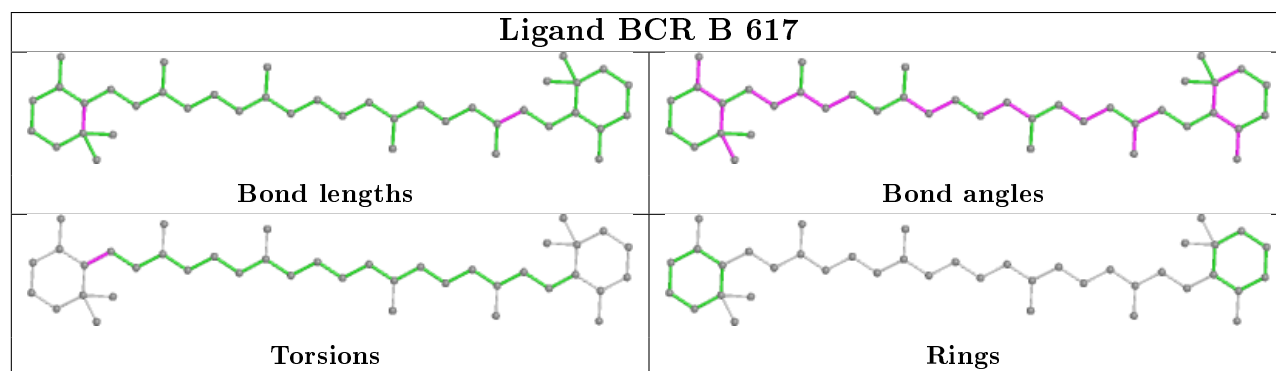
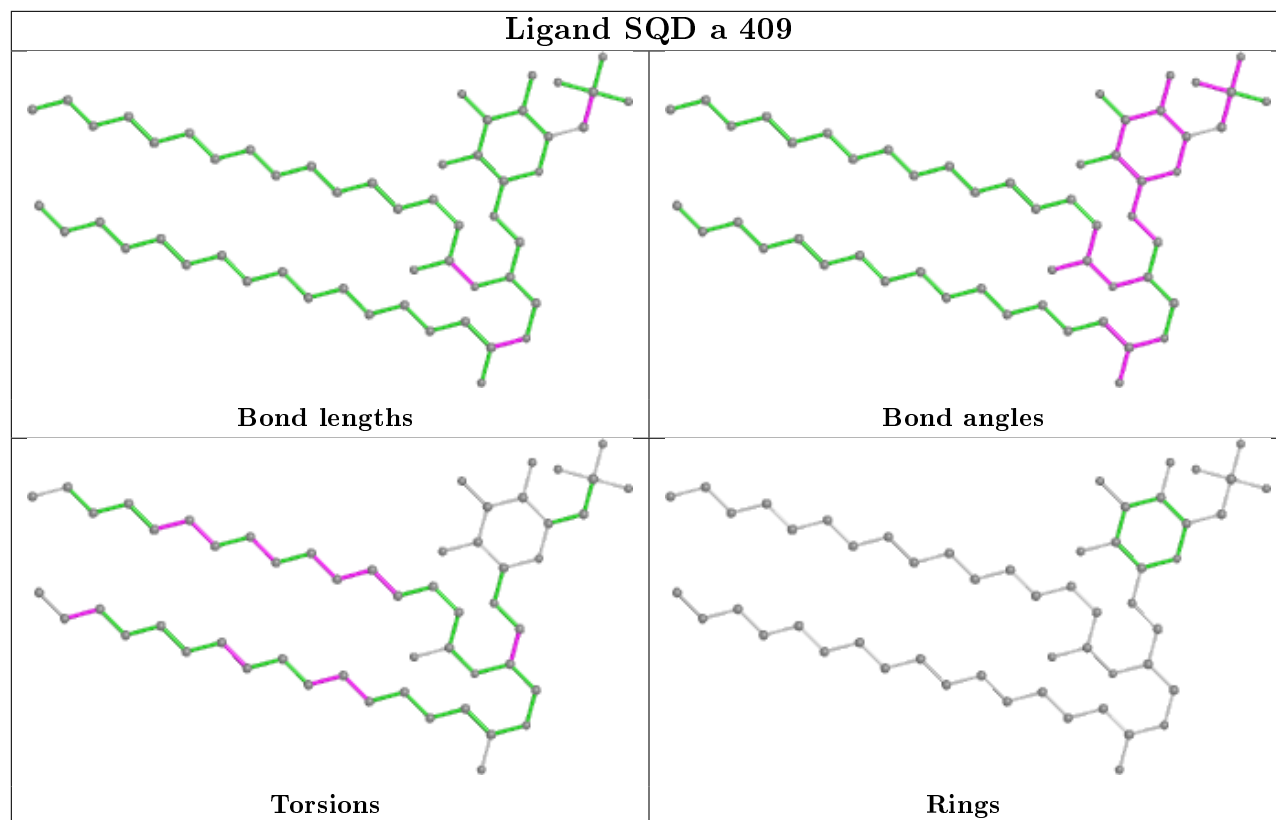


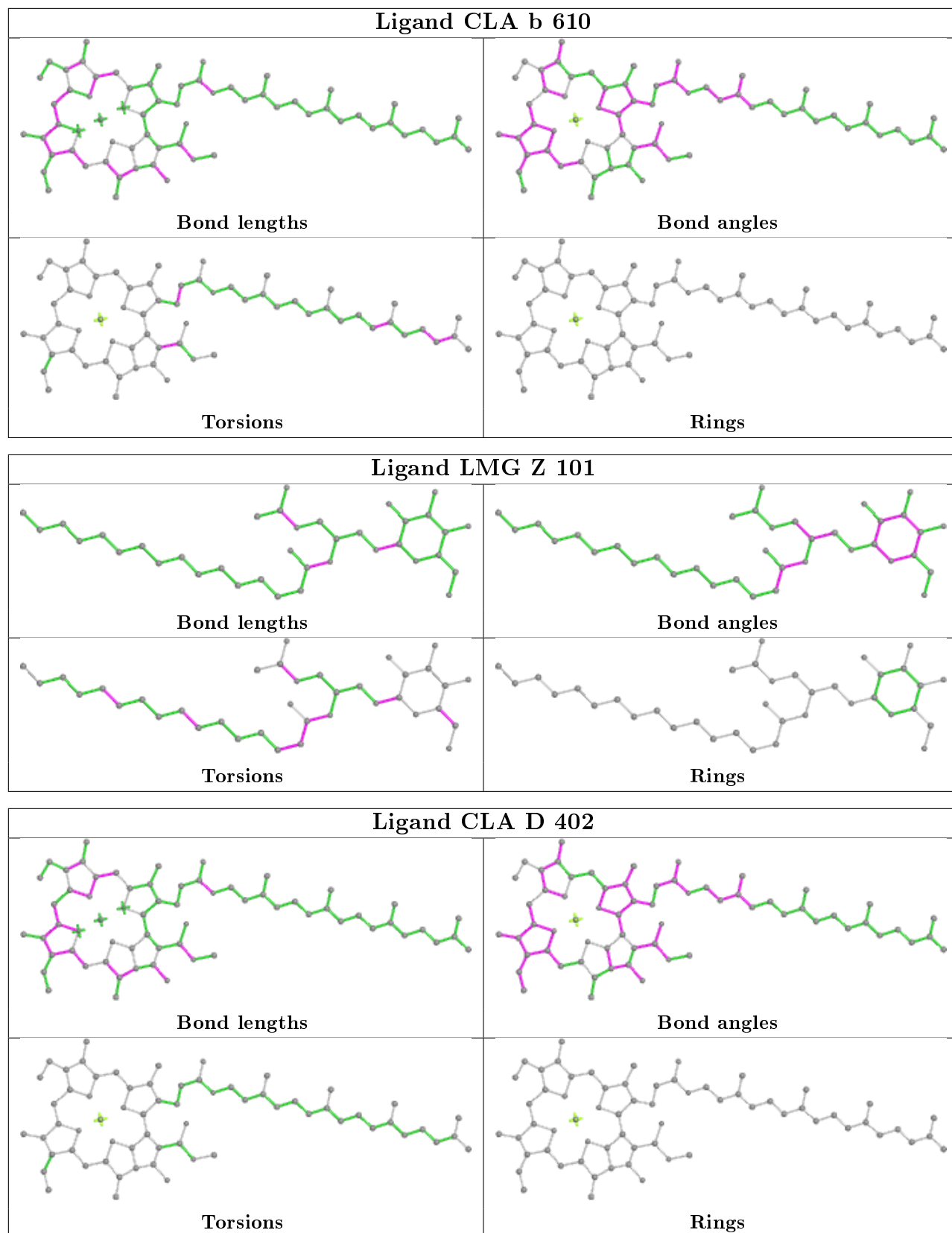


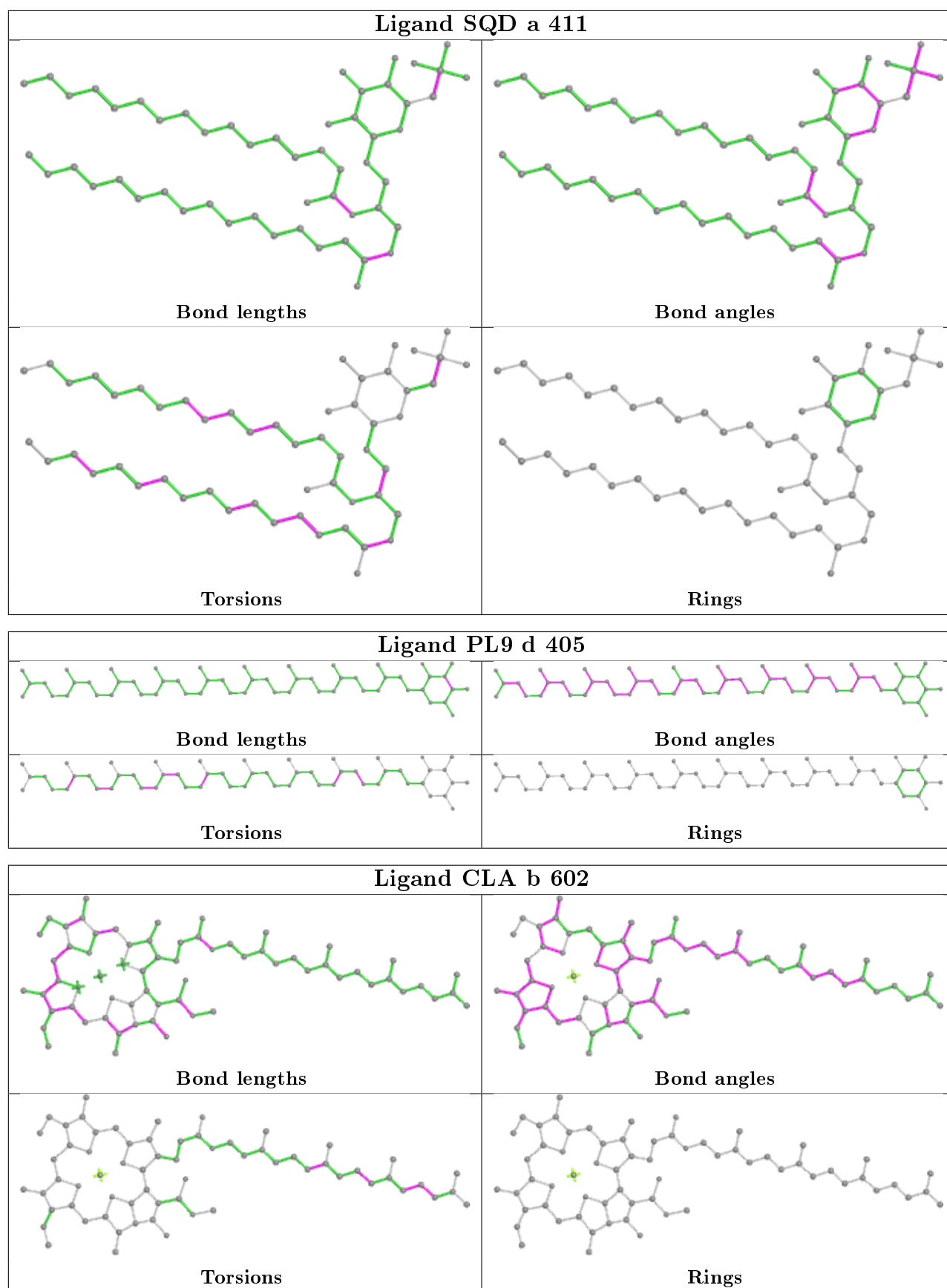


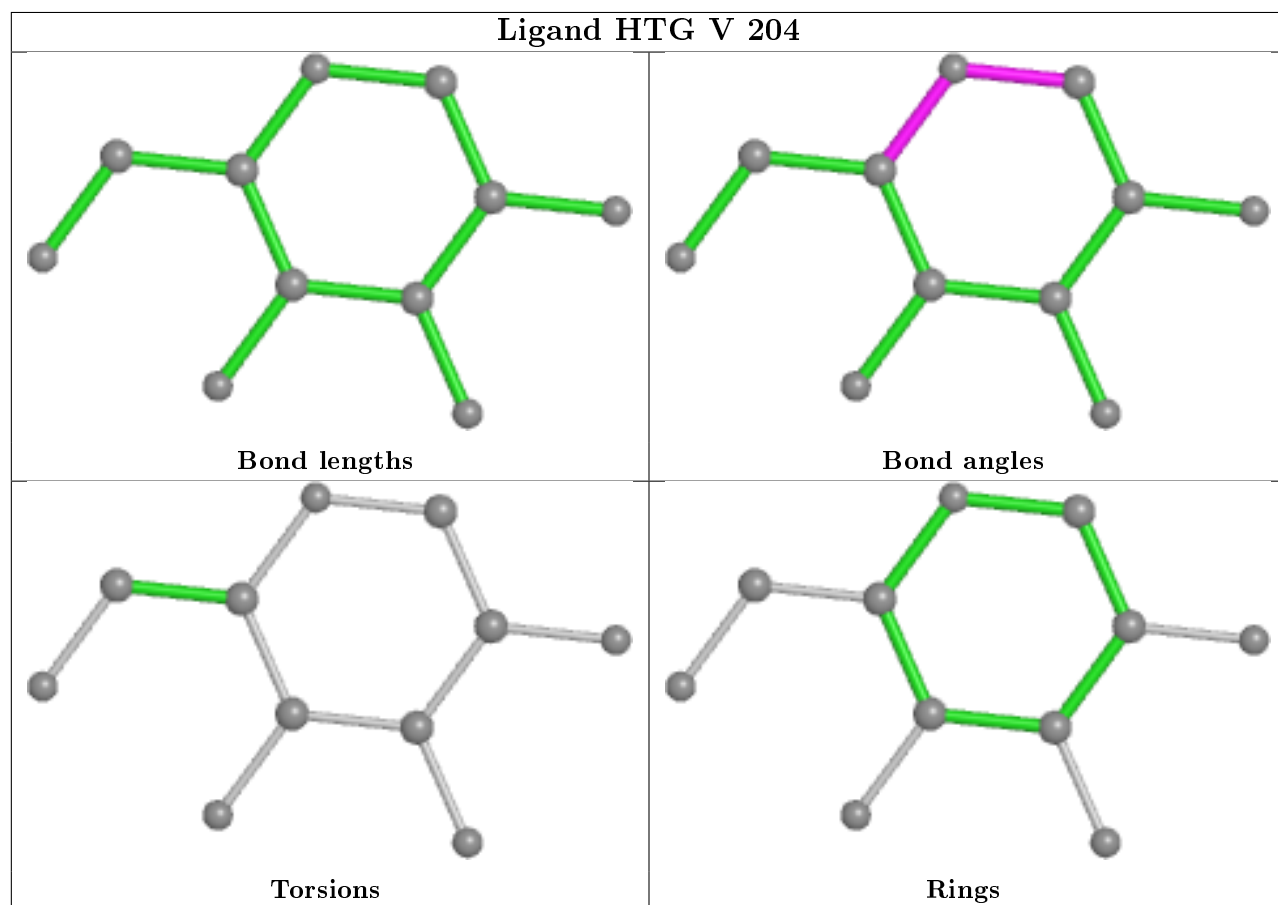
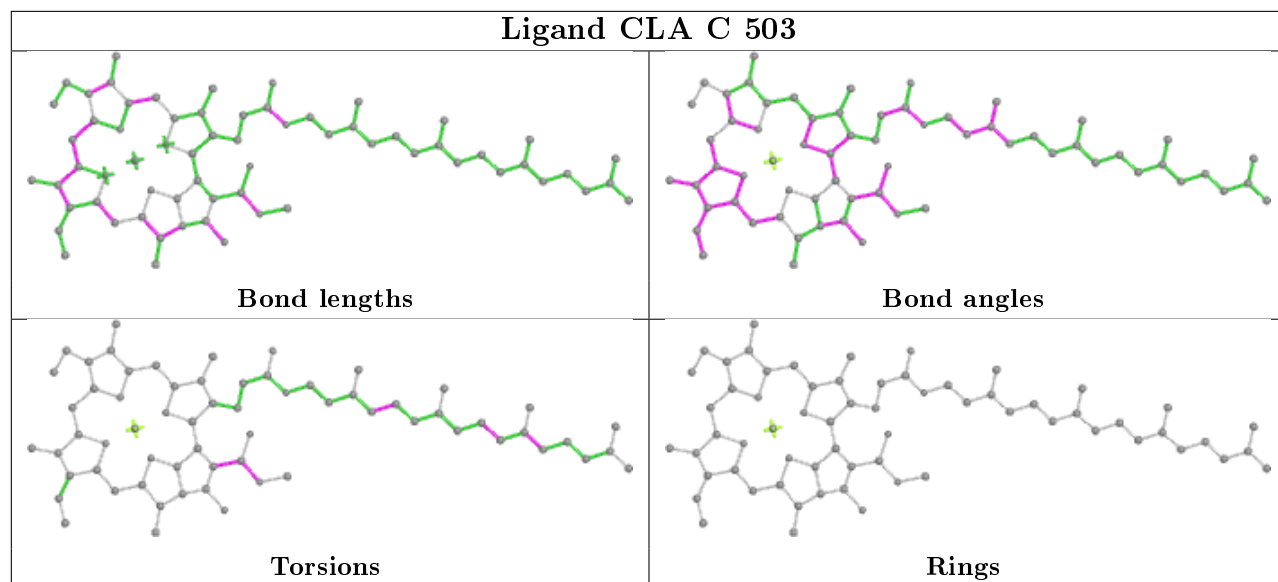


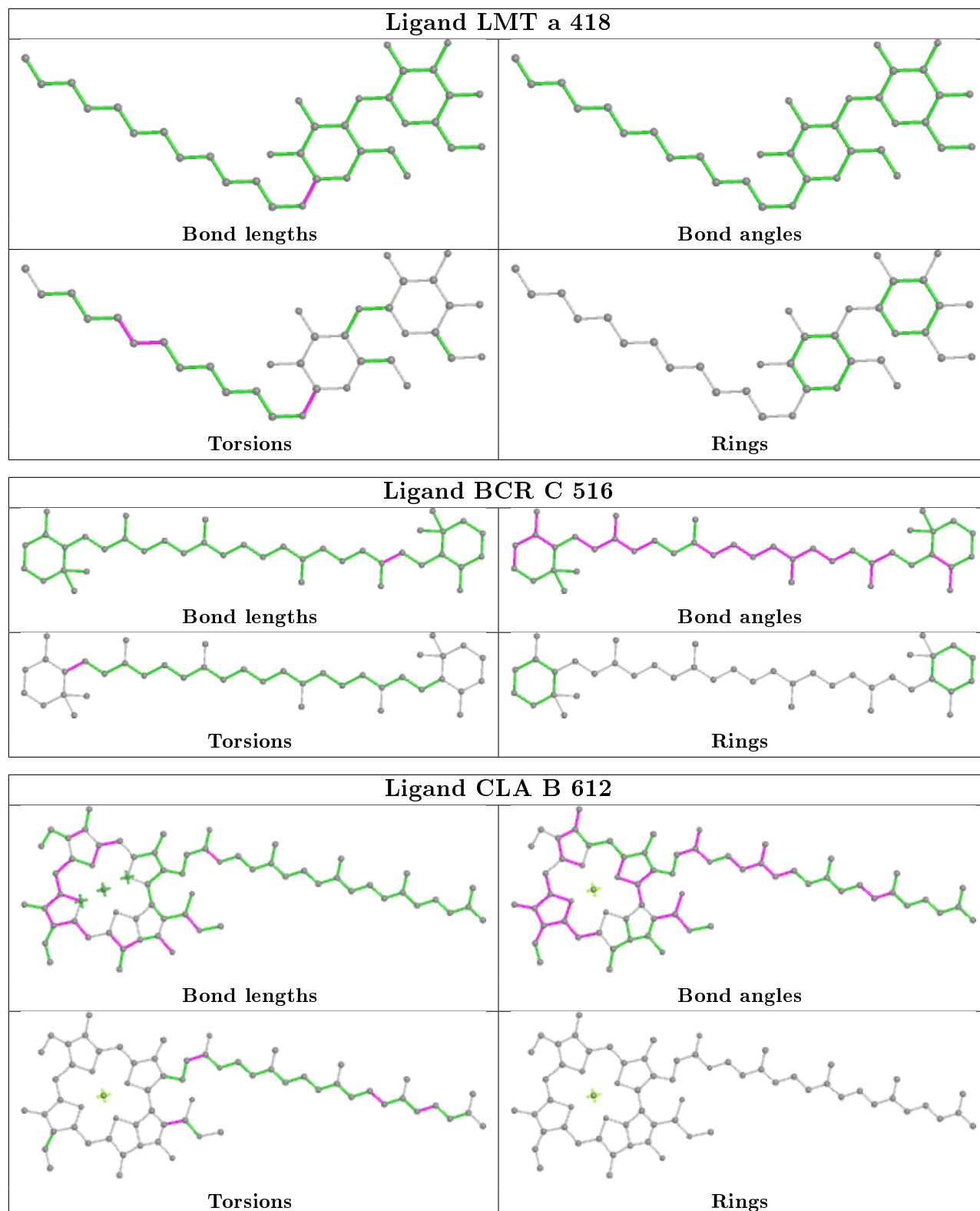


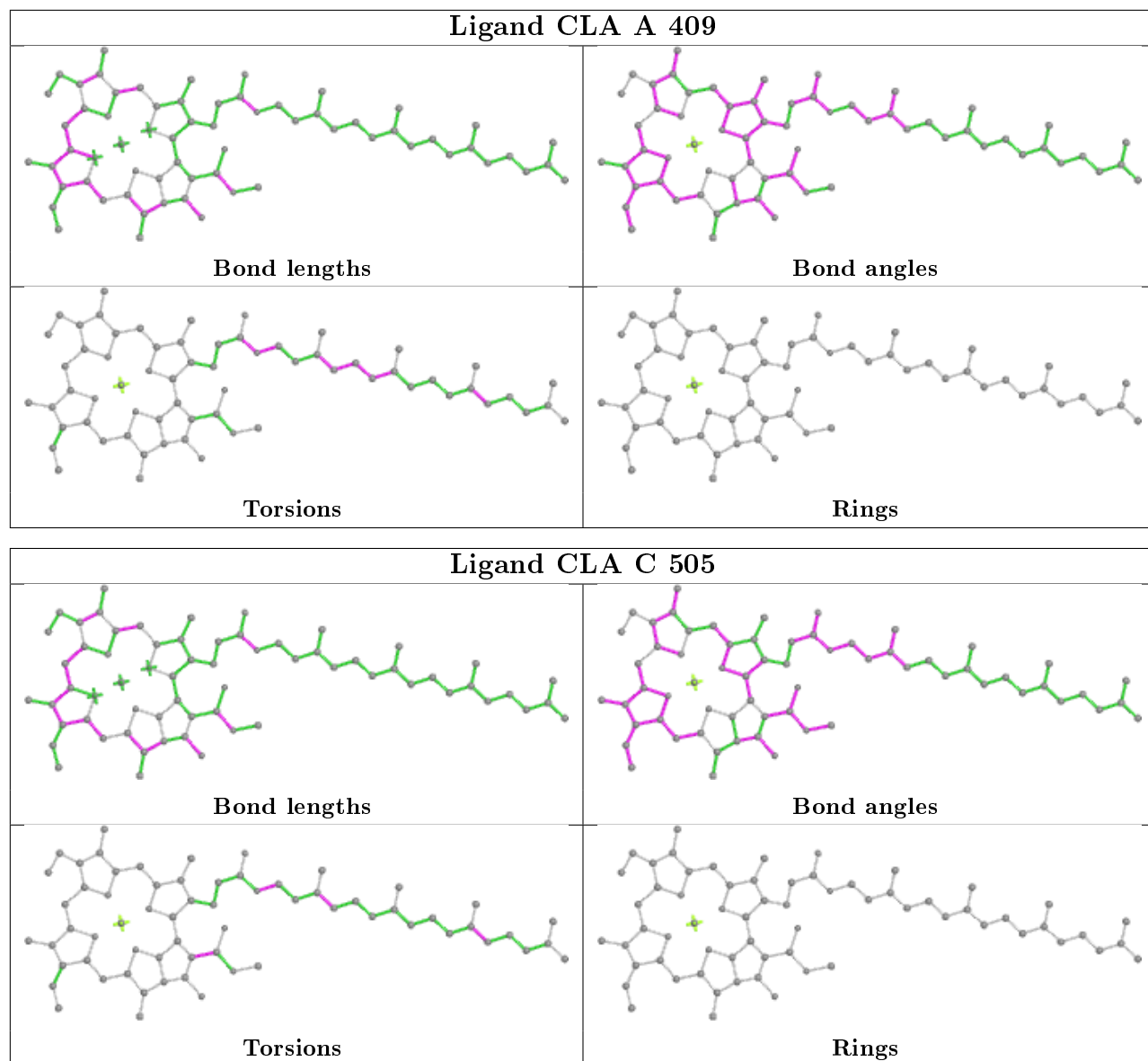


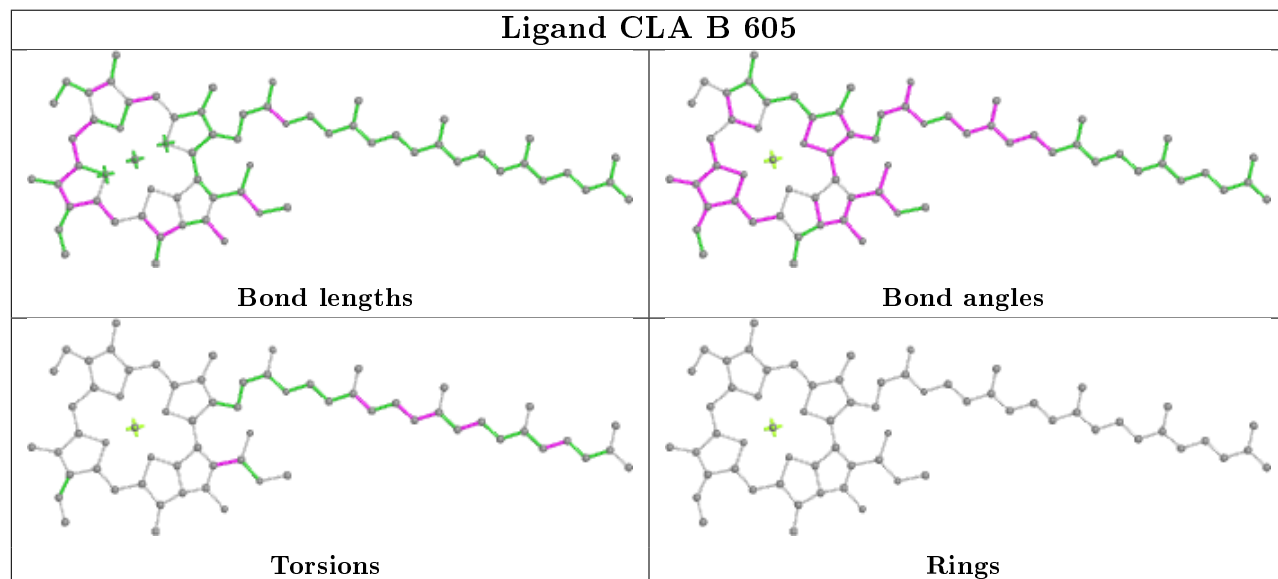
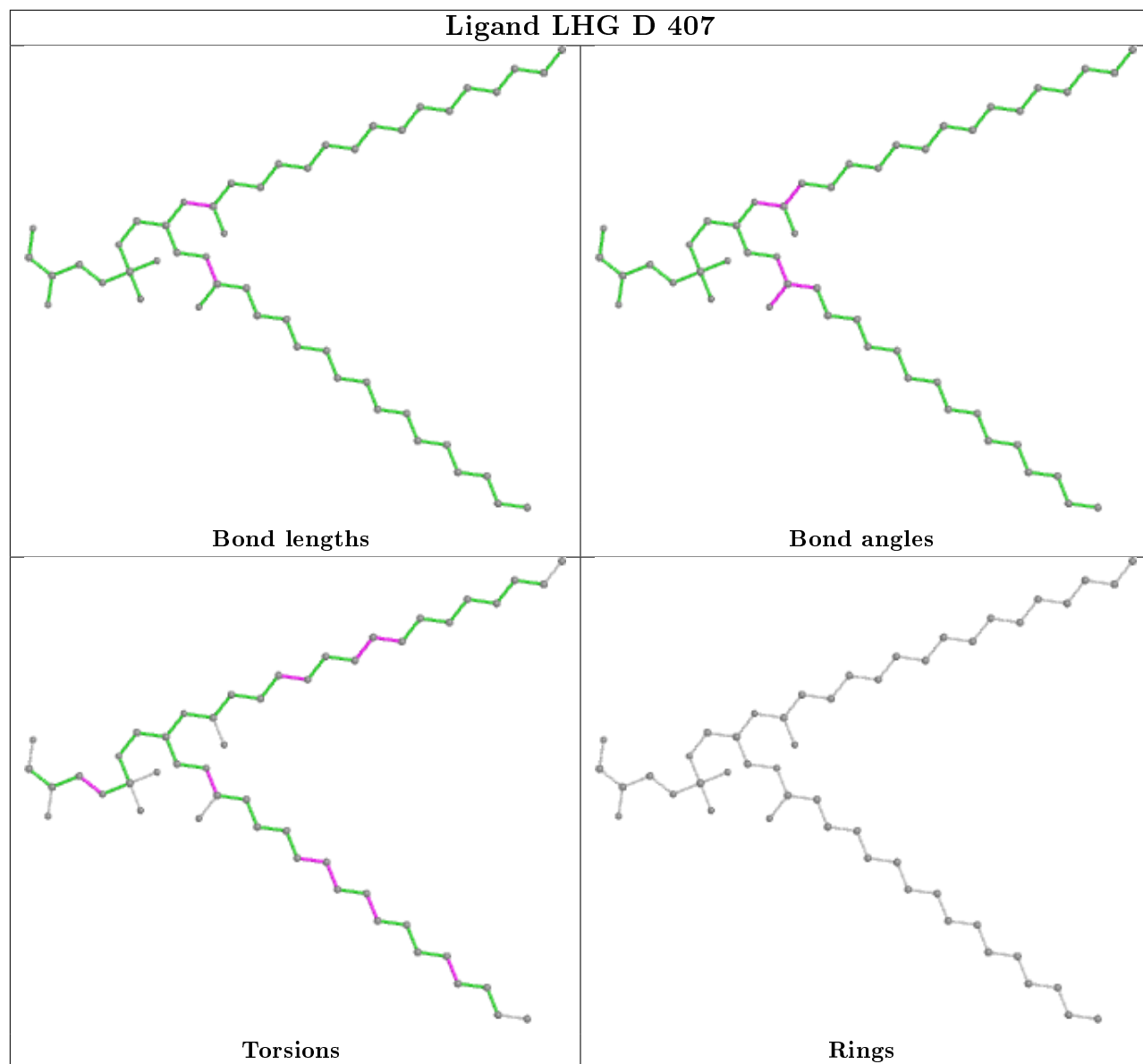


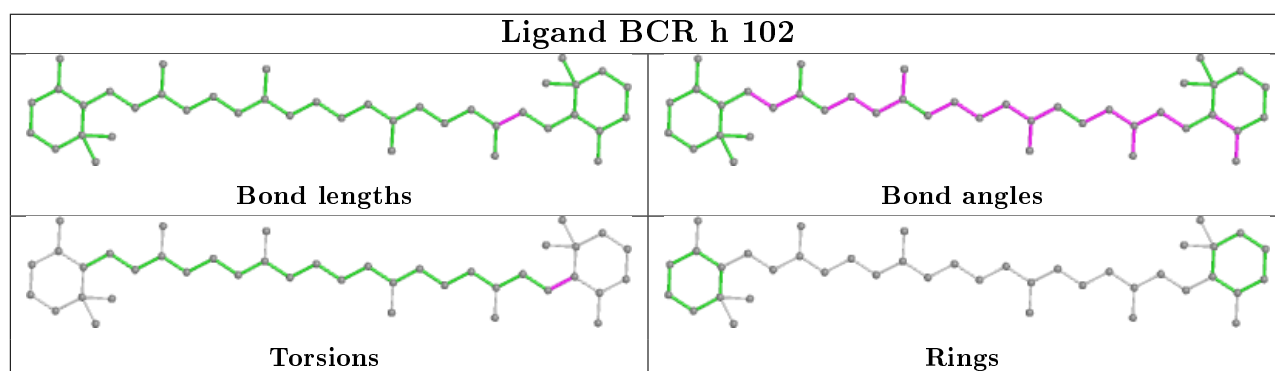
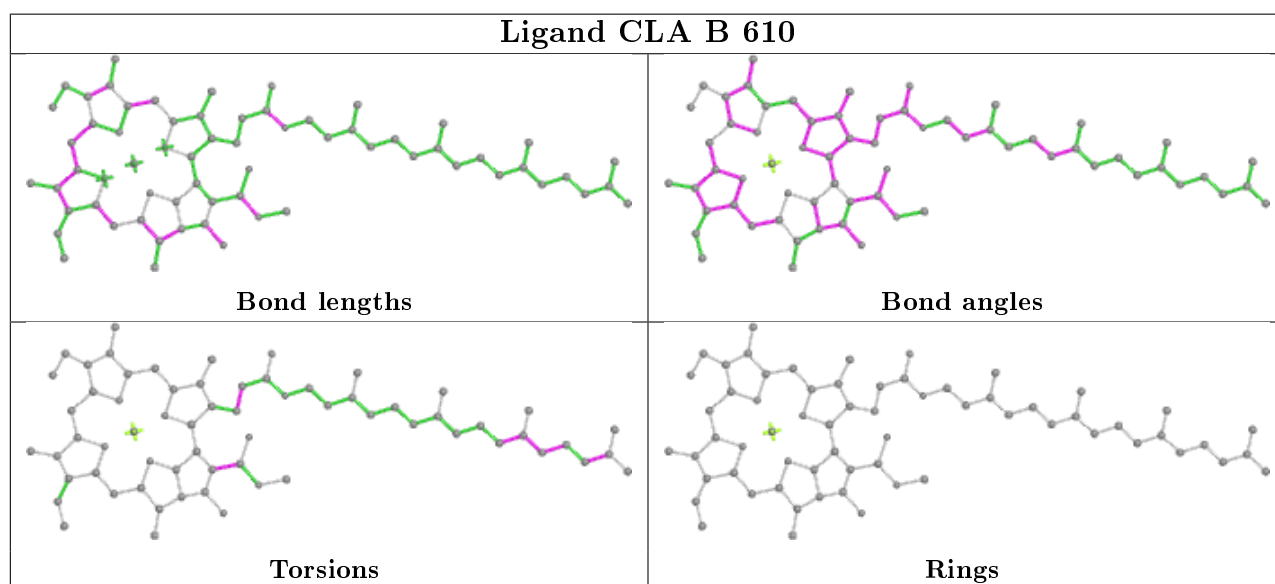
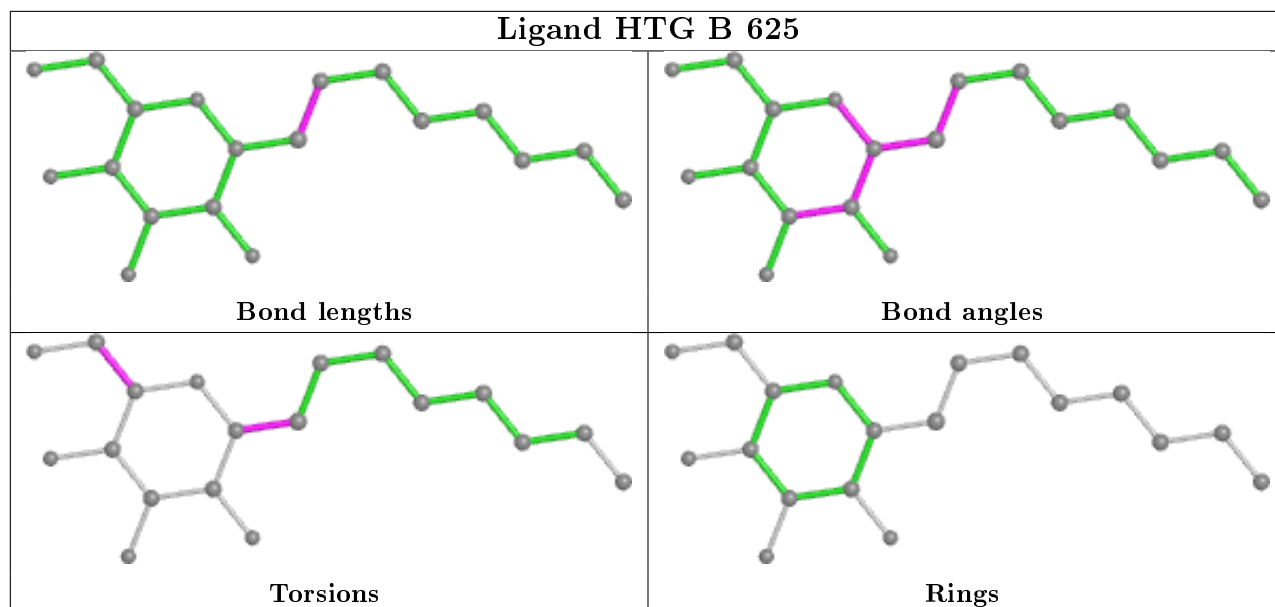


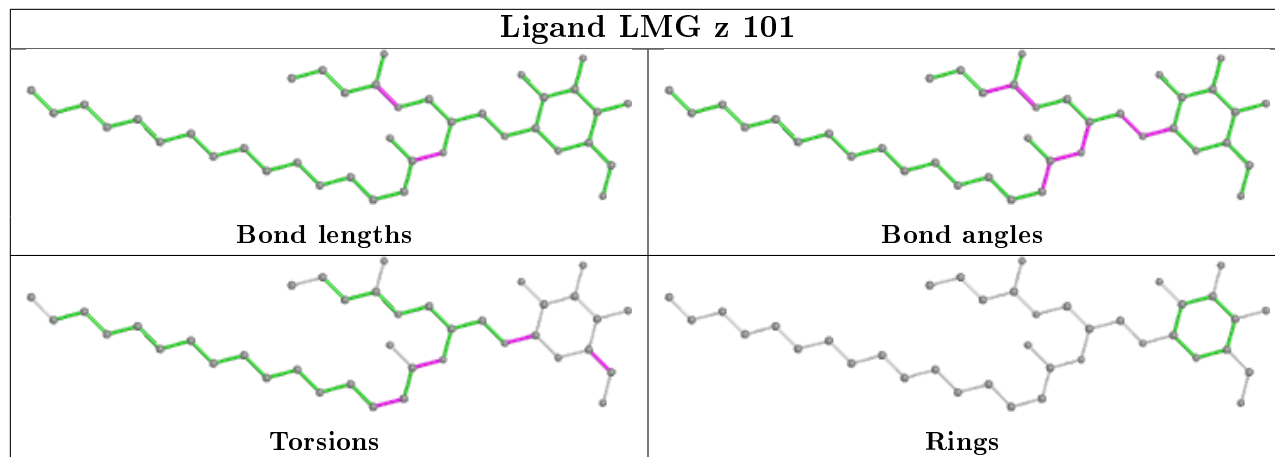
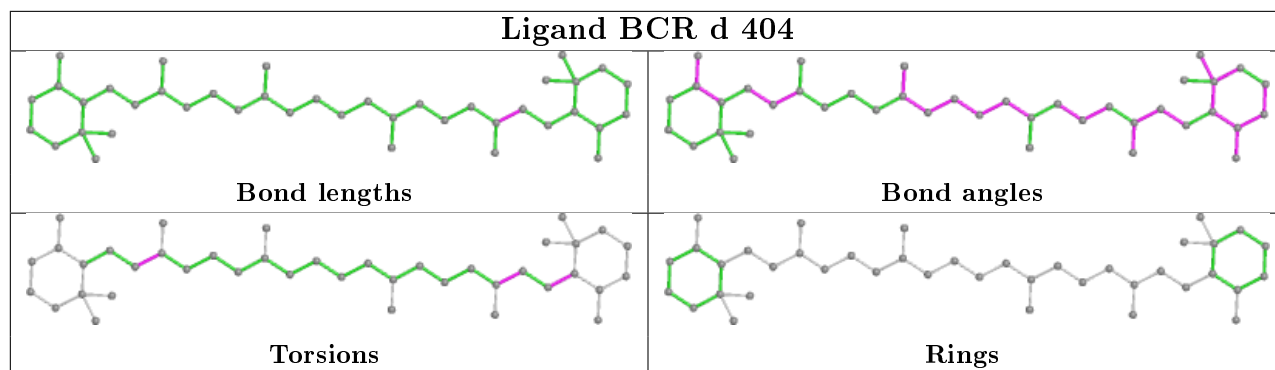


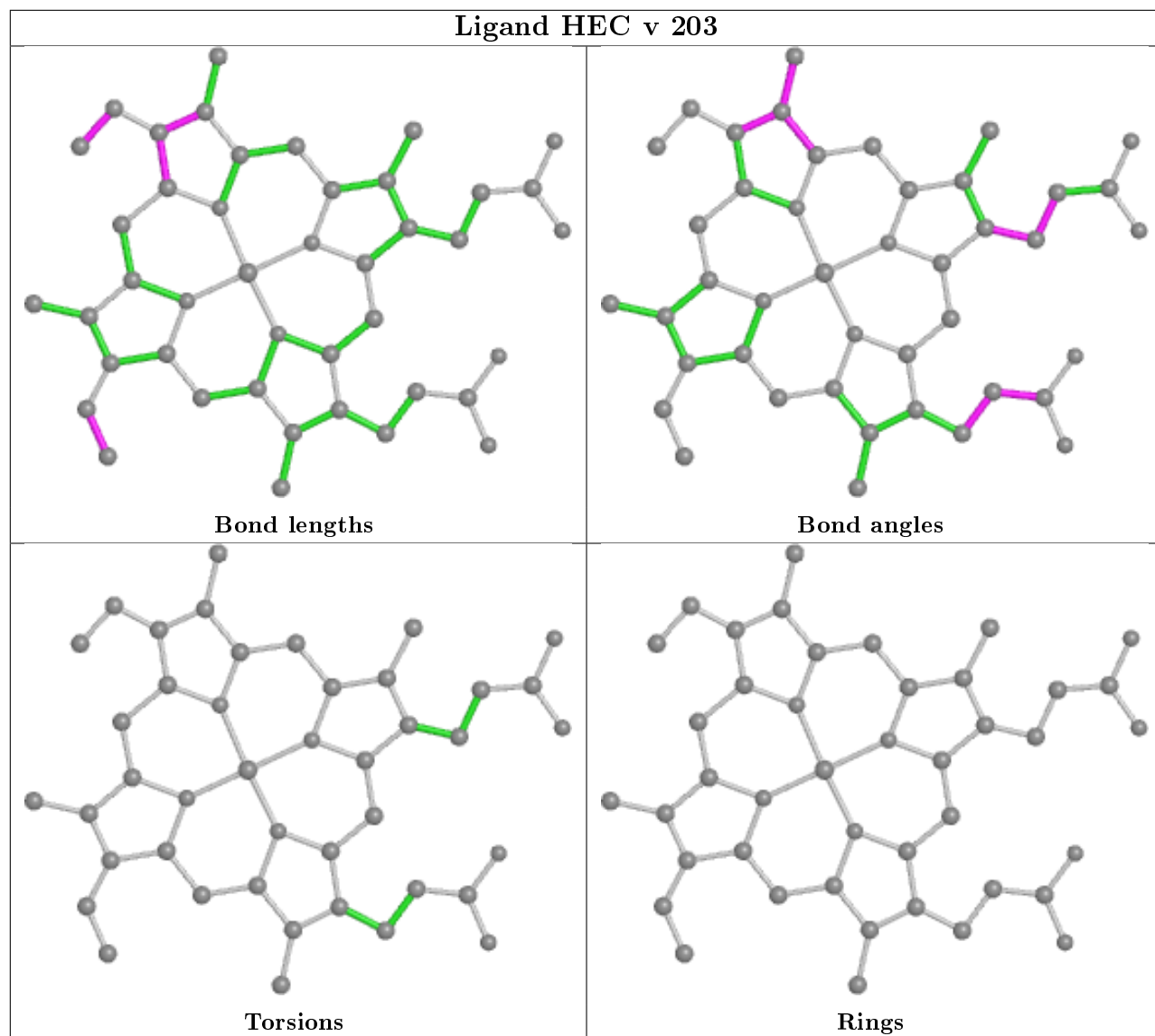


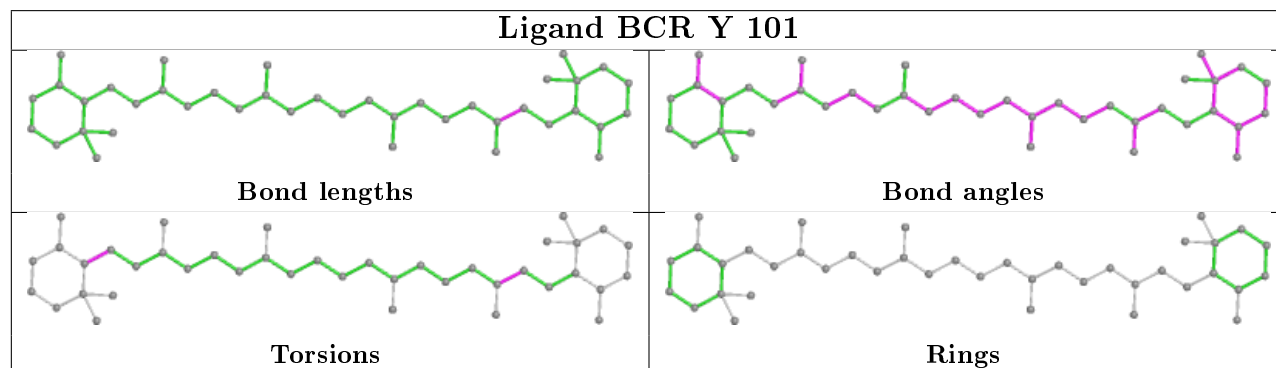
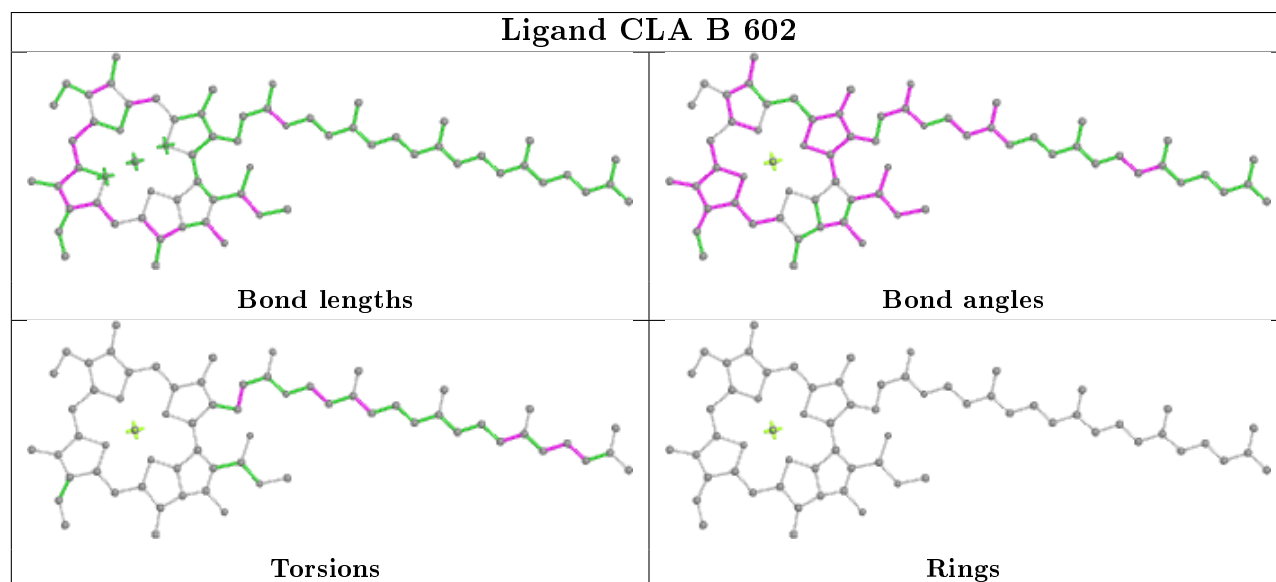
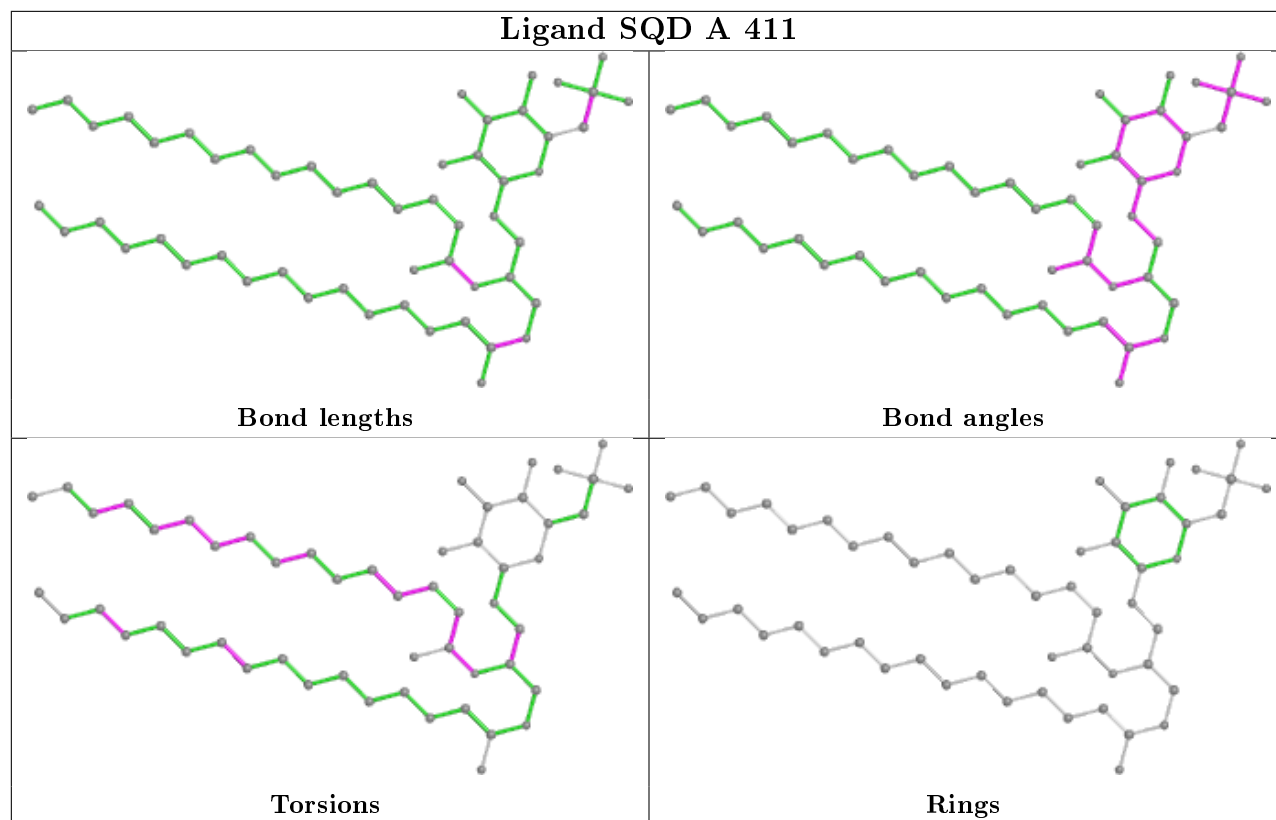


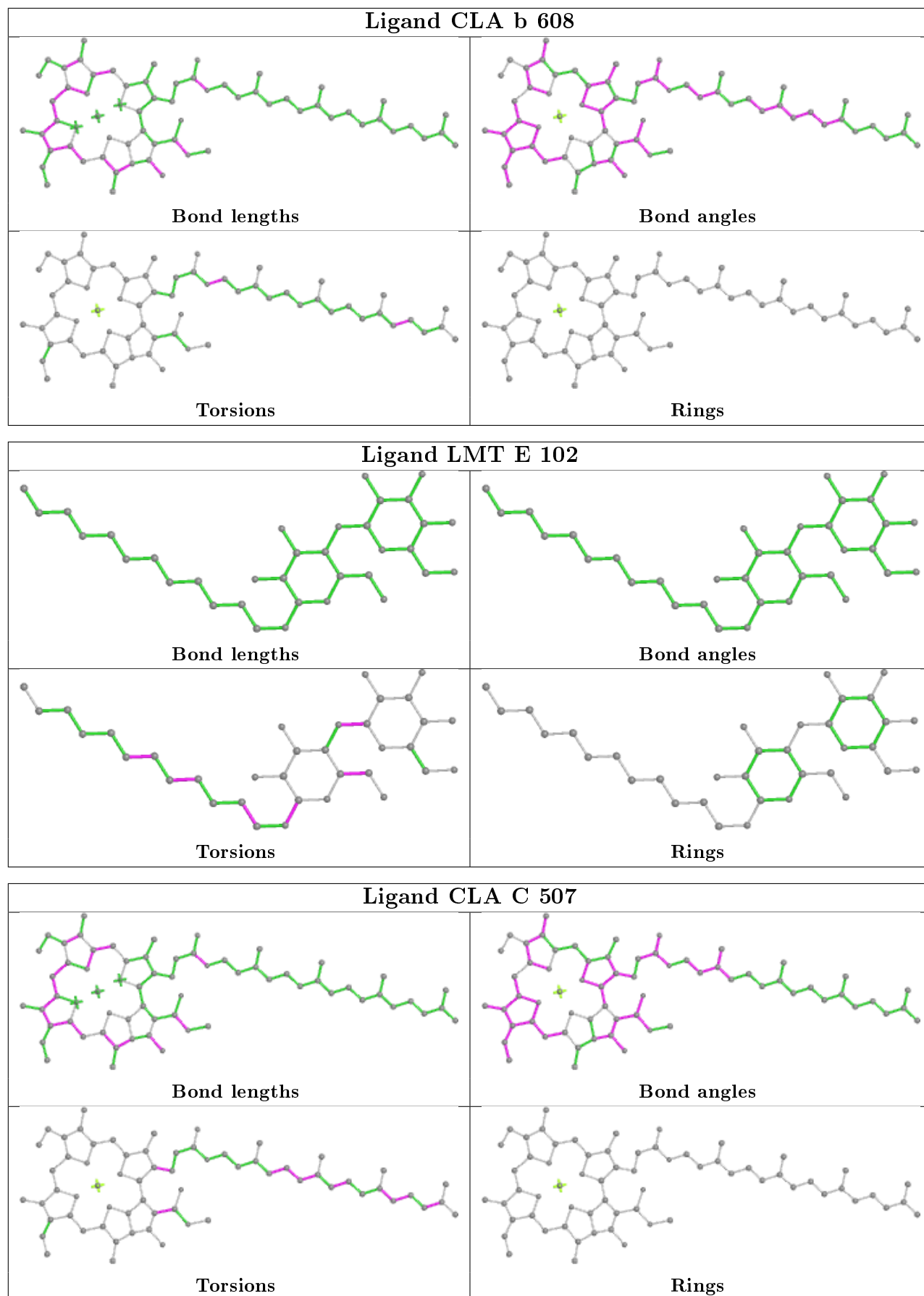


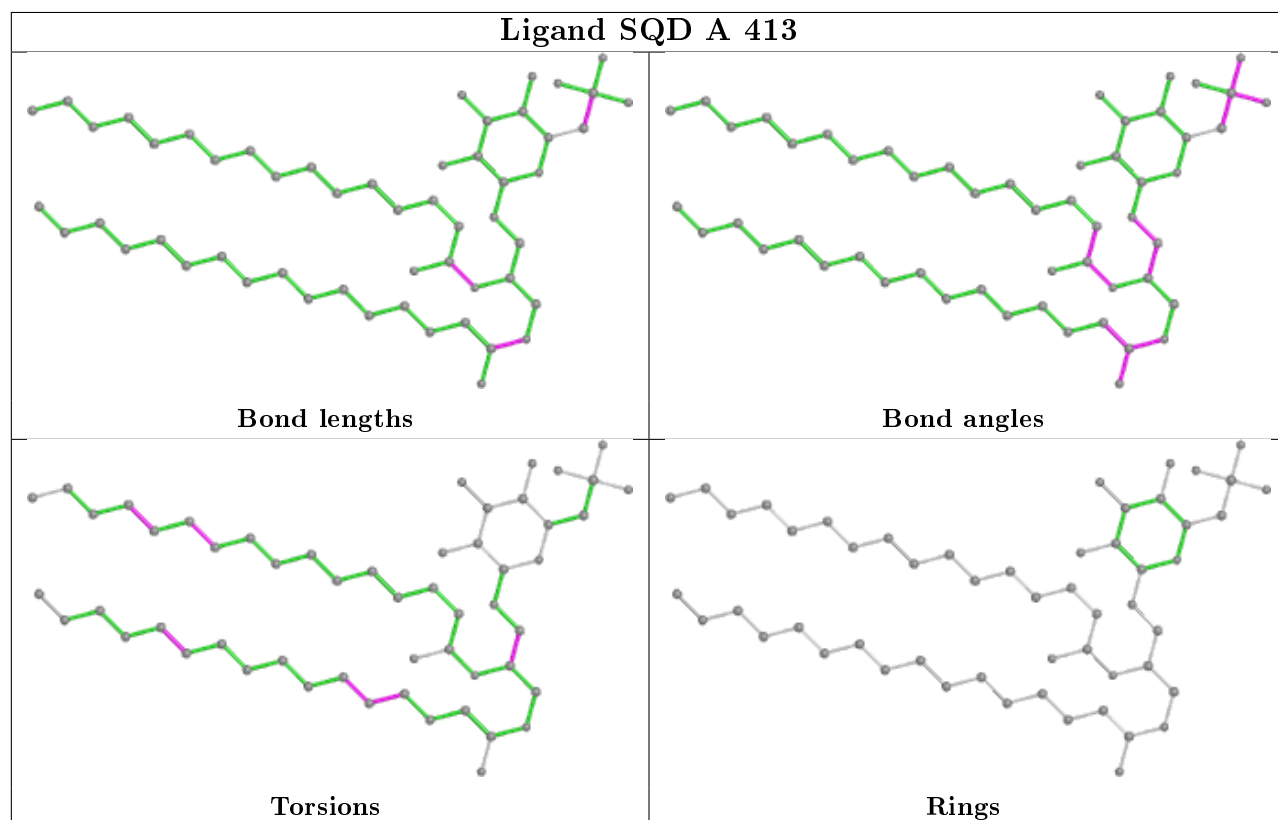
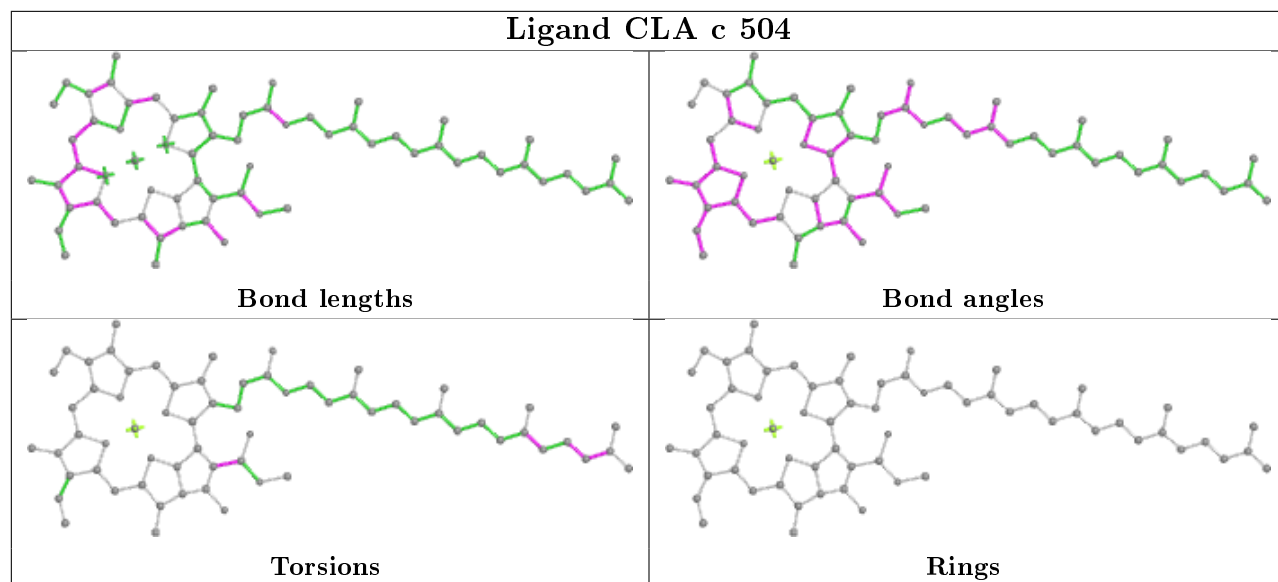


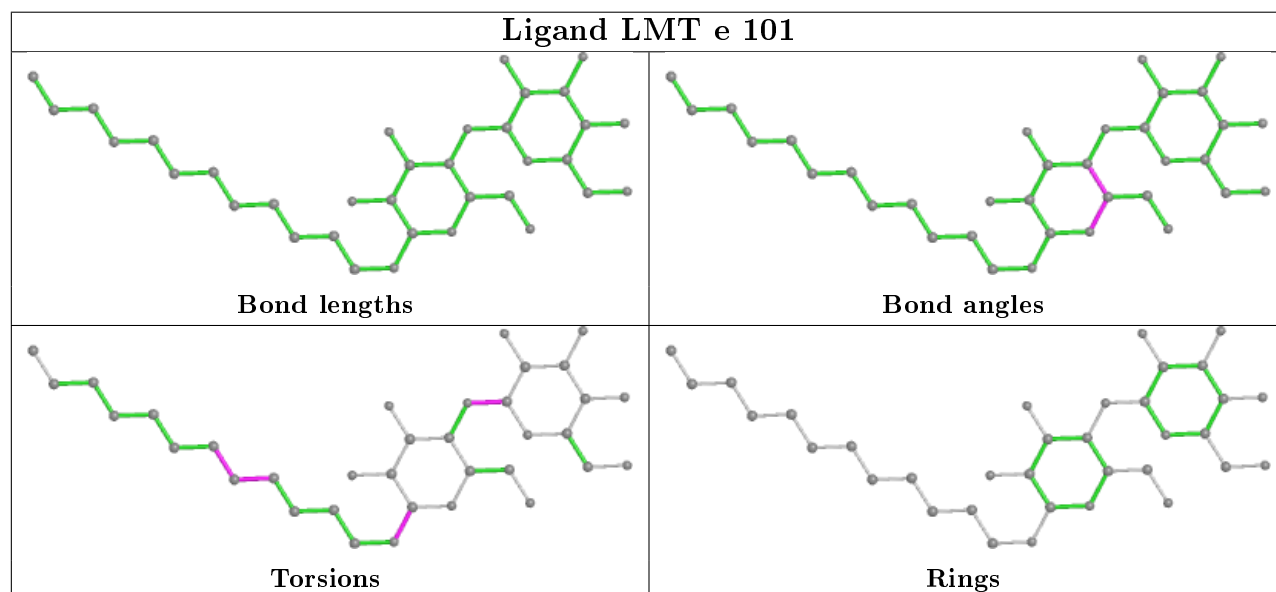
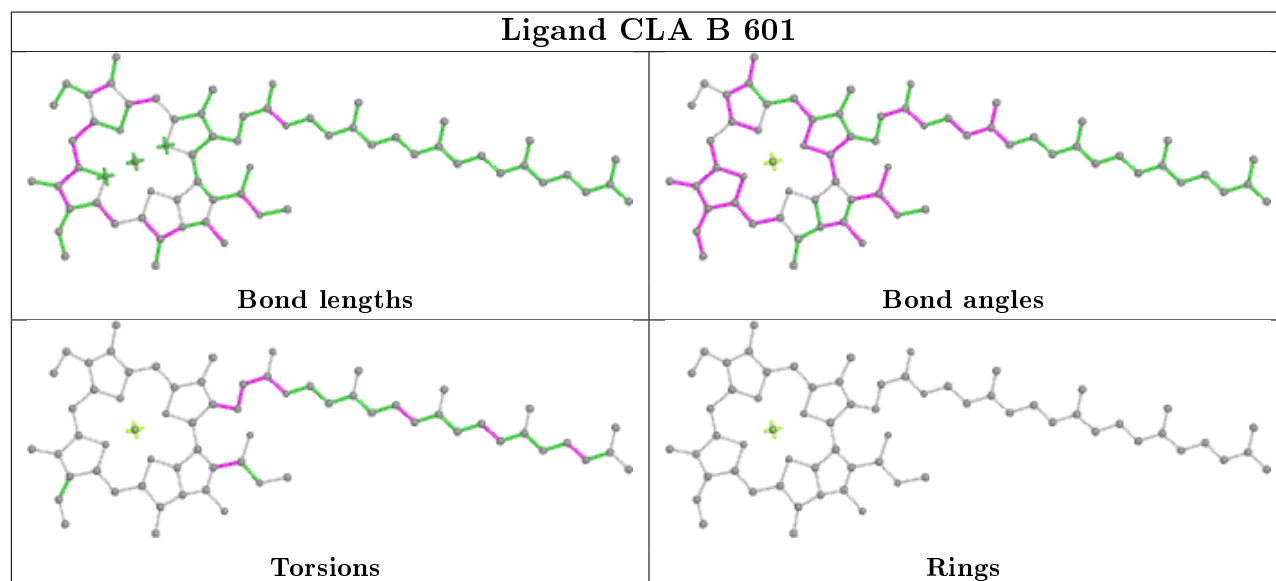
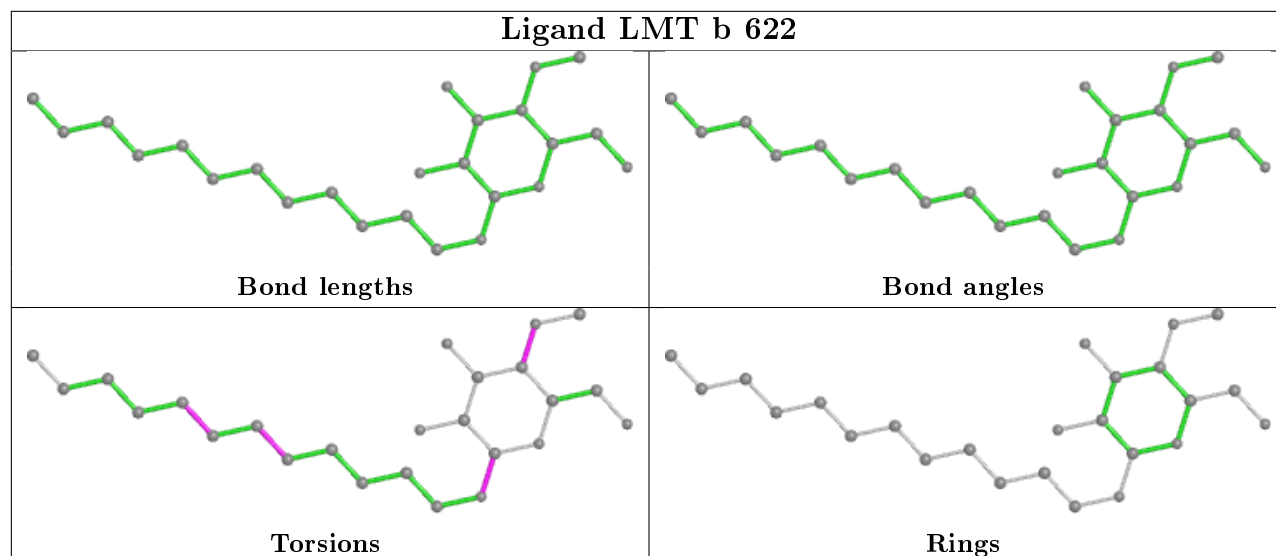


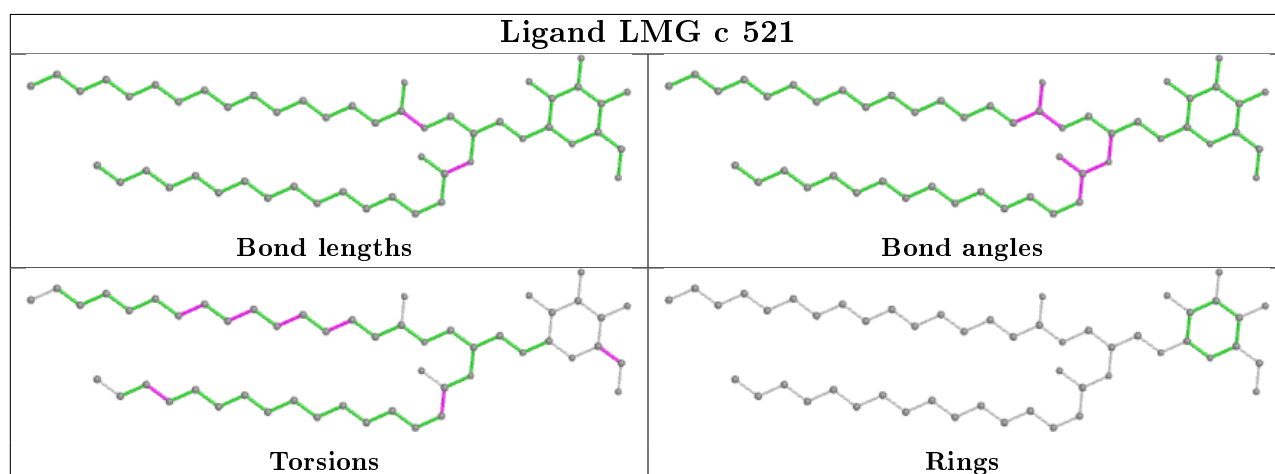
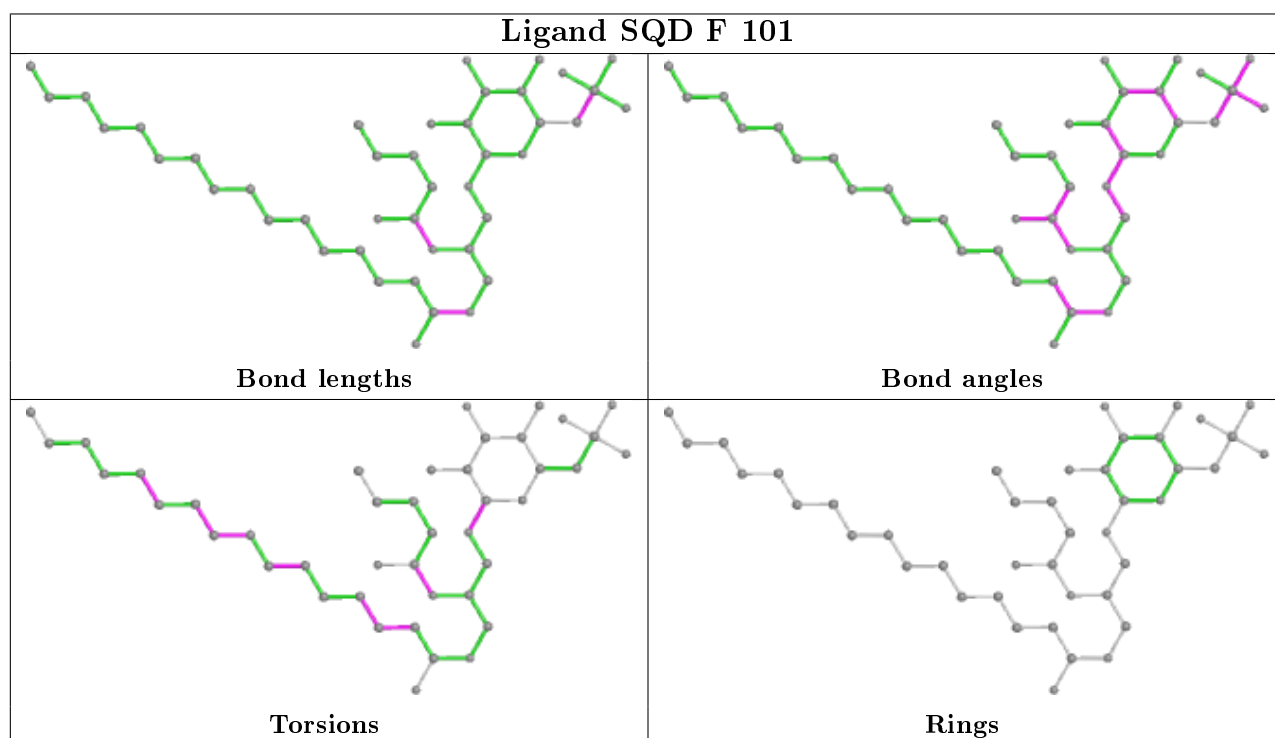
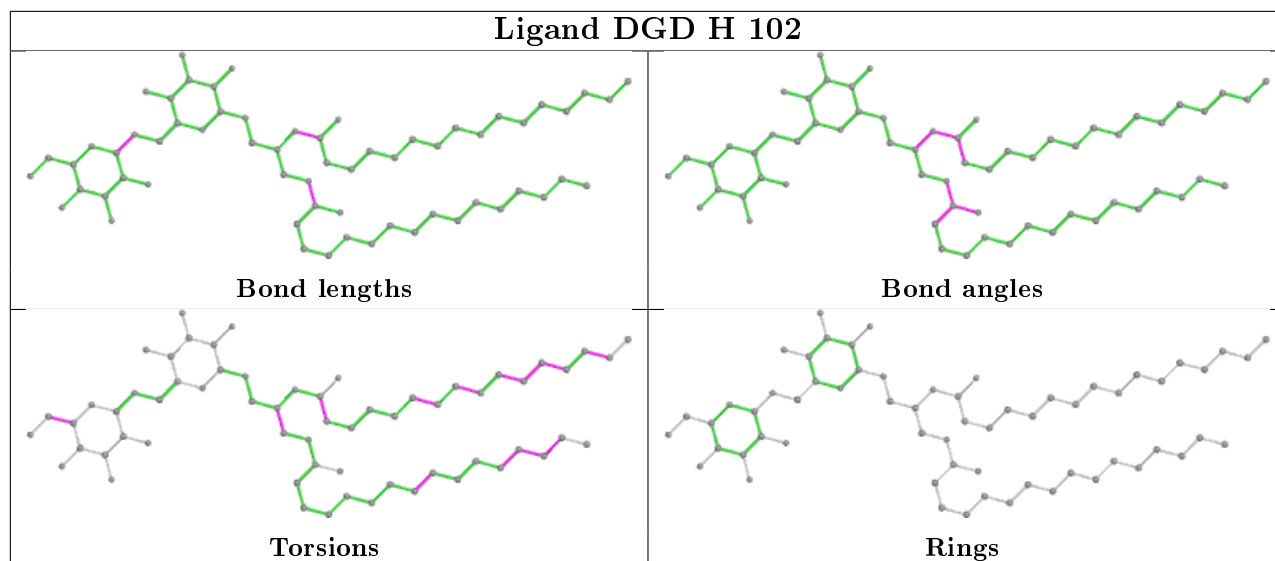


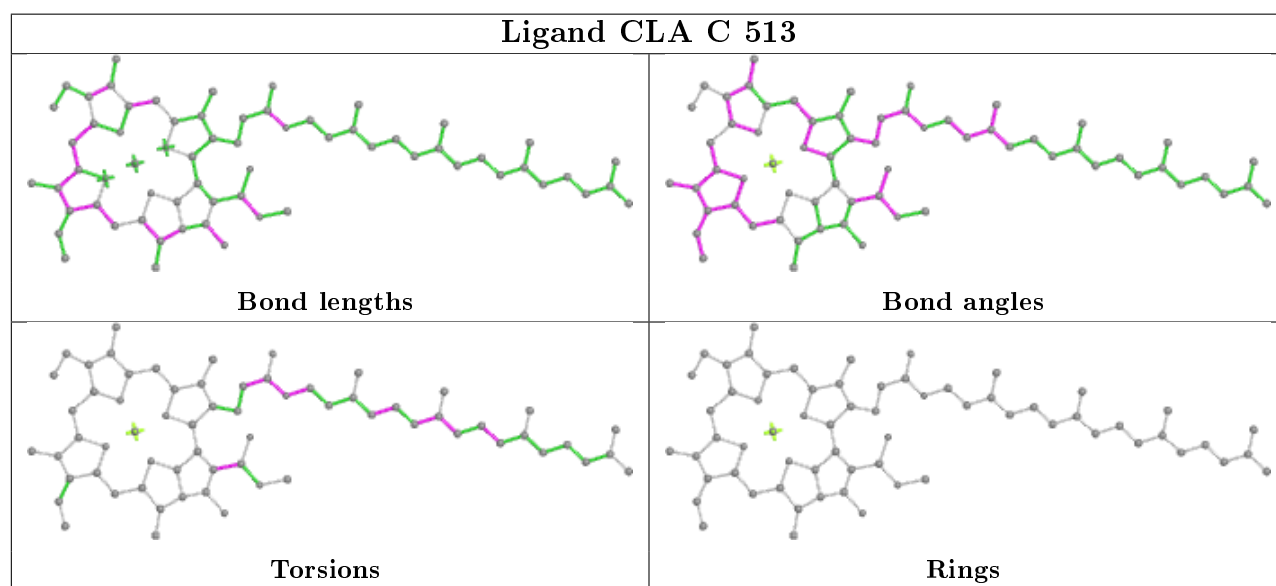
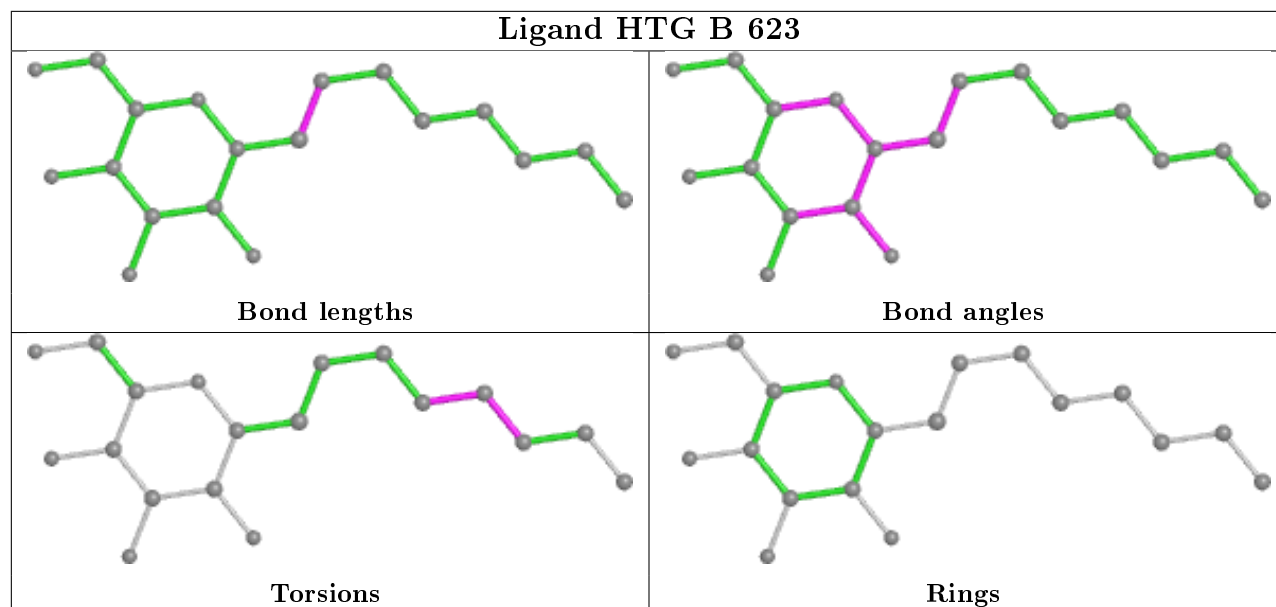


