



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2020 – 04:59 PM BST

PDB ID : 5B5E
Title : Crystal structure analysis of Photosystem II complex
Authors : Tanaka, A.; Fukushima, Y.; Kamiya, N.
Deposited on : 2016-05-02
Resolution : 1.87 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

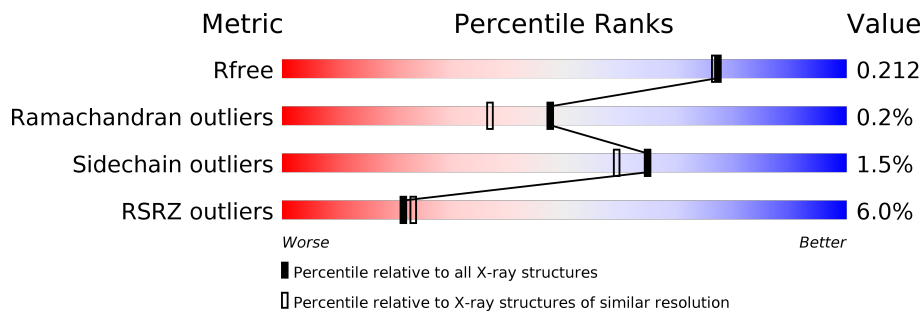
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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.



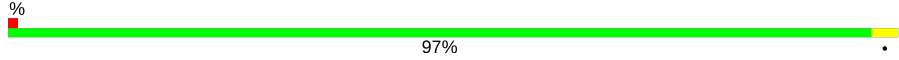
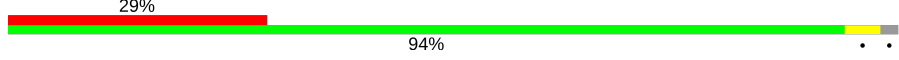
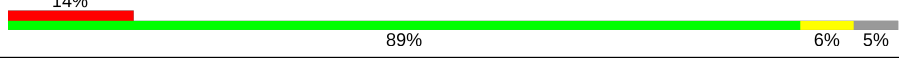


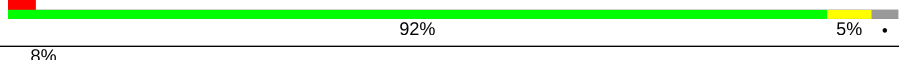
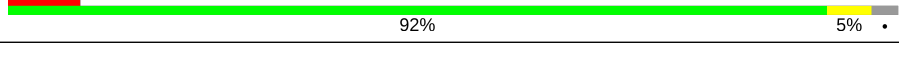
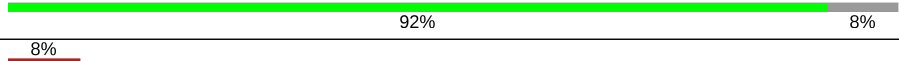
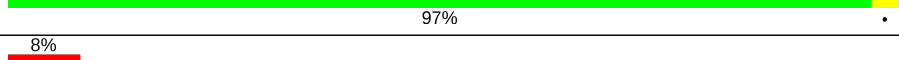
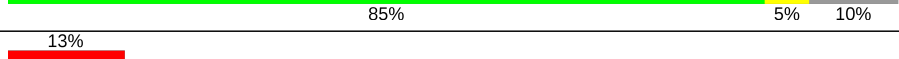
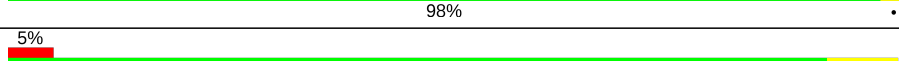
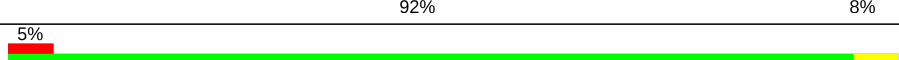
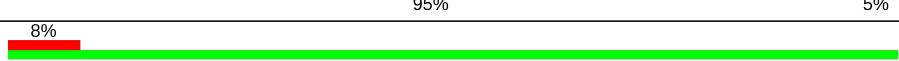
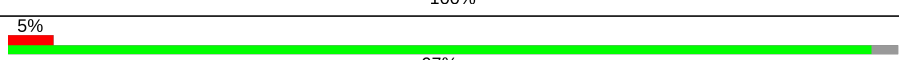
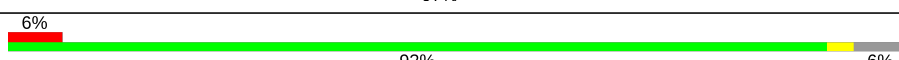
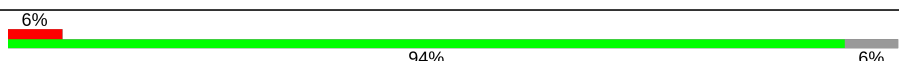
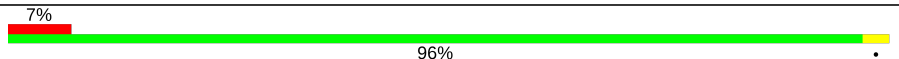
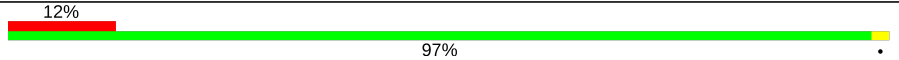

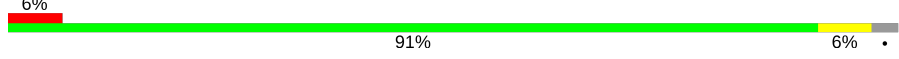
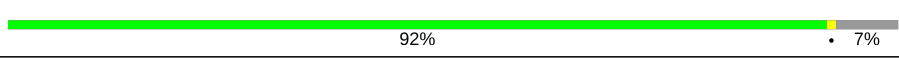
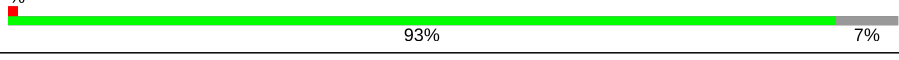
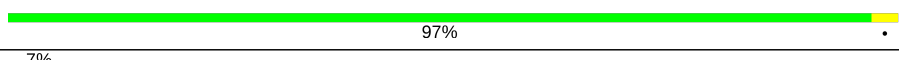
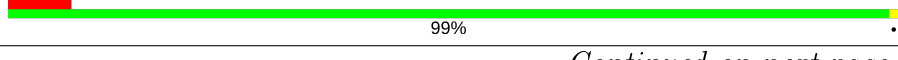

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	9470 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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

Mol	Chain	Length	Quality of chain
1	A	344	95% ..
1	a	344	95% ..
2	B	505	98% .
2	b	505	96% ..
3	C	455	97% ..
3	c	455	97% .
4	D	342	97% .

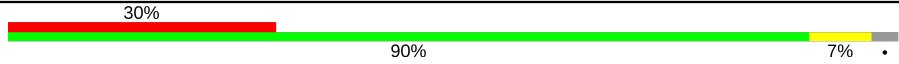
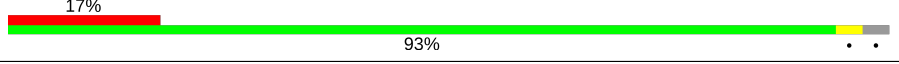
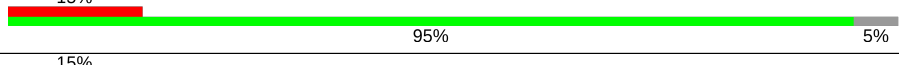
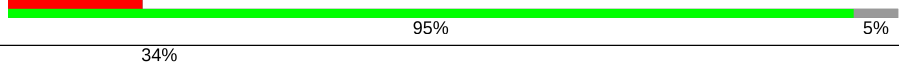
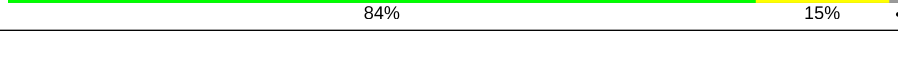
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Mol	Chain	Length	Quality of chain
4	d	342	
5	E	83	
5	e	83	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	
16	v	137	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	405	X	-	-	-
23	CLA	A	406	X	-	-	-
23	CLA	A	408	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	B	617	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	D	401	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	D	404	X	-	-	-
23	CLA	a	406	X	-	-	-
23	CLA	a	407	X	-	-	-
23	CLA	a	410	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
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23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	c	902	X	-	-	-
23	CLA	c	903	X	-	-	-
23	CLA	c	904	X	-	-	-
23	CLA	c	905	X	-	-	-
23	CLA	c	906	X	-	-	-
23	CLA	c	907	X	-	-	-
23	CLA	c	908	X	-	-	-
23	CLA	c	909	X	-	-	-
23	CLA	c	910	X	-	-	-
23	CLA	c	911	X	-	-	-
23	CLA	c	912	X	-	-	-
23	CLA	c	913	X	-	-	-
23	CLA	c	914	X	-	-	-
23	CLA	d	401	X	-	-	-
23	CLA	d	403	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	d	404	X	-	-	-
29	UNL	B	628	-	-	-	X
29	UNL	H	104	-	-	-	X
35	HTG	B	626	-	-	-	X
35	HTG	c	922	-	-	-	X

2 Entry composition [i](#)

There are 41 unique types of molecules in this entry. The entry contains 55401 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	334	2622	1718	431	458	15	0	1	0
1	a	334	2633	1727	431	460	15	0	4	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	see sequence details	UNP P51765
a	279	PRO	ARG	see sequence details	UNP P51765

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	505	3992	2619	668	692	13	0	4	0
2	b	501	3929	2582	653	681	13	0	3	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	451	3511	2297	591	610	13	0	4	0
3	c	455	3521	2305	589	614	13	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	see sequence details	UNP D0VWR7
C	20	SER	-	see sequence details	UNP D0VWR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	see sequence details	UNP D0VWR7
C	22	PHE	-	see sequence details	UNP D0VWR7
c	19	ASN	-	see sequence details	UNP D0VWR7
c	20	SER	-	see sequence details	UNP D0VWR7
c	21	ILE	-	see sequence details	UNP D0VWR7
c	22	PHE	-	see sequence details	UNP D0VWR7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	2	0
			2733	1813	446	462	12			
4	d	342	Total	C	N	O	S	0	2	0
			2733	1813	446	462	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	S	0	0	0
			651	426	103	122				
5	e	79	Total	C	N	O	S	0	0	0
			637	419	101	117				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total	C	N	O	S	0	0	0
			280	190	46	43	1			
6	f	32	Total	C	N	O	S	0	0	0
			255	173	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	63	Total	C	N	O	S	0	2	0
			511	341	83	85	2			
7	h	63	Total	C	N	O	S	0	1	0
			506	338	83	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			285	195	45	44	1			
8	i	38	Total	C	N	O	S	0	0	0
			303	205	48	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			251	171	37	42	1			
9	j	40	Total	C	N	O	S	0	0	0
			285	190	44	49	2			

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

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	see sequence details	UNP P19054
K	39	TRP	VAL	see sequence details	UNP P19054
k	33	LEU	PHE	see sequence details	UNP P19054
k	39	TRP	VAL	see sequence details	UNP P19054

- 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	0	1	0
			306	205	48	53			
11	l	36	Total	C	N	O	0	1	0
			297	200	47	50			

- 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	1	0
			264	178	38	47	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	m	34	264	178	38	47	1	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	see sequence details	UNP P12312
m	8	LEU	PHE	see sequence details	UNP P12312

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	O	243	1861	1164	311	382	4	0	2	0
13	o	243	1852	1159	310	379	4	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	T	30	256	180	36	38	2	0	0	0
14	t	31	261	183	37	39	2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
15	U	97	766	486	128	152	0	0	0
15	u	97	776	493	129	154	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	V	137	1072	680	180	208	4	0	1	0
16	v	137	1060	671	177	208	4	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	29	Total	C	N	O	S	0	0	0
			210	137	37	33	3			
17	y	29	Total	C	N	O	S	0	0	0
			207	134	37	33	3			

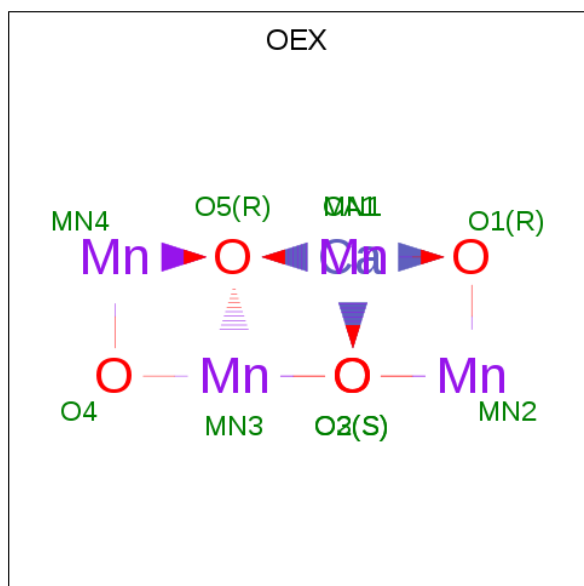
- Molecule 18 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O	S	0	1	0
			280	190	44	46				
18	x	38	Total	C	N	O	S	0	0	0
			275	185	44	46				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			468	320	71	75	2			
19	z	61	Total	C	N	O	S	0	0	0
			457	312	70	73	2			

- Molecule 20 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



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

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

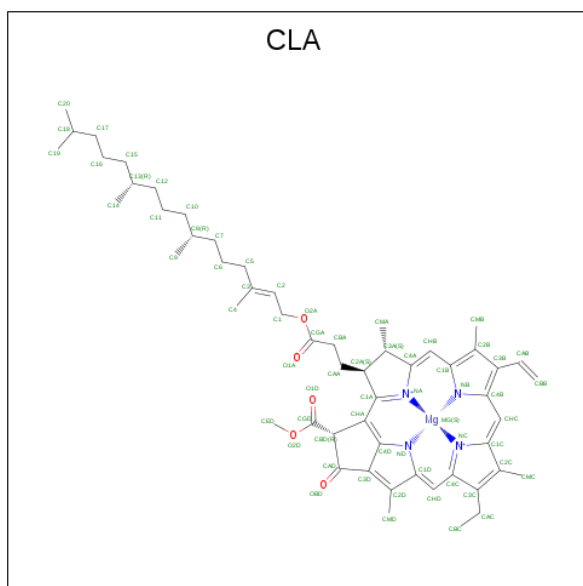
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

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

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

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



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

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

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

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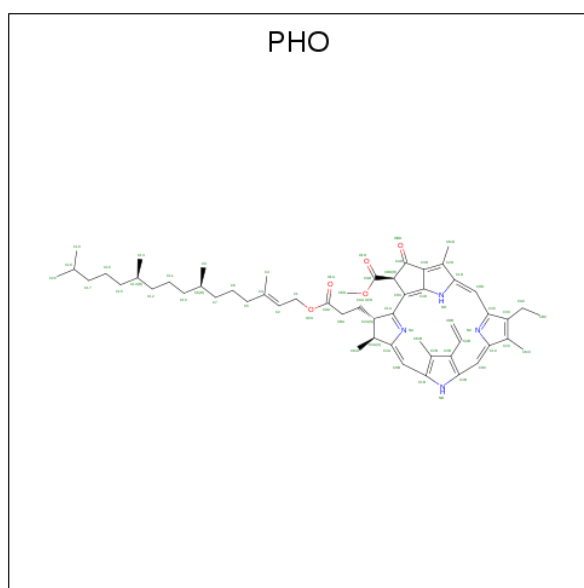
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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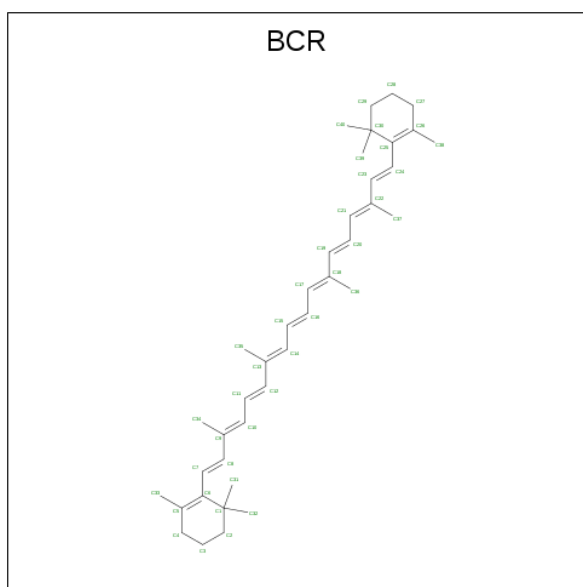
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



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

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



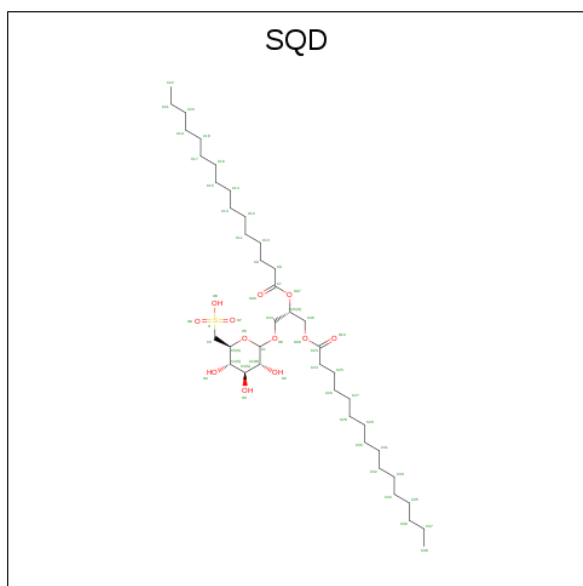
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total C 40 40	0	0
25	a	1	Total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

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

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



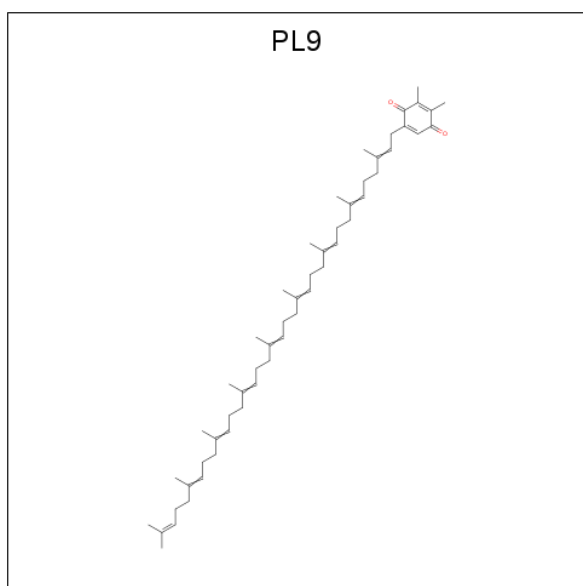
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O S 54 41 12 1	0	0
26	A	1	Total C O S 54 41 12 1	0	0
26	B	1	Total C O S 54 41 12 1	0	0
26	D	1	Total C O S 45 32 12 1	0	0
26	L	1	Total C O S 54 41 12 1	0	0

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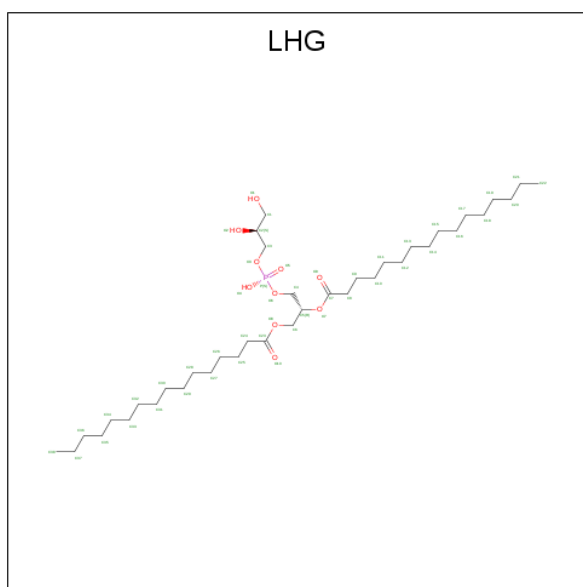
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
26	a	1	54	41	12	1	0	0
26	a	1	54	41	12	1	0	0
26	x	1	41	28	12	1	0	0

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



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

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
28	A	1	49	38	10	1	0	0
28	D	1	49	38	10	1	0	0
28	D	1	49	38	10	1	0	0
28	D	1	46	35	10	1	0	0
28	E	1	49	38	10	1	0	0
28	K	1	44	35	8	1	0	0
28	L	1	49	38	10	1	0	0
28	a	1	49	38	10	1	0	0
28	d	1	44	33	10	1	0	0
28	d	1	49	38	10	1	0	0
28	d	1	49	38	10	1	0	0
28	d	1	46	35	10	1	0	0
28	e	1	40	29	10	1	0	0
28	l	1	49	38	10	1	0	0

- Molecule 29 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

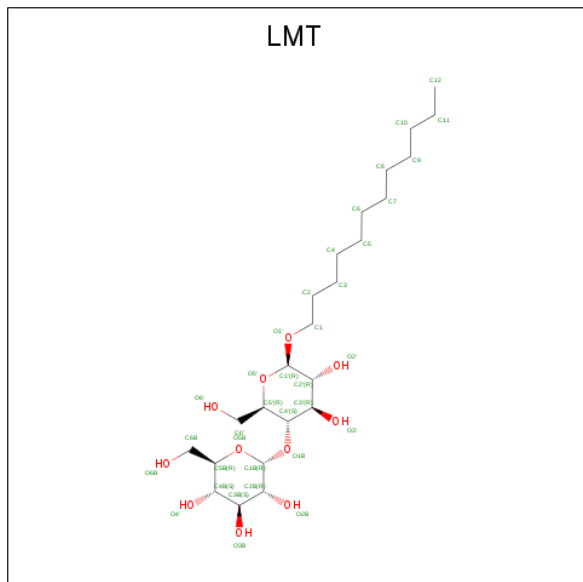
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	B	7	Total C 97 97	0	0
29	c	1	Total C 10 10	0	0
29	t	1	Total C 16 16	0	0
29	X	1	Total C 16 16	0	0
29	J	3	Total C 43 43	0	0
29	k	1	Total C 8 8	0	0
29	E	3	Total C 45 45	0	0
29	b	7	Total C 102 102	0	0
29	A	3	Total C 33 33	0	0
29	x	1	Total C 15 15	0	0
29	M	1	Total C 11 11	0	0
29	j	1	Total C 16 16	0	0
29	D	1	Total C 16 16	0	0
29	e	1	Total C 16 16	0	0
29	I	3	Total C 45 45	0	0
29	Z	2	Total C 23 23	0	0
29	a	2	Total C 16 16	0	0
29	U	1	Total C 14 14	0	0
29	m	1	Total C 11 11	0	0
29	d	2	Total C 27 27	0	0
29	H	1	Total C 14 14	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	i	4	Total C 64 64	0	0
29	C	1	Total C 11 11	0	0
29	z	1	Total C 13 13	0	0
29	T	1	Total C 13 13	0	0
29	u	2	Total C 27 27	0	0

- Molecule 30 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



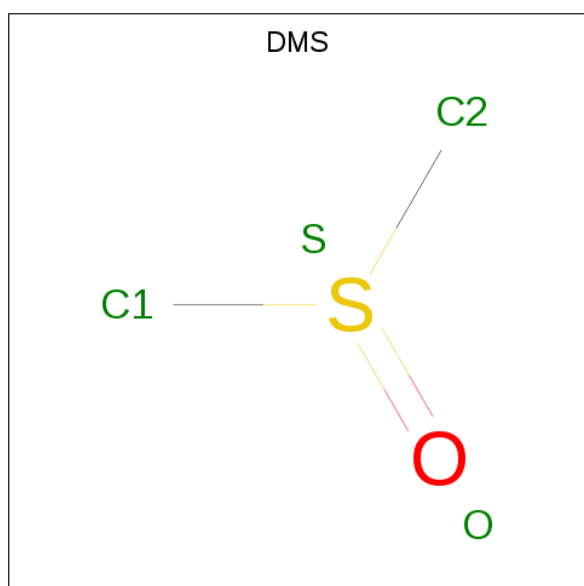
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	1	Total C O 35 24 11	0	0
30	B	1	Total C O 35 24 11	0	0
30	B	1	Total C O 24 18 6	0	0
30	B	1	Total C O 24 18 6	0	0
30	F	1	Total C O 35 24 11	0	0
30	I	1	Total C O 35 24 11	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	M	1	Total	C	O	0	0
			35	24	11		
30	T	1	Total	C	O	0	0
			24	18	6		
30	Z	1	Total	C	O	0	0
			35	24	11		
30	a	1	Total	C	O	0	0
			35	24	11		
30	a	1	Total	C	O	0	0
			35	24	11		
30	b	1	Total	C	O	0	0
			25	19	6		
30	e	1	Total	C	O	0	0
			25	19	6		
30	m	1	Total	C	O	0	0
			35	24	11		
30	m	1	Total	C	O	0	0
			35	24	11		
30	z	1	Total	C	O	0	0
			32	21	11		

- Molecule 31 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



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

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	D	1	Total 4	C 2	O 1	S 1	0	0
31	D	1	Total 4	C 2	O 1	S 1	0	0
31	D	1	Total 4	C 2	O 1	S 1	0	0
31	F	1	Total 4	C 2	O 1	S 1	0	0
31	H	1	Total 4	C 2	O 1	S 1	0	0
31	H	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	U	1	Total 4	C 2	O 1	S 1	0	0
31	U	1	Total 4	C 2	O 1	S 1	0	0
31	U	1	Total 4	C 2	O 1	S 1	0	0

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

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

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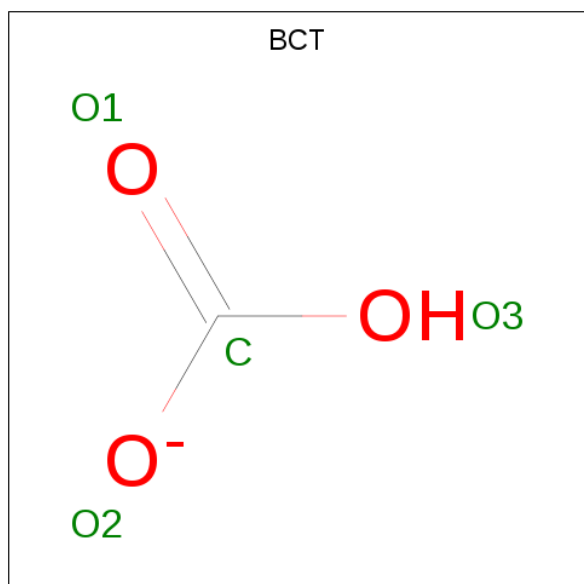
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	e	1	Total 4	C 2	O 1	S 1	0	0
31	h	1	Total 4	C 2	O 1	S 1	0	0
31	h	1	Total 4	C 2	O 1	S 1	0	0
31	h	1	Total 4	C 2	O 1	S 1	0	0
31	h	1	Total 4	C 2	O 1	S 1	0	0
31	i	1	Total 4	C 2	O 1	S 1	0	0
31	i	1	Total 4	C 2	O 1	S 1	0	0
31	k	1	Total 4	C 2	O 1	S 1	0	0
31	l	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	v	1	Total	C	O	S	0	0
			4	2	1	1		
31	v	1	Total	C	O	S	0	0
			4	2	1	1		
31	v	1	Total	C	O	S	0	0
			4	2	1	1		
31	v	1	Total	C	O	S	0	0
			4	2	1	1		
31	v	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 32 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



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

- Molecule 33 is CALCIUM ION (three-letter code: CA) (formula: Ca).

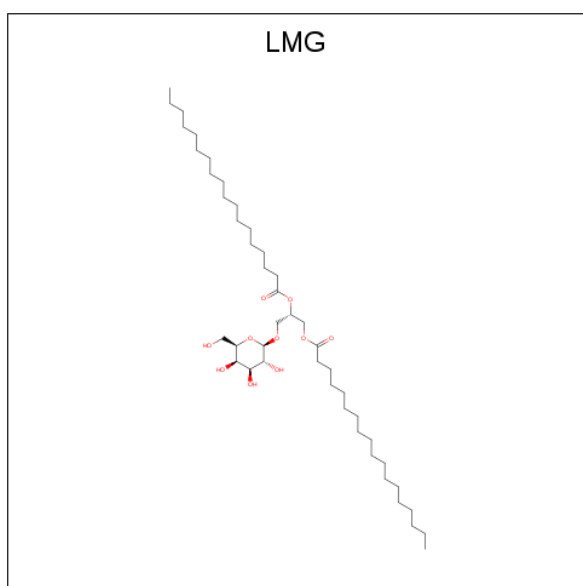
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	o	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	O	1	Total Ca 1 1	0	0
33	B	1	Total Ca 1 1	0	0
33	b	1	Total Ca 1 1	0	0
33	c	1	Total Ca 1 1	0	0

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



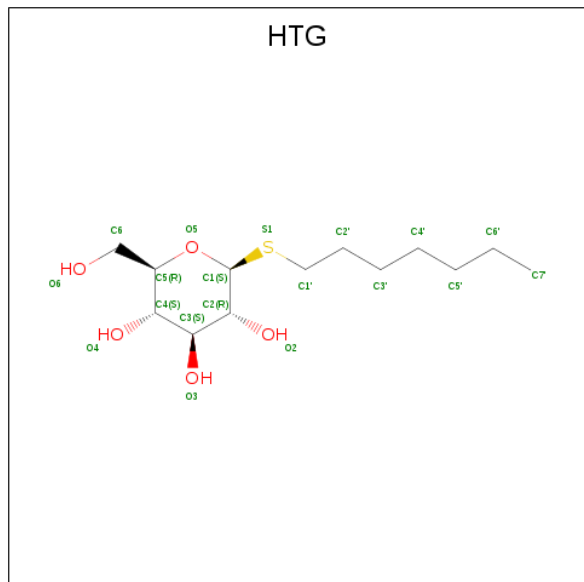
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	B	1	Total C O 51 41 10	0	0
34	C	1	Total C O 51 41 10	0	0
34	C	1	Total C O 51 41 10	0	0
34	C	1	Total C O 51 41 10	0	0
34	D	1	Total C O 51 41 10	0	0
34	J	1	Total C O 51 41 10	0	0
34	a	1	Total C O 51 41 10	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	c	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		
34	d	1	Total	C	O	0	0
			51	41	10		
34	j	1	Total	C	O	0	0
			51	41	10		
34	m	1	Total	C	O	0	0
			51	41	10		

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: C₁₃H₂₆O₅S).



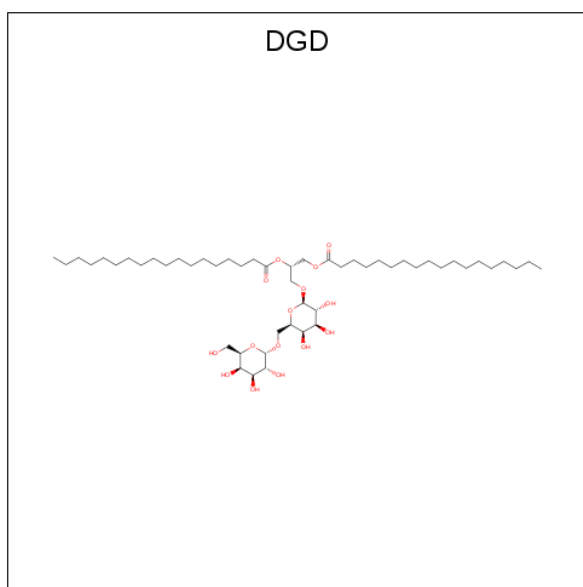
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		

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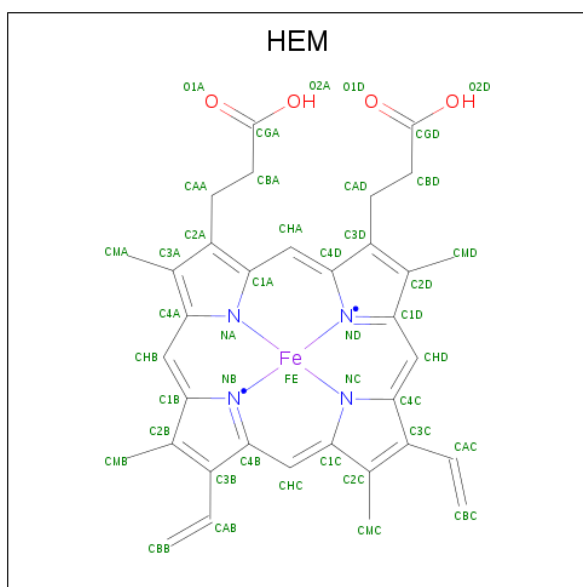
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
35	C	1	19	13	5	1	0	0
35	C	1	19	13	5	1	0	0
35	D	1	19	13	5	1	0	0
35	O	1	19	13	5	1	0	0
35	V	1	14	8	5	1	0	0
35	b	1	19	13	5	1	0	0
35	b	1	19	13	5	1	0	0
35	b	1	19	13	5	1	0	0
35	b	1	19	13	5	1	0	0
35	c	1	19	13	5	1	0	0
35	c	1	19	13	5	1	0	0
35	c	1	13	10	2	1	0	0
35	d	1	19	13	5	1	0	0
35	v	1	19	13	5	1	0	0

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



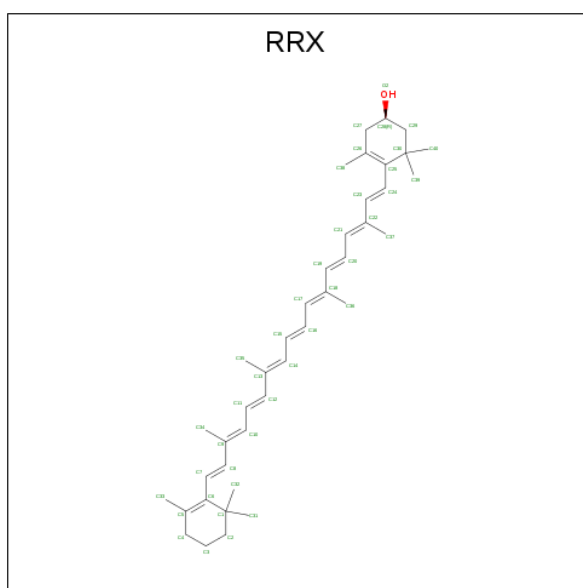
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	C	1	Total	C	O	0	0
			62	47	15		
36	C	1	Total	C	O	0	0
			62	47	15		
36	C	1	Total	C	O	0	0
			62	47	15		
36	D	1	Total	C	O	0	0
			50	41	9		
36	H	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C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

- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 38 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: C₄₀H₅₆O).

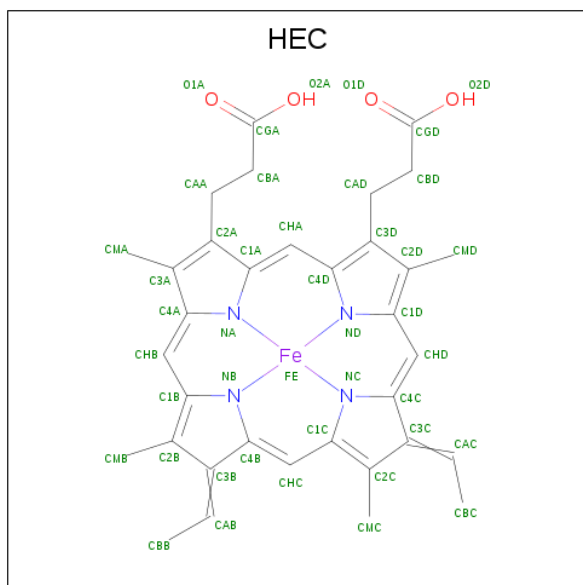


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
38	H	1	Total	C	O	0	0
			41	40	1		
38	x	1	Total	C	O	0	0
			41	40	1		

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

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

- Molecule 40 is HEME C (three-letter code: HEC) (formula: C₃₄H₃₄FeN₄O₄).



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	A	176	Total O 187 187	0	11
41	B	420	Total O 437 437	0	17
41	C	286	Total O 294 294	0	8
41	D	159	Total O 166 166	0	7
41	E	44	Total O 47 47	0	3

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	F	9	Total O 9 9	0	0
41	H	54	Total O 54 54	0	0
41	I	11	Total O 13 13	0	2
41	J	16	Total O 17 17	0	1
41	K	13	Total O 14 14	0	1
41	L	23	Total O 26 26	0	3
41	M	15	Total O 17 17	0	2
41	O	251	Total O 265 265	0	14
41	T	15	Total O 16 16	0	1
41	U	123	Total O 128 128	0	5
41	V	165	Total O 169 169	0	4
41	Y	8	Total O 8 8	0	0
41	X	14	Total O 14 14	0	0
41	Z	8	Total O 10 10	0	2
41	a	172	Total O 175 175	0	3
41	b	405	Total O 423 423	0	18
41	c	300	Total O 320 320	0	20
41	d	177	Total O 185 185	0	8
41	e	52	Total O 56 56	0	4
41	f	9	Total O 9 9	0	0
41	h	56	Total O 57 57	0	1

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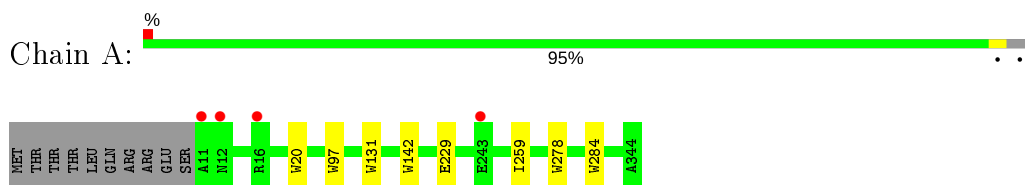
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	i	12	Total O 13 13	0	1
41	j	13	Total O 13 13	0	0
41	k	14	Total O 14 14	0	0
41	l	16	Total O 19 19	0	3
41	m	14	Total O 15 15	0	1
41	o	223	Total O 240 240	0	17
41	t	19	Total O 21 21	0	2
41	u	146	Total O 157 157	0	11
41	v	147	Total O 154 154	0	7
41	y	16	Total O 16 16	0	0
41	x	18	Total O 19 19	0	1
41	z	5	Total O 5 5	0	0

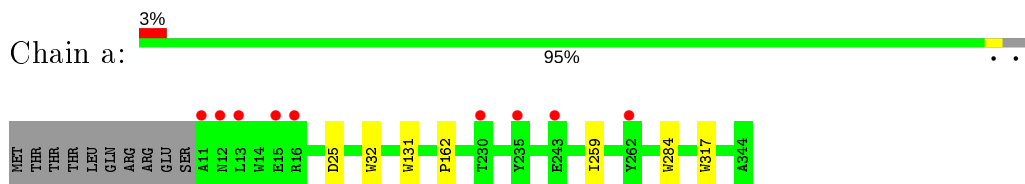
3 Residue-property plots [i](#)

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.

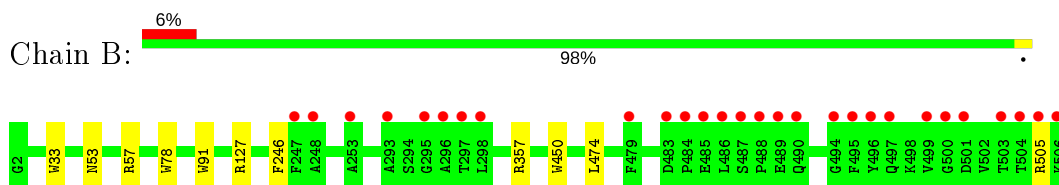
- Molecule 1: Photosystem II protein D1



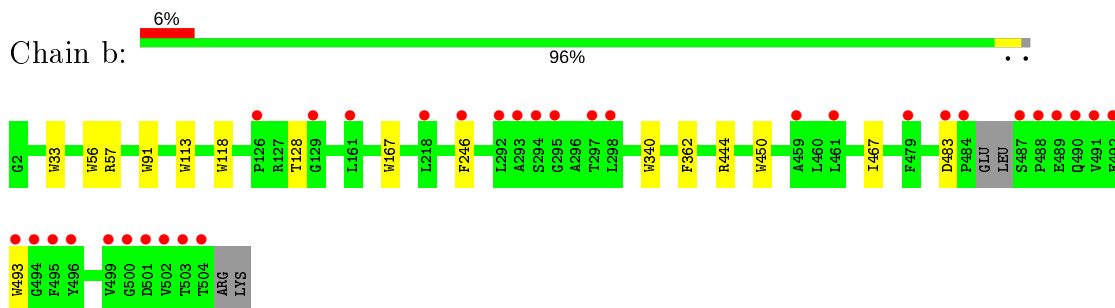
- Molecule 1: Photosystem II protein D1



- Molecule 2: Photosystem II CP47 reaction center protein

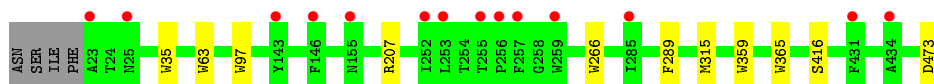


- Molecule 2: Photosystem II CP47 reaction center protein

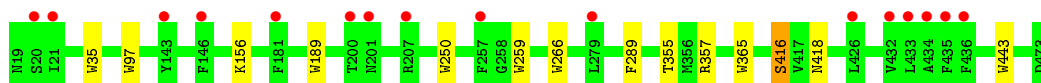


- Molecule 3: Photosystem II CP43 reaction center protein





- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 4: Photosystem II D2 protein



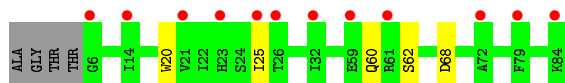
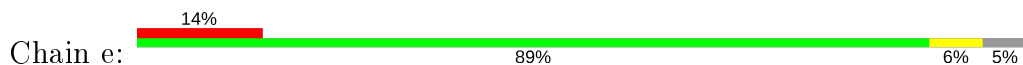
- Molecule 4: Photosystem II D2 protein



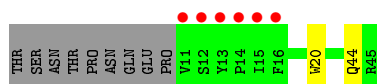
- Molecule 5: Cytochrome b559 subunit alpha



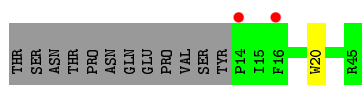
- Molecule 5: Cytochrome b559 subunit alpha



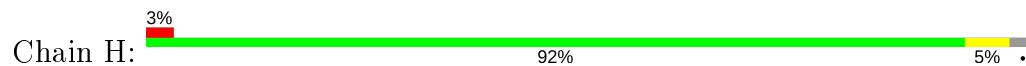
- Molecule 6: Cytochrome b559 subunit beta



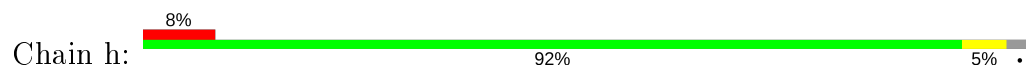
- Molecule 6: Cytochrome b559 subunit beta



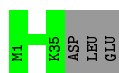
- Molecule 7: Photosystem II reaction center protein H



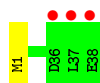
- Molecule 7: Photosystem II reaction center protein H



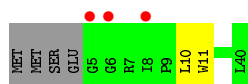
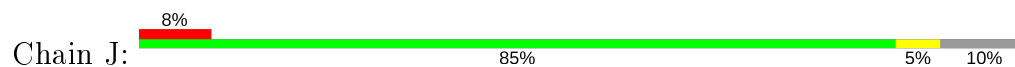
- Molecule 8: Photosystem II reaction center protein I



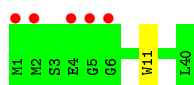
- Molecule 8: Photosystem II reaction center protein I



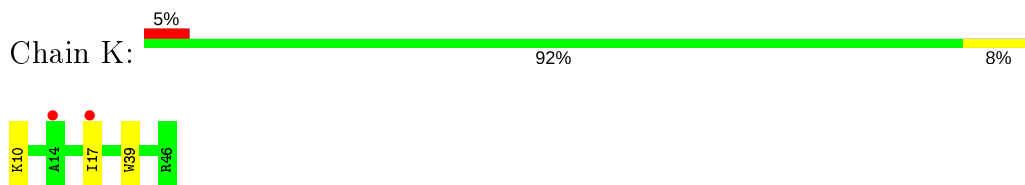
- Molecule 9: Photosystem II reaction center protein J



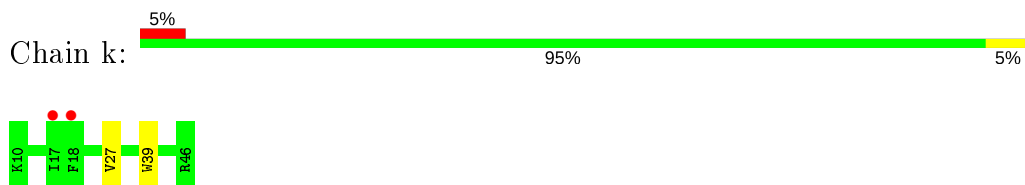
- Molecule 9: Photosystem II reaction center protein J



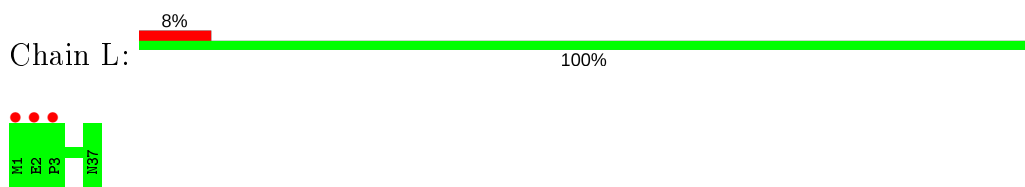
- Molecule 10: Photosystem II reaction center protein K



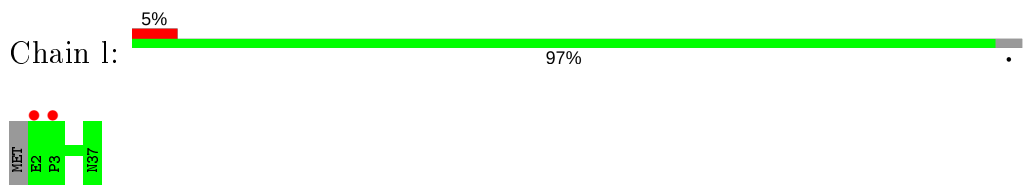
- Molecule 10: Photosystem II reaction center protein K



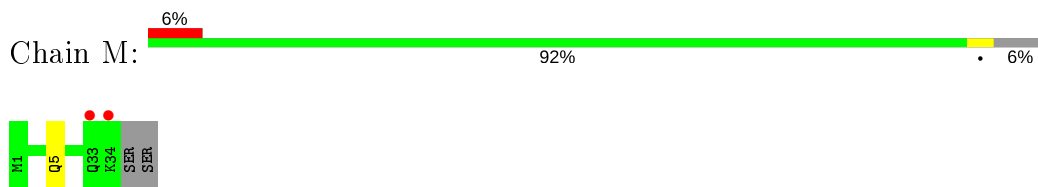
- Molecule 11: Photosystem II reaction center protein L



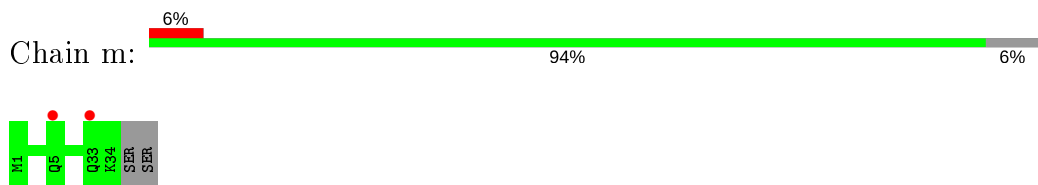
- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M

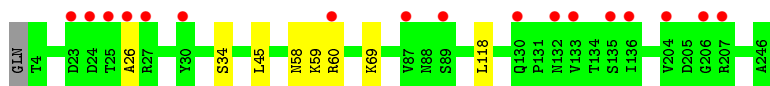


- Molecule 12: Photosystem II reaction center protein M

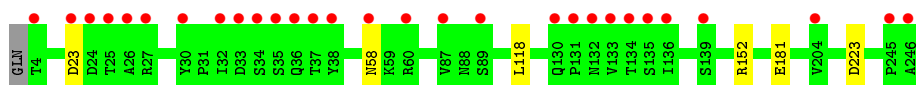


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

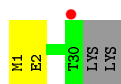
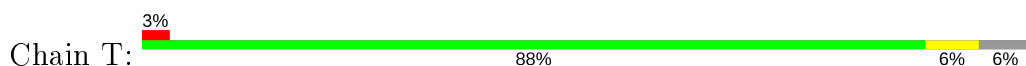




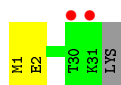
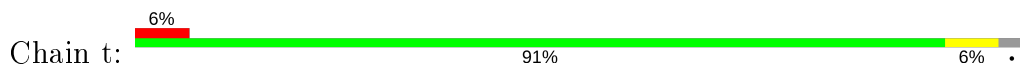
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 14: Photosystem II reaction center protein T



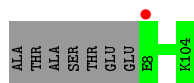
- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein



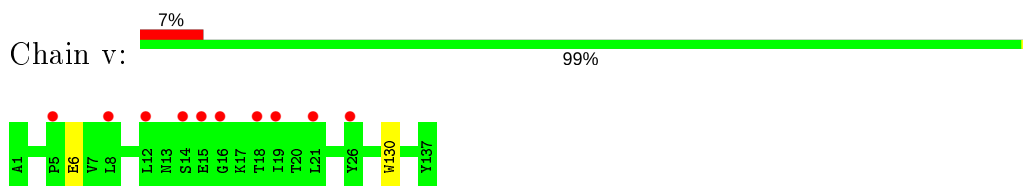
- Molecule 15: Photosystem II 12 kDa extrinsic protein



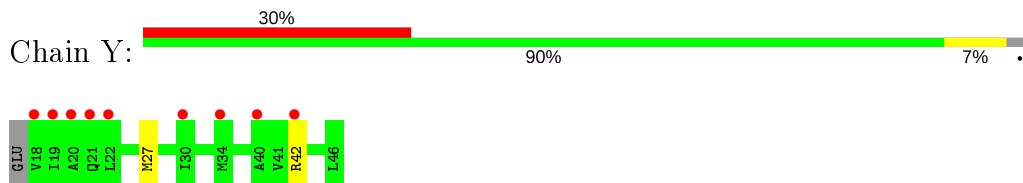
- Molecule 16: Cytochrome c-550



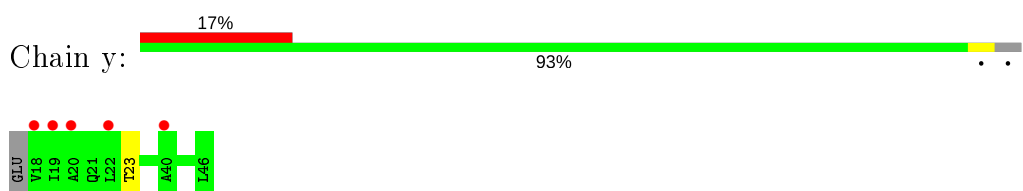
- Molecule 16: Cytochrome c-550



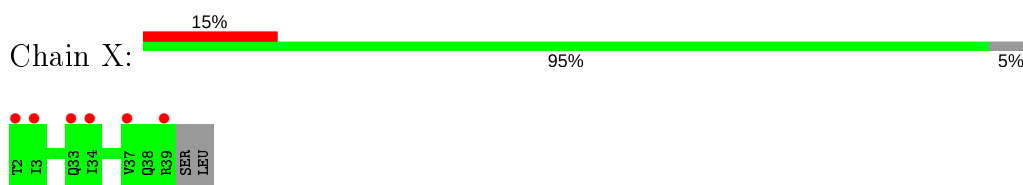
- Molecule 17: Photosystem II reaction center protein Ycf12



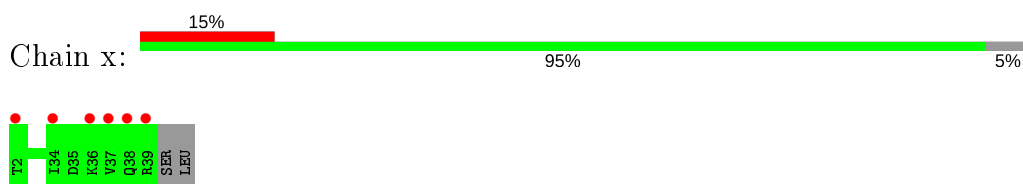
- Molecule 17: Photosystem II reaction center protein Ycf12



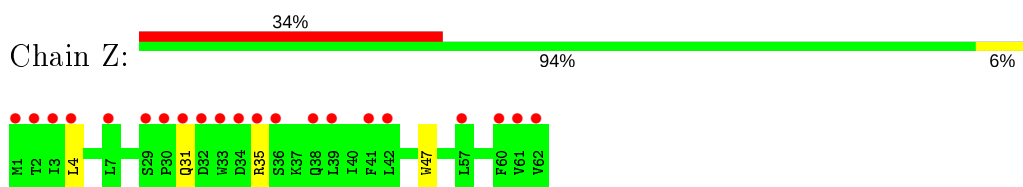
- Molecule 18: Photosystem II reaction center protein X



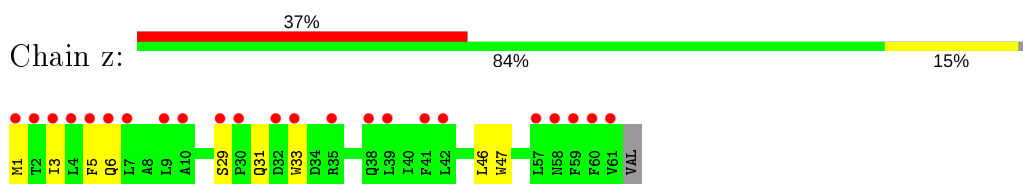
- Molecule 18: Photosystem II reaction center protein X



