



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 04:23 PM JST

PDB ID : 7YQ2  
Title : Crystal structure of photosystem II expressing psbA2 gene only  
Authors : Nakajima, Y.; Suga, M.; Shen, J.R.  
Deposited on : 2022-08-05  
Resolution : 1.90 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

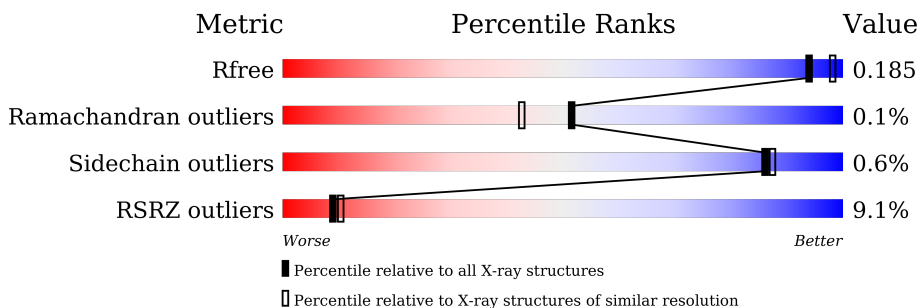
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	360	 3% 92% 7%
1	a	360	 8% 93% 7%
2	B	510	 6% 99% 5%
2	b	510	 9% 98% 7%
3	C	461	 4% 97% 7%
3	c	461	 6% 98% 7%
4	D	352	 2% 97% 7%

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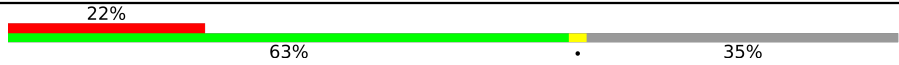

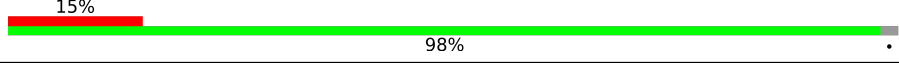
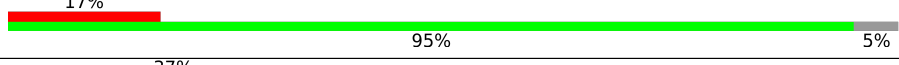
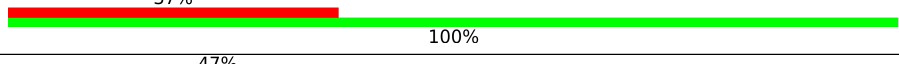
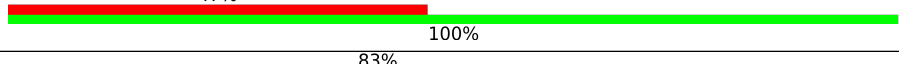
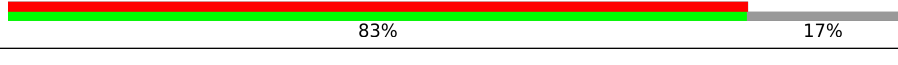


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Mol	Chain	Length	Quality of chain
4	d	352	<p>2% 96%</p>
5	E	84	<p>25% 95% 5%</p>
5	e	84	<p>18% 94% 6%</p>
6	F	45	<p>7% 76% 24%</p>
6	f	45	<p>4% 71% 29%</p>
7	H	66	<p>8% 97%</p>
7	h	66	<p>15% 97%</p>
8	I	38	<p>13% 95%</p>
8	i	38	<p>5% 95%</p>
9	J	40	<p>5% 90% 10%</p>
9	j	40	<p>98%</p>
10	K	46	<p>2% 80% 20%</p>
10	k	46	<p>4% 80% 20%</p>
11	L	37	<p>5% 100%</p>
11	l	37	<p>3% 100%</p>
12	M	36	<p>3% 94% 6%</p>
12	m	36	<p>6% 92% 6%</p>
13	O	272	<p>12% 89% 11%</p>
13	o	272	<p>13% 87% 11%</p>
14	T	32	<p>3% 91% 6%</p>
14	t	32	<p>6% 91% 6%</p>
15	U	134	<p>2% 73% 27%</p>
15	u	134	<p>2% 72% 28%</p>
16	V	163	<p>7% 83% 16%</p>
16	v	163	<p>17% 84% 16%</p>

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Mol	Chain	Length	Quality of chain
17	Y	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	R	41	

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	405	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	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	B	617	X	-	-	-
24	CLA	C	501	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	D	401	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	a	409	X	-	-	-
24	CLA	a	413	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	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	b	618	X	-	-	-
24	CLA	b	619	X	-	-	-
24	CLA	b	620	X	-	-	-
24	CLA	c	902	X	-	-	-
24	CLA	c	903	X	-	-	-
24	CLA	c	904	X	-	-	-
24	CLA	c	905	X	-	-	-
24	CLA	c	906	X	-	-	-
24	CLA	c	907	X	-	-	-
24	CLA	c	908	X	-	-	-
24	CLA	c	909	X	-	-	-
24	CLA	c	910	X	-	-	-
24	CLA	c	911	X	-	-	-
24	CLA	c	913	X	-	-	-
24	CLA	c	914	X	-	-	-
24	CLA	d	401	X	-	-	-
24	CLA	d	404	X	-	-	-
24	CLA	d	405	X	-	-	-
30	UNL	A	415	-	-	-	X
30	UNL	A	418	-	-	-	X
30	UNL	B	627	-	-	-	X
30	UNL	T	102	-	-	-	X
30	UNL	a	418	-	-	-	X
30	UNL	h	103	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	UNL	h	106	-	-	-	X
30	UNL	t	103	-	-	-	X
31	LMT	c	922	-	-	-	X
32	GOL	B	637	-	-	-	X
32	GOL	O	304	-	-	-	X
34	DMS	O	312	-	-	-	X
36	HTG	B	625	-	-	-	X
36	HTG	c	924	-	-	-	X
36	HTG	c	943	-	-	-	X
36	HTG	d	420	-	-	-	X

## 2 Entry composition

There are 43 unique types of molecules in this entry. The entry contains 55630 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II protein D1 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	334	Total	C	N	O	S	0	2	0
			2607	1712	427	455	13			
1	a	336	Total	C	N	O	S	0	3	0
			2632	1727	431	461	13			

- 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	505	Total	C	N	O	S	0	8	0
			3995	2623	665	694	13			
2	b	504	Total	C	N	O	S	0	9	0
			3961	2600	656	692	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	451	Total	C	N	O	S	0	6	0
			3507	2295	586	613	13			
3	c	456	Total	C	N	O	S	0	3	0
			3532	2314	589	616	13			

- 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	C	N	O	S	0	1	0
			2713	1799	439	463	12			
4	d	342	Total	C	N	O	S	0	2	0
			2724	1806	442	463	13			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	80	Total	C	N	O	0	1	0
			629	413	102	114			
5	e	79	Total	C	N	O	0	2	0
			644	423	102	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	32	Total	C	N	O	S	0	1	0
			263	179	44	39	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	0	0
			505	336	81	86	2			
7	h	65	Total	C	N	O	S	0	1	0
			516	343	85	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	37	Total	C	N	O	S	0	0	0
			301	205	47	48	1			
8	i	37	Total	C	N	O	S	0	0	0
			297	203	47	46	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			251	171	37	42	1			
9	j	39	Total	C	N	O	S	0	0	0
			270	182	40	46	2			

- 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
			289	201	42	46			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	k	37	289	201	42	46	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	L	37	311	209	49	52	1	0	2	0
11	l	37	305	205	48	51	1	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	M	34	270	182	39	48	1	0	1	0
12	m	34	274	184	40	49	1	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	O	243	1895	1190	313	388	4	0	10	0
13	o	243	1879	1177	311	387	4	0	5	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	T	30	264	185	36	41	2	0	1	0
14	t	30	264	185	36	41	2	0	1	0

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
15	U	98	767	487	129	151	0	0	0
15	u	97	774	491	129	154	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	V	137	Total 1089	C 691	N 181	O 213	S 4	0	4	0
16	v	137	Total 1070	C 678	N 178	O 210	S 4	0	2	0

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	Y	30	Total 218	C 144	N 35	O 36	S 3	0	0	0
17	y	30	Total 229	C 152	N 38	O 36	S 3	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
18	X	40	Total 286	C 191	N 46	O 49		0	0	0
18	x	39	Total 286	C 191	N 46	O 49		0	0	0

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

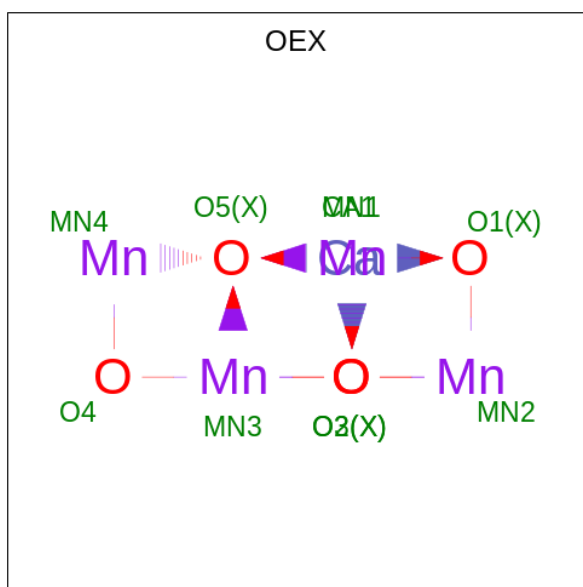
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	Z	62	Total 458	C 317	N 67	O 72	S 2	0	0	0
19	z	62	Total 455	C 312	N 67	O 74	S 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	R	34	Total 228	C 150	N 41	O 37		0	0	0

- Molecule 21 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).





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

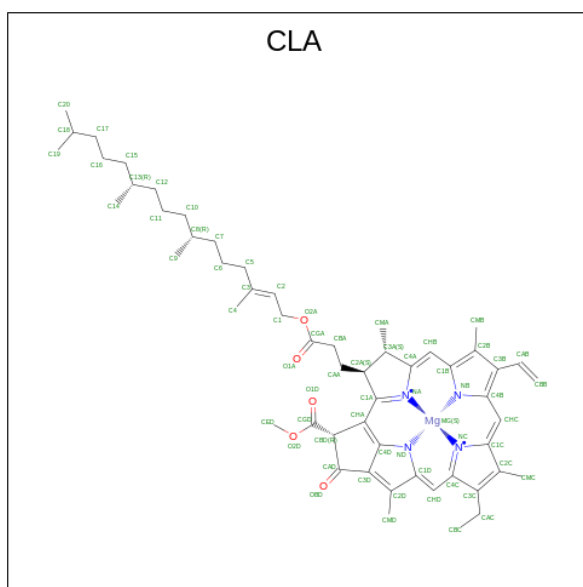
- Molecule 22 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 23 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

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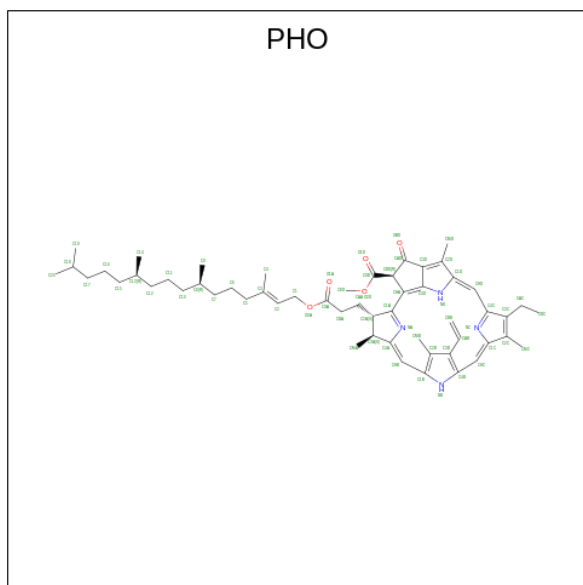
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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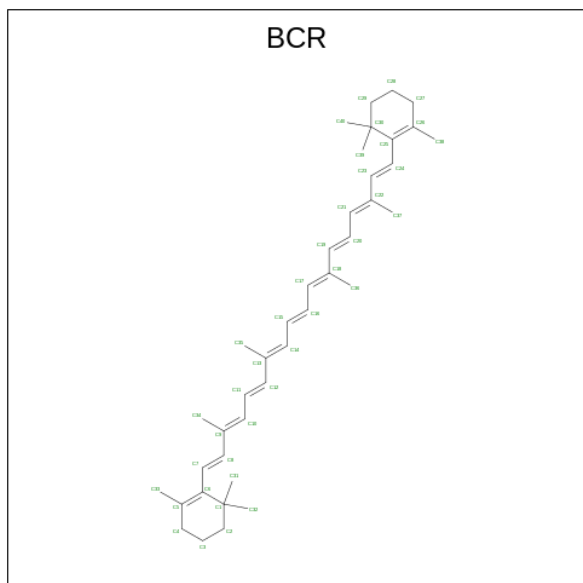
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
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	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		
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: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



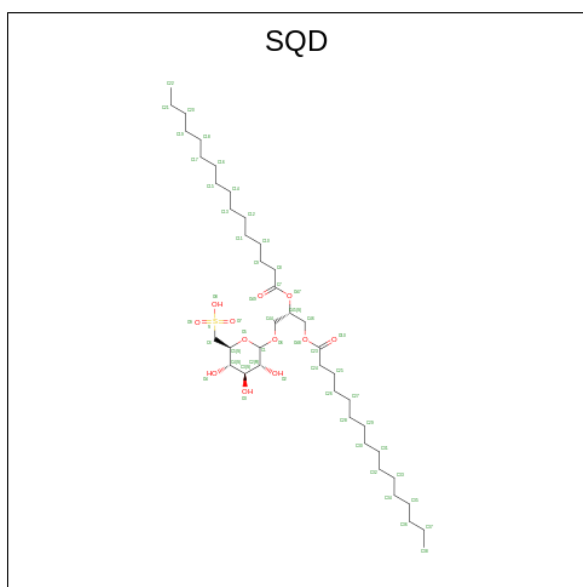
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
			Total	C	N			O	
25	A	1	Total	64	55	4	5	0	0
25	A	1	Total	64	55	4	5	0	0
25	a	1	Total	64	55	4	5	0	0
25	a	1	Total	64	55	4	5	0	0

- 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	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	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	k	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0

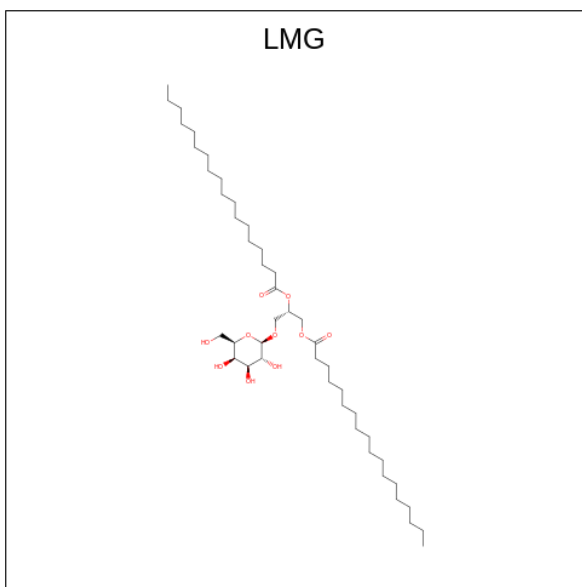
- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
27	A	1	54	41	12	1	0	0
27	A	1	54	41	12	1	0	0
27	F	1	37	25	11	1	0	0
27	a	1	54	41	12	1	0	0
27	a	1	54	41	12	1	0	0
27	b	1	54	41	12	1	0	0
27	f	1	43	30	12	1	0	0
27	l	1	54	41	12	1	0	0

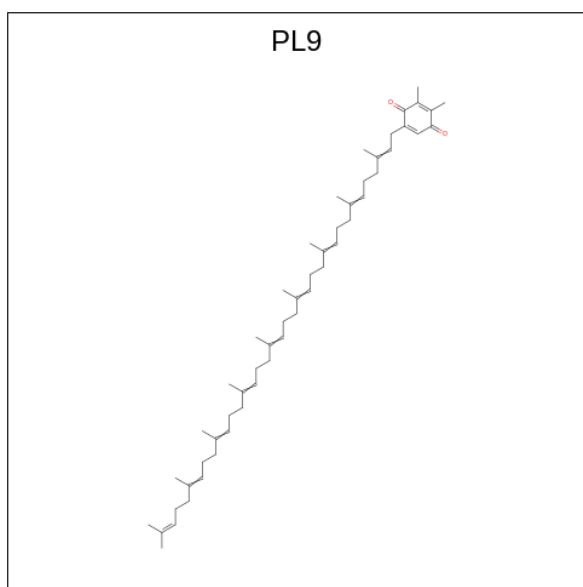
- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
28	A	1	51	41	10	0	0
28	B	1	51	41	10	0	0
28	C	1	51	41	10	0	0
28	C	1	51	41	10	0	0
28	D	1	51	41	10	0	0
28	a	1	51	41	10	0	0
28	b	1	51	41	10	0	0
28	c	1	51	41	10	0	0
28	c	1	51	41	10	0	0
28	d	1	51	41	10	0	0

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:  $C_{53}H_{80}O_2$ ) (labeled as "Ligand of Interest" by depositor).



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

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	4	Total	C	O	0	0
			57	52	5		
30	B	4	Total	C		0	0
			24	24			
30	C	3	Total	C	O	0	0
			54	49	5		
30	D	3	Total	C	O	0	0
			60	55	5		
30	E	4	Total	C		0	0
			22	22			
30	H	2	Total	C	O	0	0
			24	22	2		
30	I	7	Total	C		0	0
			79	79			
30	J	3	Total	C		0	0
			36	36			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	T	1	Total C 15 15	0	0
30	X	1	Total C 16 16	0	0
30	Z	3	Total C 20 20	0	0
30	a	2	Total C O 45 40 5	0	0
30	b	8	Total C O 87 85 2	0	0
30	c	6	Total C O 47 45 2	0	0
30	d	3	Total C O 65 58 7	0	0
30	e	2	Total C 15 15	0	0
30	h	3	Total C 29 29	0	0
30	i	5	Total C O 66 64 2	0	0
30	j	3	Total C 15 15	0	0
30	k	2	Total C O 39 34 5	0	0
30	l	1	Total C 13 13	0	0
30	m	1	Total C 11 11	0	0
30	t	1	Total C 12 12	0	0
30	y	1	Total C 4 4	0	0
30	x	4	Total C O 39 37 2	0	0

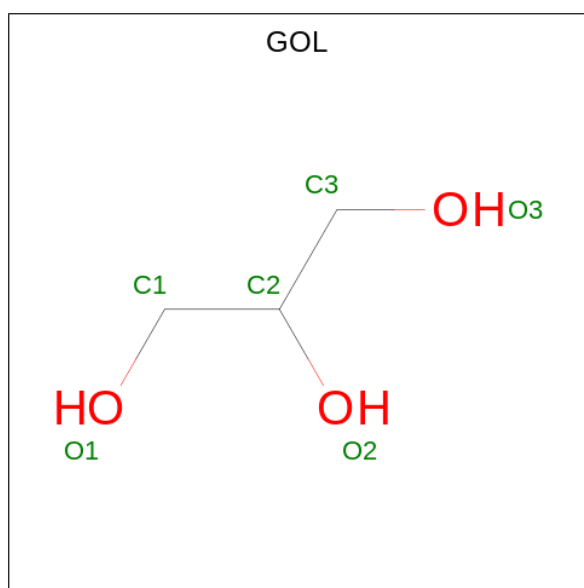
- Molecule 31 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	j	1	Total	C	O	0	0
			24	18	6		
31	m	1	Total	C	O	0	0
			35	24	11		
31	m	1	Total	C	O	0	0
			35	24	11		
31	t	1	Total	C	O	0	0
			23	18	5		
31	t	1	Total	C	O	0	0
			35	24	11		

- Molecule 32 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



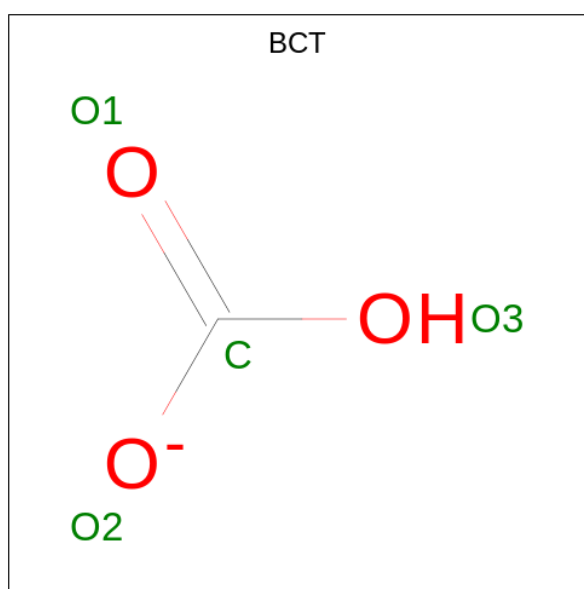
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			6	3	3		
32	B	1	Total	C	O	0	0
			6	3	3		
32	B	1	Total	C	O	0	0
			6	3	3		
32	C	1	Total	C	O	0	0
			6	3	3		
32	O	1	Total	C	O	0	0
			6	3	3		
32	V	1	Total	C	O	0	0
			6	3	3		

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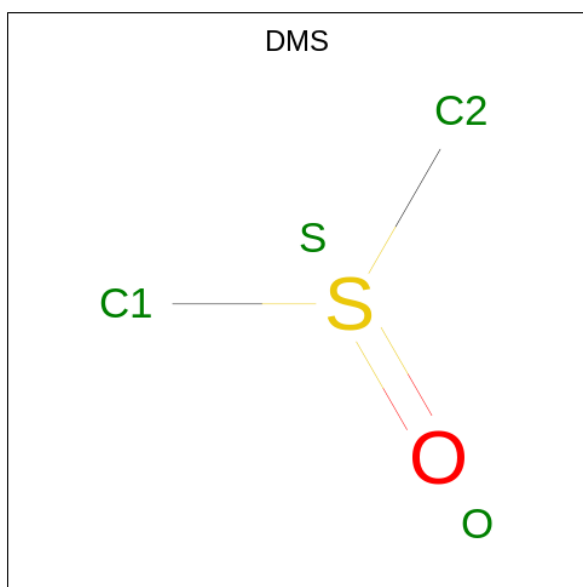
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	V	1	Total	C	O	0	0
			6	3	3		
32	a	1	Total	C	O	0	0
			6	3	3		
32	b	1	Total	C	O	0	0
			6	3	3		
32	c	1	Total	C	O	0	0
			6	3	3		

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



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

- Molecule 34 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $\text{C}_2\text{H}_6\text{OS}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	A	1	Total	C	O	S	0	0
			4	2	1	1		
34	A	1	Total	C	O	S	0	0
			4	2	1	1		
34	A	1	Total	C	O	S	0	0
			4	2	1	1		
34	A	1	Total	C	O	S	0	0
			4	2	1	1		
34	A	1	Total	C	O	S	0	0
			4	2	1	1		
34	B	1	Total	C	O	S	0	0
			4	2	1	1		
34	B	1	Total	C	O	S	0	0
			4	2	1	1		
34	B	1	Total	C	O	S	0	0
			4	2	1	1		
34	B	1	Total	C	O	S	0	0
			4	2	1	1		
34	B	1	Total	C	O	S	0	0
			4	2	1	1		
34	B	1	Total	C	O	S	0	0
			4	2	1	1		
34	B	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
34	B	1	4	2	1	1	0	0
34	B	1	4	2	1	1	0	0
34	B	1	4	2	1	1	0	0
34	C	1	4	2	1	1	0	0
34	C	1	4	2	1	1	0	0
34	C	1	4	2	1	1	0	0
34	C	1	4	2	1	1	0	0
34	C	1	4	2	1	1	0	0
34	C	1	4	2	1	1	0	0
34	C	1	4	2	1	1	0	0
34	C	1	4	2	1	1	0	0
34	C	1	4	2	1	1	0	0
34	C	1	4	2	1	1	0	0
34	C	1	4	2	1	1	0	0
34	C	1	4	2	1	1	0	0
34	D	1	4	2	1	1	0	0
34	D	1	4	2	1	1	0	0
34	D	1	4	2	1	1	0	0
34	D	1	4	2	1	1	0	0
34	H	1	4	2	1	1	0	0
34	K	1	4	2	1	1	0	0
34	L	1	4	2	1	1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	T	1	Total 4	C 2	O 1	S 1	0	0
34	U	1	Total 4	C 2	O 1	S 1	0	0
34	U	1	Total 4	C 2	O 1	S 1	0	0
34	U	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
34	V	1	4	2	1	1	0	0
34	V	1	4	2	1	1	0	0
34	V	1	4	2	1	1	0	0
34	V	1	4	2	1	1	0	0
34	a	1	4	2	1	1	0	0
34	a	1	4	2	1	1	0	0
34	a	1	4	2	1	1	0	0
34	a	1	4	2	1	1	0	0
34	a	1	4	2	1	1	0	0
34	a	1	4	2	1	1	0	0
34	a	1	4	2	1	1	0	0
34	a	1	4	2	1	1	0	0
34	b	1	4	2	1	1	0	0
34	b	1	4	2	1	1	0	0
34	b	1	4	2	1	1	0	0
34	b	1	4	2	1	1	0	0
34	b	1	4	2	1	1	0	0
34	b	1	4	2	1	1	0	0
34	b	1	4	2	1	1	0	0
34	b	1	4	2	1	1	0	0
34	b	1	4	2	1	1	0	0
34	b	1	4	2	1	1	0	0
34	b	1	4	2	1	1	0	0
34	b	1	4	2	1	1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	d	1	Total 4	C 2	O 1	S 1	0	0
34	d	1	Total 4	C 2	O 1	S 1	0	0
34	d	1	Total 4	C 2	O 1	S 1	0	0
34	d	1	Total 4	C 2	O 1	S 1	0	0
34	e	1	Total 4	C 2	O 1	S 1	0	0
34	e	1	Total 4	C 2	O 1	S 1	0	0
34	e	1	Total 4	C 2	O 1	S 1	0	0
34	h	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	i	1	Total	C	O	S	0	0
			4	2	1	1		
34	o	1	Total	C	O	S	0	0
			4	2	1	1		
34	o	1	Total	C	O	S	0	0
			4	2	1	1		
34	o	1	Total	C	O	S	0	0
			4	2	1	1		
34	o	1	Total	C	O	S	0	0
			4	2	1	1		
34	o	1	Total	C	O	S	0	0
			4	2	1	1		
34	u	1	Total	C	O	S	0	0
			4	2	1	1		
34	u	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	y	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 35 is CALCIUM ION (three-letter code: CA) (formula: Ca).

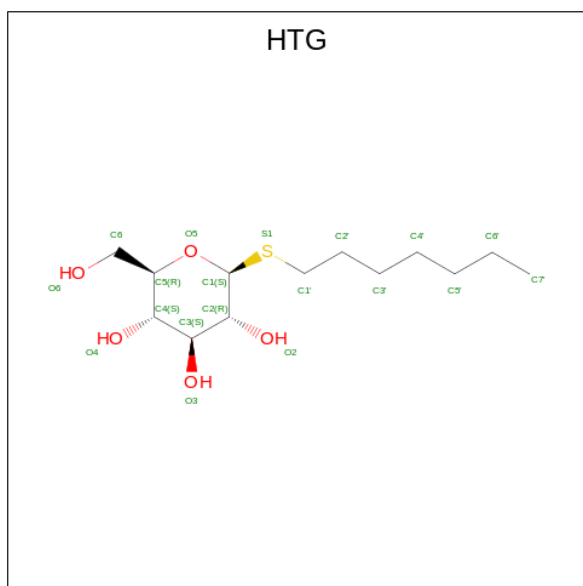
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	B	1	Total	Ca	0	0
			1	1		

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

- Molecule 36 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula:  $C_{13}H_{26}O_5S$ ).



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

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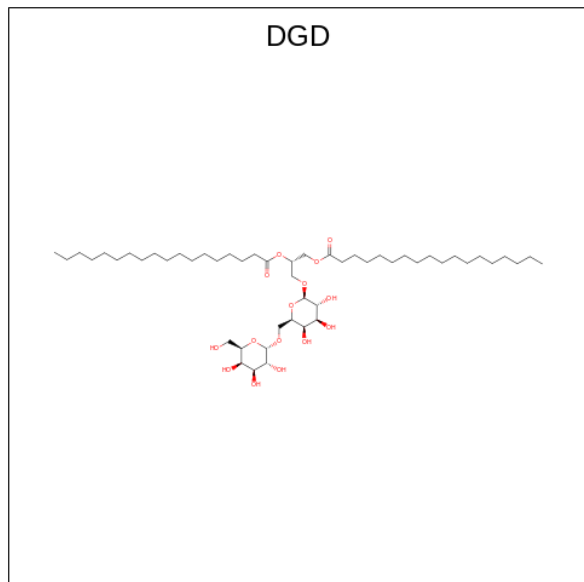
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	D	1	Total	C	O	S	0	0
			19	13	5	1		
36	O	1	Total	C	O	S	0	0
			19	13	5	1		
36	O	1	Total	C	O	S	0	0
			19	13	5	1		
36	U	1	Total	C			0	0
			4	4				
36	V	1	Total	C	O	S	0	0
			13	7	5	1		
36	V	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			17	11	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
36	d	1	Total 19	C 13	O 5	S 1	0	0
36	d	1	Total 19	C 13	O 5	S 1	0	0
36	d	1	Total 19	C 13	O 5	S 1	0	0
36	v	1	Total 19	C 13	O 5	S 1	0	0
36	y	1	Total 19	C 13	O 5	S 1	0	0

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



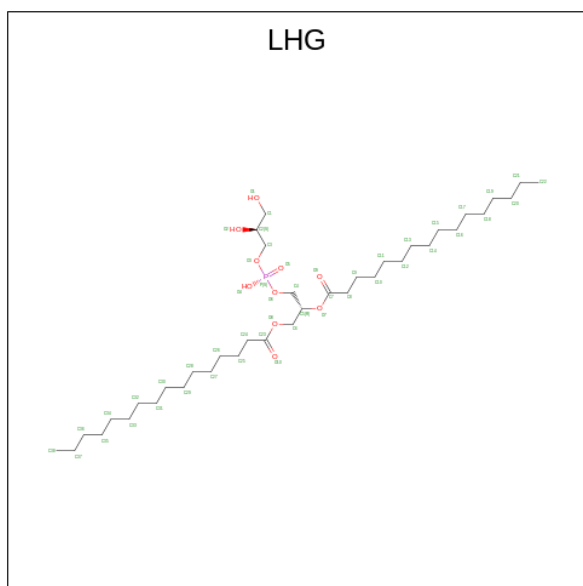
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
37	C	1	Total 62	C 47	O 15	0	0
37	C	1	Total 62	C 47	O 15	0	0
37	C	1	Total 62	C 47	O 15	0	0
37	D	1	Total 52	C 42	O 10	0	0
37	H	1	Total 62	C 47	O 15	0	0
37	c	1	Total 62	C 47	O 15	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	c	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	d	1	Total	C	O	0	0
			50	41	9		
37	h	1	Total	C	O	0	0
			62	47	15		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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
			46	35	10	1		
38	E	1	Total	C	O	P	0	0
			42	31	10	1		
38	L	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		

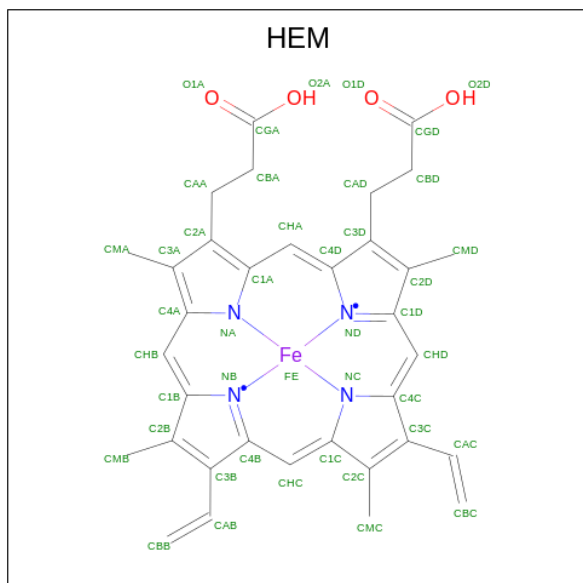
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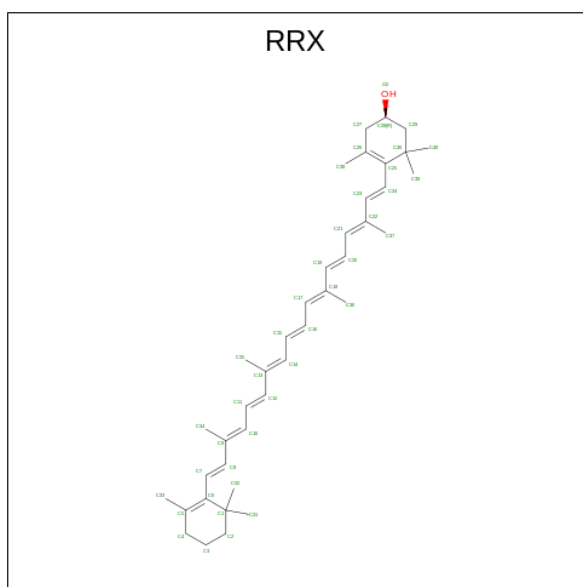
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	d	1	Total	C	O	P	0	0
			47	36	10	1		
38	l	1	Total	C	O	P	0	0
			49	38	10	1		

- 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	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
39	f	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 40 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula:  $C_{40}H_{56}O$ ).

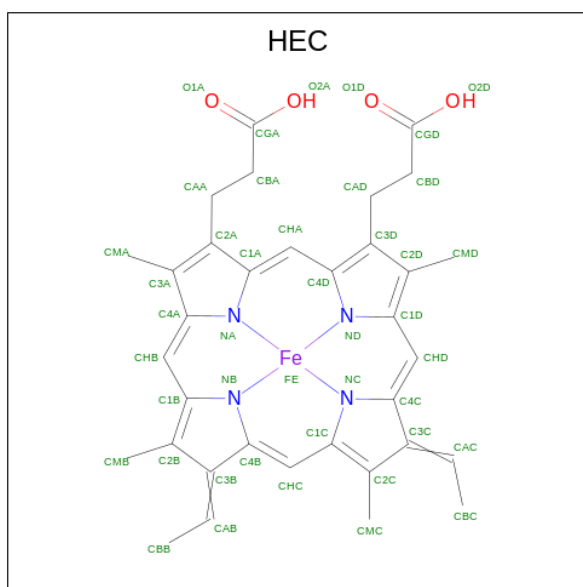


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	H	1	Total	C O	0	0
			41	40 1		
40	h	1	Total	C O	0	0
			41	40 1		

- Molecule 41 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 42 is HEME C (three-letter code: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

- Molecule 43 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
43	A	158	Total	O	0	1
			159	159		
43	B	406	Total	O	0	6
			411	411		
43	C	293	Total	O	0	2
			295	295		
43	D	173	Total	O	0	4
			177	177		
43	E	35	Total	O	0	0
			35	35		
43	F	15	Total	O	0	0
			15	15		
43	H	51	Total	O	0	0
			51	51		
43	I	11	Total	O	0	0
			11	11		
43	J	15	Total	O	0	0
			15	15		
43	K	9	Total	O	0	0
			9	9		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
43	L	16	Total O 16 16	0	0
43	M	20	Total O 20 20	0	0
43	O	217	Total O 224 224	0	7
43	T	14	Total O 14 14	0	0
43	U	116	Total O 117 117	0	1
43	V	153	Total O 157 157	0	4
43	Y	6	Total O 6 6	0	0
43	X	22	Total O 22 22	0	0
43	Z	4	Total O 4 4	0	0
43	a	157	Total O 159 159	0	2
43	b	394	Total O 399 399	0	5
43	c	316	Total O 320 320	0	5
43	d	170	Total O 172 172	0	2
43	e	38	Total O 39 39	0	1
43	f	12	Total O 12 12	0	0
43	h	51	Total O 52 52	0	1
43	i	12	Total O 12 12	0	0
43	j	12	Total O 12 12	0	0
43	k	6	Total O 6 6	0	0
43	l	20	Total O 20 20	0	0
43	m	20	Total O 20 20	0	0

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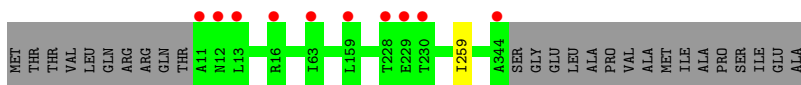
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
43	o	194	Total 198	O 198	0	4
43	t	23	Total 24	O 24	0	1
43	u	117	Total 119	O 119	0	2
43	v	116	Total 118	O 118	0	2
43	y	8	Total 8	O 8	0	0
43	x	14	Total 14	O 14	0	0
43	z	6	Total 6	O 6	0	0

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

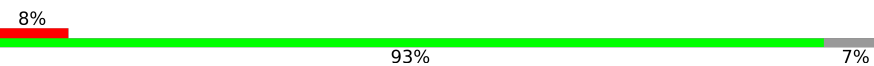
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

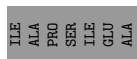
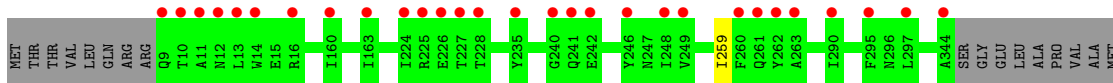
- Molecule 1: Photosystem II protein D1 2

Chain A: 



- Molecule 1: Photosystem II protein D1 2

Chain a: 



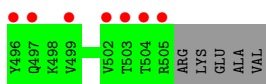
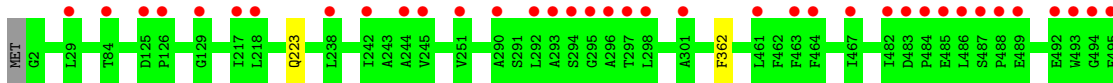
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B: 



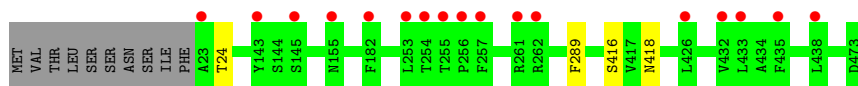
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b: 

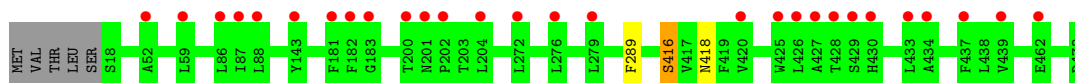


- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 



- Molecule 3: Photosystem II CP43 reaction center protein



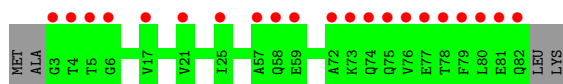
- Molecule 4: Photosystem II D2 protein



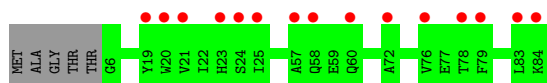
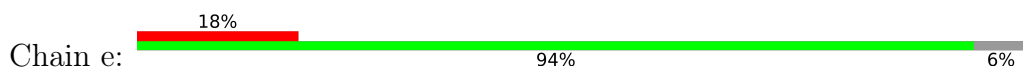
- Molecule 4: Photosystem II D2 protein



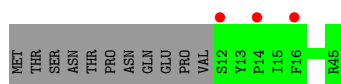
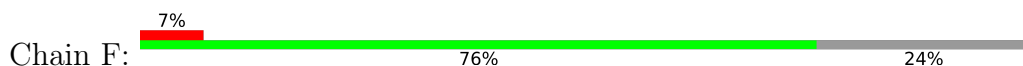
- Molecule 5: Cytochrome b559 subunit alpha



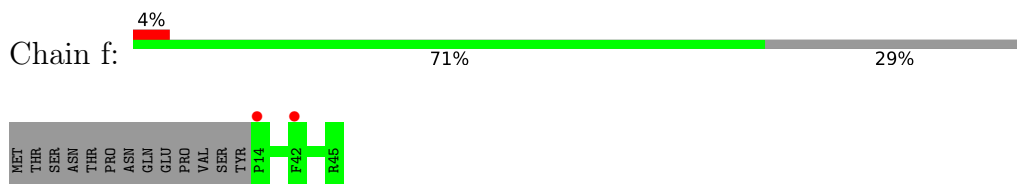
- Molecule 5: Cytochrome b559 subunit alpha



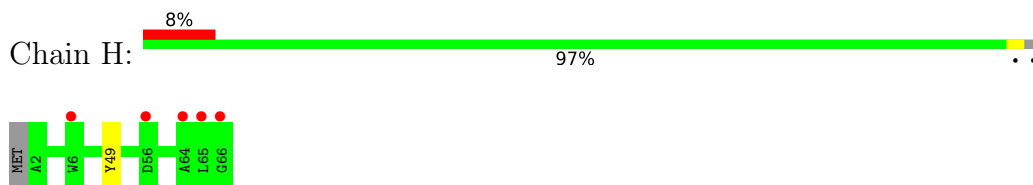
- Molecule 6: Cytochrome b559 subunit beta



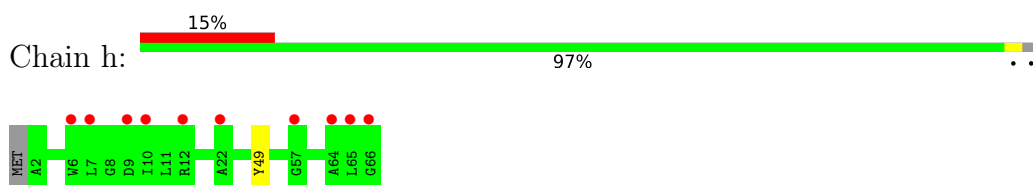
- Molecule 6: Cytochrome b559 subunit beta



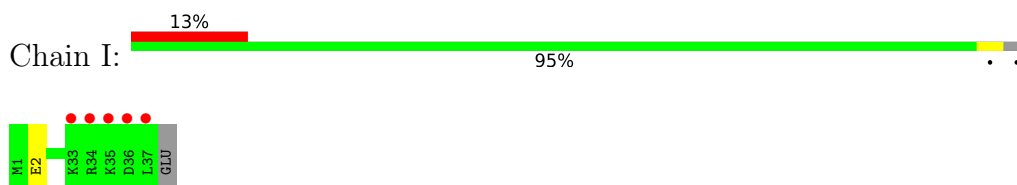
- Molecule 7: Photosystem II reaction center protein H



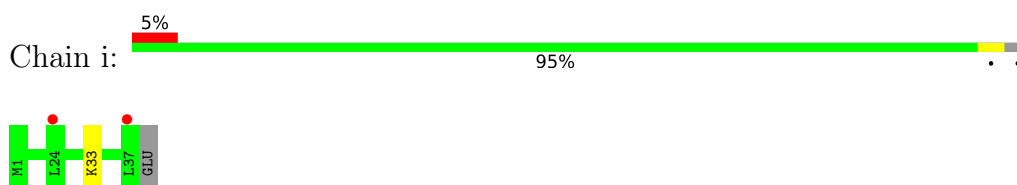
- Molecule 7: Photosystem II reaction center protein H



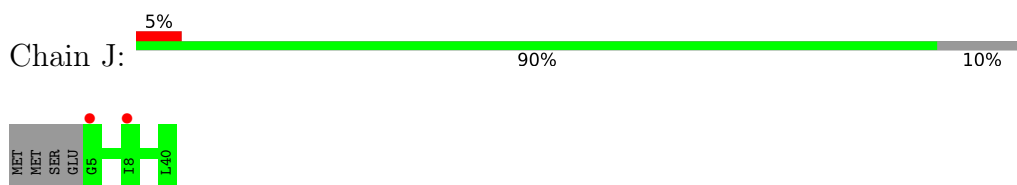
- Molecule 8: Photosystem II reaction center protein I



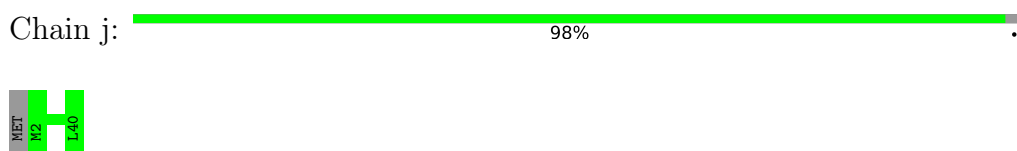
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J

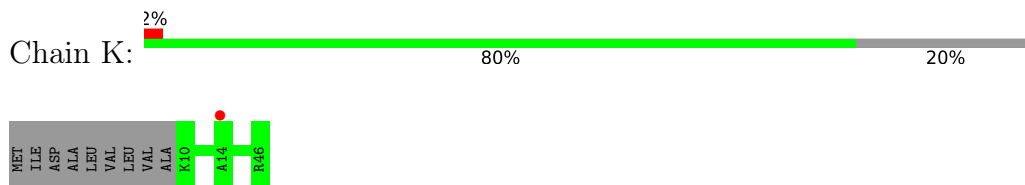


- Molecule 9: Photosystem II reaction center protein J

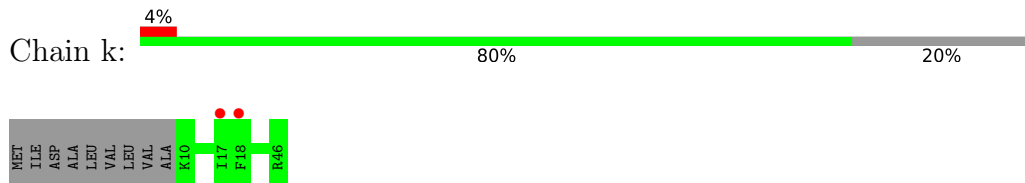




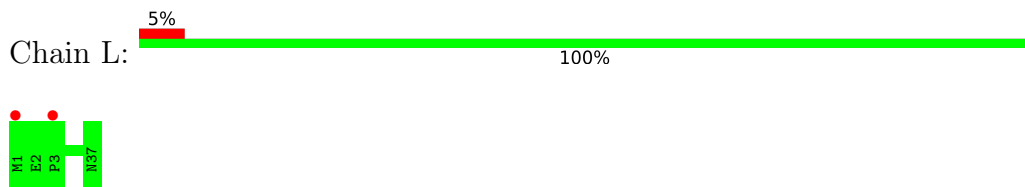
- Molecule 10: Photosystem II reaction center protein K



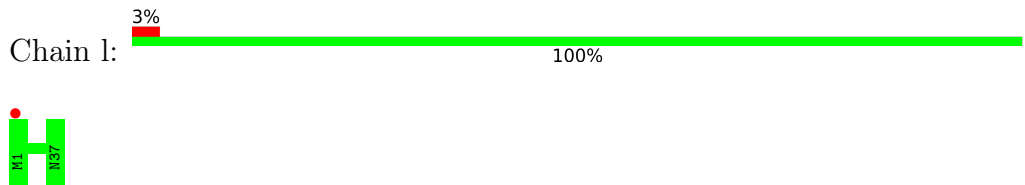
- Molecule 10: Photosystem II reaction center protein K



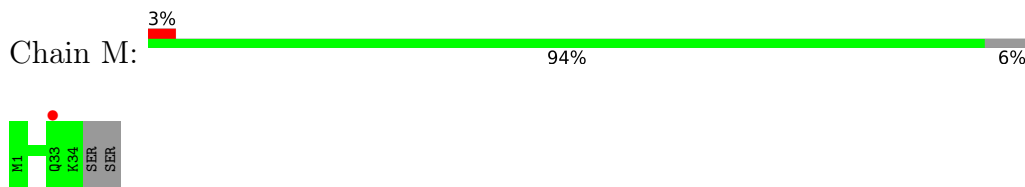
- Molecule 11: Photosystem II reaction center protein L



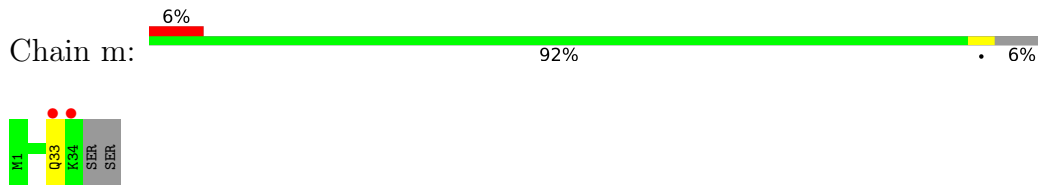
- Molecule 11: Photosystem II reaction center protein L



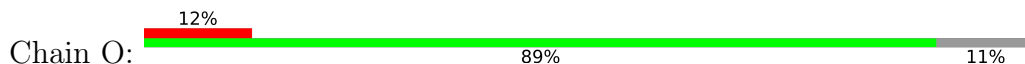
- Molecule 12: Photosystem II reaction center protein M

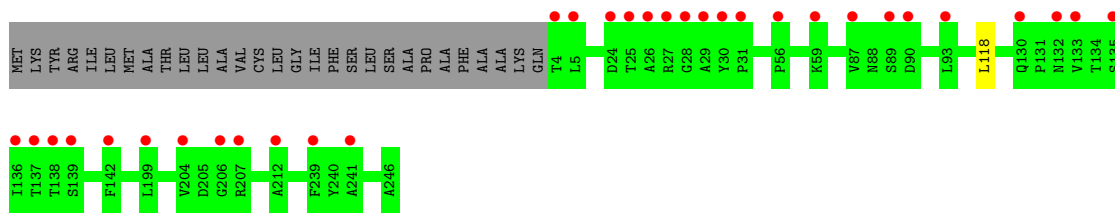


- Molecule 12: Photosystem II reaction center protein M

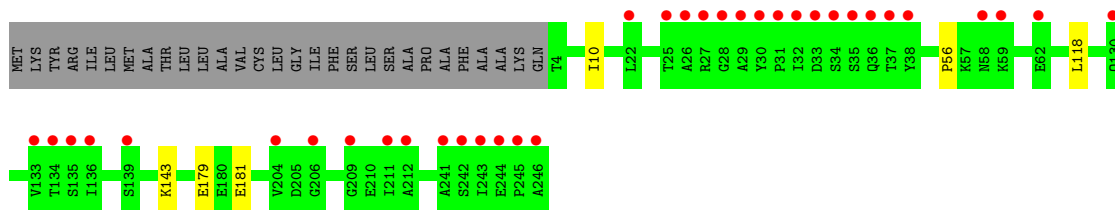
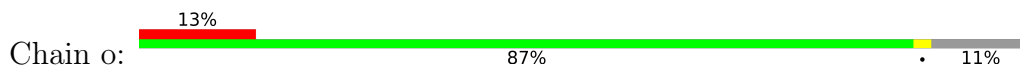


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

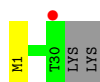
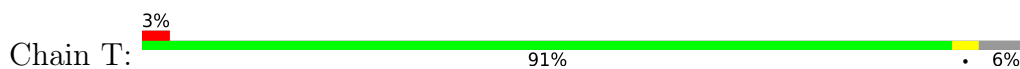




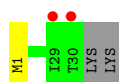
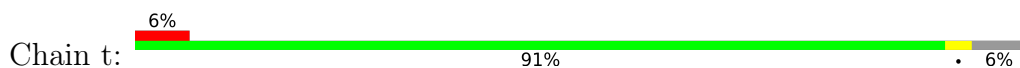
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



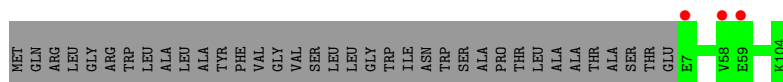
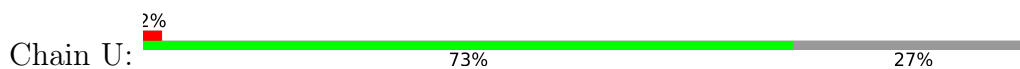
- Molecule 14: Photosystem II reaction center protein T



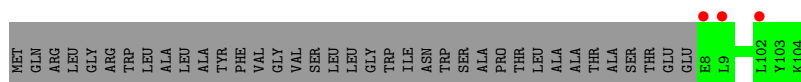
- Molecule 14: Photosystem II reaction center protein T



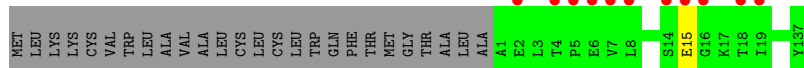
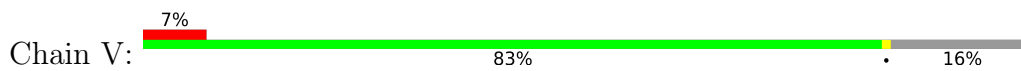
- Molecule 15: Photosystem II 12 kDa extrinsic protein



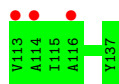
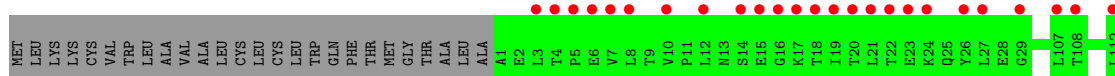
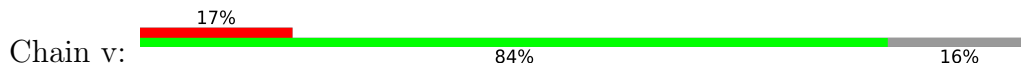
- Molecule 15: Photosystem II 12 kDa extrinsic protein



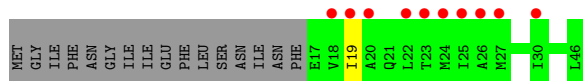
- Molecule 16: Cytochrome c-550



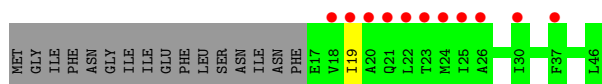
• Molecule 16: Cytochrome c-550



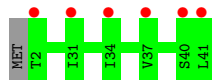
• Molecule 17: Photosystem II reaction center protein Ycf12



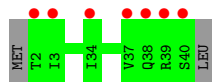
• Molecule 17: Photosystem II reaction center protein Ycf12



• Molecule 18: Photosystem II reaction center X protein

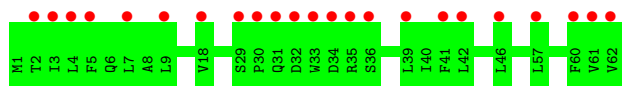


• Molecule 18: Photosystem II reaction center X protein

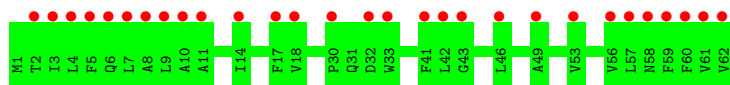


• Molecule 19: Photosystem II reaction center protein Z

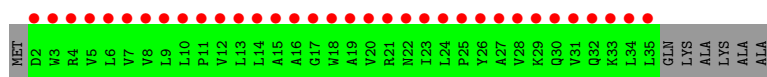
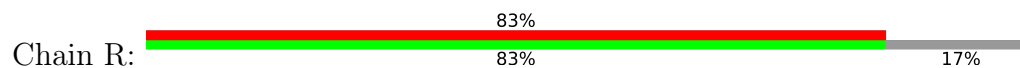




- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.14Å 228.17Å 286.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 48.98 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-1.90) 99.8 (48.98-1.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.15 (at 1.90Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660, REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.151 , 0.184 0.151 , 0.185	Depositor DCC
$R_{free}$ test set	31121 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.0	Xtrriage
Anisotropy	0.693	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 73.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	55630	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HTG, CL, HEM, OEX, LMT, PHO, UNL, FE2, PL9, BCT, FME, HEC, LHG, CA, GOL, MG, BCR, RRX, DGD, DMS, LMG, CLA, 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	0.45	0/2693	0.54	0/3680
1	a	0.43	0/2723	0.54	0/3719
2	B	0.42	0/4156	0.54	0/5665
2	b	0.41	0/4122	0.54	0/5623
3	C	0.39	0/3638	0.51	0/4954
3	c	0.39	0/3655	0.51	0/4976
4	D	0.48	0/2811	0.56	1/3833 (0.0%)
4	d	0.44	0/2825	0.54	1/3850 (0.0%)
5	E	0.37	0/651	0.49	0/892
5	e	0.32	0/669	0.49	0/913
6	F	0.36	0/284	0.46	0/387
6	f	0.37	0/274	0.44	0/372
7	H	0.36	0/518	0.51	0/706
7	h	0.32	0/532	0.48	0/723
8	I	0.31	0/298	0.43	0/403
8	i	0.33	0/294	0.47	0/398
9	J	0.36	0/257	0.47	0/349
9	j	0.33	0/276	0.49	0/374
10	K	0.34	0/299	0.43	0/412
10	k	0.33	0/299	0.45	0/412
11	L	0.47	0/324	0.53	0/441
11	l	0.48	0/315	0.48	0/428
12	M	0.41	0/266	0.53	0/363
12	m	0.39	0/270	0.51	0/368
13	O	0.37	0/1956	0.57	0/2653
13	o	0.38	0/1925	0.58	0/2611
14	T	0.48	0/266	0.53	0/362
14	t	0.42	0/266	0.52	0/362
15	U	0.40	0/778	0.55	0/1057
15	u	0.40	0/785	0.56	0/1064
16	V	0.39	0/1122	0.54	0/1522

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	v	0.32	0/1097	0.51	0/1491
17	Y	0.29	0/219	0.43	0/294
17	y	0.26	0/233	0.42	0/312
18	X	0.28	0/289	0.42	0/391
18	x	0.28	0/289	0.44	0/391
19	Z	0.31	0/459	0.39	0/630
19	z	0.29	0/456	0.37	0/626
20	R	0.26	0/232	0.46	0/321
All	All	0.40	0/42821	0.53	2/58328 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	272	LEU	CA-CB-CG	5.83	128.70	115.30
4	D	272	LEU	CA-CB-CG	5.05	126.93	115.30

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	334/360 (93%)	329 (98%)	4 (1%)	1 (0%)	41	31
1	a	337/360 (94%)	332 (98%)	4 (1%)	1 (0%)	41	31
2	B	511/510 (100%)	503 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	511/510 (100%)	503 (98%)	8 (2%)	0	100	100
3	C	455/461 (99%)	445 (98%)	8 (2%)	2 (0%)	34	24
3	c	457/461 (99%)	446 (98%)	10 (2%)	1 (0%)	47	38
4	D	341/352 (97%)	334 (98%)	7 (2%)	0	100	100
4	d	342/352 (97%)	335 (98%)	7 (2%)	0	100	100
5	E	79/84 (94%)	79 (100%)	0	0	100	100
5	e	79/84 (94%)	79 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	31/45 (69%)	31 (100%)	0	0	100	100
7	H	63/66 (96%)	59 (94%)	4 (6%)	0	100	100
7	h	64/66 (97%)	63 (98%)	1 (2%)	0	100	100
8	I	35/38 (92%)	33 (94%)	2 (6%)	0	100	100
8	i	35/38 (92%)	33 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
9	j	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	37/37 (100%)	37 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/36 (92%)	33 (100%)	0	0	100	100
12	m	33/36 (92%)	33 (100%)	0	0	100	100
13	O	251/272 (92%)	246 (98%)	5 (2%)	0	100	100
13	o	246/272 (90%)	241 (98%)	5 (2%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	96/134 (72%)	93 (97%)	3 (3%)	0	100	100
15	u	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
16	V	139/163 (85%)	136 (98%)	3 (2%)	0	100	100
16	v	137/163 (84%)	134 (98%)	3 (2%)	0	100	100
17	Y	28/46 (61%)	28 (100%)	0	0	100	100
17	y	29/46 (63%)	29 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	X	38/41 (93%)	37 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
19	z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
20	R	32/41 (78%)	32 (100%)	0	0	100	100
All	All	5292/5691 (93%)	5194 (98%)	93 (2%)	5 (0%)	51	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416	SER
1	A	259	ILE
1	a	259	ILE

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	266/290 (92%)	266 (100%)	0	100	100
1	a	271/290 (93%)	271 (100%)	0	100	100
2	B	405/407 (100%)	404 (100%)	1 (0%)	93	94
2	b	397/407 (98%)	395 (100%)	2 (0%)	88	89
3	C	357/362 (99%)	354 (99%)	3 (1%)	81	82
3	c	358/362 (99%)	355 (99%)	3 (1%)	81	82
4	D	275/283 (97%)	274 (100%)	1 (0%)	91	91
4	d	277/283 (98%)	275 (99%)	2 (1%)	84	84
5	E	65/73 (89%)	65 (100%)	0	100	100
5	e	68/73 (93%)	68 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	27/39 (69%)	27 (100%)	0	100	100
7	H	52/55 (94%)	51 (98%)	1 (2%)	57	53
7	h	54/55 (98%)	53 (98%)	1 (2%)	57	53
8	I	32/34 (94%)	31 (97%)	1 (3%)	40	32
8	i	31/34 (91%)	30 (97%)	1 (3%)	39	30
9	J	23/28 (82%)	23 (100%)	0	100	100
9	j	25/28 (89%)	25 (100%)	0	100	100
10	K	29/37 (78%)	29 (100%)	0	100	100
10	k	29/37 (78%)	29 (100%)	0	100	100
11	L	36/35 (103%)	36 (100%)	0	100	100
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	30/32 (94%)	30 (100%)	0	100	100
12	m	31/32 (97%)	30 (97%)	1 (3%)	39	30
13	O	211/228 (92%)	210 (100%)	1 (0%)	88	89
13	o	208/228 (91%)	201 (97%)	7 (3%)	37	28
14	T	27/28 (96%)	27 (100%)	0	100	100
14	t	27/28 (96%)	27 (100%)	0	100	100
15	U	81/112 (72%)	81 (100%)	0	100	100
15	u	84/112 (75%)	84 (100%)	0	100	100
16	V	121/138 (88%)	119 (98%)	2 (2%)	60	57
16	v	117/138 (85%)	117 (100%)	0	100	100
17	Y	22/37 (60%)	21 (96%)	1 (4%)	27	18
17	y	24/37 (65%)	23 (96%)	1 (4%)	30	20
18	X	30/34 (88%)	30 (100%)	0	100	100
18	x	31/34 (91%)	31 (100%)	0	100	100
19	Z	45/51 (88%)	45 (100%)	0	100	100
19	z	44/51 (86%)	44 (100%)	0	100	100
20	R	16/33 (48%)	16 (100%)	0	100	100
All	All	4289/4639 (92%)	4260 (99%)	29 (1%)	86	84

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	362	PHE
3	C	24	THR
3	C	289	PHE
3	C	418	ASN
4	D	180	ARG
7	H	49	TYR
8	I	2	GLU
13	O	118	LEU
16	V	15[A]	GLU
16	V	15[B]	GLU
17	Y	19	ILE
2	b	223	GLN
2	b	362	PHE
3	c	289	PHE
3	c	416	SER
3	c	418	ASN
4	d	90	LEU
4	d	180	ARG
7	h	49	TYR
8	i	33	LYS
12	m	33	GLN
13	o	10	ILE
13	o	56	PRO
13	o	118	LEU
13	o	143	LYS
13	o	179[A]	GLU
13	o	179[B]	GLU
13	o	181	GLU
17	y	19	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	332	GLN
17	y	21	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains

8 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	1.00	0	7,9,11	0.47	0
19	FME	z	1	19	8,9,10	0.90	0	7,9,11	1.05	0
14	FME	T	1	14	8,9,10	0.99	0	7,9,11	1.40	1 (14%)
12	FME	m	1	12	8,9,10	0.95	0	7,9,11	0.83	0
19	FME	Z	1	19	8,9,10	0.91	0	7,9,11	1.01	0
8	FME	I	1	8	8,9,10	0.91	0	7,9,11	0.97	0
14	FME	t	1	14	8,9,10	0.99	0	7,9,11	1.48	1 (14%)
8	FME	i	1	8	8,9,10	0.92	0	7,9,11	0.86	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	-	0/7/9/11	-
19	FME	z	1	19	-	2/7/9/11	-
14	FME	T	1	14	-	2/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
19	FME	Z	1	19	-	2/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
14	FME	t	1	14	-	4/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	C-CA-N	2.59	114.41	109.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	C-CA-N	2.11	113.55	109.73

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	1	FME	N-CA-CB-CG
19	Z	1	FME	CA-CB-CG-SD
14	t	1	FME	N-CA-CB-CG
14	t	1	FME	O-C-CA-CB
19	z	1	FME	CA-CB-CG-SD
19	Z	1	FME	CB-CG-SD-CE
14	t	1	FME	CB-CG-SD-CE
14	T	1	FME	C-CA-CB-CG
14	t	1	FME	C-CA-CB-CG
19	z	1	FME	C-CA-CB-CG

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 414 ligands modelled in this entry, 15 are monoatomic and 77 are unknown - leaving 322 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
26	BCR	T	101	-	41,41,41	0.71	0	56,56,56	1.69	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	B	603	-	65,73,73	2.36	19 (29%)	76,113,113	2.63	29 (38%)
24	CLA	B	614	-	65,73,73	2.31	18 (27%)	76,113,113	2.57	28 (36%)
34	DMS	c	939	-	3,3,3	2.69	1 (33%)	3,3,3	0.57	0
38	LHG	d	409	-	48,48,48	0.89	2 (4%)	51,54,54	1.15	5 (9%)
36	HTG	c	942	-	19,19,19	1.02	2 (10%)	23,24,24	1.32	4 (17%)
34	DMS	C	530	-	3,3,3	2.68	1 (33%)	3,3,3	0.56	0
36	HTG	v	211	-	19,19,19	1.06	2 (10%)	23,24,24	1.63	4 (17%)
34	DMS	y	101	-	3,3,3	2.66	1 (33%)	3,3,3	0.54	0
34	DMS	v	206	-	3,3,3	2.71	1 (33%)	3,3,3	0.55	0
37	DGD	c	918	-	63,63,67	0.82	2 (3%)	77,77,81	1.00	4 (5%)
31	LMT	A	417	-	36,36,36	0.47	0	47,47,47	1.19	3 (6%)
24	CLA	b	618	-	65,73,73	2.38	19 (29%)	76,113,113	2.60	26 (34%)
32	GOL	V	206	-	5,5,5	0.85	0	5,5,5	0.96	0
34	DMS	d	416	-	3,3,3	2.66	1 (33%)	3,3,3	0.43	0
24	CLA	b	610	-	65,73,73	2.48	18 (27%)	76,113,113	2.47	25 (32%)
24	CLA	A	406	43	65,73,73	2.34	20 (30%)	76,113,113	2.69	24 (31%)
24	CLA	b	617	-	65,73,73	2.49	19 (29%)	76,113,113	2.54	25 (32%)
34	DMS	C	534	-	3,3,3	2.65	1 (33%)	3,3,3	0.42	0
36	HTG	U	201	-	3,3,19	0.34	0	2,2,24	0.71	0
37	DGD	C	518	-	63,63,67	0.82	2 (3%)	77,77,81	0.99	4 (5%)
34	DMS	O	311	-	3,3,3	2.66	1 (33%)	3,3,3	0.57	0
36	HTG	C	536	-	19,19,19	1.09	2 (10%)	23,24,24	1.29	1 (4%)
34	DMS	B	643	-	3,3,3	2.66	1 (33%)	3,3,3	0.51	0
34	DMS	v	209	-	3,3,3	2.65	1 (33%)	3,3,3	0.52	0
31	LMT	j	102	-	24,24,36	0.54	1 (4%)	29,29,47	0.90	0
31	LMT	B	626	-	24,24,36	0.47	0	29,29,47	1.13	2 (6%)
36	HTG	C	520	-	19,19,19	1.01	2 (10%)	23,24,24	1.29	1 (4%)
34	DMS	d	418	-	3,3,3	2.66	1 (33%)	3,3,3	0.47	0
36	HTG	c	923	-	19,19,19	1.03	2 (10%)	23,24,24	1.53	2 (8%)
24	CLA	C	508	-	65,73,73	2.53	18 (27%)	76,113,113	2.45	25 (32%)
24	CLA	b	619	-	65,73,73	2.43	20 (30%)	76,113,113	2.39	27 (35%)
31	LMT	M	102	-	25,25,36	0.48	0	30,30,47	0.93	1 (3%)
21	OEX	A	401	43,3,1	0,15,15	-	-	-	-	-
27	SQD	A	412	-	53,54,54	0.96	3 (5%)	62,65,65	1.69	12 (19%)
34	DMS	A	427	-	3,3,3	2.68	1 (33%)	3,3,3	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	DMS	v	207	-	3,3,3	2.67	1 (33%)	3,3,3	0.51	0
24	CLA	C	506	-	65,73,73	2.57	20 (30%)	76,113,113	2.45	26 (34%)
34	DMS	B	647	-	3,3,3	2.67	1 (33%)	3,3,3	0.58	0
33	BCT	A	422	22	2,3,3	0.64	0	2,3,3	0.61	0
34	DMS	D	414	-	3,3,3	2.66	1 (33%)	3,3,3	0.53	0
28	LMG	a	416	-	51,51,55	0.95	3 (5%)	59,59,63	1.29	9 (15%)
25	PHO	A	408	-	51,69,69	1.75	7 (13%)	47,99,99	1.66	9 (19%)
34	DMS	D	415	-	3,3,3	2.71	1 (33%)	3,3,3	0.54	0
24	CLA	c	907	-	65,73,73	2.49	20 (30%)	76,113,113	2.46	24 (31%)
31	LMT	F	103	-	24,24,36	0.45	0	29,29,47	0.58	0
34	DMS	L	102	-	3,3,3	2.65	1 (33%)	3,3,3	0.54	0
28	LMG	C	519	-	51,51,55	0.91	2 (3%)	59,59,63	1.19	6 (10%)
34	DMS	v	203	-	3,3,3	2.63	1 (33%)	3,3,3	0.40	0
36	HTG	c	941	-	19,19,19	1.00	1 (5%)	23,24,24	1.84	5 (21%)
34	DMS	A	425	-	3,3,3	2.68	1 (33%)	3,3,3	0.59	0
34	DMS	O	312	-	3,3,3	2.67	1 (33%)	3,3,3	0.49	0
27	SQD	l	101	-	53,54,54	1.03	4 (7%)	62,65,65	1.35	5 (8%)
34	DMS	O	313	-	3,3,3	2.68	1 (33%)	3,3,3	0.55	0
24	CLA	b	607	-	65,73,73	2.43	20 (30%)	76,113,113	2.46	25 (32%)
26	BCR	b	621	-	41,41,41	0.74	0	56,56,56	1.47	9 (16%)
34	DMS	v	208	-	3,3,3	2.66	1 (33%)	3,3,3	0.51	0
34	DMS	C	527	-	3,3,3	2.64	1 (33%)	3,3,3	0.49	0
26	BCR	B	619	-	41,41,41	0.88	0	56,56,56	1.15	6 (10%)
34	DMS	O	302	-	3,3,3	2.68	1 (33%)	3,3,3	0.62	0
24	CLA	A	407	43	65,73,73	2.16	20 (30%)	76,113,113	2.65	26 (34%)
34	DMS	C	526	-	3,3,3	2.63	1 (33%)	3,3,3	0.40	0
24	CLA	c	904	-	65,73,73	2.72	20 (30%)	76,113,113	2.27	26 (34%)
34	DMS	C	528	-	3,3,3	2.69	1 (33%)	3,3,3	0.57	0
32	GOL	V	207	-	5,5,5	1.02	0	5,5,5	0.86	0
36	HTG	c	924	-	19,19,19	1.04	2 (10%)	23,24,24	1.30	2 (8%)
26	BCR	k	102	-	41,41,41	0.76	0	56,56,56	1.54	8 (14%)
31	LMT	A	421	-	36,36,36	0.43	0	47,47,47	0.99	1 (2%)
24	CLA	c	911	-	65,73,73	2.47	20 (30%)	76,113,113	2.42	23 (30%)
34	DMS	b	643	-	3,3,3	2.67	1 (33%)	3,3,3	0.54	0
42	HEC	v	202	16	32,50,50	2.33	6 (18%)	24,82,82	1.64	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	HTG	B	630	-	19,19,19	1.01	2 (10%)	23,24,24	1.35	3 (13%)
21	OEX	a	404	43,3,1	0,15,15	-	-	-		
34	DMS	o	306	-	3,3,3	2.70	1 (33%)	3,3,3	0.67	0
34	DMS	a	422	-	3,3,3	2.67	1 (33%)	3,3,3	0.50	0
28	LMG	c	921	-	51,51,55	0.96	2 (3%)	59,59,63	1.20	6 (10%)
34	DMS	H	104	7	3,3,3	2.65	1 (33%)	3,3,3	0.56	0
31	LMT	Z	101	-	36,36,36	0.42	0	47,47,47	0.91	1 (2%)
31	LMT	t	101	-	23,23,36	0.46	0	26,27,47	1.00	1 (3%)
26	BCR	B	618	-	41,41,41	0.76	0	56,56,56	1.32	5 (8%)
36	HTG	O	316	-	19,19,19	0.89	2 (10%)	23,24,24	1.29	2 (8%)
24	CLA	d	404	-	65,73,73	2.56	20 (30%)	76,113,113	2.53	26 (34%)
27	SQD	A	416	-	53,54,54	1.04	3 (5%)	62,65,65	1.11	5 (8%)
34	DMS	V	201	-	3,3,3	2.64	1 (33%)	3,3,3	0.46	0
24	CLA	B	606	-	65,73,73	2.35	20 (30%)	76,113,113	2.50	26 (34%)
24	CLA	d	405	-	65,73,73	2.29	20 (30%)	76,113,113	2.60	26 (34%)
34	DMS	V	205	-	3,3,3	2.66	1 (33%)	3,3,3	0.54	0
39	HEM	f	101	5,6	41,50,50	1.95	8 (19%)	45,82,82	1.68	8 (17%)
24	CLA	c	913	-	65,73,73	2.60	19 (29%)	76,113,113	2.51	25 (32%)
26	BCR	c	916	-	41,41,41	0.76	0	56,56,56	1.38	7 (12%)
34	DMS	c	931	-	3,3,3	2.63	1 (33%)	3,3,3	0.49	0
34	DMS	b	645	-	3,3,3	2.63	1 (33%)	3,3,3	0.49	0
32	GOL	b	637	-	5,5,5	0.91	0	5,5,5	0.97	0
28	LMG	D	409	41	51,51,55	0.83	2 (3%)	59,59,63	0.90	4 (6%)
34	DMS	A	426	-	3,3,3	2.67	1 (33%)	3,3,3	0.61	0
36	HTG	C	537	-	19,19,19	0.99	2 (10%)	23,24,24	1.48	3 (13%)
24	CLA	C	507	43	65,73,73	2.56	20 (30%)	76,113,113	2.51	25 (32%)
24	CLA	c	906	-	65,73,73	2.39	18 (27%)	76,113,113	2.36	25 (32%)
38	LHG	d	410	-	48,48,48	0.86	2 (4%)	51,54,54	0.91	3 (5%)
38	LHG	D	407	-	48,48,48	0.88	2 (4%)	51,54,54	0.91	3 (5%)
32	GOL	a	419	-	5,5,5	1.11	0	5,5,5	0.65	0
24	CLA	b	608	-	65,73,73	2.72	20 (30%)	76,113,113	2.54	25 (32%)
38	LHG	l	103	-	48,48,48	0.89	2 (4%)	51,54,54	1.04	5 (9%)
24	CLA	b	614	43	65,73,73	2.29	19 (29%)	76,113,113	2.44	25 (32%)
24	CLA	c	905	43	65,73,73	2.24	20 (30%)	76,113,113	2.65	29 (38%)
24	CLA	B	609	-	65,73,73	2.44	19 (29%)	76,113,113	2.36	24 (31%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	SQD	F	101	-	36,37,54	0.95	2 (5%)	44,47,65	1.94	9 (20%)
32	GOL	B	637	-	5,5,5	0.95	0	5,5,5	0.90	0
26	BCR	d	406	-	41,41,41	0.82	0	56,56,56	1.71	10 (17%)
34	DMS	O	310	-	3,3,3	2.67	1 (33%)	3,3,3	0.48	0
26	BCR	Y	101	-	41,41,41	0.78	0	56,56,56	1.53	10 (17%)
34	DMS	O	307	-	3,3,3	2.68	1 (33%)	3,3,3	0.51	0
36	HTG	C	521	-	19,19,19	1.05	2 (10%)	23,24,24	1.50	2 (8%)
34	DMS	b	638	-	3,3,3	2.73	1 (33%)	3,3,3	0.67	0
31	LMT	m	102	-	36,36,36	0.44	0	47,47,47	0.87	0
34	DMS	B	632	-	3,3,3	2.45	1 (33%)	3,3,3	0.38	0
24	CLA	a	413	-	65,73,73	2.20	19 (29%)	76,113,113	2.54	29 (38%)
24	CLA	B	608	43	65,73,73	2.27	18 (27%)	76,113,113	2.44	23 (30%)
37	DGD	C	516	-	63,63,67	0.83	3 (4%)	77,77,81	1.10	5 (6%)
24	CLA	a	409	-	65,73,73	2.41	20 (30%)	76,113,113	2.53	26 (34%)
34	DMS	u	202	-	3,3,3	2.61	1 (33%)	3,3,3	0.72	0
36	HTG	O	303	-	19,19,19	1.09	1 (5%)	23,24,24	1.15	2 (8%)
24	CLA	b	620	-	65,73,73	2.50	18 (27%)	76,113,113	2.55	26 (34%)
24	CLA	b	609	-	65,73,73	2.29	18 (27%)	76,113,113	2.62	25 (32%)
34	DMS	B	644	-	3,3,3	2.59	1 (33%)	3,3,3	0.32	0
36	HTG	b	627	-	19,19,19	1.11	2 (10%)	23,24,24	1.71	3 (13%)
38	LHG	L	101	-	48,48,48	0.96	2 (4%)	51,54,54	1.12	3 (5%)
24	CLA	c	912	3	65,73,73	2.39	18 (27%)	76,113,113	2.42	26 (34%)
24	CLA	B	605	-	65,73,73	2.33	20 (30%)	76,113,113	2.55	24 (31%)
34	DMS	i	106	-	3,3,3	2.67	1 (33%)	3,3,3	0.53	0
36	HTG	d	414	-	19,19,19	1.04	2 (10%)	23,24,24	1.70	3 (13%)
25	PHO	a	411	-	51,69,69	1.70	7 (13%)	47,99,99	1.72	10 (21%)
24	CLA	D	401	-	65,73,73	2.19	20 (30%)	76,113,113	2.74	25 (32%)
31	LMT	J	102	-	24,24,36	0.51	0	29,29,47	0.76	0
34	DMS	D	416	-	3,3,3	2.69	1 (33%)	3,3,3	0.56	0
36	HTG	d	420	-	19,19,19	1.01	2 (10%)	23,24,24	1.45	2 (8%)
34	DMS	c	938	-	3,3,3	2.67	1 (33%)	3,3,3	0.53	0
34	DMS	h	105	-	3,3,3	2.65	1 (33%)	3,3,3	0.37	0
34	DMS	o	305	-	3,3,3	2.65	1 (33%)	3,3,3	0.52	0
36	HTG	c	943	-	17,17,19	1.05	2 (11%)	21,22,24	1.42	1 (4%)
32	GOL	O	304	-	5,5,5	0.82	0	5,5,5	1.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	A	405	-	65,73,73	2.56	18 (27%)	76,113,113	2.47	25 (32%)
31	LMT	M	101	-	36,36,36	0.39	0	47,47,47	0.81	1 (2%)
31	LMT	c	927	-	36,36,36	0.43	0	47,47,47	0.89	3 (6%)
24	CLA	B	613	-	65,73,73	2.32	20 (30%)	76,113,113	2.40	21 (27%)
34	DMS	V	208	-	3,3,3	2.65	1 (33%)	3,3,3	0.53	0
24	CLA	b	605	43	65,73,73	2.51	19 (29%)	76,113,113	2.38	26 (34%)
28	LMG	d	412	41	51,51,55	0.90	2 (3%)	59,59,63	0.89	3 (5%)
34	DMS	T	103	-	3,3,3	2.65	1 (33%)	3,3,3	0.52	0
24	CLA	a	410	43	65,73,73	2.29	20 (30%)	76,113,113	2.62	26 (34%)
38	LHG	d	411	-	46,46,48	0.88	2 (4%)	49,52,54	1.02	4 (8%)
24	CLA	C	510	-	65,73,73	2.49	21 (32%)	76,113,113	2.51	30 (39%)
40	RRX	H	101	-	42,42,42	0.71	0	57,58,58	1.34	7 (12%)
34	DMS	O	309	-	3,3,3	2.64	1 (33%)	3,3,3	0.47	0
34	DMS	C	524	-	3,3,3	2.66	1 (33%)	3,3,3	0.50	0
24	CLA	C	512	-	65,73,73	2.58	19 (29%)	76,113,113	2.39	27 (35%)
34	DMS	b	632	-	3,3,3	2.63	1 (33%)	3,3,3	0.45	0
34	DMS	a	425	-	3,3,3	2.68	1 (33%)	3,3,3	0.52	0
34	DMS	O	305	-	3,3,3	2.67	1 (33%)	3,3,3	0.49	0
24	CLA	c	908	43	65,73,73	2.51	20 (30%)	76,113,113	2.59	28 (36%)
34	DMS	U	203	-	3,3,3	2.68	1 (33%)	3,3,3	0.86	0
31	LMT	c	922	-	36,36,36	0.50	1 (2%)	47,47,47	1.24	4 (8%)
31	LMT	B	622	-	36,36,36	0.43	0	47,47,47	1.58	10 (21%)
39	HEM	F	102	5,6	41,50,50	1.90	6 (14%)	45,82,82	1.71	7 (15%)
24	CLA	B	615	-	65,73,73	2.20	18 (27%)	76,113,113	2.64	27 (35%)
36	HTG	B	623	-	19,19,19	1.09	1 (5%)	23,24,24	1.24	1 (4%)
26	BCR	C	515	-	41,41,41	0.71	0	56,56,56	1.45	7 (12%)
37	DGD	c	917	-	63,63,67	0.84	2 (3%)	77,77,81	1.13	4 (5%)
29	PL9	A	414	-	55,55,55	0.60	1 (1%)	68,69,69	1.90	20 (29%)
31	LMT	t	102	-	36,36,36	0.43	0	47,47,47	0.85	1 (2%)
36	HTG	y	102	-	19,19,19	1.07	2 (10%)	23,24,24	1.19	1 (4%)
26	BCR	b	623	-	41,41,41	0.76	1 (2%)	56,56,56	1.46	13 (23%)
36	HTG	b	603	-	19,19,19	1.02	2 (10%)	23,24,24	1.40	3 (13%)
34	DMS	a	423	-	3,3,3	2.68	1 (33%)	3,3,3	0.66	0
34	DMS	V	214	-	3,3,3	2.66	1 (33%)	3,3,3	0.58	0
34	DMS	b	640	-	3,3,3	2.66	1 (33%)	3,3,3	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	DMS	c	930	-	3,3,3	2.53	1 (33%)	3,3,3	0.36	0
34	DMS	o	304	-	3,3,3	2.66	1 (33%)	3,3,3	0.51	0
28	LMG	b	624	-	51,51,55	0.95	2 (3%)	59,59,63	1.07	4 (6%)
34	DMS	V	211	-	3,3,3	2.68	1 (33%)	3,3,3	0.52	0
34	DMS	B	640	-	3,3,3	2.66	1 (33%)	3,3,3	0.49	0
34	DMS	a	420	-	3,3,3	2.51	1 (33%)	3,3,3	0.41	0
34	DMS	e	102	-	3,3,3	2.67	1 (33%)	3,3,3	0.56	0
34	DMS	B	634	-	3,3,3	2.69	1 (33%)	3,3,3	0.73	0
36	HTG	b	602	-	19,19,19	1.02	2 (10%)	23,24,24	1.38	3 (13%)
24	CLA	C	502	-	65,73,73	2.57	20 (30%)	76,113,113	2.49	26 (34%)
37	DGD	H	102	-	63,63,67	0.89	3 (4%)	77,77,81	0.99	7 (9%)
34	DMS	b	642	-	3,3,3	2.68	1 (33%)	3,3,3	0.53	0
31	LMT	e	101	-	24,24,36	0.46	0	29,29,47	0.64	0
34	DMS	C	532	-	3,3,3	2.68	1 (33%)	3,3,3	0.58	0
34	DMS	c	934	-	3,3,3	2.69	1 (33%)	3,3,3	0.54	0
36	HTG	B	625	-	19,19,19	1.01	1 (5%)	23,24,24	1.94	4 (17%)
34	DMS	c	926	-	3,3,3	2.67	1 (33%)	3,3,3	0.51	0
36	HTG	V	204	-	12,13,19	0.61	0	16,18,24	2.11	5 (31%)
28	LMG	c	920	-	51,51,55	0.94	2 (3%)	59,59,63	1.12	4 (6%)
34	DMS	b	644	-	3,3,3	2.63	1 (33%)	3,3,3	0.53	0
24	CLA	B	616	-	65,73,73	2.44	18 (27%)	76,113,113	2.49	24 (31%)
34	DMS	v	205	-	3,3,3	2.67	1 (33%)	3,3,3	0.56	0
37	DGD	C	517	-	63,63,67	0.81	2 (3%)	77,77,81	1.06	6 (7%)
24	CLA	c	903	-	65,73,73	2.41	18 (27%)	76,113,113	2.43	24 (31%)
34	DMS	D	413	-	3,3,3	2.59	1 (33%)	3,3,3	0.48	0
26	BCR	k	103	-	41,41,41	0.72	0	56,56,56	1.30	6 (10%)
34	DMS	V	213	-	3,3,3	2.67	1 (33%)	3,3,3	0.63	0
26	BCR	c	915	-	41,41,41	0.74	0	56,56,56	1.37	6 (10%)
34	DMS	V	212	-	3,3,3	2.68	1 (33%)	3,3,3	0.64	0
28	LMG	B	621	-	51,51,55	0.95	2 (3%)	59,59,63	1.11	5 (8%)
34	DMS	V	209	-	3,3,3	2.60	1 (33%)	3,3,3	0.58	0
36	HTG	c	928	-	19,19,19	1.07	2 (10%)	23,24,24	1.49	3 (13%)
27	SQD	a	401	-	53,54,54	1.04	3 (5%)	62,65,65	1.11	3 (4%)
24	CLA	B	612	-	65,73,73	2.46	16 (24%)	76,113,113	2.62	29 (38%)
24	CLA	B	602	43	65,73,73	2.39	21 (32%)	76,113,113	2.42	26 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	DMS	C	533	-	3,3,3	2.66	1 (33%)	3,3,3	0.48	0
34	DMS	b	631	-	3,3,3	2.38	1 (33%)	3,3,3	0.42	0
28	LMG	A	413	-	51,51,55	0.95	2 (3%)	59,59,63	1.16	6 (10%)
34	DMS	B	642	-	3,3,3	2.67	1 (33%)	3,3,3	0.57	0
32	GOL	c	929	-	5,5,5	1.00	0	5,5,5	0.93	0
24	CLA	B	617	-	65,73,73	2.40	19 (29%)	76,113,113	2.58	27 (35%)
26	BCR	a	414	-	41,41,41	0.79	0	56,56,56	1.28	4 (7%)
27	SQD	f	102	-	42,43,54	1.19	3 (7%)	51,54,65	1.49	6 (11%)
34	DMS	O	314	-	3,3,3	2.67	1 (33%)	3,3,3	0.64	0
32	GOL	C	525	-	5,5,5	0.92	0	5,5,5	0.97	0
34	DMS	u	201	-	3,3,3	2.66	1 (33%)	3,3,3	0.82	0
24	CLA	C	503	-	65,73,73	2.70	19 (29%)	76,113,113	2.37	22 (28%)
34	DMS	B	639	-	3,3,3	2.64	1 (33%)	3,3,3	0.48	0
28	LMG	C	523	-	51,51,55	0.94	2 (3%)	59,59,63	1.27	8 (13%)
24	CLA	C	501	-	65,73,73	2.32	19 (29%)	76,113,113	2.50	24 (31%)
26	BCR	A	411	-	41,41,41	0.77	0	56,56,56	1.35	4 (7%)
24	CLA	C	505	-	65,73,73	2.68	19 (29%)	76,113,113	2.26	20 (26%)
32	GOL	B	638	-	5,5,5	1.06	0	5,5,5	1.20	1 (20%)
34	DMS	c	940	-	3,3,3	2.64	1 (33%)	3,3,3	0.46	0
34	DMS	U	202	-	3,3,3	2.66	1 (33%)	3,3,3	0.49	0
34	DMS	V	210	-	3,3,3	2.67	1 (33%)	3,3,3	0.57	0
36	HTG	b	626	-	19,19,19	0.85	1 (5%)	23,24,24	1.28	3 (13%)
24	CLA	C	509	-	65,73,73	2.49	20 (30%)	76,113,113	2.46	26 (34%)
27	SQD	b	601	-	53,54,54	1.05	4 (7%)	62,65,65	1.61	12 (19%)
34	DMS	c	937	-	3,3,3	2.63	1 (33%)	3,3,3	0.56	0
34	DMS	A	423	-	3,3,3	2.42	1 (33%)	3,3,3	0.73	0
24	CLA	D	402	-	65,73,73	2.27	19 (29%)	76,113,113	2.49	25 (32%)
34	DMS	B	645	-	3,3,3	2.68	1 (33%)	3,3,3	0.62	0
38	LHG	D	406	-	48,48,48	0.82	2 (4%)	51,54,54	1.19	7 (13%)
29	PL9	a	417	-	55,55,55	0.62	1 (1%)	68,69,69	1.80	17 (25%)
33	BCT	a	408[A]	22	2,3,3	0.65	0	2,3,3	0.75	0
34	DMS	v	204	-	3,3,3	2.64	1 (33%)	3,3,3	0.53	0
34	DMS	B	633	-	3,3,3	2.60	1 (33%)	3,3,3	0.38	0
26	BCR	b	622	-	41,41,41	0.85	0	56,56,56	1.10	4 (7%)
27	SQD	a	415	-	53,54,54	0.95	3 (5%)	62,65,65	1.68	11 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	DMS	O	306	-	3,3,3	2.67	1 (33%)	3,3,3	0.47	0
33	BCT	d	402[B]	22	2,3,3	0.68	0	2,3,3	0.47	0
34	DMS	O	308	-	3,3,3	2.65	1 (33%)	3,3,3	0.47	0
34	DMS	c	935	-	3,3,3	2.67	1 (33%)	3,3,3	0.55	0
34	DMS	e	104	-	3,3,3	2.70	1 (33%)	3,3,3	0.56	0
34	DMS	o	302	-	3,3,3	2.65	1 (33%)	3,3,3	0.53	0
29	PL9	D	404	-	55,55,55	0.72	1 (1%)	68,69,69	1.58	14 (20%)
34	DMS	A	424	-	3,3,3	2.67	1 (33%)	3,3,3	0.54	0
24	CLA	c	909	-	65,73,73	2.40	18 (27%)	76,113,113	2.65	27 (35%)
34	DMS	b	639	-	3,3,3	2.66	1 (33%)	3,3,3	0.59	0
25	PHO	A	409	-	51,69,69	1.89	7 (13%)	47,99,99	1.83	8 (17%)
31	LMT	a	402	-	36,36,36	0.42	0	47,47,47	1.13	4 (8%)
38	LHG	E	101	-	41,41,48	1.03	2 (4%)	44,47,54	1.07	3 (6%)
36	HTG	B	631	-	19,19,19	0.98	1 (5%)	23,24,24	1.77	2 (8%)
26	BCR	D	403	-	41,41,41	0.83	0	56,56,56	1.68	9 (16%)
42	HEC	V	203	16	32,50,50	2.16	6 (18%)	24,82,82	1.85	5 (20%)
34	DMS	d	417	-	3,3,3	2.69	1 (33%)	3,3,3	0.55	0
34	DMS	o	307	-	3,3,3	2.68	1 (33%)	3,3,3	0.64	0
34	DMS	v	210	-	3,3,3	2.69	1 (33%)	3,3,3	0.53	0
24	CLA	B	611	43	65,73,73	2.46	19 (29%)	76,113,113	2.52	27 (35%)
24	CLA	C	513	-	65,73,73	2.42	19 (29%)	76,113,113	2.44	25 (32%)
37	DGD	c	919	-	63,63,67	0.84	2 (3%)	77,77,81	0.96	4 (5%)
24	CLA	b	611	43	65,73,73	2.31	19 (29%)	76,113,113	2.41	25 (32%)
34	DMS	d	415	-	3,3,3	2.62	1 (33%)	3,3,3	0.50	0
37	DGD	D	405	-	52,52,67	0.92	2 (3%)	60,60,81	1.17	6 (10%)
24	CLA	c	910	-	65,73,73	2.44	19 (29%)	76,113,113	2.49	28 (36%)
31	LMT	m	103	-	36,36,36	0.40	0	47,47,47	0.81	2 (4%)
34	DMS	c	936	-	3,3,3	2.66	1 (33%)	3,3,3	0.54	0
24	CLA	d	401	43	65,73,73	2.34	17 (26%)	76,113,113	2.65	29 (38%)
24	CLA	B	607	-	65,73,73	2.52	20 (30%)	76,113,113	2.49	27 (35%)
24	CLA	A	410	-	65,73,73	2.22	18 (27%)	76,113,113	2.62	26 (34%)
34	DMS	U	204	-	3,3,3	2.67	1 (33%)	3,3,3	0.50	0
34	DMS	B	641	-	3,3,3	2.66	1 (33%)	3,3,3	0.53	0
40	RRX	h	101	-	42,42,42	0.73	0	57,58,58	1.30	7 (12%)
26	BCR	K	101	-	41,41,41	0.74	0	56,56,56	1.34	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	PHO	a	412	-	51,69,69	1.80	8 (15%)	47,99,99	1.80	8 (17%)
24	CLA	C	504	43	65,73,73	2.35	19 (29%)	76,113,113	2.54	26 (34%)
34	DMS	K	102	-	3,3,3	2.65	1 (33%)	3,3,3	0.45	0
32	GOL	A	419	-	5,5,5	0.99	0	5,5,5	1.00	0
36	HTG	d	419	-	19,19,19	1.05	2 (10%)	23,24,24	1.27	1 (4%)
34	DMS	o	303	-	3,3,3	2.65	1 (33%)	3,3,3	0.46	0
34	DMS	C	531	-	3,3,3	2.67	1 (33%)	3,3,3	0.54	0
24	CLA	B	604	-	65,73,73	2.33	20 (30%)	76,113,113	2.62	26 (34%)
37	DGD	d	408	-	50,50,67	0.95	2 (4%)	58,58,81	1.38	8 (13%)
34	DMS	b	646	-	3,3,3	2.73	1 (33%)	3,3,3	0.60	0
24	CLA	B	610	-	65,73,73	2.57	18 (27%)	76,113,113	2.37	24 (31%)
34	DMS	a	424	-	3,3,3	2.66	1 (33%)	3,3,3	0.53	0
34	DMS	C	529	-	3,3,3	2.66	1 (33%)	3,3,3	0.44	0
24	CLA	b	616	-	65,73,73	2.24	18 (27%)	76,113,113	2.64	25 (32%)
26	BCR	B	636	-	41,41,41	0.72	0	56,56,56	1.58	12 (21%)
24	CLA	c	902	-	65,73,73	2.46	18 (27%)	76,113,113	2.67	27 (35%)
29	PL9	d	407	-	55,55,55	0.76	1 (1%)	68,69,69	1.51	13 (19%)
24	CLA	b	613	-	65,73,73	2.58	21 (32%)	76,113,113	2.31	23 (30%)
36	HTG	V	215	-	19,19,19	1.03	1 (5%)	23,24,24	2.17	3 (13%)
37	DGD	h	102	-	63,63,67	0.92	3 (4%)	77,77,81	0.89	3 (3%)
24	CLA	b	606	-	65,73,73	2.49	20 (30%)	76,113,113	2.50	28 (36%)
31	LMT	b	625	-	36,36,36	0.40	0	47,47,47	1.27	6 (12%)
24	CLA	b	615	-	65,73,73	2.46	18 (27%)	76,113,113	2.46	30 (39%)
36	HTG	B	624	-	19,19,19	0.78	1 (5%)	23,24,24	1.44	2 (8%)
34	DMS	c	933	-	3,3,3	2.67	1 (33%)	3,3,3	0.48	0
24	CLA	c	914	-	65,73,73	2.55	19 (29%)	76,113,113	2.33	25 (32%)
34	DMS	b	641	-	3,3,3	2.69	1 (33%)	3,3,3	0.57	0
24	CLA	C	511	3	65,73,73	2.55	18 (27%)	76,113,113	2.41	26 (34%)
34	DMS	C	535	-	3,3,3	2.71	1 (33%)	3,3,3	0.56	0
34	DMS	c	932	-	3,3,3	2.66	1 (33%)	3,3,3	0.54	0
26	BCR	C	514	-	41,41,41	0.74	0	56,56,56	1.35	7 (12%)
36	HTG	D	412	-	19,19,19	1.05	2 (10%)	23,24,24	1.46	3 (13%)
34	DMS	e	103	-	3,3,3	2.67	1 (33%)	3,3,3	0.51	0
26	BCR	B	620	-	41,41,41	0.68	0	56,56,56	1.24	7 (12%)
36	HTG	B	629	-	19,19,19	1.00	2 (10%)	23,24,24	1.46	3 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	DMS	a	421	-	3,3,3	2.65	1 (33%)	3,3,3	0.46	0
34	DMS	B	646	-	3,3,3	2.67	1 (33%)	3,3,3	0.53	0
34	DMS	b	647	-	3,3,3	2.67	1 (33%)	3,3,3	0.60	0
24	CLA	b	612	-	65,73,73	2.77	20 (30%)	76,113,113	2.40	23 (30%)
38	LHG	D	408	-	45,45,48	0.90	2 (4%)	48,51,54	0.95	4 (8%)
34	DMS	O	315	-	3,3,3	2.71	1 (33%)	3,3,3	0.60	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
26	BCR	A	411	-	-	1/29/63/63	0/2/2/2
24	CLA	C	505	-	1/1/15/20	3/37/115/115	-
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
31	LMT	t	101	-	-	3/15/31/61	0/1/1/2
32	GOL	B	638	-	-	4/4/4/4	-
36	HTG	O	316	-	-	2/10/30/30	0/1/1/1
24	CLA	d	404	-	1/1/15/20	4/37/115/115	-
26	BCR	T	101	-	-	2/29/63/63	0/2/2/2
24	CLA	B	603	-	1/1/15/20	4/37/115/115	-
27	SQD	A	416	-	-	12/49/69/69	0/1/1/1
24	CLA	B	606	-	1/1/15/20	3/37/115/115	-
24	CLA	d	405	-	1/1/15/20	5/37/115/115	-
24	CLA	B	614	-	1/1/15/20	6/37/115/115	-
38	LHG	d	409	-	-	8/53/53/53	-
39	HEM	f	101	5,6	-	1/12/54/54	-
24	CLA	c	913	-	1/1/15/20	3/37/115/115	-
36	HTG	b	626	-	-	2/10/30/30	0/1/1/1
24	CLA	C	509	-	1/1/15/20	7/37/115/115	-
24	CLA	c	908	43	1/1/15/20	5/37/115/115	-
26	BCR	c	916	-	-	3/29/63/63	0/2/2/2
27	SQD	b	601	-	-	17/49/69/69	0/1/1/1
36	HTG	c	942	-	-	2/10/30/30	0/1/1/1
31	LMT	c	922	-	-	7/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	GOL	b	637	-	-	0/4/4/4	-
36	HTG	v	211	-	-	1/10/30/30	0/1/1/1
24	CLA	D	402	-	1/1/15/20	5/37/115/115	-
28	LMG	D	409	41	-	4/46/66/70	0/1/1/1
31	LMT	B	622	-	-	6/21/61/61	0/2/2/2
38	LHG	D	406	-	-	9/53/53/53	-
39	HEM	F	102	5,6	-	3/12/54/54	-
29	PL9	a	417	-	-	11/53/73/73	0/1/1/1
24	CLA	B	615	-	1/1/15/20	4/37/115/115	-
36	HTG	C	537	-	-	2/10/30/30	0/1/1/1
36	HTG	B	623	-	-	2/10/30/30	0/1/1/1
24	CLA	C	507	43	1/1/15/20	8/37/115/115	-
37	DGD	c	918	-	-	16/51/91/95	0/2/2/2
24	CLA	c	906	-	1/1/15/20	4/37/115/115	-
31	LMT	A	417	-	-	6/21/61/61	0/2/2/2
26	BCR	b	622	-	-	0/29/63/63	0/2/2/2
27	SQD	a	415	-	-	6/49/69/69	0/1/1/1
24	CLA	b	618	-	1/1/15/20	13/37/115/115	-
26	BCR	C	515	-	-	2/29/63/63	0/2/2/2
32	GOL	V	206	-	-	4/4/4/4	-
37	DGD	c	917	-	-	13/51/91/95	0/2/2/2
29	PL9	A	414	-	-	10/53/73/73	0/1/1/1
24	CLA	b	610	-	1/1/15/20	4/37/115/115	-
31	LMT	t	102	-	-	9/21/61/61	0/2/2/2
38	LHG	d	410	-	-	11/53/53/53	-
24	CLA	A	406	43	-	5/37/115/115	-
38	LHG	D	407	-	-	5/53/53/53	-
36	HTG	y	102	-	-	3/10/30/30	0/1/1/1
32	GOL	a	419	-	-	2/4/4/4	-
24	CLA	b	617	-	1/1/15/20	2/37/115/115	-
24	CLA	b	608	-	1/1/15/20	2/37/115/115	-
38	LHG	l	103	-	-	14/53/53/53	-
26	BCR	b	623	-	-	0/29/63/63	0/2/2/2
36	HTG	U	201	-	-	0/1/1/30	-
24	CLA	b	614	43	1/1/15/20	3/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	905	43	1/1/15/20	5/37/115/115	-
37	DGD	C	518	-	-	10/51/91/95	0/2/2/2
29	PL9	D	404	-	-	2/53/73/73	0/1/1/1
36	HTG	b	603	-	-	0/10/30/30	0/1/1/1
36	HTG	C	536	-	-	1/10/30/30	0/1/1/1
24	CLA	B	609	-	-	2/37/115/115	-
27	SQD	F	101	-	-	10/31/51/69	0/1/1/1
24	CLA	c	909	-	1/1/15/20	8/37/115/115	-
25	PHO	A	409	-	-	0/37/103/103	0/5/6/6
31	LMT	a	402	-	-	7/21/61/61	0/2/2/2
32	GOL	B	637	-	-	4/4/4/4	-
38	LHG	E	101	-	-	10/46/46/53	-
28	LMG	b	624	-	-	11/46/66/70	0/1/1/1
26	BCR	d	406	-	-	4/29/63/63	0/2/2/2
31	LMT	j	102	-	-	3/15/35/61	0/1/1/2
36	HTG	B	631	-	-	1/10/30/30	0/1/1/1
31	LMT	B	626	-	-	10/15/35/61	0/1/1/2
26	BCR	D	403	-	-	7/29/63/63	0/2/2/2
42	HEC	V	203	16	-	2/10/54/54	-
36	HTG	C	520	-	-	3/10/30/30	0/1/1/1
26	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
36	HTG	c	923	-	-	1/10/30/30	0/1/1/1
24	CLA	B	611	43	1/1/15/20	3/37/115/115	-
24	CLA	C	513	-	-	6/37/115/115	-
36	HTG	C	521	-	-	2/10/30/30	0/1/1/1
37	DGD	c	919	-	-	9/51/91/95	0/2/2/2
24	CLA	C	508	-	1/1/15/20	6/37/115/115	-
24	CLA	b	611	43	1/1/15/20	1/37/115/115	-
24	CLA	b	619	-	1/1/15/20	7/37/115/115	-
31	LMT	m	102	-	-	3/21/61/61	0/2/2/2
31	LMT	M	102	-	-	7/17/37/61	0/1/1/2
37	DGD	D	405	-	-	20/47/67/95	0/1/1/2
24	CLA	a	413	-	1/1/15/20	7/37/115/115	-
24	CLA	c	910	-	1/1/15/20	8/37/115/115	-
31	LMT	m	103	-	-	2/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SQD	A	412	-	-	9/49/69/69	0/1/1/1
36	HTG	b	602	-	-	2/10/30/30	0/1/1/1
24	CLA	C	502	-	-	3/37/115/115	-
24	CLA	C	506	-	1/1/15/20	6/37/115/115	-
24	CLA	B	608	43	1/1/15/20	1/37/115/115	-
37	DGD	H	102	-	-	10/51/91/95	0/2/2/2
24	CLA	d	401	43	1/1/15/20	5/37/115/115	-
24	CLA	B	607	-	1/1/15/20	7/37/115/115	-
37	DGD	C	516	-	-	14/51/91/95	0/2/2/2
24	CLA	a	409	-	1/1/15/20	3/37/115/115	-
24	CLA	A	410	-	-	8/37/115/115	-
36	HTG	O	303	-	-	2/10/30/30	0/1/1/1
31	LMT	e	101	-	-	3/15/35/61	0/1/1/2
24	CLA	b	620	-	1/1/15/20	6/37/115/115	-
24	CLA	b	609	-	1/1/15/20	2/37/115/115	-
36	HTG	B	625	-	-	3/10/30/30	0/1/1/1
36	HTG	b	627	-	-	3/10/30/30	0/1/1/1
28	LMG	a	416	-	-	18/46/66/70	0/1/1/1
40	RRX	h	101	-	-	2/29/65/65	0/2/2/2
25	PHO	A	408	-	-	4/37/103/103	0/5/6/6
24	CLA	c	907	-	1/1/15/20	8/37/115/115	-
31	LMT	F	103	-	-	4/15/35/61	0/1/1/2
38	LHG	L	101	-	-	14/53/53/53	-
28	LMG	C	519	-	-	14/46/66/70	0/1/1/1
26	BCR	K	101	-	-	1/29/63/63	0/2/2/2
36	HTG	V	204	-	-	3/4/24/30	0/1/1/1
28	LMG	c	920	-	-	8/46/66/70	0/1/1/1
36	HTG	c	941	-	-	1/10/30/30	0/1/1/1
25	PHO	a	412	-	-	1/37/103/103	0/5/6/6
24	CLA	c	912	3	-	0/37/115/115	-
24	CLA	C	504	43	1/1/15/20	5/37/115/115	-
27	SQD	l	101	-	-	22/49/69/69	0/1/1/1
24	CLA	B	605	-	1/1/15/20	1/37/115/115	-
24	CLA	B	616	-	1/1/15/20	10/37/115/115	-
24	CLA	b	607	-	1/1/15/20	3/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	DGD	C	517	-	-	15/51/91/95	0/2/2/2
32	GOL	A	419	-	-	2/4/4/4	-
36	HTG	d	419	-	-	1/10/30/30	0/1/1/1
24	CLA	c	903	-	1/1/15/20	5/37/115/115	-
26	BCR	b	621	-	-	2/29/63/63	0/2/2/2
36	HTG	d	414	-	-	4/10/30/30	0/1/1/1
24	CLA	B	604	-	1/1/15/20	4/37/115/115	-
37	DGD	d	408	-	-	20/44/64/95	0/1/1/2
25	PHO	a	411	-	-	4/37/103/103	0/5/6/6
24	CLA	D	401	-	1/1/15/20	3/37/115/115	-
24	CLA	B	610	-	1/1/15/20	5/37/115/115	-
31	LMT	J	102	-	-	3/15/35/61	0/1/1/2
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
24	CLA	A	407	43	-	6/37/115/115	-
26	BCR	k	103	-	-	1/29/63/63	0/2/2/2
24	CLA	b	616	-	1/1/15/20	4/37/115/115	-
26	BCR	c	915	-	-	1/29/63/63	0/2/2/2
26	BCR	B	636	-	-	1/29/63/63	0/2/2/2
24	CLA	c	902	-	1/1/15/20	1/37/115/115	-
29	PL9	d	407	-	-	7/53/73/73	0/1/1/1
36	HTG	d	420	-	-	3/10/30/30	0/1/1/1
24	CLA	b	613	-	1/1/15/20	0/37/115/115	-
28	LMG	B	621	-	-	13/46/66/70	0/1/1/1
36	HTG	V	215	-	-	1/10/30/30	0/1/1/1
24	CLA	c	904	-	1/1/15/20	4/37/115/115	-
36	HTG	c	928	-	-	0/10/30/30	0/1/1/1
27	SQD	a	401	-	-	19/49/69/69	0/1/1/1
24	CLA	B	612	-	1/1/15/20	2/37/115/115	-
24	CLA	B	602	43	1/1/15/20	12/37/115/115	-
32	GOL	V	207	-	-	1/4/4/4	-
36	HTG	c	924	-	-	0/10/30/30	0/1/1/1
32	GOL	O	304	-	-	2/4/4/4	-
24	CLA	b	606	-	1/1/15/20	8/37/115/115	-
36	HTG	c	943	-	-	2/8/28/30	0/1/1/1
37	DGD	h	102	-	-	10/51/91/95	0/2/2/2
24	CLA	A	405	-	1/1/15/20	2/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	b	625	-	-	7/21/61/61	0/2/2/2
28	LMG	A	413	-	-	16/46/66/70	0/1/1/1
24	CLA	b	615	-	1/1/15/20	2/37/115/115	-
26	BCR	k	102	-	-	4/29/63/63	0/2/2/2
36	HTG	B	624	-	-	2/10/30/30	0/1/1/1
24	CLA	c	914	-	1/1/15/20	3/37/115/115	-
24	CLA	C	511	3	1/1/15/20	3/37/115/115	-
31	LMT	M	101	-	-	3/21/61/61	0/2/2/2
24	CLA	B	617	-	1/1/15/20	11/37/115/115	-
26	BCR	a	414	-	-	1/29/63/63	0/2/2/2
31	LMT	A	421	-	-	8/21/61/61	0/2/2/2
32	GOL	c	929	-	-	2/4/4/4	-
31	LMT	c	927	-	-	11/21/61/61	0/2/2/2
24	CLA	B	613	-	1/1/15/20	2/37/115/115	-
24	CLA	c	911	-	1/1/15/20	2/37/115/115	-
27	SQD	f	102	-	-	16/38/58/69	0/1/1/1
26	BCR	C	514	-	-	2/29/63/63	0/2/2/2
36	HTG	D	412	-	-	3/10/30/30	0/1/1/1
24	CLA	b	605	43	1/1/15/20	5/37/115/115	-
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
42	HEC	v	202	16	-	2/10/54/54	-
36	HTG	B	630	-	-	1/10/30/30	0/1/1/1
36	HTG	B	629	-	-	2/10/30/30	0/1/1/1
28	LMG	d	412	41	-	8/46/66/70	0/1/1/1
32	GOL	C	525	-	-	1/4/4/4	-
24	CLA	C	503	-	1/1/15/20	3/37/115/115	-
24	CLA	a	410	43	-	6/37/115/115	-
24	CLA	b	612	-	-	2/37/115/115	-
28	LMG	c	921	-	-	1/46/66/70	0/1/1/1
38	LHG	d	411	-	-	9/51/51/53	-
24	CLA	C	510	-	1/1/15/20	4/37/115/115	-
38	LHG	D	408	-	-	8/50/50/53	-
40	RRX	H	101	-	-	3/29/65/65	0/2/2/2
28	LMG	C	523	-	-	9/46/66/70	0/1/1/1
24	CLA	C	501	-	1/1/15/20	3/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	512	-	1/1/15/20	5/37/115/115	-
31	LMT	Z	101	-	-	7/21/61/61	0/2/2/2