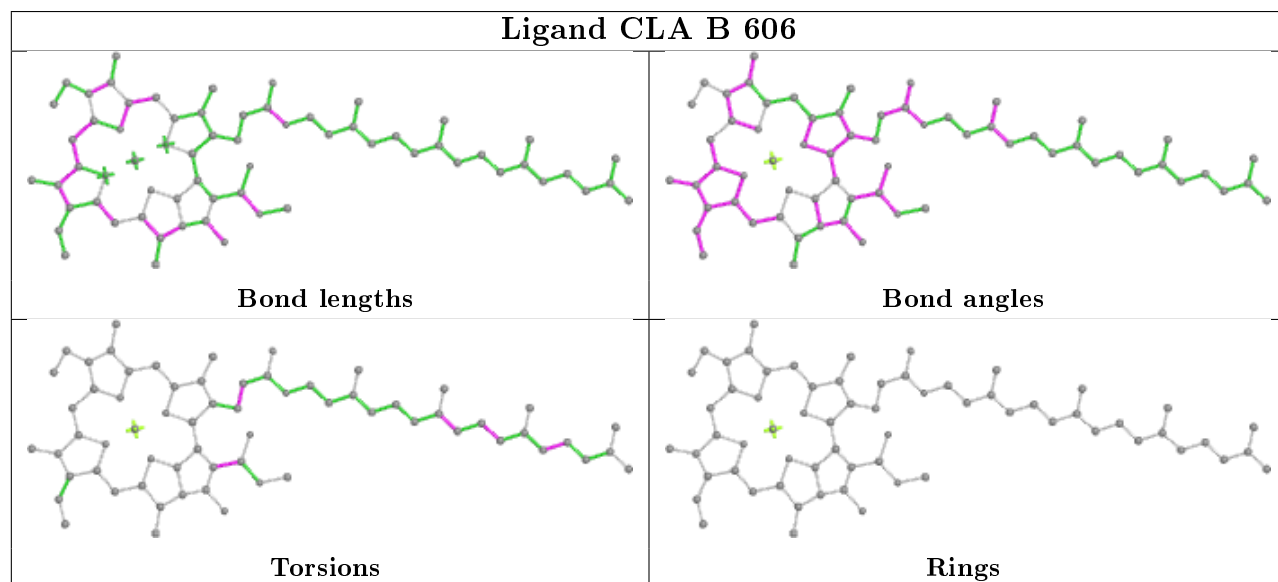
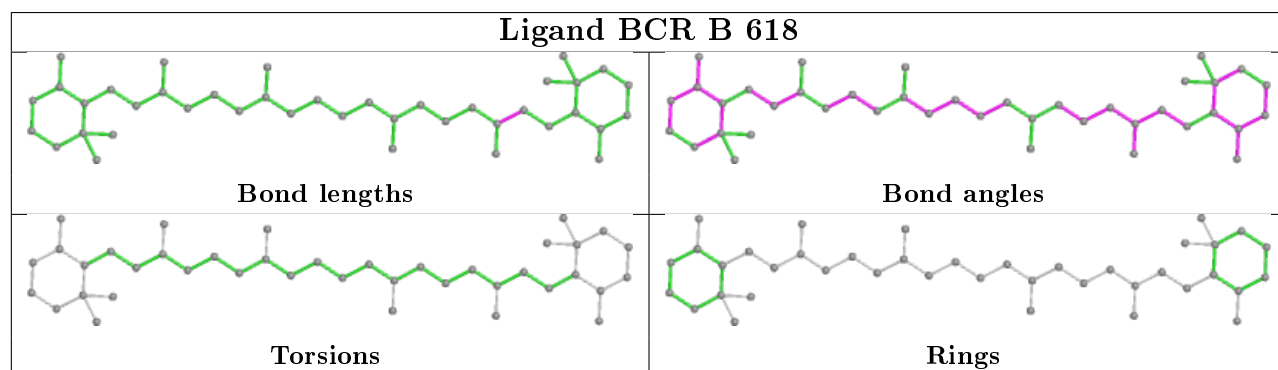
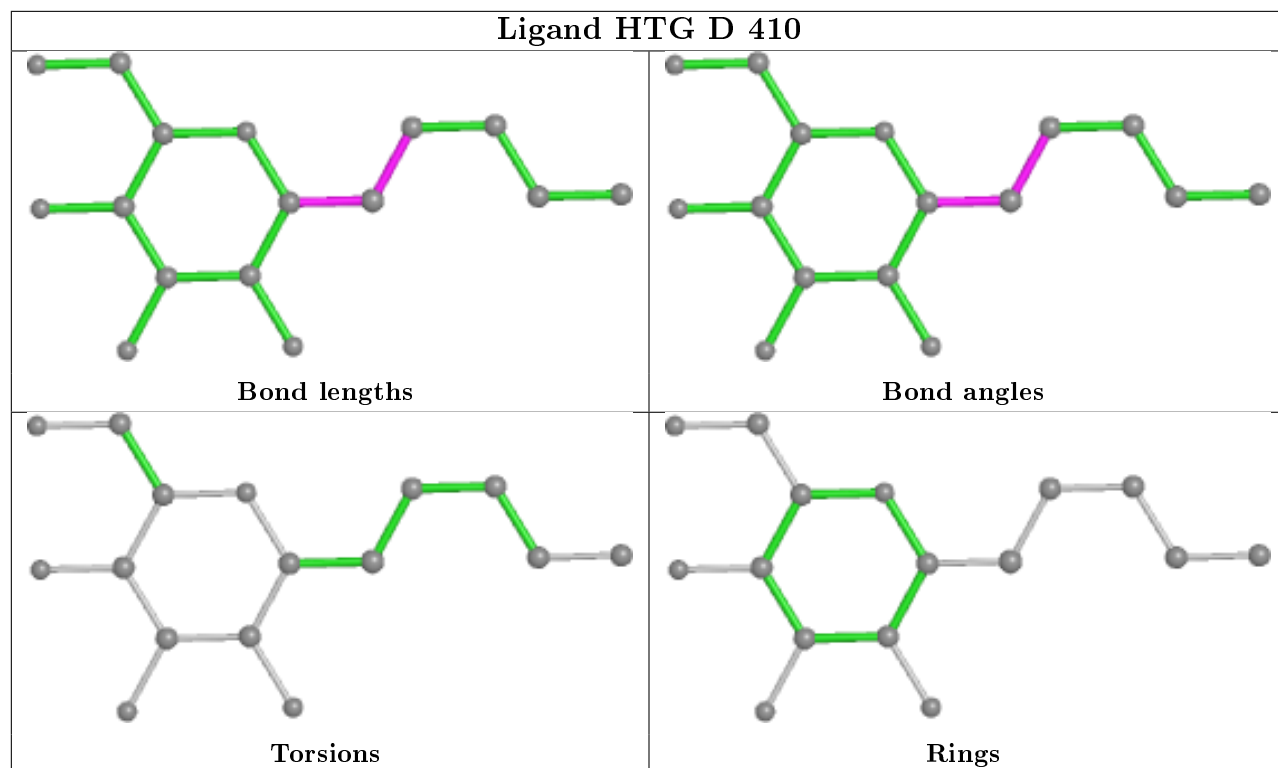


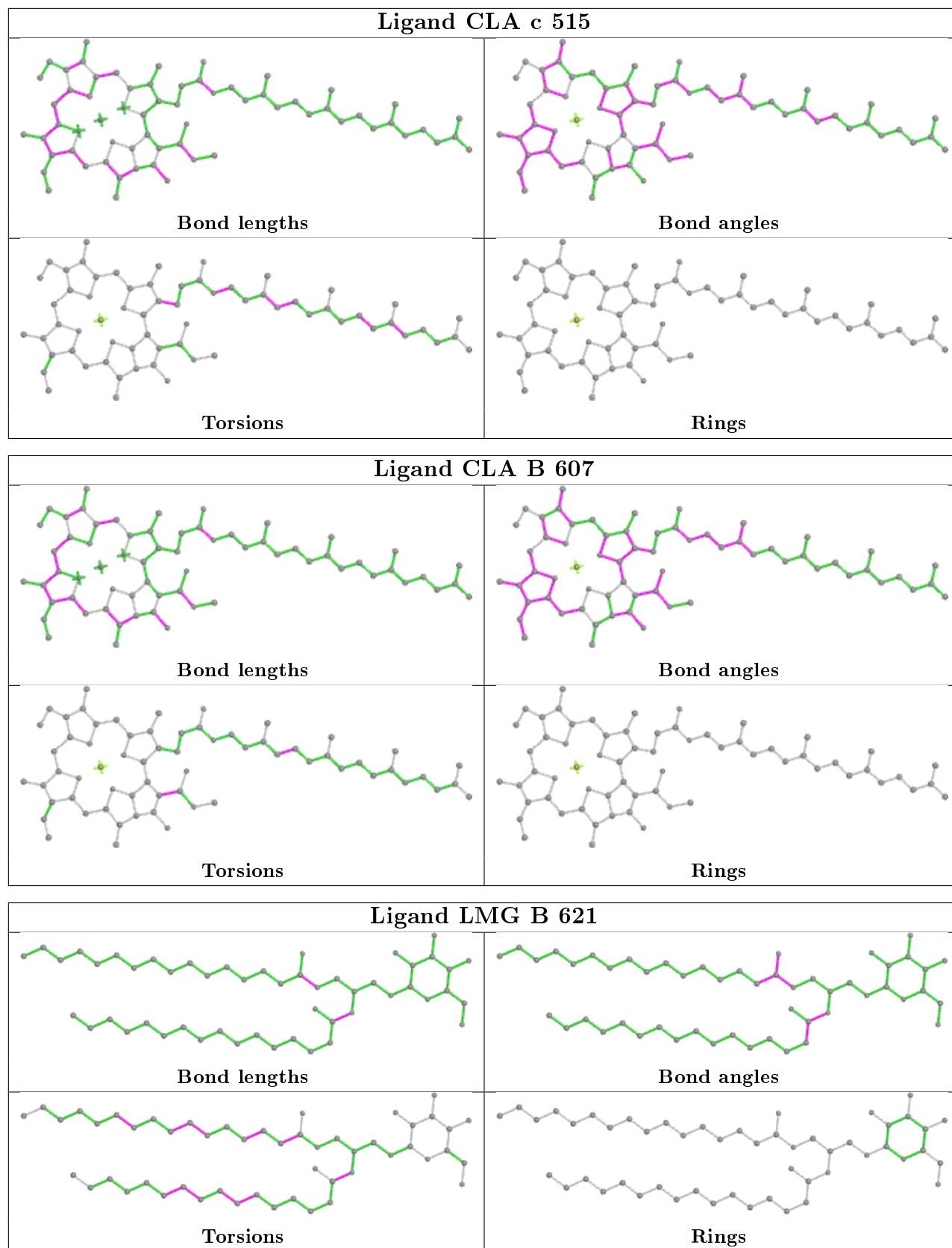


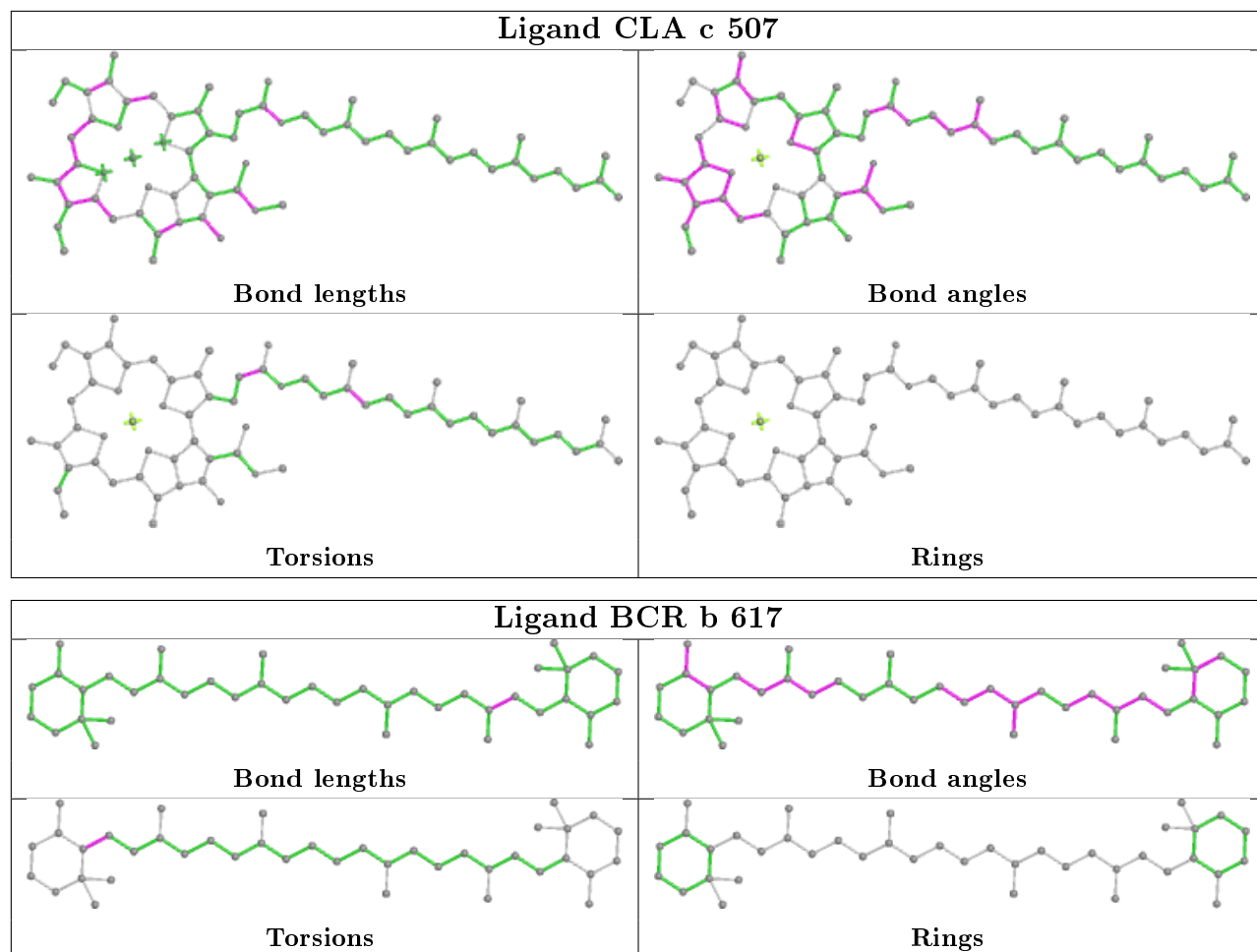


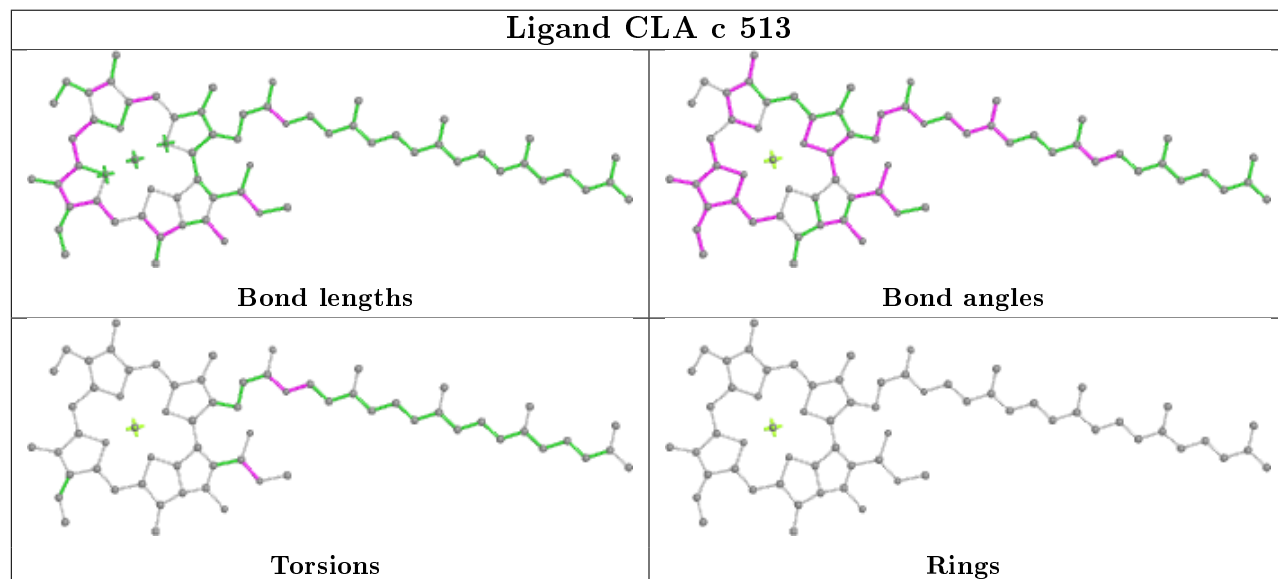
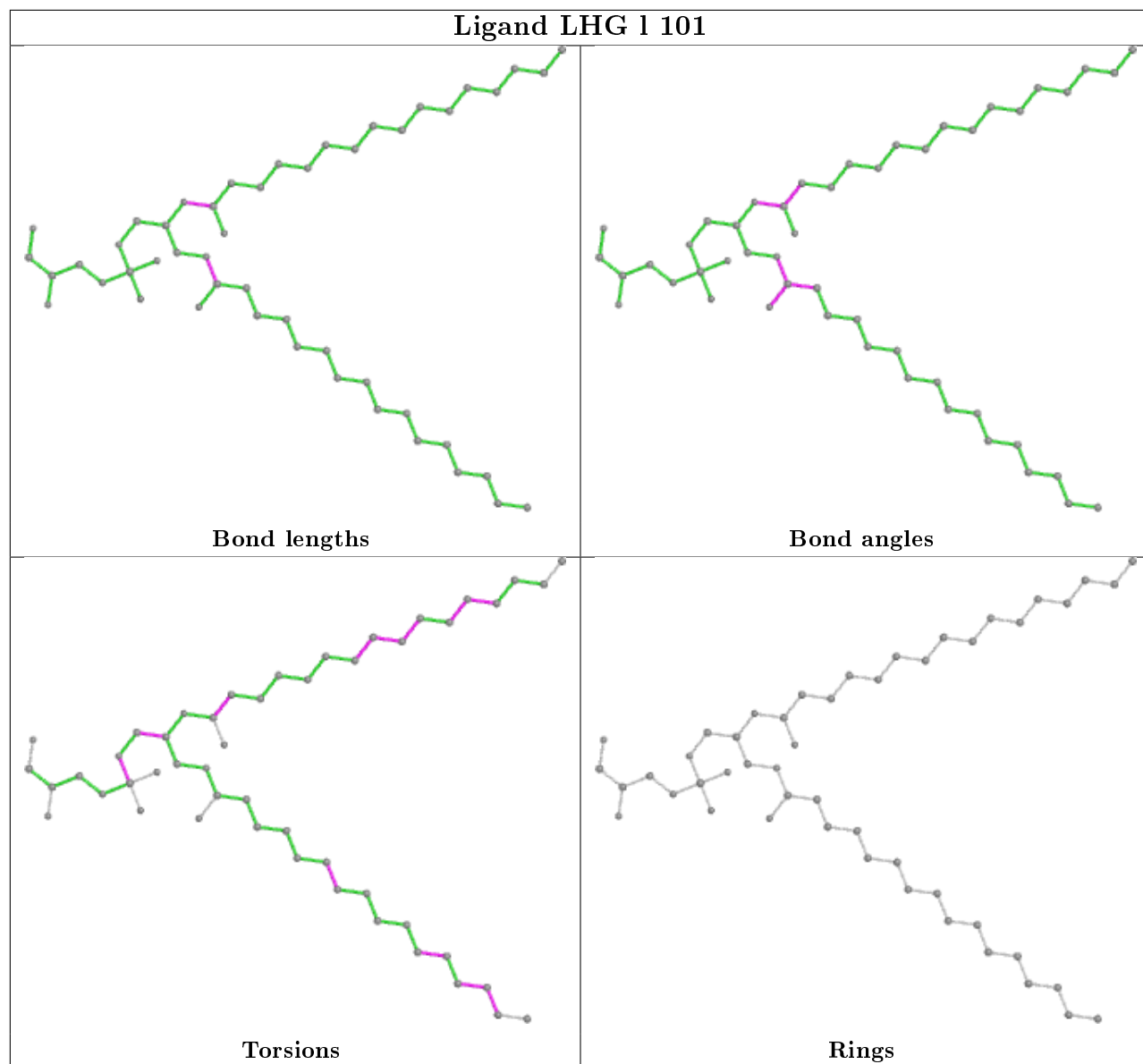


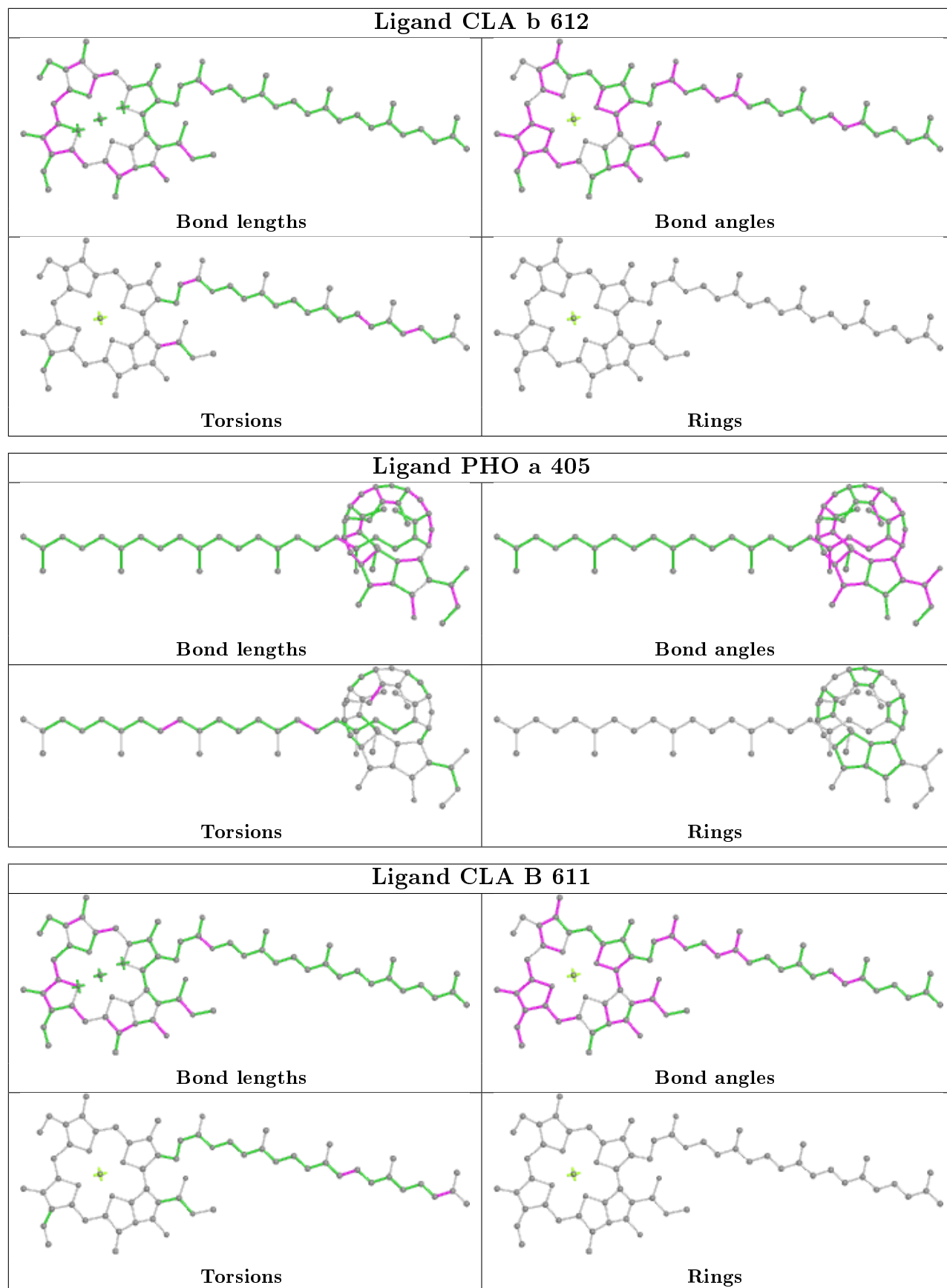


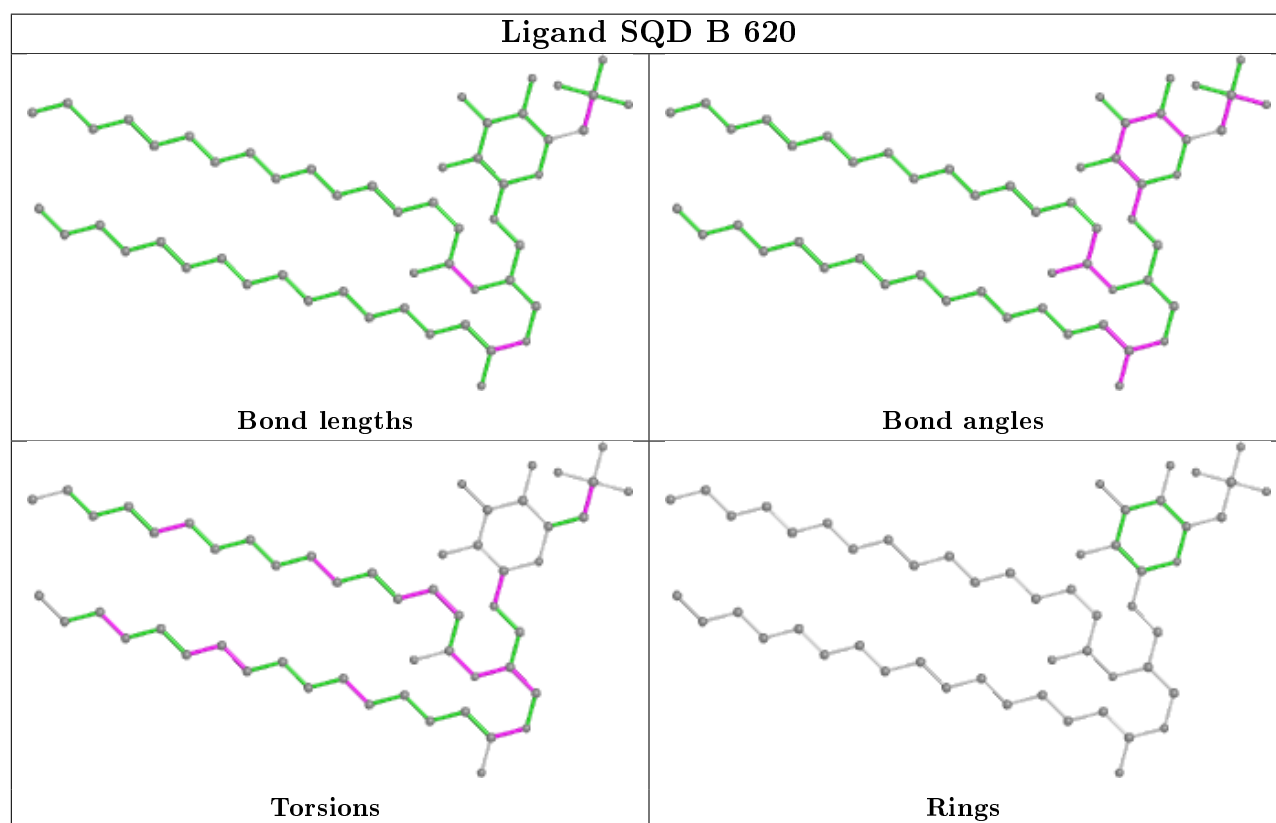
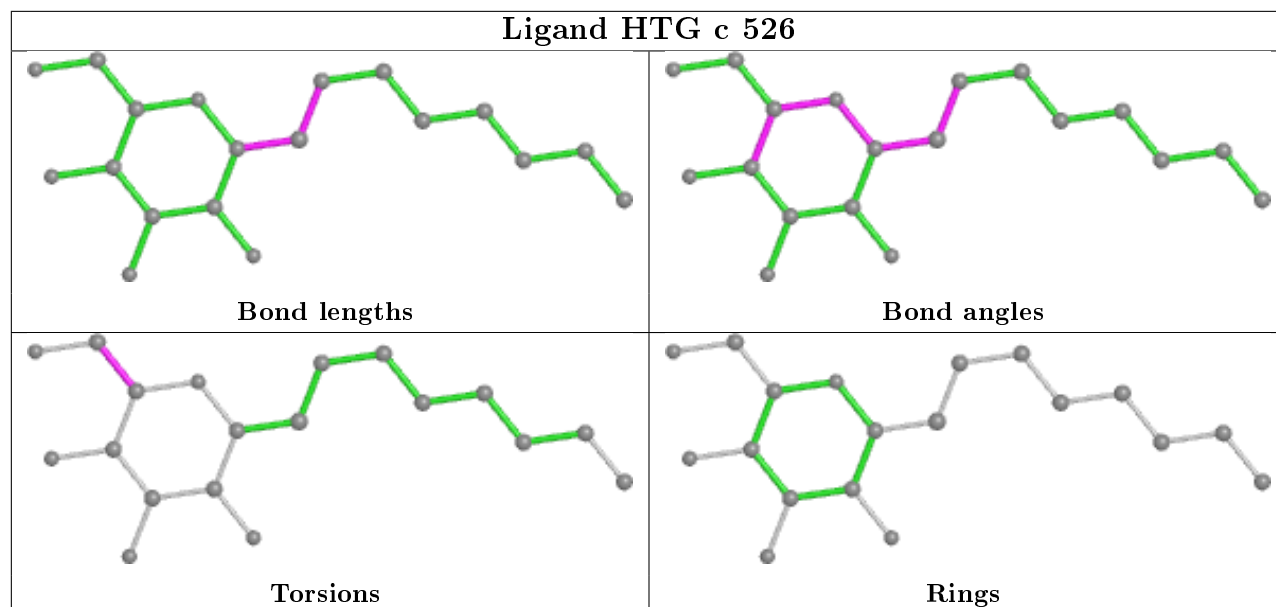


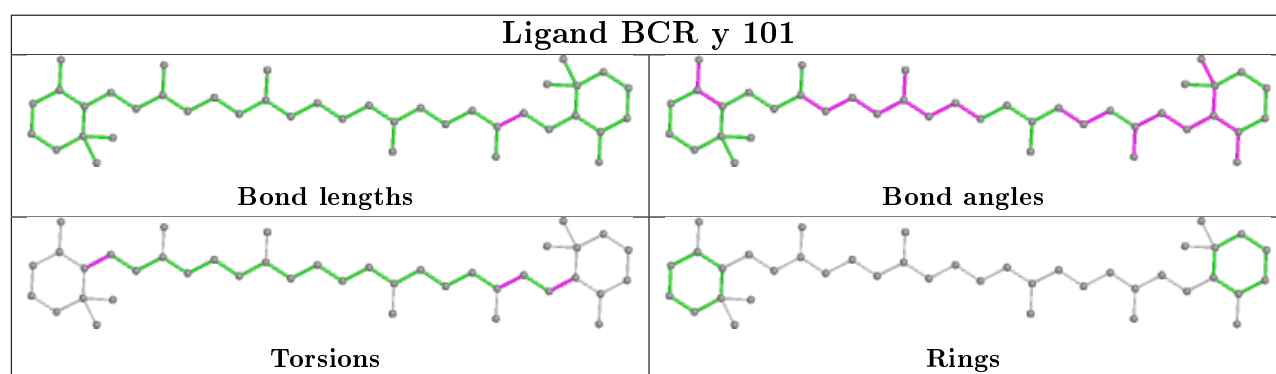
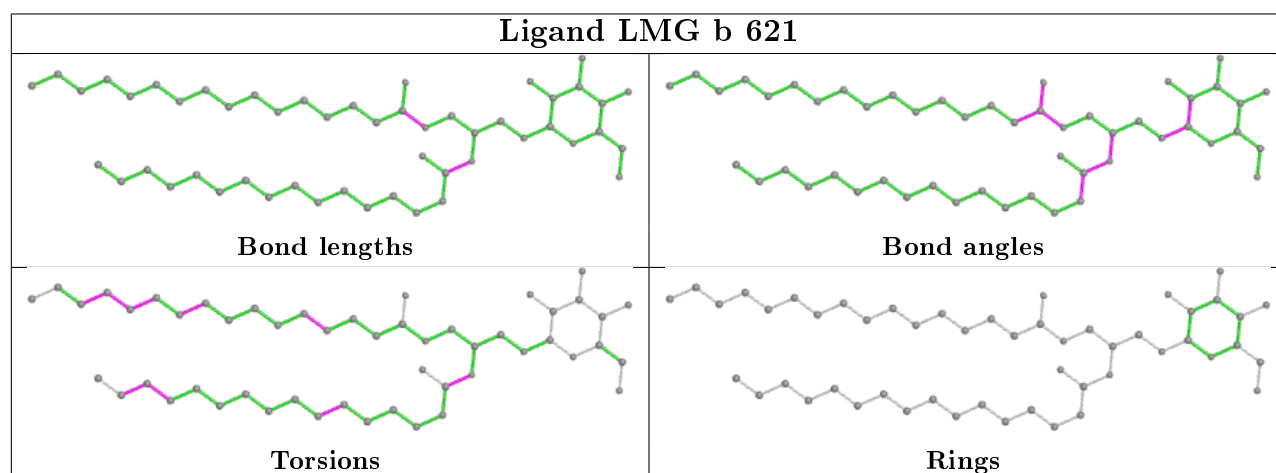
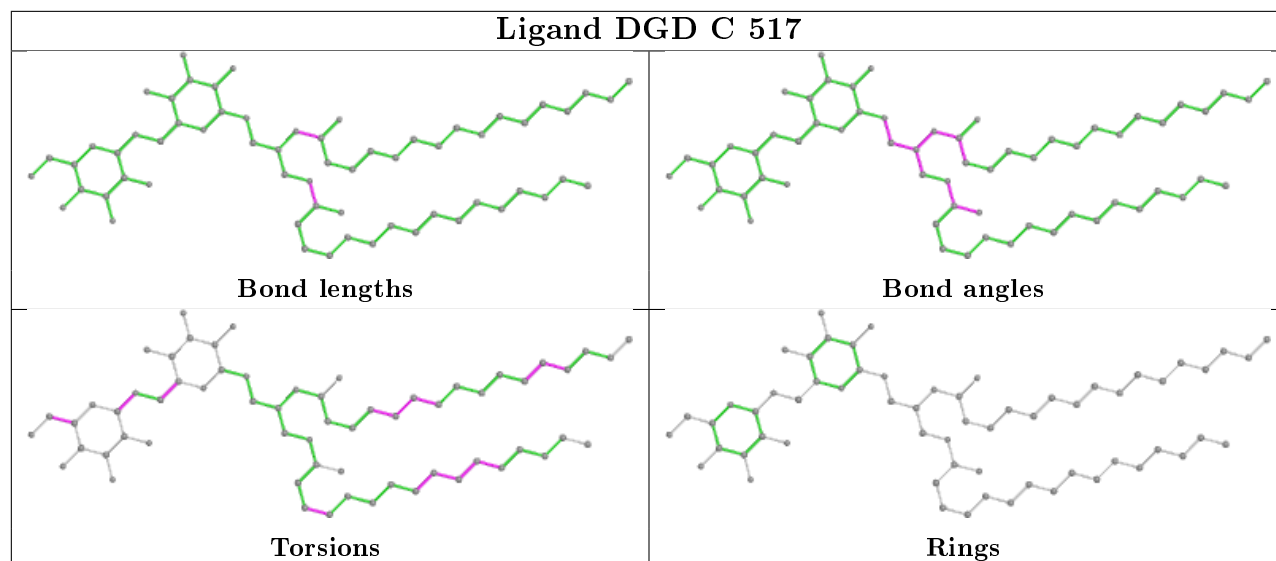


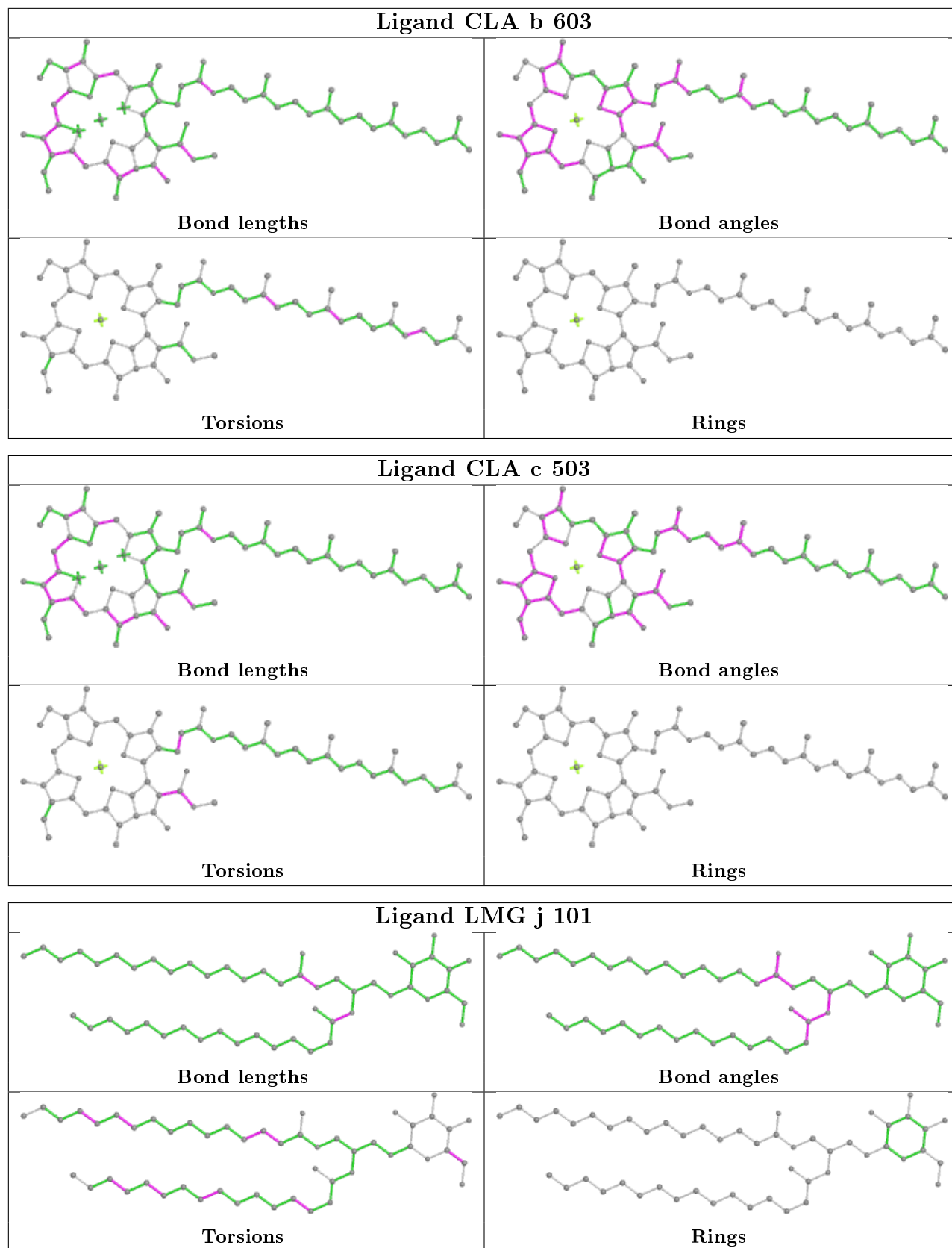


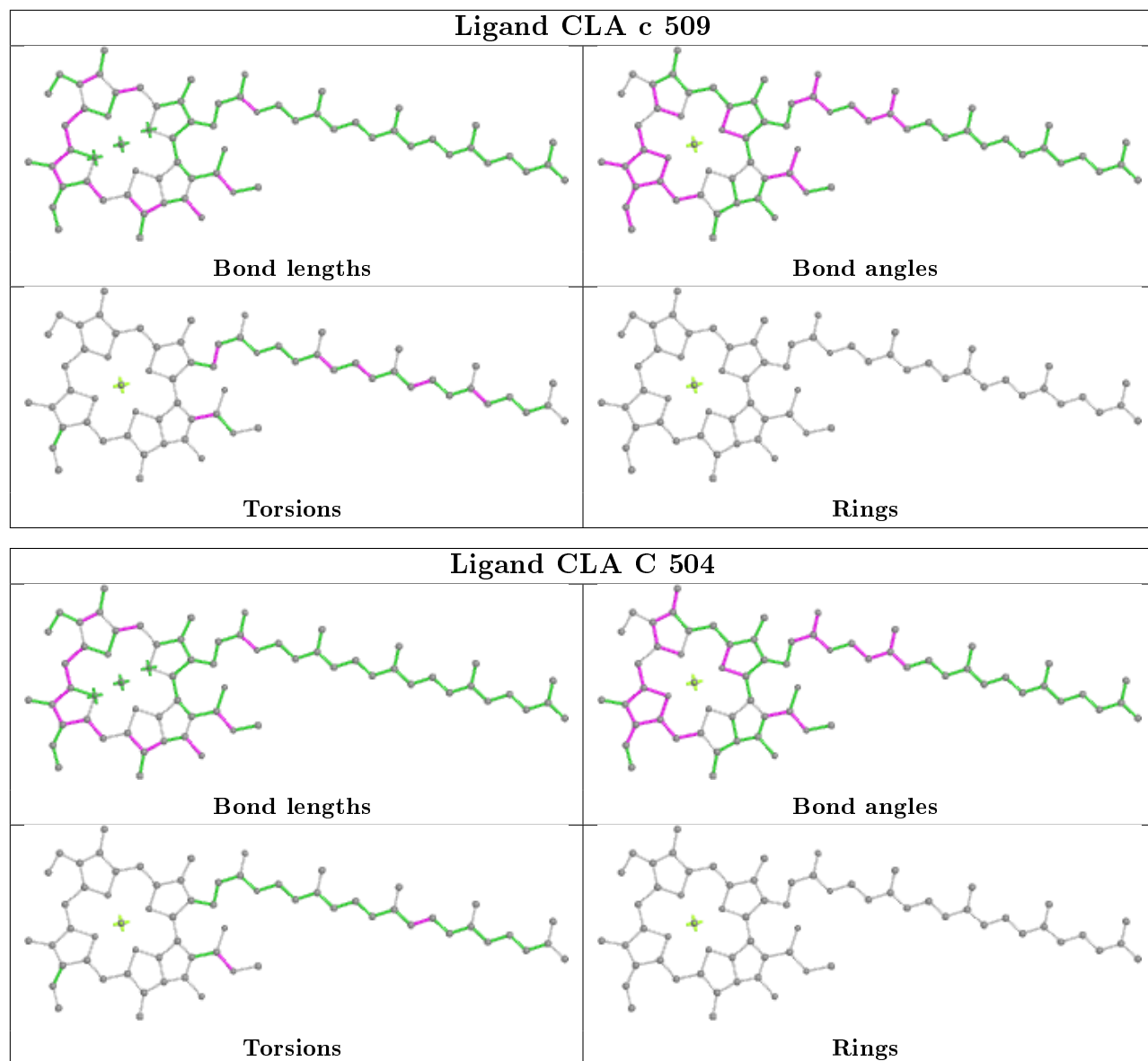


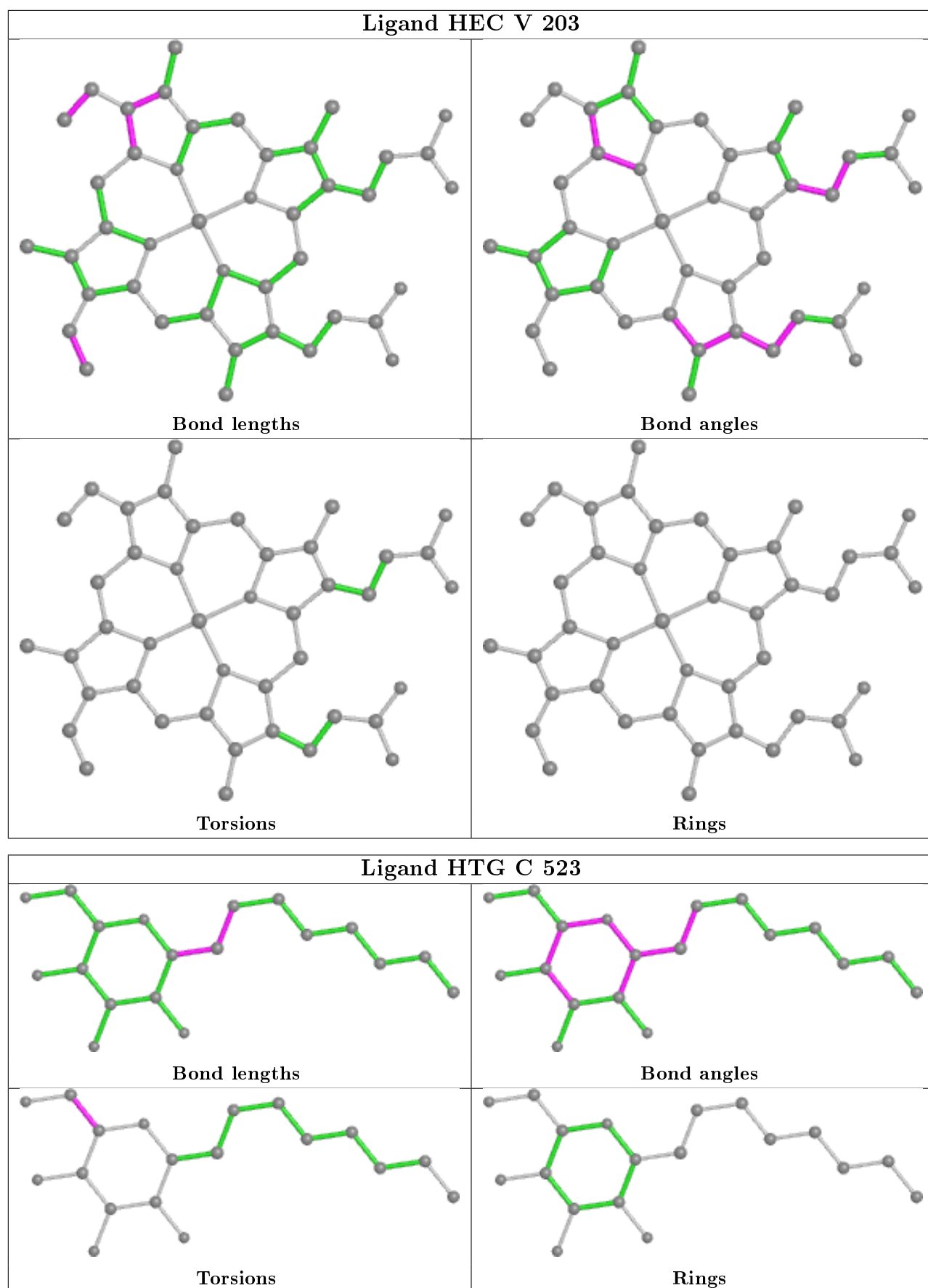


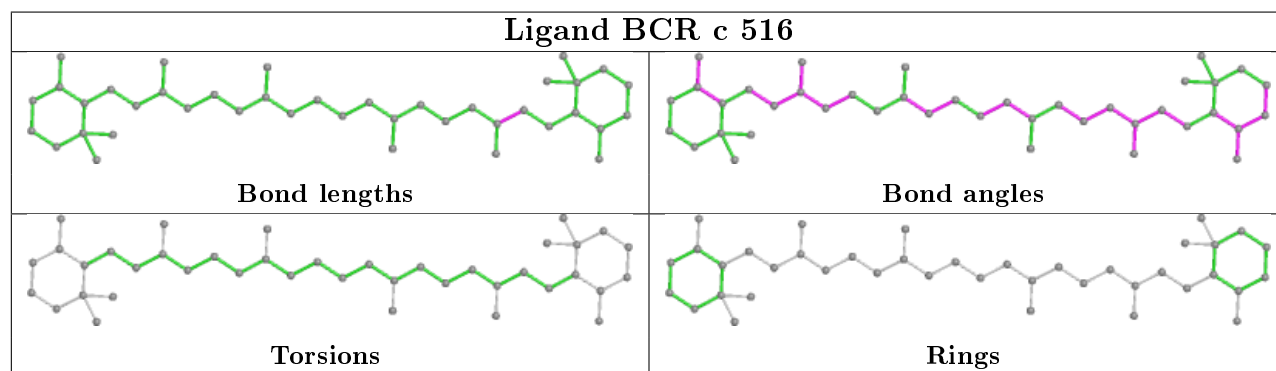
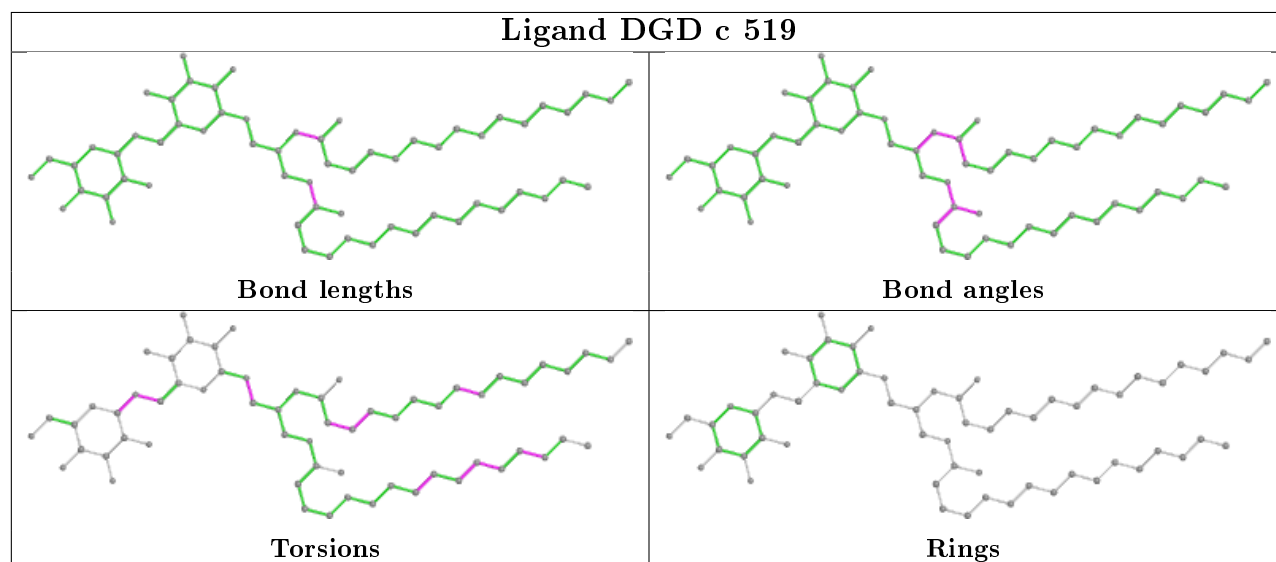
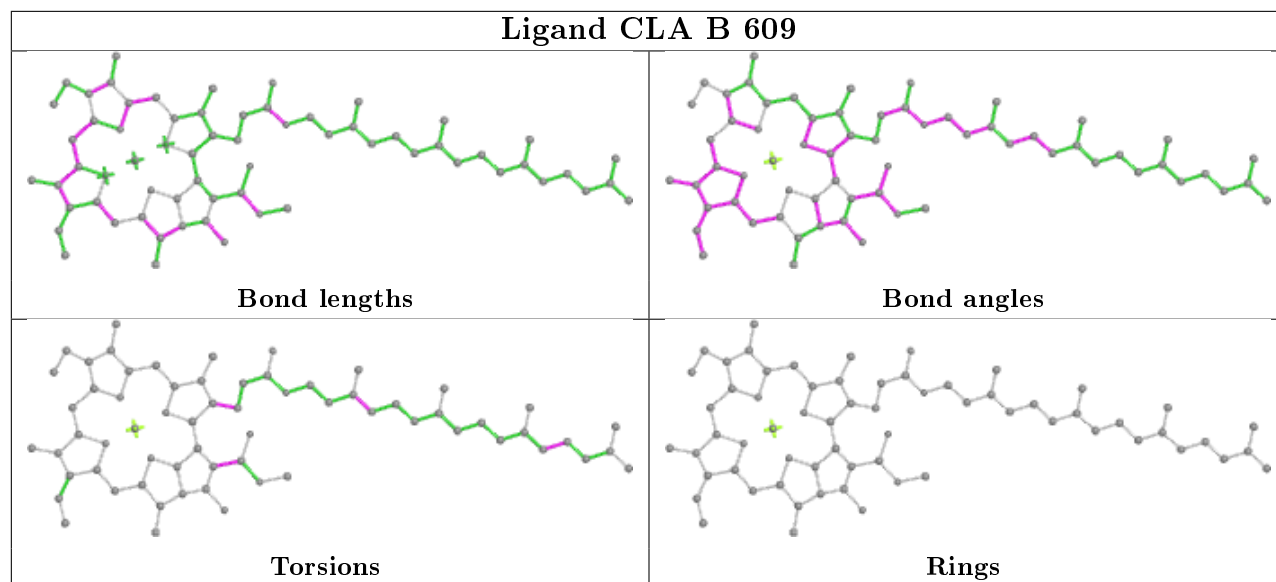


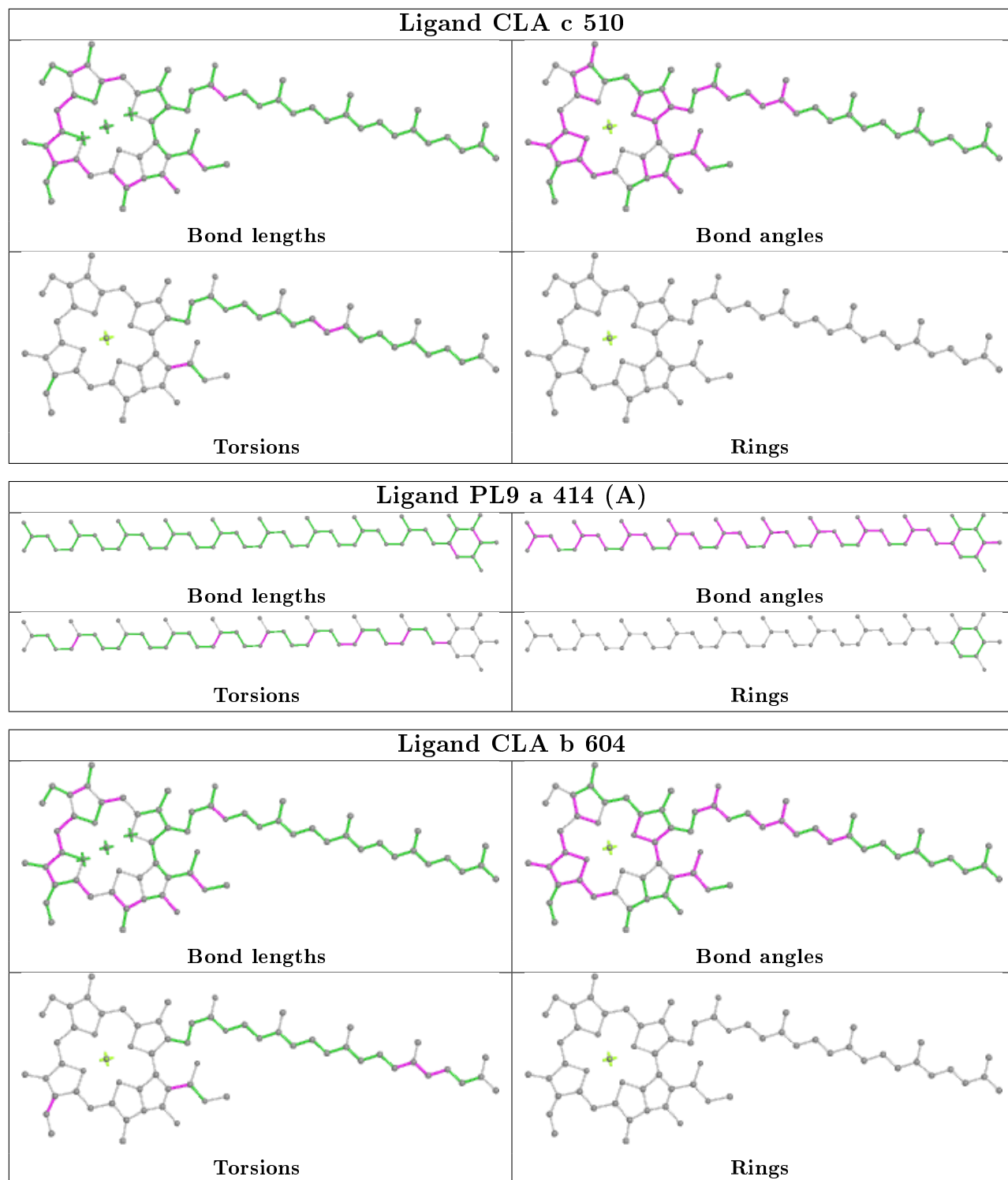


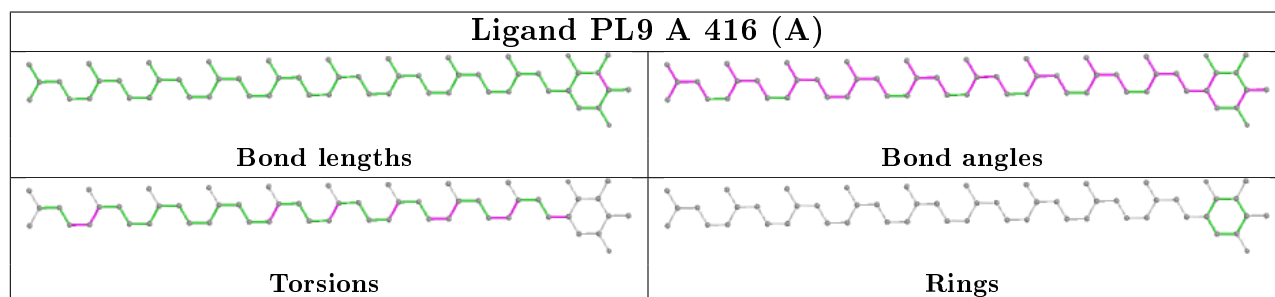
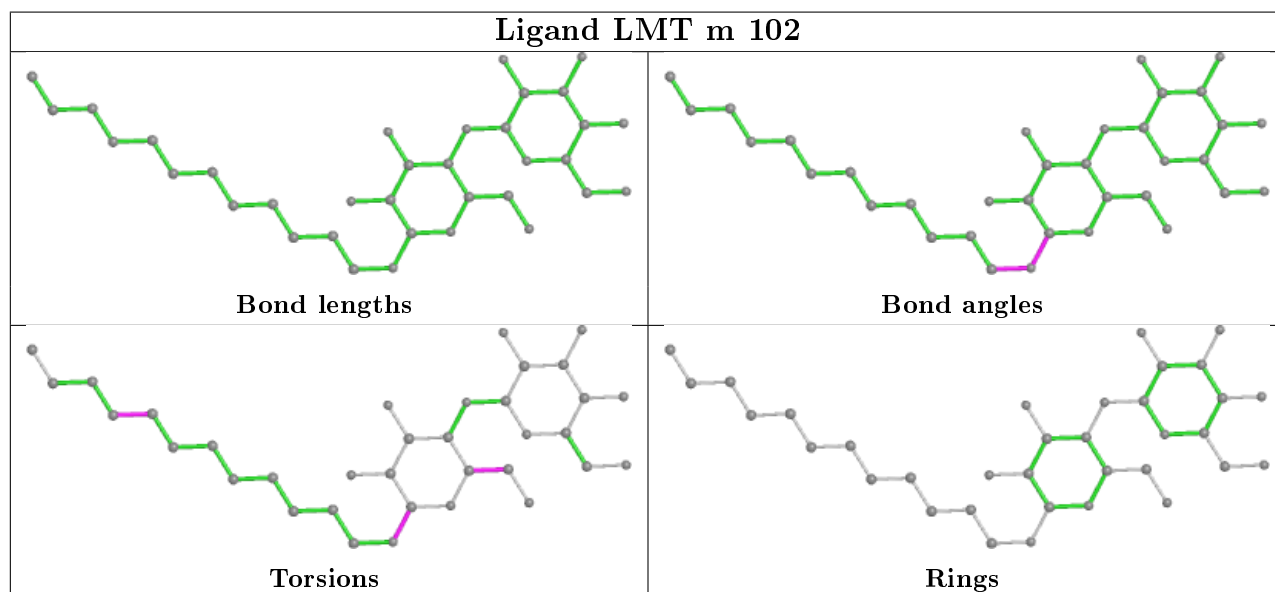
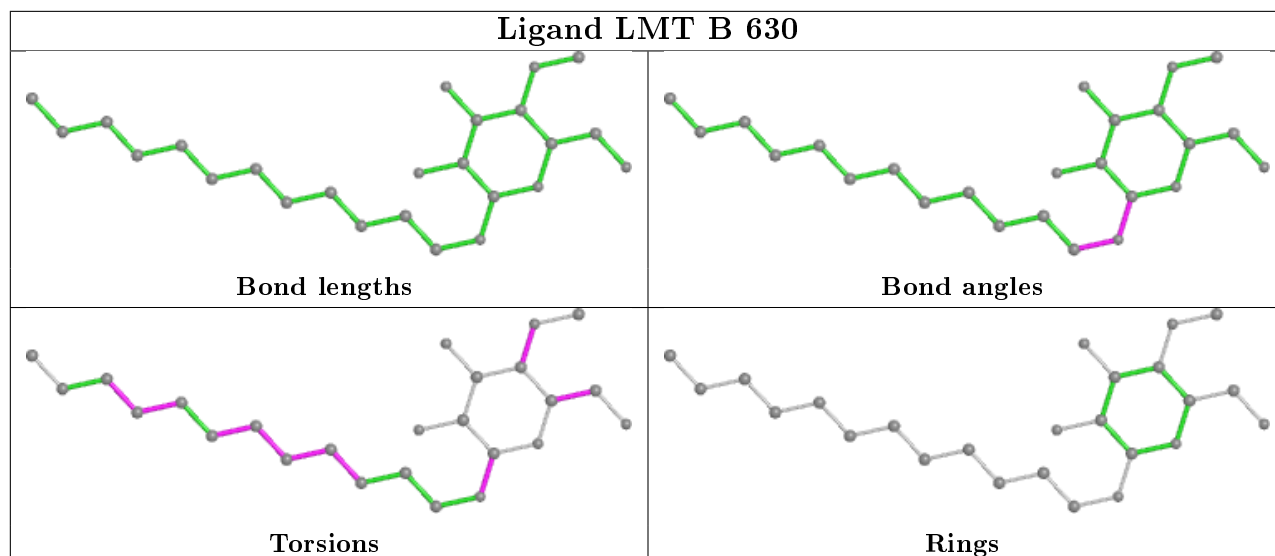


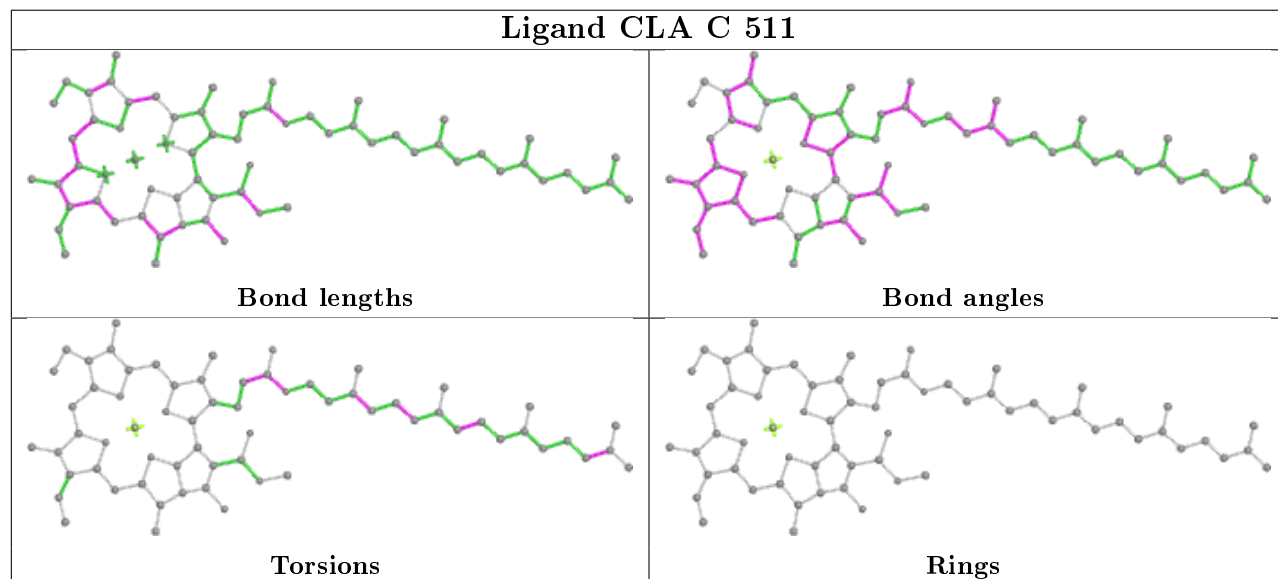
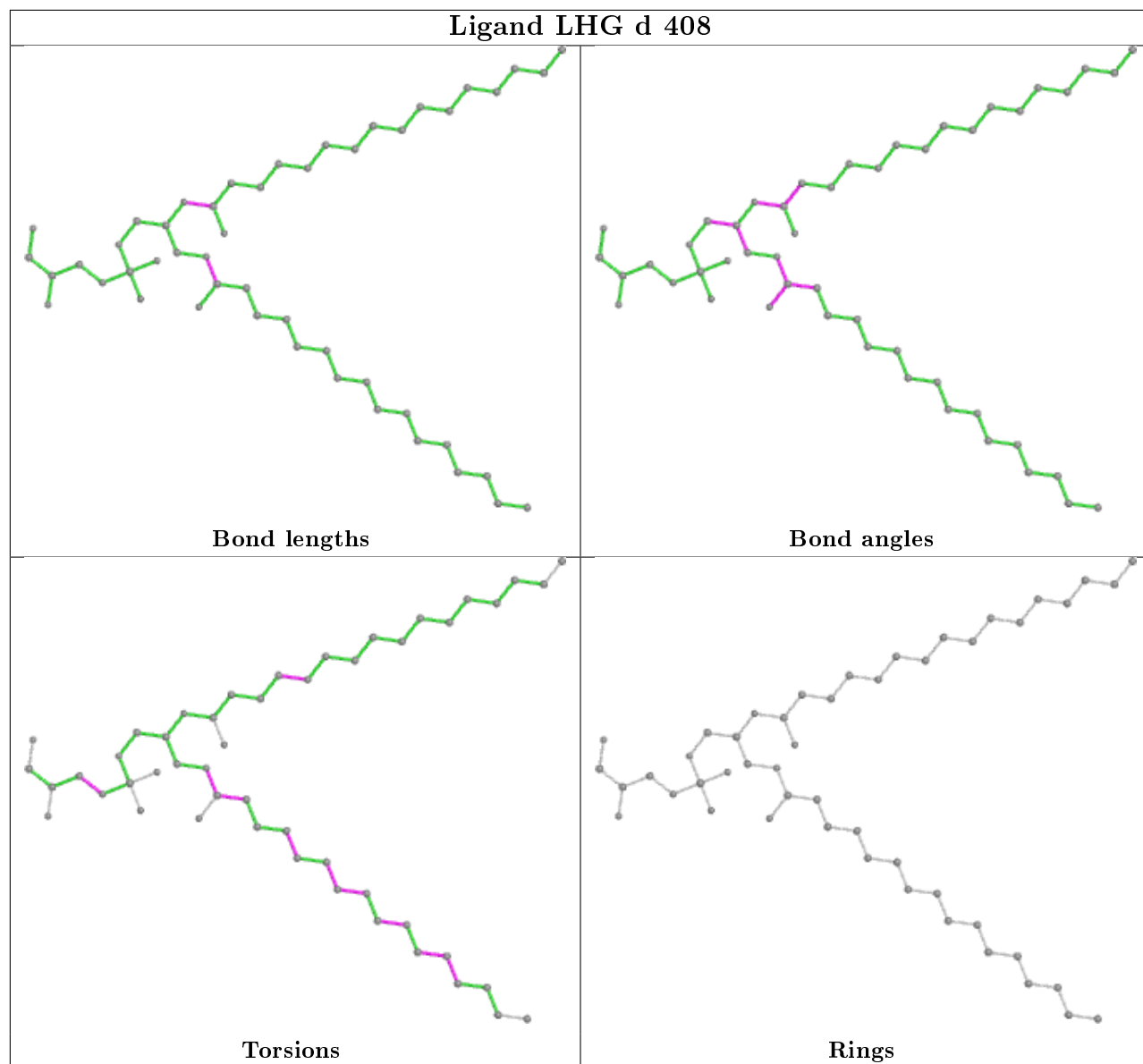


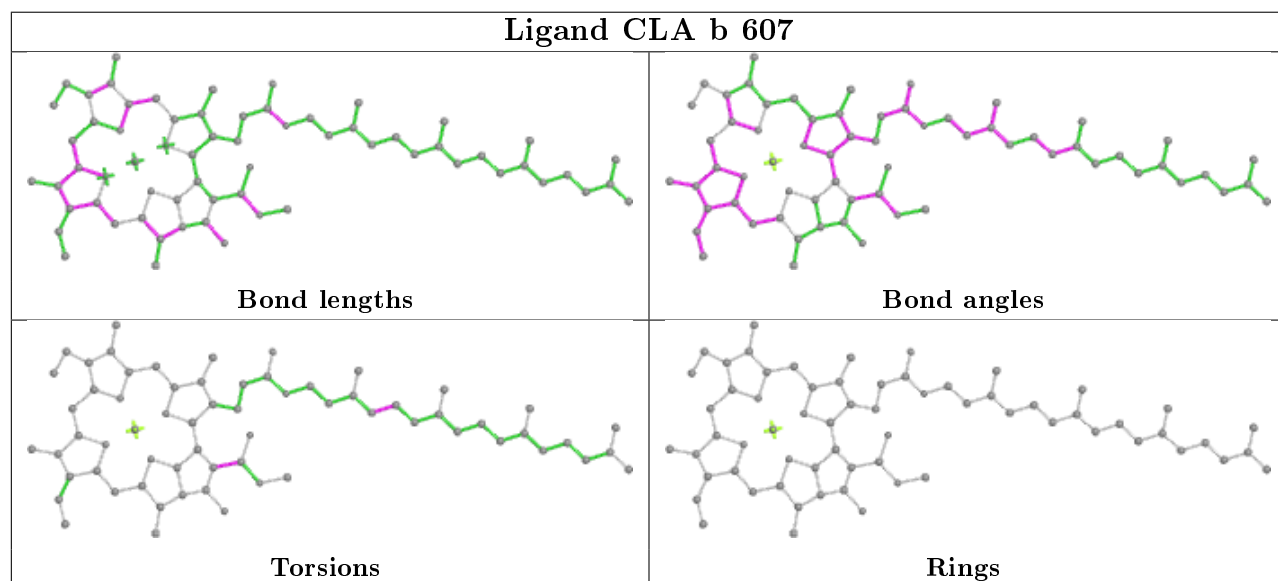
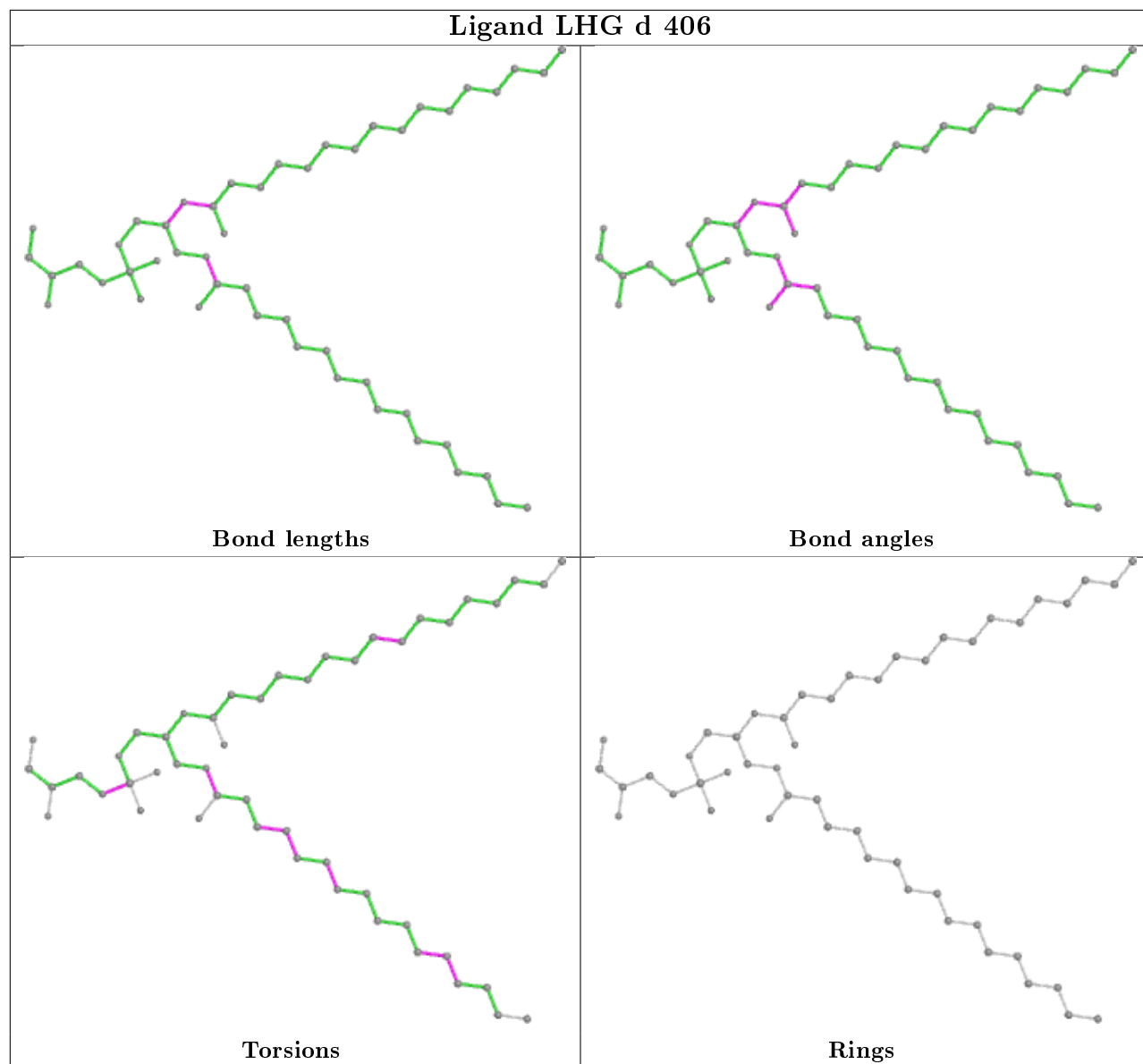