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.40Å 228.22Å 286.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.98 – 1.87 48.98 – 1.87	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.98-1.87) 99.8 (48.98-1.87)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 1.87Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.171 , 0.212 0.171 , 0.212	Depositor DCC
R_{free} test set	32518 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtrriage
Anisotropy	0.104	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 70.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	55401	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.02	5/2710 (0.2%)	0.81	1/3696 (0.0%)
1	a	0.99	4/2730 (0.1%)	0.81	1/3723 (0.0%)
2	B	0.94	4/4144 (0.1%)	0.82	4/5647 (0.1%)
2	b	0.98	9/4076 (0.2%)	0.83	3/5558 (0.1%)
3	C	0.91	6/3633 (0.2%)	0.78	1/4945 (0.0%)
3	c	0.91	9/3638 (0.2%)	0.78	1/4953 (0.0%)
4	D	1.01	4/2834 (0.1%)	0.83	2/3861 (0.1%)
4	d	1.02	8/2834 (0.3%)	0.82	1/3861 (0.0%)
5	E	0.74	1/670 (0.1%)	0.71	0/917
5	e	0.71	1/656 (0.2%)	0.73	0/896
6	F	0.83	1/289 (0.3%)	0.64	0/394
6	f	0.83	1/262 (0.4%)	0.65	0/356
7	H	0.85	1/530 (0.2%)	0.78	0/722
7	h	0.89	2/522 (0.4%)	0.79	0/711
8	I	0.66	0/282	0.67	0/381
8	i	0.68	0/300	0.67	0/406
9	J	0.80	1/257 (0.4%)	0.63	0/349
9	j	0.84	1/291 (0.3%)	0.69	0/393
10	K	0.73	1/303 (0.3%)	0.70	0/416
10	k	0.77	1/303 (0.3%)	0.71	0/416
11	L	0.94	0/316	0.80	0/430
11	l	0.98	0/307	0.80	0/418
12	M	0.78	0/270	0.75	0/369
12	m	0.72	0/270	0.74	0/369
13	O	0.78	0/1898	0.83	0/2577
13	o	0.74	0/1886	0.83	2/2562 (0.1%)
14	T	0.83	0/255	0.79	0/346
14	t	0.82	0/260	0.74	0/353
15	U	0.82	0/777	0.84	2/1055 (0.2%)
15	u	0.80	0/790	0.82	0/1071
16	V	0.88	0/1096	0.83	1/1487 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.78	1/1084 (0.1%)	0.76	0/1475
17	Y	0.54	0/211	0.71	0/282
17	y	0.51	0/208	0.63	0/278
18	X	0.61	0/286	0.73	0/387
18	x	0.60	0/278	0.71	0/376
19	Z	0.67	1/479 (0.2%)	0.67	0/656
19	z	0.63	2/468 (0.4%)	0.61	0/640
All	All	0.90	64/42403 (0.2%)	0.80	19/57732 (0.0%)

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	365	TRP	CD2-CE2	7.28	1.50	1.41
1	a	131	TRP	CD2-CE2	6.83	1.49	1.41
3	c	35	TRP	CD2-CE2	6.66	1.49	1.41
2	b	56	TRP	CD2-CE2	6.63	1.49	1.41
10	k	39	TRP	CD2-CE2	6.56	1.49	1.41
2	b	113	TRP	CD2-CE2	6.36	1.49	1.41
9	j	11	TRP	CD2-CE2	6.31	1.49	1.41
2	B	78	TRP	CD2-CE2	6.24	1.48	1.41
6	f	20	TRP	CD2-CE2	6.22	1.48	1.41
3	c	443	TRP	CD2-CE2	6.11	1.48	1.41
1	A	20	TRP	CD2-CE2	6.07	1.48	1.41
4	D	32	TRP	CD2-CE2	6.06	1.48	1.41
3	C	266	TRP	CD2-CE2	6.03	1.48	1.41
1	a	317	TRP	CD2-CE2	5.91	1.48	1.41
2	b	450	TRP	CD2-CE2	5.90	1.48	1.41
2	b	33	TRP	CD2-CE2	5.85	1.48	1.41
3	c	189	TRP	CD2-CE2	5.83	1.48	1.41
2	B	91	TRP	CD2-CE2	5.74	1.48	1.41
2	b	167	TRP	CD2-CE2	5.73	1.48	1.41
6	F	20	TRP	CD2-CE2	5.72	1.48	1.41
7	H	62	TRP	CD2-CE2	5.71	1.48	1.41
2	B	33	TRP	CD2-CE2	5.61	1.48	1.41
2	b	91	TRP	CD2-CE2	5.58	1.48	1.41
4	d	111	TRP	CD2-CE2	5.58	1.48	1.41
1	a	284	TRP	CD2-CE2	5.56	1.48	1.41
1	A	278	TRP	CD2-CE2	5.55	1.48	1.41
2	B	450	TRP	CD2-CE2	5.52	1.48	1.41
3	c	250	TRP	CD2-CE2	5.50	1.48	1.41
4	D	21	TRP	CD2-CE2	5.49	1.48	1.41
3	c	259	TRP	CD2-CE2	5.49	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	365	TRP	CD2-CE2	5.47	1.48	1.41
4	d	14	TRP	CD2-CE2	5.45	1.47	1.41
4	d	191	TRP	CD2-CE2	5.44	1.47	1.41
2	b	340	TRP	CD2-CE2	5.43	1.47	1.41
2	b	493	TRP	CD2-CE2	5.41	1.47	1.41
19	Z	47	TRP	CD2-CE2	5.41	1.47	1.41
3	C	63	TRP	CD2-CE2	5.40	1.47	1.41
9	J	11	TRP	CD2-CE2	5.40	1.47	1.41
7	h	62	TRP	CD2-CE2	5.39	1.47	1.41
1	a	32	TRP	CD2-CE2	5.36	1.47	1.41
4	d	104	TRP	CD2-CE2	5.34	1.47	1.41
1	A	142	TRP	CD2-CE2	5.33	1.47	1.41
4	d	32	TRP	CD2-CE2	5.33	1.47	1.41
16	v	130	TRP	CD2-CE2	5.33	1.47	1.41
5	E	20	TRP	CD2-CE2	5.31	1.47	1.41
3	C	359	TRP	CD2-CE2	5.29	1.47	1.41
10	K	39	TRP	CD2-CE2	5.29	1.47	1.41
3	c	365	TRP	CG-CD1	5.27	1.44	1.36
3	c	266	TRP	CD2-CE2	5.26	1.47	1.41
4	D	111	TRP	CD2-CE2	5.23	1.47	1.41
7	h	25	TRP	CD2-CE2	5.21	1.47	1.41
1	A	284	TRP	CD2-CE2	5.17	1.47	1.41
5	e	20	TRP	CD2-CE2	5.16	1.47	1.41
19	z	33	TRP	CD2-CE2	5.14	1.47	1.41
4	D	328	TRP	CD2-CE2	5.10	1.47	1.41
4	d	48	TRP	CD2-CE2	5.09	1.47	1.41
4	d	58	TRP	CD2-CE2	5.09	1.47	1.41
19	z	47	TRP	CD2-CE2	5.08	1.47	1.41
4	d	93	TRP	CD2-CE2	5.06	1.47	1.41
3	C	35	TRP	CD2-CE2	5.06	1.47	1.41
3	C	97	TRP	CD2-CE2	5.06	1.47	1.41
3	c	97	TRP	CD2-CE2	5.04	1.47	1.41
1	A	97	TRP	CD2-CE2	5.03	1.47	1.41
2	b	118	TRP	CD2-CE2	5.02	1.47	1.41

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	152	ARG	NE-CZ-NH2	-7.84	116.38	120.30
4	d	297	ASP	CB-CG-OD1	7.14	124.73	118.30
2	B	357	ARG	NE-CZ-NH2	-6.52	117.04	120.30
15	U	39	ARG	NE-CZ-NH2	-6.50	117.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	100	ASP	CB-CG-OD1	6.18	123.86	118.30
2	b	444	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	a	25	ASP	CB-CG-OD1	5.86	123.57	118.30
15	U	39	ARG	NE-CZ-NH1	5.82	123.21	120.30
16	V	99	ASP	CB-CG-OD1	5.63	123.37	118.30
13	o	223	ASP	CB-CG-OD1	5.50	123.25	118.30
4	D	297	ASP	CB-CG-OD1	5.46	123.22	118.30
2	B	57	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	131	TRP	CA-CB-CG	-5.45	103.35	113.70
2	B	57	ARG	NE-CZ-NH2	-5.34	117.63	120.30
2	b	444	ARG	NE-CZ-NH2	-5.30	117.65	120.30
2	B	474	LEU	CB-CG-CD1	-5.18	102.20	111.00
3	C	473	ASP	CB-CG-OD1	5.16	122.94	118.30
3	c	357	ARG	NE-CZ-NH1	-5.07	117.76	120.30
2	b	57	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	325 (98%)	7 (2%)	1 (0%)	41	30
1	a	336/344 (98%)	330 (98%)	5 (2%)	1 (0%)	41	30
2	B	507/505 (100%)	497 (98%)	10 (2%)	0	100	100
2	b	500/505 (99%)	490 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	453/455 (100%)	440 (97%)	12 (3%)	1 (0%)	47	37
3	c	454/455 (100%)	441 (97%)	12 (3%)	1 (0%)	47	37
4	D	342/342 (100%)	333 (97%)	8 (2%)	1 (0%)	41	30
4	d	342/342 (100%)	333 (97%)	9 (3%)	0	100	100
5	E	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
5	e	77/83 (93%)	76 (99%)	1 (1%)	0	100	100
6	F	33/44 (75%)	33 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
7	h	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
8	I	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
8	i	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
9	J	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
9	j	38/40 (95%)	38 (100%)	0	0	100	100
10	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
10	k	35/37 (95%)	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	33/36 (92%)	32 (97%)	1 (3%)	0	100	100
12	m	33/36 (92%)	32 (97%)	1 (3%)	0	100	100
13	O	243/244 (100%)	229 (94%)	11 (4%)	3 (1%)	13	4
13	o	242/244 (99%)	230 (95%)	12 (5%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	29/32 (91%)	28 (97%)	1 (3%)	0	100	100
15	U	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
15	u	96/104 (92%)	93 (97%)	3 (3%)	0	100	100
16	V	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
16	v	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
17	Y	27/30 (90%)	27 (100%)	0	0	100	100
17	y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
18	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	x	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	56 (93%)	3 (5%)	1 (2%)	9	2
19	z	59/62 (95%)	54 (92%)	3 (5%)	2 (3%)	3	0
All	All	5210/5350 (97%)	5059 (97%)	140 (3%)	11 (0%)	47	37

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	12	ARG
19	Z	31	GLN
3	c	416	SER
19	z	31	GLN
3	C	416	SER
19	z	3	ILE
13	O	26	ALA
13	O	59	LYS
13	O	60	ARG
1	A	259	ILE
1	a	259	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/279 (96%)	268 (100%)	1 (0%)	91	90
1	a	272/279 (98%)	271 (100%)	1 (0%)	91	90
2	B	403/403 (100%)	399 (99%)	4 (1%)	76	73
2	b	394/403 (98%)	389 (99%)	5 (1%)	69	64
3	C	355/356 (100%)	351 (99%)	4 (1%)	73	70
3	c	356/356 (100%)	351 (99%)	5 (1%)	67	62
4	D	278/277 (100%)	274 (99%)	4 (1%)	67	62
4	d	278/277 (100%)	276 (99%)	2 (1%)	84	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	70/72 (97%)	68 (97%)	2 (3%)	42	32
5	e	68/72 (94%)	64 (94%)	4 (6%)	19	9
6	F	28/38 (74%)	27 (96%)	1 (4%)	35	23
6	f	25/38 (66%)	25 (100%)	0	100	100
7	H	55/54 (102%)	53 (96%)	2 (4%)	35	23
7	h	54/54 (100%)	53 (98%)	1 (2%)	57	49
8	I	30/34 (88%)	30 (100%)	0	100	100
8	i	31/34 (91%)	31 (100%)	0	100	100
9	J	23/28 (82%)	22 (96%)	1 (4%)	29	17
9	j	27/28 (96%)	27 (100%)	0	100	100
10	K	30/30 (100%)	28 (93%)	2 (7%)	16	6
10	k	30/30 (100%)	29 (97%)	1 (3%)	38	26
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	34 (100%)	0	100	100
12	M	30/33 (91%)	29 (97%)	1 (3%)	38	26
12	m	30/33 (91%)	30 (100%)	0	100	100
13	O	205/207 (99%)	200 (98%)	5 (2%)	49	39
13	o	203/207 (98%)	199 (98%)	4 (2%)	55	47
14	T	25/28 (89%)	24 (96%)	1 (4%)	31	19
14	t	25/28 (89%)	24 (96%)	1 (4%)	31	19
15	U	82/89 (92%)	82 (100%)	0	100	100
15	u	84/89 (94%)	84 (100%)	0	100	100
16	V	118/117 (101%)	115 (98%)	3 (2%)	47	37
16	v	115/117 (98%)	114 (99%)	1 (1%)	78	76
17	Y	20/23 (87%)	18 (90%)	2 (10%)	7	2
17	y	19/23 (83%)	18 (95%)	1 (5%)	22	11
18	X	30/33 (91%)	30 (100%)	0	100	100
18	x	29/33 (88%)	29 (100%)	0	100	100
19	Z	49/52 (94%)	47 (96%)	2 (4%)	30	19
19	z	46/52 (88%)	41 (89%)	5 (11%)	6	2
All	All	4255/4376 (97%)	4189 (98%)	66 (2%)	65	56

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	229	GLU
2	B	53	ASN
2	B	127	ARG
2	B	246	PHE
2	B	505	ARG
3	C	207[A]	ARG
3	C	207[B]	ARG
3	C	289	PHE
3	C	315	MET
4	D	12	ARG
4	D	26	ARG
4	D	90	LEU
4	D	180	ARG
5	E	4	THR
5	E	25	ILE
6	F	44	GLN
7	H	49	TYR
7	H	63	LYS
9	J	10	LEU
10	K	10	LYS
10	K	17	ILE
12	M	5	GLN
13	O	34	SER
13	O	45	LEU
13	O	58	ASN
13	O	69	LYS
13	O	118	LEU
14	T	2	GLU
16	V	30	LYS
16	V	86	GLN
16	V	122	GLU
17	Y	27	MET
17	Y	42	ARG
19	Z	4	LEU
19	Z	35	ARG
1	a	162	PRO
2	b	128	THR
2	b	246	PHE
2	b	362	PHE
2	b	467	ILE
2	b	483	ASP
3	c	156	LYS

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Mol	Chain	Res	Type
3	c	289	PHE
3	c	355	THR
3	c	416	SER
3	c	418	ASN
4	d	24	ARG
4	d	180	ARG
5	e	25	ILE
5	e	60	GLN
5	e	62	SER
5	e	68	ASP
7	h	49	TYR
10	k	27	VAL
13	o	23	ASP
13	o	58	ASN
13	o	118	LEU
13	o	181	GLU
14	t	2	GLU
16	v	6	GLU
17	y	23	THR
19	z	1	MET
19	z	5	PHE
19	z	6	GLN
19	z	29	SER
19	z	46	LEU

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

Mol	Chain	Res	Type
2	B	53	ASN
2	B	179	GLN
2	B	331	ASN
13	O	82	GLN
16	V	34	GLN
1	a	315	ASN
2	b	53	ASN
2	b	179	GLN
2	b	331	ASN
2	b	374	ASN
3	c	201	ASN
4	d	332	GLN
6	f	44	GLN
7	h	59	ASN

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Mol	Chain	Res	Type
13	o	36	GLN
13	o	82	GLN
13	o	231	HIS
15	u	73	GLN
16	v	34	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	FME	T	1	14	8,9,10	0.53	0	7,9,11	1.70	2 (28%)
8	FME	I	1	8	8,9,10	0.75	0	7,9,11	1.04	0
8	FME	i	1	8	8,9,10	0.73	0	7,9,11	1.54	3 (42%)
14	FME	t	1	14	8,9,10	0.64	0	7,9,11	1.70	3 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	T	1	14	-	3/7/9/11	-
8	FME	I	1	8	-	2/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	CE-SD-CG	2.58	109.25	100.40
14	T	1	FME	O-C-CA	-2.49	118.27	124.78
14	t	1	FME	O-C-CA	-2.36	118.60	124.78
14	t	1	FME	CE-SD-CG	2.29	108.28	100.40
8	i	1	FME	O1-CN-N	-2.24	119.36	125.27
14	t	1	FME	C-CA-N	2.24	113.77	109.73
8	i	1	FME	C-CA-N	2.07	113.47	109.73
8	i	1	FME	O-C-CA	-2.01	119.50	124.78

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	1	FME	N-CA-CB-CG
8	I	1	FME	O1-CN-N-CA
8	i	1	FME	O1-CN-N-CA
14	t	1	FME	C-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	CB-CG-SD-CE
8	I	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 366 ligands modelled in this entry, 53 are unknown and 13 are monoatomic - leaving 300 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$
28	LHG	d	402	-	43,43,48	1.06	2 (4%)	46,49,54	0.96	3 (6%)
28	LHG	a	415	-	48,48,48	1.01	2 (4%)	51,54,54	1.07	4 (7%)
27	PL9	a	414	-	55,55,55	0.94	3 (5%)	68,69,69	1.65	16 (23%)
35	HTG	B	630	-	19,19,19	0.98	2 (10%)	23,24,24	1.32	2 (8%)
25	BCR	C	515	-	41,41,41	0.83	0	56,56,56	1.50	10 (17%)
31	DMS	V	207	-	3,3,3	2.84	1 (33%)	3,3,3	1.25	0
31	DMS	h	105	-	3,3,3	2.74	1 (33%)	3,3,3	0.68	0
23	CLA	b	605	-	59,73,73	2.00	14 (23%)	67,113,113	2.16	21 (31%)
30	LMT	m	103	-	36,36,36	0.61	1 (2%)	47,47,47	0.98	3 (6%)
28	LHG	L	101	-	48,48,48	0.97	3 (6%)	51,54,54	1.13	3 (5%)
23	CLA	C	504	-	59,73,73	2.33	13 (22%)	67,113,113	1.84	18 (26%)
31	DMS	V	210	-	3,3,3	2.71	1 (33%)	3,3,3	0.53	0
30	LMT	e	103	-	25,25,36	0.71	1 (4%)	30,30,47	1.02	3 (10%)
25	BCR	B	619	-	41,41,41	1.06	1 (2%)	56,56,56	1.17	9 (16%)
36	DGD	C	519	-	63,63,67	0.86	2 (3%)	77,77,81	1.13	8 (10%)
35	HTG	V	204	-	14,14,19	0.67	0	18,19,24	3.10	6 (33%)
23	CLA	B	604	-	59,73,73	1.83	14 (23%)	67,113,113	2.37	21 (31%)
30	LMT	B	623	-	36,36,36	0.59	0	47,47,47	1.05	3 (6%)
23	CLA	B	608	41	59,73,73	2.03	12 (20%)	67,113,113	2.08	20 (29%)
31	DMS	b	638	-	3,3,3	2.93	1 (33%)	3,3,3	1.08	0
35	HTG	c	921	-	19,19,19	0.95	2 (10%)	23,24,24	1.45	2 (8%)
37	HEM	e	105	5,6	27,50,50	2.18	9 (33%)	17,82,82	2.50	8 (47%)
23	CLA	B	613	-	59,73,73	2.11	13 (22%)	67,113,113	2.13	19 (28%)
34	LMG	D	412	-	51,51,55	1.10	2 (3%)	59,59,63	1.34	8 (13%)
23	CLA	a	407	41	59,73,73	1.82	11 (18%)	67,113,113	2.16	18 (26%)
31	DMS	i	106	-	3,3,3	2.74	1 (33%)	3,3,3	0.66	0
31	DMS	C	527	-	3,3,3	2.56	1 (33%)	3,3,3	0.63	0
23	CLA	b	602	41	59,73,73	2.26	15 (25%)	67,113,113	2.42	24 (35%)
36	DGD	h	102	-	63,63,67	0.93	3 (4%)	77,77,81	1.23	9 (11%)
37	HEM	E	105	5,6	27,50,50	2.09	10 (37%)	17,82,82	2.40	7 (41%)
31	DMS	C	529	-	3,3,3	2.55	1 (33%)	3,3,3	0.44	0
31	DMS	v	210	-	3,3,3	2.67	1 (33%)	3,3,3	0.56	0
31	DMS	l	102	-	3,3,3	2.64	1 (33%)	3,3,3	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DMS	B	647	-	3,3,3	2.72	1 (33%)	3,3,3	0.55	0
23	CLA	A	405	-	59,73,73	1.74	13 (22%)	67,113,113	2.22	25 (37%)
31	DMS	A	422	-	3,3,3	2.68	1 (33%)	3,3,3	0.84	0
25	BCR	D	405	-	41,41,41	1.10	4 (9%)	56,56,56	1.99	14 (25%)
31	DMS	V	205	-	3,3,3	2.63	1 (33%)	3,3,3	0.95	0
25	BCR	t	101	-	41,41,41	1.03	0	56,56,56	1.52	14 (25%)
34	LMG	B	622	-	51,51,55	0.99	3 (5%)	59,59,63	1.31	9 (15%)
23	CLA	c	903	-	59,73,73	1.97	10 (16%)	67,113,113	2.23	25 (37%)
27	PL9	D	406	-	55,55,55	1.02	3 (5%)	68,69,69	1.49	13 (19%)
23	CLA	D	401	41	59,73,73	1.88	14 (23%)	67,113,113	2.14	19 (28%)
31	DMS	d	419	-	3,3,3	2.69	1 (33%)	3,3,3	0.71	0
26	SQD	a	412	-	53,54,54	0.93	3 (5%)	62,65,65	2.14	13 (20%)
36	DGD	c	917	-	63,63,67	0.84	3 (4%)	77,77,81	1.24	8 (10%)
31	DMS	c	925	-	3,3,3	2.81	1 (33%)	3,3,3	0.84	0
36	DGD	d	407	-	50,50,67	1.11	2 (4%)	58,58,81	1.24	6 (10%)
31	DMS	B	649	-	3,3,3	2.71	1 (33%)	3,3,3	0.55	0
23	CLA	c	902	-	59,73,73	2.14	14 (23%)	67,113,113	2.36	15 (22%)
25	BCR	B	620	-	41,41,41	1.00	2 (4%)	56,56,56	1.57	13 (23%)
31	DMS	d	418	-	3,3,3	2.75	1 (33%)	3,3,3	0.62	0
31	DMS	v	205	-	3,3,3	2.65	1 (33%)	3,3,3	0.55	0
31	DMS	C	524	-	3,3,3	2.39	1 (33%)	3,3,3	0.94	0
28	LHG	D	411	-	45,45,48	0.98	2 (4%)	48,51,54	1.03	4 (8%)
25	BCR	b	619	-	41,41,41	1.03	2 (4%)	56,56,56	1.34	7 (12%)
31	DMS	C	533	-	3,3,3	2.67	1 (33%)	3,3,3	0.51	0
31	DMS	O	305	-	3,3,3	2.66	1 (33%)	3,3,3	0.88	0
31	DMS	H	101	-	3,3,3	2.78	1 (33%)	3,3,3	0.58	0
31	DMS	B	636	-	3,3,3	3.09	1 (33%)	3,3,3	0.77	0
31	DMS	D	417	-	3,3,3	2.99	1 (33%)	3,3,3	0.77	0
25	BCR	c	915	-	41,41,41	0.79	0	56,56,56	1.33	8 (14%)
36	DGD	c	918	-	63,63,67	0.90	2 (3%)	77,77,81	1.18	9 (11%)
35	HTG	d	413	-	19,19,19	1.18	1 (5%)	23,24,24	2.11	5 (21%)
31	DMS	b	634	-	3,3,3	2.45	1 (33%)	3,3,3	0.96	0
31	DMS	V	208	-	3,3,3	2.60	1 (33%)	3,3,3	0.41	0
31	DMS	v	207	-	3,3,3	2.72	1 (33%)	3,3,3	0.75	0
23	CLA	C	514	-	59,73,73	2.50	15 (25%)	67,113,113	2.01	15 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	606	-	59,73,73	1.94	14 (23%)	67,113,113	1.96	19 (28%)
31	DMS	V	209	-	3,3,3	2.52	1 (33%)	3,3,3	0.80	0
35	HTG	v	204	-	19,19,19	0.90	1 (5%)	23,24,24	2.78	8 (34%)
31	DMS	c	928	-	3,3,3	2.64	1 (33%)	3,3,3	0.50	0
31	DMS	O	310	-	3,3,3	2.61	1 (33%)	3,3,3	0.71	0
31	DMS	b	633	-	3,3,3	1.83	1 (33%)	3,3,3	0.60	0
26	SQD	A	410	-	53,54,54	0.99	3 (5%)	62,65,65	2.00	17 (27%)
36	DGD	C	517	-	63,63,67	0.82	2 (3%)	77,77,81	1.22	8 (10%)
30	LMT	z	101	-	32,32,36	0.63	1 (3%)	42,42,47	1.19	5 (11%)
31	DMS	k	103	-	3,3,3	2.65	1 (33%)	3,3,3	0.78	0
31	DMS	V	206	-	3,3,3	2.65	1 (33%)	3,3,3	0.77	0
31	DMS	u	204	-	3,3,3	2.76	1 (33%)	3,3,3	0.87	0
38	RRX	x	102	-	42,42,42	0.90	0	57,58,58	1.38	7 (12%)
34	LMG	d	411	-	51,51,55	1.13	3 (5%)	59,59,63	1.32	6 (10%)
23	CLA	c	912	3	59,73,73	2.46	15 (25%)	67,113,113	2.08	15 (22%)
31	DMS	U	203	-	3,3,3	2.71	1 (33%)	3,3,3	0.51	0
23	CLA	C	505	41	59,73,73	2.04	12 (20%)	67,113,113	2.15	16 (23%)
20	OEX	A	401	1,3,41	0,15,15	0.00	-	-	-	-
31	DMS	C	525	-	3,3,3	2.62	1 (33%)	3,3,3	0.90	0
23	CLA	b	614	-	59,73,73	2.00	11 (18%)	67,113,113	2.07	17 (25%)
28	LHG	d	410	-	45,45,48	1.00	2 (4%)	48,51,54	1.02	3 (6%)
25	BCR	d	405	-	41,41,41	0.99	1 (2%)	56,56,56	1.93	19 (33%)
24	PHO	a	409	-	67,69,69	1.93	15 (22%)	85,99,99	1.98	21 (24%)
23	CLA	c	907	-	59,73,73	2.01	13 (22%)	67,113,113	1.91	16 (23%)
35	HTG	C	521	-	19,19,19	0.96	2 (10%)	23,24,24	1.69	1 (4%)
23	CLA	b	608	41	59,73,73	2.07	14 (23%)	67,113,113	1.96	22 (32%)
35	HTG	b	623	-	19,19,19	1.11	2 (10%)	23,24,24	1.79	4 (17%)
31	DMS	i	105	-	3,3,3	2.69	1 (33%)	3,3,3	0.88	0
31	DMS	b	645	-	3,3,3	2.69	1 (33%)	3,3,3	0.49	0
25	BCR	B	618	-	41,41,41	1.06	1 (2%)	56,56,56	1.48	9 (16%)
26	SQD	A	415	-	53,54,54	1.03	3 (5%)	62,65,65	1.91	12 (19%)
28	LHG	l	101	-	48,48,48	0.82	2 (4%)	51,54,54	1.03	3 (5%)
23	CLA	b	606	-	59,73,73	1.84	13 (22%)	67,113,113	2.21	21 (31%)
26	SQD	L	102	-	53,54,54	1.08	3 (5%)	62,65,65	1.68	12 (19%)
30	LMT	B	644	-	24,24,36	0.34	0	29,29,47	1.26	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	508	41	59,73,73	2.36	15 (25%)	67,113,113	2.31	19 (28%)
35	HTG	b	628	-	19,19,19	0.90	1 (5%)	23,24,24	1.51	1 (4%)
23	CLA	C	509	-	59,73,73	2.34	14 (23%)	67,113,113	1.95	19 (28%)
35	HTG	O	302	-	19,19,19	1.45	3 (15%)	23,24,24	1.51	5 (21%)
23	CLA	B	610	-	59,73,73	2.00	12 (20%)	67,113,113	2.06	18 (26%)
31	DMS	V	201	-	3,3,3	2.57	1 (33%)	3,3,3	0.76	0
23	CLA	c	908	41	59,73,73	2.18	15 (25%)	67,113,113	1.97	16 (23%)
35	HTG	B	624	-	19,19,19	1.52	3 (15%)	23,24,24	1.56	4 (17%)
31	DMS	V	211	-	3,3,3	2.97	1 (33%)	3,3,3	1.05	0
25	BCR	T	101	-	41,41,41	0.90	0	56,56,56	1.81	18 (32%)
31	DMS	c	927	-	3,3,3	2.71	1 (33%)	3,3,3	1.27	1 (33%)
31	DMS	V	202	-	3,3,3	2.66	1 (33%)	3,3,3	0.81	0
31	DMS	U	204	-	3,3,3	2.88	1 (33%)	3,3,3	0.80	0
35	HTG	b	622	-	19,19,19	1.31	3 (15%)	23,24,24	1.51	4 (17%)
25	BCR	c	916	-	41,41,41	0.81	0	56,56,56	1.56	10 (17%)
23	CLA	B	615	-	59,73,73	2.09	13 (22%)	67,113,113	2.25	21 (31%)
23	CLA	b	609	-	59,73,73	2.01	11 (18%)	67,113,113	2.10	22 (32%)
30	LMT	m	104	-	36,36,36	0.56	0	47,47,47	1.24	4 (8%)
36	DGD	c	919	-	63,63,67	0.94	3 (4%)	77,77,81	1.23	10 (12%)
31	DMS	D	415	-	3,3,3	2.74	1 (33%)	3,3,3	0.69	0
28	LHG	e	101	-	39,39,48	1.16	2 (5%)	42,45,54	1.02	3 (7%)
35	HTG	D	414	-	19,19,19	0.94	1 (5%)	23,24,24	1.31	1 (4%)
31	DMS	o	303	-	3,3,3	2.68	1 (33%)	3,3,3	1.00	0
28	LHG	K	101	-	43,43,48	1.07	2 (4%)	47,48,54	1.14	5 (10%)
26	SQD	a	417	-	53,54,54	1.10	5 (9%)	62,65,65	1.35	4 (6%)
25	BCR	C	530	-	41,41,41	0.84	0	56,56,56	1.56	8 (14%)
31	DMS	v	206	-	3,3,3	2.60	1 (33%)	3,3,3	0.81	0
23	CLA	B	617	-	59,73,73	1.95	14 (23%)	67,113,113	2.01	21 (31%)
34	LMG	C	520	-	51,51,55	1.15	2 (3%)	59,59,63	1.35	9 (15%)
31	DMS	v	202	-	3,3,3	2.60	1 (33%)	3,3,3	0.32	0
31	DMS	c	924	-	3,3,3	2.36	1 (33%)	3,3,3	0.42	0
23	CLA	B	605	-	59,73,73	1.95	13 (22%)	67,113,113	1.83	16 (23%)
32	BCT	A	420	21	0,3,3	0.00	-	0,3,3	0.00	-
31	DMS	D	416	-	3,3,3	2.49	1 (33%)	3,3,3	0.88	0
31	DMS	a	401	-	3,3,3	2.71	1 (33%)	3,3,3	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DMS	d	414	-	3,3,3	2.70	1 (33%)	3,3,3	0.77	0
31	DMS	b	640	-	3,3,3	2.70	1 (33%)	3,3,3	0.83	0
31	DMS	B	637	-	3,3,3	2.27	1 (33%)	3,3,3	0.96	0
31	DMS	F	102	-	3,3,3	2.61	1 (33%)	3,3,3	0.25	0
25	BCR	j	104	-	41,41,41	0.82	0	56,56,56	1.48	11 (19%)
40	HEC	V	203	16	26,50,50	1.95	6 (23%)	18,82,82	1.70	4 (22%)
35	HTG	B	625	-	19,19,19	1.41	3 (15%)	23,24,24	2.08	8 (34%)
31	DMS	a	420	-	3,3,3	2.65	1 (33%)	3,3,3	0.36	0
28	LHG	d	409	-	48,48,48	0.79	2 (4%)	51,54,54	1.28	8 (15%)
25	BCR	a	411	-	41,41,41	1.20	3 (7%)	56,56,56	1.35	5 (8%)
31	DMS	B	642	-	3,3,3	2.92	1 (33%)	3,3,3	1.28	0
25	BCR	C	516	-	41,41,41	0.99	0	56,56,56	1.37	7 (12%)
31	DMS	h	101	-	3,3,3	2.68	1 (33%)	3,3,3	1.34	1 (33%)
23	CLA	c	910	-	59,73,73	2.43	15 (25%)	67,113,113	2.48	22 (32%)
23	CLA	d	403	-	59,73,73	1.92	12 (20%)	67,113,113	2.04	19 (28%)
23	CLA	C	510	-	59,73,73	2.30	10 (16%)	67,113,113	2.17	19 (28%)
30	LMT	F	101	-	36,36,36	0.71	1 (2%)	47,47,47	1.19	5 (10%)
31	DMS	b	637	-	3,3,3	2.68	1 (33%)	3,3,3	1.01	0
36	DGD	H	103	-	63,63,67	1.05	3 (4%)	77,77,81	1.32	7 (9%)
31	DMS	v	208	-	3,3,3	2.73	1 (33%)	3,3,3	0.73	0
34	LMG	C	531	-	51,51,55	1.03	2 (3%)	59,59,63	1.08	4 (6%)
31	DMS	u	206	-	3,3,3	2.79	1 (33%)	3,3,3	0.63	0
31	DMS	a	423	-	3,3,3	2.80	1 (33%)	3,3,3	0.82	0
31	DMS	A	419	-	3,3,3	2.75	1 (33%)	3,3,3	0.71	0
31	DMS	v	209	-	3,3,3	2.71	1 (33%)	3,3,3	0.72	0
31	DMS	u	205	-	3,3,3	2.62	1 (33%)	3,3,3	1.05	0
31	DMS	b	641	-	3,3,3	2.64	1 (33%)	3,3,3	0.75	0
28	LHG	D	409	-	48,48,48	0.85	1 (2%)	51,54,54	1.27	6 (11%)
38	RRX	H	102	-	42,42,42	0.89	1 (2%)	57,58,58	1.57	9 (15%)
31	DMS	a	421	-	3,3,3	2.68	1 (33%)	3,3,3	0.63	0
31	DMS	A	421	-	3,3,3	2.71	1 (33%)	3,3,3	0.80	0
30	LMT	b	621	-	25,25,36	0.63	1 (4%)	30,30,47	1.30	5 (16%)
31	DMS	c	933	-	3,3,3	2.67	1 (33%)	3,3,3	0.93	0
23	CLA	C	503	-	59,73,73	2.27	11 (18%)	67,113,113	1.88	15 (22%)
31	DMS	B	638	-	3,3,3	2.78	1 (33%)	3,3,3	1.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DMS	c	937	-	3,3,3	2.66	1 (33%)	3,3,3	0.62	0
23	CLA	d	401	41	59,73,73	2.01	11 (18%)	67,113,113	1.94	19 (28%)
23	CLA	C	512	3	59,73,73	2.33	14 (23%)	67,113,113	2.27	20 (29%)
23	CLA	a	406	-	59,73,73	1.92	14 (23%)	67,113,113	2.25	22 (32%)
23	CLA	B	616	-	59,73,73	2.19	16 (27%)	67,113,113	2.03	15 (22%)
23	CLA	B	603	-	59,73,73	2.21	14 (23%)	67,113,113	2.17	23 (34%)
23	CLA	b	611	41	59,73,73	2.02	15 (25%)	67,113,113	1.76	18 (26%)
31	DMS	b	643	-	3,3,3	2.68	1 (33%)	3,3,3	0.60	0
31	DMS	A	423	-	3,3,3	1.91	1 (33%)	3,3,3	0.64	0
23	CLA	A	408	-	59,73,73	1.83	15 (25%)	67,113,113	2.11	19 (28%)
31	DMS	b	647	-	3,3,3	2.75	1 (33%)	3,3,3	0.71	0
23	CLA	B	611	41	59,73,73	2.27	16 (27%)	67,113,113	2.19	17 (25%)
23	CLA	d	404	-	59,73,73	1.91	13 (22%)	67,113,113	1.99	19 (28%)
31	DMS	b	639	-	3,3,3	2.77	1 (33%)	3,3,3	1.33	1 (33%)
31	DMS	O	303	-	3,3,3	2.68	1 (33%)	3,3,3	0.57	0
23	CLA	b	604	-	59,73,73	2.14	12 (20%)	67,113,113	2.23	24 (35%)
31	DMS	B	645	-	3,3,3	2.80	1 (33%)	3,3,3	0.70	0
23	CLA	b	613	-	59,73,73	2.00	12 (20%)	67,113,113	2.07	18 (26%)
23	CLA	b	607	-	59,73,73	2.45	15 (25%)	67,113,113	1.95	18 (26%)
31	DMS	C	528	-	3,3,3	2.64	1 (33%)	3,3,3	0.71	0
23	CLA	A	406	41	59,73,73	1.72	10 (16%)	67,113,113	2.24	17 (25%)
25	BCR	b	618	-	41,41,41	0.95	0	56,56,56	1.75	13 (23%)
23	CLA	b	616	-	59,73,73	2.13	12 (20%)	67,113,113	2.19	22 (32%)
23	CLA	b	603	-	59,73,73	1.93	16 (27%)	67,113,113	2.32	27 (40%)
30	LMT	a	422	-	36,36,36	0.65	1 (2%)	47,47,47	0.95	3 (6%)
23	CLA	B	612	-	59,73,73	1.97	11 (18%)	67,113,113	2.05	18 (26%)
31	DMS	v	201	-	3,3,3	2.42	1 (33%)	3,3,3	0.47	0
31	DMS	A	424	-	3,3,3	2.76	1 (33%)	3,3,3	1.08	0
31	DMS	c	926	-	3,3,3	2.61	1 (33%)	3,3,3	0.30	0
30	LMT	Z	101	-	36,36,36	0.70	1 (2%)	47,47,47	0.90	2 (4%)
23	CLA	C	511	-	59,73,73	2.23	13 (22%)	67,113,113	1.97	16 (23%)
31	DMS	c	929	-	3,3,3	2.83	1 (33%)	3,3,3	0.69	0
23	CLA	c	904	-	59,73,73	2.63	16 (27%)	67,113,113	2.12	18 (26%)
31	DMS	b	644	-	3,3,3	2.78	1 (33%)	3,3,3	0.99	0
31	DMS	H	105	-	3,3,3	2.74	1 (33%)	3,3,3	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	913	-	59,73,73	2.43	14 (23%)	67,113,113	2.28	16 (23%)
23	CLA	B	609	-	59,73,73	1.86	13 (22%)	67,113,113	1.88	19 (28%)
23	CLA	C	506	-	59,73,73	2.16	15 (25%)	67,113,113	2.06	16 (23%)
31	DMS	h	103	-	3,3,3	2.65	1 (33%)	3,3,3	0.58	0
23	CLA	D	403	-	59,73,73	1.92	10 (16%)	67,113,113	2.43	24 (35%)
24	PHO	a	408	-	67,69,69	1.79	15 (22%)	85,99,99	1.77	17 (20%)
26	SQD	B	621	-	53,54,54	1.03	3 (5%)	62,65,65	1.60	7 (11%)
25	BCR	Y	101	-	41,41,41	0.85	0	56,56,56	1.66	15 (26%)
23	CLA	B	614	-	59,73,73	1.80	14 (23%)	67,113,113	1.85	15 (22%)
31	DMS	O	307	-	3,3,3	2.75	1 (33%)	3,3,3	0.72	0
31	DMS	O	304	-	3,3,3	2.79	1 (33%)	3,3,3	0.87	0
35	HTG	c	922	-	19,19,19	1.02	2 (10%)	23,24,24	1.74	3 (13%)
25	BCR	k	102	-	41,41,41	1.02	1 (2%)	56,56,56	1.21	8 (14%)
23	CLA	b	617	-	59,73,73	2.17	15 (25%)	67,113,113	2.05	22 (32%)
20	OEX	a	402	1,3,41	0,15,15	0.00	-	-	-	-
30	LMT	M	101	-	36,36,36	0.64	0	47,47,47	0.92	2 (4%)
31	DMS	b	636	-	3,3,3	2.74	1 (33%)	3,3,3	0.52	0
23	CLA	B	607	-	59,73,73	2.31	14 (23%)	67,113,113	2.04	16 (23%)
26	SQD	D	408	-	44,45,54	1.22	4 (9%)	53,56,65	2.21	13 (24%)
26	SQD	x	101	-	40,41,54	1.26	3 (7%)	49,52,65	1.46	9 (18%)
23	CLA	C	507	-	59,73,73	2.11	14 (23%)	67,113,113	2.20	18 (26%)
23	CLA	B	602	41	59,73,73	2.39	14 (23%)	67,113,113	2.29	18 (26%)
30	LMT	T	103	-	24,24,36	0.50	0	29,29,47	1.32	4 (13%)
30	LMT	A	416	-	36,36,36	0.84	1 (2%)	47,47,47	1.19	6 (12%)
31	DMS	B	640	-	3,3,3	2.63	1 (33%)	3,3,3	0.77	0
31	DMS	c	935	-	3,3,3	2.68	1 (33%)	3,3,3	0.74	0
28	LHG	A	412	-	48,48,48	1.05	2 (4%)	51,54,54	0.96	3 (5%)
35	HTG	c	923	-	11,12,19	0.54	0	11,11,24	1.89	2 (18%)
31	DMS	B	639	-	3,3,3	2.77	1 (33%)	3,3,3	0.89	0
31	DMS	B	648	-	3,3,3	2.49	1 (33%)	3,3,3	1.05	0
31	DMS	U	202	-	3,3,3	2.68	1 (33%)	3,3,3	1.60	1 (33%)
34	LMG	c	920	-	51,51,55	0.96	2 (3%)	59,59,63	1.31	7 (11%)
32	BCT	a	424	21	0,3,3	0.00	-	0,3,3	0.00	-
28	LHG	d	408	-	48,48,48	0.91	2 (4%)	51,54,54	1.24	3 (5%)
35	HTG	B	631	-	19,19,19	1.11	1 (5%)	23,24,24	1.25	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DMS	b	646	-	3,3,3	2.74	1 (33%)	3,3,3	0.69	0
31	DMS	o	301	-	3,3,3	2.14	1 (33%)	3,3,3	0.39	0
35	HTG	b	627	-	19,19,19	1.22	2 (10%)	23,24,24	1.49	2 (8%)
31	DMS	c	936	-	3,3,3	2.73	1 (33%)	3,3,3	0.83	0
25	BCR	A	409	-	41,41,41	1.06	4 (9%)	56,56,56	1.44	9 (16%)
36	DGD	C	518	-	63,63,67	0.95	4 (6%)	77,77,81	1.09	4 (5%)
31	DMS	h	104	-	3,3,3	2.70	1 (33%)	3,3,3	0.59	0
31	DMS	u	203	-	3,3,3	2.58	1 (33%)	3,3,3	0.92	0
27	PL9	d	406	-	55,55,55	1.05	4 (7%)	68,69,69	1.59	12 (17%)
35	HTG	C	523	-	19,19,19	1.09	2 (10%)	23,24,24	1.74	1 (4%)
28	LHG	D	410	-	48,48,48	0.83	2 (4%)	51,54,54	1.13	2 (3%)
28	LHG	E	101	-	48,48,48	1.06	2 (4%)	51,54,54	1.17	5 (9%)
31	DMS	B	641	-	3,3,3	2.82	1 (33%)	3,3,3	0.81	0
30	LMT	B	643	-	24,24,36	0.39	0	29,29,47	0.88	1 (3%)
34	LMG	C	501	-	51,51,55	0.95	2 (3%)	59,59,63	1.15	4 (6%)
31	DMS	o	304	-	3,3,3	2.76	1 (33%)	3,3,3	0.81	0
34	LMG	J	101	39	51,51,55	0.93	2 (3%)	59,59,63	0.97	4 (6%)
36	DGD	D	407	-	50,50,67	1.28	3 (6%)	58,58,81	1.74	8 (13%)
35	HTG	C	522	-	19,19,19	1.05	2 (10%)	23,24,24	1.95	4 (17%)
23	CLA	c	909	-	59,73,73	2.26	15 (25%)	67,113,113	1.87	14 (20%)
31	DMS	d	415	-	3,3,3	2.65	1 (33%)	3,3,3	0.88	0
30	LMT	a	418	-	36,36,36	0.71	1 (2%)	47,47,47	1.30	6 (12%)
35	HTG	B	626	-	19,19,19	0.94	1 (5%)	23,24,24	1.59	1 (4%)
23	CLA	c	914	-	59,73,73	2.55	14 (23%)	67,113,113	2.06	18 (26%)
31	DMS	d	416	-	3,3,3	2.68	1 (33%)	3,3,3	0.57	0
31	DMS	O	311	-	3,3,3	2.64	1 (33%)	3,3,3	0.85	0
34	LMG	j	101	39	51,51,55	0.98	4 (7%)	59,59,63	1.16	7 (11%)
31	DMS	C	526	-	3,3,3	2.73	1 (33%)	3,3,3	0.59	0
23	CLA	c	906	-	59,73,73	2.07	17 (28%)	67,113,113	1.95	20 (29%)
31	DMS	e	104	-	3,3,3	2.67	1 (33%)	3,3,3	0.58	0
34	LMG	c	930	-	51,51,55	1.07	3 (5%)	59,59,63	1.26	5 (8%)
31	DMS	c	932	-	3,3,3	2.65	1 (33%)	3,3,3	0.75	0
23	CLA	D	404	-	59,73,73	2.04	14 (23%)	67,113,113	1.94	22 (32%)
34	LMG	a	413	-	51,51,55	1.00	2 (3%)	59,59,63	1.10	4 (6%)
23	CLA	b	615	-	59,73,73	2.11	16 (27%)	67,113,113	1.87	20 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	b	620	-	41,41,41	0.90	2 (4%)	56,56,56	1.24	5 (8%)
24	PHO	D	402	-	67,69,69	1.95	14 (20%)	85,99,99	1.87	17 (20%)
31	DMS	b	642	-	3,3,3	2.70	1 (33%)	3,3,3	0.57	0
23	CLA	a	410	-	59,73,73	1.94	10 (16%)	67,113,113	2.09	21 (31%)
23	CLA	c	905	41	59,73,73	2.32	15 (25%)	67,113,113	2.33	20 (29%)
31	DMS	O	308	-	3,3,3	2.72	1 (33%)	3,3,3	0.69	0
24	PHO	A	407	-	67,69,69	1.75	11 (16%)	85,99,99	2.01	22 (25%)
31	DMS	O	306	-	3,3,3	2.70	1 (33%)	3,3,3	0.55	0
31	DMS	c	934	-	3,3,3	2.70	1 (33%)	3,3,3	0.73	0
23	CLA	c	911	-	59,73,73	1.82	10 (16%)	67,113,113	2.05	20 (29%)
40	HEC	v	203	16	26,50,50	2.27	9 (34%)	18,82,82	2.45	7 (38%)
31	DMS	O	309	-	3,3,3	2.88	1 (33%)	3,3,3	0.94	0
23	CLA	b	610	-	59,73,73	2.45	13 (22%)	67,113,113	1.76	16 (23%)
23	CLA	b	612	-	59,73,73	2.12	10 (16%)	67,113,113	2.11	21 (31%)
34	LMG	m	102	-	51,51,55	0.95	2 (3%)	59,59,63	1.33	6 (10%)
27	PL9	A	411	-	55,55,55	0.90	4 (7%)	68,69,69	1.69	14 (20%)
23	CLA	C	513	-	59,73,73	2.53	14 (23%)	67,113,113	2.08	18 (26%)
31	DMS	b	635	-	3,3,3	2.72	1 (33%)	3,3,3	0.59	0
31	DMS	B	646	-	3,3,3	2.60	1 (33%)	3,3,3	0.71	0
31	DMS	A	418	-	3,3,3	2.73	1 (33%)	3,3,3	0.65	0
23	CLA	C	502	-	59,73,73	2.05	12 (20%)	67,113,113	1.94	15 (22%)
30	LMT	I	101	-	36,36,36	0.74	1 (2%)	47,47,47	1.40	5 (10%)

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
28	LHG	d	402	-	-	24/48/48/53	-
28	LHG	a	415	-	-	20/53/53/53	-
35	HTG	C	522	-	-	5/10/30/30	0/1/1/1
35	HTG	B	630	-	-	4/10/30/30	0/1/1/1
25	BCR	C	515	-	-	3/29/63/63	0/2/2/2
23	CLA	b	605	-	3/3/20/25	5/37/135/135	-
30	LMT	m	103	-	-	10/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LHG	L	101	-	-	18/53/53/53	-
23	CLA	C	504	-	2/2/20/25	3/37/135/135	-
28	LHG	d	410	-	-	11/50/50/53	-
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
36	DGD	C	519	-	-	18/51/91/95	0/2/2/2
35	HTG	V	204	-	-	1/5/25/30	0/1/1/1
23	CLA	B	604	-	3/3/20/25	3/37/135/135	-
30	LMT	B	623	-	-	15/21/61/61	0/2/2/2
23	CLA	B	608	41	3/3/20/25	3/37/135/135	-
35	HTG	c	921	-	-	5/10/30/30	0/1/1/1
37	HEM	e	105	5,6	-	0/6/54/54	-
23	CLA	B	613	-	3/3/20/25	2/37/135/135	-
34	LMG	D	412	-	-	24/46/66/70	0/1/1/1
23	CLA	a	407	41	2/2/20/25	9/37/135/135	-
35	HTG	B	631	-	-	3/10/30/30	0/1/1/1
23	CLA	b	602	41	3/3/20/25	18/37/135/135	-
36	DGD	h	102	-	-	17/51/91/95	0/2/2/2
37	HEM	E	105	5,6	-	0/6/54/54	-
23	CLA	B	603	-	3/3/20/25	4/37/135/135	-
23	CLA	b	607	-	3/3/20/25	11/37/135/135	-
36	DGD	D	407	-	-	24/44/64/95	0/1/1/2
23	CLA	A	405	-	2/2/20/25	2/37/135/135	-
25	BCR	D	405	-	-	4/29/63/63	0/2/2/2
25	BCR	t	101	-	-	4/29/63/63	0/2/2/2
34	LMG	B	622	-	-	15/46/66/70	0/1/1/1
23	CLA	c	903	-	2/2/20/25	8/37/135/135	-
27	PL9	D	406	-	-	3/53/73/73	0/1/1/1
23	CLA	c	914	-	1/1/20/25	9/37/135/135	-
26	SQD	a	412	-	-	23/49/69/69	0/1/1/1
36	DGD	c	917	-	-	13/51/91/95	0/2/2/2
36	DGD	d	407	-	-	22/44/64/95	0/1/1/2
26	SQD	B	621	-	-	29/49/69/69	0/1/1/1
23	CLA	c	902	-	3/3/20/25	4/37/135/135	-
25	BCR	B	620	-	-	0/29/63/63	0/2/2/2
23	CLA	b	610	-	2/2/20/25	0/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LHG	D	411	-	-	15/50/50/53	-
25	BCR	b	619	-	-	1/29/63/63	0/2/2/2
25	BCR	c	915	-	-	1/29/63/63	0/2/2/2
36	DGD	c	918	-	-	16/51/91/95	0/2/2/2
35	HTG	d	413	-	-	7/10/30/30	0/1/1/1
23	CLA	B	606	-	3/3/20/25	6/37/135/135	-
35	HTG	v	204	-	-	7/10/30/30	0/1/1/1
28	LHG	d	409	-	-	10/53/53/53	-
26	SQD	A	410	-	-	20/49/69/69	0/1/1/1
23	CLA	b	609	-	1/1/20/25	1/37/135/135	-
34	LMG	d	411	-	-	25/46/66/70	0/1/1/1
23	CLA	c	912	3	2/2/20/25	1/37/135/135	-
23	CLA	B	607	-	3/3/20/25	8/37/135/135	-
23	CLA	b	614	-	3/3/20/25	3/37/135/135	-
30	LMT	e	103	-	-	6/17/37/61	0/1/1/2
25	BCR	d	405	-	-	4/29/63/63	0/2/2/2
24	PHO	a	409	-	-	6/53/103/103	0/5/6/6
23	CLA	c	907	-	2/2/20/25	10/37/135/135	-
35	HTG	C	521	-	-	3/10/30/30	0/1/1/1
36	DGD	c	919	-	-	15/51/91/95	0/2/2/2
35	HTG	b	623	-	-	8/10/30/30	0/1/1/1
25	BCR	B	618	-	-	2/29/63/63	0/2/2/2
26	SQD	A	415	-	-	24/49/69/69	0/1/1/1
28	LHG	l	101	-	-	13/53/53/53	-
23	CLA	b	606	-	3/3/20/25	6/37/135/135	-
26	SQD	L	102	-	-	27/49/69/69	0/1/1/1
30	LMT	B	644	-	-	8/15/35/61	0/1/1/2
23	CLA	C	508	41	3/3/20/25	11/37/135/135	-
35	HTG	b	628	-	-	1/10/30/30	0/1/1/1
23	CLA	C	509	-	3/3/20/25	6/37/135/135	-
35	HTG	O	302	-	-	3/10/30/30	0/1/1/1
23	CLA	B	610	-	2/2/20/25	0/37/135/135	-
23	CLA	c	908	41	3/3/20/25	10/37/135/135	-
35	HTG	B	624	-	-	4/10/30/30	0/1/1/1
25	BCR	T	101	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	506	-	2/2/20/25	2/37/135/135	-
35	HTG	b	622	-	-	4/10/30/30	0/1/1/1
25	BCR	c	916	-	-	0/29/63/63	0/2/2/2
24	PHO	a	408	-	-	5/53/103/103	0/5/6/6
30	LMT	m	104	-	-	2/21/61/61	0/2/2/2
23	CLA	C	512	3	2/2/20/25	0/37/135/135	-
23	CLA	b	611	41	3/3/20/25	7/37/135/135	-
35	HTG	D	414	-	-	3/10/30/30	0/1/1/1
28	LHG	K	101	-	-	24/45/45/53	-
26	SQD	a	417	-	-	14/49/69/69	0/1/1/1
23	CLA	B	617	-	3/3/20/25	11/37/135/135	-
34	LMG	C	520	-	-	20/46/66/70	0/1/1/1
23	CLA	B	605	-	3/3/20/25	8/37/135/135	-
25	BCR	b	620	-	-	0/29/63/63	0/2/2/2
25	BCR	j	104	-	-	2/29/63/63	0/2/2/2
40	HEC	V	203	16	-	0/6/54/54	-
35	HTG	B	625	-	-	5/10/30/30	0/1/1/1
25	BCR	a	411	-	-	1/29/63/63	0/2/2/2
23	CLA	c	910	-	3/3/20/25	9/37/135/135	-
23	CLA	d	403	-	2/2/20/25	1/37/135/135	-
23	CLA	d	401	41	1/1/20/25	7/37/135/135	-
30	LMT	F	101	-	-	11/21/61/61	0/2/2/2
36	DGD	H	103	-	-	10/51/91/95	0/2/2/2
27	PL9	A	411	-	-	14/53/73/73	0/1/1/1
34	LMG	C	531	-	-	18/46/66/70	0/1/1/1
28	LHG	D	409	-	-	9/53/53/53	-
38	RRX	H	102	-	-	0/29/65/65	0/2/2/2
28	LHG	e	101	-	-	18/44/44/53	-
23	CLA	C	503	-	1/1/20/25	6/37/135/135	-
23	CLA	C	510	-	3/3/20/25	9/37/135/135	-
23	CLA	a	406	-	3/3/20/25	6/37/135/135	-
23	CLA	B	616	-	3/3/20/25	5/37/135/135	-
35	HTG	B	626	-	-	7/10/30/30	0/1/1/1
23	CLA	D	404	-	3/3/20/25	11/37/135/135	-
23	CLA	A	408	-	2/2/20/25	18/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	611	41	3/3/20/25	5/37/135/135	-
23	CLA	d	404	-	1/1/20/25	13/37/135/135	-
23	CLA	b	604	-	3/3/20/25	5/37/135/135	-
30	LMT	A	416	-	-	7/21/61/61	0/2/2/2
23	CLA	b	613	-	3/3/20/25	3/37/135/135	-
23	CLA	A	406	41	2/2/20/25	11/37/135/135	-
25	BCR	b	618	-	-	2/29/63/63	0/2/2/2
23	CLA	b	616	-	3/3/20/25	8/37/135/135	-
23	CLA	b	603	-	3/3/20/25	2/37/135/135	-
23	CLA	C	513	-	3/3/20/25	14/37/135/135	-
23	CLA	B	612	-	3/3/20/25	5/37/135/135	-
30	LMT	Z	101	-	-	11/21/61/61	0/2/2/2
23	CLA	C	511	-	3/3/20/25	2/37/135/135	-
38	RRX	x	102	-	-	0/29/65/65	0/2/2/2
23	CLA	c	904	-	1/1/20/25	4/37/135/135	-
23	CLA	C	514	-	1/1/20/25	9/37/135/135	-
23	CLA	c	913	-	3/3/20/25	7/37/135/135	-
23	CLA	B	609	-	1/1/20/25	1/37/135/135	-
23	CLA	D	403	-	1/1/20/25	7/37/135/135	-
23	CLA	B	615	-	3/3/20/25	9/37/135/135	-
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
25	BCR	Y	101	-	-	2/29/63/63	0/2/2/2
23	CLA	B	614	-	3/3/20/25	5/37/135/135	-
35	HTG	c	922	-	-	4/10/30/30	0/1/1/1
25	BCR	k	102	-	-	2/29/63/63	0/2/2/2
23	CLA	b	617	-	3/3/20/25	19/37/135/135	-
30	LMT	M	101	-	-	0/21/61/61	0/2/2/2
23	CLA	C	505	41	3/3/20/25	9/37/135/135	-
26	SQD	D	408	-	-	19/40/60/69	0/1/1/1
26	SQD	x	101	-	-	19/36/56/69	0/1/1/1
23	CLA	C	507	-	3/3/20/25	16/37/135/135	-
23	CLA	B	602	41	2/2/20/25	19/37/135/135	-
30	LMT	T	103	-	-	7/15/35/61	0/1/1/2
23	CLA	b	615	-	3/3/20/25	13/37/135/135	-
35	HTG	c	923	-	-	4/8/10/30	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LHG	A	412	-	-	29/53/53/53	-
40	HEC	v	203	16	-	0/6/54/54	-
25	BCR	C	530	-	-	0/29/63/63	0/2/2/2
34	LMG	c	920	-	-	21/46/66/70	0/1/1/1
28	LHG	d	408	-	-	14/53/53/53	-
35	HTG	b	627	-	-	3/10/30/30	0/1/1/1
30	LMT	b	621	-	-	12/17/37/61	0/1/1/2
36	DGD	C	517	-	-	13/51/91/95	0/2/2/2
36	DGD	C	518	-	-	14/51/91/95	0/2/2/2
27	PL9	d	406	-	-	4/53/73/73	0/1/1/1
35	HTG	C	523	-	-	4/10/30/30	0/1/1/1
28	LHG	D	410	-	-	10/53/53/53	-
28	LHG	E	101	-	-	28/53/53/53	-
30	LMT	z	101	-	-	8/15/55/61	0/2/2/2
30	LMT	B	643	-	-	6/15/35/61	0/1/1/2
34	LMG	C	501	-	-	24/46/66/70	0/1/1/1
34	LMG	J	101	39	-	15/46/66/70	0/1/1/1
27	PL9	a	414	-	-	11/53/73/73	0/1/1/1
23	CLA	b	608	41	3/3/20/25	2/37/135/135	-
23	CLA	c	909	-	2/2/20/25	4/37/135/135	-
30	LMT	a	418	-	-	12/21/61/61	0/2/2/2
23	CLA	D	401	41	1/1/20/25	4/37/135/135	-
34	LMG	j	101	39	-	11/46/66/70	0/1/1/1
23	CLA	c	906	-	2/2/20/25	4/37/135/135	-
34	LMG	c	930	-	-	7/46/66/70	0/1/1/1
23	CLA	c	911	-	3/3/20/25	3/37/135/135	-
34	LMG	a	413	-	-	24/46/66/70	0/1/1/1
24	PHO	D	402	-	-	3/53/103/103	0/5/6/6
23	CLA	a	410	-	1/1/20/25	8/37/135/135	-
23	CLA	c	905	41	2/2/20/25	9/37/135/135	-
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
24	PHO	A	407	-	-	3/53/103/103	0/5/6/6
23	CLA	b	612	-	1/1/20/25	6/37/135/135	-
34	LMG	m	102	-	-	18/46/66/70	0/1/1/1
30	LMT	a	422	-	-	5/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	502	-	3/3/20/25	3/37/135/135	-
30	LMT	I	101	-	-	8/21/61/61	0/2/2/2

