



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 23, 2022 – 06:20 PM JST

PDB ID : 7YQ7
Title : Crystal structure of photosystem II expressing psbA3 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

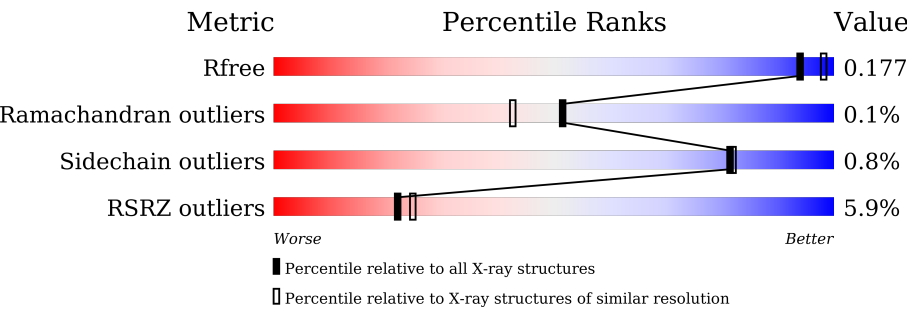
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.3
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance i

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 ≥ 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	<div><div>%</div><div>92%</div><div>7%</div></div>
1	a	360	<div><div>4%</div><div>94%</div><div>5%</div></div>
2	B	510	<div><div>4%</div><div>98%</div><div>..</div></div>
2	b	510	<div><div>6%</div><div>98%</div><div>.</div></div>
3	C	461	<div><div>%</div><div>97%</div><div>..</div></div>
3	c	461	<div><div>2%</div><div>98%</div><div>..</div></div>
4	D	352	<div><div>%</div><div>96%</div><div>..</div></div>

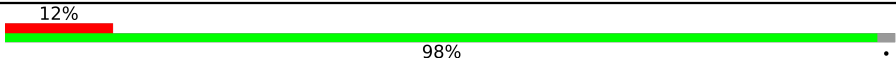
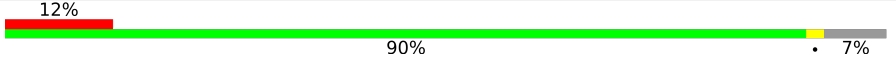
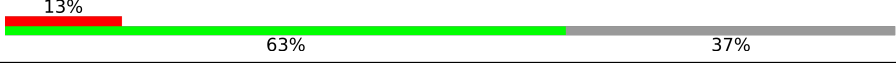
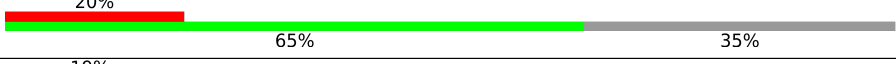
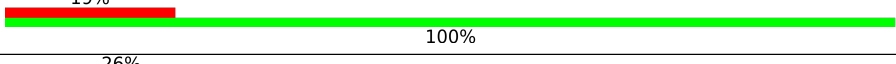
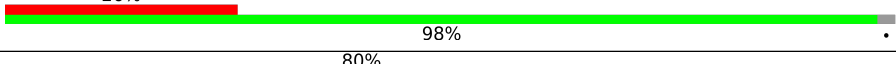
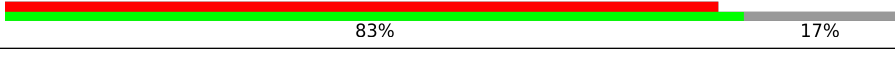
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Mol	Chain	Length	Quality of chain
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	
14	t	32	
15	U	134	
15	u	134	
16	V	163	
16	v	163	

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Mol	Chain	Length	Quality of chain
17	X	41	
17	x	41	
18	Y	46	
18	y	46	
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	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	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	B	618	X	-	-	-
24	CLA	C	503	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	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	514	X	-	-	-
24	CLA	D	405	X	-	-	-
24	CLA	D	406	X	-	-	-
24	CLA	a	409	X	-	-	-
24	CLA	a	410	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	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	503	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	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	c	514	X	-	-	-
24	CLA	d	405	X	-	-	-
24	CLA	d	406	X	-	-	-
34	DMS	C	501	-	-	-	X
34	DMS	O	308	-	-	-	X
34	DMS	o	305	-	-	-	X
34	DMS	u	203	-	-	-	X
36	HTG	B	626	-	-	-	X
36	HTG	u	201	-	-	-	X

2 Entry composition

There are 43 unique types of molecules in this entry. The entry contains 55105 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 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	1	0
			2624	1720	429	461	14			
1	a	342	Total	C	N	O	S	0	0	0
			2658	1741	436	467	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	5	0
			3994	2618	668	695	13			
2	b	504	Total	C	N	O	S	0	6	0
			3978	2609	666	690	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	450	Total	C	N	O	S	0	2	0
			3492	2284	585	610	13			
3	c	455	Total	C	N	O	S	0	4	0
			3527	2311	586	617	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	1	0
			2714	1799	441	462	12			
4	d	342	Total	C	N	O	S	0	0	0
			2722	1803	445	462	12			

- 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
			647	424	103	120			
5	e	79	Total	C	N	O	0	2	0
			642	421	103	118			

- 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	0	0
			257	175	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	1	0
			514	342	85	85	2			
7	h	65	Total	C	N	O	S	0	1	0
			519	344	86	87	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
			287	196	42	48	1			
8	i	37	Total	C	N	O	S	0	0	0
			304	206	47	50	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	37	Total	C	N	O	S	0	0	0
			256	174	38	43	1			
9	j	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	1	0
			305	205	48	51	1			
11	l	36	Total	C	N	O		0	1	0
			301	202	47	52				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	0	0
			261	174	38	48	1			
12	m	34	Total	C	N	O	S	0	1	0
			274	184	40	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	4	0
			1860	1165	310	380	5			
13	o	243	Total	C	N	O	S	0	3	0
			1848	1159	306	378	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	0	0	0
			770	489	129	152			
15	u	97	Total	C	N	O	0	0	0
			774	491	129	154			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	1	0
			1070	678	178	210	4			
16	v	137	Total	C	N	O	S	0	1	0
			1065	677	175	209	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	40	Total	C	N	O	0	1	0
			295	198	47	50			
17	x	38	Total	C	N	O	0	0	0
			275	185	44	46			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Y	29	Total	C	N	O	S	0	0	0
			206	136	34	33	3			
18	y	30	Total	C	N	O	S	0	0	0
			215	140	38	34	3			

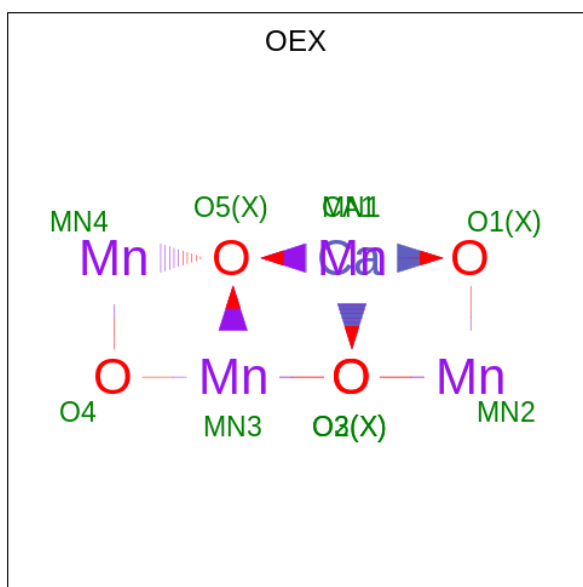
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	5	0
			495	341	74	78	2			
19	z	61	Total	C	N	O	S	0	0	0
			450	311	67	71	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	0	0	0
			206	132	38	36			

- Molecule 21 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



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

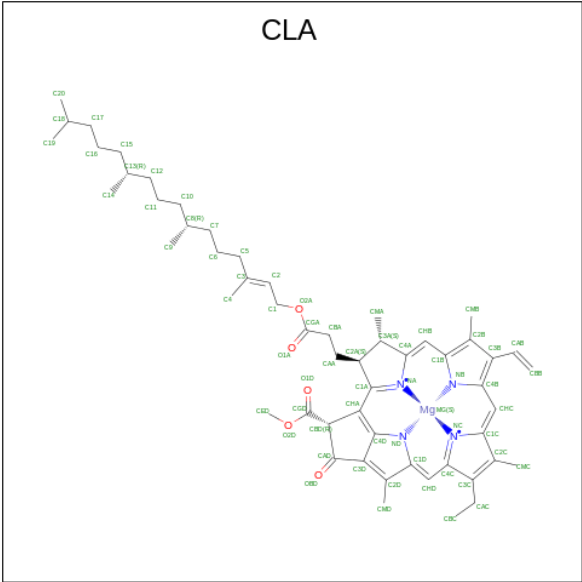
- Molecule 22 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

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

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

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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		

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

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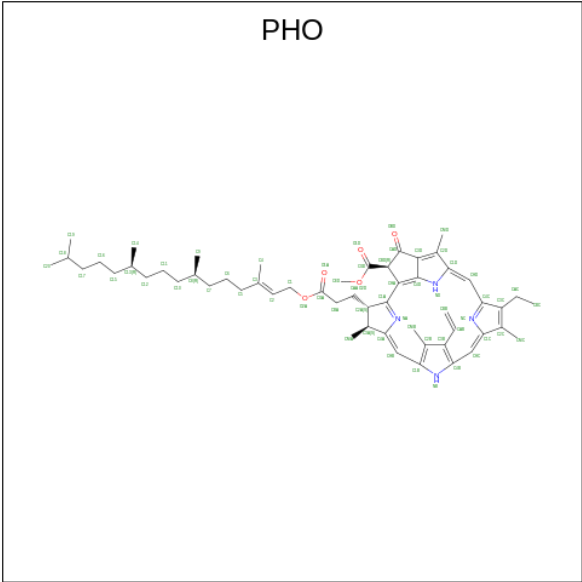
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24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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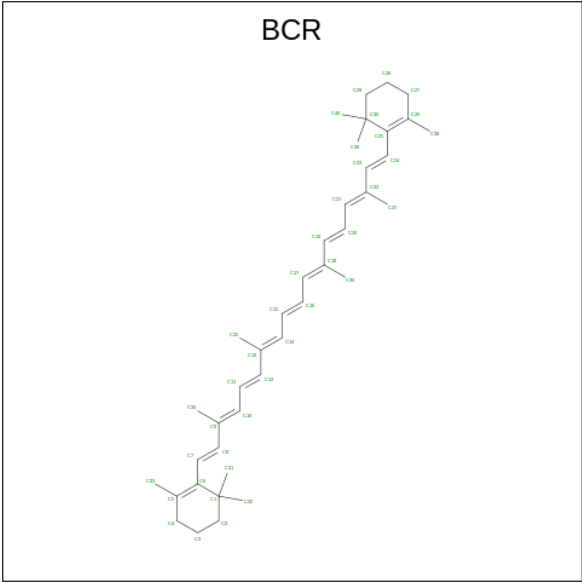
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅) (labeled as "Ligand of Interest" by depositor).



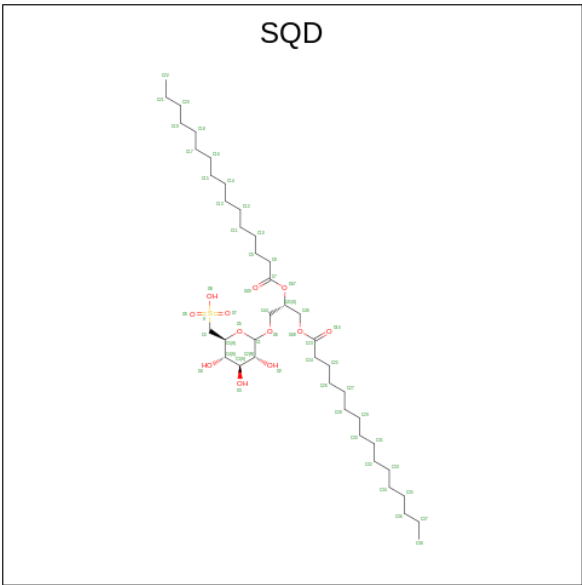
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



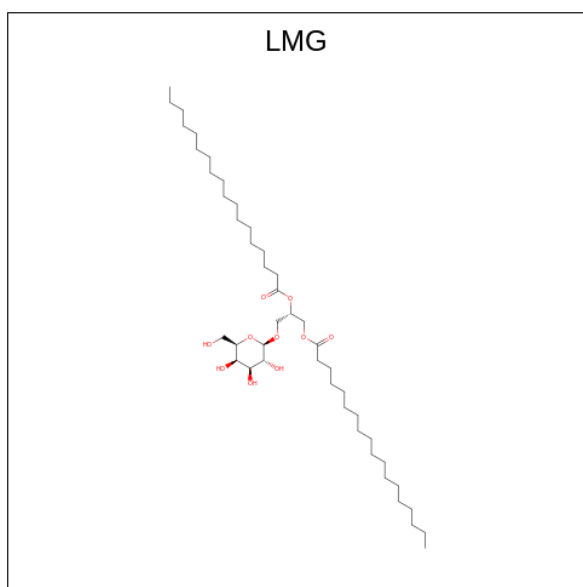
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	a	1	Total 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
26	t	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: C₄₁H₇₈O₁₂S) (labeled as "Ligand of Interest" by depositor).



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

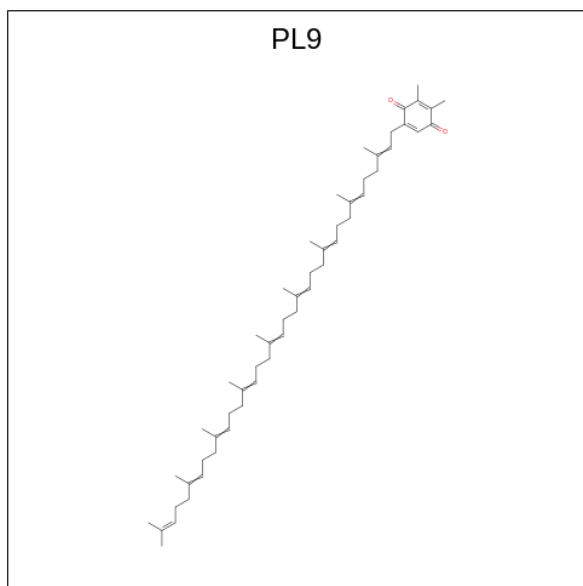
- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



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

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:

C₅₃H₈₀O₂) (labeled as "Ligand of Interest" by depositor).



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

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	5	Total	C		0	0
			39	39			
30	B	7	Total	C		0	0
			51	51			
30	C	9	Total	C	O	0	0
			85	80	5		
30	D	4	Total	C	O	0	0
			75	71	4		
30	E	2	Total	C		0	0
			22	22			
30	H	2	Total	C		0	0
			12	12			
30	I	6	Total	C		0	0
			81	81			

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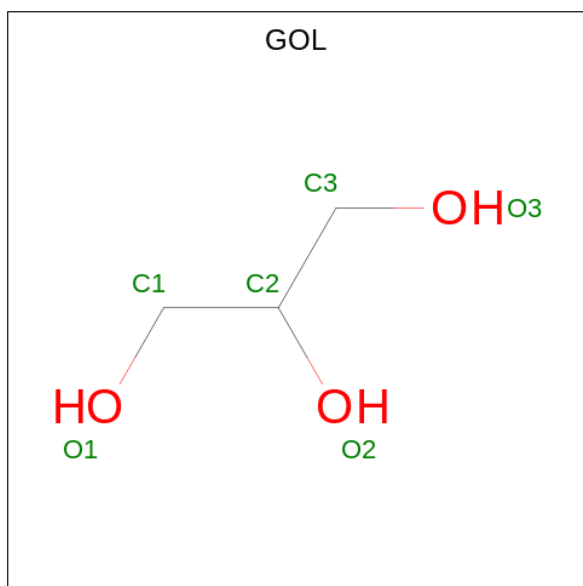
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	J	3	Total C 20 20	0	0
30	T	1	Total C 7 7	0	0
30	U	1	Total C 5 5	0	0
30	V	3	Total C 20 20	0	0
30	X	2	Total C O 44 39 5	0	0
30	Y	1	Total C 16 16	0	0
30	Z	3	Total C 15 15	0	0
30	a	2	Total C 17 17	0	0
30	b	6	Total C 53 53	0	0
30	c	5	Total C 36 36	0	0
30	d	3	Total C O 56 51 5	0	0
30	e	1	Total C 10 10	0	0
30	h	4	Total C 37 37	0	0
30	i	3	Total C 36 36	0	0
30	j	1	Total C 10 10	0	0
30	k	2	Total C O 38 33 5	0	0
30	l	1	Total C 13 13	0	0
30	m	1	Total C 8 8	0	0
30	t	1	Total C 8 8	0	0
30	x	1	Total C 11 11	0	0
30	y	1	Total C 10 10	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	z	1	Total C 6 6	0	0

- Molecule 31 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



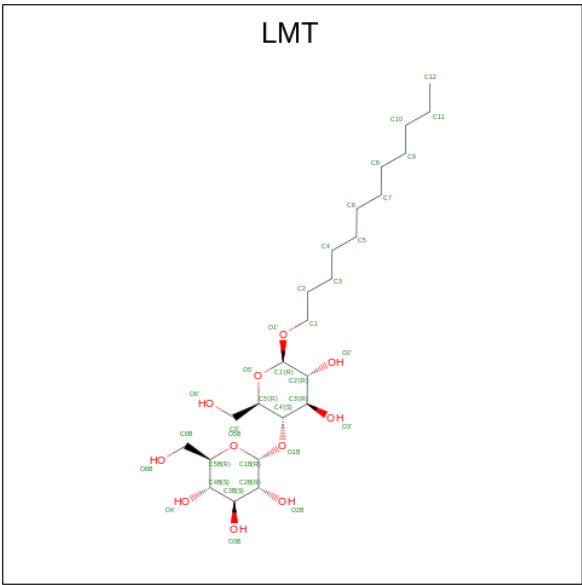
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C O 6 3 3	0	0
31	A	1	Total C O 6 3 3	0	0
31	C	1	Total C O 6 3 3	0	0
31	D	1	Total C O 6 3 3	0	0
31	O	1	Total C O 6 3 3	0	0
31	V	1	Total C O 6 3 3	0	0
31	a	1	Total C O 6 3 3	0	0
31	b	1	Total C O 6 3 3	0	0
31	b	1	Total C O 6 3 3	0	0
31	d	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	v	1	Total	C	O	0	0
			6	3	3		

- Molecule 32 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



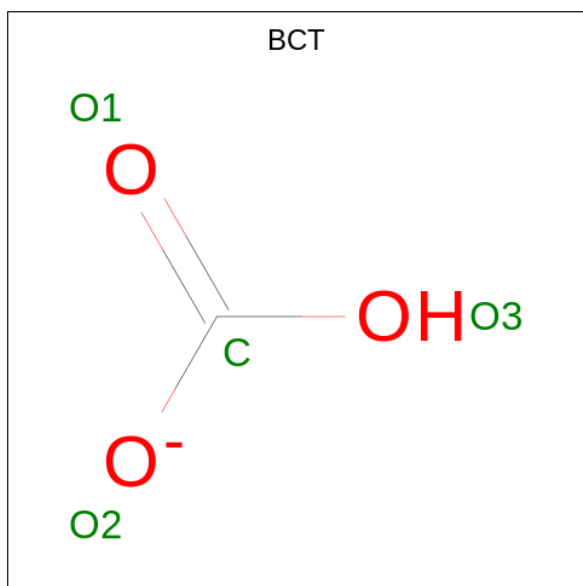
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			35	24	11		
32	B	1	Total	C	O	0	0
			35	24	11		
32	B	1	Total	C	O	0	0
			35	24	11		
32	D	1	Total	C	O	0	0
			35	24	11		
32	D	1	Total	C	O	0	0
			35	24	11		
32	F	1	Total	C	O	0	0
			35	24	11		
32	J	1	Total	C	O	0	0
			24	18	6		
32	M	1	Total	C	O	0	0
			35	24	11		
32	M	1	Total	C	O	0	0
			35	24	11		
32	a	1	Total	C	O	0	0
			35	24	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	a	1	Total	C	O	0	0
			35	24	11		
32	b	1	Total	C	O	0	0
			35	24	11		
32	b	1	Total	C	O	0	0
			35	24	11		
32	b	1	Total	C	O	0	0
			24	18	6		
32	f	1	Total	C	O	0	0
			25	19	6		
32	j	1	Total	C	O	0	0
			24	18	6		
32	m	1	Total	C	O	0	0
			35	24	11		
32	m	1	Total	C	O	0	0
			35	24	11		

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



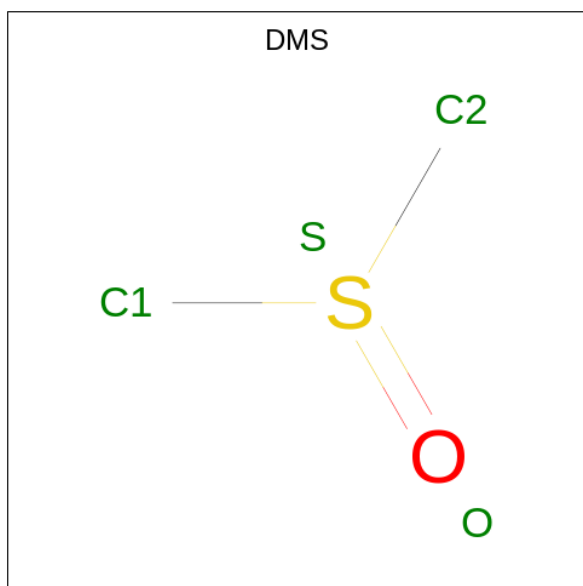
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	A	1	Total	C	O	0	1
			4	1	3		
33	D	1	Total	C	O	0	1
			4	1	3		
33	a	1	Total	C	O	0	1
			4	1	3		

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

- Molecule 34 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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	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
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	E	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	T	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
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	a	1	Total 4	C 2	O 1	S 1	0	0
34	a	1	Total 4	C 2	O 1	S 1	0	0
34	a	1	Total 4	C 2	O 1	S 1	0	0
34	a	1	Total 4	C 2	O 1	S 1	0	0
34	a	1	Total 4	C 2	O 1	S 1	0	0
34	a	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
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

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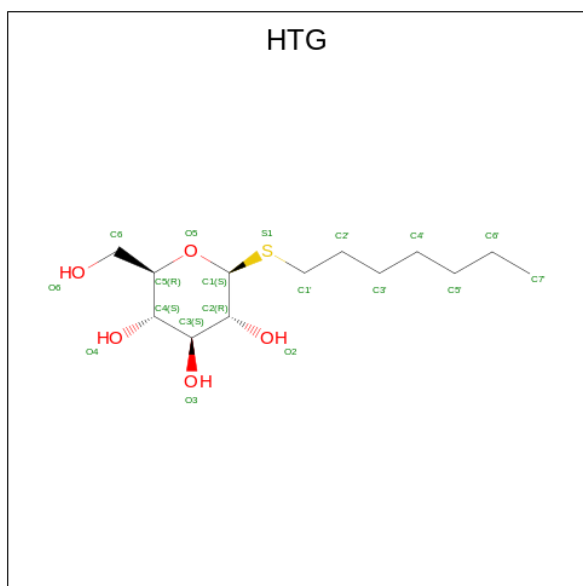
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	d	1	Total 4	C 2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

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

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

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



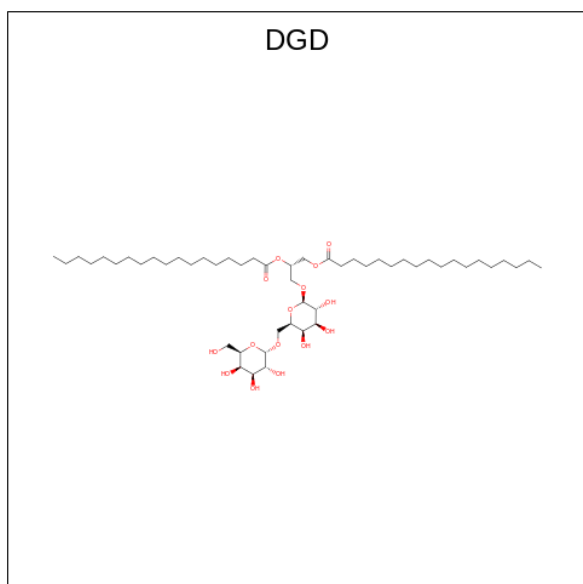
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	B	1	Total C O S 19 13 5 1	0	0
36	B	1	Total C O S 19 13 5 1	0	0
36	B	1	Total C O S 19 13 5 1	0	0
36	B	1	Total C O S 19 13 5 1	0	0
36	C	1	Total C O S 19 13 5 1	0	0
36	C	1	Total C O S 19 13 5 1	0	0

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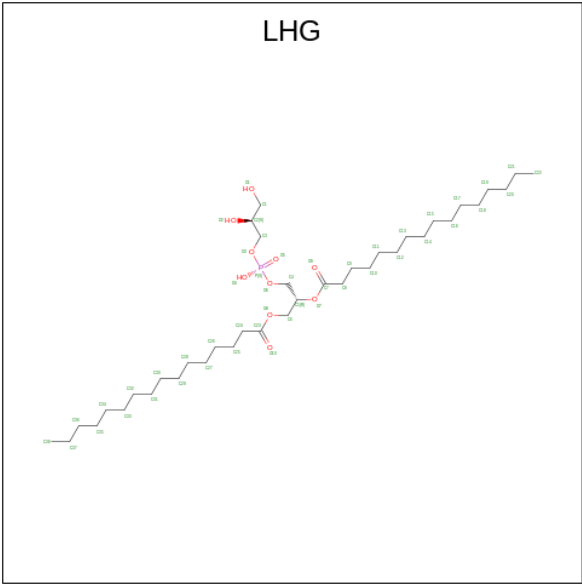
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	H	1	Total	C	O	S	0	0
			16	10	5	1		
36	O	1	Total	C	O	S	0	0
			19	13	5	1		
36	V	1	Total	C	O	S	0	0
			12	6	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	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	d	1	Total	C	O	S	0	0
			16	10	5	1		
36	o	1	Total	C	O	S	0	0
			19	13	5	1		
36	u	1	Total	C	O	S	0	0
			14	10	3	1		

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



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	C	1	Total	C	O	0	0
			62	47	15		
37	H	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
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: C₃₈H₇₅O₁₀P).



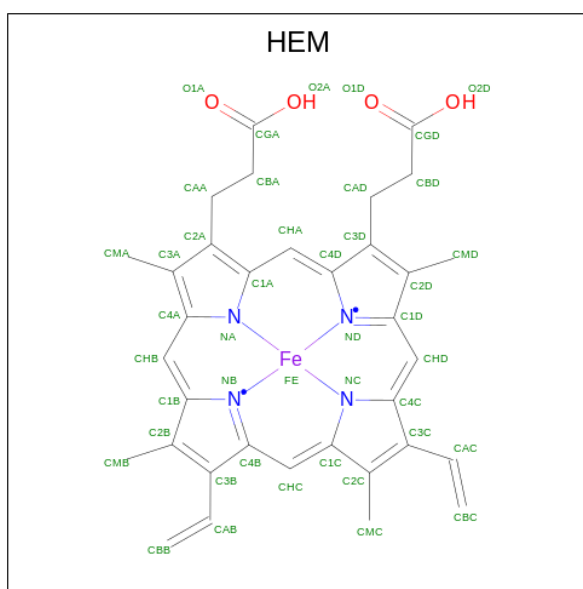
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	D	1	Total	C	O	P	0	0
			49	38	10	1		
38	D	1	Total	C	O	P	0	0
			49	38	10	1		

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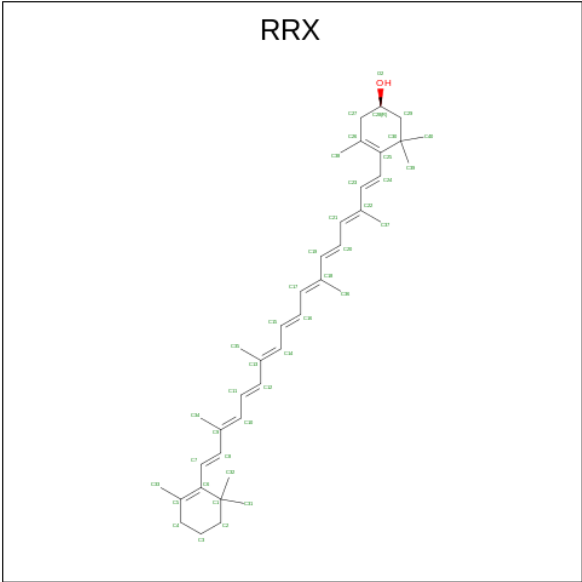
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	D	1	Total	C	O	P	0	0
			45	34	10	1		
38	E	1	Total	C	O	P	0	0
			42	31	10	1		
38	L	1	Total	C	O	P	0	0
			49	38	10	1		
38	a	1	Total	C	O	P	0	0
			42	31	10	1		
38	d	1	Total	C	O	P	0	0
			49	38	10	1		
38	d	1	Total	C	O	P	0	0
			49	38	10	1		
38	d	1	Total	C	O	P	0	0
			46	35	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
			43	34	1	4	4	
39	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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

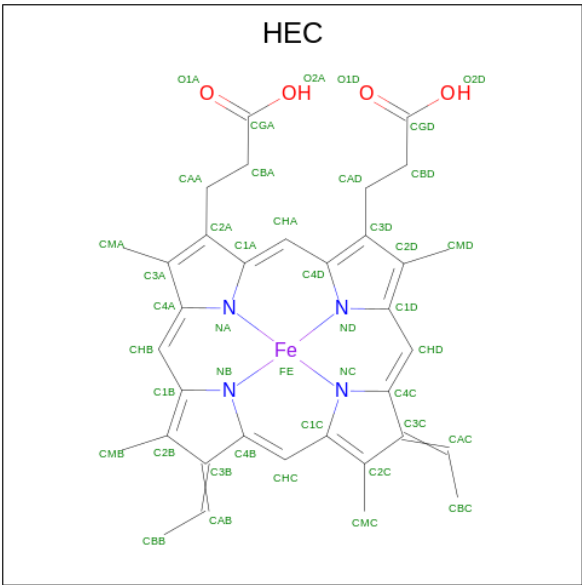


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
40	H	1	Total	C	O	0	0
			41	40	1		
40	h	1	Total	C	O	0	0
			41	40	1		

- 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: C₃₄H₃₄FeN₄O₄).



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

- Molecule 43 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
43	A	164	Total	O	0	5
			169	169		
43	B	394	Total	O	0	15
			408	408		
43	C	274	Total	O	0	8
			282	282		
43	D	171	Total	O	0	5
			176	176		
43	E	31	Total	O	0	1
			32	32		
43	F	14	Total	O	0	0
			14	14		
43	H	56	Total	O	0	0
			56	56		
43	I	9	Total	O	0	0
			9	9		
43	J	16	Total	O	0	0
			16	16		
43	K	8	Total	O	0	1
			9	9		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
43	L	20	Total O 20 20	0	1
43	M	17	Total O 19 19	0	2
43	O	197	Total O 208 208	0	13
43	T	11	Total O 11 11	0	0
43	U	99	Total O 99 99	0	1
43	V	143	Total O 146 146	0	3
43	X	16	Total O 17 17	0	1
43	Y	7	Total O 7 7	0	0
43	Z	1	Total O 1 1	0	0
43	a	184	Total O 192 192	0	9
43	b	381	Total O 390 390	0	15
43	c	285	Total O 298 298	0	12
43	d	170	Total O 176 176	0	8
43	e	33	Total O 34 34	0	1
43	f	8	Total O 9 9	0	1
43	h	55	Total O 57 57	0	2
43	i	19	Total O 21 21	0	2
43	j	15	Total O 16 16	0	2
43	k	11	Total O 11 11	0	0
43	l	15	Total O 17 17	0	3
43	m	23	Total O 26 26	0	3

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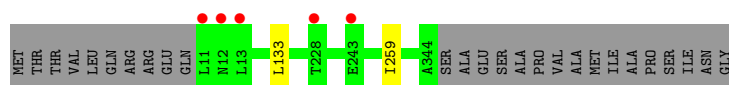
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
43	o	176	Total 188	O 188	0	12
43	t	18	Total 19	O 19	0	2
43	u	109	Total 114	O 114	0	6
43	v	112	Total 114	O 114	0	2
43	x	19	Total 19	O 19	0	0
43	y	5	Total 5	O 5	0	0
43	z	4	Total 4	O 4	0	0

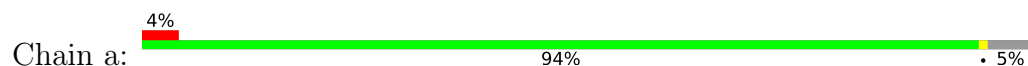
3 Residue-property plots [i](#)

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

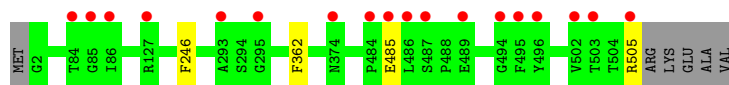
- Molecule 1: Photosystem II protein D1 3



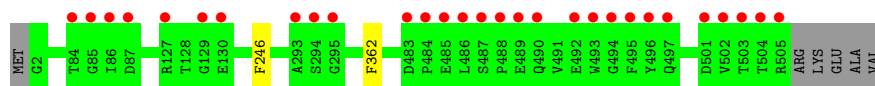
- Molecule 1: Photosystem II protein D1 3



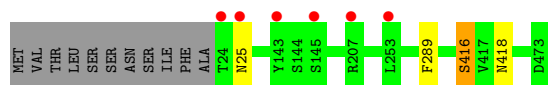
- Molecule 2: Photosystem II CP47 reaction center protein



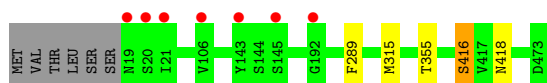
- Molecule 2: Photosystem II CP47 reaction center protein



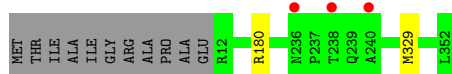
- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein



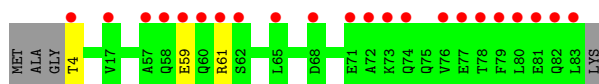
• Molecule 4: Photosystem II D2 protein



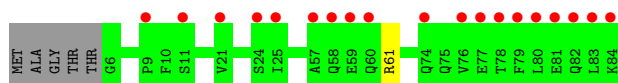
• Molecule 4: Photosystem II D2 protein



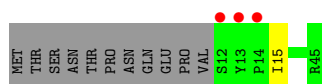
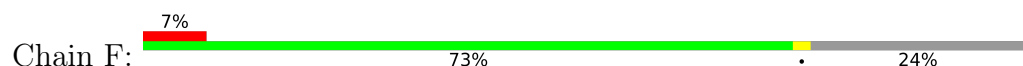
• Molecule 5: Cytochrome b559 subunit alpha



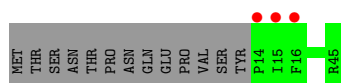
• Molecule 5: Cytochrome b559 subunit alpha



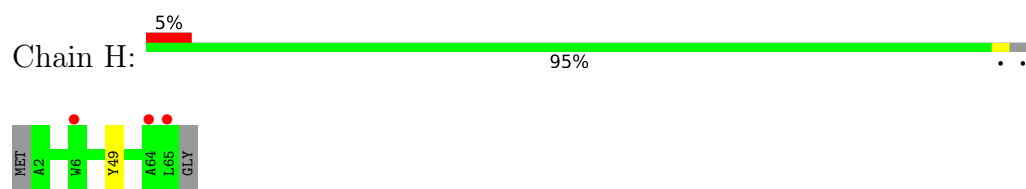
• Molecule 6: Cytochrome b559 subunit beta



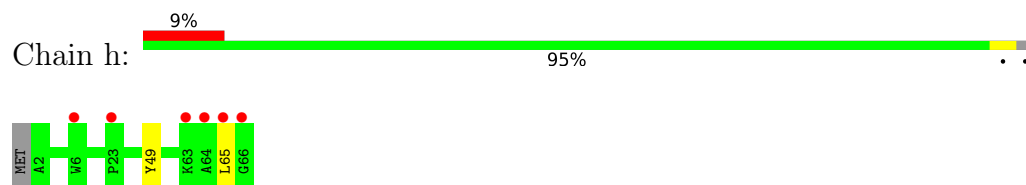
• Molecule 6: Cytochrome b559 subunit beta



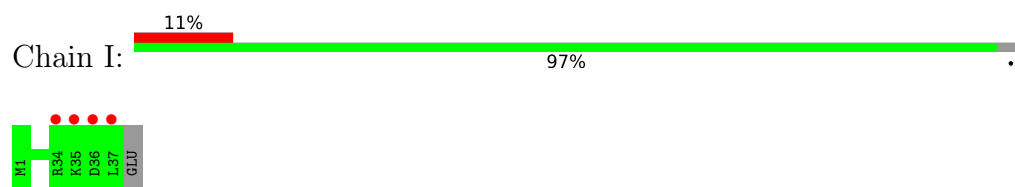
- Molecule 7: Photosystem II reaction center protein H



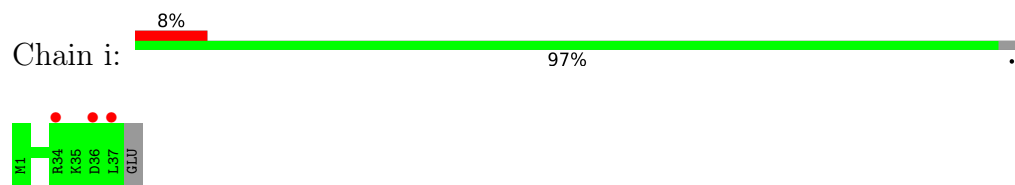
- Molecule 7: Photosystem II reaction center protein H



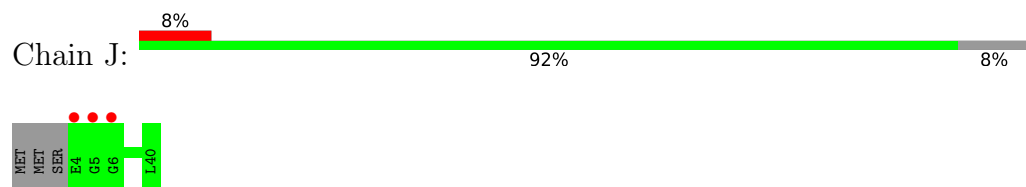
- Molecule 8: Photosystem II reaction center protein I



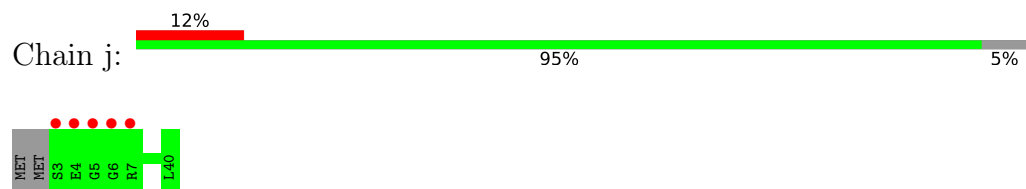
- Molecule 8: Photosystem II reaction center protein I



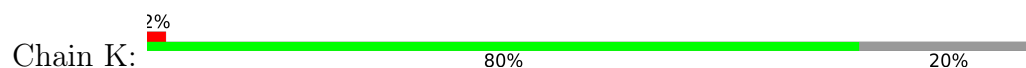
- Molecule 9: Photosystem II reaction center protein J

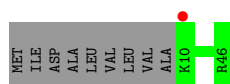


- Molecule 9: Photosystem II reaction center protein J

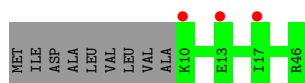
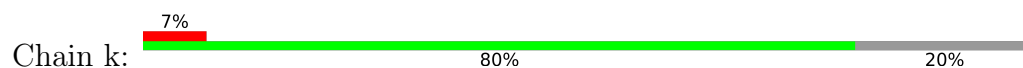


- Molecule 10: Photosystem II reaction center protein K

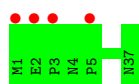




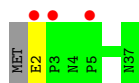
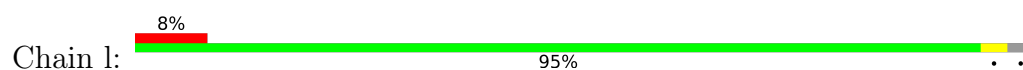
- Molecule 10: Photosystem II reaction center protein K



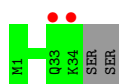
- Molecule 11: Photosystem II reaction center protein L



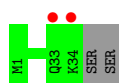
- Molecule 11: Photosystem II reaction center protein L



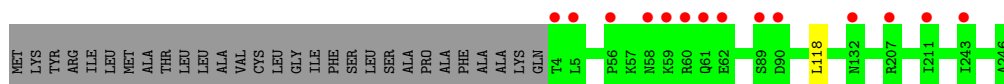
- Molecule 12: Photosystem II reaction center protein M



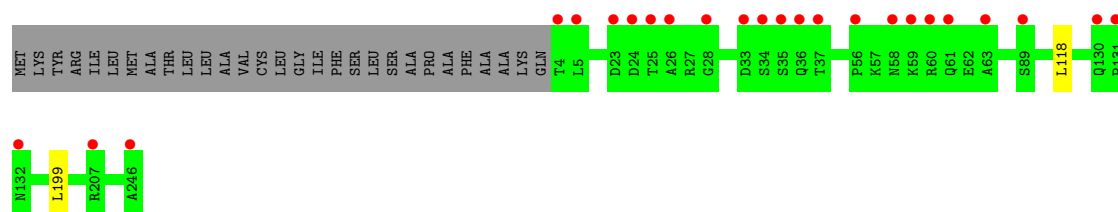
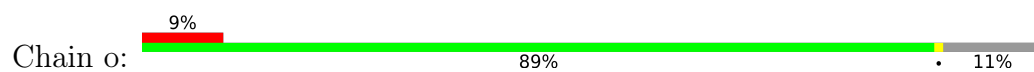
- Molecule 12: Photosystem II reaction center protein M



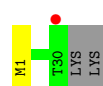
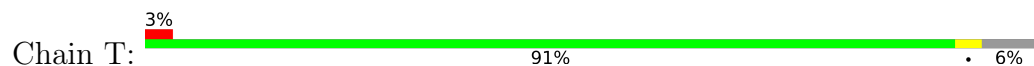
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



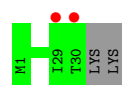
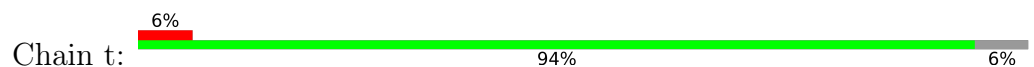
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



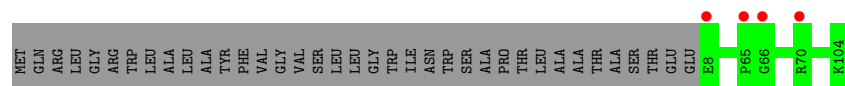
- Molecule 14: Photosystem II reaction center protein T



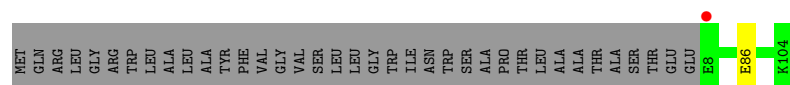
- Molecule 14: Photosystem II reaction center protein T



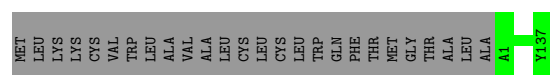
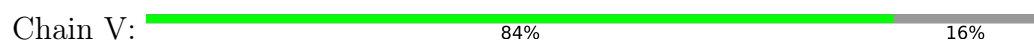
- Molecule 15: Photosystem II 12 kDa extrinsic protein



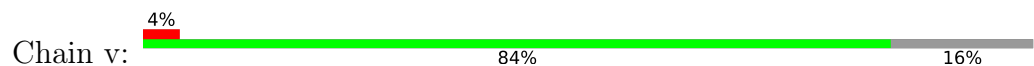
- Molecule 15: Photosystem II 12 kDa extrinsic protein

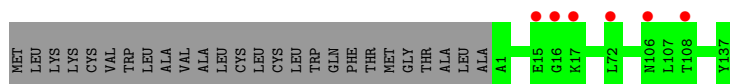


- Molecule 16: Cytochrome c-550

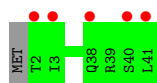


- Molecule 16: Cytochrome c-550





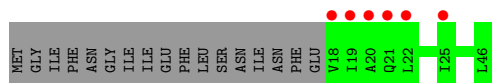
- Molecule 17: Photosystem II reaction center X protein



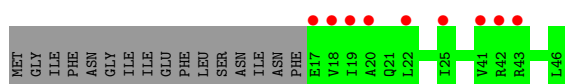
- Molecule 17: Photosystem II reaction center X protein



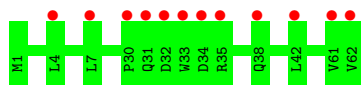
- Molecule 18: Photosystem II reaction center protein Ycf12



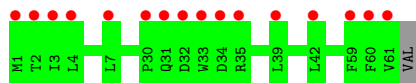
- Molecule 18: Photosystem II reaction center protein Ycf12



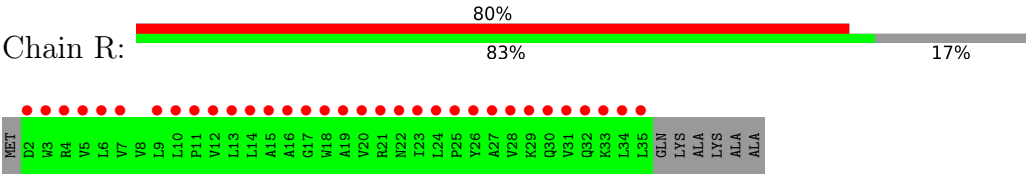
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	122.80Å 228.46Å 286.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 1.90 19.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.99-1.90) 99.6 (19.99-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, REFMAC 5.8.0103	Depositor
R, R_{free}	0.147 , 0.177 0.147 , 0.177	Depositor DCC
R_{free} test set	31327 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 78.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	55105	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, CLA, HTG, PL9, DGD, LMT, GOL, BCR, FME, MG, UNL, BCT, CL, RRX, LMG, HEM, CA, OEX, LHG, SQD, DMS, PHO, FE2

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	0.46	0/2709	0.56	0/3699
1	a	0.44	0/2743	0.54	0/3747
2	B	0.44	0/4145	0.53	0/5649
2	b	0.41	0/4134	0.53	0/5632
3	C	0.39	0/3608	0.51	0/4912
3	c	0.37	0/3653	0.50	0/4974
4	D	0.48	0/2812	0.56	0/3833
4	d	0.44	0/2817	0.53	0/3839
5	E	0.37	0/669	0.47	0/915
5	e	0.30	0/667	0.46	0/910
6	F	0.38	0/284	0.46	0/387
6	f	0.30	0/265	0.44	0/360
7	H	0.38	0/527	0.52	0/718
7	h	0.36	0/532	0.53	0/723
8	I	0.36	0/284	0.49	0/388
8	i	0.33	0/301	0.48	0/407
9	J	0.36	0/262	0.48	0/356
9	j	0.33	0/278	0.46	0/376
10	K	0.31	0/303	0.44	0/416
10	k	0.30	0/303	0.45	0/416
11	L	0.52	0/315	0.52	0/428
11	l	0.51	0/311	0.49	0/423
12	M	0.40	0/254	0.54	0/348
12	m	0.42	0/270	0.56	0/368
13	O	0.36	0/1903	0.57	0/2583
13	o	0.35	0/1888	0.57	0/2564
14	T	0.52	0/257	0.51	0/349
14	t	0.46	0/257	0.49	0/349
15	U	0.36	0/781	0.53	0/1059
15	u	0.36	0/785	0.52	0/1064
16	V	0.38	0/1091	0.52	0/1481

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.30	0/1090	0.50	0/1483
17	X	0.29	0/301	0.40	0/407
17	x	0.29	0/278	0.42	0/376
18	Y	0.28	0/207	0.43	0/278
18	y	0.26	0/216	0.42	0/289
19	Z	0.28	0/509	0.40	0/699
19	z	0.27	0/461	0.37	0/633
20	R	0.23	0/208	0.39	0/289
All	All	0.40	0/42678	0.52	0/58127

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/360 (92%)	328 (98%)	4 (1%)	1 (0%)	41	31
1	a	340/360 (94%)	335 (98%)	3 (1%)	2 (1%)	25	15
2	B	507/510 (99%)	501 (99%)	6 (1%)	0	100	100
2	b	508/510 (100%)	503 (99%)	5 (1%)	0	100	100
3	C	450/461 (98%)	440 (98%)	8 (2%)	2 (0%)	34	24
3	c	457/461 (99%)	448 (98%)	7 (2%)	2 (0%)	34	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	340/352 (97%)	334 (98%)	6 (2%)	0	100	100
4	d	340/352 (97%)	334 (98%)	6 (2%)	0	100	100
5	E	79/84 (94%)	78 (99%)	1 (1%)	0	100	100
5	e	79/84 (94%)	79 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	30/45 (67%)	30 (100%)	0	0	100	100
7	H	63/66 (96%)	59 (94%)	4 (6%)	0	100	100
7	h	64/66 (97%)	59 (92%)	4 (6%)	1 (2%)	9	2
8	I	35/38 (92%)	33 (94%)	2 (6%)	0	100	100
8	i	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
9	J	35/40 (88%)	35 (100%)	0	0	100	100
9	j	36/40 (90%)	36 (100%)	0	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	36/37 (97%)	36 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	33/36 (92%)	33 (100%)	0	0	100	100
13	O	245/272 (90%)	239 (98%)	6 (2%)	0	100	100
13	o	244/272 (90%)	237 (97%)	7 (3%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
15	u	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
16	V	136/163 (83%)	134 (98%)	2 (2%)	0	100	100
16	v	136/163 (83%)	134 (98%)	2 (2%)	0	100	100
17	X	39/41 (95%)	38 (97%)	1 (3%)	0	100	100
17	x	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	Y	27/46 (59%)	26 (96%)	1 (4%)	0	100	100
18	y	28/46 (61%)	28 (100%)	0	0	100	100
19	Z	65/62 (105%)	61 (94%)	4 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	z	59/62 (95%)	56 (95%)	3 (5%)	0	100	100
20	R	32/41 (78%)	30 (94%)	2 (6%)	0	100	100
All	All	5262/5691 (92%)	5162 (98%)	92 (2%)	8 (0%)	51	38

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	4	VAL
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
7	h	65	LEU
1	A	259	ILE
1	a	259	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/291 (93%)	269 (100%)	1 (0%)	91	91
1	a	269/291 (92%)	269 (100%)	0	100	100
2	B	405/407 (100%)	401 (99%)	4 (1%)	76	76
2	b	401/407 (98%)	399 (100%)	2 (0%)	88	89
3	C	354/362 (98%)	349 (99%)	5 (1%)	67	65
3	c	359/362 (99%)	353 (98%)	6 (2%)	60	57
4	D	276/283 (98%)	274 (99%)	2 (1%)	84	84
4	d	276/283 (98%)	274 (99%)	2 (1%)	84	84
5	E	70/73 (96%)	67 (96%)	3 (4%)	29	19
5	e	69/73 (94%)	68 (99%)	1 (1%)	67	65
6	F	28/39 (72%)	27 (96%)	1 (4%)	35	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	f	26/39 (67%)	26 (100%)	0	100	100
7	H	54/55 (98%)	53 (98%)	1 (2%)	57	53
7	h	54/55 (98%)	53 (98%)	1 (2%)	57	53
8	I	29/34 (85%)	29 (100%)	0	100	100
8	i	33/34 (97%)	33 (100%)	0	100	100
9	J	23/28 (82%)	23 (100%)	0	100	100
9	j	26/28 (93%)	26 (100%)	0	100	100
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	30 (100%)	0	100	100
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	34 (97%)	1 (3%)	42	35
12	M	28/32 (88%)	28 (100%)	0	100	100
12	m	31/32 (97%)	31 (100%)	0	100	100
13	O	205/228 (90%)	204 (100%)	1 (0%)	88	89
13	o	202/228 (89%)	200 (99%)	2 (1%)	76	76
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	83/112 (74%)	83 (100%)	0	100	100
15	u	84/112 (75%)	83 (99%)	1 (1%)	71	70
16	V	118/138 (86%)	118 (100%)	0	100	100
16	v	116/138 (84%)	116 (100%)	0	100	100
17	X	32/34 (94%)	32 (100%)	0	100	100
17	x	29/34 (85%)	28 (97%)	1 (3%)	37	28
18	Y	20/37 (54%)	20 (100%)	0	100	100
18	y	20/37 (54%)	20 (100%)	0	100	100
19	Z	49/52 (94%)	49 (100%)	0	100	100
19	z	45/52 (86%)	45 (100%)	0	100	100
20	R	11/33 (33%)	11 (100%)	0	100	100
All	All	4277/4643 (92%)	4242 (99%)	35 (1%)	81	82

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	LEU
2	B	246	PHE
2	B	362	PHE
2	B	485	GLU
2	B	505	ARG
3	C	25	ASN
3	C	289	PHE
3	C	416[A]	SER
3	C	416[B]	SER
3	C	418	ASN
4	D	180	ARG
4	D	329	MET
5	E	4	THR
5	E	59	GLU
5	E	61	ARG
6	F	15	ILE
7	H	49	TYR
13	O	118	LEU
2	b	246	PHE
2	b	362	PHE
3	c	289	PHE
3	c	315	MET
3	c	355	THR
3	c	416[A]	SER
3	c	416[B]	SER
3	c	418	ASN
4	d	180	ARG
4	d	329	MET
5	e	61	ARG
7	h	49	TYR
11	l	2	GLU
13	o	118	LEU
13	o	199	LEU
15	u	86	GLU
17	x	37	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	I	1	8	8,9,10	0.90	0	7,9,11	0.68	0
8	FME	i	1	8	8,9,10	0.88	0	7,9,11	0.98	0
14	FME	T	1	14	8,9,10	0.98	0	7,9,11	1.57	1 (14%)
12	FME	M	1	12	8,9,10	0.93	0	7,9,11	0.68	0
14	FME	t	1	14	8,9,10	0.92	0	7,9,11	1.28	0
12	FME	m	1	12	8,9,10	1.04	0	7,9,11	0.50	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
8	FME	I	1	8	-	0/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
14	FME	T	1	14	-	3/7/9/11	-
12	FME	M	1	12	-	2/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	C-CA-N	3.12	115.37	109.73

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 362 ligands modelled in this entry, 13 are monoatomic and 82 are unknown - leaving 267 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	LMT	F	103	-	36,36,36	0.46	0	47,47,47	0.79	1 (2%)
36	HTG	d	404	-	16,16,19	1.01	1 (6%)	20,21,24	1.55	1 (5%)
38	LHG	D	410	-	48,48,48	0.84	2 (4%)	51,54,54	1.21	8 (15%)
24	CLA	B	610	-	65,73,73	2.39	20 (30%)	76,113,113	2.37	24 (31%)
24	CLA	b	606	-	65,73,73	2.39	20 (30%)	76,113,113	2.44	26 (34%)
34	DMS	A	425	-	3,3,3	0.67	0	3,3,3	0.55	0
31	GOL	C	525	-	5,5,5	0.71	0	5,5,5	0.92	0
26	BCR	B	619	-	41,41,41	1.01	1 (2%)	56,56,56	1.23	3 (5%)
29	PL9	a	417	-	55,55,55	0.63	1 (1%)	68,69,69	1.92	19 (27%)
31	GOL	O	304	-	5,5,5	0.90	0	5,5,5	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	DMS	c	539	-	3,3,3	0.69	0	3,3,3	0.53	0
27	SQD	B	622	-	53,54,54	1.03	3 (5%)	62,65,65	1.51	8 (12%)
24	CLA	b	609	-	65,73,73	2.37	18 (27%)	76,113,113	2.45	24 (31%)
40	RRX	h	101	-	42,42,42	3.99	15 (35%)	57,58,58	8.73	39 (68%)
36	HTG	B	629	-	19,19,19	0.95	2 (10%)	23,24,24	1.63	1 (4%)
34	DMS	b	633	-	3,3,3	0.66	0	3,3,3	0.66	0
39	HEM	e	102	6,5	41,50,50	1.34	8 (19%)	45,82,82	1.91	11 (24%)
24	CLA	b	610	-	65,73,73	2.43	19 (29%)	76,113,113	2.44	24 (31%)
31	GOL	b	638	-	5,5,5	0.97	0	5,5,5	0.98	0
34	DMS	C	538	-	3,3,3	0.65	0	3,3,3	0.59	0
34	DMS	B	641	-	3,3,3	0.66	0	3,3,3	0.57	0
34	DMS	C	535	-	3,3,3	0.58	0	3,3,3	0.53	0
36	HTG	H	101	-	16,16,19	1.03	1 (6%)	20,21,24	1.76	4 (20%)
34	DMS	e	103	-	3,3,3	0.67	0	3,3,3	0.49	0
36	HTG	V	202	-	11,12,19	0.29	0	15,17,24	1.73	3 (20%)
26	BCR	a	414	-	41,41,41	1.05	1 (2%)	56,56,56	1.08	2 (3%)
34	DMS	u	202	-	3,3,3	0.68	0	3,3,3	0.55	0
34	DMS	C	540	-	3,3,3	0.66	0	3,3,3	0.60	0
36	HTG	B	626	-	19,19,19	0.98	1 (5%)	23,24,24	1.93	3 (13%)
34	DMS	A	424	-	3,3,3	0.64	0	3,3,3	0.56	0
36	HTG	B	630	-	19,19,19	0.97	1 (5%)	23,24,24	1.37	1 (4%)
34	DMS	B	642	-	3,3,3	0.67	0	3,3,3	0.56	0
28	LMG	c	522	-	51,51,55	0.96	2 (3%)	59,59,63	1.08	5 (8%)
27	SQD	A	411	-	53,54,54	0.94	3 (5%)	62,65,65	1.78	10 (16%)
24	CLA	B	616	-	65,73,73	2.27	21 (32%)	76,113,113	2.72	29 (38%)
34	DMS	c	529	-	3,3,3	0.67	0	3,3,3	0.61	0
34	DMS	c	531	-	3,3,3	0.67	0	3,3,3	0.39	0
28	LMG	D	413	41	51,51,55	0.83	2 (3%)	59,59,63	0.83	2 (3%)
24	CLA	D	401	43	65,73,73	2.09	19 (29%)	76,113,113	2.56	28 (36%)
27	SQD	a	401	-	53,54,54	1.04	3 (5%)	62,65,65	1.20	6 (9%)
34	DMS	c	537	-	3,3,3	0.67	0	3,3,3	0.58	0
37	DGD	c	519	-	63,63,67	0.87	2 (3%)	77,77,81	0.95	5 (6%)
38	LHG	d	410	-	48,48,48	0.87	2 (4%)	51,54,54	0.89	2 (3%)
34	DMS	D	418	-	3,3,3	0.63	0	3,3,3	0.31	0
24	CLA	a	410	43	65,73,73	2.24	18 (27%)	76,113,113	2.81	30 (39%)
34	DMS	a	403	-	3,3,3	0.66	0	3,3,3	0.52	0
27	SQD	f	802	-	42,43,54	1.17	3 (7%)	51,54,65	1.55	8 (15%)
21	OEX	a	404	43,3,1	0,15,15	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	C	509	43	65,73,73	2.48	20 (30%)	76,113,113	2.56	25 (32%)
29	PL9	A	413	-	55,55,55	0.61	2 (3%)	68,69,69	1.89	20 (29%)
31	GOL	V	207	-	5,5,5	0.89	0	5,5,5	0.95	0
34	DMS	b	643	-	3,3,3	0.63	0	3,3,3	0.60	0
34	DMS	c	538	-	3,3,3	0.64	0	3,3,3	0.41	0
24	CLA	b	612	-	65,73,73	2.44	19 (29%)	76,113,113	2.35	27 (35%)
28	LMG	z	101	-	37,37,55	0.97	2 (5%)	45,45,63	1.31	6 (13%)
34	DMS	c	535	-	3,3,3	0.70	0	3,3,3	0.53	0
36	HTG	b	603	-	19,19,19	1.06	2 (10%)	23,24,24	0.99	1 (4%)
24	CLA	a	413	-	65,73,73	2.20	18 (27%)	76,113,113	2.60	28 (36%)
24	CLA	b	619	-	65,73,73	2.25	18 (27%)	76,113,113	2.52	26 (34%)
33	BCT	A	423[B]	22	2,3,3	0.65	0	2,3,3	0.56	0
24	CLA	c	506	43	65,73,73	2.32	19 (29%)	76,113,113	2.54	29 (38%)
28	LMG	b	624	-	51,51,55	0.92	2 (3%)	59,59,63	1.12	6 (10%)
31	GOL	A	418	-	5,5,5	1.01	0	5,5,5	1.00	0
37	DGD	d	416	-	50,50,67	0.98	2 (4%)	58,58,81	1.08	4 (6%)
28	LMG	C	521	-	51,51,55	0.96	2 (3%)	59,59,63	1.13	5 (8%)
31	GOL	a	419	-	5,5,5	1.03	0	5,5,5	0.89	0
24	CLA	a	409	-	65,73,73	2.41	20 (30%)	76,113,113	2.43	25 (32%)
32	LMT	m	103	-	36,36,36	0.46	0	47,47,47	0.89	2 (4%)
27	SQD	A	415	-	53,54,54	1.00	3 (5%)	62,65,65	1.33	8 (12%)
34	DMS	h	107	-	3,3,3	0.66	0	3,3,3	0.50	0
38	LHG	D	412	-	44,44,48	0.87	2 (4%)	47,50,54	1.09	3 (6%)
24	CLA	b	607	-	65,73,73	2.44	19 (29%)	76,113,113	2.48	27 (35%)
34	DMS	O	310	-	3,3,3	0.67	0	3,3,3	0.73	0
34	DMS	c	530	-	3,3,3	0.61	0	3,3,3	0.64	0
34	DMS	B	643	-	3,3,3	0.68	0	3,3,3	0.53	0
34	DMS	V	208	-	3,3,3	0.65	0	3,3,3	0.72	0
24	CLA	b	614	43	65,73,73	2.40	19 (29%)	76,113,113	2.38	28 (36%)
24	CLA	A	405	-	65,73,73	2.36	18 (27%)	76,113,113	2.32	25 (32%)
24	CLA	B	612	43	65,73,73	2.35	20 (30%)	76,113,113	2.42	25 (32%)
32	LMT	b	629	-	24,24,36	0.49	0	29,29,47	1.25	5 (17%)
24	CLA	c	515	-	65,73,73	2.60	20 (30%)	76,113,113	2.39	24 (31%)
32	LMT	b	625	-	36,36,36	0.44	0	47,47,47	1.20	5 (10%)
34	DMS	T	103	-	3,3,3	0.66	0	3,3,3	0.65	0
34	DMS	a	422	-	3,3,3	0.74	0	3,3,3	0.28	0
34	DMS	b	644	-	3,3,3	0.66	0	3,3,3	0.67	0
24	CLA	c	504	-	65,73,73	2.53	20 (30%)	76,113,113	2.32	25 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	DMS	c	534	-	3,3,3	0.67	0	3,3,3	0.52	0
34	DMS	v	205	-	3,3,3	0.68	0	3,3,3	0.52	0
36	HTG	b	628	-	19,19,19	1.03	2 (10%)	23,24,24	1.63	3 (13%)
24	CLA	c	508	-	65,73,73	2.62	20 (30%)	76,113,113	2.41	27 (35%)
34	DMS	C	536	-	3,3,3	0.69	0	3,3,3	0.46	0
24	CLA	B	607	-	65,73,73	2.45	18 (27%)	76,113,113	2.63	24 (31%)
34	DMS	V	210	-	3,3,3	0.66	0	3,3,3	0.51	0
37	DGD	H	104	-	63,63,67	0.88	3 (4%)	77,77,81	0.97	4 (5%)
34	DMS	d	418	-	3,3,3	0.66	0	3,3,3	0.65	0
24	CLA	B	605	-	65,73,73	2.34	19 (29%)	76,113,113	2.61	25 (32%)
34	DMS	E	104	-	3,3,3	0.67	0	3,3,3	0.52	0
34	DMS	O	305	-	3,3,3	0.64	0	3,3,3	0.43	0
34	DMS	B	634	-	3,3,3	0.65	0	3,3,3	0.75	0
32	LMT	M	102	-	36,36,36	0.40	0	47,47,47	0.86	0
24	CLA	B	614	-	65,73,73	2.21	18 (27%)	76,113,113	2.49	25 (32%)
34	DMS	O	307	-	3,3,3	0.68	0	3,3,3	0.58	0
42	HEC	V	201	16	32,50,50	1.50	4 (12%)	24,82,82	1.41	3 (12%)
37	DGD	C	520	-	63,63,67	0.81	2 (3%)	77,77,81	0.98	4 (5%)
24	CLA	C	505	-	65,73,73	2.81	19 (29%)	76,113,113	2.29	23 (30%)
34	DMS	a	426	-	3,3,3	0.65	0	3,3,3	0.45	0
32	LMT	j	102	-	24,24,36	0.49	0	29,29,47	0.76	0
24	CLA	B	606	-	65,73,73	2.36	19 (29%)	76,113,113	2.47	25 (32%)
34	DMS	c	536	-	3,3,3	0.65	0	3,3,3	0.57	0
34	DMS	d	417	-	3,3,3	0.64	0	3,3,3	0.33	0
34	DMS	d	419	-	3,3,3	0.68	0	3,3,3	0.56	0
36	HTG	b	602	-	19,19,19	0.99	2 (10%)	23,24,24	1.54	1 (4%)
29	PL9	D	408	-	55,55,55	0.72	2 (3%)	68,69,69	1.56	16 (23%)
29	PL9	d	408	-	55,55,55	0.77	2 (3%)	68,69,69	1.47	13 (19%)
32	LMT	m	102	-	36,36,36	0.42	0	47,47,47	0.95	1 (2%)
25	PHO	A	407	-	51,69,69	1.70	7 (13%)	47,99,99	1.65	10 (21%)
33	BCT	D	404[A]	22	2,3,3	0.63	0	2,3,3	1.05	0
34	DMS	o	304	-	3,3,3	0.66	0	3,3,3	0.52	0
33	BCT	d	402[B]	22	2,3,3	0.61	0	2,3,3	1.15	0
24	CLA	B	611	-	65,73,73	2.47	18 (27%)	76,113,113	2.43	23 (30%)
26	BCR	d	407	-	41,41,41	1.06	1 (2%)	56,56,56	1.56	13 (23%)
34	DMS	C	539	-	3,3,3	0.64	0	3,3,3	0.69	0
36	HTG	u	201	-	10,13,19	1.18	1 (10%)	13,14,24	1.79	1 (7%)
37	DGD	c	520	-	63,63,67	0.82	2 (3%)	77,77,81	0.94	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	b	621	-	41,41,41	1.04	1 (2%)	56,56,56	1.37	7 (12%)
24	CLA	B	603	43	65,73,73	2.49	21 (32%)	76,113,113	2.45	22 (28%)
33	BCT	a	408[A]	22	2,3,3	0.66	0	2,3,3	0.53	0
34	DMS	u	203	-	3,3,3	0.61	0	3,3,3	0.76	0
26	BCR	D	407	-	41,41,41	1.05	1 (2%)	56,56,56	1.59	12 (21%)
34	DMS	o	303	-	3,3,3	0.63	0	3,3,3	0.58	0
24	CLA	A	406	43	65,73,73	2.18	19 (29%)	76,113,113	2.56	28 (36%)
24	CLA	b	618	-	65,73,73	2.21	18 (27%)	76,113,113	2.60	28 (36%)
34	DMS	a	424	-	3,3,3	0.66	0	3,3,3	0.60	0
24	CLA	b	613	-	65,73,73	2.67	19 (29%)	76,113,113	2.45	24 (31%)
26	BCR	k	103	-	41,41,41	1.00	1 (2%)	56,56,56	1.38	9 (16%)
32	LMT	a	421	-	36,36,36	0.46	0	47,47,47	1.05	5 (10%)
37	DGD	C	518	-	63,63,67	0.83	3 (4%)	77,77,81	1.07	5 (6%)
24	CLA	c	510	-	65,73,73	2.33	18 (27%)	76,113,113	2.57	24 (31%)
26	BCR	B	621	-	41,41,41	1.01	1 (2%)	56,56,56	1.24	4 (7%)
24	CLA	a	411	43	65,73,73	2.17	19 (29%)	76,113,113	2.51	26 (34%)
24	CLA	b	615	-	65,73,73	2.40	19 (29%)	76,113,113	2.57	28 (36%)
24	CLA	C	507	-	65,73,73	2.54	20 (30%)	76,113,113	2.29	21 (27%)
34	DMS	v	202	-	3,3,3	0.63	0	3,3,3	0.51	0
24	CLA	C	506	43	65,73,73	2.31	20 (30%)	76,113,113	2.61	30 (39%)
26	BCR	t	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.49	11 (19%)
32	LMT	b	626	-	36,36,36	0.39	0	47,47,47	0.97	3 (6%)
24	CLA	C	513	3	65,73,73	2.44	20 (30%)	76,113,113	2.36	26 (34%)
26	BCR	K	102	-	41,41,41	1.02	1 (2%)	56,56,56	1.35	8 (14%)
26	BCR	b	622	-	41,41,41	1.05	1 (2%)	56,56,56	1.24	6 (10%)
34	DMS	V	211	-	3,3,3	0.66	0	3,3,3	0.57	0
24	CLA	b	617	-	65,73,73	2.32	20 (30%)	76,113,113	2.52	25 (32%)
34	DMS	v	204	-	3,3,3	0.65	0	3,3,3	0.53	0
24	CLA	c	514	-	65,73,73	2.57	19 (29%)	76,113,113	2.44	29 (38%)
34	DMS	O	308	-	3,3,3	0.68	0	3,3,3	0.57	0
24	CLA	B	618	-	65,73,73	2.32	18 (27%)	76,113,113	2.55	23 (30%)
27	SQD	F	101	-	42,43,54	1.18	3 (7%)	51,54,65	1.82	9 (17%)
28	LMG	B	623	-	51,51,55	0.95	2 (3%)	59,59,63	1.21	5 (8%)
28	LMG	d	412	41	51,51,55	0.87	2 (3%)	59,59,63	0.90	3 (5%)
24	CLA	C	515	-	65,73,73	2.57	19 (29%)	76,113,113	2.40	25 (32%)
24	CLA	c	509	43	65,73,73	2.60	20 (30%)	76,113,113	2.48	24 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	DMS	C	534	-	3,3,3	0.70	0	3,3,3	0.31	0
31	GOL	A	421	-	5,5,5	0.90	0	5,5,5	1.00	0
28	LMG	C	533	-	51,51,55	0.97	2 (3%)	59,59,63	1.14	6 (10%)
26	BCR	B	620	-	41,41,41	1.01	1 (2%)	56,56,56	1.19	4 (7%)
31	GOL	d	415	-	5,5,5	0.91	0	5,5,5	0.79	0
28	LMG	i	101	-	51,51,55	0.89	2 (3%)	59,59,63	1.14	5 (8%)
36	HTG	o	301	-	19,19,19	1.02	1 (5%)	23,24,24	1.50	2 (8%)
38	LHG	D	411	-	48,48,48	0.84	2 (4%)	51,54,54	0.93	3 (5%)
25	PHO	A	408	-	51,69,69	1.86	8 (15%)	47,99,99	1.73	7 (14%)
24	CLA	D	405	-	65,73,73	2.09	19 (29%)	76,113,113	2.63	27 (35%)
24	CLA	c	503	-	65,73,73	2.48	20 (30%)	76,113,113	2.60	24 (31%)
24	CLA	c	513	3	65,73,73	2.56	19 (29%)	76,113,113	2.26	28 (36%)
27	SQD	a	415	-	53,54,54	0.93	3 (5%)	62,65,65	1.92	11 (17%)
24	CLA	B	608	-	65,73,73	2.34	17 (26%)	76,113,113	2.79	26 (34%)
26	BCR	k	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.45	9 (16%)
24	CLA	b	611	43	65,73,73	2.34	20 (30%)	76,113,113	2.42	27 (35%)
34	DMS	b	631	-	3,3,3	0.66	0	3,3,3	0.31	0
34	DMS	b	632	-	3,3,3	0.64	0	3,3,3	0.37	0
34	DMS	b	642	-	3,3,3	0.67	0	3,3,3	0.58	0
38	LHG	L	101	-	48,48,48	0.88	2 (4%)	51,54,54	1.04	4 (7%)
24	CLA	C	514	-	65,73,73	2.39	20 (30%)	76,113,113	2.45	28 (36%)
34	DMS	O	309	-	3,3,3	0.68	0	3,3,3	0.74	0
38	LHG	d	411	-	45,45,48	0.93	2 (4%)	48,51,54	1.05	4 (8%)
38	LHG	a	416	-	41,41,48	1.02	2 (4%)	44,47,54	1.01	2 (4%)
34	DMS	T	104	-	3,3,3	0.67	0	3,3,3	0.46	0
34	DMS	O	306	-	3,3,3	0.67	0	3,3,3	0.60	0
28	LMG	A	412	-	51,51,55	0.94	2 (3%)	59,59,63	1.08	3 (5%)
32	LMT	A	422	-	36,36,36	0.46	0	47,47,47	0.96	2 (4%)
26	BCR	T	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.44	12 (21%)
32	LMT	D	402	-	36,36,36	0.39	0	47,47,47	1.02	4 (8%)
25	PHO	d	401	-	51,69,69	1.82	8 (15%)	47,99,99	1.84	8 (17%)
24	CLA	D	406	-	65,73,73	2.27	19 (29%)	76,113,113	2.54	29 (38%)
31	GOL	v	203	-	5,5,5	0.91	0	5,5,5	1.09	0
34	DMS	B	632	-	3,3,3	0.67	0	3,3,3	0.40	0
24	CLA	C	503	-	65,73,73	2.40	20 (30%)	76,113,113	2.53	21 (27%)
24	CLA	b	620	-	65,73,73	2.45	18 (27%)	76,113,113	2.53	24 (31%)
34	DMS	b	641	-	3,3,3	0.68	0	3,3,3	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	DMS	O	302	-	3,3,3	0.62	0	3,3,3	0.46	0
36	HTG	c	523	-	19,19,19	0.97	2 (10%)	23,24,24	1.50	3 (13%)
34	DMS	a	425	-	3,3,3	0.65	0	3,3,3	0.58	0
38	LHG	E	101	-	41,41,48	1.03	2 (4%)	44,47,54	1.16	4 (9%)
26	BCR	C	517	-	41,41,41	1.01	1 (2%)	56,56,56	1.45	10 (17%)
24	CLA	c	512	-	65,73,73	2.33	20 (30%)	76,113,113	2.40	27 (35%)
24	CLA	b	616	-	65,73,73	2.45	19 (29%)	76,113,113	2.54	25 (32%)
24	CLA	C	511	-	65,73,73	2.49	20 (30%)	76,113,113	2.46	29 (38%)
21	OEX	A	401	43,3,1	0,15,15	-	-	-	-	-
27	SQD	b	601	-	53,54,54	1.02	4 (7%)	62,65,65	1.37	9 (14%)
37	DGD	C	519	-	63,63,67	0.83	2 (3%)	77,77,81	1.09	7 (9%)
24	CLA	C	510	-	65,73,73	2.36	19 (29%)	76,113,113	2.46	23 (30%)
24	CLA	A	409	-	65,73,73	2.26	21 (32%)	76,113,113	2.60	28 (36%)
24	CLA	C	504	-	65,73,73	2.52	20 (30%)	76,113,113	2.43	22 (28%)
34	DMS	C	501	-	3,3,3	0.68	0	3,3,3	0.58	0
36	HTG	O	303	-	19,19,19	1.01	1 (5%)	23,24,24	1.08	2 (8%)
24	CLA	B	604	-	65,73,73	2.35	20 (30%)	76,113,113	2.39	28 (36%)
24	CLA	C	508	-	65,73,73	2.49	21 (32%)	76,113,113	2.27	26 (34%)
32	LMT	B	624	-	36,36,36	0.40	0	47,47,47	1.23	5 (10%)
32	LMT	J	102	-	24,24,36	0.55	1 (4%)	29,29,47	0.93	1 (3%)
24	CLA	b	608	-	65,73,73	2.52	19 (29%)	76,113,113	2.36	23 (30%)
34	DMS	V	209	-	3,3,3	0.66	0	3,3,3	0.51	0
24	CLA	B	613	-	65,73,73	2.34	17 (26%)	76,113,113	2.45	28 (36%)
34	DMS	C	537	-	3,3,3	0.66	0	3,3,3	0.62	0
32	LMT	f	801	-	25,25,36	0.53	1 (4%)	30,30,47	0.57	0
32	LMT	D	409	-	36,36,36	0.48	0	47,47,47	1.08	4 (8%)
34	DMS	a	423	-	3,3,3	0.64	0	3,3,3	0.55	0
31	GOL	D	417	-	5,5,5	0.90	0	5,5,5	0.99	0
34	DMS	c	533	-	3,3,3	0.65	0	3,3,3	0.56	0
34	DMS	c	532	-	3,3,3	0.55	0	3,3,3	1.24	0
24	CLA	B	615	-	65,73,73	2.32	18 (27%)	76,113,113	2.51	24 (31%)
26	BCR	K	101	-	41,41,41	0.97	1 (2%)	56,56,56	1.54	12 (21%)
24	CLA	c	507	-	65,73,73	2.45	19 (29%)	76,113,113	2.34	25 (32%)
36	HTG	B	625	-	19,19,19	0.78	1 (5%)	23,24,24	1.70	4 (17%)
36	HTG	C	523	-	19,19,19	1.00	2 (10%)	23,24,24	1.60	2 (8%)
24	CLA	B	609	43	65,73,73	2.30	19 (29%)	76,113,113	2.40	24 (31%)
26	BCR	c	517	-	41,41,41	1.02	1 (2%)	56,56,56	1.34	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	d	406	-	65,73,73	2.34	20 (30%)	76,113,113	2.46	27 (35%)
32	LMT	M	101	-	36,36,36	0.44	0	47,47,47	0.99	2 (4%)
32	LMT	B	638	-	36,36,36	0.41	0	47,47,47	1.09	4 (8%)
34	DMS	B	633	-	3,3,3	0.65	0	3,3,3	0.27	0
24	CLA	B	617	-	65,73,73	2.23	20 (30%)	76,113,113	2.43	26 (34%)
37	DGD	c	518	-	63,63,67	0.86	2 (3%)	77,77,81	1.18	7 (9%)
34	DMS	B	640	-	3,3,3	0.64	0	3,3,3	0.47	0
28	LMG	c	521	-	51,51,55	0.93	2 (3%)	59,59,63	1.20	6 (10%)
38	LHG	d	409	-	48,48,48	0.83	2 (4%)	51,54,54	1.04	4 (7%)
26	BCR	C	516	-	41,41,41	1.00	1 (2%)	56,56,56	1.27	5 (8%)
24	CLA	C	512	-	65,73,73	2.37	19 (29%)	76,113,113	2.40	26 (34%)
32	LMT	a	402	-	36,36,36	0.40	0	47,47,47	0.84	1 (2%)
34	DMS	V	203	-	3,3,3	0.67	0	3,3,3	0.57	0
24	CLA	c	505	-	65,73,73	2.47	19 (29%)	76,113,113	2.33	23 (30%)
31	GOL	b	639	-	5,5,5	1.15	0	5,5,5	1.00	0
26	BCR	A	410	-	41,41,41	1.05	1 (2%)	56,56,56	1.45	13 (23%)
24	CLA	d	405	-	65,73,73	2.36	20 (30%)	76,113,113	2.41	26 (34%)
28	LMG	Z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.24	4 (8%)
39	HEM	F	102	6,5	41,50,50	1.35	5 (12%)	45,82,82	2.05	11 (24%)
38	LHG	l	102	-	48,48,48	0.86	2 (4%)	51,54,54	1.05	4 (7%)
36	HTG	C	522	-	19,19,19	1.00	2 (10%)	23,24,24	1.61	3 (13%)
24	CLA	b	605	43	65,73,73	2.49	19 (29%)	76,113,113	2.47	24 (31%)
34	DMS	o	305	-	3,3,3	0.65	0	3,3,3	0.53	0
24	CLA	c	511	-	65,73,73	2.46	19 (29%)	76,113,113	2.43	27 (35%)
36	HTG	c	524	-	19,19,19	1.01	2 (10%)	23,24,24	1.57	4 (17%)
26	BCR	b	623	-	41,41,41	1.08	1 (2%)	56,56,56	1.39	10 (17%)
26	BCR	c	516	-	41,41,41	1.06	1 (2%)	56,56,56	1.40	5 (8%)
40	RRX	H	103	-	42,42,42	4.02	15 (35%)	57,58,58	8.18	42 (73%)
42	HEC	v	201	16	32,50,50	1.51	4 (12%)	24,82,82	1.48	6 (25%)
37	DGD	h	102	-	63,63,67	0.92	4 (6%)	77,77,81	0.95	4 (5%)
34	DMS	B	639	-	3,3,3	0.66	0	3,3,3	0.51	0
25	PHO	a	412	-	51,69,69	1.73	7 (13%)	47,99,99	1.66	10 (21%)
36	HTG	b	627	-	19,19,19	0.88	1 (5%)	23,24,24	1.68	5 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LMT	F	103	-	-	10/21/61/61	0/2/2/2
36	HTG	d	404	-	-	2/7/27/30	0/1/1/1
38	LHG	D	410	-	-	5/53/53/53	-
24	CLA	b	606	-	1/1/15/20	6/37/115/115	-
24	CLA	B	610	-	-	1/37/115/115	-
31	GOL	C	525	-	-	4/4/4/4	-
26	BCR	B	619	-	-	2/29/63/63	0/2/2/2
29	PL9	a	417	-	-	12/53/73/73	0/1/1/1
31	GOL	O	304	-	-	0/4/4/4	-
27	SQD	B	622	-	-	20/49/69/69	0/1/1/1
24	CLA	b	609	-	1/1/15/20	7/37/115/115	-
40	RRX	h	101	-	-	6/29/65/65	0/2/2/2
36	HTG	B	629	-	-	3/10/30/30	0/1/1/1
39	HEM	e	102	6,5	-	6/12/54/54	-
24	CLA	b	610	-	1/1/15/20	4/37/115/115	-
31	GOL	b	638	-	-	0/4/4/4	-
36	HTG	H	101	-	-	1/7/27/30	0/1/1/1
36	HTG	V	202	-	-	0/2/22/30	0/1/1/1
26	BCR	a	414	-	-	0/29/63/63	0/2/2/2
36	HTG	B	630	-	-	0/10/30/30	0/1/1/1
36	HTG	B	626	-	-	5/10/30/30	0/1/1/1
28	LMG	c	522	-	-	13/46/66/70	0/1/1/1
27	SQD	A	411	-	-	10/49/69/69	0/1/1/1
24	CLA	B	616	-	1/1/15/20	8/37/115/115	-
28	LMG	D	413	41	-	6/46/66/70	0/1/1/1
24	CLA	D	401	43	-	3/37/115/115	-
27	SQD	a	401	-	-	18/49/69/69	0/1/1/1
37	DGD	c	519	-	-	12/51/91/95	0/2/2/2
38	LHG	d	410	-	-	8/53/53/53	-
24	CLA	a	410	43	1/1/15/20	6/37/115/115	-
27	SQD	f	802	-	-	15/38/58/69	0/1/1/1
24	CLA	C	509	43	1/1/15/20	7/37/115/115	-
29	PL9	A	413	-	-	8/53/73/73	0/1/1/1
31	GOL	V	207	-	-	2/4/4/4	-
36	HTG	b	603	-	-	1/10/30/30	0/1/1/1
24	CLA	b	612	-	-	1/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMG	z	101	-	-	8/31/51/70	0/1/1/1
24	CLA	b	619	-	1/1/15/20	4/37/115/115	-
24	CLA	a	413	-	-	10/37/115/115	-
24	CLA	c	506	43	1/1/15/20	10/37/115/115	-
28	LMG	b	624	-	-	10/46/66/70	0/1/1/1
31	GOL	A	418	-	-	4/4/4/4	-
37	DGD	d	416	-	-	14/44/64/95	0/1/1/2
28	LMG	C	521	-	-	7/46/66/70	0/1/1/1
31	GOL	a	419	-	-	2/4/4/4	-
24	CLA	a	409	-	1/1/15/20	3/37/115/115	-
32	LMT	m	103	-	-	5/21/61/61	0/2/2/2
27	SQD	A	415	-	-	15/49/69/69	0/1/1/1
38	LHG	D	412	-	-	13/49/49/53	-
24	CLA	b	607	-	1/1/15/20	5/37/115/115	-
24	CLA	b	614	43	1/1/15/20	6/37/115/115	-
24	CLA	A	405	-	1/1/15/20	4/37/115/115	-
24	CLA	B	612	43	1/1/15/20	4/37/115/115	-
32	LMT	b	629	-	-	7/15/35/61	0/1/1/2
24	CLA	c	515	-	-	4/37/115/115	-
32	LMT	b	625	-	-	7/21/61/61	0/2/2/2
36	HTG	b	628	-	-	5/10/30/30	0/1/1/1
24	CLA	c	504	-	-	5/37/115/115	-
24	CLA	c	508	-	1/1/15/20	4/37/115/115	-
24	CLA	B	607	-	1/1/15/20	5/37/115/115	-
37	DGD	H	104	-	-	13/51/91/95	0/2/2/2
24	CLA	B	605	-	1/1/15/20	6/37/115/115	-
32	LMT	M	102	-	-	1/21/61/61	0/2/2/2
24	CLA	B	614	-	1/1/15/20	0/37/115/115	-
42	HEC	V	201	16	-	2/10/54/54	-
37	DGD	C	520	-	-	6/51/91/95	0/2/2/2
24	CLA	C	505	-	1/1/15/20	3/37/115/115	-
32	LMT	j	102	-	-	2/15/35/61	0/1/1/2
24	CLA	B	606	-	1/1/15/20	3/37/115/115	-
36	HTG	b	602	-	-	2/10/30/30	0/1/1/1
29	PL9	D	408	-	-	1/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PL9	d	408	-	-	1/53/73/73	0/1/1/1
32	LMT	m	102	-	-	0/21/61/61	0/2/2/2
25	PHO	A	407	-	-	3/37/103/103	0/5/6/6
24	CLA	B	611	-	1/1/15/20	4/37/115/115	-
26	BCR	d	407	-	-	4/29/63/63	0/2/2/2
36	HTG	u	201	-	-	8/12/14/30	-
37	DGD	c	520	-	-	14/51/91/95	0/2/2/2
26	BCR	b	621	-	-	1/29/63/63	0/2/2/2
24	CLA	B	603	43	1/1/15/20	16/37/115/115	-
26	BCR	D	407	-	-	4/29/63/63	0/2/2/2
24	CLA	b	618	-	1/1/15/20	13/37/115/115	-
24	CLA	A	406	43	-	3/37/115/115	-
24	CLA	b	613	-	1/1/15/20	3/37/115/115	-
26	BCR	k	103	-	-	0/29/63/63	0/2/2/2
32	LMT	a	421	-	-	6/21/61/61	0/2/2/2
37	DGD	C	518	-	-	14/51/91/95	0/2/2/2
24	CLA	c	510	-	-	2/37/115/115	-
26	BCR	B	621	-	-	0/29/63/63	0/2/2/2
24	CLA	a	411	43	-	7/37/115/115	-
24	CLA	b	615	-	-	0/37/115/115	-
24	CLA	C	507	-	1/1/15/20	0/37/115/115	-
24	CLA	C	506	43	1/1/15/20	6/37/115/115	-
26	BCR	t	101	-	-	0/29/63/63	0/2/2/2
32	LMT	b	626	-	-	5/21/61/61	0/2/2/2
24	CLA	C	513	3	1/1/15/20	0/37/115/115	-
26	BCR	K	102	-	-	0/29/63/63	0/2/2/2
26	BCR	b	622	-	-	0/29/63/63	0/2/2/2
24	CLA	b	617	-	1/1/15/20	5/37/115/115	-
24	CLA	c	514	-	1/1/15/20	4/37/115/115	-
24	CLA	B	618	-	1/1/15/20	8/37/115/115	-
27	SQD	F	101	-	-	7/38/58/69	0/1/1/1
28	LMG	B	623	-	-	15/46/66/70	0/1/1/1
28	LMG	d	412	41	-	6/46/66/70	0/1/1/1
24	CLA	C	515	-	-	4/37/115/115	-
24	CLA	c	509	43	1/1/15/20	4/37/115/115	-
31	GOL	A	421	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMG	C	533	-	-	5/46/66/70	0/1/1/1
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
31	GOL	d	415	-	-	2/4/4/4	-
28	LMG	i	101	-	-	17/46/66/70	0/1/1/1
36	HTG	o	301	-	-	2/10/30/30	0/1/1/1
38	LHG	D	411	-	-	7/53/53/53	-
25	PHO	A	408	-	-	0/37/103/103	0/5/6/6
24	CLA	D	405	-	1/1/15/20	2/37/115/115	-
24	CLA	c	503	-	1/1/15/20	3/37/115/115	-
24	CLA	c	513	3	1/1/15/20	3/37/115/115	-
27	SQD	a	415	-	-	8/49/69/69	0/1/1/1
24	CLA	B	608	-	1/1/15/20	8/37/115/115	-
26	BCR	k	102	-	-	3/29/63/63	0/2/2/2
24	CLA	b	611	43	1/1/15/20	1/37/115/115	-
38	LHG	L	101	-	-	11/53/53/53	-
24	CLA	C	514	-	1/1/15/20	10/37/115/115	-
38	LHG	d	411	-	-	8/50/50/53	-
38	LHG	a	416	-	-	18/46/46/53	-
28	LMG	A	412	-	-	15/46/66/70	0/1/1/1
32	LMT	A	422	-	-	7/21/61/61	0/2/2/2
26	BCR	T	101	-	-	0/29/63/63	0/2/2/2
32	LMT	D	402	-	-	6/21/61/61	0/2/2/2
25	PHO	d	401	-	-	1/37/103/103	0/5/6/6
24	CLA	D	406	-	1/1/15/20	5/37/115/115	-
31	GOL	v	203	-	-	2/4/4/4	-
24	CLA	C	503	-	1/1/15/20	2/37/115/115	-
24	CLA	b	620	-	1/1/15/20	11/37/115/115	-
36	HTG	c	523	-	-	2/10/30/30	0/1/1/1
38	LHG	E	101	-	-	22/46/46/53	-
26	BCR	C	517	-	-	2/29/63/63	0/2/2/2
24	CLA	c	512	-	1/1/15/20	6/37/115/115	-
24	CLA	b	616	-	1/1/15/20	3/37/115/115	-
24	CLA	C	511	-	1/1/15/20	6/37/115/115	-
37	DGD	C	519	-	-	17/51/91/95	0/2/2/2
27	SQD	b	601	-	-	18/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	510	-	-	2/37/115/115	-
24	CLA	A	409	-	-	7/37/115/115	-
24	CLA	C	504	-	-	5/37/115/115	-
36	HTG	O	303	-	-	1/10/30/30	0/1/1/1
24	CLA	B	604	-	1/1/15/20	4/37/115/115	-
24	CLA	C	508	-	1/1/15/20	5/37/115/115	-
32	LMT	B	624	-	-	5/21/61/61	0/2/2/2
32	LMT	J	102	-	-	4/15/35/61	0/1/1/2
24	CLA	b	608	-	1/1/15/20	5/37/115/115	-
24	CLA	B	613	-	1/1/15/20	6/37/115/115	-
32	LMT	f	801	-	-	7/17/37/61	0/1/1/2
32	LMT	D	409	-	-	9/21/61/61	0/2/2/2
31	GOL	D	417	-	-	1/4/4/4	-
24	CLA	B	615	-	1/1/15/20	2/37/115/115	-
26	BCR	K	101	-	-	4/29/63/63	0/2/2/2
24	CLA	c	507	-	1/1/15/20	4/37/115/115	-
36	HTG	B	625	-	-	3/10/30/30	0/1/1/1
36	HTG	C	523	-	-	2/10/30/30	0/1/1/1
24	CLA	B	609	43	1/1/15/20	1/37/115/115	-
26	BCR	c	517	-	-	1/29/63/63	0/2/2/2
24	CLA	d	406	-	1/1/15/20	3/37/115/115	-
32	LMT	M	101	-	-	4/21/61/61	0/2/2/2
32	LMT	B	638	-	-	9/21/61/61	0/2/2/2
24	CLA	B	617	-	1/1/15/20	4/37/115/115	-
37	DGD	c	518	-	-	9/51/91/95	0/2/2/2
28	LMG	c	521	-	-	19/46/66/70	0/1/1/1
38	LHG	d	409	-	-	4/53/53/53	-
26	BCR	C	516	-	-	0/29/63/63	0/2/2/2
24	CLA	C	512	-	1/1/15/20	7/37/115/115	-
32	LMT	a	402	-	-	4/21/61/61	0/2/2/2
24	CLA	c	505	-	1/1/15/20	3/37/115/115	-
31	GOL	b	639	-	-	4/4/4/4	-
26	BCR	A	410	-	-	0/29/63/63	0/2/2/2
24	CLA	d	405	-	1/1/15/20	1/37/115/115	-
28	LMG	Z	101	-	-	11/34/54/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	HEM	F	102	6,5	-	4/12/54/54	-
38	LHG	l	102	-	-	10/53/53/53	-
36	HTG	C	522	-	-	0/10/30/30	0/1/1/1
24	CLA	b	605	43	1/1/15/20	6/37/115/115	-
24	CLA	c	511	-	1/1/15/20	5/37/115/115	-
36	HTG	c	524	-	-	2/10/30/30	0/1/1/1
26	BCR	b	623	-	-	0/29/63/63	0/2/2/2
26	BCR	c	516	-	-	1/29/63/63	0/2/2/2
40	RRX	H	103	-	-	4/29/65/65	0/2/2/2
42	HEC	v	201	16	-	2/10/54/54	-
37	DGD	h	102	-	-	8/51/91/95	0/2/2/2
25	PHO	a	412	-	-	4/37/103/103	0/5/6/6
36	HTG	b	627	-	-	3/10/30/30	0/1/1/1

All (1571) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	505	CLA	MG-NA	12.55	2.36	2.06
24	c	513	CLA	MG-NA	10.20	2.30	2.06
24	c	509	CLA	MG-NA	9.90	2.29	2.06
24	b	613	CLA	MG-NA	9.82	2.29	2.06
24	b	620	CLA	MG-NA	9.81	2.29	2.06
24	C	515	CLA	MG-NA	9.42	2.28	2.06
24	B	615	CLA	MG-NA	9.20	2.28	2.06
24	b	610	CLA	MG-NA	9.16	2.28	2.06
24	b	607	CLA	MG-NA	9.07	2.27	2.06
24	B	608	CLA	MG-NA	9.04	2.27	2.06
24	b	608	CLA	MG-NA	8.99	2.27	2.06
40	H	103	RRX	C8-C9	-8.92	1.26	1.45
24	c	514	CLA	MG-NA	8.80	2.27	2.06
40	h	101	RRX	C8-C9	-8.80	1.27	1.45
24	c	504	CLA	MG-NA	8.79	2.27	2.06
40	h	101	RRX	C19-C18	-8.75	1.27	1.45
24	c	508	CLA	MG-ND	-8.75	1.88	2.05
40	H	103	RRX	C19-C18	-8.73	1.27	1.45
40	H	103	RRX	C12-C13	-8.69	1.27	1.45
40	h	101	RRX	C12-C13	-8.62	1.27	1.45
24	b	615	CLA	MG-NA	8.60	2.26	2.06
24	C	513	CLA	MG-NA	8.29	2.26	2.06
24	B	611	CLA	MG-NA	8.21	2.25	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	606	CLA	MG-NA	8.21	2.25	2.06
24	B	613	CLA	MG-NA	8.17	2.25	2.06
24	C	507	CLA	MG-NA	8.00	2.25	2.06
24	C	514	CLA	MG-NA	7.89	2.25	2.06
24	b	611	CLA	MG-NA	7.82	2.24	2.06
24	c	505	CLA	MG-NA	7.82	2.24	2.06
24	C	509	CLA	MG-NA	7.80	2.24	2.06
40	H	103	RRX	C16-C17	-7.68	1.19	1.43
40	H	103	RRX	C20-C21	-7.65	1.19	1.43
40	h	101	RRX	C16-C17	-7.65	1.19	1.43
40	h	101	RRX	C20-C21	-7.64	1.19	1.43
24	b	619	CLA	MG-NA	7.64	2.24	2.06
24	b	609	CLA	MG-NA	7.51	2.24	2.06
24	B	617	CLA	MG-NA	7.50	2.24	2.06
24	b	616	CLA	MG-ND	-7.43	1.91	2.05
24	B	607	CLA	MG-NA	7.43	2.23	2.06
24	C	508	CLA	MG-NA	7.42	2.23	2.06
24	B	603	CLA	MG-NA	7.39	2.23	2.06
24	c	503	CLA	MG-NA	7.36	2.23	2.06
24	b	605	CLA	MG-NC	7.36	2.23	2.06
24	B	607	CLA	MG-ND	-7.19	1.91	2.05
24	c	507	CLA	MG-NA	7.19	2.23	2.06
24	c	505	CLA	MG-NC	7.17	2.23	2.06
24	c	506	CLA	MG-NA	7.16	2.23	2.06
24	c	503	CLA	MG-ND	-7.05	1.91	2.05
24	C	504	CLA	MG-NA	6.91	2.22	2.06
24	d	405	CLA	MG-NA	6.87	2.22	2.06
24	d	405	CLA	C3B-C2B	6.87	1.49	1.40
24	a	409	CLA	MG-ND	-6.85	1.92	2.05
24	c	515	CLA	MG-NC	6.83	2.22	2.06
24	C	510	CLA	MG-NA	6.81	2.22	2.06
24	c	515	CLA	MG-NA	6.76	2.22	2.06
24	c	511	CLA	MG-NA	6.74	2.22	2.06
24	B	610	CLA	MG-NA	6.73	2.22	2.06
40	H	103	RRX	O2-C28	-6.72	1.23	1.43
24	b	617	CLA	MG-NA	6.69	2.22	2.06
24	C	506	CLA	MG-NA	6.66	2.22	2.06
24	B	609	CLA	MG-NA	6.64	2.22	2.06
40	h	101	RRX	O2-C28	-6.63	1.23	1.43
24	A	405	CLA	MG-NA	6.52	2.21	2.06
24	b	615	CLA	C3B-C2B	6.52	1.49	1.40
24	C	512	CLA	MG-NA	6.50	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	618	CLA	MG-NA	6.48	2.21	2.06
40	H	103	RRX	C21-C22	-6.47	1.27	1.35
24	C	509	CLA	MG-NC	6.45	2.21	2.06
40	h	101	RRX	C21-C22	-6.44	1.27	1.35
24	C	513	CLA	C3B-C2B	6.44	1.49	1.40
24	C	515	CLA	C3B-C2B	6.44	1.49	1.40
24	b	616	CLA	MG-NA	6.44	2.21	2.06
24	c	511	CLA	C3B-C2B	6.40	1.49	1.40
24	c	514	CLA	C3B-C2B	6.39	1.49	1.40
40	H	103	RRX	C17-C18	-6.38	1.27	1.35
24	B	608	CLA	C3B-C2B	6.37	1.49	1.40
24	C	510	CLA	C3B-C2B	6.37	1.49	1.40
40	h	101	RRX	C17-C18	-6.36	1.27	1.35
24	b	613	CLA	MG-ND	-6.36	1.93	2.05
24	C	504	CLA	C3B-C2B	6.34	1.49	1.40
24	c	508	CLA	MG-NA	6.33	2.21	2.06
24	C	514	CLA	C3B-C2B	6.32	1.49	1.40
24	B	610	CLA	C3B-C2B	6.31	1.49	1.40
24	C	505	CLA	C3B-C2B	6.30	1.49	1.40
24	c	515	CLA	C3B-C2B	6.30	1.49	1.40
24	c	503	CLA	C3B-C2B	6.28	1.49	1.40
24	c	514	CLA	MG-ND	-6.28	1.93	2.05
24	C	503	CLA	MG-NA	6.27	2.21	2.06
24	b	614	CLA	MG-NC	6.26	2.21	2.06
24	c	510	CLA	C3B-C2B	6.26	1.49	1.40
24	c	515	CLA	MG-ND	-6.25	1.93	2.05
24	c	508	CLA	C1D-ND	6.24	1.45	1.37
24	b	614	CLA	C3B-C2B	6.24	1.49	1.40
24	C	509	CLA	C3B-C2B	6.24	1.49	1.40
24	C	503	CLA	C3B-C2B	6.22	1.49	1.40
24	a	410	CLA	C3B-C2B	6.21	1.49	1.40
24	d	406	CLA	C3B-C2B	6.17	1.48	1.40
24	B	618	CLA	C3B-C2B	6.16	1.48	1.40
24	b	605	CLA	C1D-ND	6.15	1.45	1.37
24	C	511	CLA	C3B-C2B	6.14	1.48	1.40
24	b	606	CLA	C3B-C2B	6.14	1.48	1.40
24	b	612	CLA	C3B-C2B	6.13	1.48	1.40
24	D	406	CLA	C3B-C2B	6.13	1.48	1.40
40	h	101	RRX	C15-C16	-6.12	1.20	1.36
40	H	103	RRX	C15-C16	-6.12	1.20	1.36
24	b	613	CLA	C1D-ND	6.11	1.45	1.37
24	C	506	CLA	C3B-C2B	6.10	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	511	CLA	MG-NC	6.10	2.20	2.06
24	C	505	CLA	C1D-ND	6.10	1.45	1.37
24	b	610	CLA	C3B-C2B	6.10	1.48	1.40
24	c	513	CLA	C3B-C2B	6.10	1.48	1.40
24	C	504	CLA	MG-ND	-6.07	1.93	2.05
24	a	411	CLA	C3B-C2B	6.06	1.48	1.40
24	C	504	CLA	C1D-ND	6.05	1.45	1.37
24	b	605	CLA	C3C-C2C	6.04	1.49	1.36
24	b	612	CLA	MG-NA	6.03	2.20	2.06
24	c	509	CLA	C3B-C2B	6.03	1.48	1.40
24	C	507	CLA	C3B-C2B	6.02	1.48	1.40
24	B	605	CLA	MG-ND	-6.01	1.93	2.05
25	A	408	PHO	C3B-C2B	6.01	1.48	1.40
24	c	515	CLA	C1D-ND	6.00	1.45	1.37
24	B	604	CLA	C3B-C2B	5.99	1.48	1.40
24	D	405	CLA	MG-NA	5.97	2.20	2.06
24	c	504	CLA	C3B-C2B	5.97	1.48	1.40
24	c	507	CLA	C3B-C2B	5.96	1.48	1.40
24	c	508	CLA	C3B-C2B	5.96	1.48	1.40
24	D	401	CLA	C3B-C2B	5.96	1.48	1.40
24	B	604	CLA	MG-NA	5.94	2.20	2.06
24	a	410	CLA	MG-NA	5.94	2.20	2.06
24	C	505	CLA	C3C-C2C	5.91	1.49	1.36
24	C	507	CLA	MG-ND	-5.91	1.94	2.05
24	B	605	CLA	C3B-C2B	5.91	1.48	1.40
24	c	512	CLA	MG-NA	5.90	2.20	2.06
24	b	608	CLA	MG-NC	5.90	2.20	2.06
24	b	611	CLA	C3B-C2B	5.89	1.48	1.40
25	A	407	PHO	C3B-C2B	5.89	1.48	1.40
24	B	613	CLA	C3B-C2B	5.89	1.48	1.40
25	a	412	PHO	C3B-C2B	5.89	1.48	1.40
24	C	511	CLA	C1D-ND	5.88	1.45	1.37
24	B	611	CLA	MG-NC	5.87	2.20	2.06
24	C	504	CLA	MG-NC	5.87	2.20	2.06
24	C	509	CLA	C1D-ND	5.87	1.45	1.37
24	c	506	CLA	C3B-C2B	5.85	1.48	1.40
24	B	603	CLA	C3C-C2C	5.85	1.49	1.36
24	B	611	CLA	MG-ND	-5.85	1.94	2.05
24	a	413	CLA	C3B-C2B	5.85	1.48	1.40
24	A	409	CLA	C3B-C2B	5.85	1.48	1.40
24	a	413	CLA	C3C-C2C	5.82	1.49	1.36
24	b	605	CLA	C3B-C2B	5.82	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	512	CLA	C3B-C2B	5.82	1.48	1.40
24	A	405	CLA	C3B-C2B	5.81	1.48	1.40
24	c	512	CLA	C3B-C2B	5.81	1.48	1.40
24	b	613	CLA	MG-NC	5.81	2.20	2.06
40	H	103	RRX	C20-C19	-5.80	1.19	1.34
24	b	616	CLA	C3B-C2B	5.80	1.48	1.40
24	B	605	CLA	MG-NA	5.80	2.20	2.06
24	A	409	CLA	MG-ND	-5.79	1.94	2.05
24	C	503	CLA	MG-ND	-5.79	1.94	2.05
24	B	609	CLA	C3B-C2B	5.79	1.48	1.40
24	c	507	CLA	MG-NC	5.78	2.20	2.06
24	B	603	CLA	C3B-C2B	5.77	1.48	1.40
24	b	609	CLA	MG-NC	5.77	2.20	2.06
24	B	603	CLA	C1D-ND	5.76	1.44	1.37
40	h	101	RRX	C20-C19	-5.75	1.19	1.34
24	B	607	CLA	C3C-C2C	5.74	1.48	1.36
24	B	614	CLA	C3B-C2B	5.74	1.48	1.40
24	c	503	CLA	C1D-ND	5.74	1.44	1.37
24	c	509	CLA	C1D-ND	5.73	1.44	1.37
24	c	508	CLA	C3C-C2C	5.72	1.48	1.36
24	c	515	CLA	C3C-C2C	5.72	1.48	1.36
40	H	103	RRX	C11-C12	-5.72	1.19	1.34
24	b	606	CLA	C3C-C2C	5.71	1.48	1.36
24	c	511	CLA	C1D-ND	5.71	1.44	1.37
24	b	614	CLA	C3C-C2C	5.71	1.48	1.36
24	b	606	CLA	MG-NA	5.70	2.19	2.06
24	B	606	CLA	C3B-C2B	5.70	1.48	1.40
24	C	515	CLA	C1D-ND	5.70	1.44	1.37
24	C	510	CLA	C3C-C2C	5.70	1.48	1.36
24	c	511	CLA	MG-NC	5.69	2.19	2.06
24	b	617	CLA	C3B-C2B	5.69	1.48	1.40
24	b	607	CLA	C3C-C2C	5.69	1.48	1.36
24	b	609	CLA	CHC-C1C	5.68	1.49	1.35
24	B	612	CLA	C3C-C2C	5.68	1.48	1.36
24	B	615	CLA	C3B-C2B	5.68	1.48	1.40
24	b	607	CLA	C3B-C2B	5.67	1.48	1.40
24	c	514	CLA	C3C-C2C	5.67	1.48	1.36
24	C	508	CLA	C3B-C2B	5.67	1.48	1.40
24	B	616	CLA	MG-NA	5.66	2.19	2.06
24	C	505	CLA	MG-NC	5.65	2.19	2.06
24	c	510	CLA	C3C-C2C	5.65	1.48	1.36
24	b	613	CLA	C3B-C2B	5.64	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	504	CLA	C3C-C2C	5.64	1.48	1.36
24	C	508	CLA	C3C-C2C	5.64	1.48	1.36
24	c	510	CLA	MG-NA	5.64	2.19	2.06
24	b	614	CLA	C1D-ND	5.63	1.44	1.37
24	a	409	CLA	C3B-C2B	5.63	1.48	1.40
24	C	511	CLA	C3C-C2C	5.62	1.48	1.36
24	c	505	CLA	C1D-ND	5.62	1.44	1.37
24	A	409	CLA	C3C-C2C	5.61	1.48	1.36
24	D	405	CLA	C3B-C2B	5.61	1.48	1.40
24	C	511	CLA	MG-NA	5.59	2.19	2.06
24	C	512	CLA	C3C-C2C	5.59	1.48	1.36
24	B	612	CLA	C3B-C2B	5.58	1.48	1.40
40	h	101	RRX	C11-C12	-5.58	1.20	1.34
24	D	406	CLA	C3C-C2C	5.58	1.48	1.36
24	C	503	CLA	C1D-ND	5.57	1.44	1.37
24	b	607	CLA	C1D-ND	5.56	1.44	1.37
24	b	606	CLA	MG-NC	5.56	2.19	2.06
24	a	410	CLA	C3C-C2C	5.55	1.48	1.36
24	c	509	CLA	C3C-C2C	5.55	1.48	1.36
24	B	612	CLA	C1D-ND	5.55	1.44	1.37
24	B	616	CLA	CHC-C1C	5.54	1.49	1.35
24	b	609	CLA	C3C-C2C	5.54	1.48	1.36
24	b	605	CLA	MG-NA	5.54	2.19	2.06
24	B	604	CLA	CHC-C1C	5.54	1.49	1.35
25	d	401	PHO	C3B-C2B	5.54	1.48	1.40
24	c	511	CLA	C3C-C2C	5.54	1.48	1.36
24	b	608	CLA	C3B-C2B	5.53	1.48	1.40
24	C	515	CLA	CHC-C1C	5.53	1.49	1.35
24	B	610	CLA	C3C-C2C	5.53	1.48	1.36
24	B	613	CLA	CHC-C1C	5.52	1.49	1.35
24	C	515	CLA	C3C-C2C	5.52	1.48	1.36
24	b	620	CLA	C3B-C2B	5.52	1.48	1.40
24	c	504	CLA	C1D-ND	5.52	1.44	1.37
24	c	512	CLA	C3C-C2C	5.51	1.48	1.36
24	C	507	CLA	C3C-C2C	5.51	1.48	1.36
24	B	609	CLA	C3C-C2C	5.50	1.48	1.36
24	B	603	CLA	MG-ND	-5.50	1.94	2.05
24	B	612	CLA	MG-NA	5.48	2.19	2.06
24	c	510	CLA	MG-ND	-5.47	1.94	2.05
24	b	612	CLA	C1D-ND	5.47	1.44	1.37
24	b	618	CLA	MG-NA	5.47	2.19	2.06
24	c	505	CLA	C3B-C2B	5.46	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	513	CLA	CHC-C1C	5.46	1.49	1.35
24	a	411	CLA	MG-NA	5.46	2.19	2.06
24	c	505	CLA	C3C-C2C	5.45	1.48	1.36
24	c	513	CLA	C3C-C2C	5.44	1.48	1.36
24	B	604	CLA	C3C-C2C	5.44	1.48	1.36
24	c	510	CLA	CHC-C1C	5.44	1.48	1.35
24	b	619	CLA	C3C-C2C	5.43	1.48	1.36
24	C	507	CLA	CHC-C1C	5.43	1.48	1.35
24	B	614	CLA	C3C-C2C	5.41	1.48	1.36
24	C	505	CLA	CHC-C1C	5.40	1.48	1.35
24	c	508	CLA	MG-NC	5.40	2.19	2.06
24	C	514	CLA	CHC-C1C	5.40	1.48	1.35
24	B	605	CLA	C3C-C2C	5.40	1.48	1.36
24	c	514	CLA	CHC-C1C	5.40	1.48	1.35
24	C	512	CLA	C1D-ND	5.40	1.44	1.37
24	a	409	CLA	C1D-ND	5.40	1.44	1.37
24	b	611	CLA	C3C-C2C	5.39	1.48	1.36
24	b	605	CLA	CHC-C1C	5.38	1.48	1.35
24	B	614	CLA	MG-NA	5.38	2.19	2.06
24	b	615	CLA	C1D-ND	5.38	1.44	1.37
24	d	405	CLA	CHC-C1C	5.38	1.48	1.35
24	C	508	CLA	C1D-ND	5.37	1.44	1.37
24	b	612	CLA	MG-ND	-5.37	1.95	2.05
24	b	618	CLA	CHC-C1C	5.37	1.48	1.35
24	c	507	CLA	C3C-C2C	5.36	1.48	1.36
24	b	620	CLA	CHC-C1C	5.36	1.48	1.35
24	a	409	CLA	MG-NC	5.36	2.19	2.06
24	b	609	CLA	C3B-C2B	5.36	1.47	1.40
24	b	618	CLA	C3B-C2B	5.36	1.47	1.40
24	C	513	CLA	C3C-C2C	5.35	1.48	1.36
24	b	606	CLA	CHC-C1C	5.35	1.48	1.35
24	A	406	CLA	MG-NA	5.35	2.19	2.06
24	b	606	CLA	C1D-ND	5.35	1.44	1.37
24	C	514	CLA	C3C-C2C	5.35	1.48	1.36
24	B	614	CLA	CHC-C1C	5.35	1.48	1.35
24	c	504	CLA	C3C-C2C	5.34	1.48	1.36
24	B	616	CLA	C3C-C2C	5.34	1.48	1.36
24	C	510	CLA	CHC-C1C	5.33	1.48	1.35
24	b	618	CLA	C3C-C2C	5.33	1.48	1.36
24	C	507	CLA	C1D-ND	5.33	1.44	1.37
24	C	513	CLA	CHC-C1C	5.33	1.48	1.35
24	a	410	CLA	MG-ND	-5.33	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	612	CLA	C3C-C2C	5.32	1.48	1.36
24	d	405	CLA	C3C-C2C	5.32	1.48	1.36
24	C	504	CLA	CHC-C1C	5.32	1.48	1.35
24	B	603	CLA	CHC-C1C	5.31	1.48	1.35
25	d	401	PHO	C3D-C2D	5.31	1.48	1.39
24	b	610	CLA	C3C-C2C	5.30	1.48	1.36
24	b	612	CLA	MG-NC	5.30	2.18	2.06
24	d	406	CLA	C3C-C2C	5.30	1.48	1.36
24	B	606	CLA	C1D-ND	5.30	1.44	1.37
24	b	619	CLA	CHC-C1C	5.30	1.48	1.35
24	a	409	CLA	C3C-C2C	5.30	1.48	1.36
24	b	614	CLA	CHC-C1C	5.29	1.48	1.35
24	C	511	CLA	MG-ND	-5.29	1.95	2.05
24	B	610	CLA	CHC-C1C	5.29	1.48	1.35
24	c	514	CLA	C1D-ND	5.29	1.44	1.37
24	C	507	CLA	MG-NC	5.29	2.18	2.06
24	A	406	CLA	C3B-C2B	5.28	1.47	1.40
40	H	103	RRX	C11-C10	-5.27	1.27	1.43
24	d	406	CLA	MG-NC	5.27	2.18	2.06
24	C	514	CLA	C1D-ND	5.27	1.44	1.37
24	A	405	CLA	C1D-ND	5.26	1.44	1.37
24	B	616	CLA	C1D-ND	5.26	1.44	1.37
24	C	506	CLA	C3C-C2C	5.26	1.47	1.36
24	B	617	CLA	CHC-C1C	5.26	1.48	1.35
24	c	503	CLA	C3C-C2C	5.26	1.47	1.36
24	b	619	CLA	C1D-ND	5.25	1.44	1.37
24	b	620	CLA	C3C-C2C	5.25	1.47	1.36
24	B	607	CLA	C3B-C2B	5.24	1.47	1.40
24	b	608	CLA	C3C-C2C	5.24	1.47	1.36
24	b	608	CLA	C1D-ND	5.24	1.44	1.37
25	A	408	PHO	C3D-C2D	5.24	1.48	1.39
24	c	506	CLA	C3C-C2C	5.23	1.47	1.36
24	c	506	CLA	CHC-C1C	5.23	1.48	1.35
24	a	411	CLA	C3C-C2C	5.23	1.47	1.36
24	c	515	CLA	CHC-C1C	5.22	1.48	1.35
24	c	508	CLA	CHC-C1C	5.22	1.48	1.35
24	c	507	CLA	MG-ND	-5.22	1.95	2.05
24	c	505	CLA	CHC-C1C	5.22	1.48	1.35
24	b	617	CLA	C1D-ND	5.21	1.44	1.37
24	C	508	CLA	CHC-C1C	5.21	1.48	1.35
24	d	405	CLA	MG-ND	-5.20	1.95	2.05
24	c	511	CLA	CHC-C1C	5.20	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	503	CLA	C3C-C2C	5.20	1.47	1.36
24	A	405	CLA	C3C-C2C	5.19	1.47	1.36
24	B	604	CLA	MG-NC	5.19	2.18	2.06
24	a	410	CLA	CHC-C1C	5.19	1.48	1.35
24	B	610	CLA	C1D-ND	5.18	1.44	1.37
24	A	405	CLA	CHC-C1C	5.17	1.48	1.35
24	B	612	CLA	CHC-C1C	5.16	1.48	1.35
24	b	607	CLA	CHC-C1C	5.16	1.48	1.35
24	A	406	CLA	C3C-C2C	5.16	1.47	1.36
24	b	615	CLA	C3C-C2C	5.16	1.47	1.36
40	h	101	RRX	C11-C10	-5.16	1.27	1.43
24	b	605	CLA	O2D-CGD	5.16	1.45	1.33
24	C	511	CLA	O2D-CGD	5.16	1.45	1.33
24	c	504	CLA	CHC-C1C	5.15	1.48	1.35
40	H	103	RRX	C15-C14	-5.15	1.27	1.43
40	h	101	RRX	C15-C14	-5.15	1.27	1.43
24	B	606	CLA	CHC-C1C	5.15	1.48	1.35
24	C	503	CLA	CHC-C1C	5.15	1.48	1.35
24	b	616	CLA	C1D-ND	5.14	1.44	1.37
24	a	409	CLA	MG-NA	5.14	2.18	2.06
24	b	617	CLA	C3C-C2C	5.14	1.47	1.36
24	b	612	CLA	CHC-C1C	5.14	1.48	1.35
24	d	406	CLA	C1D-ND	5.13	1.44	1.37
24	C	512	CLA	CHC-C1C	5.13	1.48	1.35
24	D	406	CLA	MG-NC	5.13	2.18	2.06
24	b	610	CLA	CHC-C1C	5.12	1.48	1.35
24	B	615	CLA	C3C-C2C	5.12	1.47	1.36
24	b	618	CLA	C1D-ND	5.11	1.44	1.37
24	b	608	CLA	CHC-C1C	5.11	1.48	1.35
24	B	611	CLA	C3C-C2C	5.11	1.47	1.36
24	A	409	CLA	CHC-C1C	5.11	1.48	1.35
24	b	613	CLA	O2D-CGD	5.10	1.45	1.33
24	b	613	CLA	C3C-C2C	5.10	1.47	1.36
24	B	607	CLA	CHC-C1C	5.09	1.48	1.35
24	B	605	CLA	C1D-ND	5.09	1.44	1.37
25	A	407	PHO	C3D-C2D	5.09	1.48	1.39
24	a	411	CLA	CHC-C1C	5.09	1.48	1.35
24	c	507	CLA	CHC-C1C	5.08	1.48	1.35
24	C	509	CLA	C3C-C2C	5.08	1.47	1.36
24	B	608	CLA	C3C-C2C	5.08	1.47	1.36
24	B	607	CLA	MG-NC	5.08	2.18	2.06
24	c	503	CLA	CHC-C1C	5.07	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	508	CLA	CHD-C1D	5.07	1.48	1.38
25	a	412	PHO	C3D-C2D	5.07	1.48	1.39
24	c	509	CLA	CHC-C1C	5.07	1.48	1.35
24	B	603	CLA	O2D-CGD	5.06	1.45	1.33
24	B	618	CLA	CHC-C1C	5.06	1.47	1.35
40	h	101	RRX	C23-C22	-5.05	1.35	1.45
24	C	507	CLA	CHD-C1D	5.05	1.48	1.38
24	B	605	CLA	CHC-C1C	5.05	1.47	1.35
24	C	506	CLA	CHC-C1C	5.05	1.47	1.35
24	B	616	CLA	C3B-C2B	5.04	1.47	1.40
24	B	615	CLA	C1D-ND	5.04	1.44	1.37
24	B	618	CLA	C3C-C2C	5.04	1.47	1.36
24	c	506	CLA	O2D-CGD	5.02	1.45	1.33
24	b	611	CLA	MG-NC	5.02	2.18	2.06
24	b	611	CLA	CHC-C1C	5.02	1.47	1.35
24	c	512	CLA	CHC-C1C	5.01	1.47	1.35
24	B	611	CLA	C1D-ND	5.01	1.43	1.37
24	d	406	CLA	CHC-C1C	5.01	1.47	1.35
24	C	508	CLA	MG-ND	-5.01	1.95	2.05
24	b	615	CLA	MG-ND	-5.01	1.95	2.05
24	B	604	CLA	C1D-ND	5.01	1.43	1.37
24	B	609	CLA	CHC-C1C	5.00	1.47	1.35
24	A	406	CLA	MG-ND	-5.00	1.95	2.05
24	b	616	CLA	CHC-C1C	4.99	1.47	1.35
24	c	507	CLA	CHD-C1D	4.99	1.48	1.38
24	B	615	CLA	CHC-C1C	4.98	1.47	1.35
24	b	612	CLA	O2D-CGD	4.98	1.45	1.33
24	c	509	CLA	MG-NC	4.98	2.18	2.06
24	C	515	CLA	MG-ND	-4.98	1.95	2.05
24	D	406	CLA	O2D-CGD	4.98	1.45	1.33
40	H	103	RRX	C23-C22	-4.97	1.35	1.45
24	B	618	CLA	C1D-ND	4.97	1.43	1.37
24	B	610	CLA	CHD-C1D	4.97	1.48	1.38
24	C	511	CLA	CHC-C1C	4.97	1.47	1.35
24	a	409	CLA	CHC-C1C	4.96	1.47	1.35
24	d	406	CLA	MG-ND	-4.96	1.96	2.05
24	a	413	CLA	CHC-C1C	4.96	1.47	1.35
24	C	515	CLA	O2D-CGD	4.96	1.45	1.33
24	b	608	CLA	CHD-C1D	4.95	1.48	1.38
24	B	613	CLA	C3C-C2C	4.95	1.47	1.36
24	b	608	CLA	MG-ND	-4.95	1.96	2.05
24	B	613	CLA	O2D-CGD	4.95	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	401	CLA	MG-NA	4.94	2.18	2.06
24	B	607	CLA	C1D-ND	4.94	1.43	1.37
24	c	504	CLA	O2D-CGD	4.93	1.45	1.33
24	a	413	CLA	MG-NA	4.93	2.18	2.06
26	b	623	BCR	C23-C22	-4.93	1.35	1.45
24	D	406	CLA	CHC-C1C	4.92	1.47	1.35
24	c	504	CLA	MG-NC	4.92	2.18	2.06
24	D	401	CLA	C3C-C2C	4.92	1.47	1.36
24	B	609	CLA	MG-NC	4.92	2.18	2.06
24	A	405	CLA	MG-ND	-4.92	1.96	2.05
24	c	513	CLA	CHD-C1D	4.92	1.47	1.38
24	c	512	CLA	C1D-ND	4.91	1.43	1.37
24	c	504	CLA	MG-ND	-4.91	1.96	2.05
24	b	616	CLA	C3C-C2C	4.91	1.47	1.36
24	B	617	CLA	C3B-C2B	4.90	1.47	1.40
24	C	513	CLA	C1D-ND	4.90	1.43	1.37
24	b	613	CLA	CHC-C1C	4.89	1.47	1.35
24	B	609	CLA	CHD-C1D	4.89	1.47	1.38
24	B	614	CLA	O2D-CGD	4.89	1.45	1.33
26	k	102	BCR	C23-C22	-4.89	1.35	1.45
24	B	611	CLA	C3B-C2B	4.89	1.47	1.40
24	b	614	CLA	MG-NA	4.88	2.17	2.06
24	C	508	CLA	MG-NC	4.88	2.17	2.06
24	b	620	CLA	O2D-CGD	4.87	1.45	1.33
24	b	617	CLA	O2D-CGD	4.87	1.45	1.33
24	c	515	CLA	O2D-CGD	4.86	1.45	1.33
24	c	506	CLA	C1D-ND	4.86	1.43	1.37
24	C	506	CLA	C1D-ND	4.86	1.43	1.37
24	B	607	CLA	O2D-CGD	4.85	1.45	1.33
24	A	409	CLA	C1D-ND	4.85	1.43	1.37
24	A	406	CLA	CHC-C1C	4.85	1.47	1.35
24	c	512	CLA	MG-ND	-4.85	1.96	2.05
24	C	510	CLA	O2D-CGD	4.85	1.45	1.33
24	b	615	CLA	CHC-C1C	4.84	1.47	1.35
24	C	513	CLA	O2D-CGD	4.84	1.45	1.33
24	B	611	CLA	O2D-CGD	4.83	1.45	1.33
24	b	616	CLA	O2D-CGD	4.83	1.45	1.33
25	A	408	PHO	O2D-CGD	4.83	1.45	1.33
24	b	619	CLA	O2D-CGD	4.83	1.45	1.33
24	b	610	CLA	O2D-CGD	4.82	1.45	1.33
24	B	617	CLA	C3C-C2C	4.82	1.47	1.36
24	B	612	CLA	MG-NC	4.82	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	504	CLA	O2D-CGD	4.81	1.44	1.33
24	c	508	CLA	O2D-CGD	4.81	1.44	1.33
26	c	516	BCR	C23-C22	-4.80	1.35	1.45
24	c	507	CLA	C1D-ND	4.80	1.43	1.37
26	k	103	BCR	C23-C22	-4.80	1.35	1.45
24	b	613	CLA	CHD-C1D	4.80	1.47	1.38
26	d	407	BCR	C23-C22	-4.79	1.35	1.45
24	B	618	CLA	O2D-CGD	4.79	1.44	1.33
24	B	611	CLA	CHC-C1C	4.78	1.47	1.35
24	c	514	CLA	O2D-CGD	4.78	1.44	1.33
24	b	617	CLA	CHC-C1C	4.78	1.47	1.35
24	C	509	CLA	O2D-CGD	4.77	1.44	1.33
24	D	406	CLA	C1D-ND	4.76	1.43	1.37
24	c	513	CLA	O2D-CGD	4.76	1.44	1.33
24	d	406	CLA	O2D-CGD	4.75	1.44	1.33
24	B	612	CLA	CHD-C1D	4.75	1.47	1.38
26	K	102	BCR	C23-C22	-4.75	1.35	1.45
24	a	413	CLA	O2D-CGD	4.74	1.44	1.33
24	C	510	CLA	MG-ND	-4.74	1.96	2.05
24	C	514	CLA	O2D-CGD	4.72	1.44	1.33
24	c	503	CLA	O2D-CGD	4.72	1.44	1.33
24	B	609	CLA	C1D-ND	4.71	1.43	1.37
24	C	503	CLA	O2D-CGD	4.71	1.44	1.33
24	c	515	CLA	CHD-C1D	4.71	1.47	1.38
24	d	406	CLA	MG-NA	4.71	2.17	2.06
24	C	509	CLA	CHC-C1C	4.70	1.47	1.35
24	b	605	CLA	CHD-C1D	4.69	1.47	1.38
24	B	604	CLA	MG-ND	-4.69	1.96	2.05
24	c	512	CLA	MG-NC	4.69	2.17	2.06
24	C	507	CLA	O2D-CGD	4.68	1.44	1.33
24	b	612	CLA	CHD-C1D	4.68	1.47	1.38
24	B	604	CLA	CHD-C1D	4.68	1.47	1.38
24	D	405	CLA	CHC-C1C	4.68	1.47	1.35
24	b	610	CLA	CHD-C1D	4.67	1.47	1.38
24	c	509	CLA	CHD-C1D	4.67	1.47	1.38
24	c	509	CLA	O2D-CGD	4.67	1.44	1.33
24	a	413	CLA	C1D-ND	4.67	1.43	1.37
24	c	513	CLA	C1D-ND	4.66	1.43	1.37
24	D	405	CLA	C3C-C2C	4.66	1.46	1.36
26	C	517	BCR	C23-C22	-4.66	1.35	1.45
24	B	613	CLA	C1D-ND	4.66	1.43	1.37
24	C	508	CLA	O2D-CGD	4.66	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	409	CLA	CHD-C1D	4.66	1.47	1.38
24	A	405	CLA	O2D-CGD	4.66	1.44	1.33
24	b	615	CLA	O2D-CGD	4.65	1.44	1.33
24	C	511	CLA	CHD-C1D	4.65	1.47	1.38
24	b	611	CLA	CHD-C1D	4.64	1.47	1.38
24	B	606	CLA	CHD-C1D	4.63	1.47	1.38
26	B	621	BCR	C23-C22	-4.63	1.36	1.45
25	d	401	PHO	O2D-CGD	4.63	1.44	1.33
24	c	508	CLA	CHD-C1D	4.63	1.47	1.38
24	C	509	CLA	CHD-C1D	4.62	1.47	1.38
24	C	506	CLA	MG-ND	-4.62	1.96	2.05
24	c	511	CLA	MG-ND	-4.62	1.96	2.05
24	b	607	CLA	CHD-C1D	4.62	1.47	1.38
24	C	505	CLA	CHD-C1D	4.61	1.47	1.38
24	b	614	CLA	CHD-C1D	4.60	1.47	1.38
24	c	514	CLA	CHD-C1D	4.60	1.47	1.38
24	b	608	CLA	O2D-CGD	4.60	1.44	1.33
24	b	620	CLA	CHD-C1D	4.59	1.47	1.38
24	B	608	CLA	O2D-CGD	4.59	1.44	1.33
24	b	619	CLA	OBD-CAD	4.59	1.30	1.22
24	c	505	CLA	CHD-C1D	4.59	1.47	1.38
24	b	606	CLA	O2D-CGD	4.58	1.44	1.33
24	B	608	CLA	CHC-C1C	4.58	1.46	1.35
24	A	405	CLA	CHD-C1D	4.58	1.47	1.38
25	d	401	PHO	OBD-CAD	4.57	1.28	1.22
24	b	609	CLA	O2D-CGD	4.57	1.44	1.33
24	c	512	CLA	CHD-C1D	4.57	1.47	1.38
24	a	409	CLA	CHD-C1D	4.57	1.47	1.38
24	A	409	CLA	O2D-CGD	4.57	1.44	1.33
24	B	610	CLA	MG-NC	4.56	2.17	2.06
24	c	510	CLA	C1D-ND	4.56	1.43	1.37
24	b	620	CLA	C1D-ND	4.56	1.43	1.37
25	a	412	PHO	O2D-CGD	4.55	1.44	1.33
24	A	409	CLA	MG-NC	4.54	2.17	2.06
28	C	521	LMG	O8-C28	4.54	1.46	1.33
24	C	515	CLA	CHD-C1D	4.54	1.47	1.38
24	B	605	CLA	O2D-CGD	4.54	1.44	1.33
24	B	603	CLA	MG-NC	4.53	2.17	2.06
27	F	101	SQD	O47-C7	4.53	1.47	1.34
24	B	612	CLA	MG-ND	-4.53	1.96	2.05
24	C	512	CLA	CHD-C1D	4.53	1.47	1.38
24	b	619	CLA	C3B-C2B	4.53	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	504	CLA	CHD-C1D	4.53	1.47	1.38
24	B	608	CLA	MG-ND	-4.52	1.96	2.05
24	c	511	CLA	CHD-C1D	4.52	1.47	1.38
24	c	507	CLA	O2D-CGD	4.51	1.44	1.33
24	b	609	CLA	CHD-C1D	4.51	1.47	1.38
24	C	514	CLA	CHD-C1D	4.51	1.47	1.38
24	B	613	CLA	MG-ND	-4.49	1.96	2.05
24	c	506	CLA	CHD-C1D	4.49	1.47	1.38
24	B	617	CLA	C1D-ND	4.49	1.43	1.37
24	B	606	CLA	O2D-CGD	4.49	1.44	1.33
24	b	620	CLA	O2A-CGA	4.49	1.46	1.33
28	Z	101	LMG	O8-C28	4.48	1.46	1.33
24	b	617	CLA	MG-NC	4.48	2.16	2.06
24	B	610	CLA	O2D-CGD	4.48	1.44	1.33
24	d	406	CLA	CHD-C1D	4.48	1.47	1.38
24	c	511	CLA	O2D-CGD	4.47	1.44	1.33
24	c	510	CLA	O2D-CGD	4.47	1.44	1.33
24	B	614	CLA	CHD-C1D	4.47	1.47	1.38
24	D	406	CLA	MG-NA	4.47	2.16	2.06
26	c	517	BCR	C23-C22	-4.46	1.36	1.45
24	b	614	CLA	O2D-CGD	4.46	1.44	1.33
24	b	618	CLA	O2D-CGD	4.46	1.44	1.33
24	D	406	CLA	CHD-C1D	4.46	1.47	1.38
24	B	603	CLA	O2A-CGA	4.45	1.46	1.33
24	b	606	CLA	CHD-C1D	4.45	1.47	1.38
24	B	617	CLA	O2D-CGD	4.45	1.44	1.33
24	a	413	CLA	CHD-C1D	4.44	1.47	1.38
26	T	101	BCR	C23-C22	-4.44	1.36	1.45
26	D	407	BCR	C23-C22	-4.44	1.36	1.45
27	B	622	SQD	O47-C7	4.44	1.46	1.34
24	B	608	CLA	C1D-ND	4.43	1.43	1.37
24	d	405	CLA	C1D-ND	4.43	1.43	1.37
24	B	606	CLA	C3C-C2C	4.43	1.46	1.36
25	A	407	PHO	O2D-CGD	4.43	1.44	1.33
24	B	611	CLA	CHD-C1D	4.42	1.47	1.38
24	b	616	CLA	MG-NC	4.42	2.16	2.06
24	C	503	CLA	CHD-C1D	4.41	1.47	1.38
24	B	604	CLA	O2D-CGD	4.41	1.44	1.33
24	C	506	CLA	O2D-CGD	4.41	1.44	1.33
24	a	409	CLA	O2D-CGD	4.41	1.44	1.33
24	b	607	CLA	O2D-CGD	4.40	1.43	1.33
24	b	620	CLA	MG-ND	-4.39	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	505	CLA	O2D-CGD	4.38	1.43	1.33
27	a	401	SQD	O48-C23	4.38	1.46	1.33
27	f	802	SQD	O47-C7	4.38	1.46	1.34
38	E	101	LHG	O8-C23	4.37	1.46	1.33
24	B	603	CLA	CHD-C1D	4.37	1.46	1.38
24	c	505	CLA	O2D-CGD	4.37	1.43	1.33
24	b	617	CLA	CHD-C1D	4.37	1.46	1.38
24	B	607	CLA	CHD-C1D	4.36	1.46	1.38
24	B	615	CLA	O2D-CGD	4.36	1.43	1.33
28	b	624	LMG	O8-C28	4.36	1.46	1.33
27	F	101	SQD	O48-C23	4.35	1.46	1.33
24	b	616	CLA	OBD-CAD	4.35	1.30	1.22
24	a	411	CLA	CHD-C1D	4.35	1.46	1.38
28	C	533	LMG	O7-C10	4.35	1.46	1.34
24	a	411	CLA	C1D-ND	4.35	1.43	1.37
24	C	509	CLA	MG-ND	-4.35	1.97	2.05
24	c	514	CLA	O2A-CGA	4.35	1.46	1.33
37	d	416	DGD	O1G-C1A	4.34	1.46	1.33
24	B	618	CLA	CHD-C1D	4.33	1.46	1.38
26	b	622	BCR	C23-C22	-4.33	1.36	1.45
24	B	617	CLA	CHD-C1D	4.33	1.46	1.38
28	A	412	LMG	O7-C10	4.33	1.46	1.34
24	C	512	CLA	MG-ND	-4.33	1.97	2.05
28	c	522	LMG	O8-C28	4.33	1.46	1.33
24	B	610	CLA	O2A-CGA	4.32	1.46	1.33
24	A	406	CLA	CHD-C1D	4.32	1.46	1.38
24	C	512	CLA	O2D-CGD	4.32	1.43	1.33
24	A	406	CLA	C1D-ND	4.32	1.43	1.37
26	C	516	BCR	C23-C22	-4.31	1.36	1.45
24	C	510	CLA	CHD-C1D	4.31	1.46	1.38
24	b	615	CLA	CHD-C1D	4.31	1.46	1.38
24	D	405	CLA	O2D-CGD	4.31	1.43	1.33
24	b	610	CLA	C1D-ND	4.30	1.43	1.37
24	b	611	CLA	O2D-CGD	4.30	1.43	1.33
26	B	619	BCR	C23-C22	-4.30	1.36	1.45
24	A	405	CLA	MG-NC	4.30	2.16	2.06
28	c	521	LMG	O8-C28	4.29	1.45	1.33
28	C	533	LMG	O8-C28	4.29	1.45	1.33
27	b	601	SQD	O47-C7	4.29	1.46	1.34
24	C	508	CLA	O2A-CGA	4.29	1.45	1.33
24	C	513	CLA	CHD-C1D	4.29	1.46	1.38
26	K	101	BCR	C23-C22	-4.29	1.36	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	t	101	BCR	C23-C22	-4.29	1.36	1.45
27	a	401	SQD	O47-C7	4.28	1.46	1.34
24	b	605	CLA	O2A-CGA	4.28	1.45	1.33
26	A	410	BCR	C23-C22	-4.28	1.36	1.45
28	B	623	LMG	O8-C28	4.27	1.45	1.33
24	c	515	CLA	O2A-CGA	4.27	1.45	1.33
24	B	605	CLA	MG-NC	4.27	2.16	2.06
24	b	611	CLA	MG-ND	-4.27	1.97	2.05
24	C	511	CLA	O2A-CGA	4.27	1.45	1.33
24	c	512	CLA	O2D-CGD	4.27	1.43	1.33
24	B	606	CLA	MG-NC	4.26	2.16	2.06
24	c	509	CLA	O2A-CGA	4.26	1.45	1.33
24	C	514	CLA	O2A-CGA	4.26	1.45	1.33
24	c	508	CLA	O2A-CGA	4.26	1.45	1.33
38	a	416	LHG	O8-C23	4.26	1.45	1.33
24	d	405	CLA	MG-NC	4.26	2.16	2.06
24	a	411	CLA	O2D-CGD	4.26	1.43	1.33
24	a	409	CLA	OBD-CAD	4.25	1.29	1.22
24	C	504	CLA	CHD-C1D	4.25	1.46	1.38
24	A	406	CLA	OBD-CAD	4.25	1.29	1.22
37	d	416	DGD	O2G-C1B	4.24	1.46	1.34
28	c	522	LMG	O7-C10	4.24	1.46	1.34
26	a	414	BCR	C23-C22	-4.24	1.36	1.45
24	d	405	CLA	O2A-CGA	4.24	1.45	1.33
24	b	618	CLA	O2A-CGA	4.24	1.45	1.33
24	D	401	CLA	O2D-CGD	4.22	1.43	1.33
27	A	415	SQD	O47-C7	4.22	1.46	1.34
24	B	616	CLA	CHD-C1D	4.22	1.46	1.38
24	b	616	CLA	CHD-C1D	4.20	1.46	1.38
24	c	503	CLA	CHD-C1D	4.20	1.46	1.38
24	c	510	CLA	CHD-C1D	4.20	1.46	1.38
24	C	512	CLA	MG-NC	4.20	2.16	2.06
24	c	510	CLA	MG-NC	4.19	2.16	2.06
24	C	510	CLA	O2A-CGA	4.19	1.45	1.33
24	B	613	CLA	CHD-C1D	4.19	1.46	1.38
24	C	515	CLA	O2A-CGA	4.19	1.45	1.33
27	f	802	SQD	O48-C23	4.19	1.45	1.33
24	B	616	CLA	O2D-CGD	4.18	1.43	1.33
24	A	406	CLA	O2D-CGD	4.18	1.43	1.33
24	d	405	CLA	CHD-C1D	4.18	1.46	1.38
24	C	510	CLA	C1D-ND	4.18	1.42	1.37
27	A	415	SQD	O48-C23	4.18	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	401	CLA	C1D-ND	4.18	1.42	1.37
24	B	605	CLA	O2A-CGA	4.17	1.45	1.33
38	E	101	LHG	O7-C7	4.17	1.46	1.34
24	b	606	CLA	O2A-CGA	4.17	1.45	1.33
24	B	618	CLA	O2A-CGA	4.17	1.45	1.33
24	D	405	CLA	MG-ND	-4.17	1.97	2.05
24	c	503	CLA	O2A-CGA	4.17	1.45	1.33
24	C	505	CLA	O2A-CGA	4.16	1.45	1.33
42	V	201	HEC	CBC-CAC	-4.16	1.33	1.49
42	v	201	HEC	CBC-CAC	-4.14	1.33	1.49
24	C	506	CLA	CHD-C1D	4.14	1.46	1.38
38	a	416	LHG	O7-C7	4.14	1.46	1.34
26	b	621	BCR	C23-C22	-4.14	1.37	1.45
24	B	617	CLA	O2A-CGA	4.14	1.45	1.33
24	C	508	CLA	CHD-C4C	4.14	1.48	1.39
24	c	509	CLA	CHD-C4C	4.14	1.48	1.39
24	B	611	CLA	OBD-CAD	4.13	1.29	1.22
24	b	619	CLA	O2A-CGA	4.13	1.45	1.33
24	b	614	CLA	OBD-CAD	4.13	1.29	1.22
24	B	608	CLA	O2A-CGA	4.13	1.45	1.33
24	a	410	CLA	C1D-ND	4.13	1.42	1.37
24	c	510	CLA	O2A-CGA	4.12	1.45	1.33
24	b	609	CLA	O2A-CGA	4.12	1.45	1.33
24	b	610	CLA	MG-ND	-4.11	1.97	2.05
25	A	408	PHO	OBD-CAD	4.11	1.28	1.22
24	C	504	CLA	O2A-CGA	4.11	1.45	1.33
24	B	612	CLA	O2D-CGD	4.10	1.43	1.33
24	C	511	CLA	OBD-CAD	4.10	1.29	1.22
28	z	101	LMG	O7-C10	4.10	1.45	1.34
24	a	410	CLA	O2A-CGA	4.10	1.45	1.33
24	B	615	CLA	CHD-C1D	4.09	1.46	1.38
24	D	401	CLA	CHC-C1C	4.09	1.45	1.35
28	B	623	LMG	O7-C10	4.09	1.45	1.34
24	B	617	CLA	CHD-C4C	4.08	1.48	1.39
28	A	412	LMG	O8-C28	4.07	1.45	1.33
24	b	618	CLA	CHD-C1D	4.07	1.46	1.38
24	b	617	CLA	O2A-CGA	4.07	1.45	1.33
24	B	614	CLA	MG-ND	-4.06	1.97	2.05
24	c	511	CLA	O2A-CGA	4.06	1.45	1.33
24	B	616	CLA	O2A-CGA	4.06	1.45	1.33
28	i	101	LMG	O8-C28	4.06	1.45	1.33
24	C	509	CLA	O2A-CGA	4.05	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	617	CLA	MG-ND	-4.05	1.97	2.05
24	b	605	CLA	C3D-C2D	4.04	1.50	1.39
24	b	619	CLA	CHD-C1D	4.04	1.46	1.38
24	B	618	CLA	MG-ND	-4.04	1.97	2.05
24	b	616	CLA	O2A-CGA	4.04	1.45	1.33
26	B	620	BCR	C23-C22	-4.04	1.37	1.45
24	C	503	CLA	O2A-CGA	4.04	1.45	1.33
24	b	619	CLA	C3D-C2D	4.03	1.50	1.39
24	a	413	CLA	O2A-CGA	4.03	1.45	1.33
24	c	514	CLA	MG-NC	4.03	2.15	2.06
24	C	513	CLA	MG-ND	-4.03	1.97	2.05
24	B	614	CLA	O2A-CGA	4.03	1.45	1.33
24	B	614	CLA	OBD-CAD	4.03	1.29	1.22
39	F	102	HEM	C4D-ND	-4.02	1.33	1.40
25	A	408	PHO	O2A-CGA	4.02	1.45	1.33
24	C	506	CLA	CHD-C4C	4.02	1.48	1.39
28	b	624	LMG	O7-C10	4.02	1.45	1.34
24	c	514	CLA	CHD-C4C	4.02	1.48	1.39
24	c	513	CLA	CHD-C4C	4.02	1.48	1.39
24	D	405	CLA	CHD-C1D	4.02	1.46	1.38
24	b	608	CLA	OBD-CAD	4.01	1.29	1.22
24	a	413	CLA	C3D-C2D	4.01	1.50	1.39
25	a	412	PHO	OBD-CAD	4.01	1.27	1.22
24	c	505	CLA	O2A-CGA	4.01	1.45	1.33
37	h	102	DGD	O1G-C1A	4.01	1.45	1.33
24	C	513	CLA	O2A-CGA	4.01	1.45	1.33
24	c	507	CLA	O2A-CGA	4.00	1.45	1.33
24	B	605	CLA	CHD-C1D	4.00	1.46	1.38
24	a	410	CLA	O2D-CGD	4.00	1.43	1.33
24	C	511	CLA	C3D-C2D	4.00	1.50	1.39
24	b	611	CLA	C1D-ND	4.00	1.42	1.37
24	A	405	CLA	O2A-CGA	4.00	1.45	1.33
24	a	410	CLA	CHD-C1D	4.00	1.46	1.38
24	c	513	CLA	OBD-CAD	3.99	1.29	1.22
24	c	504	CLA	CHD-C4C	3.99	1.48	1.39
24	C	506	CLA	O2A-CGA	3.99	1.45	1.33
24	c	513	CLA	O2A-CGA	3.99	1.45	1.33
28	c	521	LMG	O7-C10	3.98	1.45	1.34
24	b	607	CLA	CHD-C4C	3.98	1.48	1.39
24	b	613	CLA	CHD-C4C	3.98	1.48	1.39
24	b	606	CLA	C3D-C2D	3.98	1.50	1.39
24	B	609	CLA	CHD-C4C	3.98	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	509	CLA	MG-ND	-3.98	1.97	2.05
24	a	411	CLA	C3D-C2D	3.97	1.50	1.39
24	b	618	CLA	OBD-CAD	3.97	1.29	1.22
24	b	617	CLA	OBD-CAD	3.97	1.29	1.22
24	c	508	CLA	CHD-C4C	3.97	1.48	1.39
24	B	603	CLA	CHD-C4C	3.97	1.48	1.39
24	B	609	CLA	O2D-CGD	3.96	1.42	1.33
37	c	519	DGD	O1G-C1A	3.96	1.44	1.33
24	a	410	CLA	OBD-CAD	3.96	1.29	1.22
24	c	512	CLA	CHD-C4C	3.95	1.48	1.39
27	b	601	SQD	O48-C23	3.95	1.44	1.33
27	B	622	SQD	O48-C23	3.95	1.44	1.33
28	C	521	LMG	O7-C10	3.95	1.45	1.34
24	B	611	CLA	O2A-CGA	3.95	1.44	1.33
24	C	503	CLA	MG-NC	3.95	2.15	2.06
24	b	609	CLA	C1D-ND	3.94	1.42	1.37
37	C	518	DGD	O2G-C1B	3.94	1.45	1.34
24	c	506	CLA	C3D-C2D	3.94	1.49	1.39
24	b	606	CLA	MG-ND	-3.94	1.98	2.05
24	D	406	CLA	O2A-CGA	3.94	1.44	1.33
24	D	401	CLA	O2A-CGA	3.93	1.44	1.33
24	d	406	CLA	CHD-C4C	3.93	1.48	1.39
28	i	101	LMG	O7-C10	3.93	1.45	1.34
24	B	618	CLA	MG-NC	3.93	2.15	2.06
24	C	513	CLA	C3D-C2D	3.93	1.49	1.39
42	v	201	HEC	C2B-C3B	-3.92	1.36	1.40
37	h	102	DGD	O2G-C1B	3.92	1.45	1.34
42	V	201	HEC	C4B-C3B	3.92	1.50	1.43
24	C	512	CLA	O2A-CGA	3.92	1.44	1.33
24	b	605	CLA	CHD-C4C	3.92	1.48	1.39
24	b	607	CLA	O2A-CGA	3.92	1.44	1.33
24	A	406	CLA	O2A-CGA	3.91	1.44	1.33
24	b	612	CLA	C3D-C2D	3.91	1.49	1.39
37	c	518	DGD	O1G-C1A	3.90	1.44	1.33
24	D	401	CLA	CHD-C1D	3.90	1.46	1.38
24	c	512	CLA	OBD-CAD	3.89	1.29	1.22
28	d	412	LMG	O7-C10	3.89	1.45	1.34
24	C	513	CLA	CHD-C4C	3.89	1.48	1.39
38	d	411	LHG	O8-C23	3.89	1.44	1.33
24	D	405	CLA	C1D-ND	3.89	1.42	1.37
24	c	511	CLA	CHD-C4C	3.89	1.48	1.39
24	c	506	CLA	O2A-CGA	3.89	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	616	CLA	MG-ND	-3.88	1.98	2.05
24	b	614	CLA	C3D-C2D	3.88	1.49	1.39
24	b	612	CLA	O2A-CGA	3.88	1.44	1.33
24	C	515	CLA	CHD-C4C	3.88	1.48	1.39
24	C	510	CLA	CHD-C4C	3.88	1.48	1.39
24	C	506	CLA	MG-NC	3.88	2.15	2.06
38	L	101	LHG	O8-C23	3.87	1.44	1.33
24	c	504	CLA	C3D-C2D	3.87	1.49	1.39
37	c	518	DGD	O2G-C1B	3.87	1.45	1.34
24	C	510	CLA	C3D-C2D	3.87	1.49	1.39
37	c	520	DGD	O1G-C1A	3.87	1.44	1.33
24	C	503	CLA	OBD-CAD	3.87	1.29	1.22
24	B	614	CLA	C1D-ND	3.86	1.42	1.37
24	C	508	CLA	C3D-C2D	3.86	1.49	1.39
37	C	519	DGD	O1G-C1A	3.86	1.44	1.33
24	B	608	CLA	CHD-C1D	3.86	1.45	1.38
24	B	610	CLA	CHD-C4C	3.86	1.48	1.39
24	a	409	CLA	O2A-CGA	3.85	1.44	1.33
42	v	201	HEC	CBB-CAB	-3.85	1.35	1.49
24	b	614	CLA	O2A-CGA	3.85	1.44	1.33
24	C	505	CLA	CHD-C4C	3.85	1.48	1.39
28	Z	101	LMG	O7-C10	3.85	1.45	1.34
24	c	515	CLA	C3D-C2D	3.85	1.49	1.39
24	d	406	CLA	OBD-CAD	3.84	1.29	1.22
27	a	415	SQD	O47-C7	3.84	1.45	1.34
37	c	519	DGD	O2G-C1B	3.84	1.45	1.34
24	B	607	CLA	O2A-CGA	3.84	1.44	1.33
24	b	606	CLA	CHD-C4C	3.84	1.48	1.39
24	a	411	CLA	O2A-CGA	3.84	1.44	1.33
28	d	412	LMG	O8-C28	3.83	1.44	1.33
24	c	507	CLA	OBD-CAD	3.83	1.29	1.22
24	b	613	CLA	OBD-CAD	3.83	1.29	1.22
24	d	406	CLA	C3D-C2D	3.83	1.49	1.39
24	D	401	CLA	MG-ND	-3.83	1.98	2.05
24	B	612	CLA	CHD-C4C	3.83	1.48	1.39
24	b	613	CLA	O2A-CGA	3.83	1.44	1.33
24	C	511	CLA	CHD-C4C	3.83	1.48	1.39
24	b	615	CLA	C3D-C2D	3.83	1.49	1.39
24	b	614	CLA	CHD-C4C	3.83	1.48	1.39
24	c	511	CLA	C3D-C2D	3.83	1.49	1.39
24	C	503	CLA	CHD-C4C	3.82	1.48	1.39
24	C	512	CLA	CHD-C4C	3.82	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	514	CLA	C3D-C2D	3.82	1.49	1.39
24	B	606	CLA	MG-ND	-3.82	1.98	2.05
37	H	104	DGD	O1G-C1A	3.82	1.44	1.33
38	D	410	LHG	O8-C23	3.82	1.44	1.33
24	B	617	CLA	OBD-CAD	3.81	1.29	1.22
24	B	612	CLA	C3D-C2D	3.81	1.49	1.39
24	c	512	CLA	O2A-CGA	3.81	1.44	1.33
24	B	616	CLA	C3D-C2D	3.81	1.49	1.39
38	d	409	LHG	O8-C23	3.81	1.44	1.33
24	c	515	CLA	CHD-C4C	3.81	1.47	1.39
24	C	512	CLA	OBD-CAD	3.80	1.29	1.22
24	b	610	CLA	O2A-CGA	3.80	1.44	1.33
24	b	608	CLA	O2A-CGA	3.79	1.44	1.33
24	c	504	CLA	O2A-CGA	3.79	1.44	1.33
24	b	618	CLA	CHD-C4C	3.79	1.47	1.39
24	B	609	CLA	OBD-CAD	3.79	1.29	1.22
24	B	604	CLA	OBD-CAD	3.78	1.29	1.22
24	B	604	CLA	CHD-C4C	3.78	1.47	1.39
24	C	507	CLA	OBD-CAD	3.78	1.29	1.22
24	B	613	CLA	C3D-C2D	3.78	1.49	1.39
24	c	506	CLA	CHD-C4C	3.77	1.47	1.39
25	d	401	PHO	C3C-C2C	3.77	1.48	1.37
24	b	609	CLA	MG-ND	-3.77	1.98	2.05
24	C	505	CLA	OBD-CAD	3.77	1.29	1.22
37	C	520	DGD	O1G-C1A	3.77	1.44	1.33
24	d	405	CLA	CHD-C4C	3.77	1.47	1.39
24	d	405	CLA	O2D-CGD	3.76	1.42	1.33
36	o	301	HTG	C1'-S1	-3.76	1.76	1.81
25	A	408	PHO	CHA-CBD	-3.76	1.47	1.52
27	A	411	SQD	O48-C23	3.76	1.44	1.33
38	l	102	LHG	O8-C23	3.76	1.44	1.33
24	b	609	CLA	CHD-C4C	3.76	1.47	1.39
24	B	612	CLA	O2A-CGA	3.76	1.44	1.33
38	d	410	LHG	O8-C23	3.76	1.44	1.33
24	c	509	CLA	OBD-CAD	3.76	1.29	1.22
27	A	411	SQD	O47-C7	3.76	1.44	1.34
24	C	504	CLA	C3D-C2D	3.75	1.49	1.39
24	c	510	CLA	C3D-C2D	3.75	1.49	1.39
24	D	406	CLA	C3D-C2D	3.75	1.49	1.39
24	a	410	CLA	C3D-C2D	3.75	1.49	1.39
24	c	513	CLA	MG-ND	-3.75	1.98	2.05
24	B	613	CLA	CHD-C4C	3.74	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	513	CLA	C3D-C2D	3.74	1.49	1.39
24	A	409	CLA	OBD-CAD	3.74	1.28	1.22
24	B	615	CLA	CHD-C4C	3.74	1.47	1.39
25	d	401	PHO	O2A-CGA	3.74	1.44	1.33
27	a	415	SQD	O48-C23	3.74	1.44	1.33
24	c	506	CLA	OBD-CAD	3.73	1.28	1.22
24	B	604	CLA	O2A-CGA	3.73	1.44	1.33
24	B	610	CLA	C3D-C2D	3.73	1.49	1.39
24	C	515	CLA	C3D-C2D	3.73	1.49	1.39
24	b	607	CLA	MG-NC	3.73	2.15	2.06
36	O	303	HTG	C1'-S1	-3.73	1.76	1.81
24	B	618	CLA	C3D-C2D	3.73	1.49	1.39
24	C	506	CLA	C3D-C2D	3.73	1.49	1.39
24	a	413	CLA	CHD-C4C	3.72	1.47	1.39
24	B	611	CLA	C3D-C2D	3.72	1.49	1.39
24	C	514	CLA	MG-ND	-3.72	1.98	2.05
24	c	509	CLA	C3D-C2D	3.71	1.49	1.39
24	D	405	CLA	O2A-CGA	3.71	1.44	1.33
38	L	101	LHG	O7-C7	3.71	1.44	1.34
24	c	504	CLA	OBD-CAD	3.71	1.28	1.22
25	A	407	PHO	OBD-CAD	3.70	1.27	1.22
24	B	618	CLA	OBD-CAD	3.70	1.28	1.22
24	c	515	CLA	OBD-CAD	3.69	1.28	1.22
24	A	409	CLA	C3D-C2D	3.69	1.49	1.39
37	c	520	DGD	O2G-C1B	3.69	1.44	1.34
42	V	201	HEC	CBB-CAB	-3.69	1.35	1.49
38	d	411	LHG	O7-C7	3.69	1.44	1.34
24	C	505	CLA	C3D-C2D	3.69	1.49	1.39
24	C	507	CLA	O2A-CGA	3.69	1.44	1.33
24	c	513	CLA	MG-NC	3.69	2.15	2.06
24	d	406	CLA	O2A-CGA	3.68	1.44	1.33
24	b	608	CLA	C3D-C2D	3.67	1.49	1.39
37	H	104	DGD	O2G-C1B	3.67	1.44	1.34
24	c	503	CLA	CHD-C4C	3.67	1.47	1.39
24	b	618	CLA	C3D-C2D	3.67	1.49	1.39
36	b	603	HTG	C1'-S1	-3.67	1.76	1.81
24	b	615	CLA	O2A-CGA	3.66	1.44	1.33
24	c	503	CLA	OBD-CAD	3.66	1.28	1.22
24	c	505	CLA	C3D-C2D	3.66	1.49	1.39
24	B	606	CLA	C3D-C2D	3.66	1.49	1.39
24	C	503	CLA	C3D-C2D	3.66	1.49	1.39
24	b	610	CLA	MG-NC	3.65	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	u	201	HTG	C1'-S1	-3.65	1.76	1.81
24	c	507	CLA	C3D-C2D	3.65	1.49	1.39
24	b	611	CLA	C3D-C2D	3.64	1.49	1.39
24	b	614	CLA	MG-ND	-3.64	1.98	2.05
24	b	608	CLA	CHD-C4C	3.64	1.47	1.39
24	c	514	CLA	C3D-C2D	3.64	1.49	1.39
24	C	509	CLA	OBD-CAD	3.64	1.28	1.22
24	A	406	CLA	CHD-C4C	3.64	1.47	1.39
24	C	510	CLA	OBD-CAD	3.64	1.28	1.22
24	c	505	CLA	CHD-C4C	3.64	1.47	1.39
24	D	401	CLA	C3D-C2D	3.63	1.49	1.39
36	c	524	HTG	C1'-S1	-3.63	1.76	1.81
24	A	405	CLA	C3D-C2D	3.63	1.49	1.39
42	v	201	HEC	C4B-C3B	3.63	1.49	1.43
24	C	515	CLA	OBD-CAD	3.63	1.28	1.22
38	D	411	LHG	O8-C23	3.63	1.43	1.33
28	D	413	LMG	O8-C28	3.62	1.43	1.33
38	D	412	LHG	O7-C7	3.62	1.44	1.34
24	c	510	CLA	OBD-CAD	3.62	1.28	1.22
24	C	512	CLA	C3D-C2D	3.62	1.49	1.39
24	B	615	CLA	O2A-CGA	3.62	1.43	1.33
24	B	603	CLA	C3D-C2D	3.62	1.49	1.39
24	c	512	CLA	C3D-C2D	3.62	1.49	1.39
24	c	511	CLA	OBD-CAD	3.62	1.28	1.22
24	C	513	CLA	MG-NC	3.61	2.14	2.06
24	b	611	CLA	CHD-C4C	3.61	1.47	1.39
24	C	507	CLA	C3D-C2D	3.61	1.49	1.39
36	b	628	HTG	C1'-S1	-3.61	1.76	1.81
24	B	609	CLA	C3D-C2D	3.61	1.49	1.39
24	B	616	CLA	OBD-CAD	3.61	1.28	1.22
24	b	615	CLA	OBD-CAD	3.61	1.28	1.22
24	b	620	CLA	C3D-C2D	3.60	1.49	1.39
24	B	606	CLA	O2A-CGA	3.60	1.43	1.33
24	C	504	CLA	CHD-C4C	3.60	1.47	1.39
24	C	513	CLA	OBD-CAD	3.60	1.28	1.22
24	B	612	CLA	OBD-CAD	3.60	1.28	1.22
24	C	509	CLA	CHD-C4C	3.60	1.47	1.39
24	a	410	CLA	CHD-C4C	3.60	1.47	1.39
24	a	411	CLA	CHD-C4C	3.60	1.47	1.39
25	a	412	PHO	O2A-CGA	3.59	1.43	1.33
24	D	406	CLA	OBD-CAD	3.59	1.28	1.22
24	a	411	CLA	OBD-CAD	3.59	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	616	CLA	CHD-C4C	3.59	1.47	1.39
24	b	612	CLA	CHD-C4C	3.58	1.47	1.39
24	b	605	CLA	OBD-CAD	3.58	1.28	1.22
24	a	413	CLA	MG-NC	3.58	2.14	2.06
24	A	405	CLA	CHD-C4C	3.58	1.47	1.39
24	b	611	CLA	O2A-CGA	3.58	1.43	1.33
24	B	614	CLA	C3D-C2D	3.57	1.48	1.39
24	B	606	CLA	CHD-C4C	3.57	1.47	1.39
24	C	507	CLA	CHD-C4C	3.57	1.47	1.39
24	b	610	CLA	CHD-C4C	3.57	1.47	1.39
24	B	604	CLA	C3D-C2D	3.56	1.48	1.39
24	B	609	CLA	O2A-CGA	3.56	1.43	1.33
28	D	413	LMG	O7-C10	3.56	1.44	1.34
25	A	407	PHO	O2A-CGA	3.55	1.43	1.33
24	C	508	CLA	OBD-CAD	3.55	1.28	1.22
24	b	619	CLA	CHD-C4C	3.55	1.47	1.39
24	C	514	CLA	CHD-C4C	3.55	1.47	1.39
24	b	613	CLA	C3D-C2D	3.55	1.48	1.39
24	b	615	CLA	CHD-C4C	3.55	1.47	1.39
24	c	514	CLA	OBD-CAD	3.55	1.28	1.22
24	B	616	CLA	MG-NC	3.54	2.14	2.06
24	c	508	CLA	C3D-C2D	3.54	1.48	1.39
24	a	413	CLA	OBD-CAD	3.53	1.28	1.22
24	b	620	CLA	CHD-C4C	3.53	1.47	1.39
37	C	520	DGD	O2G-C1B	3.53	1.44	1.34
24	b	618	CLA	MG-NC	3.53	2.14	2.06
39	e	102	HEM	C4D-ND	-3.52	1.34	1.40
24	b	610	CLA	C3D-C2D	3.52	1.48	1.39
24	b	616	CLA	C3D-C2D	3.52	1.48	1.39
25	A	408	PHO	C3C-C2C	3.52	1.48	1.37
24	B	605	CLA	CHD-C4C	3.52	1.47	1.39
24	B	613	CLA	O2A-CGA	3.51	1.43	1.33
24	C	509	CLA	C3D-C2D	3.51	1.48	1.39
24	B	615	CLA	OBD-CAD	3.51	1.28	1.22
24	b	617	CLA	C3D-C2D	3.51	1.48	1.39
38	d	410	LHG	O7-C7	3.50	1.44	1.34
24	a	409	CLA	CHD-C4C	3.50	1.47	1.39
36	C	523	HTG	C1'-S1	-3.49	1.77	1.81
36	B	626	HTG	C1'-S1	-3.49	1.77	1.81
24	D	401	CLA	CHD-C4C	3.49	1.47	1.39
38	l	102	LHG	O7-C7	3.48	1.44	1.34
24	b	612	CLA	OBD-CAD	3.48	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	409	CLA	O2A-CGA	3.47	1.43	1.33
24	b	607	CLA	C3D-C2D	3.47	1.48	1.39
24	A	406	CLA	MG-NC	3.47	2.14	2.06
24	c	503	CLA	C3D-C2D	3.46	1.48	1.39
24	C	515	CLA	MG-NC	3.46	2.14	2.06
24	B	617	CLA	C3D-C2D	3.45	1.48	1.39
24	B	618	CLA	CHD-C4C	3.45	1.47	1.39
39	F	102	HEM	C1B-NB	-3.45	1.34	1.40
24	c	506	CLA	MG-ND	-3.45	1.99	2.05
24	B	610	CLA	MG-ND	-3.45	1.99	2.05
24	B	615	CLA	C3D-C2D	3.44	1.48	1.39
24	b	607	CLA	OBD-CAD	3.44	1.28	1.22
24	B	614	CLA	MG-NC	3.44	2.14	2.06
24	b	609	CLA	OBD-CAD	3.43	1.28	1.22
24	d	405	CLA	C3D-C2D	3.42	1.48	1.39
24	D	406	CLA	MG-ND	-3.42	1.99	2.05
24	B	603	CLA	OBD-CAD	3.42	1.28	1.22
38	D	412	LHG	O8-C23	3.42	1.43	1.33
25	A	407	PHO	C3C-C2C	3.41	1.47	1.37
36	C	522	HTG	C1'-S1	-3.40	1.77	1.81
24	C	505	CLA	MG-ND	-3.40	1.99	2.05
24	c	507	CLA	CHD-C4C	3.40	1.47	1.39
24	A	409	CLA	CHD-C4C	3.39	1.47	1.39
24	B	608	CLA	CHD-C4C	3.38	1.47	1.39
36	H	101	HTG	C1'-S1	-3.38	1.77	1.81
37	C	518	DGD	O1G-C1A	3.38	1.43	1.33
24	c	509	CLA	C4D-CHA	3.38	1.50	1.38
36	B	630	HTG	C1'-S1	-3.38	1.77	1.81
24	c	506	CLA	MG-NC	3.38	2.14	2.06
24	A	406	CLA	C3D-C2D	3.36	1.48	1.39
36	b	602	HTG	C1'-S1	-3.36	1.77	1.81
24	b	620	CLA	OBD-CAD	3.36	1.28	1.22
24	B	607	CLA	C3D-C2D	3.35	1.48	1.39
24	B	608	CLA	OBD-CAD	3.35	1.28	1.22
36	d	404	HTG	C1'-S1	-3.35	1.77	1.81
37	C	519	DGD	O2G-C1B	3.35	1.43	1.34
24	B	605	CLA	C3D-C2D	3.34	1.48	1.39
24	b	609	CLA	C3D-C2D	3.34	1.48	1.39
24	c	513	CLA	C1B-CHB	3.34	1.50	1.41
24	B	611	CLA	C1B-CHB	3.33	1.50	1.41
38	D	411	LHG	O7-C7	3.33	1.43	1.34
25	a	412	PHO	C3C-C2C	3.32	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	405	CLA	OBD-CAD	3.32	1.28	1.22
24	b	610	CLA	C1B-CHB	3.32	1.50	1.41
24	D	405	CLA	C3D-C2D	3.32	1.48	1.39
24	b	606	CLA	OBD-CAD	3.32	1.28	1.22
24	d	405	CLA	C1B-CHB	3.32	1.50	1.41
24	B	606	CLA	OBD-CAD	3.31	1.28	1.22
24	a	409	CLA	C3D-C2D	3.29	1.48	1.39
24	D	406	CLA	CHD-C4C	3.29	1.46	1.39
36	B	629	HTG	C1'-S1	-3.28	1.77	1.81
24	b	617	CLA	CHD-C4C	3.28	1.46	1.39
24	B	605	CLA	OBD-CAD	3.27	1.28	1.22
36	c	523	HTG	C1'-S1	-3.26	1.77	1.81
24	b	607	CLA	MG-ND	-3.25	1.99	2.05
24	b	613	CLA	C1B-CHB	3.24	1.50	1.41
24	B	610	CLA	OBD-CAD	3.23	1.28	1.22
24	D	405	CLA	OBD-CAD	3.23	1.28	1.22
24	c	503	CLA	MG-NC	3.22	2.13	2.06
24	B	607	CLA	CHD-C4C	3.22	1.46	1.39
24	B	616	CLA	C1B-NB	-3.21	1.32	1.35
25	d	401	PHO	CHA-CBD	-3.20	1.48	1.52
24	C	513	CLA	C1B-CHB	3.17	1.49	1.41
24	c	510	CLA	CHD-C4C	3.16	1.46	1.39
24	D	405	CLA	CHD-C4C	3.16	1.46	1.39
24	B	613	CLA	OBD-CAD	3.16	1.27	1.22
24	B	614	CLA	CHD-C4C	3.16	1.46	1.39
24	C	504	CLA	OBD-CAD	3.15	1.27	1.22
24	B	614	CLA	C1B-CHB	3.14	1.49	1.41
24	B	606	CLA	C4D-CHA	3.13	1.49	1.38
24	C	506	CLA	OBD-CAD	3.13	1.27	1.22
24	B	607	CLA	C1B-CHB	3.11	1.49	1.41
24	B	608	CLA	C3D-C2D	3.10	1.47	1.39
42	V	201	HEC	C2B-C3B	-3.10	1.37	1.40
24	c	504	CLA	C1B-CHB	3.09	1.49	1.41
24	C	508	CLA	C4D-CHA	3.08	1.49	1.38
24	D	406	CLA	C1B-CHB	3.08	1.49	1.41
24	B	609	CLA	MG-ND	-3.07	1.99	2.05
24	b	616	CLA	C1B-CHB	3.07	1.49	1.41
24	b	611	CLA	OBD-CAD	3.06	1.27	1.22
24	C	514	CLA	OBD-CAD	3.06	1.27	1.22
24	b	612	CLA	C1C-NC	-3.06	1.33	1.37
24	B	606	CLA	C1B-CHB	3.06	1.49	1.41
24	C	505	CLA	C4D-CHA	3.05	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	505	CLA	OBD-CAD	3.05	1.27	1.22
24	C	512	CLA	C1B-CHB	3.05	1.49	1.41
24	b	610	CLA	OBD-CAD	3.05	1.27	1.22
24	b	620	CLA	C4D-CHA	3.05	1.49	1.38
38	d	409	LHG	O7-C7	3.05	1.42	1.34
24	c	511	CLA	C1B-CHB	3.05	1.49	1.41
24	C	505	CLA	C4B-CHC	3.04	1.49	1.41
25	a	412	PHO	CHA-CBD	-3.04	1.48	1.52
24	b	608	CLA	C4D-CHA	3.03	1.49	1.38
24	C	509	CLA	C4D-CHA	3.03	1.49	1.38
24	b	617	CLA	C1C-NC	-3.02	1.33	1.37
24	B	615	CLA	C4D-CHA	3.01	1.49	1.38
24	B	607	CLA	OBD-CAD	3.01	1.27	1.22
24	C	507	CLA	C1B-CHB	3.01	1.49	1.41
24	b	616	CLA	CHD-C4C	3.00	1.46	1.39
24	A	405	CLA	C1B-CHB	3.00	1.49	1.41
24	C	505	CLA	C1C-NC	-3.00	1.33	1.37
24	c	508	CLA	OBD-CAD	2.99	1.27	1.22
24	B	611	CLA	CHD-C4C	2.99	1.46	1.39
24	C	514	CLA	MG-NC	2.99	2.13	2.06
24	C	514	CLA	C1B-CHB	2.99	1.49	1.41
24	C	505	CLA	C1B-CHB	2.98	1.49	1.41
24	C	510	CLA	MG-NC	2.98	2.13	2.06
24	B	603	CLA	C4D-CHA	2.98	1.49	1.38
24	C	503	CLA	C1B-CHB	2.98	1.49	1.41
24	C	507	CLA	C4B-CHC	2.97	1.49	1.41
24	c	514	CLA	C4D-CHA	2.97	1.49	1.38
39	e	102	HEM	C1B-NB	-2.97	1.35	1.40
24	c	509	CLA	C1B-CHB	2.96	1.49	1.41
24	c	513	CLA	C4D-CHA	2.96	1.48	1.38
24	B	615	CLA	C1B-CHB	2.95	1.49	1.41
24	b	605	CLA	MG-ND	-2.95	1.99	2.05
24	C	506	CLA	C4D-CHA	2.95	1.48	1.38
36	b	627	HTG	C1'-S1	-2.94	1.77	1.81
24	C	515	CLA	C4D-CHA	2.94	1.48	1.38
24	c	507	CLA	C1B-CHB	2.93	1.49	1.41
24	B	616	CLA	C1B-CHB	2.93	1.49	1.41
24	c	512	CLA	C1B-CHB	2.93	1.49	1.41
24	C	515	CLA	C4B-CHC	2.93	1.49	1.41
24	D	401	CLA	OBD-CAD	2.92	1.27	1.22
24	c	504	CLA	C4D-CHA	2.92	1.48	1.38
24	C	513	CLA	C4D-CHA	2.92	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	620	CLA	C1B-CHB	2.91	1.49	1.41
24	B	618	CLA	C1B-CHB	2.91	1.49	1.41
24	b	609	CLA	C4B-CHC	2.91	1.49	1.41
24	b	617	CLA	C1B-CHB	2.91	1.49	1.41
24	B	613	CLA	C4D-CHA	2.91	1.48	1.38
24	A	405	CLA	C4D-CHA	2.90	1.48	1.38
24	C	505	CLA	C1C-C2C	2.90	1.50	1.44
24	C	504	CLA	C1B-CHB	2.90	1.49	1.41
24	C	514	CLA	C4D-CHA	2.89	1.48	1.38
27	f	802	SQD	C6-S	-2.89	1.66	1.77
24	b	616	CLA	C1C-NC	-2.88	1.33	1.37
24	b	613	CLA	C4B-CHC	2.88	1.49	1.41
24	C	511	CLA	C4D-CHA	2.88	1.48	1.38
24	c	506	CLA	C4D-CHA	2.88	1.48	1.38
24	b	607	CLA	C4D-CHA	2.88	1.48	1.38
24	c	512	CLA	C4D-CHA	2.87	1.48	1.38
24	c	515	CLA	C4D-CHA	2.87	1.48	1.38
24	c	511	CLA	C4D-CHA	2.87	1.48	1.38
24	C	507	CLA	C4D-CHA	2.87	1.48	1.38
24	b	613	CLA	C4D-CHA	2.87	1.48	1.38
24	b	610	CLA	C1C-C2C	2.87	1.50	1.44
24	b	614	CLA	C4B-CHC	2.86	1.49	1.41
24	b	605	CLA	C1B-CHB	2.86	1.48	1.41
24	D	401	CLA	MG-NC	2.86	2.13	2.06
24	b	608	CLA	C1B-CHB	2.86	1.48	1.41
24	b	611	CLA	C4D-CHA	2.86	1.48	1.38
24	B	618	CLA	C1C-NC	-2.86	1.33	1.37
24	C	512	CLA	C4D-CHA	2.86	1.48	1.38
24	b	606	CLA	C1B-CHB	2.85	1.48	1.41
24	C	508	CLA	C1B-CHB	2.85	1.48	1.41
24	a	413	CLA	C4D-CHA	2.85	1.48	1.38
24	C	515	CLA	C1B-CHB	2.85	1.48	1.41
24	c	505	CLA	C1B-CHB	2.85	1.48	1.41
24	a	411	CLA	C1B-CHB	2.85	1.48	1.41
24	b	610	CLA	C4D-CHA	2.84	1.48	1.38
24	D	405	CLA	C1C-NC	-2.84	1.33	1.37
24	B	612	CLA	C1B-CHB	2.84	1.48	1.41
24	b	614	CLA	C4D-CHA	2.84	1.48	1.38
24	b	605	CLA	C4B-CHC	2.83	1.48	1.41
38	D	410	LHG	O7-C7	2.83	1.42	1.34
24	C	510	CLA	C1B-CHB	2.83	1.48	1.41
24	c	509	CLA	C4B-CHC	2.83	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	B	625	HTG	C1'-S1	-2.83	1.77	1.81
24	B	617	CLA	C1B-CHB	2.83	1.48	1.41
27	a	401	SQD	C6-S	-2.83	1.67	1.77
24	D	405	CLA	MG-NC	2.82	2.13	2.06
24	c	505	CLA	C4B-CHC	2.82	1.48	1.41
24	B	610	CLA	C4D-CHA	2.82	1.48	1.38
24	b	612	CLA	C4D-CHA	2.82	1.48	1.38
24	C	510	CLA	C4D-CHA	2.82	1.48	1.38
24	b	605	CLA	C4D-CHA	2.82	1.48	1.38
24	B	611	CLA	C4D-CHA	2.82	1.48	1.38
24	C	511	CLA	C1B-CHB	2.82	1.48	1.41
24	B	617	CLA	C4D-CHA	2.82	1.48	1.38
24	B	609	CLA	C4D-CHA	2.82	1.48	1.38
24	a	409	CLA	C1B-CHB	2.81	1.48	1.41
27	A	415	SQD	C6-S	-2.81	1.67	1.77
24	c	505	CLA	C4D-CHA	2.81	1.48	1.38
40	H	103	RRX	C24-C25	-2.80	1.35	1.45
24	B	615	CLA	MG-NC	2.80	2.12	2.06
24	c	510	CLA	C1B-CHB	2.80	1.48	1.41
24	C	504	CLA	C4D-CHA	2.80	1.48	1.38
24	c	505	CLA	MG-ND	-2.80	2.00	2.05
24	B	617	CLA	C4B-CHC	2.80	1.48	1.41
24	A	409	CLA	MG-NA	2.80	2.12	2.06
24	b	619	CLA	C4D-CHA	2.79	1.48	1.38
24	B	613	CLA	C1B-CHB	2.79	1.48	1.41
24	c	503	CLA	C4D-CHA	2.79	1.48	1.38
24	C	503	CLA	C4D-CHA	2.79	1.48	1.38
24	B	603	CLA	C1C-C2C	2.79	1.50	1.44
24	b	616	CLA	C4D-CHA	2.78	1.48	1.38
24	B	612	CLA	C4D-CHA	2.78	1.48	1.38
24	B	618	CLA	C4D-CHA	2.78	1.48	1.38
24	c	507	CLA	C4D-CHA	2.78	1.48	1.38
25	A	407	PHO	CHA-CBD	-2.78	1.49	1.52
24	a	411	CLA	C4D-CHA	2.78	1.48	1.38
24	A	405	CLA	OBD-CAD	2.77	1.27	1.22
24	D	406	CLA	C4B-CHC	2.77	1.48	1.41
24	B	610	CLA	C4B-CHC	2.77	1.48	1.41
24	A	405	CLA	C4C-C3C	2.77	1.49	1.45
24	C	504	CLA	C1C-C2C	2.77	1.49	1.44
24	d	406	CLA	C4D-CHA	2.76	1.48	1.38
24	c	513	CLA	C4B-CHC	2.76	1.48	1.41
24	D	406	CLA	C4D-CHA	2.76	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	619	CLA	MG-NC	2.76	2.12	2.06
24	B	604	CLA	C1B-CHB	2.76	1.48	1.41
24	C	507	CLA	C1C-C2C	2.75	1.49	1.44
24	b	606	CLA	C4D-CHA	2.75	1.48	1.38
24	b	615	CLA	C1B-CHB	2.75	1.48	1.41
24	B	617	CLA	MG-ND	-2.75	2.00	2.05
24	c	508	CLA	C1B-CHB	2.75	1.48	1.41
24	B	603	CLA	C4B-CHC	2.74	1.48	1.41
24	c	508	CLA	C4D-CHA	2.74	1.48	1.38
24	B	608	CLA	C4B-CHC	2.74	1.48	1.41
24	d	406	CLA	C1B-CHB	2.73	1.48	1.41
24	C	509	CLA	C1C-C2C	2.73	1.49	1.44
24	b	609	CLA	C4D-CHA	2.73	1.48	1.38
24	c	505	CLA	C1C-NC	-2.73	1.33	1.37
24	B	608	CLA	C1B-CHB	2.73	1.48	1.41
24	a	410	CLA	C1B-CHB	2.73	1.48	1.41
24	c	510	CLA	C4B-CHC	2.73	1.48	1.41
24	b	606	CLA	C1C-C2C	2.73	1.49	1.44
24	c	503	CLA	C1B-CHB	2.72	1.48	1.41
24	b	618	CLA	C1C-C2C	2.72	1.49	1.44
24	a	413	CLA	C1B-CHB	2.72	1.48	1.41
24	c	508	CLA	C1C-C2C	2.71	1.49	1.44
24	B	604	CLA	C4B-CHC	2.71	1.48	1.41
24	b	613	CLA	C1C-NC	-2.71	1.33	1.37
24	C	504	CLA	C4B-CHC	2.71	1.48	1.41
24	b	617	CLA	C4D-CHA	2.71	1.48	1.38
24	C	514	CLA	C4B-CHC	2.71	1.48	1.41
24	c	514	CLA	C4B-CHC	2.70	1.48	1.41
24	B	607	CLA	C1C-NC	-2.70	1.33	1.37
24	b	616	CLA	C1C-C2C	2.70	1.49	1.44
24	c	514	CLA	C1B-CHB	2.70	1.48	1.41
24	a	409	CLA	C4D-CHA	2.70	1.48	1.38
24	B	605	CLA	C4D-CHA	2.70	1.48	1.38
24	A	405	CLA	C4B-CHC	2.70	1.48	1.41
39	e	102	HEM	CHB-C1B	2.69	1.41	1.35
25	d	401	PHO	C3A-C2A	-2.69	1.52	1.54
24	B	609	CLA	C1B-CHB	2.69	1.48	1.41
29	a	417	PL9	C6-C5	2.69	1.49	1.35
24	B	603	CLA	C1B-CHB	2.69	1.48	1.41
24	B	608	CLA	C4D-CHA	2.69	1.48	1.38
24	b	615	CLA	C4B-CHC	2.69	1.48	1.41
24	b	618	CLA	MG-ND	-2.69	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	409	CLA	C1C-C2C	2.69	1.49	1.44
24	C	515	CLA	C1C-C2C	2.69	1.49	1.44
24	b	607	CLA	C1B-CHB	2.69	1.48	1.41
24	c	506	CLA	C1B-CHB	2.68	1.48	1.41
24	b	611	CLA	C4B-CHC	2.68	1.48	1.41
24	c	515	CLA	C1C-NC	-2.68	1.33	1.37
24	b	606	CLA	C4B-CHC	2.68	1.48	1.41
24	c	515	CLA	C1B-CHB	2.68	1.48	1.41
24	b	615	CLA	MG-NC	2.67	2.12	2.06
24	C	506	CLA	C1B-CHB	2.67	1.48	1.41
24	c	507	CLA	C4B-CHC	2.67	1.48	1.41
24	C	507	CLA	C4C-C3C	2.66	1.49	1.45
27	B	622	SQD	C6-S	-2.66	1.67	1.77
24	b	612	CLA	C1B-CHB	2.66	1.48	1.41
39	e	102	HEM	FE-NB	2.66	2.10	1.96
24	B	605	CLA	C1C-NC	-2.66	1.33	1.37
24	B	612	CLA	C4B-CHC	2.66	1.48	1.41
24	b	609	CLA	C1B-CHB	2.66	1.48	1.41
24	B	616	CLA	C4B-CHC	2.65	1.48	1.41
24	b	605	CLA	C1C-C2C	2.65	1.49	1.44
24	B	604	CLA	C4D-CHA	2.65	1.47	1.38
24	d	405	CLA	C4D-CHA	2.65	1.47	1.38
24	c	515	CLA	C4B-CHC	2.64	1.48	1.41
24	c	505	CLA	C1C-C2C	2.64	1.49	1.44
24	b	618	CLA	C1B-CHB	2.64	1.48	1.41
24	b	608	CLA	C1C-C2C	2.64	1.49	1.44
24	b	614	CLA	C1B-CHB	2.63	1.48	1.41
24	B	614	CLA	C4D-CHA	2.63	1.47	1.38
24	C	509	CLA	C1C-NC	-2.63	1.33	1.37
39	F	102	HEM	FE-NB	2.62	2.09	1.96
24	b	618	CLA	C4D-CHA	2.62	1.47	1.38
40	h	101	RRX	C24-C25	-2.61	1.35	1.45
24	c	509	CLA	C1C-C2C	2.61	1.49	1.44
24	b	612	CLA	C4B-CHC	2.61	1.48	1.41
24	C	509	CLA	C1B-CHB	2.60	1.48	1.41
24	a	411	CLA	MG-ND	-2.60	2.00	2.05
24	B	605	CLA	C4B-CHC	2.60	1.48	1.41
24	c	510	CLA	C4D-CHA	2.59	1.47	1.38
24	B	610	CLA	C1B-CHB	2.59	1.48	1.41
24	b	620	CLA	C4B-CHC	2.59	1.48	1.41
24	B	606	CLA	C4B-CHC	2.59	1.48	1.41
24	C	511	CLA	C1C-NC	-2.58	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	409	CLA	C4D-CHA	2.58	1.47	1.38
24	c	511	CLA	C1C-NC	-2.58	1.34	1.37
24	b	609	CLA	C1C-NC	-2.58	1.34	1.37
24	b	607	CLA	C1C-C2C	2.58	1.49	1.44
27	b	601	SQD	C6-S	-2.58	1.67	1.77
28	z	101	LMG	O8-C28	2.57	1.46	1.33
27	A	411	SQD	C6-S	-2.56	1.67	1.77
24	C	512	CLA	C1C-C2C	2.56	1.49	1.44
24	c	508	CLA	C4B-CHC	2.56	1.48	1.41
24	C	512	CLA	C4B-CHC	2.56	1.48	1.41
24	a	411	CLA	C1C-NC	-2.55	1.34	1.37
24	D	405	CLA	C1B-CHB	2.55	1.48	1.41
24	c	515	CLA	C1C-C2C	2.55	1.49	1.44
24	B	615	CLA	C4B-CHC	2.55	1.48	1.41
24	d	406	CLA	C4B-CHC	2.55	1.48	1.41
24	b	616	CLA	C4B-CHC	2.55	1.48	1.41
24	B	616	CLA	C4D-CHA	2.55	1.47	1.38
24	A	406	CLA	C4D-CHA	2.54	1.47	1.38
24	C	514	CLA	C1C-C2C	2.54	1.49	1.44
24	c	504	CLA	C4C-C3C	2.54	1.49	1.45
24	c	510	CLA	C1C-C2C	2.54	1.49	1.44
24	b	609	CLA	C1C-C2C	2.54	1.49	1.44
24	D	401	CLA	C4D-CHA	2.53	1.47	1.38
27	F	101	SQD	C6-S	-2.52	1.68	1.77
24	b	614	CLA	C1C-NC	-2.52	1.34	1.37
24	c	506	CLA	C4B-CHC	2.52	1.48	1.41
24	c	511	CLA	C4B-CHC	2.52	1.48	1.41
24	a	411	CLA	C4C-C3C	2.52	1.49	1.45
24	D	405	CLA	C4D-CHA	2.52	1.47	1.38
24	B	610	CLA	C1C-NC	-2.51	1.34	1.37
24	A	409	CLA	C1B-CHB	2.51	1.48	1.41
24	B	605	CLA	C1B-CHB	2.51	1.48	1.41
24	c	512	CLA	C4B-CHC	2.51	1.48	1.41
24	B	613	CLA	C4B-CHC	2.51	1.48	1.41
24	b	608	CLA	C1C-NC	-2.51	1.34	1.37
24	B	613	CLA	MG-NC	2.51	2.12	2.06
24	C	506	CLA	C1C-NC	-2.51	1.34	1.37
24	B	611	CLA	C4B-CHC	2.50	1.47	1.41
24	B	607	CLA	C4B-CHC	2.50	1.47	1.41
24	B	608	CLA	C1C-C2C	2.50	1.49	1.44
24	c	504	CLA	C4B-CHC	2.50	1.47	1.41
24	b	607	CLA	C4B-CHC	2.50	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	604	CLA	C4C-C3C	2.50	1.49	1.45
24	b	619	CLA	C4B-CHC	2.49	1.47	1.41
24	c	507	CLA	C4C-C3C	2.49	1.49	1.45
24	C	511	CLA	C1C-C2C	2.49	1.49	1.44
24	b	620	CLA	C1C-NC	-2.49	1.34	1.37
24	c	503	CLA	C4B-CHC	2.49	1.47	1.41
24	c	503	CLA	C1C-C2C	2.48	1.49	1.44
24	C	509	CLA	C4B-CHC	2.48	1.47	1.41
24	C	508	CLA	C4C-C3C	2.48	1.49	1.45
24	b	615	CLA	C4D-CHA	2.48	1.47	1.38
36	b	602	HTG	C1-S1	-2.48	1.76	1.80
24	B	609	CLA	C4B-CHC	2.48	1.47	1.41
24	b	612	CLA	C4C-C3C	2.48	1.49	1.45
24	a	411	CLA	C4B-NB	-2.48	1.33	1.35
24	C	507	CLA	C1C-NC	-2.47	1.34	1.37
29	A	413	PL9	C6-C5	2.47	1.48	1.35
24	D	405	CLA	C4C-C3C	2.47	1.49	1.45
25	A	408	PHO	C3A-C2A	-2.47	1.52	1.54
24	C	513	CLA	C1C-C2C	2.47	1.49	1.44
24	B	612	CLA	C1C-NC	-2.47	1.34	1.37
24	a	409	CLA	C4B-CHC	2.47	1.47	1.41
24	C	508	CLA	C4B-CHC	2.46	1.47	1.41
24	A	409	CLA	C4B-CHC	2.46	1.47	1.41
24	C	503	CLA	C1C-C2C	2.46	1.49	1.44
24	D	406	CLA	C1C-C2C	2.46	1.49	1.44
24	B	610	CLA	C4C-C3C	2.45	1.49	1.45
24	C	504	CLA	C1C-NC	-2.44	1.34	1.37
24	B	618	CLA	C4B-CHC	2.44	1.47	1.41
24	B	612	CLA	C4C-C3C	2.44	1.49	1.45
24	B	616	CLA	C3D-C4D	-2.44	1.38	1.44
24	C	511	CLA	C4B-CHC	2.44	1.47	1.41
24	B	607	CLA	C4D-CHA	2.43	1.47	1.38
24	D	405	CLA	C4B-CHC	2.43	1.47	1.41
24	c	507	CLA	C1C-NC	-2.43	1.34	1.37
24	c	507	CLA	C1C-C2C	2.43	1.49	1.44
24	b	610	CLA	C4B-CHC	2.43	1.47	1.41
24	b	608	CLA	C4B-CHC	2.42	1.47	1.41
24	C	503	CLA	C1C-NC	-2.42	1.34	1.37
24	b	614	CLA	C4C-C3C	2.42	1.49	1.45
24	c	506	CLA	C1C-C2C	2.42	1.49	1.44
24	C	513	CLA	C4B-CHC	2.42	1.47	1.41
24	c	513	CLA	C1C-C2C	2.42	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	406	CLA	C4C-C3C	2.41	1.49	1.45
24	C	513	CLA	C4C-C3C	2.41	1.49	1.45
24	C	510	CLA	C1C-C2C	2.41	1.49	1.44
24	a	413	CLA	C1C-C2C	2.41	1.49	1.44
36	b	603	HTG	C1-S1	-2.41	1.77	1.80
24	b	607	CLA	C4C-C3C	2.40	1.49	1.45
24	D	401	CLA	C1B-CHB	2.40	1.47	1.41
24	d	405	CLA	C4B-CHC	2.40	1.47	1.41
24	C	503	CLA	C4B-CHC	2.40	1.47	1.41
24	B	606	CLA	C3D-C4D	-2.39	1.38	1.44
27	a	415	SQD	C6-S	-2.39	1.68	1.77
24	B	611	CLA	C1C-C2C	2.38	1.49	1.44
24	c	513	CLA	C4C-C3C	2.38	1.49	1.45
24	b	613	CLA	C1C-C2C	2.37	1.49	1.44
24	c	509	CLA	C1C-NC	-2.36	1.34	1.37
24	c	505	CLA	C4C-C3C	2.36	1.49	1.45
39	F	102	HEM	CHB-C1B	2.36	1.41	1.35
24	B	612	CLA	C1C-C2C	2.36	1.49	1.44
24	B	616	CLA	C4B-NB	-2.36	1.33	1.35
24	B	611	CLA	C1C-NC	-2.36	1.34	1.37
24	B	615	CLA	C1C-NC	-2.35	1.34	1.37
24	D	401	CLA	C4B-CHC	2.35	1.47	1.41
24	c	511	CLA	C1C-C2C	2.35	1.49	1.44
24	b	617	CLA	C4C-C3C	2.35	1.49	1.45
24	B	616	CLA	C1C-C2C	2.35	1.49	1.44
24	b	620	CLA	C1C-C2C	2.35	1.49	1.44
24	a	413	CLA	C4B-CHC	2.34	1.47	1.41
29	D	408	PL9	C6-C5	2.34	1.47	1.35
24	C	512	CLA	C1C-NC	-2.34	1.34	1.37
24	c	514	CLA	C4C-C3C	2.34	1.49	1.45
37	h	102	DGD	O5D-C1E	2.34	1.44	1.40
24	B	606	CLA	C4C-C3C	2.34	1.49	1.45
24	A	406	CLA	C1B-CHB	2.33	1.47	1.41
24	d	405	CLA	C4C-C3C	2.33	1.49	1.45
24	C	503	CLA	C4C-C3C	2.33	1.49	1.45
24	b	612	CLA	C1C-C2C	2.33	1.49	1.44
24	C	511	CLA	C4C-C3C	2.33	1.49	1.45
24	b	606	CLA	C1C-NC	-2.33	1.34	1.37
24	c	511	CLA	C3D-C4D	-2.33	1.38	1.44
24	C	512	CLA	C4C-C3C	2.32	1.49	1.45
24	B	605	CLA	C1C-C2C	2.32	1.49	1.44
24	b	611	CLA	C1B-CHB	2.32	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	d	408	PL9	C6-C5	2.32	1.47	1.35
24	C	513	CLA	C1C-NC	-2.30	1.34	1.37
24	B	615	CLA	C1C-C2C	2.30	1.49	1.44
24	C	515	CLA	C1C-NC	-2.29	1.34	1.37
24	B	604	CLA	C1C-C2C	2.29	1.49	1.44
24	B	615	CLA	C4C-C3C	2.29	1.49	1.45
24	b	611	CLA	C4C-C3C	2.29	1.49	1.45
24	c	508	CLA	C1C-NC	-2.28	1.34	1.37
24	b	617	CLA	C4B-CHC	2.28	1.47	1.41
24	B	603	CLA	C1C-NC	-2.28	1.34	1.37
24	B	605	CLA	C3D-C4D	-2.28	1.39	1.44
36	C	522	HTG	C1-S1	-2.28	1.77	1.80
24	B	614	CLA	C1C-C2C	2.28	1.49	1.44
24	B	607	CLA	C1C-C2C	2.28	1.49	1.44
24	c	514	CLA	C1C-C2C	2.28	1.49	1.44
24	b	607	CLA	C1C-NC	-2.28	1.34	1.37
24	c	515	CLA	C4C-C3C	2.28	1.49	1.45
24	c	504	CLA	C1C-C2C	2.27	1.49	1.44
24	C	509	CLA	C4C-C3C	2.27	1.49	1.45
37	H	104	DGD	O5D-C1E	2.27	1.44	1.40
24	C	510	CLA	C4B-CHC	2.27	1.47	1.41
24	a	409	CLA	C1B-NB	-2.27	1.33	1.35
24	a	413	CLA	C1C-NC	-2.27	1.34	1.37
24	a	410	CLA	C4D-CHA	2.27	1.46	1.38
24	a	410	CLA	C3D-C4D	-2.27	1.39	1.44
24	B	610	CLA	C1C-C2C	2.26	1.48	1.44
24	C	506	CLA	C4B-CHC	2.26	1.47	1.41
24	C	510	CLA	C3D-C4D	-2.26	1.39	1.44
24	c	506	CLA	C1C-NC	-2.26	1.34	1.37
24	C	506	CLA	C1C-C2C	2.26	1.48	1.44
24	c	512	CLA	C1C-NC	-2.26	1.34	1.37
24	c	504	CLA	C1C-NC	-2.25	1.34	1.37
24	A	406	CLA	C4B-CHC	2.25	1.47	1.41
24	b	619	CLA	C1C-C2C	2.25	1.48	1.44
36	B	629	HTG	C1-S1	-2.24	1.77	1.80
24	c	510	CLA	C1C-NC	-2.24	1.34	1.37
24	B	614	CLA	C4B-CHC	2.24	1.47	1.41
24	C	505	CLA	C4C-C3C	2.24	1.48	1.45
24	c	503	CLA	C1C-NC	-2.24	1.34	1.37
24	B	617	CLA	C1B-NB	-2.24	1.33	1.35
24	a	409	CLA	C1C-NC	-2.23	1.34	1.37
24	b	618	CLA	C4B-CHC	2.23	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	508	CLA	C1C-NC	-2.23	1.34	1.37
24	b	613	CLA	C3D-C4D	-2.23	1.39	1.44
24	C	514	CLA	C1C-NC	-2.23	1.34	1.37
24	b	615	CLA	C4C-C3C	2.22	1.48	1.45
24	b	616	CLA	C4C-C3C	2.22	1.48	1.45
24	C	508	CLA	C1C-C2C	2.22	1.48	1.44
36	c	523	HTG	C1-S1	-2.22	1.77	1.80
24	b	614	CLA	C1C-C2C	2.22	1.48	1.44
24	b	605	CLA	C1C-NC	-2.22	1.34	1.37
24	c	506	CLA	C3D-C4D	-2.22	1.39	1.44
24	B	604	CLA	C1D-C2D	2.22	1.49	1.45
24	A	406	CLA	C1C-NC	-2.22	1.34	1.37
24	b	608	CLA	C4C-C3C	2.21	1.48	1.45
24	b	617	CLA	C1C-C2C	2.21	1.48	1.44
24	b	619	CLA	C4C-C3C	2.21	1.48	1.45
24	B	617	CLA	MG-NC	2.21	2.11	2.06
24	A	409	CLA	C1B-NB	-2.21	1.33	1.35
39	e	102	HEM	C1D-ND	-2.20	1.34	1.38
24	b	620	CLA	C3D-C4D	-2.20	1.39	1.44
24	a	409	CLA	C1C-C2C	2.20	1.48	1.44
24	B	609	CLA	C1C-NC	-2.20	1.34	1.37
24	c	512	CLA	C4C-C3C	2.20	1.48	1.45
24	C	515	CLA	C4D-ND	2.20	1.40	1.37
37	C	518	DGD	O5D-C1E	2.20	1.43	1.40
24	A	405	CLA	C1C-C2C	2.20	1.48	1.44
24	a	413	CLA	C4C-C3C	2.19	1.48	1.45
24	D	406	CLA	C4C-C3C	2.19	1.48	1.45
36	C	523	HTG	C1-S1	-2.19	1.77	1.80
24	c	503	CLA	C4C-C3C	2.19	1.48	1.45
39	F	102	HEM	C1D-ND	-2.19	1.34	1.38
24	C	514	CLA	C3D-C4D	-2.19	1.39	1.44
24	a	411	CLA	C4B-CHC	2.19	1.47	1.41
24	D	401	CLA	C3D-C4D	-2.18	1.39	1.44
24	C	514	CLA	C4C-C3C	2.18	1.48	1.45
24	a	410	CLA	C1C-NC	-2.17	1.34	1.37
24	c	514	CLA	C3D-C4D	-2.17	1.39	1.44
39	e	102	HEM	C4B-NB	-2.17	1.34	1.38
24	B	604	CLA	C1C-NC	-2.16	1.34	1.37
24	C	511	CLA	C3D-C4D	-2.16	1.39	1.44
24	C	513	CLA	C3D-C4D	-2.16	1.39	1.44
24	b	618	CLA	C4C-C3C	2.16	1.48	1.45
24	B	603	CLA	C4C-C3C	2.16	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	603	CLA	C3D-C4D	-2.15	1.39	1.44
24	B	617	CLA	C1C-C2C	2.15	1.48	1.44
24	A	409	CLA	C4C-C3C	2.15	1.48	1.45
29	d	408	PL9	C2-C3	2.15	1.40	1.34
24	B	609	CLA	C3D-C4D	-2.15	1.39	1.44
24	B	608	CLA	C1C-NC	-2.15	1.34	1.37
36	c	524	HTG	C1-S1	-2.15	1.77	1.80
24	A	406	CLA	C3D-C4D	-2.15	1.39	1.44
24	b	610	CLA	C4C-C3C	2.15	1.48	1.45
24	b	617	CLA	C3D-C4D	-2.14	1.39	1.44
24	c	512	CLA	C3D-C4D	-2.14	1.39	1.44
24	d	406	CLA	C1C-C2C	2.14	1.48	1.44
24	c	508	CLA	C3D-C4D	-2.13	1.39	1.44
24	d	406	CLA	C3D-C4D	-2.13	1.39	1.44
24	b	611	CLA	C1C-NC	-2.13	1.34	1.37
24	c	504	CLA	C3D-C4D	-2.13	1.39	1.44
24	a	411	CLA	MG-NC	2.13	2.11	2.06
36	b	628	HTG	C1-S1	-2.13	1.77	1.80
24	d	405	CLA	C1C-C2C	2.12	1.48	1.44
24	b	611	CLA	C1C-C2C	2.12	1.48	1.44
32	f	801	LMT	O1'-C1'	2.12	1.43	1.40
24	B	612	CLA	C1B-NB	-2.12	1.33	1.35
24	D	401	CLA	C4B-NB	-2.11	1.33	1.35
24	B	614	CLA	C1C-NC	-2.11	1.34	1.37
24	b	606	CLA	C4C-C3C	2.11	1.48	1.45
24	b	606	CLA	C3D-C4D	-2.11	1.39	1.44
24	B	617	CLA	C3D-C4D	-2.11	1.39	1.44
24	c	509	CLA	C4D-ND	2.10	1.40	1.37
24	c	508	CLA	C4C-C3C	2.10	1.48	1.45
24	a	409	CLA	C3D-C4D	-2.09	1.39	1.44
24	a	410	CLA	C4B-CHC	2.09	1.46	1.41
24	b	615	CLA	C1C-NC	-2.09	1.34	1.37
24	B	606	CLA	C1C-C2C	2.09	1.48	1.44
24	B	618	CLA	C3D-C4D	-2.09	1.39	1.44
24	d	405	CLA	C1C-NC	-2.08	1.34	1.37
24	b	619	CLA	C1B-CHB	2.08	1.46	1.41
24	C	503	CLA	C3D-C4D	-2.08	1.39	1.44
39	e	102	HEM	C3B-C4B	2.08	1.49	1.44
24	A	406	CLA	C4C-C3C	2.08	1.48	1.45
24	C	510	CLA	C4C-C3C	2.07	1.48	1.45
24	b	611	CLA	C3D-C4D	-2.07	1.39	1.44
24	a	410	CLA	C1C-C2C	2.07	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	504	CLA	C4C-C3C	2.07	1.48	1.45
24	b	610	CLA	C1C-NC	-2.07	1.34	1.37
24	d	406	CLA	C1B-NB	-2.07	1.33	1.35
24	C	506	CLA	C3D-C4D	-2.07	1.39	1.44
24	D	405	CLA	C1C-C2C	2.06	1.48	1.44
24	C	508	CLA	C1B-NB	-2.06	1.33	1.35
24	b	605	CLA	C3D-C4D	-2.06	1.39	1.44
24	c	503	CLA	C3D-C4D	-2.06	1.39	1.44
24	c	515	CLA	C3D-C4D	-2.05	1.39	1.44
24	A	409	CLA	C3D-C4D	-2.05	1.39	1.44
24	C	507	CLA	C3D-C4D	-2.04	1.39	1.44
24	D	406	CLA	C1C-NC	-2.04	1.34	1.37
24	B	617	CLA	C4C-C3C	2.04	1.48	1.45
24	D	401	CLA	C1C-C2C	2.04	1.48	1.44
24	A	409	CLA	C1C-NC	-2.04	1.34	1.37
24	B	616	CLA	C4C-C3C	2.03	1.48	1.45
24	C	508	CLA	C3D-C4D	-2.03	1.39	1.44
24	B	609	CLA	C1B-NB	-2.03	1.33	1.35
24	c	512	CLA	C1C-C2C	2.03	1.48	1.44
24	c	509	CLA	C1A-CHA	2.02	1.51	1.43
24	b	615	CLA	C1C-C2C	2.02	1.48	1.44
24	B	613	CLA	C1C-NC	-2.02	1.34	1.37
37	h	102	DGD	O3G-C1D	2.02	1.43	1.40
24	C	509	CLA	C3D-C4D	-2.02	1.39	1.44
27	b	601	SQD	O6-C1	2.02	1.43	1.40
24	B	610	CLA	C1B-NB	-2.01	1.33	1.35
29	D	408	PL9	C2-C3	2.01	1.39	1.34
24	c	513	CLA	C1C-NC	-2.01	1.34	1.37
24	B	603	CLA	C1D-C2D	2.01	1.49	1.45
24	b	619	CLA	C1C-NC	-2.01	1.34	1.37
24	d	405	CLA	C3D-C4D	-2.01	1.39	1.44
32	J	102	LMT	O1'-C1'	2.01	1.43	1.40
24	C	506	CLA	C4D-ND	2.01	1.40	1.37
29	A	413	PL9	C2-C3	2.01	1.39	1.34
24	C	504	CLA	C3D-C4D	-2.00	1.39	1.44
39	e	102	HEM	CHA-C4D	2.00	1.40	1.35