All (1653) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	904	CLA	MG-NA	10.97	2.32	2.06
24	C	507	CLA	MG-NA	10.43	2.31	2.06
24	C	511	CLA	MG-NA	10.27	2.30	2.06
24	C	503	CLA	MG-NA	10.00	2.30	2.06
24	b	612	CLA	MG-ND	-9.99	1.86	2.05
24	b	608	CLA	MG-ND	-9.58	1.86	2.05
24	B	607	CLA	MG-NA	9.53	2.28	2.06
24	b	615	CLA	MG-NA	9.28	2.28	2.06
24	b	608	CLA	MG-NA	9.03	2.27	2.06
24	c	908	CLA	MG-NA	8.91	2.27	2.06
24	c	913	CLA	MG-ND	-8.91	1.88	2.05
24	B	616	CLA	MG-NA	8.89	2.27	2.06
24	b	613	CLA	MG-NA	8.85	2.27	2.06
24	A	405	CLA	MG-ND	-8.82	1.88	2.05
24	C	506	CLA	MG-NA	8.63	2.26	2.06
24	b	619	CLA	MG-NA	8.52	2.26	2.06
24	B	612	CLA	MG-NA	8.50	2.26	2.06
24	C	510	CLA	MG-ND	-8.46	1.89	2.05
24	C	505	CLA	MG-ND	-8.42	1.89	2.05
24	C	508	CLA	MG-ND	-8.30	1.89	2.05
24	d	404	CLA	MG-ND	-8.30	1.89	2.05
24	c	910	CLA	MG-NA	8.30	2.26	2.06
24	b	610	CLA	MG-NA	8.21	2.25	2.06
24	C	512	CLA	MG-NA	7.96	2.25	2.06
24	d	401	CLA	MG-ND	-7.92	1.90	2.05
39	f	101	HEM	C3D-C2D	7.77	1.53	1.36
24	B	611	CLA	MG-ND	-7.76	1.90	2.05
24	C	505	CLA	MG-NA	7.74	2.24	2.06
24	c	914	CLA	MG-NC	7.72	2.24	2.06
24	c	913	CLA	MG-NA	7.65	2.24	2.06
24	b	620	CLA	MG-NA	7.65	2.24	2.06
24	C	502	CLA	MG-ND	-7.61	1.90	2.05
24	c	902	CLA	MG-ND	-7.57	1.90	2.05
39	F	102	HEM	C3D-C2D	7.55	1.52	1.36
24	b	620	CLA	MG-ND	-7.52	1.90	2.05
24	c	909	CLA	MG-ND	-7.45	1.91	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	617	CLA	MG-NA	7.40	2.23	2.06
24	c	912	CLA	MG-NA	7.29	2.23	2.06
24	B	610	CLA	MG-NC	7.28	2.23	2.06
24	b	617	CLA	MG-ND	-7.24	1.91	2.05
24	B	609	CLA	MG-NA	7.22	2.23	2.06
24	c	911	CLA	MG-ND	-7.16	1.91	2.05
24	c	911	CLA	MG-NC	7.15	2.23	2.06
24	B	610	CLA	MG-NA	7.14	2.23	2.06
24	c	907	CLA	MG-ND	-7.12	1.91	2.05
24	b	612	CLA	MG-NA	7.12	2.23	2.06
24	b	617	CLA	MG-NA	7.09	2.23	2.06
24	b	612	CLA	MG-NC	7.01	2.22	2.06
24	C	512	CLA	MG-ND	-6.99	1.91	2.05
24	B	612	CLA	MG-ND	-6.96	1.92	2.05
24	b	618	CLA	MG-ND	-6.88	1.92	2.05
24	C	501	CLA	MG-NA	6.86	2.22	2.06
24	b	615	CLA	C3B-C2B	6.80	1.49	1.40
24	A	406	CLA	MG-ND	-6.77	1.92	2.05
24	B	610	CLA	MG-ND	-6.76	1.92	2.05
24	C	509	CLA	MG-NC	6.72	2.22	2.06
24	b	620	CLA	C3B-C2B	6.68	1.49	1.40
24	b	609	CLA	MG-NA	6.65	2.22	2.06
24	c	906	CLA	MG-NA	6.64	2.22	2.06
24	d	404	CLA	MG-NA	6.62	2.22	2.06
24	b	605	CLA	MG-NC	6.62	2.22	2.06
24	B	602	CLA	MG-NA	6.62	2.22	2.06
24	c	904	CLA	MG-NC	6.61	2.22	2.06
24	C	503	CLA	MG-NC	6.59	2.21	2.06
24	c	903	CLA	MG-NA	6.56	2.21	2.06
24	b	613	CLA	MG-NC	6.54	2.21	2.06
24	b	606	CLA	MG-ND	-6.51	1.92	2.05
24	C	502	CLA	C3B-C2B	6.51	1.49	1.40
24	c	910	CLA	C3B-C2B	6.51	1.49	1.40
24	C	513	CLA	C3B-C2B	6.51	1.49	1.40
24	C	502	CLA	MG-NA	6.50	2.21	2.06
24	B	606	CLA	C3B-C2B	6.50	1.49	1.40
24	c	908	CLA	C3B-C2B	6.50	1.49	1.40
25	A	409	PHO	C3B-C2B	6.48	1.49	1.40
24	B	617	CLA	C3B-C2B	6.48	1.49	1.40
24	c	902	CLA	MG-NA	6.43	2.21	2.06
24	b	616	CLA	MG-ND	-6.43	1.93	2.05
24	A	405	CLA	C3B-C2B	6.42	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	513	CLA	MG-ND	-6.40	1.93	2.05
24	A	406	CLA	C3B-C2B	6.38	1.49	1.40
24	B	614	CLA	MG-NA	6.36	2.21	2.06
24	B	602	CLA	C3B-C2B	6.36	1.49	1.40
24	b	607	CLA	MG-NC	6.35	2.21	2.06
24	d	404	CLA	MG-NC	6.34	2.21	2.06
24	C	502	CLA	C1D-ND	6.34	1.45	1.37
24	C	511	CLA	C3B-C2B	6.34	1.49	1.40
24	C	510	CLA	MG-NA	6.31	2.21	2.06
24	D	401	CLA	MG-NA	6.29	2.21	2.06
24	C	503	CLA	C1D-ND	6.29	1.45	1.37
24	c	902	CLA	C3B-C2B	6.27	1.49	1.40
24	C	509	CLA	C3B-C2B	6.27	1.49	1.40
24	B	609	CLA	C3B-C2B	6.22	1.49	1.40
24	B	604	CLA	C3B-C2B	6.21	1.49	1.40
24	A	410	CLA	C3B-C2B	6.20	1.49	1.40
24	b	610	CLA	C3B-C2B	6.18	1.48	1.40
24	a	409	CLA	MG-ND	-6.17	1.93	2.05
24	C	508	CLA	C3B-C2B	6.17	1.48	1.40
24	b	606	CLA	C3B-C2B	6.17	1.48	1.40
42	v	202	HEC	C2B-C3B	-6.17	1.34	1.40
24	c	913	CLA	C3B-C2B	6.17	1.48	1.40
24	B	613	CLA	MG-NA	6.16	2.20	2.06
24	b	619	CLA	C3B-C2B	6.15	1.48	1.40
24	C	507	CLA	C3B-C2B	6.14	1.48	1.40
24	a	413	CLA	C3B-C2B	6.14	1.48	1.40
24	C	505	CLA	C3B-C2B	6.13	1.48	1.40
24	B	603	CLA	MG-NA	6.13	2.20	2.06
24	c	914	CLA	C3B-C2B	6.13	1.48	1.40
24	B	614	CLA	C3B-C2B	6.13	1.48	1.40
24	B	616	CLA	MG-ND	-6.12	1.93	2.05
24	C	503	CLA	MG-ND	-6.12	1.93	2.05
24	b	605	CLA	MG-NA	6.11	2.20	2.06
24	C	509	CLA	C1D-ND	6.08	1.45	1.37
24	C	504	CLA	MG-NA	6.08	2.20	2.06
24	a	410	CLA	MG-NA	6.04	2.20	2.06
24	b	605	CLA	C1D-ND	6.03	1.45	1.37
24	B	610	CLA	C1D-ND	6.03	1.45	1.37
24	d	404	CLA	C3B-C2B	6.02	1.48	1.40
24	b	614	CLA	C3B-C2B	6.01	1.48	1.40
24	B	615	CLA	MG-NA	6.01	2.20	2.06
24	b	606	CLA	C1D-ND	6.01	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	511	CLA	MG-ND	-6.00	1.93	2.05
24	B	605	CLA	C1D-ND	5.99	1.45	1.37
24	C	504	CLA	C3B-C2B	5.99	1.48	1.40
24	a	410	CLA	MG-ND	-5.99	1.93	2.05
24	c	904	CLA	C3B-C2B	5.99	1.48	1.40
24	C	506	CLA	MG-ND	-5.99	1.93	2.05
24	C	512	CLA	C3B-C2B	5.98	1.48	1.40
24	c	912	CLA	C3B-C2B	5.98	1.48	1.40
24	b	605	CLA	C3B-C2B	5.97	1.48	1.40
24	c	914	CLA	MG-ND	-5.96	1.94	2.05
24	b	607	CLA	MG-NA	5.96	2.20	2.06
24	c	914	CLA	C1D-ND	5.96	1.45	1.37
24	B	607	CLA	C3B-C2B	5.96	1.48	1.40
24	b	618	CLA	C3B-C2B	5.95	1.48	1.40
24	c	903	CLA	MG-ND	-5.94	1.94	2.05
25	A	408	PHO	C3B-C2B	5.94	1.48	1.40
24	c	903	CLA	C3B-C2B	5.94	1.48	1.40
24	C	510	CLA	C3B-C2B	5.93	1.48	1.40
24	B	605	CLA	MG-NC	5.92	2.20	2.06
24	B	607	CLA	C3C-C2C	5.92	1.49	1.36
24	c	907	CLA	C1D-ND	5.92	1.45	1.37
24	c	913	CLA	C3C-C2C	5.90	1.49	1.36
25	a	411	PHO	C3B-C2B	5.90	1.48	1.40
24	B	605	CLA	MG-ND	-5.90	1.94	2.05
24	C	503	CLA	C3B-C2B	5.89	1.48	1.40
24	C	506	CLA	C1D-ND	5.89	1.45	1.37
24	b	612	CLA	C3C-C2C	5.89	1.49	1.36
24	c	907	CLA	C3B-C2B	5.89	1.48	1.40
24	B	603	CLA	C3B-C2B	5.88	1.48	1.40
24	b	608	CLA	C1D-ND	5.88	1.45	1.37
24	B	606	CLA	MG-NA	5.87	2.20	2.06
24	C	507	CLA	C1D-ND	5.87	1.45	1.37
24	b	606	CLA	MG-NC	5.86	2.20	2.06
24	b	605	CLA	C3C-C2C	5.86	1.49	1.36
24	C	505	CLA	C1D-ND	5.83	1.45	1.37
24	c	909	CLA	C3B-C2B	5.83	1.48	1.40
24	b	612	CLA	C1D-ND	5.83	1.45	1.37
24	c	911	CLA	C3B-C2B	5.83	1.48	1.40
24	C	505	CLA	MG-NC	5.83	2.20	2.06
24	B	611	CLA	C3C-C2C	5.83	1.49	1.36
24	B	612	CLA	C1D-ND	5.82	1.44	1.37
24	B	608	CLA	C3B-C2B	5.82	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	612	CLA	C3B-C2B	5.82	1.48	1.40
24	D	401	CLA	C3B-C2B	5.81	1.48	1.40
24	C	512	CLA	C3C-C2C	5.81	1.49	1.36
24	C	508	CLA	C3C-C2C	5.78	1.49	1.36
24	c	909	CLA	C1D-ND	5.78	1.44	1.37
24	a	413	CLA	C3C-C2C	5.78	1.49	1.36
24	C	509	CLA	C3C-C2C	5.77	1.49	1.36
24	b	607	CLA	C3B-C2B	5.77	1.48	1.40
24	b	606	CLA	MG-NA	5.76	2.20	2.06
24	a	409	CLA	C1D-ND	5.76	1.44	1.37
24	a	409	CLA	MG-NA	5.76	2.20	2.06
24	c	909	CLA	C3C-C2C	5.75	1.49	1.36
24	b	608	CLA	C3C-C2C	5.74	1.48	1.36
24	b	613	CLA	C1D-ND	5.74	1.44	1.37
24	A	406	CLA	MG-NA	5.74	2.19	2.06
24	B	611	CLA	C3B-C2B	5.73	1.48	1.40
24	c	904	CLA	C1D-ND	5.73	1.44	1.37
24	c	914	CLA	C3C-C2C	5.73	1.48	1.36
24	B	613	CLA	C3B-C2B	5.72	1.48	1.40
24	c	911	CLA	C3C-C2C	5.72	1.48	1.36
24	c	909	CLA	MG-NC	5.72	2.19	2.06
24	D	402	CLA	C3C-C2C	5.72	1.48	1.36
24	c	907	CLA	C3C-C2C	5.71	1.48	1.36
24	B	616	CLA	C3B-C2B	5.69	1.48	1.40
24	C	504	CLA	MG-ND	-5.69	1.94	2.05
24	B	610	CLA	C3B-C2B	5.69	1.48	1.40
24	b	606	CLA	C3C-C2C	5.68	1.48	1.36
24	B	609	CLA	C1D-ND	5.68	1.44	1.37
24	B	611	CLA	C1D-ND	5.68	1.44	1.37
24	b	614	CLA	C3C-C2C	5.67	1.48	1.36
42	v	202	HEC	C3C-C2C	-5.67	1.34	1.40
24	b	608	CLA	MG-NC	5.67	2.19	2.06
24	b	611	CLA	C3B-C2B	5.66	1.48	1.40
24	B	602	CLA	C3C-C2C	5.66	1.48	1.36
24	b	614	CLA	MG-NA	5.66	2.19	2.06
24	C	513	CLA	MG-NA	5.65	2.19	2.06
24	d	404	CLA	C1D-ND	5.65	1.44	1.37
24	C	503	CLA	C3C-C2C	5.65	1.48	1.36
24	b	617	CLA	C3B-C2B	5.64	1.48	1.40
24	B	608	CLA	C3C-C2C	5.64	1.48	1.36
24	a	409	CLA	C3B-C2B	5.64	1.48	1.40
24	d	401	CLA	MG-NA	5.64	2.19	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	907	CLA	MG-NA	5.63	2.19	2.06
24	C	501	CLA	C1D-ND	5.62	1.44	1.37
24	B	603	CLA	C3C-C2C	5.62	1.48	1.36
24	C	501	CLA	C3B-C2B	5.60	1.48	1.40
24	A	405	CLA	MG-NC	5.60	2.19	2.06
24	b	610	CLA	MG-NC	5.60	2.19	2.06
24	b	610	CLA	C3C-C2C	5.60	1.48	1.36
24	b	609	CLA	C3B-C2B	5.59	1.48	1.40
24	A	405	CLA	MG-NA	5.59	2.19	2.06
24	c	902	CLA	C1D-ND	5.58	1.44	1.37
24	b	613	CLA	C3C-C2C	5.57	1.48	1.36
24	b	617	CLA	C1D-ND	5.57	1.44	1.37
24	C	508	CLA	MG-NC	5.57	2.19	2.06
24	a	410	CLA	C3B-C2B	5.57	1.48	1.40
24	c	905	CLA	C3B-C2B	5.56	1.48	1.40
24	A	405	CLA	C1D-ND	5.56	1.44	1.37
24	b	607	CLA	C3C-C2C	5.56	1.48	1.36
24	B	608	CLA	MG-NA	5.56	2.19	2.06
24	C	506	CLA	C3C-C2C	5.55	1.48	1.36
24	b	605	CLA	CHC-C1C	5.54	1.49	1.35
24	B	606	CLA	C3C-C2C	5.54	1.48	1.36
24	c	906	CLA	C1D-ND	5.54	1.44	1.37
24	d	405	CLA	MG-ND	-5.53	1.94	2.05
24	B	604	CLA	C3C-C2C	5.53	1.48	1.36
24	B	606	CLA	C1D-ND	5.52	1.44	1.37
24	B	603	CLA	MG-ND	-5.52	1.94	2.05
24	C	509	CLA	MG-NA	5.52	2.19	2.06
24	b	611	CLA	C3C-C2C	5.52	1.48	1.36
24	C	506	CLA	C3B-C2B	5.51	1.48	1.40
24	c	912	CLA	C3C-C2C	5.51	1.48	1.36
24	c	912	CLA	C1D-ND	5.50	1.44	1.37
24	A	405	CLA	C3C-C2C	5.50	1.48	1.36
24	c	911	CLA	C1D-ND	5.50	1.44	1.37
24	C	513	CLA	C3C-C2C	5.49	1.48	1.36
24	c	913	CLA	C1D-ND	5.49	1.44	1.37
24	b	619	CLA	C1D-ND	5.49	1.44	1.37
24	B	613	CLA	C3C-C2C	5.48	1.48	1.36
24	b	618	CLA	C3C-C2C	5.48	1.48	1.36
24	C	507	CLA	C3C-C2C	5.48	1.48	1.36
24	c	903	CLA	C3C-C2C	5.48	1.48	1.36
24	C	505	CLA	C3C-C2C	5.47	1.48	1.36
24	d	401	CLA	C3B-C2B	5.47	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	502	CLA	C3C-C2C	5.47	1.48	1.36
24	C	512	CLA	C1D-ND	5.47	1.44	1.37
24	d	405	CLA	C3B-C2B	5.46	1.47	1.40
24	a	409	CLA	C3C-C2C	5.46	1.48	1.36
24	c	904	CLA	CHC-C1C	5.46	1.49	1.35
24	C	513	CLA	C1D-ND	5.45	1.44	1.37
24	c	910	CLA	C3C-C2C	5.45	1.48	1.36
24	d	401	CLA	C3C-C2C	5.45	1.48	1.36
24	B	616	CLA	C1D-ND	5.45	1.44	1.37
24	B	615	CLA	C1D-ND	5.44	1.44	1.37
24	c	906	CLA	C3B-C2B	5.44	1.47	1.40
24	B	617	CLA	MG-ND	-5.43	1.95	2.05
24	B	607	CLA	C1D-ND	5.43	1.44	1.37
24	C	510	CLA	C1D-ND	5.43	1.44	1.37
24	B	611	CLA	CHC-C1C	5.42	1.48	1.35
24	B	607	CLA	MG-NC	5.42	2.19	2.06
24	A	410	CLA	C3C-C2C	5.42	1.48	1.36
24	B	611	CLA	MG-NC	5.42	2.19	2.06
24	B	602	CLA	C1D-ND	5.42	1.44	1.37
24	B	604	CLA	C1D-ND	5.42	1.44	1.37
24	B	617	CLA	CHC-C1C	5.41	1.48	1.35
24	b	619	CLA	C3C-C2C	5.41	1.48	1.36
24	D	402	CLA	CHC-C1C	5.40	1.48	1.35
24	c	908	CLA	C3C-C2C	5.40	1.48	1.36
24	B	602	CLA	CHC-C1C	5.40	1.48	1.35
24	a	413	CLA	CHC-C1C	5.40	1.48	1.35
24	b	609	CLA	CHC-C1C	5.40	1.48	1.35
24	b	612	CLA	C3B-C2B	5.39	1.47	1.40
24	b	614	CLA	CHC-C1C	5.39	1.48	1.35
24	B	617	CLA	C3C-C2C	5.39	1.48	1.36
24	B	605	CLA	MG-NA	5.37	2.19	2.06
24	b	617	CLA	C3C-C2C	5.37	1.48	1.36
24	C	512	CLA	CHC-C1C	5.37	1.48	1.35
24	c	904	CLA	C3C-C2C	5.36	1.48	1.36
24	d	404	CLA	C3C-C2C	5.35	1.48	1.36
24	B	603	CLA	CHC-C1C	5.35	1.48	1.35
24	D	401	CLA	C3C-C2C	5.34	1.48	1.36
24	C	503	CLA	CHC-C1C	5.34	1.48	1.35
24	B	604	CLA	MG-ND	-5.34	1.95	2.05
25	a	412	PHO	C3D-C2D	5.34	1.49	1.39
24	B	615	CLA	C3B-C2B	5.33	1.47	1.40
24	B	613	CLA	CHC-C1C	5.33	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	405	CLA	C3C-C2C	5.32	1.48	1.36
24	b	608	CLA	C3B-C2B	5.32	1.47	1.40
24	b	614	CLA	C1D-ND	5.32	1.44	1.37
24	B	604	CLA	MG-NC	5.31	2.18	2.06
24	C	508	CLA	C1D-ND	5.31	1.44	1.37
24	B	607	CLA	CHC-C1C	5.31	1.48	1.35
24	c	910	CLA	C1D-ND	5.31	1.44	1.37
24	B	609	CLA	C3C-C2C	5.31	1.48	1.36
24	c	914	CLA	CHC-C1C	5.29	1.48	1.35
42	v	202	HEC	C3D-C2D	5.28	1.53	1.37
24	b	618	CLA	CHC-C1C	5.28	1.48	1.35
24	C	505	CLA	CHC-C1C	5.27	1.48	1.35
42	V	203	HEC	C3C-C2C	-5.27	1.35	1.40
24	a	410	CLA	C3C-C2C	5.26	1.47	1.36
24	b	611	CLA	MG-NA	5.25	2.18	2.06
24	B	616	CLA	CHC-C1C	5.25	1.48	1.35
24	A	410	CLA	MG-NA	5.25	2.18	2.06
24	D	402	CLA	MG-ND	-5.25	1.95	2.05
24	b	609	CLA	C3C-C2C	5.25	1.47	1.36
24	b	616	CLA	C3C-C2C	5.24	1.47	1.36
24	A	407	CLA	C3B-C2B	5.24	1.47	1.40
24	c	905	CLA	C3C-C2C	5.24	1.47	1.36
24	B	603	CLA	C1D-ND	5.23	1.44	1.37
24	d	404	CLA	CHC-C1C	5.23	1.48	1.35
24	b	620	CLA	C3C-C2C	5.23	1.47	1.36
42	V	203	HEC	C2B-C3B	-5.23	1.35	1.40
24	C	506	CLA	O2D-CGD	5.23	1.45	1.33
24	D	402	CLA	MG-NC	5.22	2.18	2.06
24	B	606	CLA	CHC-C1C	5.22	1.48	1.35
24	B	615	CLA	C3C-C2C	5.22	1.47	1.36
24	b	610	CLA	CHC-C1C	5.22	1.48	1.35
24	C	512	CLA	MG-NC	5.22	2.18	2.06
24	b	613	CLA	O2D-CGD	5.21	1.45	1.33
24	a	410	CLA	CHC-C1C	5.21	1.48	1.35
24	c	906	CLA	C3C-C2C	5.21	1.47	1.36
24	B	605	CLA	C3C-C2C	5.20	1.47	1.36
24	D	402	CLA	C3B-C2B	5.20	1.47	1.40
24	C	510	CLA	C3C-C2C	5.20	1.47	1.36
24	b	612	CLA	CHC-C1C	5.19	1.48	1.35
24	b	620	CLA	C1D-ND	5.19	1.44	1.37
24	b	613	CLA	C3B-C2B	5.19	1.47	1.40
24	C	508	CLA	CHC-C1C	5.19	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	906	CLA	MG-ND	-5.19	1.95	2.05
24	C	506	CLA	CHC-C1C	5.19	1.48	1.35
24	C	504	CLA	C3C-C2C	5.18	1.47	1.36
24	C	502	CLA	CHC-C1C	5.18	1.48	1.35
24	b	609	CLA	C1D-ND	5.18	1.44	1.37
24	a	413	CLA	O2D-CGD	5.17	1.45	1.33
25	a	412	PHO	C3B-C2B	5.17	1.47	1.40
24	A	410	CLA	CHC-C1C	5.17	1.48	1.35
24	c	902	CLA	C3C-C2C	5.17	1.47	1.36
24	B	612	CLA	CHC-C1C	5.16	1.48	1.35
24	d	405	CLA	C1D-ND	5.16	1.44	1.37
24	b	616	CLA	C3B-C2B	5.16	1.47	1.40
24	c	912	CLA	CHC-C1C	5.15	1.48	1.35
24	c	903	CLA	O2D-CGD	5.15	1.45	1.33
24	B	605	CLA	C3B-C2B	5.15	1.47	1.40
24	C	501	CLA	CHC-C1C	5.15	1.48	1.35
24	c	903	CLA	CHC-C1C	5.15	1.48	1.35
24	c	913	CLA	CHC-C1C	5.15	1.48	1.35
24	c	905	CLA	C1D-ND	5.14	1.44	1.37
24	B	614	CLA	CHC-C1C	5.14	1.48	1.35
24	A	406	CLA	C3C-C2C	5.13	1.47	1.36
24	A	407	CLA	C3C-C2C	5.13	1.47	1.36
24	c	910	CLA	CHC-C1C	5.13	1.48	1.35
24	c	905	CLA	MG-NA	5.13	2.18	2.06
24	c	907	CLA	CHC-C1C	5.13	1.48	1.35
24	c	905	CLA	O2D-CGD	5.12	1.45	1.33
24	B	609	CLA	CHC-C1C	5.12	1.48	1.35
24	c	903	CLA	C1D-ND	5.12	1.44	1.37
24	C	511	CLA	CHC-C1C	5.12	1.48	1.35
24	C	502	CLA	O2D-CGD	5.12	1.45	1.33
24	C	502	CLA	MG-NC	5.11	2.18	2.06
24	B	617	CLA	C1D-ND	5.11	1.44	1.37
24	c	908	CLA	C1D-ND	5.11	1.44	1.37
24	C	511	CLA	C3C-C2C	5.11	1.47	1.36
24	B	614	CLA	C1D-ND	5.10	1.44	1.37
24	B	610	CLA	C3C-C2C	5.10	1.47	1.36
24	C	501	CLA	C3C-C2C	5.10	1.47	1.36
24	b	619	CLA	CHC-C1C	5.09	1.48	1.35
24	b	608	CLA	CHC-C1C	5.09	1.48	1.35
24	b	616	CLA	CHC-C1C	5.08	1.48	1.35
24	C	504	CLA	CHC-C1C	5.08	1.48	1.35
24	b	605	CLA	O2D-CGD	5.08	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	513	CLA	CHC-C1C	5.08	1.48	1.35
24	c	909	CLA	CHC-C1C	5.08	1.48	1.35
24	C	505	CLA	CHD-C1D	5.07	1.48	1.38
24	B	612	CLA	C3C-C2C	5.07	1.47	1.36
24	c	904	CLA	CHD-C1D	5.07	1.48	1.38
24	B	606	CLA	O2D-CGD	5.06	1.45	1.33
25	A	409	PHO	C3D-C2D	5.06	1.48	1.39
25	a	412	PHO	O2D-CGD	5.06	1.45	1.33
24	b	617	CLA	CHC-C1C	5.06	1.47	1.35
24	c	906	CLA	CHC-C1C	5.05	1.47	1.35
24	B	614	CLA	C3C-C2C	5.04	1.47	1.36
42	V	203	HEC	C3D-C2D	5.03	1.52	1.37
24	C	509	CLA	CHC-C1C	5.03	1.47	1.35
24	b	613	CLA	CHC-C1C	5.03	1.47	1.35
24	B	609	CLA	MG-NC	5.02	2.18	2.06
24	d	401	CLA	CHC-C1C	5.02	1.47	1.35
25	A	408	PHO	C3D-C2D	5.02	1.48	1.39
24	B	608	CLA	CHC-C1C	5.02	1.47	1.35
24	b	615	CLA	C3C-C2C	5.01	1.47	1.36
24	D	402	CLA	O2D-CGD	5.01	1.45	1.33
24	A	410	CLA	C1D-ND	5.01	1.43	1.37
24	b	610	CLA	C1D-ND	5.01	1.43	1.37
24	B	604	CLA	CHC-C1C	5.01	1.47	1.35
24	c	911	CLA	CHC-C1C	5.00	1.47	1.35
24	c	907	CLA	MG-NC	5.00	2.18	2.06
24	a	409	CLA	MG-NC	5.00	2.18	2.06
25	A	409	PHO	O2D-CGD	5.00	1.45	1.33
24	b	611	CLA	CHC-C1C	4.99	1.47	1.35
24	B	610	CLA	CHC-C1C	4.98	1.47	1.35
24	b	612	CLA	O2D-CGD	4.98	1.45	1.33
24	b	618	CLA	MG-NA	4.98	2.18	2.06
24	C	509	CLA	O2D-CGD	4.97	1.45	1.33
24	D	402	CLA	C1D-ND	4.97	1.43	1.37
24	b	611	CLA	CHD-C1D	4.97	1.48	1.38
24	b	615	CLA	C1D-ND	4.97	1.43	1.37
24	b	615	CLA	CHC-C1C	4.97	1.47	1.35
24	b	606	CLA	CHC-C1C	4.96	1.47	1.35
24	d	405	CLA	MG-NA	4.96	2.18	2.06
24	C	506	CLA	MG-NC	4.96	2.18	2.06
24	B	610	CLA	O2D-CGD	4.96	1.45	1.33
24	b	618	CLA	MG-NC	4.96	2.18	2.06
24	b	620	CLA	O2D-CGD	4.96	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	616	CLA	C1D-ND	4.96	1.43	1.37
24	c	905	CLA	CHC-C1C	4.96	1.47	1.35
24	b	618	CLA	C1D-ND	4.95	1.43	1.37
24	c	914	CLA	MG-NA	4.95	2.18	2.06
24	c	902	CLA	CHC-C1C	4.95	1.47	1.35
24	b	611	CLA	C1D-ND	4.95	1.43	1.37
24	B	616	CLA	C3C-C2C	4.94	1.47	1.36
24	b	607	CLA	CHD-C1D	4.94	1.48	1.38
24	d	405	CLA	CHC-C1C	4.93	1.47	1.35
24	A	407	CLA	CHC-C1C	4.93	1.47	1.35
24	B	614	CLA	MG-ND	-4.92	1.96	2.05
24	B	602	CLA	O2D-CGD	4.92	1.45	1.33
24	c	907	CLA	O2D-CGD	4.92	1.45	1.33
24	c	908	CLA	CHC-C1C	4.92	1.47	1.35
24	b	617	CLA	MG-NC	4.92	2.18	2.06
24	c	906	CLA	MG-NC	4.92	2.18	2.06
24	A	405	CLA	CHC-C1C	4.91	1.47	1.35
24	B	606	CLA	MG-NC	4.91	2.17	2.06
24	C	511	CLA	O2D-CGD	4.91	1.45	1.33
24	B	609	CLA	MG-ND	-4.90	1.96	2.05
24	C	504	CLA	MG-NC	4.90	2.17	2.06
24	a	410	CLA	C1D-ND	4.90	1.43	1.37
24	C	513	CLA	O2D-CGD	4.88	1.45	1.33
24	b	616	CLA	O2D-CGD	4.88	1.45	1.33
25	a	411	PHO	C3D-C2D	4.88	1.48	1.39
24	b	607	CLA	CHC-C1C	4.87	1.47	1.35
24	c	906	CLA	CHD-C1D	4.87	1.47	1.38
24	b	607	CLA	C1D-ND	4.87	1.43	1.37
24	B	613	CLA	MG-ND	-4.87	1.96	2.05
24	B	607	CLA	O2D-CGD	4.86	1.45	1.33
24	B	609	CLA	CHD-C1D	4.85	1.47	1.38
24	C	509	CLA	CHD-C1D	4.85	1.47	1.38
24	b	607	CLA	O2D-CGD	4.85	1.45	1.33
24	c	904	CLA	O2D-CGD	4.84	1.45	1.33
24	c	914	CLA	CHD-C1D	4.84	1.47	1.38
24	A	407	CLA	O2D-CGD	4.83	1.45	1.33
24	b	617	CLA	O2D-CGD	4.83	1.45	1.33
24	b	613	CLA	CHD-C1D	4.83	1.47	1.38
24	B	617	CLA	O2D-CGD	4.83	1.45	1.33
24	b	611	CLA	MG-NC	4.83	2.17	2.06
24	b	614	CLA	MG-ND	-4.83	1.96	2.05
24	B	605	CLA	CHC-C1C	4.83	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	406	CLA	C1D-ND	4.83	1.43	1.37
24	b	615	CLA	O2D-CGD	4.83	1.45	1.33
24	C	508	CLA	MG-NA	4.82	2.17	2.06
24	B	608	CLA	C1D-ND	4.82	1.43	1.37
24	b	606	CLA	O2D-CGD	4.82	1.45	1.33
24	C	510	CLA	CHC-C1C	4.81	1.47	1.35
24	c	912	CLA	CHD-C1D	4.81	1.47	1.38
24	C	504	CLA	C1D-ND	4.81	1.43	1.37
24	a	413	CLA	MG-NA	4.80	2.17	2.06
24	B	615	CLA	CHC-C1C	4.80	1.47	1.35
24	c	911	CLA	O2D-CGD	4.79	1.44	1.33
25	A	408	PHO	O2D-CGD	4.77	1.44	1.33
24	b	612	CLA	CHD-C1D	4.77	1.47	1.38
24	b	620	CLA	CHC-C1C	4.77	1.47	1.35
24	a	409	CLA	CHC-C1C	4.77	1.47	1.35
24	b	608	CLA	O2D-CGD	4.76	1.44	1.33
24	c	902	CLA	O2D-CGD	4.76	1.44	1.33
24	d	405	CLA	O2D-CGD	4.76	1.44	1.33
24	B	604	CLA	O2D-CGD	4.76	1.44	1.33
24	B	608	CLA	MG-NC	4.75	2.17	2.06
24	b	611	CLA	MG-ND	-4.75	1.96	2.05
24	B	614	CLA	O2D-CGD	4.75	1.44	1.33
24	b	610	CLA	MG-ND	-4.73	1.96	2.05
24	b	605	CLA	CHD-C1D	4.73	1.47	1.38
24	b	607	CLA	MG-ND	-4.72	1.96	2.05
24	b	609	CLA	O2D-CGD	4.72	1.44	1.33
24	c	906	CLA	O2D-CGD	4.72	1.44	1.33
24	b	615	CLA	CHD-C1D	4.71	1.47	1.38
24	B	603	CLA	O2D-CGD	4.70	1.44	1.33
25	A	409	PHO	OBD-CAD	4.70	1.28	1.22
24	C	507	CLA	O2D-CGD	4.70	1.44	1.33
24	B	613	CLA	O2D-CGD	4.70	1.44	1.33
24	C	510	CLA	O2D-CGD	4.68	1.44	1.33
24	c	914	CLA	O2D-CGD	4.67	1.44	1.33
24	b	610	CLA	O2D-CGD	4.67	1.44	1.33
24	b	611	CLA	O2D-CGD	4.67	1.44	1.33
24	C	508	CLA	O2D-CGD	4.66	1.44	1.33
24	A	410	CLA	O2D-CGD	4.66	1.44	1.33
24	c	908	CLA	O2D-CGD	4.65	1.44	1.33
24	c	907	CLA	CHD-C1D	4.64	1.47	1.38
24	B	602	CLA	CHD-C1D	4.64	1.47	1.38
24	C	507	CLA	CHC-C1C	4.64	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	504	CLA	O2D-CGD	4.64	1.44	1.33
24	C	505	CLA	O2D-CGD	4.64	1.44	1.33
24	B	611	CLA	MG-NA	4.64	2.17	2.06
24	b	606	CLA	CHD-C1D	4.63	1.47	1.38
24	d	401	CLA	C1D-ND	4.62	1.43	1.37
24	c	908	CLA	MG-ND	-4.62	1.96	2.05
24	B	608	CLA	O2D-CGD	4.62	1.44	1.33
24	b	608	CLA	CHD-C1D	4.62	1.47	1.38
24	C	512	CLA	O2D-CGD	4.62	1.44	1.33
24	b	609	CLA	MG-ND	-4.61	1.96	2.05
24	a	413	CLA	C1D-ND	4.61	1.43	1.37
24	C	511	CLA	C1D-ND	4.60	1.43	1.37
24	B	603	CLA	CHD-C1D	4.60	1.47	1.38
24	c	912	CLA	O2D-CGD	4.60	1.44	1.33
24	C	512	CLA	CHD-C1D	4.59	1.47	1.38
24	B	610	CLA	CHD-C1D	4.58	1.47	1.38
24	d	401	CLA	O2D-CGD	4.58	1.44	1.33
24	C	501	CLA	O2D-CGD	4.58	1.44	1.33
24	B	616	CLA	O2D-CGD	4.58	1.44	1.33
24	A	407	CLA	OBD-CAD	4.57	1.30	1.22
34	b	638	DMS	O-S	4.57	1.81	1.50
24	C	506	CLA	CHD-C1D	4.57	1.47	1.38
25	a	411	PHO	O2D-CGD	4.56	1.44	1.33
34	b	646	DMS	O-S	4.56	1.81	1.50
24	a	409	CLA	CHD-C1D	4.56	1.47	1.38
34	D	415	DMS	O-S	4.55	1.81	1.50
24	c	909	CLA	CHD-C1D	4.55	1.47	1.38
24	b	616	CLA	MG-NA	4.54	2.17	2.06
24	b	620	CLA	CHD-C1D	4.54	1.47	1.38
34	v	206	DMS	O-S	4.54	1.80	1.50
34	O	315	DMS	O-S	4.54	1.80	1.50
24	b	614	CLA	O2D-CGD	4.54	1.44	1.33
34	o	306	DMS	O-S	4.53	1.80	1.50
34	C	535	DMS	O-S	4.53	1.80	1.50
34	e	104	DMS	O-S	4.53	1.80	1.50
24	c	910	CLA	O2D-CGD	4.53	1.44	1.33
24	B	612	CLA	O2D-CGD	4.53	1.44	1.33
34	v	210	DMS	O-S	4.52	1.80	1.50
24	b	618	CLA	O2D-CGD	4.52	1.44	1.33
27	A	416	SQD	O48-C23	4.52	1.46	1.33
34	D	416	DMS	O-S	4.52	1.80	1.50
34	c	934	DMS	O-S	4.51	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	c	939	DMS	O-S	4.51	1.80	1.50
34	C	528	DMS	O-S	4.51	1.80	1.50
24	B	607	CLA	CHD-C1D	4.51	1.47	1.38
34	a	425	DMS	O-S	4.51	1.80	1.50
24	B	606	CLA	CHD-C1D	4.51	1.47	1.38
34	V	211	DMS	O-S	4.51	1.80	1.50
34	B	634	DMS	O-S	4.50	1.80	1.50
34	a	423	DMS	O-S	4.50	1.80	1.50
24	C	513	CLA	MG-NC	4.50	2.17	2.06
24	C	507	CLA	CHD-C1D	4.50	1.47	1.38
34	A	425	DMS	O-S	4.50	1.80	1.50
34	b	641	DMS	O-S	4.50	1.80	1.50
34	d	417	DMS	O-S	4.50	1.80	1.50
34	A	427	DMS	O-S	4.50	1.80	1.50
34	b	642	DMS	O-S	4.50	1.80	1.50
34	o	307	DMS	O-S	4.50	1.80	1.50
34	C	532	DMS	O-S	4.50	1.80	1.50
24	a	409	CLA	OBD-CAD	4.49	1.30	1.22
34	A	426	DMS	O-S	4.49	1.80	1.50
24	D	401	CLA	CHC-C1C	4.49	1.46	1.35
34	V	212	DMS	O-S	4.49	1.80	1.50
34	c	933	DMS	O-S	4.49	1.80	1.50
34	O	307	DMS	O-S	4.49	1.80	1.50
34	b	643	DMS	O-S	4.49	1.80	1.50
34	O	313	DMS	O-S	4.49	1.80	1.50
34	O	302	DMS	O-S	4.49	1.80	1.50
34	O	312	DMS	O-S	4.49	1.80	1.50
34	C	530	DMS	O-S	4.48	1.80	1.50
34	B	645	DMS	O-S	4.48	1.80	1.50
34	C	529	DMS	O-S	4.48	1.80	1.50
24	D	401	CLA	O2D-CGD	4.48	1.44	1.33
24	C	513	CLA	CHD-C1D	4.48	1.47	1.38
34	e	103	DMS	O-S	4.48	1.80	1.50
24	B	612	CLA	CHD-C1D	4.48	1.47	1.38
34	C	531	DMS	O-S	4.48	1.80	1.50
28	b	624	LMG	O8-C28	4.48	1.46	1.33
34	U	204	DMS	O-S	4.48	1.80	1.50
34	A	424	DMS	O-S	4.48	1.80	1.50
24	b	618	CLA	CHD-C1D	4.48	1.47	1.38
34	O	310	DMS	O-S	4.48	1.80	1.50
34	v	207	DMS	O-S	4.48	1.80	1.50
34	V	210	DMS	O-S	4.48	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	c	938	DMS	O-S	4.48	1.80	1.50
34	i	106	DMS	O-S	4.48	1.80	1.50
34	e	102	DMS	O-S	4.47	1.80	1.50
34	d	416	DMS	O-S	4.47	1.80	1.50
34	c	926	DMS	O-S	4.47	1.80	1.50
34	V	213	DMS	O-S	4.47	1.80	1.50
34	a	422	DMS	O-S	4.47	1.80	1.50
28	B	621	LMG	O8-C28	4.47	1.46	1.33
24	a	409	CLA	O2D-CGD	4.47	1.44	1.33
24	c	903	CLA	CHD-C1D	4.47	1.47	1.38
34	B	646	DMS	O-S	4.47	1.80	1.50
24	A	405	CLA	O2D-CGD	4.47	1.44	1.33
34	c	936	DMS	O-S	4.47	1.80	1.50
34	b	639	DMS	O-S	4.47	1.80	1.50
34	B	640	DMS	O-S	4.47	1.80	1.50
34	U	202	DMS	O-S	4.47	1.80	1.50
34	c	935	DMS	O-S	4.47	1.80	1.50
34	O	305	DMS	O-S	4.47	1.80	1.50
34	C	534	DMS	O-S	4.47	1.80	1.50
24	A	406	CLA	O2D-CGD	4.47	1.44	1.33
34	B	643	DMS	O-S	4.47	1.80	1.50
34	y	101	DMS	O-S	4.47	1.80	1.50
34	O	306	DMS	O-S	4.47	1.80	1.50
34	b	647	DMS	O-S	4.47	1.80	1.50
34	C	524	DMS	O-S	4.47	1.80	1.50
24	C	503	CLA	O2D-CGD	4.47	1.44	1.33
34	B	647	DMS	O-S	4.47	1.80	1.50
34	C	533	DMS	O-S	4.47	1.80	1.50
34	D	414	DMS	O-S	4.46	1.80	1.50
34	c	932	DMS	O-S	4.46	1.80	1.50
34	V	205	DMS	O-S	4.46	1.80	1.50
34	V	208	DMS	O-S	4.46	1.80	1.50
34	V	214	DMS	O-S	4.46	1.80	1.50
34	d	418	DMS	O-S	4.46	1.80	1.50
34	U	203	DMS	O-S	4.46	1.80	1.50
34	B	642	DMS	O-S	4.46	1.80	1.50
34	v	205	DMS	O-S	4.46	1.80	1.50
24	d	404	CLA	O2A-CGA	4.46	1.46	1.33
34	O	314	DMS	O-S	4.46	1.80	1.50
34	H	104	DMS	O-S	4.46	1.80	1.50
34	a	424	DMS	O-S	4.46	1.80	1.50
34	o	303	DMS	O-S	4.46	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	v	204	DMS	O-S	4.46	1.80	1.50
24	c	910	CLA	CHD-C1D	4.46	1.47	1.38
34	b	640	DMS	O-S	4.45	1.80	1.50
34	o	304	DMS	O-S	4.45	1.80	1.50
34	L	102	DMS	O-S	4.45	1.80	1.50
34	O	311	DMS	O-S	4.45	1.80	1.50
34	B	641	DMS	O-S	4.45	1.80	1.50
24	c	908	CLA	CHD-C1D	4.45	1.47	1.38
34	v	209	DMS	O-S	4.45	1.80	1.50
34	v	208	DMS	O-S	4.45	1.80	1.50
34	O	308	DMS	O-S	4.45	1.80	1.50
27	f	102	SQD	O47-C7	4.45	1.46	1.34
24	C	504	CLA	CHD-C1D	4.45	1.47	1.38
34	a	421	DMS	O-S	4.45	1.80	1.50
34	o	302	DMS	O-S	4.45	1.80	1.50
24	b	605	CLA	O2A-CGA	4.44	1.46	1.33
34	o	305	DMS	O-S	4.44	1.80	1.50
24	C	506	CLA	O2A-CGA	4.44	1.46	1.33
34	K	102	DMS	O-S	4.44	1.80	1.50
34	T	103	DMS	O-S	4.44	1.80	1.50
38	E	101	LHG	O8-C23	4.44	1.46	1.33
34	C	527	DMS	O-S	4.44	1.80	1.50
34	B	639	DMS	O-S	4.44	1.80	1.50
34	b	632	DMS	O-S	4.43	1.80	1.50
24	b	614	CLA	CHD-C1D	4.43	1.47	1.38
34	h	105	DMS	O-S	4.43	1.80	1.50
34	u	201	DMS	O-S	4.43	1.80	1.50
34	c	937	DMS	O-S	4.42	1.80	1.50
34	c	931	DMS	O-S	4.42	1.80	1.50
34	b	645	DMS	O-S	4.42	1.80	1.50
34	V	201	DMS	O-S	4.42	1.80	1.50
34	v	203	DMS	O-S	4.42	1.80	1.50
34	O	309	DMS	O-S	4.42	1.80	1.50
34	d	415	DMS	O-S	4.42	1.80	1.50
27	b	601	SQD	O47-C7	4.41	1.46	1.34
34	c	940	DMS	O-S	4.41	1.80	1.50
24	c	913	CLA	CHD-C1D	4.41	1.47	1.38
24	c	913	CLA	O2D-CGD	4.41	1.44	1.33
34	C	526	DMS	O-S	4.41	1.80	1.50
34	b	644	DMS	O-S	4.40	1.80	1.50
24	b	613	CLA	MG-ND	-4.40	1.97	2.05
24	A	407	CLA	CHD-C1D	4.40	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	401	SQD	O48-C23	4.39	1.46	1.33
34	B	633	DMS	O-S	4.39	1.79	1.50
34	D	413	DMS	O-S	4.38	1.79	1.50
24	C	510	CLA	CHD-C1D	4.38	1.46	1.38
24	A	406	CLA	CHC-C1C	4.37	1.46	1.35
24	c	908	CLA	O2A-CGA	4.37	1.46	1.33
34	u	202	DMS	O-S	4.36	1.79	1.50
34	V	209	DMS	O-S	4.36	1.79	1.50
24	B	615	CLA	O2D-CGD	4.36	1.43	1.33
24	C	512	CLA	O2A-CGA	4.36	1.46	1.33
24	C	503	CLA	CHD-C1D	4.35	1.46	1.38
24	c	911	CLA	CHD-C1D	4.35	1.46	1.38
24	b	619	CLA	O2D-CGD	4.35	1.43	1.33
24	B	609	CLA	O2D-CGD	4.34	1.43	1.33
24	b	620	CLA	O2A-CGA	4.33	1.46	1.33
24	B	602	CLA	O2A-CGA	4.33	1.46	1.33
24	C	509	CLA	O2A-CGA	4.32	1.46	1.33
34	B	644	DMS	O-S	4.32	1.79	1.50
28	c	921	LMG	O8-C28	4.32	1.46	1.33
24	c	909	CLA	O2D-CGD	4.32	1.43	1.33
24	b	617	CLA	CHD-C1D	4.31	1.46	1.38
24	b	619	CLA	MG-NC	4.31	2.16	2.06
25	a	412	PHO	OBD-CAD	4.31	1.28	1.22
24	d	401	CLA	CHD-C1D	4.31	1.46	1.38
27	l	101	SQD	O47-C7	4.31	1.46	1.34
24	b	619	CLA	CHD-C1D	4.31	1.46	1.38
27	a	401	SQD	O47-C7	4.30	1.46	1.34
24	A	406	CLA	CHD-C1D	4.30	1.46	1.38
24	B	604	CLA	O2A-CGA	4.29	1.45	1.33
24	C	502	CLA	CHD-C1D	4.28	1.46	1.38
28	A	413	LMG	O7-C10	4.28	1.46	1.34
27	A	416	SQD	O47-C7	4.28	1.46	1.34
27	f	102	SQD	O48-C23	4.28	1.45	1.33
24	b	607	CLA	O2A-CGA	4.27	1.45	1.33
24	C	507	CLA	O2A-CGA	4.26	1.45	1.33
24	B	611	CLA	CHD-C1D	4.26	1.46	1.38
24	c	903	CLA	MG-NC	4.26	2.16	2.06
24	c	910	CLA	MG-ND	-4.26	1.97	2.05
28	C	523	LMG	O8-C28	4.26	1.45	1.33
24	B	614	CLA	MG-NC	4.25	2.16	2.06
24	C	501	CLA	CHD-C1D	4.25	1.46	1.38
28	c	921	LMG	O7-C10	4.25	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	604	CLA	CHD-C1D	4.25	1.46	1.38
24	c	912	CLA	MG-NC	4.25	2.16	2.06
24	B	613	CLA	CHD-C1D	4.25	1.46	1.38
34	c	930	DMS	O-S	4.25	1.78	1.50
28	A	413	LMG	O8-C28	4.25	1.45	1.33
24	B	605	CLA	O2D-CGD	4.24	1.43	1.33
24	c	907	CLA	O2A-CGA	4.24	1.45	1.33
24	c	912	CLA	O2A-CGA	4.24	1.45	1.33
24	B	608	CLA	MG-ND	-4.24	1.97	2.05
24	C	508	CLA	O2A-CGA	4.23	1.45	1.33
24	c	902	CLA	CHD-C1D	4.23	1.46	1.38
24	c	905	CLA	MG-NC	4.22	2.16	2.06
24	A	407	CLA	C1D-ND	4.22	1.43	1.37
24	d	404	CLA	O2D-CGD	4.22	1.43	1.33
24	C	507	CLA	OBD-CAD	4.22	1.29	1.22
24	B	611	CLA	O2D-CGD	4.21	1.43	1.33
24	B	613	CLA	OBD-CAD	4.21	1.29	1.22
24	b	609	CLA	CHD-C1D	4.21	1.46	1.38
24	C	502	CLA	O2A-CGA	4.20	1.45	1.33
28	a	416	LMG	O7-C10	4.20	1.46	1.34
36	O	303	HTG	C1'-S1	-4.20	1.76	1.81
24	c	909	CLA	O2A-CGA	4.20	1.45	1.33
24	c	913	CLA	MG-NC	4.20	2.16	2.06
34	a	420	DMS	O-S	4.19	1.78	1.50
24	c	905	CLA	CHD-C1D	4.19	1.46	1.38
37	D	405	DGD	O1G-C1A	4.19	1.45	1.33
28	C	523	LMG	O7-C10	4.19	1.46	1.34
24	C	511	CLA	O2A-CGA	4.19	1.45	1.33
28	c	920	LMG	O8-C28	4.19	1.45	1.33
24	D	401	CLA	CHD-C1D	4.18	1.46	1.38
27	F	101	SQD	O47-C7	4.18	1.46	1.34
24	B	608	CLA	CHD-C1D	4.18	1.46	1.38
27	b	601	SQD	O48-C23	4.18	1.45	1.33
24	B	613	CLA	MG-NC	4.18	2.16	2.06
24	B	604	CLA	MG-NA	4.18	2.16	2.06
24	c	914	CLA	O2A-CGA	4.17	1.45	1.33
24	c	902	CLA	MG-NC	4.17	2.16	2.06
24	A	407	CLA	MG-ND	-4.17	1.97	2.05
24	D	401	CLA	MG-ND	-4.16	1.97	2.05
24	B	602	CLA	CHD-C4C	4.16	1.48	1.39
24	D	402	CLA	CHD-C1D	4.16	1.46	1.38
24	D	401	CLA	O2A-CGA	4.16	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	L	101	LHG	O7-C7	4.16	1.46	1.34
24	b	615	CLA	MG-ND	-4.16	1.97	2.05
28	a	416	LMG	O8-C28	4.15	1.45	1.33
24	a	410	CLA	O2D-CGD	4.15	1.43	1.33
37	d	408	DGD	O1G-C1A	4.15	1.45	1.33
24	B	609	CLA	O2A-CGA	4.15	1.45	1.33
28	c	920	LMG	O7-C10	4.15	1.46	1.34
24	b	610	CLA	O2A-CGA	4.15	1.45	1.33
24	C	508	CLA	CHD-C1D	4.14	1.46	1.38
24	d	405	CLA	O2A-CGA	4.13	1.45	1.33
37	d	408	DGD	O2G-C1B	4.13	1.46	1.34
28	b	624	LMG	O7-C10	4.13	1.45	1.34
24	d	401	CLA	O2A-CGA	4.12	1.45	1.33
34	B	632	DMS	O-S	4.12	1.78	1.50
24	c	905	CLA	MG-ND	-4.11	1.97	2.05
24	d	401	CLA	OBD-CAD	4.11	1.29	1.22
24	A	410	CLA	CHD-C1D	4.11	1.46	1.38
24	d	405	CLA	CHD-C1D	4.11	1.46	1.38
37	D	405	DGD	O2G-C1B	4.11	1.45	1.34
24	a	413	CLA	O2A-CGA	4.10	1.45	1.33
24	c	902	CLA	O2A-CGA	4.10	1.45	1.33
24	C	509	CLA	MG-ND	-4.10	1.97	2.05
24	B	616	CLA	CHD-C1D	4.10	1.46	1.38
24	B	608	CLA	CHD-C4C	4.09	1.48	1.39
24	C	501	CLA	MG-NC	4.09	2.16	2.06
24	c	910	CLA	O2A-CGA	4.09	1.45	1.33
24	B	617	CLA	O2A-CGA	4.09	1.45	1.33
24	D	401	CLA	C1D-ND	4.09	1.42	1.37
38	d	409	LHG	O8-C23	4.08	1.45	1.33
28	C	519	LMG	O8-C28	4.08	1.45	1.33
42	v	202	HEC	CBC-CAC	-4.08	1.34	1.49
24	B	613	CLA	O2A-CGA	4.07	1.45	1.33
24	B	614	CLA	CHD-C1D	4.07	1.46	1.38
24	B	617	CLA	CHD-C1D	4.07	1.46	1.38
24	B	613	CLA	C1D-ND	4.07	1.42	1.37
38	L	101	LHG	O8-C23	4.07	1.45	1.33
38	E	101	LHG	O7-C7	4.07	1.45	1.34
37	C	516	DGD	O2G-C1B	4.06	1.45	1.34
24	C	501	CLA	OBD-CAD	4.06	1.29	1.22
36	B	623	HTG	C1'-S1	-4.06	1.76	1.81
27	l	101	SQD	O48-C23	4.05	1.45	1.33
24	A	406	CLA	O2A-CGA	4.05	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	906	CLA	OBD-CAD	4.04	1.29	1.22
34	A	423	DMS	O-S	4.04	1.77	1.50
24	b	617	CLA	O2A-CGA	4.04	1.45	1.33
24	a	410	CLA	CHD-C1D	4.04	1.46	1.38
24	d	404	CLA	CHD-C1D	4.03	1.46	1.38
24	c	907	CLA	CHD-C4C	4.03	1.48	1.39
24	C	504	CLA	C3D-C2D	4.03	1.50	1.39
24	b	613	CLA	OBD-CAD	4.03	1.29	1.22
24	c	913	CLA	O2A-CGA	4.02	1.45	1.33
24	b	605	CLA	MG-ND	-4.02	1.97	2.05
37	H	102	DGD	O1G-C1A	4.02	1.45	1.33
24	C	513	CLA	O2A-CGA	4.02	1.45	1.33
24	B	605	CLA	CHD-C1D	4.02	1.46	1.38
24	C	511	CLA	CHD-C1D	4.01	1.46	1.38
24	b	613	CLA	O2A-CGA	4.01	1.45	1.33
28	B	621	LMG	O7-C10	4.01	1.45	1.34
24	C	508	CLA	OBD-CAD	4.01	1.29	1.22
24	B	602	CLA	MG-NC	4.01	2.15	2.06
24	B	611	CLA	O2A-CGA	4.00	1.45	1.33
24	A	407	CLA	MG-NC	3.99	2.15	2.06
24	b	605	CLA	CHD-C4C	3.99	1.48	1.39
38	l	103	LHG	O7-C7	3.99	1.45	1.34
24	d	405	CLA	MG-NC	3.99	2.15	2.06
24	b	619	CLA	OBD-CAD	3.99	1.29	1.22
24	c	903	CLA	C3D-C2D	3.99	1.50	1.39
24	c	912	CLA	CHD-C4C	3.98	1.48	1.39
27	a	415	SQD	O48-C23	3.98	1.45	1.33
24	a	410	CLA	OBD-CAD	3.97	1.29	1.22
24	B	615	CLA	O2A-CGA	3.97	1.44	1.33
24	b	616	CLA	O2A-CGA	3.97	1.44	1.33
24	C	501	CLA	CHD-C4C	3.97	1.48	1.39
34	b	631	DMS	O-S	3.97	1.77	1.50
24	C	507	CLA	MG-ND	-3.97	1.97	2.05
37	h	102	DGD	O2G-C1B	3.97	1.45	1.34
39	F	102	HEM	C3C-C2C	-3.96	1.34	1.40
24	B	603	CLA	OBD-CAD	3.96	1.29	1.22
24	A	405	CLA	O2A-CGA	3.96	1.44	1.33
24	A	410	CLA	O2A-CGA	3.96	1.44	1.33
24	b	612	CLA	O2A-CGA	3.96	1.44	1.33
24	B	616	CLA	O2A-CGA	3.96	1.44	1.33
37	c	917	DGD	O2G-C1B	3.95	1.45	1.34
24	B	617	CLA	C3D-C2D	3.95	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	610	CLA	CHD-C1D	3.95	1.46	1.38
24	c	904	CLA	MG-ND	-3.95	1.98	2.05
24	B	608	CLA	O2A-CGA	3.95	1.44	1.33
24	b	606	CLA	O2A-CGA	3.95	1.44	1.33
24	c	908	CLA	CHD-C4C	3.95	1.48	1.39
36	b	627	HTG	C1'-S1	-3.95	1.76	1.81
24	b	607	CLA	CHD-C4C	3.94	1.48	1.39
24	c	914	CLA	C3D-C2D	3.94	1.49	1.39
24	A	406	CLA	OBD-CAD	3.94	1.29	1.22
24	b	605	CLA	C3D-C2D	3.93	1.49	1.39
24	B	615	CLA	CHD-C1D	3.93	1.46	1.38
24	c	904	CLA	O2A-CGA	3.93	1.44	1.33
24	B	610	CLA	OBD-CAD	3.93	1.29	1.22
24	C	504	CLA	CHD-C4C	3.93	1.48	1.39
24	A	405	CLA	CHD-C1D	3.93	1.46	1.38
24	c	912	CLA	OBD-CAD	3.93	1.29	1.22
24	A	407	CLA	MG-NA	3.92	2.15	2.06
24	b	618	CLA	C3D-C2D	3.92	1.49	1.39
24	c	912	CLA	C3D-C2D	3.92	1.49	1.39
25	A	409	PHO	CHA-CBD	-3.92	1.47	1.52
24	C	511	CLA	C3D-C2D	3.92	1.49	1.39
24	a	413	CLA	CHD-C1D	3.91	1.46	1.38
24	C	505	CLA	OBD-CAD	3.91	1.29	1.22
24	a	409	CLA	CHD-C4C	3.91	1.48	1.39
24	a	410	CLA	O2A-CGA	3.91	1.44	1.33
24	b	613	CLA	CHD-C4C	3.91	1.48	1.39
28	d	412	LMG	O7-C10	3.91	1.45	1.34
37	c	919	DGD	O1G-C1A	3.91	1.44	1.33
24	B	616	CLA	OBD-CAD	3.90	1.29	1.22
24	c	914	CLA	CHD-C4C	3.90	1.48	1.39
24	C	501	CLA	O2A-CGA	3.90	1.44	1.33
24	c	906	CLA	O2A-CGA	3.89	1.44	1.33
24	B	615	CLA	C3D-C2D	3.89	1.49	1.39
24	c	905	CLA	O2A-CGA	3.89	1.44	1.33
24	c	911	CLA	MG-NA	3.89	2.15	2.06
24	C	508	CLA	C3D-C2D	3.88	1.49	1.39
24	b	606	CLA	C3D-C2D	3.88	1.49	1.39
24	b	619	CLA	C3D-C2D	3.88	1.49	1.39
24	b	616	CLA	OBD-CAD	3.88	1.29	1.22
24	b	609	CLA	O2A-CGA	3.88	1.44	1.33
24	b	619	CLA	O2A-CGA	3.88	1.44	1.33
24	C	510	CLA	CHD-C4C	3.88	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	d	411	LHG	O7-C7	3.87	1.45	1.34
24	b	613	CLA	C3D-C2D	3.87	1.49	1.39
24	b	619	CLA	MG-ND	-3.87	1.98	2.05
24	B	606	CLA	O2A-CGA	3.87	1.44	1.33
24	b	610	CLA	OBD-CAD	3.86	1.29	1.22
24	C	506	CLA	CHD-C4C	3.86	1.48	1.39
37	H	102	DGD	O2G-C1B	3.86	1.45	1.34
24	b	611	CLA	C3D-C2D	3.86	1.49	1.39
24	c	910	CLA	C3D-C2D	3.85	1.49	1.39
24	c	910	CLA	OBD-CAD	3.85	1.29	1.22
37	c	919	DGD	O2G-C1B	3.85	1.45	1.34
25	a	411	PHO	O2A-CGA	3.85	1.44	1.33
24	b	606	CLA	CHD-C4C	3.85	1.48	1.39
27	A	412	SQD	O48-C23	3.85	1.44	1.33
28	d	412	LMG	O8-C28	3.85	1.44	1.33
27	a	415	SQD	O47-C7	3.84	1.45	1.34
24	C	503	CLA	O2A-CGA	3.84	1.44	1.33
39	f	101	HEM	C3C-C2C	-3.84	1.35	1.40
27	A	412	SQD	O47-C7	3.84	1.45	1.34
24	c	910	CLA	CHD-C4C	3.83	1.48	1.39
24	b	618	CLA	O2A-CGA	3.83	1.44	1.33
24	c	904	CLA	C3D-C2D	3.83	1.49	1.39
24	b	611	CLA	O2A-CGA	3.83	1.44	1.33
24	C	509	CLA	CHD-C4C	3.83	1.48	1.39
37	h	102	DGD	O1G-C1A	3.83	1.44	1.33
24	c	913	CLA	C3D-C2D	3.83	1.49	1.39
25	a	412	PHO	O2A-CGA	3.83	1.44	1.33
24	C	509	CLA	C3D-C2D	3.82	1.49	1.39
24	b	612	CLA	OBD-CAD	3.82	1.29	1.22
24	D	402	CLA	O2A-CGA	3.82	1.44	1.33
25	A	409	PHO	O2A-CGA	3.82	1.44	1.33
24	B	603	CLA	MG-NC	3.82	2.15	2.06
24	C	502	CLA	C3D-C2D	3.82	1.49	1.39
24	C	510	CLA	MG-NC	3.81	2.15	2.06
36	D	412	HTG	C1'-S1	-3.81	1.76	1.81
24	c	909	CLA	OBD-CAD	3.81	1.29	1.22
24	C	508	CLA	CHD-C4C	3.80	1.47	1.39
36	y	102	HTG	C1'-S1	-3.80	1.76	1.81
24	B	607	CLA	CHD-C4C	3.80	1.47	1.39
24	b	615	CLA	O2A-CGA	3.79	1.44	1.33
28	C	519	LMG	O7-C10	3.79	1.45	1.34
24	b	605	CLA	OBD-CAD	3.79	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	502	CLA	OBD-CAD	3.79	1.29	1.22
24	C	512	CLA	C3D-C2D	3.78	1.49	1.39
24	a	413	CLA	C3D-C2D	3.78	1.49	1.39
24	B	606	CLA	C3D-C2D	3.78	1.49	1.39
36	d	419	HTG	C1'-S1	-3.78	1.76	1.81
24	C	506	CLA	C3D-C2D	3.78	1.49	1.39
36	C	521	HTG	C1'-S1	-3.77	1.76	1.81
24	B	611	CLA	C3D-C2D	3.77	1.49	1.39
24	C	511	CLA	OBD-CAD	3.77	1.29	1.22
24	c	903	CLA	CHD-C4C	3.77	1.47	1.39
24	C	503	CLA	C3D-C2D	3.77	1.49	1.39
24	C	513	CLA	CHD-C4C	3.77	1.47	1.39
24	C	512	CLA	CHD-C4C	3.76	1.47	1.39
24	c	905	CLA	C3D-C2D	3.76	1.49	1.39
24	a	410	CLA	C3D-C2D	3.76	1.49	1.39
24	b	608	CLA	O2A-CGA	3.76	1.44	1.33
24	B	602	CLA	C3D-C2D	3.76	1.49	1.39
24	B	607	CLA	OBD-CAD	3.76	1.29	1.22
37	C	518	DGD	O2G-C1B	3.75	1.44	1.34
37	c	917	DGD	O1G-C1A	3.75	1.44	1.33
36	c	924	HTG	C1'-S1	-3.74	1.76	1.81
24	b	616	CLA	CHD-C1D	3.74	1.45	1.38
38	D	406	LHG	O8-C23	3.74	1.44	1.33
24	c	909	CLA	C3D-C2D	3.74	1.49	1.39
24	A	405	CLA	C3D-C2D	3.74	1.49	1.39
38	D	407	LHG	O8-C23	3.73	1.44	1.33
24	A	407	CLA	O2A-CGA	3.73	1.44	1.33
24	C	510	CLA	OBD-CAD	3.73	1.28	1.22
24	c	907	CLA	C3D-C2D	3.73	1.49	1.39
24	B	615	CLA	OBD-CAD	3.73	1.28	1.22
36	C	536	HTG	C1'-S1	-3.73	1.76	1.81
24	C	507	CLA	MG-NC	3.72	2.15	2.06
24	b	618	CLA	CHD-C4C	3.72	1.47	1.39
42	V	203	HEC	CBC-CAC	-3.72	1.35	1.49
24	A	410	CLA	OBD-CAD	3.72	1.28	1.22
24	c	908	CLA	C3D-C2D	3.72	1.49	1.39
24	c	914	CLA	OBD-CAD	3.71	1.28	1.22
24	c	908	CLA	MG-NC	3.71	2.15	2.06
42	v	202	HEC	CBB-CAB	-3.71	1.35	1.49
24	C	510	CLA	C3D-C2D	3.71	1.49	1.39
38	D	408	LHG	O8-C23	3.71	1.44	1.33
25	A	408	PHO	CHA-CBD	-3.71	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	405	CLA	C3D-C2D	3.71	1.49	1.39
24	c	908	CLA	OBD-CAD	3.70	1.28	1.22
24	C	511	CLA	CHD-C4C	3.70	1.47	1.39
24	c	903	CLA	O2A-CGA	3.70	1.44	1.33
24	C	513	CLA	OBD-CAD	3.70	1.28	1.22
24	b	615	CLA	CHD-C4C	3.70	1.47	1.39
24	b	619	CLA	CHD-C4C	3.69	1.47	1.39
24	a	409	CLA	O2A-CGA	3.69	1.44	1.33
24	C	505	CLA	O2A-CGA	3.69	1.44	1.33
24	c	913	CLA	CHD-C4C	3.69	1.47	1.39
24	D	402	CLA	OBD-CAD	3.69	1.28	1.22
24	B	614	CLA	O2A-CGA	3.68	1.44	1.33
28	D	409	LMG	O8-C28	3.68	1.44	1.33
37	c	918	DGD	O2G-C1B	3.68	1.44	1.34
24	B	614	CLA	C3D-C2D	3.68	1.49	1.39
36	c	928	HTG	C1'-S1	-3.68	1.76	1.81
25	A	409	PHO	C3C-C2C	3.68	1.48	1.37
36	d	414	HTG	C1'-S1	-3.68	1.76	1.81
24	B	610	CLA	C3D-C2D	3.68	1.49	1.39
24	a	410	CLA	CHD-C4C	3.67	1.47	1.39
24	A	410	CLA	CHD-C4C	3.67	1.47	1.39
24	C	505	CLA	CHD-C4C	3.67	1.47	1.39
37	c	918	DGD	O1G-C1A	3.67	1.44	1.33
24	B	609	CLA	CHD-C4C	3.67	1.47	1.39
24	D	402	CLA	C3D-C2D	3.66	1.49	1.39
24	b	610	CLA	C3D-C2D	3.66	1.49	1.39
24	B	616	CLA	CHD-C4C	3.66	1.47	1.39
24	B	613	CLA	C3D-C2D	3.66	1.49	1.39
24	B	603	CLA	C3D-C2D	3.66	1.49	1.39
36	d	420	HTG	C1'-S1	-3.66	1.76	1.81
36	v	211	HTG	C1'-S1	-3.66	1.76	1.81
37	C	517	DGD	O2G-C1B	3.65	1.44	1.34
24	B	605	CLA	OBD-CAD	3.65	1.28	1.22
24	c	911	CLA	O2A-CGA	3.65	1.44	1.33
24	b	620	CLA	OBD-CAD	3.65	1.28	1.22
24	B	603	CLA	CHD-C4C	3.65	1.47	1.39
24	d	405	CLA	CHD-C4C	3.65	1.47	1.39
24	b	607	CLA	C3D-C2D	3.64	1.49	1.39
24	B	612	CLA	CHD-C4C	3.64	1.47	1.39
38	l	103	LHG	O8-C23	3.64	1.44	1.33
24	b	610	CLA	CHD-C4C	3.64	1.47	1.39
24	c	906	CLA	CHD-C4C	3.64	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	d	410	LHG	O8-C23	3.64	1.44	1.33
24	C	501	CLA	C3D-C2D	3.64	1.49	1.39
24	B	612	CLA	O2A-CGA	3.63	1.44	1.33
36	V	215	HTG	C1'-S1	-3.63	1.76	1.81
24	B	606	CLA	MG-ND	-3.63	1.98	2.05
25	a	412	PHO	C3C-C2C	3.63	1.48	1.37
24	b	615	CLA	C3D-C2D	3.63	1.49	1.39
24	c	904	CLA	CHD-C4C	3.63	1.47	1.39
24	b	611	CLA	CHD-C4C	3.63	1.47	1.39
24	c	911	CLA	C3D-C2D	3.63	1.49	1.39
24	c	911	CLA	CHD-C4C	3.63	1.47	1.39
24	C	513	CLA	C3D-C2D	3.63	1.49	1.39
24	A	407	CLA	C3D-C2D	3.63	1.49	1.39
24	c	903	CLA	OBD-CAD	3.62	1.28	1.22
39	f	101	HEM	C3C-CAC	3.62	1.55	1.47
38	D	408	LHG	O7-C7	3.61	1.44	1.34
24	B	609	CLA	C3D-C2D	3.61	1.49	1.39
24	c	902	CLA	CHD-C4C	3.61	1.47	1.39
24	D	402	CLA	CHD-C4C	3.61	1.47	1.39
24	C	507	CLA	CHD-C4C	3.61	1.47	1.39
24	b	609	CLA	C3D-C2D	3.60	1.49	1.39
24	c	905	CLA	CHD-C4C	3.60	1.47	1.39
24	B	603	CLA	O2A-CGA	3.60	1.43	1.33
24	C	502	CLA	CHD-C4C	3.60	1.47	1.39
24	b	617	CLA	OBD-CAD	3.59	1.28	1.22
24	B	617	CLA	MG-NC	3.59	2.14	2.06
36	c	943	HTG	C1'-S1	-3.59	1.76	1.81
24	A	410	CLA	C3D-C2D	3.59	1.48	1.39
24	b	609	CLA	CHD-C4C	3.58	1.47	1.39
38	d	410	LHG	O7-C7	3.58	1.44	1.34
24	B	605	CLA	CHD-C4C	3.58	1.47	1.39
24	B	612	CLA	OBD-CAD	3.58	1.28	1.22
24	b	614	CLA	CHD-C4C	3.58	1.47	1.39
24	b	609	CLA	MG-NC	3.58	2.14	2.06
24	c	902	CLA	C3D-C2D	3.57	1.48	1.39
38	D	407	LHG	O7-C7	3.57	1.44	1.34
24	A	405	CLA	OBD-CAD	3.57	1.28	1.22
24	D	401	CLA	CHD-C4C	3.57	1.47	1.39
24	B	610	CLA	O2A-CGA	3.57	1.43	1.33
24	C	507	CLA	C3D-C2D	3.56	1.48	1.39
24	B	616	CLA	C3D-C2D	3.55	1.48	1.39
24	d	401	CLA	C3D-C2D	3.55	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	614	CLA	C3D-C2D	3.55	1.48	1.39
24	B	615	CLA	MG-ND	-3.55	1.98	2.05
25	A	408	PHO	O2A-CGA	3.54	1.43	1.33
24	C	512	CLA	OBD-CAD	3.54	1.28	1.22
39	F	102	HEM	C3C-CAC	3.54	1.55	1.47
24	C	503	CLA	CHD-C4C	3.54	1.47	1.39
24	d	404	CLA	CHD-C4C	3.53	1.47	1.39
24	d	405	CLA	OBD-CAD	3.53	1.28	1.22
24	b	620	CLA	C3D-C2D	3.53	1.48	1.39
36	c	923	HTG	C1'-S1	-3.53	1.76	1.81
24	C	505	CLA	C3D-C2D	3.52	1.48	1.39
36	b	603	HTG	C1'-S1	-3.52	1.76	1.81
24	B	602	CLA	OBD-CAD	3.52	1.28	1.22
24	b	614	CLA	O2A-CGA	3.52	1.43	1.33
24	d	401	CLA	CHD-C4C	3.51	1.47	1.39
37	C	517	DGD	O1G-C1A	3.51	1.43	1.33
24	A	407	CLA	CHD-C4C	3.51	1.47	1.39
24	b	608	CLA	C3D-C2D	3.51	1.48	1.39
24	C	510	CLA	O2A-CGA	3.51	1.43	1.33
24	C	509	CLA	OBD-CAD	3.51	1.28	1.22
36	B	630	HTG	C1'-S1	-3.51	1.76	1.81
24	B	609	CLA	OBD-CAD	3.51	1.28	1.22
24	c	902	CLA	OBD-CAD	3.51	1.28	1.22
24	c	909	CLA	CHD-C4C	3.50	1.47	1.39
24	b	617	CLA	C3D-C2D	3.50	1.48	1.39
24	B	607	CLA	O2A-CGA	3.50	1.43	1.33
24	B	613	CLA	CHD-C4C	3.50	1.47	1.39
24	B	606	CLA	CHD-C4C	3.49	1.47	1.39
24	c	913	CLA	OBD-CAD	3.49	1.28	1.22
25	A	408	PHO	C3C-C2C	3.49	1.48	1.37
24	b	612	CLA	C3D-C2D	3.48	1.48	1.39
24	b	617	CLA	CHD-C4C	3.48	1.47	1.39
24	C	501	CLA	MG-ND	-3.48	1.98	2.05
24	b	616	CLA	C3D-C2D	3.48	1.48	1.39
36	b	602	HTG	C1'-S1	-3.47	1.77	1.81
24	B	607	CLA	C3D-C2D	3.47	1.48	1.39
24	b	612	CLA	CHD-C4C	3.47	1.47	1.39
24	A	405	CLA	CHD-C4C	3.47	1.47	1.39
24	B	604	CLA	C3D-C2D	3.47	1.48	1.39
36	C	537	HTG	C1'-S1	-3.47	1.77	1.81
24	B	606	CLA	OBD-CAD	3.47	1.28	1.22
24	c	906	CLA	C3D-C2D	3.47	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	B	625	HTG	C1'-S1	-3.46	1.77	1.81
24	b	606	CLA	OBD-CAD	3.46	1.28	1.22
24	C	506	CLA	OBD-CAD	3.46	1.28	1.22
36	B	631	HTG	C1'-S1	-3.46	1.77	1.81
24	a	413	CLA	CHD-C4C	3.45	1.47	1.39
36	c	942	HTG	C1'-S1	-3.45	1.77	1.81
36	c	941	HTG	C1'-S1	-3.45	1.77	1.81
38	d	411	LHG	O8-C23	3.45	1.43	1.33
24	B	608	CLA	C3D-C2D	3.44	1.48	1.39
24	c	904	CLA	OBD-CAD	3.44	1.28	1.22
24	B	614	CLA	CHD-C4C	3.44	1.47	1.39
24	b	616	CLA	MG-NC	3.44	2.14	2.06
24	b	614	CLA	MG-NC	3.43	2.14	2.06
24	b	615	CLA	MG-NC	3.43	2.14	2.06
25	A	408	PHO	OBD-CAD	3.42	1.27	1.22
36	C	520	HTG	C1'-S1	-3.42	1.77	1.81
24	b	607	CLA	OBD-CAD	3.42	1.28	1.22
36	B	629	HTG	C1'-S1	-3.42	1.77	1.81
37	C	518	DGD	O1G-C1A	3.42	1.43	1.33
24	C	504	CLA	O2A-CGA	3.41	1.43	1.33
24	c	907	CLA	OBD-CAD	3.41	1.28	1.22
24	B	604	CLA	CHD-C4C	3.41	1.47	1.39
24	B	614	CLA	OBD-CAD	3.41	1.28	1.22
24	c	911	CLA	OBD-CAD	3.40	1.28	1.22
37	C	516	DGD	O1G-C1A	3.40	1.43	1.33
24	B	617	CLA	CHD-C4C	3.40	1.47	1.39
24	B	612	CLA	C3D-C2D	3.39	1.48	1.39
24	A	410	CLA	MG-NC	3.38	2.14	2.06
24	C	504	CLA	OBD-CAD	3.37	1.28	1.22
24	B	611	CLA	OBD-CAD	3.37	1.28	1.22
24	A	406	CLA	CHD-C4C	3.36	1.46	1.39
24	a	413	CLA	MG-NC	3.36	2.14	2.06
24	B	605	CLA	C3D-C2D	3.36	1.48	1.39
24	b	620	CLA	CHD-C4C	3.36	1.46	1.39
24	b	615	CLA	OBD-CAD	3.35	1.28	1.22
25	a	411	PHO	C3C-C2C	3.35	1.47	1.37
28	D	409	LMG	O7-C10	3.34	1.43	1.34
24	D	401	CLA	OBD-CAD	3.34	1.28	1.22
25	a	411	PHO	OBD-CAD	3.33	1.27	1.22
24	c	905	CLA	OBD-CAD	3.32	1.28	1.22
24	d	404	CLA	OBD-CAD	3.31	1.28	1.22
24	A	406	CLA	C3D-C2D	3.31	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	404	CLA	C3D-C2D	3.29	1.48	1.39
24	c	908	CLA	C4D-CHA	3.29	1.50	1.38
24	B	611	CLA	CHD-C4C	3.28	1.46	1.39
24	B	615	CLA	CHD-C4C	3.27	1.46	1.39
39	F	102	HEM	FE-ND	3.27	2.13	1.96
24	b	618	CLA	OBD-CAD	3.26	1.28	1.22
38	d	409	LHG	O7-C7	3.26	1.43	1.34
24	b	608	CLA	C4D-CHA	3.25	1.50	1.38
24	c	904	CLA	C4D-CHA	3.25	1.49	1.38
24	B	605	CLA	O2A-CGA	3.24	1.42	1.33
24	B	608	CLA	OBD-CAD	3.24	1.28	1.22
24	B	615	CLA	MG-NC	3.22	2.13	2.06
24	b	608	CLA	OBD-CAD	3.22	1.28	1.22
24	C	505	CLA	C1B-CHB	3.22	1.49	1.41
42	V	203	HEC	CBB-CAB	-3.21	1.37	1.49
24	c	910	CLA	C1B-CHB	3.21	1.49	1.41
24	C	507	CLA	C4D-CHA	3.21	1.49	1.38
24	B	604	CLA	OBD-CAD	3.20	1.28	1.22
24	b	615	CLA	C1B-CHB	3.20	1.49	1.41
24	D	401	CLA	C3D-C2D	3.20	1.47	1.39
39	f	101	HEM	CAB-C3B	3.19	1.56	1.47
24	B	610	CLA	CHD-C4C	3.19	1.46	1.39
24	c	903	CLA	C1B-CHB	3.19	1.49	1.41
24	A	406	CLA	MG-NC	3.18	2.13	2.06
24	B	613	CLA	C1B-CHB	3.17	1.49	1.41
24	b	608	CLA	CHD-C4C	3.17	1.46	1.39
24	B	617	CLA	OBD-CAD	3.16	1.27	1.22
24	D	402	CLA	MG-NA	3.16	2.13	2.06
24	b	614	CLA	OBD-CAD	3.16	1.27	1.22
24	C	503	CLA	C4D-CHA	3.14	1.49	1.38
24	c	904	CLA	C1B-CHB	3.12	1.49	1.41
24	B	610	CLA	C1B-CHB	3.12	1.49	1.41
24	B	617	CLA	C1B-CHB	3.11	1.49	1.41
39	f	101	HEM	FE-ND	3.10	2.12	1.96
24	a	413	CLA	MG-ND	-3.09	1.99	2.05
24	b	612	CLA	C1B-CHB	3.09	1.49	1.41
24	c	910	CLA	MG-NC	3.09	2.13	2.06
24	C	503	CLA	OBD-CAD	3.08	1.27	1.22
38	D	406	LHG	O7-C7	3.08	1.43	1.34
24	a	413	CLA	OBD-CAD	3.07	1.27	1.22
24	a	409	CLA	C3D-C2D	3.07	1.47	1.39
25	a	411	PHO	CHA-CBD	-3.07	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	605	CLA	C4D-CHA	3.07	1.49	1.38
24	c	910	CLA	C4D-CHA	3.06	1.49	1.38
24	b	619	CLA	C4D-CHA	3.06	1.49	1.38
24	C	509	CLA	C1B-CHB	3.06	1.49	1.41
24	C	503	CLA	C4B-CHC	3.05	1.49	1.41
24	b	609	CLA	OBD-CAD	3.04	1.27	1.22
24	C	511	CLA	C4D-CHA	3.04	1.49	1.38
24	b	608	CLA	C1B-CHB	3.04	1.49	1.41
24	b	620	CLA	C1B-CHB	3.04	1.49	1.41
24	c	912	CLA	C1B-CHB	3.03	1.49	1.41
24	A	410	CLA	C1B-CHB	3.03	1.49	1.41
24	b	616	CLA	C1B-CHB	3.02	1.49	1.41
24	B	612	CLA	C4D-CHA	3.02	1.49	1.38
36	b	626	HTG	C1'-S1	-3.02	1.77	1.81
24	B	607	CLA	C4B-CHC	3.01	1.49	1.41
24	C	503	CLA	C1B-CHB	3.01	1.49	1.41
24	b	620	CLA	MG-NC	3.01	2.13	2.06
24	b	605	CLA	C4B-CHC	3.00	1.49	1.41
24	b	610	CLA	C4D-CHA	3.00	1.49	1.38
24	b	617	CLA	C1B-CHB	2.99	1.49	1.41
24	B	616	CLA	C4D-CHA	2.99	1.49	1.38
24	b	612	CLA	C4D-CHA	2.99	1.49	1.38
24	D	401	CLA	MG-NC	2.99	2.13	2.06
24	C	502	CLA	C1B-CHB	2.98	1.49	1.41
39	F	102	HEM	CAB-C3B	2.98	1.55	1.47
24	b	611	CLA	OBD-CAD	2.98	1.27	1.22
24	B	615	CLA	C1B-CHB	2.97	1.49	1.41
24	C	512	CLA	C4D-CHA	2.97	1.48	1.38
24	b	606	CLA	C4D-CHA	2.97	1.48	1.38
24	B	609	CLA	C4C-C3C	2.94	1.50	1.45
24	B	607	CLA	C4D-CHA	2.94	1.48	1.38
24	B	611	CLA	C1B-CHB	2.94	1.49	1.41
24	c	913	CLA	C4D-CHA	2.94	1.48	1.38
24	C	503	CLA	C1C-C2C	2.93	1.50	1.44
24	c	912	CLA	C4D-CHA	2.92	1.48	1.38
36	B	624	HTG	C1'-S1	-2.92	1.77	1.81
24	B	614	CLA	C4B-CHC	2.92	1.49	1.41
24	C	505	CLA	C4D-CHA	2.92	1.48	1.38
24	a	409	CLA	C1B-CHB	2.90	1.49	1.41
24	C	505	CLA	C4B-CHC	2.90	1.49	1.41
24	b	610	CLA	C1B-CHB	2.90	1.49	1.41
24	b	605	CLA	C4D-CHA	2.90	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	617	CLA	C1C-NC	-2.90	1.33	1.37
24	C	511	CLA	C1B-CHB	2.89	1.49	1.41
24	C	506	CLA	C4D-CHA	2.89	1.48	1.38
24	A	405	CLA	C4D-CHA	2.89	1.48	1.38
24	B	602	CLA	C4D-CHA	2.89	1.48	1.38
24	C	512	CLA	C1B-CHB	2.89	1.49	1.41
27	f	102	SQD	C6-S	-2.89	1.66	1.77
24	C	502	CLA	C4D-CHA	2.88	1.48	1.38
25	a	412	PHO	CHA-CBD	-2.88	1.48	1.52
24	C	508	CLA	C1B-CHB	2.88	1.49	1.41
24	b	615	CLA	C4D-CHA	2.88	1.48	1.38
24	B	609	CLA	C4D-CHA	2.87	1.48	1.38
36	O	316	HTG	C1'-S1	-2.87	1.77	1.81
24	c	904	CLA	C1C-C2C	2.87	1.50	1.44
24	D	402	CLA	C1B-CHB	2.87	1.49	1.41
24	B	614	CLA	C4D-CHA	2.87	1.48	1.38
24	b	611	CLA	C4D-CHA	2.87	1.48	1.38
24	C	509	CLA	C4D-CHA	2.85	1.48	1.38
24	B	606	CLA	C1B-CHB	2.85	1.48	1.41
24	C	501	CLA	C1B-CHB	2.85	1.48	1.41
24	c	908	CLA	C1B-CHB	2.85	1.48	1.41
25	a	412	PHO	C3A-C2A	-2.84	1.52	1.54
24	b	614	CLA	C4D-CHA	2.84	1.48	1.38
24	b	611	CLA	C1B-CHB	2.83	1.48	1.41
27	A	416	SQD	C6-S	-2.83	1.66	1.77
24	a	410	CLA	C1B-CHB	2.83	1.48	1.41
24	c	906	CLA	C1B-CHB	2.83	1.48	1.41
24	c	905	CLA	C4D-CHA	2.83	1.48	1.38
24	A	410	CLA	MG-ND	-2.83	2.00	2.05
24	C	510	CLA	C1B-CHB	2.83	1.48	1.41
24	c	902	CLA	C1B-CHB	2.82	1.48	1.41
24	c	904	CLA	C4B-CHC	2.82	1.48	1.41
24	b	619	CLA	C1B-CHB	2.82	1.48	1.41
24	A	410	CLA	C4D-CHA	2.82	1.48	1.38
24	B	610	CLA	C4D-CHA	2.82	1.48	1.38
24	c	909	CLA	MG-NA	2.81	2.13	2.06
24	b	605	CLA	C1B-CHB	2.81	1.48	1.41
24	c	911	CLA	C1B-CHB	2.81	1.48	1.41
24	C	512	CLA	C4B-CHC	2.81	1.48	1.41
24	B	615	CLA	C4D-CHA	2.81	1.48	1.38
24	b	616	CLA	CHD-C4C	2.81	1.45	1.39
24	A	405	CLA	C1C-C2C	2.80	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	603	CLA	C1B-CHB	2.80	1.48	1.41
24	B	610	CLA	C1C-NC	-2.80	1.33	1.37
24	c	902	CLA	C4D-CHA	2.80	1.48	1.38
24	C	501	CLA	C4D-CHA	2.80	1.48	1.38
27	A	412	SQD	C6-S	-2.80	1.67	1.77
24	b	613	CLA	C4D-CHA	2.79	1.48	1.38
24	b	613	CLA	C1B-CHB	2.79	1.48	1.41
24	B	602	CLA	C1B-CHB	2.78	1.48	1.41
24	b	613	CLA	C4B-CHC	2.78	1.48	1.41
24	C	513	CLA	C1B-CHB	2.78	1.48	1.41
24	D	401	CLA	C1B-CHB	2.78	1.48	1.41
24	B	603	CLA	C4B-CHC	2.77	1.48	1.41
24	D	402	CLA	C4D-CHA	2.77	1.48	1.38
24	d	405	CLA	C4D-CHA	2.77	1.48	1.38
24	b	606	CLA	C1B-CHB	2.76	1.48	1.41
24	c	911	CLA	C4D-CHA	2.76	1.48	1.38
24	c	912	CLA	MG-ND	-2.76	2.00	2.05
24	d	404	CLA	C4D-CHA	2.76	1.48	1.38
24	c	906	CLA	C4D-CHA	2.75	1.48	1.38
24	c	906	CLA	C4B-CHC	2.75	1.48	1.41
24	C	506	CLA	C1B-CHB	2.75	1.48	1.41
24	d	404	CLA	C1B-CHB	2.75	1.48	1.41
24	c	914	CLA	C1C-C2C	2.75	1.49	1.44
24	a	413	CLA	C1B-CHB	2.75	1.48	1.41
24	B	617	CLA	C4D-CHA	2.75	1.48	1.38
24	B	602	CLA	C4B-CHC	2.74	1.48	1.41
24	d	404	CLA	C1C-NC	-2.74	1.33	1.37
24	c	914	CLA	C4D-CHA	2.73	1.48	1.38
27	a	401	SQD	C6-S	-2.72	1.67	1.77
24	C	510	CLA	C4D-CHA	2.72	1.48	1.38
24	C	502	CLA	C1C-C2C	2.72	1.49	1.44
24	c	914	CLA	C4B-CHC	2.72	1.48	1.41
24	A	406	CLA	C4D-CHA	2.72	1.48	1.38
27	a	415	SQD	C6-S	-2.72	1.67	1.77
24	B	608	CLA	C4D-CHA	2.71	1.48	1.38
24	b	610	CLA	C4B-CHC	2.71	1.48	1.41
24	B	613	CLA	C4D-CHA	2.71	1.48	1.38
24	B	611	CLA	C4B-CHC	2.71	1.48	1.41
24	b	620	CLA	C4D-CHA	2.71	1.48	1.38
24	B	612	CLA	MG-NC	2.71	2.12	2.06
27	l	101	SQD	C6-S	-2.70	1.67	1.77
24	C	504	CLA	C4D-CHA	2.70	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	902	CLA	C1C-C2C	2.70	1.49	1.44
24	B	612	CLA	C1B-CHB	2.70	1.48	1.41
24	C	507	CLA	C1B-CHB	2.70	1.48	1.41
24	b	617	CLA	C4D-CHA	2.70	1.48	1.38
24	D	402	CLA	C4B-CHC	2.70	1.48	1.41
24	C	509	CLA	C4B-CHC	2.69	1.48	1.41
24	b	610	CLA	C1C-C2C	2.69	1.49	1.44
24	c	908	CLA	C4B-CHC	2.69	1.48	1.41
24	B	611	CLA	C4D-CHA	2.69	1.48	1.38
24	c	902	CLA	C4B-CHC	2.69	1.48	1.41
24	b	618	CLA	C1B-CHB	2.68	1.48	1.41
24	c	903	CLA	C4D-CHA	2.68	1.47	1.38
24	B	616	CLA	C1B-CHB	2.68	1.48	1.41
24	b	613	CLA	C1C-NC	-2.68	1.33	1.37
24	b	609	CLA	C4D-CHA	2.68	1.47	1.38
24	a	410	CLA	C4D-CHA	2.68	1.47	1.38
24	A	405	CLA	C1B-CHB	2.67	1.48	1.41
24	C	513	CLA	C4D-CHA	2.67	1.47	1.38
24	B	616	CLA	C4B-CHC	2.67	1.48	1.41
24	c	911	CLA	C4B-CHC	2.67	1.48	1.41
24	b	607	CLA	C4D-CHA	2.67	1.47	1.38
24	B	610	CLA	C4B-CHC	2.67	1.48	1.41
24	b	607	CLA	C1B-CHB	2.66	1.48	1.41
24	B	603	CLA	C4D-CHA	2.66	1.47	1.38
24	A	406	CLA	C1B-CHB	2.66	1.48	1.41
24	b	614	CLA	C4B-CHC	2.66	1.48	1.41
24	C	510	CLA	C4B-CHC	2.66	1.48	1.41
24	c	907	CLA	C4D-CHA	2.66	1.47	1.38
24	c	908	CLA	C1C-C2C	2.66	1.49	1.44
24	B	602	CLA	MG-ND	-2.66	2.00	2.05
24	a	410	CLA	MG-NC	2.65	2.12	2.06
24	C	506	CLA	C4B-CHC	2.65	1.48	1.41
37	h	102	DGD	O5D-C1E	2.65	1.44	1.40
24	c	906	CLA	C4C-C3C	2.65	1.49	1.45
24	B	607	CLA	C1B-CHB	2.64	1.48	1.41
27	b	601	SQD	C6-S	-2.64	1.67	1.77
24	a	409	CLA	C4D-CHA	2.64	1.47	1.38
24	b	620	CLA	C1C-NC	-2.64	1.33	1.37
24	b	605	CLA	C1C-C2C	2.64	1.49	1.44
24	b	612	CLA	C1C-NC	-2.64	1.33	1.37
24	C	513	CLA	C1C-C2C	2.64	1.49	1.44
24	C	502	CLA	C4B-CHC	2.64	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	536	HTG	C1-S1	-2.64	1.76	1.80
24	a	413	CLA	C4D-CHA	2.64	1.47	1.38
24	B	604	CLA	C4B-CHC	2.63	1.48	1.41
24	b	618	CLA	C4B-CHC	2.63	1.48	1.41
24	c	904	CLA	C4C-C3C	2.62	1.49	1.45
24	d	405	CLA	C1B-CHB	2.62	1.48	1.41
24	C	513	CLA	C4B-CHC	2.62	1.48	1.41
24	c	903	CLA	C4B-CHC	2.62	1.48	1.41
24	b	609	CLA	C4B-CHC	2.61	1.48	1.41
24	d	405	CLA	C1C-C2C	2.61	1.49	1.44
24	B	614	CLA	C1C-C2C	2.61	1.49	1.44
24	b	611	CLA	C1B-NB	-2.60	1.32	1.35
24	b	615	CLA	C4B-CHC	2.60	1.48	1.41
24	A	406	CLA	C4B-CHC	2.60	1.48	1.41
24	d	401	CLA	C1B-CHB	2.60	1.48	1.41
24	C	505	CLA	C4C-C3C	2.60	1.49	1.45
24	c	914	CLA	C1B-CHB	2.59	1.48	1.41
24	b	608	CLA	C1C-C2C	2.59	1.49	1.44
24	B	605	CLA	C4B-CHC	2.59	1.48	1.41
24	C	504	CLA	C1B-CHB	2.58	1.48	1.41
24	B	614	CLA	C1B-CHB	2.58	1.48	1.41
29	a	417	PL9	C6-C5	2.58	1.48	1.35
24	d	405	CLA	C4B-CHC	2.57	1.48	1.41
24	A	407	CLA	C4D-CHA	2.57	1.47	1.38
24	B	605	CLA	C1B-CHB	2.57	1.48	1.41
24	b	612	CLA	C4B-CHC	2.57	1.48	1.41
24	b	608	CLA	C4B-CHC	2.57	1.48	1.41
24	b	616	CLA	C4D-CHA	2.56	1.47	1.38
24	b	612	CLA	C1C-C2C	2.56	1.49	1.44
24	C	508	CLA	C4B-CHC	2.56	1.48	1.41
24	b	608	CLA	C1C-NC	-2.56	1.34	1.37
24	b	614	CLA	C4C-C3C	2.56	1.49	1.45
24	C	511	CLA	C4B-CHC	2.56	1.48	1.41
24	b	618	CLA	C4D-CHA	2.55	1.47	1.38
24	B	609	CLA	C1B-CHB	2.55	1.48	1.41
24	C	505	CLA	C1C-C2C	2.55	1.49	1.44
24	c	913	CLA	C1B-CHB	2.54	1.48	1.41
24	C	512	CLA	C1C-C2C	2.54	1.49	1.44
24	b	609	CLA	C1B-CHB	2.54	1.48	1.41
24	B	607	CLA	C1C-C2C	2.54	1.49	1.44
24	B	608	CLA	C3D-C4D	-2.54	1.38	1.44
24	B	602	CLA	C1C-C2C	2.54	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	907	CLA	C1C-NC	-2.54	1.34	1.37
24	B	609	CLA	C4B-CHC	2.54	1.48	1.41
24	C	503	CLA	C1C-NC	-2.53	1.34	1.37
24	A	410	CLA	C4B-CHC	2.53	1.48	1.41
24	B	607	CLA	MG-ND	-2.53	2.00	2.05
24	C	507	CLA	C4B-CHC	2.52	1.48	1.41
37	H	102	DGD	O5D-C1E	2.52	1.44	1.40
24	c	905	CLA	C1B-CHB	2.52	1.48	1.41
24	B	611	CLA	C4C-C3C	2.52	1.49	1.45
24	c	907	CLA	C1B-CHB	2.51	1.48	1.41
24	A	407	CLA	C1B-CHB	2.51	1.48	1.41
24	c	912	CLA	C4B-CHC	2.51	1.48	1.41
24	c	909	CLA	C1B-CHB	2.51	1.48	1.41
24	C	510	CLA	C3D-C4D	-2.51	1.38	1.44
24	A	405	CLA	C4B-CHC	2.50	1.48	1.41
24	C	508	CLA	C4C-C3C	2.50	1.49	1.45
24	B	608	CLA	C4B-CHC	2.50	1.47	1.41
36	v	211	HTG	C1-S1	-2.50	1.76	1.80
24	b	607	CLA	C1C-NC	-2.50	1.34	1.37
24	C	509	CLA	C1C-NC	-2.50	1.34	1.37
36	b	602	HTG	C1-S1	-2.49	1.76	1.80
24	C	501	CLA	C4B-CHC	2.49	1.47	1.41
24	b	607	CLA	C4B-CHC	2.49	1.47	1.41
24	C	511	CLA	C1C-C2C	2.49	1.49	1.44
24	b	619	CLA	C4B-CHC	2.49	1.47	1.41
29	d	407	PL9	C6-C5	2.48	1.48	1.35
24	C	504	CLA	C4B-CHC	2.47	1.47	1.41
24	B	608	CLA	C1B-CHB	2.47	1.47	1.41
24	b	614	CLA	C1B-CHB	2.47	1.47	1.41
24	D	401	CLA	C4B-CHC	2.47	1.47	1.41
24	B	606	CLA	C1C-C2C	2.46	1.49	1.44
24	B	612	CLA	C4B-CHC	2.46	1.47	1.41
24	C	509	CLA	C1C-C2C	2.46	1.49	1.44
24	b	616	CLA	C4B-CHC	2.46	1.47	1.41
24	B	617	CLA	C1C-NC	-2.45	1.34	1.37
24	c	906	CLA	C1C-C2C	2.45	1.49	1.44
24	b	607	CLA	C1C-C2C	2.45	1.49	1.44
24	d	401	CLA	C4D-CHA	2.45	1.47	1.38
24	b	617	CLA	C1C-C2C	2.45	1.49	1.44
29	A	414	PL9	C6-C5	2.45	1.48	1.35
24	B	606	CLA	C4D-CHA	2.45	1.47	1.38
29	D	404	PL9	C6-C5	2.44	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	c	942	HTG	C1-S1	-2.44	1.77	1.80
24	b	617	CLA	C4B-CHC	2.44	1.47	1.41
24	B	606	CLA	C1C-NC	-2.44	1.34	1.37
24	B	603	CLA	C1C-C2C	2.43	1.49	1.44
24	b	606	CLA	C1C-NC	-2.43	1.34	1.37
24	C	507	CLA	C1C-NC	-2.43	1.34	1.37
24	b	617	CLA	C4C-C3C	2.43	1.49	1.45
24	B	615	CLA	C4B-CHC	2.43	1.47	1.41
24	c	913	CLA	C4B-CHC	2.43	1.47	1.41
36	C	520	HTG	C1-S1	-2.43	1.77	1.80
24	B	606	CLA	C4B-CHC	2.42	1.47	1.41
24	C	501	CLA	C1C-C2C	2.42	1.49	1.44
24	B	611	CLA	C1C-C2C	2.42	1.49	1.44
24	b	606	CLA	C4B-CHC	2.42	1.47	1.41
36	B	629	HTG	C1-S1	-2.42	1.77	1.80
24	C	508	CLA	C4D-CHA	2.42	1.47	1.38
24	c	909	CLA	C1C-NC	-2.42	1.34	1.37
24	A	410	CLA	C1C-C2C	2.42	1.49	1.44
24	c	913	CLA	C1C-C2C	2.42	1.49	1.44
24	B	604	CLA	C1B-CHB	2.41	1.47	1.41
24	b	611	CLA	C4B-CHC	2.41	1.47	1.41
24	D	401	CLA	C1C-NC	-2.41	1.34	1.37
24	c	905	CLA	C1C-NC	-2.41	1.34	1.37
24	A	406	CLA	C1C-C2C	2.40	1.49	1.44
36	c	928	HTG	C1-S1	-2.40	1.77	1.80
24	c	908	CLA	C1C-NC	-2.40	1.34	1.37
24	A	406	CLA	C1C-NC	-2.40	1.34	1.37
24	c	912	CLA	C4C-C3C	2.40	1.49	1.45
24	d	405	CLA	C4C-C3C	2.39	1.49	1.45
24	D	402	CLA	C3D-C4D	-2.39	1.38	1.44
24	b	607	CLA	C4C-C3C	2.39	1.49	1.45
24	C	509	CLA	C4C-C3C	2.39	1.49	1.45
24	C	510	CLA	C1C-C2C	2.38	1.49	1.44
24	c	909	CLA	C4D-CHA	2.38	1.46	1.38
24	b	616	CLA	C1C-C2C	2.38	1.49	1.44
24	c	914	CLA	C4C-C3C	2.38	1.49	1.45
36	d	419	HTG	C1-S1	-2.38	1.77	1.80
24	c	905	CLA	C1C-C2C	2.37	1.49	1.44
24	c	907	CLA	C4B-CHC	2.37	1.47	1.41
36	c	923	HTG	C1-S1	-2.37	1.77	1.80
24	D	401	CLA	C4D-CHA	2.37	1.46	1.38
24	b	612	CLA	C3D-C4D	-2.37	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	611	CLA	C1C-NC	-2.36	1.34	1.37
24	C	501	CLA	C1C-NC	-2.36	1.34	1.37
36	b	603	HTG	C1-S1	-2.36	1.77	1.80
24	B	613	CLA	C1C-NC	-2.36	1.34	1.37
24	c	907	CLA	C3D-C4D	-2.36	1.38	1.44
24	B	617	CLA	C4B-CHC	2.36	1.47	1.41
24	c	911	CLA	C3D-C4D	-2.36	1.38	1.44
24	d	404	CLA	C1C-C2C	2.35	1.49	1.44
24	d	401	CLA	C4B-CHC	2.35	1.47	1.41
24	b	618	CLA	C4C-C3C	2.35	1.49	1.45
24	b	616	CLA	C1C-NC	-2.34	1.34	1.37
24	b	620	CLA	C4B-CHC	2.34	1.47	1.41
24	c	910	CLA	C4B-CHC	2.34	1.47	1.41
24	b	614	CLA	C3D-C4D	-2.34	1.38	1.44
24	B	605	CLA	C1C-C2C	2.34	1.49	1.44
24	D	402	CLA	C1C-C2C	2.34	1.49	1.44
24	C	506	CLA	C1C-NC	-2.33	1.34	1.37
24	a	413	CLA	C4B-CHC	2.33	1.47	1.41
24	b	613	CLA	C1C-C2C	2.33	1.49	1.44
42	V	203	HEC	C4B-C3B	2.32	1.47	1.43
24	A	406	CLA	C4C-C3C	2.32	1.49	1.45
24	B	610	CLA	C1C-C2C	2.32	1.49	1.44
24	B	604	CLA	C4D-CHA	2.32	1.46	1.38
24	D	401	CLA	C4C-C3C	2.31	1.49	1.45
24	a	409	CLA	C4B-CHC	2.31	1.47	1.41
24	B	615	CLA	C4C-C3C	2.31	1.49	1.45
24	c	903	CLA	C3D-C4D	-2.31	1.39	1.44
24	C	510	CLA	C4C-C3C	2.30	1.49	1.45
36	b	627	HTG	C1-S1	-2.30	1.77	1.80
24	b	609	CLA	C1C-C2C	2.30	1.49	1.44
24	C	504	CLA	C3D-C4D	-2.30	1.39	1.44
24	b	609	CLA	C1C-NC	-2.29	1.34	1.37
24	C	502	CLA	C4C-C3C	2.29	1.49	1.45
24	c	905	CLA	C4B-CHC	2.29	1.47	1.41
24	b	620	CLA	C3D-C4D	-2.29	1.39	1.44
24	a	410	CLA	C4C-C3C	2.29	1.49	1.45
24	B	604	CLA	C1C-NC	-2.28	1.34	1.37
24	c	905	CLA	C3D-C4D	-2.28	1.39	1.44
24	c	908	CLA	C4D-ND	2.27	1.40	1.37
24	b	606	CLA	C1C-C2C	2.27	1.49	1.44
24	B	613	CLA	C1C-C2C	2.27	1.49	1.44
24	c	911	CLA	C1C-NC	-2.27	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	413	CLA	C1C-C2C	2.27	1.49	1.44
24	C	506	CLA	C1C-C2C	2.27	1.49	1.44
24	A	407	CLA	C3D-C4D	-2.27	1.39	1.44
24	a	409	CLA	C4C-C3C	2.27	1.48	1.45
24	b	611	CLA	C4C-C3C	2.27	1.48	1.45
36	C	521	HTG	C1-S1	-2.26	1.77	1.80
24	A	407	CLA	C4B-CHC	2.26	1.47	1.41
36	y	102	HTG	C1-S1	-2.26	1.77	1.80
24	c	909	CLA	C4B-CHC	2.26	1.47	1.41
24	C	508	CLA	C1C-C2C	2.26	1.48	1.44
24	B	604	CLA	C3D-C4D	-2.26	1.39	1.44
24	B	604	CLA	C1C-C2C	2.26	1.48	1.44
24	C	507	CLA	C4C-C3C	2.25	1.48	1.45
24	B	613	CLA	C4B-CHC	2.25	1.47	1.41
24	c	913	CLA	C4C-C3C	2.25	1.48	1.45
24	c	903	CLA	C1C-C2C	2.25	1.48	1.44
24	c	904	CLA	C1C-NC	-2.25	1.34	1.37
24	D	401	CLA	C1C-C2C	2.25	1.48	1.44
24	A	407	CLA	C1C-NC	-2.25	1.34	1.37
24	c	912	CLA	C1C-C2C	2.25	1.48	1.44
36	c	924	HTG	C1-S1	-2.24	1.77	1.80
24	b	605	CLA	C1C-NC	-2.24	1.34	1.37
24	c	911	CLA	C4C-C3C	2.23	1.48	1.45
24	c	905	CLA	C4C-C3C	2.23	1.48	1.45
24	B	606	CLA	C3D-C4D	-2.23	1.39	1.44
24	B	602	CLA	C4C-C3C	2.23	1.48	1.45
36	B	630	HTG	C1-S1	-2.23	1.77	1.80
27	F	101	SQD	C6-S	-2.22	1.69	1.77
24	C	506	CLA	C4C-C3C	2.22	1.48	1.45
24	b	606	CLA	C4C-C3C	2.22	1.48	1.45
24	a	413	CLA	C1C-NC	-2.22	1.34	1.37
24	b	608	CLA	C4C-C3C	2.22	1.48	1.45
24	b	613	CLA	C1D-C2D	2.21	1.49	1.45
24	D	401	CLA	C3D-C4D	-2.21	1.39	1.44
24	c	907	CLA	C1C-C2C	2.21	1.48	1.44
24	d	404	CLA	C4B-CHC	2.21	1.47	1.41
24	b	607	CLA	C3D-C4D	-2.21	1.39	1.44
24	C	511	CLA	C4C-C3C	2.21	1.48	1.45
24	C	505	CLA	C1B-NB	-2.21	1.33	1.35
24	C	502	CLA	C3D-C4D	-2.21	1.39	1.44
24	A	405	CLA	C1C-NC	-2.20	1.34	1.37
24	d	404	CLA	C4C-C3C	2.20	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	910	CLA	C1C-C2C	2.20	1.48	1.44
24	b	618	CLA	C3D-C4D	-2.19	1.39	1.44
24	B	617	CLA	C3D-C4D	-2.19	1.39	1.44
24	a	409	CLA	C1C-C2C	2.18	1.48	1.44
24	a	410	CLA	C1C-NC	-2.18	1.34	1.37
24	B	615	CLA	C3D-C4D	-2.18	1.39	1.44
36	d	414	HTG	C1-S1	-2.17	1.77	1.80
24	c	913	CLA	C3D-C4D	-2.17	1.39	1.44
24	a	410	CLA	C3D-C4D	-2.17	1.39	1.44
24	C	511	CLA	C3D-C4D	-2.17	1.39	1.44
24	B	602	CLA	C1C-NC	-2.16	1.34	1.37
24	B	603	CLA	C4C-C3C	2.16	1.48	1.45
24	B	608	CLA	C4C-C3C	2.16	1.48	1.45
24	b	612	CLA	C4C-C3C	2.16	1.48	1.45
24	B	602	CLA	C1D-C2D	2.16	1.49	1.45
24	B	617	CLA	C4C-C3C	2.16	1.48	1.45
24	C	501	CLA	C4C-C3C	2.16	1.48	1.45
24	c	910	CLA	C1C-NC	-2.16	1.34	1.37
24	B	602	CLA	C3D-C4D	-2.15	1.39	1.44
24	C	513	CLA	C1C-NC	-2.15	1.34	1.37
24	b	618	CLA	C1C-C2C	2.15	1.48	1.44
24	B	616	CLA	C3D-C4D	-2.15	1.39	1.44
24	c	914	CLA	C1C-NC	-2.15	1.34	1.37
28	a	416	LMG	O1-C1	2.15	1.43	1.40
24	B	605	CLA	C3D-C4D	-2.15	1.39	1.44
24	C	504	CLA	C1C-C2C	2.15	1.48	1.44
24	C	506	CLA	C3D-C4D	-2.14	1.39	1.44
24	b	619	CLA	C3D-C4D	-2.14	1.39	1.44
24	A	406	CLA	C3D-C4D	-2.14	1.39	1.44
24	B	616	CLA	C4C-C3C	2.14	1.48	1.45
24	b	613	CLA	C3D-C4D	-2.14	1.39	1.44
24	B	605	CLA	C4D-ND	2.14	1.40	1.37
24	a	409	CLA	C1B-NB	-2.14	1.33	1.35
24	b	606	CLA	C3D-C4D	-2.14	1.39	1.44
24	c	910	CLA	C4C-C3C	2.13	1.48	1.45
36	D	412	HTG	C1-S1	-2.13	1.77	1.80
31	j	102	LMT	O1'-C1'	2.13	1.43	1.40
24	B	603	CLA	C3D-C4D	-2.13	1.39	1.44
24	C	507	CLA	C1C-C2C	2.13	1.48	1.44
39	f	101	HEM	CMB-C2B	2.13	1.55	1.50
24	C	509	CLA	C3D-C4D	-2.12	1.39	1.44
24	B	607	CLA	C3D-C4D	-2.12	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	606	CLA	C4C-C3C	2.12	1.48	1.45
24	a	409	CLA	C1C-NC	-2.11	1.34	1.37
24	b	615	CLA	C3D-C4D	-2.11	1.39	1.44
24	a	410	CLA	C4B-CHC	2.11	1.46	1.41
24	C	507	CLA	C4D-ND	2.11	1.40	1.37
36	C	537	HTG	C1-S1	-2.10	1.77	1.80
24	b	608	CLA	C3D-C4D	-2.10	1.39	1.44
24	c	911	CLA	C1C-C2C	2.10	1.48	1.44
24	b	619	CLA	C4C-C3C	2.10	1.48	1.45
24	B	609	CLA	C3D-C4D	-2.10	1.39	1.44
24	A	410	CLA	C1C-NC	-2.10	1.34	1.37
27	b	601	SQD	O6-C1	2.10	1.43	1.40
31	c	922	LMT	O1'-C1'	2.10	1.43	1.40
24	B	609	CLA	C1C-C2C	2.10	1.48	1.44
24	b	619	CLA	C1C-C2C	2.10	1.48	1.44
24	B	613	CLA	C1B-NB	-2.09	1.33	1.35
24	B	613	CLA	C4D-ND	2.09	1.40	1.37
24	c	909	CLA	C1C-C2C	2.09	1.48	1.44
24	b	615	CLA	C4C-C3C	2.09	1.48	1.45
24	C	502	CLA	C1C-NC	-2.09	1.34	1.37
24	d	401	CLA	C3D-C4D	-2.08	1.39	1.44
24	b	611	CLA	C3D-C4D	-2.08	1.39	1.44
24	b	613	CLA	C4C-C3C	2.08	1.48	1.45
24	b	605	CLA	C3D-C4D	-2.07	1.39	1.44
24	C	510	CLA	C1B-NB	-2.07	1.33	1.35
24	B	607	CLA	C4C-C3C	2.07	1.48	1.45
37	C	516	DGD	O5D-C1E	2.07	1.43	1.40
24	A	407	CLA	C1B-NB	-2.07	1.33	1.35
39	F	102	HEM	CAA-C2A	2.07	1.55	1.52
36	d	420	HTG	C1-S1	-2.07	1.77	1.80
24	a	410	CLA	C1C-C2C	2.07	1.48	1.44
39	f	101	HEM	CAA-C2A	2.07	1.55	1.52
24	C	512	CLA	C3D-C4D	-2.06	1.39	1.44
24	c	907	CLA	C4C-C3C	2.06	1.48	1.45
24	B	614	CLA	C4C-C3C	2.06	1.48	1.45
24	B	605	CLA	C4C-C3C	2.06	1.48	1.45
24	A	407	CLA	C1C-C2C	2.06	1.48	1.44
39	f	101	HEM	FE-NB	2.06	2.07	1.96
24	C	510	CLA	C1C-NC	-2.06	1.34	1.37
24	c	908	CLA	C1A-CHA	2.05	1.51	1.43
26	b	623	BCR	C30-C25	-2.05	1.50	1.53
24	C	512	CLA	C1C-NC	-2.05	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	513	CLA	C3D-C4D	-2.05	1.39	1.44
24	d	405	CLA	C3D-C4D	-2.05	1.39	1.44
42	v	202	HEC	C4D-ND	2.05	1.40	1.36
24	C	503	CLA	C4D-ND	2.04	1.40	1.37
24	b	614	CLA	C1C-C2C	2.04	1.48	1.44
24	B	616	CLA	MG-NC	2.04	2.11	2.06
24	d	404	CLA	C3D-C4D	-2.04	1.39	1.44
24	b	619	CLA	C1C-NC	-2.04	1.34	1.37
24	d	405	CLA	C1C-NC	-2.04	1.34	1.37
36	O	316	HTG	C1-S1	-2.04	1.77	1.80
27	l	101	SQD	O6-C1	2.03	1.43	1.40
24	D	402	CLA	C1C-NC	-2.03	1.34	1.37
24	b	610	CLA	C1C-NC	-2.03	1.34	1.37
24	a	413	CLA	C4C-C3C	2.02	1.48	1.45
24	d	401	CLA	C1C-C2C	2.02	1.48	1.44
24	B	604	CLA	C4C-C3C	2.01	1.48	1.45
24	C	504	CLA	C1C-NC	-2.01	1.34	1.37
36	c	943	HTG	C1-S1	-2.01	1.77	1.80
24	c	902	CLA	C1C-NC	-2.00	1.34	1.37
24	c	904	CLA	C1A-CHA	2.00	1.51	1.43
24	B	607	CLA	C4D-ND	2.00	1.40	1.37