All (1325) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	914	CLA	MG-NA	12.47	2.35	2.06
23	c	904	CLA	MG-NA	12.19	2.35	2.06
23	b	607	CLA	MG-NA	11.84	2.34	2.06
23	b	610	CLA	MG-NA	11.72	2.34	2.06
23	B	602	CLA	MG-NA	11.01	2.32	2.06
23	c	913	CLA	MG-NA	10.78	2.31	2.06
23	C	512	CLA	MG-NA	10.61	2.31	2.06
23	C	513	CLA	MG-NA	10.55	2.31	2.06
23	C	514	CLA	MG-NA	10.20	2.30	2.06
23	c	910	CLA	MG-NA	10.17	2.30	2.06
23	C	510	CLA	MG-NA	9.93	2.29	2.06
23	c	908	CLA	MG-NA	9.90	2.29	2.06
23	b	604	CLA	MG-NA	9.77	2.29	2.06
23	C	503	CLA	MG-NA	9.77	2.29	2.06
23	B	613	CLA	MG-NA	9.62	2.29	2.06
23	c	912	CLA	MG-NC	9.61	2.29	2.06
23	c	905	CLA	MG-NA	9.50	2.28	2.06
23	B	607	CLA	MG-NA	9.46	2.28	2.06
23	c	902	CLA	MG-NA	9.36	2.28	2.06
23	B	611	CLA	MG-NA	9.06	2.27	2.06
23	C	509	CLA	MG-NA	8.91	2.27	2.06
23	b	612	CLA	MG-NA	8.74	2.27	2.06
23	B	612	CLA	MG-NA	8.48	2.26	2.06
23	C	508	CLA	MG-NC	8.44	2.26	2.06
23	B	608	CLA	MG-NA	8.43	2.26	2.06
23	B	605	CLA	MG-NA	8.39	2.26	2.06
23	b	615	CLA	MG-NA	8.33	2.26	2.06
23	d	401	CLA	MG-NA	8.24	2.25	2.06
23	C	511	CLA	MG-NA	8.11	2.25	2.06
23	D	403	CLA	MG-NA	8.11	2.25	2.06
23	B	616	CLA	MG-NA	7.92	2.25	2.06
23	C	504	CLA	MG-NC	7.90	2.25	2.06
23	c	906	CLA	MG-NA	7.85	2.24	2.06
23	B	603	CLA	MG-NA	7.81	2.24	2.06
23	b	616	CLA	MG-NA	7.67	2.24	2.06
23	B	606	CLA	MG-NA	7.67	2.24	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	502	CLA	MG-NC	7.66	2.24	2.06
23	c	903	CLA	MG-NA	7.36	2.23	2.06
23	c	909	CLA	MG-NA	7.31	2.23	2.06
23	B	610	CLA	MG-NA	7.29	2.23	2.06
23	b	605	CLA	MG-NA	7.27	2.23	2.06
23	c	910	CLA	OBD-CAD	7.02	1.32	1.22
23	C	505	CLA	MG-NA	6.75	2.22	2.06
23	b	613	CLA	MG-NA	6.70	2.22	2.06
23	C	507	CLA	MG-NA	6.68	2.22	2.06
23	b	602	CLA	MG-NC	6.60	2.21	2.06
23	C	506	CLA	MG-NA	6.55	2.21	2.06
23	D	404	CLA	MG-NC	6.47	2.21	2.06
23	c	904	CLA	MG-NC	6.47	2.21	2.06
23	A	406	CLA	MG-NA	6.43	2.21	2.06
23	C	508	CLA	MG-NA	6.37	2.21	2.06
23	C	513	CLA	C3C-C2C	6.33	1.50	1.36
23	B	615	CLA	MG-NA	6.18	2.20	2.06
23	c	907	CLA	MG-NA	6.16	2.20	2.06
23	C	513	CLA	C3B-C2B	6.16	1.48	1.40
23	b	607	CLA	C3B-C2B	6.16	1.48	1.40
23	b	609	CLA	MG-NA	6.15	2.20	2.06
23	b	617	CLA	MG-NA	6.10	2.20	2.06
23	b	608	CLA	MG-NA	6.08	2.20	2.06
23	b	616	CLA	C3B-C2B	6.05	1.48	1.40
23	b	617	CLA	MG-NC	6.04	2.20	2.06
23	b	604	CLA	CHC-C1C	6.03	1.50	1.35
23	B	614	CLA	MG-NA	6.02	2.20	2.06
23	a	410	CLA	CHC-C1C	6.01	1.50	1.35
23	C	508	CLA	C3B-C2B	6.00	1.48	1.40
23	a	407	CLA	MG-NA	6.00	2.20	2.06
24	A	407	PHO	CHB-C1B	6.00	1.50	1.38
23	C	509	CLA	C3B-C2B	6.00	1.48	1.40
23	b	609	CLA	CHC-C1C	5.99	1.50	1.35
23	c	904	CLA	CHC-C1C	5.99	1.50	1.35
23	C	504	CLA	CHC-C1C	5.91	1.50	1.35
23	C	504	CLA	C3B-C2B	5.86	1.48	1.40
23	b	610	CLA	CHC-C1C	5.84	1.50	1.35
23	B	607	CLA	C3C-C2C	5.82	1.49	1.36
23	c	904	CLA	C3C-C2C	5.79	1.49	1.36
23	C	513	CLA	O2D-CGD	5.78	1.47	1.33
23	C	514	CLA	C3B-C2B	5.75	1.48	1.40
23	B	609	CLA	MG-NC	5.75	2.19	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	514	CLA	C3D-C2D	5.74	1.49	1.39
23	C	510	CLA	C3D-C2D	5.73	1.49	1.39
23	d	403	CLA	MG-NA	5.72	2.19	2.06
23	c	909	CLA	MG-NC	5.71	2.19	2.06
23	a	406	CLA	MG-NA	5.71	2.19	2.06
23	c	912	CLA	C3B-C2B	5.71	1.48	1.40
37	e	105	HEM	C3D-C2D	5.68	1.54	1.37
23	C	514	CLA	C3C-C2C	5.65	1.48	1.36
23	C	511	CLA	C3D-C2D	5.65	1.49	1.39
23	B	615	CLA	CHC-C1C	5.64	1.49	1.35
23	d	403	CLA	CHC-C1C	5.64	1.49	1.35
23	B	603	CLA	CHC-C1C	5.64	1.49	1.35
23	B	617	CLA	CHC-C1C	5.62	1.49	1.35
23	c	903	CLA	CHC-C1C	5.61	1.49	1.35
23	b	614	CLA	MG-NA	5.60	2.19	2.06
24	D	402	PHO	C3B-C2B	5.59	1.48	1.37
23	c	913	CLA	C3B-C2B	5.58	1.48	1.40
23	C	503	CLA	C3B-C2B	5.58	1.48	1.40
23	B	607	CLA	CHC-C1C	5.58	1.49	1.35
23	b	617	CLA	CHC-C1C	5.57	1.49	1.35
23	B	616	CLA	O2D-CGD	5.57	1.46	1.33
23	c	913	CLA	C3C-C2C	5.57	1.48	1.36
23	C	510	CLA	C3C-C2C	5.56	1.48	1.36
23	b	602	CLA	MG-NA	5.54	2.19	2.06
23	b	608	CLA	C3D-C2D	5.53	1.49	1.39
23	b	608	CLA	MG-NC	5.52	2.19	2.06
23	d	404	CLA	MG-NA	5.51	2.19	2.06
23	B	603	CLA	C3B-C2B	5.51	1.48	1.40
23	C	510	CLA	OBD-CAD	5.50	1.30	1.22
23	b	602	CLA	O2A-CGA	5.49	1.49	1.33
23	b	614	CLA	CHC-C1C	5.48	1.49	1.35
23	b	605	CLA	C3C-C2C	5.48	1.48	1.36
23	b	602	CLA	C3B-C2B	5.48	1.48	1.40
23	C	502	CLA	CHC-C1C	5.47	1.49	1.35
23	a	407	CLA	CHC-C1C	5.47	1.49	1.35
23	c	912	CLA	MG-NA	5.46	2.19	2.06
23	B	614	CLA	CHC-C1C	5.46	1.49	1.35
23	B	612	CLA	CHC-C1C	5.45	1.48	1.35
23	c	914	CLA	C3B-C2B	5.45	1.47	1.40
23	b	611	CLA	CHC-C1C	5.44	1.48	1.35
23	C	504	CLA	C3C-C2C	5.43	1.48	1.36
23	b	606	CLA	CHC-C1C	5.41	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	912	CLA	O2D-CGD	5.41	1.46	1.33
23	B	606	CLA	CHC-C1C	5.41	1.48	1.35
23	b	605	CLA	CHC-C1C	5.40	1.48	1.35
23	c	907	CLA	CHC-C1C	5.40	1.48	1.35
23	b	617	CLA	C3C-C2C	5.38	1.48	1.36
23	c	912	CLA	CHC-C1C	5.38	1.48	1.35
40	V	203	HEC	C3C-C2C	-5.37	1.35	1.40
23	c	902	CLA	C3B-C2B	5.37	1.47	1.40
23	B	610	CLA	CHC-C1C	5.36	1.48	1.35
23	c	909	CLA	C3B-C2B	5.35	1.47	1.40
23	c	909	CLA	CHC-C1C	5.35	1.48	1.35
23	C	507	CLA	CHC-C1C	5.34	1.48	1.35
23	C	511	CLA	OBD-CAD	5.34	1.29	1.22
23	b	603	CLA	C3C-C2C	5.34	1.48	1.36
23	b	609	CLA	C3C-C2C	5.33	1.48	1.36
23	C	507	CLA	C3B-C2B	5.33	1.47	1.40
23	c	914	CLA	CHC-C1C	5.32	1.48	1.35
23	C	511	CLA	CHC-C1C	5.31	1.48	1.35
23	b	610	CLA	C3C-C2C	5.31	1.48	1.36
23	a	406	CLA	C3C-C2C	5.31	1.48	1.36
31	B	636	DMS	O-S	5.31	1.86	1.50
23	b	611	CLA	O2D-CGD	5.30	1.46	1.33
23	b	606	CLA	MG-NA	5.30	2.18	2.06
23	C	508	CLA	C3C-C2C	5.27	1.47	1.36
23	B	611	CLA	C3C-C2C	5.27	1.47	1.36
23	C	513	CLA	CHC-C1C	5.27	1.48	1.35
23	C	506	CLA	C3C-C2C	5.27	1.47	1.36
23	c	908	CLA	C3C-C2C	5.26	1.47	1.36
23	B	604	CLA	O2D-CGD	5.25	1.46	1.33
23	c	905	CLA	C3C-C2C	5.25	1.47	1.36
23	C	509	CLA	C3D-C2D	5.24	1.48	1.39
23	b	616	CLA	C3C-C2C	5.24	1.47	1.36
23	C	514	CLA	MG-NC	5.24	2.18	2.06
23	c	914	CLA	C3C-C2C	5.23	1.47	1.36
23	b	613	CLA	C4B-NB	-5.22	1.30	1.35
23	B	613	CLA	CHC-C1C	5.22	1.48	1.35
23	c	913	CLA	CHC-C1C	5.21	1.48	1.35
23	c	909	CLA	C3D-C2D	5.21	1.48	1.39
23	b	612	CLA	CHC-C1C	5.19	1.48	1.35
23	C	505	CLA	C3C-C2C	5.18	1.47	1.36
23	C	506	CLA	OBD-CAD	5.17	1.29	1.22
23	C	503	CLA	C3D-C2D	5.17	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	603	CLA	OBD-CAD	5.16	1.29	1.22
23	c	907	CLA	O2D-CGD	5.14	1.45	1.33
24	a	409	PHO	CHB-C1B	5.14	1.48	1.38
23	b	608	CLA	C3C-C2C	5.14	1.47	1.36
35	B	624	HTG	C1'-S1	-5.14	1.74	1.81
23	c	910	CLA	C3D-C2D	5.13	1.48	1.39
23	B	602	CLA	O2A-CGA	5.13	1.48	1.33
23	C	503	CLA	O2D-CGD	5.13	1.45	1.33
23	b	602	CLA	C3C-C2C	5.13	1.47	1.36
34	C	520	LMG	O8-C28	5.13	1.48	1.33
23	C	514	CLA	CHC-C1C	5.12	1.48	1.35
40	v	203	HEC	C3B-C2B	-5.12	1.35	1.40
23	A	405	CLA	OBD-CAD	5.12	1.29	1.22
23	b	606	CLA	C3C-C2C	5.12	1.47	1.36
23	C	509	CLA	O2D-CGD	5.12	1.45	1.33
23	C	507	CLA	C3C-C2C	5.11	1.47	1.36
23	a	410	CLA	C3C-C2C	5.11	1.47	1.36
23	b	611	CLA	MG-NA	5.09	2.18	2.06
23	b	615	CLA	CHC-C1C	5.09	1.48	1.35
23	C	506	CLA	CHC-C1C	5.09	1.48	1.35
23	a	410	CLA	C3B-C2B	5.08	1.47	1.40
23	c	909	CLA	C3C-C2C	5.08	1.47	1.36
23	b	616	CLA	OBD-CAD	5.07	1.29	1.22
23	C	514	CLA	O2D-CGD	5.07	1.45	1.33
23	B	616	CLA	CHC-C1C	5.06	1.48	1.35
23	c	914	CLA	O2D-CGD	5.06	1.45	1.33
23	B	602	CLA	CHC-C1C	5.06	1.47	1.35
23	c	908	CLA	CHC-C1C	5.06	1.47	1.35
23	a	410	CLA	MG-NA	5.06	2.18	2.06
23	B	608	CLA	CHC-C1C	5.05	1.47	1.35
23	C	505	CLA	O2D-CGD	5.05	1.45	1.33
23	C	511	CLA	O2D-CGD	5.05	1.45	1.33
36	D	407	DGD	O1G-C1A	5.04	1.48	1.33
24	a	409	PHO	CHD-C1D	5.04	1.48	1.38
23	C	513	CLA	C3D-C2D	5.02	1.48	1.39
23	B	605	CLA	CHC-C1C	5.02	1.47	1.35
23	B	610	CLA	C3C-C2C	5.02	1.47	1.36
23	b	614	CLA	O2D-CGD	5.02	1.45	1.33
23	c	913	CLA	C3D-C2D	5.01	1.48	1.39
34	D	412	LMG	O8-C28	5.01	1.48	1.33
23	C	502	CLA	C3C-C2C	5.01	1.47	1.36
31	D	417	DMS	O-S	4.99	1.83	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	615	CLA	C3C-C2C	4.98	1.47	1.36
23	d	401	CLA	CHC-C1C	4.98	1.47	1.35
23	c	904	CLA	C3B-C2B	4.98	1.47	1.40
23	C	506	CLA	C3D-C2D	4.97	1.48	1.39
23	c	911	CLA	CHC-C1C	4.97	1.47	1.35
23	b	612	CLA	C3B-C2B	4.97	1.47	1.40
28	E	101	LHG	O8-C23	4.97	1.47	1.33
23	c	910	CLA	CHC-C1C	4.96	1.47	1.35
23	D	404	CLA	C3C-C2C	4.96	1.47	1.36
23	b	612	CLA	O2D-CGD	4.96	1.45	1.33
24	a	409	PHO	CHC-C1C	4.96	1.48	1.38
23	C	512	CLA	C3D-C2D	4.95	1.48	1.39
23	B	611	CLA	CHC-C1C	4.95	1.47	1.35
23	B	617	CLA	C3C-C2C	4.95	1.47	1.36
23	B	610	CLA	C3D-C2D	4.95	1.48	1.39
31	V	211	DMS	O-S	4.95	1.83	1.50
24	D	402	PHO	CHB-C1B	4.94	1.48	1.38
23	C	504	CLA	MG-NA	4.94	2.18	2.06
23	b	613	CLA	CHC-C1C	4.94	1.47	1.35
23	C	503	CLA	CHC-C1C	4.93	1.47	1.35
23	b	603	CLA	CHC-C1C	4.93	1.47	1.35
34	C	531	LMG	O7-C10	4.93	1.48	1.34
23	B	603	CLA	C3C-C2C	4.92	1.47	1.36
23	c	912	CLA	C3C-C2C	4.91	1.47	1.36
23	C	510	CLA	CHC-C1C	4.91	1.47	1.35
23	b	608	CLA	CHC-C1C	4.90	1.47	1.35
23	C	509	CLA	CHC-C1C	4.90	1.47	1.35
23	c	905	CLA	CHC-C1C	4.90	1.47	1.35
23	b	610	CLA	C3B-C2B	4.90	1.47	1.40
23	B	607	CLA	O2D-CGD	4.89	1.45	1.33
23	C	502	CLA	C3D-C2D	4.89	1.48	1.39
23	b	613	CLA	C3C-C2C	4.88	1.47	1.36
34	d	411	LMG	O7-C10	4.88	1.48	1.34
23	c	911	CLA	OBD-CAD	4.88	1.29	1.22
31	b	638	DMS	O-S	4.88	1.83	1.50
23	D	401	CLA	CHC-C1C	4.88	1.47	1.35
31	B	642	DMS	O-S	4.88	1.83	1.50
23	C	509	CLA	C3C-C2C	4.87	1.47	1.36
23	c	902	CLA	OBD-CAD	4.87	1.29	1.22
23	B	602	CLA	O2D-CGD	4.87	1.45	1.33
23	c	912	CLA	OBD-CAD	4.86	1.29	1.22
23	c	907	CLA	C3B-C2B	4.85	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	404	CLA	OBD-CAD	4.85	1.29	1.22
23	b	602	CLA	O2D-CGD	4.85	1.45	1.33
23	C	512	CLA	O2D-CGD	4.85	1.45	1.33
23	b	602	CLA	CHC-C1C	4.85	1.47	1.35
24	a	409	PHO	C1A-NA	-4.84	1.28	1.37
26	L	102	SQD	O47-C7	4.84	1.47	1.34
23	C	511	CLA	C3B-C2B	4.83	1.47	1.40
36	D	407	DGD	O2G-C1B	4.82	1.47	1.34
23	C	505	CLA	C3B-C2B	4.81	1.47	1.40
23	a	406	CLA	CHC-C1C	4.81	1.47	1.35
34	D	412	LMG	O7-C10	4.81	1.47	1.34
23	B	612	CLA	OBD-CAD	4.80	1.29	1.22
31	O	309	DMS	O-S	4.80	1.82	1.50
23	b	604	CLA	O2D-CGD	4.80	1.44	1.33
31	U	204	DMS	O-S	4.79	1.82	1.50
23	b	616	CLA	O2D-CGD	4.79	1.44	1.33
23	A	408	CLA	C3B-C2B	4.79	1.47	1.40
23	B	604	CLA	C3C-C2C	4.79	1.46	1.36
37	E	105	HEM	C3D-C2D	4.78	1.51	1.37
23	C	505	CLA	C3D-C2D	4.78	1.48	1.39
36	d	407	DGD	O2G-C1B	4.78	1.47	1.34
23	c	905	CLA	OBD-CAD	4.78	1.29	1.22
34	d	411	LMG	O8-C28	4.78	1.47	1.33
23	b	604	CLA	C3C-C2C	4.78	1.46	1.36
24	a	408	PHO	CHC-C1C	4.78	1.47	1.38
24	a	408	PHO	CHB-C1B	4.77	1.47	1.38
23	b	602	CLA	OBD-CAD	4.76	1.29	1.22
31	c	929	DMS	O-S	4.74	1.82	1.50
23	c	912	CLA	C3D-C2D	4.74	1.47	1.39
23	c	904	CLA	C3D-C2D	4.74	1.47	1.39
23	D	404	CLA	CHC-C1C	4.74	1.47	1.35
23	B	608	CLA	C3D-C2D	4.74	1.47	1.39
31	a	423	DMS	O-S	4.74	1.82	1.50
31	V	207	DMS	O-S	4.74	1.82	1.50
23	B	602	CLA	C3C-C2C	4.73	1.46	1.36
23	c	913	CLA	O2D-CGD	4.73	1.44	1.33
23	C	506	CLA	O2D-CGD	4.73	1.44	1.33
23	b	607	CLA	CHC-C1C	4.72	1.47	1.35
23	d	403	CLA	C3B-C2B	4.72	1.46	1.40
23	c	910	CLA	C3B-C2B	4.72	1.46	1.40
31	B	641	DMS	O-S	4.72	1.82	1.50
31	c	925	DMS	O-S	4.71	1.82	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	605	CLA	O2D-CGD	4.71	1.44	1.33
23	B	611	CLA	C3D-C2D	4.71	1.47	1.39
23	C	509	CLA	OBD-CAD	4.70	1.28	1.22
23	C	505	CLA	CHC-C1C	4.70	1.47	1.35
23	B	613	CLA	O2D-CGD	4.69	1.44	1.33
23	C	508	CLA	CHC-C1C	4.69	1.47	1.35
24	A	407	PHO	C3B-C2B	4.69	1.46	1.37
23	B	606	CLA	C3C-C2C	4.69	1.46	1.36
23	b	617	CLA	C3D-C2D	4.68	1.47	1.39
31	O	304	DMS	O-S	4.68	1.81	1.50
23	c	903	CLA	C3D-C2D	4.68	1.47	1.39
34	c	930	LMG	O7-C10	4.67	1.47	1.34
28	d	402	LHG	O8-C23	4.67	1.47	1.33
31	B	645	DMS	O-S	4.67	1.81	1.50
23	C	503	CLA	C3C-C2C	4.67	1.46	1.36
23	c	905	CLA	C3D-C2D	4.67	1.47	1.39
31	u	206	DMS	O-S	4.67	1.81	1.50
28	e	101	LHG	O8-C23	4.67	1.47	1.33
23	A	408	CLA	CHC-C1C	4.67	1.46	1.35
23	d	404	CLA	C3B-C2B	4.67	1.46	1.40
31	B	639	DMS	O-S	4.66	1.81	1.50
23	B	612	CLA	C3C-C2C	4.66	1.46	1.36
31	A	424	DMS	O-S	4.66	1.81	1.50
23	b	612	CLA	C3D-C2D	4.66	1.47	1.39
23	D	401	CLA	C3B-C2B	4.65	1.46	1.40
26	D	408	SQD	O47-C7	4.65	1.47	1.34
23	c	911	CLA	C3C-C2C	4.65	1.46	1.36
34	a	413	LMG	O8-C28	4.65	1.46	1.33
23	b	613	CLA	C3D-C2D	4.65	1.47	1.39
23	b	603	CLA	OBD-CAD	4.65	1.28	1.22
23	c	905	CLA	O2D-CGD	4.64	1.44	1.33
23	B	617	CLA	C3D-C2D	4.64	1.47	1.39
31	b	636	DMS	O-S	4.64	1.81	1.50
31	B	638	DMS	O-S	4.64	1.81	1.50
23	c	906	CLA	CHC-C1C	4.64	1.46	1.35
26	x	101	SQD	O47-C7	4.64	1.47	1.34
28	e	101	LHG	O7-C7	4.64	1.47	1.34
23	C	507	CLA	O2D-CGD	4.64	1.44	1.33
31	b	647	DMS	O-S	4.63	1.81	1.50
31	C	526	DMS	O-S	4.63	1.81	1.50
40	v	203	HEC	C3D-C2D	4.62	1.51	1.37
31	H	101	DMS	O-S	4.62	1.81	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	v	203	HEC	C3C-C2C	-4.62	1.35	1.40
31	H	105	DMS	O-S	4.62	1.81	1.50
23	b	605	CLA	C3D-C2D	4.62	1.47	1.39
23	a	407	CLA	C3D-C2D	4.62	1.47	1.39
23	B	607	CLA	C3D-C2D	4.62	1.47	1.39
31	u	204	DMS	O-S	4.61	1.81	1.50
23	A	405	CLA	CHC-C1C	4.61	1.46	1.35
31	o	304	DMS	O-S	4.61	1.81	1.50
23	B	616	CLA	C3C-C2C	4.61	1.46	1.36
31	b	644	DMS	O-S	4.61	1.81	1.50
23	b	607	CLA	O2D-CGD	4.60	1.44	1.33
31	O	308	DMS	O-S	4.60	1.81	1.50
23	C	512	CLA	C3C-C2C	4.60	1.46	1.36
23	B	615	CLA	OBD-CAD	4.59	1.28	1.22
31	O	307	DMS	O-S	4.59	1.81	1.50
31	d	418	DMS	O-S	4.59	1.81	1.50
24	a	408	PHO	C3C-C2C	4.59	1.46	1.36
23	B	608	CLA	C3B-C2B	4.59	1.46	1.40
31	b	639	DMS	O-S	4.59	1.81	1.50
31	D	415	DMS	O-S	4.59	1.81	1.50
23	D	404	CLA	C3B-C2B	4.59	1.46	1.40
31	d	416	DMS	O-S	4.58	1.81	1.50
31	h	105	DMS	O-S	4.58	1.81	1.50
23	d	404	CLA	C3C-C2C	4.58	1.46	1.36
23	C	512	CLA	C3B-C2B	4.58	1.46	1.40
28	a	415	LHG	O8-C23	4.58	1.46	1.33
23	B	602	CLA	OBD-CAD	4.58	1.28	1.22
23	d	403	CLA	C3C-C2C	4.58	1.46	1.36
31	i	106	DMS	O-S	4.58	1.81	1.50
31	b	646	DMS	O-S	4.57	1.81	1.50
23	b	614	CLA	C3C-C2C	4.57	1.46	1.36
31	A	418	DMS	O-S	4.57	1.81	1.50
28	A	412	LHG	O7-C7	4.57	1.47	1.34
23	B	613	CLA	C3C-C2C	4.57	1.46	1.36
31	A	419	DMS	O-S	4.57	1.81	1.50
31	V	210	DMS	O-S	4.56	1.81	1.50
31	v	209	DMS	O-S	4.56	1.81	1.50
23	b	612	CLA	C3C-C2C	4.56	1.46	1.36
23	B	602	CLA	C3B-C2B	4.56	1.46	1.40
23	c	905	CLA	MG-NC	4.56	2.17	2.06
34	B	622	LMG	O8-C28	4.56	1.46	1.33
23	C	510	CLA	O2D-CGD	4.56	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	412	LHG	O8-C23	4.55	1.46	1.33
31	v	208	DMS	O-S	4.55	1.81	1.50
23	c	907	CLA	C3C-C2C	4.55	1.46	1.36
23	B	616	CLA	MG-NC	4.55	2.17	2.06
23	b	617	CLA	O2D-CGD	4.55	1.44	1.33
31	b	635	DMS	O-S	4.55	1.81	1.50
23	C	506	CLA	C3B-C2B	4.55	1.46	1.40
23	B	617	CLA	O2D-CGD	4.55	1.44	1.33
23	b	615	CLA	C3D-C2D	4.54	1.47	1.39
31	B	647	DMS	O-S	4.54	1.80	1.50
31	A	421	DMS	O-S	4.54	1.80	1.50
31	v	207	DMS	O-S	4.54	1.80	1.50
23	c	910	CLA	O2D-CGD	4.54	1.44	1.33
23	C	504	CLA	C3D-C2D	4.53	1.47	1.39
31	h	104	DMS	O-S	4.53	1.80	1.50
31	a	401	DMS	O-S	4.52	1.80	1.50
31	i	105	DMS	O-S	4.52	1.80	1.50
23	B	614	CLA	C3C-C2C	4.52	1.46	1.36
31	U	203	DMS	O-S	4.52	1.80	1.50
23	B	609	CLA	CHC-C1C	4.52	1.46	1.35
31	d	414	DMS	O-S	4.52	1.80	1.50
31	B	649	DMS	O-S	4.52	1.80	1.50
31	c	936	DMS	O-S	4.52	1.80	1.50
31	O	303	DMS	O-S	4.52	1.80	1.50
31	b	645	DMS	O-S	4.52	1.80	1.50
31	O	306	DMS	O-S	4.52	1.80	1.50
31	o	303	DMS	O-S	4.52	1.80	1.50
31	b	640	DMS	O-S	4.51	1.80	1.50
23	c	906	CLA	C3C-C2C	4.51	1.46	1.36
31	a	420	DMS	O-S	4.51	1.80	1.50
31	b	642	DMS	O-S	4.51	1.80	1.50
23	c	902	CLA	CHC-C1C	4.51	1.46	1.35
26	D	408	SQD	O48-C23	4.50	1.46	1.33
23	D	404	CLA	C3D-C2D	4.50	1.47	1.39
23	c	906	CLA	C3D-C2D	4.50	1.47	1.39
31	c	934	DMS	O-S	4.50	1.80	1.50
26	B	621	SQD	O47-C7	4.50	1.47	1.34
34	m	102	LMG	O8-C28	4.49	1.46	1.33
31	A	422	DMS	O-S	4.49	1.80	1.50
24	a	409	PHO	O2D-CGD	4.49	1.44	1.33
23	A	406	CLA	CHC-C1C	4.49	1.46	1.35
31	O	305	DMS	O-S	4.49	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	E	101	LHG	O7-C7	4.48	1.47	1.34
23	c	914	CLA	C3D-C2D	4.48	1.47	1.39
31	v	210	DMS	O-S	4.48	1.80	1.50
24	a	409	PHO	C3B-C2B	4.48	1.46	1.37
24	D	402	PHO	CHD-C1D	4.48	1.47	1.38
28	K	101	LHG	O7-C7	4.48	1.46	1.34
31	b	643	DMS	O-S	4.48	1.80	1.50
31	a	421	DMS	O-S	4.48	1.80	1.50
31	e	104	DMS	O-S	4.48	1.80	1.50
23	b	611	CLA	C3C-C2C	4.47	1.46	1.36
28	D	409	LHG	O8-C23	4.47	1.46	1.33
23	C	513	CLA	O2A-CGA	4.47	1.46	1.33
23	b	607	CLA	C3D-C2D	4.47	1.47	1.39
23	b	614	CLA	OBD-CAD	4.46	1.28	1.22
23	C	507	CLA	C3D-C2D	4.46	1.47	1.39
31	c	933	DMS	O-S	4.46	1.80	1.50
31	d	419	DMS	O-S	4.46	1.80	1.50
23	A	405	CLA	C4C-C3C	4.46	1.52	1.45
23	b	608	CLA	O2D-CGD	4.45	1.44	1.33
31	c	935	DMS	O-S	4.45	1.80	1.50
31	C	533	DMS	O-S	4.45	1.80	1.50
31	l	102	DMS	O-S	4.45	1.80	1.50
31	F	102	DMS	O-S	4.45	1.80	1.50
23	c	905	CLA	C3B-C2B	4.45	1.46	1.40
31	h	103	DMS	O-S	4.44	1.80	1.50
31	b	641	DMS	O-S	4.44	1.80	1.50
26	x	101	SQD	O48-C23	4.44	1.46	1.33
31	h	101	DMS	O-S	4.44	1.80	1.50
31	c	937	DMS	O-S	4.44	1.80	1.50
31	k	103	DMS	O-S	4.44	1.80	1.50
24	D	402	PHO	C3C-C2C	4.44	1.46	1.36
23	b	616	CLA	CHC-C1C	4.44	1.46	1.35
23	C	508	CLA	C3D-C2D	4.43	1.47	1.39
31	O	311	DMS	O-S	4.43	1.80	1.50
31	c	926	DMS	O-S	4.43	1.80	1.50
31	d	415	DMS	O-S	4.43	1.80	1.50
31	V	206	DMS	O-S	4.43	1.80	1.50
23	b	610	CLA	C3D-C2D	4.42	1.47	1.39
31	c	932	DMS	O-S	4.42	1.80	1.50
23	B	609	CLA	O2D-CGD	4.42	1.44	1.33
23	B	604	CLA	CHC-C1C	4.42	1.46	1.35
31	c	928	DMS	O-S	4.42	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	v	205	DMS	O-S	4.42	1.80	1.50
23	D	401	CLA	CHD-C4C	4.42	1.53	1.41
23	B	603	CLA	C3D-C2D	4.41	1.47	1.39
31	c	927	DMS	O-S	4.41	1.80	1.50
31	b	637	DMS	O-S	4.41	1.80	1.50
34	C	501	LMG	O7-C10	4.40	1.46	1.34
31	C	528	DMS	O-S	4.40	1.80	1.50
23	d	404	CLA	CHC-C1C	4.40	1.46	1.35
36	d	407	DGD	O1G-C1A	4.40	1.46	1.33
23	C	508	CLA	O2D-CGD	4.39	1.43	1.33
26	a	417	SQD	O48-C23	4.39	1.46	1.33
34	c	930	LMG	O8-C28	4.39	1.46	1.33
23	C	508	CLA	OBD-CAD	4.39	1.28	1.22
23	B	610	CLA	OBD-CAD	4.39	1.28	1.22
26	a	417	SQD	O47-C7	4.38	1.46	1.34
23	c	911	CLA	O2D-CGD	4.38	1.43	1.33
23	B	609	CLA	C3B-C2B	4.38	1.46	1.40
23	d	401	CLA	C4B-NB	4.38	1.39	1.35
23	b	614	CLA	C3D-C2D	4.37	1.47	1.39
23	B	608	CLA	C3C-C2C	4.37	1.46	1.36
28	a	415	LHG	O7-C7	4.37	1.46	1.34
31	V	205	DMS	O-S	4.36	1.79	1.50
23	C	504	CLA	O2D-CGD	4.36	1.43	1.33
23	b	603	CLA	MG-NA	4.36	2.16	2.06
31	v	206	DMS	O-S	4.36	1.79	1.50
23	b	617	CLA	C3B-C2B	4.36	1.46	1.40
31	B	646	DMS	O-S	4.36	1.79	1.50
23	C	511	CLA	C3C-C2C	4.36	1.46	1.36
31	v	202	DMS	O-S	4.36	1.79	1.50
28	K	101	LHG	O8-C23	4.35	1.46	1.33
23	b	602	CLA	C3D-C2D	4.35	1.47	1.39
34	a	413	LMG	O7-C10	4.35	1.46	1.34
23	c	909	CLA	OBD-CAD	4.35	1.28	1.22
31	V	208	DMS	O-S	4.33	1.79	1.50
23	B	613	CLA	OBD-CAD	4.33	1.28	1.22
23	a	410	CLA	O2D-CGD	4.33	1.43	1.33
31	B	640	DMS	O-S	4.33	1.79	1.50
26	A	415	SQD	O48-C23	4.32	1.46	1.33
34	C	520	LMG	O7-C10	4.32	1.46	1.34
31	O	310	DMS	O-S	4.32	1.79	1.50
31	V	201	DMS	O-S	4.32	1.79	1.50
23	c	908	CLA	C3B-C2B	4.32	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	505	CLA	MG-NC	4.31	2.16	2.06
31	V	202	DMS	O-S	4.31	1.79	1.50
23	B	607	CLA	OBD-CAD	4.31	1.28	1.22
23	C	504	CLA	O2A-CGA	4.31	1.45	1.33
23	D	403	CLA	C3C-C2C	4.30	1.45	1.36
23	b	609	CLA	OBD-CAD	4.30	1.28	1.22
31	U	202	DMS	O-S	4.30	1.79	1.50
31	u	205	DMS	O-S	4.29	1.79	1.50
23	b	611	CLA	MG-NC	4.28	2.16	2.06
31	C	527	DMS	O-S	4.28	1.79	1.50
23	B	615	CLA	C1C-NC	-4.28	1.31	1.37
24	D	402	PHO	O2D-CGD	4.27	1.43	1.33
23	C	512	CLA	CHC-C1C	4.27	1.45	1.35
31	C	529	DMS	O-S	4.26	1.79	1.50
23	d	404	CLA	C3D-C2D	4.26	1.47	1.39
23	B	607	CLA	C3B-C2B	4.26	1.46	1.40
23	C	510	CLA	O2A-CGA	4.25	1.45	1.33
23	c	914	CLA	OBD-CAD	4.25	1.28	1.22
23	c	913	CLA	OBD-CAD	4.25	1.28	1.22
23	b	616	CLA	C3D-C2D	4.25	1.47	1.39
23	c	902	CLA	C3D-C2D	4.25	1.47	1.39
23	B	611	CLA	MG-NC	4.25	2.16	2.06
36	C	519	DGD	O1G-C1A	4.24	1.45	1.33
23	c	904	CLA	O2D-CGD	4.24	1.43	1.33
24	A	407	PHO	C3C-C2C	4.23	1.45	1.36
23	c	914	CLA	O2A-CGA	4.23	1.45	1.33
31	V	209	DMS	O-S	4.23	1.78	1.50
23	d	401	CLA	C3C-C2C	4.23	1.45	1.36
28	d	402	LHG	O7-C7	4.23	1.46	1.34
23	c	907	CLA	O2A-CGA	4.22	1.45	1.33
31	D	416	DMS	O-S	4.22	1.78	1.50
31	C	525	DMS	O-S	4.22	1.78	1.50
23	B	604	CLA	MG-NA	4.21	2.16	2.06
23	B	605	CLA	C3C-C2C	4.21	1.45	1.36
23	b	606	CLA	C1B-NB	-4.21	1.31	1.35
34	C	531	LMG	O8-C28	4.20	1.45	1.33
23	C	507	CLA	O2A-CGA	4.20	1.45	1.33
23	c	903	CLA	O2D-CGD	4.20	1.43	1.33
24	D	402	PHO	C1A-NA	-4.20	1.29	1.37
23	b	607	CLA	C3C-C2C	4.19	1.45	1.36
23	A	408	CLA	C3C-C2C	4.19	1.45	1.36
23	B	617	CLA	C3B-C2B	4.19	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	u	203	DMS	O-S	4.19	1.78	1.50
23	a	410	CLA	OBD-CAD	4.18	1.28	1.22
23	a	406	CLA	C3B-C2B	4.16	1.46	1.40
35	O	302	HTG	C1'-S1	-4.14	1.76	1.81
23	c	902	CLA	O2D-CGD	4.14	1.43	1.33
23	b	614	CLA	O2A-CGA	4.13	1.45	1.33
23	c	903	CLA	C3B-C2B	4.12	1.46	1.40
23	B	615	CLA	C3D-C2D	4.12	1.46	1.39
34	c	920	LMG	O7-C10	4.12	1.45	1.34
31	b	634	DMS	O-S	4.12	1.78	1.50
23	D	401	CLA	MG-NA	4.12	2.16	2.06
26	L	102	SQD	O48-C23	4.11	1.45	1.33
34	c	920	LMG	O8-C28	4.11	1.45	1.33
23	b	615	CLA	C4C-C3C	4.11	1.52	1.45
34	j	101	LMG	O8-C28	4.10	1.45	1.33
23	B	611	CLA	OBD-CAD	4.09	1.28	1.22
35	b	627	HTG	C1'-S1	-4.09	1.76	1.81
23	A	405	CLA	O2D-CGD	4.08	1.43	1.33
34	m	102	LMG	O7-C10	4.08	1.45	1.34
23	a	410	CLA	C3D-C2D	4.08	1.46	1.39
23	b	609	CLA	C4B-NB	-4.08	1.31	1.35
23	b	614	CLA	C3B-C2B	4.08	1.46	1.40
23	B	616	CLA	C3D-C2D	4.07	1.46	1.39
24	A	407	PHO	CHD-C1D	4.06	1.46	1.38
31	v	201	DMS	O-S	4.05	1.77	1.50
23	C	513	CLA	OBD-CAD	4.05	1.28	1.22
23	B	611	CLA	O2D-CGD	4.04	1.43	1.33
24	a	409	PHO	C3C-C2C	4.04	1.45	1.36
23	C	504	CLA	OBD-CAD	4.03	1.27	1.22
34	J	101	LMG	O7-C10	4.03	1.45	1.34
37	E	105	HEM	C3C-CAC	4.02	1.56	1.47
31	B	648	DMS	O-S	4.01	1.77	1.50
23	A	408	CLA	MG-NA	4.01	2.15	2.06
26	A	410	SQD	O47-C7	4.01	1.45	1.34
23	d	403	CLA	OBD-CAD	4.00	1.27	1.22
23	c	910	CLA	C3C-C2C	4.00	1.45	1.36
23	C	512	CLA	MG-NC	4.00	2.15	2.06
23	c	907	CLA	OBD-CAD	4.00	1.27	1.22
23	b	608	CLA	C3B-C2B	3.99	1.45	1.40
36	H	103	DGD	O5D-C1E	3.99	1.47	1.40
24	D	402	PHO	CHC-C1C	3.98	1.46	1.38
23	c	906	CLA	O2A-CGA	3.98	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	404	CLA	C4C-C3C	3.98	1.51	1.45
23	B	609	CLA	C3C-C2C	3.97	1.45	1.36
23	B	616	CLA	C3B-C2B	3.96	1.45	1.40
23	c	909	CLA	O2D-CGD	3.96	1.42	1.33
23	c	911	CLA	C3B-C2B	3.96	1.45	1.40
23	C	502	CLA	C3B-C2B	3.96	1.45	1.40
31	c	924	DMS	O-S	3.95	1.76	1.50
36	H	103	DGD	O2G-C1B	3.95	1.45	1.34
23	b	610	CLA	O2D-CGD	3.94	1.42	1.33
26	A	415	SQD	O47-C7	3.94	1.45	1.34
31	C	524	DMS	O-S	3.93	1.76	1.50
24	A	407	PHO	CHC-C1C	3.93	1.46	1.38
23	d	401	CLA	C3B-C2B	3.92	1.45	1.40
23	A	406	CLA	C3B-C2B	3.92	1.45	1.40
23	a	406	CLA	OBD-CAD	3.91	1.27	1.22
24	a	408	PHO	CHD-C4C	3.91	1.49	1.40
23	D	401	CLA	C4B-NB	-3.91	1.31	1.35
23	C	512	CLA	OBD-CAD	3.90	1.27	1.22
23	D	404	CLA	O2D-CGD	3.90	1.42	1.33
23	B	606	CLA	O2D-CGD	3.90	1.42	1.33
23	a	410	CLA	O2A-CGA	3.89	1.44	1.33
23	b	609	CLA	C3D-C2D	3.89	1.46	1.39
23	c	906	CLA	C3B-C2B	3.89	1.45	1.40
40	V	203	HEC	C3B-C2B	-3.87	1.36	1.40
23	b	610	CLA	OBD-CAD	3.86	1.27	1.22
23	d	401	CLA	OBD-CAD	3.86	1.27	1.22
26	a	412	SQD	O48-C23	3.86	1.44	1.33
28	L	101	LHG	O7-C7	3.86	1.45	1.34
28	d	408	LHG	O8-C23	3.85	1.44	1.33
34	C	501	LMG	O8-C28	3.85	1.44	1.33
23	B	603	CLA	O2D-CGD	3.84	1.42	1.33
23	B	615	CLA	O2D-CGD	3.84	1.42	1.33
36	c	918	DGD	O1G-C1A	3.84	1.44	1.33
37	e	105	HEM	C3B-C2B	-3.83	1.35	1.40
23	b	617	CLA	O2A-CGA	3.82	1.44	1.33
35	b	622	HTG	C1-S1	3.82	1.86	1.80
35	C	523	HTG	C1'-S1	-3.82	1.76	1.81
23	c	911	CLA	O2A-CGA	3.81	1.44	1.33
23	C	514	CLA	OBD-CAD	3.80	1.27	1.22
23	c	908	CLA	OBD-CAD	3.80	1.27	1.22
23	b	615	CLA	O2A-CGA	3.80	1.44	1.33
37	E	105	HEM	C3B-CAB	3.80	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	605	CLA	C3B-C2B	3.80	1.45	1.40
36	c	919	DGD	O1G-C1A	3.80	1.44	1.33
23	B	606	CLA	OBD-CAD	3.80	1.27	1.22
36	C	518	DGD	O1G-C1A	3.79	1.44	1.33
23	c	908	CLA	O2A-CGA	3.79	1.44	1.33
26	B	621	SQD	O48-C23	3.79	1.44	1.33
23	C	507	CLA	MG-NC	3.79	2.15	2.06
24	a	408	PHO	CHD-C1D	3.79	1.46	1.38
23	A	406	CLA	OBD-CAD	3.78	1.27	1.22
23	b	610	CLA	O2A-CGA	3.78	1.44	1.33
23	B	602	CLA	C3D-C2D	3.78	1.46	1.39
23	A	406	CLA	C3C-C2C	3.78	1.44	1.36
23	D	403	CLA	OBD-CAD	3.78	1.27	1.22
23	D	401	CLA	C3C-C2C	3.77	1.44	1.36
23	A	408	CLA	O2D-CGD	3.77	1.42	1.33
23	B	612	CLA	O2D-CGD	3.77	1.42	1.33
36	h	102	DGD	O5D-C1E	3.77	1.46	1.40
23	c	911	CLA	C3D-C2D	3.76	1.46	1.39
35	B	631	HTG	C1'-S1	-3.76	1.76	1.81
23	c	912	CLA	O2A-CGA	3.76	1.44	1.33
23	B	611	CLA	C4C-C3C	3.76	1.51	1.45
35	b	623	HTG	C1'-S1	-3.75	1.76	1.81
23	b	603	CLA	C3B-C2B	3.75	1.45	1.40
31	B	637	DMS	O-S	3.75	1.75	1.50
23	C	510	CLA	C3B-C2B	3.75	1.45	1.40
34	j	101	LMG	O7-C10	3.74	1.44	1.34
28	L	101	LHG	O8-C23	3.74	1.44	1.33
37	e	105	HEM	C3C-C2C	-3.74	1.35	1.40
23	b	604	CLA	C3D-C2D	3.73	1.46	1.39
23	b	613	CLA	OBD-CAD	3.73	1.27	1.22
23	b	611	CLA	C1B-NB	-3.73	1.31	1.35
23	c	907	CLA	C3D-C2D	3.72	1.46	1.39
23	A	406	CLA	C3D-C2D	3.72	1.46	1.39
23	b	615	CLA	C3C-C2C	3.72	1.44	1.36
23	b	607	CLA	OBD-CAD	3.72	1.27	1.22
23	C	502	CLA	O2D-CGD	3.71	1.42	1.33
23	B	615	CLA	O2A-CGA	3.71	1.44	1.33
23	D	404	CLA	MG-NA	3.71	2.15	2.06
23	A	405	CLA	C3D-C2D	3.71	1.46	1.39
23	B	617	CLA	MG-NA	3.71	2.15	2.06
26	A	410	SQD	O48-C23	3.70	1.44	1.33
23	c	903	CLA	OBD-CAD	3.69	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	403	CLA	C3B-C2B	3.69	1.45	1.40
23	C	503	CLA	C1B-CHB	3.69	1.51	1.41
23	b	611	CLA	C3B-C2B	3.68	1.45	1.40
23	c	902	CLA	C3C-C2C	3.68	1.44	1.36
23	D	404	CLA	O2A-CGA	3.67	1.44	1.33
23	B	612	CLA	C3D-C2D	3.67	1.46	1.39
24	D	402	PHO	CHC-C4B	3.66	1.49	1.40
23	B	617	CLA	O2A-CGA	3.65	1.44	1.33
23	c	903	CLA	C3C-C2C	3.65	1.44	1.36
23	d	403	CLA	C3D-C2D	3.64	1.46	1.39
23	C	505	CLA	O2A-CGA	3.64	1.44	1.33
23	b	607	CLA	C4B-CHC	3.63	1.51	1.41
23	b	609	CLA	C3B-C2B	3.63	1.45	1.40
23	c	906	CLA	OBD-CAD	3.62	1.27	1.22
23	B	617	CLA	MG-NC	3.62	2.14	2.06
35	d	413	HTG	C1'-S1	-3.62	1.76	1.81
23	B	614	CLA	O2A-CGA	3.62	1.43	1.33
23	B	605	CLA	C3B-C2B	3.62	1.45	1.40
23	C	511	CLA	O2A-CGA	3.61	1.43	1.33
23	b	603	CLA	C1B-NB	-3.61	1.32	1.35
23	B	608	CLA	OBD-CAD	3.61	1.27	1.22
28	D	411	LHG	O8-C23	3.61	1.43	1.33
23	c	910	CLA	O2A-CGA	3.60	1.43	1.33
23	C	508	CLA	O2A-CGA	3.59	1.43	1.33
23	b	617	CLA	OBD-CAD	3.59	1.27	1.22
23	a	407	CLA	O2D-CGD	3.59	1.42	1.33
26	a	412	SQD	O47-C7	3.59	1.44	1.34
23	b	612	CLA	C1B-CHB	3.58	1.51	1.41
23	D	403	CLA	O2A-CGA	3.58	1.43	1.33
23	b	606	CLA	C3D-C2D	3.58	1.45	1.39
23	b	609	CLA	O2D-CGD	3.58	1.41	1.33
23	C	509	CLA	O2A-CGA	3.56	1.43	1.33
23	b	613	CLA	C3B-C2B	3.55	1.45	1.40
23	C	512	CLA	O2A-CGA	3.55	1.43	1.33
40	V	203	HEC	CBC-CAC	-3.55	1.36	1.49
23	c	913	CLA	O2A-CGA	3.54	1.43	1.33
23	C	506	CLA	O2A-CGA	3.52	1.43	1.33
23	B	614	CLA	C4C-C3C	3.51	1.51	1.45
23	a	407	CLA	C3C-C2C	3.51	1.44	1.36
23	C	503	CLA	O2A-CGA	3.51	1.43	1.33
23	B	616	CLA	OBD-CAD	3.50	1.27	1.22
23	C	514	CLA	O2A-CGA	3.50	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	e	105	HEM	C3B-CAB	3.50	1.55	1.47
24	A	407	PHO	C1A-NA	-3.50	1.30	1.37
23	c	905	CLA	O2A-CGA	3.49	1.43	1.33
23	d	403	CLA	O2A-CGA	3.49	1.43	1.33
40	V	203	HEC	C3D-C2D	3.49	1.48	1.37
28	d	410	LHG	O8-C23	3.48	1.43	1.33
24	a	408	PHO	OBD-CAD	3.48	1.28	1.22
24	D	402	PHO	O2A-CGA	3.48	1.43	1.33
37	E	105	HEM	C3B-C2B	-3.48	1.35	1.40
23	b	611	CLA	OBD-CAD	3.47	1.27	1.22
23	c	913	CLA	C4C-C3C	3.47	1.51	1.45
34	J	101	LMG	O8-C28	3.47	1.43	1.33
23	b	611	CLA	C3D-C2D	3.46	1.45	1.39
28	D	411	LHG	O7-C7	3.46	1.44	1.34
25	a	411	BCR	C26-C25	3.46	1.40	1.34
23	B	607	CLA	MG-NC	3.45	2.14	2.06
23	B	615	CLA	MG-NC	3.45	2.14	2.06
31	o	301	DMS	O-S	3.44	1.73	1.50
23	A	408	CLA	O2A-CGA	3.44	1.43	1.33
27	a	414	PL9	C7-C3	3.43	1.54	1.51
23	c	905	CLA	C4C-C3C	3.43	1.50	1.45
23	B	610	CLA	O2D-CGD	3.43	1.41	1.33
23	A	408	CLA	C1B-CHB	3.42	1.50	1.41
23	B	611	CLA	C3B-C2B	3.42	1.45	1.40
23	b	615	CLA	C3B-C2B	3.42	1.45	1.40
23	C	502	CLA	O2A-CGA	3.41	1.43	1.33
23	b	612	CLA	O2A-CGA	3.41	1.43	1.33
23	b	615	CLA	O2D-CGD	3.41	1.41	1.33
23	a	406	CLA	C3D-C2D	3.40	1.45	1.39
35	B	625	HTG	C1-S1	3.40	1.86	1.80
23	b	606	CLA	C4B-NB	-3.40	1.32	1.35
40	v	203	HEC	CBC-CAC	-3.39	1.36	1.49
35	B	630	HTG	C1'-S1	-3.39	1.77	1.81
23	B	613	CLA	C3D-C2D	3.39	1.45	1.39
23	c	908	CLA	C3D-C2D	3.38	1.45	1.39
28	D	410	LHG	O7-C7	3.38	1.43	1.34
23	B	609	CLA	OBD-CAD	3.38	1.27	1.22
24	a	409	PHO	O2A-CGA	3.38	1.43	1.33
34	B	622	LMG	O7-C10	3.37	1.43	1.34
23	c	906	CLA	C1D-C2D	3.37	1.50	1.42
23	b	615	CLA	OBD-CAD	3.37	1.27	1.22
24	a	408	PHO	C3B-C2B	3.37	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	606	CLA	O2A-CGA	3.37	1.43	1.33
23	d	404	CLA	O2A-CGA	3.36	1.43	1.33
23	B	615	CLA	C4C-C3C	3.36	1.50	1.45
23	B	611	CLA	O2A-CGA	3.36	1.43	1.33
23	B	617	CLA	OBD-CAD	3.35	1.27	1.22
23	b	603	CLA	O2A-CGA	3.35	1.43	1.33
23	A	408	CLA	C1B-NB	3.35	1.38	1.35
23	D	403	CLA	O2D-CGD	3.34	1.41	1.33
36	c	917	DGD	O1G-C1A	3.33	1.43	1.33
23	D	403	CLA	C4B-NB	-3.32	1.32	1.35
23	B	609	CLA	C3D-C2D	3.32	1.45	1.39
37	e	105	HEM	C3C-CAC	3.32	1.54	1.47
24	D	402	PHO	C3D-C4D	-3.32	1.33	1.43
23	C	503	CLA	OBD-CAD	3.31	1.26	1.22
23	B	603	CLA	C4C-C3C	3.31	1.50	1.45
23	c	903	CLA	O2A-CGA	3.31	1.43	1.33
23	b	606	CLA	O2D-CGD	3.31	1.41	1.33
23	C	513	CLA	MG-NC	3.30	2.14	2.06
23	B	615	CLA	C1B-CHB	3.29	1.50	1.41
23	B	607	CLA	C4C-C3C	3.29	1.50	1.45
23	b	613	CLA	O2D-CGD	3.29	1.41	1.33
35	c	922	HTG	C1'-S1	-3.29	1.77	1.81
23	B	610	CLA	C3B-C2B	3.29	1.44	1.40
27	A	411	PL9	C7-C3	3.28	1.54	1.51
23	D	404	CLA	OBD-CAD	3.28	1.26	1.22
23	B	604	CLA	C3D-C2D	3.28	1.45	1.39
28	l	101	LHG	O8-C23	3.28	1.42	1.33
23	C	507	CLA	C1B-CHB	3.28	1.50	1.41
23	C	504	CLA	CHD-C4C	3.27	1.50	1.41
36	D	407	DGD	O3G-C1D	3.27	1.45	1.40
23	B	613	CLA	O2A-CGA	3.26	1.42	1.33
23	a	407	CLA	C3B-C2B	3.25	1.44	1.40
23	B	603	CLA	C4B-NB	3.25	1.38	1.35
23	b	603	CLA	O2D-CGD	3.25	1.41	1.33
23	c	909	CLA	C1C-NC	-3.25	1.33	1.37
24	D	402	PHO	OBD-CAD	3.25	1.28	1.22
23	B	609	CLA	O2A-CGA	3.25	1.42	1.33
36	C	517	DGD	O1G-C1A	3.24	1.42	1.33
23	c	909	CLA	O2A-CGA	3.24	1.42	1.33
23	a	406	CLA	O2A-CGA	3.23	1.42	1.33
23	b	604	CLA	OBD-CAD	3.23	1.26	1.22
23	A	408	CLA	MG-NC	3.21	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	H	103	DGD	O1G-C1A	3.21	1.42	1.33
23	C	502	CLA	OBD-CAD	3.21	1.26	1.22
23	b	612	CLA	MG-NC	3.20	2.13	2.06
23	B	605	CLA	O2D-CGD	3.20	1.41	1.33
23	C	506	CLA	C1B-NB	-3.20	1.32	1.35
23	B	610	CLA	O2A-CGA	3.20	1.42	1.33
35	B	625	HTG	O5-C1	3.20	1.47	1.42
36	c	918	DGD	O2G-C1B	3.20	1.43	1.34
23	D	401	CLA	C3D-C2D	3.19	1.45	1.39
23	B	604	CLA	O2A-CGA	3.19	1.42	1.33
23	a	410	CLA	C1B-CHB	3.19	1.49	1.41
23	D	404	CLA	C4C-C3C	3.19	1.50	1.45
28	D	410	LHG	O8-C23	3.18	1.42	1.33
23	c	910	CLA	C1C-NC	-3.18	1.33	1.37
23	b	610	CLA	C1B-CHB	3.18	1.49	1.41
23	C	504	CLA	C4B-CHC	3.18	1.49	1.41
23	b	609	CLA	O2A-CGA	3.17	1.42	1.33
23	b	615	CLA	C4B-CHC	3.17	1.49	1.41
23	C	509	CLA	C4C-C3C	3.17	1.50	1.45
23	B	605	CLA	O2A-CGA	3.16	1.42	1.33
23	B	616	CLA	C4C-C3C	3.16	1.50	1.45
23	c	910	CLA	MG-NC	3.16	2.13	2.06
23	c	904	CLA	C1B-CHB	3.16	1.49	1.41
24	a	408	PHO	C3D-C2D	3.15	1.47	1.39
24	A	407	PHO	O2D-CGD	3.15	1.40	1.33
23	c	914	CLA	C1B-CHB	3.15	1.49	1.41
23	a	407	CLA	O2A-CGA	3.15	1.42	1.33
24	a	408	PHO	O2D-CGD	3.15	1.40	1.33
23	c	911	CLA	MG-NA	3.15	2.13	2.06
23	c	908	CLA	O2D-CGD	3.15	1.40	1.33
23	a	407	CLA	OBD-CAD	3.15	1.26	1.22
23	B	608	CLA	O2D-CGD	3.14	1.40	1.33
35	C	522	HTG	C1'-S1	-3.13	1.77	1.81
31	A	423	DMS	O-S	3.13	1.71	1.50
24	A	407	PHO	CHD-C4C	3.13	1.47	1.40
23	D	403	CLA	CHC-C1C	3.13	1.43	1.35
23	b	613	CLA	O2A-CGA	3.11	1.42	1.33
36	C	519	DGD	O2G-C1B	3.10	1.43	1.34
23	C	513	CLA	C4C-C3C	3.09	1.50	1.45
23	A	406	CLA	O2A-CGA	3.09	1.42	1.33
23	C	512	CLA	C4C-C3C	3.08	1.50	1.45
23	B	604	CLA	OBD-CAD	3.08	1.26	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	607	CLA	C4B-CHC	3.08	1.49	1.41
23	A	408	CLA	C4C-C3C	3.08	1.50	1.45
23	c	912	CLA	C1B-CHB	3.08	1.49	1.41
23	b	609	CLA	C1B-CHB	3.07	1.49	1.41
23	B	605	CLA	C1D-C2D	3.07	1.49	1.42
35	b	627	HTG	C1-S1	-3.07	1.76	1.80
23	C	514	CLA	C4C-C3C	3.07	1.50	1.45
35	v	204	HTG	C1'-S1	-3.07	1.77	1.81
30	A	416	LMT	O1'-C1'	3.06	1.45	1.40
23	d	403	CLA	C1D-C2D	3.05	1.49	1.42
23	C	513	CLA	C1B-CHB	3.05	1.49	1.41
23	a	406	CLA	O2D-CGD	3.05	1.40	1.33
23	D	401	CLA	O2D-CGD	3.04	1.40	1.33
23	B	616	CLA	C1B-NB	-3.04	1.32	1.35
23	C	508	CLA	C4C-C3C	3.03	1.50	1.45
23	b	617	CLA	C1B-CHB	3.03	1.49	1.41
23	A	406	CLA	O2D-CGD	3.03	1.40	1.33
36	h	102	DGD	O2G-C1B	3.03	1.42	1.34
28	d	408	LHG	O7-C7	3.03	1.42	1.34
23	b	615	CLA	MG-NC	3.02	2.13	2.06
23	B	603	CLA	MG-NC	3.02	2.13	2.06
23	C	506	CLA	C4C-C3C	3.02	1.50	1.45
23	b	603	CLA	C4C-C3C	3.01	1.50	1.45
36	c	919	DGD	O2G-C2G	-3.01	1.39	1.46
23	B	614	CLA	OBD-CAD	3.00	1.26	1.22
23	c	906	CLA	O2D-CGD	3.00	1.40	1.33
23	C	508	CLA	C1D-C2D	3.00	1.49	1.42
23	d	403	CLA	O2D-CGD	2.99	1.40	1.33
23	B	606	CLA	C3B-C2B	2.99	1.44	1.40
23	A	405	CLA	C3C-C2C	2.99	1.43	1.36
23	c	904	CLA	C4C-C3C	2.99	1.50	1.45
23	D	401	CLA	OBD-CAD	2.98	1.26	1.22
35	c	921	HTG	C1'-S1	-2.98	1.77	1.81
23	c	902	CLA	O2A-CGA	2.98	1.42	1.33
23	B	605	CLA	OBD-CAD	2.97	1.26	1.22
23	B	616	CLA	O2A-CGA	2.97	1.42	1.33
25	A	409	BCR	C19-C18	2.96	1.52	1.45
23	b	615	CLA	C1C-C2C	2.96	1.50	1.44
23	B	611	CLA	C1C-NC	-2.96	1.33	1.37
23	b	616	CLA	O2A-CGA	2.95	1.42	1.33
23	B	607	CLA	O2A-CGA	2.94	1.41	1.33
23	C	504	CLA	C1C-C2C	2.94	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	511	CLA	C1C-NC	-2.93	1.33	1.37
35	O	302	HTG	O5-C1	2.93	1.47	1.42
24	D	402	PHO	C3D-C2D	2.93	1.47	1.39
23	b	614	CLA	C1C-NC	-2.93	1.33	1.37
25	b	619	BCR	C5-C6	2.93	1.39	1.34
23	b	603	CLA	C3D-C2D	2.92	1.44	1.39
30	Z	101	LMT	O1'-C1'	2.92	1.45	1.40
23	b	608	CLA	OBD-CAD	2.92	1.26	1.22
23	c	914	CLA	C1C-C2C	2.91	1.50	1.44
30	I	101	LMT	O1'-C1'	2.91	1.45	1.40
23	c	913	CLA	C1D-C2D	2.91	1.49	1.42
35	C	521	HTG	C1'-S1	-2.91	1.77	1.81
23	D	404	CLA	C1B-NB	2.91	1.37	1.35
24	a	408	PHO	C1A-NA	-2.91	1.31	1.37
23	c	904	CLA	O2A-CGA	2.90	1.41	1.33
23	D	403	CLA	CHD-C4C	2.90	1.49	1.41
23	B	603	CLA	C1B-CHB	2.90	1.49	1.41
23	C	512	CLA	C1B-CHB	2.90	1.49	1.41
23	d	401	CLA	O2A-CGA	2.90	1.41	1.33
26	A	415	SQD	C6-S	-2.90	1.66	1.77
23	b	604	CLA	C1B-NB	-2.90	1.32	1.35
35	B	626	HTG	C1'-S1	-2.89	1.77	1.81
23	a	407	CLA	C4C-C3C	2.89	1.50	1.45
23	c	902	CLA	C4C-C3C	2.89	1.50	1.45
23	C	509	CLA	MG-NC	2.89	2.13	2.06
23	A	405	CLA	O2A-CGA	2.89	1.41	1.33
23	c	912	CLA	C4C-C3C	2.88	1.50	1.45
23	c	910	CLA	C1B-CHB	2.88	1.49	1.41
26	a	417	SQD	C6-S	-2.88	1.66	1.77
24	a	409	PHO	C3D-C2D	2.88	1.47	1.39
23	b	607	CLA	C4B-NB	2.88	1.37	1.35
23	b	614	CLA	MG-NC	2.87	2.13	2.06
23	C	514	CLA	C1B-CHB	2.87	1.49	1.41
36	c	917	DGD	O2G-C1B	2.86	1.42	1.34
35	D	414	HTG	C1'-S1	-2.86	1.77	1.81
23	B	616	CLA	C1D-C2D	2.86	1.49	1.42
23	c	902	CLA	C4B-CHC	2.86	1.48	1.41
40	V	203	HEC	CBB-CAB	-2.86	1.38	1.49
23	B	608	CLA	C1B-CHB	2.85	1.48	1.41
24	A	407	PHO	O2A-CGA	2.85	1.41	1.33
25	B	618	BCR	C14-C13	2.85	1.39	1.35
27	a	414	PL9	C2-C3	2.84	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	403	CLA	C4B-NB	2.84	1.37	1.35
23	B	605	CLA	C3D-C2D	2.84	1.44	1.39
31	b	633	DMS	O-S	2.84	1.69	1.50
23	b	607	CLA	C1B-CHB	2.83	1.48	1.41
28	l	101	LHG	O7-C7	2.82	1.42	1.34
36	C	517	DGD	O2G-C1B	2.82	1.42	1.34
23	B	613	CLA	C3B-C2B	2.82	1.44	1.40
23	d	401	CLA	CHD-C4C	2.82	1.49	1.41
28	d	409	LHG	O7-C7	2.82	1.42	1.34
24	a	409	PHO	OBD-CAD	2.81	1.27	1.22
23	a	406	CLA	CHD-C4C	2.81	1.49	1.41
23	c	905	CLA	C1C-NC	-2.81	1.33	1.37
23	A	408	CLA	C1C-NC	-2.81	1.33	1.37
23	d	403	CLA	C1B-CHB	2.81	1.48	1.41
23	c	914	CLA	C1D-C2D	2.80	1.48	1.42
24	a	408	PHO	CHC-C4B	2.79	1.47	1.40
23	B	609	CLA	C4B-NB	2.79	1.37	1.35
23	b	611	CLA	C4C-C3C	2.79	1.49	1.45
23	d	401	CLA	C3D-C2D	2.79	1.44	1.39
23	C	502	CLA	C1C-NC	-2.79	1.33	1.37
23	c	908	CLA	C4B-CHC	2.78	1.48	1.41
23	C	505	CLA	CHD-C4C	2.78	1.49	1.41
23	B	612	CLA	O2A-CGA	2.77	1.41	1.33
23	D	403	CLA	C3D-C2D	2.77	1.44	1.39
28	d	410	LHG	O7-C7	2.76	1.42	1.34
23	D	401	CLA	C4B-CHC	2.76	1.48	1.41
23	B	604	CLA	C1B-CHB	2.75	1.48	1.41
25	D	405	BCR	C12-C13	2.75	1.51	1.45
23	d	404	CLA	O2D-CGD	2.75	1.39	1.33
23	b	616	CLA	CHD-C4C	2.75	1.49	1.41
36	h	102	DGD	O1G-C1A	2.75	1.41	1.33
23	C	506	CLA	CHD-C4C	2.75	1.49	1.41
23	b	606	CLA	O2A-CGA	2.75	1.41	1.33
23	c	911	CLA	C1B-CHB	2.74	1.48	1.41
23	c	907	CLA	C1C-NC	-2.74	1.33	1.37
30	a	422	LMT	O1'-C1'	2.74	1.44	1.40
23	b	605	CLA	MG-NC	2.74	2.12	2.06
36	c	919	DGD	O2G-C1B	2.74	1.42	1.34
23	B	614	CLA	C3B-C2B	2.74	1.44	1.40
23	b	602	CLA	C1B-CHB	2.73	1.48	1.41
23	D	404	CLA	C1B-CHB	2.72	1.48	1.41
23	C	509	CLA	C4B-CHC	2.72	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	606	CLA	CHD-C4C	2.72	1.48	1.41
37	E	105	HEM	C3C-C2C	-2.71	1.36	1.40
23	C	502	CLA	C4B-CHC	2.71	1.48	1.41
23	b	605	CLA	O2A-CGA	2.71	1.41	1.33
23	b	616	CLA	C1B-CHB	2.71	1.48	1.41
23	C	507	CLA	OBD-CAD	2.71	1.26	1.22
23	b	606	CLA	MG-NC	-2.71	1.99	2.06
23	B	612	CLA	C4B-CHC	2.70	1.48	1.41
35	B	624	HTG	O5-C1	2.70	1.46	1.42
23	C	511	CLA	C1B-CHB	2.70	1.48	1.41
23	b	606	CLA	OBD-CAD	2.70	1.26	1.22
23	B	608	CLA	O2A-CGA	2.69	1.41	1.33
23	a	406	CLA	C4B-NB	-2.69	1.32	1.35
23	C	508	CLA	CHD-C4C	2.69	1.48	1.41
35	B	624	HTG	C1-C2	2.69	1.58	1.53
23	c	906	CLA	C1B-CHB	2.68	1.48	1.41
35	b	628	HTG	C1'-S1	-2.68	1.78	1.81
23	B	603	CLA	CHD-C4C	2.68	1.48	1.41
26	a	412	SQD	C6-S	-2.68	1.67	1.77
23	b	605	CLA	C4C-C3C	2.68	1.49	1.45
23	B	616	CLA	C1B-CHB	2.68	1.48	1.41
23	b	603	CLA	C3B-CAB	2.67	1.53	1.47
23	b	603	CLA	C4B-NB	2.67	1.37	1.35
23	c	903	CLA	C1B-CHB	2.67	1.48	1.41
23	b	617	CLA	C4B-CHC	2.67	1.48	1.41
23	D	401	CLA	O2A-CGA	2.67	1.41	1.33
23	C	506	CLA	C4B-CHC	2.67	1.48	1.41
23	B	617	CLA	C1C-NC	-2.66	1.33	1.37
23	b	616	CLA	C4C-C3C	2.66	1.49	1.45
35	C	521	HTG	C1-S1	-2.65	1.76	1.80
23	B	602	CLA	C1D-C2D	2.65	1.48	1.42
23	b	611	CLA	C4B-CHC	2.65	1.48	1.41
23	d	404	CLA	C4B-CHC	2.65	1.48	1.41
23	C	514	CLA	CHD-C4C	2.64	1.48	1.41
23	B	604	CLA	C3B-C2B	2.64	1.44	1.40
23	c	908	CLA	C1B-CHB	2.64	1.48	1.41
23	B	605	CLA	MG-NC	2.64	2.12	2.06
23	A	408	CLA	C4B-CHC	2.64	1.48	1.41
23	D	404	CLA	C4B-CHC	2.64	1.48	1.41
23	b	610	CLA	C4B-CHC	2.64	1.48	1.41
23	B	608	CLA	C4B-CHC	2.63	1.48	1.41
37	E	105	HEM	C4B-NB	2.63	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	908	CLA	C1C-C2C	2.62	1.49	1.44
23	C	511	CLA	C4C-C3C	2.61	1.49	1.45
24	a	408	PHO	C1C-NC	-2.61	1.33	1.38
23	C	509	CLA	C1C-C2C	2.61	1.49	1.44
23	C	509	CLA	C1D-C2D	2.61	1.48	1.42
23	a	406	CLA	C1B-CHB	2.61	1.48	1.41
23	C	505	CLA	OBD-CAD	2.61	1.25	1.22
23	C	510	CLA	C1B-CHB	2.60	1.48	1.41
30	e	103	LMT	O1'-C1'	2.59	1.44	1.40
23	c	906	CLA	CHD-C4C	2.59	1.48	1.41
23	b	602	CLA	C1C-C2C	2.59	1.49	1.44
23	C	502	CLA	CHD-C4C	2.59	1.48	1.41
23	b	606	CLA	C3B-C2B	2.58	1.44	1.40
23	A	408	CLA	OBD-CAD	2.58	1.25	1.22
23	b	607	CLA	O2A-CGA	2.58	1.40	1.33
23	b	607	CLA	C1D-C2D	2.58	1.48	1.42
24	a	409	PHO	CHC-C4B	2.58	1.46	1.40
23	B	616	CLA	C1C-NC	-2.58	1.34	1.37
23	C	507	CLA	CHD-C4C	2.57	1.48	1.41
23	C	509	CLA	C1B-CHB	2.57	1.48	1.41
23	c	910	CLA	C4C-C3C	2.57	1.49	1.45
23	B	611	CLA	CHD-C4C	2.56	1.48	1.41
23	C	514	CLA	C4B-CHC	2.56	1.48	1.41
23	c	914	CLA	C4B-CHC	2.56	1.48	1.41
27	a	414	PL9	C6-C5	2.56	1.48	1.35
23	c	903	CLA	CHD-C4C	2.56	1.48	1.41
23	D	401	CLA	C4C-C3C	2.56	1.49	1.45
23	b	617	CLA	C1C-C2C	2.55	1.49	1.44
23	b	604	CLA	C1B-CHB	2.55	1.48	1.41
23	B	608	CLA	C1D-C2D	2.55	1.48	1.42
27	D	406	PL9	C6-C5	2.55	1.48	1.35
23	b	611	CLA	C1B-CHB	2.55	1.48	1.41
23	B	615	CLA	C1B-NB	-2.54	1.32	1.35
23	c	909	CLA	C4C-C3C	2.54	1.49	1.45
27	D	406	PL9	C2-C3	2.54	1.41	1.34
23	b	603	CLA	MG-NC	2.53	2.12	2.06
23	C	506	CLA	C1D-C2D	2.53	1.48	1.42
23	A	405	CLA	C4B-CHC	2.53	1.48	1.41
23	b	603	CLA	CHD-C4C	2.53	1.48	1.41
23	b	608	CLA	O2A-CGA	2.53	1.40	1.33
27	A	411	PL9	C2-C3	2.53	1.41	1.34
23	b	613	CLA	C1B-CHB	2.52	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	508	CLA	C1B-CHB	2.52	1.48	1.41
23	C	511	CLA	C4B-CHC	2.52	1.48	1.41
23	C	507	CLA	C4B-CHC	2.52	1.48	1.41
24	a	409	PHO	C3B-C4B	2.52	1.48	1.43
23	B	614	CLA	C3D-C2D	2.52	1.43	1.39
23	c	908	CLA	CHD-C4C	2.51	1.48	1.41
23	B	609	CLA	CHD-C4C	2.51	1.48	1.41
35	b	622	HTG	C1-C2	2.51	1.57	1.53
23	c	913	CLA	C1B-CHB	2.51	1.48	1.41
23	c	913	CLA	C4B-CHC	2.51	1.48	1.41
23	c	906	CLA	C4B-CHC	2.51	1.48	1.41
23	B	606	CLA	C1B-CHB	2.51	1.48	1.41
34	d	411	LMG	O1-C1	2.51	1.44	1.40
23	B	604	CLA	CHD-C4C	2.50	1.48	1.41
23	B	606	CLA	C3D-C2D	2.50	1.43	1.39
24	A	407	PHO	OBD-CAD	2.50	1.26	1.22
23	b	607	CLA	C1B-NB	2.50	1.37	1.35
36	C	518	DGD	O2G-C1B	2.50	1.41	1.34
25	b	620	BCR	C26-C25	2.49	1.38	1.34
23	b	603	CLA	C1D-C2D	2.49	1.48	1.42
23	B	602	CLA	C1B-CHB	2.49	1.47	1.41
23	c	904	CLA	C4B-CHC	2.49	1.47	1.41
36	c	917	DGD	O5D-C1E	2.49	1.44	1.40
23	C	513	CLA	C1C-C2C	2.49	1.49	1.44
37	e	105	HEM	CAA-C2A	2.49	1.55	1.52
23	d	404	CLA	C1C-NC	-2.48	1.34	1.37
23	c	911	CLA	MG-NC	2.48	2.12	2.06
27	A	411	PL9	C6-C5	2.48	1.48	1.35
23	a	406	CLA	CMD-C2D	-2.47	1.45	1.51
24	a	409	PHO	CHD-C4C	2.47	1.46	1.40
23	C	510	CLA	C4C-C3C	2.47	1.49	1.45
23	B	614	CLA	C1B-CHB	2.47	1.47	1.41
24	a	409	PHO	C4D-ND	2.47	1.41	1.36
23	d	401	CLA	C4C-C3C	2.46	1.49	1.45
23	c	904	CLA	OBD-CAD	2.46	1.25	1.22
23	B	604	CLA	CAA-C2A	2.46	1.58	1.54
23	B	602	CLA	C4B-CHC	2.46	1.47	1.41
23	B	610	CLA	C1B-CHB	2.46	1.47	1.41
23	C	502	CLA	C1D-C2D	2.45	1.48	1.42
23	c	909	CLA	C1B-CHB	2.45	1.47	1.41
23	b	605	CLA	C4B-NB	-2.45	1.33	1.35
23	b	604	CLA	C4C-C3C	2.45	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	608	CLA	C1B-CHB	2.45	1.47	1.41
38	H	102	RRX	C5-C6	2.45	1.38	1.34
24	D	402	PHO	CHD-C4C	2.45	1.46	1.40
40	v	203	HEC	CBB-CAB	-2.44	1.40	1.49
23	B	614	CLA	O2D-CGD	2.44	1.39	1.33
26	x	101	SQD	C6-S	-2.44	1.68	1.77
23	c	902	CLA	C1B-CHB	2.43	1.47	1.41
23	B	605	CLA	C1B-CHB	2.43	1.47	1.41
23	a	406	CLA	C1D-C2D	2.43	1.48	1.42
26	L	102	SQD	C6-S	-2.43	1.68	1.77
27	d	406	PL9	C23-C24	2.43	1.38	1.33
30	z	101	LMT	O1'-C1'	2.42	1.44	1.40
23	c	907	CLA	C1D-C2D	2.42	1.48	1.42
23	c	913	CLA	C1C-C2C	2.42	1.49	1.44
23	B	602	CLA	C1C-C2C	2.42	1.49	1.44
23	C	513	CLA	CHD-C4C	2.42	1.48	1.41
25	A	409	BCR	C8-C9	2.42	1.51	1.45
27	d	406	PL9	C6-C5	2.41	1.47	1.35
23	B	604	CLA	C4B-NB	2.41	1.37	1.35
23	C	508	CLA	C1C-C2C	2.41	1.49	1.44
23	C	503	CLA	C4C-C3C	2.41	1.49	1.45
23	b	607	CLA	C1C-C2C	2.41	1.49	1.44
23	b	604	CLA	O2A-CGA	2.40	1.40	1.33
23	c	912	CLA	CHD-C4C	2.40	1.48	1.41
23	b	610	CLA	C1D-C2D	2.39	1.48	1.42
27	D	406	PL9	C23-C24	2.39	1.38	1.33
37	e	105	HEM	CMA-C3A	2.38	1.56	1.51
23	c	910	CLA	CHD-C4C	2.38	1.47	1.41
23	a	407	CLA	C1B-CHB	2.38	1.47	1.41
23	B	605	CLA	CHD-C4C	2.38	1.47	1.41
24	A	407	PHO	C3D-C4D	-2.38	1.36	1.43
23	B	604	CLA	C1D-C2D	2.38	1.48	1.42
23	c	902	CLA	C1D-C2D	2.38	1.47	1.42
23	B	606	CLA	C4C-C3C	2.38	1.49	1.45
23	b	607	CLA	C4C-C3C	2.37	1.49	1.45
23	b	610	CLA	C1C-C2C	2.37	1.49	1.44
23	B	606	CLA	O1D-CGD	2.37	1.27	1.21
23	c	910	CLA	C4B-NB	2.36	1.37	1.35
23	B	615	CLA	C3B-C2B	2.36	1.43	1.40
23	a	406	CLA	O2A-C1	-2.36	1.39	1.46
23	d	403	CLA	C4B-CHC	2.36	1.47	1.41
23	B	609	CLA	C1B-CHB	2.36	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	613	CLA	C1D-C2D	2.35	1.47	1.42
23	C	506	CLA	MG-NC	2.35	2.11	2.06
24	a	409	PHO	C3D-C4D	-2.35	1.36	1.43
23	C	514	CLA	C1C-C2C	2.35	1.49	1.44
23	b	609	CLA	CHD-C4C	2.34	1.47	1.41
26	A	410	SQD	C6-S	-2.34	1.68	1.77
23	B	606	CLA	O2A-C1	-2.34	1.39	1.46
23	c	905	CLA	C1B-CHB	2.34	1.47	1.41
23	c	914	CLA	CHD-C4C	2.34	1.47	1.41
23	C	504	CLA	C4C-C3C	2.34	1.49	1.45
23	c	905	CLA	C1C-C2C	2.33	1.49	1.44
23	c	913	CLA	CHD-C4C	2.33	1.47	1.41
23	B	613	CLA	C1B-CHB	2.33	1.47	1.41
35	c	922	HTG	C1-S1	-2.33	1.77	1.80
23	c	905	CLA	C4B-CHC	2.33	1.47	1.41
23	c	905	CLA	C1D-C2D	2.33	1.47	1.42
23	C	513	CLA	C4B-CHC	2.33	1.47	1.41
23	C	505	CLA	C1D-C2D	2.32	1.47	1.42
23	b	612	CLA	C4B-NB	2.32	1.37	1.35
23	c	904	CLA	C1C-C2C	2.32	1.49	1.44
34	c	930	LMG	O1-C1	2.32	1.44	1.40
23	b	611	CLA	CHD-C4C	2.31	1.47	1.41
23	B	612	CLA	C4C-C3C	2.31	1.49	1.45
23	b	602	CLA	CHD-C4C	2.31	1.47	1.41
23	d	401	CLA	C1D-C2D	2.31	1.47	1.42
23	B	610	CLA	C1D-C2D	2.31	1.47	1.42
23	C	511	CLA	CHD-C4C	2.30	1.47	1.41
23	c	908	CLA	C1B-NB	2.30	1.37	1.35
23	c	906	CLA	C1B-NB	-2.30	1.33	1.35
23	b	617	CLA	C4C-C3C	2.30	1.49	1.45
23	b	605	CLA	C1B-CHB	2.29	1.47	1.41
23	A	405	CLA	CHD-C4C	2.29	1.47	1.41
35	c	921	HTG	C1-S1	-2.29	1.77	1.80
23	B	604	CLA	MG-NC	2.28	2.11	2.06
26	B	621	SQD	O6-C1	2.28	1.44	1.40
35	C	523	HTG	C1-S1	-2.28	1.77	1.80
23	B	609	CLA	MG-NA	2.28	2.11	2.06
25	D	405	BCR	C30-C25	-2.28	1.50	1.53
23	a	407	CLA	C4B-NB	-2.28	1.33	1.35
23	A	408	CLA	C3D-C2D	2.28	1.43	1.39
34	B	622	LMG	O7-C8	-2.27	1.40	1.46
23	D	404	CLA	C1C-C2C	2.27	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	604	CLA	C3B-C2B	2.27	1.43	1.40
23	c	904	CLA	C1D-C2D	2.27	1.47	1.42
23	B	613	CLA	CHD-C4C	2.26	1.47	1.41
37	e	105	HEM	CMC-C2C	2.26	1.56	1.51
30	m	103	LMT	O1'-C1'	2.25	1.44	1.40
26	D	408	SQD	O6-C1	2.25	1.44	1.40
28	L	101	LHG	O7-C5	-2.25	1.41	1.46
23	b	615	CLA	C1B-CHB	2.25	1.47	1.41
24	a	408	PHO	O2A-CGA	2.24	1.39	1.33
23	a	410	CLA	CHD-C4C	2.24	1.47	1.41
23	b	614	CLA	CHD-C4C	2.24	1.47	1.41
23	b	608	CLA	C4C-C3C	2.23	1.48	1.45
40	v	203	HEC	C3C-C4C	2.23	1.47	1.43
40	v	203	HEC	C1D-ND	2.23	1.40	1.36
23	c	907	CLA	C1C-C2C	2.22	1.48	1.44
23	c	912	CLA	C1D-C2D	2.22	1.47	1.42
25	B	620	BCR	C20-C21	2.22	1.50	1.43
23	C	507	CLA	C4C-C3C	2.22	1.48	1.45
23	c	912	CLA	C3D-CAD	2.22	1.51	1.46
23	c	908	CLA	C1C-NC	-2.21	1.34	1.37
23	A	405	CLA	CAA-C2A	2.21	1.58	1.54
23	B	611	CLA	C4B-CHC	2.21	1.47	1.41
23	B	617	CLA	C4C-C3C	2.21	1.48	1.45
23	b	615	CLA	C1C-NC	-2.20	1.34	1.37
23	c	909	CLA	C4B-CHC	2.20	1.47	1.41
23	b	611	CLA	O2A-CGA	2.20	1.39	1.33
23	B	603	CLA	O2A-CGA	2.20	1.39	1.33
23	c	908	CLA	C1D-C2D	2.20	1.47	1.42
23	B	606	CLA	C1C-C2C	2.20	1.48	1.44
23	b	602	CLA	C1C-NC	-2.20	1.34	1.37
37	E	105	HEM	C1D-ND	2.20	1.40	1.36
23	C	506	CLA	C1B-CHB	2.20	1.47	1.41
27	d	406	PL9	C7-C3	2.19	1.53	1.51
23	C	514	CLA	C1D-C2D	2.19	1.47	1.42
36	C	518	DGD	O2G-C2G	-2.19	1.41	1.46
23	B	610	CLA	C1B-NB	-2.19	1.33	1.35
25	D	405	BCR	C20-C21	2.19	1.50	1.43
23	D	401	CLA	C1D-C2D	2.19	1.47	1.42
23	b	602	CLA	C4C-C3C	2.18	1.48	1.45
26	D	408	SQD	C6-S	-2.18	1.69	1.77
30	b	621	LMT	O1'-C1'	2.18	1.43	1.40
23	b	606	CLA	C4B-CHC	2.18	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	411	BCR	C5-C6	2.18	1.38	1.34
23	c	902	CLA	C1C-C2C	2.18	1.48	1.44
23	b	604	CLA	CHD-C4C	2.18	1.47	1.41
40	v	203	HEC	CMC-C2C	2.18	1.56	1.51
40	V	203	HEC	CMC-C2C	2.17	1.56	1.51
23	B	611	CLA	C1C-C2C	2.17	1.48	1.44
23	c	906	CLA	MG-NC	2.17	2.11	2.06
30	F	101	LMT	O1'-C1'	2.17	1.43	1.40
23	b	605	CLA	OBD-CAD	2.17	1.25	1.22
35	b	622	HTG	O5-C1	2.17	1.45	1.42
23	b	615	CLA	C1B-NB	2.17	1.37	1.35
23	C	512	CLA	CHD-C4C	2.17	1.47	1.41
24	D	402	PHO	CHB-C4A	-2.16	1.34	1.40
23	B	616	CLA	CHD-C4C	2.16	1.47	1.41
23	b	615	CLA	CHD-C4C	2.16	1.47	1.41
28	d	409	LHG	O8-C23	2.16	1.39	1.33
23	C	512	CLA	C4B-CHC	2.16	1.47	1.41
25	b	619	BCR	C24-C25	2.16	1.52	1.45
23	B	603	CLA	C4B-CHC	2.16	1.47	1.41
23	B	606	CLA	CHD-C4C	2.15	1.47	1.41
23	b	605	CLA	C1C-C2C	2.15	1.48	1.44
37	e	105	HEM	CAD-C3D	2.15	1.56	1.52
30	a	418	LMT	O1'-C1'	2.15	1.43	1.40
35	B	630	HTG	C1-S1	-2.14	1.77	1.80
23	c	910	CLA	C1B-NB	2.14	1.37	1.35
23	B	612	CLA	C3B-C2B	2.14	1.43	1.40
23	c	914	CLA	C4C-C3C	2.14	1.48	1.45
23	d	404	CLA	MG-NC	2.14	2.11	2.06
23	A	406	CLA	C1B-CHB	2.14	1.46	1.41
25	k	102	BCR	C19-C18	2.14	1.50	1.45
23	A	405	CLA	C3B-CAB	2.13	1.52	1.47
23	B	614	CLA	C3B-CAB	2.13	1.52	1.47
23	d	404	CLA	C1C-C2C	2.13	1.48	1.44
23	B	602	CLA	C4B-NB	2.13	1.37	1.35
23	B	617	CLA	CHD-C4C	2.13	1.47	1.41
23	B	613	CLA	C4B-NB	-2.13	1.33	1.35
23	b	613	CLA	C4B-CHC	2.13	1.46	1.41
23	C	503	CLA	C4B-CHC	2.13	1.46	1.41
23	b	603	CLA	C1B-CHB	2.12	1.46	1.41
34	j	101	LMG	O7-C8	-2.12	1.41	1.46
23	D	401	CLA	C1B-CHB	2.12	1.46	1.41
25	d	405	BCR	C19-C18	2.12	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	607	CLA	C1D-C2D	2.12	1.47	1.42
34	j	101	LMG	O1-C1	2.12	1.43	1.40
23	C	508	CLA	C4B-CHC	2.12	1.46	1.41
23	b	610	CLA	C4C-C3C	2.12	1.48	1.45
23	A	405	CLA	C1B-CHB	2.11	1.46	1.41
23	C	505	CLA	C4C-C3C	2.11	1.48	1.45
23	B	608	CLA	MG-NC	2.11	2.11	2.06
35	O	302	HTG	C1-S1	2.11	1.84	1.80
23	B	617	CLA	C1B-NB	2.11	1.37	1.35
23	c	906	CLA	C1C-C2C	2.11	1.48	1.44
23	A	405	CLA	C1D-C2D	2.11	1.47	1.42
23	C	512	CLA	C1D-C2D	2.11	1.47	1.42
23	A	408	CLA	CHD-C4C	2.11	1.47	1.41
23	B	614	CLA	C1C-C2C	2.10	1.48	1.44
23	B	605	CLA	C1C-NC	-2.10	1.34	1.37
23	B	613	CLA	C4B-CHC	2.10	1.46	1.41
23	c	912	CLA	C1C-C2C	2.10	1.48	1.44
23	c	904	CLA	C1C-NC	-2.10	1.34	1.37
23	B	612	CLA	C1D-C2D	2.09	1.47	1.42
35	B	625	HTG	C1-C2	2.09	1.57	1.53
25	B	619	BCR	C24-C25	2.09	1.52	1.45
23	b	611	CLA	CAA-C2A	2.09	1.58	1.54
23	A	406	CLA	C1C-NC	-2.09	1.34	1.37
23	B	602	CLA	CHD-C4C	2.09	1.47	1.41
23	b	616	CLA	C4B-NB	2.09	1.37	1.35
26	a	417	SQD	O7-S	2.08	1.51	1.45
23	c	902	CLA	CHD-C4C	2.08	1.47	1.41
23	c	906	CLA	C4C-C3C	2.08	1.48	1.45
37	E	105	HEM	CAA-C2A	2.08	1.55	1.52
37	E	105	HEM	CMC-C2C	2.08	1.56	1.51
24	a	408	PHO	CHB-C4A	-2.07	1.34	1.40
35	b	623	HTG	C1-S1	-2.07	1.77	1.80
27	A	411	PL9	C6-C1	2.07	1.52	1.48
23	b	605	CLA	CHD-C4C	2.06	1.47	1.41
23	c	909	CLA	C1C-C2C	2.06	1.48	1.44
23	c	909	CLA	CHD-C4C	2.06	1.47	1.41
23	B	614	CLA	C1D-C2D	2.06	1.47	1.42
35	C	522	HTG	O5-C1	2.06	1.45	1.42
23	B	617	CLA	C1B-CHB	2.06	1.46	1.41
23	C	507	CLA	C1A-CHA	2.06	1.51	1.43
23	b	617	CLA	C1D-C2D	2.05	1.47	1.42
24	a	408	PHO	C3D-C4D	-2.05	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	409	BCR	C23-C22	2.04	1.50	1.45
23	b	608	CLA	C1B-NB	-2.04	1.33	1.35
23	B	611	CLA	C1-C2	2.04	1.55	1.49
25	D	405	BCR	C19-C18	2.04	1.50	1.45
25	b	620	BCR	C30-C25	-2.03	1.51	1.53
23	b	617	CLA	CHD-C4C	2.03	1.46	1.41
23	B	609	CLA	O2A-C1	-2.03	1.40	1.46
23	c	907	CLA	C4B-CHC	2.03	1.46	1.41
23	c	907	CLA	C4B-NB	2.03	1.37	1.35
40	v	203	HEC	C1A-C2A	2.03	1.47	1.42
25	B	620	BCR	C19-C18	2.02	1.50	1.45
23	b	613	CLA	CHD-C4C	2.02	1.46	1.41
36	C	518	DGD	O3G-C1D	2.02	1.43	1.40
25	a	411	BCR	C8-C9	2.02	1.50	1.45
23	B	610	CLA	C4B-CHC	2.02	1.46	1.41
23	b	602	CLA	C1D-C2D	2.02	1.47	1.42
23	B	614	CLA	C4B-NB	2.01	1.37	1.35
23	c	906	CLA	C1C-NC	-2.01	1.34	1.37
23	b	608	CLA	C4B-CHC	2.01	1.46	1.41
23	B	611	CLA	C1B-CHB	2.01	1.46	1.41
23	b	608	CLA	CHD-C4C	2.01	1.46	1.41
23	B	616	CLA	C4B-CHC	2.01	1.46	1.41
23	B	607	CLA	C1C-C2C	2.01	1.48	1.44
27	d	406	PL9	C13-C14	2.00	1.37	1.33
25	A	409	BCR	C26-C25	2.00	1.37	1.34
23	B	607	CLA	C1B-CHB	2.00	1.46	1.41
37	E	105	HEM	CMD-C2D	2.00	1.55	1.51
23	c	904	CLA	CHD-C4C	2.00	1.46	1.41
26	a	417	SQD	O9-S	2.00	1.50	1.45