All (2474) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	h	101	RRX	C20-C21-C22	21.81	158.43	127.31
40	h	101	RRX	C15-C16-C17	20.97	166.42	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	H	103	RRX	C16-C17-C18	20.52	156.60	127.31
40	h	101	RRX	C16-C17-C18	19.69	155.40	127.31
40	h	101	RRX	C15-C14-C13	19.68	155.39	127.31
40	h	101	RRX	C16-C15-C14	19.67	163.76	123.47
40	H	103	RRX	C11-C10-C9	18.75	154.06	127.31
40	h	101	RRX	C11-C10-C9	18.72	154.03	127.31
40	H	103	RRX	C15-C14-C13	18.53	153.75	127.31
40	H	103	RRX	C19-C18-C17	18.50	147.33	118.94
40	H	103	RRX	C15-C16-C17	17.46	159.24	123.47
40	H	103	RRX	C16-C15-C14	17.29	158.88	123.47
40	H	103	RRX	C20-C21-C22	16.33	150.62	127.31
40	h	101	RRX	C21-C20-C19	15.73	172.30	123.22
40	h	101	RRX	C19-C18-C17	15.04	142.03	118.94
40	h	101	RRX	C20-C19-C18	12.90	162.65	126.42
40	h	101	RRX	C10-C11-C12	12.87	163.37	123.22
40	H	103	RRX	C21-C20-C19	11.58	159.34	123.22
40	H	103	RRX	C20-C19-C18	11.35	158.30	126.42
24	B	607	CLA	C1D-ND-C4D	-11.07	98.47	106.33
40	H	103	RRX	C10-C11-C12	10.62	156.37	123.22
24	a	410	CLA	C1D-ND-C4D	-10.28	99.03	106.33
40	h	101	RRX	C23-C24-C25	10.19	155.83	127.20
24	c	503	CLA	C1D-ND-C4D	-10.18	99.11	106.33
24	A	406	CLA	C1D-ND-C4D	-10.17	99.11	106.33
40	H	103	RRX	C36-C18-C19	-10.10	102.16	118.08
24	B	608	CLA	C1D-ND-C4D	-10.09	99.17	106.33
40	h	101	RRX	C12-C13-C14	9.89	134.11	118.94
40	h	101	RRX	C8-C7-C6	9.87	154.93	127.20
24	b	616	CLA	C1D-ND-C4D	-9.84	99.35	106.33
24	b	618	CLA	C1D-ND-C4D	-9.81	99.36	106.33
24	A	409	CLA	C1D-ND-C4D	-9.79	99.38	106.33
24	D	405	CLA	C2D-C1D-ND	9.77	117.31	110.10
24	a	409	CLA	C1D-ND-C4D	-9.74	99.42	106.33
24	c	510	CLA	C1D-ND-C4D	-9.63	99.49	106.33
24	B	616	CLA	C1D-ND-C4D	-9.61	99.51	106.33
24	B	608	CLA	C2D-C1D-ND	9.59	117.17	110.10
40	H	103	RRX	C23-C24-C25	9.56	154.04	127.20
24	B	605	CLA	C1D-ND-C4D	-9.53	99.56	106.33
24	a	410	CLA	C2D-C1D-ND	9.51	117.11	110.10
40	H	103	RRX	C12-C13-C14	9.51	133.54	118.94
24	B	607	CLA	C2D-C1D-ND	9.51	117.11	110.10
24	C	504	CLA	C1D-ND-C4D	-9.50	99.59	106.33
24	C	503	CLA	C1D-ND-C4D	-9.49	99.60	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	506	CLA	C1D-ND-C4D	-9.40	99.66	106.33
24	D	406	CLA	C1D-ND-C4D	-9.39	99.66	106.33
24	B	618	CLA	C1D-ND-C4D	-9.38	99.67	106.33
24	C	510	CLA	C1D-ND-C4D	-9.38	99.67	106.33
40	H	103	RRX	C24-C23-C22	9.35	140.36	126.23
40	h	101	RRX	C24-C23-C22	9.32	140.31	126.23
24	b	620	CLA	C1D-ND-C4D	-9.30	99.73	106.33
24	b	619	CLA	C2D-C1D-ND	9.29	116.95	110.10
24	B	611	CLA	C1D-ND-C4D	-9.28	99.74	106.33
24	B	614	CLA	C1D-ND-C4D	-9.27	99.75	106.33
24	c	508	CLA	C1D-ND-C4D	-9.26	99.75	106.33
24	b	619	CLA	C1D-ND-C4D	-9.24	99.77	106.33
40	h	101	RRX	C36-C18-C17	-9.21	110.02	122.92
24	D	405	CLA	C1D-ND-C4D	-9.19	99.81	106.33
24	B	615	CLA	C2D-C1D-ND	9.18	116.87	110.10
24	b	615	CLA	C1D-ND-C4D	-9.18	99.82	106.33
24	d	406	CLA	C1D-ND-C4D	-9.17	99.82	106.33
24	b	617	CLA	C1D-ND-C4D	-9.13	99.85	106.33
24	B	615	CLA	C1D-ND-C4D	-9.10	99.87	106.33
24	c	512	CLA	C1D-ND-C4D	-9.06	99.90	106.33
24	b	613	CLA	C1D-ND-C4D	-9.05	99.91	106.33
24	c	515	CLA	C1D-ND-C4D	-9.04	99.91	106.33
24	B	603	CLA	C1D-ND-C4D	-9.01	99.93	106.33
24	a	413	CLA	C1D-ND-C4D	-9.00	99.94	106.33
24	C	515	CLA	C1D-ND-C4D	-8.98	99.95	106.33
24	c	510	CLA	C2D-C1D-ND	8.95	116.70	110.10
24	b	620	CLA	C2D-C1D-ND	8.89	116.65	110.10
40	H	103	RRX	C36-C18-C17	-8.88	110.48	122.92
24	d	405	CLA	C1D-ND-C4D	-8.87	100.03	106.33
24	B	617	CLA	C1D-ND-C4D	-8.86	100.04	106.33
24	c	505	CLA	C1D-ND-C4D	-8.86	100.04	106.33
24	b	616	CLA	C2D-C1D-ND	8.79	116.58	110.10
24	B	610	CLA	C1D-ND-C4D	-8.79	100.09	106.33
24	b	618	CLA	C2D-C1D-ND	8.77	116.57	110.10
24	c	514	CLA	C1D-ND-C4D	-8.77	100.11	106.33
24	c	506	CLA	C1D-ND-C4D	-8.75	100.12	106.33
24	A	409	CLA	C2D-C1D-ND	8.74	116.54	110.10
24	C	510	CLA	C2D-C1D-ND	8.73	116.54	110.10
24	C	509	CLA	C1D-ND-C4D	-8.73	100.13	106.33
24	b	605	CLA	C1D-ND-C4D	-8.73	100.13	106.33
24	c	507	CLA	C1D-ND-C4D	-8.73	100.14	106.33
24	b	610	CLA	C1D-ND-C4D	-8.70	100.16	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	613	CLA	C2D-C1D-ND	8.68	116.50	110.10
24	C	511	CLA	C1D-ND-C4D	-8.67	100.18	106.33
24	B	612	CLA	C1D-ND-C4D	-8.66	100.19	106.33
24	C	513	CLA	C1D-ND-C4D	-8.65	100.19	106.33
24	c	503	CLA	C2D-C1D-ND	8.63	116.46	110.10
24	C	513	CLA	C2D-C1D-ND	8.62	116.46	110.10
24	B	618	CLA	C2D-C1D-ND	8.61	116.45	110.10
24	b	615	CLA	C2D-C1D-ND	8.60	116.44	110.10
24	C	512	CLA	C1D-ND-C4D	-8.59	100.23	106.33
24	A	406	CLA	C2D-C1D-ND	8.57	116.42	110.10
24	b	609	CLA	C1D-ND-C4D	-8.57	100.25	106.33
24	b	612	CLA	C1D-ND-C4D	-8.55	100.26	106.33
40	h	101	RRX	C11-C12-C13	8.53	150.37	126.42
24	b	611	CLA	C1D-ND-C4D	-8.51	100.29	106.33
24	B	616	CLA	C2D-C1D-ND	8.50	116.37	110.10
24	b	614	CLA	C1D-ND-C4D	-8.49	100.31	106.33
24	C	506	CLA	C2D-C1D-ND	8.48	116.36	110.10
24	a	411	CLA	C1D-ND-C4D	-8.47	100.32	106.33
24	D	406	CLA	C2D-C1D-ND	8.45	116.33	110.10
40	H	103	RRX	C11-C12-C13	8.44	150.13	126.42
24	a	413	CLA	C2D-C1D-ND	8.44	116.32	110.10
24	c	511	CLA	C1D-ND-C4D	-8.41	100.36	106.33
24	C	514	CLA	C1D-ND-C4D	-8.39	100.37	106.33
24	a	411	CLA	C2D-C1D-ND	8.39	116.29	110.10
24	B	614	CLA	C2D-C1D-ND	8.39	116.28	110.10
24	B	606	CLA	C1D-ND-C4D	-8.38	100.38	106.33
24	B	611	CLA	C2D-C1D-ND	8.37	116.27	110.10
40	h	101	RRX	C4-C5-C6	8.34	134.84	122.73
24	C	505	CLA	C1D-ND-C4D	-8.33	100.42	106.33
24	b	611	CLA	C2D-C1D-ND	8.28	116.21	110.10
24	B	609	CLA	C1D-ND-C4D	-8.26	100.47	106.33
24	c	504	CLA	C1D-ND-C4D	-8.23	100.49	106.33
24	B	610	CLA	C2D-C1D-ND	8.22	116.16	110.10
24	B	612	CLA	C2D-C1D-ND	8.22	116.16	110.10
24	b	608	CLA	C2D-C1D-ND	8.22	116.16	110.10
24	b	608	CLA	C1D-ND-C4D	-8.15	100.54	106.33
24	C	509	CLA	C2D-C1D-ND	8.15	116.11	110.10
24	B	613	CLA	C1D-ND-C4D	-8.14	100.56	106.33
24	b	607	CLA	C1D-ND-C4D	-8.12	100.57	106.33
24	b	617	CLA	C2D-C1D-ND	8.11	116.08	110.10
24	b	606	CLA	C1D-ND-C4D	-8.07	100.60	106.33
24	b	609	CLA	C2D-C1D-ND	8.07	116.05	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	617	CLA	C2D-C1D-ND	8.05	116.04	110.10
40	h	101	RRX	C7-C8-C9	8.04	138.39	126.23
24	c	509	CLA	C1D-ND-C4D	-8.04	100.62	106.33
24	B	606	CLA	C2D-C1D-ND	8.03	116.02	110.10
24	C	504	CLA	C2D-C1D-ND	8.02	116.01	110.10
24	C	503	CLA	C2D-C1D-ND	8.01	116.00	110.10
40	H	103	RRX	C38-C26-C27	-7.97	99.59	114.36
24	B	605	CLA	C2D-C1D-ND	7.97	115.97	110.10
24	d	406	CLA	C2D-C1D-ND	7.97	115.97	110.10
24	c	513	CLA	C1D-ND-C4D	-7.96	100.68	106.33
24	c	505	CLA	C2D-C1D-ND	7.91	115.94	110.10
24	b	614	CLA	C2D-C1D-ND	7.89	115.92	110.10
24	C	514	CLA	C2D-C1D-ND	7.89	115.92	110.10
24	A	405	CLA	C2D-C1D-ND	7.80	115.85	110.10
24	C	505	CLA	C2D-C1D-ND	7.79	115.85	110.10
24	A	405	CLA	C1D-ND-C4D	-7.79	100.80	106.33
24	c	514	CLA	C2D-C1D-ND	7.78	115.84	110.10
24	b	610	CLA	C2D-C1D-ND	7.77	115.83	110.10
24	C	515	CLA	C2D-C1D-ND	7.76	115.83	110.10
40	H	103	RRX	C8-C9-C10	7.72	130.79	118.94
24	c	506	CLA	C2D-C1D-ND	7.66	115.75	110.10
24	a	409	CLA	C2D-C1D-ND	7.61	115.71	110.10
24	B	609	CLA	C2D-C1D-ND	7.57	115.68	110.10
24	d	405	CLA	C2D-C1D-ND	7.56	115.67	110.10
24	C	507	CLA	C1D-ND-C4D	-7.54	100.98	106.33
24	B	604	CLA	C1D-ND-C4D	-7.54	100.98	106.33
24	c	515	CLA	C2D-C1D-ND	7.53	115.65	110.10
24	c	509	CLA	C2D-C1D-ND	7.52	115.64	110.10
24	b	605	CLA	C2D-C1D-ND	7.50	115.63	110.10
24	c	512	CLA	C2D-C1D-ND	7.47	115.61	110.10
24	C	508	CLA	C1D-ND-C4D	-7.46	101.03	106.33
24	C	511	CLA	C2D-C1D-ND	7.38	115.54	110.10
24	c	508	CLA	C2D-C1D-ND	7.37	115.54	110.10
24	B	603	CLA	C2D-C1D-ND	7.34	115.52	110.10
24	b	613	CLA	C2D-C1D-ND	7.33	115.51	110.10
24	c	511	CLA	C2D-C1D-ND	7.32	115.50	110.10
24	b	612	CLA	C2D-C1D-ND	7.29	115.47	110.10
24	C	512	CLA	C2D-C1D-ND	7.27	115.46	110.10
24	D	401	CLA	C2D-C1D-ND	7.22	115.43	110.10
24	c	504	CLA	C2D-C1D-ND	7.22	115.42	110.10
36	B	626	HTG	C1'-S1-C1	7.16	113.49	100.09
24	b	606	CLA	C2D-C1D-ND	7.16	115.38	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	412	PHO	O2D-CGD-CBD	7.01	119.88	111.00
24	B	608	CLA	CMD-C2D-C1D	7.01	137.07	124.71
24	D	401	CLA	C1D-ND-C4D	-6.95	101.40	106.33
24	B	616	CLA	C1-C2-C3	-6.94	114.04	126.04
24	c	513	CLA	C2D-C1D-ND	6.86	115.16	110.10
24	B	606	CLA	CMD-C2D-C1D	6.86	136.80	124.71
24	b	613	CLA	CMD-C2D-C1D	6.85	136.79	124.71
24	B	604	CLA	C2D-C1D-ND	6.77	115.09	110.10
40	h	101	RRX	C35-C13-C14	-6.71	113.53	122.92
24	D	401	CLA	CMD-C2D-C1D	6.66	136.46	124.71
36	B	629	HTG	C1'-S1-C1	6.66	112.55	100.09
24	b	607	CLA	C2D-C1D-ND	6.66	115.01	110.10
24	c	507	CLA	C2D-C1D-ND	6.65	115.00	110.10
24	B	603	CLA	CMD-C2D-C1D	6.64	136.41	124.71
27	F	101	SQD	O6-C1-C2	6.59	118.59	108.30
24	B	615	CLA	CMD-C2D-C1D	6.59	136.32	124.71
24	c	509	CLA	O2D-CGD-CBD	6.58	122.97	111.27
24	b	617	CLA	CMD-C2D-C1D	6.56	136.28	124.71
24	c	503	CLA	CMD-C2D-C1D	6.55	136.25	124.71
40	H	103	RRX	C34-C9-C10	-6.53	113.78	122.92
24	B	604	CLA	CMD-C2D-C1D	6.48	136.13	124.71
40	h	101	RRX	C36-C18-C19	-6.46	107.89	118.08
25	A	408	PHO	O2D-CGD-CBD	6.43	119.15	111.00
24	C	503	CLA	CMD-C2D-C1D	6.43	136.05	124.71
24	C	507	CLA	CMD-C2D-C1D	6.43	136.04	124.71
40	H	103	RRX	C23-C22-C21	6.42	128.79	118.94
25	d	401	PHO	O2D-CGD-CBD	6.41	119.11	111.00
36	d	404	HTG	C1'-S1-C1	6.40	112.05	100.09
24	C	509	CLA	CMD-C2D-C1D	6.39	135.97	124.71
40	h	101	RRX	C33-C5-C4	-6.39	101.34	113.62
24	B	605	CLA	CMD-C2D-C1D	6.38	135.96	124.71
24	D	401	CLA	C2C-C1C-NC	6.37	115.94	109.97
24	c	508	CLA	CMD-C2D-C1D	6.32	135.86	124.71
25	A	407	PHO	O2D-CGD-CBD	6.32	119.00	111.00
24	C	515	CLA	CMD-C2D-C1D	6.28	135.78	124.71
24	C	508	CLA	C2D-C1D-ND	6.28	114.73	110.10
24	b	607	CLA	CMD-C2D-C1D	6.26	135.75	124.71
36	C	522	HTG	C1'-S1-C1	6.23	111.75	100.09
24	C	512	CLA	CMD-C2D-C1D	6.19	135.63	124.71
24	B	618	CLA	CMD-C2D-C1D	6.18	135.60	124.71
24	b	608	CLA	CMD-C2D-C1D	6.16	135.57	124.71
24	A	405	CLA	CMD-C2D-C1D	6.14	135.54	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	H	103	RRX	C35-C13-C14	-6.13	114.33	122.92
36	u	201	HTG	C1'-S1-C1	6.12	111.54	100.09
40	h	101	RRX	C1-C6-C5	-6.11	114.01	122.61
36	b	602	HTG	C1'-S1-C1	6.09	111.47	100.09
29	a	417	PL9	C7-C8-C9	-6.06	116.70	126.79
40	H	103	RRX	C33-C5-C6	6.06	131.34	124.53
36	C	523	HTG	C1'-S1-C1	6.05	111.40	100.09
24	c	506	CLA	O2D-CGD-CBD	6.04	122.00	111.27
24	C	507	CLA	C2D-C1D-ND	6.03	114.55	110.10
24	c	514	CLA	O2D-CGD-CBD	6.02	121.96	111.27
24	C	503	CLA	O2D-CGD-CBD	6.01	121.95	111.27
24	c	509	CLA	CMD-C2D-C1D	6.01	135.31	124.71
24	B	603	CLA	O2D-CGD-CBD	5.99	121.91	111.27
24	C	508	CLA	CMD-C2D-C1D	5.98	135.25	124.71
24	c	511	CLA	CMD-C2D-C1D	5.97	135.24	124.71
24	c	506	CLA	CMD-C2D-C1D	5.96	135.22	124.71
36	H	101	HTG	C1'-S1-C1	5.95	111.22	100.09
40	H	103	RRX	C7-C8-C9	5.91	135.17	126.23
24	b	606	CLA	O2D-CGD-CBD	5.89	121.74	111.27
27	a	415	SQD	O6-C1-C2	5.88	117.48	108.30
24	b	614	CLA	CMD-C2D-C1D	5.86	135.03	124.71
24	B	608	CLA	CHD-C1D-ND	-5.85	119.08	124.45
24	b	607	CLA	O2D-CGD-CBD	5.82	121.61	111.27
40	H	103	RRX	C8-C7-C6	5.81	143.53	127.20
24	B	614	CLA	O2D-CGD-CBD	5.81	121.59	111.27
24	c	515	CLA	CMD-C2D-C1D	5.80	134.94	124.71
36	o	301	HTG	C1'-S1-C1	5.78	110.91	100.09
24	c	507	CLA	CMD-C2D-C1D	5.78	134.89	124.71
24	c	505	CLA	CMD-C2D-C1D	5.77	134.89	124.71
24	b	611	CLA	CMD-C2D-C1D	5.76	134.87	124.71
24	C	505	CLA	CMD-C2D-C1D	5.76	134.86	124.71
24	a	409	CLA	CMD-C2D-C1D	5.76	134.86	124.71
24	B	608	CLA	O2D-CGD-CBD	5.75	121.49	111.27
24	D	406	CLA	CMD-C2D-C1D	5.75	134.85	124.71
24	b	620	CLA	O2D-CGD-CBD	5.71	121.41	111.27
27	a	415	SQD	C1-O5-C5	-5.70	102.51	113.69
24	B	606	CLA	O2D-CGD-CBD	5.68	121.35	111.27
24	b	605	CLA	O2D-CGD-CBD	5.67	121.35	111.27
24	b	605	CLA	CMD-C2D-C1D	5.66	134.69	124.71
40	h	101	RRX	C38-C26-C27	-5.65	103.89	114.36
27	A	411	SQD	O6-C1-C2	5.64	117.11	108.30
24	a	410	CLA	CHD-C4C-C3C	-5.63	116.57	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	509	CLA	O2D-CGD-CBD	5.61	121.25	111.27
24	B	609	CLA	CMD-C2D-C1D	5.61	134.59	124.71
24	C	511	CLA	CMD-C2D-C1D	5.59	134.57	124.71
24	b	620	CLA	CMD-C2D-C1D	5.57	134.53	124.71
24	B	605	CLA	O2D-CGD-CBD	5.55	121.13	111.27
36	B	630	HTG	C1'-S1-C1	5.54	110.46	100.09
24	B	617	CLA	CMD-C2D-C1D	5.54	134.48	124.71
24	D	401	CLA	C1C-C2C-C3C	-5.54	101.13	106.96
24	c	512	CLA	CMD-C2D-C1D	5.53	134.45	124.71
24	b	618	CLA	O2D-CGD-CBD	5.52	121.07	111.27
36	c	524	HTG	C1'-S1-C1	5.52	110.41	100.09
24	B	616	CLA	CMD-C2D-C1D	5.51	134.43	124.71
24	a	411	CLA	CMD-C2D-C1D	5.51	134.42	124.71
24	c	513	CLA	CMD-C2D-C1D	5.49	134.39	124.71
24	c	510	CLA	O2D-CGD-CBD	5.49	121.02	111.27
27	a	415	SQD	O47-C7-C8	5.49	123.33	111.50
24	b	617	CLA	C1-C2-C3	-5.48	116.56	126.04
36	c	523	HTG	C1'-S1-C1	5.48	110.34	100.09
24	d	406	CLA	CMD-C2D-C1D	5.48	134.37	124.71
24	B	616	CLA	CHD-C4C-C3C	-5.47	116.81	124.84
24	D	405	CLA	CMD-C2D-C1D	5.45	134.32	124.71
39	F	102	HEM	CAD-CBD-CGD	5.44	125.31	113.60
24	C	506	CLA	CMD-C2D-C1D	5.43	134.28	124.71
24	b	615	CLA	O2D-CGD-CBD	5.42	120.90	111.27
24	C	506	CLA	O2D-CGD-CBD	5.40	120.86	111.27
24	b	618	CLA	CMD-C2D-C1D	5.39	134.22	124.71
24	C	512	CLA	O2D-CGD-CBD	5.39	120.84	111.27
27	A	411	SQD	C1-O5-C5	-5.39	103.12	113.69
24	b	606	CLA	CMD-C2D-C1D	5.38	134.20	124.71
24	C	504	CLA	CMD-C2D-C1D	5.38	134.20	124.71
24	C	514	CLA	CMD-C2D-C1D	5.36	134.17	124.71
24	B	616	CLA	O2D-CGD-CBD	5.36	120.80	111.27
40	h	101	RRX	C1-C6-C7	5.34	130.88	115.78
40	h	101	RRX	C23-C22-C21	5.34	127.13	118.94
24	B	611	CLA	CMD-C2D-C1D	5.33	134.10	124.71
24	D	405	CLA	CHD-C1D-ND	-5.32	119.56	124.45
24	C	514	CLA	O2D-CGD-CBD	5.32	120.71	111.27
24	b	610	CLA	CMD-C2D-C1D	5.31	134.08	124.71
24	C	513	CLA	CMD-C2D-C1D	5.30	134.06	124.71
24	c	504	CLA	CMD-C2D-C1D	5.29	134.04	124.71
24	B	612	CLA	CMD-C2D-C1D	5.28	134.02	124.71
27	F	101	SQD	O47-C7-C8	5.27	122.87	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	413	CLA	C1-C2-C3	-5.27	116.93	126.04
24	d	405	CLA	CMD-C2D-C1D	5.26	133.99	124.71
24	a	410	CLA	CHD-C1D-ND	-5.26	119.62	124.45
24	B	618	CLA	O2D-CGD-CBD	5.24	120.58	111.27
40	H	103	RRX	C27-C26-C25	5.24	132.52	120.85
24	b	619	CLA	CMD-C2D-C1D	5.23	133.93	124.71
24	B	615	CLA	CHD-C1D-ND	-5.21	119.67	124.45
24	B	615	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
24	D	405	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
24	b	610	CLA	O2D-CGD-CBD	5.19	120.49	111.27
27	B	622	SQD	O47-C7-C8	5.17	122.64	111.50
39	e	102	HEM	CBA-CAA-C2A	-5.15	103.83	112.62
24	A	406	CLA	CMD-C2D-C1D	5.14	133.77	124.71
24	c	514	CLA	CMD-C2D-C1D	5.12	133.75	124.71
40	h	101	RRX	C8-C9-C10	5.11	126.78	118.94
39	F	102	HEM	CHC-C4B-NB	5.10	129.97	124.43
24	b	619	CLA	CHD-C4C-C3C	-5.09	117.36	124.84
24	a	410	CLA	CMD-C2D-C1D	5.09	133.68	124.71
24	B	617	CLA	O2D-CGD-CBD	5.08	120.29	111.27
24	b	612	CLA	CMD-C2D-C1D	5.07	133.66	124.71
24	b	619	CLA	C3D-C2D-C1D	-5.07	98.92	105.83
24	D	401	CLA	C3D-C2D-C1D	-5.07	98.92	105.83
24	b	609	CLA	CMD-C2D-C1D	5.06	133.63	124.71
24	A	405	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
24	B	608	CLA	C2C-C1C-NC	5.06	114.71	109.97
39	e	102	HEM	CAD-CBD-CGD	5.05	124.47	113.60
24	B	608	CLA	C3D-C2D-C1D	-5.04	98.96	105.83
24	a	413	CLA	O2D-CGD-CBD	5.03	120.21	111.27
24	D	405	CLA	C2C-C1C-NC	5.01	114.66	109.97
24	b	615	CLA	CMD-C2D-C1D	5.01	133.53	124.71
24	a	410	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
24	B	613	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
24	b	616	CLA	O2D-CGD-CBD	4.98	120.11	111.27
24	B	618	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
24	b	617	CLA	C2C-C1C-NC	4.96	114.62	109.97
24	C	513	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
24	C	507	CLA	O2D-CGD-CBD	4.94	120.04	111.27
24	c	503	CLA	O2D-CGD-CBD	4.94	120.04	111.27
24	c	504	CLA	O2D-CGD-CBD	4.92	120.01	111.27
40	H	103	RRX	C37-C22-C23	-4.92	110.33	118.08
24	A	409	CLA	CMD-C2D-C1D	4.92	133.38	124.71
24	b	620	CLA	C3D-C2D-C1D	-4.90	99.15	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	409	CLA	O2D-CGD-CBD	4.90	119.97	111.27
24	a	411	CLA	C2C-C1C-NC	4.90	114.56	109.97
24	C	504	CLA	O2D-CGD-CBD	4.86	119.91	111.27
24	c	507	CLA	O2D-CGD-CBD	4.86	119.91	111.27
27	A	411	SQD	C1-C2-C3	-4.85	99.90	110.00
24	B	608	CLA	CHD-C4C-C3C	-4.84	117.72	124.84
24	C	509	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
24	A	406	CLA	C2C-C1C-NC	4.81	114.48	109.97
24	B	605	CLA	CHD-C4C-C3C	-4.80	117.78	124.84
27	a	415	SQD	C1-C2-C3	-4.80	100.00	110.00
24	B	607	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
24	c	507	CLA	C2C-C1C-NC	4.79	114.46	109.97
24	C	514	CLA	CHD-C4C-C3C	-4.78	117.81	124.84
27	b	601	SQD	O47-C7-C8	4.78	121.80	111.50
36	b	628	HTG	C1'-S1-C1	4.78	109.02	100.09
24	B	618	CLA	CHD-C4C-C3C	-4.77	117.83	124.84
24	b	620	CLA	CHD-C4C-C3C	-4.75	117.86	124.84
24	B	613	CLA	CMD-C2D-C1D	4.75	133.08	124.71
40	h	101	RRX	C37-C22-C23	-4.75	110.60	118.08
24	B	614	CLA	CMD-C2D-C1D	4.75	133.08	124.71
24	C	510	CLA	CMD-C2D-C1D	4.74	133.06	124.71
24	B	607	CLA	C3D-C4D-ND	4.73	117.89	110.24
36	B	625	HTG	C1'-S1-C1	4.73	108.94	100.09
24	b	611	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
24	c	510	CLA	C3D-C2D-C1D	-4.72	99.40	105.83
24	a	411	CLA	CHD-C1D-ND	-4.71	120.12	124.45
37	c	518	DGD	O2G-C1B-C2B	4.71	121.65	111.50
24	a	413	CLA	CMD-C2D-C1D	4.70	133.00	124.71
24	C	509	CLA	C2C-C1C-NC	4.70	114.38	109.97
24	b	611	CLA	O2D-CGD-CBD	4.69	119.61	111.27
24	b	616	CLA	CMD-C2D-C1D	4.69	132.97	124.71
24	B	614	CLA	CHD-C4C-C3C	-4.69	117.95	124.84
24	B	606	CLA	C3D-C2D-C1D	-4.69	99.44	105.83
24	B	615	CLA	C2C-C1C-NC	4.68	114.36	109.97
24	c	503	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
24	a	411	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
24	a	410	CLA	C2C-C1C-NC	4.66	114.34	109.97
24	B	610	CLA	CMD-C2D-C1D	4.66	132.92	124.71
24	D	401	CLA	CHD-C4C-C3C	-4.65	118.00	124.84
24	b	615	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
27	f	802	SQD	O47-C7-C8	4.63	121.49	111.50
24	B	609	CLA	C3D-C2D-C1D	-4.63	99.51	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	510	CLA	CHD-C4C-C3C	-4.63	118.04	124.84
38	E	101	LHG	O7-C7-C8	4.62	121.46	111.50
24	b	609	CLA	O2D-CGD-CBD	4.62	119.47	111.27
28	C	533	LMG	O7-C10-C11	4.61	121.45	111.50
24	C	510	CLA	C3D-C2D-C1D	-4.61	99.53	105.83
24	C	506	CLA	C1C-C2C-C3C	-4.61	102.11	106.96
24	C	511	CLA	O2D-CGD-CBD	4.61	119.45	111.27
24	A	406	CLA	C3D-C4D-ND	4.60	117.68	110.24
24	c	503	CLA	CHD-C1D-ND	-4.60	120.22	124.45
24	b	615	CLA	CHD-C4C-C3C	-4.60	118.08	124.84
24	C	514	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
24	b	608	CLA	O2D-CGD-CBD	4.60	119.44	111.27
24	D	406	CLA	CHD-C4C-C3C	-4.60	118.08	124.84
24	b	617	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
24	c	510	CLA	CMD-C2D-C1D	4.59	132.81	124.71
24	b	616	CLA	C3C-C4C-NC	4.59	115.72	110.57
24	c	505	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
24	B	612	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
24	b	615	CLA	C2C-C1C-NC	4.57	114.26	109.97
24	a	413	CLA	CHD-C4C-C3C	-4.57	118.12	124.84
24	a	410	CLA	C3D-C4D-ND	4.57	117.63	110.24
40	H	103	RRX	C31-C1-C6	4.56	117.69	110.30
24	b	614	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
24	a	413	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
24	a	413	CLA	C2C-C1C-NC	4.55	114.23	109.97
24	b	616	CLA	CHD-C4C-C3C	-4.54	118.16	124.84
24	B	607	CLA	CMD-C2D-C1D	4.54	132.72	124.71
24	d	406	CLA	C2C-C1C-NC	4.54	114.22	109.97
24	b	618	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
24	D	406	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
24	B	604	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
24	b	617	CLA	CHD-C1D-ND	-4.53	120.30	124.45
24	C	506	CLA	C1-C2-C3	-4.52	118.22	126.04
24	B	604	CLA	CAA-C2A-C3A	-4.51	100.42	112.78
24	B	617	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
24	d	406	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
24	c	511	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
24	B	606	CLA	CHD-C1D-ND	-4.49	120.33	124.45
40	H	103	RRX	C29-C28-C27	4.49	116.45	110.30
24	B	605	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
24	B	616	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
24	b	618	CLA	CHD-C4C-C3C	-4.48	118.26	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	607	CLA	O2D-CGD-CBD	4.47	119.22	111.27
24	C	504	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
24	B	609	CLA	C2C-C1C-NC	4.45	114.14	109.97
24	c	509	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
24	A	409	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
24	B	609	CLA	C1C-C2C-C3C	-4.44	102.29	106.96
24	D	401	CLA	CHD-C1D-ND	-4.44	120.38	124.45
24	b	613	CLA	C3D-C2D-C1D	-4.44	99.78	105.83
24	b	605	CLA	C3D-C2D-C1D	-4.44	99.78	105.83
24	C	503	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
24	C	510	CLA	O2D-CGD-CBD	4.43	119.15	111.27
24	b	606	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
24	B	617	CLA	CHD-C4C-C3C	-4.42	118.35	124.84
39	e	102	HEM	C1B-NB-C4B	4.42	109.63	105.07
24	C	506	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
26	d	407	BCR	C24-C23-C22	-4.41	119.57	126.23
24	B	618	CLA	CHD-C1D-ND	-4.41	120.40	124.45
27	A	411	SQD	O47-C7-C8	4.41	121.00	111.50
24	c	506	CLA	CHD-C1D-ND	-4.40	120.41	124.45
24	c	513	CLA	CHD-C1D-ND	-4.40	120.41	124.45
24	c	506	CLA	C4-C3-C5	4.40	122.67	115.27
24	C	509	CLA	C4A-NA-C1A	4.40	108.68	106.71
24	b	620	CLA	CHD-C1D-ND	-4.40	120.42	124.45
24	d	405	CLA	C2C-C1C-NC	4.39	114.09	109.97
24	c	507	CLA	C3D-C4D-ND	4.39	117.34	110.24
24	b	609	CLA	C3D-C2D-C1D	-4.39	99.84	105.83
24	d	406	CLA	O2D-CGD-CBD	4.39	119.06	111.27
24	b	608	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
27	B	622	SQD	O6-C1-C2	4.38	115.14	108.30
24	B	613	CLA	CHD-C4C-C3C	-4.38	118.41	124.84
24	B	609	CLA	O2D-CGD-CBD	4.37	119.04	111.27
24	b	608	CLA	C1C-C2C-C3C	-4.37	102.36	106.96
24	C	512	CLA	CHD-C4C-C3C	-4.37	118.42	124.84
24	b	609	CLA	C4-C3-C5	4.37	122.62	115.27
24	B	611	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
24	C	505	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
24	B	616	CLA	O2D-CGD-O1D	-4.36	115.32	123.84
24	B	603	CLA	C3D-C2D-C1D	-4.35	99.89	105.83
24	c	508	CLA	C3D-C2D-C1D	-4.35	99.89	105.83
29	A	413	PL9	C37-C38-C39	-4.35	117.18	127.66
26	B	619	BCR	C33-C5-C6	-4.35	119.65	124.53
24	C	515	CLA	C3D-C2D-C1D	-4.35	99.90	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	605	CLA	C1-C2-C3	-4.34	118.53	126.04
24	B	611	CLA	CHD-C4C-C3C	-4.34	118.46	124.84
24	C	506	CLA	C2C-C1C-NC	4.34	114.03	109.97
40	H	103	RRX	C33-C5-C4	-4.34	105.29	113.62
24	b	610	CLA	CHD-C4C-C3C	-4.33	118.47	124.84
24	c	506	CLA	CHD-C4C-C3C	-4.33	118.48	124.84
39	F	102	HEM	C1B-NB-C4B	4.32	109.54	105.07
24	C	506	CLA	CHD-C4C-C3C	-4.32	118.48	124.84
24	B	610	CLA	C3D-C2D-C1D	-4.32	99.93	105.83
24	b	618	CLA	CHD-C1D-ND	-4.32	120.48	124.45
24	b	612	CLA	C1-C2-C3	-4.32	118.58	126.04
24	B	604	CLA	O2D-CGD-CBD	4.31	118.93	111.27
24	c	515	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
28	B	623	LMG	O7-C10-C11	4.30	120.78	111.50
24	A	406	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
28	c	522	LMG	O7-C10-C11	4.30	120.77	111.50
26	t	101	BCR	C33-C5-C6	-4.30	119.70	124.53
24	b	618	CLA	C3D-C4D-ND	4.29	117.19	110.24
26	K	101	BCR	C33-C5-C6	-4.29	119.71	124.53
24	a	411	CLA	O2D-CGD-CBD	4.29	118.89	111.27
24	B	617	CLA	CHD-C1D-ND	-4.29	120.51	124.45
24	B	608	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
24	D	406	CLA	C3D-C4D-ND	4.29	117.17	110.24
24	C	511	CLA	C3D-C2D-C1D	-4.28	99.99	105.83
24	C	515	CLA	CHD-C1D-ND	-4.28	120.52	124.45
28	A	412	LMG	O7-C10-C11	4.28	120.72	111.50
24	b	619	CLA	O2D-CGD-CBD	4.28	118.87	111.27
24	c	512	CLA	C2C-C1C-NC	4.27	113.98	109.97
24	A	409	CLA	CHD-C4C-C3C	-4.27	118.56	124.84
24	c	514	CLA	C3D-C2D-C1D	-4.27	100.01	105.83
24	B	614	CLA	C3D-C4D-ND	4.27	117.14	110.24
24	B	615	CLA	CHD-C4C-C3C	-4.27	118.57	124.84
24	b	608	CLA	C2C-C1C-NC	4.26	113.97	109.97
27	A	411	SQD	O9-S-C6	4.26	112.00	106.94
24	B	604	CLA	C2C-C1C-NC	4.26	113.96	109.97
24	C	510	CLA	CHD-C4C-C3C	-4.26	118.58	124.84
24	C	509	CLA	C1C-C2C-C3C	-4.26	102.48	106.96
28	b	624	LMG	O7-C10-C11	4.25	120.66	111.50
24	c	510	CLA	C3D-C4D-ND	4.25	117.11	110.24
24	C	510	CLA	CHD-C1D-ND	-4.24	120.56	124.45
24	a	409	CLA	C3D-C4D-ND	4.24	117.10	110.24
24	c	504	CLA	C3D-C2D-C1D	-4.24	100.05	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	615	CLA	C1C-C2C-C3C	-4.24	102.50	106.96
36	b	627	HTG	C1'-S1-C1	4.24	108.01	100.09
24	C	503	CLA	C2C-C1C-NC	4.23	113.94	109.97
24	c	506	CLA	C3D-C2D-C1D	-4.23	100.05	105.83
24	a	409	CLA	C2C-C1C-NC	4.23	113.94	109.97
24	c	509	CLA	CHD-C4C-C3C	-4.23	118.62	124.84
36	b	628	HTG	O5-C1-C2	4.23	115.63	110.31
24	a	413	CLA	CHD-C1D-ND	-4.22	120.57	124.45
24	D	405	CLA	CHD-C4C-C3C	-4.22	118.64	124.84
24	d	406	CLA	CHD-C1D-ND	-4.21	120.58	124.45
24	b	605	CLA	CHD-C4C-C3C	-4.21	118.66	124.84
24	C	508	CLA	C2C-C1C-NC	4.20	113.91	109.97
25	A	408	PHO	C1-C2-C3	-4.20	118.77	126.04
24	d	406	CLA	C1C-C2C-C3C	-4.20	102.54	106.96
24	C	503	CLA	CHD-C1D-ND	-4.20	120.59	124.45
24	d	405	CLA	O2D-CGD-CBD	4.20	118.73	111.27
24	b	616	CLA	C3D-C2D-C1D	-4.19	100.11	105.83
24	D	406	CLA	O2D-CGD-CBD	4.19	118.71	111.27
24	B	607	CLA	CHD-C4C-C3C	-4.18	118.69	124.84
24	c	511	CLA	O2D-CGD-CBD	4.17	118.68	111.27
28	i	101	LMG	O7-C10-C11	4.17	120.48	111.50
24	b	611	CLA	C2C-C1C-NC	4.17	113.88	109.97
24	d	406	CLA	C3D-C4D-ND	4.16	116.97	110.24
24	C	509	CLA	CHD-C4C-C3C	-4.16	118.72	124.84
24	C	511	CLA	C2C-C1C-NC	4.16	113.87	109.97
36	V	202	HTG	O5-C1-C2	-4.16	105.08	110.31
24	c	509	CLA	C1C-C2C-C3C	-4.16	102.59	106.96
24	A	409	CLA	C3D-C4D-ND	4.16	116.96	110.24
24	b	610	CLA	C3D-C2D-C1D	-4.15	100.16	105.83
24	C	510	CLA	C3D-C4D-ND	4.14	116.94	110.24
24	B	607	CLA	C3C-C4C-NC	4.14	115.22	110.57
24	b	609	CLA	O2D-CGD-O1D	-4.13	115.76	123.84
24	c	515	CLA	O2D-CGD-CBD	4.13	118.61	111.27
24	b	616	CLA	C2C-C1C-NC	4.13	113.84	109.97
25	d	401	PHO	C1-C2-C3	-4.13	118.90	126.04
24	c	510	CLA	C3C-C4C-NC	4.13	115.20	110.57
24	C	504	CLA	C1-C2-C3	-4.12	118.92	126.04
24	B	612	CLA	CHD-C4C-C3C	-4.12	118.79	124.84
24	D	406	CLA	C2C-C1C-NC	4.11	113.83	109.97
24	C	504	CLA	C3D-C4D-ND	4.11	116.88	110.24
24	A	405	CLA	C2C-C1C-NC	4.11	113.82	109.97
37	d	416	DGD	O2G-C1B-C2B	4.10	120.34	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	504	CLA	C2C-C1C-NC	4.10	113.81	109.97
24	D	405	CLA	C3C-C4C-NC	4.10	115.17	110.57
24	B	616	CLA	C3D-C4D-ND	4.10	116.87	110.24
40	H	103	RRX	C35-C13-C12	-4.10	111.61	118.08
24	a	413	CLA	C3D-C4D-ND	4.10	116.87	110.24
24	B	612	CLA	C2C-C1C-NC	4.10	113.81	109.97
24	b	612	CLA	C3D-C2D-C1D	-4.09	100.24	105.83
24	d	405	CLA	O2D-CGD-O1D	-4.09	115.83	123.84
24	c	511	CLA	C1-C2-C3	-4.09	118.97	126.04
24	a	411	CLA	CHD-C4C-C3C	-4.09	118.83	124.84
24	b	606	CLA	CHD-C4C-C3C	-4.09	118.83	124.84
24	c	503	CLA	O2D-CGD-O1D	-4.09	115.85	123.84
24	c	510	CLA	C1-C2-C3	-4.08	118.98	126.04
24	C	504	CLA	CHD-C4C-C3C	-4.08	118.84	124.84
24	B	614	CLA	C3D-C2D-C1D	-4.08	100.26	105.83
24	a	411	CLA	C3D-C4D-ND	4.08	116.84	110.24
24	B	609	CLA	CBC-CAC-C3C	-4.08	101.19	112.43
24	D	406	CLA	CHD-C1D-ND	-4.08	120.71	124.45
24	B	612	CLA	CMA-C3A-C4A	-4.07	100.82	111.77
24	C	503	CLA	C3D-C4D-ND	4.07	116.83	110.24
24	d	405	CLA	C3D-C4D-ND	4.07	116.82	110.24
40	H	103	RRX	C30-C25-C26	-4.07	116.88	122.61
24	C	508	CLA	CHD-C1D-ND	-4.07	120.72	124.45
24	B	605	CLA	C2C-C1C-NC	4.07	113.78	109.97
24	c	512	CLA	C3D-C4D-ND	4.07	116.82	110.24
24	C	506	CLA	CHD-C1D-ND	-4.07	120.72	124.45
24	C	512	CLA	C3D-C2D-C1D	-4.07	100.28	105.83
24	C	515	CLA	O2D-CGD-CBD	4.07	118.49	111.27
24	c	503	CLA	C3D-C4D-ND	4.06	116.81	110.24
24	B	605	CLA	C3D-C4D-ND	4.06	116.81	110.24
27	a	415	SQD	C45-O47-C7	-4.06	107.79	117.79
24	b	609	CLA	CHD-C4C-C3C	-4.06	118.88	124.84
24	c	506	CLA	C3D-C4D-ND	4.05	116.80	110.24
27	a	401	SQD	O47-C7-C8	4.05	120.23	111.50
27	B	622	SQD	O7-S-C6	4.05	111.75	106.94
24	A	409	CLA	C2C-C1C-NC	4.05	113.77	109.97
27	f	802	SQD	O5-C5-C4	4.04	117.03	109.69
24	D	405	CLA	O2D-CGD-CBD	4.03	118.44	111.27
24	b	607	CLA	C3D-C2D-C1D	-4.03	100.33	105.83
24	b	611	CLA	CHD-C1D-ND	-4.03	120.75	124.45
27	b	601	SQD	O6-C1-C2	4.03	114.59	108.30
36	B	626	HTG	O5-C1-C2	4.03	115.38	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	606	CLA	C2C-C1C-NC	4.03	113.75	109.97
24	B	618	CLA	C3D-C4D-ND	4.02	116.74	110.24
24	b	619	CLA	C2C-C1C-NC	4.02	113.73	109.97
24	C	513	CLA	CHD-C4C-C3C	-4.02	118.94	124.84
24	b	612	CLA	C3D-C4D-ND	4.01	116.73	110.24
24	B	603	CLA	CHD-C1D-ND	-4.01	120.77	124.45
24	b	616	CLA	C4-C3-C5	4.00	122.01	115.27
24	b	607	CLA	CHD-C4C-C3C	-4.00	118.96	124.84
24	C	513	CLA	C2C-C1C-NC	4.00	113.72	109.97
24	B	603	CLA	CHD-C4C-C3C	-4.00	118.96	124.84
24	b	611	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
24	d	405	CLA	C3D-C2D-C1D	-4.00	100.38	105.83
24	B	606	CLA	CAC-C3C-C4C	3.99	129.99	124.81
24	a	409	CLA	C3D-C2D-C1D	-3.99	100.38	105.83
24	b	607	CLA	C2C-C1C-NC	3.99	113.71	109.97
24	a	410	CLA	C1C-C2C-C3C	-3.99	102.76	106.96
26	k	102	BCR	C33-C5-C6	-3.99	120.05	124.53
24	C	515	CLA	CHD-C4C-C3C	-3.99	118.98	124.84
24	b	619	CLA	C1D-CHD-C4C	-3.98	117.47	126.06
27	A	415	SQD	O47-C7-C8	3.98	120.08	111.50
24	B	614	CLA	C3C-C4C-NC	3.97	115.03	110.57
24	c	515	CLA	C2C-C1C-NC	3.97	113.69	109.97
24	c	503	CLA	C2C-C1C-NC	3.97	113.69	109.97
24	C	507	CLA	C2C-C1C-NC	3.96	113.68	109.97
24	b	613	CLA	O2D-CGD-CBD	3.96	118.31	111.27
24	c	511	CLA	CHD-C4C-C3C	-3.96	119.02	124.84
24	B	605	CLA	C1D-CHD-C4C	-3.96	117.52	126.06
24	c	515	CLA	C3D-C4D-ND	3.96	116.64	110.24
24	c	509	CLA	C2C-C1C-NC	3.95	113.68	109.97
24	c	510	CLA	C2C-C1C-NC	3.95	113.68	109.97
24	b	618	CLA	C1C-C2C-C3C	-3.95	102.80	106.96
24	B	616	CLA	C1D-CHD-C4C	-3.95	117.53	126.06
32	b	625	LMT	C1B-O5B-C5B	3.95	121.44	113.69
36	B	625	HTG	C1-C2-C3	3.95	118.39	110.59
24	b	618	CLA	O2D-CGD-O1D	-3.95	116.12	123.84
37	c	519	DGD	O2G-C1B-C2B	3.94	120.00	111.50
24	C	505	CLA	O2D-CGD-CBD	3.94	118.28	111.27
24	c	508	CLA	C3D-C4D-ND	3.94	116.61	110.24
29	D	408	PL9	C40-C39-C41	3.94	121.90	115.27
26	D	407	BCR	C38-C26-C25	-3.94	120.11	124.53
24	b	617	CLA	C3D-C4D-ND	3.93	116.60	110.24
24	b	618	CLA	C2C-C1C-NC	3.93	113.66	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	508	CLA	C3D-C2D-C1D	-3.93	100.47	105.83
24	b	607	CLA	C4-C3-C5	3.93	121.88	115.27
27	B	622	SQD	C3-C4-C5	3.92	117.24	110.24
24	B	605	CLA	C1C-C2C-C3C	-3.92	102.83	106.96
24	B	603	CLA	C3D-C4D-ND	3.92	116.58	110.24
37	C	519	DGD	O2G-C1B-C2B	3.92	119.95	111.50
24	b	612	CLA	C2C-C1C-NC	3.92	113.64	109.97
24	B	607	CLA	C2C-C1C-NC	3.92	113.64	109.97
24	b	610	CLA	C2C-C1C-NC	3.91	113.64	109.97
24	c	506	CLA	C2C-C1C-NC	3.91	113.64	109.97
24	c	504	CLA	C1C-C2C-C3C	-3.91	102.85	106.96
24	b	616	CLA	C3D-C4D-ND	3.91	116.56	110.24
24	C	505	CLA	C2C-C1C-NC	3.91	113.63	109.97
27	a	415	SQD	C44-O6-C1	-3.90	106.11	113.74
24	C	508	CLA	C1C-C2C-C3C	-3.90	102.86	106.96
24	b	605	CLA	C3D-C4D-ND	3.90	116.54	110.24
24	C	511	CLA	C3D-C4D-ND	3.90	116.54	110.24
24	C	506	CLA	C3D-C4D-ND	3.90	116.54	110.24
24	B	611	CLA	C2C-C1C-NC	3.90	113.62	109.97
26	T	101	BCR	C33-C5-C6	-3.89	120.16	124.53
28	C	521	LMG	O7-C10-C11	3.89	119.89	111.50
24	b	610	CLA	CHD-C1D-ND	-3.89	120.88	124.45
24	B	617	CLA	C3D-C4D-ND	3.89	116.53	110.24
24	a	410	CLA	CBC-CAC-C3C	-3.89	101.72	112.43
24	b	615	CLA	C3D-C4D-ND	3.89	116.52	110.24
39	F	102	HEM	CBA-CAA-C2A	-3.88	106.00	112.62
24	B	606	CLA	CHD-C4C-C3C	-3.88	119.14	124.84
24	a	410	CLA	C1D-CHD-C4C	-3.88	117.69	126.06
36	b	627	HTG	C1-C2-C3	3.88	118.25	110.59
24	b	613	CLA	C2C-C1C-NC	3.87	113.60	109.97
24	b	606	CLA	C3D-C4D-ND	3.87	116.50	110.24
24	B	603	CLA	C2C-C1C-NC	3.87	113.60	109.97
24	a	409	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
24	c	503	CLA	CHD-C4C-C3C	-3.87	119.16	124.84
26	c	516	BCR	C33-C5-C6	-3.87	120.19	124.53
28	c	521	LMG	O7-C10-C11	3.87	119.83	111.50
24	B	603	CLA	C1C-C2C-C3C	-3.86	102.89	106.96
24	c	507	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
24	B	617	CLA	CAC-C3C-C4C	3.86	129.82	124.81
24	b	619	CLA	CHD-C1D-ND	-3.86	120.91	124.45
24	C	513	CLA	CHD-C1D-ND	-3.86	120.91	124.45
24	b	615	CLA	C1D-CHD-C4C	-3.86	117.74	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	505	CLA	CHD-C4C-C3C	-3.85	119.17	124.84
24	b	607	CLA	C1D-CHD-C4C	-3.85	117.75	126.06
24	c	504	CLA	O2D-CGD-O1D	-3.85	116.31	123.84
24	b	615	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
24	c	512	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
24	c	509	CLA	C4A-NA-C1A	3.84	108.43	106.71
24	B	613	CLA	CAC-C3C-C4C	3.84	129.80	124.81
40	h	101	RRX	C34-C9-C10	-3.84	117.54	122.92
24	C	512	CLA	C2C-C1C-NC	3.84	113.57	109.97
24	B	614	CLA	CHD-C1D-ND	-3.84	120.92	124.45
24	b	610	CLA	C3D-C4D-ND	3.84	116.45	110.24
27	F	101	SQD	C44-O6-C1	-3.84	106.24	113.74
24	B	611	CLA	C3D-C4D-ND	3.83	116.44	110.24
24	A	406	CLA	CHD-C4C-C3C	-3.83	119.21	124.84
24	b	609	CLA	CHD-C1D-ND	-3.83	120.93	124.45
29	A	413	PL9	C20-C19-C21	3.83	121.72	115.27
24	b	613	CLA	C3D-C4D-ND	3.83	116.44	110.24
24	B	612	CLA	C3C-C4C-NC	3.83	114.87	110.57
24	c	512	CLA	C3D-C2D-C1D	-3.83	100.61	105.83
24	B	608	CLA	C3C-C4C-NC	3.83	114.86	110.57
24	B	611	CLA	CBC-CAC-C3C	-3.83	101.88	112.43
24	b	607	CLA	C1C-C2C-C3C	-3.83	102.94	106.96
24	c	505	CLA	CHD-C4C-C3C	-3.82	119.22	124.84
24	A	406	CLA	C3B-C4B-NB	3.82	114.15	109.21
24	b	613	CLA	CBC-CAC-C3C	-3.82	101.91	112.43
24	b	614	CLA	C2C-C1C-NC	3.82	113.55	109.97
24	b	609	CLA	C3D-C4D-ND	3.81	116.41	110.24
24	B	611	CLA	C3C-C4C-NC	3.81	114.85	110.57
24	B	613	CLA	C2C-C1C-NC	3.81	113.54	109.97
24	C	505	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
28	C	521	LMG	O8-C28-C29	3.81	123.86	111.91
25	d	401	PHO	C1A-C2A-C3A	-3.81	99.22	102.84
24	B	610	CLA	CHD-C4C-C3C	-3.81	119.25	124.84
24	C	512	CLA	C3D-C4D-ND	3.80	116.39	110.24
26	B	620	BCR	C29-C30-C25	3.80	116.33	110.48
39	e	102	HEM	CHC-C4B-NB	3.79	128.55	124.43
24	A	409	CLA	C3C-C4C-NC	3.79	114.83	110.57
24	c	513	CLA	C3D-C2D-C1D	-3.79	100.66	105.83
24	D	405	CLA	C3D-C4D-ND	3.79	116.37	110.24
24	b	613	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
24	D	401	CLA	CBC-CAC-C3C	-3.78	102.01	112.43
27	f	802	SQD	C1-O5-C5	3.78	121.11	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	505	CLA	C3D-C4D-ND	3.78	116.35	110.24
24	b	615	CLA	CBC-CAC-C3C	-3.78	102.02	112.43
24	A	406	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
26	C	517	BCR	C3-C4-C5	-3.77	107.34	114.08
26	D	407	BCR	C24-C23-C22	-3.77	120.53	126.23
28	c	521	LMG	O8-C28-C29	3.77	123.74	111.91
24	B	608	CLA	C3D-C4D-ND	3.77	116.34	110.24
25	d	401	PHO	C4-C3-C5	3.77	121.61	115.27
24	C	509	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
24	B	610	CLA	C3D-C4D-ND	3.76	116.33	110.24
24	C	511	CLA	C1-C2-C3	-3.76	119.53	126.04
24	B	610	CLA	C2C-C1C-NC	3.76	113.50	109.97
24	b	611	CLA	C3D-C4D-ND	3.76	116.32	110.24
24	B	611	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
24	c	505	CLA	C2C-C1C-NC	3.76	113.49	109.97
24	B	609	CLA	C3D-C4D-ND	3.76	116.31	110.24
24	B	605	CLA	O2D-CGD-O1D	-3.75	116.50	123.84
24	c	509	CLA	CHD-C1D-ND	-3.75	121.01	124.45
24	C	503	CLA	C1C-C2C-C3C	-3.75	103.01	106.96
24	b	616	CLA	C4C-C3C-C2C	-3.75	101.43	106.90
24	b	607	CLA	CAA-C2A-C3A	-3.75	102.51	112.78
24	C	511	CLA	C1C-C2C-C3C	-3.75	103.02	106.96
24	b	619	CLA	C3D-C4D-ND	3.75	116.30	110.24
24	b	618	CLA	CBC-CAC-C3C	-3.75	102.10	112.43
24	b	606	CLA	CAA-C2A-C3A	-3.75	102.52	112.78
24	C	515	CLA	C3D-C4D-ND	3.74	116.29	110.24
24	c	513	CLA	C4-C3-C5	3.74	121.56	115.27
24	c	513	CLA	C3D-C4D-ND	3.74	116.28	110.24
24	c	512	CLA	CHD-C4C-C3C	-3.74	119.35	124.84
24	a	410	CLA	C3C-C4C-NC	3.73	114.76	110.57
24	c	512	CLA	CHD-C1D-ND	-3.73	121.03	124.45
24	C	510	CLA	C2C-C1C-NC	3.73	113.47	109.97
39	F	102	HEM	CBD-CAD-C3D	-3.73	102.27	112.63
24	b	615	CLA	C1-C2-C3	-3.73	119.59	126.04
38	a	416	LHG	O7-C7-C8	3.73	119.54	111.50
24	b	617	CLA	C1C-C2C-C3C	-3.73	103.04	106.96
24	c	503	CLA	C1C-C2C-C3C	-3.73	103.04	106.96
24	b	614	CLA	CHD-C4C-C3C	-3.72	119.37	124.84
24	C	503	CLA	O2D-CGD-O1D	-3.72	116.56	123.84
24	b	605	CLA	C4-C3-C5	3.72	121.53	115.27
29	A	413	PL9	C22-C23-C24	-3.72	118.70	127.66
24	b	610	CLA	C1C-C2C-C3C	-3.72	103.05	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	406	CLA	O2D-CGD-CBD	3.71	117.87	111.27
24	c	511	CLA	C3D-C4D-ND	3.71	116.24	110.24
24	D	406	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
27	A	415	SQD	O48-C23-C24	3.71	123.54	111.91
24	B	616	CLA	C2C-C1C-NC	3.71	113.44	109.97
24	B	604	CLA	CHD-C1D-ND	-3.70	121.05	124.45
24	A	409	CLA	CHD-C1D-ND	-3.70	121.06	124.45
24	c	508	CLA	C1D-CHD-C4C	-3.69	118.09	126.06
24	b	614	CLA	O2D-CGD-CBD	3.69	117.83	111.27
24	b	620	CLA	C3C-C4C-NC	3.69	114.71	110.57
24	B	604	CLA	C3D-C4D-ND	3.68	116.20	110.24
24	c	506	CLA	C1C-C2C-C3C	-3.68	103.08	106.96
36	V	202	HTG	C1-C2-C3	-3.68	103.32	110.59
29	a	417	PL9	C10-C9-C11	3.68	121.46	115.27
24	C	507	CLA	C3C-C4C-NC	3.68	114.70	110.57
24	b	617	CLA	CHD-C4C-C3C	-3.68	119.43	124.84
27	a	415	SQD	O8-S-C6	3.68	111.60	105.74
24	a	413	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
24	C	511	CLA	C16-C15-C13	-3.68	104.03	115.92
24	c	508	CLA	O2D-CGD-CBD	3.68	117.80	111.27
24	b	617	CLA	C3C-C4C-NC	3.67	114.69	110.57
24	C	514	CLA	CHD-C1D-ND	-3.67	121.08	124.45
24	C	514	CLA	C2C-C1C-NC	3.67	113.41	109.97
24	c	507	CLA	C3C-C4C-NC	3.67	114.68	110.57
24	B	612	CLA	C3D-C4D-ND	3.67	116.17	110.24
24	b	615	CLA	O2D-CGD-O1D	-3.67	116.67	123.84
24	b	620	CLA	C3D-C4D-ND	3.66	116.16	110.24
24	c	512	CLA	O2D-CGD-CBD	3.66	117.78	111.27
24	b	620	CLA	C4C-C3C-C2C	-3.66	101.57	106.90
24	C	505	CLA	C1D-CHD-C4C	-3.66	118.17	126.06
40	h	101	RRX	C35-C13-C12	-3.66	112.32	118.08
40	h	101	RRX	C29-C28-C27	3.65	115.31	110.30
24	b	608	CLA	CHD-C1D-ND	-3.65	121.10	124.45
24	A	405	CLA	CHD-C4C-C3C	-3.65	119.47	124.84
24	b	614	CLA	C3D-C4D-ND	3.65	116.14	110.24
24	b	606	CLA	O2D-CGD-O1D	-3.65	116.71	123.84
24	c	504	CLA	C3D-C4D-ND	3.64	116.13	110.24
24	A	406	CLA	C3C-C4C-NC	3.64	114.66	110.57
24	B	614	CLA	C2C-C1C-NC	3.64	113.38	109.97
24	B	618	CLA	C2C-C1C-NC	3.64	113.38	109.97
24	D	401	CLA	CAA-C2A-C3A	-3.63	102.83	112.78
24	c	511	CLA	C2C-C1C-NC	3.63	113.38	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	504	CLA	C3C-C4C-NC	3.63	114.64	110.57
24	B	616	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
24	a	410	CLA	C3B-C4B-NB	3.62	113.89	109.21
24	c	514	CLA	C3D-C4D-ND	3.62	116.09	110.24
24	b	605	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
24	C	507	CLA	C3D-C4D-ND	3.61	116.08	110.24
24	B	606	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
24	a	409	CLA	CHD-C4C-C3C	-3.61	119.53	124.84
29	A	413	PL9	C27-C28-C29	-3.61	118.96	127.66
24	B	607	CLA	C4C-C3C-C2C	-3.61	101.64	106.90
24	D	401	CLA	O2D-CGD-CBD	3.61	117.68	111.27
24	C	504	CLA	O2D-CGD-O1D	-3.60	116.79	123.84
24	C	510	CLA	C3C-C4C-NC	3.60	114.61	110.57
24	C	507	CLA	C3D-C2D-C1D	-3.60	100.92	105.83
24	D	401	CLA	CMC-C2C-C1C	3.60	130.52	125.04
24	a	411	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
24	a	409	CLA	C1D-CHD-C4C	-3.60	118.30	126.06
24	b	607	CLA	C3D-C4D-ND	3.60	116.06	110.24
24	C	507	CLA	CHD-C4C-C3C	-3.59	119.56	124.84
24	c	508	CLA	CHD-C4C-C3C	-3.59	119.56	124.84
24	C	506	CLA	C3B-C4B-NB	3.59	113.85	109.21
24	B	612	CLA	C4C-C3C-C2C	-3.59	101.67	106.90
24	B	605	CLA	CAA-C2A-C3A	-3.59	102.96	112.78
24	B	610	CLA	CMA-C3A-C4A	-3.57	102.17	111.77
39	e	102	HEM	CHB-C1B-NB	3.57	128.79	124.38
24	c	514	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
24	b	613	CLA	CHD-C4C-C3C	-3.57	119.60	124.84
40	h	101	RRX	C7-C6-C5	-3.57	112.82	121.46
24	A	406	CLA	CHD-C1D-ND	-3.56	121.18	124.45
24	b	620	CLA	C1D-CHD-C4C	-3.56	118.38	126.06
24	b	612	CLA	C4C-C3C-C2C	-3.56	101.71	106.90
24	c	509	CLA	C1D-CHD-C4C	-3.56	118.38	126.06
24	d	405	CLA	C1C-C2C-C3C	-3.56	103.22	106.96
24	c	514	CLA	C2C-C1C-NC	3.56	113.30	109.97
26	b	621	BCR	C7-C8-C9	-3.56	120.86	126.23
24	C	508	CLA	C3D-C4D-ND	3.55	115.99	110.24
24	B	613	CLA	C1D-CHD-C4C	-3.55	118.39	126.06
24	b	612	CLA	C3C-C4C-NC	3.55	114.56	110.57
24	C	503	CLA	C1D-CHD-C4C	-3.54	118.41	126.06
24	C	503	CLA	C3B-C4B-NB	3.54	113.79	109.21
24	B	609	CLA	CAA-C2A-C3A	-3.54	103.08	112.78
24	c	511	CLA	C1C-C2C-C3C	-3.54	103.23	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	510	CLA	CHD-C1D-ND	-3.54	121.20	124.45
24	C	514	CLA	C1D-CHD-C4C	-3.53	118.44	126.06
28	z	101	LMG	O7-C10-C11	3.53	119.11	111.50
40	h	101	RRX	C30-C25-C26	-3.53	117.64	122.61
29	a	417	PL9	C32-C33-C34	-3.53	119.17	127.66
24	b	606	CLA	CHD-C1D-ND	-3.53	121.21	124.45
25	d	401	PHO	CMB-C2B-C3B	3.53	131.28	124.68
32	A	422	LMT	O1B-C4'-C3'	3.53	116.66	107.28
24	C	504	CLA	C2C-C1C-NC	3.53	113.28	109.97
24	a	411	CLA	C3B-C4B-NB	3.52	113.77	109.21
24	C	514	CLA	C3C-C4C-NC	3.52	114.52	110.57
24	b	605	CLA	C1D-CHD-C4C	-3.52	118.46	126.06
28	B	623	LMG	O8-C28-C29	3.52	122.96	111.91
25	A	407	PHO	C4A-C3A-C2A	-3.52	99.49	102.84
24	B	605	CLA	C3C-C4C-NC	3.52	114.52	110.57
24	C	513	CLA	C3D-C4D-ND	3.52	115.92	110.24
24	c	515	CLA	C1C-C2C-C3C	-3.51	103.26	106.96
26	D	407	BCR	C28-C27-C26	-3.51	107.81	114.08
24	D	401	CLA	C3C-C4C-NC	3.51	114.51	110.57
24	A	405	CLA	CHD-C1D-ND	-3.50	121.24	124.45
24	a	413	CLA	C3C-C4C-NC	3.50	114.49	110.57
26	b	622	BCR	C29-C30-C25	3.50	115.86	110.48
24	B	611	CLA	C1D-CHD-C4C	-3.49	118.52	126.06
24	d	405	CLA	CHD-C1D-ND	-3.49	121.24	124.45
24	c	514	CLA	C1-C2-C3	-3.49	120.00	126.04
24	C	514	CLA	C3D-C4D-ND	3.49	115.88	110.24
24	D	406	CLA	C4-C3-C5	3.49	121.14	115.27
24	d	405	CLA	C1-C2-C3	-3.49	120.01	126.04
24	A	409	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
24	B	613	CLA	C1-C2-C3	-3.48	120.03	126.04
24	c	510	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
24	c	515	CLA	C1D-CHD-C4C	-3.47	118.57	126.06
24	c	504	CLA	CHD-C4C-C3C	-3.47	119.74	124.84
24	b	609	CLA	C3C-C4C-NC	3.47	114.46	110.57
36	b	603	HTG	C1'-S1-C1	3.47	106.58	100.09
24	b	608	CLA	CHD-C4C-C3C	-3.47	119.74	124.84
24	c	515	CLA	C3C-C4C-NC	3.47	114.46	110.57
29	A	413	PL9	C53-C6-C1	3.46	122.07	114.99
24	C	512	CLA	CHD-C1D-ND	-3.46	121.27	124.45
24	d	405	CLA	C3C-C4C-NC	3.46	114.45	110.57
24	c	506	CLA	CBC-CAC-C3C	-3.46	102.89	112.43
24	C	503	CLA	CHD-C4C-C3C	-3.46	119.75	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	417	PL9	C20-C19-C21	3.46	121.09	115.27
26	d	407	BCR	C28-C27-C26	-3.46	107.90	114.08
24	C	512	CLA	C3C-C4C-NC	3.46	114.45	110.57
24	D	401	CLA	C3D-C4D-ND	3.45	115.81	110.24
24	B	617	CLA	C1D-CHD-C4C	-3.45	118.63	126.06
24	B	604	CLA	C1C-C2C-C3C	-3.44	103.33	106.96
24	C	513	CLA	C1-O2A-CGA	3.44	125.48	116.44
24	c	505	CLA	O2D-CGD-CBD	3.44	117.38	111.27
24	b	608	CLA	C4A-NA-C1A	3.44	108.25	106.71
24	a	413	CLA	C3B-C4B-NB	3.44	113.65	109.21
24	a	411	CLA	CBC-CAC-C3C	-3.44	102.95	112.43
24	D	405	CLA	C4C-C3C-C2C	-3.44	101.89	106.90
24	b	610	CLA	C3C-C4C-NC	3.44	114.42	110.57
38	L	101	LHG	O7-C7-C8	3.43	118.90	111.50
24	C	513	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
26	b	623	BCR	C15-C14-C13	-3.43	122.41	127.31
24	b	617	CLA	C3B-C4B-NB	3.43	113.65	109.21
24	D	406	CLA	C3C-C4C-NC	3.43	114.42	110.57
24	b	620	CLA	O2D-CGD-O1D	-3.43	117.14	123.84
24	B	617	CLA	CMC-C2C-C1C	3.43	130.26	125.04
24	B	618	CLA	C3C-C4C-NC	3.43	114.41	110.57
24	A	405	CLA	C1D-CHD-C4C	-3.43	118.67	126.06
24	B	613	CLA	CMC-C2C-C1C	3.43	130.25	125.04
29	A	413	PL9	C32-C33-C34	-3.43	119.41	127.66
24	c	510	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
24	c	508	CLA	C3C-C4C-NC	3.42	114.41	110.57
24	B	618	CLA	C4C-C3C-C2C	-3.42	101.91	106.90
24	C	504	CLA	C1D-CHD-C4C	-3.42	118.68	126.06
32	M	101	LMT	C1-O1'-C1'	-3.42	108.18	113.84
24	a	411	CLA	C3C-C4C-NC	3.41	114.40	110.57
32	D	409	LMT	C1B-O5B-C5B	3.41	120.38	113.69
24	b	614	CLA	C4C-C3C-C2C	-3.41	101.93	106.90
24	c	513	CLA	CHD-C4C-C3C	-3.41	119.83	124.84
24	b	609	CLA	C1C-C2C-C3C	-3.41	103.38	106.96
24	B	612	CLA	O2D-CGD-CBD	3.40	117.32	111.27
40	h	101	RRX	C34-C9-C8	-3.40	112.71	118.08
24	b	612	CLA	CHD-C4C-C3C	-3.40	119.84	124.84
24	A	405	CLA	C3C-C4C-NC	3.40	114.39	110.57
24	b	616	CLA	C3B-C4B-NB	3.40	113.61	109.21
24	C	507	CLA	C4C-C3C-C2C	-3.40	101.94	106.90
24	b	610	CLA	C1D-CHD-C4C	-3.40	118.72	126.06
24	C	509	CLA	C3C-C4C-NC	3.40	114.38	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	506	CLA	O2D-CGD-O1D	-3.40	117.19	123.84
24	c	511	CLA	O2D-CGD-O1D	-3.40	117.19	123.84
24	C	509	CLA	C4-C3-C5	3.40	120.99	115.27
24	C	503	CLA	CAC-C3C-C4C	3.40	129.22	124.81
24	b	606	CLA	CMA-C3A-C4A	-3.40	102.64	111.77
24	b	608	CLA	C3B-C4B-NB	3.40	113.60	109.21
26	A	410	BCR	C38-C26-C25	-3.39	120.72	124.53
24	B	610	CLA	C4C-C3C-C2C	-3.39	101.96	106.90
24	C	508	CLA	O2D-CGD-CBD	3.39	117.29	111.27
24	d	406	CLA	CHD-C4C-C3C	-3.39	119.86	124.84
24	c	514	CLA	C1D-CHD-C4C	-3.39	118.75	126.06
24	c	514	CLA	CHD-C4C-C3C	-3.38	119.87	124.84
24	D	401	CLA	CMA-C3A-C4A	-3.38	102.69	111.77
38	d	411	LHG	O7-C7-C8	3.38	118.78	111.50
24	A	409	CLA	O2D-CGD-O1D	-3.38	117.23	123.84
24	C	504	CLA	C1C-C2C-C3C	-3.38	103.41	106.96
24	c	505	CLA	C1C-C2C-C3C	-3.38	103.41	106.96
24	b	605	CLA	CHD-C1D-ND	-3.37	121.36	124.45
24	C	509	CLA	C1-C2-C3	-3.37	120.21	126.04
29	D	408	PL9	C25-C24-C26	3.37	120.94	115.27
24	b	616	CLA	C1D-CHD-C4C	-3.37	118.79	126.06
26	K	102	BCR	C7-C8-C9	-3.37	121.14	126.23
27	a	401	SQD	O48-C23-C24	3.37	122.48	111.91
24	c	513	CLA	C1C-C2C-C3C	-3.37	103.42	106.96
24	a	413	CLA	CAA-C2A-C3A	-3.37	103.56	112.78
24	c	513	CLA	O2D-CGD-CBD	3.37	117.25	111.27
24	B	603	CLA	C1D-CHD-C4C	-3.37	118.80	126.06
24	B	612	CLA	C1D-CHD-C4C	-3.37	118.80	126.06
24	b	619	CLA	C1C-C2C-C3C	-3.36	103.42	106.96
24	c	503	CLA	C1D-CHD-C4C	-3.36	118.80	126.06
24	b	611	CLA	CHD-C4C-C3C	-3.36	119.90	124.84
24	a	410	CLA	CAA-C2A-C3A	-3.36	103.57	112.78
24	B	604	CLA	C3C-C4C-NC	3.36	114.34	110.57
24	b	614	CLA	C3C-C4C-NC	3.36	114.34	110.57
24	c	507	CLA	CHD-C1D-ND	-3.36	121.37	124.45
37	C	518	DGD	O2G-C1B-C2B	3.36	118.74	111.50
24	C	511	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
24	B	610	CLA	C3C-C4C-NC	3.36	114.33	110.57
38	l	102	LHG	O7-C7-C8	3.36	118.73	111.50
27	b	601	SQD	O8-S-C6	3.35	111.08	105.74
24	c	508	CLA	C2C-C1C-NC	3.35	113.11	109.97
24	B	615	CLA	C3D-C4D-ND	3.35	115.65	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	415	SQD	O47-C7-O49	-3.35	115.61	123.70
27	F	101	SQD	C1-C2-C3	-3.35	103.03	110.00
24	B	618	CLA	C1D-CHD-C4C	-3.35	118.84	126.06
24	c	507	CLA	C3D-C2D-C1D	-3.34	101.27	105.83
24	B	607	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
24	B	610	CLA	O2D-CGD-CBD	3.34	117.20	111.27
24	b	607	CLA	CHD-C1D-ND	-3.34	121.38	124.45
24	b	613	CLA	C1D-CHD-C4C	-3.34	118.86	126.06
24	D	406	CLA	C1D-CHD-C4C	-3.34	118.86	126.06
24	c	506	CLA	C1D-CHD-C4C	-3.34	118.86	126.06
24	b	605	CLA	C2C-C1C-NC	3.34	113.10	109.97
27	F	101	SQD	O7-S-C6	3.34	110.90	106.94
24	C	511	CLA	C3B-C4B-NB	3.34	113.52	109.21
24	B	613	CLA	C3C-C4C-NC	3.33	114.31	110.57
24	B	603	CLA	C4-C3-C5	3.33	120.88	115.27
29	d	408	PL9	C40-C39-C41	3.33	120.88	115.27
24	c	510	CLA	C4C-C3C-C2C	-3.33	102.05	106.90
29	a	417	PL9	C30-C29-C31	3.33	120.87	115.27
40	h	101	RRX	C27-C26-C25	3.33	128.26	120.85
24	B	614	CLA	C4C-C3C-C2C	-3.33	102.05	106.90
24	D	405	CLA	C1C-C2C-C3C	-3.32	103.46	106.96
24	A	409	CLA	CMA-C3A-C4A	-3.32	102.84	111.77
39	F	102	HEM	CHB-C1B-NB	3.32	128.49	124.38
24	a	410	CLA	O2D-CGD-CBD	3.32	117.17	111.27
24	B	611	CLA	O2D-CGD-CBD	3.32	117.17	111.27
24	a	409	CLA	C3C-C4C-NC	3.32	114.30	110.57
38	D	410	LHG	O8-C23-O10	-3.32	115.21	123.59
24	C	510	CLA	C1C-C2C-C3C	-3.32	103.47	106.96
28	c	521	LMG	C8-O7-C10	-3.32	109.62	117.79
26	k	102	BCR	C15-C14-C13	-3.32	122.57	127.31
29	a	417	PL9	C42-C43-C44	-3.32	119.67	127.66
24	b	606	CLA	C1D-CHD-C4C	-3.32	118.90	126.06
24	B	613	CLA	C3D-C4D-ND	3.32	115.60	110.24
24	A	405	CLA	CAA-C2A-C3A	-3.32	103.70	112.78
24	B	610	CLA	CMB-C2B-C3B	3.31	130.88	124.68
24	b	606	CLA	C1C-C2C-C3C	-3.31	103.47	106.96
24	C	511	CLA	CHD-C1D-ND	-3.31	121.41	124.45
24	A	409	CLA	CBC-CAC-C3C	-3.31	103.30	112.43
28	Z	101	LMG	O7-C10-C11	3.31	118.64	111.50
24	C	506	CLA	C1D-CHD-C4C	-3.31	118.91	126.06
24	b	618	CLA	C1-C2-C3	-3.31	120.32	126.04
24	d	405	CLA	CHD-C4C-C3C	-3.31	119.98	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	513	CLA	C3C-C4C-NC	3.31	114.28	110.57
24	B	607	CLA	C1D-CHD-C4C	-3.31	118.92	126.06
37	c	518	DGD	C3G-C2G-C1G	-3.31	103.97	111.79
24	B	609	CLA	C3B-C4B-NB	3.31	113.48	109.21
25	a	412	PHO	CMA-C3A-C4A	-3.31	107.14	114.38
24	c	513	CLA	C2C-C1C-NC	3.30	113.07	109.97
24	c	513	CLA	CAC-C3C-C4C	3.30	129.09	124.81
24	b	606	CLA	C3C-C4C-NC	3.30	114.27	110.57
24	B	605	CLA	CHD-C1D-ND	-3.30	121.42	124.45
24	B	609	CLA	CHD-C4C-C3C	-3.30	119.99	124.84
24	D	405	CLA	C1-C2-C3	-3.30	120.34	126.04
24	C	515	CLA	C1D-CHD-C4C	-3.29	118.95	126.06
24	C	512	CLA	C1C-C2C-C3C	-3.29	103.49	106.96
24	b	612	CLA	CHD-C1D-ND	-3.29	121.43	124.45
24	b	615	CLA	C3C-C4C-NC	3.29	114.26	110.57
24	C	512	CLA	C1D-CHD-C4C	-3.28	118.97	126.06
24	b	607	CLA	C5-C3-C2	-3.28	114.48	121.12
24	C	512	CLA	C3B-C4B-NB	3.28	113.45	109.21
24	B	608	CLA	C1D-CHD-C4C	-3.28	118.98	126.06
24	C	510	CLA	C3B-C4B-NB	3.28	113.44	109.21
24	b	619	CLA	CBC-CAC-C3C	-3.28	103.40	112.43
24	b	613	CLA	CHD-C1D-ND	-3.27	121.45	124.45
24	c	503	CLA	C3B-C4B-NB	3.27	113.44	109.21
26	C	516	BCR	C33-C5-C6	-3.27	120.86	124.53
24	C	505	CLA	C3D-C4D-ND	3.26	115.52	110.24
24	B	612	CLA	O2A-CGA-CBA	3.26	122.15	111.91
26	c	516	BCR	C16-C17-C18	-3.26	122.66	127.31
24	b	612	CLA	CMA-C3A-C4A	-3.26	103.02	111.77
24	b	608	CLA	C3D-C4D-ND	3.26	115.51	110.24
24	b	612	CLA	CMB-C2B-C3B	3.26	130.77	124.68
24	B	612	CLA	CAC-C3C-C4C	3.26	129.03	124.81
24	b	606	CLA	C2C-C1C-NC	3.25	113.02	109.97
24	b	616	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
24	B	604	CLA	CHD-C4C-C3C	-3.25	120.06	124.84
38	D	412	LHG	O7-C7-C8	3.25	118.51	111.50
24	B	609	CLA	CHD-C1D-ND	-3.25	121.47	124.45
24	A	409	CLA	C3B-C4B-NB	3.25	113.41	109.21
24	C	511	CLA	CHD-C4C-C3C	-3.25	120.07	124.84
24	B	607	CLA	C4-C3-C5	3.24	120.73	115.27
24	A	405	CLA	CAC-C3C-C4C	3.24	129.02	124.81
24	C	508	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
24	b	609	CLA	C2C-C1C-NC	3.24	113.01	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	608	CLA	C3B-C4B-NB	3.24	113.40	109.21
24	A	406	CLA	CAC-C3C-C4C	3.24	129.01	124.81
24	C	514	CLA	C1-O2A-CGA	3.24	124.94	116.44
29	A	413	PL9	C15-C14-C16	3.24	120.72	115.27
24	a	409	CLA	C3B-C4B-NB	3.23	113.39	109.21
29	A	413	PL9	C7-C8-C9	-3.23	121.41	126.79
24	B	616	CLA	CHD-C1D-ND	-3.23	121.48	124.45
36	O	303	HTG	C1'-S1-C1	3.23	106.13	100.09
24	C	515	CLA	C1C-C2C-C3C	-3.23	103.56	106.96
24	b	618	CLA	C3B-C4B-NB	3.23	113.38	109.21
24	B	610	CLA	C1D-CHD-C4C	-3.22	119.10	126.06
24	c	515	CLA	CHD-C4C-C3C	-3.22	120.10	124.84
37	C	519	DGD	C2G-O2G-C1B	-3.22	109.85	117.79
24	C	509	CLA	C3D-C4D-ND	3.22	115.45	110.24
24	B	618	CLA	CBC-CAC-C3C	-3.22	103.56	112.43
37	h	102	DGD	O2G-C1B-C2B	3.22	118.44	111.50
24	c	505	CLA	C1D-CHD-C4C	-3.22	119.11	126.06
24	b	619	CLA	C3C-C4C-NC	3.22	114.18	110.57
24	b	619	CLA	C4-C3-C5	3.21	120.68	115.27
24	D	405	CLA	C3B-C4B-NB	3.21	113.36	109.21
24	B	603	CLA	C3C-C4C-NC	3.21	114.17	110.57
24	C	503	CLA	CBC-CAC-C3C	-3.21	103.58	112.43
24	A	409	CLA	C1-C2-C3	-3.21	120.49	126.04
24	c	507	CLA	CHD-C4C-C3C	-3.21	120.12	124.84
24	C	508	CLA	CAA-C2A-C3A	-3.21	104.00	112.78
24	c	515	CLA	C4C-C3C-C2C	-3.21	102.22	106.90
24	c	503	CLA	C3C-C4C-NC	3.21	114.17	110.57
24	D	405	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
40	h	101	RRX	C3-C4-C5	-3.21	108.35	114.08
24	C	507	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
24	C	509	CLA	CBC-CAC-C3C	-3.20	103.60	112.43
24	A	409	CLA	C1D-CHD-C4C	-3.20	119.15	126.06
24	b	610	CLA	CMC-C2C-C1C	3.20	129.91	125.04
24	A	406	CLA	CBC-CAC-C3C	-3.20	103.61	112.43
24	B	607	CLA	C1C-C2C-C3C	-3.20	103.60	106.96
24	C	513	CLA	C3B-C4B-NB	3.19	113.34	109.21
26	C	516	BCR	C7-C8-C9	-3.19	121.41	126.23
24	b	617	CLA	C4C-C3C-C2C	-3.19	102.24	106.90
24	B	614	CLA	O2A-C1-C2	-3.19	100.24	108.64
29	a	417	PL9	C27-C28-C29	-3.19	119.97	127.66
24	B	604	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
24	B	609	CLA	C1D-CHD-C4C	-3.19	119.17	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	615	CLA	C3B-C4B-NB	3.19	113.33	109.21
29	a	417	PL9	C22-C23-C24	-3.19	119.98	127.66
24	C	507	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
29	d	408	PL9	C53-C6-C1	3.19	121.51	114.99
24	c	511	CLA	C16-C15-C13	-3.19	105.62	115.92
24	a	411	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
29	a	417	PL9	C37-C38-C39	-3.18	120.00	127.66
26	D	407	BCR	C29-C30-C25	3.18	115.38	110.48
24	B	613	CLA	CHD-C1D-ND	-3.18	121.53	124.45
24	B	606	CLA	C3D-C4D-ND	3.18	115.38	110.24
24	C	504	CLA	C4C-C3C-C2C	-3.18	102.27	106.90
24	b	620	CLA	C1-O2A-CGA	3.17	124.77	116.44
24	C	504	CLA	CBC-CAC-C3C	-3.17	103.68	112.43
24	B	608	CLA	CAA-C2A-C3A	-3.17	104.09	112.78
24	C	507	CLA	CHD-C1D-ND	-3.17	121.54	124.45
24	b	613	CLA	C1-C2-C3	-3.17	120.56	126.04
24	A	405	CLA	C3D-C4D-ND	3.17	115.36	110.24
24	C	512	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
24	c	508	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
24	B	613	CLA	O2D-CGD-CBD	3.17	116.90	111.27
40	H	103	RRX	C34-C9-C8	-3.17	113.09	118.08
24	B	608	CLA	O2D-CGD-O1D	-3.16	117.65	123.84
24	C	515	CLA	C4-C3-C5	3.16	120.59	115.27
24	b	607	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
24	A	405	CLA	CAA-C2A-C1A	-3.16	101.62	111.97
24	b	608	CLA	C3C-C4C-NC	3.16	114.11	110.57
24	c	515	CLA	CMB-C2B-C3B	3.16	130.59	124.68
38	d	411	LHG	O8-C23-C24	3.16	121.82	111.91
24	c	511	CLA	C1-O2A-CGA	3.16	124.73	116.44
24	B	603	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
27	A	411	SQD	C44-O6-C1	-3.15	107.58	113.74
36	C	523	HTG	C1-O5-C5	3.15	118.40	112.58
24	c	511	CLA	CHD-C1D-ND	-3.15	121.56	124.45
24	C	508	CLA	C1-C2-C3	-3.15	120.59	126.04
24	c	509	CLA	C3D-C4D-ND	3.15	115.34	110.24
24	b	609	CLA	C4C-C3C-C2C	-3.15	102.30	106.90
24	C	513	CLA	CAC-C3C-C4C	3.15	128.89	124.81
24	C	514	CLA	C4C-C3C-C2C	-3.14	102.31	106.90
24	c	511	CLA	C1D-CHD-C4C	-3.14	119.28	126.06
24	A	406	CLA	C1D-CHD-C4C	-3.14	119.28	126.06
24	c	512	CLA	C3B-C4B-NB	3.14	113.27	109.21
24	c	514	CLA	CBC-CAC-C3C	-3.14	103.78	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	616	CLA	CAC-C3C-C4C	3.14	128.88	124.81
28	Z	101	LMG	O6-C5-C4	3.13	115.38	109.69
24	c	505	CLA	C3C-C4C-NC	3.13	114.08	110.57
24	C	505	CLA	C1-C2-C3	-3.13	120.63	126.04
24	c	504	CLA	CHD-C1D-ND	-3.13	121.58	124.45
32	B	624	LMT	C1-O1'-C1'	-3.13	108.65	113.84
28	i	101	LMG	C8-O7-C10	-3.12	110.10	117.79
24	b	618	CLA	C1-O2A-CGA	3.12	124.64	116.44
24	B	611	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
24	c	508	CLA	C1C-C2C-C3C	-3.12	103.68	106.96
24	C	515	CLA	C3C-C4C-NC	3.12	114.07	110.57
24	B	607	CLA	O2A-CGA-O1A	-3.12	115.72	123.59
38	d	409	LHG	O8-C23-O10	-3.12	115.73	123.59
24	B	615	CLA	CED-O2D-CGD	3.12	122.98	115.94
24	B	610	CLA	O2A-CGA-CBA	3.11	121.68	111.91
24	c	508	CLA	CHD-C1D-ND	-3.11	121.59	124.45
24	c	506	CLA	C3C-C4C-NC	3.11	114.06	110.57
24	b	613	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
24	A	405	CLA	C4C-C3C-C2C	-3.11	102.36	106.90
24	c	511	CLA	C3C-C4C-NC	3.11	114.06	110.57
24	b	614	CLA	CAC-C3C-C4C	3.11	128.84	124.81
24	a	409	CLA	CAA-C2A-C1A	-3.11	101.79	111.97
24	b	605	CLA	C1-O2A-CGA	3.11	124.59	116.44
26	d	407	BCR	C38-C26-C25	-3.11	121.04	124.53
24	D	401	CLA	C1D-CHD-C4C	-3.10	119.36	126.06
36	b	627	HTG	C6-C5-C4	-3.10	105.74	113.00
24	B	614	CLA	C1D-CHD-C4C	-3.10	119.37	126.06
24	b	607	CLA	O2A-CGA-O1A	-3.10	115.77	123.59
24	d	406	CLA	C3B-C4B-NB	3.10	113.22	109.21
26	C	517	BCR	C15-C14-C13	-3.10	122.89	127.31
24	C	511	CLA	C3C-C4C-NC	3.09	114.04	110.57
24	b	615	CLA	CAC-C3C-C4C	3.09	128.82	124.81
24	A	409	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
24	C	510	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
24	C	510	CLA	C1D-CHD-C4C	-3.09	119.39	126.06
40	H	103	RRX	C40-C30-C29	-3.09	95.18	109.05
24	B	614	CLA	C1C-C2C-C3C	-3.08	103.71	106.96
24	B	615	CLA	C3C-C4C-NC	3.08	114.03	110.57
24	B	605	CLA	C3B-C4B-NB	3.08	113.19	109.21
24	c	508	CLA	CBC-CAC-C3C	-3.08	103.93	112.43
24	a	410	CLA	CMA-C3A-C2A	-3.08	101.40	113.83
24	c	506	CLA	C3B-C4B-NB	3.08	113.19	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	504	CLA	C1D-CHD-C4C	-3.08	119.41	126.06
24	c	514	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
24	C	514	CLA	C1C-C2C-C3C	-3.08	103.72	106.96
24	a	413	CLA	CMA-C3A-C2A	-3.08	101.41	113.83
24	b	606	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
24	c	505	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
26	A	410	BCR	C28-C27-C26	-3.08	108.58	114.08
24	b	614	CLA	C1D-CHD-C4C	-3.08	119.42	126.06
24	C	505	CLA	C3C-C4C-NC	3.08	114.02	110.57
40	H	103	RRX	C39-C30-C25	3.07	115.28	110.30
24	B	618	CLA	C3B-C4B-NB	3.07	113.18	109.21
24	C	507	CLA	CHA-C1A-NA	-3.07	119.37	126.40
24	a	410	CLA	CHC-C1C-C2C	-3.07	118.23	126.72
24	b	612	CLA	CAC-C3C-C4C	3.07	128.79	124.81
24	c	513	CLA	C1-O2A-CGA	3.07	124.49	116.44
24	c	509	CLA	CBC-CAC-C3C	-3.07	103.98	112.43
26	b	621	BCR	C29-C30-C25	3.06	115.20	110.48
24	C	508	CLA	CHD-C4C-C3C	-3.06	120.34	124.84
39	F	102	HEM	CHD-C1D-ND	3.06	127.76	124.43
24	C	507	CLA	CAC-C3C-C4C	3.06	128.78	124.81
24	c	511	CLA	C3B-C4B-NB	3.06	113.16	109.21
24	A	405	CLA	C1C-C2C-C3C	-3.06	103.74	106.96
24	a	413	CLA	C1D-CHD-C4C	-3.06	119.47	126.06
24	C	505	CLA	CHD-C1D-ND	-3.05	121.65	124.45
24	b	607	CLA	CBC-CAC-C3C	-3.05	104.03	112.43
24	B	604	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
24	B	616	CLA	C3C-C4C-NC	3.05	113.99	110.57
24	c	507	CLA	C4C-C3C-C2C	-3.05	102.46	106.90
24	c	512	CLA	C4-C3-C5	3.04	120.39	115.27
24	c	509	CLA	O1D-CGD-CBD	-3.04	118.25	124.48
24	c	505	CLA	O2A-CGA-CBA	3.04	121.46	111.91
24	C	506	CLA	CBC-CAC-C3C	-3.04	104.04	112.43
25	A	408	PHO	C4-C3-C5	3.04	120.39	115.27
24	c	510	CLA	C1D-CHD-C4C	-3.04	119.50	126.06
24	b	620	CLA	CAC-C3C-C4C	3.04	128.75	124.81
24	c	512	CLA	C11-C10-C8	-3.04	106.11	115.92
24	D	401	CLA	C3B-C4B-NB	3.04	113.13	109.21
24	a	413	CLA	CBC-CAC-C3C	-3.03	104.08	112.43
24	B	613	CLA	CBC-CAC-C3C	-3.03	104.08	112.43
24	b	611	CLA	C3C-C4C-NC	3.03	113.97	110.57
27	A	415	SQD	O9-S-C6	3.03	110.54	106.94
24	a	413	CLA	C4C-C3C-C2C	-3.03	102.48	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	512	CLA	C1D-CHD-C4C	-3.03	119.53	126.06
24	C	511	CLA	C1D-CHD-C4C	-3.02	119.54	126.06
24	C	511	CLA	C7-C6-C5	-3.02	105.15	113.36
24	C	514	CLA	CBA-CAA-C2A	-3.02	104.95	113.86
26	c	516	BCR	C15-C14-C13	-3.02	123.00	127.31
24	b	606	CLA	C4-C3-C5	3.02	120.35	115.27
24	a	411	CLA	O2A-CGA-O1A	-3.02	115.98	123.59
24	C	514	CLA	CBC-CAC-C3C	-3.02	104.11	112.43
24	C	508	CLA	CAC-C3C-C4C	3.02	128.72	124.81
24	C	513	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
24	B	616	CLA	CHD-C4C-NC	3.01	128.95	124.20
24	C	512	CLA	C4-C3-C5	3.01	120.34	115.27
24	C	505	CLA	C4A-NA-C1A	3.01	108.06	106.71
24	C	509	CLA	C1-O2A-CGA	3.01	124.34	116.44
29	d	408	PL9	C7-C8-C9	-3.01	121.78	126.79
26	D	407	BCR	C7-C8-C9	-3.01	121.69	126.23
24	A	409	CLA	C4-C3-C5	3.01	120.33	115.27
24	b	616	CLA	C1C-C2C-C3C	-3.01	103.80	106.96
24	C	515	CLA	C2C-C1C-NC	3.01	112.79	109.97
27	b	601	SQD	O48-C23-C24	3.01	121.34	111.91
24	b	613	CLA	C3C-C4C-NC	3.00	113.94	110.57
24	D	405	CLA	CAA-C2A-C3A	-3.00	104.55	112.78
24	b	611	CLA	CBC-CAC-C3C	-3.00	104.15	112.43
24	c	507	CLA	CAC-C3C-C4C	3.00	128.70	124.81
26	d	407	BCR	C7-C8-C9	-3.00	121.70	126.23
25	A	407	PHO	C1A-C2A-C3A	-3.00	99.99	102.84
24	B	613	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
26	k	103	BCR	C7-C8-C9	-2.99	121.71	126.23
24	d	405	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
38	D	412	LHG	O8-C23-O10	-2.99	116.04	123.59
24	B	613	CLA	C1C-C2C-C3C	-2.99	103.81	106.96
24	b	606	CLA	CMA-C3A-C2A	-2.99	101.77	113.83
24	C	513	CLA	C1D-CHD-C4C	-2.99	119.61	126.06
24	C	511	CLA	CAC-C3C-C4C	2.99	128.69	124.81
24	d	406	CLA	CAC-C3C-C4C	2.99	128.69	124.81
24	b	605	CLA	C3C-C4C-NC	2.99	113.92	110.57
28	B	623	LMG	O7-C10-O9	-2.98	116.49	123.70
27	A	415	SQD	C1-O5-C5	-2.98	107.84	113.69
24	b	609	CLA	CMB-C2B-C1B	2.98	133.04	128.46
39	F	102	HEM	C4D-ND-C1D	2.98	108.15	105.07
24	c	504	CLA	O2A-CGA-O1A	-2.98	116.08	123.59
24	B	608	CLA	C4-C3-C5	2.98	120.28	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	C	518	DGD	O3G-C3G-C2G	-2.98	103.72	110.90
24	B	606	CLA	C1D-CHD-C4C	-2.97	119.65	126.06
38	d	409	LHG	O8-C23-C24	2.97	121.23	111.91
24	B	610	CLA	CAC-C3C-C4C	2.97	128.66	124.81
24	C	505	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
24	B	616	CLA	O2A-CGA-CBA	2.97	121.22	111.91
26	t	101	BCR	C7-C8-C9	-2.97	121.75	126.23
24	B	606	CLA	CMC-C2C-C1C	2.96	129.55	125.04
24	b	607	CLA	C3B-C4B-NB	2.96	113.04	109.21
32	b	629	LMT	O1'-C1'-C2'	2.96	112.93	108.30
24	D	401	CLA	CMA-C3A-C2A	-2.96	101.88	113.83
24	b	614	CLA	O2A-CGA-CBA	2.96	121.20	111.91
24	C	509	CLA	C3B-C4B-NB	2.96	113.04	109.21
24	C	507	CLA	C1-C2-C3	-2.96	120.92	126.04
24	c	515	CLA	C1-C2-C3	-2.96	120.93	126.04
24	c	512	CLA	C1-C2-C3	-2.96	120.93	126.04
24	b	615	CLA	CHD-C1D-ND	-2.95	121.74	124.45
24	B	610	CLA	C1C-C2C-C3C	-2.95	103.85	106.96
24	c	503	CLA	CMC-C2C-C1C	2.95	129.53	125.04
24	c	504	CLA	CMC-C2C-C1C	2.95	129.53	125.04
24	b	614	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
29	d	408	PL9	C15-C14-C16	2.95	120.23	115.27
24	B	612	CLA	CHD-C1D-ND	-2.95	121.75	124.45
24	B	616	CLA	O2A-CGA-O1A	-2.95	116.16	123.59
24	b	614	CLA	C1C-C2C-C3C	-2.95	103.86	106.96
24	C	515	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
26	K	102	BCR	C10-C11-C12	-2.94	114.03	123.22
24	b	610	CLA	C1-C2-C3	-2.94	120.95	126.04
24	B	605	CLA	O2A-CGA-CBA	2.94	121.14	111.91
25	A	408	PHO	C1A-C2A-C3A	-2.94	100.04	102.84
24	C	509	CLA	CMC-C2C-C1C	2.94	129.52	125.04
26	c	517	BCR	C7-C8-C9	-2.94	121.79	126.23
25	A	408	PHO	C4A-C3A-C2A	-2.94	100.04	102.84
24	d	406	CLA	C1D-CHD-C4C	-2.94	119.72	126.06
24	c	509	CLA	C3C-C4C-NC	2.94	113.87	110.57
24	c	508	CLA	O2A-CGA-O1A	-2.94	116.17	123.59
24	b	606	CLA	CMB-C2B-C3B	2.94	130.17	124.68
24	B	607	CLA	CHD-C1D-ND	-2.94	121.75	124.45
24	B	616	CLA	CMC-C2C-C1C	2.94	129.51	125.04
24	c	512	CLA	C3C-C4C-NC	2.94	113.86	110.57
24	B	608	CLA	O2A-CGA-O1A	-2.93	116.19	123.59
24	A	406	CLA	C4C-C3C-C2C	-2.93	102.62	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	409	CLA	O2A-CGA-O1A	-2.93	116.19	123.59
27	A	415	SQD	O48-C23-O10	-2.93	116.20	123.59
26	k	103	BCR	C24-C23-C22	-2.93	121.81	126.23
24	c	509	CLA	C4-C3-C5	2.93	120.20	115.27
37	C	520	DGD	O3G-C3G-C2G	-2.93	103.84	110.90
24	c	514	CLA	CBA-CAA-C2A	-2.93	105.22	113.86
24	c	515	CLA	C3B-C4B-NB	2.93	112.99	109.21
28	C	533	LMG	O6-C5-C4	2.92	115.00	109.69
24	b	619	CLA	C1-C2-C3	-2.92	120.99	126.04
24	b	618	CLA	C3C-C4C-NC	2.92	113.85	110.57
24	c	508	CLA	C1-C2-C3	-2.92	120.99	126.04
24	B	612	CLA	O2A-CGA-O1A	-2.92	116.22	123.59
24	a	409	CLA	CAA-C2A-C3A	-2.92	104.79	112.78
25	a	412	PHO	C1A-C2A-C3A	-2.92	100.06	102.84
24	d	405	CLA	CAA-C2A-C3A	-2.91	104.80	112.78
24	A	406	CLA	C4-C3-C5	2.91	120.17	115.27
26	c	517	BCR	C38-C26-C25	-2.91	121.26	124.53
24	c	508	CLA	C3B-C4B-NB	2.91	112.98	109.21
24	b	612	CLA	C1C-C2C-C3C	-2.91	103.90	106.96
24	a	413	CLA	C4-C3-C5	2.91	120.17	115.27
24	a	411	CLA	CAA-C2A-C3A	-2.91	104.81	112.78
24	b	614	CLA	CHD-C1D-ND	-2.91	121.78	124.45
24	B	617	CLA	C2C-C1C-NC	2.91	112.69	109.97
29	D	408	PL9	C10-C9-C11	2.91	120.16	115.27
24	b	614	CLA	C1-C2-C3	-2.90	121.02	126.04
24	d	405	CLA	C3B-C4B-NB	2.90	112.97	109.21
24	c	511	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
24	C	503	CLA	C3C-C4C-NC	2.90	113.83	110.57
24	C	511	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
24	B	610	CLA	CHD-C1D-ND	-2.90	121.79	124.45
26	K	102	BCR	C33-C5-C6	-2.90	121.27	124.53
24	B	612	CLA	C1C-C2C-C3C	-2.90	103.91	106.96
24	b	619	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
36	B	625	HTG	C6-C5-C4	-2.90	106.22	113.00
24	B	611	CLA	C1-O2A-CGA	2.90	124.04	116.44
24	a	409	CLA	CHD-C1D-ND	-2.90	121.79	124.45
32	b	625	LMT	O5B-C1B-C2B	2.89	116.47	110.35
24	b	609	CLA	O2A-CGA-O1A	-2.89	116.29	123.59
24	c	511	CLA	CMC-C2C-C1C	2.89	129.44	125.04
24	D	406	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
24	c	505	CLA	CHD-C1D-ND	-2.89	121.80	124.45
42	v	201	HEC	CBA-CAA-C2A	-2.89	107.74	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	607	CLA	O2A-CGA-CBA	2.89	120.97	111.91
24	c	513	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
24	c	509	CLA	C3B-C4B-NB	2.89	112.94	109.21
24	B	617	CLA	C3C-C4C-NC	2.89	113.81	110.57
24	b	610	CLA	C3B-C4B-NB	2.88	112.94	109.21
24	b	609	CLA	C1D-CHD-C4C	-2.88	119.84	126.06
24	C	507	CLA	C1D-CHD-C4C	-2.88	119.84	126.06
24	b	613	CLA	CMA-C3A-C4A	-2.88	104.03	111.77
27	A	411	SQD	C45-O47-C7	-2.88	110.70	117.79
24	d	406	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
28	i	101	LMG	C7-O1-C1	-2.88	108.12	113.74
26	C	517	BCR	C8-C7-C6	-2.87	119.13	127.20
26	d	407	BCR	C29-C30-C25	2.87	114.90	110.48
24	b	612	CLA	O2D-CGD-CBD	2.87	116.37	111.27
42	V	201	HEC	CBD-CAD-C3D	-2.87	107.72	112.62
24	C	507	CLA	CMA-C3A-C4A	-2.87	104.06	111.77
25	A	408	PHO	CMB-C2B-C3B	2.87	130.04	124.68
29	a	417	PL9	C53-C6-C1	2.87	120.85	114.99
24	b	618	CLA	C1D-CHD-C4C	-2.86	119.88	126.06
24	B	605	CLA	C4C-C3C-C2C	-2.86	102.72	106.90
24	C	508	CLA	C1D-CHD-C4C	-2.86	119.89	126.06
32	B	638	LMT	C1'-C2'-C3'	2.86	115.95	110.00
24	C	503	CLA	CMC-C2C-C1C	2.86	129.39	125.04
24	b	614	CLA	CAA-C2A-C3A	-2.86	104.96	112.78
24	a	410	CLA	C1-C2-C3	-2.86	121.10	126.04
37	h	102	DGD	O1G-C1A-O1A	-2.85	116.39	123.59
24	B	616	CLA	C3B-C4B-NB	2.85	112.90	109.21
24	c	509	CLA	CMC-C2C-C1C	2.85	129.38	125.04
24	b	612	CLA	C4-C3-C5	2.85	120.07	115.27
24	d	405	CLA	O2A-CGA-CBA	2.85	120.85	111.91
26	b	621	BCR	C33-C5-C6	-2.85	121.33	124.53
24	C	514	CLA	CMB-C2B-C3B	2.85	130.01	124.68
24	B	606	CLA	C3B-C4B-NB	2.85	112.89	109.21
24	C	510	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
24	B	617	CLA	C4A-NA-C1A	2.84	107.98	106.71
27	f	802	SQD	C3-C4-C5	2.84	115.31	110.24
24	B	614	CLA	C3B-C4B-NB	2.84	112.89	109.21
24	c	514	CLA	C1-O2A-CGA	2.84	123.91	116.44
28	Z	101	LMG	O8-C28-C29	2.84	120.83	111.91
24	c	505	CLA	C1-C2-C3	-2.84	121.13	126.04
24	A	406	CLA	CMC-C2C-C1C	2.84	129.37	125.04
24	A	409	CLA	CMB-C2B-C3B	2.84	130.00	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	604	CLA	C4-C3-C5	2.84	120.05	115.27
24	a	409	CLA	CAC-C3C-C4C	2.84	128.50	124.81
26	c	517	BCR	C33-C5-C6	-2.84	121.34	124.53
26	K	101	BCR	C8-C7-C6	-2.83	119.24	127.20
24	C	515	CLA	CAA-C2A-C3A	-2.83	105.02	112.78
24	B	605	CLA	CMC-C2C-C1C	2.83	129.35	125.04
24	c	507	CLA	C1D-CHD-C4C	-2.83	119.95	126.06
24	c	514	CLA	CHD-C1D-ND	-2.83	121.85	124.45
24	b	609	CLA	CHA-C1A-NA	-2.83	119.91	126.40
24	C	508	CLA	C3B-C4B-NB	2.83	112.87	109.21
24	B	610	CLA	CAA-C2A-C3A	-2.83	105.03	112.78
24	c	506	CLA	CMC-C2C-C1C	2.83	129.35	125.04
24	a	409	CLA	CMB-C2B-C3B	2.83	129.97	124.68
24	C	508	CLA	C4-C3-C5	2.83	120.03	115.27
24	d	405	CLA	C1D-CHD-C4C	-2.83	119.95	126.06
24	c	514	CLA	C3C-C4C-NC	2.83	113.74	110.57
24	B	618	CLA	O2A-CGA-CBA	2.83	120.78	111.91
24	b	612	CLA	C3B-C4B-NB	2.83	112.86	109.21
24	c	515	CLA	CAC-C3C-C4C	2.83	128.48	124.81
24	B	612	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
24	b	605	CLA	C4C-C3C-C2C	-2.82	102.78	106.90
24	B	617	CLA	C4-C3-C5	2.82	120.02	115.27
24	a	410	CLA	CHD-C4C-NC	2.82	128.65	124.20
26	K	101	BCR	C38-C26-C25	-2.82	121.36	124.53
24	b	617	CLA	C1-O2A-CGA	2.82	123.85	116.44
29	d	408	PL9	C37-C38-C39	-2.82	120.87	127.66
40	H	103	RRX	C31-C1-C32	-2.82	99.87	108.53
24	b	617	CLA	CAC-C3C-C4C	2.82	128.47	124.81
24	c	504	CLA	CHA-C1A-NA	-2.82	119.95	126.40
24	B	607	CLA	C1-C2-C3	-2.82	121.17	126.04
24	c	504	CLA	C3B-C4B-NB	2.82	112.85	109.21
29	D	408	PL9	C51-C49-C50	2.81	120.81	114.60
24	d	405	CLA	C4-C3-C5	2.81	120.00	115.27
24	B	615	CLA	CMA-C3A-C4A	-2.81	104.22	111.77
24	a	411	CLA	C4-C3-C5	2.81	120.00	115.27
24	b	619	CLA	C3B-C4B-NB	2.81	112.84	109.21
38	D	411	LHG	O7-C7-C8	2.81	117.55	111.50
24	B	603	CLA	C4C-C3C-C2C	-2.81	102.81	106.90
24	B	611	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
24	B	609	CLA	C4-C3-C5	2.80	119.99	115.27
29	A	413	PL9	C25-C24-C26	2.80	119.99	115.27
24	C	514	CLA	C4-C3-C5	2.80	119.99	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	D	412	LHG	O8-C23-C24	2.80	120.71	111.91
27	f	802	SQD	O48-C23-C24	2.80	120.70	111.91
37	H	104	DGD	O2G-C1B-C2B	2.80	117.54	111.50
24	B	610	CLA	C3B-C4B-NB	2.80	112.83	109.21
26	A	410	BCR	C15-C14-C13	-2.80	123.31	127.31
24	c	509	CLA	CBA-CAA-C2A	-2.80	105.59	113.86
24	a	410	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
24	B	605	CLA	O2A-CGA-O1A	-2.80	116.53	123.59
24	D	406	CLA	CMB-C2B-C3B	2.80	129.91	124.68
24	b	607	CLA	C3C-C4C-NC	2.80	113.71	110.57
24	a	409	CLA	O2D-CGD-CBD	2.79	116.23	111.27
24	b	610	CLA	O2A-CGA-O1A	-2.79	116.54	123.59
24	d	406	CLA	CMB-C2B-C3B	2.79	129.90	124.68
28	z	101	LMG	C1-C2-C3	2.79	115.81	110.00
24	d	406	CLA	O2A-CGA-O1A	-2.79	116.55	123.59
26	K	102	BCR	C24-C23-C22	-2.79	122.02	126.23
39	e	102	HEM	CHA-C4D-ND	2.79	127.82	124.38
24	c	507	CLA	CBC-CAC-C3C	-2.79	104.75	112.43
24	B	604	CLA	C1D-CHD-C4C	-2.78	120.05	126.06
24	D	401	CLA	O2A-CGA-O1A	-2.78	116.57	123.59
24	c	507	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
24	B	604	CLA	CAC-C3C-C4C	2.78	128.42	124.81
24	c	503	CLA	CBC-CAC-C3C	-2.78	104.76	112.43
24	b	605	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
24	B	604	CLA	CMA-C3A-C4A	-2.78	104.30	111.77
24	B	617	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
37	C	518	DGD	C3G-C2G-C1G	-2.78	105.21	111.79
24	A	406	CLA	O2A-CGA-O1A	-2.78	116.58	123.59
24	a	410	CLA	CMB-C2B-C3B	2.78	129.88	124.68
24	c	512	CLA	CBC-CAC-C3C	-2.78	104.77	112.43
24	a	411	CLA	C1D-CHD-C4C	-2.78	120.07	126.06
24	C	512	CLA	O1D-CGD-CBD	-2.78	118.80	124.48
24	D	405	CLA	C4-C3-C5	2.78	119.94	115.27
24	B	608	CLA	CHA-C1A-NA	-2.78	120.04	126.40
26	B	619	BCR	C7-C8-C9	-2.77	122.05	126.23
24	B	608	CLA	CMB-C2B-C3B	2.77	129.86	124.68
24	b	613	CLA	C4A-NA-C1A	2.77	107.95	106.71
25	a	412	PHO	CMC-C2C-C3C	2.77	130.16	124.94
24	d	406	CLA	C4-C3-C5	2.77	119.93	115.27
28	b	624	LMG	O7-C10-O9	-2.77	117.01	123.70
24	c	508	CLA	CAA-C2A-C3A	-2.77	105.20	112.78
24	B	606	CLA	C3C-C4C-NC	2.77	113.67	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	z	101	LMG	C7-O1-C1	-2.77	108.33	113.74
40	H	103	RRX	O2-C28-C29	2.77	115.30	109.80
27	A	415	SQD	C1-C2-C3	-2.77	104.24	110.00
24	B	604	CLA	CMA-C3A-C2A	-2.76	102.68	113.83
24	c	512	CLA	CMA-C3A-C4A	-2.76	104.34	111.77
36	B	625	HTG	C1-O5-C5	2.76	117.68	112.58
24	b	615	CLA	C3B-C4B-NB	2.76	112.78	109.21
24	B	613	CLA	C3B-C4B-NB	2.76	112.78	109.21
24	b	615	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
26	d	407	BCR	C33-C5-C6	-2.76	121.43	124.53
40	H	103	RRX	C38-C26-C25	2.76	127.63	124.53
24	B	616	CLA	CMA-C3A-C2A	-2.76	102.69	113.83
26	b	622	BCR	C28-C27-C26	-2.76	109.15	114.08
36	H	101	HTG	O5-C5-C4	2.75	114.70	109.69
24	c	503	CLA	C4C-C3C-C2C	-2.75	102.88	106.90
24	B	606	CLA	O1D-CGD-CBD	-2.75	118.85	124.48
24	b	612	CLA	O2A-CGA-O1A	-2.75	116.65	123.59
24	c	514	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
24	b	620	CLA	CBC-CAC-C3C	-2.75	104.85	112.43
29	a	417	PL9	C17-C18-C19	-2.75	121.04	127.66
25	d	401	PHO	O2D-CGD-O1D	-2.75	118.47	123.84
24	D	406	CLA	O2A-CGA-O1A	-2.75	116.66	123.59
24	B	615	CLA	CBC-CAC-C3C	-2.75	104.86	112.43
26	C	516	BCR	C16-C17-C18	-2.75	123.39	127.31
24	b	615	CLA	CHC-C1C-C2C	-2.75	119.13	126.72
32	D	402	LMT	O5'-C5'-C4'	2.74	115.54	109.75
24	b	610	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
29	A	413	PL9	C42-C43-C44	-2.74	121.06	127.66
38	d	411	LHG	O8-C23-O10	-2.74	116.67	123.59
24	C	513	CLA	CBC-CAC-C3C	-2.74	104.87	112.43
24	b	620	CLA	C2C-C1C-NC	2.74	112.54	109.97
24	d	406	CLA	CMC-C2C-C1C	2.74	129.21	125.04
36	c	524	HTG	C1-O5-C5	2.74	117.63	112.58
24	B	611	CLA	C3B-C4B-NB	2.73	112.74	109.21
37	c	519	DGD	O1G-C1A-C2A	2.73	120.48	111.91
24	b	614	CLA	CMA-C3A-C4A	-2.73	104.43	111.77
24	C	506	CLA	C11-C10-C8	-2.73	107.09	115.92
24	c	513	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
24	c	503	CLA	CAC-C3C-C4C	2.73	128.35	124.81
24	c	512	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
24	a	409	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
36	c	524	HTG	O5-C5-C4	2.72	114.64	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	608	CLA	CMC-C2C-C1C	2.72	129.19	125.04
26	b	623	BCR	C2-C1-C6	2.71	114.66	110.48
24	a	410	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
27	F	101	SQD	O9-S-C6	2.71	110.16	106.94
24	D	406	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
24	b	613	CLA	C4C-C3C-C2C	-2.71	102.94	106.90
37	H	104	DGD	O1G-C1A-C2A	2.71	120.42	111.91
24	a	411	CLA	CHC-C1C-C2C	-2.71	119.22	126.72
24	c	509	CLA	CHA-C1A-NA	-2.71	120.19	126.40
24	c	508	CLA	C4-C3-C5	2.71	119.83	115.27
24	c	504	CLA	O2A-CGA-CBA	2.71	120.40	111.91
24	B	608	CLA	C6-C7-C8	-2.71	107.17	115.92
24	B	617	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
36	b	627	HTG	C1-O5-C5	2.71	117.57	112.58
24	c	510	CLA	C3B-C4B-NB	2.70	112.71	109.21
36	b	628	HTG	C1-C2-C3	2.70	115.93	110.59
29	A	413	PL9	C37-C36-C34	-2.70	104.09	112.98
24	b	619	CLA	CHD-C4C-NC	2.70	128.46	124.20
24	A	405	CLA	CMA-C3A-C4A	-2.70	104.52	111.77
24	C	511	CLA	O2A-CGA-CBA	2.70	120.38	111.91
24	B	613	CLA	O2A-CGA-O1A	-2.70	116.79	123.59
24	C	505	CLA	CHA-C1A-NA	-2.69	120.23	126.40
24	c	504	CLA	C4-C3-C5	2.69	119.80	115.27
24	a	409	CLA	CMA-C3A-C4A	-2.69	104.54	111.77
24	b	612	CLA	C1D-CHD-C4C	-2.69	120.25	126.06
27	b	601	SQD	O7-S-C6	2.69	110.14	106.94
24	B	617	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
24	B	606	CLA	O2A-CGA-O1A	-2.69	116.81	123.59
37	c	520	DGD	O1G-C1A-C2A	2.69	120.34	111.91
24	b	607	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
37	c	518	DGD	O2G-C1B-O1B	-2.69	117.21	123.70
38	d	410	LHG	O7-C7-C8	2.69	117.29	111.50
38	E	101	LHG	C5-O7-C7	-2.68	111.19	117.79
32	B	624	LMT	C1B-O5B-C5B	2.68	118.95	113.69
24	C	513	CLA	CMC-C2C-C1C	2.68	129.12	125.04
24	D	406	CLA	C3B-C4B-NB	2.68	112.67	109.21
24	b	611	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
24	a	410	CLA	O2A-CGA-CBA	2.68	120.32	111.91
24	B	616	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
24	A	409	CLA	CMC-C2C-C1C	2.68	129.12	125.04
24	c	513	CLA	C3C-C4C-NC	2.68	113.57	110.57
24	c	509	CLA	O2D-CGD-O1D	-2.68	118.60	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	619	CLA	O2D-CGD-O1D	-2.68	118.61	123.84
24	C	508	CLA	CBC-CAC-C3C	-2.68	105.06	112.43
24	c	504	CLA	C3C-C4C-NC	2.67	113.57	110.57
24	c	515	CLA	CHD-C1D-ND	-2.67	122.00	124.45
24	C	506	CLA	C1-O2A-CGA	2.67	123.46	116.44
24	A	406	CLA	C1-C2-C3	-2.67	121.42	126.04
40	h	101	RRX	C39-C30-C25	2.67	114.63	110.30
24	b	618	CLA	O2A-CGA-O1A	-2.67	116.86	123.59
24	c	514	CLA	CMB-C2B-C3B	2.67	129.66	124.68
24	C	510	CLA	C4-C3-C5	2.66	119.75	115.27
24	d	405	CLA	CHC-C1C-C2C	-2.66	119.35	126.72
24	B	610	CLA	CMA-C3A-C2A	-2.66	103.09	113.83
24	c	515	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
27	A	415	SQD	O8-S-C6	2.66	109.98	105.74
26	t	101	BCR	C11-C10-C9	-2.66	123.51	127.31
25	d	401	PHO	CMC-C2C-C3C	2.66	129.96	124.94
24	c	503	CLA	CMB-C2B-C3B	2.66	129.66	124.68
28	c	522	LMG	C8-O7-C10	-2.66	111.24	117.79
24	c	505	CLA	C4A-NA-C1A	2.66	107.90	106.71
29	a	417	PL9	C40-C39-C41	2.66	119.75	115.27
28	z	101	LMG	C9-C8-C7	-2.66	105.50	111.79
24	B	616	CLA	CMB-C2B-C3B	2.66	129.65	124.68
24	d	406	CLA	C3C-C4C-NC	2.66	113.55	110.57
24	B	608	CLA	C4C-C3C-C2C	-2.66	103.03	106.90
24	B	618	CLA	O2D-CGD-O1D	-2.66	118.65	123.84
24	d	405	CLA	O2A-CGA-O1A	-2.65	116.89	123.59
24	c	505	CLA	CBC-CAC-C3C	-2.65	105.11	112.43
24	c	506	CLA	C4C-C3C-C2C	-2.65	103.03	106.90
24	C	509	CLA	C4C-C3C-C2C	-2.65	103.03	106.90
24	a	411	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
29	a	417	PL9	C45-C44-C46	2.65	119.73	115.27
29	D	408	PL9	C53-C6-C1	2.65	120.41	114.99
24	c	504	CLA	C4C-C3C-C2C	-2.65	103.04	106.90
24	A	406	CLA	CAA-C2A-C3A	-2.65	105.53	112.78
26	T	101	BCR	C21-C20-C19	-2.65	114.95	123.22
24	c	513	CLA	CMC-C2C-C1C	2.65	129.07	125.04
26	C	517	BCR	C33-C5-C6	-2.64	121.56	124.53
24	c	513	CLA	C1D-CHD-C4C	-2.64	120.35	126.06
24	B	613	CLA	C17-C16-C15	-2.64	101.09	113.24
26	K	102	BCR	C11-C10-C9	-2.64	123.54	127.31
26	k	103	BCR	C33-C5-C6	-2.64	121.56	124.53
24	a	410	CLA	O2A-CGA-O1A	-2.64	116.93	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	605	CLA	CMB-C2B-C3B	2.64	129.62	124.68
26	K	101	BCR	C37-C22-C23	2.64	122.23	118.08
24	b	617	CLA	O2A-CGA-CBA	2.64	120.18	111.91
24	C	503	CLA	C4C-C3C-C2C	-2.64	103.06	106.90
24	b	614	CLA	C4-C3-C5	2.63	119.70	115.27
27	a	415	SQD	O9-S-C6	2.63	110.07	106.94
26	A	410	BCR	C33-C5-C6	-2.63	121.57	124.53
27	A	411	SQD	O8-S-C6	2.63	109.93	105.74
24	b	610	CLA	C4-C3-C5	2.63	119.70	115.27
29	A	413	PL9	C45-C44-C46	2.63	119.70	115.27
26	k	102	BCR	C16-C17-C18	-2.63	123.56	127.31
24	b	615	CLA	C4A-NA-C1A	2.63	107.89	106.71
24	B	618	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
24	C	510	CLA	CMB-C2B-C3B	2.63	129.59	124.68
24	c	506	CLA	O1D-CGD-CBD	-2.63	119.11	124.48
24	b	605	CLA	CBC-CAC-C3C	-2.63	105.19	112.43
24	b	611	CLA	C3B-C4B-NB	2.63	112.61	109.21
24	D	405	CLA	CAC-C3C-C4C	2.63	128.22	124.81
29	a	417	PL9	C35-C34-C36	2.62	119.69	115.27
24	c	508	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
24	C	515	CLA	O2A-CGA-CBA	2.62	120.14	111.91
24	b	618	CLA	CMC-C2C-C1C	2.62	129.03	125.04
24	C	509	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
24	c	511	CLA	CBC-CAC-C3C	-2.62	105.20	112.43
26	k	103	BCR	C11-C10-C9	-2.62	123.57	127.31
24	C	508	CLA	C4C-C3C-C2C	-2.62	103.08	106.90
24	c	505	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
24	C	506	CLA	CAA-C2A-C3A	-2.62	105.61	112.78
24	a	411	CLA	CMB-C2B-C3B	2.62	129.58	124.68
25	a	412	PHO	O2D-CGD-O1D	-2.62	118.72	123.84
24	b	607	CLA	CMA-C3A-C2A	-2.62	103.27	113.83
24	B	614	CLA	O1D-CGD-CBD	-2.62	119.13	124.48
29	a	417	PL9	C25-C24-C26	2.62	119.67	115.27
29	a	417	PL9	C12-C13-C14	-2.62	121.36	127.66
24	a	413	CLA	CED-O2D-CGD	2.62	121.85	115.94
29	d	408	PL9	C36-C37-C38	-2.61	103.30	111.88
24	b	616	CLA	O2A-C1-C2	-2.61	101.78	108.64
24	c	515	CLA	C4-C3-C5	2.61	119.66	115.27
26	k	103	BCR	C20-C21-C22	-2.61	123.59	127.31
24	b	606	CLA	C3B-C4B-NB	2.61	112.58	109.21
27	f	802	SQD	C44-O6-C1	-2.61	108.65	113.74
37	C	519	DGD	O2G-C1B-O1B	-2.61	117.40	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	517	BCR	C21-C20-C19	-2.61	115.09	123.22
24	c	507	CLA	C3B-C4B-NB	2.60	112.58	109.21
26	B	620	BCR	C28-C27-C26	-2.60	109.43	114.08
29	D	408	PL9	C37-C38-C39	-2.60	121.39	127.66
24	D	406	CLA	CMC-C2C-C1C	2.60	129.00	125.04
24	c	504	CLA	CAC-C3C-C4C	2.60	128.19	124.81
24	d	405	CLA	CMA-C3A-C4A	-2.60	104.78	111.77
28	z	101	LMG	C1-O6-C5	2.60	118.80	113.69
24	b	608	CLA	C1D-CHD-C4C	-2.60	120.44	126.06
26	c	517	BCR	C3-C4-C5	-2.60	109.43	114.08
24	a	413	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
38	D	411	LHG	O8-C23-O10	-2.60	117.03	123.59
24	B	605	CLA	CMA-C3A-C2A	-2.60	103.35	113.83
24	B	611	CLA	CHA-C1A-NA	-2.60	120.45	126.40
24	b	620	CLA	C3B-C4B-NB	2.60	112.57	109.21
24	D	405	CLA	CMA-C3A-C4A	-2.60	104.80	111.77
24	C	510	CLA	O2A-CGA-O1A	-2.60	117.04	123.59
24	C	508	CLA	C3C-C4C-NC	2.59	113.48	110.57
24	c	510	CLA	O2A-CGA-O1A	-2.59	117.05	123.59
24	B	605	CLA	CBC-CAC-C3C	-2.59	105.28	112.43
27	a	401	SQD	O48-C23-O10	-2.59	117.05	123.59
38	D	410	LHG	O8-C23-C24	2.59	120.03	111.91
24	c	504	CLA	C4A-NA-C1A	2.59	107.87	106.71
24	a	411	CLA	C1-C2-C3	-2.59	121.57	126.04
37	H	104	DGD	O1G-C1A-O1A	-2.59	117.06	123.59
32	a	421	LMT	C1B-C2B-C3B	2.59	115.39	110.00
24	C	512	CLA	CMB-C2B-C3B	2.59	129.52	124.68
36	H	101	HTG	C6-C5-C4	-2.59	106.94	113.00
24	D	406	CLA	C1-C2-C3	-2.59	121.57	126.04
24	A	409	CLA	CMA-C3A-C2A	-2.59	103.40	113.83
27	A	411	SQD	O47-C7-O49	-2.59	117.45	123.70
24	B	616	CLA	OBD-CAD-C3D	-2.59	122.30	128.52
24	c	515	CLA	O2A-CGA-CBA	2.59	120.02	111.91
27	B	622	SQD	O5-C5-C4	2.58	114.39	109.69
26	C	517	BCR	C2-C1-C6	2.58	114.46	110.48
24	B	604	CLA	C3B-C4B-NB	2.58	112.54	109.21
25	A	407	PHO	O2D-CGD-O1D	-2.58	118.80	123.84
24	D	405	CLA	C1D-CHD-C4C	-2.58	120.50	126.06
24	b	612	CLA	O2A-CGA-CBA	2.58	119.99	111.91
26	K	101	BCR	C15-C14-C13	-2.57	123.64	127.31
24	b	608	CLA	O2A-CGA-O1A	-2.57	117.10	123.59
24	C	515	CLA	O2D-CGD-O1D	-2.57	118.81	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	614	CLA	C4-C3-C5	2.57	119.60	115.27
28	d	412	LMG	O7-C10-C11	2.57	117.04	111.50
24	C	504	CLA	C3B-C4B-NB	2.57	112.53	109.21
24	A	405	CLA	CHC-C1C-C2C	-2.57	119.62	126.72
32	b	629	LMT	O5'-C5'-C4'	2.57	114.36	109.69
24	B	618	CLA	CAC-C3C-C4C	2.57	128.14	124.81
27	a	415	SQD	O48-C23-C24	2.57	119.96	111.91
24	c	506	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
24	b	611	CLA	CAA-C2A-C3A	-2.56	105.75	112.78
24	c	508	CLA	O2A-CGA-CBA	2.56	119.96	111.91
26	K	101	BCR	C2-C1-C6	2.56	114.43	110.48
29	D	408	PL9	C40-C39-C38	-2.56	117.10	123.68
24	B	605	CLA	C1-O2A-CGA	2.56	123.16	116.44
24	C	514	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
27	b	601	SQD	O47-C7-O49	-2.56	117.52	123.70
26	b	621	BCR	C2-C1-C6	2.56	114.42	110.48
32	b	626	LMT	O5B-C5B-C4B	2.56	114.34	109.69
28	C	521	LMG	C8-O7-C10	-2.56	111.50	117.79
24	a	410	CLA	CMA-C3A-C4A	-2.56	104.90	111.77
24	D	405	CLA	CMC-C2C-C1C	2.56	128.93	125.04
24	c	514	CLA	C3B-C4B-NB	2.55	112.51	109.21
24	A	405	CLA	CMB-C2B-C3B	2.55	129.46	124.68
24	B	612	CLA	C3B-C4B-NB	2.55	112.51	109.21
24	d	406	CLA	CBC-CAC-C3C	-2.55	105.39	112.43
24	b	608	CLA	C4C-C3C-C2C	-2.55	103.18	106.90
24	c	513	CLA	C3B-C4B-NB	2.55	112.51	109.21
24	B	603	CLA	O2A-CGA-CBA	2.55	119.92	111.91
24	b	610	CLA	CHA-C1A-NA	-2.55	120.55	126.40
24	C	515	CLA	C1-C2-C3	-2.55	121.63	126.04
24	a	411	CLA	O2A-CGA-CBA	2.55	119.92	111.91
24	c	513	CLA	C6-C5-C3	-2.55	106.77	113.45
24	c	510	CLA	CBC-CAC-C3C	-2.55	105.40	112.43
24	c	510	CLA	C1-O2A-CGA	2.55	123.14	116.44
26	C	516	BCR	C11-C10-C9	-2.55	123.67	127.31
26	c	517	BCR	C15-C14-C13	-2.55	123.67	127.31
26	k	102	BCR	C10-C11-C12	-2.55	115.26	123.22
28	D	413	LMG	O8-C28-O10	-2.55	117.16	123.59
32	D	409	LMT	C1B-C2B-C3B	2.55	115.30	110.00
37	d	416	DGD	C1D-O6D-C5D	2.55	118.05	113.67
29	D	408	PL9	C35-C34-C36	2.55	119.56	115.27
24	B	616	CLA	O2A-C1-C2	2.55	115.32	108.64
28	z	101	LMG	O6-C1-C2	2.54	115.73	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	615	CLA	C4C-C3C-C2C	-2.54	103.19	106.90
24	a	413	CLA	CAC-C3C-C4C	2.54	128.11	124.81
25	a	412	PHO	C4-C3-C5	2.54	119.55	115.27
24	c	505	CLA	CAC-C3C-C4C	2.54	128.11	124.81
29	A	413	PL9	C10-C9-C11	2.54	119.54	115.27
24	b	618	CLA	O2A-CGA-CBA	2.54	119.88	111.91
24	B	614	CLA	CAC-C3C-C4C	2.54	128.10	124.81
29	D	408	PL9	C22-C23-C24	-2.54	121.55	127.66
38	L	101	LHG	O8-C23-C24	2.54	119.86	111.91
24	C	514	CLA	C1-C2-C3	-2.53	121.66	126.04
24	a	410	CLA	C4-C3-C5	2.53	119.53	115.27
38	d	409	LHG	O7-C7-C8	2.53	116.96	111.50
24	b	608	CLA	O2A-CGA-CBA	2.53	119.86	111.91
24	c	505	CLA	O2A-CGA-O1A	-2.53	117.20	123.59
32	b	629	LMT	C3'-C4'-C5'	2.53	114.75	110.24
26	t	101	BCR	C38-C26-C25	-2.53	121.69	124.53
24	C	515	CLA	CBC-CAC-C3C	-2.53	105.46	112.43
39	e	102	HEM	CHD-C1D-ND	2.53	127.18	124.43
24	a	413	CLA	O2A-CGA-O1A	-2.53	117.21	123.59
24	b	608	CLA	CHA-C1A-NA	-2.53	120.61	126.40
24	c	507	CLA	CMC-C2C-C1C	2.53	128.89	125.04
24	C	506	CLA	C3C-C4C-NC	2.52	113.40	110.57
28	b	624	LMG	O8-C28-C29	2.52	119.81	111.91
24	B	607	CLA	C3B-C4B-NB	2.52	112.47	109.21
26	T	101	BCR	C29-C28-C27	-2.52	105.75	111.38
24	D	405	CLA	CHC-C1C-C2C	-2.51	119.77	126.72
24	c	510	CLA	CMB-C2B-C3B	2.51	129.38	124.68
32	b	626	LMT	C1-O1'-C1'	-2.51	109.68	113.84
24	b	613	CLA	C4-C3-C5	2.51	119.49	115.27
24	b	608	CLA	C16-C15-C13	-2.51	107.81	115.92
26	T	101	BCR	C28-C27-C26	-2.51	109.60	114.08
24	c	512	CLA	CAC-C3C-C4C	2.51	128.06	124.81
24	B	607	CLA	CMA-C3A-C2A	-2.51	103.72	113.83
24	B	613	CLA	CHC-C1C-C2C	-2.50	119.79	126.72
24	D	401	CLA	CHC-C1C-C2C	-2.50	119.79	126.72
38	E	101	LHG	O8-C23-C24	2.50	119.77	111.91
37	C	519	DGD	O1G-C1A-C2A	2.50	119.76	111.91
24	B	604	CLA	CBC-CAC-C3C	-2.50	105.53	112.43
24	b	618	CLA	CAA-C2A-C3A	-2.50	105.93	112.78
24	a	413	CLA	CMA-C3A-C4A	-2.50	105.06	111.77
24	B	612	CLA	CMB-C2B-C3B	2.50	129.35	124.68
26	B	619	BCR	C29-C30-C25	2.50	114.32	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	610	CLA	CAC-C3C-C4C	2.50	128.05	124.81
27	B	622	SQD	O48-C23-C24	2.50	119.74	111.91
37	c	520	DGD	O2G-C1B-C2B	2.49	116.88	111.50
29	d	408	PL9	C31-C32-C33	-2.49	103.68	111.88
24	C	509	CLA	CMB-C2B-C3B	2.49	129.34	124.68
26	c	516	BCR	C7-C8-C9	-2.49	122.47	126.23
26	K	102	BCR	C20-C21-C22	-2.49	123.76	127.31
24	C	511	CLA	C4-C3-C5	2.49	119.46	115.27
26	T	101	BCR	C36-C18-C19	2.49	122.00	118.08
38	D	410	LHG	O7-C7-O9	-2.49	117.69	123.70
24	c	506	CLA	C7-C6-C5	-2.49	106.60	113.36
24	C	515	CLA	CMB-C2B-C3B	2.49	129.33	124.68
40	H	103	RRX	C32-C1-C6	-2.49	106.27	110.30
32	B	624	LMT	O1B-C4'-C5'	-2.49	102.64	109.45
24	c	509	CLA	C4C-C3C-C2C	-2.48	103.28	106.90
39	F	102	HEM	CHA-C4D-ND	2.48	127.45	124.38
24	C	510	CLA	CHC-C1C-C2C	-2.48	119.85	126.72
24	B	603	CLA	C3B-C4B-NB	2.48	112.42	109.21
24	b	612	CLA	CAA-C2A-C3A	-2.48	105.98	112.78
24	A	405	CLA	C3B-C4B-NB	2.48	112.42	109.21
24	b	611	CLA	CED-O2D-CGD	2.48	121.55	115.94
40	H	103	RRX	C7-C6-C5	-2.48	115.45	121.46
24	b	611	CLA	CAA-C2A-C1A	-2.48	103.85	111.97
28	B	623	LMG	O8-C28-O10	-2.48	117.33	123.59
24	C	513	CLA	C4-C3-C5	2.48	119.44	115.27
24	B	607	CLA	CHA-C1A-NA	-2.48	120.72	126.40
24	A	409	CLA	CAA-C2A-C3A	-2.48	105.99	112.78
24	B	617	CLA	CHC-C1C-C2C	-2.48	119.87	126.72
36	B	626	HTG	C1-C2-C3	2.48	115.48	110.59
26	t	101	BCR	C15-C16-C17	-2.48	118.40	123.47
26	b	623	BCR	C37-C22-C23	2.47	121.98	118.08
40	h	101	RRX	C40-C30-C29	-2.47	97.94	109.05
38	D	410	LHG	O8-C6-C5	-2.47	101.23	108.43
24	c	505	CLA	C3B-C4B-NB	2.47	112.41	109.21
24	c	510	CLA	CAC-C3C-C2C	2.47	131.76	127.53
24	A	406	CLA	CMA-C3A-C4A	-2.47	105.13	111.77
24	B	611	CLA	C4-C3-C5	2.47	119.43	115.27
24	D	406	CLA	CMA-C3A-C4A	-2.47	105.14	111.77
24	a	409	CLA	CHC-C1C-C2C	-2.47	119.89	126.72
24	b	611	CLA	O2A-CGA-O1A	-2.47	117.36	123.59
24	c	514	CLA	CHA-C1A-NA	-2.47	120.75	126.40
24	C	506	CLA	C4-C3-C5	2.47	119.42	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	t	101	BCR	C29-C28-C27	-2.47	105.86	111.38
24	c	513	CLA	CBC-CAC-C3C	-2.47	105.63	112.43
24	B	613	CLA	CHA-C1A-NA	-2.47	120.75	126.40
24	c	510	CLA	O2A-CGA-CBA	2.47	119.64	111.91
26	A	410	BCR	C31-C1-C6	-2.47	106.30	110.30
24	b	609	CLA	C11-C10-C8	-2.47	107.95	115.92
29	d	408	PL9	C10-C9-C11	2.46	119.42	115.27
24	b	606	CLA	CBC-CAC-C3C	-2.46	105.64	112.43
26	k	102	BCR	C2-C1-C6	2.46	114.27	110.48
24	C	514	CLA	C3B-C4B-NB	2.46	112.39	109.21
24	C	511	CLA	CBC-CAC-C3C	-2.46	105.65	112.43
24	C	512	CLA	CBC-CAC-C3C	-2.46	105.65	112.43
24	b	617	CLA	CMC-C2C-C1C	2.46	128.78	125.04
24	c	508	CLA	CAC-C3C-C4C	2.46	128.00	124.81
24	b	614	CLA	C3B-C4B-NB	2.46	112.39	109.21
24	C	510	CLA	CHA-C1A-NA	-2.46	120.77	126.40
24	b	613	CLA	C3B-C4B-NB	2.46	112.39	109.21
24	B	614	CLA	O2A-CGA-CBA	2.46	119.62	111.91
27	F	101	SQD	O48-C23-C24	2.46	119.61	111.91
24	c	503	CLA	O2A-CGA-O1A	-2.46	117.39	123.59
24	D	401	CLA	O2A-CGA-CBA	2.46	119.61	111.91
24	B	607	CLA	CAA-C2A-C3A	-2.45	106.06	112.78
32	a	421	LMT	C1'-O5'-C5'	2.45	118.50	113.69
24	c	505	CLA	CMC-C2C-C1C	2.45	128.77	125.04
24	b	605	CLA	CAA-C2A-C3A	-2.45	106.06	112.78
24	C	508	CLA	CHC-C1C-C2C	-2.45	119.94	126.72
24	C	514	CLA	CMA-C3A-C4A	-2.45	105.19	111.77
28	c	522	LMG	O8-C28-C29	2.45	119.60	111.91
40	h	101	RRX	C30-C29-C28	-2.45	108.11	113.64
24	B	615	CLA	CMC-C2C-C1C	2.45	128.77	125.04
24	b	613	CLA	CMC-C2C-C1C	2.45	128.77	125.04
24	d	406	CLA	CHC-C1C-C2C	-2.45	119.95	126.72
24	B	618	CLA	C4-C3-C5	2.44	119.38	115.27
24	B	608	CLA	O2A-CGA-CBA	2.44	119.57	111.91
38	a	416	LHG	O8-C23-C24	2.44	119.57	111.91
24	c	506	CLA	CAC-C3C-C4C	2.44	127.98	124.81
24	B	614	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
26	t	101	BCR	C1-C6-C7	2.44	122.69	115.78
24	c	511	CLA	CAC-C3C-C4C	2.44	127.98	124.81
24	B	613	CLA	CMB-C2B-C3B	2.44	129.24	124.68
32	B	638	LMT	C1'-O5'-C5'	2.44	118.48	113.69
24	B	606	CLA	O2A-CGA-CBA	2.44	119.56	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	609	CLA	CMB-C2B-C3B	2.44	129.24	124.68
25	A	407	PHO	CBA-CAA-C2A	-2.43	106.70	113.81
24	a	410	CLA	C6-C5-C3	-2.43	107.07	113.45
24	a	409	CLA	CMC-C2C-C1C	2.43	128.74	125.04
24	B	618	CLA	CHC-C1C-C2C	-2.43	119.99	126.72
26	C	517	BCR	C40-C30-C25	-2.43	106.36	110.30
27	a	401	SQD	O9-S-C6	2.43	109.83	106.94
24	C	514	CLA	OBD-CAD-C3D	-2.43	122.67	128.52
24	D	406	CLA	CAC-C3C-C4C	2.43	127.96	124.81
29	A	413	PL9	C35-C34-C36	2.43	119.36	115.27
26	b	622	BCR	C37-C22-C21	-2.43	119.52	122.92
27	F	101	SQD	O47-C7-O49	-2.43	117.83	123.70
24	d	406	CLA	CAA-C2A-C3A	-2.43	106.13	112.78
24	B	606	CLA	CHC-C1C-C2C	-2.43	120.01	126.72
24	B	609	CLA	CHC-C1C-C2C	-2.43	120.01	126.72
28	C	533	LMG	C3-C4-C5	2.43	114.56	110.24
24	C	512	CLA	O2A-CGA-CBA	2.43	119.52	111.91
24	B	617	CLA	C11-C10-C8	-2.42	108.08	115.92
27	b	601	SQD	O48-C23-O10	-2.42	117.47	123.59
39	e	102	HEM	CBD-CAD-C3D	-2.42	105.89	112.63
24	B	613	CLA	C7-C6-C5	-2.42	106.78	113.36
24	c	515	CLA	CAA-C2A-C3A	-2.42	106.14	112.78
24	c	513	CLA	CHA-C1A-NA	-2.42	120.85	126.40
24	B	612	CLA	CHA-C1A-NA	-2.42	120.85	126.40
32	b	629	LMT	C1-O1'-C1'	-2.42	109.83	113.84
24	D	406	CLA	CAA-C2A-C3A	-2.42	106.16	112.78
32	B	624	LMT	O5B-C5B-C4B	2.42	114.08	109.69
26	a	414	BCR	C7-C8-C9	-2.42	122.58	126.23
24	b	611	CLA	C1D-CHD-C4C	-2.41	120.85	126.06
24	b	619	CLA	CHA-C1A-NA	-2.41	120.87	126.40
24	c	512	CLA	CHC-C1C-C2C	-2.41	120.04	126.72
24	B	617	CLA	C3B-C4B-NB	2.41	112.33	109.21
24	C	505	CLA	CMC-C2C-C1C	2.41	128.71	125.04
37	d	416	DGD	O1G-C1A-C2A	2.41	119.47	111.91
26	K	101	BCR	C10-C11-C12	-2.41	115.70	123.22
24	B	609	CLA	C3C-C4C-NC	2.41	113.27	110.57
24	C	503	CLA	O2A-CGA-O1A	-2.41	117.52	123.59
24	b	615	CLA	CMB-C2B-C3B	2.41	129.18	124.68
24	b	620	CLA	O2A-CGA-CBA	2.41	119.45	111.91
24	D	405	CLA	CMA-C3A-C2A	-2.40	104.14	113.83
24	C	511	CLA	CMC-C2C-C1C	2.40	128.70	125.04
24	b	611	CLA	CAC-C3C-C4C	2.40	127.92	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	610	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
39	F	102	HEM	O2A-CGA-CBA	2.40	121.73	114.03
26	T	101	BCR	C37-C22-C21	-2.40	119.56	122.92
24	C	505	CLA	CAC-C3C-C4C	2.40	127.92	124.81
25	d	401	PHO	C4A-C3A-C2A	-2.40	100.56	102.84
24	c	507	CLA	CHA-C1A-NA	-2.40	120.91	126.40
24	c	514	CLA	CMA-C3A-C4A	-2.39	105.34	111.77
32	a	421	LMT	C1B-O5B-C5B	2.39	118.39	113.69
24	B	613	CLA	C4-C3-C5	2.39	119.29	115.27
24	b	610	CLA	O2A-CGA-CBA	2.39	119.41	111.91
24	b	610	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
24	D	401	CLA	OBD-CAD-C3D	-2.39	122.77	128.52
29	A	413	PL9	C7-C3-C4	2.39	118.82	116.88
29	A	413	PL9	C30-C29-C31	2.39	119.29	115.27
24	C	508	CLA	CHA-C1A-NA	-2.39	120.93	126.40
24	B	606	CLA	C4C-C3C-C2C	-2.39	103.42	106.90
24	B	606	CLA	CHA-C1A-NA	-2.38	120.94	126.40
37	c	518	DGD	C2G-O2G-C1B	-2.38	111.93	117.79
26	B	621	BCR	C38-C26-C25	-2.38	121.86	124.53
24	B	616	CLA	C1-O2A-CGA	2.38	122.68	116.44
32	a	421	LMT	O5B-C1B-C2B	2.38	115.38	110.35
24	C	509	CLA	CHD-C1D-ND	-2.38	122.27	124.45
24	c	505	CLA	C4-C3-C5	2.37	119.27	115.27
28	A	412	LMG	O8-C28-C29	2.37	119.36	111.91
24	C	507	CLA	C4-C3-C5	2.37	119.26	115.27
24	C	504	CLA	CHD-C1D-ND	-2.37	122.28	124.45
24	c	508	CLA	CGD-CBD-CAD	-2.37	103.06	110.73
26	t	101	BCR	C7-C6-C5	-2.37	115.73	121.46
24	B	615	CLA	C1D-CHD-C4C	-2.37	120.95	126.06
24	a	409	CLA	CMA-C3A-C2A	-2.36	104.29	113.83
24	B	604	CLA	O2A-CGA-O1A	-2.36	117.62	123.59
24	B	615	CLA	O2A-CGA-O1A	-2.36	117.62	123.59
26	D	407	BCR	C29-C28-C27	-2.36	106.09	111.38
24	B	608	CLA	CHC-C1C-C2C	-2.36	120.18	126.72
24	C	504	CLA	CHA-C1A-NA	-2.36	120.99	126.40
24	b	618	CLA	CMA-C3A-C2A	-2.36	104.30	113.83
24	b	619	CLA	CAC-C3C-C4C	2.36	127.88	124.81
28	c	522	LMG	O6-C5-C4	2.36	113.98	109.69
26	D	407	BCR	C15-C14-C13	-2.36	123.94	127.31
24	c	510	CLA	C4-C3-C5	2.36	119.24	115.27
24	A	406	CLA	CMB-C2B-C3B	2.36	129.09	124.68
24	C	504	CLA	CMB-C2B-C3B	2.36	129.09	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	407	PHO	CMC-C2C-C3C	2.36	129.39	124.94
24	C	508	CLA	CMC-C2C-C1C	2.36	128.63	125.04
24	B	612	CLA	C4-C3-C5	2.36	119.23	115.27
24	b	613	CLA	CHA-C1A-NA	-2.36	121.00	126.40
24	B	612	CLA	CAA-C2A-C3A	-2.36	106.33	112.78
24	a	413	CLA	O2A-CGA-CBA	2.35	119.29	111.91
24	b	608	CLA	CMB-C2B-C3B	2.35	129.08	124.68
37	h	102	DGD	O1G-C1A-C2A	2.35	119.29	111.91
24	b	619	CLA	C1-O2A-CGA	2.35	122.62	116.44
24	b	606	CLA	CAC-C3C-C2C	2.35	131.55	127.53
24	C	505	CLA	C3B-C4B-NB	2.35	112.25	109.21
24	B	617	CLA	CMB-C2B-C1B	2.35	132.07	128.46
24	B	607	CLA	CMC-C2C-C1C	2.35	128.61	125.04
26	k	103	BCR	C10-C11-C12	-2.35	115.90	123.22
24	d	406	CLA	C4C-C3C-C2C	-2.34	103.48	106.90
24	B	604	CLA	CHA-C1A-NA	-2.34	121.03	126.40
24	b	617	CLA	CMA-C3A-C4A	-2.34	105.48	111.77
24	D	405	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
24	c	512	CLA	O2A-CGA-CBA	2.34	119.26	111.91
24	C	515	CLA	C3B-C4B-NB	2.34	112.24	109.21
24	a	409	CLA	O2A-CGA-CBA	2.34	119.25	111.91
24	B	616	CLA	CBC-CAC-C3C	-2.34	105.98	112.43
24	D	406	CLA	O2A-CGA-CBA	2.34	119.25	111.91
24	B	604	CLA	CMB-C2B-C3B	2.34	129.05	124.68
28	C	533	LMG	O8-C28-C29	2.34	119.24	111.91
24	D	405	CLA	O2A-CGA-CBA	2.34	119.24	111.91
24	C	506	CLA	CHC-C1C-C2C	-2.33	120.26	126.72
29	D	408	PL9	C7-C8-C9	-2.33	122.91	126.79
42	v	201	HEC	O2A-CGA-O1A	-2.33	117.48	123.30
26	b	623	BCR	C16-C17-C18	-2.33	123.98	127.31
24	A	405	CLA	OBD-CAD-C3D	-2.33	122.91	128.52
25	A	408	PHO	O2D-CGD-O1D	-2.33	119.28	123.84
26	D	407	BCR	C39-C30-C25	-2.33	106.52	110.30
25	A	407	PHO	CMA-C3A-C4A	-2.33	109.27	114.38
24	b	614	CLA	CAA-CBA-CGA	-2.33	106.44	113.25
24	B	611	CLA	CMA-C3A-C4A	-2.33	105.51	111.77
38	l	102	LHG	O8-C23-O10	-2.33	117.72	123.59
29	D	408	PL9	C12-C13-C14	-2.33	122.05	127.66
24	c	507	CLA	C11-C10-C8	-2.33	108.39	115.92
24	C	513	CLA	CMB-C2B-C3B	2.32	129.03	124.68
40	h	101	RRX	C40-C30-C25	-2.32	106.53	110.30
27	B	622	SQD	O47-C7-O49	-2.32	118.09	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	517	BCR	C7-C8-C9	-2.32	122.73	126.23
24	b	617	CLA	C1D-CHD-C4C	-2.32	121.05	126.06
24	B	603	CLA	CMC-C2C-C1C	2.32	128.57	125.04
26	a	414	BCR	C37-C22-C21	-2.32	119.67	122.92
24	a	411	CLA	CAC-C3C-C4C	2.32	127.82	124.81
24	C	506	CLA	C16-C15-C13	-2.32	108.42	115.92
36	H	101	HTG	C1-O5-C5	2.32	116.86	112.58
28	A	412	LMG	O6-C5-C4	2.32	113.91	109.69
24	C	511	CLA	C6-C5-C3	-2.32	107.38	113.45
24	b	609	CLA	O2A-CGA-CBA	2.32	119.18	111.91
26	B	621	BCR	C39-C30-C25	-2.32	106.54	110.30
25	A	407	PHO	C1-C2-C3	-2.32	122.04	126.04
24	C	513	CLA	O2D-CGD-CBD	2.32	115.38	111.27
24	c	514	CLA	C4-C3-C5	2.31	119.16	115.27
28	b	624	LMG	C9-C8-C7	-2.31	106.32	111.79
26	d	407	BCR	C10-C11-C12	-2.31	116.00	123.22
24	d	406	CLA	C1-C2-C3	-2.31	122.04	126.04
24	c	511	CLA	C16-C17-C18	-2.31	105.08	115.98
24	C	508	CLA	CED-O2D-CGD	2.31	121.17	115.94
24	A	405	CLA	O2D-CGD-CBD	2.31	115.38	111.27
24	B	604	CLA	CHC-C1C-C2C	-2.31	120.33	126.72
24	C	506	CLA	CMC-C2C-C1C	2.31	128.56	125.04
39	e	102	HEM	O2D-CGD-CBD	2.31	121.45	114.03
26	b	622	BCR	C38-C26-C25	-2.31	121.93	124.53
38	D	410	LHG	C6-O8-C23	2.31	125.67	117.12
32	b	625	LMT	O5'-C5'-C4'	2.31	114.62	109.75
24	C	503	CLA	CHC-C1C-C2C	-2.31	120.34	126.72
24	B	617	CLA	CHD-C4C-NC	2.31	127.84	124.20
24	B	613	CLA	CMA-C3A-C2A	-2.31	104.52	113.83
39	F	102	HEM	C4B-C3B-C2B	-2.31	105.28	107.11
24	c	503	CLA	O2A-CGA-CBA	2.30	119.14	111.91
27	a	415	SQD	O48-C23-O10	-2.30	117.78	123.59
24	b	609	CLA	CED-O2D-CGD	2.30	121.15	115.94
24	d	406	CLA	CHA-C1A-NA	-2.30	121.12	126.40
24	c	514	CLA	O2A-CGA-CBA	2.30	119.13	111.91
24	B	615	CLA	CMB-C2B-C3B	2.30	128.98	124.68
26	c	516	BCR	C11-C10-C9	-2.30	124.03	127.31
24	c	504	CLA	CBC-CAC-C3C	-2.30	106.09	112.43
40	H	103	RRX	C28-C27-C26	-2.30	107.27	111.85
24	c	515	CLA	CHA-C1A-NA	-2.30	121.13	126.40
24	b	615	CLA	CMA-C3A-C4A	-2.30	105.59	111.77
27	F	101	SQD	C1-O5-C5	-2.30	109.18	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	v	201	HEC	O2D-CGD-CBD	2.30	121.40	114.03
32	J	102	LMT	O5'-C1'-O1'	-2.29	104.54	109.97
27	A	415	SQD	O6-C1-C2	2.29	111.89	108.30
24	c	503	CLA	C1-C2-C3	-2.29	122.08	126.04
37	d	416	DGD	O6D-C5D-C4D	2.29	113.64	109.52
24	B	613	CLA	O2A-CGA-CBA	2.29	119.11	111.91
26	d	407	BCR	C15-C14-C13	-2.29	124.04	127.31
24	C	513	CLA	C11-C10-C8	-2.29	108.51	115.92
24	b	620	CLA	O2A-C1-C2	2.29	114.66	108.64
37	C	518	DGD	O1G-C1A-O1A	-2.29	117.81	123.59
24	b	616	CLA	CHD-C1D-C2D	-2.29	120.67	125.48
24	C	505	CLA	CBC-CAC-C3C	-2.29	106.11	112.43
29	d	408	PL9	C27-C28-C29	-2.29	122.14	127.66
24	B	615	CLA	O2A-CGA-CBA	2.29	119.10	111.91
24	b	618	CLA	CHC-C1C-C2C	-2.29	120.38	126.72
24	c	506	CLA	C5-C3-C2	-2.29	116.48	121.12
24	b	609	CLA	CBC-CAC-C3C	-2.29	106.12	112.43
24	D	406	CLA	C6-C7-C8	-2.29	108.52	115.92
24	C	512	CLA	CHC-C1C-C2C	-2.29	120.39	126.72
24	b	617	CLA	C7-C6-C5	-2.29	107.14	113.36
36	o	301	HTG	O5-C5-C6	2.29	112.12	106.44
24	B	608	CLA	CMC-C2C-C1C	2.29	128.52	125.04
28	c	521	LMG	O8-C28-O10	-2.29	117.82	123.59
24	D	406	CLA	CBC-CAC-C3C	-2.29	106.13	112.43
24	b	615	CLA	O2A-CGA-CBA	2.29	119.08	111.91
24	C	512	CLA	CMA-C3A-C4A	-2.29	105.63	111.77
24	C	506	CLA	CMB-C2B-C3B	2.29	128.96	124.68
24	b	605	CLA	C3B-C4B-NB	2.29	112.17	109.21
26	T	101	BCR	C1-C6-C7	2.29	122.24	115.78
24	c	513	CLA	O2A-CGA-CBA	2.29	119.08	111.91
26	T	101	BCR	C20-C21-C22	-2.28	124.05	127.31
37	c	518	DGD	O5D-C6D-C5D	-2.28	104.82	109.05
26	K	101	BCR	C2-C3-C4	2.28	116.48	111.38
24	b	605	CLA	C4A-NA-C1A	2.28	107.73	106.71
24	c	504	CLA	CMB-C2B-C3B	2.28	128.95	124.68
24	B	608	CLA	CAC-C3C-C4C	2.28	127.77	124.81
24	B	618	CLA	CMB-C2B-C3B	2.28	128.94	124.68
24	C	507	CLA	C1-O2A-CGA	2.28	122.43	116.44
42	v	201	HEC	CBD-CAD-C3D	-2.28	108.73	112.62
24	a	409	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
26	b	623	BCR	C38-C26-C25	-2.28	121.97	124.53
24	C	510	CLA	O2A-CGA-CBA	2.28	119.06	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	521	LMG	O8-C28-O10	-2.28	117.85	123.59
24	C	506	CLA	CHD-C4C-NC	2.28	127.79	124.20
36	c	523	HTG	C1-O5-C5	2.27	116.78	112.58
24	C	505	CLA	O2D-CGD-O1D	-2.27	119.39	123.84
37	c	520	DGD	O1G-C1A-O1A	-2.27	117.85	123.59
24	B	612	CLA	CHC-C1C-C2C	-2.27	120.43	126.72
24	C	504	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
32	a	402	LMT	O5'-C5'-C4'	2.27	114.54	109.75
24	C	509	CLA	CHA-C1A-NA	-2.27	121.20	126.40
24	c	515	CLA	CMC-C2C-C1C	2.27	128.49	125.04
24	B	610	CLA	O2A-CGA-O1A	-2.27	117.88	123.59
24	c	507	CLA	O2A-CGA-CBA	2.26	119.01	111.91
24	a	411	CLA	CMA-C3A-C2A	-2.26	104.70	113.83
38	L	101	LHG	O8-C23-O10	-2.26	117.88	123.59
24	b	614	CLA	CMB-C2B-C3B	2.26	128.91	124.68
40	H	103	RRX	C1-C6-C7	2.26	122.18	115.78
26	D	407	BCR	C38-C26-C27	2.26	117.96	113.62
24	A	409	CLA	CAC-C3C-C4C	2.26	127.74	124.81
24	b	617	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
32	B	638	LMT	O5'-C1'-O1'	-2.26	104.63	109.97
24	C	503	CLA	O2A-CGA-CBA	2.26	118.99	111.91
32	b	625	LMT	O5B-C5B-C4B	2.26	113.79	109.69
24	b	618	CLA	CHD-C4C-NC	2.26	127.76	124.20
36	C	522	HTG	O5-C1-C2	2.26	113.15	110.31
38	D	410	LHG	C5-O7-C7	-2.25	112.24	117.79
32	m	103	LMT	O1'-C1'-C2'	2.25	111.82	108.30
26	b	622	BCR	C15-C16-C17	-2.25	118.86	123.47
26	c	517	BCR	C37-C22-C23	2.25	121.63	118.08
24	B	614	CLA	CHC-C1C-C2C	-2.25	120.49	126.72
24	b	610	CLA	CBC-CAC-C3C	-2.25	106.22	112.43
42	V	201	HEC	CBA-CAA-C2A	-2.25	108.81	112.60
38	d	409	LHG	O7-C7-O9	-2.25	118.26	123.70
38	l	102	LHG	C6-C5-C4	-2.25	106.47	111.79
24	C	506	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
26	b	623	BCR	C21-C20-C19	-2.25	116.20	123.22
24	b	618	CLA	C4C-C3C-C2C	-2.25	103.62	106.90
24	C	514	CLA	CHC-C1C-C2C	-2.25	120.51	126.72
24	C	515	CLA	CMC-C2C-C1C	2.25	128.46	125.04
24	b	611	CLA	CHC-C1C-C2C	-2.25	120.51	126.72
24	b	606	CLA	O2A-CGA-CBA	2.24	118.95	111.91
26	D	407	BCR	C37-C22-C21	-2.24	119.78	122.92
24	B	610	CLA	CHC-C1C-C2C	-2.24	120.51	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	409	CLA	CHC-C1C-C2C	-2.24	120.52	126.72
26	C	517	BCR	C38-C26-C25	-2.24	122.01	124.53
24	C	510	CLA	CBC-CAC-C3C	-2.24	106.25	112.43
26	T	101	BCR	C7-C6-C5	-2.24	116.03	121.46
24	c	507	CLA	C4-C3-C5	2.24	119.04	115.27
26	D	407	BCR	C10-C11-C12	-2.24	116.22	123.22
24	A	406	CLA	O2A-CGA-CBA	2.24	118.94	111.91
24	b	617	CLA	CBC-CAC-C3C	-2.24	106.26	112.43
24	B	611	CLA	CED-O2D-CGD	2.24	121.00	115.94
24	C	506	CLA	C4C-C3C-C2C	-2.24	103.64	106.90
24	C	504	CLA	CAC-C3C-C4C	2.24	127.71	124.81
24	B	603	CLA	CMB-C2B-C3B	2.24	128.86	124.68
24	B	609	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
24	d	405	CLA	CMA-C3A-C2A	-2.23	104.81	113.83
26	k	102	BCR	C21-C20-C19	-2.23	116.24	123.22
24	c	514	CLA	CHC-C1C-C2C	-2.23	120.54	126.72
27	b	601	SQD	C3-C4-C5	2.23	114.22	110.24
24	A	409	CLA	C6-C7-C8	-2.23	108.70	115.92
24	C	509	CLA	OBD-CAD-C3D	-2.23	123.15	128.52
24	D	401	CLA	C4-C3-C5	2.23	119.03	115.27
29	a	417	PL9	C2-C3-C4	2.23	121.87	118.80
26	k	103	BCR	C16-C17-C18	-2.23	124.13	127.31
24	c	513	CLA	C4A-NA-C1A	2.23	107.71	106.71
24	B	615	CLA	CAC-C3C-C4C	2.23	127.70	124.81
28	i	101	LMG	O8-C28-C29	2.23	118.90	111.91
24	b	620	CLA	CHA-C1A-NA	-2.23	121.30	126.40
26	t	101	BCR	C37-C22-C21	-2.23	119.81	122.92
24	B	610	CLA	C11-C12-C13	-2.22	108.73	115.92
24	C	511	CLA	CMB-C2B-C3B	2.22	128.84	124.68
32	b	625	LMT	C1-O1'-C1'	-2.22	110.16	113.84
24	a	413	CLA	CHC-C1C-C2C	-2.22	120.58	126.72
28	d	412	LMG	O8-C28-O10	-2.22	117.99	123.59
24	A	406	CLA	CHC-C1C-C2C	-2.22	120.58	126.72
37	C	520	DGD	O6E-C1E-O5D	-2.22	104.72	109.97
24	b	612	CLA	CHC-C1C-C2C	-2.22	120.58	126.72
24	B	611	CLA	CHD-C1D-ND	-2.22	122.42	124.45
24	b	613	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
24	B	603	CLA	CBC-CAC-C3C	-2.22	106.31	112.43
24	c	511	CLA	C4A-NA-C1A	2.22	107.70	106.71
24	b	611	CLA	CMB-C2B-C3B	2.22	128.83	124.68
24	B	609	CLA	C1-O2A-CGA	2.22	122.26	116.44
38	D	411	LHG	O8-C23-C24	2.22	118.86	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	618	CLA	C4-C3-C5	2.21	119.00	115.27
24	b	614	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
24	c	506	CLA	C1-O2A-CGA	2.21	122.25	116.44
38	D	410	LHG	C25-C24-C23	-2.21	105.57	113.62
24	B	617	CLA	CHA-C1A-NA	-2.21	121.33	126.40
24	c	510	CLA	CHC-C1C-C2C	-2.21	120.60	126.72
32	B	638	LMT	O5'-C1'-C2'	2.21	115.03	110.35
29	d	408	PL9	C30-C29-C31	2.21	118.99	115.27
24	b	612	CLA	CMA-C3A-C2A	-2.21	104.92	113.83
29	d	408	PL9	C42-C43-C44	-2.21	122.34	127.66
36	c	524	HTG	C6-C5-C4	-2.21	107.83	113.00
29	d	408	PL9	C12-C13-C14	-2.21	122.34	127.66
37	c	519	DGD	O1G-C1A-O1A	-2.21	118.02	123.59
24	B	618	CLA	CHA-C1A-NA	-2.21	121.35	126.40
26	b	623	BCR	C7-C8-C9	-2.21	122.90	126.23
24	B	614	CLA	C1-C2-C3	-2.21	122.23	126.04
24	b	618	CLA	CMA-C3A-C4A	-2.21	105.85	111.77
24	B	606	CLA	C16-C15-C13	-2.20	108.80	115.92
24	b	619	CLA	CMB-C2B-C1B	2.20	131.85	128.46
24	C	512	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
24	b	611	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
24	c	503	CLA	CHC-C1C-C2C	-2.20	120.64	126.72
24	b	616	CLA	CHC-C1C-C2C	-2.20	120.64	126.72
32	D	402	LMT	C1B-O1B-C4'	-2.20	112.52	117.96
37	c	518	DGD	O3G-C3G-C2G	-2.20	105.60	110.90
24	B	606	CLA	C4-C3-C5	2.20	118.97	115.27
24	C	513	CLA	C6-C7-C8	-2.20	108.82	115.92
42	V	201	HEC	O2D-CGD-CBD	2.20	121.08	114.03
26	T	101	BCR	C3-C4-C5	-2.20	110.16	114.08
26	b	623	BCR	C10-C11-C12	-2.20	116.37	123.22
24	B	614	CLA	CMB-C2B-C3B	2.20	128.78	124.68
24	C	509	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
24	b	619	CLA	CHC-C1C-C2C	-2.19	120.66	126.72
27	B	622	SQD	O8-S-C6	2.19	109.23	105.74
28	C	533	LMG	C8-O7-C10	-2.19	112.39	117.79
26	C	516	BCR	C38-C26-C25	-2.19	122.07	124.53
24	c	511	CLA	CMB-C2B-C3B	2.19	128.78	124.68
24	b	611	CLA	C4-C3-C5	2.19	118.96	115.27
32	M	101	LMT	O1'-C1'-C2'	2.19	111.72	108.30
25	A	407	PHO	CMB-C2B-C3B	2.19	128.78	124.68
32	b	629	LMT	O5'-C1'-C2'	-2.19	105.71	110.35
24	c	506	CLA	C1-C2-C3	-2.19	122.26	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	603	CLA	CHA-C1A-NA	-2.19	121.39	126.40
24	b	619	CLA	C11-C10-C8	-2.19	108.85	115.92
24	b	612	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
24	C	514	CLA	CHD-C4C-NC	2.18	127.65	124.20
26	B	620	BCR	C37-C22-C21	-2.18	119.86	122.92
24	c	508	CLA	CHA-C1A-NA	-2.18	121.40	126.40
29	D	408	PL9	C36-C37-C38	-2.18	104.70	111.88
37	c	518	DGD	O1G-C1G-C2G	-2.18	102.08	108.43
24	b	615	CLA	C7-C6-C5	-2.18	107.43	113.36
24	b	615	CLA	CHA-C1A-NA	-2.18	121.40	126.40
26	B	621	BCR	C3-C4-C5	-2.18	110.18	114.08
27	A	411	SQD	O48-C23-O10	-2.18	118.09	123.59
26	b	623	BCR	C11-C10-C9	-2.18	124.20	127.31
24	c	512	CLA	C1-O2A-CGA	2.18	122.16	116.44
29	A	413	PL9	C17-C18-C19	-2.18	122.41	127.66
24	B	609	CLA	C1-C2-C3	-2.18	122.28	126.04
24	D	401	CLA	CHA-C1A-NA	-2.18	121.41	126.40
27	b	601	SQD	C44-O6-C1	-2.18	109.48	113.74
24	B	604	CLA	C1-C2-C3	-2.18	122.28	126.04
32	m	103	LMT	C1-O1'-C1'	-2.18	110.23	113.84
26	A	410	BCR	C37-C22-C21	-2.17	119.88	122.92
24	b	614	CLA	CHC-C1C-C2C	-2.17	120.71	126.72
24	B	609	CLA	C4C-C3C-C2C	-2.17	103.73	106.90
24	c	513	CLA	CMB-C2B-C3B	2.17	128.75	124.68
28	c	521	LMG	C30-C29-C28	-2.17	105.72	113.62
38	d	410	LHG	O8-C23-O10	-2.17	118.11	123.59
24	B	615	CLA	C1-C2-C3	-2.17	122.29	126.04
24	C	508	CLA	CMB-C2B-C3B	2.17	128.74	124.68
24	b	611	CLA	O2A-CGA-CBA	2.17	118.72	111.91
24	b	612	CLA	CHA-C1A-NA	-2.17	121.43	126.40
29	D	408	PL9	C20-C19-C21	2.17	118.92	115.27
27	a	401	SQD	C3-C4-C5	2.17	114.11	110.24
32	A	422	LMT	C1'-O5'-C5'	2.17	117.94	113.69
24	B	605	CLA	CHD-C4C-NC	2.17	127.62	124.20
24	a	410	CLA	CAC-C3C-C4C	2.17	127.62	124.81
24	B	608	CLA	CBC-CAC-C3C	-2.17	106.46	112.43
24	b	616	CLA	O2A-CGA-CBA	2.16	118.70	111.91
24	b	616	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
32	D	409	LMT	O1B-C1B-O5B	-2.16	104.63	110.67
29	a	417	PL9	C7-C3-C2	-2.16	120.46	123.30
37	h	102	DGD	C6D-C5D-C4D	2.16	116.60	112.09
24	B	616	CLA	CAA-C2A-C3A	-2.16	106.87	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	506	CLA	O2A-CGA-CBA	2.16	118.68	111.91
24	B	616	CLA	CHC-C1C-C2C	-2.16	120.75	126.72
24	b	617	CLA	CED-O2D-CGD	2.16	120.82	115.94
24	c	512	CLA	CMB-C2B-C3B	2.16	128.71	124.68
26	t	101	BCR	C28-C27-C26	-2.16	110.23	114.08
24	C	513	CLA	C4A-NA-C1A	2.16	107.67	106.71
29	D	408	PL9	C27-C28-C29	-2.16	122.47	127.66
40	H	103	RRX	C2-C1-C6	2.15	113.80	110.48
28	B	623	LMG	C9-C8-C7	-2.15	106.69	111.79
24	C	513	CLA	CHA-C1A-NA	-2.15	121.47	126.40
24	B	618	CLA	CHD-C4C-NC	2.15	127.60	124.20
24	C	514	CLA	O2A-CGA-CBA	2.15	118.66	111.91
24	D	406	CLA	CMA-C3A-C2A	-2.15	105.14	113.83
24	C	512	CLA	CMA-C3A-C2A	-2.15	105.15	113.83
26	b	622	BCR	C8-C7-C6	-2.15	121.16	127.20
24	B	612	CLA	CAA-CBA-CGA	-2.15	106.97	113.25
26	K	101	BCR	C16-C15-C14	-2.15	119.07	123.47
24	D	401	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
26	T	101	BCR	C15-C16-C17	-2.15	119.07	123.47
24	D	405	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
37	C	520	DGD	C6B-C5B-C4B	-2.15	103.51	114.42
28	C	521	LMG	O7-C10-O9	-2.15	118.51	123.70
24	c	514	CLA	C4A-NA-C1A	2.15	107.67	106.71
26	A	410	BCR	C40-C30-C25	-2.15	106.81	110.30
28	D	413	LMG	O8-C28-C29	2.15	118.65	111.91
26	T	101	BCR	C11-C10-C9	-2.15	124.25	127.31
24	B	606	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
29	a	417	PL9	C51-C49-C50	2.15	119.34	114.60
24	C	515	CLA	CHA-C1A-NA	-2.14	121.49	126.40
36	b	627	HTG	O6-C6-C5	-2.14	103.93	111.29
24	B	609	CLA	CMC-C2C-C1C	2.14	128.31	125.04
26	t	101	BCR	C35-C13-C12	2.14	121.46	118.08
24	C	513	CLA	CHC-C1C-C2C	-2.14	120.79	126.72
24	b	616	CLA	CMC-C2C-C1C	2.14	128.30	125.04
25	a	412	PHO	CMB-C2B-C3B	2.14	128.69	124.68
38	D	410	LHG	O7-C7-C8	2.14	116.11	111.50
26	b	621	BCR	C3-C4-C5	-2.14	110.25	114.08
37	c	519	DGD	O2G-C1B-O1B	-2.14	118.53	123.70
32	a	421	LMT	O1B-C4'-C3'	2.14	112.97	107.28
24	b	615	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
24	C	512	CLA	CAA-C2A-C3A	-2.14	106.92	112.78
24	B	617	CLA	CBC-CAC-C3C	-2.14	106.54	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	i	101	LMG	O7-C10-O9	-2.14	118.54	123.70
28	b	624	LMG	O1-C7-C8	-2.14	105.74	110.90
26	k	102	BCR	C37-C22-C23	2.14	121.44	118.08
24	d	405	CLA	CAC-C3C-C4C	2.13	127.58	124.81
36	C	522	HTG	C1-O5-C5	2.13	116.52	112.58
24	C	506	CLA	OBD-CAD-C3D	-2.13	123.39	128.52
24	b	610	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
24	c	508	CLA	CMB-C2B-C3B	2.13	128.67	124.68
24	a	410	CLA	CHB-C4A-NA	2.13	127.46	124.51
24	C	511	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
24	B	617	CLA	CHC-C1C-NC	2.13	127.44	124.20
39	e	102	HEM	C4D-ND-C1D	2.13	107.27	105.07
37	C	519	DGD	O1G-C1A-O1A	-2.13	118.22	123.59
25	A	407	PHO	C16-C17-C18	-2.13	105.94	115.98
24	D	406	CLA	CHC-C1C-C2C	-2.13	120.83	126.72
24	B	605	CLA	CHC-C1C-C2C	-2.13	120.83	126.72
37	C	520	DGD	C6D-C5D-C4D	-2.13	107.65	112.09
24	C	515	CLA	CMA-C3A-C4A	-2.13	106.06	111.77
24	c	511	CLA	O2A-CGA-CBA	2.13	118.58	111.91
26	c	517	BCR	C37-C22-C21	-2.12	119.95	122.92
24	b	606	CLA	C11-C10-C8	-2.12	109.06	115.92
24	a	410	CLA	CHC-C1C-NC	2.12	127.42	124.20
37	c	520	DGD	O3G-C3G-C2G	-2.12	105.78	110.90
24	C	512	CLA	CAC-C3C-C4C	2.12	127.56	124.81
26	C	517	BCR	C21-C20-C19	-2.12	116.60	123.22
24	a	413	CLA	CMC-C2C-C1C	2.12	128.27	125.04
24	C	506	CLA	C6-C7-C8	-2.12	109.08	115.92
24	b	605	CLA	O1D-CGD-CBD	-2.12	120.16	124.48
24	b	611	CLA	C1-C2-C3	-2.12	122.39	126.04
24	C	504	CLA	CMC-C2C-C1C	2.11	128.26	125.04
24	c	509	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
24	b	618	CLA	CAC-C3C-C4C	2.11	127.55	124.81
24	b	607	CLA	CAC-C3C-C4C	2.11	127.55	124.81
26	A	410	BCR	C7-C8-C9	-2.11	123.05	126.23
24	A	406	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
24	b	616	CLA	CMA-C3A-C4A	-2.11	106.10	111.77
24	b	612	CLA	C11-C12-C13	-2.11	109.10	115.92
26	A	410	BCR	C20-C21-C22	-2.11	124.30	127.31
26	B	620	BCR	C37-C22-C23	2.11	121.40	118.08
38	l	102	LHG	C10-C9-C8	-2.11	105.61	113.19
26	A	410	BCR	C35-C13-C14	-2.11	119.97	122.92
24	b	614	CLA	CHA-C1A-NA	-2.11	121.57	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	609	CLA	OBD-CAD-C3D	-2.11	123.45	128.52
24	A	409	CLA	C2A-C1A-CHA	-2.11	120.17	123.86
28	c	521	LMG	O7-C10-O9	-2.11	118.61	123.70
24	B	615	CLA	CHC-C1C-C2C	-2.11	120.89	126.72
26	K	102	BCR	C38-C26-C25	-2.11	122.16	124.53
24	c	512	CLA	CMC-C2C-C1C	2.11	128.25	125.04
29	A	413	PL9	C40-C39-C41	2.10	118.81	115.27
26	k	102	BCR	C35-C13-C14	-2.10	119.97	122.92
24	b	615	CLA	CHD-C4C-NC	2.10	127.52	124.20
24	B	616	CLA	C4-C3-C2	-2.10	118.28	123.68
27	f	802	SQD	O47-C7-O49	-2.10	118.62	123.70
24	c	515	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
24	C	511	CLA	CBA-CAA-C2A	2.10	120.07	113.86
42	v	201	HEC	O2A-CGA-CBA	2.10	120.78	114.03
24	B	604	CLA	CAA-CBA-CGA	-2.10	107.12	113.25
24	c	506	CLA	CHC-C1C-C2C	-2.10	120.92	126.72
24	c	506	CLA	CMB-C2B-C3B	2.10	128.60	124.68
24	d	405	CLA	CHA-C1A-NA	-2.10	121.59	126.40
24	b	607	CLA	CMC-C2C-C1C	2.10	128.23	125.04
24	b	615	CLA	CMC-C2C-C1C	2.09	128.23	125.04
24	b	620	CLA	OBD-CAD-C3D	-2.09	123.48	128.52
32	b	626	LMT	O1B-C4'-C3'	2.09	112.85	107.28
29	D	408	PL9	C42-C43-C44	-2.09	122.62	127.66
24	C	514	CLA	CMC-C2C-C1C	2.09	128.23	125.04
24	c	508	CLA	CMC-C2C-C1C	2.09	128.23	125.04
24	B	611	CLA	C1-C2-C3	-2.09	122.42	126.04
24	b	620	CLA	CMA-C3A-C4A	-2.09	106.15	111.77
24	b	605	CLA	CMC-C2C-C1C	2.09	128.22	125.04
24	B	613	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
37	C	519	DGD	C3B-C2B-C1B	-2.09	106.02	113.62
24	D	401	CLA	C1-C2-C3	-2.09	122.43	126.04
37	C	519	DGD	C3G-O3G-C1D	-2.09	109.66	113.74
25	a	412	PHO	C4A-C3A-C2A	-2.09	100.85	102.84
24	B	614	CLA	CMA-C3A-C4A	-2.09	106.16	111.77
24	D	401	CLA	CHD-C4C-NC	2.09	127.49	124.20
24	c	511	CLA	CHA-C1A-NA	-2.09	121.62	126.40
26	K	102	BCR	C2-C1-C6	2.09	113.69	110.48
26	k	103	BCR	C2-C1-C6	2.09	113.69	110.48
36	O	303	HTG	C1-O5-C5	2.09	116.43	112.58
24	D	406	CLA	CHD-C4C-NC	2.08	127.49	124.20
42	v	201	HEC	CMC-C2C-C1C	-2.08	125.26	128.46
24	B	607	CLA	CHD-C1D-C2D	-2.08	121.11	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	f	802	SQD	O7-S-C6	2.08	109.41	106.94
24	c	514	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
32	B	624	LMT	O1'-C1'-C2'	2.08	111.55	108.30
24	c	512	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
24	b	606	CLA	CAA-CBA-CGA	-2.08	107.17	113.25
24	B	611	CLA	CMC-C2C-C1C	2.08	128.21	125.04
24	D	405	CLA	CHA-C1A-NA	-2.08	121.63	126.40
24	c	507	CLA	CMA-C3A-C4A	-2.08	106.18	111.77
26	C	517	BCR	C29-C28-C27	-2.08	106.73	111.38
24	c	511	CLA	C4-C3-C5	2.08	118.77	115.27
24	A	405	CLA	CHA-C1A-NA	-2.08	121.64	126.40
24	b	613	CLA	CMB-C2B-C1B	2.08	131.66	128.46
36	V	202	HTG	C1-O5-C5	-2.08	108.75	112.57
24	D	401	CLA	CAC-C3C-C4C	2.08	127.50	124.81
24	b	620	CLA	CHC-C1C-C2C	-2.08	120.98	126.72
37	H	104	DGD	C3G-C2G-C1G	-2.07	106.88	111.79
37	c	519	DGD	O6E-C5E-C6E	2.07	111.59	106.44
24	a	411	CLA	CHA-C1A-NA	-2.07	121.66	126.40
24	C	512	CLA	CHA-C1A-NA	-2.07	121.66	126.40
24	a	409	CLA	C1-C2-C3	-2.07	122.46	126.04
24	b	609	CLA	CMC-C2C-C1C	2.07	128.19	125.04
24	b	617	CLA	CHC-C1C-C2C	-2.07	121.01	126.72
24	c	508	CLA	CHC-C1C-C2C	-2.06	121.01	126.72
24	b	607	CLA	C7-C6-C5	-2.06	107.75	113.36
29	d	408	PL9	C8-C7-C3	2.06	117.81	111.98
24	C	513	CLA	O2D-CGD-O1D	-2.06	119.80	123.84
39	e	102	HEM	CHA-C4D-C3D	-2.06	121.45	125.33
24	c	507	CLA	CHC-C1C-C2C	-2.06	121.02	126.72
26	d	407	BCR	C39-C30-C25	-2.06	106.96	110.30
26	b	621	BCR	C15-C14-C13	-2.06	124.37	127.31
29	A	413	PL9	C51-C49-C50	2.06	119.15	114.60
28	C	533	LMG	O7-C10-O9	-2.06	118.73	123.70
32	D	402	LMT	C4B-C3B-C2B	-2.06	107.23	110.82
24	b	619	CLA	CMC-C2C-C1C	2.06	128.17	125.04
24	c	513	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
24	A	405	CLA	O2A-CGA-CBA	2.05	118.34	111.91
24	b	616	CLA	CED-O2D-CGD	2.05	120.58	115.94
28	b	624	LMG	C30-C29-C28	-2.05	106.16	113.62
24	b	620	CLA	CHD-C4C-NC	2.05	127.43	124.20
38	L	101	LHG	C6-C5-C4	-2.05	106.94	111.79
24	b	607	CLA	C6-C7-C8	-2.05	109.30	115.92
24	C	505	CLA	O2A-CGA-CBA	2.05	118.34	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	406	CLA	CMA-C3A-C2A	-2.05	105.56	113.83
32	D	409	LMT	C1'-C2'-C3'	2.05	114.26	110.00
24	d	406	CLA	O2A-CGA-CBA	2.05	118.33	111.91
24	C	514	CLA	CHA-C1A-NA	-2.05	121.71	126.40
37	C	518	DGD	O2G-C1B-O1B	-2.05	118.75	123.70
24	B	607	CLA	CAC-C3C-C4C	2.05	127.47	124.81
24	c	514	CLA	CAC-C3C-C4C	2.05	127.47	124.81
24	B	609	CLA	OBD-CAD-C3D	-2.05	123.59	128.52
24	C	511	CLA	CHA-C1A-NA	-2.05	121.71	126.40
26	k	103	BCR	C38-C26-C25	-2.04	122.23	124.53
24	C	511	CLA	CHC-C1C-C2C	-2.04	121.07	126.72
29	A	413	PL9	O1-C4-C3	-2.04	118.47	120.72
24	b	605	CLA	CED-O2D-CGD	2.04	120.56	115.94
28	Z	101	LMG	C1-O6-C5	2.04	117.70	113.69
24	c	514	CLA	C11-C12-C13	-2.04	109.32	115.92
37	c	520	DGD	C2G-O2G-C1B	-2.04	112.77	117.79
24	b	611	CLA	CMC-C2C-C1C	2.04	128.15	125.04
24	B	604	CLA	O2A-CGA-CBA	2.04	118.31	111.91
24	B	615	CLA	CHA-C1A-NA	-2.04	121.73	126.40
24	B	614	CLA	CMC-C2C-C1C	2.04	128.15	125.04
26	K	101	BCR	C33-C5-C4	2.04	117.53	113.62
24	A	406	CLA	CED-O2D-CGD	2.04	120.55	115.94
24	b	606	CLA	CHC-C1C-C2C	-2.04	121.09	126.72
24	b	617	CLA	CMA-C3A-C2A	-2.04	105.61	113.83
24	d	405	CLA	CMB-C2B-C3B	2.04	128.49	124.68
24	B	603	CLA	C1-O2A-CGA	2.04	121.78	116.44
24	b	614	CLA	O2A-C1-C2	2.03	113.98	108.64
24	C	510	CLA	CAA-C2A-C3A	-2.03	107.21	112.78
24	A	405	CLA	CMC-C2C-C1C	2.03	128.14	125.04
24	c	509	CLA	CHD-C4C-NC	2.03	127.41	124.20
38	d	411	LHG	O7-C7-O9	-2.03	118.79	123.70
24	c	506	CLA	CMA-C3A-C2A	-2.03	105.64	113.83
26	A	410	BCR	C29-C28-C27	-2.03	106.84	111.38
24	A	406	CLA	CHA-C1A-NA	-2.03	121.75	126.40
24	b	608	CLA	CHC-C1C-C2C	-2.03	121.11	126.72
24	c	507	CLA	C1-C2-C3	-2.03	122.53	126.04
24	C	515	CLA	C6-C7-C8	-2.03	109.36	115.92
26	d	407	BCR	C3-C4-C5	-2.03	110.46	114.08
26	B	621	BCR	C24-C23-C22	-2.03	123.17	126.23
24	C	508	CLA	CMA-C3A-C4A	-2.03	106.32	111.77
24	b	616	CLA	C11-C10-C8	-2.03	109.37	115.92
24	b	614	CLA	C11-C12-C13	-2.03	109.37	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	507	CLA	CHC-C1C-C2C	-2.02	121.12	126.72
24	c	513	CLA	CHC-C1C-C2C	-2.02	121.12	126.72
36	c	523	HTG	O5-C5-C4	2.02	113.37	109.69
28	d	412	LMG	O8-C28-C29	2.02	118.26	111.91
29	D	408	PL9	C47-C48-C49	-2.02	120.84	127.75
25	a	412	PHO	CBA-CAA-C2A	-2.02	107.90	113.81
26	k	102	BCR	C8-C7-C6	-2.02	121.53	127.20
24	b	607	CLA	CHC-C1C-C2C	-2.02	121.13	126.72
24	c	503	CLA	C1-O2A-CGA	2.02	121.75	116.44
32	D	402	LMT	C1'-O5'-C5'	2.02	117.65	113.69
24	c	504	CLA	CHC-C1C-C2C	-2.02	121.14	126.72
24	c	506	CLA	CHD-C4C-NC	2.02	127.38	124.20
26	A	410	BCR	C2-C1-C6	2.02	113.59	110.48
24	C	505	CLA	C4-C3-C5	2.02	118.67	115.27
26	K	101	BCR	C1-C6-C7	2.02	121.48	115.78
24	c	506	CLA	C6-C5-C3	2.02	118.74	113.45
26	K	101	BCR	C29-C28-C27	-2.02	106.87	111.38
27	a	401	SQD	O5-C5-C4	2.02	113.35	109.69
26	d	407	BCR	C38-C26-C27	2.01	117.49	113.62
24	c	513	CLA	O2A-C1-C2	-2.01	103.34	108.64
32	F	103	LMT	C1B-O5B-C5B	2.01	117.64	113.69
26	d	407	BCR	C34-C9-C10	-2.01	120.10	122.92
26	b	623	BCR	C16-C15-C14	-2.01	119.35	123.47
24	A	405	CLA	CMA-C3A-C2A	-2.01	105.71	113.83
26	A	410	BCR	C8-C7-C6	-2.01	121.55	127.20
24	c	512	CLA	CHA-C1A-NA	-2.01	121.79	126.40
26	D	407	BCR	C37-C22-C23	2.01	121.25	118.08
24	B	606	CLA	C6-C5-C3	-2.01	108.19	113.45
26	d	407	BCR	C29-C28-C27	-2.01	106.89	111.38
24	a	413	CLA	CHD-C4C-NC	2.01	127.37	124.20
28	c	522	LMG	O7-C10-O9	-2.01	118.86	123.70
25	a	412	PHO	O1D-CGD-CBD	-2.00	121.40	124.74
32	m	102	LMT	C1'-O5'-C5'	-2.00	109.75	113.69
24	b	608	CLA	O2D-CGD-O1D	-2.00	119.92	123.84
38	E	101	LHG	O7-C7-O9	-2.00	118.86	123.70
26	b	621	BCR	C21-C20-C19	-2.00	116.97	123.22