All (2413) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	909	CLA	C1D-ND-C4D	-11.30	98.31	106.33
24	D	401	CLA	C1D-ND-C4D	-11.21	98.37	106.33
24	b	616	CLA	C1D-ND-C4D	-10.86	98.62	106.33
24	A	406	CLA	C1D-ND-C4D	-10.74	98.71	106.33
24	c	902	CLA	C1D-ND-C4D	-10.67	98.75	106.33
24	d	401	CLA	C1D-ND-C4D	-10.49	98.88	106.33
24	a	409	CLA	C1D-ND-C4D	-10.32	99.00	106.33
24	B	605	CLA	C1D-ND-C4D	-10.28	99.03	106.33
24	a	410	CLA	C1D-ND-C4D	-10.26	99.05	106.33
24	d	404	CLA	C1D-ND-C4D	-10.25	99.06	106.33
24	B	604	CLA	C1D-ND-C4D	-10.17	99.11	106.33
24	b	617	CLA	C1D-ND-C4D	-10.15	99.12	106.33
24	A	407	CLA	C1D-ND-C4D	-10.14	99.13	106.33
24	B	612	CLA	C1D-ND-C4D	-10.01	99.23	106.33
24	B	614	CLA	C1D-ND-C4D	-9.99	99.24	106.33
24	D	401	CLA	C2D-C1D-ND	9.94	117.43	110.10
24	B	615	CLA	C1D-ND-C4D	-9.88	99.32	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	502	CLA	C1D-ND-C4D	-9.87	99.32	106.33
24	b	609	CLA	C1D-ND-C4D	-9.86	99.33	106.33
24	B	613	CLA	C1D-ND-C4D	-9.84	99.34	106.33
24	A	410	CLA	C1D-ND-C4D	-9.82	99.36	106.33
24	c	905	CLA	C1D-ND-C4D	-9.78	99.39	106.33
24	B	614	CLA	C2D-C1D-ND	9.76	117.30	110.10
24	b	612	CLA	C1D-ND-C4D	-9.68	99.46	106.33
24	c	909	CLA	C2D-C1D-ND	9.67	117.23	110.10
24	b	616	CLA	C2D-C1D-ND	9.66	117.22	110.10
24	A	405	CLA	C1D-ND-C4D	-9.65	99.48	106.33
24	d	405	CLA	C1D-ND-C4D	-9.64	99.49	106.33
24	B	606	CLA	C1D-ND-C4D	-9.62	99.50	106.33
24	C	508	CLA	C1D-ND-C4D	-9.61	99.51	106.33
24	b	608	CLA	C1D-ND-C4D	-9.60	99.52	106.33
24	B	610	CLA	C1D-ND-C4D	-9.59	99.52	106.33
24	A	406	CLA	C2D-C1D-ND	9.58	117.17	110.10
24	B	608	CLA	C1D-ND-C4D	-9.55	99.55	106.33
24	C	513	CLA	C1D-ND-C4D	-9.55	99.55	106.33
24	B	616	CLA	C1D-ND-C4D	-9.53	99.56	106.33
24	B	617	CLA	C1D-ND-C4D	-9.53	99.56	106.33
24	b	618	CLA	C1D-ND-C4D	-9.45	99.62	106.33
24	b	620	CLA	C1D-ND-C4D	-9.42	99.64	106.33
24	C	504	CLA	C1D-ND-C4D	-9.41	99.65	106.33
24	B	603	CLA	C1D-ND-C4D	-9.37	99.68	106.33
24	D	402	CLA	C1D-ND-C4D	-9.35	99.69	106.33
24	C	501	CLA	C1D-ND-C4D	-9.28	99.74	106.33
24	c	911	CLA	C1D-ND-C4D	-9.26	99.76	106.33
24	c	913	CLA	C1D-ND-C4D	-9.22	99.78	106.33
24	c	903	CLA	C1D-ND-C4D	-9.22	99.79	106.33
24	c	907	CLA	C1D-ND-C4D	-9.22	99.79	106.33
24	c	902	CLA	C2D-C1D-ND	9.20	116.88	110.10
24	b	609	CLA	C2D-C1D-ND	9.15	116.85	110.10
24	A	410	CLA	C2D-C1D-ND	9.14	116.84	110.10
24	B	615	CLA	C2D-C1D-ND	9.10	116.81	110.10
24	b	617	CLA	C2D-C1D-ND	9.09	116.81	110.10
24	B	617	CLA	C2D-C1D-ND	9.07	116.78	110.10
24	B	611	CLA	C1D-ND-C4D	-9.06	99.90	106.33
24	C	510	CLA	C1D-ND-C4D	-9.05	99.91	106.33
24	b	608	CLA	C2D-C1D-ND	9.02	116.75	110.10
24	B	616	CLA	C2D-C1D-ND	8.98	116.72	110.10
24	B	612	CLA	C2D-C1D-ND	8.92	116.68	110.10
24	d	405	CLA	C2D-C1D-ND	8.91	116.67	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	613	CLA	C1D-ND-C4D	-8.90	100.02	106.33
24	C	512	CLA	C1D-ND-C4D	-8.87	100.03	106.33
24	B	611	CLA	C2D-C1D-ND	8.85	116.62	110.10
24	b	614	CLA	C1D-ND-C4D	-8.84	100.06	106.33
24	c	910	CLA	C1D-ND-C4D	-8.82	100.07	106.33
24	d	401	CLA	C2D-C1D-ND	8.81	116.60	110.10
24	a	413	CLA	C1D-ND-C4D	-8.81	100.08	106.33
24	a	410	CLA	C2D-C1D-ND	8.81	116.59	110.10
24	c	908	CLA	C1D-ND-C4D	-8.79	100.09	106.33
24	B	605	CLA	C2D-C1D-ND	8.77	116.56	110.10
24	b	606	CLA	C1D-ND-C4D	-8.76	100.11	106.33
24	c	914	CLA	C1D-ND-C4D	-8.75	100.12	106.33
24	C	506	CLA	C1D-ND-C4D	-8.73	100.13	106.33
24	c	912	CLA	C1D-ND-C4D	-8.72	100.14	106.33
24	b	610	CLA	C1D-ND-C4D	-8.68	100.17	106.33
24	B	607	CLA	C1D-ND-C4D	-8.68	100.17	106.33
36	V	215	HTG	C1'-S1-C1	8.67	116.31	100.09
24	b	607	CLA	C1D-ND-C4D	-8.65	100.19	106.33
24	B	609	CLA	C1D-ND-C4D	-8.65	100.19	106.33
24	C	503	CLA	C1D-ND-C4D	-8.65	100.19	106.33
24	C	509	CLA	C1D-ND-C4D	-8.65	100.19	106.33
24	B	613	CLA	C2D-C1D-ND	8.63	116.47	110.10
24	d	404	CLA	C2D-C1D-ND	8.56	116.41	110.10
24	C	507	CLA	C1D-ND-C4D	-8.51	100.29	106.33
24	A	407	CLA	C2D-C1D-ND	8.50	116.37	110.10
24	c	910	CLA	C2D-C1D-ND	8.49	116.36	110.10
24	b	615	CLA	C1D-ND-C4D	-8.48	100.31	106.33
24	c	906	CLA	C1D-ND-C4D	-8.47	100.32	106.33
24	C	508	CLA	C2D-C1D-ND	8.44	116.32	110.10
24	b	605	CLA	C1D-ND-C4D	-8.42	100.35	106.33
24	C	511	CLA	C2D-C1D-ND	8.41	116.30	110.10
24	b	620	CLA	C2D-C1D-ND	8.41	116.30	110.10
24	C	511	CLA	C1D-ND-C4D	-8.40	100.37	106.33
24	b	619	CLA	C1D-ND-C4D	-8.40	100.37	106.33
24	C	505	CLA	C1D-ND-C4D	-8.40	100.37	106.33
24	c	905	CLA	C2D-C1D-ND	8.40	116.29	110.10
24	C	504	CLA	C2D-C1D-ND	8.38	116.28	110.10
24	a	413	CLA	C2D-C1D-ND	8.37	116.27	110.10
24	a	409	CLA	C2D-C1D-ND	8.36	116.26	110.10
24	B	606	CLA	C2D-C1D-ND	8.36	116.26	110.10
24	c	913	CLA	C2D-C1D-ND	8.35	116.26	110.10
24	b	611	CLA	C1D-ND-C4D	-8.34	100.41	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	618	CLA	C2D-C1D-ND	8.31	116.22	110.10
24	C	502	CLA	C2D-C1D-ND	8.30	116.22	110.10
24	A	405	CLA	C2D-C1D-ND	8.29	116.21	110.10
24	C	503	CLA	C2D-C1D-ND	8.29	116.21	110.10
24	B	602	CLA	C1D-ND-C4D	-8.25	100.47	106.33
24	B	604	CLA	C2D-C1D-ND	8.21	116.16	110.10
24	c	908	CLA	C2D-C1D-ND	8.18	116.13	110.10
24	B	610	CLA	C2D-C1D-ND	8.16	116.12	110.10
24	b	614	CLA	C2D-C1D-ND	8.16	116.12	110.10
24	C	501	CLA	C2D-C1D-ND	8.16	116.12	110.10
24	b	610	CLA	C2D-C1D-ND	8.16	116.12	110.10
24	C	507	CLA	C2D-C1D-ND	8.14	116.11	110.10
24	b	611	CLA	C2D-C1D-ND	8.12	116.09	110.10
24	c	903	CLA	C2D-C1D-ND	7.99	115.99	110.10
24	b	615	CLA	C2D-C1D-ND	7.95	115.96	110.10
24	B	608	CLA	C2D-C1D-ND	7.95	115.96	110.10
24	C	513	CLA	C2D-C1D-ND	7.93	115.94	110.10
24	C	512	CLA	C2D-C1D-ND	7.91	115.93	110.10
24	B	609	CLA	C2D-C1D-ND	7.83	115.87	110.10
24	B	607	CLA	C2D-C1D-ND	7.82	115.86	110.10
24	c	904	CLA	C2D-C1D-ND	7.80	115.85	110.10
24	D	402	CLA	C2D-C1D-ND	7.78	115.84	110.10
24	b	619	CLA	C2D-C1D-ND	7.78	115.83	110.10
24	B	603	CLA	C2D-C1D-ND	7.73	115.80	110.10
24	C	506	CLA	C2D-C1D-ND	7.62	115.72	110.10
24	b	606	CLA	C2D-C1D-ND	7.56	115.68	110.10
24	b	612	CLA	C2D-C1D-ND	7.55	115.67	110.10
24	c	907	CLA	C2D-C1D-ND	7.48	115.62	110.10
24	c	904	CLA	C1D-ND-C4D	-7.45	101.04	106.33
24	c	912	CLA	C2D-C1D-ND	7.37	115.53	110.10
24	C	510	CLA	C2D-C1D-ND	7.34	115.51	110.10
36	B	631	HTG	C1'-S1-C1	7.30	113.75	100.09
24	b	618	CLA	C1-C2-C3	-7.22	113.56	126.04
24	b	605	CLA	C2D-C1D-ND	7.21	115.42	110.10
24	c	914	CLA	C2D-C1D-ND	7.20	115.41	110.10
24	c	911	CLA	C2D-C1D-ND	7.16	115.38	110.10
25	a	411	PHO	O2D-CGD-CBD	7.15	120.05	111.00
24	C	509	CLA	C2D-C1D-ND	7.10	115.33	110.10
24	c	908	CLA	O2D-CGD-CBD	7.06	123.82	111.27
24	b	613	CLA	C2D-C1D-ND	6.96	115.23	110.10
36	B	625	HTG	C1'-S1-C1	6.95	113.09	100.09
24	B	602	CLA	CMD-C2D-C1D	6.88	136.84	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	412	PHO	O2D-CGD-CBD	6.82	119.64	111.00
24	C	505	CLA	C2D-C1D-ND	6.82	115.13	110.10
24	B	602	CLA	C2D-C1D-ND	6.81	115.12	110.10
24	c	906	CLA	C2D-C1D-ND	6.80	115.12	110.10
24	B	607	CLA	CMD-C2D-C1D	6.74	136.59	124.71
25	A	408	PHO	O2D-CGD-CBD	6.73	119.52	111.00
24	C	506	CLA	CMD-C2D-C1D	6.59	136.33	124.71
24	b	607	CLA	C2D-C1D-ND	6.55	114.93	110.10
27	F	101	SQD	O6-C1-C2	6.50	118.45	108.30
25	A	409	PHO	O2D-CGD-CBD	6.47	119.19	111.00
24	B	605	CLA	CMD-C2D-C1D	6.44	136.06	124.71
24	B	612	CLA	CMD-C2D-C1D	6.43	136.05	124.71
24	d	404	CLA	CMD-C2D-C1D	6.42	136.02	124.71
24	C	507	CLA	CMD-C2D-C1D	6.40	135.99	124.71
24	c	907	CLA	CMD-C2D-C1D	6.40	135.99	124.71
24	D	401	CLA	CMD-C2D-C1D	6.40	135.99	124.71
24	C	509	CLA	CMD-C2D-C1D	6.37	135.94	124.71
24	C	503	CLA	CMD-C2D-C1D	6.33	135.87	124.71
24	b	608	CLA	O2D-CGD-CBD	6.32	122.49	111.27
24	c	905	CLA	CMD-C2D-C1D	6.31	135.83	124.71
24	b	606	CLA	CMD-C2D-C1D	6.23	135.69	124.71
24	B	603	CLA	CMD-C2D-C1D	6.22	135.68	124.71
24	c	906	CLA	CMD-C2D-C1D	6.22	135.67	124.71
24	D	402	CLA	CMD-C2D-C1D	6.18	135.60	124.71
24	C	510	CLA	CMD-C2D-C1D	6.13	135.51	124.71
36	d	414	HTG	C1'-S1-C1	6.11	111.53	100.09
24	b	613	CLA	CMD-C2D-C1D	6.06	135.39	124.71
24	c	902	CLA	CMD-C2D-C1D	6.06	135.39	124.71
24	C	501	CLA	CMD-C2D-C1D	6.00	135.29	124.71
24	b	617	CLA	CMD-C2D-C1D	5.99	135.27	124.71
24	b	609	CLA	CMD-C2D-C1D	5.97	135.23	124.71
24	b	608	CLA	CMD-C2D-C1D	5.96	135.22	124.71
24	b	605	CLA	O2D-CGD-CBD	5.94	121.82	111.27
24	b	614	CLA	CMD-C2D-C1D	5.94	135.18	124.71
24	B	604	CLA	O2D-CGD-CBD	5.92	121.79	111.27
24	b	619	CLA	CMD-C2D-C1D	5.91	135.13	124.71
24	C	501	CLA	O2D-CGD-CBD	5.90	121.75	111.27
24	b	605	CLA	CMD-C2D-C1D	5.89	135.10	124.71
24	C	510	CLA	O2D-CGD-CBD	5.89	121.73	111.27
27	a	415	SQD	O6-C1-C2	5.86	117.45	108.30
24	b	620	CLA	O2D-CGD-CBD	5.85	121.67	111.27
24	C	507	CLA	O2D-CGD-CBD	5.85	121.66	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	608	CLA	CMD-C2D-C1D	5.84	135.01	124.71
24	b	611	CLA	CMD-C2D-C1D	5.81	134.95	124.71
24	C	504	CLA	CMD-C2D-C1D	5.81	134.94	124.71
36	d	420	HTG	C1'-S1-C1	5.79	110.91	100.09
24	C	513	CLA	CMD-C2D-C1D	5.78	134.90	124.71
24	c	911	CLA	CMD-C2D-C1D	5.77	134.88	124.71
24	B	604	CLA	CMD-C2D-C1D	5.76	134.86	124.71
24	C	505	CLA	CMD-C2D-C1D	5.73	134.81	124.71
24	A	407	CLA	CMD-C2D-C1D	5.70	134.76	124.71
24	c	912	CLA	CMD-C2D-C1D	5.70	134.75	124.71
24	B	602	CLA	O2D-CGD-CBD	5.69	121.39	111.27
24	A	406	CLA	CMD-C2D-C1D	5.69	134.74	124.71
24	a	409	CLA	CMD-C2D-C1D	5.67	134.71	124.71
27	b	601	SQD	O6-C1-C2	5.62	117.08	108.30
24	B	615	CLA	CMD-C2D-C1D	5.61	134.60	124.71
24	b	607	CLA	O2D-CGD-CBD	5.61	121.23	111.27
24	d	401	CLA	CMD-C2D-C1D	5.61	134.59	124.71
24	A	410	CLA	CMD-C2D-C1D	5.60	134.58	124.71
24	c	904	CLA	CMD-C2D-C1D	5.59	134.57	124.71
24	B	617	CLA	O2D-CGD-CBD	5.59	121.20	111.27
39	f	101	HEM	C4D-ND-C1D	5.58	110.84	105.07
36	c	923	HTG	C1'-S1-C1	5.55	110.47	100.09
24	b	610	CLA	CMD-C2D-C1D	5.54	134.47	124.71
24	c	905	CLA	O2D-CGD-CBD	5.53	121.10	111.27
24	B	616	CLA	CMD-C2D-C1D	5.50	134.41	124.71
36	C	521	HTG	C1'-S1-C1	5.50	110.38	100.09
24	c	910	CLA	CMD-C2D-C1D	5.50	134.40	124.71
24	C	502	CLA	CMD-C2D-C1D	5.49	134.39	124.71
24	B	614	CLA	CMD-C2D-C1D	5.48	134.38	124.71
24	A	405	CLA	CMD-C2D-C1D	5.47	134.35	124.71
24	b	607	CLA	CMD-C2D-C1D	5.45	134.31	124.71
24	C	511	CLA	CMD-C2D-C1D	5.44	134.30	124.71
24	B	610	CLA	CMD-C2D-C1D	5.43	134.28	124.71
24	d	405	CLA	CMD-C2D-C1D	5.43	134.28	124.71
24	c	903	CLA	O2D-CGD-CBD	5.41	120.89	111.27
24	b	612	CLA	CMD-C2D-C1D	5.41	134.24	124.71
24	B	603	CLA	O2D-CGD-CBD	5.41	120.87	111.27
24	b	609	CLA	CHD-C1D-ND	-5.38	119.51	124.45
24	c	908	CLA	CMD-C2D-C1D	5.36	134.16	124.71
27	f	102	SQD	O47-C7-C8	5.36	123.05	111.50
24	C	509	CLA	O2D-CGD-CBD	5.36	120.78	111.27
27	A	412	SQD	O6-C1-C2	5.35	116.66	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	409	PHO	C1-C2-C3	-5.32	116.84	126.04
24	C	502	CLA	O2D-CGD-CBD	5.32	120.71	111.27
24	c	913	CLA	CMD-C2D-C1D	5.30	134.06	124.71
36	c	943	HTG	C1'-S1-C1	5.30	110.01	100.09
24	c	913	CLA	O2D-CGD-CBD	5.29	120.67	111.27
24	B	614	CLA	C3D-C2D-C1D	-5.28	98.63	105.83
42	V	203	HEC	CBD-CAD-C3D	-5.27	103.62	112.62
36	D	412	HTG	C1'-S1-C1	5.25	109.92	100.09
24	b	610	CLA	O2D-CGD-CBD	5.25	120.59	111.27
24	b	616	CLA	CHD-C4C-C3C	-5.24	117.13	124.84
24	B	611	CLA	O2D-CGD-CBD	5.23	120.56	111.27
24	c	906	CLA	O2D-CGD-CBD	5.20	120.51	111.27
24	b	618	CLA	CMD-C2D-C1D	5.20	133.88	124.71
24	B	611	CLA	CMD-C2D-C1D	5.18	133.84	124.71
24	C	512	CLA	CMD-C2D-C1D	5.18	133.84	124.71
24	a	410	CLA	CMD-C2D-C1D	5.17	133.83	124.71
24	b	615	CLA	CMD-C2D-C1D	5.17	133.83	124.71
36	B	629	HTG	C1'-S1-C1	5.16	109.75	100.09
24	b	606	CLA	O2D-CGD-CBD	5.16	120.44	111.27
24	D	401	CLA	CHD-C1D-ND	-5.16	119.71	124.45
24	B	617	CLA	CMD-C2D-C1D	5.15	133.79	124.71
36	b	627	HTG	C1'-S1-C1	5.15	109.72	100.09
24	b	620	CLA	CMD-C2D-C1D	5.14	133.77	124.71
24	A	406	CLA	C2C-C1C-NC	5.13	114.78	109.97
36	d	419	HTG	C1'-S1-C1	5.12	109.66	100.09
39	F	102	HEM	C4D-ND-C1D	5.11	110.35	105.07
24	b	609	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
26	d	406	BCR	C38-C26-C25	-5.07	118.83	124.53
24	a	413	CLA	C1-C2-C3	-5.06	117.28	126.04
36	V	204	HTG	C1-O5-C5	5.06	121.91	112.58
24	c	914	CLA	CMD-C2D-C1D	5.04	133.59	124.71
36	b	603	HTG	C1'-S1-C1	5.03	109.50	100.09
24	A	410	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
24	B	611	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
24	A	406	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
24	B	616	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
24	B	606	CLA	CHD-C4C-C3C	-4.99	117.50	124.84
24	C	508	CLA	CMD-C2D-C1D	4.97	133.48	124.71
24	b	611	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
24	B	605	CLA	O2D-CGD-CBD	4.97	120.09	111.27
24	b	614	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
24	B	615	CLA	C2C-C1C-NC	4.96	114.62	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	C	520	HTG	C1'-S1-C1	4.96	109.36	100.09
24	B	617	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
24	c	902	CLA	O2D-CGD-CBD	4.95	120.06	111.27
36	C	536	HTG	C1'-S1-C1	4.94	109.33	100.09
27	A	412	SQD	O47-C7-C8	4.92	122.10	111.50
24	B	615	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
24	D	401	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
24	d	405	CLA	C1-C2-C3	-4.89	117.59	126.04
24	a	410	CLA	O2D-CGD-CBD	4.88	119.93	111.27
24	C	503	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
24	b	608	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
24	d	405	CLA	C3D-C2D-C1D	-4.87	99.19	105.83
29	a	417	PL9	C7-C8-C9	-4.87	118.69	126.79
24	A	407	CLA	C3D-C4D-ND	4.86	118.10	110.24
37	d	408	DGD	C3D-C4D-C5D	4.86	117.34	109.77
24	B	615	CLA	CHD-C4C-C3C	-4.85	117.71	124.84
24	B	602	CLA	CHD-C1D-ND	-4.85	120.00	124.45
36	c	924	HTG	C1'-S1-C1	4.84	109.15	100.09
24	D	401	CLA	C2C-C1C-NC	4.84	114.51	109.97
24	B	612	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
24	B	609	CLA	CMD-C2D-C1D	4.83	133.23	124.71
36	c	941	HTG	C1'-S1-C1	4.82	109.11	100.09
24	C	511	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
24	b	617	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
24	a	413	CLA	CMD-C2D-C1D	4.82	133.20	124.71
24	b	616	CLA	CMD-C2D-C1D	4.81	133.19	124.71
24	c	902	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
29	A	414	PL9	C7-C8-C9	-4.77	118.85	126.79
24	D	402	CLA	O2D-CGD-CBD	4.77	119.74	111.27
24	c	904	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
24	C	507	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
24	B	608	CLA	C2C-C1C-NC	4.74	114.42	109.97
24	b	615	CLA	O2D-CGD-CBD	4.73	119.68	111.27
36	C	537	HTG	C1'-S1-C1	4.73	108.94	100.09
27	b	601	SQD	O47-C7-C8	4.72	121.67	111.50
24	c	909	CLA	C3D-C4D-ND	4.72	117.87	110.24
24	b	619	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
24	c	909	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
36	c	941	HTG	C1-O5-C5	4.70	121.25	112.58
24	C	507	CLA	C2C-C1C-NC	4.70	114.37	109.97
24	b	616	CLA	C3C-C4C-NC	4.69	115.83	110.57
24	B	606	CLA	C3D-C2D-C1D	-4.67	99.46	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	605	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
24	b	606	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
24	A	407	CLA	CHD-C1D-ND	-4.67	120.17	124.45
24	a	410	CLA	C3D-C4D-ND	4.66	117.78	110.24
24	a	413	CLA	O2D-CGD-CBD	4.66	119.54	111.27
24	c	905	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
24	B	614	CLA	CHD-C4C-C3C	-4.64	118.02	124.84
24	B	609	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
24	c	910	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
24	d	405	CLA	O2D-CGD-CBD	4.64	119.50	111.27
26	k	102	BCR	C33-C5-C6	-4.63	119.33	124.53
26	d	406	BCR	C24-C23-C22	-4.63	119.24	126.23
24	C	512	CLA	O2D-CGD-CBD	4.63	119.49	111.27
24	C	504	CLA	CHD-C1D-ND	-4.62	120.21	124.45
26	T	101	BCR	C33-C5-C6	-4.61	119.35	124.53
24	B	612	CLA	CHD-C4C-C3C	-4.61	118.06	124.84
24	a	413	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
24	B	616	CLA	CHD-C4C-C3C	-4.61	118.06	124.84
28	C	519	LMG	O7-C10-C11	4.61	121.43	111.50
24	c	902	CLA	CHD-C1D-ND	-4.60	120.22	124.45
24	d	401	CLA	C3D-C4D-ND	4.60	117.68	110.24
24	B	607	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
24	d	401	CLA	C2C-C1C-NC	4.60	114.28	109.97
37	c	917	DGD	O2G-C1B-C2B	4.60	121.41	111.50
24	b	616	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
24	b	607	CLA	C2C-C1C-NC	4.59	114.27	109.97
28	C	523	LMG	O7-C10-C11	4.59	121.40	111.50
24	c	907	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
24	C	508	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
24	C	506	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
24	D	401	CLA	C3D-C4D-ND	4.58	117.65	110.24
24	C	509	CLA	C1-C2-C3	-4.58	118.12	126.04
24	b	620	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
24	B	606	CLA	CMD-C2D-C1D	4.57	132.77	124.71
29	D	404	PL9	C40-C39-C41	4.56	122.95	115.27
27	a	415	SQD	O47-C7-C8	4.56	121.32	111.50
24	A	410	CLA	CHD-C1D-ND	-4.56	120.27	124.45
24	b	610	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
24	A	407	CLA	C2C-C1C-NC	4.55	114.24	109.97
36	B	624	HTG	C1'-S1-C1	4.55	108.60	100.09
24	C	502	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
24	d	404	CLA	C3D-C2D-C1D	-4.53	99.65	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	406	CLA	C1C-C2C-C3C	-4.53	102.19	106.96
24	c	903	CLA	CHD-C4C-C3C	-4.53	118.18	124.84
24	A	410	CLA	CHD-C4C-C3C	-4.52	118.19	124.84
24	b	615	CLA	C3D-C2D-C1D	-4.52	99.67	105.83
24	D	402	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
24	B	605	CLA	C2C-C1C-NC	4.51	114.20	109.97
24	c	908	CLA	C4A-NA-C1A	4.51	108.73	106.71
24	A	407	CLA	O2D-CGD-CBD	4.51	119.28	111.27
24	c	909	CLA	O2D-CGD-CBD	4.50	119.27	111.27
24	B	608	CLA	C3D-C2D-C1D	-4.50	99.68	105.83
24	C	503	CLA	C1-C2-C3	-4.50	118.25	126.04
24	B	607	CLA	CHD-C4C-C3C	-4.50	118.22	124.84
24	C	501	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
24	C	504	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
26	D	403	BCR	C38-C26-C25	-4.48	119.49	124.53
24	a	409	CLA	C2C-C1C-NC	4.48	114.17	109.97
24	B	608	CLA	C1C-C2C-C3C	-4.48	102.25	106.96
24	a	410	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
24	C	503	CLA	CHD-C4C-C3C	-4.47	118.27	124.84
37	D	405	DGD	O2G-C1B-C2B	4.47	121.13	111.50
27	l	101	SQD	O47-C7-C8	4.46	121.11	111.50
24	a	409	CLA	C3D-C2D-C1D	-4.45	99.75	105.83
24	d	401	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
24	C	508	CLA	O2D-CGD-CBD	4.45	119.17	111.27
28	a	416	LMG	O7-C10-C11	4.45	121.08	111.50
24	B	609	CLA	C2C-C1C-NC	4.44	114.14	109.97
24	a	413	CLA	C2C-C1C-NC	4.44	114.13	109.97
31	A	417	LMT	C1'-O5'-C5'	4.43	122.39	113.69
24	d	405	CLA	C2C-C1C-NC	4.43	114.12	109.97
24	B	604	CLA	C3D-C4D-ND	4.43	117.41	110.24
24	a	413	CLA	CHD-C4C-C3C	-4.43	118.33	124.84
24	A	405	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
24	b	618	CLA	C3D-C2D-C1D	-4.42	99.79	105.83
28	c	921	LMG	O7-C10-C11	4.42	121.03	111.50
24	D	402	CLA	C3D-C4D-ND	4.42	117.38	110.24
24	A	406	CLA	CHD-C1D-ND	-4.41	120.40	124.45
24	b	616	CLA	C3D-C4D-ND	4.41	117.38	110.24
24	c	913	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
26	C	515	BCR	C7-C8-C9	-4.40	119.59	126.23
24	B	607	CLA	O2D-CGD-CBD	4.39	119.08	111.27
24	c	903	CLA	CMD-C2D-C1D	4.39	132.46	124.71
26	b	623	BCR	C24-C23-C22	-4.39	119.60	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	902	CLA	C3D-C4D-ND	4.39	117.34	110.24
24	B	610	CLA	C3D-C2D-C1D	-4.39	99.84	105.83
24	b	609	CLA	CHD-C4C-C3C	-4.38	118.40	124.84
26	D	403	BCR	C24-C23-C22	-4.38	119.62	126.23
24	C	508	CLA	C3D-C4D-ND	4.37	117.31	110.24
24	d	405	CLA	CHD-C4C-C3C	-4.37	118.42	124.84
24	B	606	CLA	C3D-C4D-ND	4.37	117.30	110.24
31	c	922	LMT	O5'-C5'-C4'	4.36	118.95	109.75
24	B	602	CLA	CHD-C4C-C3C	-4.36	118.42	124.84
24	D	402	CLA	CHD-C1D-ND	-4.36	120.45	124.45
24	c	908	CLA	C3D-C2D-C1D	-4.35	99.89	105.83
24	c	911	CLA	C2C-C1C-NC	4.35	114.05	109.97
24	c	905	CLA	C3D-C4D-ND	4.35	117.28	110.24
24	C	507	CLA	CHD-C4C-C3C	-4.35	118.44	124.84
36	B	630	HTG	C1'-S1-C1	4.35	108.22	100.09
24	B	608	CLA	C3D-C4D-ND	4.35	117.27	110.24
31	B	622	LMT	C1-O1'-C1'	-4.34	106.64	113.84
36	b	627	HTG	O5-C1-C2	4.34	115.77	110.31
36	b	602	HTG	C1'-S1-C1	4.33	108.20	100.09
24	c	902	CLA	CHD-C4C-C3C	-4.33	118.47	124.84
24	B	613	CLA	C3D-C4D-ND	4.33	117.25	110.24
24	b	607	CLA	C1C-C2C-C3C	-4.33	102.40	106.96
24	C	513	CLA	C3D-C2D-C1D	-4.32	99.93	105.83
24	A	406	CLA	C3D-C4D-ND	4.32	117.23	110.24
27	a	401	SQD	O47-C7-C8	4.32	120.82	111.50
26	B	636	BCR	C15-C16-C17	-4.32	114.62	123.47
24	C	501	CLA	CHD-C1D-ND	-4.32	120.49	124.45
24	C	512	CLA	C3D-C2D-C1D	-4.31	99.94	105.83
24	b	605	CLA	C3D-C2D-C1D	-4.31	99.94	105.83
27	A	412	SQD	C1-O5-C5	-4.31	105.23	113.69
24	b	607	CLA	C3D-C4D-ND	4.31	117.21	110.24
24	c	911	CLA	C3D-C4D-ND	4.31	117.21	110.24
26	B	636	BCR	C33-C5-C6	-4.31	119.69	124.53
24	A	407	CLA	CHD-C4C-C3C	-4.31	118.51	124.84
24	b	617	CLA	C2C-C1C-NC	4.31	114.01	109.97
24	B	604	CLA	C2C-C1C-NC	4.30	114.00	109.97
24	B	614	CLA	CHD-C1D-ND	-4.30	120.50	124.45
24	c	903	CLA	C3D-C2D-C1D	-4.30	99.97	105.83
24	b	615	CLA	CHD-C4C-C3C	-4.29	118.53	124.84
28	A	413	LMG	O7-C10-C11	4.29	120.75	111.50
37	C	516	DGD	O2G-C1B-C2B	4.29	120.75	111.50
24	B	605	CLA	C1C-C2C-C3C	-4.29	102.45	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	513	CLA	C3D-C4D-ND	4.28	117.17	110.24
24	d	401	CLA	CHD-C1D-ND	-4.28	120.52	124.45
24	b	618	CLA	C3D-C4D-ND	4.28	117.16	110.24
37	d	408	DGD	O2G-C1B-C2B	4.28	120.72	111.50
24	B	604	CLA	C3D-C2D-C1D	-4.27	100.00	105.83
24	B	603	CLA	C3D-C4D-ND	4.27	117.14	110.24
24	B	603	CLA	C3D-C2D-C1D	-4.27	100.01	105.83
36	c	942	HTG	C1'-S1-C1	4.26	108.07	100.09
24	A	407	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
42	v	202	HEC	CBD-CAD-C3D	-4.25	105.36	112.62
24	C	509	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
24	B	602	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
24	C	505	CLA	O2D-CGD-CBD	4.25	118.82	111.27
24	c	903	CLA	C2C-C1C-NC	4.25	113.95	109.97
24	d	405	CLA	CHD-C1D-ND	-4.25	120.55	124.45
24	C	504	CLA	C1C-C2C-C3C	-4.24	102.50	106.96
24	B	613	CLA	O2D-CGD-CBD	4.24	118.80	111.27
24	c	910	CLA	CHD-C4C-C3C	-4.24	118.61	124.84
24	A	406	CLA	CHD-C4C-C3C	-4.24	118.61	124.84
24	C	504	CLA	O2D-CGD-CBD	4.23	118.79	111.27
24	c	908	CLA	CHD-C4C-C3C	-4.23	118.62	124.84
27	F	101	SQD	O7-S-C6	4.23	111.97	106.94
24	C	506	CLA	C2C-C1C-NC	4.23	113.94	109.97
24	B	611	CLA	CAC-C3C-C4C	4.23	130.29	124.81
24	c	906	CLA	C2C-C1C-NC	4.23	113.93	109.97
24	B	611	CLA	C3C-C4C-NC	4.23	115.31	110.57
31	t	101	LMT	C1-O1'-C1'	-4.22	106.84	113.84
24	b	613	CLA	C3D-C4D-ND	4.22	117.06	110.24
24	B	609	CLA	O2D-CGD-CBD	4.22	118.76	111.27
24	A	405	CLA	C3D-C4D-ND	4.21	117.06	110.24
27	l	101	SQD	O6-C1-C2	4.21	114.88	108.30
24	C	509	CLA	C2C-C1C-NC	4.21	113.92	109.97
24	c	903	CLA	C3D-C4D-ND	4.21	117.04	110.24
24	c	910	CLA	C2C-C1C-NC	4.20	113.91	109.97
24	c	912	CLA	CHD-C4C-C3C	-4.20	118.67	124.84
24	C	504	CLA	C3D-C4D-ND	4.20	117.03	110.24
24	b	607	CLA	O2D-CGD-O1D	-4.20	115.63	123.84
24	d	401	CLA	CHD-C4C-C3C	-4.19	118.68	124.84
24	b	620	CLA	CHD-C4C-C3C	-4.19	118.68	124.84
24	c	909	CLA	CHD-C4C-C3C	-4.19	118.69	124.84
28	c	920	LMG	O7-C10-C11	4.19	120.53	111.50
27	F	101	SQD	C44-O6-C1	-4.18	105.57	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	409	CLA	C3D-C4D-ND	4.18	117.00	110.24
24	B	615	CLA	C3D-C4D-ND	4.17	116.98	110.24
24	d	405	CLA	C1C-C2C-C3C	-4.17	102.57	106.96
24	C	502	CLA	C3D-C4D-ND	4.17	116.98	110.24
24	c	902	CLA	O2D-CGD-O1D	-4.16	115.69	123.84
36	B	625	HTG	O5-C1-C2	4.16	115.55	110.31
24	b	606	CLA	C2C-C1C-NC	4.16	113.87	109.97
24	C	512	CLA	CHD-C4C-C3C	-4.16	118.73	124.84
24	D	402	CLA	CHD-C4C-C3C	-4.16	118.73	124.84
29	a	417	PL9	C22-C23-C24	-4.16	117.65	127.66
24	B	604	CLA	CHD-C4C-C3C	-4.16	118.73	124.84
24	b	618	CLA	O2D-CGD-CBD	4.16	118.65	111.27
24	b	619	CLA	C2C-C1C-NC	4.15	113.86	109.97
24	B	609	CLA	CMA-C3A-C4A	-4.15	100.62	111.77
24	C	511	CLA	CHD-C4C-C3C	-4.15	118.75	124.84
24	c	905	CLA	C2C-C1C-NC	4.14	113.86	109.97
24	C	511	CLA	C2C-C1C-NC	4.14	113.85	109.97
24	B	615	CLA	C1C-C2C-C3C	-4.14	102.60	106.96
24	B	611	CLA	C4C-C3C-C2C	-4.14	100.86	106.90
24	b	607	CLA	CAA-C2A-C3A	-4.14	101.45	112.78
24	b	613	CLA	C3D-C2D-C1D	-4.14	100.19	105.83
24	c	902	CLA	C1C-C2C-C3C	-4.14	102.61	106.96
39	F	102	HEM	CBD-CAD-C3D	-4.14	101.13	112.63
24	C	508	CLA	C2C-C1C-NC	4.14	113.85	109.97
24	b	612	CLA	CMA-C3A-C4A	-4.14	100.66	111.77
24	A	410	CLA	C2C-C1C-NC	4.13	113.84	109.97
27	F	101	SQD	C1-C2-C3	-4.13	101.39	110.00
24	c	907	CLA	C3D-C4D-ND	4.13	116.92	110.24
24	d	404	CLA	C2C-C1C-NC	4.13	113.84	109.97
26	b	621	BCR	C15-C14-C13	-4.13	121.42	127.31
24	a	410	CLA	C2C-C1C-NC	4.13	113.84	109.97
26	D	403	BCR	C7-C8-C9	-4.12	120.00	126.23
24	A	407	CLA	C1C-C2C-C3C	-4.12	102.63	106.96
24	d	404	CLA	C3D-C4D-ND	4.11	116.89	110.24
24	C	510	CLA	C3D-C2D-C1D	-4.11	100.22	105.83
24	B	607	CLA	C4-C3-C5	4.11	122.18	115.27
24	C	509	CLA	C1C-C2C-C3C	-4.11	102.64	106.96
24	b	615	CLA	C1-C2-C3	-4.11	118.94	126.04
24	c	908	CLA	C1C-C2C-C3C	-4.10	102.64	106.96
24	b	612	CLA	C3D-C4D-ND	4.10	116.88	110.24
24	b	605	CLA	CHD-C4C-C3C	-4.10	118.81	124.84
24	B	612	CLA	O2D-CGD-CBD	4.10	118.56	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	914	CLA	C3D-C2D-C1D	-4.10	100.23	105.83
24	b	611	CLA	C2C-C1C-NC	4.10	113.81	109.97
24	A	405	CLA	CMB-C2B-C3B	4.10	132.35	124.68
24	C	505	CLA	CAC-C3C-C4C	4.10	130.13	124.81
24	c	909	CLA	CMD-C2D-C1D	4.09	131.93	124.71
24	c	907	CLA	C2C-C1C-NC	4.09	113.81	109.97
27	a	415	SQD	C1-O5-C5	-4.09	105.65	113.69
24	c	912	CLA	O2D-CGD-CBD	4.09	118.54	111.27
24	B	603	CLA	CHD-C1D-ND	-4.09	120.69	124.45
24	c	905	CLA	C1C-C2C-C3C	-4.09	102.66	106.96
24	C	506	CLA	O2D-CGD-CBD	4.09	118.54	111.27
24	b	618	CLA	C2C-C1C-NC	4.09	113.80	109.97
24	B	613	CLA	C3D-C2D-C1D	-4.09	100.25	105.83
24	d	401	CLA	C1C-C2C-C3C	-4.09	102.66	106.96
24	c	905	CLA	CHD-C4C-C3C	-4.09	118.83	124.84
37	c	918	DGD	O2G-C1B-C2B	4.08	120.29	111.50
36	y	102	HTG	C1'-S1-C1	4.08	107.72	100.09
24	c	903	CLA	C1C-C2C-C3C	-4.08	102.67	106.96
24	c	911	CLA	O2D-CGD-CBD	4.08	118.51	111.27
24	c	902	CLA	CMC-C2C-C1C	4.07	131.24	125.04
24	b	619	CLA	CHD-C4C-C3C	-4.07	118.86	124.84
24	C	510	CLA	C2C-C1C-NC	4.07	113.78	109.97
24	b	608	CLA	C2C-C1C-NC	4.07	113.78	109.97
24	c	914	CLA	C3D-C4D-ND	4.07	116.82	110.24
24	C	501	CLA	O2D-CGD-O1D	-4.07	115.88	123.84
26	Y	101	BCR	C33-C5-C6	-4.07	119.96	124.53
24	C	507	CLA	C1C-C2C-C3C	-4.07	102.68	106.96
24	C	513	CLA	CHD-C4C-C3C	-4.06	118.86	124.84
24	B	613	CLA	CHD-C4C-C3C	-4.06	118.87	124.84
24	B	607	CLA	CHD-C1D-ND	-4.05	120.73	124.45
24	c	914	CLA	O2D-CGD-CBD	4.05	118.47	111.27
24	b	614	CLA	O2D-CGD-CBD	4.05	118.46	111.27
24	c	911	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
24	B	603	CLA	CHD-C4C-C3C	-4.05	118.89	124.84
24	A	407	CLA	CBC-CAC-C3C	-4.05	101.28	112.43
24	b	608	CLA	C1C-C2C-C3C	-4.04	102.70	106.96
24	b	611	CLA	CHD-C4C-C3C	-4.04	118.90	124.84
24	C	501	CLA	C2C-C1C-NC	4.04	113.76	109.97
24	B	603	CLA	O2D-CGD-O1D	-4.04	115.94	123.84
24	d	404	CLA	O2D-CGD-CBD	4.04	118.44	111.27
24	B	616	CLA	C2C-C1C-NC	4.03	113.75	109.97
24	c	913	CLA	C1C-C2C-C3C	-4.03	102.72	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	617	CLA	C3D-C4D-ND	4.03	116.76	110.24
24	b	612	CLA	C3D-C2D-C1D	-4.03	100.33	105.83
24	b	609	CLA	C3D-C4D-ND	4.03	116.75	110.24
24	b	609	CLA	O2D-CGD-CBD	4.03	118.42	111.27
24	c	912	CLA	C4-C3-C5	4.02	122.03	115.27
24	B	607	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
24	b	610	CLA	C4-C3-C5	4.02	122.03	115.27
24	A	410	CLA	C4-C3-C5	4.02	122.03	115.27
24	C	506	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
24	c	912	CLA	C3D-C4D-ND	4.02	116.74	110.24
24	c	913	CLA	C2C-C1C-NC	4.02	113.73	109.97
24	C	510	CLA	C3D-C4D-ND	4.01	116.73	110.24
24	C	508	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
24	c	905	CLA	CHD-C1D-ND	-4.01	120.77	124.45
24	c	912	CLA	C3D-C2D-C1D	-4.01	100.36	105.83
24	b	616	CLA	C2C-C1C-NC	4.00	113.72	109.97
24	A	410	CLA	C3D-C4D-ND	4.00	116.71	110.24
36	c	928	HTG	O5-C1-C2	4.00	115.34	110.31
24	A	410	CLA	C1C-C2C-C3C	-3.99	102.76	106.96
26	T	101	BCR	C15-C16-C17	-3.99	115.31	123.47
24	c	908	CLA	CHD-C1D-ND	-3.98	120.79	124.45
24	a	409	CLA	CAC-C3C-C4C	3.98	129.98	124.81
24	c	903	CLA	O2D-CGD-O1D	-3.98	116.06	123.84
24	a	410	CLA	CHD-C1D-ND	-3.98	120.80	124.45
24	b	614	CLA	CHD-C4C-C3C	-3.97	119.01	124.84
24	c	908	CLA	C2C-C1C-NC	3.97	113.69	109.97
24	C	504	CLA	C2C-C1C-NC	3.97	113.69	109.97
39	F	102	HEM	CBA-CAA-C2A	-3.96	105.85	112.62
24	B	606	CLA	C3C-C4C-NC	3.96	115.01	110.57
29	A	414	PL9	C22-C23-C24	-3.96	118.12	127.66
24	B	617	CLA	C3D-C4D-ND	3.96	116.64	110.24
24	C	509	CLA	O2D-CGD-O1D	-3.95	116.11	123.84
24	c	912	CLA	C2C-C1C-NC	3.95	113.67	109.97
24	B	616	CLA	C1D-CHD-C4C	-3.95	117.54	126.06
24	B	613	CLA	CMD-C2D-C1D	3.95	131.67	124.71
24	C	503	CLA	C1C-C2C-C3C	-3.95	102.81	106.96
24	a	410	CLA	CHD-C4C-C3C	-3.94	119.04	124.84
24	B	603	CLA	CAA-C2A-C3A	-3.94	101.99	112.78
36	V	204	HTG	C1-C2-C3	-3.94	102.81	110.59
24	C	501	CLA	C3D-C4D-ND	3.94	116.60	110.24
24	b	620	CLA	C1D-CHD-C4C	-3.94	117.57	126.06
24	b	620	CLA	C3C-C4C-NC	3.93	114.97	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	606	CLA	C2C-C1C-NC	3.92	113.65	109.97
24	B	610	CLA	C3D-C4D-ND	3.92	116.58	110.24
24	c	913	CLA	CHD-C4C-C3C	-3.92	119.07	124.84
24	b	616	CLA	O2D-CGD-CBD	3.92	118.24	111.27
24	B	606	CLA	C1D-CHD-C4C	-3.92	117.60	126.06
24	A	407	CLA	C3B-C4B-NB	3.92	114.28	109.21
24	b	610	CLA	CHD-C4C-C3C	-3.92	119.08	124.84
24	b	614	CLA	C2C-C1C-NC	3.91	113.64	109.97
24	B	612	CLA	CMC-C2C-C1C	3.91	131.00	125.04
36	v	211	HTG	C1-C2-C3	-3.91	102.87	110.59
24	B	603	CLA	C2C-C1C-NC	3.90	113.63	109.97
24	B	611	CLA	CHD-C4C-C3C	-3.90	119.10	124.84
24	a	413	CLA	C3D-C4D-ND	3.90	116.55	110.24
24	C	502	CLA	C1-C2-C3	-3.90	119.30	126.04
24	b	620	CLA	C3B-C4B-NB	3.90	114.25	109.21
24	c	909	CLA	C2C-C1C-NC	3.90	113.62	109.97
24	B	614	CLA	C1C-C2C-C3C	-3.90	102.86	106.96
24	c	902	CLA	C2C-C1C-NC	3.90	113.62	109.97
24	B	614	CLA	C3D-C4D-ND	3.90	116.54	110.24
24	d	405	CLA	C3D-C4D-ND	3.90	116.54	110.24
24	c	911	CLA	C3D-C2D-C1D	-3.89	100.52	105.83
24	c	906	CLA	C3D-C2D-C1D	-3.89	100.53	105.83
25	a	412	PHO	C1-C2-C3	-3.88	119.33	126.04
24	D	401	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
24	B	617	CLA	CHD-C4C-C3C	-3.88	119.14	124.84
24	B	610	CLA	C2C-C1C-NC	3.88	113.61	109.97
24	A	410	CLA	CBC-CAC-C3C	-3.88	101.75	112.43
27	f	102	SQD	C1-O5-C5	3.87	121.29	113.69
24	C	509	CLA	C3D-C4D-ND	3.87	116.50	110.24
27	l	101	SQD	O7-S-C6	3.87	111.54	106.94
27	A	412	SQD	C45-O47-C7	-3.87	108.26	117.79
26	Y	101	BCR	C38-C26-C25	-3.87	120.18	124.53
24	a	409	CLA	C1C-C2C-C3C	-3.86	102.89	106.96
24	B	612	CLA	C3D-C4D-ND	3.86	116.49	110.24
24	c	913	CLA	CBA-CAA-C2A	-3.86	102.47	113.86
26	K	101	BCR	C33-C5-C6	-3.86	120.20	124.53
24	B	602	CLA	C3D-C4D-ND	3.86	116.48	110.24
24	D	401	CLA	CHD-C4C-C3C	-3.86	119.17	124.84
24	A	405	CLA	C2C-C1C-NC	3.86	113.58	109.97
24	b	606	CLA	O2D-CGD-O1D	-3.86	116.30	123.84
24	B	615	CLA	C1D-CHD-C4C	-3.85	117.75	126.06
24	c	909	CLA	C1D-CHD-C4C	-3.85	117.76	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	405	CLA	C3C-C4C-NC	3.84	114.88	110.57
24	B	606	CLA	O2D-CGD-CBD	3.84	118.09	111.27
24	C	513	CLA	O2D-CGD-CBD	3.83	118.07	111.27
24	B	614	CLA	C2C-C1C-NC	3.83	113.56	109.97
24	b	611	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
24	B	605	CLA	CHD-C1D-ND	-3.82	120.94	124.45
24	C	506	CLA	CHD-C1D-ND	-3.82	120.94	124.45
24	b	606	CLA	C3D-C4D-ND	3.82	116.42	110.24
24	c	906	CLA	C3D-C4D-ND	3.82	116.42	110.24
26	c	915	BCR	C33-C5-C6	-3.82	120.24	124.53
24	B	612	CLA	CHD-C1D-ND	-3.82	120.95	124.45
24	b	609	CLA	O2D-CGD-O1D	-3.81	116.39	123.84
24	b	620	CLA	C3D-C4D-ND	3.81	116.40	110.24
24	B	610	CLA	CHD-C4C-C3C	-3.81	119.24	124.84
24	a	413	CLA	CHD-C1D-ND	-3.80	120.96	124.45
24	B	605	CLA	C3D-C4D-ND	3.80	116.39	110.24
24	B	605	CLA	CHD-C4C-C3C	-3.80	119.25	124.84
36	B	623	HTG	C1'-S1-C1	3.80	107.20	100.09
24	B	607	CLA	C2C-C1C-NC	3.80	113.53	109.97
36	c	941	HTG	O5-C5-C4	3.80	116.59	109.69
24	b	620	CLA	C2C-C1C-NC	3.80	113.53	109.97
24	b	619	CLA	CHD-C1D-ND	-3.79	120.97	124.45
24	b	610	CLA	C2C-C1C-NC	3.79	113.53	109.97
24	b	618	CLA	CHD-C4C-C3C	-3.79	119.27	124.84
24	c	906	CLA	CHD-C4C-C3C	-3.79	119.27	124.84
24	c	909	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
31	a	402	LMT	C1B-O5B-C5B	3.79	121.13	113.69
24	b	618	CLA	CAC-C3C-C4C	3.78	129.72	124.81
26	A	411	BCR	C33-C5-C6	-3.78	120.28	124.53
24	a	413	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
36	c	928	HTG	C1'-S1-C1	3.77	107.15	100.09
24	B	604	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
24	C	501	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
24	c	910	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
29	A	414	PL9	C32-C33-C34	-3.77	118.58	127.66
24	c	904	CLA	C2C-C1C-NC	3.77	113.50	109.97
24	b	606	CLA	CHD-C1D-ND	-3.77	120.99	124.45
24	b	610	CLA	C1C-C2C-C3C	-3.77	103.00	106.96
24	b	615	CLA	C2C-C1C-NC	3.77	113.50	109.97
24	c	913	CLA	C1D-CHD-C4C	-3.77	117.94	126.06
38	E	101	LHG	O7-C7-C8	3.76	119.61	111.50
24	b	609	CLA	C1C-C2C-C3C	-3.76	103.01	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	621	BCR	C7-C8-C9	-3.75	120.56	126.23
27	F	101	SQD	O47-C7-C8	3.75	119.59	111.50
24	a	409	CLA	C1D-CHD-C4C	-3.75	117.97	126.06
37	C	517	DGD	O2G-C1B-C2B	3.74	119.57	111.50
24	b	605	CLA	C3D-C4D-ND	3.74	116.29	110.24
24	c	913	CLA	C3D-C4D-ND	3.74	116.28	110.24
24	c	907	CLA	CHD-C4C-C3C	-3.73	119.35	124.84
24	b	614	CLA	C3D-C4D-ND	3.73	116.28	110.24
24	b	610	CLA	C3C-C4C-NC	3.72	114.75	110.57
24	B	617	CLA	O2A-CGA-CBA	3.72	123.59	111.91
24	A	406	CLA	CBC-CAC-C3C	-3.72	102.18	112.43
26	k	102	BCR	C15-C14-C13	-3.72	122.00	127.31
24	B	612	CLA	C1D-CHD-C4C	-3.72	118.04	126.06
24	D	401	CLA	C3C-C4C-NC	3.71	114.73	110.57
24	b	619	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
24	B	617	CLA	C1D-CHD-C4C	-3.71	118.06	126.06
24	c	907	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
28	a	416	LMG	C7-O1-C1	-3.71	106.50	113.74
24	c	910	CLA	O2D-CGD-CBD	3.70	117.85	111.27
24	b	609	CLA	C2C-C1C-NC	3.70	113.44	109.97
24	C	502	CLA	O2D-CGD-O1D	-3.70	116.60	123.84
24	b	619	CLA	C4-C3-C5	3.70	121.50	115.27
27	f	102	SQD	O7-S-C6	3.70	111.34	106.94
24	C	512	CLA	C3D-C4D-ND	3.70	116.22	110.24
24	b	611	CLA	C3D-C4D-ND	3.70	116.22	110.24
26	T	101	BCR	C7-C8-C9	-3.69	120.66	126.23
27	a	401	SQD	O8-S-C6	3.69	111.61	105.74
24	B	609	CLA	C3D-C4D-ND	3.68	116.20	110.24
38	L	101	LHG	O7-C7-C8	3.68	119.44	111.50
24	C	506	CLA	CHD-C4C-C3C	-3.68	119.43	124.84
24	C	506	CLA	C3D-C4D-ND	3.68	116.19	110.24
26	B	618	BCR	C33-C5-C6	-3.68	120.40	124.53
31	c	922	LMT	C1'-O5'-C5'	3.68	120.91	113.69
24	C	501	CLA	CHD-C4C-C3C	-3.68	119.44	124.84
24	c	914	CLA	C1-C2-C3	-3.68	119.69	126.04
24	c	914	CLA	C1D-CHD-C4C	-3.67	118.15	126.06
24	A	407	CLA	C1-C2-C3	-3.67	119.70	126.04
26	d	406	BCR	C33-C5-C6	-3.66	120.41	124.53
24	b	612	CLA	C2C-C1C-NC	3.66	113.40	109.97
24	c	912	CLA	CHD-C1D-ND	-3.66	121.09	124.45
24	b	613	CLA	O2D-CGD-CBD	3.66	117.78	111.27
24	c	905	CLA	CBC-CAC-C3C	-3.66	102.35	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	502	CLA	CHD-C4C-C3C	-3.66	119.47	124.84
24	c	903	CLA	C1D-CHD-C4C	-3.66	118.17	126.06
24	c	912	CLA	C1C-C2C-C3C	-3.65	103.11	106.96
24	b	617	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
24	C	510	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
24	C	507	CLA	C4A-NA-C1A	3.65	108.35	106.71
24	b	612	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
24	d	401	CLA	C1D-CHD-C4C	-3.65	118.19	126.06
24	c	910	CLA	CHD-C1D-ND	-3.64	121.11	124.45
26	C	514	BCR	C33-C5-C6	-3.64	120.44	124.53
24	A	407	CLA	C4-C3-C5	3.64	121.39	115.27
24	C	505	CLA	C3D-C2D-C1D	-3.64	100.87	105.83
24	C	510	CLA	CHD-C4C-C3C	-3.63	119.50	124.84
24	B	610	CLA	C3C-C4C-NC	3.63	114.64	110.57
24	B	603	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
37	c	919	DGD	O2G-C1B-C2B	3.63	119.32	111.50
24	B	604	CLA	O2D-CGD-O1D	-3.63	116.75	123.84
24	C	502	CLA	C2C-C1C-NC	3.62	113.37	109.97
29	D	404	PL9	C42-C43-C44	-3.62	118.94	127.66
24	A	406	CLA	CMA-C3A-C4A	-3.62	102.04	111.77
24	c	907	CLA	CHD-C1D-ND	-3.62	121.13	124.45
29	a	417	PL9	C32-C33-C34	-3.62	118.94	127.66
28	C	519	LMG	C8-O7-C10	-3.62	108.88	117.79
24	b	613	CLA	C2C-C1C-NC	3.62	113.36	109.97
24	B	609	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
24	A	405	CLA	CAA-C2A-C3A	-3.61	102.88	112.78
24	c	913	CLA	CBC-CAC-C3C	-3.61	102.47	112.43
40	H	101	RRX	C24-C23-C22	-3.61	120.78	126.23
24	c	911	CLA	CMA-C3A-C4A	-3.61	102.07	111.77
24	C	504	CLA	CMC-C2C-C1C	3.61	130.54	125.04
24	d	404	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
24	b	615	CLA	C4A-NA-C1A	3.61	108.33	106.71
24	B	612	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
24	C	502	CLA	C1C-C2C-C3C	-3.61	103.17	106.96
36	v	211	HTG	C1'-S1-C1	3.60	106.83	100.09
26	D	403	BCR	C28-C27-C26	-3.60	107.64	114.08
29	A	414	PL9	C53-C6-C1	3.60	122.34	114.99
24	B	616	CLA	C3D-C4D-ND	3.59	116.05	110.24
24	b	619	CLA	C3D-C4D-ND	3.59	116.05	110.24
29	A	414	PL9	C37-C38-C39	-3.59	119.01	127.66
24	B	613	CLA	C3C-C4C-NC	3.59	114.60	110.57
24	c	907	CLA	C1D-CHD-C4C	-3.59	118.31	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	610	CLA	C3D-C4D-ND	3.59	116.04	110.24
36	b	626	HTG	C1'-S1-C1	3.59	106.80	100.09
37	C	518	DGD	O2G-C1B-C2B	3.58	119.23	111.50
24	b	617	CLA	CHD-C1D-ND	-3.58	121.16	124.45
27	a	415	SQD	O8-S-C6	3.58	111.45	105.74
27	b	601	SQD	C3-C4-C5	3.58	116.63	110.24
24	C	501	CLA	CBC-CAC-C3C	-3.58	102.56	112.43
24	b	605	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
27	a	415	SQD	C1-C2-C3	-3.58	102.55	110.00
24	C	512	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
24	b	607	CLA	C3D-C2D-C1D	-3.58	100.95	105.83
31	B	626	LMT	C1'-O5'-C5'	3.58	120.71	113.69
24	A	405	CLA	CHD-C4C-C3C	-3.58	119.58	124.84
24	b	612	CLA	C3C-C4C-NC	3.57	114.58	110.57
39	f	101	HEM	CBD-CAD-C3D	-3.57	102.69	112.63
39	f	101	HEM	CBA-CAA-C2A	-3.57	106.52	112.62
24	B	611	CLA	C3D-C4D-ND	3.57	116.01	110.24
24	A	406	CLA	C3B-C4B-NB	3.57	113.83	109.21
24	c	904	CLA	CHD-C4C-C3C	-3.57	119.59	124.84
24	B	603	CLA	C1-C2-C3	-3.56	119.88	126.04
24	c	908	CLA	C3D-C4D-ND	3.56	115.99	110.24
24	C	505	CLA	C2C-C1C-NC	3.56	113.31	109.97
24	D	401	CLA	O2D-CGD-CBD	3.56	117.59	111.27
24	c	910	CLA	C3D-C4D-ND	3.55	115.99	110.24
24	C	513	CLA	C1D-CHD-C4C	-3.55	118.39	126.06
24	C	511	CLA	C3C-C4C-NC	3.55	114.55	110.57
27	A	416	SQD	O47-C7-C8	3.55	119.15	111.50
24	C	513	CLA	C1C-C2C-C3C	-3.55	103.23	106.96
24	C	505	CLA	C3D-C4D-ND	3.55	115.98	110.24
24	c	905	CLA	C3B-C4B-NB	3.55	113.80	109.21
24	c	914	CLA	C2C-C1C-NC	3.54	113.29	109.97
24	A	405	CLA	C1D-CHD-C4C	-3.54	118.42	126.06
24	C	508	CLA	CHD-C4C-C3C	-3.54	119.64	124.84
24	b	620	CLA	C4C-C3C-C2C	-3.54	101.74	106.90
24	B	612	CLA	C2C-C1C-NC	3.54	113.29	109.97
24	C	512	CLA	C1C-C2C-C3C	-3.53	103.24	106.96
24	b	617	CLA	C4-C3-C5	3.53	121.21	115.27
24	C	511	CLA	C1D-CHD-C4C	-3.53	118.44	126.06
24	c	906	CLA	C3C-C4C-NC	3.53	114.53	110.57
24	B	602	CLA	C1C-C2C-C3C	-3.53	103.25	106.96
24	b	619	CLA	C1D-CHD-C4C	-3.53	118.44	126.06
24	c	912	CLA	C1D-CHD-C4C	-3.53	118.45	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	d	408	DGD	O6D-C5D-C4D	3.53	115.85	109.52
24	b	608	CLA	C3C-C4C-NC	3.53	114.53	110.57
24	c	907	CLA	CAA-C2A-C3A	-3.53	103.12	112.78
24	C	507	CLA	C1D-CHD-C4C	-3.52	118.46	126.06
24	d	404	CLA	C3C-C4C-NC	3.52	114.52	110.57
24	C	513	CLA	C2C-C1C-NC	3.52	113.27	109.97
29	d	407	PL9	C7-C8-C9	-3.52	120.93	126.79
24	B	608	CLA	CBC-CAC-C3C	-3.51	102.75	112.43
24	C	505	CLA	C3C-C4C-NC	3.51	114.51	110.57
24	B	612	CLA	CBC-CAC-C3C	-3.51	102.75	112.43
24	a	410	CLA	C3C-C4C-NC	3.51	114.51	110.57
24	B	613	CLA	C2C-C1C-NC	3.51	113.26	109.97
24	c	904	CLA	C1D-CHD-C4C	-3.51	118.48	126.06
24	B	616	CLA	O2D-CGD-CBD	3.51	117.51	111.27
24	C	511	CLA	CAC-C3C-C4C	3.51	129.37	124.81
24	A	410	CLA	CMA-C3A-C4A	-3.51	102.34	111.77
24	A	410	CLA	O2D-CGD-CBD	3.51	117.50	111.27
24	d	401	CLA	CBC-CAC-C3C	-3.51	102.76	112.43
24	c	911	CLA	C1-C2-C3	-3.51	119.98	126.04
24	c	910	CLA	C4A-NA-C1A	3.51	108.28	106.71
24	b	617	CLA	CHD-C4C-C3C	-3.51	119.69	124.84
27	A	412	SQD	O9-S-C6	3.51	111.11	106.94
24	b	615	CLA	C3D-C4D-ND	3.51	115.91	110.24
28	b	624	LMG	O7-C10-C11	3.51	119.06	111.50
25	A	409	PHO	C4-C3-C5	3.50	121.17	115.27
36	v	211	HTG	O5-C1-C2	-3.50	105.90	110.31
24	b	606	CLA	C1C-C2C-C3C	-3.50	103.27	106.96
24	b	611	CLA	CHD-C1D-ND	-3.50	121.23	124.45
24	B	610	CLA	C1D-CHD-C4C	-3.50	118.50	126.06
24	B	615	CLA	O2D-CGD-CBD	3.50	117.49	111.27
31	A	417	LMT	O5'-C5'-C4'	3.50	117.13	109.75
24	B	607	CLA	C1D-CHD-C4C	-3.50	118.51	126.06
24	B	609	CLA	CMB-C2B-C3B	3.50	131.22	124.68
24	b	616	CLA	C1D-CHD-C4C	-3.50	118.52	126.06
24	c	912	CLA	C4A-NA-C1A	3.49	108.28	106.71
24	C	504	CLA	CHD-C4C-C3C	-3.49	119.71	124.84
26	B	618	BCR	C7-C8-C9	-3.49	120.96	126.23
29	D	404	PL9	C36-C37-C38	-3.49	100.41	111.88
24	C	511	CLA	CHD-C1D-ND	-3.49	121.25	124.45
24	A	406	CLA	C3C-C4C-NC	3.49	114.48	110.57
24	b	618	CLA	C1D-CHD-C4C	-3.49	118.54	126.06
24	b	615	CLA	CAC-C3C-C4C	3.49	129.33	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	613	CLA	C1C-C2C-C3C	-3.48	103.29	106.96
24	b	613	CLA	CHD-C1D-ND	-3.48	121.25	124.45
24	c	910	CLA	C1D-CHD-C4C	-3.48	118.55	126.06
24	C	511	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
24	B	606	CLA	C4-C3-C5	3.48	121.13	115.27
24	c	905	CLA	C4-C3-C5	3.48	121.12	115.27
24	b	614	CLA	C1D-CHD-C4C	-3.48	118.56	126.06
24	B	608	CLA	CAC-C3C-C4C	3.48	129.32	124.81
24	c	911	CLA	C1-O2A-CGA	3.47	125.56	116.44
24	C	511	CLA	C3D-C4D-ND	3.47	115.86	110.24
24	B	602	CLA	C2C-C1C-NC	3.47	113.22	109.97
24	d	401	CLA	C3C-C4C-NC	3.47	114.47	110.57
24	a	410	CLA	C3B-C4B-NB	3.47	113.70	109.21
24	B	604	CLA	C3C-C4C-NC	3.47	114.46	110.57
24	b	618	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
24	b	617	CLA	C3C-C4C-NC	3.47	114.46	110.57
24	A	405	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
24	b	616	CLA	C3B-C4B-NB	3.46	113.69	109.21
31	B	622	LMT	O1B-C4'-C3'	3.46	116.49	107.28
24	c	906	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
24	a	410	CLA	CBC-CAC-C3C	-3.46	102.90	112.43
24	a	410	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
26	C	515	BCR	C15-C14-C13	-3.46	122.38	127.31
24	B	606	CLA	C4C-C3C-C2C	-3.45	101.87	106.90
24	B	602	CLA	C1D-CHD-C4C	-3.45	118.61	126.06
24	c	904	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
24	B	614	CLA	C3C-C4C-NC	3.45	114.44	110.57
24	c	914	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
24	b	617	CLA	C3B-C4B-NB	3.45	113.67	109.21
24	c	907	CLA	O2D-CGD-CBD	3.45	117.39	111.27
38	d	409	LHG	O8-C23-C24	3.45	122.72	111.91
29	A	414	PL9	C27-C28-C29	-3.44	119.37	127.66
24	b	607	CLA	C4-C3-C5	3.44	121.05	115.27
24	b	616	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
27	f	102	SQD	O5-C5-C4	3.43	115.93	109.69
24	C	504	CLA	C4-C3-C5	3.43	121.04	115.27
24	B	604	CLA	C1D-CHD-C4C	-3.43	118.66	126.06
24	c	909	CLA	O2D-CGD-O1D	-3.43	117.14	123.84
26	B	618	BCR	C24-C23-C22	-3.43	121.06	126.23
25	A	408	PHO	C1A-C2A-C3A	-3.43	99.58	102.84
24	b	616	CLA	C4C-C3C-C2C	-3.42	101.91	106.90
28	B	621	LMG	O7-C10-C11	3.42	118.88	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	409	CLA	CAA-C2A-C1A	-3.42	100.76	111.97
24	c	904	CLA	C3C-C4C-NC	3.42	114.41	110.57
24	c	910	CLA	C3B-C4B-NB	3.42	113.63	109.21
24	a	413	CLA	CBC-CAC-C3C	-3.42	103.01	112.43
24	A	410	CLA	C1D-CHD-C4C	-3.42	118.69	126.06
24	c	912	CLA	C1-O2A-CGA	3.41	125.40	116.44
24	b	620	CLA	CBC-CAC-C3C	-3.41	103.02	112.43
24	c	914	CLA	CMB-C2B-C3B	3.41	131.06	124.68
42	V	203	HEC	CMB-C2B-C1B	-3.41	123.22	128.46
24	B	608	CLA	O2D-CGD-CBD	3.41	117.33	111.27
24	a	413	CLA	C3C-C4C-NC	3.41	114.40	110.57
24	B	611	CLA	CAA-C2A-C3A	-3.41	103.44	112.78
24	C	505	CLA	CHD-C4C-C3C	-3.41	119.83	124.84
24	B	611	CLA	CMA-C3A-C4A	-3.41	102.61	111.77
24	B	604	CLA	CAA-C2A-C3A	-3.40	103.46	112.78
24	b	611	CLA	C1D-CHD-C4C	-3.40	118.72	126.06
24	b	615	CLA	O2D-CGD-O1D	-3.40	117.19	123.84
24	C	503	CLA	C1D-CHD-C4C	-3.40	118.73	126.06
24	C	502	CLA	C3C-C4C-NC	3.40	114.38	110.57
24	C	509	CLA	CHD-C4C-C3C	-3.40	119.85	124.84
25	a	412	PHO	CMB-C2B-C3B	3.40	131.03	124.68
25	a	412	PHO	C4-C3-C5	3.40	120.98	115.27
24	b	616	CLA	C4-C3-C5	3.39	120.98	115.27
36	V	215	HTG	O5-C1-C2	3.39	114.58	110.31
24	B	616	CLA	C1C-C2C-C3C	-3.39	103.40	106.96
27	A	416	SQD	O48-C23-C24	3.39	122.53	111.91
24	d	405	CLA	C1D-CHD-C4C	-3.38	118.76	126.06
24	B	617	CLA	C4C-C3C-C2C	-3.38	101.97	106.90
29	d	407	PL9	C37-C38-C39	-3.38	119.52	127.66
36	d	414	HTG	O5-C1-C2	3.38	114.56	110.31
38	d	409	LHG	O8-C23-O10	-3.38	115.07	123.59
26	T	101	BCR	C12-C13-C14	-3.37	113.76	118.94
24	B	603	CLA	C3C-C4C-NC	3.37	114.35	110.57
24	c	909	CLA	C3C-C4C-NC	3.37	114.35	110.57
24	b	611	CLA	O2D-CGD-CBD	3.37	117.25	111.27
24	b	605	CLA	C1C-C2C-C3C	-3.37	103.42	106.96
24	a	410	CLA	C1D-CHD-C4C	-3.37	118.80	126.06
24	b	615	CLA	C1D-CHD-C4C	-3.36	118.81	126.06
24	D	402	CLA	C4-C3-C5	3.36	120.92	115.27
24	b	608	CLA	C1D-CHD-C4C	-3.36	118.81	126.06
24	b	611	CLA	O2A-CGA-O1A	-3.36	115.11	123.59
25	A	409	PHO	CMB-C2B-C3B	3.36	130.96	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	903	CLA	O2A-CGA-O1A	-3.36	115.12	123.59
36	O	316	HTG	C1'-S1-C1	3.36	106.37	100.09
24	D	402	CLA	O2D-CGD-O1D	-3.35	117.28	123.84
24	B	617	CLA	C2C-C1C-NC	3.35	113.11	109.97
24	C	503	CLA	C2C-C1C-NC	3.35	113.11	109.97
24	C	503	CLA	O2D-CGD-CBD	3.35	117.22	111.27
24	B	615	CLA	O2A-CGA-O1A	-3.35	115.14	123.59
24	c	906	CLA	C1D-CHD-C4C	-3.35	118.84	126.06
24	B	603	CLA	CMA-C3A-C4A	-3.35	102.78	111.77
24	B	615	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
24	B	614	CLA	C1-C2-C3	-3.34	120.27	126.04
24	B	605	CLA	C3B-C4B-NB	3.34	113.52	109.21
24	B	607	CLA	C3D-C4D-ND	3.34	115.64	110.24
24	C	507	CLA	C3C-C4C-NC	3.33	114.31	110.57
24	B	608	CLA	CHD-C1D-ND	-3.33	121.39	124.45
26	c	915	BCR	C38-C26-C25	-3.33	120.79	124.53
24	b	606	CLA	CHD-C4C-C3C	-3.33	119.94	124.84
24	c	903	CLA	C3C-C4C-NC	3.33	114.31	110.57
24	B	613	CLA	C1C-C2C-C3C	-3.33	103.46	106.96
24	b	615	CLA	C1C-C2C-C3C	-3.33	103.46	106.96
24	c	905	CLA	C1D-CHD-C4C	-3.33	118.88	126.06
24	c	904	CLA	C4A-NA-C1A	3.33	108.20	106.71
24	b	607	CLA	CBC-CAC-C3C	-3.33	103.26	112.43
24	C	510	CLA	C4-C3-C5	3.33	120.87	115.27
24	c	911	CLA	CHD-C4C-C3C	-3.33	119.95	124.84
24	b	620	CLA	CAC-C3C-C4C	3.32	129.12	124.81
38	l	103	LHG	O7-C7-C8	3.32	118.67	111.50
27	a	415	SQD	C45-O47-C7	-3.32	109.61	117.79
24	A	406	CLA	C1D-CHD-C4C	-3.32	118.89	126.06
26	a	414	BCR	C33-C5-C6	-3.32	120.80	124.53
24	c	908	CLA	CMC-C2C-C1C	3.32	130.10	125.04
24	B	610	CLA	C1C-C2C-C3C	-3.32	103.47	106.96
24	b	610	CLA	C1D-CHD-C4C	-3.32	118.89	126.06
24	C	513	CLA	CHD-C1D-ND	-3.32	121.40	124.45
24	C	501	CLA	C1D-CHD-C4C	-3.32	118.90	126.06
24	b	606	CLA	C1D-CHD-C4C	-3.32	118.90	126.06
24	B	616	CLA	CHD-C1D-ND	-3.32	121.41	124.45
24	D	401	CLA	C1-C2-C3	-3.32	120.31	126.04
24	C	504	CLA	O2A-CGA-O1A	-3.31	115.23	123.59
24	C	506	CLA	CBC-CAC-C3C	-3.31	103.30	112.43
24	c	909	CLA	C3B-C4B-NB	3.31	113.49	109.21
24	C	505	CLA	C4C-C3C-C2C	-3.31	102.07	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	609	CLA	C4-C3-C5	3.31	120.84	115.27
24	c	908	CLA	C1D-CHD-C4C	-3.31	118.92	126.06
24	B	603	CLA	C1D-CHD-C4C	-3.31	118.92	126.06
36	c	928	HTG	C1-O5-C5	3.31	118.68	112.58
24	b	607	CLA	CHD-C1D-ND	-3.30	121.42	124.45
24	a	409	CLA	CHD-C1D-ND	-3.30	121.42	124.45
24	C	505	CLA	C1D-CHD-C4C	-3.30	118.94	126.06
24	a	409	CLA	C3B-C4B-NB	3.30	113.47	109.21
24	b	611	CLA	C3B-C4B-NB	3.30	113.47	109.21
24	c	910	CLA	C16-C15-C13	-3.30	105.26	115.92
24	B	609	CLA	C1D-CHD-C4C	-3.30	118.95	126.06
24	D	402	CLA	C3C-C4C-NC	3.29	114.27	110.57
24	A	406	CLA	O2D-CGD-CBD	3.29	117.12	111.27
26	K	101	BCR	C24-C23-C22	-3.29	121.26	126.23
24	b	609	CLA	C1-C2-C3	-3.29	120.35	126.04
39	F	102	HEM	C4B-CHC-C1C	3.29	126.90	122.56
24	C	512	CLA	C3C-C4C-NC	3.29	114.26	110.57
24	c	914	CLA	CHD-C4C-C3C	-3.29	120.01	124.84
36	O	303	HTG	C1'-S1-C1	3.29	106.24	100.09
24	b	613	CLA	CHD-C4C-C3C	-3.29	120.01	124.84
24	d	404	CLA	C1-C2-C3	-3.28	120.36	126.04
24	B	605	CLA	C3C-C4C-NC	3.28	114.25	110.57
24	b	609	CLA	C3C-C4C-NC	3.28	114.25	110.57
24	b	608	CLA	C3D-C4D-ND	3.28	115.55	110.24
24	B	617	CLA	C3B-C4B-NB	3.28	113.45	109.21
24	c	913	CLA	C1-O2A-CGA	3.28	125.05	116.44
24	B	617	CLA	C3C-C4C-NC	3.28	114.25	110.57
37	C	516	DGD	O3G-C3G-C2G	-3.28	102.99	110.90
24	C	510	CLA	C3B-C4B-NB	3.28	113.44	109.21
24	b	606	CLA	C3C-C4C-NC	3.27	114.24	110.57
36	C	537	HTG	C1-O5-C5	3.27	118.61	112.58
24	a	413	CLA	CAA-C2A-C3A	-3.27	103.82	112.78
24	B	615	CLA	C3B-C4B-NB	3.27	113.44	109.21
24	d	405	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
24	C	508	CLA	C3C-C4C-NC	3.27	114.23	110.57
24	b	607	CLA	O2A-CGA-CBA	3.26	122.15	111.91
24	D	401	CLA	C3B-C4B-NB	3.26	113.43	109.21
26	C	514	BCR	C7-C8-C9	-3.26	121.31	126.23
38	d	411	LHG	O7-C7-C8	3.26	118.53	111.50
24	B	613	CLA	C3B-C4B-NB	3.26	113.42	109.21
24	b	612	CLA	C4C-C3C-C2C	-3.25	102.16	106.90
24	C	506	CLA	C1D-CHD-C4C	-3.25	119.04	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	510	CLA	CHD-C1D-ND	-3.25	121.47	124.45
24	C	503	CLA	C3C-C4C-NC	3.25	114.22	110.57
24	b	614	CLA	C3C-C4C-NC	3.25	114.21	110.57
27	a	415	SQD	O9-S-C6	3.25	110.80	106.94
24	b	606	CLA	CAA-C2A-C3A	-3.25	103.89	112.78
27	A	412	SQD	C1-C2-C3	-3.24	103.24	110.00
24	b	608	CLA	CHD-C4C-C3C	-3.24	120.07	124.84
29	A	414	PL9	C10-C9-C11	3.24	120.73	115.27
40	h	101	RRX	C38-C26-C25	-3.24	120.89	124.53
24	C	511	CLA	CBC-CAC-C3C	-3.24	103.49	112.43
24	d	404	CLA	C3B-C4B-NB	3.24	113.40	109.21
24	A	407	CLA	CMC-C2C-C1C	3.24	129.97	125.04
24	B	608	CLA	C3B-C4B-NB	3.24	113.39	109.21
29	D	404	PL9	C7-C8-C9	-3.24	121.41	126.79
28	c	921	LMG	C3-C4-C5	3.24	116.01	110.24
24	c	904	CLA	O2D-CGD-CBD	3.23	117.02	111.27
24	B	617	CLA	C1-C2-C3	-3.23	120.45	126.04
29	d	407	PL9	C10-C9-C11	3.23	120.71	115.27
26	C	515	BCR	C38-C26-C25	-3.23	120.90	124.53
24	c	914	CLA	C3C-C4C-NC	3.23	114.19	110.57
24	C	512	CLA	C2C-C1C-NC	3.22	112.99	109.97
24	d	405	CLA	C3C-C4C-NC	3.22	114.19	110.57
24	b	615	CLA	CHD-C1D-ND	-3.22	121.49	124.45
24	c	911	CLA	C1D-CHD-C4C	-3.22	119.11	126.06
24	C	507	CLA	C1-C2-C3	-3.22	120.47	126.04
24	B	611	CLA	C2C-C1C-NC	3.22	112.99	109.97
24	c	908	CLA	C4-C3-C5	3.22	120.68	115.27
27	b	601	SQD	O7-S-C6	3.22	110.76	106.94
24	C	510	CLA	C1D-CHD-C4C	-3.21	119.12	126.06
24	C	503	CLA	CMC-C2C-C1C	3.21	129.93	125.04
24	C	513	CLA	C3C-C4C-NC	3.21	114.17	110.57
24	B	616	CLA	C3B-C4B-NB	3.21	113.36	109.21
24	b	614	CLA	C4C-C3C-C2C	-3.21	102.22	106.90
24	C	502	CLA	C1D-CHD-C4C	-3.20	119.14	126.06
25	a	412	PHO	C1A-C2A-C3A	-3.20	99.80	102.84
24	b	617	CLA	C4C-C3C-C2C	-3.19	102.24	106.90
24	D	402	CLA	C1C-C2C-C3C	-3.19	103.60	106.96
24	c	910	CLA	O2D-CGD-O1D	-3.19	117.59	123.84
24	c	907	CLA	C3B-C4B-NB	3.19	113.33	109.21
24	C	509	CLA	CHD-C1D-ND	-3.19	121.52	124.45
26	k	103	BCR	C33-C5-C6	-3.18	120.95	124.53
24	B	608	CLA	CAA-C2A-C3A	-3.18	104.06	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	610	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
24	a	410	CLA	CAC-C3C-C4C	3.18	128.94	124.81
24	C	504	CLA	C1D-CHD-C4C	-3.18	119.19	126.06
24	d	405	CLA	CMC-C2C-C1C	3.18	129.88	125.04
24	b	607	CLA	C1D-CHD-C4C	-3.18	119.20	126.06
24	c	906	CLA	CHD-C1D-ND	-3.18	121.53	124.45
24	B	610	CLA	CAC-C3C-C4C	3.18	128.93	124.81
24	b	619	CLA	C3B-C4B-NB	3.18	113.32	109.21
24	C	507	CLA	CHD-C1D-ND	-3.18	121.54	124.45
36	V	204	HTG	C4-C3-C2	-3.18	105.28	110.82
31	B	622	LMT	C6'-C5'-C4'	-3.17	104.09	113.33
29	a	417	PL9	C17-C18-C19	-3.17	120.03	127.66
24	B	604	CLA	CHD-C1D-ND	-3.17	121.55	124.45
24	b	620	CLA	O2A-CGA-CBA	3.16	121.84	111.91
24	B	615	CLA	C4-C3-C5	3.16	120.59	115.27
24	c	903	CLA	CHD-C1D-ND	-3.16	121.55	124.45
24	C	510	CLA	C3C-C4C-NC	3.16	114.11	110.57
24	b	606	CLA	C3B-C4B-NB	3.15	113.29	109.21
24	c	912	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
24	D	402	CLA	C2C-C1C-NC	3.15	112.92	109.97
24	B	617	CLA	CAC-C3C-C4C	3.15	128.90	124.81
24	c	907	CLA	CBC-CAC-C3C	-3.15	103.75	112.43
25	A	409	PHO	C1A-C2A-C3A	-3.15	99.84	102.84
37	d	408	DGD	C2G-O2G-C1B	-3.15	110.04	117.79
24	B	607	CLA	O2A-CGA-O1A	-3.15	115.65	123.59
24	C	501	CLA	CAC-C3C-C4C	3.14	128.89	124.81
24	d	404	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
24	D	401	CLA	CAA-C2A-C3A	-3.14	104.18	112.78
29	a	417	PL9	C37-C38-C39	-3.14	120.10	127.66
24	c	911	CLA	C3C-C4C-NC	3.14	114.09	110.57
24	c	907	CLA	C3C-C4C-NC	3.14	114.09	110.57
24	b	612	CLA	C1D-CHD-C4C	-3.14	119.29	126.06
24	B	613	CLA	C4C-C3C-C2C	-3.14	102.33	106.90
24	B	604	CLA	C3B-C4B-NB	3.13	113.26	109.21
36	V	204	HTG	O5-C5-C4	3.13	115.38	109.69
38	L	101	LHG	O8-C23-C24	3.13	121.74	111.91
24	c	913	CLA	C3C-C4C-NC	3.13	114.08	110.57
24	c	911	CLA	C3B-C4B-NB	3.13	113.25	109.21
26	b	621	BCR	C33-C5-C6	-3.13	121.02	124.53
24	d	401	CLA	C3B-C4B-NB	3.13	113.25	109.21
24	A	407	CLA	C3C-C4C-NC	3.12	114.08	110.57
24	C	504	CLA	CBC-CAC-C3C	-3.12	103.82	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	612	CLA	CAC-C3C-C4C	3.12	128.86	124.81
40	H	101	RRX	C38-C26-C25	-3.12	121.03	124.53
24	B	613	CLA	CHD-C1D-ND	-3.11	121.59	124.45
26	c	916	BCR	C38-C26-C25	-3.11	121.03	124.53
27	b	601	SQD	C1-C2-C3	-3.11	103.52	110.00
24	a	410	CLA	C4-C3-C5	3.11	120.50	115.27
24	b	614	CLA	CAC-C3C-C4C	3.11	128.85	124.81
24	C	511	CLA	CMC-C2C-C1C	3.11	129.78	125.04
24	A	407	CLA	C1D-CHD-C4C	-3.11	119.35	126.06
27	b	601	SQD	O8-S-C6	3.10	110.68	105.74
26	C	515	BCR	C33-C5-C6	-3.10	121.05	124.53
29	a	417	PL9	C20-C19-C21	3.10	120.49	115.27
24	B	612	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
24	A	410	CLA	C3B-C4B-NB	3.10	113.22	109.21
26	D	403	BCR	C33-C5-C6	-3.10	121.05	124.53
24	c	908	CLA	CBC-CAC-C3C	-3.10	103.89	112.43
26	k	103	BCR	C24-C23-C22	-3.10	121.55	126.23
26	d	406	BCR	C7-C8-C9	-3.10	121.56	126.23
24	b	607	CLA	O2A-CGA-O1A	-3.10	115.78	123.59
24	b	609	CLA	C1D-CHD-C4C	-3.10	119.38	126.06
24	b	618	CLA	C3C-C4C-NC	3.09	114.04	110.57
40	H	101	RRX	C7-C8-C9	-3.09	121.56	126.23
24	b	608	CLA	C3B-C4B-NB	3.09	113.21	109.21
24	C	509	CLA	C1D-CHD-C4C	-3.09	119.39	126.06
24	a	410	CLA	C4C-C3C-C2C	-3.09	102.40	106.90
24	B	616	CLA	CHA-C1A-NA	-3.09	119.33	126.40
24	b	605	CLA	CHD-C1D-ND	-3.09	121.62	124.45
24	c	902	CLA	C1D-CHD-C4C	-3.09	119.40	126.06
24	c	906	CLA	CAC-C3C-C4C	3.08	128.81	124.81
24	B	611	CLA	C1D-CHD-C4C	-3.08	119.41	126.06
29	A	414	PL9	C20-C19-C21	3.08	120.45	115.27
31	B	622	LMT	O5'-C1'-O1'	-3.08	102.68	109.97
26	c	915	BCR	C15-C14-C13	-3.08	122.91	127.31
24	d	404	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
24	d	401	CLA	CHC-C1C-C2C	-3.08	118.20	126.72
27	b	601	SQD	O48-C23-C24	3.08	121.57	111.91
24	b	610	CLA	CMC-C2C-C1C	3.08	129.73	125.04
24	c	910	CLA	C3C-C4C-NC	3.08	114.02	110.57
27	F	101	SQD	C1-O5-C5	-3.08	107.65	113.69
26	c	915	BCR	C7-C8-C9	-3.07	121.59	126.23
28	B	621	LMG	C9-C8-C7	-3.07	104.52	111.79
24	c	902	CLA	CBC-CAC-C3C	-3.07	103.96	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	405	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
29	a	417	PL9	C30-C29-C31	3.07	120.44	115.27
24	C	503	CLA	C3D-C4D-ND	3.07	115.20	110.24
24	B	606	CLA	C1C-C2C-C3C	-3.07	103.73	106.96
24	B	615	CLA	C3C-C4C-NC	3.07	114.01	110.57
24	b	613	CLA	C3C-C4C-NC	3.07	114.01	110.57
24	b	606	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
24	b	612	CLA	CHD-C4C-C3C	-3.06	120.34	124.84
29	a	417	PL9	C42-C43-C44	-3.06	120.28	127.66
26	T	101	BCR	C35-C13-C12	3.06	122.90	118.08
24	C	511	CLA	C3B-C4B-NB	3.06	113.17	109.21
24	A	407	CLA	O2A-CGA-O1A	-3.06	115.87	123.59
24	b	606	CLA	C4-C3-C5	3.06	120.42	115.27
24	D	401	CLA	C4C-C3C-C2C	-3.05	102.44	106.90
24	a	413	CLA	C3B-C4B-NB	3.05	113.16	109.21
24	C	504	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
26	c	916	BCR	C33-C5-C6	-3.05	121.10	124.53
24	b	607	CLA	CHD-C4C-C3C	-3.05	120.35	124.84
24	c	908	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
24	b	614	CLA	CHD-C1D-ND	-3.05	121.65	124.45
24	c	903	CLA	O2A-CGA-CBA	3.05	121.47	111.91
24	c	902	CLA	C3C-C4C-NC	3.05	113.99	110.57
24	c	908	CLA	C3B-C4B-NB	3.04	113.15	109.21
27	A	416	SQD	O9-S-C6	3.04	110.56	106.94
28	c	921	LMG	O6-C5-C4	3.04	115.22	109.69
24	d	404	CLA	CHD-C1D-ND	-3.04	121.66	124.45
24	C	511	CLA	C4-C3-C5	3.04	120.39	115.27
24	B	606	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
24	c	904	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
28	A	413	LMG	C1-O6-C5	3.03	119.64	113.69
26	B	636	BCR	C21-C20-C19	-3.03	113.75	123.22
24	b	614	CLA	C1C-C2C-C3C	-3.03	103.77	106.96
29	a	417	PL9	C27-C28-C29	-3.03	120.37	127.66
24	b	618	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
24	b	612	CLA	O2A-CGA-CBA	3.03	121.40	111.91
28	B	621	LMG	O8-C28-C29	3.03	121.40	111.91
26	B	620	BCR	C2-C1-C6	3.02	115.14	110.48
31	B	626	LMT	O5'-C5'-C4'	3.02	115.19	109.69
24	b	610	CLA	O2A-CGA-O1A	-3.02	115.97	123.59
24	B	616	CLA	C3C-C4C-NC	3.02	113.96	110.57
24	b	608	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
24	c	908	CLA	O1D-CGD-CBD	-3.02	118.31	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	605	CLA	C1D-CHD-C4C	-3.01	119.56	126.06
24	C	509	CLA	C3B-C4B-NB	3.01	113.11	109.21
24	D	402	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
24	B	604	CLA	CMB-C2B-C3B	3.01	130.31	124.68
24	C	508	CLA	C1D-CHD-C4C	-3.01	119.56	126.06
24	B	612	CLA	C3B-C4B-NB	3.01	113.10	109.21
24	b	617	CLA	C4A-NA-C1A	3.01	108.06	106.71
24	B	605	CLA	O2A-CGA-O1A	-3.01	116.00	123.59
24	b	605	CLA	C2C-C1C-NC	3.01	112.79	109.97
26	C	514	BCR	C38-C26-C25	-3.00	121.15	124.53
24	C	505	CLA	C1C-C2C-C3C	-3.00	103.80	106.96
24	b	613	CLA	C4C-C3C-C2C	-3.00	102.52	106.90
31	A	421	LMT	C1B-O5B-C5B	3.00	119.58	113.69
24	B	617	CLA	O2A-CGA-O1A	-3.00	116.02	123.59
24	b	612	CLA	C3B-C4B-NB	3.00	113.09	109.21
24	B	616	CLA	CBC-CAC-C3C	-3.00	104.17	112.43
24	c	906	CLA	C4C-C3C-C2C	-2.99	102.53	106.90
27	a	415	SQD	C44-O6-C1	-2.99	107.89	113.74
24	A	410	CLA	C3C-C4C-NC	2.99	113.92	110.57
24	A	406	CLA	CAA-C2A-C3A	-2.99	104.59	112.78
24	C	501	CLA	CMC-C2C-C1C	2.99	129.59	125.04
24	b	605	CLA	C4-C3-C5	2.99	120.30	115.27
24	c	909	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
24	c	914	CLA	C4C-C3C-C2C	-2.99	102.55	106.90
24	c	907	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
24	C	507	CLA	CBC-CAC-C3C	-2.98	104.20	112.43
24	B	602	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
26	c	916	BCR	C7-C8-C9	-2.98	121.73	126.23
26	Y	101	BCR	C15-C14-C13	-2.98	123.06	127.31
26	T	101	BCR	C15-C14-C13	2.98	131.56	127.31
24	a	409	CLA	CHD-C4C-C3C	-2.97	120.47	124.84
24	b	613	CLA	CBC-CAC-C3C	-2.97	104.23	112.43
24	c	904	CLA	CHD-C1D-ND	-2.97	121.72	124.45
24	C	505	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
40	H	101	RRX	C16-C17-C18	-2.97	123.07	127.31
24	d	401	CLA	O2D-CGD-CBD	2.97	116.55	111.27
24	C	509	CLA	O2A-CGA-CBA	2.97	121.23	111.91
24	b	611	CLA	C3C-C4C-NC	2.97	113.90	110.57
37	h	102	DGD	O2G-C1B-C2B	2.97	117.90	111.50
24	C	507	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
24	C	507	CLA	C3D-C4D-ND	2.97	115.04	110.24
24	B	610	CLA	C3B-C4B-NB	2.97	113.04	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	911	CLA	CBC-CAC-C3C	-2.96	104.26	112.43
24	c	911	CLA	C4-C3-C5	2.96	120.26	115.27
24	B	609	CLA	CHD-C4C-C3C	-2.96	120.48	124.84
24	C	506	CLA	C3C-C4C-NC	2.96	113.89	110.57
24	d	405	CLA	C3B-C4B-NB	2.96	113.04	109.21
28	C	523	LMG	C1-O6-C5	2.96	119.50	113.69
24	C	508	CLA	O2A-CGA-O1A	-2.96	116.12	123.59
24	B	609	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
24	b	619	CLA	CHA-C1A-NA	-2.96	119.62	126.40
29	a	417	PL9	C53-C6-C1	2.96	121.03	114.99
26	B	636	BCR	C11-C10-C9	-2.95	123.09	127.31
24	B	617	CLA	CHD-C1D-ND	-2.95	121.74	124.45
37	C	517	DGD	O1G-C1A-C2A	2.95	121.17	111.91
24	A	405	CLA	CMC-C2C-C1C	2.95	129.53	125.04
24	B	612	CLA	C1-C2-C3	-2.95	120.94	126.04
26	b	623	BCR	C3-C4-C5	-2.95	108.81	114.08
24	C	507	CLA	C3B-C4B-NB	2.94	113.02	109.21
24	c	902	CLA	C3B-C4B-NB	2.94	113.02	109.21
24	c	907	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
24	B	613	CLA	C1D-CHD-C4C	-2.94	119.72	126.06
24	B	603	CLA	O2A-CGA-O1A	-2.94	116.17	123.59
24	B	606	CLA	C3B-C4B-NB	2.93	113.00	109.21
24	D	401	CLA	O2A-CGA-CBA	2.93	121.12	111.91
24	A	405	CLA	C3B-C4B-NB	2.93	113.00	109.21
28	c	920	LMG	C8-O7-C10	-2.93	110.58	117.79
26	D	403	BCR	C29-C30-C25	2.93	114.99	110.48
26	a	414	BCR	C7-C8-C9	-2.93	121.81	126.23
24	C	510	CLA	C1-C2-C3	-2.93	120.98	126.04
24	B	616	CLA	CAC-C3C-C4C	2.93	128.61	124.81
24	B	604	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
24	c	912	CLA	CBC-CAC-C3C	-2.92	104.37	112.43
24	b	610	CLA	CHD-C1D-ND	-2.92	121.77	124.45
24	B	607	CLA	C3C-C4C-NC	2.92	113.85	110.57
24	c	904	CLA	CHA-C1A-NA	-2.92	119.71	126.40
24	C	502	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
24	B	613	CLA	CAC-C3C-C4C	2.92	128.60	124.81
24	C	511	CLA	CHA-C1A-NA	-2.92	119.72	126.40
24	c	912	CLA	C3B-C4B-NB	2.92	112.98	109.21
24	b	610	CLA	CMB-C2B-C3B	2.92	130.13	124.68
24	C	508	CLA	CHD-C1D-ND	-2.92	121.78	124.45
24	a	413	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
24	C	511	CLA	O2D-CGD-CBD	2.91	116.45	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	609	CLA	C3C-C4C-NC	2.91	113.84	110.57
24	b	619	CLA	C7-C6-C5	-2.91	105.45	113.36
24	b	605	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
24	A	410	CLA	CMA-C3A-C2A	-2.91	102.08	113.83
24	b	612	CLA	O2A-CGA-O1A	-2.91	116.25	123.59
24	b	618	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
24	B	610	CLA	CBC-CAC-C3C	-2.91	104.41	112.43
24	D	401	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
24	C	512	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
24	b	610	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
36	C	521	HTG	C1-O5-C5	2.91	117.94	112.58
24	A	407	CLA	CAA-C2A-C3A	-2.91	104.82	112.78
24	B	613	CLA	CMC-C2C-C1C	2.91	129.46	125.04
24	B	615	CLA	CBC-CAC-C3C	-2.90	104.42	112.43
39	f	101	HEM	C4B-CHC-C1C	2.90	126.39	122.56
24	c	913	CLA	C4-C3-C5	2.90	120.15	115.27
24	c	909	CLA	C1-C2-C3	-2.90	121.03	126.04
24	c	904	CLA	CMC-C2C-C1C	2.90	129.45	125.04
24	a	413	CLA	C1D-CHD-C4C	-2.90	119.81	126.06
24	a	409	CLA	CAA-C2A-C3A	-2.89	104.85	112.78
24	c	908	CLA	C3C-C4C-NC	2.89	113.82	110.57
24	c	910	CLA	C1-C2-C3	-2.89	121.04	126.04
29	A	414	PL9	C45-C44-C46	2.89	120.14	115.27
24	B	609	CLA	CAC-C3C-C4C	2.89	128.56	124.81
24	b	616	CLA	CHD-C1D-ND	-2.89	121.80	124.45
24	C	511	CLA	C1-O2A-CGA	2.89	124.03	116.44
28	C	523	LMG	C8-O7-C10	-2.89	110.67	117.79
24	c	913	CLA	C3B-C4B-NB	2.89	112.94	109.21
24	b	619	CLA	C3C-C4C-NC	2.89	113.81	110.57
40	H	101	RRX	C10-C11-C12	-2.88	114.22	123.22
24	B	614	CLA	C1D-CHD-C4C	-2.88	119.84	126.06
24	b	613	CLA	C4-C3-C5	2.88	120.12	115.27
24	C	504	CLA	C3C-C4C-NC	2.88	113.80	110.57
24	B	606	CLA	O2A-CGA-O1A	-2.88	116.32	123.59
24	c	910	CLA	CBC-CAC-C3C	-2.88	104.50	112.43
24	B	615	CLA	CHD-C1D-ND	-2.88	121.81	124.45
24	A	405	CLA	CAA-C2A-C1A	-2.87	102.56	111.97
38	D	406	LHG	C5-O7-C7	-2.87	110.72	117.79
38	d	411	LHG	O8-C23-O10	-2.87	116.34	123.59
38	d	409	LHG	O7-C7-C8	2.87	117.69	111.50
24	C	510	CLA	C1-O2A-CGA	2.87	123.97	116.44
24	d	404	CLA	O2A-CGA-CBA	2.87	120.91	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	507	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
24	C	503	CLA	CBC-CAC-C3C	-2.87	104.53	112.43
24	C	505	CLA	CHA-C1A-NA	-2.86	119.84	126.40
24	A	405	CLA	CMA-C3A-C4A	-2.86	104.08	111.77
24	C	510	CLA	O1D-CGD-CBD	-2.86	118.63	124.48
24	b	613	CLA	C1D-CHD-C4C	-2.86	119.89	126.06
24	C	508	CLA	O2A-CGA-CBA	2.86	120.88	111.91
29	d	407	PL9	C42-C43-C44	-2.86	120.78	127.66
24	B	603	CLA	C3B-C4B-NB	2.86	112.91	109.21
24	d	404	CLA	C4-C3-C5	2.86	120.08	115.27
26	K	101	BCR	C7-C8-C9	-2.86	121.92	126.23
37	D	405	DGD	O1G-C1A-C2A	2.85	120.86	111.91
24	b	606	CLA	CBC-CAC-C3C	-2.85	104.57	112.43
24	B	612	CLA	C3C-C4C-NC	2.85	113.77	110.57
24	C	510	CLA	CBC-CAC-C3C	-2.85	104.58	112.43
24	b	617	CLA	CAC-C3C-C4C	2.85	128.50	124.81
24	C	505	CLA	C4A-NA-C1A	2.84	107.98	106.71
24	b	605	CLA	C3C-C4C-NC	2.84	113.76	110.57
24	c	907	CLA	O2A-CGA-O1A	-2.84	116.42	123.59
36	b	602	HTG	C1-O5-C5	2.84	117.82	112.58
24	B	609	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
24	a	413	CLA	C4-C3-C5	2.84	120.05	115.27
24	C	501	CLA	C3B-C4B-NB	2.84	112.88	109.21
24	C	502	CLA	CAC-C3C-C4C	2.84	128.49	124.81
24	C	506	CLA	CAA-C2A-C3A	-2.84	105.00	112.78
24	D	402	CLA	C1D-CHD-C4C	-2.84	119.94	126.06
37	C	518	DGD	O3G-C3G-C2G	-2.84	104.06	110.90
24	B	612	CLA	C4A-NA-C1A	2.83	107.98	106.71
26	B	636	BCR	C35-C13-C12	2.83	122.54	118.08
24	C	506	CLA	C1-C2-C3	-2.83	121.14	126.04
24	C	511	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
24	b	606	CLA	CMB-C2B-C3B	2.83	129.97	124.68
24	C	502	CLA	CBC-CAC-C3C	-2.83	104.64	112.43
24	B	615	CLA	CAC-C3C-C4C	2.83	128.48	124.81
24	c	911	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
24	A	406	CLA	CHC-C1C-C2C	-2.83	118.90	126.72
24	b	618	CLA	CBC-CAC-C3C	-2.82	104.64	112.43
26	c	915	BCR	C16-C17-C18	-2.82	123.28	127.31
24	C	508	CLA	CAA-C2A-C3A	-2.82	105.05	112.78
24	C	502	CLA	CED-O2D-CGD	2.82	122.32	115.94
24	b	605	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
24	B	615	CLA	C1-O2A-CGA	2.82	123.84	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	513	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
26	B	636	BCR	C12-C13-C14	-2.82	114.62	118.94
24	C	510	CLA	CAC-C3C-C4C	2.82	128.46	124.81
27	f	102	SQD	O48-C23-C24	2.82	120.74	111.91
28	c	920	LMG	O8-C28-C29	2.81	120.74	111.91
24	B	609	CLA	O2A-CGA-CBA	2.81	120.74	111.91
26	b	621	BCR	C3-C4-C5	-2.81	109.06	114.08
25	a	411	PHO	CMC-C2C-C3C	2.81	130.24	124.94
29	a	417	PL9	C15-C14-C16	2.81	120.00	115.27
24	b	607	CLA	C3C-C4C-NC	2.81	113.72	110.57
24	c	905	CLA	C3C-C4C-NC	2.81	113.72	110.57
24	C	513	CLA	C4-C3-C5	2.81	120.00	115.27
24	d	401	CLA	C4-C3-C5	2.81	119.99	115.27
24	B	614	CLA	C3B-C4B-NB	2.81	112.84	109.21
24	c	903	CLA	C3B-C4B-NB	2.81	112.84	109.21
42	v	202	HEC	C1D-C2D-C3D	-2.81	105.04	107.00
24	B	616	CLA	C11-C10-C8	-2.81	106.85	115.92
24	b	614	CLA	C3B-C4B-NB	2.81	112.84	109.21
24	c	909	CLA	CAA-C2A-C3A	-2.80	105.10	112.78
24	B	603	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
24	a	409	CLA	CMB-C2B-C3B	2.80	129.92	124.68
24	b	607	CLA	C3B-C4B-NB	2.80	112.83	109.21
24	C	512	CLA	C1-O2A-CGA	2.80	123.79	116.44
24	B	608	CLA	C1D-CHD-C4C	-2.80	120.03	126.06
24	B	608	CLA	C1-O2A-CGA	2.80	123.78	116.44
28	C	519	LMG	O8-C28-C29	2.79	120.68	111.91
24	c	914	CLA	C4-C3-C5	2.79	119.97	115.27
24	c	905	CLA	O2A-CGA-O1A	-2.79	116.54	123.59
24	c	906	CLA	CBC-CAC-C3C	-2.79	104.73	112.43
36	b	626	HTG	C1-C2-C3	2.79	116.10	110.59
24	C	513	CLA	O2A-CGA-CBA	2.79	120.67	111.91
31	a	402	LMT	O5B-C5B-C4B	2.79	114.76	109.69
24	b	611	CLA	CBC-CAC-C3C	-2.79	104.74	112.43
24	a	409	CLA	O2A-CGA-CBA	2.79	120.66	111.91
24	C	503	CLA	C4C-C3C-C2C	-2.79	102.84	106.90
29	A	414	PL9	C15-C14-C16	2.79	119.96	115.27
37	C	517	DGD	O1G-C1A-O1A	-2.78	116.56	123.59
24	B	610	CLA	CMC-C2C-C1C	2.78	129.28	125.04
24	b	620	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
24	b	615	CLA	C3C-C4C-NC	2.78	113.69	110.57
24	a	410	CLA	C1-C2-C3	-2.78	121.23	126.04
42	V	203	HEC	CBA-CAA-C2A	-2.78	107.92	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	502	CLA	CMC-C2C-C1C	2.78	129.28	125.04
24	B	613	CLA	C4-C3-C5	2.78	119.95	115.27
24	C	512	CLA	CBC-CAC-C3C	-2.78	104.76	112.43
25	a	411	PHO	O2D-CGD-O1D	-2.78	118.40	123.84
24	b	609	CLA	O2A-CGA-O1A	-2.78	116.58	123.59
29	A	414	PL9	C37-C36-C34	-2.78	103.84	112.98
24	C	504	CLA	CAC-C3C-C4C	2.78	128.41	124.81
24	b	620	CLA	C1C-C2C-C3C	-2.78	104.04	106.96
36	B	624	HTG	C1-C2-C3	2.77	116.07	110.59
24	b	611	CLA	CMC-C2C-C1C	2.77	129.26	125.04
27	F	101	SQD	C3-C4-C5	2.77	115.18	110.24
24	C	508	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
24	b	609	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
24	C	504	CLA	C3B-C4B-NB	2.77	112.79	109.21
24	A	410	CLA	CMC-C2C-C1C	2.77	129.26	125.04
24	C	510	CLA	CMA-C3A-C4A	-2.77	104.33	111.77
26	B	619	BCR	C11-C10-C9	-2.77	123.36	127.31
24	A	405	CLA	CMA-C3A-C2A	-2.77	102.67	113.83
24	c	904	CLA	C3D-C4D-ND	2.76	114.71	110.24
24	b	615	CLA	CMB-C2B-C3B	2.76	129.85	124.68
24	B	615	CLA	CMB-C2B-C3B	2.76	129.85	124.68
24	d	404	CLA	CAA-C2A-C3A	-2.76	105.22	112.78
24	a	409	CLA	C3C-C4C-NC	2.76	113.67	110.57
24	C	506	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
24	C	505	CLA	CMC-C2C-C1C	2.76	129.24	125.04
24	a	409	CLA	O2A-CGA-O1A	-2.76	116.63	123.59
25	a	411	PHO	CMB-C2B-C3B	2.76	129.84	124.68
29	d	407	PL9	C15-C14-C16	2.76	119.91	115.27
38	d	411	LHG	O8-C23-C24	2.76	120.56	111.91
24	b	612	CLA	CHA-C1A-NA	-2.76	120.09	126.40
24	B	616	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
24	B	615	CLA	CMC-C2C-C1C	2.75	129.23	125.04
24	B	611	CLA	O2A-CGA-CBA	2.75	120.54	111.91
24	c	905	CLA	CMC-C2C-C1C	2.75	129.23	125.04
26	C	515	BCR	C23-C24-C25	-2.75	119.48	127.20
24	c	914	CLA	C3B-C4B-NB	2.75	112.77	109.21
24	C	506	CLA	C3B-C4B-NB	2.75	112.76	109.21
36	B	630	HTG	C1-O5-C5	2.75	117.65	112.58
24	b	619	CLA	CBC-CAC-C3C	-2.75	104.85	112.43
24	D	402	CLA	CMC-C2C-C1C	2.75	129.22	125.04
28	b	624	LMG	C9-C8-C7	-2.75	105.29	111.79
36	O	316	HTG	C6-C5-C4	-2.74	106.58	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	620	CLA	CMB-C2B-C3B	2.74	129.81	124.68
24	c	913	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
24	b	619	CLA	C1-O2A-CGA	2.74	123.64	116.44
40	h	101	RRX	C7-C8-C9	-2.74	122.09	126.23
24	B	614	CLA	CMC-C2C-C1C	2.74	129.21	125.04
24	b	609	CLA	CMC-C2C-C1C	2.74	129.21	125.04
24	c	906	CLA	C3B-C4B-NB	2.74	112.75	109.21
24	a	410	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
24	a	413	CLA	CMA-C3A-C2A	-2.73	102.81	113.83
24	C	509	CLA	C3C-C4C-NC	2.73	113.63	110.57
24	B	602	CLA	O2A-CGA-CBA	2.73	120.47	111.91
24	B	602	CLA	C3C-C4C-NC	2.73	113.63	110.57
38	D	408	LHG	O7-C7-C8	2.72	117.37	111.50
24	C	513	CLA	CBC-CAC-C3C	-2.72	104.92	112.43
24	C	510	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
24	c	910	CLA	CMC-C2C-C1C	2.72	129.19	125.04
24	a	410	CLA	O2A-CGA-O1A	-2.72	116.72	123.59
24	c	910	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
24	A	410	CLA	CAA-C2A-C3A	-2.72	105.33	112.78
24	b	615	CLA	C3B-C4B-NB	2.72	112.73	109.21
24	c	905	CLA	CAC-C3C-C4C	2.72	128.34	124.81
24	B	606	CLA	CHD-C1D-ND	-2.72	121.96	124.45
24	B	614	CLA	CED-O2D-CGD	2.72	122.08	115.94
24	d	401	CLA	CMA-C3A-C2A	-2.72	102.87	113.83
24	B	613	CLA	CMB-C2B-C3B	2.71	129.76	124.68
37	C	516	DGD	C3G-C2G-C1G	-2.71	105.37	111.79
24	b	606	CLA	CMA-C3A-C2A	-2.71	102.89	113.83
24	B	609	CLA	C3B-C4B-NB	2.71	112.72	109.21
40	h	101	RRX	C20-C21-C22	-2.71	123.44	127.31
24	a	409	CLA	CHC-C1C-C2C	-2.71	119.22	126.72
25	a	411	PHO	C4A-C3A-C2A	-2.71	100.26	102.84
24	b	608	CLA	O1D-CGD-CBD	-2.71	118.94	124.48
31	A	417	LMT	C1B-O1B-C4'	-2.71	111.27	117.96
26	k	103	BCR	C8-C7-C6	-2.71	119.60	127.20
24	B	617	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
24	b	609	CLA	CBC-CAC-C3C	-2.71	104.97	112.43
26	B	636	BCR	C16-C15-C14	2.70	129.01	123.47
24	B	616	CLA	CMC-C2C-C1C	2.70	129.15	125.04
24	b	608	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
24	B	614	CLA	CBC-CAC-C3C	-2.70	104.99	112.43
24	B	611	CLA	CAA-CBA-CGA	-2.70	105.36	113.25
24	B	607	CLA	O2D-CGD-O1D	-2.70	118.56	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	404	CLA	CAC-C3C-C4C	2.70	128.31	124.81
24	C	509	CLA	CMB-C2B-C3B	2.70	129.73	124.68
24	D	401	CLA	C1D-CHD-C4C	-2.70	120.24	126.06
24	b	615	CLA	C4C-C3C-C2C	-2.70	102.97	106.90
27	a	415	SQD	O47-C7-O49	-2.69	117.19	123.70
24	D	402	CLA	CAC-C3C-C4C	2.69	128.31	124.81
24	b	619	CLA	CMB-C2B-C3B	2.69	129.72	124.68
24	B	602	CLA	C4C-C3C-C2C	-2.69	102.97	106.90
25	A	408	PHO	CBA-CAA-C2A	-2.69	105.95	113.81
24	c	912	CLA	C3C-C4C-NC	2.69	113.59	110.57
24	B	617	CLA	CBC-CAC-C3C	-2.69	105.03	112.43
24	B	610	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
24	B	616	CLA	C4C-C3C-C2C	-2.68	102.98	106.90
24	C	501	CLA	C3C-C4C-NC	2.68	113.58	110.57
26	b	623	BCR	C32-C1-C6	-2.68	105.95	110.30
24	b	616	CLA	CMC-C2C-C1C	2.68	129.12	125.04
27	A	412	SQD	O47-C7-O49	-2.68	117.22	123.70
24	B	617	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
37	c	917	DGD	C2G-O2G-C1B	-2.68	111.19	117.79
38	D	406	LHG	O8-C23-O10	-2.68	116.83	123.59
24	B	611	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
24	B	604	CLA	CMA-C3A-C2A	-2.68	103.03	113.83
24	C	506	CLA	C4C-C3C-C2C	-2.68	103.00	106.90
24	B	615	CLA	O2A-CGA-CBA	2.68	120.31	111.91
24	d	401	CLA	CAA-C2A-C3A	-2.68	105.45	112.78
26	A	411	BCR	C38-C26-C25	-2.67	121.53	124.53
24	C	512	CLA	CMA-C3A-C4A	-2.67	104.59	111.77
24	B	603	CLA	O2A-CGA-CBA	2.67	120.29	111.91
25	a	412	PHO	C4A-C3A-C2A	-2.67	100.30	102.84
24	b	611	CLA	C4C-C3C-C2C	-2.67	103.01	106.90
24	A	410	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
24	B	614	CLA	CMA-C3A-C4A	-2.67	104.61	111.77
25	A	409	PHO	C4A-C3A-C2A	-2.67	100.30	102.84
24	b	605	CLA	O2A-C1-C2	-2.67	101.63	108.64
24	B	614	CLA	O2A-CGA-O1A	-2.66	116.87	123.59
29	A	414	PL9	C25-C24-C26	2.66	119.75	115.27
29	A	414	PL9	C17-C18-C19	-2.66	121.25	127.66
37	H	102	DGD	O1G-C1A-C2A	2.66	120.27	111.91
24	b	608	CLA	CHA-C1A-NA	-2.66	120.30	126.40
24	B	605	CLA	C1-C2-C3	-2.66	121.44	126.04
24	B	602	CLA	C1-C2-C3	-2.66	121.44	126.04
24	d	404	CLA	C1D-CHD-C4C	-2.66	120.33	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	605	CLA	CBC-CAC-C3C	-2.66	105.11	112.43
24	C	513	CLA	CAC-C3C-C4C	2.66	128.26	124.81
40	h	101	RRX	C10-C11-C12	-2.66	114.93	123.22
40	h	101	RRX	C24-C23-C22	-2.66	122.22	126.23
24	C	508	CLA	CMC-C2C-C1C	2.65	129.08	125.04
24	B	605	CLA	O2A-CGA-CBA	2.65	120.23	111.91
24	d	404	CLA	CHD-C4C-C3C	-2.65	120.94	124.84
24	B	603	CLA	C4-C3-C5	2.65	119.73	115.27
24	C	513	CLA	C3B-C4B-NB	2.65	112.64	109.21
24	b	614	CLA	CMA-C3A-C4A	-2.65	104.65	111.77
24	b	605	CLA	C1-O2A-CGA	2.65	123.39	116.44
26	k	102	BCR	C10-C11-C12	-2.65	114.95	123.22
24	C	506	CLA	C4-C3-C5	2.65	119.73	115.27
29	a	417	PL9	C10-C9-C11	2.65	119.72	115.27
24	c	904	CLA	O2A-C1-C2	-2.65	101.68	108.64
27	a	401	SQD	O48-C23-C24	2.65	120.21	111.91
24	b	618	CLA	O2A-CGA-O1A	-2.64	116.92	123.59
24	C	509	CLA	C4C-C3C-C2C	-2.64	103.04	106.90
25	a	411	PHO	C1A-C2A-C3A	-2.64	100.32	102.84
24	A	407	CLA	CAC-C3C-C4C	2.64	128.24	124.81
26	C	514	BCR	C11-C10-C9	-2.64	123.54	127.31
24	b	611	CLA	CAA-C2A-C1A	-2.64	103.32	111.97
24	b	610	CLA	CAC-C3C-C4C	2.64	128.24	124.81
24	B	616	CLA	CHC-C1C-C2C	-2.64	119.42	126.72
24	A	406	CLA	CMA-C3A-C2A	-2.64	103.18	113.83
24	B	614	CLA	C1-O2A-CGA	2.64	123.37	116.44
24	C	503	CLA	CHA-C1A-NA	-2.64	120.36	126.40
42	v	202	HEC	CMB-C2B-C1B	-2.64	124.41	128.46
24	b	618	CLA	C3B-C4B-NB	2.63	112.62	109.21
24	C	504	CLA	OBD-CAD-C3D	-2.63	122.18	128.52
27	A	412	SQD	O8-S-C6	2.63	109.93	105.74
24	a	410	CLA	CAA-C2A-C3A	-2.63	105.57	112.78
38	D	406	LHG	O7-C7-C8	2.63	117.17	111.50
24	b	617	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
24	B	602	CLA	CBC-CAC-C3C	-2.63	105.18	112.43
24	c	904	CLA	C1-C2-C3	-2.63	121.50	126.04
24	c	904	CLA	C1-O2A-CGA	2.63	123.34	116.44
26	K	101	BCR	C38-C26-C25	-2.63	121.58	124.53
24	b	614	CLA	C1-C2-C3	-2.62	121.50	126.04
24	b	610	CLA	C3B-C4B-NB	2.62	112.60	109.21
26	b	623	BCR	C38-C26-C25	-2.62	121.58	124.53
24	A	406	CLA	O2D-CGD-O1D	-2.62	118.71	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	604	CLA	CAC-C3C-C4C	2.62	128.21	124.81
24	b	619	CLA	C4C-C3C-C2C	-2.62	103.08	106.90
29	D	404	PL9	C12-C13-C14	-2.62	121.36	127.66
37	c	919	DGD	O1G-C1A-C2A	2.62	120.12	111.91
24	c	913	CLA	CHD-C1D-ND	-2.61	122.05	124.45
24	c	913	CLA	CHA-C1A-NA	-2.61	120.42	126.40
24	b	610	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
36	C	537	HTG	O5-C5-C4	2.61	114.43	109.69
29	d	407	PL9	C12-C13-C14	-2.61	121.38	127.66
24	c	912	CLA	CMC-C2C-C1C	2.61	129.01	125.04
24	b	608	CLA	O2A-CGA-CBA	2.61	120.09	111.91
24	B	604	CLA	CBC-CAC-C3C	-2.61	105.24	112.43
28	c	921	LMG	O8-C28-C29	2.61	120.09	111.91
24	C	504	CLA	CAA-C2A-C3A	-2.61	105.64	112.78
26	k	102	BCR	C16-C17-C18	-2.61	123.59	127.31
28	a	416	LMG	O6-C5-C4	2.61	114.43	109.69
24	b	617	CLA	CMA-C3A-C4A	-2.61	104.77	111.77
29	d	407	PL9	C25-C24-C26	2.60	119.65	115.27
24	B	614	CLA	C4C-C3C-C2C	-2.60	103.10	106.90
29	A	414	PL9	C30-C29-C31	2.60	119.65	115.27
24	c	910	CLA	CAC-C3C-C4C	2.60	128.19	124.81
24	a	410	CLA	O2A-CGA-CBA	2.60	120.08	111.91
24	B	612	CLA	CMB-C2B-C3B	2.60	129.55	124.68
25	a	412	PHO	CMC-C2C-C3C	2.60	129.85	124.94
29	A	414	PL9	C42-C43-C44	-2.60	121.39	127.66
24	C	512	CLA	CHA-C1A-NA	-2.60	120.44	126.40
24	C	510	CLA	CMC-C2C-C1C	2.60	129.00	125.04
24	A	406	CLA	C4C-C3C-C2C	-2.60	103.11	106.90
40	H	101	RRX	C20-C21-C22	-2.60	123.60	127.31
24	B	611	CLA	C1-C2-C3	-2.60	121.55	126.04
24	B	602	CLA	CAA-C2A-C3A	-2.60	105.67	112.78
24	c	912	CLA	C4C-C3C-C2C	-2.60	103.11	106.90
24	C	512	CLA	C1-C2-C3	-2.59	121.56	126.04
42	v	202	HEC	CBA-CAA-C2A	-2.59	108.23	112.60
39	F	102	HEM	C1B-NB-C4B	2.59	107.75	105.07
24	a	413	CLA	CMA-C3A-C4A	-2.59	104.80	111.77
24	C	512	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
24	C	509	CLA	C16-C15-C13	-2.59	107.54	115.92
26	b	622	BCR	C38-C26-C25	-2.59	121.62	124.53
24	B	612	CLA	CHC-C1C-C2C	-2.59	119.57	126.72
27	F	101	SQD	C45-O47-C7	-2.59	111.43	117.79
24	A	410	CLA	O2A-CGA-CBA	2.58	120.02	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	607	CLA	CMC-C2C-C1C	2.58	128.97	125.04
26	k	102	BCR	C38-C26-C25	-2.58	121.63	124.53
24	B	607	CLA	C3B-C4B-NB	2.58	112.55	109.21
24	a	413	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
26	b	622	BCR	C8-C7-C6	-2.58	119.95	127.20
24	d	405	CLA	C4-C3-C5	2.58	119.61	115.27
26	b	623	BCR	C15-C14-C13	-2.58	123.63	127.31
24	B	606	CLA	CMC-C2C-C1C	2.58	128.97	125.04
24	b	618	CLA	CHC-C1C-C2C	-2.58	119.58	126.72
24	c	909	CLA	C4-C3-C5	2.58	119.61	115.27
26	T	101	BCR	C21-C20-C19	-2.58	115.17	123.22
24	C	507	CLA	CHA-C1A-NA	-2.58	120.49	126.40
38	E	101	LHG	O8-C23-C24	2.57	119.98	111.91
24	d	405	CLA	C4C-C3C-C2C	-2.57	103.15	106.90
26	A	411	BCR	C20-C21-C22	-2.57	123.64	127.31
24	b	617	CLA	O2A-CGA-CBA	2.57	119.98	111.91
24	C	510	CLA	C11-C10-C8	-2.57	107.60	115.92
38	D	406	LHG	O8-C23-C24	2.57	119.98	111.91
24	d	404	CLA	CHA-C1A-NA	-2.57	120.51	126.40
31	c	927	LMT	C1B-O1B-C4'	-2.57	111.60	117.96
24	B	604	CLA	O2A-CGA-CBA	2.57	119.98	111.91
28	c	921	LMG	C8-O7-C10	-2.57	111.46	117.79
24	B	615	CLA	C7-C6-C5	-2.57	106.38	113.36
24	C	513	CLA	CMC-C2C-C1C	2.57	128.95	125.04
24	b	615	CLA	CBC-CAC-C3C	-2.57	105.35	112.43
24	b	611	CLA	CHC-C1C-C2C	-2.57	119.62	126.72
24	b	608	CLA	C4A-NA-C1A	2.57	107.86	106.71
26	k	103	BCR	C20-C21-C22	-2.57	123.65	127.31
24	c	903	CLA	C4C-C3C-C2C	-2.56	103.16	106.90
24	C	508	CLA	C3B-C4B-NB	2.56	112.52	109.21
24	b	616	CLA	C16-C15-C13	-2.56	107.64	115.92
26	k	103	BCR	C11-C10-C9	-2.56	123.66	127.31
24	c	912	CLA	C1-C2-C3	-2.56	121.61	126.04
25	A	408	PHO	CMB-C2B-C3B	2.56	129.46	124.68
38	d	410	LHG	O7-C7-C8	2.56	117.01	111.50
37	h	102	DGD	C6D-C5D-C4D	2.56	117.43	112.09
24	b	620	CLA	C1-C2-C3	-2.56	121.62	126.04
24	b	618	CLA	O2A-CGA-CBA	2.56	119.93	111.91
24	d	401	CLA	C4C-C3C-C2C	-2.56	103.17	106.90
36	B	631	HTG	C1-O5-C5	2.56	117.29	112.58
26	B	636	BCR	C23-C24-C25	-2.56	120.03	127.20
37	H	102	DGD	O2G-C1B-C2B	2.55	117.01	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	406	BCR	C3-C4-C5	-2.55	109.52	114.08
24	B	616	CLA	C6-C7-C8	-2.55	107.66	115.92
24	C	511	CLA	O2A-C1-C2	-2.55	101.92	108.64
26	C	515	BCR	C21-C20-C19	-2.55	115.25	123.22
24	b	614	CLA	CHC-C1C-C2C	-2.55	119.66	126.72
24	B	603	CLA	CMB-C2B-C3B	2.55	129.45	124.68
24	c	914	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
24	B	604	CLA	O2A-CGA-O1A	-2.55	117.15	123.59
24	A	405	CLA	CAC-C3C-C4C	2.55	128.12	124.81
24	c	914	CLA	CAA-C2A-C3A	-2.55	105.79	112.78
24	c	905	CLA	C4C-C3C-C2C	-2.55	103.18	106.90
24	B	603	CLA	CBC-CAC-C3C	-2.55	105.40	112.43
24	b	615	CLA	CHC-C1C-C2C	-2.55	119.67	126.72
24	C	503	CLA	CHD-C1D-ND	-2.55	122.11	124.45
24	b	606	CLA	CMA-C3A-C4A	-2.55	104.93	111.77
37	C	518	DGD	O6E-C1E-O5D	-2.55	103.94	109.97
29	D	404	PL9	C30-C29-C31	2.54	119.55	115.27
26	D	403	BCR	C38-C26-C27	2.54	118.50	113.62
26	a	414	BCR	C15-C14-C13	-2.54	123.68	127.31
37	C	516	DGD	O1G-C1A-O1A	-2.54	117.17	123.59
24	d	401	CLA	CMA-C3A-C4A	-2.54	104.94	111.77
24	d	401	CLA	CAC-C3C-C4C	2.54	128.10	124.81
24	B	608	CLA	CMB-C2B-C3B	2.54	129.43	124.68
24	b	609	CLA	C3B-C4B-NB	2.54	112.49	109.21
24	D	401	CLA	CBC-CAC-C3C	-2.54	105.44	112.43
24	b	614	CLA	CAA-C2A-C3A	-2.53	105.84	112.78
24	B	615	CLA	CHD-C4C-NC	2.53	128.20	124.20
25	A	408	PHO	CMA-C3A-C4A	-2.53	108.83	114.38
26	d	406	BCR	C38-C26-C27	2.53	118.48	113.62
24	c	906	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
24	a	409	CLA	C4C-C3C-C2C	-2.53	103.21	106.90
24	b	614	CLA	CMB-C2B-C3B	2.53	129.41	124.68
24	B	617	CLA	C6-C5-C3	-2.53	106.82	113.45
27	a	415	SQD	O48-C23-C24	2.53	119.84	111.91
24	c	906	CLA	CMC-C2C-C1C	2.53	128.89	125.04
24	b	616	CLA	O2A-CGA-CBA	2.53	119.84	111.91
38	D	408	LHG	O8-C23-O10	-2.53	117.21	123.59
24	B	614	CLA	C4-C3-C5	2.53	119.52	115.27
38	d	410	LHG	O8-C23-O10	-2.53	117.22	123.59
26	b	621	BCR	C24-C23-C22	-2.52	122.42	126.23
24	b	610	CLA	CHA-C1A-NA	-2.52	120.62	126.40
26	B	636	BCR	C15-C14-C13	2.52	130.91	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	507	CLA	CMB-C2B-C3B	2.52	129.40	124.68
24	c	910	CLA	C11-C12-C13	-2.52	107.77	115.92
24	b	606	CLA	CHA-C1A-NA	-2.52	120.63	126.40
24	d	405	CLA	CAC-C3C-C4C	2.52	128.08	124.81
24	B	611	CLA	C3B-C4B-NB	2.52	112.47	109.21
27	A	412	SQD	O48-C23-C24	2.52	119.81	111.91
26	A	411	BCR	C15-C14-C13	-2.52	123.72	127.31
25	a	411	PHO	CBA-CAA-C2A	-2.52	106.46	113.81
24	b	612	CLA	CMA-C3A-C2A	-2.52	103.67	113.83
24	b	607	CLA	C4C-C3C-C2C	-2.52	103.23	106.90
24	b	620	CLA	CHD-C1D-ND	-2.52	122.14	124.45
31	b	625	LMT	O5'-C1'-C2'	-2.52	105.02	110.35
24	B	607	CLA	O2A-CGA-CBA	2.52	119.80	111.91
24	C	510	CLA	CHC-C1C-C2C	-2.51	119.77	126.72
24	c	906	CLA	CHA-C1A-NA	-2.51	120.64	126.40
24	b	607	CLA	CMA-C3A-C2A	-2.51	103.69	113.83
38	D	407	LHG	O7-C7-C8	2.51	116.92	111.50
24	C	513	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
24	B	615	CLA	CHC-C1C-C2C	-2.51	119.78	126.72
26	B	619	BCR	C29-C28-C27	-2.51	105.77	111.38
24	c	909	CLA	CBC-CAC-C3C	-2.51	105.52	112.43
25	a	412	PHO	O2D-CGD-O1D	-2.51	118.93	123.84
24	c	904	CLA	CAC-C3C-C4C	2.51	128.06	124.81
39	f	101	HEM	CMA-C3A-C4A	-2.51	124.61	128.46
24	B	612	CLA	CHA-C1A-NA	-2.51	120.66	126.40
24	B	607	CLA	C4C-C3C-C2C	-2.50	103.25	106.90
24	A	406	CLA	CMB-C2B-C3B	2.50	129.36	124.68
24	a	410	CLA	CMA-C3A-C2A	-2.50	103.74	113.83
24	d	401	CLA	O2A-CGA-O1A	-2.50	117.28	123.59
36	b	603	HTG	O5-C1-C2	2.50	113.46	110.31
24	b	613	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
24	a	413	CLA	O2A-CGA-CBA	2.50	119.74	111.91
24	C	508	CLA	C4-C3-C5	2.50	119.47	115.27
24	B	606	CLA	CMB-C2B-C3B	2.50	129.35	124.68
24	C	510	CLA	CMB-C2B-C3B	2.49	129.35	124.68
26	Y	101	BCR	C16-C17-C18	-2.49	123.75	127.31
24	c	909	CLA	CMB-C2B-C3B	2.49	129.34	124.68
24	C	508	CLA	CMB-C2B-C3B	2.49	129.34	124.68
24	A	410	CLA	CMB-C2B-C3B	2.49	129.33	124.68
28	d	412	LMG	O8-C28-O10	-2.49	117.31	123.59
24	C	509	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
24	c	902	CLA	CAC-C3C-C4C	2.49	128.03	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	619	CLA	CMC-C2C-C1C	2.49	128.82	125.04
24	c	906	CLA	C1-O2A-CGA	2.48	122.96	116.44
26	c	916	BCR	C3-C4-C5	-2.48	109.64	114.08
24	c	914	CLA	CED-O2D-CGD	2.48	121.55	115.94
24	d	405	CLA	CAA-C2A-C3A	-2.48	105.98	112.78
24	C	504	CLA	CMB-C2B-C3B	2.48	129.32	124.68
38	E	101	LHG	C5-O7-C7	-2.48	111.68	117.79
24	b	613	CLA	CHA-C1A-NA	-2.48	120.72	126.40
24	b	617	CLA	C1D-CHD-C4C	-2.48	120.71	126.06
24	d	405	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
24	B	614	CLA	O2A-CGA-CBA	2.48	119.69	111.91
24	A	410	CLA	O2A-CGA-O1A	-2.48	117.34	123.59
24	B	607	CLA	CMB-C2B-C3B	2.48	129.31	124.68
24	c	908	CLA	O2A-CGA-CBA	2.48	119.68	111.91
24	b	615	CLA	CMC-C2C-C1C	2.47	128.80	125.04
24	c	907	CLA	O2A-CGA-CBA	2.47	119.67	111.91
29	D	404	PL9	C20-C19-C21	2.47	119.43	115.27
38	d	410	LHG	O8-C23-C24	2.47	119.66	111.91
24	b	619	CLA	CAC-C3C-C4C	2.47	128.02	124.81
24	B	605	CLA	C4C-C3C-C2C	-2.47	103.30	106.90
24	D	401	CLA	CAC-C3C-C4C	2.47	128.01	124.81
24	A	405	CLA	CHD-C1D-ND	-2.47	122.18	124.45
27	F	101	SQD	O9-S-C6	2.47	109.87	106.94
24	b	616	CLA	C5-C3-C2	-2.47	116.12	121.12
27	l	101	SQD	O48-C23-C24	2.47	119.65	111.91
37	c	917	DGD	O2G-C1B-O1B	-2.47	117.74	123.70
24	b	610	CLA	CBC-CAC-C3C	-2.47	105.63	112.43
31	c	922	LMT	C1B-O5B-C5B	2.46	118.53	113.69
24	B	609	CLA	O2A-CGA-O1A	-2.46	117.37	123.59
24	A	407	CLA	C4C-C3C-C2C	-2.46	103.31	106.90
24	a	409	CLA	C4-C3-C5	2.46	119.41	115.27
24	c	907	CLA	C4-C3-C5	2.46	119.41	115.27
24	C	502	CLA	C3B-C4B-NB	2.46	112.39	109.21
26	B	620	BCR	C15-C14-C13	-2.46	123.80	127.31
24	C	503	CLA	C4A-NA-C1A	2.46	107.81	106.71
26	B	636	BCR	C1-C6-C7	2.46	122.73	115.78
24	D	402	CLA	CAA-C2A-C3A	-2.46	106.05	112.78
24	b	608	CLA	C6-C7-C8	-2.46	107.98	115.92
28	a	416	LMG	O1-C1-C2	2.46	112.14	108.30
24	B	612	CLA	CHD-C4C-NC	2.45	128.07	124.20
24	c	913	CLA	CHC-C1C-C2C	-2.45	119.93	126.72
24	B	608	CLA	C3C-C4C-NC	2.45	113.32	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	513	CLA	C11-C10-C8	-2.45	107.99	115.92
24	A	410	CLA	C4C-C3C-C2C	-2.45	103.33	106.90
42	v	202	HEC	CMC-C2C-C1C	-2.45	124.70	128.46
24	C	501	CLA	C4C-C3C-C2C	-2.45	103.33	106.90
24	B	616	CLA	C4-C3-C5	2.45	119.39	115.27
24	B	602	CLA	C3B-C4B-NB	2.45	112.37	109.21
24	c	902	CLA	C4-C3-C5	2.44	119.38	115.27
24	b	611	CLA	CAA-C2A-C3A	-2.44	106.08	112.78
24	B	602	CLA	C4-C3-C5	2.44	119.38	115.27
36	b	602	HTG	O5-C5-C4	2.44	114.13	109.69
24	c	903	CLA	CMC-C2C-C1C	2.44	128.76	125.04
25	A	409	PHO	O2D-CGD-O1D	-2.44	119.06	123.84
36	B	629	HTG	O5-C5-C4	2.44	114.13	109.69
24	b	619	CLA	CED-O2D-CGD	2.44	121.45	115.94
39	f	101	HEM	C1B-NB-C4B	2.44	107.59	105.07
26	c	916	BCR	C15-C14-C13	-2.44	123.83	127.31
24	a	410	CLA	CHC-C1C-C2C	-2.44	119.98	126.72
24	C	506	CLA	CMC-C2C-C1C	2.44	128.75	125.04
24	b	612	CLA	C11-C10-C8	-2.44	108.05	115.92
24	c	908	CLA	C4C-C3C-C2C	-2.44	103.35	106.90
24	d	405	CLA	CBC-CAC-C3C	-2.43	105.72	112.43
24	C	512	CLA	C4-C3-C5	2.43	119.36	115.27
27	f	102	SQD	O47-C7-O49	-2.43	117.82	123.70
24	c	908	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
24	b	613	CLA	CED-O2D-CGD	2.43	121.44	115.94
24	b	619	CLA	C5-C3-C2	-2.43	116.20	121.12
24	b	612	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
24	d	404	CLA	CMA-C3A-C2A	-2.43	104.03	113.83
24	c	905	CLA	O1D-CGD-CBD	-2.43	119.52	124.48
37	D	405	DGD	O6D-C5D-C4D	2.43	114.10	109.69
24	C	511	CLA	CMB-C2B-C3B	2.43	129.22	124.68
24	d	401	CLA	C6-C5-C3	-2.43	107.09	113.45
26	K	101	BCR	C10-C11-C12	-2.43	115.65	123.22
24	b	618	CLA	CHD-C1D-ND	-2.43	122.22	124.45
24	b	611	CLA	O2A-CGA-CBA	2.42	119.52	111.91
24	C	509	CLA	CBC-CAC-C3C	-2.42	105.75	112.43
27	b	601	SQD	C44-O6-C1	-2.42	109.00	113.74
24	C	512	CLA	CBA-CAA-C2A	-2.42	106.71	113.86
24	a	413	CLA	CMB-C2B-C3B	2.42	129.21	124.68
27	b	601	SQD	O5-C5-C4	2.42	114.09	109.69
24	B	603	CLA	C11-C10-C8	-2.42	108.10	115.92
24	C	506	CLA	CHA-C1A-NA	-2.42	120.86	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	H	101	RRX	C29-C28-C27	-2.42	106.99	110.30
24	B	606	CLA	C1-C2-C3	-2.42	121.86	126.04
24	c	904	CLA	C3B-C4B-NB	2.42	112.33	109.21
24	C	512	CLA	C3B-C4B-NB	2.42	112.33	109.21
42	V	203	HEC	C1D-C2D-C3D	-2.42	105.31	107.00
24	b	619	CLA	O2D-CGD-CBD	2.41	115.56	111.27
24	b	612	CLA	CMB-C2B-C3B	2.41	129.19	124.68
24	B	608	CLA	CHD-C4C-C3C	-2.41	121.29	124.84
24	b	608	CLA	CHD-C1D-C2D	-2.41	120.42	125.48
24	b	617	CLA	O2D-CGD-CBD	2.41	115.55	111.27
24	B	608	CLA	CHC-C1C-C2C	-2.41	120.06	126.72
24	C	508	CLA	CHC-C1C-C2C	-2.41	120.06	126.72
24	c	904	CLA	C4-C3-C5	2.41	119.33	115.27
24	b	618	CLA	CMB-C2B-C3B	2.41	129.19	124.68
26	b	623	BCR	C2-C1-C6	2.41	114.19	110.48
24	b	618	CLA	CAA-C2A-C3A	-2.41	106.19	112.78
24	B	610	CLA	CED-O2D-CGD	2.41	121.38	115.94
26	c	916	BCR	C21-C20-C19	-2.41	115.71	123.22
24	b	612	CLA	CBC-CAC-C3C	-2.41	105.80	112.43
24	C	503	CLA	O2A-CGA-O1A	-2.40	117.52	123.59
28	C	523	LMG	O6-C5-C4	2.40	114.06	109.69
26	d	406	BCR	C15-C14-C13	-2.40	123.88	127.31
24	c	907	CLA	CGD-CBD-CAD	-2.40	102.95	110.73
24	B	615	CLA	C4C-C3C-C2C	-2.40	103.40	106.90
24	C	505	CLA	C3B-C4B-NB	2.40	112.31	109.21
24	C	512	CLA	CHD-C1D-ND	-2.40	122.25	124.45
24	B	611	CLA	CHA-C1A-NA	-2.40	120.91	126.40
24	C	508	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
28	C	523	LMG	C3-C4-C5	2.40	114.51	110.24
24	D	401	CLA	CHC-C1C-C2C	-2.40	120.09	126.72
28	a	416	LMG	C1-O6-C5	2.40	118.39	113.69
38	L	101	LHG	O8-C23-O10	-2.39	117.55	123.59
36	c	924	HTG	C1-O5-C5	2.39	117.00	112.58
36	c	941	HTG	C3-C4-C5	2.39	114.51	110.24
24	c	913	CLA	O1D-CGD-CBD	-2.39	119.59	124.48
31	Z	101	LMT	C1B-O1B-C4'	-2.39	112.04	117.96
36	D	412	HTG	O5-C5-C4	2.39	114.04	109.69
24	B	603	CLA	CMA-C3A-C2A	-2.39	104.18	113.83
24	B	611	CLA	C4-C3-C5	2.39	119.29	115.27
28	d	412	LMG	O7-C10-C11	2.39	116.65	111.50
24	b	606	CLA	C1-C2-C3	-2.39	121.91	126.04
24	B	612	CLA	C4C-C3C-C2C	-2.39	103.42	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	613	CLA	O2D-CGD-O1D	-2.38	119.17	123.84
24	c	907	CLA	CHC-C1C-C2C	-2.38	120.12	126.72
37	D	405	DGD	O2G-C1B-O1B	-2.38	117.94	123.70
38	D	407	LHG	O8-C23-O10	-2.38	117.58	123.59
24	a	409	CLA	O2D-CGD-CBD	2.38	115.50	111.27
24	c	907	CLA	CMB-C2B-C3B	2.38	129.14	124.68
31	a	402	LMT	C3B-C4B-C5B	2.38	114.49	110.24
26	T	101	BCR	C7-C6-C5	-2.38	115.69	121.46
24	D	402	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
24	B	611	CLA	CHD-C1D-ND	-2.38	122.27	124.45
24	c	909	CLA	CHD-C1D-C2D	-2.38	120.49	125.48
24	c	909	CLA	CHB-C4A-NA	2.38	127.80	124.51
29	A	414	PL9	C51-C49-C50	2.38	119.85	114.60
24	b	620	CLA	CHC-C1C-C2C	-2.38	120.15	126.72
36	O	303	HTG	O2-C2-C3	-2.38	104.86	110.35
31	b	625	LMT	C3'-C4'-C5'	2.38	116.37	110.93
24	c	909	CLA	CHD-C1D-ND	-2.37	122.27	124.45
24	B	602	CLA	CHD-C4C-NC	2.37	127.94	124.20
24	C	507	CLA	O2A-CGA-CBA	2.37	119.35	111.91
24	C	502	CLA	C1-O2A-CGA	2.37	122.67	116.44
24	C	513	CLA	C1-C2-C3	-2.37	121.94	126.04
40	h	101	RRX	C16-C15-C14	-2.37	118.62	123.47
24	c	914	CLA	CMC-C2C-C1C	2.37	128.65	125.04
29	a	417	PL9	C40-C39-C41	2.37	119.25	115.27
24	b	614	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
24	c	912	CLA	CHC-C1C-C2C	-2.37	120.18	126.72
24	b	613	CLA	C1-C2-C3	-2.36	121.95	126.04
24	d	401	CLA	CAA-CBA-CGA	2.36	120.16	113.25
24	b	612	CLA	OBD-CAD-C3D	-2.36	122.83	128.52
24	c	902	CLA	C4C-C3C-C2C	-2.36	103.45	106.90
24	c	904	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
26	Y	101	BCR	C24-C23-C22	-2.36	122.67	126.23
24	c	912	CLA	CAC-C3C-C4C	2.36	127.87	124.81
37	C	516	DGD	O6D-C5D-C6D	2.36	111.43	106.67
31	b	625	LMT	O1'-C1'-C2'	-2.36	104.62	108.30
24	B	602	CLA	CMC-C2C-C1C	2.36	128.63	125.04
24	b	610	CLA	O2A-CGA-CBA	2.36	119.31	111.91
26	C	514	BCR	C23-C24-C25	-2.36	120.58	127.20
28	C	523	LMG	O8-C28-C29	2.36	119.30	111.91
24	a	409	CLA	CMA-C3A-C2A	-2.36	104.32	113.83
24	C	506	CLA	CMB-C2B-C3B	2.36	129.09	124.68
24	b	611	CLA	CAC-C3C-C4C	2.36	127.87	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b	625	LMT	O2'-C2'-C1'	2.35	115.77	110.05
26	T	101	BCR	C3-C4-C5	-2.35	109.88	114.08
26	k	103	BCR	C3-C4-C5	-2.35	109.88	114.08
24	b	609	CLA	CMA-C3A-C4A	-2.35	105.45	111.77
24	C	501	CLA	C4-C3-C5	2.35	119.23	115.27
24	b	620	CLA	CMA-C3A-C4A	-2.35	105.45	111.77
26	T	101	BCR	C1-C6-C7	2.35	122.43	115.78
24	A	407	CLA	O2A-CGA-CBA	2.35	119.28	111.91
38	D	408	LHG	O8-C23-C24	2.35	119.28	111.91
24	b	605	CLA	CHA-C1A-NA	-2.35	121.02	126.40
24	c	909	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
38	D	407	LHG	O8-C23-C24	2.35	119.28	111.91
24	D	402	CLA	C1-C2-C3	-2.35	121.98	126.04
36	c	923	HTG	C1-O5-C5	2.35	116.91	112.58
31	B	622	LMT	O2'-C2'-C1'	-2.35	104.34	110.05
29	d	407	PL9	C53-C6-C1	2.35	119.79	114.99
24	B	610	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
24	B	607	CLA	CBC-CAC-C3C	-2.34	105.97	112.43
28	D	409	LMG	O7-C10-C11	2.34	116.55	111.50
29	a	417	PL9	C45-C44-C46	2.34	119.21	115.27
24	b	616	CLA	CED-O2D-CGD	2.34	121.23	115.94
24	B	607	CLA	CHA-C1A-NA	-2.34	121.03	126.40
24	C	502	CLA	O2A-C1-C2	2.34	114.79	108.64
24	c	910	CLA	O2A-CGA-CBA	2.34	119.25	111.91
28	D	409	LMG	C9-C8-C7	-2.34	106.25	111.79
27	b	601	SQD	O47-C7-O49	-2.34	118.05	123.70
24	b	618	CLA	CMA-C3A-C4A	-2.34	105.48	111.77
24	B	608	CLA	CMC-C2C-C1C	2.34	128.60	125.04
24	D	402	CLA	C3B-C4B-NB	2.34	112.23	109.21
24	c	908	CLA	CHA-C1A-NA	-2.34	121.05	126.40
29	a	417	PL9	C51-C49-C50	2.34	119.77	114.60
29	D	404	PL9	C25-C24-C26	2.34	119.20	115.27
26	T	101	BCR	C23-C24-C25	-2.34	120.64	127.20
24	c	912	CLA	O2A-CGA-CBA	2.34	119.24	111.91
24	B	607	CLA	CHD-C4C-NC	2.33	127.88	124.20
39	f	101	HEM	CMC-C2C-C3C	2.33	129.04	124.68
24	b	620	CLA	CHA-C1A-NA	-2.33	121.05	126.40
24	b	606	CLA	CAC-C3C-C4C	2.33	127.84	124.81
26	k	102	BCR	C23-C24-C25	-2.33	120.65	127.20
24	b	618	CLA	CED-O2D-CGD	2.33	121.21	115.94
38	D	406	LHG	O8-C6-C5	-2.33	101.65	108.43
24	c	914	CLA	O2A-CGA-CBA	2.33	119.22	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	c	919	DGD	O3G-C3G-C2G	-2.33	105.28	110.90
29	a	417	PL9	C35-C34-C36	2.33	119.19	115.27
24	A	410	CLA	CHD-C4C-NC	2.33	127.87	124.20
24	b	605	CLA	CAA-C2A-C3A	-2.33	106.41	112.78
37	H	102	DGD	C3G-C2G-C1G	-2.32	106.29	111.79
37	c	918	DGD	O1G-C1A-O1A	-2.32	117.72	123.59
26	B	619	BCR	C15-C16-C17	-2.32	118.71	123.47
24	B	605	CLA	CHA-C1A-NA	-2.32	121.08	126.40
24	b	619	CLA	C11-C10-C8	-2.32	108.41	115.92
24	c	911	CLA	CHC-C1C-C2C	-2.32	120.30	126.72
24	b	616	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
24	c	911	CLA	CMB-C2B-C3B	2.32	129.02	124.68
37	C	518	DGD	C2G-O2G-C1B	-2.32	112.08	117.79
24	c	902	CLA	C1-C2-C3	-2.32	122.03	126.04
31	M	102	LMT	C1-O1'-C1'	-2.32	110.00	113.84
37	D	405	DGD	C2G-O2G-C1B	-2.32	112.08	117.79
24	b	608	CLA	C4-C3-C5	2.32	119.17	115.27
26	T	101	BCR	C11-C10-C9	-2.32	124.00	127.31
24	d	401	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
24	B	603	CLA	CAA-CBA-CGA	-2.31	106.49	113.25
24	a	409	CLA	CMA-C3A-C4A	-2.31	105.55	111.77
27	A	416	SQD	O8-S-C6	2.31	109.43	105.74
24	B	609	CLA	CHD-C1D-ND	-2.31	122.33	124.45
26	B	636	BCR	C7-C6-C5	-2.31	115.86	121.46
38	D	406	LHG	O7-C7-O9	-2.31	118.11	123.70
24	b	606	CLA	C7-C6-C5	-2.31	107.08	113.36
29	D	404	PL9	C51-C49-C50	2.31	119.71	114.60
26	Y	101	BCR	C10-C11-C12	-2.31	116.01	123.22
24	B	603	CLA	CHC-C1C-C2C	-2.31	120.33	126.72
25	A	408	PHO	C4-C3-C5	2.31	119.16	115.27
25	A	408	PHO	O2D-CGD-O1D	-2.31	119.32	123.84
24	b	610	CLA	C5-C3-C2	-2.31	116.45	121.12
24	b	617	CLA	CMC-C2C-C1C	2.31	128.55	125.04
24	B	609	CLA	CHA-C1A-NA	-2.31	121.11	126.40
24	c	905	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
31	b	625	LMT	O5B-C5B-C4B	2.31	113.88	109.69
36	b	603	HTG	C1-O5-C5	2.31	116.83	112.58
24	B	617	CLA	CMA-C3A-C4A	-2.30	105.59	111.77
31	B	622	LMT	O2B-C2B-C1B	-2.30	104.45	110.05
24	b	611	CLA	CAA-CBA-CGA	2.30	119.97	113.25
37	H	102	DGD	O1G-C1A-O1A	-2.30	117.79	123.59
27	A	412	SQD	C44-O6-C1	-2.30	109.25	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	610	CLA	CMA-C3A-C4A	-2.30	105.60	111.77
24	c	910	CLA	C16-C17-C18	-2.30	105.16	115.98
24	C	501	CLA	C1-O2A-CGA	2.30	122.47	116.44
24	C	504	CLA	C4C-C3C-C2C	-2.30	103.55	106.90
24	B	610	CLA	CHA-C1A-NA	-2.29	121.14	126.40
24	C	511	CLA	CHC-C1C-C2C	-2.29	120.38	126.72
24	c	905	CLA	CHC-C1C-C2C	-2.29	120.38	126.72
26	b	621	BCR	C11-C10-C9	-2.29	124.04	127.31
36	d	414	HTG	C1-C2-C3	2.29	115.12	110.59
24	C	512	CLA	O2A-CGA-CBA	2.29	119.10	111.91
24	B	610	CLA	C4-C3-C5	2.29	119.12	115.27
24	C	502	CLA	CHD-C1D-ND	-2.29	122.35	124.45
24	d	404	CLA	CMA-C3A-C4A	-2.29	105.62	111.77
24	B	608	CLA	C4C-C3C-C2C	-2.29	103.56	106.90
24	b	620	CLA	C4-C3-C5	2.29	119.12	115.27
37	c	918	DGD	O1G-C1A-C2A	2.29	119.09	111.91
27	A	412	SQD	O48-C23-O10	-2.29	117.82	123.59
24	b	614	CLA	C11-C12-C13	-2.29	108.53	115.92
24	c	910	CLA	CHC-C1C-C2C	-2.29	120.40	126.72
24	c	905	CLA	C11-C10-C8	-2.28	108.54	115.92
26	B	620	BCR	C23-C24-C25	-2.28	120.79	127.20
24	b	618	CLA	CMC-C2C-C1C	2.28	128.51	125.04
24	b	615	CLA	CMA-C3A-C4A	-2.28	105.65	111.77
24	B	614	CLA	CMB-C2B-C3B	2.28	128.94	124.68
31	t	102	LMT	O1B-C1B-C2B	2.28	114.00	108.10
28	A	413	LMG	O6-C5-C4	2.28	113.83	109.69
24	B	604	CLA	CMC-C2C-C1C	2.27	128.50	125.04
24	C	506	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
26	K	101	BCR	C11-C10-C9	-2.27	124.07	127.31
24	A	405	CLA	O2A-CGA-CBA	2.27	119.03	111.91
31	c	922	LMT	C1'-C2'-C3'	-2.27	105.27	110.00
24	B	617	CLA	C4-C3-C5	2.27	119.09	115.27
26	B	620	BCR	C24-C23-C22	-2.27	122.80	126.23
24	c	902	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
25	a	411	PHO	C1-C2-C3	-2.27	122.12	126.04
24	c	903	CLA	CHA-C1A-NA	-2.27	121.20	126.40
24	C	507	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
24	b	615	CLA	OBD-CAD-C3D	-2.27	123.06	128.52
24	a	410	CLA	CMB-C2B-C3B	2.27	128.92	124.68
24	D	401	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
24	b	613	CLA	C3B-C4B-NB	2.27	112.14	109.21
26	k	102	BCR	C34-C9-C8	2.26	121.64	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	618	BCR	C15-C14-C13	-2.26	124.08	127.31
24	b	616	CLA	CAC-C3C-C4C	2.26	127.75	124.81
24	B	604	CLA	C4-C3-C5	2.26	119.08	115.27
37	C	517	DGD	O2G-C1B-O1B	-2.26	118.24	123.70
29	D	404	PL9	C27-C28-C29	-2.26	122.22	127.66
24	B	614	CLA	C7-C6-C5	-2.26	107.23	113.36
26	B	619	BCR	C3-C4-C5	-2.26	110.05	114.08
39	F	102	HEM	CMC-C2C-C3C	2.25	128.90	124.68
24	c	914	CLA	CAC-C3C-C4C	2.25	127.73	124.81
24	c	910	CLA	CHA-C1A-NA	-2.25	121.24	126.40
29	A	414	PL9	C12-C13-C14	-2.25	122.23	127.66
37	d	408	DGD	O1G-C1A-C2A	2.25	118.98	111.91
31	B	622	LMT	C3B-C4B-C5B	2.25	114.25	110.24
24	C	508	CLA	CAC-C3C-C4C	2.25	127.73	124.81
28	a	416	LMG	C3-C4-C5	2.25	114.25	110.24
24	B	607	CLA	O2A-C1-C2	-2.25	102.73	108.64
28	C	519	LMG	O8-C28-O10	-2.25	117.92	123.59
24	B	605	CLA	C6-C5-C3	-2.25	107.56	113.45
24	a	409	CLA	CBC-CAC-C3C	-2.25	106.24	112.43
24	B	607	CLA	CAA-C2A-C3A	-2.24	106.64	112.78
26	B	618	BCR	C21-C20-C19	-2.24	116.22	123.22
29	D	404	PL9	C31-C32-C33	-2.24	104.51	111.88
24	c	913	CLA	CAC-C3C-C2C	2.24	131.36	127.53
24	C	505	CLA	C1-O2A-CGA	2.24	122.32	116.44
24	B	617	CLA	CAA-CBA-CGA	-2.24	106.71	113.25
24	d	401	CLA	CHB-C4A-NA	2.24	127.61	124.51
24	C	510	CLA	CHA-C1A-NA	-2.24	121.27	126.40
24	a	413	CLA	CED-O2D-CGD	2.24	121.00	115.94
24	B	612	CLA	CAA-C2A-C3A	-2.24	106.65	112.78
37	H	102	DGD	C6D-C5D-C4D	2.24	116.77	112.09
26	B	620	BCR	C28-C27-C26	-2.24	110.08	114.08
24	A	407	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
38	d	409	LHG	C5-O7-C7	-2.23	112.29	117.79
24	B	605	CLA	CHC-C1C-C2C	-2.23	120.55	126.72
24	b	605	CLA	C1-C2-C3	-2.23	122.18	126.04
24	a	413	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
29	d	407	PL9	C35-C34-C36	2.23	119.02	115.27
39	F	102	HEM	C3B-C2B-C1B	2.23	108.14	106.49
24	b	605	CLA	CMB-C2B-C3B	2.23	128.85	124.68
36	B	629	HTG	C3-C4-C5	2.23	114.21	110.24
24	c	907	CLA	CHA-C1A-NA	-2.23	121.30	126.40
24	c	902	CLA	C1-O2A-CGA	2.22	122.28	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	620	CLA	O1D-CGD-CBD	-2.22	119.93	124.48
24	C	503	CLA	O2A-CGA-CBA	2.22	118.89	111.91
24	b	612	CLA	O2D-CGD-CBD	2.22	115.22	111.27
29	d	407	PL9	O1-C4-C3	-2.22	118.27	120.72
28	b	624	LMG	C30-C29-C28	-2.22	105.54	113.62
24	b	607	CLA	CMB-C2B-C3B	2.22	128.83	124.68
24	b	609	CLA	CHA-C1A-NA	-2.22	121.31	126.40
29	A	414	PL9	C25-C24-C23	-2.22	117.98	123.68
24	c	904	CLA	O2A-CGA-CBA	2.22	118.87	111.91
24	c	903	CLA	CHC-C1C-C2C	-2.22	120.59	126.72
24	C	511	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
24	c	908	CLA	C7-C6-C5	-2.22	107.34	113.36
24	b	613	CLA	CMA-C3A-C4A	-2.22	105.81	111.77
24	B	607	CLA	C6-C7-C8	-2.22	108.75	115.92
24	d	405	CLA	C6-C7-C8	-2.22	108.76	115.92
24	B	609	CLA	OBD-CAD-C3D	-2.22	123.19	128.52
24	b	616	CLA	O2D-CGD-O1D	-2.22	119.51	123.84
36	V	215	HTG	C1-C2-C3	2.21	114.96	110.59
25	A	408	PHO	C4A-C3A-C2A	-2.21	100.73	102.84
24	d	401	CLA	O2A-CGA-CBA	2.21	118.85	111.91
24	c	909	CLA	CAC-C3C-C2C	2.21	131.31	127.53
24	D	402	CLA	O2A-CGA-CBA	2.21	118.84	111.91
24	b	617	CLA	CBC-CAC-C3C	-2.21	106.34	112.43
26	b	623	BCR	C8-C7-C6	-2.21	121.00	127.20
24	C	513	CLA	CHC-C1C-C2C	-2.21	120.61	126.72
24	D	402	CLA	CHB-C4A-NA	2.21	127.56	124.51
28	A	413	LMG	O8-C28-C29	2.21	118.83	111.91
28	C	523	LMG	O6-C1-C2	2.21	115.02	110.35
24	A	405	CLA	O2D-CGD-CBD	2.21	115.19	111.27
24	b	620	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
24	d	404	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
37	c	917	DGD	O6D-C1D-O3G	-2.20	104.75	109.97
24	b	617	CLA	CHC-C1C-C2C	-2.20	120.63	126.72
38	D	406	LHG	C25-C24-C23	-2.20	105.61	113.62
37	H	102	DGD	C3B-C2B-C1B	-2.20	105.62	113.62
24	B	617	CLA	CHC-C1C-C2C	-2.20	120.63	126.72
26	d	406	BCR	C16-C15-C14	-2.20	118.97	123.47
24	b	613	CLA	CAC-C3C-C4C	2.20	127.67	124.81
27	a	415	SQD	O48-C23-O10	-2.20	118.04	123.59
26	C	515	BCR	C37-C22-C23	2.20	121.54	118.08
24	b	605	CLA	CMC-C2C-C1C	2.20	128.38	125.04
38	l	103	LHG	O8-C23-C24	2.20	118.80	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	401	CLA	CHA-C1A-NA	-2.20	121.37	126.40
24	b	615	CLA	C7-C6-C5	-2.19	107.40	113.36
24	c	912	CLA	CHD-C4C-NC	2.19	127.66	124.20
24	B	606	CLA	CAC-C3C-C4C	2.19	127.66	124.81
24	B	606	CLA	CMA-C3A-C2A	-2.19	104.98	113.83
24	b	619	CLA	C1-C2-C3	-2.19	122.25	126.04
24	C	507	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
24	A	410	CLA	C4-C3-C2	-2.19	118.07	123.68
26	b	622	BCR	C37-C22-C21	-2.19	119.86	122.92
24	c	906	CLA	O2A-CGA-CBA	2.19	118.77	111.91
24	B	609	CLA	CMA-C3A-C2A	-2.19	105.01	113.83
24	B	616	CLA	CHD-C4C-NC	2.19	127.65	124.20
24	A	405	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
24	B	613	CLA	O2A-CGA-CBA	2.18	118.76	111.91
31	B	622	LMT	C1B-O5B-C5B	2.18	117.98	113.69
24	C	512	CLA	CMC-C2C-C1C	2.18	128.36	125.04
24	d	405	CLA	CHC-C1C-C2C	-2.18	120.69	126.72
38	l	103	LHG	O4-P-O5	2.18	123.03	112.24
24	C	510	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
24	a	413	CLA	CHC-C1C-C2C	-2.18	120.69	126.72
24	c	910	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
26	Y	101	BCR	C21-C20-C19	-2.18	116.41	123.22
28	B	621	LMG	O7-C10-O9	-2.18	118.43	123.70
24	c	909	CLA	CMC-C2C-C1C	2.18	128.36	125.04
24	B	602	CLA	CMB-C2B-C3B	2.18	128.76	124.68
24	B	614	CLA	CMA-C3A-C2A	-2.18	105.04	113.83
24	b	619	CLA	CHC-C1C-C2C	-2.18	120.69	126.72
24	A	405	CLA	CHA-C1A-NA	-2.18	121.41	126.40
24	A	407	CLA	CHC-C1C-C2C	-2.18	120.70	126.72
24	b	605	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
24	c	904	CLA	C7-C6-C5	-2.17	107.45	113.36
26	D	403	BCR	C29-C28-C27	-2.17	106.52	111.38
24	b	615	CLA	O2A-CGA-O1A	-2.17	118.10	123.59
24	B	604	CLA	CHC-C1C-C2C	-2.17	120.71	126.72
24	C	506	CLA	O2A-CGA-CBA	2.17	118.73	111.91
24	C	502	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
24	c	909	CLA	C6-C7-C8	-2.17	108.90	115.92
38	d	409	LHG	O7-C7-O9	-2.17	118.46	123.70
27	A	416	SQD	O48-C23-O10	-2.17	118.12	123.59
24	b	615	CLA	O2A-CGA-CBA	2.17	118.71	111.91
24	b	614	CLA	O2A-CGA-CBA	2.17	118.71	111.91
27	b	601	SQD	O48-C23-O10	-2.17	118.12	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	619	BCR	C2-C1-C6	2.17	113.82	110.48
24	B	607	CLA	C5-C3-C2	-2.17	116.73	121.12
24	b	615	CLA	CHA-C1A-NA	-2.17	121.44	126.40
24	a	409	CLA	CMC-C2C-C1C	2.17	128.34	125.04
24	C	502	CLA	CMB-C2B-C3B	2.16	128.73	124.68
24	B	609	CLA	CHC-C1C-C2C	-2.16	120.74	126.72
24	B	605	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
24	A	406	CLA	O2A-CGA-CBA	2.16	118.69	111.91
24	b	606	CLA	CHC-C1C-C2C	-2.16	120.74	126.72
26	b	623	BCR	C28-C27-C26	-2.16	110.22	114.08
24	C	513	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
24	B	611	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
24	b	610	CLA	C6-C5-C3	-2.16	107.79	113.45
28	C	523	LMG	O7-C10-O9	-2.16	118.48	123.70
24	b	608	CLA	CHC-C1C-C2C	-2.16	120.75	126.72
29	a	417	PL9	C25-C24-C26	2.16	118.90	115.27
36	v	211	HTG	C1-O5-C5	-2.16	108.60	112.58
24	c	904	CLA	CBC-CAC-C3C	-2.16	106.48	112.43
24	C	506	CLA	CAC-C3C-C4C	2.16	127.61	124.81
24	d	401	CLA	CHC-C1C-NC	2.16	127.48	124.20
26	D	403	BCR	C30-C25-C24	2.16	121.88	115.78
24	C	512	CLA	C4A-NA-C1A	2.16	107.68	106.71
37	H	102	DGD	O4D-C4D-C3D	-2.16	105.36	110.35
24	B	608	CLA	CAA-CBA-CGA	2.15	119.55	113.25
24	B	602	CLA	CHA-C1A-NA	-2.15	121.47	126.40
24	B	605	CLA	CMC-C2C-C1C	2.15	128.32	125.04
24	b	616	CLA	CHD-C1D-C2D	-2.15	120.97	125.48
37	h	102	DGD	O1G-C1A-O1A	-2.15	118.16	123.59
24	C	501	CLA	C1-C2-C3	-2.15	122.32	126.04
24	c	914	CLA	CHD-C1D-ND	-2.15	122.48	124.45
24	B	612	CLA	C4-C3-C5	2.15	118.89	115.27
25	A	408	PHO	O1D-CGD-CBD	-2.15	121.16	124.74
24	c	909	CLA	CHC-C1C-C2C	-2.15	120.78	126.72
24	C	502	CLA	CHA-C1A-NA	-2.15	121.48	126.40
24	b	614	CLA	CHA-C1A-NA	-2.15	121.48	126.40
26	B	636	BCR	C3-C4-C5	-2.15	110.25	114.08
24	c	906	CLA	CMA-C3A-C4A	-2.15	106.00	111.77
24	B	608	CLA	C2A-C1A-CHA	-2.15	120.11	123.86
24	C	508	CLA	C1-C2-C3	-2.14	122.33	126.04
24	a	413	CLA	OBD-CAD-C3D	-2.14	123.36	128.52
24	B	604	CLA	C1-O2A-CGA	2.14	122.07	116.44
24	C	506	CLA	CHC-C1C-C2C	-2.14	120.80	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	c	920	LMG	O7-C10-O9	-2.14	118.53	123.70
24	B	602	CLA	CHC-C1C-C2C	-2.14	120.81	126.72
24	b	616	CLA	CHC-C1C-C2C	-2.14	120.81	126.72
24	C	504	CLA	O2A-CGA-CBA	2.14	118.61	111.91
24	c	906	CLA	C6-C7-C8	-2.14	109.01	115.92
29	d	407	PL9	C51-C49-C50	2.14	119.32	114.60
24	C	501	CLA	CHC-C1C-C2C	-2.14	120.81	126.72
24	B	606	CLA	CMA-C3A-C4A	-2.14	106.03	111.77
26	b	623	BCR	C16-C15-C14	-2.14	119.10	123.47
24	b	617	CLA	CHA-C1A-NA	-2.14	121.51	126.40
26	c	916	BCR	C23-C24-C25	-2.13	121.21	127.20
24	c	906	CLA	CHC-C1C-C2C	-2.13	120.82	126.72
24	b	615	CLA	C11-C12-C13	-2.13	109.03	115.92
24	B	603	CLA	CHA-C1A-NA	-2.13	121.52	126.40
38	l	103	LHG	O8-C23-O10	-2.13	118.21	123.59
24	D	402	CLA	CMA-C3A-C2A	-2.13	105.23	113.83
37	d	408	DGD	C4D-C3D-C2D	2.13	114.54	110.82
28	b	624	LMG	O8-C28-C29	2.13	118.59	111.91
24	b	611	CLA	C1-C2-C3	-2.13	122.36	126.04
28	D	409	LMG	C7-O1-C1	-2.13	109.58	113.74
24	B	606	CLA	OBD-CAD-C3D	-2.13	123.40	128.52
36	D	412	HTG	C1-O5-C5	2.13	116.50	112.58
24	C	504	CLA	C5-C3-C2	-2.13	116.81	121.12
24	c	905	CLA	OBD-CAD-C3D	-2.12	123.41	128.52
24	b	609	CLA	C7-C6-C5	-2.12	107.59	113.36
24	C	510	CLA	C6-C7-C8	-2.12	109.06	115.92
26	Y	101	BCR	C1-C6-C7	2.12	121.78	115.78
24	C	510	CLA	OBD-CAD-C3D	-2.12	123.41	128.52
24	c	908	CLA	C1-C2-C3	-2.12	122.37	126.04
26	b	622	BCR	C29-C28-C27	-2.12	106.64	111.38
27	b	601	SQD	O6-C44-C45	2.12	116.01	110.90
28	C	519	LMG	O7-C10-O9	-2.12	118.58	123.70
24	D	401	CLA	CMA-C3A-C2A	-2.12	105.28	113.83
36	B	625	HTG	C1-C2-C3	2.12	114.78	110.59
24	B	615	CLA	CMA-C3A-C2A	-2.12	105.28	113.83
24	B	610	CLA	CHD-C1D-C2D	-2.12	121.04	125.48
36	c	941	HTG	C1-C2-C3	-2.12	106.41	110.59
24	C	504	CLA	CMA-C3A-C4A	-2.12	106.08	111.77
24	B	614	CLA	CHA-C1A-NA	-2.12	121.55	126.40
24	C	509	CLA	CMC-C2C-C1C	2.12	128.26	125.04
24	C	512	CLA	CHC-C1C-C2C	-2.12	120.87	126.72
31	B	622	LMT	O1B-C4'-C5'	-2.12	103.65	109.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	605	CLA	C3B-C4B-NB	2.11	111.94	109.21
24	B	611	CLA	C1C-C2C-C3C	-2.11	104.73	106.96
24	B	611	CLA	CHB-C4A-NA	2.11	127.43	124.51
26	b	621	BCR	C28-C27-C26	-2.11	110.30	114.08
32	B	638	GOL	C3-C2-C1	-2.11	103.49	111.70
31	b	625	LMT	C1'-C2'-C3'	2.11	114.39	110.00
26	B	620	BCR	C7-C8-C9	-2.11	123.05	126.23
24	b	617	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
24	b	606	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
24	C	505	CLA	CHC-C1C-C2C	-2.11	120.89	126.72
24	b	615	CLA	CHD-C4C-NC	2.11	127.53	124.20
24	d	404	CLA	CMC-C2C-C1C	2.11	128.25	125.04
26	B	619	BCR	C38-C26-C25	-2.10	122.17	124.53
24	C	503	CLA	C3B-C4B-NB	2.10	111.93	109.21
24	A	406	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
24	c	911	CLA	C6-C7-C8	-2.10	109.13	115.92
24	a	410	CLA	CHA-C1A-NA	-2.10	121.59	126.40
24	c	913	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
29	d	407	PL9	C50-C49-C48	-2.10	116.58	122.65
37	C	517	DGD	O6E-C5E-C6E	2.10	111.65	106.44
31	c	927	LMT	O1B-C1B-C2B	2.10	113.53	108.10
24	B	610	CLA	O2D-CGD-CBD	2.10	114.99	111.27
24	c	902	CLA	O2A-CGA-CBA	2.10	118.48	111.91
26	C	514	BCR	C20-C21-C22	-2.10	124.32	127.31
26	b	623	BCR	C11-C10-C9	-2.10	124.32	127.31
24	b	607	CLA	C1-O2A-CGA	2.09	121.94	116.44
24	C	511	CLA	O2A-CGA-CBA	2.09	118.48	111.91
28	a	416	LMG	C8-O7-C10	-2.09	112.64	117.79
24	C	507	CLA	CMC-C2C-C1C	2.09	128.22	125.04
24	B	612	CLA	C7-C6-C5	-2.09	107.68	113.36
28	C	519	LMG	C12-C11-C10	-2.09	106.01	113.62
39	f	101	HEM	C3B-C2B-C1B	2.09	108.04	106.49
24	c	902	CLA	CHC-C1C-C2C	-2.09	120.94	126.72
24	d	405	CLA	O2A-CGA-CBA	2.09	118.47	111.91
42	V	203	HEC	CMB-C2B-C3B	2.09	128.28	125.82
24	c	910	CLA	CMB-C2B-C3B	2.09	128.59	124.68
24	B	611	CLA	CHD-C1D-C2D	-2.09	121.10	125.48
24	c	905	CLA	C11-C12-C13	-2.09	109.17	115.92
24	B	614	CLA	CHD-C4C-NC	2.09	127.50	124.20
24	B	605	CLA	CAA-CBA-CGA	-2.09	107.16	113.25
24	c	902	CLA	CMB-C2B-C3B	2.09	128.58	124.68
24	B	617	CLA	O1D-CGD-CBD	-2.09	120.22	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	903	CLA	CMB-C2B-C3B	2.08	128.58	124.68
24	c	911	CLA	CHA-C1A-NA	-2.08	121.62	126.40
31	m	103	LMT	C1-O1'-C1'	-2.08	110.38	113.84
24	D	401	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
24	b	607	CLA	CHC-C1C-C2C	-2.08	120.96	126.72
24	A	406	CLA	CAA-C2A-C1A	-2.08	105.15	111.97
36	c	942	HTG	O5-C5-C4	2.08	113.47	109.69
24	b	606	CLA	O2A-CGA-CBA	2.08	118.44	111.91
24	C	501	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
24	B	606	CLA	CHD-C4C-NC	2.08	127.48	124.20
25	A	409	PHO	C4-C3-C2	-2.08	118.34	123.68
24	B	617	CLA	CHA-C1A-NA	-2.08	121.64	126.40
24	C	509	CLA	CHC-C1C-C2C	-2.08	120.97	126.72
26	b	623	BCR	C21-C20-C19	-2.08	116.73	123.22
26	c	915	BCR	C21-C20-C19	-2.08	116.73	123.22
36	V	204	HTG	O2-C2-C1	2.08	114.08	110.27
37	c	918	DGD	O2G-C1B-O1B	-2.08	118.69	123.70
24	C	513	CLA	CMB-C2B-C3B	2.07	128.56	124.68
24	c	908	CLA	CHC-C1C-C2C	-2.07	120.98	126.72
24	C	503	CLA	C4-C3-C5	2.07	118.76	115.27
26	a	414	BCR	C24-C23-C22	-2.07	123.10	126.23
24	b	614	CLA	CAA-CBA-CGA	-2.07	107.20	113.25
36	b	626	HTG	C1-O5-C5	2.07	116.40	112.58
24	B	612	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
28	d	412	LMG	O8-C28-C29	2.07	118.41	111.91
24	b	607	CLA	C5-C3-C2	-2.07	116.93	121.12
24	B	613	CLA	CBC-CAC-C3C	-2.07	106.72	112.43
27	l	101	SQD	O47-C7-O49	-2.07	118.70	123.70
24	C	507	CLA	C1-O2A-CGA	2.07	121.87	116.44
24	c	912	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
37	d	408	DGD	C3G-C2G-C1G	-2.07	106.90	111.79
26	B	620	BCR	C3-C4-C5	-2.07	110.39	114.08
24	b	608	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
24	C	509	CLA	C4-C3-C5	2.06	118.74	115.27
24	C	512	CLA	OBD-CAD-C3D	-2.06	123.56	128.52
36	d	420	HTG	C1-O5-C5	2.06	116.38	112.58
24	C	510	CLA	C4-C3-C2	-2.06	118.39	123.68
37	d	408	DGD	O2G-C1B-O1B	-2.06	118.72	123.70
38	D	408	LHG	O4-P-O5	2.06	122.42	112.24
36	c	942	HTG	C6-C5-C4	-2.06	108.19	113.00
24	c	913	CLA	CHB-C4A-NA	2.06	127.36	124.51
29	D	404	PL9	O2-C1-C6	-2.06	117.03	120.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	414	PL9	O1-C4-C3	-2.06	118.46	120.72
28	D	409	LMG	O8-C28-O10	-2.06	118.40	123.59
24	b	609	CLA	CHC-C1C-C2C	-2.06	121.04	126.72
24	C	509	CLA	CAC-C3C-C4C	2.06	127.48	124.81
24	c	914	CLA	CMA-C3A-C4A	-2.05	106.25	111.77
24	B	611	CLA	CMC-C2C-C1C	2.05	128.16	125.04
24	D	402	CLA	CHC-C1C-C2C	-2.05	121.05	126.72
28	a	416	LMG	O7-C10-O9	-2.05	118.75	123.70
24	c	905	CLA	C1-O2A-CGA	2.05	121.83	116.44
29	D	404	PL9	C10-C9-C11	2.05	118.72	115.27
26	k	102	BCR	C1-C6-C7	2.05	121.58	115.78
24	c	914	CLA	CHA-C1A-NA	-2.05	121.70	126.40
26	b	621	BCR	C10-C11-C12	-2.05	116.83	123.22
24	C	501	CLA	CMB-C2B-C3B	2.05	128.51	124.68
24	b	605	CLA	CHD-C4C-NC	2.05	127.43	124.20
38	l	103	LHG	C10-C9-C8	-2.05	105.83	113.19
24	A	405	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
24	B	605	CLA	O2D-CGD-O1D	-2.05	119.84	123.84
25	a	411	PHO	CMA-C3A-C4A	-2.04	109.90	114.38
31	c	927	LMT	O5B-C1B-C2B	-2.04	106.02	110.35
24	B	603	CLA	O2A-C1-C2	-2.04	103.26	108.64
38	d	411	LHG	O7-C7-O9	-2.04	118.76	123.70
24	b	613	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
28	a	416	LMG	O8-C28-C29	2.04	118.31	111.91
37	C	517	DGD	C9B-C8B-C7B	-2.04	104.06	114.42
24	B	610	CLA	C1-O2A-CGA	2.04	121.80	116.44
36	c	942	HTG	C3-C4-C5	2.04	113.88	110.24
28	A	413	LMG	C8-O7-C10	-2.04	112.77	117.79
24	C	502	CLA	OBD-CAD-C3D	-2.04	123.61	128.52
29	D	404	PL9	C15-C14-C16	2.04	118.70	115.27
24	c	905	CLA	CMB-C2B-C3B	2.04	128.49	124.68
24	c	903	CLA	CBC-CAC-C3C	-2.04	106.81	112.43
36	b	627	HTG	C3-C4-C5	-2.04	106.60	110.24
24	B	612	CLA	C1-O2A-CGA	2.04	121.79	116.44
26	d	406	BCR	C10-C11-C12	-2.04	116.86	123.22
24	a	413	CLA	CAC-C3C-C4C	2.04	127.45	124.81
24	B	606	CLA	C7-C6-C5	-2.04	107.83	113.36
24	A	407	CLA	CHD-C4C-NC	2.03	127.41	124.20
29	d	407	PL9	C45-C44-C46	2.03	118.69	115.27
24	b	609	CLA	O2A-CGA-CBA	2.03	118.29	111.91
24	b	611	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
24	A	407	CLA	CMA-C3A-C2A	-2.03	105.64	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	902	CLA	CHD-C4C-NC	2.03	127.40	124.20
24	c	905	CLA	O2A-CGA-CBA	2.03	118.27	111.91
24	b	608	CLA	C11-C12-C13	-2.03	109.36	115.92
24	c	911	CLA	CHD-C1D-ND	-2.03	122.59	124.45
28	B	621	LMG	O4-C4-C3	-2.03	105.67	110.35
28	c	921	LMG	O7-C10-O9	-2.03	118.81	123.70
24	B	614	CLA	CHC-C1C-C2C	-2.02	121.12	126.72
26	C	514	BCR	C8-C7-C6	-2.02	121.52	127.20
24	B	602	CLA	CAC-C3C-C4C	2.02	127.43	124.81
26	b	621	BCR	C16-C17-C18	-2.02	124.43	127.31
26	b	623	BCR	C33-C5-C6	-2.02	122.26	124.53
31	a	402	LMT	O5 <sup>1</sup> -C5 <sup>1</sup> -C4 <sup>1</sup>	2.02	114.01	109.75
37	D	405	DGD	C3G-C2G-C1G	-2.02	107.01	111.79
24	d	405	CLA	CMA-C3A-C4A	-2.02	106.34	111.77
31	m	103	LMT	C1B-O1B-C4 <sup>1</sup>	-2.02	112.97	117.96
37	c	919	DGD	O1G-C1A-O1A	-2.02	118.50	123.59
40	h	101	RRX	C33-C5-C6	-2.02	122.26	124.53
24	c	908	CLA	CAC-C3C-C4C	2.02	127.43	124.81
24	C	511	CLA	C4A-NA-C1A	2.02	107.61	106.71
31	M	101	LMT	C1 <sup>1</sup> -O5 <sup>1</sup> -C5 <sup>1</sup>	-2.01	109.73	113.69
31	B	622	LMT	C3 <sup>1</sup> -C4 <sup>1</sup> -C5 <sup>1</sup>	2.01	115.54	110.93
26	Y	101	BCR	C37-C22-C23	2.01	121.25	118.08
24	C	509	CLA	CHA-C1A-NA	-2.01	121.79	126.40
24	a	413	CLA	CHB-C4A-NA	2.01	127.30	124.51
26	d	406	BCR	C40-C30-C25	-2.01	107.03	110.30
26	b	623	BCR	C2-C3-C4	-2.01	106.89	111.38
25	a	411	PHO	C7-C6-C5	-2.01	107.90	113.36
24	c	913	CLA	CMA-C3A-C4A	-2.01	106.37	111.77
29	A	414	PL9	C40-C39-C41	2.01	118.65	115.27
24	c	908	CLA	CHD-C4C-NC	2.01	127.37	124.20
24	d	404	CLA	CBC-CAC-C3C	-2.01	106.90	112.43
24	c	903	CLA	CHD-C4C-NC	2.01	127.37	124.20
24	c	905	CLA	C2A-C1A-CHA	-2.01	120.35	123.86
24	c	902	CLA	CHA-C1A-NA	-2.01	121.81	126.40
36	B	630	HTG	C4-C3-C2	-2.01	107.32	110.82
24	c	906	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
24	b	608	CLA	C1-C2-C3	-2.00	122.58	126.04
27	A	412	SQD	O9-S-O7	-2.00	107.02	113.95
24	C	508	CLA	CHA-C1A-NA	-2.00	121.81	126.40
28	A	413	LMG	O7-C10-O9	-2.00	118.86	123.70
24	D	401	CLA	OBD-CAD-C3D	-2.00	123.70	128.52
26	Y	101	BCR	C16-C15-C14	-2.00	119.38	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	903	CLA	C4-C3-C5	2.00	118.64	115.27
36	B	625	HTG	C3-C4-C5	-2.00	106.67	110.24

All (61) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	405	CLA	ND
24	B	602	CLA	ND
24	B	603	CLA	ND
24	B	604	CLA	ND
24	B	605	CLA	ND
24	B	606	CLA	ND
24	B	607	CLA	ND
24	B	608	CLA	ND
24	B	610	CLA	ND
24	B	611	CLA	ND
24	B	612	CLA	ND
24	B	613	CLA	ND
24	B	614	CLA	ND
24	B	615	CLA	ND
24	B	616	CLA	ND
24	B	617	CLA	ND
24	C	501	CLA	ND
24	C	503	CLA	ND
24	C	504	CLA	ND
24	C	505	CLA	ND
24	C	506	CLA	ND
24	C	507	CLA	ND
24	C	508	CLA	ND
24	C	509	CLA	ND
24	C	510	CLA	ND
24	C	511	CLA	ND
24	C	512	CLA	ND
24	D	401	CLA	ND
24	D	402	CLA	ND
24	a	409	CLA	ND
24	a	413	CLA	ND
24	b	605	CLA	ND
24	b	606	CLA	ND
24	b	607	CLA	ND
24	b	608	CLA	ND
24	b	609	CLA	ND

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Mol	Chain	Res	Type	Atom
24	b	610	CLA	ND
24	b	611	CLA	ND
24	b	613	CLA	ND
24	b	614	CLA	ND
24	b	615	CLA	ND
24	b	616	CLA	ND
24	b	617	CLA	ND
24	b	618	CLA	ND
24	b	619	CLA	ND
24	b	620	CLA	ND
24	c	902	CLA	ND
24	c	903	CLA	ND
24	c	904	CLA	ND
24	c	905	CLA	ND
24	c	906	CLA	ND
24	c	907	CLA	ND
24	c	908	CLA	ND
24	c	909	CLA	ND
24	c	910	CLA	ND
24	c	911	CLA	ND
24	c	913	CLA	ND
24	c	914	CLA	ND
24	d	401	CLA	ND
24	d	404	CLA	ND
24	d	405	CLA	ND

All (1032) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	406	CLA	CHA-CBD-CGD-O1D
24	B	606	CLA	C2-C3-C5-C6
24	B	606	CLA	C4-C3-C5-C6
24	B	607	CLA	CHA-CBD-CGD-O1D
24	B	607	CLA	CHA-CBD-CGD-O2D
24	B	615	CLA	CHA-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O2D
24	C	508	CLA	CHA-CBD-CGD-O1D
24	C	513	CLA	C1A-C2A-CAA-CBA
24	C	513	CLA	C3A-C2A-CAA-CBA
24	b	610	CLA	CHA-CBD-CGD-O1D
24	b	610	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	b	618	CLA	CHA-CBD-CGD-O1D
24	b	618	CLA	CHA-CBD-CGD-O2D
24	b	618	CLA	CAD-CBD-CGD-O1D
24	b	618	CLA	CAD-CBD-CGD-O2D
24	c	909	CLA	CHA-CBD-CGD-O1D
24	c	909	CLA	CHA-CBD-CGD-O2D
24	d	405	CLA	C2-C3-C5-C6
24	d	405	CLA	C4-C3-C5-C6
26	D	403	BCR	C7-C8-C9-C34
26	D	403	BCR	C21-C22-C23-C24
26	D	403	BCR	C37-C22-C23-C24
26	Y	101	BCR	C21-C22-C23-C24
26	Y	101	BCR	C37-C22-C23-C24
26	d	406	BCR	C37-C22-C23-C24
27	A	416	SQD	O6-C44-C45-O47
27	A	416	SQD	C5-C6-S-O8
27	a	401	SQD	O6-C44-C45-O47
27	a	401	SQD	O5-C5-C6-S
27	b	601	SQD	O5-C1-O6-C44
27	b	601	SQD	O49-C7-O47-C45
27	f	102	SQD	O49-C7-O47-C45
27	f	102	SQD	C8-C7-O47-C45
27	f	102	SQD	C5-C6-S-O7
27	l	101	SQD	O5-C1-O6-C44
27	l	101	SQD	O49-C7-O47-C45
28	A	413	LMG	C2-C1-O1-C7
28	A	413	LMG	O6-C1-O1-C7
28	a	416	LMG	O9-C10-O7-C8
28	a	416	LMG	C11-C10-O7-C8
29	A	414	PL9	C14-C16-C17-C18
29	A	414	PL9	C25-C24-C26-C27
29	a	417	PL9	C28-C29-C31-C32
29	a	417	PL9	C30-C29-C31-C32
31	A	417	LMT	C2'-C1'-O1'-C1
31	A	417	LMT	O5'-C1'-O1'-C1
31	A	421	LMT	C2'-C1'-O1'-C1
31	A	421	LMT	O5'-C1'-O1'-C1
31	B	626	LMT	C2'-C1'-O1'-C1
31	B	626	LMT	O5'-C1'-O1'-C1
31	F	103	LMT	C2'-C1'-O1'-C1
31	F	103	LMT	O5'-C1'-O1'-C1
31	J	102	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
31	J	102	LMT	O5'-C1'-O1'-C1
31	M	102	LMT	C2'-C1'-O1'-C1
31	M	102	LMT	O5'-C1'-O1'-C1
31	a	402	LMT	O5'-C1'-O1'-C1
31	b	625	LMT	C2'-C1'-O1'-C1
31	b	625	LMT	O5'-C1'-O1'-C1
31	c	922	LMT	C2'-C1'-O1'-C1
31	c	922	LMT	O5'-C1'-O1'-C1
31	c	927	LMT	C2'-C1'-O1'-C1
31	c	927	LMT	O5'-C1'-O1'-C1
31	c	927	LMT	C2-C1-O1'-C1'
31	e	101	LMT	C2'-C1'-O1'-C1
31	e	101	LMT	O5'-C1'-O1'-C1
31	j	102	LMT	C2'-C1'-O1'-C1
31	j	102	LMT	O5'-C1'-O1'-C1
31	m	102	LMT	C2-C1-O1'-C1'
31	t	101	LMT	C2-C1-O1'-C1'
31	t	102	LMT	C2'-C1'-O1'-C1
31	t	102	LMT	O5'-C1'-O1'-C1
32	A	419	GOL	O1-C1-C2-C3
32	B	637	GOL	C1-C2-C3-O3
32	V	206	GOL	C1-C2-C3-O3
32	a	419	GOL	O1-C1-C2-C3
32	c	929	GOL	O1-C1-C2-C3
36	B	625	HTG	O5-C1-S1-C1'
36	C	520	HTG	C2'-C1'-S1-C1
36	V	204	HTG	O5-C1-S1-C1'
36	V	215	HTG	O5-C1-S1-C1'
36	b	627	HTG	O5-C1-S1-C1'
36	c	942	HTG	C2-C1-S1-C1'
36	c	942	HTG	O5-C1-S1-C1'
36	y	102	HTG	C2-C1-S1-C1'
36	y	102	HTG	O5-C1-S1-C1'
36	y	102	HTG	C2'-C1'-S1-C1
37	D	405	DGD	C2B-C1B-O2G-C2G
37	D	405	DGD	O1B-C1B-O2G-C2G
37	d	408	DGD	C2B-C1B-O2G-C2G
37	d	408	DGD	C2D-C1D-O3G-C3G
37	d	408	DGD	O6D-C1D-O3G-C3G
38	E	101	LHG	O7-C5-C6-O8
38	L	101	LHG	C4-O6-P-O3
38	L	101	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
38	L	101	LHG	C4-O6-P-O5
38	d	409	LHG	O1-C1-C2-C3
38	l	103	LHG	C4-O6-P-O3
38	l	103	LHG	C4-O6-P-O4
38	l	103	LHG	C4-O6-P-O5
31	b	625	LMT	C3'-C4'-O1B-C1B
31	t	102	LMT	O5B-C1B-O1B-C4'
31	B	622	LMT	C3'-C4'-O1B-C1B
31	t	102	LMT	C2B-C1B-O1B-C4'
37	d	408	DGD	O1A-C1A-O1G-C1G
37	d	408	DGD	O1B-C1B-O2G-C2G
27	b	601	SQD	C8-C7-O47-C45
27	l	101	SQD	C8-C7-O47-C45
37	D	405	DGD	O6D-C5D-C6D-O5D
37	D	405	DGD	C4D-C5D-C6D-O5D
24	B	607	CLA	C2A-CAA-CBA-CGA
37	d	408	DGD	C2A-C1A-O1G-C1G
31	m	103	LMT	C1-C2-C3-C4
26	B	636	BCR	C13-C14-C15-C16
26	T	101	BCR	C13-C14-C15-C16
31	c	927	LMT	O5B-C5B-C6B-O6B
31	t	102	LMT	O5'-C5'-C6'-O6'
24	D	402	CLA	C3-C5-C6-C7
31	M	101	LMT	O5B-C5B-C6B-O6B
36	d	420	HTG	O5-C5-C6-O6
24	B	604	CLA	C5-C6-C7-C8
24	c	904	CLA	C10-C11-C12-C13
24	b	618	CLA	C4-C3-C5-C6
29	a	417	PL9	C20-C19-C21-C22
24	b	618	CLA	C2-C3-C5-C6
29	A	414	PL9	C23-C24-C26-C27
29	a	417	PL9	C18-C19-C21-C22
36	B	625	HTG	O5-C5-C6-O6
36	V	204	HTG	O5-C5-C6-O6
36	b	627	HTG	O5-C5-C6-O6
29	D	404	PL9	C39-C41-C42-C43
31	c	927	LMT	C4B-C5B-C6B-O6B
24	c	907	CLA	C13-C15-C16-C17
36	B	625	HTG	C4-C5-C6-O6
36	b	627	HTG	C4-C5-C6-O6
24	A	410	CLA	C13-C15-C16-C17
27	F	101	SQD	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
27	l	101	SQD	C23-C24-C25-C26
24	A	410	CLA	C11-C12-C13-C14
24	B	617	CLA	C14-C13-C15-C16
24	C	509	CLA	C11-C10-C8-C9
24	c	910	CLA	C6-C7-C8-C9
24	C	504	CLA	C10-C11-C12-C13
26	d	406	BCR	C21-C22-C23-C24
27	l	101	SQD	C7-C8-C9-C10
37	C	518	DGD	C1A-C2A-C3A-C4A
37	c	918	DGD	C1A-C2A-C3A-C4A
24	c	907	CLA	C15-C16-C17-C18
24	B	617	CLA	C5-C6-C7-C8
24	C	507	CLA	C15-C16-C17-C18
24	b	618	CLA	C5-C6-C7-C8
24	b	619	CLA	C5-C6-C7-C8
37	d	408	DGD	C1B-C2B-C3B-C4B
31	c	927	LMT	O5B-C1B-O1B-C4'
36	d	414	HTG	O5-C5-C6-O6
24	B	616	CLA	C5-C6-C7-C8
24	c	908	CLA	C5-C6-C7-C8
32	O	304	GOL	O2-C2-C3-O3
38	d	409	LHG	O1-C1-C2-O2
27	f	102	SQD	C23-C24-C25-C26
28	a	416	LMG	C10-C11-C12-C13
37	d	408	DGD	C1A-C2A-C3A-C4A
24	C	508	CLA	C5-C6-C7-C8
24	B	617	CLA	C12-C13-C15-C16
24	b	610	CLA	C2A-CAA-CBA-CGA
24	D	402	CLA	C8-C10-C11-C12
31	t	102	LMT	C4'-C5'-C6'-O6'
31	Z	101	LMT	O5'-C1'-O1'-C1
29	a	417	PL9	C9-C11-C12-C13
36	V	204	HTG	C4-C5-C6-O6
24	B	617	CLA	C10-C11-C12-C13
24	c	904	CLA	C5-C6-C7-C8
24	c	910	CLA	C8-C10-C11-C12
38	E	101	LHG	C4-O6-P-O3
36	c	941	HTG	C1'-C2'-C3'-C4'
29	A	414	PL9	C20-C19-C21-C22
31	c	927	LMT	C2B-C1B-O1B-C4'
27	f	102	SQD	C7-C8-C9-C10
31	Z	101	LMT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
37	c	919	DGD	CBA-CCA-CDA-CEA
38	L	101	LHG	C14-C15-C16-C17
24	A	406	CLA	C2C-C3C-CAC-CBC
28	C	519	LMG	C30-C31-C32-C33
28	C	519	LMG	C37-C38-C39-C40
28	D	409	LMG	C20-C21-C22-C23
31	Z	101	LMT	C3-C4-C5-C6
37	c	918	DGD	CAA-CBA-CCA-CDA
38	l	103	LHG	C14-C15-C16-C17
28	B	621	LMG	C17-C18-C19-C20
28	B	621	LMG	C33-C34-C35-C36
28	b	624	LMG	C17-C18-C19-C20
28	b	624	LMG	C33-C34-C35-C36
37	D	405	DGD	C8B-C9B-CAB-CBB
37	H	102	DGD	C6A-C7A-C8A-C9A
38	L	101	LHG	C27-C28-C29-C30
24	C	510	CLA	C8-C10-C11-C12
28	d	412	LMG	C15-C16-C17-C18
37	C	517	DGD	C9A-CAA-CBA-CCA
37	c	917	DGD	C9A-CAA-CBA-CCA
37	h	102	DGD	C6A-C7A-C8A-C9A
27	A	412	SQD	C9-C10-C11-C12
36	b	626	HTG	C3'-C4'-C5'-C6'
37	H	102	DGD	C9A-CAA-CBA-CCA
38	D	406	LHG	C29-C30-C31-C32
38	l	103	LHG	C27-C28-C29-C30
31	B	626	LMT	O1'-C1-C2-C3
31	j	102	LMT	O1'-C1-C2-C3
37	c	918	DGD	CCB-CDB-CEB-CFB
31	Z	101	LMT	C2'-C1'-O1'-C1
28	A	413	LMG	C37-C38-C39-C40
28	C	519	LMG	C17-C18-C19-C20
36	B	624	HTG	C3'-C4'-C5'-C6'
37	H	102	DGD	CCA-CDA-CEA-CFA
38	d	411	LHG	C29-C30-C31-C32
24	C	508	CLA	C13-C15-C16-C17
24	D	402	CLA	C16-C17-C18-C19
27	A	416	SQD	C14-C15-C16-C17
28	B	621	LMG	C15-C16-C17-C18
28	d	412	LMG	C20-C21-C22-C23
37	D	405	DGD	C7B-C8B-C9B-CAB
38	d	411	LHG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
24	C	504	CLA	C11-C10-C8-C9
24	a	410	CLA	C6-C7-C8-C9
24	c	905	CLA	C14-C13-C15-C16
27	A	416	SQD	C16-C17-C18-C19
28	b	624	LMG	C15-C16-C17-C18
37	D	405	DGD	C3B-C4B-C5B-C6B
24	B	602	CLA	C2A-CAA-CBA-CGA
26	k	102	BCR	C37-C22-C23-C24
27	f	102	SQD	C28-C29-C30-C31
32	B	637	GOL	O1-C1-C2-C3
32	B	638	GOL	O1-C1-C2-C3
32	B	638	GOL	C1-C2-C3-O3
32	O	304	GOL	C1-C2-C3-O3
32	V	206	GOL	O1-C1-C2-C3
36	D	412	HTG	C1'-C2'-C3'-C4'
38	D	406	LHG	O1-C1-C2-C3
38	d	411	LHG	O1-C1-C2-C3
24	B	607	CLA	C13-C15-C16-C17
28	A	413	LMG	C13-C14-C15-C16
27	a	401	SQD	C33-C34-C35-C36
28	A	413	LMG	C38-C39-C40-C41
28	B	621	LMG	C29-C30-C31-C32
37	C	517	DGD	CAB-CBB-CCB-CDB
37	c	918	DGD	C3A-C4A-C5A-C6A
38	L	101	LHG	C13-C14-C15-C16
38	l	103	LHG	C13-C14-C15-C16
28	a	416	LMG	O6-C1-O1-C7
27	F	101	SQD	C9-C10-C11-C12
31	M	102	LMT	O1'-C1-C2-C3
37	C	518	DGD	C3A-C4A-C5A-C6A
37	D	405	DGD	C6B-C7B-C8B-C9B
38	D	406	LHG	C25-C26-C27-C28
38	d	409	LHG	C27-C28-C29-C30
27	a	401	SQD	C24-C25-C26-C27
28	b	624	LMG	C39-C40-C41-C42
31	t	102	LMT	C5-C6-C7-C8
37	C	516	DGD	C3B-C4B-C5B-C6B
37	c	919	DGD	C2A-C3A-C4A-C5A
24	b	620	CLA	C10-C11-C12-C13
27	b	601	SQD	C15-C16-C17-C18
38	L	101	LHG	C31-C32-C33-C34
31	A	421	LMT	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
28	A	413	LMG	C11-C12-C13-C14
28	B	621	LMG	C35-C36-C37-C38
38	d	409	LHG	C29-C30-C31-C32
24	B	610	CLA	C3A-C2A-CAA-CBA
31	a	402	LMT	C2-C1-O1'-C1'
31	b	625	LMT	C2-C1-O1'-C1'
27	a	401	SQD	C30-C31-C32-C33
27	a	415	SQD	C34-C35-C36-C37
28	B	621	LMG	C39-C40-C41-C42
38	d	410	LHG	C30-C31-C32-C33
38	l	103	LHG	C31-C32-C33-C34
37	D	405	DGD	CAB-CBB-CCB-CDB
38	d	409	LHG	C30-C31-C32-C33
24	a	413	CLA	C3-C5-C6-C7
31	c	927	LMT	O1'-C1-C2-C3
29	a	417	PL9	C25-C24-C26-C27
29	d	407	PL9	C43-C44-C46-C47
28	c	920	LMG	C36-C37-C38-C39
32	A	419	GOL	O1-C1-C2-O2
32	B	637	GOL	O1-C1-C2-O2
32	B	638	GOL	O1-C1-C2-O2
32	a	419	GOL	O1-C1-C2-O2
32	c	929	GOL	O1-C1-C2-O2
28	B	621	LMG	C14-C15-C16-C17
37	h	102	DGD	C7A-C8A-C9A-CAA
27	l	101	SQD	C28-C29-C30-C31
24	c	909	CLA	C13-C15-C16-C17
38	D	406	LHG	C28-C29-C30-C31
31	c	927	LMT	C1-C2-C3-C4
24	B	602	CLA	CBA-CGA-O2A-C1
31	b	625	LMT	C1-C2-C3-C4
27	b	601	SQD	C13-C14-C15-C16
26	B	618	BCR	C1-C6-C7-C8
26	B	618	BCR	C5-C6-C7-C8
26	D	403	BCR	C23-C24-C25-C26
26	D	403	BCR	C23-C24-C25-C30
26	Y	101	BCR	C1-C6-C7-C8
26	Y	101	BCR	C5-C6-C7-C8
26	d	406	BCR	C23-C24-C25-C26
26	d	406	BCR	C23-C24-C25-C30
26	k	102	BCR	C1-C6-C7-C8
26	k	102	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	a	401	SQD	C34-C35-C36-C37
28	b	624	LMG	C14-C15-C16-C17
24	B	616	CLA	C10-C11-C12-C13
31	B	622	LMT	C1-C2-C3-C4
38	E	101	LHG	C8-C7-O7-C5
31	A	417	LMT	C2-C3-C4-C5
37	C	518	DGD	CBA-CCA-CDA-CEA
37	c	917	DGD	C6A-C7A-C8A-C9A
27	b	601	SQD	C31-C32-C33-C34
28	a	416	LMG	C13-C14-C15-C16
31	F	103	LMT	C4-C5-C6-C7
24	B	602	CLA	C4-C3-C5-C6
29	a	417	PL9	C15-C14-C16-C17
24	B	602	CLA	C2-C3-C5-C6
24	C	504	CLA	C11-C12-C13-C15
24	C	506	CLA	C6-C7-C8-C10
24	c	905	CLA	C12-C13-C15-C16
29	a	417	PL9	C13-C14-C16-C17
37	C	517	DGD	C6A-C7A-C8A-C9A
24	b	618	CLA	C10-C11-C12-C13
27	a	415	SQD	C12-C13-C14-C15
37	c	918	DGD	CBA-CCA-CDA-CEA
28	b	624	LMG	C35-C36-C37-C38
31	J	102	LMT	O1'-C1-C2-C3
37	c	918	DGD	C9A-CAA-CBA-CCA
31	A	417	LMT	C3-C4-C5-C6
31	c	927	LMT	C4-C5-C6-C7
36	C	537	HTG	C3'-C4'-C5'-C6'
37	h	102	DGD	C5B-C6B-C7B-C8B
27	a	415	SQD	C11-C12-C13-C14
27	a	415	SQD	C15-C16-C17-C18
37	D	405	DGD	C2B-C3B-C4B-C5B
37	C	516	DGD	C1B-C2B-C3B-C4B
38	D	406	LHG	C7-C8-C9-C10
28	A	413	LMG	C11-C10-O7-C8
28	C	519	LMG	C11-C10-O7-C8
37	c	919	DGD	C6B-C7B-C8B-C9B
24	b	607	CLA	C5-C6-C7-C8
28	C	519	LMG	O9-C10-O7-C8
38	E	101	LHG	O9-C7-O7-C5
36	B	629	HTG	O5-C5-C6-O6
27	F	101	SQD	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
27	f	102	SQD	C33-C34-C35-C36
37	d	408	DGD	CBB-CCB-CDB-CEB
31	c	922	LMT	O5'-C5'-C6'-O6'
29	d	407	PL9	C45-C44-C46-C47
29	A	414	PL9	C18-C19-C21-C22
24	A	410	CLA	C6-C7-C8-C9
24	C	508	CLA	C11-C10-C8-C9
24	C	509	CLA	C14-C13-C15-C16
24	c	909	CLA	C14-C13-C15-C16
37	H	102	DGD	C7A-C8A-C9A-CAA
31	m	103	LMT	C11-C10-C9-C8
31	c	927	LMT	C5-C6-C7-C8
24	B	602	CLA	O1A-CGA-O2A-C1
24	B	602	CLA	C1A-C2A-CAA-CBA
24	B	610	CLA	C1A-C2A-CAA-CBA
24	B	612	CLA	C1A-C2A-CAA-CBA
24	C	511	CLA	C1A-C2A-CAA-CBA
24	c	907	CLA	C1A-C2A-CAA-CBA
36	B	630	HTG	O5-C5-C6-O6
27	A	416	SQD	C13-C14-C15-C16
31	B	626	LMT	C1-C2-C3-C4
28	c	920	LMG	C28-C29-C30-C31
37	C	516	DGD	O6E-C5E-C6E-O5E
28	C	519	LMG	C35-C36-C37-C38
38	L	101	LHG	O6-C4-C5-C6
37	C	518	DGD	C9A-CAA-CBA-CCA
36	b	626	HTG	C2'-C3'-C4'-C5'
37	C	518	DGD	CAA-CBA-CCA-CDA
37	c	917	DGD	O6E-C5E-C6E-O5E
24	D	402	CLA	C16-C17-C18-C20
31	M	102	LMT	C4-C5-C6-C7
28	C	523	LMG	C4-C5-C6-O5
38	D	407	LHG	C1-C2-C3-O3
29	A	414	PL9	C13-C14-C16-C17
31	B	626	LMT	C6-C7-C8-C9
36	C	520	HTG	C2'-C3'-C4'-C5'
28	D	409	LMG	C11-C12-C13-C14
28	a	416	LMG	C36-C37-C38-C39
37	D	405	DGD	CDA-CEA-CFA-CGA
24	B	603	CLA	C15-C16-C17-C18
27	A	416	SQD	O6-C44-C45-C46
27	a	401	SQD	O6-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
36	C	536	HTG	C1'-C2'-C3'-C4'
37	c	918	DGD	C2G-C3G-O3G-C1D
37	c	918	DGD	C5D-C6D-O5D-C1E
28	a	416	LMG	C15-C16-C17-C18
28	a	416	LMG	O6-C5-C6-O5
24	C	503	CLA	C15-C16-C17-C18
24	c	911	CLA	C8-C10-C11-C12
36	v	211	HTG	C4'-C5'-C6'-C7'
37	C	516	DGD	C4B-C5B-C6B-C7B
28	d	412	LMG	O6-C5-C6-O5
32	B	638	GOL	O2-C2-C3-O3
31	M	101	LMT	C4B-C5B-C6B-O6B
36	b	602	HTG	O5-C5-C6-O6
37	C	516	DGD	O6D-C5D-C6D-O5D
24	b	620	CLA	C4-C3-C5-C6
29	A	414	PL9	C15-C14-C16-C17
28	C	523	LMG	C17-C18-C19-C20
28	a	416	LMG	C40-C41-C42-C43
37	C	517	DGD	C1B-C2B-C3B-C4B
28	D	409	LMG	O6-C5-C6-O5
31	B	626	LMT	O5'-C5'-C6'-O6'
36	D	412	HTG	O5-C5-C6-O6
24	C	509	CLA	C2-C1-O2A-CGA
36	d	414	HTG	C4-C5-C6-O6
31	a	402	LMT	C3-C4-C5-C6
37	c	918	DGD	CDB-CEB-CFB-CGB
37	c	918	DGD	C7A-C8A-C9A-CAA
37	D	405	DGD	C2D-C1D-O3G-C3G
27	l	101	SQD	C9-C10-C11-C12
28	C	519	LMG	O1-C7-C8-O7
28	a	416	LMG	O7-C8-C9-O8
37	c	919	DGD	CBB-CCB-CDB-CEB
28	A	413	LMG	O9-C10-O7-C8
38	d	410	LHG	C35-C36-C37-C38
38	l	103	LHG	C28-C29-C30-C31
29	A	414	PL9	C30-C29-C31-C32
24	A	410	CLA	C6-C7-C8-C10
24	B	616	CLA	C12-C13-C15-C16
24	C	508	CLA	C11-C10-C8-C7
24	C	509	CLA	C12-C13-C15-C16
24	b	618	CLA	C6-C7-C8-C10
24	b	620	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	b	620	CLA	C11-C12-C13-C15
24	c	909	CLA	C12-C13-C15-C16
29	a	417	PL9	C23-C24-C26-C27
38	L	101	LHG	C28-C29-C30-C31
24	B	602	CLA	C6-C7-C8-C9
24	B	604	CLA	C6-C7-C8-C9
24	B	617	CLA	C11-C10-C8-C9
24	C	507	CLA	C14-C13-C15-C16
24	b	619	CLA	C11-C10-C8-C9
24	b	620	CLA	C11-C12-C13-C14
24	c	907	CLA	C14-C13-C15-C16
24	c	908	CLA	C11-C10-C8-C9
37	C	516	DGD	C2A-C3A-C4A-C5A
37	D	405	DGD	CBB-CCB-CDB-CEB
36	d	420	HTG	C4-C5-C6-O6
26	D	403	BCR	C7-C8-C9-C10
26	k	102	BCR	C21-C22-C23-C24
28	B	621	LMG	C40-C41-C42-C43
36	D	412	HTG	C4'-C5'-C6'-C7'
31	M	102	LMT	C1-C2-C3-C4
37	C	518	DGD	C7A-C8A-C9A-CAA
37	h	102	DGD	CDA-CEA-CFA-CGA
27	a	401	SQD	C11-C10-C9-C8
38	d	410	LHG	C11-C10-C9-C8
38	l	103	LHG	O6-C4-C5-C6
38	D	408	LHG	C30-C31-C32-C33
24	c	914	CLA	C10-C11-C12-C13
37	c	917	DGD	CBA-CCA-CDA-CEA
29	d	407	PL9	C40-C39-C41-C42
29	A	414	PL9	C28-C29-C31-C32
37	C	516	DGD	CDA-CEA-CFA-CGA
38	D	407	LHG	O2-C2-C3-O3
28	C	523	LMG	C29-C30-C31-C32
28	d	412	LMG	C14-C15-C16-C17
37	H	102	DGD	C5B-C6B-C7B-C8B
31	B	622	LMT	C2-C1-O1'-C1'
31	Z	101	LMT	C2-C1-O1'-C1'
27	b	601	SQD	C26-C27-C28-C29
28	c	920	LMG	C10-C11-C12-C13
27	b	601	SQD	C44-C45-C46-O48
27	f	102	SQD	C44-C45-C46-O48
27	l	101	SQD	C44-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
28	a	416	LMG	C7-C8-C9-O8
24	d	401	CLA	C2C-C3C-CAC-CBC
37	c	919	DGD	C5B-C6B-C7B-C8B
37	d	408	DGD	CDB-CEB-CFB-CGB
31	M	102	LMT	C11-C10-C9-C8
38	d	411	LHG	C28-C29-C30-C31
28	C	519	LMG	C36-C37-C38-C39
37	H	102	DGD	CDA-CEA-CFA-CGA
32	V	206	GOL	O2-C2-C3-O3
37	c	919	DGD	C9B-CAB-CBB-CCB
38	d	409	LHG	C23-C24-C25-C26
37	C	516	DGD	C4A-C5A-C6A-C7A
31	a	402	LMT	C9-C10-C11-C12
27	A	412	SQD	O6-C44-C45-O47
27	f	102	SQD	O47-C45-C46-O48
37	C	518	DGD	CDB-CEB-CFB-CGB
24	b	612	CLA	C13-C15-C16-C17
28	B	621	LMG	C18-C19-C20-C21
38	d	410	LHG	C28-C29-C30-C31
24	d	404	CLA	C2-C1-O2A-CGA
36	O	316	HTG	C2'-C3'-C4'-C5'
24	a	413	CLA	C5-C6-C7-C8
27	F	101	SQD	C12-C13-C14-C15
31	b	625	LMT	C11-C10-C9-C8
37	d	408	DGD	CCB-CDB-CEB-CFB
24	b	614	CLA	C2A-CAA-CBA-CGA
26	b	621	BCR	C1-C6-C7-C8
26	b	621	BCR	C5-C6-C7-C8
26	c	916	BCR	C1-C6-C7-C8
26	c	916	BCR	C5-C6-C7-C8
40	H	101	RRX	C23-C24-C25-C30
24	B	607	CLA	C8-C10-C11-C12
24	B	617	CLA	C8-C10-C11-C12
28	c	920	LMG	C20-C21-C22-C23
24	c	909	CLA	C16-C17-C18-C20
28	b	624	LMG	C28-C29-C30-C31
27	F	101	SQD	C11-C12-C13-C14
28	b	624	LMG	C18-C19-C20-C21
37	h	102	DGD	O2G-C1B-C2B-C3B
24	B	602	CLA	C6-C7-C8-C10
24	B	604	CLA	C6-C7-C8-C10
24	B	616	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
24	B	617	CLA	C11-C10-C8-C7
24	C	506	CLA	C12-C13-C15-C16
24	C	507	CLA	C12-C13-C15-C16
24	C	513	CLA	C12-C13-C15-C16
24	a	410	CLA	C6-C7-C8-C10
24	a	413	CLA	C11-C10-C8-C7
24	b	618	CLA	C12-C13-C15-C16
24	b	619	CLA	C11-C10-C8-C7
24	c	907	CLA	C12-C13-C15-C16
24	c	908	CLA	C11-C10-C8-C7
24	c	913	CLA	C12-C13-C15-C16
28	c	920	LMG	C14-C15-C16-C17
37	H	102	DGD	CAA-CBA-CCA-CDA
27	F	101	SQD	O47-C45-C46-O48
37	C	517	DGD	C7A-C8A-C9A-CAA
31	B	622	LMT	C11-C10-C9-C8
38	D	407	LHG	C32-C33-C34-C35
37	H	102	DGD	O2G-C1B-C2B-C3B
28	B	621	LMG	C36-C37-C38-C39
24	B	617	CLA	CAD-CBD-CGD-O2D
24	C	503	CLA	CAD-CBD-CGD-O2D
24	b	608	CLA	CAD-CBD-CGD-O2D
24	c	904	CLA	CAD-CBD-CGD-O2D
24	c	907	CLA	CAD-CBD-CGD-O2D
24	c	910	CLA	CAD-CBD-CGD-O2D
24	c	913	CLA	CAD-CBD-CGD-O2D
24	d	405	CLA	CAD-CBD-CGD-O2D
27	b	601	SQD	C46-C45-O47-C7
37	C	516	DGD	C7B-C8B-C9B-CAB
28	C	523	LMG	C16-C17-C18-C19
28	C	523	LMG	O6-C1-O1-C7
24	a	413	CLA	C8-C10-C11-C12
29	d	407	PL9	C38-C39-C41-C42
27	b	601	SQD	C11-C10-C9-C8
25	a	412	PHO	C2C-C3C-CAC-CBC
28	C	519	LMG	C7-C8-C9-O8
38	E	101	LHG	C4-C5-C6-O8
36	B	623	HTG	C4-C5-C6-O6
28	A	413	LMG	C29-C30-C31-C32
37	c	917	DGD	O6D-C5D-C6D-O5D
27	A	416	SQD	C24-C23-O48-C46
27	F	101	SQD	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
24	B	602	CLA	CHA-CBD-CGD-O1D
24	B	602	CLA	CHA-CBD-CGD-O2D
24	C	502	CLA	CHA-CBD-CGD-O1D
24	C	502	CLA	CHA-CBD-CGD-O2D
24	C	507	CLA	CHA-CBD-CGD-O1D
24	C	507	CLA	CHA-CBD-CGD-O2D
24	C	508	CLA	CHA-CBD-CGD-O2D
24	b	605	CLA	CHA-CBD-CGD-O1D
24	c	908	CLA	CHA-CBD-CGD-O1D
24	c	908	CLA	CHA-CBD-CGD-O2D
31	a	402	LMT	C6-C7-C8-C9
27	b	601	SQD	O47-C45-C46-O48
27	l	101	SQD	O47-C45-C46-O48
28	d	412	LMG	C36-C37-C38-C39
38	D	408	LHG	C28-C29-C30-C31
37	C	517	DGD	C8A-C9A-CAA-CBA
38	D	406	LHG	O1-C1-C2-O2
36	C	537	HTG	C2'-C3'-C4'-C5'
27	l	101	SQD	C24-C25-C26-C27
31	a	402	LMT	C4-C5-C6-C7
27	A	412	SQD	C7-C8-C9-C10
24	C	505	CLA	C2-C3-C5-C6
24	b	619	CLA	C8-C10-C11-C12
24	C	506	CLA	C11-C10-C8-C9
24	b	618	CLA	C14-C13-C15-C16
24	c	913	CLA	C14-C13-C15-C16
37	C	516	DGD	C4D-C5D-C6D-O5D
37	H	102	DGD	C6B-C7B-C8B-C9B
27	f	102	SQD	C5-C6-S-O8
37	C	517	DGD	C6B-C7B-C8B-C9B
31	b	625	LMT	C6-C7-C8-C9
32	V	207	GOL	O1-C1-C2-C3
36	C	521	HTG	S1-C1'-C2'-C3'
31	B	626	LMT	C7-C8-C9-C10
36	B	629	HTG	C4'-C5'-C6'-C7'
24	c	909	CLA	C1A-C2A-CAA-CBA
27	a	401	SQD	C25-C26-C27-C28
38	D	408	LHG	C2-C3-O3-P
38	d	411	LHG	C2-C3-O3-P
36	b	602	HTG	C2'-C3'-C4'-C5'
24	C	511	CLA	O1A-CGA-O2A-C1
27	A	416	SQD	O10-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
38	E	101	LHG	C4-O6-P-O5
24	c	903	CLA	C16-C17-C18-C20
31	M	101	LMT	C1-C2-C3-C4
24	B	602	CLA	C5-C6-C7-C8
24	b	608	CLA	C13-C15-C16-C17
31	F	103	LMT	C3-C4-C5-C6
37	C	518	DGD	CAB-CBB-CCB-CDB
24	B	614	CLA	C15-C16-C17-C18
24	A	405	CLA	C2C-C3C-CAC-CBC
28	a	416	LMG	C17-C18-C19-C20
31	m	102	LMT	O1'-C1-C2-C3
37	d	408	DGD	CAA-CBA-CCA-CDA
24	B	602	CLA	CAD-CBD-CGD-O1D
24	B	610	CLA	CAD-CBD-CGD-O1D
24	C	502	CLA	CAD-CBD-CGD-O1D
24	b	605	CLA	CAD-CBD-CGD-O1D
24	b	609	CLA	CAD-CBD-CGD-O1D
24	c	903	CLA	CAD-CBD-CGD-O1D
27	A	416	SQD	C5-C6-S-O7
27	A	416	SQD	C5-C6-S-O9
27	f	102	SQD	C5-C6-S-O9
36	B	624	HTG	C2'-C3'-C4'-C5'
36	C	520	HTG	S1-C1'-C2'-C3'
28	d	412	LMG	C35-C36-C37-C38
31	Z	101	LMT	O1'-C1-C2-C3
27	a	401	SQD	C28-C29-C30-C31
36	d	419	HTG	C2'-C3'-C4'-C5'
38	D	406	LHG	C11-C10-C9-C8
24	C	507	CLA	C11-C10-C8-C7
24	b	617	CLA	C12-C13-C15-C16
24	c	906	CLA	C12-C13-C15-C16
24	c	907	CLA	C11-C10-C8-C7
36	C	521	HTG	C2-C1-S1-C1'
36	O	316	HTG	C2-C1-S1-C1'
38	L	101	LHG	O6-C4-C5-O7
38	l	103	LHG	O6-C4-C5-O7
37	C	518	DGD	CBB-CCB-CDB-CEB
37	h	102	DGD	CDB-CEB-CFB-CGB
24	A	406	CLA	C4C-C3C-CAC-CBC
28	c	920	LMG	C39-C40-C41-C42
27	a	401	SQD	C15-C16-C17-C18
28	A	413	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
37	c	917	DGD	C8A-C9A-CAA-CBA
27	a	415	SQD	O6-C44-C45-O47
27	b	601	SQD	O6-C44-C45-O47
28	A	413	LMG	O1-C7-C8-O7
28	C	519	LMG	O7-C8-C9-O8
38	D	408	LHG	C14-C15-C16-C17
37	C	517	DGD	C2G-C3G-O3G-C1D
37	C	517	DGD	C5D-C6D-O5D-C1E
24	B	617	CLA	C16-C17-C18-C19
37	c	918	DGD	CBB-CCB-CDB-CEB
27	l	101	SQD	C11-C10-C9-C8
24	B	616	CLA	C14-C13-C15-C16
24	C	512	CLA	C11-C12-C13-C14
24	C	513	CLA	C14-C13-C15-C16
24	a	413	CLA	C11-C10-C8-C9
24	b	618	CLA	C6-C7-C8-C9
24	c	904	CLA	C11-C10-C8-C9
24	a	409	CLA	C2C-C3C-CAC-CBC
32	B	637	GOL	O2-C2-C3-O3
28	A	413	LMG	C35-C36-C37-C38
36	d	420	HTG	C2'-C3'-C4'-C5'
27	l	101	SQD	C16-C17-C18-C19
24	b	610	CLA	C10-C11-C12-C13
37	c	918	DGD	C5A-C6A-C7A-C8A
27	A	412	SQD	O49-C7-O47-C45
37	C	517	DGD	C2A-C3A-C4A-C5A
37	D	405	DGD	CAA-CBA-CCA-CDA
36	c	943	HTG	C1'-C2'-C3'-C4'
37	d	408	DGD	CCA-CDA-CEA-CFA
24	b	619	CLA	C16-C17-C18-C19
27	A	412	SQD	C11-C12-C13-C14
28	a	416	LMG	C16-C17-C18-C19
27	a	401	SQD	C19-C20-C21-C22
27	l	101	SQD	C26-C27-C28-C29
28	C	523	LMG	C35-C36-C37-C38
27	l	101	SQD	C46-C45-O47-C7
31	B	622	LMT	C5'-C4'-O1B-C1B
28	B	621	LMG	O9-C10-O7-C8
31	t	101	LMT	O1'-C1-C2-C3
37	c	917	DGD	C4D-C5D-C6D-O5D
37	d	408	DGD	C3A-C4A-C5A-C6A
24	b	615	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
26	C	515	BCR	C23-C24-C25-C30
40	H	101	RRX	C23-C24-C25-C26
36	d	414	HTG	C4'-C5'-C6'-C7'
28	a	416	LMG	O8-C28-C29-C30
24	c	909	CLA	C16-C17-C18-C19
27	A	412	SQD	C8-C7-O47-C45
28	B	621	LMG	C11-C10-O7-C8
27	b	601	SQD	C9-C10-C11-C12
27	l	101	SQD	C12-C13-C14-C15
37	C	517	DGD	C3A-C4A-C5A-C6A
37	c	917	DGD	C2A-C3A-C4A-C5A
27	a	401	SQD	C2-C1-O6-C44
28	C	523	LMG	O1-C7-C8-O7
38	D	407	LHG	C3-O3-P-O6
38	d	410	LHG	C3-O3-P-O6
37	c	918	DGD	CAB-CBB-CCB-CDB
38	E	101	LHG	C14-C15-C16-C17
27	a	415	SQD	O6-C44-C45-C46
28	C	519	LMG	O1-C7-C8-C9
27	a	401	SQD	C9-C10-C11-C12
31	a	402	LMT	C11-C10-C9-C8
24	b	607	CLA	C6-C7-C8-C10
37	d	408	DGD	C2A-C3A-C4A-C5A
37	D	405	DGD	CCA-CDA-CEA-CFA
24	c	907	CLA	C11-C10-C8-C9
24	b	615	CLA	C16-C17-C18-C19
27	b	601	SQD	C16-C17-C18-C19
24	B	616	CLA	C8-C10-C11-C12
28	c	921	LMG	O6-C5-C6-O5
27	a	401	SQD	C23-C24-C25-C26
28	A	413	LMG	C21-C22-C23-C24
37	h	102	DGD	CBB-CCB-CDB-CEB
24	B	613	CLA	C13-C15-C16-C17
24	b	606	CLA	C8-C10-C11-C12
38	d	410	LHG	C1-C2-C3-O3
24	A	410	CLA	C4-C3-C5-C6
32	V	206	GOL	O1-C1-C2-O2
38	d	411	LHG	O1-C1-C2-O2
27	A	412	SQD	C30-C31-C32-C33
27	b	601	SQD	C35-C36-C37-C38
31	A	417	LMT	C4-C5-C6-C7
36	O	303	HTG	C2'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
27	a	401	SQD	O5-C1-O6-C44
37	c	918	DGD	O6E-C1E-O5D-C6D
27	b	601	SQD	C10-C11-C12-C13
24	B	610	CLA	C2-C3-C5-C6
25	a	411	PHO	C2-C3-C5-C6
31	A	421	LMT	C7-C8-C9-C10
38	l	103	LHG	C17-C18-C19-C20
24	B	614	CLA	C2-C1-O2A-CGA
37	C	517	DGD	C2E-C1E-O5D-C6D
37	D	405	DGD	O1G-C1G-C2G-O2G
31	t	102	LMT	O5B-C5B-C6B-O6B
37	c	917	DGD	CAB-CBB-CCB-CDB
38	l	103	LHG	C12-C13-C14-C15
24	b	611	CLA	C3A-C2A-CAA-CBA
24	b	612	CLA	C3A-C2A-CAA-CBA
24	B	616	CLA	C16-C17-C18-C19
28	c	920	LMG	C37-C38-C39-C40
38	l	103	LHG	C10-C11-C12-C13
24	B	610	CLA	C4-C3-C5-C6
25	a	411	PHO	C4-C3-C5-C6
37	C	516	DGD	C8A-C9A-CAA-CBA
38	L	101	LHG	C17-C18-C19-C20
29	A	414	PL9	C4-C3-C7-C8
29	a	417	PL9	C4-C3-C7-C8
24	B	617	CLA	C6-C7-C8-C9
24	C	506	CLA	C14-C13-C15-C16
24	b	617	CLA	C14-C13-C15-C16
24	b	620	CLA	C11-C10-C8-C9
24	b	619	CLA	C16-C17-C18-C20
36	d	414	HTG	C2'-C3'-C4'-C5'
37	c	917	DGD	C6B-C7B-C8B-C9B
27	a	401	SQD	C18-C19-C20-C21
31	M	102	LMT	C7-C8-C9-C10
36	O	303	HTG	C3'-C4'-C5'-C6'
27	A	412	SQD	O6-C44-C45-C46
37	D	405	DGD	O1G-C1G-C2G-C3G
24	b	606	CLA	C3-C5-C6-C7
28	C	523	LMG	C14-C15-C16-C17
31	A	417	LMT	C4'-C5'-C6'-O6'
24	B	617	CLA	C16-C17-C18-C20
37	C	517	DGD	O6E-C1E-O5D-C6D
28	A	413	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
28	B	621	LMG	C31-C32-C33-C34
38	L	101	LHG	C10-C11-C12-C13
24	C	509	CLA	C16-C17-C18-C20
24	A	407	CLA	C12-C13-C15-C16
24	D	401	CLA	C12-C13-C15-C16
24	a	410	CLA	C11-C10-C8-C7
24	b	606	CLA	C6-C7-C8-C10
24	c	910	CLA	C12-C13-C15-C16
28	A	413	LMG	C31-C32-C33-C34
38	d	409	LHG	C3-O3-P-O6
31	B	626	LMT	C5-C6-C7-C8
31	c	922	LMT	O1'-C1-C2-C3
38	L	101	LHG	C12-C13-C14-C15
24	b	616	CLA	C8-C10-C11-C12
37	h	102	DGD	C9B-CAB-CBB-CCB
31	e	101	LMT	C1-C2-C3-C4
38	d	411	LHG	C11-C10-C9-C8
24	A	405	CLA	C4C-C3C-CAC-CBC
38	d	410	LHG	O2-C2-C3-O3
24	d	401	CLA	C4C-C3C-CAC-CBC
24	b	609	CLA	C8-C10-C11-C12
28	b	624	LMG	C40-C41-C42-C43
31	t	102	LMT	C6-C7-C8-C9
24	b	606	CLA	C13-C15-C16-C17
27	F	101	SQD	C44-C45-C46-O48
24	A	410	CLA	C3-C5-C6-C7
24	a	409	CLA	C2-C1-O2A-CGA
24	a	413	CLA	C2-C1-O2A-CGA
36	B	623	HTG	O5-C5-C6-O6
24	B	607	CLA	C11-C12-C13-C14
24	b	607	CLA	C6-C7-C8-C9
28	b	624	LMG	O9-C10-O7-C8
24	B	616	CLA	C16-C17-C18-C20
38	E	101	LHG	O10-C23-O8-C6
26	A	411	BCR	C1-C6-C7-C8
26	C	514	BCR	C1-C6-C7-C8
26	C	515	BCR	C1-C6-C7-C8
26	K	101	BCR	C1-C6-C7-C8
26	c	915	BCR	C1-C6-C7-C8
26	k	103	BCR	C1-C6-C7-C8
24	B	609	CLA	C13-C15-C16-C17
28	C	519	LMG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
28	b	624	LMG	C31-C32-C33-C34
24	B	614	CLA	C10-C11-C12-C13
38	d	411	LHG	C33-C34-C35-C36
38	D	408	LHG	O10-C23-O8-C6
40	H	101	RRX	C9-C10-C11-C12
40	h	101	RRX	C9-C10-C11-C12
29	a	417	PL9	C45-C44-C46-C47
25	A	408	PHO	C2-C3-C5-C6
24	B	603	CLA	C8-C10-C11-C12
37	C	516	DGD	C5D-C6D-O5D-C1E
37	c	917	DGD	C5D-C6D-O5D-C1E
27	l	101	SQD	C27-C28-C29-C30
42	v	202	HEC	CAD-CBD-CGD-O2D
28	A	413	LMG	C18-C19-C20-C21
31	A	421	LMT	C3-C4-C5-C6
37	d	408	DGD	C4A-C5A-C6A-C7A
24	C	511	CLA	CBA-CGA-O2A-C1
37	d	408	DGD	CDA-CEA-CFA-CGA
37	c	917	DGD	C1B-C2B-C3B-C4B
27	f	102	SQD	C25-C26-C27-C28
42	V	203	HEC	CAD-CBD-CGD-O2D
42	v	202	HEC	CAD-CBD-CGD-O1D
24	C	506	CLA	C4-C3-C5-C6
24	c	914	CLA	C4-C3-C5-C6
24	A	410	CLA	C11-C12-C13-C15
24	B	611	CLA	C11-C10-C8-C7
24	b	606	CLA	C15-C16-C17-C18
37	c	918	DGD	C2E-C1E-O5D-C6D
27	l	101	SQD	C24-C23-O48-C46
27	l	101	SQD	O48-C23-C24-C25
28	a	416	LMG	C32-C33-C34-C35
24	B	616	CLA	C4-C3-C5-C6
24	C	513	CLA	C4-C3-C5-C6
24	D	402	CLA	C4-C3-C5-C6
24	c	905	CLA	C4-C3-C5-C6
37	C	516	DGD	C9A-CAA-CBA-CCA
42	V	203	HEC	CAD-CBD-CGD-O1D
24	B	612	CLA	C2-C3-C5-C6
24	C	507	CLA	C11-C10-C8-C9
24	b	614	CLA	C11-C12-C13-C14
24	c	903	CLA	C14-C13-C15-C16
24	c	906	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	c	910	CLA	C14-C13-C15-C16
24	B	609	CLA	C3A-C2A-CAA-CBA
37	h	102	DGD	C9A-CAA-CBA-CCA
37	d	408	DGD	O1G-C1A-C2A-C3A
24	B	604	CLA	CAD-CBD-CGD-O2D
24	B	605	CLA	CAD-CBD-CGD-O2D
24	B	611	CLA	CAD-CBD-CGD-O2D
24	B	613	CLA	CAD-CBD-CGD-O2D
24	B	614	CLA	CAD-CBD-CGD-O2D
24	C	501	CLA	CAD-CBD-CGD-O2D
24	C	512	CLA	CAD-CBD-CGD-O2D
24	b	614	CLA	CAD-CBD-CGD-O2D
24	b	616	CLA	CAD-CBD-CGD-O2D
24	c	914	CLA	CAD-CBD-CGD-O2D
25	A	408	PHO	CAD-CBD-CGD-O2D
25	a	411	PHO	CAD-CBD-CGD-O2D
24	c	903	CLA	C16-C17-C18-C19
27	l	101	SQD	O10-C23-O48-C46
37	C	516	DGD	C7A-C8A-C9A-CAA
31	B	626	LMT	C3-C4-C5-C6
37	c	919	DGD	O1G-C1A-C2A-C3A
26	c	916	BCR	C7-C8-C9-C10
29	d	407	PL9	C39-C41-C42-C43
38	d	410	LHG	C33-C34-C35-C36
28	C	523	LMG	O1-C7-C8-C9
38	E	101	LHG	C26-C27-C28-C29
31	A	421	LMT	C11-C10-C9-C8
24	C	512	CLA	O2A-C1-C2-C3
24	b	605	CLA	O2A-C1-C2-C3
24	b	606	CLA	O2A-C1-C2-C3
24	c	910	CLA	O2A-C1-C2-C3
24	d	404	CLA	O2A-C1-C2-C3
25	A	408	PHO	O2A-C1-C2-C3
25	a	411	PHO	O2A-C1-C2-C3
24	a	409	CLA	C4C-C3C-CAC-CBC
37	h	102	DGD	C6B-C7B-C8B-C9B
38	D	408	LHG	C19-C20-C21-C22
28	a	416	LMG	O7-C10-C11-C12
24	A	406	CLA	CHA-CBD-CGD-O2D
24	A	407	CLA	CHA-CBD-CGD-O1D
24	A	407	CLA	CHA-CBD-CGD-O2D
24	B	603	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	B	603	CLA	CHA-CBD-CGD-O2D
24	B	615	CLA	CHA-CBD-CGD-O2D
24	C	509	CLA	CHA-CBD-CGD-O1D
24	a	410	CLA	CHA-CBD-CGD-O1D
24	a	410	CLA	CHA-CBD-CGD-O2D
24	b	605	CLA	CHA-CBD-CGD-O2D
24	b	606	CLA	CHA-CBD-CGD-O1D
24	c	903	CLA	CHA-CBD-CGD-O2D
24	d	401	CLA	CHA-CBD-CGD-O2D
28	C	519	LMG	C38-C39-C40-C41
29	d	407	PL9	C13-C14-C16-C17
24	B	607	CLA	C10-C11-C12-C13
37	D	405	DGD	O2G-C1B-C2B-C3B
38	D	406	LHG	O8-C23-C24-C25
27	f	102	SQD	O6-C44-C45-O47
24	C	513	CLA	O1A-CGA-O2A-C1
36	B	631	HTG	C3'-C4'-C5'-C6'
24	C	504	CLA	C15-C16-C17-C18
28	a	416	LMG	C21-C22-C23-C24
24	B	611	CLA	C2A-CAA-CBA-CGA
24	c	910	CLA	C16-C17-C18-C20
38	d	410	LHG	O1-C1-C2-O2
28	C	519	LMG	C19-C20-C21-C22
38	D	408	LHG	C24-C23-O8-C6
37	c	917	DGD	O2G-C1B-C2B-C3B
39	F	102	HEM	CAD-CBD-CGD-O1D
24	C	510	CLA	C2-C3-C5-C6
24	C	512	CLA	CAA-CBA-CGA-O2A
24	A	407	CLA	C6-C7-C8-C9
24	A	407	CLA	C14-C13-C15-C16
24	B	616	CLA	C6-C7-C8-C9
37	D	405	DGD	C1B-C2B-C3B-C4B
28	d	412	LMG	C13-C14-C15-C16
24	a	413	CLA	C10-C11-C12-C13
24	B	614	CLA	CAA-CBA-CGA-O2A
27	a	401	SQD	C4-C5-C6-S
29	d	407	PL9	C11-C12-C13-C14
38	E	101	LHG	C24-C23-O8-C6
37	c	919	DGD	O1A-C1A-C2A-C3A
27	A	416	SQD	C28-C29-C30-C31
32	C	525	GOL	O1-C1-C2-C3
38	d	410	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
24	C	510	CLA	CAA-CBA-CGA-O2A
31	Z	101	LMT	C5-C6-C7-C8
24	b	605	CLA	C1A-C2A-CAA-CBA
24	A	406	CLA	C15-C16-C17-C18
28	d	412	LMG	C16-C17-C18-C19
31	B	622	LMT	C6-C7-C8-C9
38	D	408	LHG	C17-C18-C19-C20
24	D	401	CLA	C2-C1-O2A-CGA
27	b	601	SQD	O6-C44-C45-C46
24	C	501	CLA	C2A-CAA-CBA-CGA
24	C	507	CLA	C2A-CAA-CBA-CGA
37	d	408	DGD	CBA-CCA-CDA-CEA
27	l	101	SQD	O10-C23-C24-C25
37	C	517	DGD	O2G-C1B-C2B-C3B
28	a	416	LMG	O9-C10-C11-C12
37	d	408	DGD	O1A-C1A-C2A-C3A
38	D	407	LHG	C3-O3-P-O5
24	C	512	CLA	CAA-CBA-CGA-O1A
31	m	102	LMT	O5'-C5'-C6'-O6'
26	C	514	BCR	C5-C6-C7-C8
26	D	403	BCR	C1-C6-C7-C8
26	a	414	BCR	C1-C6-C7-C8
40	h	101	RRX	C23-C24-C25-C30
36	c	943	HTG	C2'-C3'-C4'-C5'
27	a	401	SQD	O48-C23-C24-C25
24	b	618	CLA	C2A-CAA-CBA-CGA
24	c	902	CLA	C2A-CAA-CBA-CGA
31	A	421	LMT	C4-C5-C6-C7
31	t	101	LMT	C2-C3-C4-C5
24	C	505	CLA	C4-C3-C5-C6
39	F	102	HEM	CAA-CBA-CGA-O1A
24	B	606	CLA	CAD-CBD-CGD-O1D
24	B	608	CLA	CAD-CBD-CGD-O1D
24	C	504	CLA	CAD-CBD-CGD-O1D
24	C	506	CLA	CAD-CBD-CGD-O1D
24	c	905	CLA	CAD-CBD-CGD-O1D
24	d	401	CLA	CAD-CBD-CGD-O1D
27	f	102	SQD	O5-C5-C6-S
27	l	101	SQD	C5-C6-S-O7
37	H	102	DGD	C9B-CAB-CBB-CCB
38	l	103	LHG	O7-C7-C8-C9
24	a	410	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	b	606	CLA	C6-C7-C8-C9
24	c	905	CLA	C11-C12-C13-C14
24	d	405	CLA	C14-C13-C15-C16
37	c	919	DGD	CDB-CEB-CFB-CGB
24	d	404	CLA	C16-C17-C18-C20
24	b	616	CLA	CAA-CBA-CGA-O2A
24	c	906	CLA	CAA-CBA-CGA-O2A
28	D	409	LMG	O7-C10-C11-C12
38	d	411	LHG	O8-C23-C24-C25
31	A	421	LMT	C5-C6-C7-C8
27	f	102	SQD	O47-C7-C8-C9
39	F	102	HEM	CAD-CBD-CGD-O2D
31	c	922	LMT	C2-C3-C4-C5
37	D	405	DGD	C2A-C3A-C4A-C5A
24	c	906	CLA	CAA-CBA-CGA-O1A
25	A	408	PHO	C4-C3-C5-C6
24	A	407	CLA	C6-C7-C8-C10
24	A	410	CLA	C2-C3-C5-C6
24	C	509	CLA	C11-C10-C8-C7
24	c	910	CLA	C6-C7-C8-C10
24	d	404	CLA	C11-C12-C13-C15
24	d	405	CLA	C12-C13-C15-C16
36	c	923	HTG	C2-C1-S1-C1'
27	F	101	SQD	O47-C7-C8-C9
38	L	101	LHG	O7-C7-C8-C9
24	C	503	CLA	C10-C11-C12-C13
24	D	401	CLA	C2C-C3C-CAC-CBC
27	A	416	SQD	C23-C24-C25-C26
38	d	409	LHG	C7-C8-C9-C10
26	T	101	BCR	C11-C12-C13-C14
24	B	614	CLA	CAA-CBA-CGA-O1A
27	F	101	SQD	O49-C7-C8-C9
27	f	102	SQD	O49-C7-C8-C9
38	D	406	LHG	O10-C23-C24-C25
39	f	101	HEM	CAD-CBD-CGD-O1D
37	C	518	DGD	CDA-CEA-CFA-CGA
31	B	626	LMT	C2-C1-O1'-C1'
24	c	911	CLA	CAA-CBA-CGA-O2A
37	c	918	DGD	CDA-CEA-CFA-CGA
38	d	410	LHG	C26-C27-C28-C29
24	C	510	CLA	CAA-CBA-CGA-O1A
27	l	101	SQD	C30-C31-C32-C33

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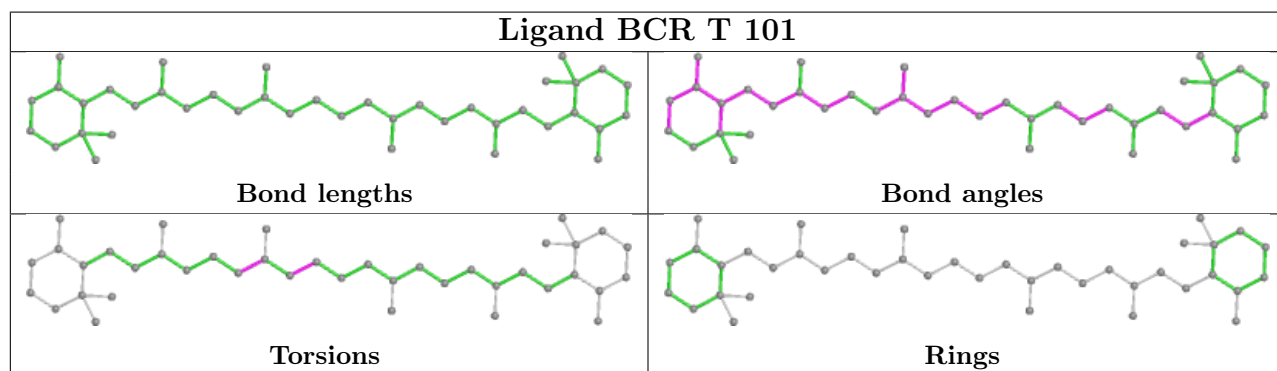
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Mol	Chain	Res	Type	Atoms
24	b	619	CLA	C10-C11-C12-C13
24	d	401	CLA	C15-C16-C17-C18
24	C	501	CLA	CAA-CBA-CGA-O2A
24	C	505	CLA	CAA-CBA-CGA-O2A
28	c	920	LMG	O7-C10-C11-C12
31	c	922	LMT	C2B-C1B-O1B-C4'
27	A	412	SQD	C13-C14-C15-C16
24	b	616	CLA	CAA-CBA-CGA-O1A
37	C	517	DGD	O1B-C1B-C2B-C3B
29	D	404	PL9	C45-C44-C46-C47
31	c	922	LMT	O5B-C1B-O1B-C4'

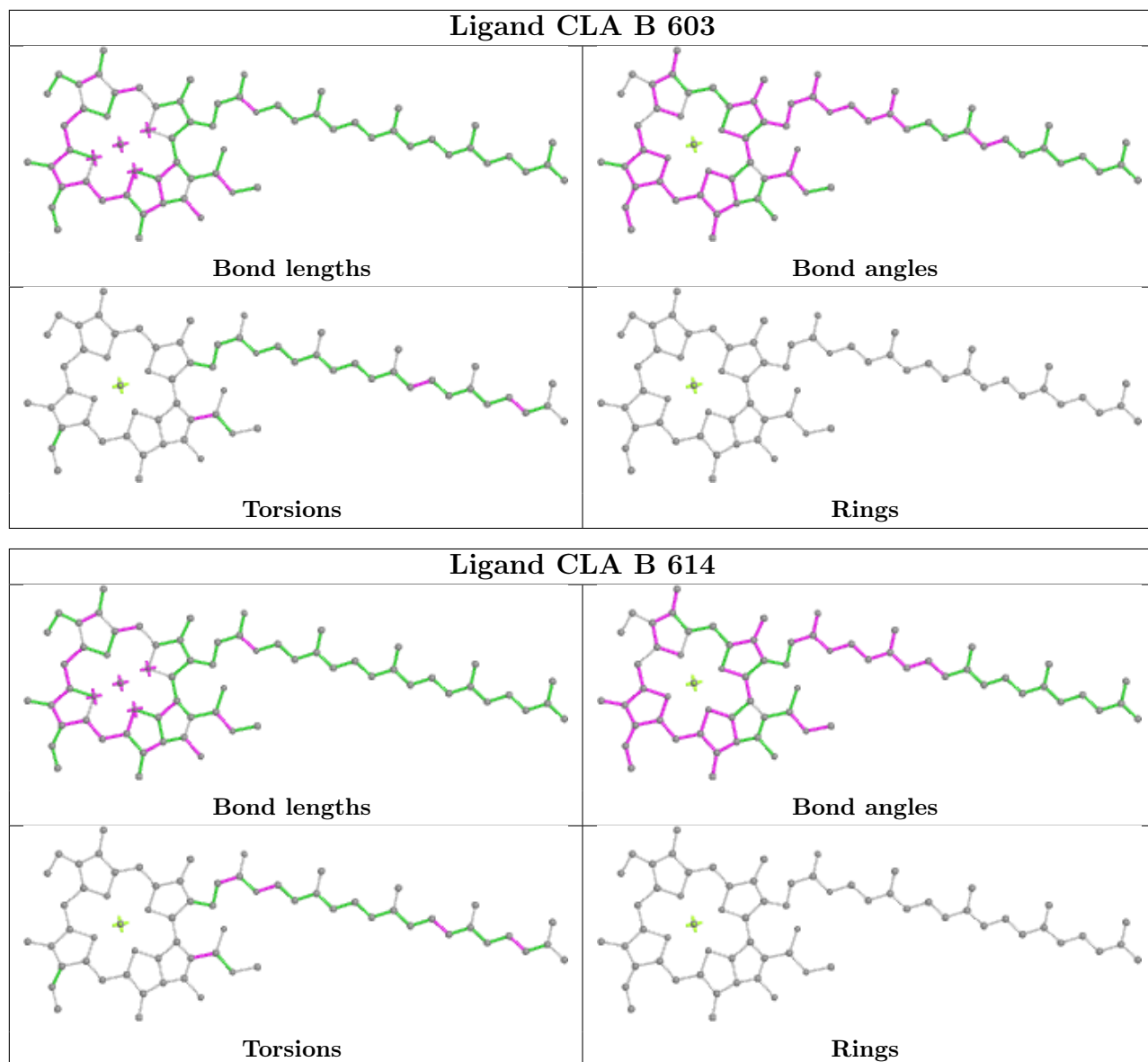
There are no ring outliers.