All (2141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	905	CLA	C4A-NA-C1A	12.36	112.26	106.71
23	c	910	CLA	C4A-NA-C1A	12.30	112.23	106.71
23	C	512	CLA	C4A-NA-C1A	11.20	111.74	106.71
23	c	902	CLA	C4A-NA-C1A	11.01	111.66	106.71
23	b	612	CLA	C4A-NA-C1A	10.40	111.38	106.71
23	c	904	CLA	C4A-NA-C1A	9.94	111.18	106.71
23	c	913	CLA	C4A-NA-C1A	9.90	111.16	106.71
23	C	508	CLA	C4A-NA-C1A	9.48	110.97	106.71
35	v	204	HTG	C1'-S1-C1	9.28	117.46	100.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	408	SQD	O6-C1-C2	9.05	122.43	108.30
23	B	616	CLA	C4A-NA-C1A	8.93	110.72	106.71
23	b	602	CLA	C4A-NA-C1A	8.89	110.70	106.71
23	A	406	CLA	C4A-NA-C1A	8.75	110.64	106.71
23	B	604	CLA	C2C-C1C-NC	8.55	117.98	109.97
23	c	912	CLA	C4A-NA-C1A	8.44	110.50	106.71
23	C	510	CLA	C4A-NA-C1A	8.40	110.48	106.71
23	a	407	CLA	C2C-C1C-NC	8.39	117.83	109.97
23	C	513	CLA	C4A-NA-C1A	8.20	110.39	106.71
23	C	507	CLA	C4A-NA-C1A	8.19	110.39	106.71
23	b	605	CLA	C4A-NA-C1A	8.05	110.33	106.71
23	C	505	CLA	C4A-NA-C1A	8.04	110.32	106.71
26	a	412	SQD	O6-C1-C2	8.03	120.85	108.30
23	C	514	CLA	C4A-NA-C1A	7.97	110.29	106.71
35	V	204	HTG	O5-C1-C2	-7.89	100.39	110.31
23	c	909	CLA	C4A-NA-C1A	7.79	110.21	106.71
23	D	403	CLA	C2C-C1C-NC	7.74	117.22	109.97
35	d	413	HTG	C1'-S1-C1	7.60	114.30	100.09
23	c	903	CLA	C4A-NA-C1A	7.58	110.12	106.71
23	D	403	CLA	C4A-NA-C1A	7.54	110.10	106.71
23	C	509	CLA	C4A-NA-C1A	7.48	110.07	106.71
35	C	523	HTG	C1'-S1-C1	7.46	114.04	100.09
23	c	914	CLA	C4A-NA-C1A	7.44	110.05	106.71
23	B	602	CLA	C4A-NA-C1A	7.36	110.02	106.71
26	a	412	SQD	O9-S-C6	7.30	115.62	106.94
37	E	105	HEM	CBD-CAD-C3D	-7.29	99.05	112.48
23	B	607	CLA	C4A-NA-C1A	7.28	109.98	106.71
24	A	407	PHO	CMD-C2D-C1D	7.27	136.27	125.06
23	B	611	CLA	C4A-NA-C1A	7.26	109.97	106.71
23	B	602	CLA	O2D-CGD-CBD	7.25	124.15	111.27
23	b	614	CLA	C4A-NA-C1A	7.19	109.94	106.71
35	C	521	HTG	C1'-S1-C1	7.15	113.47	100.09
23	B	615	CLA	C4A-NA-C1A	7.08	109.89	106.71
23	A	406	CLA	C2C-C1C-NC	6.98	116.52	109.97
35	b	623	HTG	C1'-S1-C1	6.96	113.11	100.09
23	B	613	CLA	C4A-NA-C1A	6.83	109.78	106.71
23	d	404	CLA	C2C-C1C-NC	6.81	116.35	109.97
23	b	604	CLA	C2C-C1C-NC	6.80	116.34	109.97
23	C	506	CLA	C2C-C1C-NC	6.80	116.34	109.97
23	D	404	CLA	C4A-NA-C1A	6.76	109.75	106.71
25	D	405	BCR	C7-C8-C9	-6.74	116.05	126.23
35	V	204	HTG	C1'-S1-C1	6.73	113.03	100.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	511	CLA	CHD-C4C-C3C	-6.59	115.15	124.84
23	C	506	CLA	C4A-NA-C1A	6.58	109.67	106.71
23	b	606	CLA	CHD-C4C-C3C	-6.57	115.18	124.84
23	D	401	CLA	CMD-C2D-C3D	6.53	136.90	124.68
23	C	502	CLA	O2D-CGD-CBD	6.50	122.83	111.27
23	C	505	CLA	C2C-C1C-NC	6.48	116.04	109.97
23	d	401	CLA	C2C-C1C-NC	6.45	116.01	109.97
35	B	626	HTG	C1'-S1-C1	6.40	112.07	100.09
26	A	415	SQD	O6-C1-C2	6.36	118.23	108.30
23	B	602	CLA	CHD-C4C-C3C	-6.36	115.49	124.84
23	b	602	CLA	O2D-CGD-CBD	6.36	122.56	111.27
23	C	511	CLA	C4A-NA-C1A	6.35	109.56	106.71
23	B	606	CLA	CHD-C4C-C3C	-6.34	115.52	124.84
23	c	911	CLA	CHD-C4C-C3C	-6.33	115.54	124.84
23	b	613	CLA	C2C-C1C-NC	6.31	115.88	109.97
23	B	603	CLA	C4A-NA-C1A	6.29	109.53	106.71
24	a	409	PHO	CMD-C2D-C1D	6.29	134.75	125.06
35	c	922	HTG	C1'-S1-C1	6.27	111.82	100.09
23	b	615	CLA	C4A-NA-C1A	6.27	109.53	106.71
35	b	628	HTG	C1'-S1-C1	6.23	111.75	100.09
23	c	908	CLA	C4A-NA-C1A	6.23	109.51	106.71
23	d	403	CLA	C2C-C1C-NC	6.21	115.79	109.97
23	B	615	CLA	O2D-CGD-O1D	-6.18	111.76	123.84
35	C	522	HTG	C1'-S1-C1	6.15	111.58	100.09
23	C	511	CLA	C2C-C1C-NC	6.13	115.71	109.97
26	A	415	SQD	C1-O5-C5	-6.12	101.68	113.69
23	C	510	CLA	C2C-C1C-NC	6.11	115.69	109.97
23	B	608	CLA	C2C-C1C-NC	6.10	115.68	109.97
23	B	615	CLA	CHD-C4C-C3C	-6.09	115.88	124.84
23	B	613	CLA	CAC-C3C-C4C	6.09	132.71	124.81
23	B	610	CLA	CHD-C4C-C3C	-6.07	115.91	124.84
26	a	412	SQD	C1-O5-C5	-6.07	101.77	113.69
23	b	614	CLA	C2C-C1C-NC	6.07	115.65	109.97
23	B	604	CLA	C1C-C2C-C3C	-6.04	100.60	106.96
23	B	605	CLA	C2C-C1C-NC	6.02	115.62	109.97
23	B	614	CLA	C4A-NA-C1A	6.00	109.41	106.71
23	b	613	CLA	CHD-C4C-C3C	-5.99	116.03	124.84
23	B	604	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
23	C	502	CLA	O2D-CGD-O1D	-5.96	112.19	123.84
23	B	616	CLA	C2C-C1C-NC	5.94	115.54	109.97
23	c	902	CLA	C2C-C1C-NC	5.94	115.54	109.97
23	A	405	CLA	C1D-CHD-C4C	-5.91	114.75	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	621	SQD	O7-S-C6	5.91	113.97	106.94
23	B	604	CLA	O2D-CGD-CBD	5.90	121.75	111.27
23	c	914	CLA	CHD-C4C-C3C	-5.88	116.19	124.84
23	C	507	CLA	CHD-C4C-C3C	-5.87	116.21	124.84
23	a	406	CLA	C1D-CHD-C4C	-5.81	114.89	122.56
23	a	407	CLA	C1C-C2C-C3C	-5.81	100.85	106.96
23	C	512	CLA	C2C-C1C-NC	5.81	115.41	109.97
23	B	613	CLA	C2C-C1C-NC	5.77	115.38	109.97
23	c	903	CLA	CHD-C4C-C3C	-5.76	116.38	124.84
23	B	612	CLA	C2C-C1C-NC	5.75	115.36	109.97
25	b	618	BCR	C7-C8-C9	-5.74	117.56	126.23
23	B	617	CLA	C2C-C1C-NC	5.74	115.34	109.97
26	A	410	SQD	C1-C2-C3	-5.72	98.08	110.00
35	v	204	HTG	O5-C1-C2	-5.72	103.12	110.31
26	A	415	SQD	O9-S-C6	5.71	113.73	106.94
23	B	609	CLA	C2C-C1C-NC	5.70	115.31	109.97
23	a	410	CLA	CAC-C3C-C4C	5.67	132.17	124.81
23	b	605	CLA	C2C-C1C-NC	5.67	115.28	109.97
23	C	503	CLA	C2C-C1C-NC	5.64	115.26	109.97
23	B	610	CLA	C2C-C1C-NC	5.64	115.25	109.97
23	A	408	CLA	C4A-NA-C1A	5.64	109.24	106.71
23	A	405	CLA	CMD-C2D-C3D	5.64	135.22	124.68
30	I	101	LMT	O1B-C4'-C3'	5.63	122.27	107.28
23	b	603	CLA	C2C-C1C-NC	5.63	115.25	109.97
23	b	609	CLA	C2C-C1C-NC	5.63	115.24	109.97
24	A	407	PHO	C3D-C2D-C1D	-5.62	97.68	105.87
23	A	406	CLA	CAC-C3C-C4C	5.60	132.08	124.81
23	C	505	CLA	C1C-C2C-C3C	-5.60	101.07	106.96
35	c	923	HTG	C1'-S1-C1	5.58	108.98	101.40
23	D	401	CLA	C2C-C1C-NC	5.54	115.16	109.97
23	b	617	CLA	C4A-NA-C1A	5.53	109.19	106.71
23	c	908	CLA	CHD-C4C-C3C	-5.53	116.72	124.84
23	c	906	CLA	C2C-C1C-NC	5.52	115.15	109.97
23	D	403	CLA	C3C-C4C-NC	5.52	116.76	110.57
24	a	408	PHO	C3D-C2D-C1D	-5.50	97.85	105.87
23	B	612	CLA	C4A-NA-C1A	5.49	109.18	106.71
23	B	611	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
25	d	405	BCR	C24-C23-C22	-5.48	117.95	126.23
23	c	906	CLA	C4A-NA-C1A	5.48	109.17	106.71
35	D	414	HTG	C1'-S1-C1	5.47	110.31	100.09
23	D	403	CLA	C1C-C2C-C3C	-5.46	101.22	106.96
23	b	609	CLA	CAC-C3C-C4C	5.42	131.84	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	405	CLA	C2C-C1C-NC	5.41	115.04	109.97
26	A	410	SQD	O9-S-C6	5.39	113.34	106.94
23	B	607	CLA	C2C-C1C-NC	5.38	115.01	109.97
23	C	508	CLA	C2C-C1C-NC	5.36	114.99	109.97
36	D	407	DGD	O3G-C1D-C2D	5.36	116.67	108.30
23	b	606	CLA	C2C-C1C-NC	5.36	114.99	109.97
23	B	611	CLA	C2C-C1C-NC	5.35	114.99	109.97
23	c	902	CLA	CHD-C4C-C3C	-5.35	116.98	124.84
23	a	410	CLA	C2C-C1C-NC	5.34	114.97	109.97
23	d	401	CLA	C4A-NA-C1A	5.33	109.10	106.71
23	b	616	CLA	CMD-C2D-C3D	5.33	134.66	124.68
24	D	402	PHO	CMD-C2D-C1D	5.32	133.26	125.06
23	B	607	CLA	CHD-C4C-C3C	-5.31	117.03	124.84
40	v	203	HEC	CBD-CAD-C3D	-5.31	102.69	112.49
35	C	522	HTG	C1-O5-C5	5.31	122.37	112.58
23	C	508	CLA	O2D-CGD-CBD	5.29	120.67	111.27
23	c	912	CLA	CHD-C4C-C3C	-5.28	117.08	124.84
23	b	603	CLA	C4A-NA-C1A	-5.23	104.35	106.71
23	B	615	CLA	C2C-C1C-NC	5.23	114.87	109.97
23	A	406	CLA	C1C-C2C-C3C	-5.23	101.46	106.96
23	C	507	CLA	O2D-CGD-CBD	5.22	120.55	111.27
26	A	410	SQD	O47-C7-C8	5.22	122.75	111.50
37	e	105	HEM	CBA-CAA-C2A	-5.22	102.86	112.49
23	D	403	CLA	CMC-C2C-C1C	5.21	132.97	125.04
23	b	606	CLA	CAC-C3C-C4C	5.20	131.56	124.81
36	D	407	DGD	O2G-C1B-C2B	5.20	122.71	111.50
26	D	408	SQD	C1-O5-C5	-5.20	103.48	113.69
25	c	916	BCR	C24-C23-C22	-5.19	118.39	126.23
24	a	409	PHO	O2D-CGD-CBD	5.18	120.48	111.27
23	C	508	CLA	C1C-C2C-C3C	-5.18	101.51	106.96
23	c	906	CLA	CHD-C4C-C3C	-5.16	117.25	124.84
25	C	530	BCR	C24-C23-C22	-5.15	118.45	126.23
23	b	610	CLA	C2C-C1C-NC	5.12	114.77	109.97
23	B	603	CLA	C2C-C1C-NC	5.11	114.76	109.97
23	c	903	CLA	CMD-C2D-C3D	5.11	134.23	124.68
23	B	617	CLA	CAC-C3C-C4C	5.09	131.41	124.81
23	b	604	CLA	CHD-C4C-C3C	-5.09	117.36	124.84
23	c	907	CLA	CHD-C4C-C3C	-5.08	117.37	124.84
23	b	616	CLA	C2C-C1C-NC	5.07	114.72	109.97
23	A	408	CLA	C2C-C1C-NC	5.06	114.72	109.97
23	c	913	CLA	CHD-C4C-C3C	-5.06	117.40	124.84
24	a	408	PHO	CMD-C2D-C1D	5.04	132.83	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	502	CLA	CHD-C4C-C3C	-5.04	117.43	124.84
36	d	407	DGD	O2G-C1B-C2B	5.03	122.33	111.50
23	b	614	CLA	CHD-C4C-C3C	-5.03	117.45	124.84
23	b	613	CLA	C3C-C4C-NC	5.02	116.20	110.57
23	b	608	CLA	C2C-C1C-NC	5.02	114.67	109.97
25	C	515	BCR	C38-C26-C25	-5.01	118.90	124.53
23	D	403	CLA	CHD-C4C-C3C	-5.01	117.48	124.84
23	a	410	CLA	O2D-CGD-CBD	5.00	120.15	111.27
23	C	502	CLA	C2C-C1C-NC	5.00	114.65	109.97
26	L	102	SQD	O47-C7-C8	4.99	122.26	111.50
23	a	406	CLA	CHD-C4C-C3C	-4.99	117.51	124.84
23	a	410	CLA	CHD-C4C-C3C	-4.98	117.52	124.84
23	D	401	CLA	CAC-C3C-C4C	4.98	131.27	124.81
23	b	603	CLA	CMB-C2B-C3B	4.98	133.99	124.68
23	B	606	CLA	C2C-C1C-NC	4.98	114.64	109.97
23	B	617	CLA	CHD-C4C-C3C	-4.98	117.52	124.84
23	B	612	CLA	CAC-C3C-C4C	4.97	131.26	124.81
23	C	506	CLA	C1C-C2C-C3C	-4.96	101.74	106.96
28	E	101	LHG	O7-C7-C8	4.95	122.18	111.50
23	B	614	CLA	C2C-C1C-NC	4.95	114.61	109.97
23	B	602	CLA	CHD-C4C-NC	4.93	131.97	124.20
23	a	406	CLA	C4A-NA-C1A	4.92	108.92	106.71
23	a	410	CLA	CMD-C2D-C3D	4.91	133.87	124.68
23	b	604	CLA	C1C-C2C-C3C	-4.90	101.80	106.96
23	c	913	CLA	C2C-C1C-NC	4.88	114.55	109.97
23	b	614	CLA	C1-C2-C3	-4.88	117.60	126.04
23	b	607	CLA	CHD-C4C-C3C	-4.87	117.68	124.84
23	d	404	CLA	C1C-C2C-C3C	-4.87	101.84	106.96
24	D	402	PHO	C3D-C2D-C1D	-4.87	98.78	105.87
23	b	606	CLA	C4-C3-C5	4.86	123.45	115.27
23	c	913	CLA	O2D-CGD-CBD	4.86	119.91	111.27
26	A	410	SQD	O6-C1-C2	4.85	115.88	108.30
26	a	412	SQD	O47-C7-C8	4.85	121.94	111.50
24	A	407	PHO	C2D-C1D-ND	4.84	117.10	109.79
23	d	404	CLA	CHD-C4C-C3C	-4.84	117.73	124.84
23	B	615	CLA	CHD-C4C-NC	4.83	131.81	124.20
23	C	504	CLA	C4A-NA-C1A	4.83	108.88	106.71
26	D	408	SQD	C1-C2-C3	-4.83	99.94	110.00
23	c	910	CLA	C2C-C1C-NC	4.82	114.48	109.97
23	C	507	CLA	C2C-C1C-NC	4.82	114.48	109.97
28	a	415	LHG	O7-C7-C8	4.81	121.86	111.50
23	b	602	CLA	CHD-C4C-C3C	-4.80	117.78	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	405	CLA	CAC-C3C-C4C	4.80	131.04	124.81
27	D	406	PL9	C40-C39-C41	4.80	123.35	115.27
23	C	504	CLA	CHD-C4C-C3C	-4.80	117.78	124.84
24	A	407	PHO	C2C-C1C-NC	4.80	117.03	109.79
23	b	616	CLA	CHD-C4C-C3C	-4.80	117.79	124.84
23	B	608	CLA	C1C-C2C-C3C	-4.77	101.94	106.96
26	L	102	SQD	O7-S-C6	4.77	112.61	106.94
23	B	606	CLA	CAC-C3C-C4C	4.76	130.99	124.81
23	A	408	CLA	C4-C3-C5	4.75	123.25	115.27
23	C	506	CLA	CHD-C4C-C3C	-4.75	117.86	124.84
23	c	902	CLA	C1C-C2C-C3C	-4.74	101.97	106.96
35	b	627	HTG	C1'-S1-C1	4.74	108.96	100.09
23	c	907	CLA	C4A-NA-C1A	4.74	108.83	106.71
34	d	411	LMG	O7-C10-C11	4.73	121.69	111.50
23	b	602	CLA	C2C-C1C-NC	4.72	114.40	109.97
23	C	511	CLA	CHD-C4C-NC	4.72	131.64	124.20
34	c	930	LMG	O7-C10-C11	4.72	121.68	111.50
23	c	907	CLA	C2C-C1C-NC	4.72	114.39	109.97
23	b	616	CLA	C1D-CHD-C4C	-4.72	116.33	122.56
23	a	406	CLA	C2C-C1C-NC	4.72	114.39	109.97
23	c	912	CLA	C2C-C1C-NC	4.71	114.39	109.97
26	B	621	SQD	O6-C1-C2	4.71	115.66	108.30
26	a	412	SQD	C1-C2-C3	-4.71	100.18	110.00
23	C	510	CLA	C1C-C2C-C3C	-4.71	102.01	106.96
23	B	612	CLA	CHD-C4C-C3C	-4.71	117.92	124.84
23	b	615	CLA	O2D-CGD-CBD	4.70	119.61	111.27
25	T	101	BCR	C38-C26-C25	-4.69	119.26	124.53
23	b	603	CLA	CMD-C2D-C3D	4.69	133.45	124.68
27	A	411	PL9	C53-C6-C1	4.69	124.57	114.99
40	v	203	HEC	CMB-C2B-C1B	-4.69	121.26	128.46
23	c	907	CLA	O2D-CGD-CBD	4.68	119.59	111.27
23	c	908	CLA	O2D-CGD-CBD	4.67	119.57	111.27
23	B	612	CLA	C1-C2-C3	-4.67	117.96	126.04
23	b	617	CLA	CHD-C4C-C3C	-4.66	117.98	124.84
23	b	604	CLA	O2D-CGD-O1D	-4.66	114.72	123.84
23	b	605	CLA	CMD-C2D-C3D	4.66	133.39	124.68
35	B	630	HTG	C1'-S1-C1	4.66	108.80	100.09
23	b	607	CLA	C2C-C1C-NC	4.65	114.33	109.97
35	c	921	HTG	C1'-S1-C1	4.65	108.79	100.09
36	D	407	DGD	C4D-C3D-C2D	4.65	118.94	110.82
23	c	905	CLA	CAC-C3C-C4C	4.65	130.84	124.81
23	b	613	CLA	CAC-C3C-C4C	4.64	130.83	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	405	BCR	C24-C23-C22	-4.64	119.23	126.23
23	c	911	CLA	C2C-C1C-NC	4.63	114.31	109.97
23	b	602	CLA	C1-O2A-CGA	4.63	128.60	116.44
23	c	904	CLA	CHD-C4C-C3C	-4.62	118.04	124.84
36	D	407	DGD	O1G-C1A-C2A	4.62	126.40	111.91
23	b	614	CLA	C1C-C2C-C3C	-4.62	102.10	106.96
25	B	618	BCR	C15-C14-C13	-4.60	120.74	127.31
23	B	610	CLA	CMD-C2D-C3D	4.59	133.26	124.68
23	b	611	CLA	C2C-C1C-NC	4.58	114.27	109.97
23	D	401	CLA	CHD-C4C-C3C	-4.58	118.11	124.84
23	B	607	CLA	C1C-C2C-C3C	-4.58	102.14	106.96
36	H	103	DGD	O1G-C1A-O1A	-4.58	112.04	123.59
23	C	503	CLA	C4A-NA-C1A	4.58	108.76	106.71
23	C	512	CLA	C1C-C2C-C3C	-4.57	102.16	106.96
25	B	620	BCR	C38-C26-C25	-4.56	119.40	124.53
23	c	904	CLA	C2C-C1C-NC	4.56	114.25	109.97
23	c	912	CLA	O2D-CGD-O1D	-4.56	114.93	123.84
23	B	608	CLA	CMB-C2B-C3B	4.56	133.21	124.68
23	c	907	CLA	C1C-C2C-C3C	-4.55	102.17	106.96
23	b	609	CLA	CMD-C2D-C3D	4.55	133.18	124.68
23	B	610	CLA	C3C-C4C-NC	4.54	115.66	110.57
23	b	616	CLA	C1C-C2C-C3C	-4.54	102.19	106.96
23	C	513	CLA	CMD-C2D-C3D	4.53	133.16	124.68
23	b	604	CLA	O2D-CGD-CBD	4.53	119.32	111.27
23	d	403	CLA	CHD-C4C-C3C	-4.53	118.18	124.84
23	d	401	CLA	C1C-C2C-C3C	-4.52	102.20	106.96
36	C	517	DGD	O3G-C3G-C2G	-4.52	99.98	110.90
23	C	514	CLA	C1C-C2C-C3C	-4.52	102.21	106.96
25	C	516	BCR	C7-C8-C9	-4.51	119.41	126.23
23	b	605	CLA	C1C-C2C-C3C	-4.51	102.22	106.96
23	b	606	CLA	CMD-C2D-C3D	4.50	133.10	124.68
24	a	409	PHO	C1-C2-C3	-4.50	118.26	126.04
23	b	610	CLA	CHD-C4C-C3C	-4.50	118.22	124.84
23	b	612	CLA	C2C-C1C-NC	4.50	114.19	109.97
23	d	403	CLA	O2D-CGD-O1D	-4.50	115.04	123.84
23	c	910	CLA	CAC-C3C-C4C	4.49	130.63	124.81
23	B	603	CLA	C1C-C2C-C3C	-4.49	102.24	106.96
23	B	608	CLA	C4A-NA-C1A	4.49	108.72	106.71
23	C	503	CLA	O2D-CGD-CBD	4.48	119.22	111.27
25	D	405	BCR	C40-C30-C25	-4.48	103.04	110.30
40	V	203	HEC	CBD-CAD-C3D	-4.47	104.23	112.49
34	C	531	LMG	O7-C10-C11	4.47	121.14	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	504	CLA	C1C-C2C-C3C	-4.47	102.26	106.96
23	a	407	CLA	CAC-C3C-C4C	4.46	130.60	124.81
23	a	406	CLA	C1C-C2C-C3C	-4.46	102.27	106.96
23	b	603	CLA	C1C-C2C-C3C	-4.46	102.27	106.96
23	B	613	CLA	C1C-C2C-C3C	-4.45	102.28	106.96
23	b	607	CLA	C1-C2-C3	-4.44	118.36	126.04
37	e	105	HEM	CBD-CAD-C3D	-4.44	104.30	112.48
24	a	408	PHO	C2C-C1C-NC	4.44	116.49	109.79
23	C	514	CLA	C2C-C1C-NC	4.44	114.13	109.97
23	C	505	CLA	O2D-CGD-CBD	4.44	119.15	111.27
35	V	204	HTG	C1-C2-C3	-4.43	101.84	110.59
25	Y	101	BCR	C33-C5-C6	-4.42	119.56	124.53
23	C	510	CLA	O2D-CGD-CBD	4.42	119.12	111.27
26	A	410	SQD	C1-O5-C5	-4.41	105.03	113.69
23	C	513	CLA	CHD-C4C-C3C	-4.41	118.36	124.84
26	a	417	SQD	C1-O5-C5	-4.40	105.05	113.69
35	v	204	HTG	O5-C1-S1	4.39	120.33	109.82
23	b	605	CLA	CHD-C4C-C3C	-4.39	118.39	124.84
30	F	101	LMT	C1B-O5B-C5B	4.39	122.30	113.69
35	B	624	HTG	C1'-S1-C1	4.39	108.29	100.09
23	D	403	CLA	O2D-CGD-O1D	-4.38	115.28	123.84
23	d	404	CLA	C3B-C4B-NB	4.37	114.87	109.21
24	D	402	PHO	C1-C2-C3	-4.37	118.48	126.04
23	B	611	CLA	C1D-CHD-C4C	-4.37	116.79	122.56
23	A	408	CLA	O2D-CGD-CBD	4.36	119.02	111.27
23	D	401	CLA	C1C-C2C-C3C	-4.36	102.37	106.96
23	b	613	CLA	C4A-NA-C1A	4.36	108.67	106.71
23	B	609	CLA	C1C-C2C-C3C	-4.36	102.38	106.96
23	B	611	CLA	O2D-CGD-CBD	4.34	118.97	111.27
26	D	408	SQD	O47-C7-C8	4.34	120.84	111.50
23	c	903	CLA	C2C-C1C-NC	4.32	114.02	109.97
36	c	918	DGD	O2G-C1B-C2B	4.32	120.80	111.50
24	a	408	PHO	C2D-C1D-ND	4.31	116.30	109.79
23	C	503	CLA	CHD-C4C-C3C	-4.31	118.50	124.84
23	c	912	CLA	C1C-C2C-C3C	-4.30	102.44	106.96
23	b	616	CLA	O2D-CGD-O1D	-4.30	115.44	123.84
23	B	603	CLA	C4D-C3D-CAD	4.30	110.87	108.47
23	b	607	CLA	O2D-CGD-CBD	4.30	118.90	111.27
23	B	611	CLA	O2D-CGD-O1D	-4.30	115.44	123.84
34	m	102	LMG	C9-C8-C7	-4.29	101.64	111.79
28	A	412	LHG	O7-C7-C8	4.29	120.74	111.50
28	K	101	LHG	O7-C7-C8	4.29	120.74	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	913	CLA	C1C-C2C-C3C	-4.28	102.45	106.96
23	b	608	CLA	CHD-C4C-C3C	-4.27	118.56	124.84
23	B	615	CLA	CHB-C4A-NA	4.27	130.42	124.51
23	b	602	CLA	C1C-C2C-C3C	-4.26	102.47	106.96
23	b	612	CLA	CHD-C4C-C3C	-4.26	118.58	124.84
23	B	614	CLA	CHD-C4C-C3C	-4.25	118.59	124.84
23	B	602	CLA	C1C-C2C-C3C	-4.25	102.49	106.96
24	a	409	PHO	C2B-C1B-NB	4.25	116.20	109.79
27	d	406	PL9	O1-C4-C3	-4.25	116.04	120.72
23	a	407	CLA	C3C-C4C-NC	4.23	115.32	110.57
28	D	409	LHG	O8-C23-O10	-4.23	112.91	123.59
38	H	102	RRX	C24-C23-C22	-4.23	119.85	126.23
23	B	607	CLA	O2D-CGD-O1D	-4.22	115.59	123.84
23	b	602	CLA	C4D-C3D-CAD	4.22	110.82	108.47
23	c	914	CLA	O2D-CGD-CBD	4.21	118.75	111.27
24	a	409	PHO	C3D-C2D-C1D	-4.21	99.74	105.87
23	A	408	CLA	CHD-C4C-C3C	-4.21	118.65	124.84
23	B	616	CLA	C1C-C2C-C3C	-4.21	102.53	106.96
23	B	616	CLA	CHD-C4C-C3C	-4.20	118.66	124.84
23	c	910	CLA	CHD-C4C-C3C	-4.20	118.66	124.84
26	L	102	SQD	C3-C4-C5	4.19	117.72	110.24
26	a	417	SQD	O47-C7-C8	4.19	120.53	111.50
23	c	908	CLA	C1C-C2C-C3C	-4.19	102.55	106.96
23	B	608	CLA	CHD-C4C-C3C	-4.18	118.69	124.84
23	C	503	CLA	C1C-C2C-C3C	-4.17	102.57	106.96
28	D	409	LHG	O8-C23-C24	4.17	124.99	111.91
23	a	407	CLA	O2D-CGD-CBD	4.16	118.66	111.27
23	c	905	CLA	C2C-C1C-NC	4.16	113.86	109.97
38	x	102	RRX	C33-C5-C6	-4.15	119.87	124.53
23	b	607	CLA	C1C-C2C-C3C	-4.15	102.59	106.96
23	c	908	CLA	C2C-C1C-NC	4.15	113.86	109.97
23	b	609	CLA	CHD-C4C-C3C	-4.15	118.74	124.84
23	a	406	CLA	C4-C3-C5	4.15	122.24	115.27
30	T	103	LMT	C1'-C2'-C3'	4.14	118.63	110.00
23	b	608	CLA	CAC-C3C-C4C	4.14	130.19	124.81
23	c	902	CLA	O2D-CGD-O1D	-4.13	115.76	123.84
23	D	404	CLA	C2C-C1C-NC	4.13	113.84	109.97
35	B	625	HTG	C1'-S1-C1	4.13	107.81	100.09
26	A	410	SQD	O3-C3-C4	4.13	119.89	110.35
25	B	618	BCR	C7-C8-C9	-4.13	120.00	126.23
27	d	406	PL9	C40-C39-C41	4.12	122.21	115.27
23	b	607	CLA	C4A-NA-C1A	4.12	108.56	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	415	SQD	C1-C2-C3	-4.12	101.42	110.00
23	B	605	CLA	O2D-CGD-O1D	-4.12	115.79	123.84
23	d	403	CLA	C4-C3-C5	4.12	122.20	115.27
23	b	609	CLA	C1C-C2C-C3C	-4.11	102.64	106.96
23	c	911	CLA	O2D-CGD-CBD	4.11	118.57	111.27
23	c	910	CLA	C3B-C4B-NB	4.11	114.52	109.21
23	B	602	CLA	C2C-C1C-NC	4.11	113.82	109.97
23	c	911	CLA	C1C-C2C-C3C	-4.10	102.64	106.96
27	a	414	PL9	C53-C6-C1	4.10	123.37	114.99
28	d	408	LHG	O8-C23-O10	-4.10	113.25	123.59
23	c	911	CLA	C1D-CHD-C4C	-4.10	117.15	122.56
34	m	102	LMG	O7-C10-C11	4.09	120.32	111.50
23	C	504	CLA	C2C-C1C-NC	4.09	113.80	109.97
24	a	409	PHO	C2D-C1D-ND	4.09	115.96	109.79
23	C	513	CLA	C1-O2A-CGA	4.08	127.15	116.44
23	d	403	CLA	C1C-C2C-C3C	-4.08	102.67	106.96
23	b	615	CLA	O2D-CGD-O1D	-4.07	115.88	123.84
23	B	606	CLA	C3C-C4C-NC	4.07	115.14	110.57
23	C	514	CLA	O2D-CGD-O1D	-4.07	115.88	123.84
23	C	509	CLA	C1C-C2C-C3C	-4.07	102.68	106.96
24	D	402	PHO	C2D-C1D-ND	4.06	115.92	109.79
27	A	411	PL9	C30-C29-C31	4.06	122.11	115.27
23	a	407	CLA	CHD-C4C-C3C	-4.06	118.87	124.84
23	C	505	CLA	CHD-C4C-C3C	-4.06	118.87	124.84
23	c	906	CLA	CBC-CAC-C3C	-4.06	101.25	112.43
24	A	407	PHO	C4D-ND-C1D	-4.05	99.47	106.76
23	d	401	CLA	CHD-C4C-C3C	-4.05	118.88	124.84
23	b	604	CLA	CAC-C3C-C4C	4.05	130.06	124.81
25	b	619	BCR	C29-C30-C25	4.05	116.71	110.48
23	B	610	CLA	CAC-C3C-C4C	4.05	130.06	124.81
24	A	407	PHO	O2D-CGD-CBD	4.04	118.45	111.27
28	d	408	LHG	O8-C23-C24	4.04	124.58	111.91
23	C	509	CLA	C2C-C1C-NC	4.04	113.75	109.97
23	a	406	CLA	CAC-C3C-C4C	4.03	130.04	124.81
23	B	602	CLA	CMC-C2C-C1C	4.03	131.17	125.04
23	b	604	CLA	C4A-NA-C1A	4.02	108.52	106.71
23	c	903	CLA	C1D-CHD-C4C	-4.02	117.25	122.56
24	A	407	PHO	C1C-C2C-C3C	-4.02	101.89	106.51
25	A	409	BCR	C38-C26-C25	-4.01	120.02	124.53
25	D	405	BCR	C38-C26-C25	-4.01	120.03	124.53
23	B	609	CLA	CHD-C4C-C3C	-4.01	118.95	124.84
23	b	602	CLA	C1D-CHD-C4C	-4.01	117.27	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	405	CLA	C3C-C4C-NC	4.00	115.06	110.57
23	C	508	CLA	CHD-C4C-C3C	-4.00	118.96	124.84
23	b	607	CLA	C1-O2A-CGA	4.00	126.94	116.44
40	v	203	HEC	C1D-C2D-C3D	-4.00	104.21	107.00
34	C	520	LMG	O7-C10-C11	4.00	120.11	111.50
24	D	402	PHO	CAC-C3C-C4C	3.99	129.58	125.22
23	b	611	CLA	C1C-C2C-C3C	-3.99	102.76	106.96
27	d	406	PL9	C7-C8-C9	-3.98	120.16	126.79
35	B	625	HTG	C1-C2-C3	3.98	118.45	110.59
23	c	909	CLA	CMD-C2D-C3D	3.97	132.11	124.68
23	c	914	CLA	CMD-C2D-C3D	3.97	132.10	124.68
35	V	204	HTG	C1-O5-C5	-3.97	105.27	112.58
23	b	606	CLA	CMC-C2C-C1C	3.96	131.08	125.04
23	c	911	CLA	CMD-C2D-C3D	3.96	132.09	124.68
23	A	405	CLA	C4-C3-C5	3.96	121.93	115.27
30	a	418	LMT	C1-O1'-C1'	3.96	120.41	113.84
23	c	906	CLA	C1C-C2C-C3C	-3.96	102.80	106.96
23	B	615	CLA	O2D-CGD-CBD	3.96	118.30	111.27
23	c	910	CLA	C1C-C2C-C3C	-3.95	102.81	106.96
23	B	617	CLA	CMD-C2D-C3D	3.94	132.05	124.68
23	A	406	CLA	CHD-C4C-C3C	-3.94	119.05	124.84
23	c	903	CLA	O2D-CGD-CBD	3.94	118.27	111.27
23	B	615	CLA	CAC-C3C-C4C	3.94	129.92	124.81
23	b	617	CLA	CMB-C2B-C3B	3.93	132.03	124.68
23	b	606	CLA	CHD-C4C-NC	3.93	130.39	124.20
23	B	614	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
23	C	502	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
23	b	608	CLA	O2D-CGD-CBD	3.92	118.24	111.27
30	b	621	LMT	O5'-C5'-C4'	3.92	118.02	109.75
23	B	608	CLA	CED-O2D-CGD	3.92	124.79	115.94
23	B	609	CLA	C4D-C3D-CAD	3.91	110.65	108.47
23	C	513	CLA	O2D-CGD-CBD	3.91	118.21	111.27
38	H	102	RRX	C38-C26-C25	-3.90	120.15	124.53
23	D	403	CLA	CAC-C3C-C4C	3.90	129.86	124.81
28	D	411	LHG	O4-P-O5	3.89	131.47	112.24
23	C	509	CLA	CAC-C3C-C4C	3.89	129.86	124.81
23	c	905	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
25	A	409	BCR	C7-C8-C9	-3.87	120.38	126.23
23	a	406	CLA	O2D-CGD-O1D	-3.87	116.27	123.84
26	L	102	SQD	O6-C1-C2	3.87	114.35	108.30
23	b	603	CLA	C1D-CHD-C4C	-3.87	117.45	122.56
25	b	618	BCR	C33-C5-C6	-3.87	120.18	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	412	SQD	O5-C1-C2	-3.87	102.17	110.35
23	b	608	CLA	C1C-C2C-C3C	-3.86	102.89	106.96
27	a	414	PL9	C37-C38-C39	-3.86	118.36	127.66
23	C	507	CLA	CMD-C2D-C3D	3.86	131.90	124.68
36	C	518	DGD	O2G-C1B-C2B	3.86	119.82	111.50
23	b	608	CLA	C4-C3-C5	3.86	121.76	115.27
23	b	617	CLA	O2D-CGD-CBD	3.86	118.12	111.27
24	a	409	PHO	C4C-C3C-C2C	-3.86	102.52	106.78
23	C	510	CLA	C1-C2-C3	-3.85	119.38	126.04
23	B	617	CLA	O2D-CGD-CBD	3.85	118.11	111.27
25	b	618	BCR	C24-C23-C22	-3.85	120.42	126.23
35	B	631	HTG	C1'-S1-C1	3.84	107.28	100.09
23	C	506	CLA	CAC-C3C-C4C	3.84	129.79	124.81
28	e	101	LHG	O7-C7-C8	3.84	119.78	111.50
23	B	609	CLA	O2D-CGD-CBD	3.84	118.09	111.27
23	c	905	CLA	C4-C3-C5	3.84	121.73	115.27
23	b	614	CLA	CAC-C3C-C4C	3.84	129.79	124.81
23	B	612	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
23	b	609	CLA	O2D-CGD-CBD	3.84	118.08	111.27
23	b	602	CLA	O2D-CGD-O1D	-3.83	116.35	123.84
23	b	604	CLA	C4-C3-C5	3.83	121.72	115.27
23	D	401	CLA	C1D-CHD-C4C	-3.83	117.51	122.56
27	A	411	PL9	C7-C3-C4	3.83	119.99	116.88
23	B	606	CLA	C4-C3-C5	3.83	121.71	115.27
23	C	510	CLA	CHD-C4C-C3C	-3.82	119.23	124.84
35	V	204	HTG	O5-C1-S1	3.82	118.95	109.82
23	D	404	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
23	B	603	CLA	CMD-C2D-C3D	3.81	131.81	124.68
23	c	914	CLA	C2C-C1C-NC	3.81	113.54	109.97
23	B	603	CLA	CHD-C4C-C3C	-3.81	119.24	124.84
23	B	604	CLA	C3B-C4B-NB	3.81	114.13	109.21
26	B	621	SQD	O47-C7-C8	3.81	119.70	111.50
36	c	917	DGD	O5D-C6D-C5D	-3.80	102.01	109.05
23	B	604	CLA	CHC-C1C-NC	-3.80	118.43	124.20
23	B	611	CLA	CAA-CBA-CGA	-3.80	102.15	113.25
25	t	101	BCR	C28-C27-C26	-3.80	107.30	114.08
23	C	508	CLA	C4-C3-C5	3.80	121.66	115.27
23	c	908	CLA	CHD-C4C-NC	3.80	130.18	124.20
24	D	402	PHO	C2B-C1B-NB	3.79	115.51	109.79
23	c	909	CLA	C2A-C1A-CHA	-3.79	117.23	123.86
23	C	514	CLA	CMD-C2D-C3D	3.79	131.77	124.68
23	B	603	CLA	O2D-CGD-CBD	3.79	118.00	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	603	CLA	O2D-CGD-O1D	-3.79	116.43	123.84
23	c	904	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
23	a	406	CLA	CMD-C2D-C3D	3.78	131.75	124.68
23	c	913	CLA	CHD-C4C-NC	3.78	130.16	124.20
34	D	412	LMG	O7-C10-C11	3.78	119.64	111.50
34	C	520	LMG	O8-C28-C29	3.78	123.75	111.91
35	B	625	HTG	C1-O5-C5	3.77	119.54	112.58
23	A	405	CLA	C3B-C4B-NB	3.77	114.08	109.21
23	B	605	CLA	O2D-CGD-CBD	3.76	117.96	111.27
23	B	607	CLA	O2D-CGD-CBD	3.76	117.95	111.27
23	D	401	CLA	O2D-CGD-CBD	3.76	117.94	111.27
23	C	512	CLA	CMD-C2D-C3D	3.76	131.71	124.68
23	B	605	CLA	CHD-C4C-C3C	-3.76	119.32	124.84
23	b	610	CLA	CAC-C3C-C4C	3.75	129.68	124.81
23	c	909	CLA	CHD-C4C-C3C	-3.75	119.32	124.84
26	B	621	SQD	C1-O5-C5	-3.75	106.33	113.69
23	B	603	CLA	CMB-C2B-C3B	3.75	131.69	124.68
23	A	406	CLA	C3B-C4B-NB	3.74	114.05	109.21
23	c	912	CLA	CHD-C4C-NC	3.74	130.10	124.20
23	b	610	CLA	C1C-C2C-C3C	-3.74	103.03	106.96
23	c	910	CLA	CMD-C2D-C3D	3.73	131.66	124.68
23	b	617	CLA	O2D-CGD-O1D	-3.73	116.55	123.84
26	L	102	SQD	O9-S-C6	3.72	111.36	106.94
36	D	407	DGD	C3D-C4D-C5D	3.72	115.56	109.77
24	a	409	PHO	O2D-CGD-O1D	-3.72	116.57	123.84
23	C	508	CLA	O2D-CGD-O1D	-3.72	116.57	123.84
23	B	604	CLA	C3C-C4C-NC	3.72	114.74	110.57
23	b	603	CLA	CHD-C4C-C3C	-3.71	119.38	124.84
23	B	605	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
23	c	911	CLA	C4D-C3D-CAD	3.71	110.54	108.47
23	c	910	CLA	O2D-CGD-CBD	3.71	117.86	111.27
25	B	619	BCR	C29-C30-C25	3.71	116.19	110.48
23	A	408	CLA	CHB-C4A-NA	3.71	129.64	124.51
23	b	603	CLA	C1-C2-C3	-3.71	119.63	126.04
23	B	610	CLA	O2D-CGD-CBD	3.70	117.85	111.27
25	d	405	BCR	C38-C26-C25	-3.70	120.37	124.53
23	d	404	CLA	CHD-C4C-NC	3.70	130.03	124.20
23	a	406	CLA	C2A-C1A-CHA	-3.70	117.40	123.86
25	a	411	BCR	C38-C26-C25	-3.69	120.38	124.53
23	c	903	CLA	CHD-C4C-NC	3.69	130.02	124.20
34	c	920	LMG	O8-C28-C29	3.69	123.48	111.91
28	d	402	LHG	O7-C7-C8	3.69	119.45	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	609	CLA	CMB-C2B-C3B	3.69	131.58	124.68
23	B	610	CLA	C2A-C1A-CHA	-3.68	117.42	123.86
30	m	104	LMT	C1'-O5'-C5'	-3.68	106.46	113.69
23	b	607	CLA	O2D-CGD-O1D	-3.68	116.64	123.84
34	B	622	LMG	O7-C10-C11	3.68	119.43	111.50
23	c	911	CLA	CHD-C4C-NC	3.67	129.99	124.20
23	C	509	CLA	C4-C3-C5	3.66	121.43	115.27
23	b	603	CLA	C4D-C3D-CAD	3.66	110.51	108.47
23	C	509	CLA	CHD-C4C-C3C	-3.66	119.46	124.84
24	a	408	PHO	C1C-C2C-C3C	-3.66	102.31	106.51
24	A	407	PHO	C3C-C4C-NC	3.66	115.95	110.28
25	Y	101	BCR	C38-C26-C25	-3.65	120.42	124.53
23	C	513	CLA	CED-O2D-CGD	3.65	124.20	115.94
23	c	905	CLA	CHD-C4C-C3C	-3.65	119.47	124.84
34	c	930	LMG	O1-C1-C2	3.65	114.00	108.30
23	b	609	CLA	O2D-CGD-O1D	-3.65	116.70	123.84
23	A	408	CLA	CAC-C3C-C4C	3.65	129.54	124.81
23	b	606	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
23	c	909	CLA	C1C-C2C-C3C	-3.64	103.12	106.96
30	F	101	LMT	C2'-C3'-C4'	3.64	118.00	109.68
23	D	404	CLA	CAC-C3C-C4C	3.64	129.53	124.81
23	C	509	CLA	O2D-CGD-O1D	-3.64	116.73	123.84
23	B	610	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
26	D	408	SQD	C3-C4-C5	3.63	116.72	110.24
23	b	616	CLA	C4A-NA-C1A	3.63	108.34	106.71
26	A	415	SQD	O47-C7-C8	3.63	119.32	111.50
23	A	406	CLA	O2D-CGD-CBD	3.62	117.71	111.27
23	c	905	CLA	C3B-C4B-NB	3.62	113.89	109.21
23	b	602	CLA	O2A-CGA-CBA	3.62	123.28	111.91
23	c	913	CLA	O2D-CGD-O1D	-3.62	116.76	123.84
23	b	605	CLA	CAC-C3C-C4C	3.62	129.51	124.81
34	c	920	LMG	C8-O7-C10	-3.62	108.88	117.79
23	c	902	CLA	CHD-C4C-NC	3.62	129.90	124.20
23	b	605	CLA	O2D-CGD-CBD	3.62	117.70	111.27
23	b	616	CLA	C2A-C1A-CHA	-3.62	117.54	123.86
25	b	620	BCR	C24-C23-C22	-3.61	120.78	126.23
36	h	102	DGD	O2G-C1B-C2B	3.61	119.28	111.50
23	c	914	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
23	b	609	CLA	C1D-CHD-C4C	-3.61	117.80	122.56
23	C	504	CLA	CMC-C2C-C1C	3.60	130.53	125.04
23	b	617	CLA	O1D-CGD-CBD	-3.60	117.11	124.48
23	C	511	CLA	O2D-CGD-CBD	3.60	117.67	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	613	CLA	O2D-CGD-O1D	-3.60	116.80	123.84
24	a	408	PHO	C4C-C3C-C2C	-3.60	102.80	106.78
23	c	910	CLA	CMC-C2C-C1C	3.59	130.51	125.04
23	c	903	CLA	OBD-CAD-C3D	-3.59	122.02	127.98
34	D	412	LMG	O1-C1-C2	3.59	113.91	108.30
23	b	608	CLA	CMD-C2D-C3D	3.59	131.40	124.68
25	c	915	BCR	C7-C8-C9	-3.58	120.82	126.23
23	b	603	CLA	O2D-CGD-CBD	3.58	117.63	111.27
23	b	617	CLA	CAC-C3C-C4C	3.58	129.45	124.81
23	b	604	CLA	CMC-C2C-C1C	3.57	130.48	125.04
23	a	406	CLA	CHC-C1C-C2C	-3.57	116.85	126.72
24	D	402	PHO	C4C-C3C-C2C	-3.57	102.83	106.78
23	B	611	CLA	C4C-C3C-C2C	-3.57	101.70	106.90
23	b	603	CLA	C4-C3-C5	3.57	121.27	115.27
27	d	406	PL9	C15-C14-C16	3.56	121.27	115.27
23	B	608	CLA	CBC-CAC-C3C	-3.56	102.61	112.43
23	c	913	CLA	C1-C2-C3	-3.56	119.88	126.04
23	b	605	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
23	b	613	CLA	C1C-C2C-C3C	-3.56	103.22	106.96
23	D	403	CLA	C1D-CHD-C4C	-3.56	117.86	122.56
23	C	507	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
23	c	914	CLA	CMB-C2B-C3B	3.55	131.32	124.68
23	C	513	CLA	C2C-C1C-NC	3.55	113.30	109.97
23	b	617	CLA	C3B-C4B-NB	3.54	113.79	109.21
23	a	410	CLA	C4-C3-C5	3.54	121.23	115.27
23	c	904	CLA	C4-C3-C5	3.54	121.22	115.27
24	D	402	PHO	C4D-ND-C1D	-3.53	100.41	106.76
23	B	602	CLA	C1-O2A-CGA	3.53	125.72	116.44
25	d	405	BCR	C39-C30-C25	-3.53	104.57	110.30
23	b	615	CLA	C1C-C2C-C3C	-3.53	103.24	106.96
23	B	608	CLA	CMD-C2D-C3D	3.53	131.29	124.68
26	x	101	SQD	O48-C23-C24	3.53	122.97	111.91
36	H	103	DGD	O2G-C1B-C2B	3.52	119.10	111.50
23	D	401	CLA	C4-C3-C5	3.52	121.20	115.27
35	d	413	HTG	O5-C1-C2	3.52	114.75	110.31
23	b	603	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
23	A	408	CLA	O2D-CGD-O1D	-3.52	116.95	123.84
23	c	902	CLA	O2D-CGD-CBD	3.52	117.52	111.27
25	T	101	BCR	C15-C16-C17	-3.52	116.27	123.47
26	x	101	SQD	C1-O5-C5	3.52	120.59	113.69
26	L	102	SQD	O48-C23-C24	3.51	122.93	111.91
23	b	615	CLA	O2A-CGA-O1A	-3.51	114.73	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	609	CLA	C3B-C4B-NB	3.51	113.74	109.21
23	C	506	CLA	CMC-C2C-C1C	3.51	130.38	125.04
23	B	605	CLA	C3C-C4C-NC	3.50	114.50	110.57
25	b	618	BCR	C15-C16-C17	-3.50	116.30	123.47
26	A	415	SQD	O48-C23-C24	3.50	122.89	111.91
34	a	413	LMG	O8-C28-C29	3.50	122.89	111.91
23	B	609	CLA	O2D-CGD-O1D	-3.50	117.00	123.84
23	B	613	CLA	O2D-CGD-CBD	3.48	117.46	111.27
23	B	610	CLA	C1-C2-C3	-3.48	120.02	126.04
23	B	617	CLA	O2D-CGD-O1D	-3.48	117.04	123.84
23	d	403	CLA	C3B-C4B-NB	3.48	113.71	109.21
23	b	606	CLA	O2D-CGD-CBD	3.48	117.45	111.27
23	C	506	CLA	O2D-CGD-CBD	3.48	117.44	111.27
23	b	604	CLA	C3C-C4C-NC	3.47	114.47	110.57
23	c	911	CLA	C3C-C4C-NC	3.47	114.47	110.57
23	b	612	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
23	b	603	CLA	CHC-C1C-NC	-3.47	118.94	124.20
23	B	614	CLA	C3B-C4B-NB	3.47	113.70	109.21
34	a	413	LMG	O7-C10-C11	3.47	118.98	111.50
25	T	101	BCR	C23-C24-C25	-3.47	117.46	127.20
23	b	616	CLA	C4D-C3D-CAD	3.47	110.40	108.47
23	b	617	CLA	C4-C3-C5	3.47	121.11	115.27
25	T	101	BCR	C35-C13-C12	3.47	123.54	118.08
24	a	409	PHO	C4D-ND-C1D	-3.47	100.53	106.76
23	a	410	CLA	O2D-CGD-O1D	-3.46	117.08	123.84
23	a	406	CLA	C5-C3-C2	-3.46	114.12	121.12
23	c	903	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
23	b	609	CLA	O2A-CGA-O1A	-3.46	114.87	123.59
23	c	914	CLA	O2A-CGA-CBA	3.46	122.75	111.91
23	c	912	CLA	C1-O2A-CGA	3.45	125.51	116.44
23	B	614	CLA	CAC-C3C-C4C	3.45	129.29	124.81
23	B	607	CLA	CHD-C4C-NC	3.45	129.64	124.20
26	B	621	SQD	O5-C5-C4	-3.45	103.43	109.69
23	C	513	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
28	E	101	LHG	O8-C23-C24	3.45	122.73	111.91
23	b	603	CLA	CMC-C2C-C1C	3.45	130.29	125.04
25	a	411	BCR	C24-C23-C22	-3.45	121.03	126.23
38	H	102	RRX	C7-C8-C9	-3.45	121.03	126.23
36	h	102	DGD	O1G-C1A-O1A	-3.44	114.91	123.59
23	b	606	CLA	C3C-C4C-NC	3.44	114.43	110.57
23	B	604	CLA	CMB-C2B-C3B	3.44	131.11	124.68
23	b	610	CLA	O2D-CGD-CBD	3.44	117.38	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	611	CLA	CHD-C4C-C3C	-3.44	119.79	124.84
23	C	507	CLA	O2D-CGD-O1D	-3.44	117.12	123.84
28	L	101	LHG	O4-P-O5	3.44	129.22	112.24
26	D	408	SQD	O9-S-C6	3.43	111.02	106.94
23	b	616	CLA	CAC-C3C-C4C	3.43	129.26	124.81
23	b	610	CLA	C4A-NA-C1A	3.43	108.25	106.71
24	a	408	PHO	C2B-C1B-NB	3.43	114.97	109.79
38	H	102	RRX	C10-C11-C12	-3.43	112.52	123.22
23	c	907	CLA	CHD-C4C-NC	3.42	129.60	124.20
23	C	508	CLA	CBC-CAC-C3C	-3.42	103.00	112.43
23	B	617	CLA	C3C-C4C-NC	3.42	114.41	110.57
35	b	622	HTG	C1-C2-C3	3.42	117.34	110.59
23	c	903	CLA	O2D-CGD-O1D	-3.42	117.16	123.84
23	A	408	CLA	C3B-C4B-NB	3.41	113.62	109.21
35	b	622	HTG	C1-O5-C5	3.41	118.86	112.58
26	D	408	SQD	C44-O6-C1	-3.40	107.09	113.74
23	C	509	CLA	C5-C3-C2	-3.40	114.24	121.12
23	A	405	CLA	CHD-C4C-C3C	-3.39	119.85	124.84
23	C	504	CLA	O2D-CGD-CBD	3.39	117.28	111.27
36	D	407	DGD	C3G-O3G-C1D	3.39	120.35	113.74
23	b	611	CLA	C4A-NA-C1A	3.39	108.23	106.71
23	a	407	CLA	C1-C2-C3	-3.39	120.19	126.04
24	a	408	PHO	C3C-C4C-NC	3.39	115.53	110.28
23	B	613	CLA	CAC-C3C-C2C	-3.38	121.74	127.53
24	A	407	PHO	C2B-C1B-NB	3.38	114.90	109.79
38	x	102	RRX	C16-C17-C18	-3.38	122.49	127.31
36	C	518	DGD	O2G-C1B-O1B	-3.37	115.55	123.70
28	L	101	LHG	O7-C7-C8	3.37	118.77	111.50
23	B	606	CLA	C1-C2-C3	-3.37	120.21	126.04
23	b	603	CLA	C1B-CHB-C4A	-3.37	123.44	130.12
23	B	605	CLA	CAC-C3C-C4C	3.37	129.19	124.81
23	b	612	CLA	O2D-CGD-CBD	3.37	117.26	111.27
23	c	913	CLA	C1-O2A-CGA	3.37	125.28	116.44
23	b	611	CLA	O2D-CGD-CBD	3.37	117.25	111.27
26	x	101	SQD	O47-C7-C8	3.37	120.19	110.80
23	B	615	CLA	C3B-C4B-NB	3.36	113.56	109.21
23	c	914	CLA	CHD-C4C-NC	3.36	129.50	124.20
23	D	404	CLA	CHD-C4C-C3C	-3.36	119.90	124.84
23	B	602	CLA	C4D-C3D-CAD	3.36	110.34	108.47
23	c	911	CLA	C4A-NA-C1A	3.36	108.22	106.71
24	D	402	PHO	CMB-C2B-C1B	3.36	130.23	125.06
23	d	403	CLA	C2A-C1A-CHA	-3.36	117.99	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	507	CLA	CHD-C4C-NC	3.35	129.49	124.20
23	b	613	CLA	O2D-CGD-CBD	3.35	117.23	111.27
23	C	504	CLA	C4-C3-C5	3.35	120.91	115.27
23	c	913	CLA	CBC-CAC-C3C	-3.35	103.20	112.43
23	C	509	CLA	CHB-C4A-NA	3.35	129.14	124.51
26	A	410	SQD	O47-C7-O49	-3.34	115.62	123.70
23	b	610	CLA	C3C-C4C-NC	3.34	114.32	110.57
23	B	609	CLA	C4A-NA-C1A	3.34	108.21	106.71
23	B	604	CLA	C2A-C1A-CHA	-3.34	118.02	123.86
23	C	504	CLA	CMB-C2B-C3B	3.34	130.93	124.68
23	C	502	CLA	C2A-C1A-CHA	-3.34	118.02	123.86
23	C	514	CLA	C2A-C1A-CHA	-3.34	118.02	123.86
23	B	608	CLA	C1-C2-C3	-3.34	120.27	126.04
23	b	616	CLA	CMC-C2C-C1C	3.33	130.11	125.04
23	c	914	CLA	C3C-C4C-NC	3.33	114.31	110.57
24	A	407	PHO	O2D-CGD-O1D	-3.33	117.33	123.84
23	B	604	CLA	CMC-C2C-C1C	3.33	130.11	125.04
23	C	507	CLA	CMC-C2C-C1C	3.33	130.11	125.04
23	b	607	CLA	CAC-C3C-C4C	3.33	129.13	124.81
23	c	909	CLA	C2C-C1C-NC	3.33	113.09	109.97
23	C	507	CLA	C3C-C4C-NC	3.32	114.30	110.57
23	c	904	CLA	C1-C2-C3	-3.32	120.30	126.04
23	d	403	CLA	C4D-C3D-CAD	3.32	110.32	108.47
23	B	604	CLA	CMD-C2D-C3D	3.32	130.89	124.68
24	a	409	PHO	C4-C3-C5	3.32	120.85	115.27
23	B	604	CLA	C4A-NA-C1A	3.32	108.20	106.71
23	c	908	CLA	CBC-CAC-C3C	-3.32	103.29	112.43
23	b	612	CLA	C1C-C2C-C3C	-3.32	103.47	106.96
23	B	612	CLA	O2D-CGD-CBD	3.32	117.16	111.27
25	D	405	BCR	C36-C18-C19	3.31	123.30	118.08
23	b	613	CLA	CMC-C2C-C1C	3.31	130.09	125.04
23	c	907	CLA	C2A-C1A-CHA	-3.31	118.07	123.86
27	a	414	PL9	C3-C4-C5	3.31	122.91	118.60
23	C	514	CLA	O2D-CGD-CBD	3.31	117.15	111.27
23	C	514	CLA	CHD-C4C-C3C	-3.31	119.98	124.84
23	C	503	CLA	C16-C17-C18	-3.30	100.41	115.98
36	d	407	DGD	C3D-C4D-C5D	3.30	114.92	109.77
23	a	410	CLA	C3C-C4C-NC	3.30	114.27	110.57
23	B	605	CLA	CED-O2D-CGD	3.30	123.39	115.94
25	d	405	BCR	C15-C14-C13	-3.30	122.61	127.31
24	D	402	PHO	C3C-C4C-NC	3.29	115.38	110.28
23	b	615	CLA	C2C-C1C-NC	3.29	113.06	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L	102	SQD	C4-C3-C2	3.29	116.56	110.82
23	b	614	CLA	CHD-C4C-NC	3.29	129.38	124.20
23	C	512	CLA	CHD-C4C-C3C	-3.28	120.01	124.84
35	v	204	HTG	O3-C3-C2	3.28	117.94	110.35
23	C	508	CLA	CMC-C2C-C1C	3.28	130.04	125.04
25	D	405	BCR	C29-C30-C25	3.28	115.53	110.48
23	c	904	CLA	CMD-C2D-C3D	3.28	130.81	124.68
36	c	919	DGD	O3G-C3G-C2G	-3.27	103.00	110.90
23	B	615	CLA	C4C-C3C-C2C	-3.26	102.14	106.90
23	C	510	CLA	CAC-C3C-C4C	3.26	129.04	124.81
25	B	620	BCR	C23-C24-C25	-3.26	118.04	127.20
24	A	407	PHO	C4C-C3C-C2C	-3.26	103.17	106.78
23	B	613	CLA	C4-C3-C5	3.26	120.76	115.27
23	b	617	CLA	C2C-C1C-NC	3.26	113.03	109.97
36	H	103	DGD	O1G-C1A-C2A	3.26	122.14	111.91
25	C	530	BCR	C11-C10-C9	-3.26	122.66	127.31
40	v	203	HEC	CMC-C2C-C1C	-3.26	123.46	128.46
23	B	616	CLA	CMD-C2D-C3D	3.26	130.77	124.68
25	b	619	BCR	C38-C26-C25	-3.25	120.87	124.53
23	b	616	CLA	OBD-CAD-CBD	3.25	130.54	125.89
37	e	105	HEM	CAD-CBD-CGD	3.25	118.12	112.67
23	D	403	CLA	CMD-C2D-C3D	3.25	130.76	124.68
23	b	608	CLA	CHD-C4C-NC	3.25	129.32	124.20
34	C	501	LMG	O1-C1-C2	3.25	113.38	108.30
25	B	620	BCR	C33-C5-C6	-3.25	120.88	124.53
23	C	505	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
28	D	409	LHG	O4-P-O5	3.25	128.28	112.24
23	b	611	CLA	CMD-C2D-C3D	3.24	130.75	124.68
25	j	104	BCR	C38-C26-C25	-3.24	120.89	124.53
23	B	617	CLA	C4A-NA-C1A	3.24	108.16	106.71
24	a	409	PHO	C3C-C4C-NC	3.24	115.30	110.28
23	B	603	CLA	CHD-C4C-NC	3.24	129.30	124.20
34	c	920	LMG	O7-C10-C11	3.23	118.47	111.50
24	a	408	PHO	CMC-C2C-C1C	3.23	130.04	125.06
23	C	504	CLA	CHD-C4C-NC	3.23	129.30	124.20
27	d	406	PL9	C3-C4-C5	3.23	122.80	118.60
23	b	617	CLA	CMD-C2D-C3D	3.23	130.72	124.68
23	B	607	CLA	O2A-CGA-O1A	-3.23	115.45	123.59
25	A	409	BCR	C15-C16-C17	-3.23	116.86	123.47
23	C	503	CLA	C3B-C4B-NB	3.23	113.38	109.21
23	C	510	CLA	C4-C3-C5	3.23	120.70	115.27
23	A	408	CLA	C5-C3-C2	-3.22	114.59	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	411	BCR	C15-C16-C17	-3.22	116.87	123.47
23	a	407	CLA	O2A-CGA-CBA	3.22	122.02	111.91
23	C	505	CLA	C4-C3-C5	3.22	120.69	115.27
25	C	530	BCR	C33-C5-C6	-3.22	120.91	124.53
23	D	404	CLA	CBC-CAC-C3C	-3.22	103.57	112.43
23	b	615	CLA	C2A-C1A-CHA	-3.21	118.25	123.86
23	B	608	CLA	CAC-C3C-C4C	3.21	128.97	124.81
25	d	405	BCR	C29-C30-C25	3.21	115.42	110.48
23	b	607	CLA	CMD-C2D-C3D	3.21	130.68	124.68
23	B	602	CLA	O1D-CGD-CBD	-3.20	117.93	124.48
23	B	611	CLA	O2A-CGA-O1A	-3.20	115.51	123.59
23	C	502	CLA	CHD-C4C-NC	3.20	129.25	124.20
25	T	101	BCR	C7-C8-C9	-3.20	121.41	126.23
23	c	902	CLA	C3B-C4B-NB	3.20	113.34	109.21
23	B	608	CLA	C3B-C4B-NB	3.19	113.34	109.21
24	a	408	PHO	CMB-C2B-C1B	3.19	129.98	125.06
23	d	403	CLA	CMD-C2D-C3D	3.19	130.64	124.68
24	D	402	PHO	CED-O2D-CGD	3.19	123.15	115.94
23	b	615	CLA	CHD-C4C-C3C	-3.19	120.15	124.84
23	b	603	CLA	C1-O2A-CGA	3.19	124.81	116.44
25	d	405	BCR	C11-C10-C9	-3.19	122.76	127.31
23	B	612	CLA	CMD-C2D-C3D	3.19	130.64	124.68
25	C	530	BCR	C38-C26-C25	-3.19	120.95	124.53
23	A	408	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
23	B	606	CLA	CMC-C2C-C1C	3.18	129.89	125.04
23	B	605	CLA	O2A-CGA-O1A	-3.18	115.57	123.59
23	B	611	CLA	CAC-C3C-C2C	3.18	132.97	127.53
27	a	414	PL9	C37-C36-C34	-3.18	102.53	112.98
23	c	909	CLA	C7-C6-C5	-3.17	104.74	113.36
23	b	611	CLA	O2D-CGD-O1D	-3.17	117.63	123.84
23	c	907	CLA	C4D-C3D-CAD	3.17	110.24	108.47
24	a	408	PHO	O2D-CGD-O1D	-3.17	117.64	123.84
23	A	405	CLA	C2A-C1A-CHA	-3.17	118.32	123.86
28	e	101	LHG	O8-C23-C24	3.17	121.85	111.91
24	a	409	PHO	C2C-C1C-NC	3.17	114.57	109.79
35	b	627	HTG	C2'-C1'-S1	-3.16	102.19	112.40
23	b	611	CLA	CMC-C2C-C1C	3.16	129.85	125.04
23	B	606	CLA	CMD-C2D-C3D	3.16	130.59	124.68
23	c	905	CLA	O2D-CGD-CBD	3.16	116.88	111.27
23	B	611	CLA	C3C-C4C-NC	3.16	114.11	110.57
23	B	617	CLA	C4C-C3C-C2C	-3.16	102.30	106.90
23	B	609	CLA	CAC-C3C-C4C	3.16	128.91	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	402	PHO	C2C-C1C-NC	3.15	114.55	109.79
23	C	510	CLA	C3C-C4C-NC	3.15	114.11	110.57
23	C	505	CLA	CHD-C4C-NC	3.15	129.17	124.20
23	B	604	CLA	CHD-C4C-NC	3.15	129.17	124.20
36	D	407	DGD	O1G-C1A-O1A	-3.15	115.64	123.59
23	B	606	CLA	CHD-C4C-NC	3.15	129.16	124.20
23	D	404	CLA	C4D-C3D-CAD	3.15	110.22	108.47
23	a	406	CLA	O2A-CGA-CBA	3.14	121.78	111.91
23	B	613	CLA	CMC-C2C-C1C	3.14	129.83	125.04
23	c	910	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
23	C	506	CLA	O2A-CGA-O1A	-3.14	115.66	123.59
23	c	914	CLA	CMC-C2C-C1C	3.14	129.82	125.04
23	b	616	CLA	OBD-CAD-C3D	-3.14	122.77	127.98
25	C	515	BCR	C15-C14-C13	-3.14	122.83	127.31
25	c	915	BCR	C20-C21-C22	-3.14	122.83	127.31
23	B	614	CLA	O2A-CGA-CBA	3.14	121.76	111.91
23	b	616	CLA	CHD-C4C-NC	3.14	129.15	124.20
34	D	412	LMG	C1-C2-C3	-3.13	103.47	110.00
27	A	411	PL9	C3-C4-C5	3.13	122.67	118.60
23	d	404	CLA	O2D-CGD-CBD	3.13	116.83	111.27
25	Y	101	BCR	C7-C8-C9	-3.13	121.51	126.23
23	b	606	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
23	D	404	CLA	C2A-C1A-CHA	-3.13	118.39	123.86
23	d	404	CLA	C4A-NA-C1A	3.13	108.11	106.71
23	d	401	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
23	B	603	CLA	OBD-CAD-C3D	-3.12	122.80	127.98
23	d	401	CLA	CBC-CAC-C3C	-3.12	103.83	112.43
23	b	617	CLA	O2A-CGA-CBA	3.11	121.68	111.91
23	B	614	CLA	CHD-C4C-NC	3.11	129.11	124.20
34	B	622	LMG	C9-C8-C7	-3.11	104.42	111.79
23	B	613	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
25	B	620	BCR	C2-C1-C6	3.11	115.27	110.48
23	d	403	CLA	CAC-C3C-C4C	3.11	128.85	124.81
23	B	610	CLA	CED-O2D-CGD	3.11	122.97	115.94
23	b	616	CLA	C4-C3-C5	3.11	120.50	115.27
25	T	101	BCR	C12-C13-C14	-3.10	114.18	118.94
23	b	611	CLA	C1D-CHD-C4C	-3.10	118.46	122.56
23	A	406	CLA	C3C-C4C-NC	3.10	114.05	110.57
34	c	920	LMG	O1-C7-C8	-3.10	103.42	110.90
23	b	605	CLA	CMC-C2C-C1C	3.10	129.76	125.04
23	C	513	CLA	C4-C3-C5	3.10	120.48	115.27
23	A	405	CLA	OBD-CAD-C3D	-3.10	122.84	127.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	511	CLA	C1C-C2C-C3C	-3.10	103.70	106.96
34	C	520	LMG	O6-C5-C6	3.10	114.14	106.44
30	A	416	LMT	O1'-C1'-C2'	3.10	113.14	108.30
23	c	906	CLA	CMB-C2B-C3B	3.09	130.47	124.68
23	d	403	CLA	C1D-CHD-C4C	-3.09	118.48	122.56
35	B	625	HTG	C4-C3-C2	3.09	116.22	110.82
36	c	917	DGD	O3G-C3G-C2G	-3.09	103.45	110.90
23	C	514	CLA	O2A-CGA-CBA	3.08	121.58	111.91
26	B	621	SQD	O9-S-C6	3.08	110.60	106.94
23	B	610	CLA	OBD-CAD-C3D	-3.08	122.87	127.98
23	C	503	CLA	CAC-C3C-C4C	3.08	128.80	124.81
23	B	611	CLA	CHD-C4C-NC	3.08	129.05	124.20
23	b	612	CLA	OBD-CAD-CBD	-3.07	121.50	125.89
35	B	625	HTG	O4-C4-C5	3.07	116.92	109.30
23	B	606	CLA	C1C-C2C-C3C	-3.07	103.73	106.96
23	C	508	CLA	CHD-C4C-NC	3.07	129.04	124.20
23	c	910	CLA	CHD-C4C-NC	3.07	129.03	124.20
23	B	613	CLA	C1D-CHD-C4C	3.06	126.60	122.56
23	B	602	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
36	c	917	DGD	O2G-C1B-C2B	3.06	118.10	111.50
23	c	906	CLA	CHD-C4C-NC	3.06	129.03	124.20
23	b	609	CLA	C4A-NA-C1A	3.06	108.08	106.71
23	C	510	CLA	O2A-CGA-CBA	3.06	121.51	111.91
28	d	409	LHG	O7-C7-O9	-3.06	116.31	123.70
34	d	411	LMG	O6-C5-C6	3.05	114.03	106.44
23	b	606	CLA	C1-C2-C3	-3.05	120.77	126.04
23	d	403	CLA	O2A-CGA-O1A	-3.05	115.90	123.59
25	C	515	BCR	C32-C1-C6	-3.05	105.36	110.30
23	C	507	CLA	C1-C2-C3	-3.05	120.77	126.04
23	A	405	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
23	C	506	CLA	CMB-C2B-C3B	3.04	130.37	124.68
23	c	904	CLA	CHD-C4C-NC	3.04	129.00	124.20
23	C	512	CLA	O2D-CGD-CBD	3.04	116.67	111.27
23	c	902	CLA	CMC-C2C-C1C	3.04	129.67	125.04
36	C	517	DGD	O5D-C6D-C5D	-3.03	103.43	109.05
23	b	611	CLA	C3B-C4B-NB	3.03	113.13	109.21
23	B	611	CLA	C3B-C4B-NB	3.03	113.13	109.21
23	b	615	CLA	CBC-CAC-C3C	-3.03	104.07	112.43
23	A	408	CLA	C2A-C1A-CHA	-3.03	118.56	123.86
23	C	507	CLA	CMB-C2B-C3B	3.03	130.35	124.68
23	D	404	CLA	O2A-CGA-O1A	-3.03	115.94	123.59
23	B	603	CLA	OBD-CAD-CBD	3.03	130.22	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	603	CLA	CBC-CAC-C3C	-3.03	104.08	112.43
23	a	407	CLA	O2A-CGA-O1A	-3.03	115.95	123.59
23	b	605	CLA	C6-C5-C3	-3.03	105.52	113.45
23	B	609	CLA	CMC-C2C-C1C	3.03	129.65	125.04
23	C	512	CLA	C3B-C4B-NB	3.03	113.12	109.21
23	C	513	CLA	C3C-C4C-NC	3.02	113.96	110.57
26	L	102	SQD	O5-C1-C2	-3.02	103.95	110.35
25	j	104	BCR	C33-C5-C6	-3.02	121.14	124.53
28	d	409	LHG	O7-C7-C8	3.02	118.01	111.50
36	h	102	DGD	O3G-C1D-C2D	3.02	113.02	108.30
23	D	401	CLA	CBC-CAC-C3C	-3.02	104.11	112.43
23	a	406	CLA	CMB-C2B-C3B	3.02	130.32	124.68
23	c	906	CLA	O2D-CGD-CBD	3.02	116.63	111.27
23	C	508	CLA	OBD-CAD-C3D	-3.02	122.97	127.98
25	Y	101	BCR	C24-C23-C22	-3.02	121.68	126.23
23	D	403	CLA	O2D-CGD-CBD	3.02	116.63	111.27
23	D	401	CLA	CHC-C1C-C2C	-3.01	118.39	126.72
23	a	406	CLA	CHD-C4C-NC	3.01	128.95	124.20
23	b	602	CLA	C5-C3-C2	-3.01	115.03	121.12
23	B	611	CLA	CMD-C2D-C3D	3.00	130.29	124.68
28	d	409	LHG	O8-C23-O10	-3.00	116.02	123.59
23	D	404	CLA	C3B-C4B-NB	3.00	113.09	109.21
23	B	610	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
25	C	516	BCR	C37-C22-C23	3.00	122.80	118.08
30	a	422	LMT	C1B-O5B-C5B	2.99	119.55	113.69
23	B	613	CLA	CHD-C4C-C3C	-2.99	120.45	124.84
36	c	918	DGD	O2G-C1B-O1B	-2.98	116.49	123.70
30	Z	101	LMT	C1'-O5'-C5'	2.98	119.55	113.69
23	B	617	CLA	C1C-C2C-C3C	-2.98	103.82	106.96
27	A	411	PL9	C25-C24-C26	2.98	120.29	115.27
23	b	611	CLA	CMB-C2B-C3B	2.98	130.25	124.68
23	a	406	CLA	CHC-C1C-NC	2.98	128.72	124.20
23	b	605	CLA	CMB-C2B-C3B	2.98	130.25	124.68
23	c	907	CLA	C3B-C4B-NB	2.97	113.06	109.21
23	d	403	CLA	C3C-C4C-NC	2.97	113.91	110.57
34	C	520	LMG	O8-C28-O10	-2.97	116.09	123.59
25	c	916	BCR	C36-C18-C19	2.97	122.76	118.08
23	B	616	CLA	C1-O2A-CGA	2.97	124.23	116.44
23	c	905	CLA	C4D-C3D-CAD	2.97	110.12	108.47
23	B	615	CLA	O2A-CGA-O1A	-2.97	116.11	123.59
23	a	410	CLA	C1C-C2C-C3C	-2.97	103.84	106.96
23	b	613	CLA	CMD-C2D-C3D	2.96	130.22	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	k	102	BCR	C7-C8-C9	-2.96	121.76	126.23
23	C	512	CLA	C4D-C3D-CAD	2.96	110.12	108.47
23	b	617	CLA	C1C-C2C-C3C	-2.96	103.84	106.96
23	d	404	CLA	C2A-C1A-CHA	-2.96	118.69	123.86
23	A	408	CLA	CHD-C4C-NC	2.96	128.86	124.20
35	O	302	HTG	C1-O5-C5	2.96	118.03	112.58
23	C	507	CLA	CAC-C3C-C4C	2.95	128.64	124.81
23	B	608	CLA	CMB-C2B-C1B	-2.95	123.92	128.46
23	b	617	CLA	CED-O2D-CGD	2.95	122.62	115.94
23	c	908	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
23	B	608	CLA	CHD-C4C-NC	2.95	128.85	124.20
23	D	401	CLA	CMB-C2B-C3B	2.95	130.20	124.68
30	I	101	LMT	O3'-C3'-C4'	2.95	117.77	109.94
23	C	510	CLA	O2A-CGA-O1A	-2.95	116.15	123.59
23	c	902	CLA	CAC-C3C-C4C	2.95	128.63	124.81
23	B	611	CLA	C1C-C2C-C3C	-2.95	103.86	106.96
23	b	602	CLA	CMD-C2D-C3D	2.94	130.19	124.68
23	D	401	CLA	CMC-C2C-C1C	2.94	129.52	125.04
40	v	203	HEC	CMB-C2B-C3B	2.94	129.28	125.82
23	b	607	CLA	CHD-C4C-NC	2.94	128.84	124.20
23	c	912	CLA	O2D-CGD-CBD	2.94	116.49	111.27
23	B	616	CLA	C3B-C4B-NB	2.94	113.01	109.21
25	d	405	BCR	C16-C15-C14	-2.94	117.45	123.47
34	C	520	LMG	O8-C9-C8	2.94	116.99	108.43
28	d	408	LHG	C6-O8-C23	2.94	128.00	117.12
23	c	912	CLA	CBC-CAC-C3C	-2.94	104.34	112.43
23	C	507	CLA	C1D-CHD-C4C	-2.93	118.69	122.56
23	c	903	CLA	C3B-C4B-NB	2.93	113.00	109.21
23	b	615	CLA	CAC-C3C-C4C	2.93	128.62	124.81
23	c	906	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
23	c	910	CLA	C4D-C3D-CAD	2.93	110.10	108.47
23	c	913	CLA	CBA-CAA-C2A	-2.93	105.22	113.86
24	D	402	PHO	CBA-CAA-C2A	-2.93	105.22	113.86
25	c	916	BCR	C7-C8-C9	-2.93	121.81	126.23
35	B	625	HTG	O2-C2-C3	-2.93	103.59	110.35
23	C	511	CLA	CAC-C3C-C4C	2.92	128.60	124.81
23	b	605	CLA	C1D-CHD-C4C	-2.92	118.70	122.56
23	C	506	CLA	CMD-C2D-C3D	2.92	130.15	124.68
23	c	912	CLA	CMC-C2C-C1C	2.92	129.48	125.04
23	B	607	CLA	CMB-C2B-C1B	2.92	132.95	128.46
23	b	602	CLA	CHD-C4C-NC	2.92	128.80	124.20
27	a	414	PL9	C20-C19-C21	2.91	120.17	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	609	CLA	CMC-C2C-C1C	2.91	129.47	125.04
23	A	406	CLA	CMB-C2B-C3B	2.91	130.12	124.68
36	C	518	DGD	C2G-O2G-C1B	-2.91	110.62	117.79
23	b	604	CLA	O2A-CGA-O1A	-2.91	116.25	123.59
34	c	920	LMG	O3-C3-C4	-2.91	103.63	110.35
23	b	604	CLA	O2A-C1-C2	-2.91	101.00	108.64
23	B	611	CLA	O2A-CGA-CBA	2.91	121.03	111.91
23	B	614	CLA	C2A-C1A-CHA	-2.91	118.78	123.86
23	D	404	CLA	CED-O2D-CGD	2.90	122.50	115.94
23	B	614	CLA	O2A-CGA-O1A	-2.90	116.27	123.59
23	B	603	CLA	C1-C2-C3	-2.90	121.03	126.04
23	C	514	CLA	CMB-C2B-C3B	2.90	130.10	124.68
25	b	619	BCR	C8-C7-C6	-2.89	119.08	127.20
26	A	410	SQD	O48-C23-O10	-2.89	116.29	123.59
26	A	415	SQD	O6-C44-C45	-2.89	103.92	110.90
30	A	416	LMT	O2'-C2'-C1'	2.89	117.07	110.05
38	x	102	RRX	C24-C23-C22	-2.89	121.87	126.23
23	b	616	CLA	O2D-CGD-CBD	2.89	116.40	111.27
23	c	903	CLA	CMC-C2C-C1C	2.89	129.44	125.04
27	A	411	PL9	C10-C9-C11	2.89	120.13	115.27
23	c	905	CLA	CHB-C4A-NA	2.88	128.50	124.51
40	v	203	HEC	CAD-CBD-CGD	-2.88	107.84	112.67
23	B	617	CLA	CED-O2D-CGD	2.88	122.45	115.94
37	e	105	HEM	C4C-C3C-C2C	2.88	108.91	106.90
23	B	617	CLA	CBC-CAC-C3C	-2.88	104.50	112.43
23	B	612	CLA	CHD-C4C-NC	2.88	128.74	124.20
23	B	616	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
23	c	910	CLA	O2A-CGA-CBA	2.87	120.92	111.91
23	A	406	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
36	C	517	DGD	O1G-C1A-O1A	-2.87	116.35	123.59
24	a	409	PHO	CED-O2D-CGD	2.87	122.43	115.94
34	j	101	LMG	C9-C8-C7	-2.87	105.00	111.79
24	A	407	PHO	C7-C6-C5	-2.86	105.59	113.36
23	B	612	CLA	C1D-CHD-C4C	-2.86	118.78	122.56
23	B	613	CLA	CAA-CBA-CGA	-2.86	104.90	113.25
28	L	101	LHG	C6-C5-C4	-2.86	105.03	111.79
23	d	404	CLA	C1-C2-C3	-2.86	121.10	126.04
30	m	103	LMT	C1'-O5'-C5'	2.86	119.30	113.69
23	a	407	CLA	CHC-C1C-C2C	-2.86	118.82	126.72
23	A	405	CLA	CHC-C1C-C2C	-2.85	118.83	126.72
23	b	608	CLA	C2A-C1A-CHA	-2.85	118.87	123.86
23	A	405	CLA	C7-C6-C5	-2.85	105.61	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	604	CLA	CMD-C2D-C3D	2.85	130.01	124.68
38	H	102	RRX	C16-C17-C18	-2.85	123.24	127.31
23	C	505	CLA	C3B-C4B-NB	2.85	112.89	109.21
23	a	407	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
36	c	918	DGD	O1G-C1A-O1A	-2.85	116.41	123.59
27	D	406	PL9	C10-C9-C11	2.85	120.06	115.27
23	b	608	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
23	c	911	CLA	O2A-CGA-O1A	-2.85	116.41	123.59
23	c	908	CLA	C4-C3-C5	2.85	120.06	115.27
25	C	515	BCR	C11-C10-C9	-2.84	123.25	127.31
24	A	407	PHO	C4A-NA-C1A	2.84	110.44	108.14
23	B	614	CLA	O1D-CGD-CBD	2.84	130.30	124.48
23	B	607	CLA	C3B-C4B-NB	2.84	112.88	109.21
23	D	403	CLA	C3B-C4B-NB	2.84	112.88	109.21