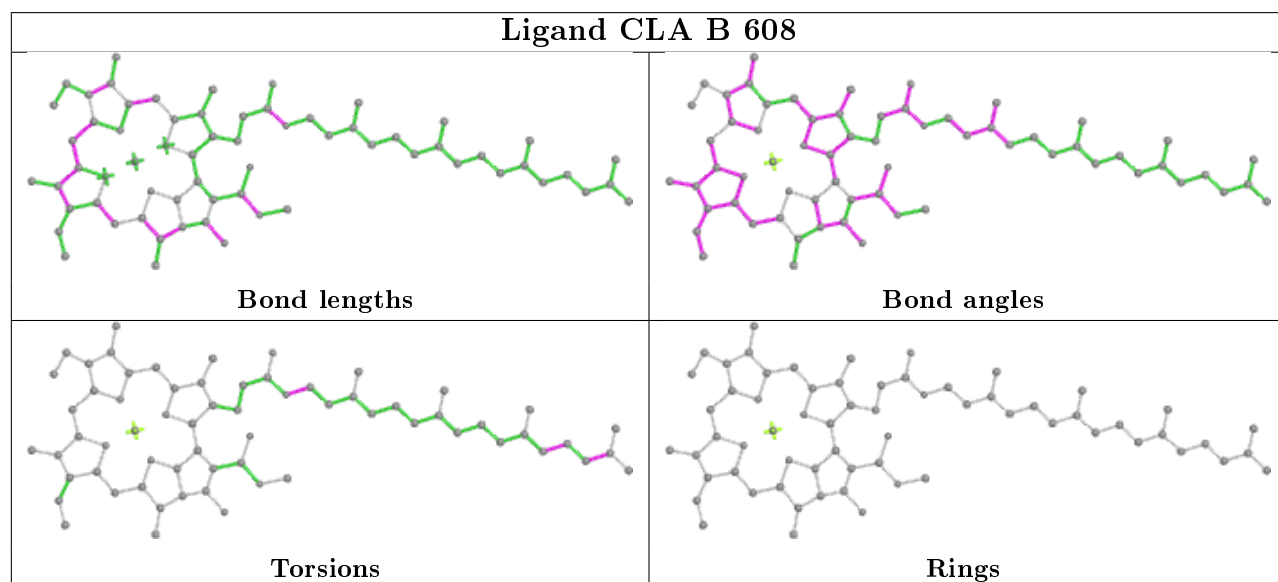
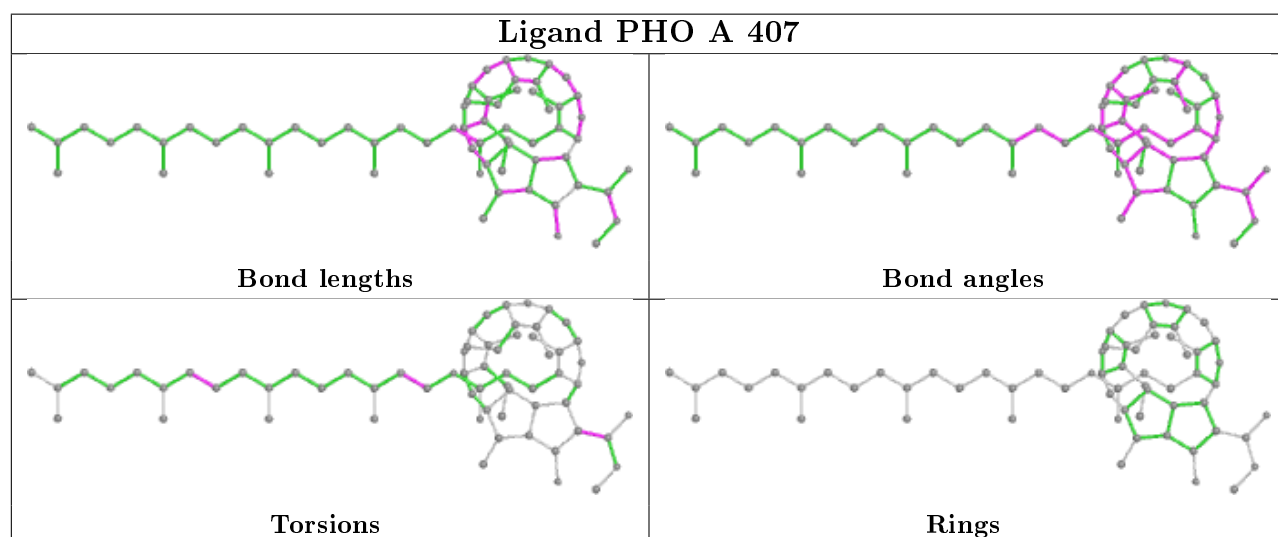
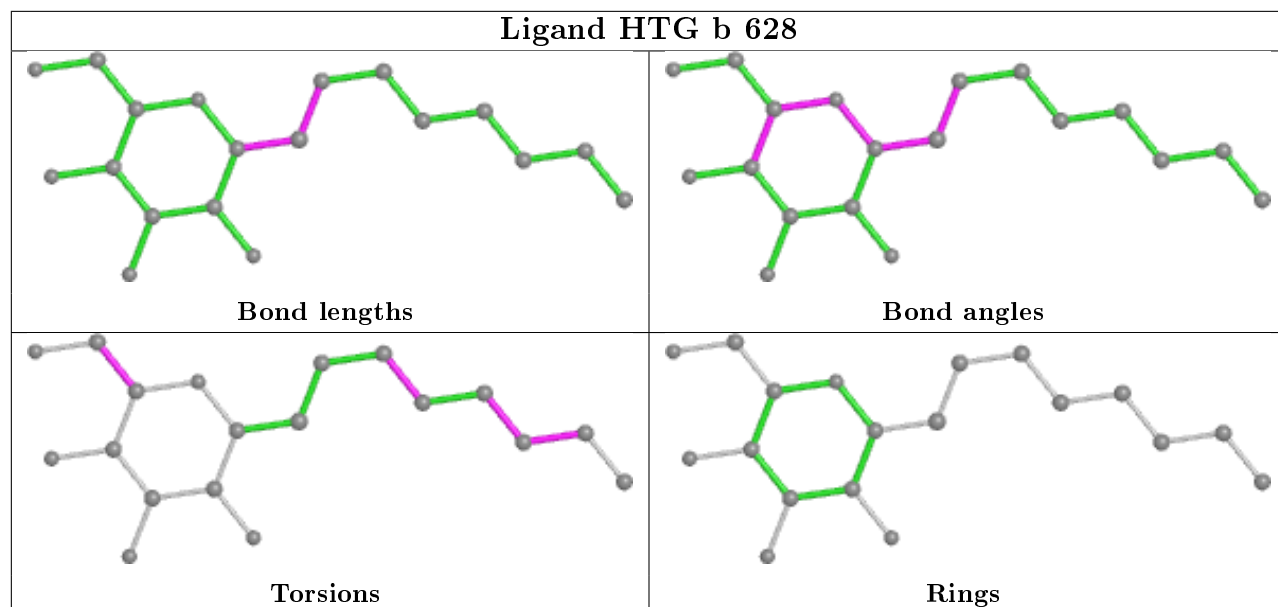


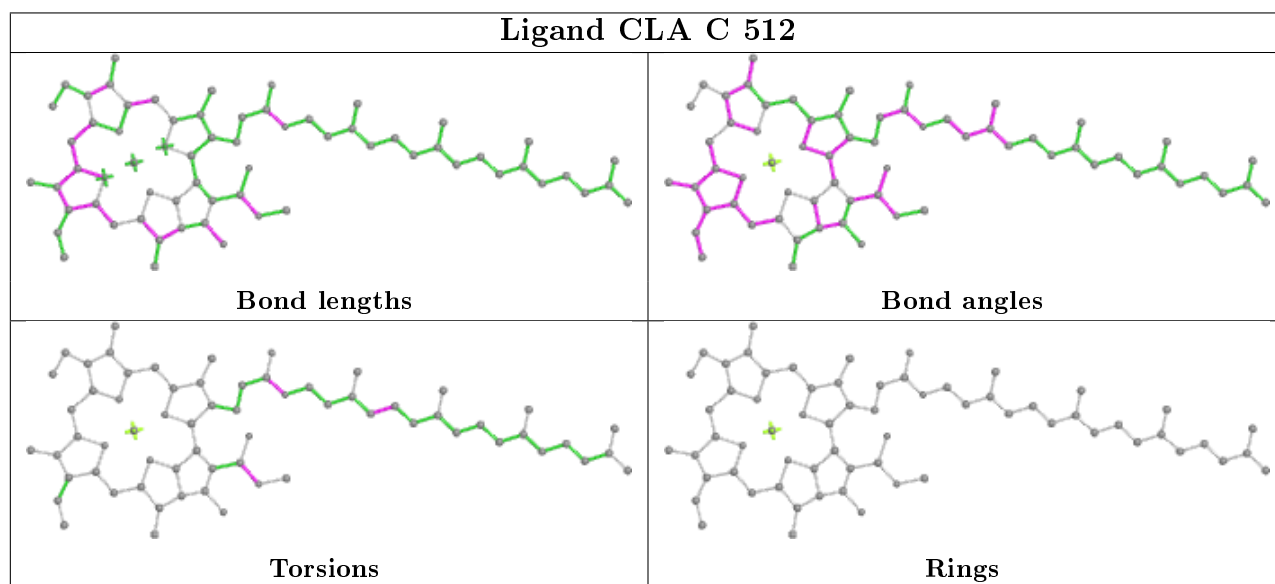
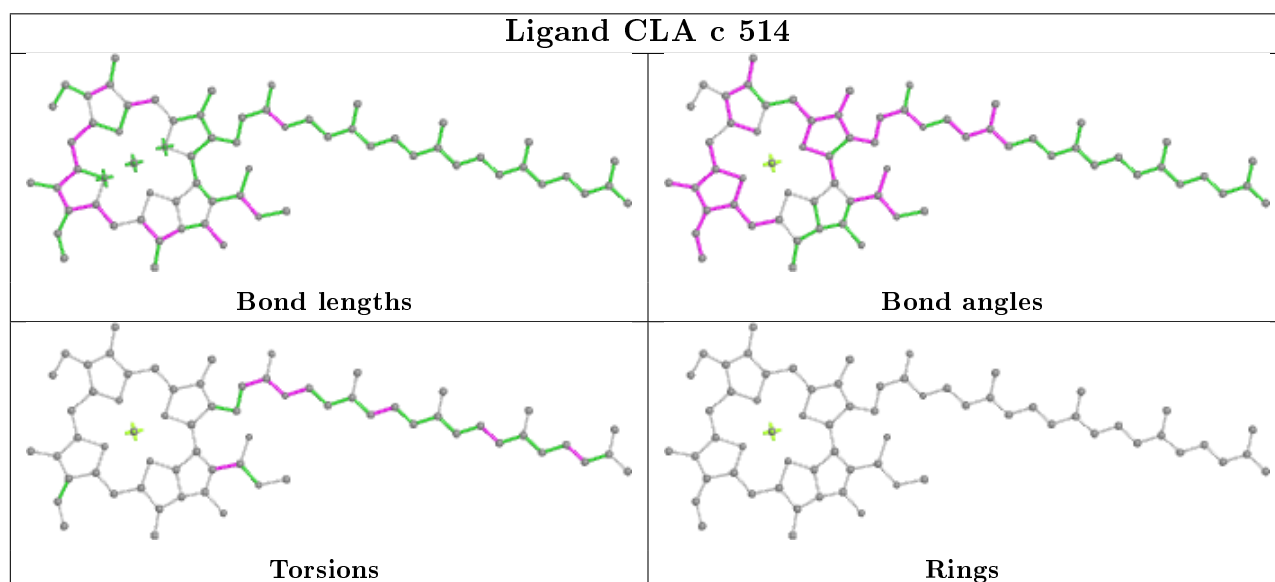
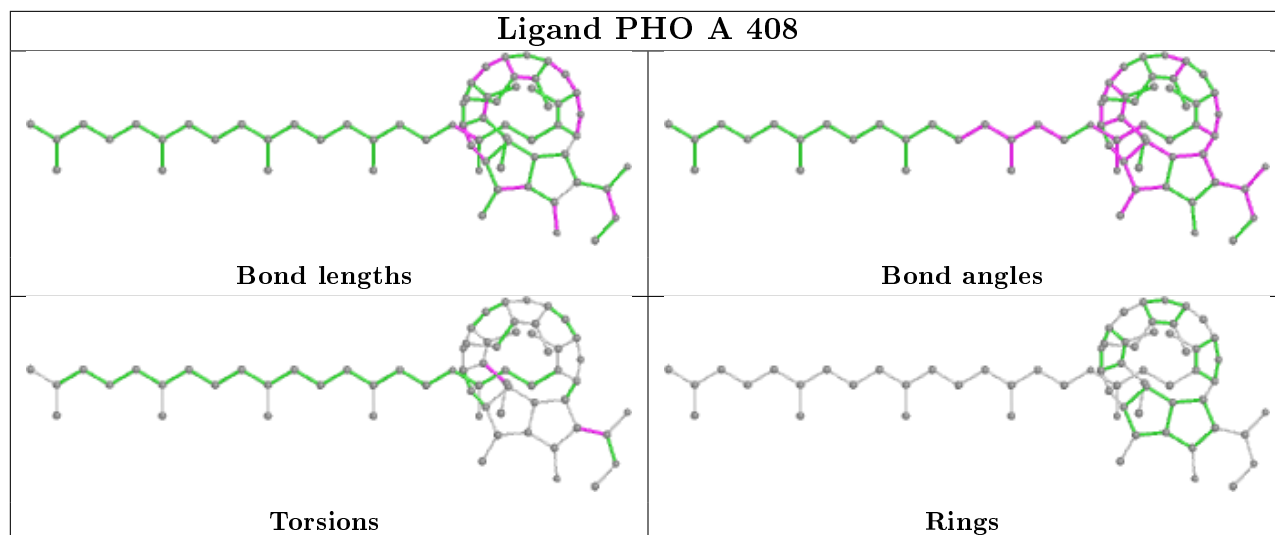


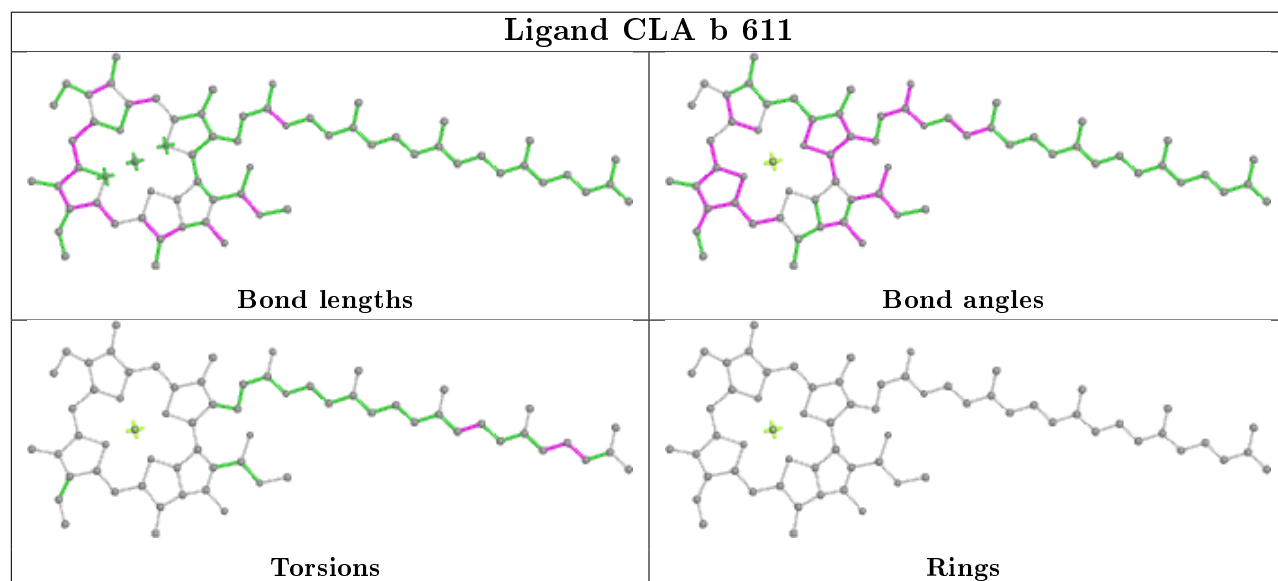
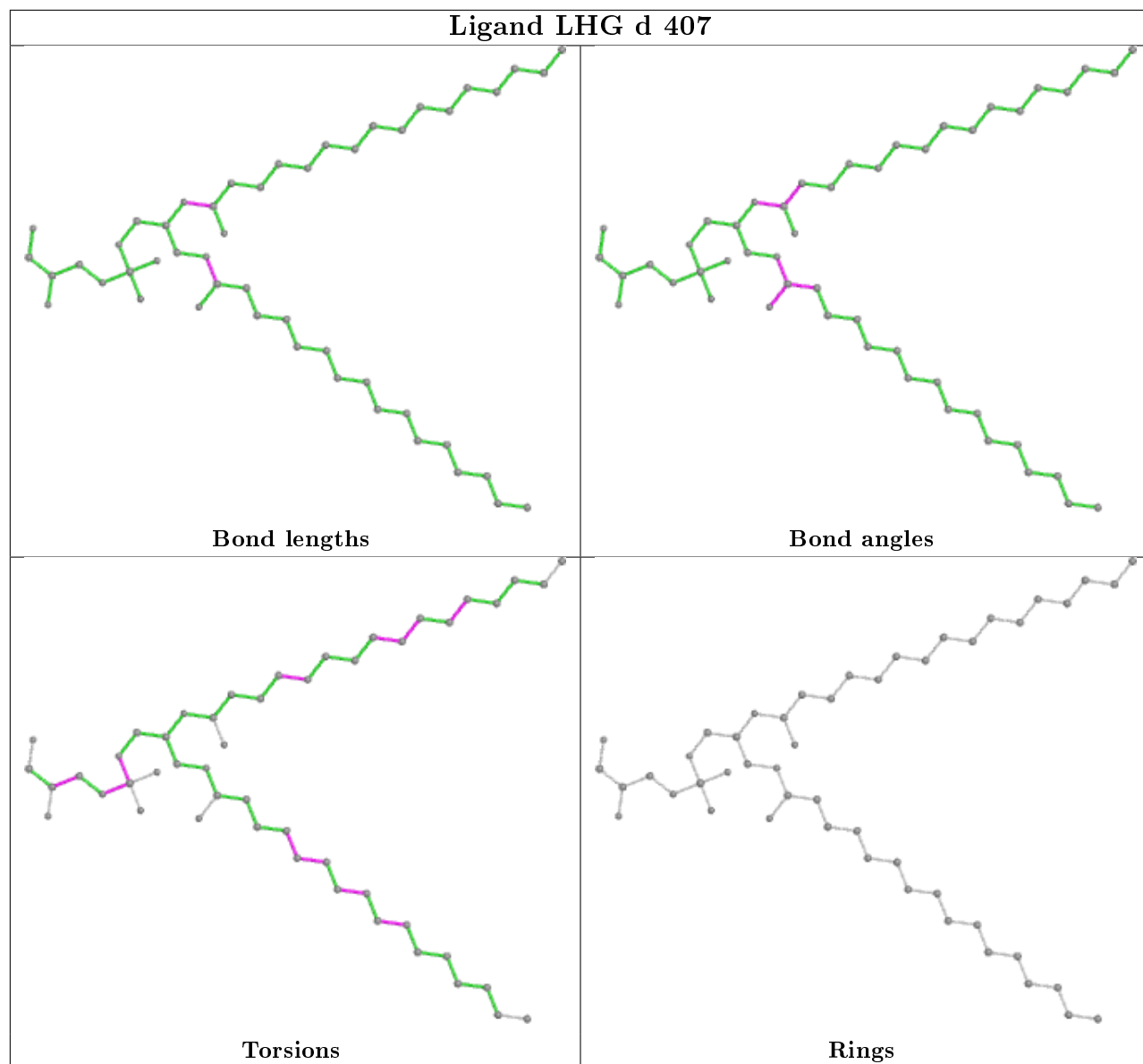


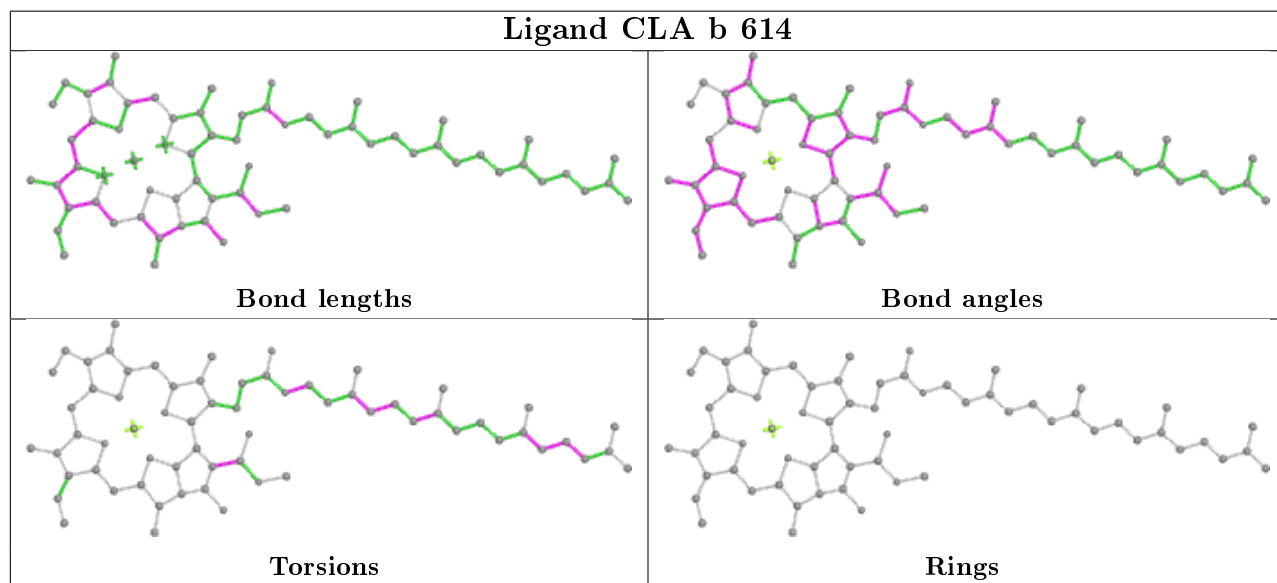
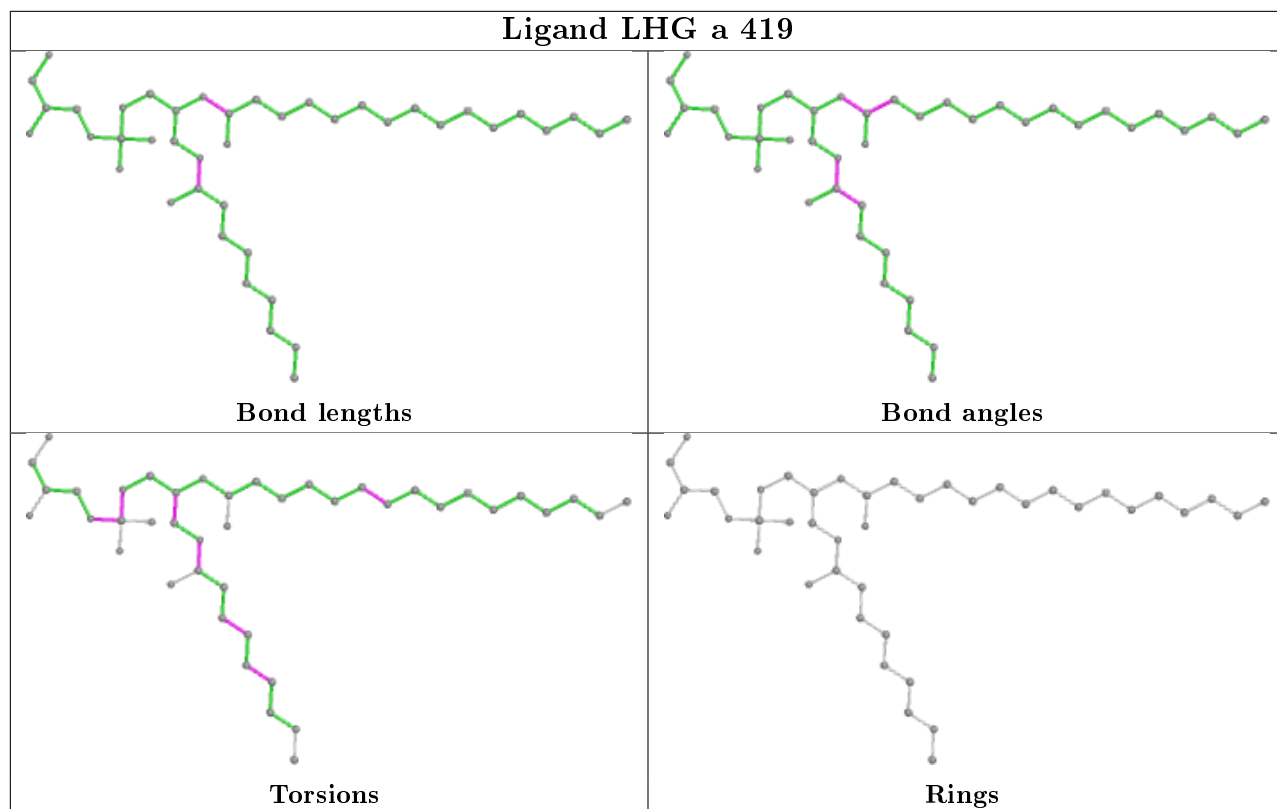
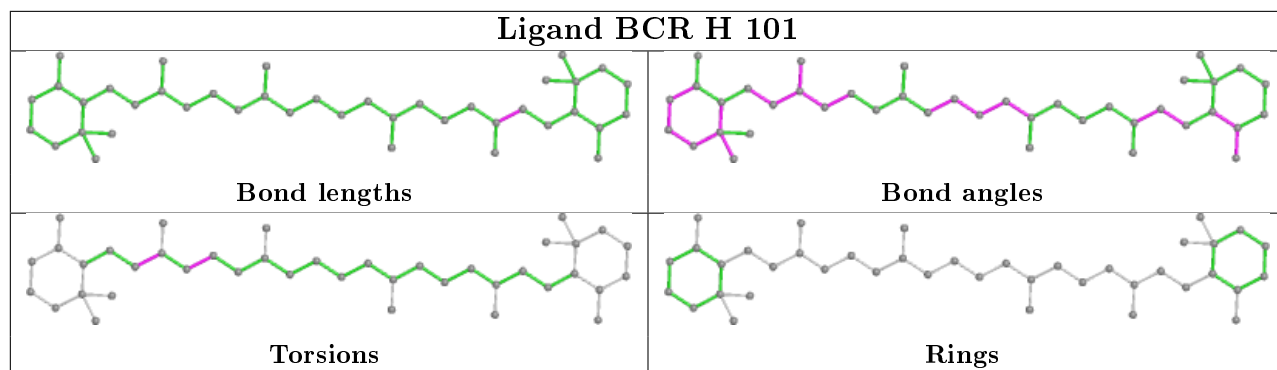


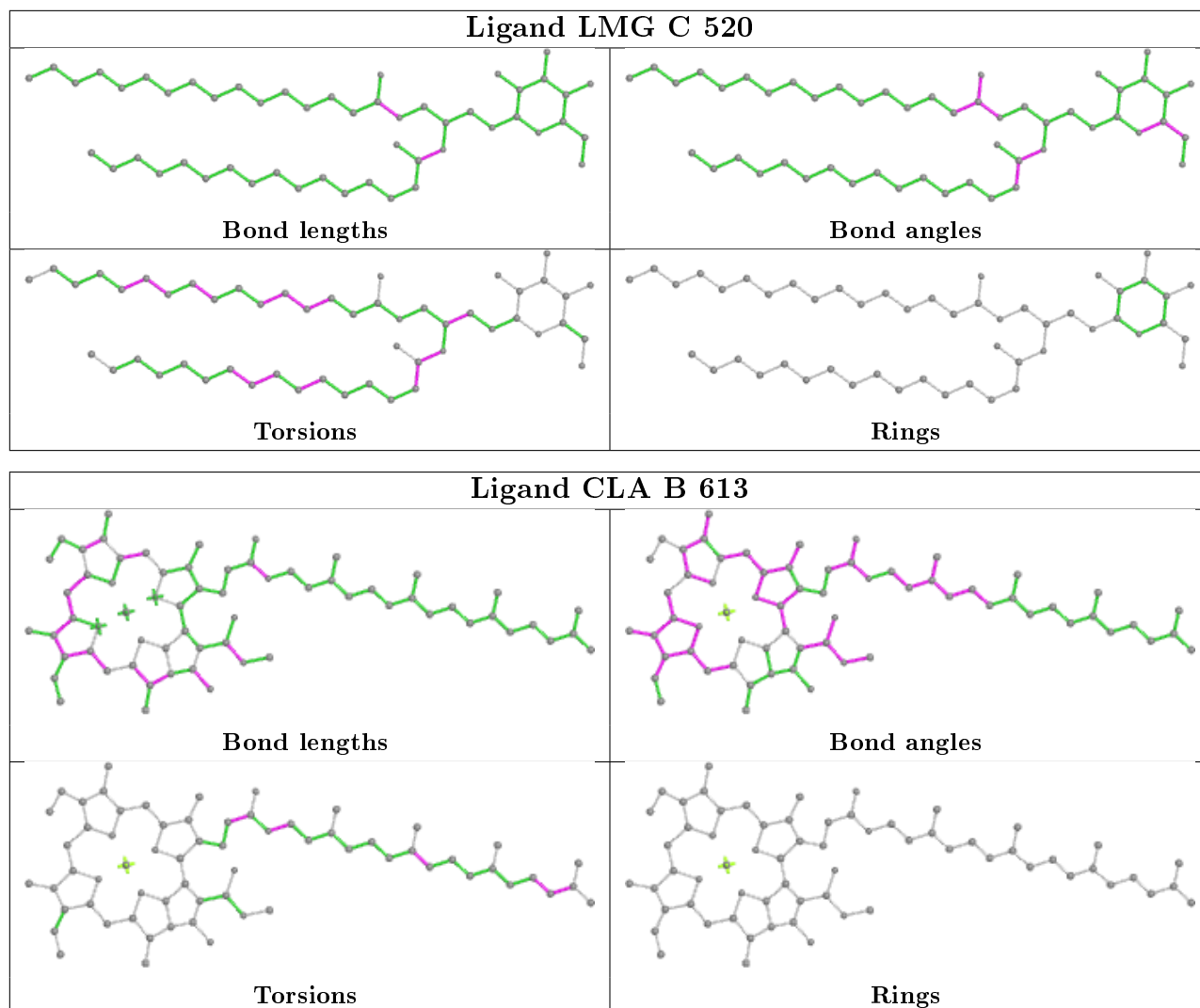


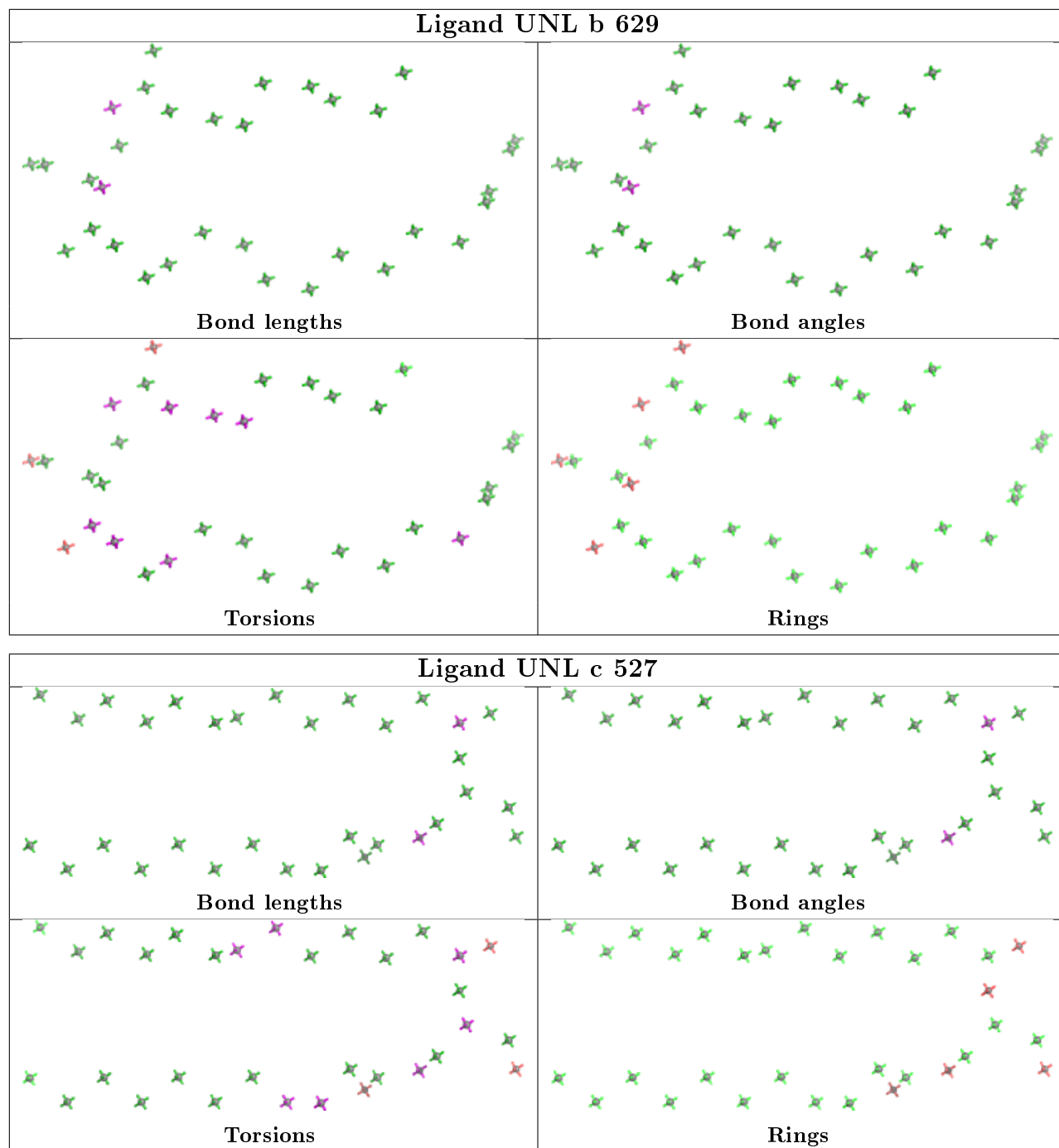


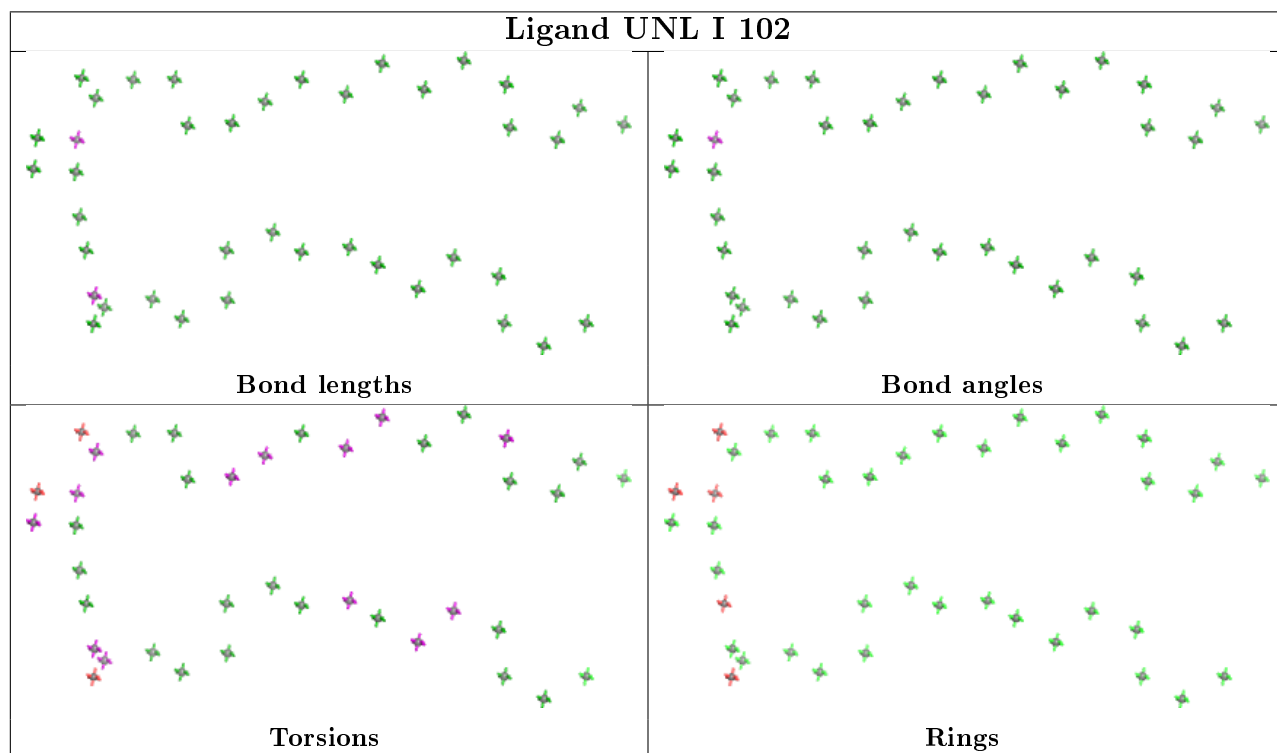
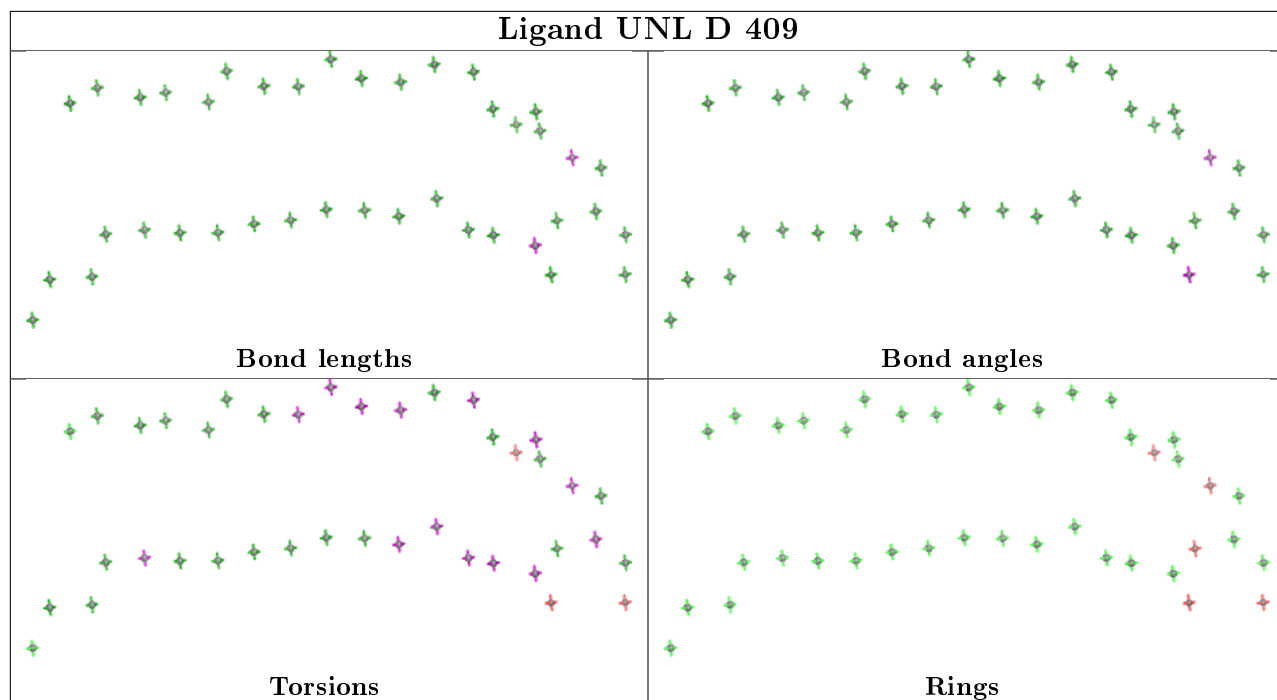


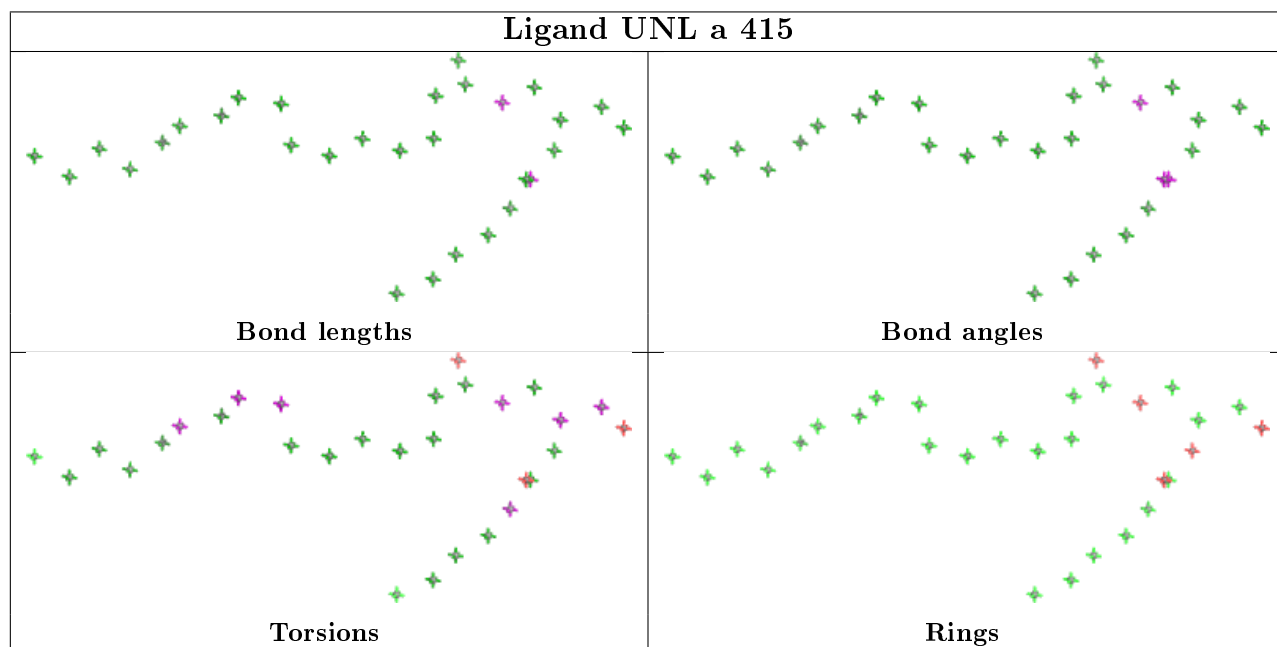
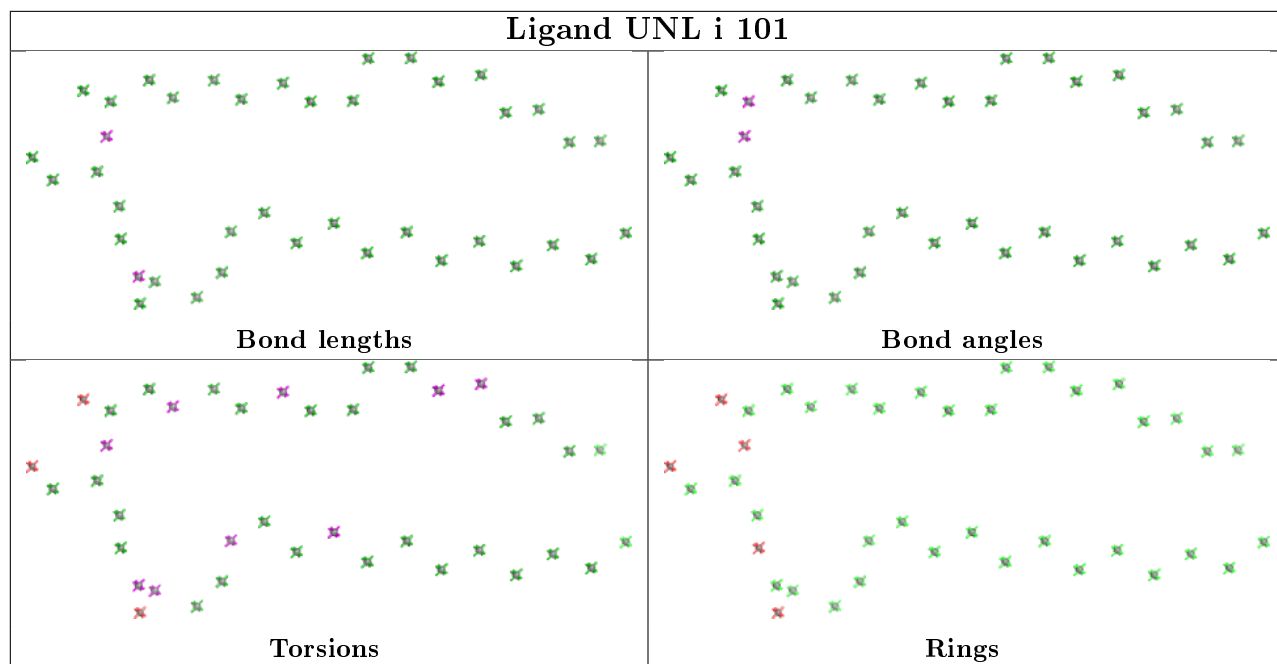


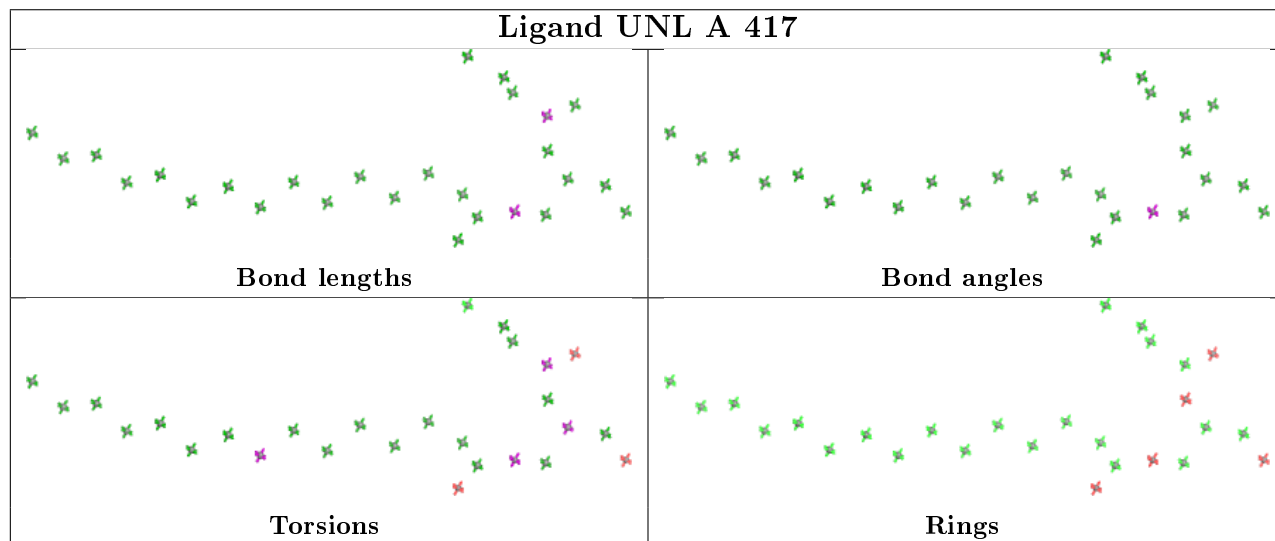
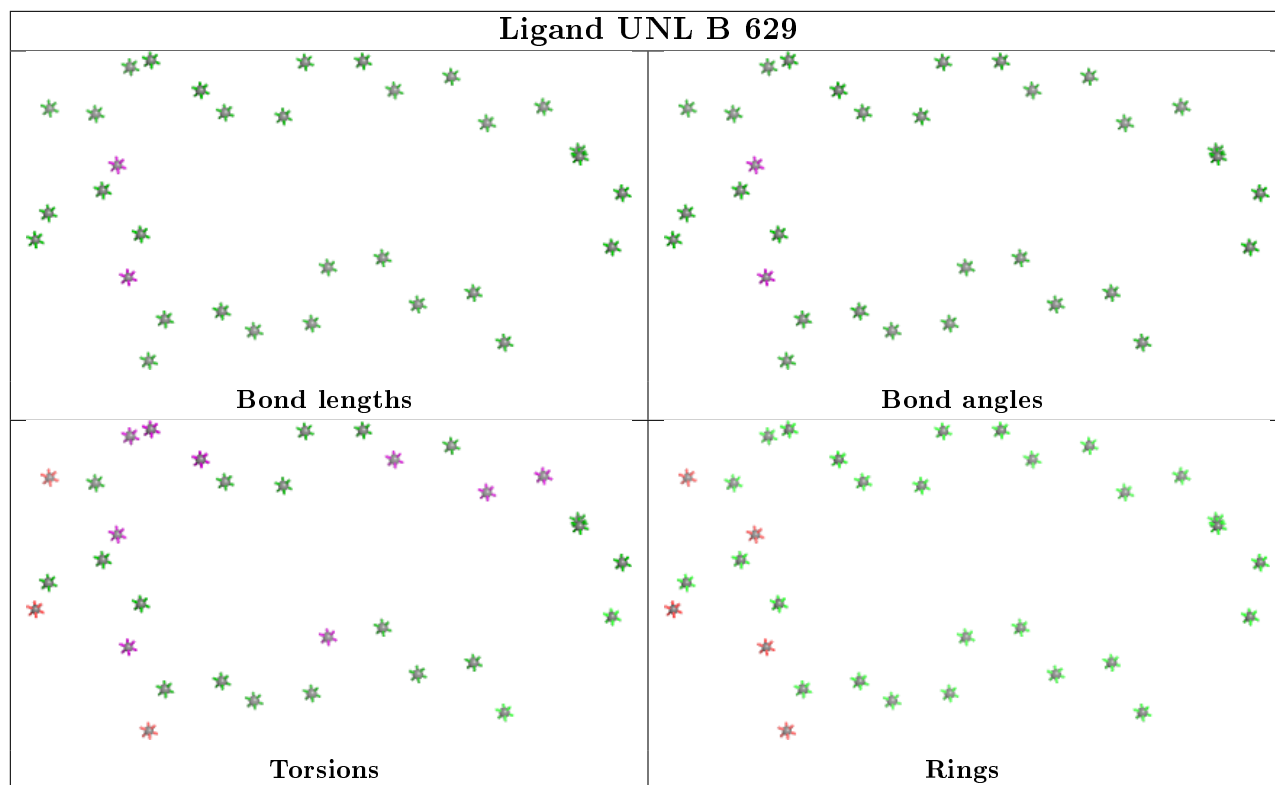


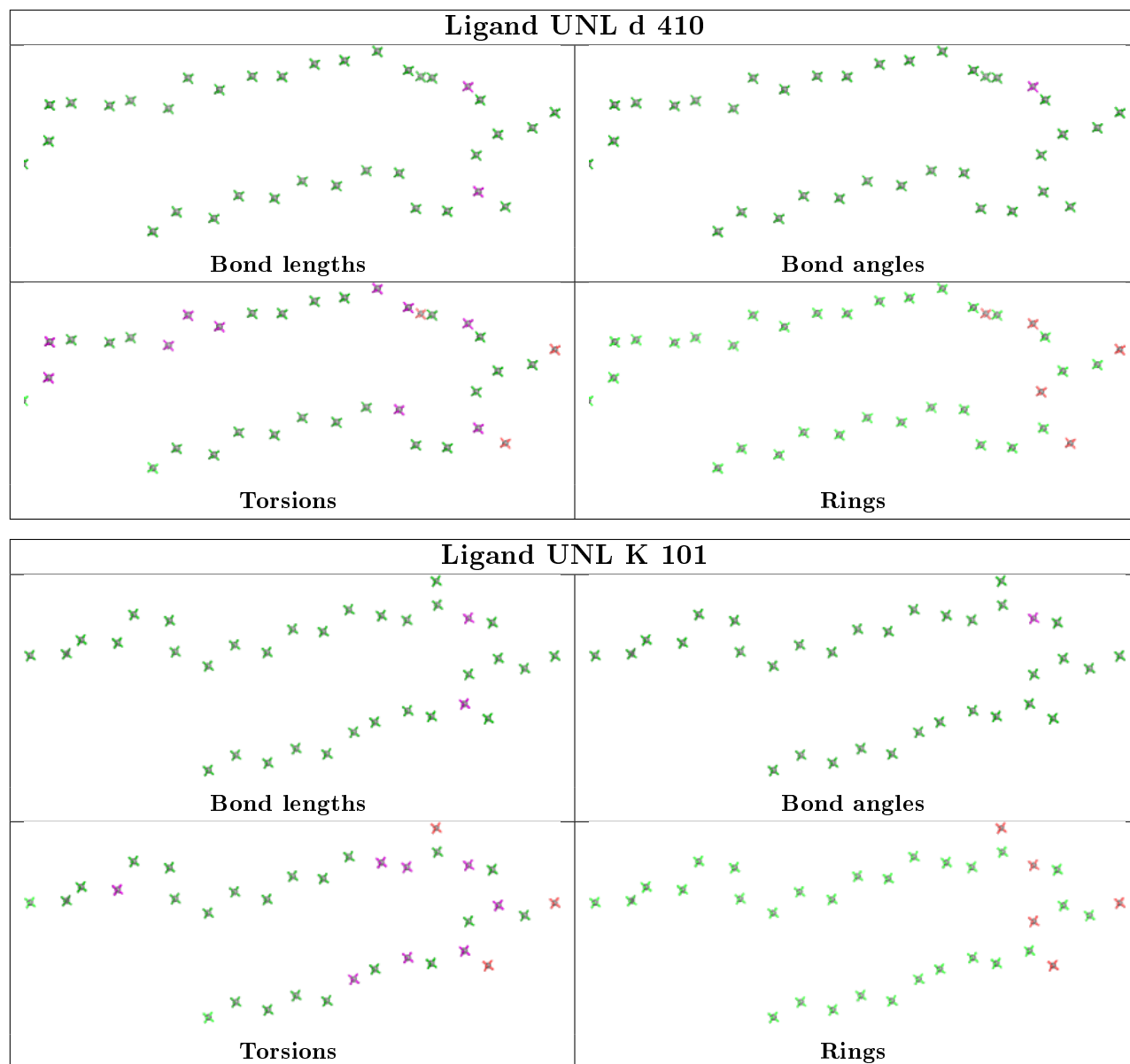












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	334/344 (97%)	1.51	76 (22%) 0 1	40, 48, 69, 120	1 (0%)
1	a	334/344 (97%)	1.77	109 (32%) 0 0	41, 52, 84, 120	0
2	B	504/505 (99%)	1.66	154 (30%) 0 0	41, 53, 83, 128	0
2	b	504/505 (99%)	1.83	167 (33%) 0 0	44, 57, 97, 149	0
3	C	451/455 (99%)	1.83	162 (35%) 0 0	43, 59, 81, 142	0
3	c	455/455 (100%)	1.97	190 (41%) 0 0	48, 67, 90, 129	0
4	D	342/342 (100%)	1.45	88 (25%) 0 1	38, 49, 68, 139	0
4	d	341/342 (99%)	1.62	104 (30%) 0 0	43, 55, 78, 147	0
5	E	81/84 (96%)	2.35	40 (49%) 0 0	53, 70, 100, 151	0
5	e	79/84 (94%)	3.52	61 (77%) 0 0	62, 78, 122, 140	0
6	F	34/44 (77%)	1.45	10 (29%) 0 0	52, 63, 90, 117	0
6	f	31/44 (70%)	2.68	15 (48%) 0 0	62, 68, 100, 140	0
7	H	64/65 (98%)	1.93	24 (37%) 0 0	49, 62, 81, 129	0
7	h	64/65 (98%)	2.21	28 (43%) 0 0	58, 69, 95, 147	0
8	I	37/38 (97%)	2.05	12 (32%) 0 0	55, 62, 127, 147	0
8	i	37/38 (97%)	2.00	15 (40%) 0 0	57, 66, 123, 138	0
9	J	38/39 (97%)	2.17	16 (42%) 0 0	51, 71, 129, 175	0
9	j	39/39 (100%)	2.85	24 (61%) 0 0	56, 80, 149, 175	0
10	K	37/37 (100%)	1.70	13 (35%) 0 0	60, 67, 89, 101	0
10	k	37/37 (100%)	2.37	25 (67%) 0 0	70, 77, 101, 117	0
11	L	36/37 (97%)	1.88	10 (27%) 0 0	41, 47, 109, 162	0
11	l	36/37 (97%)	1.50	7 (19%) 1 2	43, 48, 103, 152	0
12	M	32/36 (88%)	1.37	6 (18%) 1 2	43, 49, 74, 134	0
12	m	33/36 (91%)	1.48	4 (12%) 4 7	43, 50, 86, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	1.92	80 (32%) 0 0	40, 63, 115, 176	0
13	o	243/244 (99%)	2.05	96 (39%) 0 0	44, 65, 121, 161	0
14	T	29/32 (90%)	1.17	3 (10%) 6 10	42, 49, 81, 115	0
14	t	29/32 (90%)	1.13	2 (6%) 16 24	43, 50, 81, 130	0
15	U	96/104 (92%)	1.81	36 (37%) 0 0	47, 60, 90, 101	0
15	u	97/104 (93%)	1.36	20 (20%) 1 1	51, 62, 84, 121	0
16	V	137/137 (100%)	1.53	33 (24%) 0 1	46, 57, 82, 112	0
16	v	137/137 (100%)	2.40	74 (54%) 0 0	52, 71, 104, 137	0
17	X	38/40 (95%)	2.46	22 (57%) 0 0	59, 71, 96, 126	0
17	x	38/40 (95%)	3.14	25 (65%) 0 0	65, 78, 117, 154	0
18	Y	29/30 (96%)	4.41	24 (82%) 0 0	73, 87, 140, 155	0
18	y	29/30 (96%)	4.02	24 (82%) 0 0	79, 97, 126, 136	0
19	Z	62/62 (100%)	3.93	51 (82%) 0 0	67, 84, 131, 173	0
19	z	62/62 (100%)	4.79	55 (88%) 0 0	83, 99, 148, 185	0
20	R	34/34 (100%)	6.44	34 (100%) 0 0	97, 125, 149, 154	0
All	All	5283/5384 (98%)	1.95	1939 (36%) 0 0	38, 59, 104, 185	1 (0%)

All (1939) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	b	494	GLY	15.0
11	L	2	GLU	12.7
19	z	33	TRP	12.5
18	Y	19	ILE	12.3
6	f	15	ILE	12.3
18	Y	20	ALA	12.1
13	O	61	GLN	11.6
19	z	3	ILE	11.5
2	b	504	THR	11.4
2	B	494	GLY	11.3
19	z	30	PRO	10.3
17	x	2	THR	9.9
18	y	41	VAL	9.9
20	R	18	TRP	9.7
2	b	487	SER	9.4
1	a	11	ALA	9.4
19	Z	31	GLN	9.4

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Mol	Chain	Res	Type	RSRZ
17	x	38	GLN	9.3
19	z	31	GLN	9.2
18	Y	18	VAL	9.1
19	z	34	ASP	9.1
2	b	502	VAL	9.1
7	h	65	LEU	9.0
12	M	33	GLN	9.0
20	R	6	LEU	9.0
20	R	23	ILE	8.9
19	Z	33	TRP	8.9
2	b	503	THR	8.7
19	z	2	THR	8.7
2	b	496	TYR	8.5
20	R	24	LEU	8.5
2	b	495	PHE	8.5
20	R	7	VAL	8.4
3	c	200	THR	8.4
2	b	493	TRP	8.3
19	z	61	VAL	8.3
2	B	496	TYR	8.3
19	Z	42	LEU	8.3
20	R	28	VAL	8.2
2	b	295	GLY	8.2
20	R	27	ALA	8.1
9	j	6	ARG	8.1
9	J	4	GLY	8.0
2	b	293	ALA	8.0
1	A	13	LEU	7.9
19	Z	34	ASP	7.9
19	Z	30	PRO	7.9
13	O	133	VAL	7.8
18	Y	23	THR	7.8
11	l	3	PRO	7.8
16	v	16	GLY	7.8
19	z	39	LEU	7.7
7	h	64	ALA	7.7
19	Z	38	GLN	7.7
4	d	14	TRP	7.6
13	o	140	THR	7.6
5	e	20	TRP	7.6
2	B	293	ALA	7.6
9	j	4	GLY	7.5

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Mol	Chain	Res	Type	RSRZ
20	R	25	PRO	7.5
8	I	36	ASP	7.5
20	R	3	TRP	7.5
3	c	24	THR	7.4
19	z	60	PHE	7.4
8	i	36	ASP	7.4
20	R	31	VAL	7.4
20	R	11	PRO	7.4
17	x	37	VAL	7.4
8	I	38	GLU	7.3
18	y	19	ILE	7.3
19	z	50	LEU	7.3
16	V	16	GLY	7.3
19	z	7	LEU	7.3
5	e	79	PHE	7.2
20	R	13	LEU	7.2
2	b	497	GLN	7.2
13	O	27	ARG	7.2
13	o	208	THR	7.2
13	o	133	VAL	7.2
20	R	32	GLN	7.2
19	Z	35	ARG	7.2
3	c	203	THR	7.1
5	e	6	GLY	7.1
13	o	134	THR	7.1
3	C	30	SER	7.1
16	v	14	SER	7.0
5	e	19	TYR	7.0
9	J	3	GLU	7.0
19	z	35	ARG	6.9
5	E	4	THR	6.9
5	e	15	THR	6.9
19	z	25	VAL	6.9
19	Z	1	MET	6.9
16	v	19	ILE	6.9
3	c	143	TYR	6.9
20	R	26	TYR	6.9
2	B	487	SER	6.9
13	o	132	ASN	6.9
19	Z	41	PHE	6.9
19	Z	3	ILE	6.9
12	m	33	GLN	6.9

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Mol	Chain	Res	Type	RSRZ
2	b	296	ALA	6.9
3	C	193	GLY	6.9
2	B	495	PHE	6.8
3	c	101	PRO	6.8
13	O	139	SER	6.8
3	C	207	ARG	6.8
5	e	21	VAL	6.8
3	C	257	PHE	6.7
8	i	37	LEU	6.7
19	Z	4	LEU	6.7
5	E	17	VAL	6.7
3	C	155	ASN	6.7
5	E	84	LYS	6.7
20	R	35	LEU	6.7
13	o	35	SER	6.6
20	R	33	LYS	6.6
13	O	25	THR	6.6
20	R	21	ARG	6.6
4	D	11	GLU	6.6
13	o	58	ASN	6.6
4	D	238	THR	6.6
13	O	23	ASP	6.6
2	b	129	GLY	6.6
13	o	139	SER	6.5
5	e	34	GLY	6.5
19	z	10	ALA	6.5
2	B	295	GLY	6.5
4	d	17	ILE	6.5
9	J	7	ILE	6.5
4	d	12	ARG	6.5
13	o	33	ASP	6.5
20	R	14	LEU	6.5
5	e	74	GLN	6.4
3	c	248	GLY	6.4
13	O	131	PRO	6.4
3	c	23	ALA	6.4
2	B	290	ALA	6.4
5	E	22	ILE	6.3
19	z	32	ASP	6.3
19	z	38	GLN	6.3
18	y	22	LEU	6.3
13	O	208	THR	6.3

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Mol	Chain	Res	Type	RSRZ
19	Z	32	ASP	6.3
7	H	65	LEU	6.2
17	X	38	GLN	6.2
19	z	5	PHE	6.2
8	i	38	GLU	6.2
13	o	41	ALA	6.2
3	c	258	GLY	6.2
9	j	9	LEU	6.2
13	o	204	VAL	6.2
13	o	37	THR	6.2
18	y	20	ALA	6.1
13	O	137	THR	6.1
13	o	209	GLY	6.1
12	m	34	LYS	6.1
13	o	207	ARG	6.1
17	x	9	GLY	6.1
5	E	5	THR	6.1
2	b	491	VAL	6.1
19	z	43	GLY	6.1
13	O	130	GLN	6.1
20	R	10	LEU	6.1
3	c	193	GLY	6.1
19	z	1	MET	6.1
18	y	23	THR	6.0
19	z	42	LEU	6.0
6	f	20	TRP	6.0
19	z	46	LEU	6.0
20	R	2	ASP	6.0
3	c	201	ASN	6.0
20	R	22	ASN	6.0
13	O	26	ALA	6.0
7	h	23	PRO	6.0
20	R	34	LEU	6.0
13	o	4	THR	6.0
13	o	246	ALA	6.0
1	A	12	ASN	6.0
13	o	36	GLN	5.9
3	C	433	LEU	5.9
3	c	205	ASP	5.9
19	z	41	PHE	5.9
13	O	91	GLY	5.9
2	b	482	ILE	5.9

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Mol	Chain	Res	Type	RSRZ
13	o	32	ILE	5.9
18	y	37	PHE	5.9
16	v	15	GLU	5.9
5	E	83	LEU	5.9
13	O	59	LYS	5.9
19	z	29	SER	5.9
4	d	13	GLY	5.9
13	O	58	ASN	5.9
3	c	433	LEU	5.9
4	d	159	ILE	5.9
13	o	27	ARG	5.9
20	R	4	ARG	5.9
10	k	14	ALA	5.8
16	v	17	LYS	5.8
16	v	22	THR	5.8
3	c	426	LEU	5.8
6	F	14	PRO	5.8
13	o	24	ASP	5.8
1	a	15	GLU	5.8
5	e	39	SER	5.8
19	z	57	LEU	5.8
19	z	40	ILE	5.7
5	E	25	ILE	5.7
3	c	182	PHE	5.7
19	Z	36	SER	5.7
18	Y	24	MET	5.7
16	v	5	PRO	5.7
3	c	181	PHE	5.7
20	R	12	VAL	5.7
5	e	22	ILE	5.7
5	e	24	SER	5.7
1	A	11	ALA	5.6
7	H	6	TRP	5.6
3	C	438	LEU	5.6
13	o	31	PRO	5.6
16	v	108	THR	5.6
1	a	326	LEU	5.6
13	o	63	ALA	5.6
19	Z	61	VAL	5.6
18	Y	26	ALA	5.6
7	H	64	ALA	5.6
9	j	5	GLY	5.6

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Mol	Chain	Res	Type	RSRZ
13	o	59	LYS	5.6
3	C	258	GLY	5.5
2	b	501	ASP	5.5
5	e	17	VAL	5.5
5	e	25	ILE	5.5
2	b	294	SER	5.5
19	z	36	SER	5.5
2	B	297	THR	5.5
3	C	201	ASN	5.5
2	B	504	THR	5.5
6	f	16	PHE	5.5
13	O	134	THR	5.5
17	x	3	ILE	5.5
3	C	279	LEU	5.4
3	C	437	PHE	5.4
3	C	285	ILE	5.4
9	J	6	ARG	5.4
19	Z	25	VAL	5.4
2	b	288	VAL	5.4
9	j	7	ILE	5.4
2	b	290	ALA	5.4
2	B	292	LEU	5.4
17	X	2	THR	5.4
1	A	339	PHE	5.4
2	b	483	ASP	5.3
3	c	438	LEU	5.3
20	R	29	LYS	5.3
18	y	24	MET	5.3
19	Z	26	ALA	5.3
5	e	71	GLU	5.3
9	j	3	GLU	5.3
3	C	131	TYR	5.3
2	B	294	SER	5.3
13	o	21	THR	5.3
16	v	13	ASN	5.3
3	c	257	PHE	5.3
19	z	59	PHE	5.3
3	c	194	GLY	5.3
3	c	142	GLU	5.3
20	R	15	ALA	5.3
13	O	132	ASN	5.3
3	c	144	SER	5.3

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Mol	Chain	Res	Type	RSRZ
19	z	8	ALA	5.3
2	b	488	PRO	5.3
2	B	502	VAL	5.2
5	e	84	LYS	5.2
13	O	24	ASP	5.2
13	O	90	ASP	5.2
7	h	6	TRP	5.2
13	O	36	GLN	5.2
1	a	341	LEU	5.2
13	o	91	GLY	5.2
3	C	181	PHE	5.2
13	O	89	SER	5.2
18	Y	41	VAL	5.2
1	A	326	LEU	5.2
20	R	8	VAL	5.2
2	B	296	ALA	5.2
2	B	247	PHE	5.1
3	C	439	VAL	5.1
3	c	250	TRP	5.1
13	o	25	THR	5.1
11	L	7	ARG	5.1
13	O	138	THR	5.1
13	o	205	ASP	5.1
15	U	102	LEU	5.1
18	y	18	VAL	5.1
4	d	16	ASP	5.1
13	o	202	ALA	5.1
18	Y	43	ARG	5.1
3	c	159	THR	5.0
15	u	68	THR	5.0
1	a	228	THR	5.0
6	F	13	TYR	5.0
5	e	42	LEU	5.0
17	x	33	GLN	5.0
1	A	341	LEU	5.0
2	B	245	VAL	5.0
5	E	21	VAL	5.0
2	B	497	GLN	5.0
3	C	281	MET	5.0
3	c	202	PRO	5.0
19	Z	37	LYS	5.0
3	C	162	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
19	Z	45	GLY	5.0
13	O	63	ALA	5.0
16	v	4	THR	5.0
15	U	73	GLN	5.0
9	J	2	SER	5.0
6	f	19	ARG	4.9
2	b	463	PHE	4.9
10	k	16	ALA	4.9
4	d	154	VAL	4.9
15	u	66	GLY	4.9
3	c	260	ALA	4.9
4	d	158	LEU	4.9
1	a	12	ASN	4.9
1	a	14	TRP	4.9
13	o	137	THR	4.9
3	c	190	ALA	4.9
4	D	17	ILE	4.9
16	v	6	GLU	4.9
13	o	29	ALA	4.9
3	C	28	GLN	4.9
5	e	14	ILE	4.9
14	t	29	ILE	4.9
17	X	15	LEU	4.9
3	c	255	THR	4.9
13	o	60	ARG	4.9
13	O	56	PRO	4.8
13	O	62	GLU	4.8
17	x	15	LEU	4.8
19	z	4	LEU	4.8
8	I	37	LEU	4.8
13	O	141	ASP	4.8
17	x	36	LYS	4.8
9	j	12	VAL	4.8
16	v	9	THR	4.8
2	b	252	VAL	4.8
5	e	33	ALA	4.8
20	R	5	VAL	4.8
2	b	505	ARG	4.8
18	Y	22	LEU	4.8
2	b	301	ALA	4.8
2	B	486	LEU	4.8
3	C	317	PHE	4.7

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Mol	Chain	Res	Type	RSRZ
7	H	5	THR	4.7
13	O	140	THR	4.7
3	c	206	PRO	4.7
13	O	88	ASN	4.7
16	v	135	VAL	4.7
1	a	297	LEU	4.7
3	c	279	LEU	4.7
13	O	28	GLY	4.7
19	Z	15	LEU	4.7
2	b	250	PHE	4.7
2	b	245	VAL	4.7
20	R	17	GLY	4.7
2	B	488	PRO	4.7
11	L	3	PRO	4.7
13	O	21	THR	4.7
9	j	10	TRP	4.7
2	B	289	GLN	4.7
3	C	341	LEU	4.7
5	e	29	ALA	4.7
2	b	460	LEU	4.7
4	D	346	LEU	4.7
4	d	352	LEU	4.7
2	b	128	THR	4.7
5	e	60	GLN	4.7
19	Z	39	LEU	4.6
8	i	2	GLU	4.6
3	c	21	ILE	4.6
3	c	147	PHE	4.6
3	c	207	ARG	4.6
2	b	489	GLU	4.6
4	D	159	ILE	4.6
18	y	40	ALA	4.6
19	Z	23	VAL	4.6
19	Z	2	THR	4.6
5	e	81	GLU	4.6
2	b	247	PHE	4.6
13	o	38	TYR	4.6
4	D	352	LEU	4.6
17	x	34	ILE	4.6
13	o	130	GLN	4.6
20	R	20	VAL	4.6
15	U	80	GLU	4.6

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Mol	Chain	Res	Type	RSRZ
13	o	6	THR	4.6
16	v	113	VAL	4.6
17	x	4	THR	4.6
18	Y	21	GLN	4.5
2	b	251	VAL	4.5
19	Z	62	VAL	4.5
2	B	505	ARG	4.5
12	m	31	SER	4.5
2	b	249	ALA	4.5
3	c	60	ILE	4.5
19	z	45	GLY	4.5
3	C	200	THR	4.5
3	C	253	LEU	4.5
7	h	46	LEU	4.5
11	L	6	ASN	4.5
2	b	291	SER	4.5
5	e	78	THR	4.5
19	Z	29	SER	4.5
13	O	4	THR	4.5
3	c	251	HIS	4.5
18	y	21	GLN	4.5
13	O	30	TYR	4.5
2	b	297	THR	4.5
15	U	68	THR	4.5
2	b	486	LEU	4.5
16	v	107	LEU	4.5
16	V	6	GLU	4.5
8	I	6	ILE	4.5
2	B	250	PHE	4.4
2	B	458	PHE	4.4
3	C	276	LEU	4.4
4	d	20	ASP	4.4
1	a	248	ILE	4.4
5	e	10	PHE	4.4
1	A	343[A]	LEU	4.4
17	X	37	VAL	4.4
13	o	56	PRO	4.4
4	d	325	ILE	4.4
3	C	143	TYR	4.4
3	c	22	PHE	4.4
11	l	5	PRO	4.4
18	Y	42	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
3	c	145	SER	4.4
1	a	261	GLN	4.4
2	B	248	ALA	4.4
3	C	442	LEU	4.4
19	Z	52	LEU	4.4
2	b	186	GLY	4.4
5	e	26	THR	4.4
19	z	6	GLN	4.4
5	e	36	LEU	4.4
5	E	81	GLU	4.4
2	B	242	ILE	4.4
20	R	19	ALA	4.4
13	O	22	LEU	4.3
15	U	101	GLY	4.3
5	E	12	ASP	4.3
8	I	34	ARG	4.3
3	C	25	ASN	4.3
16	v	23	GLU	4.3
3	c	87	ILE	4.3
3	C	145[A]	SER	4.3
3	C	153	ASP	4.3
7	h	13	PRO	4.3
2	b	246	PHE	4.3
5	e	83	LEU	4.3
6	f	37	ILE	4.3
2	b	286	ARG	4.3
15	U	104	LYS	4.3
18	Y	34	MET	4.3
1	a	295	PHE	4.3
3	C	435	PHE	4.3
5	E	36	LEU	4.3
1	a	330	VAL	4.3
2	B	288	VAL	4.3
17	x	39	ARG	4.3
9	J	8	PRO	4.3
13	o	206	GLY	4.3
3	C	432	VAL	4.3
9	j	14	THR	4.3
18	Y	37	PHE	4.3
1	a	13	LEU	4.3
3	c	401	LEU	4.3
4	d	122	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
18	Y	38	LEU	4.3
3	C	288	CYS	4.2
2	b	458	PHE	4.2
3	c	158	THR	4.2
15	U	64	ILE	4.2
3	c	442	LEU	4.2
1	A	228	THR	4.2
13	o	89	SER	4.2
13	o	90	ASP	4.2
13	o	64	GLU	4.2
4	d	346	LEU	4.2
5	e	16	SER	4.2
13	O	200	ASN	4.2
1	a	120	LEU	4.2
5	e	72	ALA	4.2
4	D	14	TRP	4.2
1	a	258	LEU	4.2
3	c	261	ARG	4.2
11	l	7	ARG	4.2
13	O	205	ASP	4.2
16	v	20	THR	4.2
16	V	7	VAL	4.2
18	y	27	MET	4.1
18	y	34	MET	4.1
2	B	461	LEU	4.1
5	e	7	GLU	4.1
1	a	321	ILE	4.1
2	b	467	ILE	4.1
13	o	34	SER	4.1
18	y	43	ARG	4.1
1	a	188	ALA	4.1
2	b	130[A]	GLU	4.1
5	e	11	SER	4.1
3	C	23	ALA	4.1
20	R	16	ALA	4.1
5	E	23	HIS	4.1
20	R	30	GLN	4.1
17	x	5	PRO	4.1
2	b	461	LEU	4.1
19	z	62	VAL	4.1
3	C	60	ILE	4.1
3	C	282	MET	4.1

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Mol	Chain	Res	Type	RSRZ
7	h	42	LEU	4.1
18	y	30	ILE	4.1
3	C	100	GLY	4.1
3	c	282	MET	4.1
5	e	57	ALA	4.0
2	B	485	GLU	4.0
1	a	262	TYR	4.0
2	B	300	GLU	4.0
2	B	350	GLU	4.0
2	b	456	ALA	4.0
4	d	238	THR	4.0
16	v	28	GLU	4.0
2	b	292	LEU	4.0
2	B	490	GLN	4.0
5	E	57	ALA	4.0
19	z	49	ALA	4.0
2	B	251	VAL	4.0
3	c	153	ASP	4.0
5	e	23	HIS	4.0
3	c	437	PHE	4.0
3	c	148	GLY	4.0
3	C	262	ARG	4.0
15	U	63	ASN	4.0
5	E	20	TRP	4.0
3	c	404	LEU	4.0
2	b	244	ALA	4.0
3	c	431	PHE	4.0
3	C	27	ASP	4.0
18	Y	44	GLY	4.0
7	h	56	ASP	4.0
3	C	135	ARG	4.0
9	j	8	PRO	3.9
16	v	8	LEU	3.9
5	E	78	THR	3.9
19	z	54	VAL	3.9
8	I	10	ILE	3.9
16	v	69	ILE	3.9
18	Y	30	ILE	3.9
1	a	16	ARG	3.9
2	b	484	PRO	3.9
16	V	50	PRO	3.9
3	C	251	HIS	3.9