All (56) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	405	CLA	ND
24	B	603	CLA	ND

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Mol	Chain	Res	Type	Atom
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	609	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	B	618	CLA	ND
24	C	503	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	511	CLA	ND
24	C	512	CLA	ND
24	C	513	CLA	ND
24	C	514	CLA	ND
24	D	405	CLA	ND
24	D	406	CLA	ND
24	a	409	CLA	ND
24	a	410	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
24	b	610	CLA	ND
24	b	611	CLA	ND
24	b	613	CLA	ND
24	b	614	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

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Mol	Chain	Res	Type	Atom
24	c	503	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	511	CLA	ND
24	c	512	CLA	ND
24	c	513	CLA	ND
24	c	514	CLA	ND
24	d	405	CLA	ND
24	d	406	CLA	ND

All (1021) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	607	CLA	C2-C3-C5-C6
24	B	608	CLA	CHA-CBD-CGD-O1D
24	B	608	CLA	CHA-CBD-CGD-O2D
24	B	616	CLA	CHA-CBD-CGD-O1D
24	B	616	CLA	CHA-CBD-CGD-O2D
24	B	616	CLA	CAD-CBD-CGD-O1D
24	B	616	CLA	CAD-CBD-CGD-O2D
24	C	506	CLA	C11-C12-C13-C14
24	C	510	CLA	CHA-CBD-CGD-O1D
24	C	510	CLA	CHA-CBD-CGD-O2D
24	b	610	CLA	CHA-CBD-CGD-O2D
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	506	CLA	C2-C3-C5-C6
24	c	506	CLA	C4-C3-C5-C6
24	c	510	CLA	CHA-CBD-CGD-O1D
24	c	510	CLA	CHA-CBD-CGD-O2D
24	c	511	CLA	C2-C1-O2A-CGA
24	c	512	CLA	C11-C12-C13-C14
26	D	407	BCR	C21-C22-C23-C24
26	D	407	BCR	C37-C22-C23-C24
26	K	101	BCR	C1-C6-C7-C8
26	K	101	BCR	C5-C6-C7-C8
26	d	407	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
26	d	407	BCR	C37-C22-C23-C24
26	k	102	BCR	C1-C6-C7-C8
26	k	102	BCR	C5-C6-C7-C8
27	A	415	SQD	O6-C44-C45-O47
27	B	622	SQD	O49-C7-O47-C45
27	F	101	SQD	O49-C7-O47-C45
27	F	101	SQD	C8-C7-O47-C45
27	a	401	SQD	O6-C44-C45-O47
27	a	401	SQD	C5-C6-S-O7
27	a	401	SQD	C5-C6-S-O8
27	a	401	SQD	C5-C6-S-O9
27	b	601	SQD	O5-C1-O6-C44
27	b	601	SQD	O49-C7-O47-C45
27	f	802	SQD	C8-C7-O47-C45
27	f	802	SQD	C5-C6-S-O7
28	Z	101	LMG	C11-C10-O7-C8
28	i	101	LMG	C11-C10-O7-C8
28	z	101	LMG	C11-C10-O7-C8
29	A	413	PL9	C18-C19-C21-C22
29	A	413	PL9	C20-C19-C21-C22
29	a	417	PL9	C14-C16-C17-C18
31	A	418	GOL	O1-C1-C2-C3
31	C	525	GOL	C1-C2-C3-O3
31	a	419	GOL	C1-C2-C3-O3
31	b	639	GOL	O1-C1-C2-C3
31	v	203	GOL	O1-C1-C2-C3
32	A	422	LMT	C2'-C1'-O1'-C1
32	A	422	LMT	O5'-C1'-O1'-C1
32	B	638	LMT	O5'-C1'-O1'-C1
32	D	402	LMT	C2'-C1'-O1'-C1
32	D	402	LMT	O5'-C1'-O1'-C1
32	D	409	LMT	C2'-C1'-O1'-C1
32	D	409	LMT	O5'-C1'-O1'-C1
32	F	103	LMT	C2'-C1'-O1'-C1
32	F	103	LMT	O5'-C1'-O1'-C1
32	J	102	LMT	C2'-C1'-O1'-C1
32	J	102	LMT	O5'-C1'-O1'-C1
32	a	402	LMT	O5'-C1'-O1'-C1
32	b	626	LMT	C2'-C1'-O1'-C1
32	b	626	LMT	O5'-C1'-O1'-C1
32	b	629	LMT	C2'-C1'-O1'-C1
32	b	629	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
32	f	801	LMT	C2'-C1'-O1'-C1
32	j	102	LMT	C2'-C1'-O1'-C1
32	j	102	LMT	O5'-C1'-O1'-C1
32	m	103	LMT	O5'-C1'-O1'-C1
32	m	103	LMT	C2-C1-O1'-C1'
36	B	625	HTG	C2'-C1'-S1-C1
36	B	626	HTG	O5-C1-S1-C1'
36	b	627	HTG	C2'-C1'-S1-C1
36	b	628	HTG	O5-C1-S1-C1'
36	u	201	HTG	S1-C1-C2-O2
36	u	201	HTG	O5-C1-C2-O2
36	u	201	HTG	O2-C2-C3-O3
37	d	416	DGD	C2D-C1D-O3G-C3G
37	d	416	DGD	O6D-C1D-O3G-C3G
38	E	101	LHG	O1-C1-C2-C3
38	E	101	LHG	C3-O3-P-O4
38	E	101	LHG	C3-O3-P-O5
38	E	101	LHG	C3-O3-P-O6
38	L	101	LHG	C4-O6-P-O4
38	L	101	LHG	C4-O6-P-O5
38	a	416	LHG	C3-O3-P-O4
38	a	416	LHG	O10-C23-O8-C6
38	a	416	LHG	C24-C23-O8-C6
38	d	410	LHG	O2-C2-C3-O3
38	d	410	LHG	C3-O3-P-O4
38	d	410	LHG	C4-O6-P-O4
38	l	102	LHG	C4-O6-P-O4
38	l	102	LHG	C4-O6-P-O5
40	H	103	RRX	C11-C10-C9-C8
40	h	101	RRX	C11-C10-C9-C8
40	h	101	RRX	C7-C8-C9-C34
40	h	101	RRX	C1-C6-C7-C8
32	A	422	LMT	C3'-C4'-O1B-C1B
27	f	802	SQD	O10-C23-O48-C46
32	b	625	LMT	O5B-C1B-O1B-C4'
27	f	802	SQD	C24-C23-O48-C46
27	f	802	SQD	O49-C7-O47-C45
28	Z	101	LMG	O9-C10-O7-C8
28	i	101	LMG	O9-C10-O7-C8
28	z	101	LMG	O9-C10-O7-C8
24	a	413	CLA	C3-C5-C6-C7
24	B	613	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	B	622	SQD	C8-C7-O47-C45
27	b	601	SQD	C8-C7-O47-C45
32	J	102	LMT	O5'-C5'-C6'-O6'
24	B	607	CLA	C4-C3-C5-C6
24	b	607	CLA	C4-C3-C5-C6
24	B	608	CLA	C2A-CAA-CBA-CGA
24	B	616	CLA	C3-C5-C6-C7
36	u	201	HTG	C1-C2-C3-O3
38	E	101	LHG	O2-C2-C3-O3
38	a	416	LHG	O2-C2-C3-O3
24	B	618	CLA	C3-C5-C6-C7
24	b	618	CLA	C3-C5-C6-C7
28	c	522	LMG	O6-C5-C6-O5
28	A	412	LMG	C11-C10-O7-C8
28	C	533	LMG	O6-C5-C6-O5
28	c	522	LMG	C4-C5-C6-O5
36	d	404	HTG	C4-C5-C6-O6
28	A	412	LMG	O9-C10-O7-C8
32	b	625	LMT	C4B-C5B-C6B-O6B
36	d	404	HTG	O5-C5-C6-O6
24	B	616	CLA	C4-C3-C5-C6
24	C	509	CLA	C4-C3-C5-C6
24	a	413	CLA	C4-C3-C5-C6
29	A	413	PL9	C25-C24-C26-C27
29	a	417	PL9	C20-C19-C21-C22
29	a	417	PL9	C30-C29-C31-C32
32	b	629	LMT	C4'-C5'-C6'-O6'
24	B	616	CLA	C2-C3-C5-C6
24	C	509	CLA	C2-C3-C5-C6
24	a	413	CLA	C2-C3-C5-C6
24	b	607	CLA	C2-C3-C5-C6
29	A	413	PL9	C23-C24-C26-C27
29	a	417	PL9	C18-C19-C21-C22
29	a	417	PL9	C28-C29-C31-C32
24	b	610	CLA	C2A-CAA-CBA-CGA
36	u	201	HTG	O5-C1-C2-C3
32	F	103	LMT	O5'-C5'-C6'-O6'
32	J	102	LMT	C4'-C5'-C6'-O6'
27	B	622	SQD	O5-C1-O6-C44
32	f	801	LMT	O5'-C1'-O1'-C1
36	B	626	HTG	C4-C5-C6-O6
32	a	421	LMT	C3'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
38	D	411	LHG	C1-C2-C3-O3
32	F	103	LMT	C4'-C5'-C6'-O6'
38	d	411	LHG	C12-C13-C14-C15
32	B	638	LMT	C2'-C1'-O1'-C1
36	B	626	HTG	O5-C5-C6-O6
24	A	409	CLA	C14-C13-C15-C16
24	B	603	CLA	C11-C10-C8-C9
24	B	608	CLA	C11-C12-C13-C14
24	B	618	CLA	C6-C7-C8-C9
24	B	618	CLA	C11-C10-C8-C9
24	C	514	CLA	C11-C12-C13-C14
37	C	520	DGD	C8A-C9A-CAA-CBA
28	b	624	LMG	C28-C29-C30-C31
37	C	519	DGD	C1A-C2A-C3A-C4A
24	b	607	CLA	C5-C6-C7-C8
38	d	411	LHG	C10-C11-C12-C13
36	c	524	HTG	O5-C5-C6-O6
37	c	518	DGD	C8A-C9A-CAA-CBA
24	B	603	CLA	C10-C11-C12-C13
24	B	617	CLA	C10-C11-C12-C13
24	b	618	CLA	C8-C10-C11-C12
31	A	418	GOL	O1-C1-C2-O2
27	B	622	SQD	C7-C8-C9-C10
38	D	412	LHG	C7-C8-C9-C10
38	d	409	LHG	C23-C24-C25-C26
24	c	506	CLA	C10-C11-C12-C13
32	B	638	LMT	O1'-C1-C2-C3
24	B	603	CLA	C11-C10-C8-C7
24	B	605	CLA	C6-C7-C8-C10
24	C	506	CLA	C11-C12-C13-C15
24	B	603	CLA	C8-C10-C11-C12
24	B	618	CLA	C10-C11-C12-C13
24	C	508	CLA	C10-C11-C12-C13
24	a	411	CLA	C13-C15-C16-C17
24	b	618	CLA	C10-C11-C12-C13
32	f	801	LMT	O1'-C1-C2-C3
29	A	413	PL9	C9-C11-C12-C13
32	a	421	LMT	O5'-C5'-C6'-O6'
32	b	625	LMT	O5B-C5B-C6B-O6B
24	B	618	CLA	C8-C10-C11-C12
24	C	515	CLA	C8-C10-C11-C12
32	b	629	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
32	a	421	LMT	C4'-C5'-C6'-O6'
37	d	416	DGD	C2B-C1B-O2G-C2G
27	A	415	SQD	C16-C17-C18-C19
24	A	409	CLA	C15-C16-C17-C18
24	B	618	CLA	C5-C6-C7-C8
24	b	620	CLA	C10-C11-C12-C13
38	L	101	LHG	C4-O6-P-O3
38	d	410	LHG	C3-O3-P-O6
38	l	102	LHG	C4-O6-P-O3
36	b	628	HTG	C1'-C2'-C3'-C4'
36	b	628	HTG	O5-C5-C6-O6
28	c	521	LMG	C10-C11-C12-C13
37	d	416	DGD	O1B-C1B-O2G-C2G
24	a	413	CLA	C5-C6-C7-C8
24	b	618	CLA	C5-C6-C7-C8
24	b	620	CLA	C3-C5-C6-C7
28	d	412	LMG	O6-C5-C6-O5
27	B	622	SQD	C23-C24-C25-C26
28	i	101	LMG	C11-C12-C13-C14
32	D	409	LMT	C6-C7-C8-C9
38	E	101	LHG	C25-C26-C27-C28
40	h	101	RRX	C11-C10-C9-C34
27	a	401	SQD	C26-C27-C28-C29
37	C	518	DGD	C5A-C6A-C7A-C8A
37	C	518	DGD	C6A-C7A-C8A-C9A
38	L	101	LHG	C13-C14-C15-C16
38	l	102	LHG	C13-C14-C15-C16
38	l	102	LHG	C30-C31-C32-C33
27	a	401	SQD	C18-C19-C20-C21
28	c	522	LMG	C16-C17-C18-C19
37	h	102	DGD	CBA-CCA-CDA-CEA
27	B	622	SQD	C18-C19-C20-C21
27	a	415	SQD	C16-C17-C18-C19
38	D	411	LHG	O2-C2-C3-O3
38	L	101	LHG	C14-C15-C16-C17
27	f	802	SQD	C2-C1-O6-C44
28	A	412	LMG	C2-C1-O1-C7
40	H	103	RRX	C12-C13-C14-C15
27	b	601	SQD	C10-C11-C12-C13
28	c	521	LMG	C31-C32-C33-C34
28	d	412	LMG	C15-C16-C17-C18
37	C	518	DGD	C8A-C9A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
37	C	520	DGD	CBB-CCB-CDB-CEB
38	l	102	LHG	C14-C15-C16-C17
24	C	504	CLA	C16-C17-C18-C20
28	Z	101	LMG	C15-C16-C17-C18
28	c	522	LMG	C15-C16-C17-C18
37	H	104	DGD	C6A-C7A-C8A-C9A
38	E	101	LHG	C26-C27-C28-C29
24	C	515	CLA	C6-C7-C8-C9
24	b	620	CLA	C11-C12-C13-C14
24	c	513	CLA	C6-C7-C8-C9
27	f	802	SQD	C23-C24-C25-C26
36	o	301	HTG	C3'-C4'-C5'-C6'
27	a	401	SQD	C25-C26-C27-C28
28	A	412	LMG	C30-C31-C32-C33
31	A	418	GOL	C1-C2-C3-O3
31	C	525	GOL	O1-C1-C2-C3
31	V	207	GOL	O1-C1-C2-C3
31	b	639	GOL	C1-C2-C3-O3
31	d	415	GOL	O1-C1-C2-C3
38	a	416	LHG	O9-C7-O7-C5
38	a	416	LHG	C8-C7-O7-C5
27	A	411	SQD	C9-C10-C11-C12
27	A	411	SQD	C11-C12-C13-C14
28	d	412	LMG	C13-C14-C15-C16
37	H	104	DGD	CBB-CCB-CDB-CEB
37	c	520	DGD	C2A-C3A-C4A-C5A
38	L	101	LHG	C30-C31-C32-C33
38	l	102	LHG	C31-C32-C33-C34
24	c	507	CLA	C16-C17-C18-C20
28	A	412	LMG	O6-C1-O1-C7
36	B	625	HTG	C3'-C4'-C5'-C6'
38	d	409	LHG	C27-C28-C29-C30
27	B	622	SQD	C10-C11-C12-C13
32	b	629	LMT	C7-C8-C9-C10
37	c	519	DGD	C5A-C6A-C7A-C8A
38	E	101	LHG	C18-C19-C20-C21
24	a	410	CLA	C15-C16-C17-C18
32	B	638	LMT	C2-C1-O1'-C1'
28	A	412	LMG	C17-C18-C19-C20
38	D	412	LHG	C27-C28-C29-C30
27	A	411	SQD	C14-C15-C16-C17
37	C	519	DGD	C9A-CAA-CBA-CCA

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Mol	Chain	Res	Type	Atoms
38	d	409	LHG	C30-C31-C32-C33
28	d	412	LMG	C14-C15-C16-C17
38	D	412	LHG	C15-C16-C17-C18
38	d	411	LHG	C29-C30-C31-C32
37	c	520	DGD	CBA-CCA-CDA-CEA
24	B	611	CLA	C2-C3-C5-C6
24	C	512	CLA	C2-C3-C5-C6
27	a	401	SQD	C10-C11-C12-C13
32	D	402	LMT	C2-C3-C4-C5
31	V	207	GOL	O1-C1-C2-O2
31	a	419	GOL	O2-C2-C3-O3
24	B	616	CLA	C8-C10-C11-C12
28	B	623	LMG	C30-C31-C32-C33
28	z	101	LMG	C14-C15-C16-C17
37	c	520	DGD	C9B-CAB-CBB-CCB
38	a	416	LHG	C24-C25-C26-C27
28	b	624	LMG	C31-C32-C33-C34
28	A	412	LMG	C19-C20-C21-C22
28	c	521	LMG	C30-C31-C32-C33
37	H	104	DGD	C7A-C8A-C9A-CAA
37	c	520	DGD	C6B-C7B-C8B-C9B
27	A	411	SQD	C13-C14-C15-C16
28	B	623	LMG	C39-C40-C41-C42
24	B	603	CLA	C2-C1-O2A-CGA
24	C	509	CLA	C2-C1-O2A-CGA
24	C	511	CLA	C2-C1-O2A-CGA
24	b	620	CLA	C2-C1-O2A-CGA
27	A	415	SQD	C15-C16-C17-C18
28	B	623	LMG	C15-C16-C17-C18
27	a	401	SQD	C9-C10-C11-C12
28	c	522	LMG	C37-C38-C39-C40
32	D	402	LMT	C6-C7-C8-C9
27	F	101	SQD	C23-C24-C25-C26
27	b	601	SQD	C23-C24-C25-C26
26	B	619	BCR	C1-C6-C7-C8
26	B	619	BCR	C5-C6-C7-C8
40	h	101	RRX	C5-C6-C7-C8
38	d	410	LHG	C32-C33-C34-C35
24	B	618	CLA	C13-C15-C16-C17
24	c	509	CLA	C5-C6-C7-C8
28	b	624	LMG	C34-C35-C36-C37
32	F	103	LMT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
32	b	626	LMT	C4-C5-C6-C7
28	B	623	LMG	C33-C34-C35-C36
24	b	618	CLA	C13-C15-C16-C17
24	C	508	CLA	C11-C12-C13-C15
24	C	515	CLA	C6-C7-C8-C10
24	a	413	CLA	C11-C12-C13-C15
24	b	605	CLA	C6-C7-C8-C10
24	b	620	CLA	C11-C12-C13-C15
24	c	506	CLA	C11-C12-C13-C15
24	c	513	CLA	C6-C7-C8-C10
36	u	201	HTG	S1-C1'-C2'-C3'
24	a	413	CLA	C16-C17-C18-C20
27	a	401	SQD	C31-C32-C33-C34
28	C	521	LMG	C39-C40-C41-C42
27	A	411	SQD	C33-C34-C35-C36
27	A	415	SQD	C31-C32-C33-C34
27	B	622	SQD	C28-C29-C30-C31
28	Z	101	LMG	C10-C11-C12-C13
28	d	412	LMG	C38-C39-C40-C41
38	E	101	LHG	C24-C23-O8-C6
32	f	801	LMT	C4'-C5'-C6'-O6'
27	f	802	SQD	O5-C1-O6-C44
28	B	623	LMG	C14-C15-C16-C17
38	d	409	LHG	C29-C30-C31-C32
28	B	623	LMG	C11-C10-O7-C8
28	c	521	LMG	C11-C10-O7-C8
28	i	101	LMG	C19-C20-C21-C22
24	C	505	CLA	C10-C11-C12-C13
28	B	623	LMG	O9-C10-O7-C8
32	D	409	LMT	C4-C5-C6-C7
37	C	519	DGD	C2E-C1E-O5D-C6D
24	b	619	CLA	C10-C11-C12-C13
32	B	638	LMT	O5B-C5B-C6B-O6B
37	d	416	DGD	C5B-C6B-C7B-C8B
32	a	421	LMT	C3-C4-C5-C6
37	c	520	DGD	C8B-C9B-CAB-CBB
24	B	611	CLA	C4-C3-C5-C6
28	C	533	LMG	C28-C29-C30-C31
36	B	629	HTG	C2'-C3'-C4'-C5'
38	E	101	LHG	C24-C25-C26-C27
24	B	605	CLA	C6-C7-C8-C9
24	C	508	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	b	605	CLA	C6-C7-C8-C9
24	c	506	CLA	C11-C12-C13-C14
28	i	101	LMG	C31-C32-C33-C34
32	F	103	LMT	C7-C8-C9-C10
32	M	101	LMT	O5B-C5B-C6B-O6B
27	B	622	SQD	C9-C10-C11-C12
37	C	519	DGD	C3B-C4B-C5B-C6B
24	A	409	CLA	C16-C17-C18-C20
24	C	504	CLA	C16-C17-C18-C19
24	a	413	CLA	C16-C17-C18-C19
24	c	507	CLA	C16-C17-C18-C19
28	c	521	LMG	O9-C10-O7-C8
24	b	617	CLA	C13-C15-C16-C17
38	a	416	LHG	C3-O3-P-O6
32	B	624	LMT	C3'-C4'-O1B-C1B
37	c	518	DGD	C3B-C4B-C5B-C6B
27	F	101	SQD	C33-C34-C35-C36
38	D	410	LHG	C26-C27-C28-C29
36	b	602	HTG	O5-C5-C6-O6
36	b	627	HTG	C2'-C3'-C4'-C5'
37	C	518	DGD	O6D-C5D-C6D-O5D
32	D	409	LMT	C2B-C1B-O1B-C4'
32	A	422	LMT	O5B-C5B-C6B-O6B
38	d	410	LHG	C1-C2-C3-O3
32	B	624	LMT	C5'-C4'-O1B-C1B
24	b	620	CLA	CBD-CGD-O2D-CED
28	i	101	LMG	C33-C34-C35-C36
27	a	415	SQD	O6-C44-C45-C46
28	z	101	LMG	O1-C7-C8-C9
37	d	416	DGD	C1G-C2G-C3G-O3G
28	C	533	LMG	C8-C7-O1-C1
37	C	519	DGD	C2G-C3G-O3G-C1D
37	c	519	DGD	C2G-C3G-O3G-C1D
37	c	519	DGD	C5D-C6D-O5D-C1E
38	L	101	LHG	C29-C30-C31-C32
37	C	519	DGD	CAA-CBA-CCA-CDA
37	H	104	DGD	CDA-CEA-CFA-CGA
37	C	518	DGD	O6E-C5E-C6E-O5E
38	E	101	LHG	O10-C23-O8-C6
37	c	519	DGD	C8B-C9B-CAB-CBB
37	C	519	DGD	C8A-C9A-CAA-CBA
36	H	101	HTG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
37	c	518	DGD	O6E-C5E-C6E-O5E
31	C	525	GOL	O1-C1-C2-O2
31	v	203	GOL	O1-C1-C2-O2
38	E	101	LHG	O1-C1-C2-O2
32	b	626	LMT	C9-C10-C11-C12
32	D	409	LMT	O5B-C1B-O1B-C4'
36	B	629	HTG	O5-C5-C6-O6
24	C	512	CLA	C4-C3-C5-C6
29	A	413	PL9	C15-C14-C16-C17
27	A	415	SQD	C23-C24-C25-C26
37	h	102	DGD	C7A-C8A-C9A-CAA
28	D	413	LMG	O6-C5-C6-O5
32	B	638	LMT	O5'-C5'-C6'-O6'
24	b	617	CLA	C15-C16-C17-C18
28	c	521	LMG	C40-C41-C42-C43
36	o	301	HTG	C2'-C3'-C4'-C5'
27	A	415	SQD	C35-C36-C37-C38
32	b	625	LMT	C4-C5-C6-C7
27	A	415	SQD	C34-C35-C36-C37
27	B	622	SQD	C24-C25-C26-C27
28	i	101	LMG	C16-C17-C18-C19
36	B	625	HTG	C1'-C2'-C3'-C4'
24	c	509	CLA	C10-C11-C12-C13
24	a	410	CLA	C2C-C3C-CAC-CBC
27	A	411	SQD	O6-C44-C45-O47
27	a	415	SQD	O6-C44-C45-O47
28	c	521	LMG	C15-C16-C17-C18
37	H	104	DGD	CDB-CEB-CFB-CGB
37	h	102	DGD	CBB-CCB-CDB-CEB
32	f	801	LMT	C4-C5-C6-C7
38	D	411	LHG	C14-C15-C16-C17
28	c	522	LMG	C28-C29-C30-C31
27	B	622	SQD	C30-C31-C32-C33
24	A	409	CLA	C12-C13-C15-C16
24	C	506	CLA	C12-C13-C15-C16
24	b	607	CLA	C6-C7-C8-C10
24	c	511	CLA	C11-C12-C13-C15
29	A	413	PL9	C13-C14-C16-C17
28	b	624	LMG	C36-C37-C38-C39
24	C	506	CLA	C14-C13-C15-C16
24	b	607	CLA	C6-C7-C8-C9
24	b	618	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
32	a	421	LMT	C5'-C4'-O1B-C1B
37	C	519	DGD	C2B-C3B-C4B-C5B
27	B	622	SQD	C24-C23-O48-C46
24	b	617	CLA	C10-C11-C12-C13
28	B	623	LMG	C16-C17-C18-C19
37	d	416	DGD	CDA-CEA-CFA-CGA
38	D	412	LHG	C10-C11-C12-C13
38	d	410	LHG	C11-C10-C9-C8
24	c	515	CLA	C10-C11-C12-C13
32	M	101	LMT	O1'-C1-C2-C3
28	B	623	LMG	C40-C41-C42-C43
28	D	413	LMG	C12-C13-C14-C15
37	c	519	DGD	C2B-C3B-C4B-C5B
38	a	416	LHG	C13-C14-C15-C16
29	a	417	PL9	C12-C11-C9-C10
24	C	511	CLA	C5-C6-C7-C8
27	A	415	SQD	C25-C26-C27-C28
27	b	601	SQD	C28-C29-C30-C31
38	d	411	LHG	C32-C33-C34-C35
28	D	413	LMG	C39-C40-C41-C42
28	b	624	LMG	C37-C38-C39-C40
37	h	102	DGD	C5B-C6B-C7B-C8B
32	D	409	LMT	C2-C1-O1'-C1'
32	M	101	LMT	C2-C1-O1'-C1'
27	a	415	SQD	C30-C31-C32-C33
24	c	506	CLA	C15-C16-C17-C18
27	A	411	SQD	O6-C44-C45-C46
27	B	622	SQD	C44-C45-C46-O48
27	a	401	SQD	O6-C44-C45-C46
27	b	601	SQD	C44-C45-C46-O48
28	B	623	LMG	C7-C8-C9-O8
38	a	416	LHG	C4-C5-C6-O8
37	C	518	DGD	C1B-C2B-C3B-C4B
38	a	416	LHG	C23-C24-C25-C26
24	B	612	CLA	C15-C16-C17-C18
28	c	522	LMG	C11-C12-C13-C14
37	C	519	DGD	C9B-CAB-CBB-CCB
37	H	104	DGD	C5B-C6B-C7B-C8B
31	C	525	GOL	O2-C2-C3-O3
31	b	639	GOL	O1-C1-C2-O2
27	F	101	SQD	C24-C25-C26-C27
37	C	519	DGD	C7A-C8A-C9A-CAA

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Mol	Chain	Res	Type	Atoms
24	A	409	CLA	C16-C17-C18-C19
37	h	102	DGD	O2G-C1B-C2B-C3B
27	a	401	SQD	C19-C20-C21-C22
28	C	521	LMG	C36-C37-C38-C39
32	f	801	LMT	C3-C4-C5-C6
38	L	101	LHG	C12-C13-C14-C15
28	c	522	LMG	O7-C8-C9-O8
24	a	409	CLA	C2C-C3C-CAC-CBC
28	C	533	LMG	C29-C30-C31-C32
24	b	609	CLA	C10-C11-C12-C13
38	a	416	LHG	C1-C2-C3-O3
27	b	601	SQD	C34-C35-C36-C37
36	b	602	HTG	C4'-C5'-C6'-C7'
24	B	603	CLA	C14-C13-C15-C16
24	b	620	CLA	C11-C10-C8-C9
24	c	506	CLA	C14-C13-C15-C16
32	a	402	LMT	C11-C10-C9-C8
28	z	101	LMG	C15-C16-C17-C18
27	a	401	SQD	C34-C35-C36-C37
24	b	614	CLA	C2A-CAA-CBA-CGA
24	b	618	CLA	C16-C17-C18-C20
26	C	517	BCR	C1-C6-C7-C8
26	C	517	BCR	C5-C6-C7-C8
26	D	407	BCR	C23-C24-C25-C26
26	D	407	BCR	C23-C24-C25-C30
26	d	407	BCR	C23-C24-C25-C26
26	d	407	BCR	C23-C24-C25-C30
28	c	521	LMG	C37-C38-C39-C40
28	i	101	LMG	C29-C30-C31-C32
28	i	101	LMG	C35-C36-C37-C38
32	A	422	LMT	C3-C4-C5-C6
38	l	102	LHG	C12-C13-C14-C15
36	C	523	HTG	S1-C1'-C2'-C3'
27	B	622	SQD	O10-C23-O48-C46
38	D	412	LHG	C25-C26-C27-C28
38	d	411	LHG	C28-C29-C30-C31
24	B	603	CLA	C6-C7-C8-C10
24	B	608	CLA	C11-C10-C8-C7
24	B	608	CLA	C11-C12-C13-C15
24	B	618	CLA	C11-C10-C8-C7
24	C	514	CLA	C11-C12-C13-C15
24	c	512	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
24	d	406	CLA	C11-C10-C8-C7
29	a	417	PL9	C12-C11-C9-C8
27	A	415	SQD	C27-C28-C29-C30
27	f	802	SQD	C31-C32-C33-C34
38	E	101	LHG	C19-C20-C21-C22
37	d	416	DGD	C2A-C1A-O1G-C1G
32	B	638	LMT	C5'-C4'-O1B-C1B
24	C	511	CLA	C10-C11-C12-C13
36	b	603	HTG	O5-C1-S1-C1'
24	B	603	CLA	CBA-CGA-O2A-C1
37	c	520	DGD	C3B-C4B-C5B-C6B
24	C	505	CLA	CAD-CBD-CGD-O2D
24	C	512	CLA	CAD-CBD-CGD-O2D
24	D	406	CLA	CAD-CBD-CGD-O2D
24	c	503	CLA	CAD-CBD-CGD-O2D
24	c	511	CLA	CAD-CBD-CGD-O2D
24	d	406	CLA	CAD-CBD-CGD-O2D
25	A	407	PHO	CAD-CBD-CGD-O2D
27	B	622	SQD	C46-C45-O47-C7
39	F	102	HEM	C2B-C3B-CAB-CBB
39	e	102	HEM	C2B-C3B-CAB-CBB
28	c	521	LMG	C16-C17-C18-C19
36	B	629	HTG	C4'-C5'-C6'-C7'
28	B	623	LMG	C17-C18-C19-C20
37	C	519	DGD	O6E-C1E-O5D-C6D
37	c	519	DGD	O6E-C1E-O5D-C6D
27	A	415	SQD	O6-C44-C45-C46
28	A	412	LMG	O1-C7-C8-C9
38	d	411	LHG	C2-C3-O3-P
24	B	603	CLA	O1A-CGA-O2A-C1
24	b	620	CLA	C15-C16-C17-C18
24	A	406	CLA	C16-C17-C18-C20
24	C	514	CLA	C16-C17-C18-C19
28	b	624	LMG	C16-C17-C18-C19
38	E	101	LHG	C1-C2-C3-O3
24	B	603	CLA	CHA-CBD-CGD-O1D
24	B	603	CLA	CHA-CBD-CGD-O2D
24	C	504	CLA	CHA-CBD-CGD-O1D
24	C	504	CLA	CHA-CBD-CGD-O2D
24	C	506	CLA	CHA-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	b	605	CLA	CHA-CBD-CGD-O1D
24	b	606	CLA	CHA-CBD-CGD-O1D
24	c	504	CLA	CHA-CBD-CGD-O1D
24	c	504	CLA	CHA-CBD-CGD-O2D
24	c	509	CLA	CHA-CBD-CGD-O1D
24	c	509	CLA	CHA-CBD-CGD-O2D
27	b	601	SQD	C2-C1-O6-C44
37	c	519	DGD	C2E-C1E-O5D-C6D
28	Z	101	LMG	C11-C12-C13-C14
37	c	520	DGD	C8A-C9A-CAA-CBA
27	B	622	SQD	O47-C45-C46-O48
27	b	601	SQD	O47-C45-C46-O48
28	Z	101	LMG	O1-C7-C8-O7
37	d	416	DGD	O2G-C2G-C3G-O3G
38	a	416	LHG	O7-C5-C6-O8
28	A	412	LMG	C35-C36-C37-C38
24	B	606	CLA	C13-C15-C16-C17
24	b	614	CLA	C8-C10-C11-C12
37	C	519	DGD	C6A-C7A-C8A-C9A
31	d	415	GOL	O1-C1-C2-O2
27	a	401	SQD	C11-C10-C9-C8
32	F	103	LMT	C2B-C1B-O1B-C4'
24	B	603	CLA	CAA-CBA-CGA-O2A
24	C	512	CLA	C6-C7-C8-C9
24	C	512	CLA	C8-C10-C11-C12
27	f	802	SQD	C5-C6-S-O8
37	d	416	DGD	O1A-C1A-O1G-C1G
26	K	101	BCR	C37-C22-C23-C24
26	K	101	BCR	C21-C22-C23-C24
37	h	102	DGD	CDB-CEB-CFB-CGB
27	F	101	SQD	C7-C8-C9-C10
37	C	518	DGD	C4D-C5D-C6D-O5D
37	c	519	DGD	C4A-C5A-C6A-C7A
24	B	607	CLA	C10-C11-C12-C13
38	D	412	LHG	C2-C3-O3-P
32	B	638	LMT	C3'-C4'-O1B-C1B
38	D	411	LHG	C4-O6-P-O4
38	a	416	LHG	C3-O3-P-O5
38	l	102	LHG	O6-C4-C5-C6
38	D	410	LHG	C29-C30-C31-C32
38	D	412	LHG	C28-C29-C30-C31
37	c	519	DGD	CAA-CBA-CCA-CDA

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Mol	Chain	Res	Type	Atoms
24	B	603	CLA	CAD-CBD-CGD-O1D
24	B	607	CLA	CAD-CBD-CGD-O1D
24	C	504	CLA	CAD-CBD-CGD-O1D
24	C	506	CLA	CAD-CBD-CGD-O1D
24	b	605	CLA	CAD-CBD-CGD-O1D
24	b	609	CLA	CAD-CBD-CGD-O1D
24	b	613	CLA	CAD-CBD-CGD-O1D
24	c	504	CLA	CAD-CBD-CGD-O1D
27	f	802	SQD	C5-C6-S-O9
28	C	521	LMG	C10-C11-C12-C13
37	c	518	DGD	O6D-C5D-C6D-O5D
27	f	802	SQD	C29-C30-C31-C32
28	d	412	LMG	C19-C20-C21-C22
32	A	422	LMT	C7-C8-C9-C10
24	D	406	CLA	C11-C10-C8-C7
24	b	608	CLA	C11-C10-C8-C7
24	c	506	CLA	C12-C13-C15-C16
36	B	626	HTG	C2-C1-S1-C1'
36	C	523	HTG	C2-C1-S1-C1'
36	b	628	HTG	C2-C1-S1-C1'
36	c	523	HTG	C2-C1-S1-C1'
28	B	623	LMG	C11-C12-C13-C14
24	C	511	CLA	C8-C10-C11-C12
28	C	521	LMG	C32-C33-C34-C35
36	c	524	HTG	C4-C5-C6-O6
28	A	412	LMG	O1-C7-C8-O7
28	z	101	LMG	O1-C7-C8-O7
28	i	101	LMG	C10-C11-C12-C13
28	i	101	LMG	C32-C33-C34-C35
37	C	520	DGD	C3B-C4B-C5B-C6B
37	C	519	DGD	C5D-C6D-O5D-C1E
32	B	624	LMT	O5B-C1B-O1B-C4'
32	b	625	LMT	C5-C6-C7-C8
24	b	614	CLA	C15-C16-C17-C18
24	B	603	CLA	C6-C7-C8-C9
24	B	608	CLA	C11-C10-C8-C9
24	c	508	CLA	C11-C10-C8-C9
24	c	511	CLA	C11-C12-C13-C14
24	d	406	CLA	C11-C10-C8-C9
27	b	601	SQD	C13-C14-C15-C16
24	b	618	CLA	C16-C17-C18-C19
32	b	629	LMT	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
28	Z	101	LMG	O7-C10-C11-C12
28	i	101	LMG	C36-C37-C38-C39
28	c	522	LMG	C38-C39-C40-C41
36	O	303	HTG	C3'-C4'-C5'-C6'
37	H	104	DGD	CCA-CDA-CEA-CFA
24	b	605	CLA	CAA-CBA-CGA-O2A
37	H	104	DGD	O2G-C1B-C2B-C3B
27	a	401	SQD	C16-C17-C18-C19
37	C	519	DGD	CBA-CCA-CDA-CEA
27	b	601	SQD	C46-C45-O47-C7
32	a	402	LMT	C1-C2-C3-C4
24	A	405	CLA	C2-C1-O2A-CGA
24	a	409	CLA	C2-C1-O2A-CGA
24	a	413	CLA	C2-C1-O2A-CGA
24	c	504	CLA	C2-C1-O2A-CGA
27	b	601	SQD	C24-C25-C26-C27
38	D	412	LHG	C9-C10-C11-C12
27	A	415	SQD	C24-C23-O48-C46
27	b	601	SQD	C24-C23-O48-C46
24	b	609	CLA	C4-C3-C5-C6
26	b	621	BCR	C1-C6-C7-C8
40	H	103	RRX	C23-C24-C25-C30
24	a	409	CLA	C4C-C3C-CAC-CBC
24	B	604	CLA	C16-C17-C18-C19
27	a	415	SQD	C8-C7-O47-C45
29	D	408	PL9	C39-C41-C42-C43
29	d	408	PL9	C39-C41-C42-C43
27	b	601	SQD	O10-C23-O48-C46
28	B	623	LMG	O7-C8-C9-O8
28	i	101	LMG	O1-C7-C8-O7
32	F	103	LMT	O5B-C1B-O1B-C4'
38	D	411	LHG	C3-O3-P-O6
38	a	416	LHG	C4-O6-P-O3
38	L	101	LHG	C16-C17-C18-C19
28	Z	101	LMG	O1-C7-C8-C9
24	C	512	CLA	C6-C7-C8-C10
24	a	411	CLA	C11-C10-C8-C7
24	b	617	CLA	C12-C13-C15-C16
36	b	627	HTG	C3'-C4'-C5'-C6'
24	A	409	CLA	C11-C10-C8-C9
24	D	406	CLA	C11-C10-C8-C9
24	a	411	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
38	E	101	LHG	C28-C29-C30-C31
28	Z	101	LMG	C29-C28-O8-C9
38	d	411	LHG	O1-C1-C2-C3
28	C	521	LMG	C21-C22-C23-C24
28	D	413	LMG	C18-C19-C20-C21
28	i	101	LMG	C20-C21-C22-C23
37	c	519	DGD	C8A-C9A-CAA-CBA
29	a	417	PL9	C15-C14-C16-C17
32	M	101	LMT	O5'-C5'-C6'-O6'
24	b	609	CLA	C2-C3-C5-C6
25	a	412	PHO	C2-C3-C5-C6
32	D	402	LMT	C1-C2-C3-C4
37	C	518	DGD	C2A-C3A-C4A-C5A
39	e	102	HEM	CAD-CBD-CGD-O1D
28	C	533	LMG	C4-C5-C6-O5
27	b	601	SQD	C12-C13-C14-C15
24	b	620	CLA	O1D-CGD-O2D-CED
32	b	625	LMT	C7-C8-C9-C10
24	B	610	CLA	C13-C15-C16-C17
36	b	628	HTG	C4-C5-C6-O6
32	D	402	LMT	C9-C10-C11-C12
37	H	104	DGD	C9A-CAA-CBA-CCA
38	L	101	LHG	O6-C4-C5-C6
24	c	513	CLA	O1A-CGA-O2A-C1
27	A	415	SQD	O10-C23-O48-C46
32	a	421	LMT	O1'-C1-C2-C3
32	B	638	LMT	C9-C10-C11-C12
37	c	520	DGD	O1A-C1A-O1G-C1G
24	D	406	CLA	C4-C3-C5-C6
37	c	518	DGD	C4D-C5D-C6D-O5D
24	B	613	CLA	C2-C3-C5-C6
24	b	613	CLA	C2-C3-C5-C6
24	c	512	CLA	C2-C3-C5-C6
29	a	417	PL9	C13-C14-C16-C17
24	C	514	CLA	O1A-CGA-O2A-C1
27	F	101	SQD	C30-C31-C32-C33
27	f	802	SQD	C24-C25-C26-C27
38	E	101	LHG	C9-C10-C11-C12
37	C	518	DGD	CDA-CEA-CFA-CGA
38	l	102	LHG	C16-C17-C18-C19
24	D	405	CLA	C2-C1-O2A-CGA
24	a	413	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	B	612	CLA	C2A-CAA-CBA-CGA
38	E	101	LHG	O7-C5-C6-O8
24	B	611	CLA	C3A-C2A-CAA-CBA
24	a	410	CLA	C4C-C3C-CAC-CBC
37	d	416	DGD	CAA-CBA-CCA-CDA
39	F	102	HEM	CAD-CBD-CGD-O1D
25	a	412	PHO	C4-C3-C5-C6
29	a	417	PL9	C25-C24-C26-C27
32	f	801	LMT	O5'-C5'-C6'-O6'
24	a	413	CLA	C14-C13-C15-C16
24	b	620	CLA	C6-C7-C8-C9
24	c	511	CLA	O1A-CGA-O2A-C1
28	A	412	LMG	C7-C8-C9-O8
28	c	522	LMG	C7-C8-C9-O8
28	Z	101	LMG	O10-C28-O8-C9
37	H	104	DGD	C9B-CAB-CBB-CCB
24	B	606	CLA	O2A-C1-C2-C3
27	A	415	SQD	O5-C1-O6-C44
27	a	401	SQD	O5-C1-O6-C44
38	D	412	LHG	C31-C32-C33-C34
27	A	415	SQD	C14-C15-C16-C17
28	c	521	LMG	C29-C30-C31-C32
39	e	102	HEM	CAA-CBA-CGA-O1A
42	V	201	HEC	CAD-CBD-CGD-O1D
42	v	201	HEC	CAD-CBD-CGD-O1D
24	A	409	CLA	C11-C10-C8-C7
24	a	411	CLA	C12-C13-C15-C16
24	c	507	CLA	C2-C3-C5-C6
27	A	411	SQD	C7-C8-C9-C10
37	d	416	DGD	C9A-CAA-CBA-CCA
24	C	503	CLA	C2A-CAA-CBA-CGA
37	H	104	DGD	CAA-CBA-CCA-CDA
37	c	520	DGD	C7B-C8B-C9B-CAB
37	c	520	DGD	C2A-C1A-O1G-C1G
27	B	622	SQD	C11-C10-C9-C8
27	A	411	SQD	C25-C26-C27-C28
32	b	625	LMT	C3-C4-C5-C6
38	D	412	LHG	C24-C25-C26-C27
39	F	102	HEM	CAD-CBD-CGD-O2D
28	C	521	LMG	C33-C34-C35-C36
39	e	102	HEM	CAD-CBD-CGD-O2D
28	C	521	LMG	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
28	c	521	LMG	C39-C40-C41-C42
24	C	514	CLA	C8-C10-C11-C12
24	b	606	CLA	C13-C15-C16-C17
28	z	101	LMG	C10-C11-C12-C13
27	A	415	SQD	C2-C1-O6-C44
37	H	104	DGD	O1G-C1G-C2G-O2G
27	b	601	SQD	C31-C32-C33-C34
28	c	522	LMG	C17-C18-C19-C20
39	e	102	HEM	CAA-CBA-CGA-O2A
24	b	619	CLA	C16-C17-C18-C19
29	a	417	PL9	C19-C21-C22-C23
24	d	405	CLA	C2-C1-O2A-CGA
42	v	201	HEC	CAD-CBD-CGD-O2D
24	B	605	CLA	C11-C12-C13-C14
28	D	413	LMG	C16-C17-C18-C19
28	A	412	LMG	O8-C28-C29-C30
24	b	614	CLA	C16-C17-C18-C19
42	V	201	HEC	CAD-CBD-CGD-O2D
24	C	515	CLA	C3-C5-C6-C7
26	c	516	BCR	C1-C6-C7-C8
26	c	517	BCR	C1-C6-C7-C8
37	C	520	DGD	C8B-C9B-CAB-CBB
28	i	101	LMG	O1-C7-C8-C9
37	c	520	DGD	C1B-C2B-C3B-C4B
24	c	512	CLA	C4-C3-C5-C6
24	c	515	CLA	C4-C3-C5-C6
26	k	102	BCR	C21-C22-C23-C24
38	D	412	LHG	C11-C10-C9-C8
25	A	407	PHO	C2-C3-C5-C6
37	C	519	DGD	C5B-C6B-C7B-C8B
37	c	518	DGD	C5D-C6D-O5D-C1E
28	Z	101	LMG	C18-C19-C20-C21
24	B	604	CLA	C16-C17-C18-C20
24	b	619	CLA	C16-C17-C18-C20
28	i	101	LMG	C40-C41-C42-C43
38	E	101	LHG	O6-C4-C5-O7
24	C	505	CLA	C5-C6-C7-C8
24	b	609	CLA	C13-C15-C16-C17
27	a	415	SQD	C10-C11-C12-C13
24	b	613	CLA	C4-C3-C5-C6
38	D	410	LHG	C25-C26-C27-C28
24	B	608	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	a	411	CLA	C6-C7-C8-C10
24	c	508	CLA	C11-C10-C8-C7
24	b	606	CLA	C8-C10-C11-C12
36	B	626	HTG	S1-C1'-C2'-C3'
31	A	418	GOL	O2-C2-C3-O3
27	a	401	SQD	C11-C12-C13-C14
27	a	401	SQD	C2-C1-O6-C44
24	b	614	CLA	C16-C17-C18-C20
28	c	522	LMG	C30-C31-C32-C33
37	C	520	DGD	CBA-CCA-CDA-CEA
32	D	409	LMT	C7-C8-C9-C10
37	h	102	DGD	O1G-C1G-C2G-O2G
32	A	422	LMT	C9-C10-C11-C12
27	b	601	SQD	C18-C19-C20-C21
27	f	802	SQD	C30-C31-C32-C33
38	d	411	LHG	C14-C15-C16-C17
24	c	505	CLA	C2A-CAA-CBA-CGA
36	c	523	HTG	O5-C1-S1-C1'
37	C	518	DGD	C3A-C4A-C5A-C6A
28	b	624	LMG	O8-C28-C29-C30
24	B	603	CLA	C4-C3-C5-C6
24	D	406	CLA	C10-C11-C12-C13
24	c	515	CLA	C2-C3-C5-C6
38	E	101	LHG	C15-C16-C17-C18
24	B	613	CLA	C11-C12-C13-C14
24	b	608	CLA	C11-C10-C8-C9
24	b	617	CLA	C11-C12-C13-C14
24	c	504	CLA	C14-C13-C15-C16
24	c	514	CLA	CAA-CBA-CGA-O2A
24	B	606	CLA	CAD-CBD-CGD-O2D
24	B	612	CLA	CAD-CBD-CGD-O2D
24	C	503	CLA	CAD-CBD-CGD-O2D
24	C	508	CLA	CAD-CBD-CGD-O2D
24	b	608	CLA	CAD-CBD-CGD-O2D
24	b	614	CLA	CAD-CBD-CGD-O2D
24	b	616	CLA	CAD-CBD-CGD-O2D
24	b	620	CLA	CAD-CBD-CGD-O2D
24	c	505	CLA	CAD-CBD-CGD-O2D
24	c	514	CLA	CAD-CBD-CGD-O2D
25	a	412	PHO	CAD-CBD-CGD-O2D
28	c	521	LMG	C20-C21-C22-C23
27	a	415	SQD	O49-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
27	B	622	SQD	C27-C28-C29-C30
28	c	521	LMG	C12-C13-C14-C15
37	C	518	DGD	O2G-C1B-C2B-C3B
40	h	101	RRX	C6-C7-C8-C9
29	A	413	PL9	C45-C44-C46-C47
24	c	512	CLA	C8-C10-C11-C12
24	B	603	CLA	C2-C3-C5-C6
38	a	416	LHG	O8-C23-C24-C25
25	d	401	PHO	C2C-C3C-CAC-CBC
37	c	519	DGD	CDB-CEB-CFB-CGB
28	c	521	LMG	O7-C10-C11-C12
37	c	520	DGD	O1G-C1A-C2A-C3A
24	D	405	CLA	C2C-C3C-CAC-CBC
37	d	416	DGD	C6A-C7A-C8A-C9A
28	c	521	LMG	C17-C18-C19-C20
28	c	522	LMG	C36-C37-C38-C39
24	B	615	CLA	O2A-C1-C2-C3
24	b	606	CLA	O2A-C1-C2-C3
24	b	608	CLA	O2A-C1-C2-C3
25	a	412	PHO	O2A-C1-C2-C3
39	F	102	HEM	C4B-C3B-CAB-CBB
39	e	102	HEM	C4B-C3B-CAB-CBB
37	d	416	DGD	C7B-C8B-C9B-CAB
24	D	401	CLA	C2C-C3C-CAC-CBC
28	A	412	LMG	C22-C23-C24-C25
24	B	604	CLA	CHA-CBD-CGD-O1D
24	B	604	CLA	CHA-CBD-CGD-O2D
24	C	511	CLA	CHA-CBD-CGD-O1D
24	D	401	CLA	CHA-CBD-CGD-O1D
24	D	401	CLA	CHA-CBD-CGD-O2D
24	a	410	CLA	CHA-CBD-CGD-O2D
24	b	605	CLA	CHA-CBD-CGD-O2D
24	b	606	CLA	CHA-CBD-CGD-O2D
24	b	610	CLA	CHA-CBD-CGD-O1D
24	b	616	CLA	CHA-CBD-CGD-O1D
24	C	514	CLA	CAA-CBA-CGA-O2A
28	b	624	LMG	C17-C18-C19-C20
32	m	103	LMT	O5B-C5B-C6B-O6B
28	B	623	LMG	C35-C36-C37-C38
38	D	410	LHG	C7-C8-C9-C10
37	c	518	DGD	O1A-C1A-O1G-C1G
32	M	102	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
32	B	624	LMT	C2B-C1B-O1B-C4'
37	C	519	DGD	O6D-C5D-C6D-O5D
24	C	509	CLA	C2A-CAA-CBA-CGA
32	b	626	LMT	O5B-C1B-O1B-C4'
27	a	415	SQD	C7-C8-C9-C10
24	a	410	CLA	C11-C10-C8-C7
24	c	512	CLA	C11-C10-C8-C7
24	b	606	CLA	C15-C16-C17-C18
24	C	509	CLA	C11-C10-C8-C9
24	a	410	CLA	C11-C10-C8-C9
24	a	411	CLA	C11-C10-C8-C9
32	F	103	LMT	C3-C4-C5-C6
32	m	103	LMT	C4B-C5B-C6B-O6B
24	C	514	CLA	CBA-CGA-O2A-C1
37	c	520	DGD	C2B-C3B-C4B-C5B
27	A	411	SQD	C10-C11-C12-C13
24	c	503	CLA	C2A-CAA-CBA-CGA
24	c	514	CLA	CAA-CBA-CGA-O1A
24	A	405	CLA	C2C-C3C-CAC-CBC
31	D	417	GOL	C1-C2-C3-O3
38	E	101	LHG	C13-C14-C15-C16
24	c	508	CLA	C15-C16-C17-C18
37	C	520	DGD	CAA-CBA-CCA-CDA
24	c	505	CLA	C1A-C2A-CAA-CBA
36	u	201	HTG	C4'-C5'-C6'-C7'
37	c	520	DGD	O1A-C1A-C2A-C3A
24	c	515	CLA	C2-C1-O2A-CGA
36	u	201	HTG	C2'-C3'-C4'-C5'
24	B	617	CLA	C5-C6-C7-C8
28	c	521	LMG	O9-C10-C11-C12
38	a	416	LHG	O10-C23-C24-C25
28	c	521	LMG	O1-C7-C8-C9
37	C	518	DGD	CAB-CBB-CCB-CDB
28	A	412	LMG	C40-C41-C42-C43
28	b	624	LMG	C29-C30-C31-C32
28	c	521	LMG	C21-C22-C23-C24
24	A	405	CLA	C16-C17-C18-C19
24	B	605	CLA	C5-C6-C7-C8
24	b	619	CLA	C5-C6-C7-C8
24	A	405	CLA	C4C-C3C-CAC-CBC
32	m	103	LMT	C3-C4-C5-C6
28	A	412	LMG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
25	A	407	PHO	C4-C3-C5-C6
37	C	518	DGD	O1B-C1B-C2B-C3B
32	D	409	LMT	C1-C2-C3-C4
38	D	411	LHG	C3-O3-P-O5
38	d	410	LHG	C4-O6-P-O5
32	F	103	LMT	C6-C7-C8-C9
37	C	518	DGD	O6E-C1E-O5D-C6D
40	H	103	RRX	C11-C10-C9-C34
38	D	411	LHG	C12-C13-C14-C15
37	c	519	DGD	C9A-CAA-CBA-CCA
28	c	521	LMG	C36-C37-C38-C39
37	h	102	DGD	O1B-C1B-C2B-C3B
32	a	402	LMT	C6-C7-C8-C9
37	c	518	DGD	C4A-C5A-C6A-C7A
24	B	605	CLA	CAD-CBD-CGD-O1D
24	B	609	CLA	CAD-CBD-CGD-O1D
24	B	611	CLA	CAD-CBD-CGD-O1D
24	B	613	CLA	CAD-CBD-CGD-O1D
24	C	508	CLA	CAD-CBD-CGD-O1D
24	b	611	CLA	CAD-CBD-CGD-O1D
24	b	616	CLA	CAD-CBD-CGD-O1D
24	c	506	CLA	CAD-CBD-CGD-O1D
24	c	508	CLA	CAD-CBD-CGD-O1D
27	B	622	SQD	O5-C5-C6-S
27	B	622	SQD	C5-C6-S-O7
27	f	802	SQD	O5-C5-C6-S
24	c	514	CLA	O1A-CGA-O2A-C1
24	C	512	CLA	CAA-CBA-CGA-O2A
24	A	406	CLA	C14-C13-C15-C16
24	B	617	CLA	C14-C13-C15-C16
24	C	511	CLA	C14-C13-C15-C16
24	C	514	CLA	C11-C10-C8-C9
24	a	411	CLA	C14-C13-C15-C16
24	b	609	CLA	C11-C12-C13-C14
31	b	639	GOL	O2-C2-C3-O3
37	C	519	DGD	O2G-C1B-C2B-C3B
38	D	410	LHG	O8-C23-C24-C25
28	b	624	LMG	C35-C36-C37-C38
28	B	623	LMG	C29-C30-C31-C32
37	c	518	DGD	CAA-CBA-CCA-CDA
38	D	412	LHG	C19-C20-C21-C22
28	z	101	LMG	C19-C20-C21-C22

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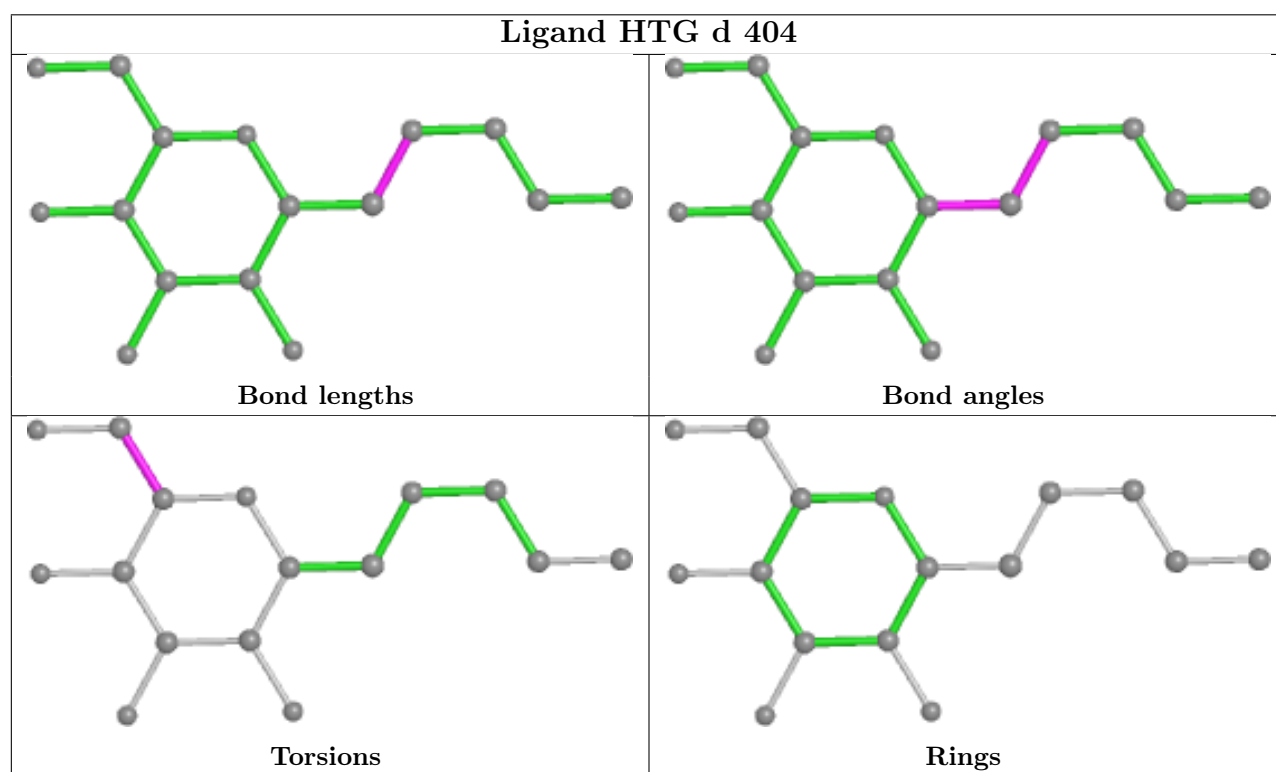
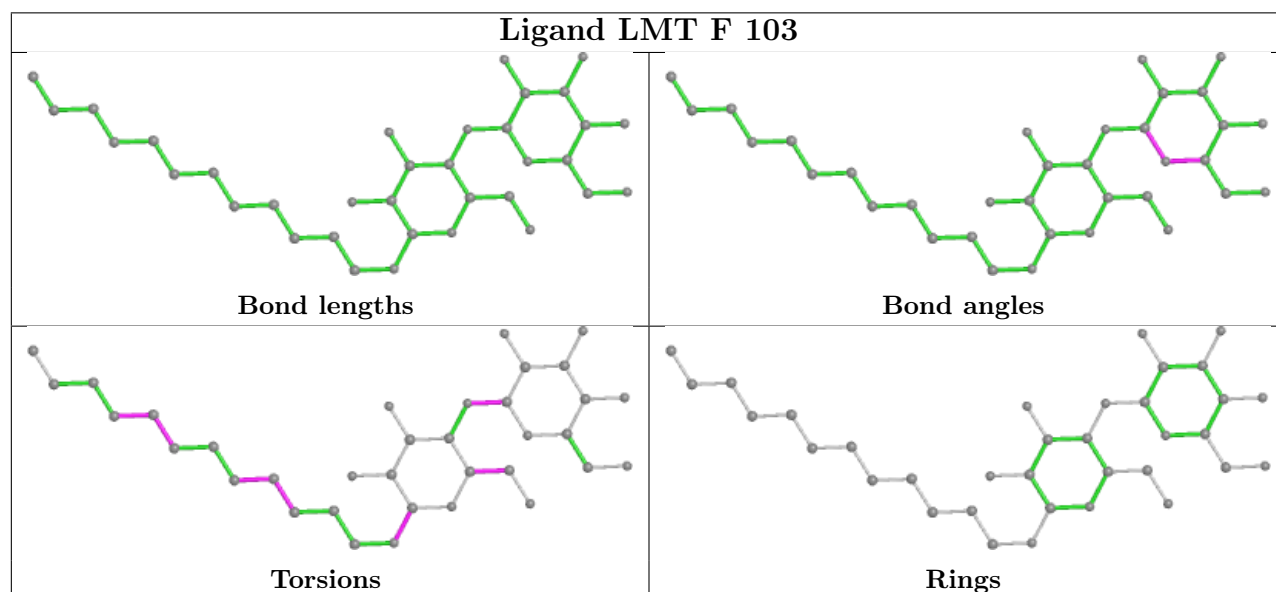
Mol	Chain	Res	Type	Atoms
24	c	507	CLA	CAA-CBA-CGA-O2A
38	E	101	LHG	O8-C23-C24-C25
24	c	506	CLA	C8-C10-C11-C12
28	D	413	LMG	C19-C20-C21-C22
24	A	406	CLA	C12-C13-C15-C16
24	B	605	CLA	C11-C12-C13-C15
24	B	612	CLA	C11-C10-C8-C7
24	B	613	CLA	C11-C10-C8-C7
24	B	613	CLA	C11-C12-C13-C15
24	B	615	CLA	C12-C13-C15-C16
24	B	617	CLA	C12-C13-C15-C16
24	C	514	CLA	C11-C10-C8-C7
24	b	608	CLA	C11-C12-C13-C15
24	b	609	CLA	C11-C12-C13-C15
24	b	610	CLA	C12-C13-C15-C16
24	b	618	CLA	C11-C10-C8-C7
29	a	417	PL9	C23-C24-C26-C27
37	H	104	DGD	C6B-C7B-C8B-C9B
38	E	101	LHG	O10-C23-C24-C25
32	b	629	LMT	C2-C1-O1'-C1'
32	B	624	LMT	O5'-C1'-O1'-C1
38	D	412	LHG	C13-C14-C15-C16
38	a	416	LHG	C18-C19-C20-C21
24	b	612	CLA	C13-C15-C16-C17
24	c	503	CLA	CAA-CBA-CGA-O2A
38	L	101	LHG	O7-C7-C8-C9
24	B	607	CLA	C13-C15-C16-C17
24	C	514	CLA	CAA-CBA-CGA-O1A
28	i	101	LMG	O7-C10-C11-C12

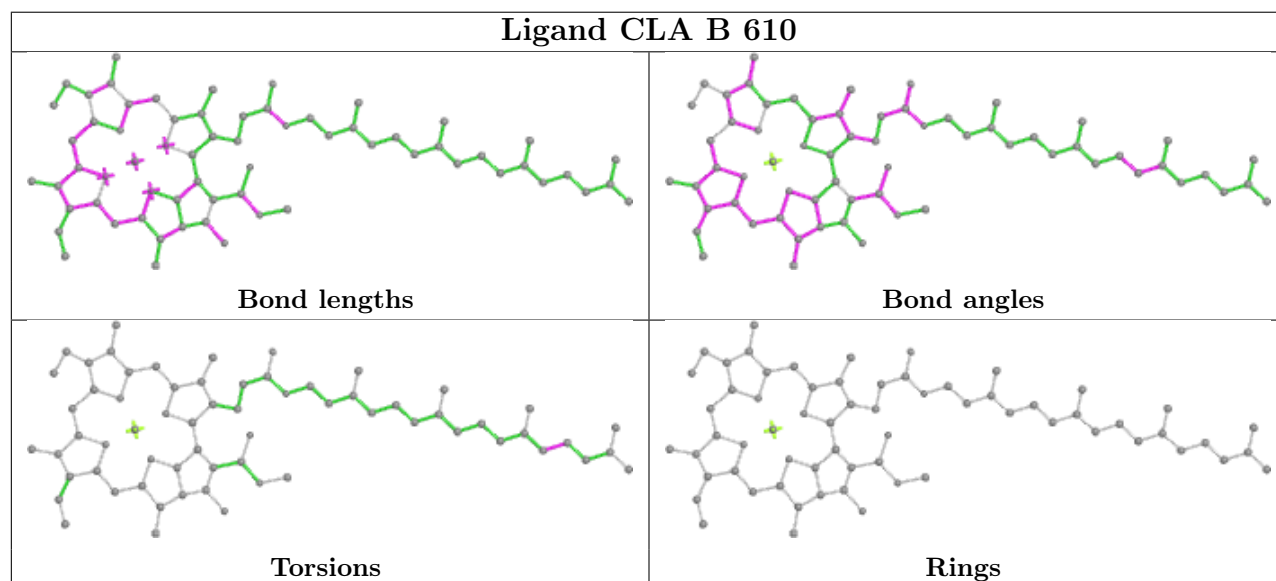
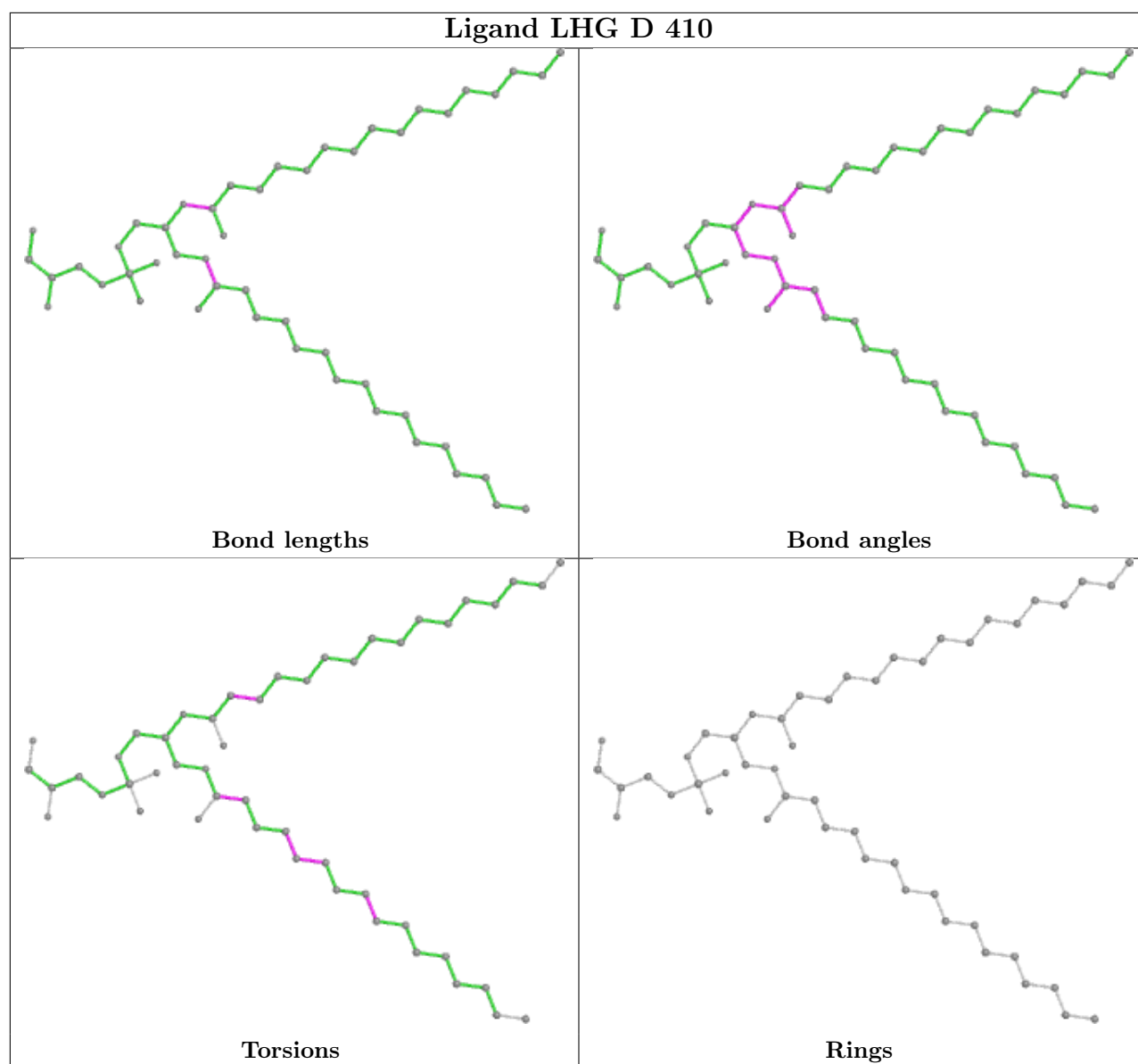
There are no ring outliers.