30	m	103	LMT	C1B-O1B-C4'	-2.84	110.93	117.96
38	x	102	RRX	C38-C26-C25	-2.84	121.34	124.53
23	B	614	CLA	CBC-CAC-C3C	-2.84	104.60	112.43
35	d	413	HTG	C1-O5-C5	2.84	117.82	112.58
35	c	922	HTG	C4-C3-C2	2.84	115.78	110.82
23	A	405	CLA	CMB-C2B-C3B	2.84	129.99	124.68
23	b	609	CLA	CED-O2D-CGD	2.84	122.35	115.94
34	d	411	LMG	O8-C28-C29	2.84	120.81	111.91
23	C	514	CLA	CBC-CAC-C3C	-2.84	104.61	112.43
23	C	504	CLA	C1D-CHD-C4C	-2.84	118.82	122.56
27	a	414	PL9	C25-C24-C26	2.83	120.04	115.27
23	b	604	CLA	C4D-C3D-CAD	-2.83	106.89	108.47
23	B	610	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
25	D	405	BCR	C28-C27-C26	-2.83	109.02	114.08
23	a	410	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
23	b	611	CLA	O2A-CGA-O1A	-2.83	116.46	123.59
30	e	103	LMT	C1-O1'-C1'	2.83	118.53	113.84
23	C	506	CLA	C1-O2A-CGA	2.83	123.86	116.44
23	A	406	CLA	OBD-CAD-CBD	-2.83	121.86	125.89
23	b	606	CLA	C2A-C1A-CHA	-2.83	118.92	123.86
23	b	616	CLA	C1-O2A-CGA	2.83	123.86	116.44
26	D	408	SQD	O48-C23-C24	2.82	120.77	111.91
26	A	410	SQD	O48-C23-C24	2.82	120.76	111.91
23	d	401	CLA	CED-O2D-CGD	2.82	122.31	115.94
23	c	906	CLA	CMC-C2C-C1C	2.82	129.33	125.04
25	b	620	BCR	C7-C8-C9	-2.82	121.98	126.23
23	a	407	CLA	CMB-C2B-C3B	2.82	129.95	124.68
25	Y	101	BCR	C21-C20-C19	-2.82	114.43	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	606	CLA	OBD-CAD-C3D	-2.82	123.31	127.98
26	a	417	SQD	O6-C1-C2	2.82	112.70	108.30
23	a	410	CLA	OBD-CAD-C3D	-2.81	123.31	127.98
23	c	914	CLA	C2A-C1A-CHA	-2.81	118.94	123.86
27	D	406	PL9	C12-C13-C14	-2.81	120.89	127.66
23	b	612	CLA	CBC-CAC-C3C	-2.81	104.68	112.43
23	c	911	CLA	C4-C3-C5	2.81	120.00	115.27
34	C	531	LMG	O8-C28-C29	2.81	120.73	111.91
25	C	516	BCR	C33-C5-C6	-2.81	121.37	124.53
23	b	606	CLA	C3D-CAD-CBD	2.81	111.30	107.61
23	c	913	CLA	CAC-C3C-C4C	2.81	128.46	124.81
26	D	408	SQD	O7-S-C6	2.81	110.28	106.94
26	x	101	SQD	O8-S-C6	2.81	110.21	105.74
25	T	101	BCR	C20-C21-C22	-2.81	123.31	127.31
23	C	513	CLA	OBD-CAD-C3D	-2.81	123.32	127.98
23	A	408	CLA	CED-O2D-CGD	2.81	122.28	115.94
24	D	402	PHO	C4A-NA-C1A	2.81	110.41	108.14
35	O	302	HTG	C4-C3-C2	2.81	115.72	110.82
26	x	101	SQD	O5-C5-C4	2.81	114.79	109.69
28	a	415	LHG	O8-C23-C24	2.80	120.71	111.91
23	b	610	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
23	C	503	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
27	A	411	PL9	C45-C44-C46	2.80	119.98	115.27
34	c	920	LMG	O8-C28-O10	-2.80	116.53	123.59
23	C	509	CLA	C4D-C3D-CAD	2.80	110.03	108.47
23	c	904	CLA	O2A-CGA-CBA	2.79	120.68	111.91
23	c	903	CLA	CAC-C3C-C4C	2.79	128.44	124.81
35	B	624	HTG	O3-C3-C2	2.79	116.81	110.35
23	a	406	CLA	O2A-CGA-O1A	-2.79	116.55	123.59
23	c	908	CLA	CMD-C2D-C3D	2.79	129.90	124.68
23	b	608	CLA	O2A-C1-C2	-2.79	101.30	108.64
23	b	602	CLA	C1-C2-C3	2.79	130.87	126.04
23	d	404	CLA	C6-C5-C3	-2.79	106.14	113.45
23	D	401	CLA	C3B-C4B-NB	2.79	112.81	109.21
23	B	608	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
23	C	510	CLA	C3B-C4B-NB	2.79	112.81	109.21
27	a	414	PL9	C7-C8-C9	-2.79	122.16	126.79
34	m	102	LMG	O7-C10-O9	-2.78	116.97	123.70
25	t	101	BCR	C38-C26-C25	-2.78	121.40	124.53
23	a	407	CLA	C4A-NA-C1A	2.78	107.96	106.71
23	b	611	CLA	CAC-C3C-C4C	2.78	128.42	124.81
23	B	602	CLA	O2A-CGA-CBA	2.78	120.63	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	608	CLA	C2A-C1A-CHA	-2.78	119.00	123.86
23	B	609	CLA	C3C-C4C-NC	2.78	113.69	110.57
23	B	616	CLA	C1D-CHD-C4C	-2.78	118.89	122.56
23	C	506	CLA	CHD-C4C-NC	2.77	128.58	124.20
23	B	612	CLA	CBC-CAC-C3C	-2.77	104.78	112.43
23	C	504	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
35	C	522	HTG	O5-C5-C4	2.77	114.73	109.69
23	C	510	CLA	CMD-C2D-C3D	2.77	129.86	124.68
25	t	101	BCR	C35-C13-C12	2.77	122.44	118.08
23	b	606	CLA	CMB-C2B-C3B	2.77	129.86	124.68
23	c	909	CLA	CMA-C3A-C4A	-2.77	104.33	111.77
28	A	412	LHG	O8-C23-C24	2.77	120.59	111.91
27	A	411	PL9	C51-C49-C50	2.77	120.71	114.60
25	D	405	BCR	C29-C28-C27	-2.76	105.20	111.38
26	A	410	SQD	O9-S-O7	-2.76	104.38	113.95
23	B	613	CLA	CMB-C2B-C3B	2.76	129.85	124.68
30	a	418	LMT	O5'-C5'-C4'	2.76	115.57	109.75
25	c	916	BCR	C16-C17-C18	-2.76	123.37	127.31
25	B	618	BCR	C33-C5-C6	-2.76	121.43	124.53
34	d	411	LMG	O6-C1-O1	2.76	116.50	109.97
23	c	905	CLA	O2A-C1-C2	-2.75	101.40	108.64
23	b	610	CLA	CBC-CAC-C3C	-2.75	104.84	112.43
23	b	613	CLA	C4-C3-C5	2.75	119.90	115.27
23	c	909	CLA	CHD-C4C-NC	2.75	128.54	124.20
23	C	511	CLA	O2A-CGA-O1A	-2.75	116.65	123.59
23	A	408	CLA	CMD-C2D-C3D	2.75	129.82	124.68
36	C	517	DGD	C1E-O6E-C5E	2.75	119.08	113.69
30	m	103	LMT	O1'-C1'-C2'	2.75	112.59	108.30
36	c	919	DGD	C6B-C5B-C4B	-2.75	100.48	114.42
23	B	609	CLA	CMD-C2D-C3D	2.75	129.82	124.68
25	d	405	BCR	C2-C1-C6	2.75	114.71	110.48
23	c	904	CLA	CBC-CAC-C3C	-2.74	104.86	112.43
23	B	606	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
23	c	904	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
23	b	608	CLA	C3B-C4B-NB	2.74	112.75	109.21
23	c	912	CLA	CMD-C2D-C3D	2.74	129.80	124.68
25	D	405	BCR	C33-C5-C6	-2.74	121.45	124.53
23	c	912	CLA	C4-C3-C5	2.74	119.88	115.27
23	C	505	CLA	OBD-CAD-C3D	-2.74	123.44	127.98
37	E	105	HEM	CMC-C2C-C3C	2.74	129.80	124.68
24	a	408	PHO	C4A-NA-C1A	2.74	110.35	108.14
23	B	615	CLA	C1-C2-C3	-2.73	121.31	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	401	CLA	CHD-C4C-NC	2.73	128.51	124.20
23	B	605	CLA	C4D-C3D-CAD	2.73	109.99	108.47
34	j	101	LMG	O7-C10-C11	2.73	117.39	111.50
23	C	510	CLA	CMB-C2B-C1B	2.73	132.66	128.46
23	b	606	CLA	C5-C3-C2	-2.73	115.59	121.12
36	d	407	DGD	O1G-C1A-O1A	-2.73	116.70	123.59
23	B	604	CLA	O2A-CGA-O1A	-2.73	116.71	123.59
23	D	403	CLA	C2A-C1A-CHA	-2.73	119.09	123.86
23	c	906	CLA	C3C-C4C-NC	2.73	113.63	110.57
23	C	511	CLA	C3B-C4B-NB	2.73	112.73	109.21
23	d	401	CLA	CMB-C2B-C3B	2.73	129.78	124.68
23	C	512	CLA	C1-O2A-CGA	2.73	123.59	116.44
30	a	418	LMT	C1B-O1B-C4'	-2.72	111.23	117.96
23	c	902	CLA	CHB-C4A-NA	2.72	128.28	124.51
23	C	513	CLA	CMB-C2B-C3B	2.72	129.77	124.68
24	a	409	PHO	CAA-C2A-C1A	-2.72	105.30	112.33
23	C	508	CLA	OBD-CAD-CBD	2.72	129.78	125.89
23	b	617	CLA	CHD-C4C-NC	2.72	128.49	124.20
38	H	102	RRX	C40-C30-C25	-2.72	105.89	110.30
23	c	908	CLA	O2A-CGA-CBA	2.71	120.42	111.91
28	d	402	LHG	O8-C23-C24	2.71	120.41	111.91
25	B	620	BCR	C24-C23-C22	-2.71	122.14	126.23
23	B	617	CLA	C3B-C4B-NB	2.70	112.71	109.21
37	e	105	HEM	CMD-C2D-C1D	-2.70	124.31	128.46
27	D	406	PL9	C36-C37-C38	-2.70	103.00	111.88
23	b	617	CLA	CMB-C2B-C1B	-2.70	124.31	128.46
36	C	519	DGD	O1G-C1A-C2A	2.70	120.38	111.91
23	C	513	CLA	C4C-C3C-C2C	-2.70	102.97	106.90
23	a	410	CLA	CMB-C2B-C3B	2.69	129.72	124.68
23	b	602	CLA	OBD-CAD-C3D	-2.69	123.51	127.98
23	b	615	CLA	CMD-C2D-C3D	2.69	129.72	124.68
23	c	909	CLA	CHB-C4A-NA	2.69	128.24	124.51
27	A	411	PL9	C7-C8-C9	-2.69	122.31	126.79
23	A	405	CLA	OBD-CAD-CBD	2.69	129.74	125.89
23	c	905	CLA	CHD-C4C-NC	2.69	128.44	124.20
23	c	913	CLA	CMC-C2C-C1C	2.69	129.13	125.04
35	b	622	HTG	O2-C2-C1	2.69	115.20	110.27
23	B	609	CLA	CMB-C2B-C3B	2.69	129.70	124.68
23	c	910	CLA	C1-C2-C3	-2.69	121.40	126.04
23	d	403	CLA	O2A-CGA-CBA	2.68	120.33	111.91
35	v	204	HTG	C1-C2-C3	-2.68	105.29	110.59
25	t	101	BCR	C2-C3-C4	-2.68	105.38	111.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	414	PL9	C15-C14-C16	2.68	119.78	115.27
34	d	411	LMG	C8-O7-C10	-2.68	111.19	117.79
23	B	610	CLA	CHD-C4C-NC	2.68	128.43	124.20
23	c	910	CLA	C6-C5-C3	-2.68	106.43	113.45
25	C	515	BCR	C33-C5-C6	-2.68	121.52	124.53
23	D	404	CLA	CMB-C2B-C3B	2.68	129.69	124.68
25	A	409	BCR	C28-C27-C26	-2.68	109.30	114.08
23	C	512	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
23	b	614	CLA	C2A-C1A-CHA	-2.67	119.19	123.86
23	c	904	CLA	O2A-CGA-O1A	-2.67	116.85	123.59
25	j	104	BCR	C35-C13-C12	2.67	122.28	118.08
23	b	613	CLA	C2A-C1A-CHA	-2.67	119.20	123.86
34	m	102	LMG	C30-C29-C28	-2.67	103.92	113.62
36	c	917	DGD	O2G-C1B-O1B	-2.67	117.26	123.70
23	C	506	CLA	C3C-C4C-NC	2.67	113.56	110.57
30	I	101	LMT	C3'-C4'-C5'	-2.66	104.82	110.93
27	D	406	PL9	C36-C34-C33	-2.66	115.73	121.12
23	b	615	CLA	C3B-C4B-NB	2.66	112.65	109.21
23	d	401	CLA	C3B-C4B-NB	2.66	112.65	109.21
23	b	602	CLA	CED-O2D-CGD	2.66	121.96	115.94
23	B	606	CLA	C2A-C1A-CHA	-2.66	119.21	123.86
38	H	102	RRX	C34-C9-C8	2.66	122.27	118.08
25	D	405	BCR	C2-C3-C4	2.66	117.32	111.38
23	b	608	CLA	C4D-C3D-CAD	-2.66	106.99	108.47
30	B	643	LMT	C1-O1'-C1'	-2.66	109.43	113.84
26	a	412	SQD	O9-S-O7	-2.66	104.75	113.95
25	C	530	BCR	C20-C21-C22	-2.66	123.52	127.31
28	d	410	LHG	O7-C7-O9	-2.65	117.29	123.70
35	c	922	HTG	C1-C2-C3	2.65	115.83	110.59
23	B	615	CLA	CHC-C1C-NC	-2.65	120.18	124.20
23	A	405	CLA	C4A-NA-C1A	-2.65	105.51	106.71
25	C	530	BCR	C7-C8-C9	-2.65	122.23	126.23
23	b	609	CLA	C3C-C4C-NC	2.65	113.54	110.57
23	B	602	CLA	C2A-C1A-CHA	-2.65	119.23	123.86
23	a	406	CLA	C3C-C4C-NC	2.65	113.54	110.57
23	c	906	CLA	CAC-C3C-C4C	2.65	128.25	124.81
34	m	102	LMG	O8-C28-C29	2.65	120.22	111.91
34	C	520	LMG	O5-C6-C5	-2.65	102.21	111.29
23	C	508	CLA	CMB-C2B-C3B	2.65	129.63	124.68
36	d	407	DGD	O1G-C1A-C2A	2.64	120.20	111.91
23	C	507	CLA	C4-C3-C5	2.64	119.71	115.27
26	A	410	SQD	C45-O47-C7	-2.64	111.29	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	405	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
23	b	617	CLA	C4-C3-C2	-2.64	116.91	123.68
23	b	603	CLA	OBD-CAD-C3D	-2.63	123.61	127.98
23	b	617	CLA	C4C-C3C-C2C	-2.63	103.06	106.90
23	B	616	CLA	CMB-C2B-C3B	2.63	129.60	124.68
25	d	405	BCR	C32-C1-C6	2.63	114.57	110.30
23	a	407	CLA	C2A-C1A-CHA	-2.63	119.26	123.86
23	C	511	CLA	O1D-CGD-CBD	-2.63	119.10	124.48
30	B	644	LMT	C1-O1'-C1'	-2.63	109.48	113.84
26	D	408	SQD	O4-C4-C3	-2.63	104.27	110.35
34	B	622	LMG	O7-C10-O9	-2.63	117.35	123.70
25	b	618	BCR	C28-C27-C26	-2.63	109.38	114.08
23	B	604	CLA	CBA-CAA-C2A	2.63	121.62	113.86
34	C	501	LMG	O7-C10-C11	2.63	117.16	111.50
23	b	602	CLA	C4-C3-C5	2.62	119.69	115.27
35	O	302	HTG	C1'-S1-C1	2.62	105.00	100.09
26	a	412	SQD	O5-C1-O6	2.62	116.19	109.97
23	b	603	CLA	C3C-C4C-NC	2.62	113.51	110.57
23	B	609	CLA	C1D-CHD-C4C	-2.62	119.10	122.56
23	B	604	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
23	C	507	CLA	C4C-C3C-C2C	-2.62	103.08	106.90
23	C	509	CLA	O2A-CGA-O1A	-2.62	116.99	123.59
30	z	101	LMT	C1B-C2B-C3B	-2.62	104.55	110.00
23	c	911	CLA	C2A-C1A-CHA	-2.62	119.29	123.86
23	b	613	CLA	C4C-C3C-C2C	-2.61	103.09	106.90
23	a	407	CLA	C4D-C3D-CAD	-2.61	107.01	108.47
23	D	404	CLA	O2D-CGD-CBD	2.61	115.91	111.27
23	b	611	CLA	CHD-C4C-NC	2.61	128.32	124.20
23	B	617	CLA	C1-O2A-CGA	2.61	123.29	116.44
35	c	921	HTG	C3-C4-C5	2.61	114.89	110.24
25	b	618	BCR	C23-C22-C21	-2.61	114.94	118.94
28	D	410	LHG	O7-C7-O9	-2.61	117.41	123.70
25	t	101	BCR	C2-C1-C6	2.61	114.49	110.48
23	B	603	CLA	CHB-C4A-NA	2.60	128.11	124.51
26	x	101	SQD	O7-S-C6	2.60	110.03	106.94
23	D	404	CLA	CMA-C3A-C4A	-2.60	104.78	111.77
23	B	607	CLA	CMC-C2C-C3C	2.60	133.18	126.12
35	B	625	HTG	O5-C1-C2	-2.60	107.04	110.31
23	C	503	CLA	CHD-C4C-NC	2.60	128.30	124.20
23	C	502	CLA	CHC-C1C-NC	-2.60	120.26	124.20
25	B	620	BCR	C32-C1-C6	-2.60	106.09	110.30
35	V	204	HTG	O2-C2-C1	2.60	115.04	110.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	x	101	SQD	O48-C23-O10	-2.60	117.04	123.59
36	h	102	DGD	O5D-C1E-C2E	2.59	112.35	108.30
28	K	101	LHG	O8-C23-C24	2.59	120.05	111.91
30	m	104	LMT	O1'-C1-C2	-2.59	100.47	109.56
23	B	616	CLA	CHD-C4C-NC	2.59	128.29	124.20
25	c	915	BCR	C11-C10-C9	-2.59	123.61	127.31
23	d	401	CLA	OBD-CAD-C3D	-2.59	123.68	127.98
25	B	619	BCR	C11-C10-C9	-2.59	123.61	127.31
23	B	613	CLA	C2A-C1A-CHA	-2.59	119.33	123.86
25	t	101	BCR	C29-C28-C27	-2.59	105.59	111.38
23	b	608	CLA	CMC-C2C-C1C	2.59	128.98	125.04
23	c	908	CLA	O2A-CGA-O1A	-2.59	117.06	123.59
23	a	410	CLA	CED-O2D-CGD	2.59	121.79	115.94
30	A	416	LMT	O5'-C5'-C4'	2.58	115.19	109.75
23	c	907	CLA	C4-C3-C5	2.58	119.61	115.27
24	A	407	PHO	CED-O2D-CGD	2.58	121.77	115.94
25	Y	101	BCR	C15-C16-C17	-2.58	118.20	123.47
23	C	511	CLA	CMD-C2D-C3D	2.58	129.50	124.68
23	B	610	CLA	CMB-C2B-C3B	2.58	129.50	124.68
23	b	602	CLA	CBC-CAC-C3C	-2.57	105.33	112.43
23	b	605	CLA	C3C-C4C-NC	2.57	113.46	110.57
23	b	617	CLA	C3C-C4C-NC	2.57	113.46	110.57
23	D	404	CLA	C4-C3-C5	2.57	119.60	115.27
23	d	401	CLA	CMD-C2D-C3D	2.57	129.49	124.68
23	b	610	CLA	C4C-C3C-C2C	-2.57	103.15	106.90
23	b	616	CLA	C3B-C4B-NB	2.57	112.53	109.21
35	B	631	HTG	C1-O5-C5	2.57	117.31	112.58
23	C	505	CLA	CAC-C3C-C4C	2.56	128.14	124.81
23	b	608	CLA	C4A-NA-C1A	2.56	107.86	106.71
23	A	406	CLA	CAC-C3C-C2C	-2.56	123.14	127.53
23	b	603	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
25	c	916	BCR	C29-C30-C25	2.56	114.42	110.48
23	b	615	CLA	CHB-C4A-NA	2.56	128.05	124.51
36	C	517	DGD	CDB-CCB-CBB	-2.56	101.43	114.42
23	B	608	CLA	O2D-CGD-CBD	2.56	115.81	111.27
28	A	412	LHG	O8-C23-O10	-2.56	117.14	123.59
23	c	911	CLA	C4C-C3C-C2C	-2.56	103.17	106.90
36	c	918	DGD	O3D-C3D-C2D	-2.56	104.44	110.35
25	j	104	BCR	C15-C14-C13	-2.56	123.66	127.31
36	H	103	DGD	O4D-C4D-C3D	-2.56	104.44	110.35
23	d	401	CLA	C1D-CHD-C4C	-2.55	119.19	122.56
30	B	644	LMT	C4'-C3'-C2'	-2.55	106.37	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	408	PHO	C7-C6-C5	-2.55	106.43	113.36
34	B	622	LMG	C30-C29-C28	-2.55	104.34	113.62
23	d	404	CLA	C6-C7-C8	-2.55	107.67	115.92
37	E	105	HEM	CMA-C3A-C4A	-2.55	124.55	128.46
23	b	615	CLA	CHD-C4C-NC	2.54	128.21	124.20
27	a	414	PL9	C10-C9-C11	2.54	119.55	115.27
23	C	508	CLA	C3B-C4B-NB	2.54	112.50	109.21
23	b	610	CLA	C1-O2A-CGA	2.54	123.11	116.44
25	j	104	BCR	C16-C15-C14	-2.54	118.27	123.47
27	A	411	PL9	C17-C18-C19	-2.54	121.54	127.66
23	C	508	CLA	C4D-C3D-CAD	2.54	109.89	108.47
23	b	602	CLA	C3C-C4C-NC	2.54	113.42	110.57
25	d	405	BCR	C36-C18-C19	2.54	122.08	118.08
36	c	919	DGD	O1G-C1G-C2G	-2.54	101.05	108.43
23	B	615	CLA	CMC-C2C-C1C	2.54	128.90	125.04
34	J	101	LMG	O8-C28-O10	-2.54	117.19	123.59
23	b	607	CLA	O2A-CGA-O1A	-2.54	117.19	123.59
23	b	614	CLA	O2A-CGA-CBA	2.54	119.87	111.91
23	b	612	CLA	CAC-C3C-C4C	2.54	128.10	124.81
25	k	102	BCR	C11-C10-C9	-2.54	123.69	127.31
30	A	416	LMT	O5B-C5B-C6B	2.53	112.73	106.44
23	B	604	CLA	O1D-CGD-CBD	-2.53	119.30	124.48
23	c	914	CLA	C4C-C3C-C2C	-2.53	103.21	106.90
23	a	410	CLA	CHD-C4C-NC	2.53	128.19	124.20
27	D	406	PL9	C53-C6-C1	2.53	120.17	114.99
23	C	514	CLA	CHD-C4C-NC	2.53	128.19	124.20
36	c	917	DGD	CDB-CCB-CBB	-2.53	101.58	114.42
24	D	402	PHO	C1C-C2C-C3C	-2.53	103.61	106.51
23	B	603	CLA	C4-C3-C5	2.53	119.52	115.27
24	a	408	PHO	CHD-C1D-ND	-2.53	119.32	124.58
23	C	509	CLA	C2A-C1A-CHA	-2.53	119.44	123.86
23	b	605	CLA	C3B-C4B-NB	2.52	112.47	109.21
23	B	605	CLA	C6-C5-C3	-2.52	106.84	113.45
23	c	913	CLA	CMD-C2D-C3D	2.52	129.40	124.68
25	C	516	BCR	C3-C4-C5	-2.52	109.57	114.08
36	c	919	DGD	O1G-C1A-C2A	2.52	119.82	111.91
23	d	401	CLA	O2A-C1-C2	-2.52	102.01	108.64
23	b	614	CLA	CHC-C1C-NC	-2.52	120.38	124.20
23	C	513	CLA	C1-C2-C3	-2.52	121.69	126.04
23	C	508	CLA	C1-O2A-CGA	2.52	123.05	116.44
23	C	511	CLA	C4C-C3C-C2C	-2.51	103.23	106.90
27	D	406	PL9	C40-C39-C38	-2.51	117.23	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	402	PHO	O2D-CGD-CBD	2.51	115.73	111.27
28	d	410	LHG	O7-C7-C8	2.51	116.92	111.50
25	T	101	BCR	C37-C22-C21	2.51	126.44	122.92
23	d	403	CLA	C4A-NA-C1A	2.51	107.83	106.71
25	k	102	BCR	C3-C4-C5	-2.51	109.59	114.08
23	b	607	CLA	C3C-C4C-NC	2.51	113.39	110.57
25	D	405	BCR	C10-C11-C12	-2.51	115.39	123.22
34	a	413	LMG	O8-C28-O10	-2.51	117.26	123.59
36	c	917	DGD	C6D-O5D-C1E	-2.51	108.84	113.74
23	c	904	CLA	OBD-CAD-C3D	-2.50	123.82	127.98
23	C	507	CLA	OBD-CAD-C3D	-2.50	123.82	127.98
23	c	914	CLA	CED-O2D-CGD	2.50	121.60	115.94
23	c	903	CLA	C16-C17-C18	-2.50	104.19	115.98
23	C	502	CLA	C1-O2A-CGA	2.50	123.01	116.44
23	c	904	CLA	CAC-C3C-C4C	2.50	128.06	124.81
23	C	514	CLA	C4-C3-C5	2.50	119.48	115.27
23	B	605	CLA	C4C-C3C-C2C	-2.50	103.25	106.90
23	c	907	CLA	CBC-CAC-C3C	-2.50	105.54	112.43
35	B	624	HTG	O3-C3-C4	-2.50	104.57	110.35
23	b	606	CLA	C4A-NA-C1A	-2.50	105.58	106.71
26	A	415	SQD	O5-C1-C2	-2.50	105.06	110.35
25	B	619	BCR	C30-C25-C26	-2.50	119.10	122.61
30	z	101	LMT	C1B-O1B-C4'	-2.50	111.78	117.96
26	A	415	SQD	O48-C23-O10	-2.50	117.29	123.59
30	m	104	LMT	C3'-C4'-C5'	-2.50	105.20	110.93
23	b	604	CLA	C5-C3-C2	-2.49	116.07	121.12
23	b	612	CLA	CMB-C2B-C3B	2.49	129.34	124.68
28	l	101	LHG	O8-C23-O10	-2.49	117.31	123.59
23	b	605	CLA	CHD-C4C-NC	2.49	128.12	124.20
25	t	101	BCR	C34-C9-C8	2.49	121.99	118.08
23	c	914	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
30	z	101	LMT	O1'-C1'-C2'	2.48	111.06	108.15
23	b	610	CLA	CMD-C2D-C3D	2.48	129.32	124.68
27	D	406	PL9	C27-C28-C29	-2.48	121.68	127.66
25	a	411	BCR	C8-C7-C6	-2.48	120.23	127.20
23	b	612	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
25	T	101	BCR	C21-C20-C19	-2.48	115.48	123.22
23	C	510	CLA	CHB-C4A-NA	2.48	127.94	124.51
23	D	403	CLA	CMB-C2B-C3B	2.48	129.32	124.68
36	C	517	DGD	C3D-C4D-C5D	-2.48	105.82	110.24
23	B	610	CLA	CBC-CAC-C3C	-2.48	105.60	112.43
23	c	904	CLA	C4C-C3C-C2C	-2.48	103.29	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	e	105	HEM	CMD-C2D-C3D	2.48	129.61	124.94
25	b	620	BCR	C23-C24-C25	-2.47	120.25	127.20
23	B	612	CLA	C3C-C4C-NC	2.47	113.34	110.57
23	D	404	CLA	C6-C7-C8	-2.47	107.92	115.92
27	A	411	PL9	O2-C1-C2	-2.47	116.11	121.78
25	c	916	BCR	C11-C10-C9	-2.47	123.78	127.31
23	b	612	CLA	C3C-C4C-NC	2.47	113.34	110.57
25	k	102	BCR	C38-C26-C25	-2.47	121.76	124.53
24	A	407	PHO	C1C-NC-C4C	-2.46	101.87	106.51
23	b	609	CLA	C3B-C4B-NB	2.46	112.40	109.21
25	c	916	BCR	C21-C20-C19	-2.46	115.53	123.22
25	B	620	BCR	C37-C22-C21	2.46	126.37	122.92
23	C	513	CLA	O1D-CGD-CBD	-2.46	119.45	124.48
23	C	505	CLA	CMC-C2C-C1C	2.46	128.79	125.04
23	c	911	CLA	CHB-C4A-NA	2.46	127.92	124.51
23	d	404	CLA	CMB-C2B-C1B	2.46	132.25	128.46
36	c	919	DGD	O3D-C3D-C4D	2.46	116.04	110.35
23	C	512	CLA	C4-C3-C5	2.46	119.41	115.27
23	D	401	CLA	C3C-C4C-NC	2.46	113.33	110.57
23	A	405	CLA	O2A-CGA-O1A	-2.46	117.39	123.59
23	D	403	CLA	CAA-CBA-CGA	-2.46	106.07	113.25
24	a	408	PHO	C4D-ND-C1D	-2.46	102.34	106.76
25	A	409	BCR	C24-C23-C22	-2.46	122.52	126.23
23	c	902	CLA	C4-C3-C5	2.46	119.40	115.27
23	B	617	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
23	b	604	CLA	CHD-C4C-NC	2.46	128.07	124.20
23	c	910	CLA	C12-C11-C10	-2.46	101.96	113.24
23	c	906	CLA	C11-C10-C8	-2.45	107.99	115.92
23	c	903	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
28	E	101	LHG	O7-C7-O9	-2.45	117.77	123.70
23	a	410	CLA	CBC-CAC-C3C	-2.45	105.67	112.43
34	c	930	LMG	C3-C4-C5	2.45	114.61	110.24
37	e	105	HEM	CMA-C3A-C4A	-2.45	124.70	128.46
23	B	607	CLA	C3C-C4C-NC	2.45	113.32	110.57
24	D	402	PHO	CHC-C1C-C2C	-2.45	119.57	125.73
23	C	502	CLA	C3C-C4C-NC	2.45	113.31	110.57
23	a	406	CLA	O2D-CGD-CBD	2.45	115.61	111.27
23	b	607	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
23	b	617	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
23	c	912	CLA	O2A-CGA-CBA	2.44	119.57	111.91
23	c	911	CLA	C3B-C4B-NB	2.44	112.36	109.21
25	Y	101	BCR	C4-C5-C6	2.44	126.27	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	C	531	LMG	O6-C5-C6	2.44	112.50	106.44
30	a	418	LMT	O2'-C2'-C3'	-2.44	104.71	110.35
23	b	602	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
34	C	501	LMG	O8-C28-C29	2.44	119.56	111.91
26	a	412	SQD	O8-S-C6	2.44	109.62	105.74
23	b	613	CLA	O2A-CGA-CBA	2.44	119.55	111.91
23	A	408	CLA	O2A-C1-C2	-2.44	102.23	108.64
23	b	606	CLA	C1D-CHD-C4C	-2.44	119.34	122.56
27	d	406	PL9	C22-C23-C24	-2.43	121.80	127.66
23	c	903	CLA	C16-C15-C13	-2.43	108.05	115.92
26	a	412	SQD	O47-C7-O49	-2.43	117.82	123.70
28	D	409	LHG	C11-C10-C9	-2.43	102.07	114.42
34	C	531	LMG	O8-C28-O10	-2.43	117.45	123.59
23	b	612	CLA	C2A-C1A-CHA	-2.43	119.60	123.86
36	H	103	DGD	C2G-O2G-C1B	-2.43	111.81	117.79
27	d	406	PL9	C7-C3-C4	2.43	118.85	116.88
23	d	404	CLA	CAC-C3C-C4C	2.43	127.96	124.81
28	d	410	LHG	O4-P-O5	2.43	124.25	112.24
23	C	508	CLA	C11-C10-C8	-2.43	108.07	115.92
35	b	623	HTG	C4-C3-C2	2.43	115.06	110.82
28	D	409	LHG	O7-C7-O9	-2.43	117.84	123.70
40	V	203	HEC	CMB-C2B-C1B	-2.43	124.74	128.46
23	B	606	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
23	b	616	CLA	C11-C10-C8	-2.42	108.08	115.92
36	h	102	DGD	C6D-C5D-C4D	2.42	117.15	112.09
23	B	617	CLA	CHD-C4C-NC	2.42	128.02	124.20
25	T	101	BCR	C2-C1-C6	2.42	114.21	110.48
23	b	607	CLA	C11-C10-C8	-2.42	108.09	115.92
25	t	101	BCR	C7-C8-C9	-2.42	122.58	126.23
23	C	504	CLA	CMD-C2D-C3D	2.42	129.21	124.68
23	B	615	CLA	OBD-CAD-C3D	-2.42	123.97	127.98
23	b	608	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
23	C	505	CLA	CMD-C2D-C3D	2.42	129.20	124.68
23	d	404	CLA	CBC-CAC-C3C	-2.42	105.77	112.43
34	c	930	LMG	O8-C28-C29	2.42	119.49	111.91
30	B	644	LMT	C1'-C2'-C3'	-2.42	104.97	110.00
25	d	405	BCR	C34-C9-C10	-2.41	119.54	122.92
25	c	916	BCR	C32-C1-C6	-2.41	106.38	110.30
23	B	613	CLA	CMD-C2D-C3D	2.41	129.19	124.68
25	t	101	BCR	C33-C5-C6	-2.41	121.82	124.53
26	L	102	SQD	O47-C7-O49	-2.41	117.87	123.70
25	A	409	BCR	C10-C11-C12	-2.41	115.69	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	C	520	LMG	O7-C10-O9	-2.41	117.87	123.70
26	D	408	SQD	O48-C23-O10	-2.41	117.50	123.59
26	D	408	SQD	O5-C1-O6	2.41	115.69	109.97
34	c	920	LMG	O5-C6-C5	-2.41	103.02	111.29
23	B	606	CLA	O2D-CGD-CBD	2.41	115.55	111.27
38	x	102	RRX	C16-C15-C14	-2.41	118.54	123.47
23	b	614	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
23	c	906	CLA	C1-O2A-CGA	2.41	122.76	116.44
25	t	101	BCR	C1-C6-C7	2.41	122.58	115.78
30	z	101	LMT	O1B-C1B-C2B	2.40	114.33	108.10
23	b	613	CLA	C5-C3-C2	-2.40	116.25	121.12
23	C	512	CLA	CBC-CAC-C3C	-2.40	105.81	112.43
31	U	202	DMS	O-S-C1	2.40	118.80	106.54
23	C	504	CLA	C5-C3-C2	-2.40	116.26	121.12
28	d	409	LHG	C34-C33-C32	-2.40	102.23	114.42
23	D	401	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
24	A	407	PHO	CBA-CAA-C2A	-2.40	106.78	113.86
23	B	616	CLA	CBC-CAC-C3C	-2.40	105.82	112.43
27	a	414	PL9	C45-C44-C46	2.40	119.30	115.27
23	c	903	CLA	O2A-CGA-CBA	2.40	119.43	111.91
40	V	203	HEC	C1D-C2D-C3D	-2.40	105.33	107.00
27	a	414	PL9	C17-C18-C19	-2.40	121.89	127.66
23	D	401	CLA	OBD-CAD-C3D	-2.40	124.00	127.98
25	Y	101	BCR	C39-C30-C25	-2.40	106.41	110.30
30	B	623	LMT	C1B-O5B-C5B	2.39	118.39	113.69
23	c	906	CLA	CMD-C2D-C3D	2.39	129.16	124.68
23	C	506	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
23	C	511	CLA	C4-C3-C5	2.39	119.29	115.27
23	c	906	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
23	c	910	CLA	CHB-C4A-NA	2.39	127.82	124.51
23	d	401	CLA	C3C-C4C-NC	2.39	113.25	110.57
25	k	102	BCR	C24-C23-C22	-2.39	122.63	126.23
23	b	604	CLA	CMA-C3A-C4A	2.39	118.19	111.77
24	a	409	PHO	C16-C15-C13	-2.39	108.21	115.92
23	b	609	CLA	C4-C3-C5	2.38	119.28	115.27
23	D	403	CLA	C14-C13-C15	-2.38	102.66	111.29
23	c	910	CLA	C1-O2A-CGA	2.38	122.69	116.44
36	h	102	DGD	O2G-C1B-O1B	-2.38	117.94	123.70
25	C	515	BCR	C24-C23-C22	-2.38	122.64	126.23
25	B	618	BCR	C24-C23-C22	-2.38	122.64	126.23
24	A	407	PHO	C1-C2-C3	-2.38	121.93	126.04
26	x	101	SQD	C3-C4-C5	2.38	114.48	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	d	411	LMG	O8-C28-O10	-2.38	117.59	123.59
26	A	410	SQD	C3-C4-C5	2.38	114.48	110.24
23	b	612	CLA	C7-C6-C5	-2.38	106.91	113.36
40	v	203	HEC	CMC-C2C-C3C	2.38	128.61	125.82
23	b	609	CLA	C5-C3-C2	-2.38	116.31	121.12
25	B	620	BCR	C7-C8-C9	-2.38	122.64	126.23
28	d	409	LHG	C32-C31-C30	-2.38	102.37	114.42
23	a	407	CLA	C3B-C4B-NB	2.37	112.28	109.21
23	c	905	CLA	C2A-C1A-CHA	-2.37	119.71	123.86
23	c	908	CLA	C16-C17-C18	-2.37	104.81	115.98
23	c	903	CLA	C3C-C4C-NC	2.37	113.22	110.57
23	d	404	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
27	a	414	PL9	C42-C43-C44	-2.37	121.96	127.66
23	C	510	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
30	a	422	LMT	O1'-C1'-C2'	2.36	112.00	108.30
25	d	405	BCR	C16-C17-C18	-2.36	123.94	127.31
27	D	406	PL9	C35-C34-C36	2.36	119.25	115.27
23	c	909	CLA	C4C-C3C-C2C	-2.36	103.45	106.90
23	C	504	CLA	CAC-C3C-C4C	2.36	127.87	124.81
23	b	605	CLA	OBD-CAD-C3D	-2.36	124.06	127.98
25	Y	101	BCR	C29-C30-C25	2.36	114.11	110.48
23	a	410	CLA	O2A-CGA-CBA	2.36	119.31	111.91
37	e	105	HEM	CMC-C2C-C3C	2.36	129.09	124.68
23	b	606	CLA	C4C-C3C-C2C	-2.36	103.46	106.90
23	C	511	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
25	b	618	BCR	C29-C28-C27	-2.35	106.12	111.38
27	A	411	PL9	C15-C14-C16	2.35	119.23	115.27
27	d	406	PL9	C36-C34-C33	-2.35	116.36	121.12
23	B	616	CLA	C4C-C3C-C2C	-2.35	103.47	106.90
23	c	910	CLA	CAA-CBA-CGA	-2.35	106.38	113.25
26	A	410	SQD	O5-C1-C2	-2.35	105.37	110.35
23	C	511	CLA	C3C-C4C-NC	2.35	113.21	110.57
23	b	603	CLA	OBD-CAD-CBD	2.35	129.25	125.89
23	B	613	CLA	C14-C13-C15	-2.35	102.78	111.29
23	b	617	CLA	CBC-CAC-C3C	-2.35	105.96	112.43
28	K	101	LHG	O4-P-O5	2.35	119.87	110.68
23	b	605	CLA	CHC-C1C-C2C	-2.35	120.23	126.72
30	T	103	LMT	C4'-C3'-C2'	2.35	114.92	110.82
26	A	415	SQD	O7-S-C6	-2.35	104.15	106.94
23	C	510	CLA	C1-O2A-CGA	2.35	122.60	116.44
25	C	516	BCR	C24-C23-C22	-2.34	122.69	126.23
34	B	622	LMG	O8-C28-O10	-2.34	117.68	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406	CLA	CBC-CAC-C3C	-2.34	105.97	112.43
25	D	405	BCR	C2-C1-C6	2.34	114.09	110.48
28	d	409	LHG	O8-C23-C24	2.34	119.26	111.91
26	x	101	SQD	O6-C1-C2	2.34	111.96	108.30
36	C	517	DGD	O2G-C1B-O1B	-2.34	118.04	123.70
23	C	502	CLA	CBC-CAC-C3C	-2.34	105.98	112.43
23	b	612	CLA	CHD-C4C-NC	2.34	127.89	124.20
23	C	506	CLA	O2A-CGA-CBA	2.34	119.25	111.91
23	B	615	CLA	C1C-C2C-C3C	-2.34	104.50	106.96
23	C	512	CLA	CHB-C4A-NA	2.34	127.75	124.51
23	d	403	CLA	CED-O2D-CGD	2.34	121.22	115.94
23	C	514	CLA	CED-O2D-CGD	2.34	121.22	115.94
23	C	502	CLA	C4C-C3C-C2C	-2.33	103.49	106.90
23	B	608	CLA	CMC-C2C-C3C	2.33	132.46	126.12
23	b	609	CLA	C11-C10-C8	-2.33	108.37	115.92
23	A	405	CLA	O2A-CGA-CBA	2.33	119.23	111.91
36	d	407	DGD	O6D-C5D-C4D	2.33	113.70	109.52
28	D	410	LHG	O4-P-O5	2.33	123.76	112.24
23	b	608	CLA	C1-C2-C3	-2.33	122.01	126.04
36	d	407	DGD	O2G-C1B-O1B	-2.33	118.07	123.70
23	b	603	CLA	C2A-C1A-CHA	-2.33	119.79	123.86
23	B	614	CLA	C7-C6-C5	-2.33	107.04	113.36
27	d	406	PL9	C31-C32-C33	-2.33	104.23	111.88
25	T	101	BCR	C33-C5-C6	-2.33	121.92	124.53
34	m	102	LMG	O8-C28-O10	-2.33	117.72	123.59
23	B	615	CLA	C4-C3-C5	2.33	119.18	115.27
23	B	602	CLA	C4-C3-C5	2.32	119.18	115.27
25	C	530	BCR	C39-C30-C25	-2.32	106.53	110.30
23	b	614	CLA	CMD-C2D-C3D	2.32	129.02	124.68
23	b	609	CLA	C4C-C3C-C2C	-2.32	103.51	106.90
36	c	919	DGD	O2G-C2G-C1G	-2.32	100.00	108.40
23	B	606	CLA	CMB-C2B-C3B	2.32	129.02	124.68
23	c	905	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
25	B	619	BCR	C29-C28-C27	-2.32	106.19	111.38
23	c	905	CLA	CMC-C2C-C1C	2.32	128.57	125.04
25	c	916	BCR	C15-C14-C13	-2.32	124.00	127.31
27	d	406	PL9	C36-C37-C38	-2.32	104.26	111.88
23	b	612	CLA	C1-C2-C3	-2.32	122.03	126.04
26	L	102	SQD	O48-C23-O10	-2.32	117.75	123.59
23	b	602	CLA	O1A-CGA-CBA	-2.32	114.70	123.73
23	B	607	CLA	C4-C3-C5	2.32	119.17	115.27
23	B	607	CLA	C4C-C3C-C2C	-2.31	103.52	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	603	CLA	CMA-C3A-C4A	-2.31	105.55	111.77
25	T	101	BCR	C3-C4-C5	-2.31	109.94	114.08
37	E	105	HEM	CAD-CBD-CGD	2.31	116.55	112.67
23	C	512	CLA	CMB-C2B-C1B	2.31	132.02	128.46
36	c	917	DGD	O1G-C1G-C2G	-2.31	101.70	108.43
28	d	409	LHG	O2-C2-C3	-2.31	101.45	109.56
23	B	608	CLA	C1-O2A-CGA	2.31	122.51	116.44
23	B	602	CLA	C1D-CHD-C4C	-2.31	119.51	122.56
23	b	614	CLA	C3C-C4C-NC	2.31	113.16	110.57
34	B	622	LMG	O8-C28-C29	2.31	119.15	111.91
35	c	923	HTG	O5-C1-S1	-2.31	107.51	113.87
23	C	503	CLA	C3C-C4C-NC	2.31	113.16	110.57
23	B	606	CLA	O2A-C1-C2	-2.30	102.58	108.64
25	k	102	BCR	C8-C7-C6	-2.30	120.74	127.20
25	Y	101	BCR	C10-C11-C12	-2.30	116.03	123.22
28	a	415	LHG	O8-C23-O10	-2.30	117.78	123.59
30	b	621	LMT	C6'-C5'-C4'	-2.30	106.63	113.33
25	c	916	BCR	C35-C13-C14	-2.30	119.70	122.92
38	H	102	RRX	C16-C15-C14	-2.30	118.76	123.47
23	d	401	CLA	O2D-CGD-CBD	2.30	115.35	111.27
23	c	902	CLA	O2A-CGA-O1A	-2.30	117.80	123.59
23	b	604	CLA	C3B-C4B-NB	2.30	112.18	109.21
35	B	625	HTG	C3-C4-C5	-2.30	106.14	110.24
25	C	516	BCR	C15-C14-C13	-2.30	124.03	127.31
23	d	404	CLA	C4-C3-C5	2.29	119.13	115.27
28	E	101	LHG	O8-C23-O10	-2.29	117.80	123.59
23	c	912	CLA	C4D-C3D-CAD	2.29	109.75	108.47
23	d	404	CLA	CBA-CAA-C2A	-2.29	107.09	113.86
23	A	405	CLA	CMA-C3A-C4A	-2.29	105.61	111.77
25	b	618	BCR	C35-C13-C12	2.29	121.69	118.08
26	B	621	SQD	O9-S-O7	-2.29	106.02	113.95
24	A	407	PHO	CHC-C1C-C2C	-2.29	119.97	125.73
23	B	613	CLA	O2A-CGA-CBA	2.29	119.09	111.91
23	b	614	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
23	d	401	CLA	CHD-C4C-NC	2.29	127.81	124.20
23	c	911	CLA	O2A-CGA-CBA	2.29	119.09	111.91
25	d	405	BCR	C15-C16-C17	-2.29	118.79	123.47
35	b	623	HTG	C1-O5-C5	-2.29	108.36	112.58
23	b	615	CLA	CED-O2D-CGD	2.28	121.10	115.94
25	C	515	BCR	C16-C17-C18	-2.28	124.05	127.31
27	a	414	PL9	C22-C23-C24	-2.28	122.16	127.66
34	J	101	LMG	O7-C10-O9	-2.28	118.19	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	620	BCR	C38-C26-C25	-2.28	121.97	124.53
31	b	639	DMS	C2-S-C1	2.28	110.18	98.44
23	B	613	CLA	C3B-C4B-NB	2.28	112.16	109.21
23	b	617	CLA	OBD-CAD-C3D	-2.28	124.19	127.98
25	b	618	BCR	C23-C24-C25	-2.28	120.80	127.20
23	C	505	CLA	CBC-CAC-C3C	-2.28	106.14	112.43
23	c	907	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
23	b	605	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
38	x	102	RRX	C7-C8-C9	-2.28	122.80	126.23
25	a	411	BCR	C7-C8-C9	-2.28	122.80	126.23
23	b	613	CLA	CMB-C2B-C3B	2.28	128.94	124.68
23	C	502	CLA	CMD-C2D-C3D	2.28	128.94	124.68
23	A	408	CLA	C4C-C3C-C2C	-2.28	103.58	106.90
25	B	619	BCR	C2-C1-C6	2.27	113.98	110.48
36	c	918	DGD	O1G-C1A-C2A	2.27	119.04	111.91
23	b	604	CLA	C1-C2-C3	-2.27	122.11	126.04
23	c	902	CLA	C3C-C4C-NC	2.27	113.12	110.57
25	B	618	BCR	C16-C15-C14	-2.27	118.82	123.47
23	B	605	CLA	C3B-C4B-NB	2.27	112.15	109.21
23	c	913	CLA	O2A-CGA-CBA	2.27	119.03	111.91
25	Y	101	BCR	C37-C22-C23	2.27	121.65	118.08
25	b	619	BCR	C15-C16-C17	-2.27	118.82	123.47
23	c	905	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
23	b	610	CLA	CED-O2D-CGD	2.27	121.07	115.94
27	a	414	PL9	C27-C28-C29	-2.27	122.19	127.66
23	B	603	CLA	C16-C15-C13	-2.27	108.58	115.92
23	B	603	CLA	C1-O2A-CGA	2.27	122.40	116.44
30	Z	101	LMT	O5'-C5'-C4'	2.27	114.53	109.75
23	B	612	CLA	C4-C3-C5	2.27	119.08	115.27
36	C	519	DGD	C3D-C4D-C5D	-2.27	106.20	110.24
36	C	519	DGD	O3D-C3D-C2D	-2.26	105.11	110.35
25	c	915	BCR	C33-C5-C6	-2.26	121.99	124.53
23	b	608	CLA	C7-C6-C5	-2.26	107.21	113.36
25	B	619	BCR	C8-C7-C6	-2.26	120.85	127.20
23	C	503	CLA	CHC-C1C-C2C	-2.26	120.46	126.72
23	A	405	CLA	C1C-C2C-C3C	-2.26	104.58	106.96
26	A	410	SQD	O2-C2-C1	2.26	115.54	110.05
25	j	104	BCR	C15-C16-C17	-2.26	118.84	123.47
35	O	302	HTG	C1-C2-C3	2.26	115.05	110.59
23	C	504	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
23	B	613	CLA	CED-O2D-CGD	2.26	121.04	115.94
23	c	903	CLA	C4-C3-C5	2.26	119.07	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	b	623	HTG	O5-C5-C6	2.26	112.05	106.44
23	b	614	CLA	C7-C6-C5	-2.26	107.23	113.36
34	j	101	LMG	C1-O6-C5	2.25	118.11	113.69
28	d	402	LHG	O8-C23-O10	-2.25	117.90	123.59
23	b	602	CLA	C3B-C4B-NB	2.25	112.12	109.21
23	B	617	CLA	CMB-C2B-C3B	2.25	128.89	124.68
25	A	409	BCR	C8-C7-C6	-2.25	120.88	127.20
23	b	603	CLA	CAA-CBA-CGA	-2.25	106.68	113.25
23	C	510	CLA	CMC-C2C-C3C	2.25	132.22	126.12
28	D	411	LHG	O7-C7-C8	2.25	116.35	111.50
23	A	406	CLA	CHC-C1C-C2C	-2.25	120.51	126.72
35	b	622	HTG	O2-C2-C3	-2.25	105.15	110.35
27	d	406	PL9	C40-C39-C38	-2.25	117.92	123.68
23	b	605	CLA	CGD-CBD-CAD	-2.25	103.46	110.73
24	a	409	PHO	CHB-C1B-C2B	-2.25	120.08	125.73
23	b	611	CLA	C4-C3-C5	2.25	119.05	115.27
23	b	611	CLA	C6-C5-C3	-2.25	107.57	113.45
34	D	412	LMG	O1-C7-C8	-2.24	105.48	110.90
37	E	105	HEM	C1D-C2D-C3D	-2.24	105.44	107.00
23	c	903	CLA	C2A-C1A-CHA	-2.24	119.94	123.86
23	B	609	CLA	C2A-C1A-CHA	-2.24	119.94	123.86
30	F	101	LMT	O4'-C4B-C5B	2.24	114.86	109.30
24	A	407	PHO	CBC-CAC-C3C	-2.24	106.25	112.43
23	b	609	CLA	CHC-C1C-C2C	-2.24	120.52	126.72
23	b	606	CLA	CHB-C4A-NA	2.24	127.61	124.51
25	A	409	BCR	C20-C19-C18	-2.24	120.12	126.42
27	a	414	PL9	C40-C39-C41	2.24	119.04	115.27
23	d	403	CLA	C5-C3-C2	-2.24	116.59	121.12
23	c	909	CLA	C3B-C4B-NB	2.24	112.10	109.21
27	d	406	PL9	C35-C34-C36	2.24	119.03	115.27
30	M	101	LMT	C1'-O5'-C5'	-2.24	109.30	113.69
23	B	615	CLA	CMA-C3A-C4A	-2.24	105.76	111.77
36	h	102	DGD	C6E-C5E-C4E	2.24	118.24	113.00
34	a	413	LMG	O1-C1-C2	2.24	111.79	108.30
30	B	623	LMT	C3B-C4B-C5B	2.23	114.22	110.24
23	B	615	CLA	O2A-CGA-CBA	2.23	118.92	111.91
25	j	104	BCR	C40-C30-C25	-2.23	106.68	110.30
25	c	915	BCR	C28-C27-C26	-2.23	110.09	114.08
38	x	102	RRX	O2-C28-C27	-2.23	104.90	109.68
23	b	610	CLA	C4-C3-C5	2.23	119.02	115.27
34	j	101	LMG	C31-C30-C29	-2.23	105.18	113.19
23	b	616	CLA	CMB-C2B-C3B	2.23	128.85	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	c	917	DGD	C1E-O6E-C5E	2.23	118.06	113.69
24	a	408	PHO	CHD-C4C-C3C	-2.23	119.97	124.49
23	C	512	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
25	Y	101	BCR	C8-C9-C10	-2.22	115.53	118.94
26	A	415	SQD	C3-C4-C5	2.22	114.20	110.24
23	D	403	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
27	a	414	PL9	C16-C14-C13	-2.22	116.62	121.12
27	D	406	PL9	C11-C9-C8	-2.22	116.62	121.12
25	j	104	BCR	C34-C9-C8	2.22	121.58	118.08
23	C	504	CLA	CHC-C1C-NC	-2.22	120.83	124.20
23	C	507	CLA	C2A-C3A-C4A	-2.22	98.28	101.87
36	h	102	DGD	CDA-CCA-CBA	-2.22	103.16	114.42
23	b	612	CLA	O2A-C1-C2	-2.22	102.80	108.64
23	a	410	CLA	C1-C2-C3	-2.22	122.21	126.04
23	c	912	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
36	C	519	DGD	C3G-C2G-C1G	-2.22	106.54	111.79
26	L	102	SQD	O6-C44-C45	2.22	116.25	110.90
25	B	620	BCR	C8-C7-C6	-2.22	120.98	127.20
23	D	404	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
36	c	919	DGD	O1G-C1A-O1A	-2.21	118.00	123.59
23	B	604	CLA	CED-O2D-CGD	2.21	120.94	115.94
23	A	405	CLA	C4D-C3D-CAD	2.21	109.70	108.47
23	b	608	CLA	CGD-CBD-CAD	-2.21	103.57	110.73
23	c	914	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
34	C	501	LMG	O6-C1-C2	-2.21	105.67	110.35
23	C	509	CLA	O2D-CGD-CBD	2.21	115.20	111.27
25	c	915	BCR	C29-C28-C27	-2.21	106.44	111.38
23	B	606	CLA	CHC-C1C-NC	-2.21	120.85	124.20
25	b	619	BCR	C37-C22-C21	-2.21	119.83	122.92
23	D	404	CLA	CMD-C2D-C3D	2.21	128.81	124.68
23	b	616	CLA	C3C-C4C-NC	2.21	113.05	110.57
23	c	908	CLA	C3C-C4C-NC	2.21	113.05	110.57
23	a	406	CLA	C3B-C4B-NB	2.21	112.06	109.21
23	B	605	CLA	CGD-CBD-CAD	-2.21	103.59	110.73
23	c	904	CLA	CMC-C2C-C1C	2.20	128.40	125.04
23	B	604	CLA	C6-C5-C3	2.20	119.23	113.45
23	c	913	CLA	CMB-C2B-C3B	2.20	128.80	124.68
23	C	504	CLA	O2A-CGA-CBA	2.20	118.82	111.91
25	B	620	BCR	C10-C11-C12	-2.20	116.35	123.22
25	Y	101	BCR	C38-C26-C27	2.20	117.84	113.62
28	D	411	LHG	O8-C23-O10	-2.20	118.04	123.59
23	C	502	CLA	C1-C2-C3	-2.20	122.24	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	602	CLA	C3B-C4B-NB	2.20	112.05	109.21
23	A	406	CLA	CMC-C2C-C1C	2.20	128.39	125.04
28	d	409	LHG	C13-C12-C11	-2.20	103.26	114.42
23	A	405	CLA	C5-C3-C2	-2.20	116.67	121.12
25	d	405	BCR	C7-C8-C9	-2.20	122.91	126.23
25	b	619	BCR	C30-C25-C26	-2.20	119.52	122.61
36	C	519	DGD	C4E-C3E-C2E	-2.20	106.99	110.82
25	C	530	BCR	C16-C17-C18	-2.20	124.18	127.31
23	d	404	CLA	O2A-C1-C2	-2.20	102.86	108.64
23	B	616	CLA	C3C-C4C-NC	2.20	113.03	110.57
23	a	407	CLA	CMC-C2C-C3C	2.20	132.08	126.12
23	C	508	CLA	CED-O2D-CGD	2.20	120.90	115.94
23	C	512	CLA	CAC-C3C-C4C	2.19	127.66	124.81
28	K	101	LHG	P-O6-C4	2.19	124.34	118.30
23	c	903	CLA	C6-C5-C3	-2.19	107.71	113.45
34	D	412	LMG	O8-C28-C29	2.19	118.79	111.91
23	B	612	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
30	M	101	LMT	O1'-C1-C2	-2.19	101.89	109.56
34	C	520	LMG	O1-C7-C8	-2.19	105.61	110.90
25	B	618	BCR	C20-C21-C22	-2.19	124.19	127.31
23	d	401	CLA	CHC-C1C-C2C	-2.19	120.67	126.72
34	j	101	LMG	O2-C2-C1	-2.19	104.73	110.05
23	B	606	CLA	C3B-C4B-NB	2.19	112.04	109.21
25	d	405	BCR	C2-C3-C4	2.19	116.27	111.38
23	D	404	CLA	CHD-C4C-NC	2.19	127.65	124.20
24	a	409	PHO	C11-C12-C13	-2.19	108.85	115.92
23	b	609	CLA	CHD-C4C-NC	2.19	127.65	124.20
23	B	603	CLA	CAC-C3C-C4C	2.19	127.65	124.81
23	b	614	CLA	CBC-CAC-C3C	-2.19	106.40	112.43
25	T	101	BCR	C40-C30-C25	-2.19	106.75	110.30
30	B	644	LMT	C1'-O5'-C5'	2.19	117.98	113.69
23	b	603	CLA	O2A-CGA-CBA	2.19	118.77	111.91
23	C	513	CLA	CHD-C4C-NC	2.19	127.65	124.20
23	B	617	CLA	CHB-C4A-NA	2.18	127.53	124.51
23	c	908	CLA	C11-C12-C13	-2.18	108.86	115.92
23	d	401	CLA	C6-C7-C8	-2.18	108.86	115.92
23	b	612	CLA	C6-C5-C3	2.18	119.18	113.45
23	c	902	CLA	C4D-C3D-CAD	2.18	109.69	108.47
25	k	102	BCR	C34-C9-C10	-2.18	119.87	122.92
25	B	618	BCR	C21-C20-C19	-2.18	116.41	123.22
23	D	403	CLA	CBC-CAC-C3C	-2.18	106.42	112.43
23	b	613	CLA	CHD-C4C-NC	2.18	127.64	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	604	CLA	C7-C6-C5	-2.18	107.44	113.36
35	v	204	HTG	O5-C5-C4	2.18	113.65	109.69
30	z	101	LMT	C1B-O5B-C5B	-2.18	109.42	113.69
36	C	519	DGD	O2G-C1B-O1B	-2.18	118.44	123.70
23	c	905	CLA	C4C-C3C-C2C	-2.18	103.73	106.90
23	a	410	CLA	CMC-C2C-C1C	2.17	128.35	125.04
23	C	514	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
34	j	101	LMG	C6-C5-C4	2.17	118.10	113.00
25	t	101	BCR	C8-C9-C10	-2.17	115.61	118.94
25	d	405	BCR	C30-C25-C24	2.17	121.92	115.78
34	c	930	LMG	O7-C10-O9	-2.17	118.45	123.70
26	a	412	SQD	C44-O6-C1	-2.17	109.50	113.74
23	C	509	CLA	OBD-CAD-CBD	-2.17	122.79	125.89
23	C	513	CLA	CHB-C4A-NA	2.17	127.52	124.51
23	b	615	CLA	C1-O2A-CGA	2.17	122.14	116.44
28	l	101	LHG	C6-C5-C4	-2.17	106.65	111.79
40	V	203	HEC	C3B-C4B-NB	-2.17	106.85	110.94
23	c	907	CLA	C3C-C4C-NC	2.17	113.00	110.57
23	a	410	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
23	b	602	CLA	OBD-CAD-CBD	2.17	128.99	125.89
25	T	101	BCR	C34-C9-C8	2.17	121.49	118.08
25	t	101	BCR	C12-C13-C14	-2.17	115.62	118.94
23	b	615	CLA	OBD-CAD-C3D	-2.17	124.39	127.98
23	b	615	CLA	O2A-CGA-CBA	2.16	118.70	111.91
23	B	608	CLA	CHC-C1C-NC	-2.16	120.92	124.20
23	A	406	CLA	C4-C3-C5	2.16	118.91	115.27
23	d	403	CLA	CHD-C4C-NC	2.16	127.61	124.20
36	H	103	DGD	O5E-C6E-C5E	-2.16	103.87	111.29
23	c	907	CLA	CMC-C2C-C1C	2.16	128.33	125.04
30	b	621	LMT	C1-O1'-C1'	-2.16	110.26	113.84
23	C	505	CLA	C7-C6-C5	-2.16	107.50	113.36
36	C	517	DGD	O5D-C1E-C2E	-2.16	104.93	108.30
30	F	101	LMT	C1'-C2'-C3'	2.16	114.49	110.00
23	B	615	CLA	C4D-C3D-CAD	2.16	109.67	108.47
24	A	407	PHO	O2A-CGA-O1A	-2.16	118.15	123.59
28	E	101	LHG	C6-O8-C23	2.16	125.10	117.12
23	b	607	CLA	C7-C6-C5	-2.16	107.51	113.36
37	E	105	HEM	CBA-CAA-C2A	-2.15	108.51	112.49
28	K	101	LHG	O8-C23-O10	-2.15	118.15	123.59
26	a	412	SQD	O48-C23-C24	2.15	118.67	111.91
25	B	620	BCR	C16-C17-C18	-2.15	124.24	127.31
23	C	509	CLA	C3C-C4C-NC	2.15	112.98	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	511	CLA	CHC-C1C-C2C	-2.15	120.77	126.72
25	A	409	BCR	C39-C30-C25	-2.15	106.81	110.30
26	A	410	SQD	O8-S-C6	2.15	109.16	105.74
25	j	104	BCR	C8-C9-C10	-2.15	115.64	118.94
23	C	506	CLA	C7-C6-C5	-2.15	107.53	113.36
23	A	406	CLA	C2A-C1A-CHA	-2.15	120.10	123.86
30	B	623	LMT	O5B-C5B-C4B	2.15	113.59	109.69
30	e	103	LMT	O5'-C5'-C4'	2.15	114.28	109.75
30	e	103	LMT	O1'-C1'-C2'	2.14	111.65	108.30
23	c	908	CLA	C7-C6-C5	-2.14	107.54	113.36
24	a	409	PHO	CHD-C1D-ND	-2.14	120.12	124.58
23	c	910	CLA	CMB-C2B-C1B	2.14	131.76	128.46
23	A	408	CLA	CBA-CAA-C2A	-2.14	107.54	113.86
23	c	907	CLA	CGD-CBD-CAD	-2.14	103.79	110.73
25	b	618	BCR	C8-C7-C6	-2.14	121.19	127.20
36	c	919	DGD	O3G-C1D-C2D	-2.14	104.96	108.30
23	B	614	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
23	C	509	CLA	CMB-C2B-C3B	2.14	128.68	124.68
25	C	515	BCR	C34-C9-C8	2.14	121.44	118.08
36	c	918	DGD	O6E-C5E-C6E	2.14	111.75	106.44
30	a	418	LMT	O2'-C2'-C1'	2.14	115.23	110.05
23	b	608	CLA	O2A-CGA-CBA	2.14	118.61	111.91
25	d	405	BCR	C34-C9-C8	2.13	121.44	118.08
25	t	101	BCR	C7-C6-C5	-2.13	116.29	121.46
34	B	622	LMG	O1-C7-C8	-2.13	105.75	110.90
25	b	618	BCR	C11-C10-C9	-2.13	124.27	127.31
30	I	101	LMT	C1B-O1B-C4'	2.13	123.24	117.96
23	b	604	CLA	O2A-CGA-CBA	2.13	118.60	111.91
34	J	101	LMG	O6-C1-C2	2.13	114.86	110.35
23	A	408	CLA	CMC-C2C-C3C	2.13	131.90	126.12
23	B	605	CLA	C4-C3-C5	2.13	118.85	115.27
23	c	904	CLA	C3C-C4C-NC	2.13	112.96	110.57
38	H	102	RRX	C32-C1-C6	2.13	113.75	110.30
23	C	509	CLA	C4C-C3C-C2C	-2.13	103.80	106.90
25	k	102	BCR	C34-C9-C8	2.13	121.43	118.08
23	D	404	CLA	O2A-CGA-CBA	2.13	118.58	111.91
23	b	604	CLA	CHC-C1C-NC	-2.13	120.98	124.20
36	c	918	DGD	O4E-C4E-C3E	-2.13	105.43	110.35
30	b	621	LMT	C3'-C4'-C5'	2.13	115.80	110.93
23	B	607	CLA	C4D-C3D-CAD	2.13	109.66	108.47
36	C	519	DGD	O2G-C1B-C2B	2.12	116.08	111.50
25	T	101	BCR	C29-C28-C27	-2.12	106.63	111.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	618	BCR	C32-C1-C6	-2.12	106.85	110.30
23	B	615	CLA	CMB-C2B-C1B	2.12	131.73	128.46
25	d	405	BCR	C32-C1-C2	-2.12	100.41	108.91
25	j	104	BCR	C29-C30-C25	2.12	113.75	110.48
23	C	509	CLA	CHD-C4C-NC	2.12	127.55	124.20
25	B	618	BCR	C34-C9-C10	-2.12	119.95	122.92
24	a	409	PHO	C1C-C2C-C3C	-2.12	104.07	106.51
23	B	612	CLA	C4C-C3C-C2C	-2.12	103.81	106.90
25	c	915	BCR	C15-C16-C17	-2.12	119.13	123.47
23	c	914	CLA	C1D-CHD-C4C	-2.12	119.76	122.56
23	B	603	CLA	C1D-CHD-C4C	-2.12	119.76	122.56
23	C	512	CLA	OBD-CAD-C3D	-2.12	124.46	127.98
35	d	413	HTG	C2'-C1'-S1	-2.12	105.56	112.40
36	C	519	DGD	C3A-C2A-C1A	-2.12	105.92	113.62
23	C	510	CLA	C4C-C3C-C2C	-2.12	103.81	106.90
23	D	403	CLA	CBA-CAA-C2A	-2.12	107.62	113.86
23	C	505	CLA	C1-O2A-CGA	2.12	122.00	116.44
23	A	405	CLA	C16-C15-C13	-2.11	109.09	115.92
25	t	101	BCR	C21-C20-C19	-2.11	116.62	123.22
25	b	619	BCR	C8-C9-C10	-2.11	115.70	118.94
23	b	607	CLA	CMB-C2B-C1B	2.11	131.71	128.46
23	b	605	CLA	O2A-CGA-CBA	2.11	118.53	111.91
25	B	619	BCR	C39-C30-C25	-2.11	106.88	110.30
35	B	630	HTG	O5-C5-C6	2.11	111.68	106.44
26	L	102	SQD	O9-S-O7	-2.11	106.65	113.95
27	D	406	PL9	O2-C1-C6	-2.11	116.94	120.59
23	b	609	CLA	C6-C5-C3	-2.11	107.93	113.45
23	B	616	CLA	C11-C10-C8	-2.11	109.11	115.92
25	T	101	BCR	C28-C27-C26	-2.11	110.31	114.08
25	c	915	BCR	C37-C22-C23	2.11	121.40	118.08
23	B	602	CLA	CAC-C3C-C4C	2.11	127.54	124.81
23	a	406	CLA	C1-C2-C3	-2.11	122.40	126.04
30	A	416	LMT	C1B-O5B-C5B	2.11	117.82	113.69
23	B	617	CLA	C4-C3-C2	-2.11	118.28	123.68
30	T	103	LMT	O5'-C1'-C2'	2.10	114.80	110.35
25	B	618	BCR	C37-C22-C23	2.10	121.39	118.08
23	D	403	CLA	OBD-CAD-C3D	-2.10	124.49	127.98
23	B	611	CLA	CMC-C2C-C3C	2.10	131.82	126.12
34	J	101	LMG	O7-C10-C11	2.10	116.03	111.50
23	b	603	CLA	C7-C6-C5	-2.10	107.66	113.36
36	c	919	DGD	CEA-CDA-CCA	-2.10	103.77	114.42
23	b	614	CLA	C3B-C4B-NB	2.10	111.92	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	604	CLA	C2A-C1A-CHA	-2.10	120.19	123.86
25	T	101	BCR	C1-C6-C7	2.10	121.70	115.78
23	b	611	CLA	C1-O2A-CGA	2.09	121.94	116.44
23	d	404	CLA	CMC-C2C-C3C	2.09	131.80	126.12
23	c	909	CLA	OBD-CAD-CBD	2.09	128.89	125.89
23	B	617	CLA	O2A-C1-C2	2.09	114.14	108.64
25	T	101	BCR	C7-C6-C5	-2.09	116.39	121.46
23	b	611	CLA	OBD-CAD-C3D	-2.09	124.51	127.98
23	a	410	CLA	C3B-C4B-NB	2.09	111.92	109.21
23	b	603	CLA	C2A-C3A-C4A	-2.09	98.49	101.87
23	b	608	CLA	CBC-CAC-C3C	-2.09	106.66	112.43
23	a	410	CLA	C2A-C1A-CHA	-2.09	120.20	123.86
23	C	504	CLA	C3C-C4C-NC	2.09	112.92	110.57
28	a	415	LHG	O7-C7-O9	-2.09	118.65	123.70
34	B	622	LMG	C18-C17-C16	-2.09	103.82	114.42
23	C	512	CLA	O2A-C1-C2	-2.09	103.14	108.64
23	b	608	CLA	CED-O2D-CGD	2.09	120.66	115.94
23	c	906	CLA	CED-O2D-CGD	2.09	120.66	115.94
23	B	610	CLA	OBD-CAD-CBD	2.09	128.88	125.89
23	c	904	CLA	C7-C6-C5	-2.09	107.69	113.36
23	B	612	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
23	b	604	CLA	C4C-C3C-C2C	-2.09	103.85	106.90
30	m	104	LMT	C1-O1'-C1'	2.09	117.30	113.84
26	D	408	SQD	O5-C5-C4	2.08	113.48	109.69
25	B	619	BCR	C33-C5-C6	-2.08	122.19	124.53
28	e	101	LHG	O8-C23-O10	-2.08	118.33	123.59
23	B	603	CLA	C3B-C4B-NB	2.08	111.90	109.21
36	h	102	DGD	O3G-C3G-C2G	-2.08	105.88	110.90
23	b	615	CLA	CMB-C2B-C1B	2.08	131.66	128.46
23	b	610	CLA	C1-C2-C3	-2.08	122.44	126.04
23	b	607	CLA	O2A-CGA-CBA	2.08	118.44	111.91
23	c	906	CLA	O2A-CGA-CBA	2.08	118.43	111.91
35	v	204	HTG	O4-C4-C3	-2.08	105.54	110.35
23	c	906	CLA	C4C-C3C-C2C	-2.08	103.87	106.90
23	B	609	CLA	C1-O2A-CGA	2.08	121.90	116.44
34	B	622	LMG	C38-C37-C36	-2.08	103.88	114.42
36	c	918	DGD	C2G-O2G-C1B	-2.08	112.68	117.79
23	c	905	CLA	CMD-C2D-C3D	2.07	128.56	124.68
23	D	403	CLA	C4C-C3C-C2C	-2.07	103.88	106.90
25	b	618	BCR	C20-C19-C18	-2.07	120.59	126.42
23	b	602	CLA	C4C-C3C-C2C	-2.07	103.88	106.90
26	A	410	SQD	O3-C3-C2	-2.07	105.56	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	D	412	LMG	C3-C4-C5	2.07	113.93	110.24
23	c	903	CLA	C1-C2-C3	-2.07	122.46	126.04
25	B	620	BCR	C38-C26-C27	2.07	117.59	113.62
36	D	407	DGD	O2G-C1B-O1B	-2.07	118.70	123.70
26	A	410	SQD	C44-O6-C1	-2.07	109.70	113.74
24	a	409	PHO	CHD-C4C-C3C	-2.07	120.29	124.49
23	C	508	CLA	CAC-C3C-C4C	2.07	127.49	124.81
26	A	415	SQD	C46-O48-C23	2.07	124.77	117.12
23	C	503	CLA	CMD-C2D-C3D	2.07	128.54	124.68
25	C	516	BCR	C38-C26-C25	-2.06	122.21	124.53
27	A	411	PL9	C16-C14-C13	-2.06	116.94	121.12
30	F	101	LMT	O5B-C5B-C6B	2.06	111.56	106.44
23	A	405	CLA	CED-O2D-CGD	2.06	120.60	115.94
23	B	609	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
35	d	413	HTG	O5-C1-S1	-2.06	104.91	109.82
23	C	502	CLA	CMB-C2B-C3B	2.06	128.53	124.68
23	B	605	CLA	O2A-CGA-CBA	2.06	118.36	111.91
25	j	104	BCR	C10-C11-C12	-2.06	116.80	123.22
23	B	614	CLA	C1-C2-C3	-2.05	122.49	126.04
23	B	604	CLA	C1B-CHB-C4A	-2.05	126.05	130.12
23	c	907	CLA	O2A-CGA-CBA	2.05	118.35	111.91
30	I	101	LMT	C2'-C3'-C4'	-2.05	104.99	109.68
23	D	404	CLA	CMC-C2C-C1C	2.05	128.16	125.04
23	b	610	CLA	CHD-C4C-NC	2.05	127.44	124.20
23	B	612	CLA	C3B-C4B-NB	2.05	111.86	109.21
23	c	903	CLA	C4C-C3C-C2C	-2.05	103.91	106.90
23	c	910	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
28	D	409	LHG	C6-O8-C23	2.05	124.72	117.12
23	c	905	CLA	CBC-CAC-C3C	-2.05	106.78	112.43
28	l	101	LHG	O4-P-O5	2.05	122.38	112.24
23	c	911	CLA	O2D-CGD-O1D	-2.05	119.83	123.84
23	B	603	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
27	D	406	PL9	C27-C26-C24	-2.05	106.24	112.98
24	a	409	PHO	CMB-C2B-C1B	2.05	128.22	125.06
23	a	406	CLA	CMC-C2C-C3C	2.05	131.68	126.12
23	C	503	CLA	C4-C3-C5	2.05	118.72	115.27
25	D	405	BCR	C36-C18-C17	-2.05	120.06	122.92
23	b	612	CLA	CHB-C4A-NA	2.05	127.34	124.51
31	h	101	DMS	O-S-C2	2.05	116.99	106.54
23	B	609	CLA	C11-C10-C8	-2.05	109.30	115.92
35	v	204	HTG	O5-C5-C6	2.05	111.53	106.44
23	c	905	CLA	CMB-C2B-C3B	2.05	128.51	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	515	BCR	C8-C7-C6	-2.05	121.46	127.20
25	B	619	BCR	C28-C27-C26	-2.04	110.43	114.08
36	c	919	DGD	C3E-C4E-C5E	-2.04	106.59	110.24
27	A	411	PL9	C20-C19-C21	2.04	118.71	115.27
34	D	412	LMG	O6-C5-C4	2.04	113.41	109.69
35	C	522	HTG	O5-C1-C2	2.04	112.88	110.31
23	B	607	CLA	O2A-CGA-CBA	2.04	118.32	111.91
23	B	617	CLA	O2A-CGA-CBA	2.04	118.31	111.91
23	d	403	CLA	O1D-CGD-CBD	2.04	128.66	124.48
23	c	906	CLA	CHC-C1C-NC	-2.04	121.11	124.20
23	C	503	CLA	CBC-CAC-C3C	-2.04	106.81	112.43
23	D	403	CLA	CHC-C1C-C2C	-2.04	121.08	126.72
24	A	407	PHO	CHD-C1D-ND	-2.04	120.34	124.58
25	d	405	BCR	C10-C11-C12	-2.04	116.86	123.22
26	a	417	SQD	O6-C44-C45	-2.04	105.98	110.90
30	a	418	LMT	O5B-C5B-C4B	2.04	113.39	109.69
23	c	909	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
30	T	103	LMT	O6'-C6'-C5'	-2.03	104.32	111.29
23	b	613	CLA	CHB-C4A-NA	2.03	127.32	124.51
23	B	603	CLA	CMA-C3A-C4A	-2.03	106.31	111.77
23	d	401	CLA	CGD-CBD-CAD	-2.03	104.16	110.73
23	b	605	CLA	C6-C7-C8	-2.03	109.35	115.92
23	c	914	CLA	CAC-C3C-C4C	2.03	127.44	124.81
23	b	612	CLA	C14-C13-C15	-2.03	103.95	111.29
23	c	911	CLA	O2A-C1-C2	-2.03	103.31	108.64
23	D	401	CLA	CAC-C3C-C2C	-2.03	124.06	127.53
23	C	512	CLA	C1D-CHD-C4C	-2.03	119.88	122.56
34	j	101	LMG	O1-C7-C8	-2.03	106.01	110.90
28	D	411	LHG	O7-C7-O9	-2.03	118.81	123.70
23	B	608	CLA	C7-C6-C5	-2.03	107.86	113.36
23	B	602	CLA	CHB-C4A-NA	2.02	127.31	124.51
23	C	512	CLA	CHD-C4C-NC	2.02	127.39	124.20
23	c	911	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
23	c	903	CLA	CHB-C4A-NA	2.02	127.31	124.51
34	D	412	LMG	C8-O7-C10	-2.02	112.81	117.79
36	c	918	DGD	O5D-C1E-C2E	-2.02	105.15	108.30
25	b	620	BCR	C16-C15-C14	-2.02	119.34	123.47
23	b	612	CLA	C4C-C3C-C2C	-2.02	103.95	106.90
36	H	103	DGD	O4D-C4D-C5D	2.02	114.31	109.30
34	C	520	LMG	C9-C8-C7	-2.02	107.01	111.79
30	A	416	LMT	O3B-C3B-C4B	2.02	115.02	110.35
23	b	616	CLA	C1-C2-C3	-2.02	122.55	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	O	302	HTG	O2-C2-C3	-2.02	105.69	110.35
23	a	407	CLA	C1B-CHB-C4A	-2.02	126.12	130.12
23	D	404	CLA	C4C-C3C-C2C	-2.02	103.96	106.90
23	b	615	CLA	C4-C3-C5	2.02	118.66	115.27
31	c	927	DMS	O-S-C1	2.01	116.82	106.54
23	c	903	CLA	OBD-CAD-CBD	2.01	128.77	125.89
37	E	105	HEM	C3C-C4C-NC	-2.01	107.14	110.94
25	C	515	BCR	C23-C24-C25	-2.01	121.55	127.20
25	Y	101	BCR	C2-C1-C6	-2.01	107.38	110.48
36	C	518	DGD	O5D-C6D-C5D	2.01	112.77	109.05
25	B	620	BCR	C16-C15-C14	-2.01	119.36	123.47
23	b	603	CLA	C3B-C4B-NB	2.01	111.81	109.21
26	a	412	SQD	O48-C23-O10	-2.01	118.52	123.59
24	a	408	PHO	O2D-CGD-CBD	2.01	114.84	111.27
30	a	422	LMT	O2'-C2'-C1'	2.01	114.92	110.05
35	B	624	HTG	O2-C2-C3	-2.01	105.71	110.35
23	B	604	CLA	O2A-CGA-CBA	2.01	118.20	111.91
23	B	610	CLA	C7-C6-C5	-2.01	107.91	113.36
27	D	406	PL9	C31-C32-C33	-2.01	105.29	111.88
23	c	910	CLA	C4C-C3C-C2C	-2.01	103.97	106.90
25	Y	101	BCR	C20-C21-C22	-2.01	124.45	127.31
24	A	407	PHO	CMB-C2B-C1B	2.01	128.15	125.06
23	D	401	CLA	CBA-CAA-C2A	-2.01	107.94	113.86
23	C	513	CLA	O2D-CGD-O1D	-2.00	119.92	123.84
23	B	606	CLA	C1D-CHD-C4C	-2.00	119.91	122.56
23	D	403	CLA	C4D-C3D-CAD	2.00	109.59	108.47
23	C	509	CLA	OBD-CAD-C3D	2.00	131.31	127.98
23	B	609	CLA	CHD-C4C-NC	2.00	127.36	124.20
25	D	405	BCR	C38-C26-C27	2.00	117.46	113.62
30	b	621	LMT	C1'-O5'-C5'	2.00	117.62	113.69
23	B	612	CLA	C15-C13-C12	-2.00	101.61	112.13
23	D	403	CLA	CED-O2D-CGD	2.00	120.46	115.94