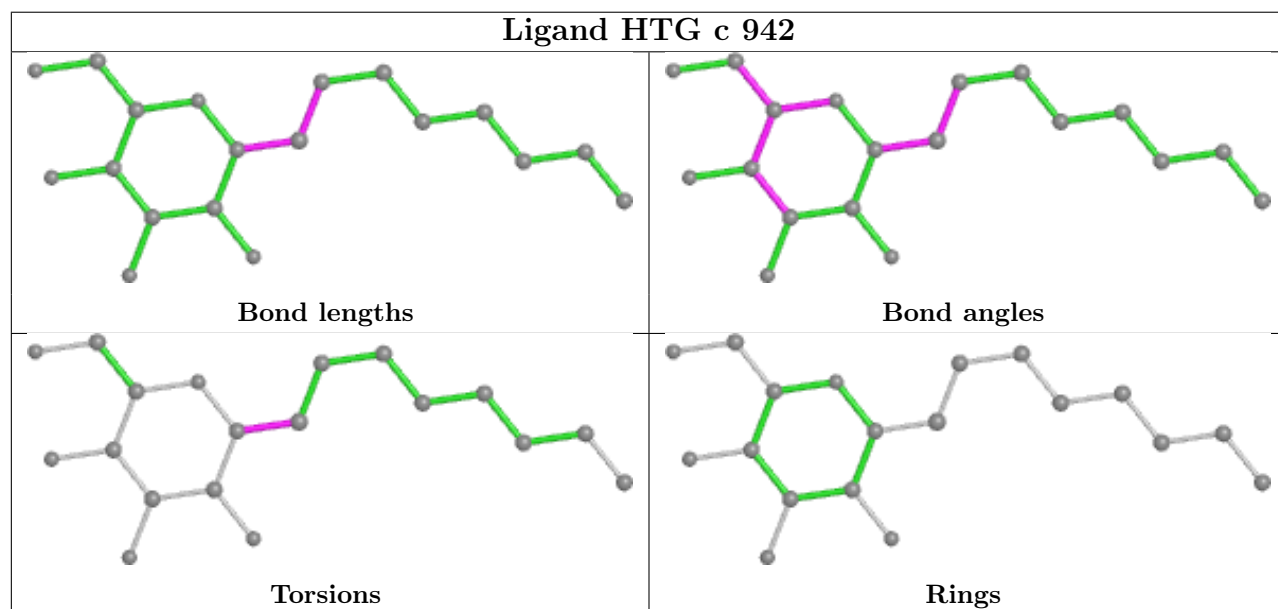
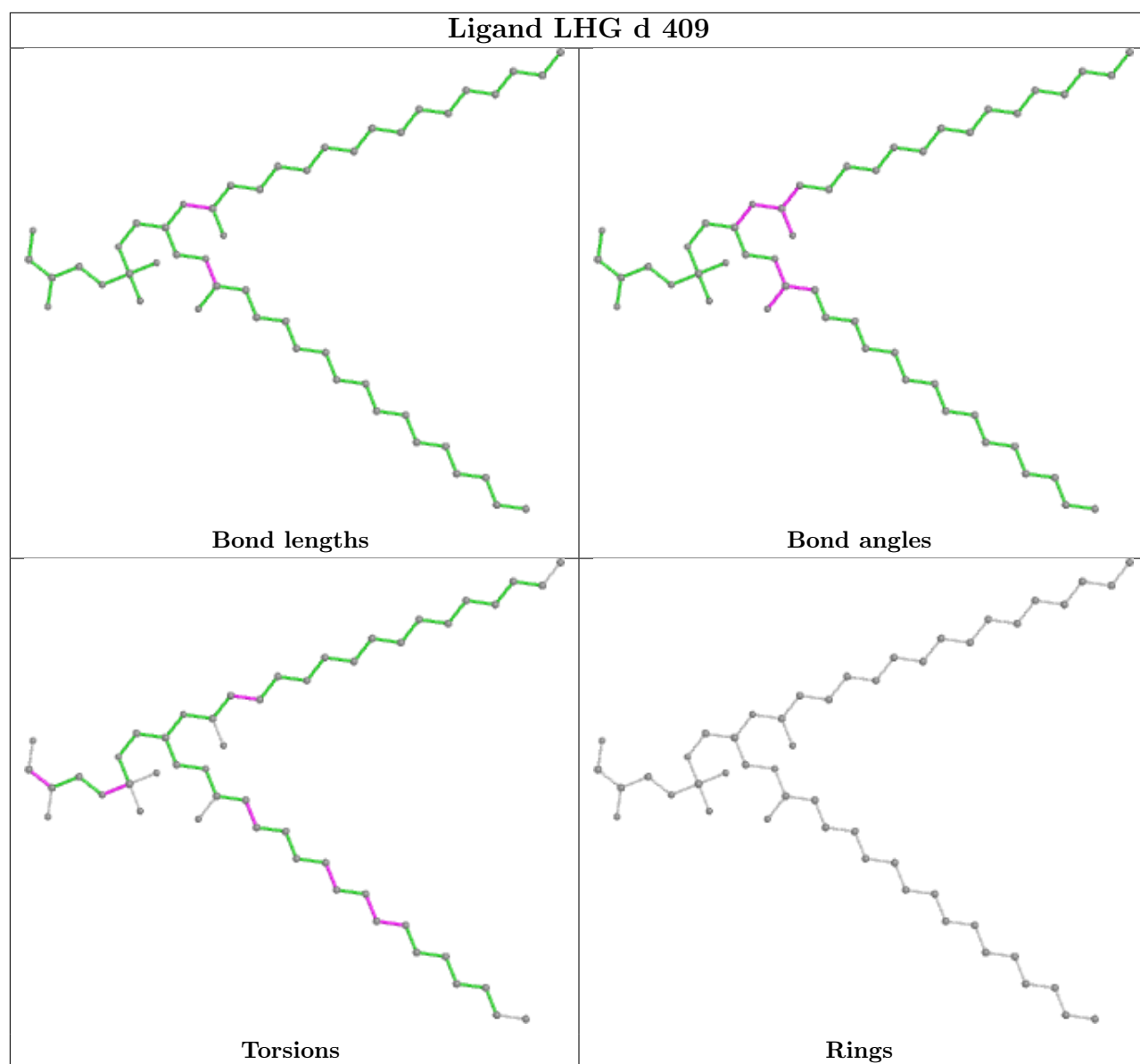
No monomer is involved in short contacts.

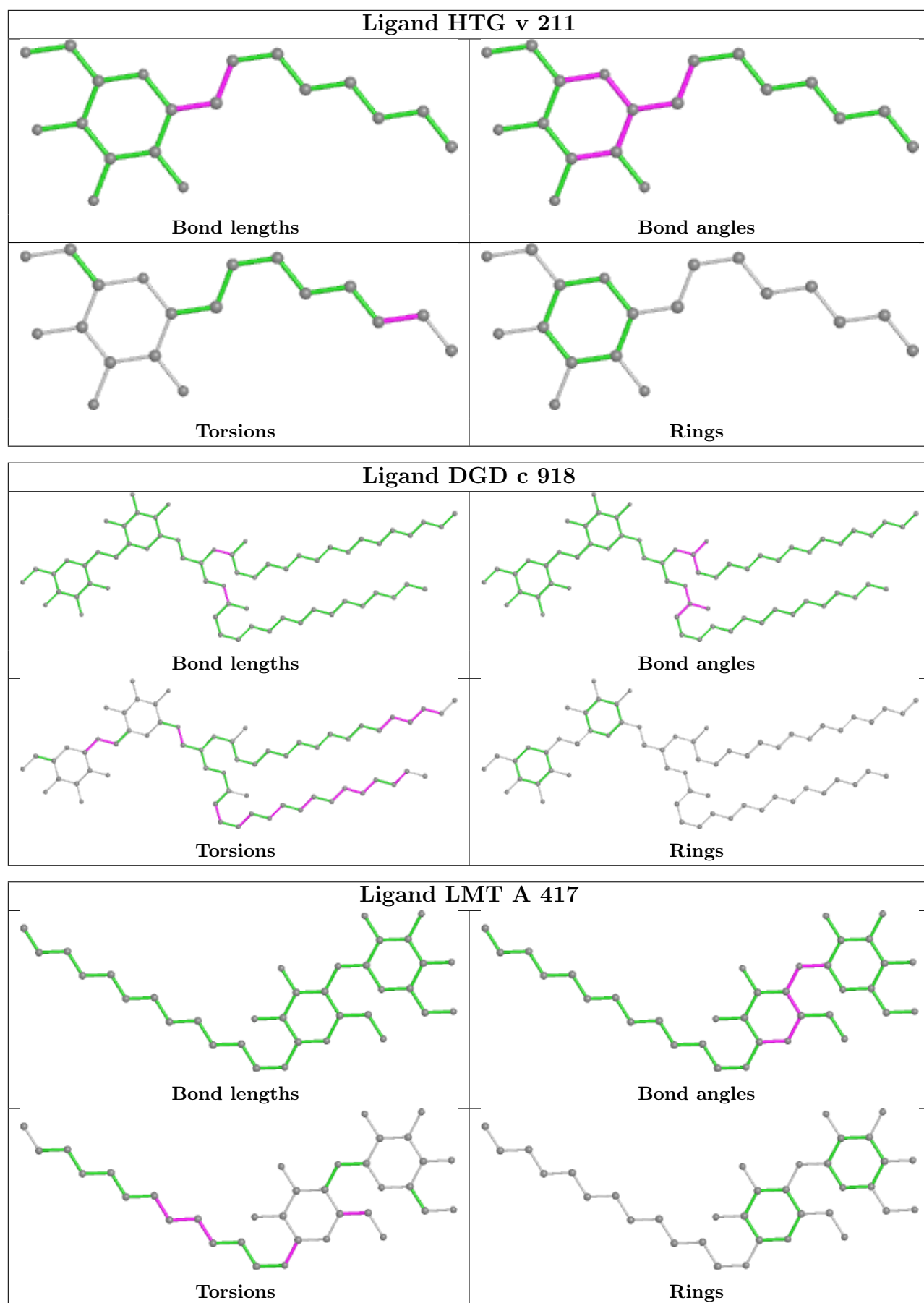
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

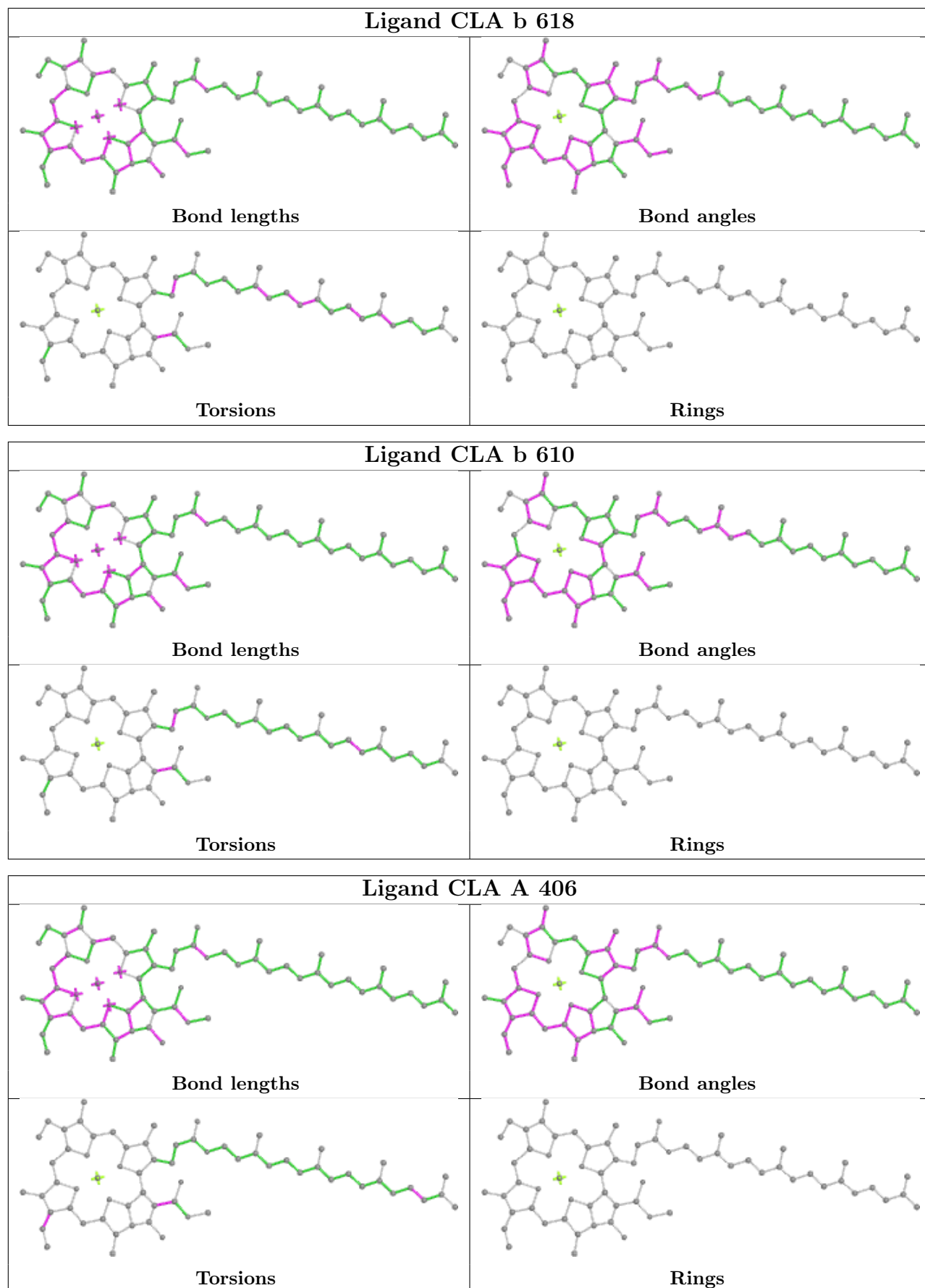


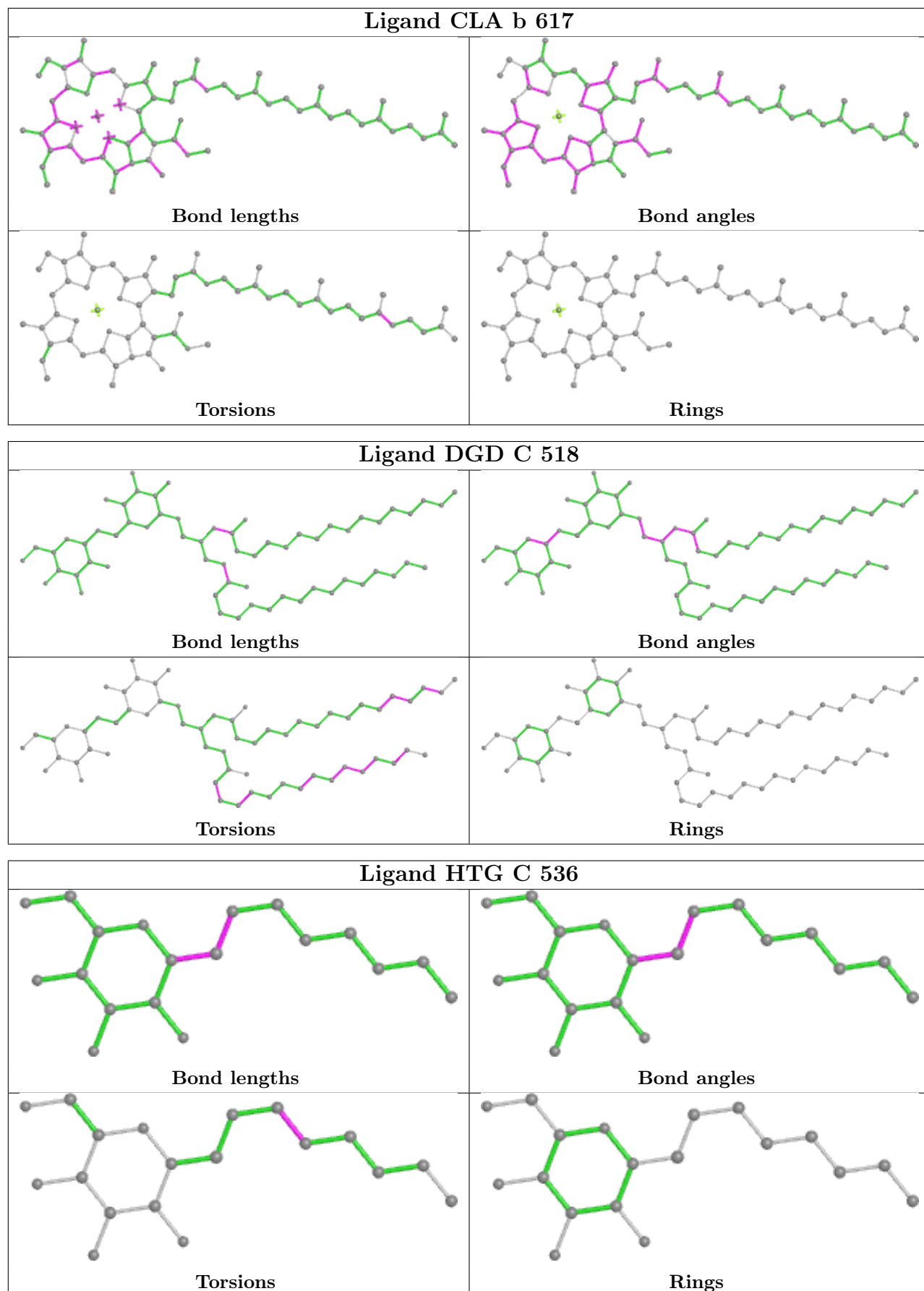


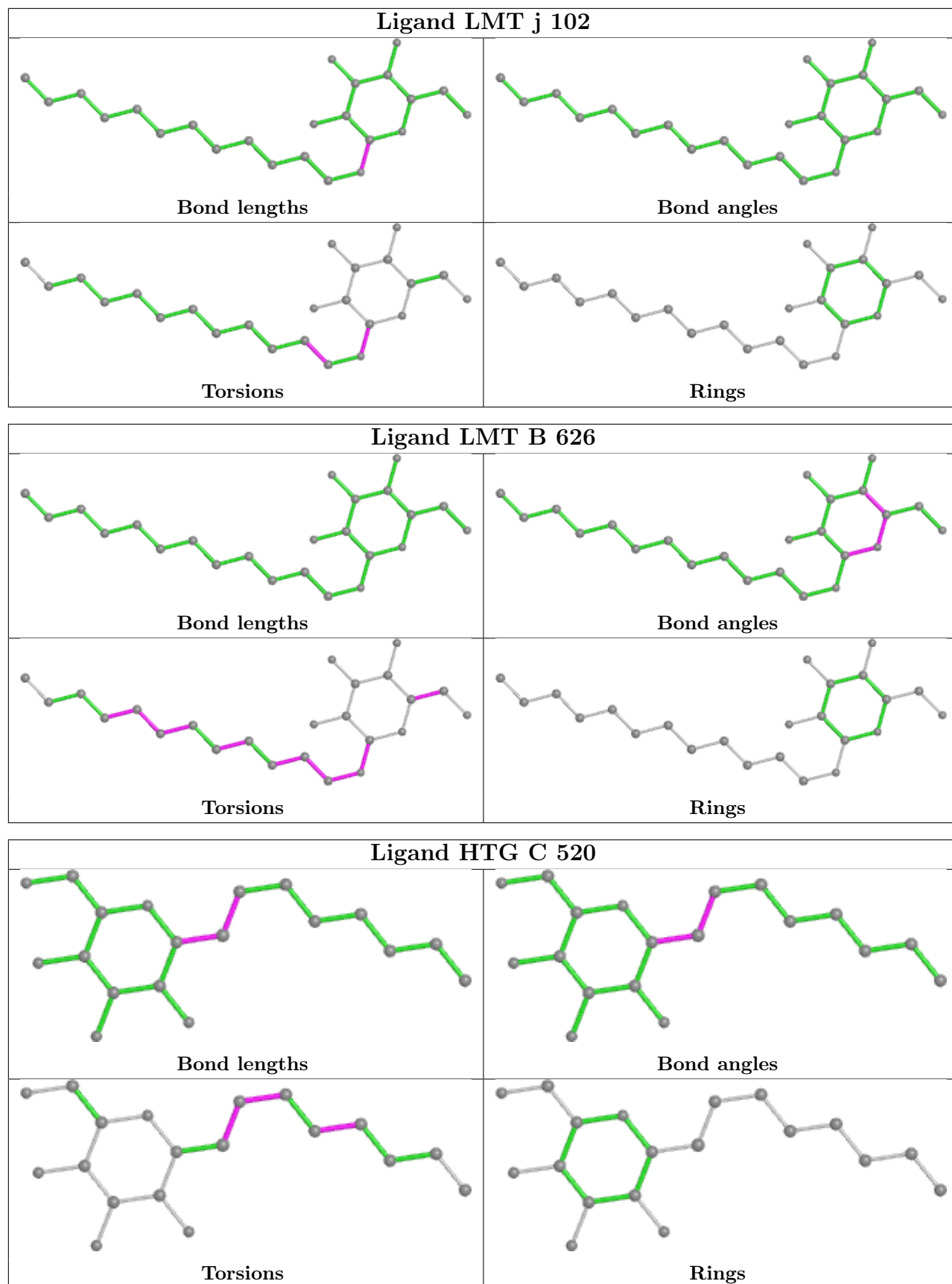


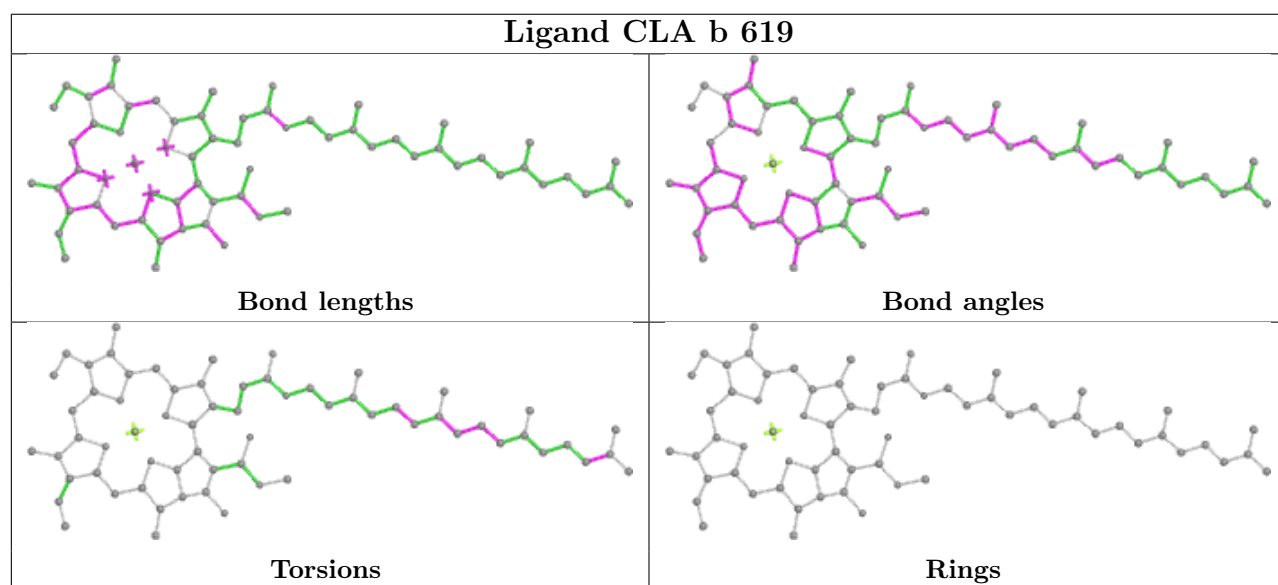
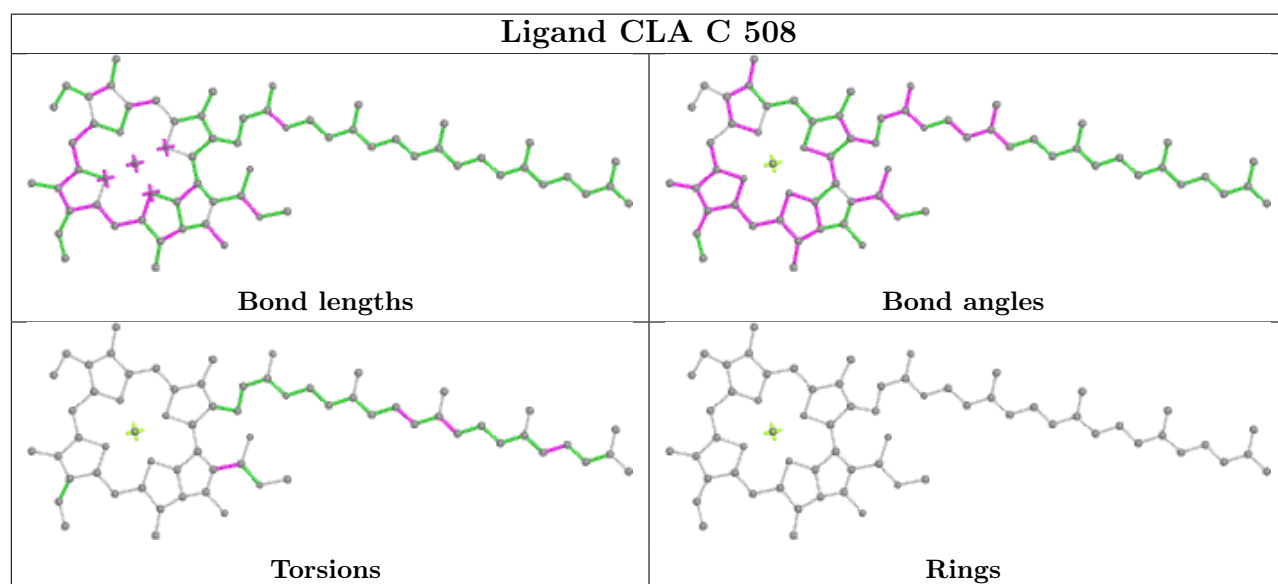
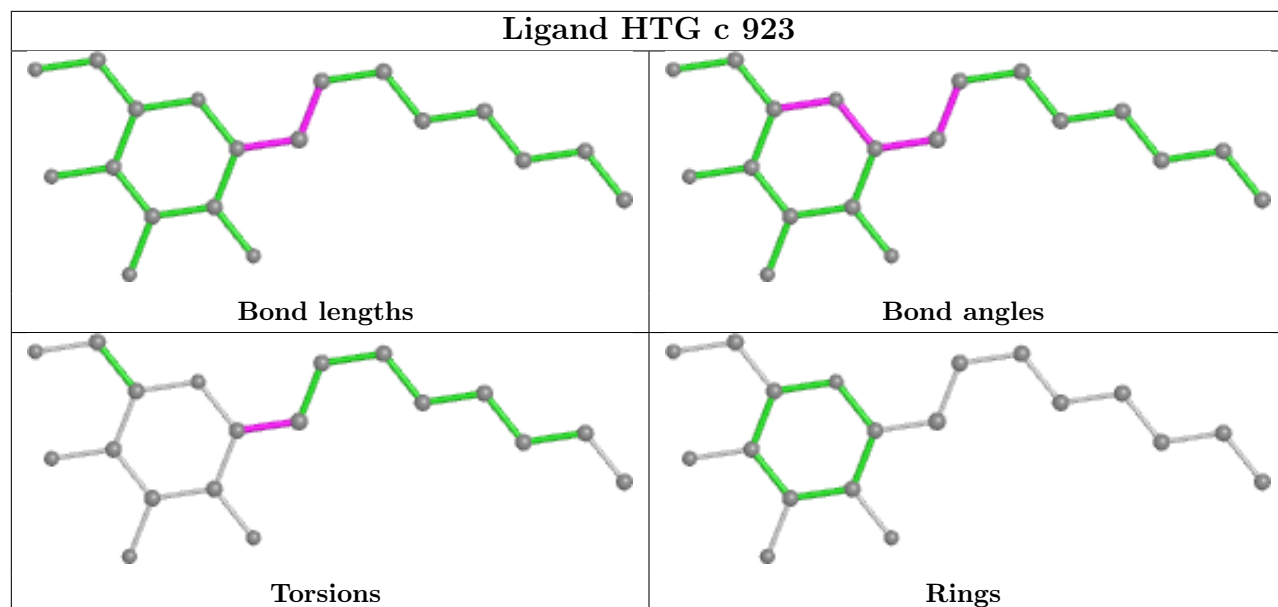


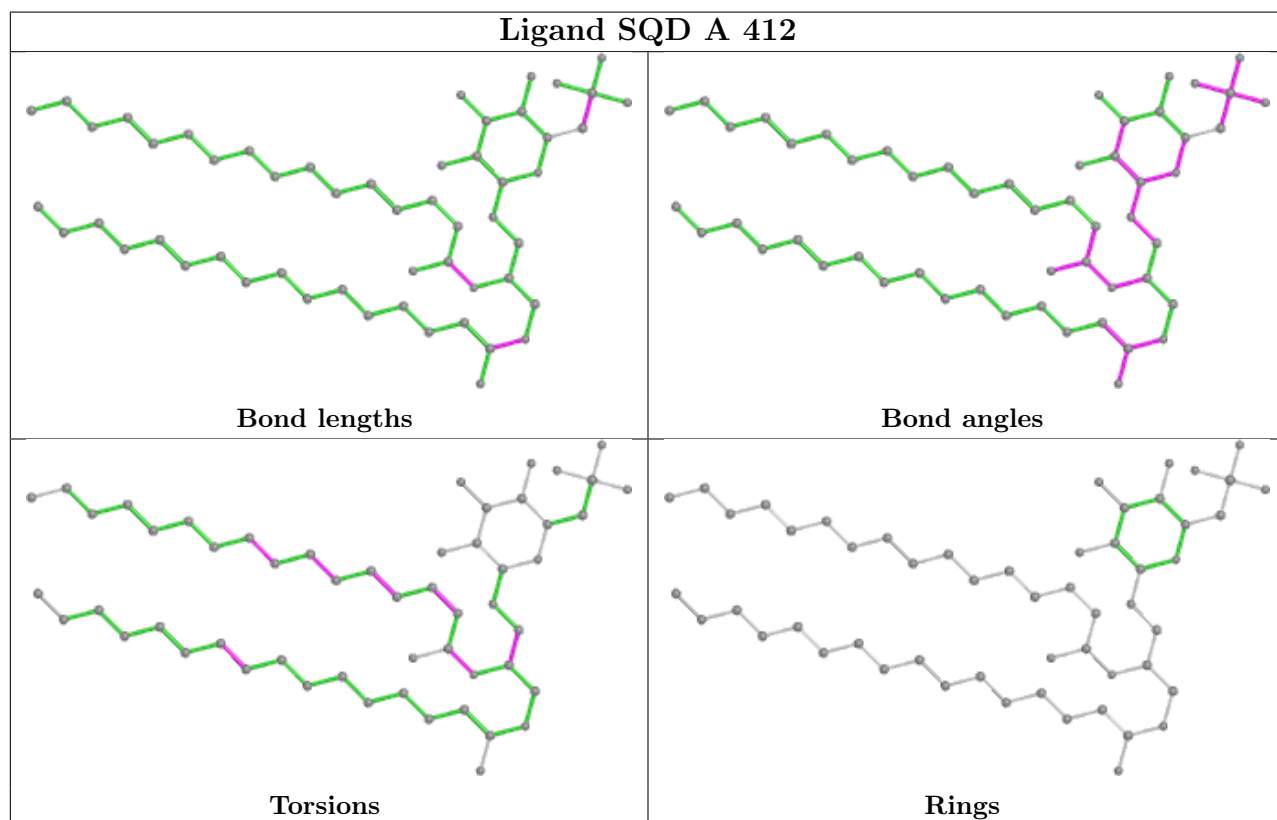
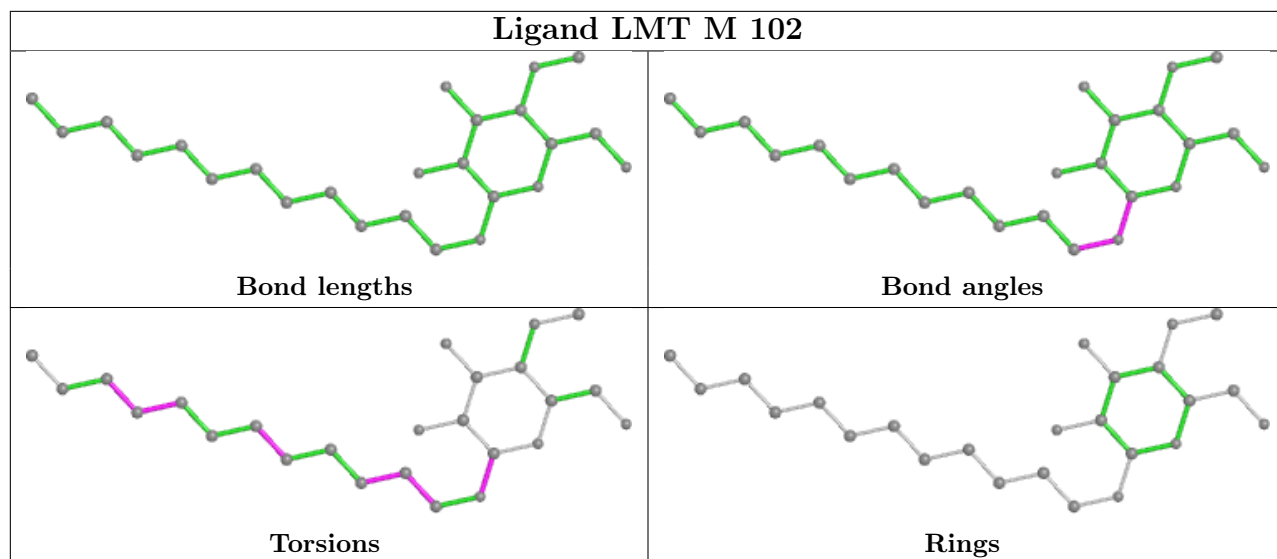




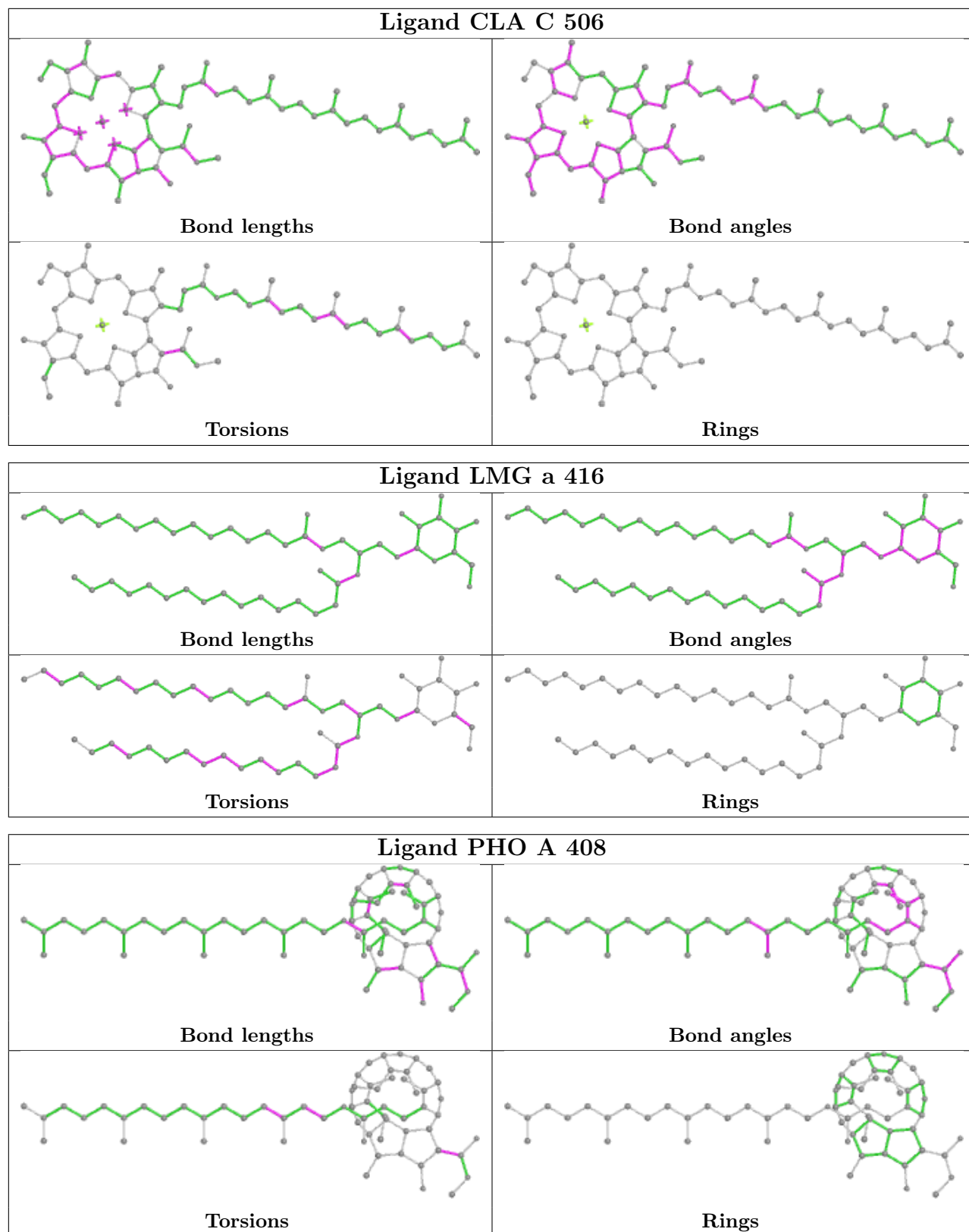


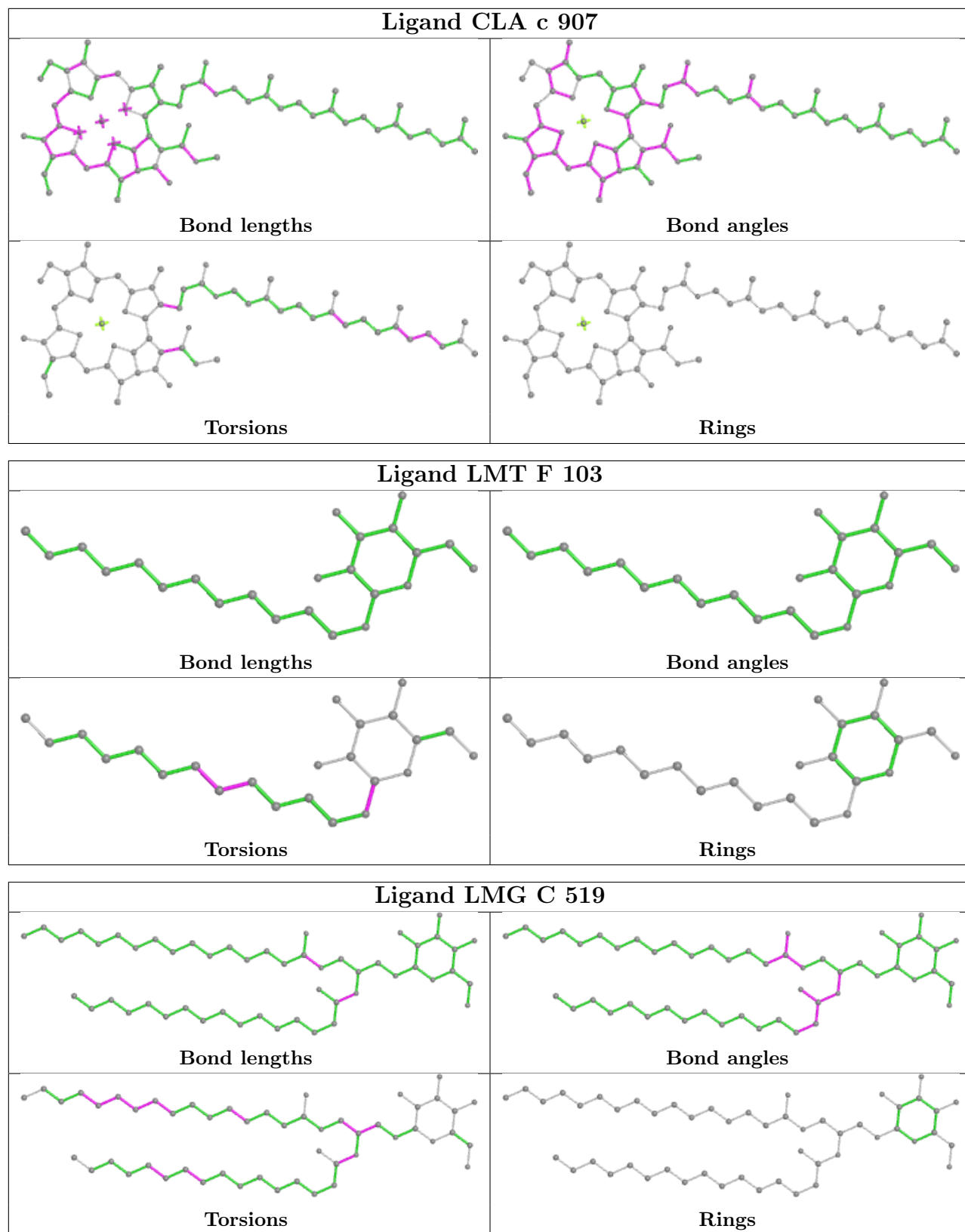


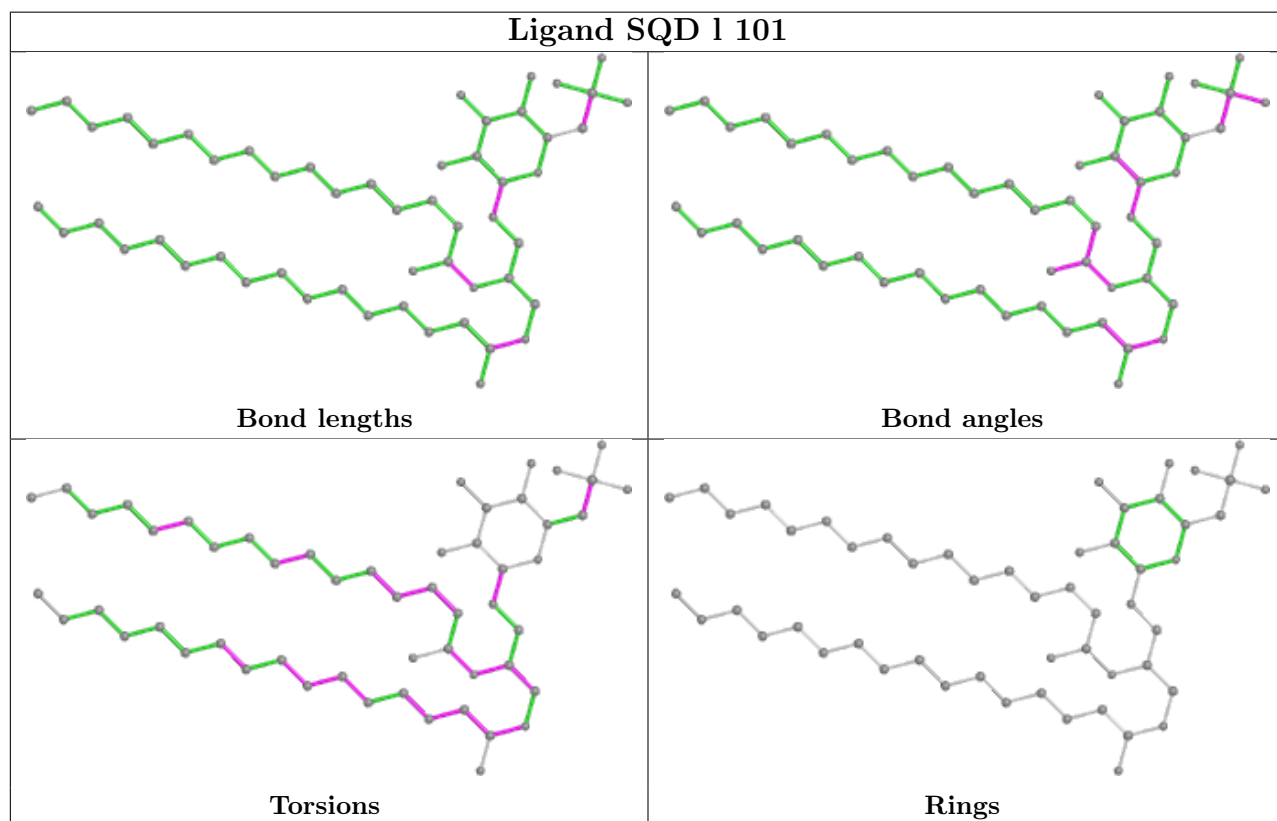
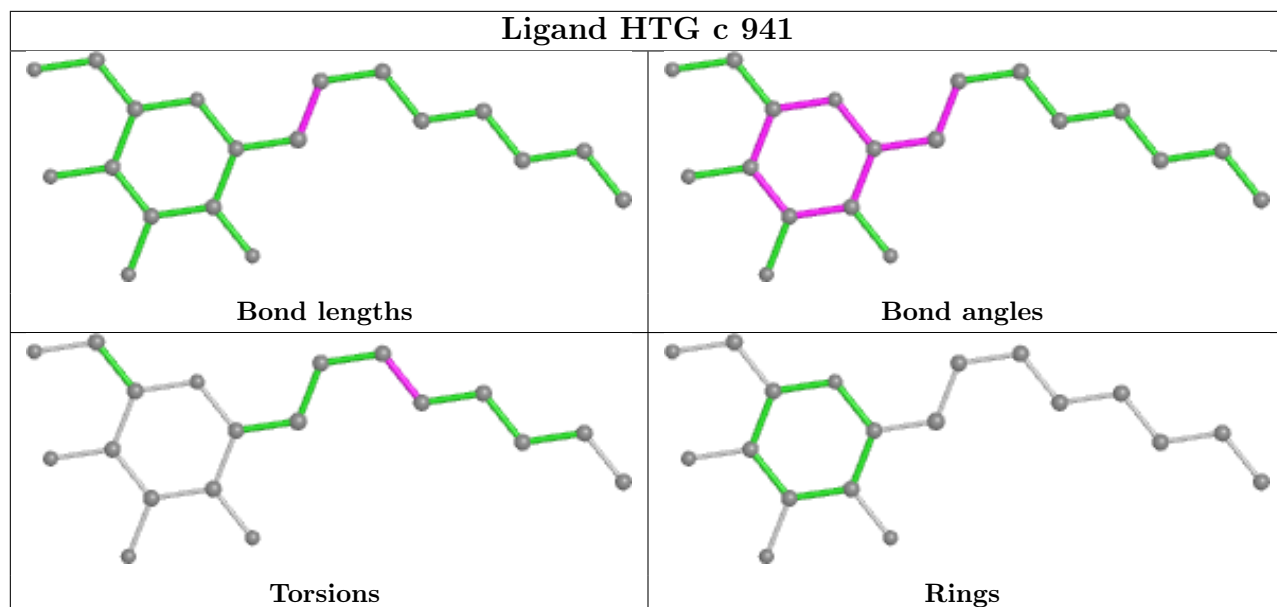


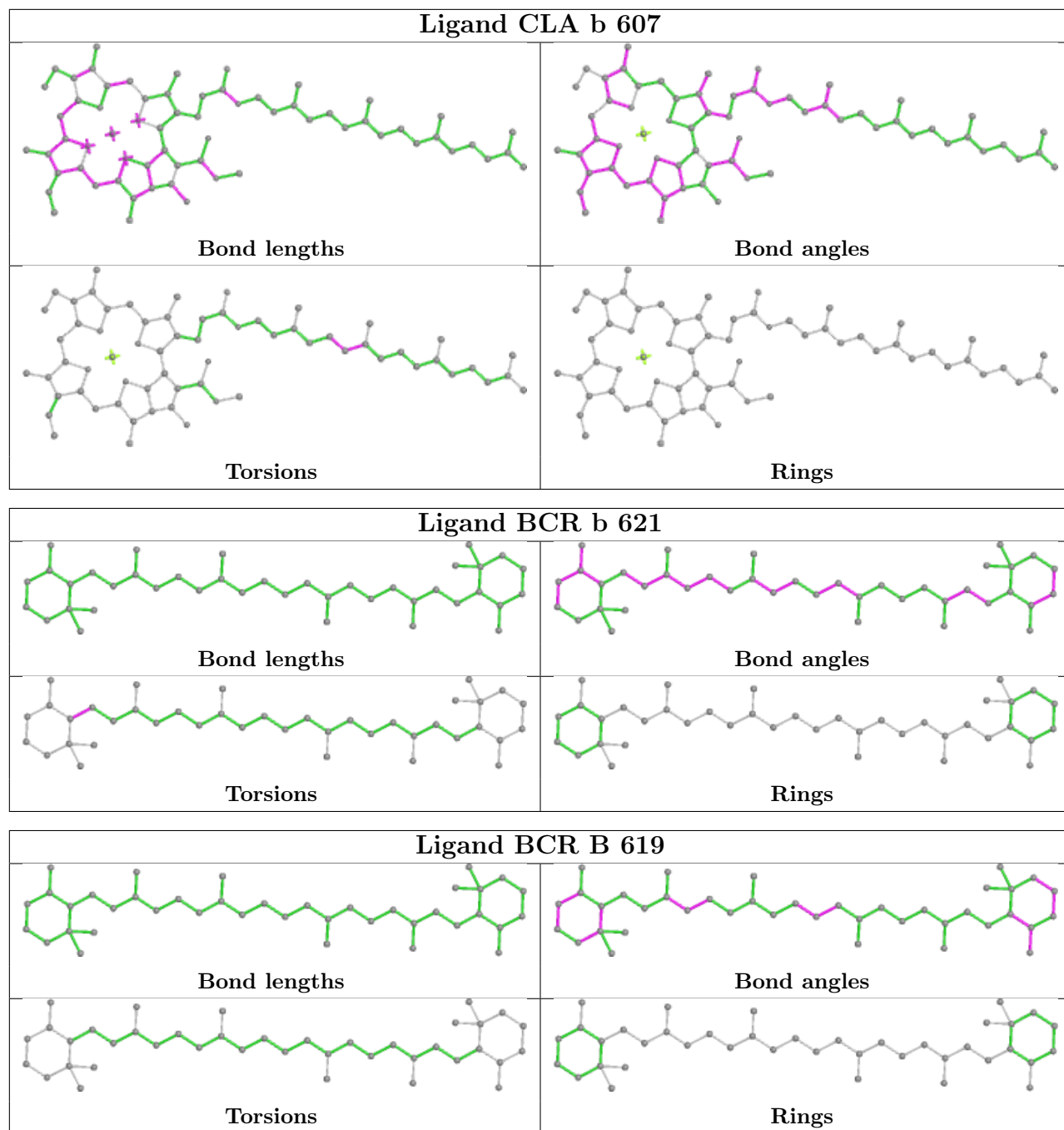


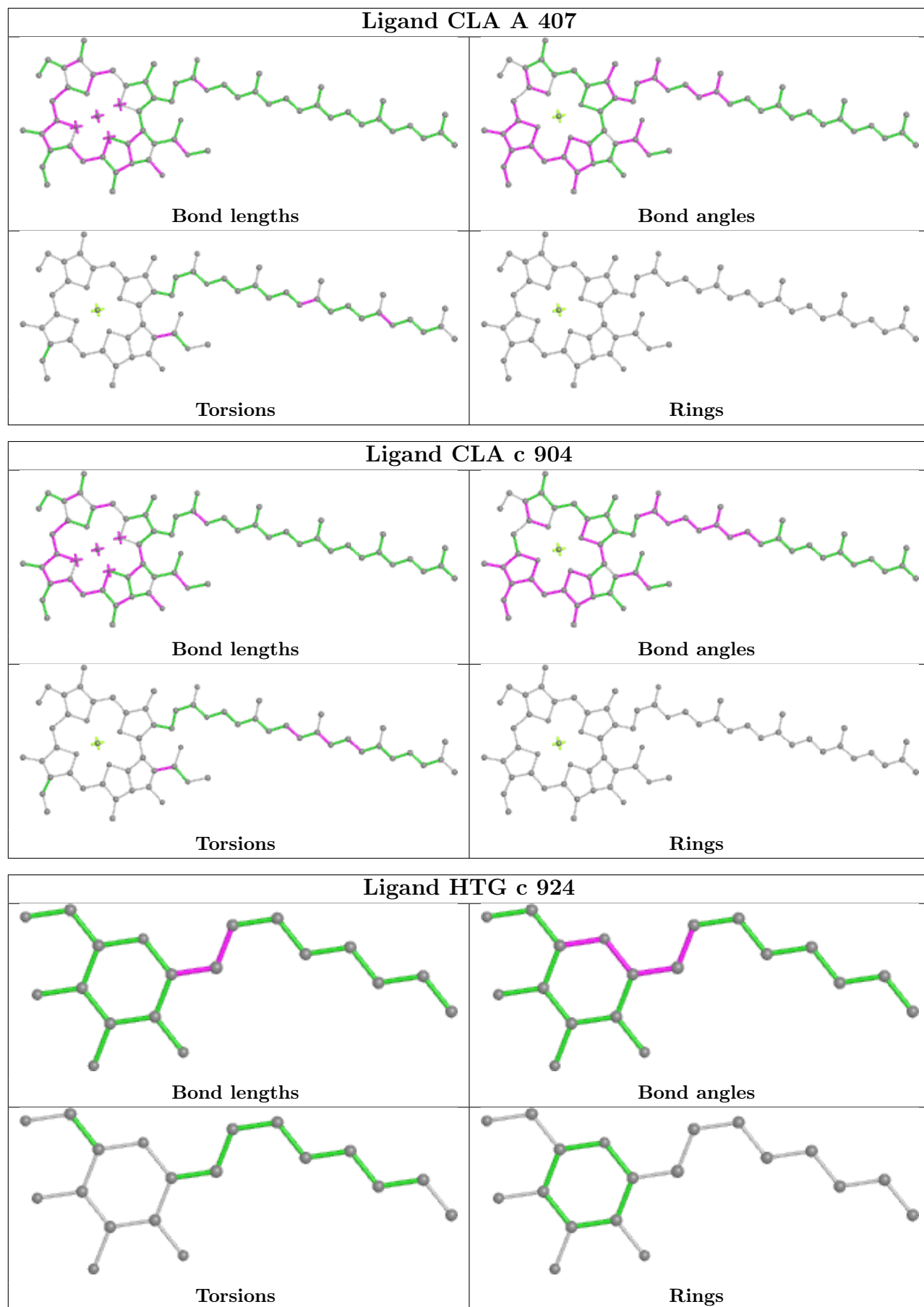


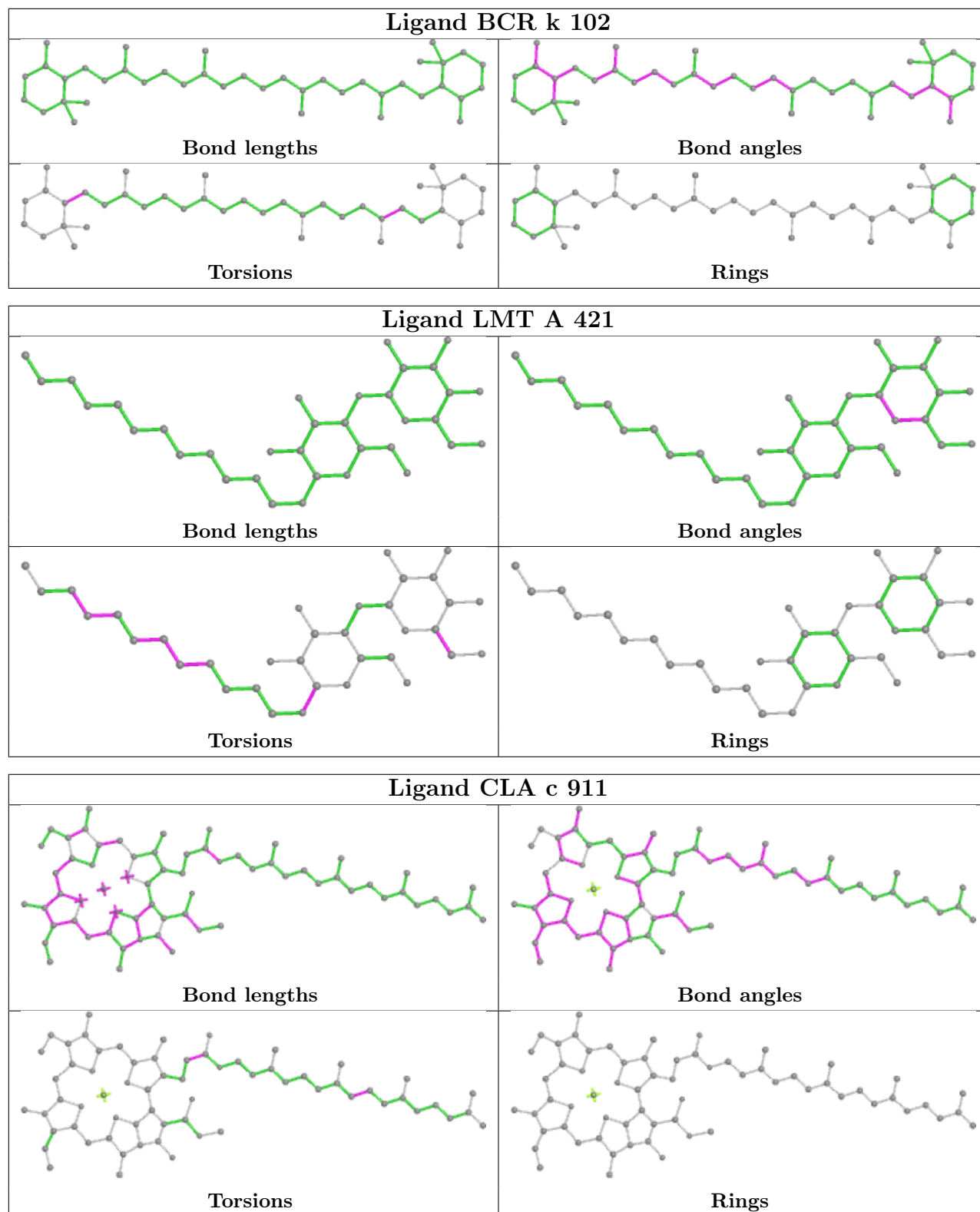


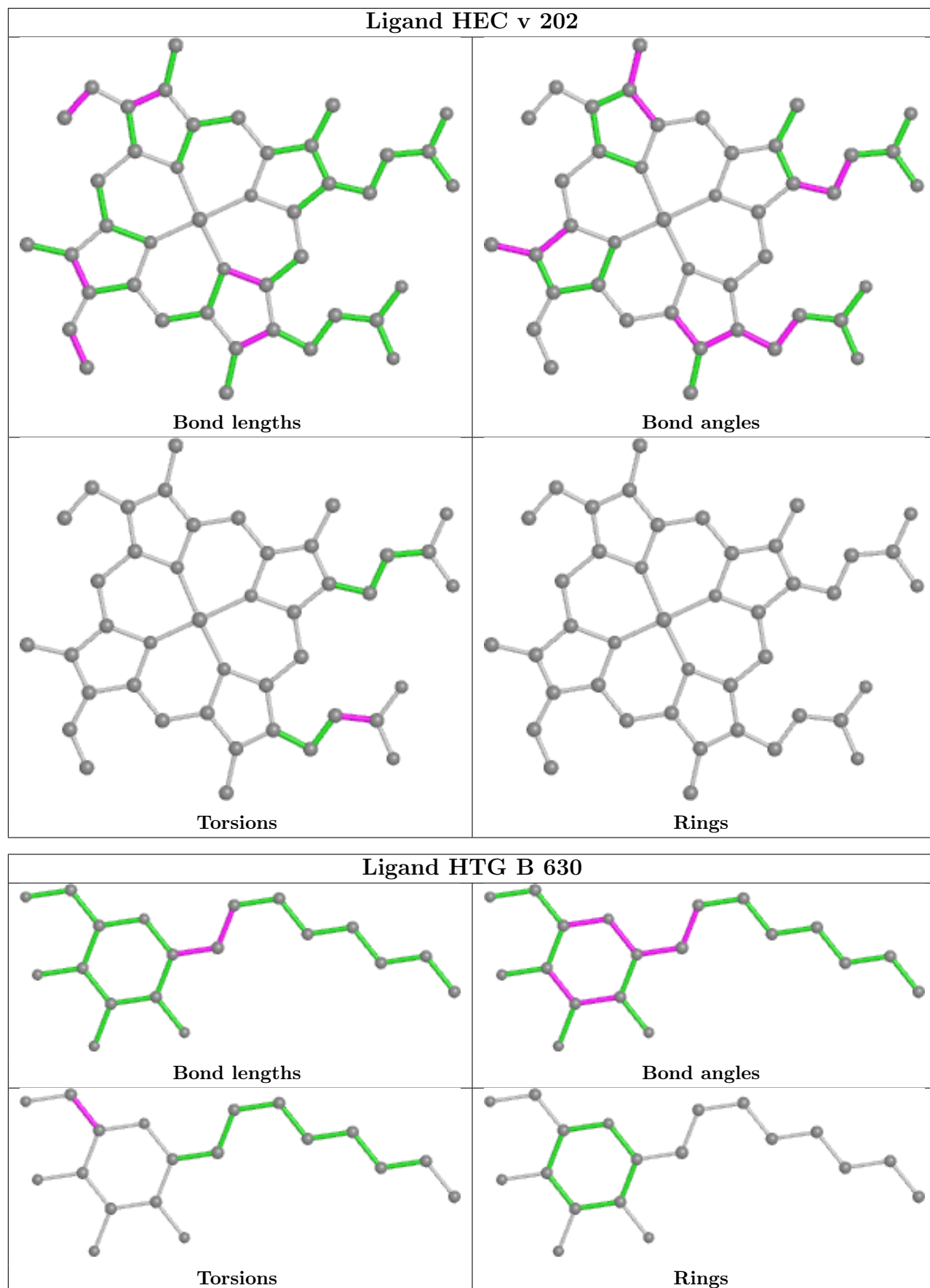


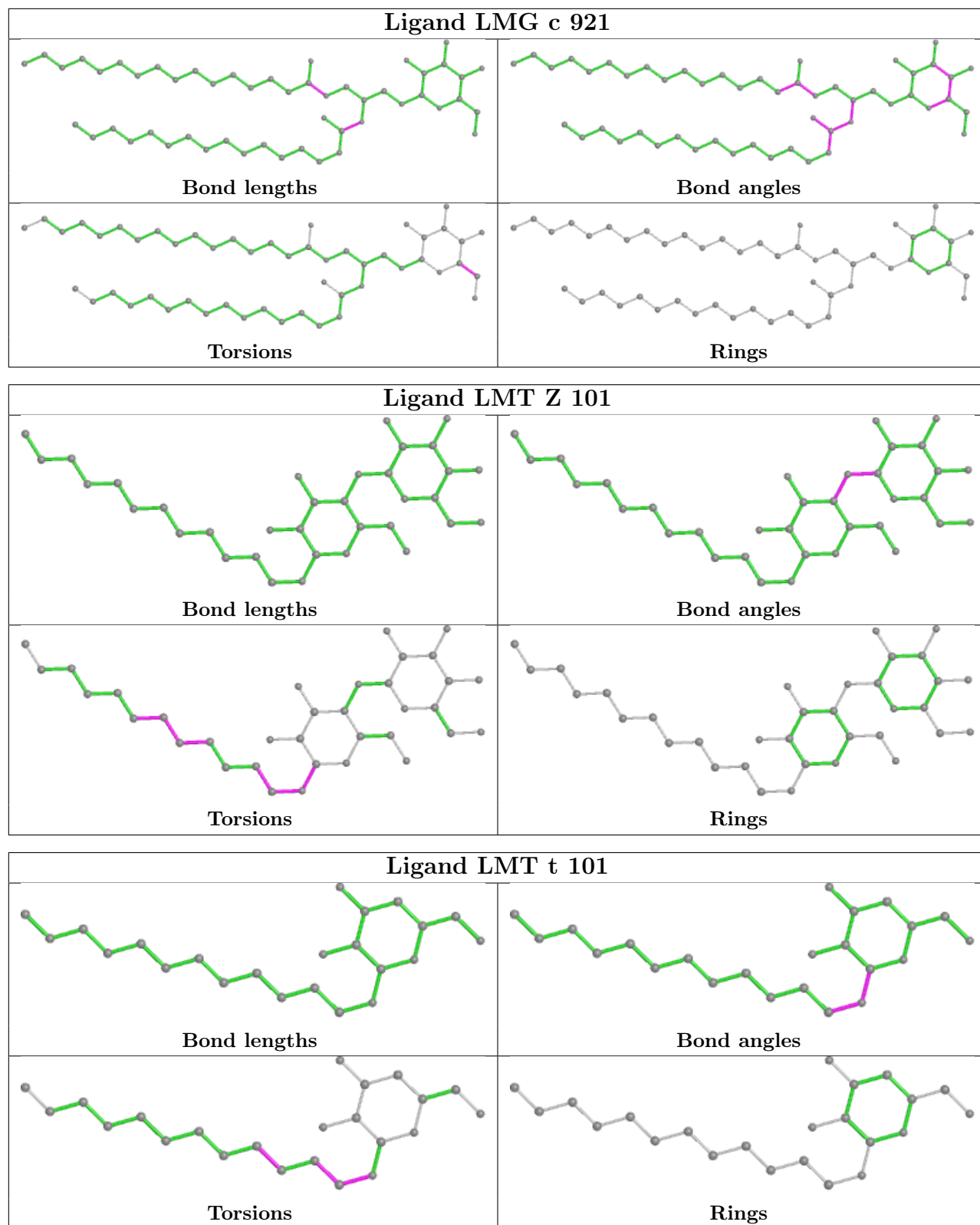




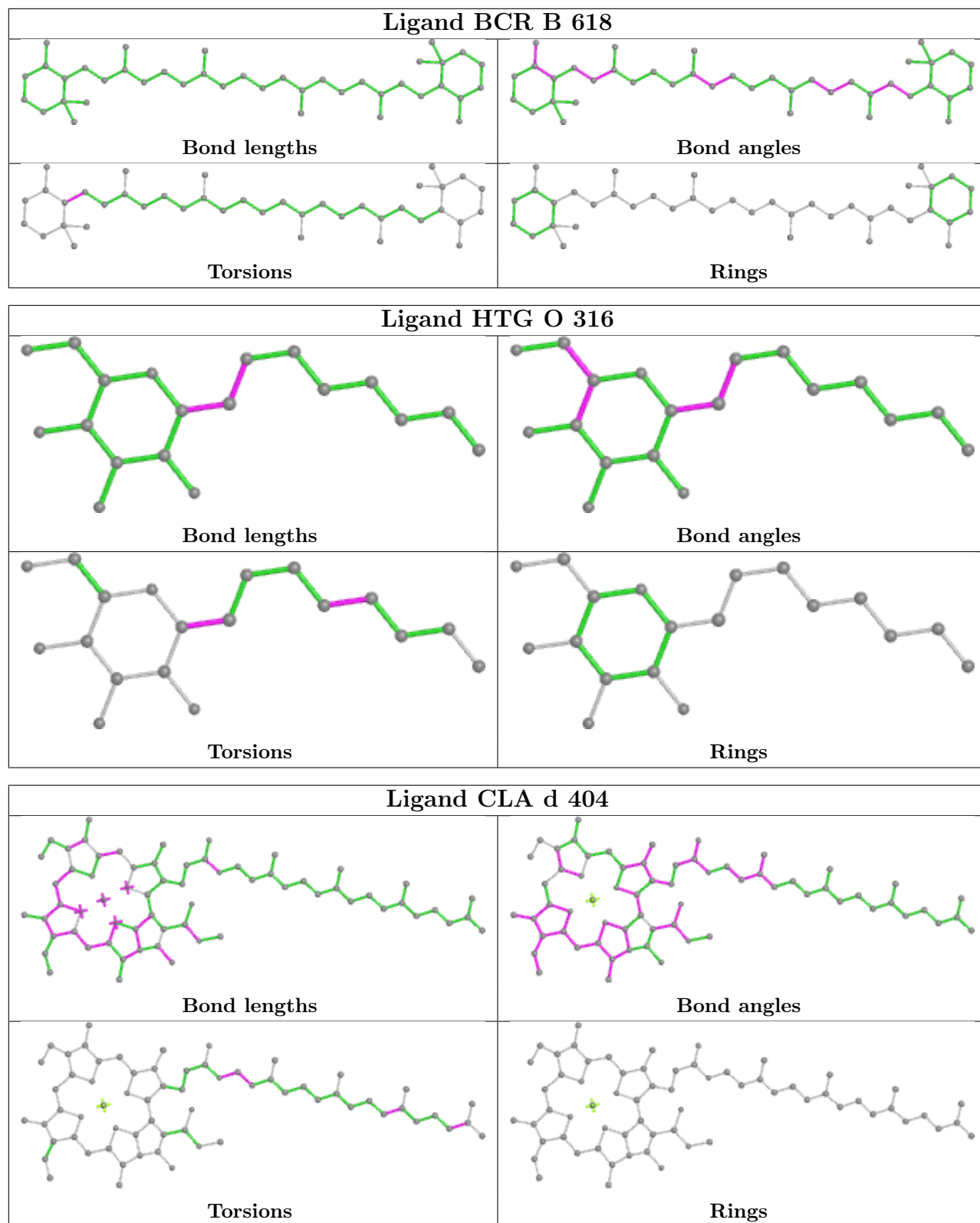


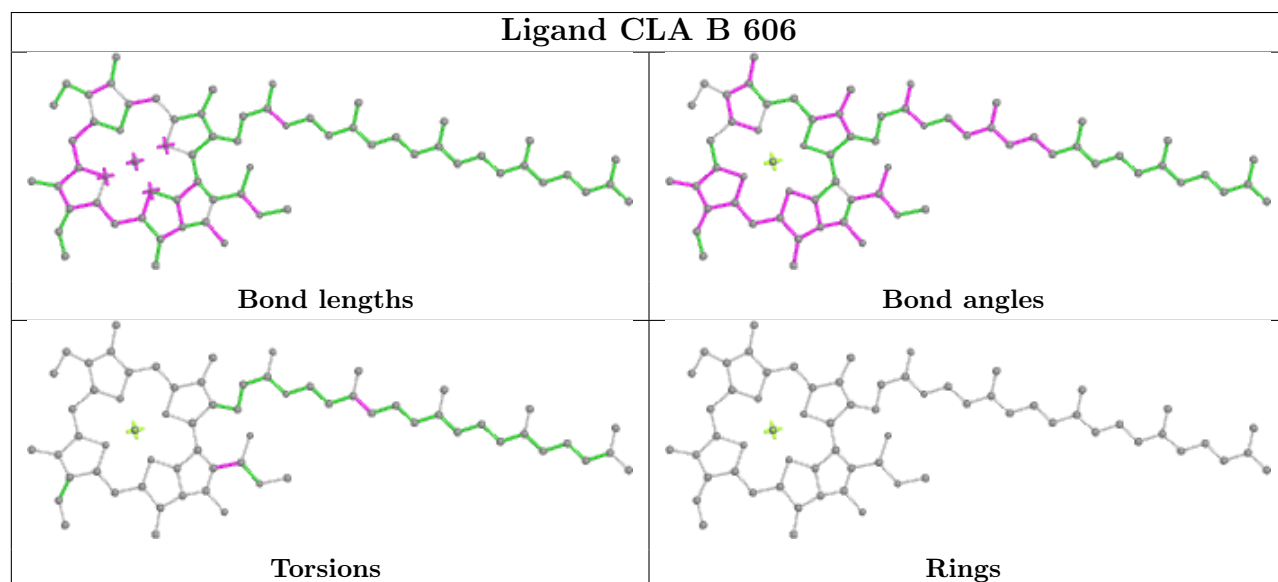
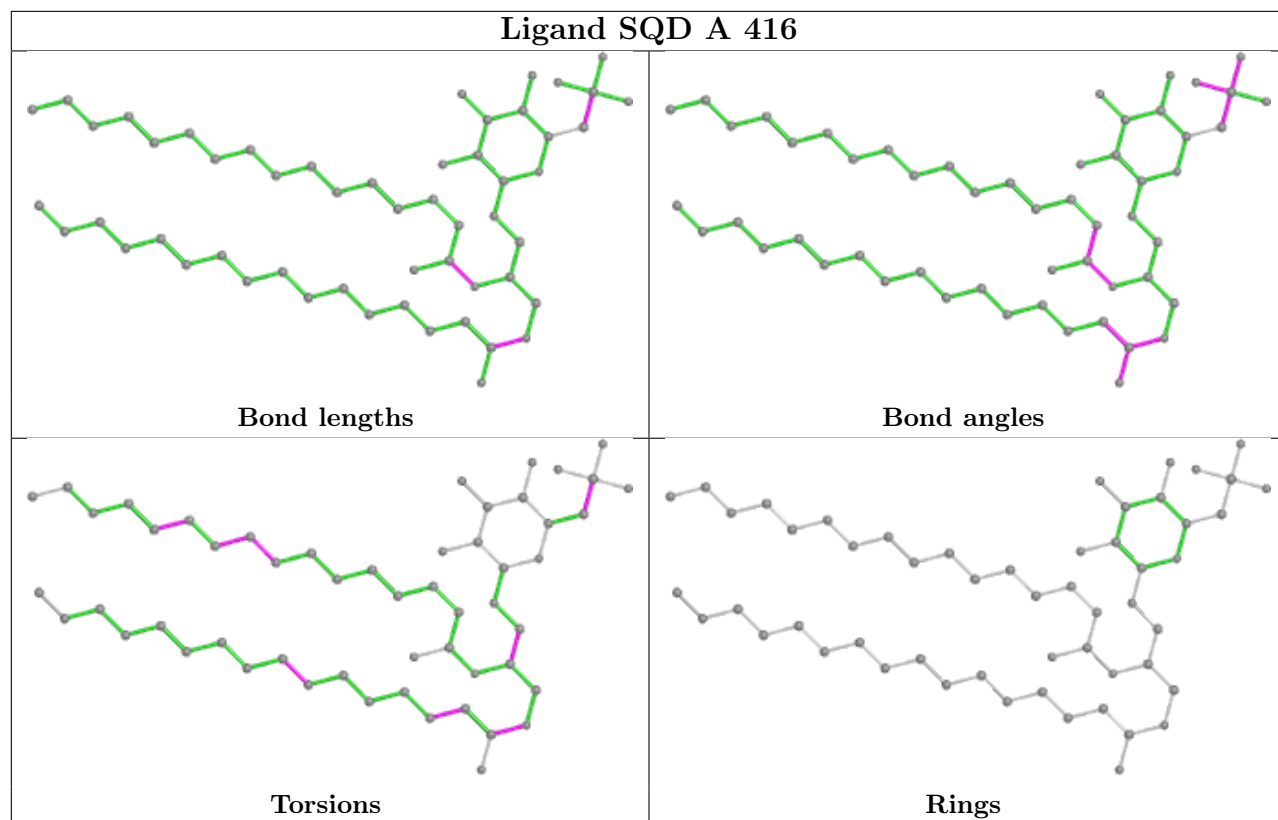


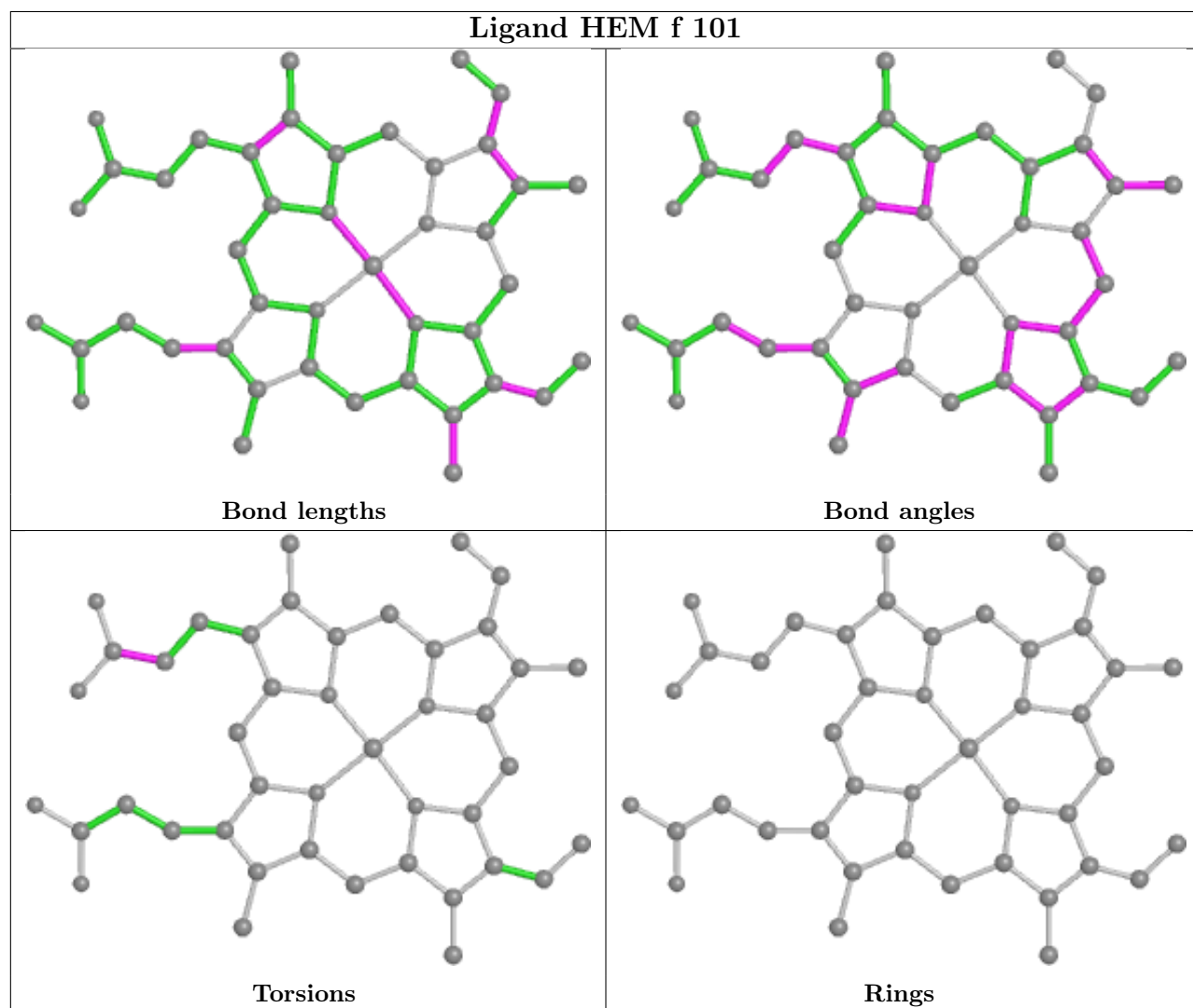
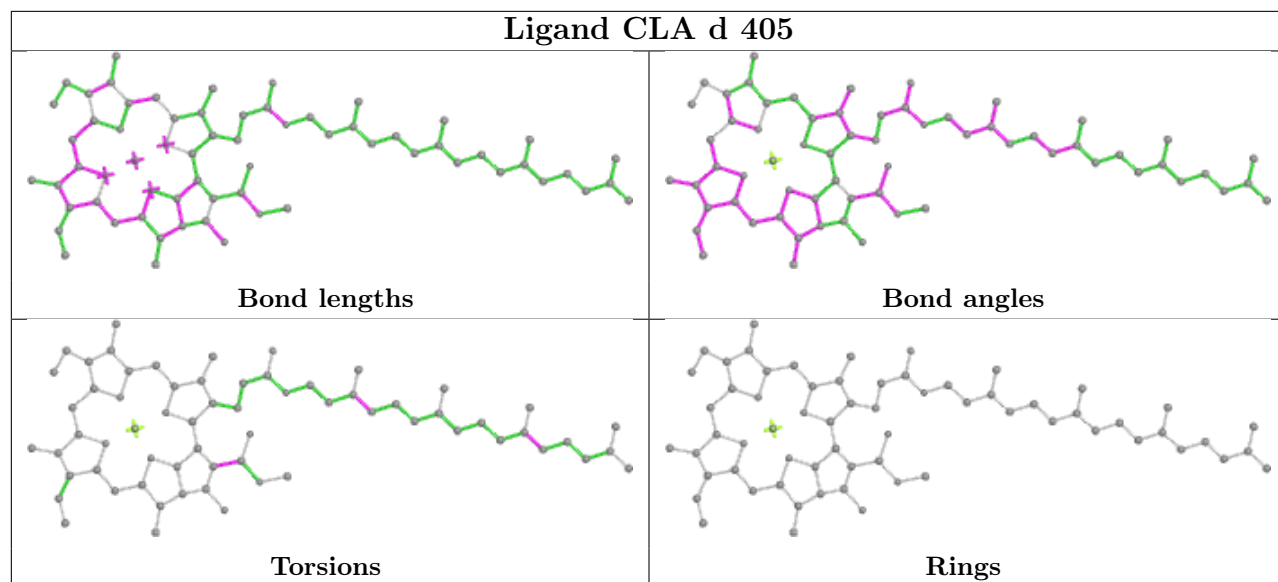


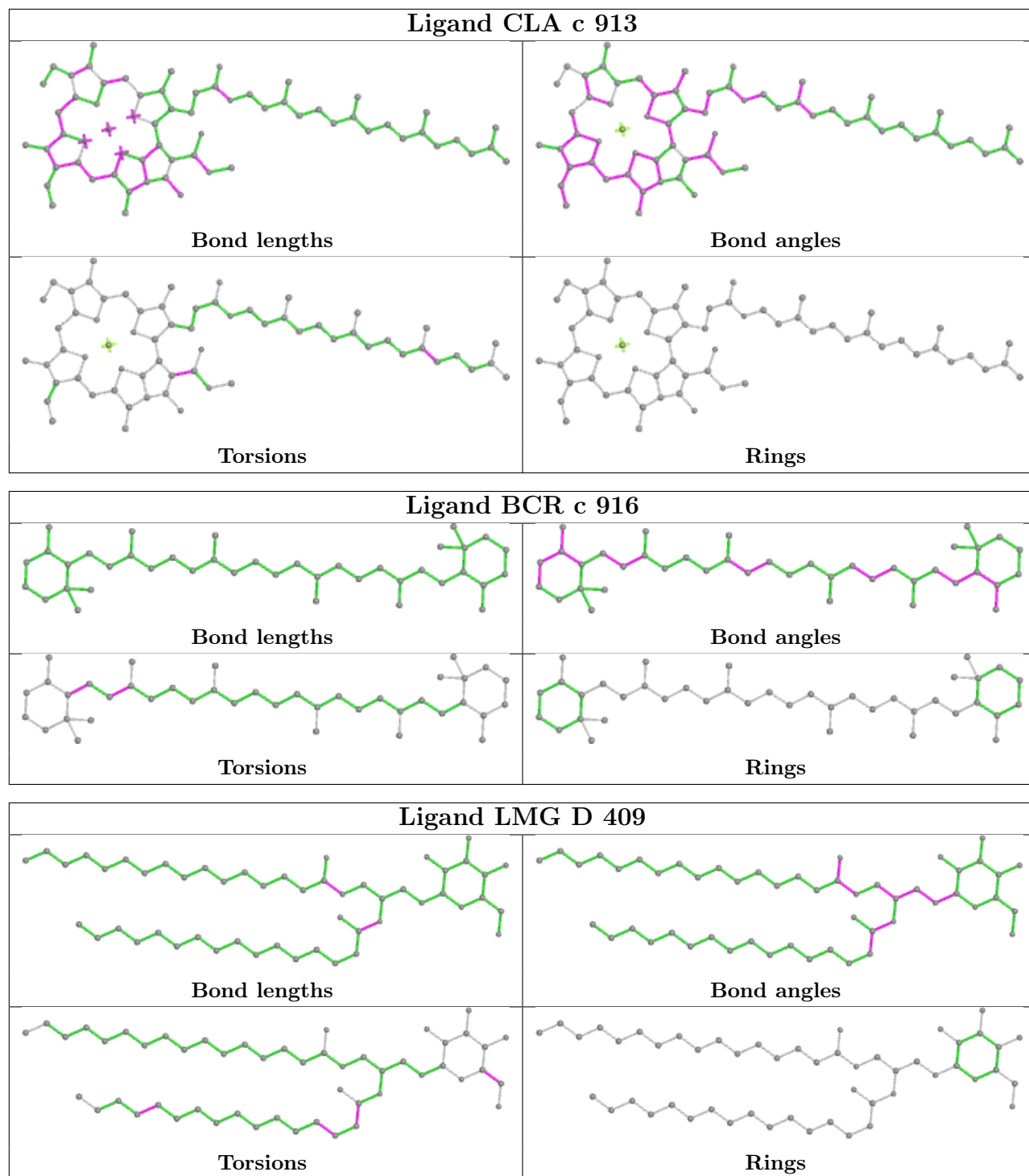


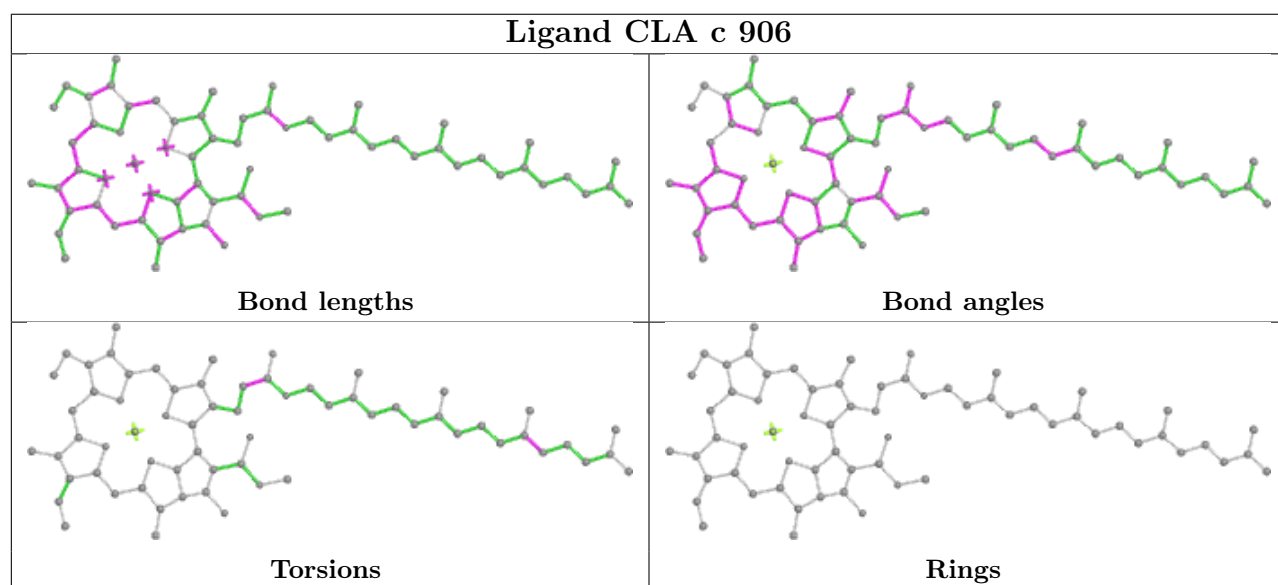
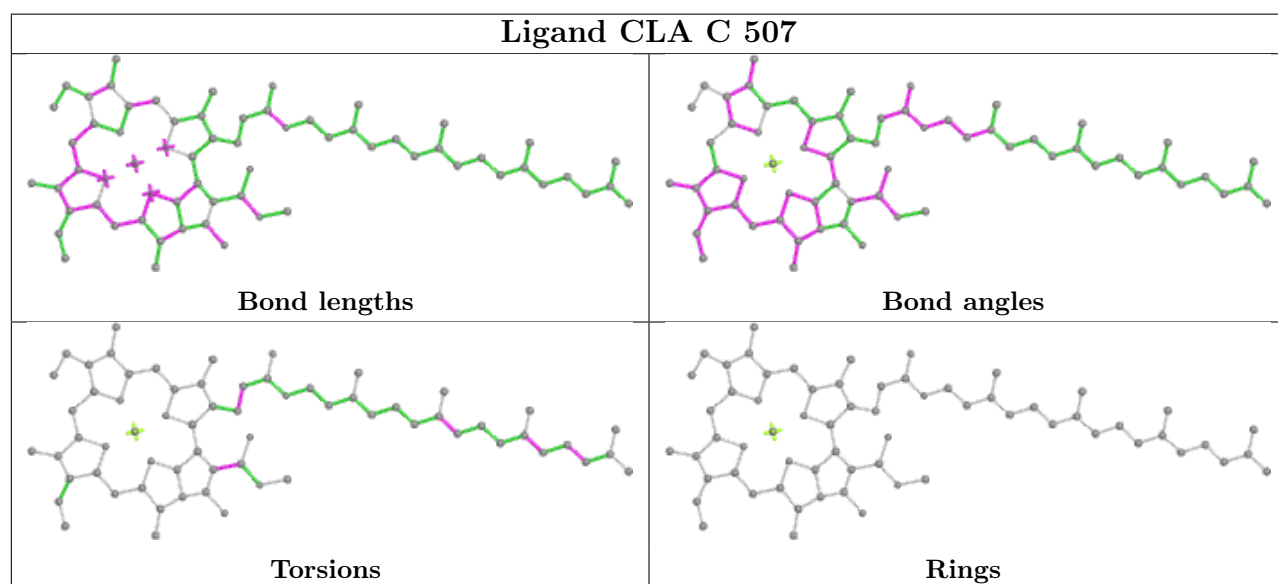
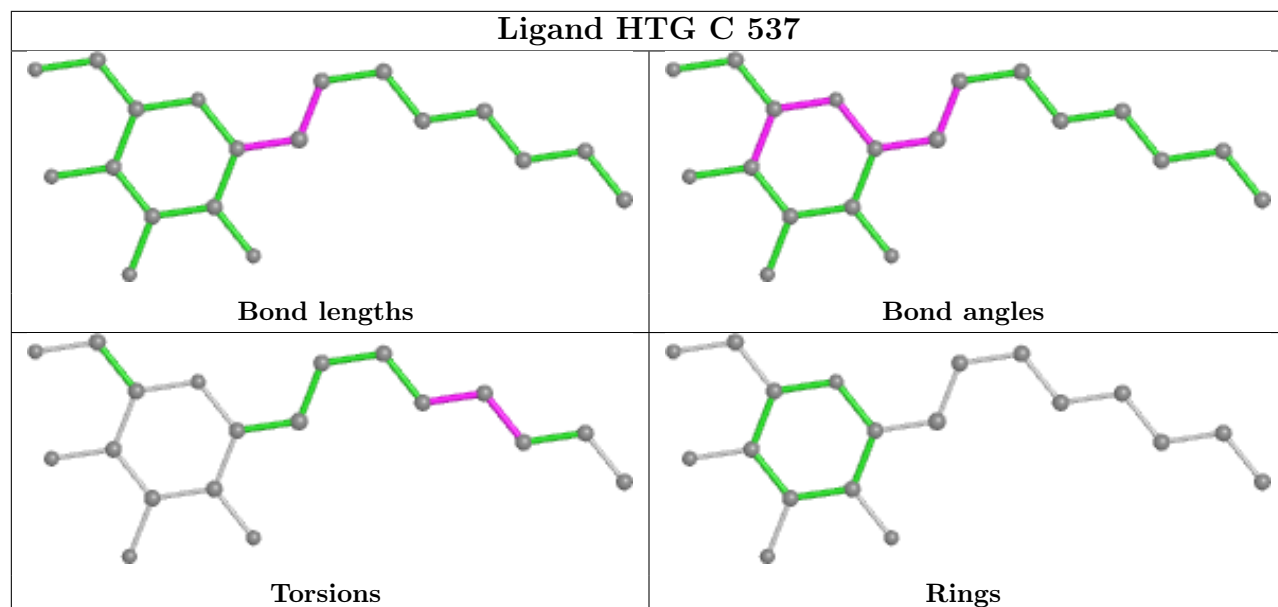


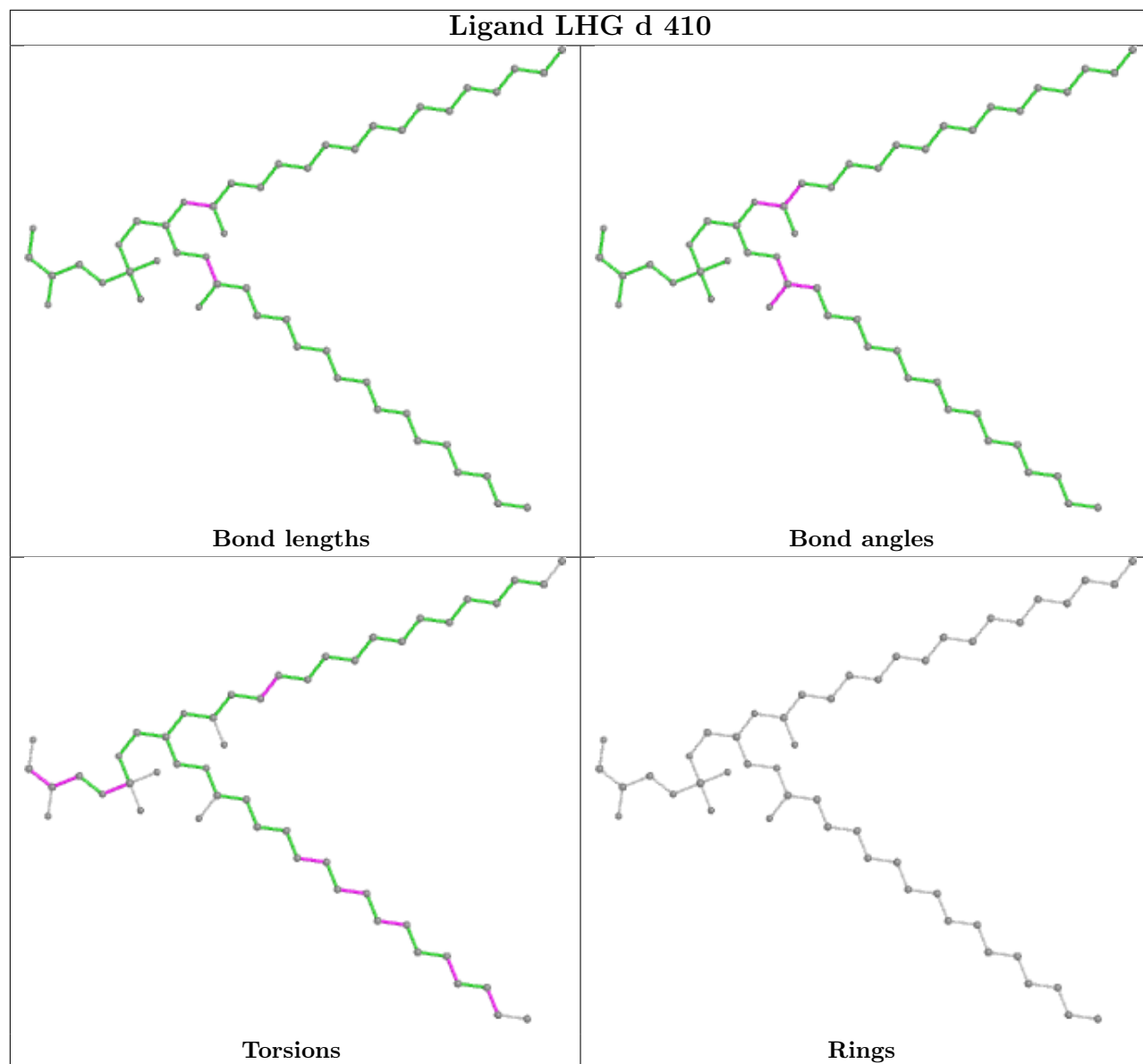


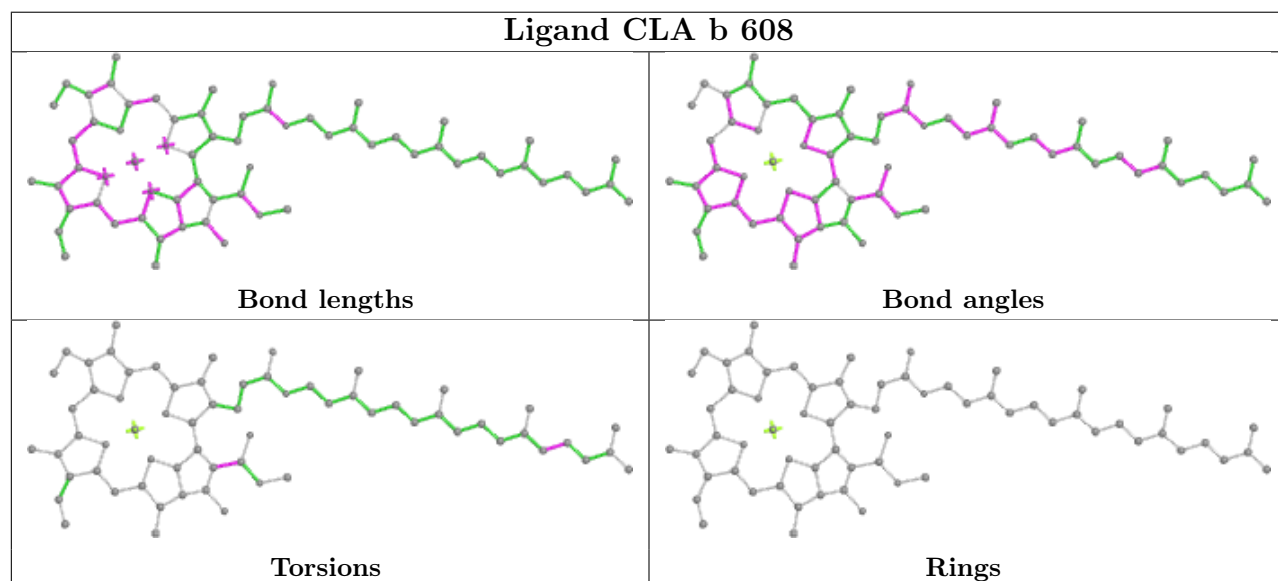
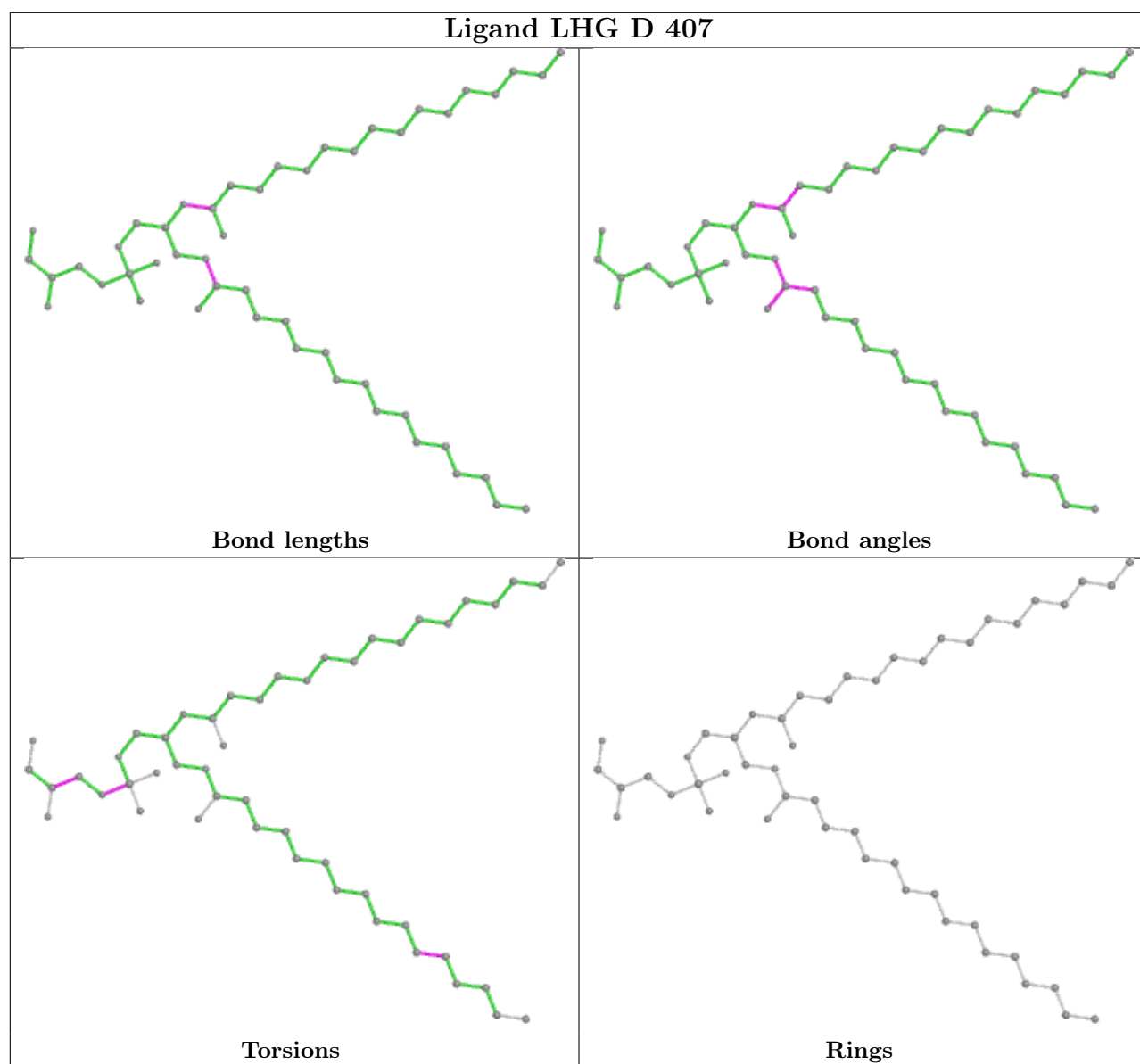


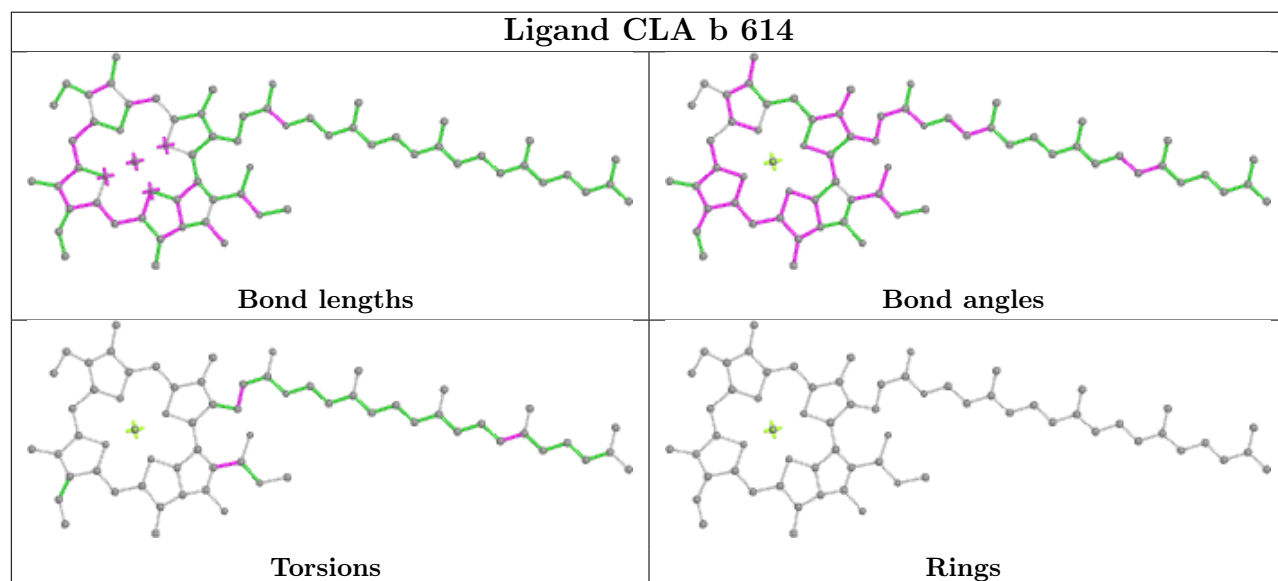
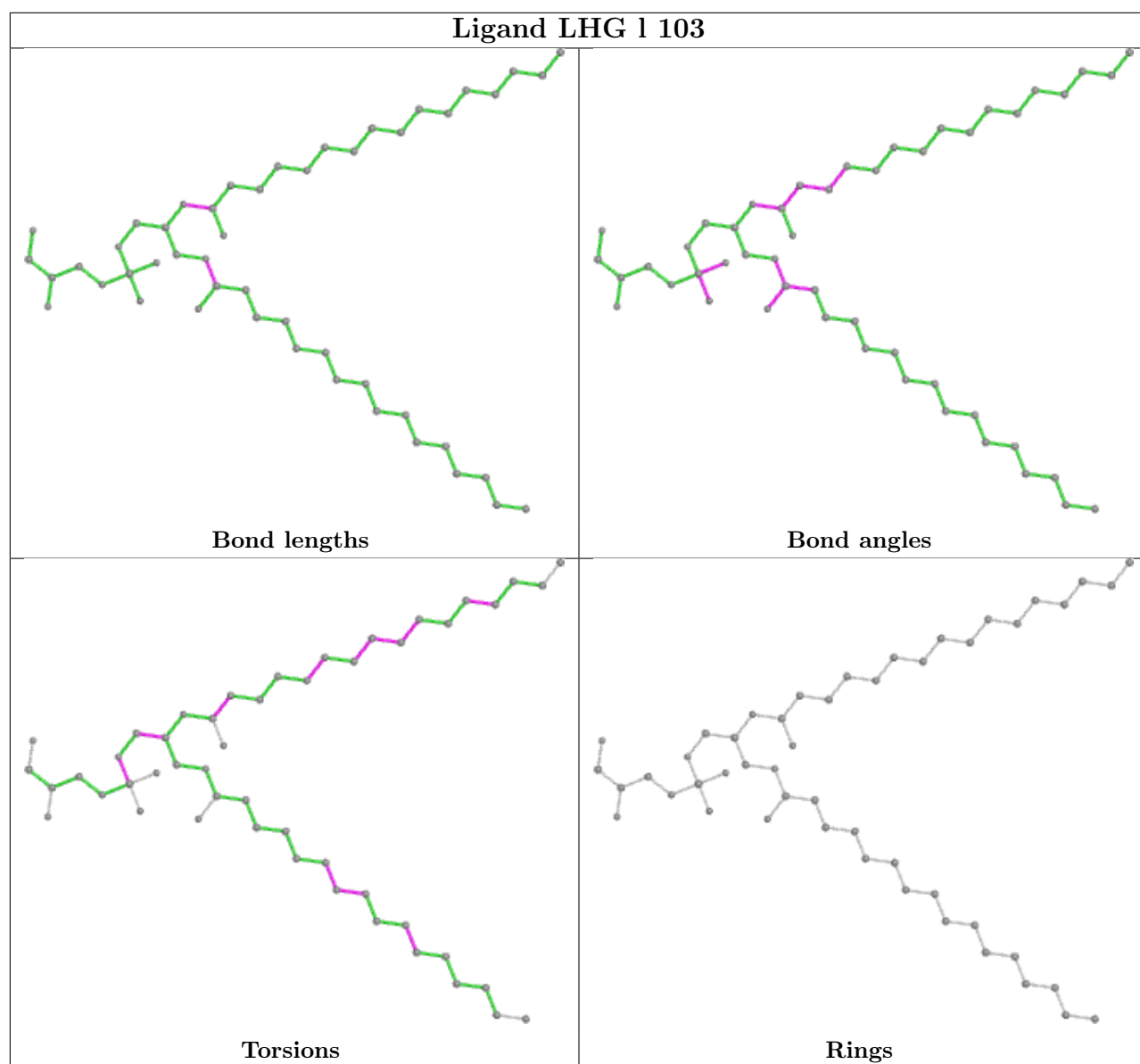




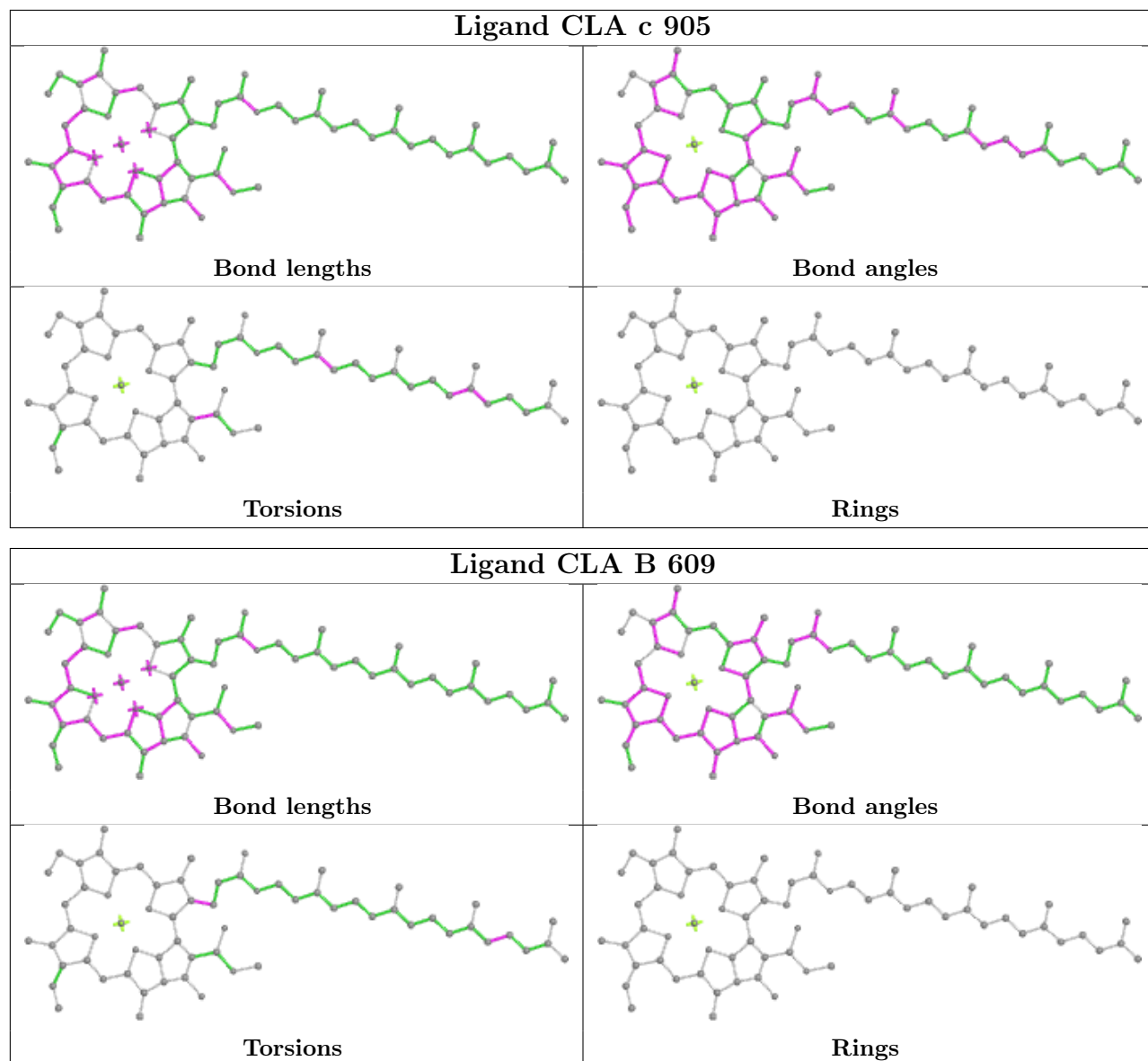


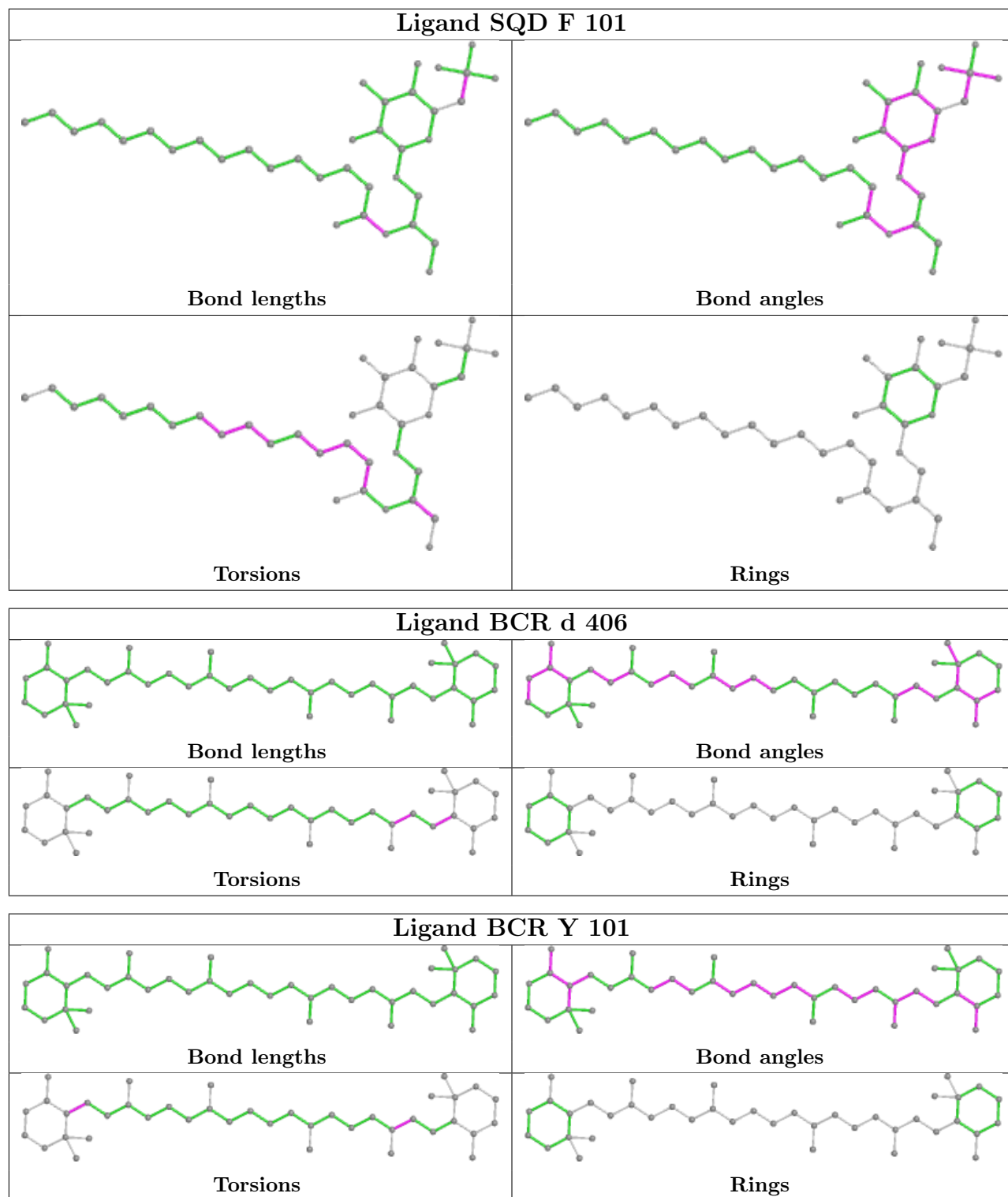


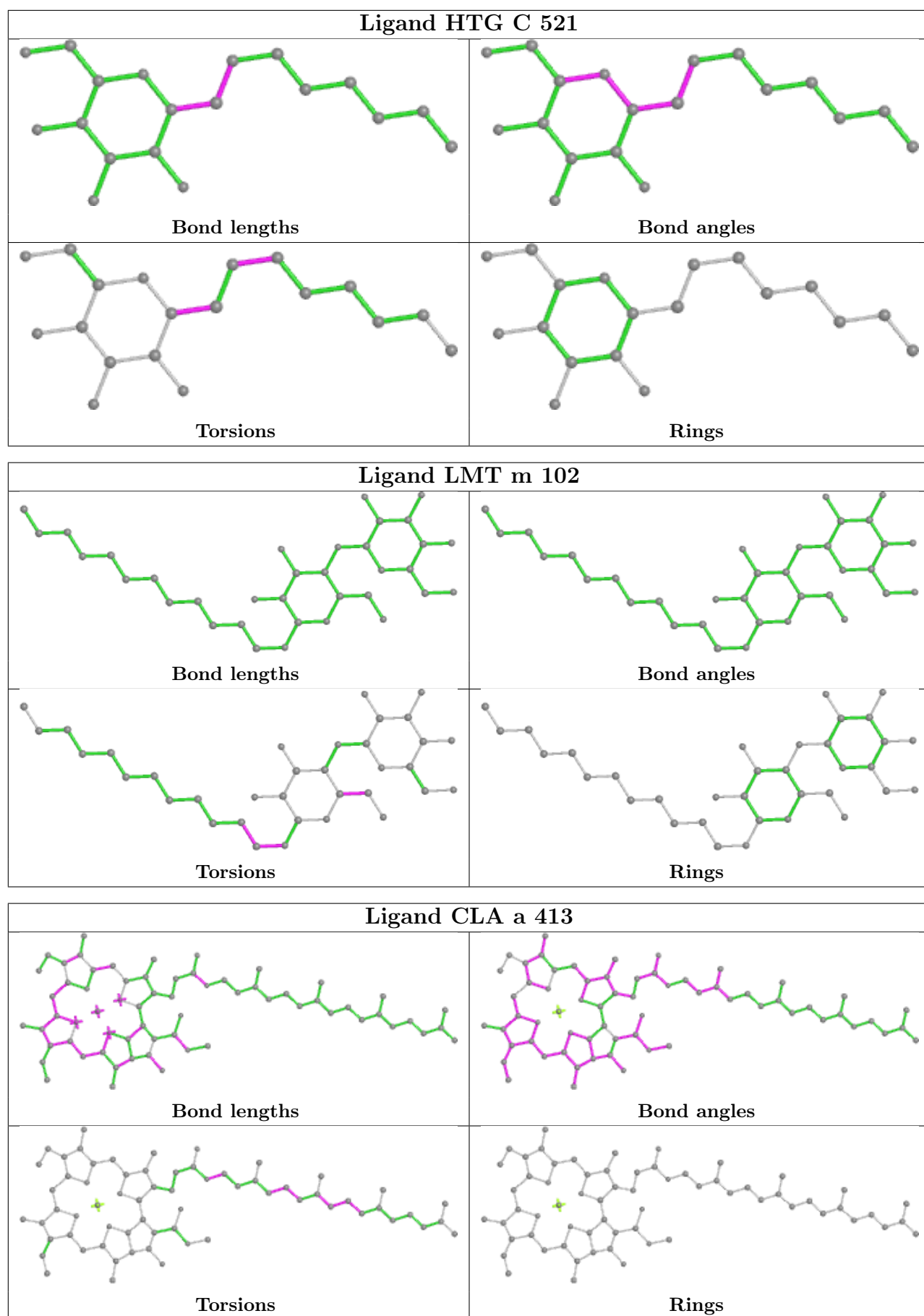


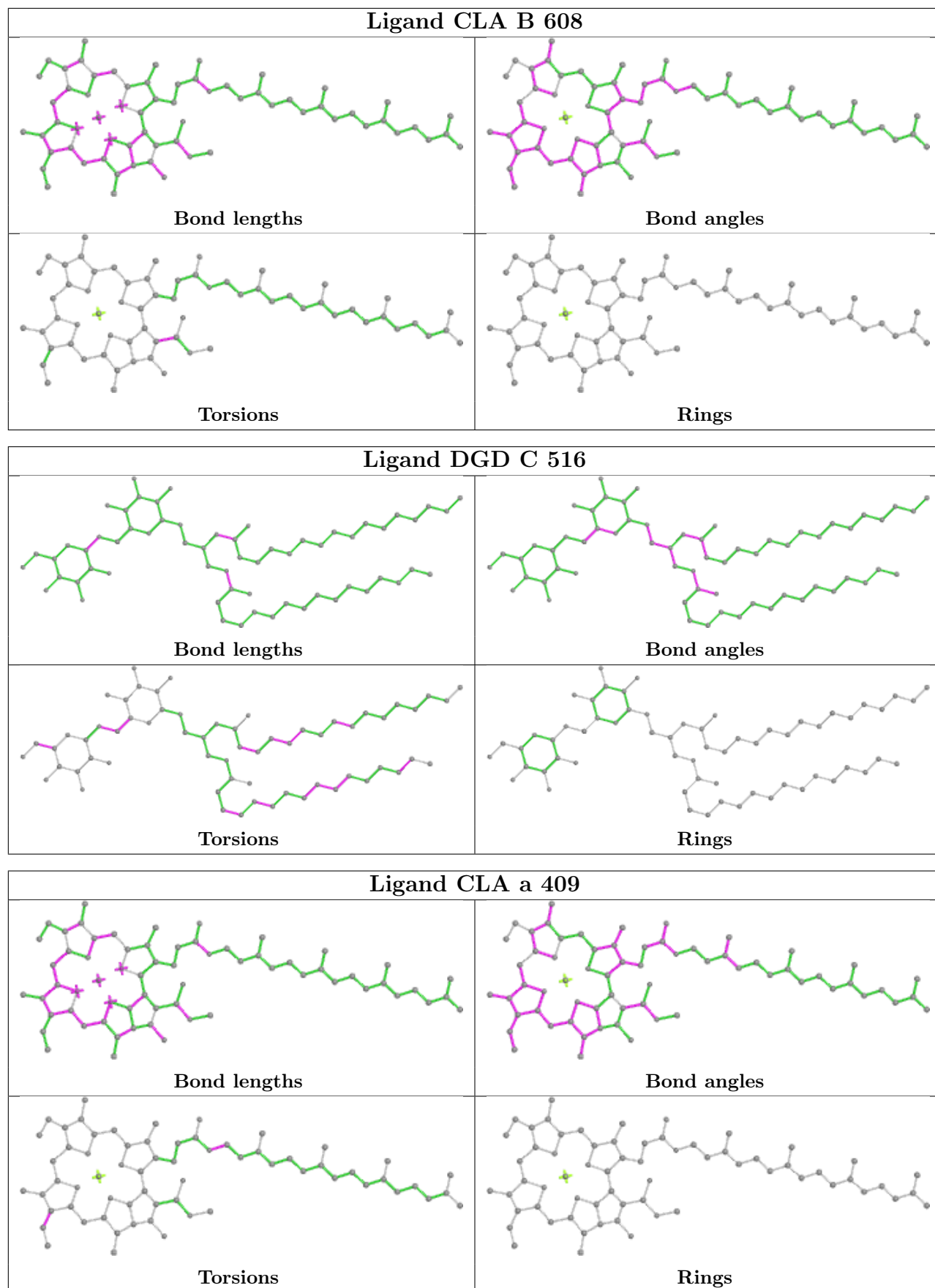


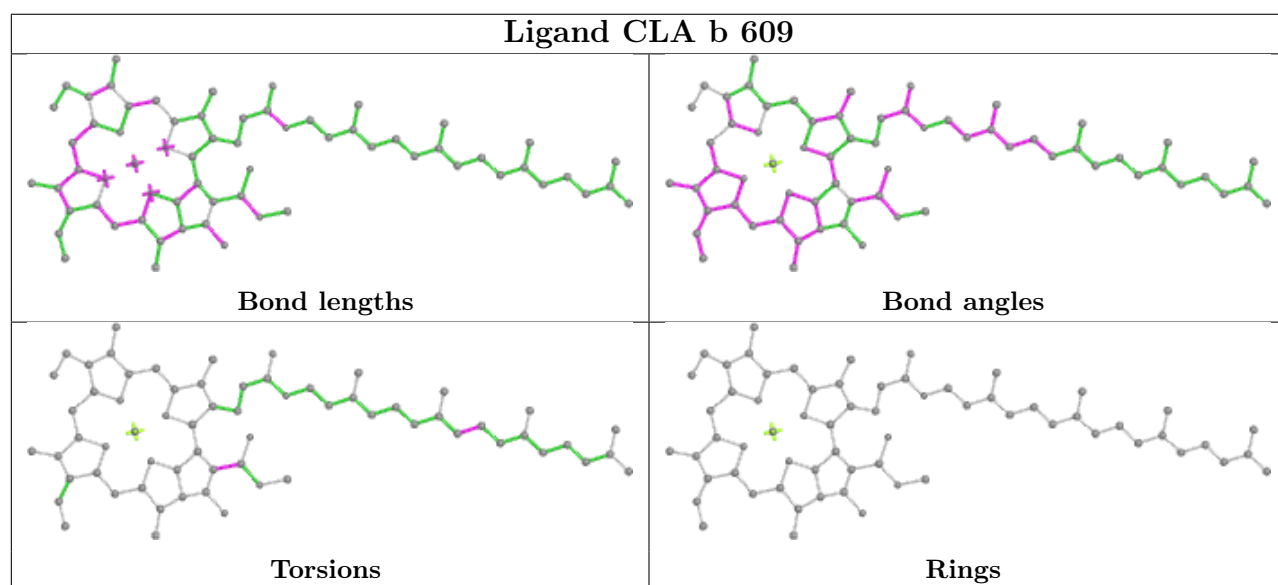
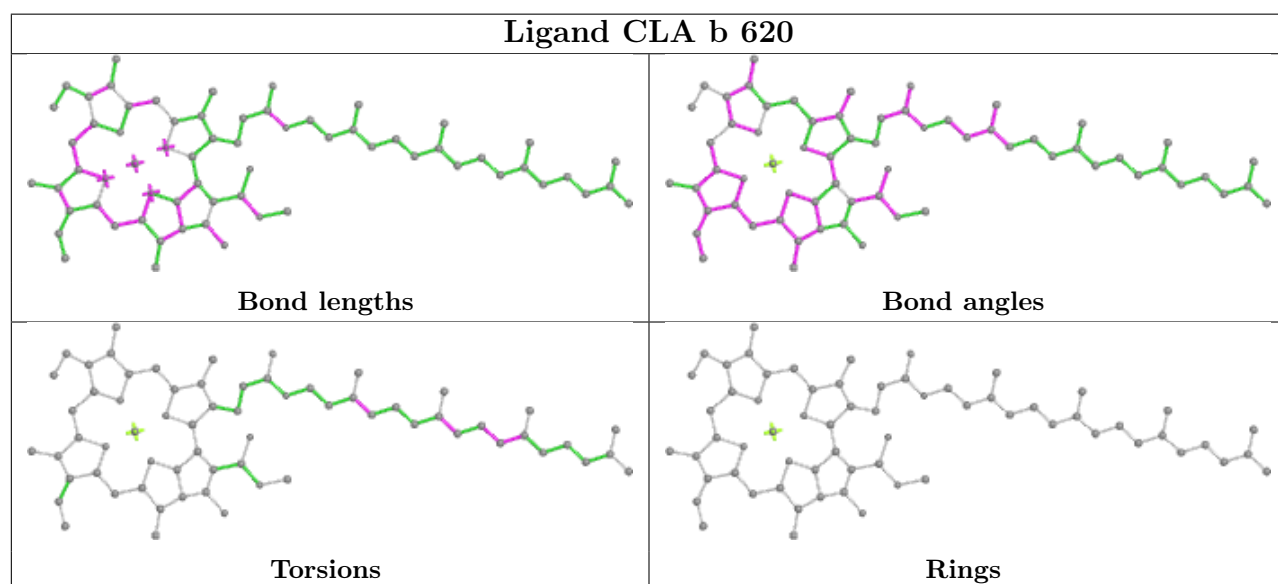
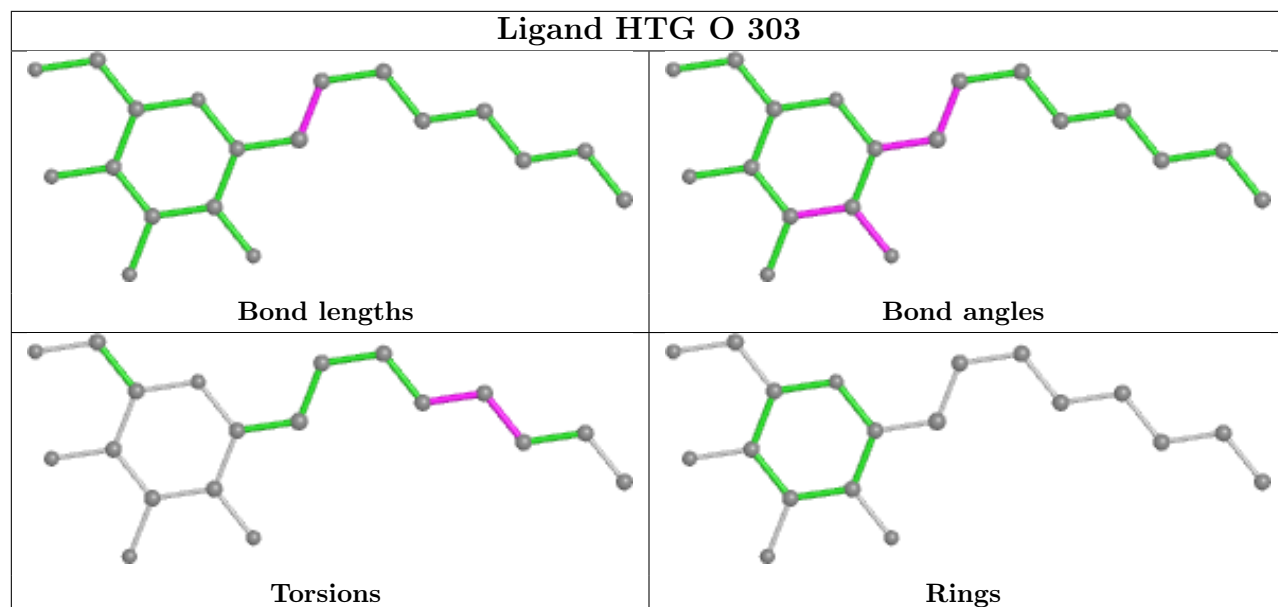


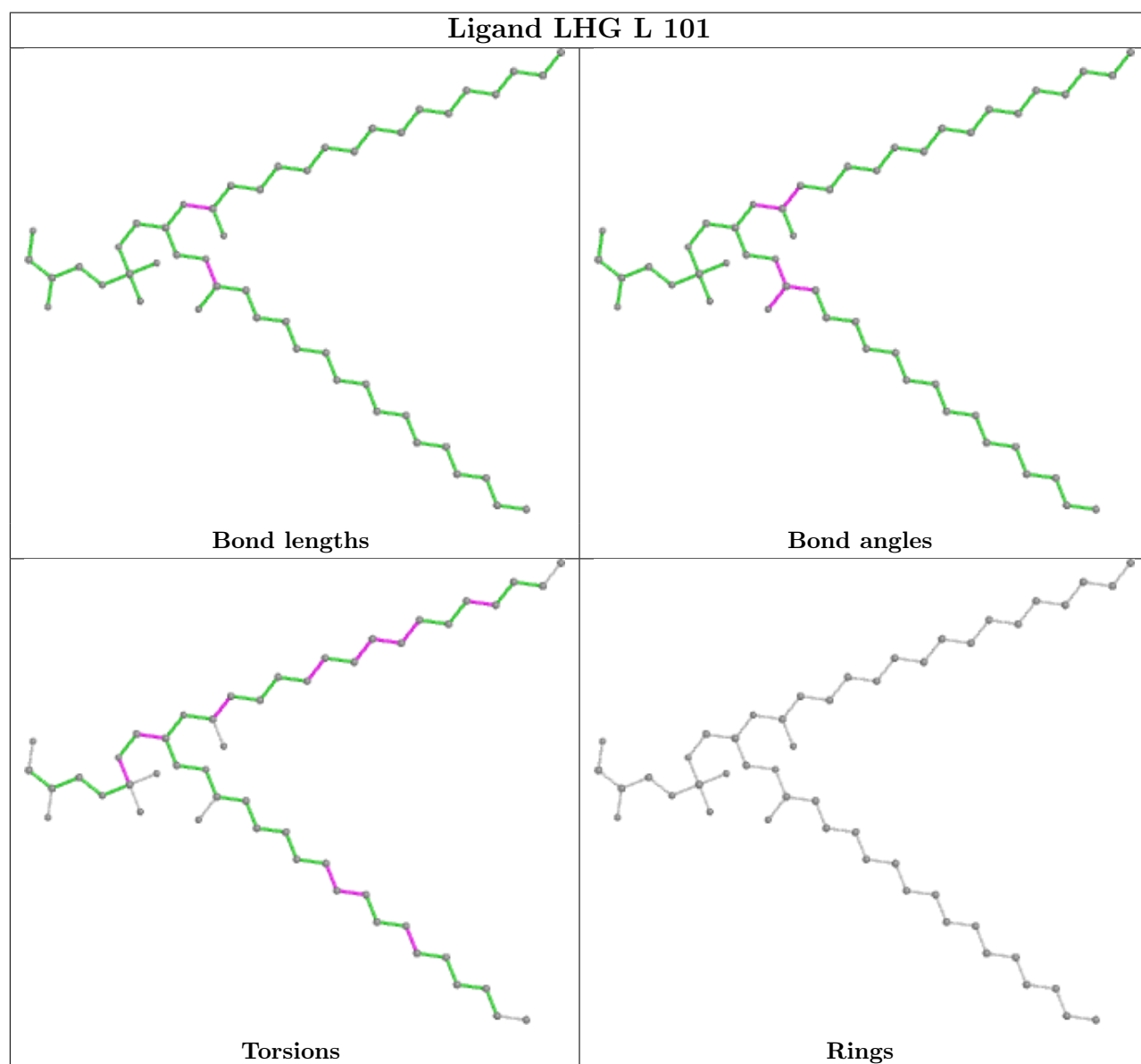
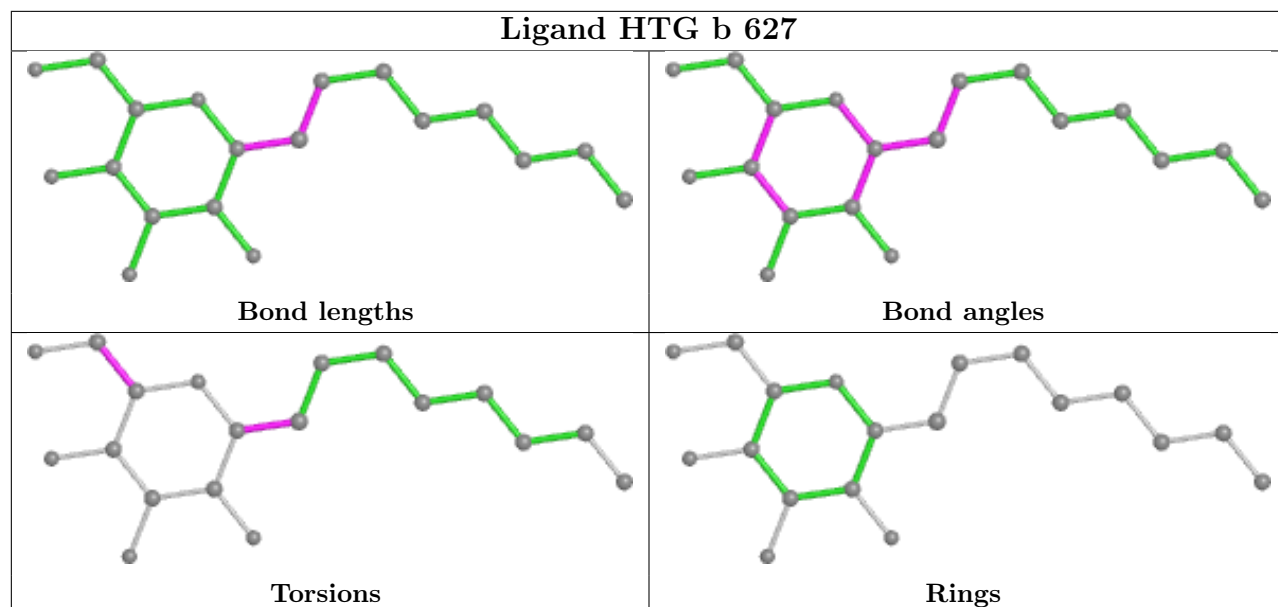