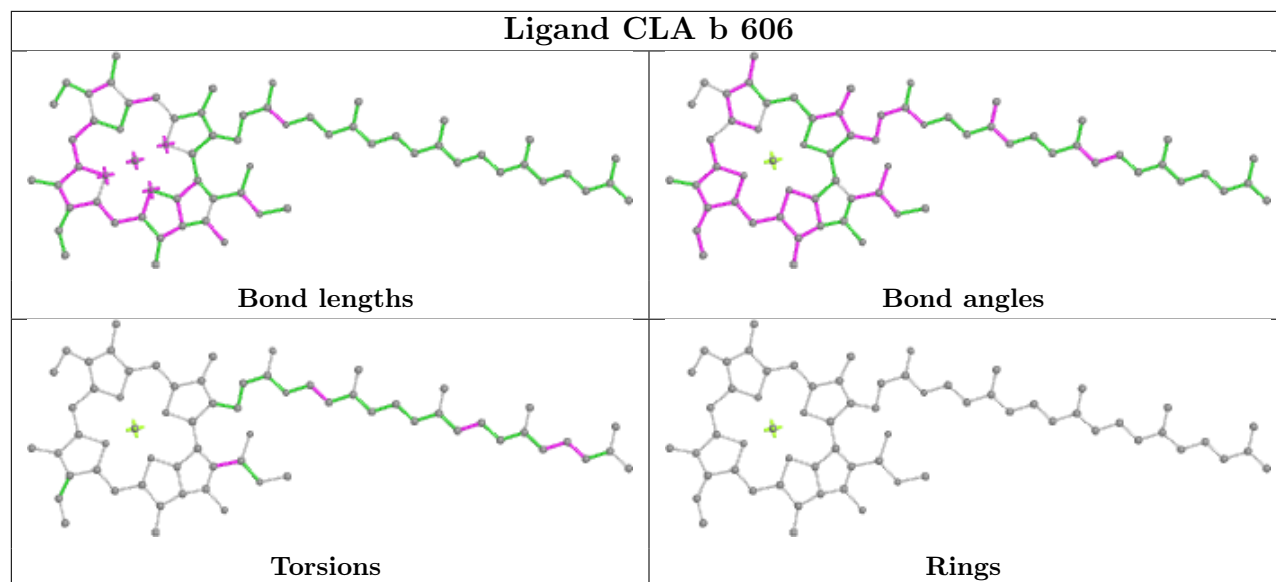
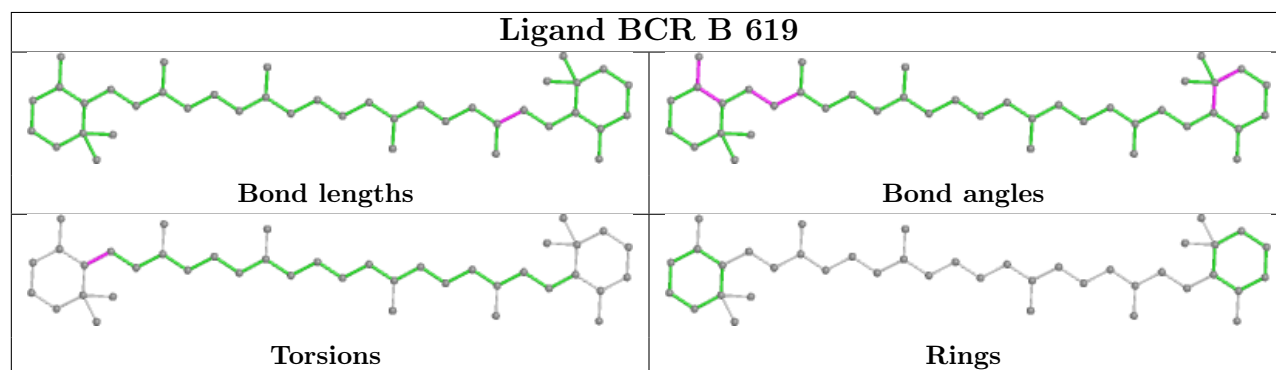
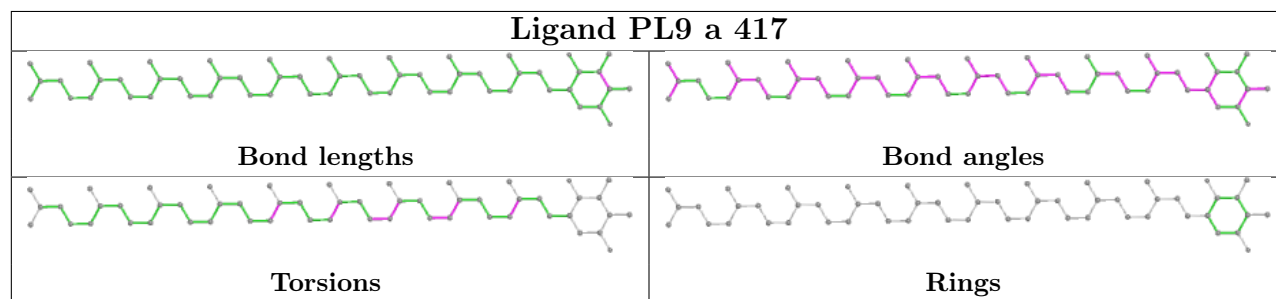
No monomer is involved in short contacts.

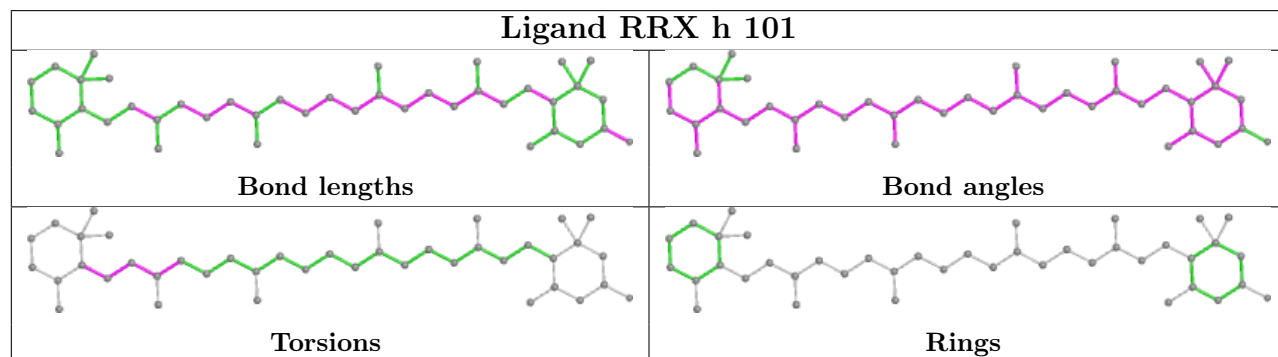
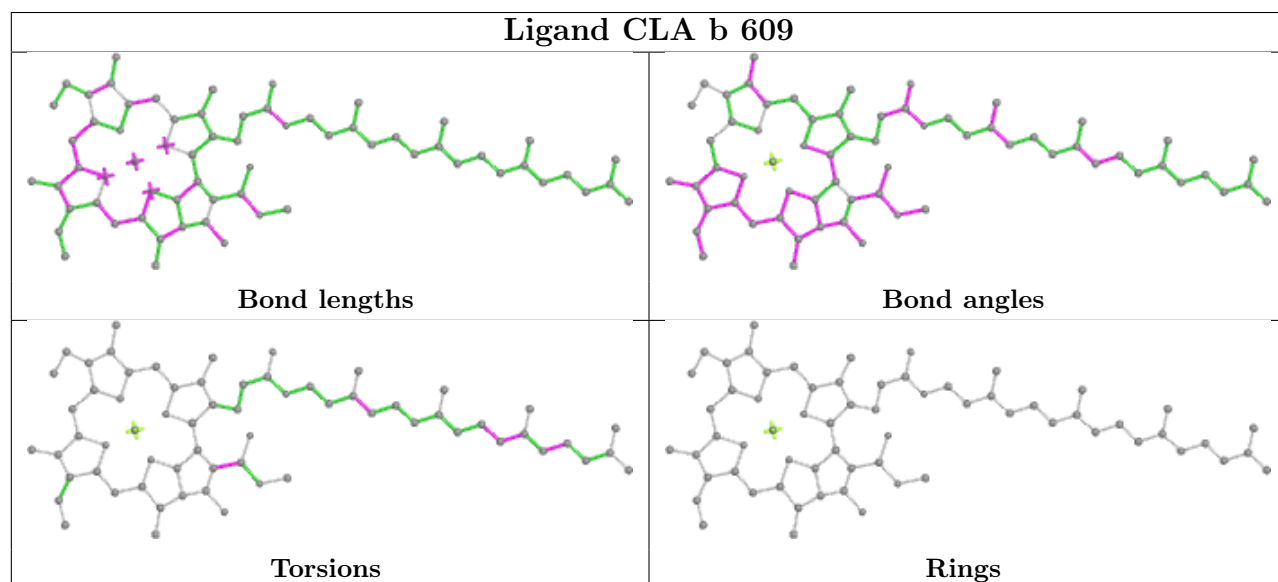
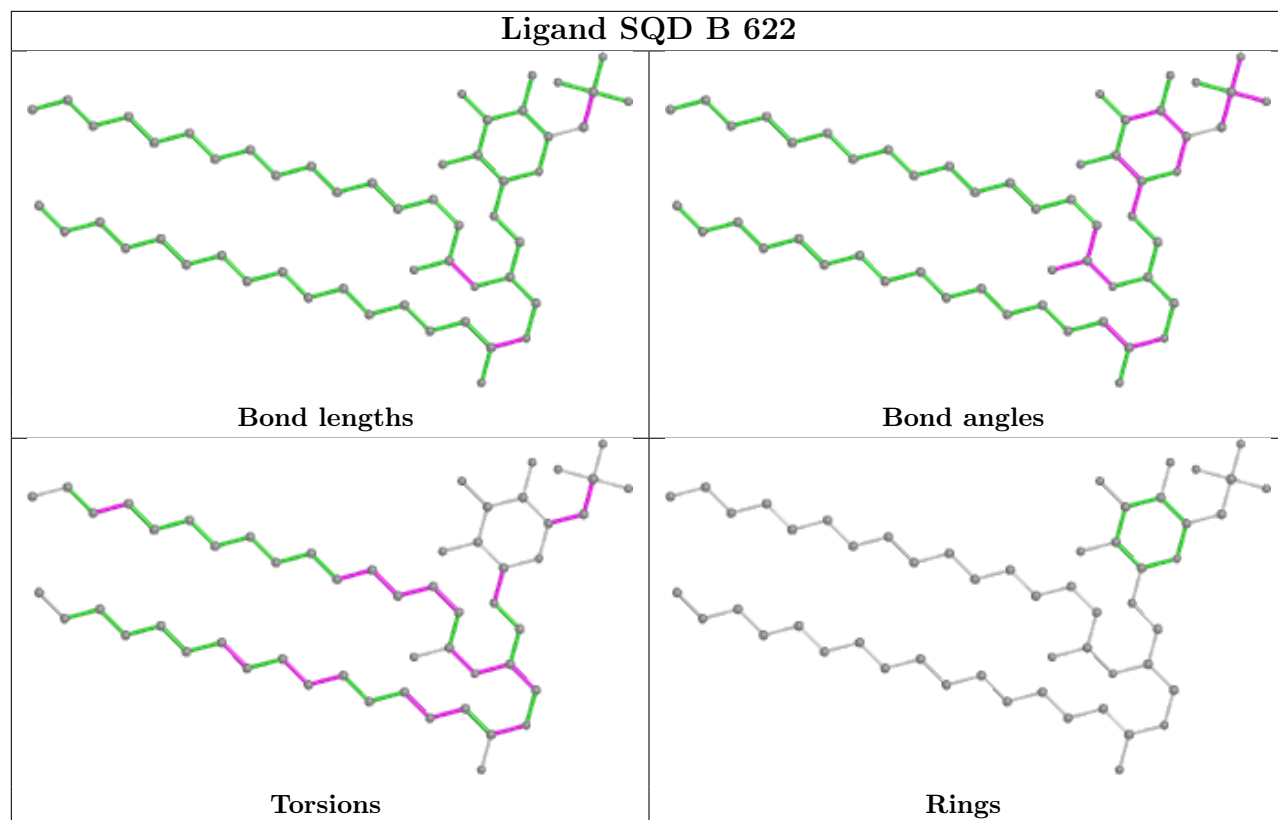
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

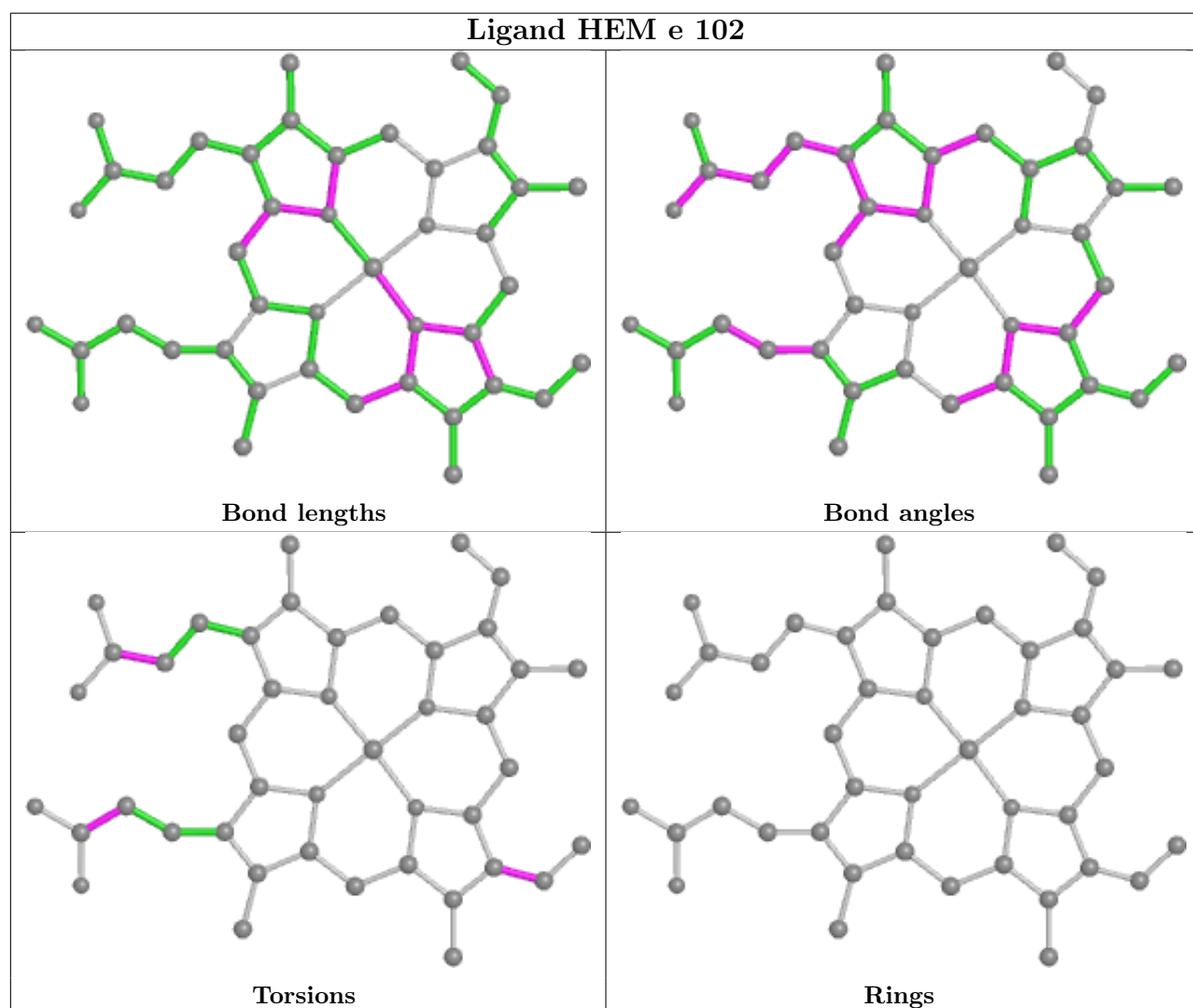
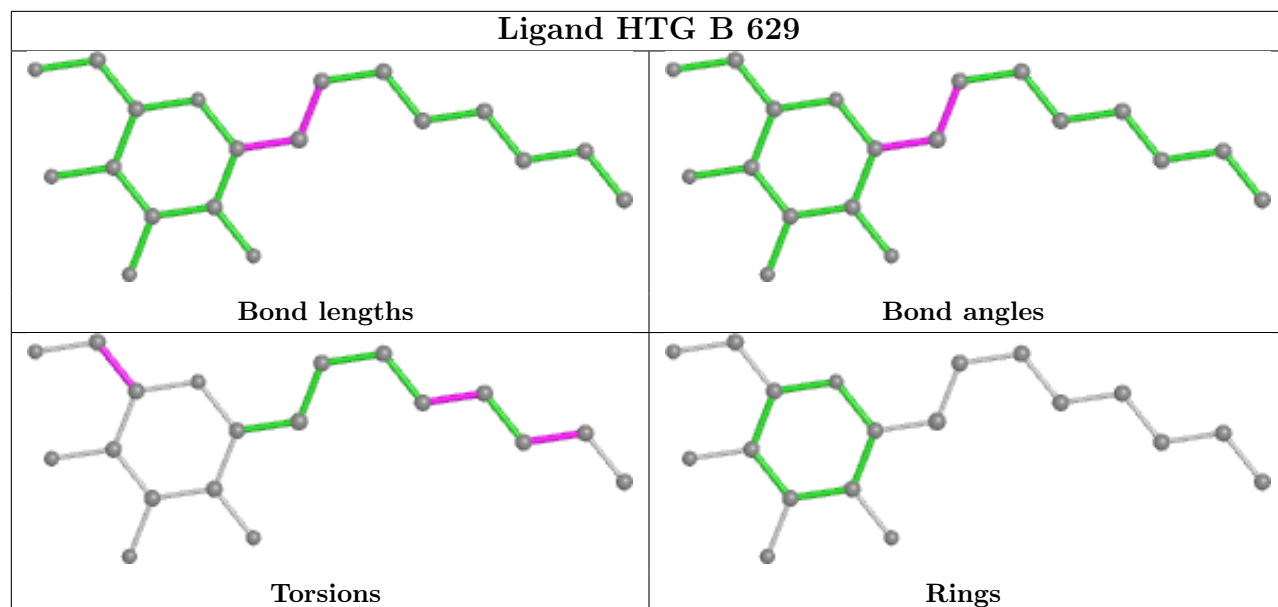
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



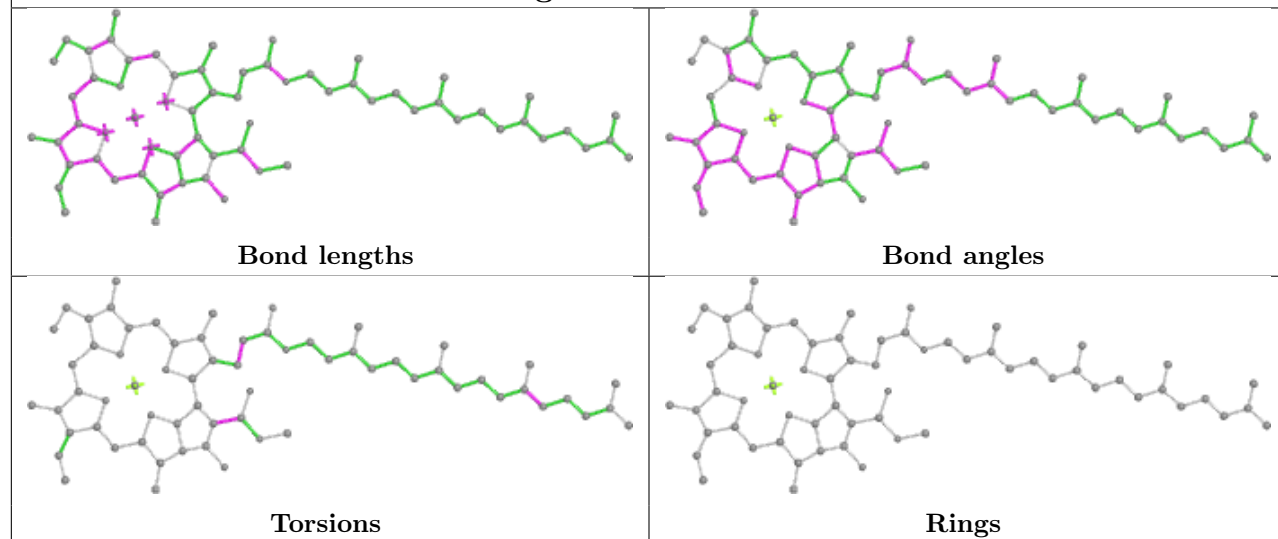


Ligand CLA b 606**Ligand BCR B 619****Ligand PL9 a 417**

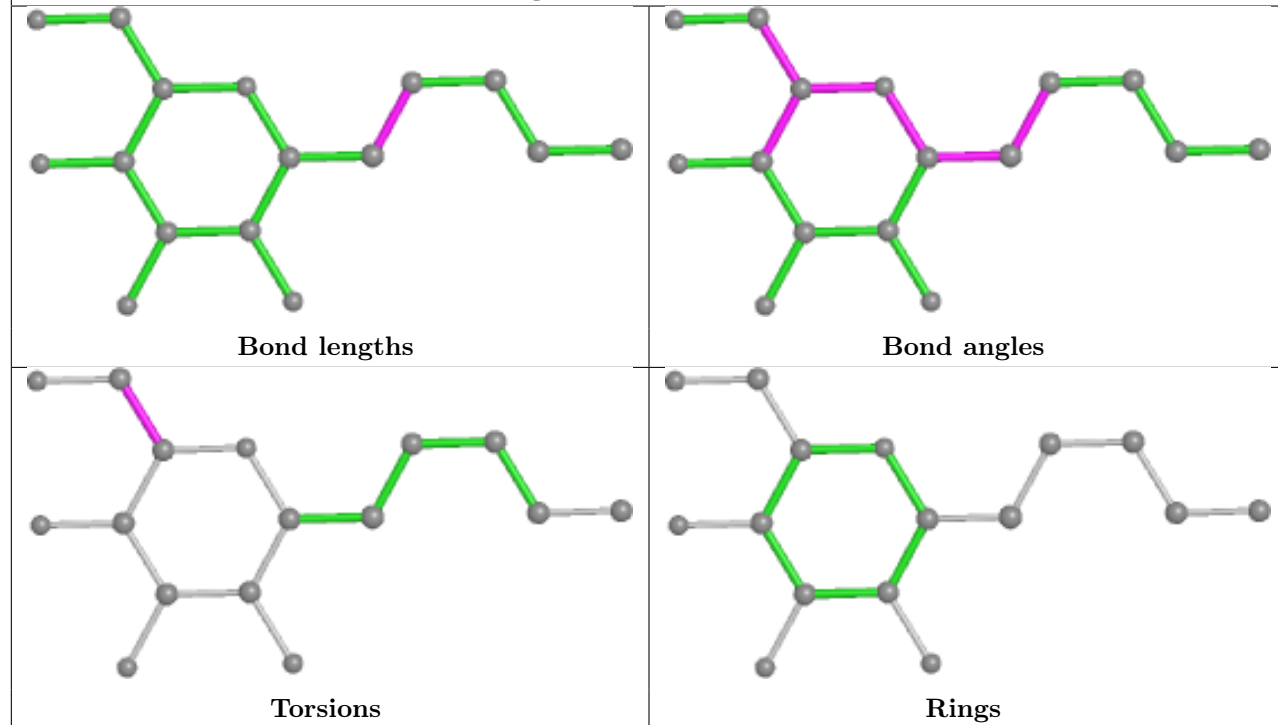


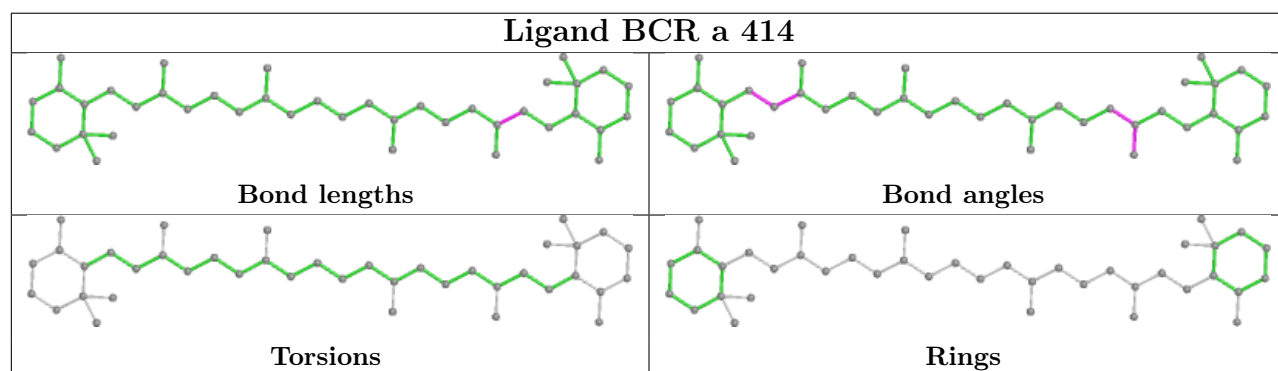
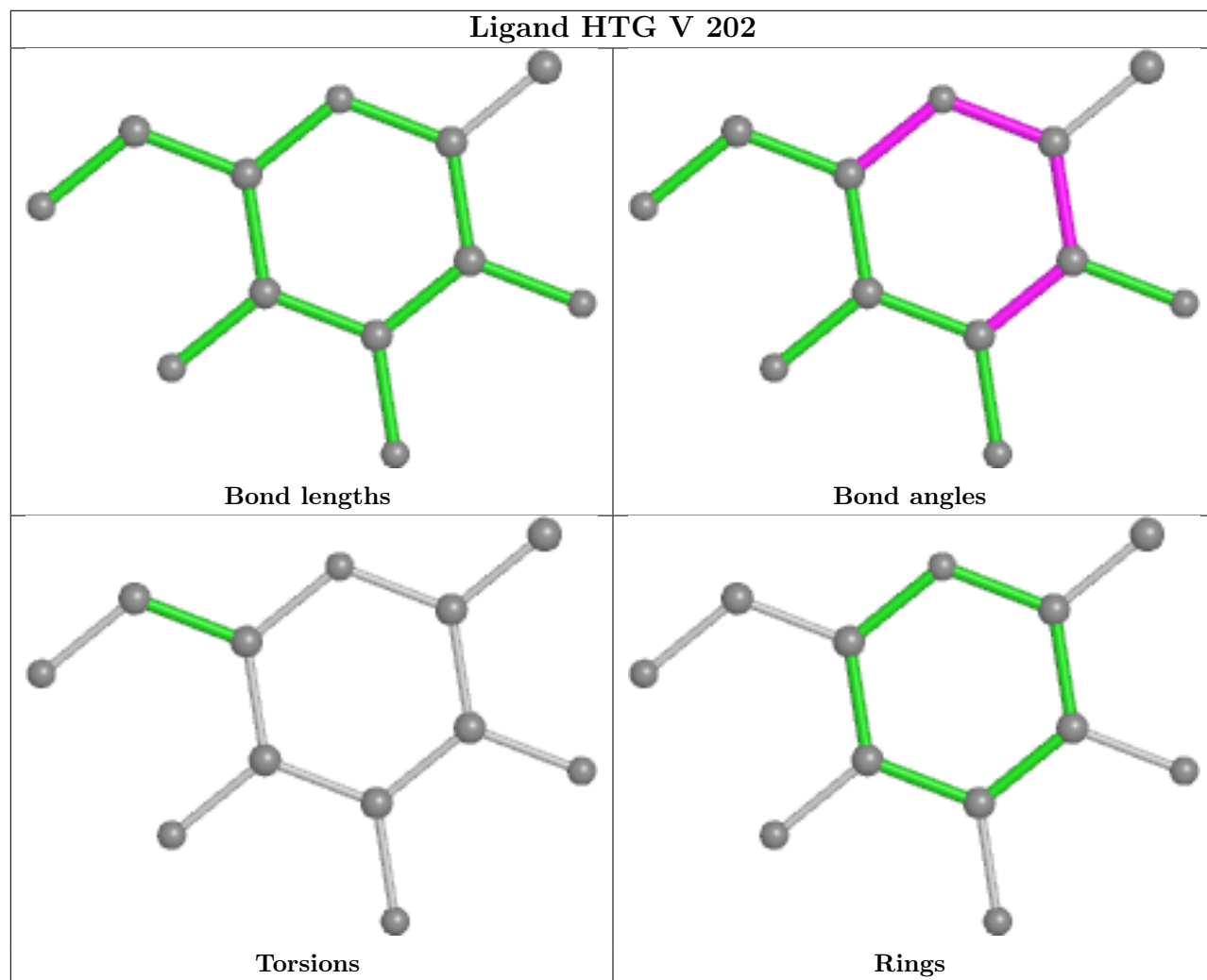


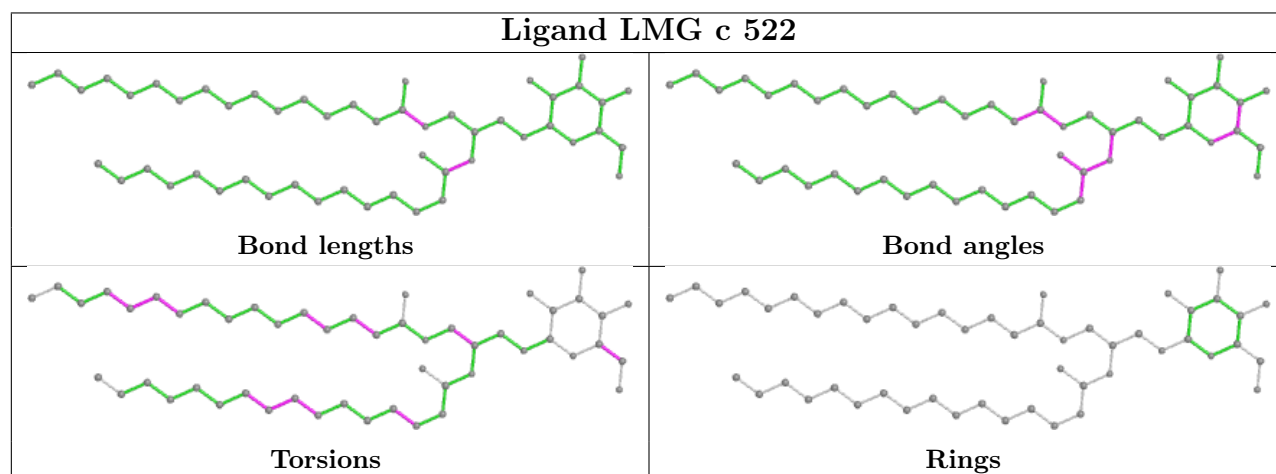
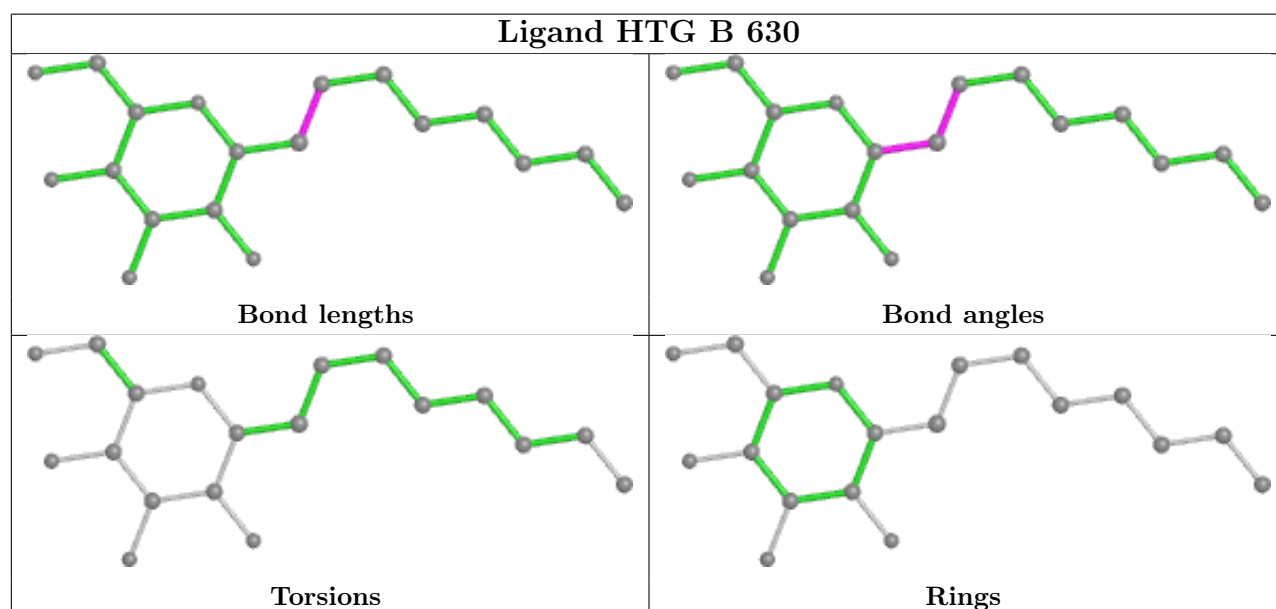
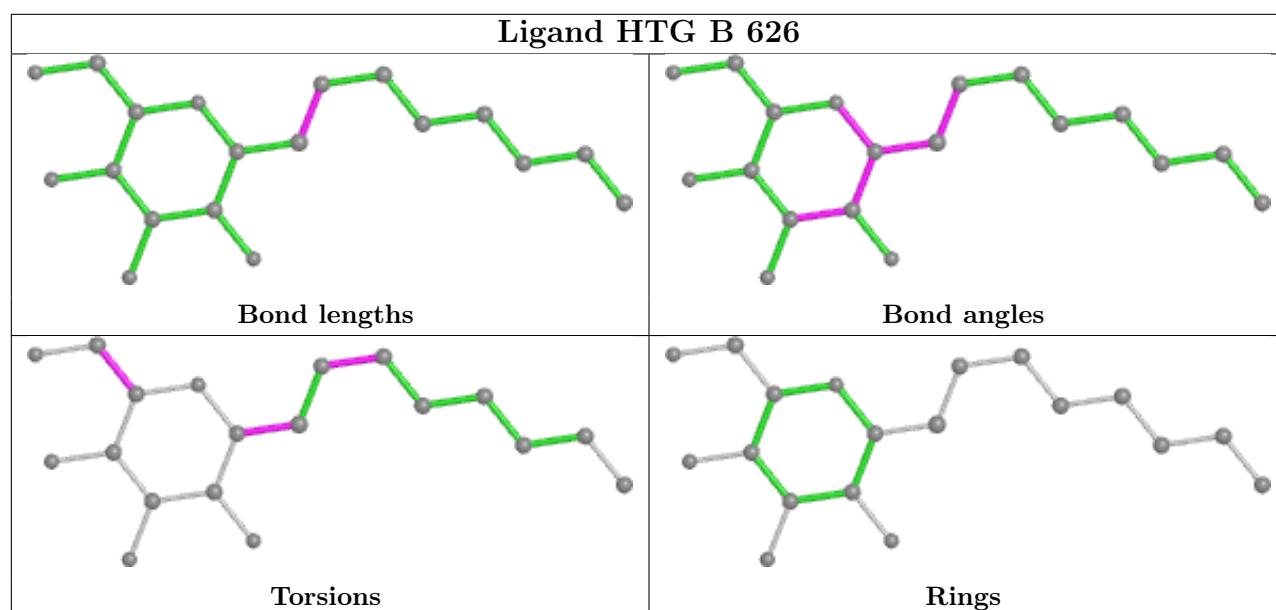
Ligand CLA b 610

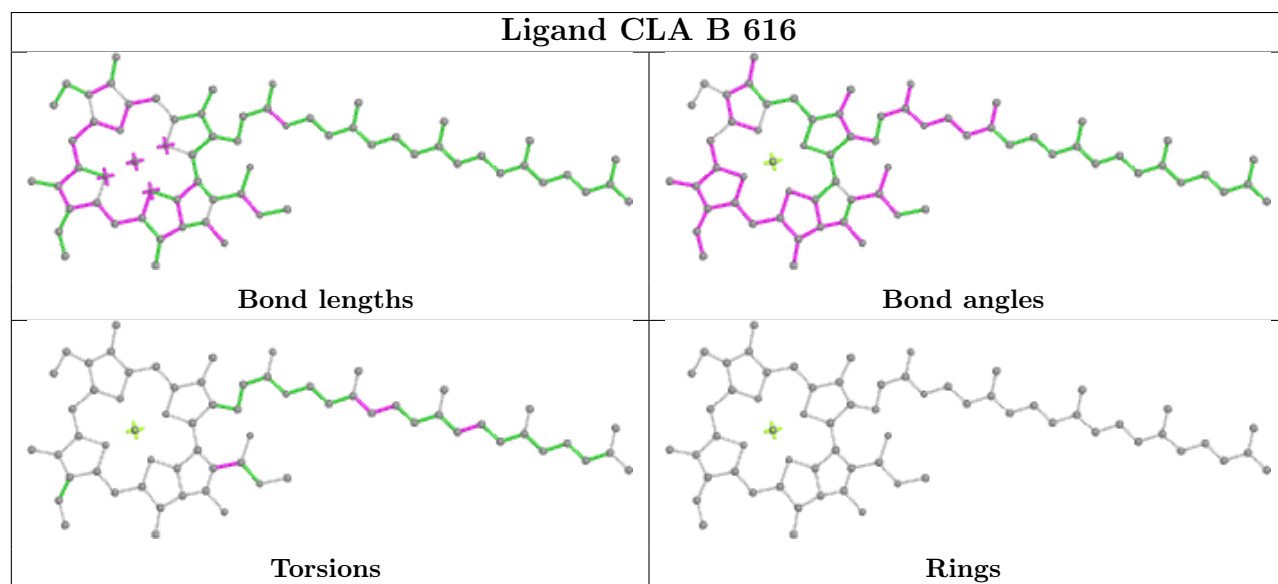
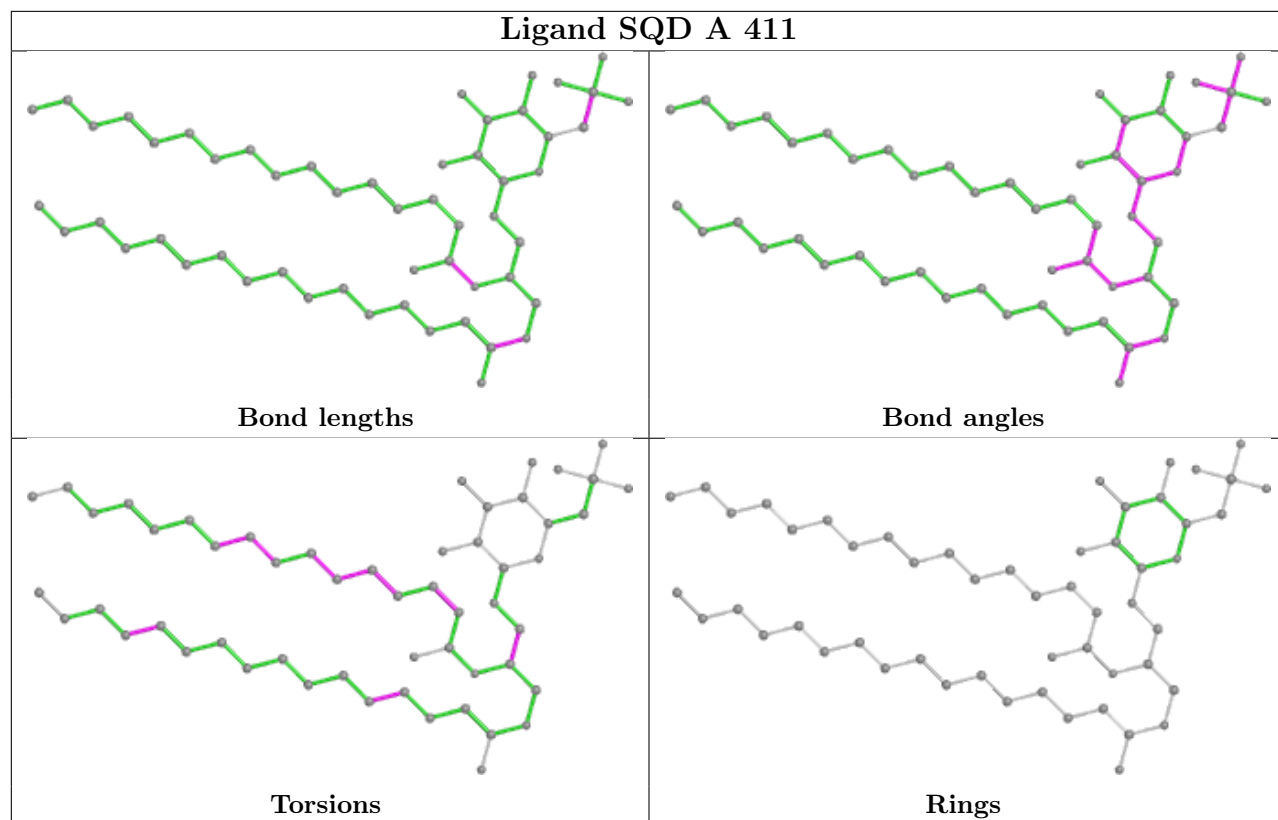


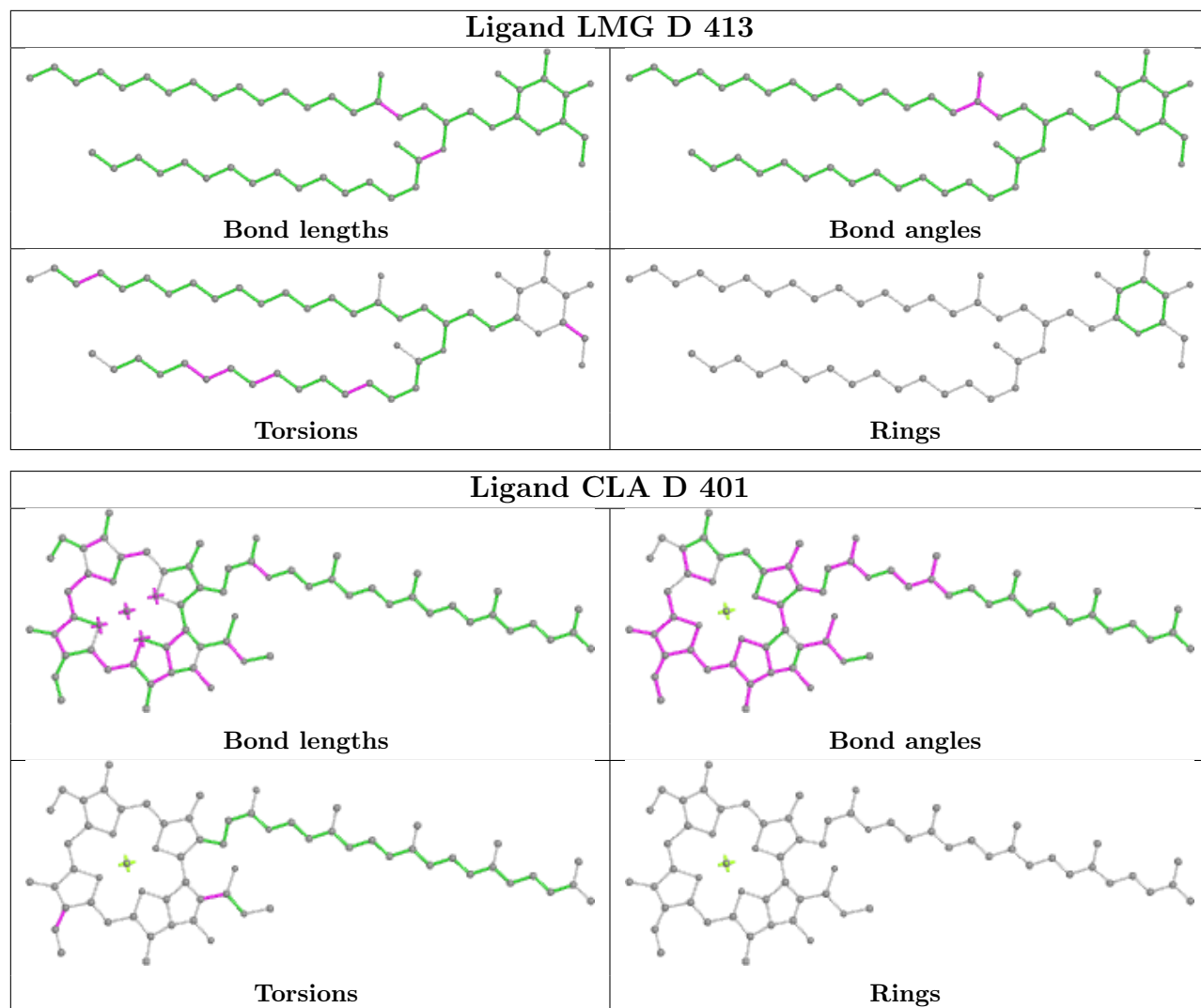
Ligand HTG H 101

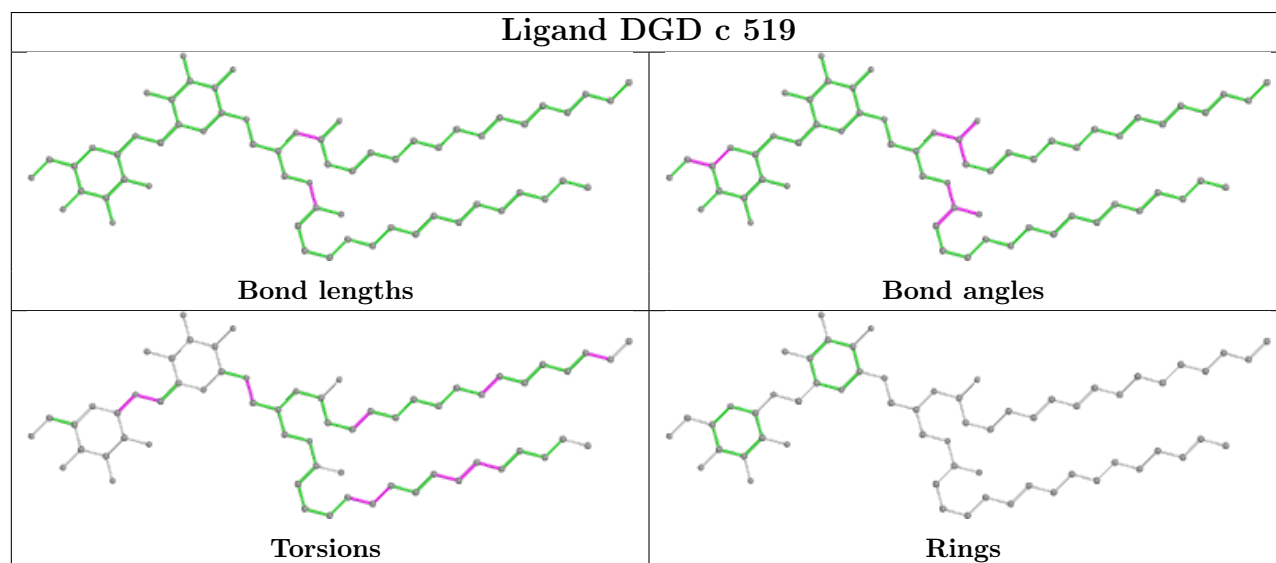
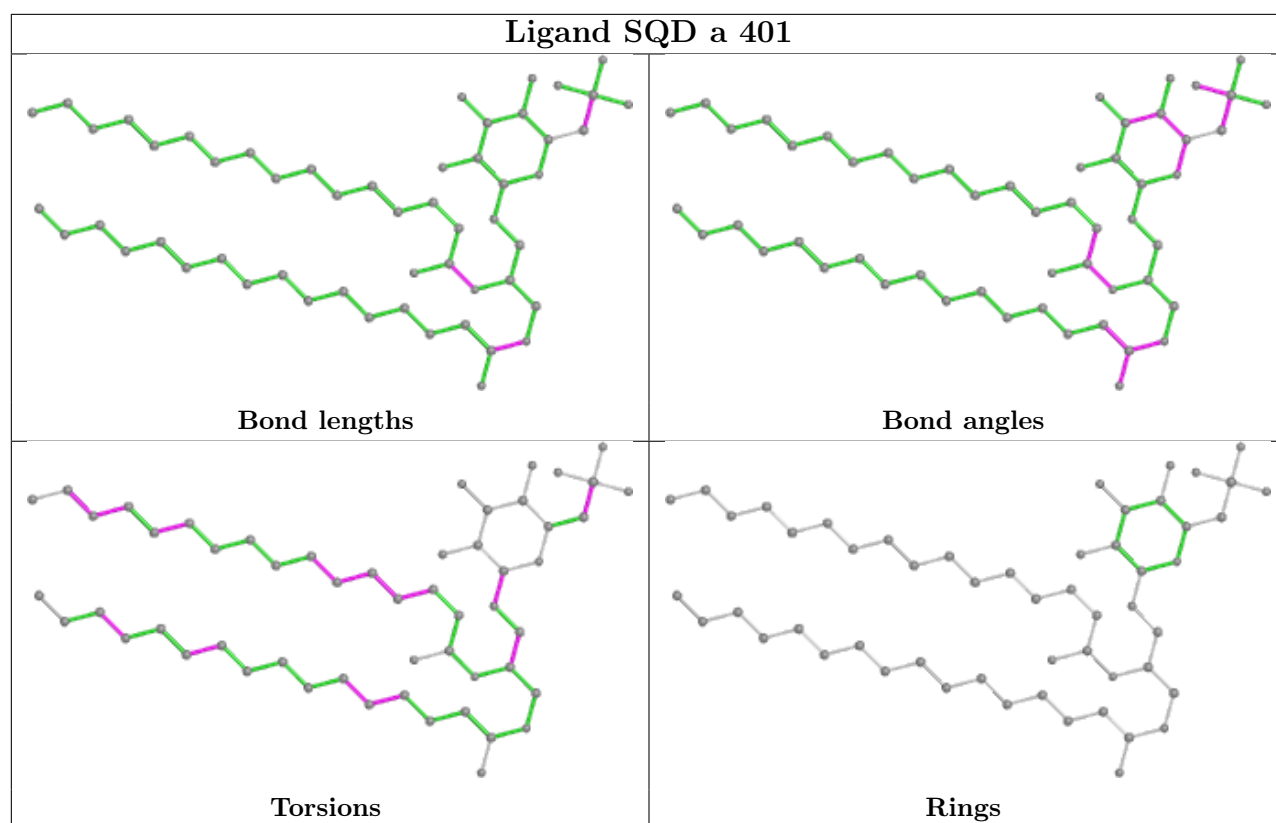




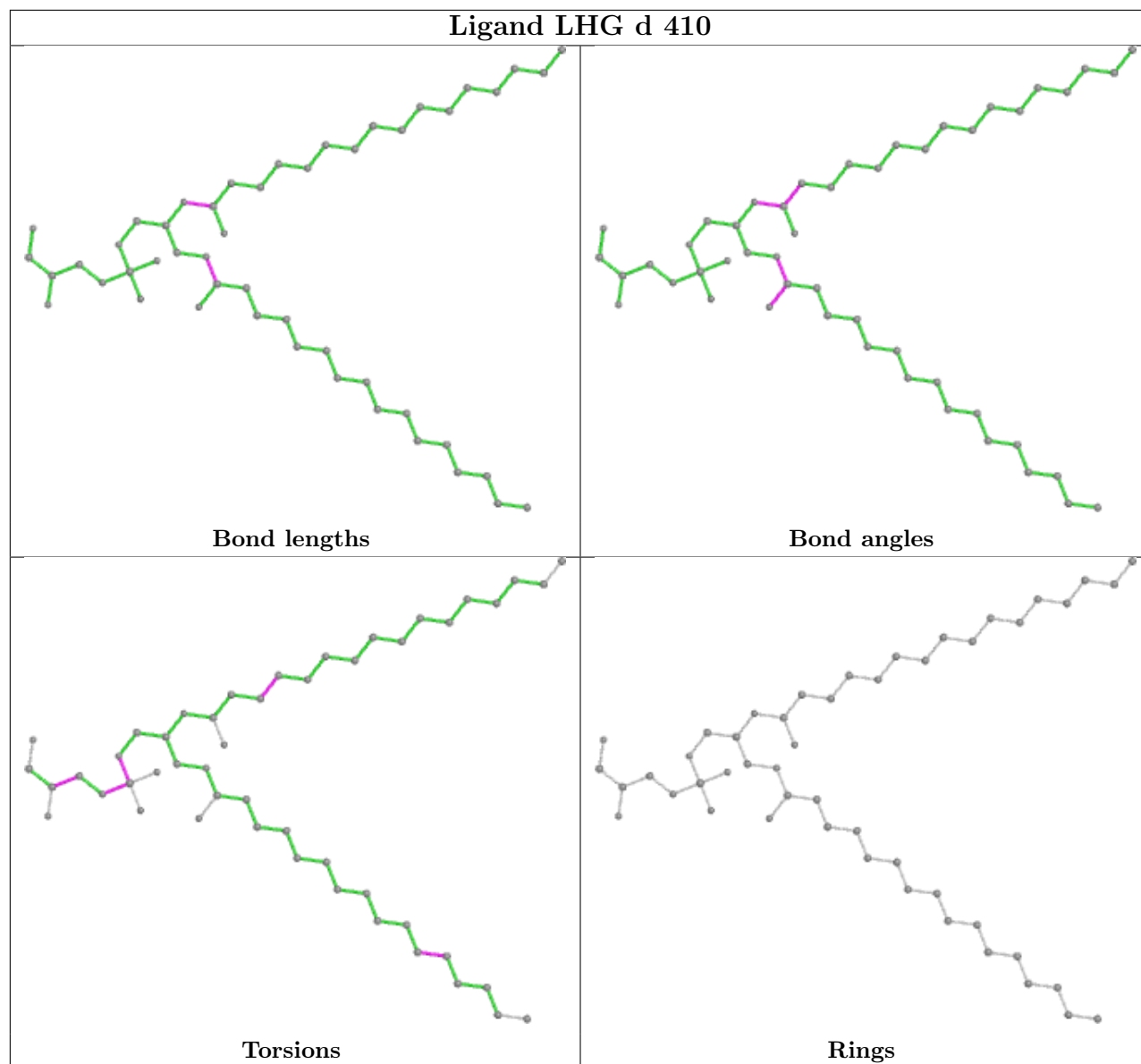




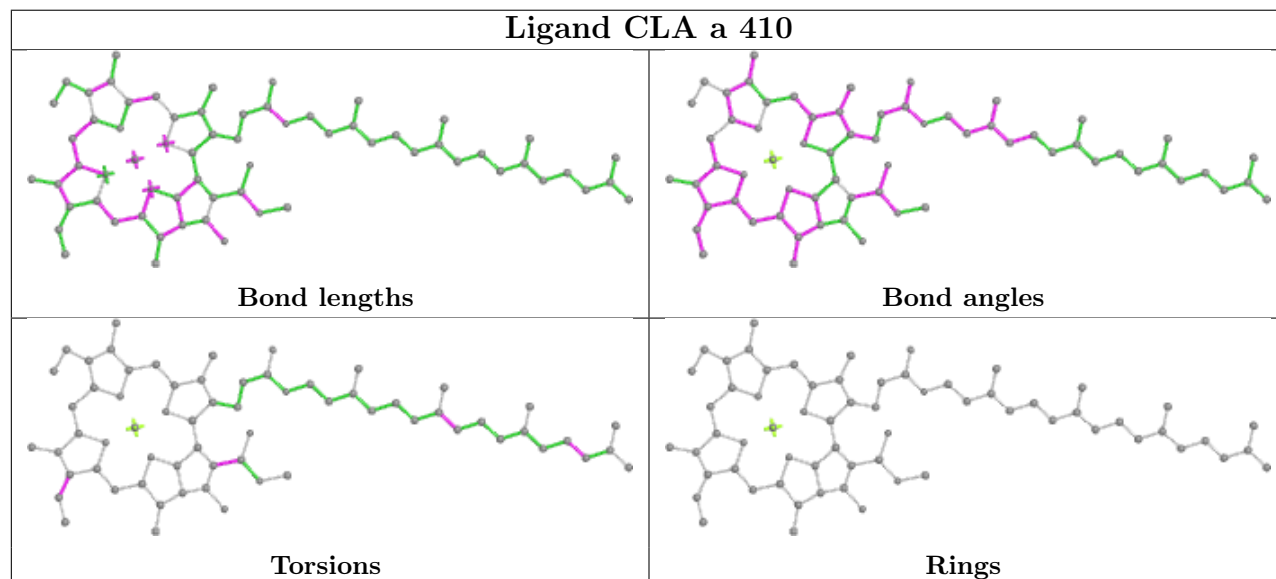


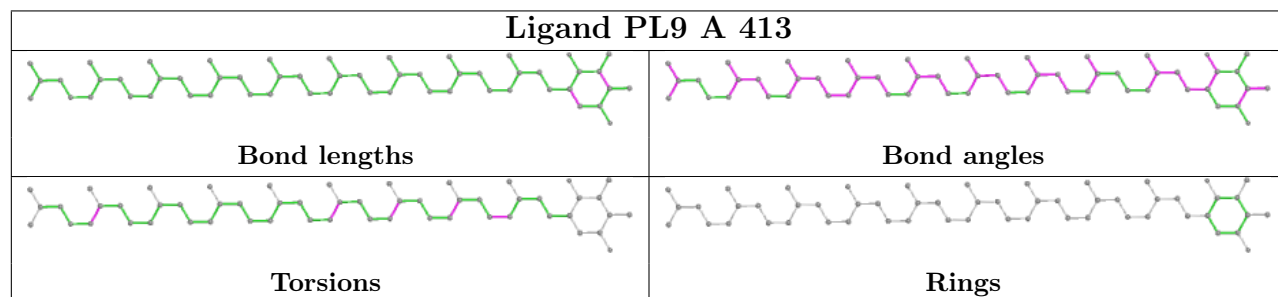
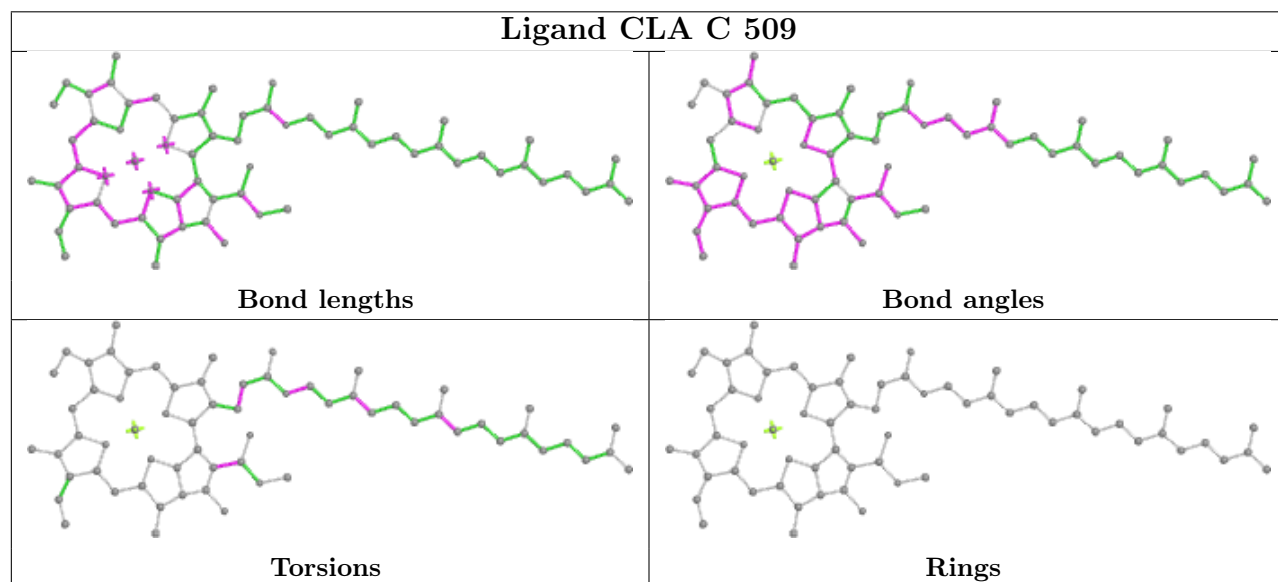
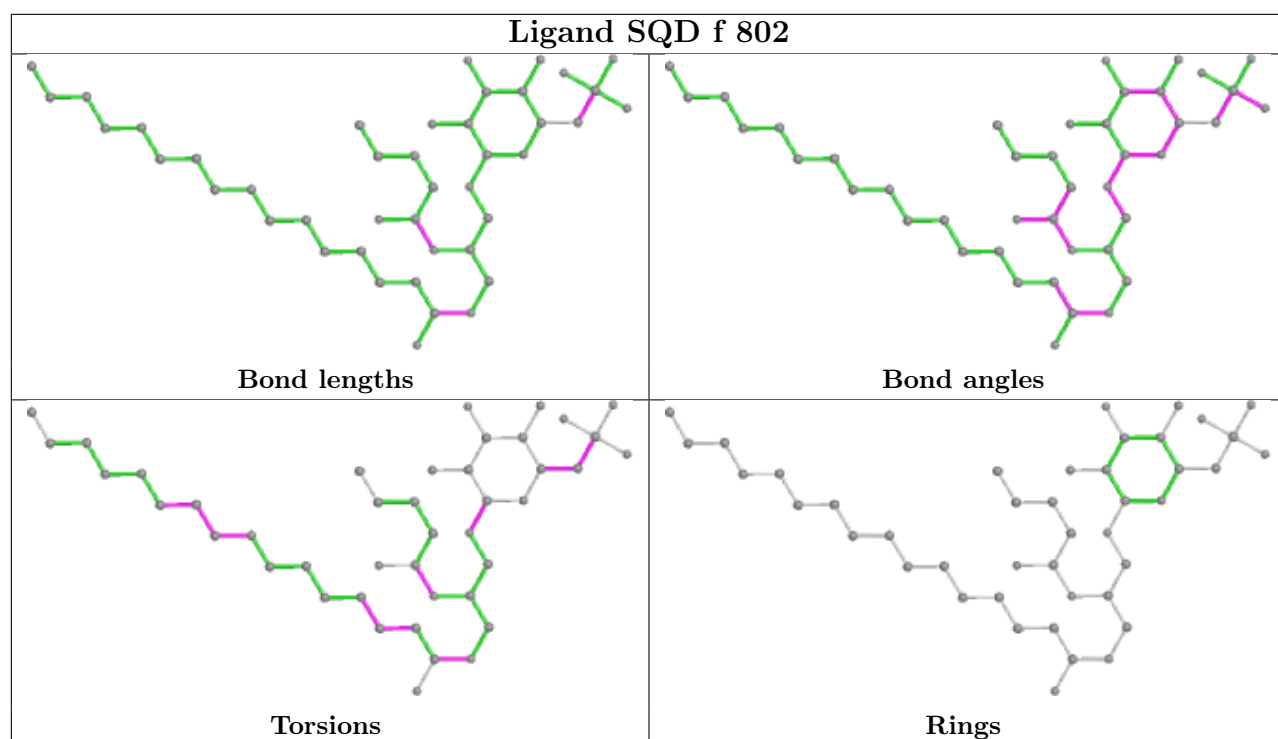


Ligand LHG d 410

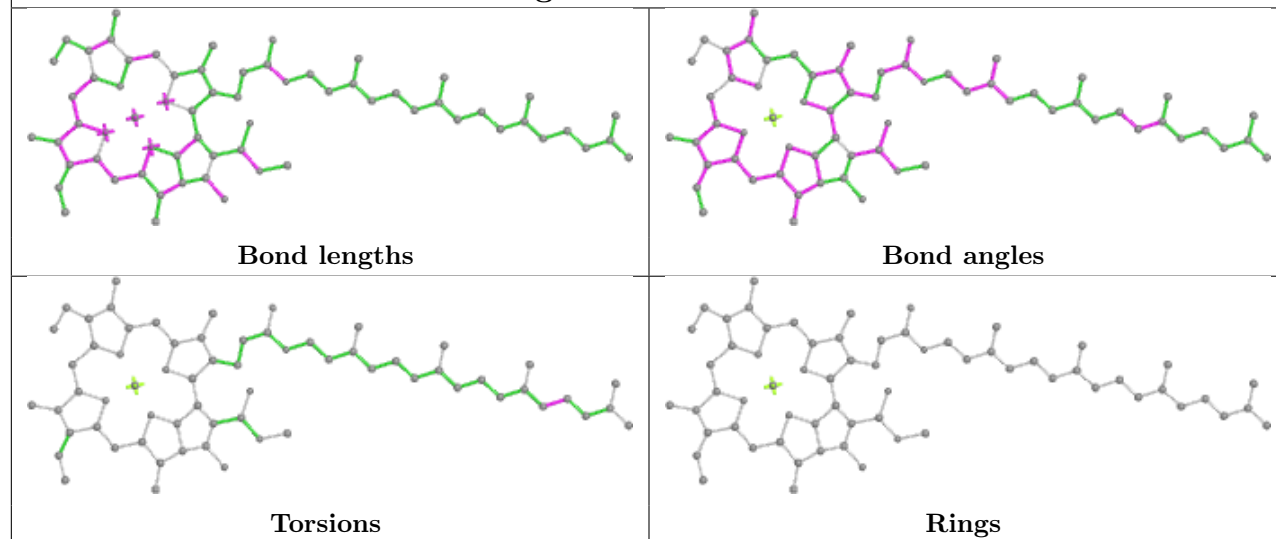


Ligand CLA a 410

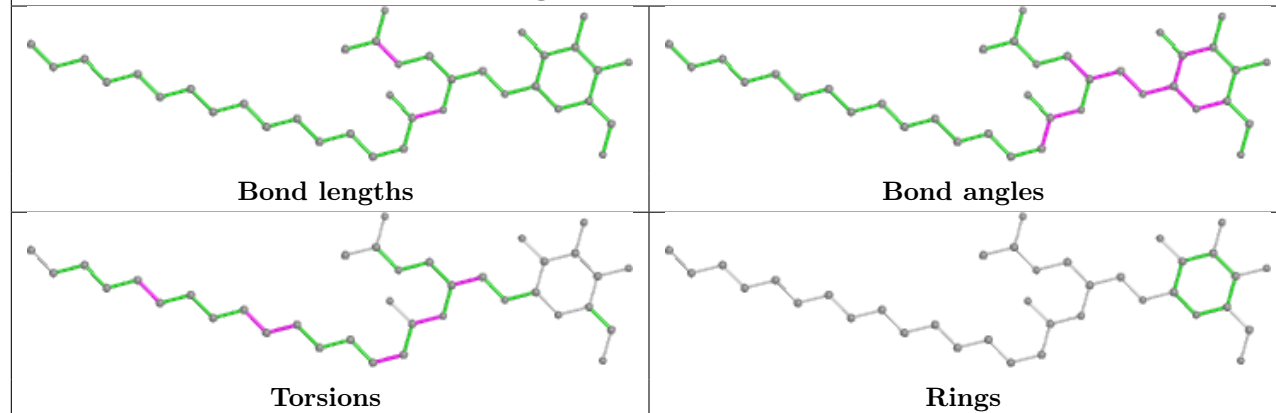




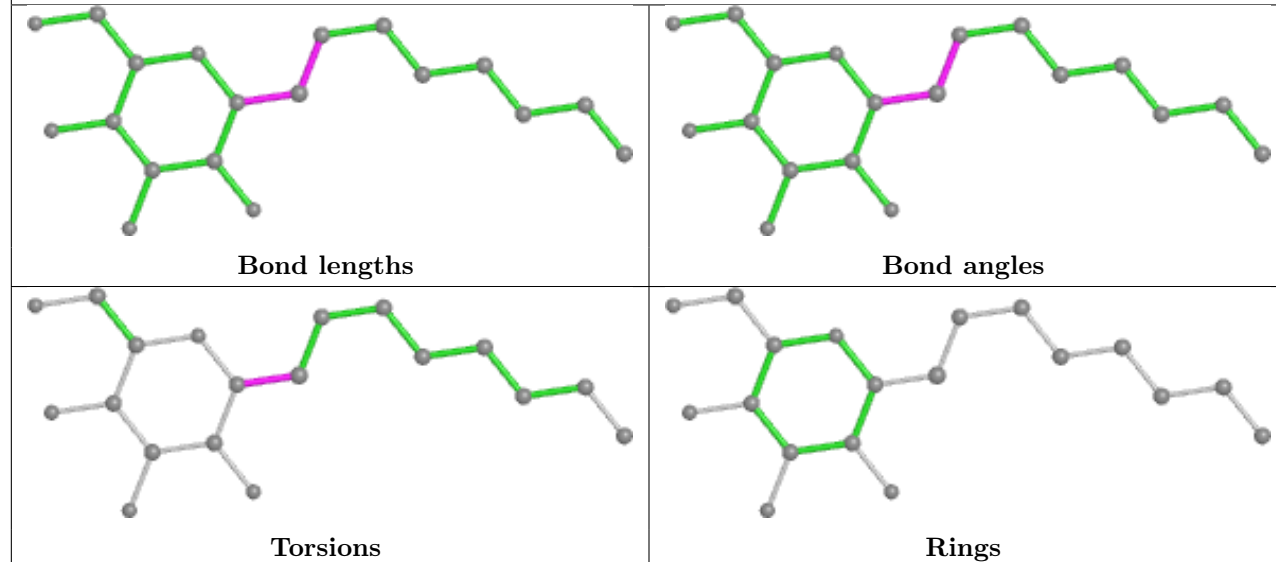
Ligand CLA b 612



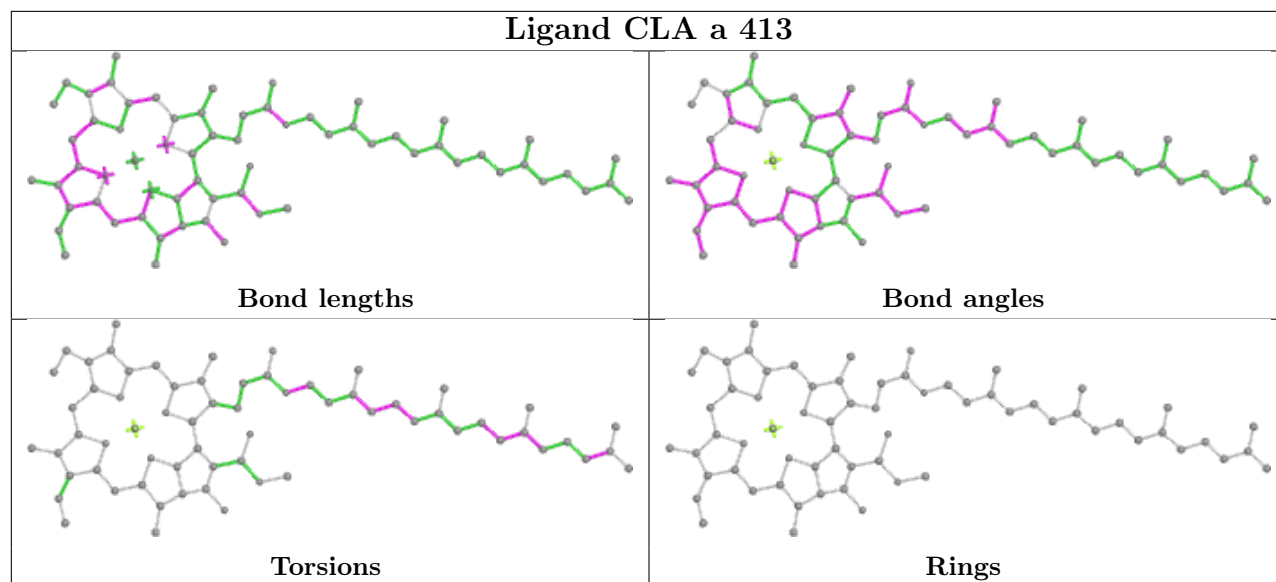
Ligand LMG z 101



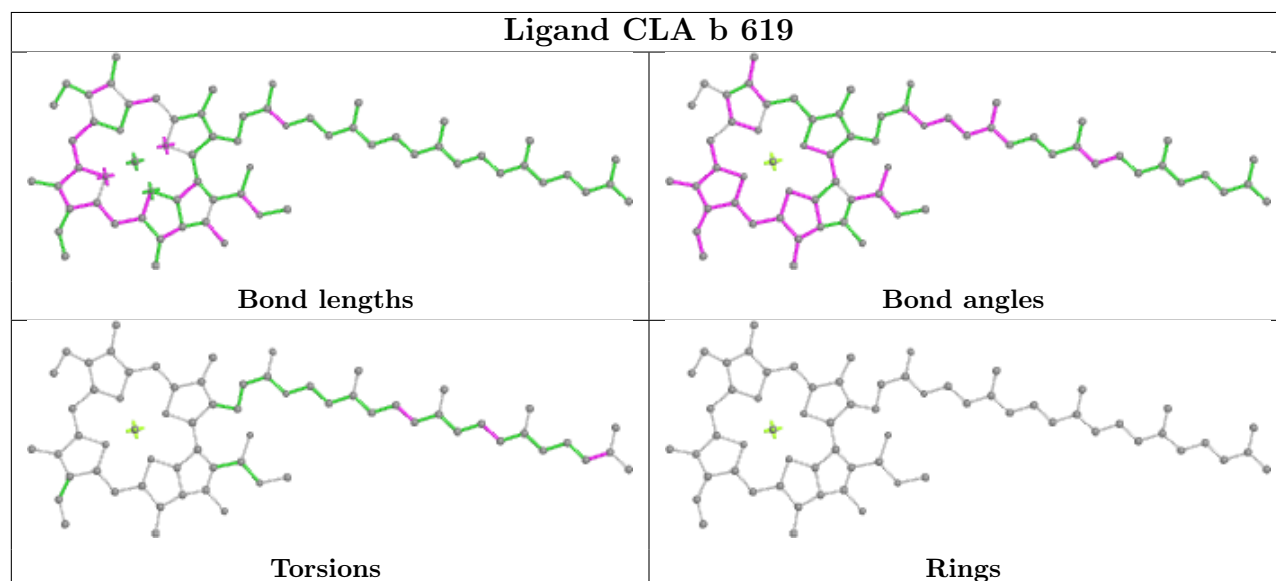
Ligand HTG b 603



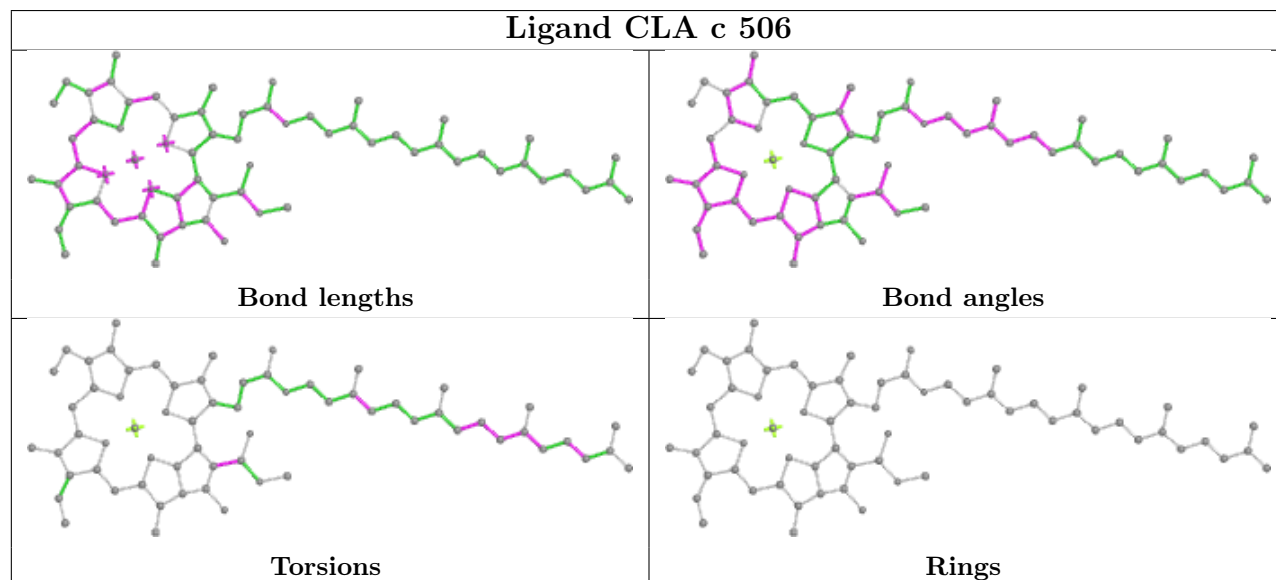
Ligand CLA a 413

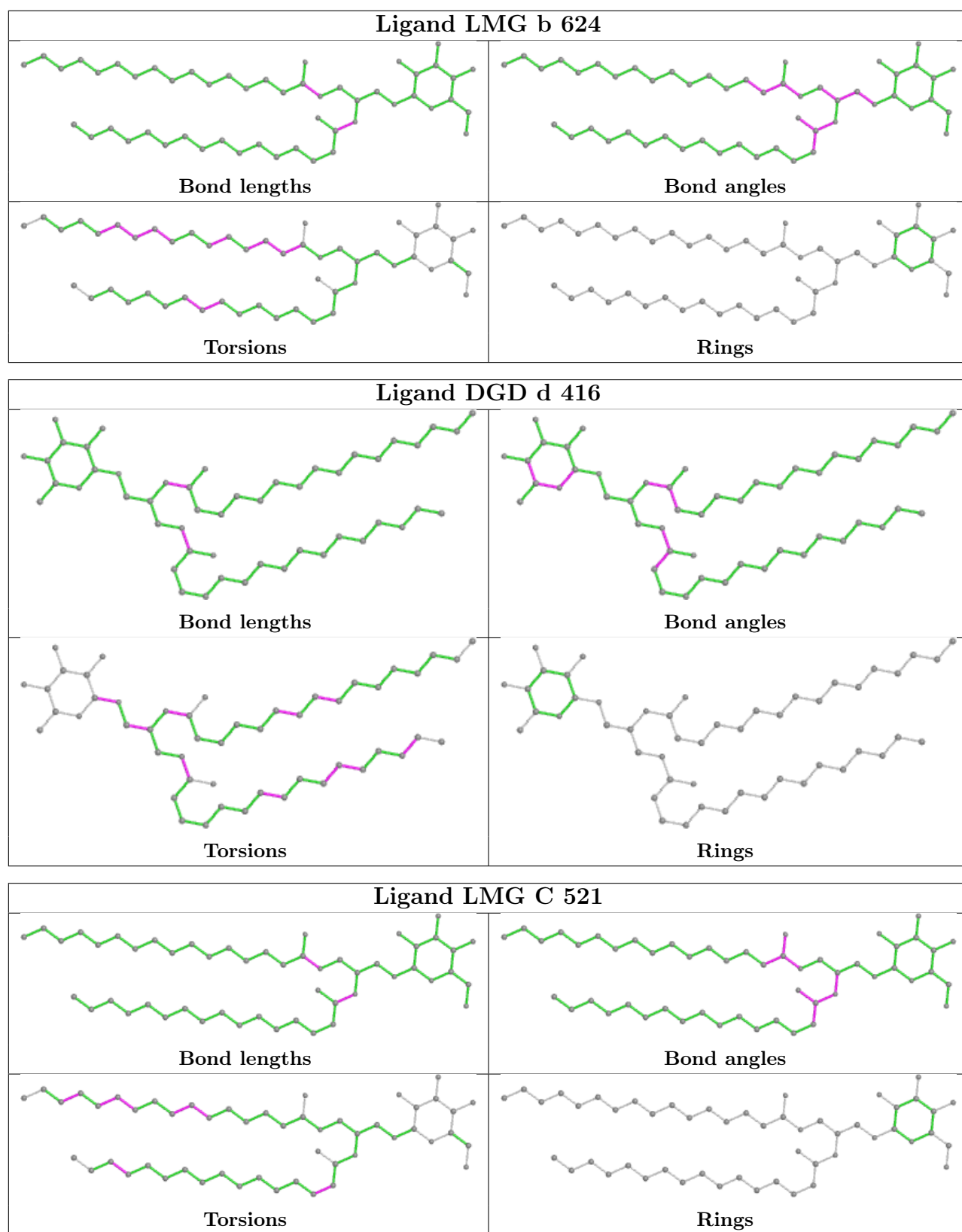


Ligand CLA b 619

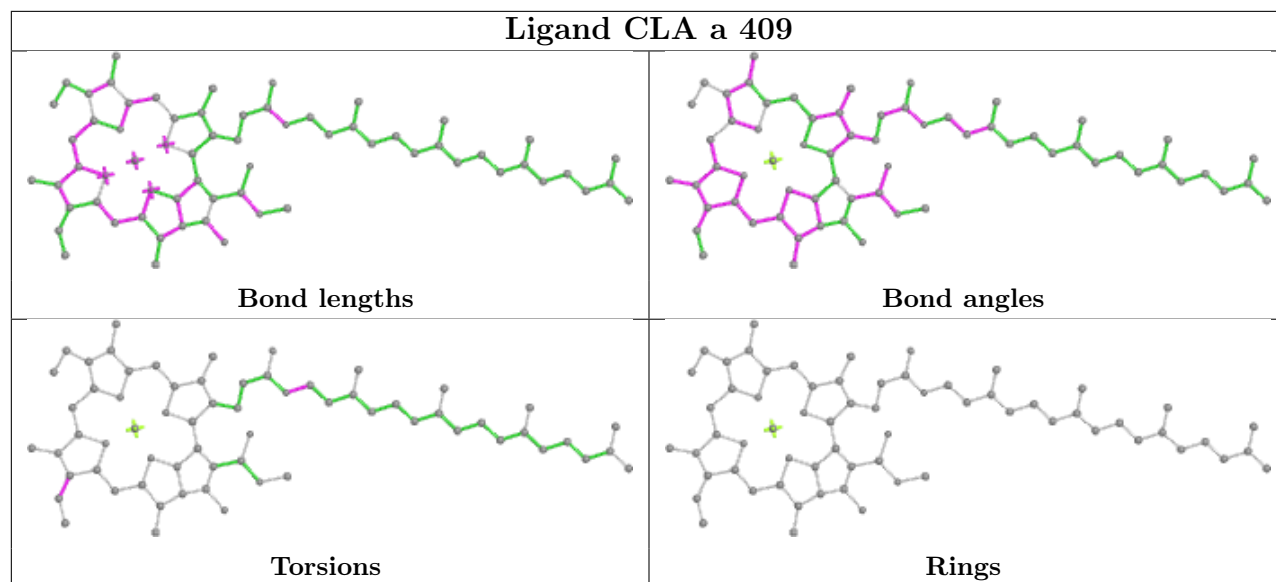


Ligand CLA c 506

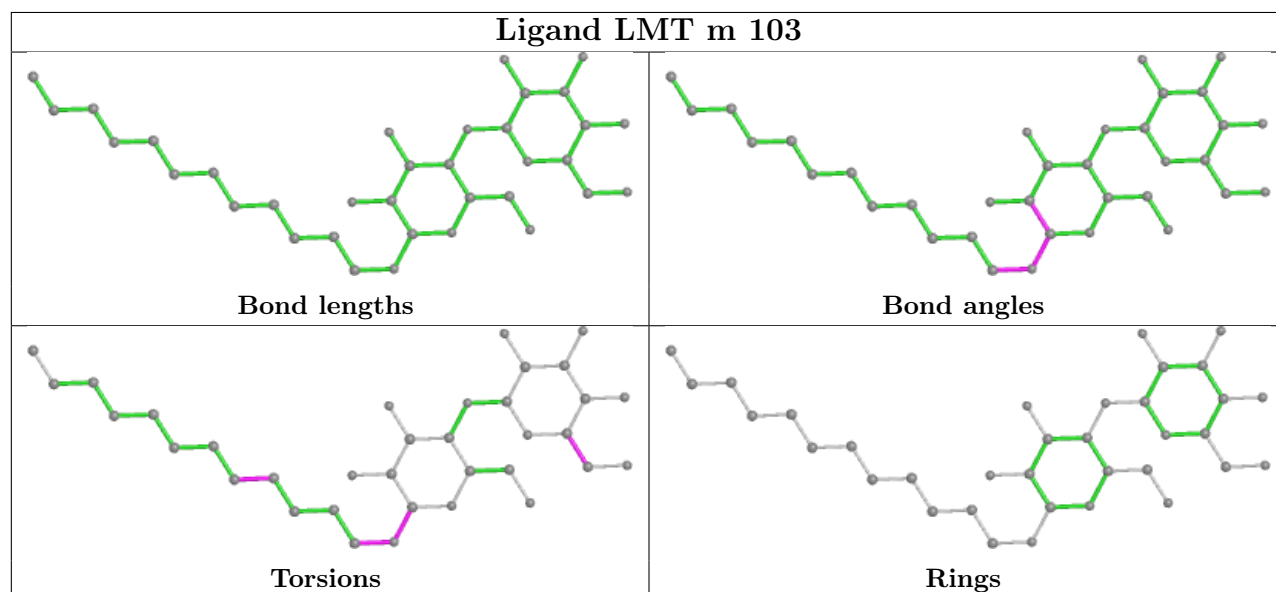


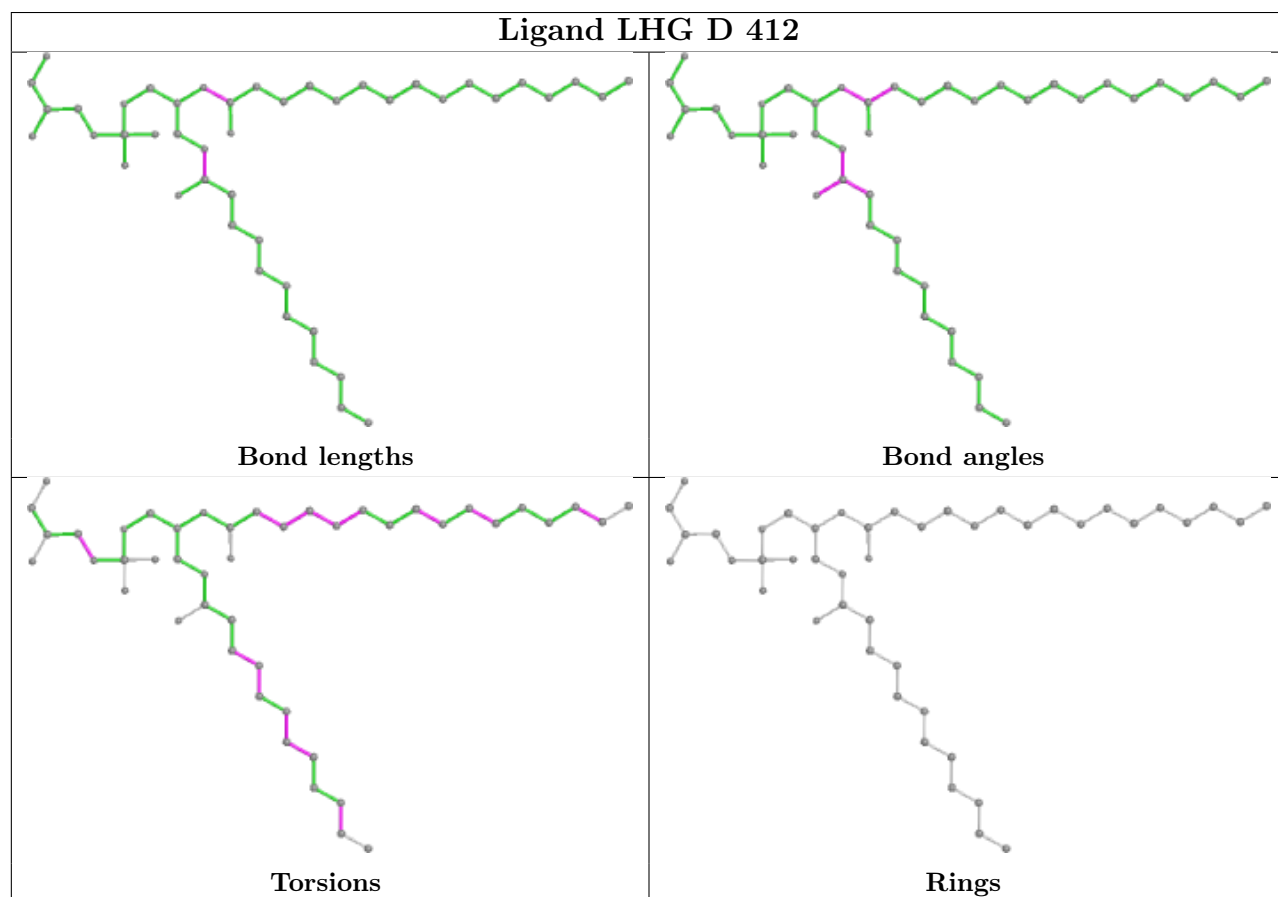
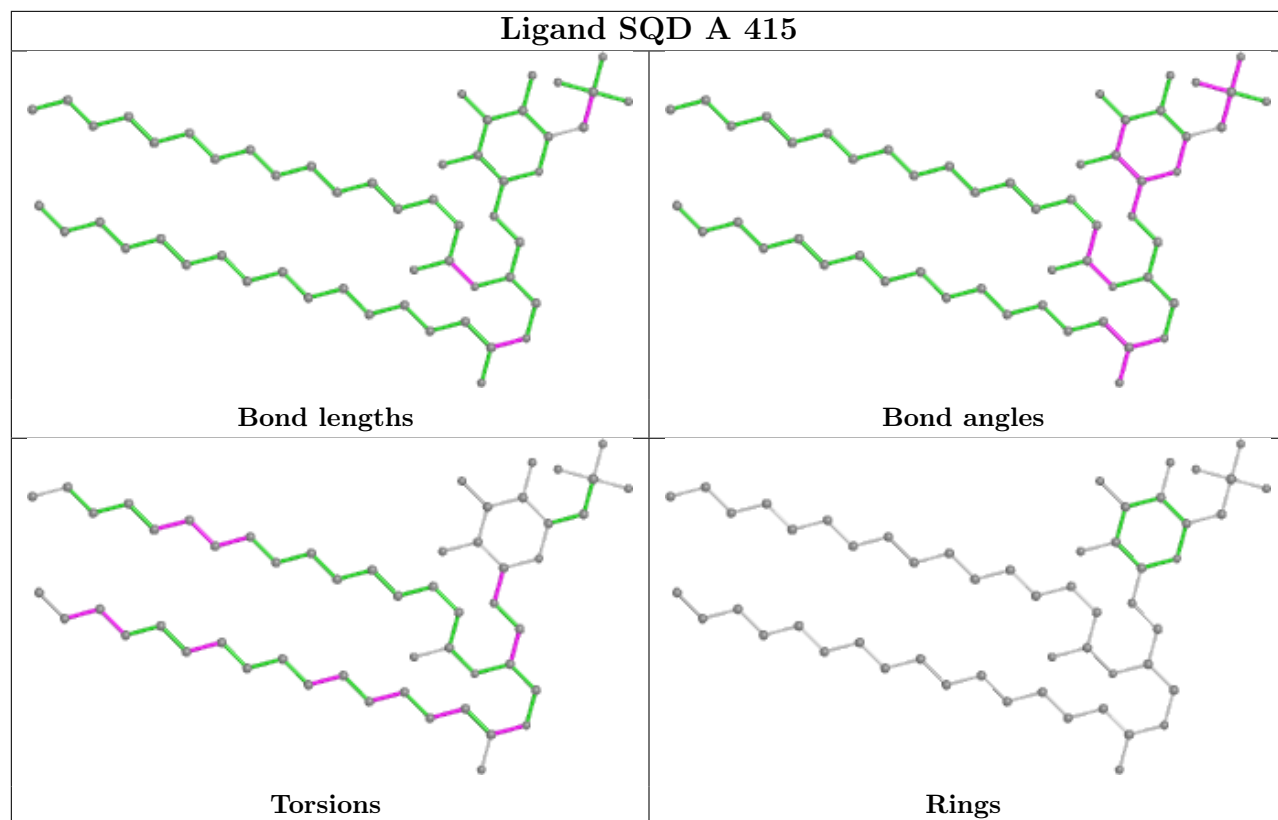


Ligand CLA a 409

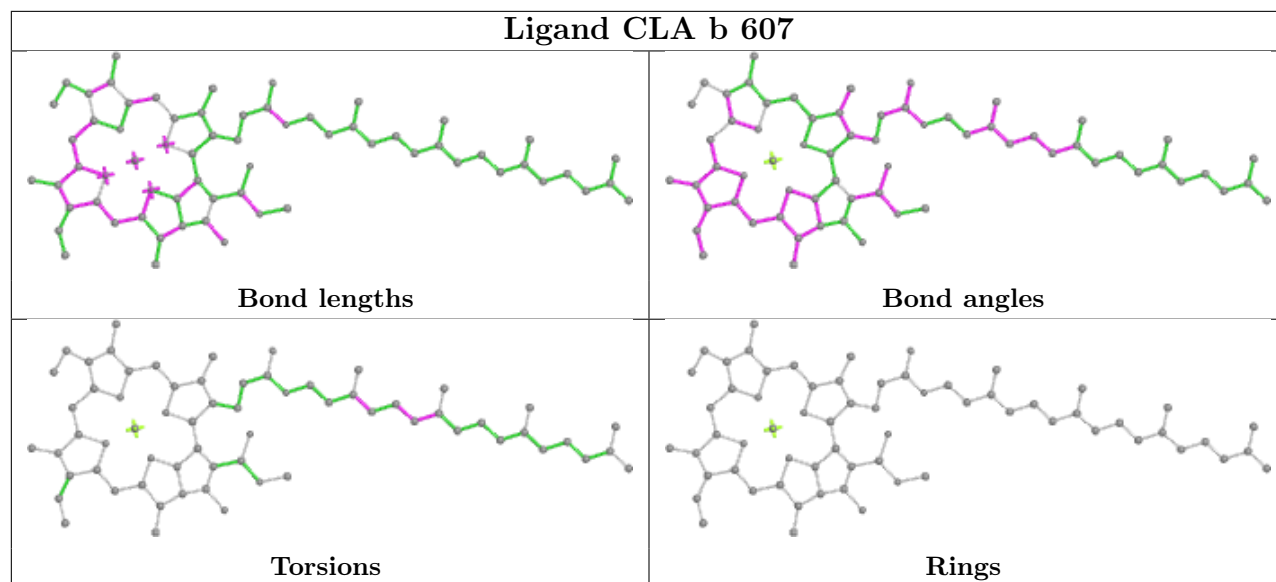


Ligand LMT m 103

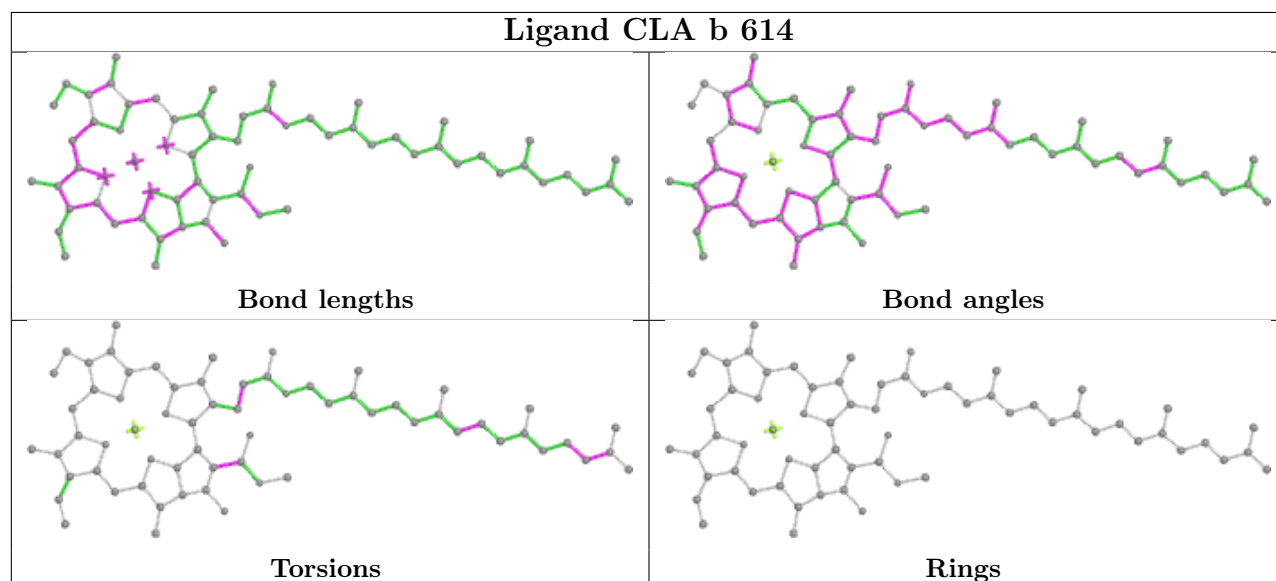




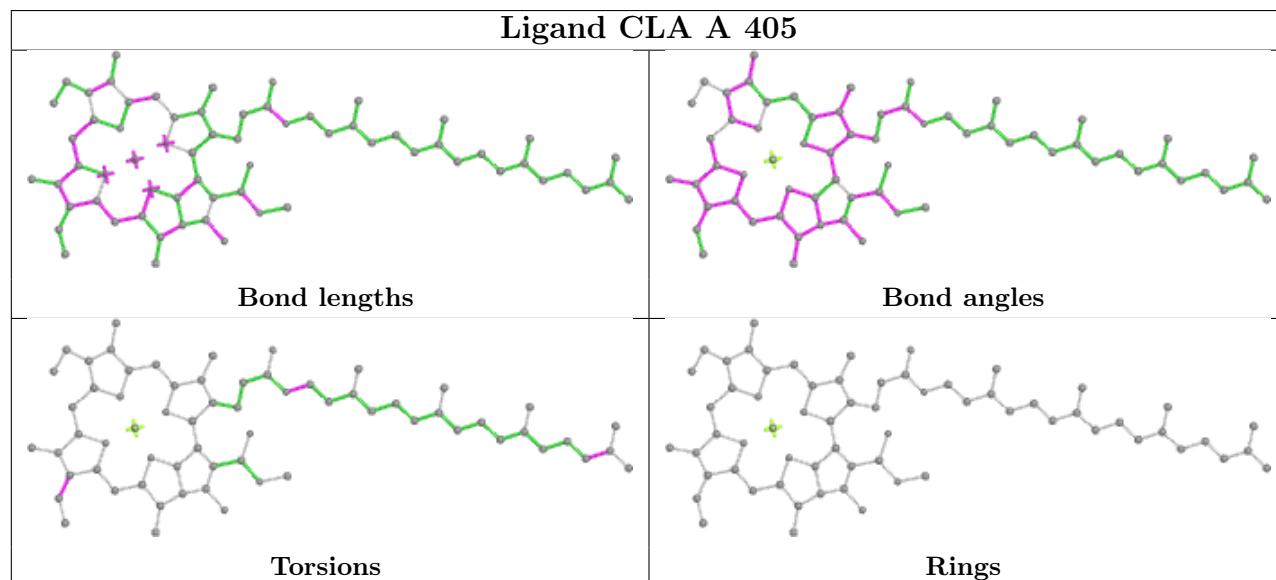
Ligand CLA b 607



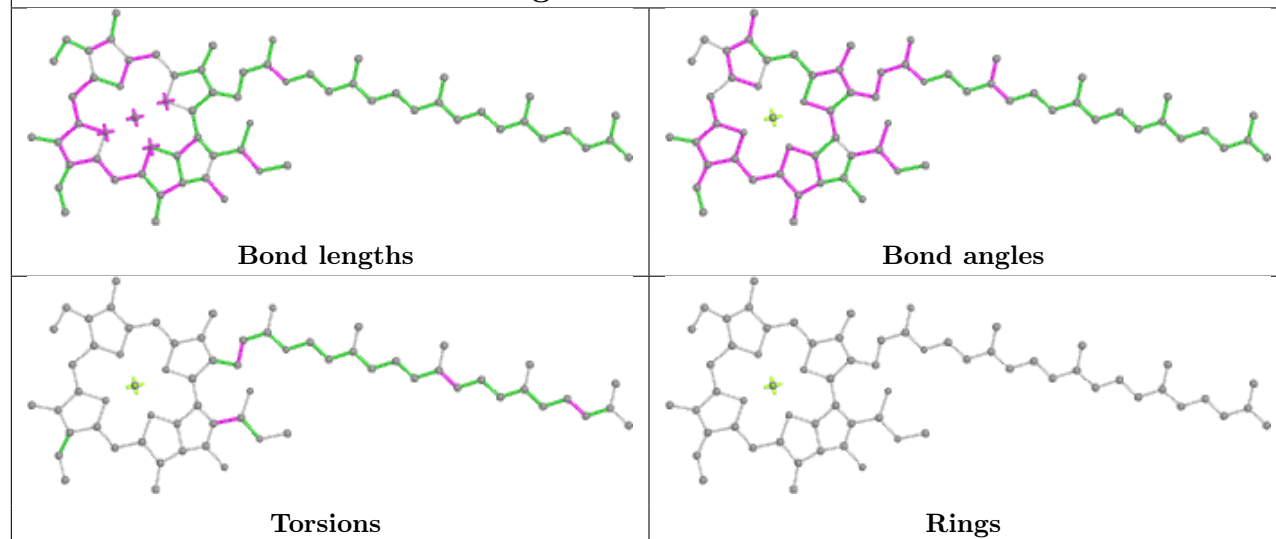
Ligand CLA b 614



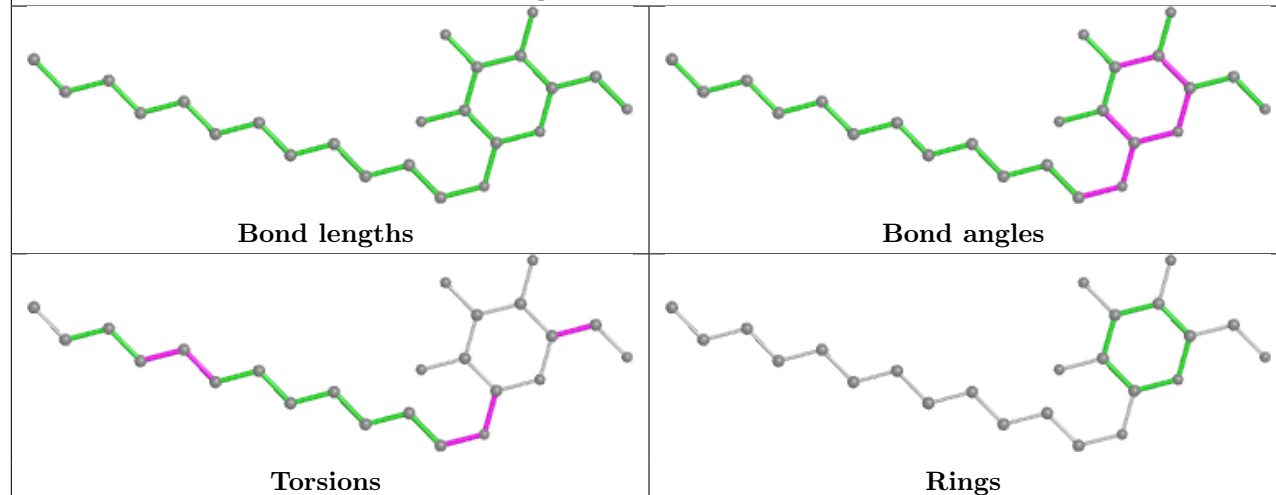
Ligand CLA A 405



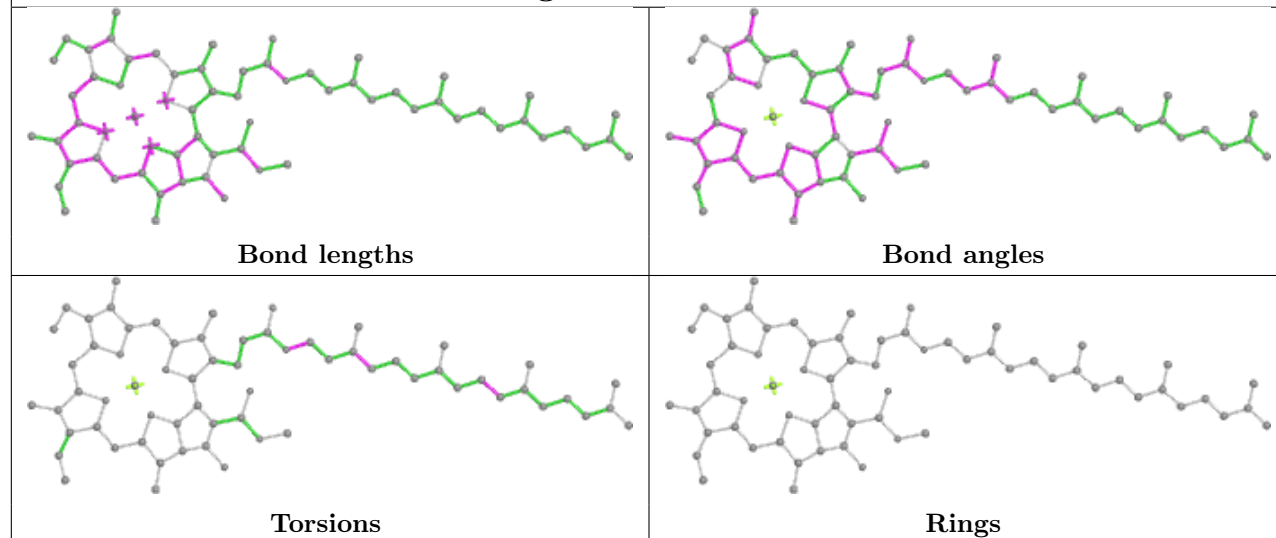
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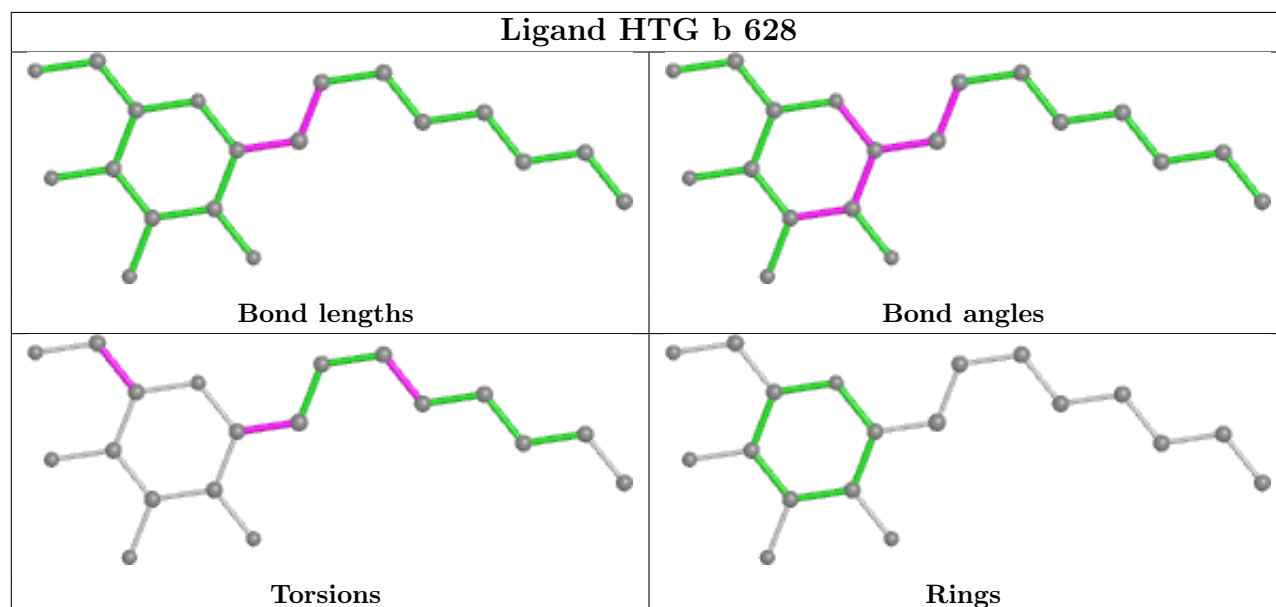
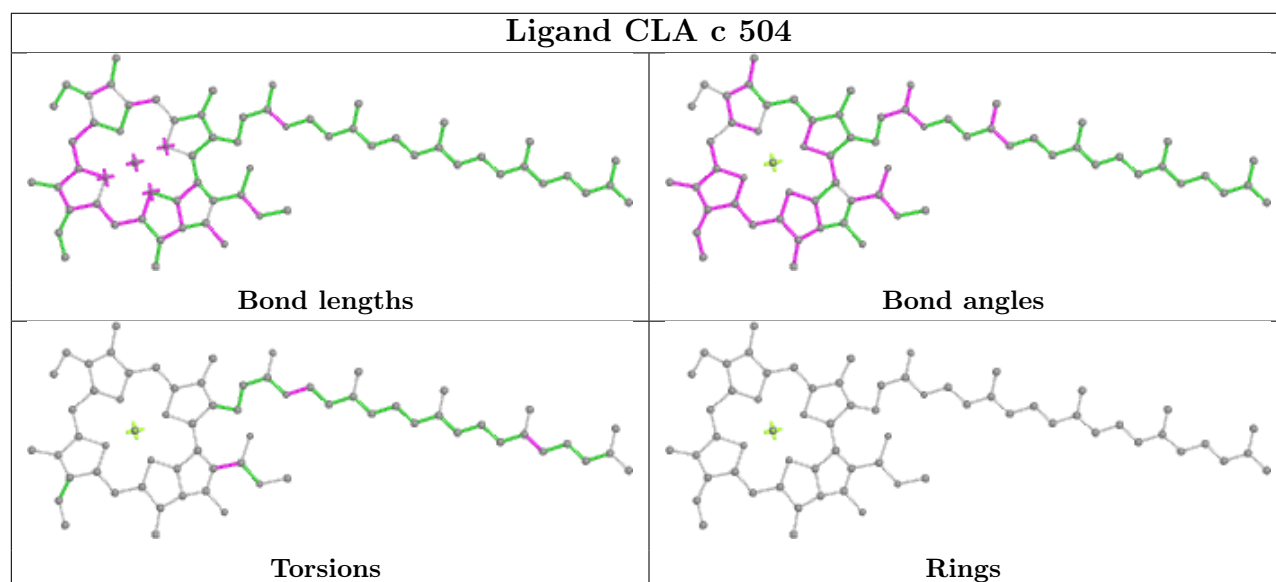
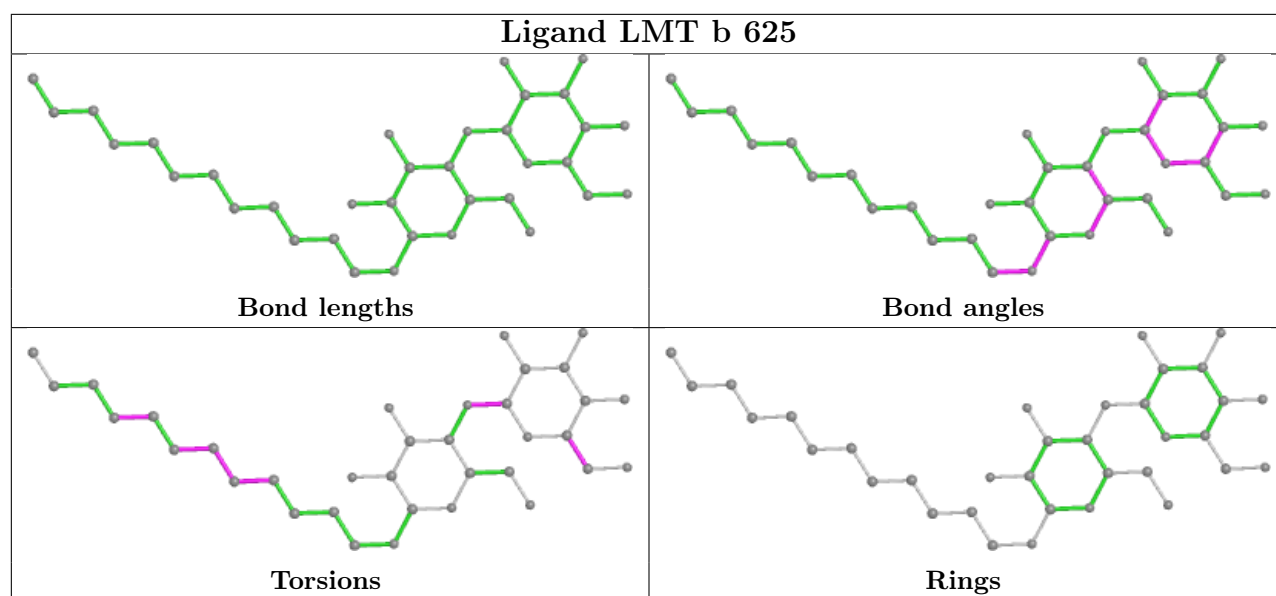


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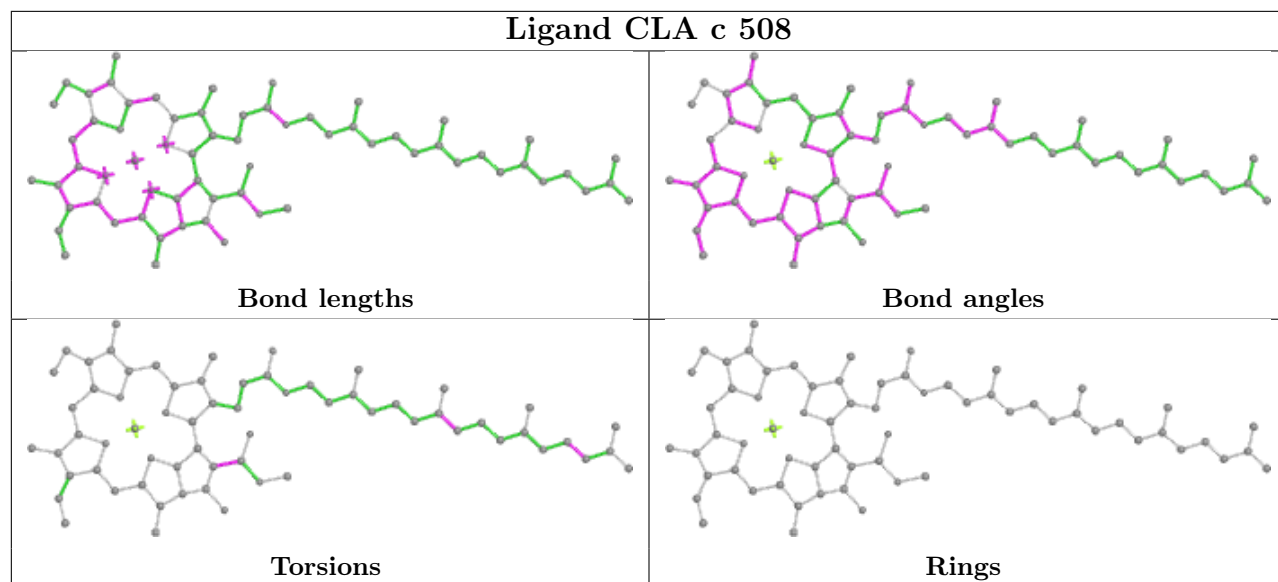


Ligand CLA c 515

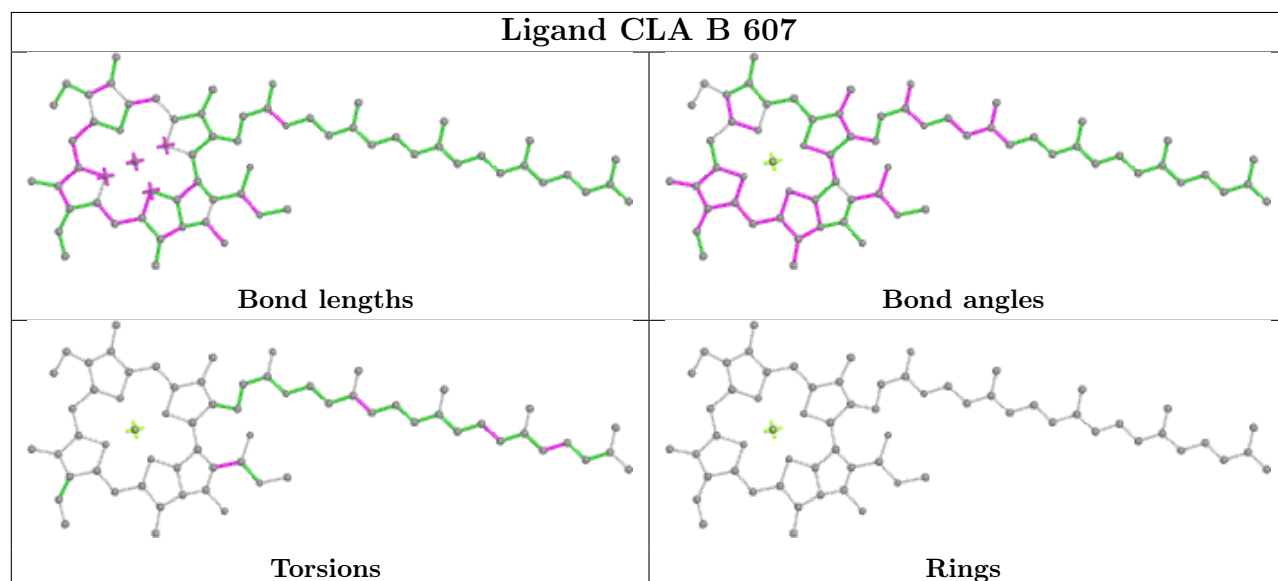




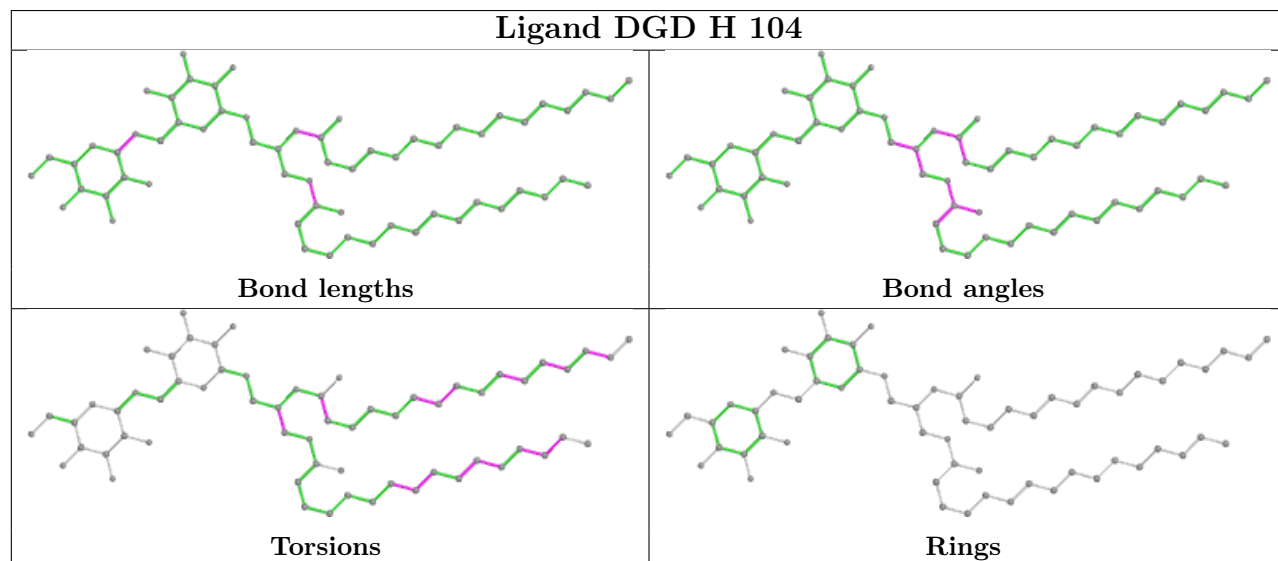
Ligand CLA c 508



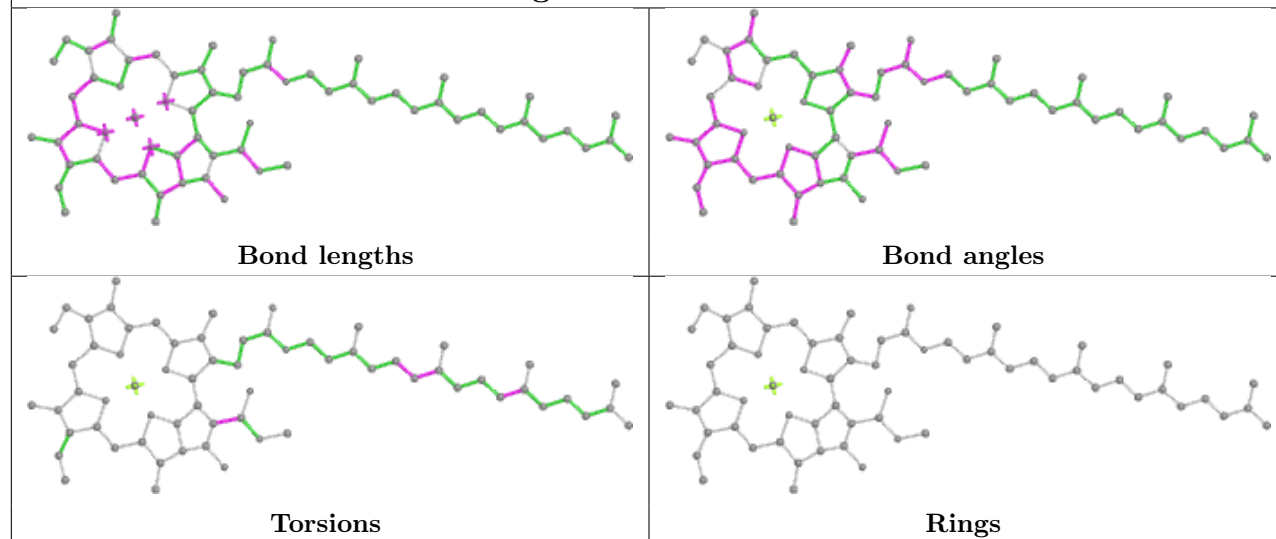
Ligand CLA B 607



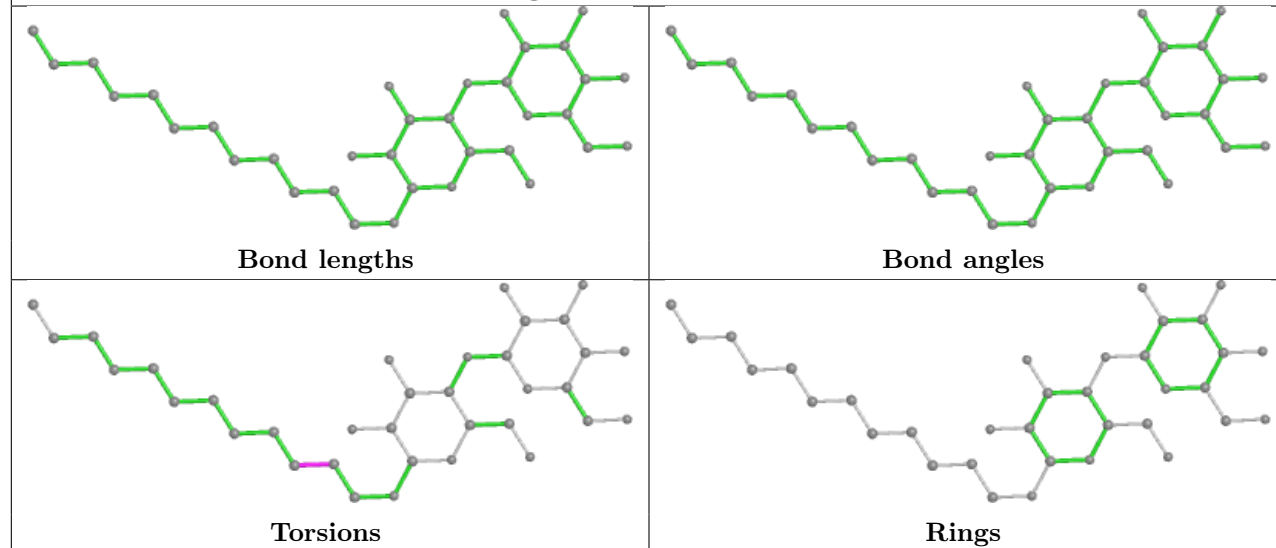
Ligand DGD H 104



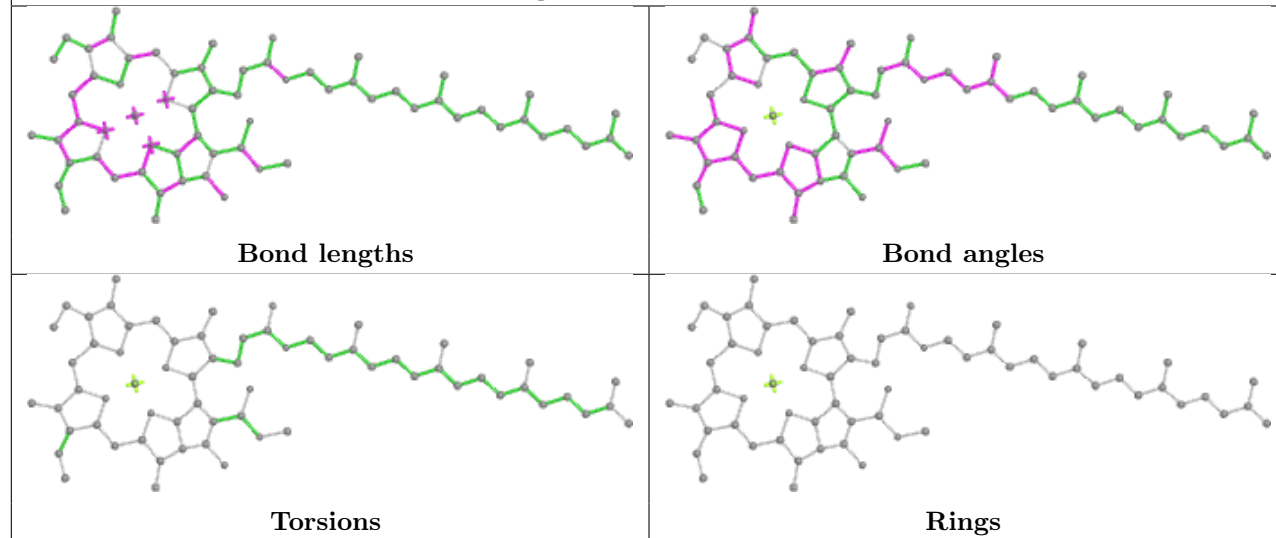
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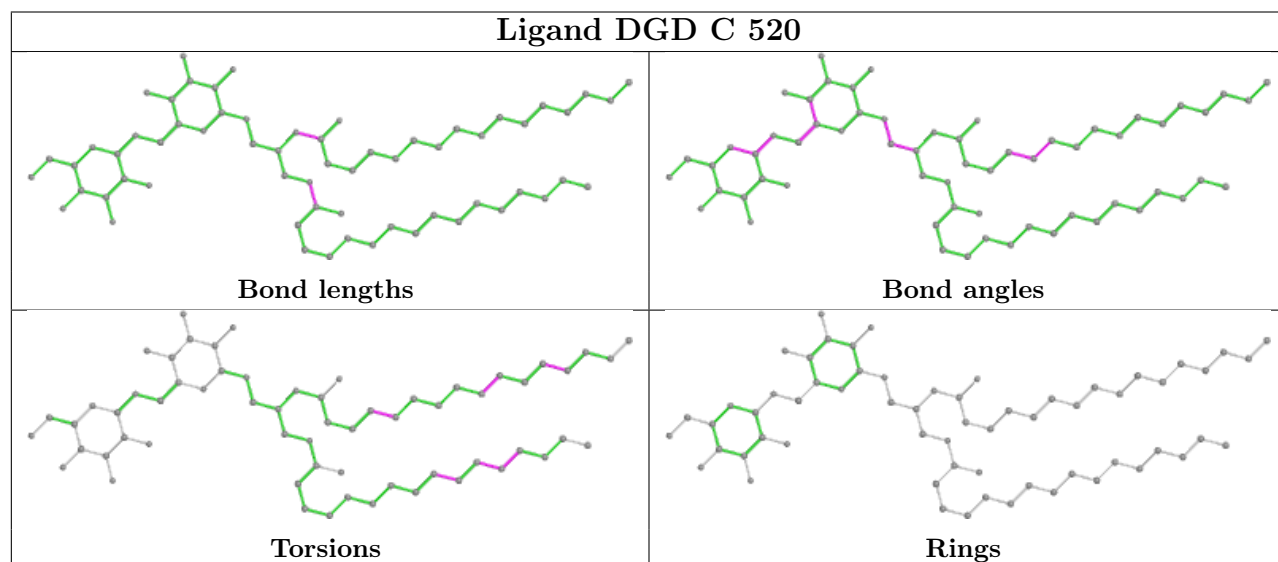
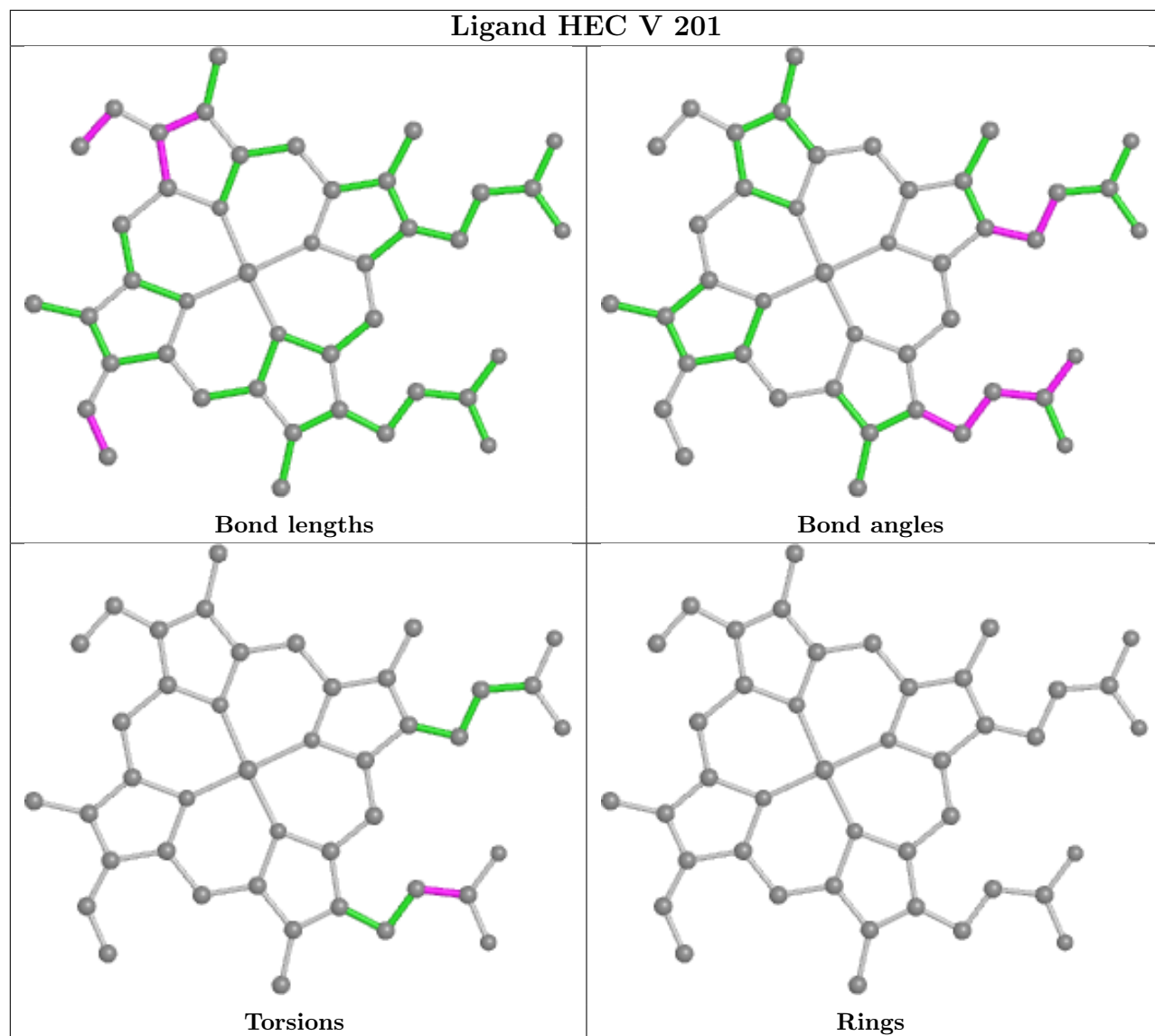


Ligand LMT M 102

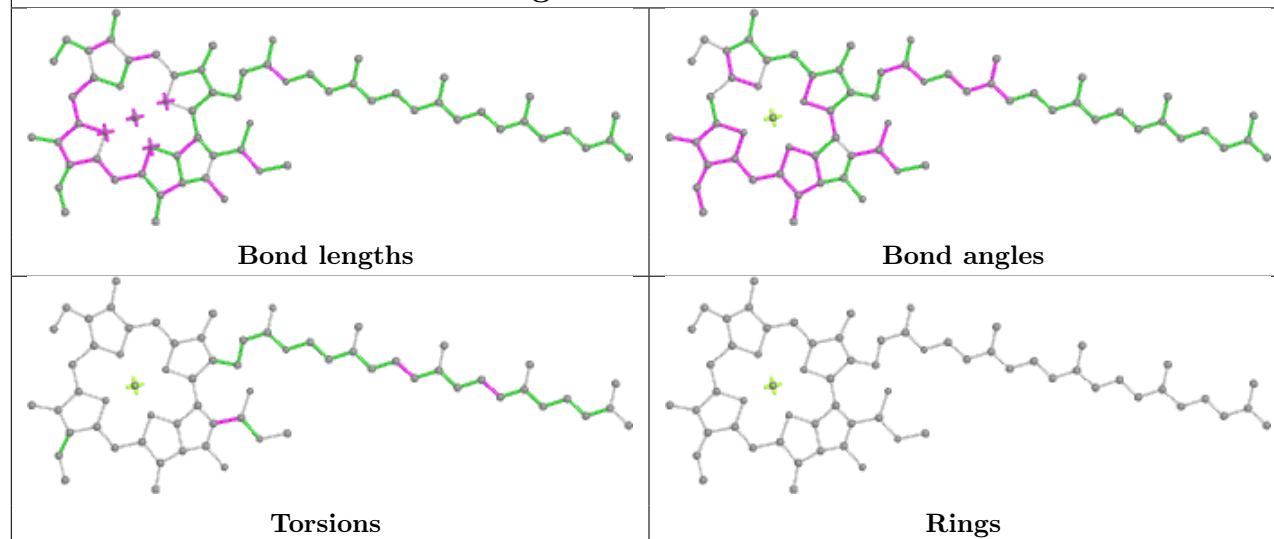


Ligand CLA B 614

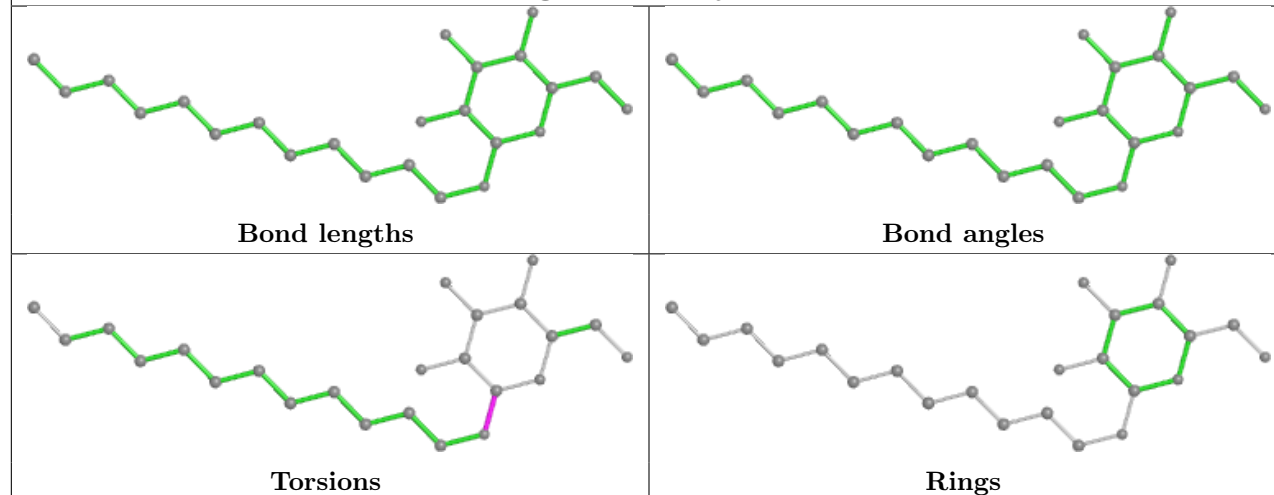




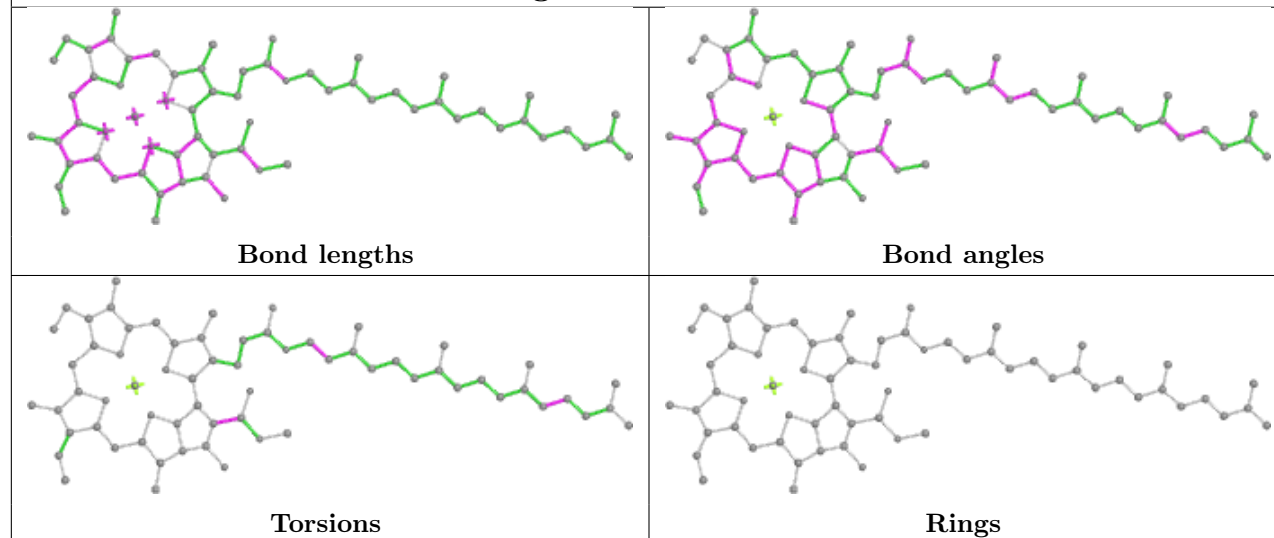
Ligand CLA C 505

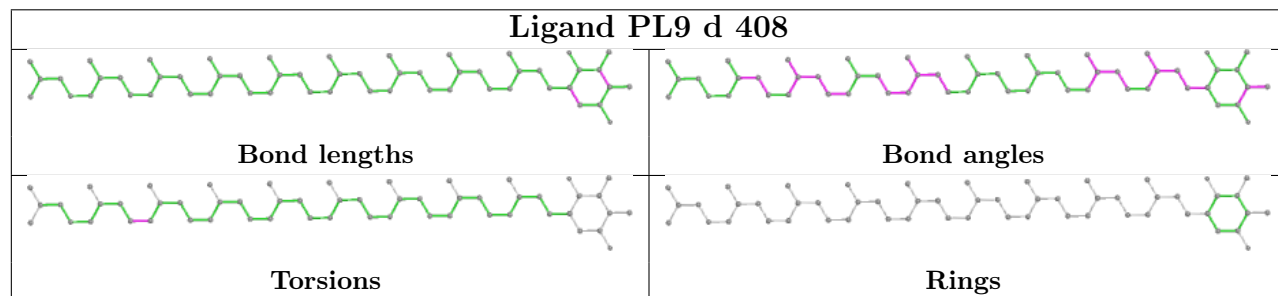
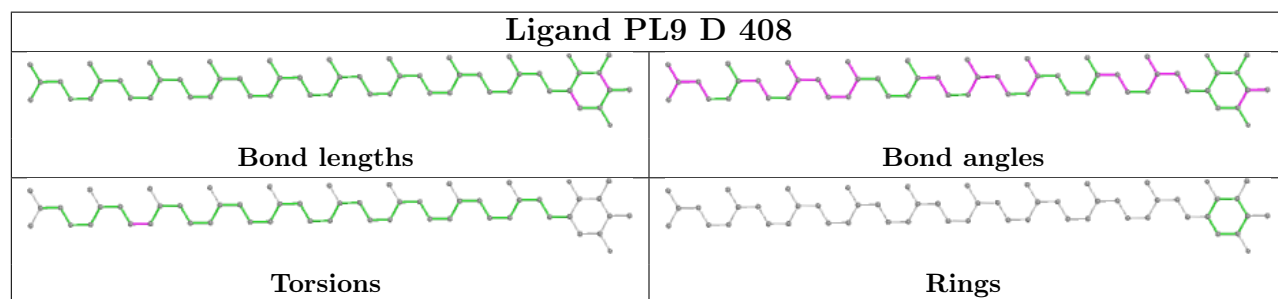
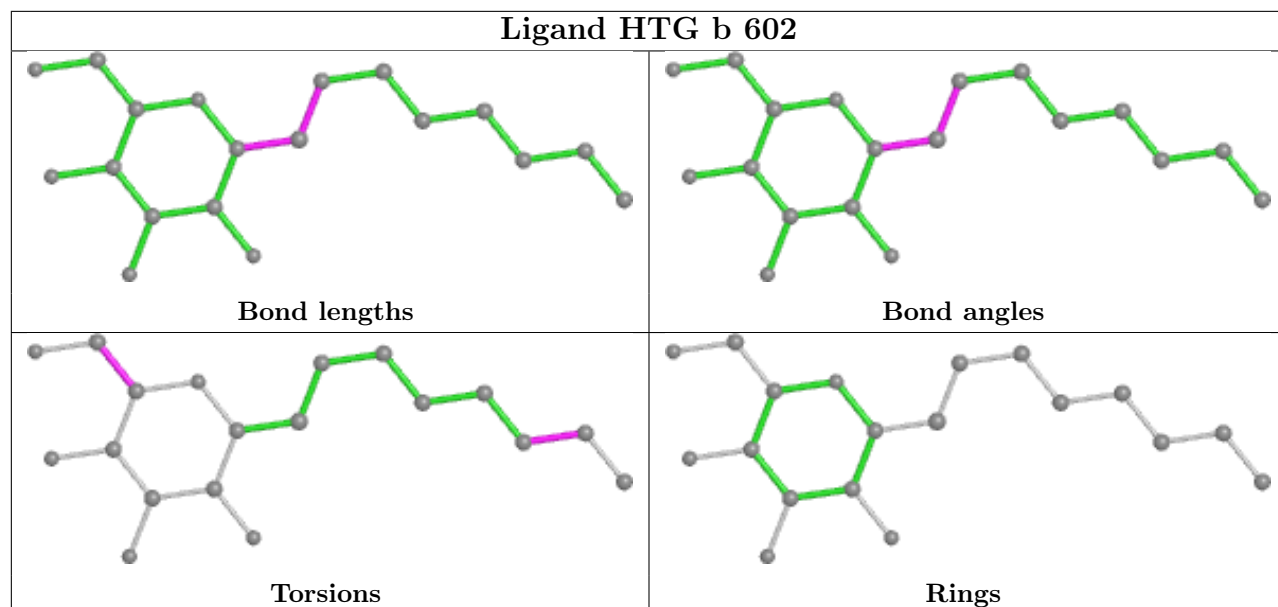