All (169) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	b	605	CLA	NC
23	b	605	CLA	ND
23	b	605	CLA	NA
23	C	504	CLA	NC
23	C	504	CLA	NA
23	a	407	CLA	NC

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Mol	Chain	Res	Type	Atom
23	a	407	CLA	NA
23	A	405	CLA	NC
23	A	405	CLA	NA
23	c	912	CLA	NC
23	c	912	CLA	NA
23	d	403	CLA	ND
23	d	403	CLA	NA
23	B	605	CLA	NC
23	B	605	CLA	ND
23	B	605	CLA	NA
23	c	910	CLA	NC
23	c	910	CLA	ND
23	c	910	CLA	NA
23	a	406	CLA	NC
23	a	406	CLA	ND
23	a	406	CLA	NA
23	b	613	CLA	NA
23	b	613	CLA	NC
23	b	613	CLA	ND
23	A	406	CLA	NC
23	A	406	CLA	NA
23	C	513	CLA	NC
23	C	513	CLA	ND
23	C	513	CLA	NA
23	B	602	CLA	NC
23	B	602	CLA	ND
23	C	514	CLA	NC
23	D	403	CLA	ND
23	B	614	CLA	NC
23	B	614	CLA	ND
23	B	614	CLA	NA
23	b	615	CLA	NC
23	b	615	CLA	ND
23	b	615	CLA	NA
23	a	410	CLA	NC
23	B	604	CLA	NC
23	B	604	CLA	ND
23	B	604	CLA	NA
23	B	613	CLA	NA
23	B	613	CLA	NC
23	B	613	CLA	ND
23	B	603	CLA	NC