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Mol	Chain	Res	Type	RSRZ
1	a	63	ILE	3.9
5	e	58	GLN	3.9
2	B	249	ALA	3.9
17	X	23	LEU	3.9
13	o	198	SER	3.9
3	C	158	THR	3.9
3	c	254	THR	3.9
3	C	210	PHE	3.9
5	E	79	PHE	3.9
19	Z	60	PHE	3.9
1	a	320	ILE	3.9
2	b	242	ILE	3.9
16	v	78	ASN	3.9
16	V	52	LEU	3.9
16	v	72	LEU	3.9
18	y	38	LEU	3.9
4	d	27	PHE	3.9
1	a	160	ILE	3.9
5	e	28	PRO	3.9
2	b	243	ALA	3.9
18	y	31	ALA	3.9
8	I	3	THR	3.9
14	T	30	THR	3.9
3	C	436	PHE	3.9
19	Z	17	PHE	3.9
2	b	485	GLU	3.9
4	d	21	TRP	3.9
3	c	285	ILE	3.9
13	O	60	ARG	3.9
10	k	41	ALA	3.9
1	a	343[A]	LEU	3.9
3	C	426	LEU	3.9
4	d	321	LEU	3.9
16	v	27	LEU	3.9
19	z	37	LYS	3.8
2	B	161	LEU	3.8
2	b	348	ASN	3.8
4	d	162	LEU	3.8
19	Z	46	LEU	3.8
3	C	142	GLU	3.8
1	A	160	ILE	3.8
13	o	241	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
5	E	15	THR	3.8
8	i	6	ILE	3.8
10	K	16	ALA	3.8
2	b	298	LEU	3.8
4	D	90	LEU	3.8
5	e	40	THR	3.8
14	t	30	THR	3.8
15	u	103	TYR	3.8
3	c	25	ASN	3.8
1	A	330	VAL	3.8
1	a	184	ILE	3.8
11	L	5	PRO	3.8
13	O	92	SER	3.8
19	Z	27	TYR	3.8
2	b	248	ALA	3.8
5	e	53	ASP	3.8
5	e	27	ILE	3.8
18	Y	25	ILE	3.8
2	B	410	THR	3.8
2	B	298	LEU	3.8
5	E	35	TRP	3.8
9	j	2	SER	3.8
2	B	503	THR	3.7
3	c	166	ILE	3.7
3	c	259	TRP	3.7
18	y	44	GLY	3.7
17	x	26	ALA	3.7
17	X	36	LYS	3.7
3	C	401	LEU	3.7
3	C	206	PRO	3.7
3	C	192	GLY	3.7
2	B	383	PHE	3.7
13	O	203	LYS	3.7
4	d	119	ALA	3.7
16	v	7	VAL	3.7
18	Y	36	ILE	3.7
2	b	350	GLU	3.7
1	A	16	ARG	3.7
3	c	249	ILE	3.7
13	O	35	SER	3.7
16	V	14	SER	3.7
10	K	33	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
8	I	2	GLU	3.7
16	v	99	ASP	3.7
2	b	462	PHE	3.7
18	y	33	PRO	3.7
16	v	25	GLN	3.7
11	l	2	GLU	3.7
13	o	200	ASN	3.7
19	Z	5	PHE	3.7
13	O	31	PRO	3.7
19	z	27	TYR	3.7
4	d	287	VAL	3.7
2	B	460	LEU	3.6
4	d	127	LEU	3.6
13	O	34	SER	3.6
2	B	252	VAL	3.6
3	c	378	ASN	3.6
3	c	410[A]	VAL	3.6
19	z	58	ASN	3.6
3	c	119	LEU	3.6
5	e	65	LEU	3.6
13	o	237	GLY	3.6
16	v	114	ALA	3.6
10	k	17	ILE	3.6
13	O	87	VAL	3.6
13	O	240	TYR	3.6
13	o	10	ILE	3.6
2	b	499	VAL	3.6
5	E	16	SER	3.6
3	C	32	GLY	3.6
4	D	351	ALA	3.6
3	c	384	ILE	3.6
3	c	88	LEU	3.6
9	J	10	TRP	3.6
19	z	52	LEU	3.6
3	c	424	SER	3.6
5	e	18	ARG	3.6
15	u	8	GLU	3.6
4	D	287	VAL	3.6
9	j	15	VAL	3.6
17	X	28	LEU	3.6
13	o	28	GLY	3.6
4	D	233	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	454	ALA	3.6
3	C	159	THR	3.6
18	y	26	ALA	3.6
5	e	82	GLN	3.6
2	b	162	PHE	3.6
3	C	284	PHE	3.6
4	d	284	ILE	3.6
7	h	10	ILE	3.6
16	V	45	ILE	3.6
16	V	135	VAL	3.6
19	Z	7	LEU	3.6
2	B	493	TRP	3.6
10	k	39	TRP	3.6
13	o	61	GLN	3.6
3	c	284	PHE	3.5
4	d	120	PHE	3.5
3	c	429	SER	3.5
1	a	259	ILE	3.5
13	O	32	ILE	3.5
1	A	120	LEU	3.5
1	A	145	VAL	3.5
2	B	452	THR	3.5
2	b	398	THR	3.5
7	H	2	ALA	3.5
17	X	4	THR	3.5
4	d	169	PHE	3.5
4	D	89	LEU	3.5
2	b	492	GLU	3.5
2	b	454	ALA	3.5
3	c	427	ALA	3.5
2	b	206	GLY	3.5
15	U	57	SER	3.5
17	X	32	SER	3.5
2	b	300	GLU	3.5
1	A	159	LEU	3.5
4	d	123	ILE	3.5
4	d	144	ILE	3.5
4	d	320	LEU	3.5
13	o	22	LEU	3.5
13	o	96	VAL	3.5
3	C	427	ALA	3.5
16	V	99	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
2	b	241	SER	3.5
5	e	59	GLU	3.5
3	c	95	LEU	3.5
19	z	14	ILE	3.5
3	c	208	VAL	3.5
13	o	245	PRO	3.5
13	o	138	THR	3.5
4	D	151	ALA	3.5
17	x	30	ALA	3.5
1	a	231	GLU	3.5
15	U	103	TYR	3.5
1	A	331	MET	3.5
5	E	13	ILE	3.5
1	a	331	MET	3.4
1	A	121[A]	LEU	3.4
1	A	338	ASN	3.4
3	C	43	ILE	3.4
13	O	202	ALA	3.4
7	h	51	SER	3.4
2	b	127	ARG	3.4
15	U	59	GLU	3.4
16	v	26	TYR	3.4
10	k	20	PRO	3.4
13	o	57	LYS	3.4
2	b	256	MET	3.4
3	C	35	TRP	3.4
1	A	163	ILE	3.4
1	a	89	ILE	3.4
2	b	452	THR	3.4
3	c	59	LEU	3.4
7	H	42	LEU	3.4
6	f	36	ALA	3.4
1	a	238	LYS	3.4
1	a	340	PRO	3.4
13	o	131	PRO	3.4
1	A	151	LEU	3.4
1	A	295	PHE	3.4
2	b	383	PHE	3.4
4	d	188	PHE	3.4
3	c	191	PRO	3.4
15	U	65	PRO	3.4
2	b	498	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	a	163	ILE	3.4
8	i	21	PHE	3.4
18	y	28	ILE	3.4
4	D	154	VAL	3.4
7	H	18	TYR	3.4
1	a	286	ALA	3.4
3	C	95	LEU	3.4
3	c	414	ILE	3.4
4	D	144	ILE	3.4
18	Y	40	ALA	3.4
10	k	38	VAL	3.4
2	b	163	GLY	3.4
3	C	139	THR	3.4
16	V	18	THR	3.4
1	a	328	MET	3.4
3	c	240	ILE	3.4
4	D	36	LEU	3.4
4	D	234	ALA	3.4
1	a	224	ILE	3.4
2	b	126	PRO	3.3
16	v	79	PRO	3.3
1	a	19	ASN	3.3
2	B	456	ALA	3.3
3	c	64	ALA	3.3
15	u	73	GLN	3.3
3	C	431	PHE	3.3
3	c	43	ILE	3.3
3	c	209	ILE	3.3
4	d	157	PHE	3.3
3	c	117	VAL	3.3
3	c	198	VAL	3.3
13	O	135	SER	3.3
3	C	57	ALA	3.3
3	C	140	LEU	3.3
18	Y	39	LEU	3.3
2	B	366	PHE	3.3
2	b	479	PHE	3.3
3	c	92	ILE	3.3
10	k	28	ILE	3.3
9	j	34	GLY	3.3
1	a	67	VAL	3.3
6	f	24	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	14	TRP	3.3
5	E	40	THR	3.3
3	C	286	ALA	3.3
4	d	151	ALA	3.3
16	v	98	ALA	3.3
16	v	136	TYR	3.3
3	C	42	LEU	3.3
3	C	59	LEU	3.3
3	c	86	LEU	3.3
4	D	158	LEU	3.3
15	u	101	GLY	3.3
2	B	463	PHE	3.3
2	B	464	PHE	3.3
13	o	39	ARG	3.3
2	B	179	GLN	3.3
3	c	20	SER	3.3
13	O	201	VAL	3.3
2	B	483	ASP	3.3
5	e	12	ASP	3.3
7	h	5	THR	3.3
2	b	373	LYS	3.3
5	e	8	ARG	3.3
3	c	170	ILE	3.3
4	D	270	PHE	3.3
13	o	243	ILE	3.3
15	U	60	ASP	3.3
3	c	197	ARG	3.3
9	J	5	GLY	3.3
3	c	204	LEU	3.3
9	j	18	MET	3.3
16	v	137	TYR	3.3
6	F	15	ILE	3.3
13	o	201	VAL	3.3
5	E	26	THR	3.3
13	O	37	THR	3.3
17	X	13	GLY	3.2
1	a	294	ALA	3.2
2	B	256	MET	3.2
15	u	65	PRO	3.2
1	a	290	ILE	3.2
3	c	350	ILE	3.2
18	Y	35	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
19	Z	48	ILE	3.2
2	B	462	PHE	3.2
3	c	439	VAL	3.2
2	b	289	GLN	3.2
2	B	489	GLU	3.2
16	V	94	SER	3.2
3	C	318	LEU	3.2
1	A	63	ILE	3.2
2	B	265	ILE	3.2
6	F	42	PHE	3.2
2	b	223	GLN	3.2
6	f	28	VAL	3.2
2	b	449	GLY	3.2
16	V	63	THR	3.2
15	u	28	ASN	3.2
2	b	121	GLU	3.2
4	d	115	ALA	3.2
15	U	70	ARG	3.2
4	D	116	LEU	3.2
13	o	157	LEU	3.2
19	z	47	TRP	3.2
7	h	57	GLY	3.2
2	b	457	VAL	3.2
13	O	129	THR	3.2
4	d	18	LEU	3.2
8	I	4	LEU	3.2
1	A	15	GLU	3.2
13	o	62	GLU	3.2
15	U	56	GLU	3.2
3	C	283	GLY	3.2
7	h	9	ASP	3.2
10	k	18	PHE	3.2
16	V	13	ASN	3.2
18	Y	45	ASN	3.2
2	B	457	VAL	3.2
3	C	29	GLU	3.2
3	c	141	GLU	3.2
3	C	337	LEU	3.2
2	B	413	ASP	3.2
15	u	64	ILE	3.2
2	B	65	PHE	3.2
1	A	281	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
16	v	64	PRO	3.2
4	D	12	ARG	3.2
13	o	9	ASP	3.2
3	C	404	LEU	3.2
16	v	110	LYS	3.2
15	U	32	ILE	3.1
17	X	33	GLN	3.1
2	b	464	PHE	3.1
4	d	146	PHE	3.1
6	F	16	PHE	3.1
16	V	81	THR	3.1
17	x	11	PHE	3.1
3	c	425	TRP	3.1
3	c	187	ASP	3.1
9	j	19	GLY	3.1
3	c	276	LEU	3.1
4	d	116	LEU	3.1
14	T	14	ILE	3.1
4	d	15	PHE	3.1
4	d	153	PHE	3.1
2	B	484	PRO	3.1
7	h	18	TYR	3.1
10	k	15	TYR	3.1
15	U	58	VAL	3.1
9	j	13	ALA	3.1
16	V	96	ARG	3.1
17	x	35	ASP	3.1
19	Z	10	ALA	3.1
2	b	490	GLN	3.1
3	c	28	GLN	3.1
3	c	31	SER	3.1
4	D	150	ILE	3.1
4	D	213	ILE	3.1
1	a	242	GLU	3.1
3	C	101	PRO	3.1
13	O	55	GLU	3.1
19	z	51	VAL	3.1
15	U	85	THR	3.1
17	X	35	ASP	3.1
17	X	34	ILE	3.1
2	b	268	PHE	3.1
3	c	136	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
2	b	185	TRP	3.1
3	C	104	GLU	3.1
5	E	59	GLU	3.1
15	U	86	GLU	3.1
2	b	413	ASP	3.1
7	H	46	LEU	3.1
3	C	24	THR	3.1
9	j	11	ILE	3.1
3	c	171	GLY	3.1
4	d	345	VAL	3.1
1	a	288	LEU	3.1
2	b	238	LEU	3.1
3	c	253	LEU	3.1
11	L	19	LEU	3.1
2	B	449	GLY	3.1
4	D	123	ILE	3.1
1	A	336	ALA	3.1
2	B	253	ALA	3.1
2	B	453	PHE	3.1
3	C	331	ALA	3.1
3	c	317	PHE	3.1
5	e	43	ALA	3.1
19	z	11	ALA	3.1
4	D	276	VAL	3.0
16	v	42	VAL	3.0
2	B	258	TYR	3.0
1	a	42	LEU	3.0
3	C	254	THR	3.0
3	C	272	LEU	3.0
3	c	428	THR	3.0
9	J	14	THR	3.0
16	v	132	GLY	3.0
1	a	116	ILE	3.0
7	H	10	ILE	3.0
1	A	123	ALA	3.0
10	K	14	ALA	3.0
17	x	8	LYS	3.0
4	D	291	LEU	3.0
4	d	279	LEU	3.0
17	X	22	GLY	3.0
1	a	336	ALA	3.0
2	B	301	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
3	C	414	ILE	3.0
4	d	259	ILE	3.0
12	m	32	GLN	3.0
10	k	34	ALA	3.0
15	u	86	GLU	3.0
2	B	478	VAL	3.0
3	C	144	SER	3.0
3	c	54	VAL	3.0
4	D	28	VAL	3.0
2	B	402	TYR	3.0
4	D	324	GLY	3.0
4	D	162	LEU	3.0
4	D	210	LEU	3.0
13	o	229	GLU	3.0
5	e	13	ILE	3.0
10	K	28	ILE	3.0
3	C	358	PHE	3.0
2	B	62	VAL	3.0
3	c	227	VAL	3.0
3	c	353	GLY	3.0
16	v	18	THR	3.0
19	Z	49	ALA	3.0
1	a	232	SER	3.0
2	B	241	SER	3.0
2	B	162	PHE	3.0
3	c	358	PHE	3.0
5	E	74	GLN	3.0
5	e	45	ASP	3.0
8	i	3	THR	3.0
3	C	88	LEU	3.0
19	Z	14	ILE	3.0
8	i	26	GLY	3.0
13	o	83	GLY	3.0
2	b	65	PHE	3.0
3	c	420	VAL	3.0
16	v	11	PRO	3.0
17	x	27	VAL	3.0
3	C	26	ARG	3.0
4	d	182	LEU	2.9
13	O	5	LEU	2.9
13	O	93	LEU	2.9
16	v	12	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
13	o	227	ALA	2.9
3	C	184	GLY	2.9
3	C	252	ILE	2.9
4	d	163	GLY	2.9
7	H	8	GLY	2.9
1	A	285	PHE	2.9
5	e	31	PHE	2.9
2	b	30	VAL	2.9
3	C	63	TRP	2.9
3	C	225	VAL	2.9
3	c	29	GLU	2.9
3	C	204	LEU	2.9
3	c	356	MET	2.9
4	d	25	ASP	2.9
3	c	235	GLY	2.9
3	c	199	ILE	2.9
4	d	178	ILE	2.9
16	v	24	LYS	2.9
19	Z	40	ILE	2.9
1	a	252	HIS	2.9
3	c	168	LEU	2.9
4	d	183	LEU	2.9
11	L	23	LEU	2.9
13	o	5	LEU	2.9
13	o	92	SER	2.9
2	B	349	LYS	2.9
2	b	402	TYR	2.9
16	v	106	ASN	2.9
19	z	13	VAL	2.9
2	B	254	GLY	2.9
16	v	21	LEU	2.9
1	a	309	ALA	2.9
2	B	244	ALA	2.9
3	c	246	ALA	2.9
9	j	16	ALA	2.9
1	a	46	ILE	2.9
13	o	211	ILE	2.9
1	a	243	GLU	2.9
4	D	130	PHE	2.9
1	a	281	VAL	2.9
1	a	327	GLY	2.9
1	A	218	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	185	TRP	2.9
2	b	39	LEU	2.9
4	d	150	ILE	2.9
2	b	411	PHE	2.9
4	d	204	VAL	2.9
13	O	204	VAL	2.9
17	X	20	VAL	2.9
1	A	242	GLU	2.9
1	A	288	LEU	2.9
2	B	304	ALA	2.9
4	d	74	LEU	2.9
4	d	143	ALA	2.9
15	U	75	LEU	2.9
3	c	63	TRP	2.9
3	c	195	ASP	2.9
7	H	12[A]	ARG	2.9
4	d	256	ILE	2.8
15	U	74	ILE	2.8
5	E	24	SER	2.8
13	O	128	SER	2.8
1	A	33	PHE	2.8
11	L	4	ASN	2.8
10	K	24	VAL	2.8
2	B	39	LEU	2.8
4	D	19	ASP	2.8
4	D	321	LEU	2.8
10	K	46	ARG	2.8
1	A	38	ILE	2.8
3	C	92	ILE	2.8
3	C	277	GLY	2.8
3	c	412[A]	THR	2.8
4	D	284	ILE	2.8
5	e	41	GLY	2.8
11	l	8	GLN	2.8
16	v	2	GLU	2.8
1	a	339	PHE	2.8
2	B	268	PHE	2.8
13	o	141	ASP	2.8
1	a	28	LEU	2.8
2	B	238	LEU	2.8
2	B	267	LEU	2.8
3	C	168	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
16	v	116	ALA	2.8
2	B	396	GLY	2.8
2	b	189	GLY	2.8
3	C	280	SER	2.8
4	d	147	SER	2.8
4	d	160	TYR	2.8
5	E	39	SER	2.8
19	z	16	SER	2.8
3	C	224	ILE	2.8
2	b	87	ASP	2.8
2	B	30	VAL	2.8
19	Z	18	VAL	2.8
19	z	18	VAL	2.8
13	O	64	GLU	2.8
13	o	55	GLU	2.8
2	b	63	LEU	2.8
3	c	157	MET	2.8
4	d	329	MET	2.8
7	H	30	LEU	2.8
2	B	403	GLY	2.8
13	O	237	GLY	2.8
1	a	176	ILE	2.8
1	a	225	ARG	2.8
4	D	259	ILE	2.8
13	o	30	TYR	2.8
1	a	283	VAL	2.8
2	B	376	VAL	2.8
17	X	26	ALA	2.8
3	C	137	PRO	2.8
19	Z	24	PRO	2.8
1	a	311	GLY	2.8
1	a	230	THR	2.8
2	b	412	THR	2.8
15	U	19	THR	2.8
16	V	15	GLU	2.8
17	x	31	ILE	2.8
1	A	19	ASN	2.8
1	a	158	PHE	2.8
1	a	145	VAL	2.8
6	f	18	VAL	2.8
3	C	396	MET	2.8
3	c	50	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
15	U	79	LEU	2.8
17	X	6	SER	2.8
17	x	7	LEU	2.8
2	B	130[A]	GLU	2.8
3	C	428	THR	2.8
13	o	94	THR	2.8
3	c	385	GLN	2.8
2	b	425	ILE	2.8
13	o	136	ILE	2.8
3	C	259	TRP	2.8
2	B	246	PHE	2.7
2	b	125	ASP	2.7
3	C	182	PHE	2.7
3	c	314	ALA	2.7
4	d	286	VAL	2.7
3	C	463	SER	2.7
16	v	71	GLY	2.7
2	B	474	LEU	2.7
16	V	48	THR	2.7
1	A	53	ILE	2.7
1	A	143	ILE	2.7
4	d	100	ASP	2.7
13	O	38	TYR	2.7
5	E	29	ALA	2.7
6	F	12	SER	2.7
16	v	62	ALA	2.7
17	x	32	SER	2.7
2	b	399	VAL	2.7
1	A	258	LEU	2.7
2	b	29	LEU	2.7
3	c	175	LEU	2.7
3	c	281	MET	2.7
2	B	373	LYS	2.7
2	b	435	GLU	2.7
5	e	77	GLU	2.7
7	h	63	LYS	2.7
8	I	33	LYS	2.7
2	b	374	ASN	2.7
16	v	45	ILE	2.7
2	B	465	GLY	2.7
2	b	415	PRO	2.7
3	C	256	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	a	300	PHE	2.7
2	b	61	PHE	2.7
4	D	257	PHE	2.7
1	A	200	LEU	2.7
1	a	200	LEU	2.7
4	d	49	LEU	2.7
13	O	157	LEU	2.7
7	h	28	THR	2.7
3	C	205	ASP	2.7
2	B	467	ILE	2.7
2	B	481	GLY	2.7
3	C	429	SER	2.7
3	C	309	ALA	2.7
3	c	340	TYR	2.7
2	B	124	ARG	2.7
3	C	146	PHE	2.7
19	Z	56	VAL	2.7
1	a	218	LEU	2.7
2	b	109	LEU	2.7
2	b	407	ASN	2.7
3	c	242	LEU	2.7
20	R	9	LEU	2.7
2	B	129	GLY	2.7
3	C	141	GLU	2.7
3	c	137	PRO	2.7
3	C	263	ALA	2.7
4	D	115	ALA	2.7
6	f	38	ALA	2.7
13	o	78	LEU	2.7
19	Z	53	VAL	2.7
1	a	18	CYS	2.7
5	E	71	GLU	2.7
7	H	25	TRP	2.7
7	H	54	ILE	2.7
2	B	501	ASP	2.7
4	d	327	ALA	2.7
11	l	6	ASN	2.7
4	d	241	GLU	2.7
3	c	272	LEU	2.7
4	D	277	THR	2.7
7	H	58	VAL	2.7
9	J	24	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
16	v	10	VAL	2.7
17	X	11	PHE	2.7
19	Z	59	PHE	2.7
5	e	48	GLY	2.7
2	B	450	TRP	2.6
16	V	97	SER	2.6
13	O	33	ASP	2.6
1	A	321	ILE	2.6
14	T	21	ILE	2.6
2	b	320	ALA	2.6
13	O	127	ALA	2.6
1	a	186	PHE	2.6
3	c	131	TYR	2.6
2	B	12	LEU	2.6
2	b	62	VAL	2.6
3	C	352	GLY	2.6
3	c	192	GLY	2.6
3	c	213[A]	LEU	2.6
16	v	121	VAL	2.6
19	Z	50	LEU	2.6
19	z	12	LEU	2.6
3	C	424	SER	2.6
5	e	73	LYS	2.6
2	B	285	ASN	2.6
6	F	20	TRP	2.6
5	E	82	GLN	2.6
3	C	459	ILE	2.6
4	D	256	ILE	2.6
7	H	45	ILE	2.6
15	U	76	ARG	2.6
1	a	197	PHE	2.6
3	C	196	VAL	2.6
4	d	156	VAL	2.6
16	v	134	LYS	2.6
1	A	127	MET	2.6
9	j	1	MET	2.6
1	a	196	PRO	2.6
2	b	155	ALA	2.6
3	C	87	ILE	2.6
2	B	163	GLY	2.6
3	c	409[A]	GLY	2.6
8	I	35	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
3	c	188	THR	2.6
6	F	17	THR	2.6
13	o	23	ASP	2.6
1	a	159	LEU	2.6
3	C	208	VAL	2.6
4	D	49	LEU	2.6
4	d	185	PHE	2.6
4	d	339	PHE	2.6
5	E	58	GLN	2.6
6	f	41	GLN	2.6
16	V	64	PRO	2.6
16	v	102	PRO	2.6
1	A	324	ALA	2.6
2	b	253	ALA	2.6
2	b	304	ALA	2.6
3	C	270	ALA	2.6
10	k	42	ALA	2.6
1	a	143	ILE	2.6
4	D	325	ILE	2.6
5	E	34	GLY	2.6
1	A	144	CYS	2.6
3	C	255	THR	2.6
2	b	303	SER	2.6
3	c	19	ASN	2.6
3	c	30	SER	2.6
12	M	31	SER	2.6
2	b	324	LEU	2.6
3	c	90	PRO	2.6
4	D	209	LEU	2.6
4	d	130	PHE	2.6
4	d	171	PRO	2.6
11	L	17	LEU	2.6
13	o	20	PRO	2.6
3	C	261	ARG	2.6
7	h	12	ARG	2.6
3	c	270	ALA	2.6
4	D	170	ALA	2.6
7	h	22	ALA	2.6
18	Y	31	ALA	2.6
19	z	26	ALA	2.6
2	B	128	THR	2.6
3	c	291	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
5	e	35	TRP	2.6
3	c	288	CYS	2.6
4	d	24	ARG	2.6
2	b	218	LEU	2.6
10	K	25	LEU	2.6
13	o	93	LEU	2.6
16	V	126	LEU	2.6
19	Z	12	LEU	2.6
1	A	49	VAL	2.6
1	a	285	PHE	2.6
4	d	126	MET	2.6
3	c	286	ALA	2.6
1	a	245	THR	2.5
2	b	239[A]	SER	2.5
4	D	280	TRP	2.5
19	Z	47	TRP	2.5
1	a	121[A]	LEU	2.5
2	B	63	LEU	2.5
4	D	293	LEU	2.5
4	d	293	LEU	2.5
13	O	85	LEU	2.5
1	A	205	VAL	2.5
2	b	363	PHE	2.5
3	c	396	MET	2.5
13	O	196	GLN	2.5
2	B	387	GLU	2.5
1	a	324	ALA	2.5
3	C	278	ALA	2.5
3	C	445	ALA	2.5
18	y	35	ILE	2.5
1	A	231	GLU	2.5
2	B	120	LEU	2.5
2	b	119	ASP	2.5
3	C	86	LEU	2.5
3	c	341	LEU	2.5
4	D	20	ASP	2.5
19	Z	6	GLN	2.5
15	u	9	LEU	2.5
1	A	328	MET	2.5
3	C	157	MET	2.5
9	J	20	VAL	2.5
5	e	61	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
16	v	96	ARG	2.5
2	b	459	ALA	2.5
1	A	290	ILE	2.5
2	B	425	ILE	2.5
16	v	88	ILE	2.5
17	x	24	THR	2.5
6	f	29	PRO	2.5
16	v	70	GLU	2.5
2	B	372	ASP	2.5
2	b	103	LEU	2.5
3	C	165	LEU	2.5
1	A	158	PHE	2.5
3	c	196	VAL	2.5
4	D	156	VAL	2.5
10	K	30	VAL	2.5
13	o	88	ASN	2.5
1	A	152	ALA	2.5
3	c	302	TYR	2.5
4	D	141	TYR	2.5
13	O	153	THR	2.5
15	u	85	THR	2.5
5	e	32	ILE	2.5
8	i	10	ILE	2.5
16	v	93	PRO	2.5
9	j	25	GLY	2.5
19	Z	19	MET	2.5
2	b	362	PHE	2.5
2	B	291	SER	2.5
3	c	57	ALA	2.5
5	E	19	TYR	2.5
13	o	226	GLY	2.5
15	U	18	GLY	2.5
4	d	89	LEU	2.5
13	O	70	LEU	2.5
1	A	155	PHE	2.5
2	B	399	VAL	2.5
3	C	61	VAL	2.5
7	h	60	VAL	2.5
3	C	443	TRP	2.5
3	c	450	ALA	2.5
2	B	384	ARG	2.5
2	b	68	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	a	227	THR	2.5
7	h	17	GLU	2.5
16	v	123	PRO	2.5
3	c	430	HIS	2.5
19	Z	22	GLY	2.5
2	b	98	LEU	2.5
5	E	42	LEU	2.5
1	A	197	PHE	2.4
1	a	49	VAL	2.4
2	B	356	VAL	2.4
3	C	190	ALA	2.4
3	C	407	VAL	2.4
3	c	436	PHE	2.4
3	c	462[A]	GLU	2.4
10	k	13	GLU	2.4
2	b	410	THR	2.4
4	D	328	TRP	2.4
3	c	162	GLY	2.4
16	v	84	GLY	2.4
19	z	48	ILE	2.4
1	A	41	LEU	2.4
2	b	161	LEU	2.4
2	b	480	SER	2.4
4	D	348	ARG	2.4
4	D	289	LEU	2.4
4	d	155	SER	2.4
7	H	17	GLU	2.4
8	i	4	LEU	2.4
13	o	199	LEU	2.4
1	A	280	VAL	2.4
1	a	152	ALA	2.4
1	a	280	VAL	2.4
2	b	212	ALA	2.4
3	c	309	ALA	2.4
6	f	21	VAL	2.4
15	U	13	VAL	2.4
12	M	29	THR	2.4
16	V	46	THR	2.4
1	a	307[A]	ILE	2.4
13	o	210	GLU	2.4
15	u	104	LYS	2.4
17	x	6	SER	2.4

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Mol	Chain	Res	Type	RSRZ
19	Z	44	SER	2.4
4	d	92	LEU	2.4
19	Z	57	LEU	2.4
1	A	340	PRO	2.4
1	a	33	PHE	2.4
4	D	341	PHE	2.4
15	U	84	VAL	2.4
15	u	81	HIS	2.4
2	b	255	THR	2.4
2	B	286	ARG	2.4
8	i	34	ARG	2.4
10	k	19	ASP	2.4
1	A	147	TYR	2.4
10	k	10	LYS	2.4
1	a	38	ILE	2.4
2	B	407	ASN	2.4
3	c	173	LEU	2.4
7	H	43	LEU	2.4
9	J	35	LEU	2.4
1	a	127	MET	2.4
4	d	148	ALA	2.4
15	U	81	HIS	2.4
19	Z	28	ALA	2.4
1	a	306	VAL	2.4
2	B	61	PHE	2.4
3	C	54	VAL	2.4
3	C	410[A]	VAL	2.4
3	c	176	VAL	2.4
4	d	75	THR	2.4
13	o	193	THR	2.4
16	v	97	SER	2.4
2	b	450	TRP	2.4
3	C	250	TRP	2.4
15	U	36	ILE	2.4
16	v	68	ASN	2.4
1	A	114	LEU	2.4
10	k	35	LEU	2.4
15	u	102	LEU	2.4
1	a	233	ALA	2.4
2	B	243	ALA	2.4
2	b	375	GLY	2.4
7	H	63	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
4	d	330	ALA	2.4
16	v	74	ASP	2.4
2	b	222	PRO	2.4
17	X	30	ALA	2.4
2	B	411	PHE	2.4
3	C	109	PHE	2.4
5	e	38	VAL	2.4
13	o	197	ILE	2.4
3	C	197	ARG	2.4
2	b	89	GLY	2.4
2	b	254	GLY	2.4
3	c	58	GLY	2.4
5	E	6	GLY	2.4
3	C	125	LEU	2.4
19	z	9	LEU	2.4
1	A	287	ALA	2.4
1	a	149	ALA	2.4
3	C	434	ALA	2.4
13	o	183	ALA	2.4
2	B	255	THR	2.4
3	C	287	THR	2.4
13	O	214	THR	2.4
1	a	185[A]	VAL	2.4
2	b	151	PHE	2.4
10	k	30	VAL	2.4
13	O	66	VAL	2.4
13	o	65	PHE	2.4
3	C	339	LYS	2.3
1	a	323	ARG	2.3
17	X	39	ARG	2.3
2	B	165	GLY	2.3
8	I	26	GLY	2.3
13	O	226	GLY	2.3
3	C	425	TRP	2.3
1	A	209	ALA	2.3
2	b	471	ALA	2.3
3	C	314	ALA	2.3
3	c	42	LEU	2.3
3	c	49	LEU	2.3
3	c	161	LEU	2.3
4	D	119	ALA	2.3
1	A	238[A]	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
3	c	397	THR	2.3
1	A	249	VAL	2.3
1	a	168	PHE	2.3
3	c	435	PHE	2.3
4	D	30	VAL	2.3
4	D	120	PHE	2.3
4	D	236	ASN	2.3
11	l	10	VAL	2.3
2	b	224	ARG	2.3
19	z	17	PHE	2.3
3	C	136	GLY	2.3
1	a	60	ILE	2.3
2	B	101	ILE	2.3
3	c	237	HIS	2.3
15	U	77	GLU	2.3
16	v	90	GLU	2.3
2	b	225	LEU	2.3
7	h	20	LYS	2.3
15	u	17	LEU	2.3
16	V	24	LYS	2.3
7	H	32	ALA	2.3
3	c	139	THR	2.3
16	V	51	SER	2.3
2	b	181	VAL	2.3
4	d	196	PHE	2.3
5	e	37	PHE	2.3
7	h	58	VAL	2.3
2	b	283	GLU	2.3
2	b	351	GLY	2.3
16	v	47	LYS	2.3
2	B	482	ILE	2.3
4	d	213	ILE	2.3
2	B	447	PRO	2.3
1	a	325	ASN	2.3
2	B	224	ARG	2.3
2	B	273	TYR	2.3
3	C	450	ALA	2.3
3	c	337	LEU	2.3
4	d	44	ALA	2.3
4	d	229	ALA	2.3
5	E	33	ALA	2.3
3	C	275	SER	2.3

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Mol	Chain	Res	Type	RSRZ
19	z	44	SER	2.3
2	B	257	TRP	2.3
2	B	139	PHE	2.3
2	B	219	VAL	2.3
2	B	237	VAL	2.3
2	B	451	PHE	2.3
2	b	366	PHE	2.3
3	C	152	LYS	2.3
9	j	24	VAL	2.3
9	j	17	GLY	2.3
17	X	9	GLY	2.3
2	B	180	PRO	2.3
7	h	4	ARG	2.3
16	v	50	PRO	2.3
1	A	250	ALA	2.3
2	B	97	ALA	2.3
13	o	181	GLU	2.3
16	v	38	ALA	2.3
2	B	109	LEU	2.3
2	b	27	THR	2.3
3	C	175	LEU	2.3
4	D	91	LEU	2.3
13	O	6	THR	2.3
4	D	126	MET	2.3
3	c	102	GLY	2.3
9	J	17	GLY	2.3
12	M	32	GLN	2.3
4	d	48	TRP	2.3
2	b	455	HIS	2.3
16	V	92	HIS	2.3
19	z	53	VAL	2.3
10	k	46	ARG	2.3
13	o	54	GLU	2.3
2	B	415	PRO	2.3
2	b	187	PRO	2.3
1	A	259	ILE	2.3
3	C	199	ILE	2.3
16	V	47	LYS	2.3
16	v	100	ILE	2.3
3	c	172	ALA	2.3
3	c	278	ALA	2.3
1	A	245	THR	2.3

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Mol	Chain	Res	Type	RSRZ
4	D	122	LEU	2.3
4	D	319	LEU	2.3
5	e	80	LEU	2.3
19	Z	9	LEU	2.3
10	K	15	TYR	2.3
3	C	440	GLY	2.3
3	c	67	MET	2.3
4	D	281	MET	2.3
1	A	185[A]	VAL	2.3
4	d	328	TRP	2.3
2	B	374	ASN	2.3
4	D	16	ASP	2.3
16	v	67	ASP	2.3
1	a	318	ALA	2.3
2	b	207	ILE	2.3
2	b	240	SER	2.3
3	c	120	ILE	2.3
4	D	147	SER	2.3
4	D	148	ALA	2.3
9	J	13	ALA	2.3
2	b	133	LEU	2.2
2	b	370	LEU	2.2
4	d	291	LEU	2.2
11	L	22	LEU	2.2
13	O	207	ARG	2.2
15	u	23	GLU	2.2
1	a	293	MET	2.2
1	A	337[A]	HIS	2.2
16	V	40	CYS	2.2
1	a	315	ASN	2.2
8	i	35	LYS	2.2
3	C	383	ASP	2.2
5	e	68	ASP	2.2
3	C	292	PHE	2.2
4	d	175	VAL	2.2
3	c	256	PRO	2.2
7	h	29	PRO	2.2
2	B	381	ILE	2.2
3	C	260	ALA	2.2
4	D	216	ALA	2.2
9	j	23	ILE	2.2
3	C	47	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	148	GLY	2.2
4	d	102	THR	2.2
3	C	161	LEU	2.2
3	C	377	LEU	2.2
4	D	182	LEU	2.2
4	D	272	LEU	2.2
4	d	289	LEU	2.2
7	h	30	LEU	2.2
13	o	125	LEU	2.2
18	y	39	LEU	2.2
2	B	330	MET	2.2
3	c	212	TYR	2.2
4	D	160	TYR	2.2
2	B	397	VAL	2.2
10	K	27	VAL	2.2
2	B	426	PHE	2.2
13	o	84	GLU	2.2
13	o	128	SER	2.2
1	a	220	THR	2.2
3	C	399	ALA	2.2
3	c	459	ILE	2.2
4	D	249	ALA	2.2
1	a	193	LEU	2.2
4	d	63	LEU	2.2
4	D	329	MET	2.2
1	A	229	GLU	2.2
15	U	71	GLN	2.2
2	b	258	TYR	2.2
7	H	49	TYR	2.2
2	B	126	PRO	2.2
2	b	131	PRO	2.2
3	c	130	VAL	2.2
4	D	136	VAL	2.2
8	i	8	VAL	2.2
10	K	38	VAL	2.2
1	A	124	SER	2.2
1	a	221[A]	SER	2.2
4	d	179	PHE	2.2
13	O	215	PHE	2.2
13	o	213	GLY	2.2
2	B	468	TRP	2.2
3	c	312	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
16	v	130	TRP	2.2
2	B	369	ILE	2.2
3	C	430	HIS	2.2
13	o	180	GLU	2.2
4	D	205	LEU	2.2
4	D	271	MET	2.2
2	B	270	PRO	2.2
2	b	414	PRO	2.2
3	C	340	TYR	2.2
16	V	102	PRO	2.2
16	V	136	TYR	2.2
2	b	417	VAL	2.2
3	C	296	VAL	2.2
4	D	286	VAL	2.2
2	b	451	PHE	2.2
4	D	235	PHE	2.2
1	a	154	ALA	2.2
1	a	296	ASN	2.2
2	B	438	ASN	2.2
5	e	75	GLN	2.2
13	O	154	ALA	2.2
16	V	49	ASN	2.2
2	b	468	TRP	2.2
3	c	252	ILE	2.2
1	a	275	LEU	2.2
4	D	279	LEU	2.2
4	D	320	LEU	2.2
4	d	36	LEU	2.2
4	d	209	LEU	2.2
12	M	22	LEU	2.2
13	o	182	LEU	2.2
3	C	342	MET	2.2
2	B	351	GLY	2.2
2	b	397	VAL	2.2
3	c	352	GLY	2.2
7	H	26	GLY	2.2
1	a	206	PHE	2.2
3	c	155	ASN	2.2
10	K	22	VAL	2.2
13	o	87	VAL	2.2
4	d	173	PHE	2.2
13	O	29	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	50	ILE	2.2
1	A	125	CYS	2.2
4	D	35	ILE	2.2
13	O	172	ILE	2.2
15	u	74	ILE	2.2
15	U	67	LEU	2.2
3	C	356	MET	2.2
4	d	347	PRO	2.2
13	O	217[A]	SER	2.2
1	A	327	GLY	2.2
13	O	206	GLY	2.2
15	u	18	GLY	2.2
1	a	58	VAL	2.1
2	B	178	VAL	2.1
3	c	56	HIS	2.1
3	c	167	VAL	2.1
4	D	152	VAL	2.1
3	c	289	PHE	2.1
4	D	143	ALA	2.1
4	d	217	THR	2.1
4	d	283	ALA	2.1
7	H	28	THR	2.1
1	A	28	LEU	2.1
2	B	29	LEU	2.1
13	O	224	ASP	2.1
2	B	88	PRO	2.1
7	H	29	PRO	2.1
16	v	94	SER	2.1
1	A	164	GLY	2.1
3	c	128	GLY	2.1
2	B	127	ARG	2.1
5	E	8	ARG	2.1
5	E	18	ARG	2.1
3	c	114	VAL	2.1
3	c	231	GLU	2.1
3	c	233	VAL	2.1
4	D	227	GLU	2.1
4	d	227	GLU	2.1
1	A	149	ALA	2.1
4	d	341	PHE	2.1
5	E	72	ALA	2.1
15	U	34	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
16	v	56	THR	2.1
2	b	80	ILE	2.1
13	O	10	ILE	2.1
13	o	118	LEU	2.1
16	v	112	LEU	2.1
2	B	186	GLY	2.1
3	C	211	GLY	2.1
9	J	34	GLY	2.1
18	y	32	GLY	2.1
13	O	225	MET	2.1
2	B	263	THR	2.1
3	c	290	VAL	2.1
2	B	119	ASP	2.1
2	B	125	ASP	2.1
4	d	38	PHE	2.1
1	A	320	ILE	2.1
2	b	500	GLY	2.1
3	C	134	ILE	2.1
4	d	215	GLY	2.1
10	k	21	LEU	2.1
10	k	44	GLY	2.1
13	o	135	SER	2.1
13	o	172	ILE	2.1
2	b	214	LEU	2.1
3	c	118	HIS	2.1
16	v	92	HIS	2.1
4	d	40	CYS	2.1
16	v	40	CYS	2.1
6	F	44	GLN	2.1
2	B	111	ALA	2.1
3	c	61	VAL	2.1
3	c	113	VAL	2.1
4	D	204	VAL	2.1
6	f	27	ALA	2.1
15	U	55	TYR	2.1
19	z	56	VAL	2.1
1	a	229	GLU	2.1
2	B	144	PHE	2.1
3	c	218	PHE	2.1
8	i	19	PHE	2.1
16	v	29	GLY	2.1
17	X	31	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	a	137	LEU	2.1
10	K	35	LEU	2.1
17	x	28	LEU	2.1
1	a	214[A]	MET	2.1
2	B	455	HIS	2.1
3	C	67	MET	2.1
3	C	94	THR	2.1
10	k	36	ALA	2.1
13	O	165	ALA	2.1
16	V	4	THR	2.1
3	c	124	VAL	2.1
19	z	20	VAL	2.1
3	C	297	TYR	2.1
3	C	351	PHE	2.1
3	c	271	TYR	2.1
3	c	283	GLY	2.1
3	c	310	SER	2.1
4	D	121	GLY	2.1
4	D	163	GLY	2.1
3	C	422	PRO	2.1
1	A	60	ILE	2.1
2	b	217	ILE	2.1
3	C	209	ILE	2.1
3	C	319	ILE	2.1
4	d	37	LEU	2.1
6	F	37	ILE	2.1
9	j	21	ILE	2.1
13	O	136	ILE	2.1
2	b	352	GLU	2.1
4	d	180	ARG	2.1
2	b	159	THR	2.1
2	b	271	THR	2.1
3	c	335	THR	2.1
4	D	350	ASN	2.1
5	e	49	THR	2.1
7	h	59	ASN	2.1
1	a	156	ALA	2.1
3	c	37	ALA	2.1
16	V	17	LYS	2.1
1	A	148	SER	2.1
3	C	290	VAL	2.1
4	D	105	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
4	d	46	GLY	2.1
4	d	276	VAL	2.1
15	U	50	VAL	2.1
2	b	93	PHE	2.1
2	b	453	PHE	2.1
5	E	28	PRO	2.1
10	k	29	PRO	2.1
2	B	87	ASP	2.0
1	A	184	ILE	2.0
2	B	324	LEU	2.0
2	b	315	ILE	2.0
3	C	249	ILE	2.0
3	c	69	LEU	2.0
5	e	30	LEU	2.0
9	J	11	ILE	2.0
10	k	25	LEU	2.0
16	v	95	LEU	2.0
17	x	29	ILE	2.0
4	d	322	ASN	2.0
4	d	277	THR	2.0
15	u	44	THR	2.0
2	b	160	GLY	2.0
3	C	66	ALA	2.0
3	c	226	SER	2.0
4	D	206	GLY	2.0
4	d	237	PRO	2.0
8	i	28	PRO	2.0
3	c	239	TRP	2.0
3	c	244	CYS	2.0
4	d	167	TRP	2.0
13	O	19	CYS	2.0
13	o	19	CYS	2.0
1	a	106	LEU	2.0
2	B	103	LEU	2.0
2	B	315	ILE	2.0
2	b	474	LEU	2.0
3	c	174	LEU	2.0
3	c	185	LEU	2.0
3	c	467	LEU	2.0
16	V	107	LEU	2.0
1	a	267[A]	ASN	2.0
6	f	40	MET	2.0

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Mol	Chain	Res	Type	RSRZ
19	z	19	MET	2.0
2	b	465	GLY	2.0
4	d	187	GLY	2.0
1	a	123	ALA	2.0
3	c	177	ALA	2.0
10	k	12	PRO	2.0
18	y	42	ARG	2.0
2	b	237	VAL	2.0
3	C	444	HIS	2.0
3	c	225	VAL	2.0
10	k	43	VAL	2.0
16	V	134	LYS	2.0
1	a	265[A]	PHE	2.0
2	B	78	TRP	2.0
2	B	118	TRP	2.0
2	b	144	PHE	2.0
4	d	253	TRP	2.0
2	B	149	LEU	2.0
7	h	39	LEU	2.0
12	M	23	ILE	2.0
18	Y	46	LEU	2.0
1	a	183	MET	2.0
1	a	289	GLY	2.0
3	c	371	GLY	2.0
2	B	239[A]	SER	2.0
2	b	371	THR	2.0
2	b	416	THR	2.0
5	E	62[A]	SER	2.0
7	h	27	THR	2.0
4	D	283	ALA	2.0
13	o	26	ALA	2.0
15	U	20	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	FME	I	1	10/11	0.81	0.25	46,65,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	FME	i	1	10/11	0.81	0.28	59,64,77,78	0
12	FME	M	1	10/11	0.84	0.26	34,56,91,100	0
14	FME	T	1	10/11	0.88	0.19	44,50,74,88	0
12	FME	m	1	10/11	0.89	0.20	47,60,91,103	0
14	FME	t	1	10/11	0.89	0.17	43,51,75,84	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
35	HTG	c	523	19/19	-0.05	0.60	118,144,148,169	0
34	LMT	b	622	25/35	0.02	0.59	88,117,159,160	0
37	CA	V	201	1/1	0.13	0.20	141,141,141,141	0
35	HTG	c	526	19/19	0.13	0.58	114,161,170,200	0
35	HTG	b	625	19/19	0.16	0.45	91,138,154,196	0
32	UNL	i	101	40/-	0.20	0.44	77,109,164,165	0
34	LMT	B	622	35/35	0.21	0.46	78,125,142,144	0
32	UNL	b	629	33/-	0.22	0.40	72,108,162,162	0
34	LMT	m	102	35/35	0.22	0.45	63,95,117,121	0
33	LMG	c	522	51/55	0.23	0.53	80,127,154,158	0
34	LMT	I	101	35/35	0.23	0.47	110,145,160,162	0
27	SQD	f	101	43/54	0.24	0.51	118,136,170,175	0
32	UNL	A	417	28/-	0.24	0.44	98,110,128,144	0
35	HTG	D	410	16/19	0.24	0.50	82,121,136,138	0
38	LHG	a	419	42/49	0.24	0.51	78,141,167,179	0
34	LMT	A	359	35/35	0.26	0.55	73,134,144,148	0
33	LMG	C	521	51/55	0.27	0.46	68,121,155,157	0
34	LMT	e	101	35/35	0.27	0.67	121,166,181,186	0
35	HTG	h	101	16/19	0.28	0.50	98,133,140,163	0
34	LMT	a	359	35/35	0.28	0.50	65,144,151,154	0
32	UNL	B	629	33/-	0.29	0.46	57,103,166,173	0
32	UNL	K	101	34/-	0.30	0.61	83,119,134,150	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	LMT	M	101	35/35	0.31	0.41	61,99,123,126	0
35	HTG	B	625	19/19	0.31	0.34	82,167,178,238	0
33	LMG	Z	101	37/55	0.33	0.44	77,129,150,151	0
38	LHG	E	101	42/49	0.34	0.45	72,118,132,132	0
32	UNL	a	415	30/-	0.34	0.41	98,115,136,146	0
34	LMT	a	418	35/35	0.35	0.49	113,136,151,151	0
33	LMG	z	101	39/55	0.38	0.42	84,133,148,153	0
27	SQD	b	620	54/54	0.40	0.44	68,93,144,152	0
34	LMT	M	103	35/35	0.42	0.38	68,146,169,171	0
33	LMG	a	417	51/55	0.42	0.52	76,100,122,129	0
34	LMT	B	630	25/35	0.43	0.47	54,89,147,148	0
35	HTG	C	522	19/19	0.45	0.36	112,123,133,150	0
35	HTG	C	523	19/19	0.45	0.56	84,153,166,186	0
32	UNL	I	102	40/-	0.46	0.39	66,113,156,158	0
27	SQD	B	620	54/54	0.46	0.43	65,93,132,134	0
32	UNL	d	410	36/-	0.46	0.58	73,100,136,140	0
33	LMG	A	418	51/55	0.47	0.50	61,97,118,121	0
35	HTG	b	624	19/19	0.48	0.44	114,128,145,170	0
36	DGD	h	103	62/66	0.49	0.50	52,66,78,86	0
35	HTG	b	628	19/19	0.49	0.33	61,82,106,112	0
27	SQD	a	411	54/54	0.49	0.43	72,95,139,149	0
34	LMT	b	630	25/35	0.50	0.42	57,81,151,153	0
32	UNL	c	527	32/-	0.50	0.37	93,125,140,143	0
35	HTG	b	623	19/19	0.50	0.40	68,88,130,131	0
27	SQD	A	413	54/54	0.54	0.42	63,91,128,137	0
34	LMT	E	102	35/35	0.57	0.44	119,145,171,173	0
32	UNL	j	102	10/-	0.58	0.58	87,106,117,118	0
35	HTG	B	624	19/19	0.58	0.36	71,103,114,115	0
32	UNL	D	409	40/-	0.59	0.43	67,93,136,140	0
33	LMG	B	621	51/55	0.60	0.41	53,72,94,108	0
24	CLA	C	514	65/65	0.61	0.31	60,81,122,127	0
33	LMG	b	621	51/55	0.62	0.36	53,74,105,124	0
33	LMG	c	521	51/55	0.63	0.39	68,101,145,156	0
35	HTG	B	623	19/19	0.63	0.34	70,88,128,128	0
24	CLA	B	609	65/65	0.63	0.30	47,57,73,80	0
24	CLA	b	602	65/65	0.63	0.37	51,62,79,88	0
28	GOL	a	416	6/6	0.64	0.36	55,82,84,86	0
36	DGD	H	102	62/66	0.65	0.48	46,63,76,78	0
24	CLA	c	515	65/65	0.65	0.33	70,91,134,138	0
27	SQD	A	411	54/54	0.65	0.41	55,86,123,126	0
31	PL9	a	414[A]	55/55	0.66	0.43	97,107,120,124	55

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
31	PL9	a	414[B]	55/55	0.66	0.43	97,107,120,124	55
33	LMG	C	520	51/55	0.66	0.41	56,90,127,140	0
27	SQD	F	101	43/54	0.67	0.32	81,114,134,137	0
35	HTG	B	628	19/19	0.67	0.26	65,80,89,95	0
32	UNL	x	101	18/-	0.67	0.27	70,85,105,106	0
34	LMT	t	101	26/35	0.67	0.28	71,110,152,153	0
36	DGD	C	518	62/66	0.68	0.36	48,67,127,131	0
32	UNL	m	101	10/-	0.69	0.55	69,78,80,84	0
24	CLA	b	609	65/65	0.69	0.31	50,61,83,99	0
24	CLA	C	505	65/65	0.69	0.40	42,56,103,113	0
28	GOL	v	202	6/6	0.70	0.75	75,86,94,96	0
38	LHG	l	101	49/49	0.70	0.32	50,60,74,91	0
24	CLA	c	505	65/65	0.70	0.40	58,67,77,83	0
24	CLA	C	504	65/65	0.70	0.40	47,58,76,85	0
24	CLA	B	602	65/65	0.71	0.34	45,55,80,84	0
26	BCR	h	102	40/40	0.71	0.24	56,70,80,81	0
37	CA	O	301	1/1	0.71	0.32	119,119,119,119	0
24	CLA	c	512	65/65	0.71	0.39	50,65,81,92	0
31	PL9	A	416[B]	55/55	0.72	0.39	66,93,108,113	55
24	CLA	C	512	65/65	0.72	0.23	52,63,79,86	0
36	DGD	c	518	62/66	0.72	0.37	49,67,95,103	0
31	PL9	A	416[A]	55/55	0.72	0.39	66,93,107,111	55
28	GOL	a	410	6/6	0.73	0.31	79,81,90,95	0
24	CLA	c	507	65/65	0.73	0.29	49,61,91,95	0
28	GOL	b	627	6/6	0.73	0.29	97,106,113,116	0
24	CLA	b	601	65/65	0.73	0.30	58,85,115,130	0
36	DGD	C	517	62/66	0.73	0.40	43,63,104,106	0
24	CLA	b	603	65/65	0.74	0.38	46,56,85,92	0
24	CLA	c	513	65/65	0.74	0.24	57,71,91,97	0
36	DGD	c	519	62/66	0.74	0.34	56,73,136,145	0
32	UNL	X	101	18/-	0.74	0.26	57,76,100,100	0
27	SQD	a	409	54/54	0.75	0.30	63,85,127,131	0
24	CLA	c	508	65/65	0.75	0.26	60,72,120,133	0
24	CLA	C	513	65/65	0.75	0.25	60,73,118,123	0
38	LHG	D	357	49/49	0.76	0.49	49,64,86,102	0
24	CLA	a	350	65/65	0.76	0.27	36,46,63,77	0
24	CLA	B	605	65/65	0.76	0.32	39,48,65,68	0
24	CLA	C	506	65/65	0.76	0.36	49,57,92,100	0
33	LMG	J	101	51/55	0.76	0.30	48,73,119,126	0
24	CLA	b	615	65/65	0.76	0.22	46,59,81,86	0
24	CLA	B	611	65/65	0.76	0.33	37,47,63,73	0
24	CLA	C	507	65/65	0.76	0.27	53,69,137,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CLA	b	614	65/65	0.76	0.25	41,49,116,120	0
24	CLA	c	510	65/65	0.76	0.29	53,63,141,145	0
33	LMG	j	101	51/55	0.77	0.27	60,70,121,138	0
24	CLA	B	606	65/65	0.77	0.25	41,52,104,114	0
24	CLA	B	608	65/65	0.77	0.35	41,54,68,71	0
24	CLA	b	608	65/65	0.77	0.40	46,58,81,84	0
24	CLA	b	606	65/65	0.77	0.24	45,58,114,129	0
39	HEM	E	103	43/43	0.77	0.26	60,70,80,93	0
24	CLA	C	509	65/65	0.77	0.34	44,57,115,131	0
24	CLA	B	612	65/65	0.78	0.32	35,47,57,74	0
36	DGD	C	519	62/66	0.78	0.28	43,60,94,116	0
24	CLA	b	610	65/65	0.78	0.33	47,58,73,75	0
24	CLA	c	514	65/65	0.78	0.26	59,80,123,128	0
24	CLA	A	405	65/65	0.78	0.26	34,45,54,63	0
24	CLA	b	612	65/65	0.78	0.34	43,54,64,75	0
24	CLA	A	404	65/65	0.78	0.27	36,43,66,80	0
28	GOL	V	202	6/6	0.78	0.74	64,74,85,92	0
24	CLA	C	502	65/65	0.79	0.32	48,59,73,83	0
32	UNL	d	409	17/-	0.79	0.65	68,83,111,114	0
24	CLA	B	601	65/65	0.79	0.30	53,77,112,132	0
24	CLA	B	614	65/65	0.79	0.26	38,49,103,113	0
38	LHG	d	407	49/49	0.79	0.36	48,59,73,85	0
26	BCR	H	101	40/40	0.79	0.20	50,65,77,82	0
38	LHG	d	406	49/49	0.79	0.37	50,66,90,106	0
38	LHG	L	101	49/49	0.79	0.36	45,55,67,96	0
38	LHG	D	407	49/49	0.79	0.42	53,61,120,125	0
24	CLA	c	504	65/65	0.80	0.36	45,65,86,89	0
24	CLA	b	605	65/65	0.80	0.33	43,52,70,74	0
38	LHG	d	408	49/49	0.80	0.34	53,68,121,125	0
24	CLA	C	511	65/65	0.80	0.42	49,61,74,88	0
24	CLA	c	509	65/65	0.81	0.25	56,70,86,92	0
24	CLA	B	615	65/65	0.81	0.20	37,52,74,83	0
24	CLA	A	406	65/65	0.81	0.24	36,47,110,116	0
24	CLA	C	508	65/65	0.81	0.29	49,60,80,82	0
24	CLA	c	511	65/65	0.81	0.31	51,69,82,89	0
24	CLA	D	402	65/65	0.81	0.24	31,45,68,82	0
37	CA	b	626	1/1	0.81	0.51	151,151,151,151	0
24	CLA	B	607	65/65	0.81	0.30	32,45,71,78	0
24	CLA	a	403	65/65	0.81	0.29	36,48,69,86	0
24	CLA	a	404	65/65	0.81	0.26	42,53,126,133	0
24	CLA	c	506	65/65	0.81	0.34	51,66,116,125	0
32	UNL	J	102	10/-	0.81	0.50	77,81,99,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CLA	B	613	65/65	0.81	0.36	37,47,94,103	0
24	CLA	B	604	65/65	0.82	0.37	34,46,123,127	0
35	HTG	V	204	11/19	0.82	0.49	104,117,122,125	0
37	CA	c	525	1/1	0.82	0.16	92,92,92,92	0
39	HEM	e	102	43/43	0.82	0.42	67,93,128,137	0
24	CLA	b	611	65/65	0.82	0.28	41,52,73,82	0
24	CLA	b	616	65/65	0.82	0.21	50,60,124,127	0
26	BCR	y	101	40/40	0.82	0.16	58,74,88,88	0
24	CLA	d	403	65/65	0.82	0.20	46,64,132,137	0
24	CLA	b	607	65/65	0.82	0.30	35,49,77,87	0
25	PHO	a	406	64/64	0.82	0.29	41,55,63,65	0
32	UNL	M	102	10/-	0.83	0.47	62,72,86,92	0
26	BCR	c	516	40/40	0.83	0.21	77,86,93,96	0
32	UNL	D	408	17/-	0.83	0.56	66,85,107,110	0
38	LHG	D	406	49/49	0.83	0.40	47,57,76,93	0
24	CLA	d	402	65/65	0.83	0.28	39,48,74,86	0
24	CLA	B	603	65/65	0.83	0.34	42,52,69,76	0
36	DGD	c	520	62/66	0.84	0.28	55,64,100,116	0
26	BCR	B	618	40/40	0.84	0.34	44,57,70,77	0
28	GOL	C	525	6/6	0.84	0.39	66,73,76,78	0
26	BCR	T	101	40/40	0.84	0.33	46,57,68,72	0
24	CLA	B	610	65/65	0.84	0.30	43,53,64,80	0
26	BCR	k	101	40/40	0.84	0.26	58,73,84,90	0
37	CA	v	201	1/1	0.84	0.18	123,123,123,123	0
24	CLA	c	503	65/65	0.84	0.31	56,66,79,86	0
41	HEC	V	203	43/43	0.84	0.19	39,52,58,60	0
37	CA	o	301	1/1	0.85	0.23	108,108,108,108	0
26	BCR	d	404	40/40	0.85	0.20	53,67,96,98	0
26	BCR	b	618	40/40	0.85	0.36	44,60,73,75	0
24	CLA	D	403	65/65	0.85	0.21	44,58,139,144	0
24	CLA	C	503	65/65	0.85	0.37	47,55,78,95	0
24	CLA	b	613	65/65	0.85	0.33	42,49,101,106	0
24	CLA	b	604	65/65	0.85	0.35	37,50,122,128	0
40	MG	J	103	1/1	0.86	0.20	61,61,61,61	0
24	CLA	B	616	65/65	0.86	0.19	45,58,147,153	0
26	BCR	K	102	40/40	0.86	0.22	56,67,74,81	0
26	BCR	C	515	40/40	0.86	0.16	63,75,82,85	0
25	PHO	A	407	64/64	0.86	0.30	35,45,54,58	0
25	PHO	A	408	64/64	0.87	0.27	37,49,57,60	0
41	HEC	v	203	43/43	0.87	0.17	51,64,72,78	0
24	CLA	A	409	65/65	0.87	0.21	42,53,136,144	0
26	BCR	D	404	40/40	0.87	0.22	46,61,94,95	0

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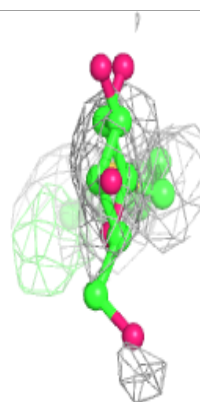
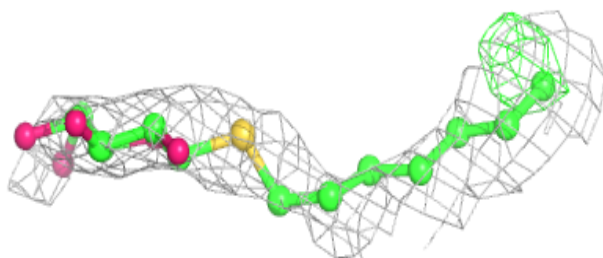
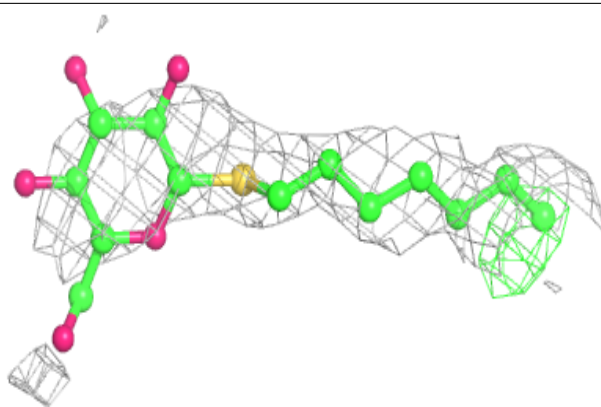
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
26	BCR	a	408	40/40	0.87	0.22	42,52,65,68	0
26	BCR	b	619	40/40	0.88	0.20	51,62,81,84	0
26	BCR	b	617	40/40	0.88	0.25	45,52,63,63	0
26	BCR	t	102	40/40	0.88	0.31	45,60,76,80	0
24	CLA	C	510	65/65	0.88	0.33	49,60,81,91	0
26	BCR	B	619	40/40	0.88	0.17	45,57,80,87	0
28	GOL	B	627	6/6	0.88	0.34	58,77,85,87	0
26	BCR	C	516	40/40	0.88	0.30	53,62,72,81	0
26	BCR	c	517	40/40	0.89	0.20	56,67,80,81	0
28	GOL	A	412	6/6	0.89	0.17	80,82,86,98	0
23	BCT	A	403[B]	4/4	0.89	0.23	55,61,62,78	4
31	PL9	d	405	55/55	0.89	0.29	41,50,66,85	0
23	BCT	A	403[A]	4/4	0.89	0.23	58,60,60,69	4
26	BCR	Y	101	40/40	0.89	0.18	57,68,74,81	0
25	PHO	a	405	64/64	0.90	0.30	41,49,56,64	0
26	BCR	B	617	40/40	0.90	0.29	44,52,59,65	0
24	CLA	a	407	65/65	0.90	0.19	44,57,134,140	0
28	GOL	c	502	6/6	0.91	0.55	68,70,71,75	0
26	BCR	A	410	40/40	0.91	0.22	42,51,61,62	0
23	BCT	a	420[A]	4/4	0.92	0.21	58,63,63,68	4
23	BCT	a	420[B]	4/4	0.92	0.21	54,63,64,72	4
31	PL9	D	405	55/55	0.92	0.34	37,49,62,78	0
29	OEX	a	412[A]	10/10	0.92	0.24	50,55,61,74	10
30	OEY	A	415[B]	11/11	0.92	0.23	43,49,55,56	11
40	MG	j	103	1/1	0.92	0.18	64,64,64,64	0
30	OEY	a	413[B]	11/11	0.93	0.24	50,54,58,74	11
29	OEX	A	414[A]	10/10	0.93	0.23	44,48,55,59	10
37	CA	c	524	1/1	0.94	0.20	78,78,78,78	0
28	GOL	B	626	6/6	0.95	0.34	85,88,90,95	0
22	CL	a	347	1/1	0.97	0.28	53,53,53,53	0
22	CL	A	347	1/1	0.98	0.37	49,49,49,49	0
22	CL	a	402	1/1	0.98	0.40	51,51,51,51	0
22	CL	A	402	1/1	0.98	0.32	44,44,44,44	0
37	CA	C	524	1/1	0.99	0.19	72,72,72,72	0
21	FE2	A	401[B]	1/1	0.99	0.05	60,60,60,60	1
21	FE2	a	401[B]	1/1	0.99	0.07	60,60,60,60	1
21	FE2	a	401[A]	1/1	0.99	0.07	60,60,60,60	1
21	FE2	A	401[A]	1/1	0.99	0.05	62,62,62,62	1

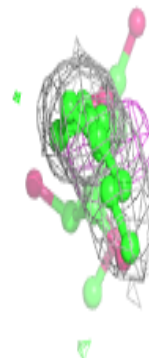
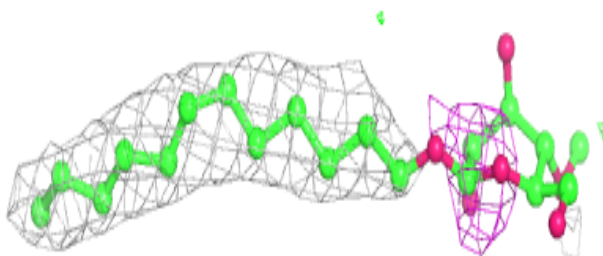
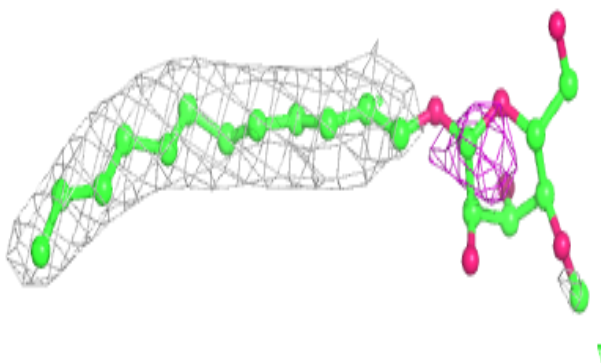
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HTG c 523:

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

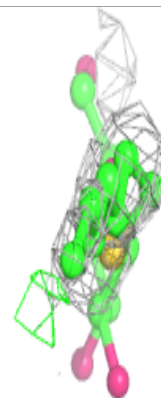
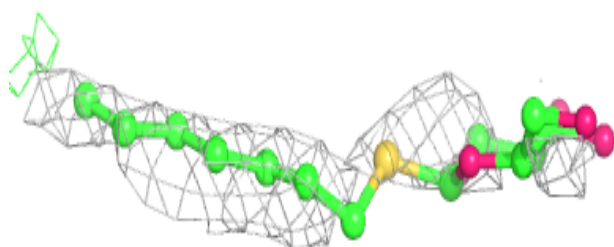
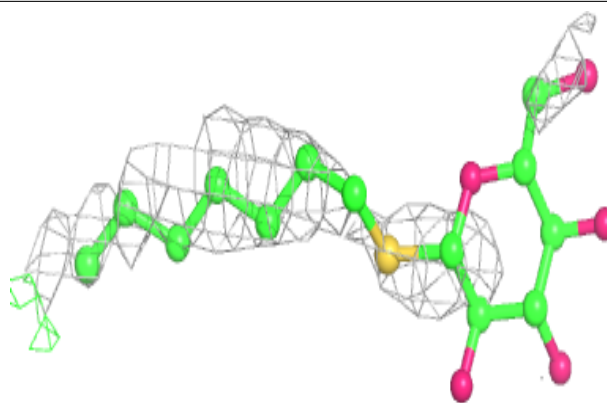
**Electron density around LMT b 622:**

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

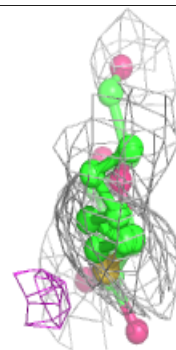
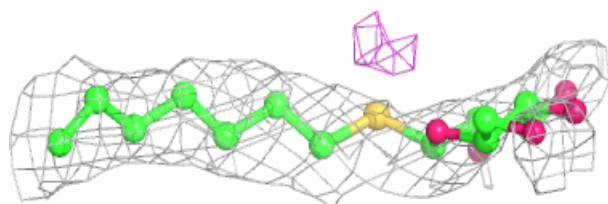
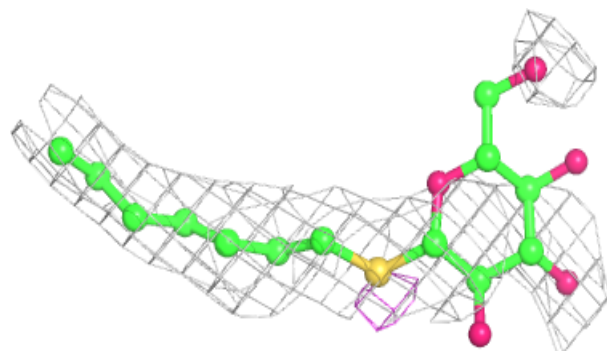


Electron density around HTG c 526:

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

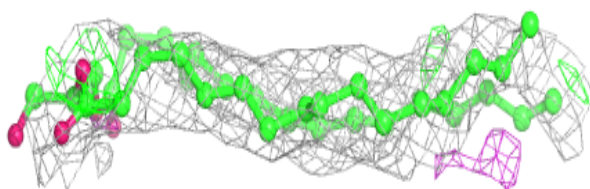
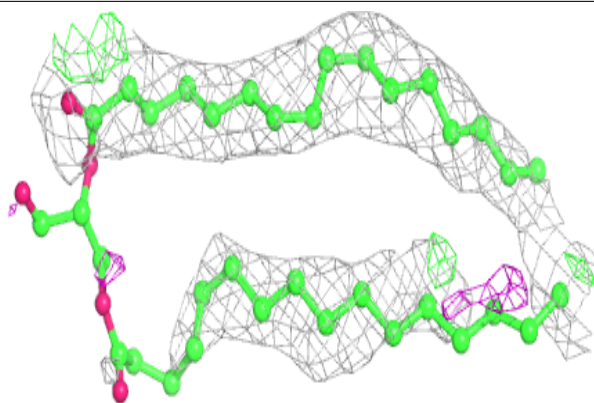
**Electron density around HTG b 625:**

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

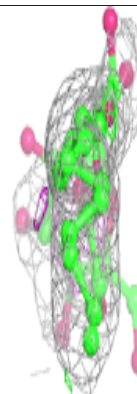
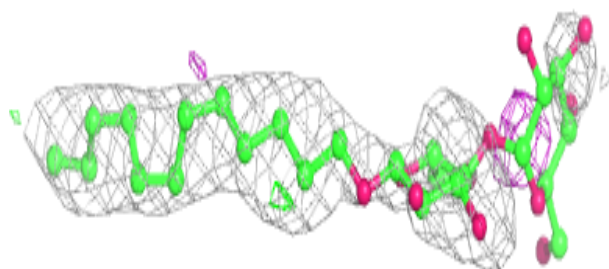
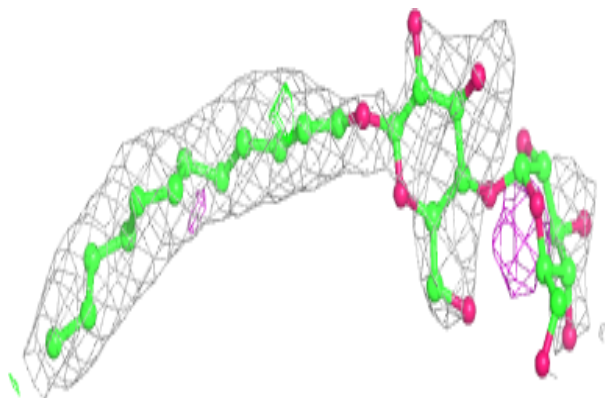


Electron density around UNL i 101:

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

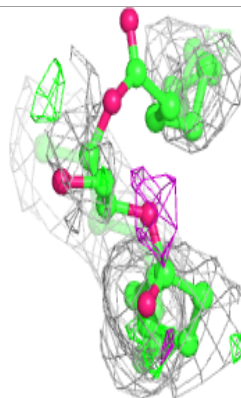
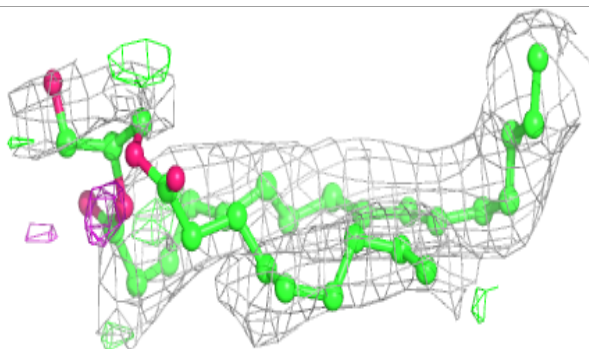
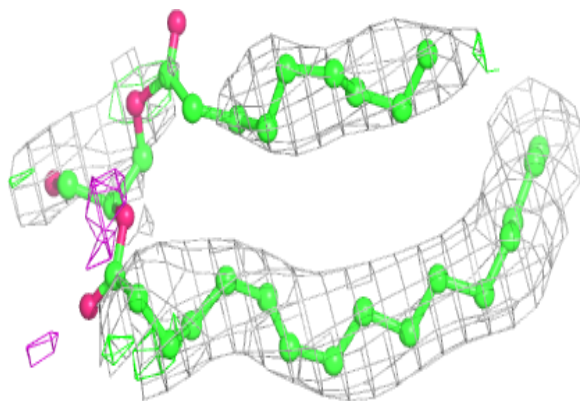
**Electron density around LMT B 622:**

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

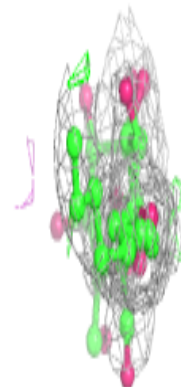
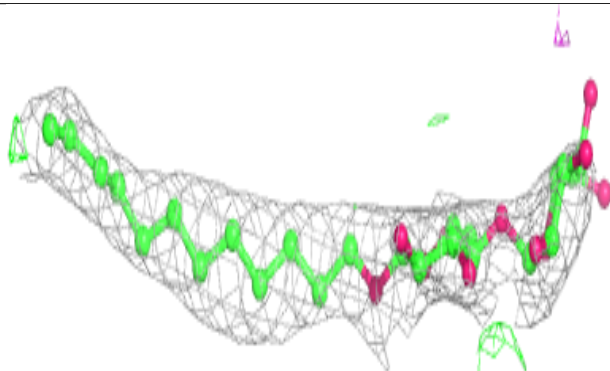
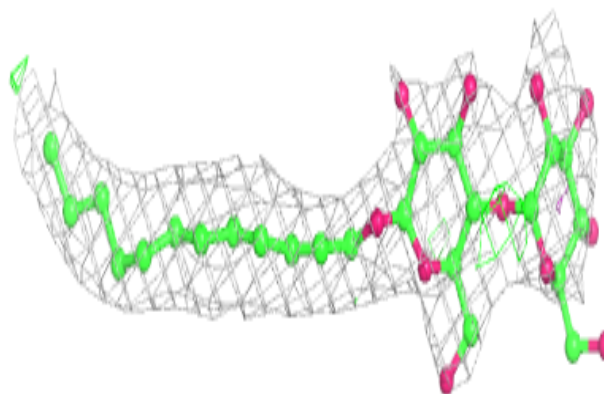


Electron density around UNL b 629:

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

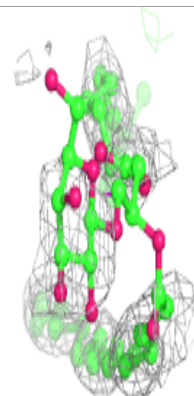
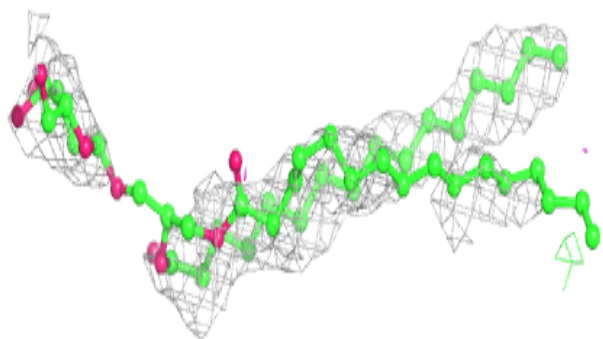
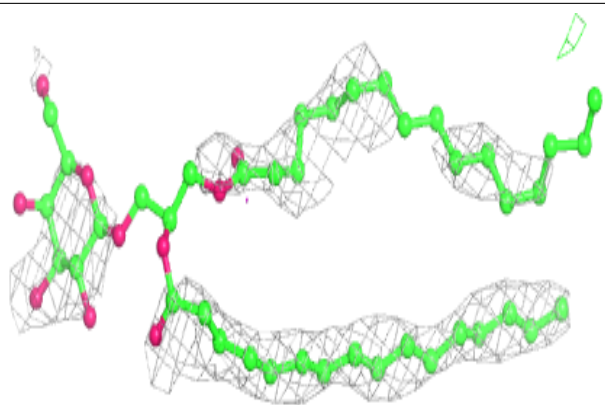
**Electron density around LMT m 102:**

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

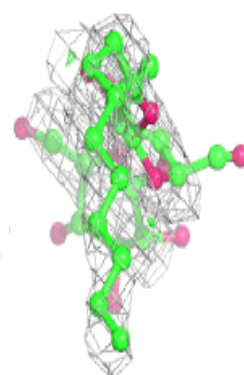
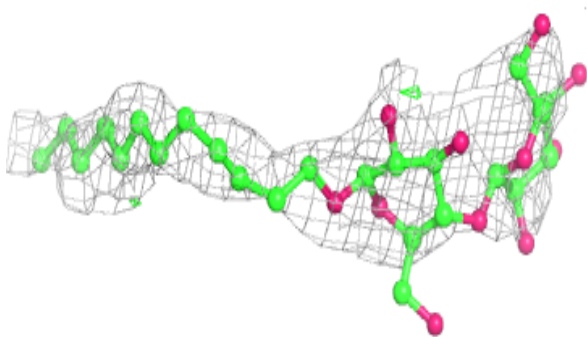
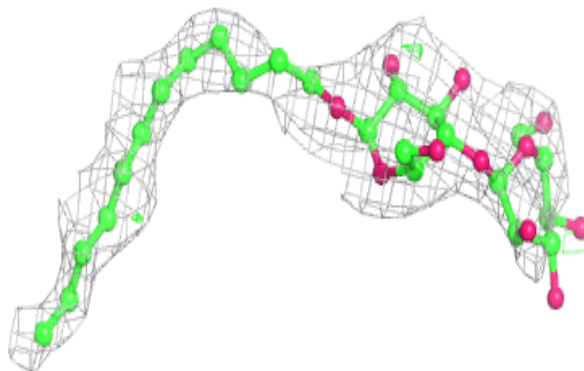


Electron density around LMG c 522:

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

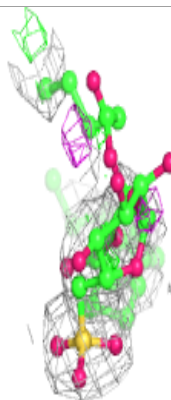
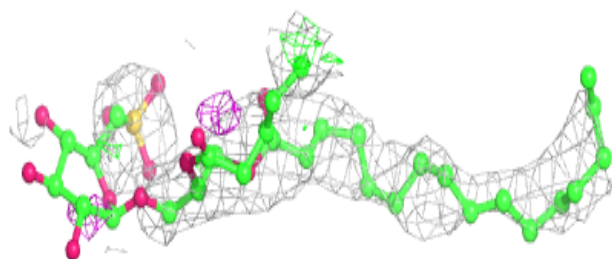
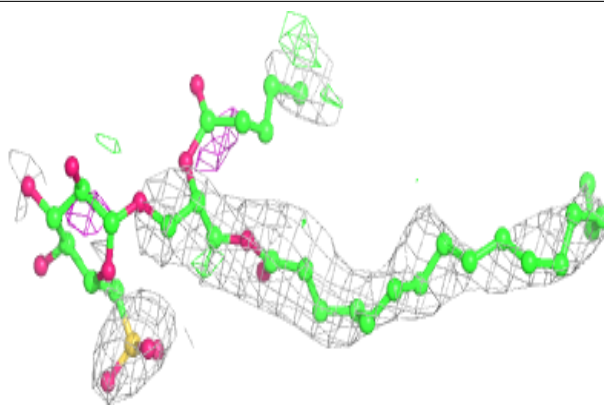
**Electron density around LMT I 101:**

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

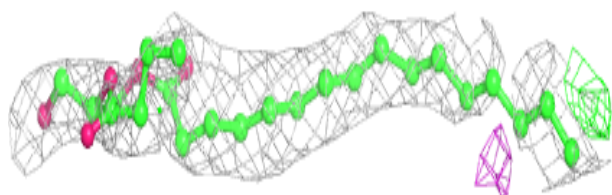
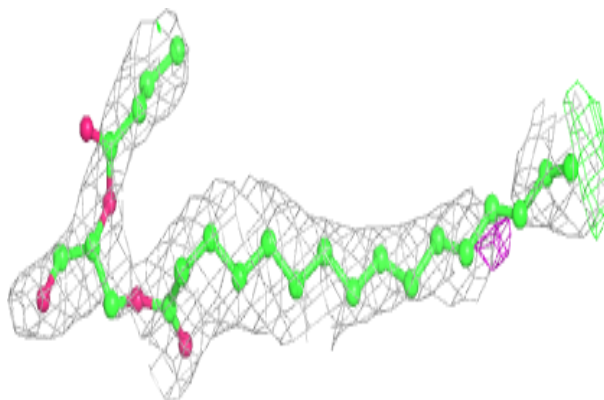