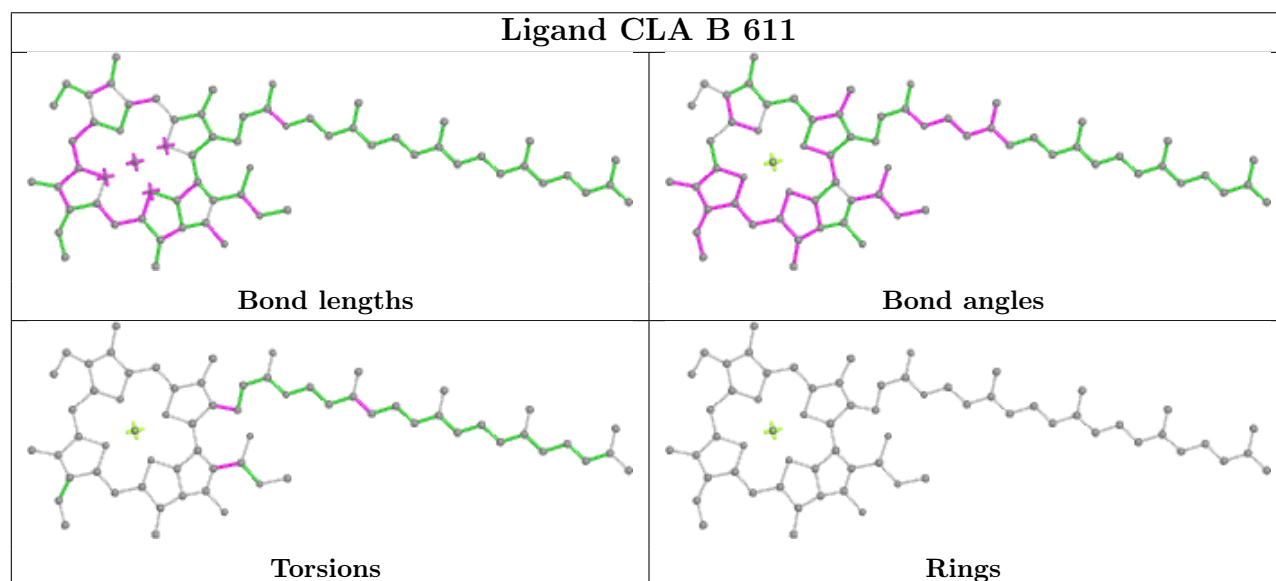
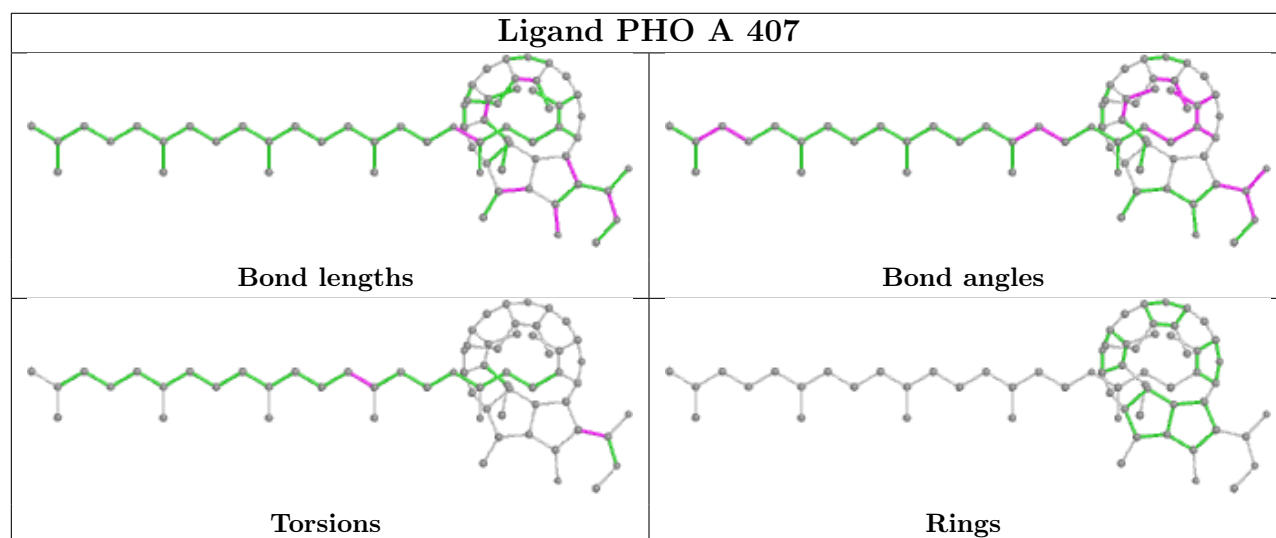
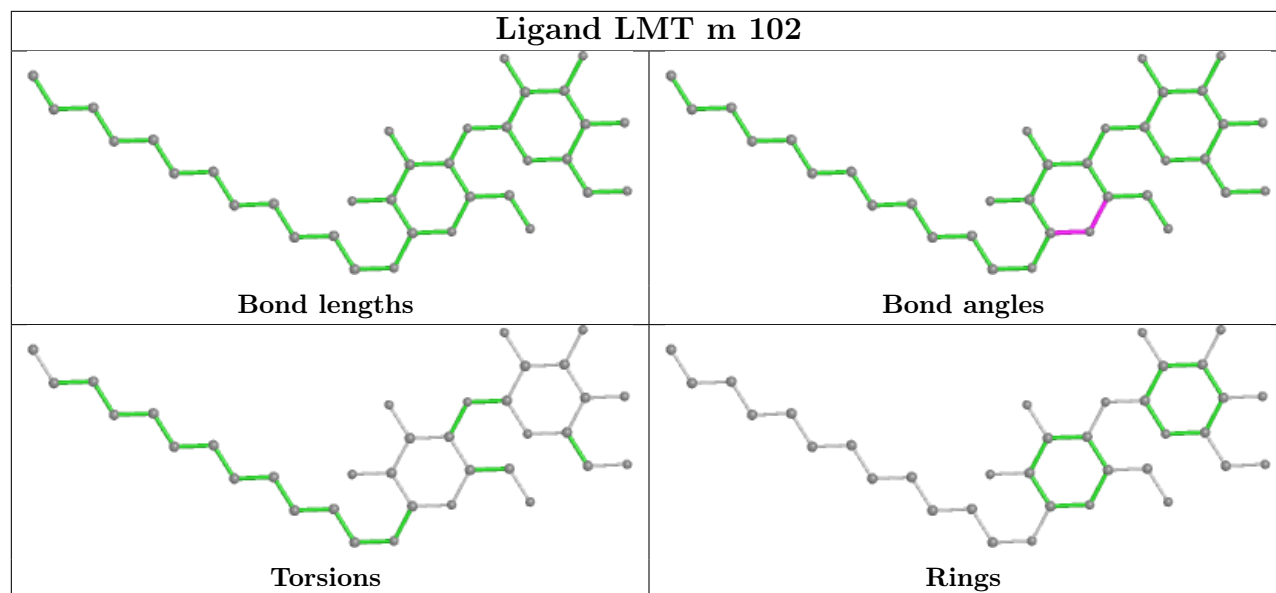
Ligand LMT j 102

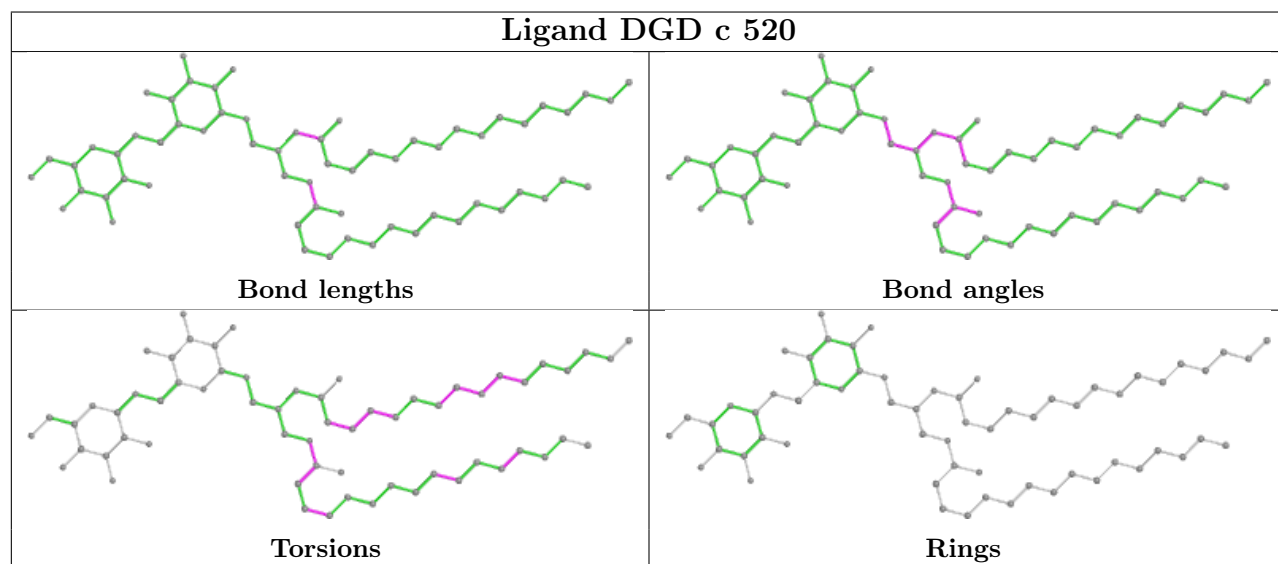
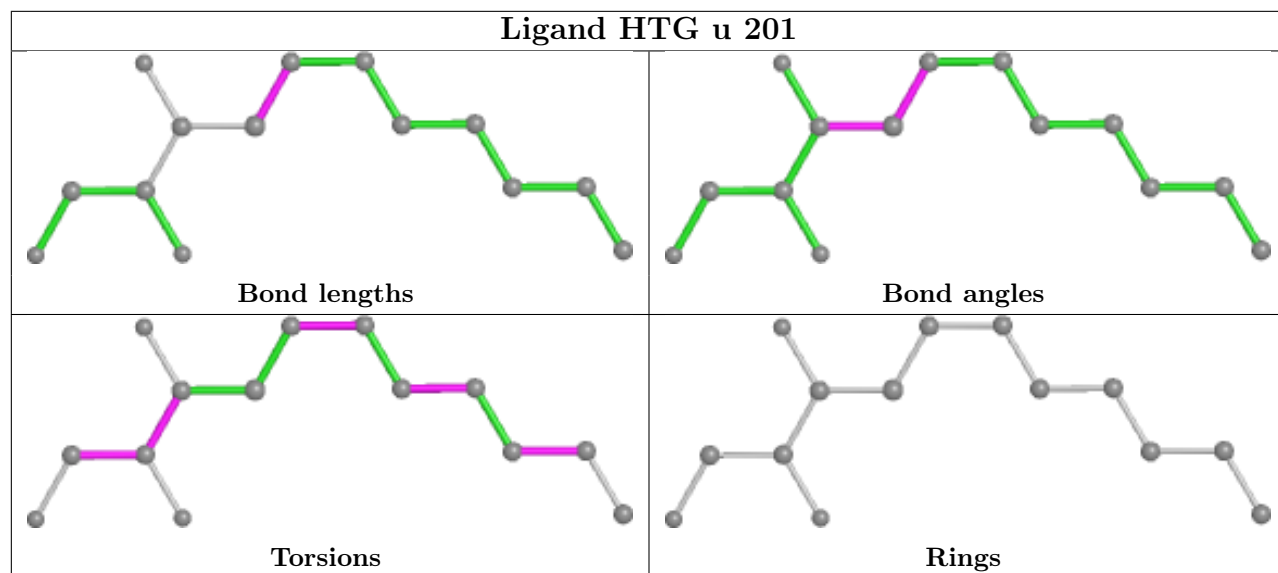
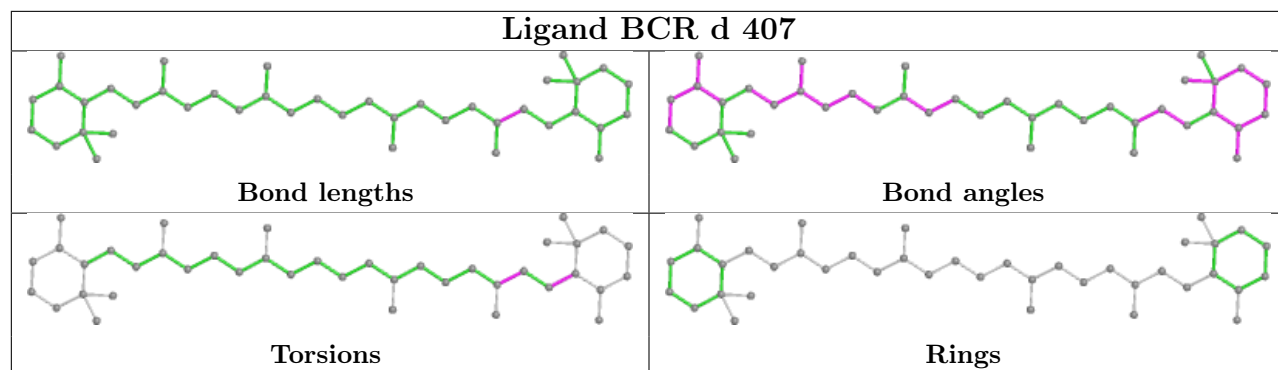


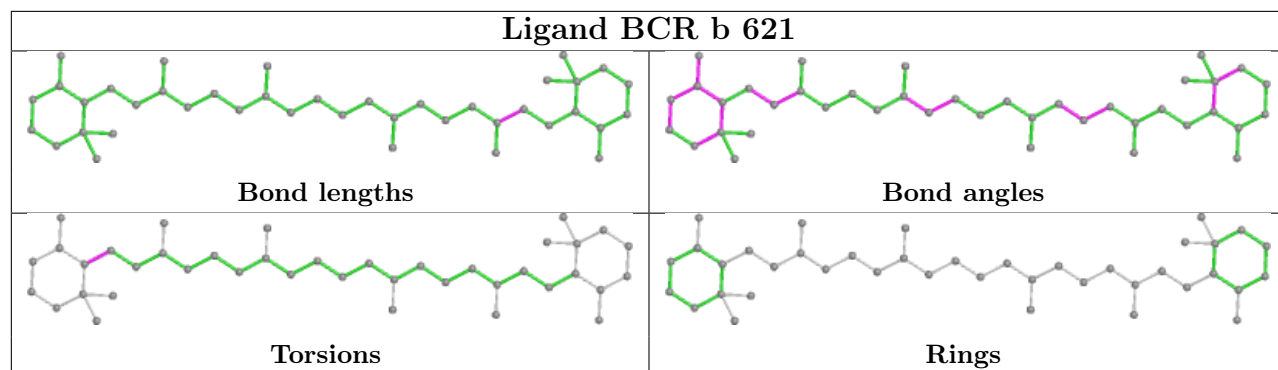
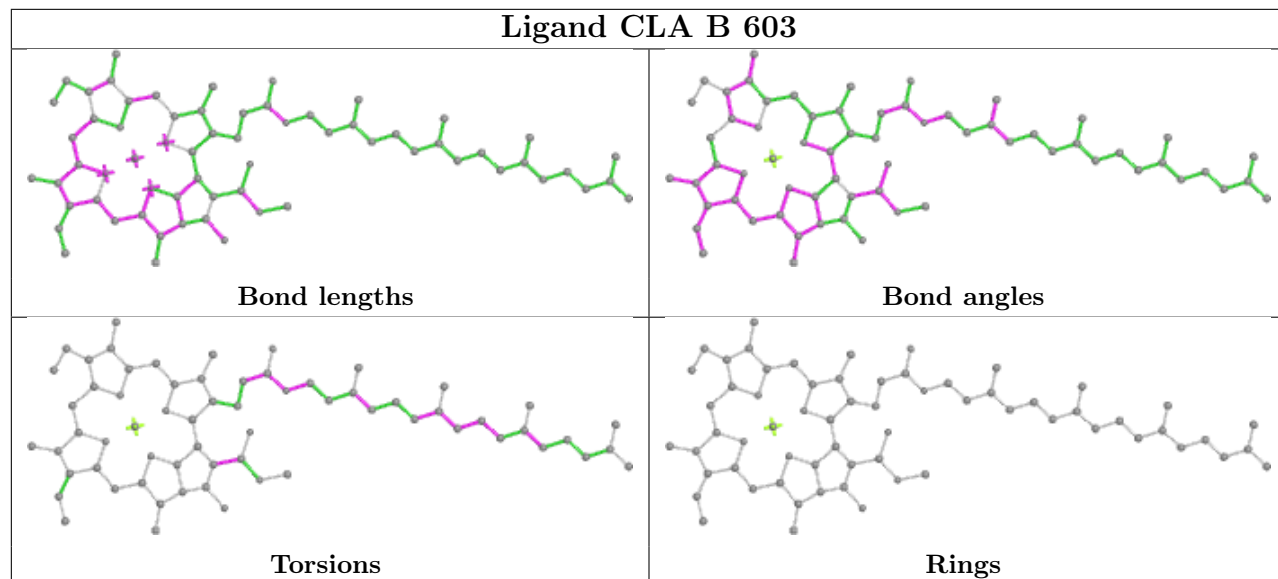
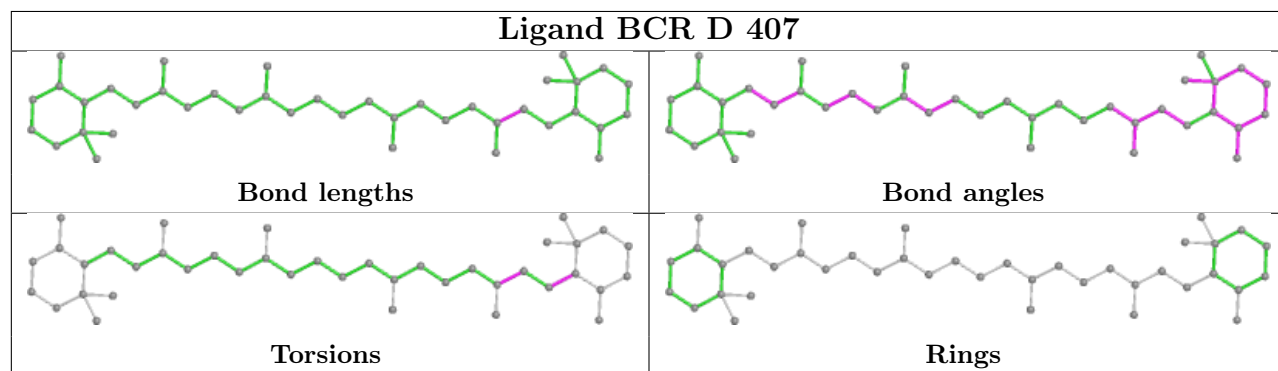
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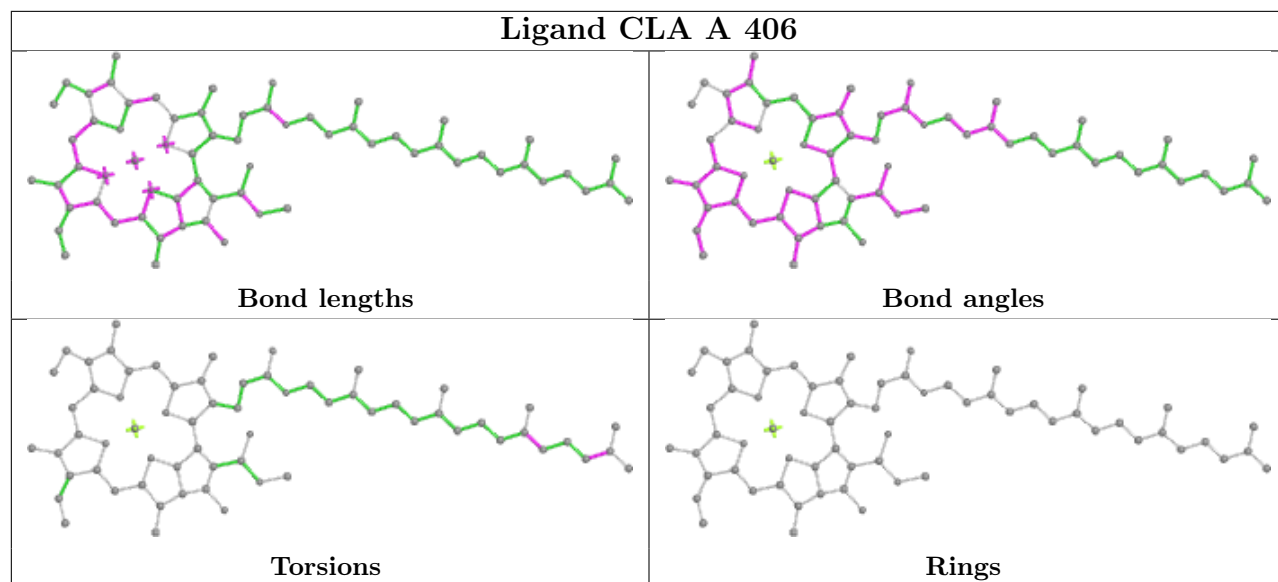




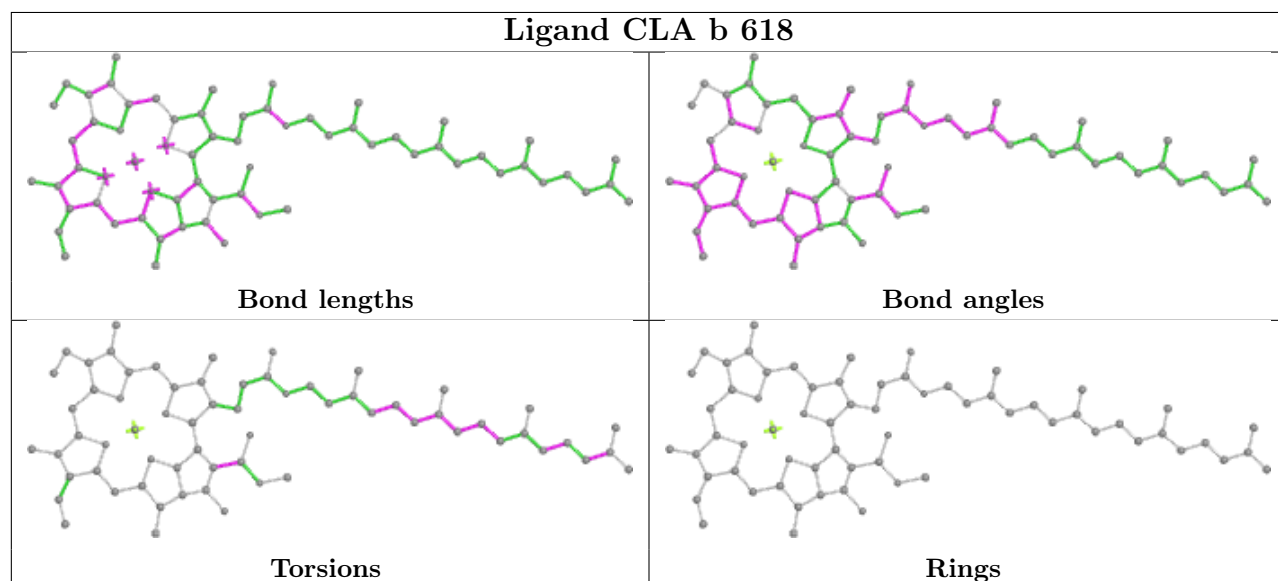


Ligand BCR b 621**Ligand CLA B 603****Ligand BCR D 407**

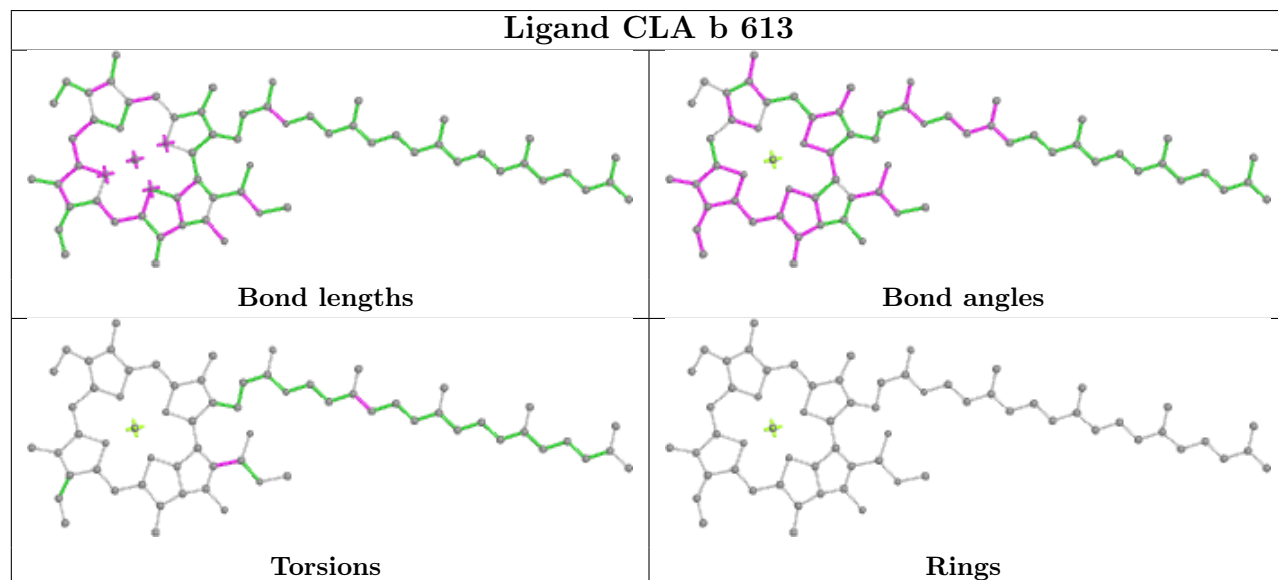
Ligand CLA A 406

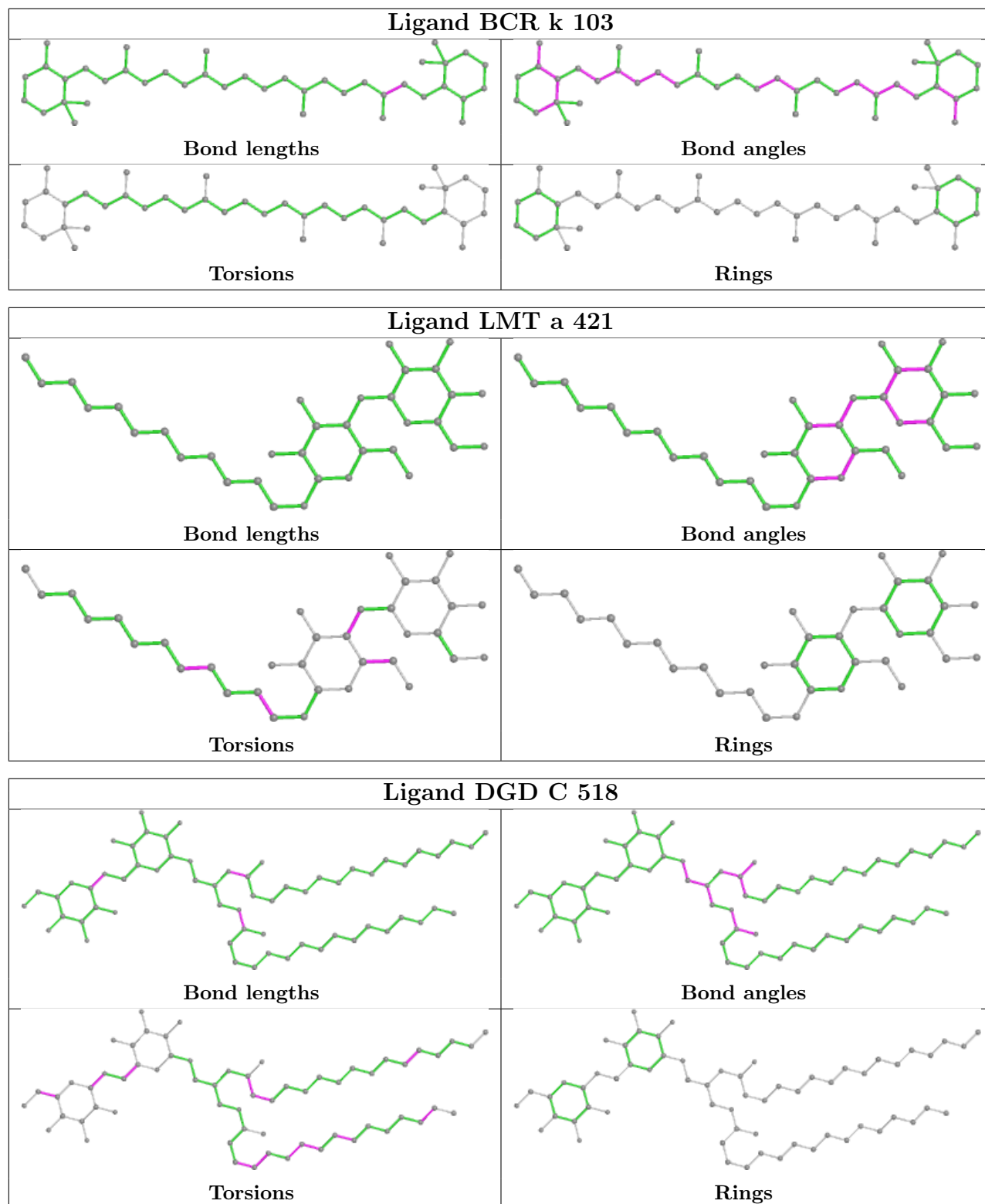


Ligand CLA b 618

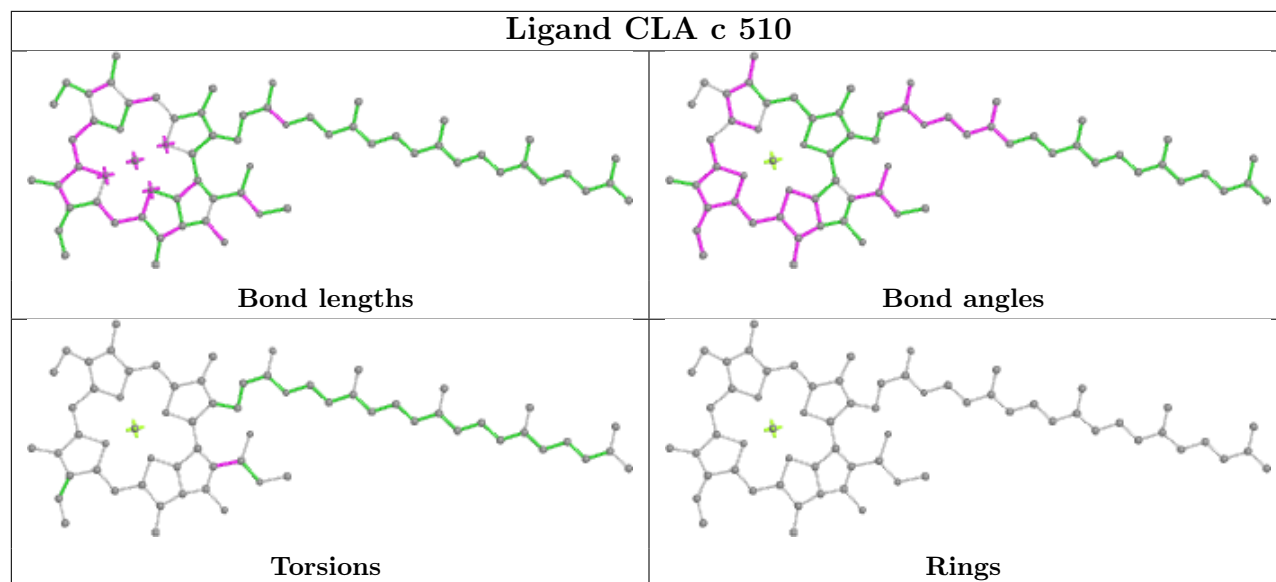


Ligand CLA b 613

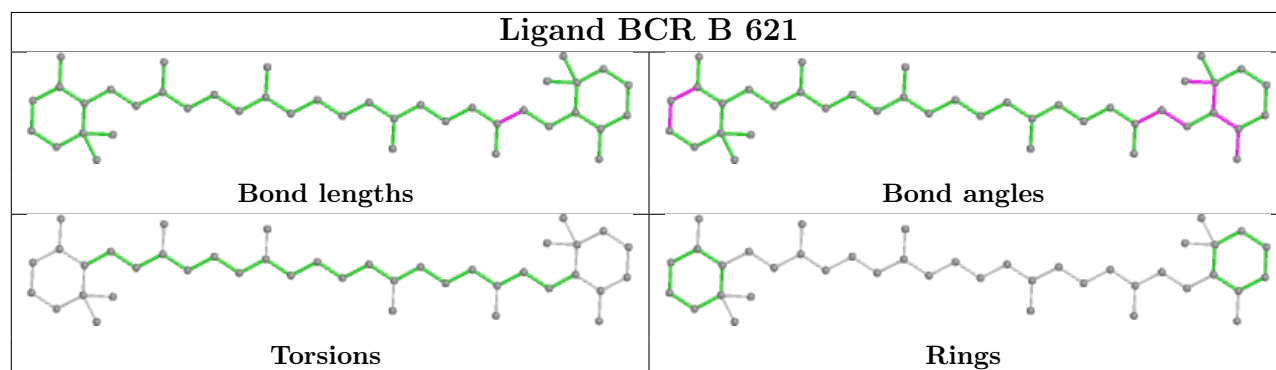




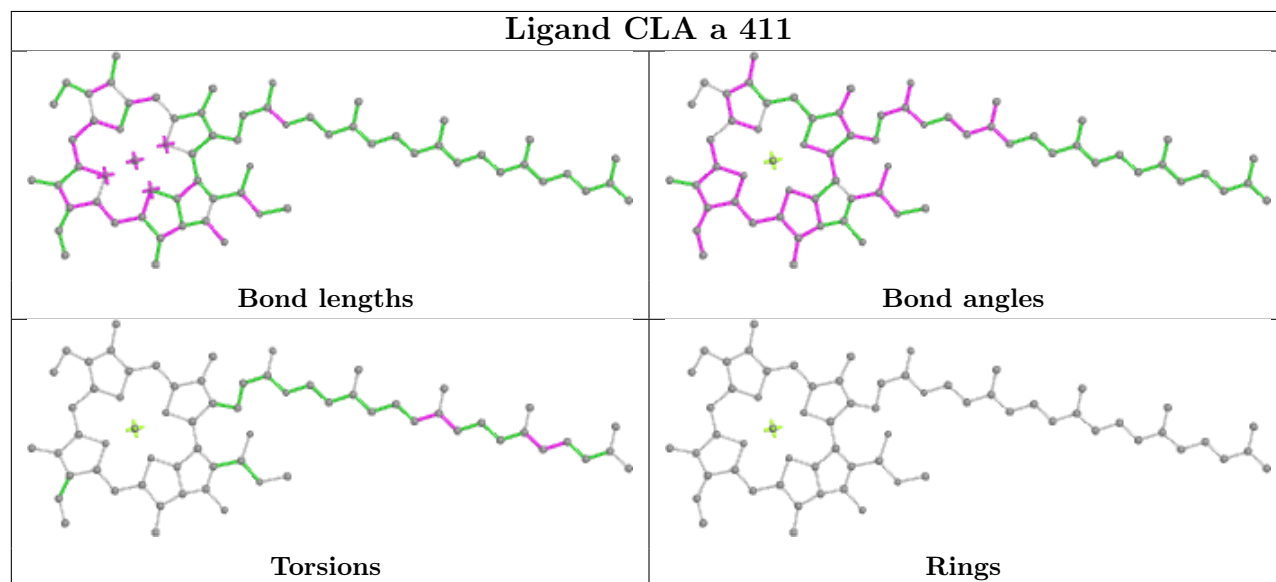
Ligand CLA c 510



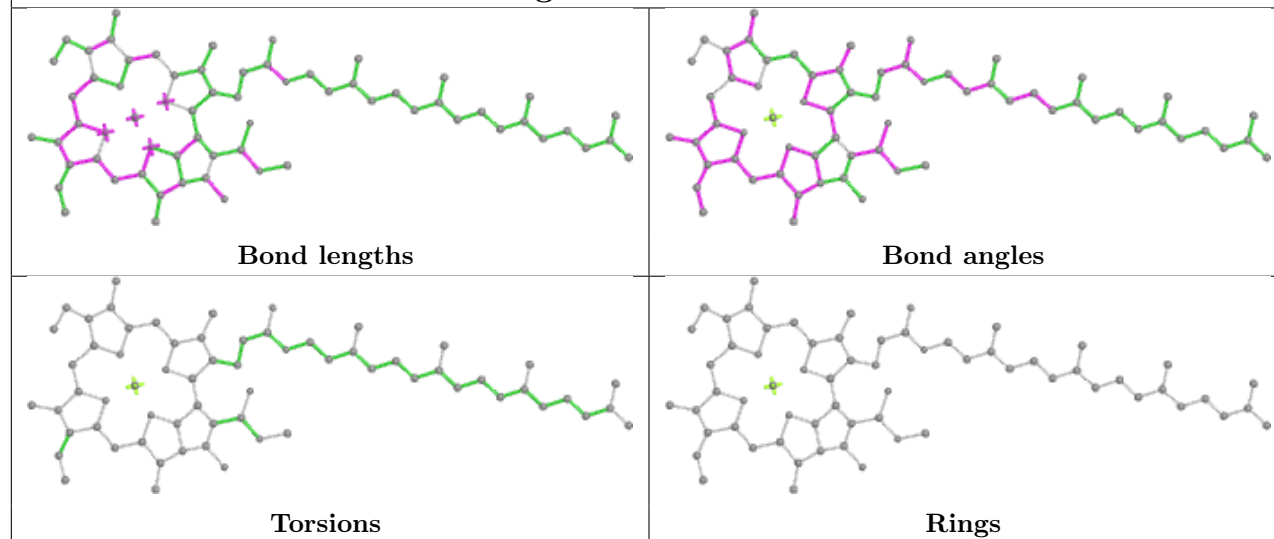
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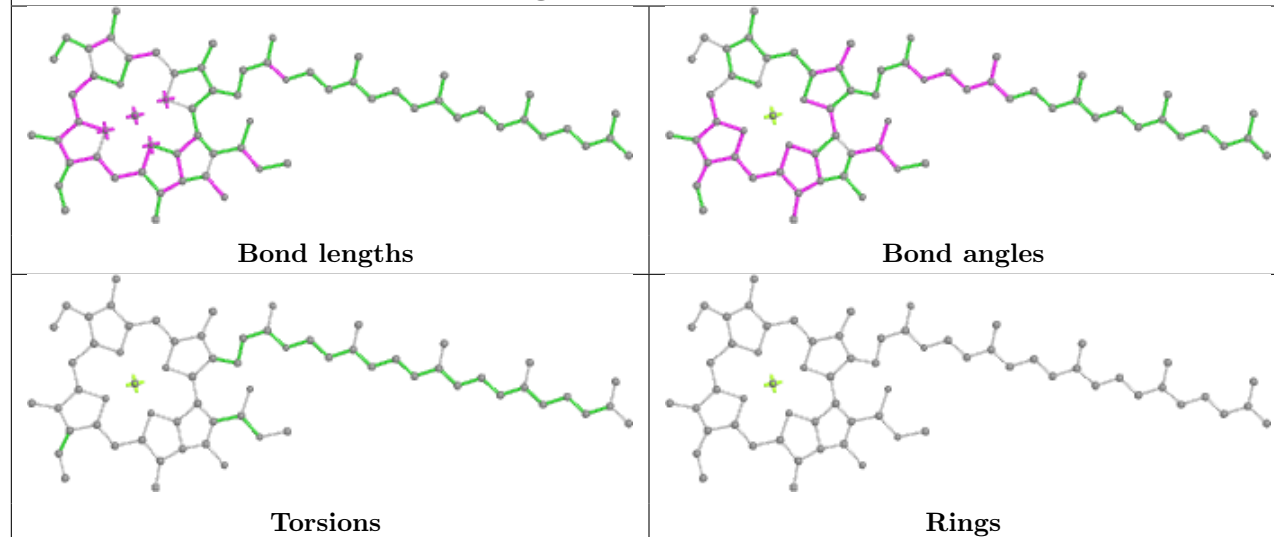
Ligand CLA a 411



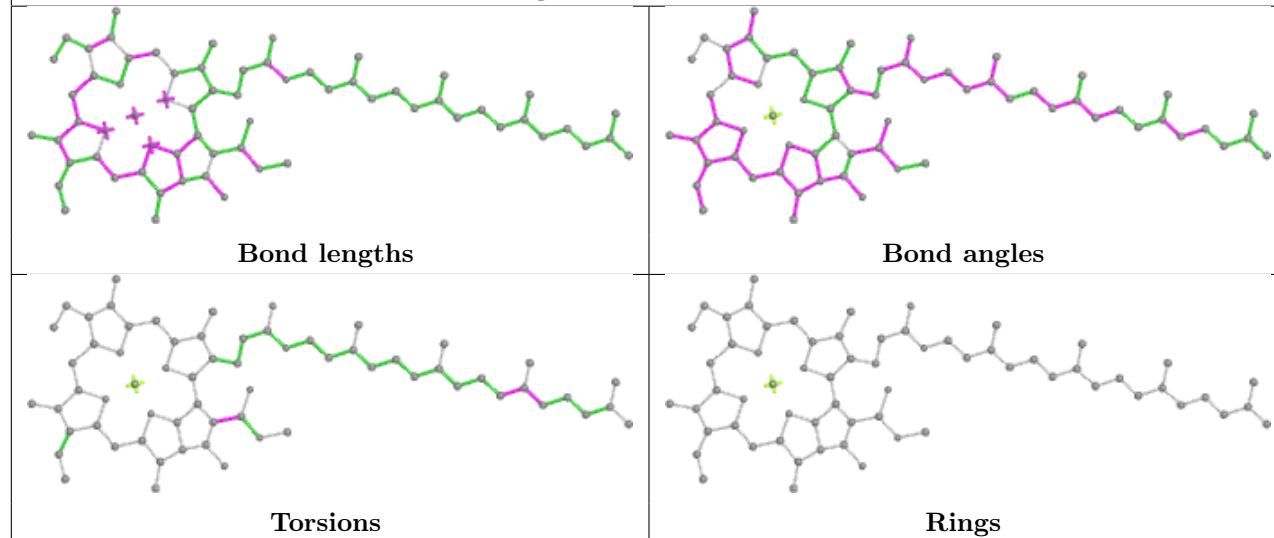
Ligand CLA b 615



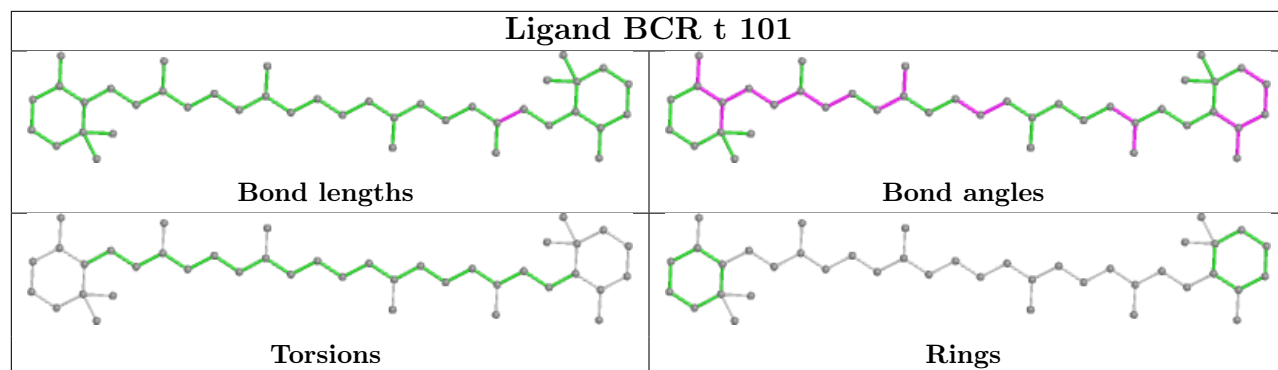
Ligand CLA C 507



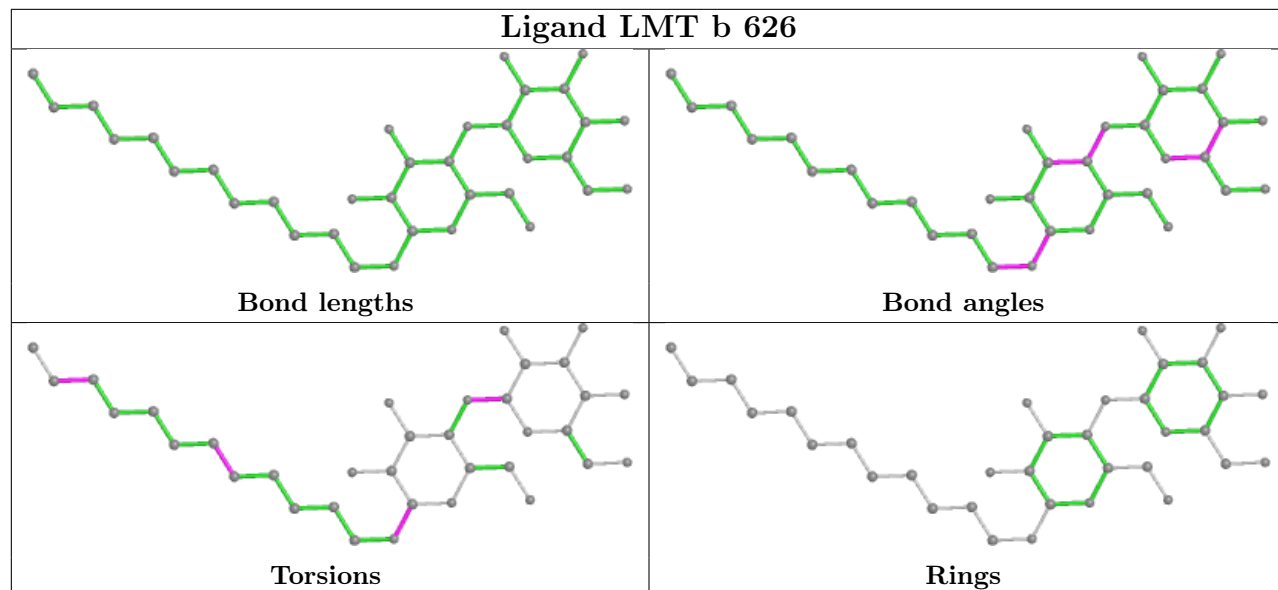
Ligand CLA C 506



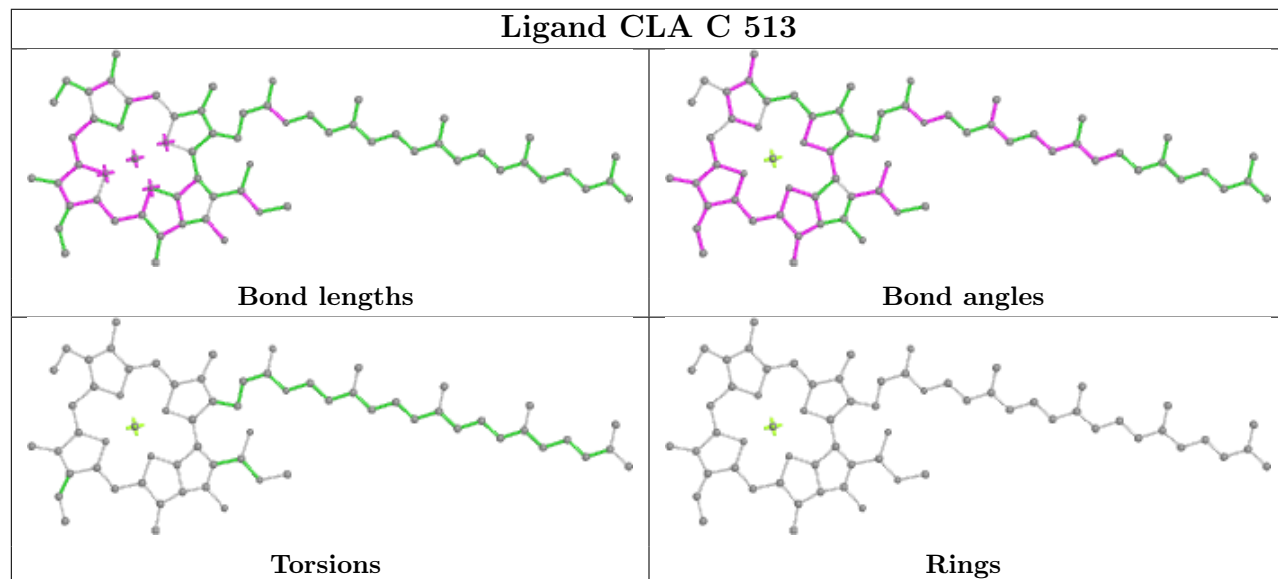
Ligand BCR t 101

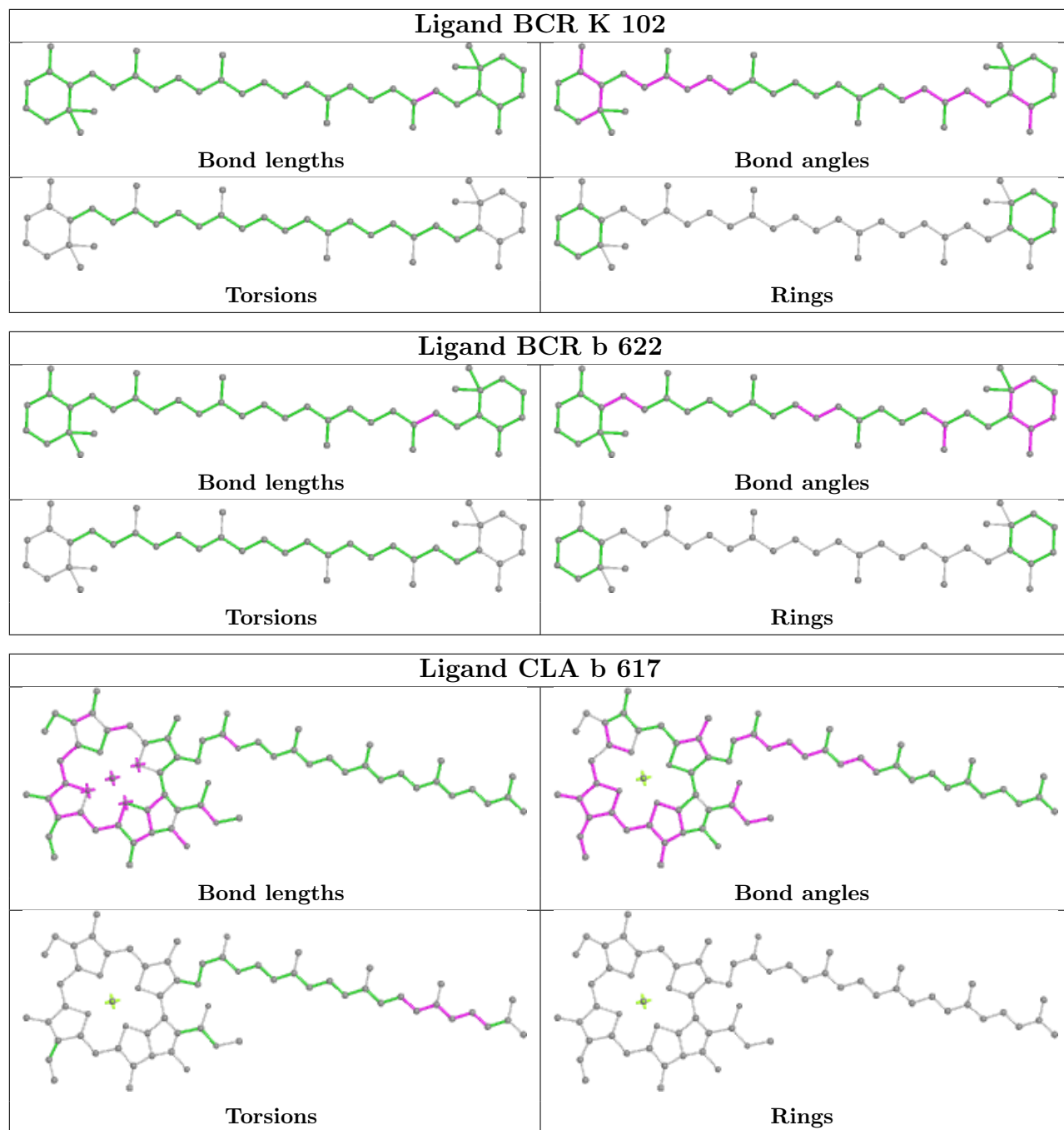


Ligand LMT b 626

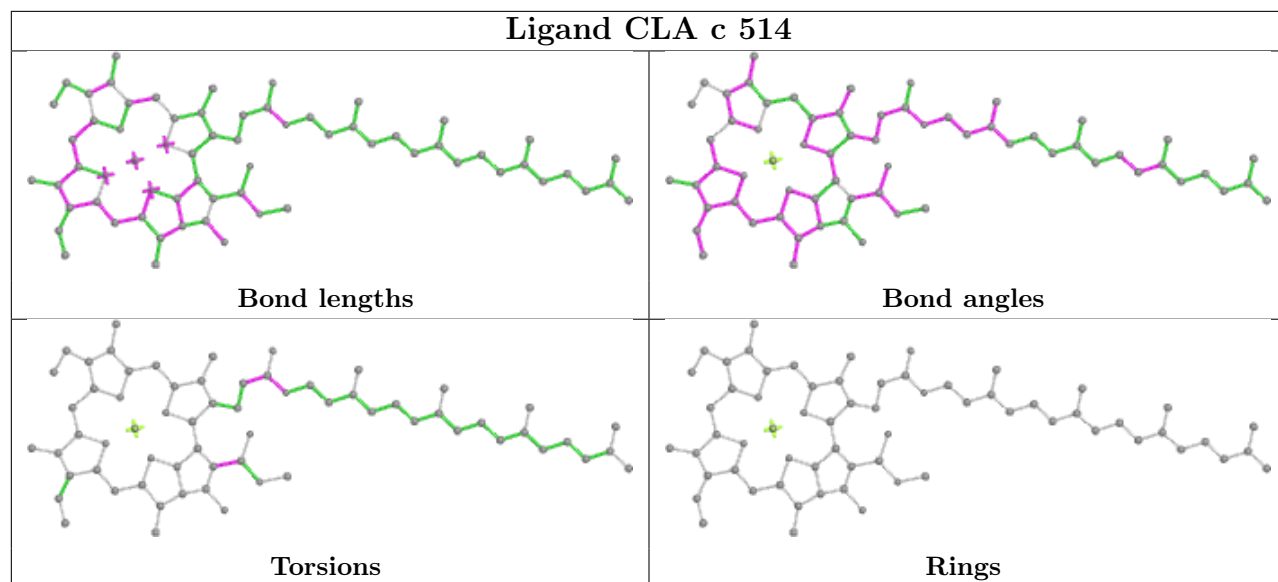


Ligand CLA C 513

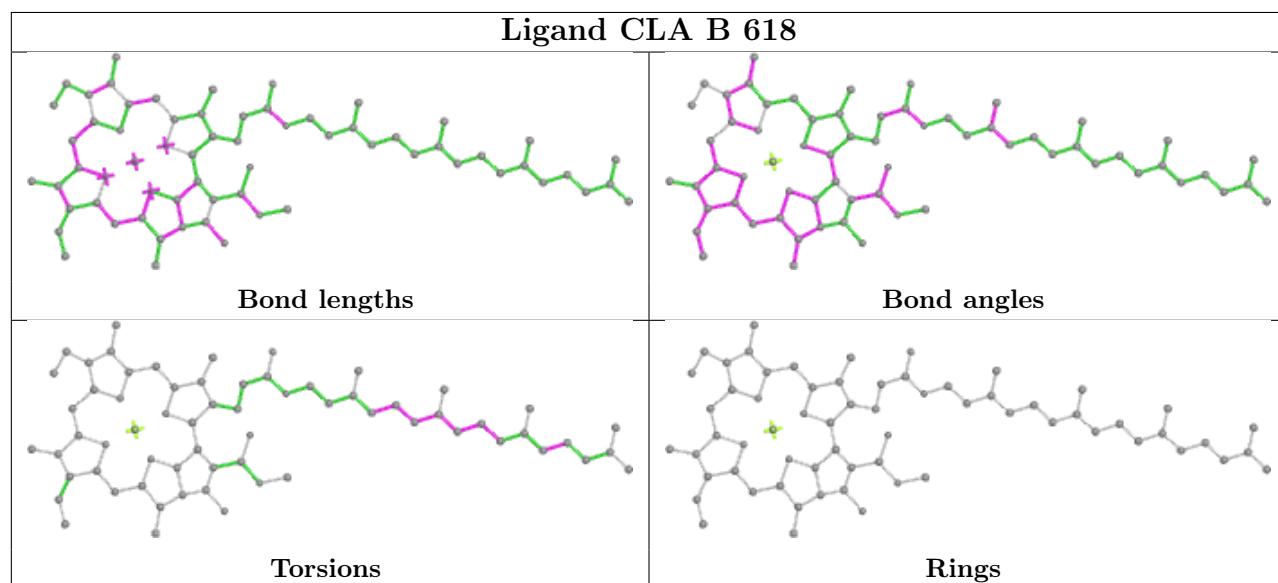


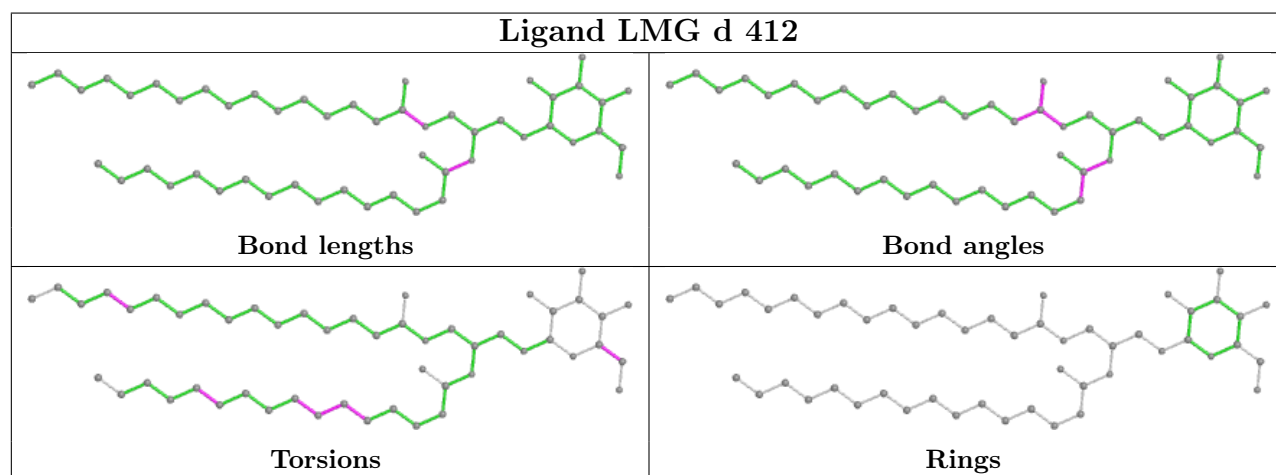
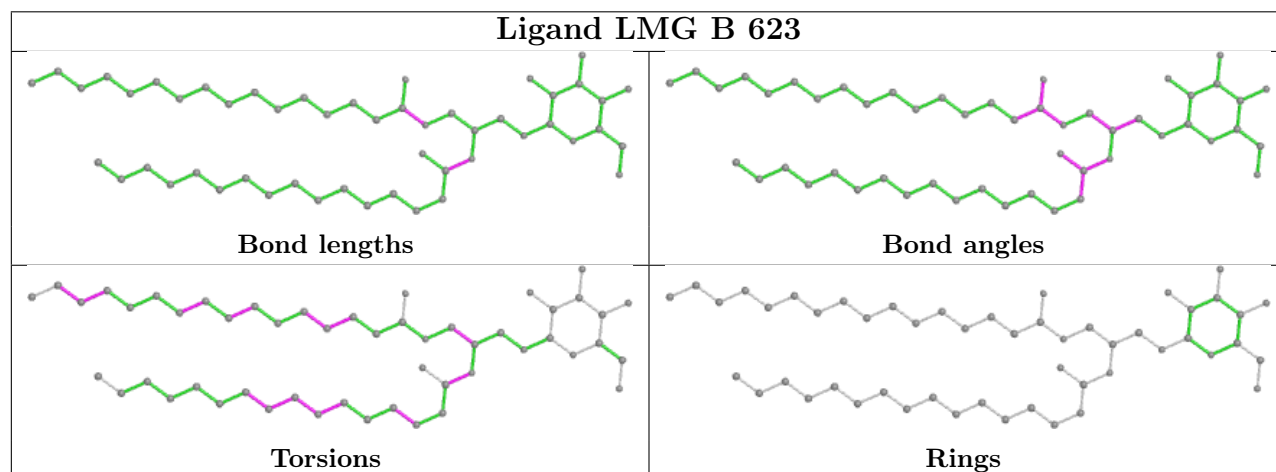
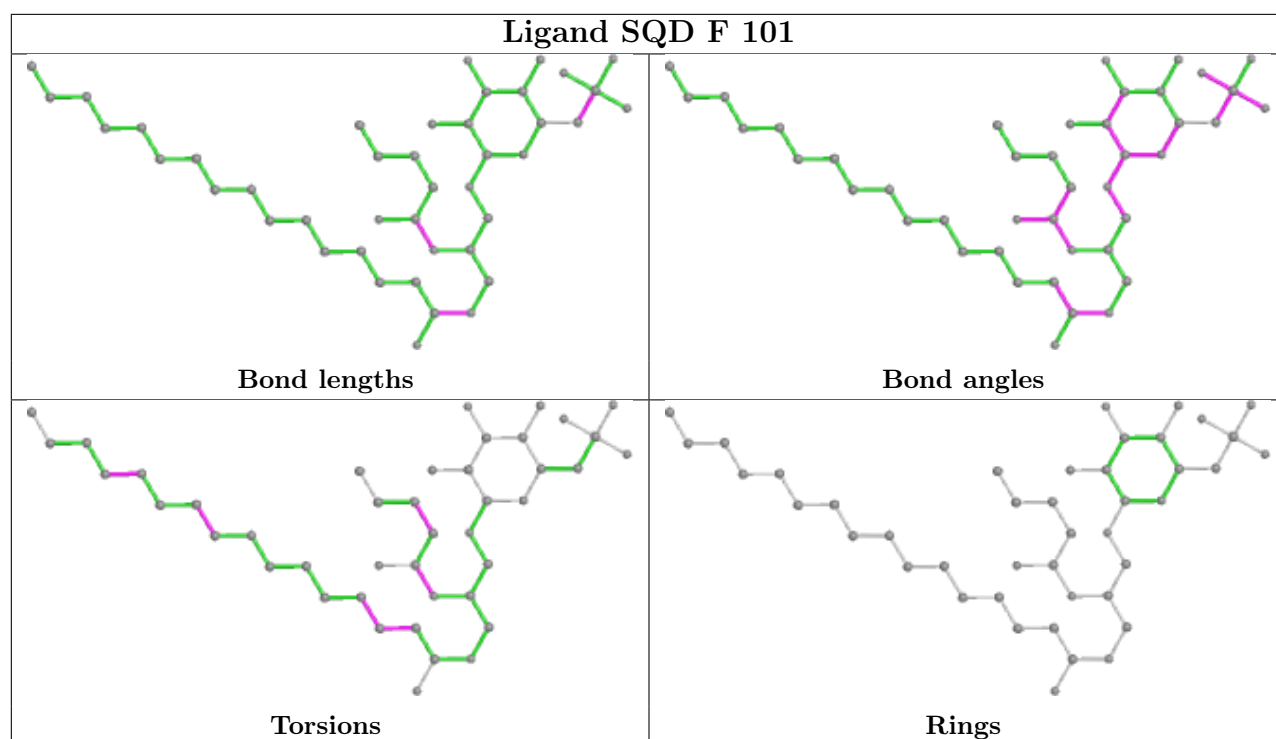


Ligand CLA c 514

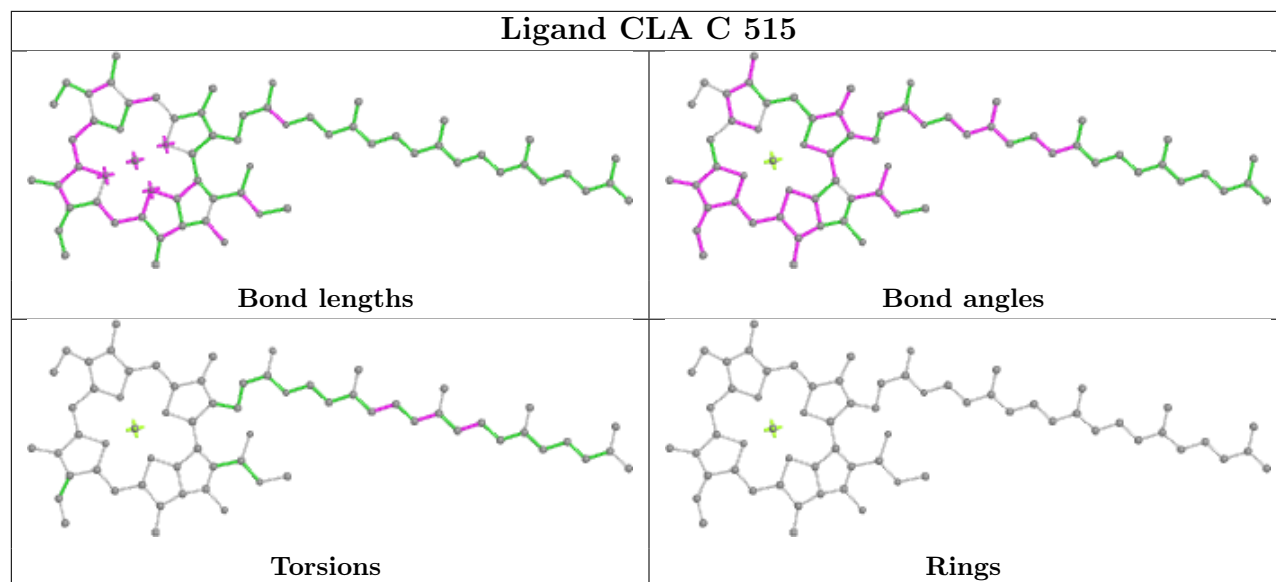


Ligand CLA B 618

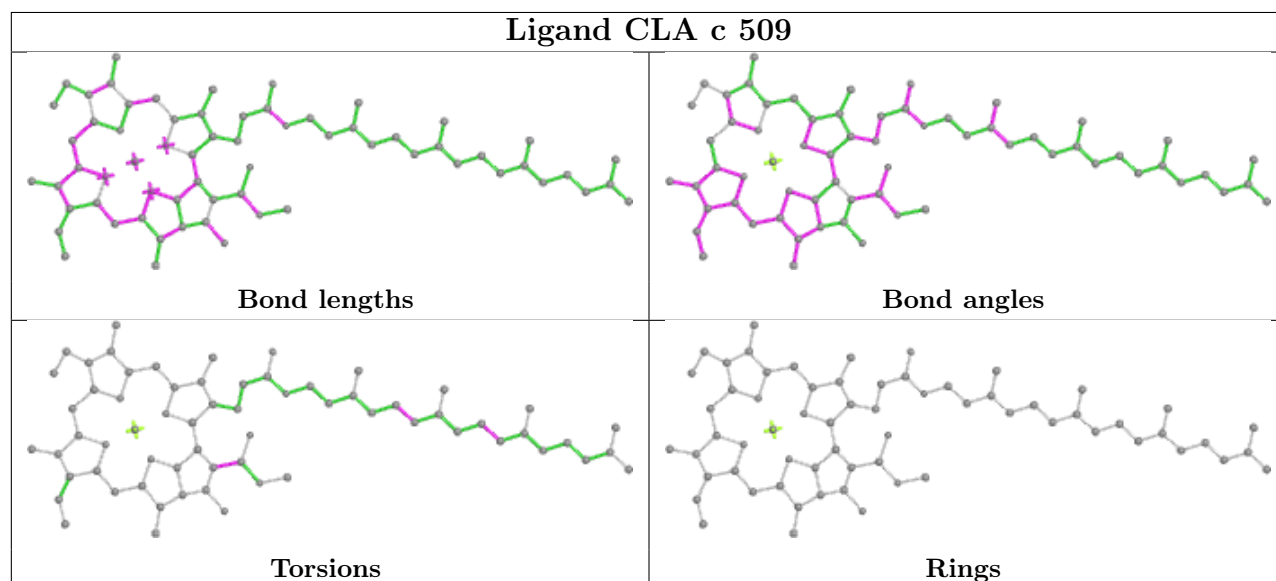




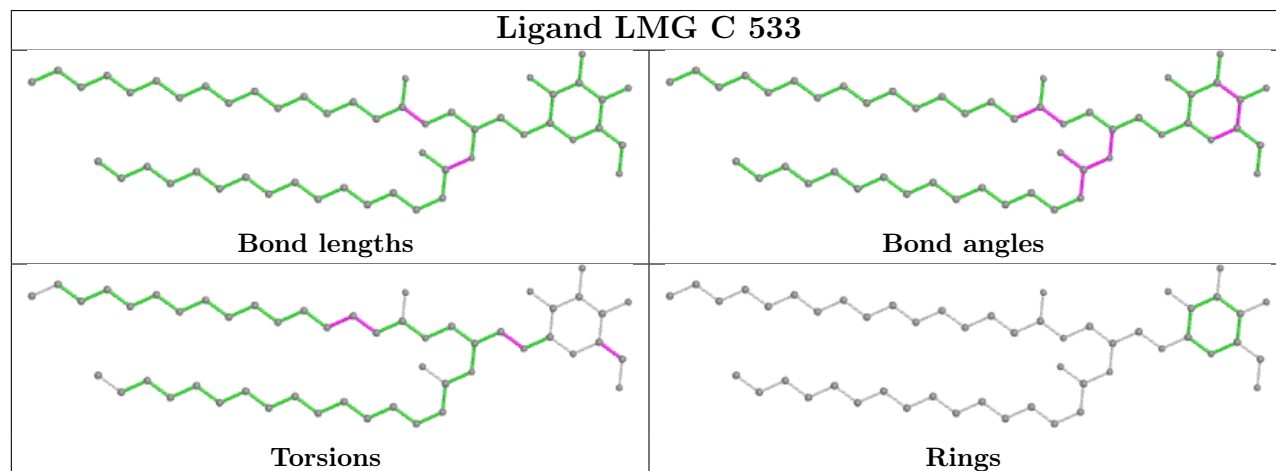
Ligand CLA C 515

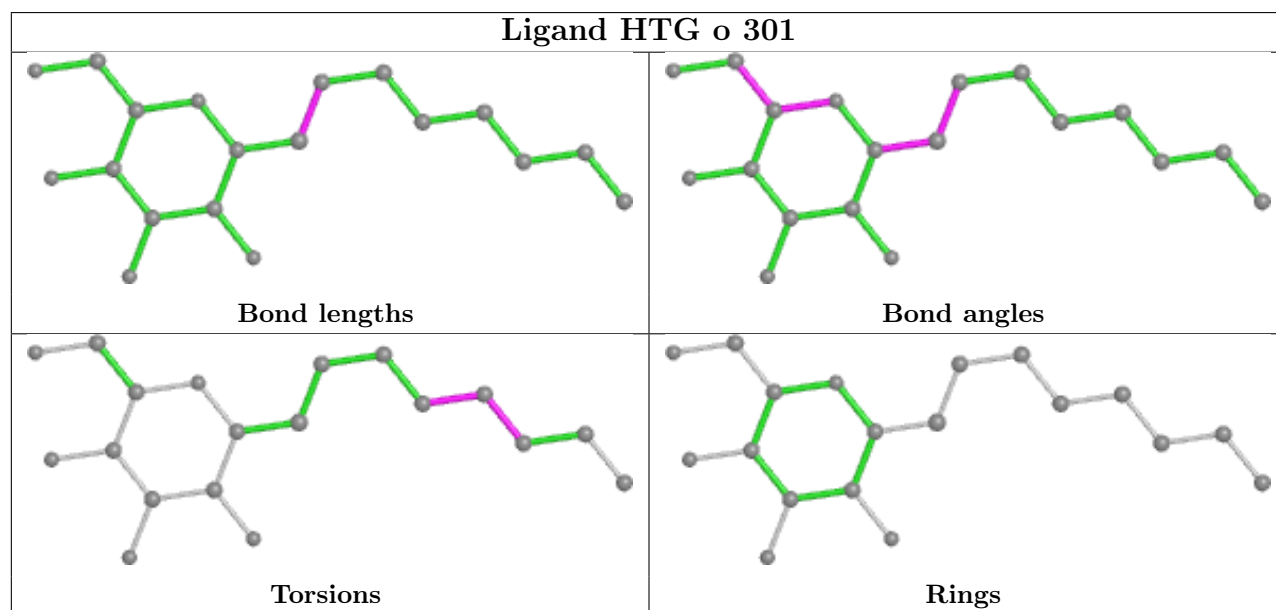
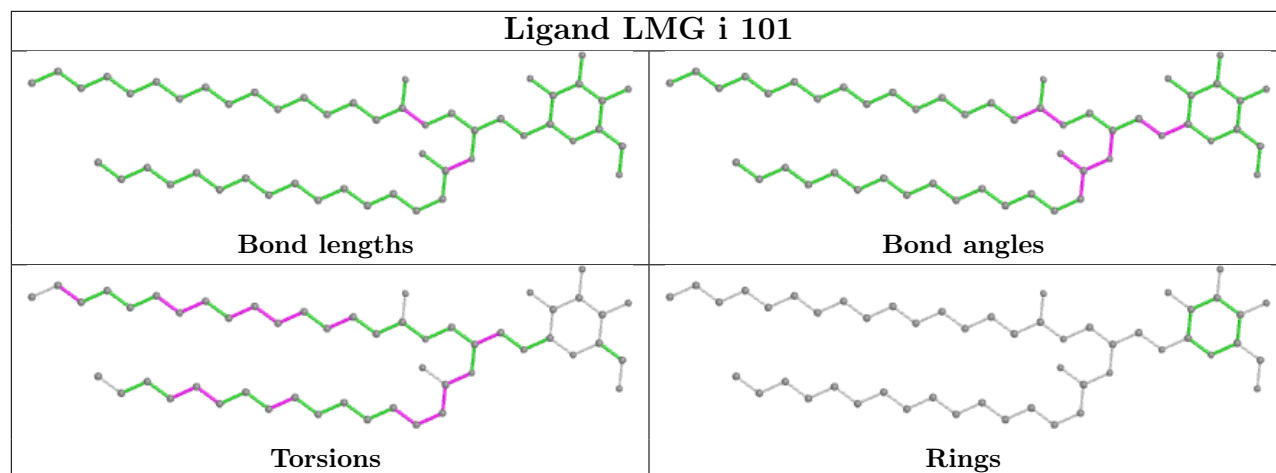
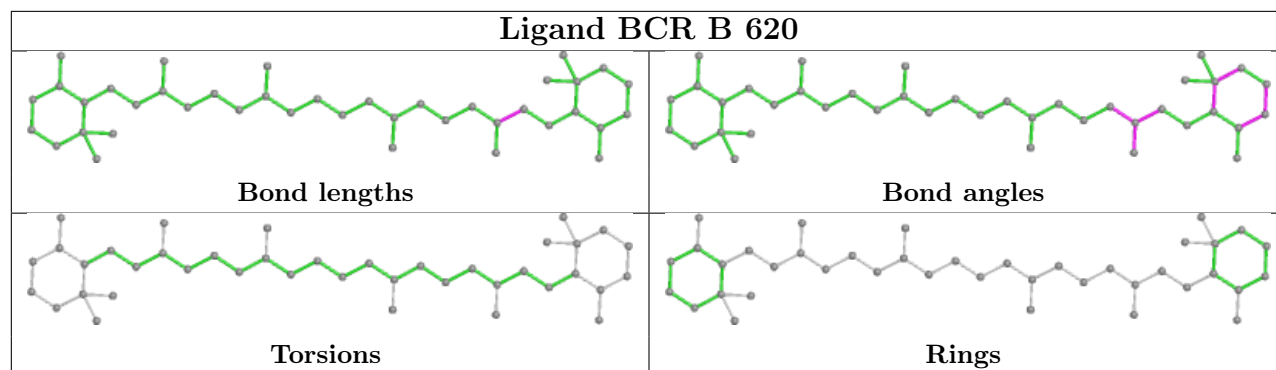


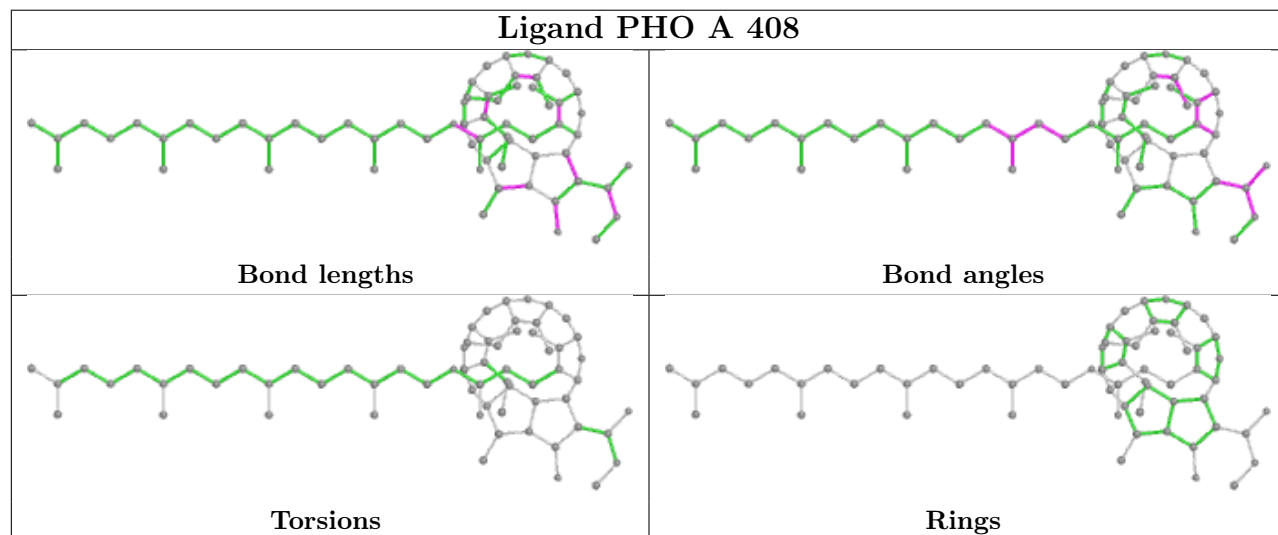
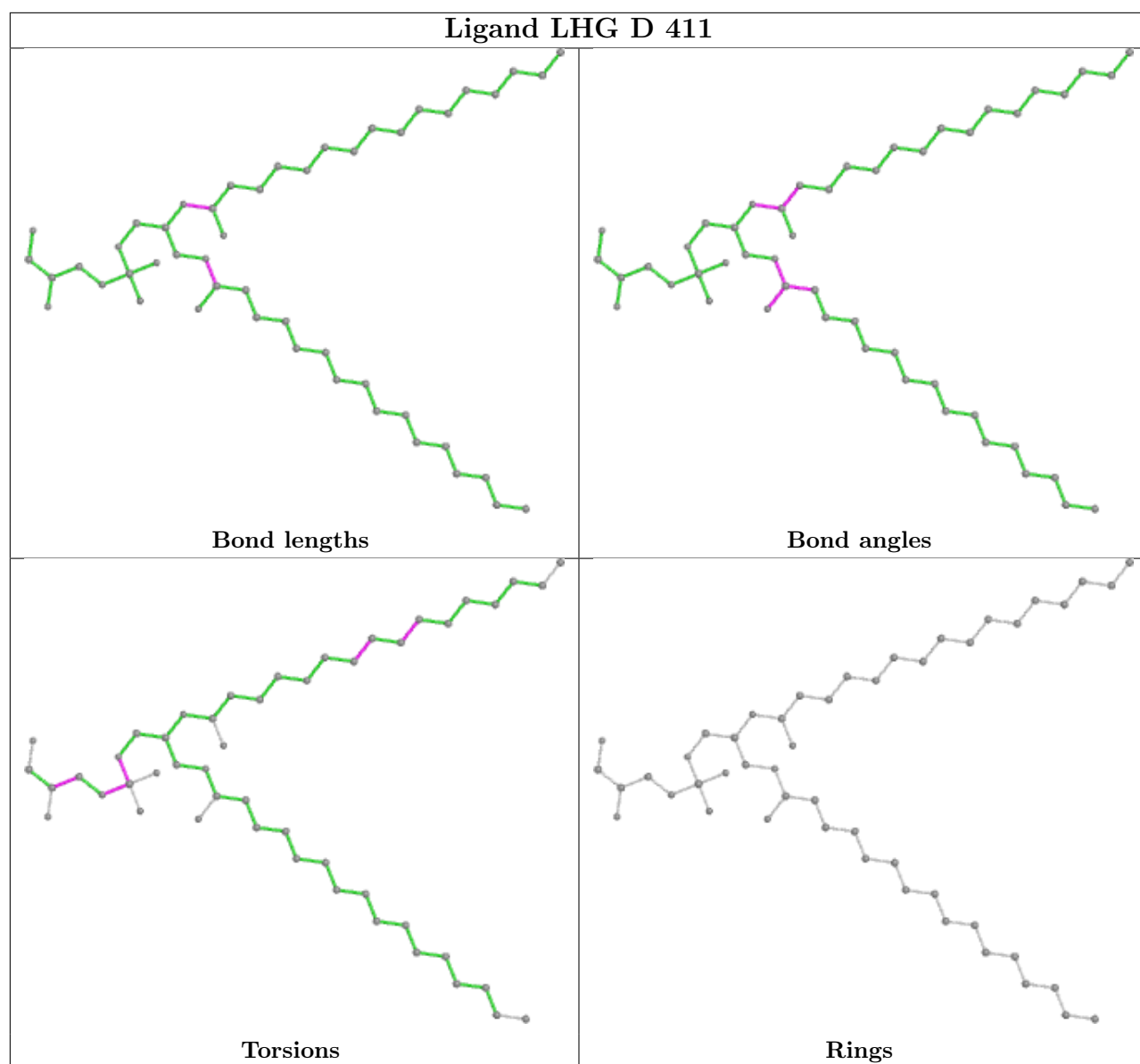
Ligand CLA c 509



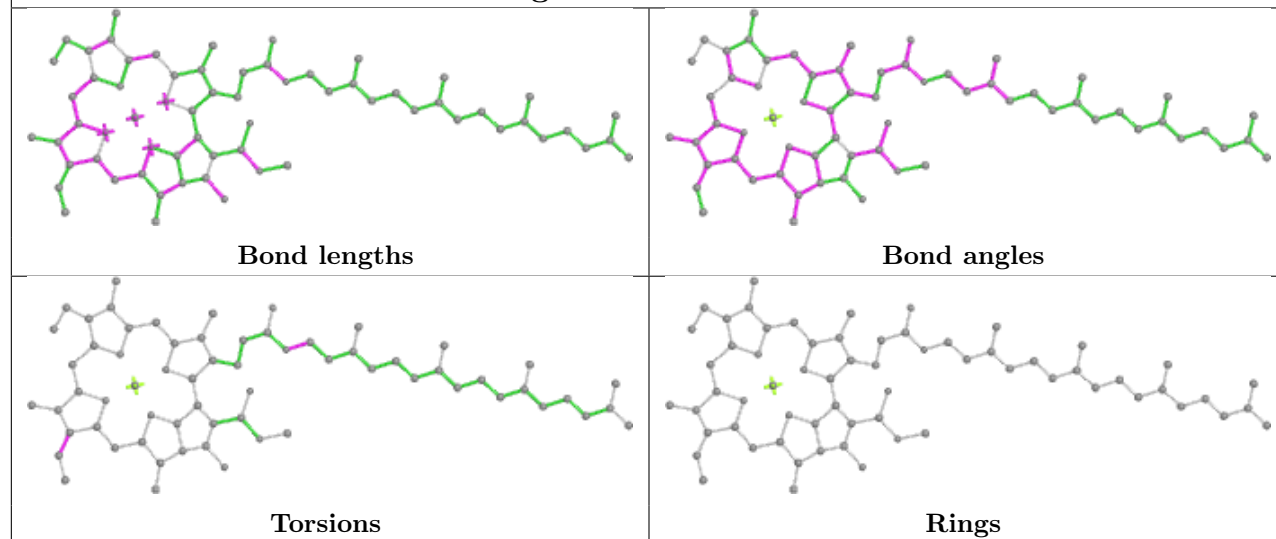
Ligand LMG C 533



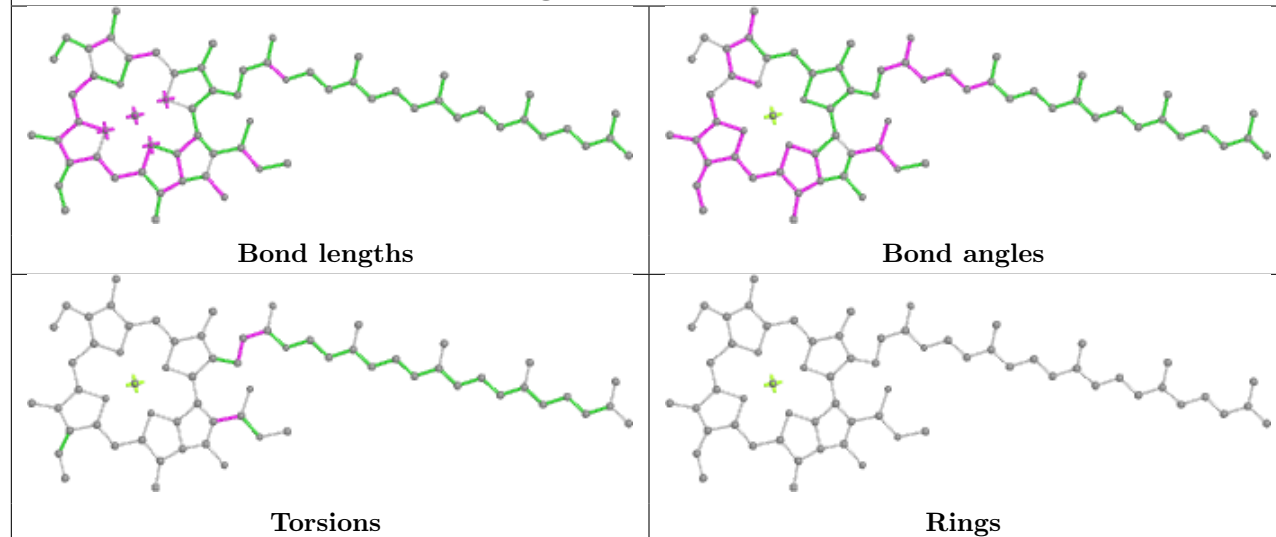




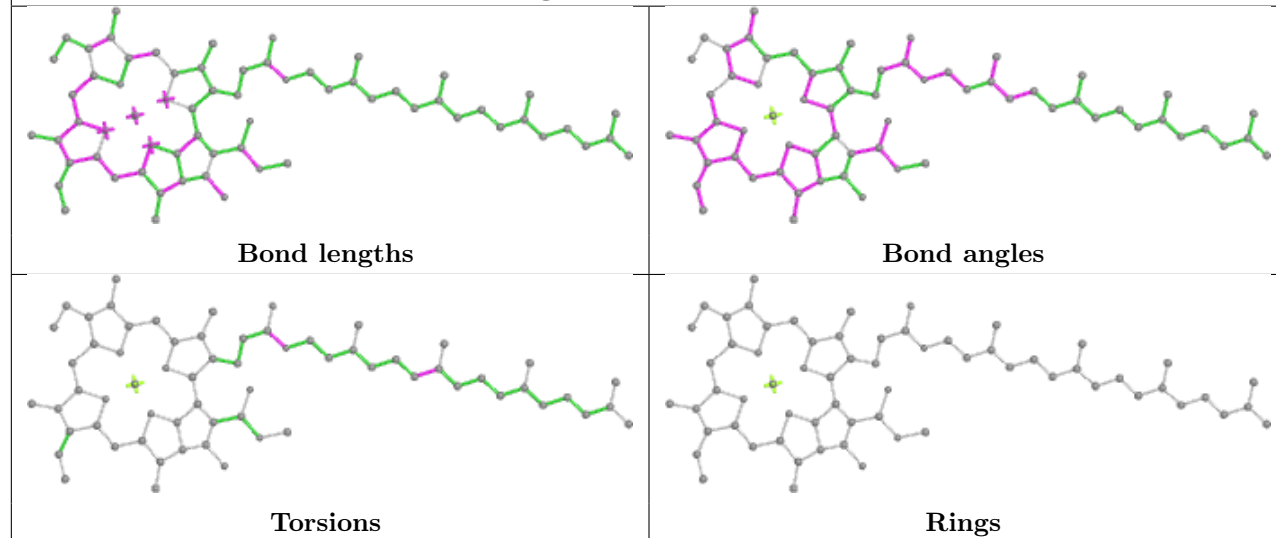
Ligand CLA D 405

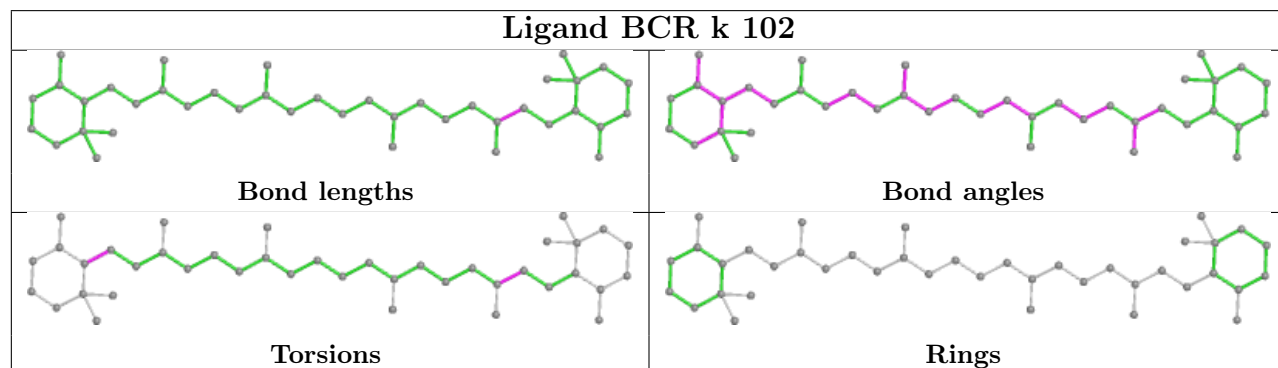
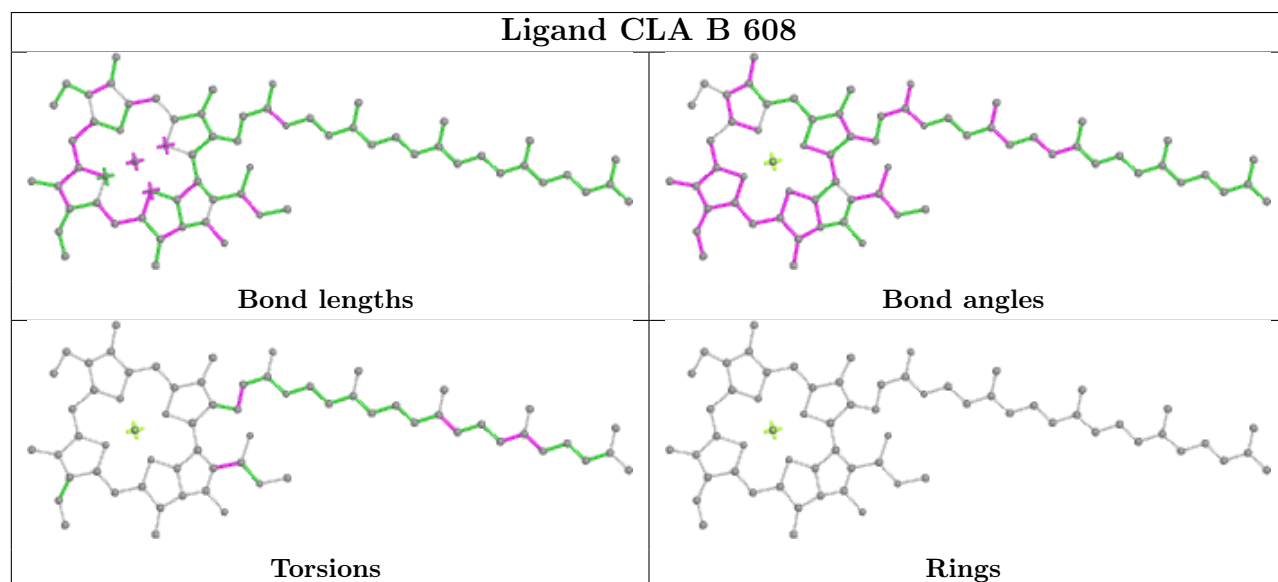
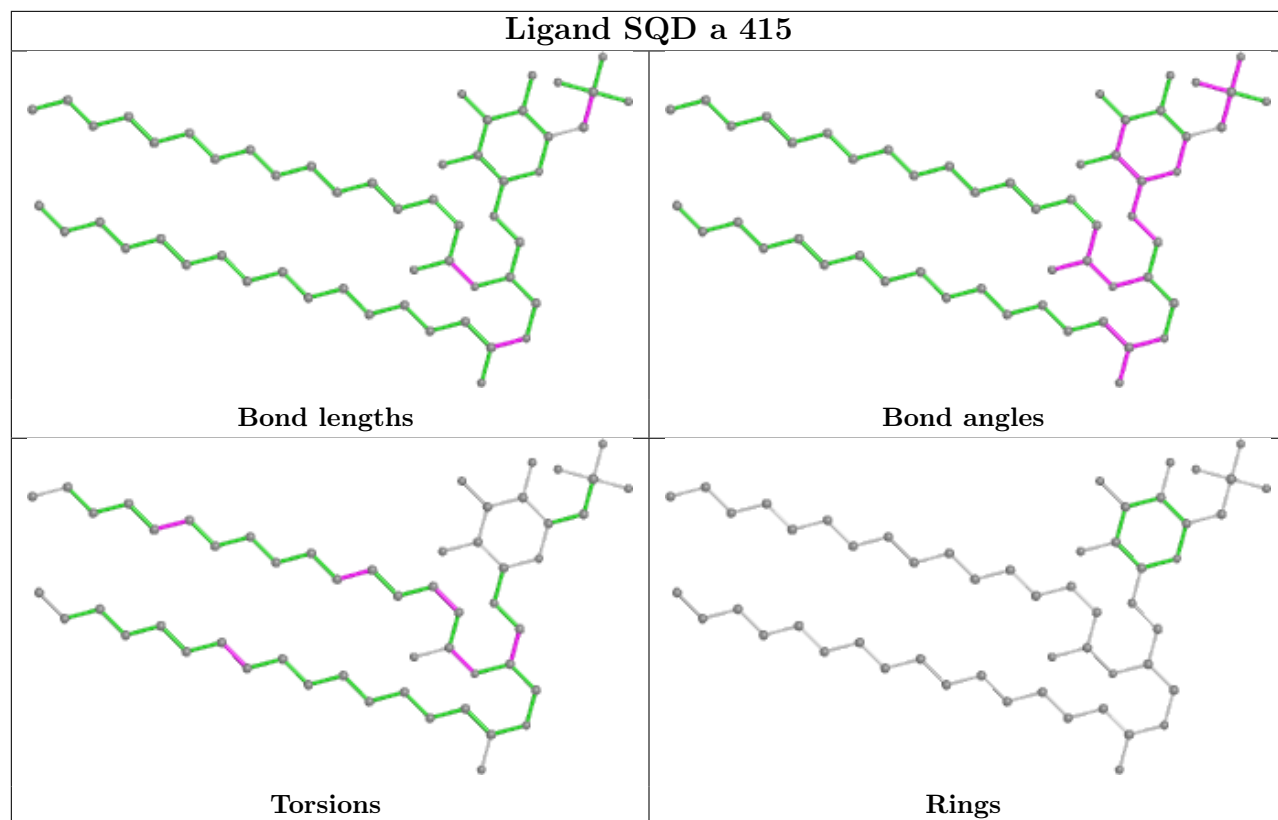


Ligand CLA c 503

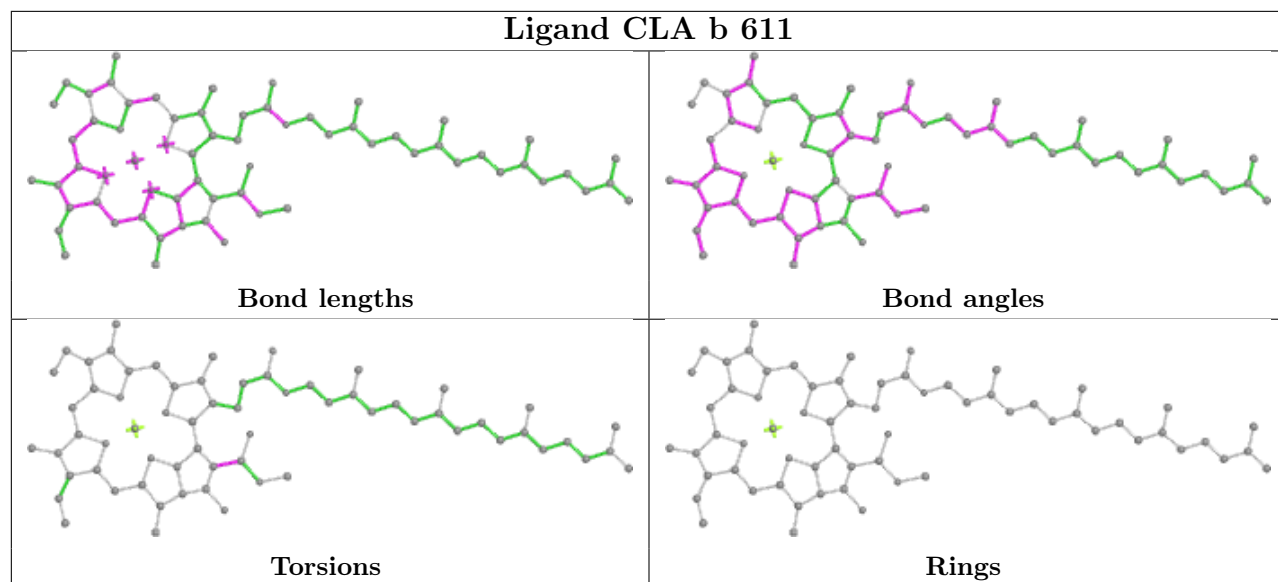


Ligand CLA c 513

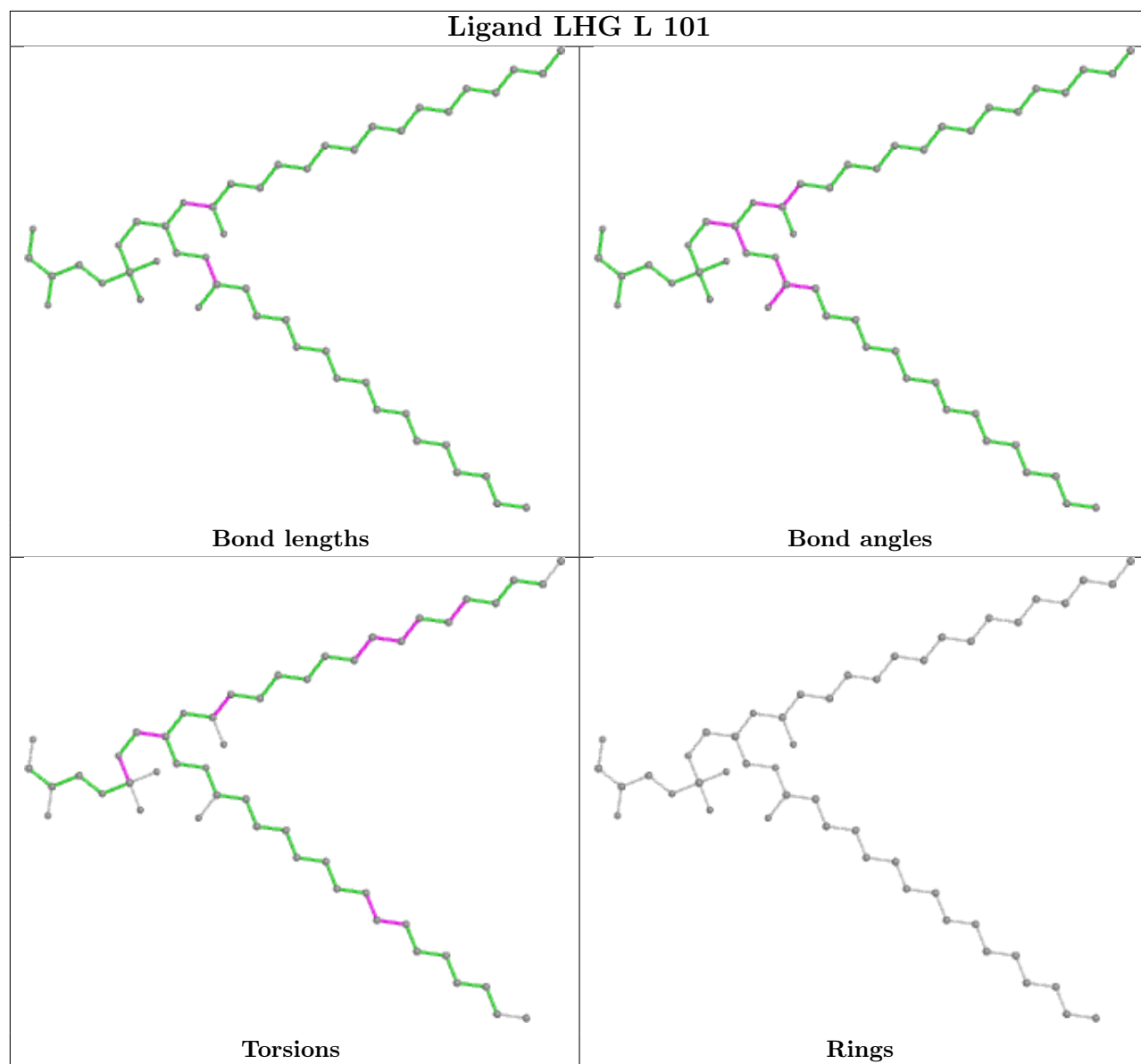




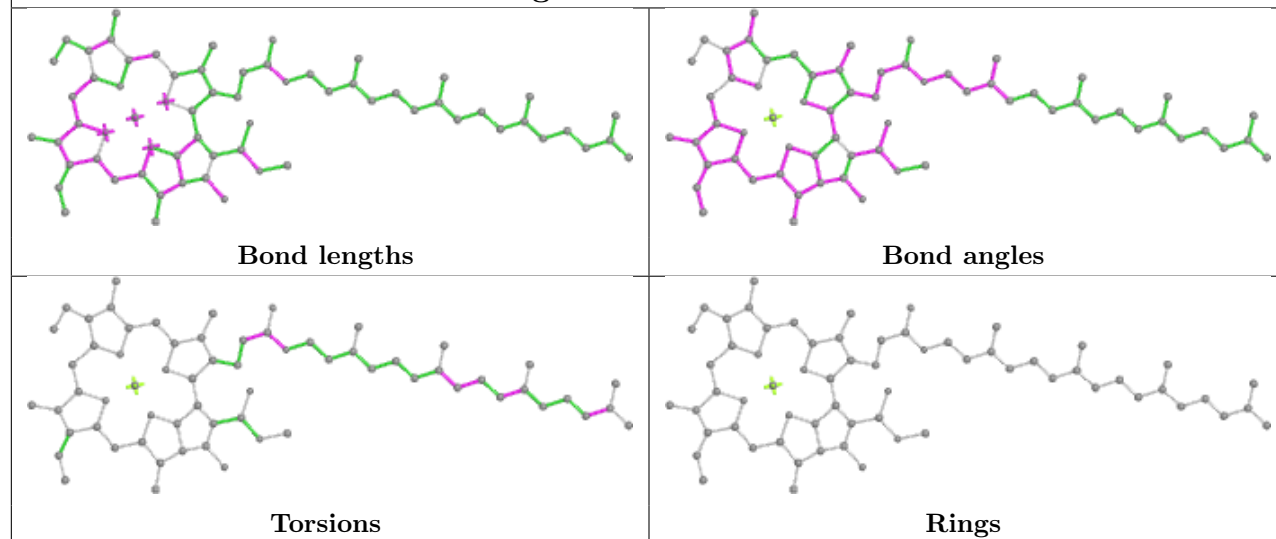
Ligand CLA b 611



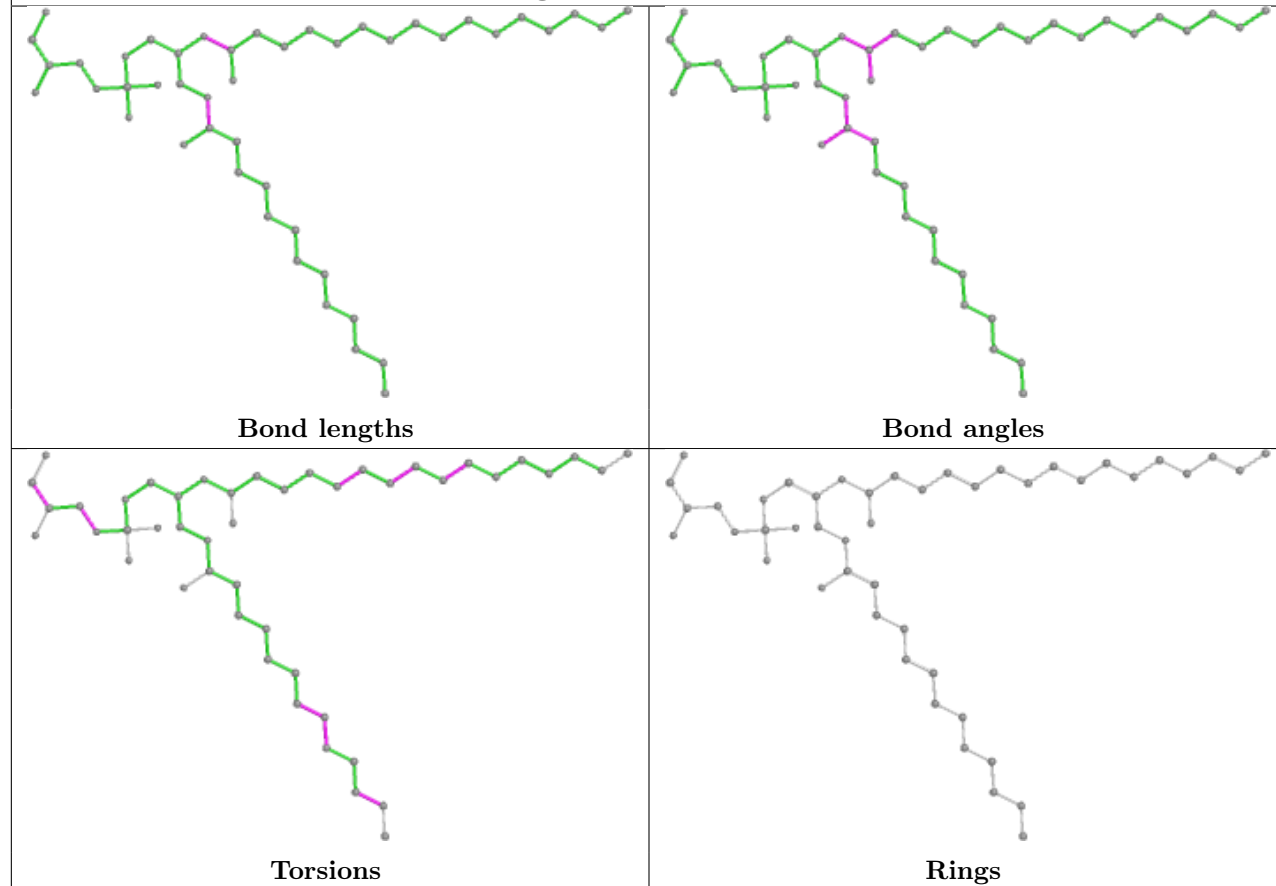
Ligand LHG L 101

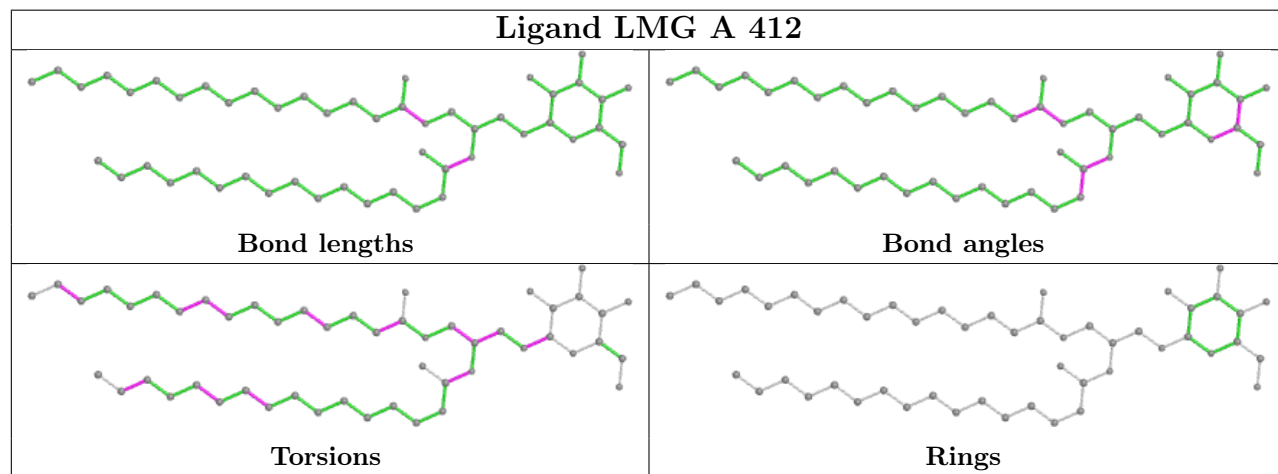
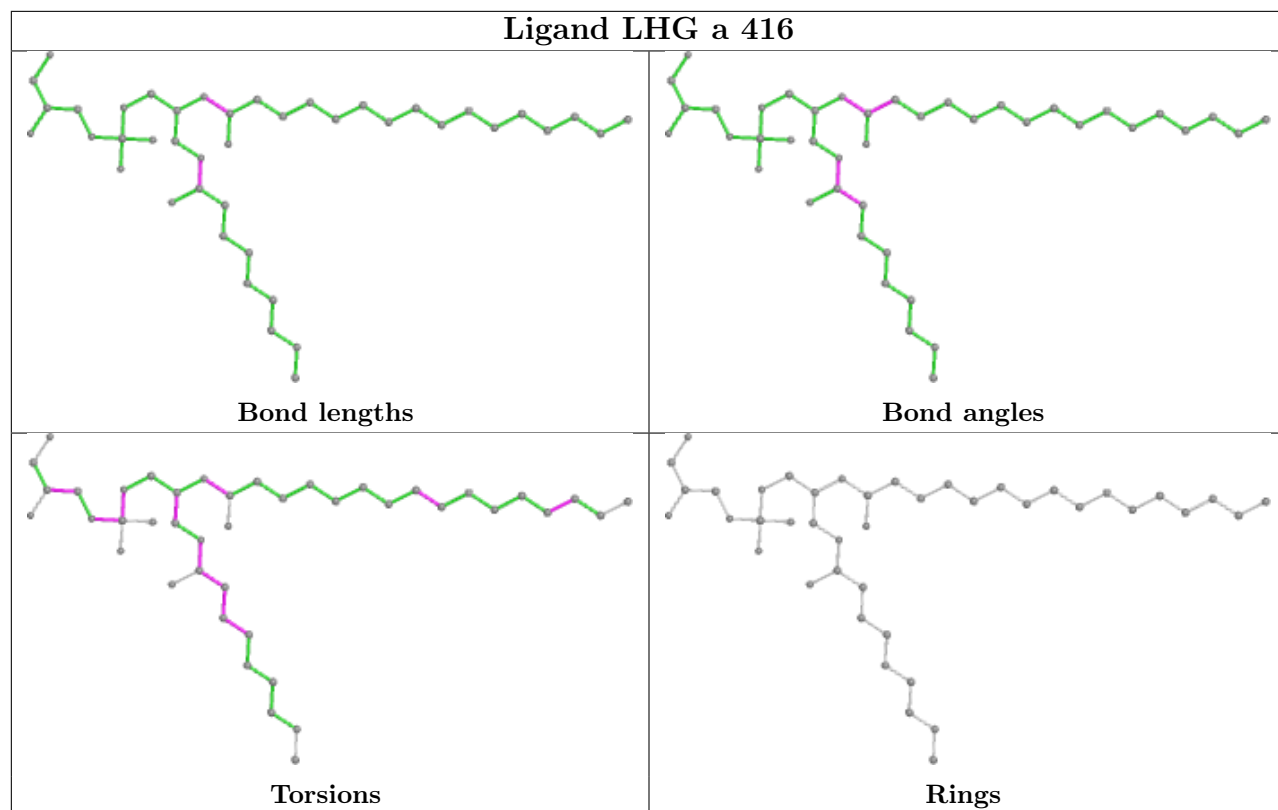


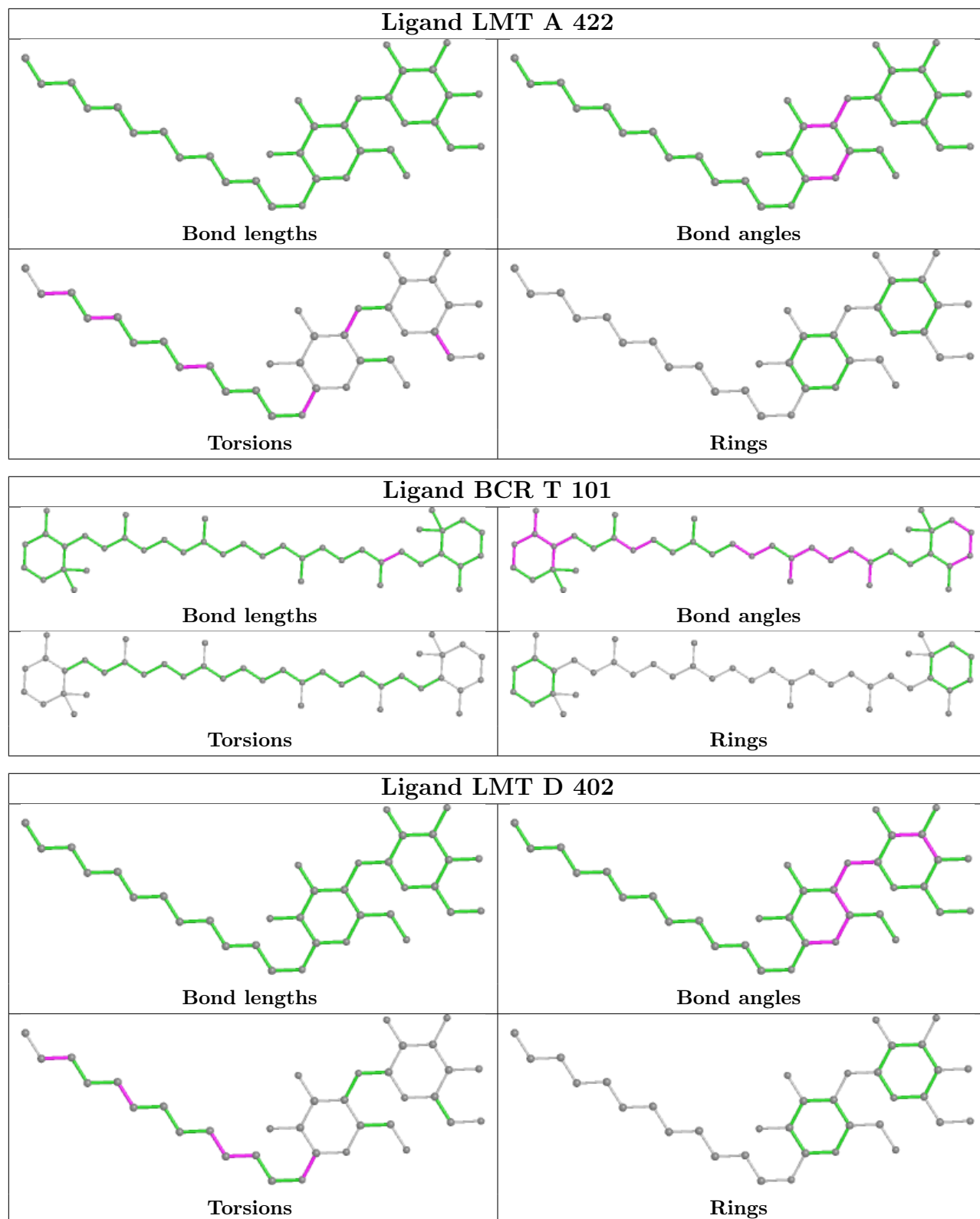
Ligand CLA C 514

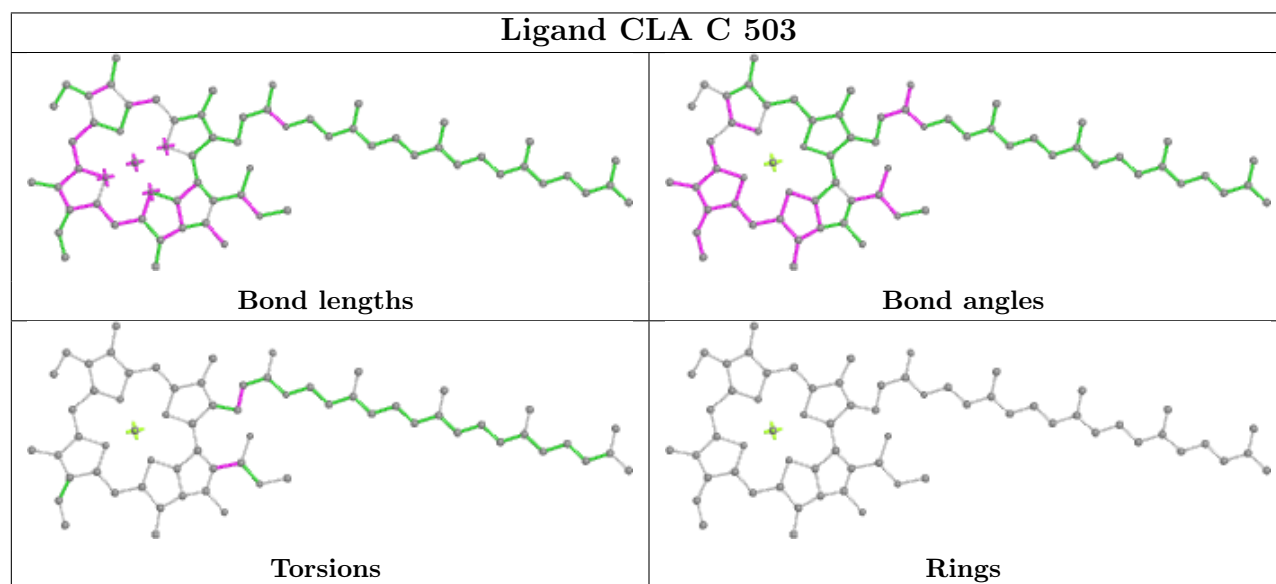
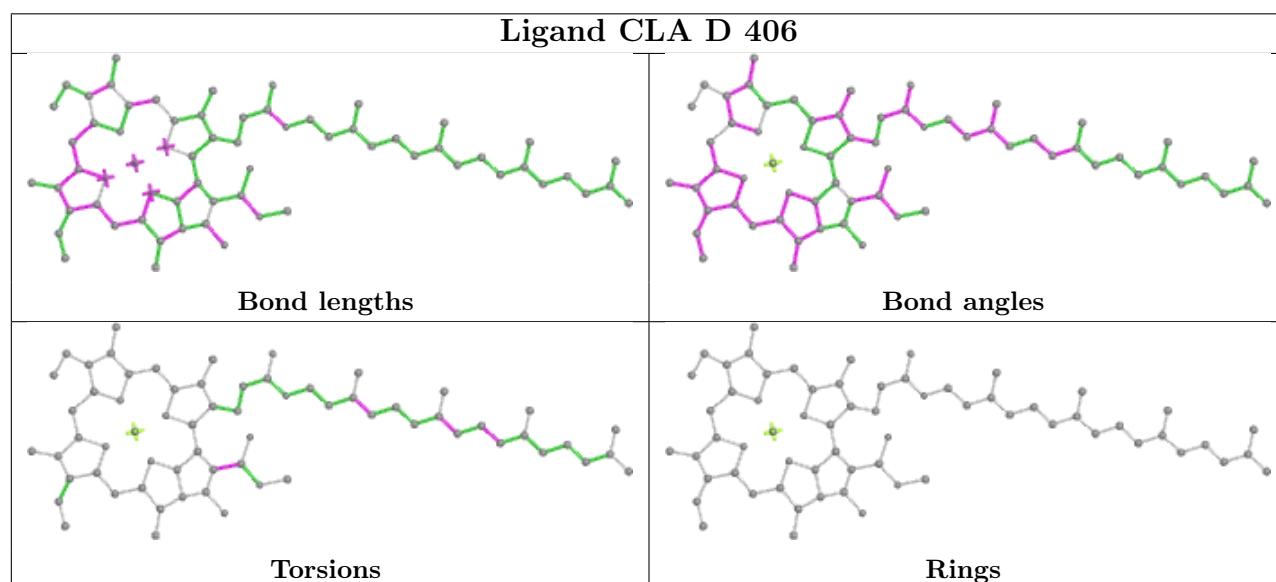
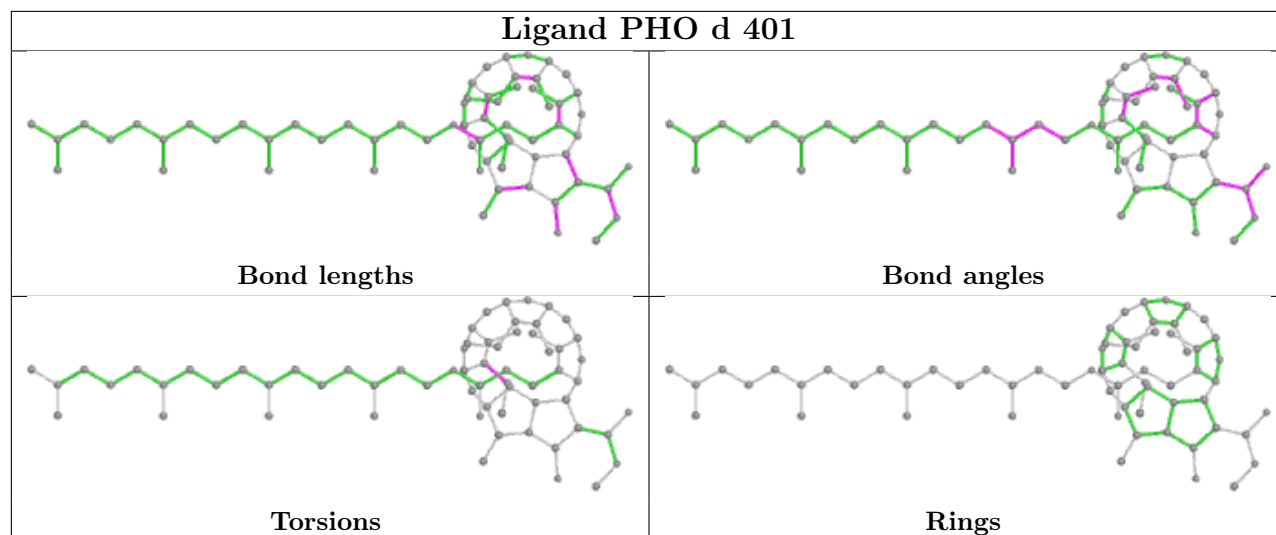


Ligand LHG d 411

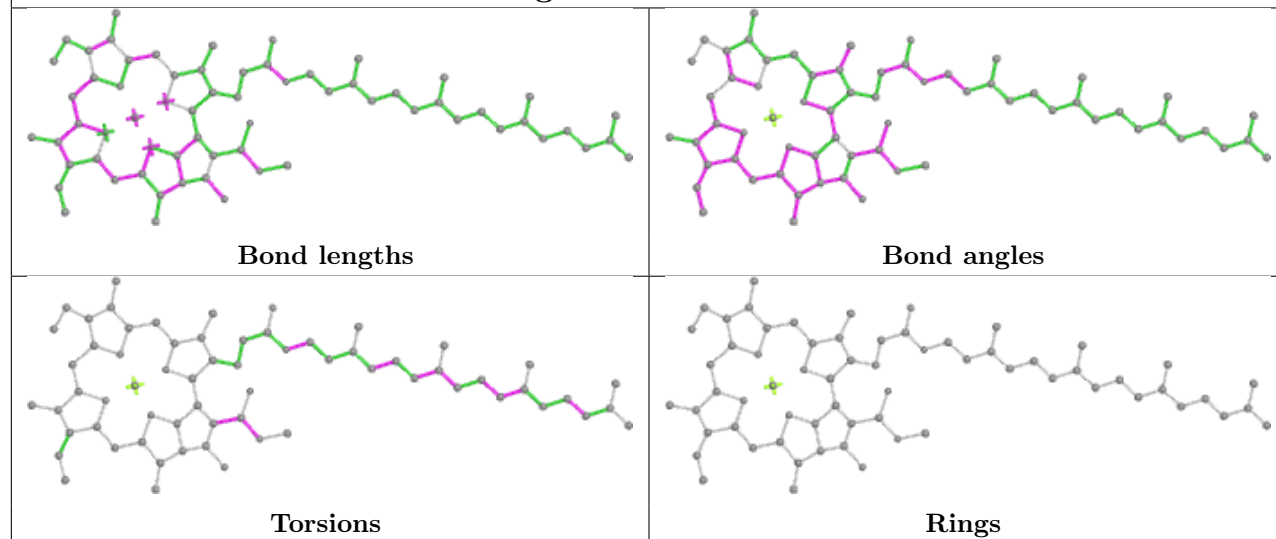




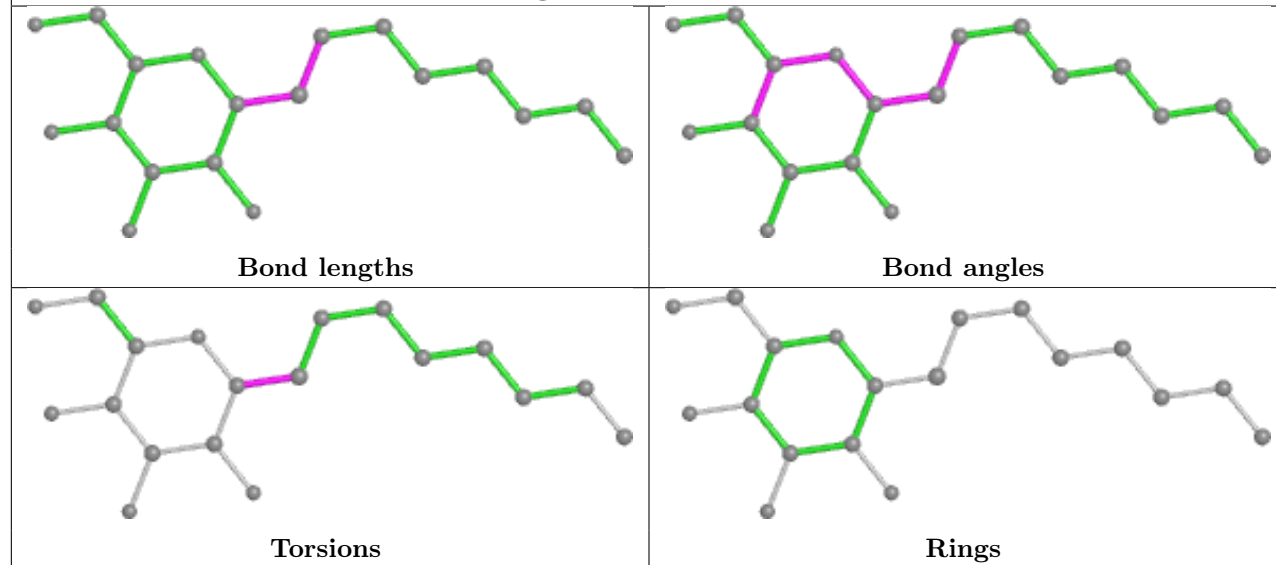


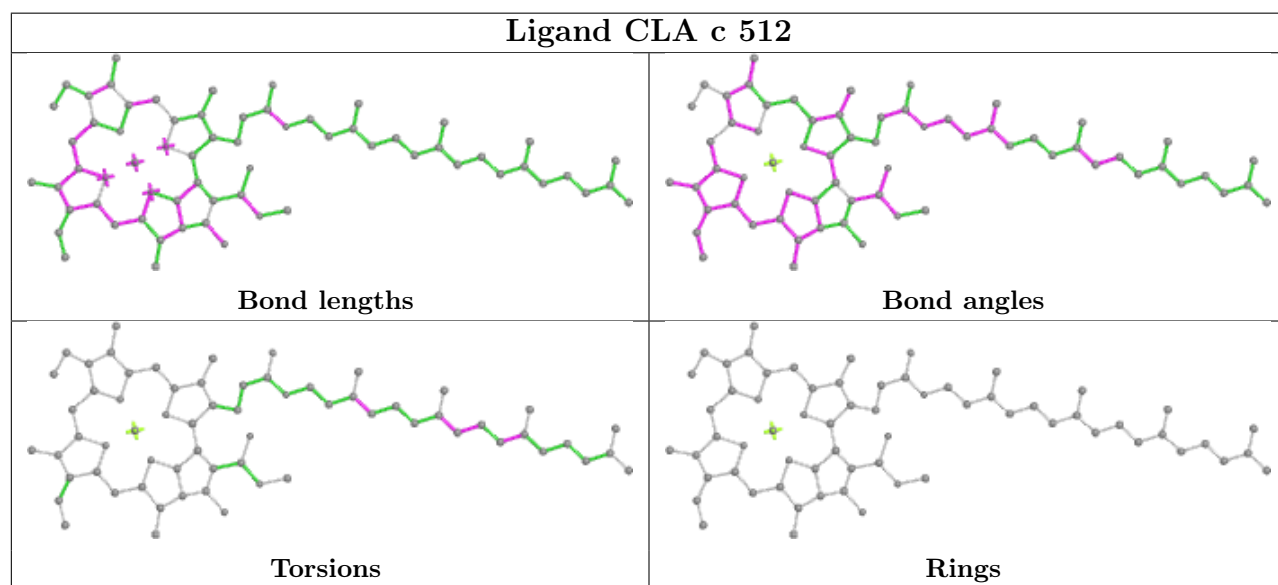
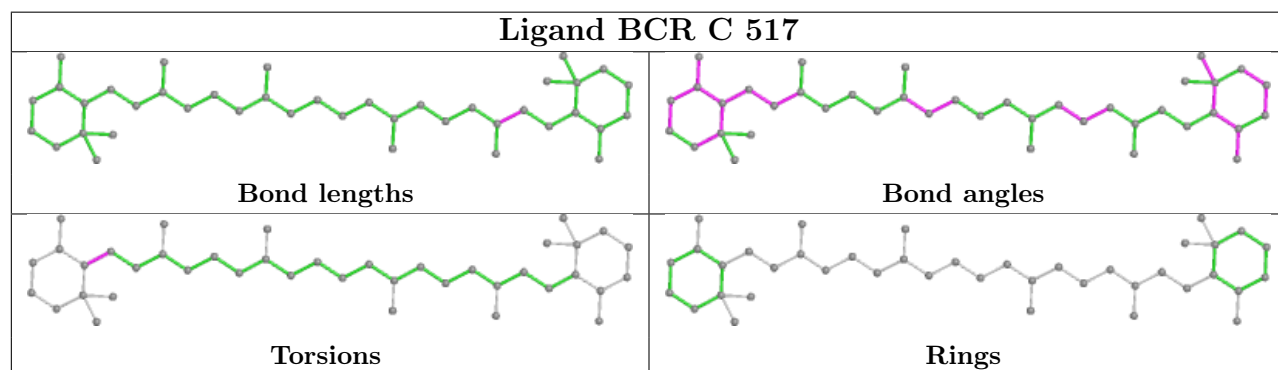
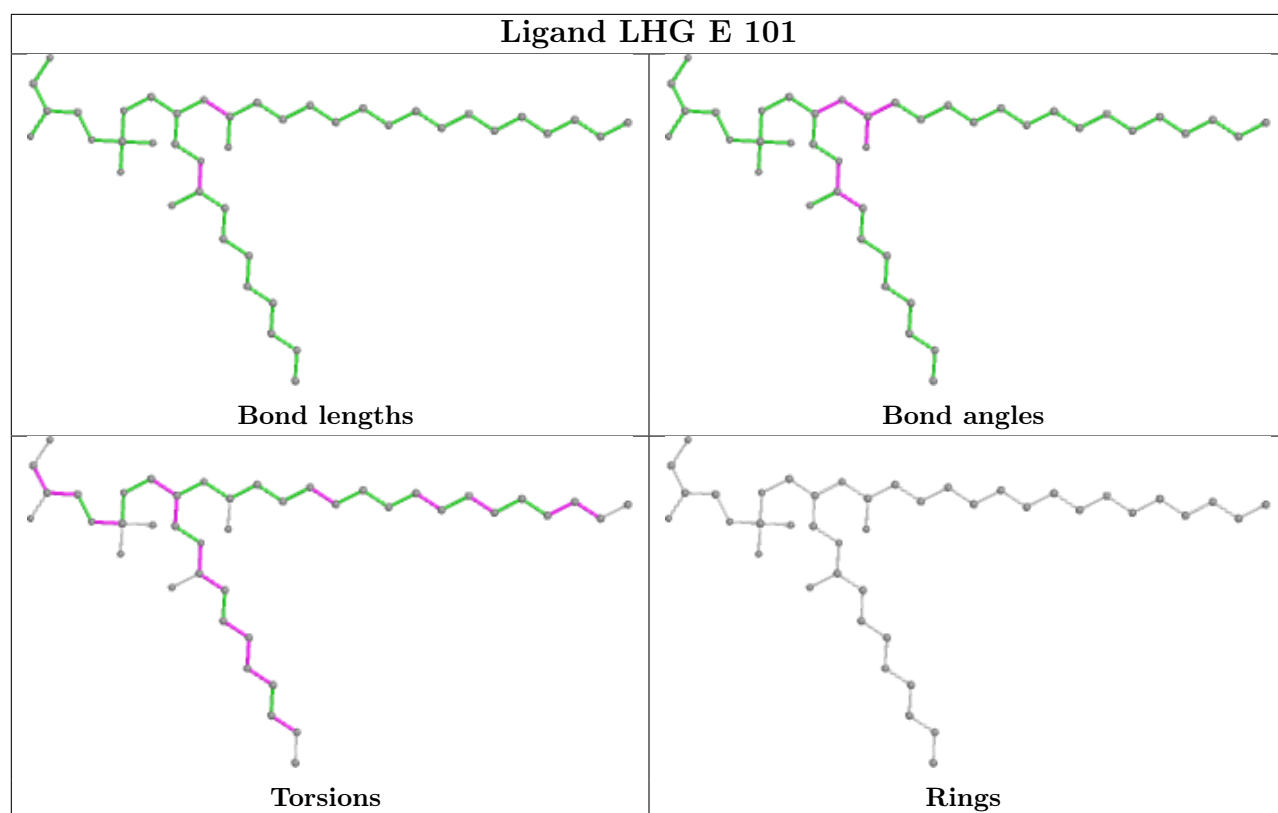


Ligand CLA b 620

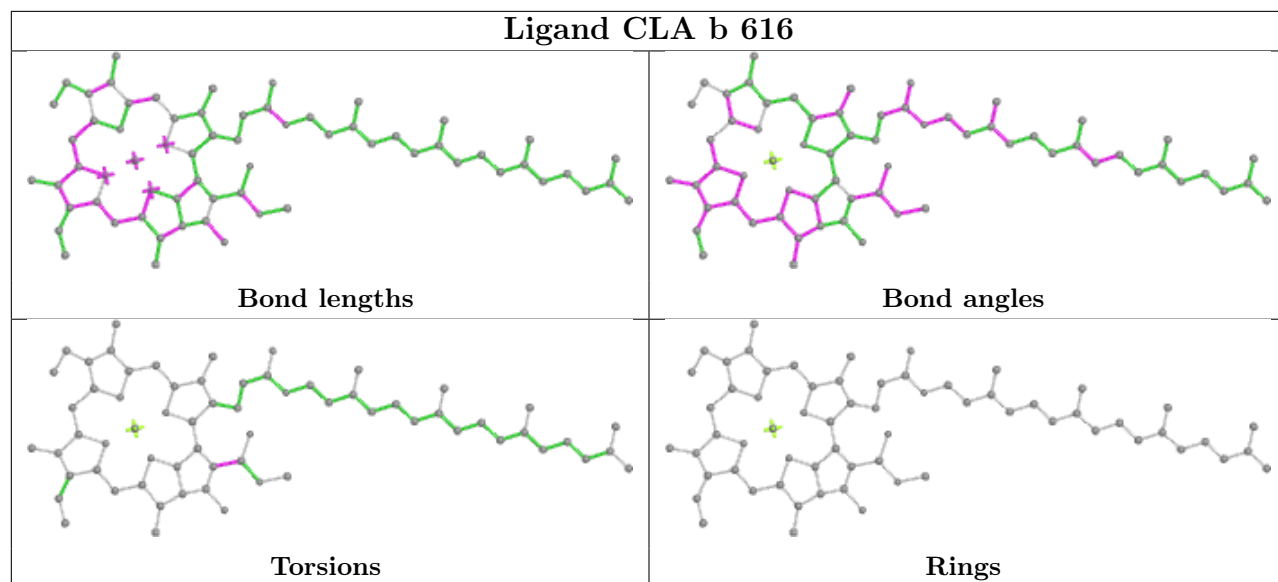


Ligand HTG c 523

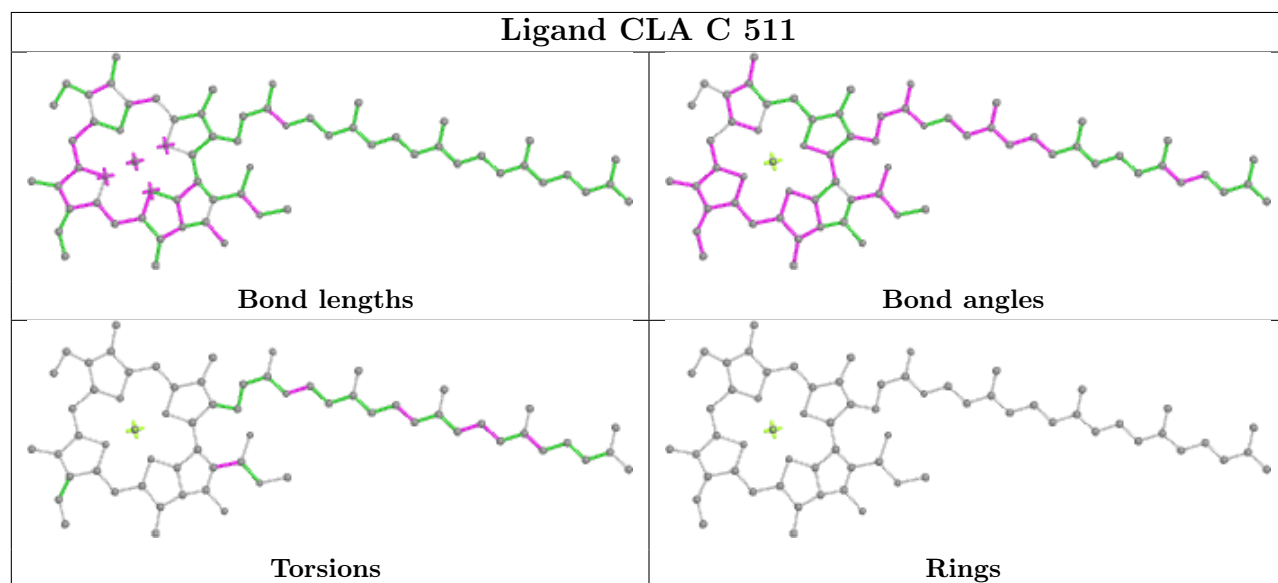


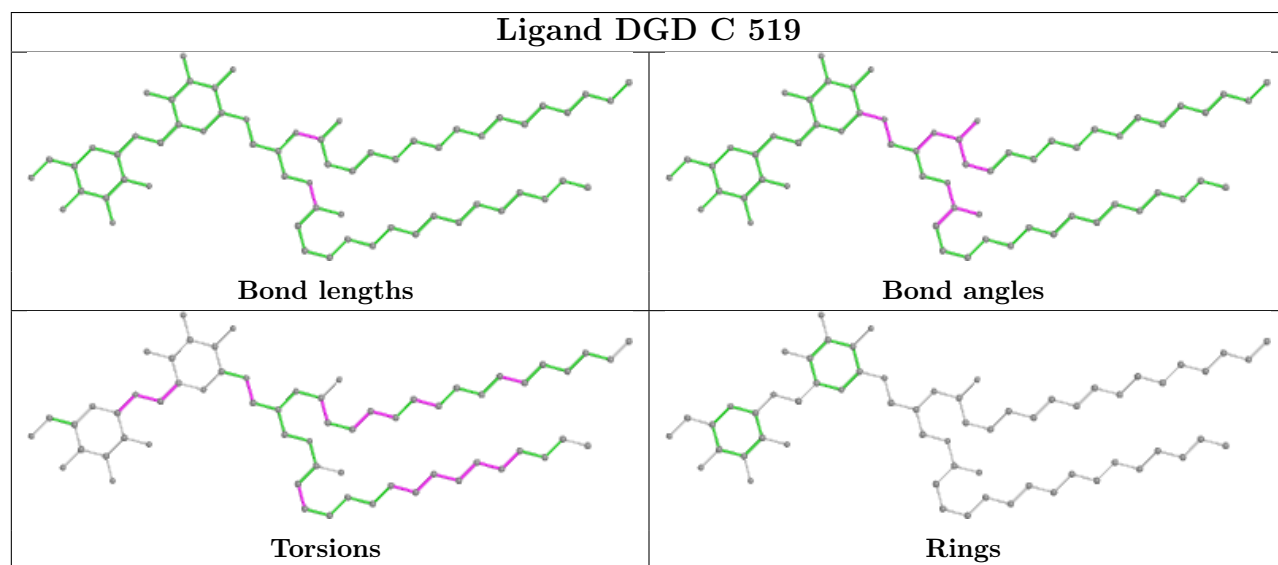
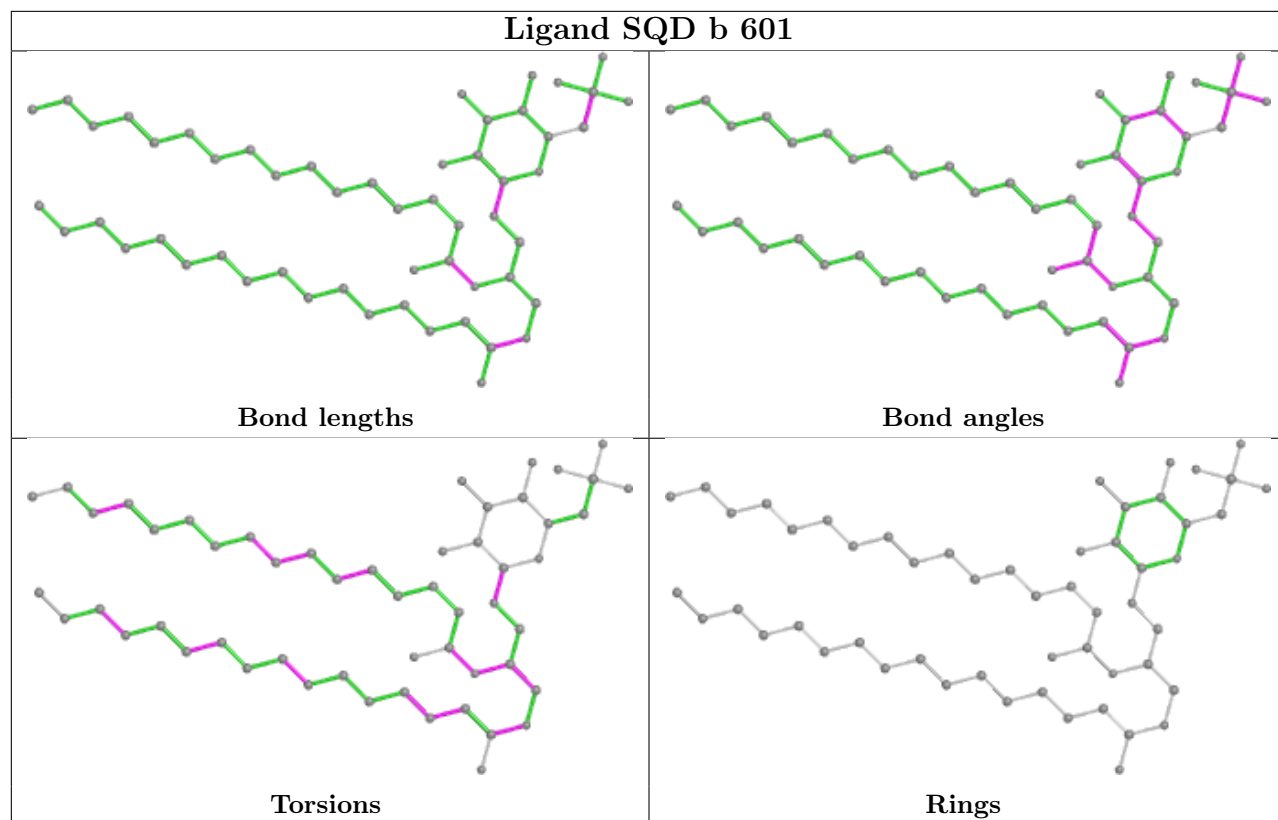


Ligand CLA b 616

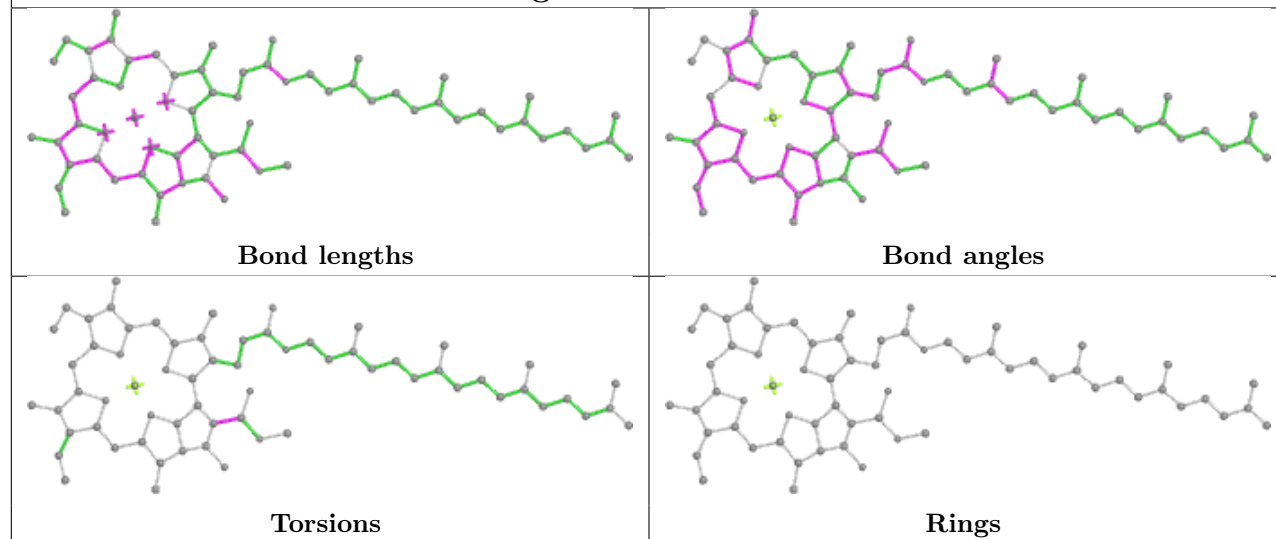


Ligand CLA C 511

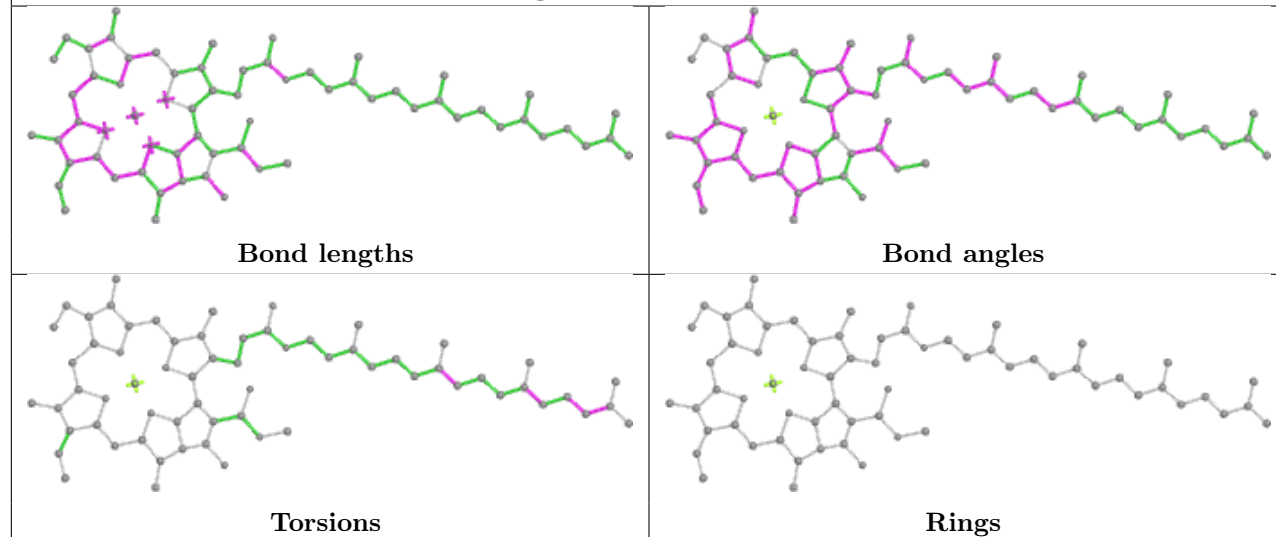




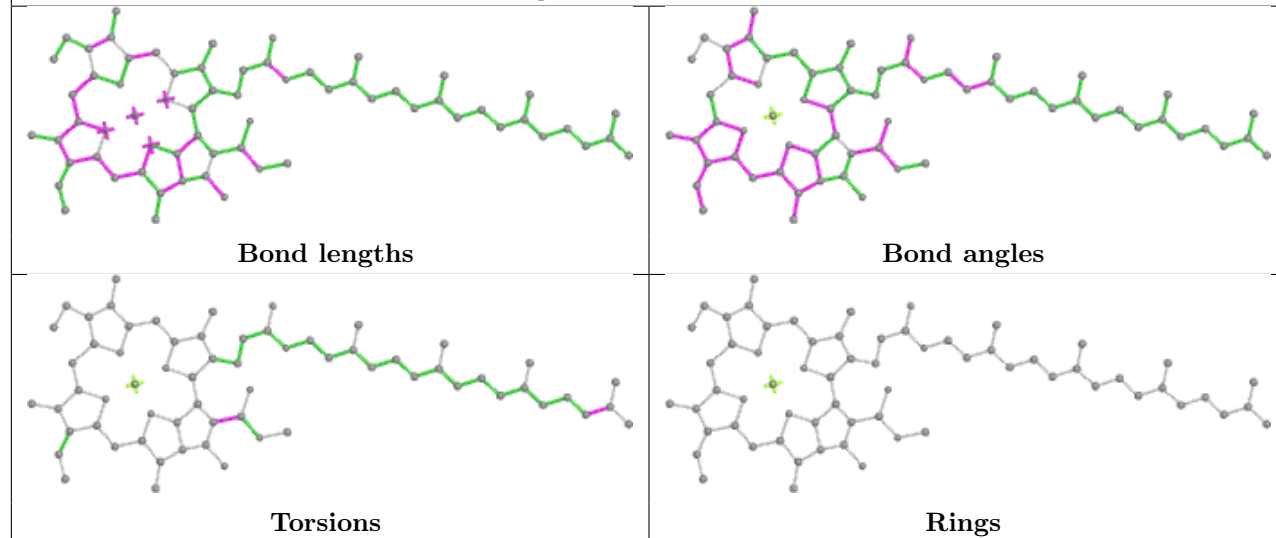
Ligand CLA C 510

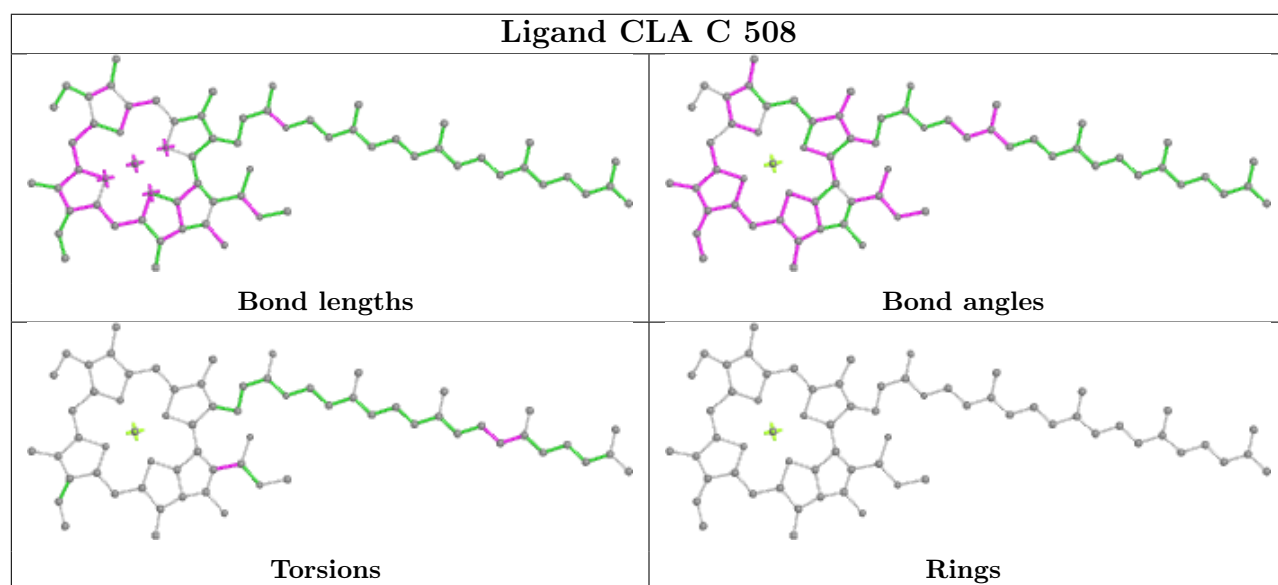
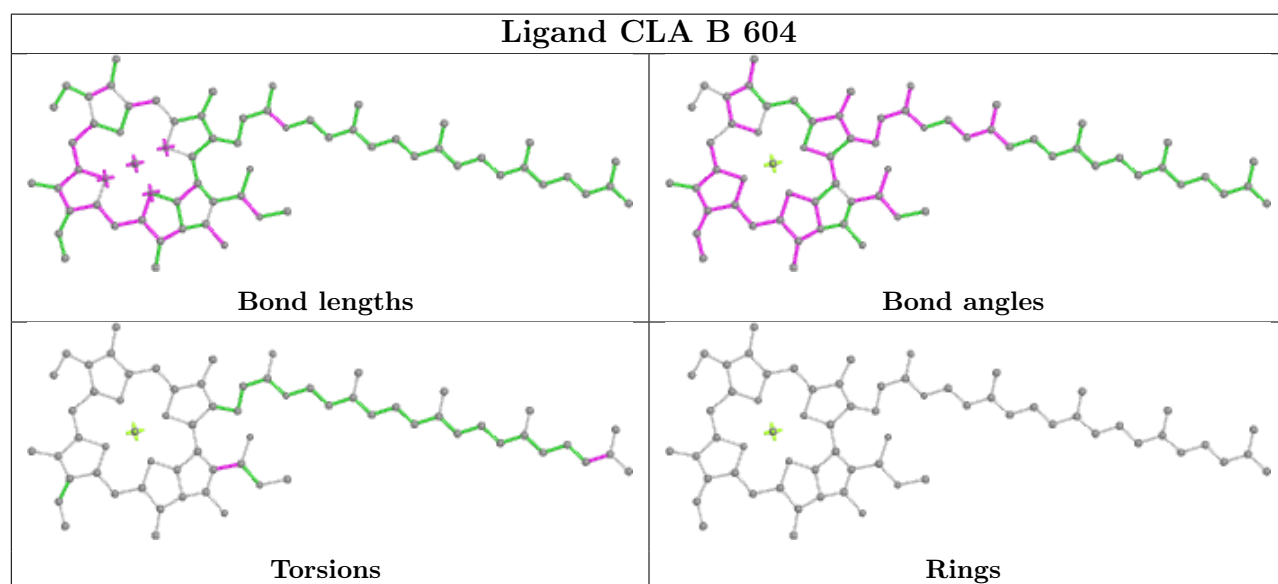
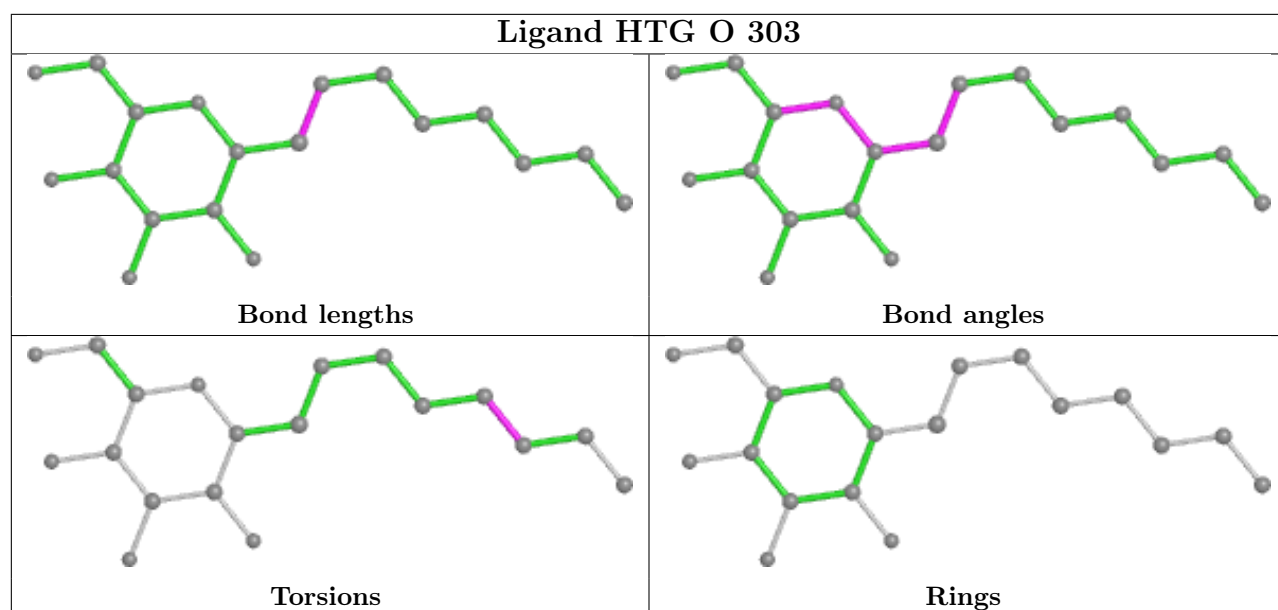