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Mol	Chain	Res	Type	Atom
23	B	603	CLA	ND
23	B	603	CLA	NA
23	b	607	CLA	NC
23	b	607	CLA	ND
23	b	607	CLA	NA
23	c	903	CLA	NC
23	c	903	CLA	NA
23	D	401	CLA	NA
23	c	902	CLA	NC
23	c	902	CLA	ND
23	c	902	CLA	NA
23	C	505	CLA	NC
23	C	505	CLA	ND
23	C	505	CLA	NA
23	b	614	CLA	NC
23	b	614	CLA	ND
23	b	614	CLA	NA
23	c	907	CLA	ND
23	c	907	CLA	NA
23	c	908	CLA	NC
23	c	908	CLA	ND
23	c	908	CLA	NA
23	C	510	CLA	NC
23	C	510	CLA	NA
23	C	510	CLA	ND
23	B	616	CLA	NC
23	B	616	CLA	ND
23	B	616	CLA	NA
23	c	911	CLA	NC
23	c	911	CLA	ND
23	c	911	CLA	NA
23	A	408	CLA	NC
23	A	408	CLA	NA
23	B	609	CLA	NC
23	B	615	CLA	NC
23	B	615	CLA	ND
23	B	615	CLA	NA
23	c	909	CLA	NC
23	c	909	CLA	NA
23	C	502	CLA	NC
23	C	502	CLA	ND
23	C	502	CLA	NA

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Mol	Chain	Res	Type	Atom
23	B	606	CLA	NC
23	B	606	CLA	ND
23	B	606	CLA	NA
23	b	602	CLA	NC
23	b	602	CLA	ND
23	b	602	CLA	NA
23	C	508	CLA	NC
23	C	508	CLA	ND
23	C	508	CLA	NA
23	b	609	CLA	NC
23	b	606	CLA	NC
23	b	606	CLA	ND
23	b	606	CLA	NA
23	C	509	CLA	NC
23	C	509	CLA	ND
23	C	509	CLA	NA
23	b	611	CLA	NC
23	b	611	CLA	ND
23	b	611	CLA	NA
23	C	507	CLA	NC
23	C	507	CLA	ND
23	C	507	CLA	NA
23	d	401	CLA	NA
23	d	404	CLA	NC
23	b	604	CLA	NC
23	b	604	CLA	ND
23	b	604	CLA	NA
23	B	612	CLA	NC
23	B	612	CLA	ND
23	B	612	CLA	NA
23	C	511	CLA	NA
23	C	511	CLA	NC
23	C	511	CLA	ND
23	c	904	CLA	NC
23	c	913	CLA	NC
23	c	913	CLA	ND
23	c	913	CLA	NA
23	b	617	CLA	NC
23	b	617	CLA	ND
23	b	617	CLA	NA
23	c	914	CLA	NC
23	D	404	CLA	NC

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Mol	Chain	Res	Type	Atom
23	D	404	CLA	ND
23	D	404	CLA	NA
23	C	506	CLA	ND
23	C	506	CLA	NA
23	B	608	CLA	NC
23	B	608	CLA	ND
23	B	608	CLA	NA
23	b	610	CLA	NC
23	b	610	CLA	NA
23	B	607	CLA	NC
23	B	607	CLA	ND
23	B	607	CLA	NA
23	B	610	CLA	NC
23	B	610	CLA	NA
23	C	512	CLA	NC
23	C	512	CLA	NA
23	B	617	CLA	NC
23	B	617	CLA	ND
23	B	617	CLA	NA
23	C	503	CLA	NA
23	B	611	CLA	NC
23	B	611	CLA	ND
23	B	611	CLA	NA
23	b	616	CLA	NC
23	b	616	CLA	ND
23	b	616	CLA	NA
23	b	603	CLA	NC
23	b	603	CLA	ND
23	b	603	CLA	NA
23	b	608	CLA	NC
23	b	608	CLA	ND
23	b	608	CLA	NA
23	c	906	CLA	ND
23	c	906	CLA	NA
23	c	905	CLA	NC
23	c	905	CLA	NA
23	b	612	CLA	NC