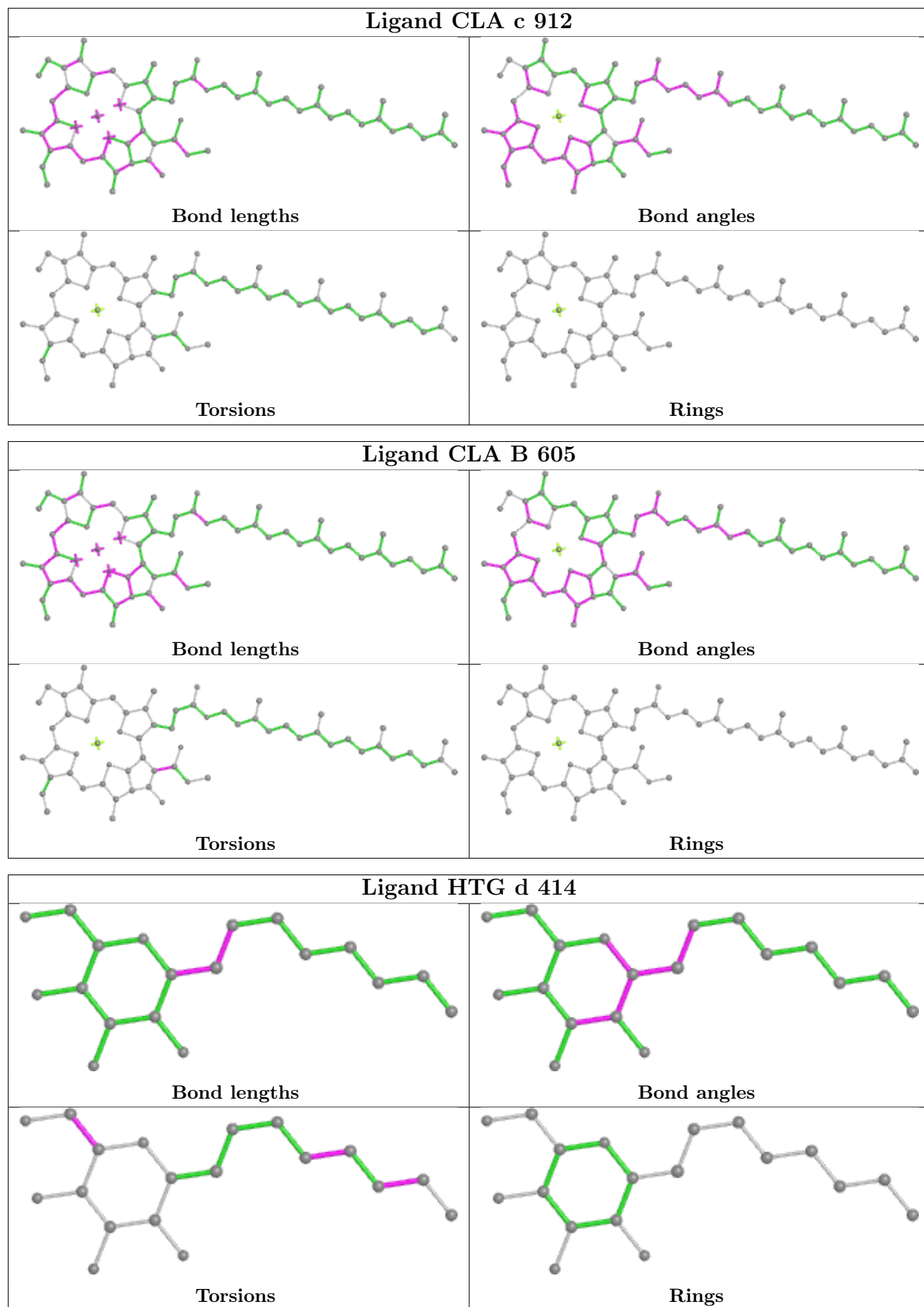


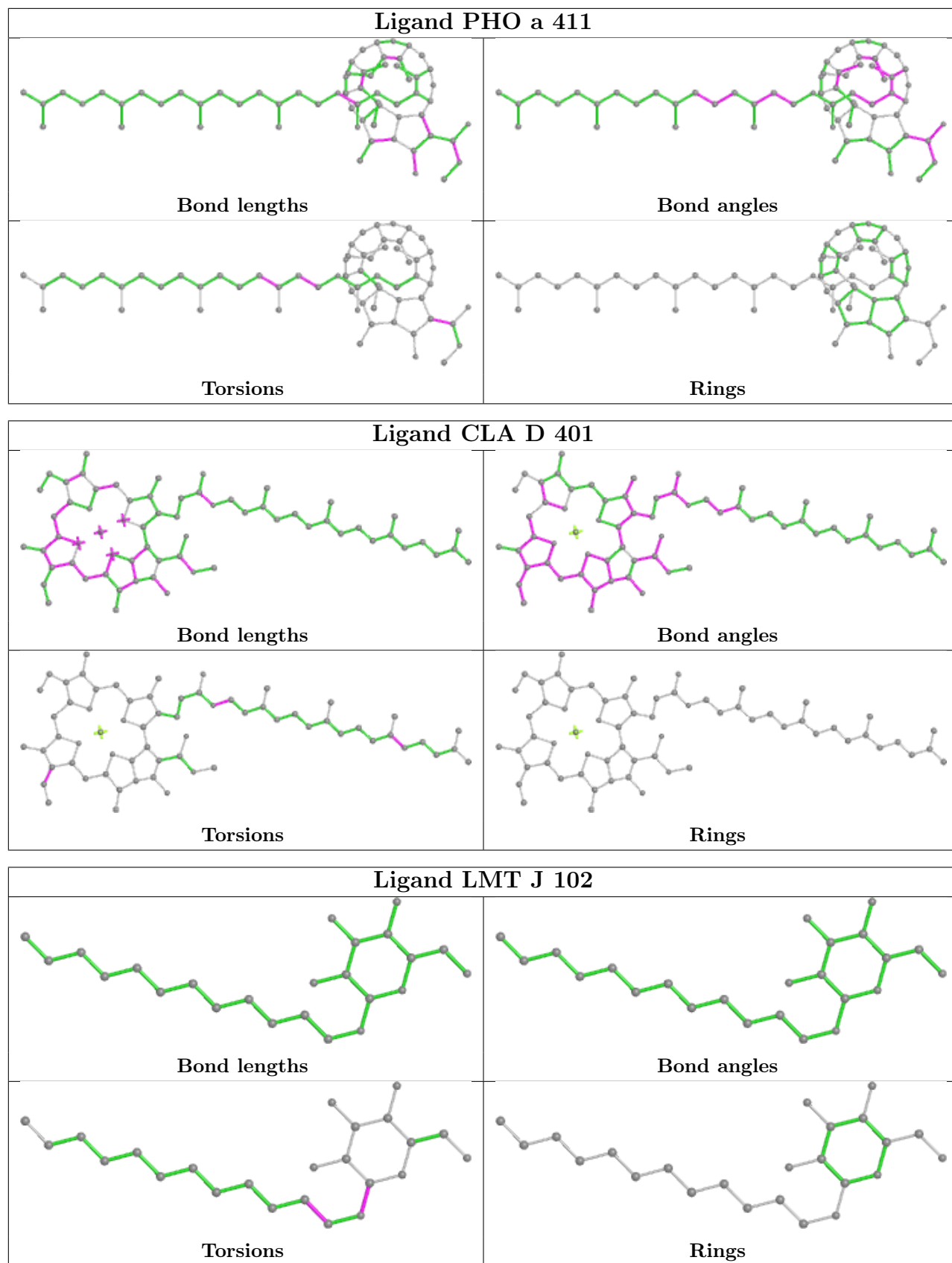




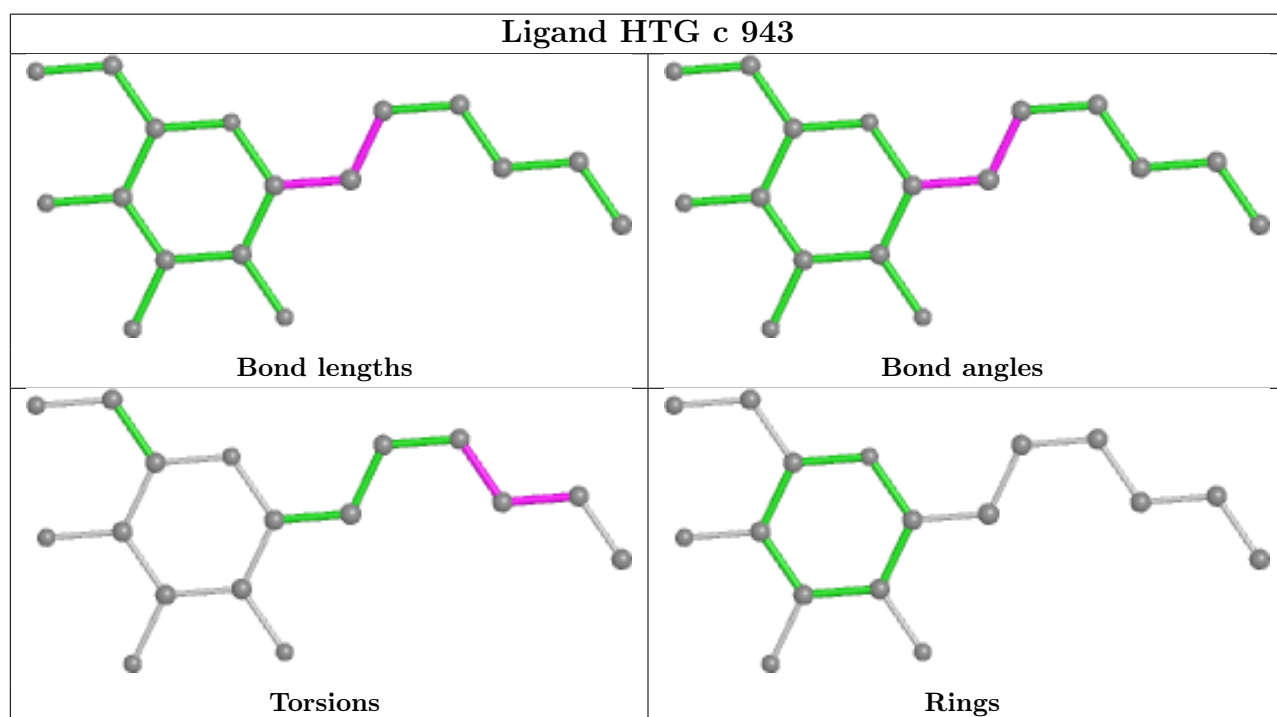
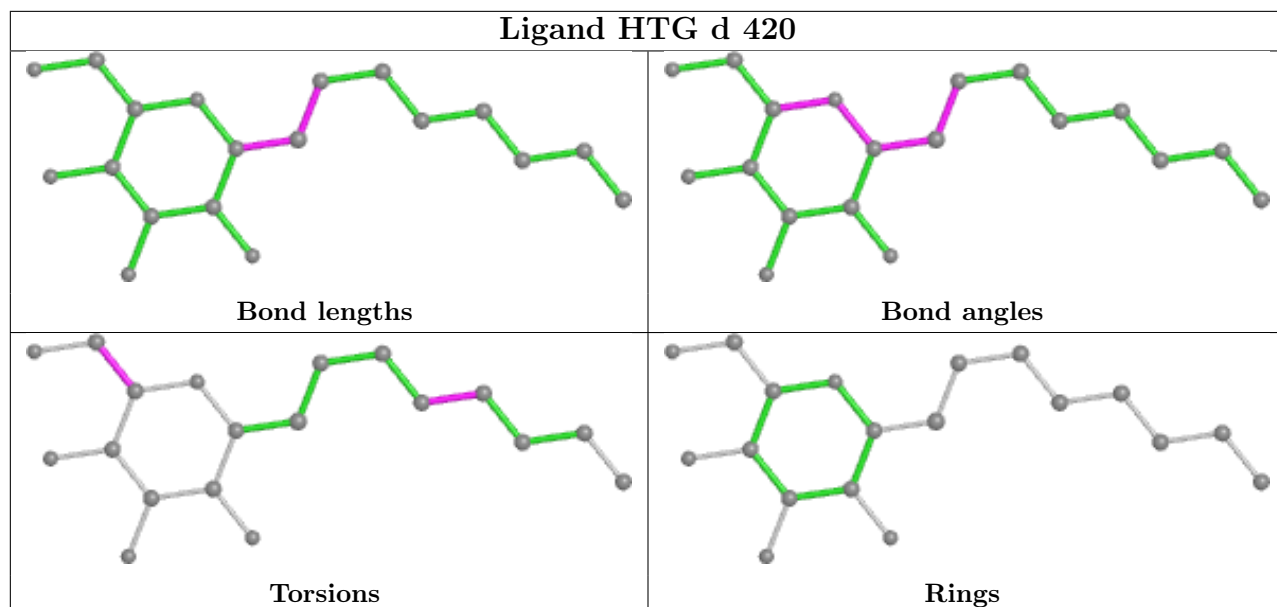


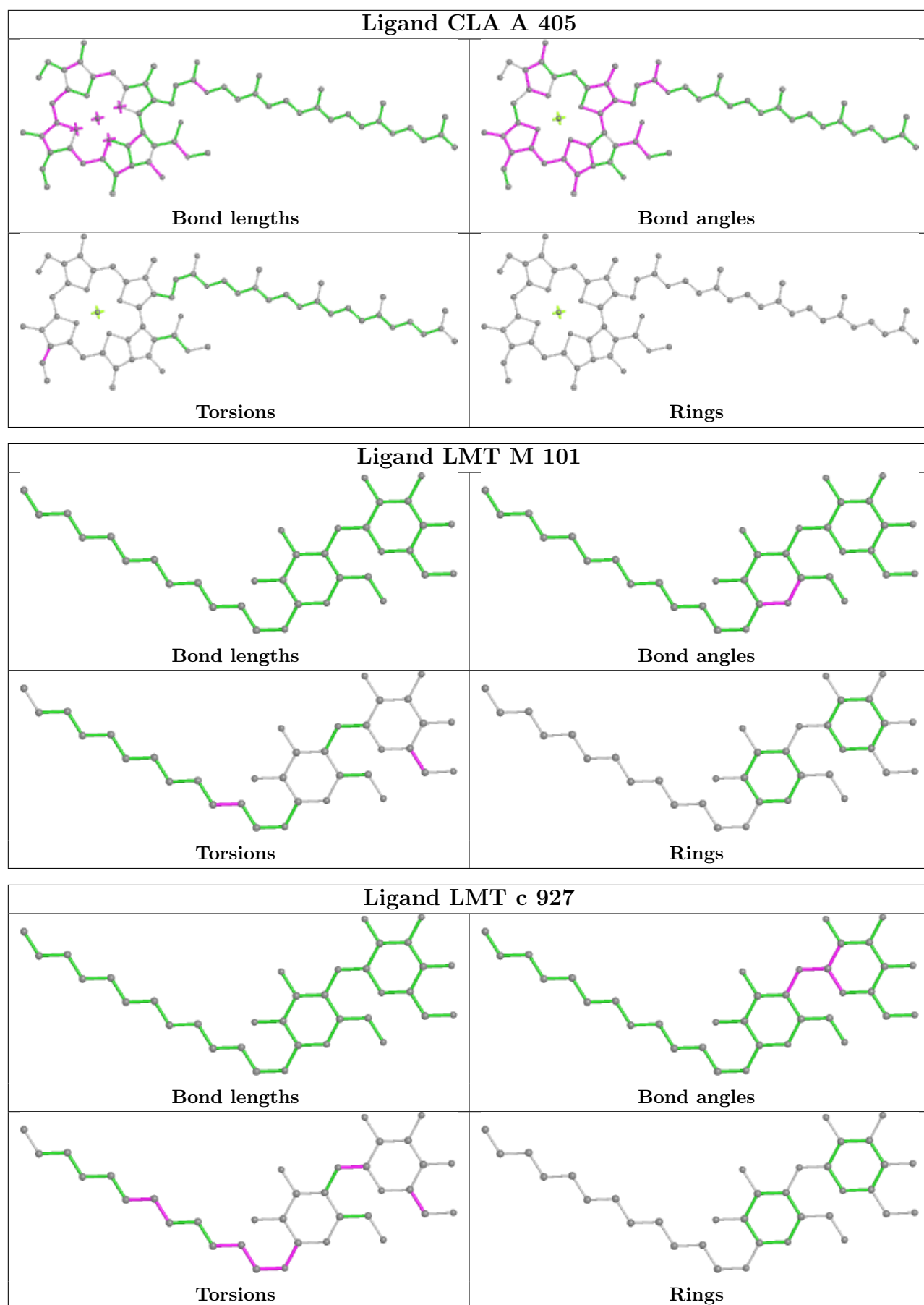


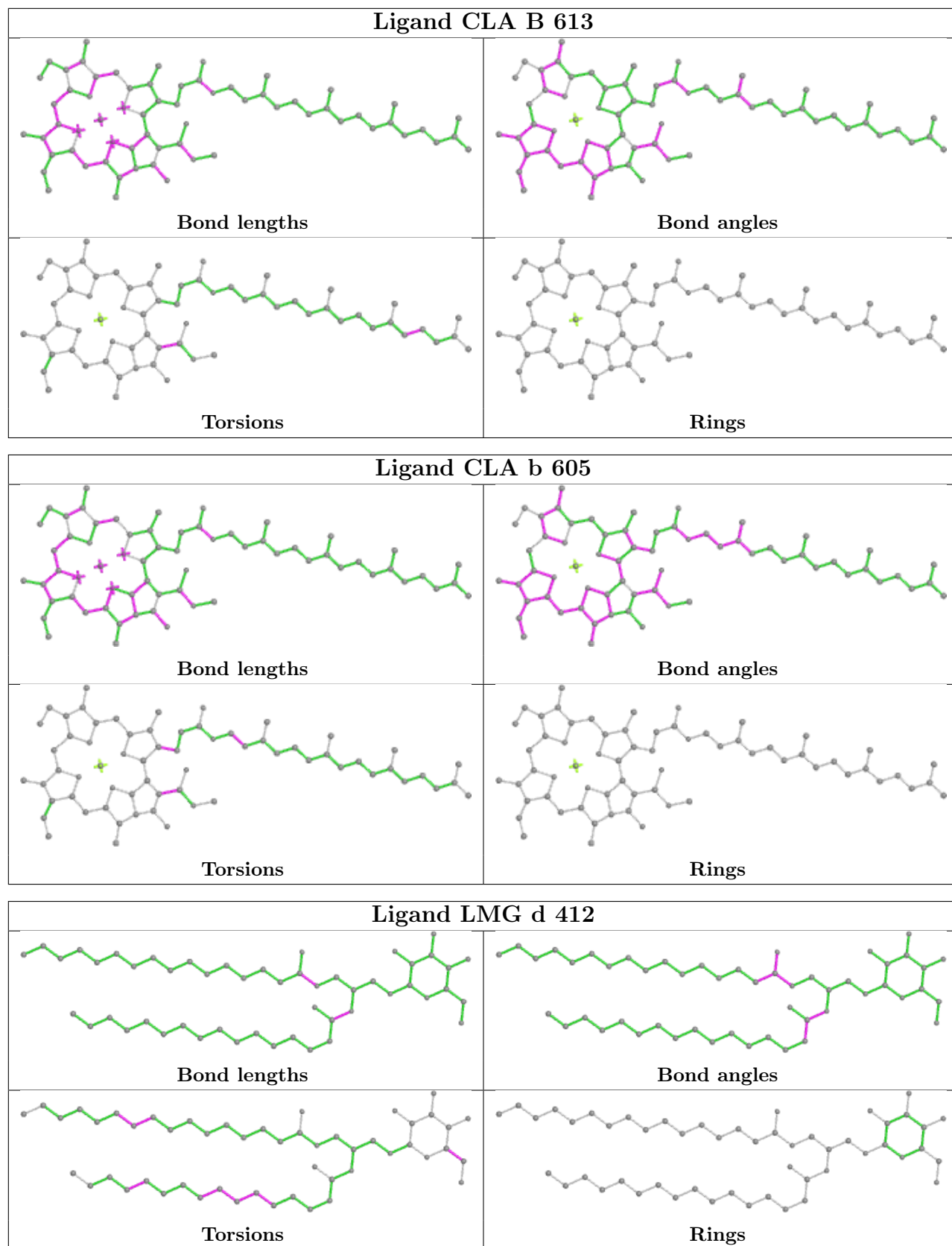


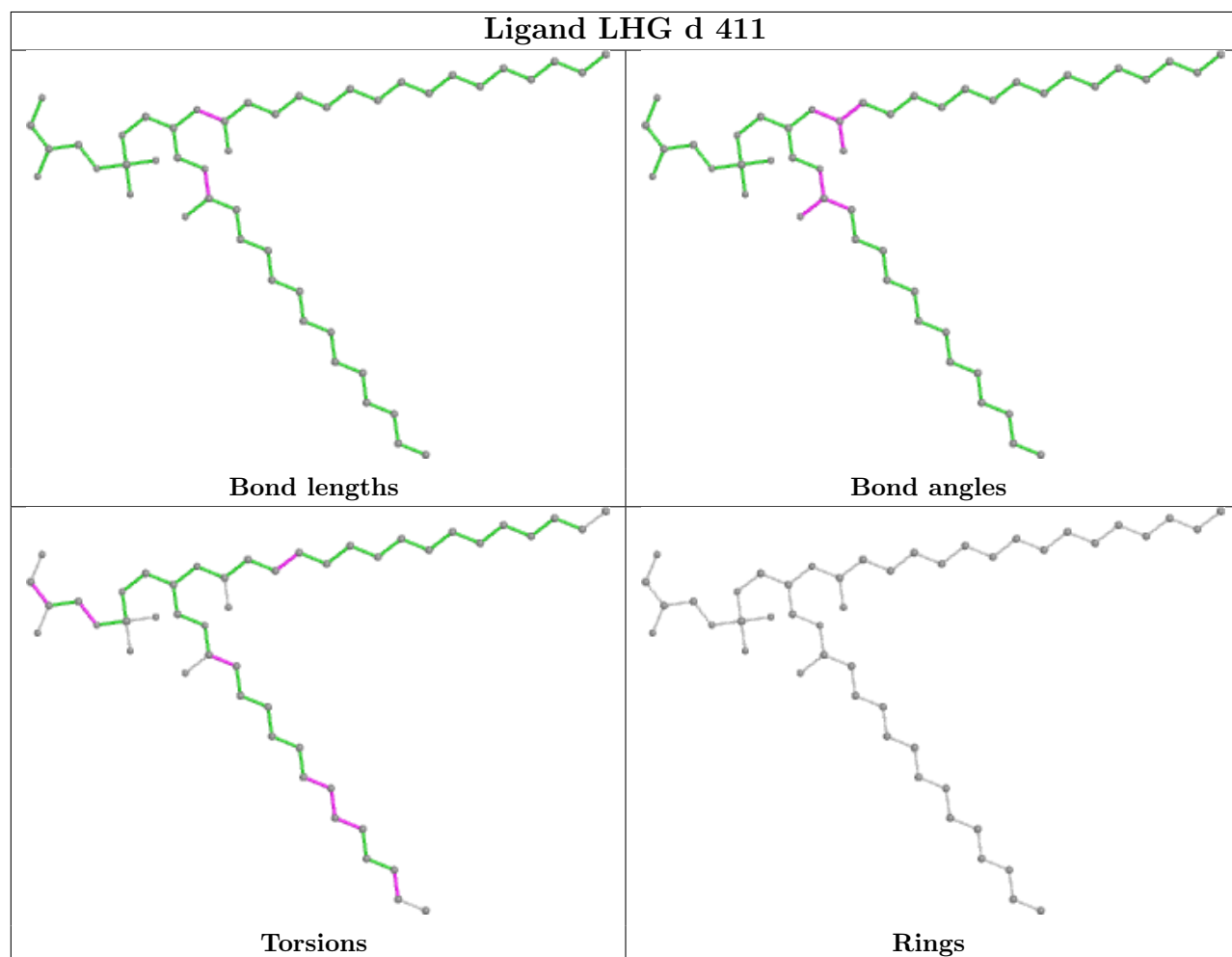
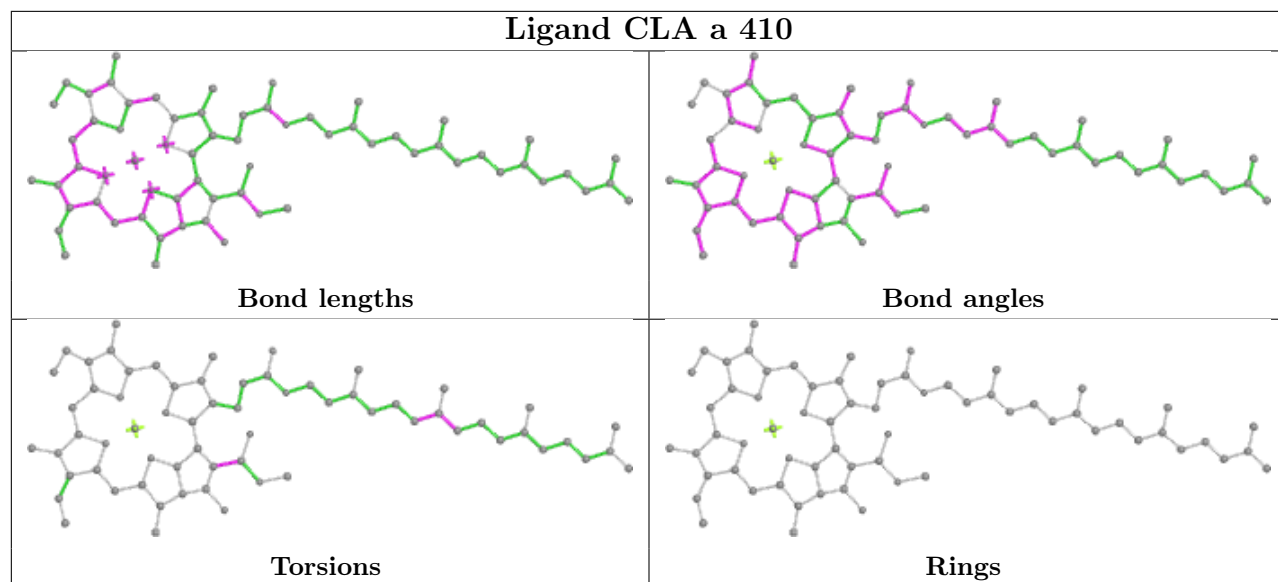


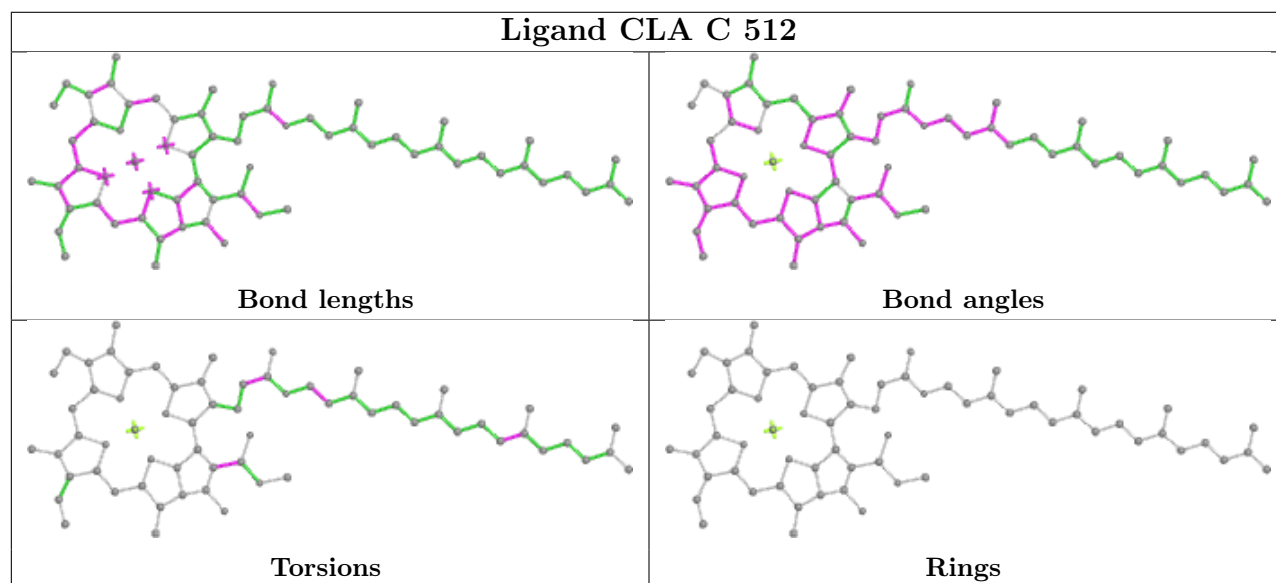
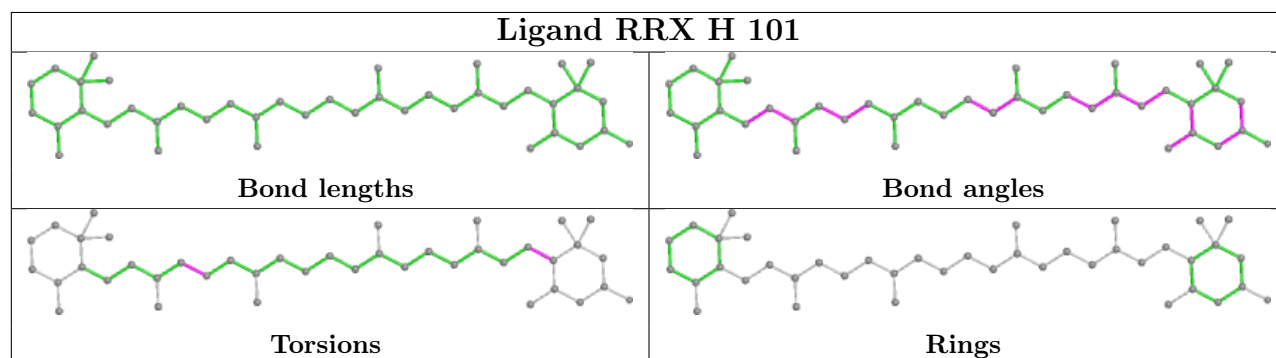
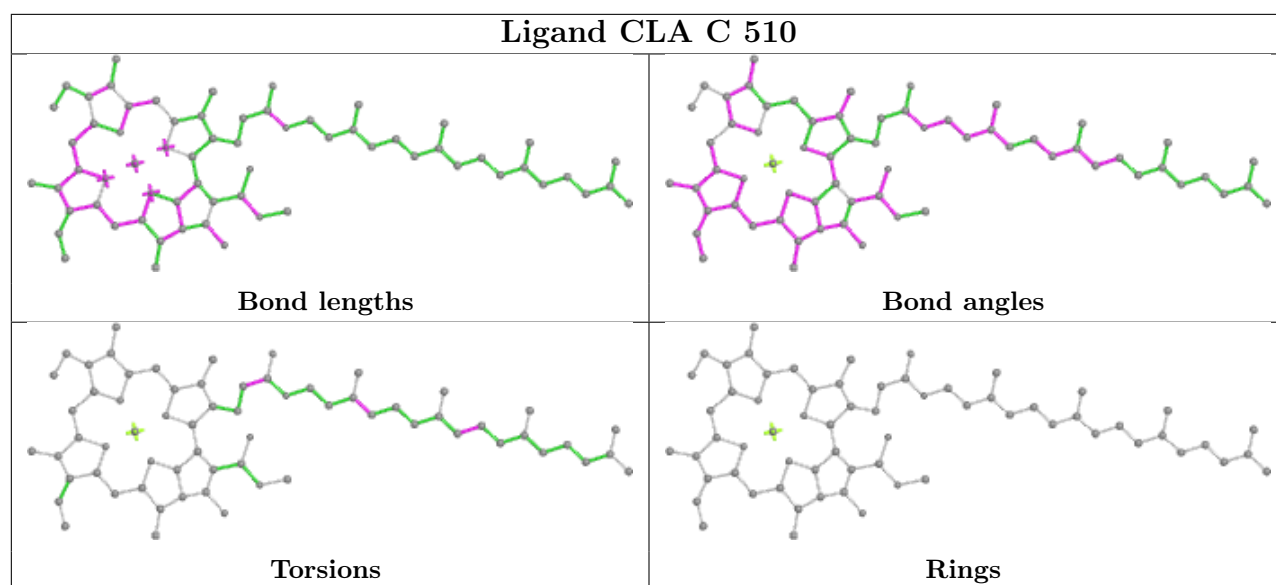


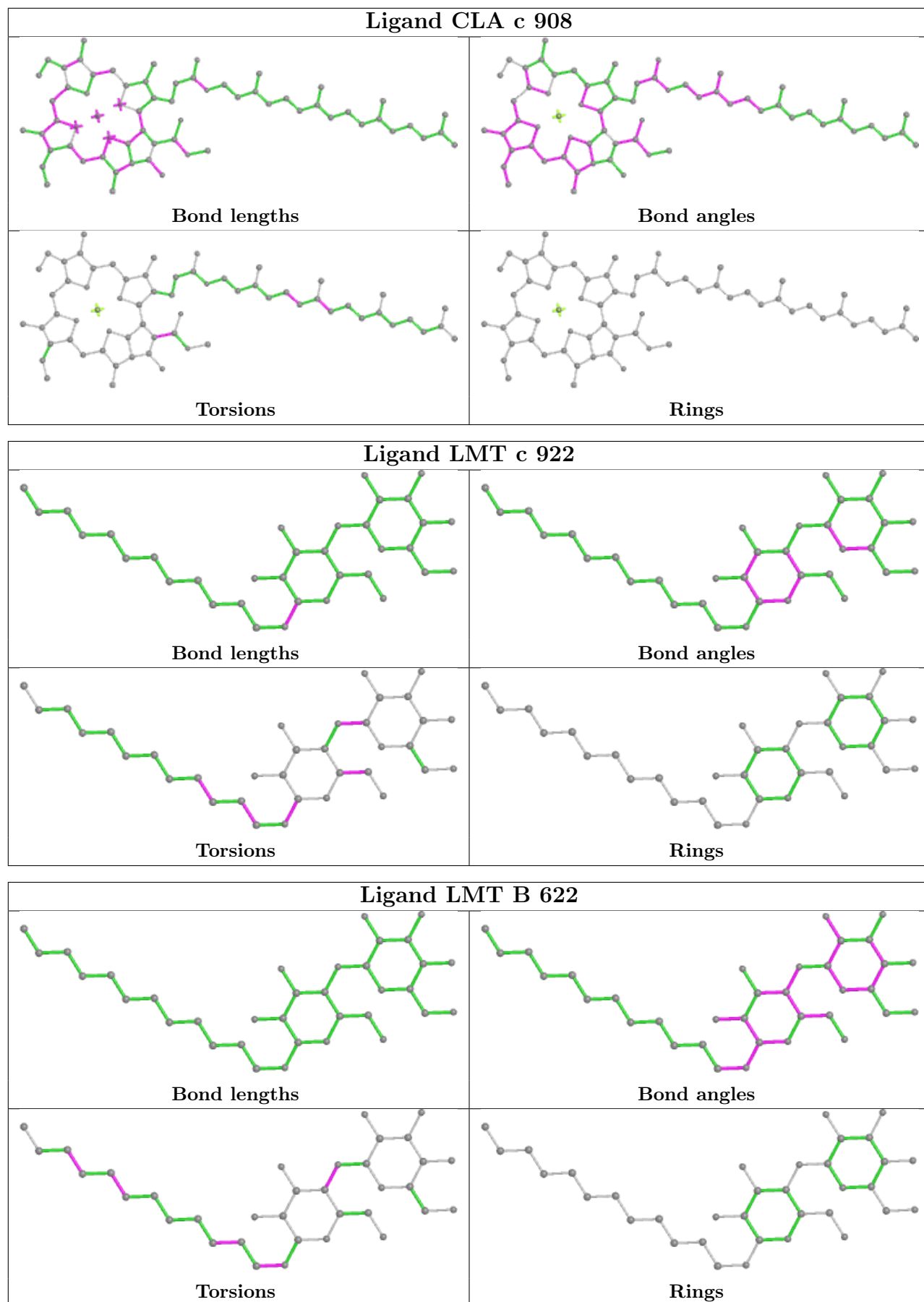


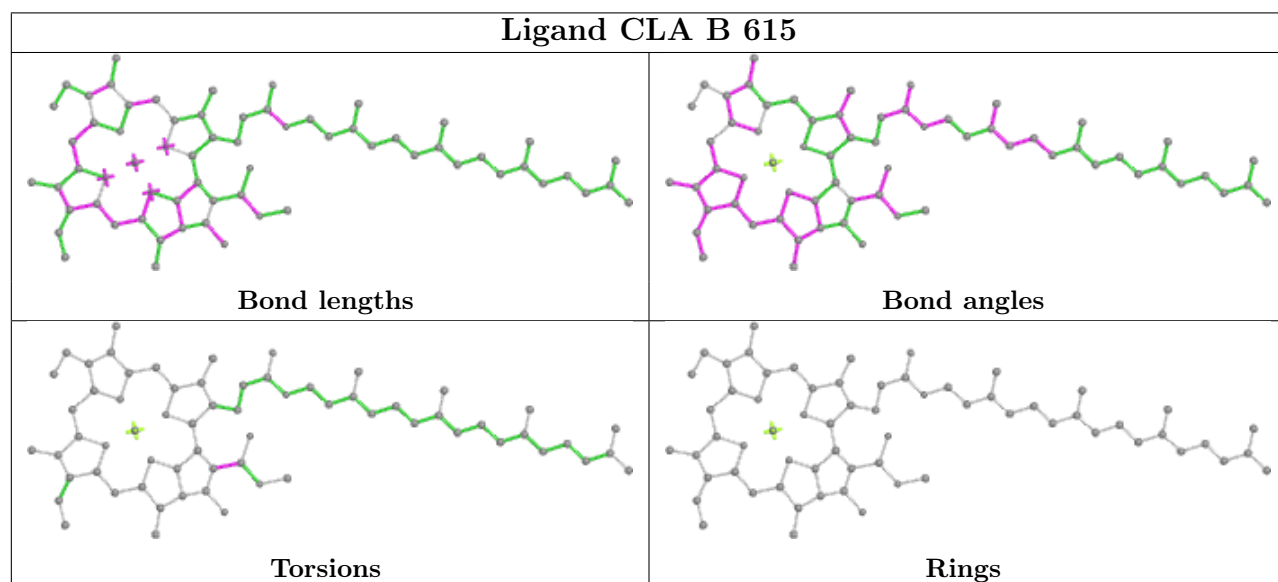
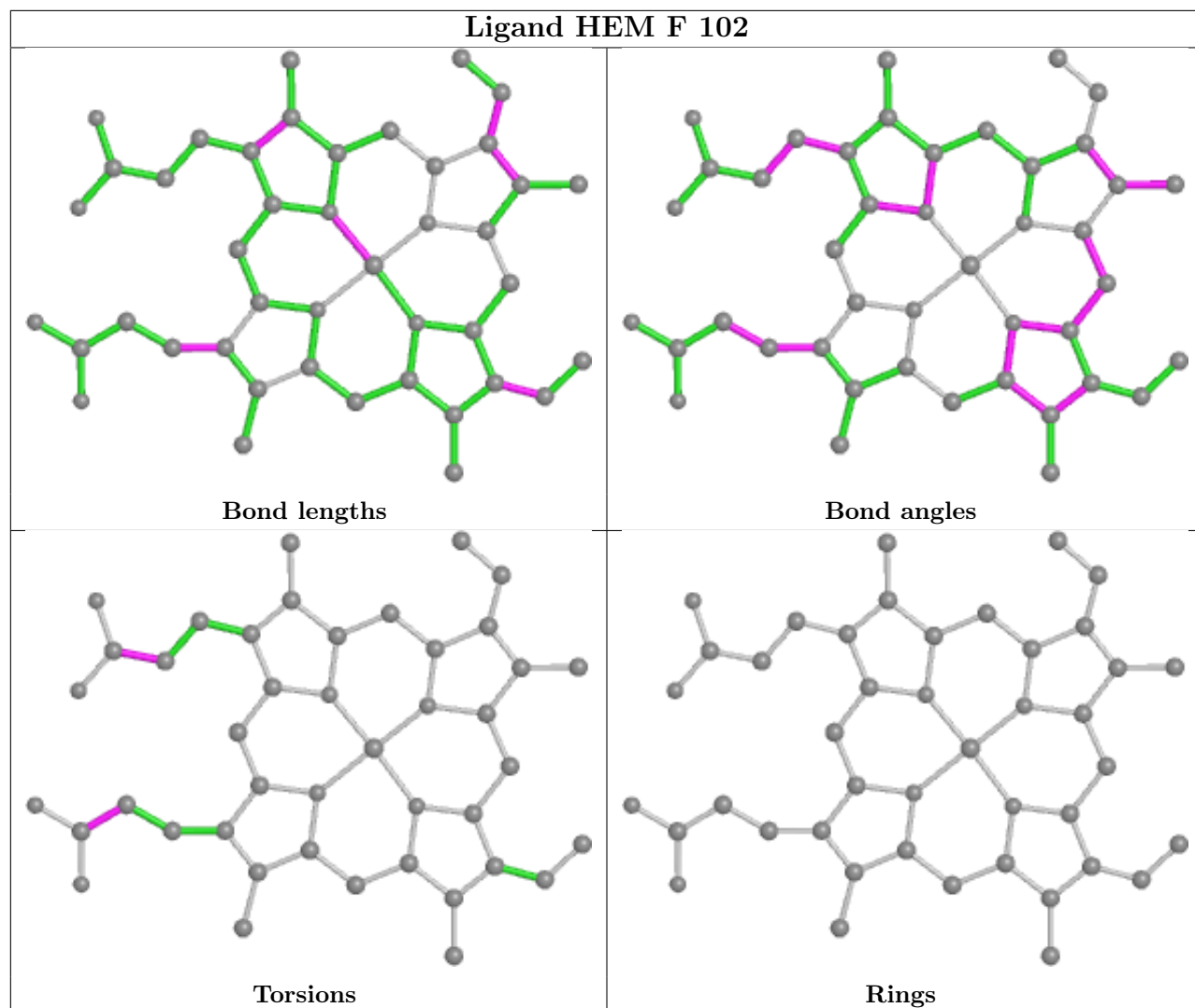


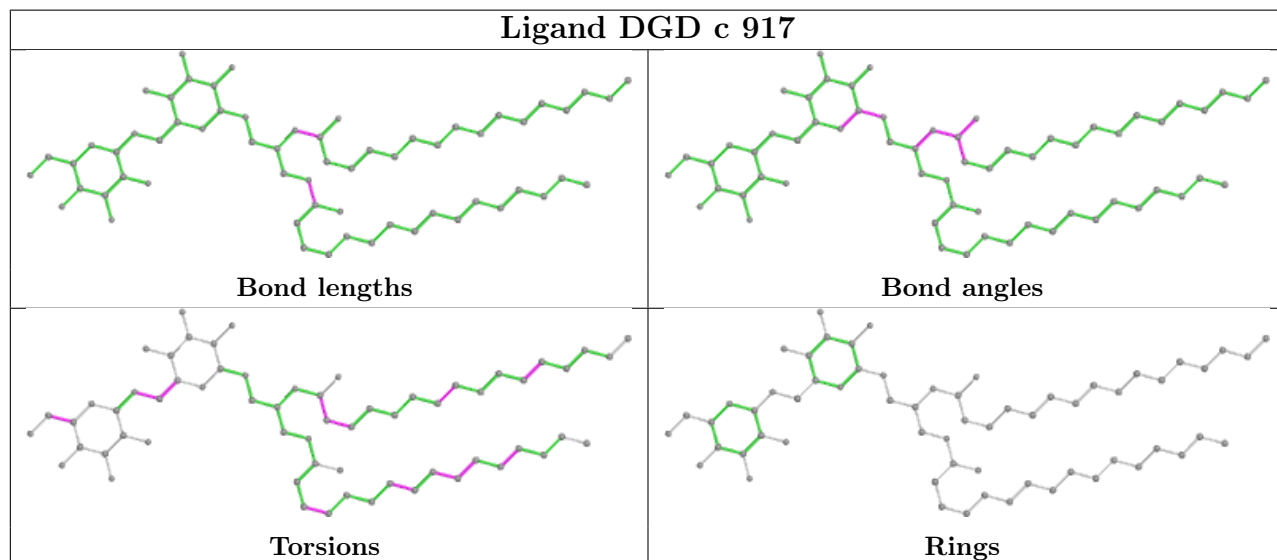
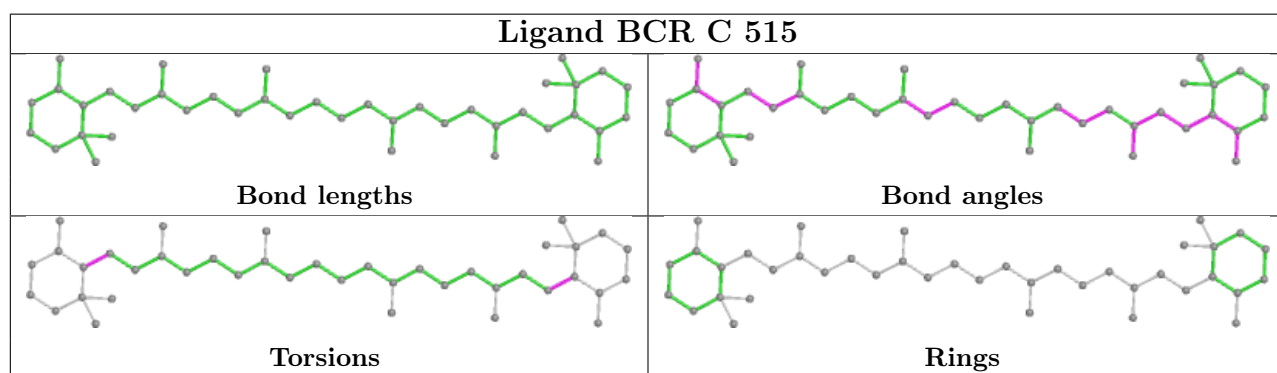
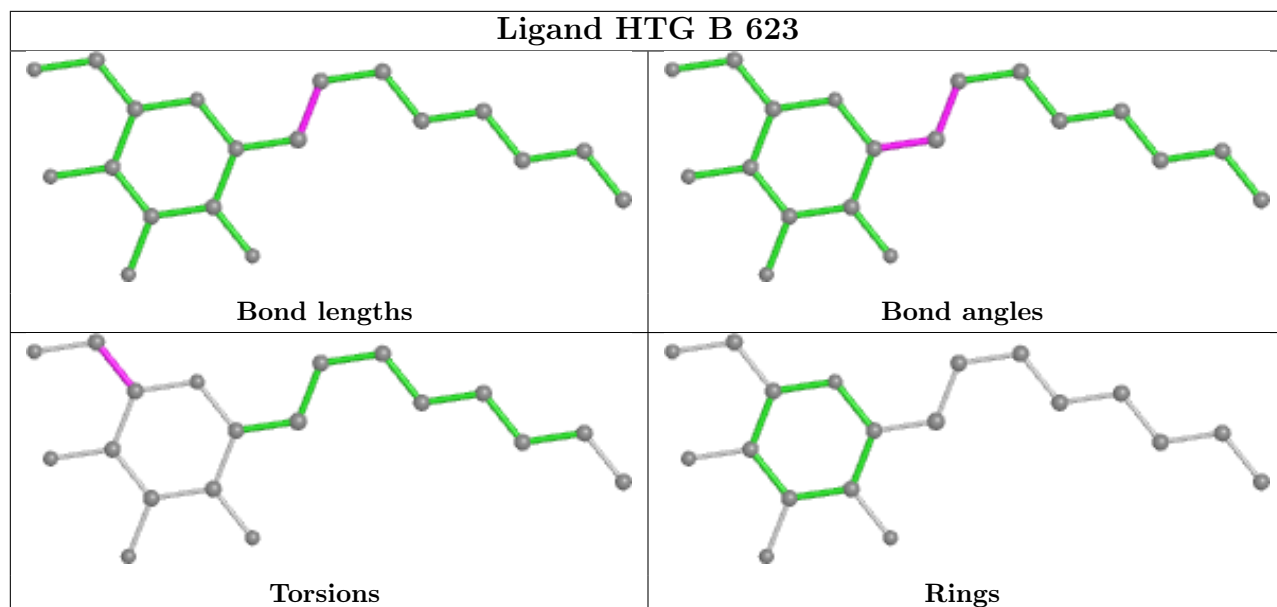




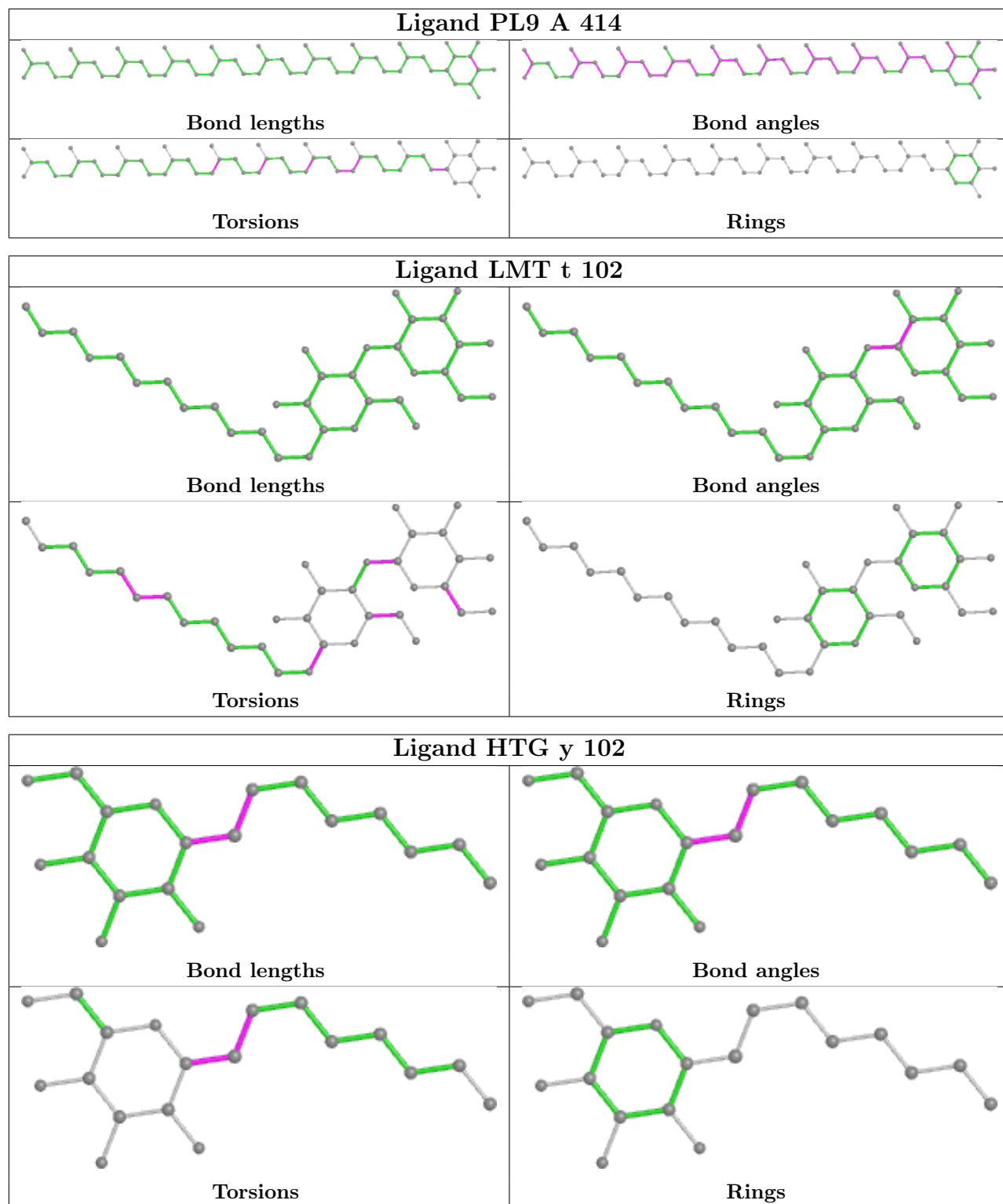


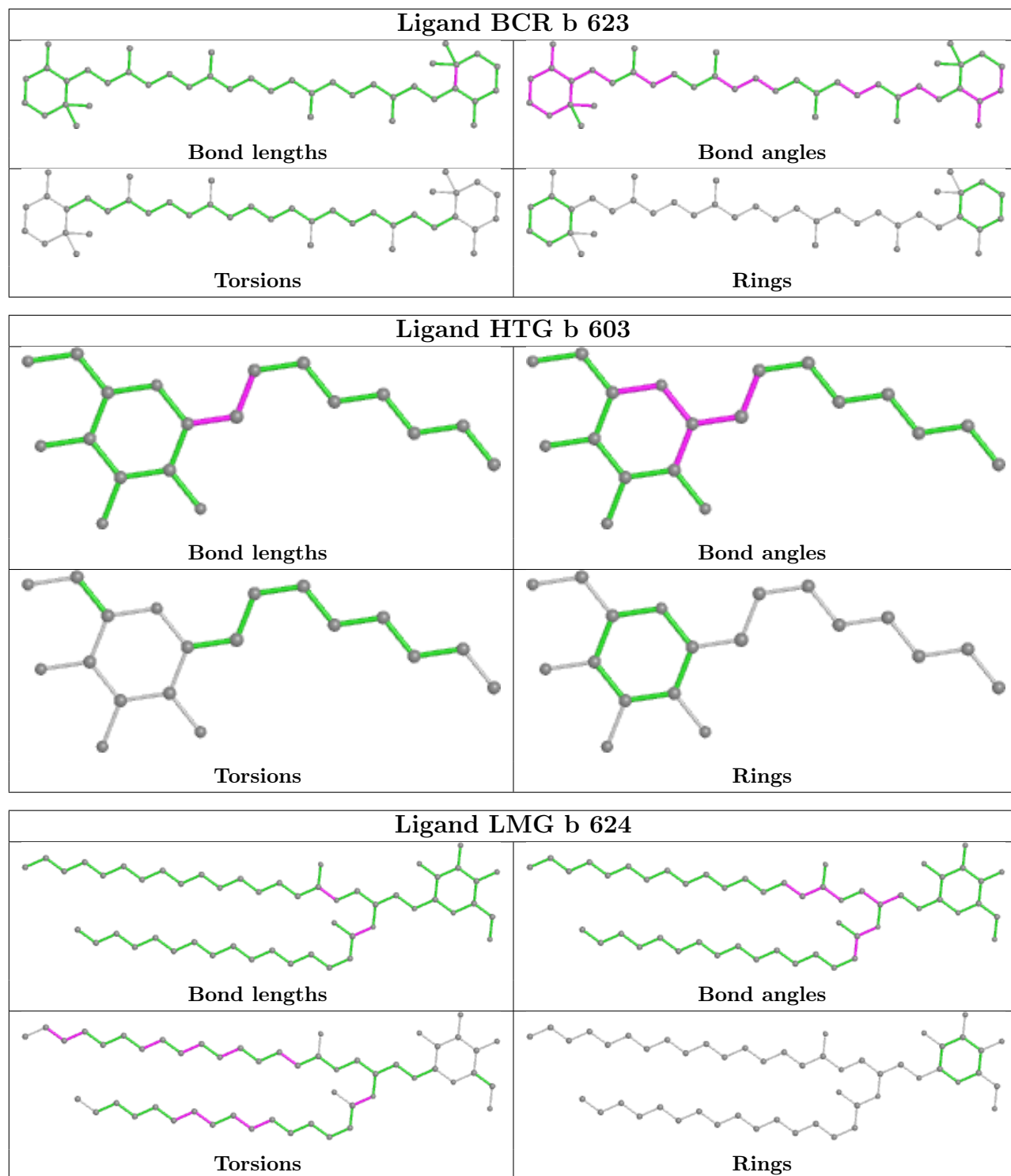


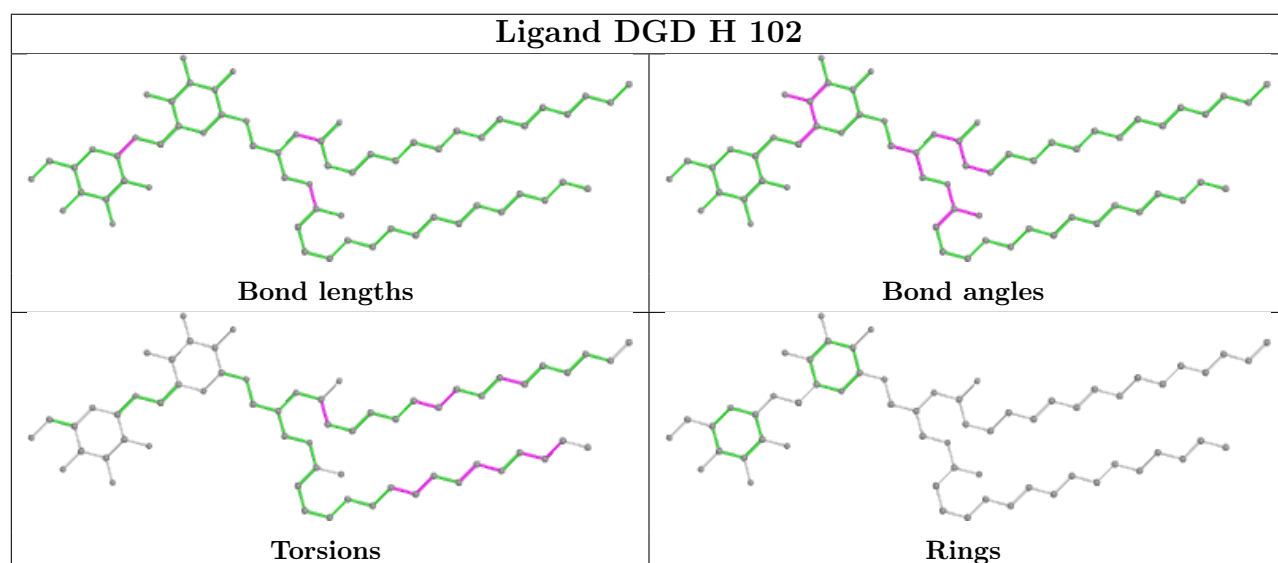
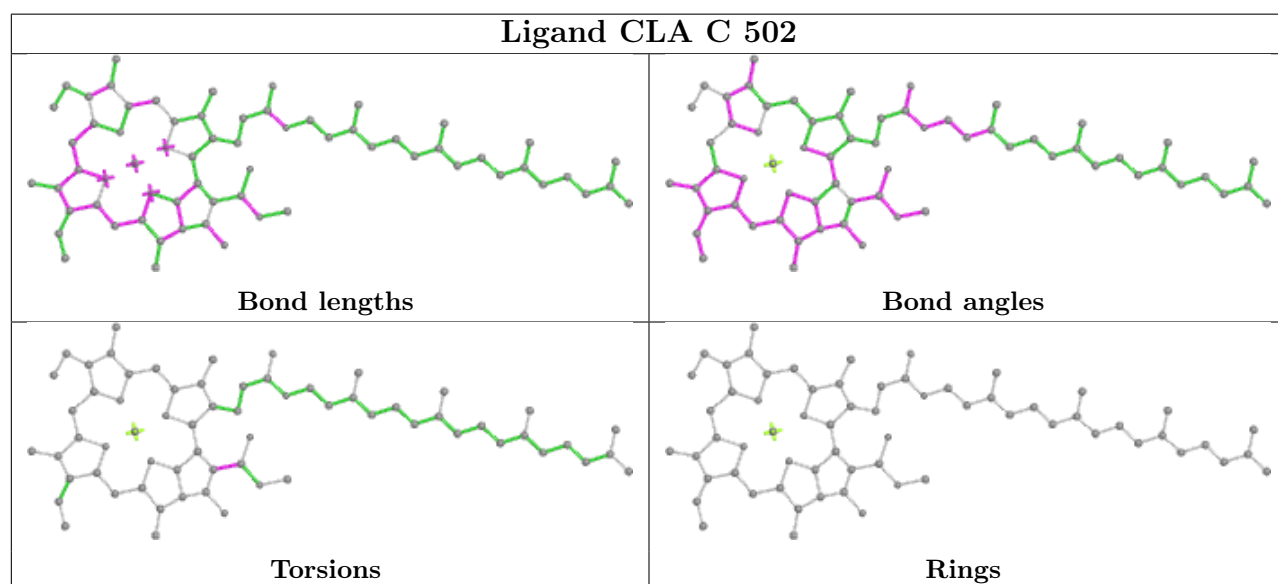
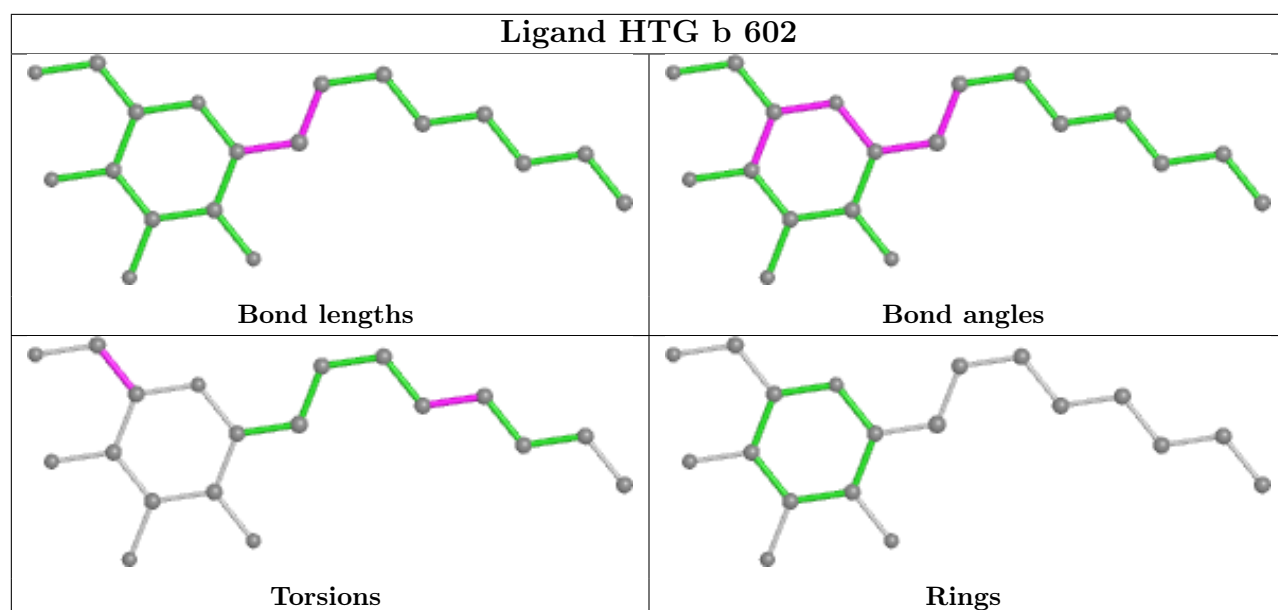


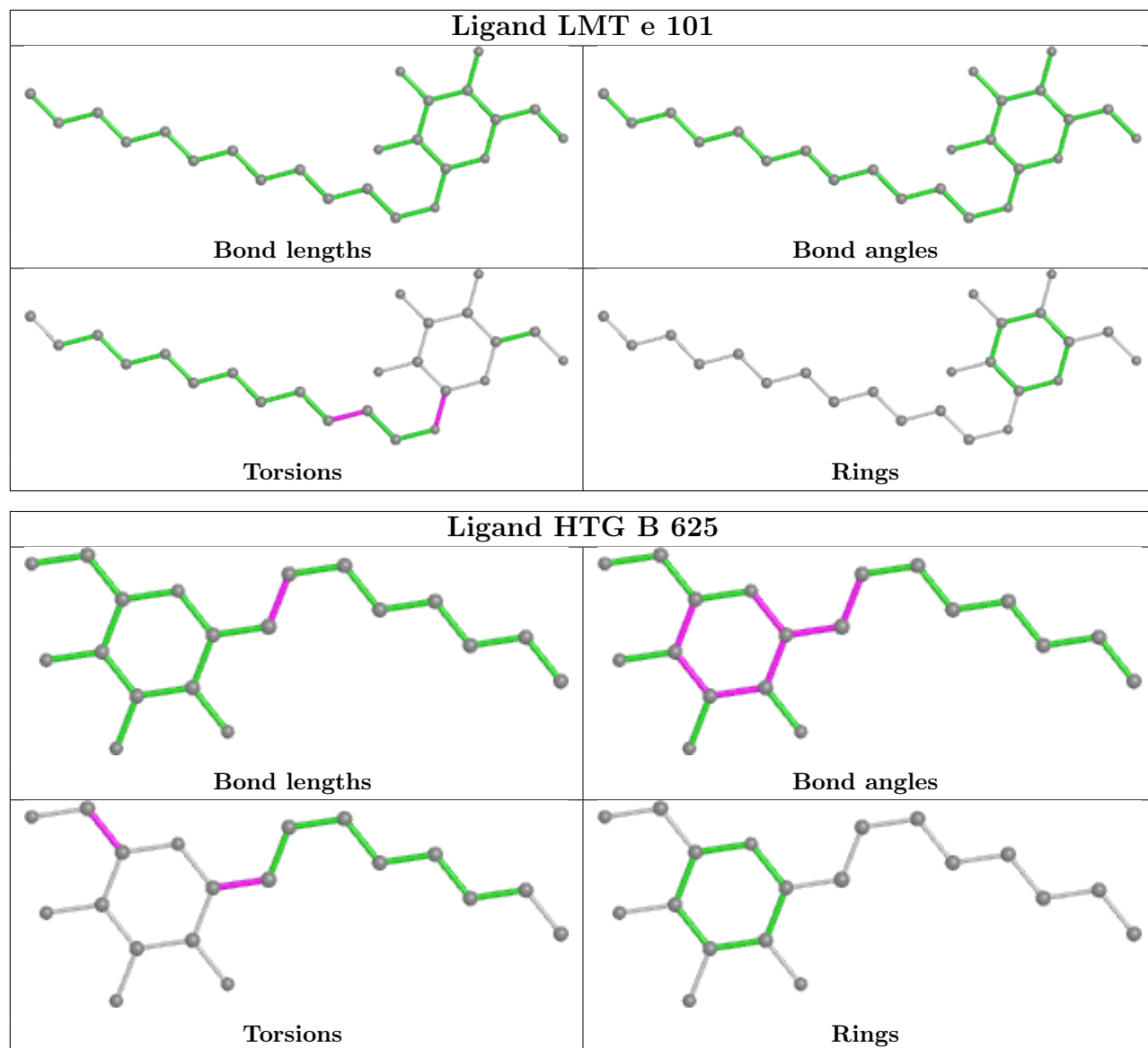


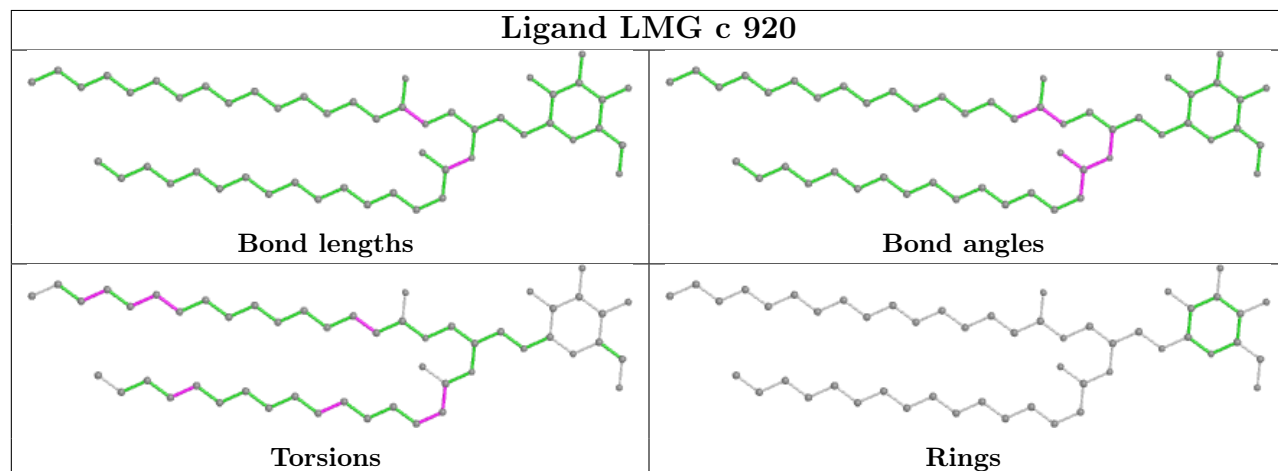
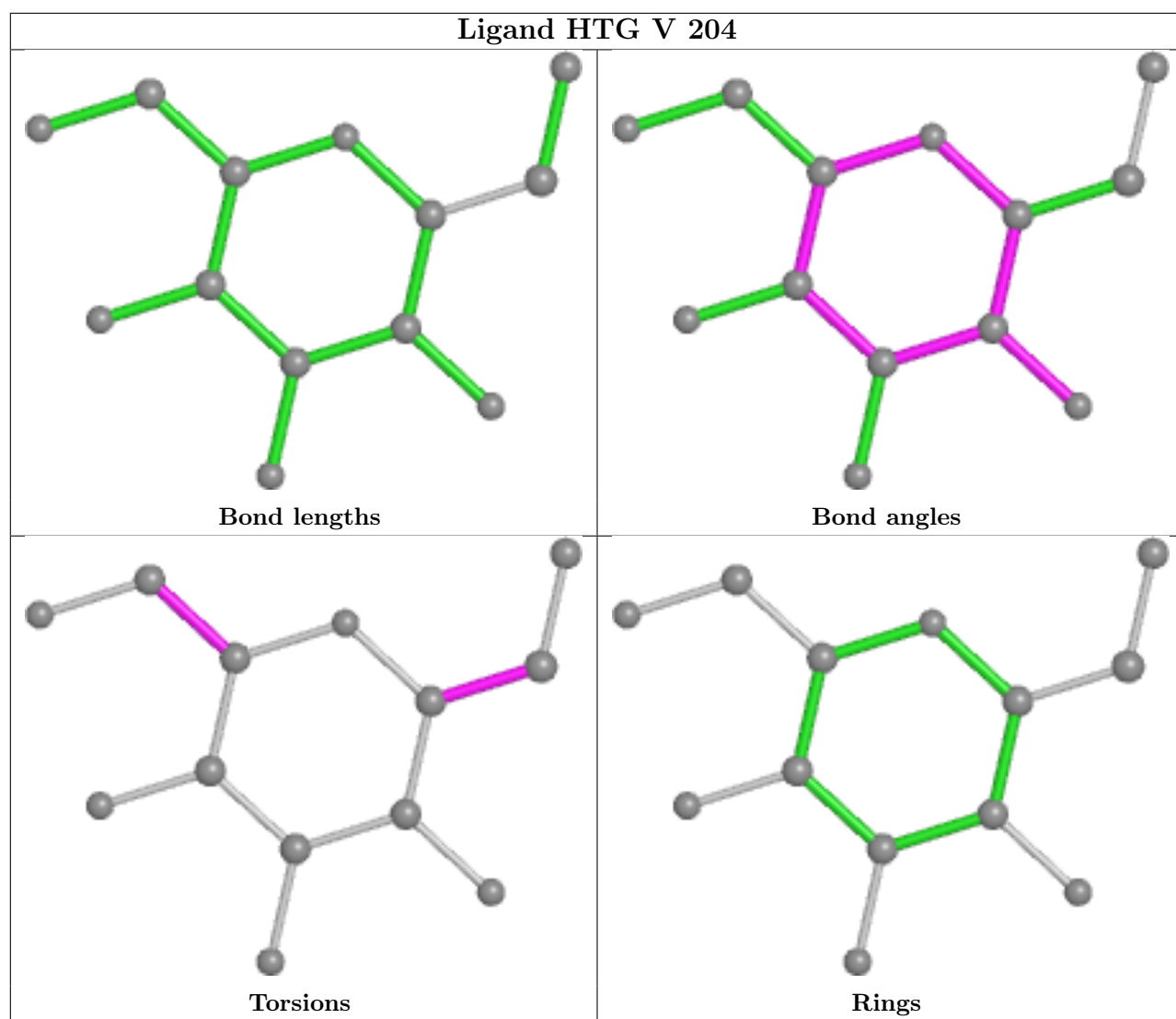


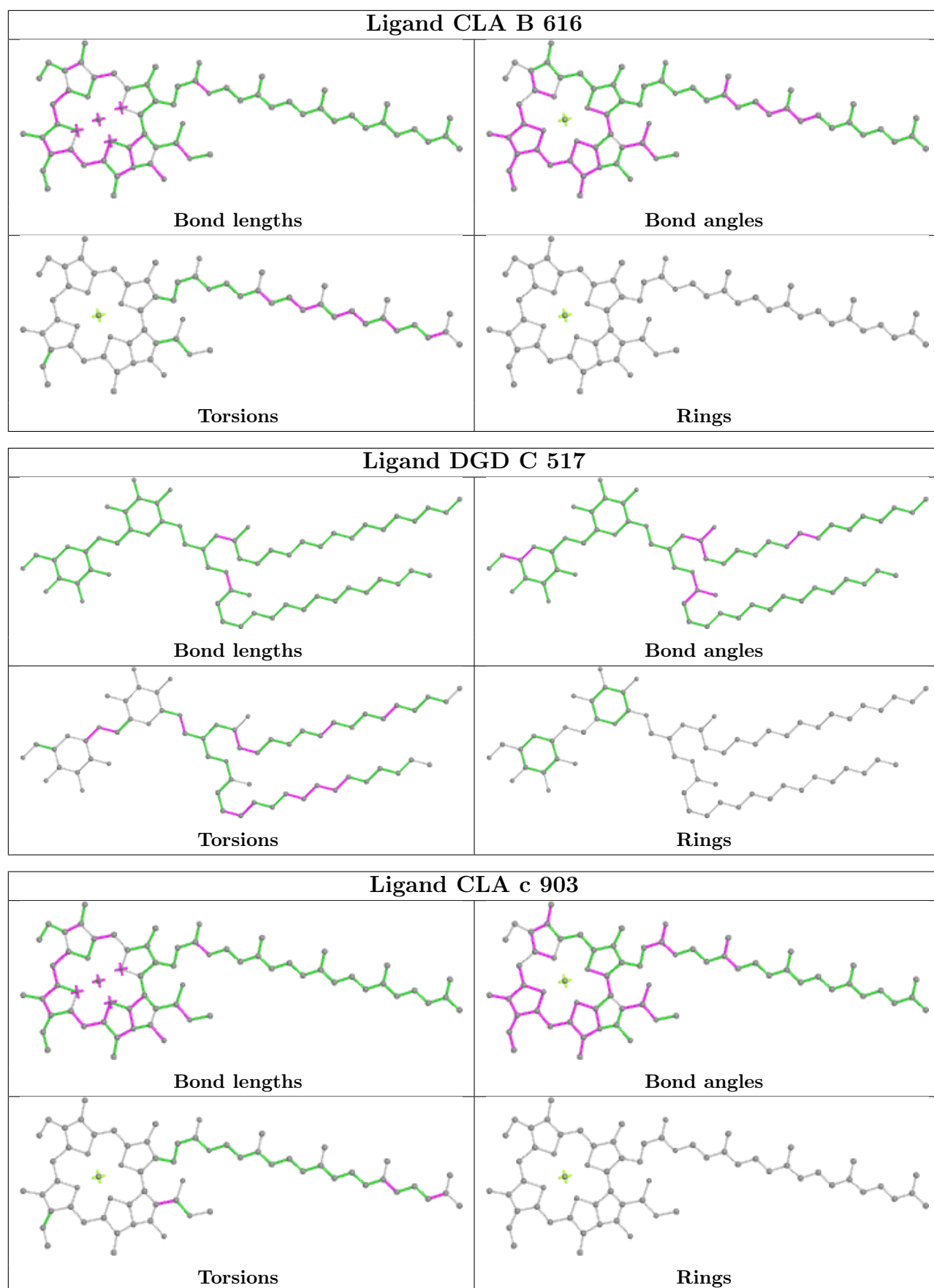


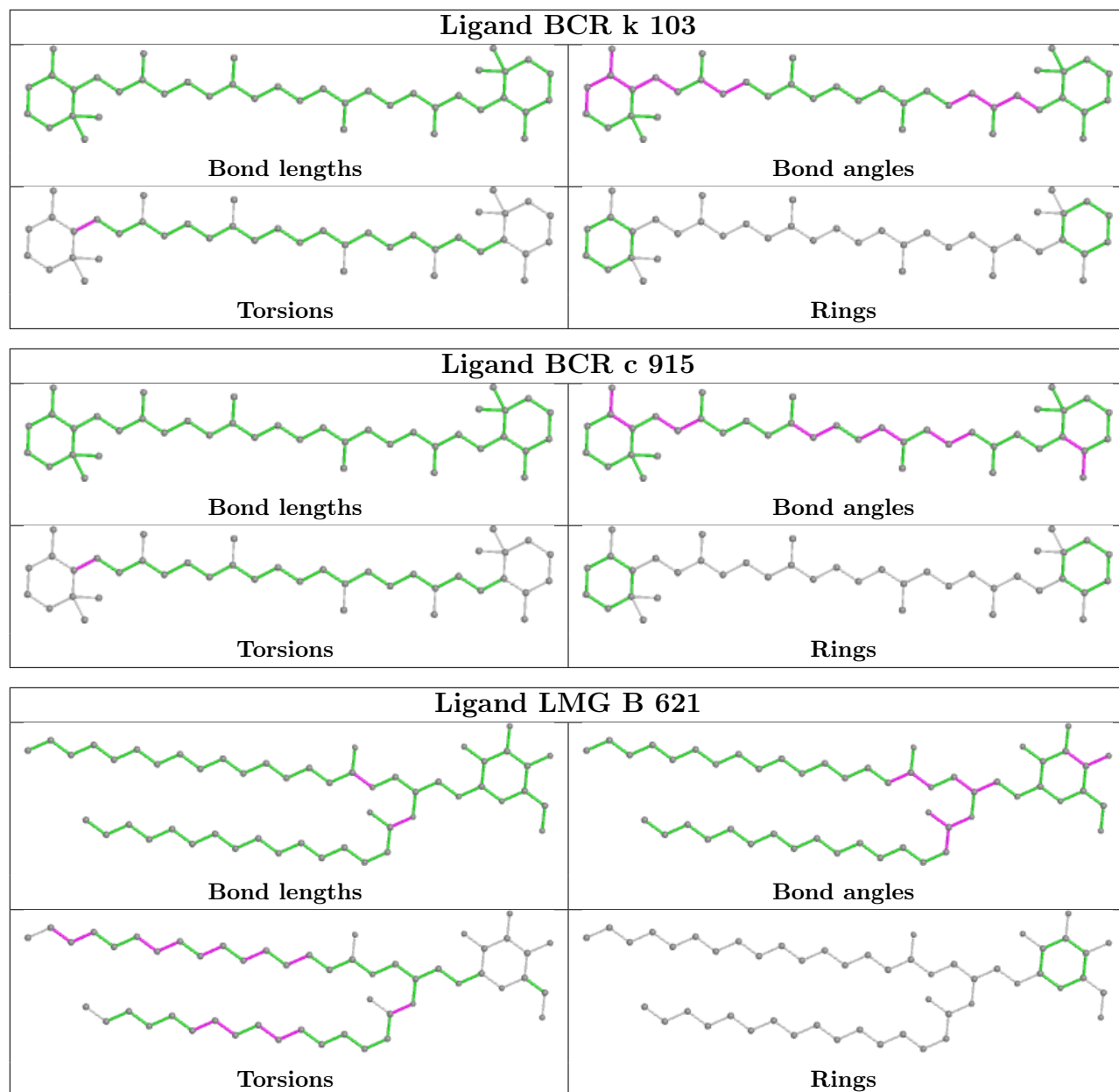


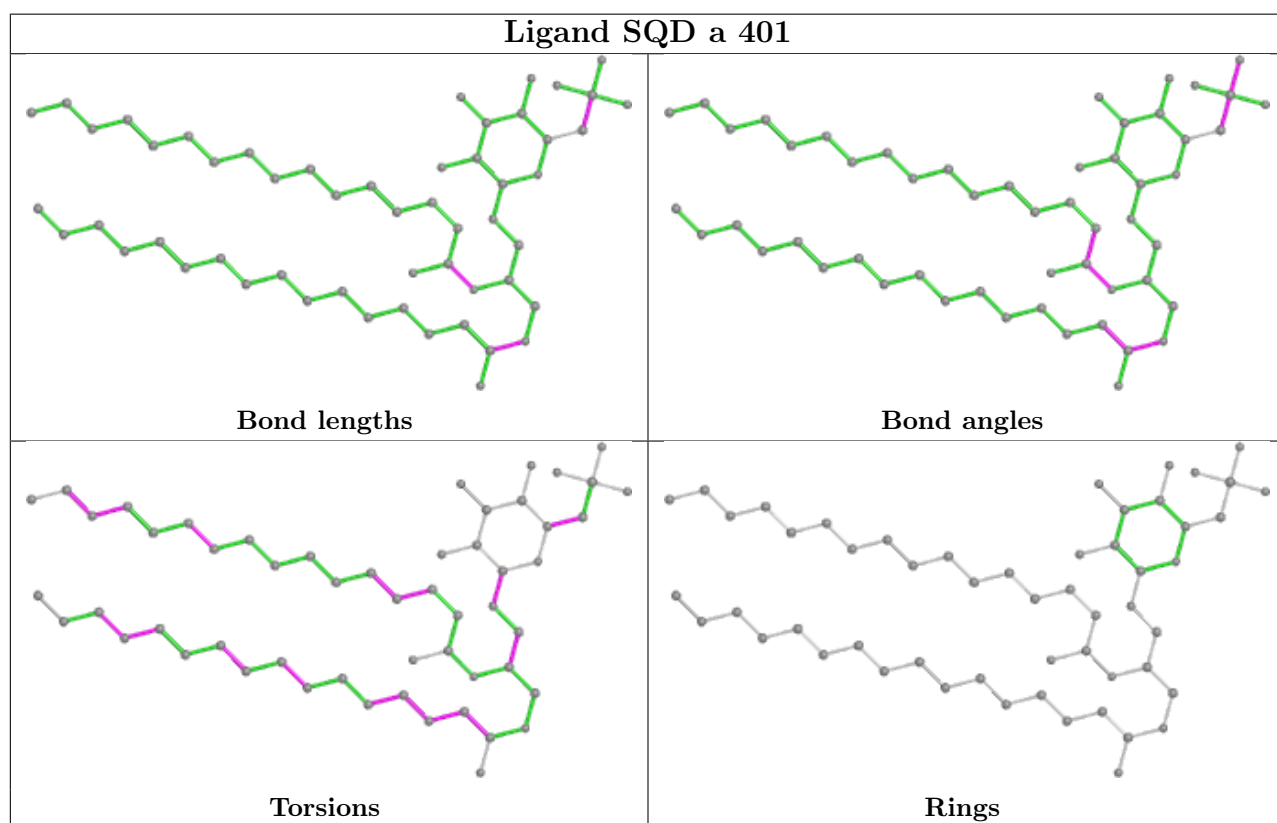
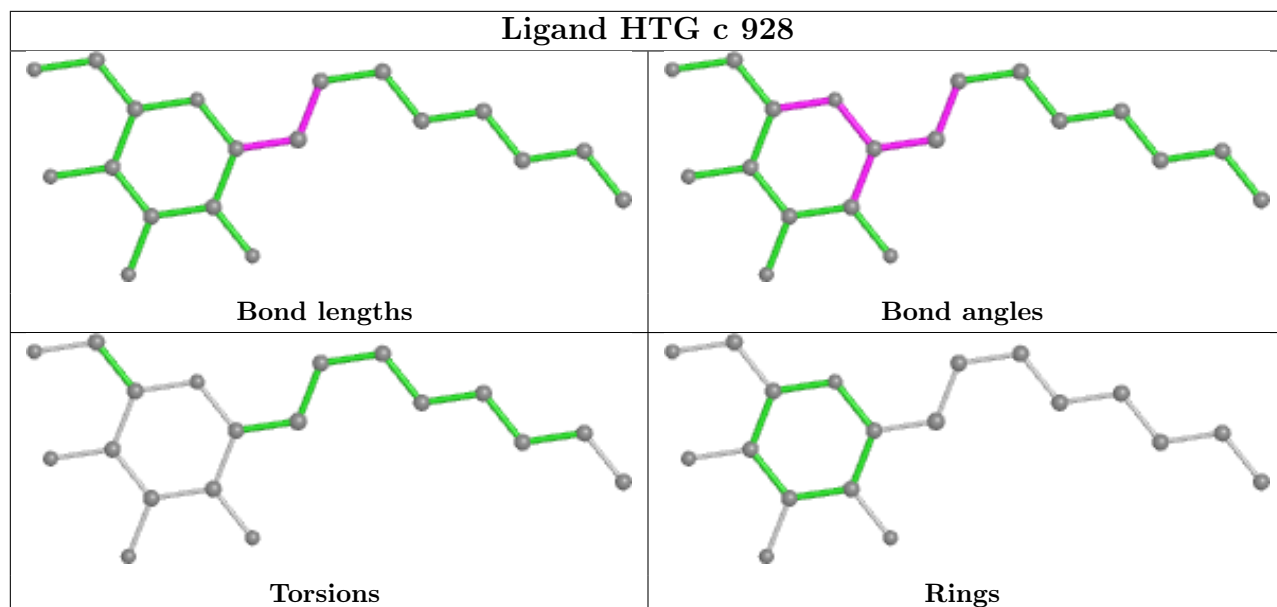




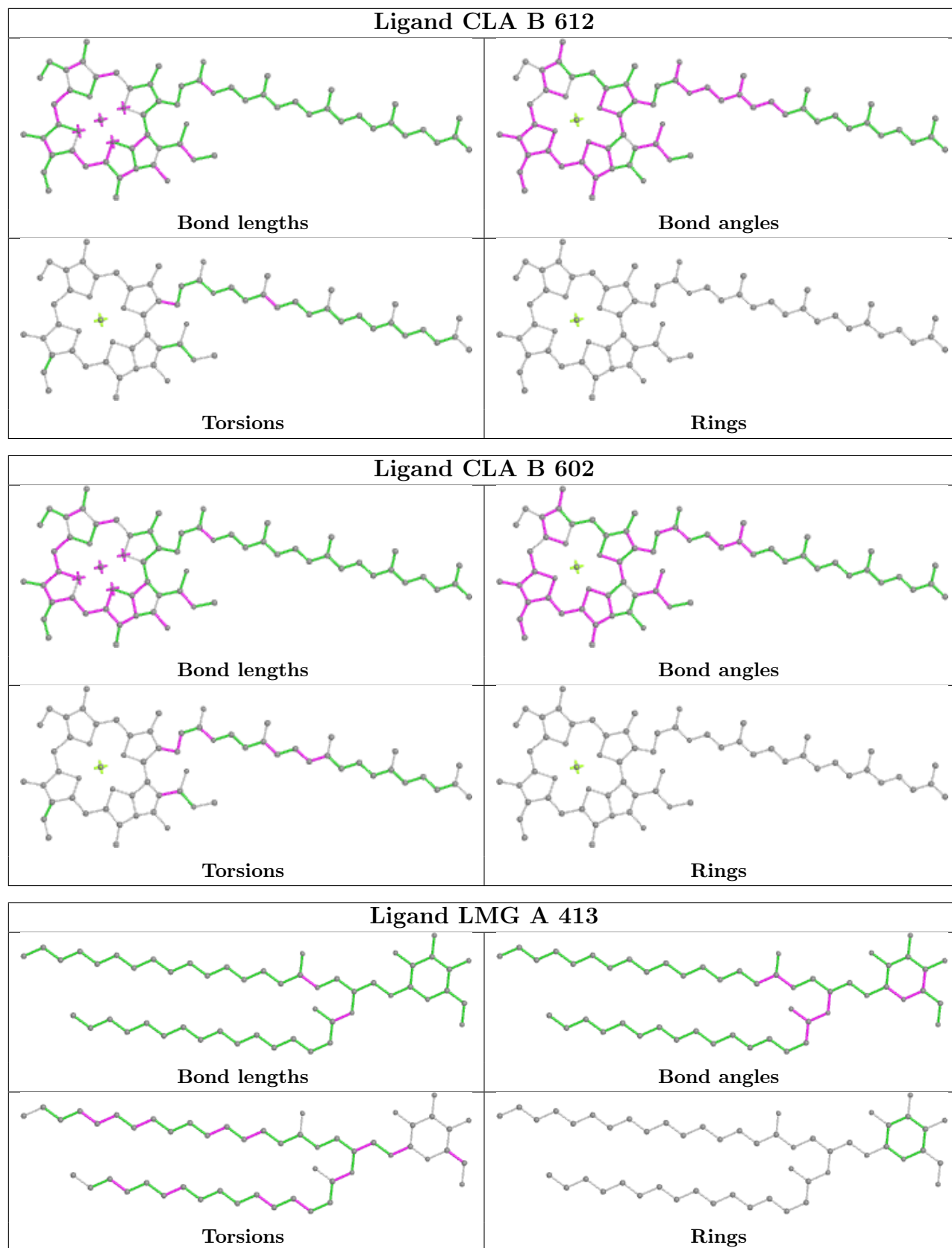


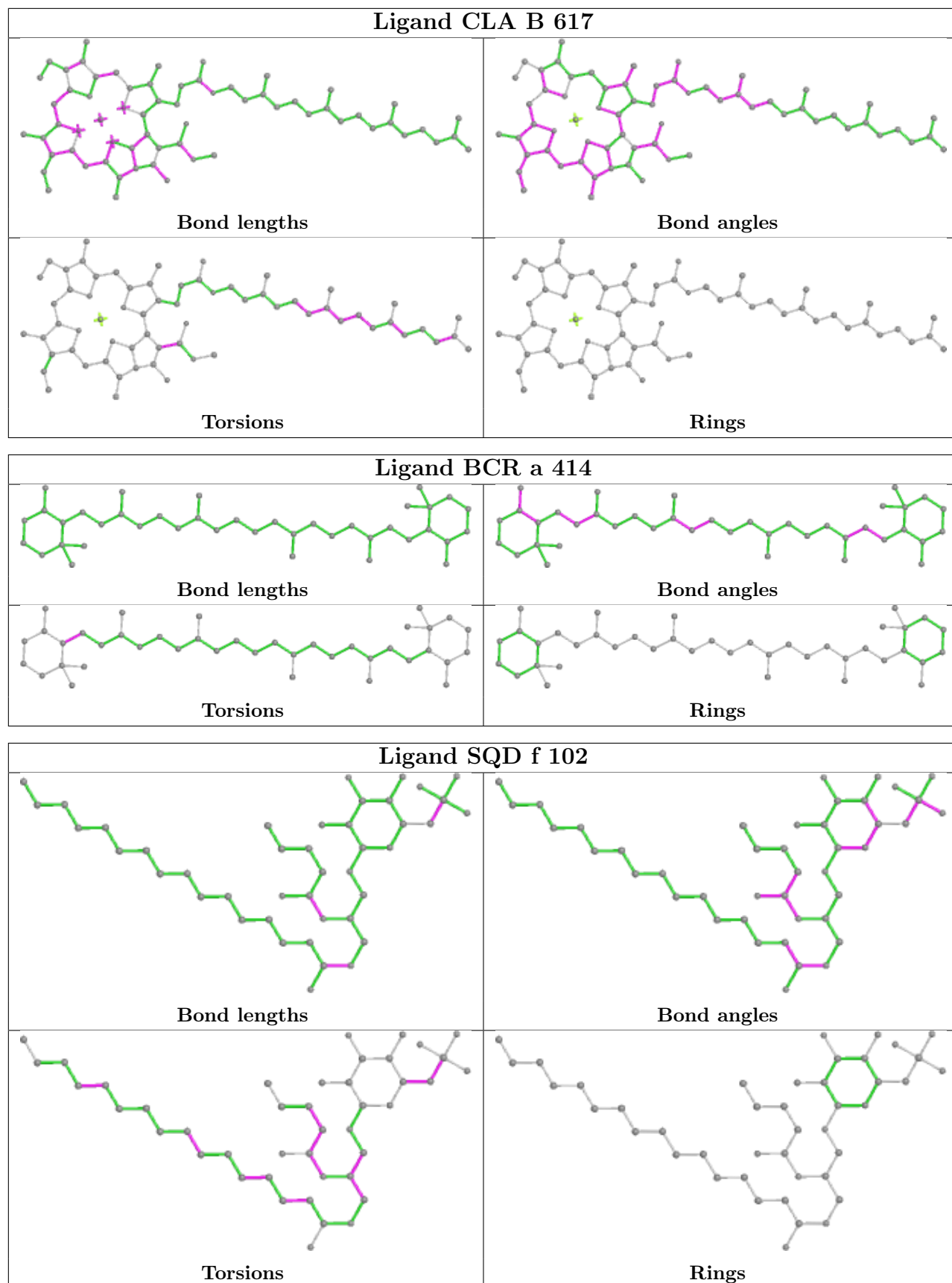


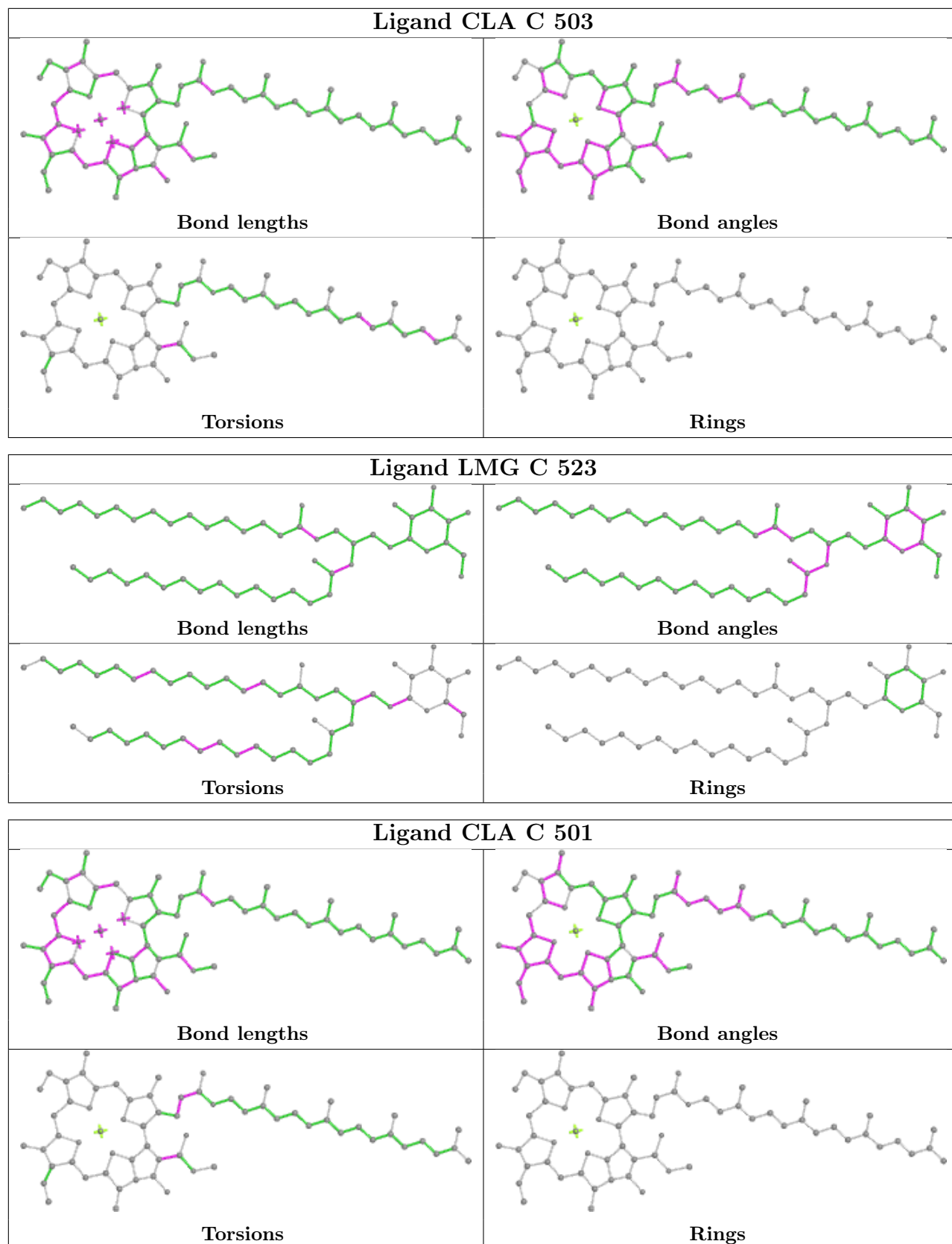


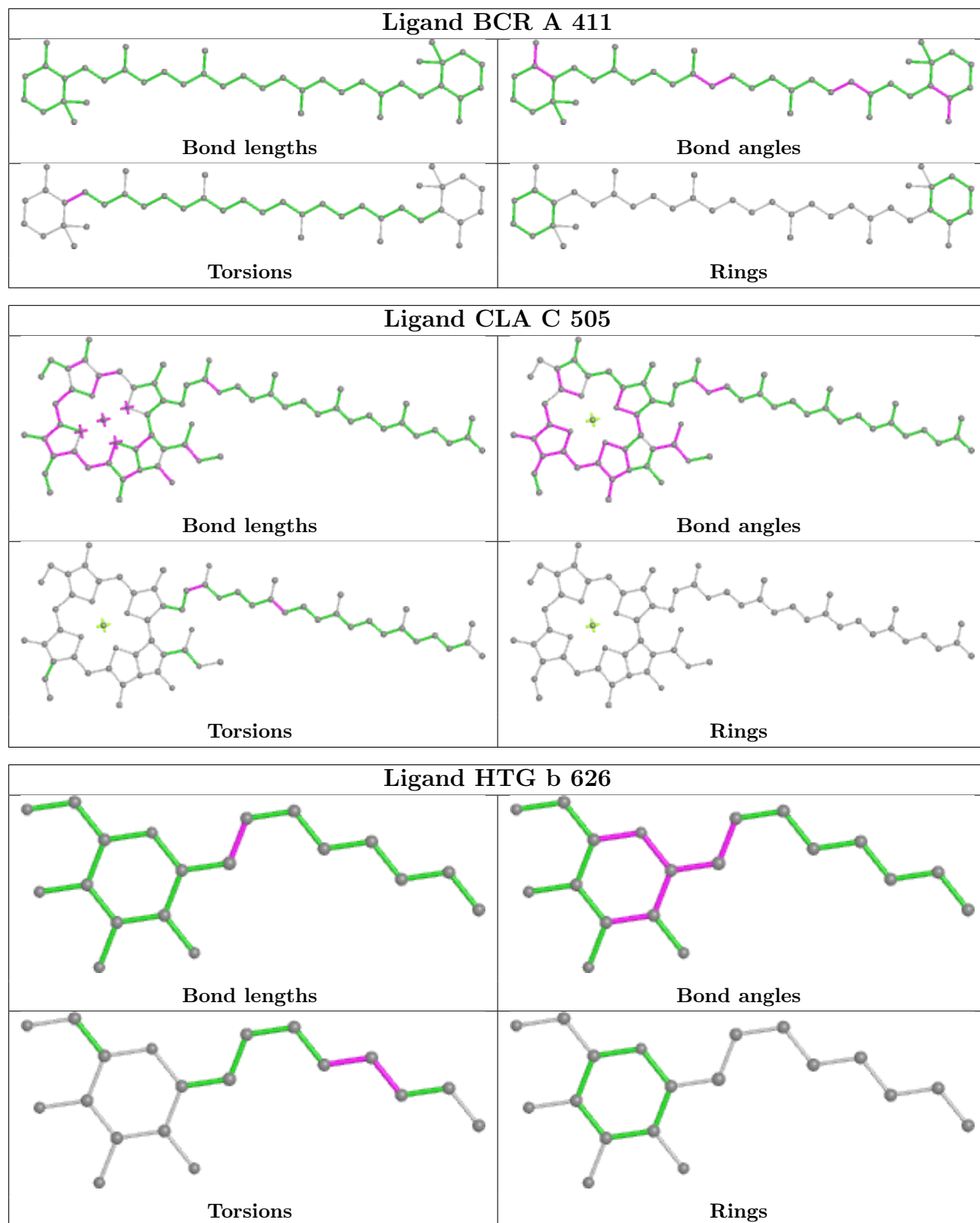


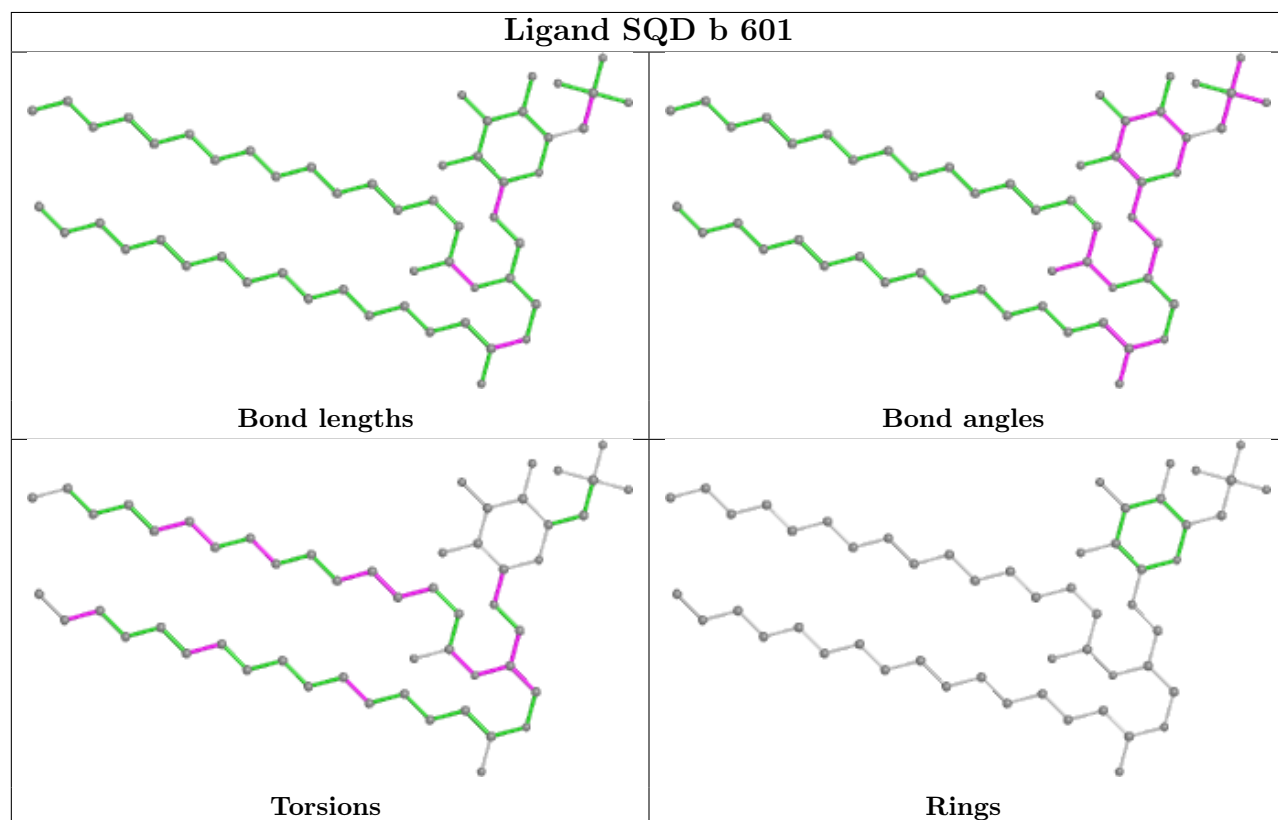
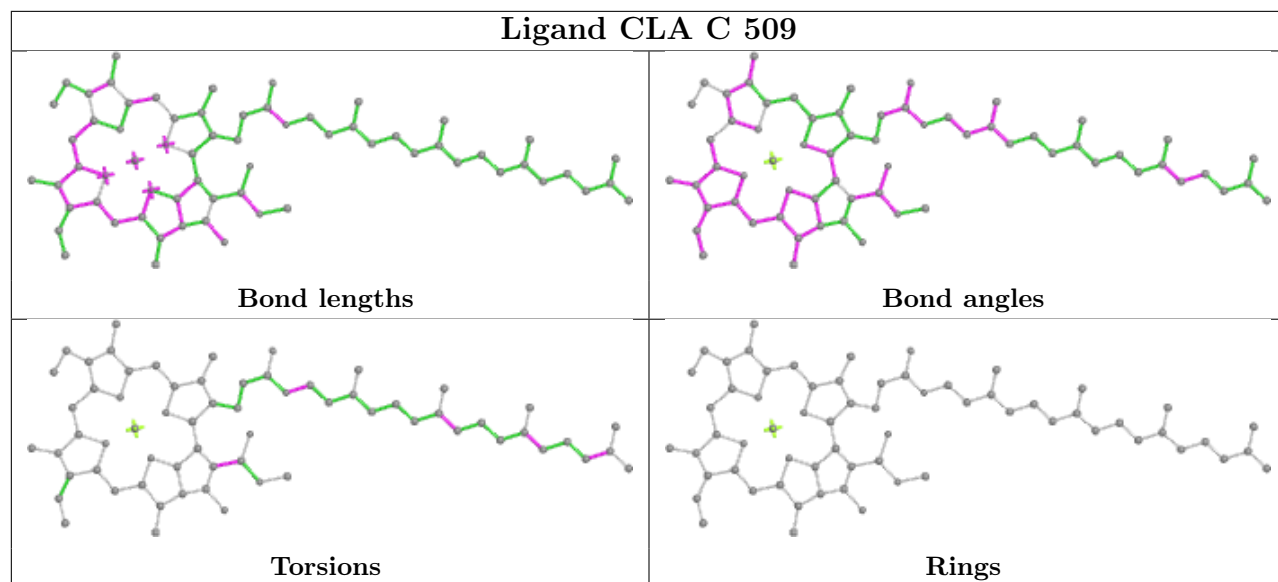


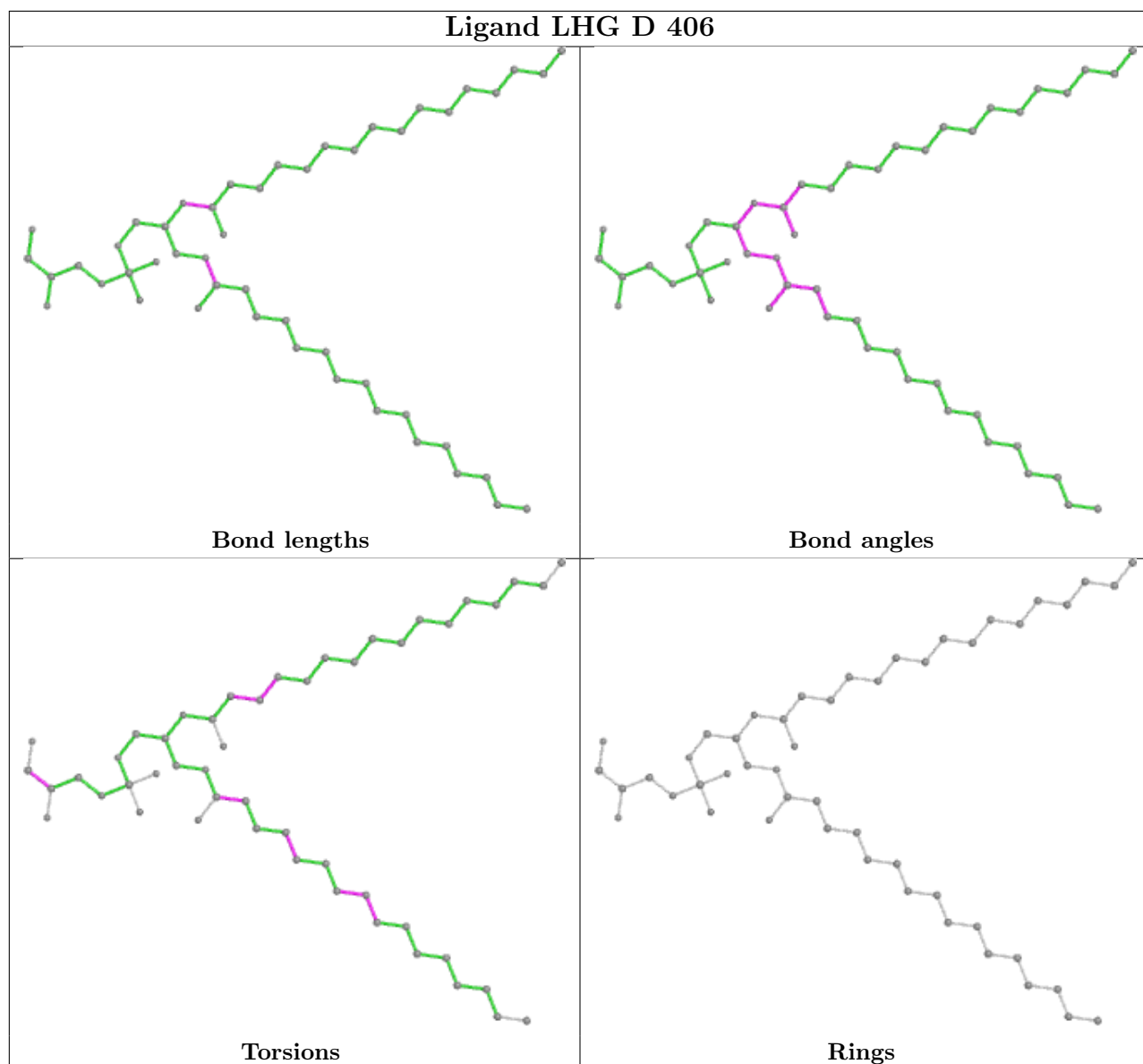
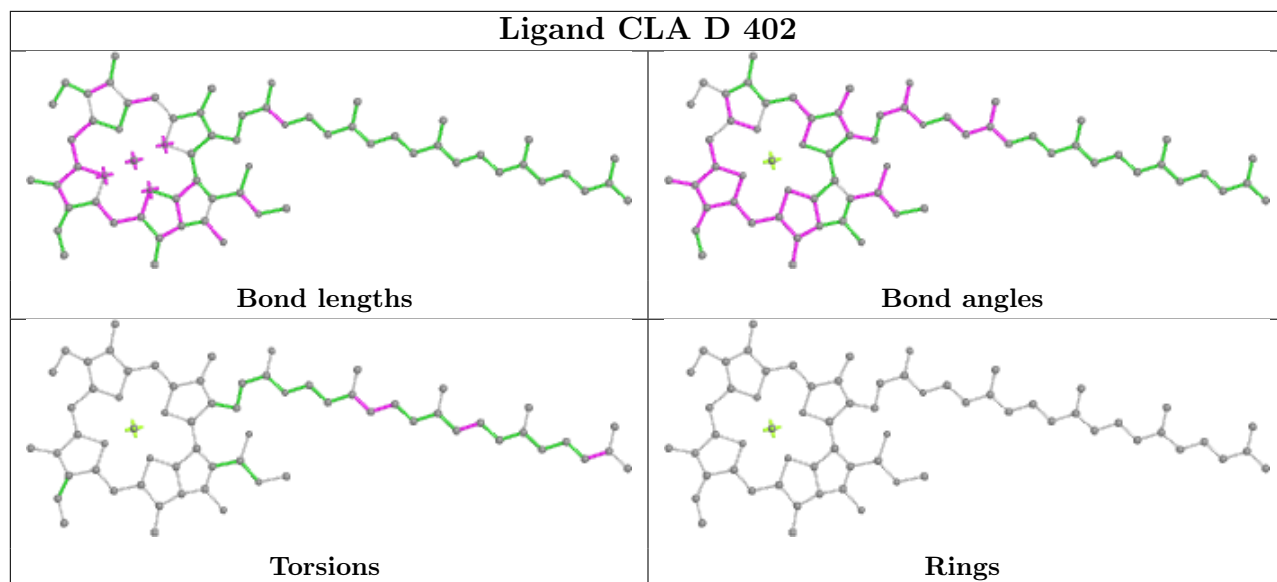


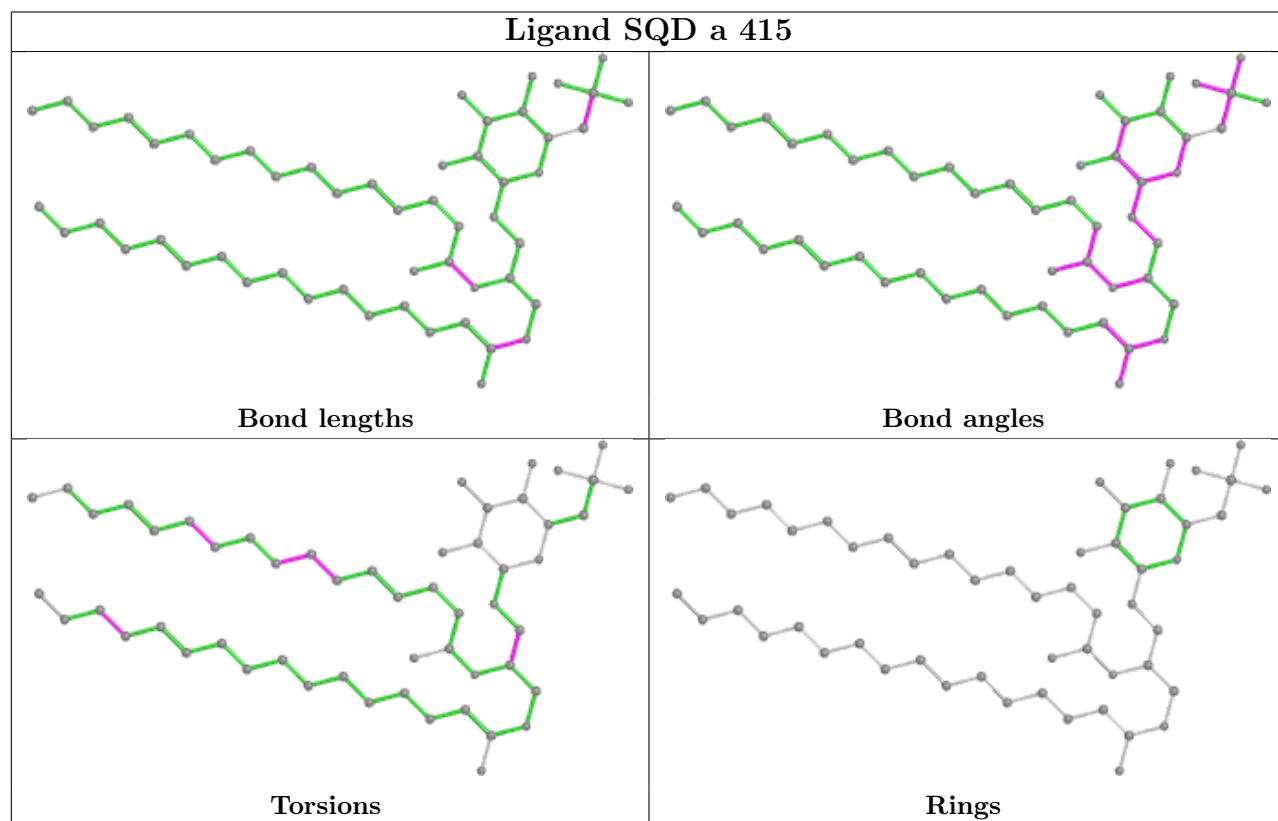
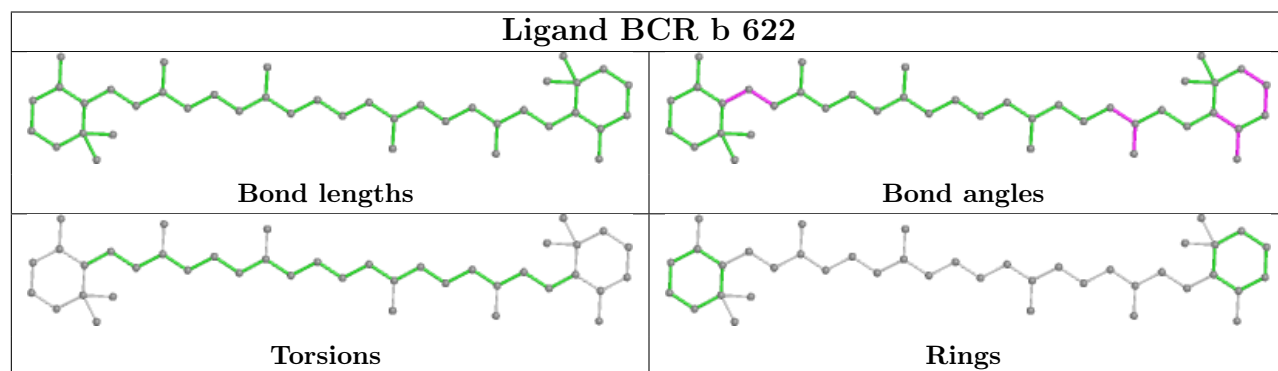
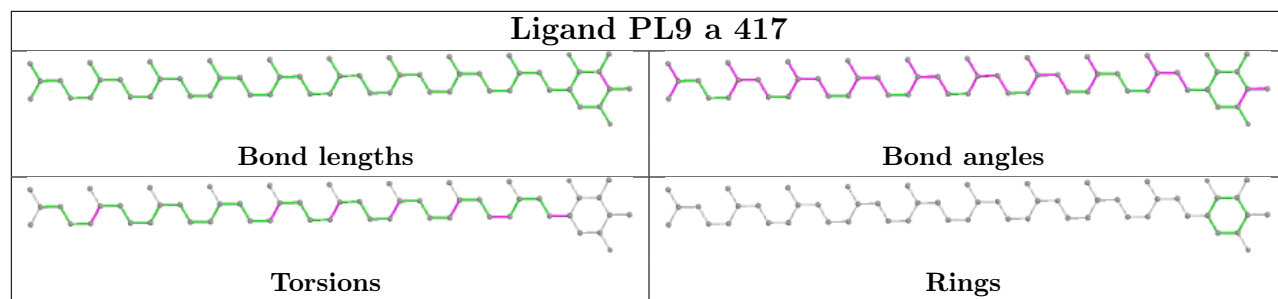


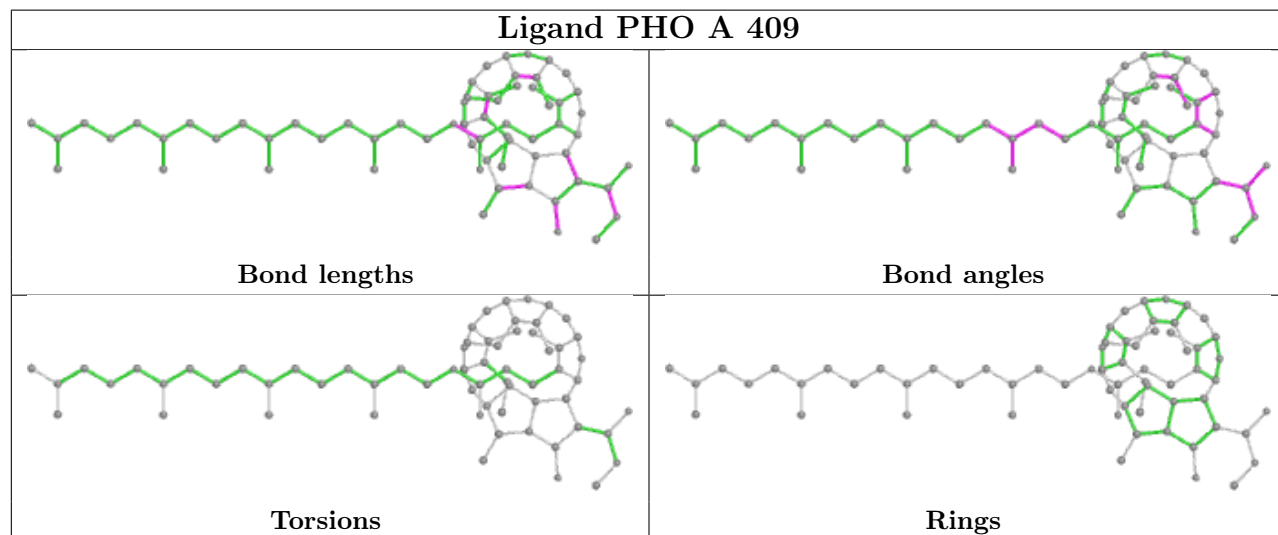
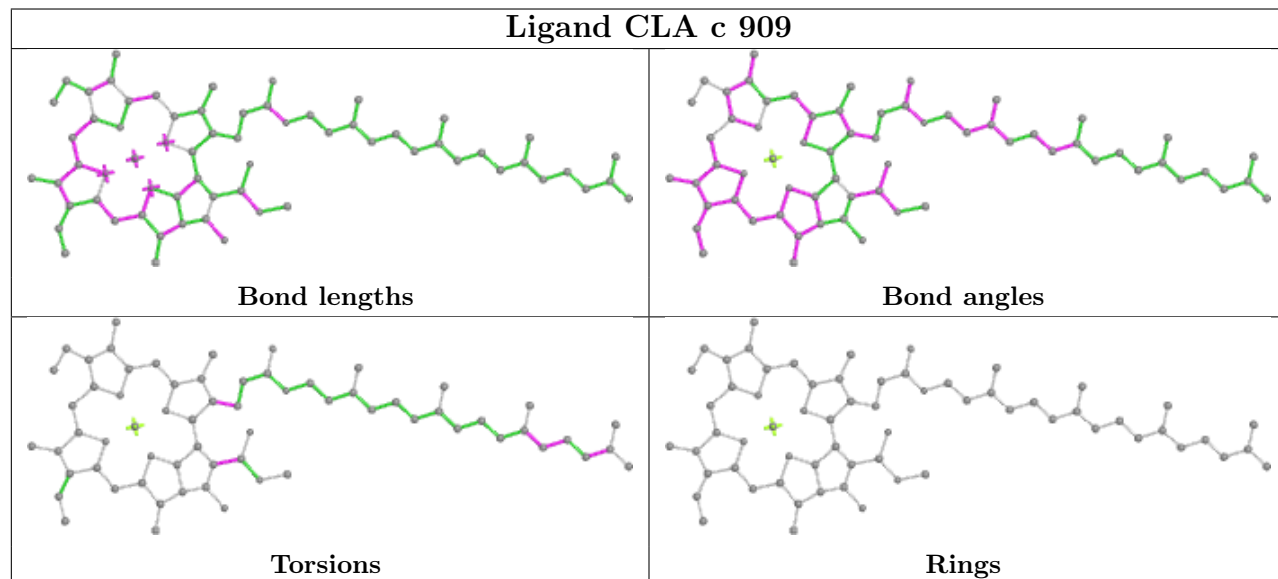
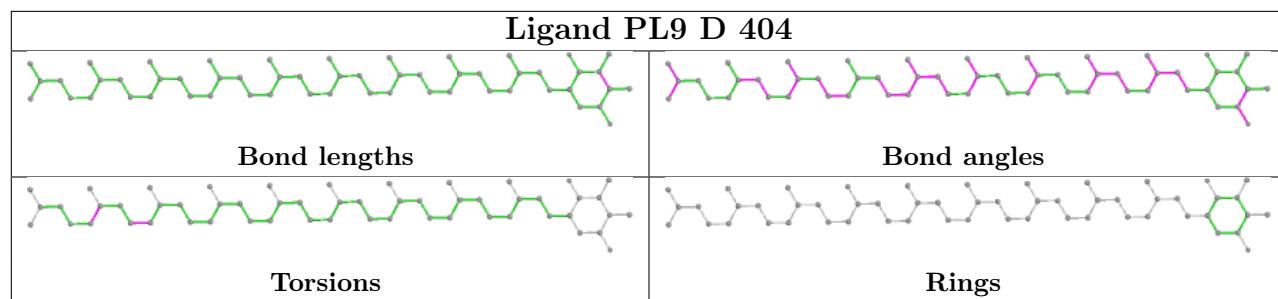




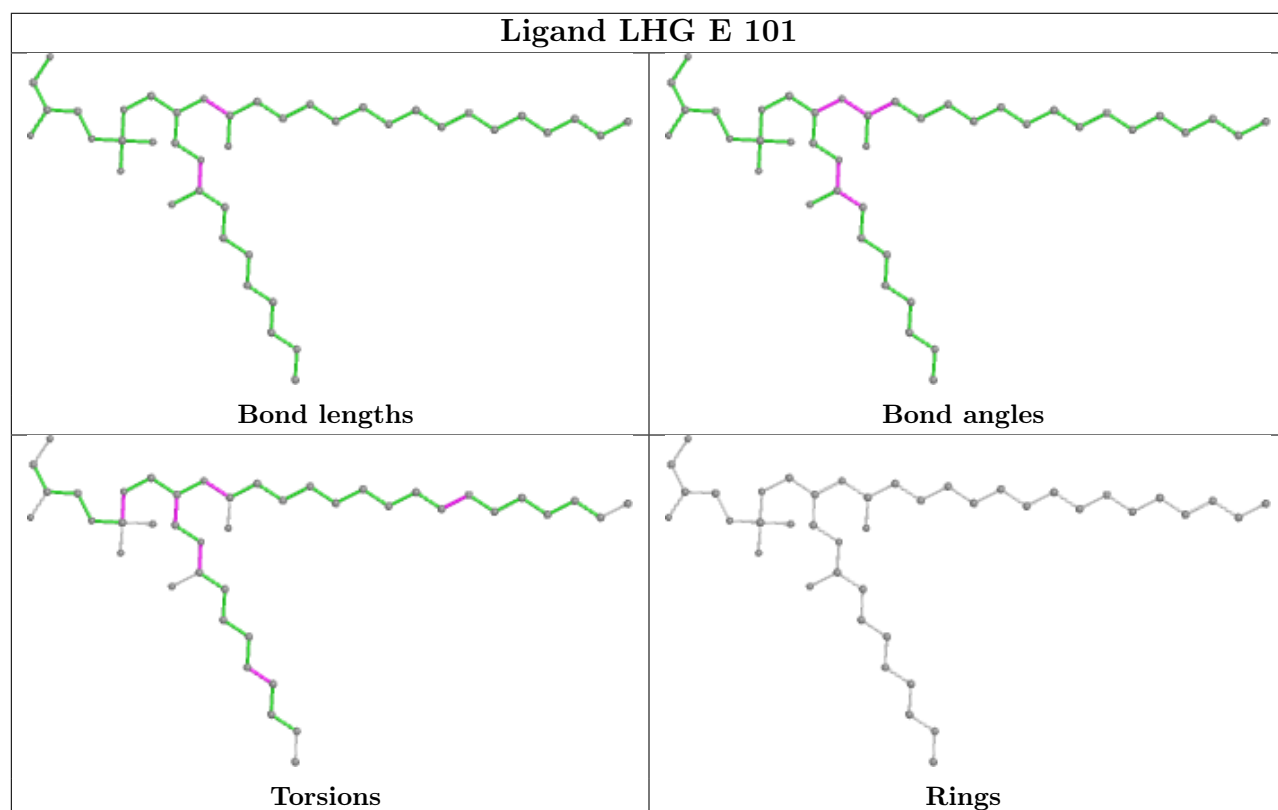
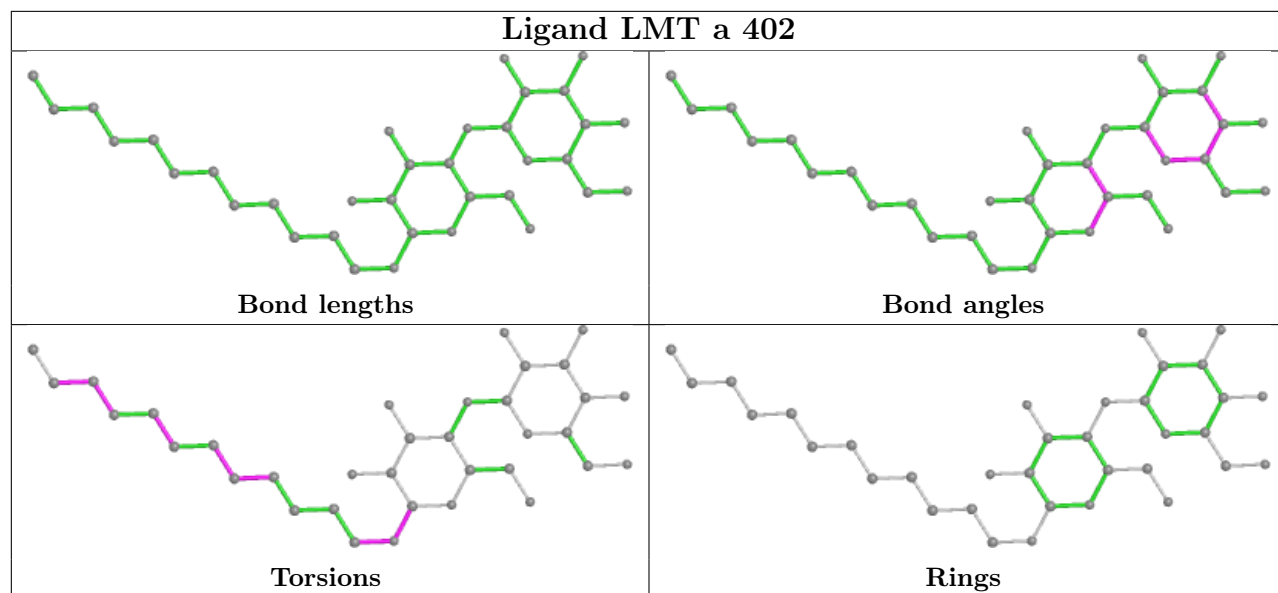


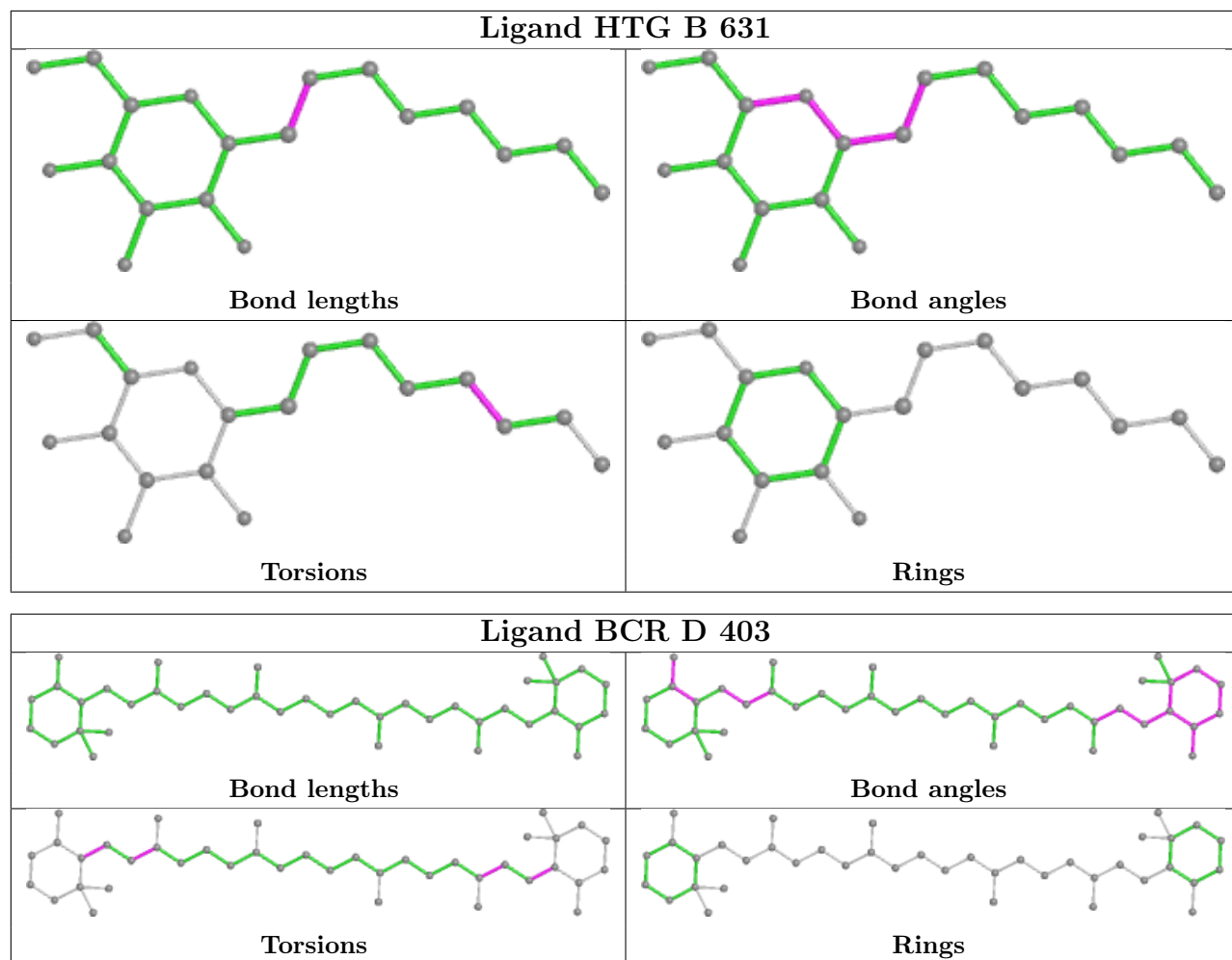


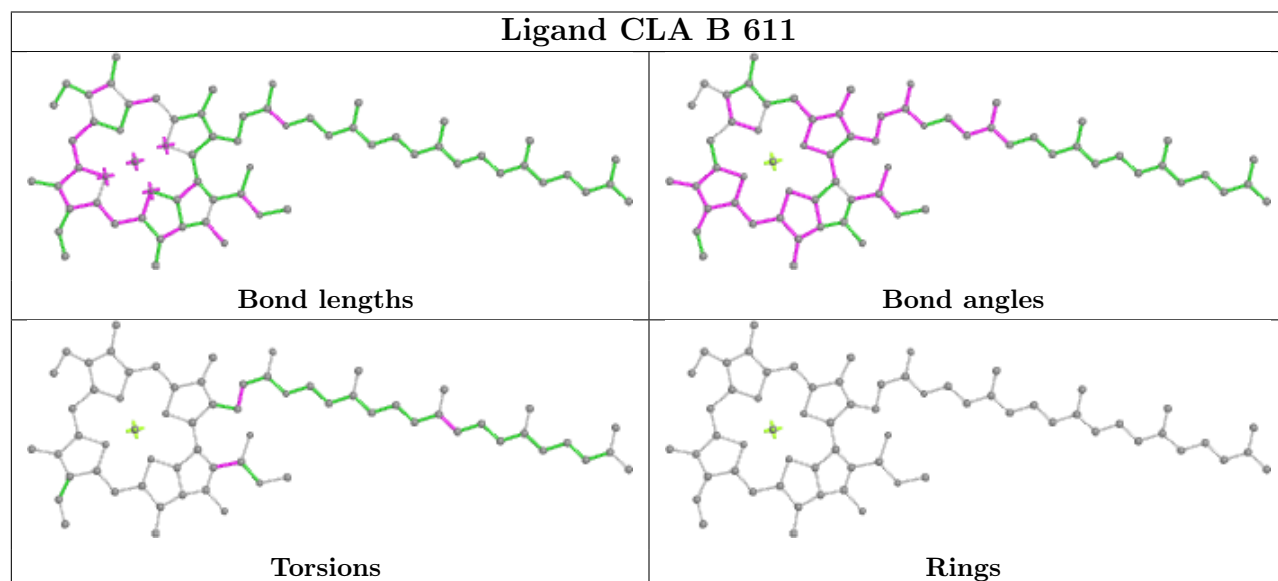
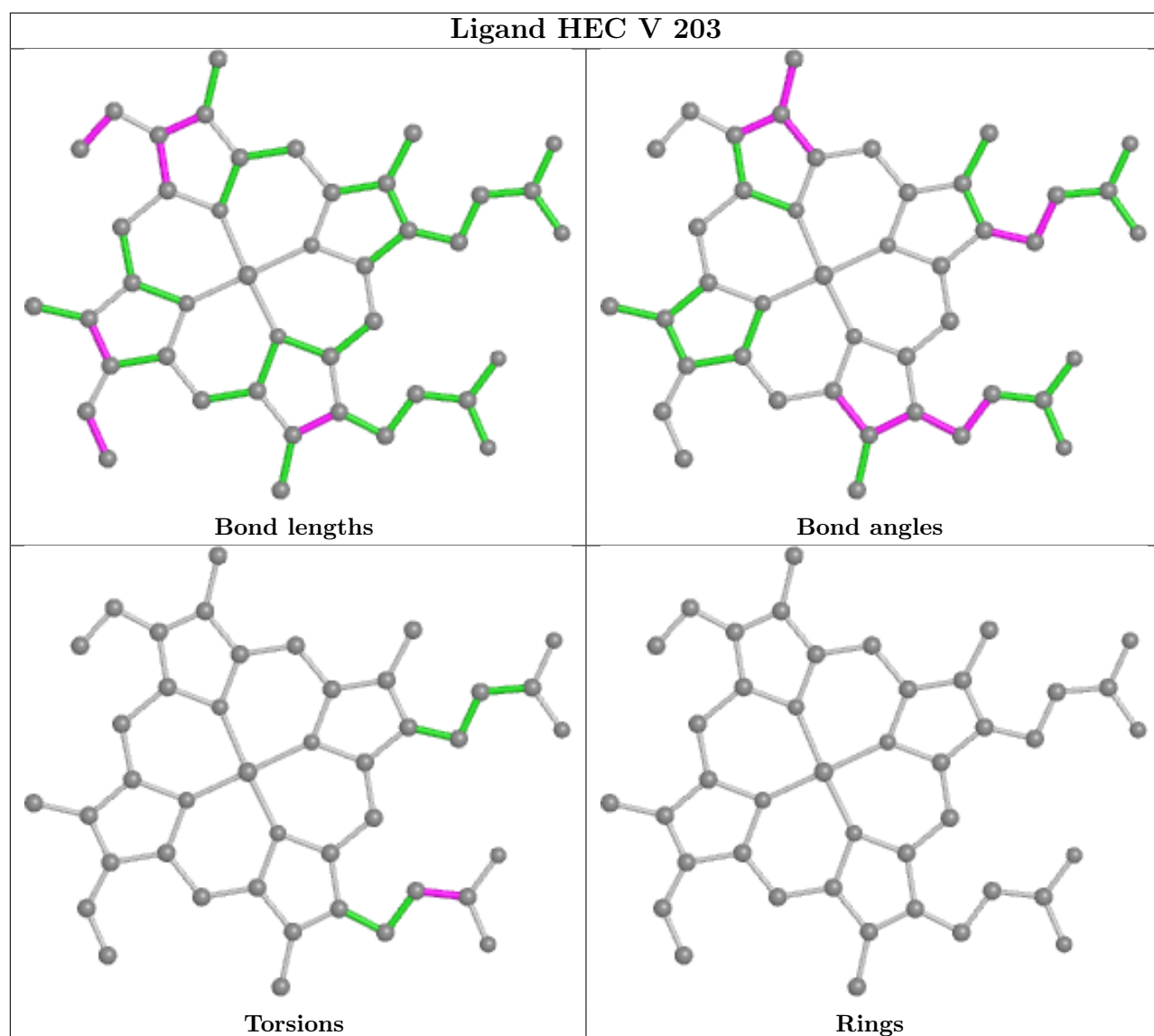