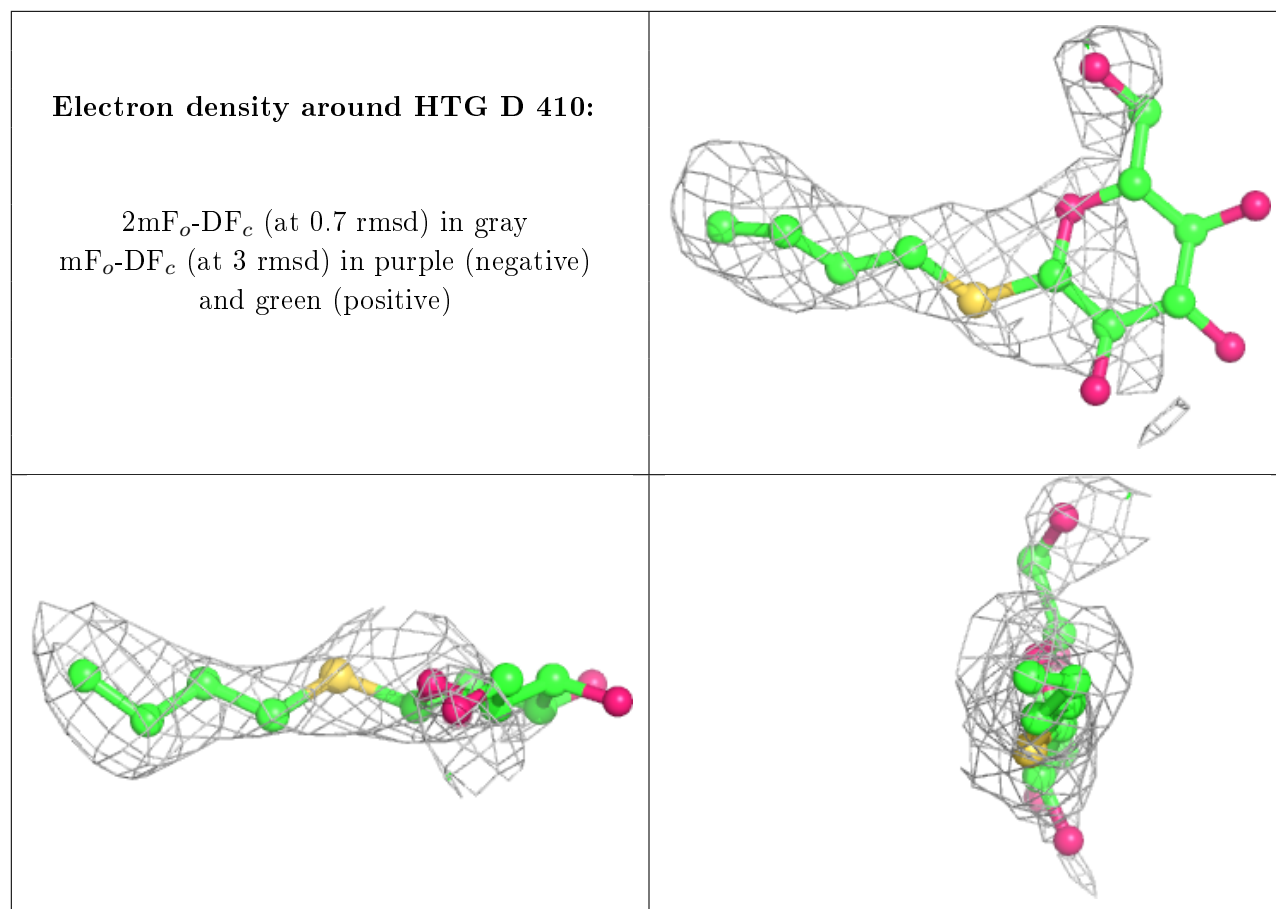
Electron density around SQD f 101:

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

**Electron density around UNL A 417:**

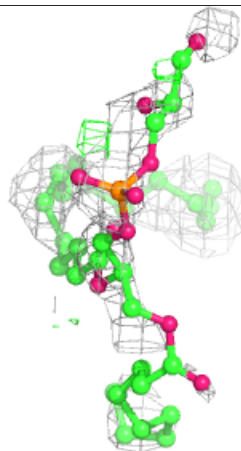
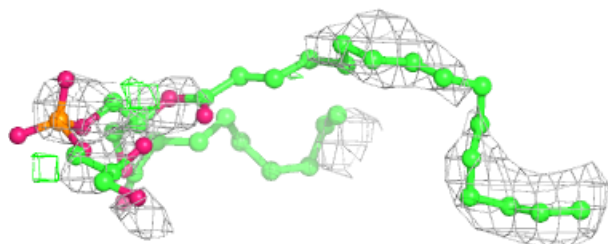
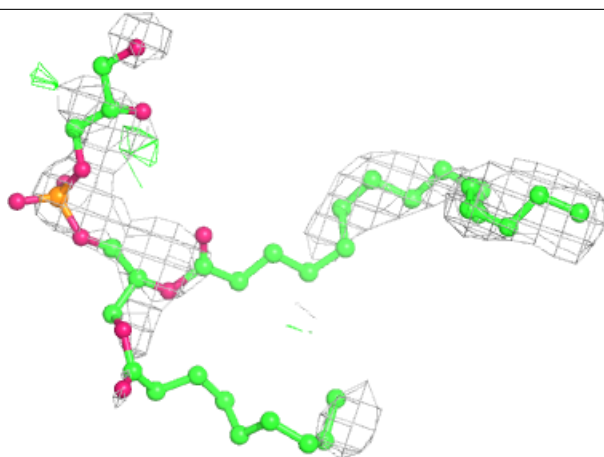
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



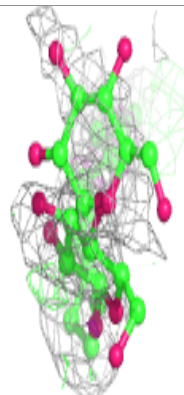
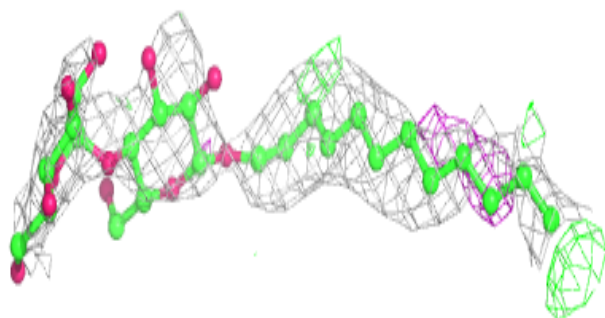
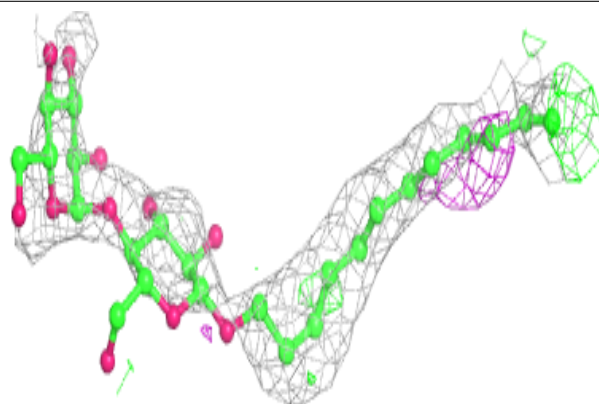


Electron density around LHG a 419:

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

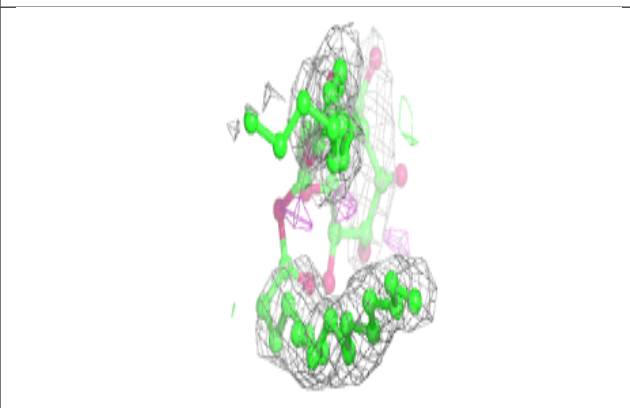
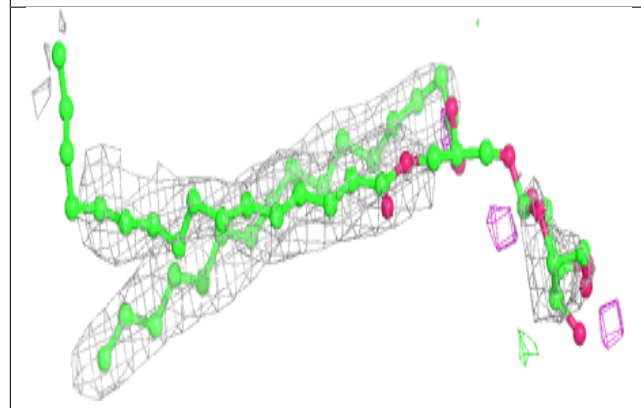
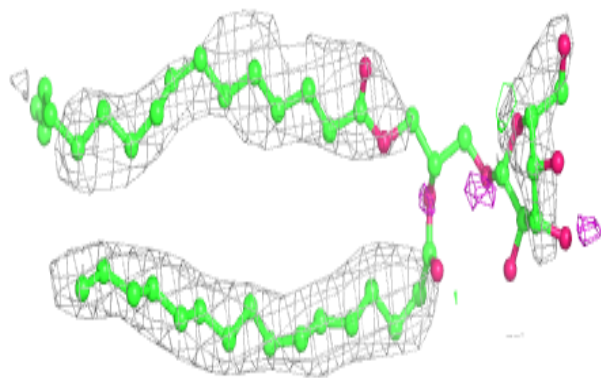
**Electron density around LMT A 359:**

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

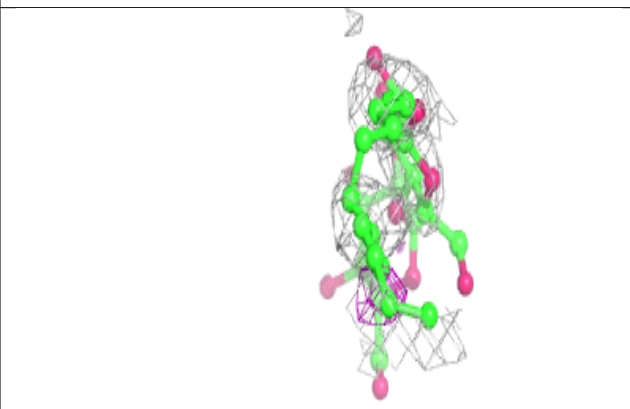
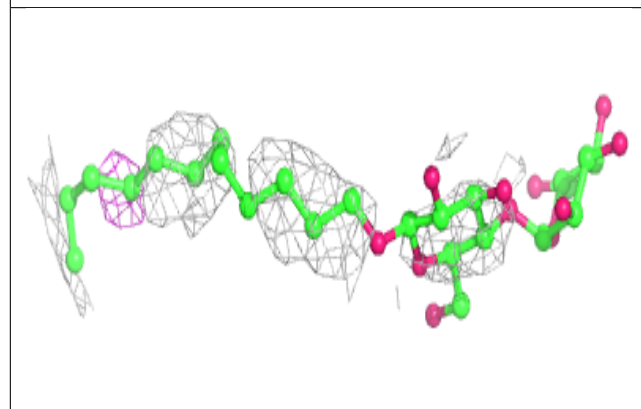
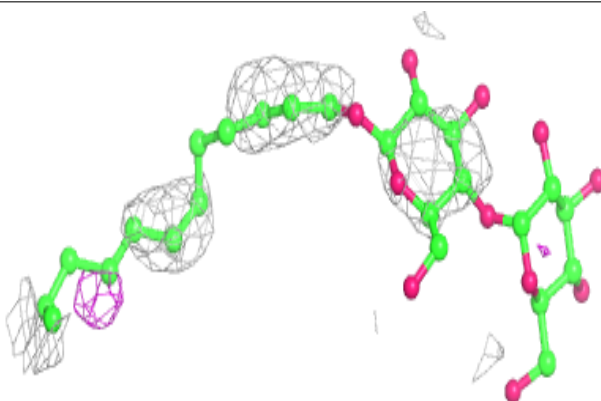


Electron density around LMG C 521:

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

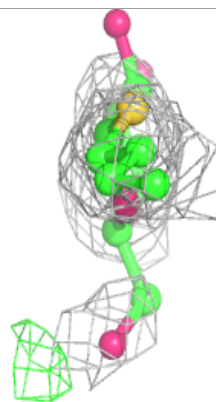
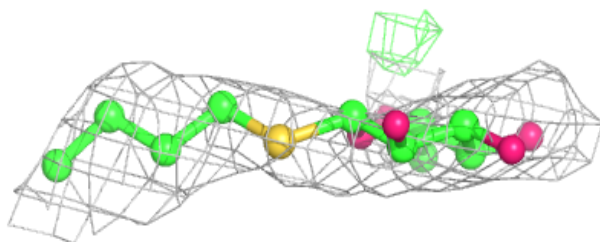
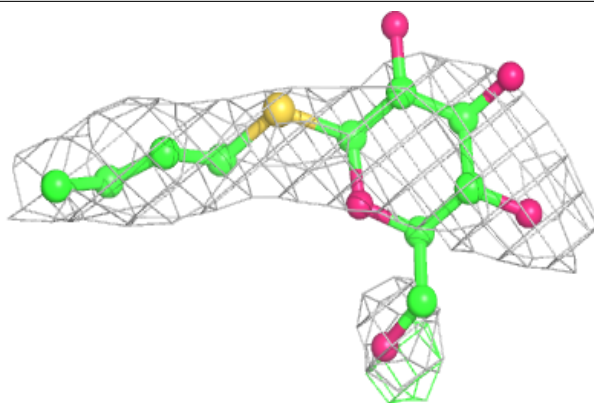
**Electron density around LMT e 101:**

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

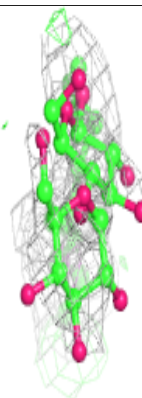
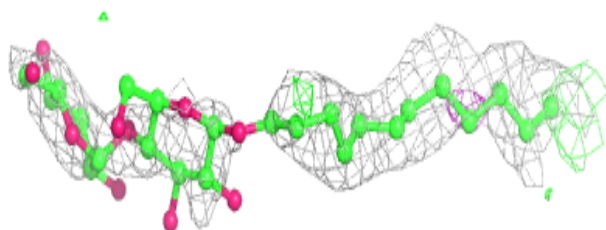
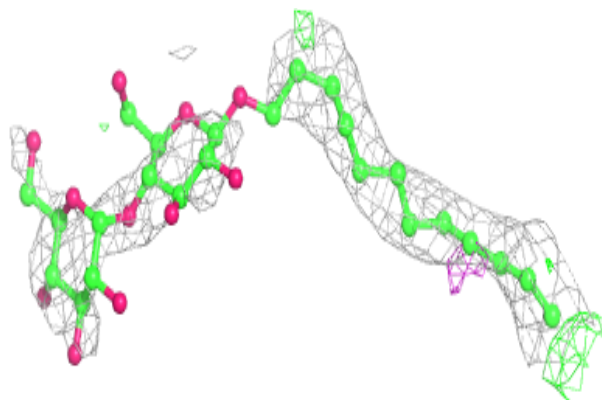


Electron density around HTG h 101:

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

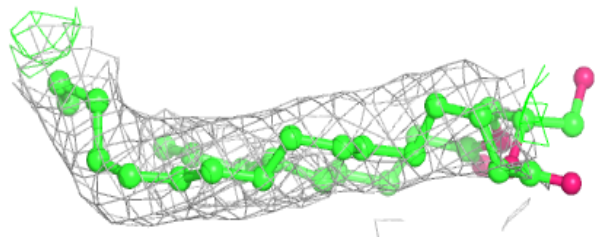
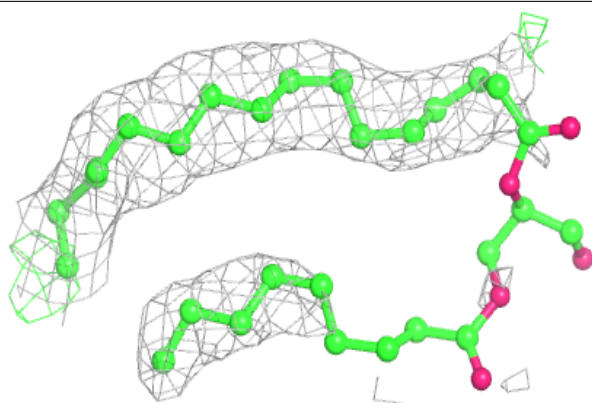
**Electron density around LMT a 359:**

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

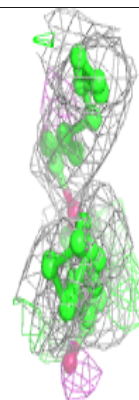
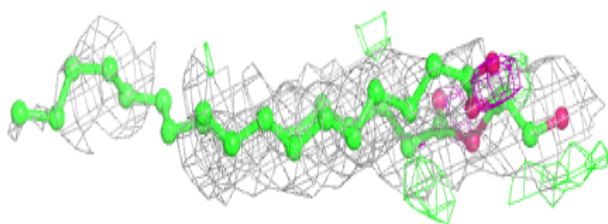
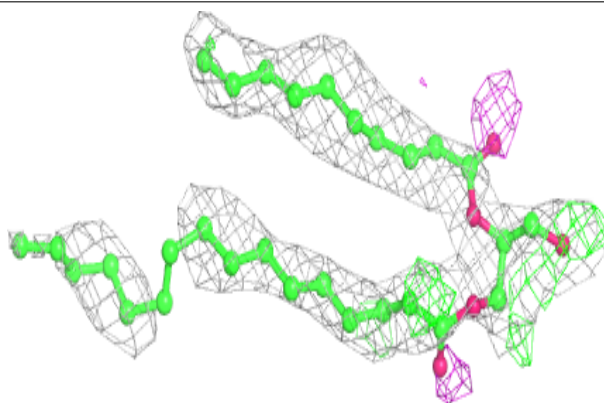


Electron density around UNL B 629:

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

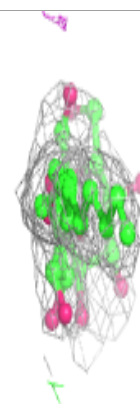
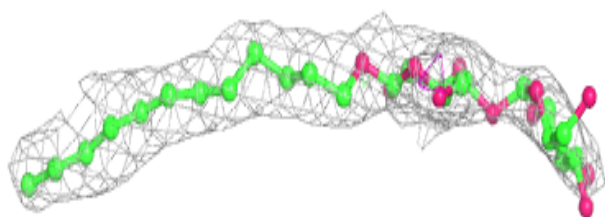
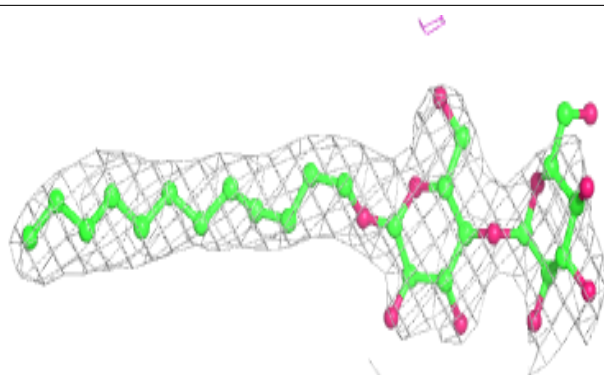
**Electron density around UNL K 101:**

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

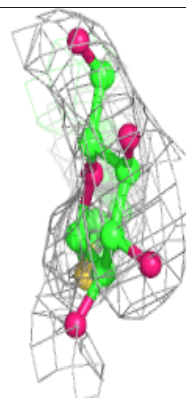
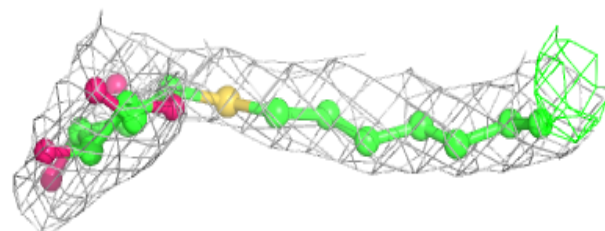
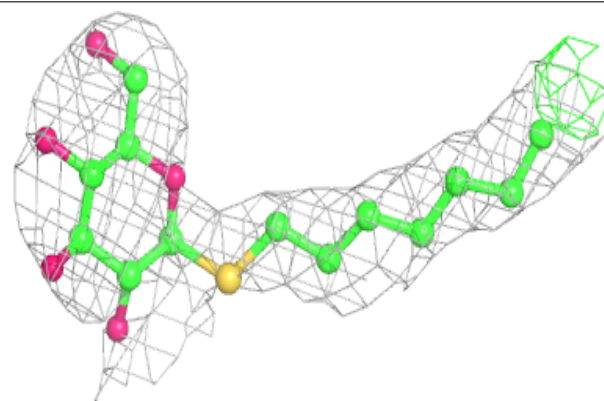


Electron density around LMT M 101:

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

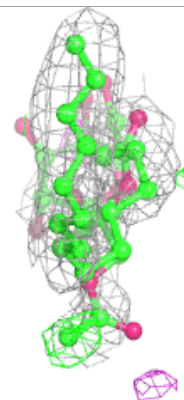
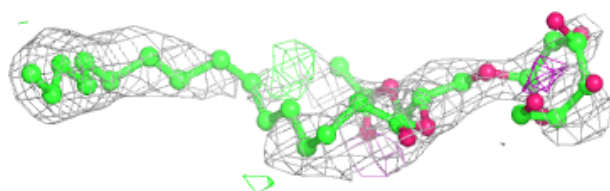
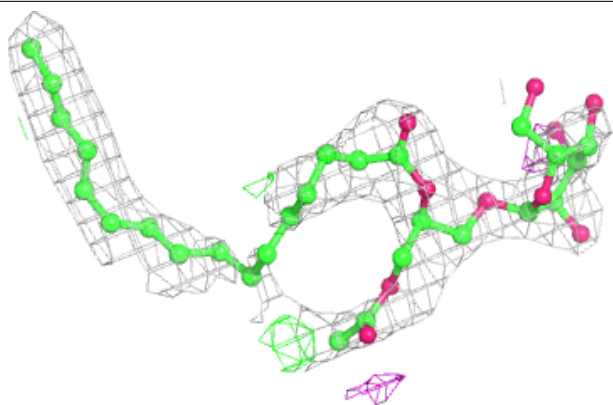
**Electron density around HTG B 625:**

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

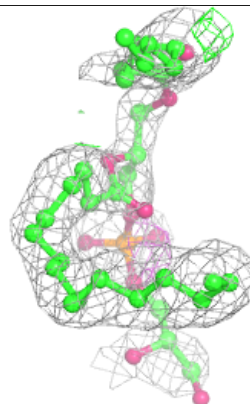
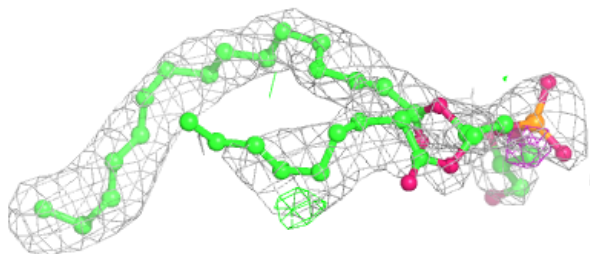
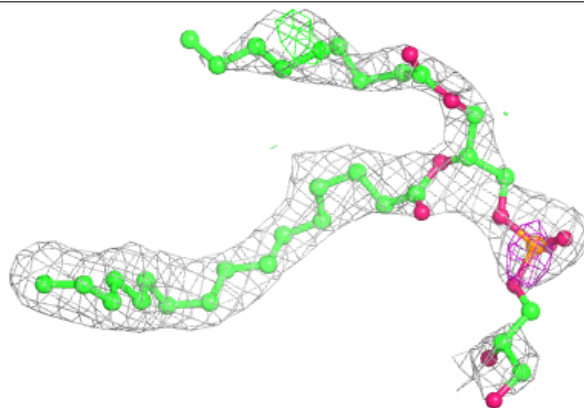


Electron density around LMG Z 101:

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

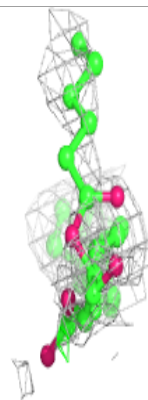
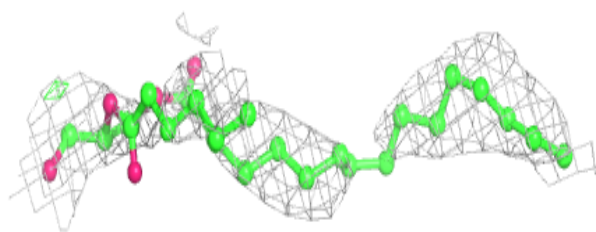
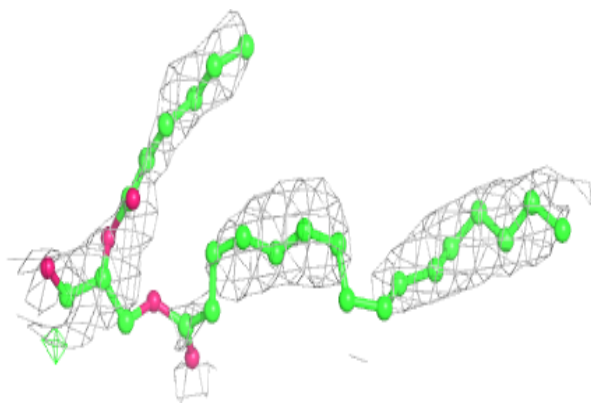
**Electron density around LHG E 101:**

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

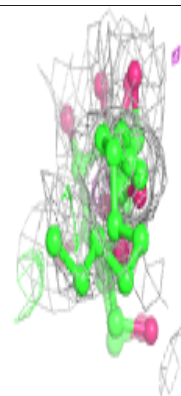
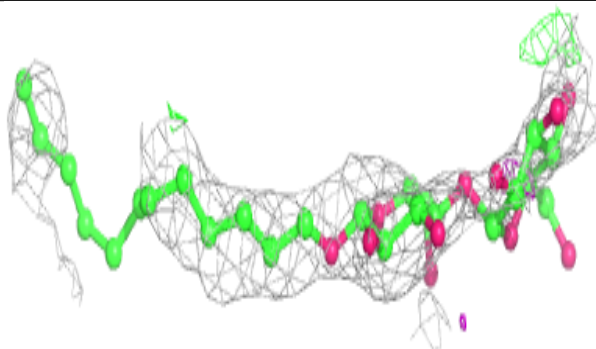
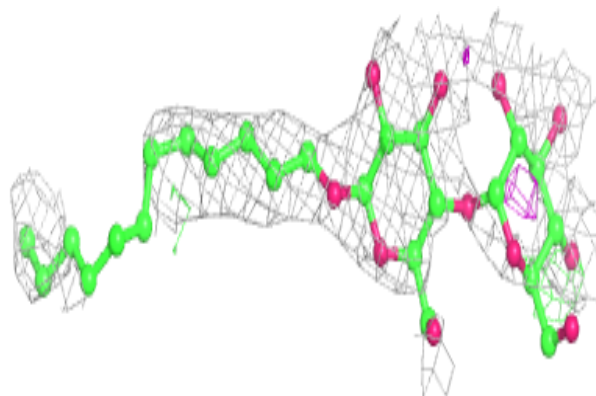


Electron density around UNL a 415:

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

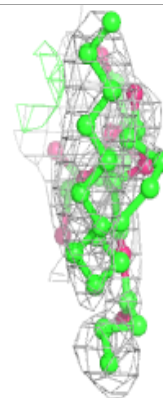
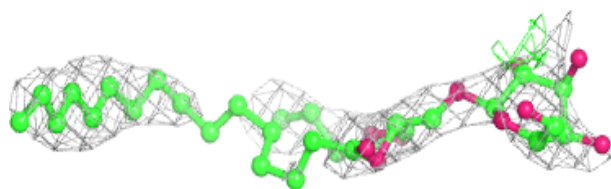
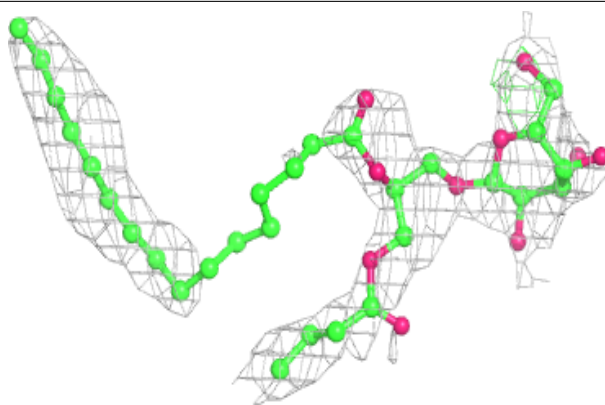
**Electron density around LMT a 418:**

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

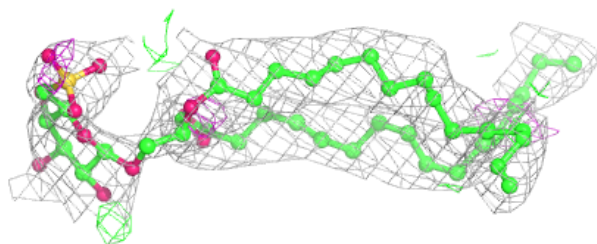
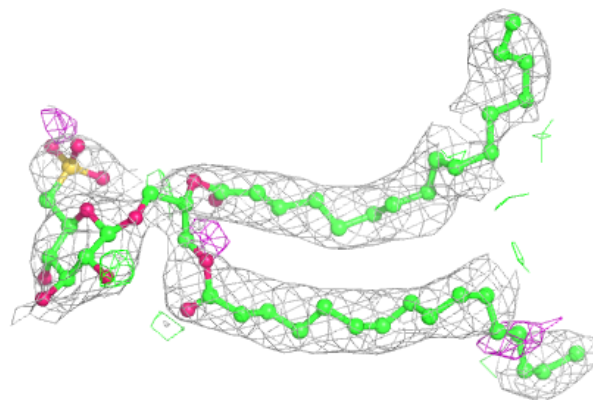


Electron density around LMG z 101:

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

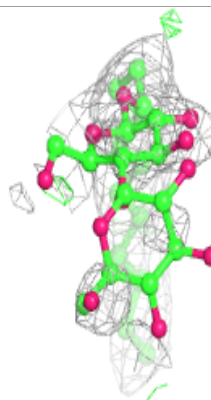
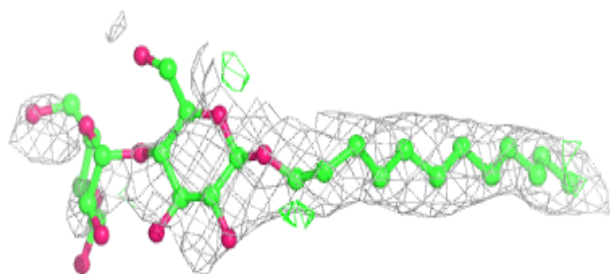
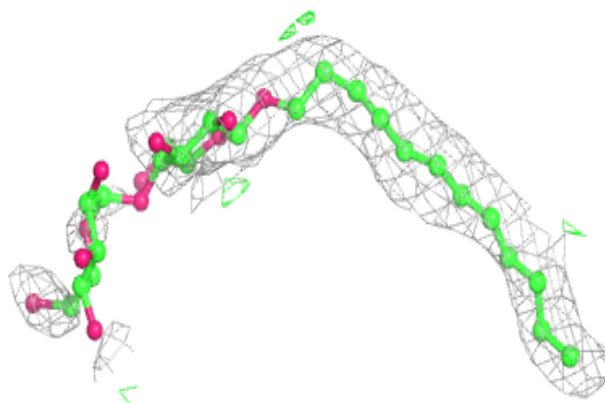
**Electron density around SQD b 620:**

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

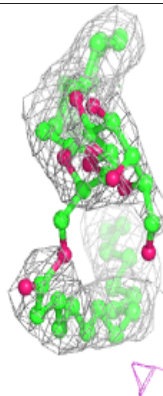
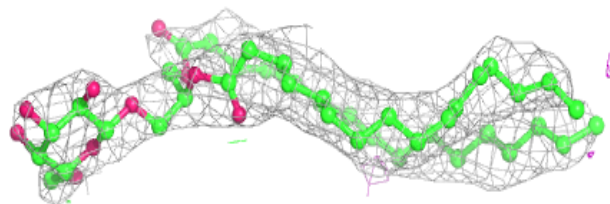
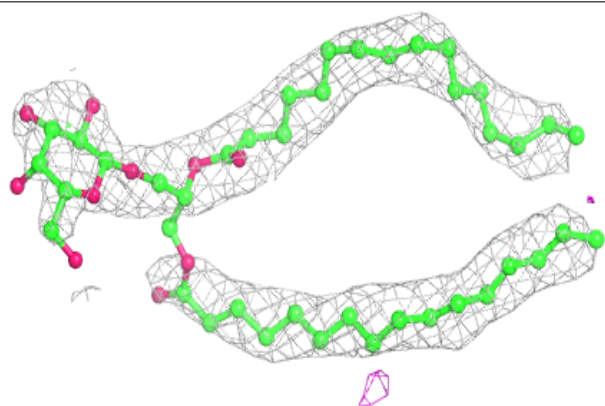


Electron density around LMT M 103:

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

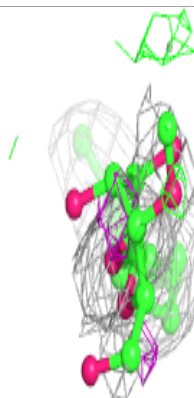
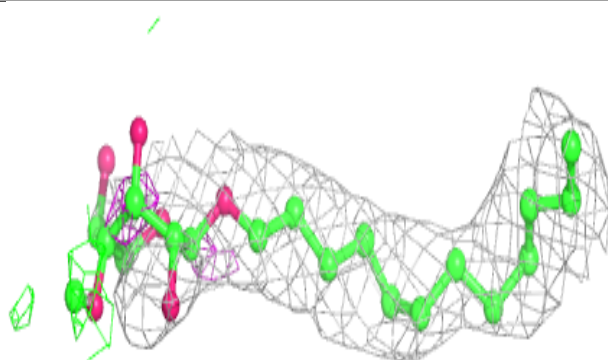
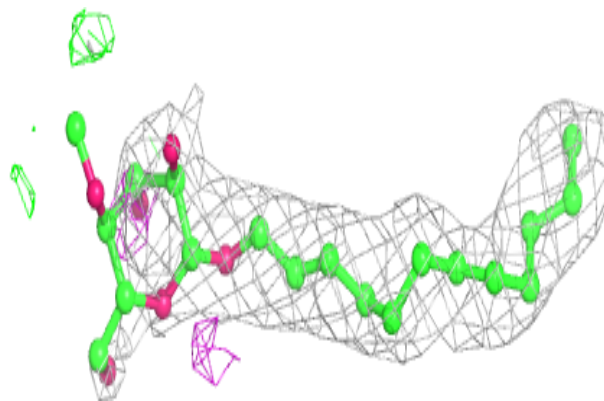
**Electron density around LMG a 417:**

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

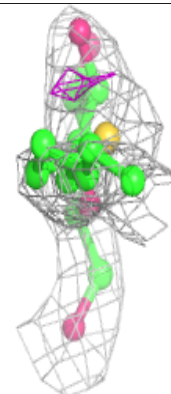
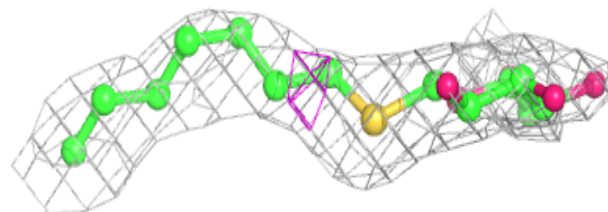
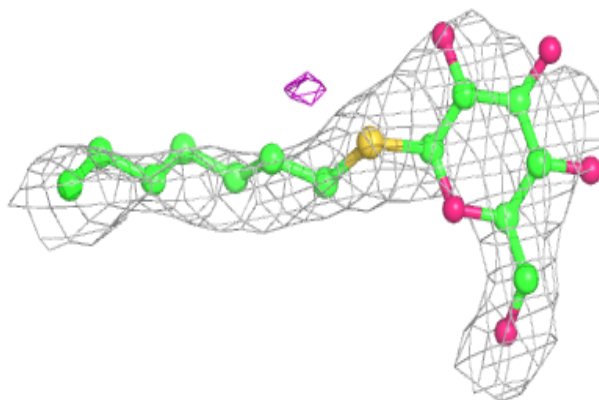


Electron density around LMT B 630:

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

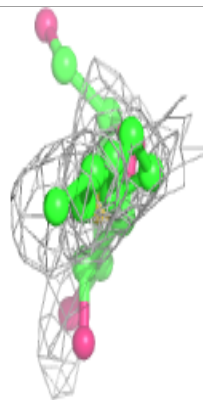
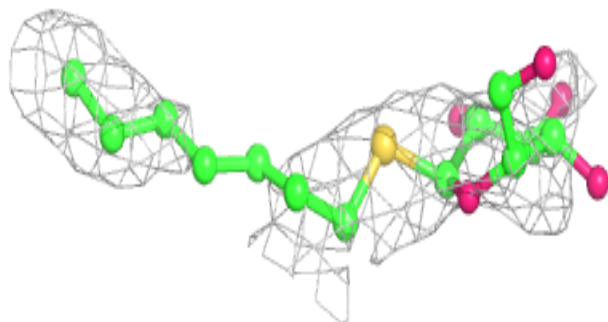
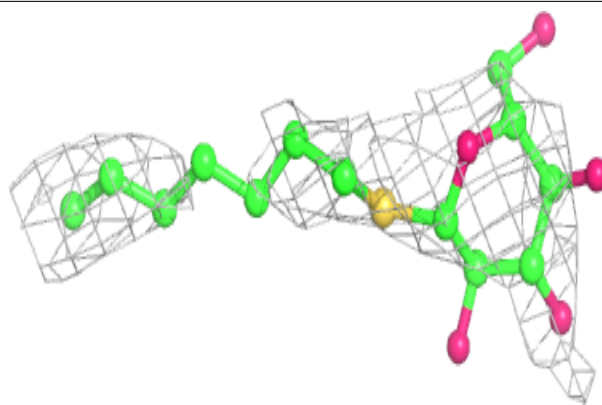
**Electron density around HTG C 522:**

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

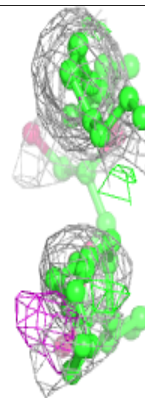
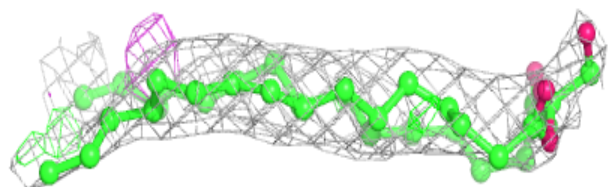
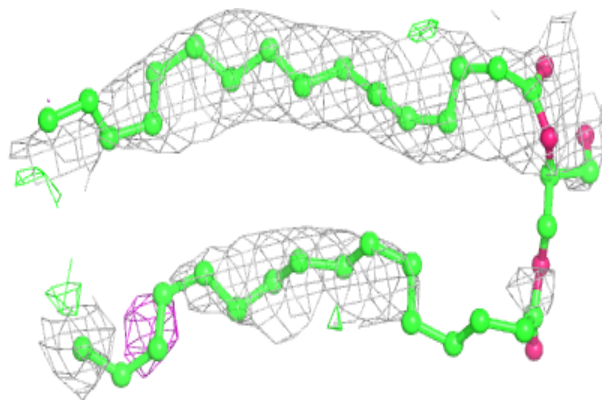


Electron density around HTG C 523:

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

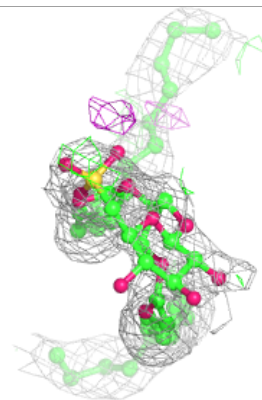
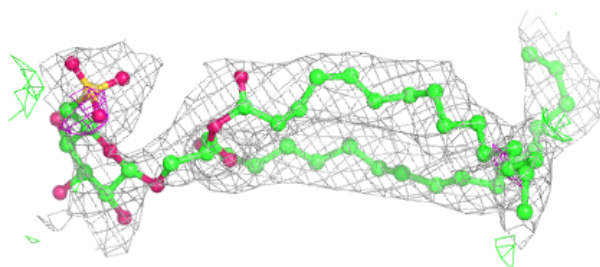
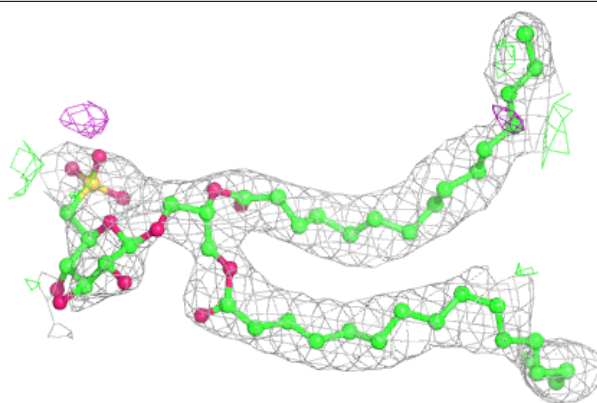
**Electron density around UNL I 102:**

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

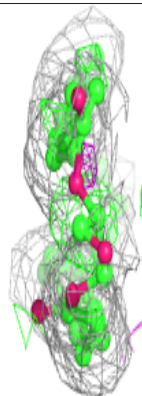
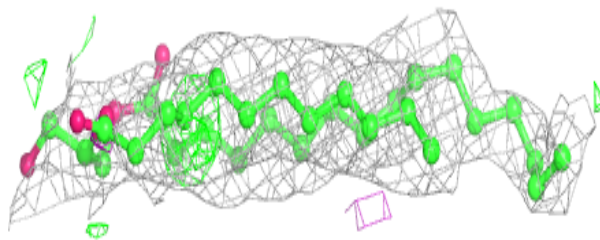
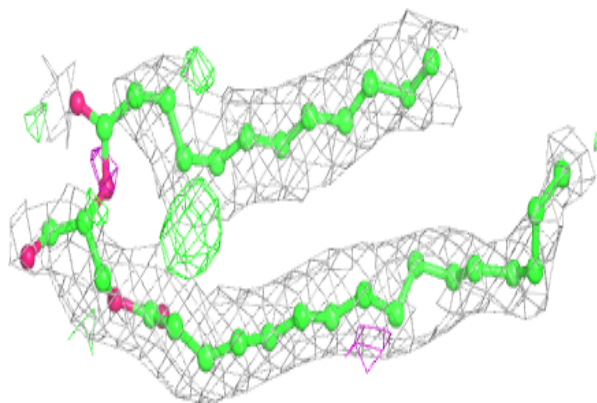


Electron density around SQD B 620:

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

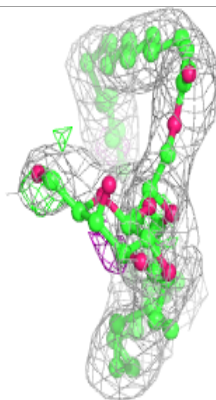
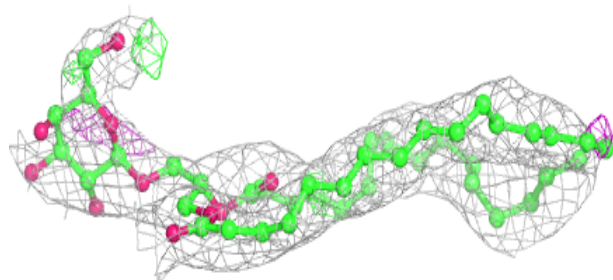
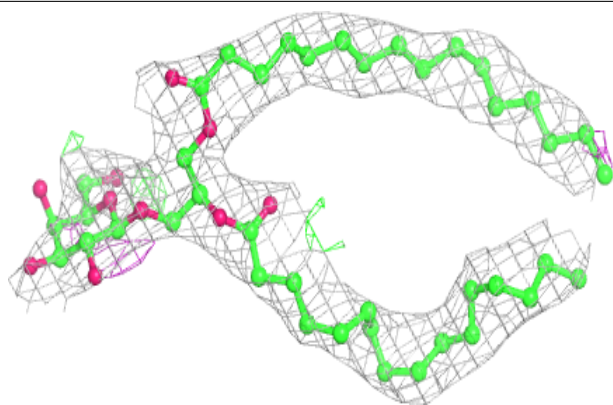
**Electron density around UNL d 410:**

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

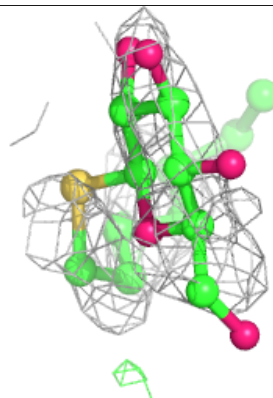
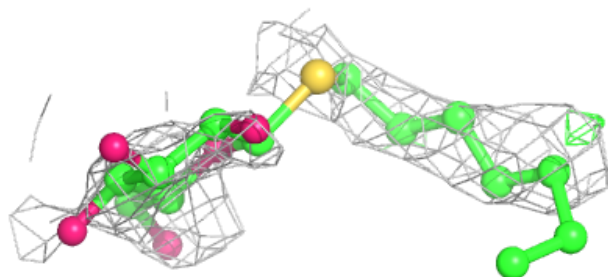
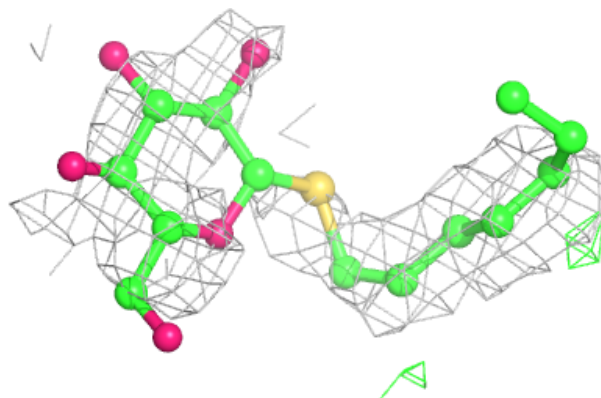


Electron density around LMG A 418:

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

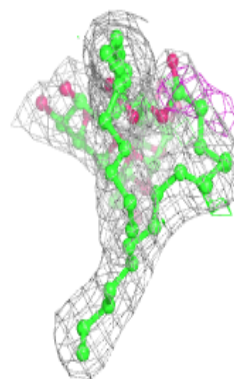
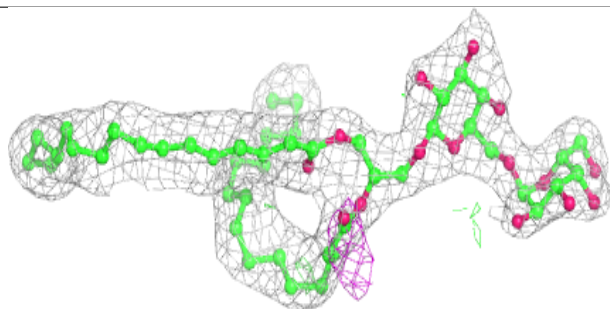
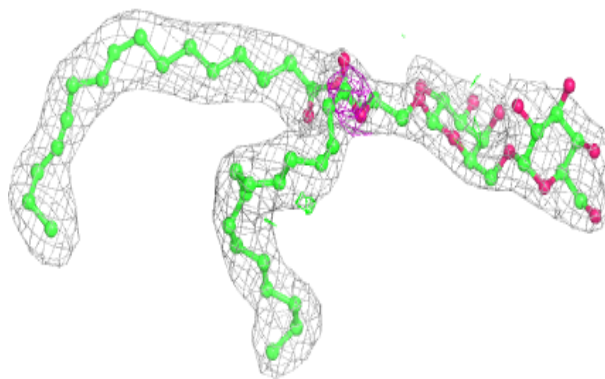
**Electron density around HTG b 624:**

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

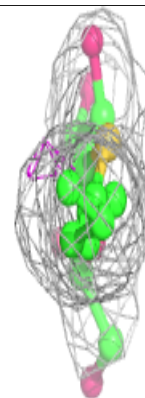
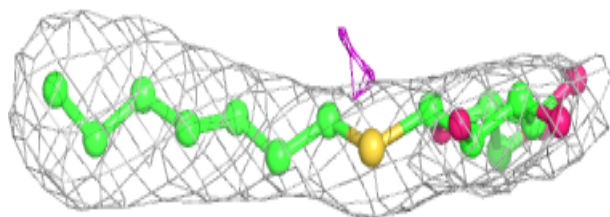
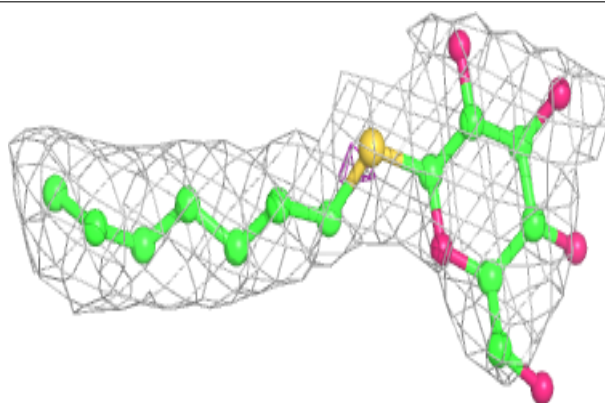


Electron density around DGD h 103:

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

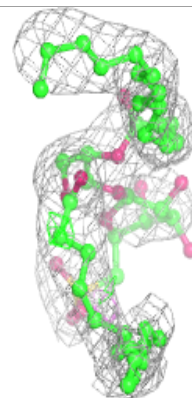
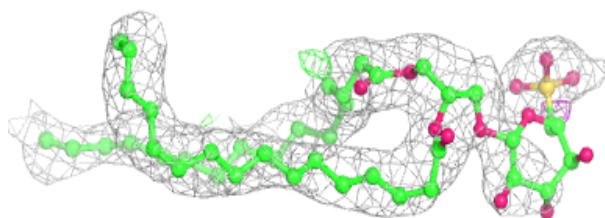
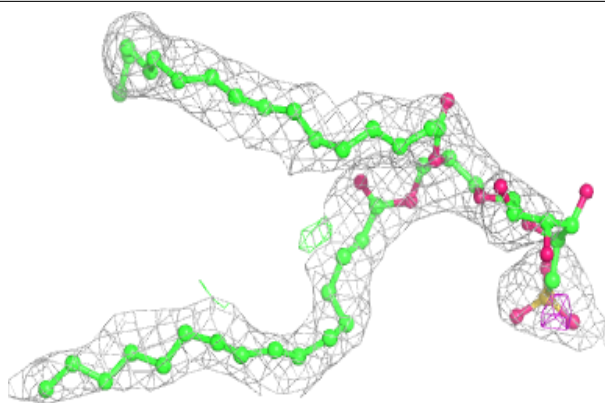
**Electron density around HTG b 628:**

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

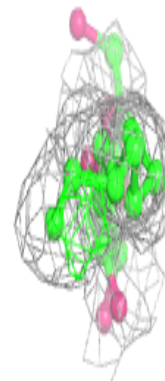
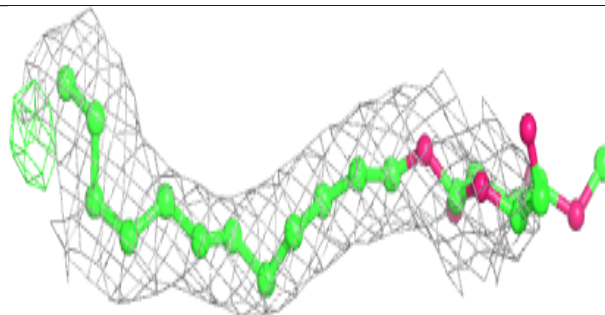
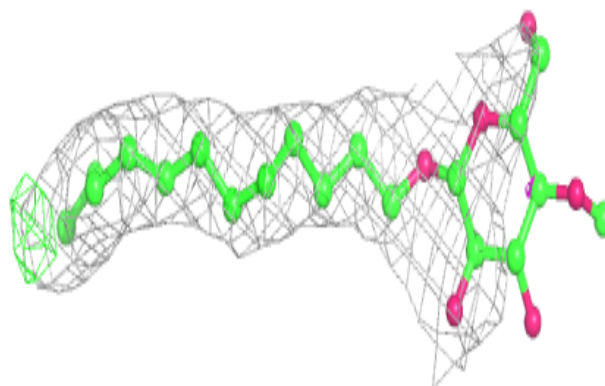


Electron density around SQD a 411:

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

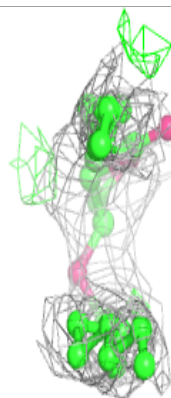
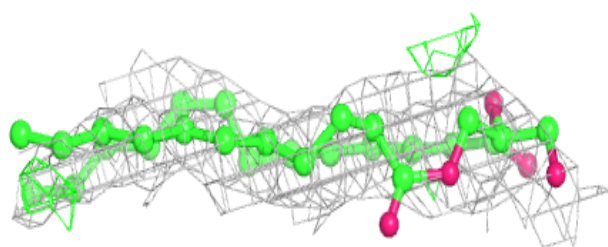
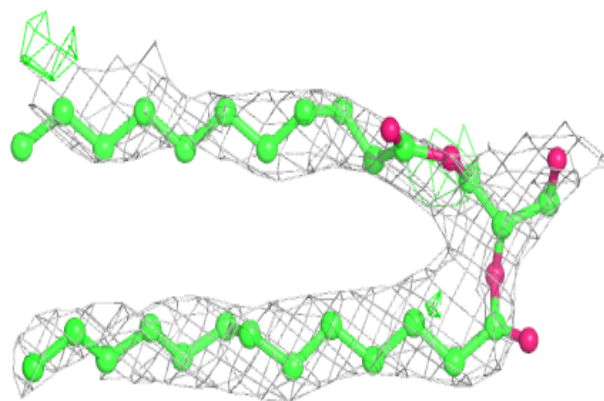
**Electron density around LMT b 630:**

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

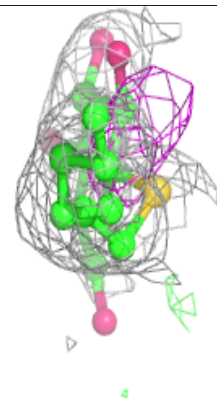
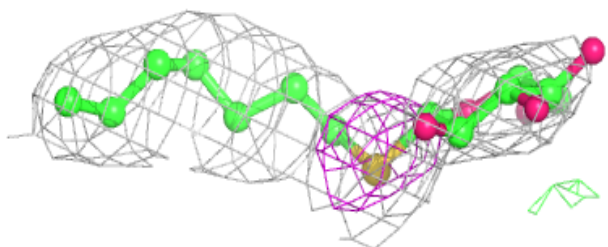
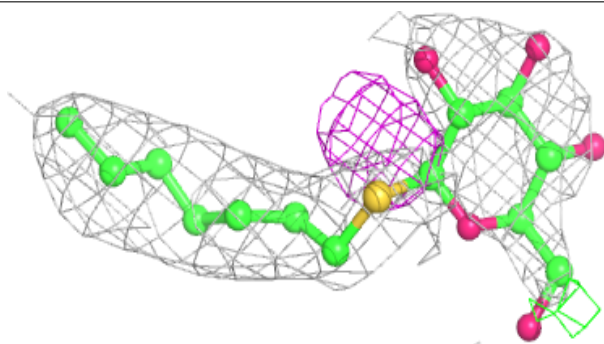


Electron density around UNL c 527:

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

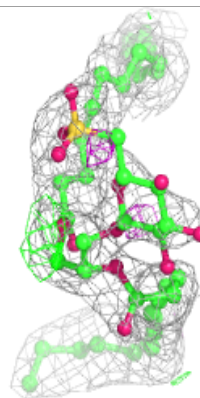
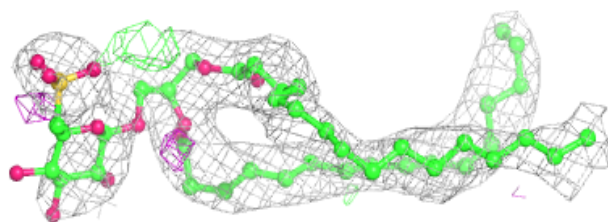
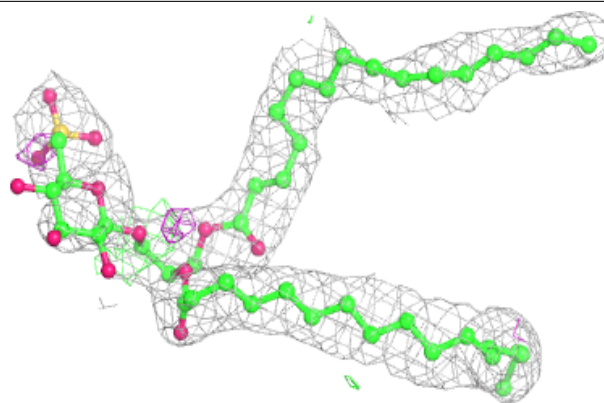
**Electron density around HTG b 623:**

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

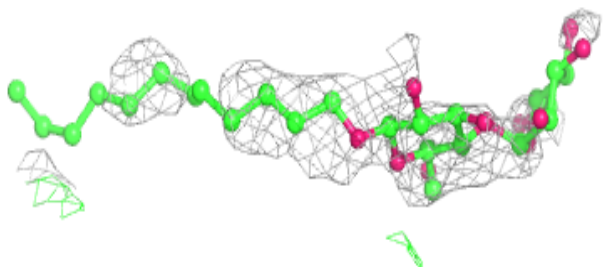
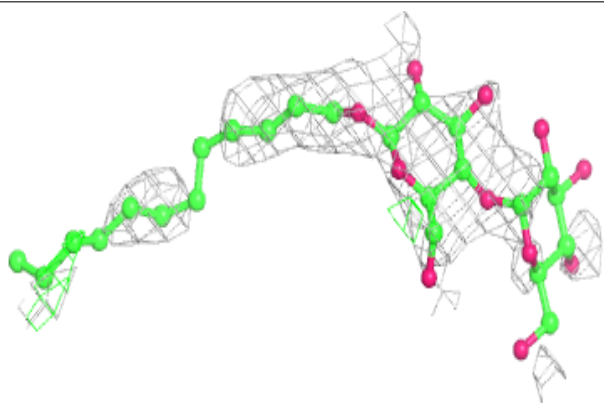


Electron density around SQD A 413:

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

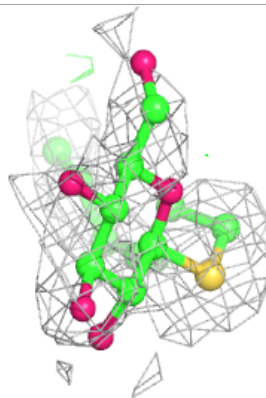
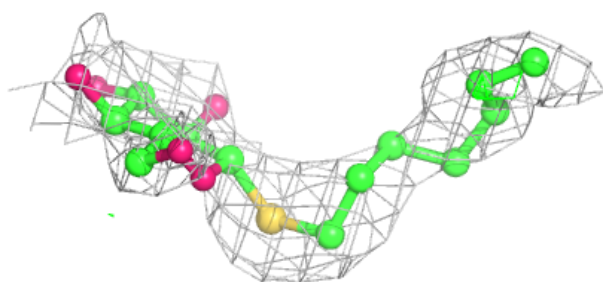
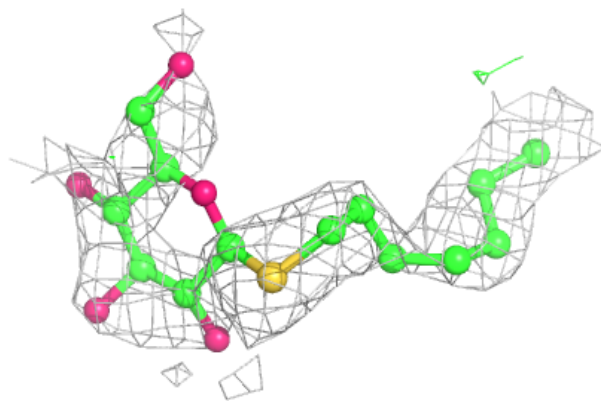
**Electron density around LMT E 102:**

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

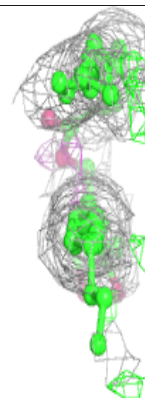
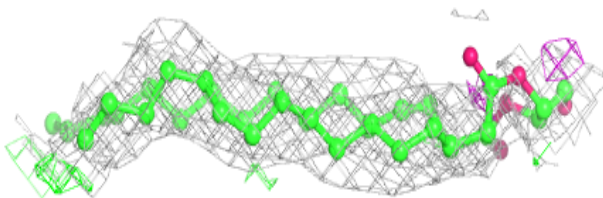
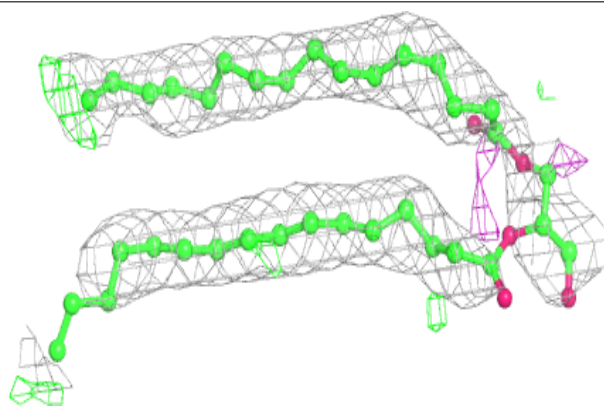


Electron density around HTG B 624:

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

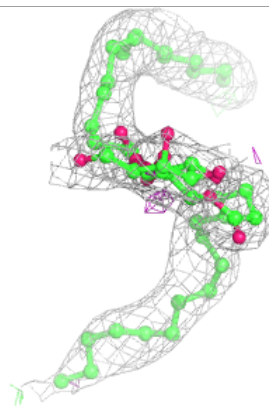
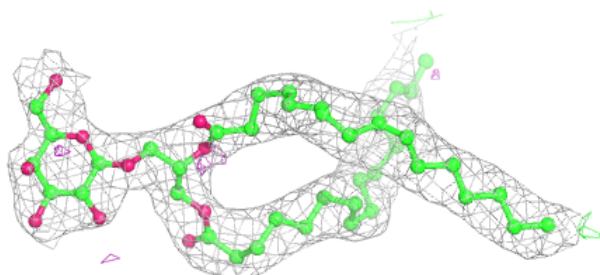
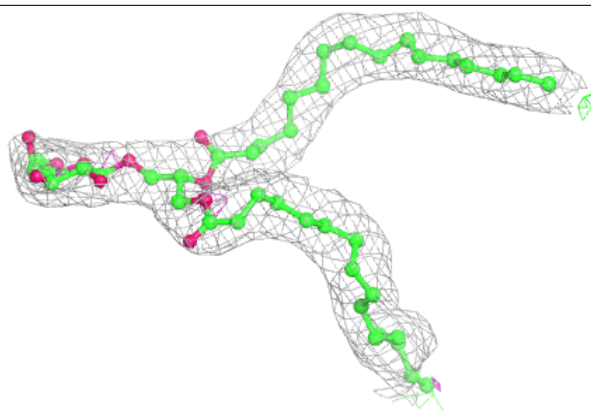
**Electron density around UNL D 409:**

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

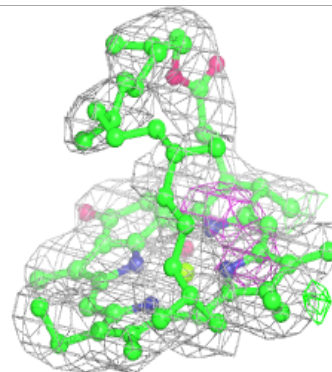
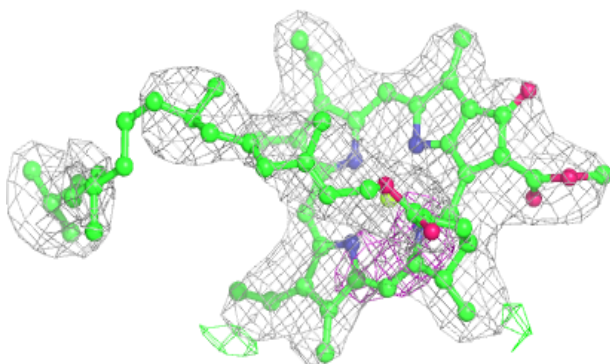
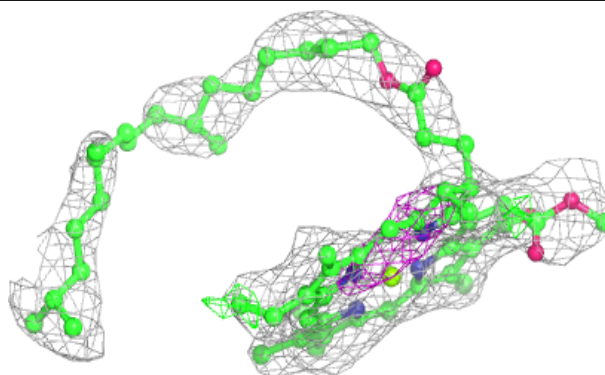


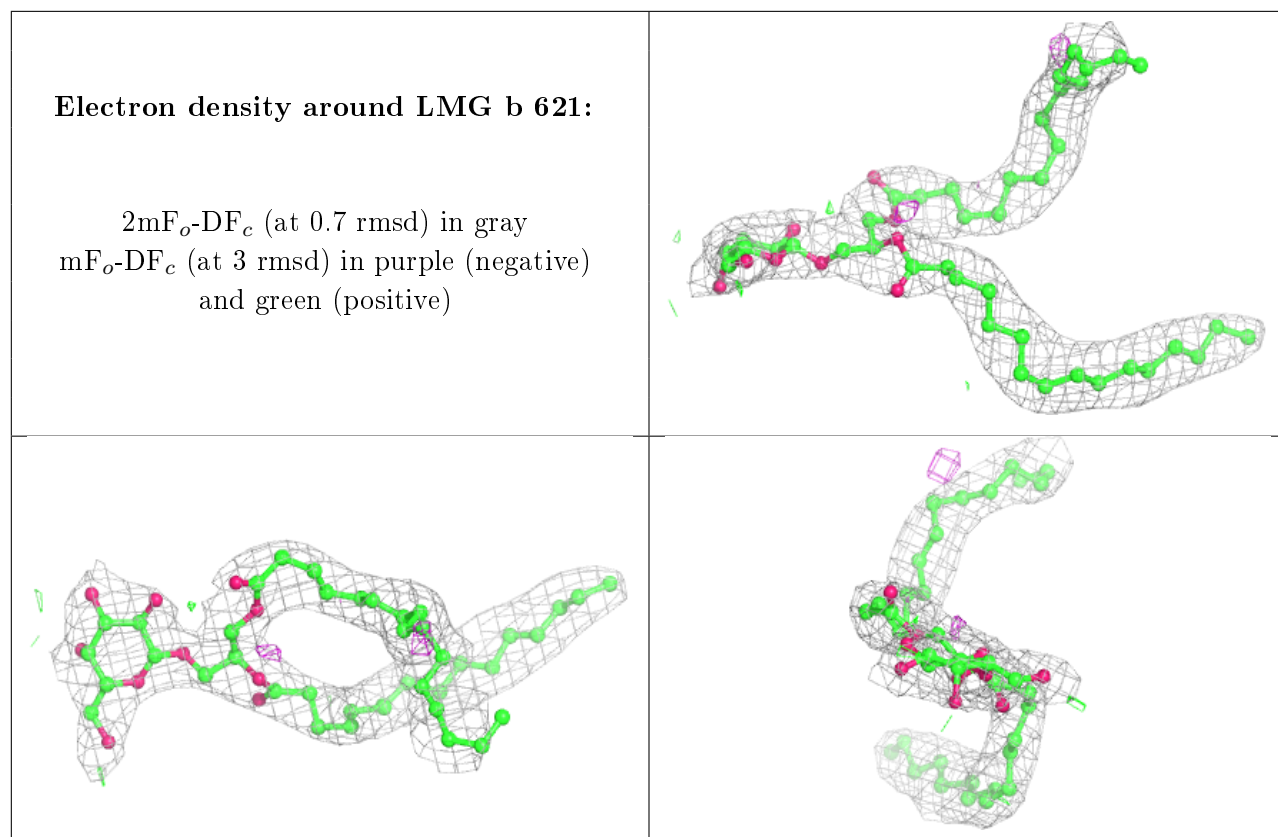
Electron density around LMG B 621:

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

**Electron density around CLA C 514:**

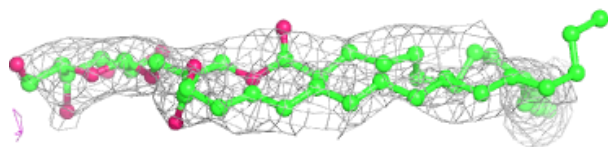
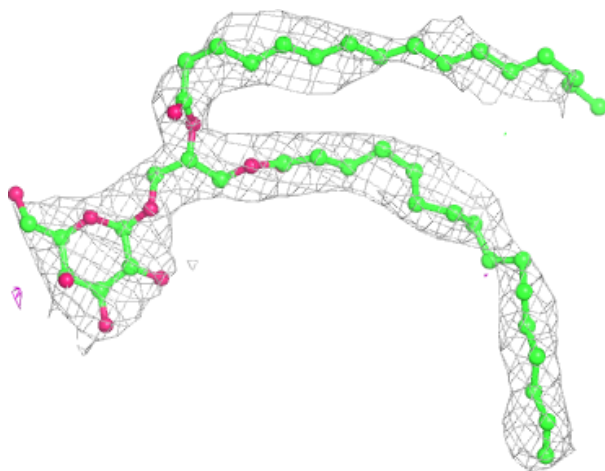
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





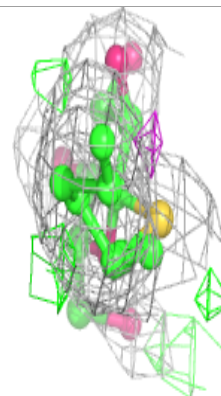
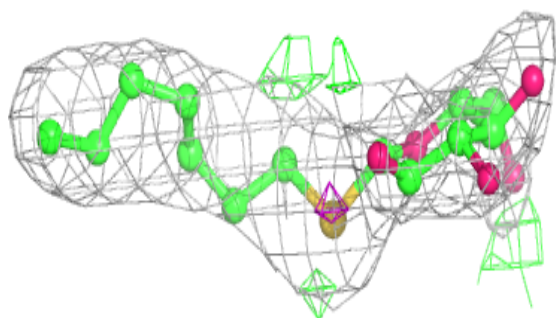
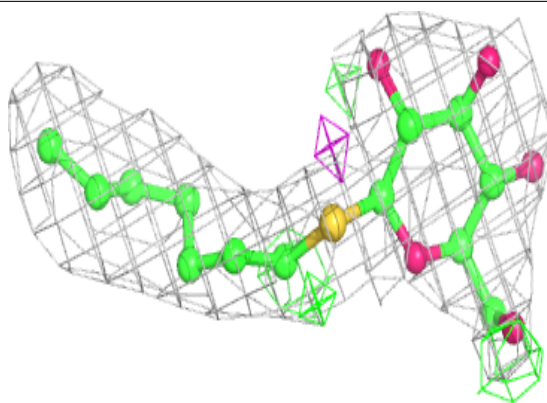
Electron density around LMG c 521:

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

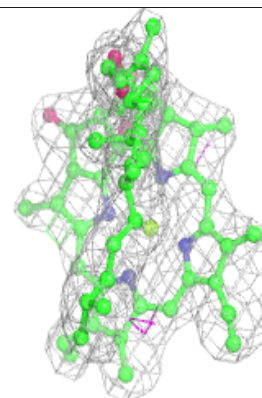
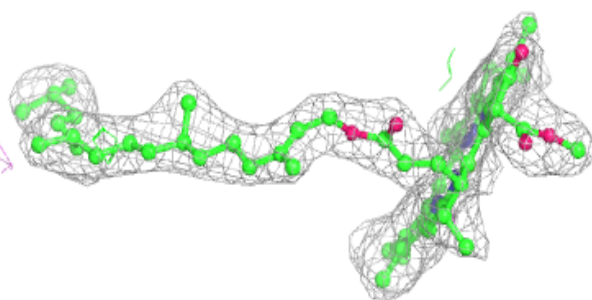
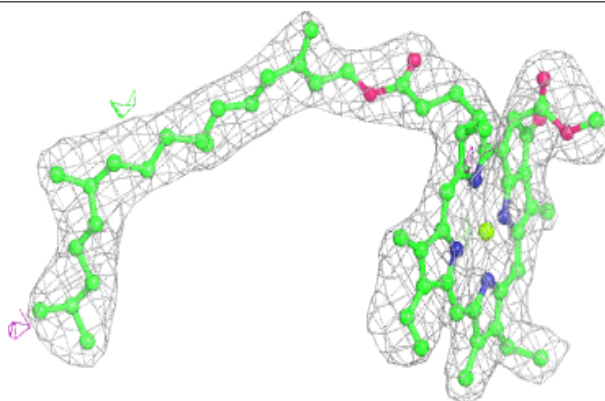


Electron density around HTG B 623:

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

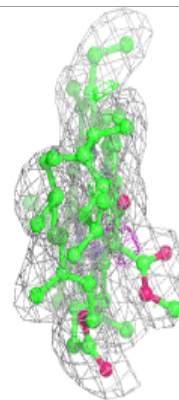
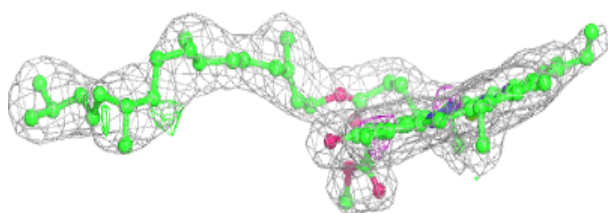
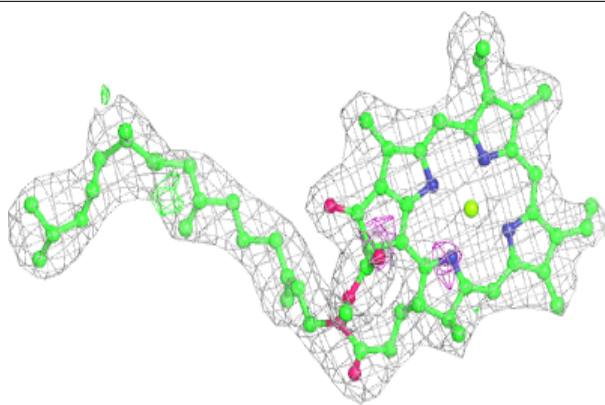
**Electron density around CLA B 609:**

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

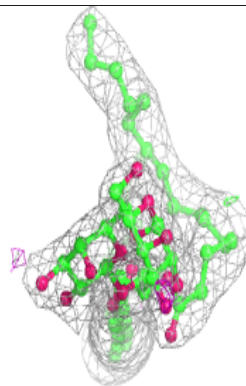
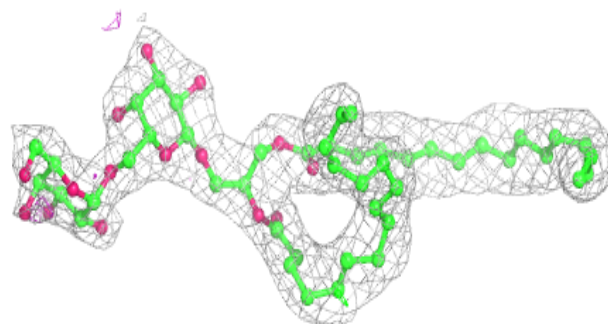
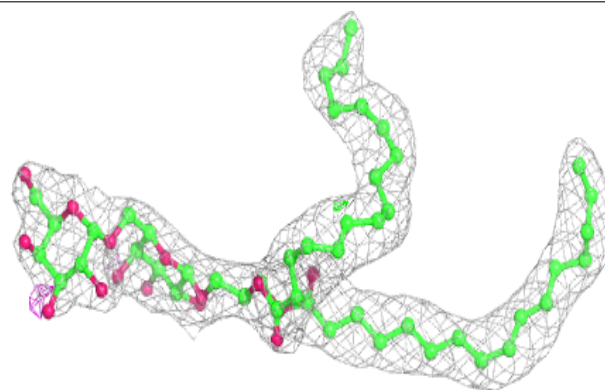


Electron density around CLA b 602:

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

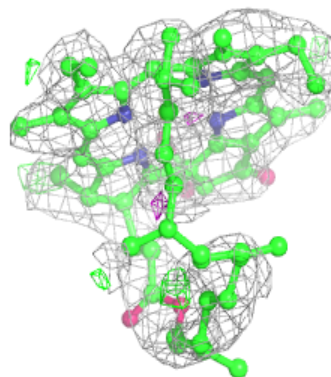
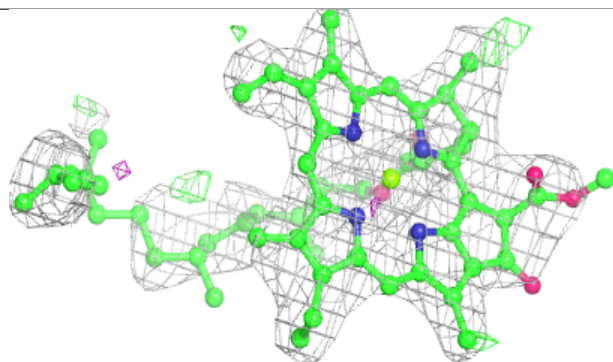
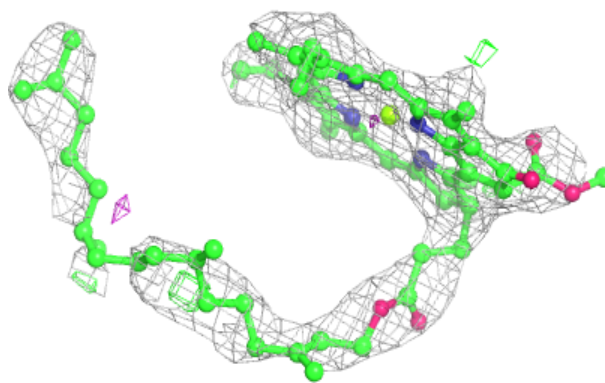
**Electron density around DGD H 102:**

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



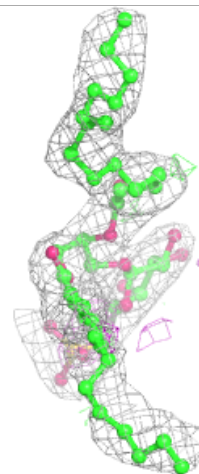
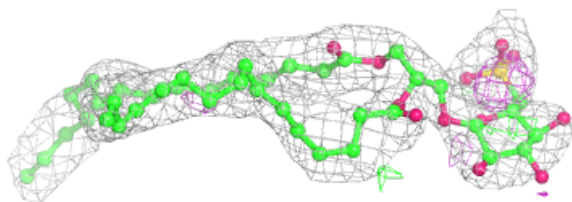
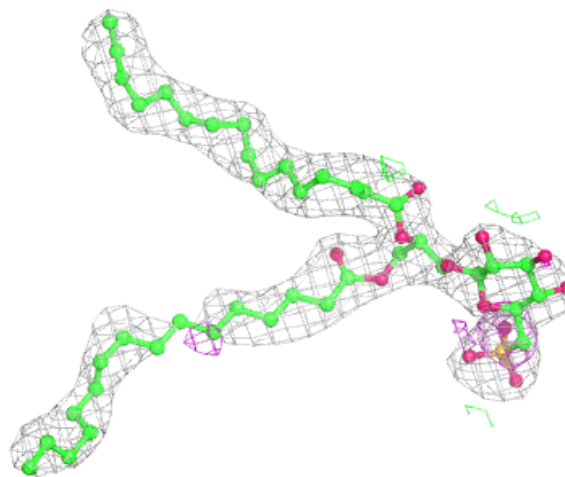
Electron density around CLA c 515:

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



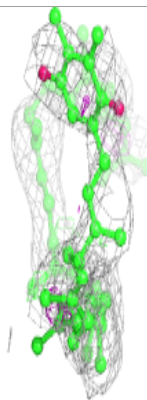
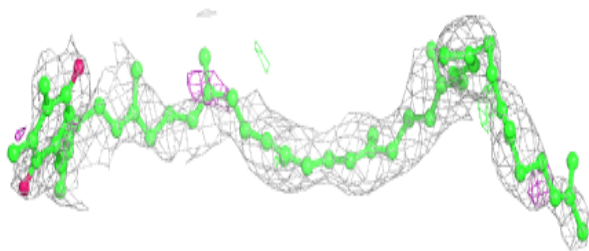
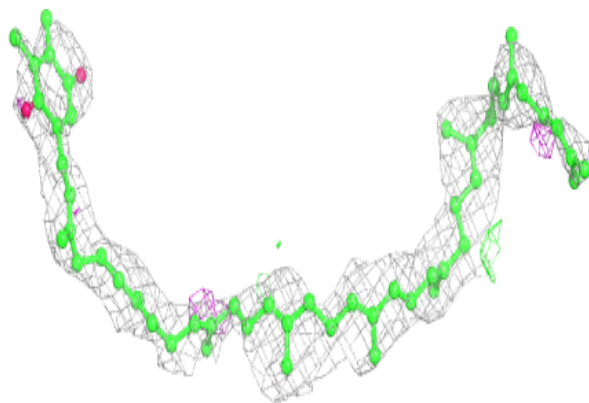
Electron density around SQD A 411:

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

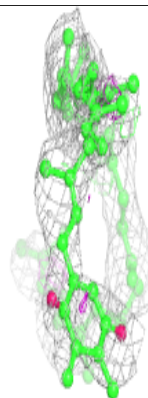
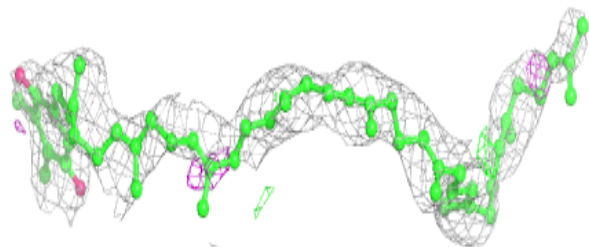
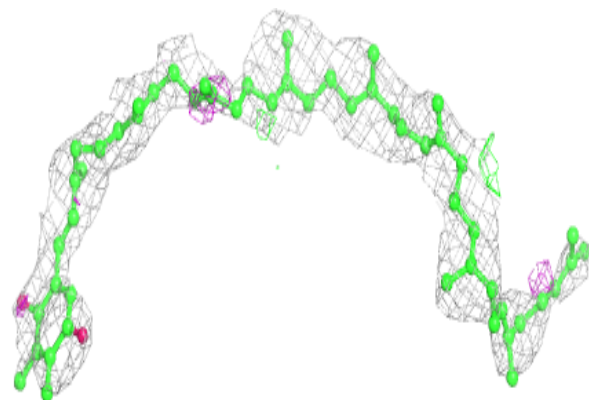


Electron density around PL9 a 414 (A):

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

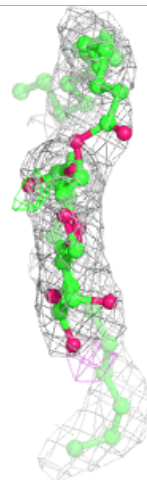
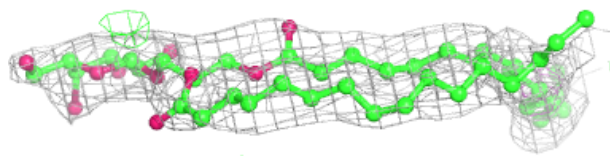
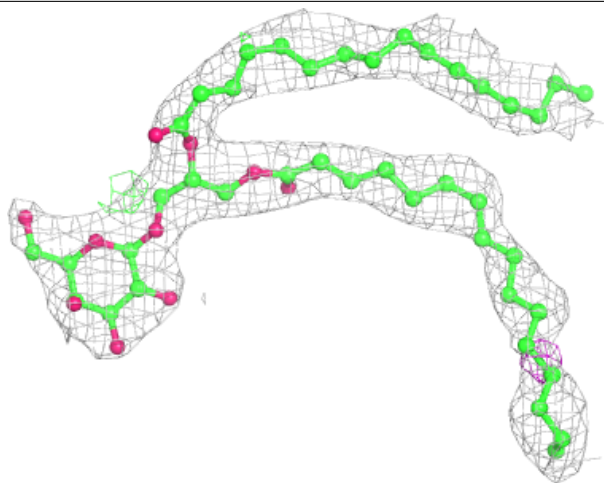
**Electron density around PL9 a 414 (B):**

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



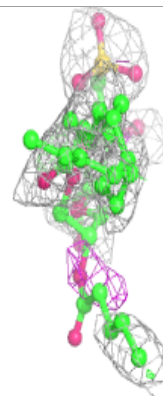
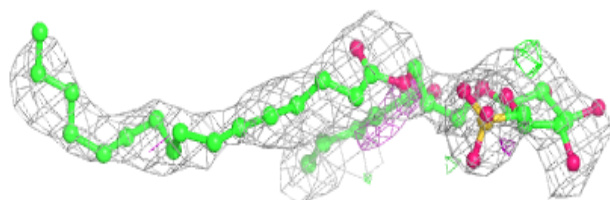
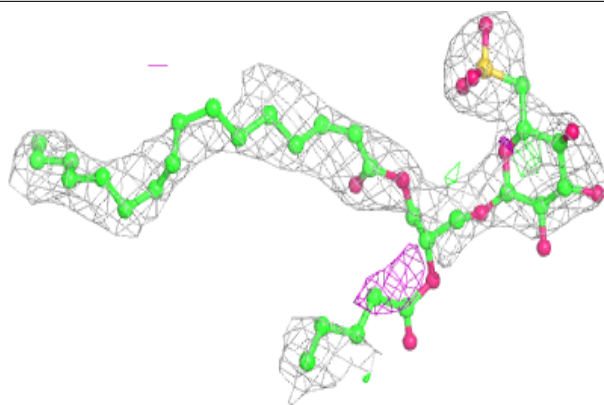
Electron density around LMG C 520:

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

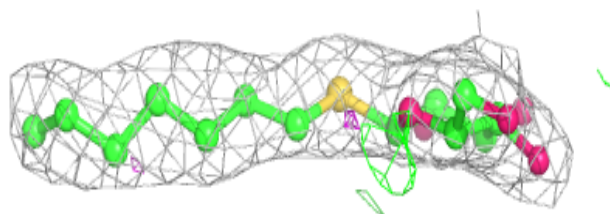
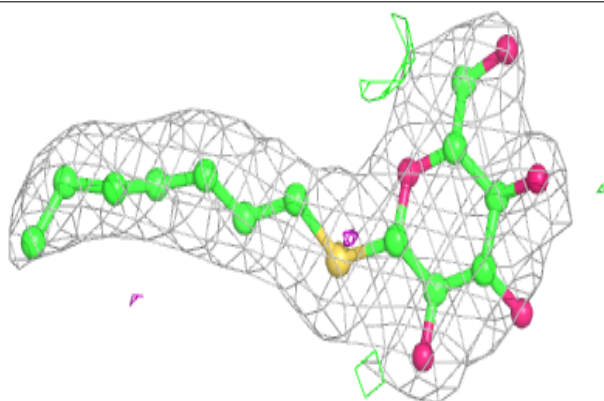


Electron density around SQD F 101:

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

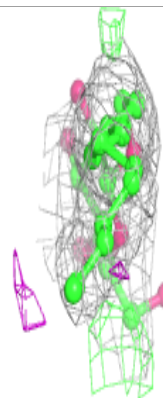
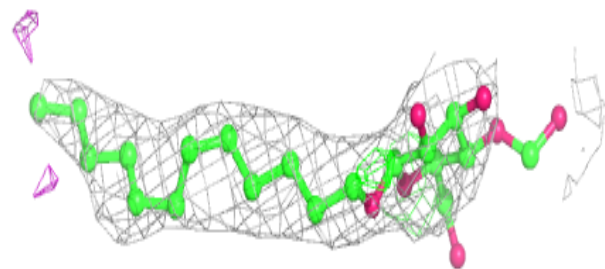
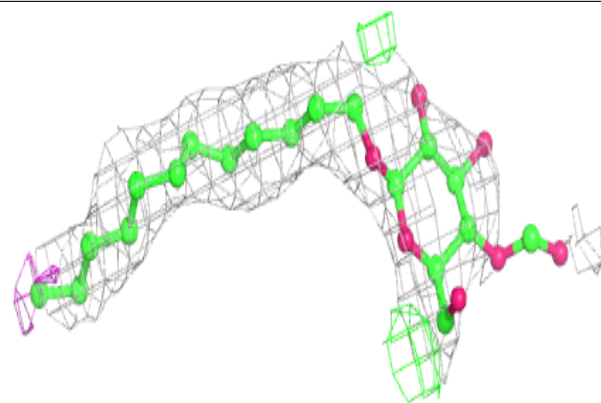
**Electron density around HTG B 628:**

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

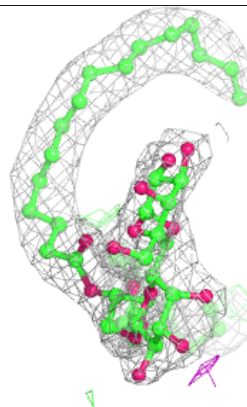
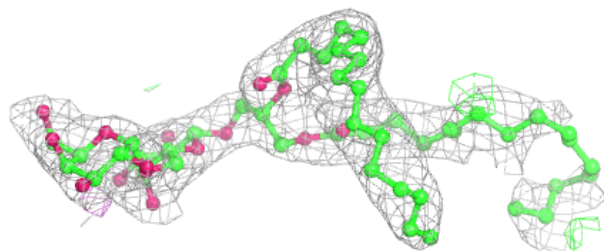
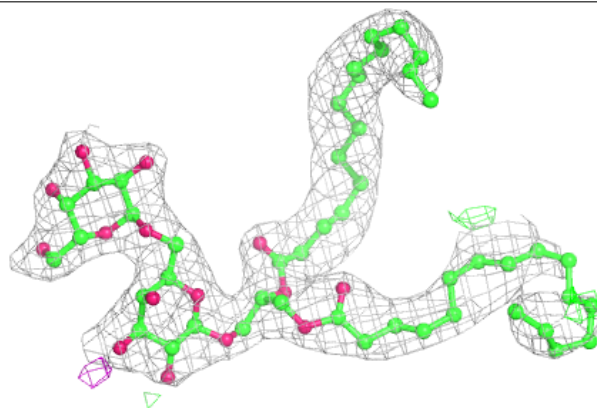


Electron density around LMT t 101:

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

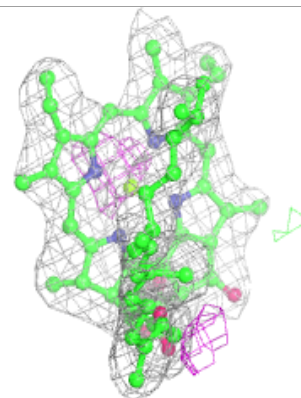
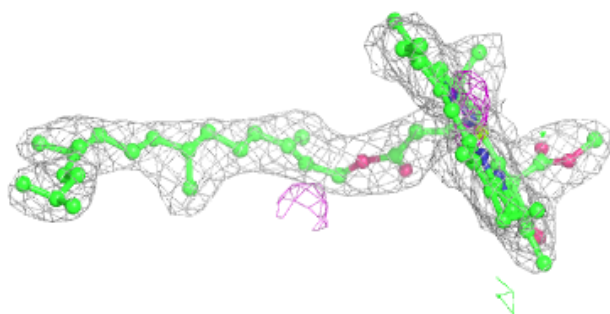
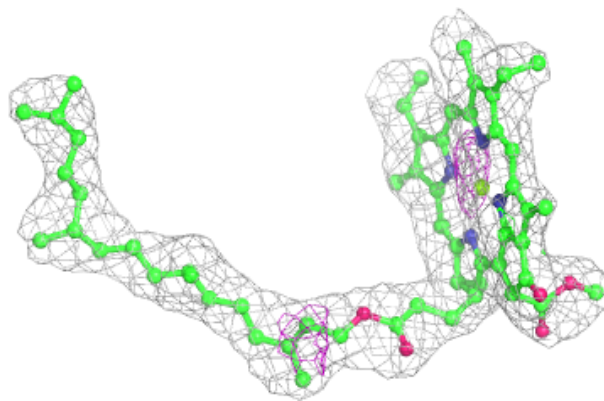
**Electron density around DGD C 518:**

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

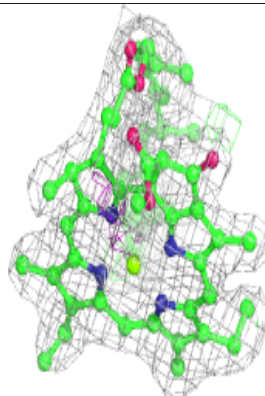
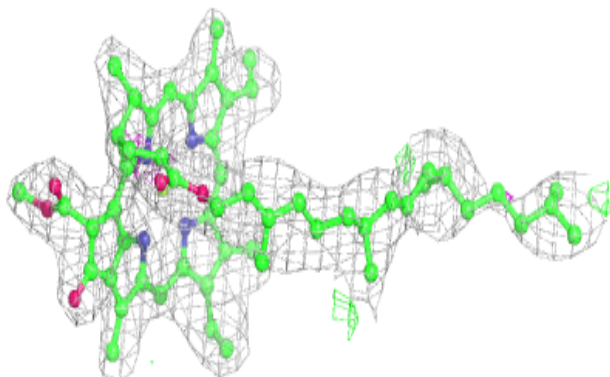
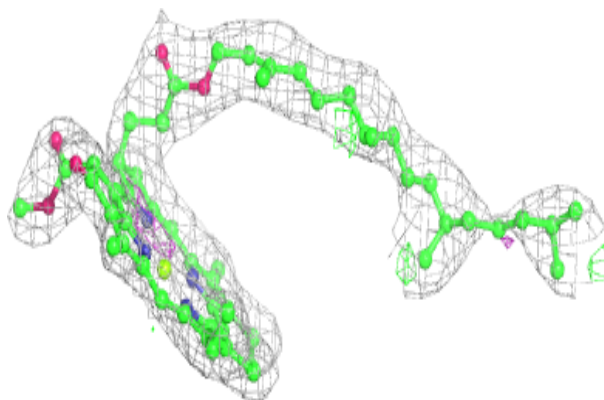


Electron density around CLA b 609:

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

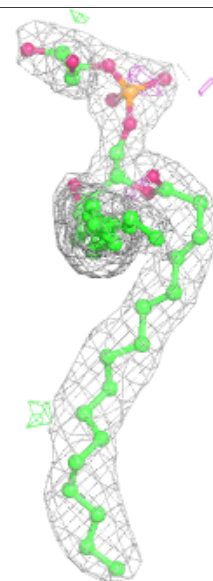
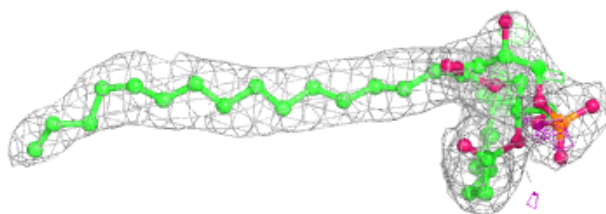
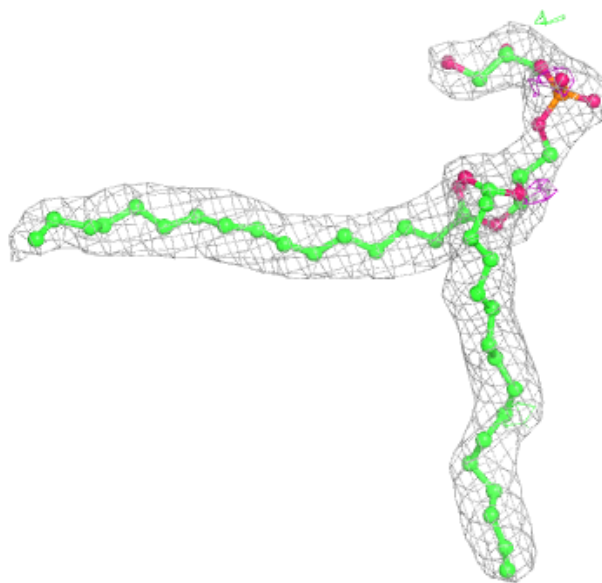
**Electron density around CLA C 505:**

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



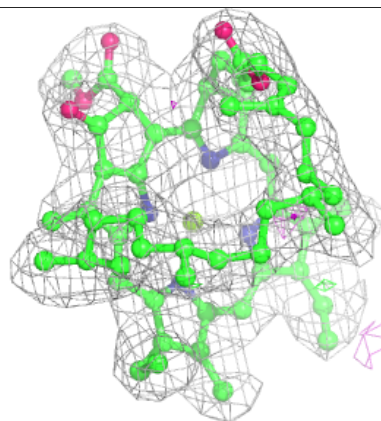
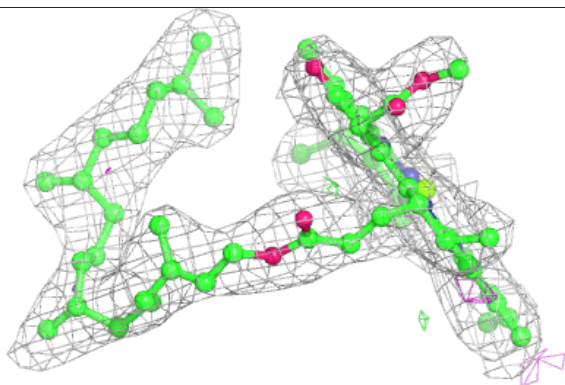
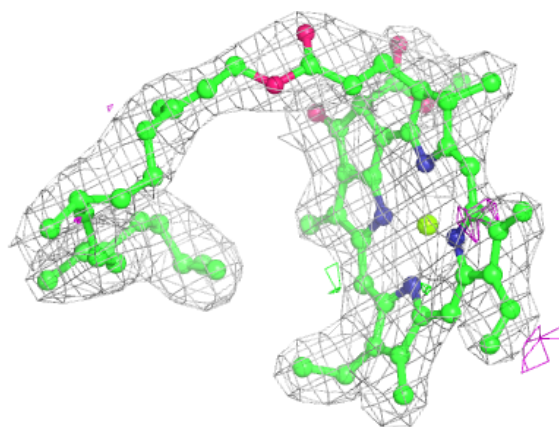
Electron density around LHG 1 101:

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



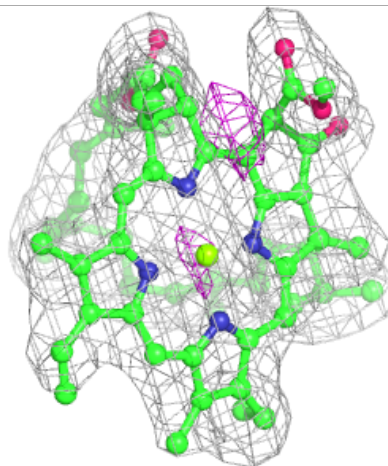
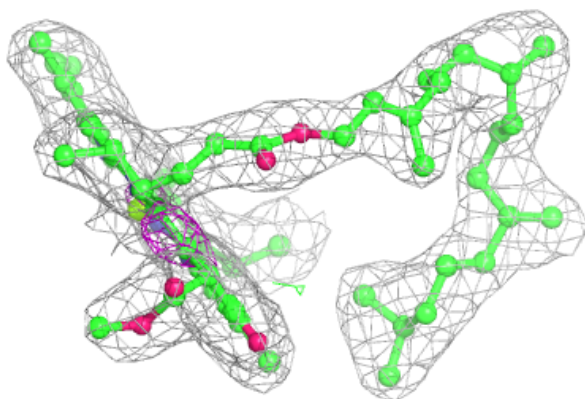
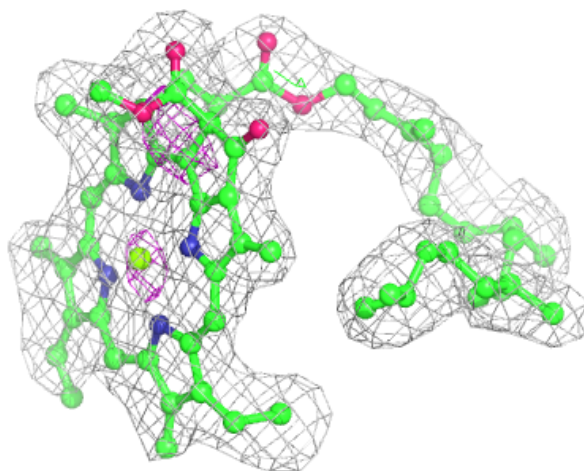
Electron density around CLA c 505:

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



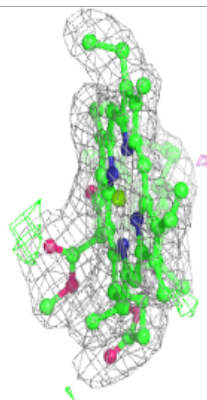
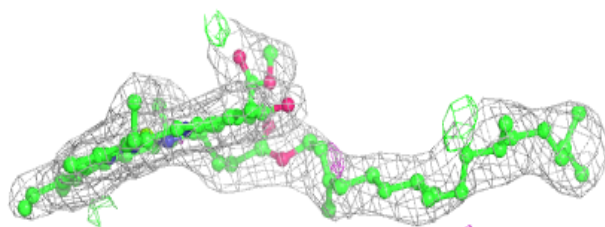
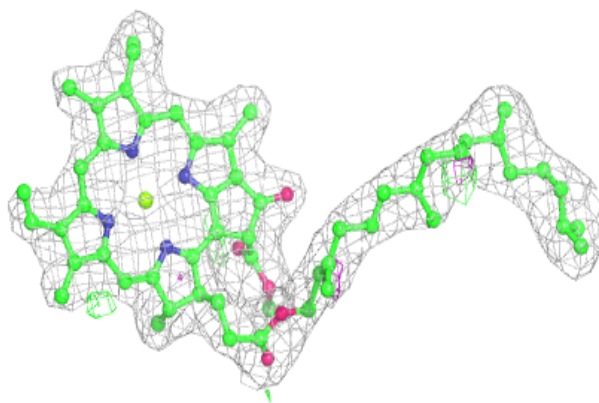
Electron density around CLA C 504:

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

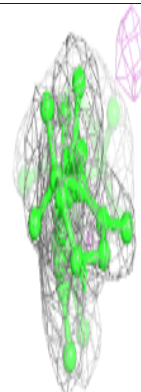
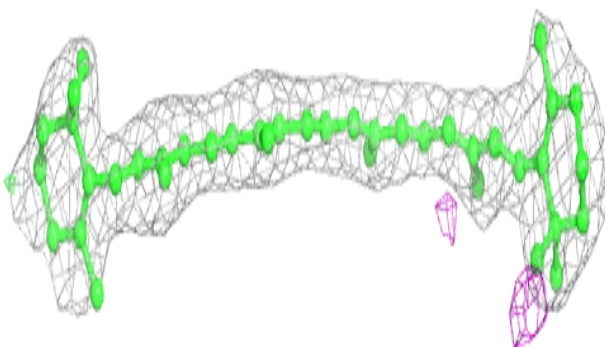
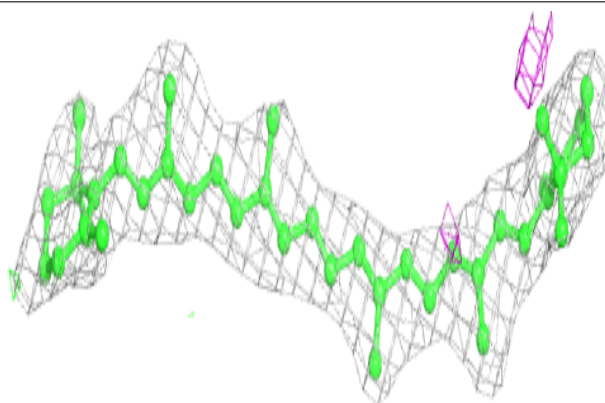


Electron density around CLA B 602:

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

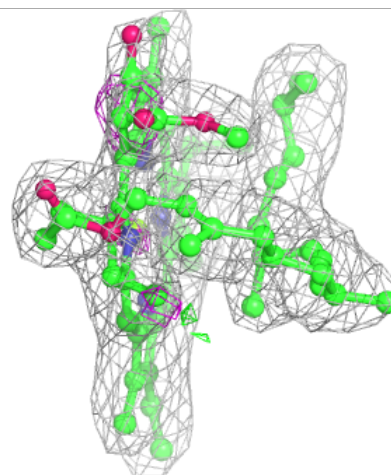
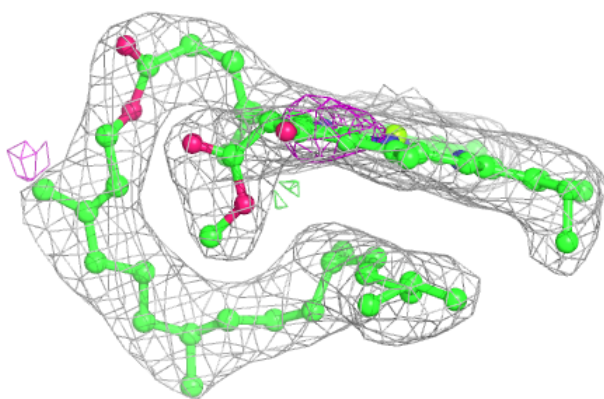
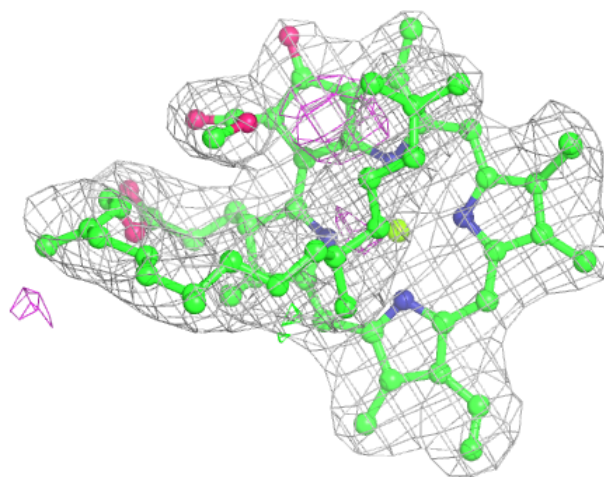
**Electron density around BCR h 102:**

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



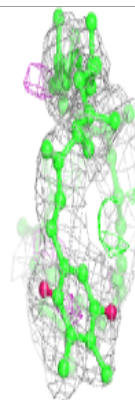
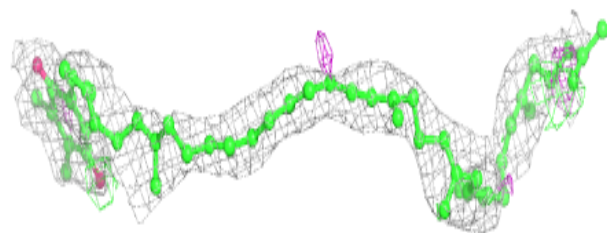
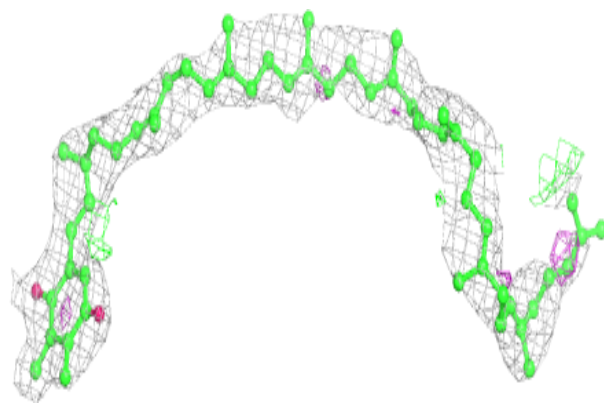
Electron density around CLA c 512:

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

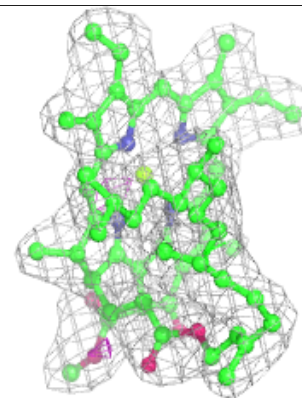
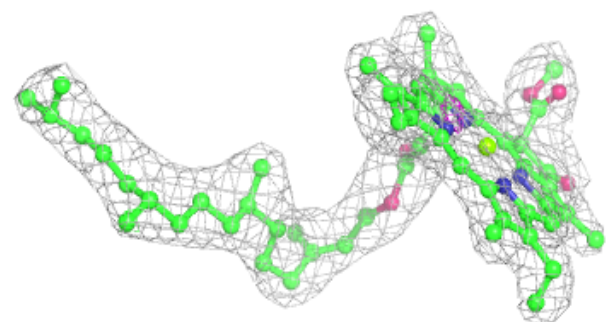
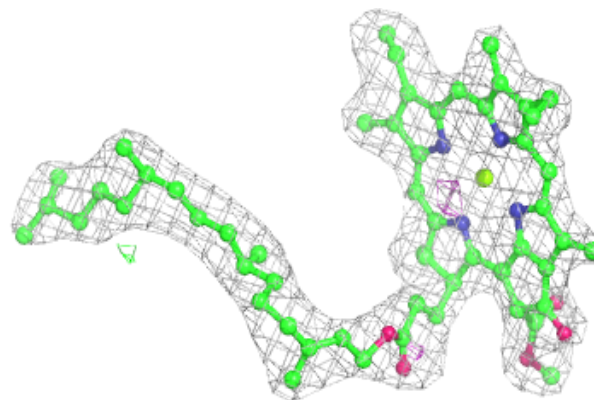


Electron density around PL9 A 416 (B):

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

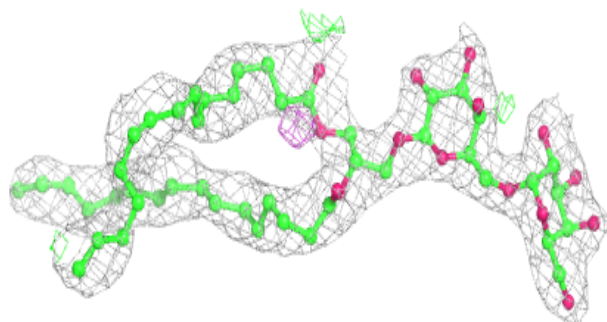
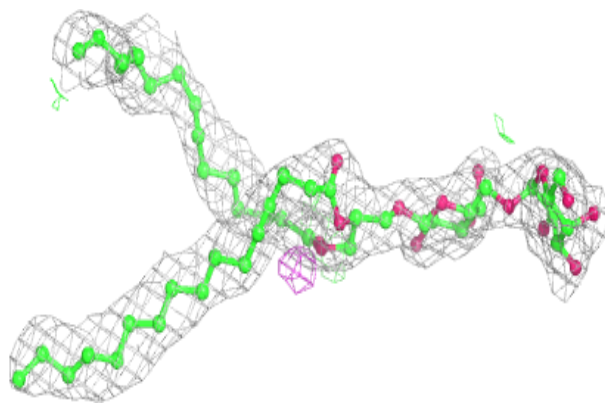
**Electron density around CLA C 512:**

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

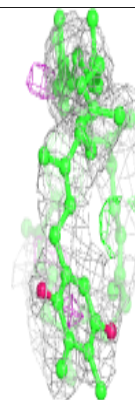
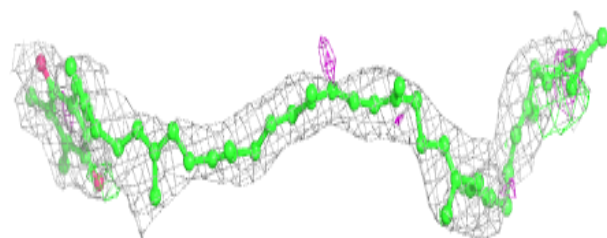
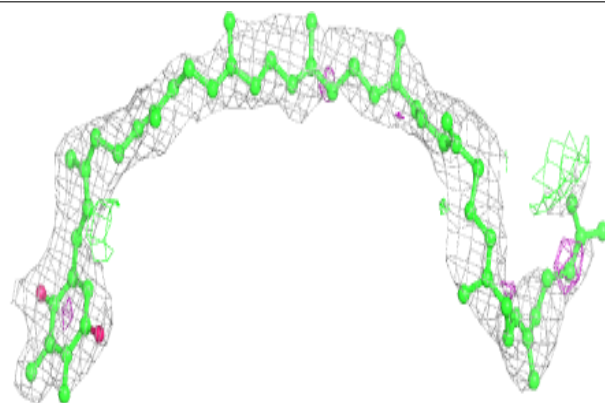


Electron density around DGD c 518:

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

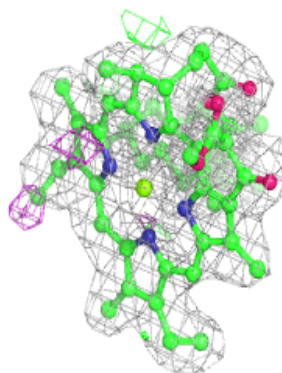
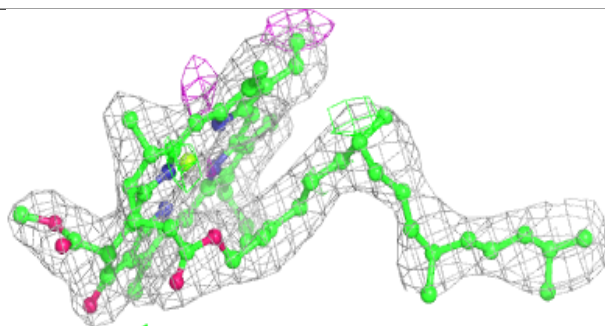
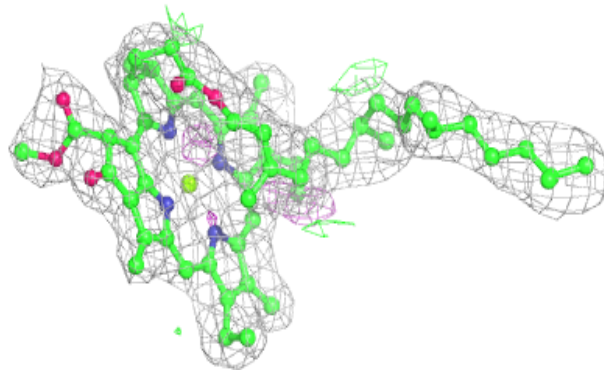
**Electron density around PL9 A 416 (A):**

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



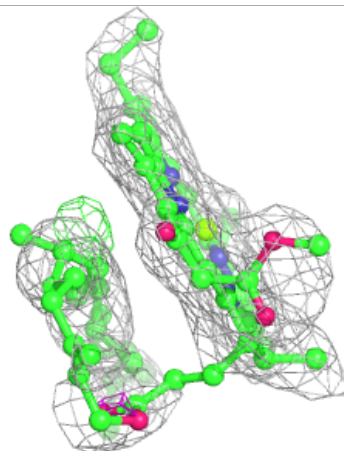
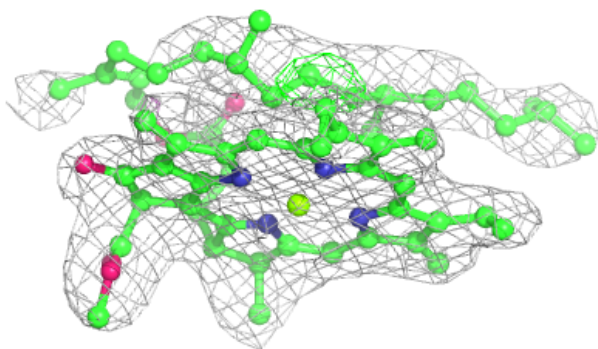
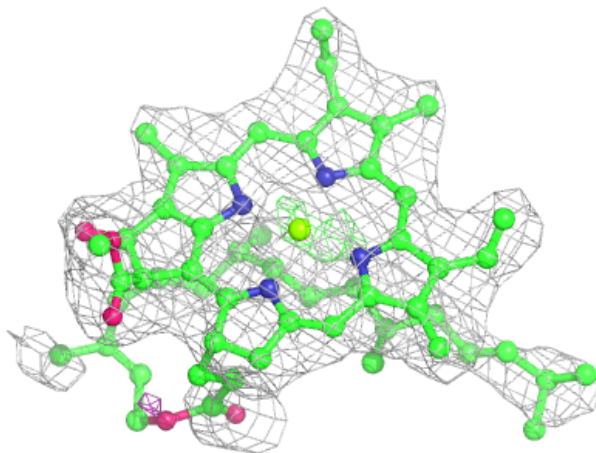
Electron density around CLA c 507:

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



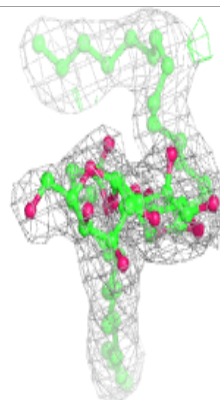
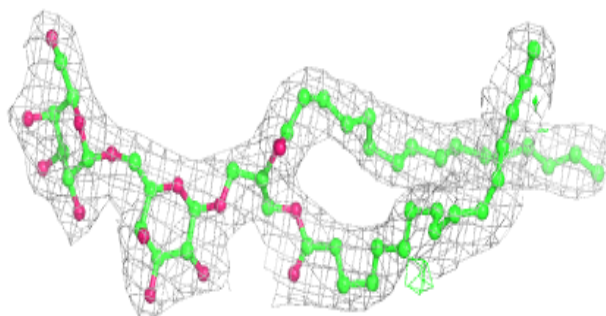
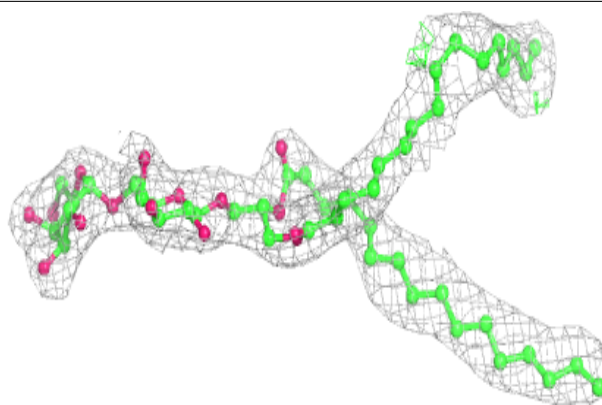
Electron density around CLA b 601:

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

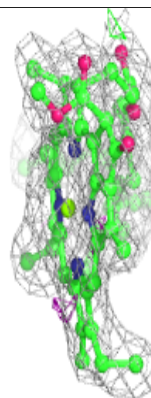
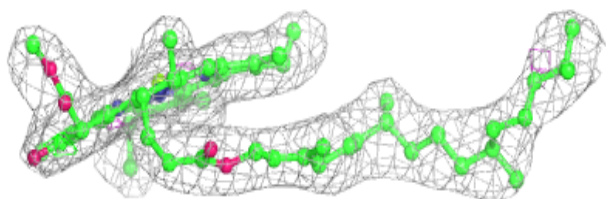
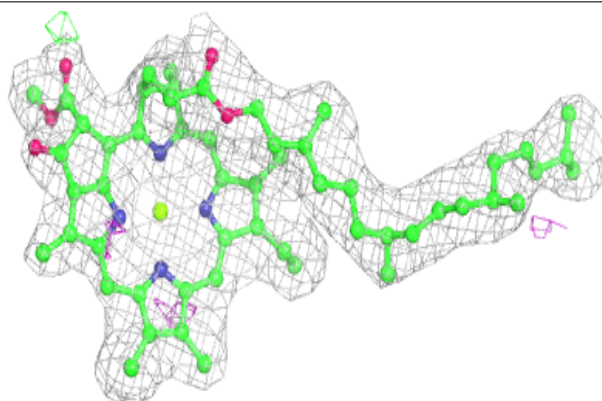


Electron density around DGD C 517:

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

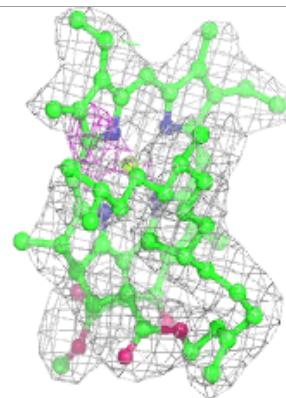
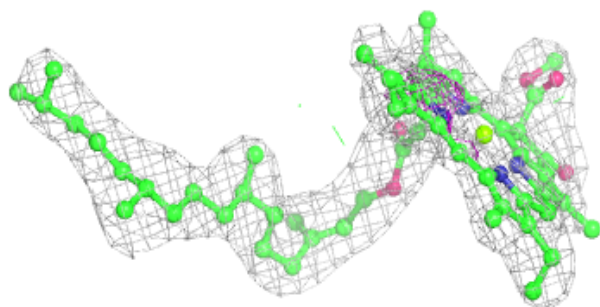
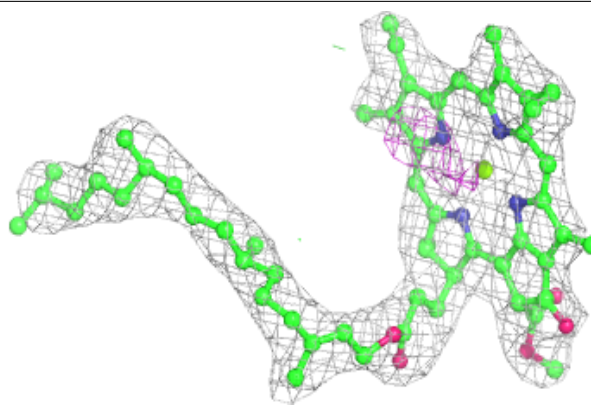
**Electron density around CLA b 603:**

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

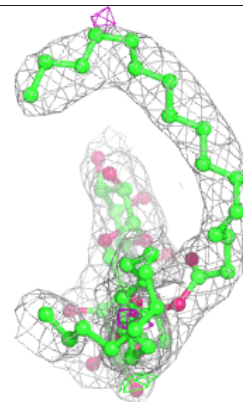
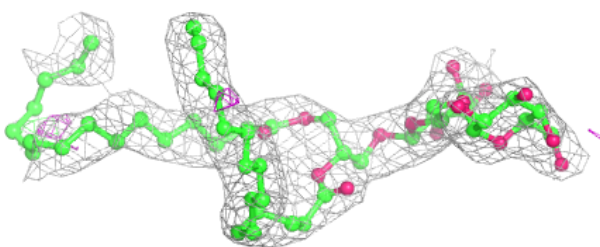
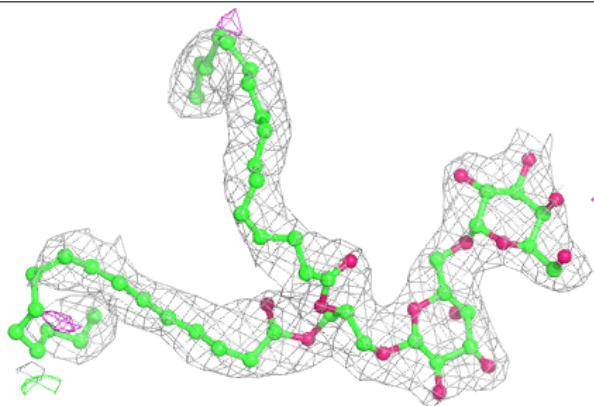


Electron density around CLA c 513:

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

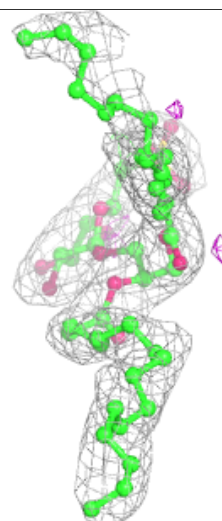
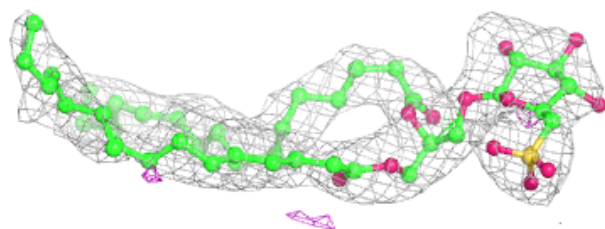
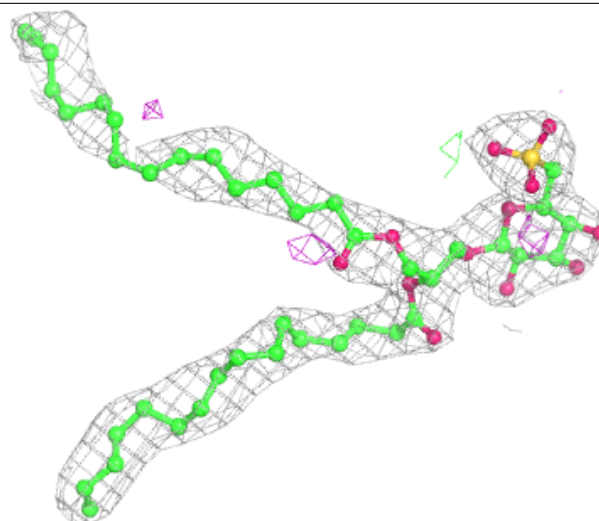
**Electron density around DGD c 519:**

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



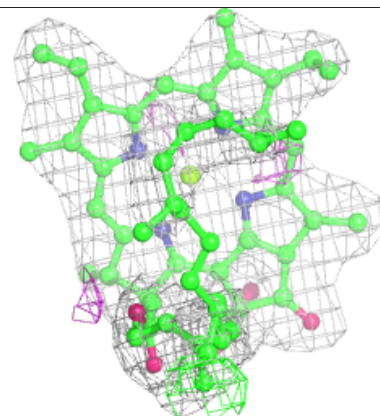
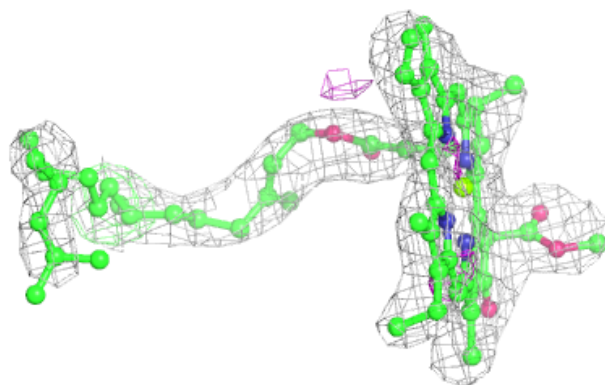
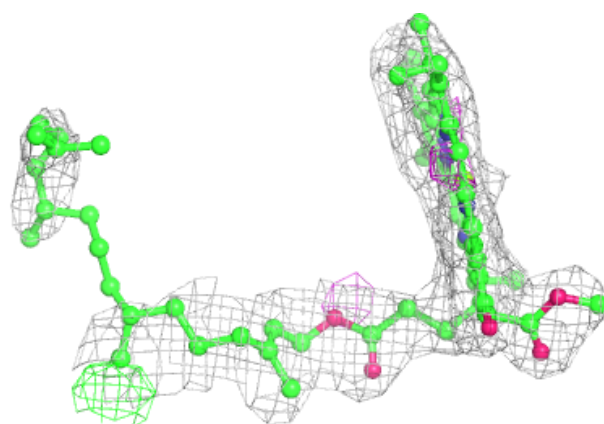
Electron density around SQD a 409:

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



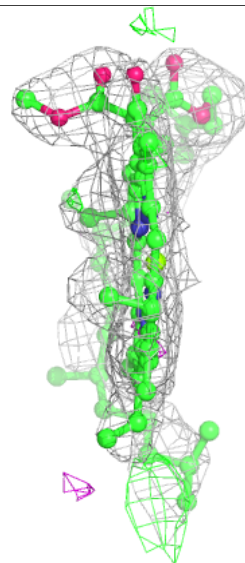
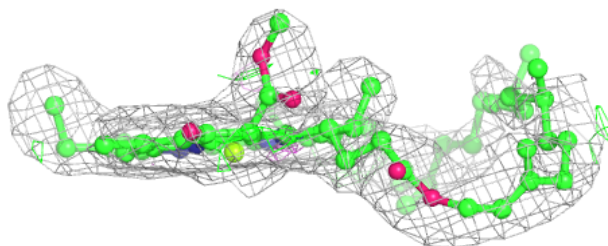
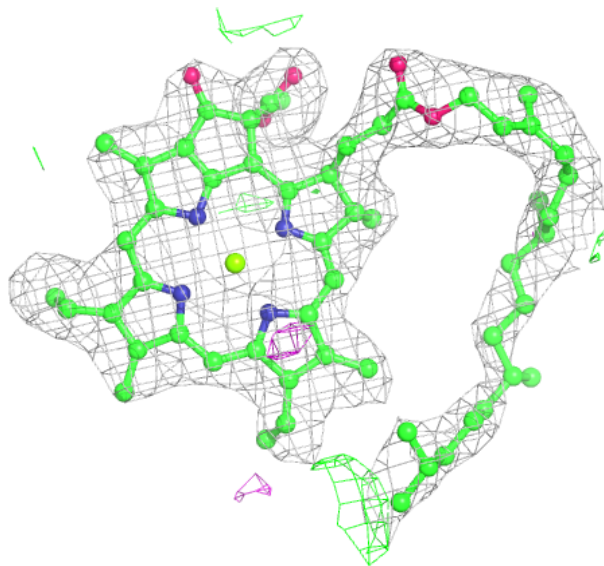
Electron density around CLA c 508:

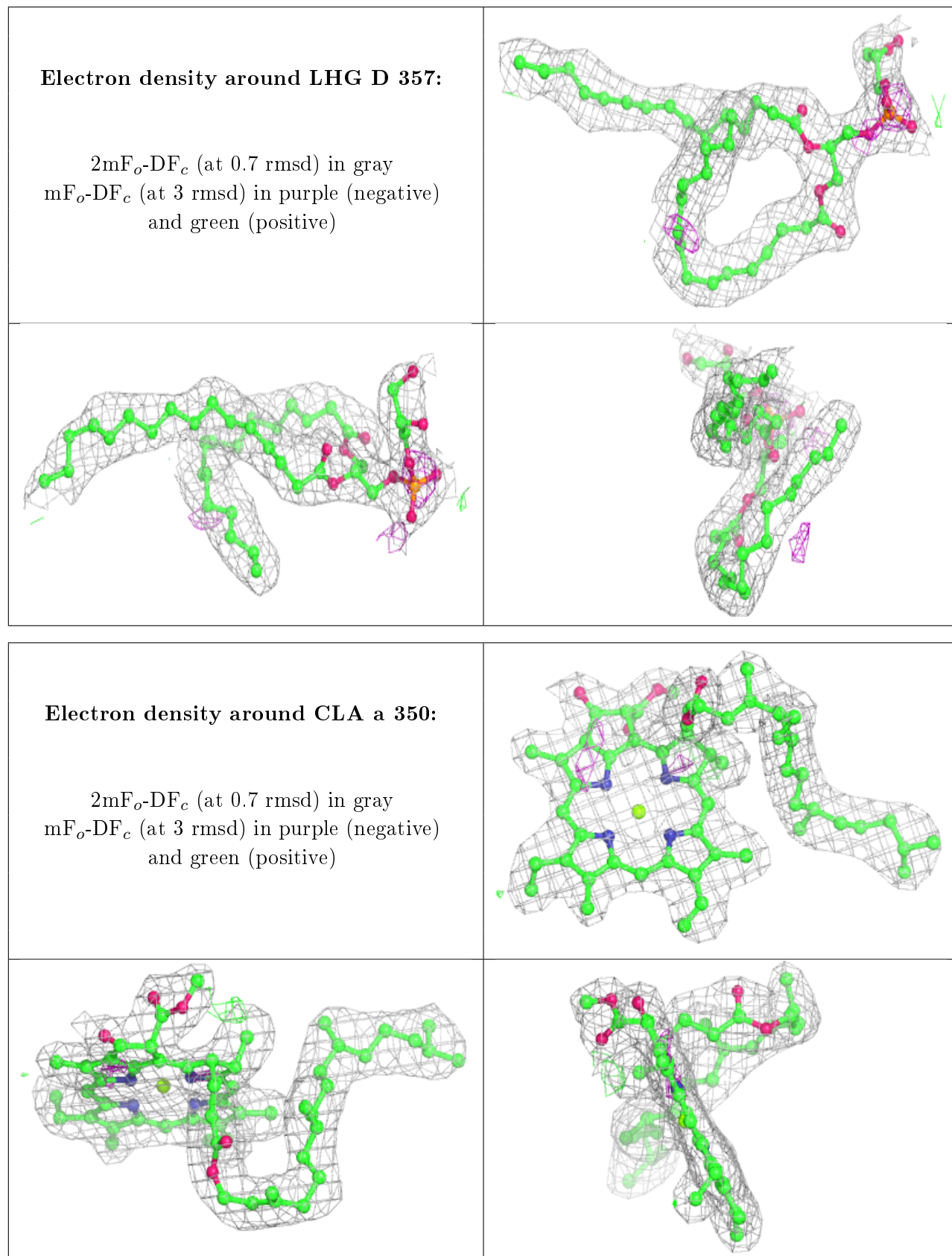
$2mF_o-DF_c$ (at 0.7 rnsd) in gray
 mF_o-DF_c (at 3 rnsd) in purple (negative)
and green (positive)



Electron density around CLA C 513:

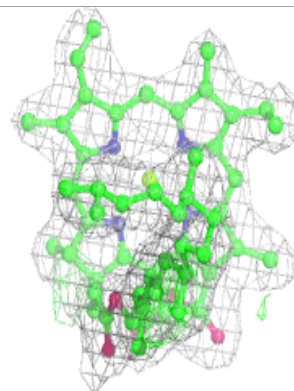
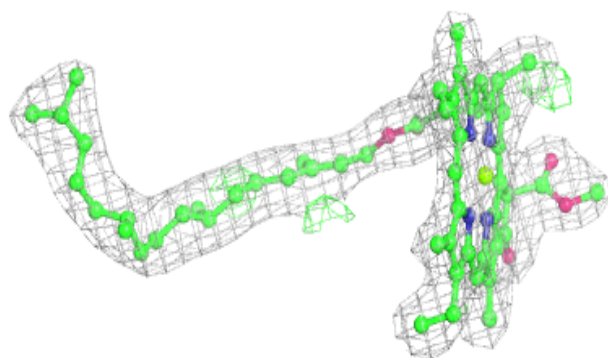
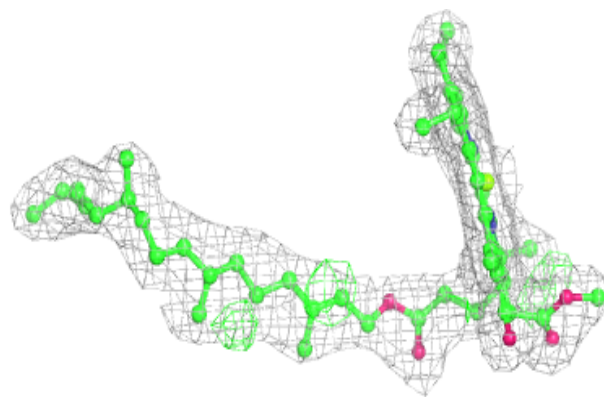
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



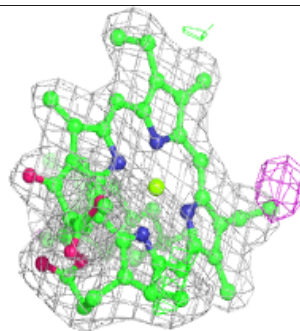
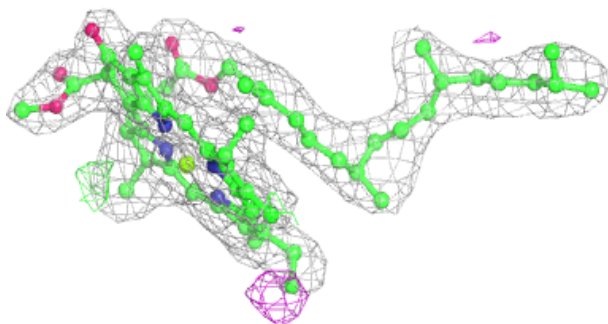
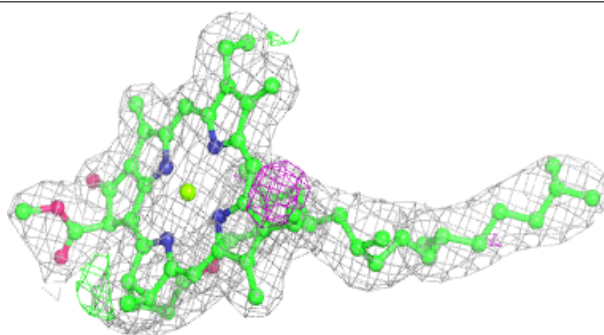


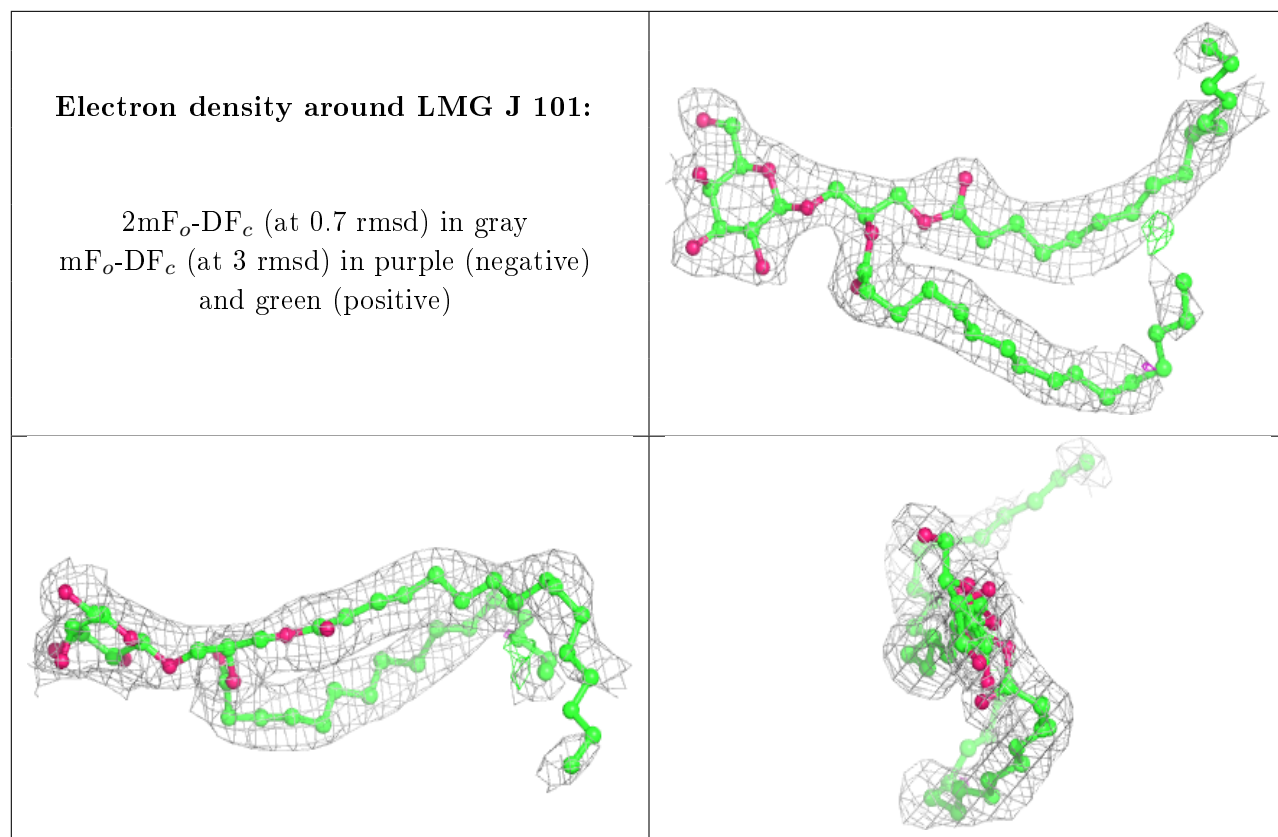
Electron density around CLA B 605:

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

**Electron density around CLA C 506:**

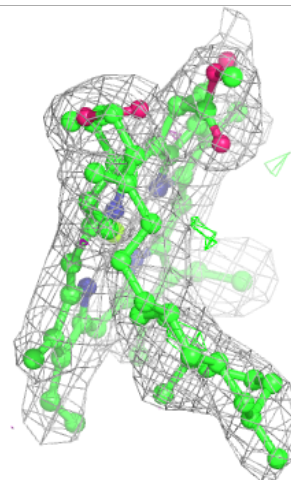
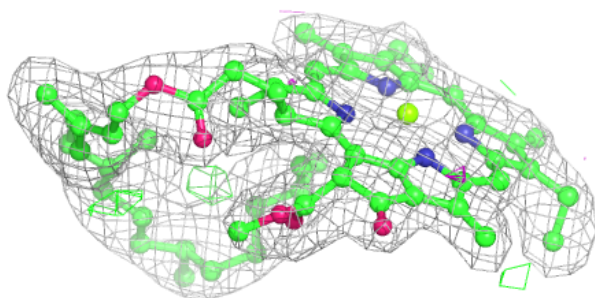
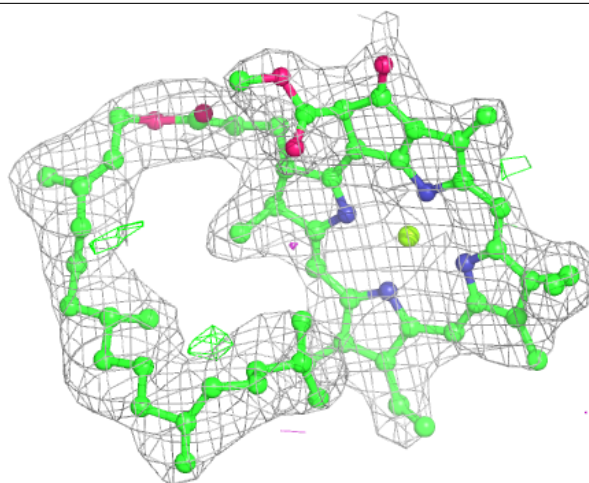
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





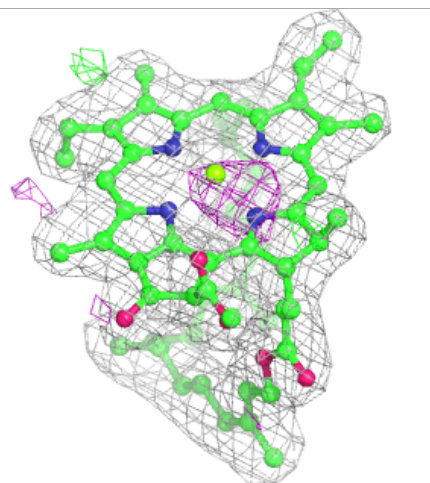
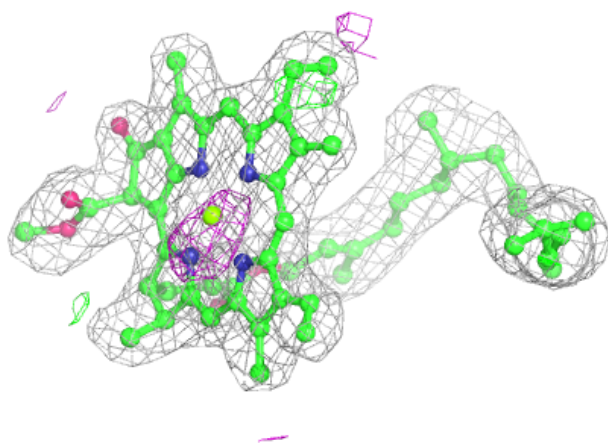
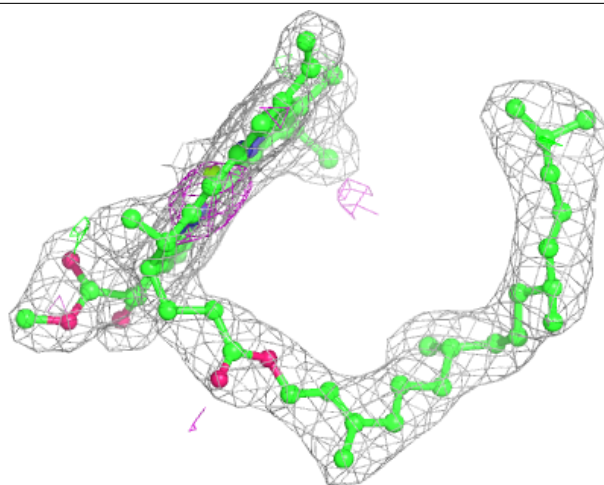
Electron density around CLA b 615:

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



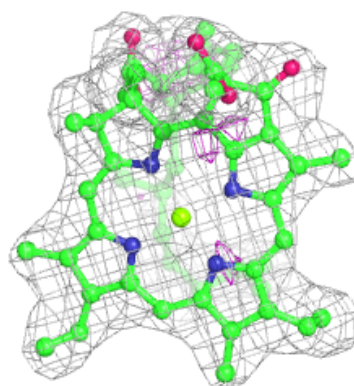
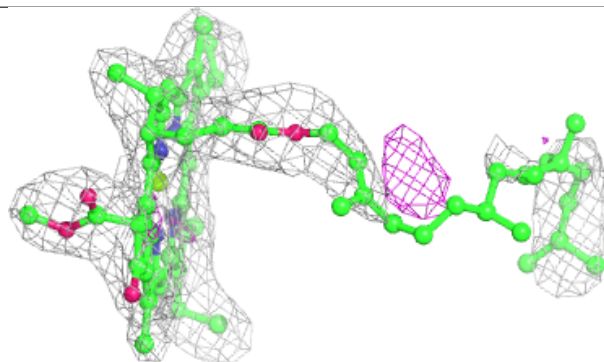
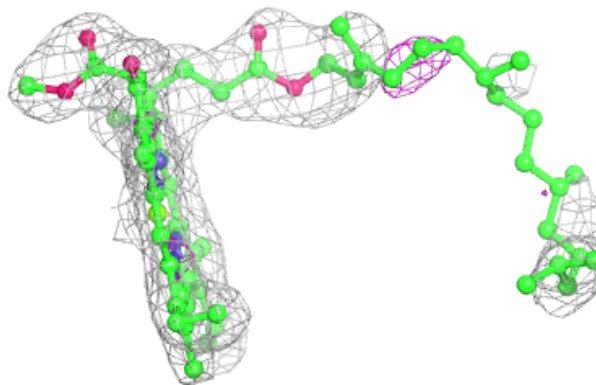
Electron density around CLA B 611:

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

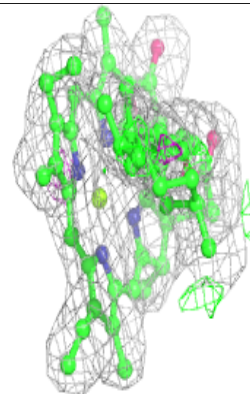
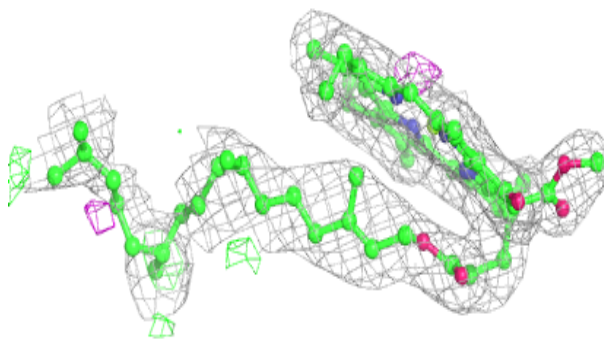
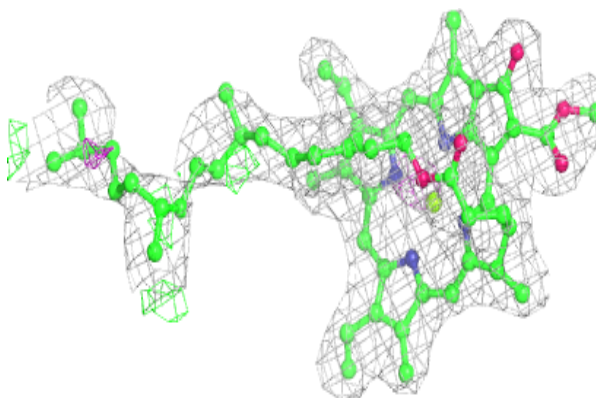


Electron density around CLA C 507:

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

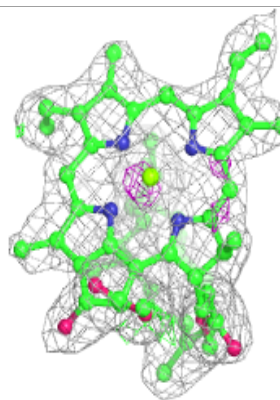
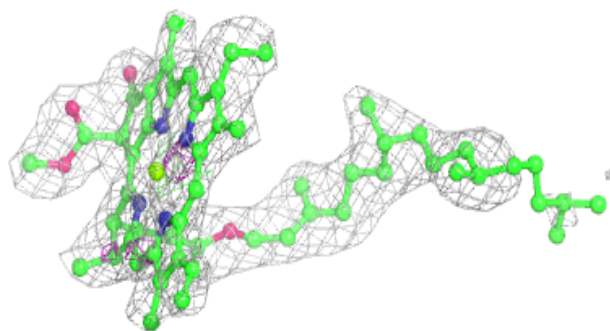
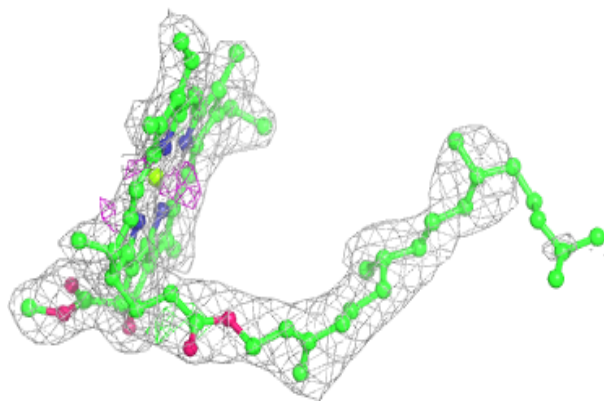
**Electron density around CLA b 614:**

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

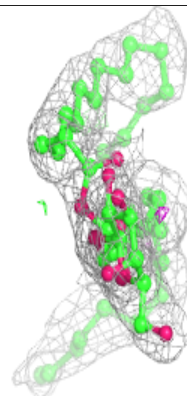
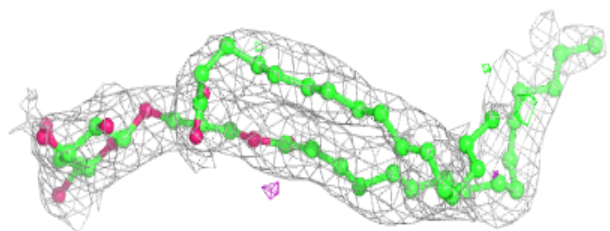
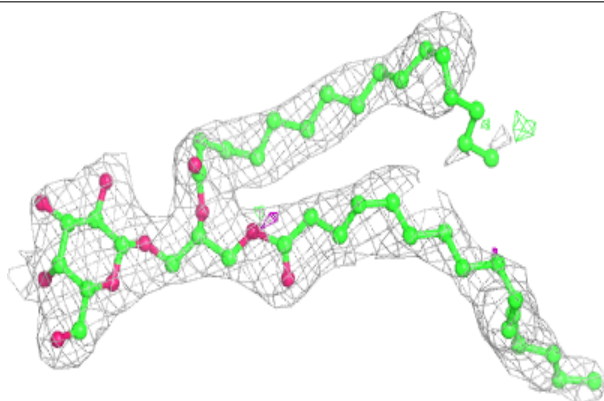


Electron density around CLA c 510:

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

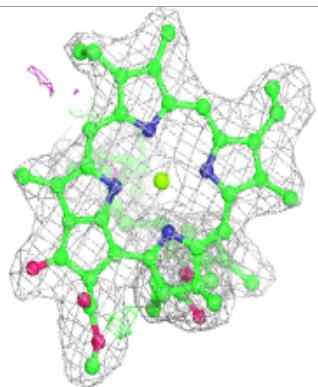
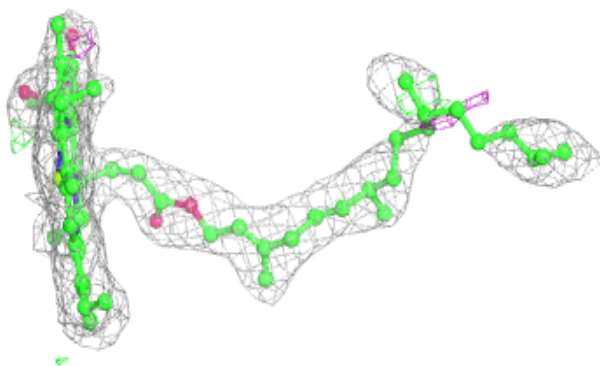
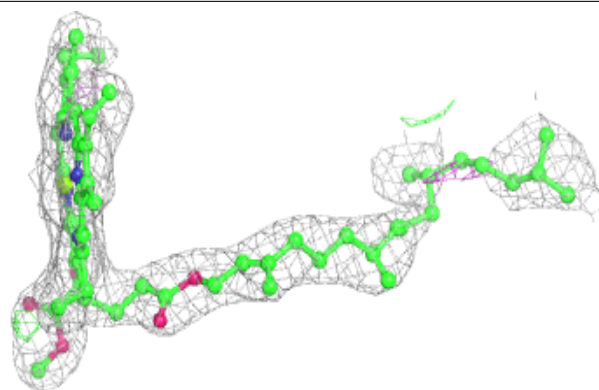
**Electron density around LMG j 101:**

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

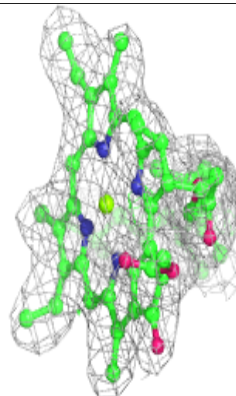
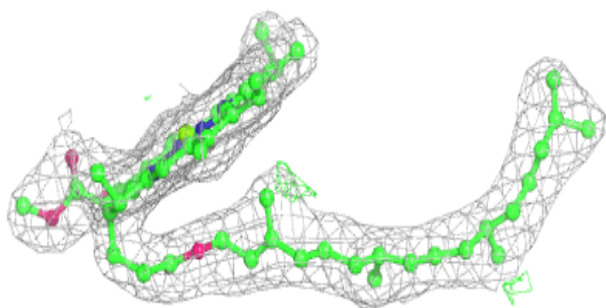
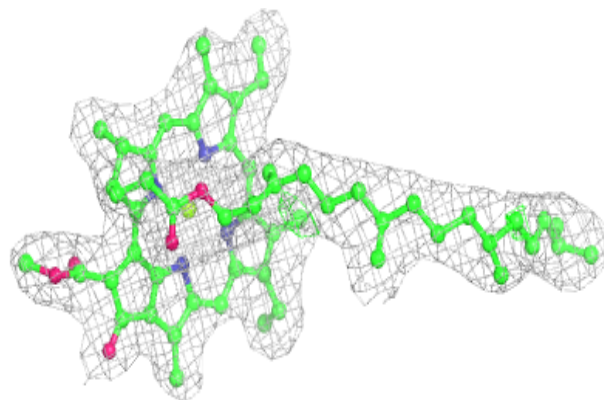


Electron density around CLA B 606:

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

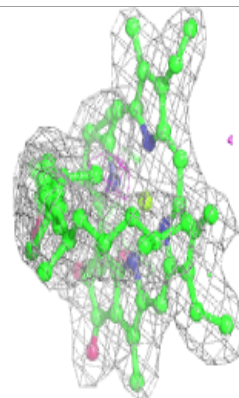
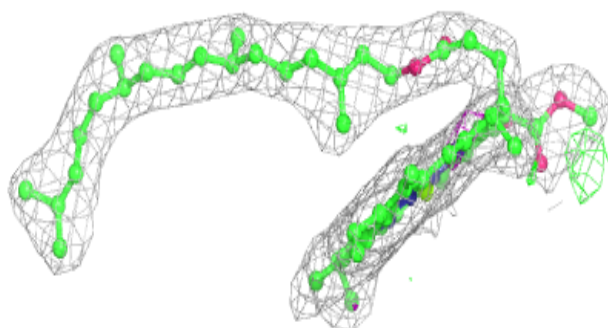
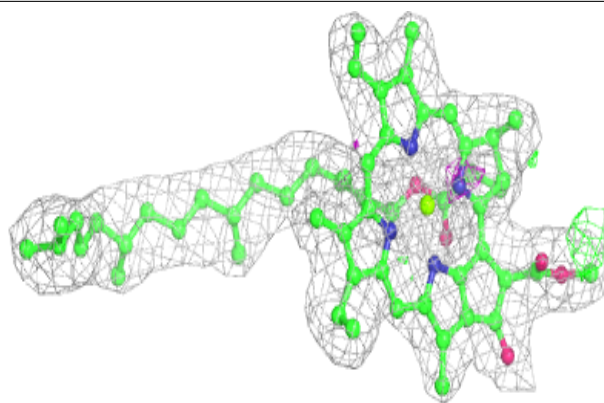
**Electron density around CLA B 608:**