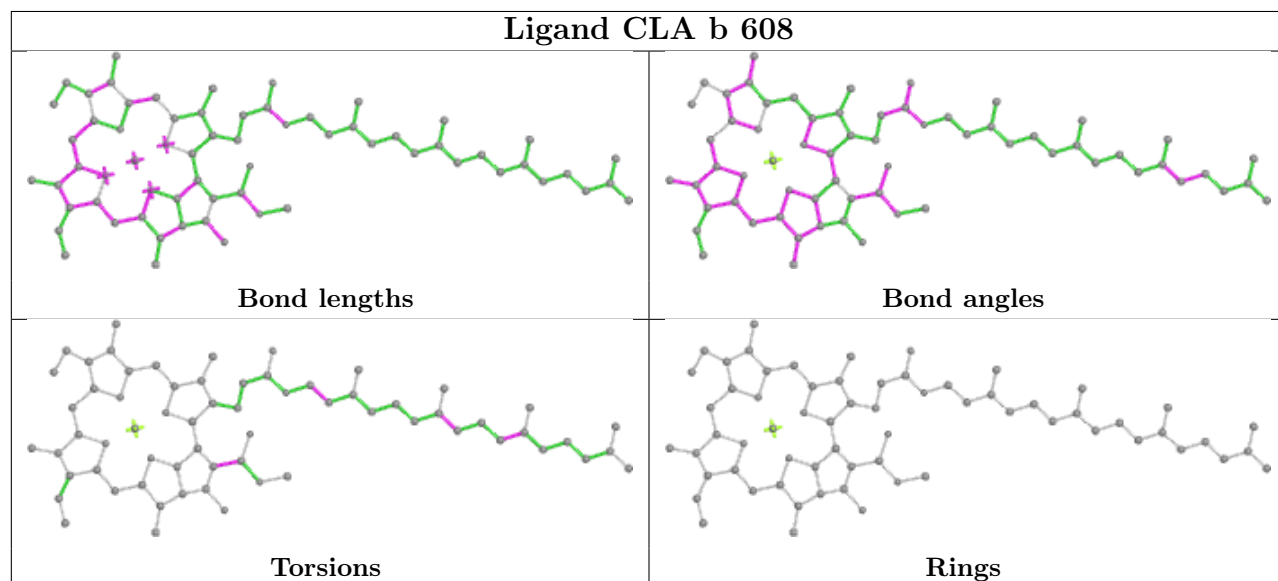
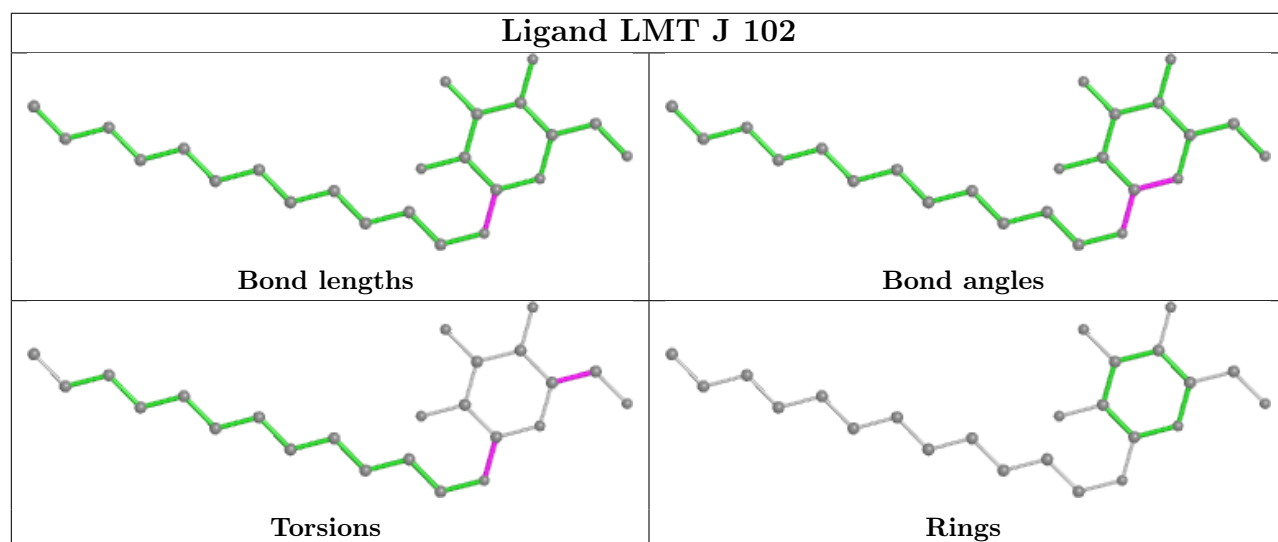
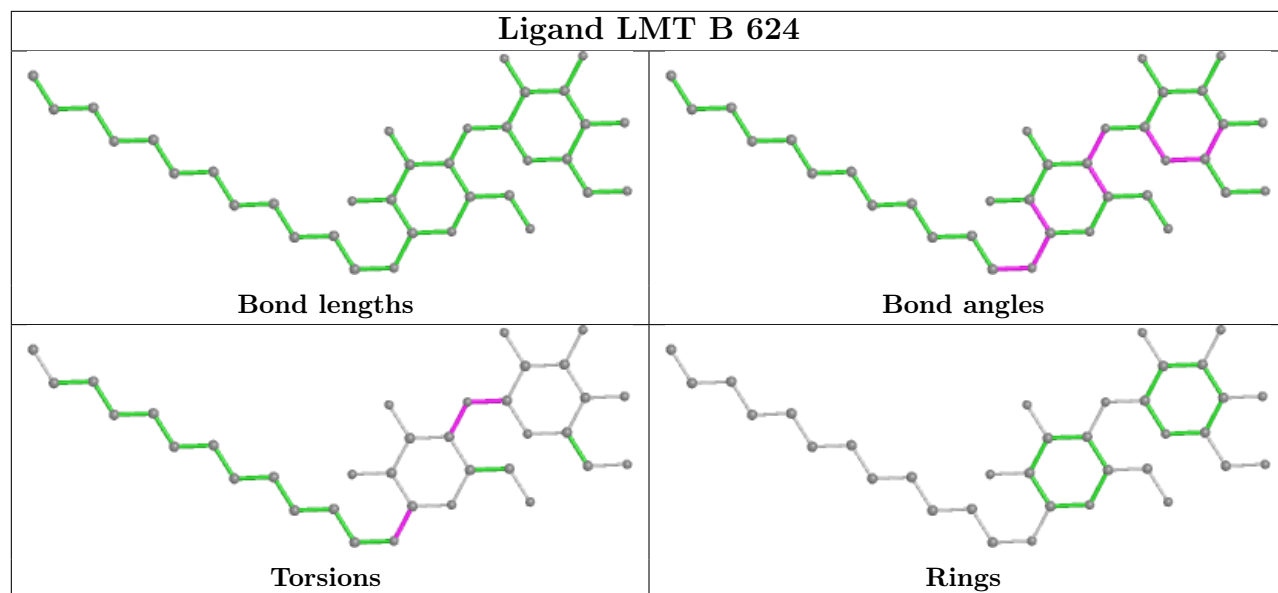
Ligand CLA A 409



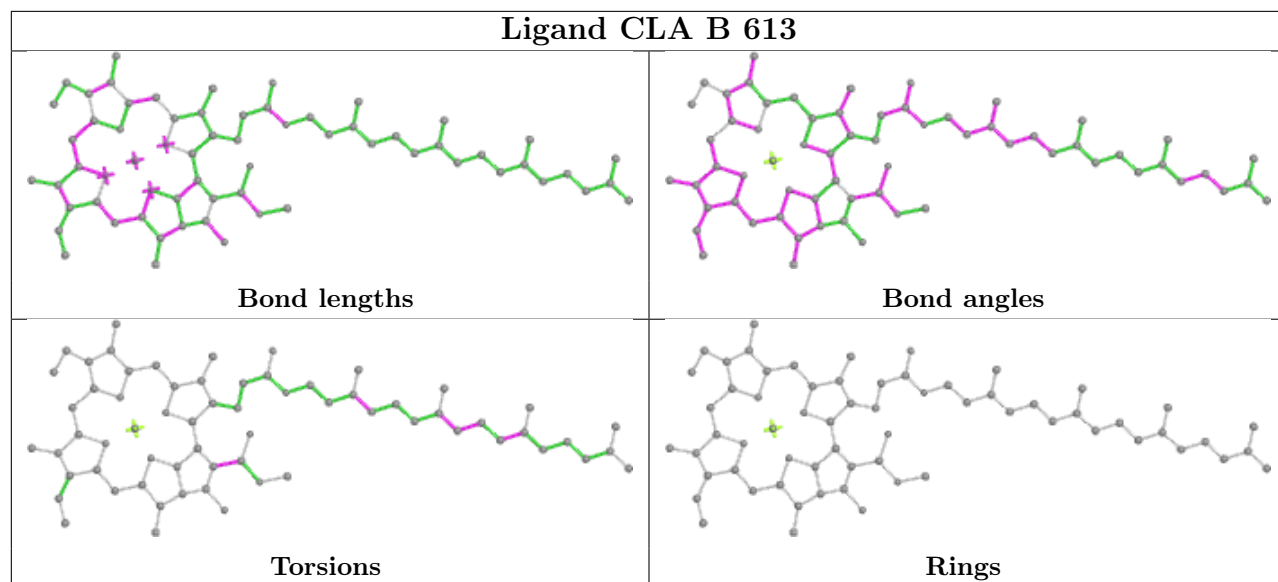
Ligand CLA C 504



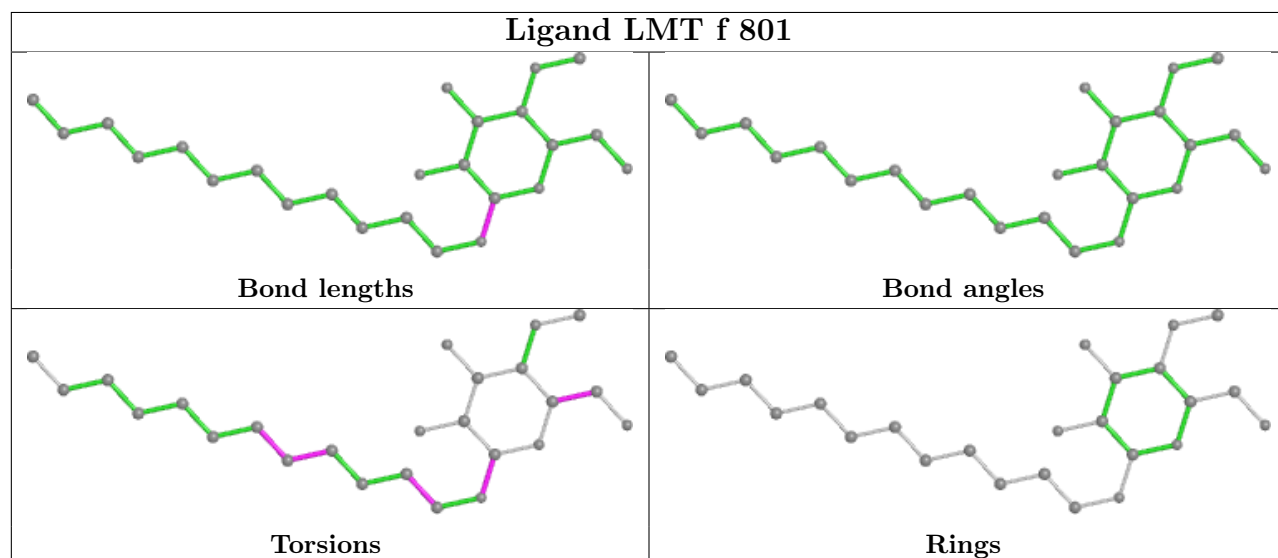




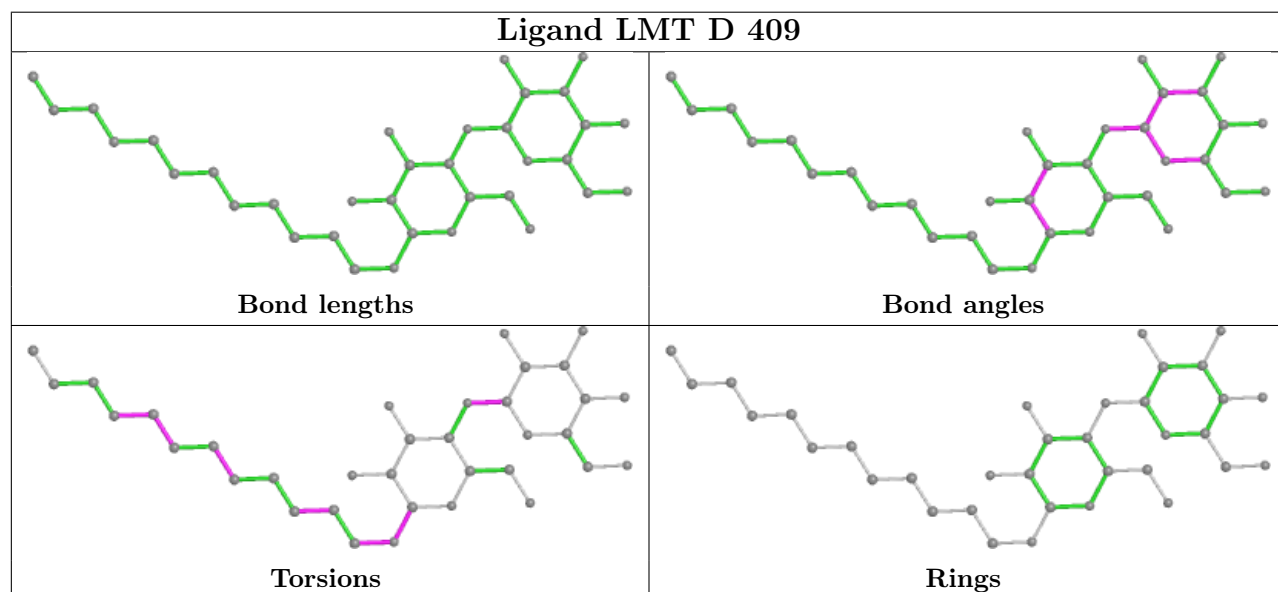
Ligand CLA B 613



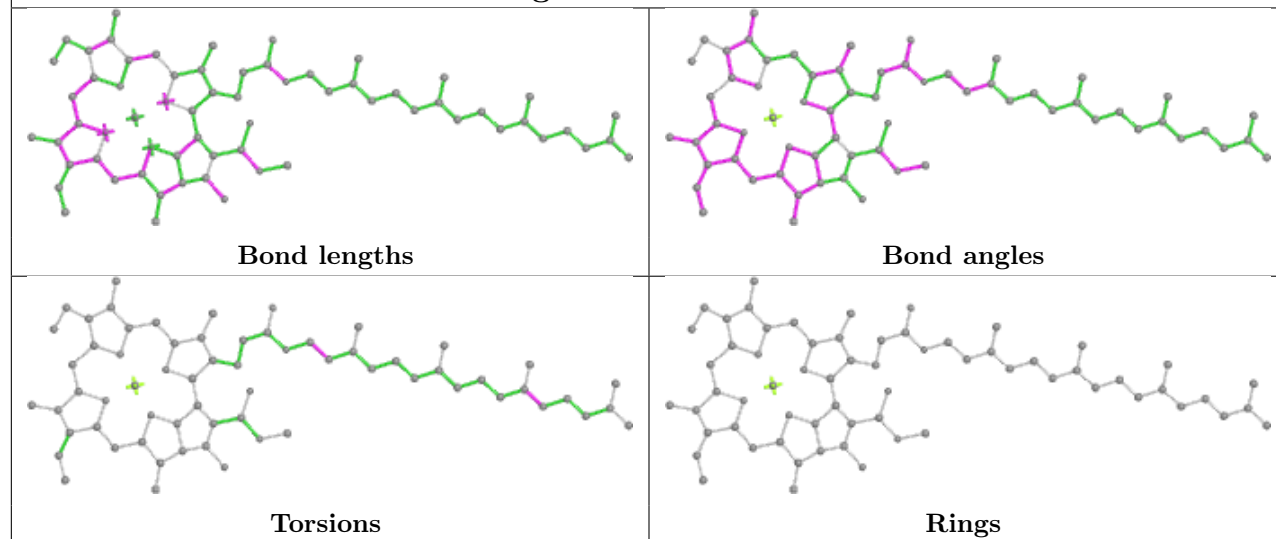
Ligand LMT f 801



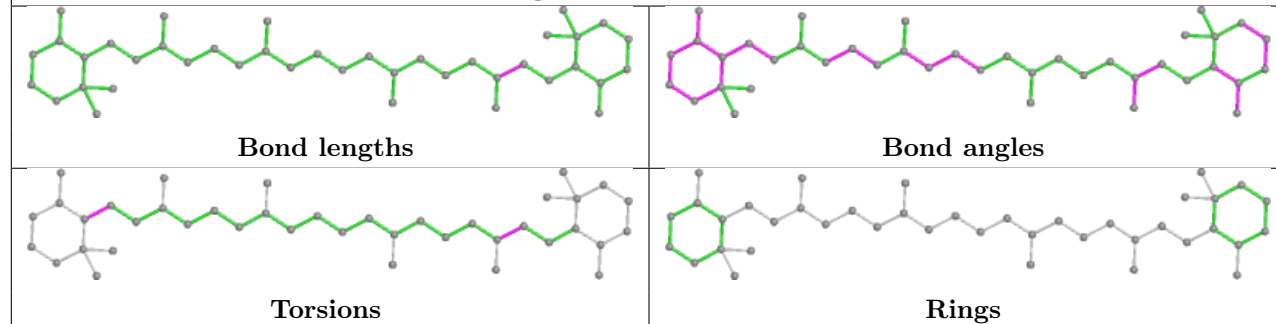
Ligand LMT D 409



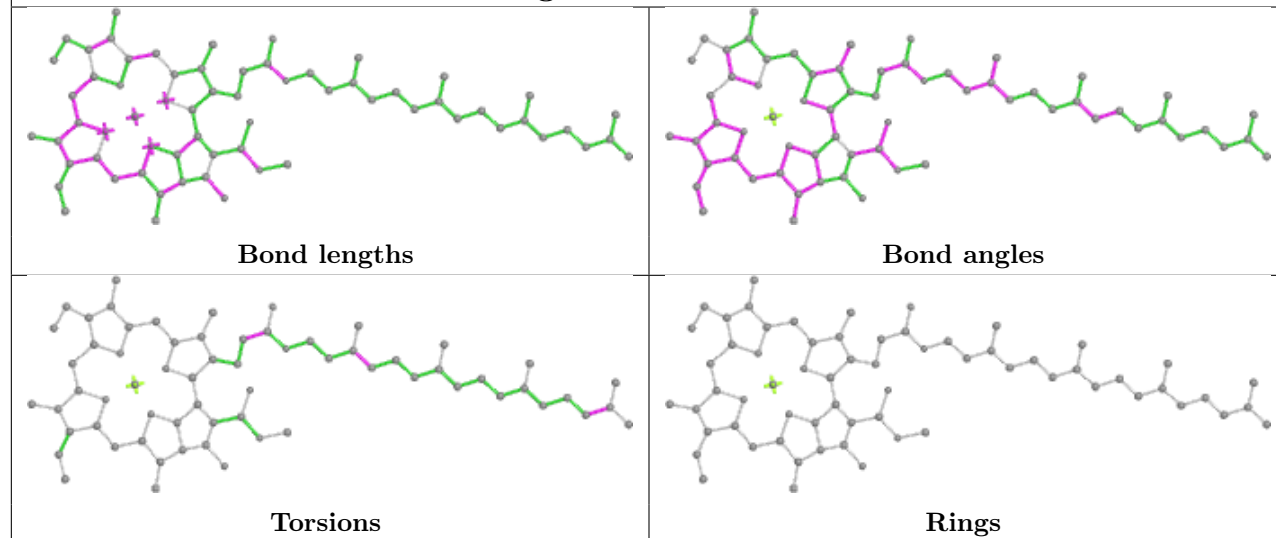
Ligand CLA B 615

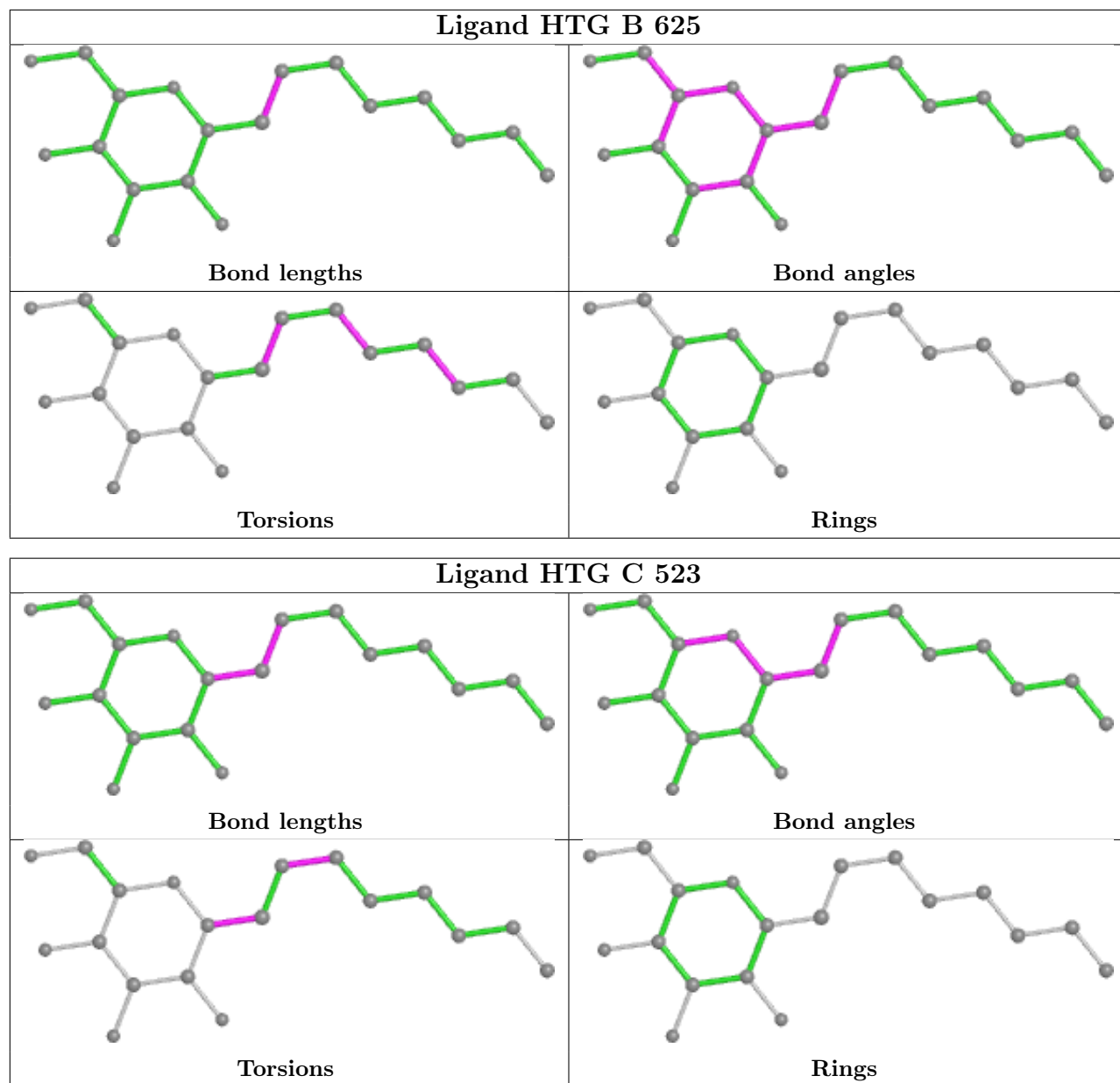


Ligand BCR K 101

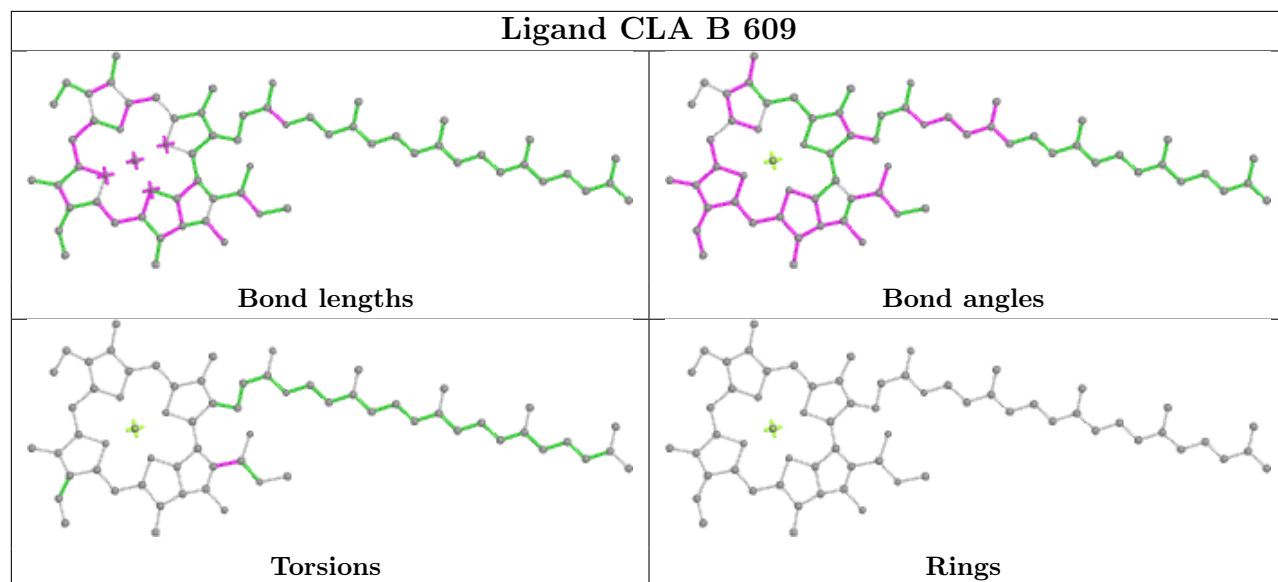


Ligand CLA c 507

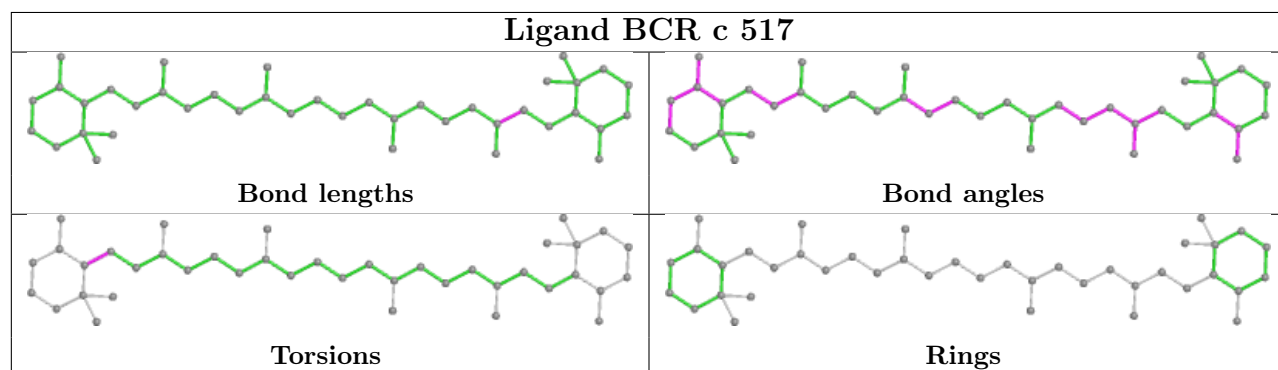




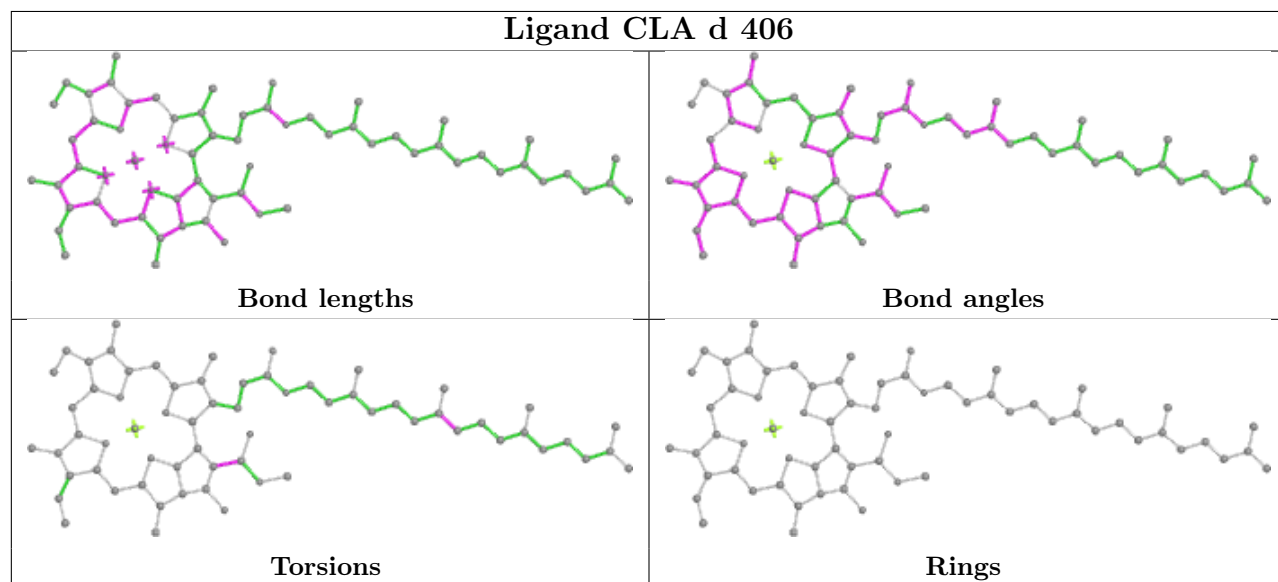
Ligand CLA B 609

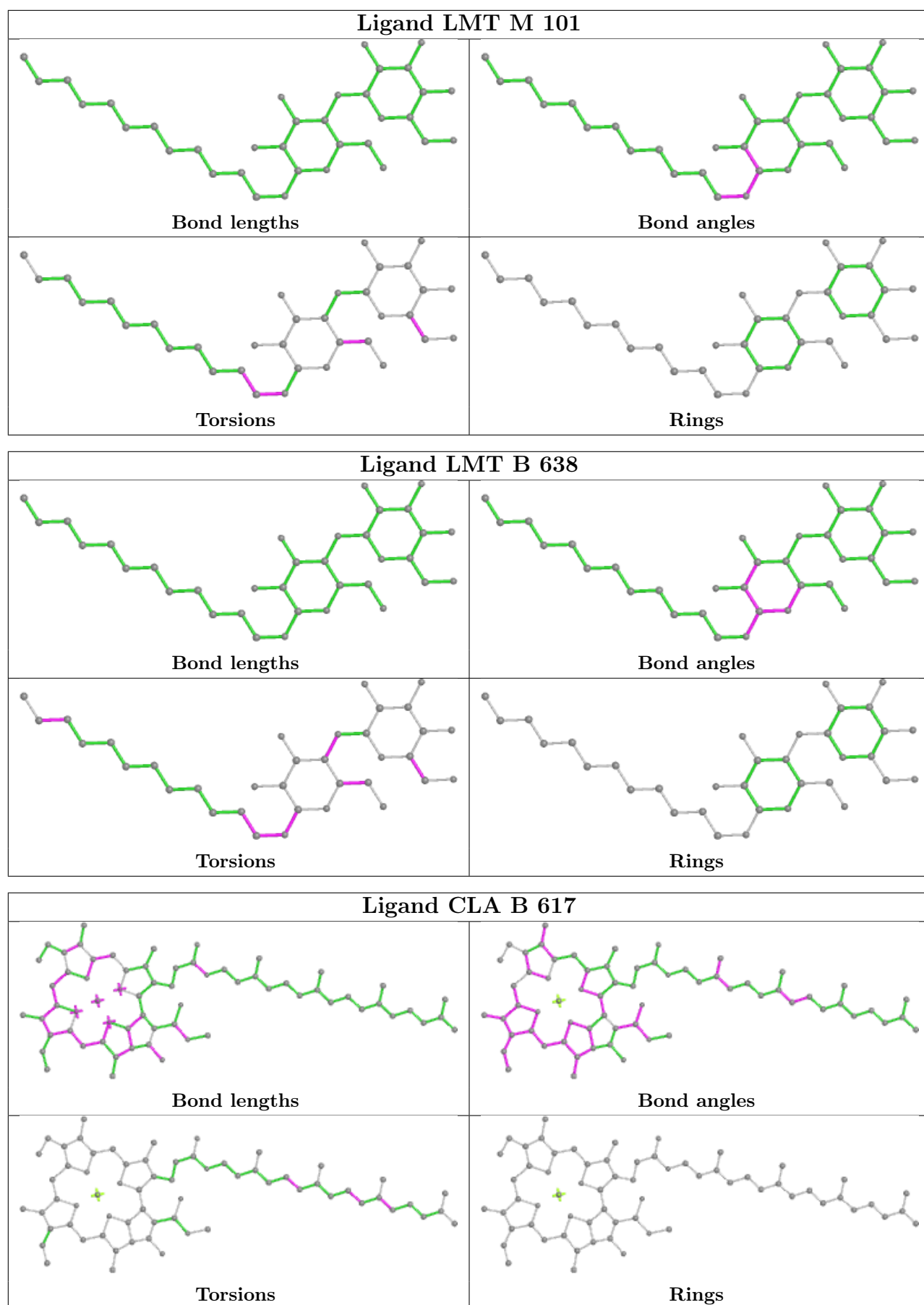


Ligand BCR c 517

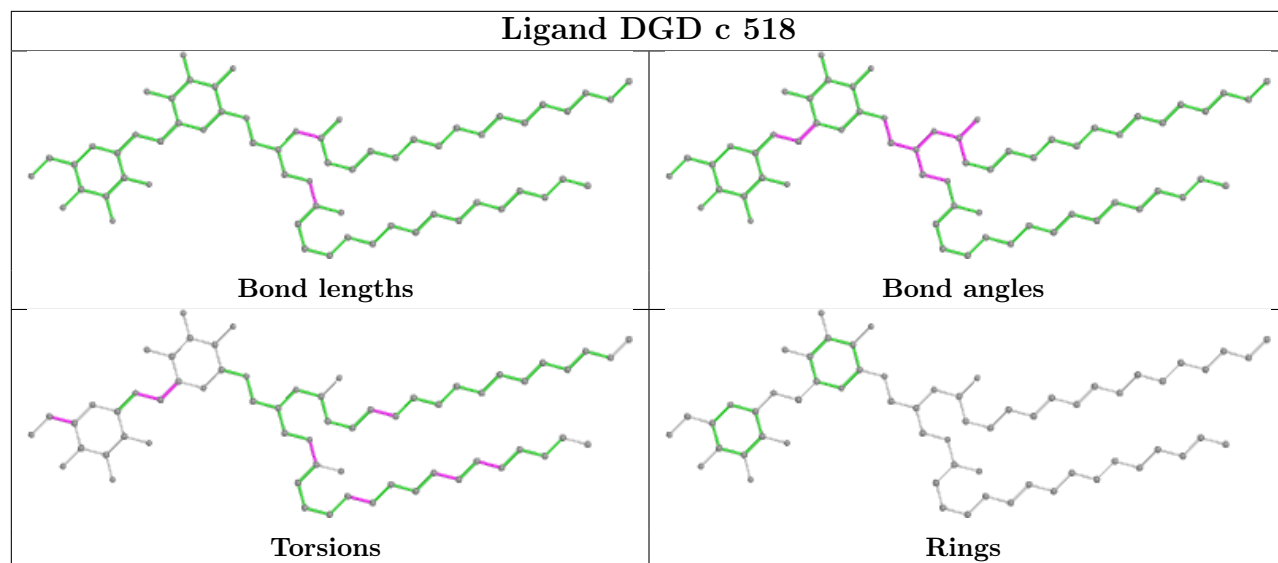


Ligand CLA d 406

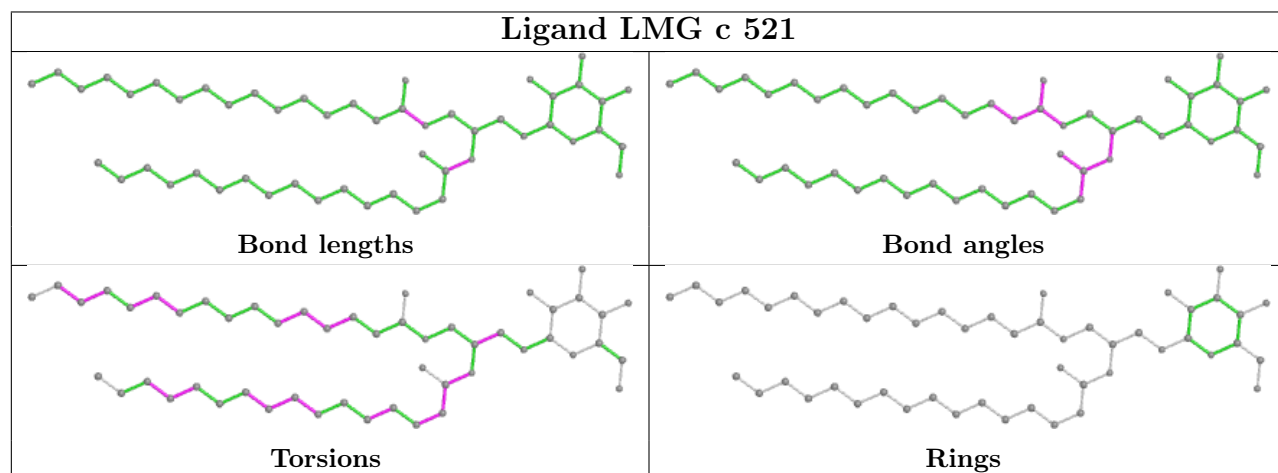




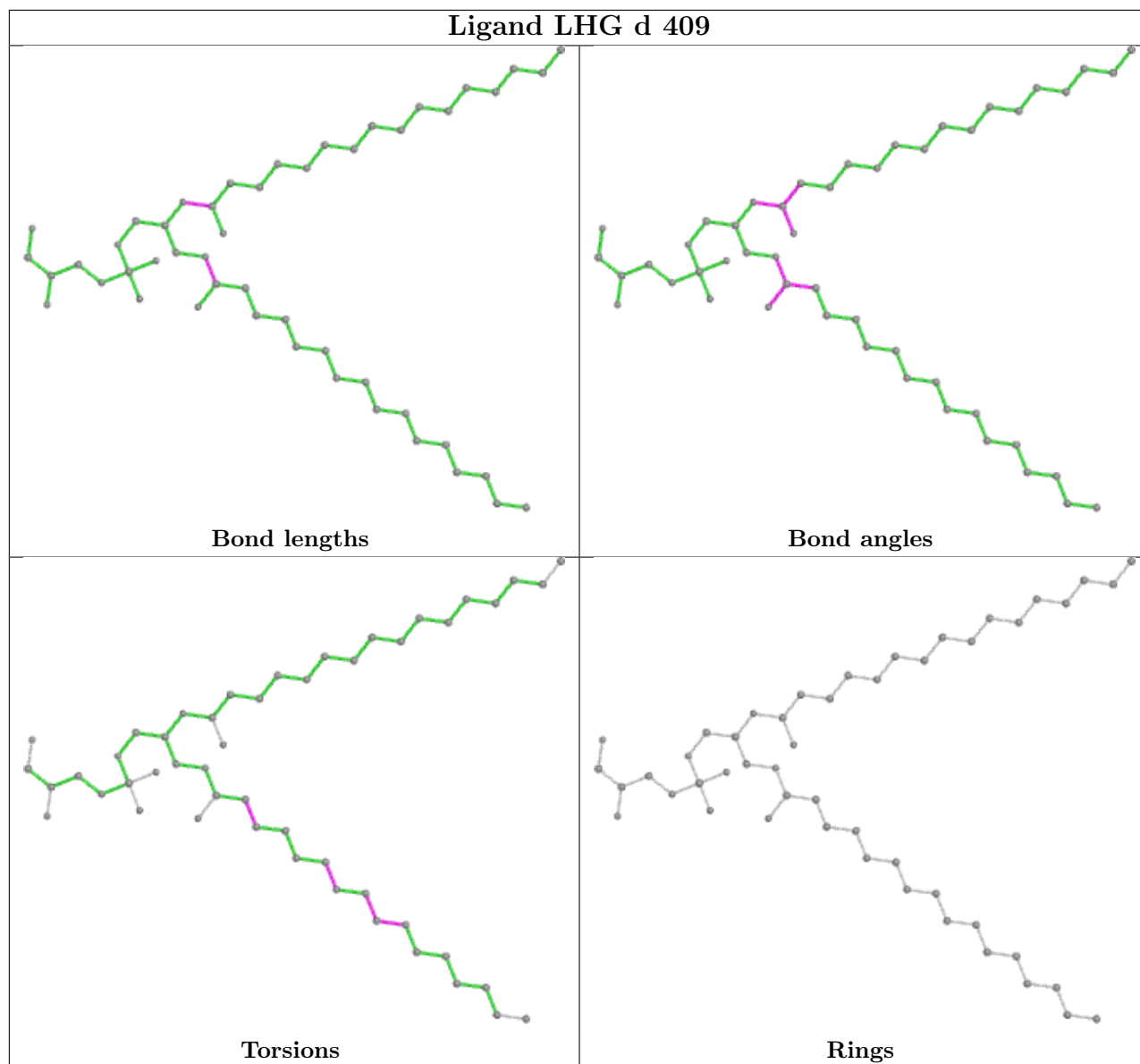
Ligand DGD c 518



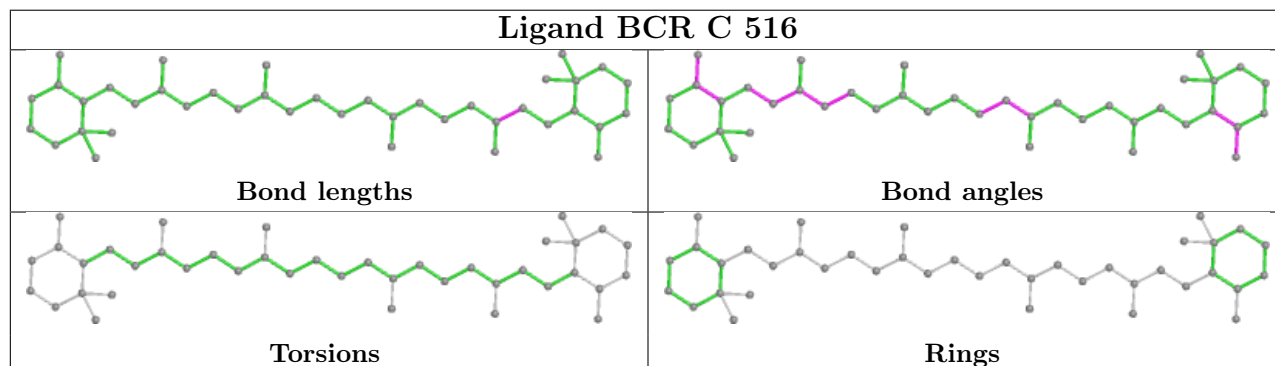
Ligand LMG c 521



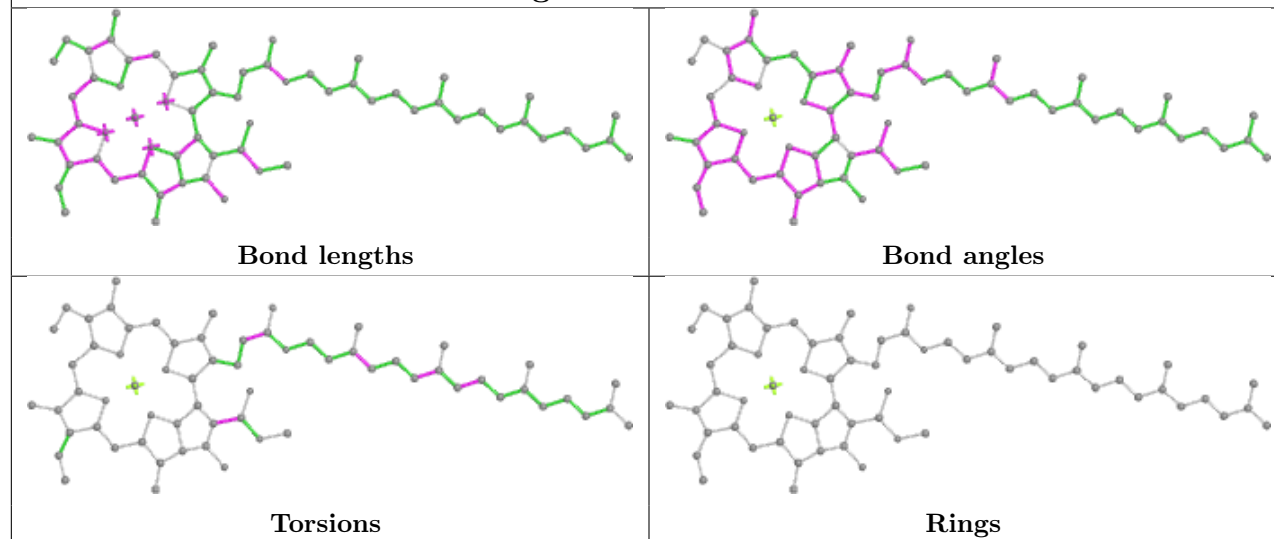
Ligand LHG d 409



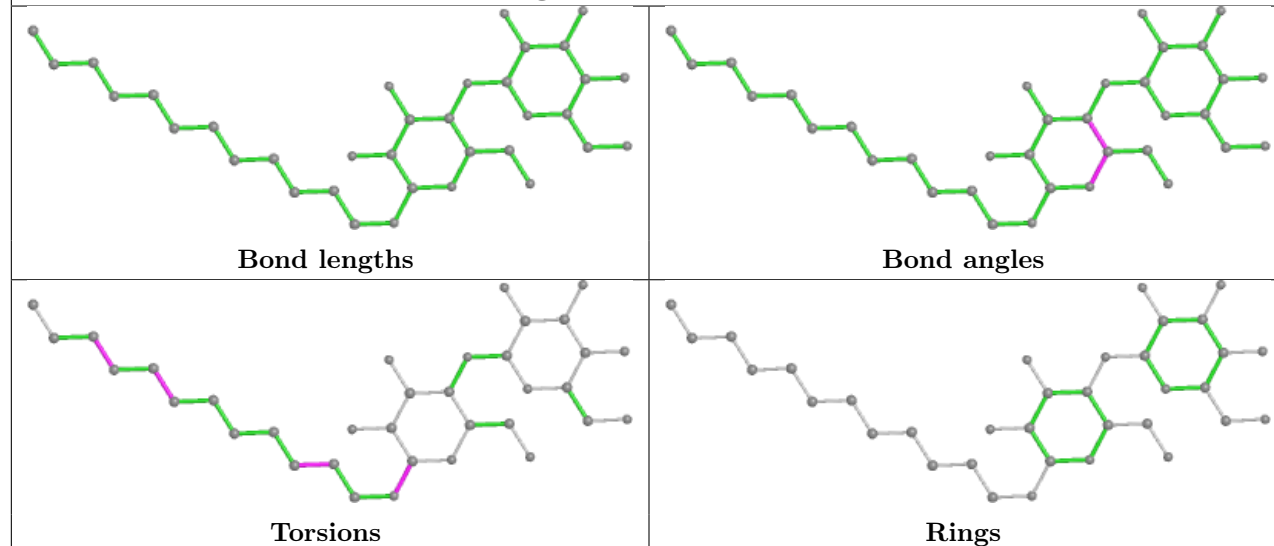
Ligand BCR C 516



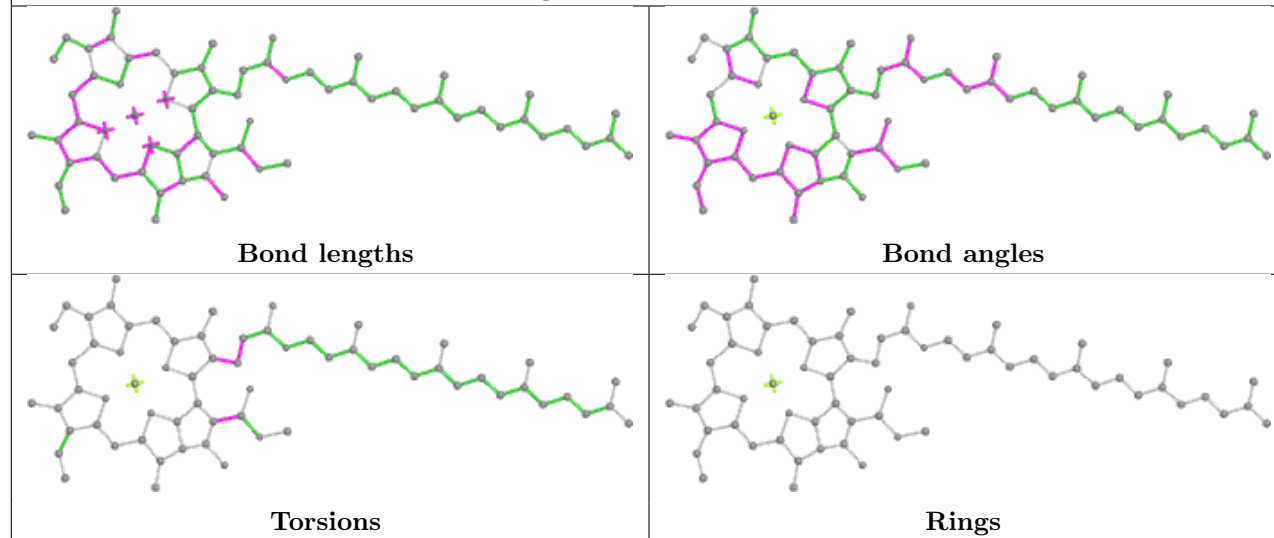
Ligand CLA C 512

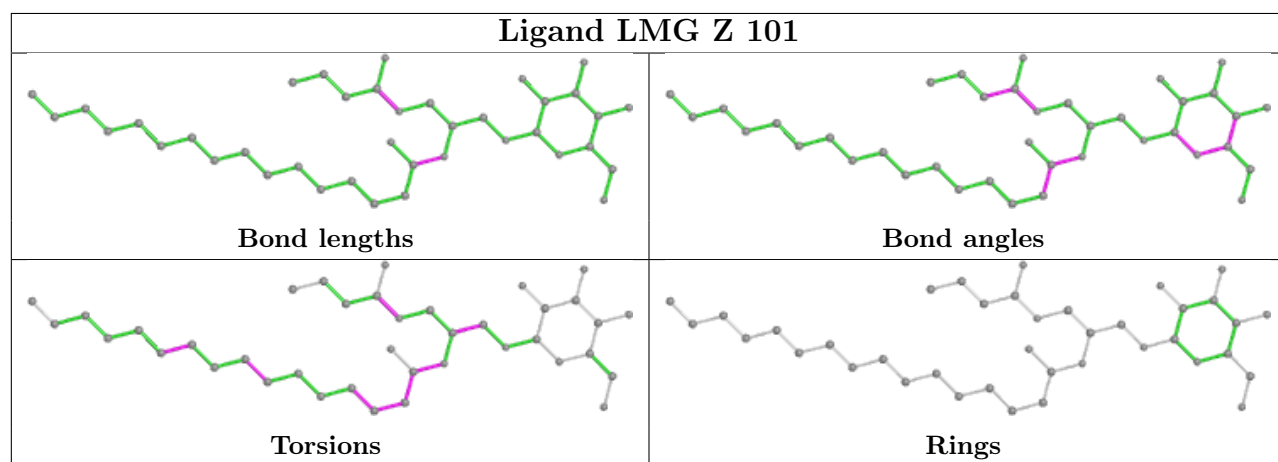
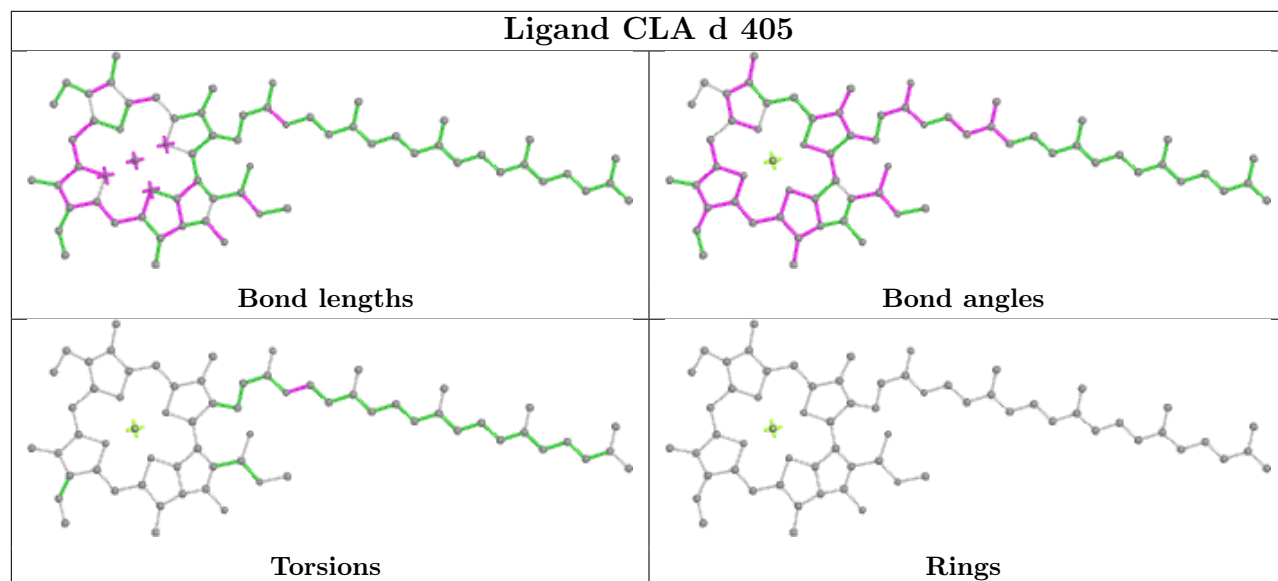
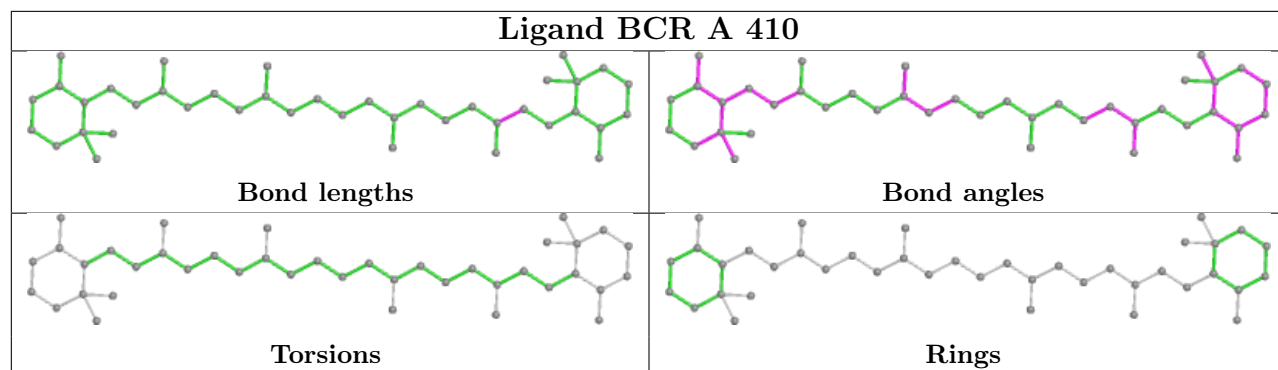


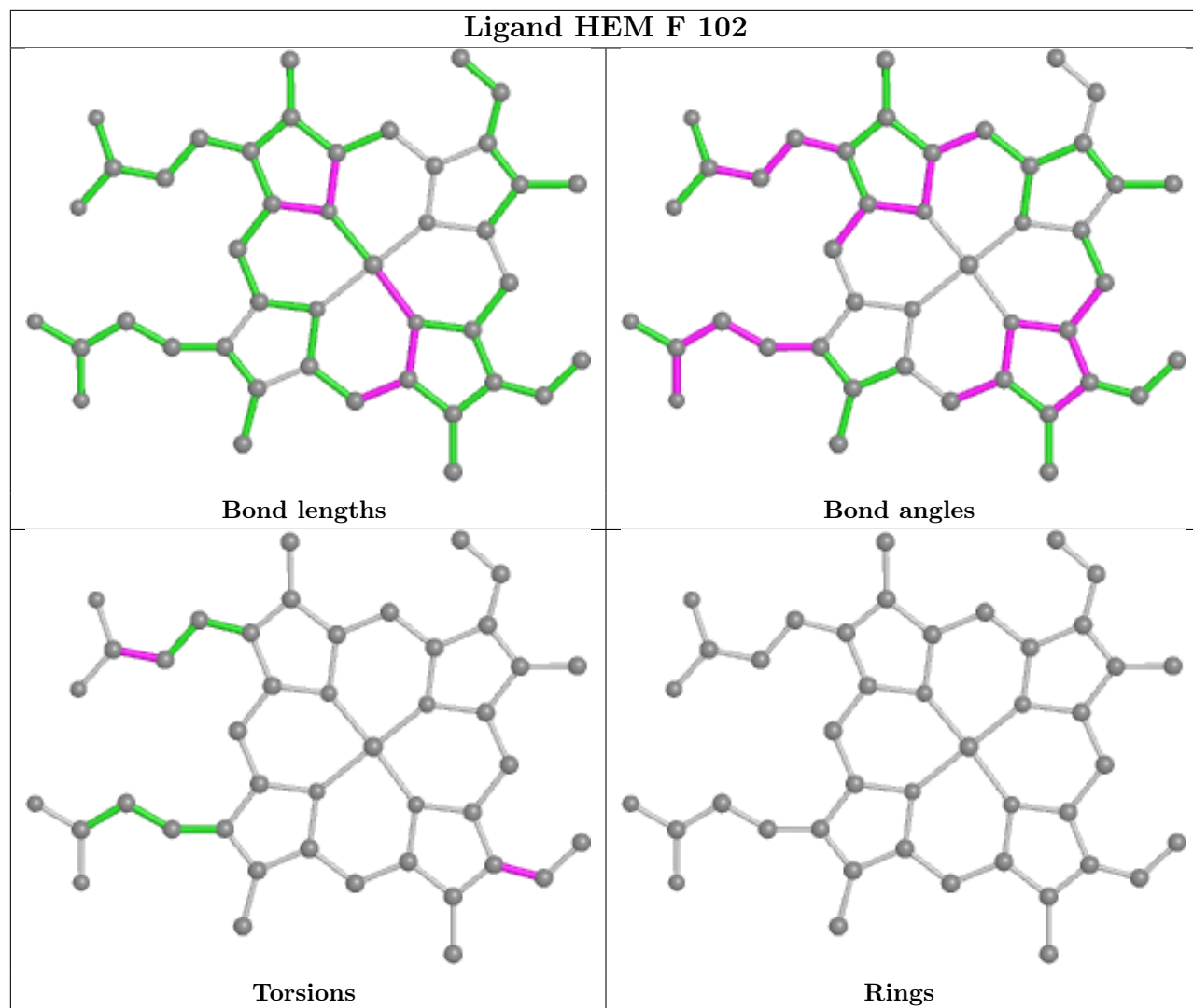
Ligand LMT a 402

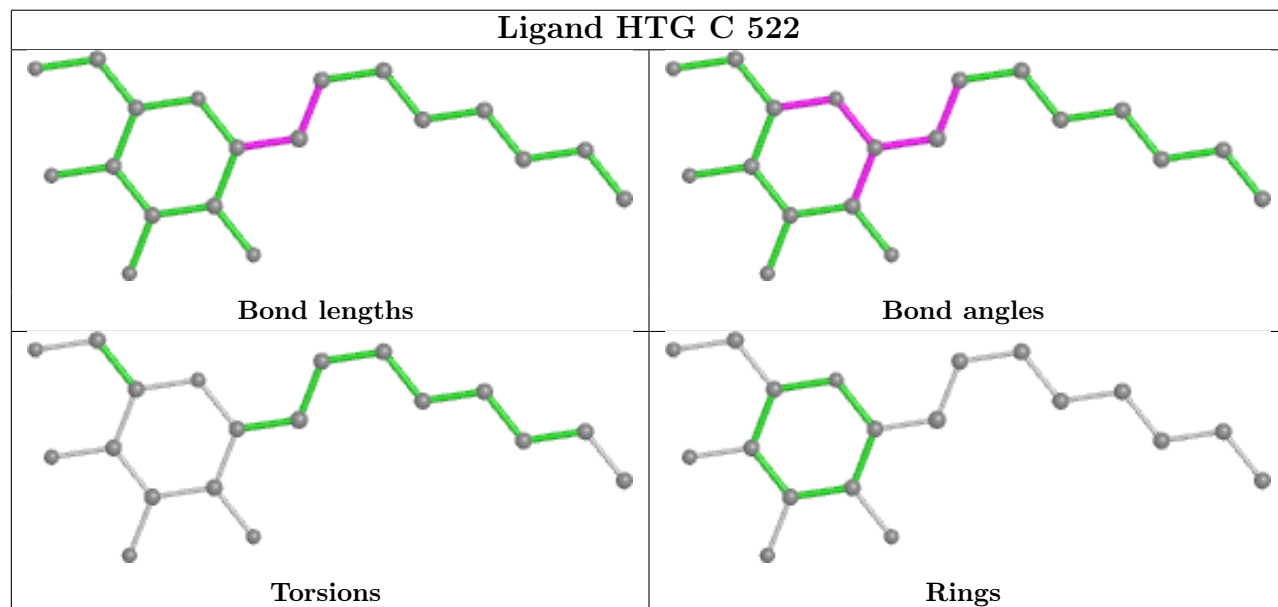
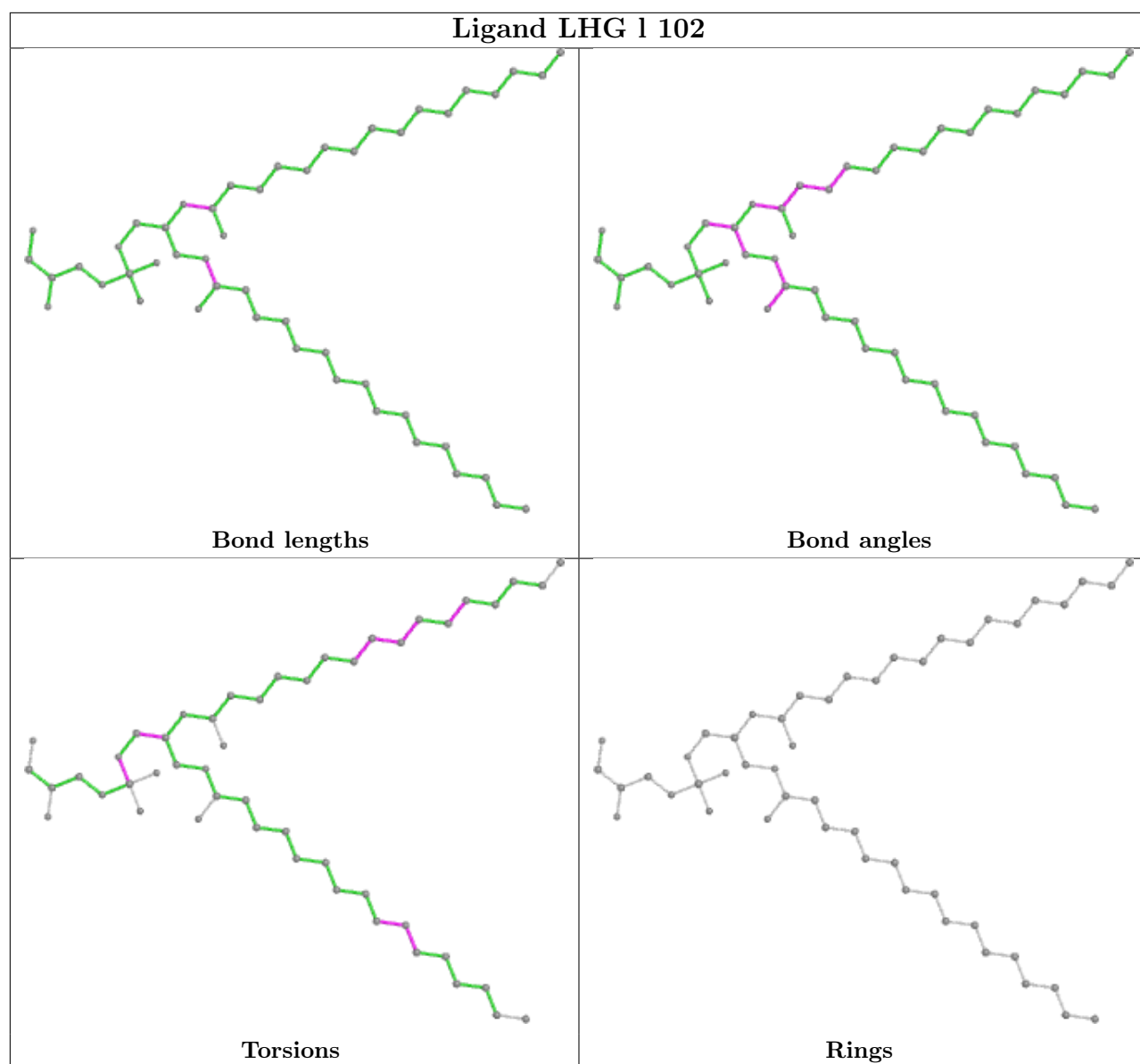


Ligand CLA c 505

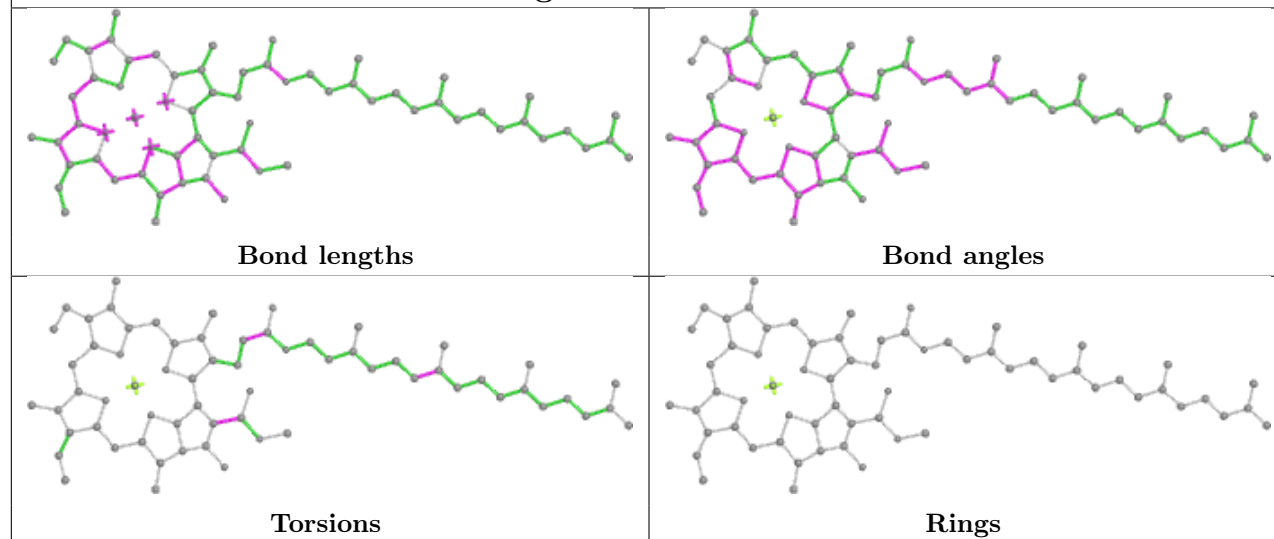




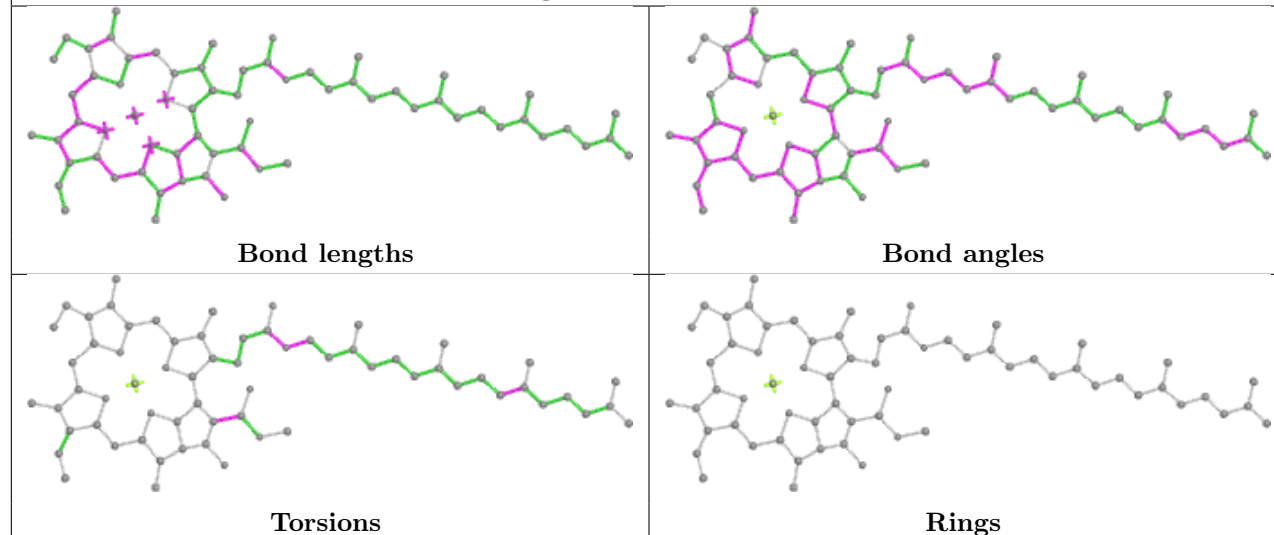




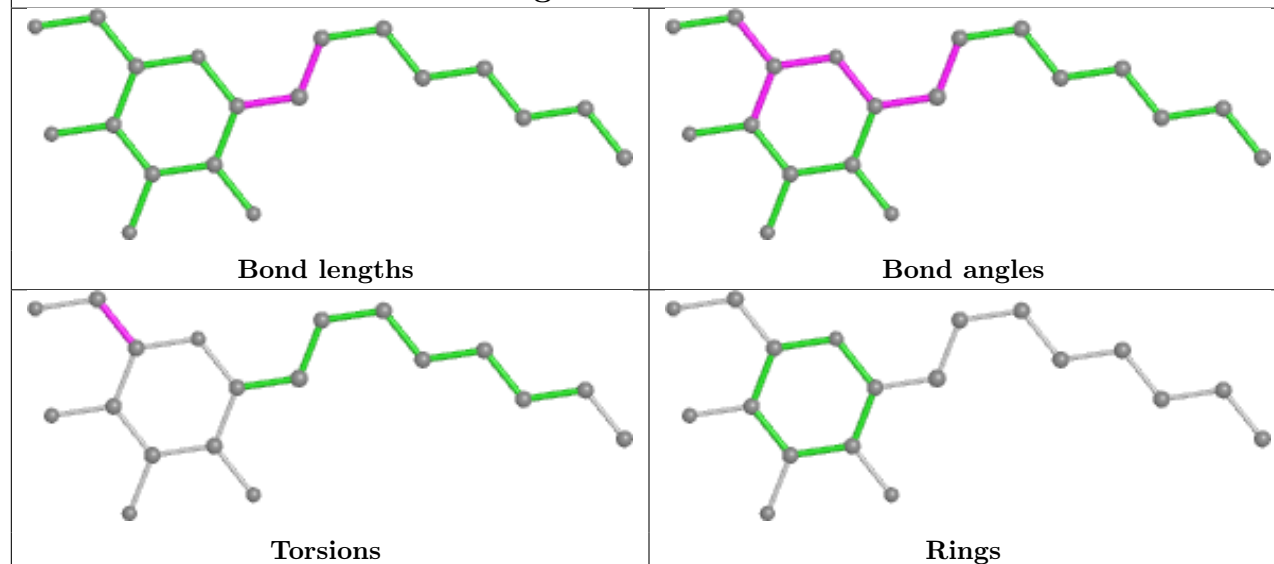
Ligand CLA b 605

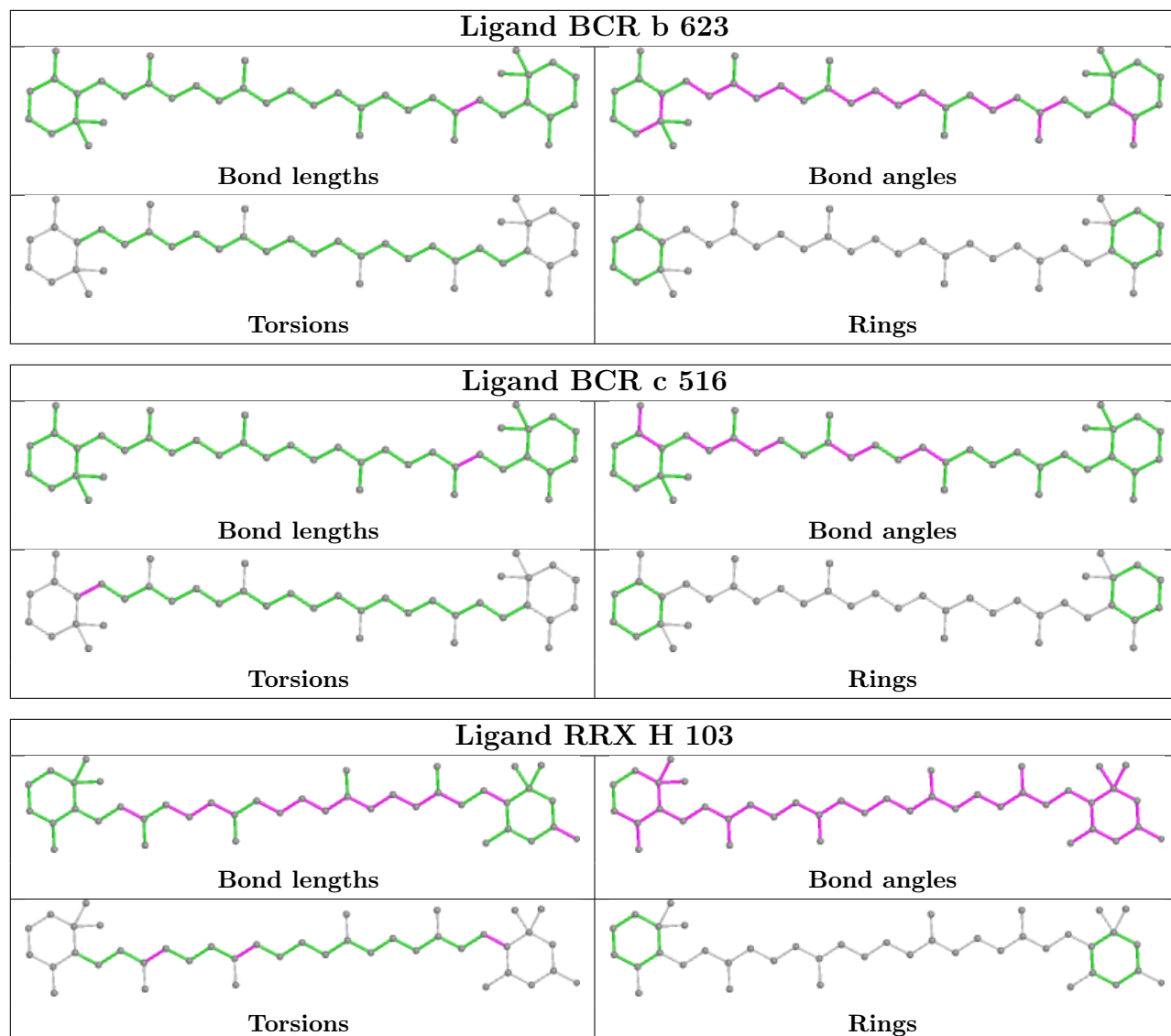


Ligand CLA c 511

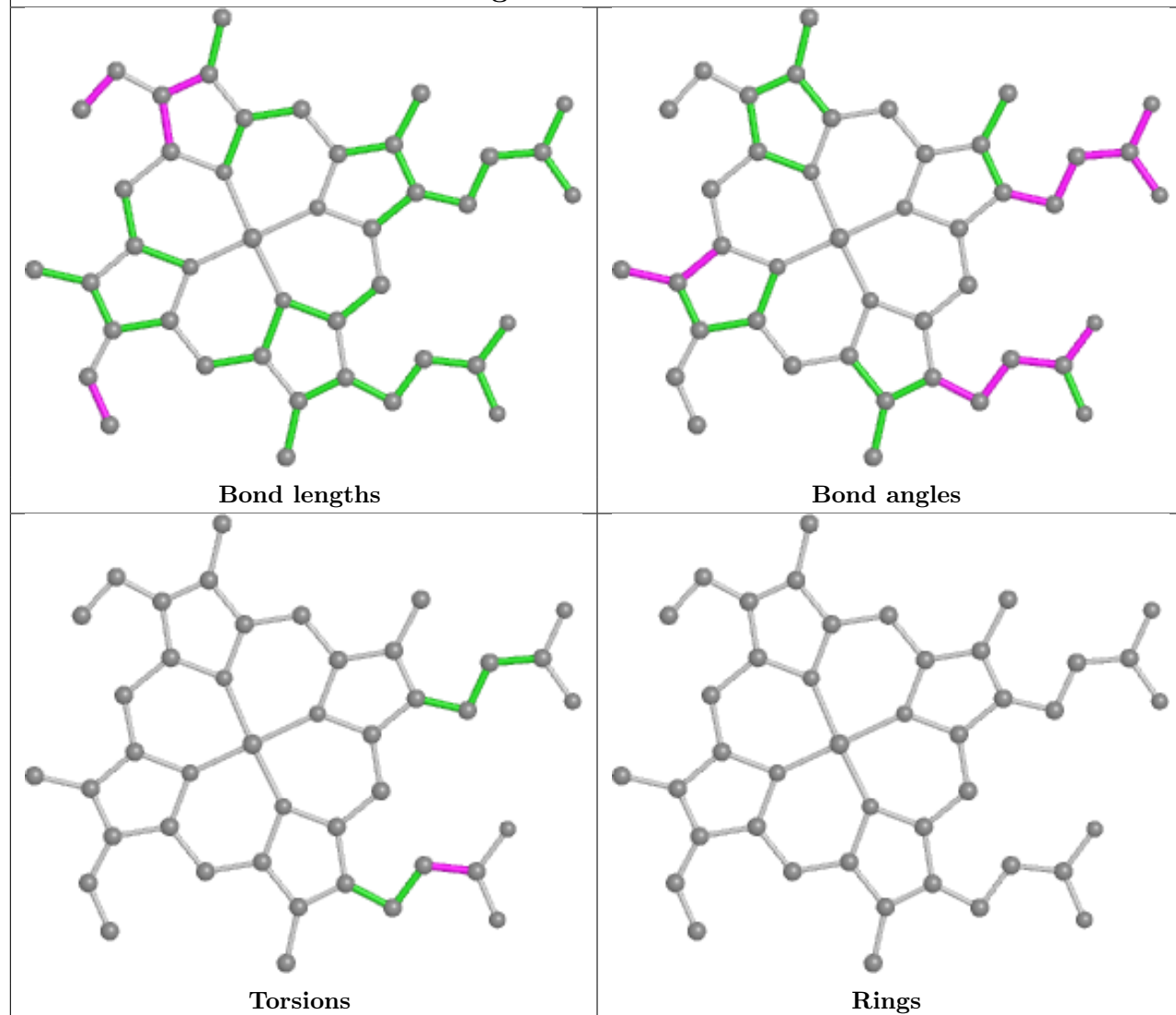


Ligand HTG c 524

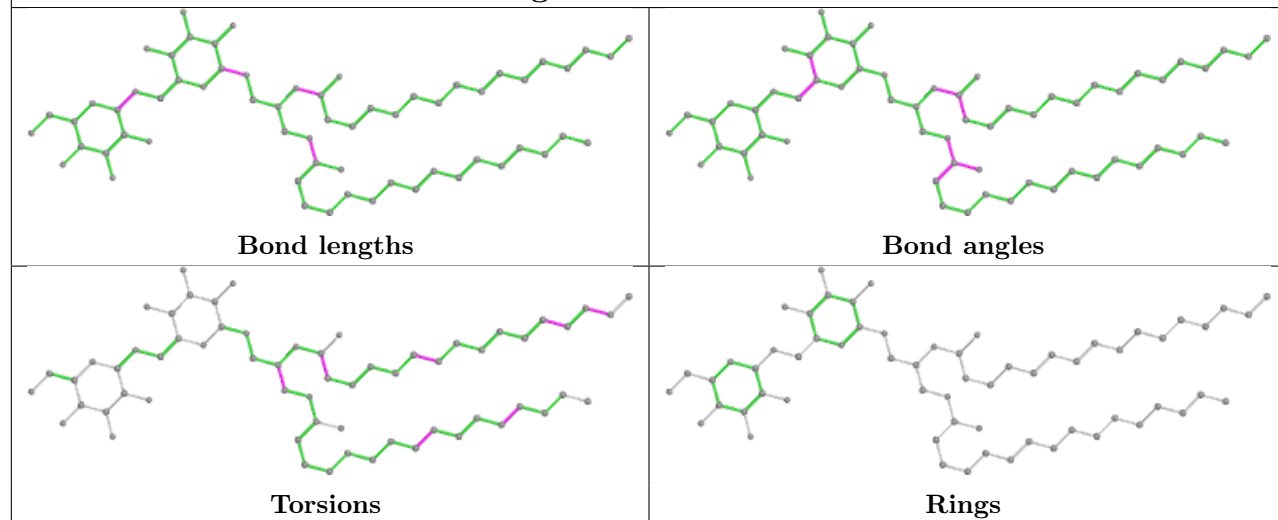


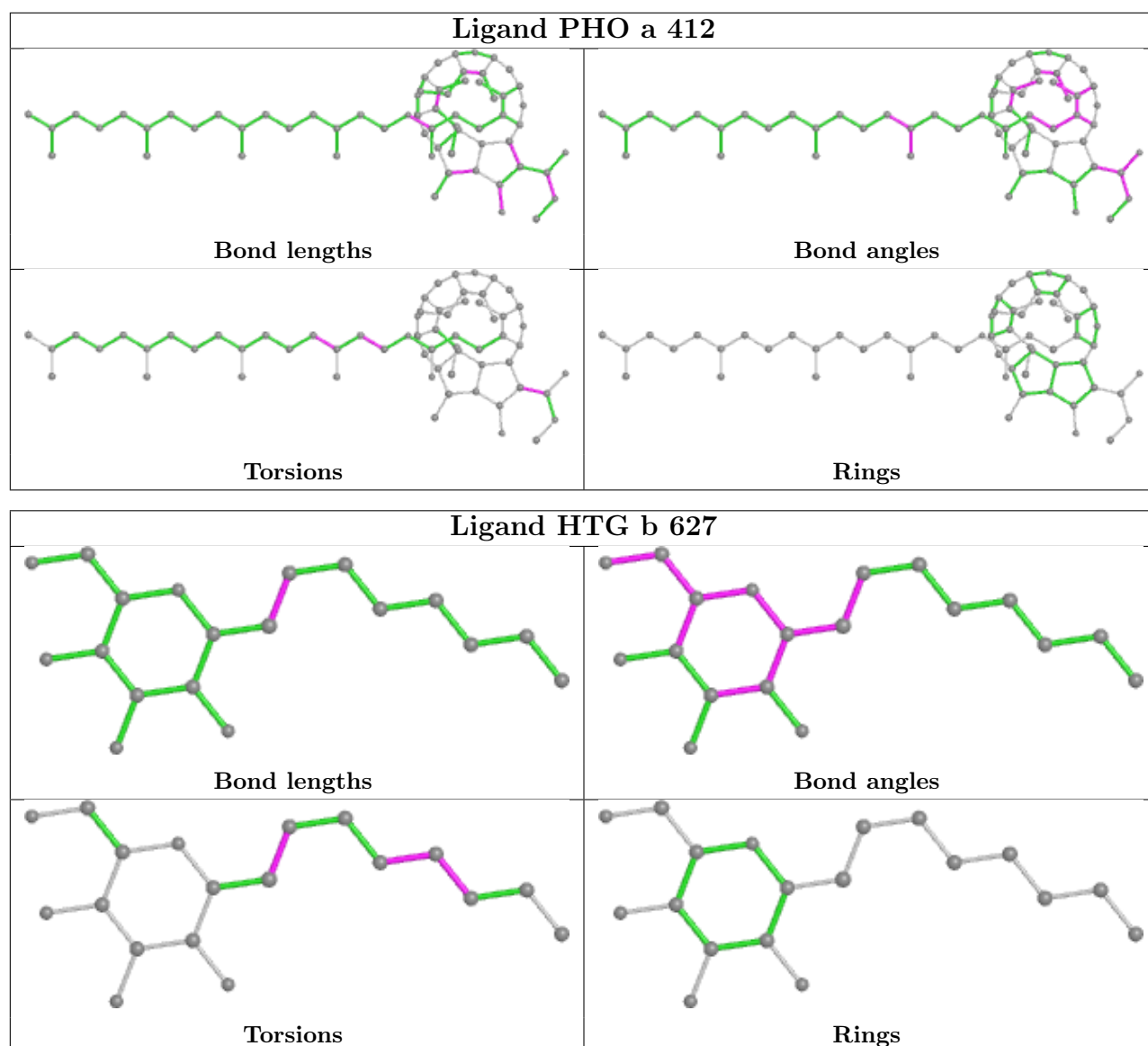


Ligand HEC v 201



Ligand DGD h 102





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/360 (92%)	-0.71	5 (1%) 73 76	21, 28, 47, 90	0
1	a	342/360 (95%)	-0.51	13 (3%) 40 43	22, 30, 62, 142	0
2	B	504/510 (98%)	-0.50	18 (3%) 42 45	23, 33, 57, 122	0
2	b	504/510 (98%)	-0.34	29 (5%) 23 25	24, 35, 67, 147	0
3	C	450/461 (97%)	-0.55	6 (1%) 77 79	26, 37, 55, 93	0
3	c	455/461 (98%)	-0.46	7 (1%) 73 76	30, 41, 57, 114	0
4	D	341/352 (96%)	-0.75	3 (0%) 84 85	21, 28, 45, 92	0
4	d	342/352 (97%)	-0.66	7 (2%) 65 68	23, 32, 53, 119	0
5	E	80/84 (95%)	0.80	22 (27%) 0 0	33, 49, 106, 133	0
5	e	79/84 (94%)	0.84	19 (24%) 0 0	39, 54, 96, 126	0
6	F	34/45 (75%)	-0.16	3 (8%) 10 11	32, 41, 64, 96	0
6	f	32/45 (71%)	-0.11	3 (9%) 8 9	36, 43, 91, 120	0
7	H	64/66 (96%)	-0.06	3 (4%) 31 34	29, 40, 53, 136	0
7	h	65/66 (98%)	0.14	6 (9%) 9 10	34, 43, 58, 147	0
8	I	36/38 (94%)	0.14	4 (11%) 5 6	32, 42, 98, 126	0
8	i	36/38 (94%)	-0.09	3 (8%) 11 13	32, 40, 85, 116	0
9	J	37/40 (92%)	-0.26	3 (8%) 12 13	31, 41, 106, 122	0
9	j	38/40 (95%)	0.14	5 (13%) 3 3	36, 47, 85, 104	0
10	K	37/46 (80%)	-0.42	1 (2%) 54 57	35, 42, 67, 71	0
10	k	37/46 (80%)	-0.09	3 (8%) 12 13	39, 48, 72, 87	0
11	L	37/37 (100%)	-0.21	4 (10%) 5 6	21, 26, 78, 100	0
11	l	36/37 (97%)	-0.34	3 (8%) 11 13	23, 26, 79, 112	0
12	M	33/36 (91%)	-0.55	2 (6%) 21 24	24, 29, 59, 110	0
12	m	33/36 (91%)	-0.58	2 (6%) 21 24	24, 29, 59, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/272 (89%)	-0.18	14 (5%) 23 25	23, 41, 72, 114	0
13	o	243/272 (89%)	0.09	24 (9%) 7 8	26, 44, 78, 127	0
14	T	29/32 (90%)	-0.53	1 (3%) 45 48	23, 26, 49, 117	0
14	t	29/32 (90%)	-0.32	2 (6%) 16 19	25, 28, 55, 85	0
15	U	97/134 (72%)	-0.20	4 (4%) 37 40	29, 40, 68, 107	0
15	u	97/134 (72%)	-0.24	1 (1%) 82 84	33, 43, 62, 126	0
16	V	137/163 (84%)	-0.48	0 100 100	27, 36, 57, 84	0
16	v	137/163 (84%)	-0.20	6 (4%) 34 37	34, 49, 77, 99	0
17	X	40/41 (97%)	0.07	5 (12%) 3 4	36, 46, 80, 99	0
17	x	38/41 (92%)	0.26	5 (13%) 3 3	41, 50, 98, 113	0
18	Y	29/46 (63%)	1.30	6 (20%) 1 1	43, 54, 91, 119	0
18	y	30/46 (65%)	1.17	9 (30%) 0 0	51, 63, 102, 111	0
19	Z	62/62 (100%)	0.41	12 (19%) 1 1	44, 55, 90, 101	0
19	z	61/62 (98%)	0.94	16 (26%) 0 0	52, 65, 107, 126	0
20	R	34/41 (82%)	5.30	33 (97%) 0 0	70, 121, 137, 141	0
All	All	5292/5691 (92%)	-0.29	312 (5%) 22 25	21, 37, 75, 147	0

All (312) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	h	66	GLY	11.3
7	h	64	ALA	10.5
20	R	18	TRP	9.2
2	b	486	LEU	8.8
2	b	494	GLY	8.8
2	b	495	PHE	8.3
18	Y	18	VAL	8.1
1	a	3	THR	8.0
18	Y	19	ILE	8.0
20	R	28	VAL	7.8
20	R	27	ALA	7.8
20	R	31	VAL	7.7
20	R	3	TRP	7.7
20	R	23	ILE	7.5
8	I	37	LEU	7.4
20	R	6	LEU	7.2
18	y	18	VAL	7.2

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Mol	Chain	Res	Type	RSRZ
1	a	5	LEU	7.2
1	a	4	VAL	7.1
13	o	4	THR	7.1
8	I	36	ASP	7.0
20	R	34	LEU	7.0
1	A	11	LEU	6.8
17	X	41	LEU	6.6
20	R	26	TYR	6.6
20	R	14	LEU	6.6
13	o	246	ALA	6.4
14	T	30	THR	6.4
20	R	32	GLN	6.3
5	E	83	LEU	6.3
7	H	65	LEU	6.3
20	R	25	PRO	6.3
5	E	76	VAL	6.2
20	R	13	LEU	6.2
20	R	30	GLN	6.0
7	H	64	ALA	5.9
13	O	4	THR	5.9
17	x	38	GLN	5.7
20	R	24	LEU	5.7
11	L	1	MET	5.6
7	h	65	LEU	5.6
18	Y	20	ALA	5.5
20	R	15	ALA	5.5
17	x	2	THR	5.4
19	z	1	MET	5.4
20	R	20	VAL	5.3
2	b	502	VAL	5.3
11	L	3	PRO	5.3
8	I	34	ARG	5.2
20	R	7	VAL	5.2
6	f	14	PRO	5.2
17	x	37	VAL	5.1
19	z	60	PHE	5.1
18	y	19	ILE	5.0
12	M	34	LYS	5.0
18	Y	22	LEU	5.0
20	R	16	ALA	4.9
13	o	59	LYS	4.9
20	R	5	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
1	a	8	ARG	4.8
2	b	493	TRP	4.8
1	A	13	LEU	4.8
20	R	35	LEU	4.8
5	E	59	GLU	4.8
5	E	79	PHE	4.8
20	R	2	ASP	4.8
4	d	238	THR	4.8
13	o	35	SER	4.8
5	E	82	GLN	4.8
8	i	36	ASP	4.7
14	t	30	THR	4.7
19	z	32	ASP	4.6
19	Z	33[A]	TRP	4.6
2	b	485	GLU	4.6
19	z	30	PRO	4.6
2	b	504	THR	4.6
6	F	12	SER	4.6
1	a	262	TYR	4.5
14	t	29	ILE	4.5
6	f	16	PHE	4.5
3	c	21	ILE	4.5
11	l	3	PRO	4.5
5	e	81	GLU	4.5
20	R	33	LYS	4.5
17	X	40	SER	4.4
5	E	57	ALA	4.4
5	E	81	GLU	4.4
20	R	9	LEU	4.4
18	y	22	LEU	4.4
19	z	33	TRP	4.3
9	j	6	GLY	4.3
5	E	80	LEU	4.3
2	b	503	THR	4.3
19	Z	62	VAL	4.3
2	b	505	ARG	4.3
16	v	17	LYS	4.2
5	E	78	THR	4.2
19	Z	32[A]	ASP	4.2
20	R	22	ASN	4.2
20	R	17	GLY	4.2
2	b	496	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
15	u	8	GLU	4.1
19	z	2	THR	4.1
7	h	63	LYS	4.1
3	c	20	SER	4.1
13	o	61	GLN	4.1
5	e	84	LYS	4.1
5	e	25	ILE	4.1
1	a	6	GLN	4.0
13	o	36	GLN	4.0
5	e	83	LEU	4.0
17	x	34	ILE	4.0
2	b	85	GLY	4.0
4	D	238	THR	4.0
8	I	35	LYS	4.0
13	O	56	PRO	4.0
5	E	72	ALA	4.0
4	d	237	PRO	3.9
2	b	487	SER	3.9
11	l	2	GLU	3.9
5	E	77	GLU	3.9
9	j	5	GLY	3.9
4	d	236	ASN	3.8
5	e	60	GLN	3.8
17	X	2	THR	3.8
19	z	34	ASP	3.8
2	b	293	ALA	3.8
20	R	19	ALA	3.8
5	e	59	GLU	3.8
11	L	2	GLU	3.8
18	Y	25	ILE	3.8
2	b	127	ARG	3.8
3	C	24	THR	3.7
2	b	484	PRO	3.7
2	B	494	GLY	3.7
2	b	86	ILE	3.7
2	B	485	GLU	3.7
7	H	6	TRP	3.7
3	c	143	TYR	3.6
12	m	33	GLN	3.6
19	Z	4	LEU	3.6
13	o	33	ASP	3.6
19	z	7	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
19	z	61	VAL	3.6
4	d	11	GLU	3.6
9	J	4	GLU	3.6
15	U	8	GLU	3.5
3	C	25	ASN	3.5
3	C	207	ARG	3.5
13	O	61	GLN	3.5
20	R	10	LEU	3.5
10	k	10	LYS	3.4
19	z	3	ILE	3.4
2	b	129	GLY	3.4
18	y	17	GLU	3.4
13	o	60	ARG	3.4
1	a	7	ARG	3.4
20	R	12	VAL	3.4
15	U	65	PRO	3.4
17	x	39	ARG	3.4
2	B	295	GLY	3.4
13	o	58	ASN	3.3
13	o	56	PRO	3.3
18	y	25	ILE	3.2
5	e	78	THR	3.2
1	A	243	GLU	3.2
19	Z	7	LEU	3.2
5	E	17	VAL	3.2
13	o	34	SER	3.2
5	e	82	GLN	3.2
11	L	5	PRO	3.2
19	z	31	GLN	3.1
13	o	63	ALA	3.1
9	j	3	SER	3.1
12	M	33	GLN	3.1
9	j	4	GLU	3.1
20	R	21	ARG	3.1
5	E	73	LYS	3.1
5	e	77	GLU	3.1
6	F	13	TYR	3.1
5	e	58	GLN	3.1
2	B	484	PRO	3.1
2	b	295	GLY	3.1
13	O	5	LEU	3.0
19	z	42	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
4	d	240	ALA	3.0
18	Y	21	GLN	3.0
19	z	59	PHE	3.0
18	y	41	VAL	3.0
19	Z	38	GLN	3.0
5	e	21	VAL	3.0
13	o	37	THR	2.9
3	C	143	TYR	2.9
16	v	72	LEU	2.9
20	R	29	LYS	2.9
2	b	497	GLN	2.9
13	O	58	ASN	2.9
5	e	74	GLN	2.9
19	Z	31[A]	GLN	2.9
2	b	492	GLU	2.9
2	B	86	ILE	2.9
2	B	489	GLU	2.8
10	k	13	GLU	2.8
13	o	26	ALA	2.8
8	i	34	ARG	2.8
17	X	3	ILE	2.8
3	c	19	ASN	2.8
2	B	503	THR	2.8
19	Z	35	ARG	2.8
1	a	235	TYR	2.8
5	e	57	ALA	2.7
6	F	14	PRO	2.7
2	B	505	ARG	2.7
2	B	487	SER	2.7
1	a	12	ASN	2.7
2	B	495	PHE	2.7
9	J	6	GLY	2.7
5	E	60	GLN	2.7
17	X	38	GLN	2.7
9	J	5	GLY	2.7
5	E	74	GLN	2.7
5	E	65	LEU	2.7
13	o	25	THR	2.7
4	D	240	ALA	2.7
18	y	20	ALA	2.7
2	B	502	VAL	2.7
13	O	89	SER	2.7

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Mol	Chain	Res	Type	RSRZ
5	E	71	GLU	2.6
13	O	132	ASN	2.6
2	B	486	LEU	2.6
1	a	11	LEU	2.6
13	o	5	LEU	2.6
1	a	9	GLU	2.6
2	B	293	ALA	2.6
13	o	23	ASP	2.6
13	O	62	GLU	2.6
13	o	207	ARG	2.6
16	v	106	ASN	2.6
13	o	24	ASP	2.6
19	Z	30[A]	PRO	2.6
2	B	85	GLY	2.6
2	b	488	PRO	2.5
10	k	17	ILE	2.5
8	i	37	LEU	2.5
3	c	192	GLY	2.5
5	e	11	SER	2.5
3	C	145	SER	2.5
13	O	243	ILE	2.5
4	d	107	LEU	2.5
9	j	7	ARG	2.5
19	z	35	ARG	2.5
5	E	4	THR	2.4
19	Z	42	LEU	2.4
13	o	130	GLN	2.4
2	b	483	ASP	2.4
2	b	489	GLU	2.4
13	O	60	ARG	2.4
2	b	501	ASP	2.4
5	e	24	SER	2.4
11	l	5	PRO	2.4
7	h	6	TRP	2.4
3	c	106	VAL	2.4
3	c	145[A]	SER	2.3
16	v	15	GLU	2.3
2	b	87	ASP	2.3
1	a	10	GLN	2.3
6	f	15	ILE	2.3
18	y	43	ARG	2.3
2	b	84	THR	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	253	LEU	2.3
4	d	12	ARG	2.3
13	O	90	ASP	2.3
19	Z	34	ASP	2.3
2	b	490	GLN	2.3
13	O	207	ARG	2.3
15	U	66	GLY	2.2
2	b	130	GLU	2.2
12	m	34	LYS	2.2
7	h	23	PRO	2.2
13	O	211	ILE	2.2
13	O	59	LYS	2.2
19	z	4	LEU	2.2
1	A	12	ASN	2.2
13	o	132	ASN	2.2
18	y	42	ARG	2.2
19	z	39	LEU	2.2
2	B	496	TYR	2.2
16	v	108	THR	2.2
5	E	61	ARG	2.2
1	A	228	THR	2.2
16	v	16	GLY	2.2
5	E	58	GLN	2.2
5	e	76	VAL	2.2
5	e	79	PHE	2.1
20	R	11	PRO	2.1
2	b	294	SER	2.1
2	B	127	ARG	2.1
2	B	84	THR	2.1
5	E	62[A]	SER	2.1
4	D	236	ASN	2.1
13	o	131	PRO	2.1
1	a	242	GLU	2.1
5	e	9	PRO	2.1
15	U	70	ARG	2.1
5	E	68	ASP	2.1
10	K	10	LYS	2.1
20	R	4	ARG	2.0
2	B	374	ASN	2.0
19	Z	61	VAL	2.0
13	o	28	GLY	2.0
13	o	89	SER	2.0

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Mol	Chain	Res	Type	RSRZ
5	e	80	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	t	1	10/11	0.95	0.08	27,32,61,65	0
14	FME	T	1	10/11	0.96	0.08	25,32,60,61	0
12	FME	M	1	10/11	0.96	0.12	28,38,66,77	0
12	FME	m	1	10/11	0.97	0.10	29,37,67,73	0
8	FME	i	1	10/11	0.97	0.12	31,39,45,51	0
8	FME	I	1	10/11	0.98	0.07	32,39,44,49	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
30	UNL	I	106	10/-	0.29	0.40	63,88,93,94	0
36	HTG	d	404	16/19	0.47	0.34	63,100,108,111	0
36	HTG	H	101	16/19	0.48	0.30	63,123,128,130	0
34	DMS	v	205	4/4	0.48	0.37	129,131,133,136	0
32	LMT	j	102	24/35	0.51	0.27	64,83,130,132	0
34	DMS	u	203	4/4	0.52	0.40	60,81,82,87	0
30	UNL	V	206	7/-	0.55	0.24	75,86,100,101	0
31	GOL	O	304	6/6	0.56	0.26	80,88,90,92	0
30	UNL	C	527	8/-	0.56	0.24	87,99,102,102	0
37	DGD	d	416	50/66	0.56	0.32	81,99,118,119	0
36	HTG	u	201	14/19	0.57	0.42	63,93,113,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	HTG	B	630	19/19	0.57	0.25	53,112,124,125	0
32	LMT	M	101	35/35	0.58	0.28	50,115,142,145	0
32	LMT	F	103	35/35	0.59	0.37	74,113,128,129	0
30	UNL	X	102	10/-	0.59	0.28	70,77,82,84	0
36	HTG	b	603	19/19	0.60	0.22	56,104,122,125	0
30	UNL	E	102	12/-	0.60	0.31	66,75,95,97	0
30	UNL	D	416	16/-	0.60	0.26	78,82,87,88	0
32	LMT	J	102	24/35	0.60	0.24	56,70,106,110	0
30	UNL	h	104	16/-	0.61	0.29	65,75,101,101	0
34	DMS	B	641	4/4	0.61	0.33	123,126,128,129	0
36	HTG	B	626	19/19	0.61	0.41	56,115,122,124	0
34	DMS	C	539	4/4	0.62	0.35	99,100,102,106	0
30	UNL	C	528	7/-	0.62	0.39	54,74,76,77	0
30	UNL	b	640	13/-	0.63	0.36	73,90,108,109	0
30	UNL	C	524	28/-	0.63	0.20	55,73,107,110	0
30	UNL	V	204	8/-	0.63	0.30	49,66,70,71	0
30	UNL	h	105	10/-	0.64	0.21	70,85,94,97	0
30	UNL	h	103	7/-	0.64	0.25	78,80,84,85	0
34	DMS	O	308	4/4	0.64	0.44	107,116,120,120	0
36	HTG	b	628	19/19	0.65	0.26	60,120,129,130	0
28	LMG	Z	101	39/55	0.65	0.27	52,91,115,120	0
32	LMT	a	421	35/35	0.65	0.37	89,107,136,139	0
30	UNL	X	101	34/-	0.65	0.25	37,74,119,123	0
30	UNL	k	101	30/-	0.66	0.20	59,87,110,113	0
30	UNL	J	103	8/-	0.66	0.22	70,72,74,75	0
32	LMT	B	638	35/35	0.66	0.25	42,110,127,128	0
34	DMS	C	501	4/4	0.66	0.48	129,130,133,134	0
36	HTG	c	524	19/19	0.67	0.37	70,95,108,112	0
34	DMS	o	305	4/4	0.67	0.41	123,128,128,131	0
38	LHG	a	416	42/49	0.67	0.28	64,113,146,149	0
30	UNL	I	105	16/-	0.68	0.23	70,80,84,88	0
30	UNL	j	103	10/-	0.68	0.20	63,68,76,77	0
30	UNL	c	526	4/-	0.68	0.26	67,72,73,74	0
30	UNL	c	528	8/-	0.69	0.33	61,79,81,84	0
30	UNL	Z	102	5/-	0.69	0.20	61,63,66,69	0
30	UNL	C	532	10/-	0.69	0.32	82,86,88,89	0
34	DMS	O	306	4/4	0.69	0.26	106,111,111,112	0
28	LMG	c	522	51/55	0.69	0.26	46,91,109,123	0
32	LMT	D	409	35/35	0.69	0.34	73,105,130,134	0
30	UNL	J	105	6/-	0.70	0.20	78,83,85,85	0
32	LMT	m	103	35/35	0.70	0.22	51,107,122,129	0
32	LMT	B	624	35/35	0.70	0.22	55,82,98,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	LMT	b	629	24/35	0.70	0.23	47,74,124,126	0
30	UNL	c	501	8/-	0.71	0.15	63,73,83,84	0
30	UNL	b	630	10/-	0.71	0.22	80,85,90,91	0
34	DMS	a	424	4/4	0.71	0.23	110,112,113,114	0
32	LMT	b	626	35/35	0.71	0.25	38,102,128,130	0
32	LMT	b	625	35/35	0.72	0.23	55,102,123,127	0
34	DMS	b	644	4/4	0.72	0.33	119,122,123,124	0
32	LMT	a	402	35/35	0.72	0.27	43,84,103,110	0
34	DMS	B	639	4/4	0.72	0.34	111,114,115,115	0
30	UNL	B	628	6/-	0.72	0.30	55,60,66,69	0
31	GOL	b	638	6/6	0.73	0.21	88,94,100,100	0
30	UNL	h	106	4/-	0.73	0.19	69,70,72,74	0
32	LMT	f	801	25/35	0.73	0.31	73,101,111,114	0
34	DMS	O	302	4/4	0.73	0.32	104,111,113,118	0
30	UNL	I	103	16/-	0.73	0.20	53,72,92,94	0
27	SQD	B	622	54/54	0.73	0.20	43,72,113,116	0
30	UNL	B	635	4/-	0.73	0.20	67,72,73,78	0
30	UNL	A	417	12/-	0.74	0.20	77,79,82,83	0
30	UNL	y	101	10/-	0.74	0.15	83,85,87,88	0
30	UNL	B	601	4/-	0.74	0.27	70,71,72,74	0
34	DMS	c	537	4/4	0.74	0.37	115,117,119,122	0
34	DMS	d	419	4/4	0.74	0.23	106,112,113,114	0
28	LMG	C	533	51/55	0.74	0.22	43,88,98,101	0
36	HTG	c	523	19/19	0.75	0.23	87,103,110,114	0
36	HTG	B	625	19/19	0.75	0.24	34,61,77,79	0
34	DMS	O	310	4/4	0.75	0.30	89,93,96,97	0
32	LMT	A	422	35/35	0.76	0.31	76,95,118,119	0
28	LMG	z	101	37/55	0.76	0.21	50,105,120,121	0
30	UNL	a	420	7/-	0.76	0.24	61,67,71,74	0
30	UNL	B	631	11/-	0.77	0.27	63,70,103,106	0
30	UNL	C	529	8/-	0.77	0.20	75,78,82,84	0
30	UNL	i	103	10/-	0.77	0.14	54,64,75,76	0
30	UNL	I	104	16/-	0.77	0.24	69,82,85,85	0
30	UNL	Z	104	5/-	0.77	0.20	67,70,78,78	0
30	UNL	i	104	10/-	0.78	0.22	69,72,77,81	0
30	UNL	A	414	10/-	0.78	0.25	67,79,83,83	0
34	DMS	v	204	4/4	0.78	0.20	127,130,131,132	0
38	LHG	E	101	42/49	0.78	0.25	58,83,103,104	0
34	DMS	b	643	4/4	0.78	0.33	113,115,117,117	0
34	DMS	T	103	4/4	0.79	0.21	89,96,101,104	0
36	HTG	C	523	19/19	0.79	0.26	59,93,111,113	0
27	SQD	b	601	54/54	0.79	0.19	46,64,119,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	LMT	D	402	35/35	0.79	0.22	50,91,100,105	0
34	DMS	a	403	4/4	0.80	0.18	101,106,108,108	0
30	UNL	b	637	7/-	0.80	0.15	59,63,77,83	0
30	UNL	C	530	4/-	0.80	0.14	69,73,78,80	0
30	UNL	Y	101	16/-	0.80	0.25	75,81,88,88	0
30	UNL	c	525	10/-	0.80	0.27	65,70,85,89	0
32	LMT	m	102	35/35	0.80	0.19	33,59,77,79	0
30	UNL	I	102	7/-	0.81	0.15	66,69,73,74	0
30	UNL	E	103	10/-	0.81	0.19	70,73,77,78	0
34	DMS	A	425	4/4	0.81	0.25	113,114,116,117	0
30	UNL	m	101	8/-	0.81	0.22	48,50,54,58	0
30	UNL	B	637	6/-	0.82	0.20	69,71,75,79	0
34	DMS	V	210	4/4	0.82	0.18	123,123,125,127	0
32	LMT	M	102	35/35	0.82	0.16	36,58,72,75	0
36	HTG	b	627	19/19	0.82	0.30	39,62,87,91	0
27	SQD	a	401	54/54	0.82	0.17	44,67,92,99	0
29	PL9	a	417	55/55	0.82	0.18	55,70,98,100	0
34	DMS	E	104	4/4	0.83	0.19	122,125,125,126	0
34	DMS	b	641	4/4	0.83	0.29	85,91,95,97	0
30	UNL	d	414	10/-	0.83	0.21	67,74,78,80	0
29	PL9	A	413	55/55	0.83	0.18	45,65,92,96	0
30	UNL	b	634	12/-	0.83	0.22	58,68,84,85	0
28	LMG	i	101	51/55	0.84	0.18	53,68,86,93	0
34	DMS	O	309	4/4	0.84	0.25	97,101,102,103	0
30	UNL	a	418	10/-	0.84	0.20	73,77,86,90	0
34	DMS	C	540	4/4	0.84	0.27	123,124,124,124	0
34	DMS	c	538	4/4	0.84	0.22	122,123,123,124	0
30	UNL	H	102	4/-	0.84	0.18	67,67,72,76	0
30	UNL	H	105	8/-	0.84	0.12	64,69,75,75	0
36	HTG	b	602	19/19	0.84	0.16	46,71,81,82	0
30	UNL	D	414	39/-	0.84	0.17	42,64,108,112	0
30	UNL	i	102	16/-	0.85	0.18	45,52,86,88	0
34	DMS	C	535	4/4	0.85	0.24	46,62,66,70	0
34	DMS	T	104	4/4	0.85	0.23	119,119,120,122	0
34	DMS	V	203	4/4	0.85	0.18	110,111,113,115	0
31	GOL	D	417	6/6	0.85	0.23	75,77,79,85	0
30	UNL	D	403	5/-	0.85	0.17	61,66,69,72	0
31	GOL	V	207	6/6	0.85	0.15	67,71,73,75	0
34	DMS	A	424	4/4	0.85	0.24	109,112,114,115	0
30	UNL	Z	103	5/-	0.85	0.19	58,67,76,78	0
31	GOL	b	639	6/6	0.85	0.36	41,60,66,74	0
31	GOL	v	203	6/6	0.85	0.16	65,73,75,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
27	SQD	A	415	54/54	0.86	0.15	39,58,89,92	0
34	DMS	C	538	4/4	0.86	0.34	96,97,101,107	0
27	SQD	f	802	43/54	0.86	0.24	59,85,114,121	0
28	LMG	B	623	51/55	0.86	0.14	34,50,66,71	0
30	UNL	A	419	8/-	0.86	0.15	62,71,73,74	0
30	UNL	J	104	6/-	0.86	0.12	57,58,60,62	0
30	UNL	C	502	4/-	0.87	0.16	67,67,68,69	0
30	UNL	b	635	7/-	0.87	0.14	49,51,57,57	0
34	DMS	c	529	4/4	0.87	0.24	87,99,100,101	0
30	UNL	B	636	6/-	0.87	0.21	67,69,69,71	0
36	HTG	B	629	19/19	0.87	0.14	44,80,103,108	0
30	UNL	c	527	6/-	0.87	0.15	76,77,78,78	0
36	HTG	C	522	19/19	0.87	0.20	75,88,95,96	0
28	LMG	A	412	51/55	0.87	0.15	51,66,85,92	0
34	DMS	b	633	4/4	0.87	0.14	78,79,87,91	0
30	UNL	k	104	8/-	0.87	0.15	63,67,77,81	0
28	LMG	C	521	51/55	0.88	0.18	34,66,96,101	0
30	UNL	A	416	3/-	0.88	0.09	68,68,72,74	0
30	UNL	z	102	6/-	0.88	0.18	77,79,79,80	0
34	DMS	O	307	4/4	0.88	0.30	93,98,99,102	0
34	DMS	C	537	4/4	0.88	0.18	91,93,94,95	0
34	DMS	a	425	4/4	0.88	0.18	79,91,92,99	0
26	BCR	d	407	40/40	0.88	0.12	32,40,69,72	0
30	UNL	b	636	4/-	0.88	0.09	61,63,66,66	0
30	UNL	e	101	10/-	0.88	0.12	64,67,69,70	0
28	LMG	c	521	51/55	0.89	0.15	39,69,95,97	0
34	DMS	c	534	4/4	0.89	0.31	108,111,112,114	0
34	DMS	c	536	4/4	0.89	0.27	105,108,108,109	0
30	UNL	B	627	14/-	0.89	0.16	50,56,68,70	0
30	UNL	U	201	5/-	0.89	0.14	52,55,68,73	0
28	LMG	d	412	51/55	0.89	0.13	33,45,84,94	0
30	UNL	l	101	13/-	0.89	0.17	42,51,74,75	0
30	UNL	I	101	16/-	0.90	0.15	39,54,68,70	0
31	GOL	a	419	6/6	0.90	0.15	53,57,60,64	0
36	HTG	V	202	12/19	0.90	0.23	51,59,78,102	0
34	DMS	B	643	4/4	0.90	0.22	87,92,94,95	0
30	UNL	d	403	32/-	0.90	0.15	45,62,113,118	0
30	UNL	A	420	6/-	0.90	0.16	31,50,66,74	0
24	CLA	B	603	65/65	0.90	0.12	33,47,99,108	0
40	RRX	h	101	41/41	0.90	0.10	29,46,55,66	0
28	LMG	b	624	51/55	0.91	0.12	35,50,61,74	0
27	SQD	F	101	43/54	0.91	0.19	47,81,103,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	HTG	O	303	19/19	0.91	0.12	36,44,56,60	0
30	UNL	d	413	14/-	0.91	0.12	40,50,58,63	0
34	DMS	b	642	4/4	0.91	0.16	101,102,104,105	0
34	DMS	B	642	4/4	0.91	0.36	95,96,98,101	0
24	CLA	b	620	65/65	0.91	0.13	28,38,101,102	0
24	CLA	b	605	65/65	0.91	0.14	39,50,99,105	0
30	UNL	C	526	6/-	0.92	0.09	64,68,77,79	0
34	DMS	u	202	4/4	0.92	0.16	86,88,88,90	0
31	GOL	d	415	6/6	0.92	0.20	47,58,64,67	0
31	GOL	A	421	6/6	0.92	0.18	62,81,86,87	0
24	CLA	B	618	65/65	0.92	0.14	24,34,96,96	0
34	DMS	V	211	4/4	0.92	0.16	102,102,102,102	0
24	CLA	C	515	65/65	0.92	0.12	38,50,90,94	0
34	DMS	a	423	4/4	0.92	0.21	91,92,95,102	0
36	HTG	o	301	19/19	0.92	0.13	39,48,52,59	0
27	SQD	a	415	54/54	0.92	0.14	38,53,94,97	0
30	UNL	V	205	5/-	0.92	0.30	57,62,63,74	0
34	DMS	d	418	4/4	0.92	0.20	80,89,93,93	0
26	BCR	D	407	40/40	0.92	0.11	28,36,67,69	0
34	DMS	o	303	4/4	0.92	0.28	105,109,109,110	0
24	CLA	C	514	65/65	0.93	0.10	37,47,79,81	0
28	LMG	D	413	51/55	0.93	0.12	29,39,100,108	0
34	DMS	e	103	4/4	0.93	0.27	96,98,98,100	0
34	DMS	h	107	4/4	0.93	0.31	125,127,128,129	0
24	CLA	c	514	65/65	0.93	0.10	39,47,78,82	0
30	UNL	T	102	7/-	0.93	0.22	52,60,79,80	0
34	DMS	B	634	4/4	0.93	0.14	78,80,81,83	0
26	BCR	C	516	40/40	0.93	0.09	40,46,51,52	0
34	DMS	v	202	4/4	0.93	0.20	97,97,103,108	0
34	DMS	B	640	4/4	0.93	0.18	107,110,112,114	0
34	DMS	c	539	4/4	0.93	0.25	77,79,80,89	0
24	CLA	D	406	65/65	0.94	0.10	26,34,98,102	0
34	DMS	c	531	4/4	0.94	0.28	92,93,94,97	0
24	CLA	c	515	65/65	0.94	0.11	42,54,86,92	0
26	BCR	B	621	40/40	0.94	0.08	29,35,46,50	0
24	CLA	B	608	65/65	0.94	0.09	23,32,67,71	0
26	BCR	C	517	40/40	0.94	0.10	31,42,53,56	0
24	CLA	b	610	65/65	0.94	0.09	26,35,83,91	0
34	DMS	V	208	4/4	0.94	0.31	76,81,83,84	0
31	GOL	C	525	6/6	0.94	0.15	38,43,58,63	0
26	BCR	K	101	40/40	0.94	0.09	35,41,47,49	0
26	BCR	K	102	40/40	0.94	0.12	32,39,47,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
26	BCR	a	414	40/40	0.94	0.08	23,31,38,41	0
30	UNL	C	531	10/-	0.94	0.24	70,73,94,97	0
26	BCR	c	516	40/40	0.94	0.09	47,54,64,65	0
34	DMS	a	426	4/4	0.94	0.13	105,106,106,107	0
26	BCR	c	517	40/40	0.94	0.10	32,41,49,50	0
37	DGD	C	519	62/66	0.94	0.11	29,38,88,97	0
37	DGD	H	104	62/66	0.94	0.11	26,37,47,57	0
37	DGD	c	519	62/66	0.94	0.10	34,43,90,100	0
24	CLA	C	508	65/65	0.94	0.09	38,47,94,101	0
37	DGD	h	102	62/66	0.94	0.10	30,38,51,59	0
26	BCR	t	101	40/40	0.94	0.09	23,34,47,52	0
27	SQD	A	411	54/54	0.94	0.12	40,53,86,87	0
40	RRX	H	103	41/41	0.94	0.08	27,41,53,60	0
24	CLA	c	508	65/65	0.94	0.09	36,47,88,92	0
33	BCT	d	402[B]	4/4	0.95	0.11	28,31,36,38	4
37	DGD	c	518	62/66	0.95	0.09	29,37,85,91	0
26	BCR	B	620	40/40	0.95	0.08	24,32,56,63	0
34	DMS	o	304	4/4	0.95	0.18	98,102,102,102	0
24	CLA	a	411	65/65	0.95	0.10	23,30,89,94	0
38	LHG	D	410	49/49	0.95	0.10	24,38,53,61	0
26	BCR	b	622	40/40	0.95	0.08	23,32,49,52	0
26	BCR	k	102	40/40	0.95	0.08	36,43,54,57	0
38	LHG	d	409	49/49	0.95	0.11	30,42,52,55	0
30	UNL	x	101	11/-	0.95	0.20	40,44,63,64	0
37	DGD	C	520	62/66	0.95	0.10	25,36,71,82	0
34	DMS	D	418	4/4	0.96	0.19	71,78,84,86	0
26	BCR	T	101	40/40	0.96	0.07	23,33,46,49	0
24	CLA	b	614	65/65	0.96	0.07	25,33,40,51	0
29	PL9	D	408	55/55	0.96	0.09	19,27,35,39	0
24	CLA	b	616	65/65	0.96	0.08	24,29,40,44	0
29	PL9	d	408	55/55	0.96	0.08	21,27,36,45	0
26	BCR	b	623	40/40	0.96	0.08	28,37,51,53	0
24	CLA	b	618	65/65	0.96	0.08	20,29,78,85	0
24	CLA	b	619	65/65	0.96	0.08	26,35,53,57	0
24	CLA	C	511	65/65	0.96	0.09	30,38,58,63	0
24	CLA	c	503	65/65	0.96	0.08	31,41,53,61	0
26	BCR	k	103	40/40	0.96	0.10	35,46,55,59	0
34	DMS	V	209	4/4	0.96	0.21	95,97,98,103	0
24	CLA	c	505	65/65	0.96	0.08	34,41,49,67	0
24	CLA	c	506	65/65	0.96	0.08	30,37,84,89	0
24	CLA	C	513	65/65	0.96	0.09	29,40,46,50	0
24	CLA	c	509	65/65	0.96	0.09	31,38,59,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CLA	c	510	65/65	0.96	0.09	27,35,96,109	0
24	CLA	c	512	65/65	0.96	0.08	28,37,50,58	0
24	CLA	c	513	65/65	0.96	0.08	33,41,52,54	0
34	DMS	b	632	4/4	0.96	0.11	70,74,76,84	0
24	CLA	B	616	65/65	0.96	0.09	21,29,80,89	0
30	UNL	t	102	8/-	0.96	0.16	50,57,68,71	0
24	CLA	A	409	65/65	0.96	0.09	23,31,98,103	0
24	CLA	d	406	65/65	0.96	0.09	31,38,92,94	0
25	PHO	A	408	64/64	0.96	0.09	21,27,35,41	0
26	BCR	A	410	40/40	0.96	0.08	24,30,37,38	0
34	DMS	c	530	4/4	0.96	0.27	73,76,80,83	0
26	BCR	B	619	40/40	0.96	0.07	21,30,37,39	0
34	DMS	c	533	4/4	0.96	0.15	96,97,102,104	0
24	CLA	C	505	65/65	0.96	0.07	29,36,44,51	0
37	DGD	c	520	62/66	0.96	0.08	31,40,68,76	0
24	CLA	C	506	65/65	0.96	0.08	26,32,71,77	0
24	CLA	a	413	65/65	0.96	0.10	25,32,90,93	0
24	CLA	B	611	65/65	0.96	0.10	26,33,40,44	0
38	LHG	D	412	45/49	0.96	0.09	29,34,56,60	0
34	DMS	C	536	4/4	0.96	0.24	58,60,65,69	0
30	UNL	D	415	15/-	0.96	0.11	41,45,53,59	0
24	CLA	b	606	65/65	0.96	0.08	27,35,45,51	0
24	CLA	C	510	65/65	0.96	0.08	25,33,94,111	0
24	CLA	b	613	65/65	0.96	0.10	30,36,43,60	0
24	CLA	C	503	65/65	0.97	0.07	29,37,51,59	0
24	CLA	c	511	65/65	0.97	0.09	30,40,59,62	0
24	CLA	C	504	65/65	0.97	0.07	26,33,45,50	0
24	CLA	B	606	65/65	0.97	0.08	19,27,64,70	0
24	CLA	B	607	65/65	0.97	0.08	22,28,39,45	0
24	CLA	b	607	65/65	0.97	0.07	25,33,42,44	0
24	CLA	b	608	65/65	0.97	0.08	21,28,64,70	0
24	CLA	b	609	65/65	0.97	0.08	22,29,40,45	0
25	PHO	a	412	64/64	0.97	0.08	20,26,30,31	0
34	DMS	c	532	4/4	0.97	0.14	43,53,53,63	0
24	CLA	C	507	65/65	0.97	0.07	27,36,61,65	0
24	CLA	b	611	65/65	0.97	0.07	21,27,39,44	0
34	DMS	c	535	4/4	0.97	0.18	63,65,67,68	0
24	CLA	A	405	65/65	0.97	0.08	18,24,33,45	0
24	CLA	C	509	65/65	0.97	0.07	31,38,57,61	0
24	CLA	b	615	65/65	0.97	0.07	21,27,47,51	0
37	DGD	C	518	62/66	0.97	0.08	26,32,87,94	0
31	GOL	A	418	6/6	0.97	0.17	56,62,66,76	0

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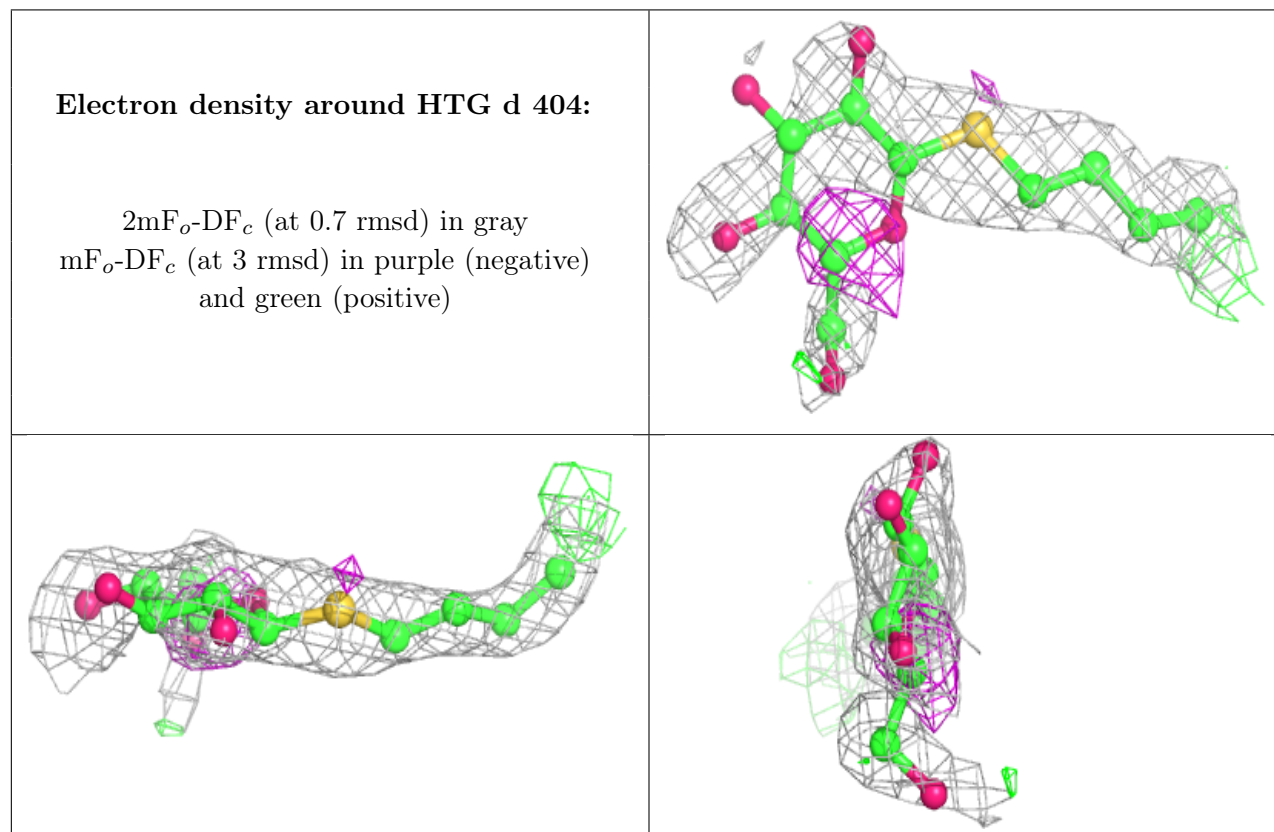
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CLA	B	609	65/65	0.97	0.07	17,27,40,50	0
24	CLA	A	406	65/65	0.97	0.08	20,26,97,101	0
24	CLA	C	512	65/65	0.97	0.07	28,34,45,51	0
33	BCT	A	423[B]	4/4	0.97	0.10	23,31,38,38	4
33	BCT	D	404[A]	4/4	0.97	0.10	27,35,36,41	4
33	BCT	a	408[A]	4/4	0.97	0.10	25,35,36,36	4
24	CLA	B	612	65/65	0.97	0.08	24,29,45,53	0
24	CLA	B	604	65/65	0.97	0.07	24,32,37,44	0
24	CLA	B	617	65/65	0.97	0.07	25,32,53,59	0
34	DMS	B	633	4/4	0.97	0.11	58,61,66,68	0
38	LHG	L	101	49/49	0.97	0.10	27,34,55,59	0
24	CLA	D	405	65/65	0.97	0.08	17,23,44,47	0
24	CLA	c	507	65/65	0.97	0.07	29,35,61,73	0
38	LHG	d	410	49/49	0.97	0.10	26,32,59,68	0
38	LHG	d	411	46/49	0.97	0.10	32,36,67,74	0
38	LHG	l	102	49/49	0.97	0.09	25,35,56,64	0
39	HEM	e	102	43/43	0.97	0.09	39,50,74,89	0
24	CLA	B	605	65/65	0.97	0.07	24,30,39,42	0
24	CLA	a	409	65/65	0.97	0.09	21,26,40,51	0
41	MG	j	101	1/1	0.97	0.14	43,43,43,43	0
42	HEC	v	201	43/43	0.97	0.09	35,40,45,49	0
24	CLA	B	615	65/65	0.98	0.06	19,26,56,63	0
25	PHO	A	407	64/64	0.98	0.07	19,25,28,31	0
24	CLA	b	617	65/65	0.98	0.07	21,27,64,71	0
24	CLA	D	401	65/65	0.98	0.06	16,22,30,43	0
26	BCR	b	621	40/40	0.98	0.06	22,31,40,42	0
38	LHG	D	411	49/49	0.98	0.10	22,32,48,55	0
25	PHO	d	401	64/64	0.98	0.09	24,31,37,40	0
24	CLA	B	610	65/65	0.98	0.07	23,30,38,45	0
24	CLA	b	612	65/65	0.98	0.06	25,31,42,48	0
24	CLA	B	613	65/65	0.98	0.07	18,26,43,50	0
35	CA	O	301	1/1	0.98	0.04	58,58,58,58	0
35	CA	b	604	1/1	0.98	0.15	52,52,52,52	0
35	CA	c	502	1/1	0.98	0.06	49,49,49,49	0
35	CA	o	302	1/1	0.98	0.06	57,57,57,57	0
39	HEM	F	102	43/43	0.98	0.08	37,44,54,60	0
24	CLA	c	504	65/65	0.98	0.07	27,36,48,55	0
34	DMS	d	417	4/4	0.98	0.11	69,74,75,78	0
24	CLA	B	614	65/65	0.98	0.07	21,28,35,41	0
24	CLA	a	410	65/65	0.98	0.06	20,25,38,45	0
42	HEC	V	201	43/43	0.98	0.07	27,31,36,40	0
24	CLA	d	405	65/65	0.98	0.08	20,26,48,57	0

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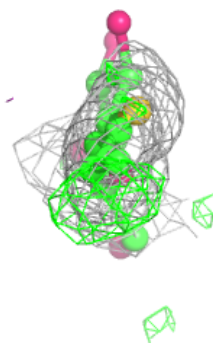
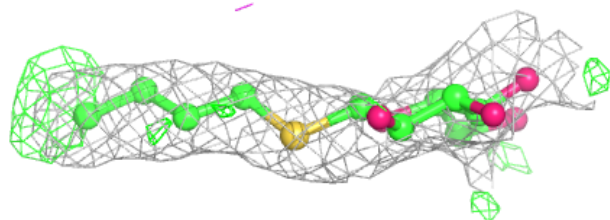
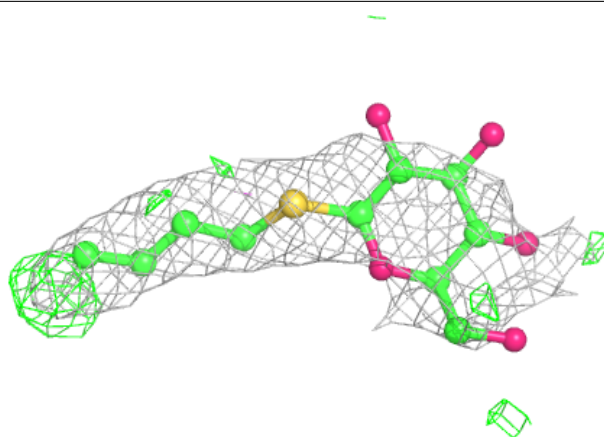
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	DMS	B	632	4/4	0.99	0.05	25,28,32,37	0
34	DMS	O	305	4/4	0.99	0.05	29,35,37,44	0
34	DMS	C	534	4/4	0.99	0.06	45,45,48,51	0
41	MG	J	101	1/1	0.99	0.02	34,34,34,34	0
34	DMS	a	422	4/4	0.99	0.06	29,35,39,45	0
34	DMS	b	631	4/4	0.99	0.06	29,34,36,40	0
35	CA	B	602	1/1	0.99	0.20	53,53,53,53	0
22	FE2	A	402	1/1	1.00	0.03	30,30,30,30	0
22	FE2	a	405	1/1	1.00	0.04	31,31,31,31	0
23	CL	A	403	1/1	1.00	0.04	27,27,27,27	0
23	CL	A	404	1/1	1.00	0.05	28,28,28,28	0
23	CL	a	406	1/1	1.00	0.03	31,31,31,31	0
23	CL	a	407	1/1	1.00	0.05	33,33,33,33	0
21	OEX	A	401	10/10	1.00	0.04	24,27,29,31	0
21	OEX	a	404	10/10	1.00	0.03	27,30,31,32	0

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

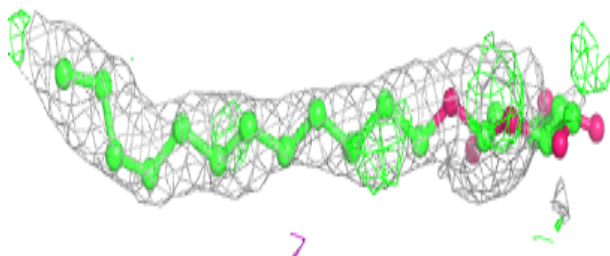
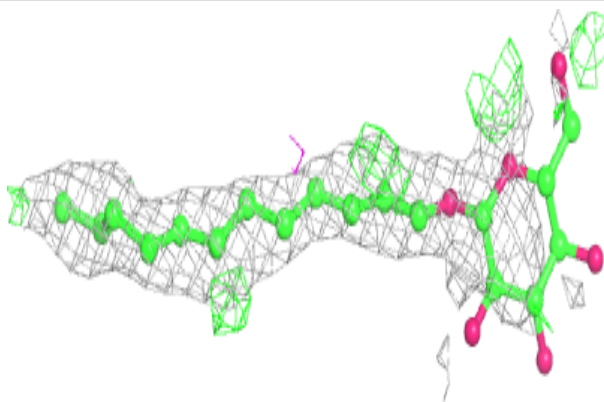


Electron density around HTG H 101:

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

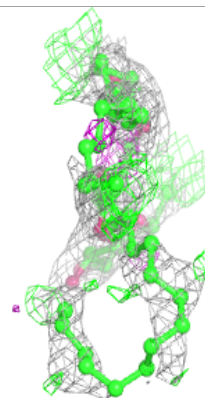
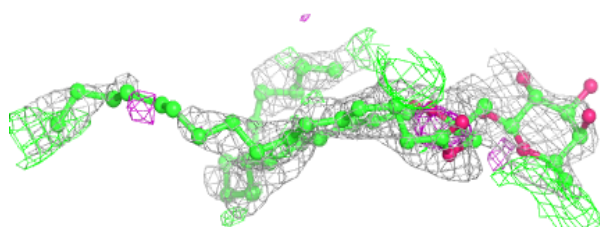
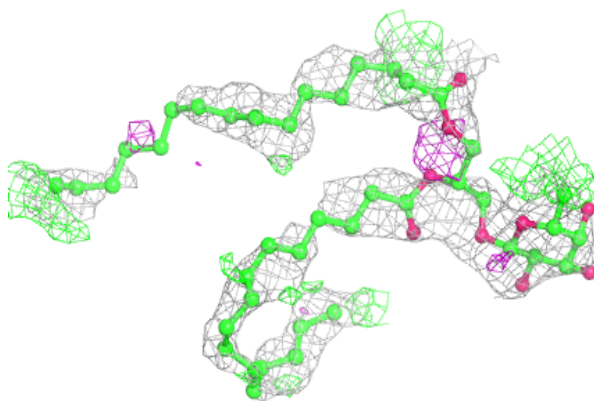
**Electron density around LMT j 102:**

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

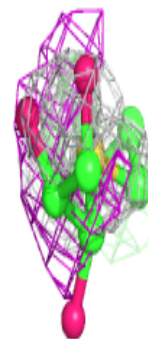
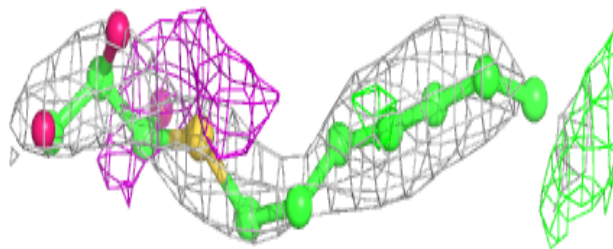
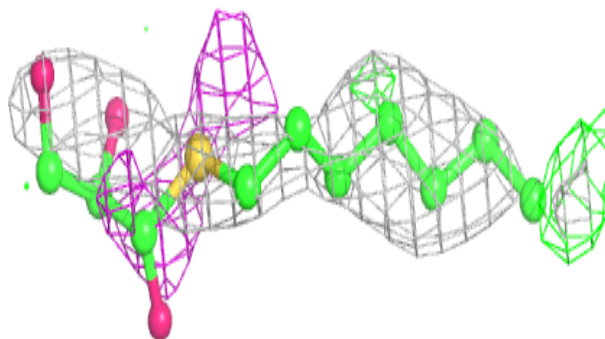


Electron density around DGD d 416:

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

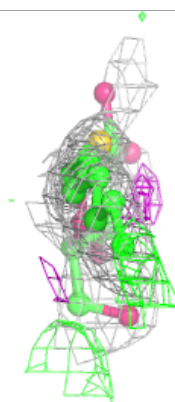
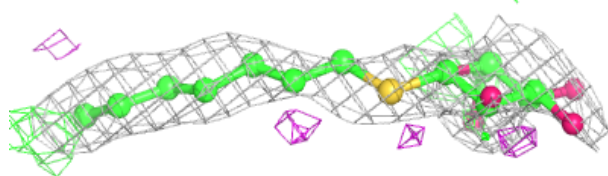
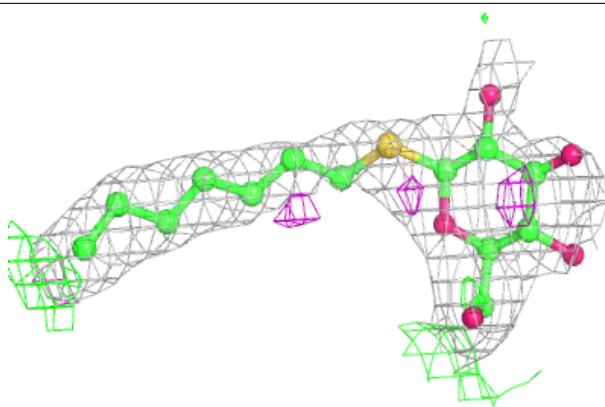
**Electron density around HTG u 201:**

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

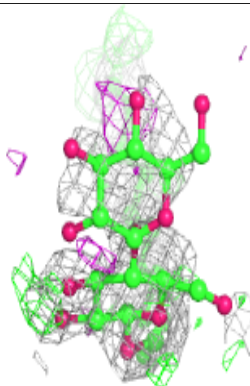
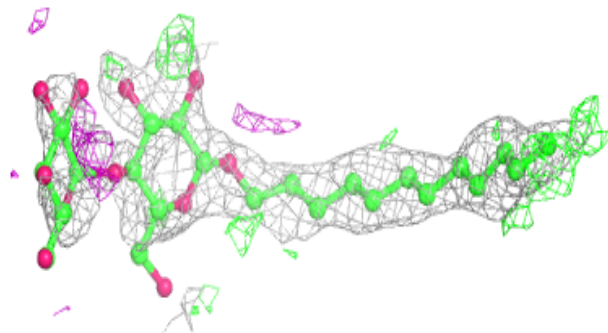
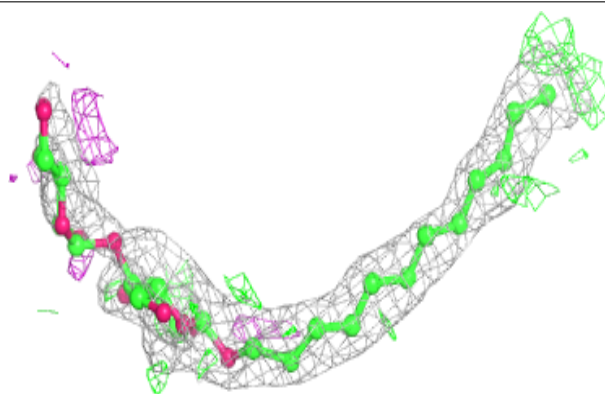


Electron density around HTG B 630:

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

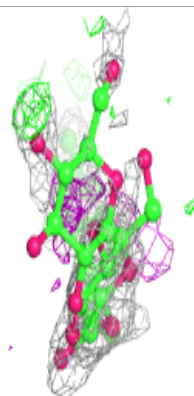
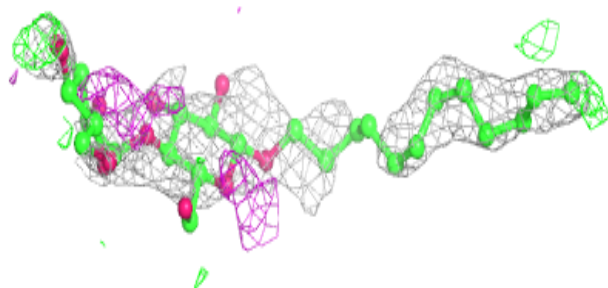
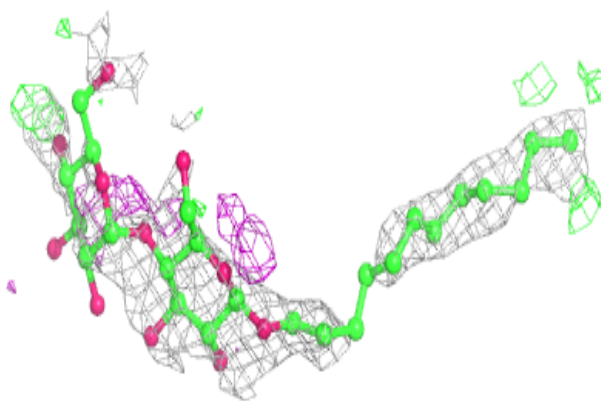
**Electron density around LMT M 101:**

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

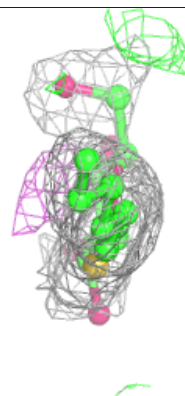
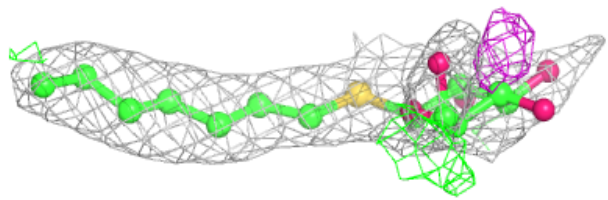
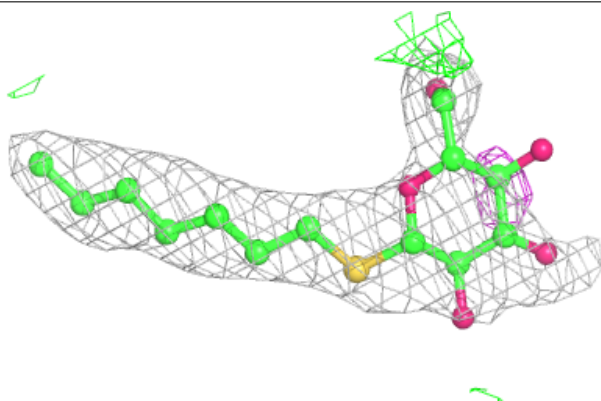


Electron density around LMT F 103:

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

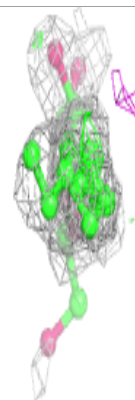
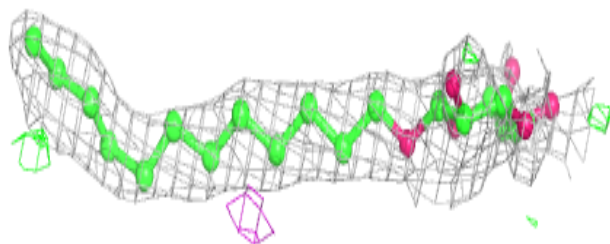
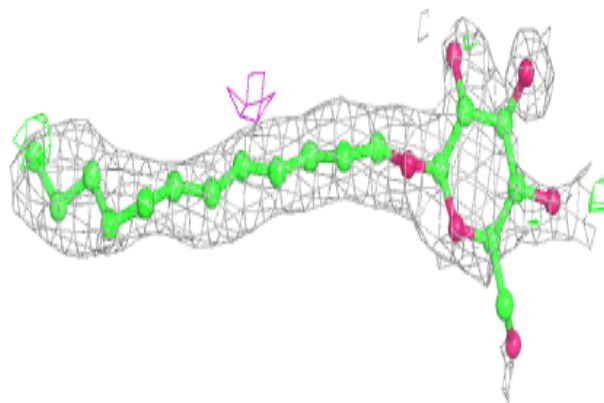
**Electron density around HTG b 603:**