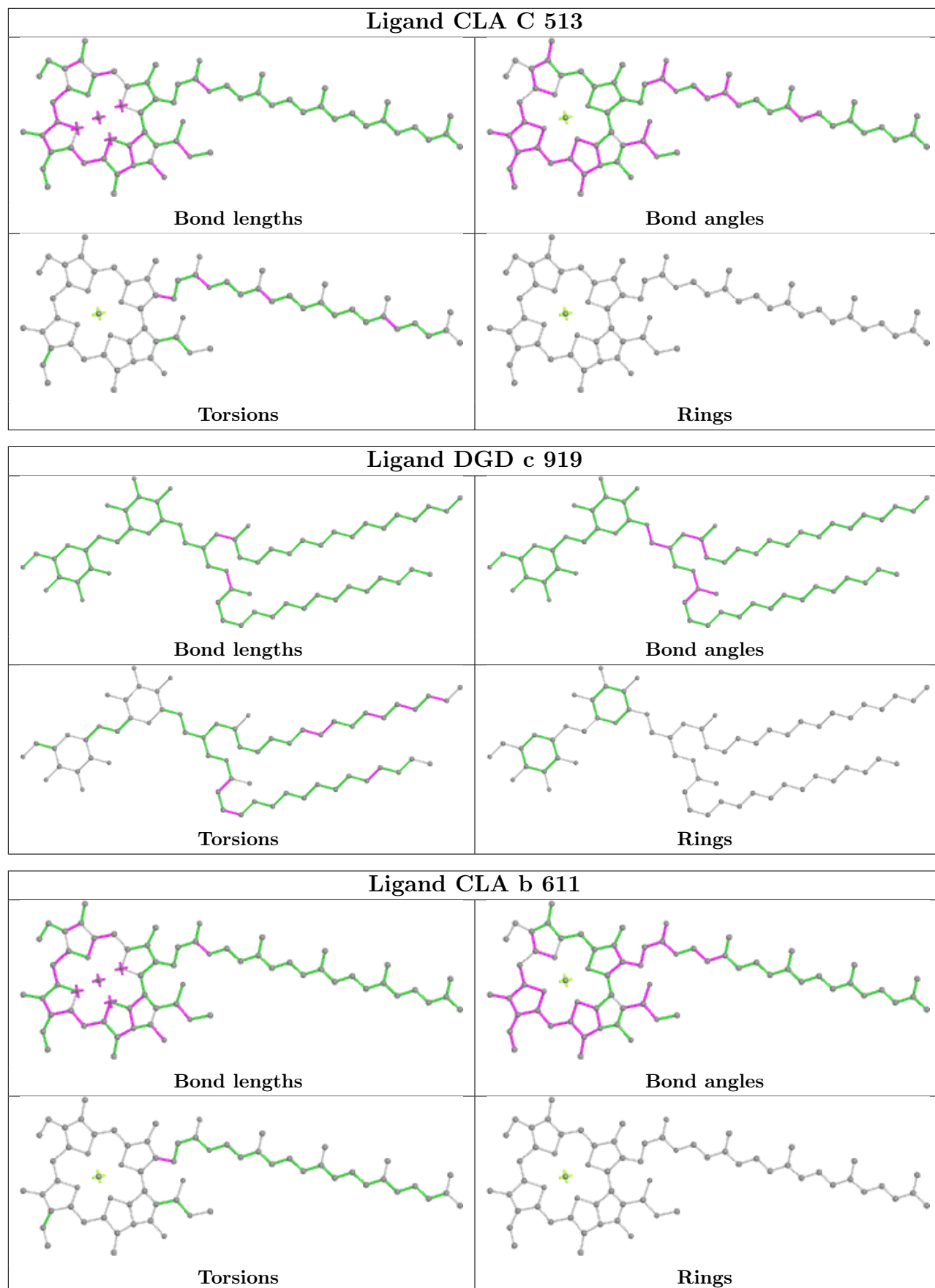


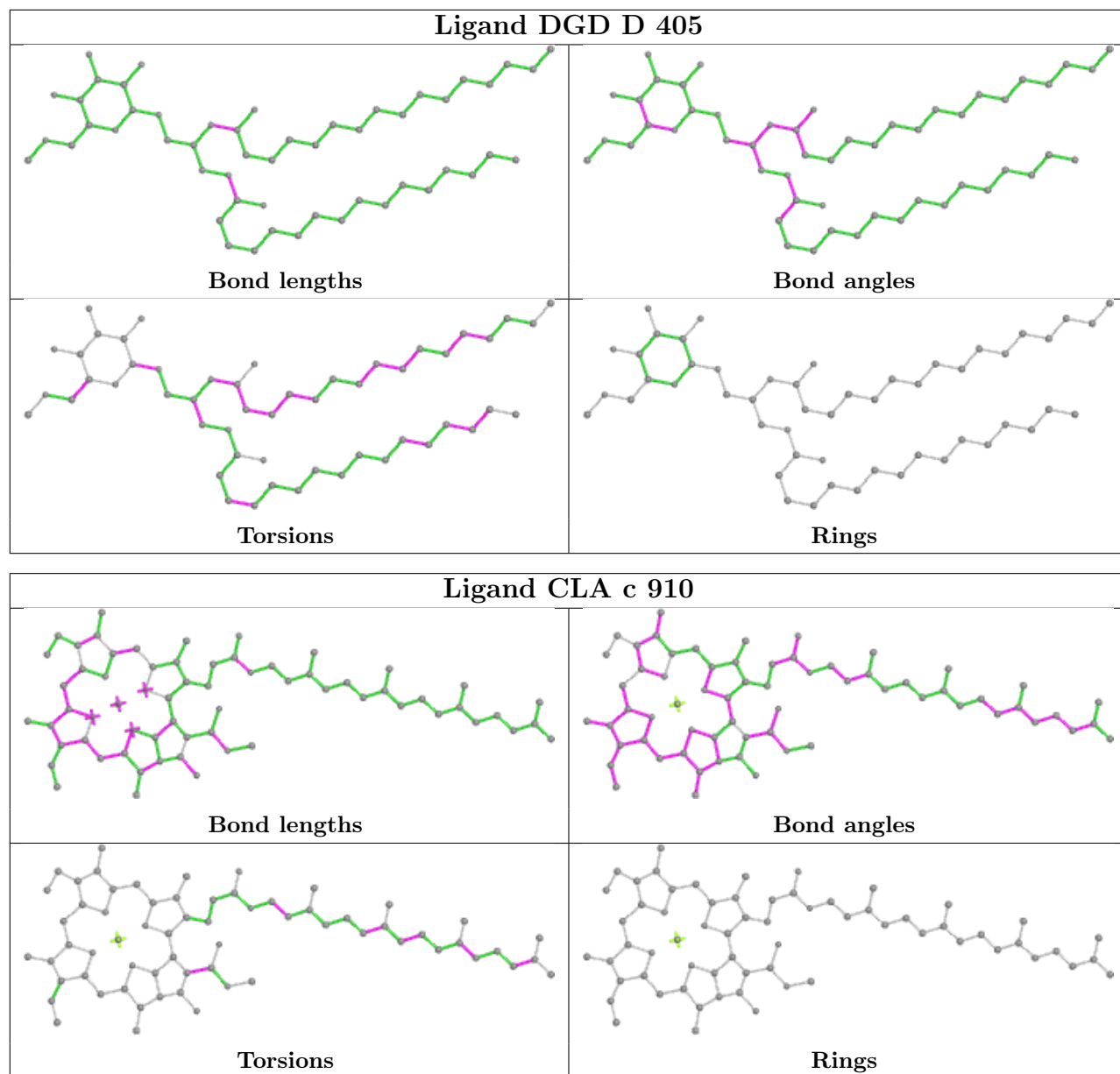


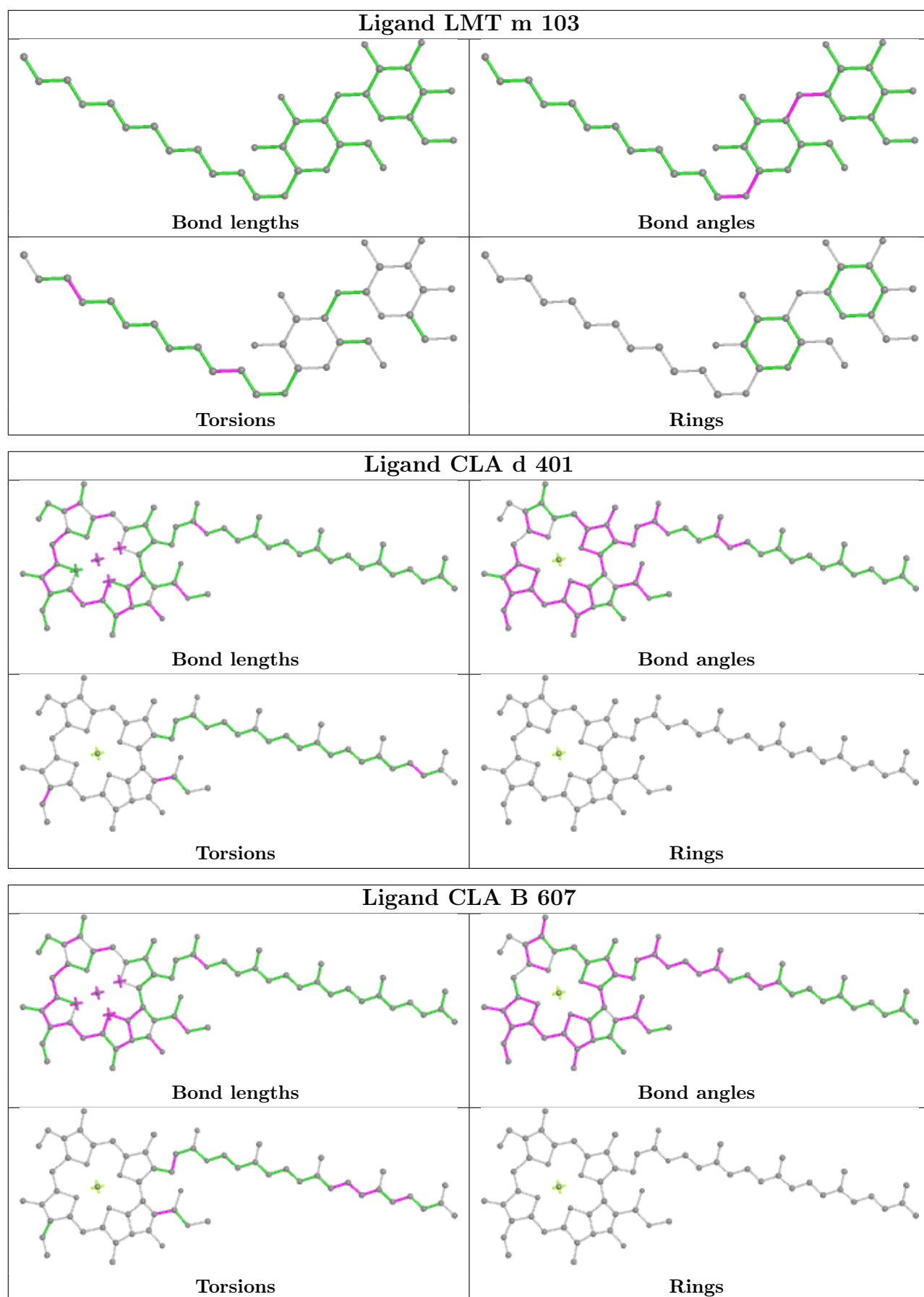


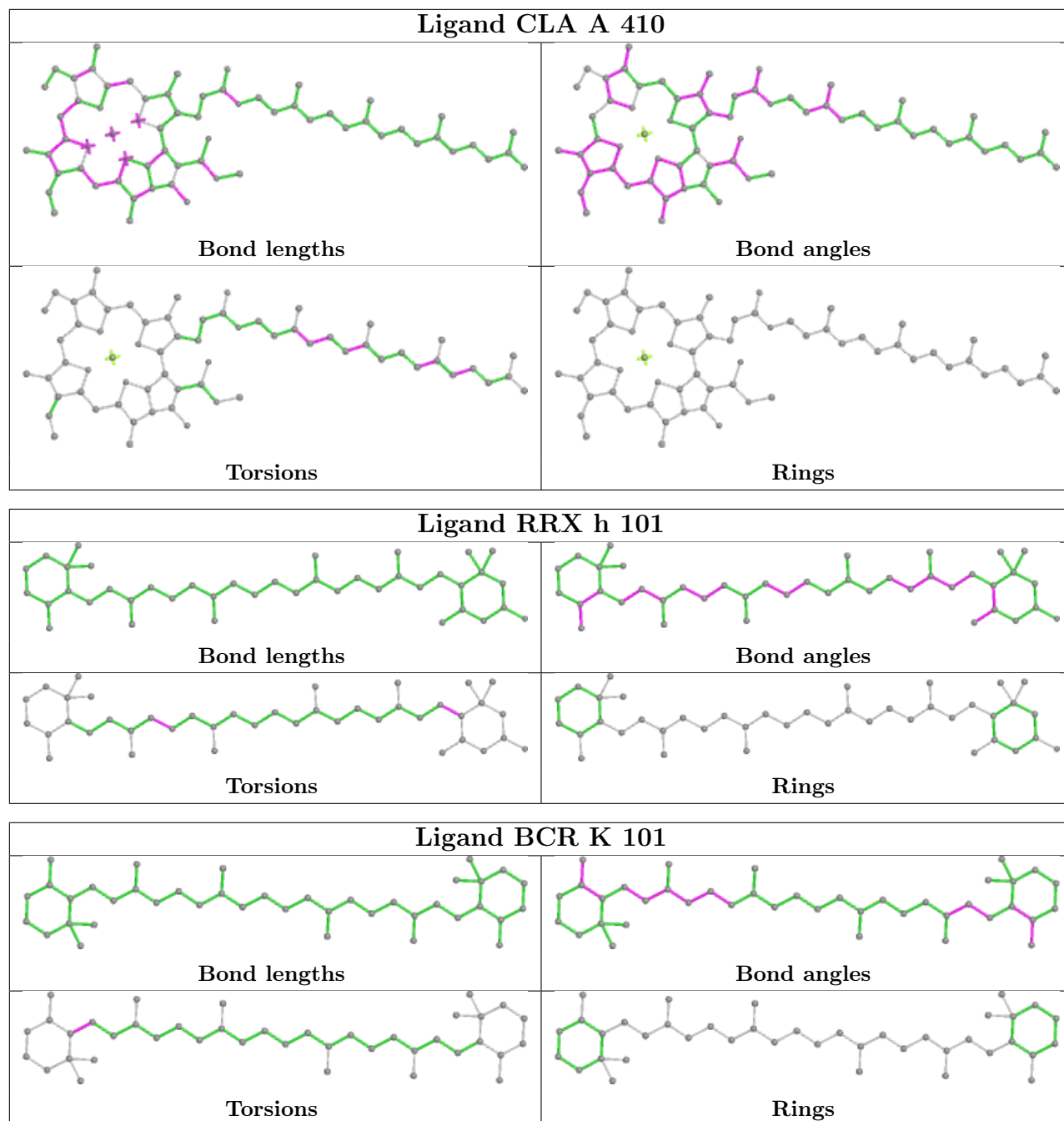


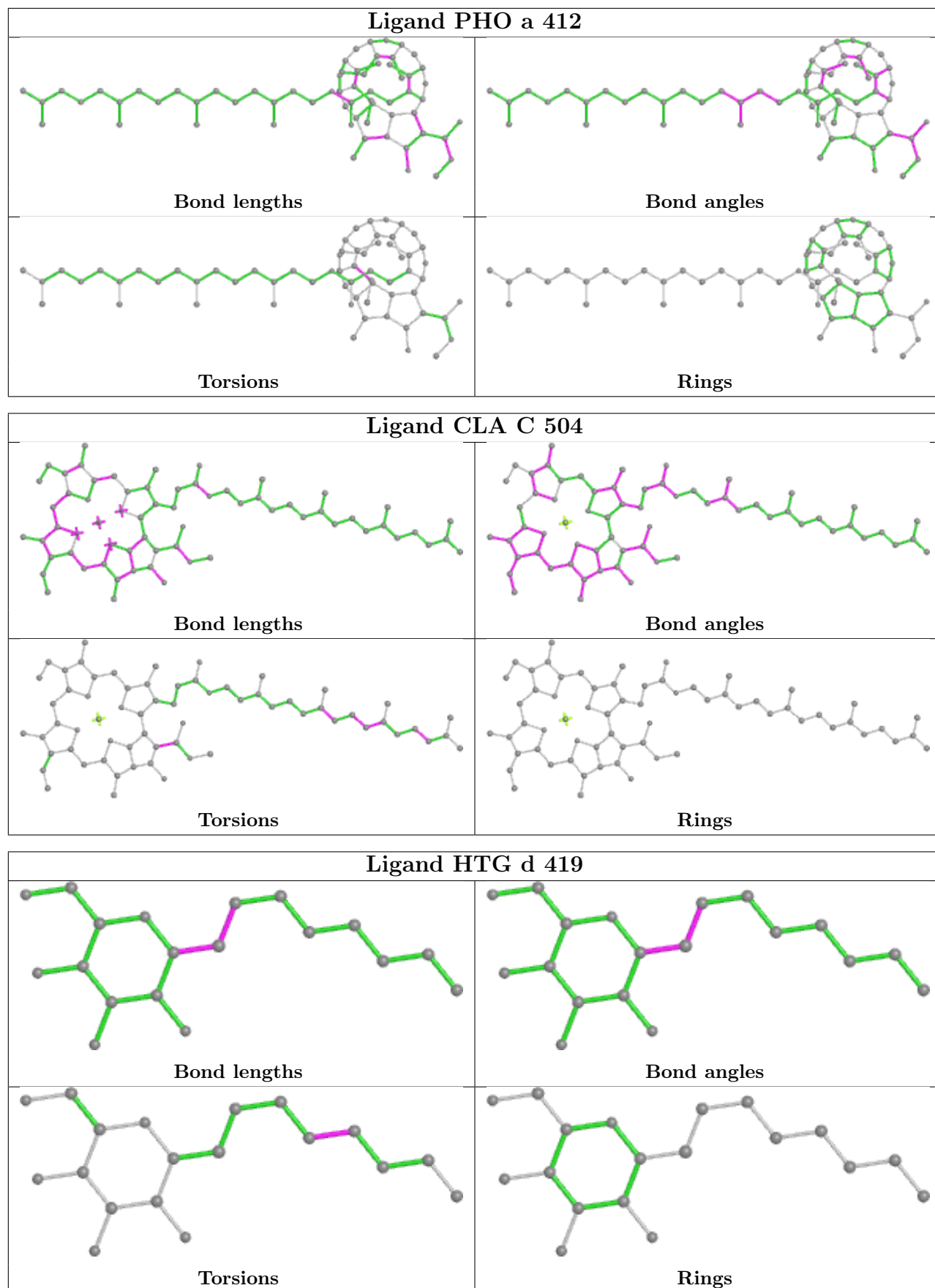




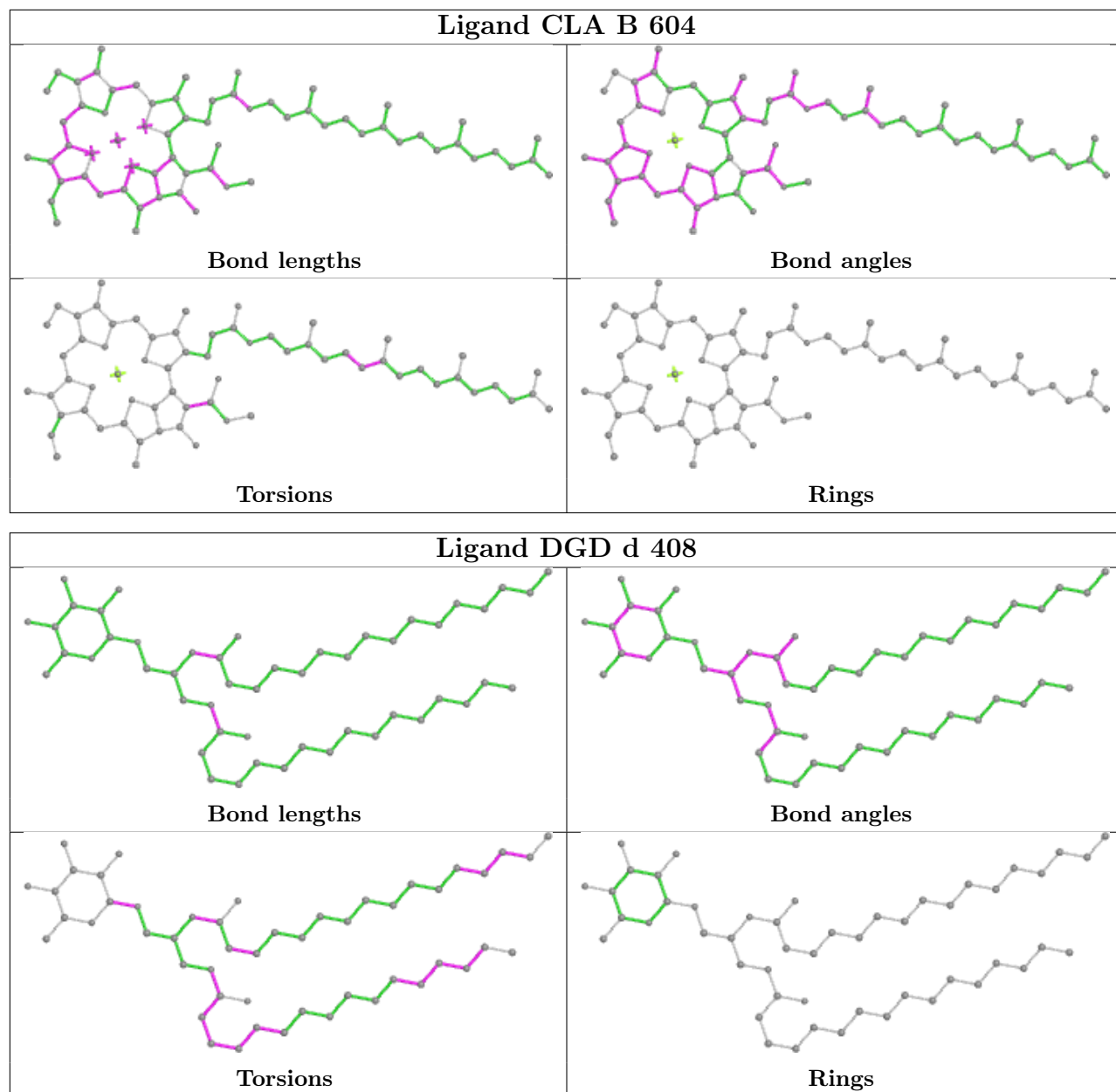


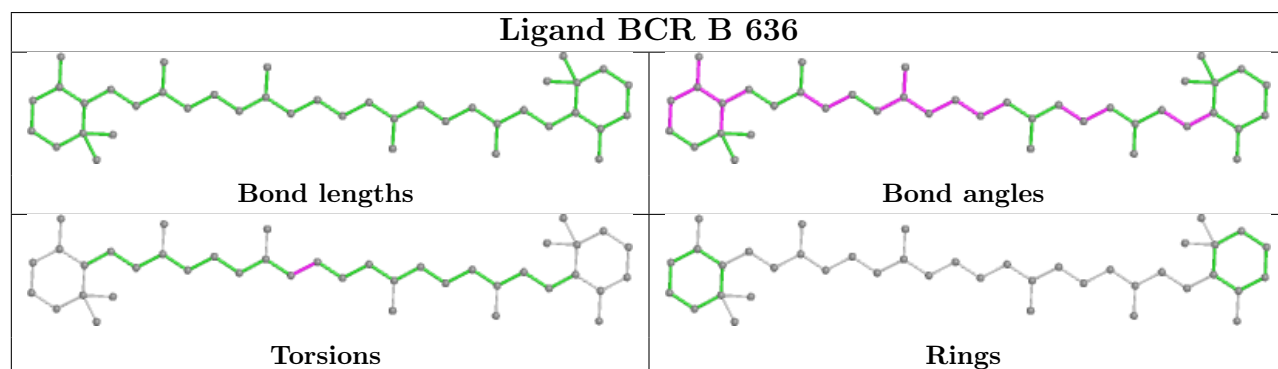
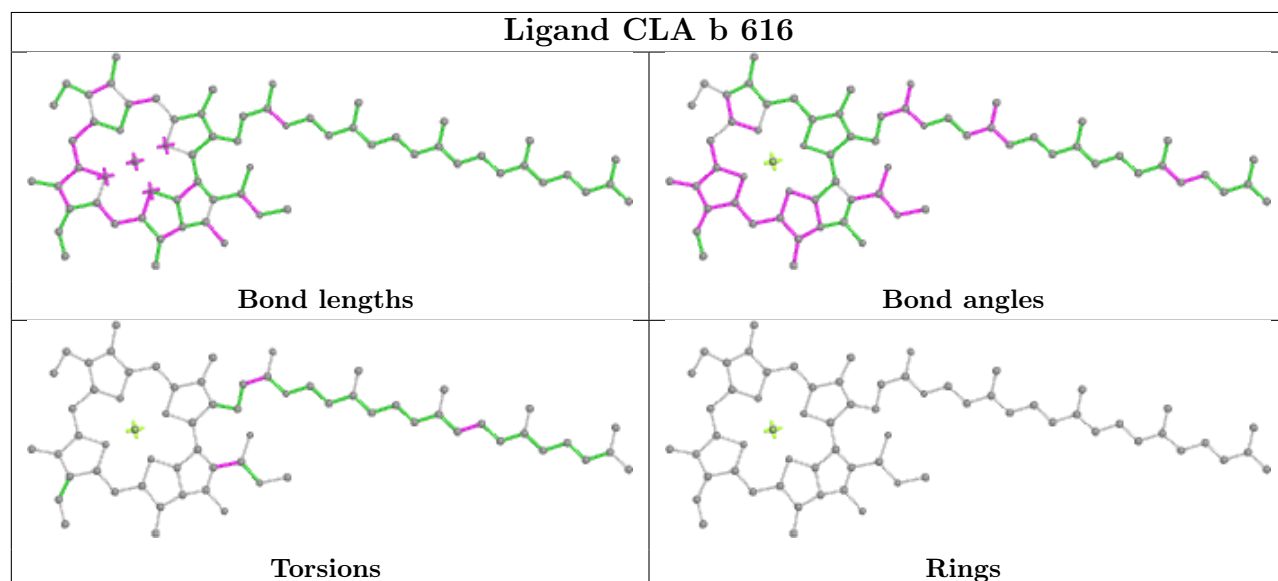
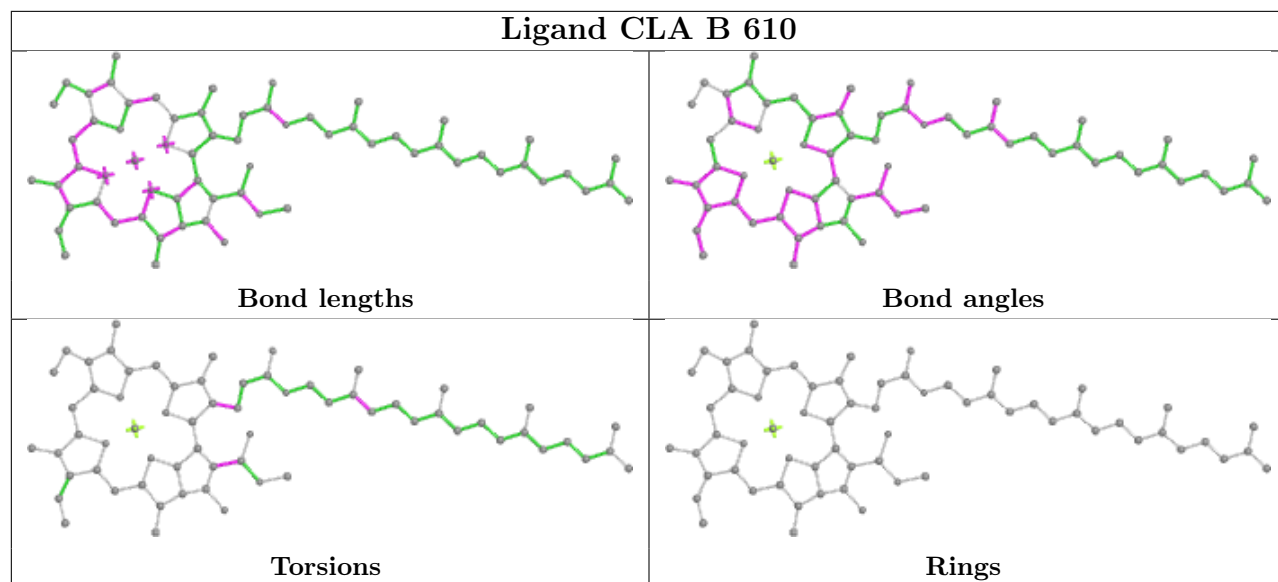


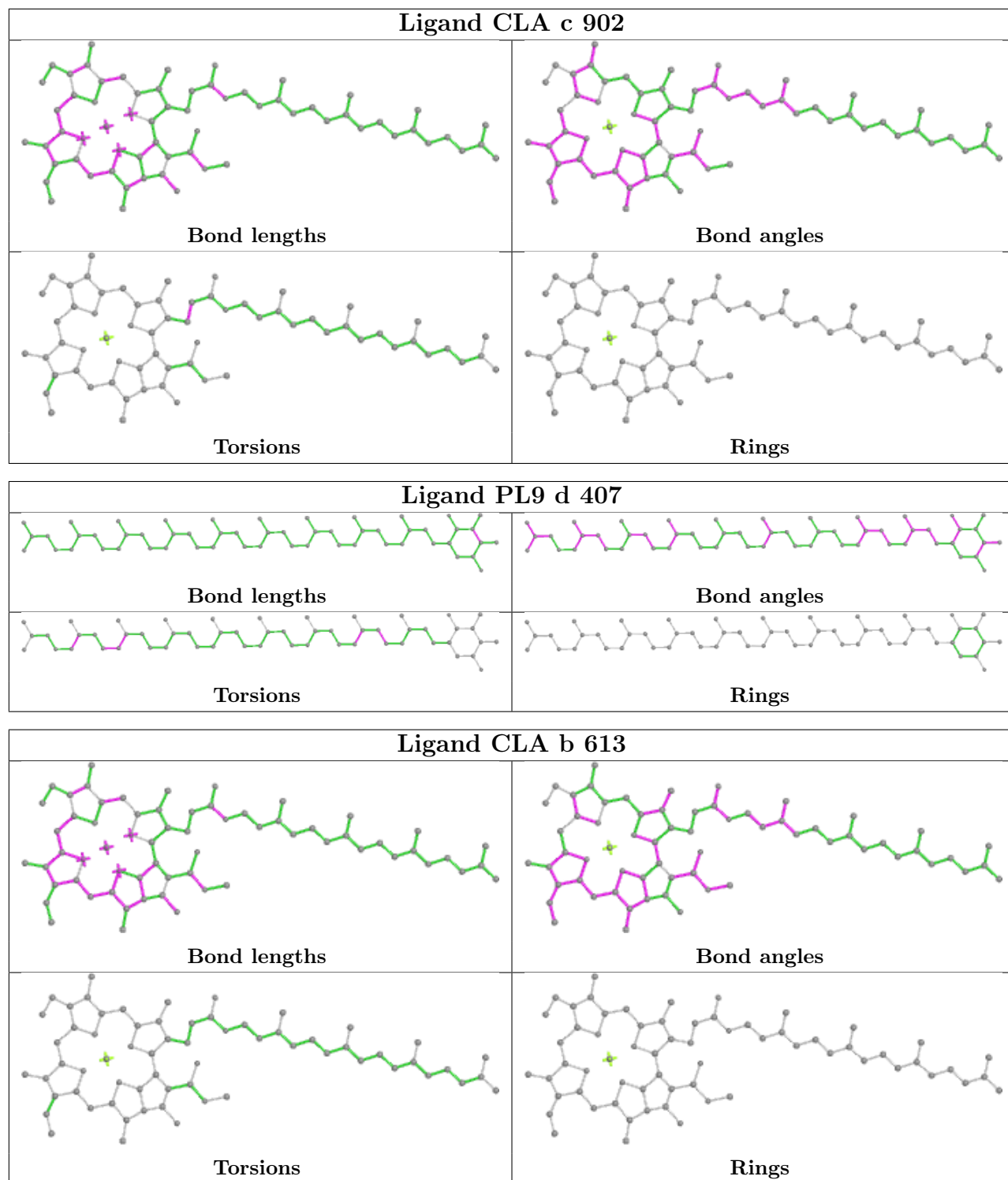


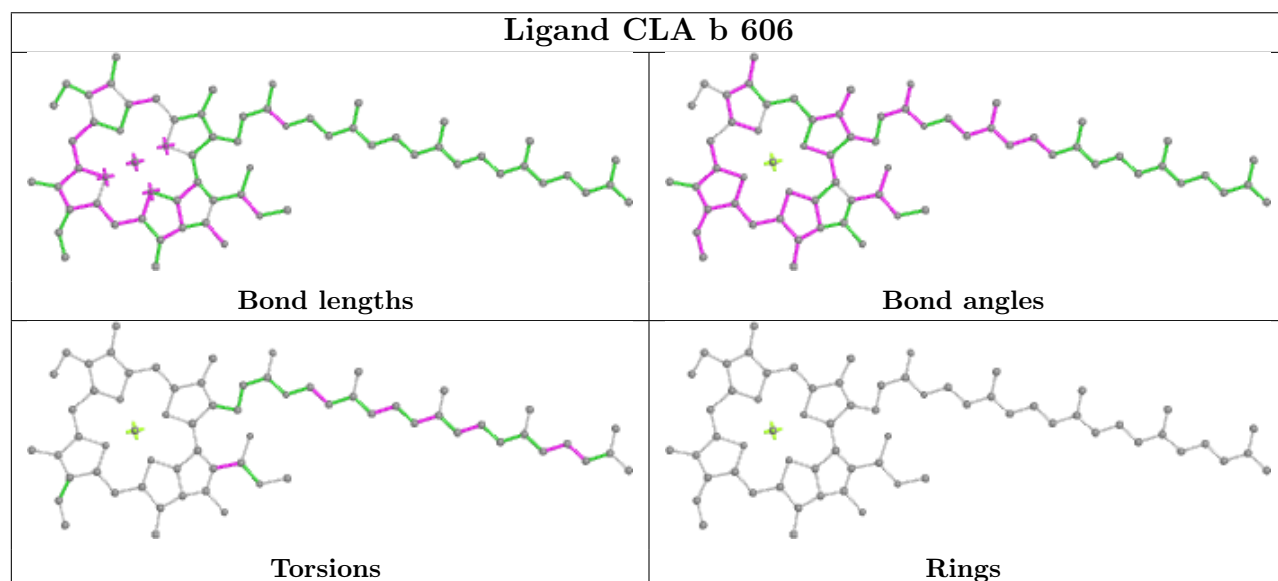
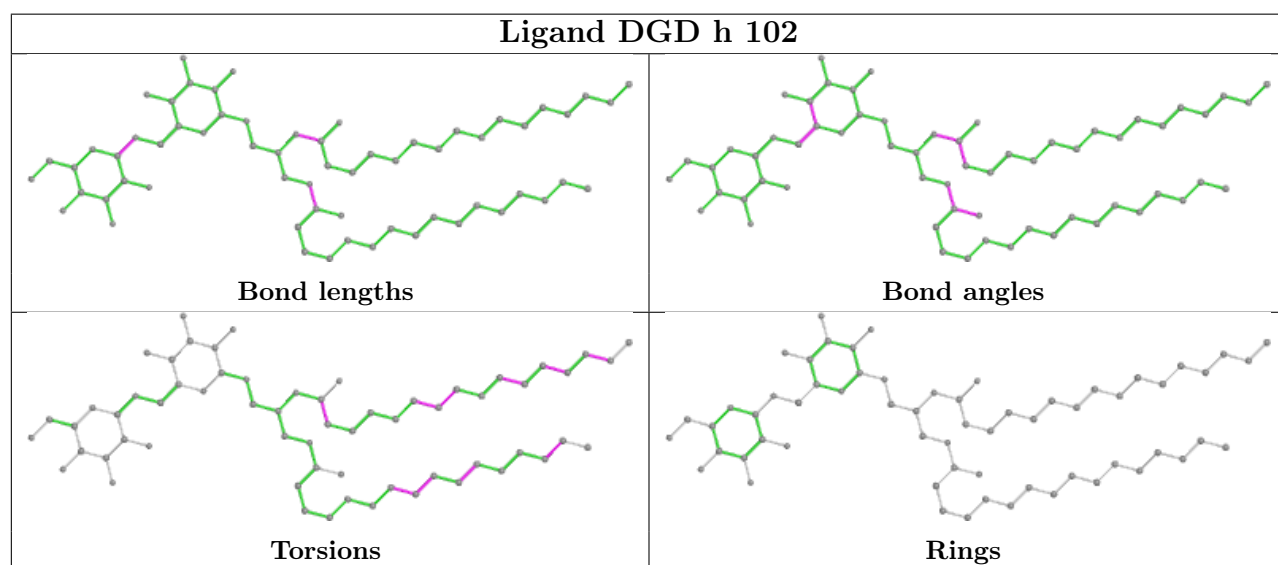
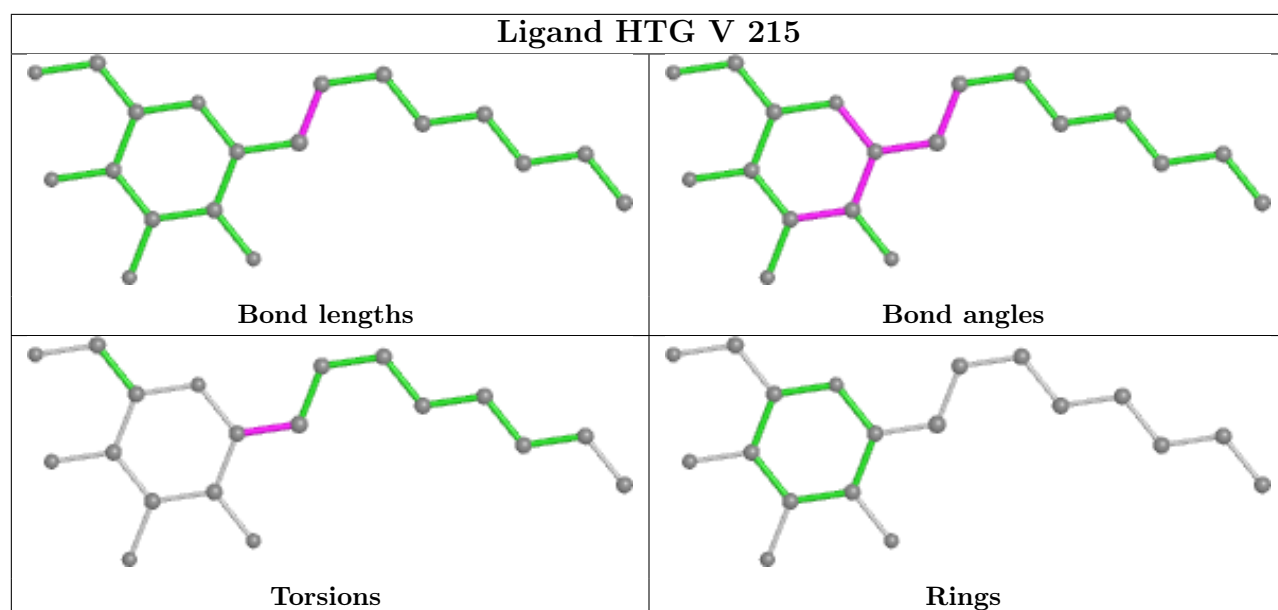


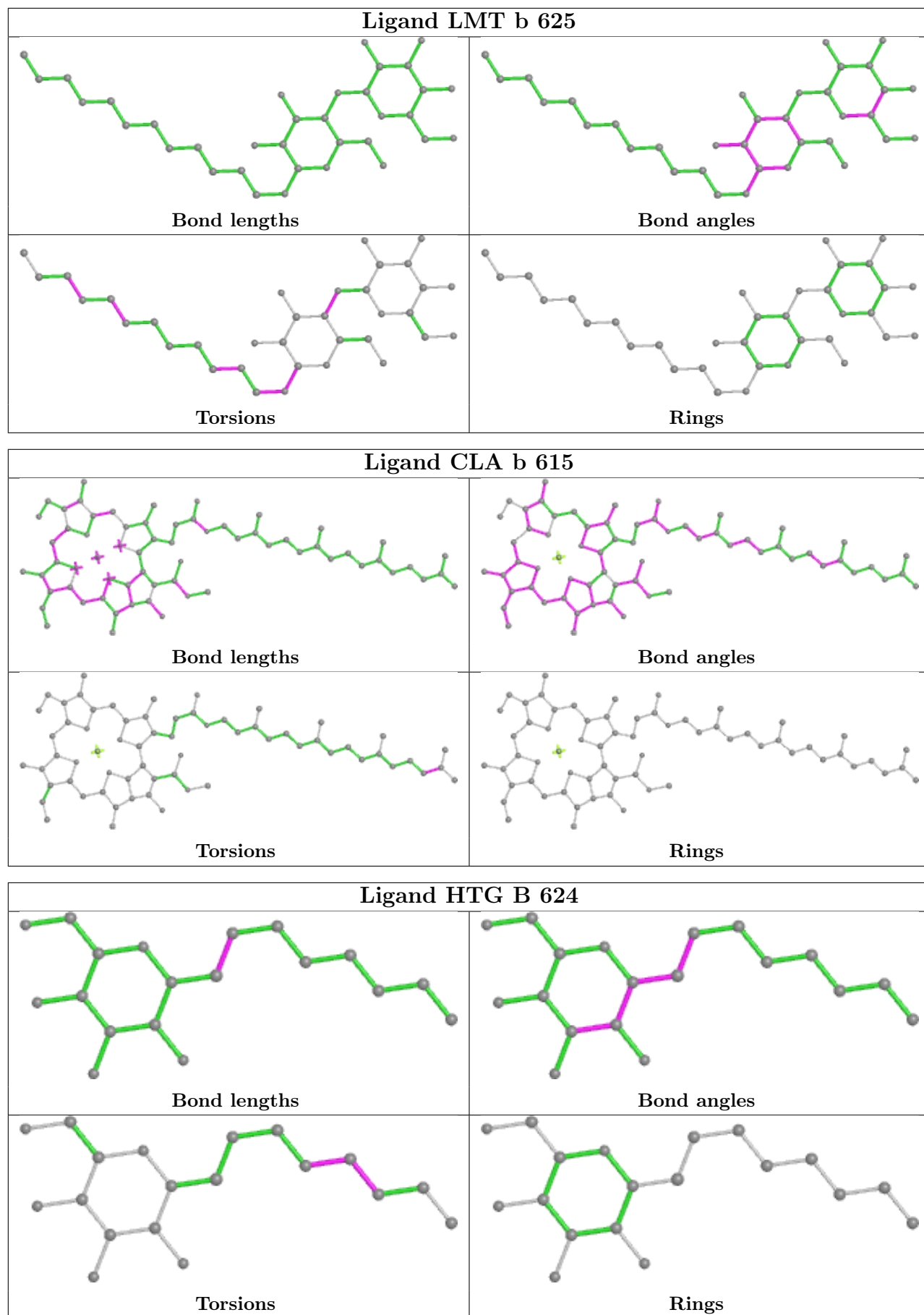


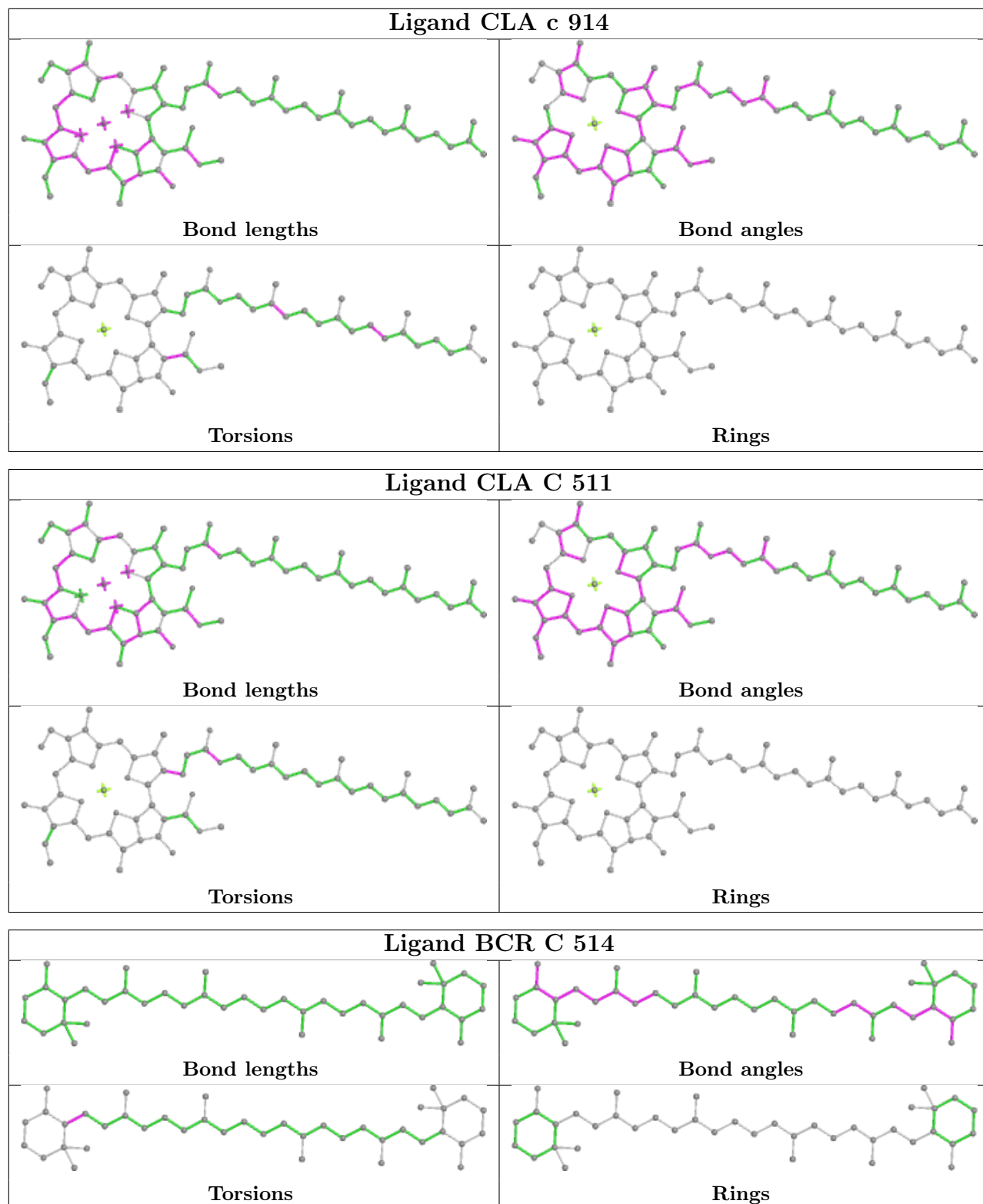


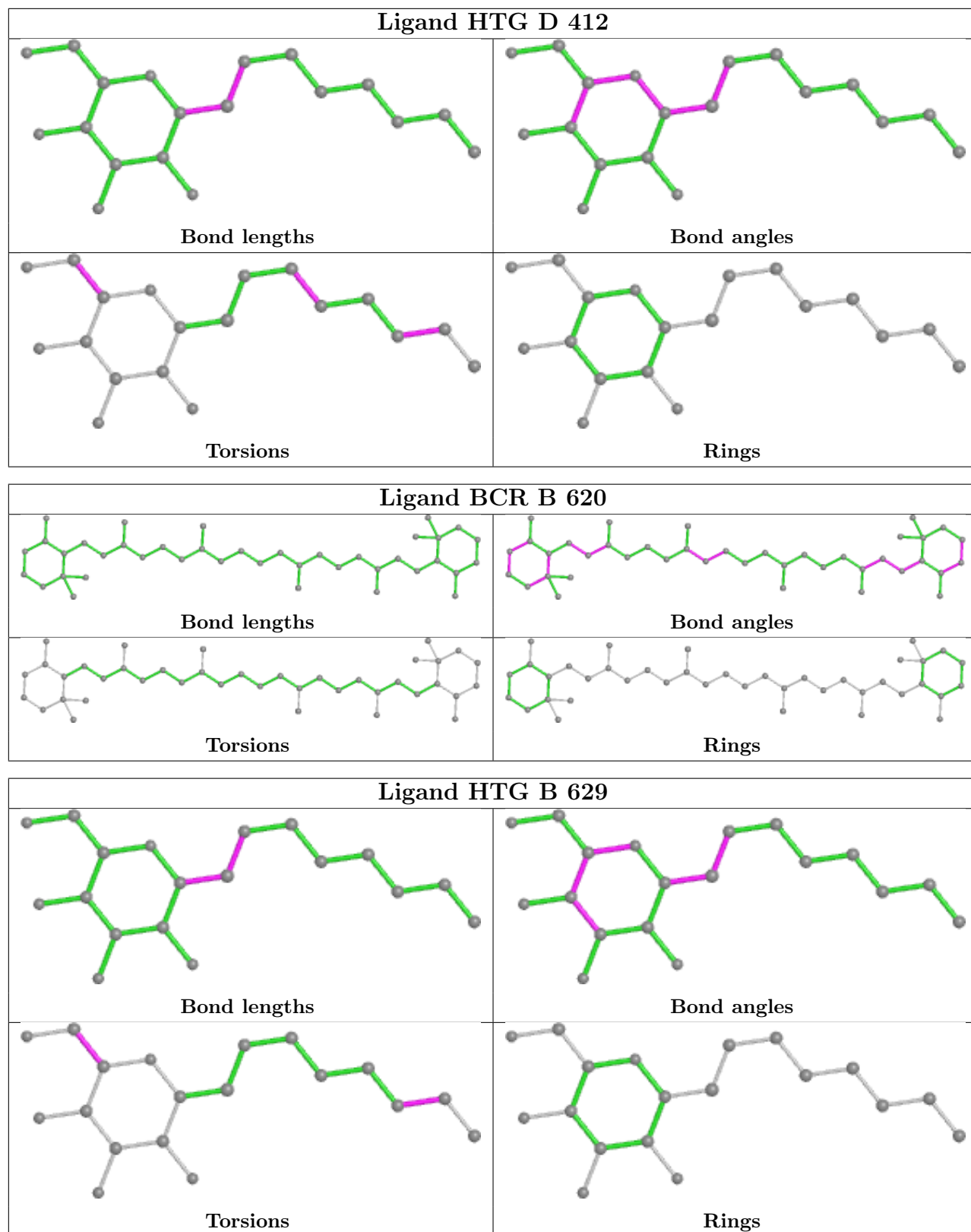


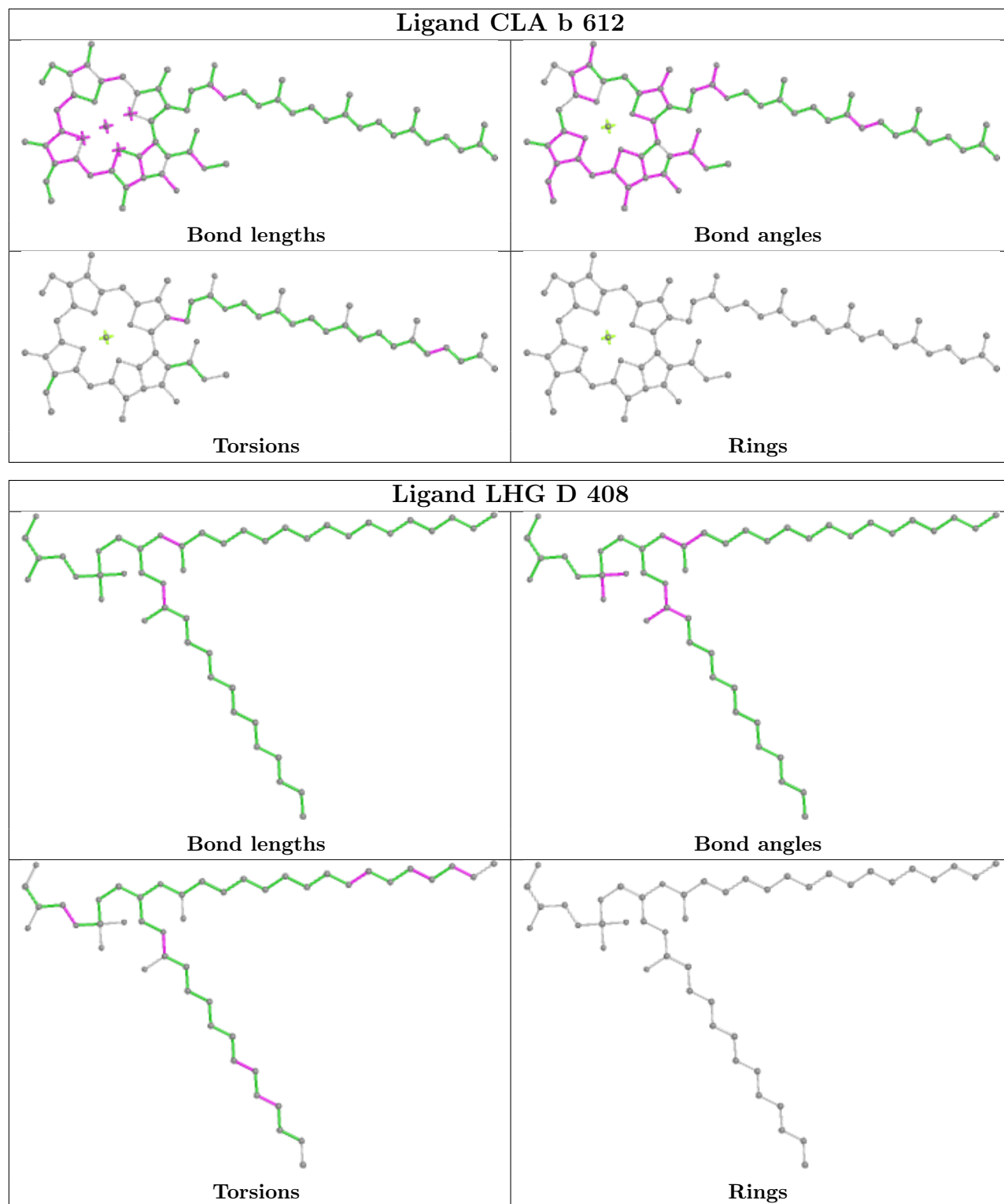












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.



## 5.8 Polymer linkage issues

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	334/360 (92%)	-0.04	10 (2%) 50 53	24, 30, 52, 108	0
1	a	336/360 (93%)	0.23	29 (8%) 10 12	26, 32, 66, 131	0
2	B	505/510 (99%)	0.11	33 (6%) 18 21	26, 35, 61, 93	0
2	b	504/510 (98%)	0.17	44 (8%) 10 11	27, 38, 70, 153	0
3	C	451/461 (97%)	-0.02	17 (3%) 40 43	27, 40, 57, 104	0
3	c	456/461 (98%)	0.23	28 (6%) 21 24	30, 43, 59, 112	0
4	D	342/352 (97%)	-0.17	6 (1%) 68 71	24, 31, 48, 116	0
4	d	342/352 (97%)	-0.20	6 (1%) 68 71	25, 34, 52, 104	0
5	E	80/84 (95%)	0.98	21 (26%) 0 0	33, 54, 100, 124	0
5	e	79/84 (94%)	0.84	15 (18%) 1 1	39, 52, 98, 121	0
6	F	34/45 (75%)	-0.06	3 (8%) 10 11	35, 42, 64, 94	0
6	f	32/45 (71%)	-0.18	2 (6%) 20 22	37, 43, 82, 101	0
7	H	65/66 (98%)	0.21	5 (7%) 13 15	32, 43, 64, 121	0
7	h	65/66 (98%)	0.78	10 (15%) 2 2	35, 47, 62, 133	0
8	I	36/38 (94%)	0.47	5 (13%) 2 3	39, 46, 115, 133	0
8	i	36/38 (94%)	0.27	2 (5%) 24 27	37, 45, 86, 108	0
9	J	36/40 (90%)	-0.29	2 (5%) 24 27	33, 46, 85, 103	0
9	j	39/40 (97%)	-0.12	0 100 100	38, 49, 64, 71	0
10	K	37/46 (80%)	-0.04	1 (2%) 54 57	40, 46, 61, 68	0
10	k	37/46 (80%)	0.09	2 (5%) 25 29	40, 50, 69, 82	0
11	L	37/37 (100%)	-0.36	2 (5%) 25 29	25, 29, 75, 116	0
11	l	37/37 (100%)	-0.03	1 (2%) 54 57	26, 30, 83, 121	0
12	M	33/36 (91%)	-0.47	1 (3%) 50 53	27, 32, 75, 105	0
12	m	33/36 (91%)	0.02	2 (6%) 21 24	28, 33, 73, 86	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/272 (89%)	0.35	32 (13%) 3 3	24, 42, 69, 115	0
13	o	243/272 (89%)	0.39	35 (14%) 2 2	27, 44, 80, 109	0
14	T	29/32 (90%)	-0.34	1 (3%) 45 48	25, 30, 51, 120	0
14	t	29/32 (90%)	0.30	2 (6%) 16 19	27, 31, 59, 101	0
15	U	98/134 (73%)	-0.05	3 (3%) 49 51	30, 38, 61, 115	0
15	u	97/134 (72%)	-0.31	3 (3%) 49 51	34, 44, 61, 123	0
16	V	137/163 (84%)	-0.10	11 (8%) 12 13	30, 37, 58, 70	0
16	v	137/163 (84%)	0.55	28 (20%) 1 1	35, 50, 70, 87	0
17	Y	30/46 (65%)	1.61	10 (33%) 0 0	47, 60, 102, 111	0
17	y	30/46 (65%)	1.93	11 (36%) 0 0	50, 64, 96, 105	0
18	X	40/41 (97%)	1.20	6 (15%) 2 2	41, 50, 92, 125	0
18	x	39/41 (95%)	0.89	7 (17%) 1 1	44, 52, 113, 137	0
19	Z	61/62 (98%)	1.90	23 (37%) 0 0	45, 55, 85, 112	0
19	z	61/62 (98%)	2.55	29 (47%) 0 0	51, 64, 105, 121	0
20	R	34/41 (82%)	5.82	34 (100%) 0 0	60, 94, 119, 124	0
All	All	5294/5691 (93%)	0.23	482 (9%) 9 10	24, 39, 72, 153	0

All (482) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	X	41	LEU	15.0
8	I	37	LEU	12.9
2	b	486	LEU	12.4
7	h	65	LEU	11.2
20	R	18	TRP	9.9
20	R	35	LEU	9.9
7	h	64	ALA	9.9
20	R	31	VAL	9.6
20	R	34	LEU	9.5
19	z	4	LEU	9.0
13	o	246	ALA	9.0
20	R	3	TRP	8.3
18	x	2	THR	8.2
17	y	18	VAL	8.2
19	z	3	ILE	8.1
2	b	485	GLU	8.0
2	b	495	PHE	7.5

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Mol	Chain	Res	Type	RSRZ
17	y	19	ILE	7.3
5	E	79	PHE	7.2
19	z	5	PHE	7.1
20	R	14	LEU	7.0
18	x	40	SER	7.0
20	R	16	ALA	6.9
2	b	496	TYR	6.9
2	B	486	LEU	6.8
19	z	9	LEU	6.8
20	R	28	VAL	6.7
1	A	11	ALA	6.7
17	Y	18	VAL	6.7
2	b	487	SER	6.7
17	Y	19	ILE	6.6
20	R	10	LEU	6.6
20	R	32	GLN	6.6
19	Z	3	ILE	6.6
7	H	64	ALA	6.6
16	v	26	TYR	6.6
20	R	23	ILE	6.6
19	z	2	THR	6.5
18	X	40	SER	6.4
20	R	27	ALA	6.4
2	b	493	TRP	6.2
5	E	72	ALA	6.2
1	a	11	ALA	6.2
20	R	5	VAL	6.1
1	a	10	THR	6.0
17	y	25	ILE	6.0
7	h	66	GLY	6.0
2	B	479	PHE	6.0
8	I	36	ASP	6.0
2	b	484	PRO	5.9
2	b	488	PRO	5.9
20	R	7	VAL	5.9
5	E	76	VAL	5.9
19	z	61	VAL	5.9
20	R	13	LEU	5.9
20	R	24	LEU	5.9
1	a	13	LEU	5.8
19	Z	33	TRP	5.7
2	b	494	GLY	5.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
20	R	6	LEU	5.7
20	R	30	GLN	5.6
7	H	65	LEU	5.6
20	R	25	PRO	5.6
2	B	487	SER	5.6
20	R	33	LYS	5.6
2	b	504	THR	5.5
18	X	2	THR	5.5
20	R	12	VAL	5.4
20	R	17	GLY	5.4
14	t	29	ILE	5.3
15	U	7	GLU	5.2
7	h	6	TRP	5.2
4	D	238	THR	5.2
19	z	10	ALA	5.2
2	b	295	GLY	5.1
19	Z	32	ASP	5.1
20	R	26	TYR	5.1
17	Y	25	ILE	5.1
20	R	15	ALA	5.1
17	y	22	LEU	5.1
1	A	12	ASN	5.1
19	z	62	VAL	5.1
19	z	7	LEU	5.0
18	x	37	VAL	5.0
19	z	60	PHE	5.0
2	b	502	VAL	5.0
5	E	78	THR	4.9
2	b	293	ALA	4.8
13	o	36	GLN	4.8
3	c	200	THR	4.8
17	y	20	ALA	4.8
13	o	37	THR	4.8
19	z	57	LEU	4.7
3	c	201	ASN	4.6
2	B	502	VAL	4.6
1	a	235	TYR	4.5
15	u	8	GLU	4.5
20	R	19	ALA	4.5
4	d	238	THR	4.5
14	t	30	THR	4.5
2	b	505	ARG	4.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
20	R	9	LEU	4.4
19	Z	31	GLN	4.4
3	C	143	TYR	4.4
13	o	34	SER	4.4
17	Y	20	ALA	4.4
19	Z	36	SER	4.3
4	D	11	GLU	4.3
16	v	21	LEU	4.3
19	z	6	GLN	4.3
20	R	22	ASN	4.2
2	B	496	TYR	4.2
10	k	18	PHE	4.2
5	E	74	GLN	4.2
13	o	245	PRO	4.2
3	c	143	TYR	4.2
1	A	230	THR	4.2
5	E	57	ALA	4.2
13	o	35	SER	4.1
4	d	240	ALA	4.1
18	x	38	GLN	4.1
5	E	80	LEU	4.1
20	R	29	LYS	4.1
18	x	3	ILE	4.1
16	v	3	LEU	4.1
19	z	53	VAL	4.1
5	E	17	VAL	4.0
20	R	2	ASP	4.0
13	O	136	ILE	4.0
1	A	229	GLU	4.0
13	O	4	THR	4.0
2	b	298	LEU	3.9
19	Z	62	VAL	3.9
13	O	137	THR	3.9
5	e	57	ALA	3.9
7	h	10	ILE	3.9
2	b	503	THR	3.9
2	b	129	GLY	3.9
20	R	20	VAL	3.9
1	a	260	PHE	3.8
2	b	296	ALA	3.8
8	I	34	ARG	3.8
19	z	8	ALA	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	c	183	GLY	3.8
2	b	294	SER	3.8
17	Y	22	LEU	3.8
5	E	73	LYS	3.7
2	B	495	PHE	3.7
2	b	489	GLU	3.7
2	b	483	ASP	3.7
4	d	236	ASN	3.7
5	e	60	GLN	3.7
12	M	33	GLN	3.6
19	Z	4	LEU	3.6
5	E	77	GLU	3.6
18	x	39	ARG	3.6
13	O	135	SER	3.6
1	a	225	ARG	3.6
16	v	19	ILE	3.6
13	O	30	TYR	3.6
13	O	204	VAL	3.6
3	c	181	PHE	3.6
18	x	34	ILE	3.6
1	a	242	GLU	3.6
3	c	279	LEU	3.6
2	b	126	PRO	3.6
19	z	41	PHE	3.5
2	B	494	GLY	3.5
19	Z	30	PRO	3.5
13	o	211	ILE	3.5
19	z	59	PHE	3.5
19	Z	2	THR	3.5
13	o	25	THR	3.5
14	T	30	THR	3.5
17	y	24	MET	3.5
16	V	19	ILE	3.4
19	z	11	ALA	3.4
3	c	426	LEU	3.4
19	Z	35	ARG	3.4
13	O	132	ASN	3.4
13	o	28	GLY	3.4
13	O	27	ARG	3.4
5	E	21	VAL	3.4
5	e	21	VAL	3.4
13	O	56	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
13	o	38	TYR	3.3
3	c	182	PHE	3.3
3	C	145[A]	SER	3.3
6	F	12	SER	3.3
13	o	30	TYR	3.3
11	l	1	MET	3.3
5	E	81	GLU	3.3
3	C	253	LEU	3.3
7	H	66	GLY	3.3
19	Z	61	VAL	3.3
20	R	8	VAL	3.3
13	o	26	ALA	3.3
13	o	58	ASN	3.3
1	a	297	LEU	3.3
3	C	155	ASN	3.2
7	h	7	LEU	3.2
5	E	82	GLN	3.2
5	e	76	VAL	3.2
19	Z	29	SER	3.2
1	a	224	ILE	3.2
2	b	238	LEU	3.1
19	Z	9	LEU	3.1
19	Z	42	LEU	3.1
1	a	9	GLN	3.1
2	B	253	ALA	3.1
1	A	16	ARG	3.1
2	b	242	ILE	3.1
16	v	8	LEU	3.1
2	B	505	ARG	3.1
13	o	134	THR	3.1
13	O	26	ALA	3.1
19	z	56	VAL	3.1
2	b	292	LEU	3.1
3	c	204	LEU	3.1
2	B	295	GLY	3.1
16	v	4	THR	3.1
3	c	86	LEU	3.1
19	Z	5	PHE	3.1
19	z	42	LEU	3.1
3	C	23	ALA	3.1
10	K	14	ALA	3.1
4	d	237	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	13	LEU	3.0
3	c	276	LEU	3.0
13	o	33	ASP	3.0
20	R	11	PRO	3.0
12	m	33	GLN	3.0
1	a	14	TRP	3.0
3	c	433	LEU	3.0
19	Z	34	ASP	3.0
1	a	240	GLY	3.0
16	v	16	GLY	3.0
1	a	248	ILE	3.0
5	E	75	GLN	3.0
16	V	15[A]	GLU	3.0
17	y	21	GLN	3.0
1	a	263	ALA	3.0
16	v	27	LEU	3.0
17	y	37	PHE	3.0
19	z	18	VAL	3.0
2	b	499	VAL	2.9
19	z	46	LEU	2.9
3	c	87	ILE	2.9
16	v	15	GLU	2.9
2	b	245	VAL	2.9
16	v	22	THR	2.9
13	O	5	LEU	2.9
12	m	34	LYS	2.9
2	B	485	GLU	2.9
2	b	492	GLU	2.9
1	a	261	GLN	2.9
16	V	8	LEU	2.9
1	A	63	ILE	2.9
1	A	344	ALA	2.9
13	o	27	ARG	2.9
18	X	37	VAL	2.9
3	c	59	LEU	2.9
3	c	272	LEU	2.9
16	v	5	PRO	2.9
18	X	34	ILE	2.9
19	z	58	ASN	2.9
6	f	14	PRO	2.8
13	O	24	ASP	2.8
19	Z	46	LEU	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
13	o	243	ILE	2.8
1	a	228	THR	2.8
3	C	255	THR	2.8
4	d	241	GLU	2.8
5	E	59	GLU	2.8
13	O	93	LEU	2.8
1	A	228	THR	2.8
16	v	18	THR	2.8
2	B	293	ALA	2.8
17	y	26	ALA	2.8
2	B	503	THR	2.8
2	b	297	THR	2.8
19	z	33	TRP	2.8
2	B	488	PRO	2.8
5	e	25	ILE	2.8
16	V	18	THR	2.8
9	J	8	ILE	2.8
18	X	31	ILE	2.8
13	O	139	SER	2.8
3	c	427	ALA	2.7
1	a	295	PHE	2.7
19	Z	41	PHE	2.7
2	B	484	PRO	2.7
1	A	159	LEU	2.7
13	o	22	LEU	2.7
16	v	12	LEU	2.7
1	a	344	ALA	2.7
19	z	30	PRO	2.7
1	a	226	GLU	2.7
5	e	72	ALA	2.7
5	e	24	SER	2.7
19	Z	7	LEU	2.7
19	z	32	ASP	2.7
2	b	244	ALA	2.7
13	o	135	SER	2.7
3	C	257	PHE	2.7
7	H	6	TRP	2.7
20	R	21	ARG	2.7
13	O	25	THR	2.7
19	z	14	ILE	2.6
5	e	20	TRP	2.6
16	V	7	VAL	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	D	122	LEU	2.6
3	c	429	SER	2.6
3	c	434	ALA	2.6
13	o	32	ILE	2.6
13	o	136	ILE	2.6
3	C	182	PHE	2.6
8	i	37	LEU	2.6
19	Z	39	LEU	2.6
1	a	163	ILE	2.6
16	v	113	VAL	2.6
16	V	4	THR	2.6
4	D	45	LEU	2.6
13	O	133	VAL	2.6
16	v	10	VAL	2.6
5	E	6	GLY	2.6
2	b	461	LEU	2.6
11	L	3	PRO	2.6
4	D	114	ILE	2.6
2	B	251	VAL	2.6
16	V	5	PRO	2.5
17	Y	30	ILE	2.5
16	v	14	SER	2.5
13	O	212	ALA	2.5
16	v	114	ALA	2.5
6	F	16	PHE	2.5
2	B	298	LEU	2.5
2	b	218	LEU	2.5
17	Y	24	MET	2.5
1	a	12	ASN	2.5
2	b	290	ALA	2.5
13	O	31	PRO	2.5
1	a	16	ARG	2.5
11	L	1	MET	2.5
19	Z	60	PHE	2.5
2	b	29	LEU	2.5
5	e	83	LEU	2.5
2	b	497	GLN	2.5
5	E	5	THR	2.5
2	B	290	ALA	2.5
5	E	3	GLY	2.5
19	z	43	GLY	2.5
5	e	58	GLN	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	c	462	GLU	2.4
20	R	4	ARG	2.4
2	B	247	PHE	2.4
17	Y	26	ALA	2.4
2	B	242	ILE	2.4
5	e	78	THR	2.4
2	b	463	PHE	2.4
7	h	12	ARG	2.4
5	e	84	LYS	2.4
13	O	138	THR	2.4
13	o	139	SER	2.4
17	Y	27	MET	2.4
2	B	483	ASP	2.4
17	Y	23	THR	2.4
3	C	261	ARG	2.4
3	C	262	ARG	2.4
3	C	435	PHE	2.4
13	O	142	PHE	2.4
2	B	84	THR	2.4
13	o	31	PRO	2.4
13	O	130	GLN	2.4
13	o	133	VAL	2.4
1	a	246	TYR	2.3
1	a	227	THR	2.3
7	h	57	GLY	2.3
1	a	249	VAL	2.3
16	v	7	VAL	2.3
2	B	248	ALA	2.3
13	o	241	ALA	2.3
13	O	206	GLY	2.3
16	v	24	LYS	2.3
13	o	242	SER	2.3
5	E	58	GLN	2.3
13	o	204	VAL	2.3
19	Z	18	VAL	2.3
13	o	206	GLY	2.3
3	c	88	LEU	2.3
13	O	199	LEU	2.3
19	Z	57	LEU	2.3
3	c	202	PRO	2.3
16	v	23	GLU	2.3
2	b	301	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
13	o	212	ALA	2.3
16	v	112	LEU	2.3
13	O	239	PHE	2.3
3	c	425	TRP	2.3
16	v	116	ALA	2.3
13	o	209	GLY	2.2
16	v	6	GLU	2.2
13	O	90	ASP	2.2
3	C	438	LEU	2.2
13	o	130	GLN	2.2
10	k	17	ILE	2.2
2	B	489	GLU	2.2
13	o	62	GLU	2.2
2	B	29	LEU	2.2
3	C	433	LEU	2.2
13	O	59	LYS	2.2
13	o	59	LYS	2.2
1	a	262	TYR	2.2
2	B	462	PHE	2.2
5	e	79	PHE	2.2
13	o	29	ALA	2.2
3	c	430	HIS	2.2
2	b	467	ILE	2.2
16	v	107	LEU	2.2
6	f	42	PHE	2.2
16	v	29	GLY	2.2
15	U	58	VAL	2.2
7	h	9	ASP	2.2
2	B	482	ILE	2.2
8	I	35	LYS	2.2
3	C	254	THR	2.2
16	v	108	THR	2.2
3	c	52	ALA	2.2
5	e	19	TYR	2.2
13	O	207	ARG	2.2
3	C	432	VAL	2.2
4	d	154	VAL	2.2
6	F	14	PRO	2.1
13	O	89	SER	2.1
15	u	9	LEU	2.1
16	V	6	GLU	2.1
13	O	28	GLY	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	459	ALA	2.1
7	H	56	ASP	2.1
7	h	22	ALA	2.1
1	a	241	GLN	2.1
3	c	420	VAL	2.1
15	U	59	GLU	2.1
2	B	504	THR	2.1
2	b	84	THR	2.1
8	i	24	LEU	2.1
13	O	29	ALA	2.1
16	V	14	SER	2.1
5	e	23	HIS	2.1
19	z	17	PHE	2.1
2	B	500	GLY	2.1
16	V	16	GLY	2.1
2	b	217	ILE	2.1
13	o	244	GLU	2.1
2	B	296	ALA	2.1
19	z	49	ALA	2.1
2	b	125	ASP	2.1
1	a	160	ILE	2.1
3	C	426	LEU	2.1
3	C	256	PRO	2.1
9	J	5	GLY	2.1
5	E	4	THR	2.1
8	I	33	LYS	2.1
16	v	17	LYS	2.1
17	y	23	THR	2.1
13	O	87	VAL	2.1
13	O	241	ALA	2.1
2	b	251	VAL	2.0
2	b	464	PHE	2.0
3	c	439	VAL	2.0
1	a	290	ILE	2.0
16	V	2[A]	GLU	2.0
3	c	437	PHE	2.0
4	D	240	ALA	2.0
2	B	33	TRP	2.0
2	b	482	ILE	2.0
5	E	25	ILE	2.0
15	u	102	LEU	2.0
17	y	30[A]	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	297	THR	2.0
3	c	428	THR	2.0
16	v	20	THR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
19	FME	Z	1	10/11	0.90	0.23	68,82,98,101	0
19	FME	z	1	10/11	0.90	0.34	98,112,120,122	0
14	FME	t	1	10/11	0.95	0.09	30,34,59,63	0
14	FME	T	1	10/11	0.95	0.10	30,39,62,64	0
8	FME	i	1	10/11	0.97	0.13	31,40,44,47	0
12	FME	m	1	10/11	0.98	0.07	33,42,69,78	0
12	FME	M	1	10/11	0.98	0.11	31,40,71,76	0
8	FME	I	1	10/11	0.98	0.07	34,43,49,50	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
30	UNL	A	415	36/-	0.37	0.46	75,99,113,114	0
36	HTG	c	941	19/19	0.39	0.34	67,133,141,142	0
30	UNL	c	947	6/-	0.43	0.31	71,80,83,85	0
30	UNL	h	103	9/-	0.47	0.47	81,86,109,110	0
30	UNL	J	105	8/-	0.51	0.21	80,94,98,99	0
30	UNL	i	105	12/-	0.52	0.37	77,86,88,89	0
37	DGD	D	405	52/66	0.55	0.36	74,102,120,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
30	UNL	a	418	40/-	0.56	0.52	79,99,122,125	0
31	LMT	m	103	35/35	0.56	0.31	53,125,136,137	0
30	UNL	b	633	9/-	0.57	0.22	76,81,87,88	0
31	LMT	j	102	24/35	0.58	0.23	66,84,120,122	0
30	UNL	b	634	9/-	0.60	0.37	99,103,113,114	0
30	UNL	I	106	9/-	0.60	0.18	76,80,87,87	0
30	UNL	c	944	4/-	0.62	0.28	76,77,78,81	0
31	LMT	b	625	35/35	0.62	0.26	59,119,133,139	0
37	DGD	d	408	50/66	0.63	0.34	81,99,121,130	0
36	HTG	d	420	19/19	0.64	0.42	85,115,118,118	0
27	SQD	l	101	54/54	0.64	0.26	48,77,116,117	0
31	LMT	A	417	35/35	0.64	0.31	55,92,108,115	0
30	UNL	e	106	11/-	0.65	0.18	83,87,92,94	0
31	LMT	t	101	23/35	0.65	0.28	60,95,135,138	0
32	GOL	O	304	6/6	0.65	0.40	89,90,92,96	0
36	HTG	b	627	19/19	0.65	0.25	69,113,125,128	0
31	LMT	e	101	24/35	0.66	0.31	94,101,125,127	0
31	LMT	A	421	35/35	0.66	0.37	84,100,131,132	0
31	LMT	J	102	24/35	0.66	0.25	64,86,118,120	0
36	HTG	y	102	19/19	0.66	0.23	84,115,122,124	0
30	UNL	J	103	12/-	0.66	0.25	69,79,83,84	0
31	LMT	c	922	35/35	0.66	0.45	85,117,122,126	0
36	HTG	c	924	19/19	0.67	0.50	69,99,118,118	0
34	DMS	c	939	4/4	0.67	0.35	112,114,119,120	0
34	DMS	B	646	4/4	0.67	0.26	109,114,115,116	0
36	HTG	b	603	19/19	0.68	0.19	64,103,118,120	0
30	UNL	J	104	16/-	0.68	0.26	75,83,91,91	0
34	DMS	i	106	4/4	0.68	0.27	125,125,125,127	0
36	HTG	B	631	19/19	0.68	0.36	71,107,118,120	0
30	UNL	h	106	11/-	0.69	0.50	72,75,78,79	0
30	UNL	k	104	9/-	0.69	0.18	69,82,89,90	0
30	UNL	c	948	18/-	0.70	0.29	79,89,113,114	0
30	UNL	I	105	9/-	0.70	0.27	70,73,81,83	0
30	UNL	A	428	4/-	0.71	0.35	64,66,70,71	0
31	LMT	M	101	35/35	0.71	0.19	42,70,85,89	0
30	UNL	b	635	9/-	0.71	0.30	59,82,90,90	0
36	HTG	c	943	17/19	0.71	0.44	76,122,129,130	0
30	UNL	y	103	4/-	0.71	0.14	81,82,84,85	0
30	UNL	b	630	10/-	0.71	0.17	71,82,85,85	0
28	LMG	C	523	51/55	0.71	0.30	47,94,109,114	0
31	LMT	B	626	24/35	0.71	0.19	47,73,114,118	0
31	LMT	a	402	35/35	0.72	0.28	49,96,119,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
30	UNL	h	104	9/-	0.72	0.20	68,74,84,85	0
30	UNL	E	104	5/-	0.72	0.22	59,64,67,69	0
34	DMS	O	307	4/4	0.72	0.30	113,113,115,121	0
27	SQD	a	401	54/54	0.73	0.19	55,80,106,110	0
36	HTG	B	625	19/19	0.73	0.47	64,112,121,124	0
30	UNL	C	522	34/-	0.73	0.30	68,94,102,106	0
36	HTG	d	419	19/19	0.73	0.30	75,100,110,113	0
36	HTG	C	521	19/19	0.73	0.30	58,93,110,117	0
36	HTG	V	215	19/19	0.73	0.30	100,116,127,128	0
30	UNL	c	946	4/-	0.73	0.37	83,83,83,84	0
31	LMT	t	102	35/35	0.73	0.24	43,91,116,118	0
28	LMG	a	416	51/55	0.74	0.27	54,73,92,98	0
30	UNL	d	421	11/-	0.74	0.29	77,88,95,95	0
30	UNL	A	420	9/-	0.74	0.36	85,95,111,112	0
30	UNL	x	102	8/-	0.74	0.25	77,80,86,88	0
38	LHG	E	101	42/49	0.74	0.27	53,100,110,112	0
30	UNL	b	636	11/-	0.75	0.27	70,77,83,83	0
30	UNL	Z	104	8/-	0.75	0.35	69,83,102,103	0
36	HTG	D	412	19/19	0.75	0.29	68,112,130,130	0
30	UNL	l	102	13/-	0.75	0.30	55,61,77,83	0
36	HTG	B	630	19/19	0.75	0.23	56,109,116,118	0
30	UNL	A	418	8/-	0.76	0.41	70,75,82,82	0
30	UNL	b	648	5/-	0.76	0.32	73,74,76,77	0
31	LMT	m	102	35/35	0.76	0.22	34,64,85,88	0
30	UNL	T	102	15/-	0.76	0.50	78,86,92,93	0
36	HTG	C	537	19/19	0.77	0.35	84,109,123,126	0
36	HTG	d	414	19/19	0.77	0.21	67,100,117,120	0
34	DMS	d	417	4/4	0.77	0.26	106,109,109,110	0
30	UNL	I	107	11/-	0.77	0.26	65,78,88,88	0
30	UNL	b	629	16/-	0.77	0.28	59,83,97,99	0
29	PL9	A	414	55/55	0.77	0.27	53,68,102,104	0
34	DMS	c	936	4/4	0.77	0.25	119,124,124,124	0
30	UNL	B	627	8/-	0.77	0.50	63,68,78,83	0
34	DMS	A	425	4/4	0.78	0.28	94,101,101,104	0
30	UNL	I	104	12/-	0.78	0.22	70,80,92,93	0
31	LMT	Z	101	35/35	0.78	0.22	52,104,121,123	0
29	PL9	a	417	55/55	0.78	0.23	50,78,101,105	0
30	UNL	c	945	4/-	0.78	0.27	77,77,77,78	0
30	UNL	C	539	16/-	0.78	0.22	76,79,102,107	0
32	GOL	B	637	6/6	0.78	0.50	61,67,75,80	0
34	DMS	y	101	4/4	0.78	0.17	116,122,123,124	0
27	SQD	b	601	54/54	0.78	0.22	46,73,108,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	LMT	F	103	24/35	0.79	0.29	85,90,119,121	0
30	UNL	t	103	12/-	0.79	0.51	64,74,83,86	0
34	DMS	D	415	4/4	0.79	0.24	83,93,97,99	0
30	UNL	C	538	4/-	0.79	0.23	74,76,77,82	0
34	DMS	O	312	4/4	0.79	0.51	101,103,104,106	0
31	LMT	B	622	35/35	0.79	0.19	48,85,97,99	0
36	HTG	c	928	19/19	0.79	0.34	74,98,122,126	0
30	UNL	j	105	5/-	0.79	0.29	66,67,73,74	0
34	DMS	B	645	4/4	0.80	0.25	103,104,107,107	0
30	UNL	H	103	6/-	0.80	0.14	65,66,79,81	0
30	UNL	Z	102	6/-	0.80	0.23	61,72,75,77	0
30	UNL	I	102	12/-	0.80	0.23	70,82,95,98	0
28	LMG	A	413	51/55	0.80	0.24	49,74,97,102	0
34	DMS	T	103	4/4	0.80	0.28	112,112,112,112	0
34	DMS	U	202	4/4	0.80	0.42	105,108,108,110	0
30	UNL	x	104	9/-	0.80	0.19	93,95,99,102	0
34	DMS	O	302	4/4	0.81	0.21	101,104,107,108	0
36	HTG	c	942	19/19	0.81	0.22	52,78,94,100	0
30	UNL	Z	103	6/-	0.81	0.31	73,84,87,88	0
30	UNL	D	410	40/-	0.81	0.20	46,67,103,106	0
36	HTG	O	316	19/19	0.81	0.21	47,71,81,84	0
34	DMS	v	210	4/4	0.81	0.30	119,119,120,120	0
34	DMS	O	315	4/4	0.81	0.28	96,96,98,99	0
30	UNL	H	105	18/-	0.81	0.19	51,67,98,103	0
30	UNL	d	403	36/-	0.81	0.22	47,67,99,107	0
30	UNL	B	628	6/-	0.81	0.16	68,69,79,82	0
28	LMG	c	921	51/55	0.82	0.23	47,94,101,104	0
32	GOL	C	525	6/6	0.82	0.16	89,91,92,93	0
34	DMS	B	647	4/4	0.82	0.25	107,108,110,113	0
34	DMS	C	530	4/4	0.82	0.21	89,96,97,99	0
30	UNL	x	101	18/-	0.82	0.20	51,65,90,92	0
36	HTG	B	624	19/19	0.82	0.20	34,53,75,76	0
27	SQD	A	416	54/54	0.82	0.18	50,70,89,95	0
34	DMS	C	534	4/4	0.83	0.31	112,116,117,120	0
31	LMT	c	927	35/35	0.83	0.19	49,97,104,111	0
36	HTG	v	211	19/19	0.83	0.24	63,84,98,102	0
30	UNL	B	635	6/-	0.83	0.34	70,73,75,79	0
30	UNL	k	101	30/-	0.83	0.20	62,90,106,111	0
34	DMS	v	205	4/4	0.83	0.25	90,95,98,106	0
34	DMS	b	645	4/4	0.83	0.28	103,110,111,111	0
40	RRX	h	101	41/41	0.83	0.16	31,44,61,71	0
30	UNL	E	102	5/-	0.84	0.17	76,76,76,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
30	UNL	x	103	4/-	0.84	0.16	74,75,83,84	0
36	HTG	B	623	19/19	0.84	0.19	46,59,69,72	0
34	DMS	C	532	4/4	0.84	0.28	96,99,100,102	0
30	UNL	i	101	8/-	0.84	0.38	63,67,75,81	0
34	DMS	o	307	4/4	0.84	0.18	89,91,91,93	0
34	DMS	c	926	4/4	0.84	0.36	107,110,110,111	0
28	LMG	B	621	51/55	0.85	0.17	39,54,71,82	0
34	DMS	O	314	4/4	0.85	0.27	81,87,87,88	0
34	DMS	H	104	4/4	0.85	0.32	109,109,112,116	0
28	LMG	b	624	51/55	0.85	0.20	44,56,78,89	0
30	UNL	i	104	16/-	0.85	0.29	65,72,83,83	0
34	DMS	e	103	4/4	0.85	0.20	106,108,108,111	0
34	DMS	a	425	4/4	0.85	0.23	116,120,120,121	0
36	HTG	b	602	19/19	0.85	0.14	51,67,78,83	0
36	HTG	C	520	19/19	0.86	0.25	81,93,101,105	0
30	UNL	E	103	8/-	0.86	0.23	65,78,79,79	0
36	HTG	C	536	19/19	0.86	0.32	66,106,124,126	0
30	UNL	e	105	4/-	0.86	0.13	74,77,79,82	0
34	DMS	o	306	4/4	0.86	0.36	84,85,89,90	0
34	DMS	U	204	4/4	0.86	0.33	134,135,136,136	0
30	UNL	E	105	4/-	0.86	0.15	60,62,69,72	0
34	DMS	b	639	4/4	0.86	0.28	90,100,102,102	0
30	UNL	c	925	11/-	0.87	0.14	74,77,85,85	0
30	UNL	b	628	18/-	0.87	0.14	51,61,81,95	0
34	DMS	b	643	4/4	0.87	0.21	113,118,118,120	0
32	GOL	c	929	6/6	0.87	0.22	77,89,93,94	0
34	DMS	b	646	4/4	0.87	0.40	74,83,84,85	0
31	LMT	M	102	25/35	0.87	0.19	40,67,106,110	0
34	DMS	D	414	4/4	0.87	0.22	102,104,106,107	0
30	UNL	i	102	18/-	0.87	0.17	44,68,93,96	0
30	UNL	D	417	4/-	0.87	0.51	57,66,66,70	0
36	HTG	c	923	19/19	0.87	0.28	84,98,100,102	0
34	DMS	K	102	4/4	0.87	0.15	95,106,107,109	0
34	DMS	V	212	4/4	0.87	0.44	86,96,99,99	0
36	HTG	O	303	19/19	0.88	0.17	46,56,64,64	0
32	GOL	V	207	6/6	0.88	0.22	78,85,88,96	0
36	HTG	B	629	19/19	0.88	0.16	46,70,92,97	0
34	DMS	A	427	4/4	0.88	0.26	82,88,89,89	0
34	DMS	b	638	4/4	0.88	0.20	58,80,83,83	0
36	HTG	b	626	19/19	0.88	0.23	41,52,95,99	0
34	DMS	v	207	4/4	0.88	0.32	111,114,114,114	0
34	DMS	B	644	4/4	0.88	0.22	56,75,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
34	DMS	b	641	4/4	0.88	0.22	89,91,92,95	0
34	DMS	O	309	4/4	0.88	0.36	98,101,102,105	0
30	UNL	i	103	12/-	0.88	0.20	67,75,83,87	0
34	DMS	O	311	4/4	0.89	0.31	93,96,97,98	0
34	DMS	a	422	4/4	0.89	0.25	91,94,96,98	0
34	DMS	C	529	4/4	0.89	0.15	100,103,104,105	0
30	UNL	I	103	12/-	0.89	0.12	60,63,84,84	0
34	DMS	A	424	4/4	0.89	0.21	95,98,100,101	0
34	DMS	C	533	4/4	0.89	0.19	121,122,123,125	0
26	BCR	k	103	40/40	0.89	0.14	37,46,54,59	0
34	DMS	U	203	4/4	0.89	0.18	40,60,64,66	0
40	RRX	H	101	41/41	0.89	0.12	30,41,56,63	0
30	UNL	a	403	5/-	0.89	0.50	73,73,74,75	0
30	UNL	B	648	4/-	0.90	0.10	66,70,70,71	0
34	DMS	o	305	4/4	0.90	0.32	94,102,106,107	0
34	DMS	B	642	4/4	0.90	0.14	104,106,109,111	0
24	CLA	B	610	65/65	0.90	0.12	30,36,43,46	0
34	DMS	b	640	4/4	0.90	0.20	69,91,92,97	0
34	DMS	C	535	4/4	0.90	0.22	66,79,83,89	0
32	GOL	a	419	6/6	0.90	0.15	55,59,59,60	0
32	GOL	b	637	6/6	0.90	0.32	92,92,94,96	0
24	CLA	c	904	65/65	0.90	0.19	35,44,50,62	0
34	DMS	C	524	4/4	0.90	0.21	105,107,108,108	0
34	DMS	L	102	4/4	0.90	0.48	106,110,111,112	0
37	DGD	h	102	62/66	0.90	0.16	34,42,51,63	0
30	UNL	j	103	6/-	0.90	0.17	72,80,86,88	0
34	DMS	V	214	4/4	0.90	0.32	102,102,104,106	0
30	UNL	d	413	18/-	0.90	0.24	42,57,77,85	0
34	DMS	v	206	4/4	0.91	0.17	55,68,74,84	0
28	LMG	c	920	51/55	0.91	0.16	41,72,98,99	0
34	DMS	v	209	4/4	0.91	0.26	110,110,110,111	0
30	UNL	D	411	16/-	0.91	0.26	44,51,73,74	0
34	DMS	a	424	4/4	0.91	0.26	102,104,105,105	0
34	DMS	o	304	4/4	0.91	0.33	83,88,90,94	0
24	CLA	c	913	65/65	0.91	0.15	40,49,84,89	0
38	LHG	D	406	49/49	0.91	0.17	36,50,67,81	0
30	UNL	X	101	16/-	0.91	0.16	48,57,70,73	0
38	LHG	d	409	49/49	0.91	0.23	38,50,61,67	0
34	DMS	V	205	4/4	0.91	0.32	94,98,98,100	0
27	SQD	f	102	43/54	0.91	0.18	50,91,111,117	0
24	CLA	b	613	65/65	0.92	0.11	32,38,44,57	0
30	UNL	m	101	11/-	0.92	0.27	56,67,78,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	DMS	B	639	4/4	0.92	0.18	87,90,93,95	0
34	DMS	B	641	4/4	0.92	0.18	107,108,110,110	0
24	CLA	B	603	65/65	0.92	0.14	27,34,44,49	0
34	DMS	B	643	4/4	0.92	0.34	100,104,106,106	0
34	DMS	c	935	4/4	0.92	0.32	101,101,101,102	0
24	CLA	C	513	65/65	0.92	0.14	43,54,86,88	0
34	DMS	O	313	4/4	0.92	0.27	101,106,108,111	0
36	HTG	V	204	13/19	0.92	0.21	49,59,79,86	0
37	DGD	H	102	62/66	0.92	0.20	27,40,51,53	0
28	LMG	C	519	51/55	0.92	0.17	36,80,92,97	0
35	CA	V	202	1/1	0.92	0.15	89,89,89,89	0
35	CA	b	604	1/1	0.92	0.05	52,52,52,52	0
34	DMS	d	418	4/4	0.92	0.29	74,75,76,78	0
26	BCR	B	619	40/40	0.92	0.17	28,37,54,62	0
38	LHG	l	103	49/49	0.92	0.17	32,42,66,69	0
34	DMS	e	104	4/4	0.92	0.23	88,94,96,98	0
26	BCR	c	915	40/40	0.92	0.15	47,58,64,66	0
26	BCR	Y	101	40/40	0.93	0.10	40,44,48,54	0
34	DMS	a	423	4/4	0.93	0.21	63,76,79,85	0
34	DMS	C	531	4/4	0.93	0.11	109,111,113,116	0
26	BCR	a	414	40/40	0.93	0.11	27,33,39,41	0
34	DMS	h	105	4/4	0.93	0.19	52,53,61,80	0
26	BCR	b	622	40/40	0.93	0.17	31,39,57,64	0
24	CLA	c	903	65/65	0.93	0.22	29,38,50,61	0
24	CLA	C	512	65/65	0.93	0.10	43,50,90,92	0
30	UNL	j	104	4/-	0.93	0.29	74,75,76,78	0
32	GOL	V	206	6/6	0.93	0.31	58,69,71,83	0
37	DGD	C	517	62/66	0.93	0.14	31,43,92,101	0
34	DMS	v	203	4/4	0.93	0.25	87,94,95,96	0
26	BCR	B	636	40/40	0.93	0.14	29,41,59,59	0
27	SQD	F	101	37/54	0.93	0.22	45,71,88,92	0
26	BCR	C	514	40/40	0.93	0.11	41,49,57,57	0
34	DMS	v	208	4/4	0.93	0.25	86,89,94,98	0
34	DMS	V	211	4/4	0.93	0.12	94,94,96,99	0
26	BCR	C	515	40/40	0.93	0.10	33,42,50,54	0
34	DMS	c	937	4/4	0.93	0.13	99,101,103,103	0
34	DMS	c	938	4/4	0.93	0.27	97,97,100,104	0
26	BCR	T	101	40/40	0.93	0.14	29,42,60,63	0
27	SQD	a	415	54/54	0.94	0.14	35,65,85,87	0
24	CLA	C	507	65/65	0.94	0.11	36,42,57,66	0
24	CLA	c	914	65/65	0.94	0.17	41,53,89,96	0
25	PHO	A	409	64/64	0.94	0.15	24,30,37,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
36	HTG	U	201	4/19	0.94	0.12	49,51,51,56	0
26	BCR	B	618	40/40	0.94	0.17	27,35,41,41	0
24	CLA	B	607	65/65	0.94	0.11	28,34,65,71	0
24	CLA	B	602	65/65	0.94	0.23	35,52,105,110	0
24	CLA	b	605	65/65	0.94	0.18	40,54,102,107	0
24	CLA	b	606	65/65	0.94	0.11	31,36,46,56	0
26	BCR	K	101	40/40	0.94	0.10	34,43,48,49	0
24	CLA	b	610	65/65	0.94	0.10	29,37,71,80	0
34	DMS	u	202	4/4	0.94	0.23	68,80,81,86	0
24	CLA	B	615	65/65	0.94	0.13	24,32,86,95	0
24	CLA	b	614	65/65	0.94	0.10	30,36,42,61	0
24	CLA	b	619	65/65	0.94	0.10	29,37,58,65	0
32	GOL	A	419	6/6	0.94	0.20	59,61,62,66	0
29	PL9	d	407	55/55	0.94	0.15	22,29,43,56	0
32	GOL	B	638	6/6	0.94	0.32	39,58,69,73	0
26	BCR	b	623	40/40	0.94	0.12	32,41,55,58	0
24	CLA	b	620	65/65	0.94	0.13	30,41,98,102	0
34	DMS	D	416	4/4	0.94	0.19	93,94,97,98	0
26	BCR	d	406	40/40	0.94	0.10	34,41,69,72	0
35	CA	v	201	1/1	0.94	0.09	104,104,104,104	0
26	BCR	k	102	40/40	0.94	0.09	40,45,54,55	0
37	DGD	c	918	62/66	0.94	0.17	36,44,99,109	0
24	CLA	c	902	65/65	0.94	0.11	33,42,54,60	0
34	DMS	b	647	4/4	0.94	0.17	72,73,79,79	0
27	SQD	A	412	54/54	0.94	0.13	35,64,79,85	0
34	DMS	c	933	4/4	0.94	0.16	108,111,113,114	0
34	DMS	O	306	4/4	0.94	0.20	78,82,86,86	0
38	LHG	d	410	49/49	0.94	0.15	27,33,53,64	0
24	CLA	C	503	65/65	0.94	0.13	32,39,46,56	0
24	CLA	C	506	65/65	0.94	0.11	37,52,90,94	0
24	CLA	c	908	65/65	0.94	0.12	32,42,59,61	0
34	DMS	o	303	4/4	0.95	0.34	92,94,95,101	0
34	DMS	V	213	4/4	0.95	0.09	76,84,85,86	0
28	LMG	D	409	51/55	0.95	0.18	32,43,99,106	0
24	CLA	c	912	65/65	0.95	0.10	34,43,52,58	0
24	CLA	C	501	65/65	0.95	0.14	30,39,53,61	0
34	DMS	u	201	4/4	0.95	0.14	52,64,66,70	0
26	BCR	c	916	40/40	0.95	0.09	38,43,54,57	0
24	CLA	B	611	65/65	0.95	0.15	26,35,43,50	0
28	LMG	d	412	51/55	0.95	0.10	35,45,89,94	0
24	CLA	d	405	65/65	0.95	0.10	33,39,102,107	0
33	BCT	a	408[A]	4/4	0.95	0.07	31,38,39,41	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	BCT	d	402[B]	4/4	0.95	0.09	34,37,37,40	4
29	PL9	D	404	55/55	0.95	0.10	23,29,38,51	0
34	DMS	b	644	4/4	0.95	0.22	63,65,67,78	0
24	CLA	C	504	65/65	0.95	0.13	27,35,80,83	0
30	UNL	I	101	14/-	0.95	0.15	46,53,70,73	0
34	DMS	B	633	4/4	0.95	0.19	48,49,56,58	0
24	CLA	B	612	65/65	0.95	0.15	25,30,46,54	0
24	CLA	B	604	65/65	0.95	0.15	28,33,40,42	0
34	DMS	c	934	4/4	0.95	0.17	73,80,82,84	0
24	CLA	b	618	65/65	0.95	0.17	24,33,88,91	0
37	DGD	c	917	62/66	0.95	0.14	28,39,84,88	0
24	CLA	C	508	65/65	0.95	0.12	28,37,95,108	0
24	CLA	C	510	65/65	0.95	0.14	31,39,51,58	0
26	BCR	D	403	40/40	0.95	0.17	33,41,69,73	0
24	CLA	C	511	65/65	0.95	0.08	33,44,51,54	0
24	CLA	B	616	65/65	0.95	0.11	26,35,53,65	0
38	LHG	L	101	49/49	0.95	0.12	30,41,64,71	0
24	CLA	B	617	65/65	0.95	0.10	30,36,105,109	0
34	DMS	C	528	4/4	0.95	0.11	81,81,83,83	0
24	CLA	c	907	65/65	0.95	0.10	39,48,81,85	0
26	BCR	b	621	40/40	0.95	0.16	31,37,48,53	0
24	CLA	D	402	65/65	0.95	0.11	29,37,102,104	0
24	CLA	c	905	65/65	0.96	0.16	32,40,72,81	0
24	CLA	b	611	65/65	0.96	0.12	23,31,44,50	0
24	CLA	B	605	65/65	0.96	0.21	23,29,61,62	0
24	CLA	c	909	65/65	0.96	0.18	31,37,91,96	0
35	CA	c	901	1/1	0.96	0.06	52,52,52,52	0
34	DMS	a	421	4/4	0.96	0.12	78,84,85,89	0
24	CLA	c	910	65/65	0.96	0.25	34,40,58,64	0
34	DMS	O	305	4/4	0.96	0.10	81,82,85,88	0
34	DMS	e	102	4/4	0.96	0.15	95,95,96,99	0
24	CLA	C	509	65/65	0.96	0.12	34,41,63,67	0
24	CLA	b	616	65/65	0.96	0.18	25,33,41,42	0
37	DGD	C	516	62/66	0.96	0.17	27,38,90,95	0
34	DMS	C	527	4/4	0.96	0.19	72,74,75,77	0
37	DGD	C	518	62/66	0.96	0.12	28,37,80,85	0
24	CLA	b	617	65/65	0.96	0.21	25,31,71,77	0
24	CLA	a	413	65/65	0.96	0.11	26,34,107,111	0
24	CLA	C	505	65/65	0.96	0.13	32,39,57,63	0
34	DMS	b	642	4/4	0.96	0.08	57,63,69,73	0
24	CLA	C	502	65/65	0.96	0.14	29,36,48,63	0
24	CLA	b	607	65/65	0.96	0.12	28,35,41,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
26	BCR	B	620	40/40	0.96	0.09	30,37,52,55	0
34	DMS	B	634	4/4	0.96	0.11	63,64,64,65	0
24	CLA	b	608	65/65	0.96	0.17	25,31,69,74	0
34	DMS	B	640	4/4	0.96	0.30	77,78,82,86	0
34	DMS	c	931	4/4	0.96	0.24	88,88,89,92	0
34	DMS	c	932	4/4	0.96	0.16	80,88,88,89	0
34	DMS	V	201	4/4	0.96	0.21	75,76,79,88	0
24	CLA	B	608	65/65	0.96	0.12	23,29,44,50	0
34	DMS	V	210	4/4	0.97	0.09	69,71,76,76	0
24	CLA	b	612	65/65	0.97	0.14	28,35,42,45	0
24	CLA	c	906	65/65	0.97	0.12	30,37,66,74	0
24	CLA	A	406	65/65	0.97	0.08	20,26,38,53	0
24	CLA	a	410	65/65	0.97	0.13	26,32,89,95	0
24	CLA	b	615	65/65	0.97	0.20	25,31,51,55	0
34	DMS	c	940	4/4	0.97	0.22	58,63,64,66	0
34	DMS	d	415	4/4	0.97	0.20	63,66,70,74	0
24	CLA	B	606	65/65	0.97	0.19	25,30,43,46	0
24	CLA	c	911	65/65	0.97	0.26	30,39,51,61	0
24	CLA	A	407	65/65	0.97	0.15	21,29,89,95	0
24	CLA	B	613	65/65	0.97	0.19	24,31,37,41	0
34	DMS	O	308	4/4	0.97	0.18	80,83,84,90	0
24	CLA	B	614	65/65	0.97	0.19	21,30,67,76	0
34	DMS	O	310	4/4	0.97	0.53	88,89,90,94	0
34	DMS	o	302	4/4	0.97	0.10	71,74,78,80	0
24	CLA	d	401	65/65	0.97	0.12	21,27,41,51	0
24	CLA	A	410	65/65	0.97	0.09	26,35,99,104	0
37	DGD	c	919	62/66	0.97	0.10	32,40,76,82	0
33	BCT	A	422	4/4	0.97	0.07	37,37,48,55	0
25	PHO	A	408	64/64	0.97	0.10	21,28,33,36	0
24	CLA	b	609	65/65	0.97	0.13	25,33,44,49	0
38	LHG	D	407	49/49	0.97	0.11	25,34,48,65	0
38	LHG	D	408	46/49	0.97	0.11	32,39,72,77	0
25	PHO	a	411	64/64	0.97	0.11	24,28,33,38	0
25	PHO	a	412	64/64	0.97	0.12	26,33,41,43	0
26	BCR	A	411	40/40	0.97	0.12	27,33,41,45	0
34	DMS	v	204	4/4	0.97	0.14	55,57,58,64	0
38	LHG	d	411	47/49	0.97	0.13	32,39,87,92	0
24	CLA	B	609	65/65	0.97	0.14	27,33,40,44	0
39	HEM	F	102	43/43	0.97	0.08	38,48,56,60	0
39	HEM	f	101	43/43	0.97	0.11	42,50,65,84	0
34	DMS	D	413	4/4	0.97	0.20	62,65,67,73	0
24	CLA	D	401	65/65	0.97	0.13	20,26,41,46	0

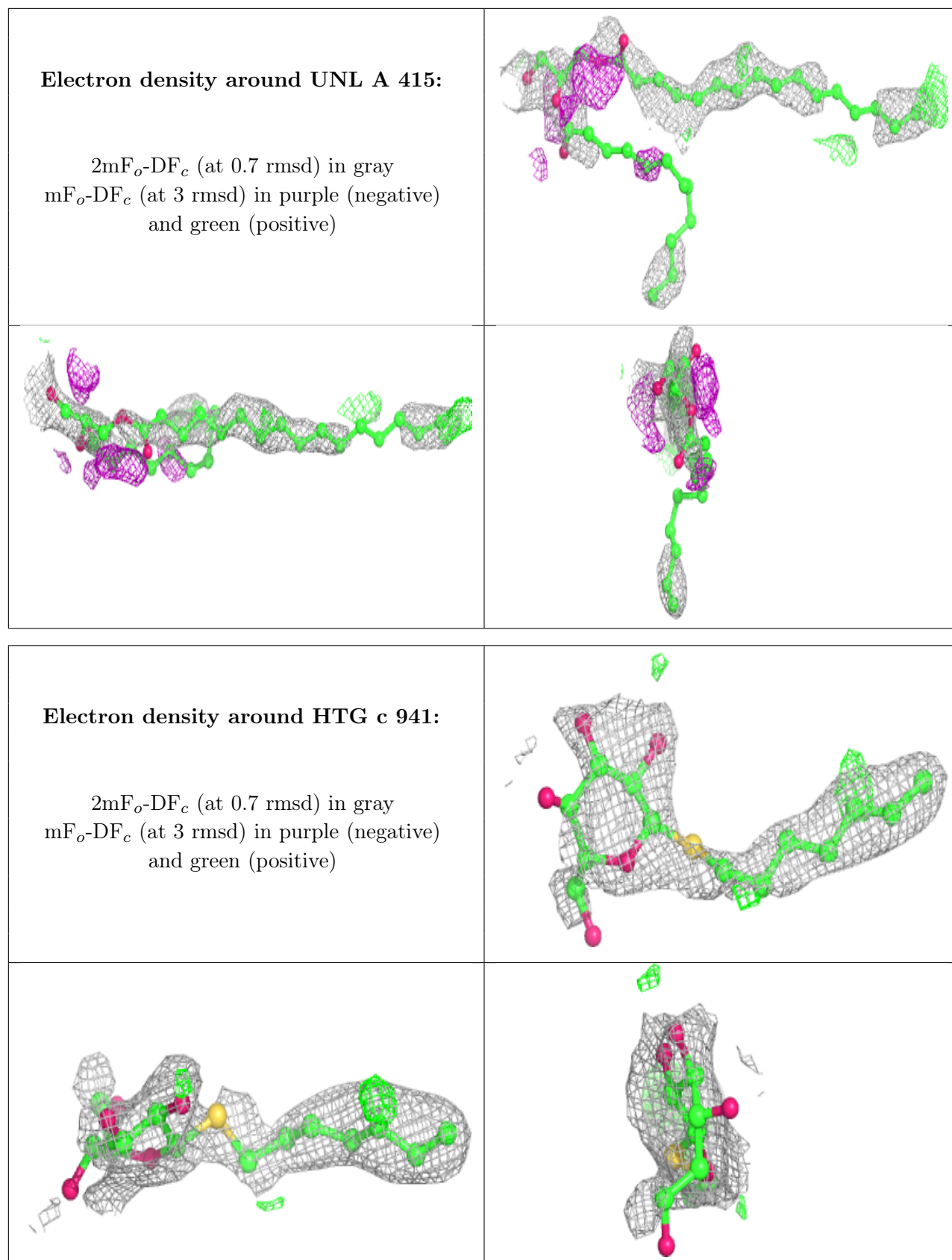
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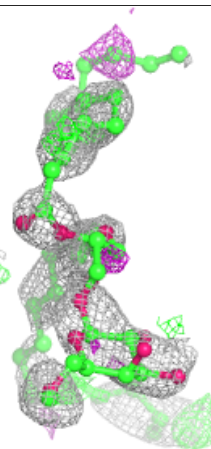
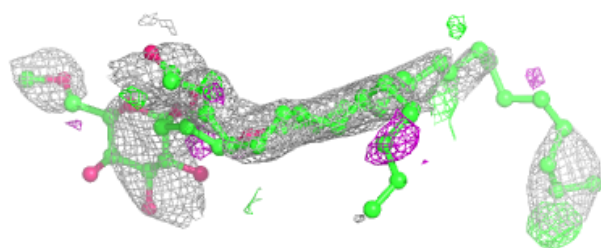
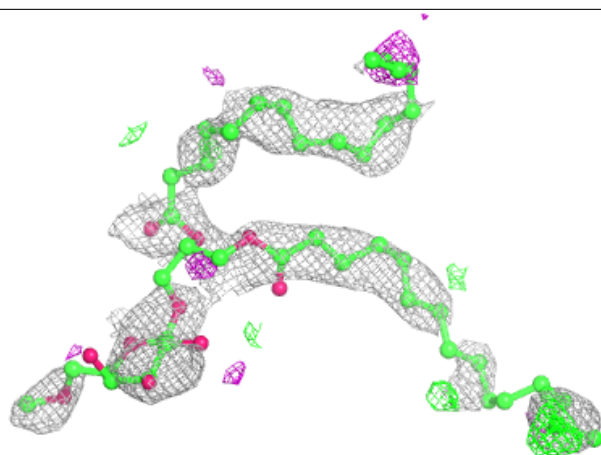
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
41	MG	j	101	1/1	0.97	0.18	44,44,44,44	0
42	HEC	v	202	43/43	0.97	0.10	35,41,47,48	0
24	CLA	d	404	65/65	0.98	0.13	23,28,50,57	0
34	DMS	d	416	4/4	0.98	0.13	62,64,65,72	0
34	DMS	V	209	4/4	0.98	0.12	50,59,66,67	0
34	DMS	C	526	4/4	0.98	0.12	44,46,46,50	0
24	CLA	A	405	65/65	0.98	0.10	22,26,33,54	0
35	CA	o	301	1/1	0.98	0.08	55,55,55,55	0
24	CLA	a	409	65/65	0.98	0.14	23,28,37,50	0
34	DMS	A	426	4/4	0.98	0.11	81,86,86,88	0
42	HEC	V	203	43/43	0.98	0.07	27,31,37,40	0
34	DMS	b	632	4/4	0.98	0.09	61,63,64,65	0
35	CA	O	301	1/1	0.99	0.15	56,56,56,56	0
34	DMS	V	208	4/4	0.99	0.09	50,53,56,57	0
34	DMS	B	632	4/4	0.99	0.14	28,31,33,34	0
21	OEX	A	401	10/10	0.99	0.10	25,28,31,31	0
34	DMS	a	420	4/4	0.99	0.07	34,35,35,42	0
34	DMS	b	631	4/4	0.99	0.14	34,34,37,43	0
41	MG	J	101	1/1	0.99	0.08	36,36,36,36	0
34	DMS	c	930	4/4	0.99	0.10	46,49,49,50	0
34	DMS	A	423	4/4	0.99	0.11	31,34,37,48	0
35	CA	B	601	1/1	0.99	0.09	51,51,51,51	0
21	OEX	a	404	10/10	1.00	0.08	29,32,33,34	0
22	FE2	A	402	1/1	1.00	0.04	33,33,33,33	0
22	FE2	a	405	1/1	1.00	0.07	33,33,33,33	0
23	CL	A	403	1/1	1.00	0.10	26,26,26,26	0
23	CL	A	404	1/1	1.00	0.14	29,29,29,29	0
23	CL	a	406	1/1	1.00	0.10	29,29,29,29	0
23	CL	a	407	1/1	1.00	0.18	34,34,34,34	0

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

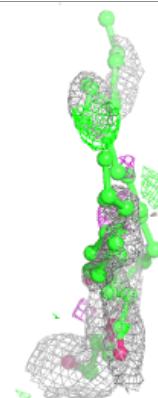
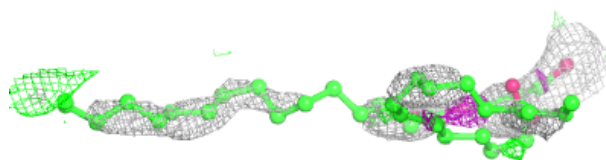
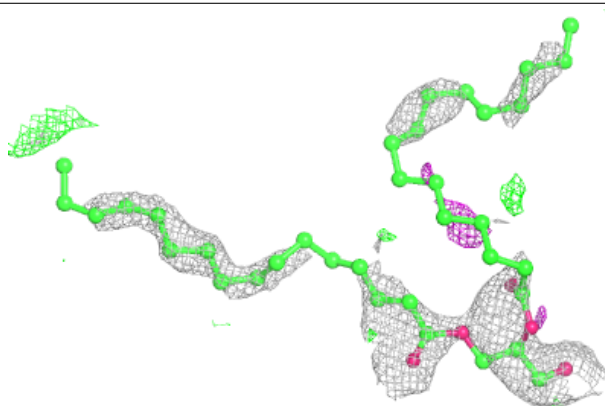


**Electron density around DGD D 405:**

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

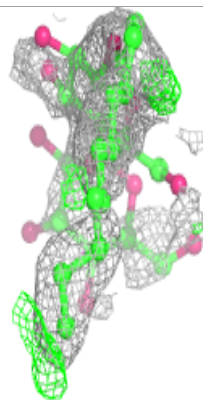
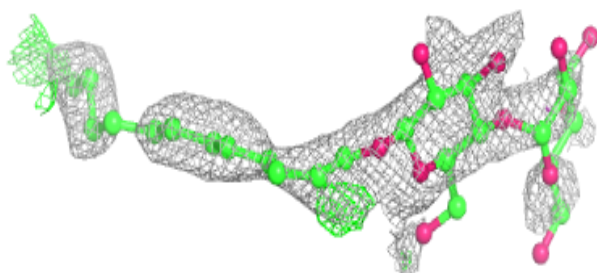
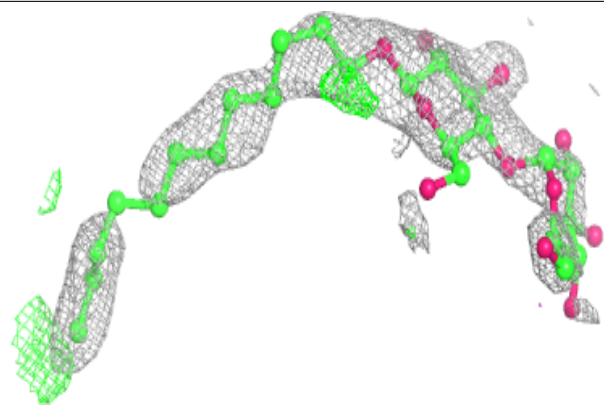
**Electron density around UNL a 418:**

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

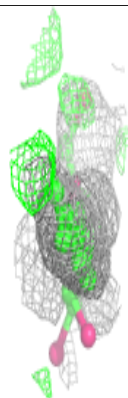
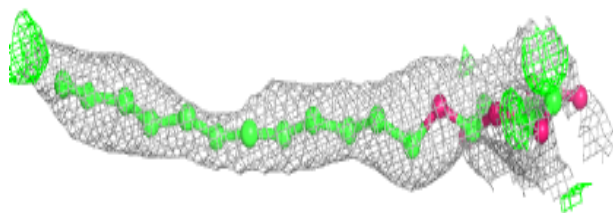
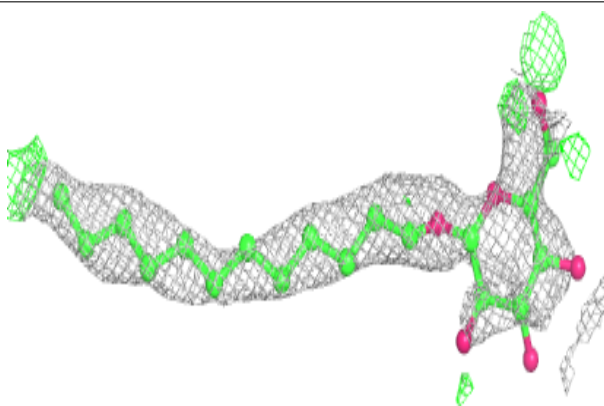


**Electron density around LMT m 103:**

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

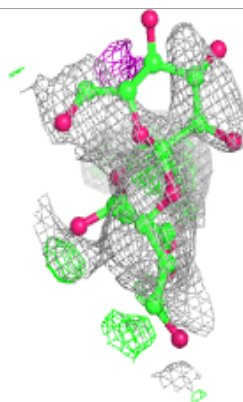
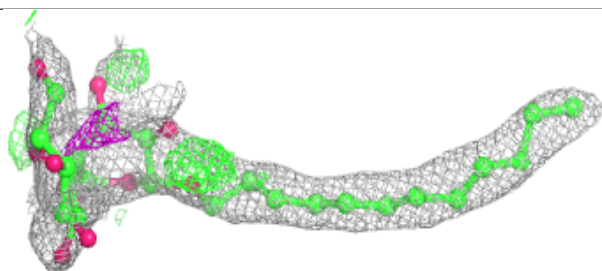
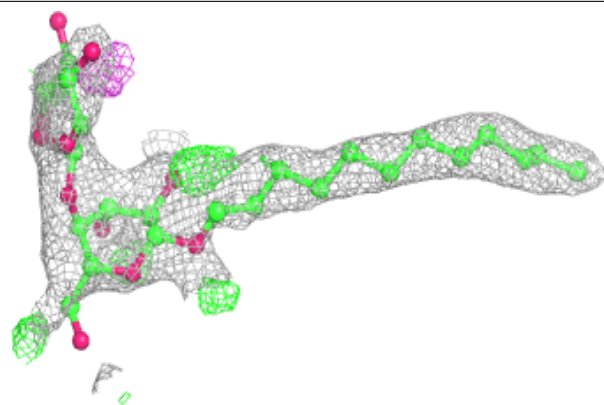
**Electron density around LMT j 102:**

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

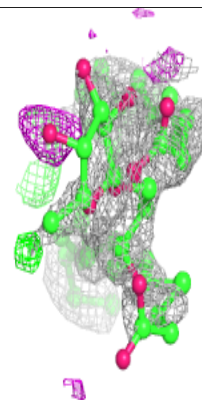
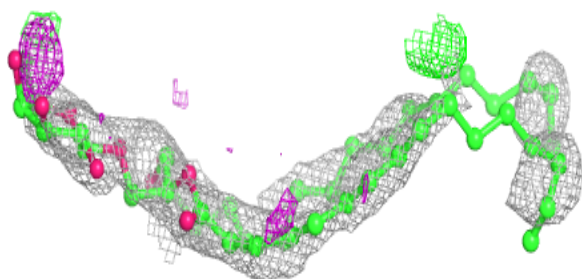
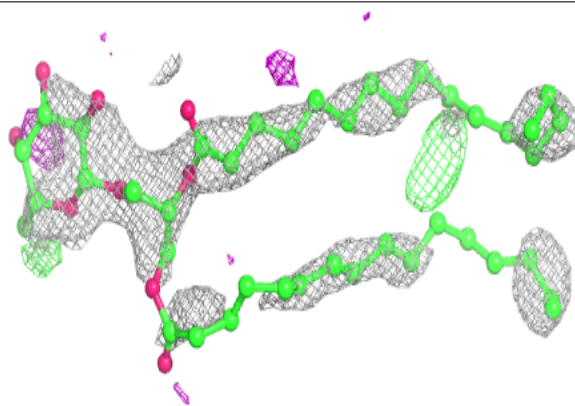


**Electron density around LMT b 625:**

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

**Electron density around DGD d 408:**

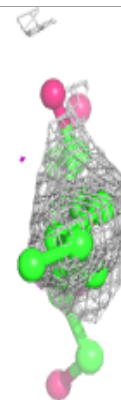
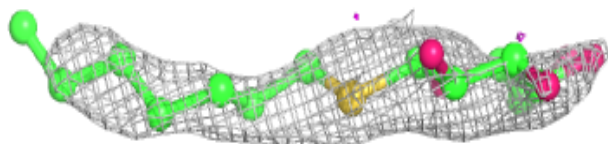
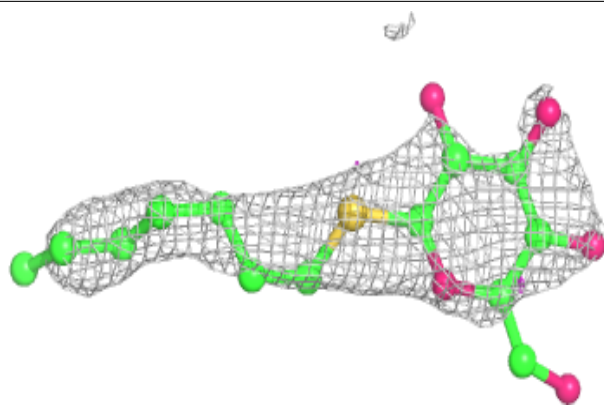
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



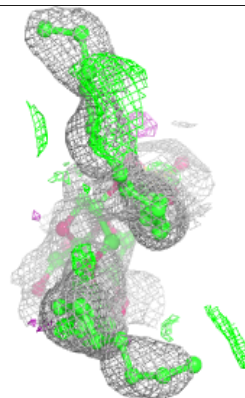
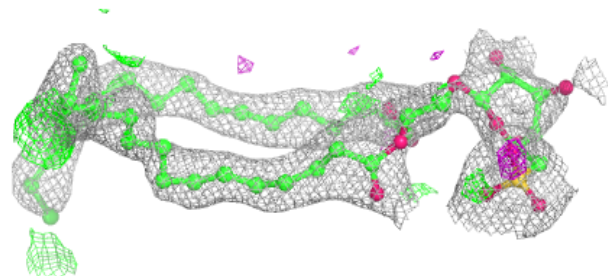
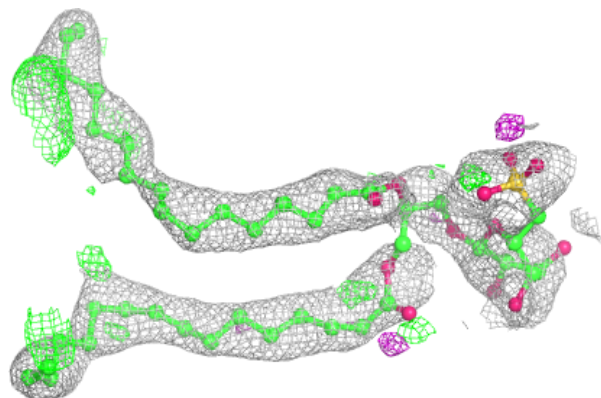


**Electron density around HTG d 420:**

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

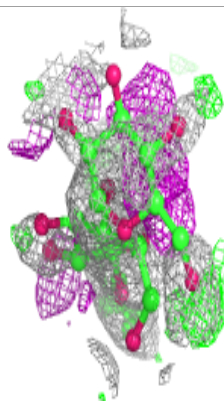
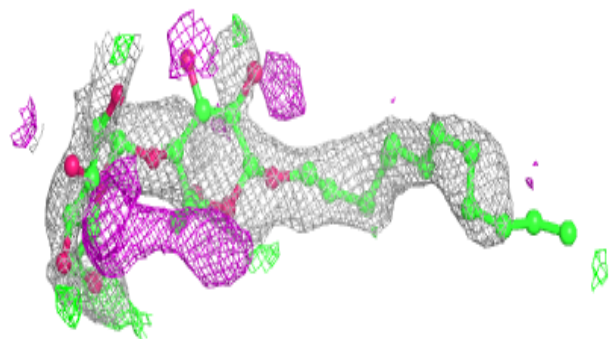
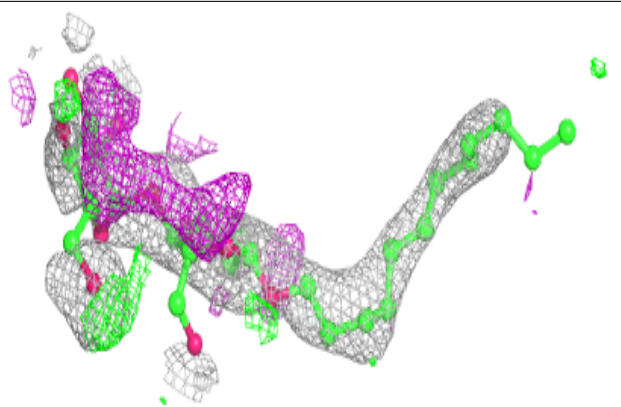
**Electron density around SQD l 101:**

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

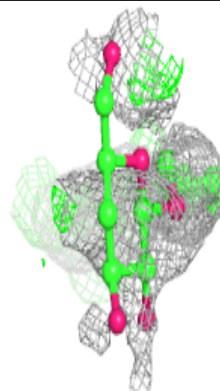
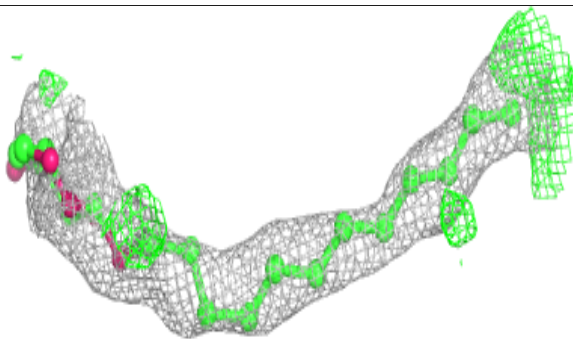
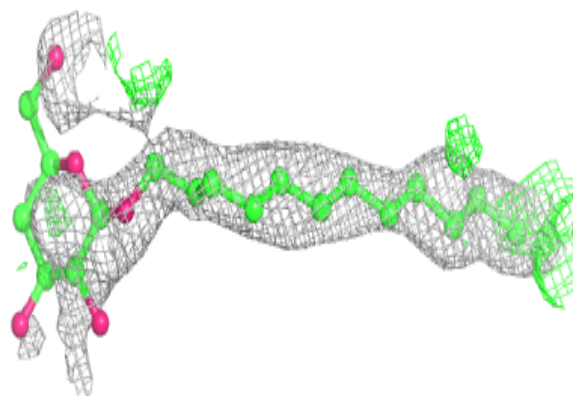


**Electron density around LMT A 417:**

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

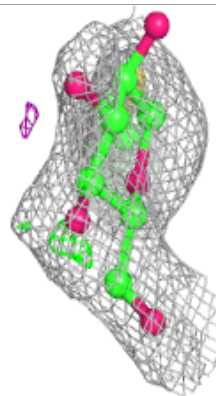
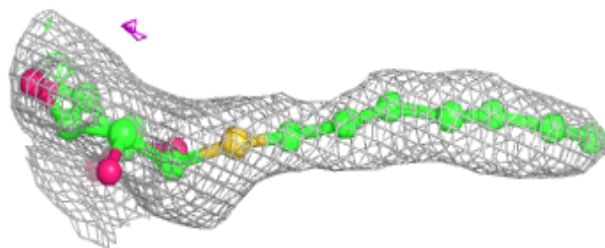
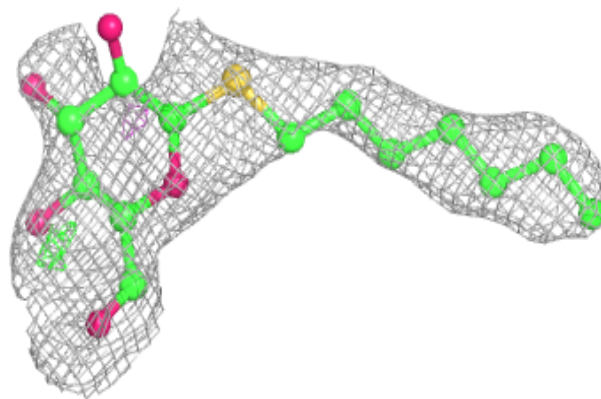
**Electron density around LMT t 101:**

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

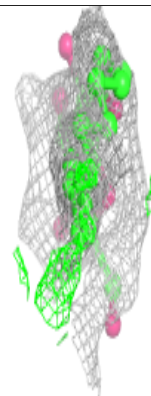
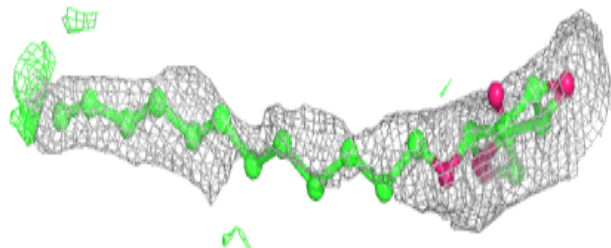
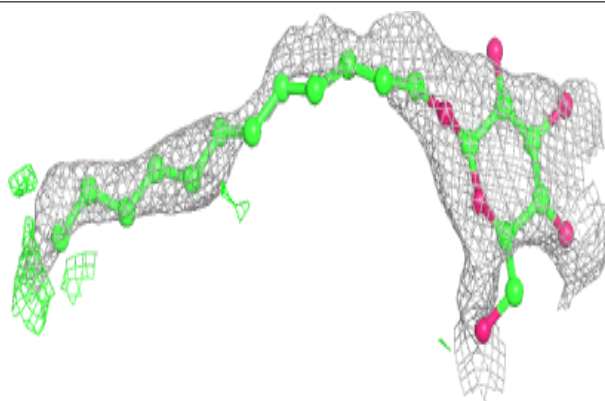


**Electron density around HTG b 627:**

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

**Electron density around LMT e 101:**

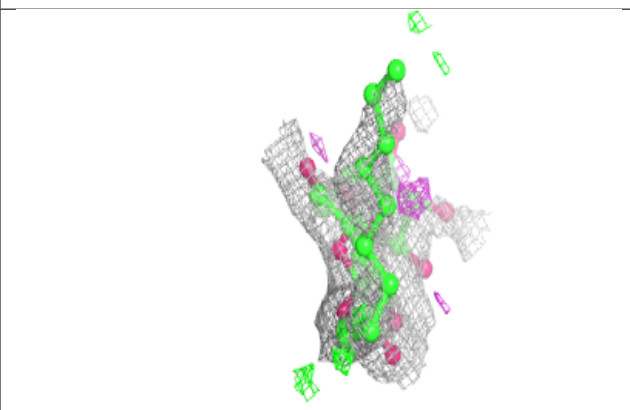
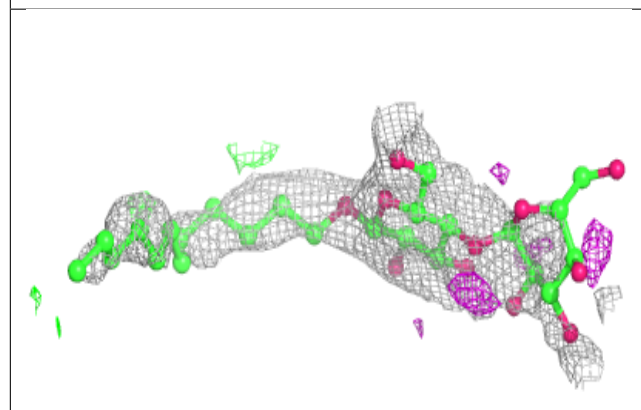
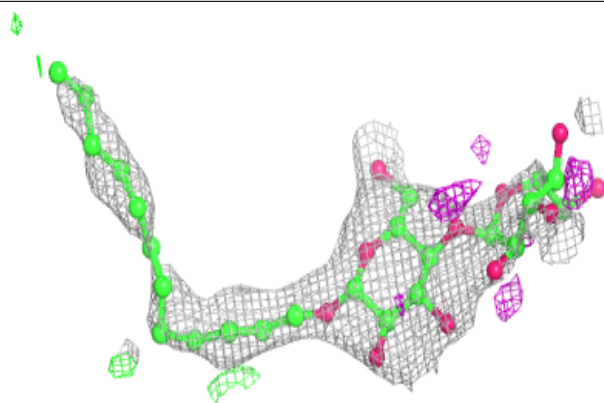
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



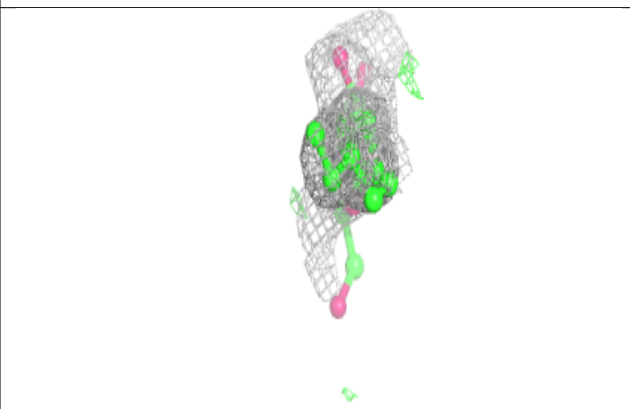
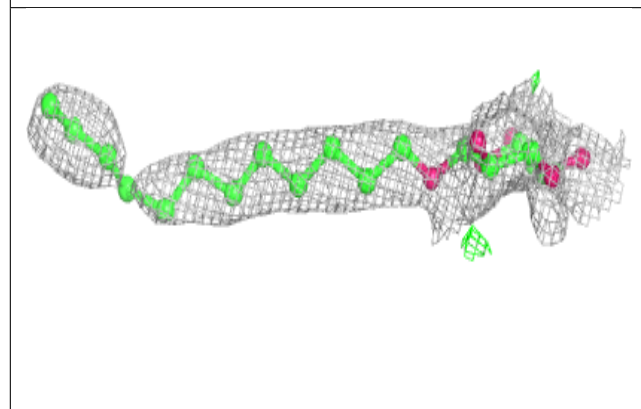
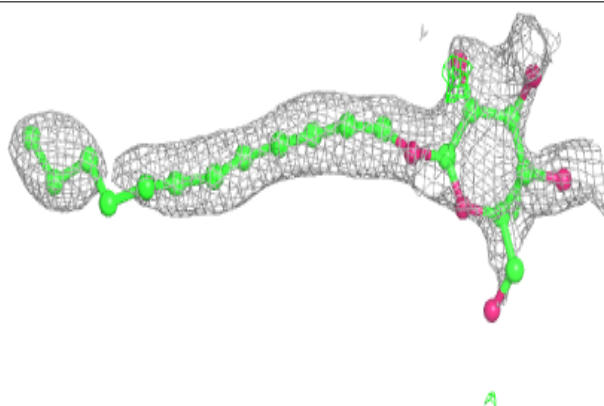


**Electron density around LMT A 421:**

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

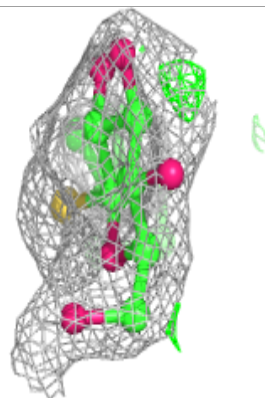
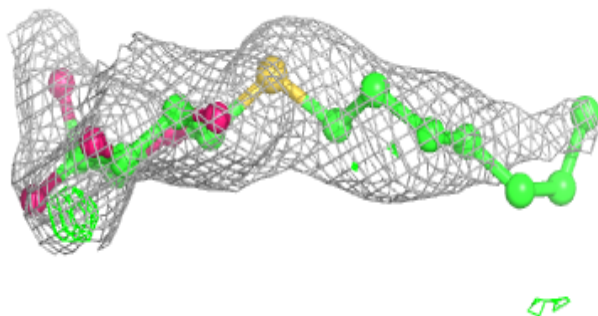
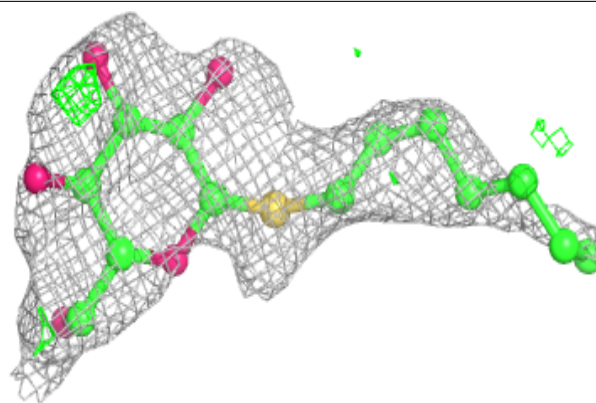
**Electron density around LMT J 102:**

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

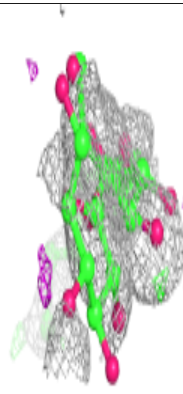
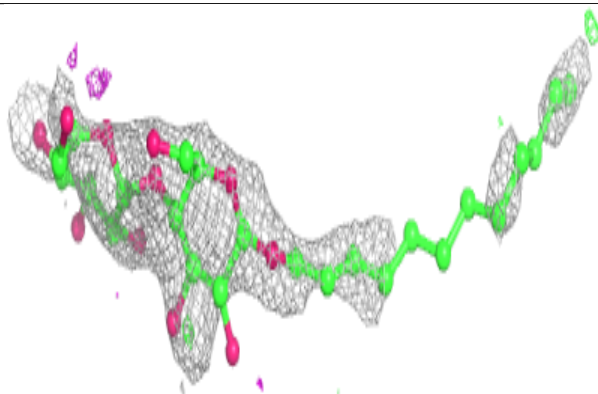
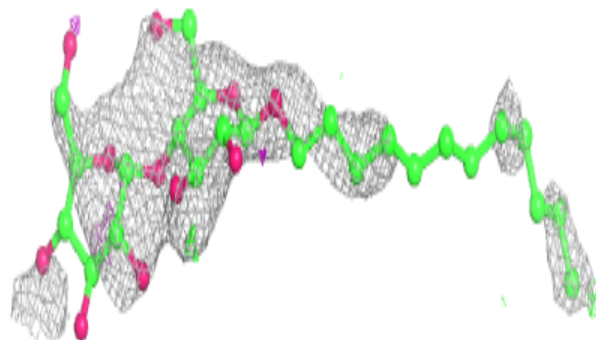


**Electron density around HTG y 102:**

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

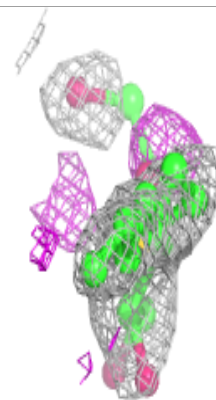
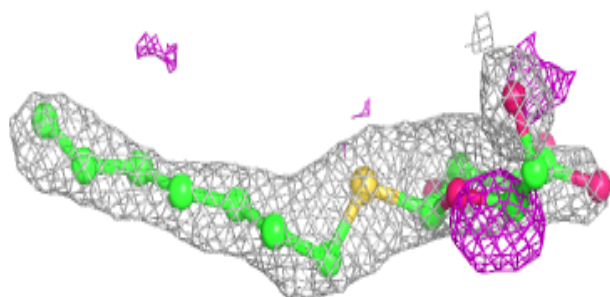
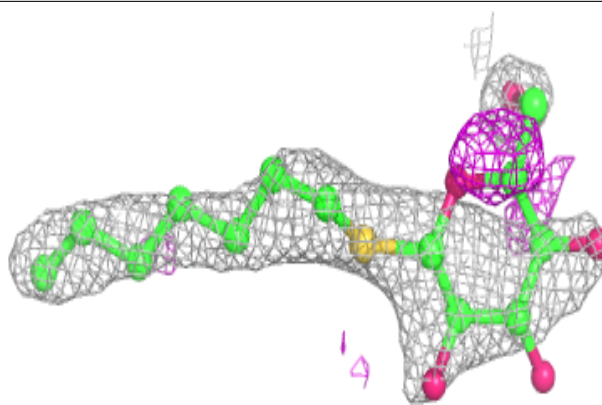
**Electron density around LMT c 922:**

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

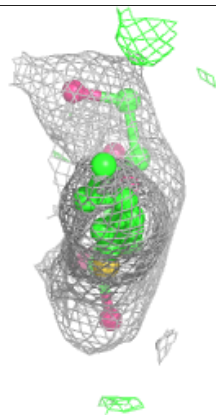
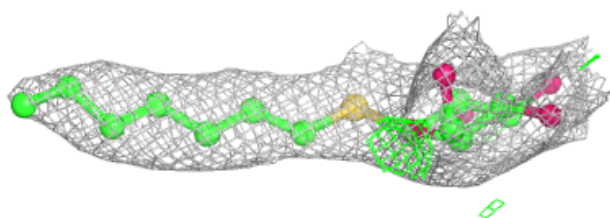
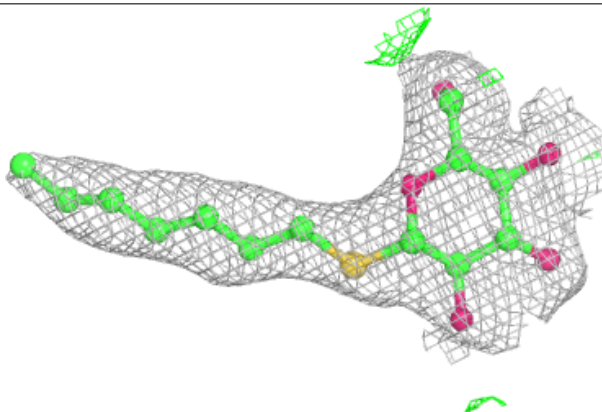


**Electron density around HTG c 924:**

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

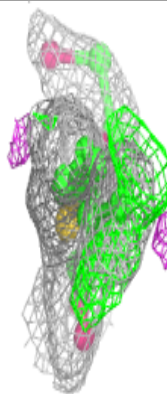
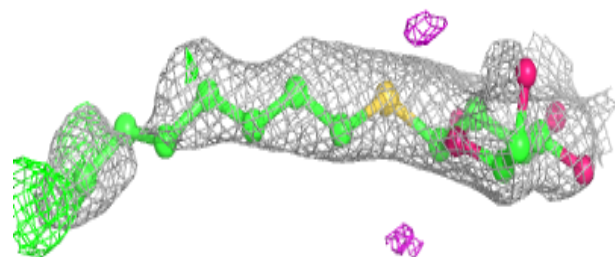
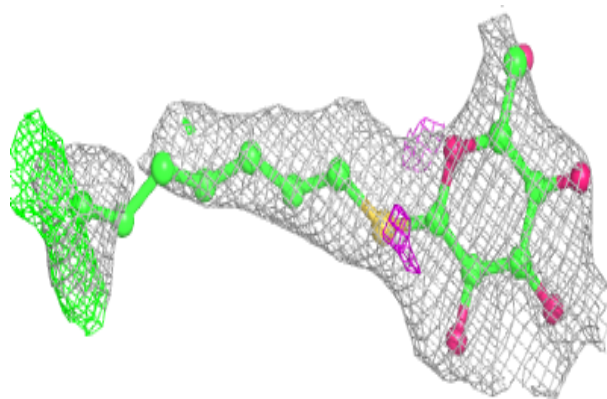
**Electron density around HTG b 603:**

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

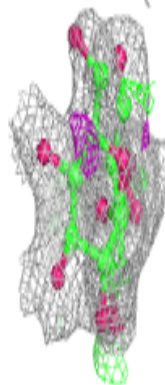
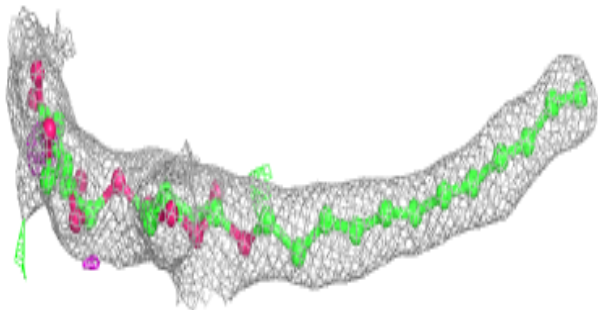
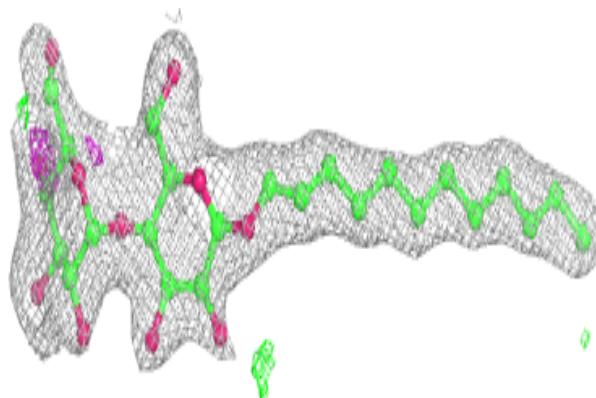


**Electron density around HTG B 631:**

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

**Electron density around LMT M 101:**

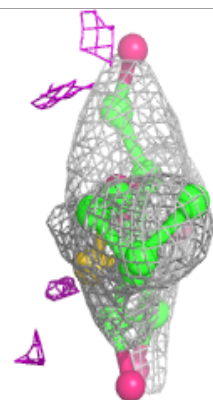
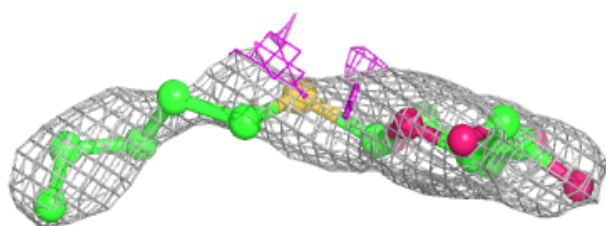
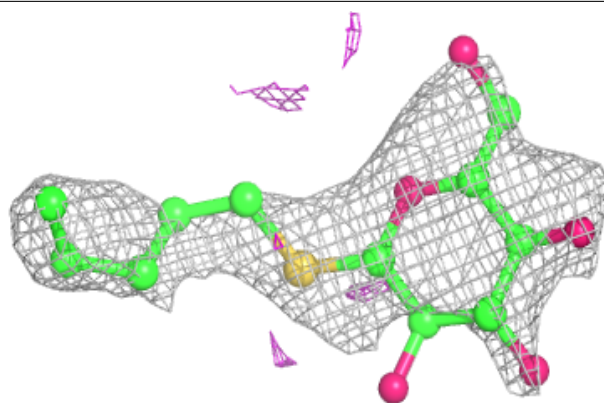
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



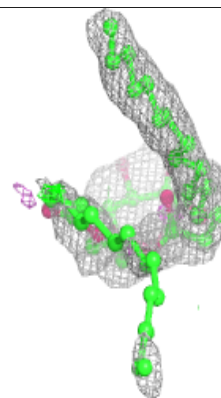
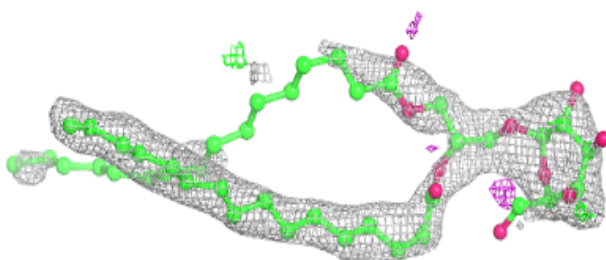
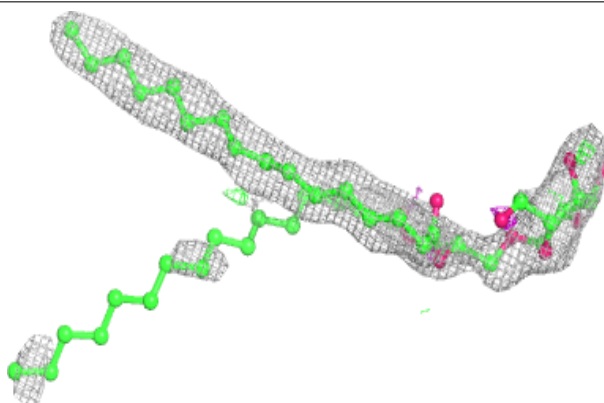


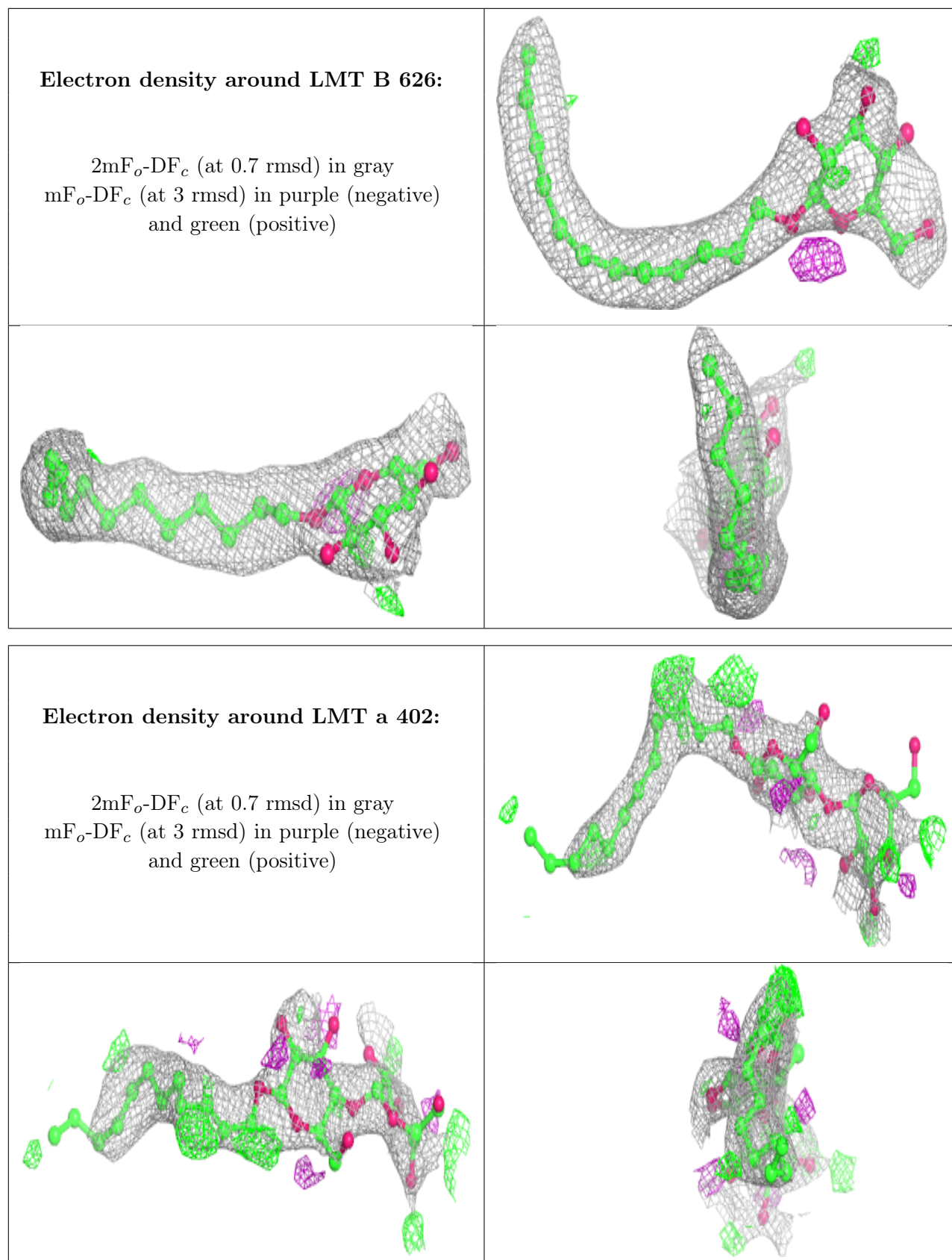
**Electron density around HTG c 943:**

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

**Electron density around LMG C 523:**

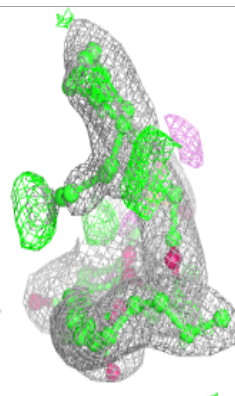
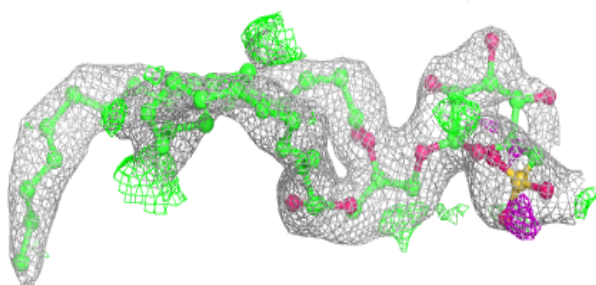
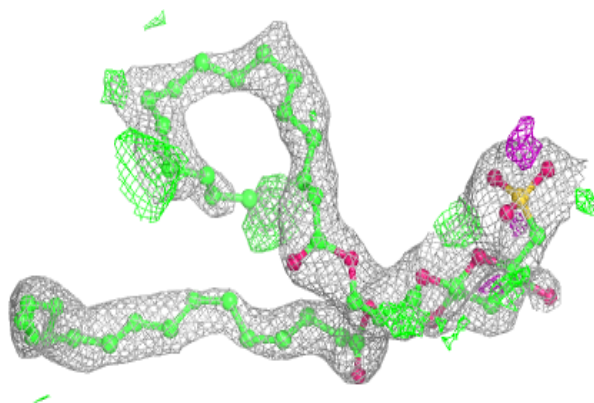
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



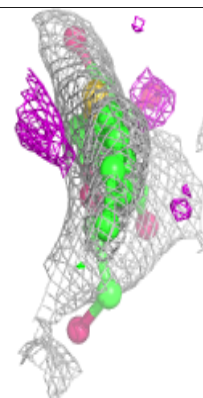
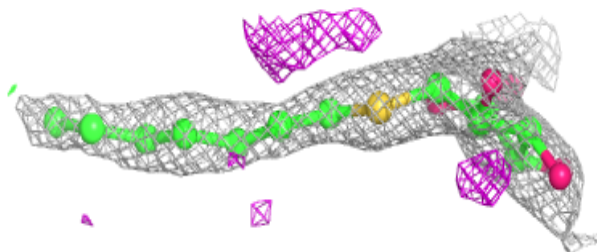
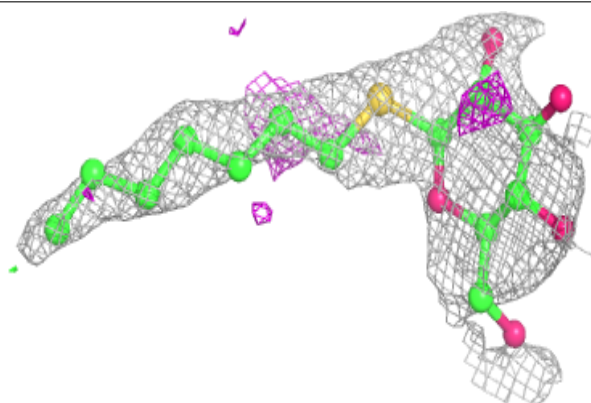


**Electron density around SQD a 401:**

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

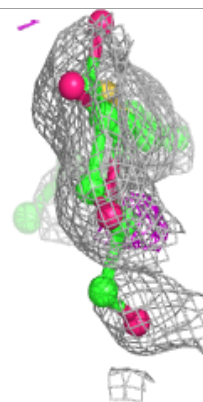
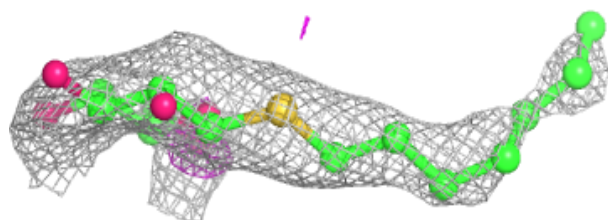
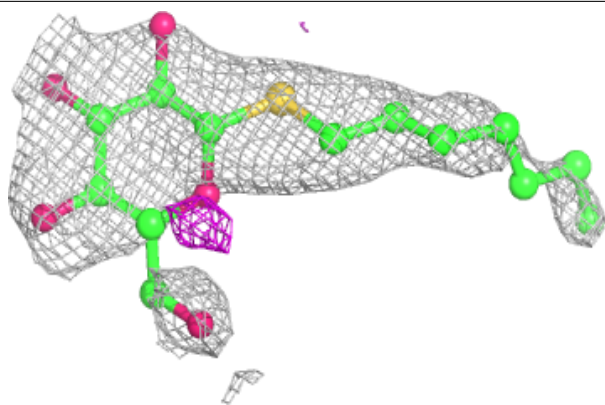
**Electron density around HTG B 625:**

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

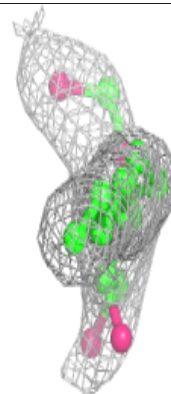
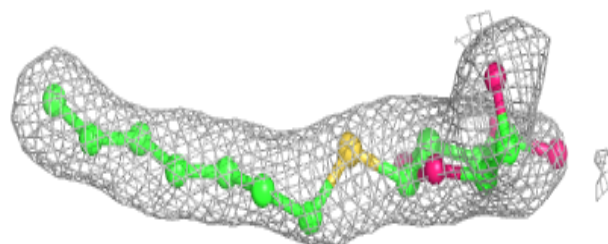
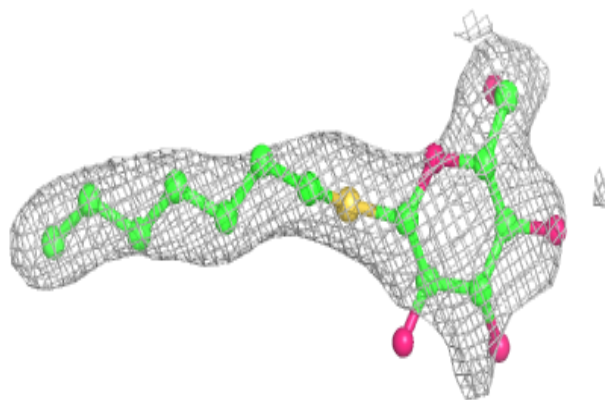


**Electron density around HTG d 419:**

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

**Electron density around HTG C 521:**

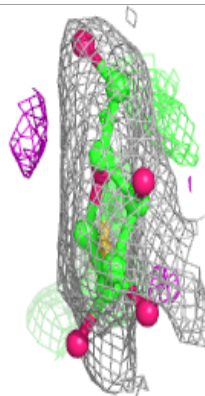
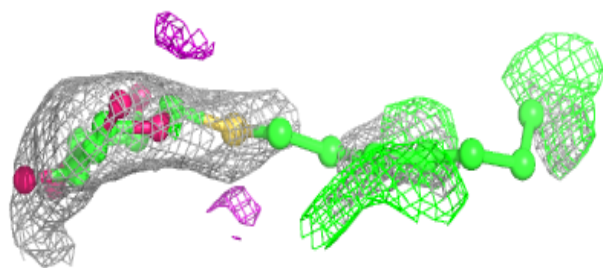
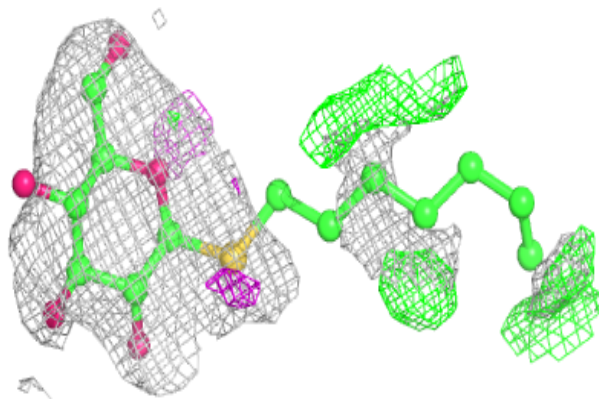
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



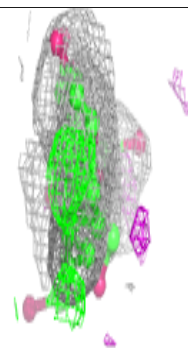
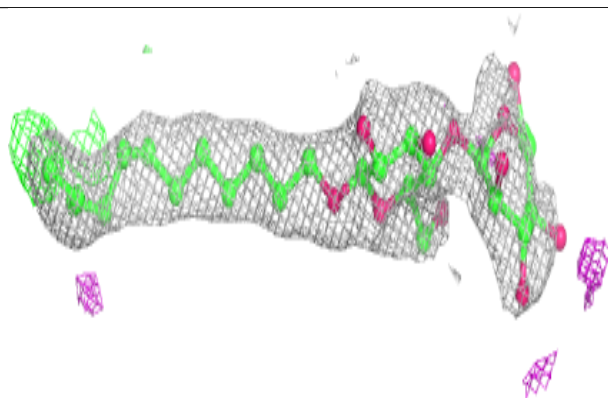
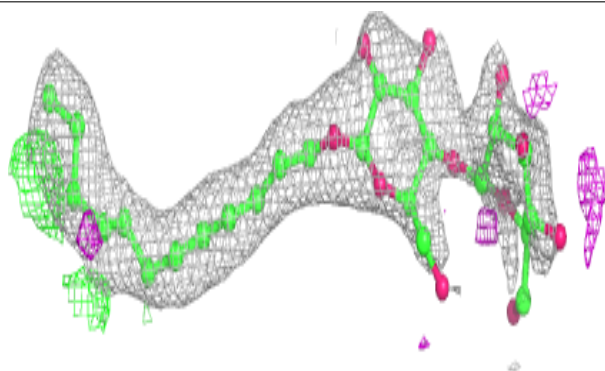


**Electron density around HTG V 215:**

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

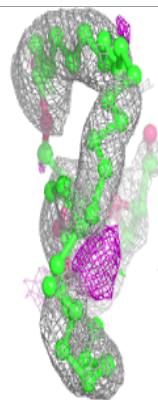
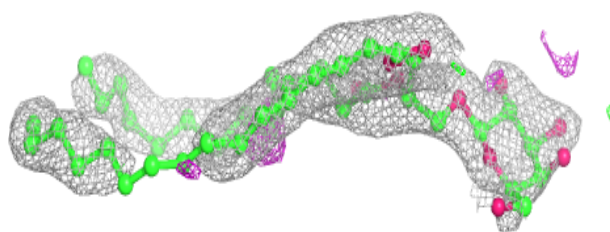
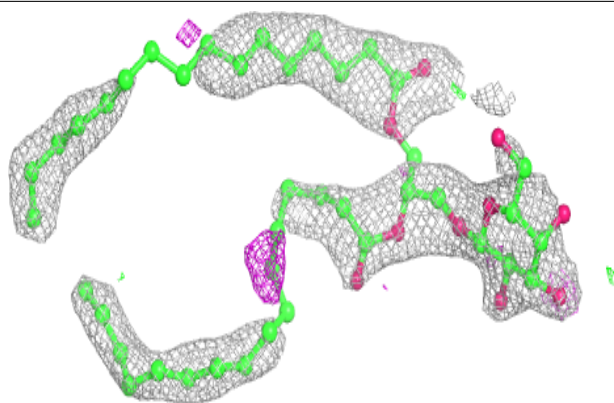
**Electron density around LMT t 102:**