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

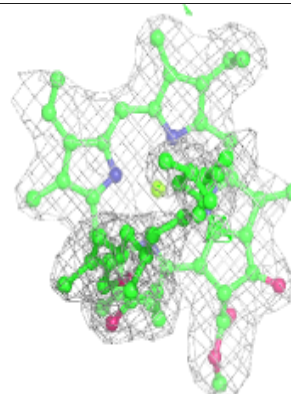
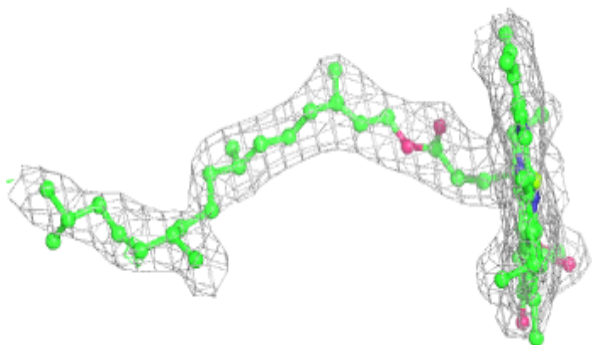
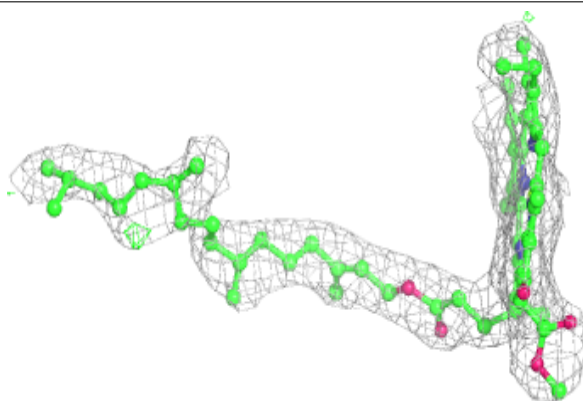


Electron density around CLA b 608:

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

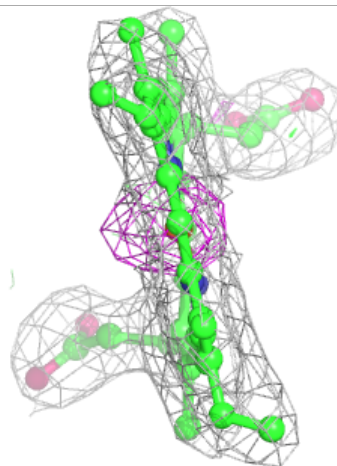
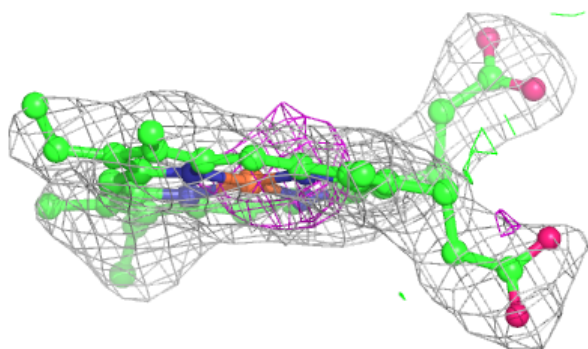
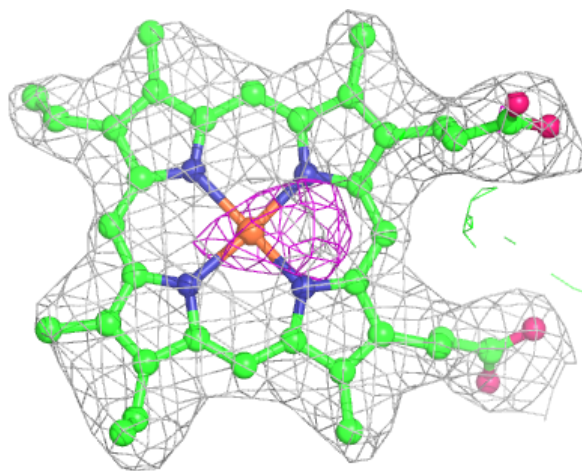
**Electron density around CLA b 606:**

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



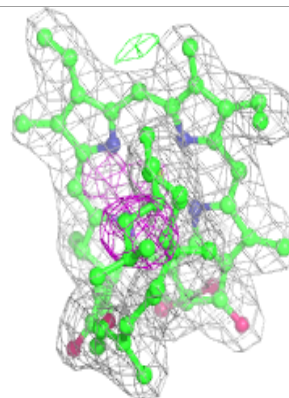
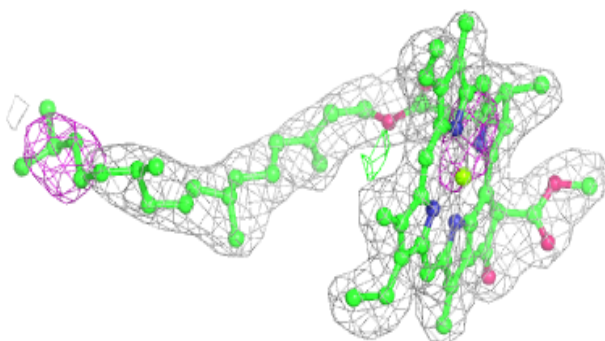
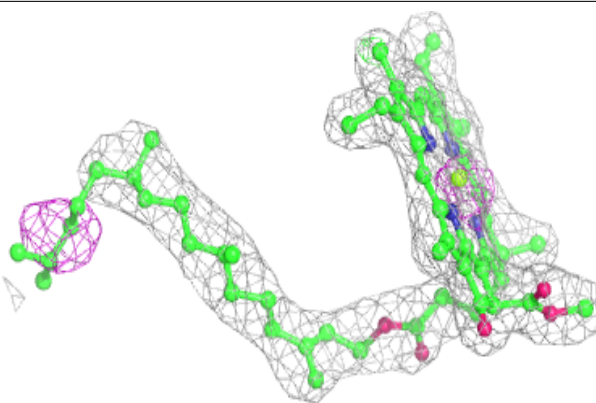
Electron density around HEM E 103:

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

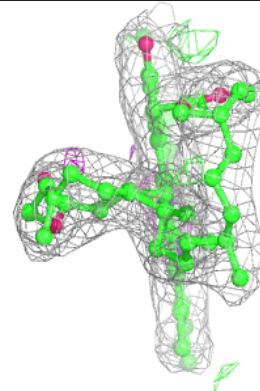
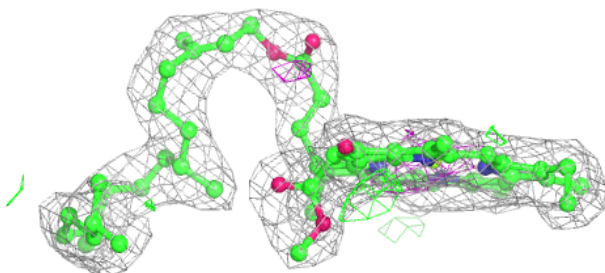
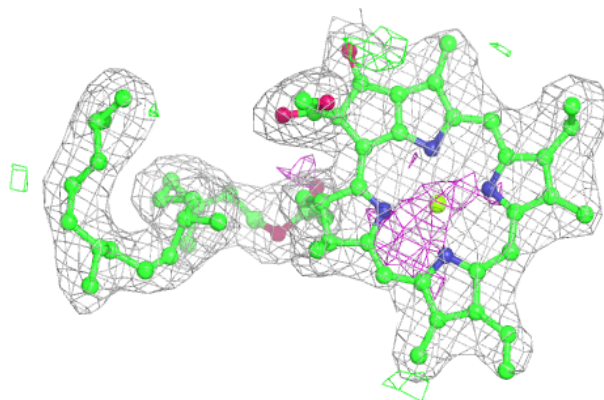


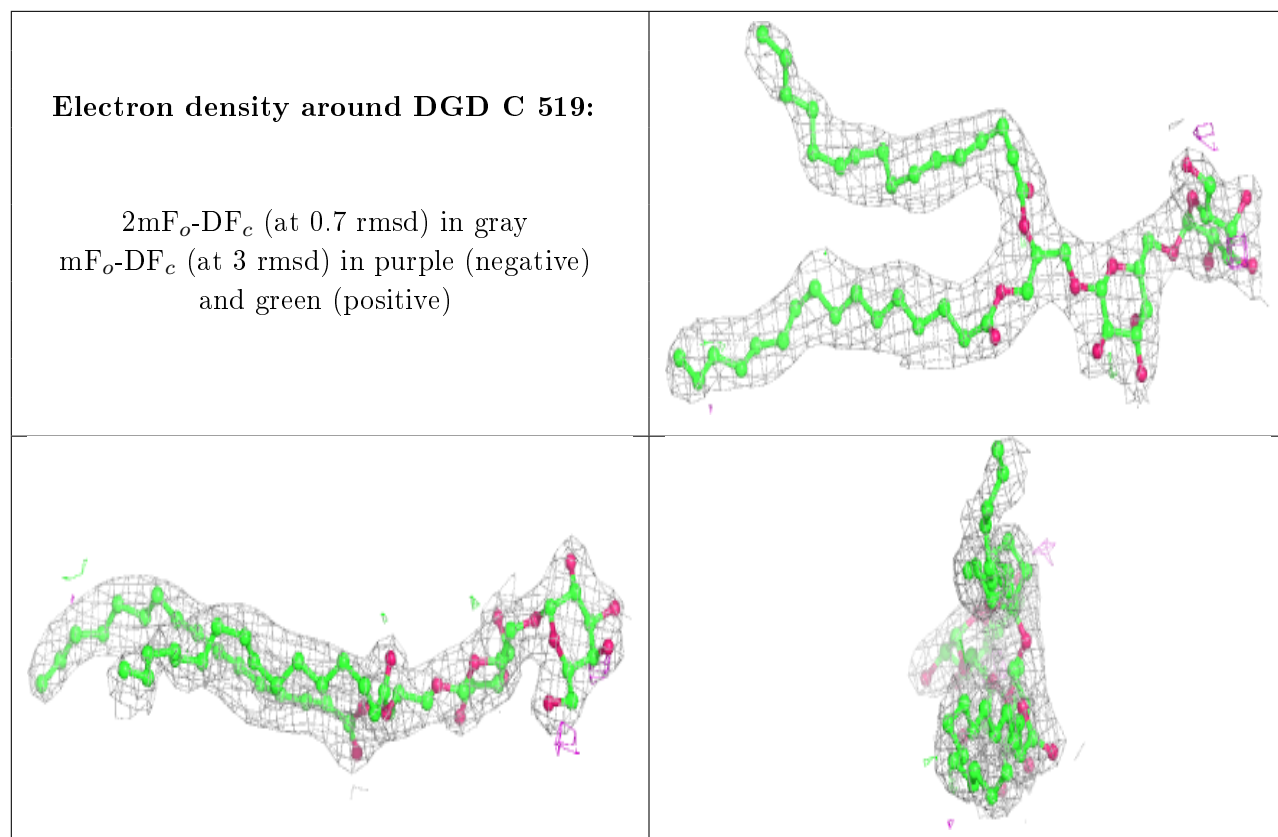
Electron density around CLA C 509:

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

**Electron density around CLA B 612:**

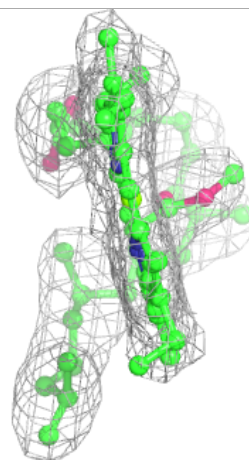
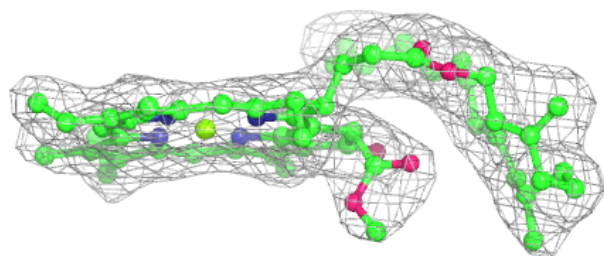
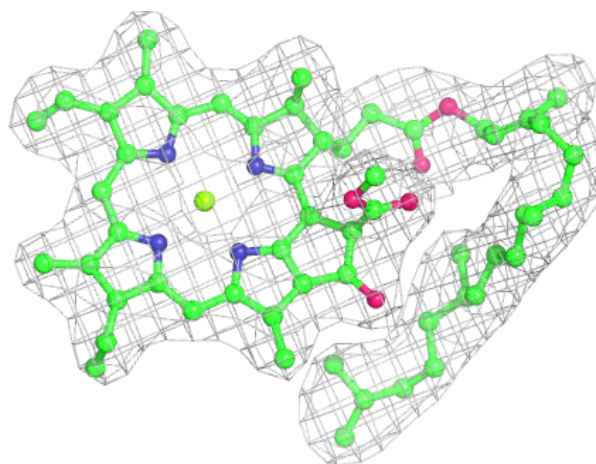
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





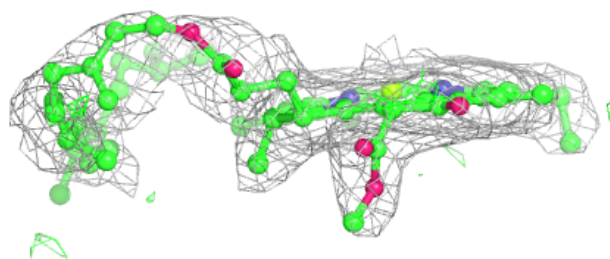
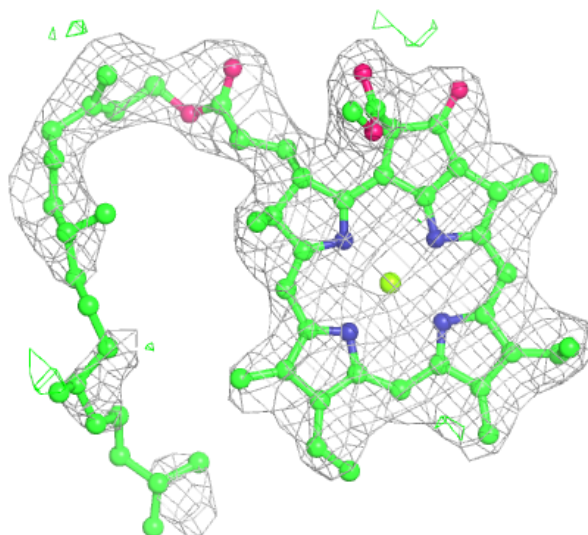
Electron density around CLA b 610:

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



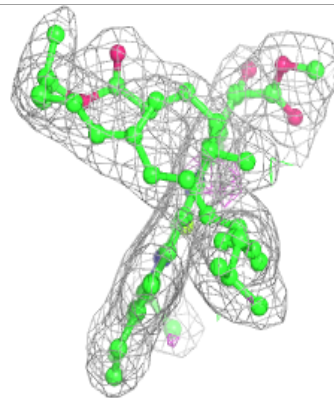
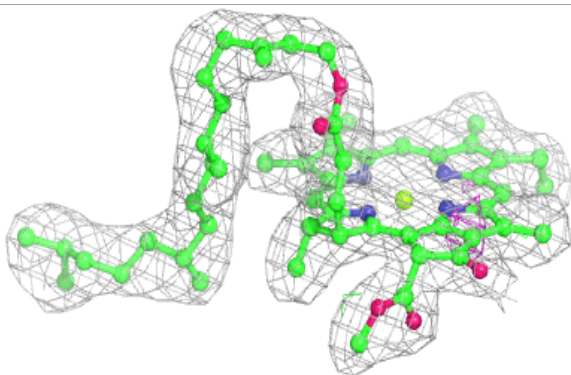
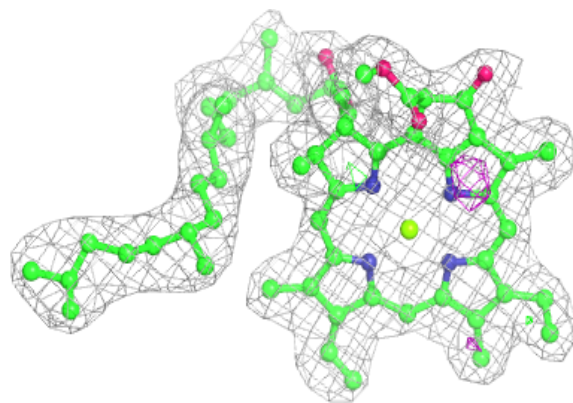
Electron density around CLA c 514:

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

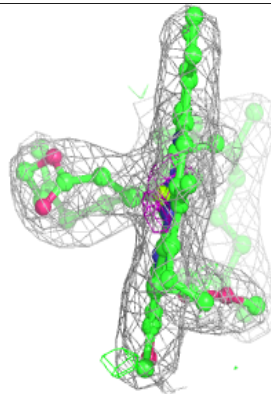
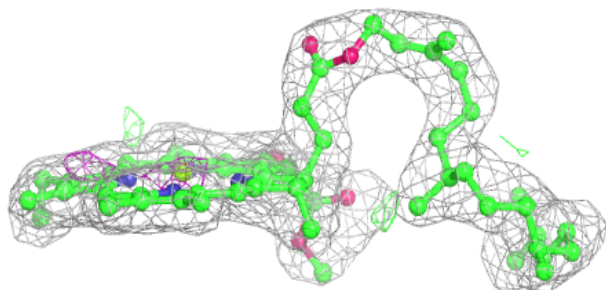
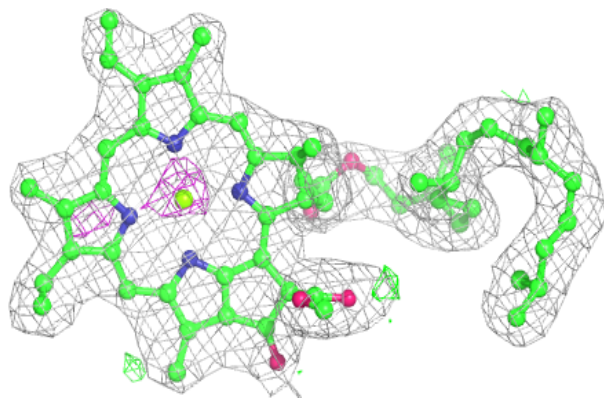


Electron density around CLA A 405:

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

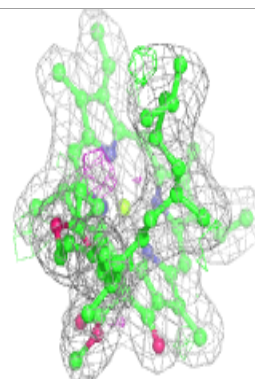
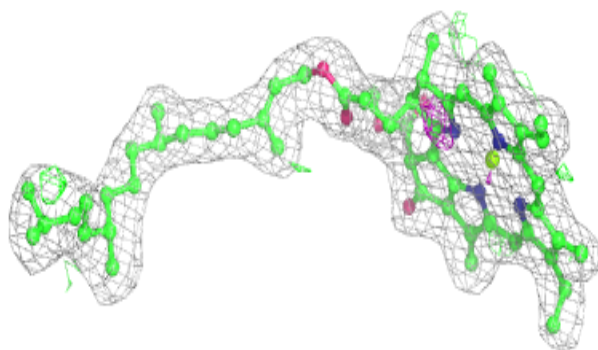
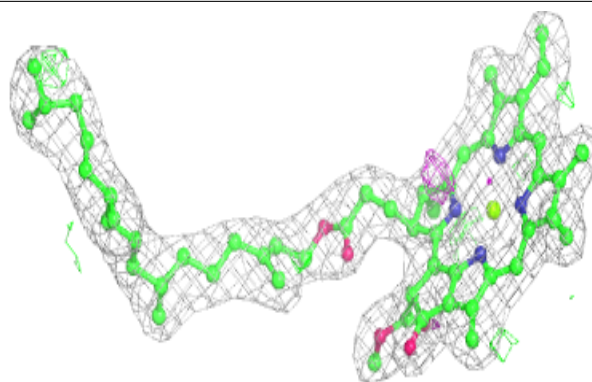
**Electron density around CLA b 612:**

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

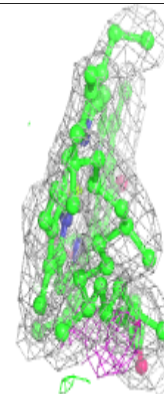
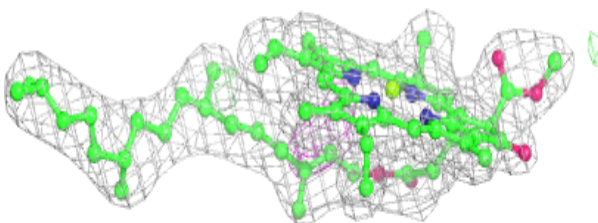
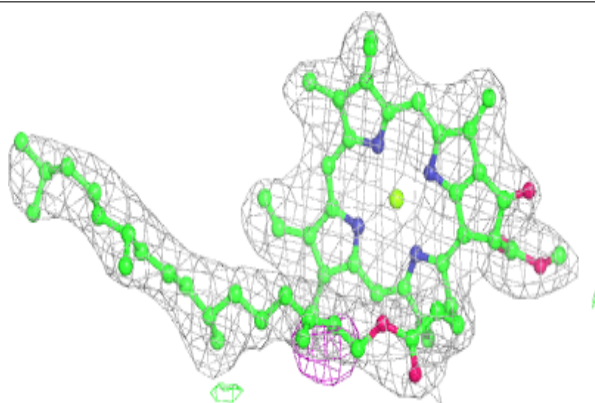


Electron density around CLA A 404:

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

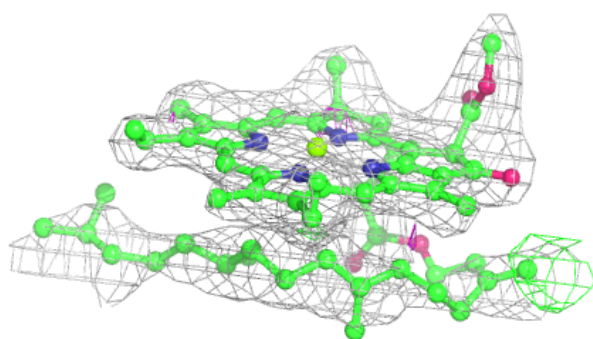
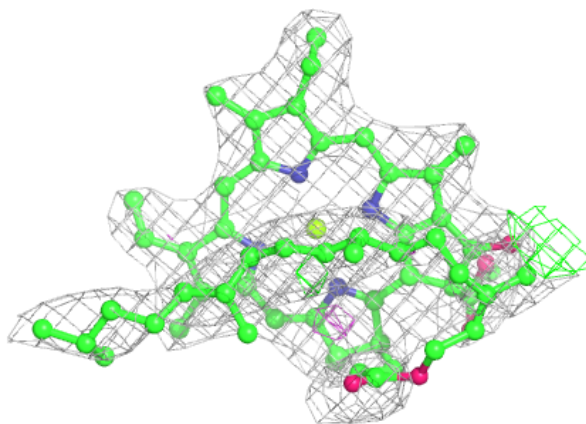
**Electron density around CLA C 502:**

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

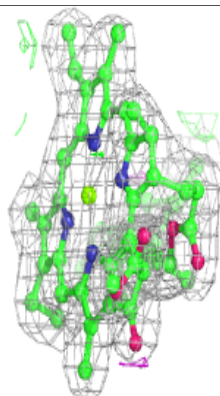
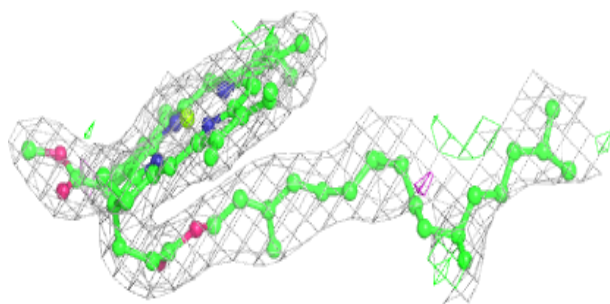
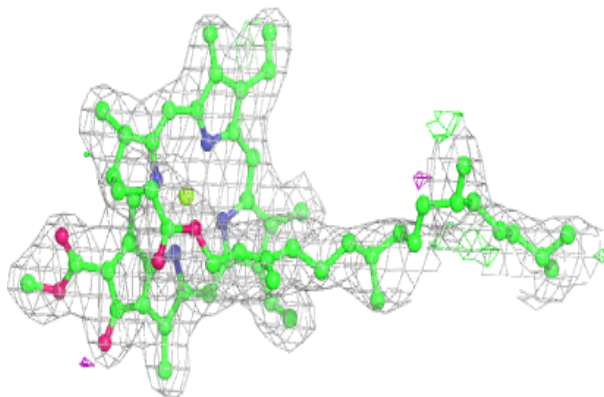


Electron density around CLA B 601:

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

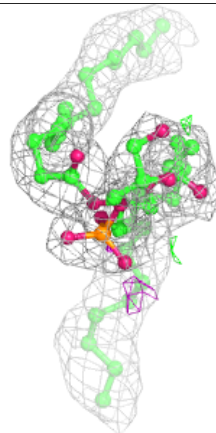
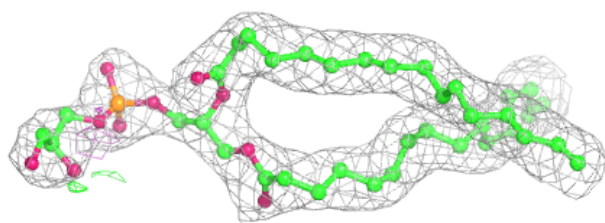
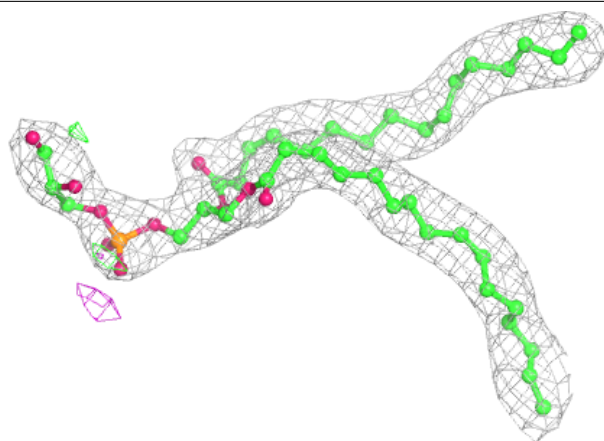
**Electron density around CLA B 614:**

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

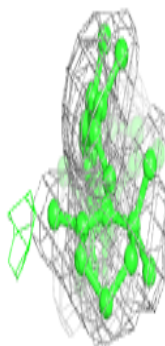
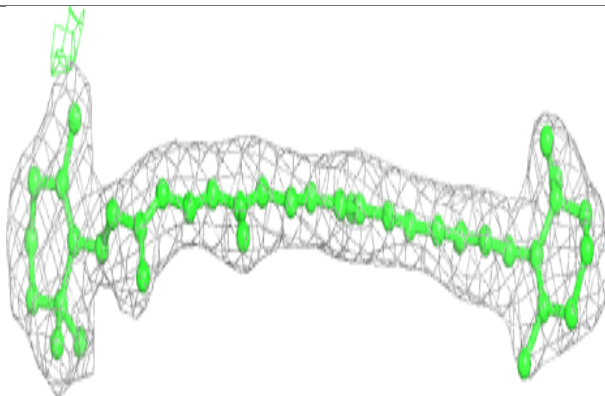
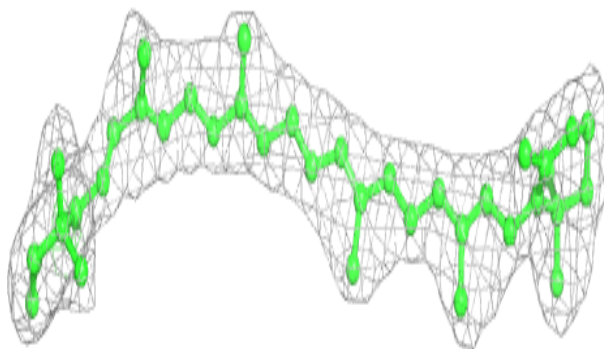


Electron density around LHG d 407:

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

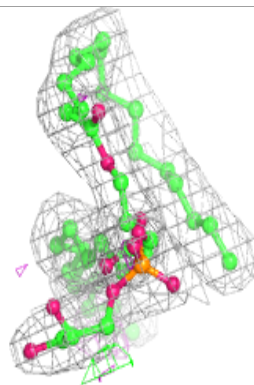
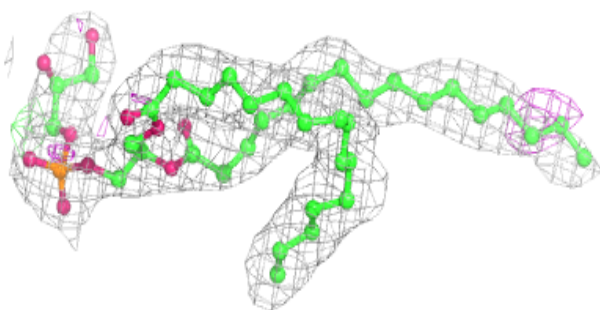
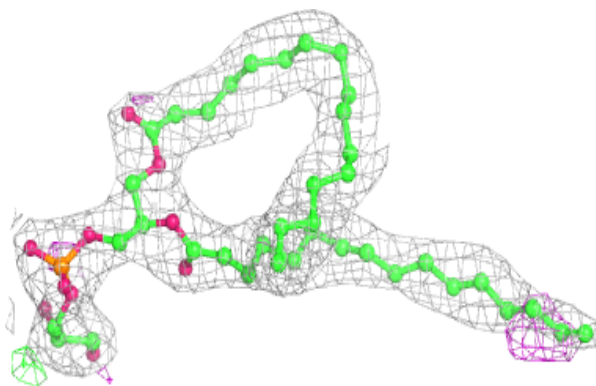
**Electron density around BCR H 101:**

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



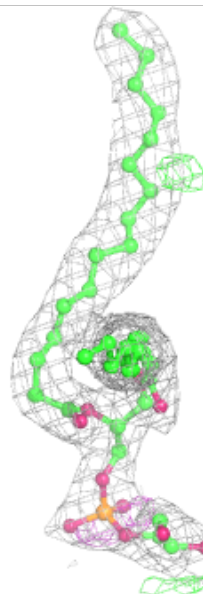
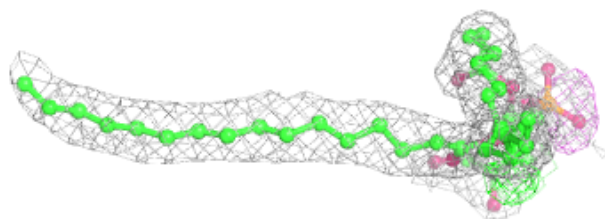
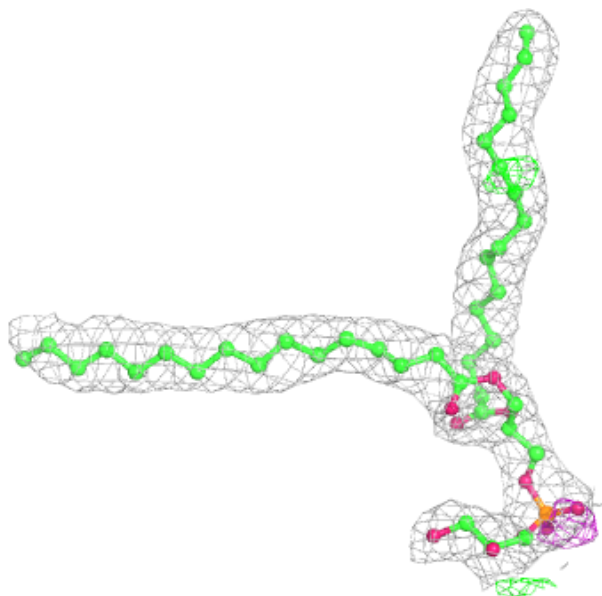
Electron density around LHG d 406:

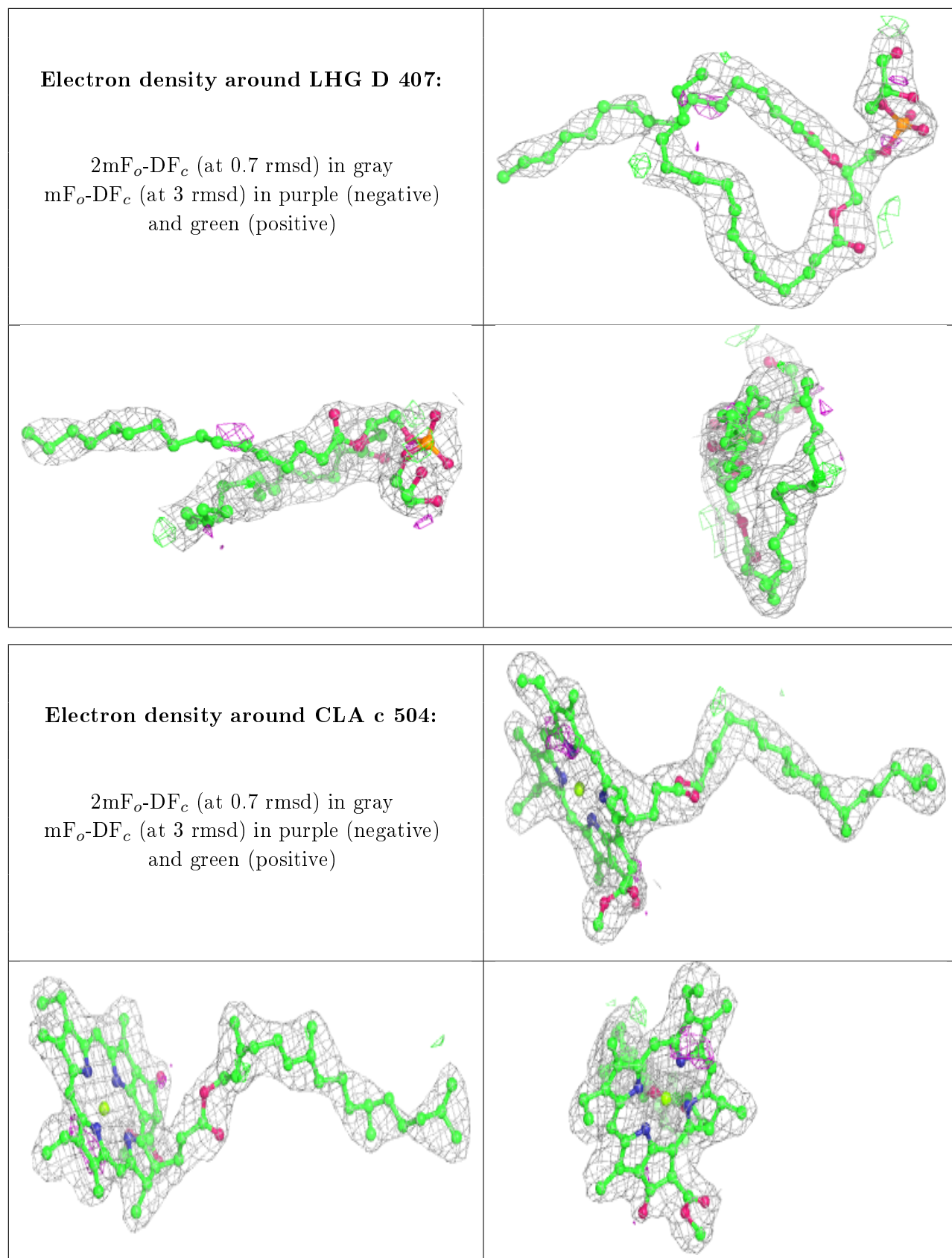
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LHG L 101:

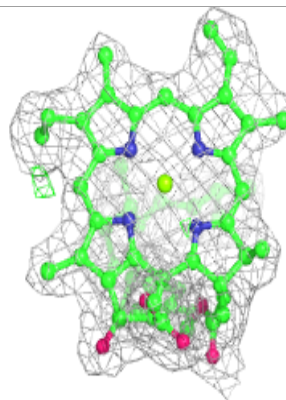
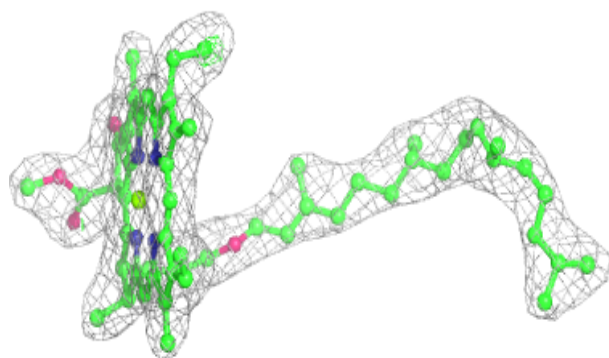
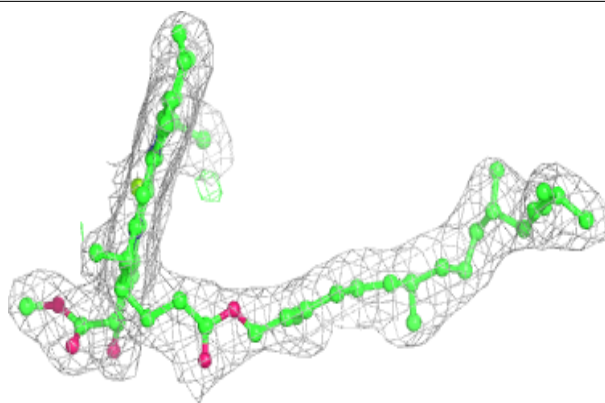
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



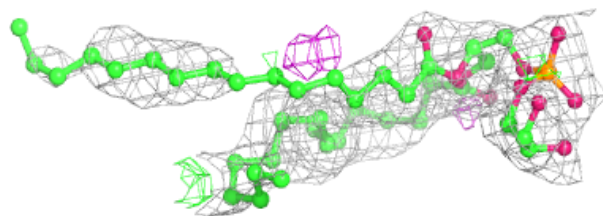
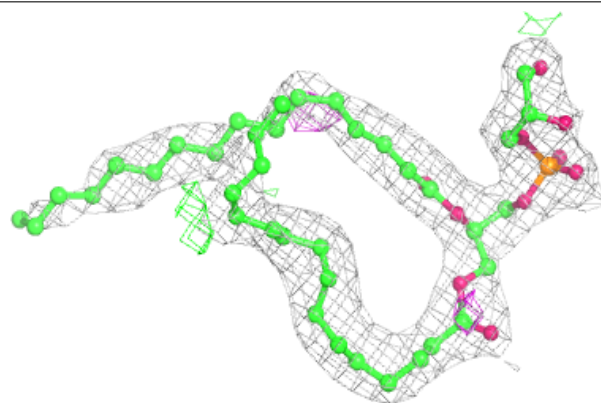


Electron density around CLA b 605:

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

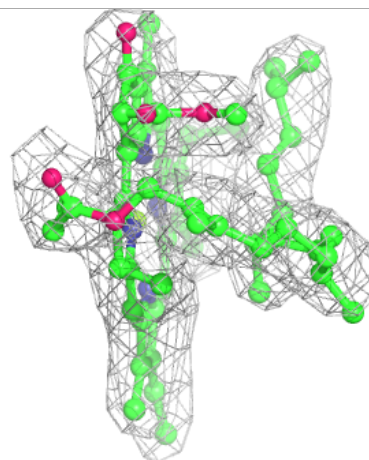
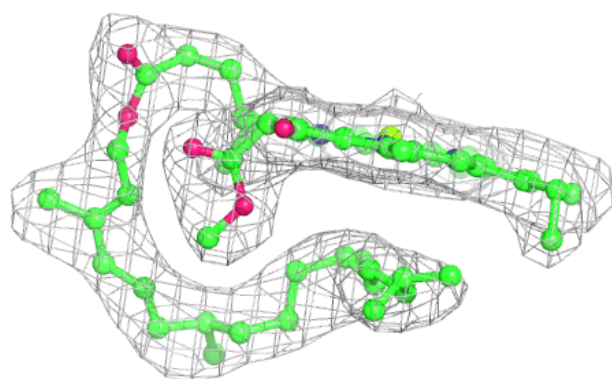
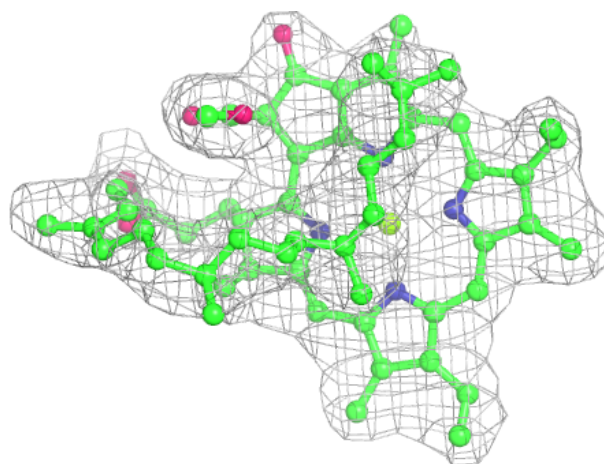
**Electron density around LHG d 408:**

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



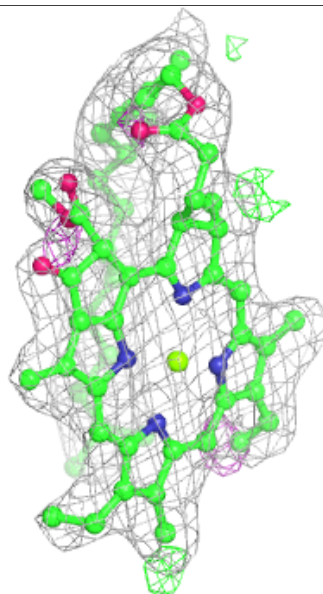
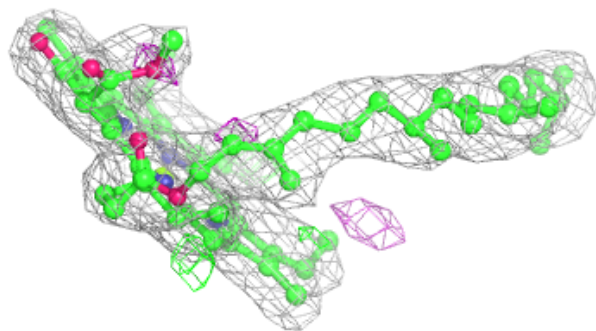
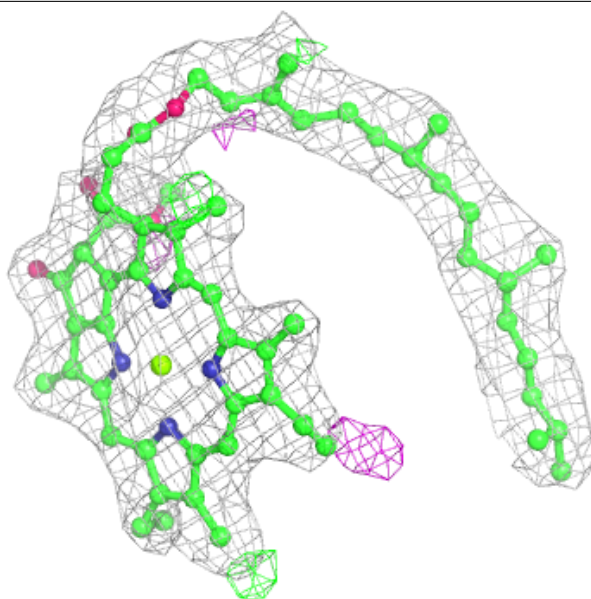
Electron density around CLA C 511:

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



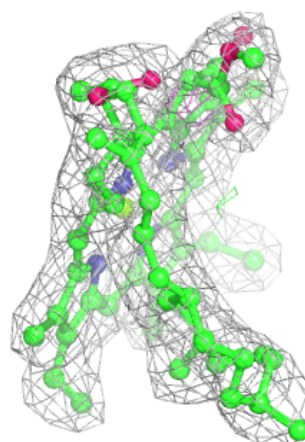
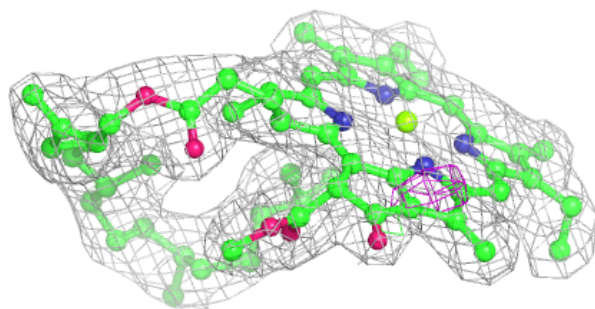
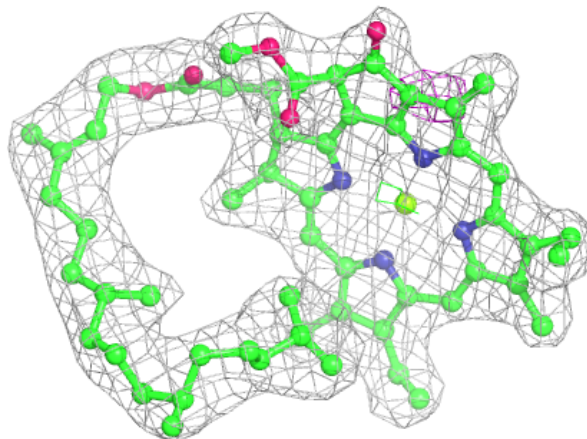
Electron density around CLA c 509:

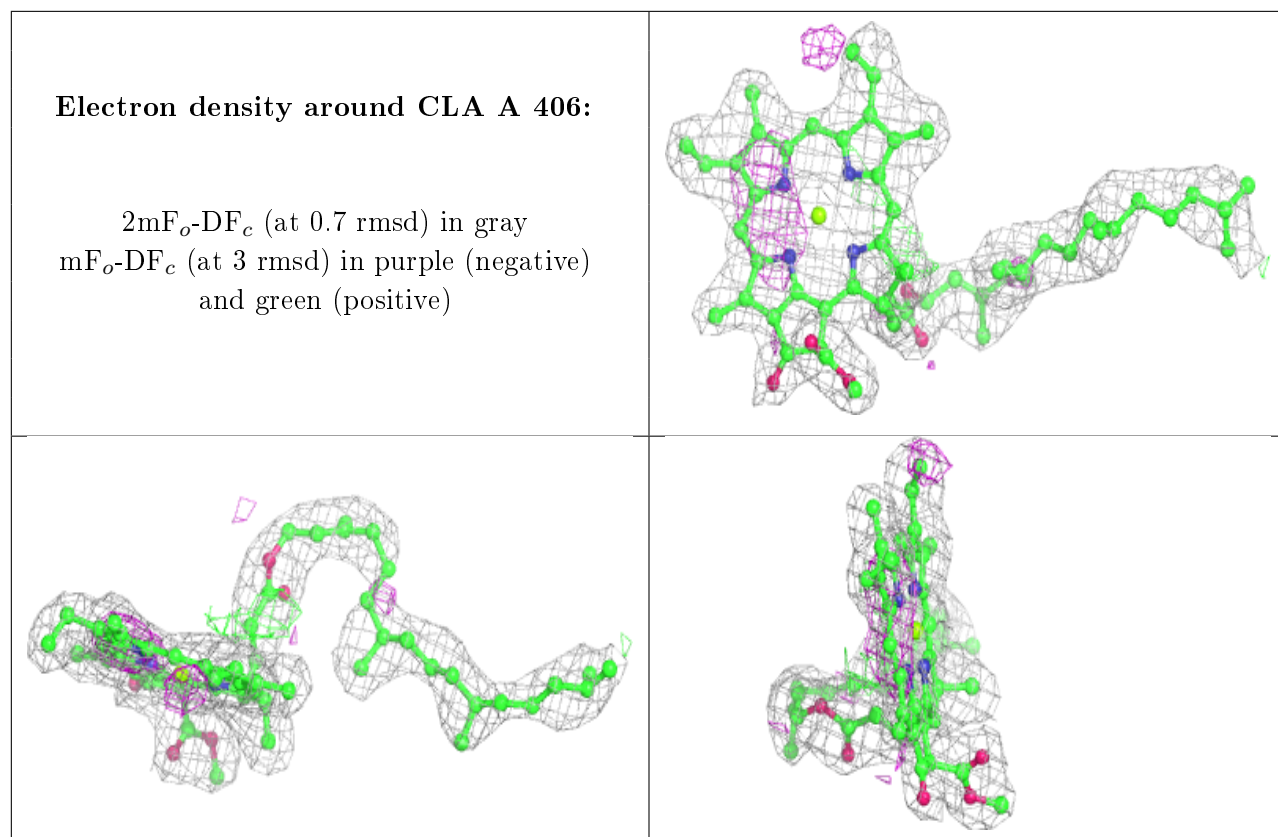
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 615:

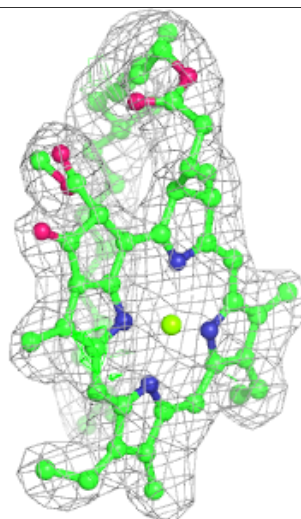
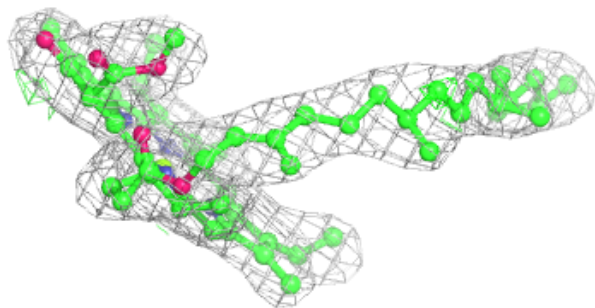
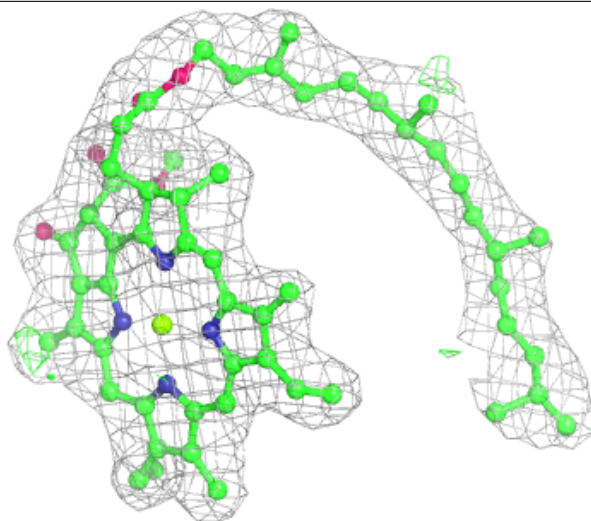
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





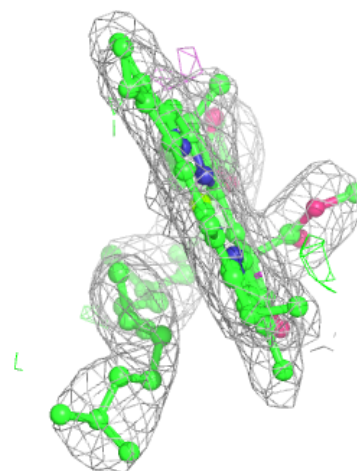
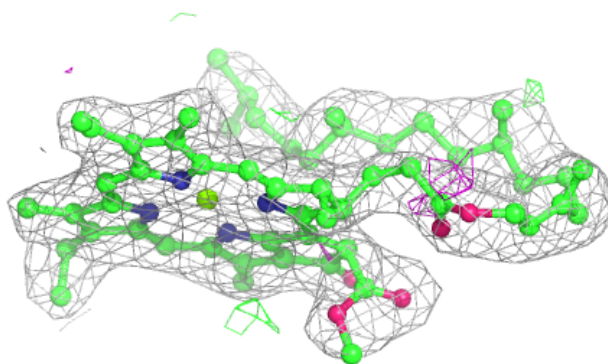
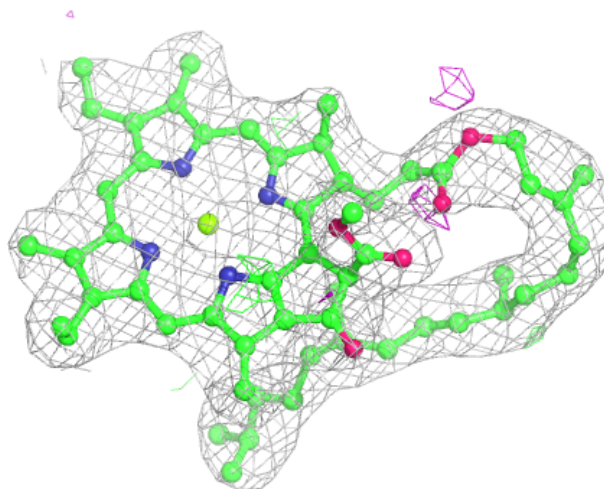
Electron density around CLA C 508:

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



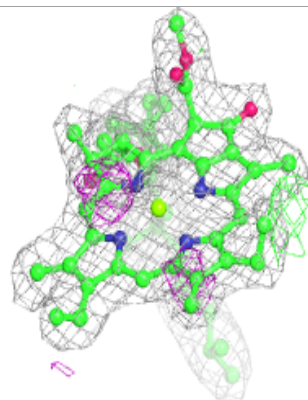
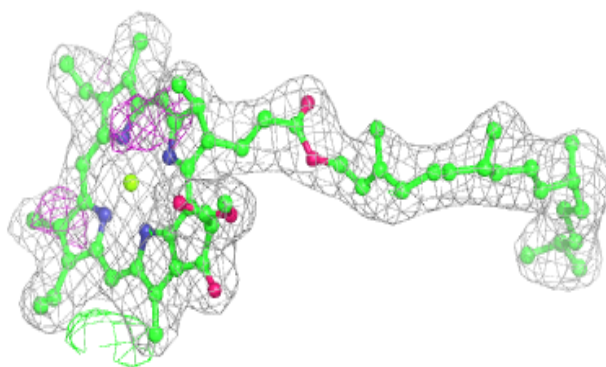
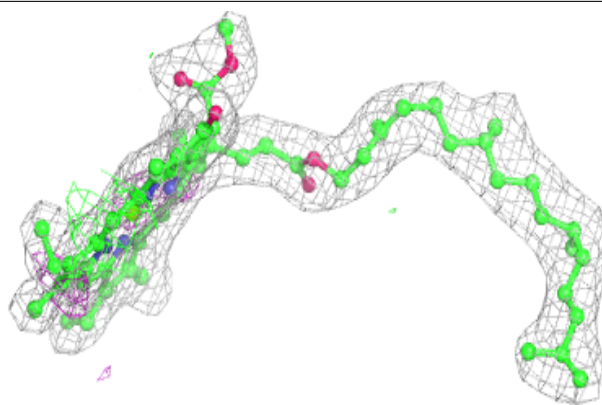
Electron density around CLA c 511:

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

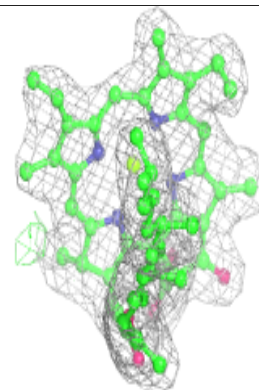
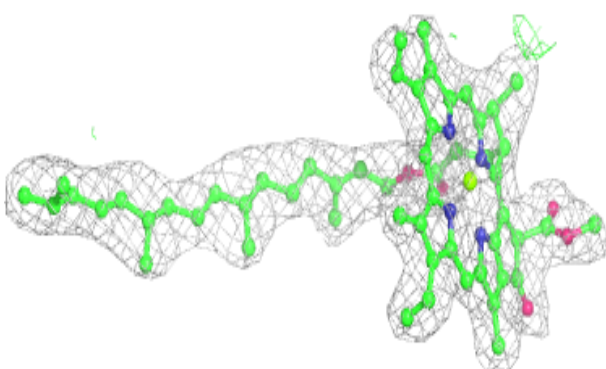
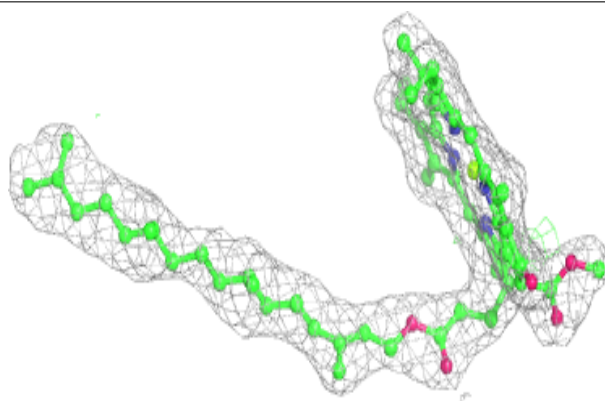


Electron density around CLA D 402:

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

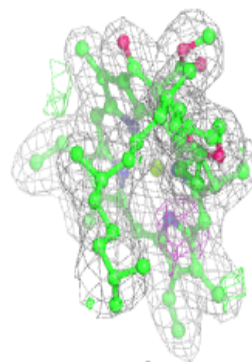
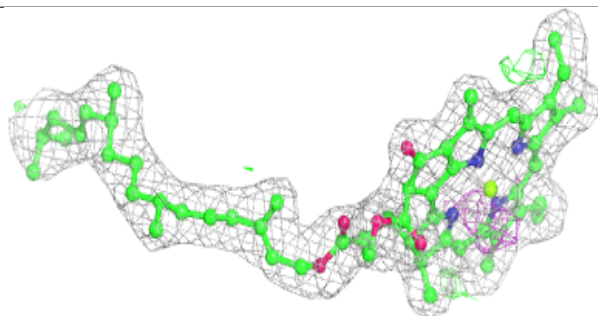
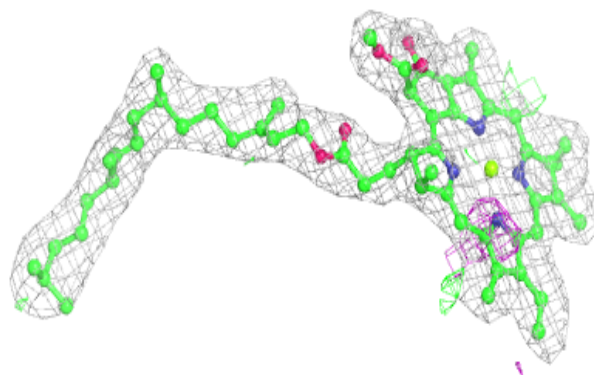
**Electron density around CLA B 607:**

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

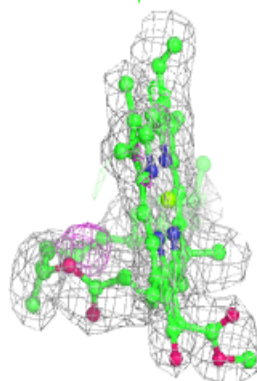
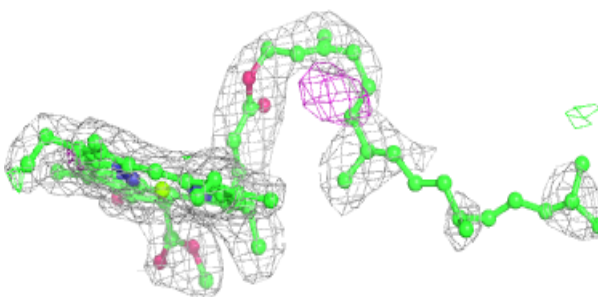
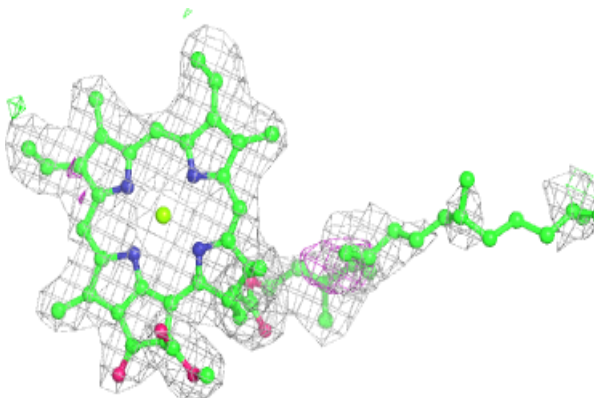


Electron density around CLA a 403:

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

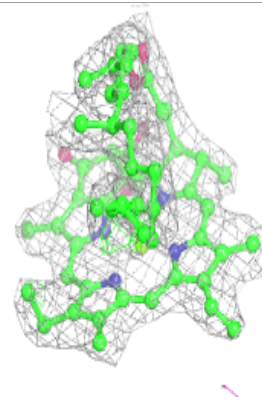
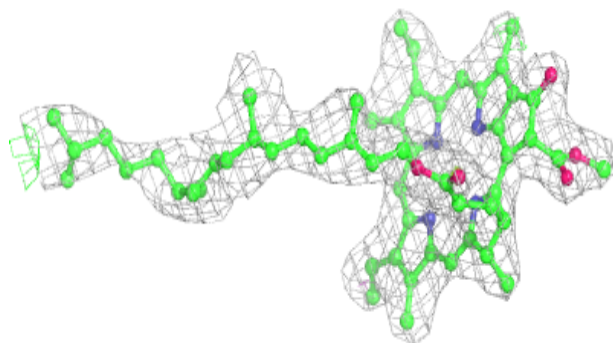
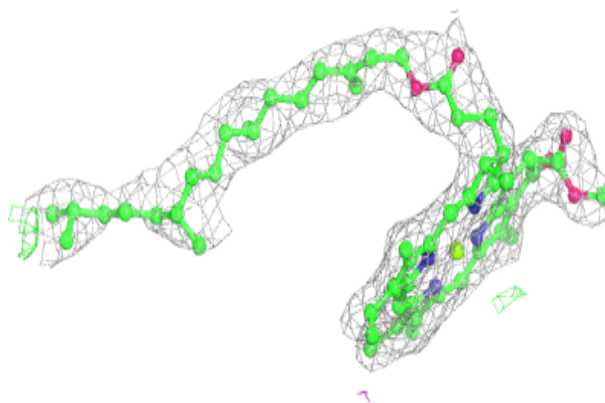
**Electron density around CLA a 404:**

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



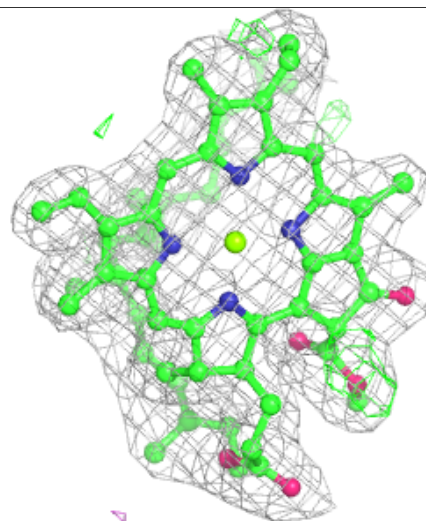
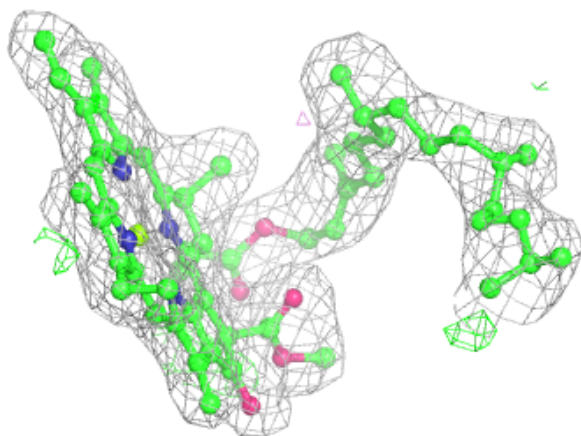
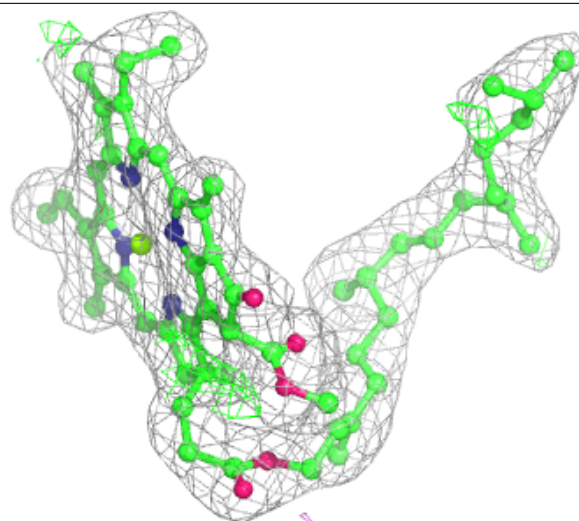
Electron density around CLA c 506:

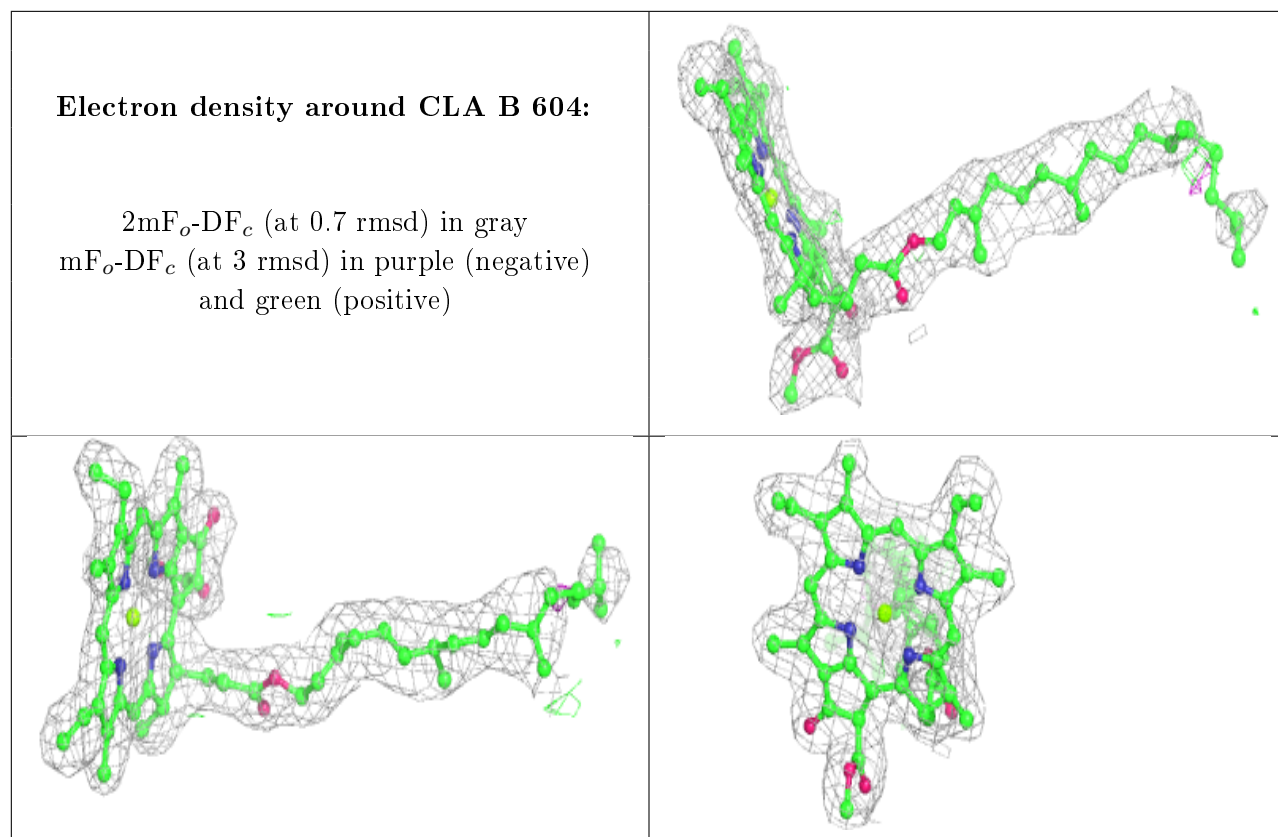
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 613:

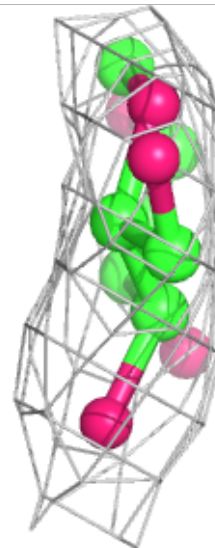
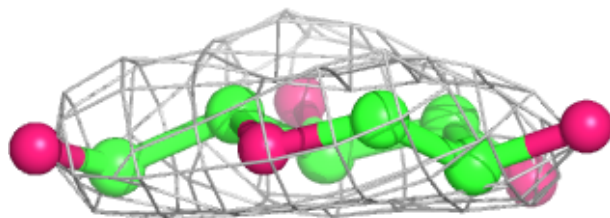
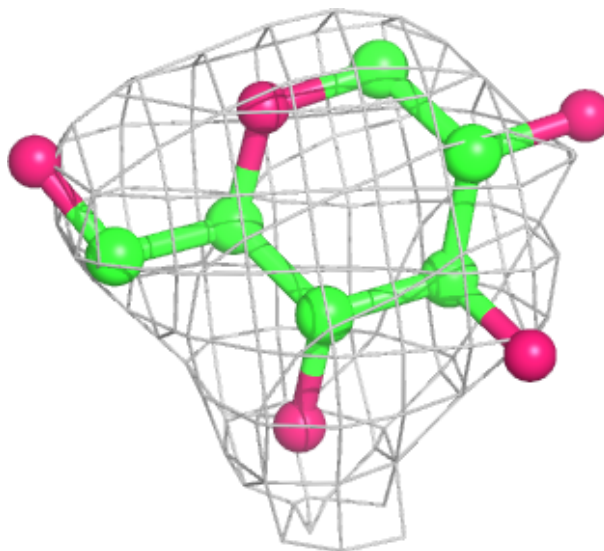
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

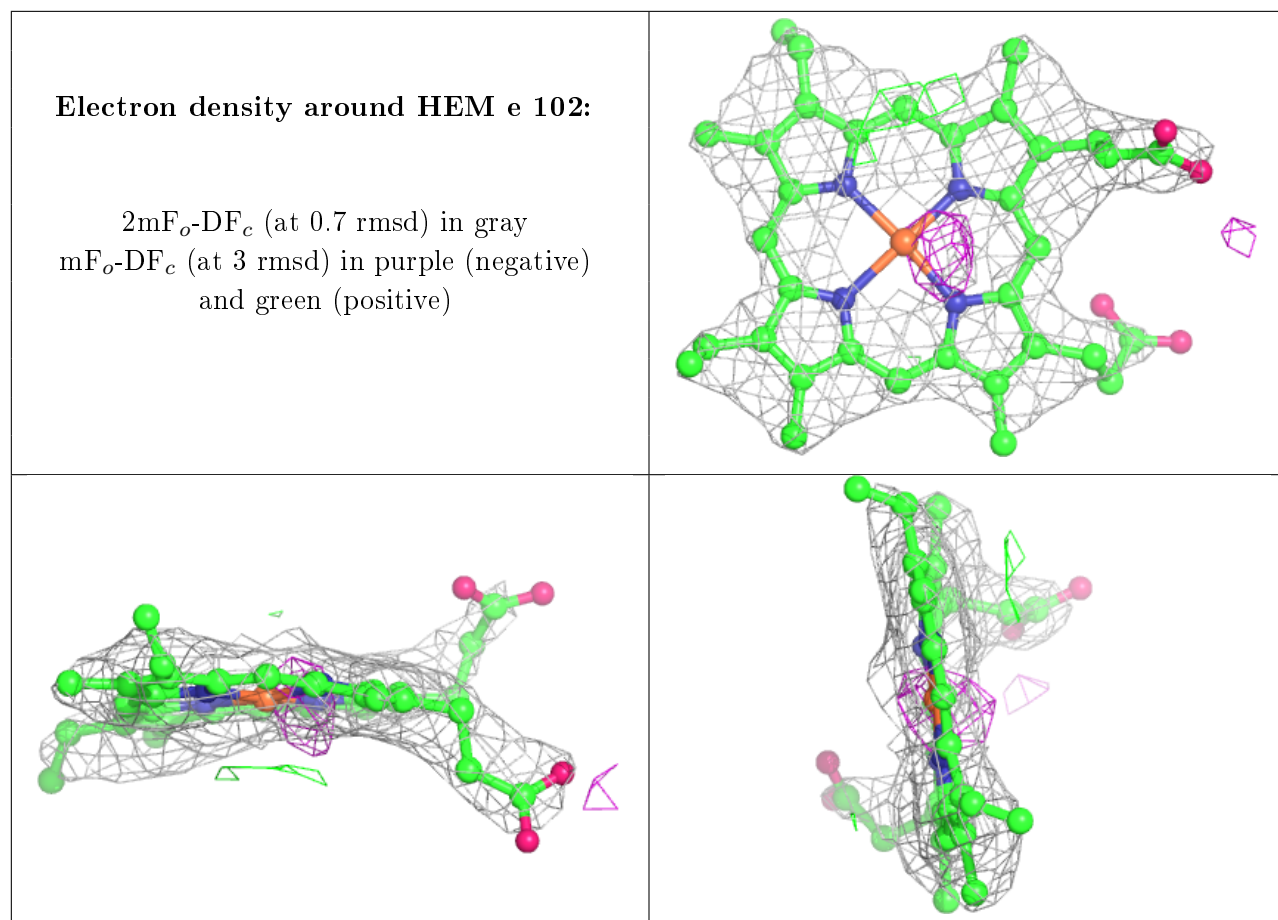




Electron density around HTG V 204:

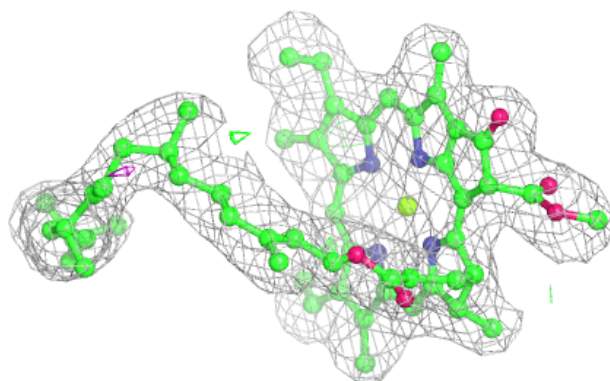
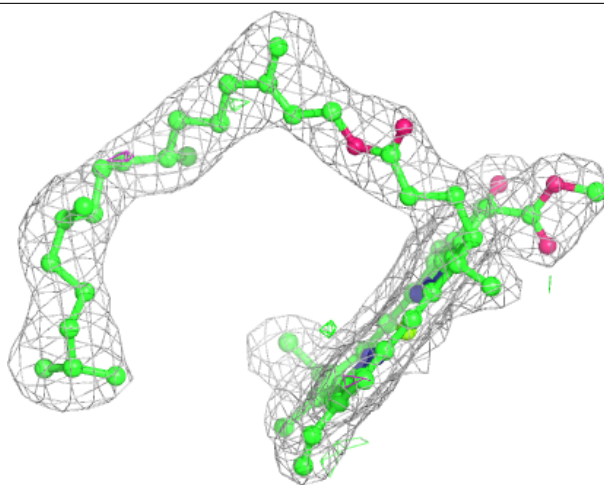
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





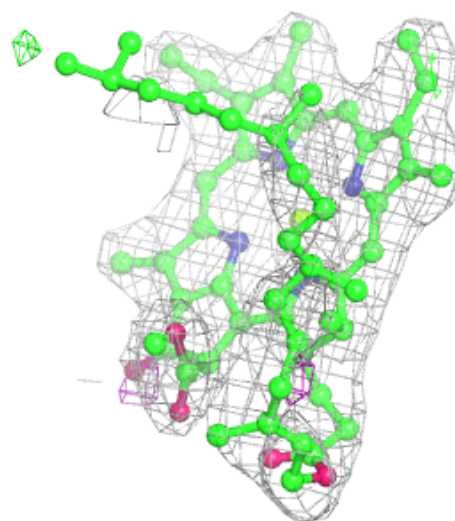
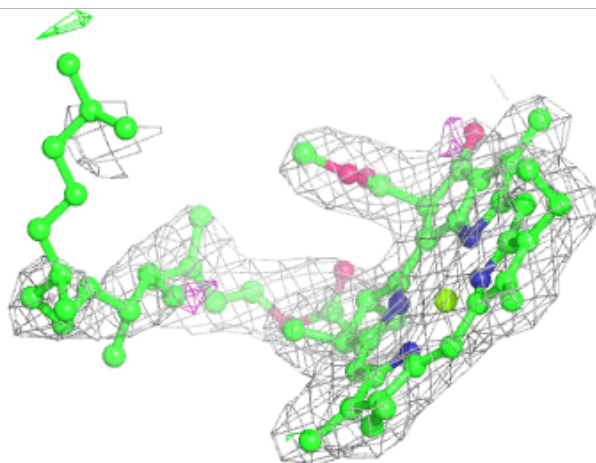
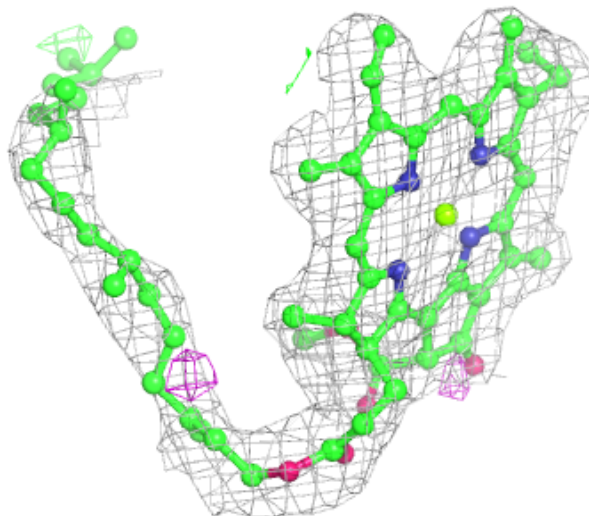
Electron density around CLA b 611:

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



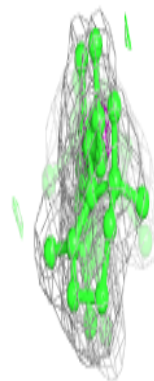
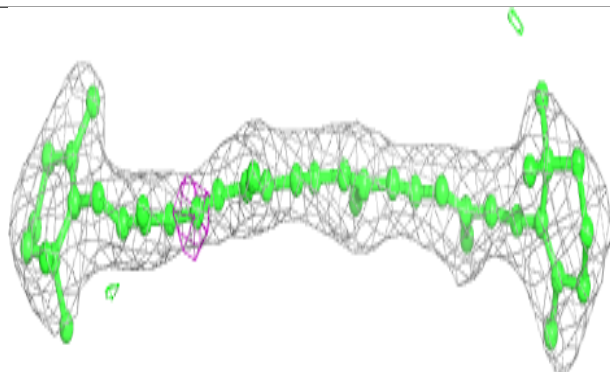
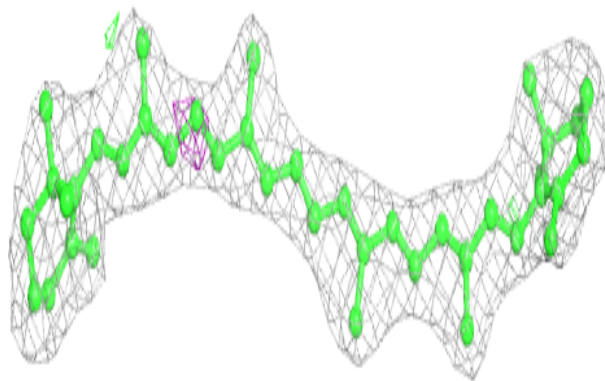
Electron density around CLA b 616:

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

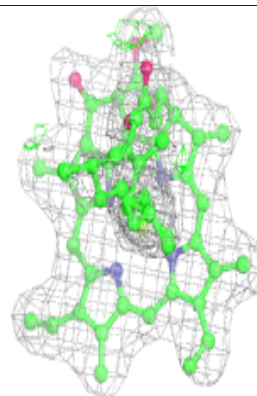
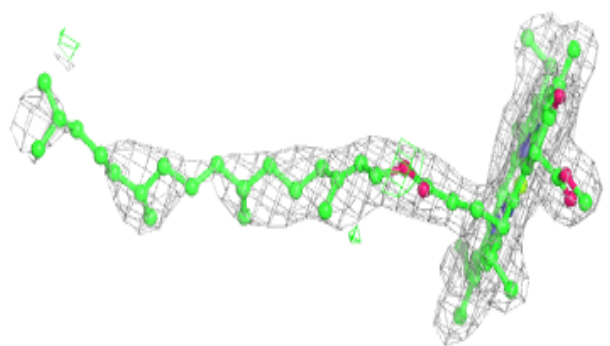
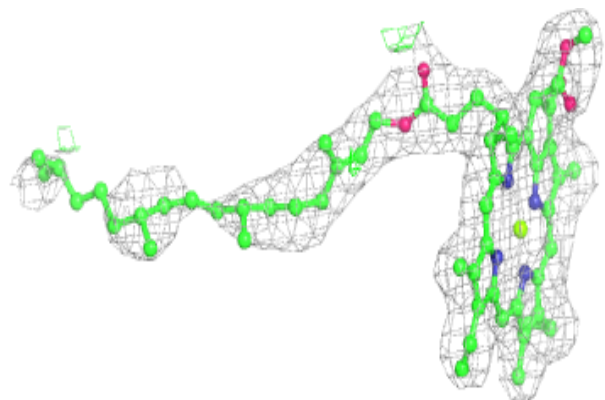


Electron density around BCR y 101:

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

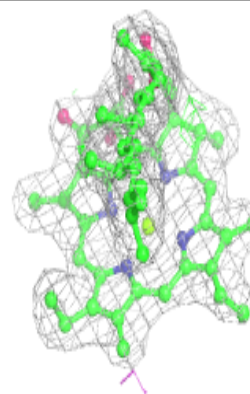
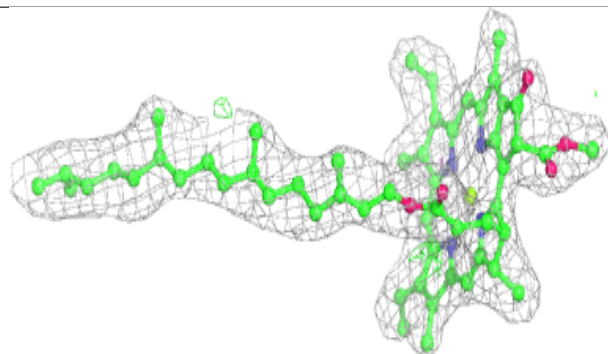
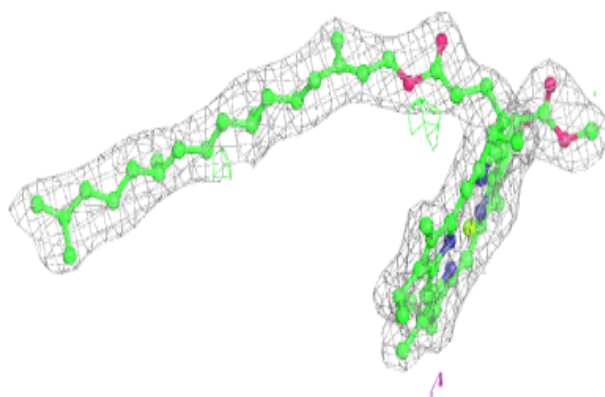
**Electron density around CLA d 403:**

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



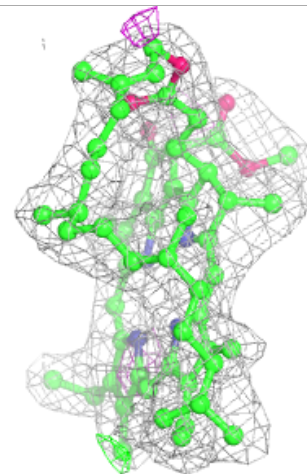
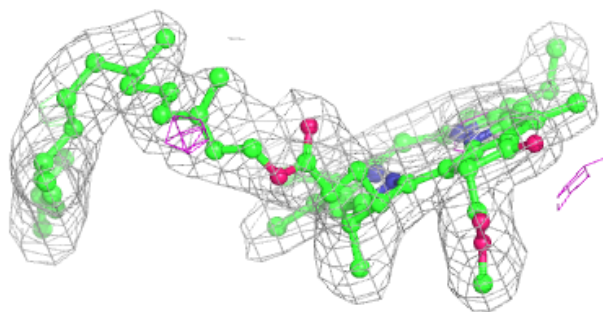
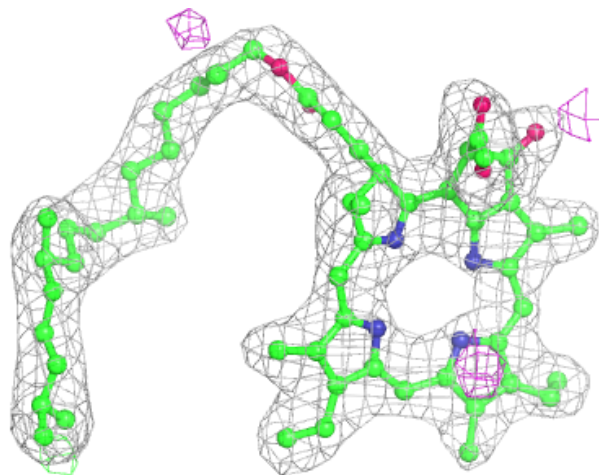
Electron density around CLA b 607:

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



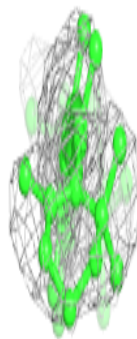
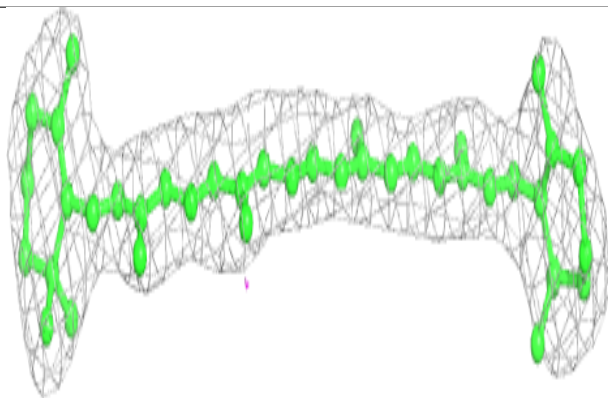
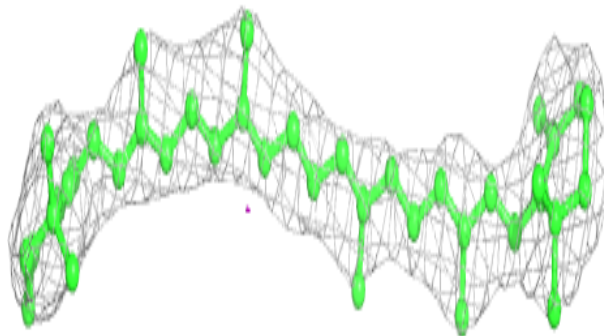
Electron density around PHO a 406:

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

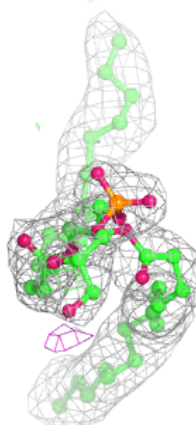
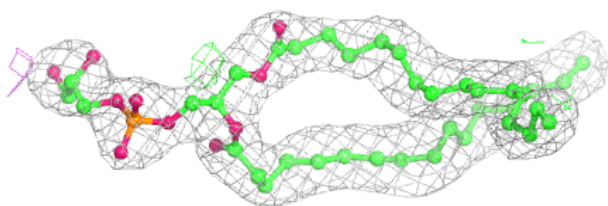
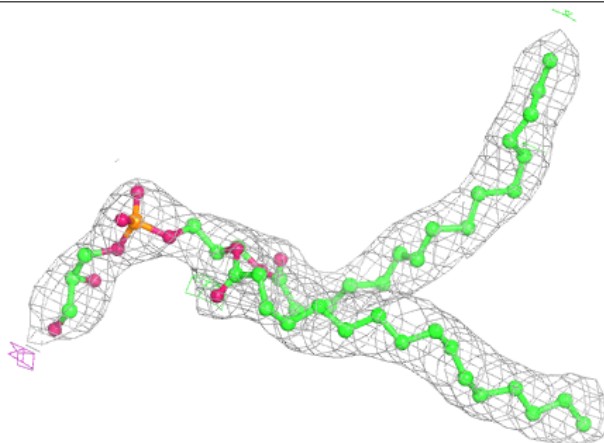


Electron density around BCR c 516:

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

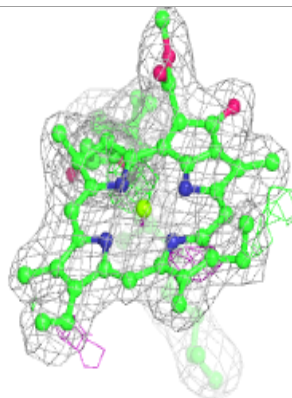
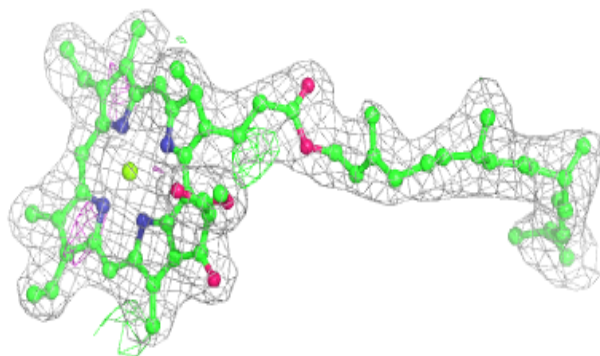
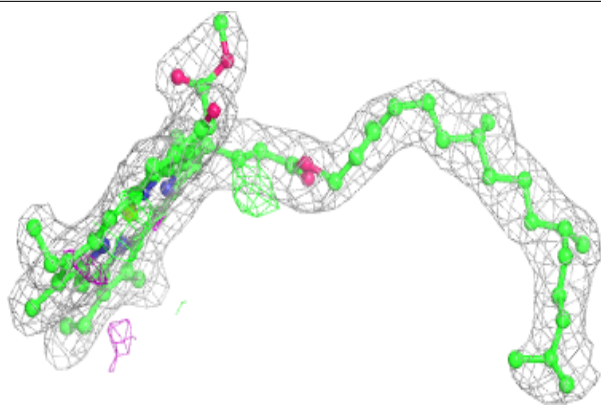
**Electron density around LHG D 406:**

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

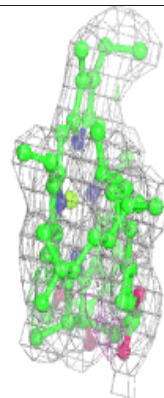
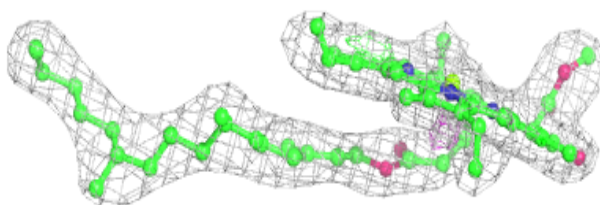
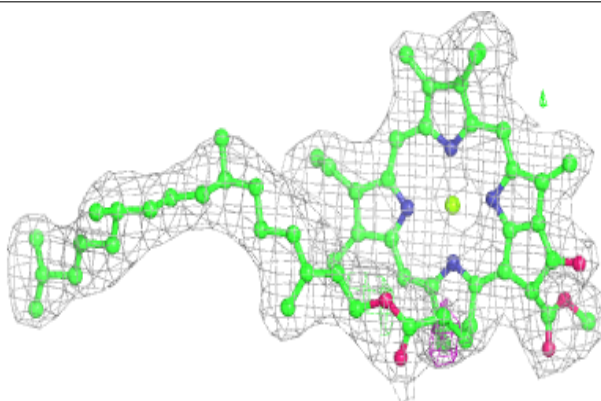


Electron density around CLA d 402:

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

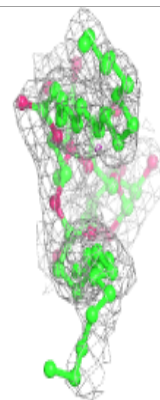
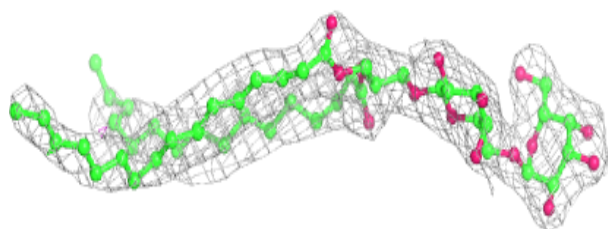
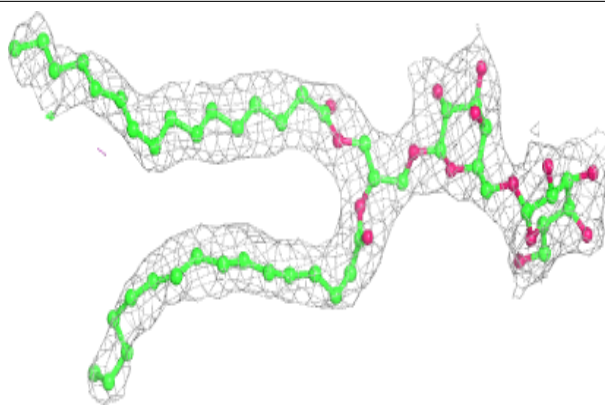
**Electron density around CLA B 603:**

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

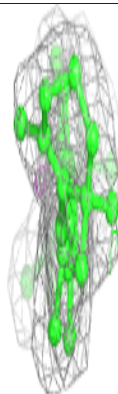
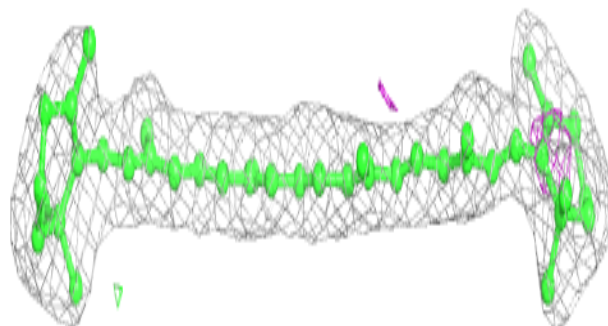
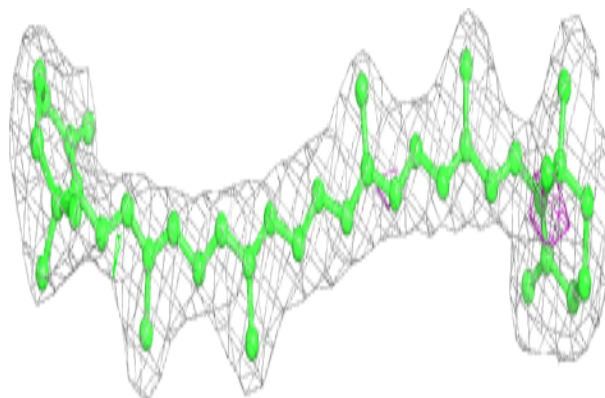


Electron density around DGD c 520:

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

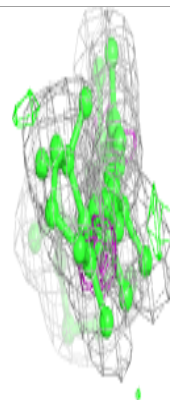
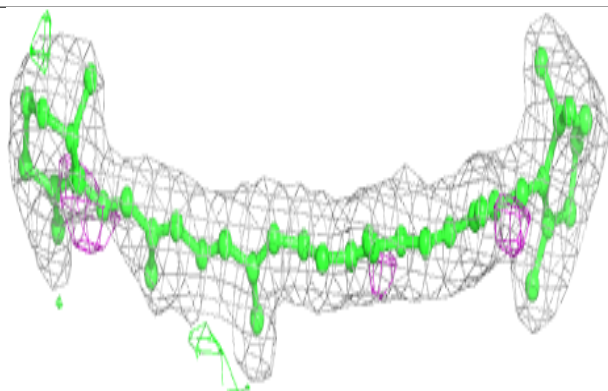
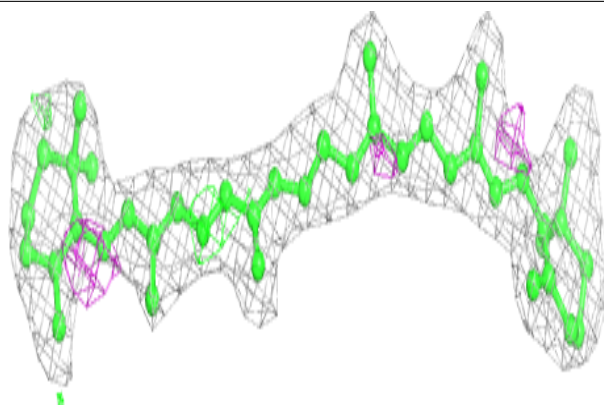
**Electron density around BCR B 618:**

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

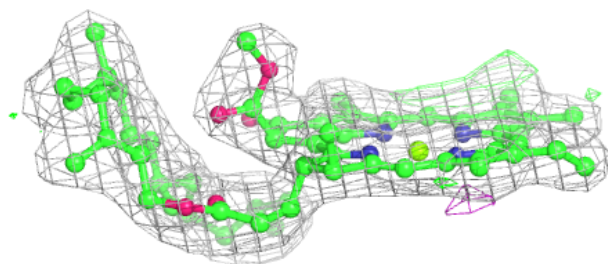
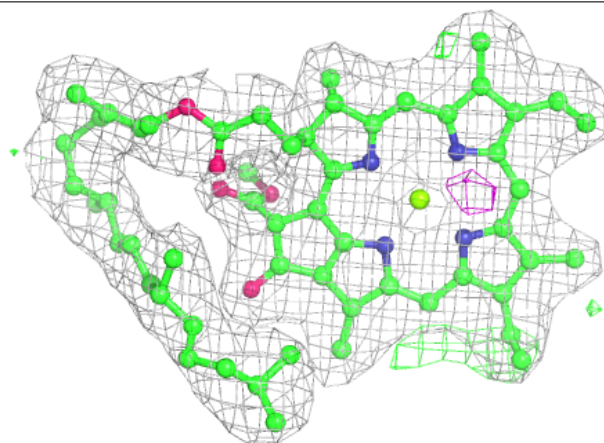


Electron density around BCR T 101:

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

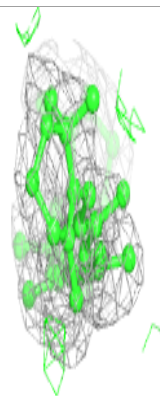
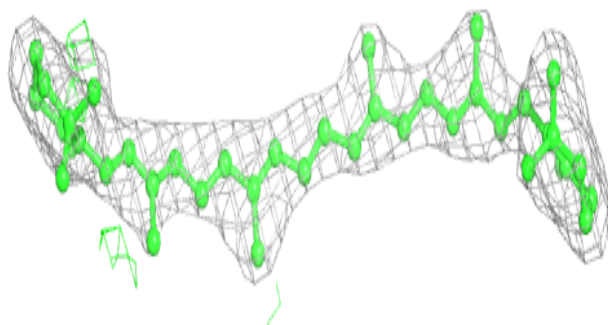
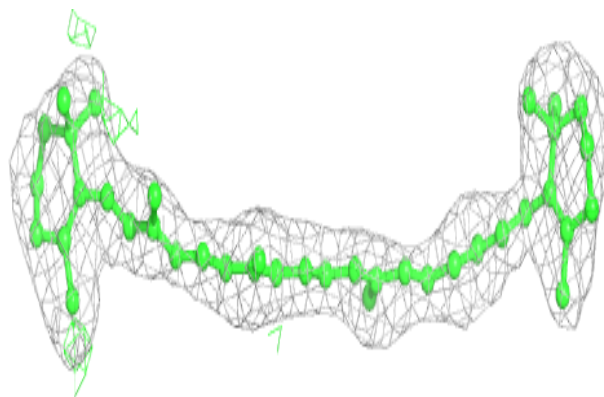
**Electron density around CLA B 610:**

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

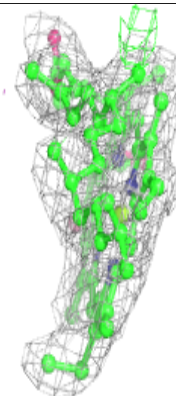
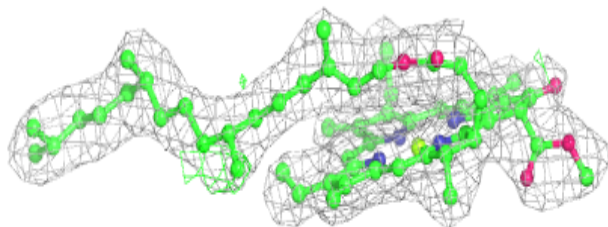
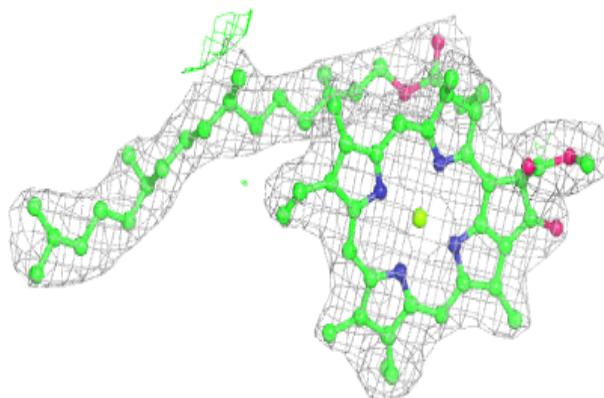


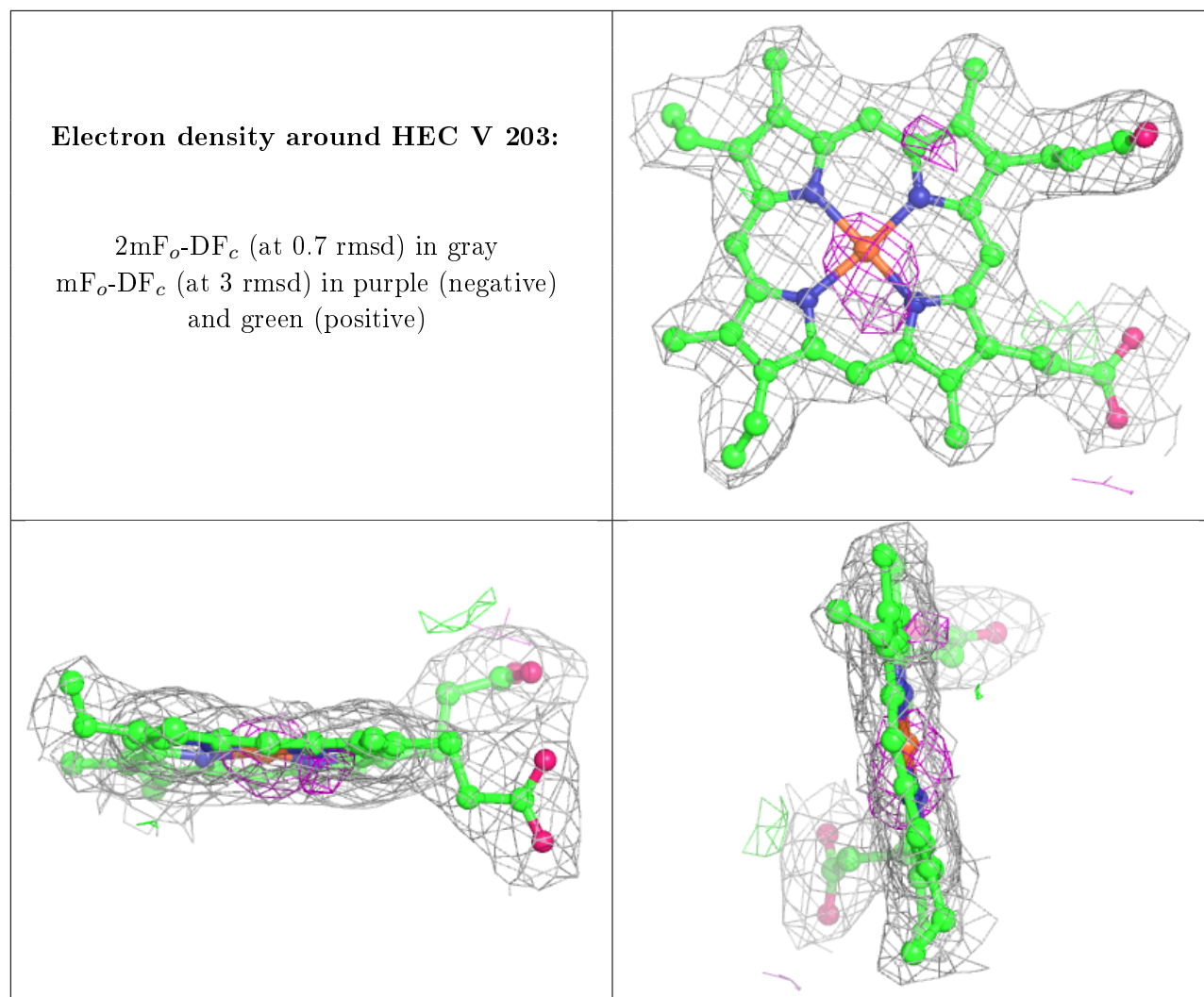
Electron density around BCR k 101:

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

**Electron density around CLA c 503:**

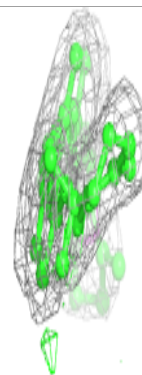
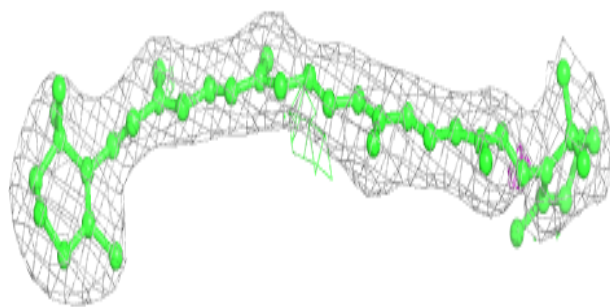
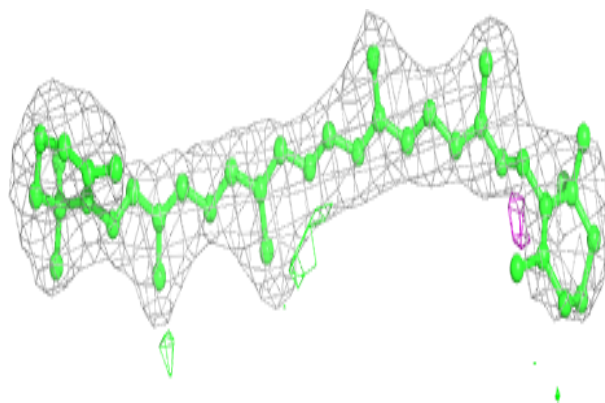
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



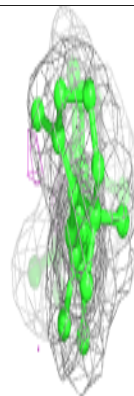
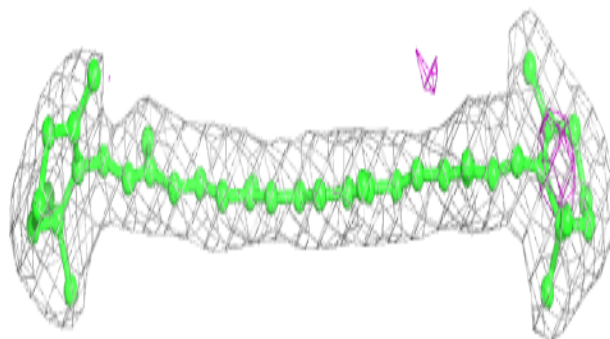
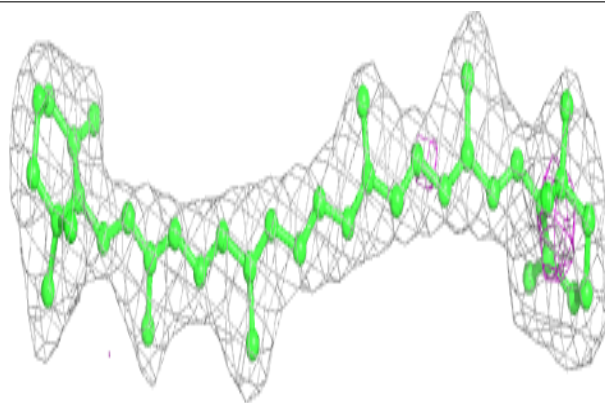


Electron density around BCR d 404:

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

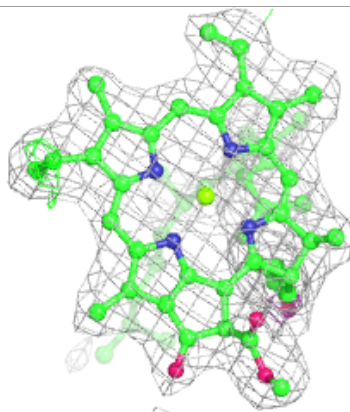
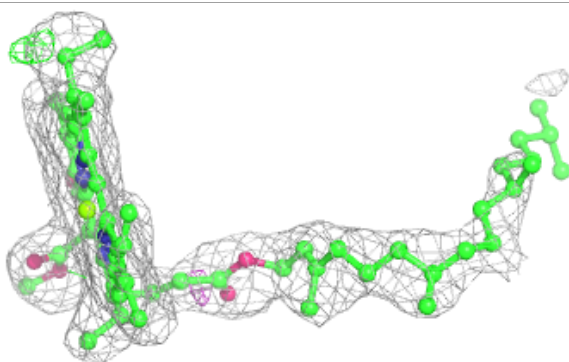
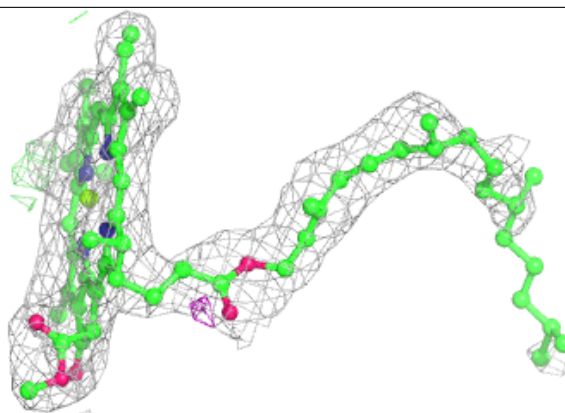
**Electron density around BCR b 618:**

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

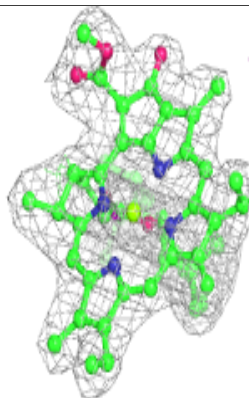
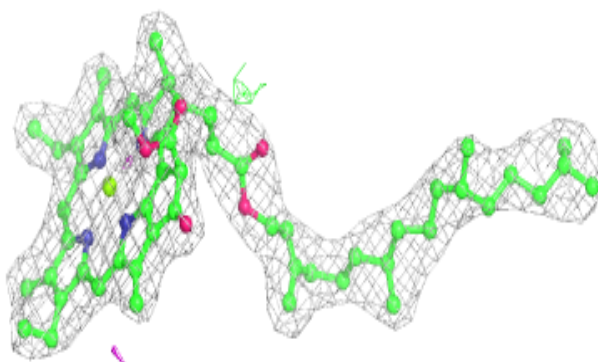
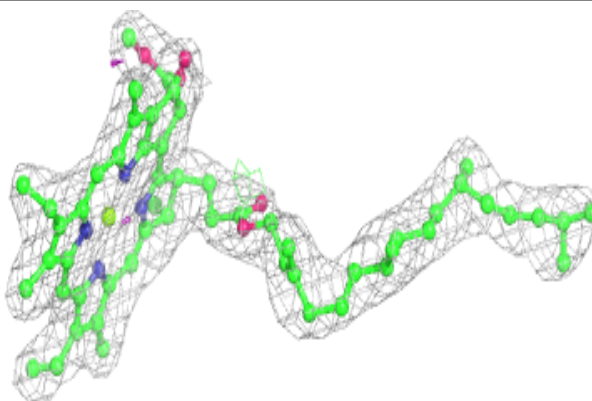


Electron density around CLA D 403:

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

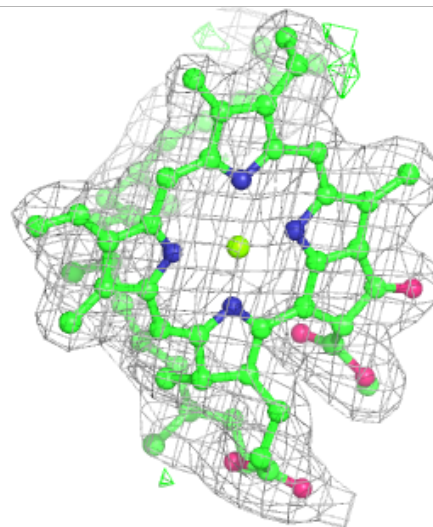
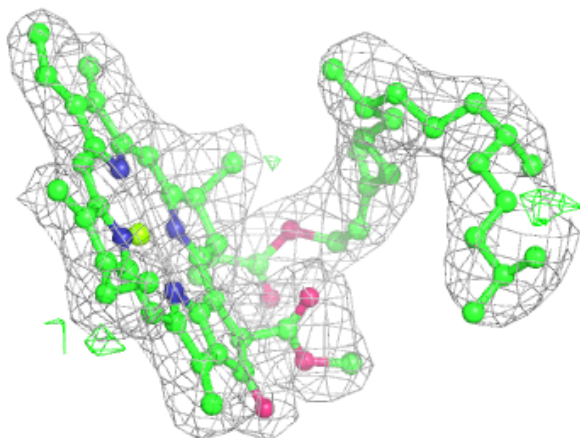
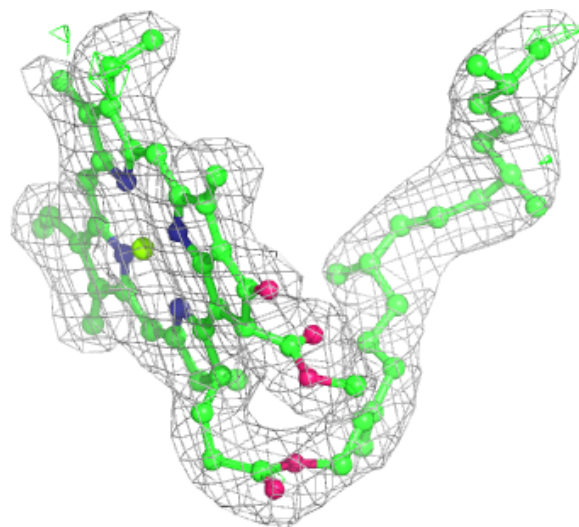
**Electron density around CLA C 503:**

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



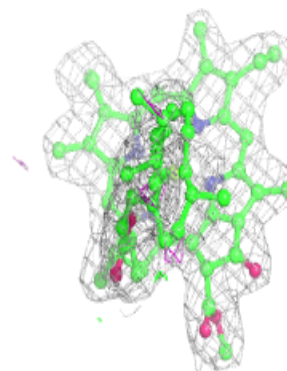
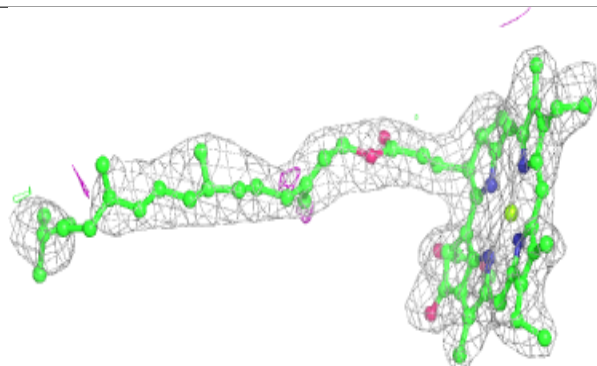
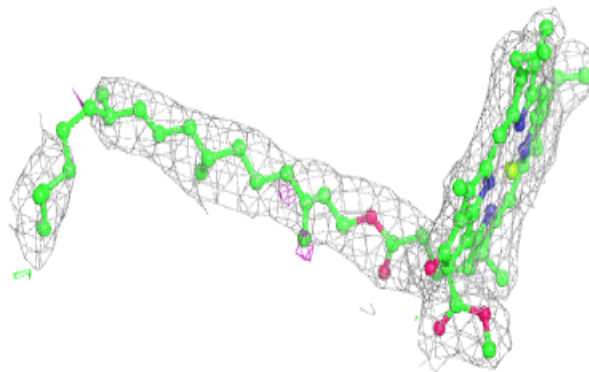
Electron density around CLA b 613:

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



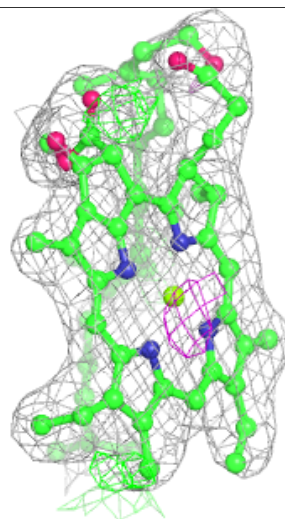
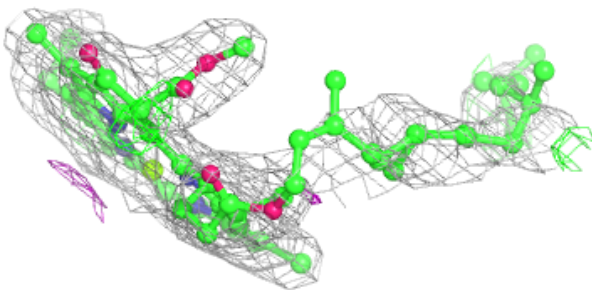
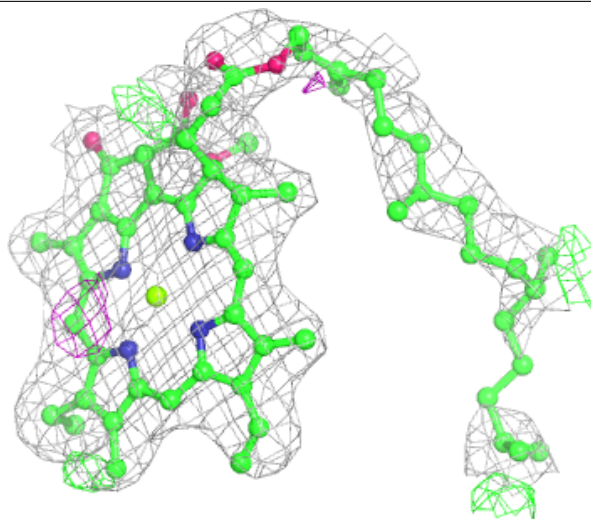
Electron density around CLA b 604:

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



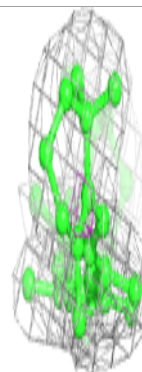
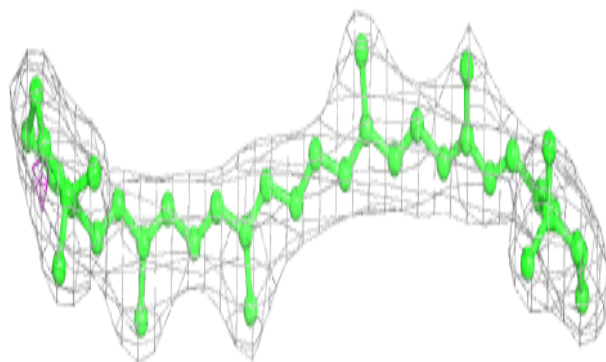
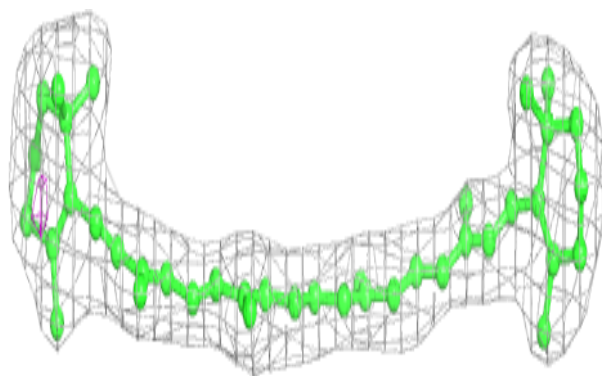
Electron density around CLA B 616:

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

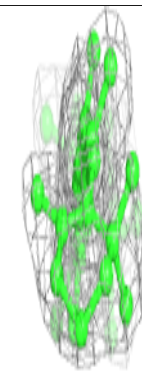
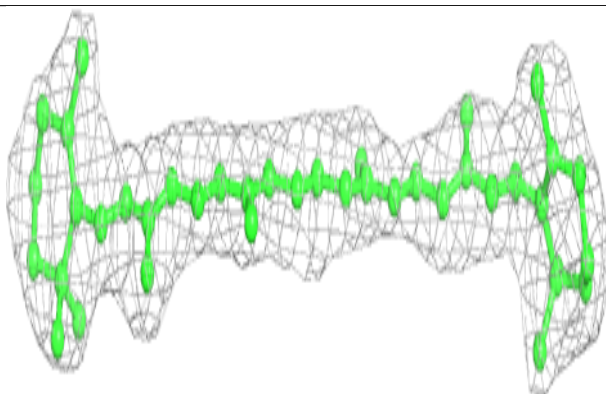
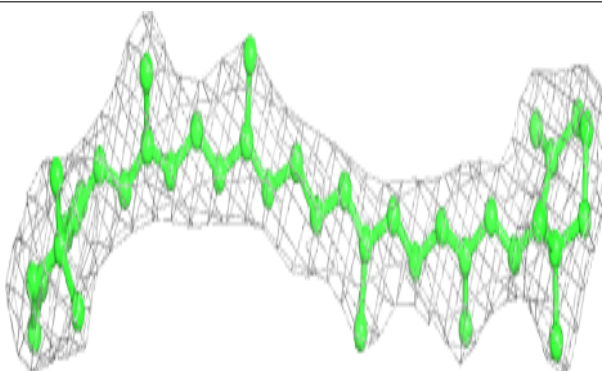


Electron density around BCR K 102:

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

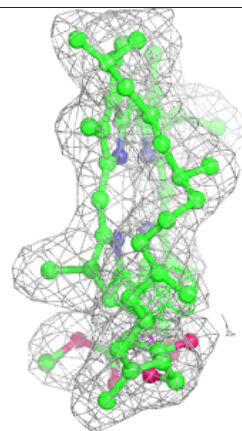
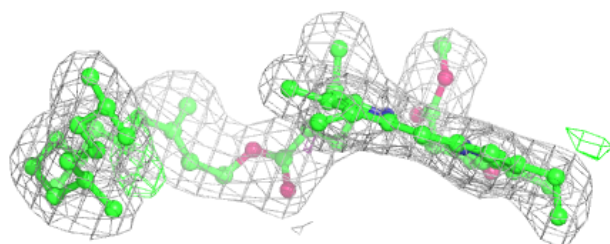
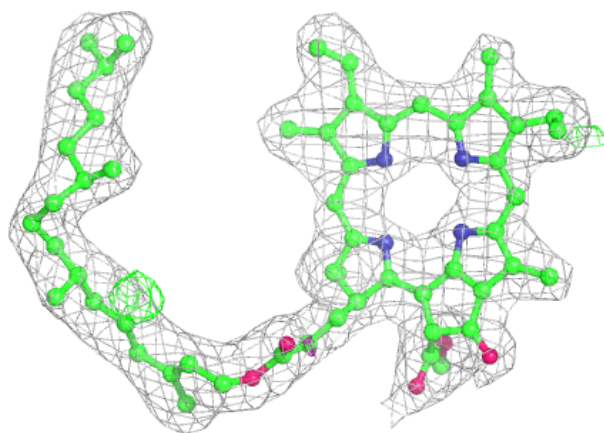
**Electron density around BCR C 515:**

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



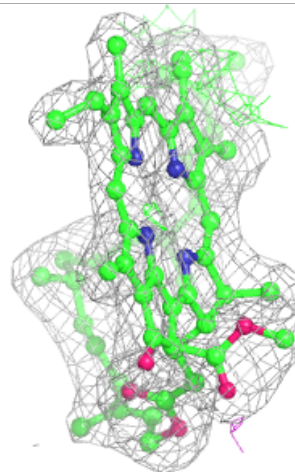
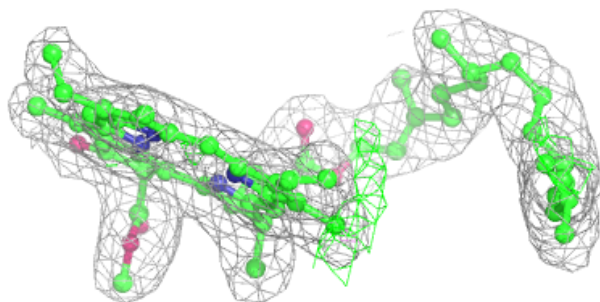
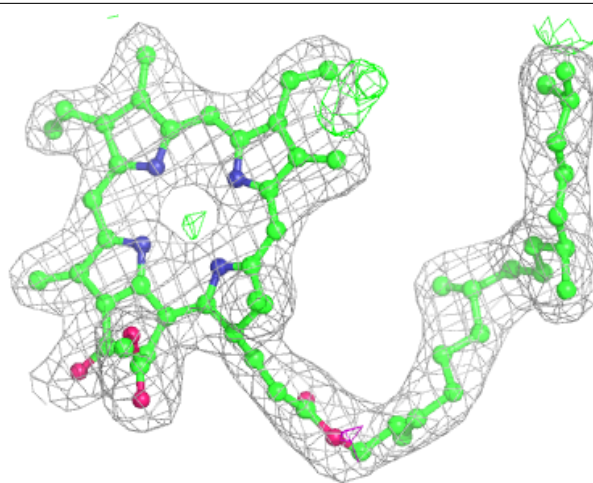
Electron density around PHO A 407:

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



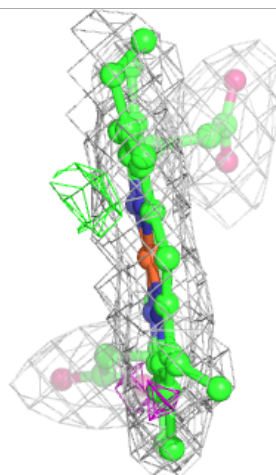
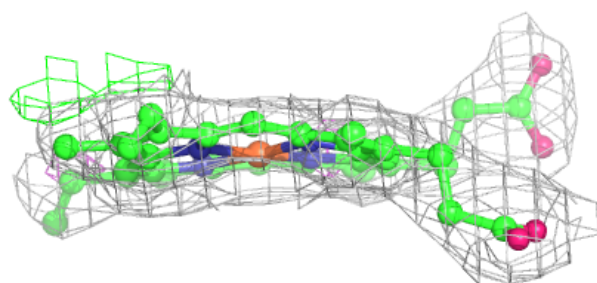
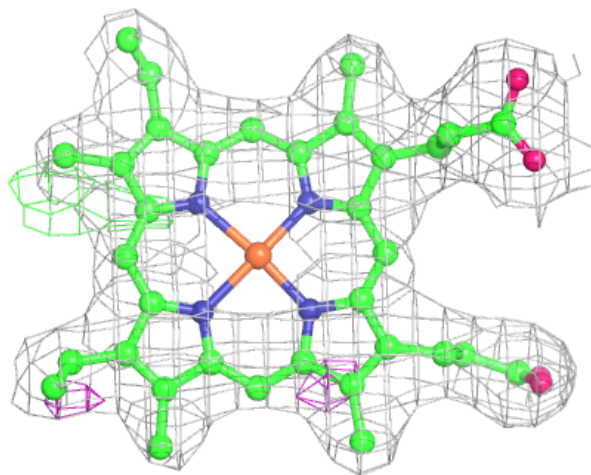
Electron density around PHO A 408:

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



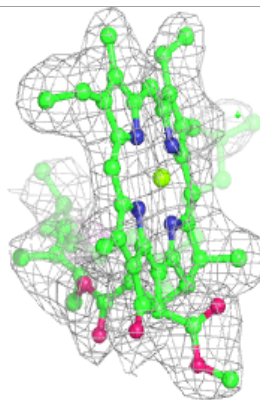
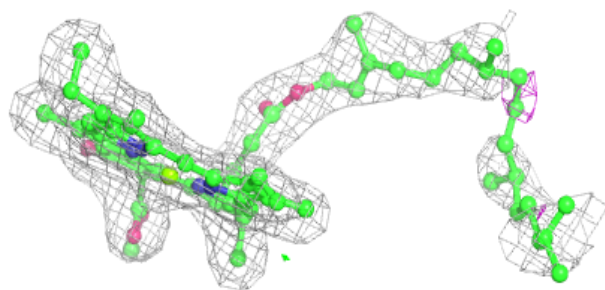
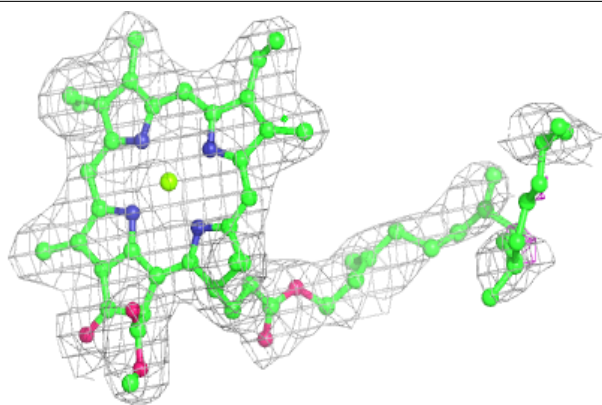
Electron density around HEC v 203:

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

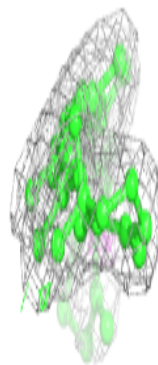
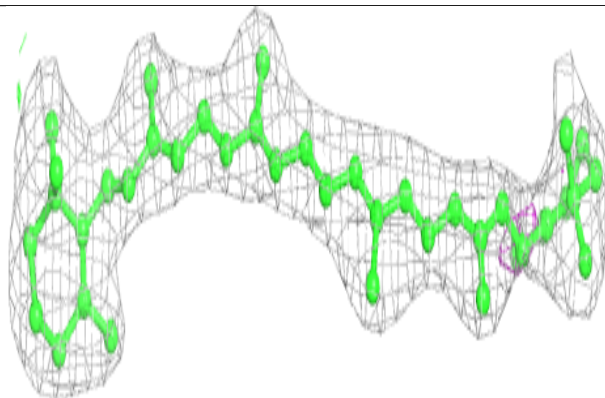
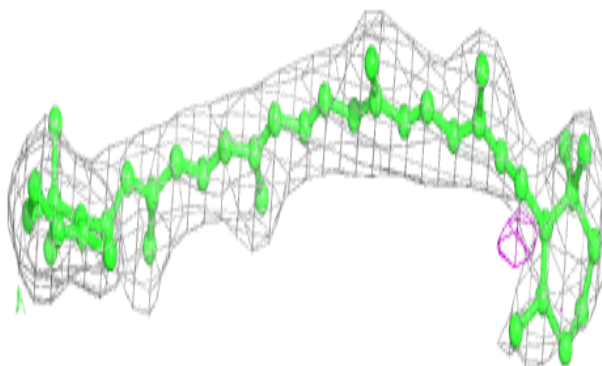


Electron density around CLA A 409:

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

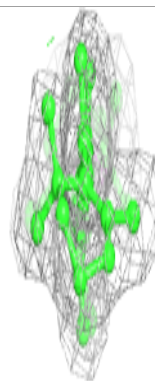
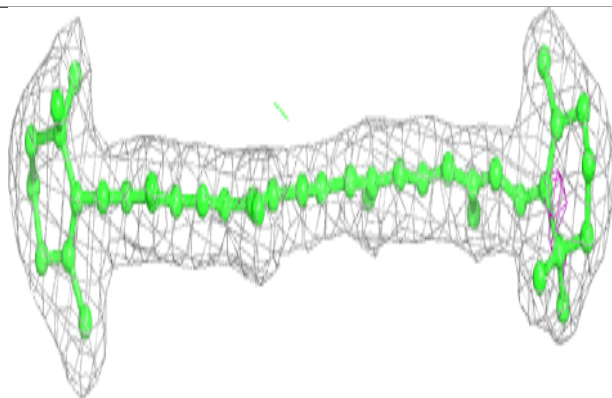
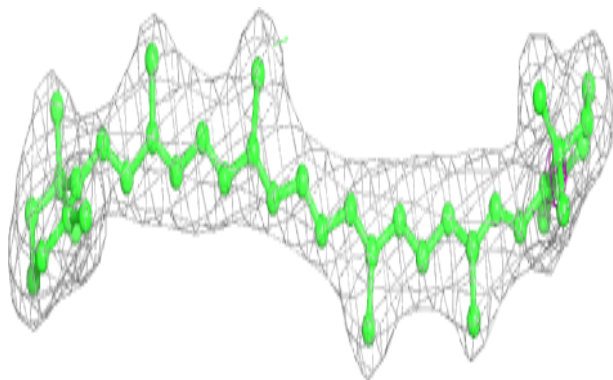
**Electron density around BCR D 404:**

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

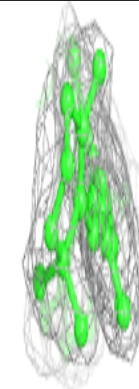
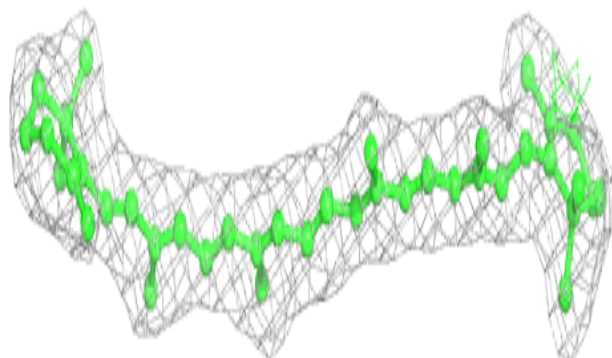
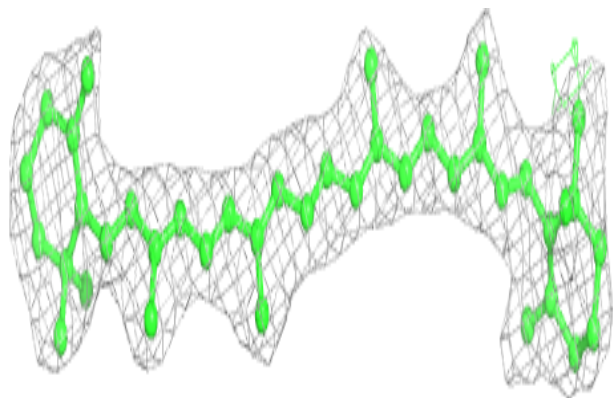


Electron density around BCR a 408:

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

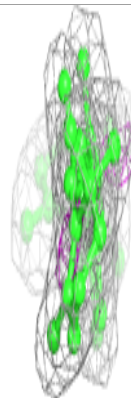
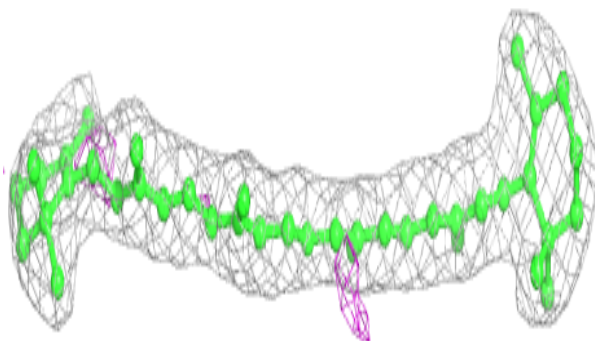
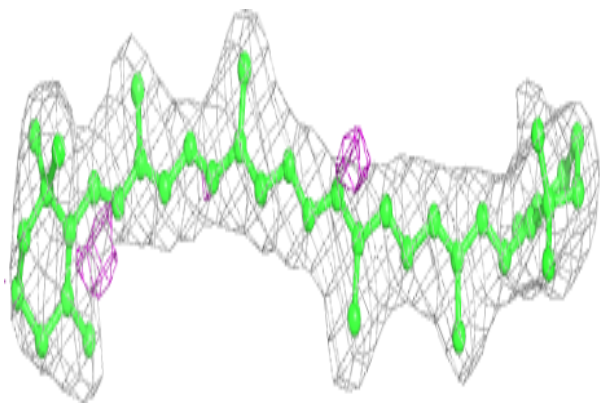
**Electron density around BCR b 619:**

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

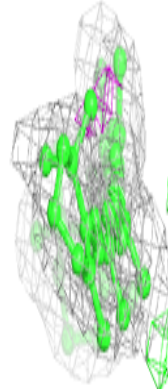
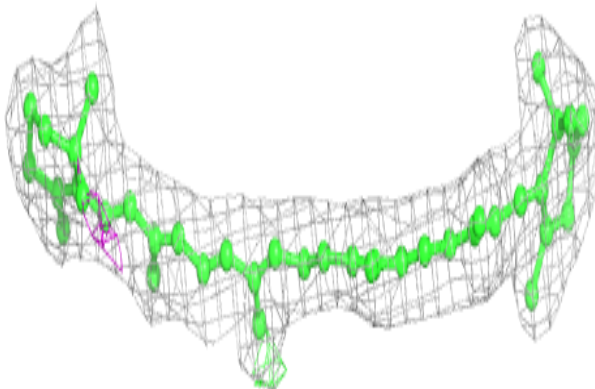
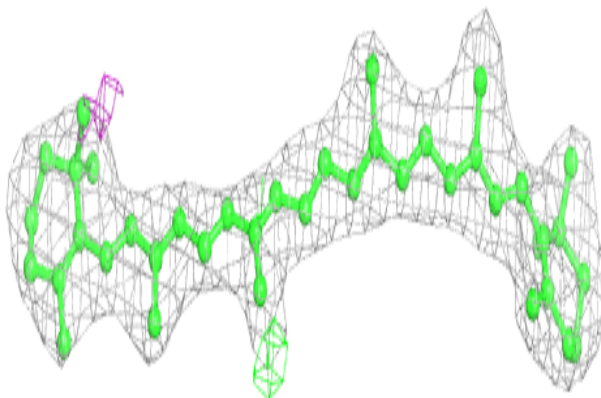


Electron density around BCR b 617:

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

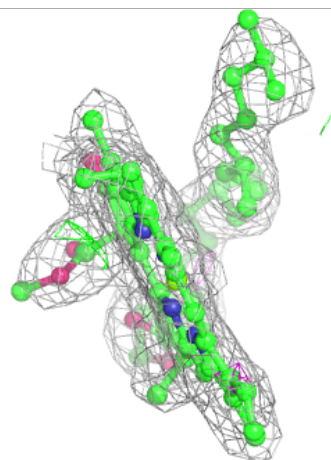
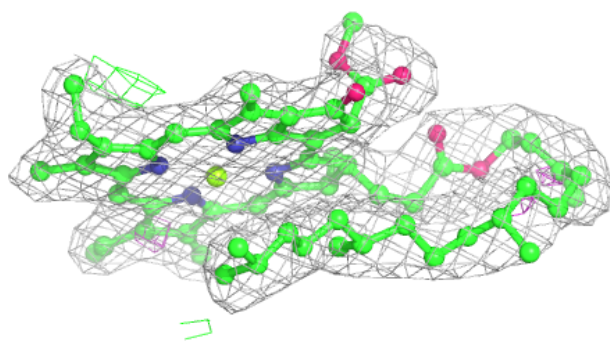
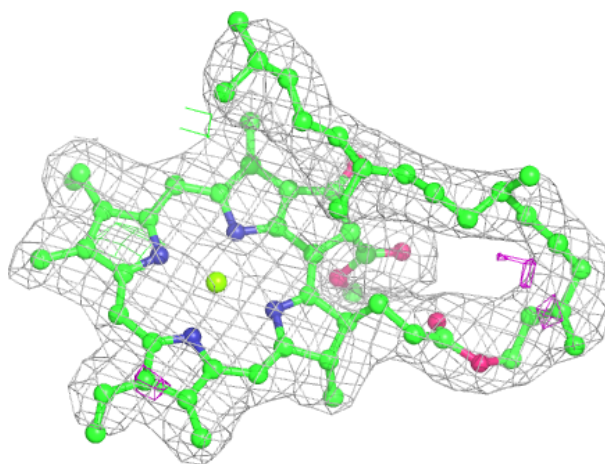
**Electron density around BCR t 102:**

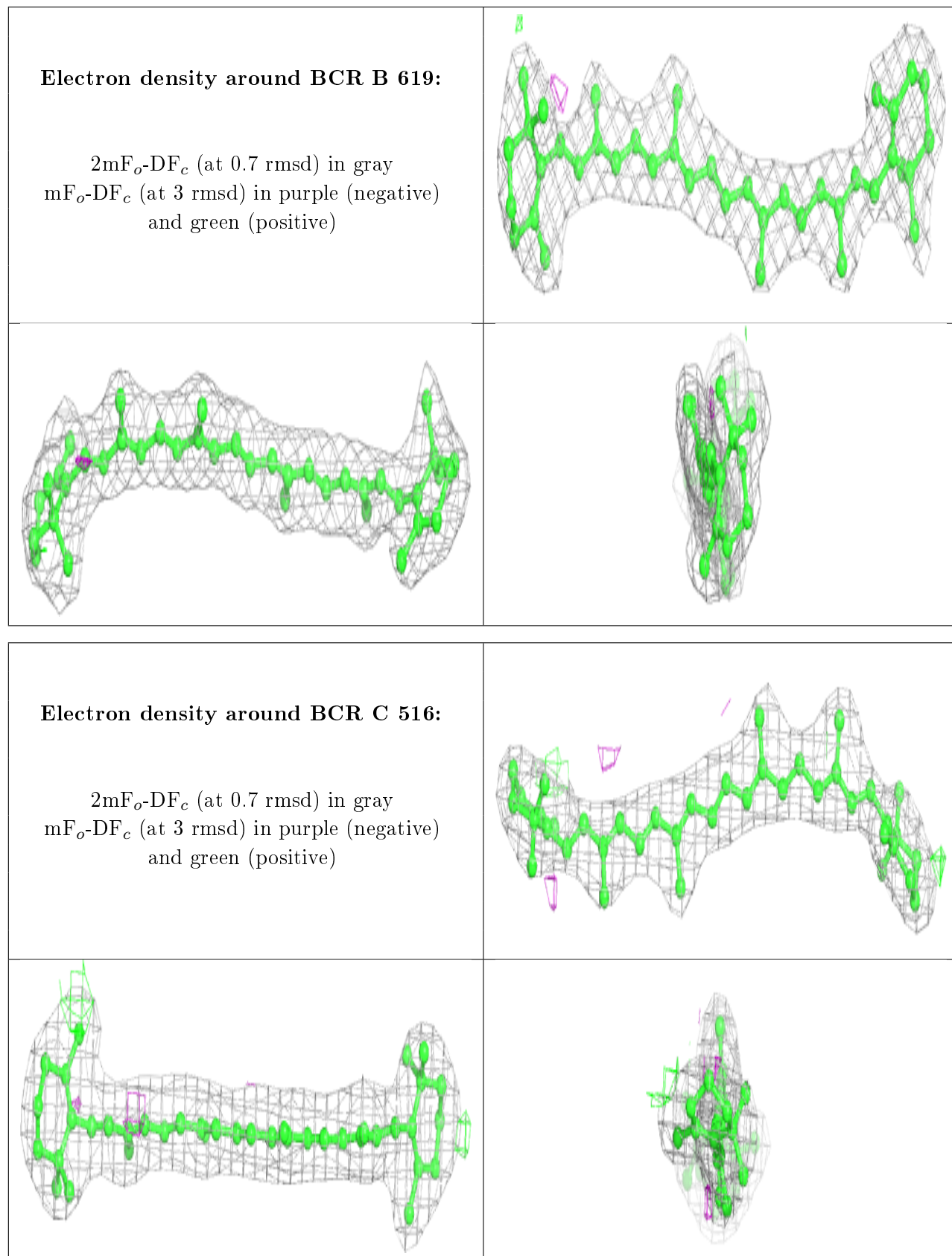
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA C 510:

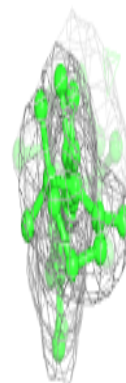
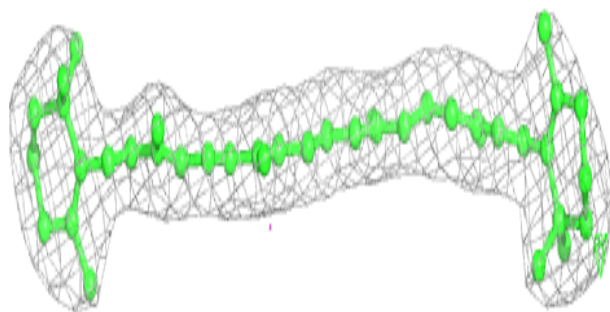
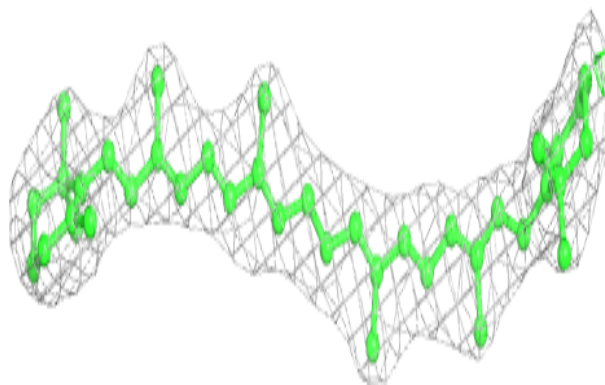
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



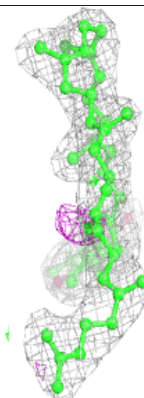
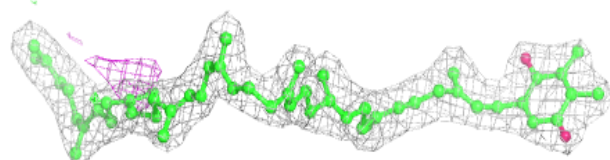
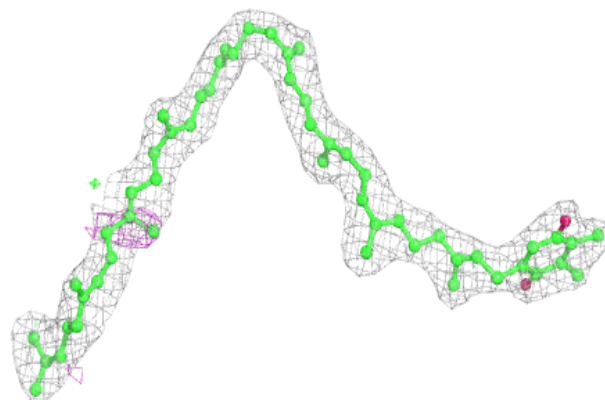


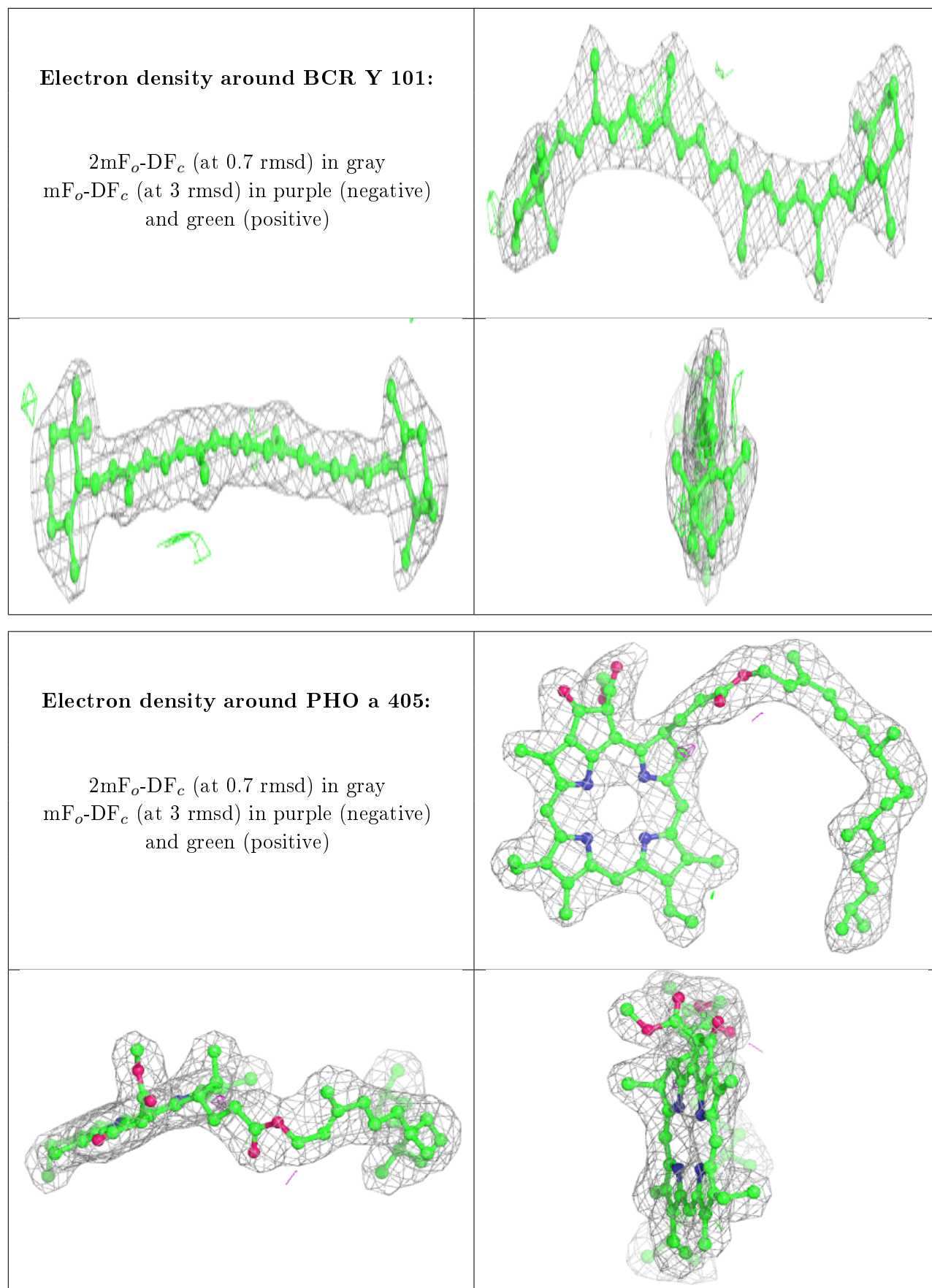
Electron density around BCR c 517:

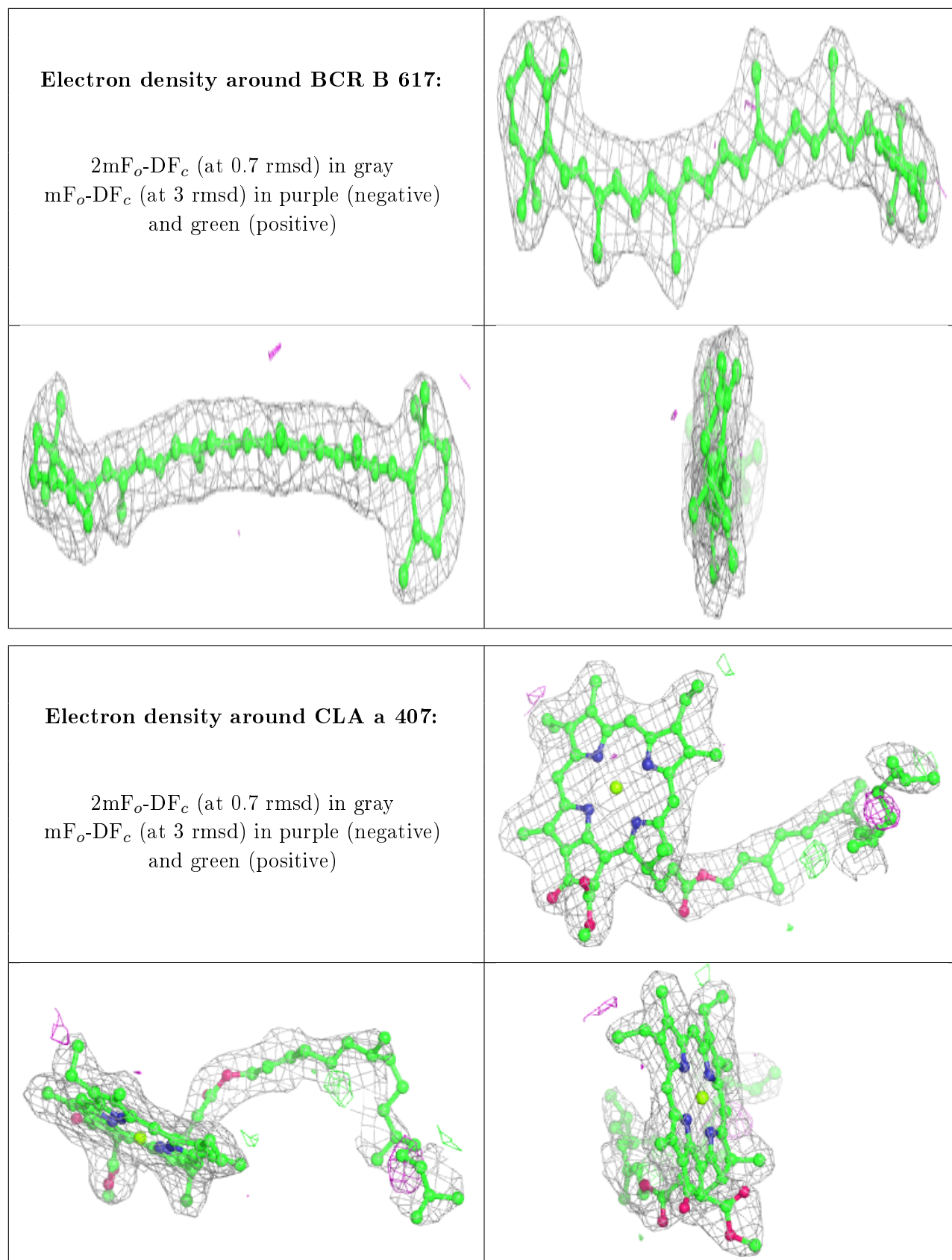
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

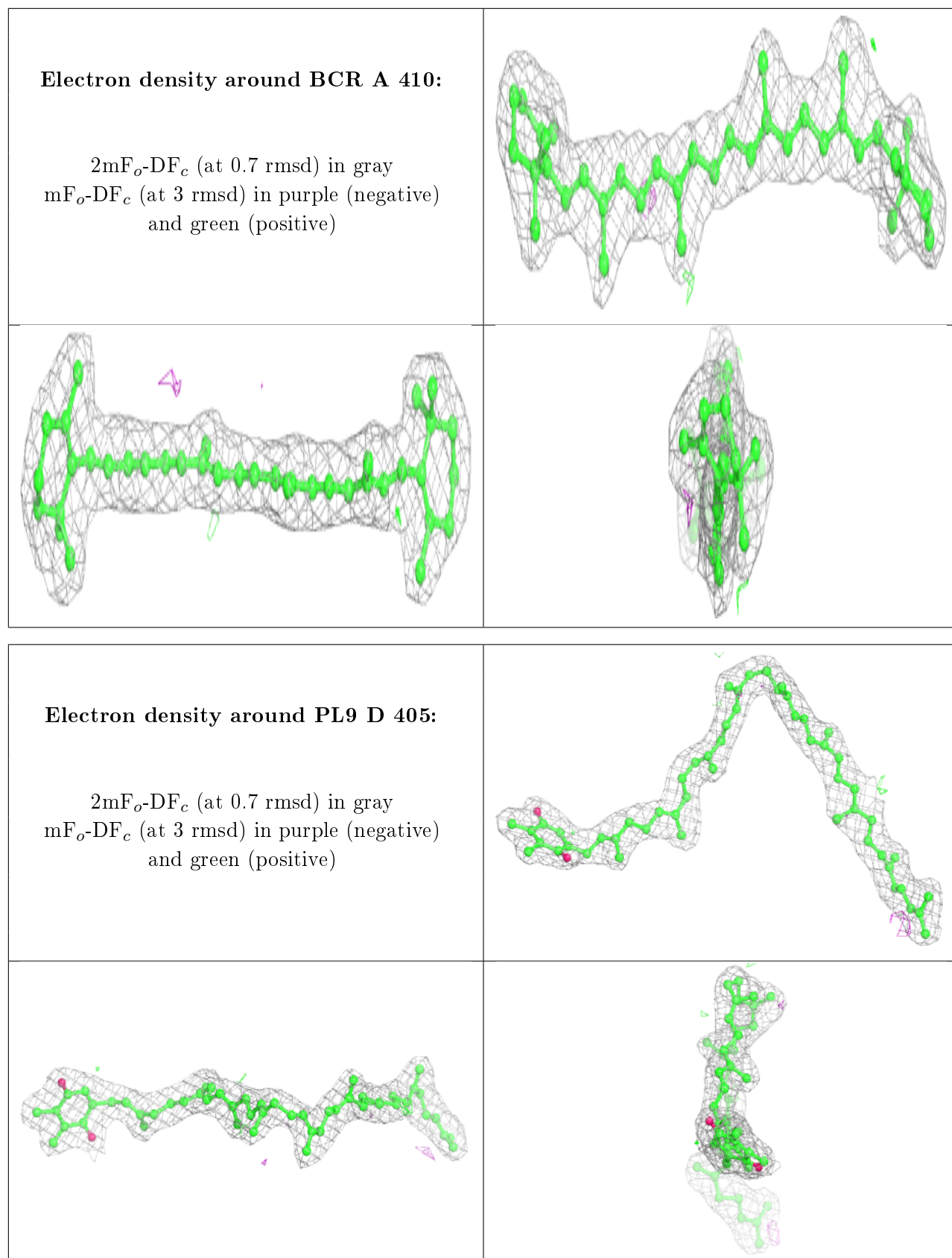
**Electron density around PL9 d 405:**

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









6.5 Other polymers [i](#)

There are no such residues in this entry.