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

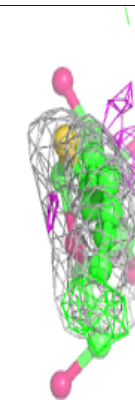
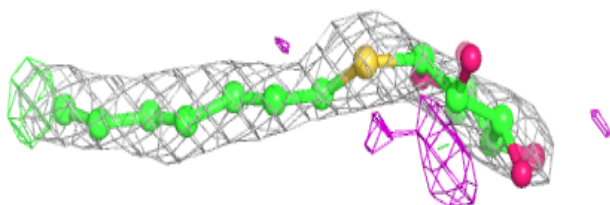
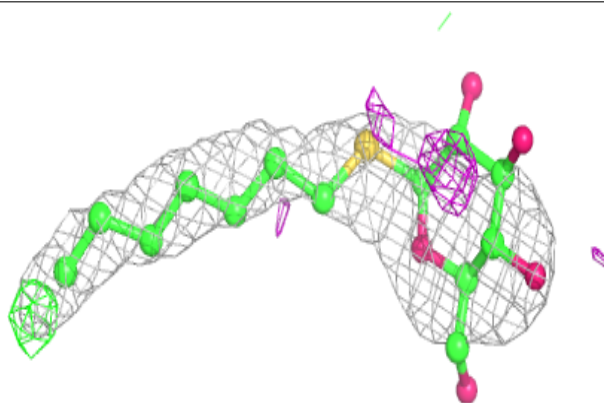


Electron density around LMT J 102:

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

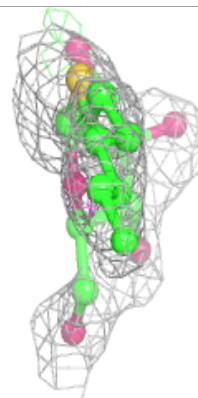
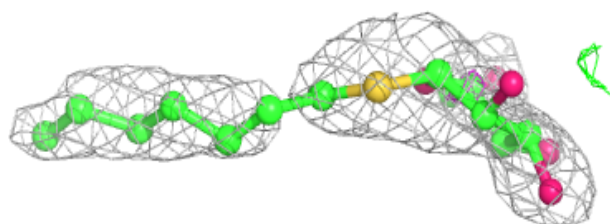
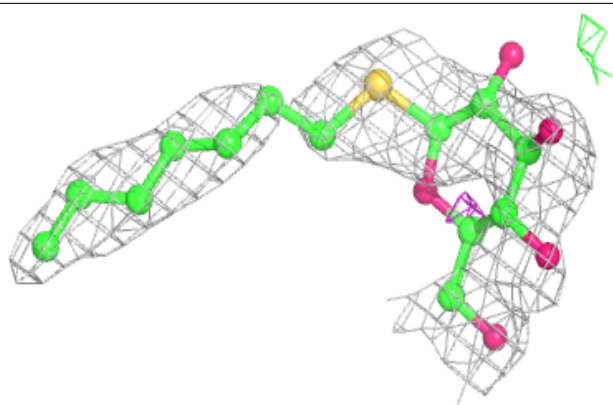
**Electron density around HTG B 626:**

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

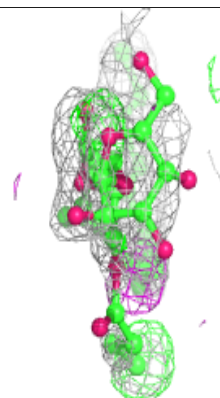
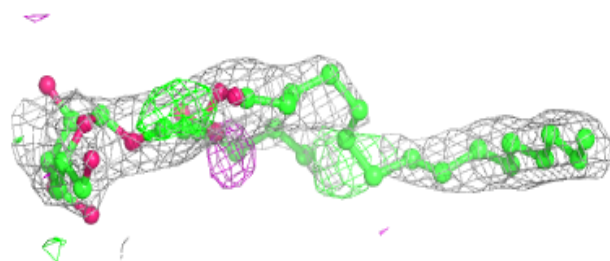
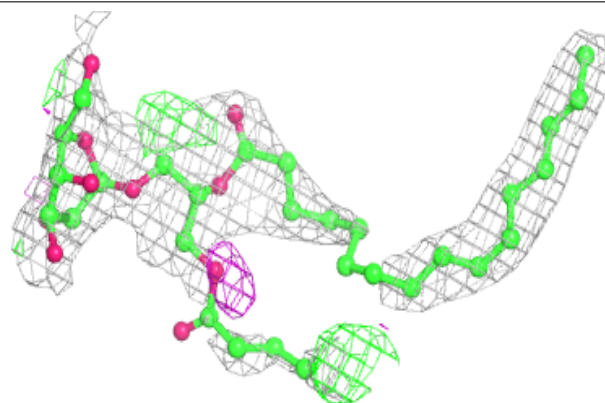


Electron density around HTG b 628:

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

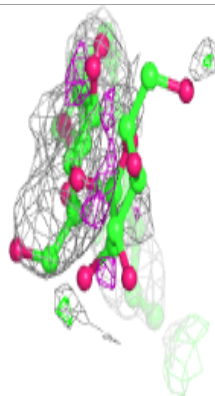
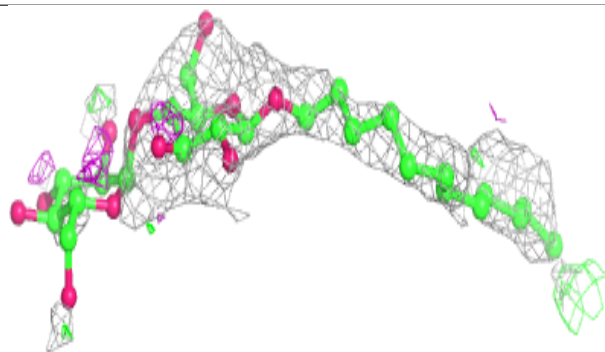
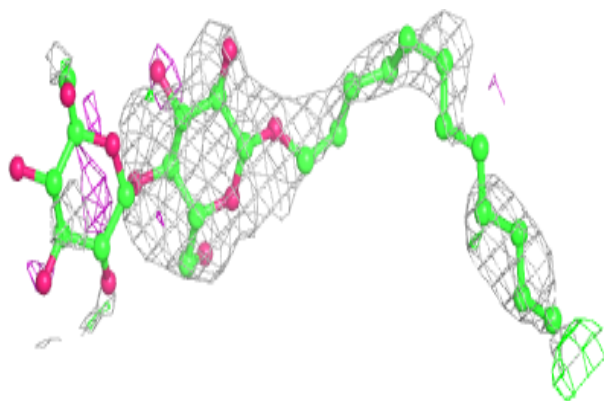
**Electron density around LMG Z 101:**

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

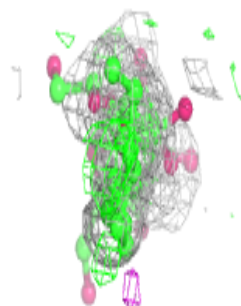
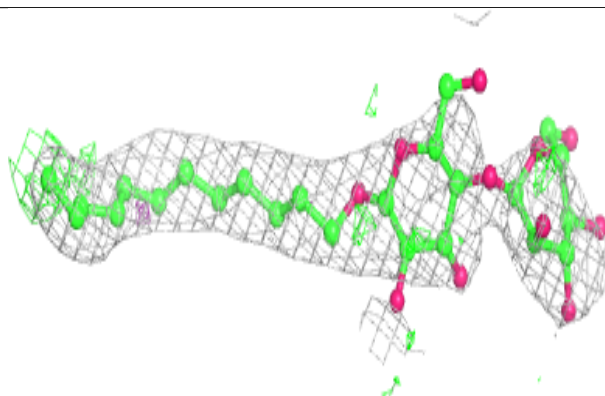
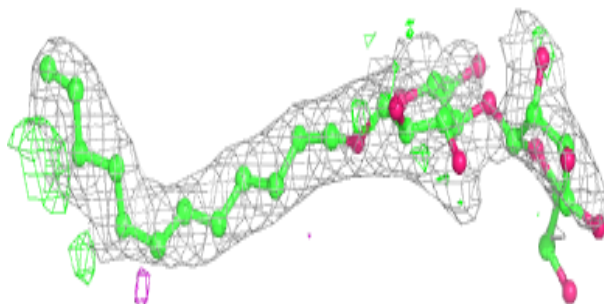


Electron density around LMT a 421:

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

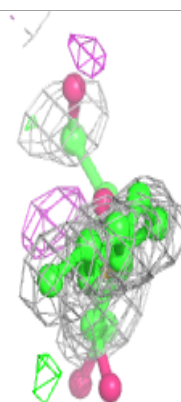
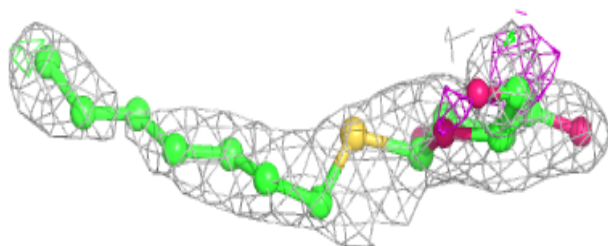
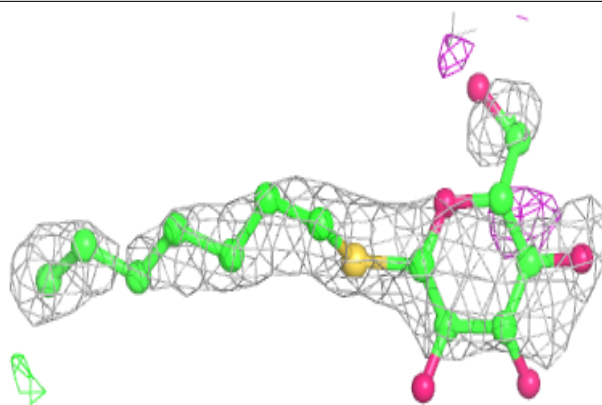
**Electron density around LMT B 638:**

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

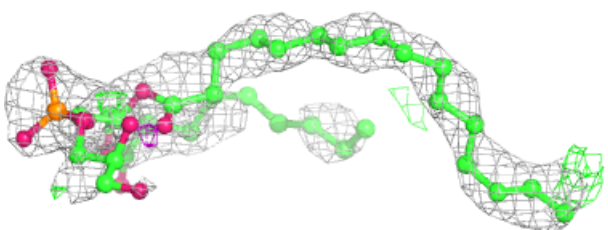
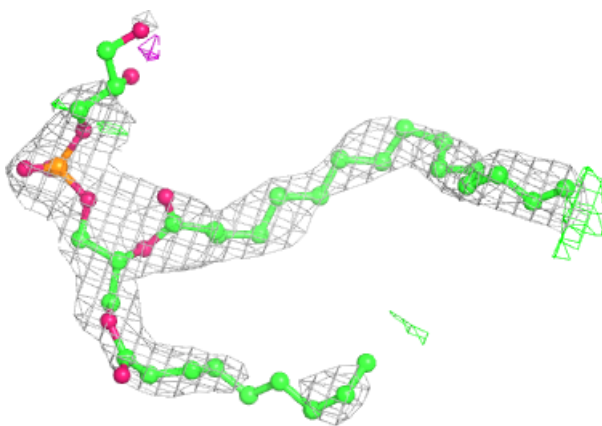


Electron density around HTG c 524:

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

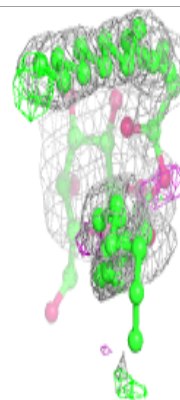
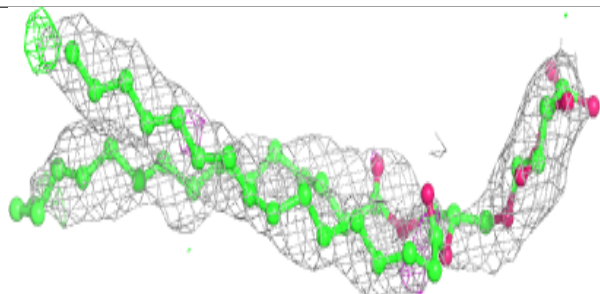
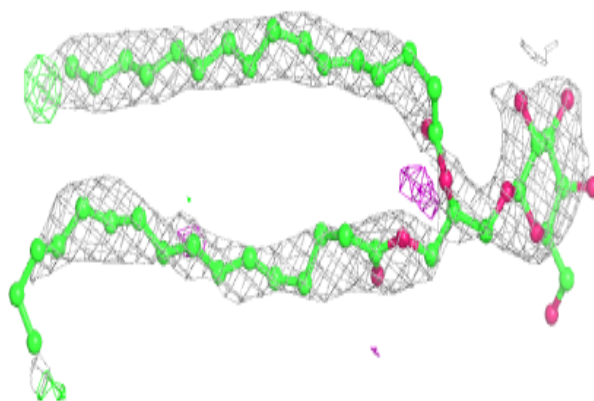
**Electron density around LHG a 416:**

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

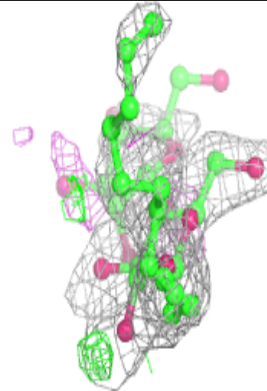
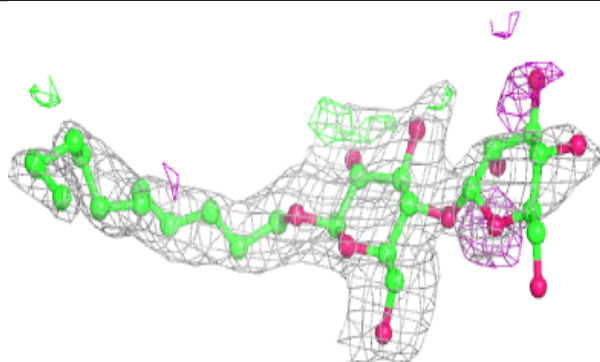
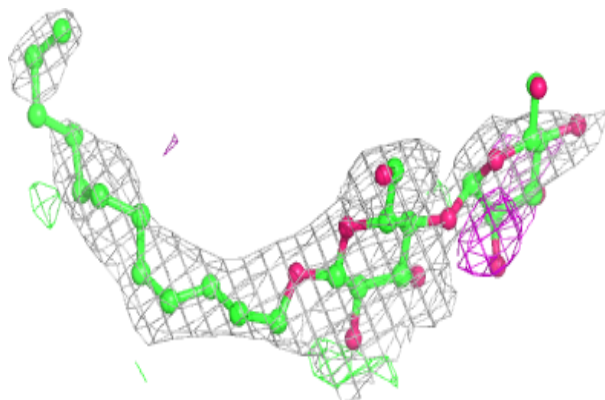


Electron density around LMG c 522:

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

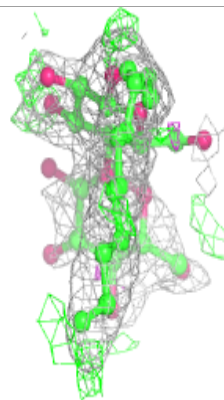
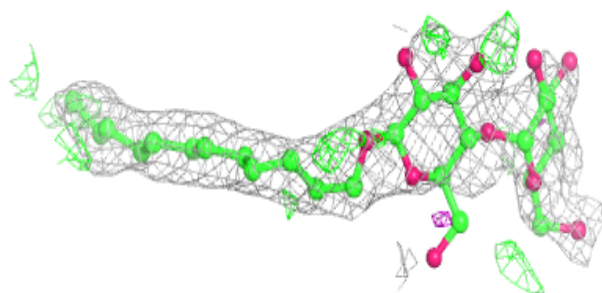
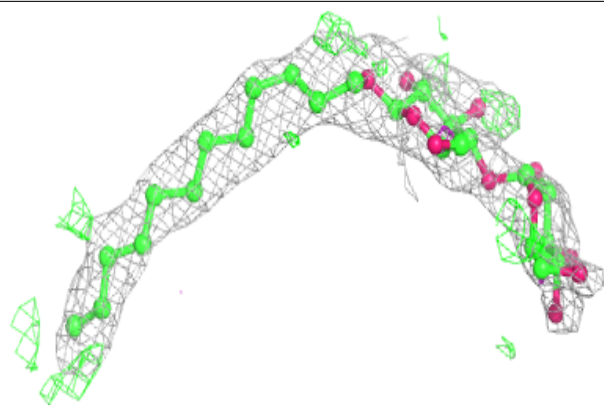
**Electron density around LMT D 409:**

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

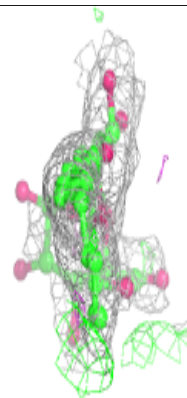
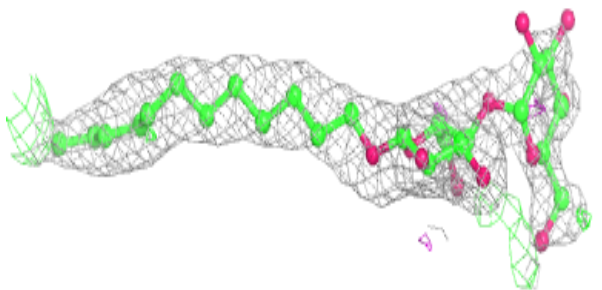
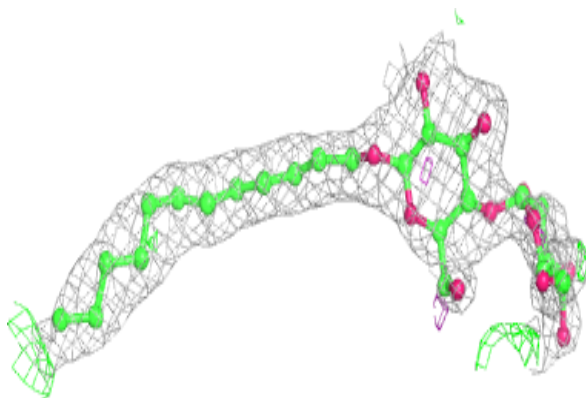


Electron density around LMT m 103:

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

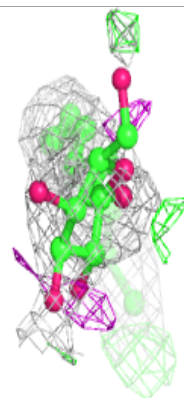
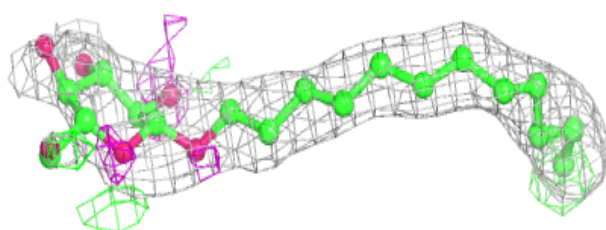
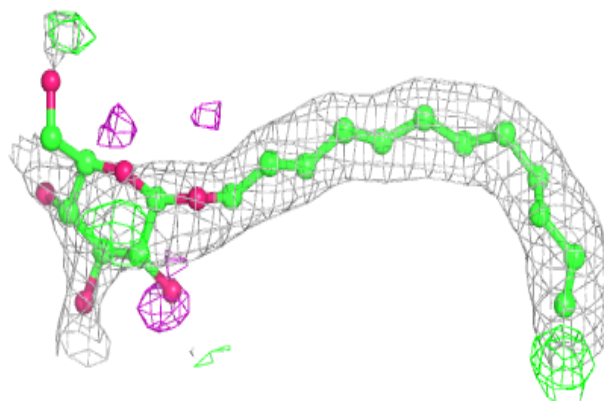
**Electron density around LMT B 624:**

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

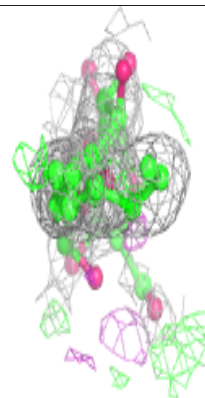
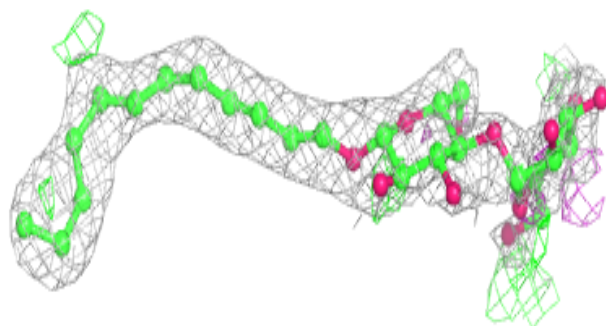
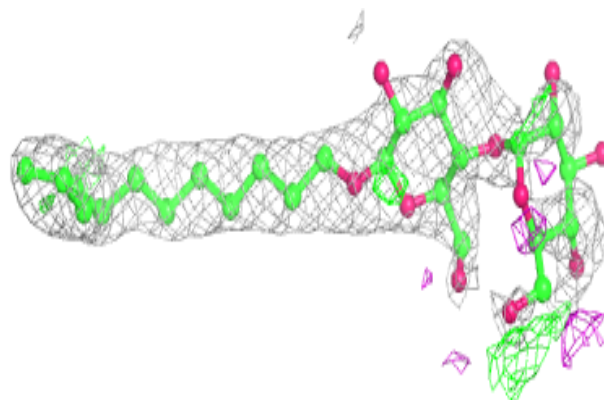


Electron density around LMT b 629:

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

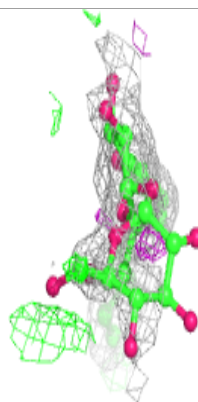
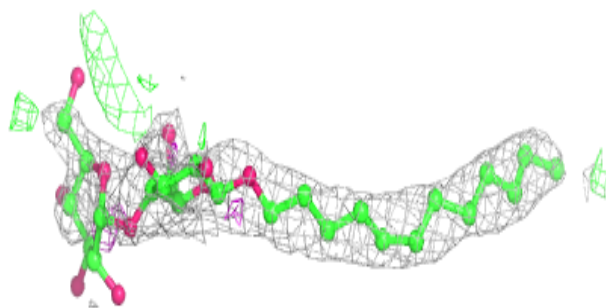
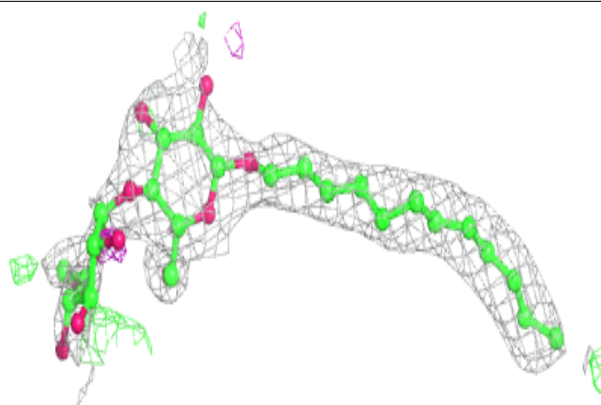
**Electron density around LMT b 626:**

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

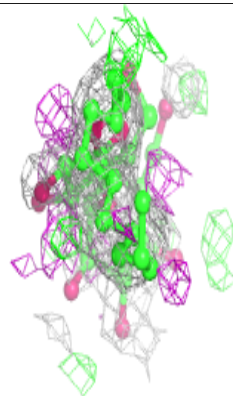
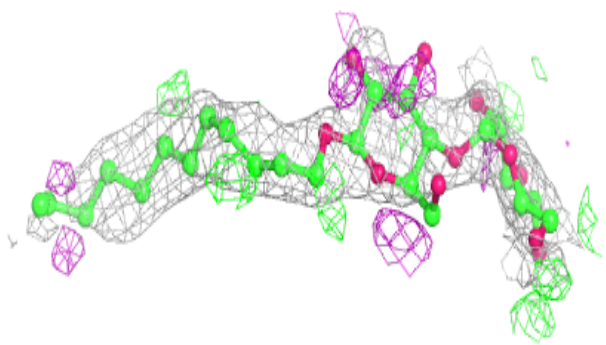
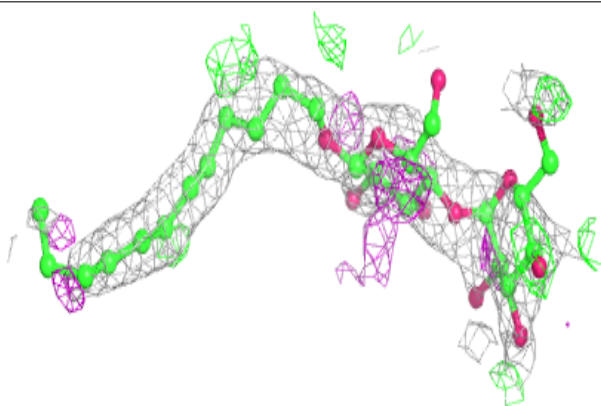


Electron density around LMT b 625:

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

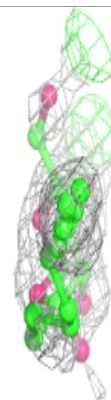
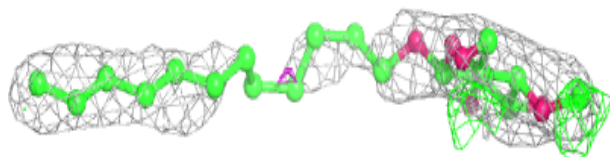
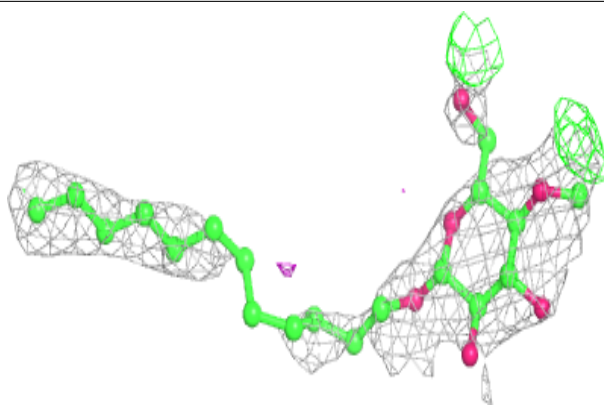
**Electron density around LMT a 402:**

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

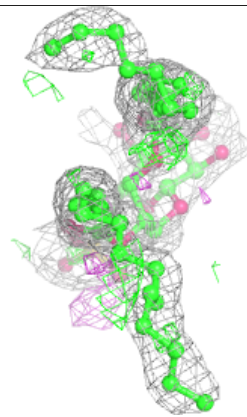
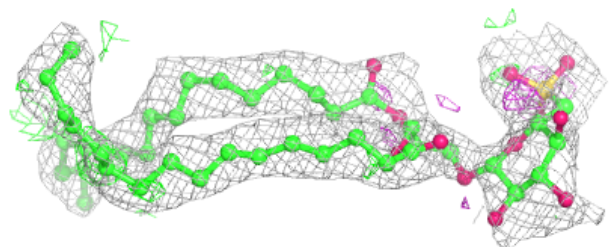
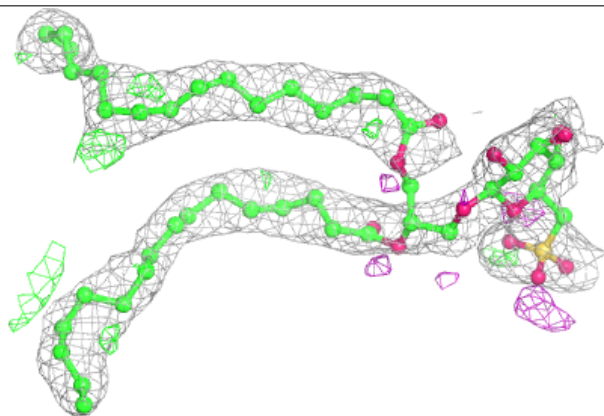


Electron density around LMT f 801:

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

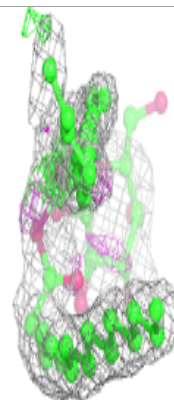
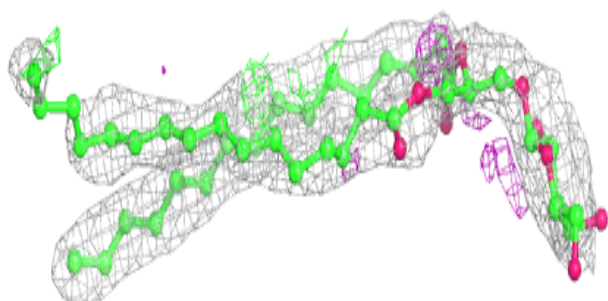
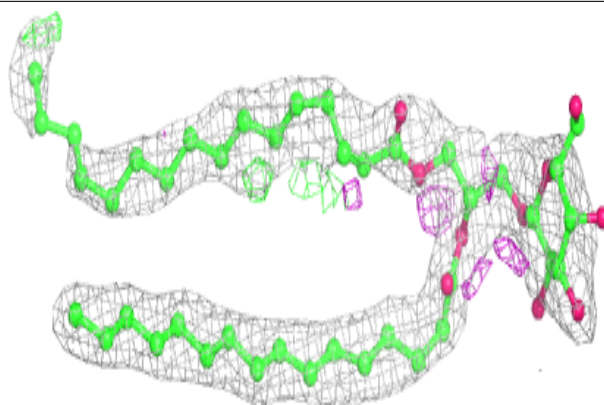
**Electron density around SQD B 622:**

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

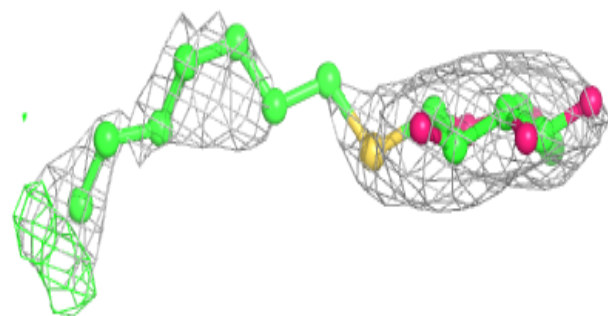
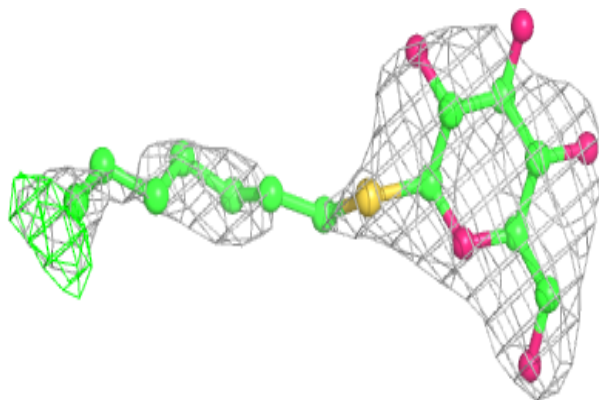


Electron density around LMG C 533:

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

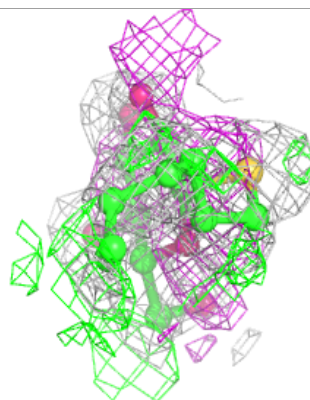
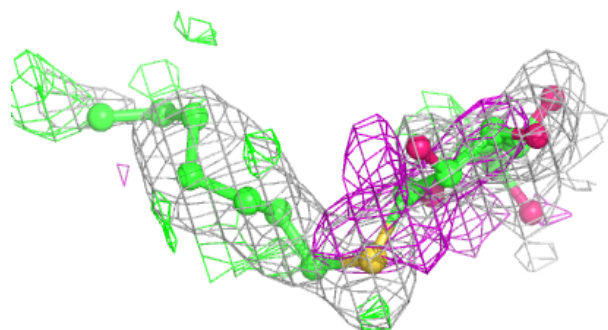
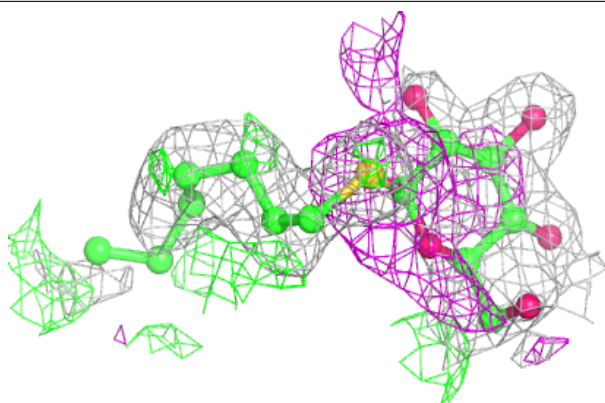
**Electron density around HTG c 523:**

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

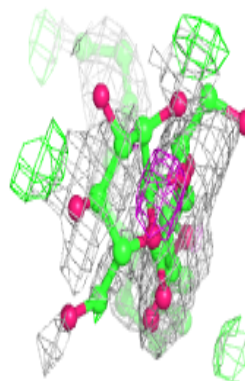
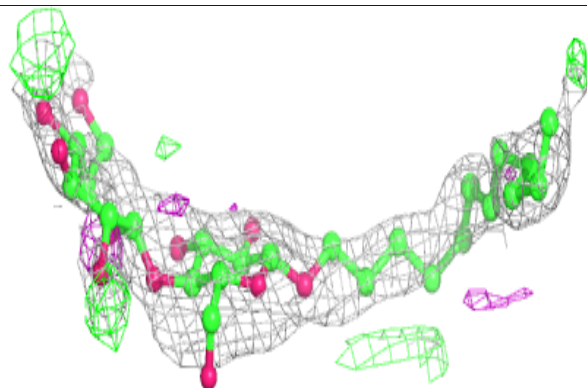
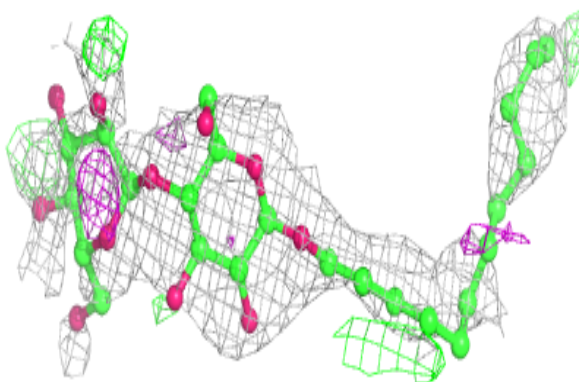


Electron density around HTG B 625:

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

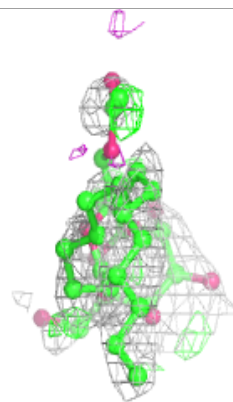
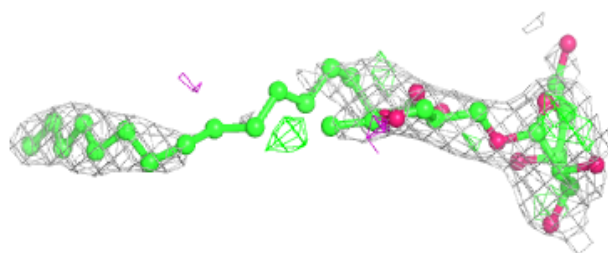
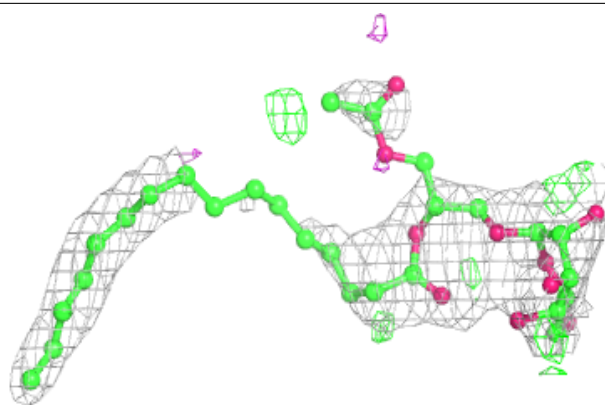
**Electron density around LMT A 422:**

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

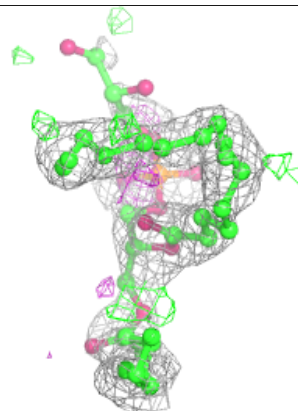
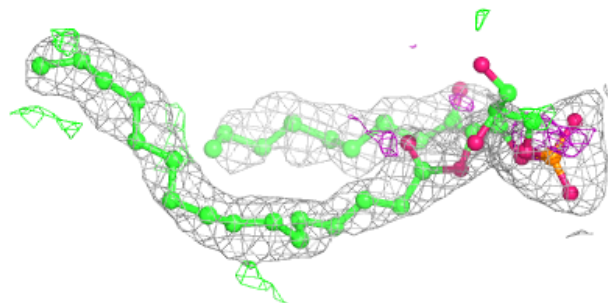
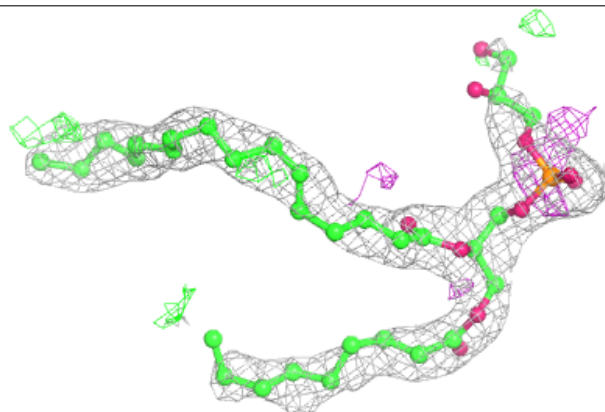


Electron density around LMG z 101:

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

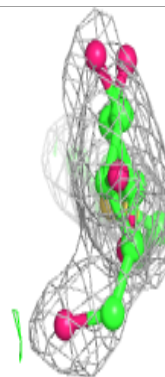
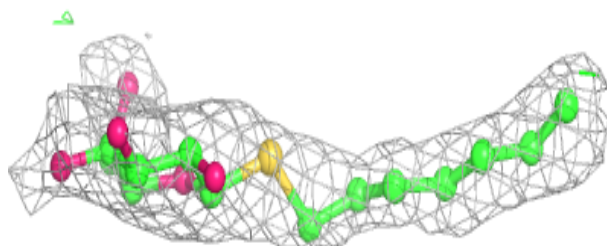
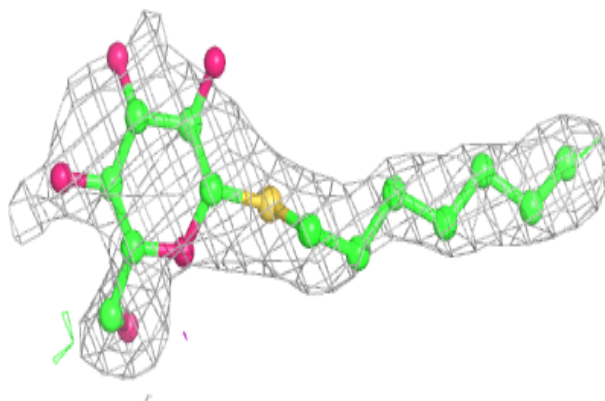
**Electron density around LHG E 101:**

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

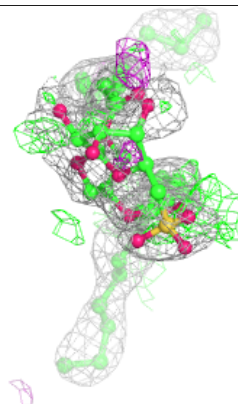
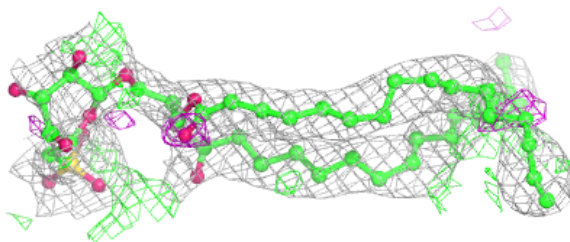
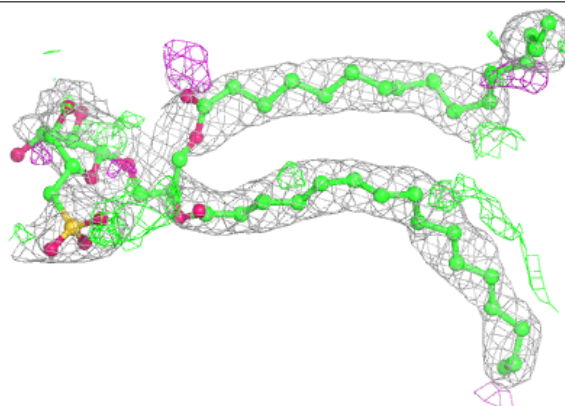


Electron density around HTG C 523:

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

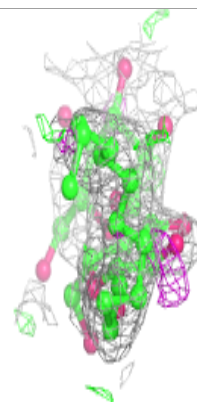
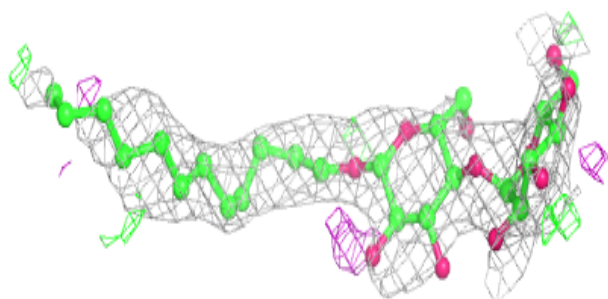
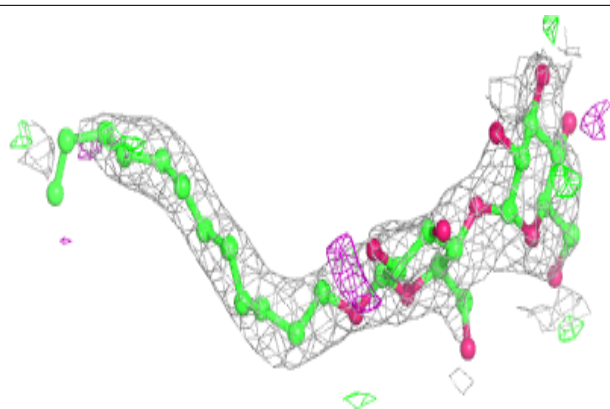
**Electron density around SQD b 601:**

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

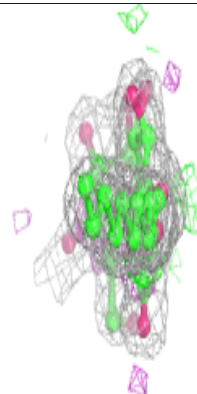
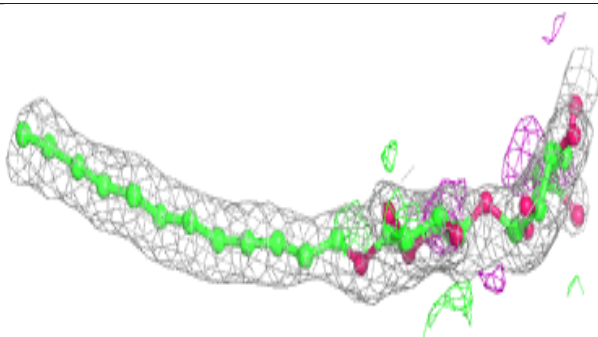
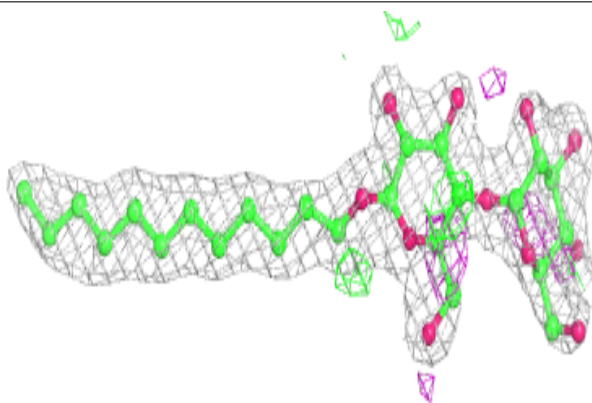


Electron density around LMT D 402:

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

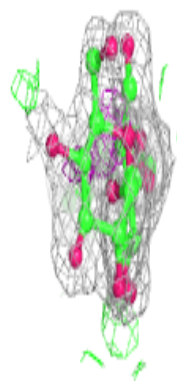
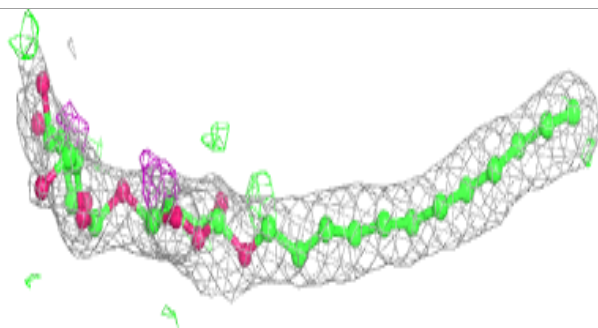
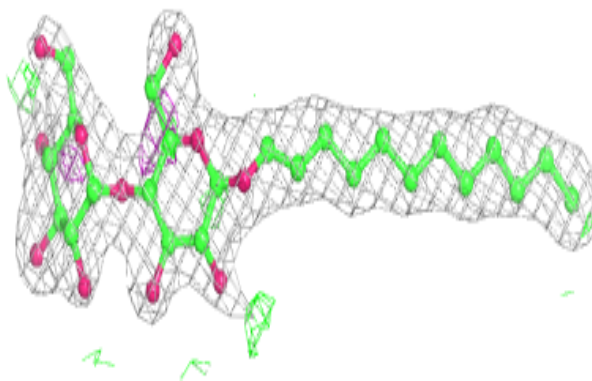
**Electron density around LMT m 102:**

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

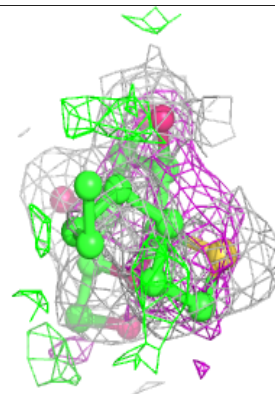
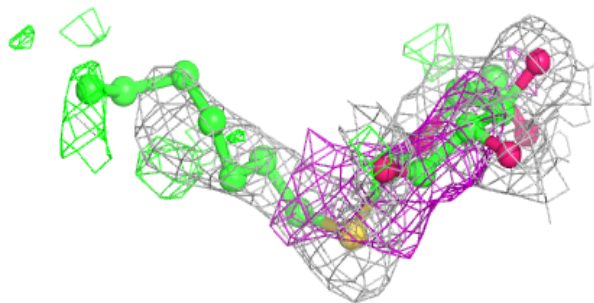
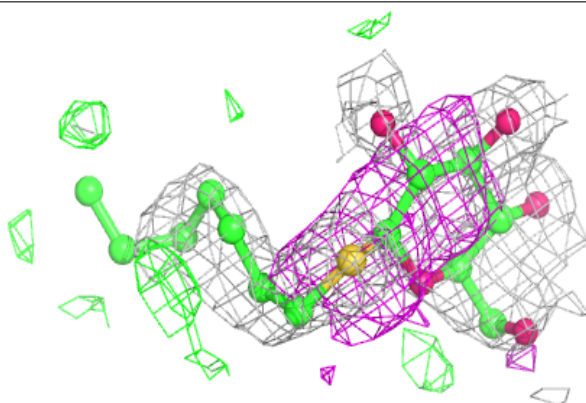


Electron density around LMT M 102:

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

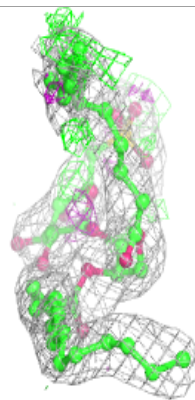
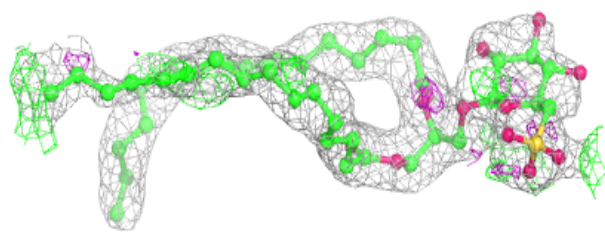
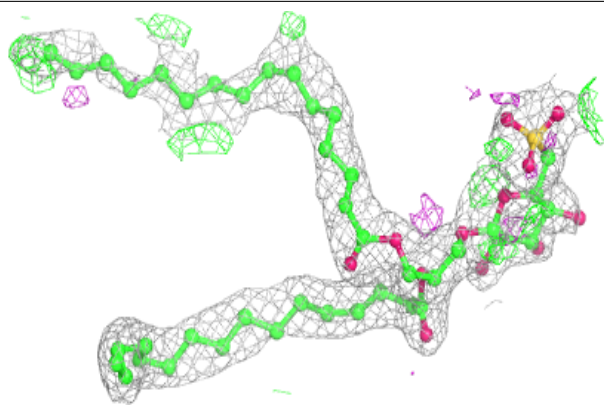
**Electron density around HTG b 627:**

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

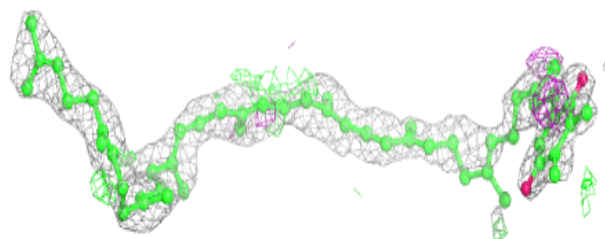
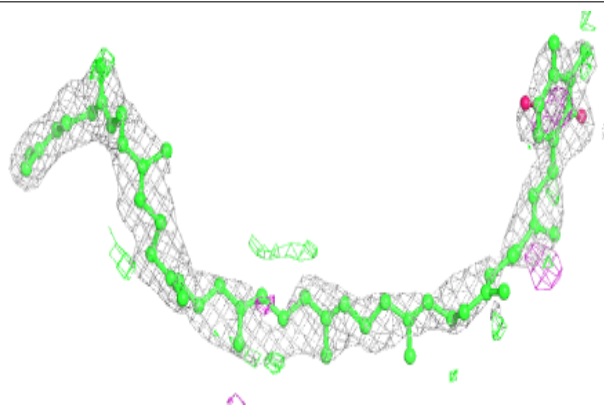


Electron density around SQD a 401:

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

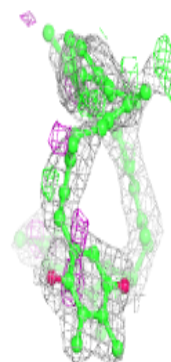
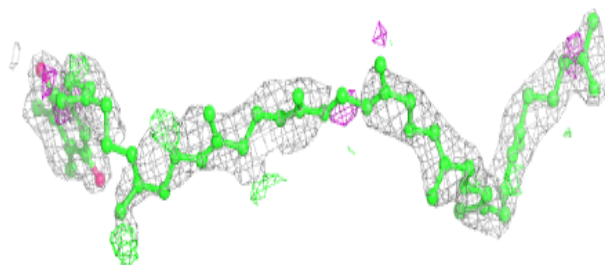
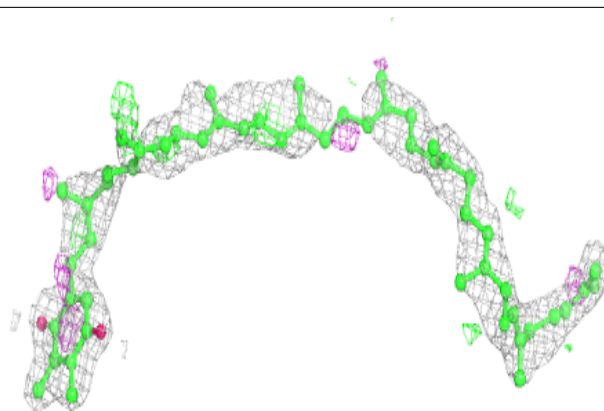
**Electron density around PL9 a 417:**

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

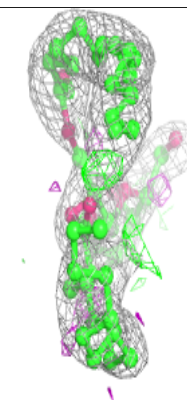
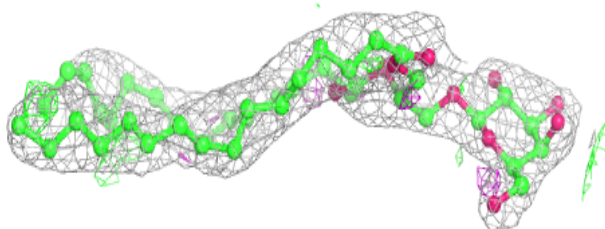
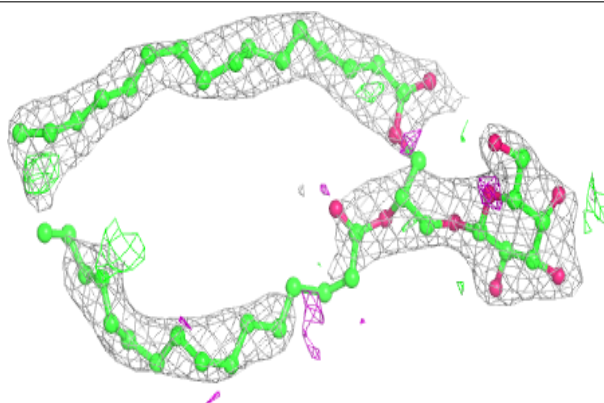


Electron density around PL9 A 413:

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

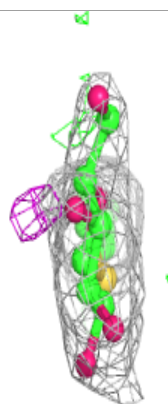
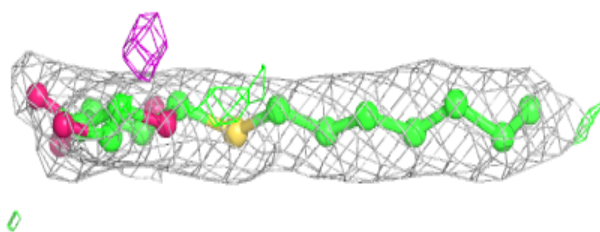
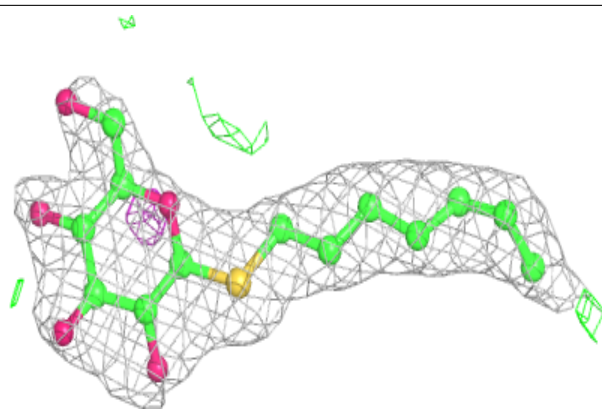
**Electron density around LMG i 101:**

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

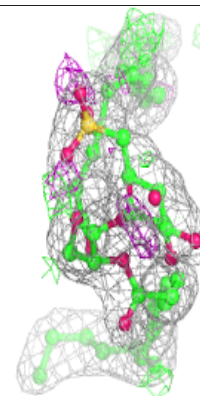
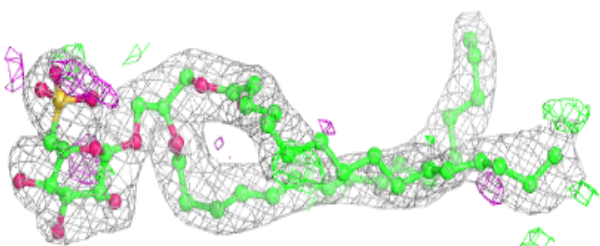
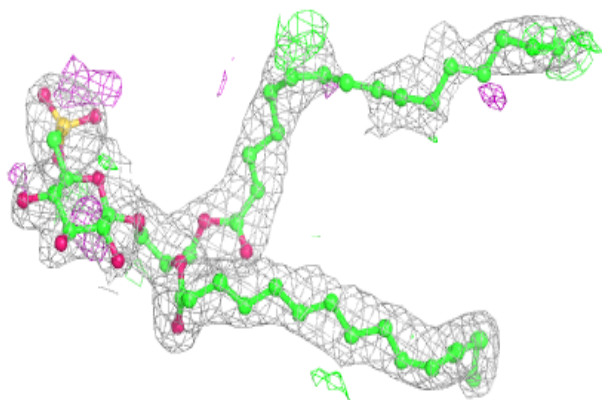


Electron density around HTG b 602:

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

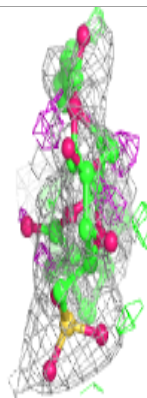
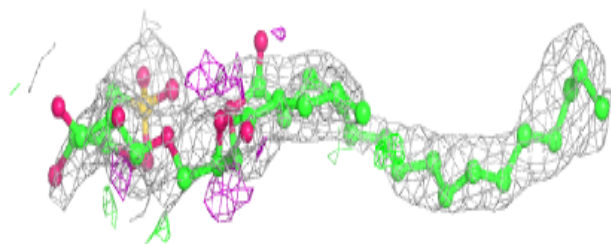
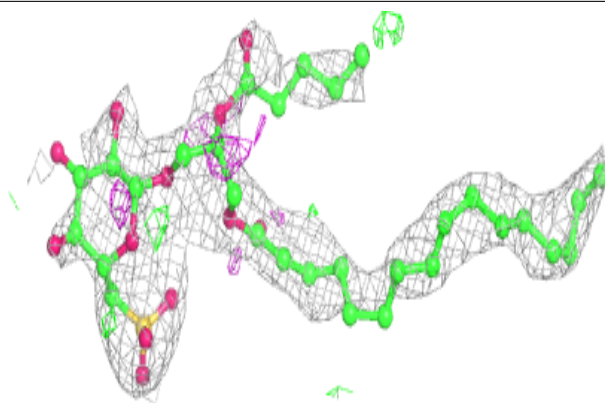
**Electron density around SQD A 415:**

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

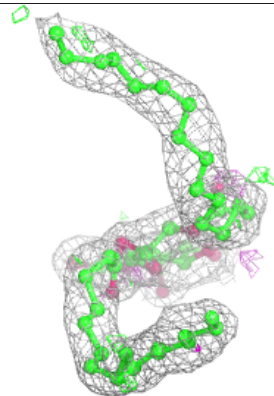
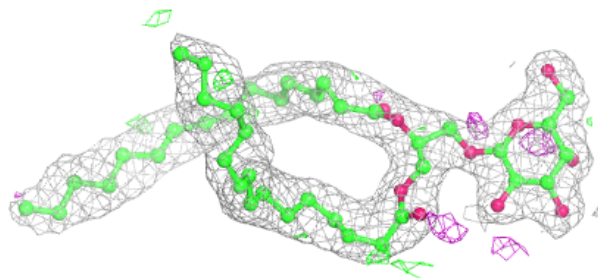
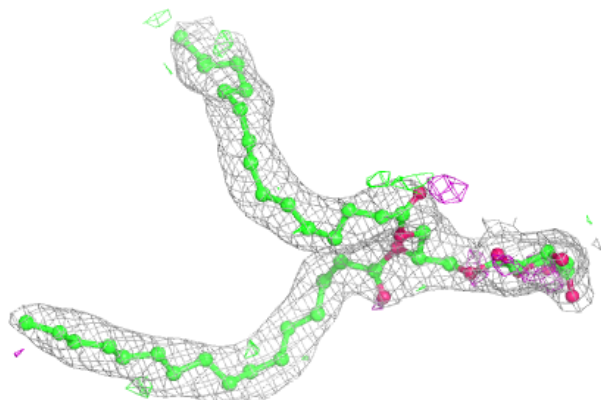


Electron density around SQD f 802:

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

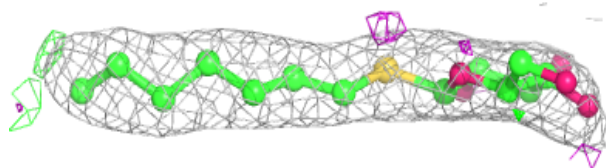
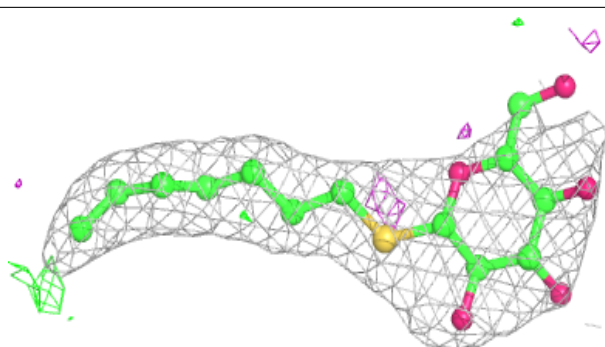
**Electron density around LMG B 623:**

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

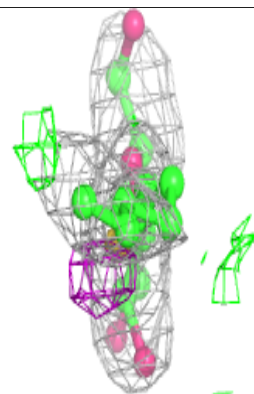
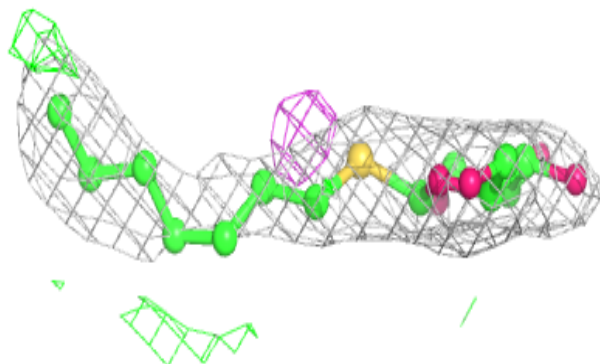
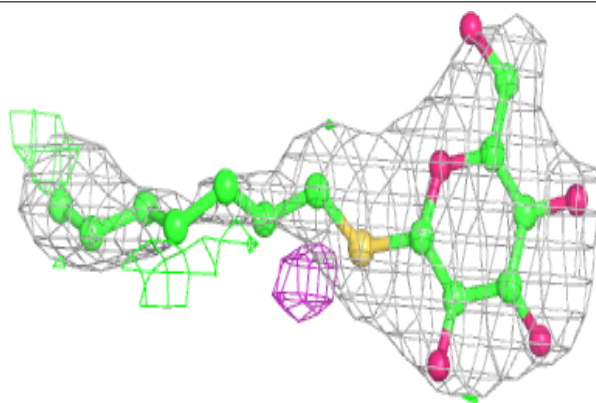


Electron density around HTG B 629:

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

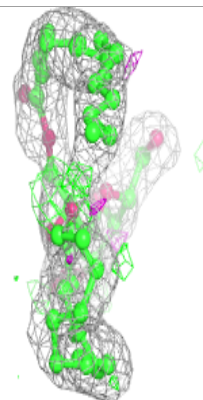
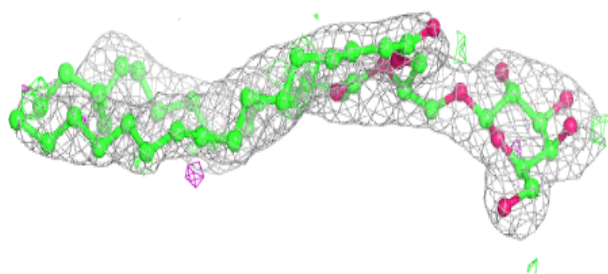
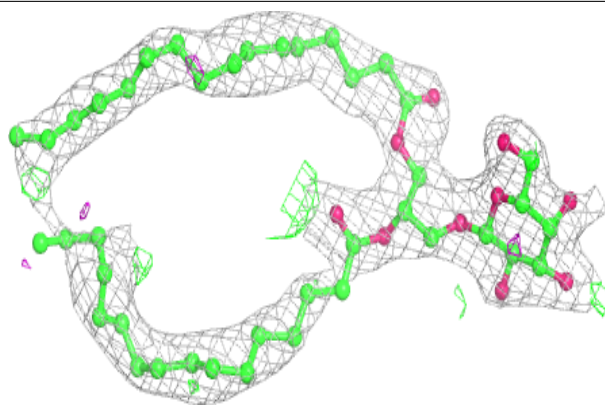
**Electron density around HTG C 522:**

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

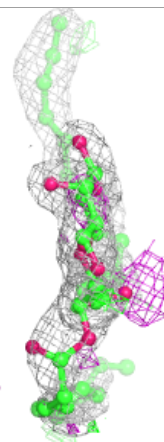
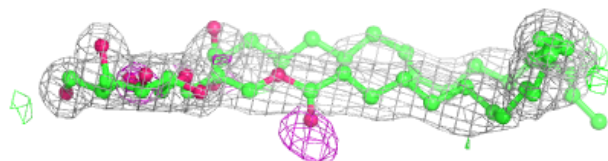
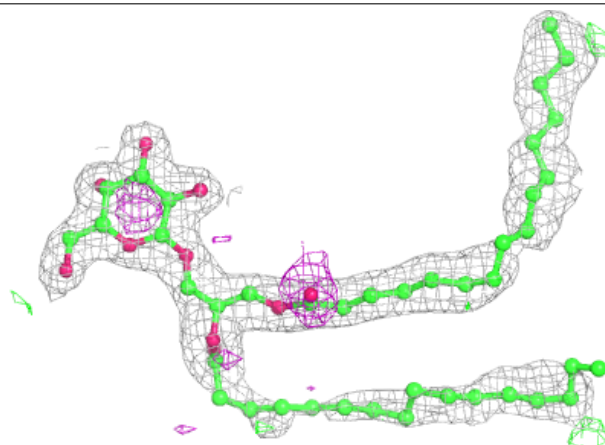


Electron density around LMG A 412:

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

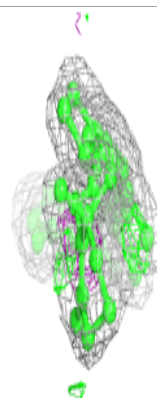
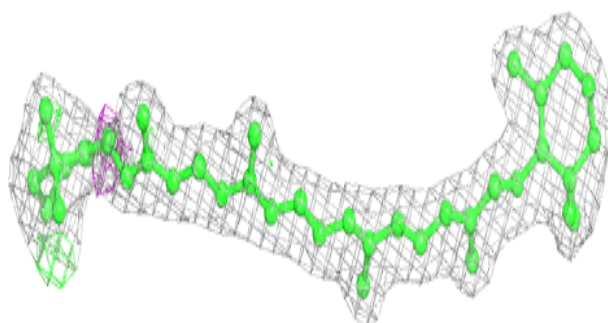
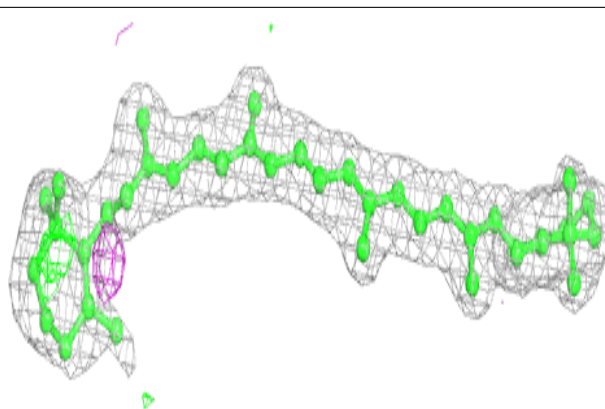
**Electron density around LMG C 521:**

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

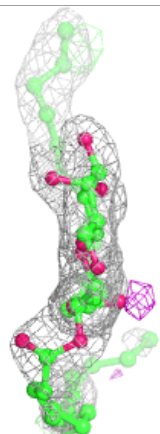
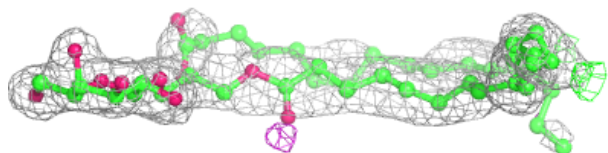
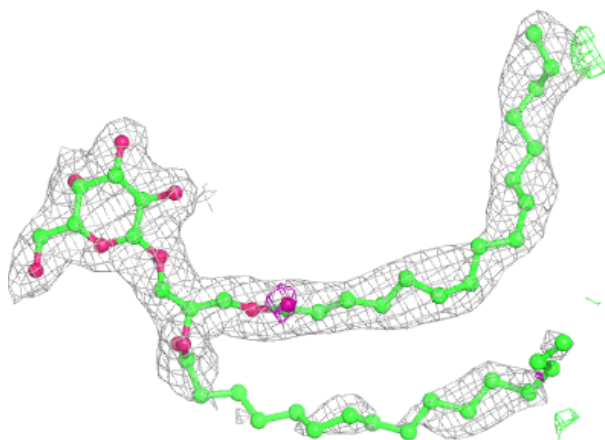


Electron density around BCR d 407:

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

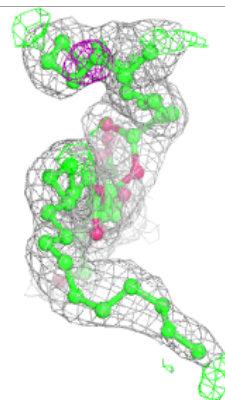
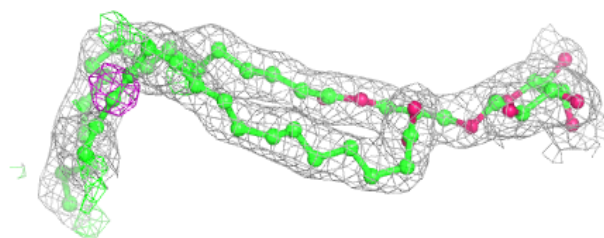
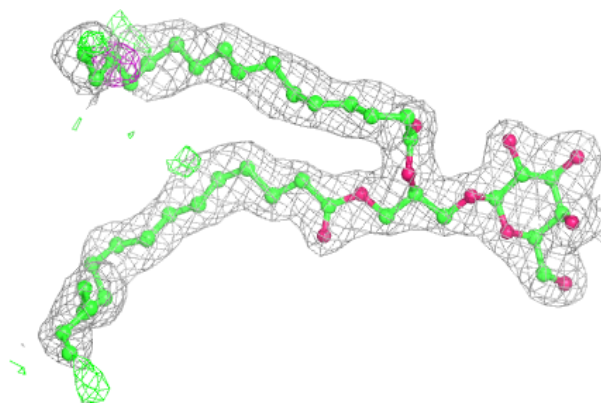
**Electron density around LMG c 521:**

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



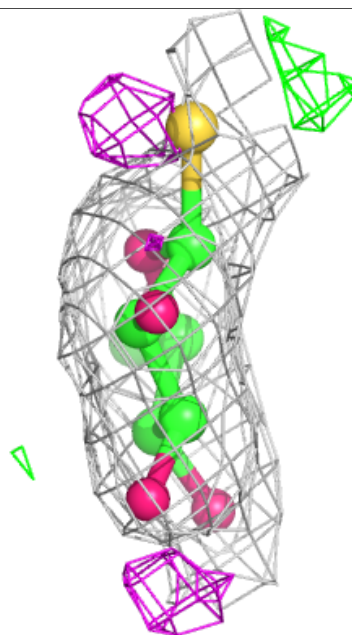
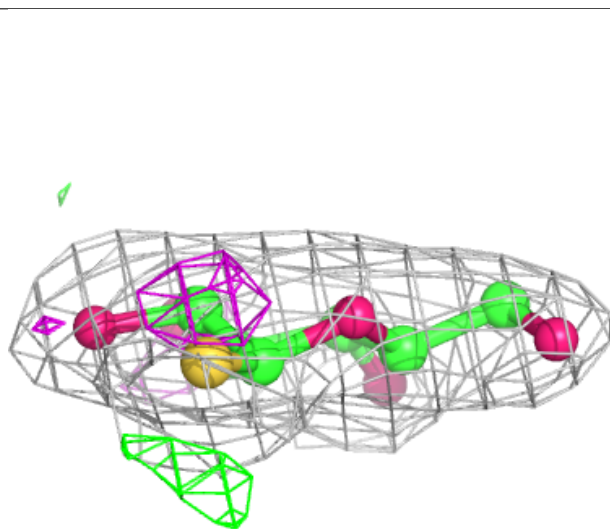
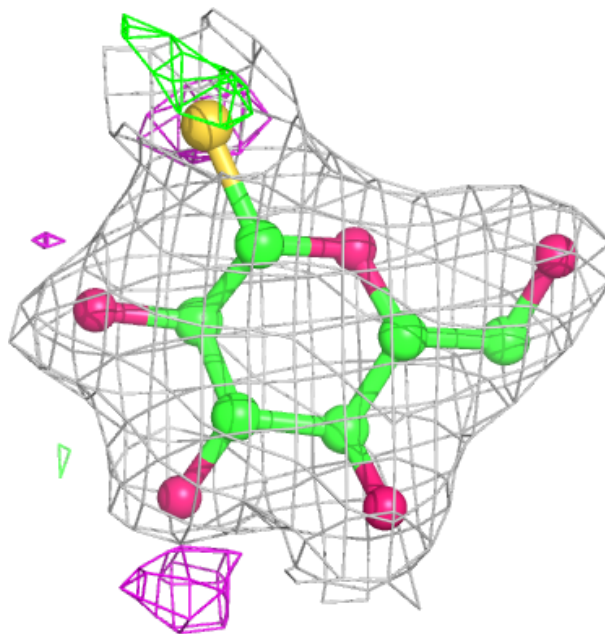
Electron density around LMG d 412:

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



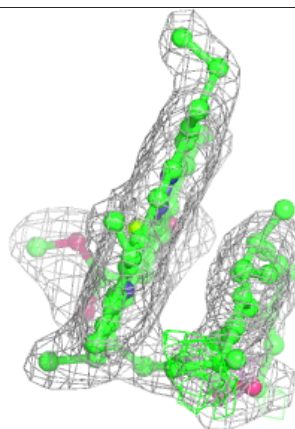
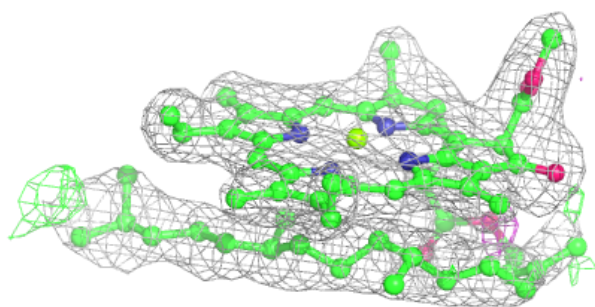
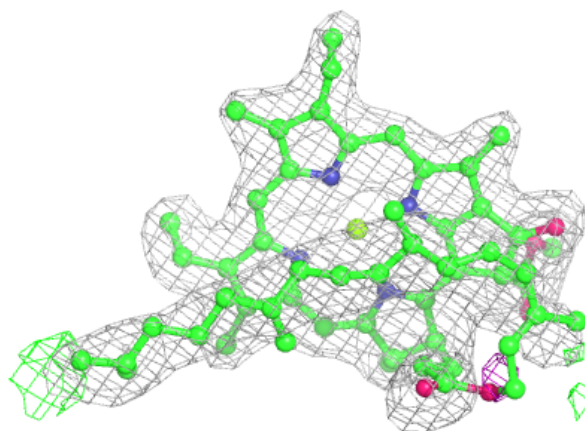
Electron density around HTG V 202:

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

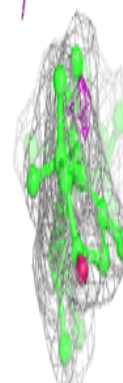
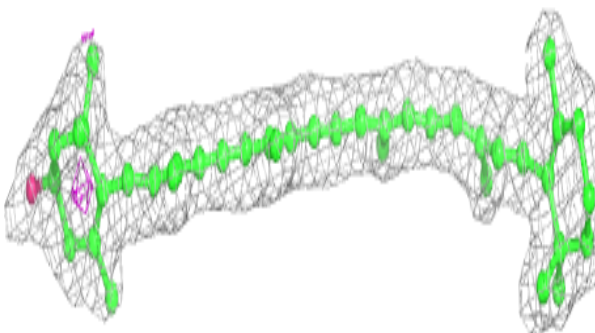
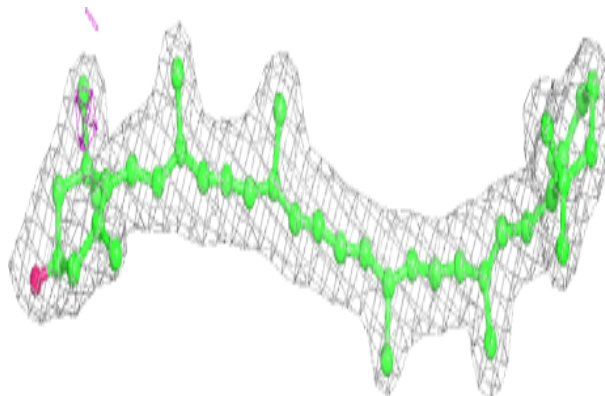


Electron density around CLA B 603:

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

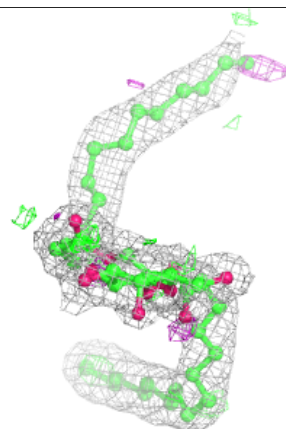
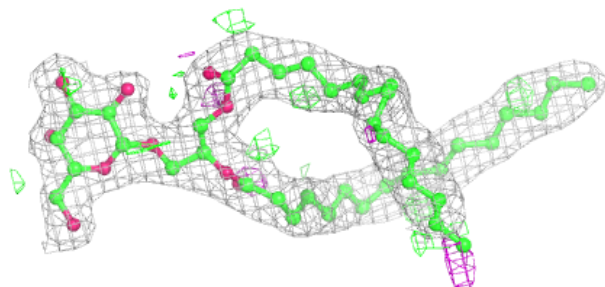
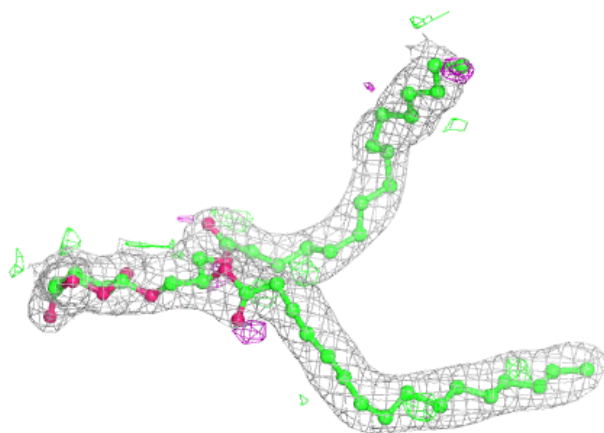
**Electron density around RRX h 101:**

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

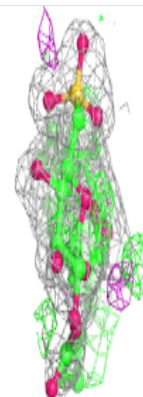
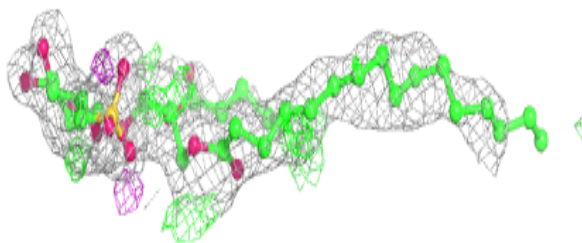
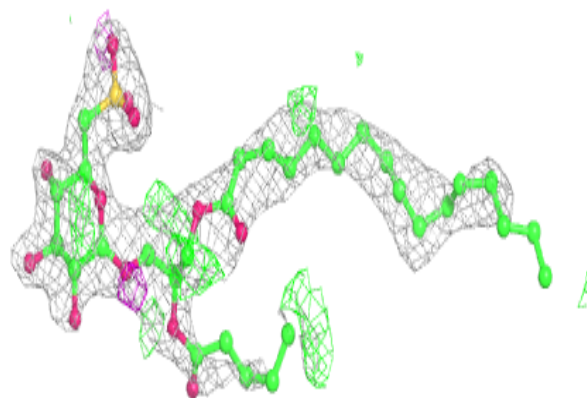


Electron density around LMG b 624:

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

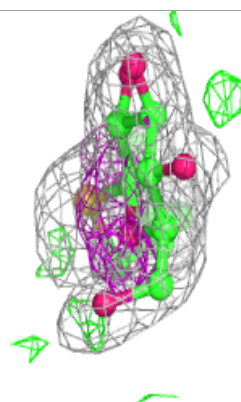
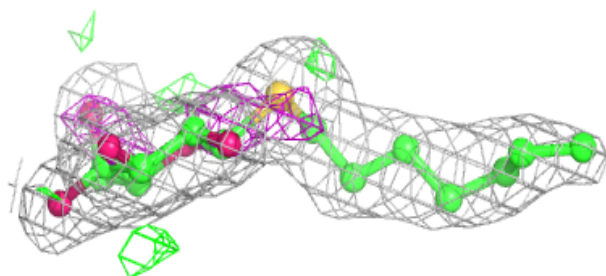
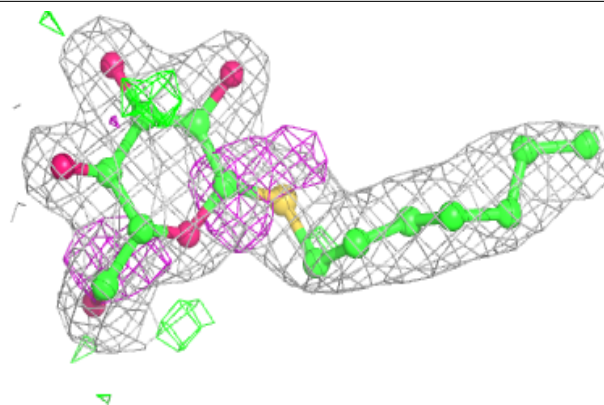
**Electron density around SQD F 101:**

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



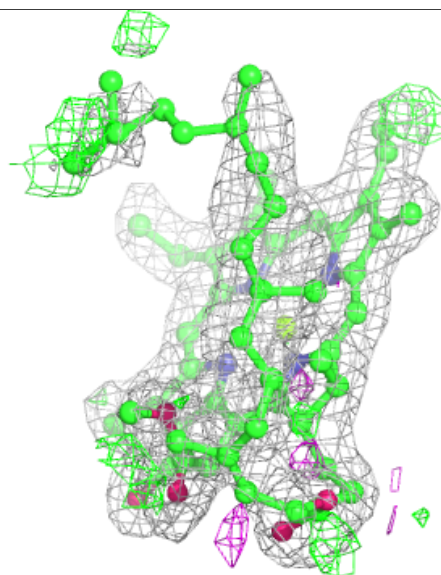
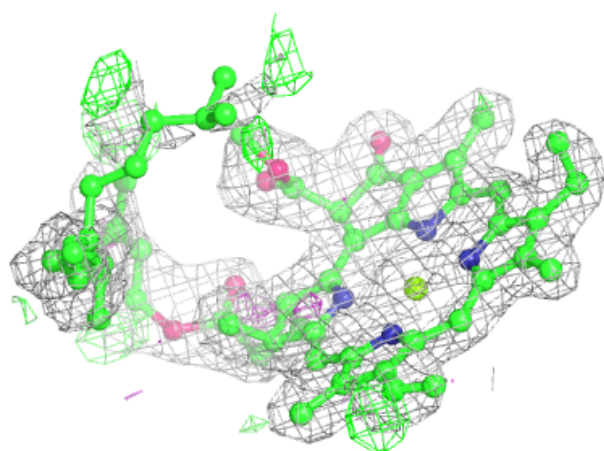
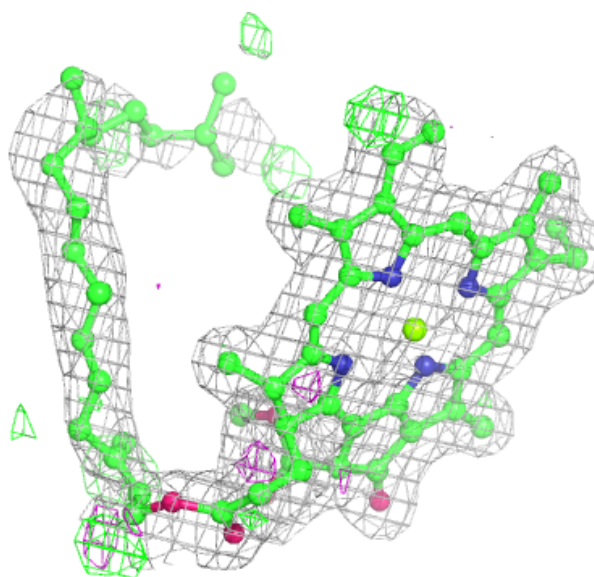
Electron density around HTG O 303:

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



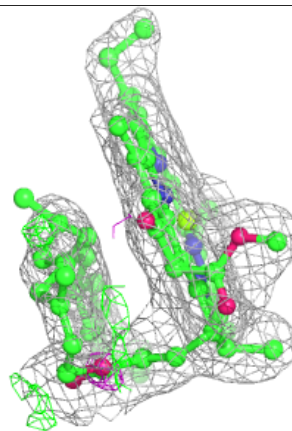
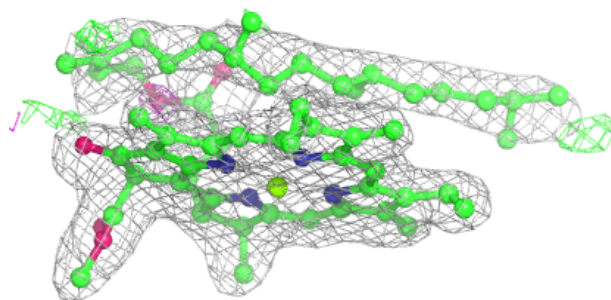
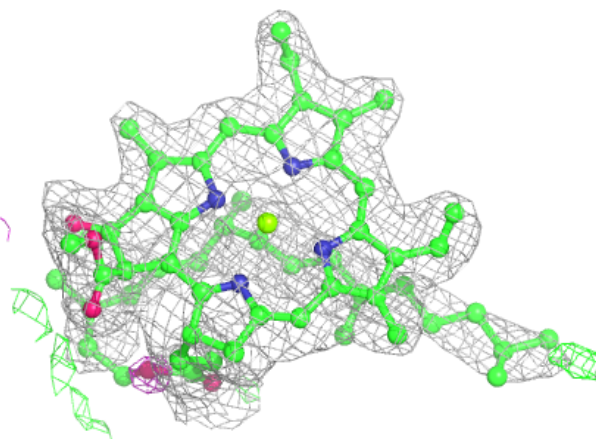
Electron density around CLA b 620:

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



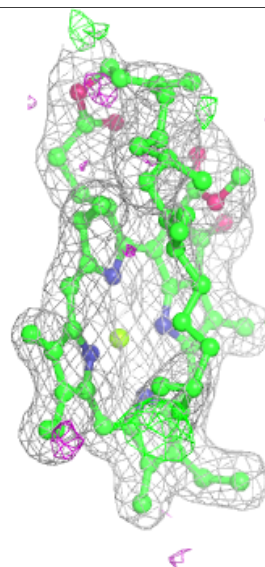
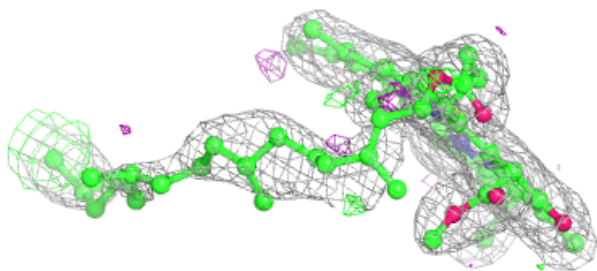
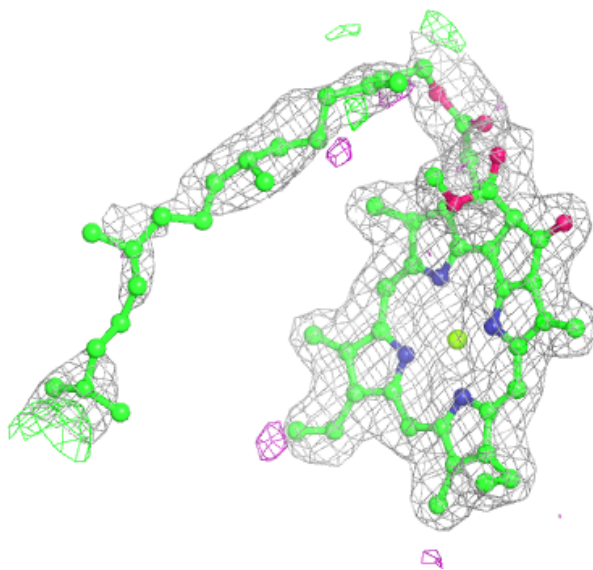
Electron density around CLA b 605:

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



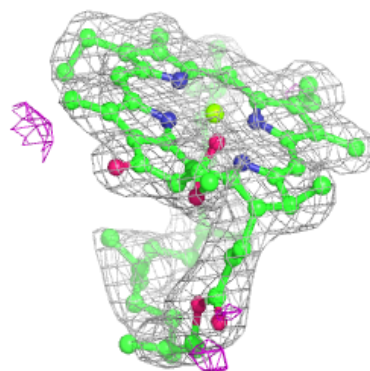
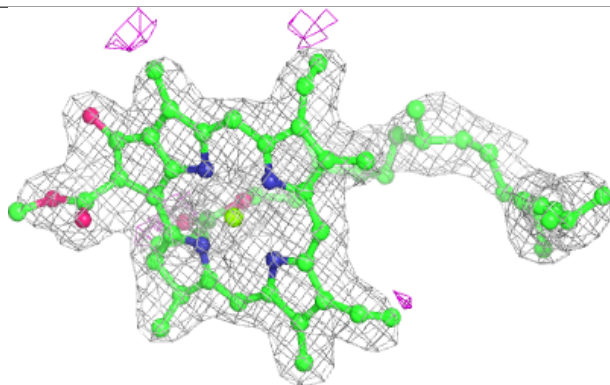
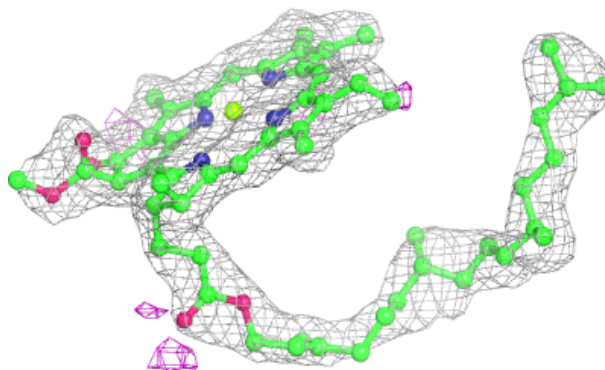
Electron density around CLA B 618:

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

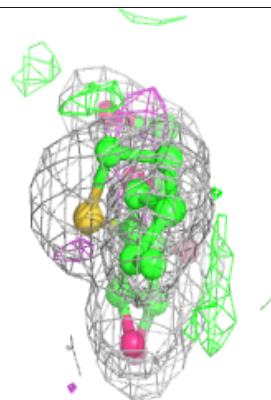
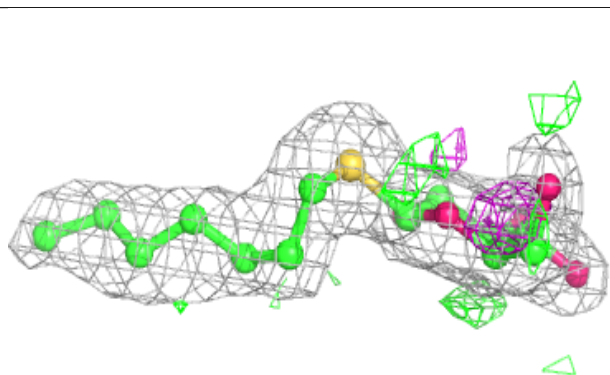
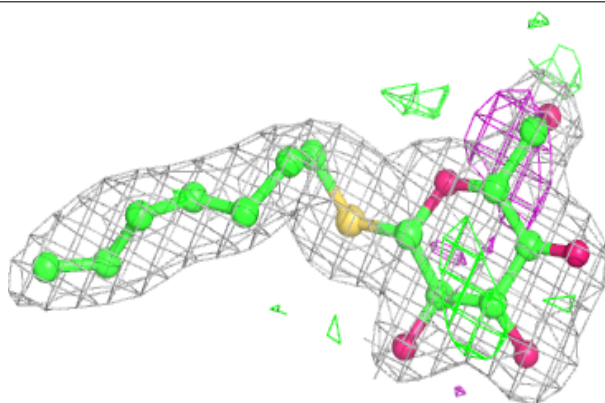


Electron density around CLA C 515:

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

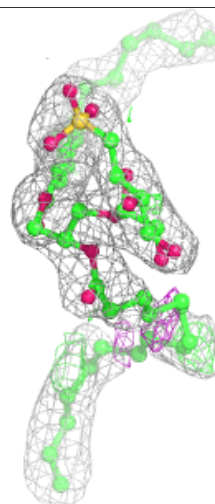
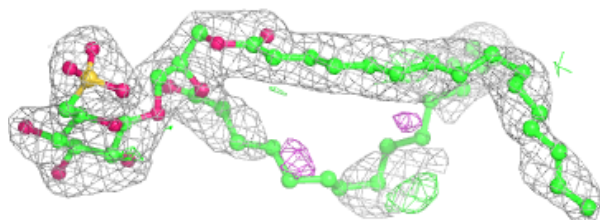
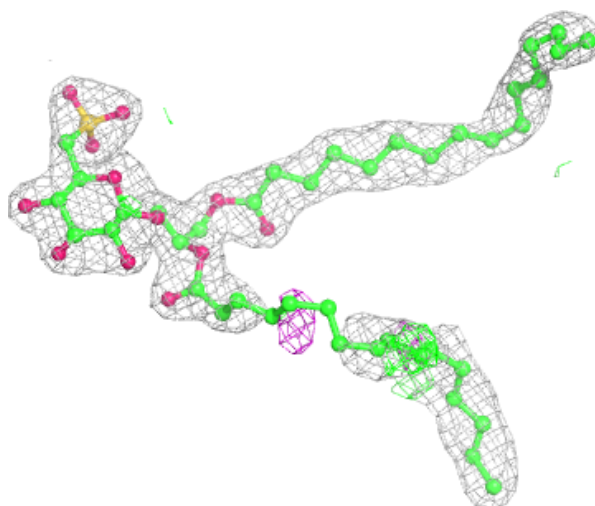
**Electron density around HTG o 301:**

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



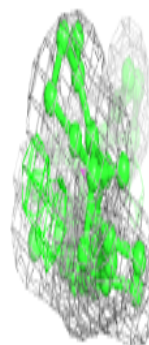
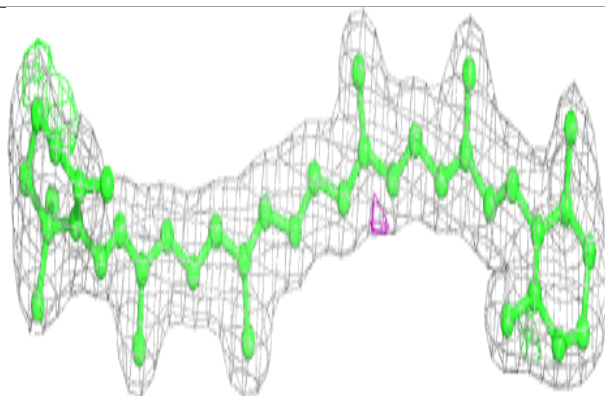
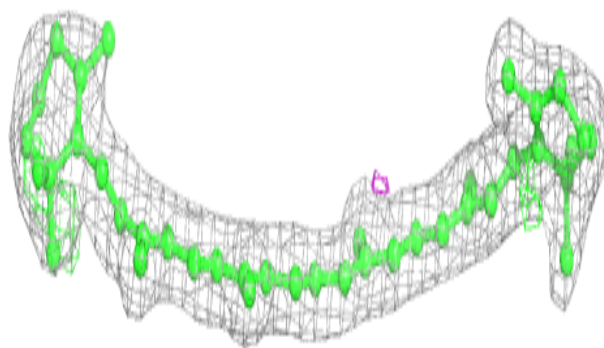
Electron density around SQD a 415:

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



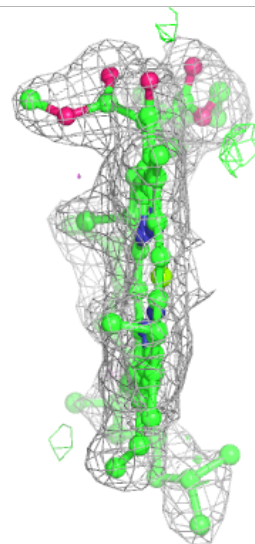
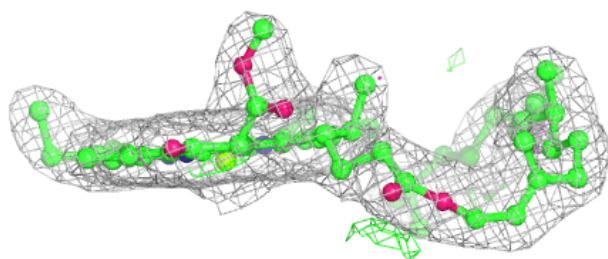
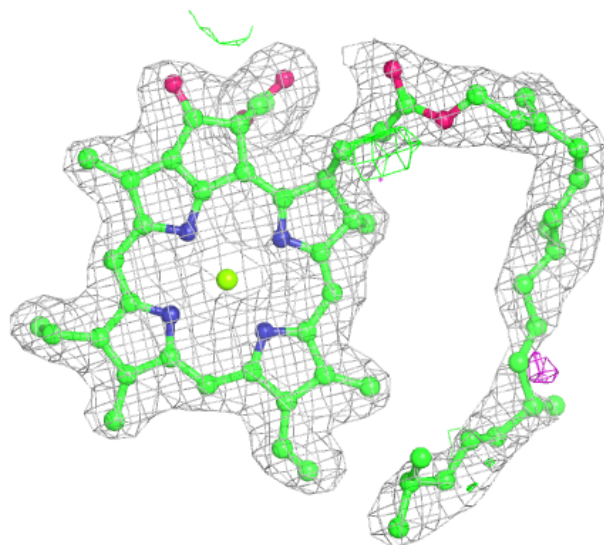
Electron density around BCR D 407:

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



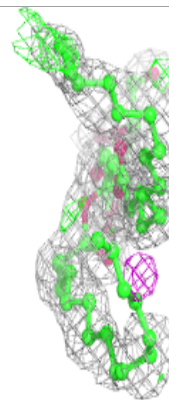
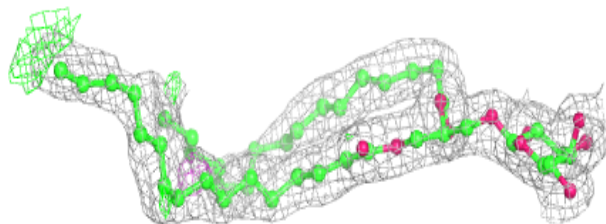
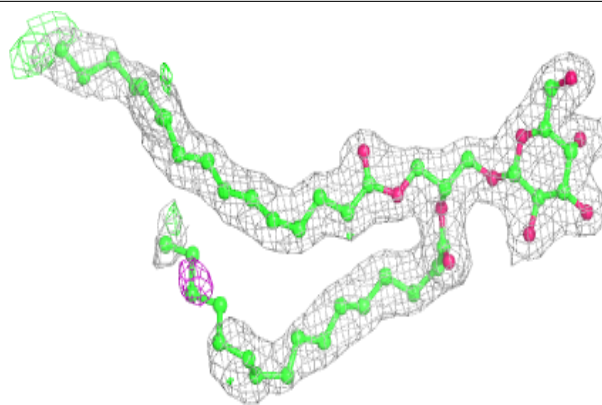
Electron density around CLA C 514:

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



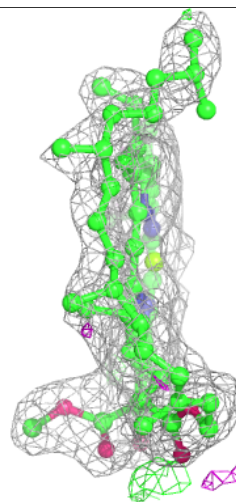
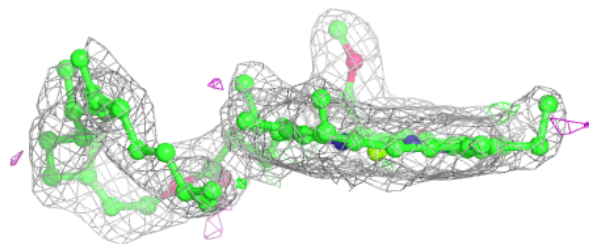
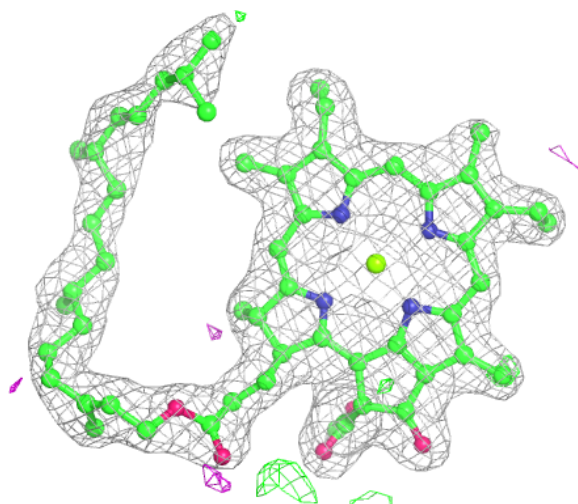
Electron density around LMG D 413:

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



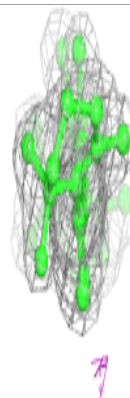
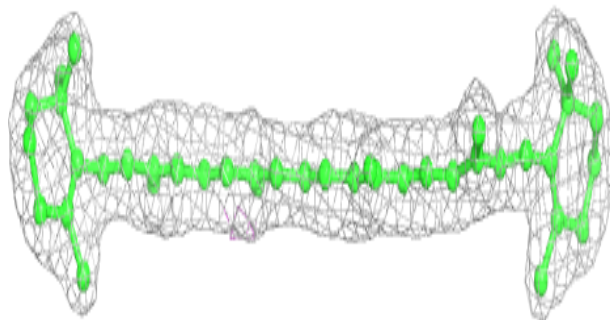
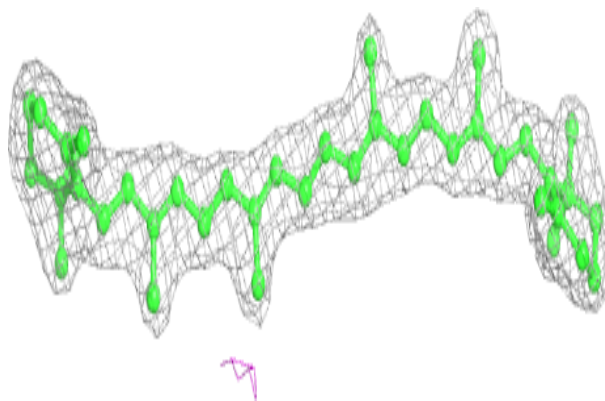
Electron density around CLA c 514:

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

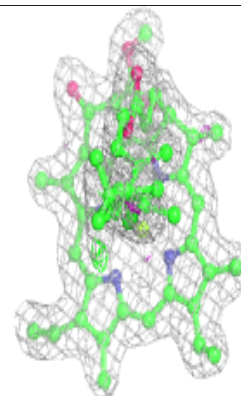
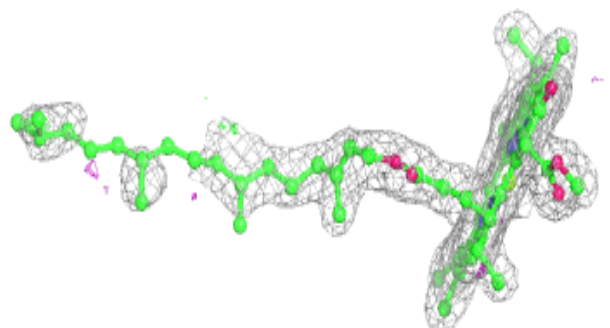
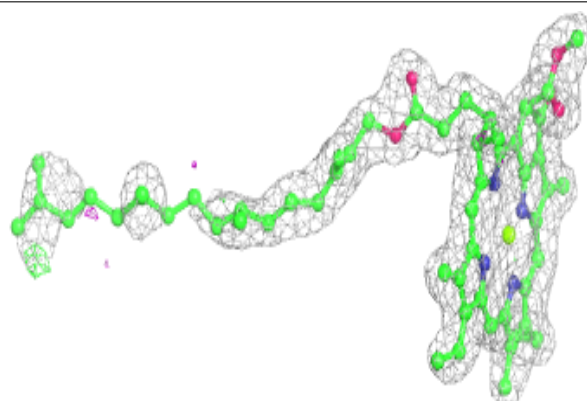


Electron density around BCR C 516:

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

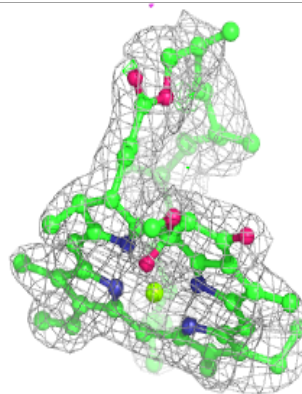
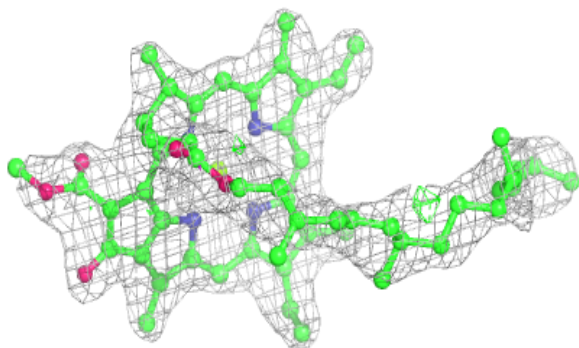
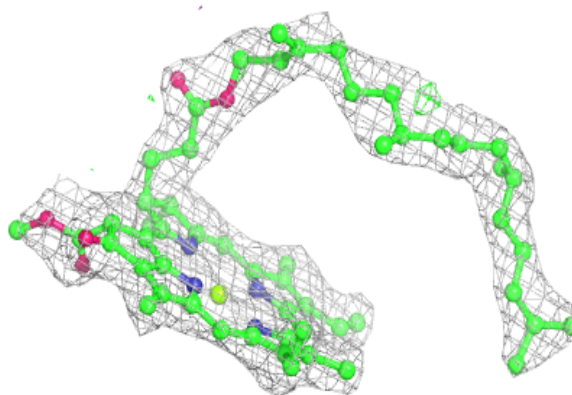
**Electron density around CLA D 406:**

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

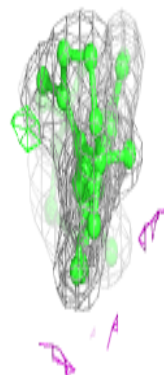
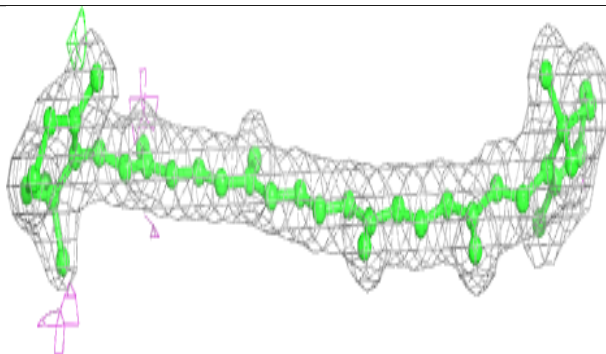
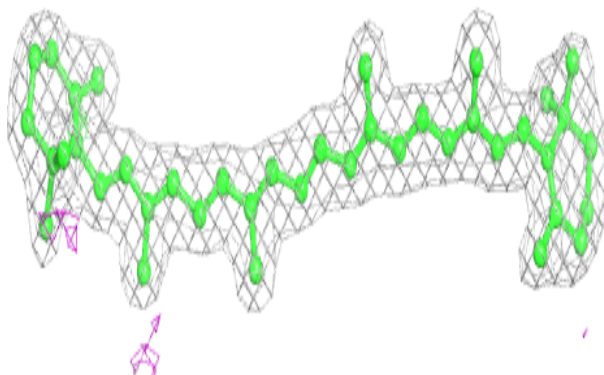


Electron density around CLA c 515:

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

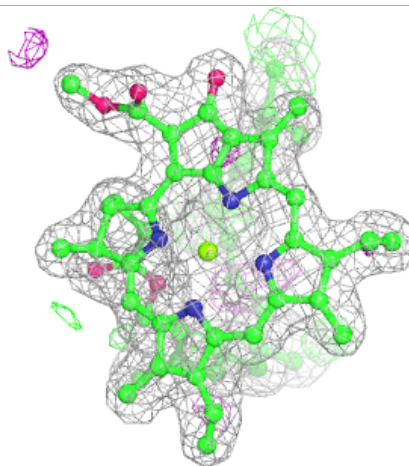
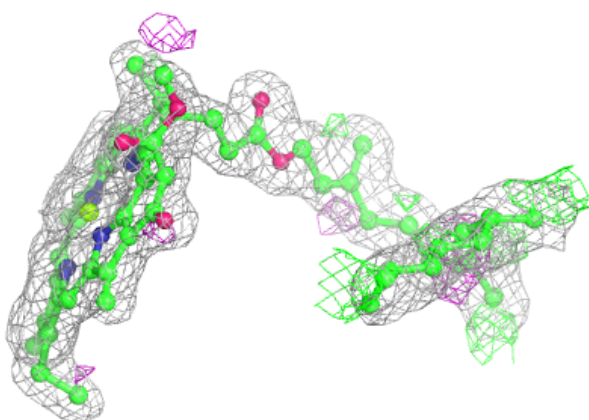
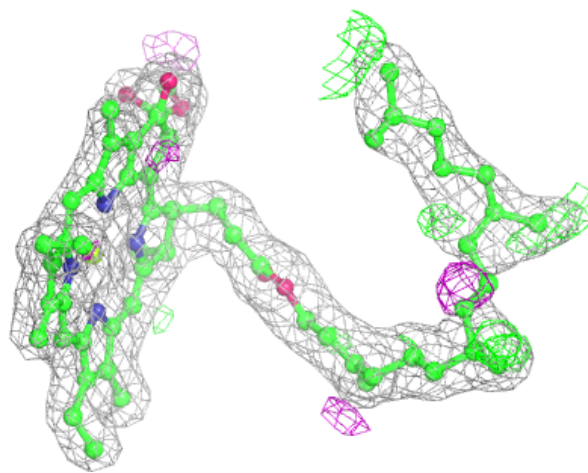
**Electron density around BCR B 621:**

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



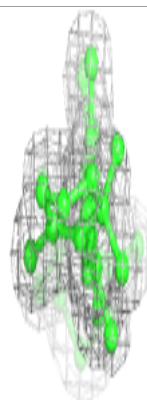
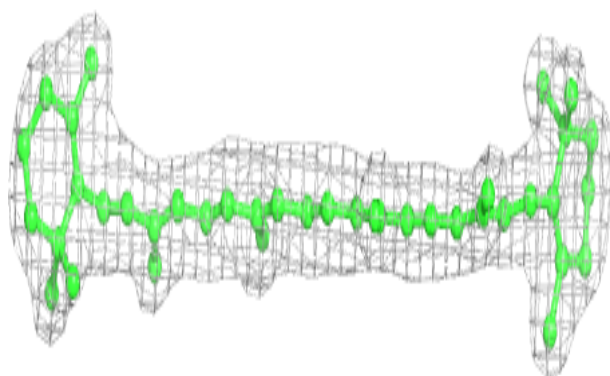
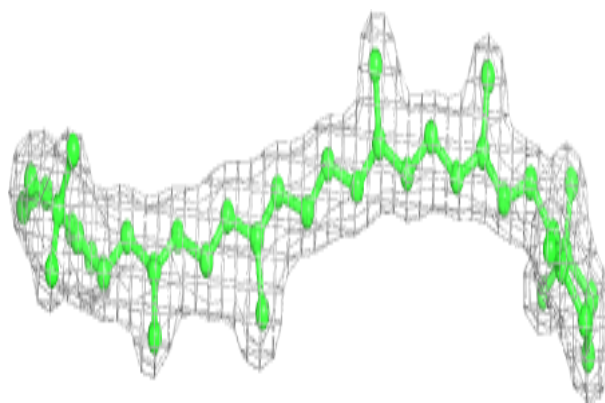
Electron density around CLA B 608:

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

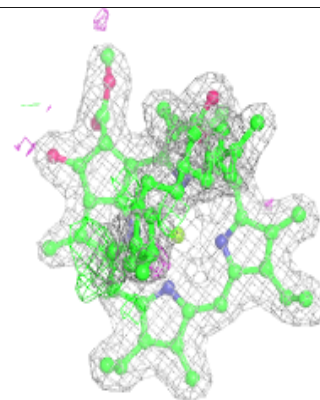
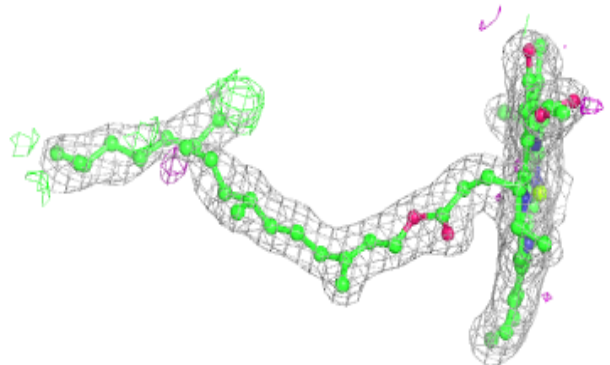
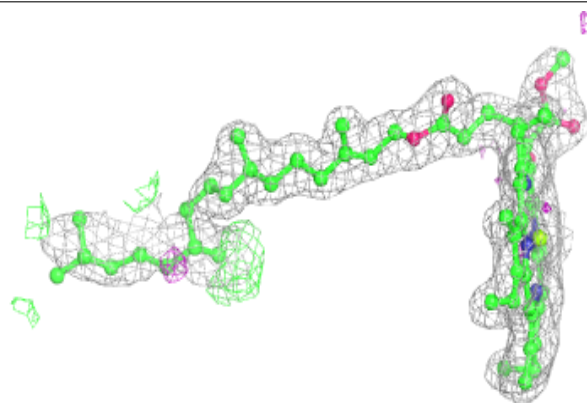


Electron density around BCR C 517:

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

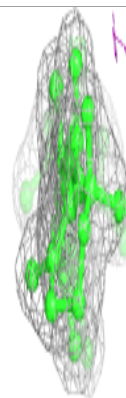
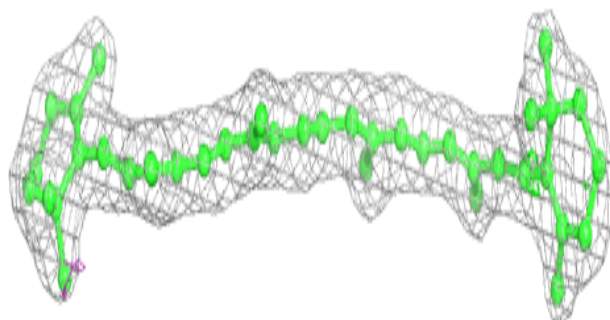
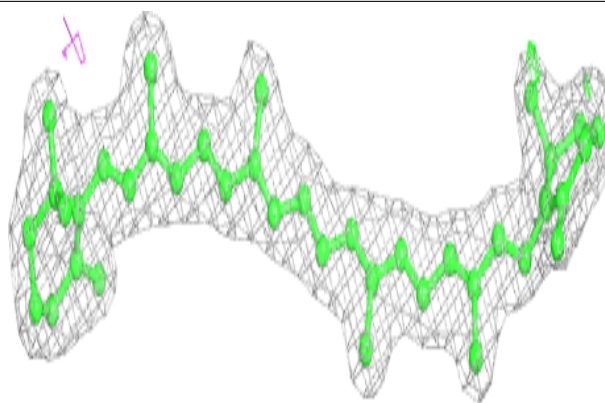
**Electron density around CLA b 610:**

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

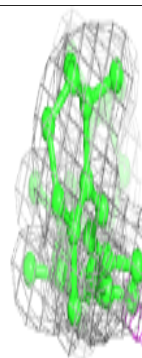
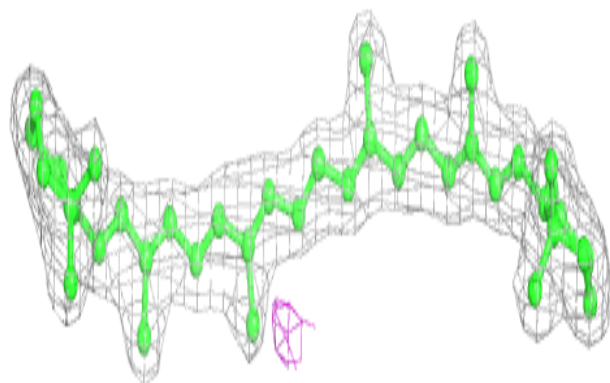
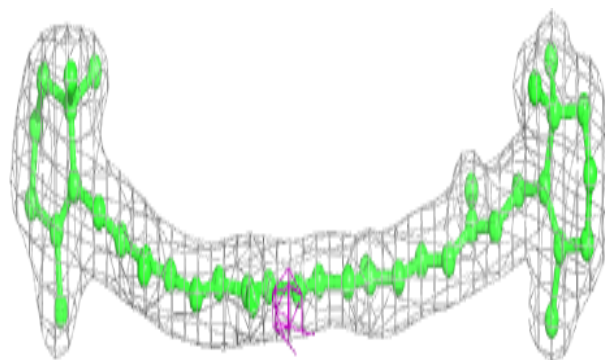


Electron density around BCR K 101:

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

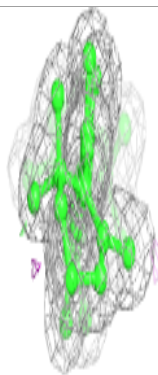
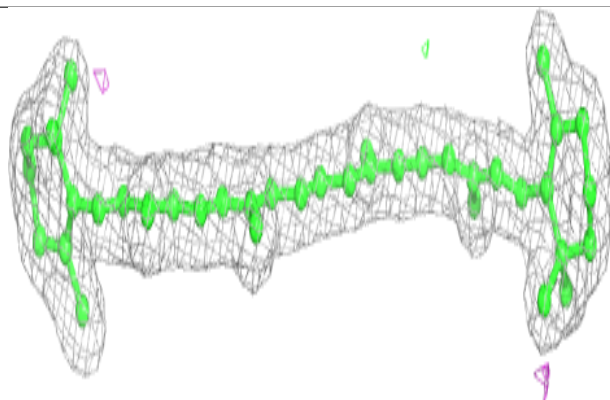
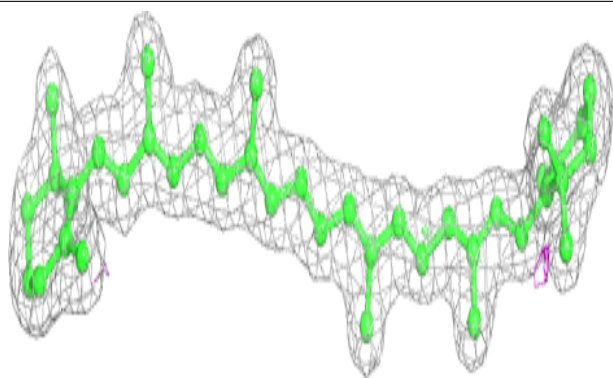
**Electron density around BCR K 102:**

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

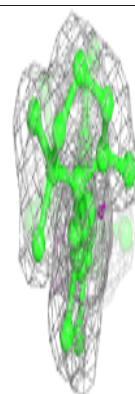
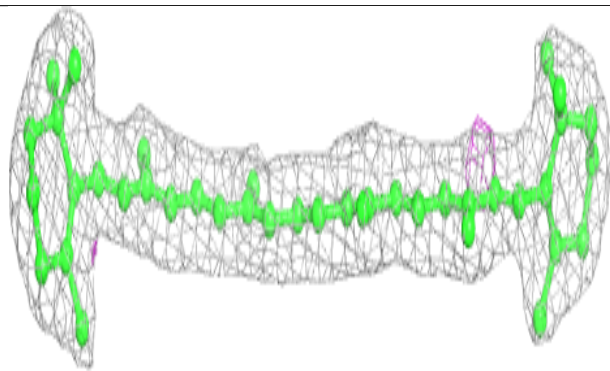
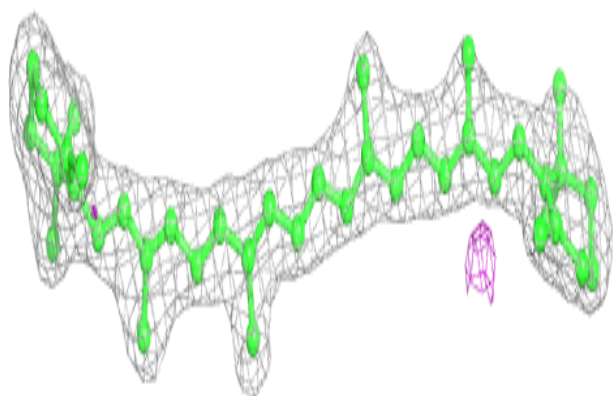


Electron density around BCR a 414:

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

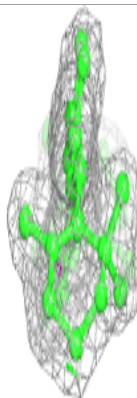
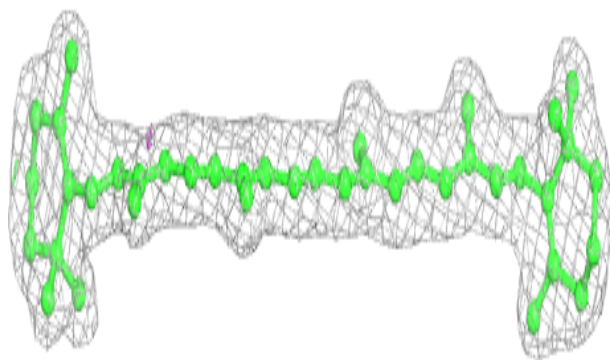
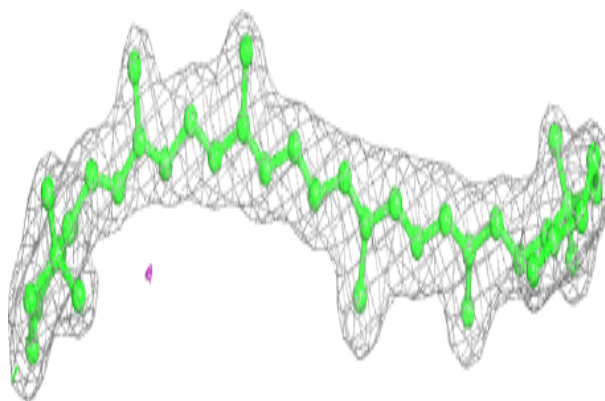
**Electron density around BCR c 516:**

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

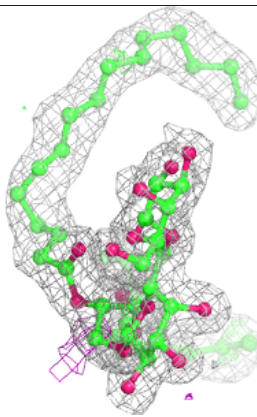
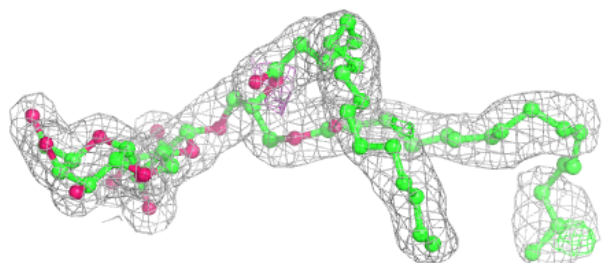
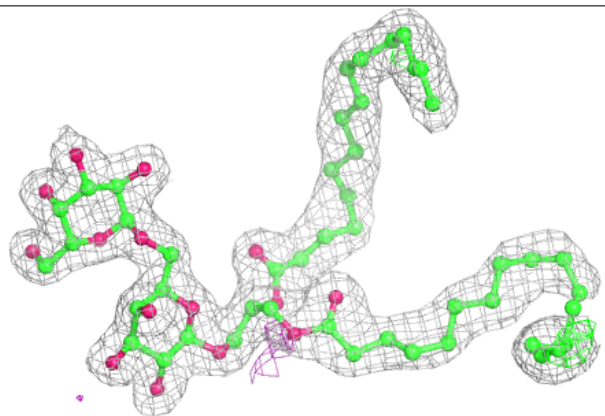


Electron density around BCR c 517:

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

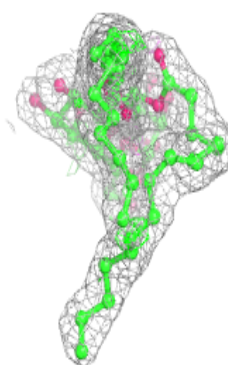
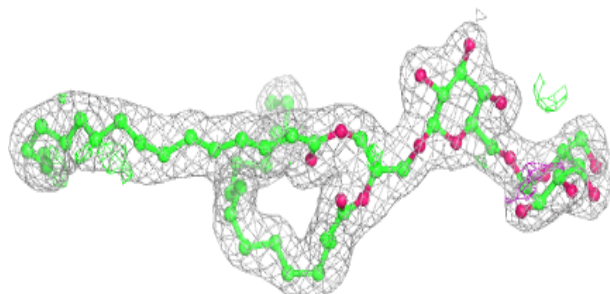
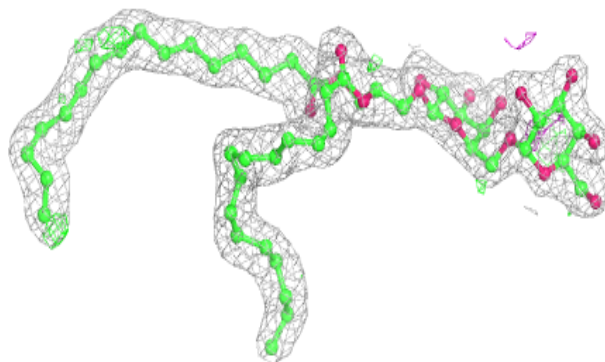
**Electron density around DGD C 519:**

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

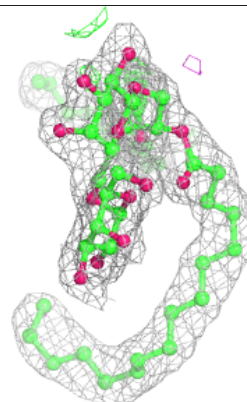
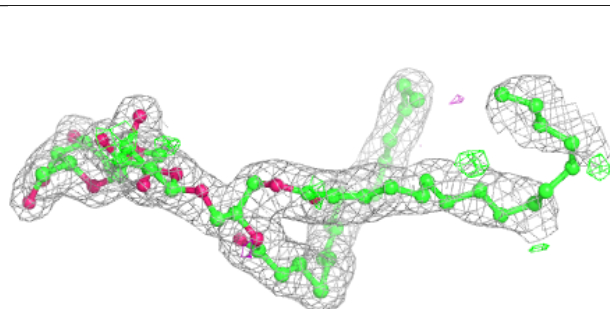
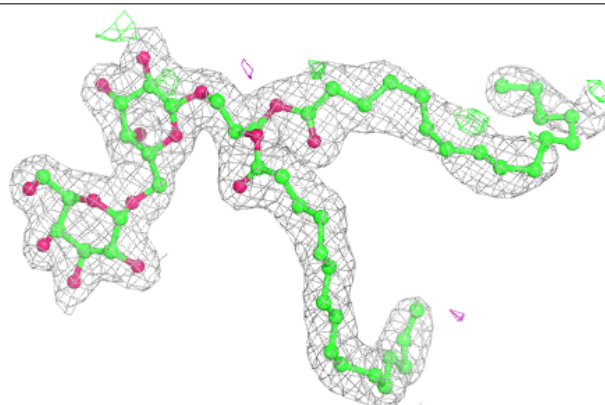


Electron density around DGD H 104:

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

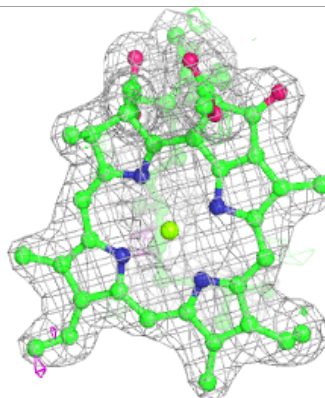
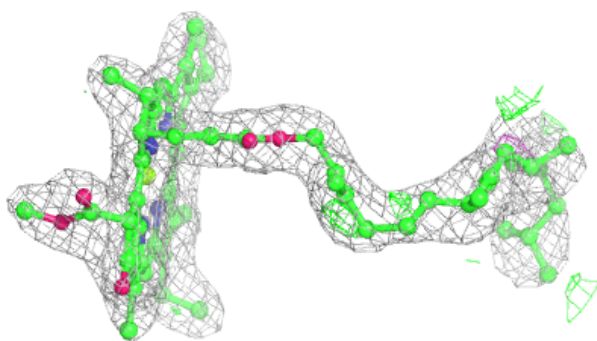
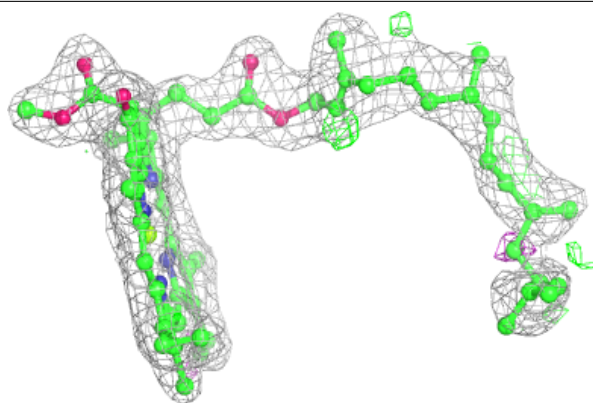
**Electron density around DGD c 519:**

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

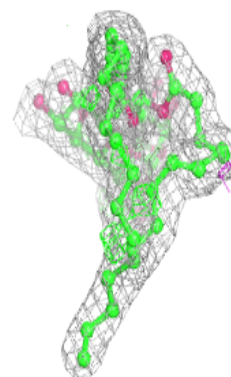
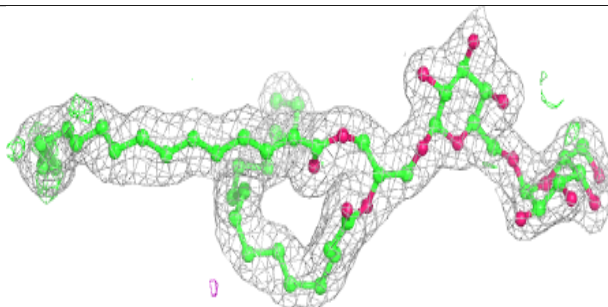
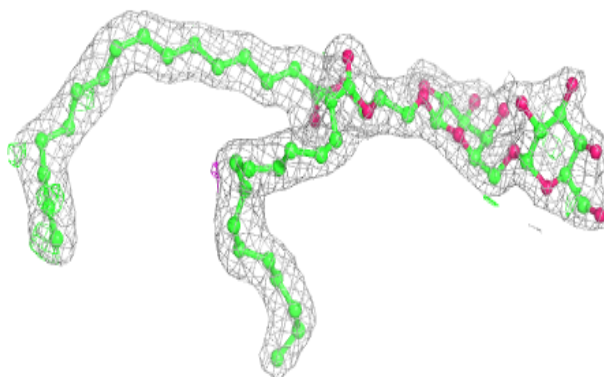


Electron density around CLA C 508:

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

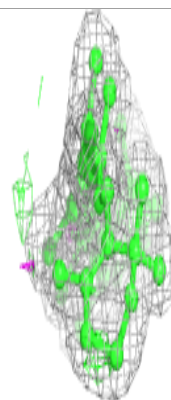
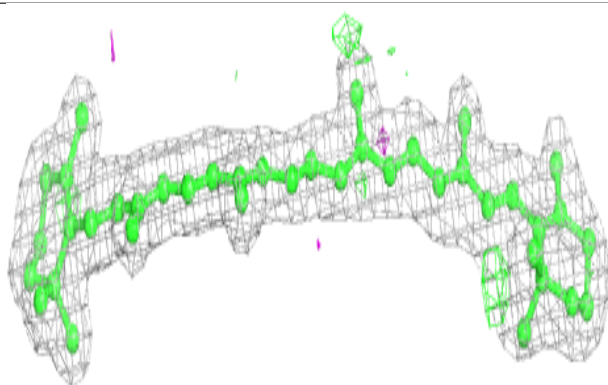
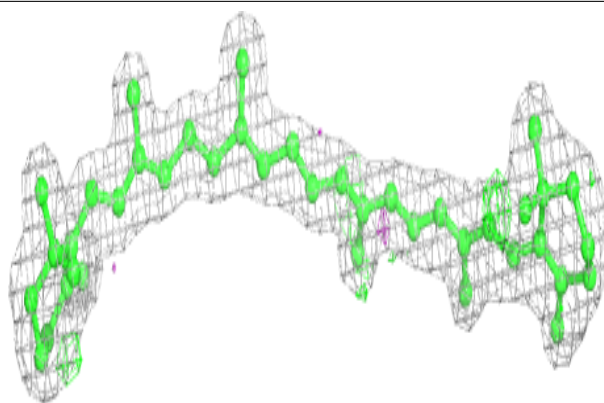
**Electron density around DGD h 102:**

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

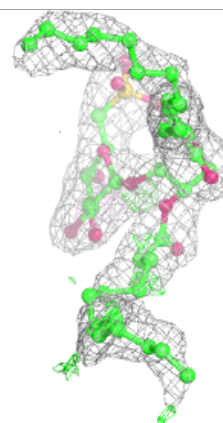
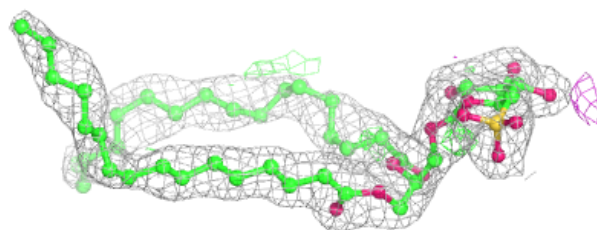
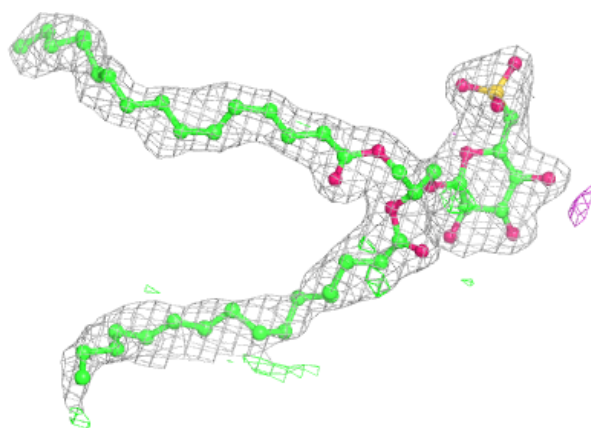


Electron density around BCR t 101:

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

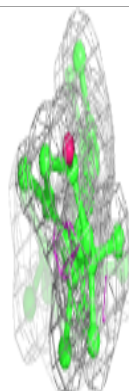
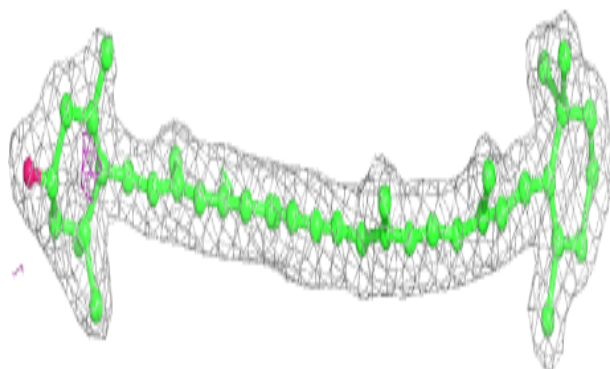
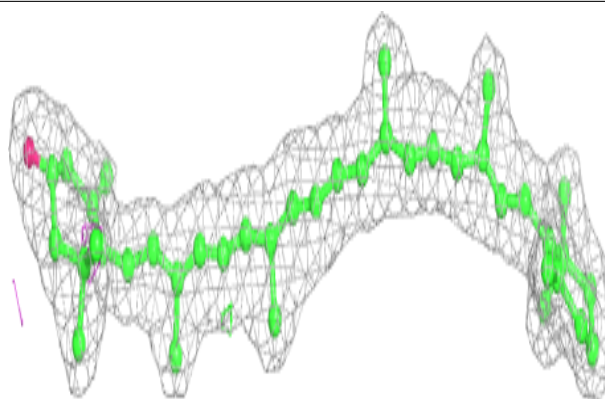
**Electron density around SQD A 411:**

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

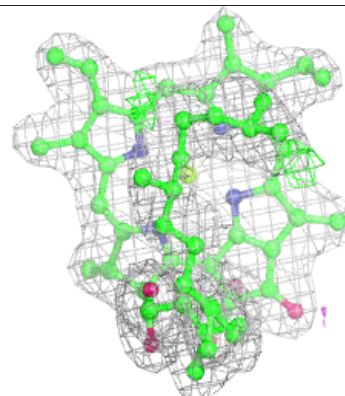
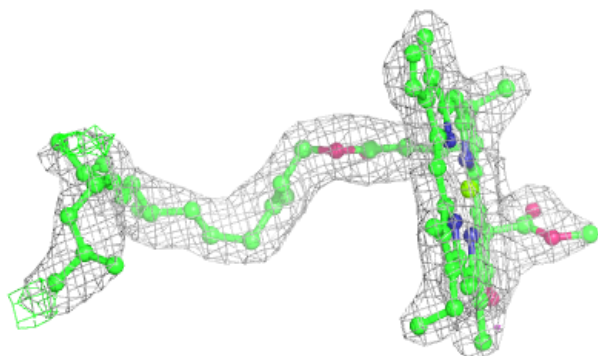
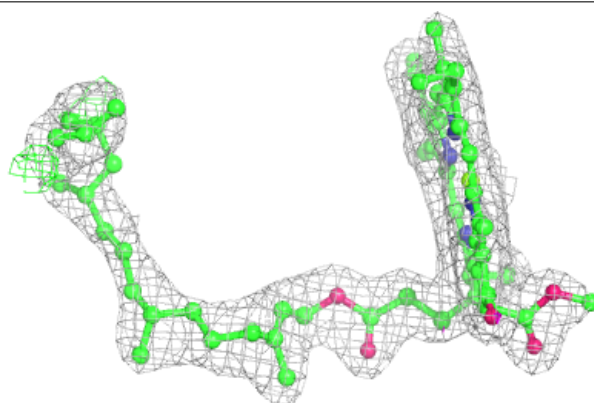


Electron density around RRX H 103:

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

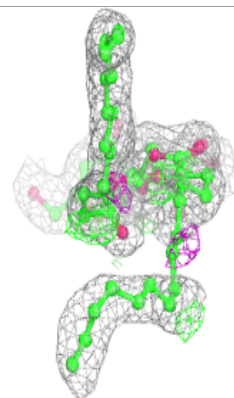
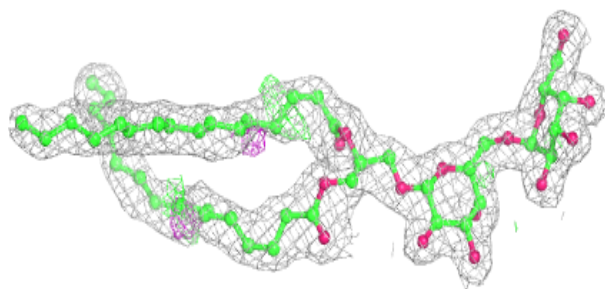
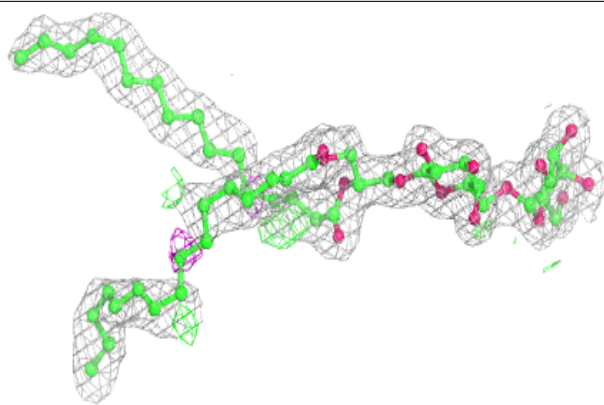
**Electron density around CLA c 508:**

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

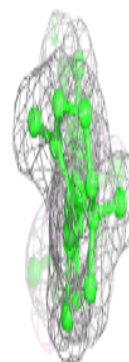
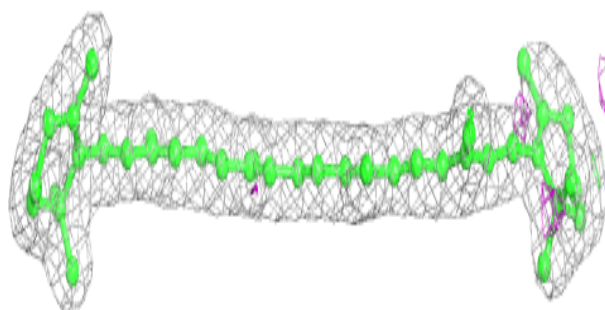
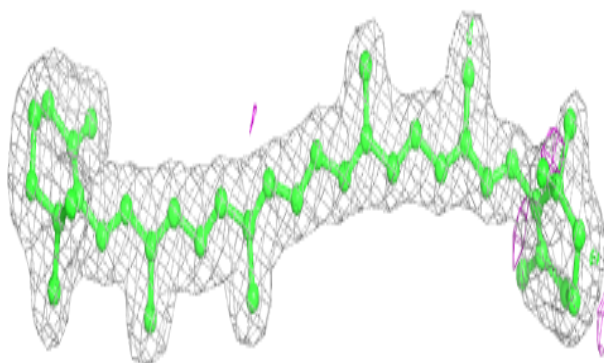


Electron density around DGD c 518:

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

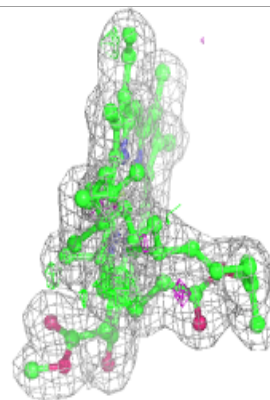
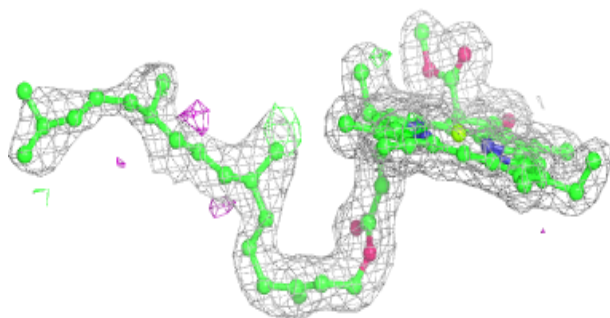
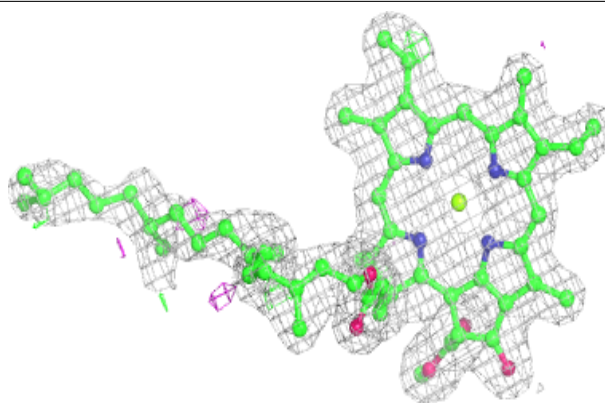
**Electron density around BCR B 620:**

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

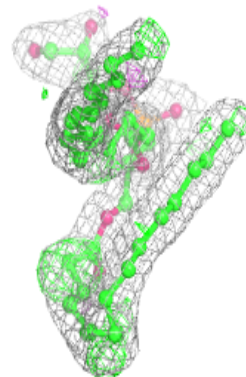
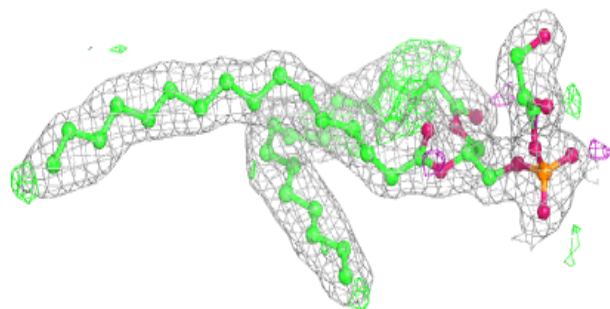
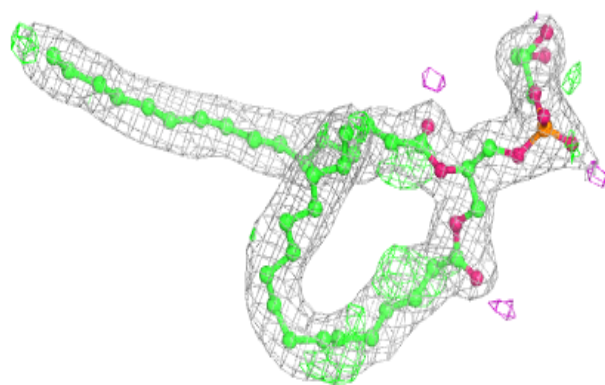


Electron density around CLA a 411:

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

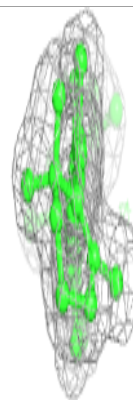
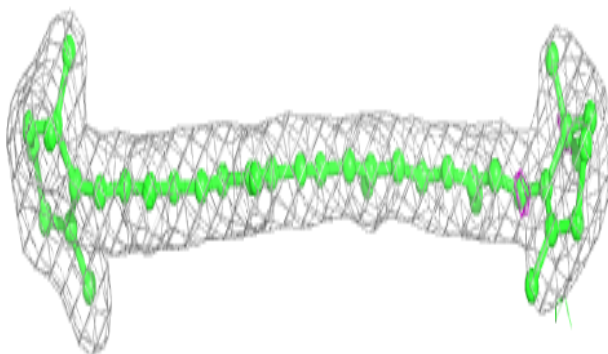
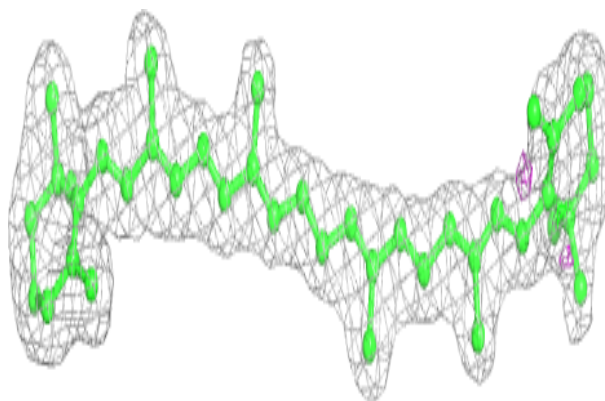
**Electron density around LHG D 410:**

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

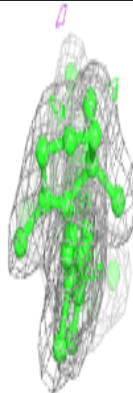
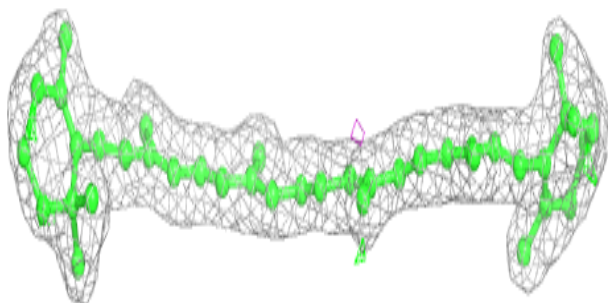
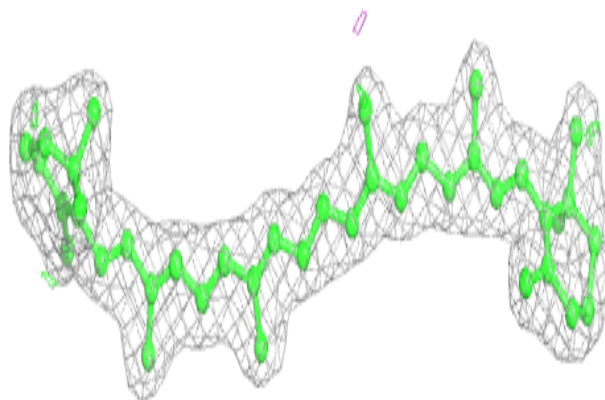


Electron density around BCR b 622:

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

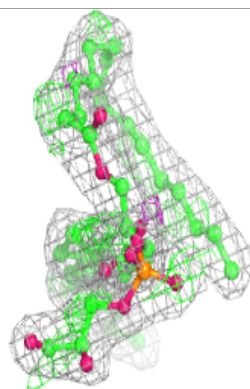
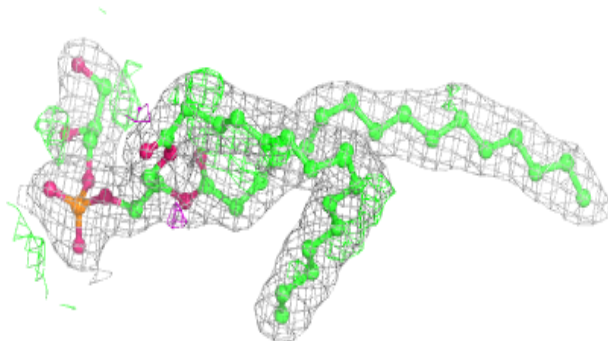
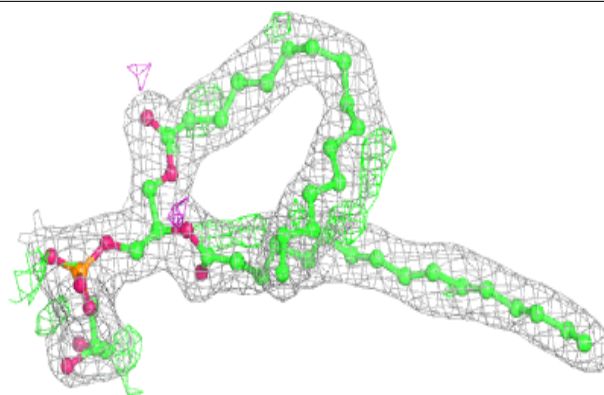
**Electron density around BCR k 102:**