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

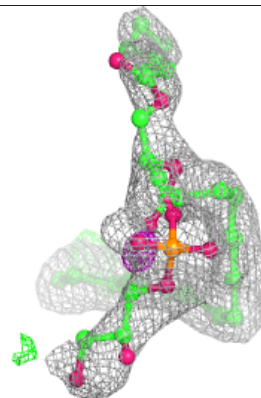
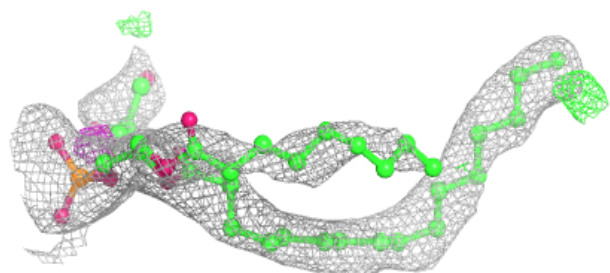
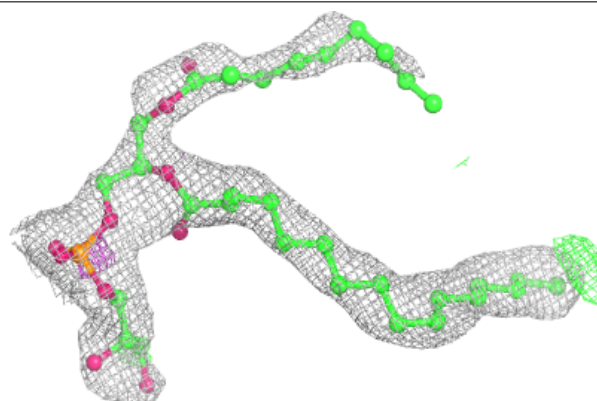


**Electron density around LMG a 416:**

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

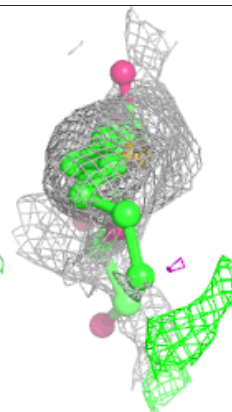
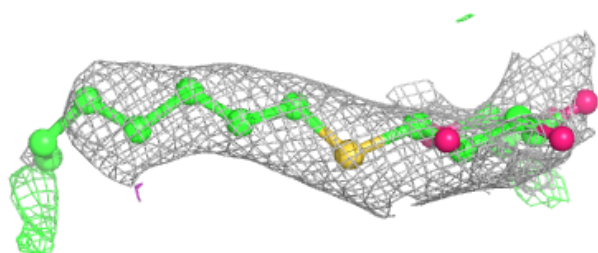
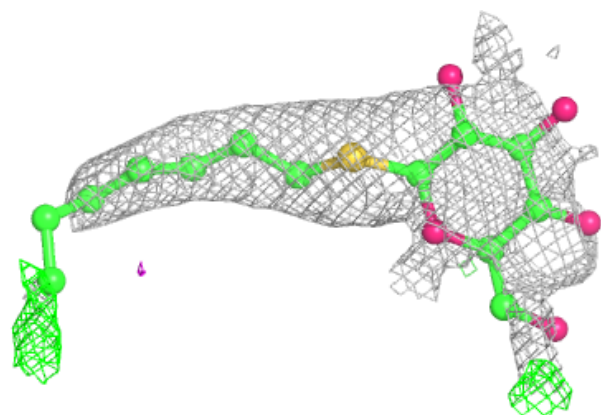
**Electron density around LHG E 101:**

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

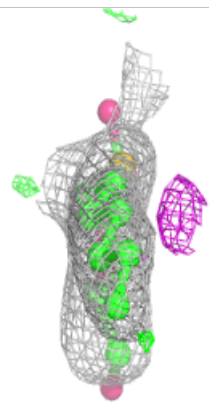
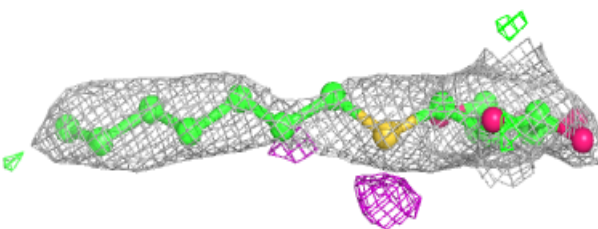
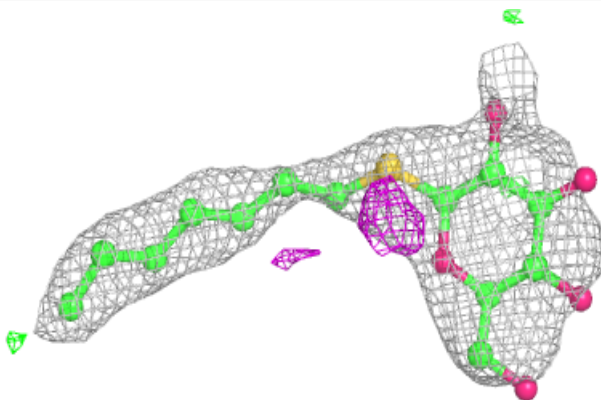


**Electron density around HTG D 412:**

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

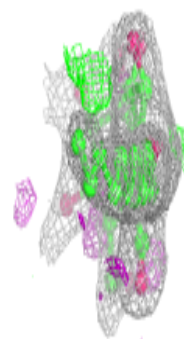
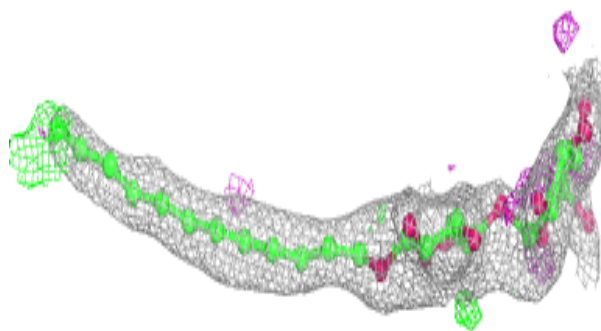
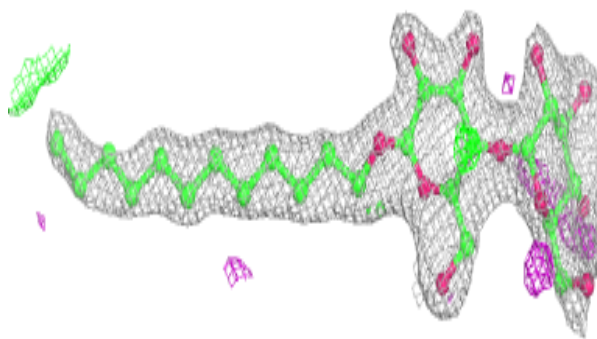
**Electron density around HTG B 630:**

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

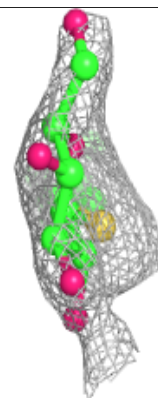
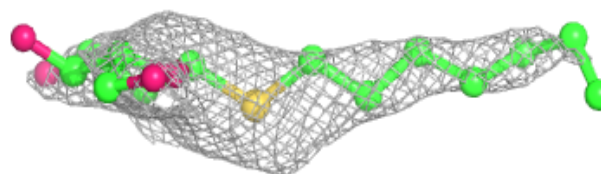
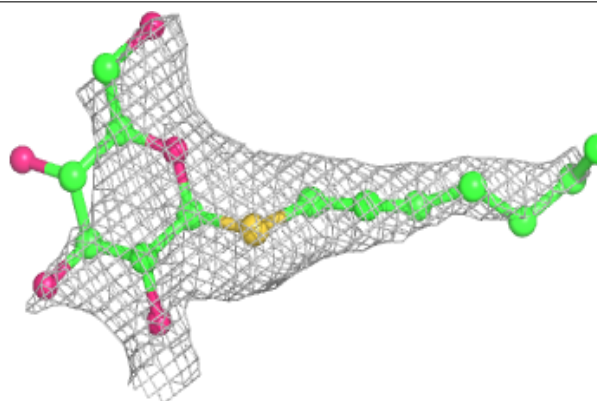


**Electron density around LMT m 102:**

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

**Electron density around HTG C 537:**

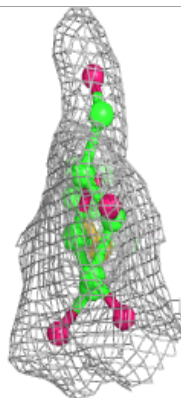
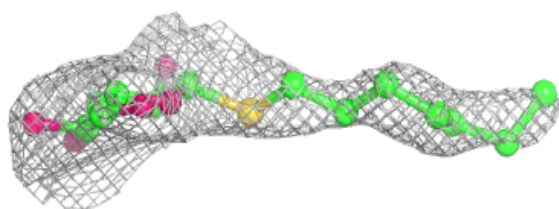
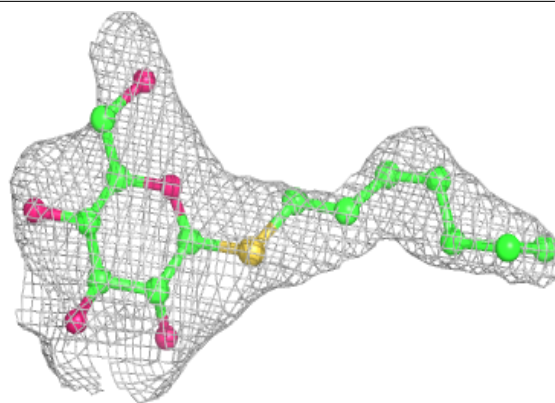
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



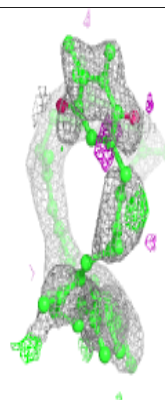
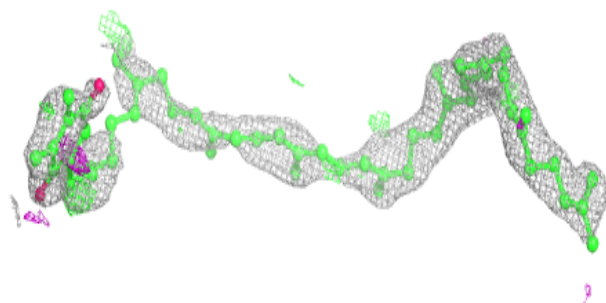
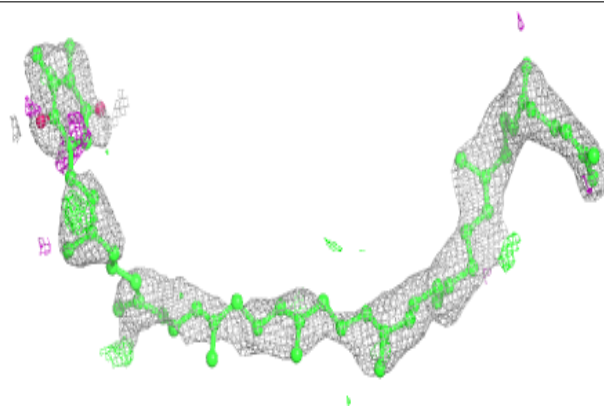


**Electron density around HTG d 414:**

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

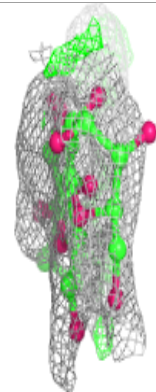
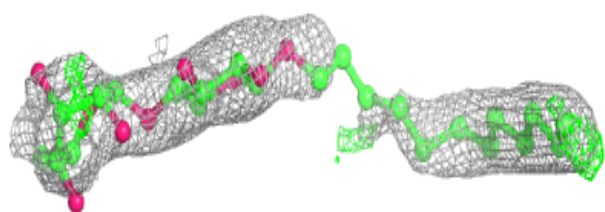
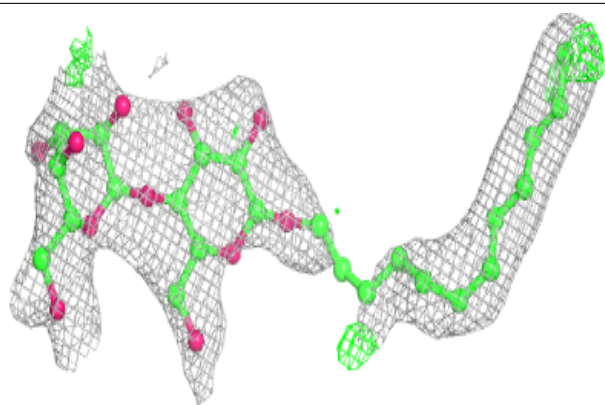
**Electron density around PL9 A 414:**

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

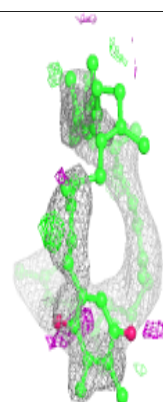
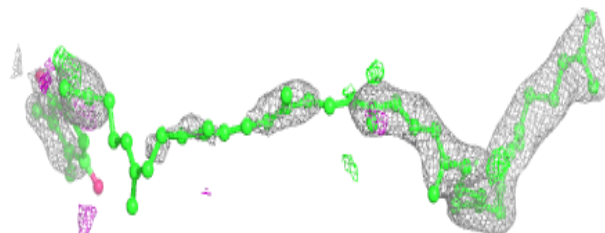
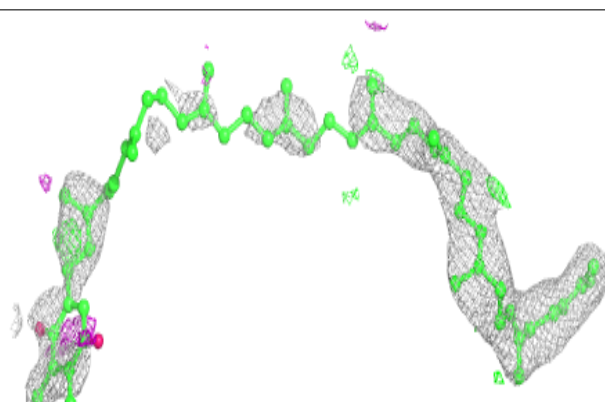


**Electron density around LMT Z 101:**

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

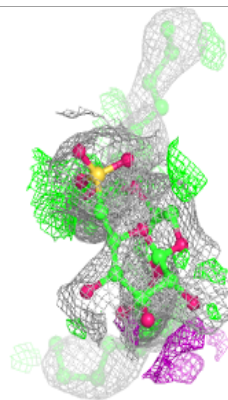
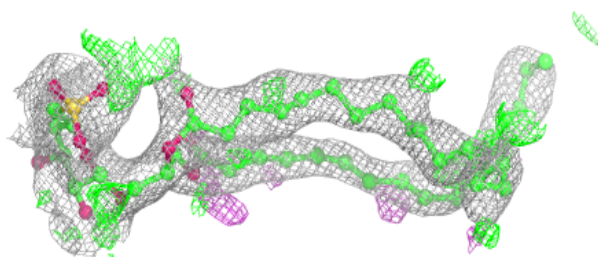
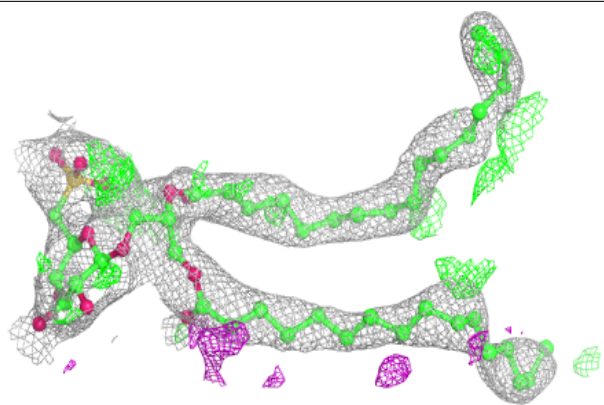
**Electron density around PL9 a 417:**

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

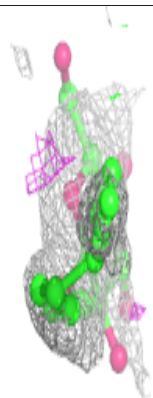
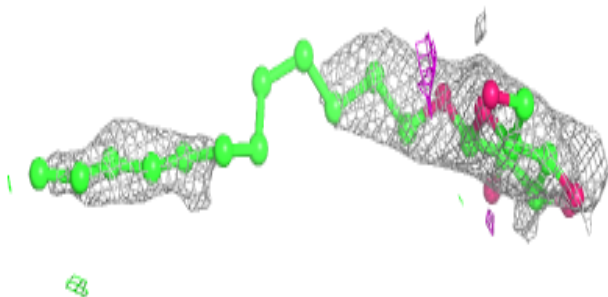
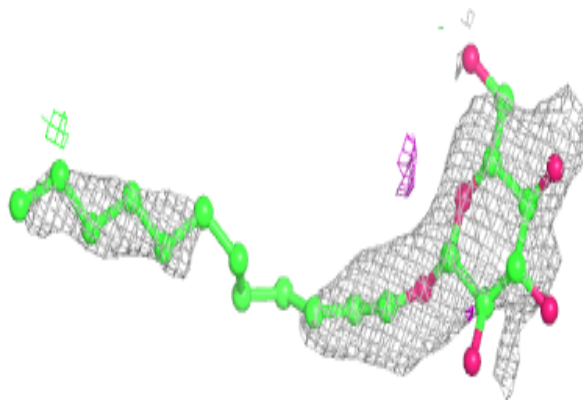


**Electron density around SQD b 601:**

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

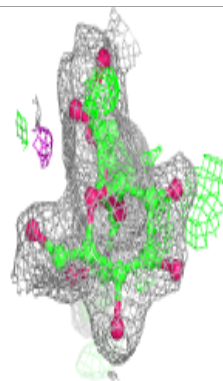
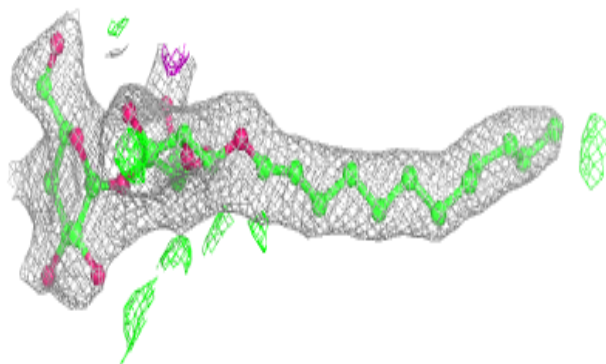
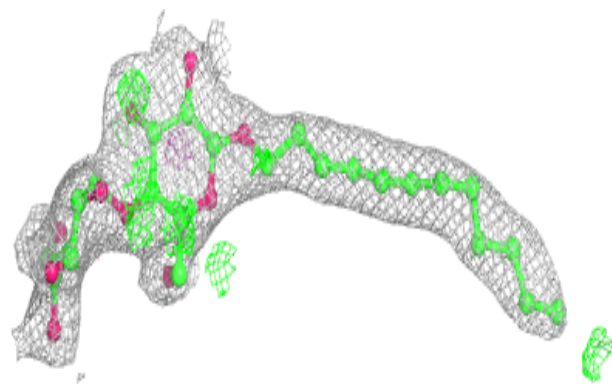
**Electron density around LMT F 103:**

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

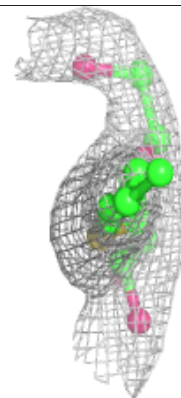
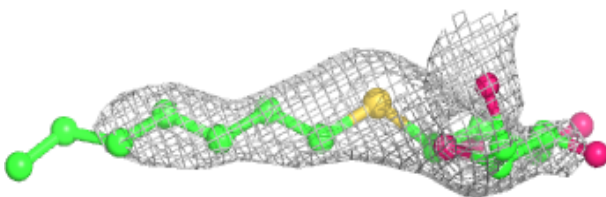
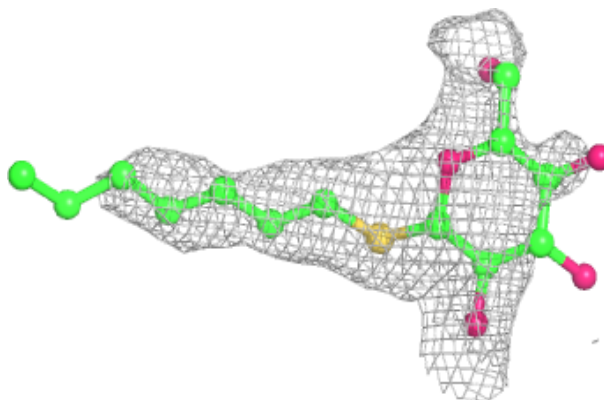


**Electron density around LMT B 622:**

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

**Electron density around HTG c 928:**

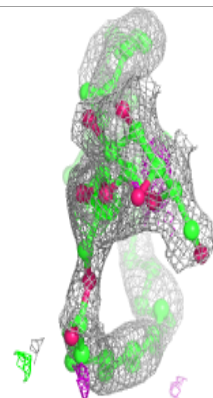
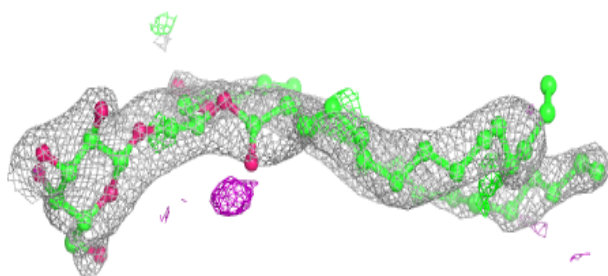
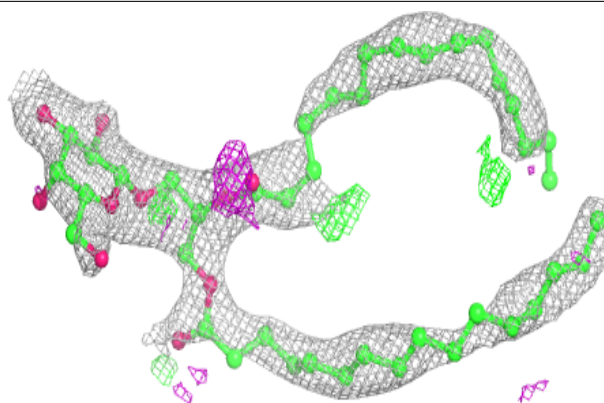
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



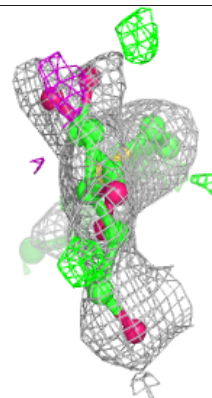
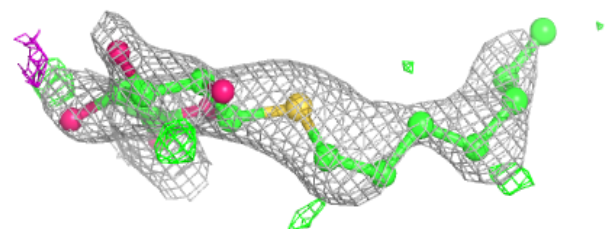
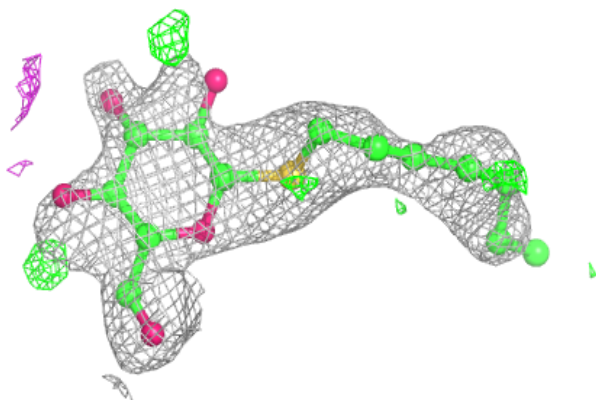


**Electron density around LMG A 413:**

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

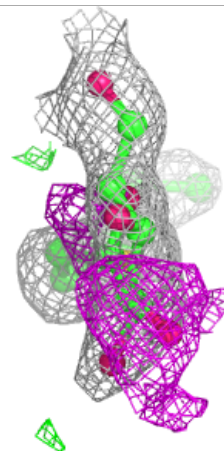
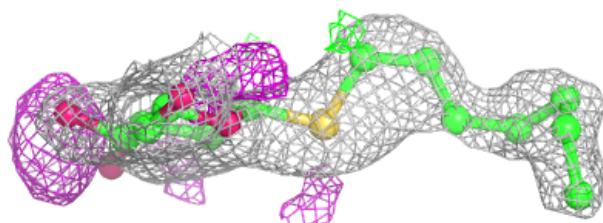
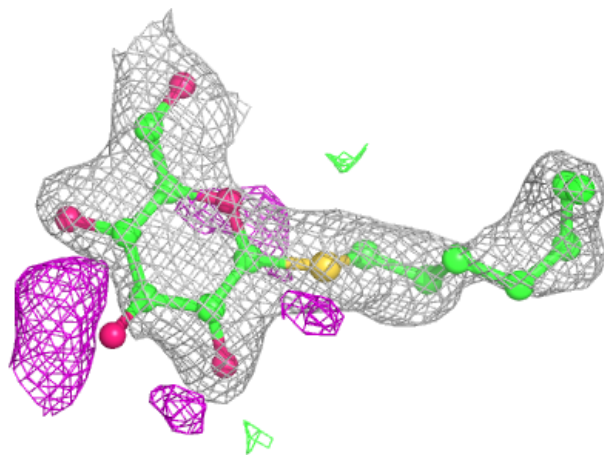
**Electron density around HTG c 942:**

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



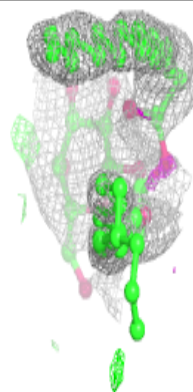
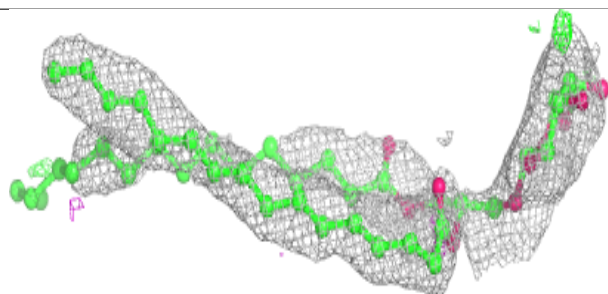
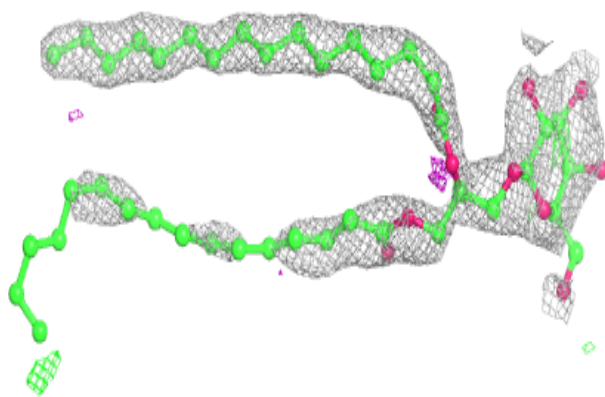
**Electron density around HTG O 316:**

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

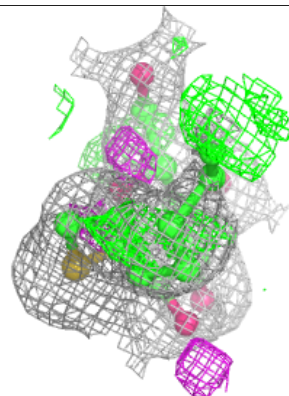
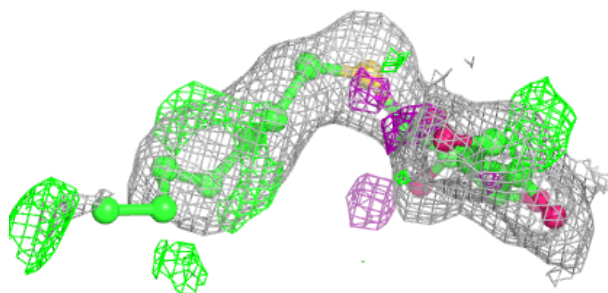
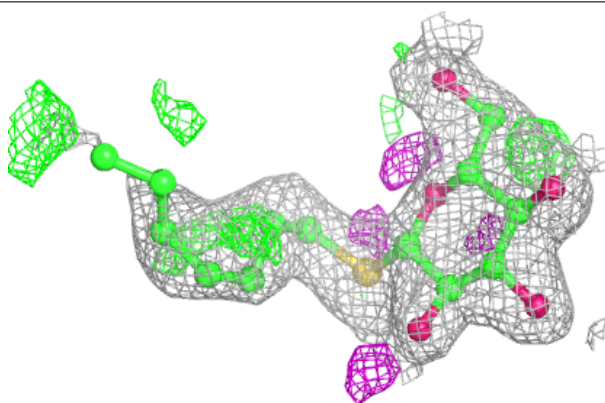


**Electron density around LMG c 921:**

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

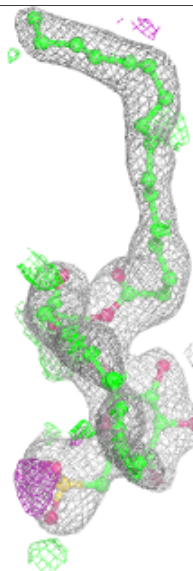
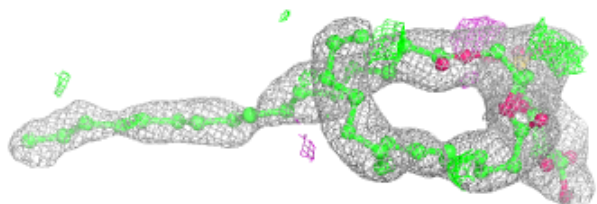
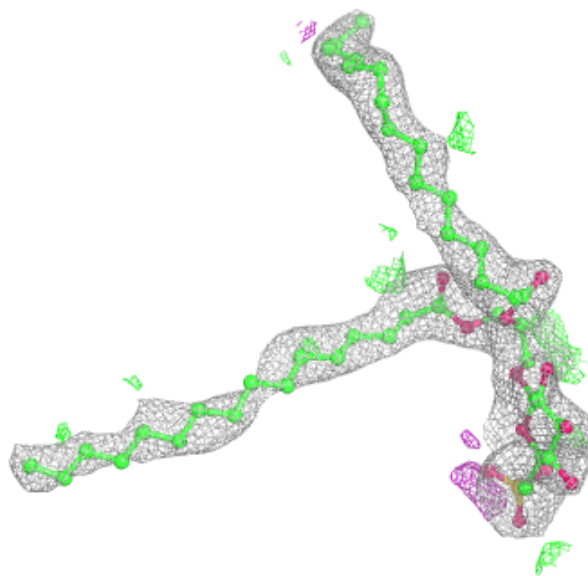
**Electron density around HTG B 624:**

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



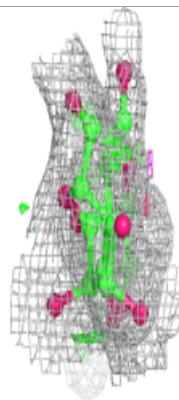
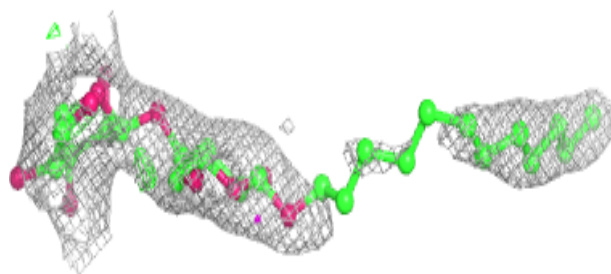
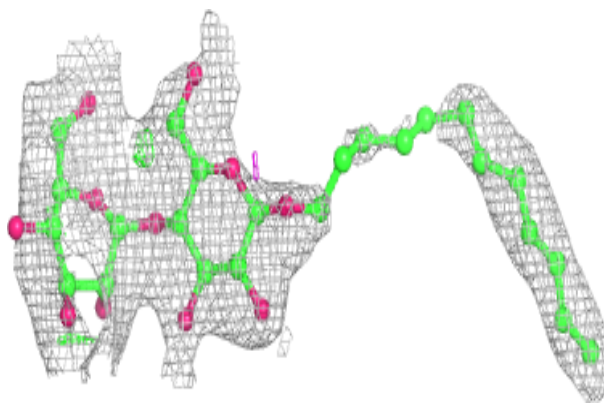
**Electron density around SQD A 416:**

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

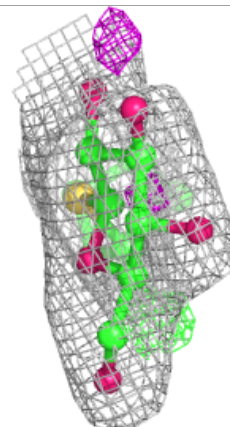
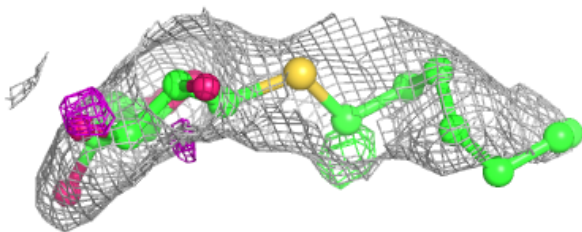
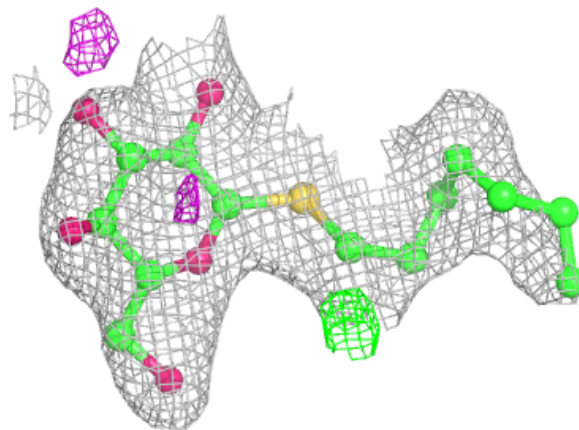


**Electron density around LMT c 927:**

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

**Electron density around HTG v 211:**

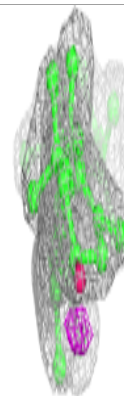
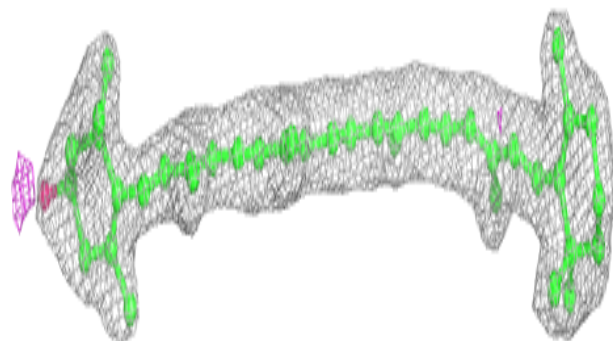
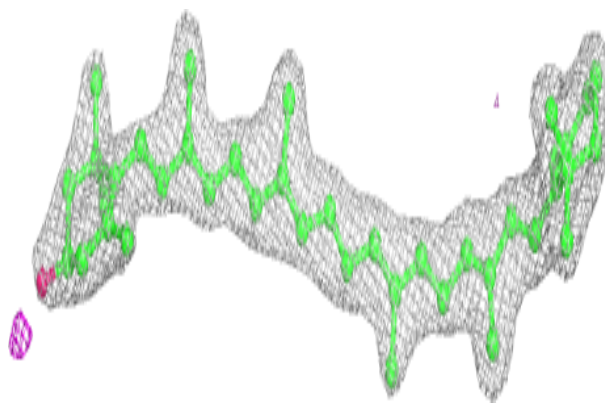
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



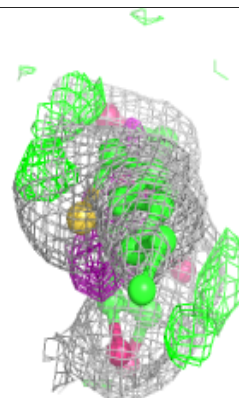
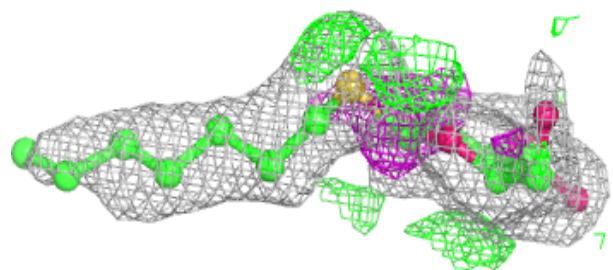
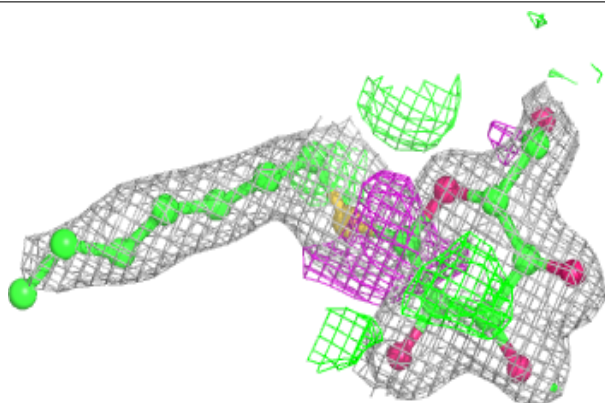


**Electron density around RRX h 101:**

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

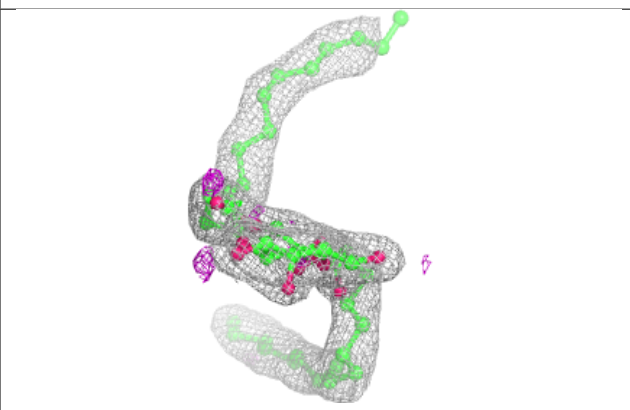
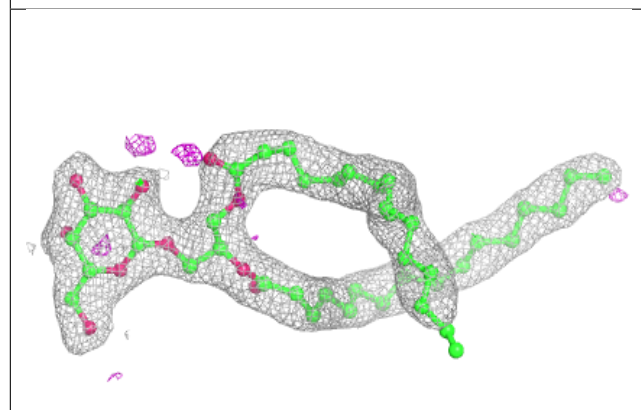
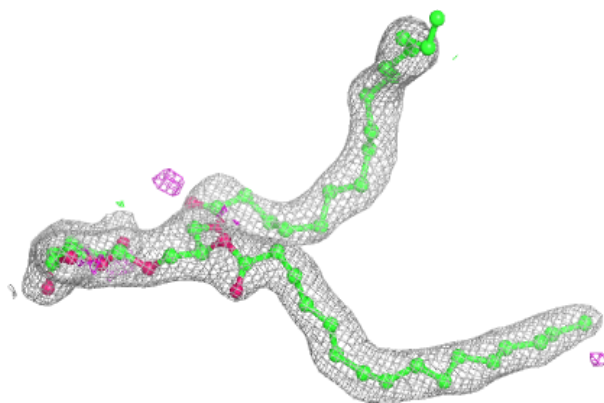
**Electron density around HTG B 623:**

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

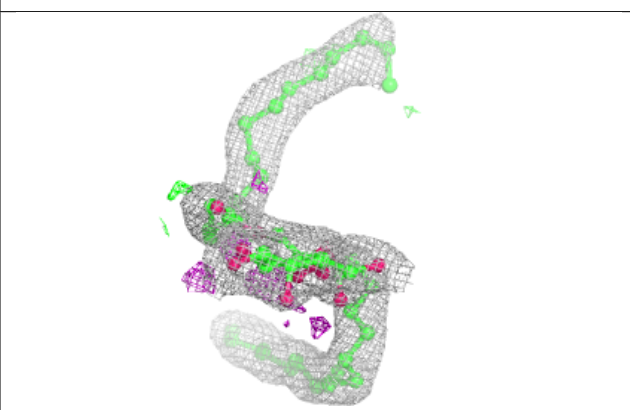
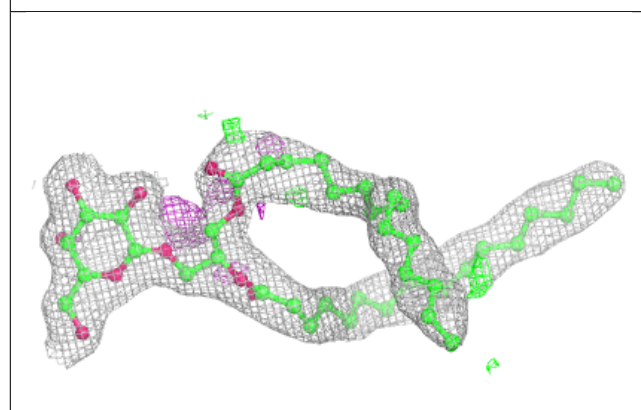
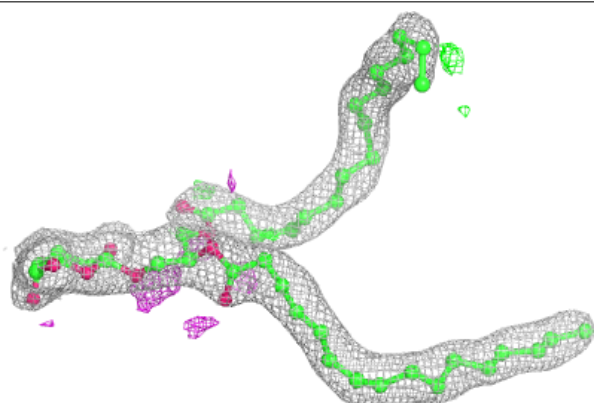


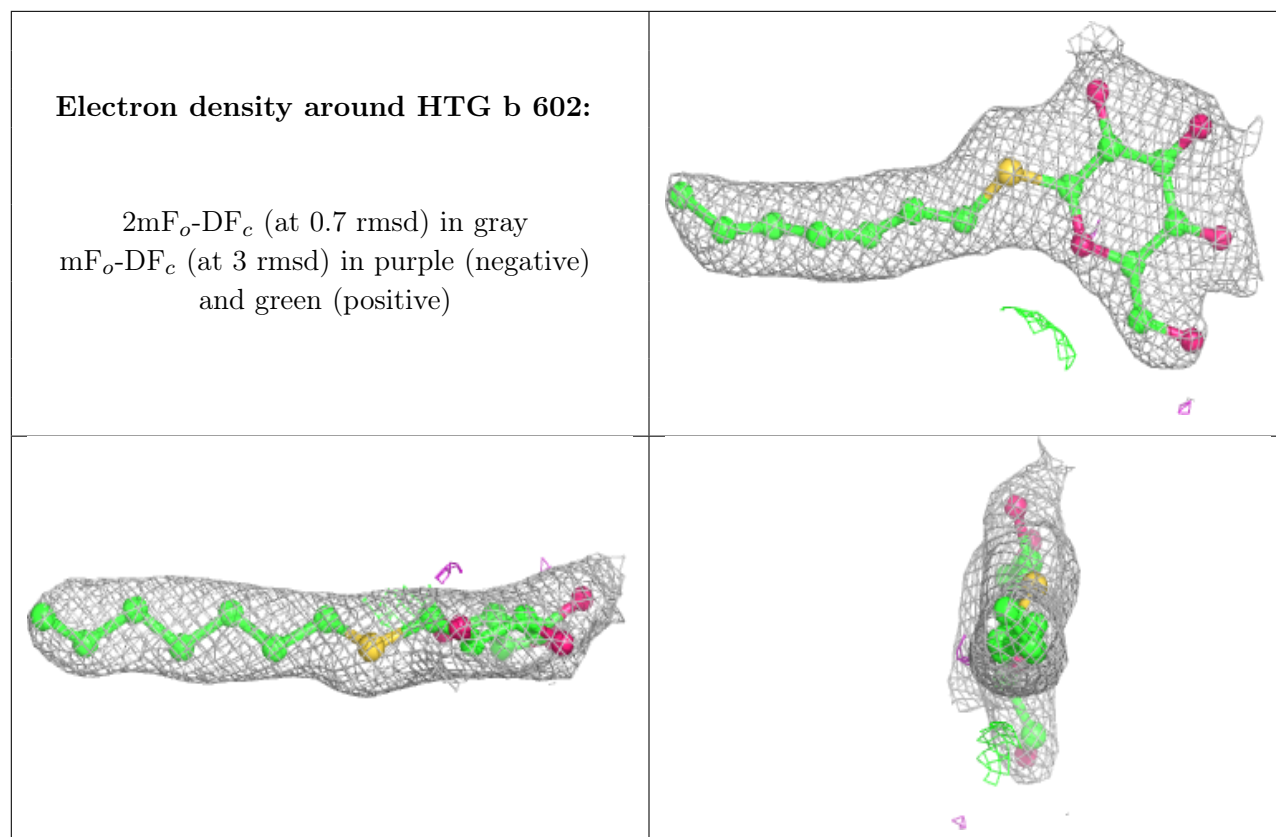
**Electron density around LMG B 621:**

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

**Electron density around LMG 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)

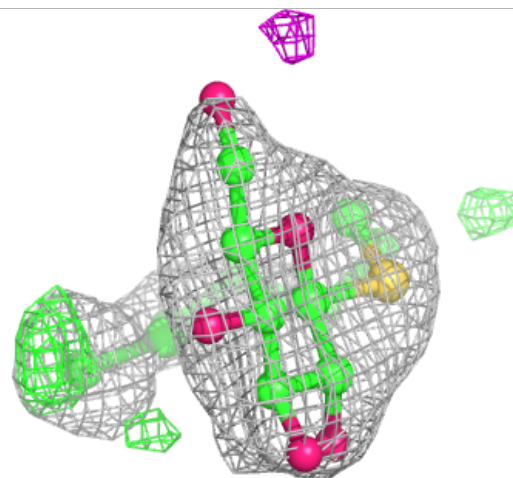
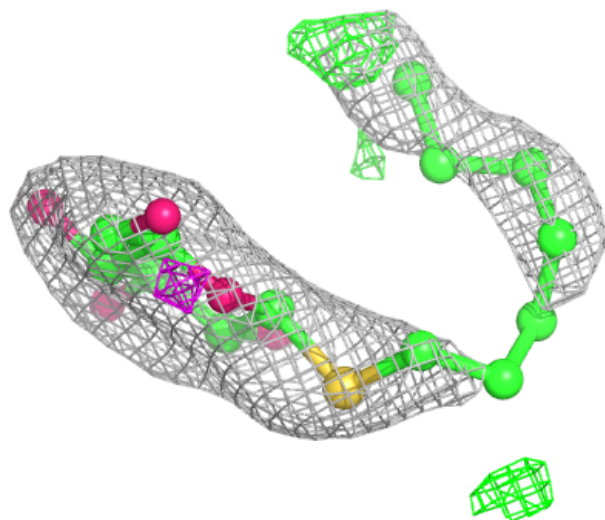
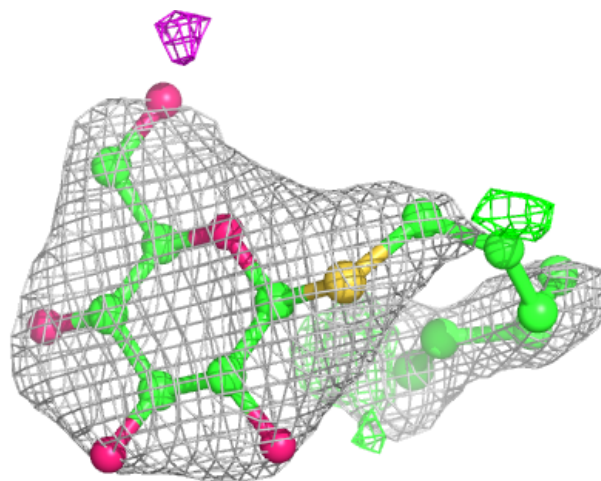






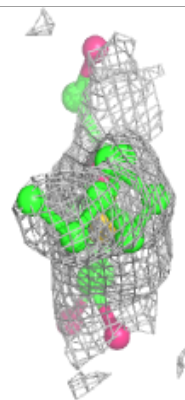
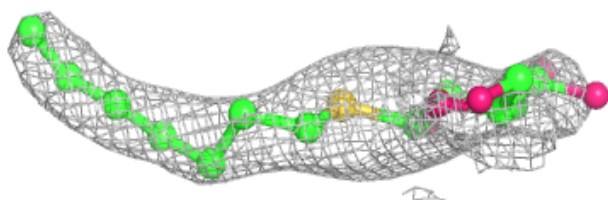
**Electron density around HTG C 520:**

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

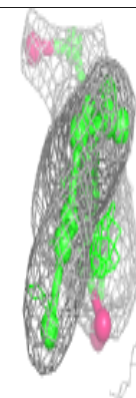
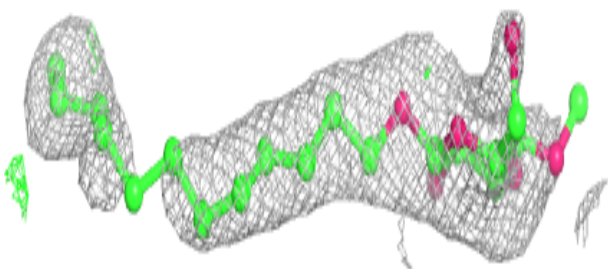
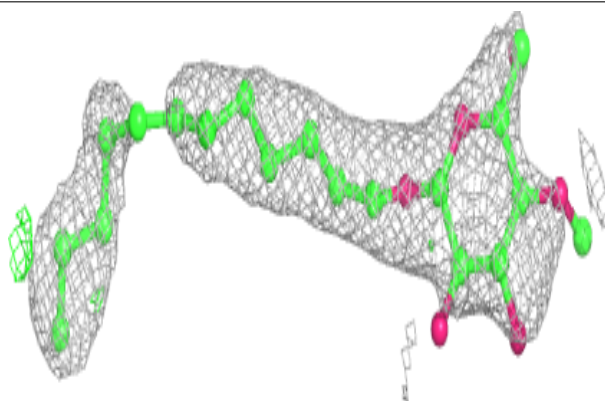


**Electron density around HTG C 536:**

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

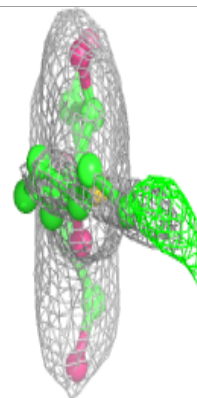
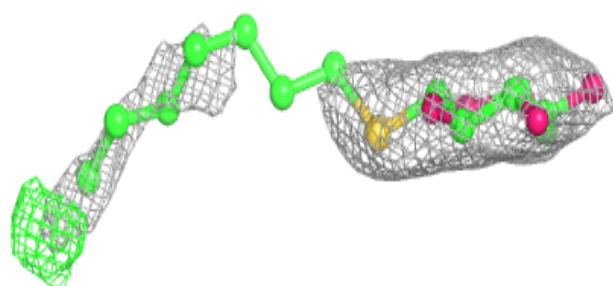
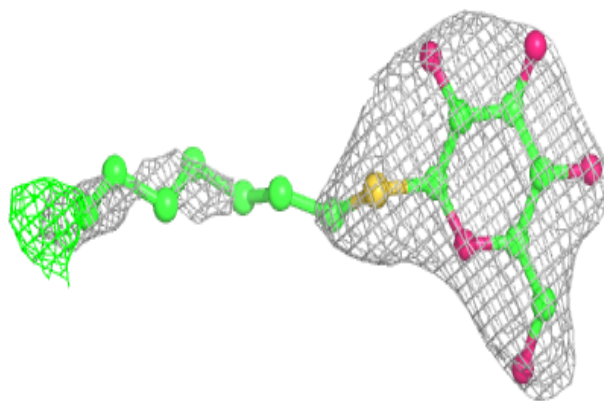
**Electron density around LMT M 102:**

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

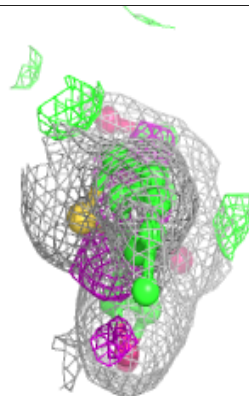
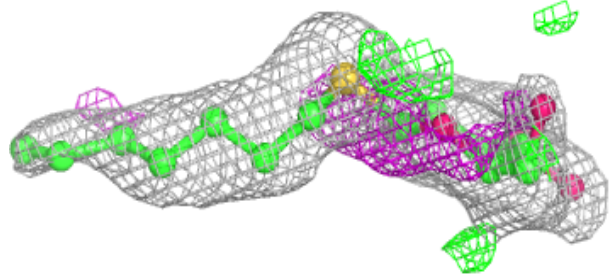
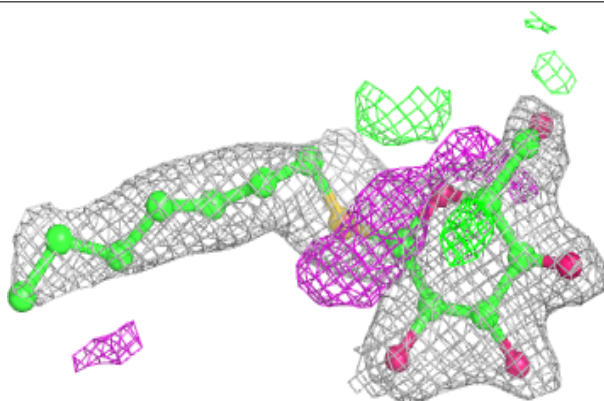


**Electron density around HTG c 923:**

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

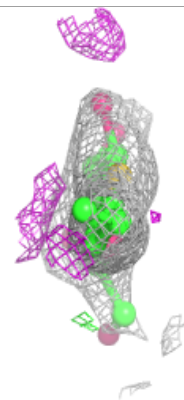
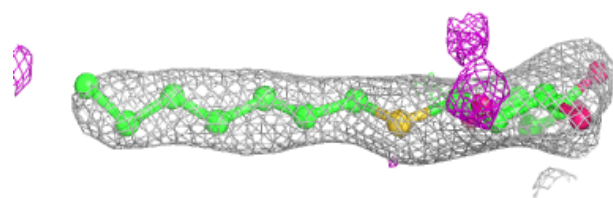
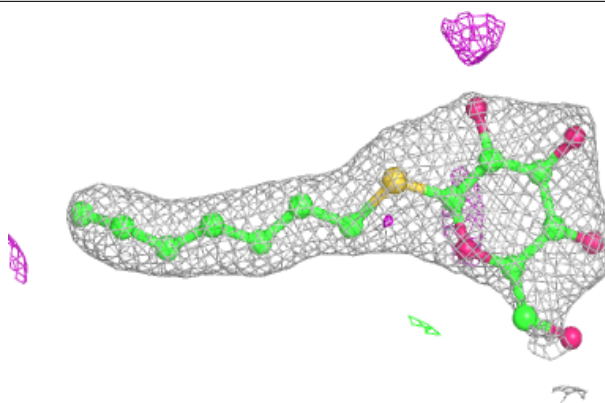
**Electron density around HTG O 303:**

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

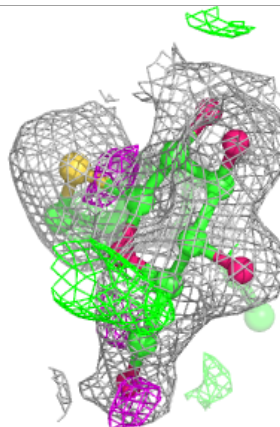
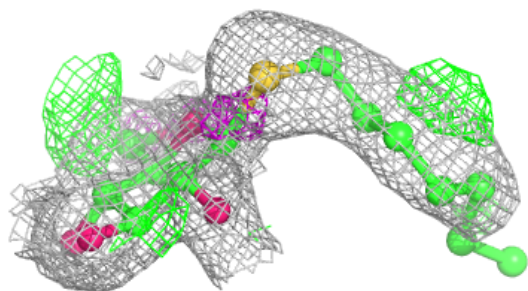
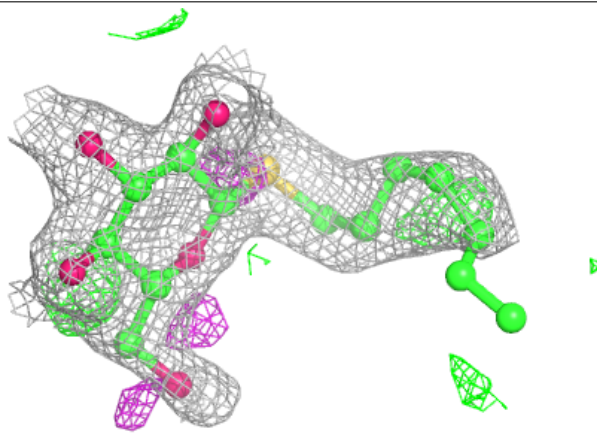


**Electron density around HTG B 629:**

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

**Electron density around HTG b 626:**

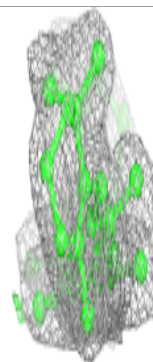
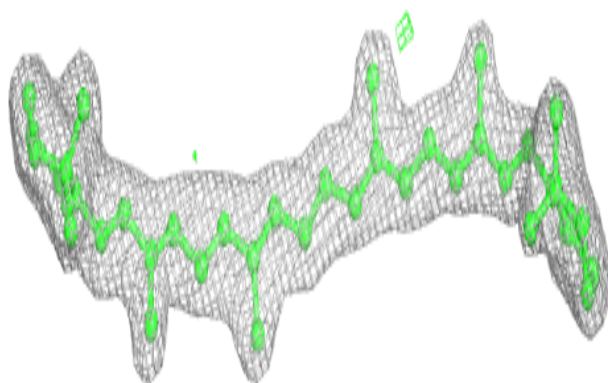
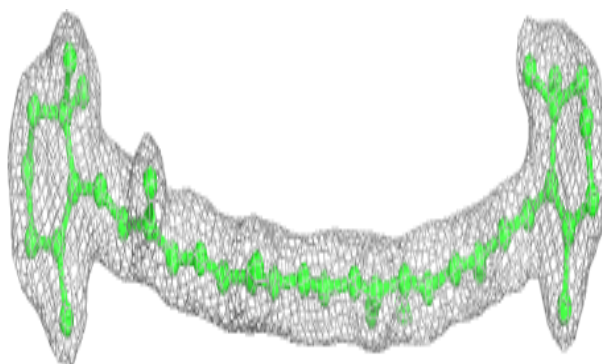
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



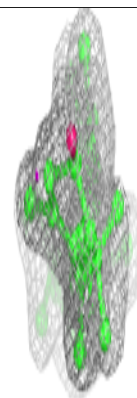
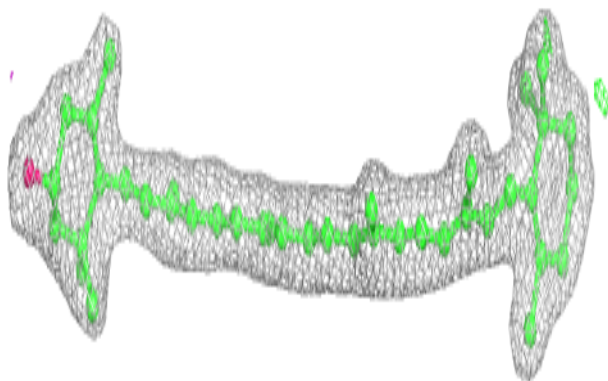
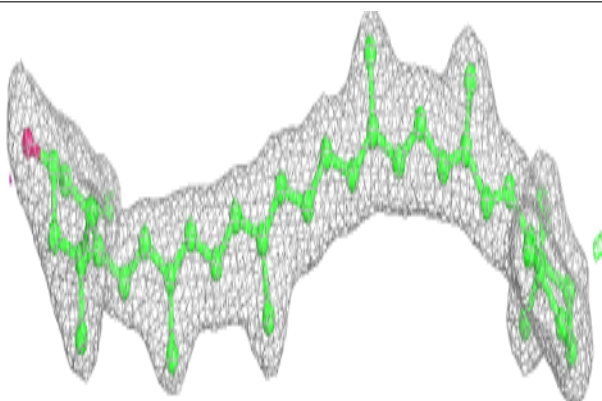


**Electron density around BCR k 103:**

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

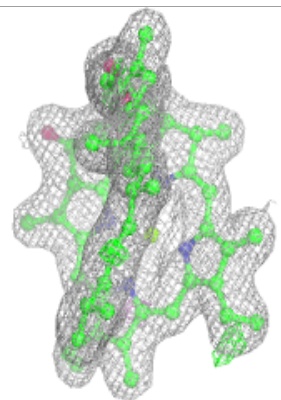
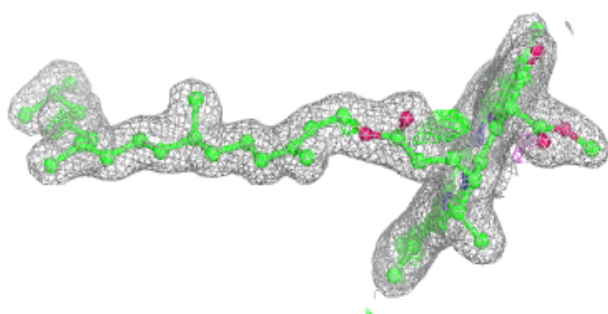
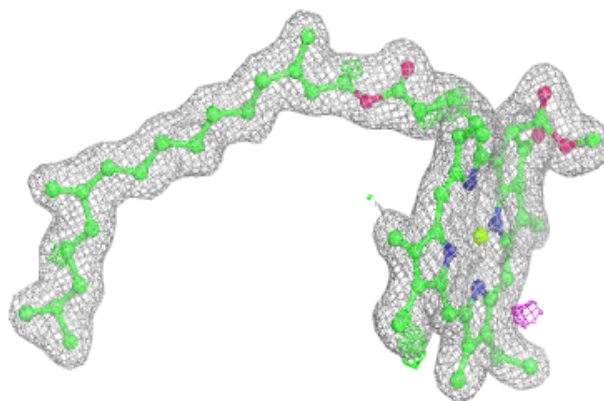
**Electron density around RRX H 101:**

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

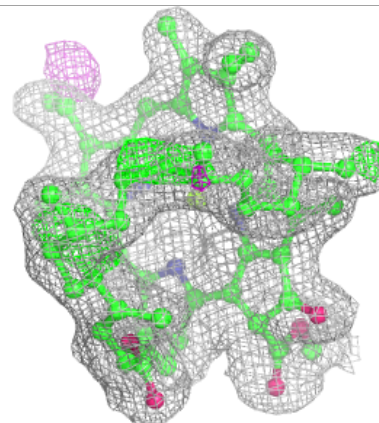
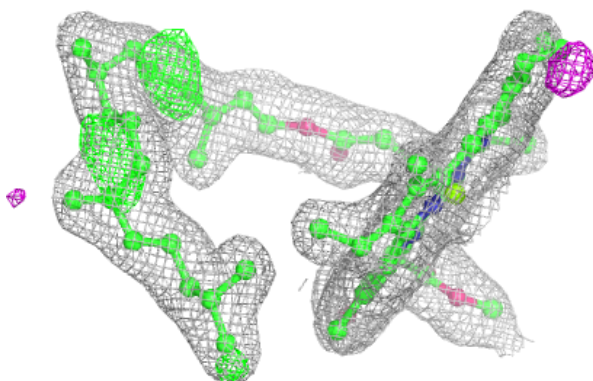
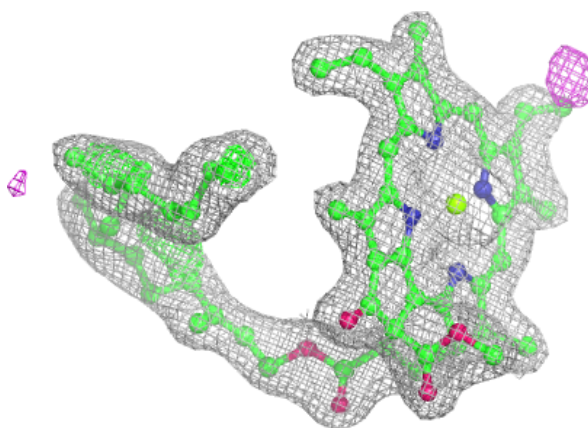


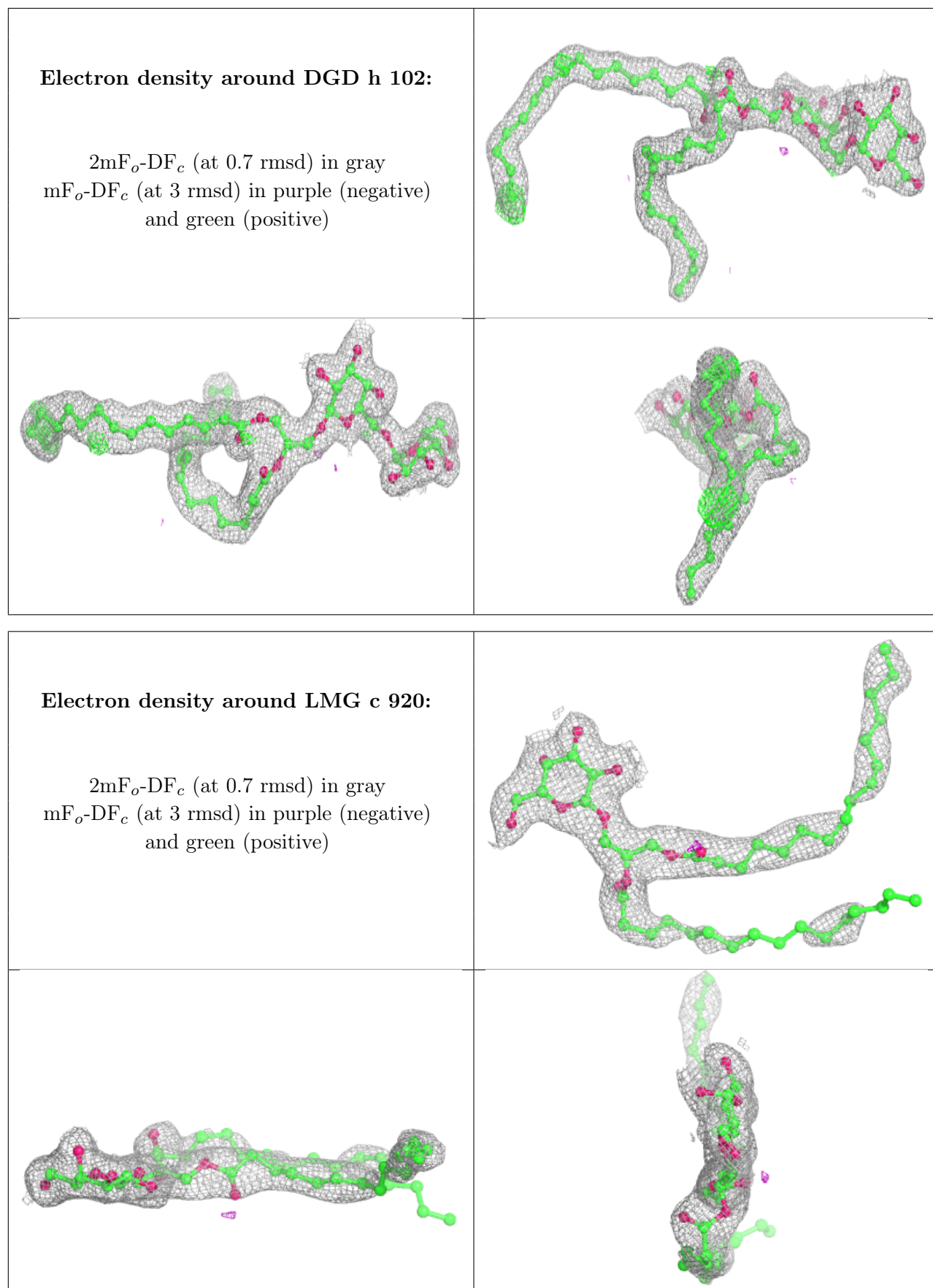
**Electron density around CLA B 610:**

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

**Electron density around CLA c 904:**

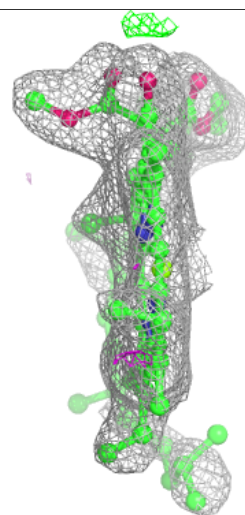
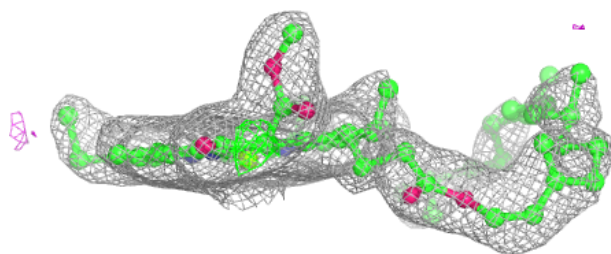
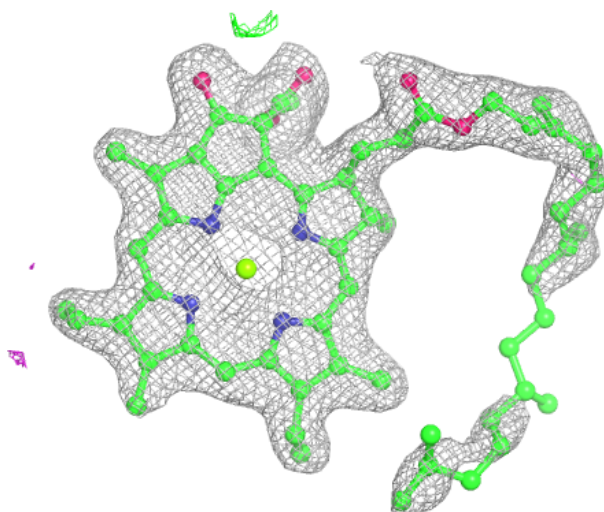
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



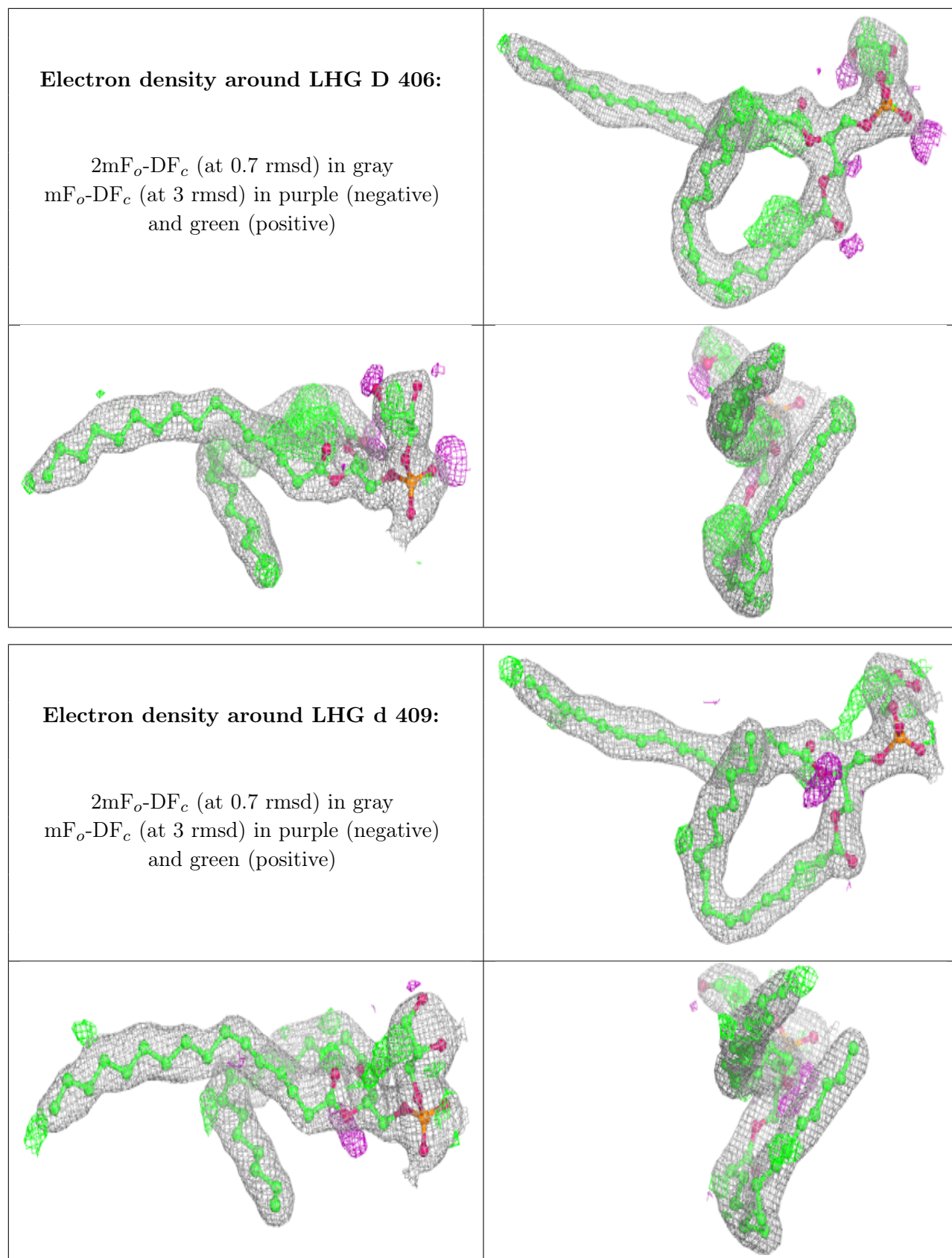


**Electron density around CLA c 913:**

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

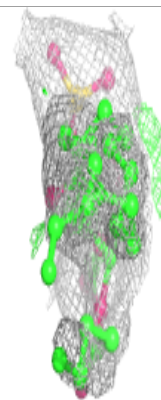
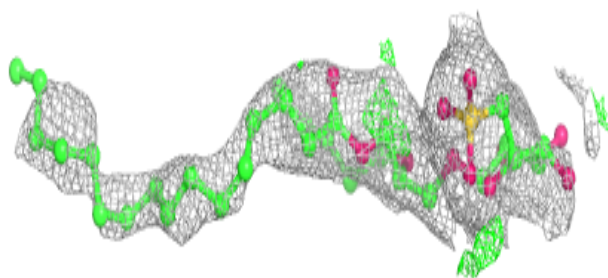
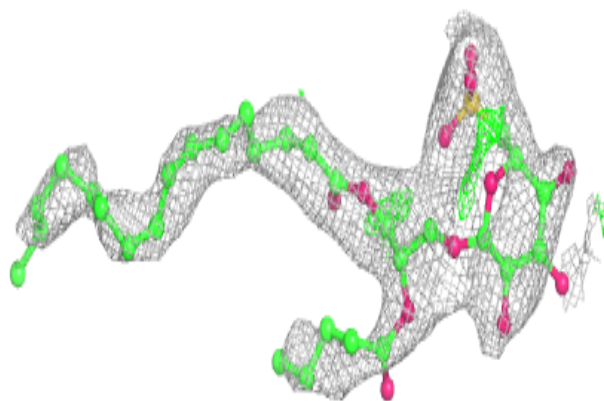




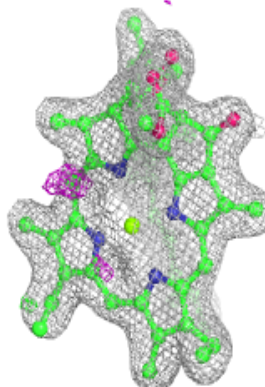
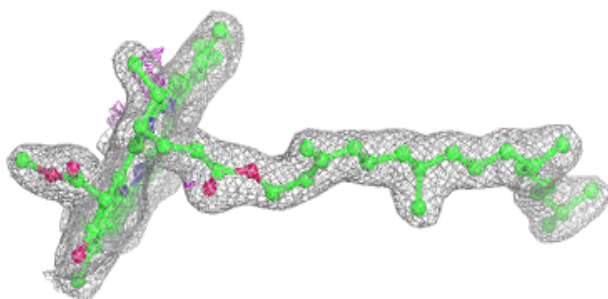
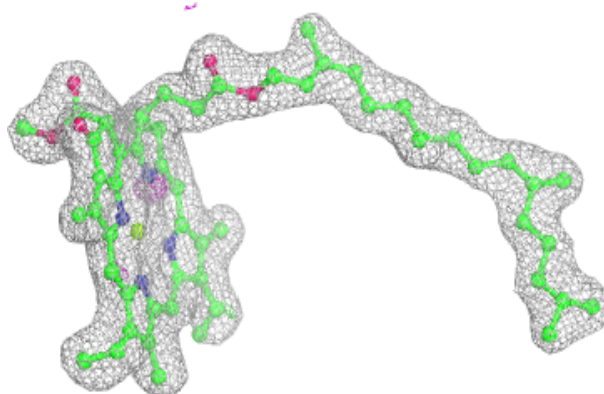


**Electron density around SQD f 102:**

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

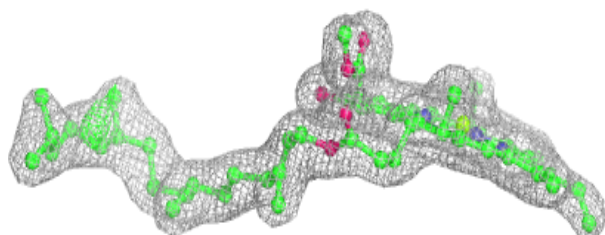
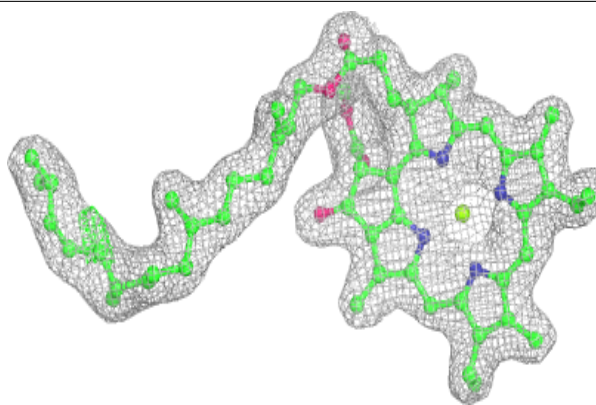
**Electron density around CLA b 613:**

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

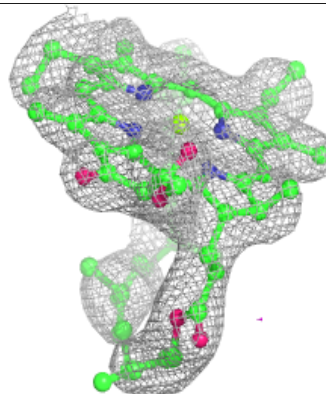
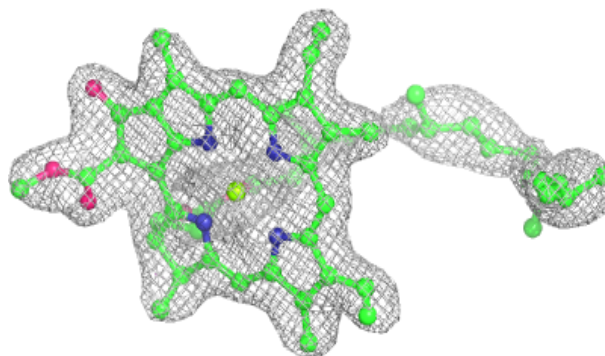
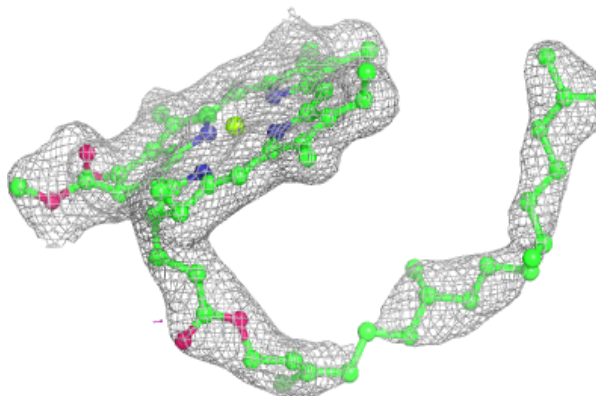


**Electron density around CLA B 603:**

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

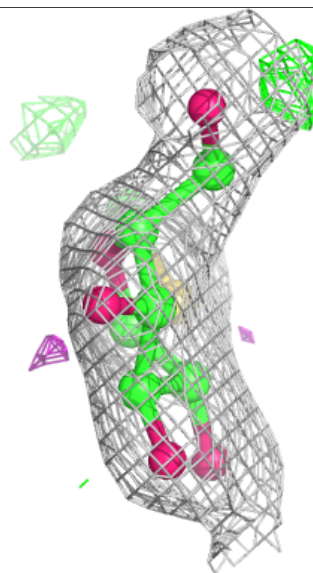
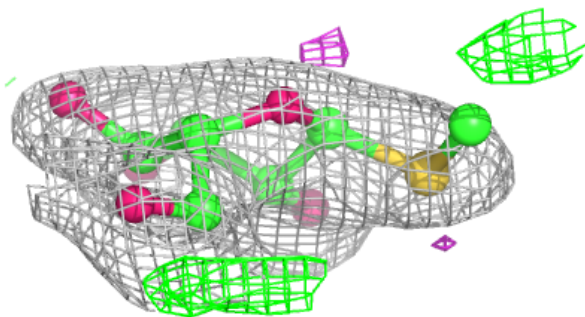
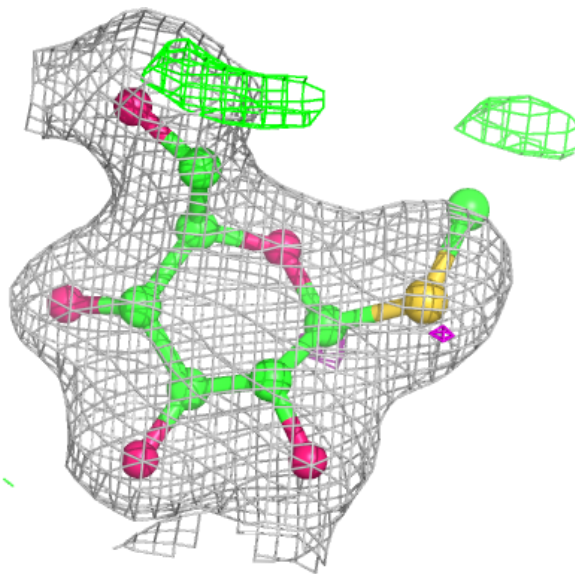
**Electron density around CLA C 513:**

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



**Electron density around HTG V 204:**

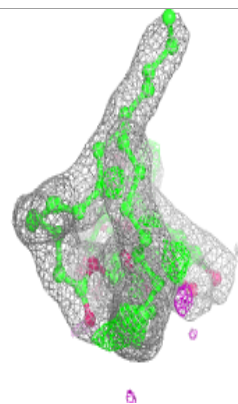
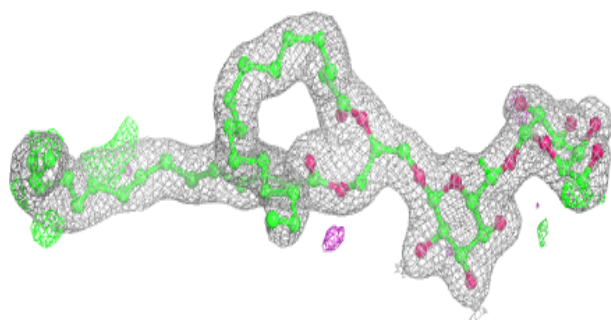
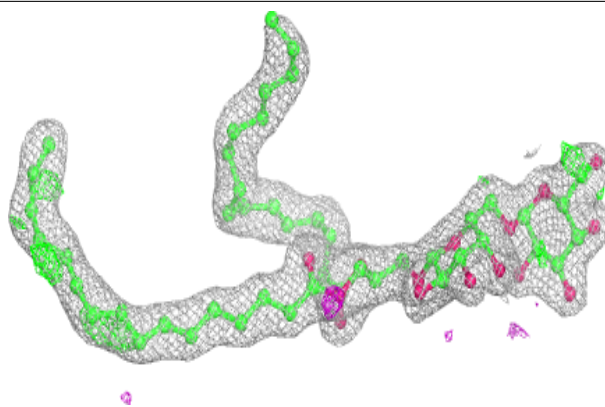
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



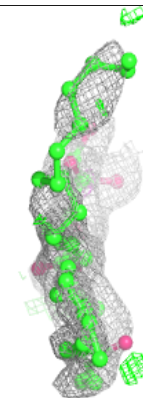
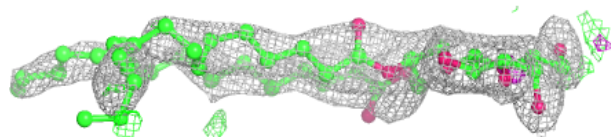
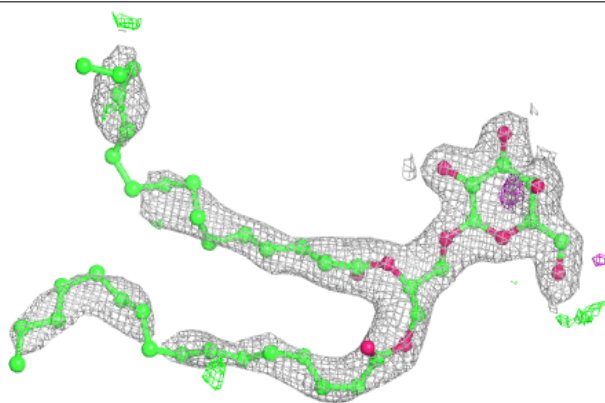


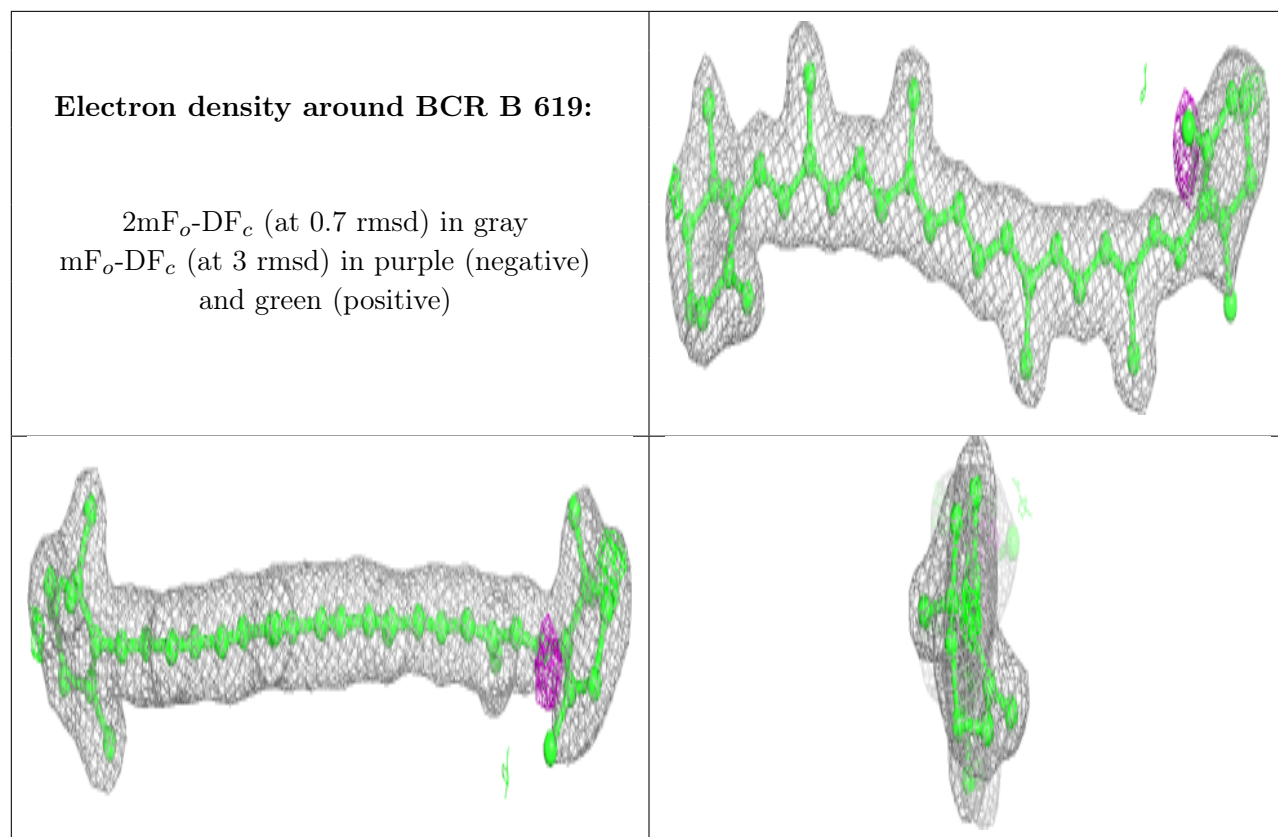
**Electron density around DGD H 102:**

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

**Electron density around LMG C 519:**

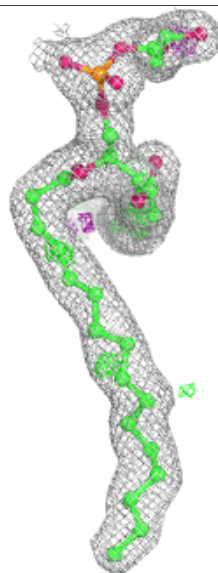
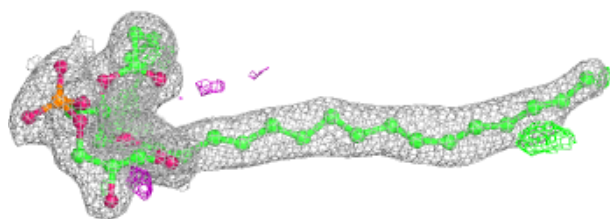
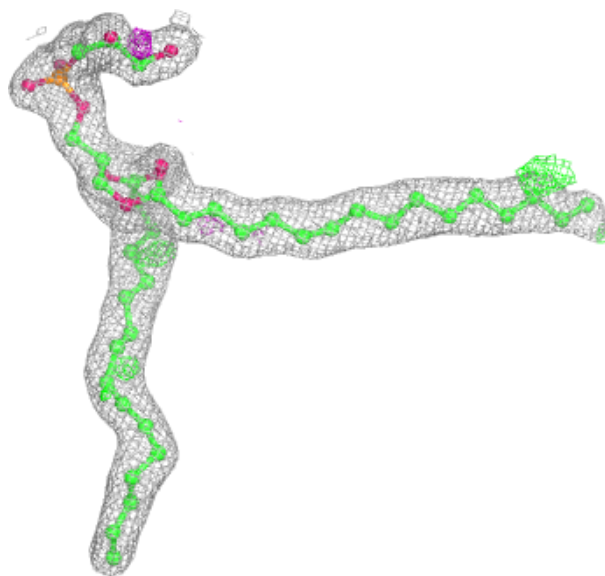
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





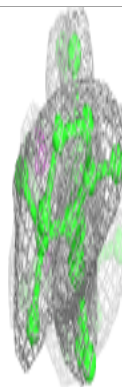
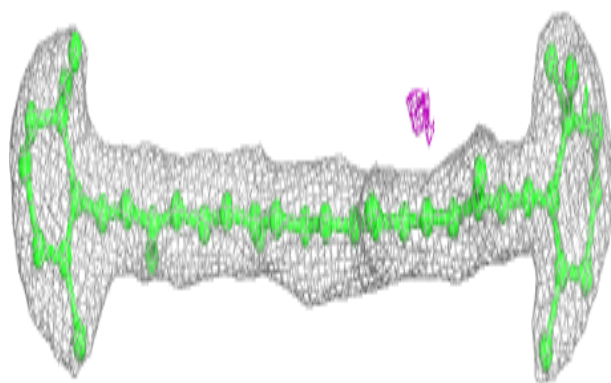
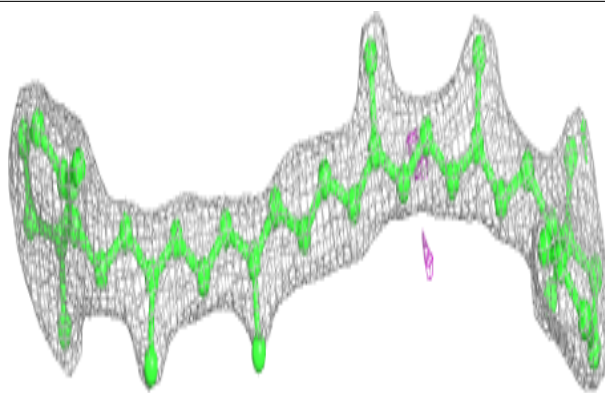
**Electron density around LHG 1 103:**

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

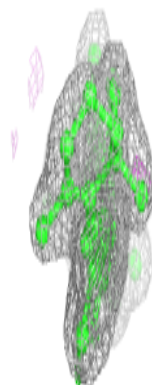
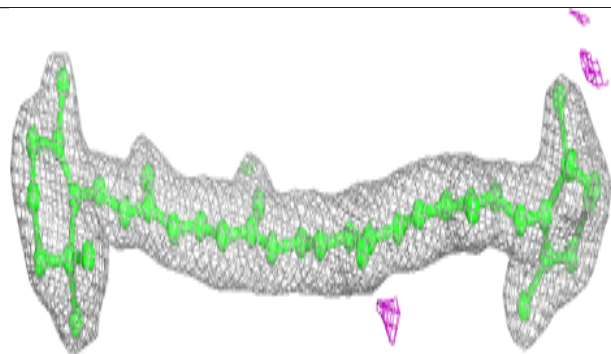
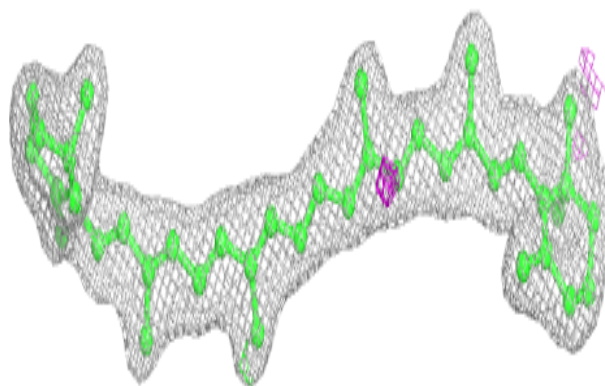


**Electron density around BCR c 915:**

$2mF_o-DF_c$  (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:**

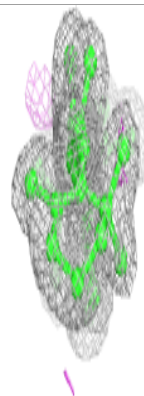
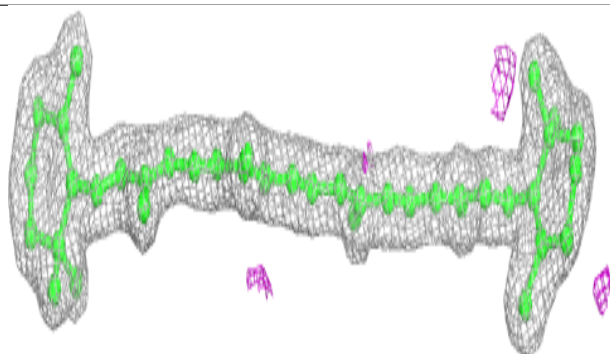
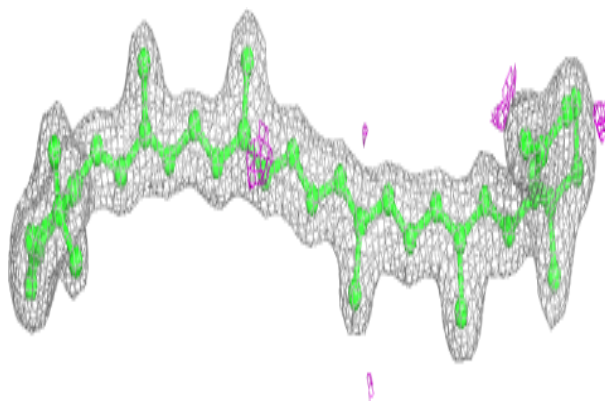
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



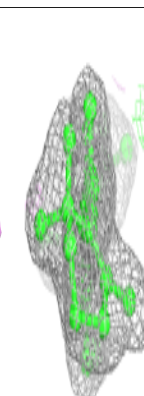
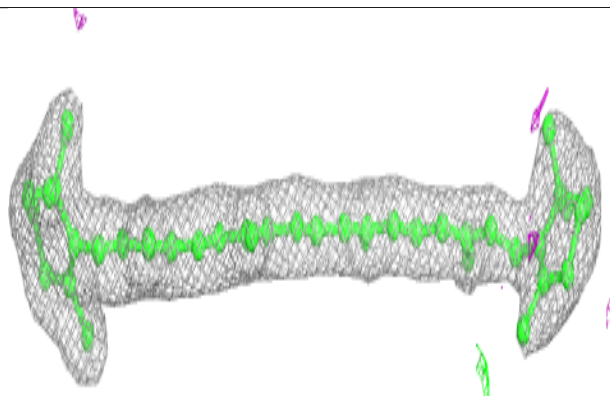
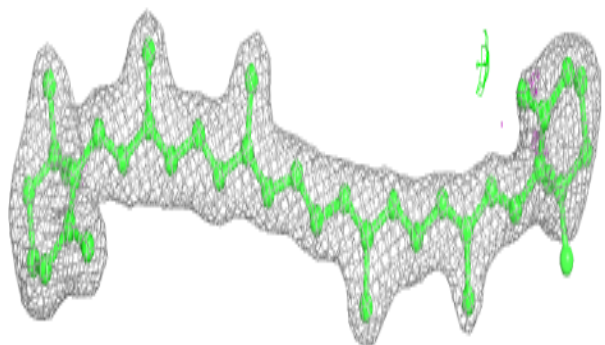


**Electron density around BCR a 414:**

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

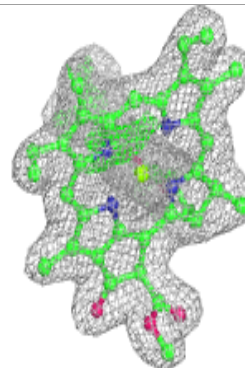
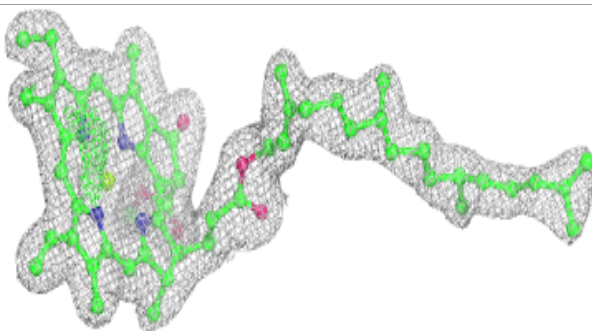
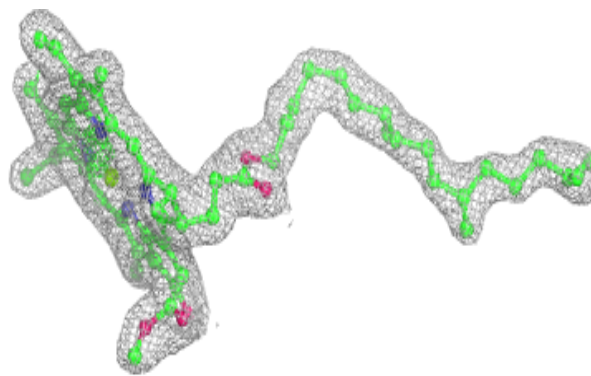
**Electron density around BCR b 622:**

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



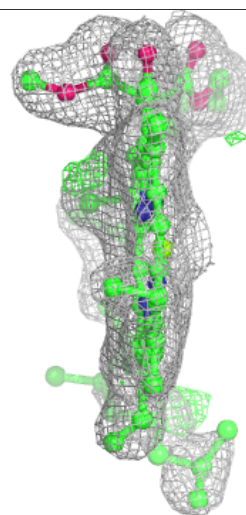
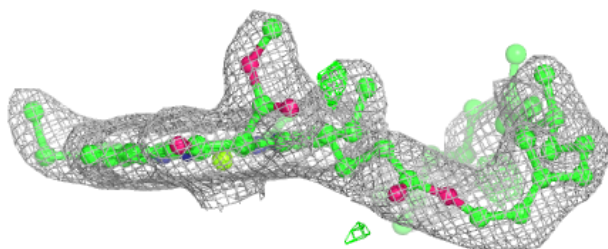
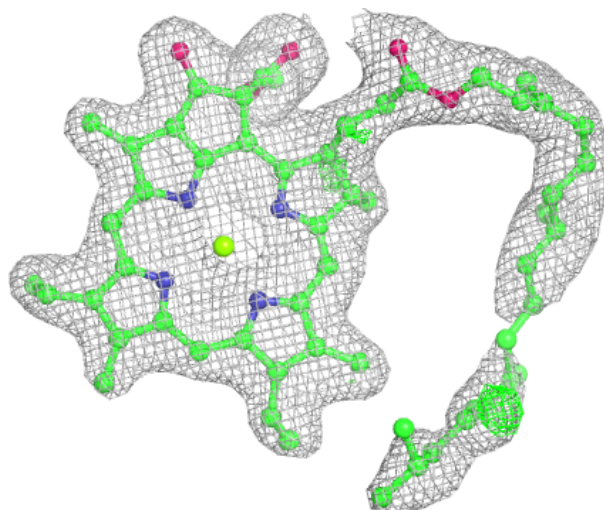
**Electron density around CLA c 903:**

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



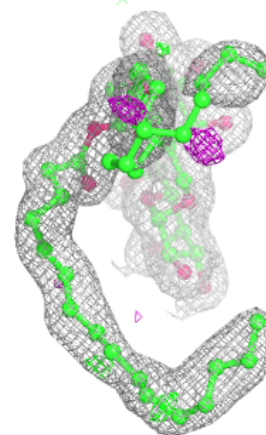
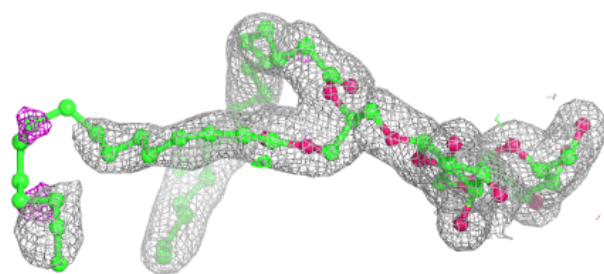
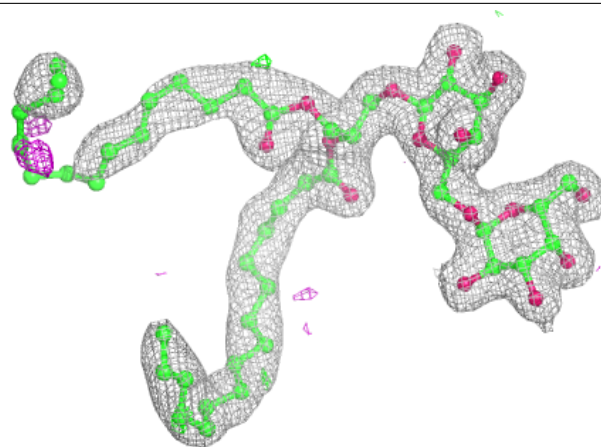
**Electron density around CLA C 512:**

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

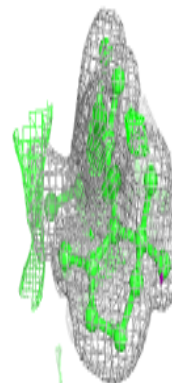
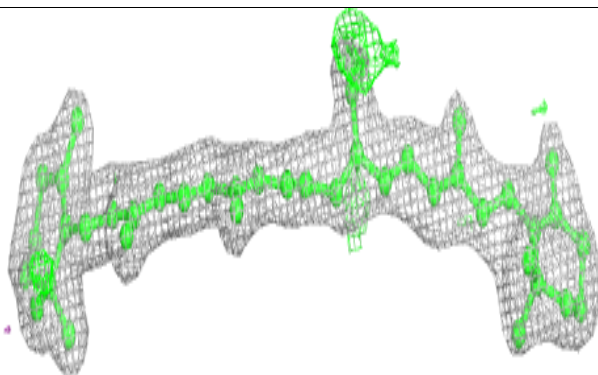
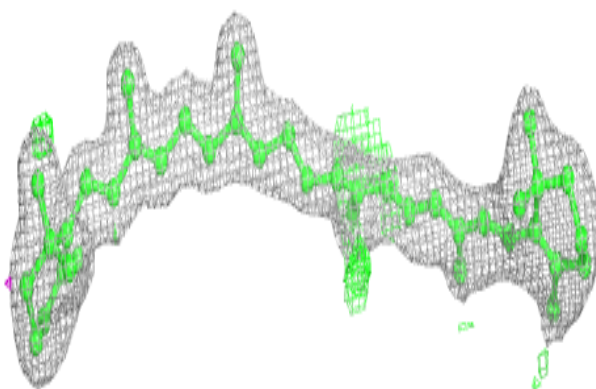


**Electron density around DGD C 517:**

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

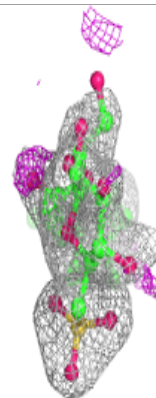
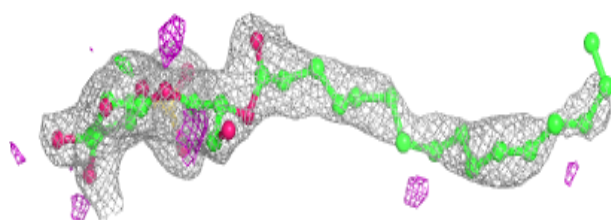
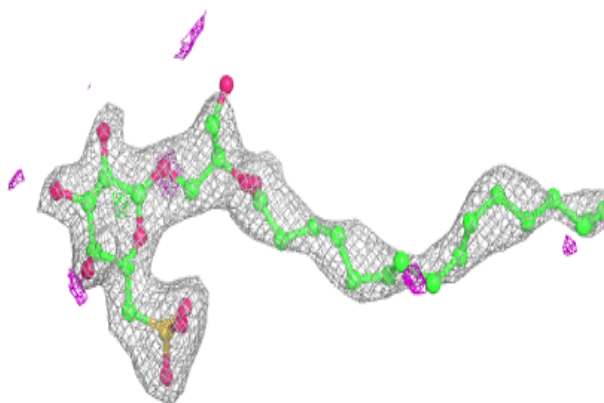
**Electron density around BCR B 636:**

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

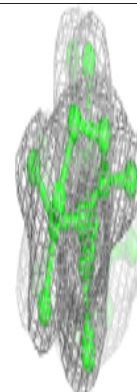
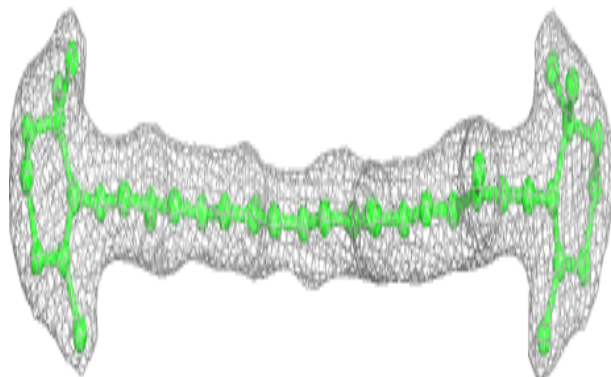
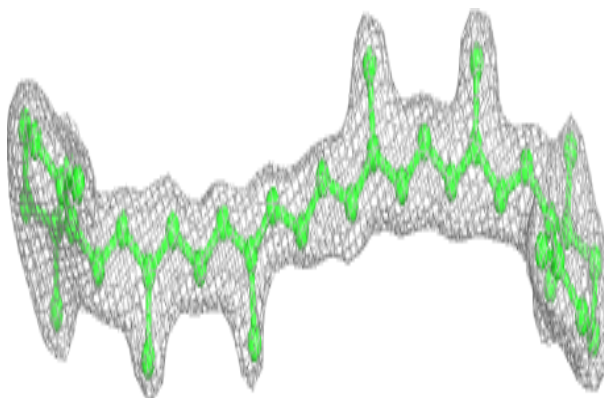


**Electron density around SQD F 101:**

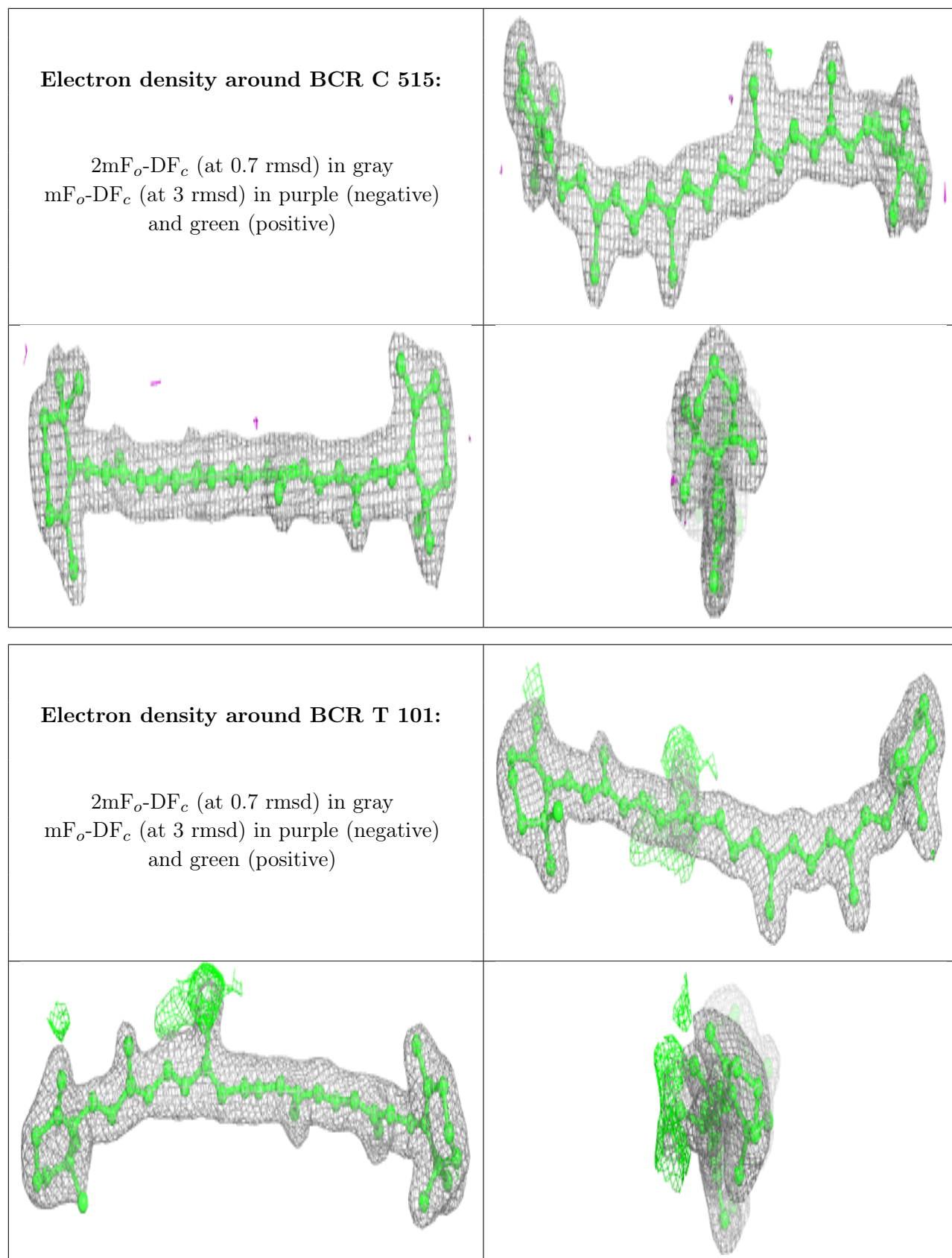
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around BCR C 514:**

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

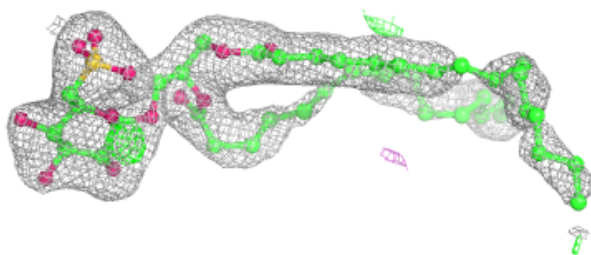
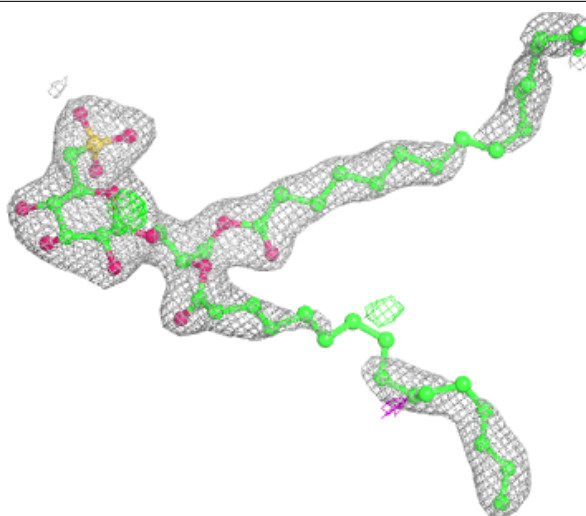






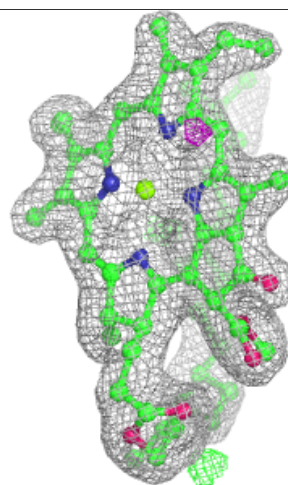
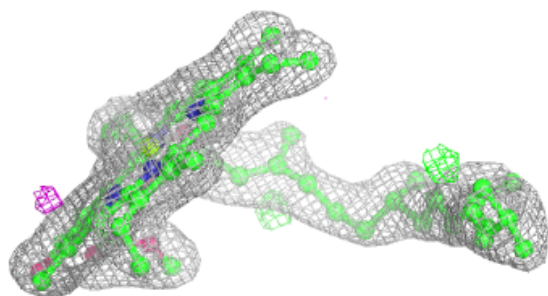
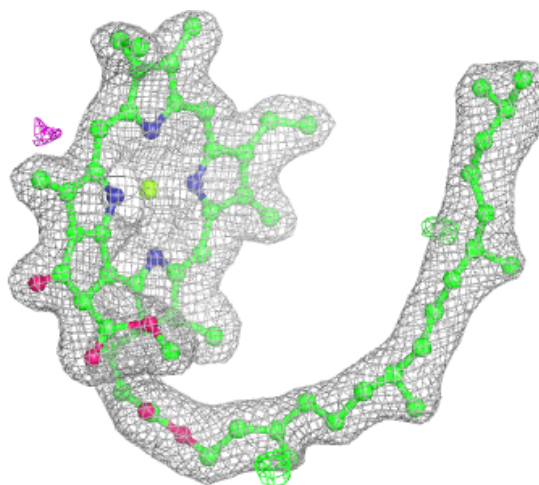
**Electron density around SQD a 415:**

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



**Electron density around CLA C 507:**

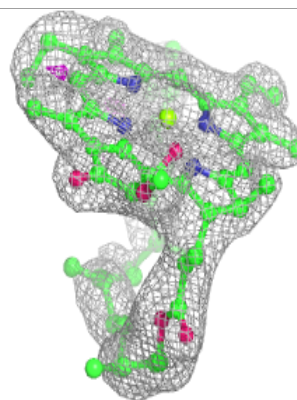
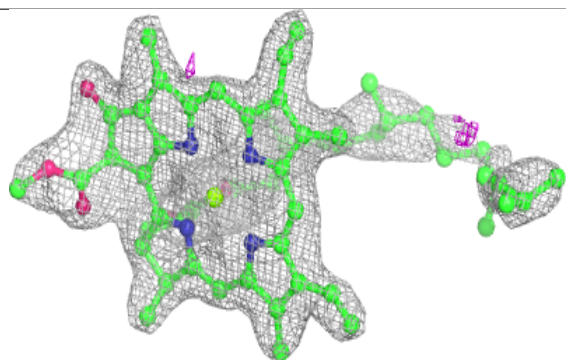
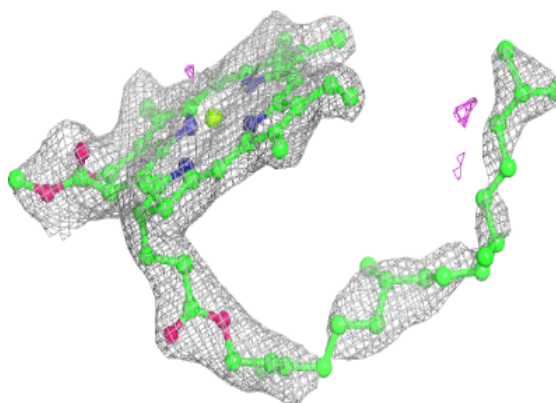
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





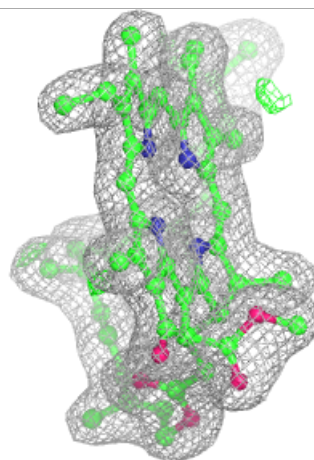
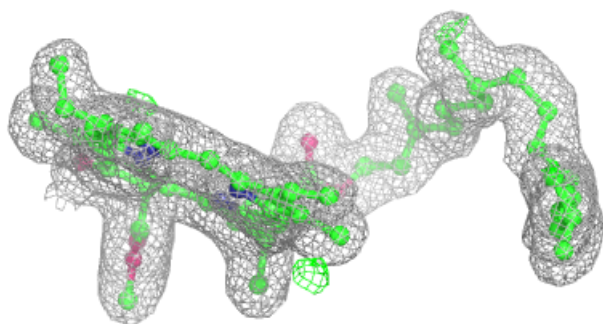
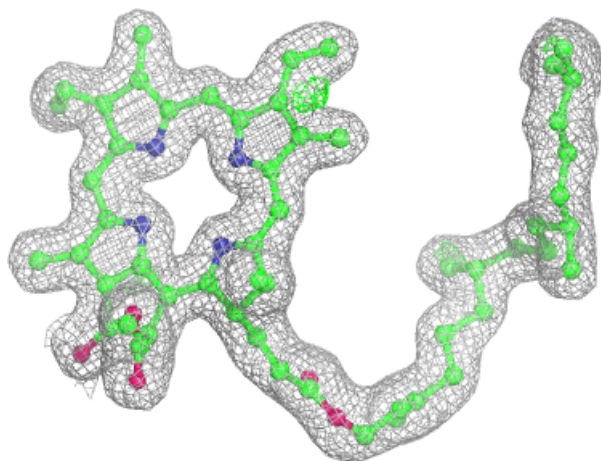
**Electron density around CLA c 914:**

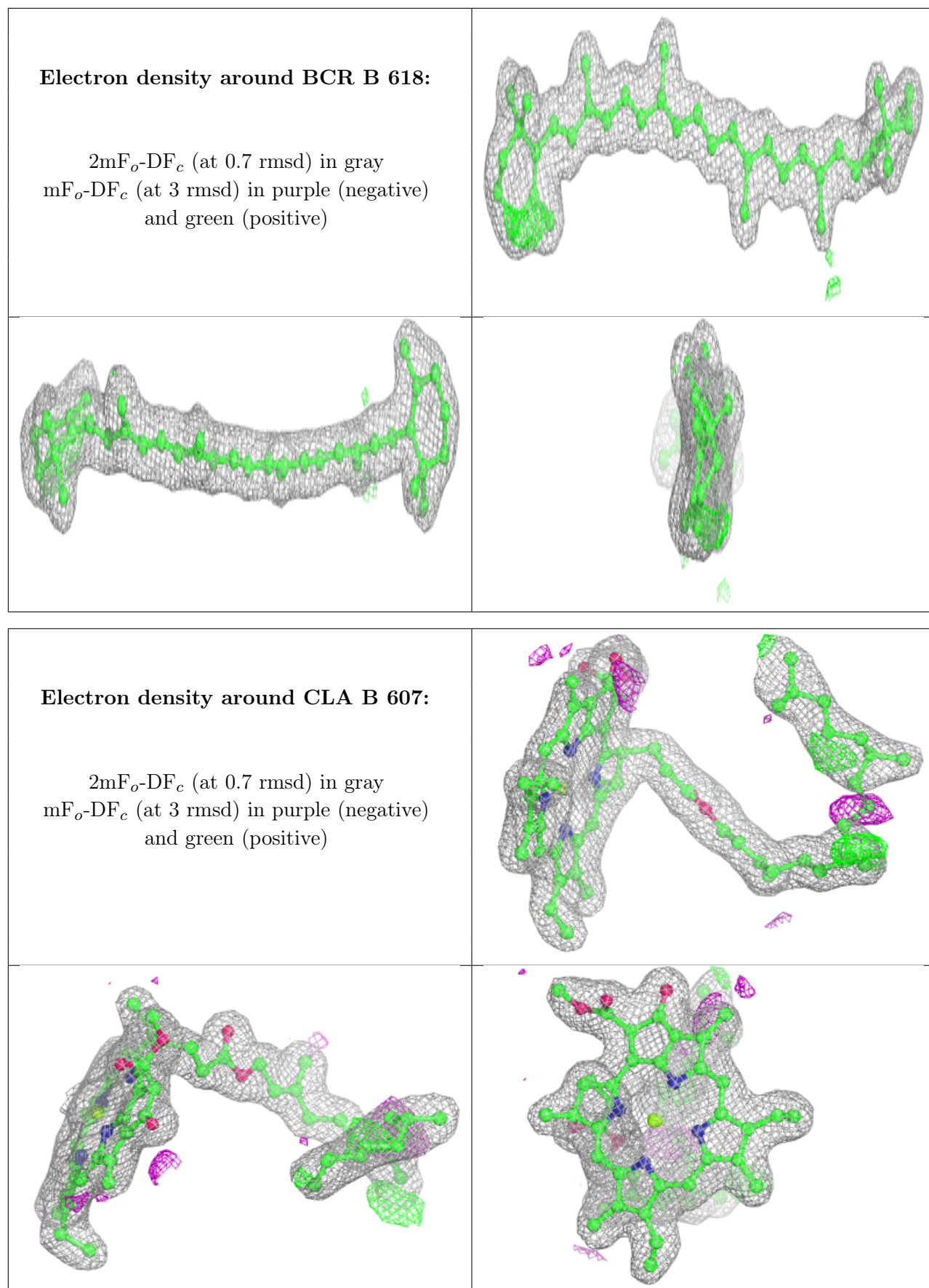
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PHO A 409:**

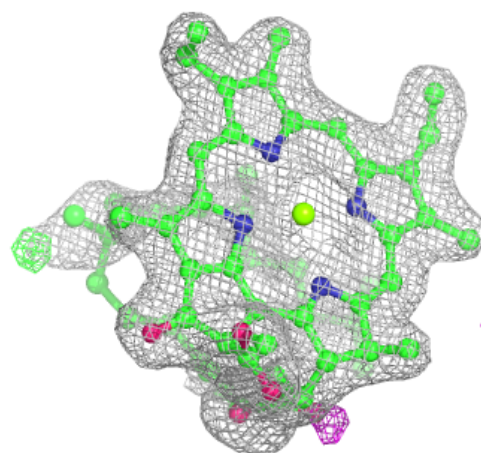
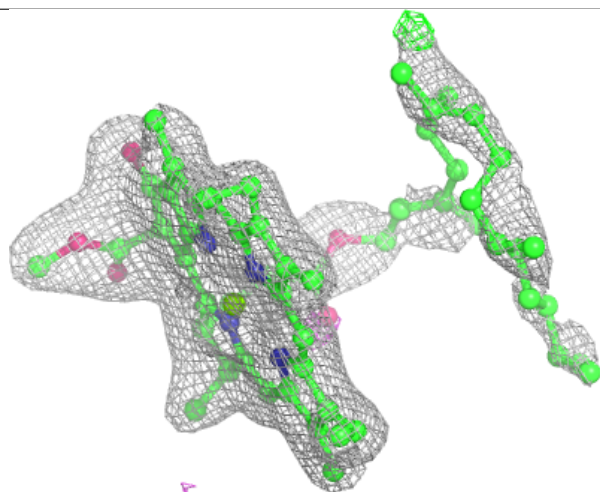
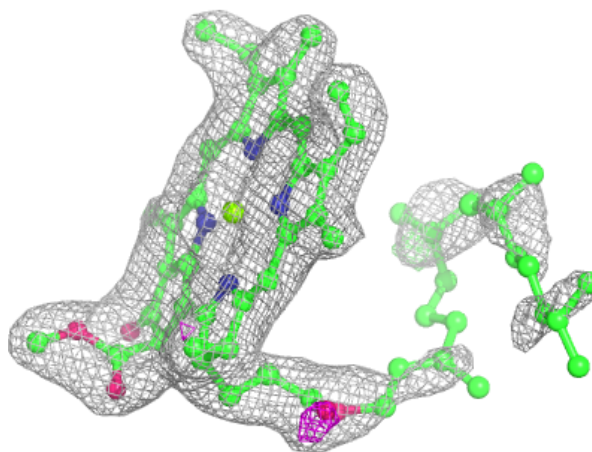
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





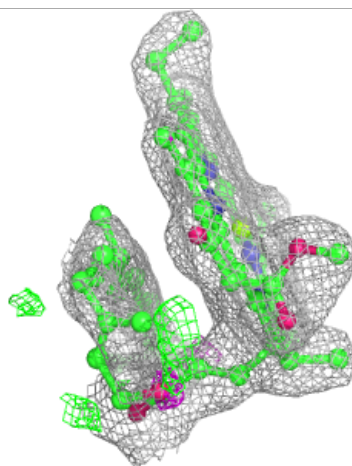
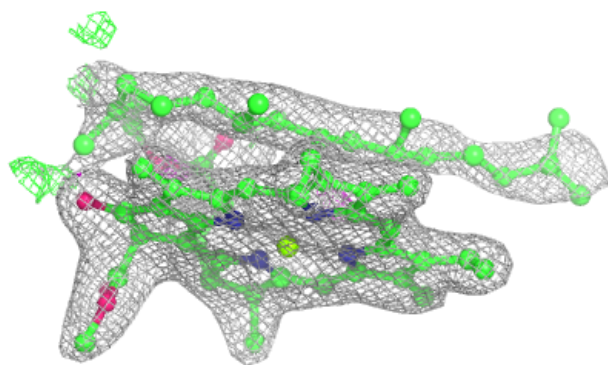
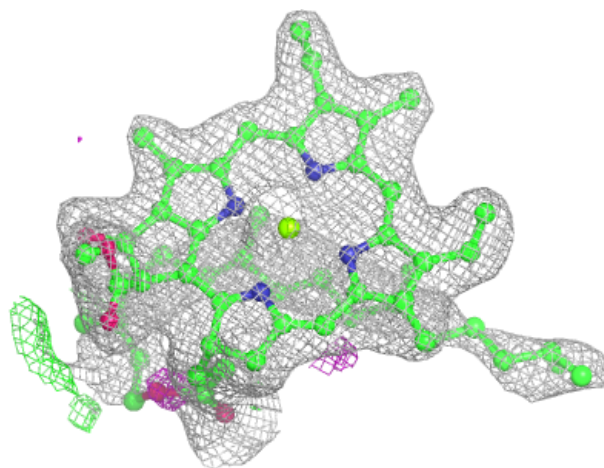
**Electron density around CLA B 602:**

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



**Electron density around CLA b 605:**

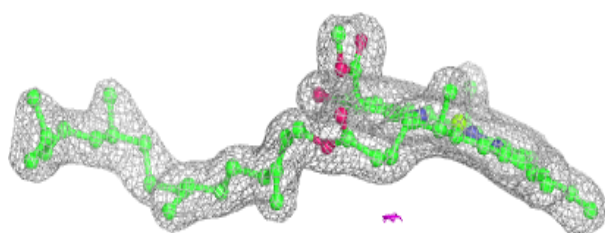
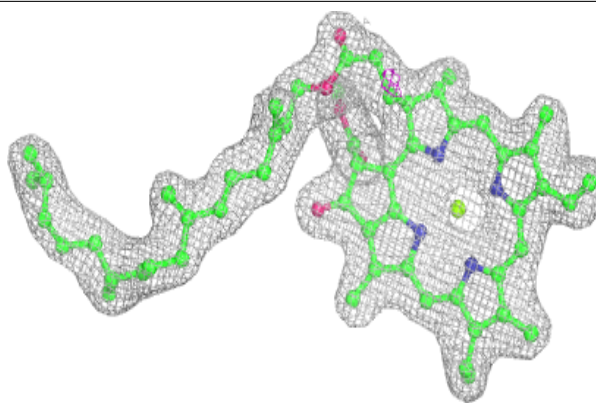
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



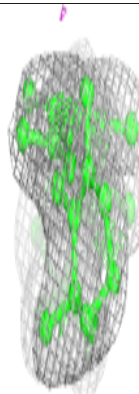
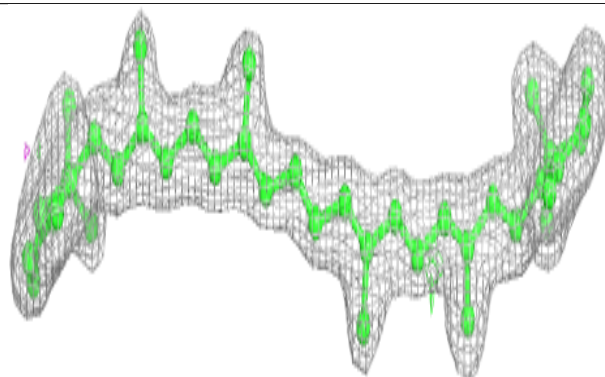
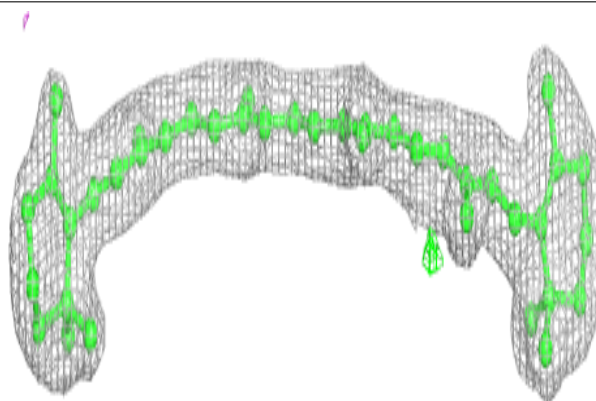


**Electron density around CLA b 606:**

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

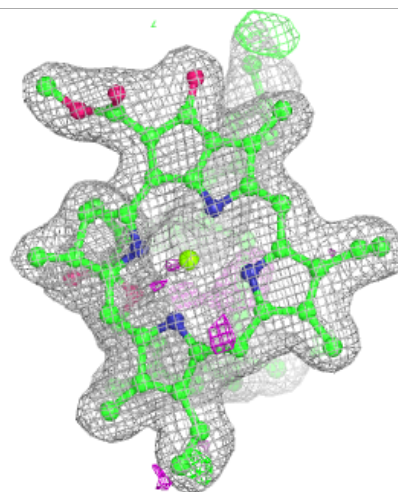
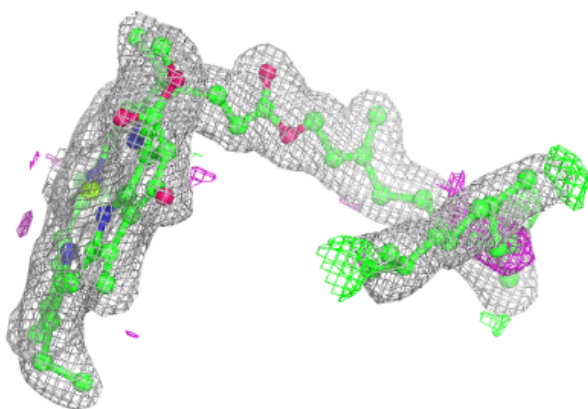
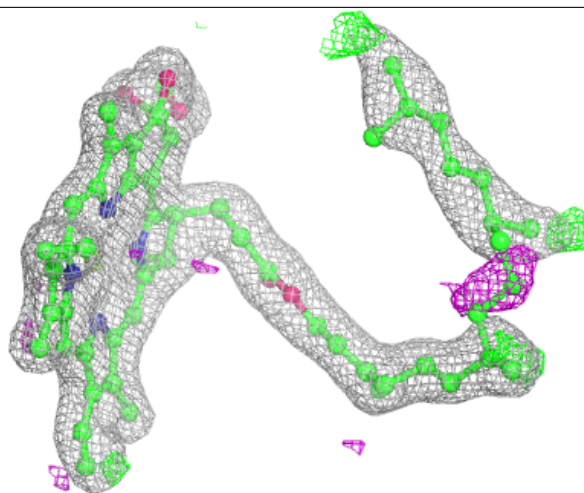
**Electron density around BCR K 101:**

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



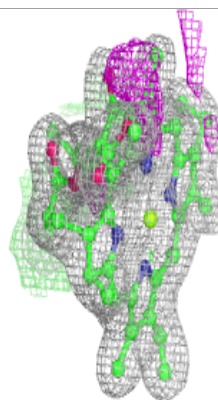
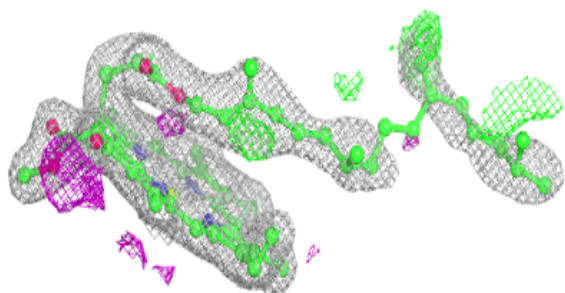
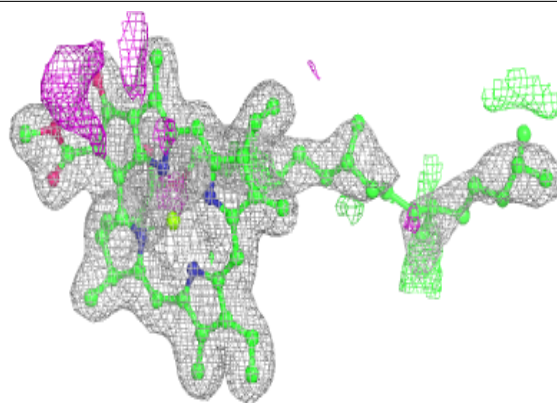
**Electron density around CLA b 610:**

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

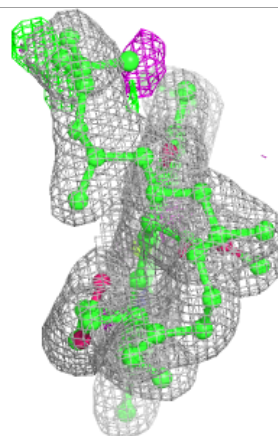
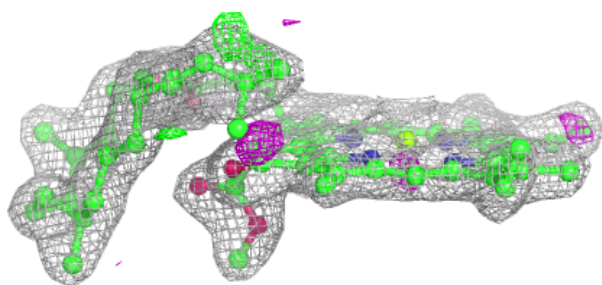
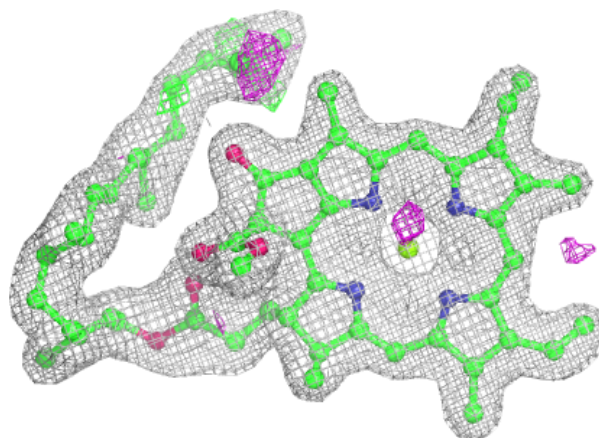


**Electron density around CLA B 615:**

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

**Electron density around CLA b 614:**

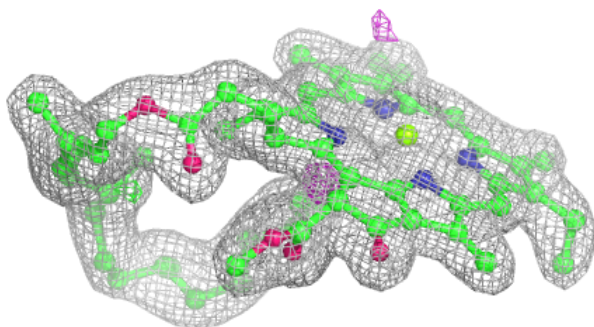
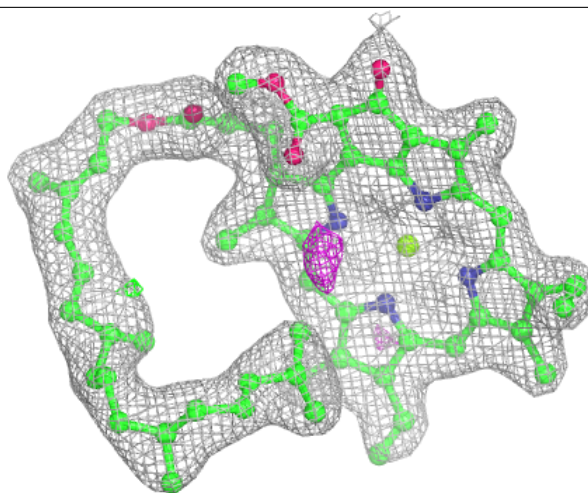
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





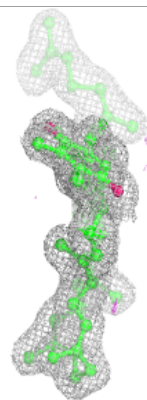
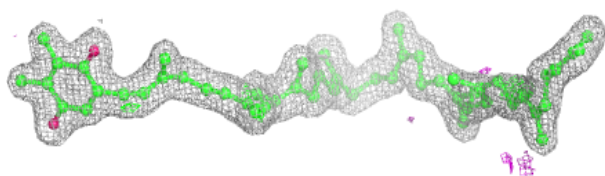
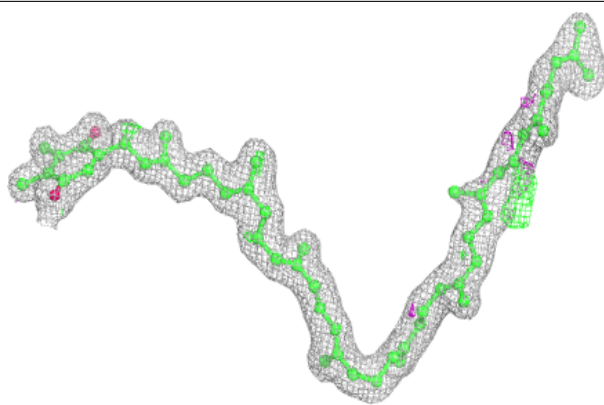
**Electron density around CLA b 619:**

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

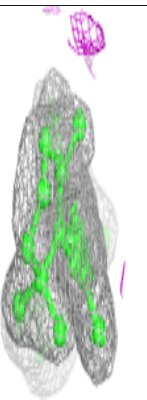
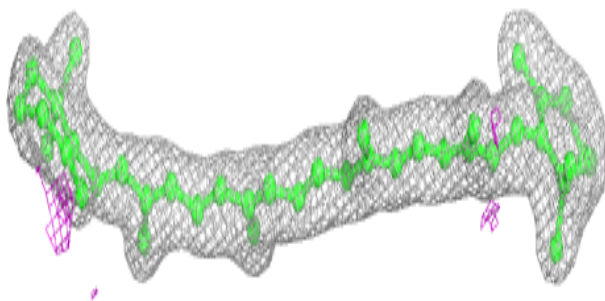
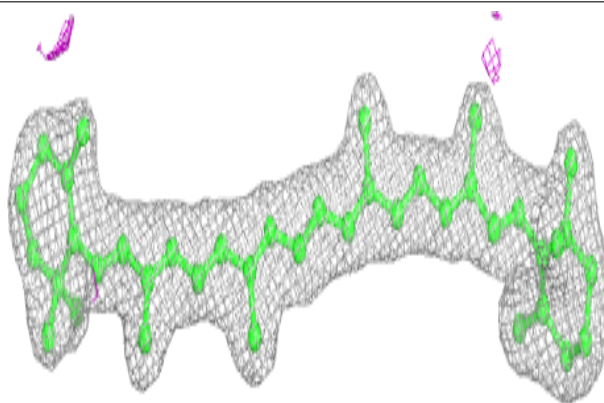


**Electron density around PL9 d 407:**

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

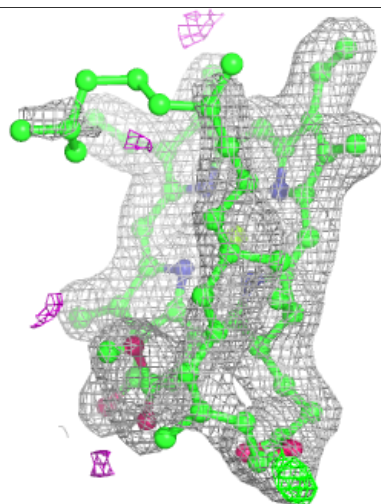
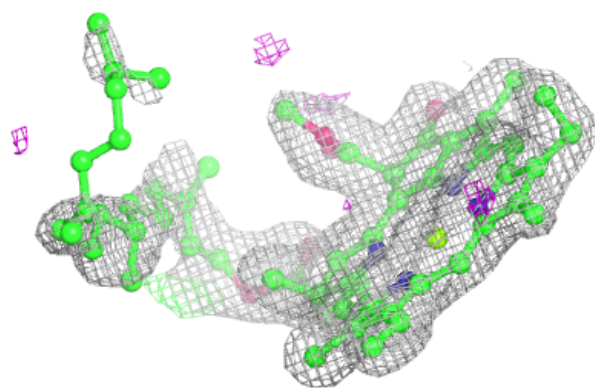
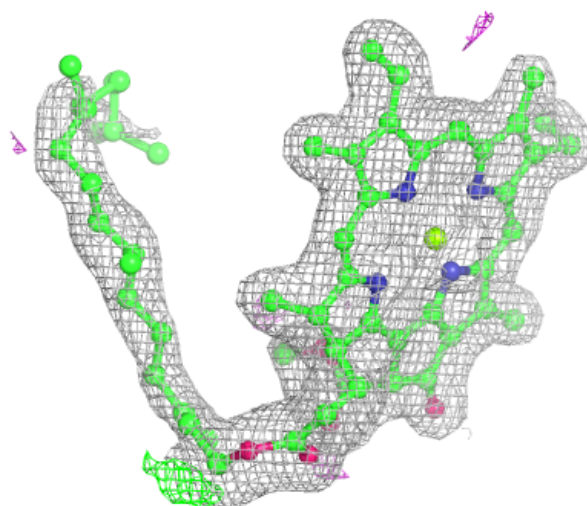
**Electron density around BCR b 623:**

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



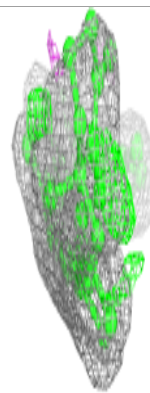
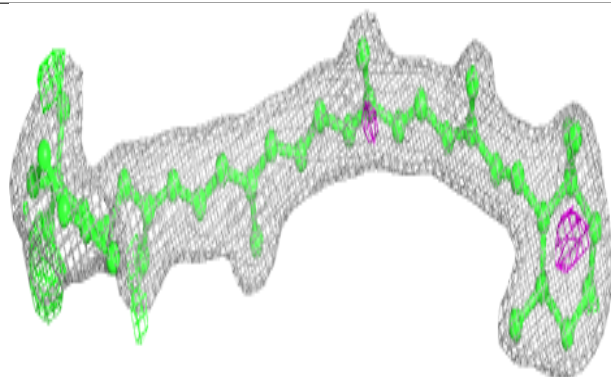
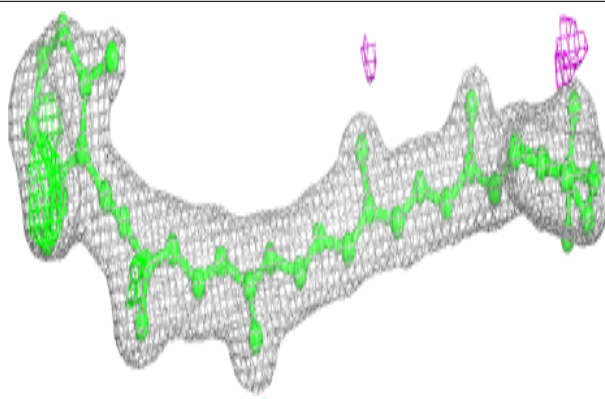
**Electron density around CLA b 620:**

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

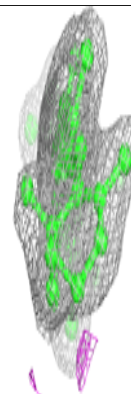
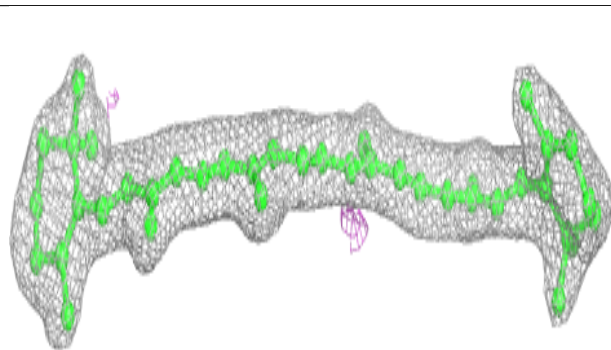
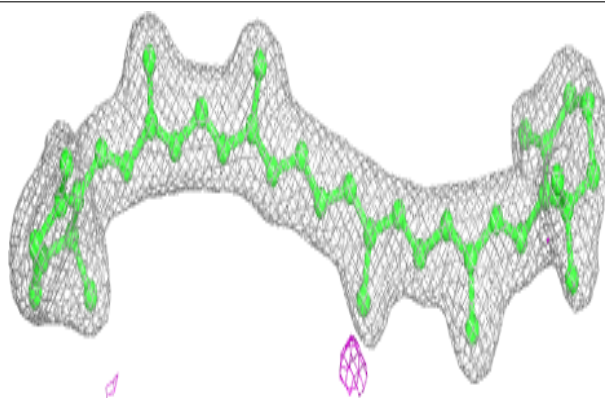


**Electron density around BCR d 406:**

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

**Electron density around BCR k 102:**

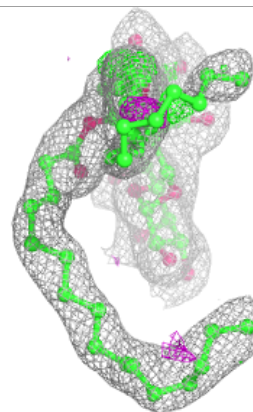
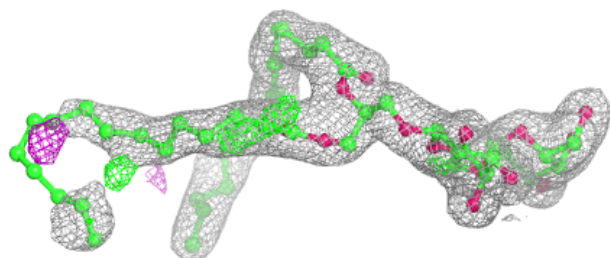
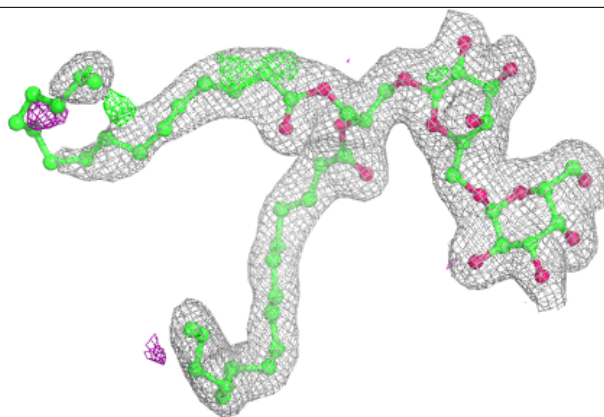
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



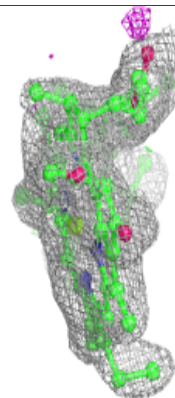
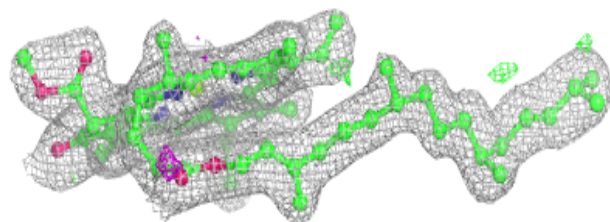
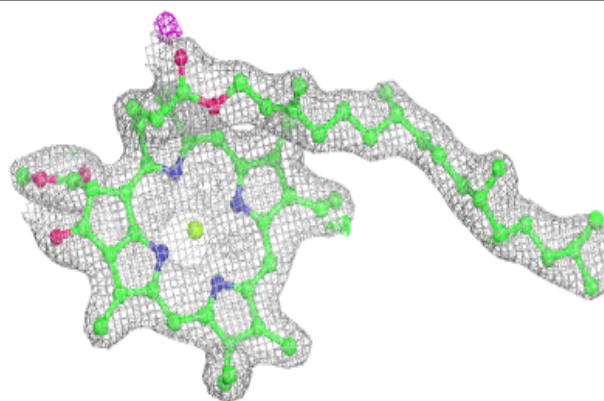


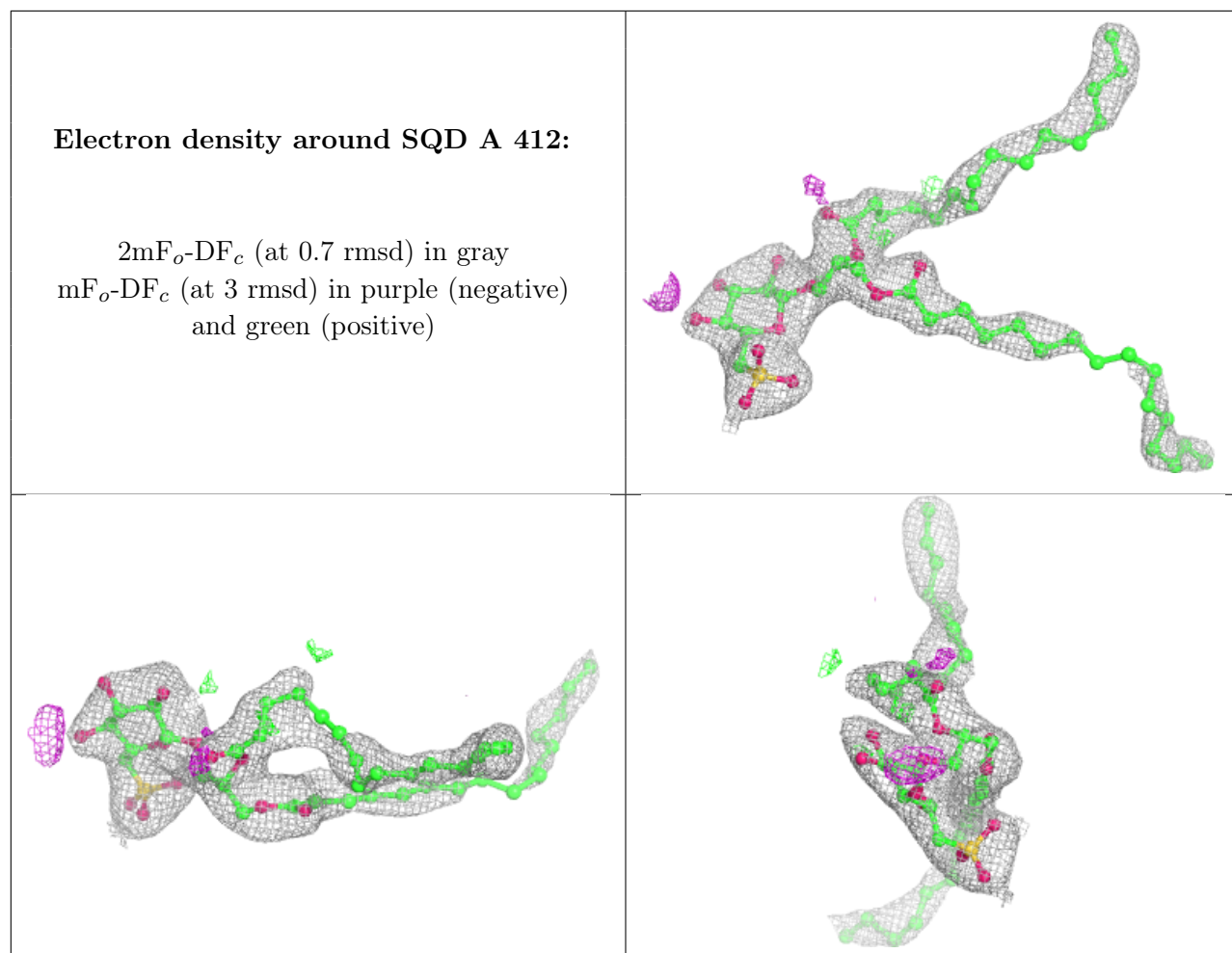
**Electron density around DGD c 918:**

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

**Electron density around CLA c 902:**

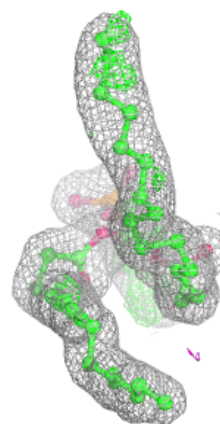
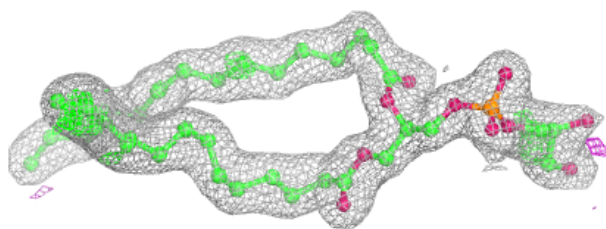
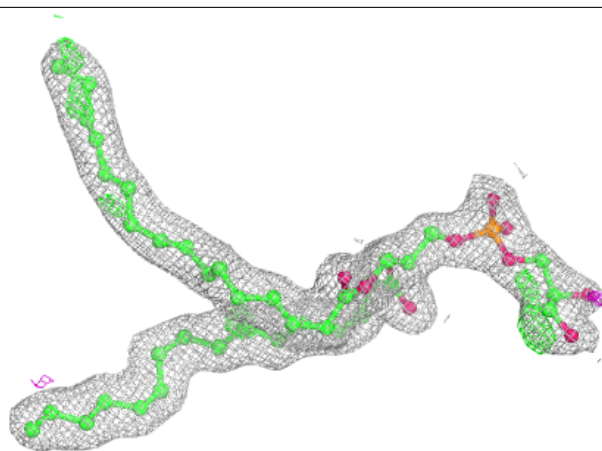
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





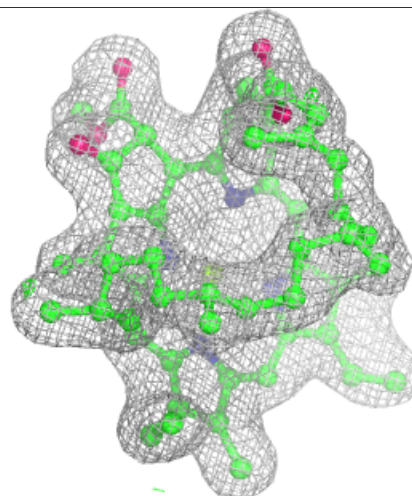
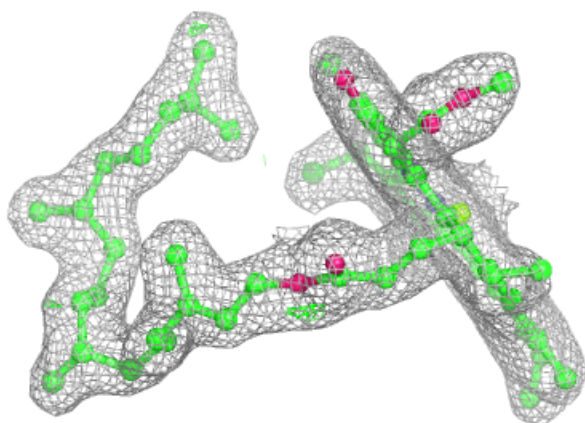
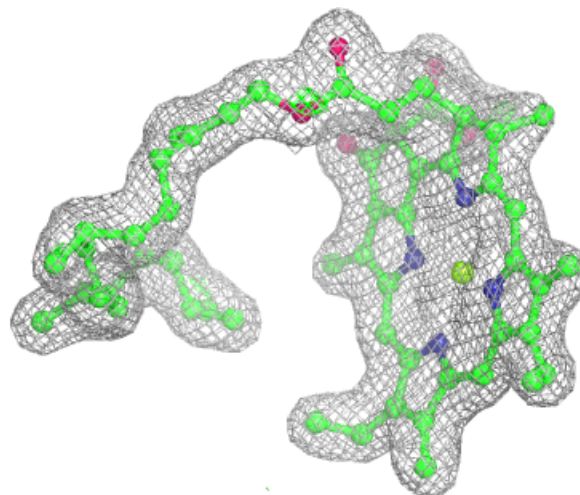
**Electron density around LHG d 410:**

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



**Electron density around CLA C 503:**

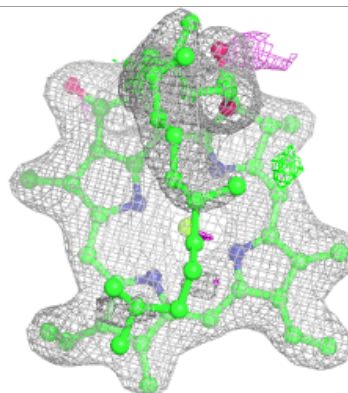
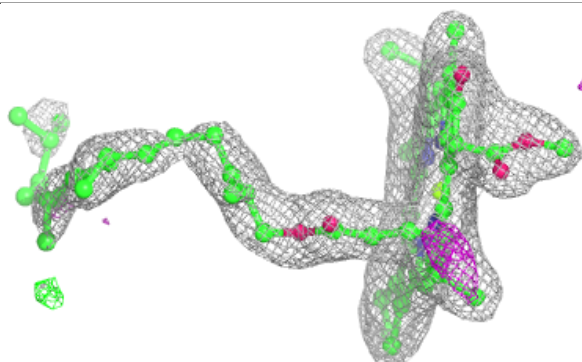
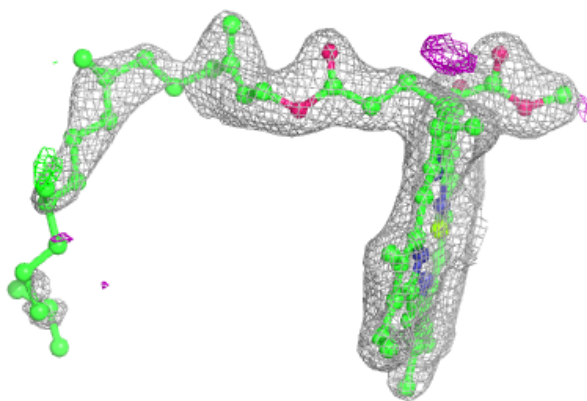
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





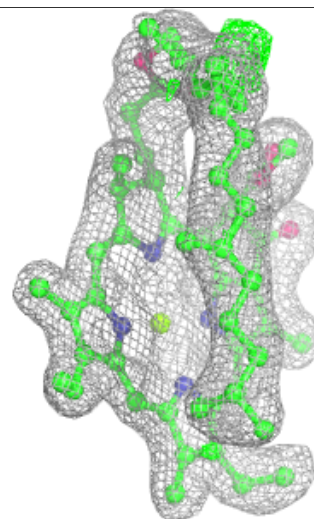
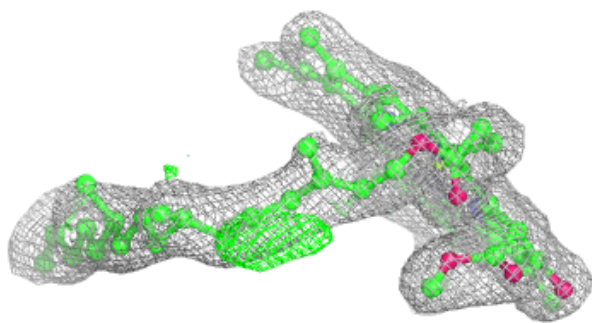
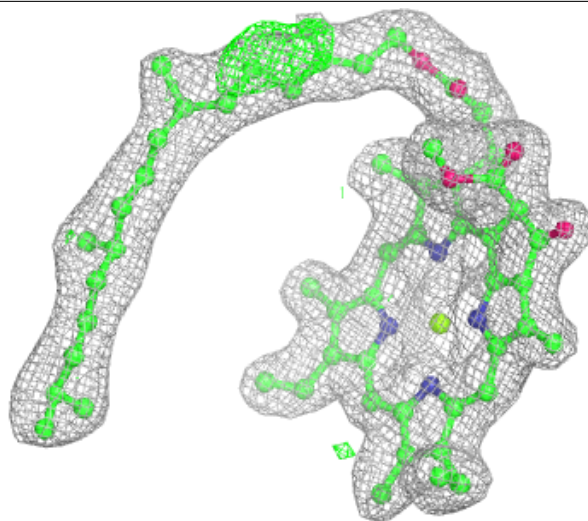
**Electron density around CLA C 506:**

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



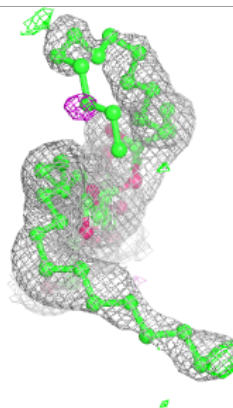
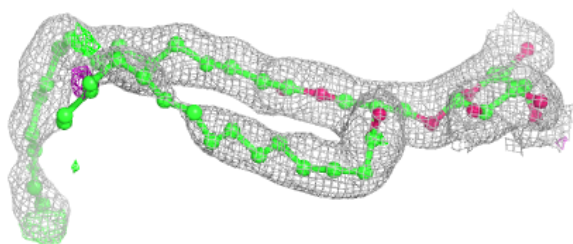
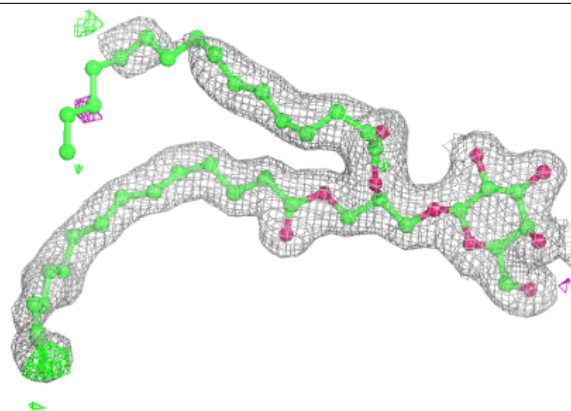
**Electron density around CLA c 908:**

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

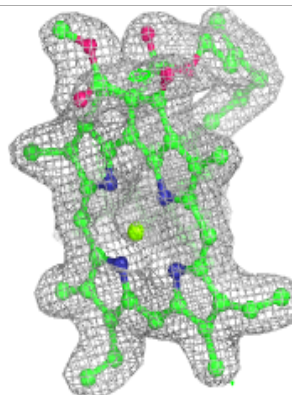
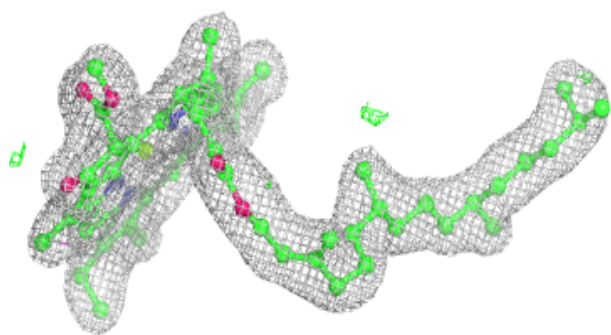
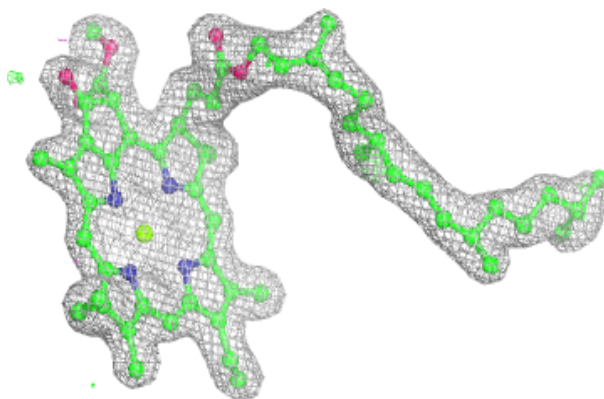


**Electron density around LMG D 409:**

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

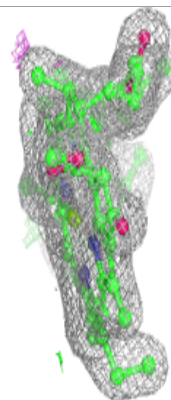
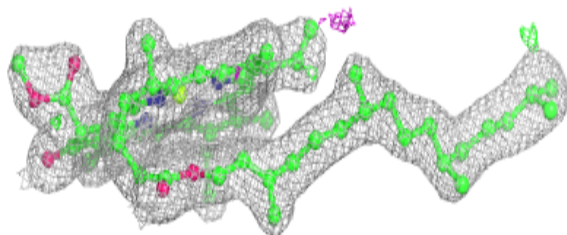
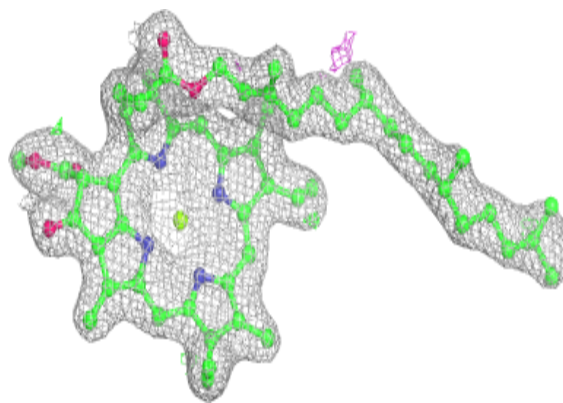
**Electron density around CLA c 912:**

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

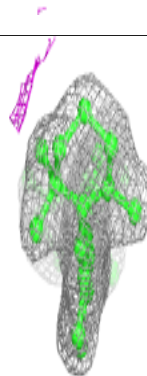
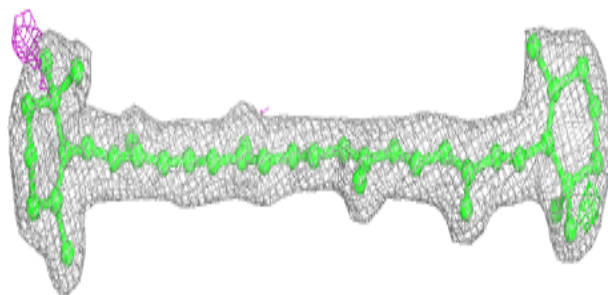
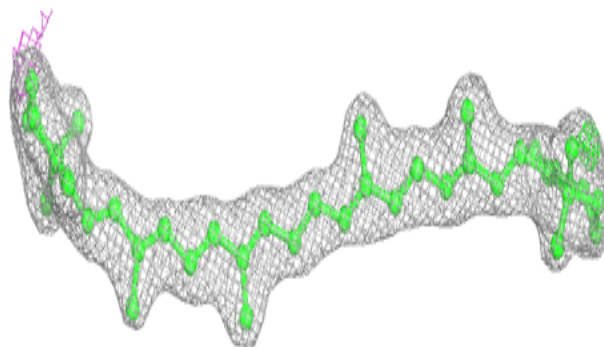


**Electron density around CLA C 501:**

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

**Electron density around BCR c 916:**

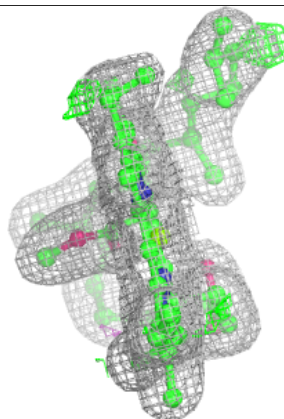
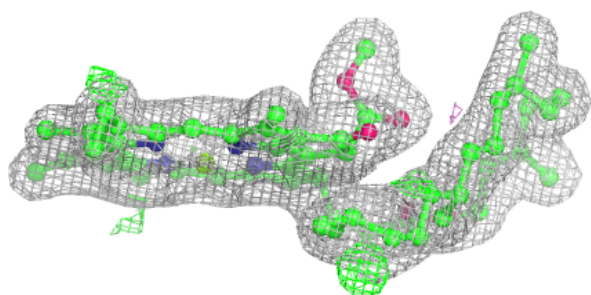
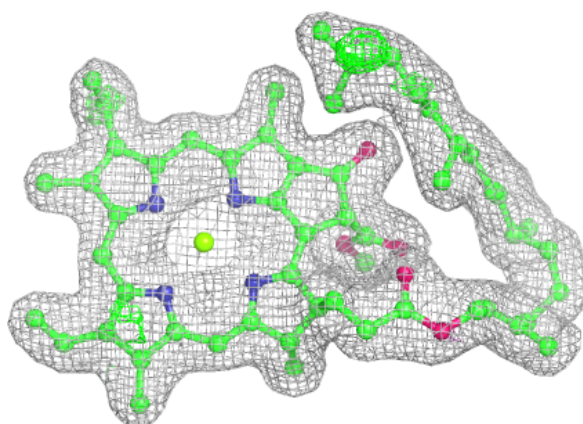
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



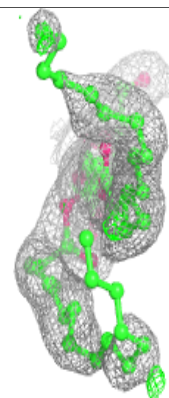
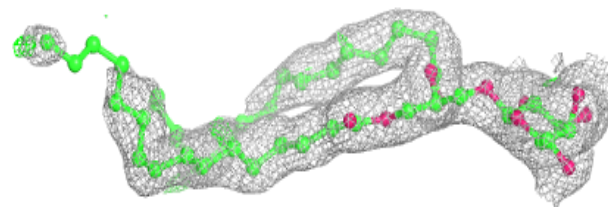
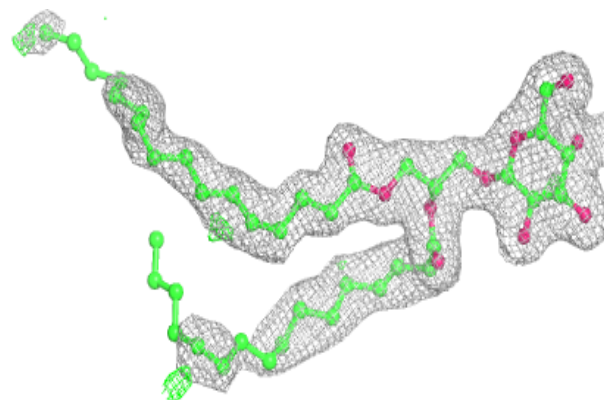


**Electron density around CLA B 611:**

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

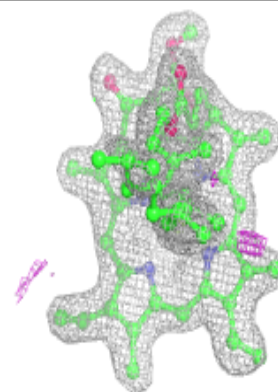
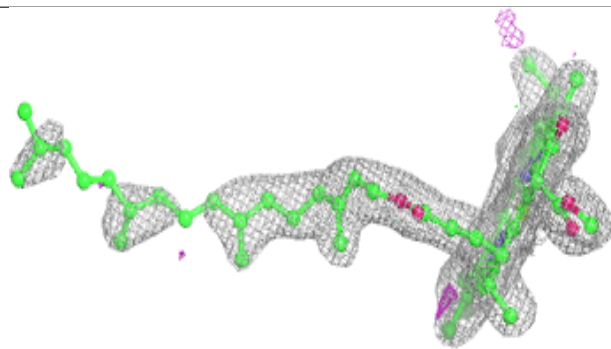
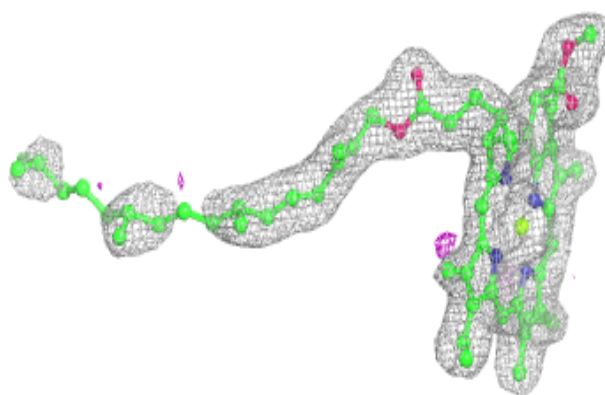
**Electron density around LMG d 412:**

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

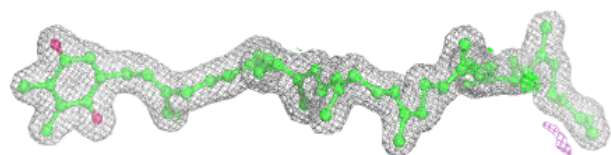
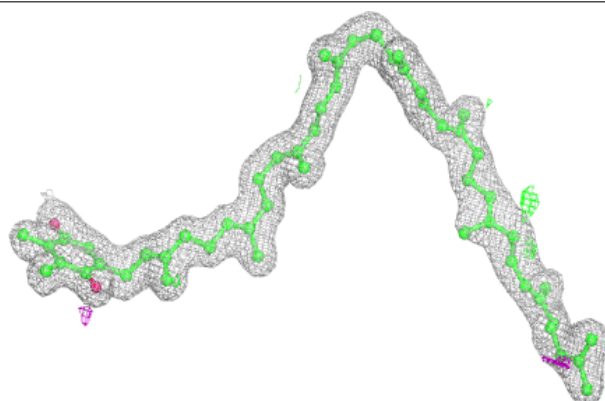


**Electron density around CLA d 405:**

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

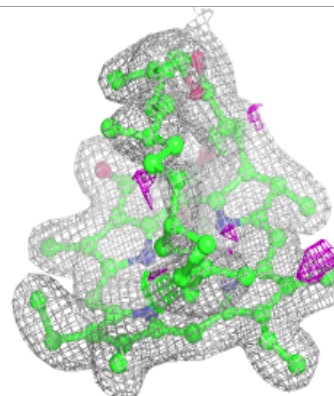
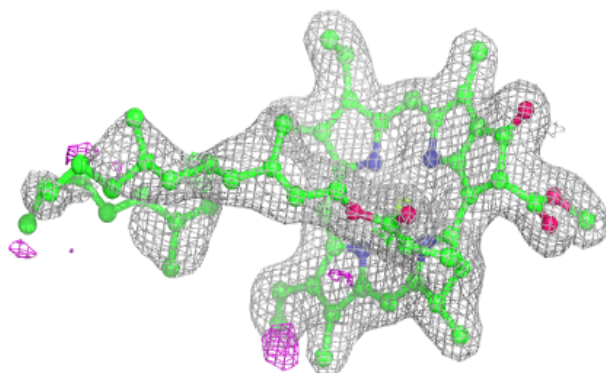
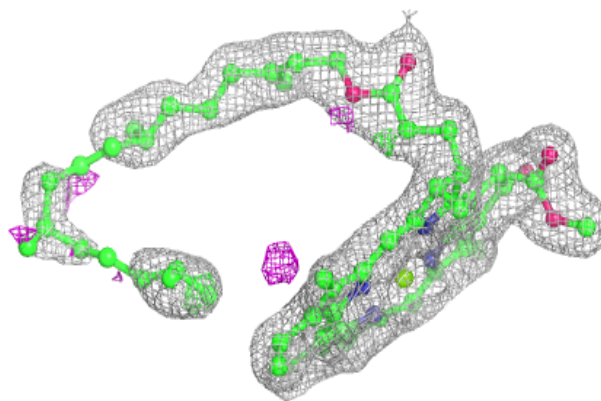
**Electron density around PL9 D 404:**

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



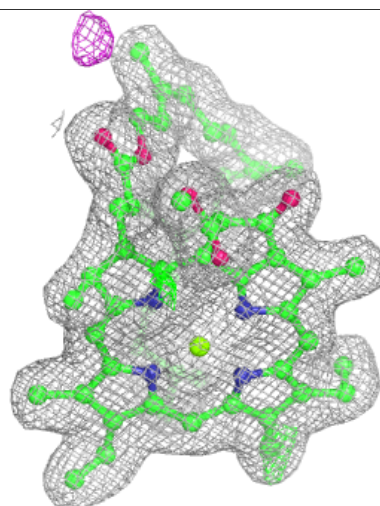
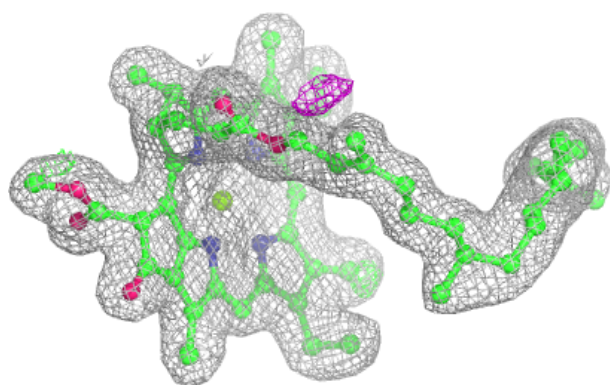
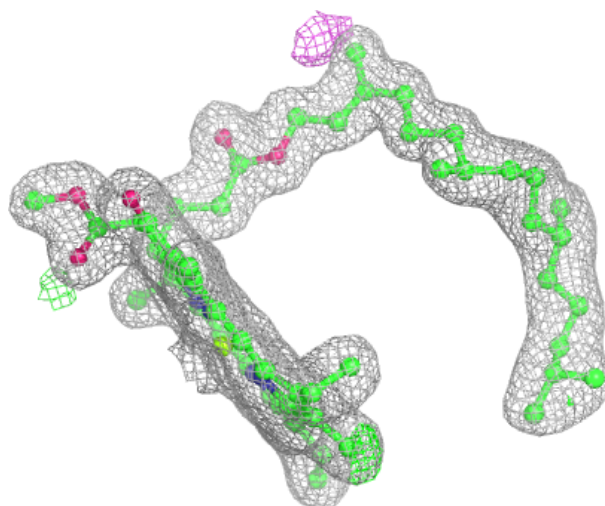
**Electron density around CLA C 504:**

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



**Electron density around CLA B 612:**

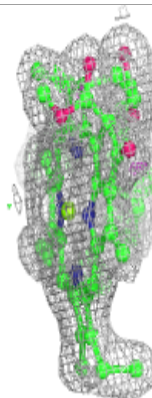
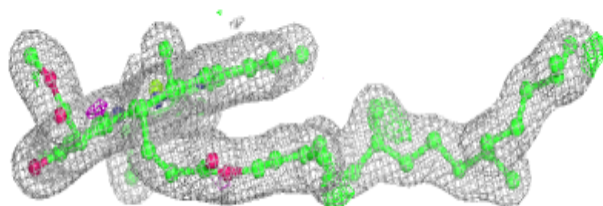
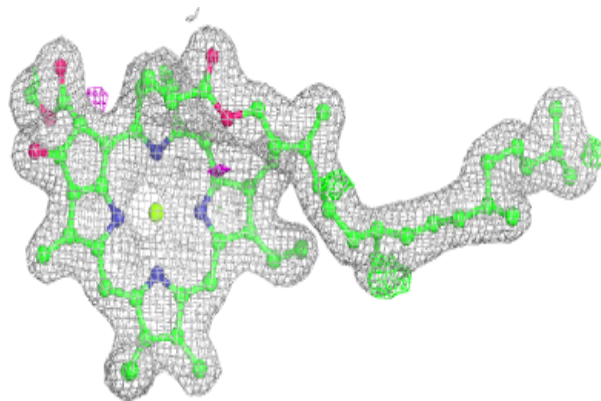
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



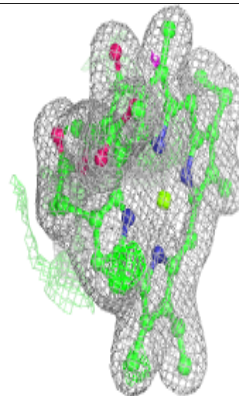
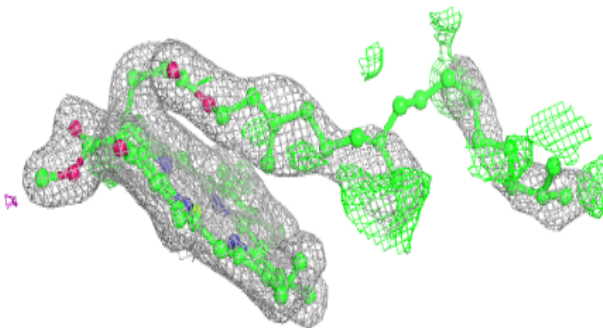
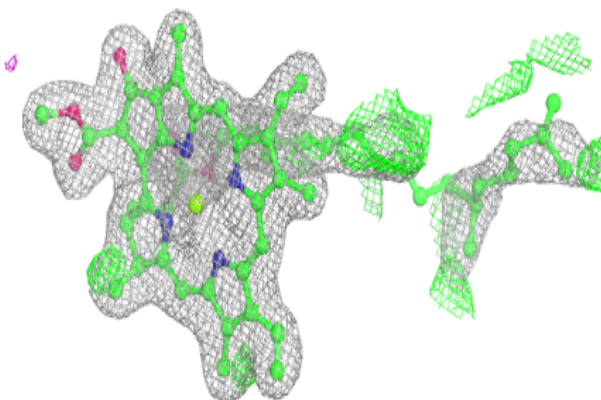


**Electron density around CLA B 604:**

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

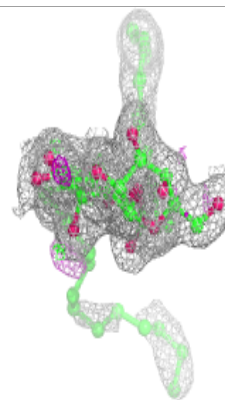
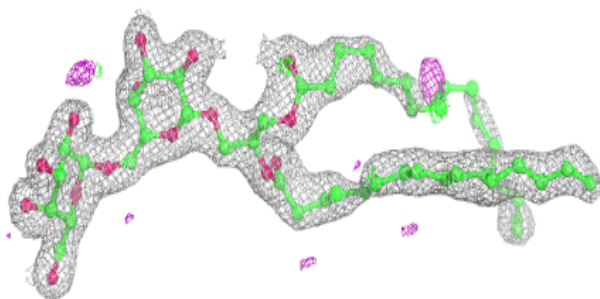
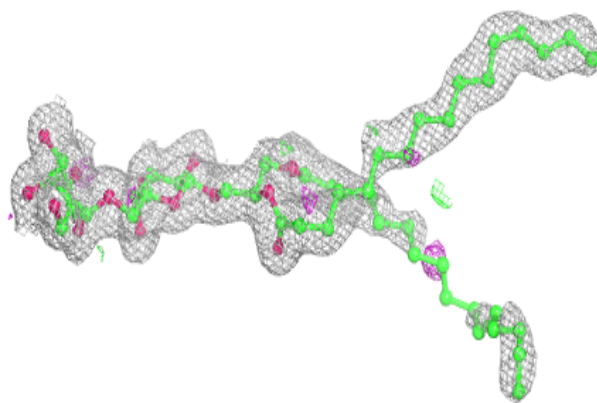
**Electron density around CLA b 618:**

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

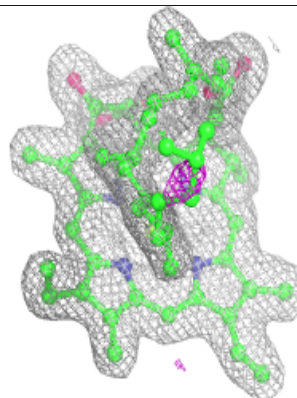
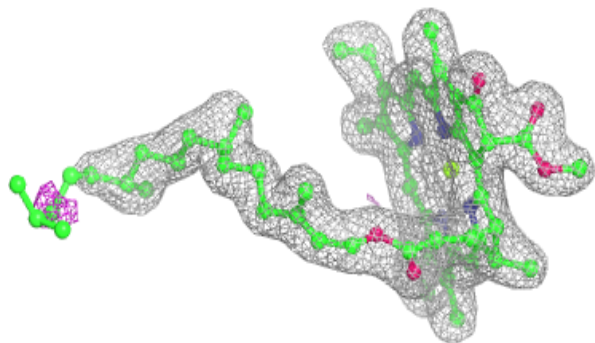
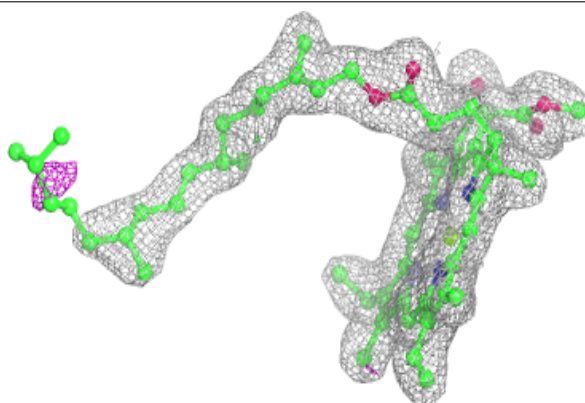


**Electron density around DGD c 917:**

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

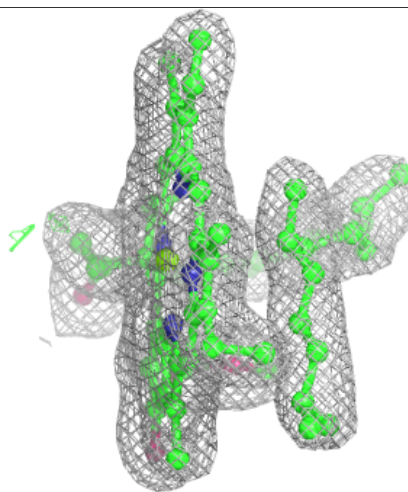
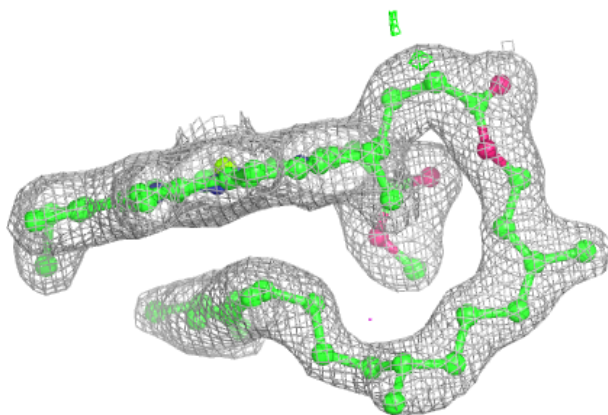
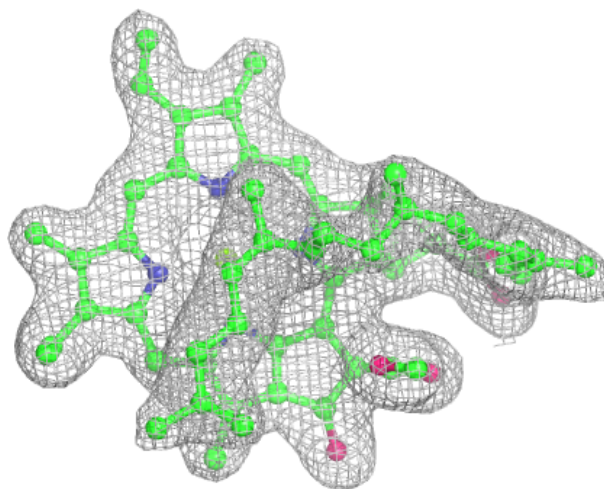
**Electron density around CLA C 508:**

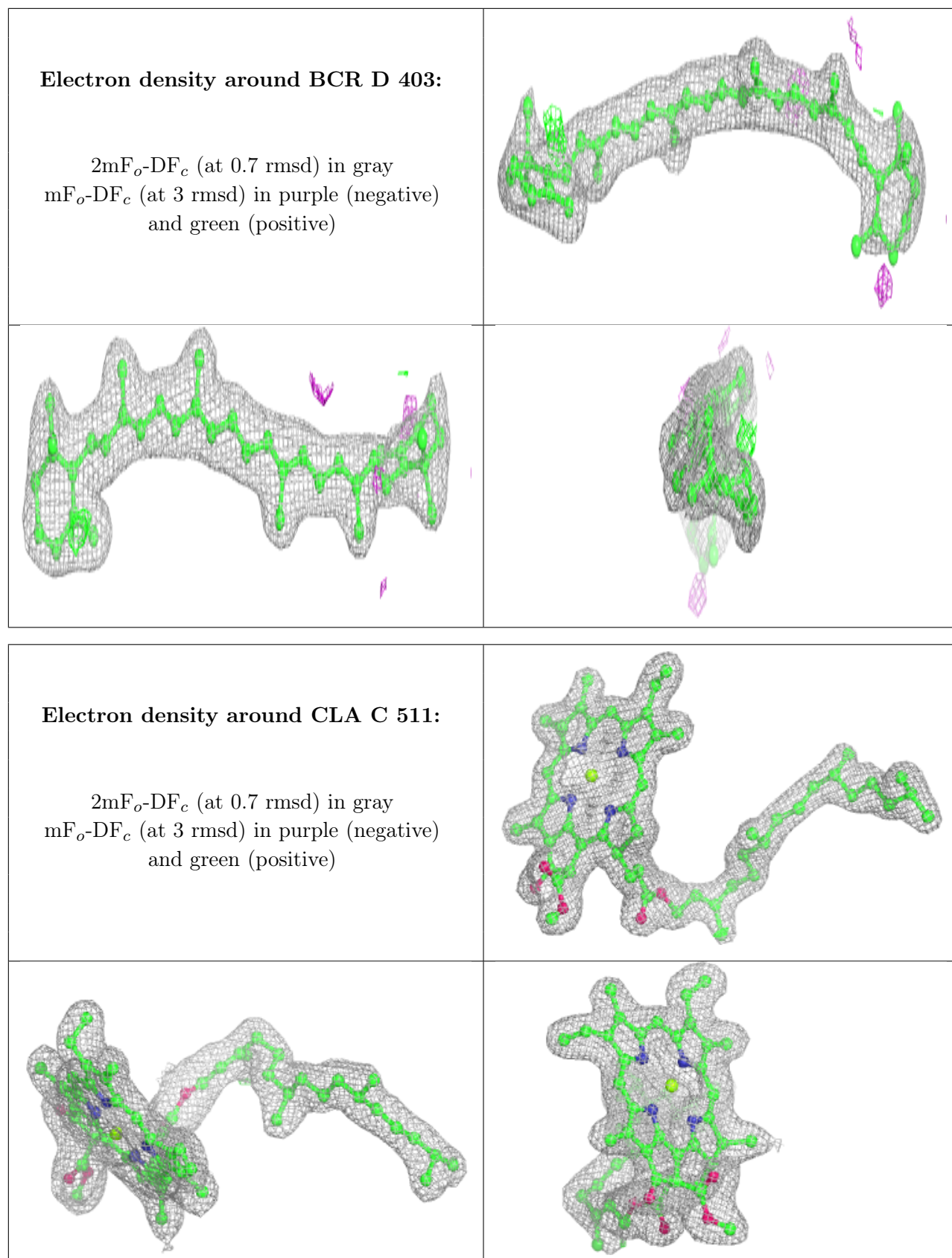
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA C 510:**

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

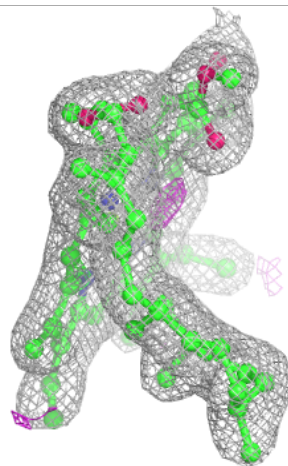
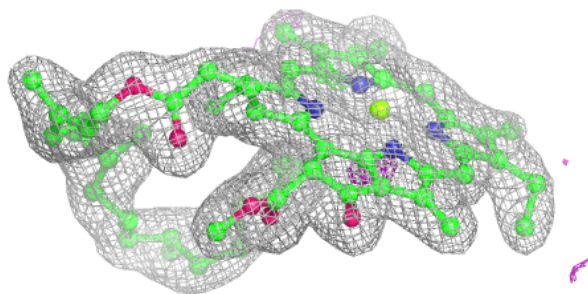
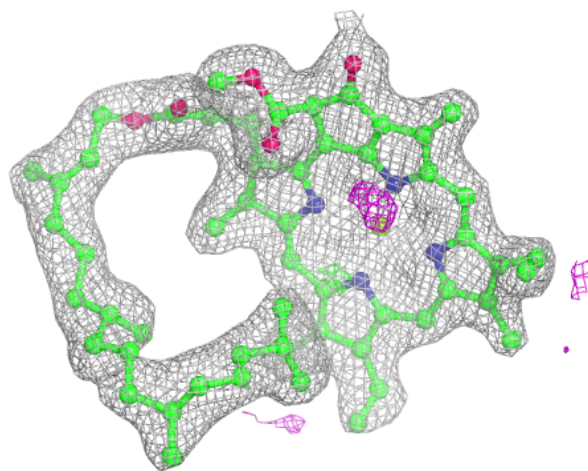






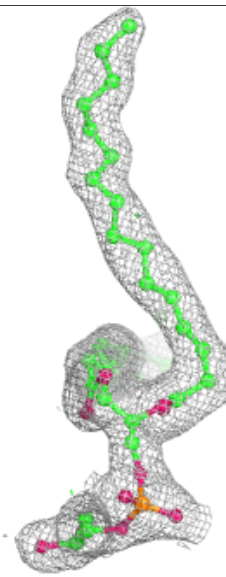
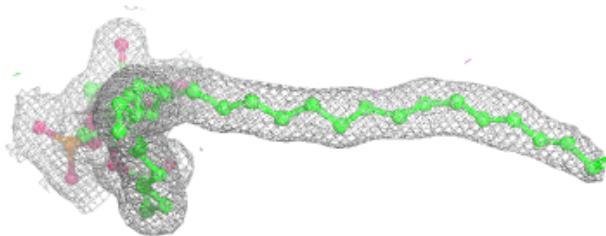
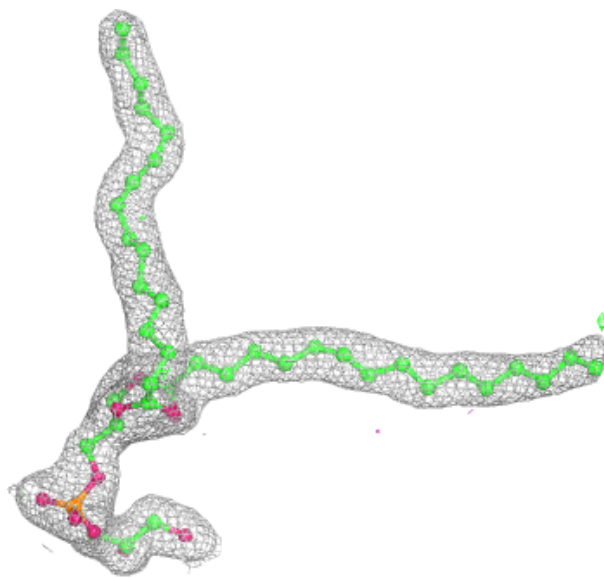
**Electron density around CLA B 616:**

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



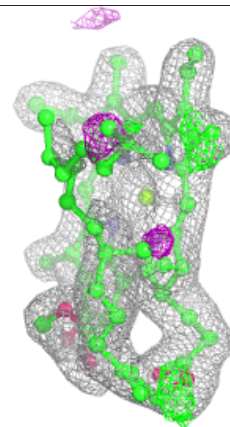
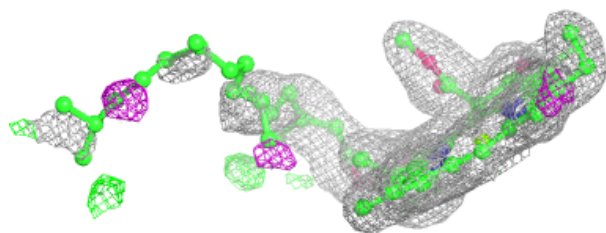
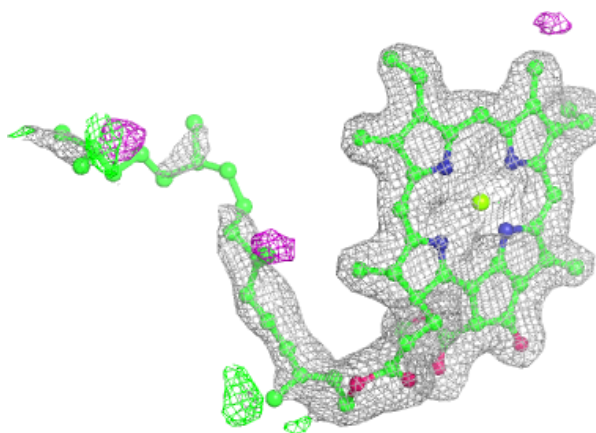
**Electron density around LHG L 101:**

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

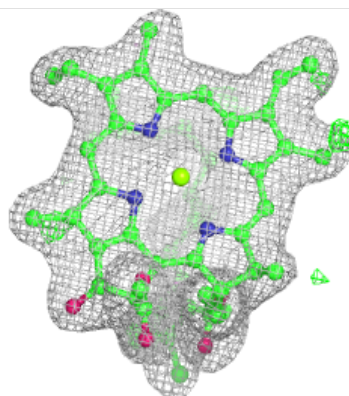
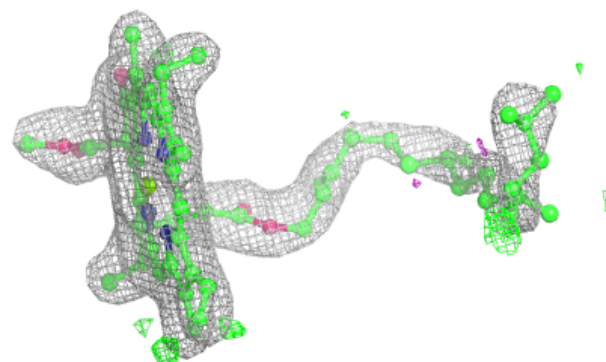
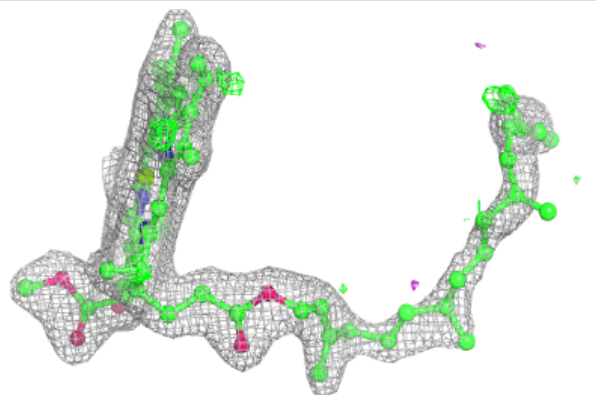


**Electron density around CLA B 617:**

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

**Electron density around CLA c 907:**

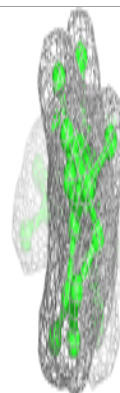
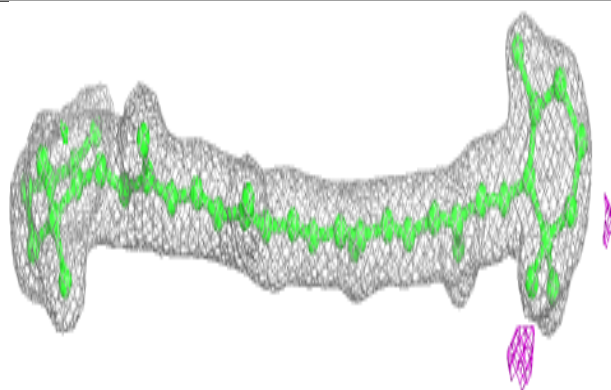
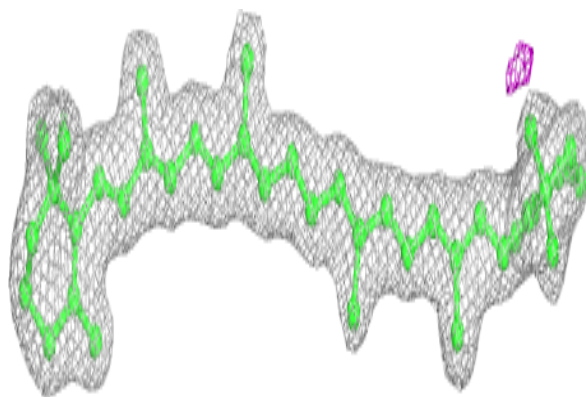
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



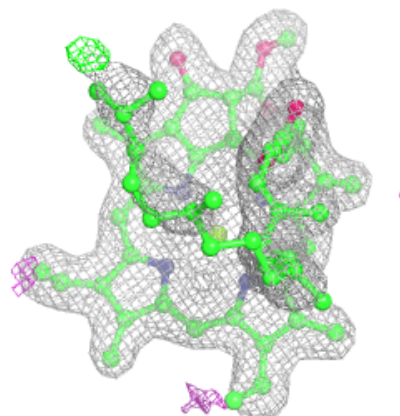
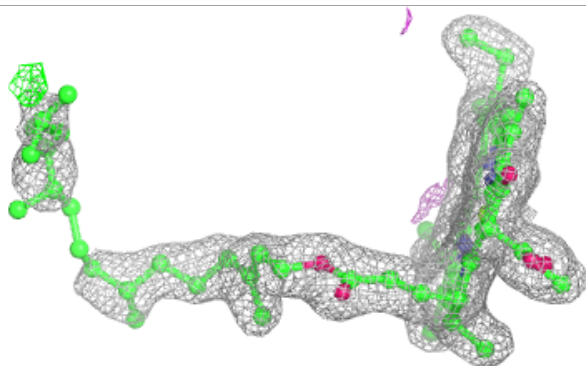
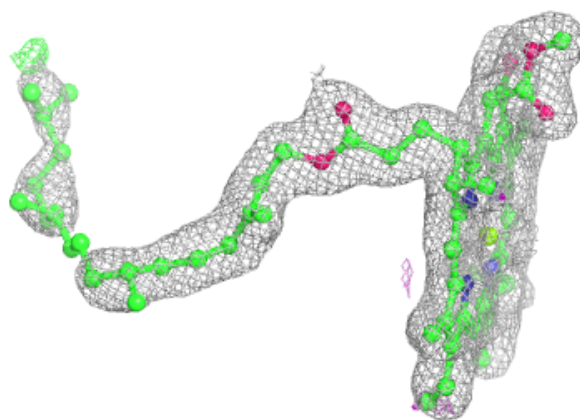


**Electron density around BCR b 621:**

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

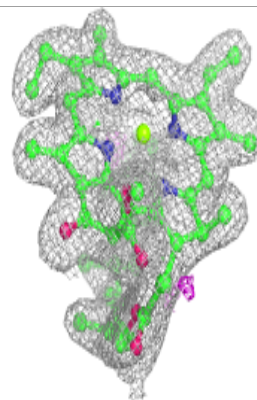
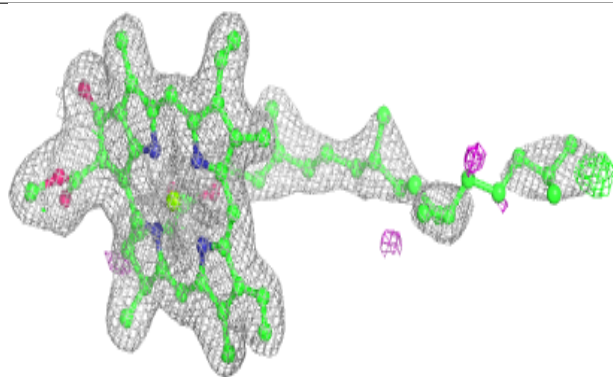
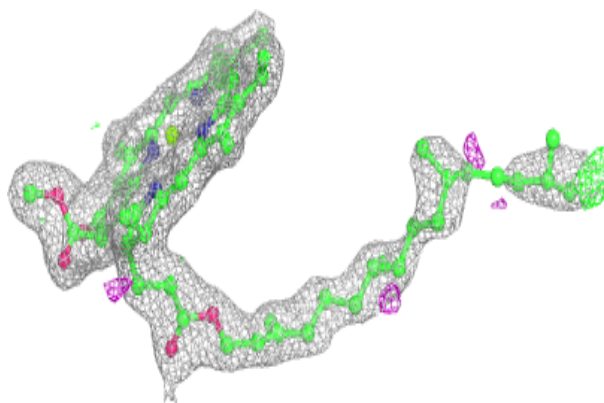
**Electron density around CLA D 402:**

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

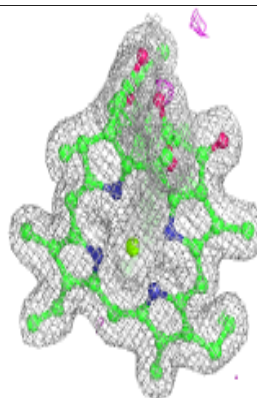
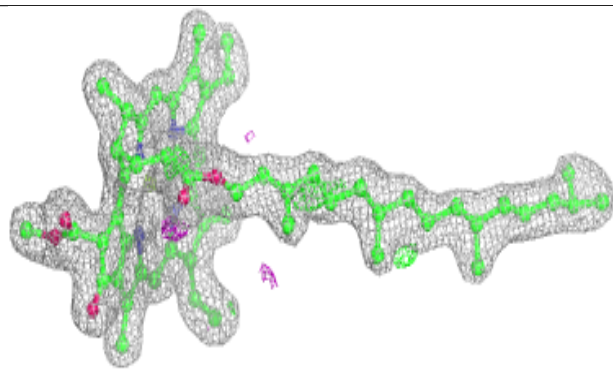
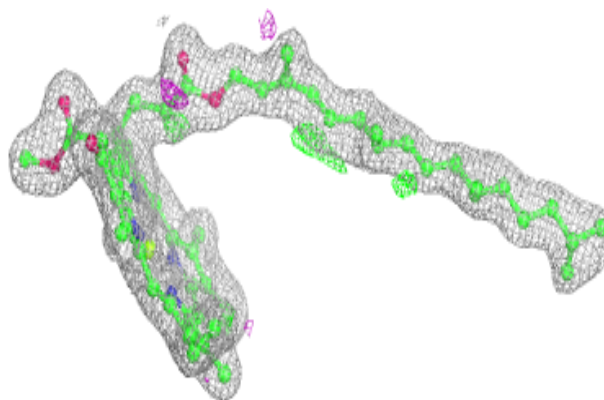


**Electron density around CLA c 905:**

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

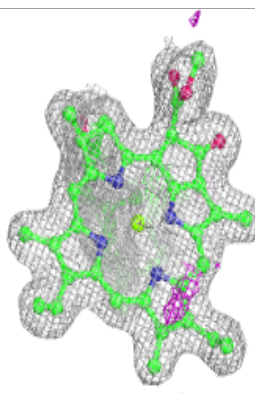
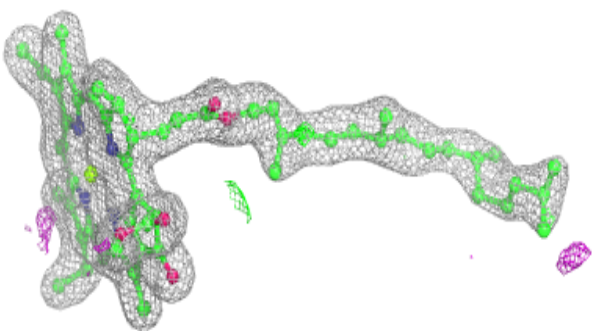
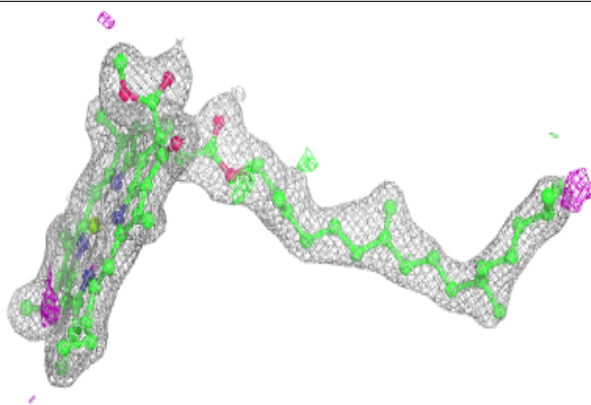
**Electron density around CLA b 611:**

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

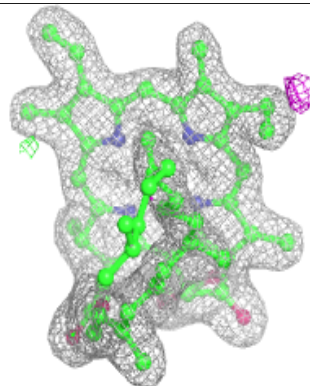
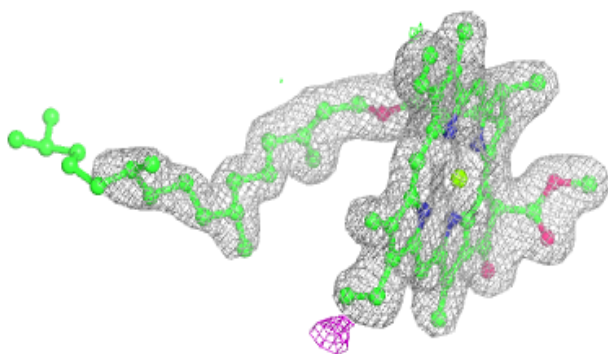
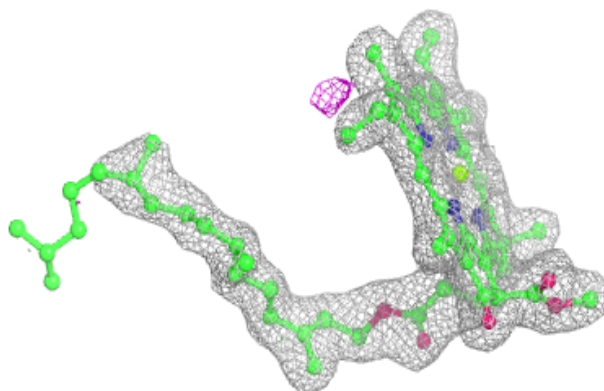


**Electron density around CLA B 605:**

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

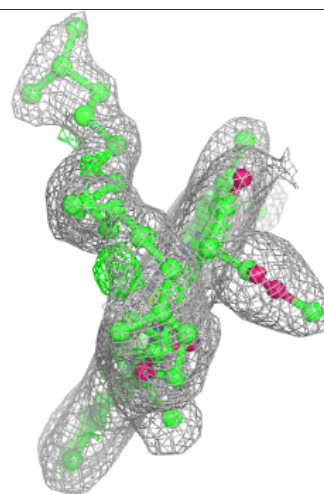
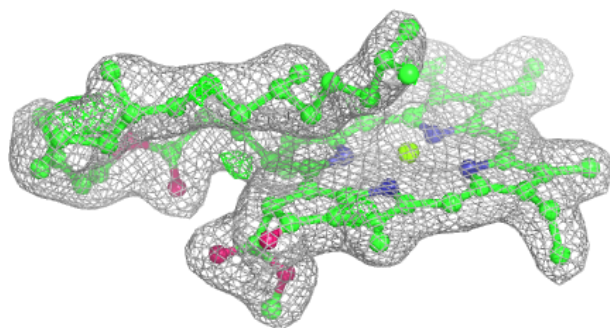
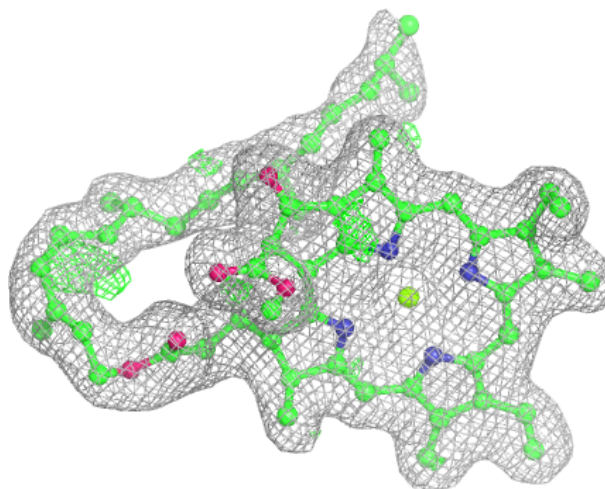
**Electron density around CLA c 909:**

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



**Electron density around CLA c 910:**

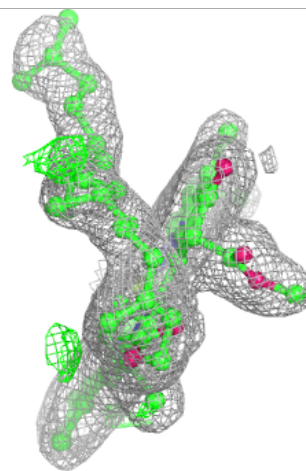
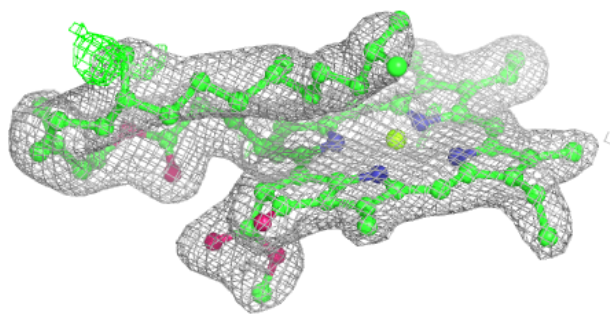
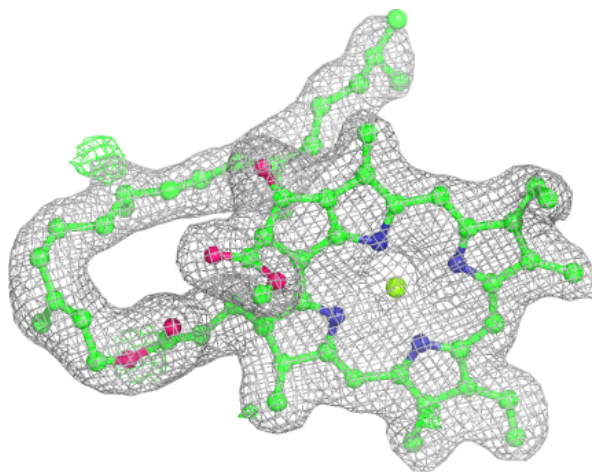
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





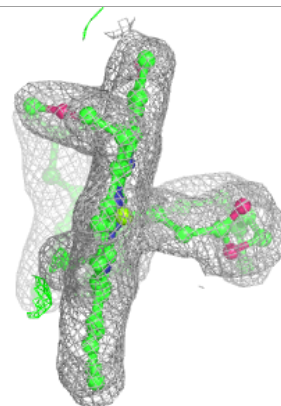
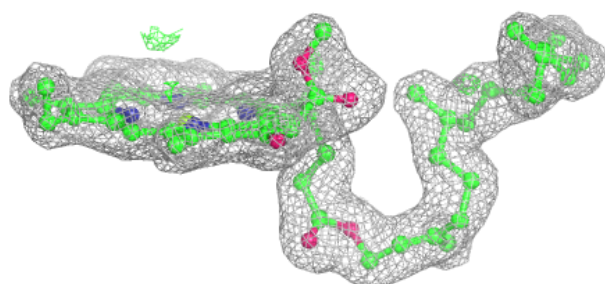
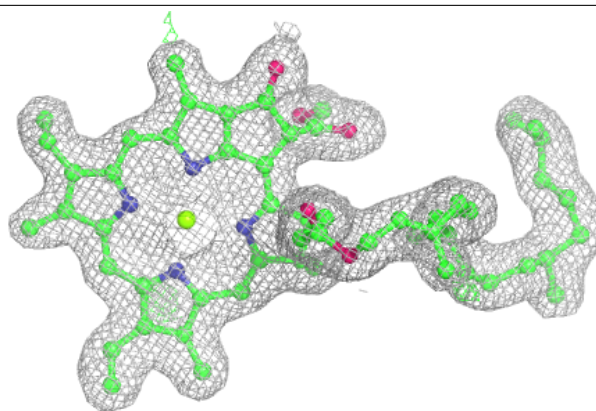
**Electron density around CLA C 509:**

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

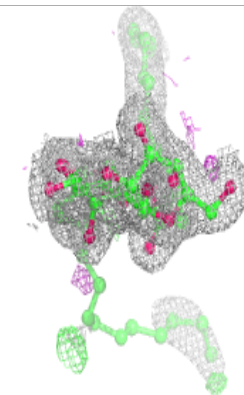
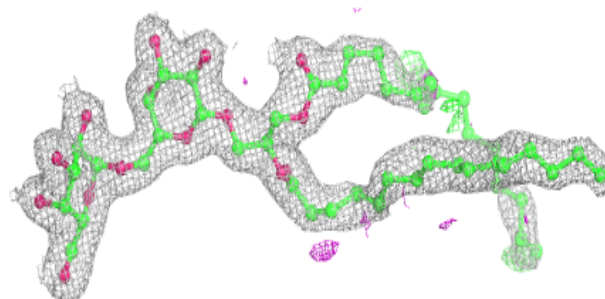
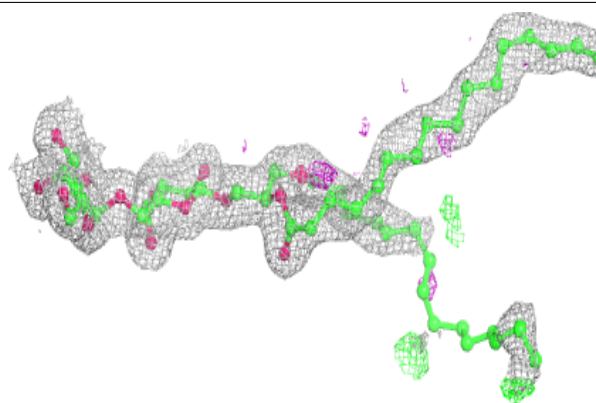


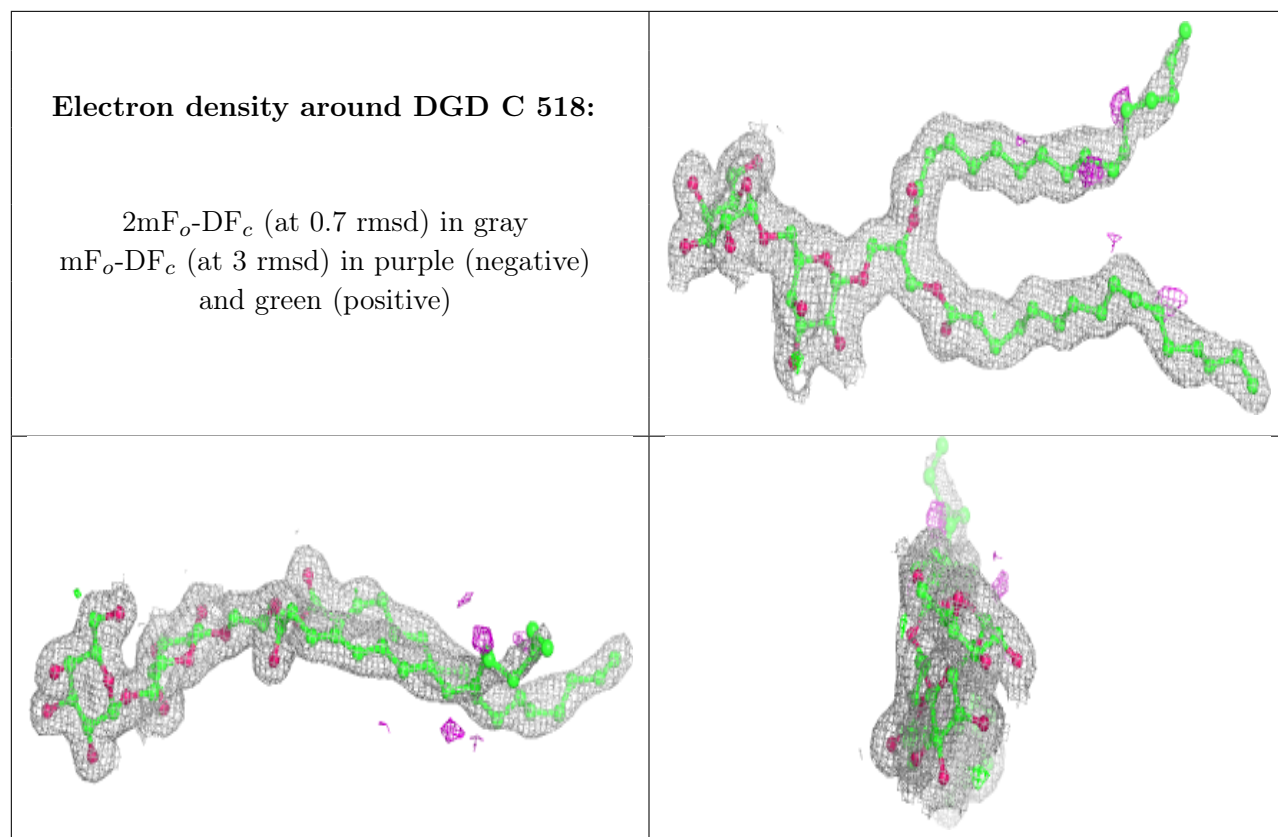
**Electron density around CLA b 616:**

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

**Electron density around DGD C 516:**

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

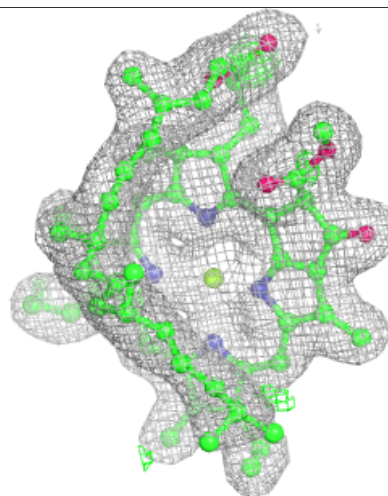
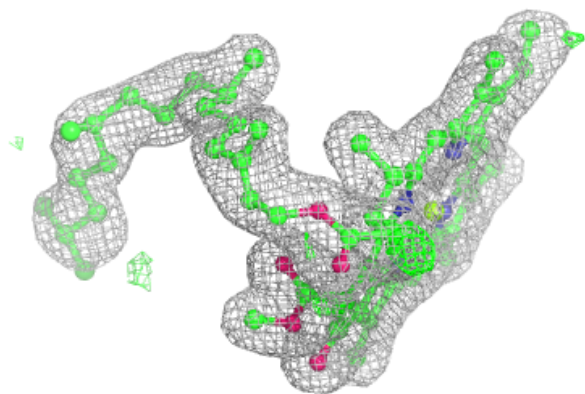
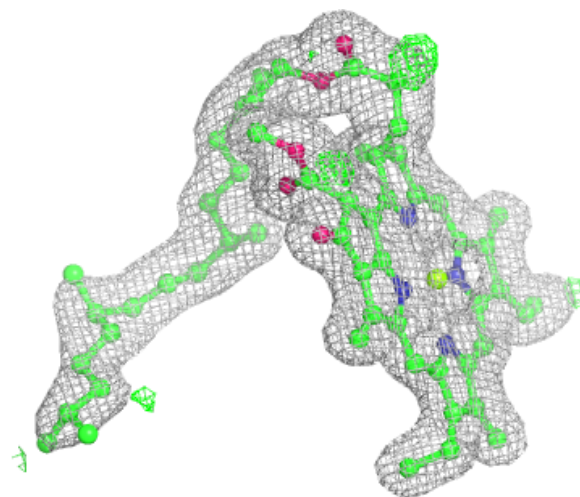






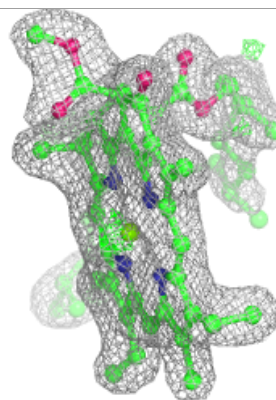
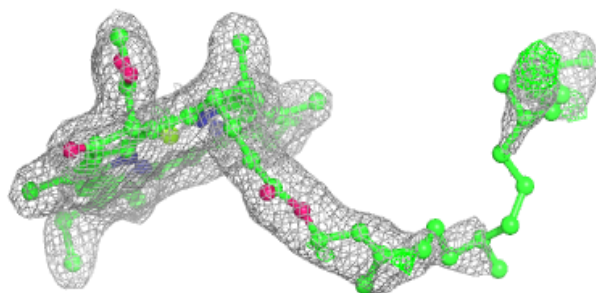
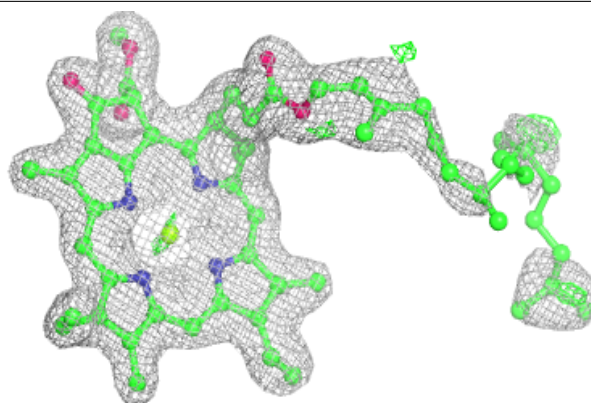
**Electron density around CLA b 617:**

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

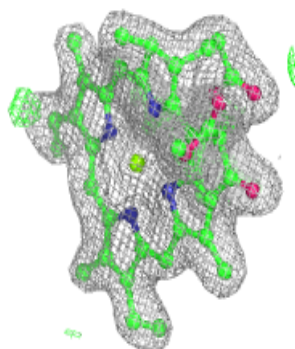
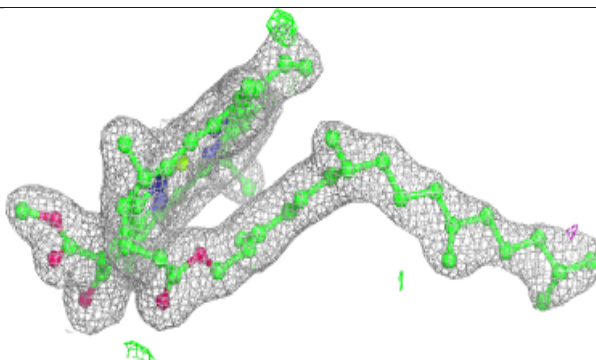
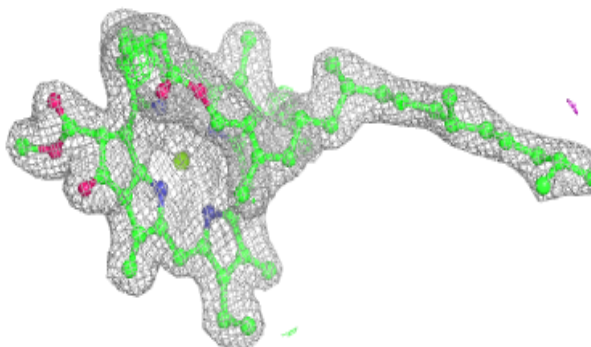


**Electron density around CLA a 413:**

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

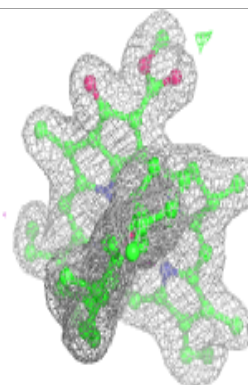
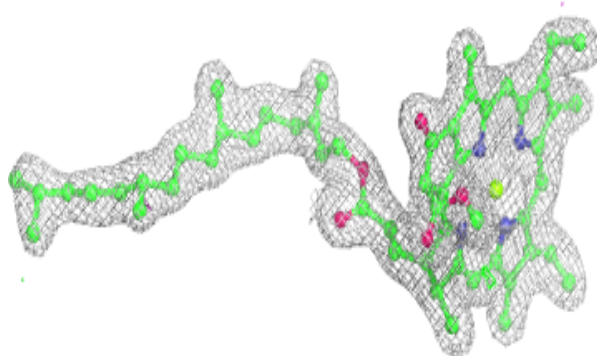
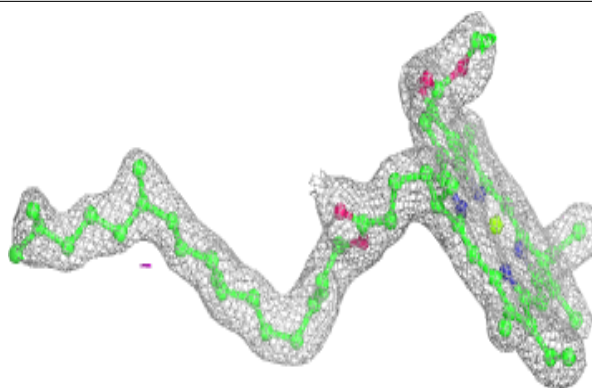
**Electron density around CLA C 505:**

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

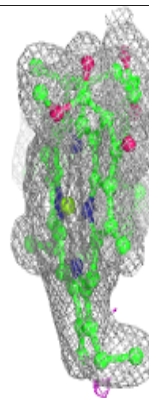
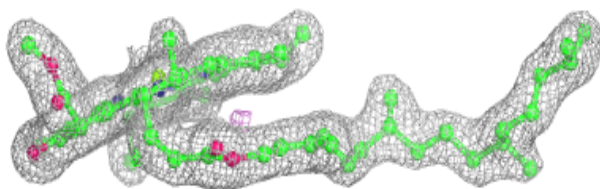
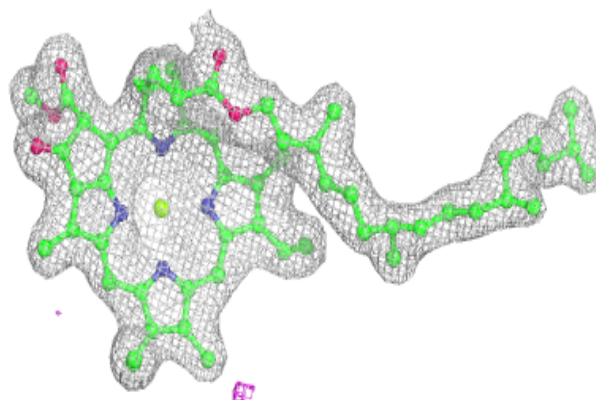


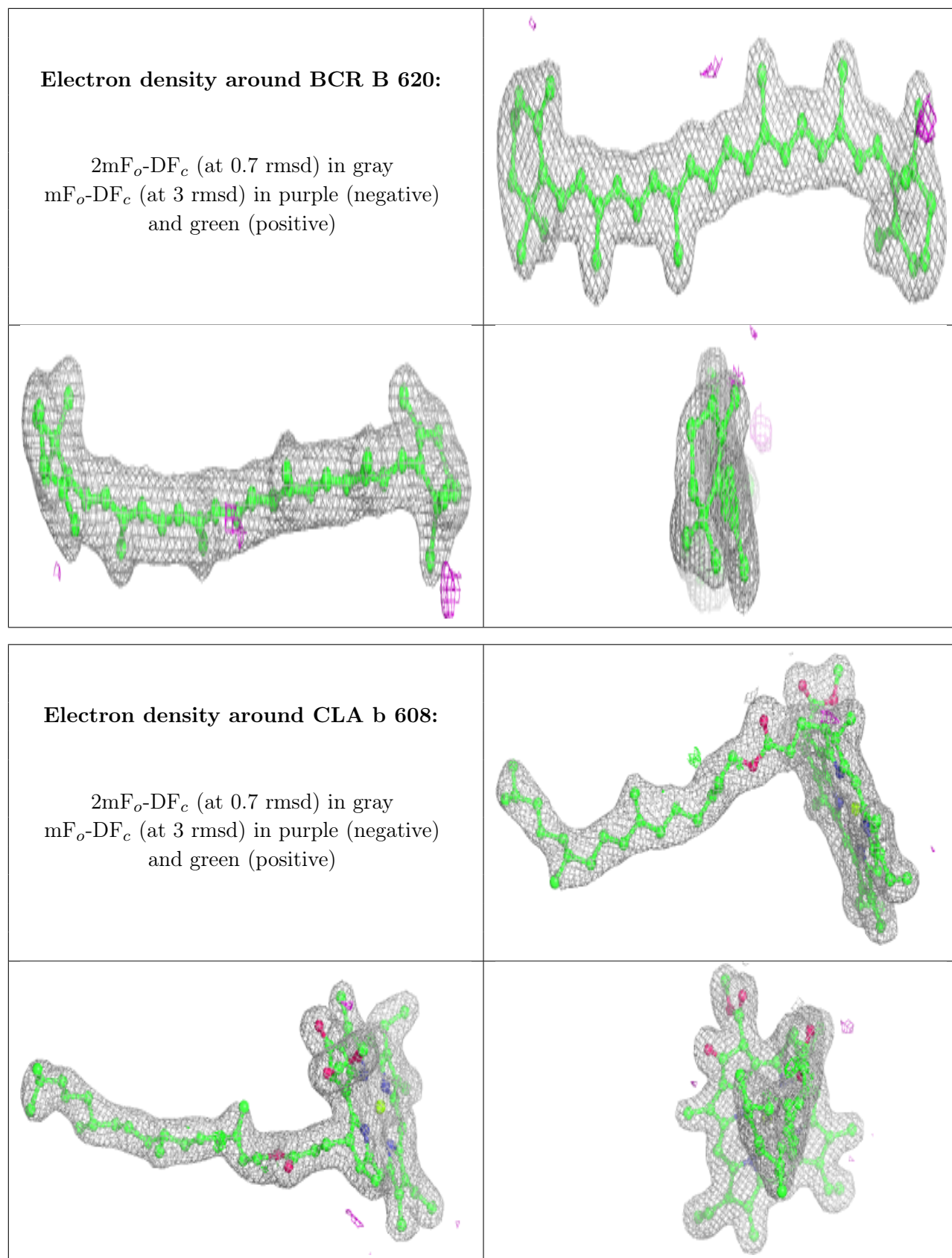
**Electron density around CLA C 502:**

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

**Electron density around CLA b 607:**

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

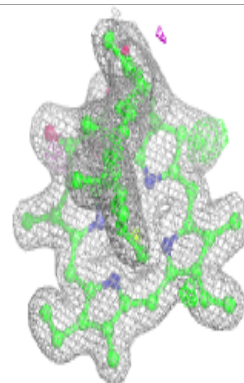
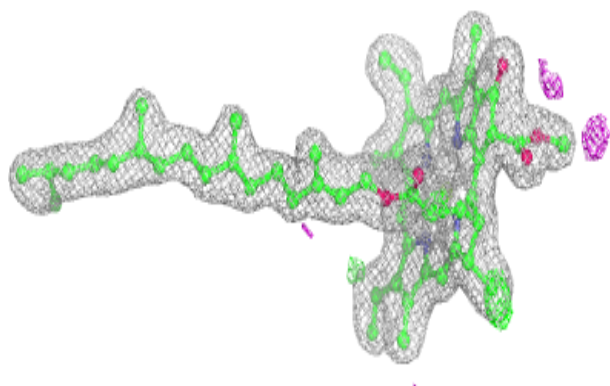
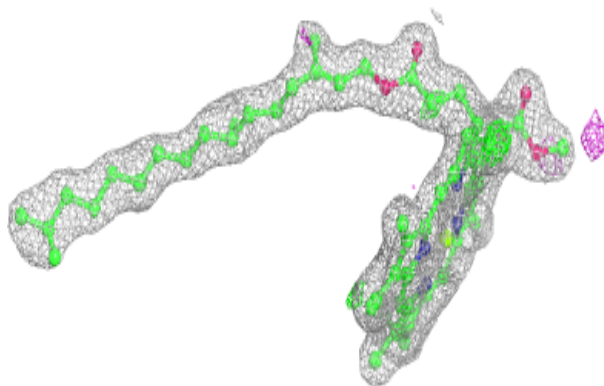




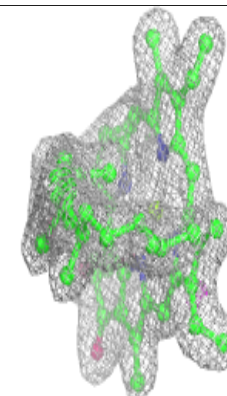
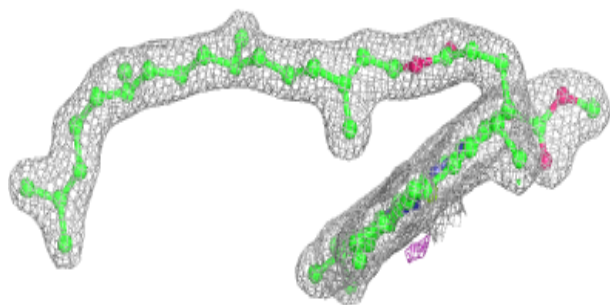
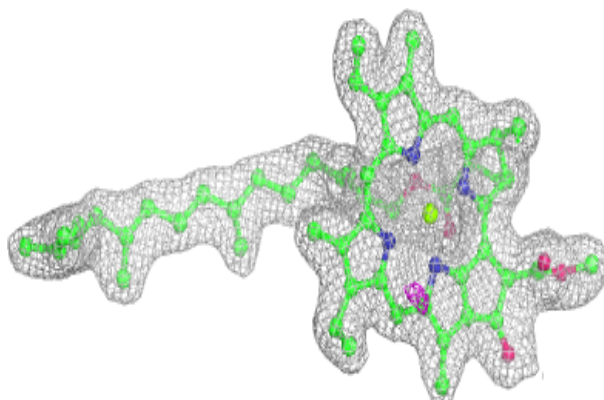


**Electron density around CLA B 608:**

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

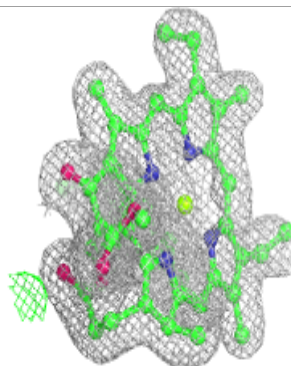
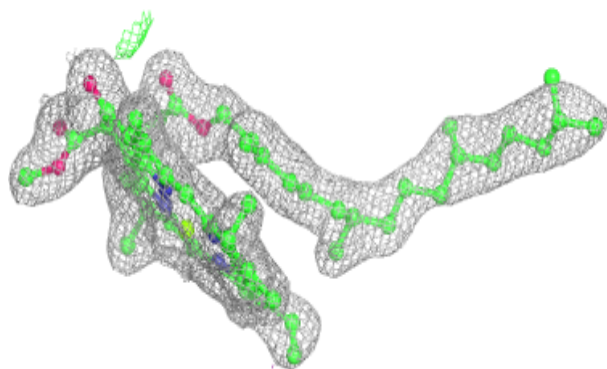
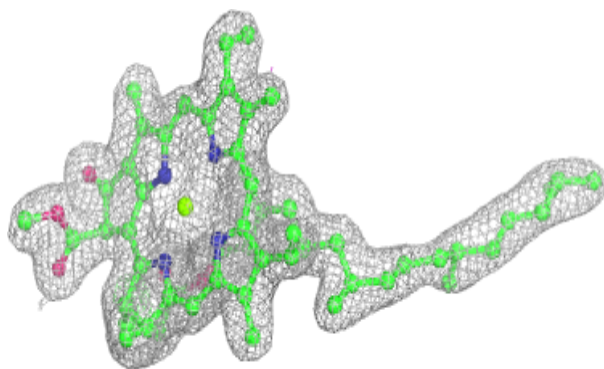
**Electron density around CLA b 612:**

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

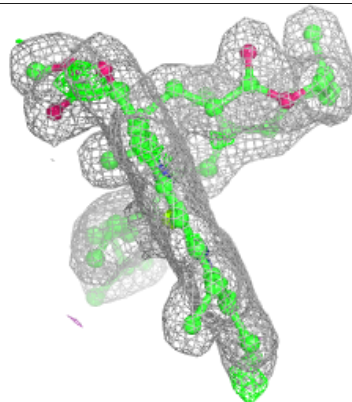
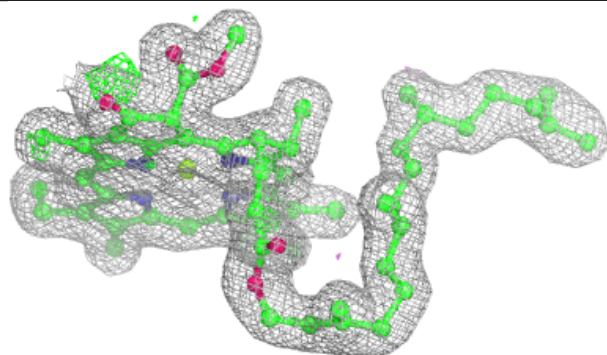
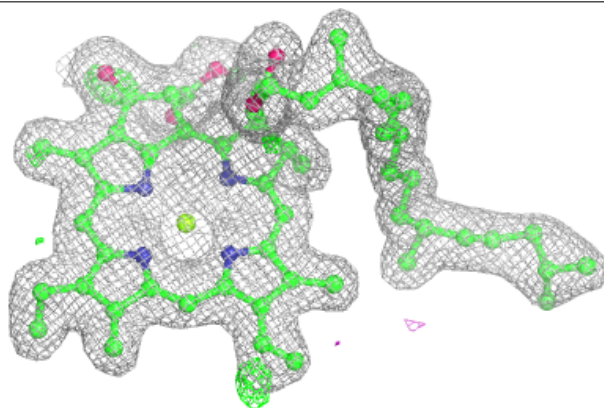


**Electron density around CLA c 906:**

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

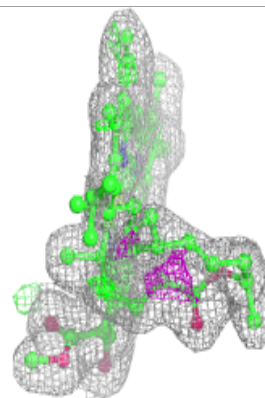
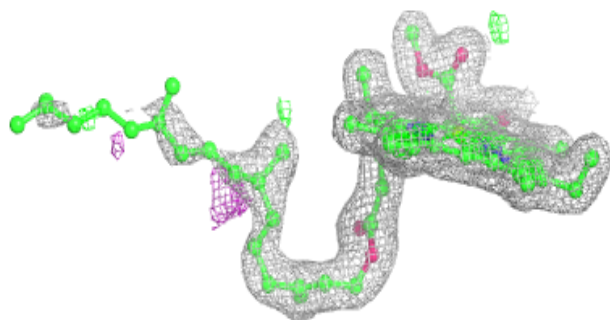
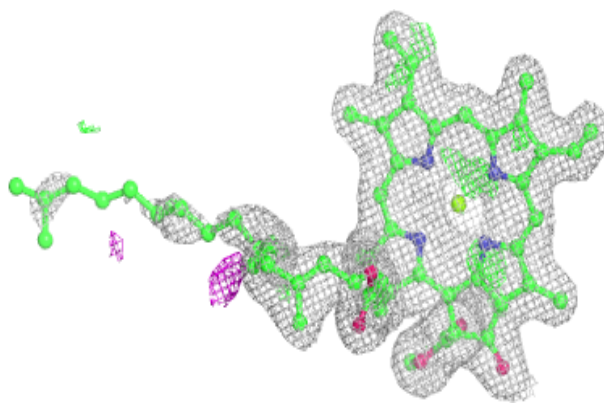
**Electron density around CLA A 406:**

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



**Electron density around CLA a 410:**

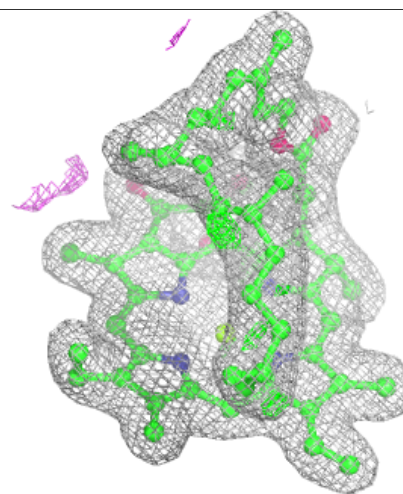
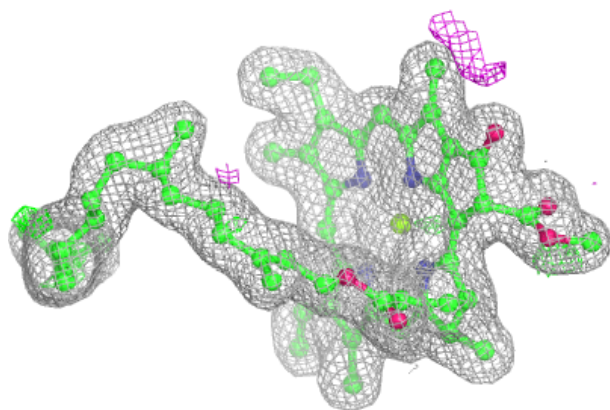
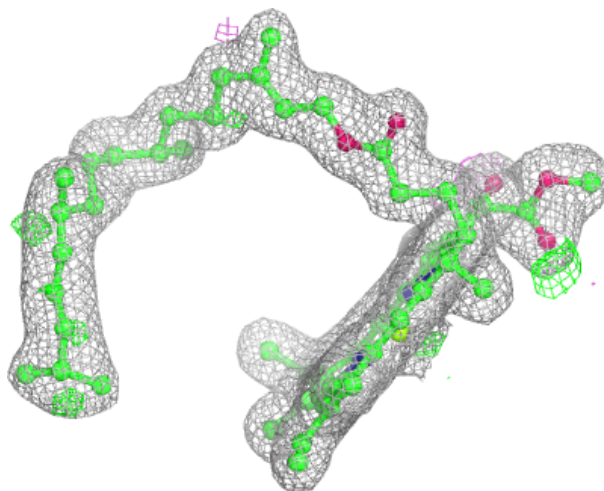
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

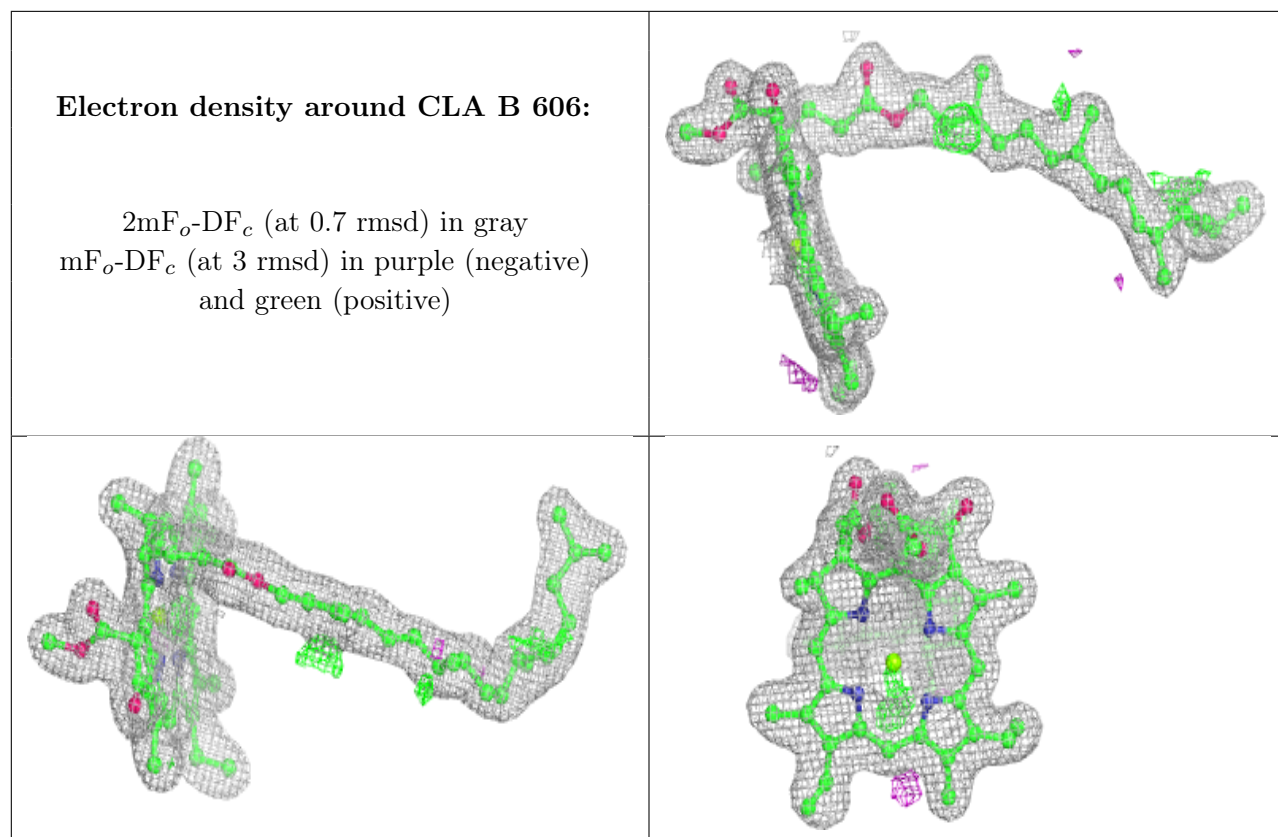




**Electron density around CLA b 615:**

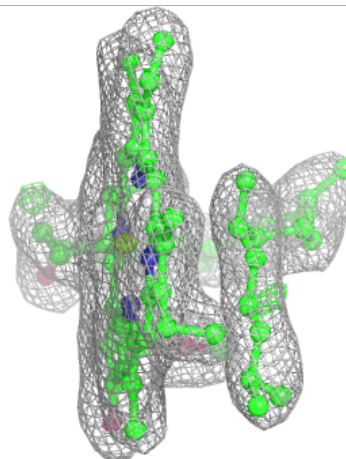
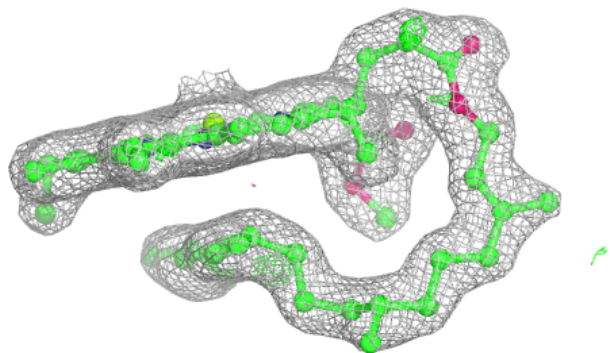
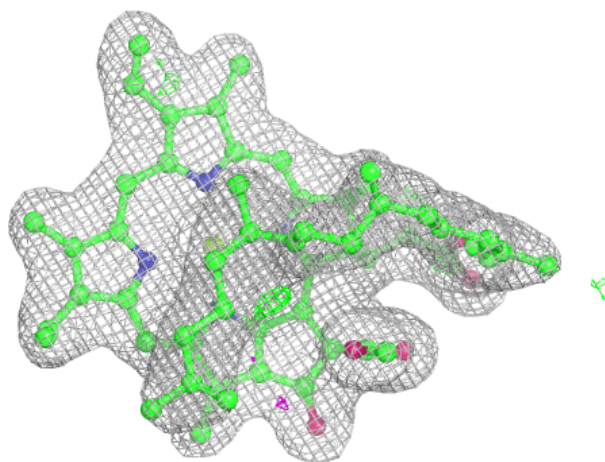
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





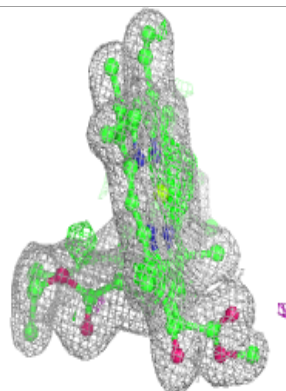
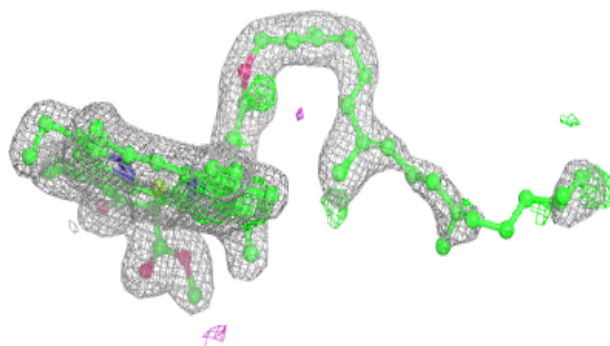
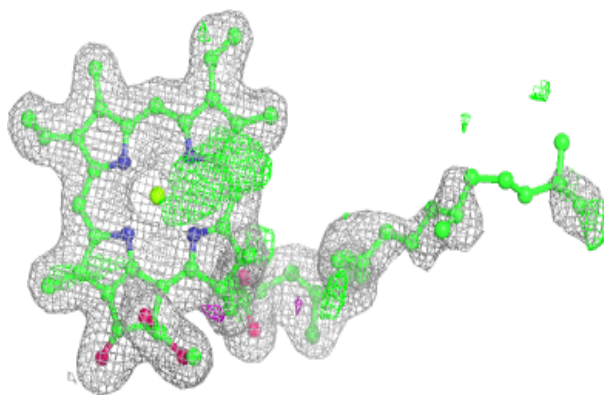
**Electron density around CLA c 911:**

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

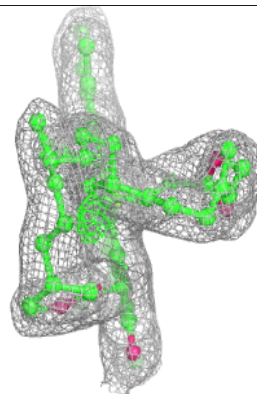
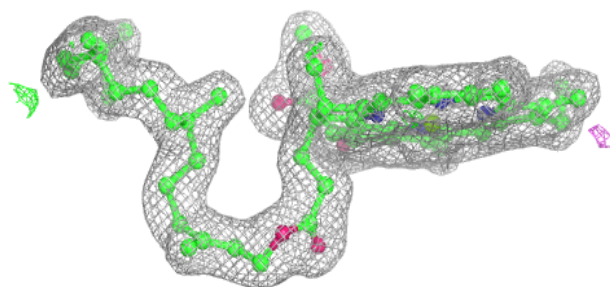
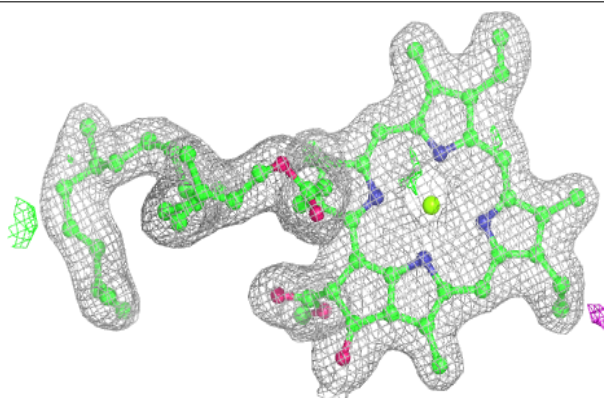


**Electron density around CLA A 407:**

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

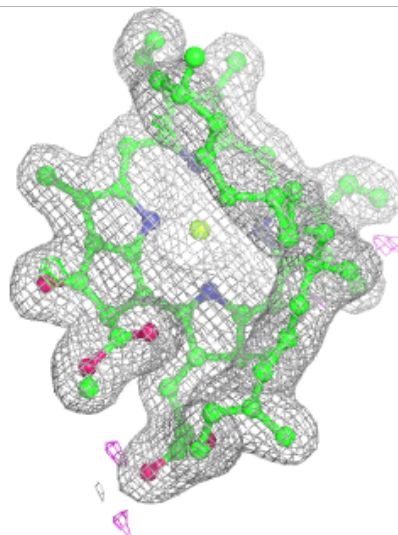
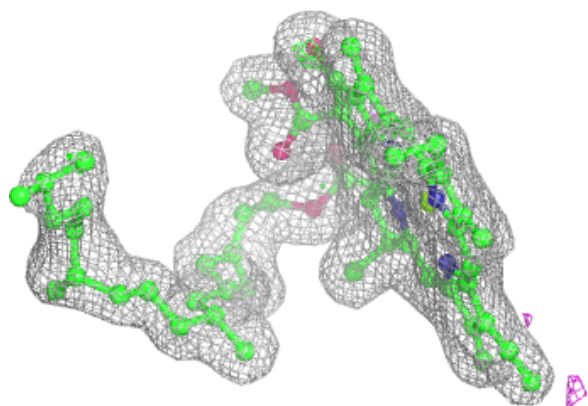
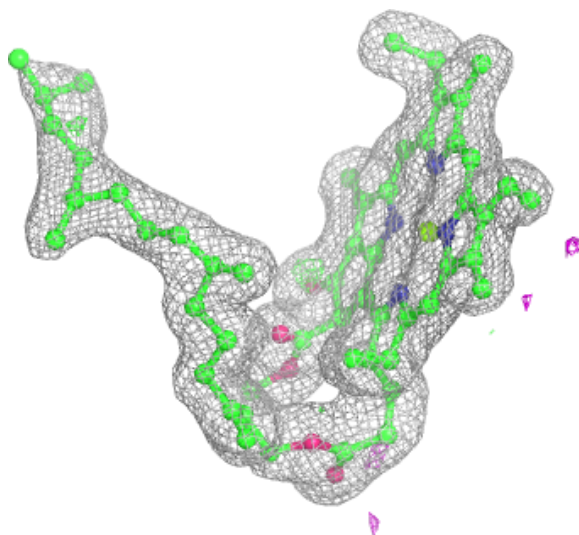
**Electron density around CLA B 613:**

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



**Electron density around CLA B 614:**

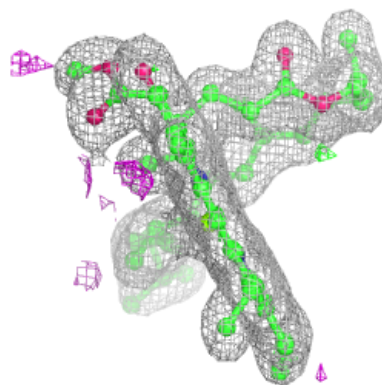
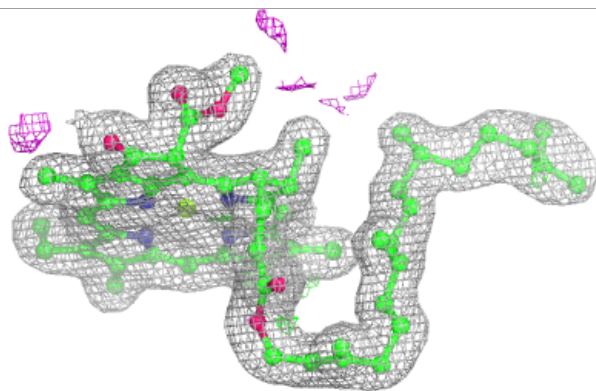
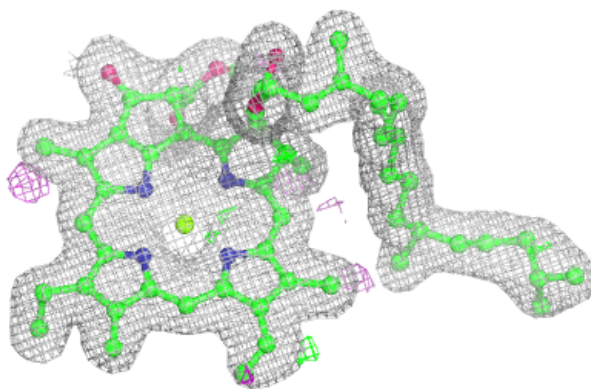
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



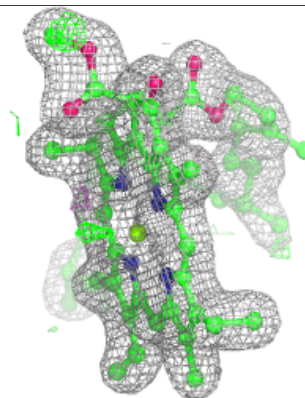
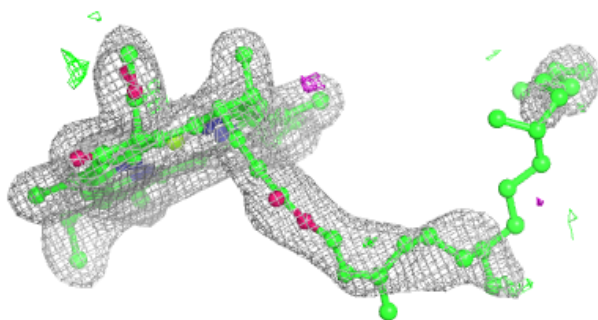
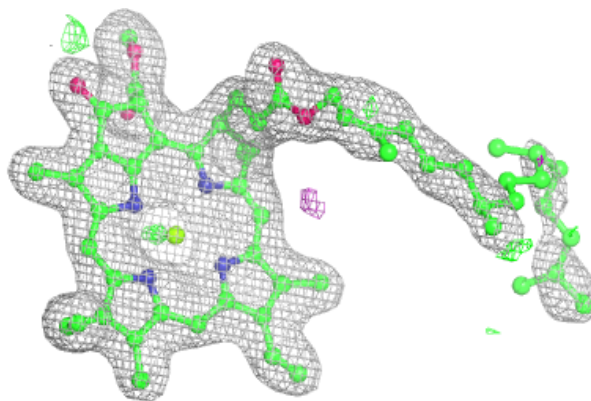


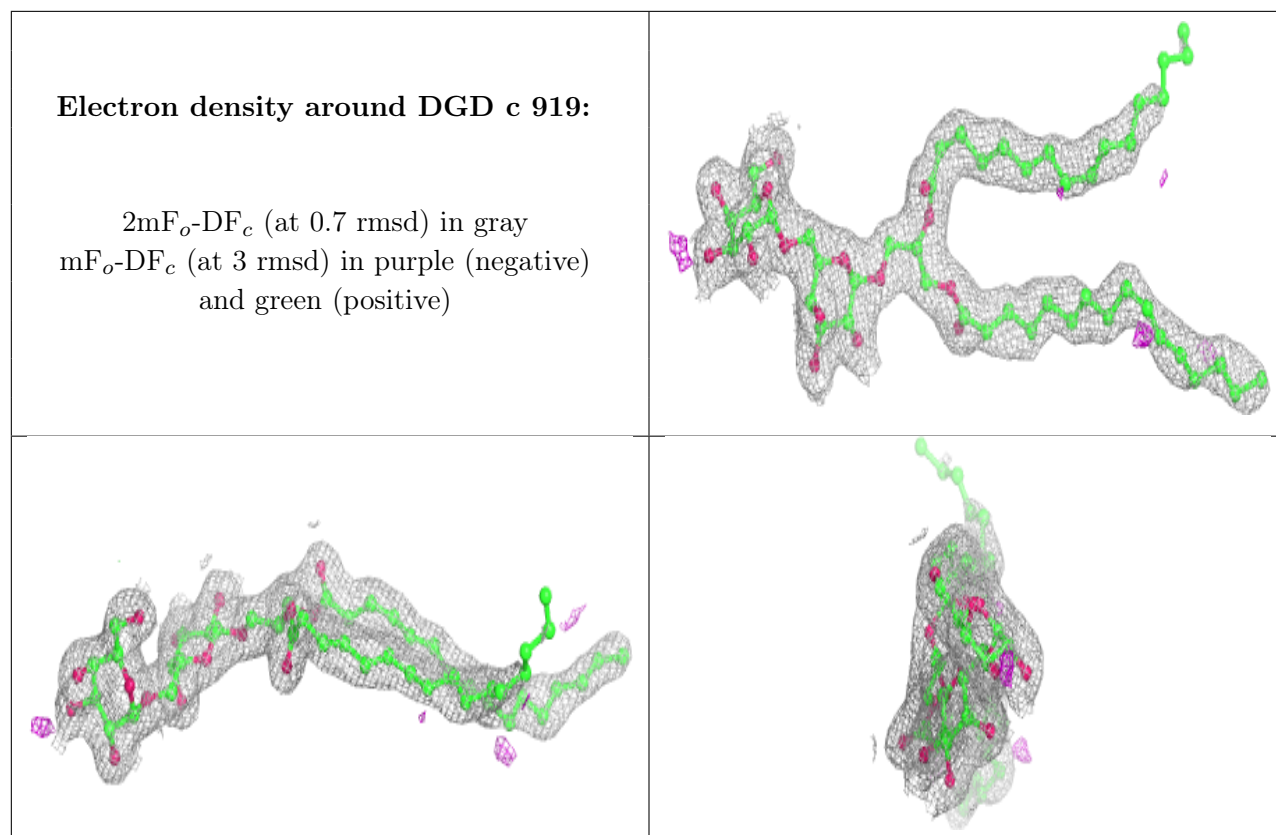
**Electron density around CLA d 401:**

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

**Electron density around CLA A 410:**

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

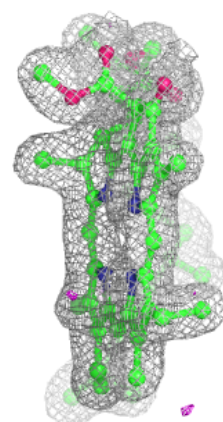
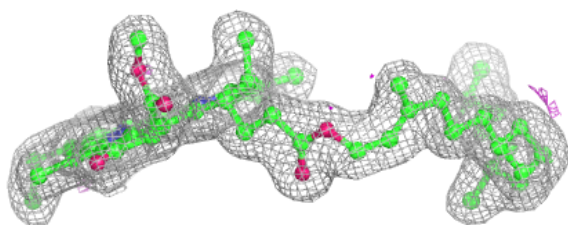
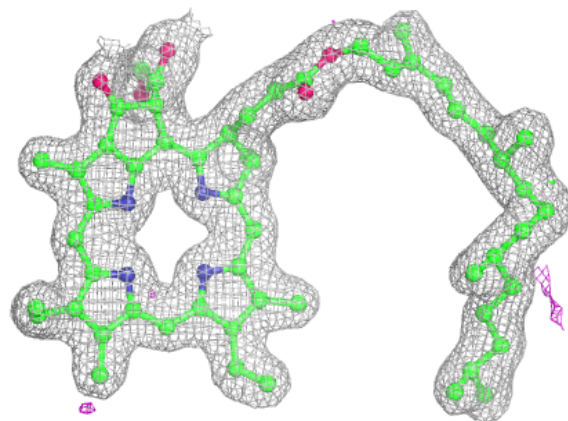






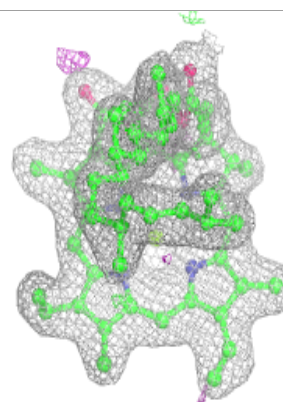
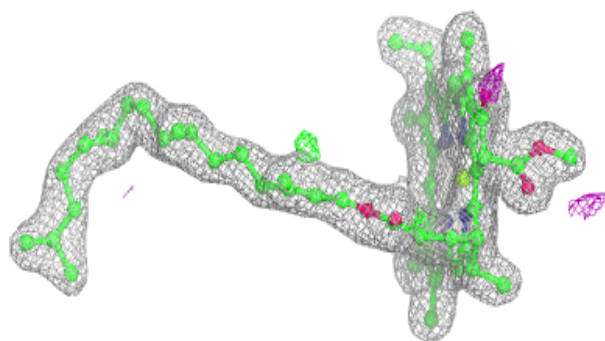
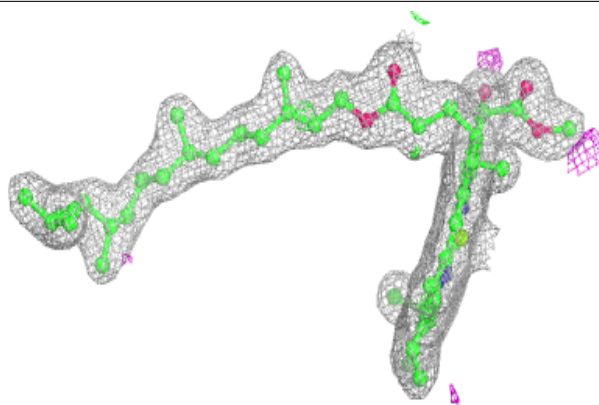
**Electron density around PHO A 408:**

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

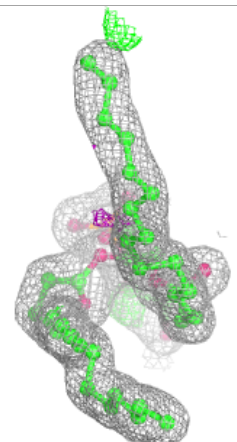
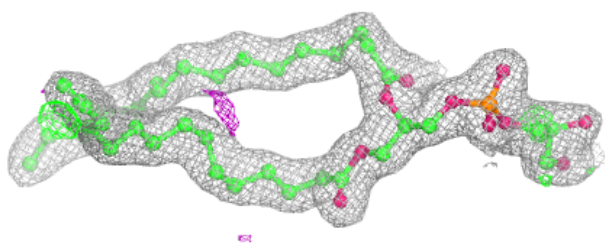
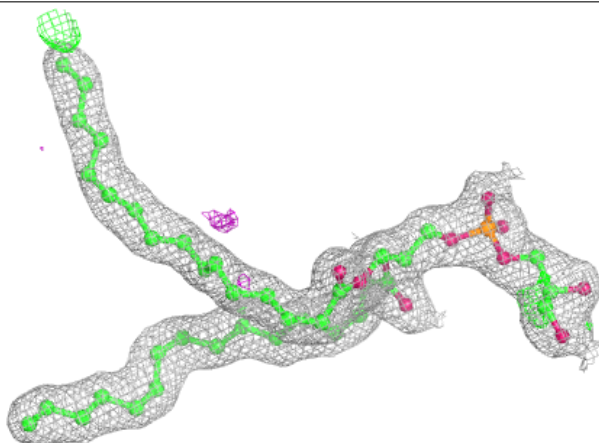


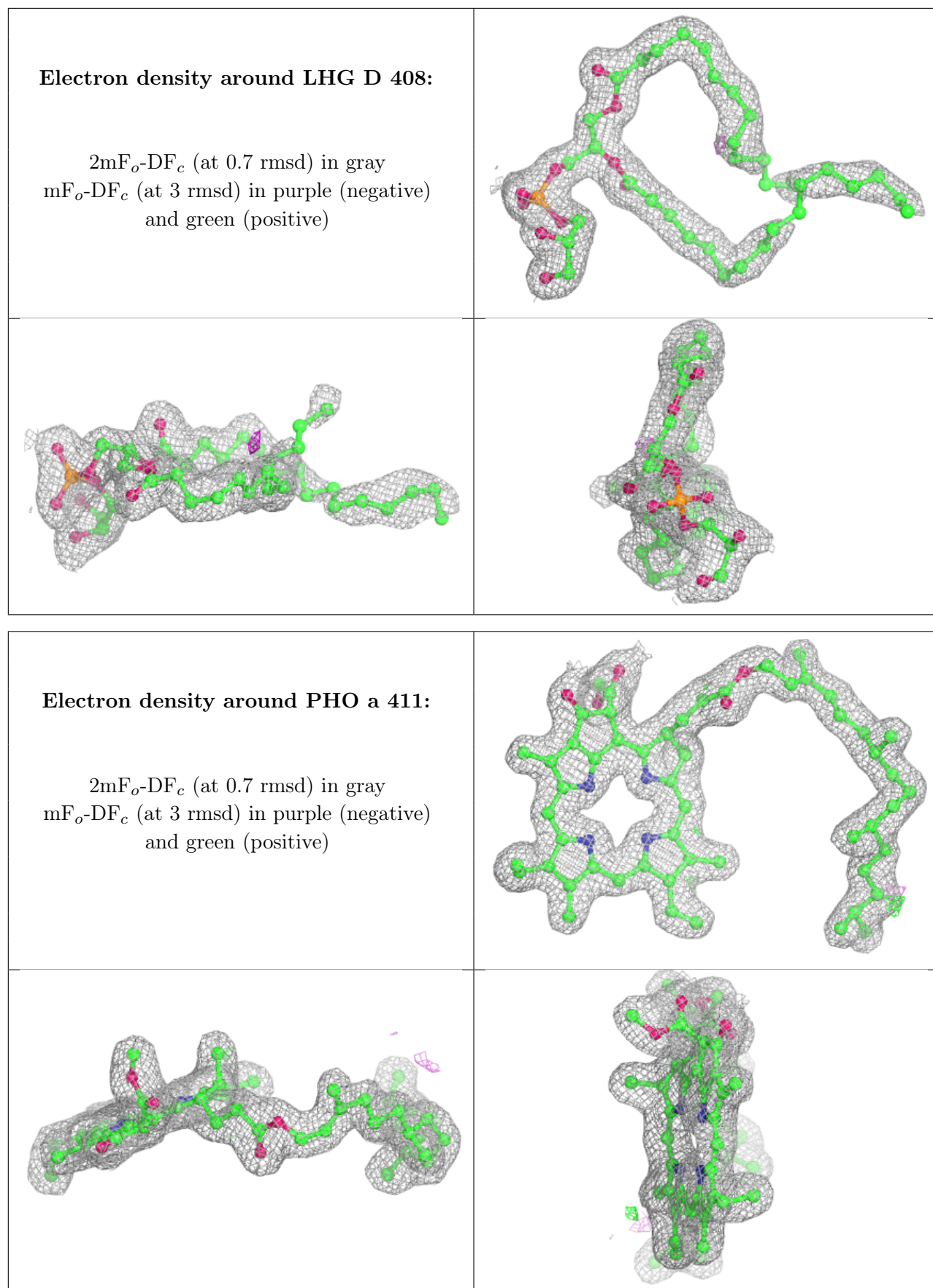
**Electron density around CLA b 609:**

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

**Electron density around LHG D 407:**

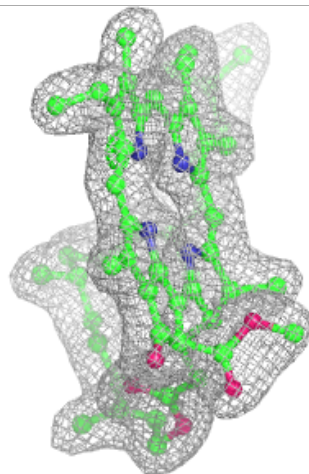
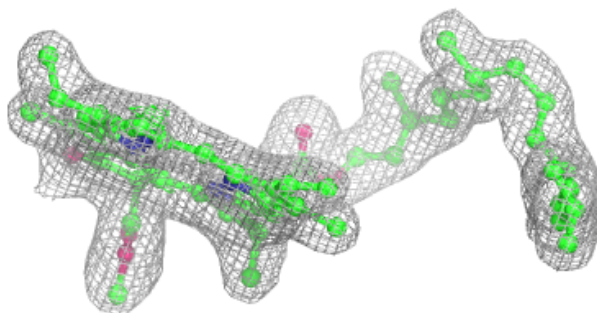
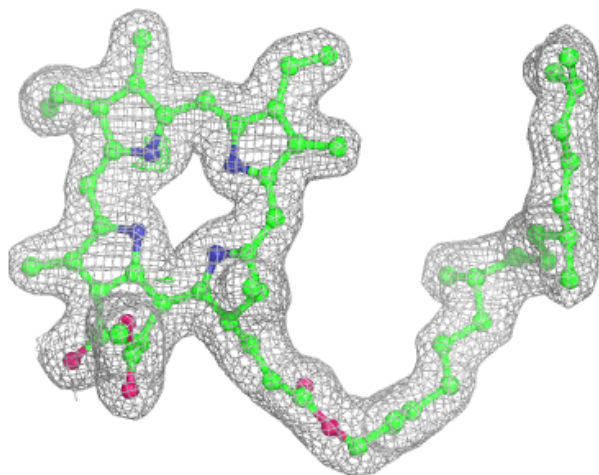
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



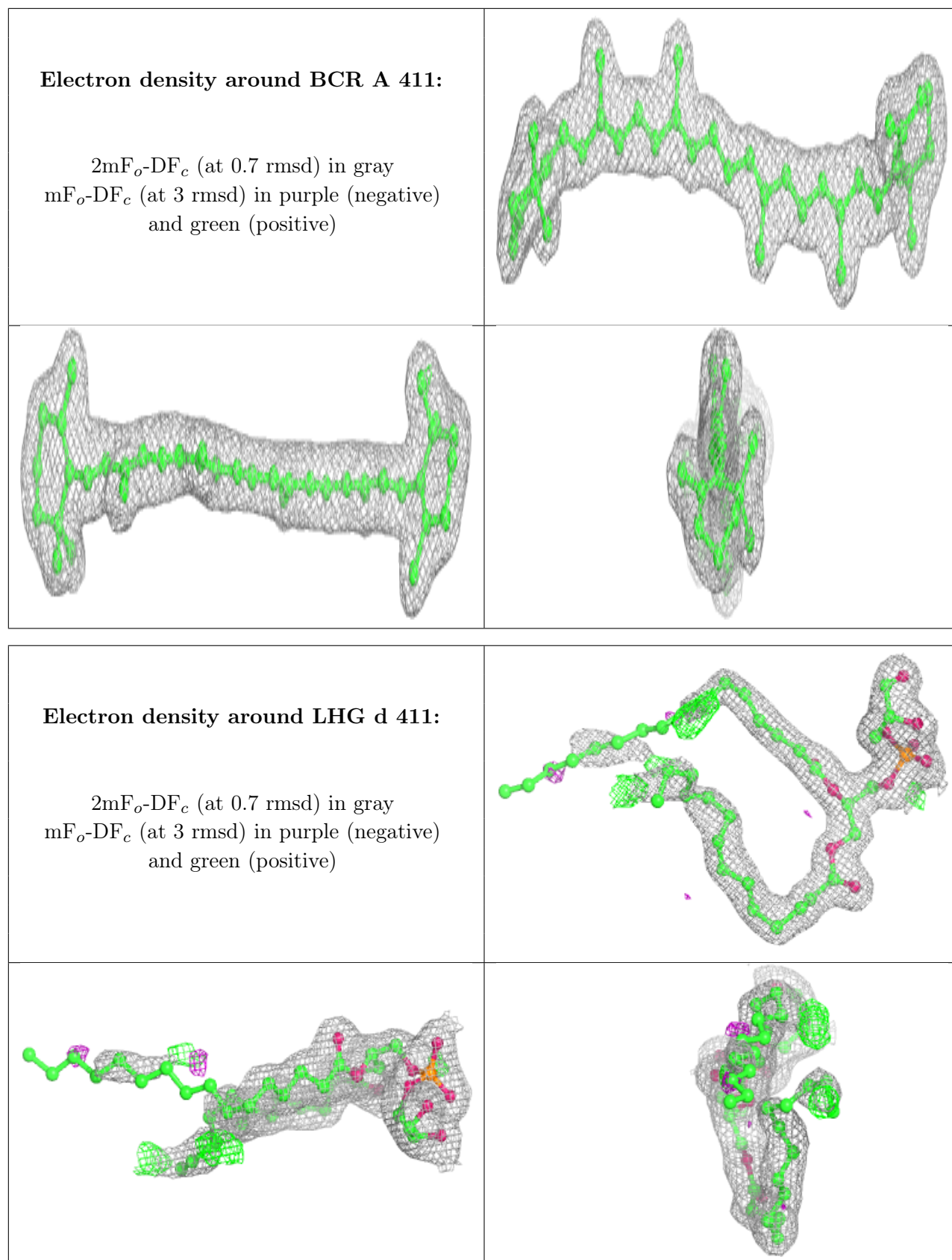


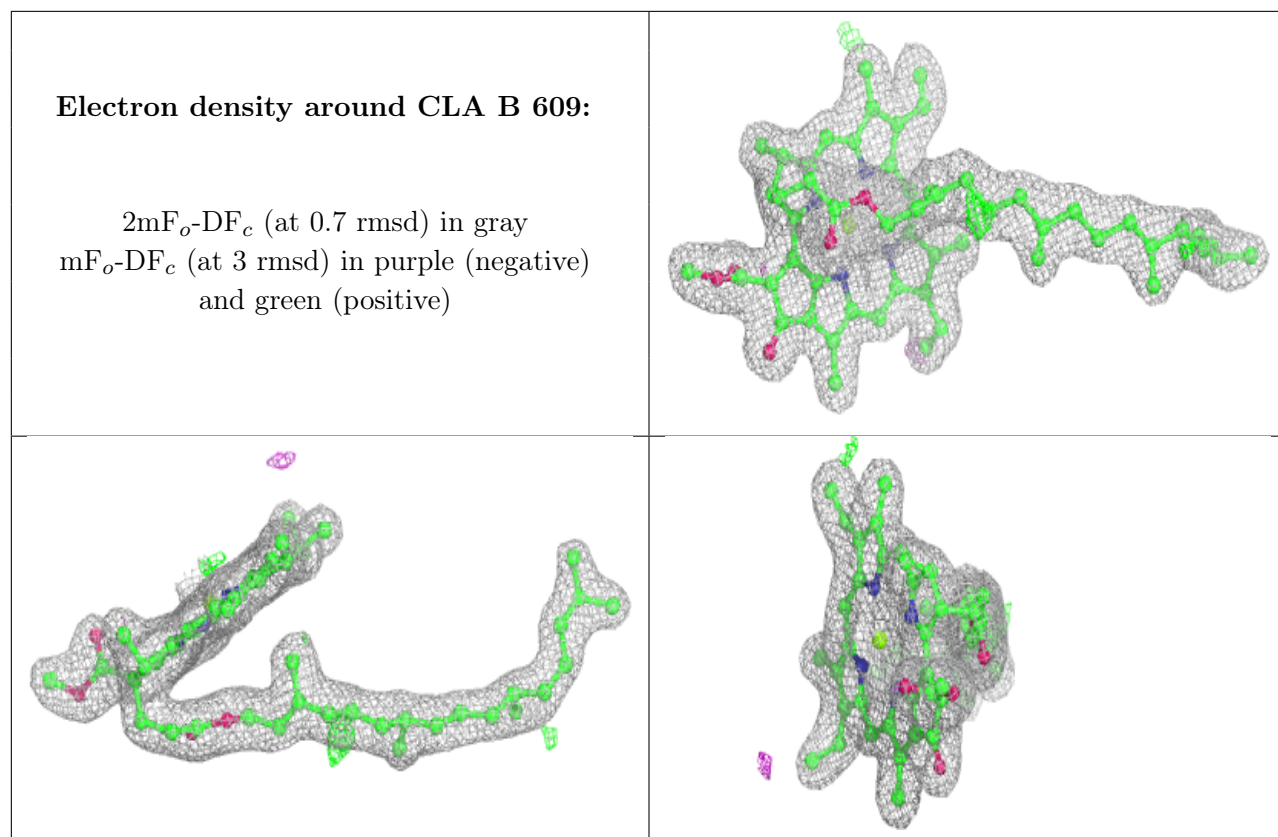
**Electron density around PHO a 412:**

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



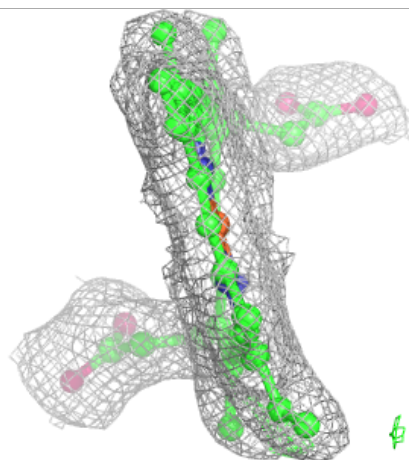
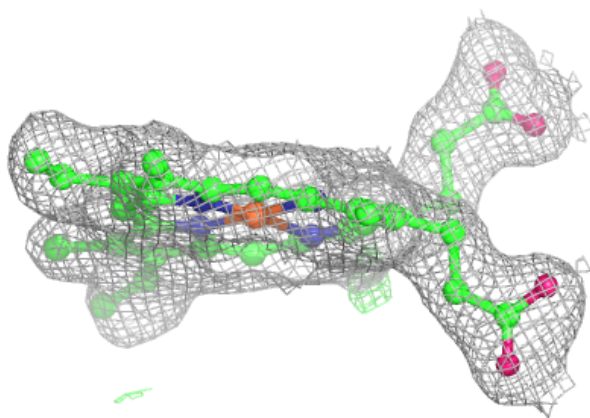
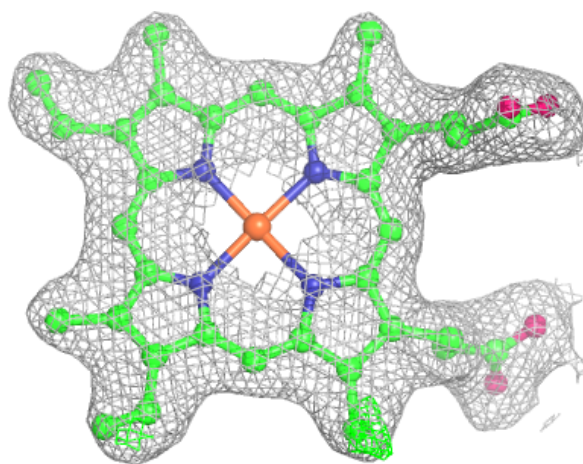






**Electron density around HEM F 102:**

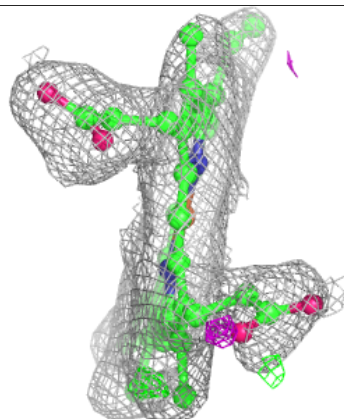
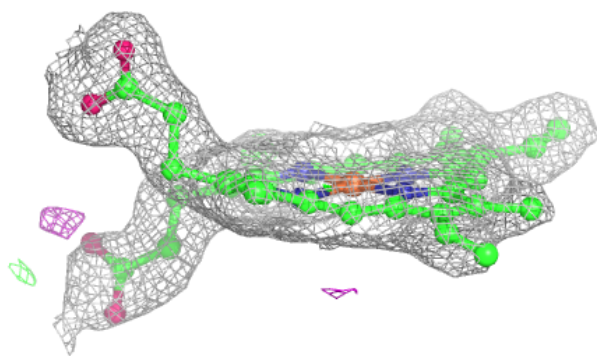
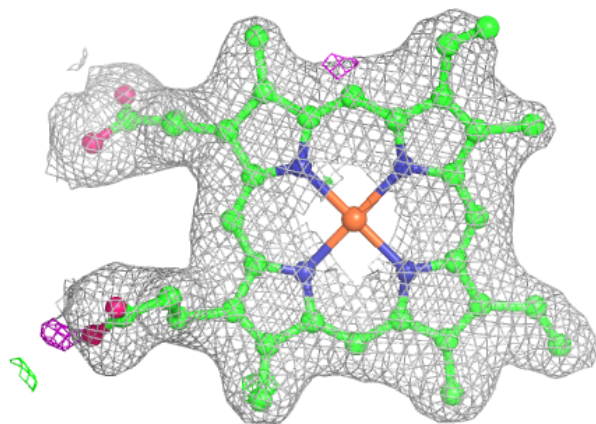
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



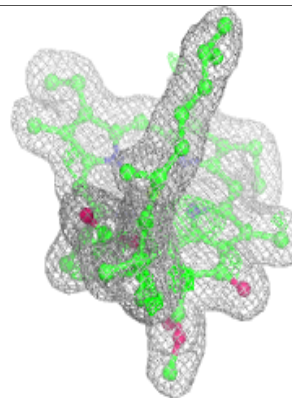
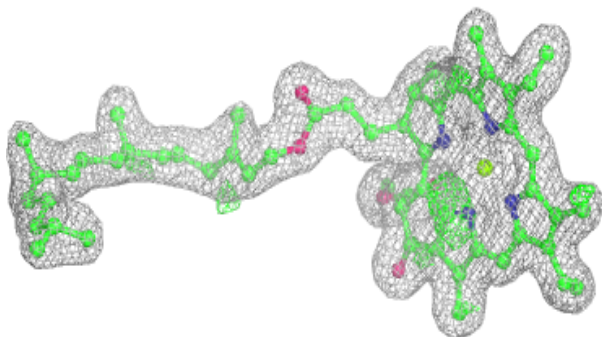
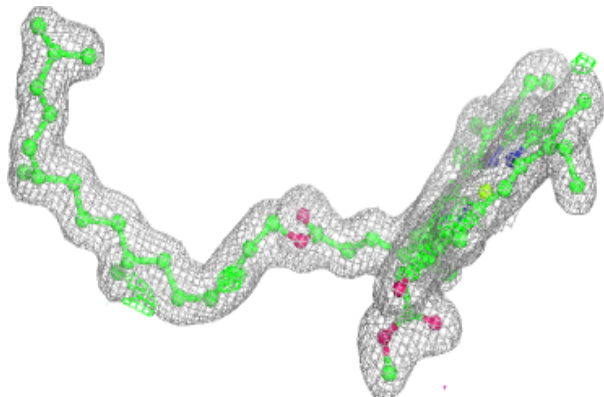


**Electron density around HEM f 101:**

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

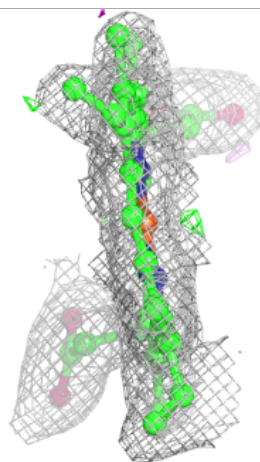
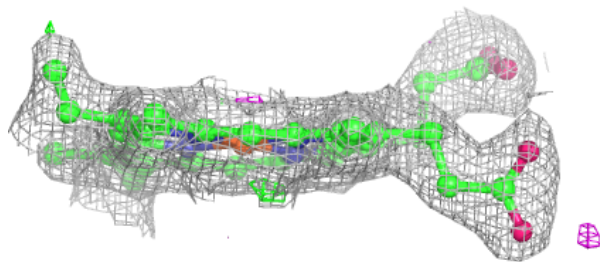
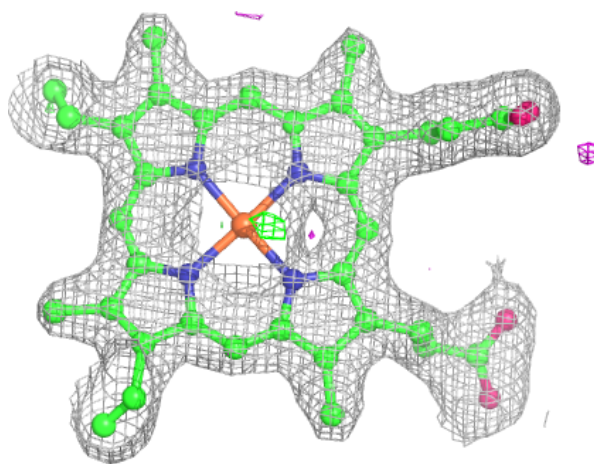
**Electron density around CLA D 401:**

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



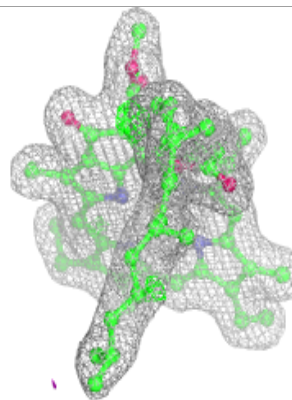
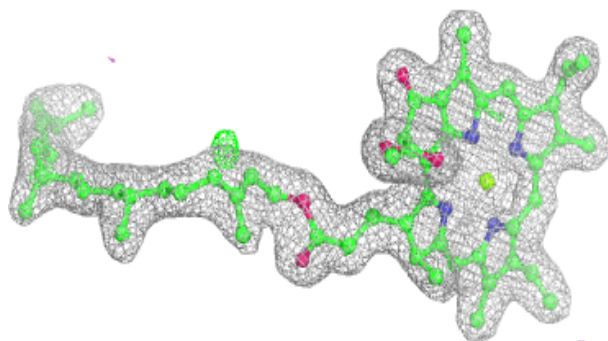
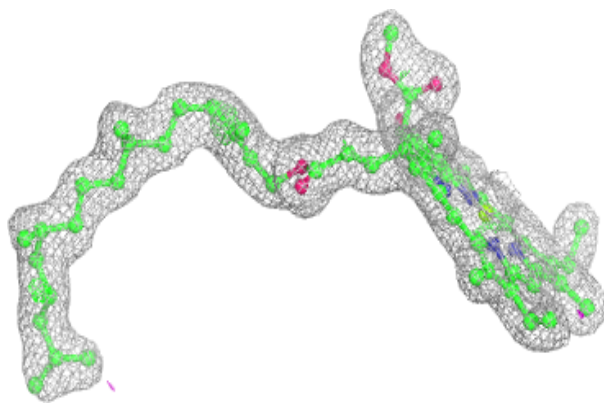
**Electron density around HEC v 202:**

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

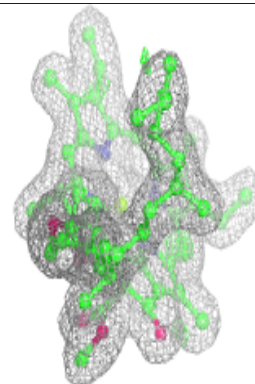
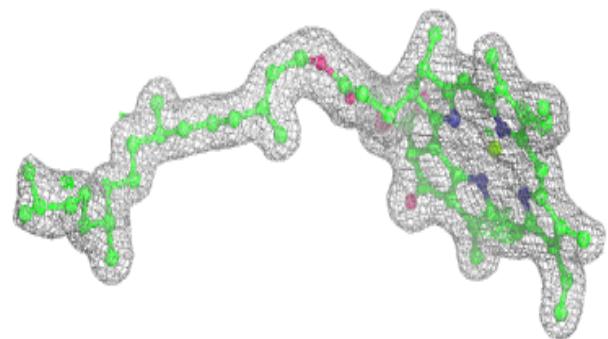
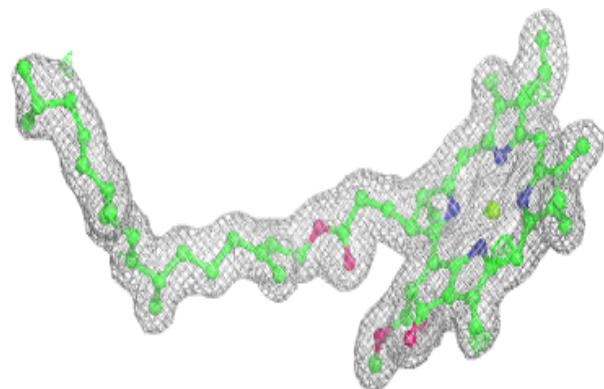


**Electron density around CLA d 404:**

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

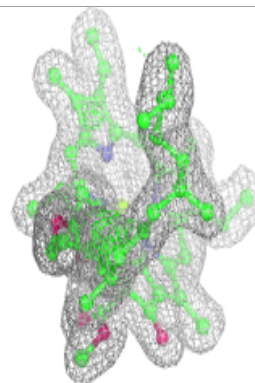
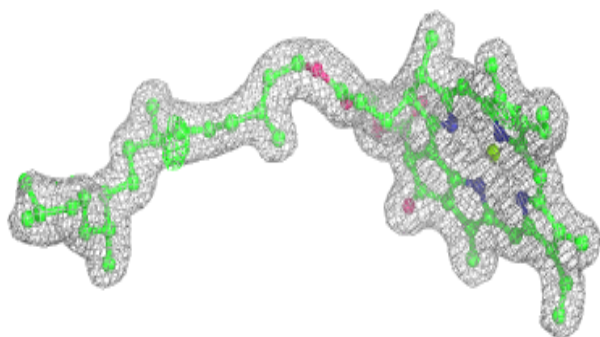
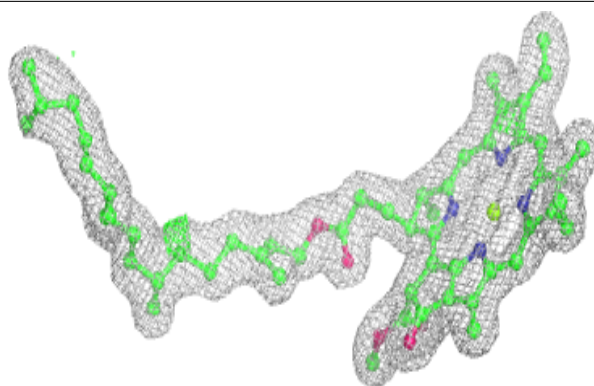
**Electron density around CLA A 405:**

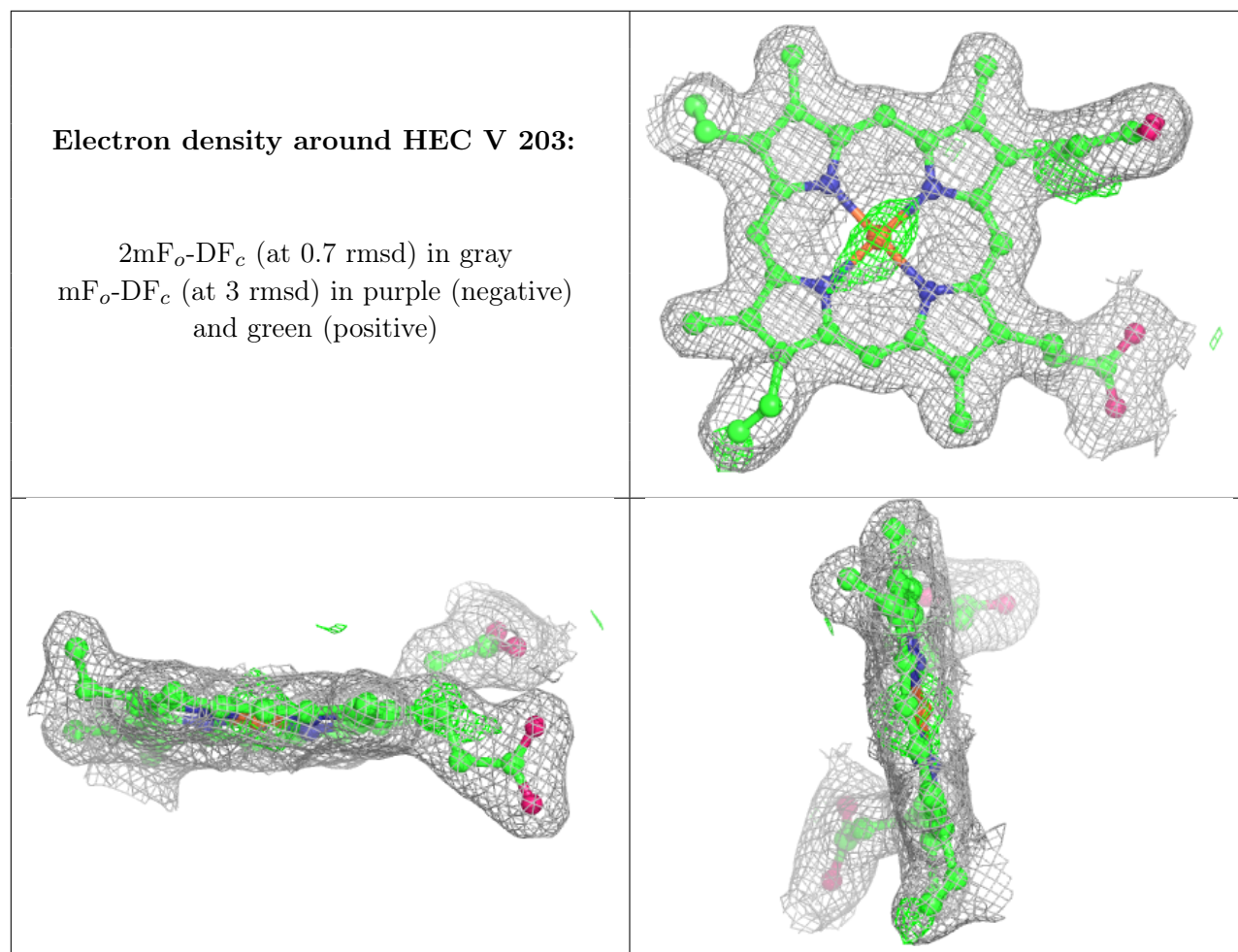
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA a 409:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.