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

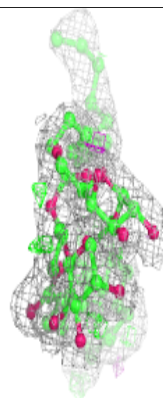
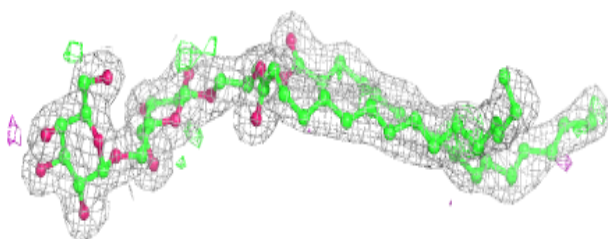
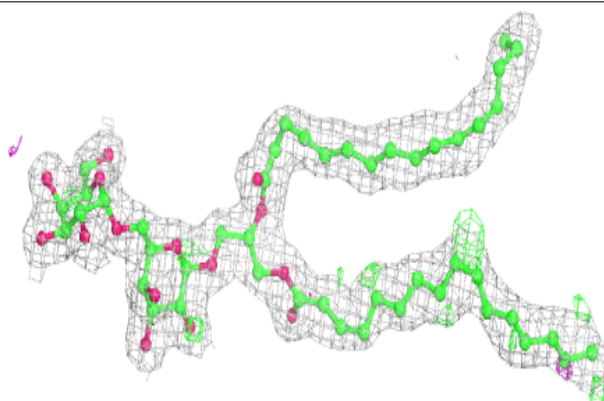


Electron density around LHG d 409:

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

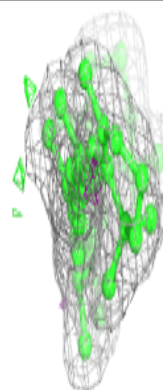
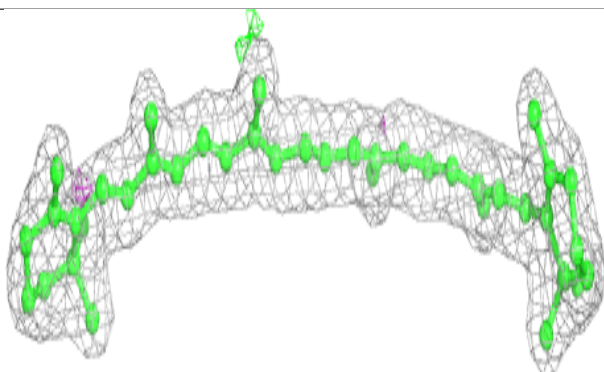
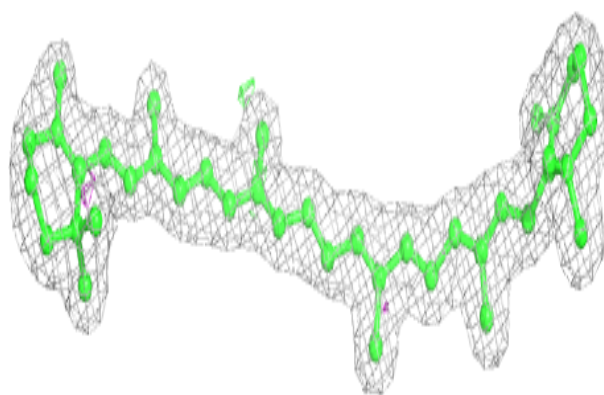
**Electron density around DGD C 520:**

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

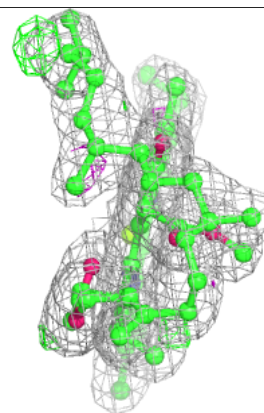
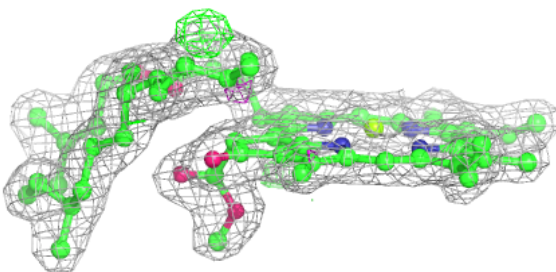
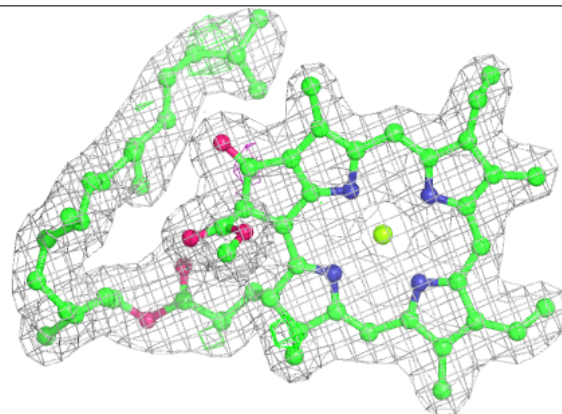


Electron density around BCR T 101:

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

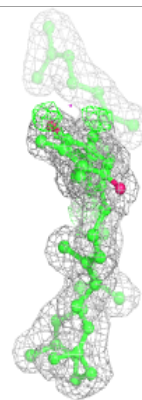
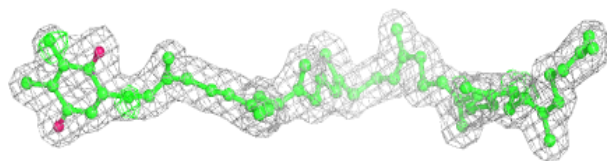
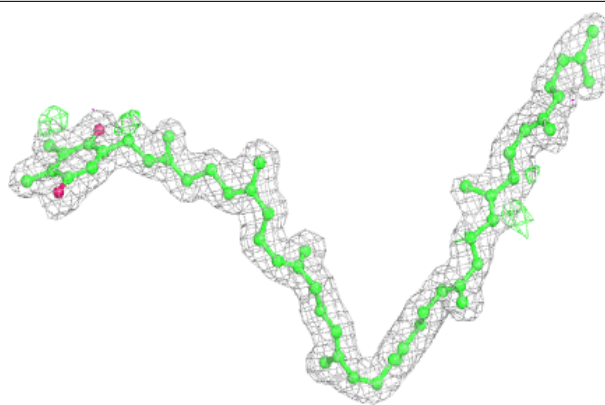
**Electron density around CLA b 614:**

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

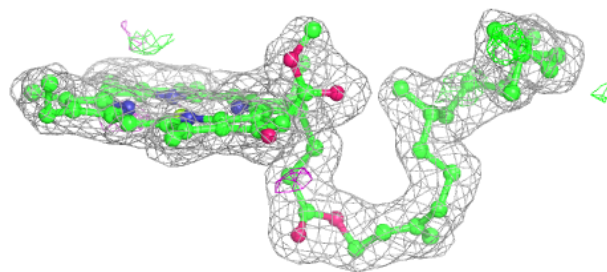
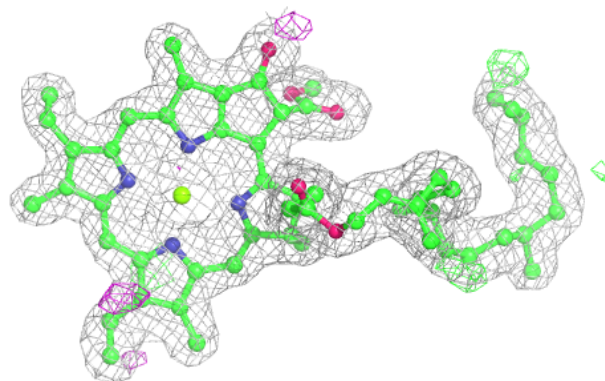


Electron density around PL9 D 408:

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

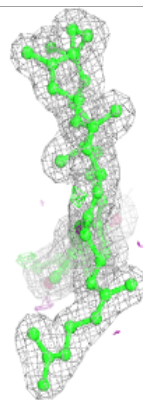
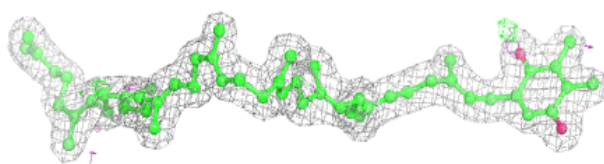
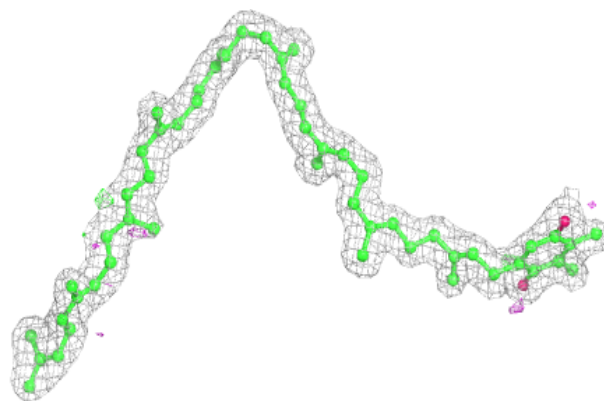
**Electron density around CLA b 616:**

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

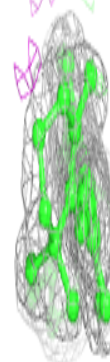
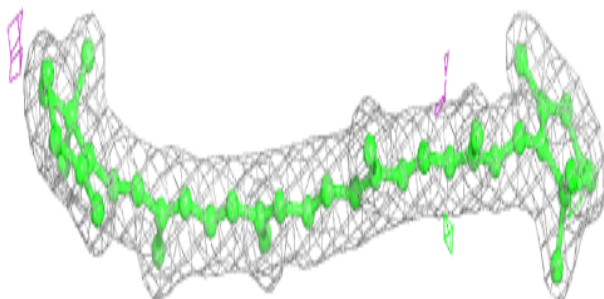
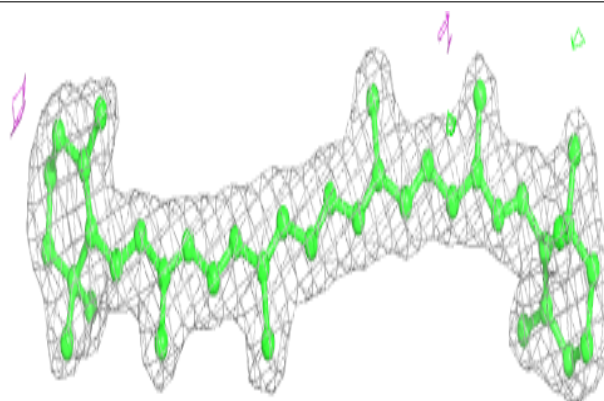


Electron density around PL9 d 408:

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

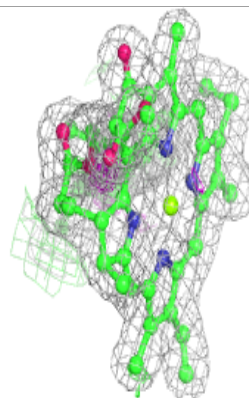
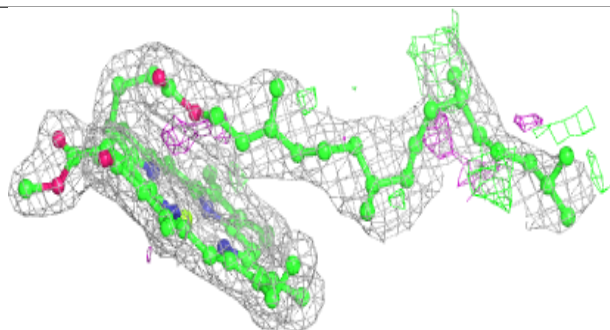
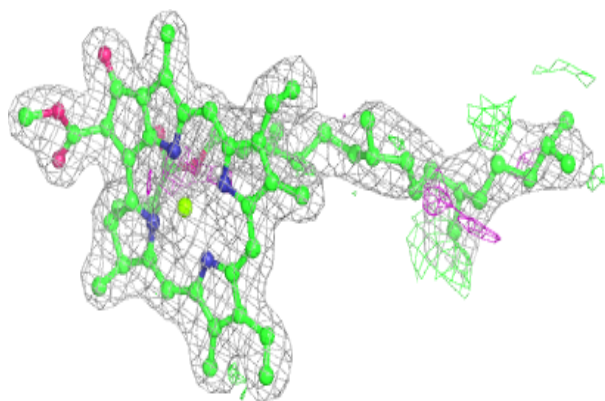
**Electron density around BCR b 623:**

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



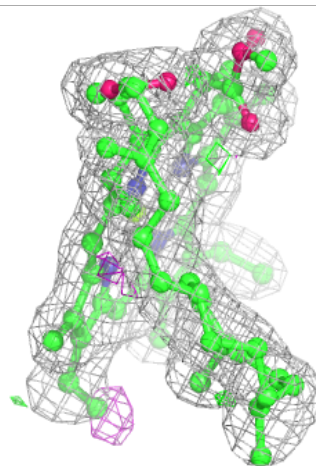
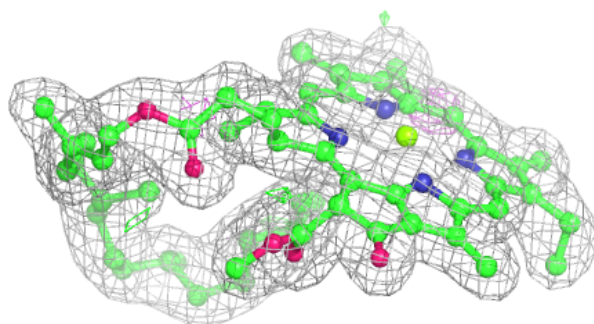
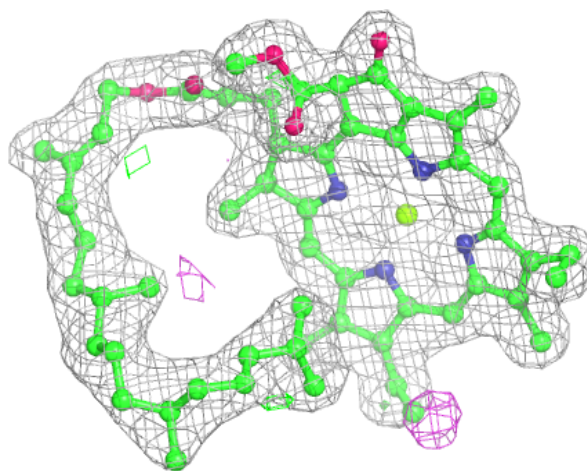
Electron density around CLA b 618:

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



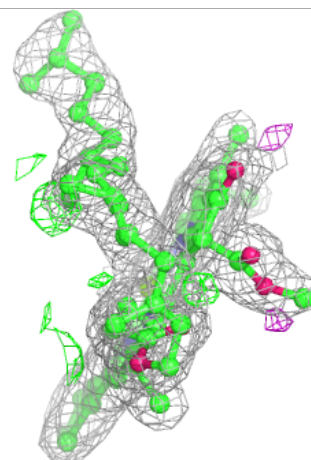
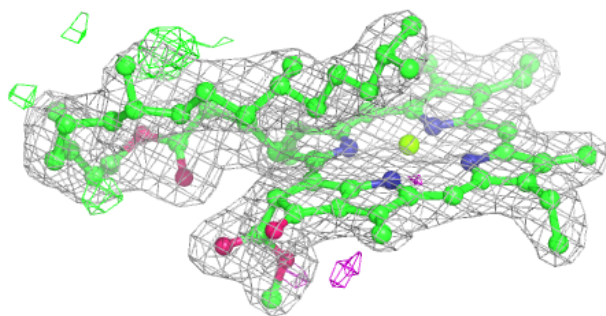
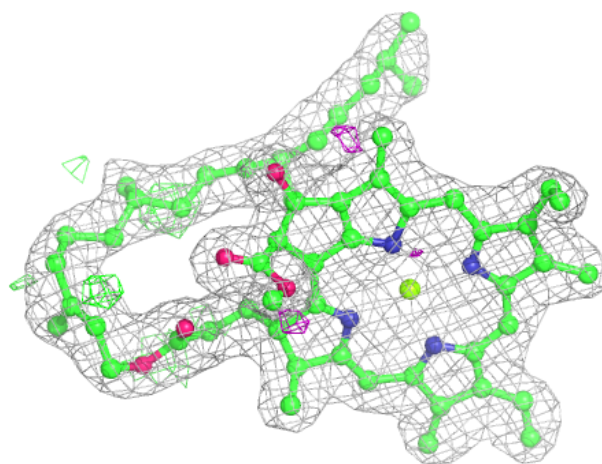
Electron density around CLA b 619:

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



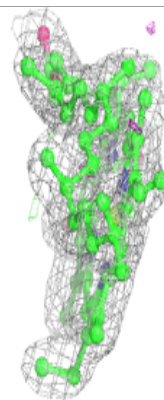
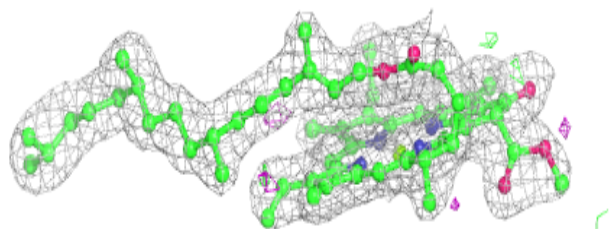
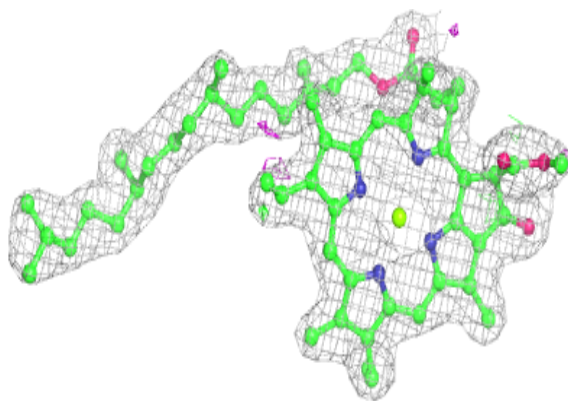
Electron density around CLA C 511:

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

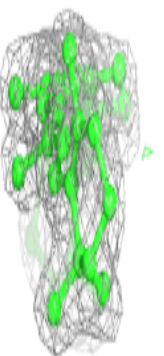
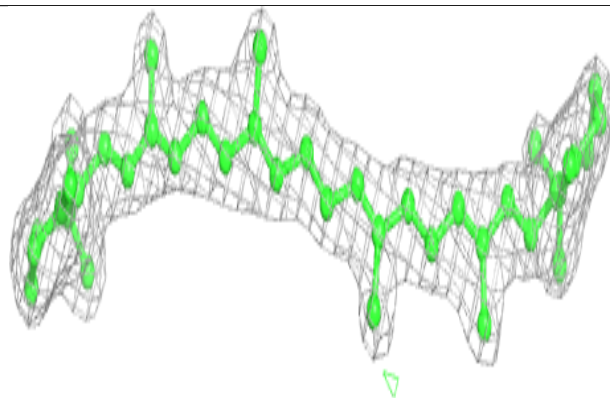
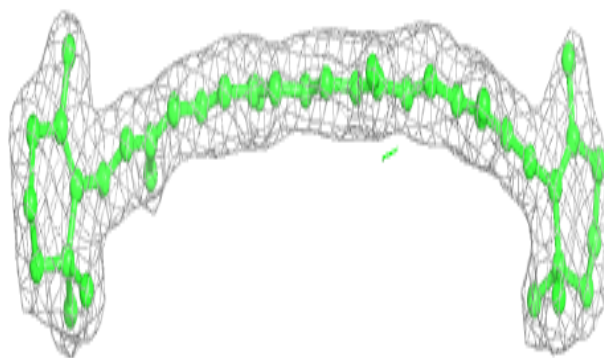


Electron density around CLA c 503:

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

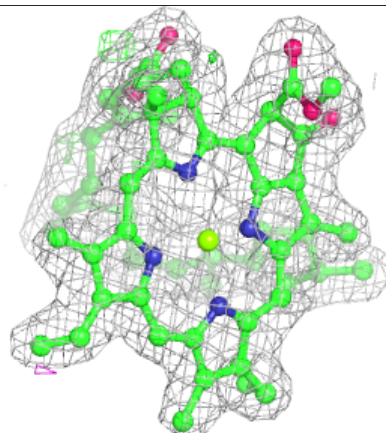
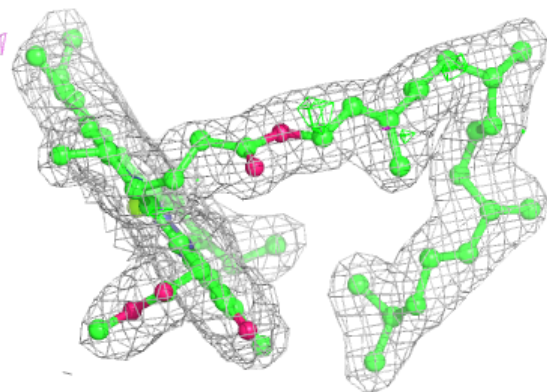
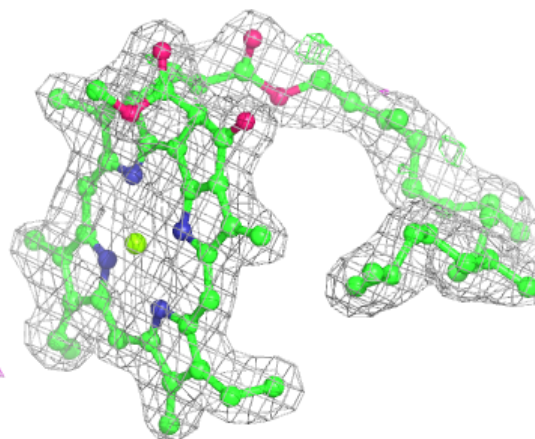
**Electron density around BCR k 103:**

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

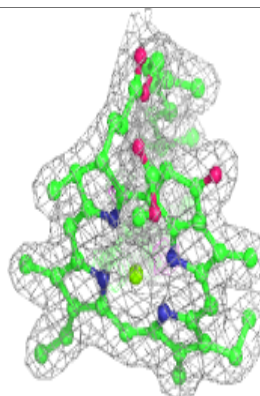
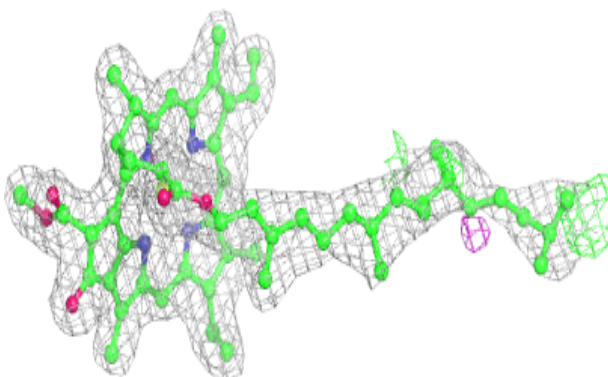
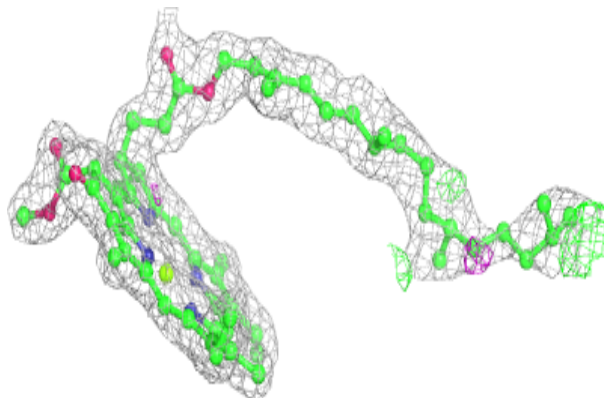


Electron density around CLA c 505:

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

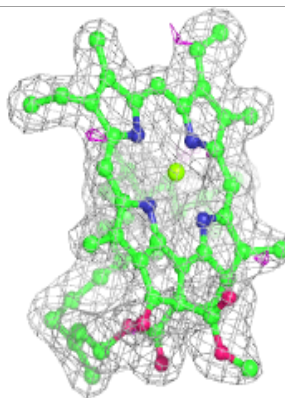
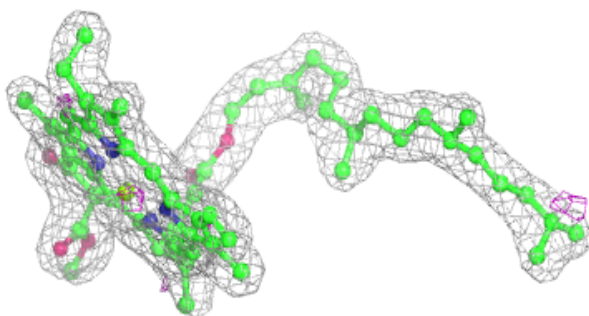
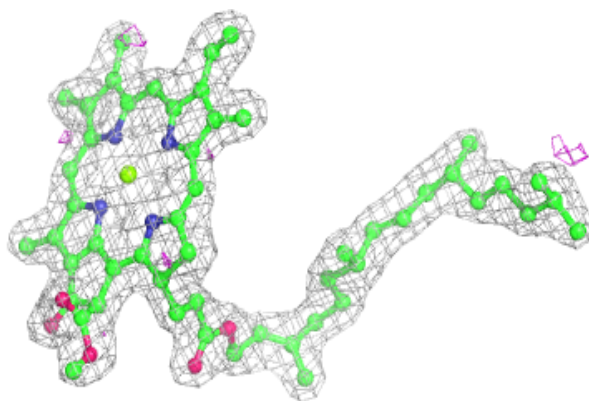
**Electron density around CLA c 506:**

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



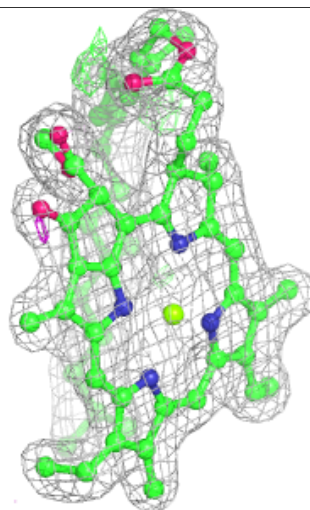
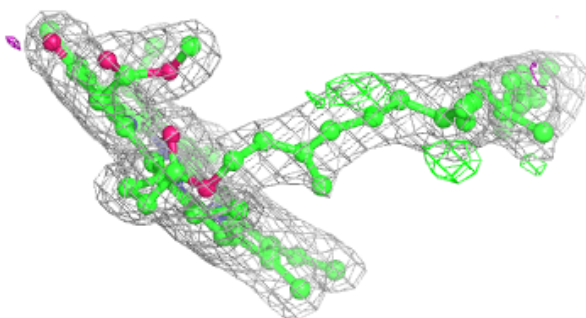
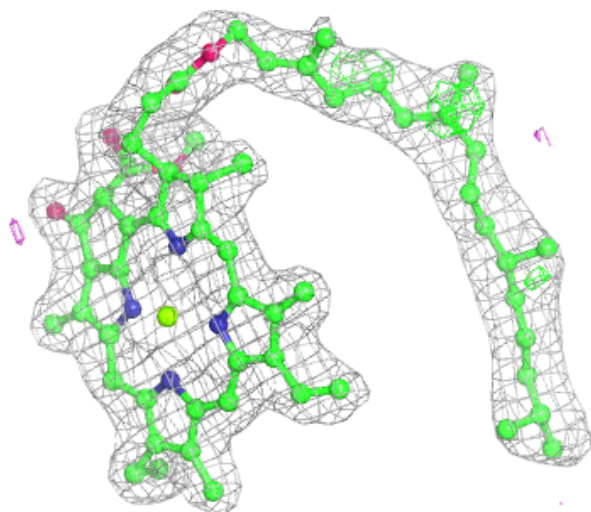
Electron density around CLA C 513:

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



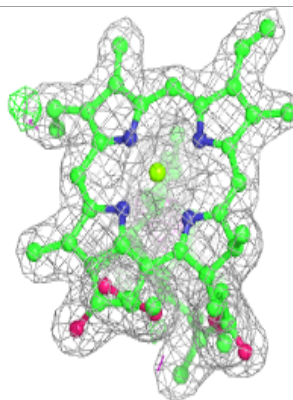
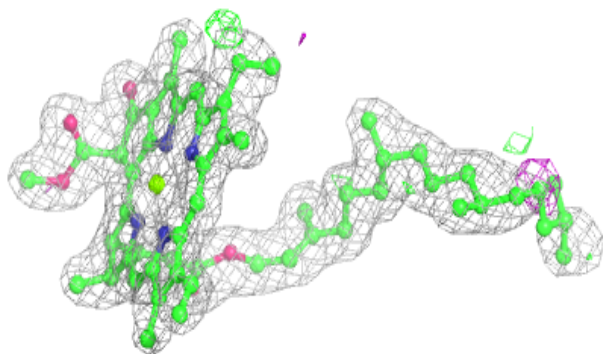
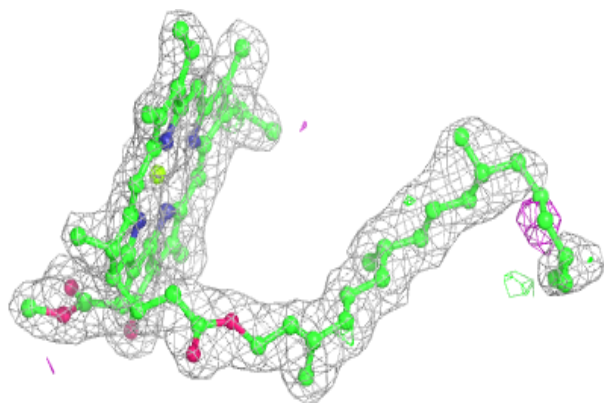
Electron density around CLA c 509:

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



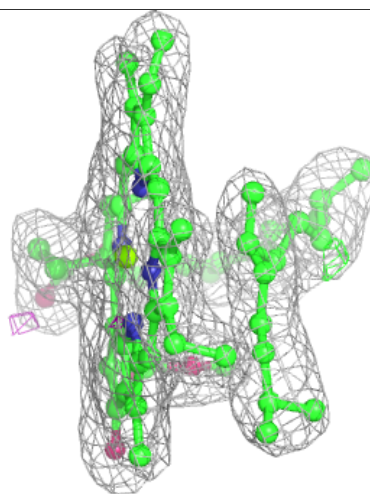
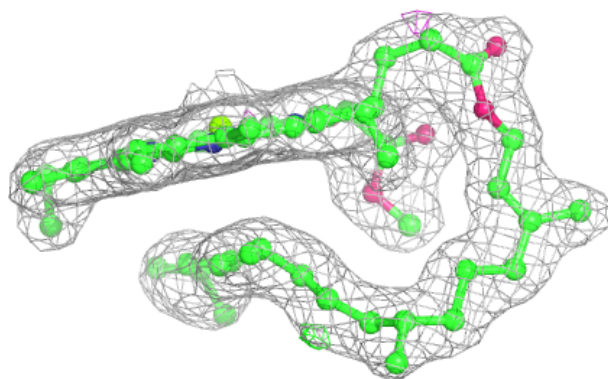
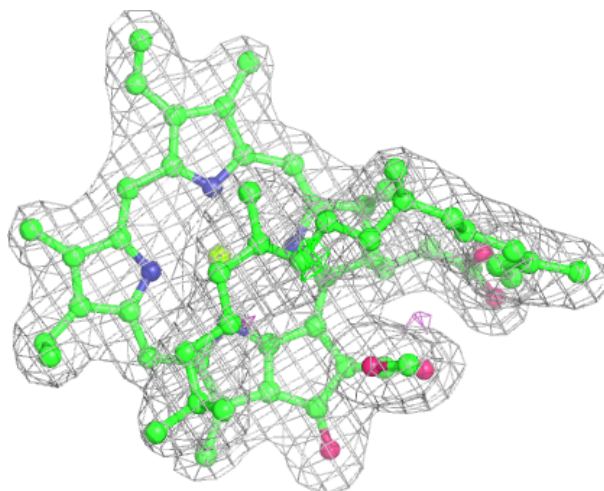
Electron density around CLA c 510:

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



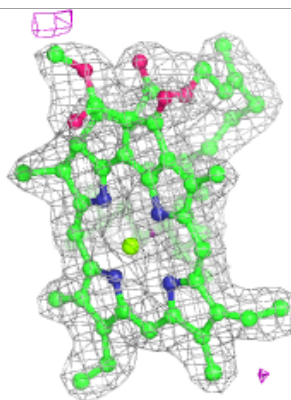
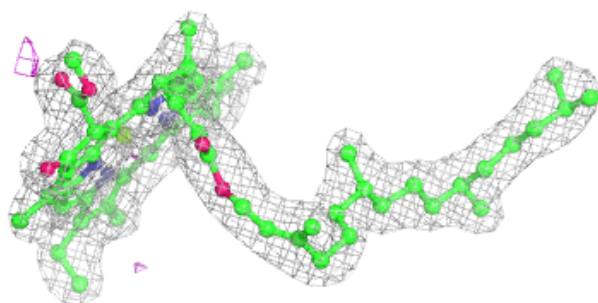
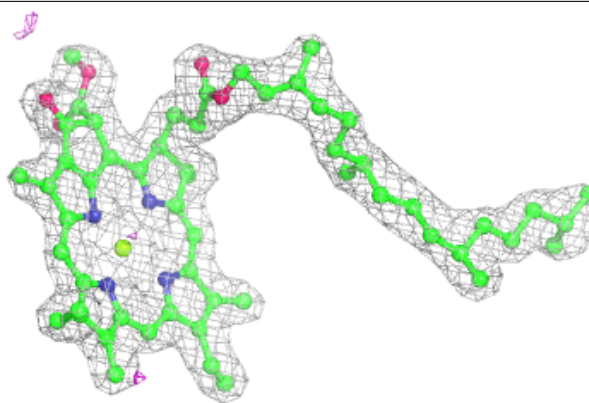
Electron density around CLA c 512:

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

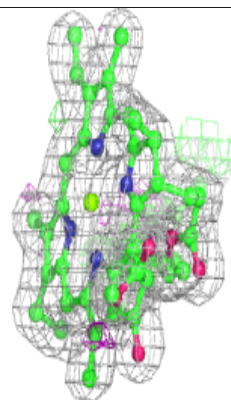
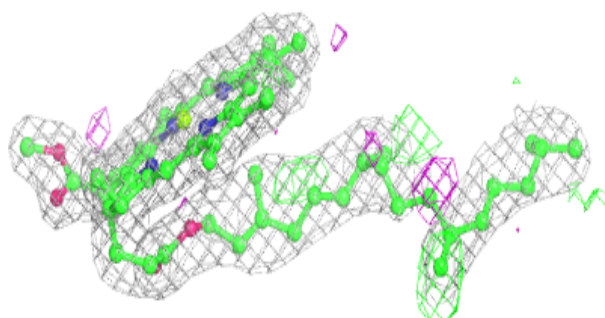
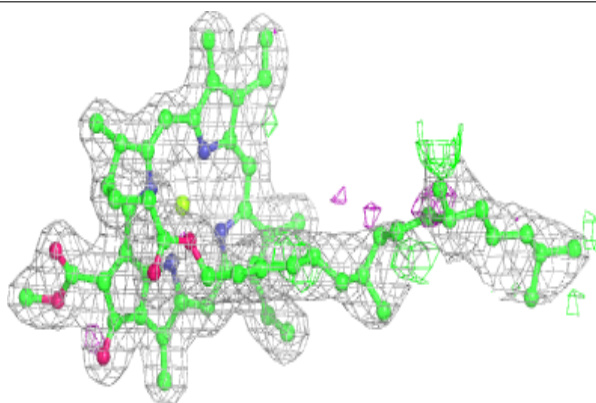


Electron density around CLA c 513:

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

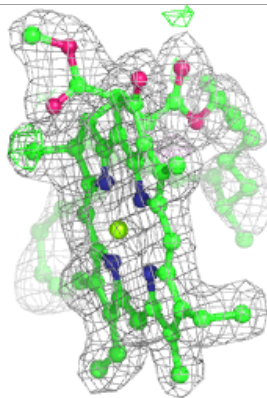
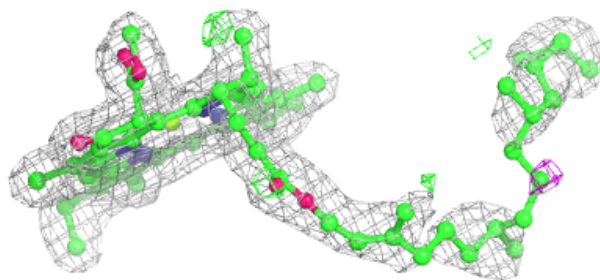
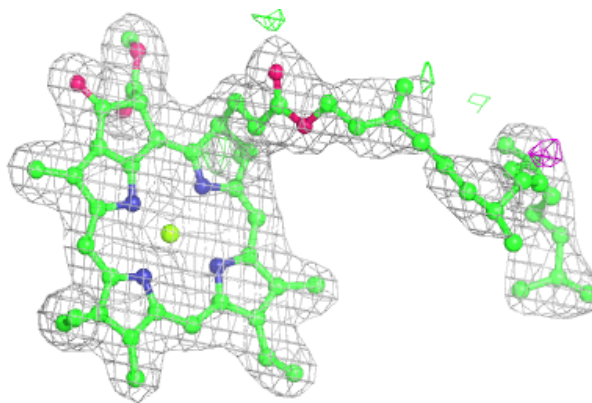
**Electron density around CLA B 616:**

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

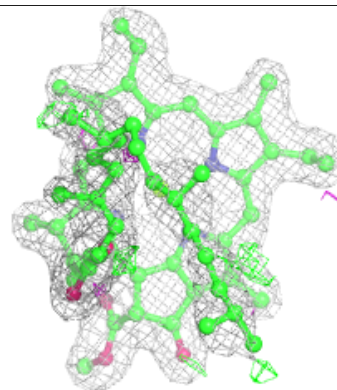
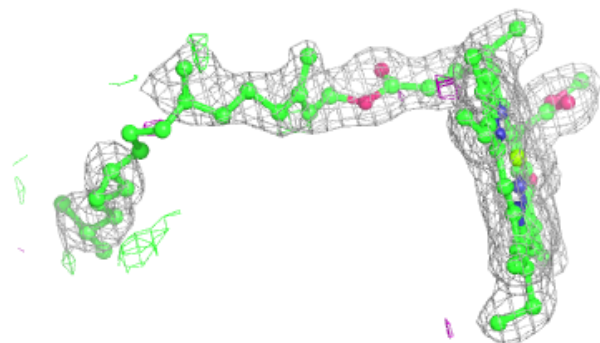
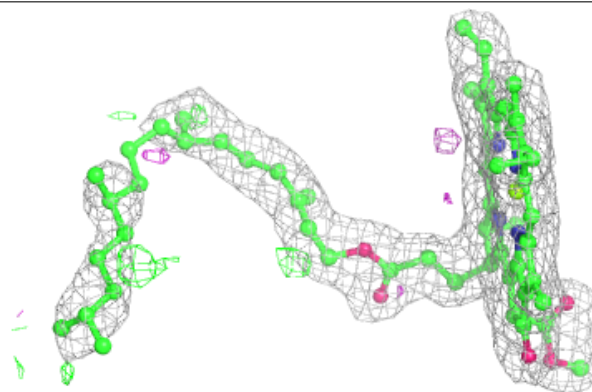


Electron density around CLA A 409:

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

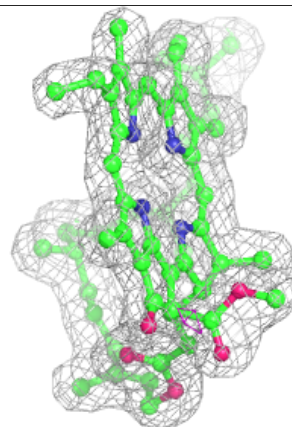
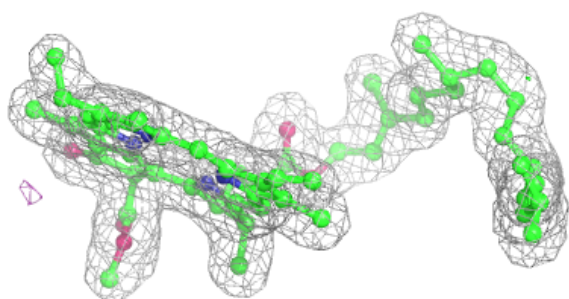
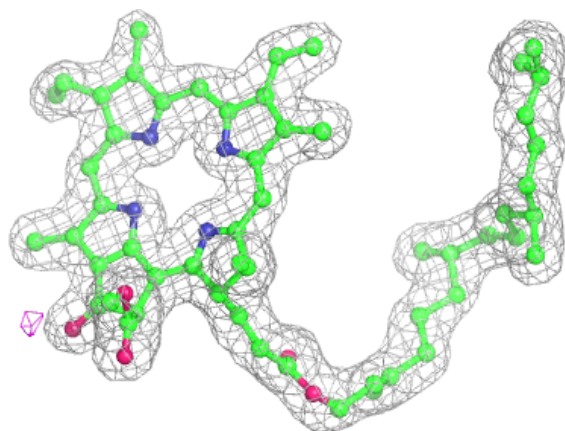
**Electron density around CLA d 406:**

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

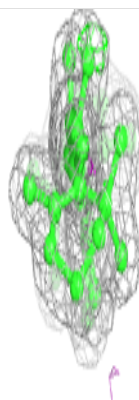
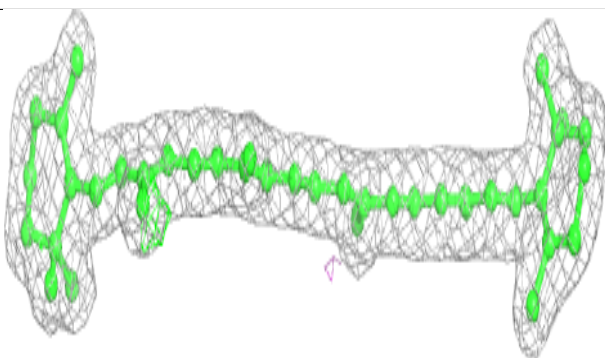
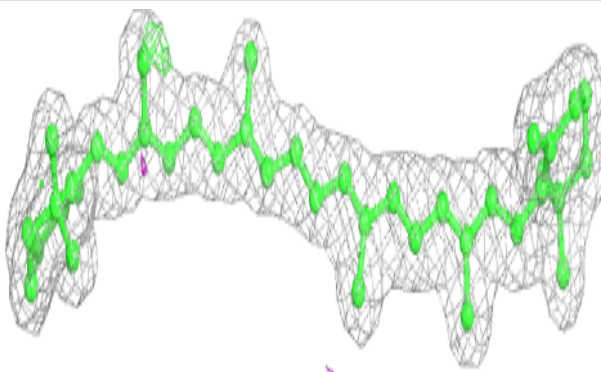


Electron density around PHO A 408:

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

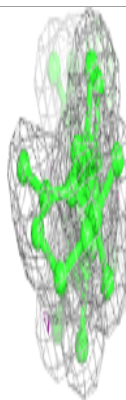
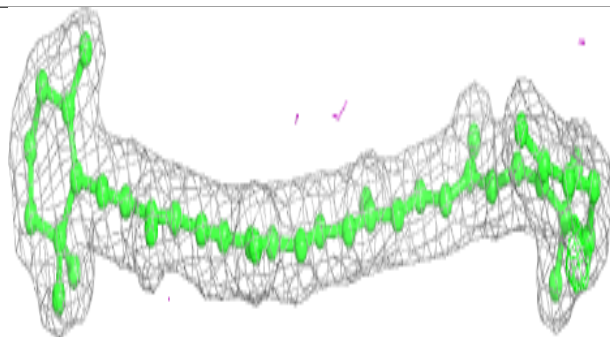
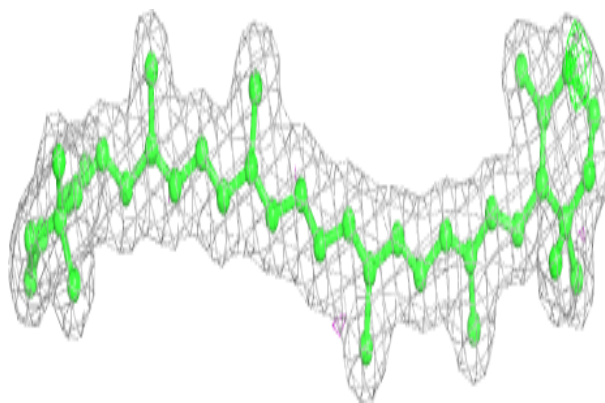
**Electron density around BCR A 410:**

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



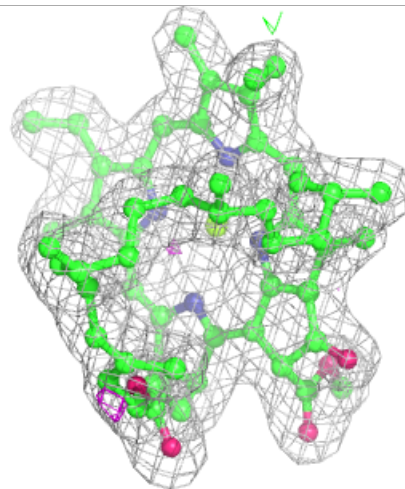
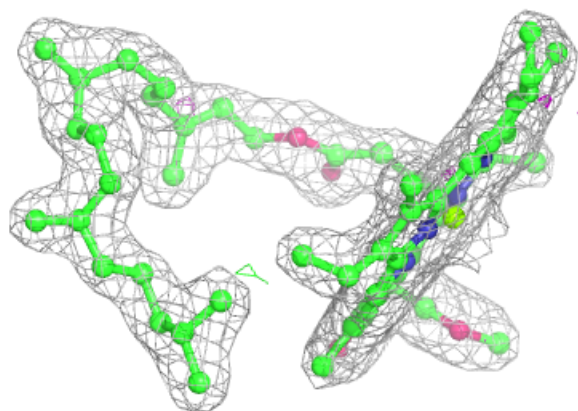
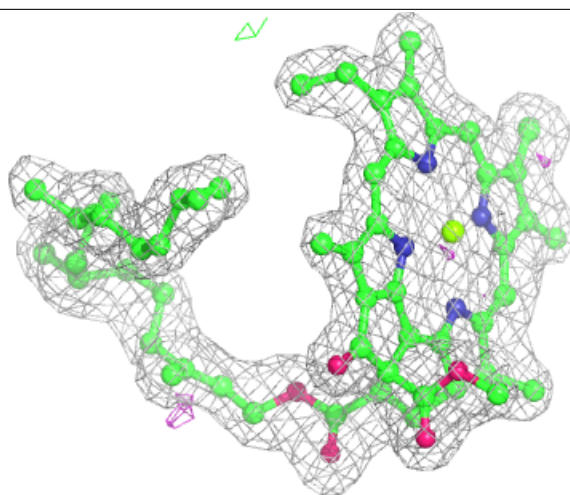
Electron density around BCR B 619:

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



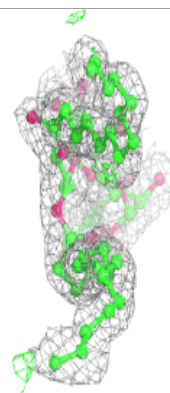
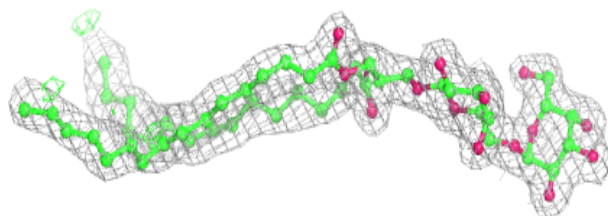
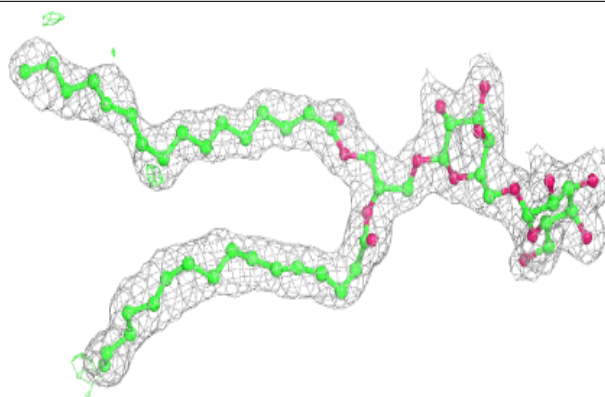
Electron density around CLA C 505:

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

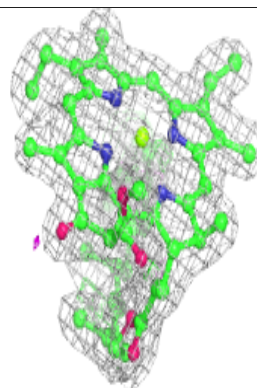
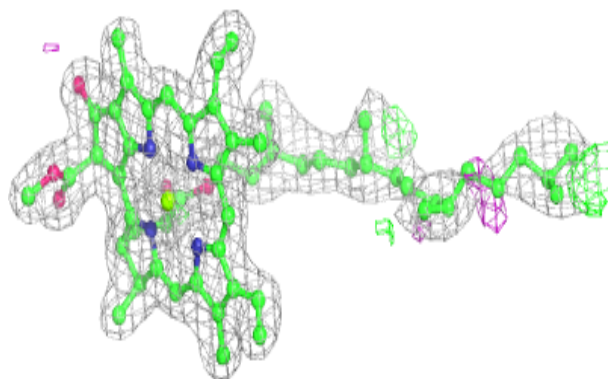
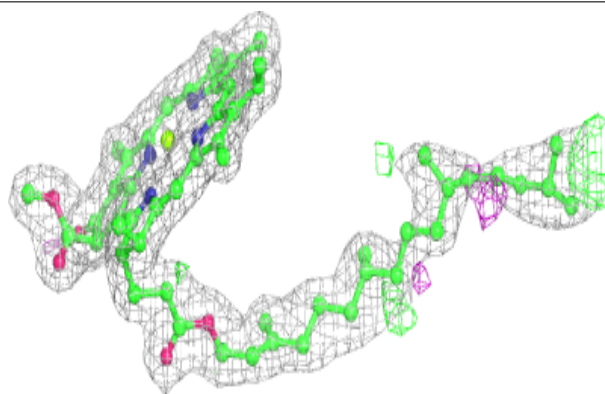


Electron density around DGD c 520:

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

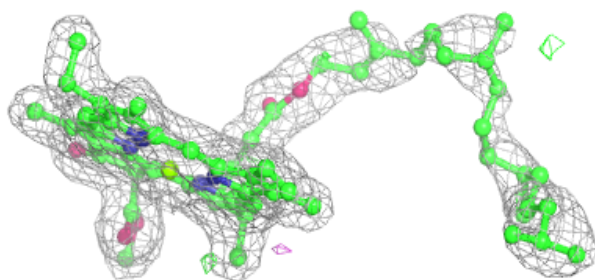
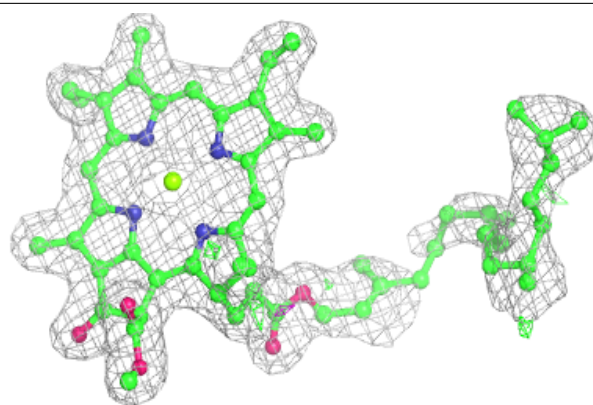
**Electron density around CLA C 506:**

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

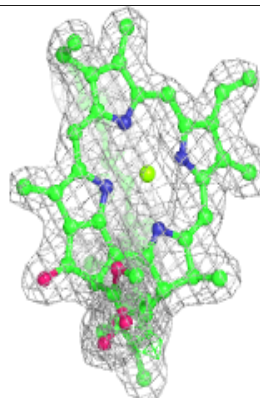
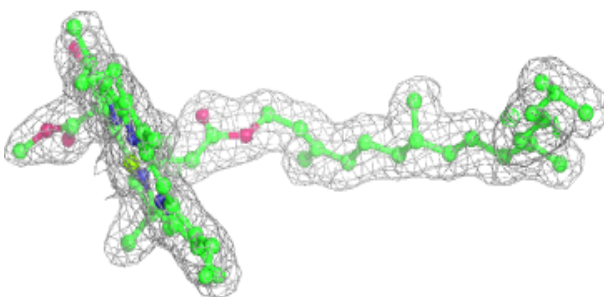
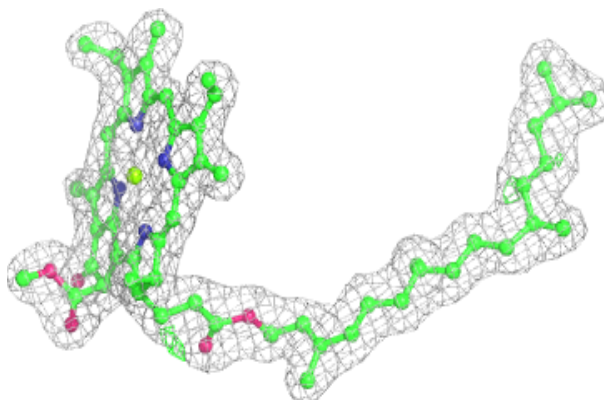


Electron density around CLA a 413:

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

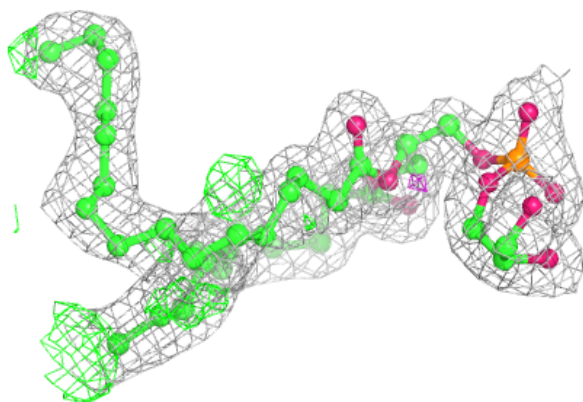
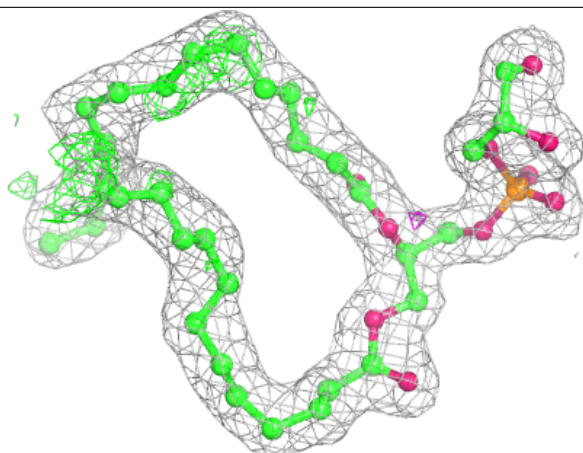
**Electron density around CLA B 611:**

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

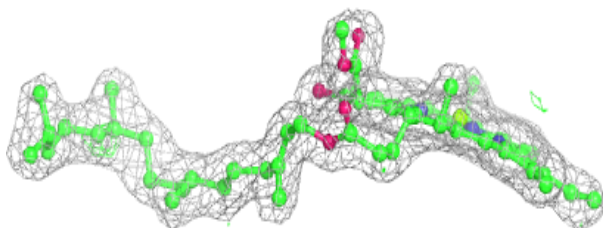
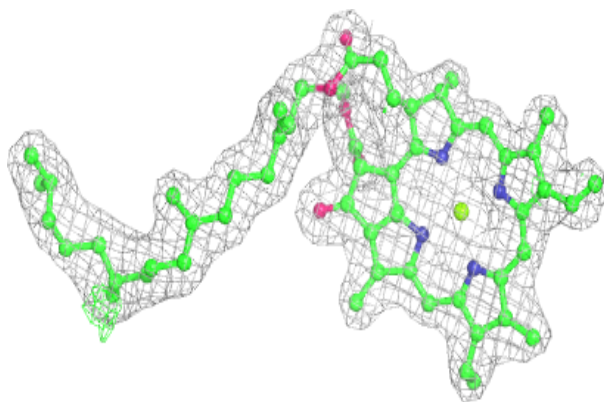


Electron density around LHG D 412:

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

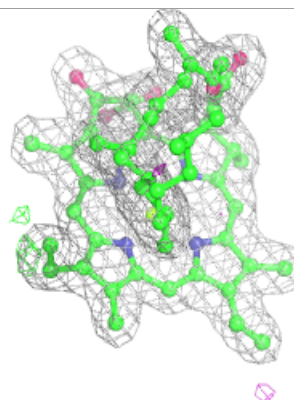
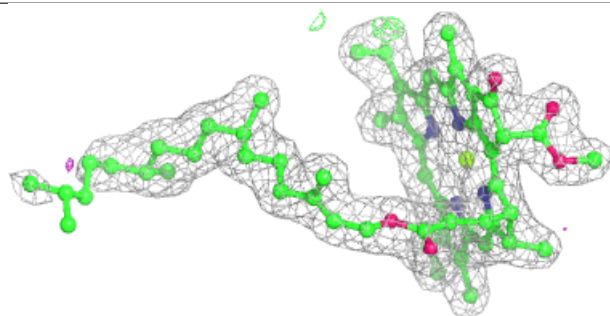
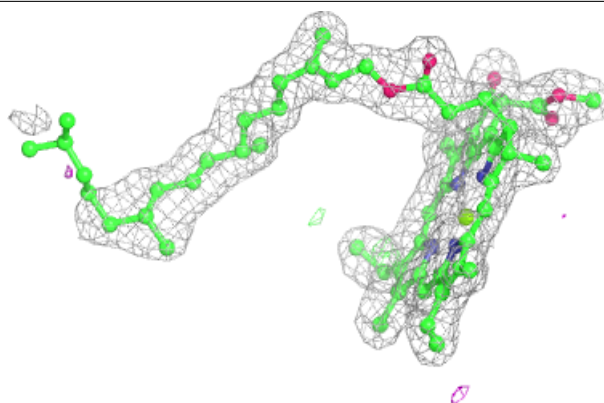
**Electron density around CLA b 606:**

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

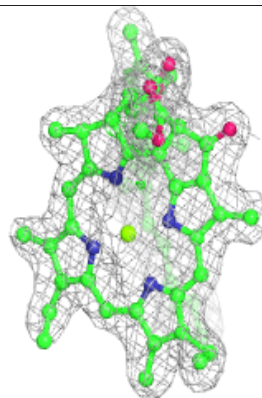
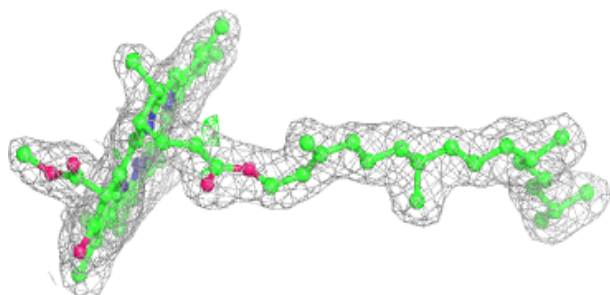
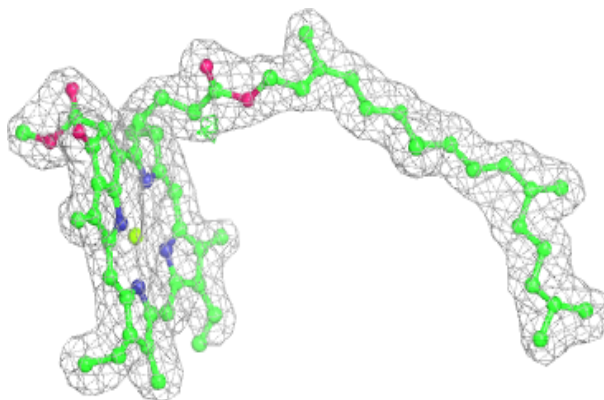


Electron density around CLA C 510:

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

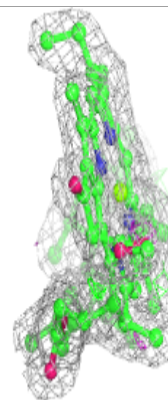
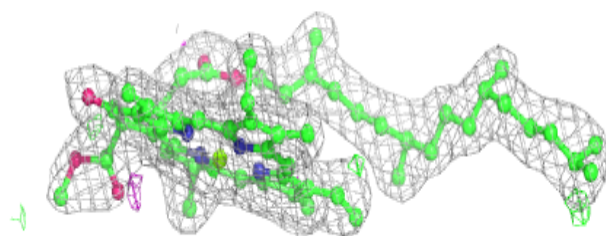
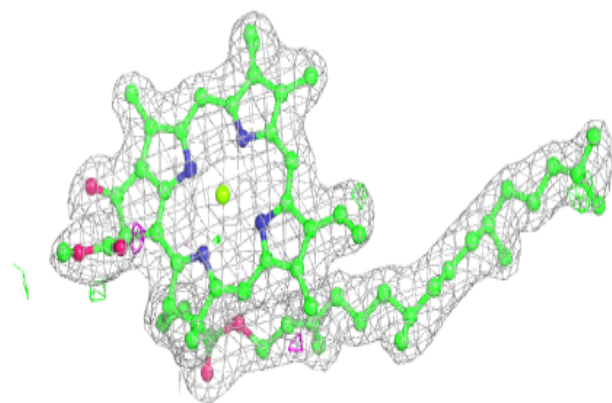
**Electron density around CLA b 613:**

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



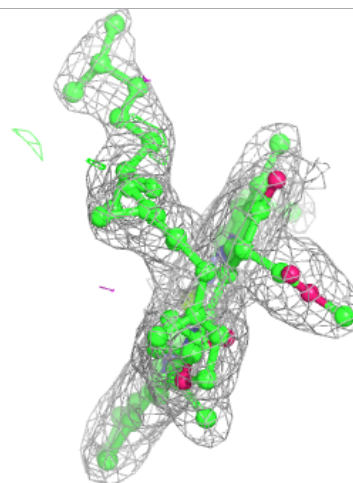
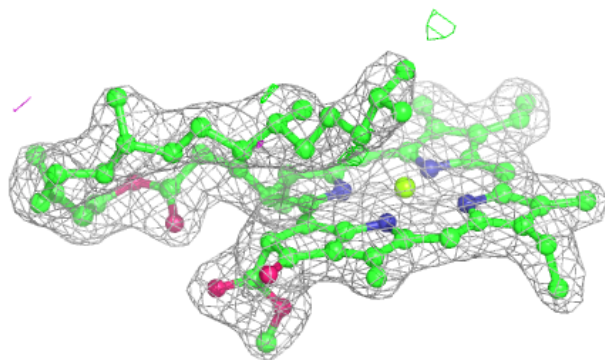
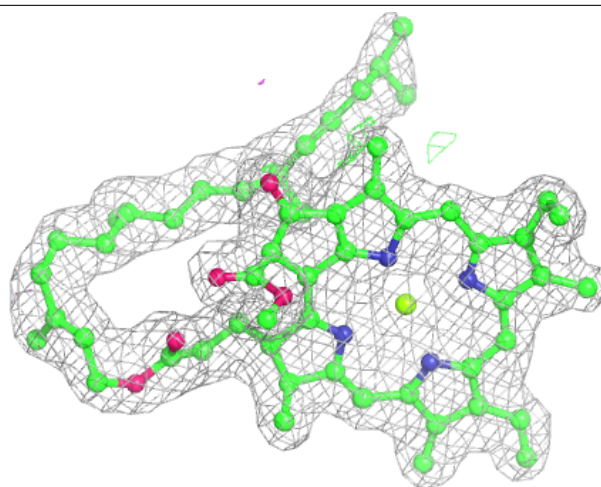
Electron density around CLA C 503:

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



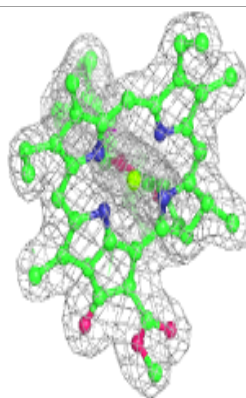
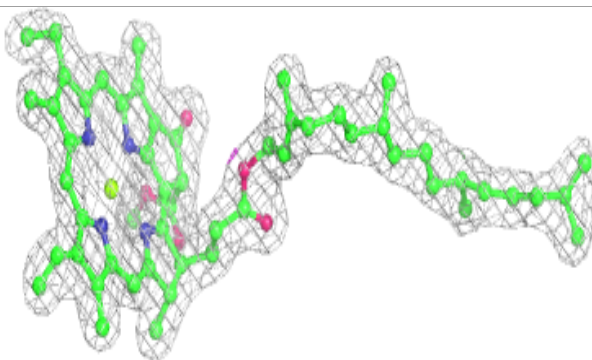
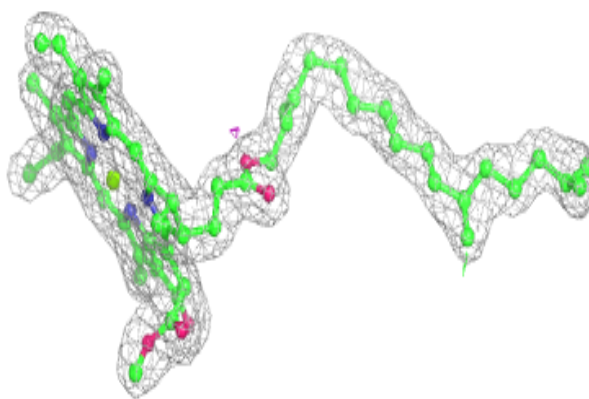
Electron density around CLA c 511:

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

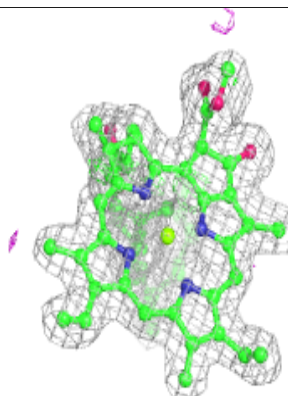
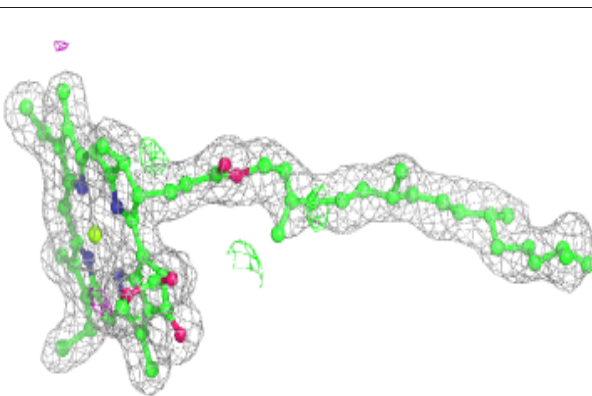
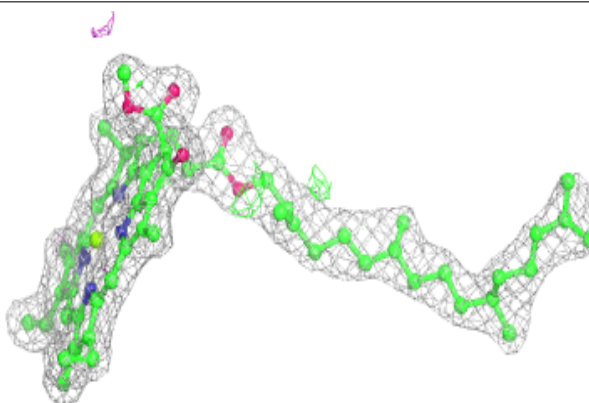


Electron density around CLA C 504:

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

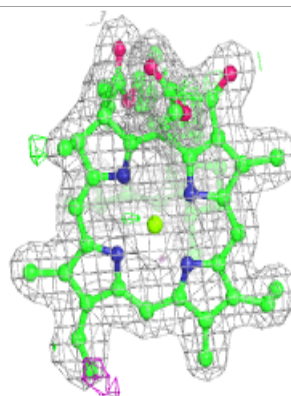
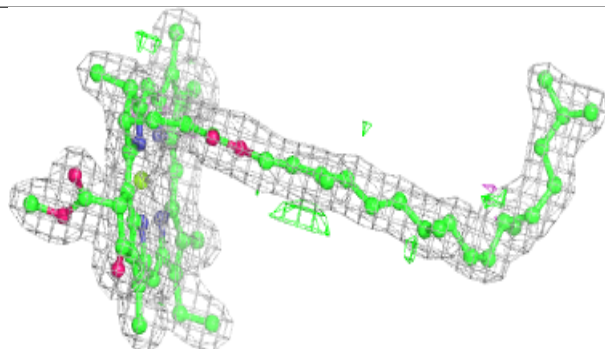
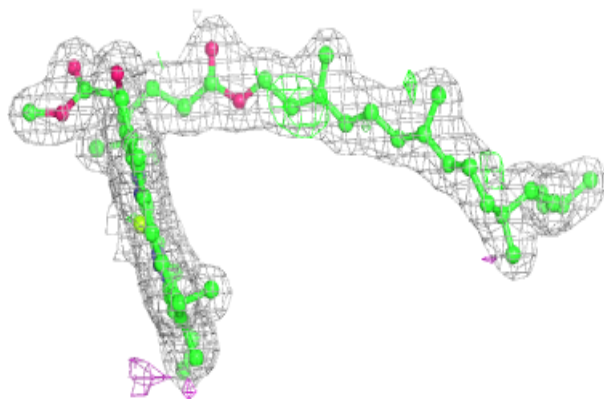
**Electron density around CLA B 606:**

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

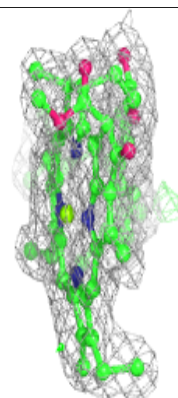
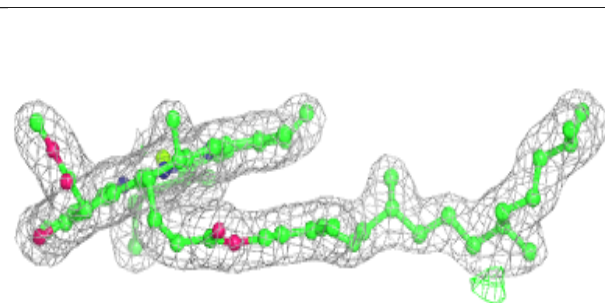
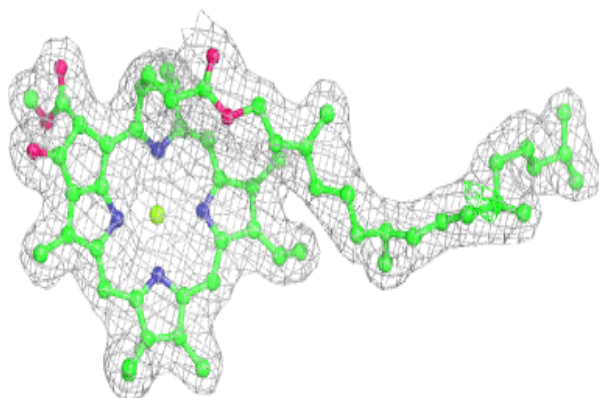


Electron density around CLA B 607:

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

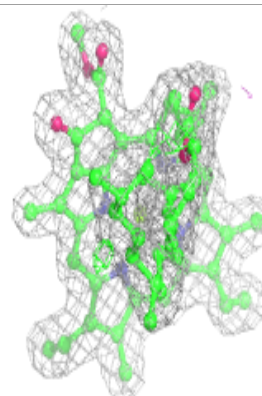
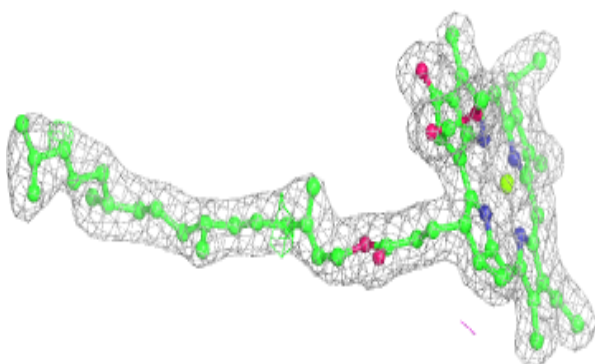
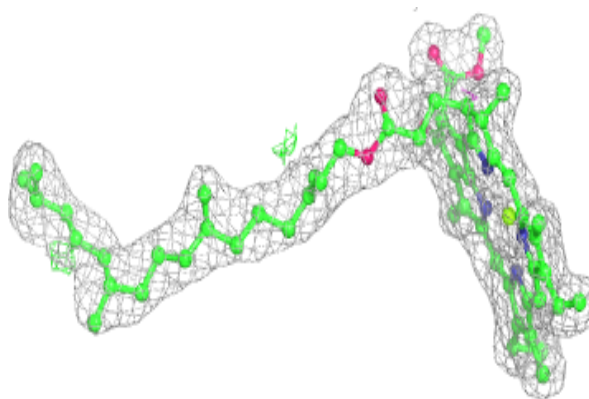
**Electron density around CLA b 607:**

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

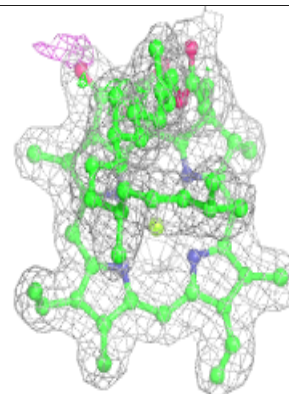
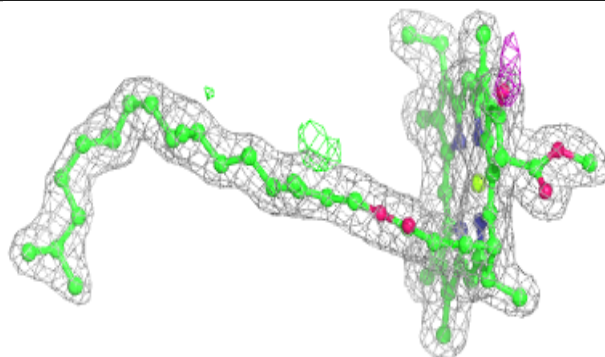
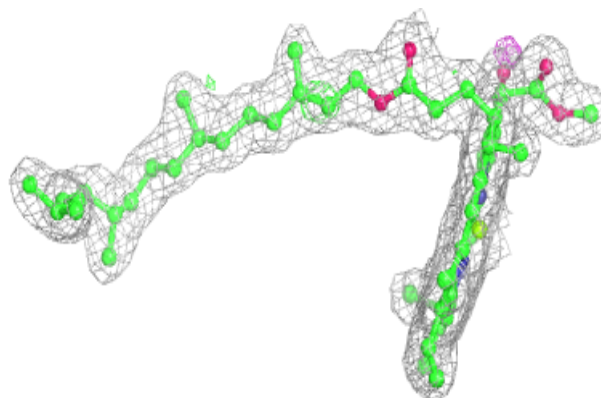


Electron density around CLA b 608:

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

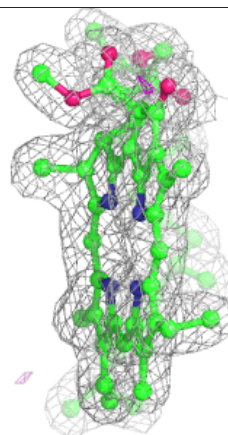
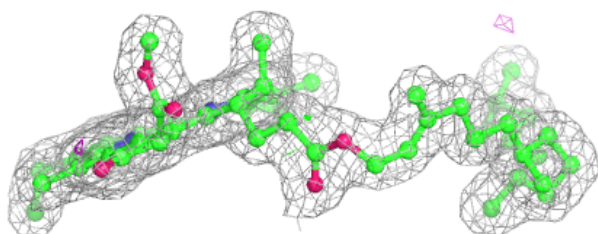
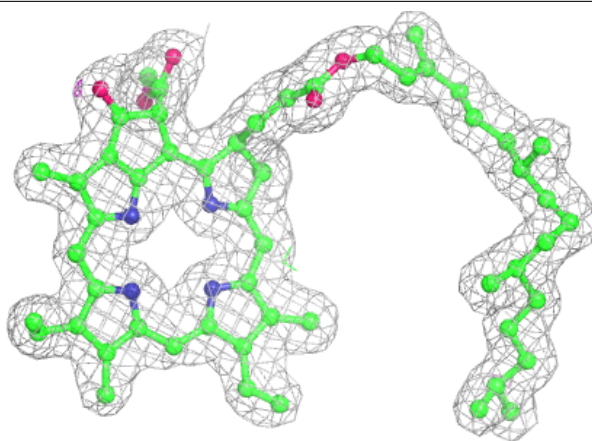
**Electron density around CLA b 609:**

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

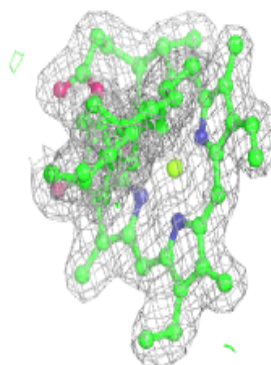
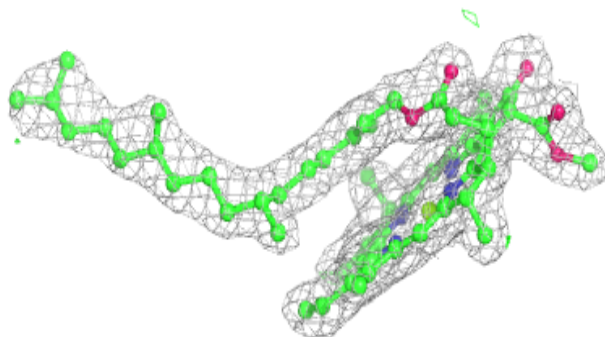
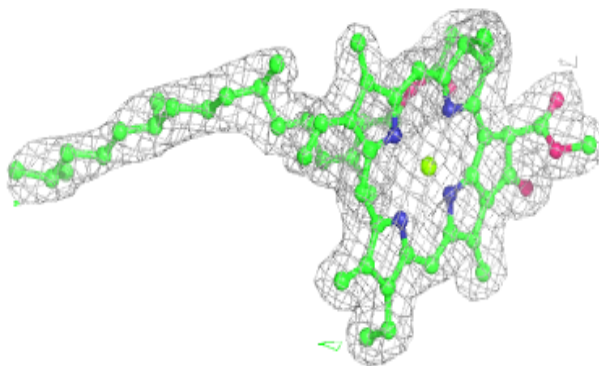


Electron density around PHO a 412:

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

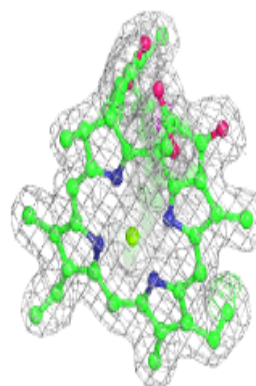
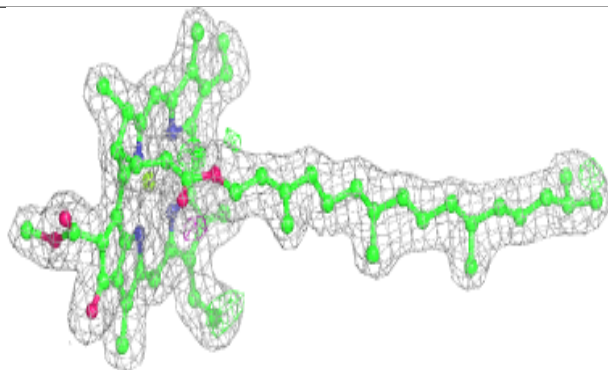
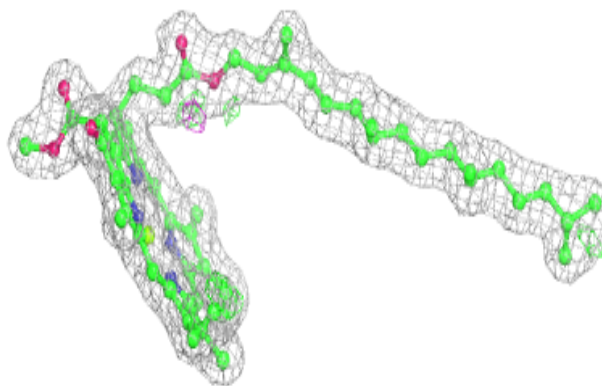
**Electron density around CLA C 507:**

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

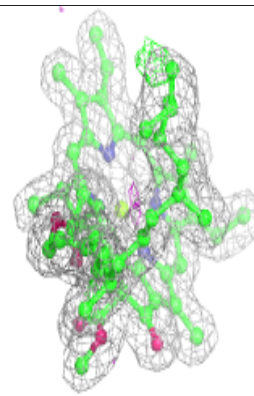
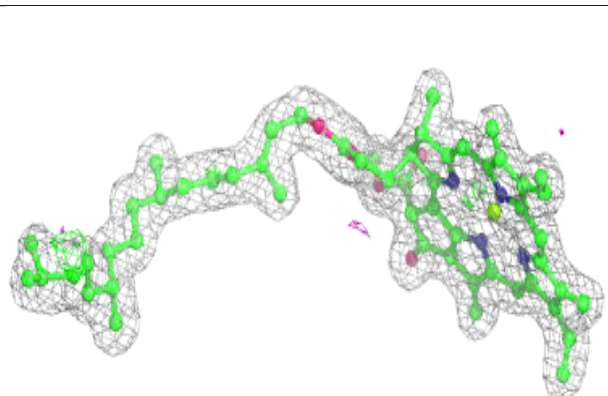
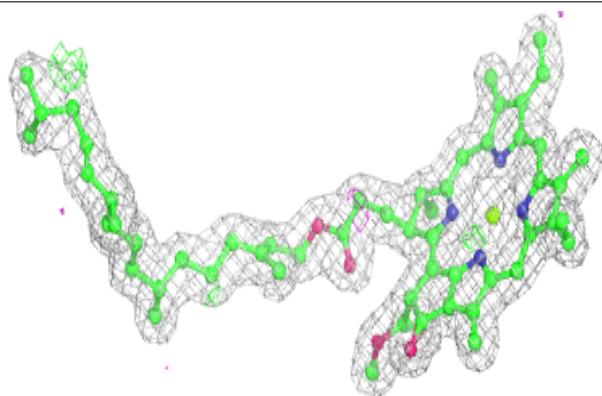


Electron density around CLA b 611:

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

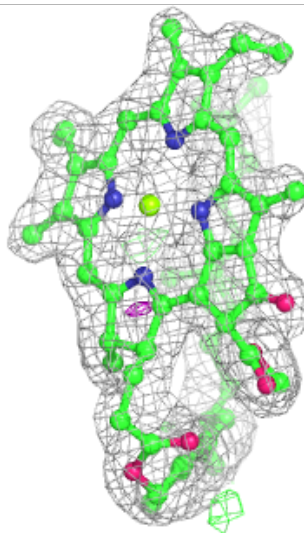
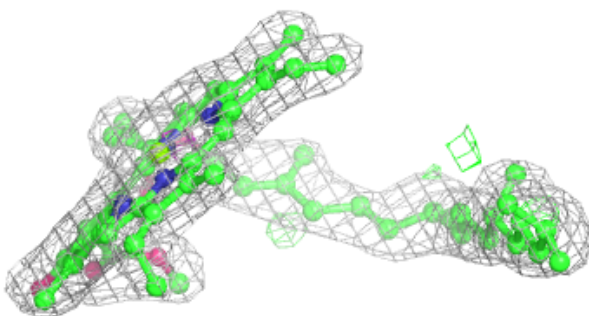
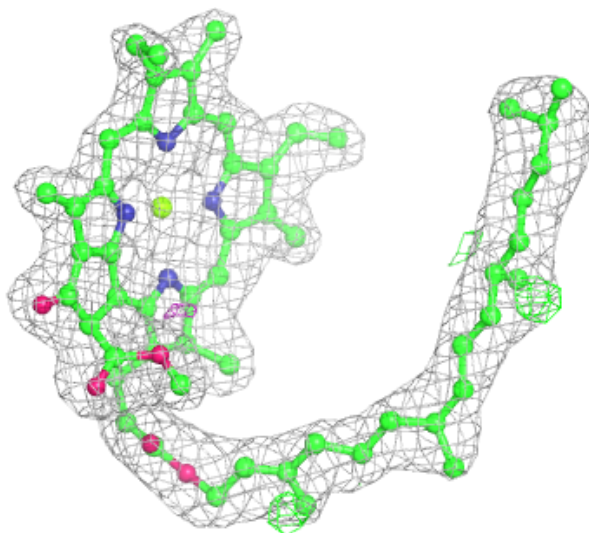
**Electron density around CLA A 405:**

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



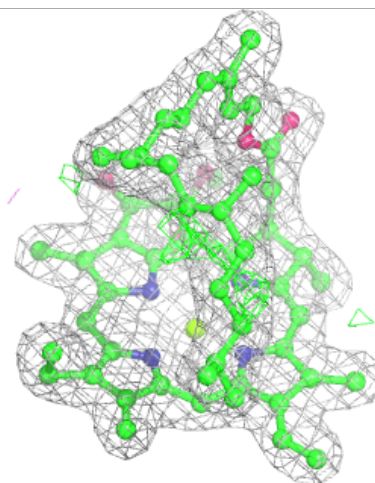
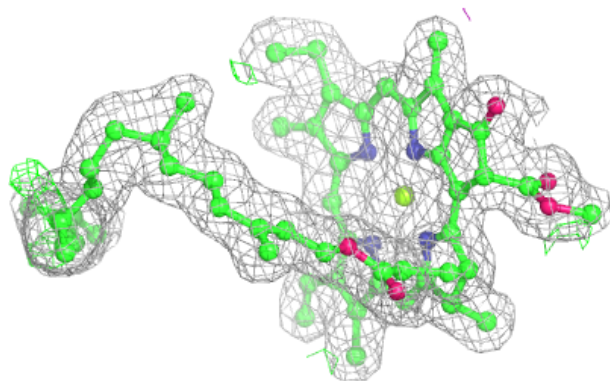
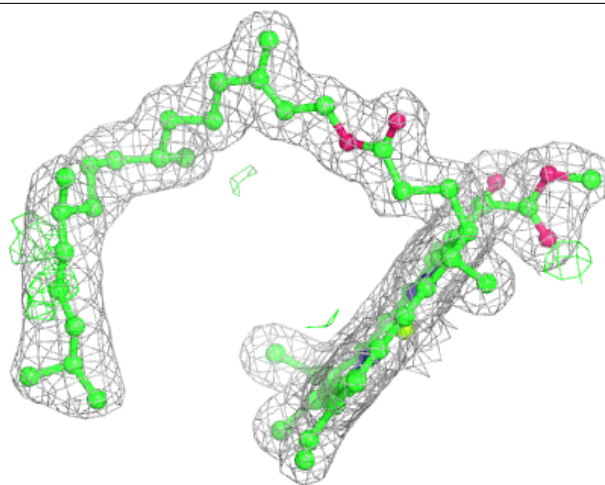
Electron density around CLA C 509:

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



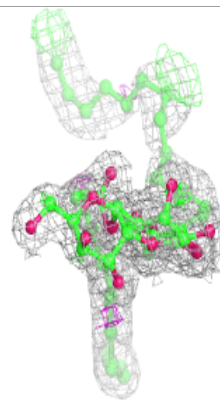
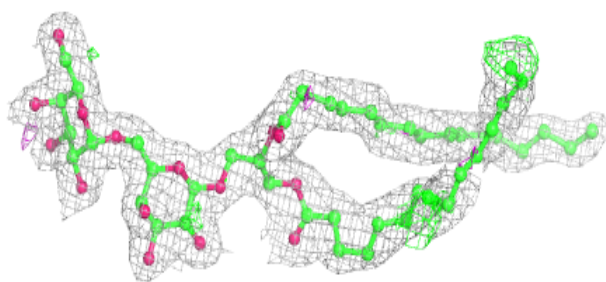
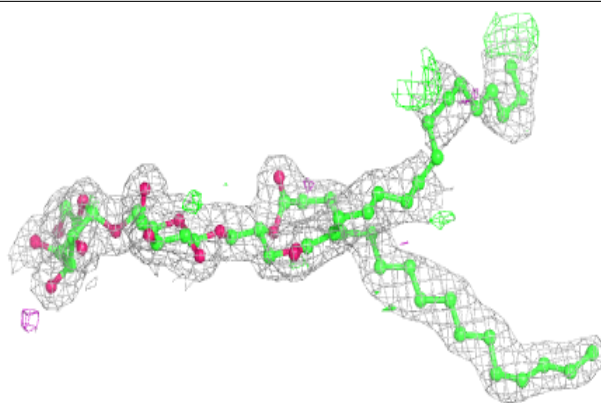
Electron density around CLA b 615:

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

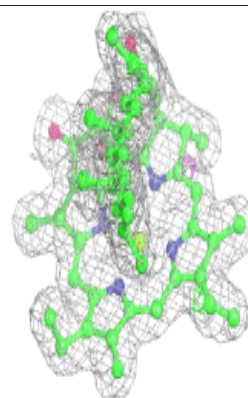
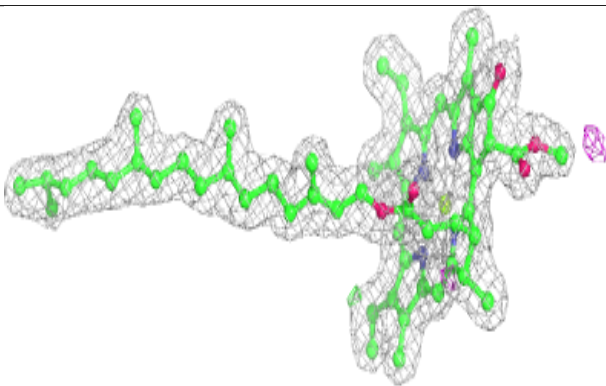
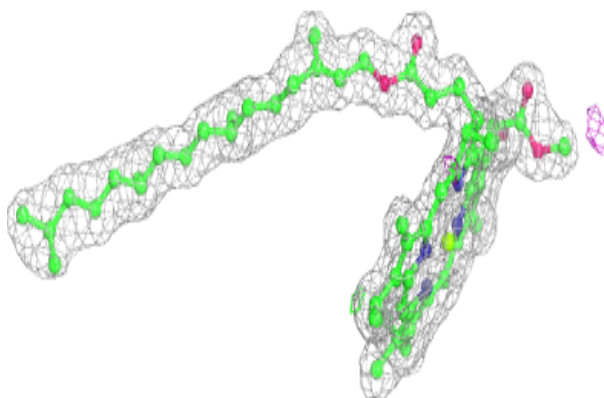


Electron density around DGD C 518:

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

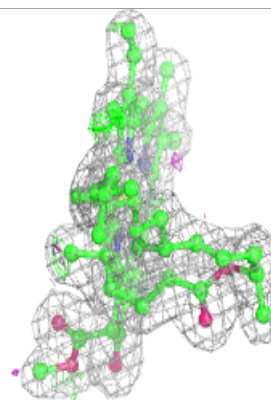
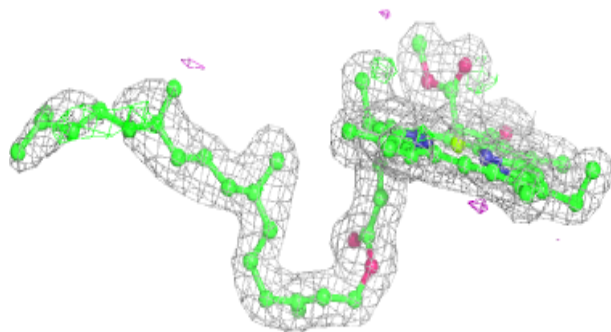
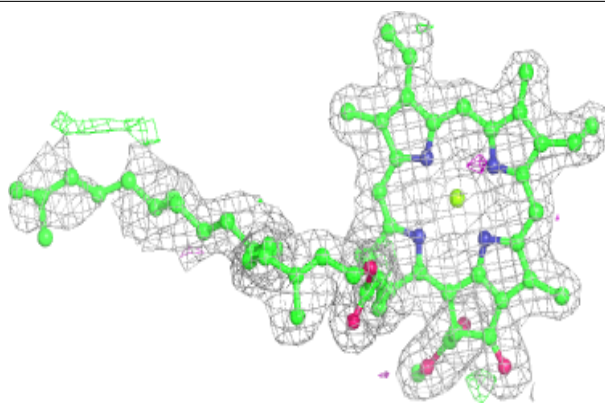
**Electron density around CLA B 609:**

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



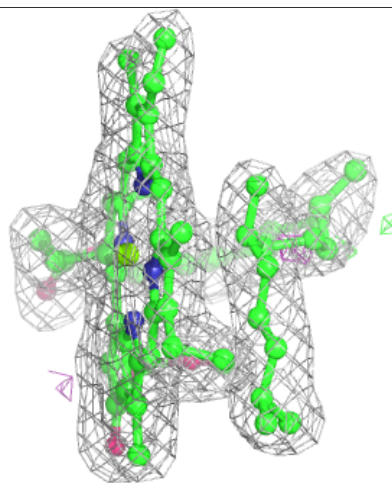
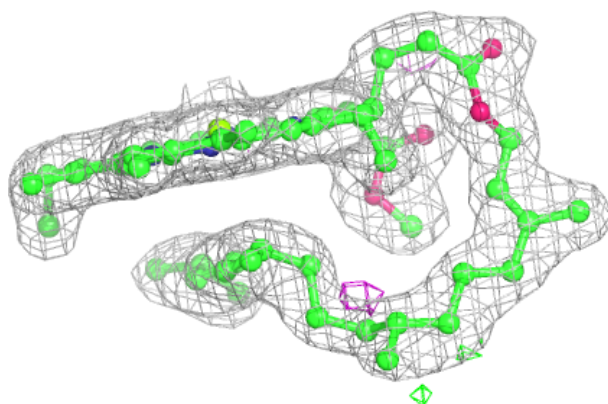
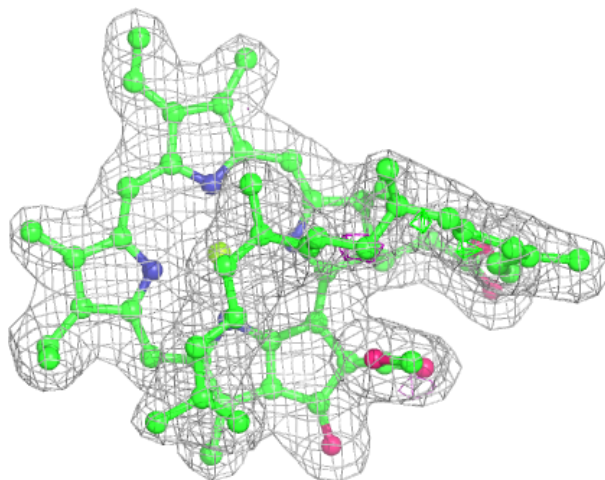
Electron density around CLA A 406:

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



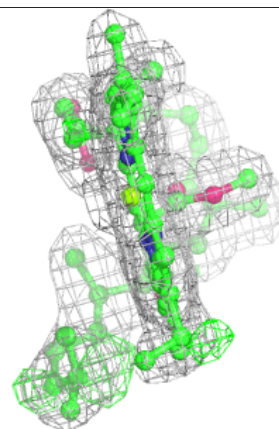
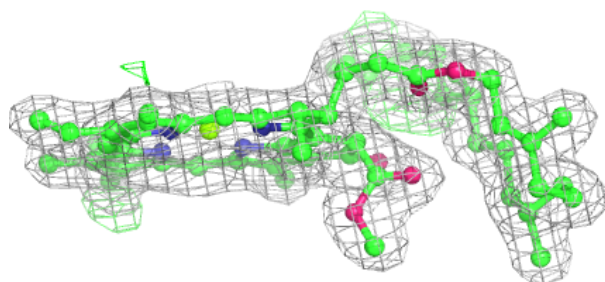
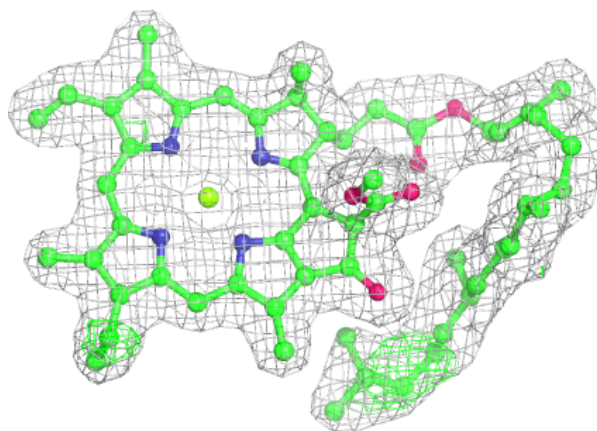
Electron density around CLA C 512:

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

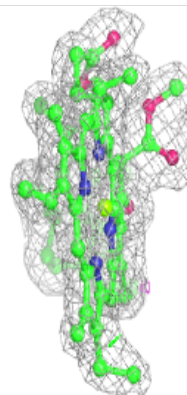
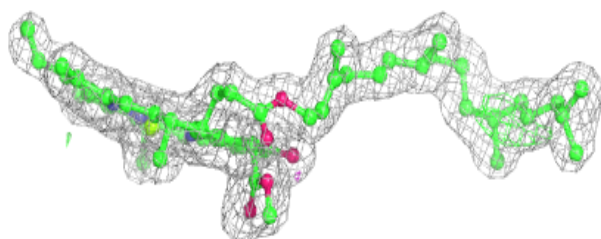
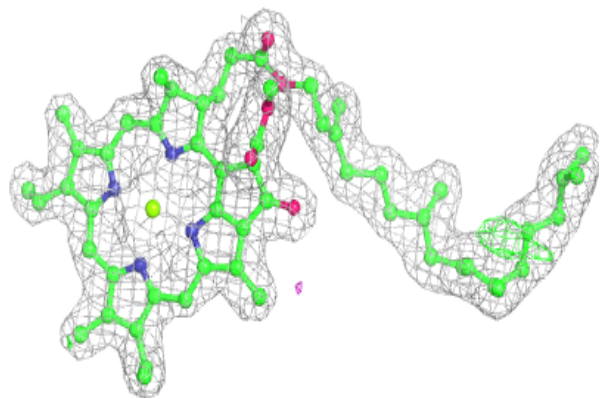


Electron density around CLA B 612:

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

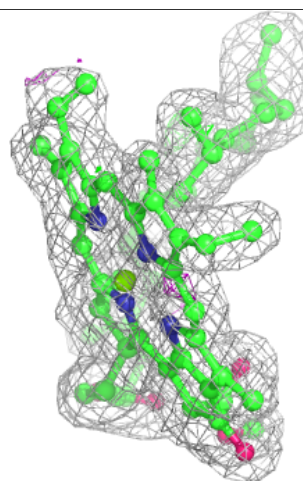
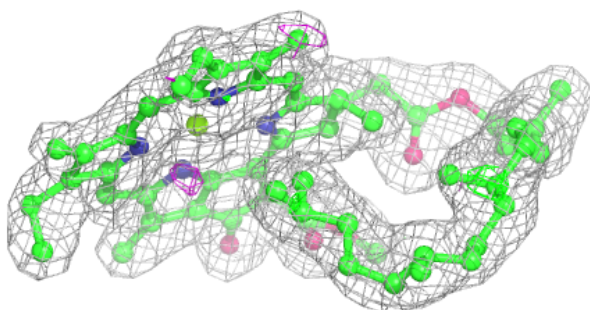
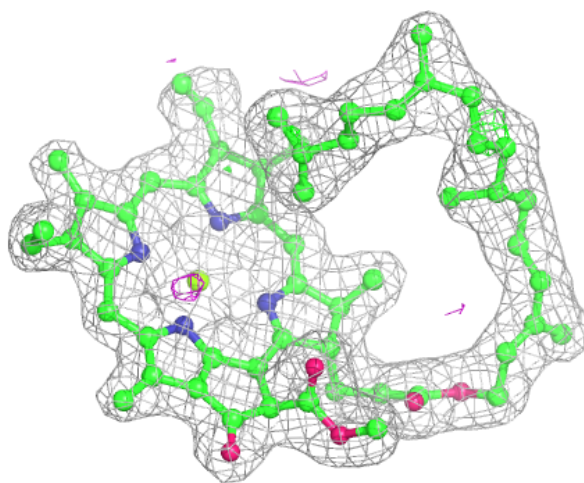
**Electron density around CLA B 604:**

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



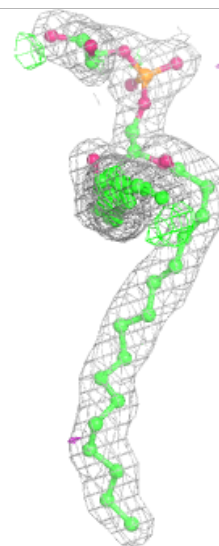
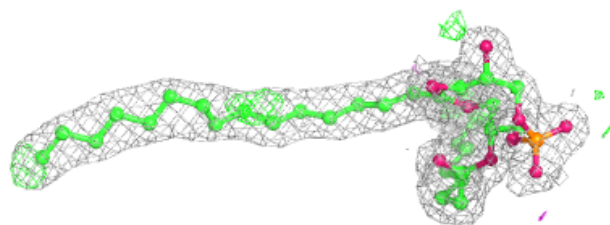
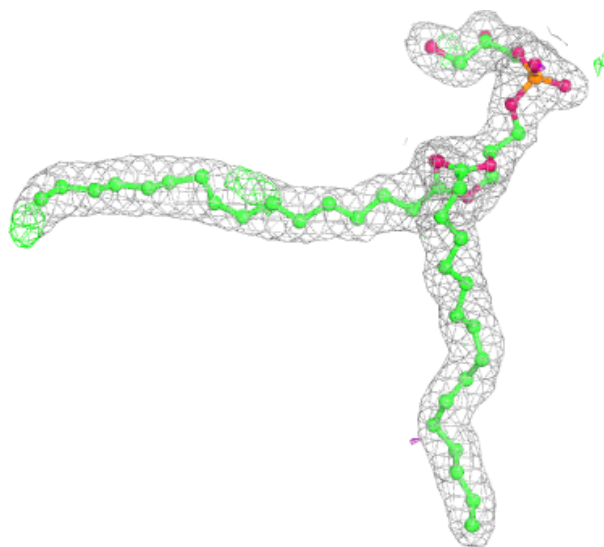
Electron density around CLA B 617:

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



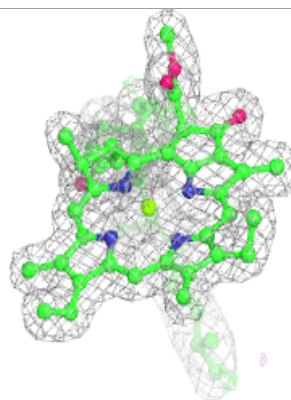
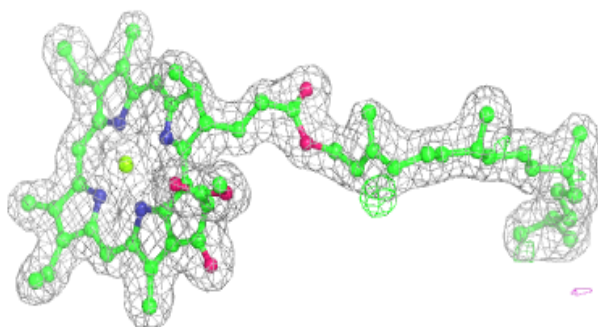
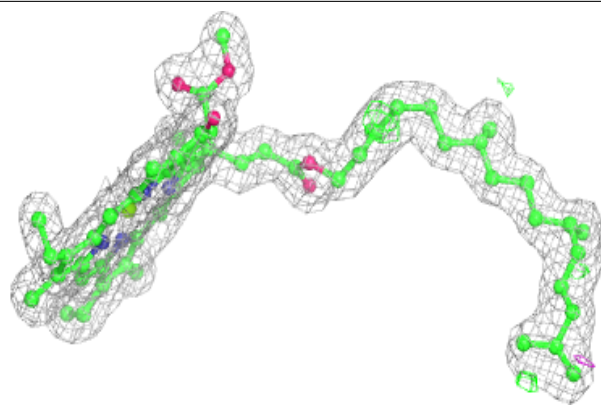
Electron density around LHG L 101:

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

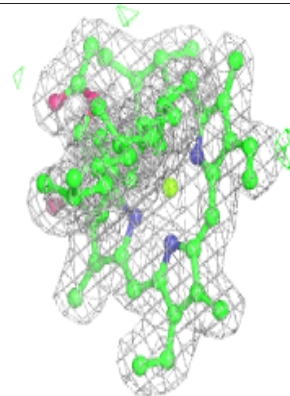
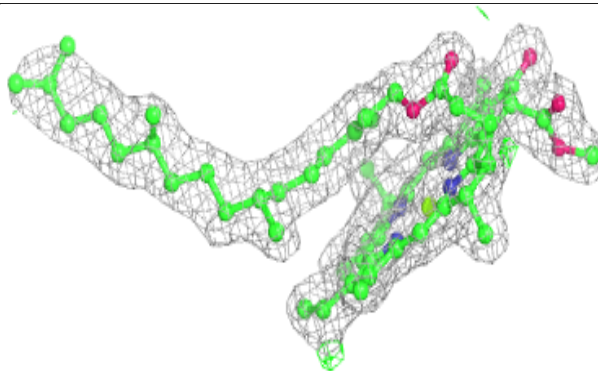
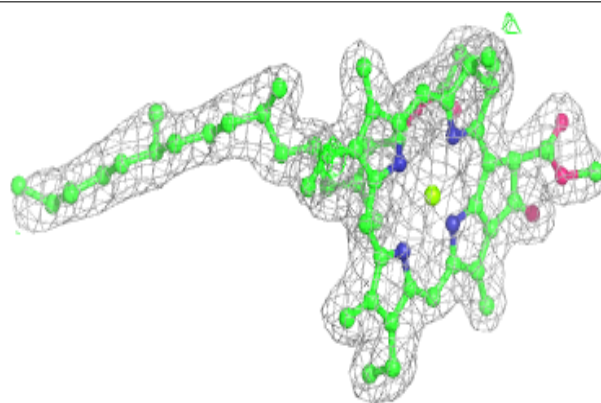


Electron density around CLA D 405:

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

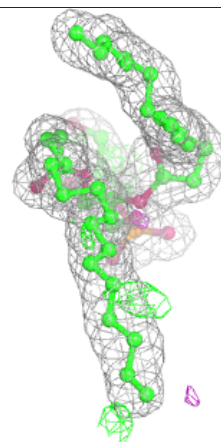
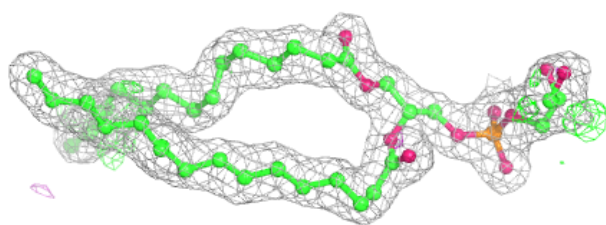
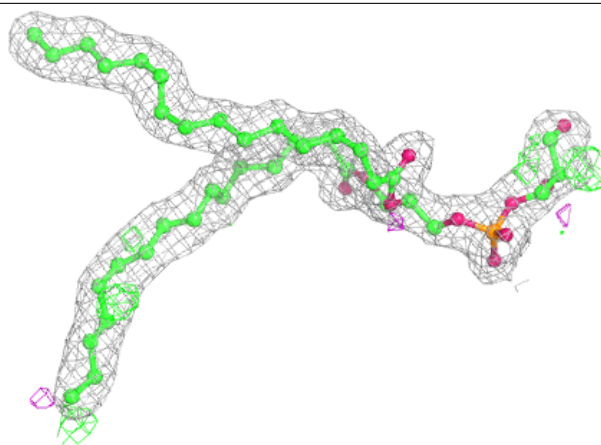
**Electron density around CLA c 507:**

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



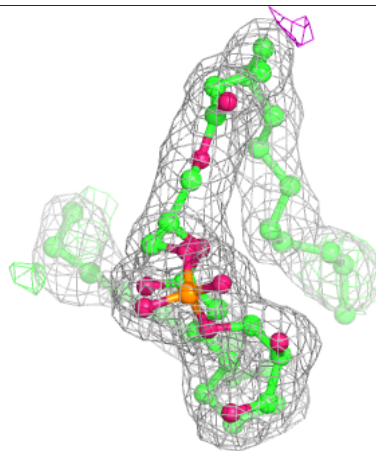
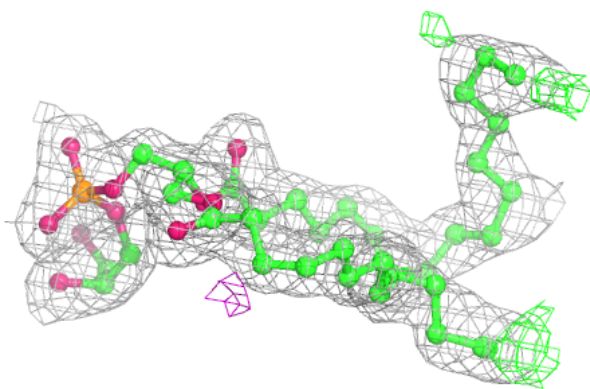
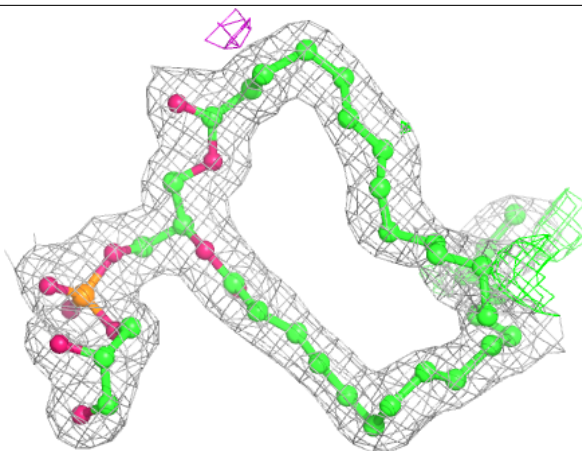
Electron density around LHG d 410:

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



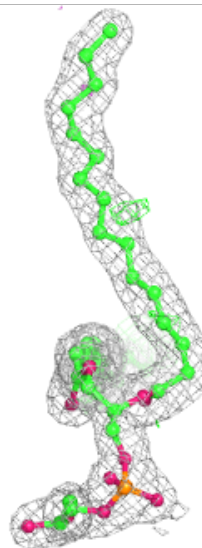
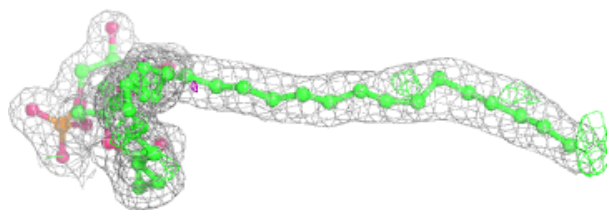
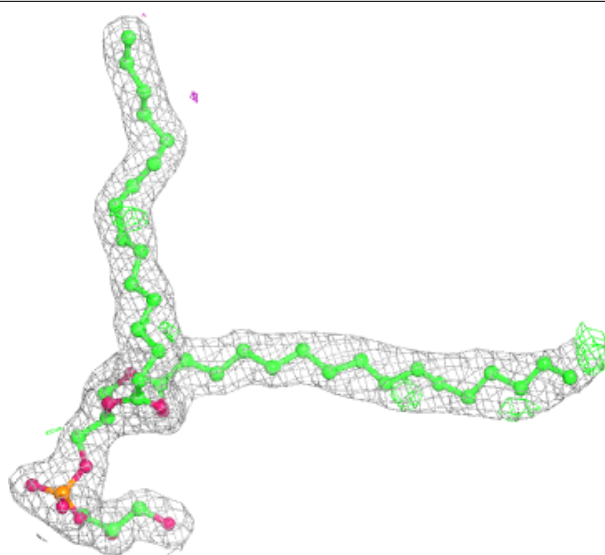
Electron density around LHG d 411:

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



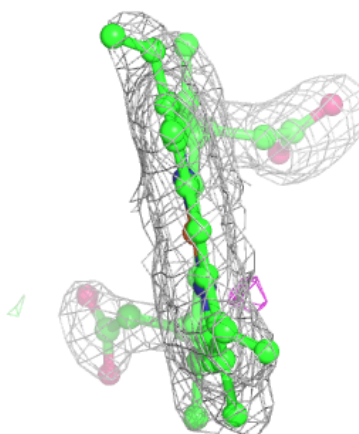
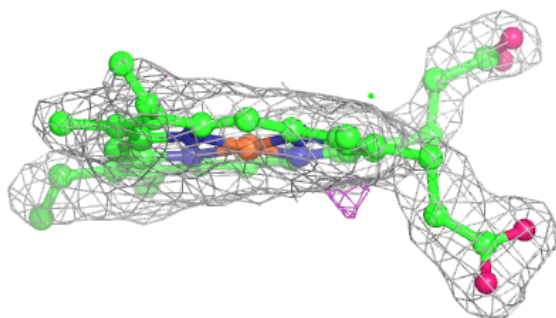
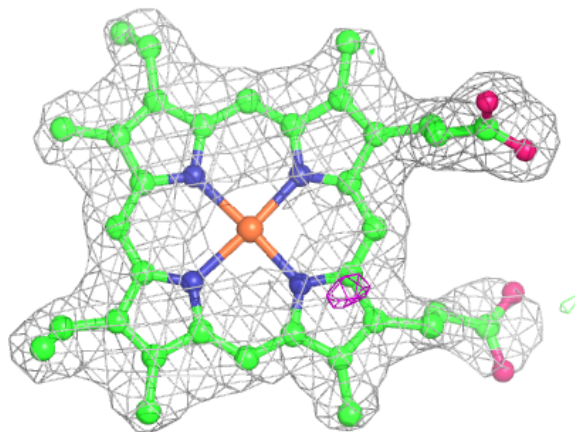
Electron density around LHG 1 102:

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



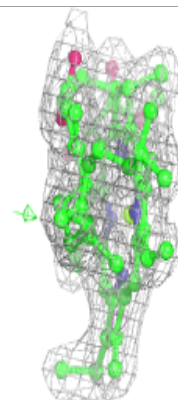
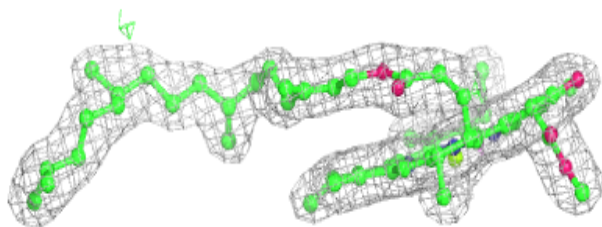
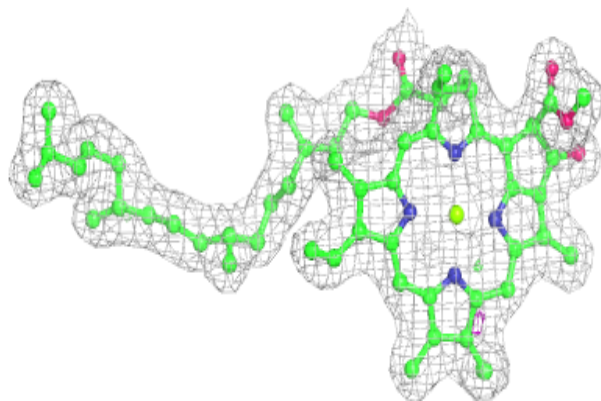
Electron density around HEM e 102:

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

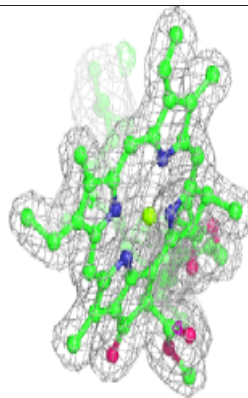
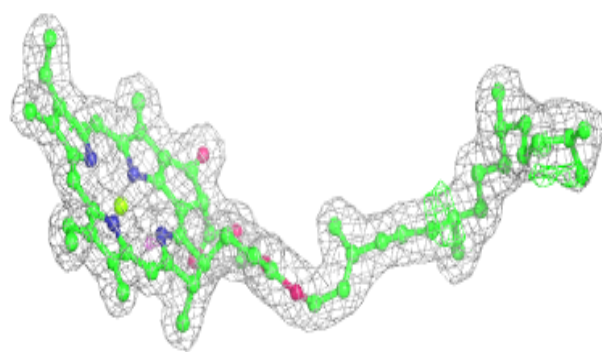
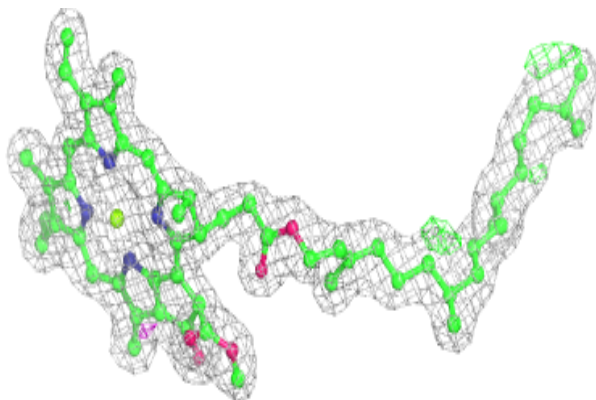


Electron density around CLA B 605:

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

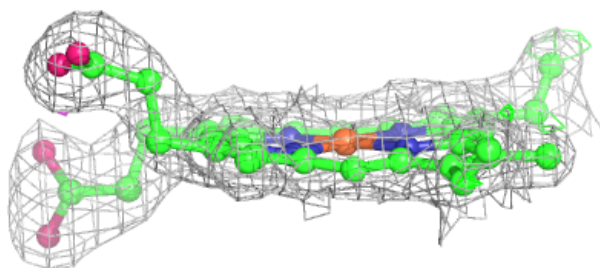
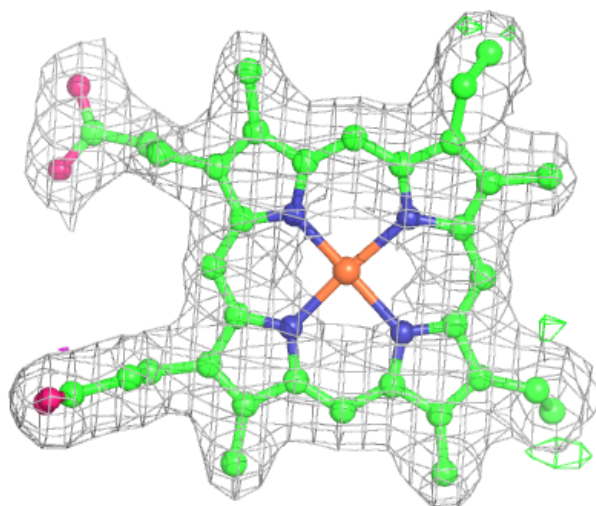
**Electron density around CLA a 409:**

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



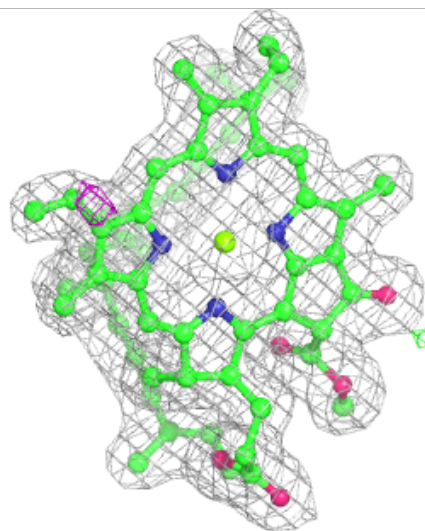
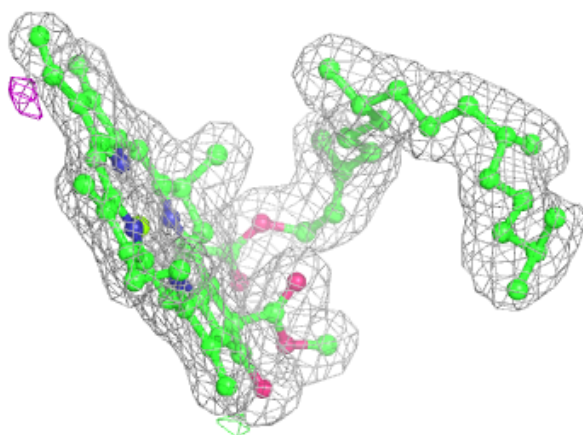
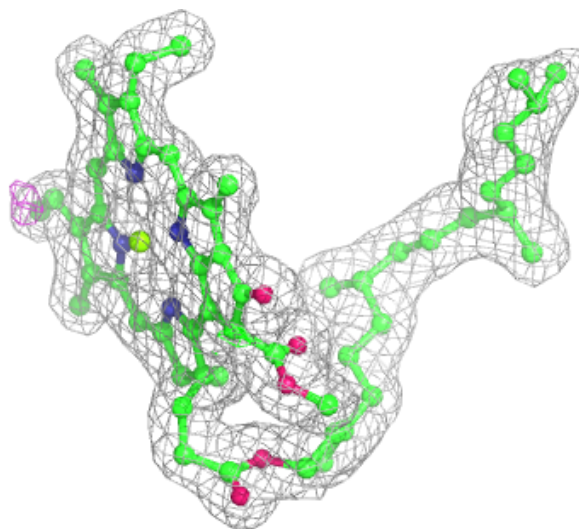
Electron density around HEC v 201:

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



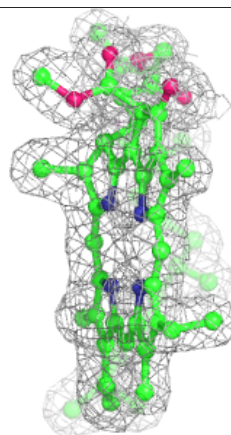
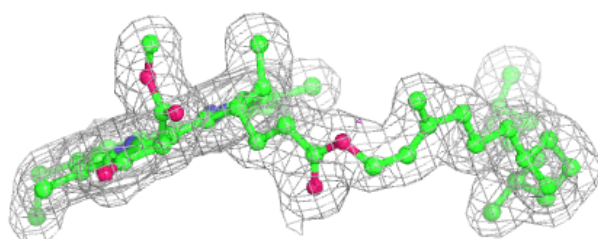
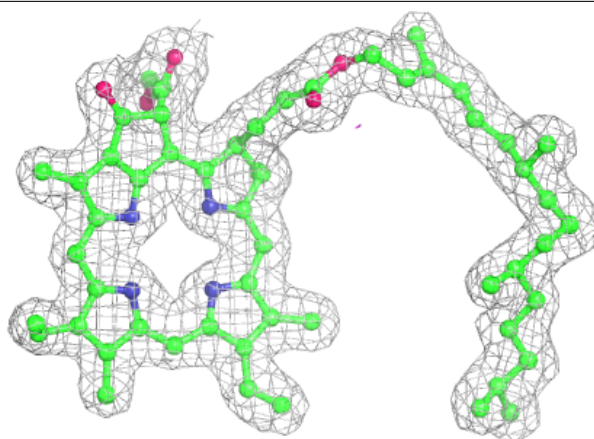
Electron density around CLA B 615:

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



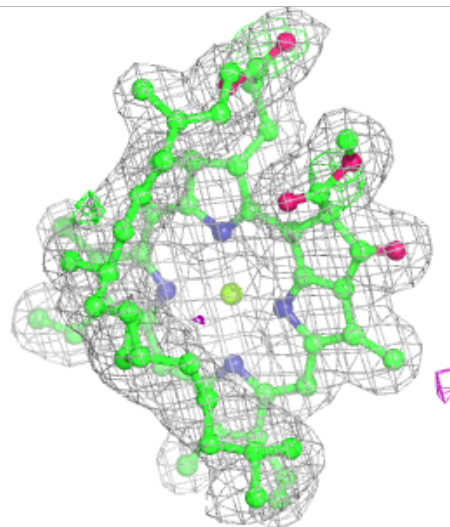
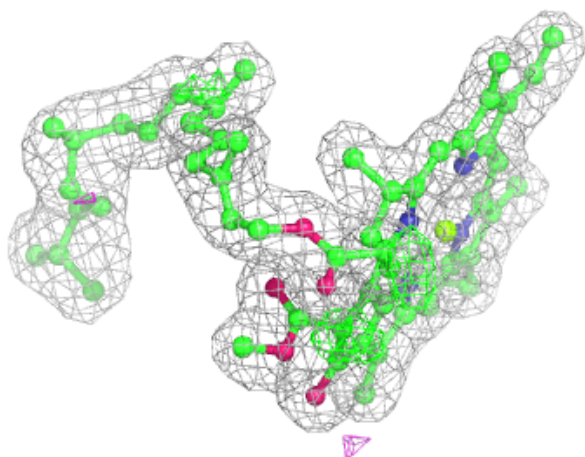
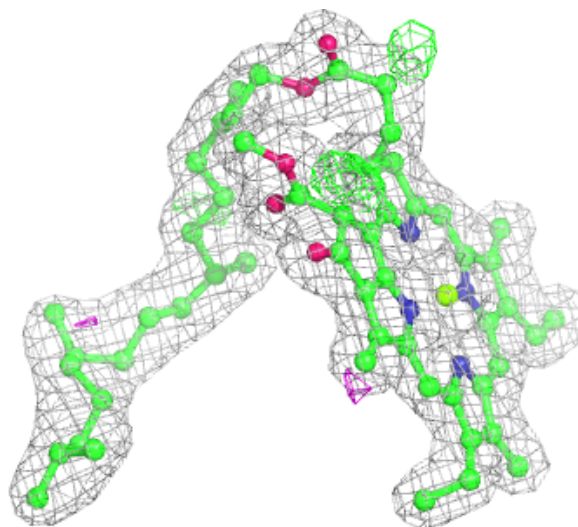
Electron density around PHO A 407:

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



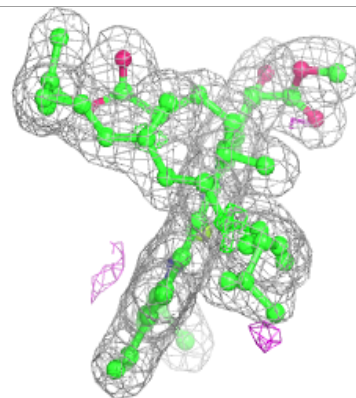
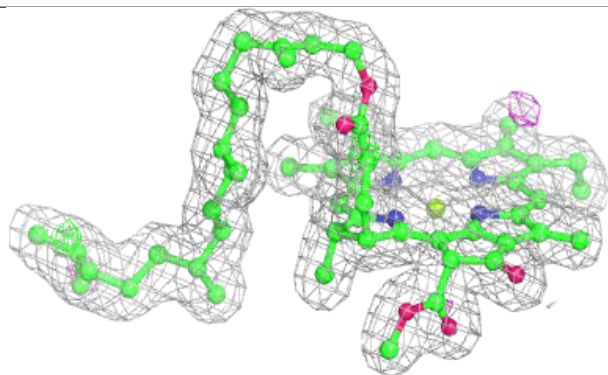
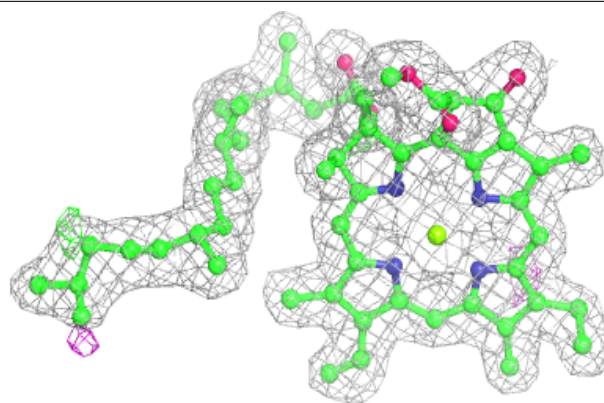
Electron density around CLA b 617:

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

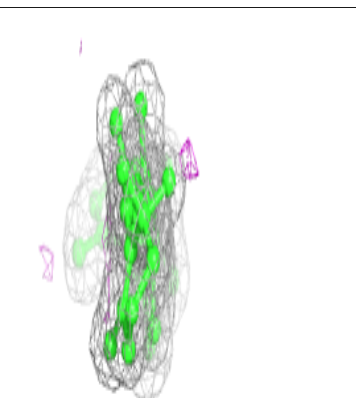
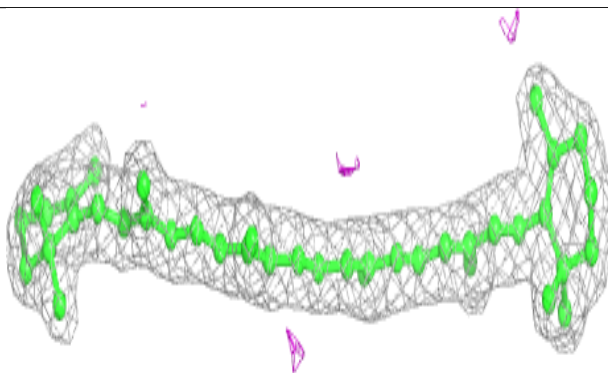
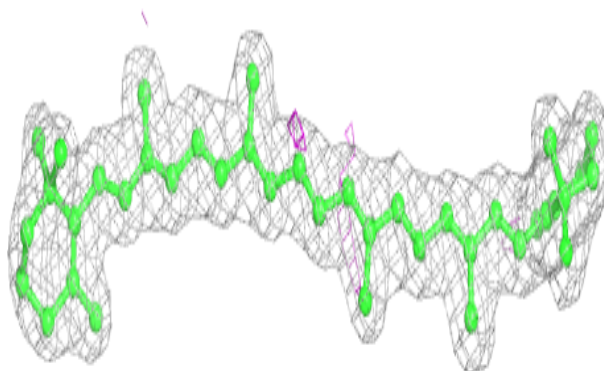


Electron density around CLA D 401:

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

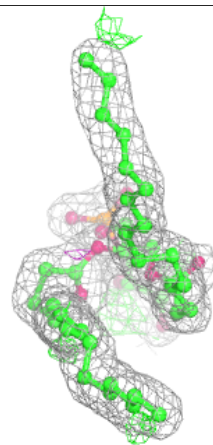
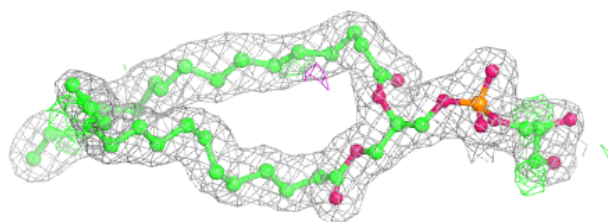
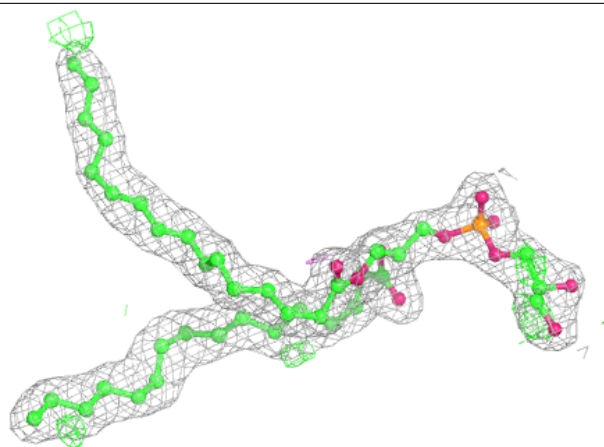
**Electron density around BCR b 621:**

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



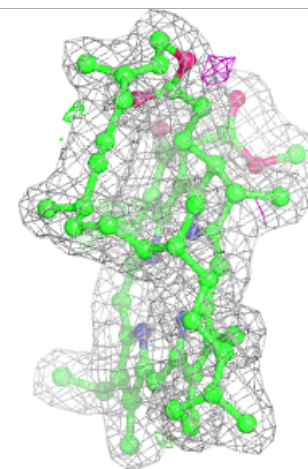
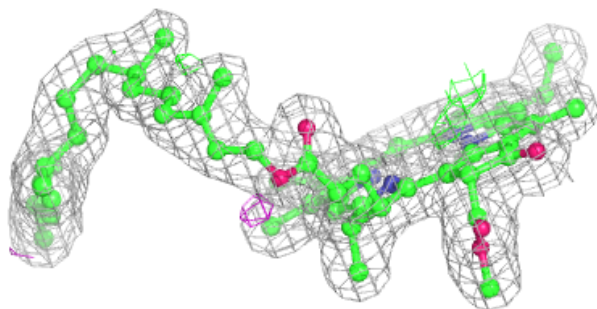
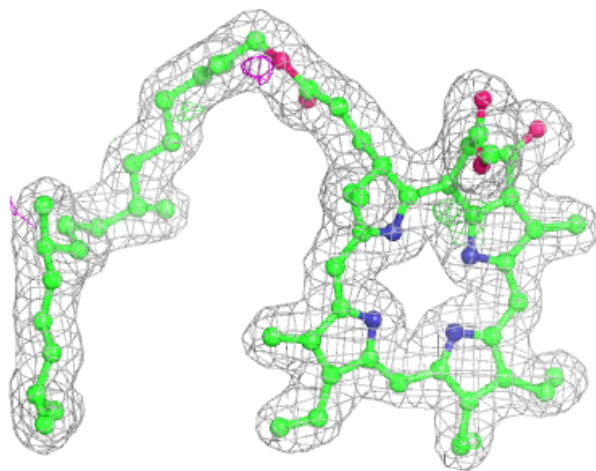
Electron density around LHG D 411:

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



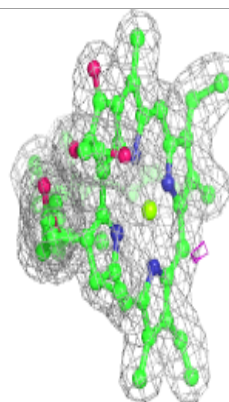
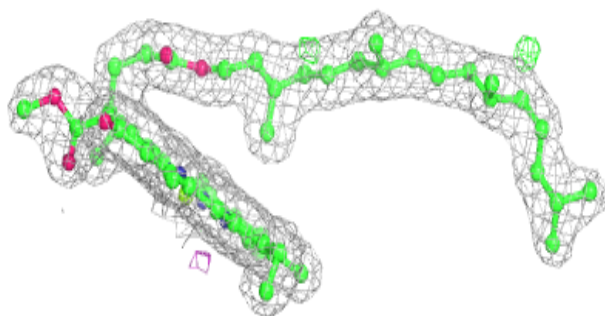
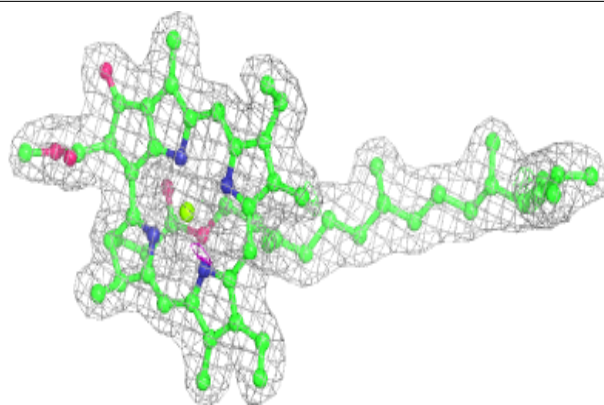
Electron density around PHO d 401:

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

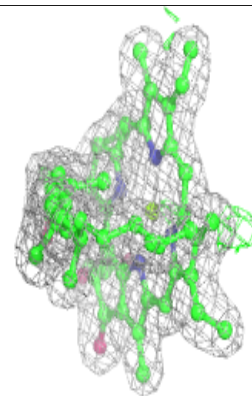
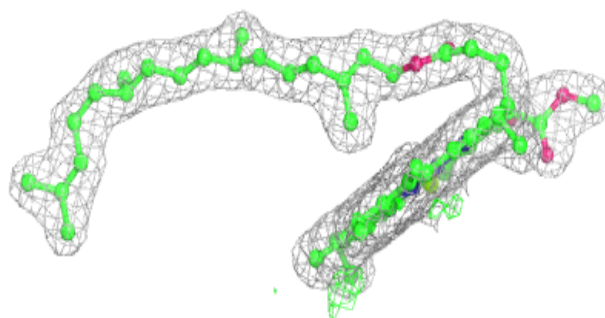
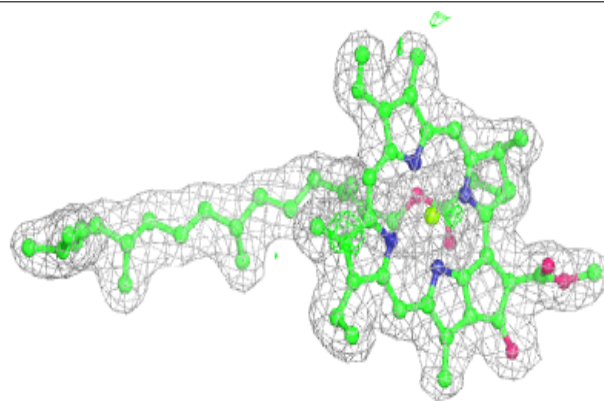


Electron density around CLA B 610:

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

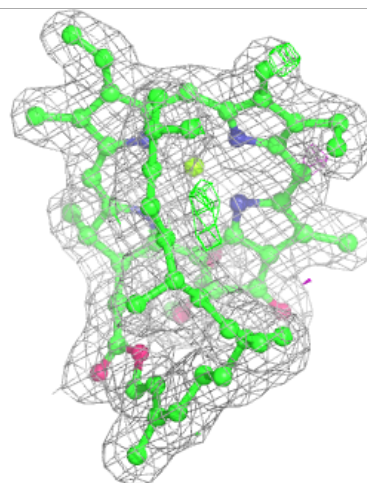
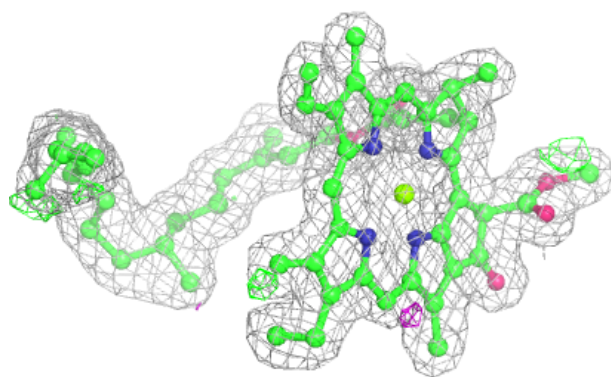
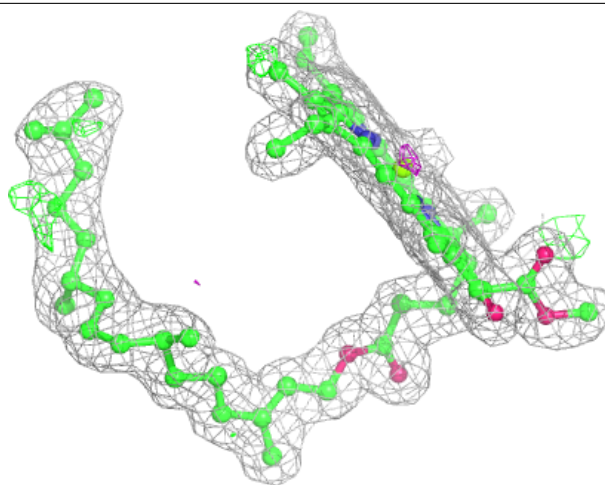
**Electron density around CLA b 612:**

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



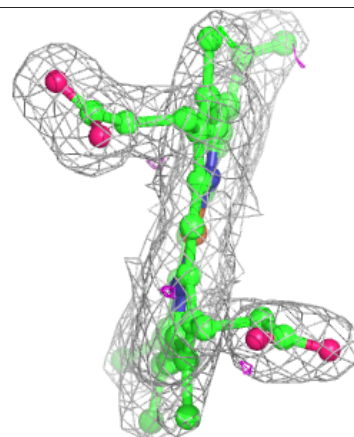
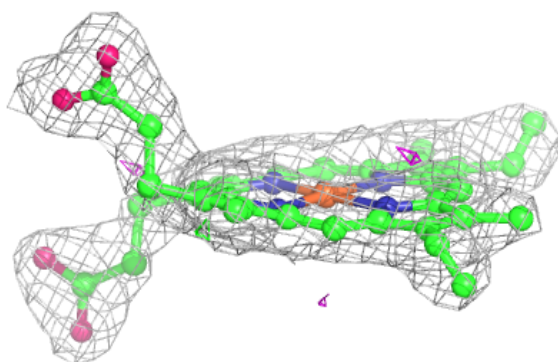
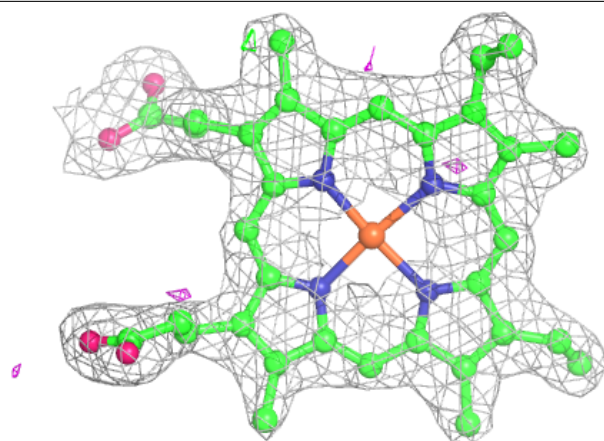
Electron density around CLA B 613:

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

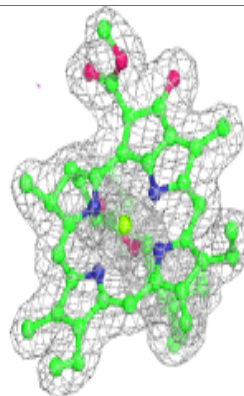
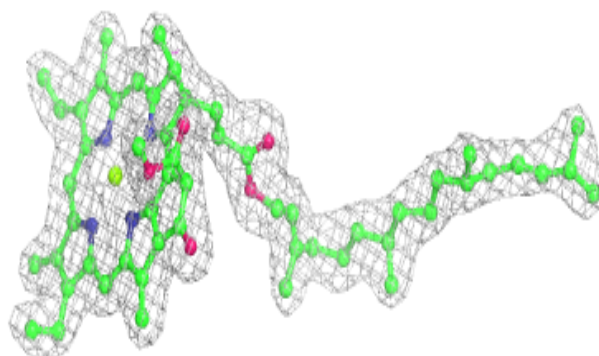
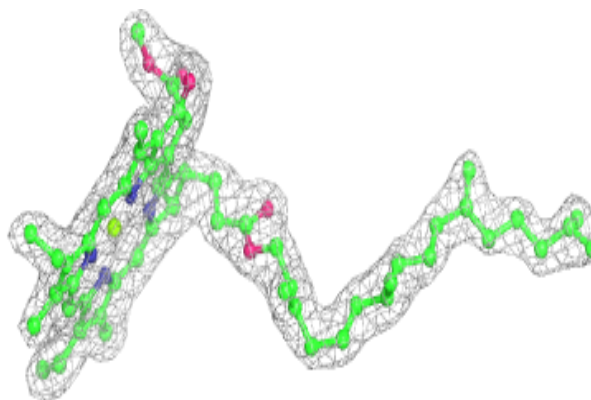


Electron density around HEM F 102:

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

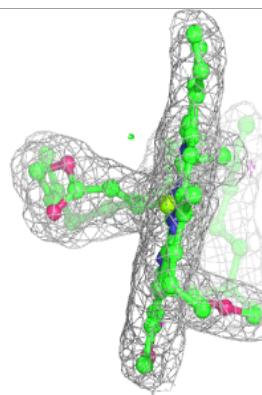
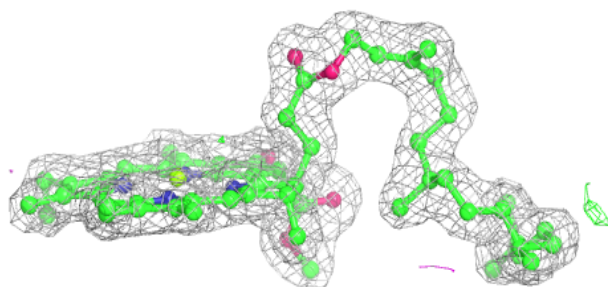
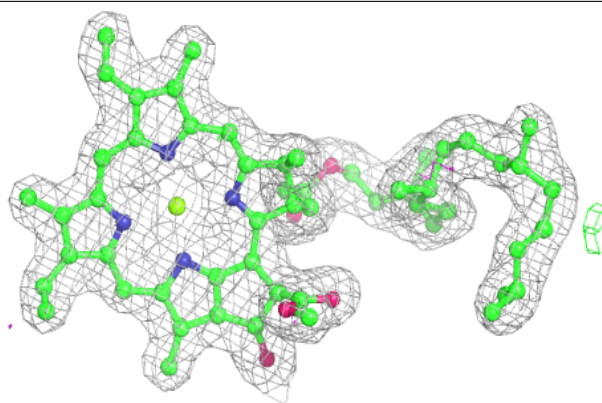
**Electron density around CLA c 504:**

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

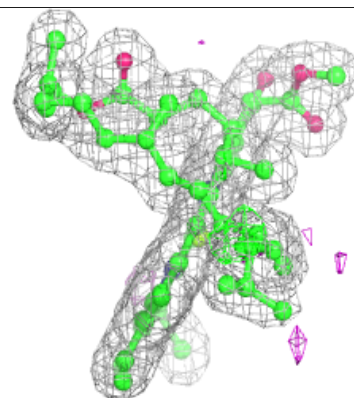
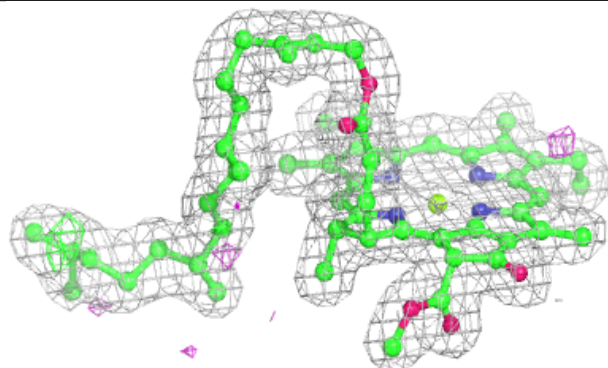
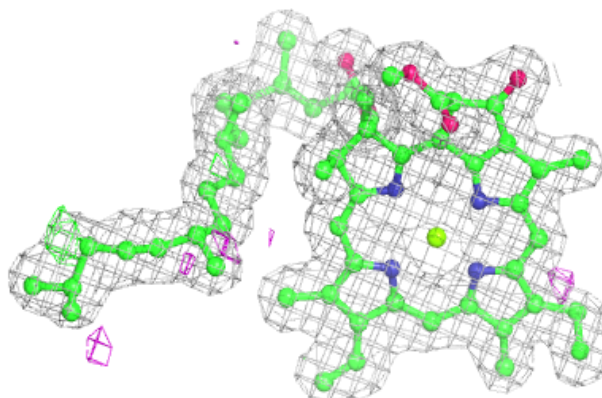


Electron density around CLA B 614:

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

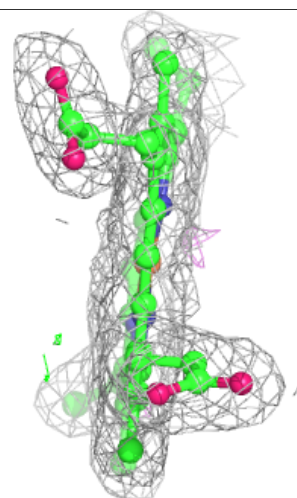
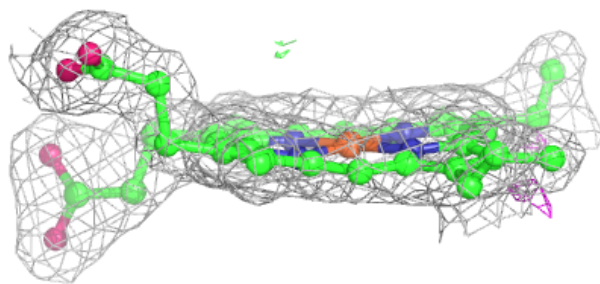
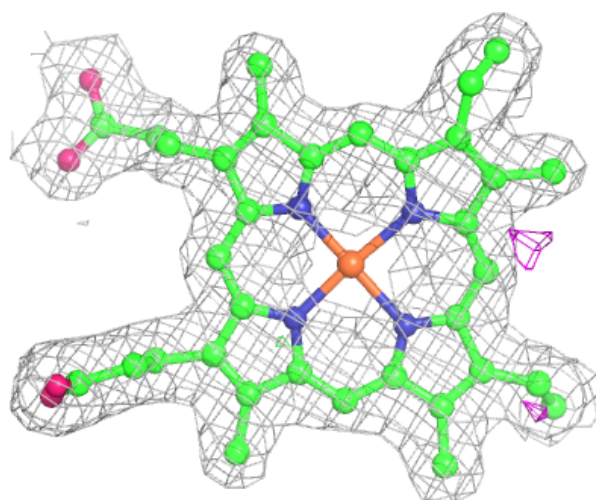
**Electron density around CLA a 410:**

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



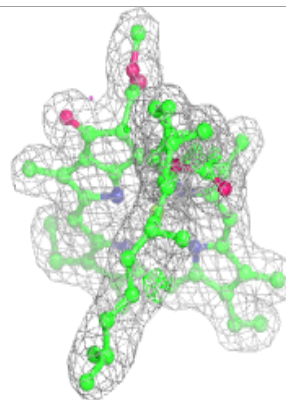
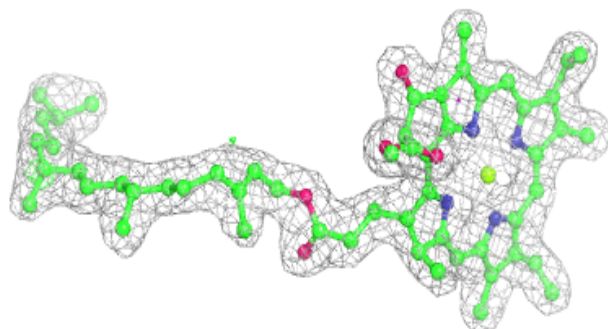
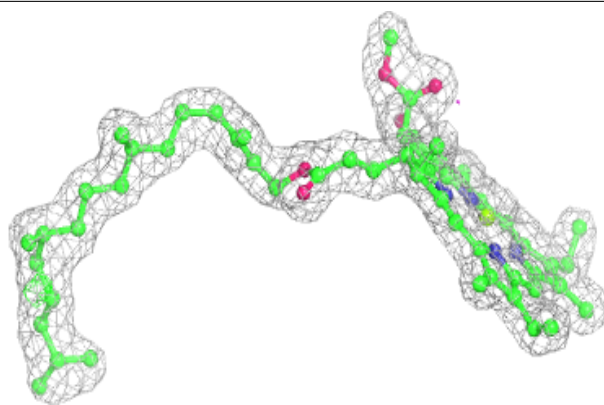
Electron density around HEC V 201:

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



Electron density around CLA d 405:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.