All (1567) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	m	103	LMT	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
25	D	405	BCR	C21-C22-C23-C24
25	D	405	BCR	C37-C22-C23-C24
25	t	101	BCR	C11-C12-C13-C14
25	t	101	BCR	C11-C12-C13-C35
35	v	204	HTG	C2'-C1'-S1-C1
34	d	411	LMG	C2-C1-O1-C7
34	d	411	LMG	O6-C1-O1-C7
34	d	411	LMG	C8-C9-O8-C28
34	d	411	LMG	C11-C10-O7-C8
35	C	521	HTG	C2'-C1'-S1-C1
28	l	101	LHG	C4-O6-P-O4
26	L	102	SQD	O5-C1-O6-C44
26	L	102	SQD	O49-C7-O47-C45
35	B	626	HTG	O5-C1-S1-C1'
23	B	602	CLA	CHA-CBD-CGD-O1D
23	B	602	CLA	CHA-CBD-CGD-O2D
23	B	602	CLA	CAD-CBD-CGD-O1D
23	b	615	CLA	CHA-CBD-CGD-O2D
23	b	615	CLA	CAD-CBD-CGD-O1D
30	e	103	LMT	C2'-C1'-O1'-C1
30	e	103	LMT	O5'-C1'-O1'-C1
34	D	412	LMG	C11-C10-O7-C8
23	B	603	CLA	CHA-CBD-CGD-O2D
23	b	607	CLA	CHA-CBD-CGD-O1D
23	b	607	CLA	CHA-CBD-CGD-O2D
23	D	401	CLA	CHA-CBD-CGD-O1D
25	d	405	BCR	C37-C22-C23-C24
25	d	405	BCR	C23-C24-C25-C30
28	e	101	LHG	C4-O6-P-O3
26	a	417	SQD	C2-C1-O6-C44
26	a	417	SQD	O5-C1-O6-C44
26	a	417	SQD	O6-C44-C45-O47
23	A	408	CLA	C2-C3-C5-C6
23	A	408	CLA	C4-C3-C5-C6
35	C	522	HTG	C2-C1-S1-C1'
35	C	522	HTG	O5-C1-S1-C1'
23	B	615	CLA	CHA-CBD-CGD-O2D
23	B	615	CLA	CAD-CBD-CGD-O1D
28	A	412	LHG	C4-O6-P-O4
28	A	412	LHG	C4-O6-P-O5
28	A	412	LHG	C8-C7-O7-C5
23	c	909	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
34	C	501	LMG	C2-C1-O1-C7
34	C	501	LMG	O6-C1-O1-C7
28	d	402	LHG	O1-C1-C2-C3
23	B	606	CLA	C2-C3-C5-C6
23	B	606	CLA	C4-C3-C5-C6
23	b	602	CLA	C2-C1-O2A-CGA
23	b	602	CLA	CHA-CBD-CGD-O1D
23	b	602	CLA	CHA-CBD-CGD-O2D
23	b	602	CLA	CAD-CBD-CGD-O1D
36	D	407	DGD	C2A-C1A-O1G-C1G
36	D	407	DGD	O1A-C1A-O1G-C1G
36	D	407	DGD	C2B-C1B-O2G-C2G
36	D	407	DGD	C2D-C1D-O3G-C3G
35	d	413	HTG	O5-C1-S1-C1'
35	d	413	HTG	C2'-C1'-S1-C1
35	b	623	HTG	C2-C1-S1-C1'
35	b	623	HTG	O5-C1-S1-C1'
23	C	509	CLA	CHA-CBD-CGD-O1D
28	K	101	LHG	C4-O6-P-O4
28	K	101	LHG	O9-C7-O7-C5
28	K	101	LHG	C8-C7-O7-C5
23	C	507	CLA	C1A-C2A-CAA-CBA
35	c	921	HTG	C2-C1-S1-C1'
35	c	921	HTG	O5-C1-S1-C1'
35	B	625	HTG	C2'-C1'-S1-C1
27	A	411	PL9	C9-C11-C12-C13
27	A	411	PL9	C24-C26-C27-C28
27	A	411	PL9	C28-C29-C31-C32
27	A	411	PL9	C30-C29-C31-C32
36	d	407	DGD	C2B-C1B-O2G-C2G
36	d	407	DGD	O1B-C1B-O2G-C2G
30	Z	101	LMT	C2'-C1'-O1'-C1
23	b	617	CLA	O2A-C1-C2-C3
23	b	617	CLA	C2-C3-C5-C6
23	b	617	CLA	C4-C3-C5-C6
28	a	415	LHG	C4-O6-P-O3
28	a	415	LHG	C4-O6-P-O4
28	L	101	LHG	C4-O6-P-O3
28	L	101	LHG	C4-O6-P-O4
28	L	101	LHG	C4-O6-P-O5
26	x	101	SQD	C5-C6-S-O8
26	x	101	SQD	C5-C6-S-O9

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Mol	Chain	Res	Type	Atoms
28	d	409	LHG	O1-C1-C2-C3
26	A	415	SQD	C2-C1-O6-C44
26	A	415	SQD	O6-C44-C45-O47
23	b	603	CLA	CHA-CBD-CGD-O1D
35	C	523	HTG	O5-C1-S1-C1'
28	D	410	LHG	C4-O6-P-O4
28	E	101	LHG	C3-O3-P-O4
28	E	101	LHG	O6-C4-C5-O7
30	b	621	LMT	C3'-C4'-O1B-C1B
34	d	411	LMG	O10-C28-O8-C9
28	E	101	LHG	O10-C23-O8-C6
30	m	103	LMT	C4B-C5B-C6B-O6B
30	I	101	LMT	C3'-C4'-O1B-C1B
28	E	101	LHG	C24-C23-O8-C6
28	d	402	LHG	O10-C23-O8-C6
23	b	602	CLA	O1A-CGA-O2A-C1
26	D	408	SQD	O10-C23-O48-C46
23	B	611	CLA	C15-C16-C17-C18
23	C	514	CLA	CBD-CGD-O2D-CED
34	d	411	LMG	O9-C10-O7-C8
34	D	412	LMG	O9-C10-O7-C8
28	A	412	LHG	O9-C7-O7-C5
36	D	407	DGD	O1B-C1B-O2G-C2G
35	v	204	HTG	C1'-C2'-C3'-C4'
23	B	605	CLA	C3-C5-C6-C7
23	B	602	CLA	C3-C5-C6-C7
23	B	615	CLA	C3-C5-C6-C7
34	d	411	LMG	C29-C28-O8-C9
28	d	402	LHG	C24-C23-O8-C6
23	b	602	CLA	CBA-CGA-O2A-C1
26	D	408	SQD	C24-C23-O48-C46
26	L	102	SQD	C8-C7-O47-C45
28	E	101	LHG	C8-C7-O7-C5
23	b	613	CLA	C13-C15-C16-C17
34	m	102	LMG	C37-C38-C39-C40
34	C	501	LMG	C29-C28-O8-C9
36	d	407	DGD	C2A-C1A-O1G-C1G
30	T	103	LMT	O5'-C5'-C6'-O6'
30	B	623	LMT	O5B-C5B-C6B-O6B
23	b	617	CLA	O1D-CGD-O2D-CED
35	v	204	HTG	S1-C1'-C2'-C3'
35	C	521	HTG	S1-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
30	m	103	LMT	O5B-C5B-C6B-O6B
30	a	418	LMT	O5B-C5B-C6B-O6B
28	E	101	LHG	O9-C7-O7-C5
34	C	501	LMG	O10-C28-O8-C9
28	E	101	LHG	O2-C2-C3-O3
23	A	408	CLA	C3-C5-C6-C7
36	d	407	DGD	O1A-C1A-O1G-C1G
35	B	631	HTG	O5-C5-C6-O6
30	F	101	LMT	O5'-C5'-C6'-O6'
23	b	616	CLA	C13-C15-C16-C17
36	C	517	DGD	C4A-C5A-C6A-C7A
35	B	626	HTG	O5-C5-C6-O6
30	T	103	LMT	C4'-C5'-C6'-O6'
28	d	410	LHG	C30-C31-C32-C33
34	a	413	LMG	C15-C16-C17-C18
28	a	415	LHG	C17-C18-C19-C20
35	B	630	HTG	S1-C1'-C2'-C3'
30	z	101	LMT	C4'-C5'-C6'-O6'
30	B	623	LMT	C4B-C5B-C6B-O6B
30	Z	101	LMT	C5-C6-C7-C8
34	D	412	LMG	O6-C5-C6-O5
35	v	204	HTG	O5-C5-C6-O6
30	a	418	LMT	C4B-C5B-C6B-O6B
30	m	103	LMT	O5'-C1'-O1'-C1
30	Z	101	LMT	O5'-C1'-O1'-C1
26	A	415	SQD	O5-C1-O6-C44
27	a	414	PL9	C19-C21-C22-C23
27	a	414	PL9	C24-C26-C27-C28
36	d	407	DGD	C2A-C3A-C4A-C5A
26	B	621	SQD	C31-C32-C33-C34
28	D	411	LHG	C30-C31-C32-C33
35	b	623	HTG	C4-C5-C6-O6
36	c	919	DGD	C2B-C3B-C4B-C5B
26	B	621	SQD	C24-C23-O48-C46
23	b	617	CLA	CBA-CGA-O2A-C1
23	c	914	CLA	CBA-CGA-O2A-C1
30	B	644	LMT	O5'-C5'-C6'-O6'
35	v	204	HTG	C4-C5-C6-O6
35	c	923	HTG	C1'-C2'-C3'-C4'
35	B	631	HTG	C4-C5-C6-O6
30	F	101	LMT	C4'-C5'-C6'-O6'
34	C	501	LMG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	b	615	CLA	C5-C6-C7-C8
23	C	507	CLA	C15-C16-C17-C18
28	d	409	LHG	O2-C2-C3-O3
28	D	410	LHG	O2-C2-C3-O3
28	E	101	LHG	C23-C24-C25-C26
34	D	412	LMG	C2-C1-O1-C7
23	c	914	CLA	O1A-CGA-O2A-C1
30	z	101	LMT	O5'-C5'-C6'-O6'
23	B	602	CLA	C11-C10-C8-C9
23	B	602	CLA	C14-C13-C15-C16
23	b	607	CLA	C14-C13-C15-C16
23	C	505	CLA	C11-C12-C13-C14
23	c	907	CLA	C6-C7-C8-C9
23	b	602	CLA	C11-C10-C8-C9
23	b	617	CLA	C6-C7-C8-C9
23	b	616	CLA	O1D-CGD-O2D-CED
25	d	405	BCR	C21-C22-C23-C24
28	e	101	LHG	C18-C19-C20-C21
28	D	409	LHG	C23-C24-C25-C26
23	C	513	CLA	C15-C16-C17-C18
23	a	410	CLA	C8-C10-C11-C12
23	C	507	CLA	C10-C11-C12-C13
30	Z	101	LMT	O5'-C5'-C6'-O6'
23	B	605	CLA	C13-C15-C16-C17
23	c	910	CLA	C13-C15-C16-C17
35	D	414	HTG	C1'-C2'-C3'-C4'
35	B	625	HTG	C1'-C2'-C3'-C4'
23	B	602	CLA	C10-C11-C12-C13
23	b	617	CLA	C5-C6-C7-C8
23	b	617	CLA	C15-C16-C17-C18
23	B	607	CLA	C10-C11-C12-C13
23	c	902	CLA	O1D-CGD-O2D-CED
34	C	520	LMG	C10-C11-C12-C13
28	e	101	LHG	C23-C24-C25-C26
34	c	920	LMG	C28-C29-C30-C31
28	K	101	LHG	C23-C24-C25-C26
34	c	930	LMG	C10-C11-C12-C13
28	a	415	LHG	C7-C8-C9-C10
26	A	415	SQD	C23-C24-C25-C26
34	C	531	LMG	C28-C29-C30-C31
30	e	103	LMT	O1'-C1-C2-C3
23	c	910	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	B	602	CLA	C13-C15-C16-C17
23	D	403	CLA	C15-C16-C17-C18
23	A	408	CLA	C10-C11-C12-C13
28	A	412	LHG	C24-C23-O8-C6
28	d	402	LHG	C5-C6-O8-C23
30	F	101	LMT	O1'-C1-C2-C3
34	J	101	LMG	O6-C5-C6-O5
23	b	607	CLA	C10-C11-C12-C13
23	d	404	CLA	C15-C16-C17-C18
23	b	617	CLA	C13-C15-C16-C17
36	D	407	DGD	C1B-C2B-C3B-C4B
28	a	415	LHG	C23-C24-C25-C26
23	b	612	CLA	C13-C15-C16-C17
23	a	407	CLA	C6-C7-C8-C10
23	b	607	CLA	C6-C7-C8-C10
23	A	408	CLA	C6-C7-C8-C10
23	d	404	CLA	C11-C10-C8-C7
23	B	607	CLA	C6-C7-C8-C10
23	b	607	CLA	C2A-CAA-CBA-CGA
23	B	607	CLA	C2A-CAA-CBA-CGA
24	D	402	PHO	C2C-C3C-CAC-CBC
30	B	644	LMT	C4'-C5'-C6'-O6'
30	B	644	LMT	O5'-C1'-O1'-C1
23	c	914	CLA	C10-C11-C12-C13
27	a	414	PL9	C9-C11-C12-C13
36	d	407	DGD	C1A-C2A-C3A-C4A
28	E	101	LHG	C7-C8-C9-C10
35	b	622	HTG	S1-C1'-C2'-C3'
35	b	623	HTG	S1-C1'-C2'-C3'
30	B	623	LMT	O1'-C1-C2-C3
23	b	602	CLA	C3-C5-C6-C7
23	B	614	CLA	C8-C10-C11-C12
23	A	408	CLA	C13-C15-C16-C17
26	B	621	SQD	O10-C23-O48-C46
23	b	617	CLA	O1A-CGA-O2A-C1
30	m	103	LMT	O1'-C1-C2-C3
23	B	612	CLA	C15-C16-C17-C18
34	D	412	LMG	C4-C5-C6-O5
26	D	408	SQD	C8-C7-O47-C45
23	b	615	CLA	C8-C10-C11-C12
23	b	615	CLA	C10-C11-C12-C13
23	B	616	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	B	617	CLA	C15-C16-C17-C18
28	l	101	LHG	C4-O6-P-O3
28	A	412	LHG	C4-O6-P-O3
28	d	402	LHG	C3-O3-P-O6
28	a	415	LHG	C3-O3-P-O6
28	E	101	LHG	C3-O3-P-O6
26	B	621	SQD	C23-C24-C25-C26
35	b	623	HTG	C1'-C2'-C3'-C4'
23	B	615	CLA	C5-C6-C7-C8
28	D	410	LHG	C1-C2-C3-O3
26	D	408	SQD	O49-C7-O47-C45
23	C	514	CLA	C8-C10-C11-C12
23	B	615	CLA	C8-C10-C11-C12
23	c	914	CLA	C16-C17-C18-C19
35	b	623	HTG	O5-C5-C6-O6
30	I	101	LMT	O1'-C1-C2-C3
36	c	919	DGD	C8A-C9A-CAA-CBA
28	D	411	LHG	C11-C12-C13-C14
23	C	504	CLA	O1D-CGD-O2D-CED
25	t	101	BCR	C13-C14-C15-C16
25	T	101	BCR	C13-C14-C15-C16
36	C	518	DGD	C1A-C2A-C3A-C4A
28	D	411	LHG	C17-C18-C19-C20
26	a	412	SQD	C18-C19-C20-C21
26	a	417	SQD	C34-C35-C36-C37
35	C	523	HTG	C2'-C3'-C4'-C5'
34	C	501	LMG	C11-C10-O7-C8
35	c	922	HTG	O5-C5-C6-O6
23	C	510	CLA	C3-C5-C6-C7
28	D	411	LHG	C28-C29-C30-C31
28	e	101	LHG	C14-C15-C16-C17
34	c	920	LMG	C39-C40-C41-C42
34	C	501	LMG	C13-C14-C15-C16
34	C	501	LMG	C39-C40-C41-C42
34	B	622	LMG	C11-C12-C13-C14
30	a	418	LMT	O1'-C1-C2-C3
28	E	101	LHG	C25-C26-C27-C28
28	E	101	LHG	C29-C30-C31-C32
28	E	101	LHG	C31-C32-C33-C34
34	a	413	LMG	C11-C12-C13-C14
36	C	519	DGD	C7A-C8A-C9A-CAA
36	C	519	DGD	C9B-CAB-CBB-CCB

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Mol	Chain	Res	Type	Atoms
28	d	410	LHG	C14-C15-C16-C17
26	a	412	SQD	C9-C10-C11-C12
26	a	412	SQD	C13-C14-C15-C16
28	d	408	LHG	C30-C31-C32-C33
28	A	412	LHG	C12-C13-C14-C15
34	C	501	LMG	C18-C19-C20-C21
34	C	501	LMG	C21-C22-C23-C24
28	D	409	LHG	C31-C32-C33-C34
34	J	101	LMG	C17-C18-C19-C20
28	a	415	LHG	C15-C16-C17-C18
36	c	919	DGD	CAA-CBA-CCA-CDA
26	A	415	SQD	C17-C18-C19-C20
30	a	418	LMT	C3-C4-C5-C6
34	C	531	LMG	C29-C30-C31-C32
34	C	531	LMG	C30-C31-C32-C33
26	D	408	SQD	C24-C25-C26-C27
34	C	501	LMG	O9-C10-O7-C8
28	e	101	LHG	C24-C25-C26-C27
34	C	501	LMG	C11-C12-C13-C14
34	C	501	LMG	C37-C38-C39-C40
28	K	101	LHG	C31-C32-C33-C34
36	C	518	DGD	CAA-CBA-CCA-CDA
28	a	415	LHG	C9-C10-C11-C12
30	a	418	LMT	C7-C8-C9-C10
23	D	401	CLA	O1D-CGD-O2D-CED
23	A	408	CLA	O1D-CGD-O2D-CED
30	m	103	LMT	C7-C8-C9-C10
28	D	411	LHG	C14-C15-C16-C17
28	D	411	LHG	C29-C30-C31-C32
26	A	410	SQD	C29-C30-C31-C32
26	B	621	SQD	C9-C10-C11-C12
26	B	621	SQD	C29-C30-C31-C32
34	c	920	LMG	C21-C22-C23-C24
28	K	101	LHG	C25-C26-C27-C28
36	C	518	DGD	C8A-C9A-CAA-CBA
28	L	101	LHG	C11-C12-C13-C14
34	a	413	LMG	C18-C19-C20-C21
26	A	410	SQD	C11-C12-C13-C14
34	C	520	LMG	C20-C21-C22-C23
34	c	920	LMG	C19-C20-C21-C22
36	D	407	DGD	C2B-C3B-C4B-C5B
36	D	407	DGD	C6B-C7B-C8B-C9B

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Mol	Chain	Res	Type	Atoms
36	C	518	DGD	C5A-C6A-C7A-C8A
34	m	102	LMG	C20-C21-C22-C23
36	c	919	DGD	C6A-C7A-C8A-C9A
34	C	531	LMG	C38-C39-C40-C41
34	D	412	LMG	C28-C29-C30-C31
26	L	102	SQD	C2-C1-O6-C44
30	B	644	LMT	C2'-C1'-O1'-C1
30	b	621	LMT	C2'-C1'-O1'-C1
36	C	519	DGD	CBA-CCA-CDA-CEA
28	D	411	LHG	C15-C16-C17-C18
26	L	102	SQD	C10-C11-C12-C13
34	D	412	LMG	C29-C30-C31-C32
28	e	101	LHG	C13-C14-C15-C16
28	e	101	LHG	C16-C17-C18-C19
36	C	517	DGD	C9A-CAA-CBA-CCA
34	c	930	LMG	C39-C40-C41-C42
36	h	102	DGD	C7A-C8A-C9A-CAA
23	D	404	CLA	C15-C16-C17-C18
23	c	903	CLA	C16-C17-C18-C19
23	C	507	CLA	C16-C17-C18-C20
23	c	914	CLA	C4-C3-C5-C6
26	L	102	SQD	C12-C13-C14-C15
26	a	412	SQD	C29-C30-C31-C32
35	B	626	HTG	C3'-C4'-C5'-C6'
30	I	101	LMT	C4-C5-C6-C7
28	A	412	LHG	C11-C10-C9-C8
34	c	920	LMG	C17-C18-C19-C20
34	c	920	LMG	C34-C35-C36-C37
34	C	501	LMG	C17-C18-C19-C20
36	D	407	DGD	C8A-C9A-CAA-CBA
34	B	622	LMG	C16-C17-C18-C19
36	C	517	DGD	C4B-C5B-C6B-C7B
34	m	102	LMG	C31-C32-C33-C34
26	x	101	SQD	C28-C29-C30-C31
28	E	101	LHG	C12-C13-C14-C15
23	a	407	CLA	C11-C12-C13-C14
23	A	406	CLA	C6-C7-C8-C9
23	C	513	CLA	C14-C13-C15-C16
23	A	408	CLA	C11-C12-C13-C14
34	a	413	LMG	C10-C11-C12-C13
26	A	410	SQD	C17-C18-C19-C20
26	A	410	SQD	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
28	d	410	LHG	C28-C29-C30-C31
26	L	102	SQD	C11-C10-C9-C8
26	L	102	SQD	C17-C18-C19-C20
28	A	412	LHG	C16-C17-C18-C19
34	c	920	LMG	C11-C12-C13-C14
34	c	920	LMG	C13-C14-C15-C16
36	c	918	DGD	C7A-C8A-C9A-CAA
36	c	918	DGD	C9A-CAA-CBA-CCA
36	C	518	DGD	CCA-CDA-CEA-CFA
28	a	415	LHG	C13-C14-C15-C16
28	L	101	LHG	C27-C28-C29-C30
23	c	907	CLA	C10-C11-C12-C13
28	A	412	LHG	O10-C23-O8-C6
30	T	103	LMT	C7-C8-C9-C10
34	D	412	LMG	C36-C37-C38-C39
34	c	920	LMG	C29-C30-C31-C32
28	a	415	LHG	C11-C12-C13-C14
30	a	422	LMT	C7-C8-C9-C10
28	d	410	LHG	O1-C1-C2-C3
28	d	408	LHG	O1-C1-C2-C3
35	B	630	HTG	C1'-C2'-C3'-C4'
23	B	617	CLA	C3-C5-C6-C7
26	x	101	SQD	O49-C7-O47-C45
23	C	507	CLA	C5-C6-C7-C8
26	x	101	SQD	C8-C7-O47-C45
34	C	520	LMG	C19-C20-C21-C22
34	C	520	LMG	C39-C40-C41-C42
28	A	412	LHG	C32-C33-C34-C35
35	B	625	HTG	C3'-C4'-C5'-C6'
36	c	918	DGD	C1A-C2A-C3A-C4A
26	a	417	SQD	C29-C30-C31-C32
28	A	412	LHG	C13-C14-C15-C16
28	A	412	LHG	C14-C15-C16-C17
34	c	920	LMG	C14-C15-C16-C17
35	b	628	HTG	C3'-C4'-C5'-C6'
28	D	409	LHG	C29-C30-C31-C32
35	c	923	HTG	C2'-C3'-C4'-C5'
30	a	418	LMT	C11-C10-C9-C8
28	D	410	LHG	C32-C33-C34-C35
34	a	413	LMG	C13-C14-C15-C16
34	a	413	LMG	C33-C34-C35-C36
23	a	406	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
23	A	406	CLA	C16-C17-C18-C19
23	B	602	CLA	C16-C17-C18-C20
23	c	907	CLA	C16-C17-C18-C19
23	c	907	CLA	C16-C17-C18-C20
23	C	509	CLA	C16-C17-C18-C20
23	C	507	CLA	C16-C17-C18-C19
23	b	617	CLA	C16-C17-C18-C19
23	c	914	CLA	C16-C17-C18-C20
23	C	503	CLA	C16-C17-C18-C20
36	D	407	DGD	O6D-C1D-O3G-C3G
36	C	519	DGD	C8A-C9A-CAA-CBA
34	C	520	LMG	C31-C32-C33-C34
30	B	644	LMT	C11-C10-C9-C8
34	B	622	LMG	C38-C39-C40-C41
35	b	623	HTG	C3'-C4'-C5'-C6'
34	J	101	LMG	C18-C19-C20-C21
34	J	101	LMG	C36-C37-C38-C39
30	Z	101	LMT	O5B-C5B-C6B-O6B
26	a	412	SQD	C31-C32-C33-C34
23	a	406	CLA	C2C-C3C-CAC-CBC
28	A	412	LHG	C27-C28-C29-C30
28	A	412	LHG	C29-C30-C31-C32
34	c	920	LMG	C18-C19-C20-C21
28	d	402	LHG	C25-C26-C27-C28
30	F	101	LMT	C11-C10-C9-C8
34	c	930	LMG	C35-C36-C37-C38
26	x	101	SQD	C30-C31-C32-C33
36	c	919	DGD	C4A-C5A-C6A-C7A
26	A	415	SQD	C9-C10-C11-C12
26	A	415	SQD	C25-C26-C27-C28
26	A	415	SQD	C27-C28-C29-C30
34	C	531	LMG	C16-C17-C18-C19
34	C	501	LMG	C10-C11-C12-C13
26	a	412	SQD	C16-C17-C18-C19
26	B	621	SQD	C16-C17-C18-C19
34	B	622	LMG	C39-C40-C41-C42
34	j	101	LMG	C31-C32-C33-C34
36	d	407	DGD	C7A-C8A-C9A-CAA
28	L	101	LHG	C29-C30-C31-C32
34	d	411	LMG	C11-C12-C13-C14
26	a	412	SQD	C34-C35-C36-C37
30	z	101	LMT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
36	d	407	DGD	C7B-C8B-C9B-CAB
36	C	517	DGD	C2B-C3B-C4B-C5B
28	E	101	LHG	C27-C28-C29-C30
23	c	907	CLA	C15-C16-C17-C18
30	e	103	LMT	C2-C1-O1'-C1'
36	C	519	DGD	C2A-C3A-C4A-C5A
28	l	101	LHG	C30-C31-C32-C33
26	a	412	SQD	C27-C28-C29-C30
34	C	520	LMG	C17-C18-C19-C20
28	d	408	LHG	C29-C30-C31-C32
26	a	417	SQD	C25-C26-C27-C28
36	c	918	DGD	C3A-C4A-C5A-C6A
36	c	918	DGD	C5A-C6A-C7A-C8A
36	d	407	DGD	C6A-C7A-C8A-C9A
36	d	407	DGD	C6B-C7B-C8B-C9B
36	H	103	DGD	C7A-C8A-C9A-CAA
28	E	101	LHG	C17-C18-C19-C20
23	B	615	CLA	O1D-CGD-O2D-CED
23	A	406	CLA	C16-C17-C18-C20
34	d	411	LMG	C38-C39-C40-C41
36	c	917	DGD	C2B-C3B-C4B-C5B
30	B	644	LMT	C7-C8-C9-C10
36	C	518	DGD	C9A-CAA-CBA-CCA
34	a	413	LMG	C21-C22-C23-C24
36	D	407	DGD	O1G-C1G-C2G-C3G
30	B	643	LMT	C1-C2-C3-C4
35	C	523	HTG	C1'-C2'-C3'-C4'
36	C	517	DGD	C8A-C9A-CAA-CBA
36	h	102	DGD	CAA-CBA-CCA-CDA
30	B	623	LMT	C3-C4-C5-C6
30	B	623	LMT	C7-C8-C9-C10
28	E	101	LHG	C33-C34-C35-C36
23	b	615	CLA	C3-C5-C6-C7
26	B	621	SQD	C28-C29-C30-C31
34	J	101	LMG	C19-C20-C21-C22
27	a	414	PL9	C15-C14-C16-C17
34	C	520	LMG	C29-C28-O8-C9
35	B	626	HTG	C4-C5-C6-O6
27	a	414	PL9	C13-C14-C16-C17
27	D	406	PL9	C28-C29-C31-C32
28	d	402	LHG	O1-C1-C2-O2
26	A	410	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
34	C	520	LMG	C12-C13-C14-C15
28	d	408	LHG	C15-C16-C17-C18
28	d	402	LHG	C29-C30-C31-C32
36	C	518	DGD	C3A-C4A-C5A-C6A
30	a	422	LMT	C3-C4-C5-C6
23	C	513	CLA	C16-C17-C18-C19
23	b	616	CLA	C16-C17-C18-C19
30	A	416	LMT	C3-C4-C5-C6
34	c	920	LMG	C15-C16-C17-C18
34	c	920	LMG	C16-C17-C18-C19
34	c	920	LMG	C12-C13-C14-C15
34	j	101	LMG	C37-C38-C39-C40
28	E	101	LHG	C34-C35-C36-C37
26	D	408	SQD	C23-C24-C25-C26
28	d	409	LHG	C1-C2-C3-O3
26	B	621	SQD	C13-C14-C15-C16
36	c	917	DGD	C9A-CAA-CBA-CCA
26	x	101	SQD	C34-C35-C36-C37
36	c	919	DGD	CBB-CCB-CDB-CEB
26	D	408	SQD	C26-C27-C28-C29
30	A	416	LMT	C1-C2-C3-C4
23	B	617	CLA	C2-C1-O2A-CGA
35	B	626	HTG	C1'-C2'-C3'-C4'
35	b	622	HTG	C2'-C3'-C4'-C5'
34	B	622	LMG	C37-C38-C39-C40
35	d	413	HTG	C3'-C4'-C5'-C6'
23	b	605	CLA	C13-C15-C16-C17
23	b	604	CLA	C5-C6-C7-C8
30	F	101	LMT	C1-C2-C3-C4
30	b	621	LMT	C4'-C5'-C6'-O6'
26	A	410	SQD	C33-C34-C35-C36
34	C	520	LMG	C34-C35-C36-C37
36	c	917	DGD	C4B-C5B-C6B-C7B
36	D	407	DGD	C7B-C8B-C9B-CAB
28	K	101	LHG	C14-C15-C16-C17
36	d	407	DGD	C4B-C5B-C6B-C7B
26	x	101	SQD	C32-C33-C34-C35
25	C	515	BCR	C23-C24-C25-C26
25	C	515	BCR	C23-C24-C25-C30
25	B	618	BCR	C1-C6-C7-C8
25	B	618	BCR	C5-C6-C7-C8
25	Y	101	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	Y	101	BCR	C5-C6-C7-C8
25	d	405	BCR	C23-C24-C25-C26
28	K	101	LHG	C32-C33-C34-C35
36	d	407	DGD	CCA-CDA-CEA-CFA
36	h	102	DGD	C6B-C7B-C8B-C9B
28	L	101	LHG	C10-C11-C12-C13
36	C	519	DGD	C9A-CAA-CBA-CCA
28	d	408	LHG	C25-C26-C27-C28
36	c	917	DGD	C7A-C8A-C9A-CAA
26	D	408	SQD	C28-C29-C30-C31
23	C	510	CLA	C10-C11-C12-C13
23	b	602	CLA	C15-C16-C17-C18
26	a	417	SQD	C26-C27-C28-C29
28	A	412	LHG	C17-C18-C19-C20
27	D	406	PL9	C30-C29-C31-C32
23	B	605	CLA	C6-C7-C8-C10
23	D	403	CLA	C12-C13-C15-C16
23	a	410	CLA	C12-C13-C15-C16
23	B	604	CLA	C6-C7-C8-C10
23	c	903	CLA	C11-C12-C13-C15
23	b	614	CLA	C11-C12-C13-C15
23	A	408	CLA	C12-C13-C15-C16
23	c	914	CLA	C2-C3-C5-C6
23	b	612	CLA	C12-C13-C15-C16
34	C	520	LMG	O10-C28-O8-C9
28	A	412	LHG	C33-C34-C35-C36
34	C	501	LMG	C12-C13-C14-C15
34	B	622	LMG	C13-C14-C15-C16
36	c	919	DGD	C2A-C3A-C4A-C5A
36	H	103	DGD	C9B-CAB-CBB-CCB
23	B	607	CLA	C8-C10-C11-C12
23	c	905	CLA	C13-C15-C16-C17
23	b	617	CLA	C16-C17-C18-C20
23	B	607	CLA	O1D-CGD-O2D-CED
34	B	622	LMG	C10-C11-C12-C13
26	x	101	SQD	C24-C23-O48-C46
34	d	411	LMG	C18-C19-C20-C21
28	d	410	LHG	C29-C30-C31-C32
30	T	103	LMT	O1'-C1-C2-C3
34	B	622	LMG	C29-C30-C31-C32
28	K	101	LHG	C18-C19-C20-C21
30	F	101	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
30	Z	101	LMT	O1'-C1-C2-C3
26	A	415	SQD	C26-C27-C28-C29
30	B	644	LMT	C4-C5-C6-C7
34	c	920	LMG	C35-C36-C37-C38
26	x	101	SQD	C27-C28-C29-C30
26	D	408	SQD	C30-C31-C32-C33
26	D	408	SQD	C7-C8-C9-C10
28	A	412	LHG	C25-C26-C27-C28
36	D	407	DGD	C7A-C8A-C9A-CAA
30	F	101	LMT	C6-C7-C8-C9
28	E	101	LHG	C18-C19-C20-C21
30	z	101	LMT	C4B-C5B-C6B-O6B
30	B	623	LMT	C1-C2-C3-C4
30	a	418	LMT	C1-C2-C3-C4
23	a	406	CLA	C4C-C3C-CAC-CBC
30	B	643	LMT	C7-C8-C9-C10
30	b	621	LMT	O5'-C1'-O1'-C1
23	b	607	CLA	C15-C16-C17-C18
26	a	412	SQD	C12-C13-C14-C15
34	D	412	LMG	C11-C12-C13-C14
34	B	622	LMG	C32-C33-C34-C35
26	A	410	SQD	C18-C19-C20-C21
26	a	417	SQD	C30-C31-C32-C33
36	D	407	DGD	CCA-CDA-CEA-CFA
36	c	918	DGD	CAA-CBA-CCA-CDA
28	K	101	LHG	C26-C27-C28-C29
28	K	101	LHG	C28-C29-C30-C31
24	a	409	PHO	C2C-C3C-CAC-CBC
30	b	621	LMT	C7-C8-C9-C10
35	c	922	HTG	C4-C5-C6-O6
35	c	921	HTG	C4-C5-C6-O6
35	C	522	HTG	S1-C1'-C2'-C3'
23	C	504	CLA	C8-C10-C11-C12
30	Z	101	LMT	C4-C5-C6-C7
26	A	415	SQD	C15-C16-C17-C18
34	C	531	LMG	C18-C19-C20-C21
36	c	917	DGD	C5B-C6B-C7B-C8B
26	a	417	SQD	C27-C28-C29-C30
28	d	402	LHG	C18-C19-C20-C21
28	K	101	LHG	C33-C34-C35-C36
28	a	415	LHG	C12-C13-C14-C15
34	C	531	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
26	A	410	SQD	O6-C44-C45-O47
26	a	412	SQD	O6-C44-C45-O47
28	E	101	LHG	C10-C11-C12-C13
23	b	616	CLA	C16-C17-C18-C20
36	c	917	DGD	O6D-C5D-C6D-O5D
36	C	519	DGD	CAA-CBA-CCA-CDA
34	C	520	LMG	C11-C12-C13-C14
36	C	517	DGD	O6E-C5E-C6E-O5E
34	C	531	LMG	O6-C5-C6-O5
23	B	617	CLA	C13-C15-C16-C17
23	b	606	CLA	C2-C3-C5-C6
27	A	411	PL9	C4-C3-C7-C8
30	F	101	LMT	C5-C6-C7-C8
23	a	407	CLA	C6-C7-C8-C9
23	B	605	CLA	C6-C7-C8-C9
23	a	410	CLA	C14-C13-C15-C16
23	B	604	CLA	C6-C7-C8-C9
23	A	408	CLA	C6-C7-C8-C9
23	d	404	CLA	C11-C10-C8-C9
23	d	404	CLA	C14-C13-C15-C16
23	B	612	CLA	C14-C13-C15-C16
23	b	617	CLA	C14-C13-C15-C16
23	b	615	CLA	O1D-CGD-O2D-CED
35	B	624	HTG	C3'-C4'-C5'-C6'
36	c	918	DGD	C2B-C3B-C4B-C5B
28	d	402	LHG	C16-C17-C18-C19
35	D	414	HTG	C3'-C4'-C5'-C6'
28	a	415	LHG	C10-C11-C12-C13
34	j	101	LMG	O6-C5-C6-O5
26	A	410	SQD	C14-C15-C16-C17
30	T	103	LMT	C4-C5-C6-C7
25	T	101	BCR	C11-C12-C13-C14
26	x	101	SQD	O10-C23-O48-C46
28	a	415	LHG	C8-C7-O7-C5
34	a	413	LMG	C11-C10-O7-C8
34	C	520	LMG	C37-C38-C39-C40
28	A	412	LHG	C26-C27-C28-C29
36	C	517	DGD	C6A-C7A-C8A-C9A
36	H	103	DGD	CCA-CDA-CEA-CFA
23	B	614	CLA	C10-C11-C12-C13
35	b	622	HTG	C3'-C4'-C5'-C6'
30	Z	101	LMT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
36	c	919	DGD	CBA-CCA-CDA-CEA
30	e	103	LMT	C1-C2-C3-C4
23	c	911	CLA	C8-C10-C11-C12
23	A	408	CLA	C15-C16-C17-C18
23	b	616	CLA	C10-C11-C12-C13
28	E	101	LHG	O6-C4-C5-C6
23	C	513	CLA	O1D-CGD-O2D-CED
26	L	102	SQD	C23-C24-C25-C26
30	A	416	LMT	C11-C10-C9-C8
28	a	415	LHG	C14-C15-C16-C17
34	C	531	LMG	C17-C18-C19-C20
23	C	503	CLA	C16-C17-C18-C19
36	C	519	DGD	C6B-C7B-C8B-C9B
26	A	410	SQD	C15-C16-C17-C18
28	K	101	LHG	C11-C12-C13-C14
36	h	102	DGD	CCB-CDB-CEB-CFB
36	H	103	DGD	C5B-C6B-C7B-C8B
23	C	514	CLA	C3-C5-C6-C7
26	A	410	SQD	C32-C33-C34-C35
34	m	102	LMG	C15-C16-C17-C18
23	b	615	CLA	C4-C3-C5-C6
24	a	408	PHO	C4-C3-C5-C6
34	d	411	LMG	C36-C37-C38-C39
34	c	920	LMG	C20-C21-C22-C23
36	C	518	DGD	C2B-C3B-C4B-C5B
34	C	531	LMG	C15-C16-C17-C18
28	E	101	LHG	C32-C33-C34-C35
30	z	101	LMT	C2B-C1B-O1B-C4'
34	C	520	LMG	C21-C22-C23-C24
36	h	102	DGD	C9B-CAB-CBB-CCB
28	L	101	LHG	C25-C26-C27-C28
34	C	531	LMG	C19-C20-C21-C22
34	d	411	LMG	C19-C20-C21-C22
34	C	520	LMG	C38-C39-C40-C41
30	e	103	LMT	C2-C3-C4-C5
28	e	101	LHG	C15-C16-C17-C18
26	a	417	SQD	C35-C36-C37-C38
36	c	917	DGD	O6E-C5E-C6E-O5E
30	m	104	LMT	O5'-C5'-C6'-O6'
26	B	621	SQD	C44-C45-C46-O48
26	a	417	SQD	O6-C44-C45-C46
34	C	501	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
28	K	101	LHG	C16-C17-C18-C19
26	A	415	SQD	O6-C44-C45-C46
26	D	408	SQD	O6-C44-C45-C46
28	E	101	LHG	C4-C5-C6-O8
28	K	101	LHG	C35-C36-C37-C38
36	d	407	DGD	C3A-C4A-C5A-C6A
36	c	918	DGD	C2G-C3G-O3G-C1D
36	C	518	DGD	C2G-C3G-O3G-C1D
36	C	518	DGD	C5D-C6D-O5D-C1E
34	c	930	LMG	C8-C7-O1-C1
34	C	531	LMG	C8-C7-O1-C1
26	A	410	SQD	C30-C31-C32-C33
28	d	402	LHG	C24-C25-C26-C27
30	a	418	LMT	C6-C7-C8-C9
23	C	510	CLA	C13-C15-C16-C17
28	D	411	LHG	C19-C20-C21-C22
28	d	410	LHG	C13-C14-C15-C16
26	a	412	SQD	C11-C12-C13-C14
26	B	621	SQD	C14-C15-C16-C17
28	K	101	LHG	C30-C31-C32-C33
34	a	413	LMG	C35-C36-C37-C38
36	h	102	DGD	O2G-C1B-C2B-C3B
36	h	102	DGD	CDB-CEB-CFB-CGB
26	x	101	SQD	C31-C32-C33-C34
30	B	623	LMT	C9-C10-C11-C12
36	H	103	DGD	CDB-CEB-CFB-CGB
23	C	503	CLA	O1D-CGD-O2D-CED
26	B	621	SQD	C12-C13-C14-C15
34	C	520	LMG	C16-C17-C18-C19
28	e	101	LHG	C26-C27-C28-C29
35	D	414	HTG	C4'-C5'-C6'-C7'
36	c	919	DGD	CDB-CEB-CFB-CGB
28	d	408	LHG	O1-C1-C2-O2
30	z	101	LMT	C3-C4-C5-C6
34	a	413	LMG	C34-C35-C36-C37
34	D	412	LMG	O10-C28-O8-C9
36	C	519	DGD	CDB-CEB-CFB-CGB
26	B	621	SQD	C34-C35-C36-C37
28	K	101	LHG	C10-C11-C12-C13
30	B	623	LMT	C6-C7-C8-C9
30	m	103	LMT	O5'-C5'-C6'-O6'
30	I	101	LMT	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
27	A	411	PL9	C15-C14-C16-C17
27	A	411	PL9	C18-C19-C21-C22
23	B	602	CLA	C16-C17-C18-C19
23	c	903	CLA	C16-C17-C18-C20
23	b	602	CLA	C16-C17-C18-C19
34	D	412	LMG	C29-C28-O8-C9
35	b	622	HTG	C4'-C5'-C6'-C7'
30	a	422	LMT	C4-C5-C6-C7
23	b	609	CLA	C13-C15-C16-C17
26	a	412	SQD	C19-C20-C21-C22
36	c	917	DGD	CDA-CEA-CFA-CGA
26	A	415	SQD	C16-C17-C18-C19
26	A	415	SQD	C35-C36-C37-C38
36	H	103	DGD	CBB-CCB-CDB-CEB
34	a	413	LMG	C40-C41-C42-C43
35	C	522	HTG	O5-C5-C6-O6
23	c	910	CLA	C2-C1-O2A-CGA
23	C	510	CLA	C2-C1-O2A-CGA
26	x	101	SQD	C29-C30-C31-C32
26	D	408	SQD	C9-C10-C11-C12
28	D	411	LHG	C18-C19-C20-C21
28	e	101	LHG	C11-C10-C9-C8
30	B	643	LMT	O1'-C1-C2-C3
34	a	413	LMG	C17-C18-C19-C20
28	d	402	LHG	O7-C7-C8-C9
30	B	643	LMT	C3-C4-C5-C6
26	x	101	SQD	C26-C27-C28-C29
23	c	908	CLA	C5-C6-C7-C8
23	a	410	CLA	O1D-CGD-O2D-CED
28	d	402	LHG	C23-C24-C25-C26
36	C	518	DGD	C2E-C1E-O5D-C6D
28	d	402	LHG	C10-C11-C12-C13
34	J	101	LMG	C37-C38-C39-C40
36	H	103	DGD	O2G-C1B-C2B-C3B
34	d	411	LMG	O1-C7-C8-O7
26	D	408	SQD	O6-C44-C45-O47
30	A	416	LMT	C9-C10-C11-C12
30	b	621	LMT	C9-C10-C11-C12
28	a	415	LHG	O9-C7-O7-C5
26	B	621	SQD	C19-C20-C21-C22
34	J	101	LMG	C12-C13-C14-C15
36	h	102	DGD	CBB-CCB-CDB-CEB

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Mol	Chain	Res	Type	Atoms
36	c	919	DGD	C8B-C9B-CAB-CBB
27	A	411	PL9	C20-C19-C21-C22
34	D	412	LMG	C21-C22-C23-C24
30	b	621	LMT	C6-C7-C8-C9
23	C	513	CLA	C12-C13-C15-C16
23	B	602	CLA	C11-C10-C8-C7
23	B	602	CLA	C11-C12-C13-C15
23	B	602	CLA	C12-C13-C15-C16
23	C	505	CLA	C11-C12-C13-C15
23	C	509	CLA	C11-C10-C8-C7
23	C	507	CLA	C6-C7-C8-C10
23	C	507	CLA	C11-C12-C13-C15
27	A	411	PL9	C13-C14-C16-C17
23	d	404	CLA	C12-C13-C15-C16
23	c	913	CLA	C11-C10-C8-C7
23	b	617	CLA	C12-C13-C15-C16
36	h	102	DGD	C5B-C6B-C7B-C8B
30	b	621	LMT	C5-C6-C7-C8
23	C	513	CLA	C11-C10-C8-C9
23	B	602	CLA	C11-C12-C13-C14
23	C	508	CLA	C11-C12-C13-C14
23	C	509	CLA	C11-C10-C8-C9
23	b	611	CLA	C11-C12-C13-C14
23	C	507	CLA	C11-C12-C13-C14
23	c	905	CLA	C11-C12-C13-C14
30	b	621	LMT	C1-C2-C3-C4
30	A	416	LMT	C2-C3-C4-C5
25	T	101	BCR	C11-C12-C13-C35
28	d	402	LHG	C30-C31-C32-C33
35	b	627	HTG	C3'-C4'-C5'-C6'
34	a	413	LMG	C14-C15-C16-C17
35	C	521	HTG	C3'-C4'-C5'-C6'
30	I	101	LMT	C9-C10-C11-C12
36	D	407	DGD	CBA-CCA-CDA-CEA
35	c	921	HTG	C2'-C3'-C4'-C5'
36	d	407	DGD	C5A-C6A-C7A-C8A
36	C	517	DGD	C7B-C8B-C9B-CAB
36	C	517	DGD	O6D-C5D-C6D-O5D
28	E	101	LHG	C1-C2-C3-O3
23	c	904	CLA	C8-C10-C11-C12
26	L	102	SQD	C34-C35-C36-C37
30	B	623	LMT	C3'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
28	d	408	LHG	C23-C24-C25-C26
36	C	517	DGD	C1A-C2A-C3A-C4A
23	B	616	CLA	C5-C6-C7-C8
28	d	402	LHG	C26-C27-C28-C29
26	D	408	SQD	C33-C34-C35-C36
23	C	508	CLA	C16-C17-C18-C20
24	a	408	PHO	C8-C10-C11-C12
23	a	410	CLA	C3-C5-C6-C7
34	d	411	LMG	C20-C21-C22-C23
28	D	409	LHG	C25-C26-C27-C28
34	a	413	LMG	C20-C21-C22-C23
34	a	413	LMG	C31-C32-C33-C34
28	d	410	LHG	C10-C11-C12-C13
23	b	602	CLA	C4-C3-C5-C6
23	b	602	CLA	C2-C3-C5-C6
26	a	412	SQD	C24-C25-C26-C27
26	B	621	SQD	C17-C18-C19-C20
36	D	407	DGD	CDB-CEB-CFB-CGB
23	a	406	CLA	C15-C16-C17-C18
30	B	623	LMT	C2-C3-C4-C5
30	a	418	LMT	C2-C3-C4-C5
23	D	404	CLA	C16-C17-C18-C20
26	a	412	SQD	C26-C27-C28-C29
26	B	621	SQD	C30-C31-C32-C33
26	L	102	SQD	C7-C8-C9-C10
36	c	918	DGD	CDA-CEA-CFA-CGA
35	B	625	HTG	C4'-C5'-C6'-C7'
28	a	415	LHG	C29-C30-C31-C32
30	a	422	LMT	C5-C6-C7-C8
30	T	103	LMT	C2-C1-O1'-C1'
30	Z	101	LMT	C2-C1-O1'-C1'
30	B	623	LMT	C2-C1-O1'-C1'
26	A	410	SQD	C35-C36-C37-C38
36	h	102	DGD	CDA-CEA-CFA-CGA
34	J	101	LMG	C10-C11-C12-C13
23	B	613	CLA	C13-C15-C16-C17
26	a	412	SQD	C17-C18-C19-C20
23	B	614	CLA	C15-C16-C17-C18
23	c	913	CLA	C15-C16-C17-C18
23	B	607	CLA	C13-C15-C16-C17
26	A	410	SQD	O6-C44-C45-C46
34	d	411	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
34	d	411	LMG	C7-C8-C9-O8
26	L	102	SQD	C44-C45-C46-O48
26	a	412	SQD	O6-C44-C45-C46
34	D	412	LMG	O1-C7-C8-C9
34	D	412	LMG	C7-C8-C9-O8
28	A	412	LHG	C4-C5-C6-O8
34	a	413	LMG	C7-C8-C9-O8
35	d	413	HTG	C2'-C3'-C4'-C5'
26	x	101	SQD	C25-C26-C27-C28
36	c	919	DGD	CCB-CDB-CEB-CFB
28	L	101	LHG	C9-C10-C11-C12
23	C	514	CLA	O2A-C1-C2-C3
23	a	410	CLA	C10-C11-C12-C13
30	B	623	LMT	C11-C10-C9-C8
26	a	412	SQD	C10-C11-C12-C13
23	c	905	CLA	C4-C3-C5-C6
23	b	602	CLA	C16-C17-C18-C20
27	d	406	PL9	C43-C44-C46-C47
36	D	407	DGD	C2A-C3A-C4A-C5A
30	a	422	LMT	O1'-C1-C2-C3
36	C	519	DGD	CDA-CEA-CFA-CGA
23	c	909	CLA	C15-C16-C17-C18
26	a	412	SQD	C25-C26-C27-C28
23	B	611	CLA	C8-C10-C11-C12
34	D	412	LMG	C37-C38-C39-C40
28	d	402	LHG	C9-C10-C11-C12
34	c	930	LMG	C40-C41-C42-C43
36	c	919	DGD	C3A-C4A-C5A-C6A
26	A	415	SQD	C11-C12-C13-C14
34	a	413	LMG	O9-C10-O7-C8
23	C	508	CLA	C16-C17-C18-C19
23	D	404	CLA	C16-C17-C18-C19
35	d	413	HTG	C4'-C5'-C6'-C7'
24	D	402	PHO	C4C-C3C-CAC-CBC
28	D	411	LHG	C16-C17-C18-C19
30	F	101	LMT	C2-C3-C4-C5
26	D	408	SQD	C10-C11-C12-C13
23	A	405	CLA	C2C-C3C-CAC-CBC
34	j	101	LMG	C36-C37-C38-C39
26	L	102	SQD	O47-C45-C46-O48
26	B	621	SQD	O47-C45-C46-O48
34	D	412	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
34	C	501	LMG	O1-C7-C8-O7
28	l	101	LHG	C31-C32-C33-C34
23	C	513	CLA	C16-C17-C18-C20
23	C	509	CLA	C16-C17-C18-C19
34	m	102	LMG	C33-C34-C35-C36
26	A	415	SQD	C34-C35-C36-C37
34	d	411	LMG	C35-C36-C37-C38
34	C	520	LMG	C15-C16-C17-C18
28	e	101	LHG	C19-C20-C21-C22
35	C	522	HTG	C2'-C3'-C4'-C5'
36	D	407	DGD	CBB-CCB-CDB-CEB
23	D	403	CLA	C2-C1-O2A-CGA
30	B	623	LMT	C5'-C4'-O1B-C1B
28	d	409	LHG	C11-C10-C9-C8
23	a	410	CLA	C11-C10-C8-C9
23	A	408	CLA	C11-C10-C8-C9
23	b	602	CLA	C14-C13-C15-C16
23	c	913	CLA	C11-C10-C8-C9
23	D	404	CLA	C14-C13-C15-C16
24	a	409	PHO	C6-C7-C8-C9
23	B	617	CLA	C11-C12-C13-C14
23	B	617	CLA	C14-C13-C15-C16
28	L	101	LHG	C24-C25-C26-C27
34	C	520	LMG	C36-C37-C38-C39
23	D	403	CLA	C2C-C3C-CAC-CBC
28	d	408	LHG	C32-C33-C34-C35
30	B	644	LMT	C3-C4-C5-C6
30	A	416	LMT	C4-C5-C6-C7
36	d	407	DGD	C5B-C6B-C7B-C8B
36	h	102	DGD	CBA-CCA-CDA-CEA
23	c	910	CLA	C16-C17-C18-C19
30	z	101	LMT	O5B-C5B-C6B-O6B
25	D	405	BCR	C23-C24-C25-C26
25	D	405	BCR	C23-C24-C25-C30
25	b	618	BCR	C5-C6-C7-C8
23	B	612	CLA	C13-C15-C16-C17
36	d	407	DGD	CCB-CDB-CEB-CFB
26	B	621	SQD	O49-C7-O47-C45
34	d	411	LMG	C12-C13-C14-C15
23	a	406	CLA	C16-C17-C18-C20
34	d	411	LMG	C32-C33-C34-C35
36	d	407	DGD	CDA-CEA-CFA-CGA

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Mol	Chain	Res	Type	Atoms
27	a	414	PL9	C30-C29-C31-C32
28	A	412	LHG	C28-C29-C30-C31
34	m	102	LMG	C36-C37-C38-C39
23	a	407	CLA	C11-C10-C8-C7
23	C	513	CLA	C11-C10-C8-C7
23	C	514	CLA	C6-C7-C8-C10
27	a	414	PL9	C28-C29-C31-C32
23	a	410	CLA	C11-C10-C8-C7
23	C	505	CLA	C12-C13-C15-C16
23	c	907	CLA	C11-C10-C8-C7
23	A	408	CLA	C11-C10-C8-C7
23	b	602	CLA	C11-C12-C13-C15
23	C	508	CLA	C11-C12-C13-C15
23	d	404	CLA	C6-C7-C8-C10
23	D	404	CLA	C11-C12-C13-C15
23	D	404	CLA	C12-C13-C15-C16
23	B	617	CLA	C12-C13-C15-C16
23	c	905	CLA	C11-C12-C13-C15
35	b	627	HTG	C4'-C5'-C6'-C7'
34	m	102	LMG	C19-C20-C21-C22
28	E	101	LHG	C35-C36-C37-C38
23	C	507	CLA	C13-C15-C16-C17
23	b	617	CLA	C8-C10-C11-C12
30	Z	101	LMT	C1-C2-C3-C4
26	B	621	SQD	C10-C11-C12-C13
36	c	917	DGD	C4D-C5D-C6D-O5D
26	a	417	SQD	C11-C12-C13-C14
35	B	631	HTG	C2'-C1'-S1-C1
28	K	101	LHG	C19-C20-C21-C22
28	d	408	LHG	C18-C19-C20-C21
23	b	605	CLA	C16-C17-C18-C20
36	D	407	DGD	C9A-CAA-CBA-CCA
28	K	101	LHG	C15-C16-C17-C18
34	a	413	LMG	C16-C17-C18-C19
34	C	501	LMG	C22-C23-C24-C25
36	h	102	DGD	CCA-CDA-CEA-CFA
26	B	621	SQD	C46-C45-O47-C7
23	B	605	CLA	CAD-CBD-CGD-O2D
23	a	406	CLA	CAD-CBD-CGD-O2D
23	B	602	CLA	CAD-CBD-CGD-O2D
23	b	615	CLA	CAD-CBD-CGD-O2D
23	c	911	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	A	407	PHO	CAD-CBD-CGD-O2D
23	c	904	CLA	CAD-CBD-CGD-O2D
23	c	914	CLA	CAD-CBD-CGD-O2D
23	D	404	CLA	CAD-CBD-CGD-O2D
24	a	409	PHO	CAD-CBD-CGD-O2D
24	a	408	PHO	CAD-CBD-CGD-O2D
34	m	102	LMG	C35-C36-C37-C38
28	d	409	LHG	C32-C33-C34-C35
34	j	101	LMG	C34-C35-C36-C37
27	A	411	PL9	C25-C24-C26-C27
34	D	412	LMG	O6-C1-O1-C7
26	B	621	SQD	C18-C19-C20-C21
34	J	101	LMG	C35-C36-C37-C38
30	Z	101	LMT	C4'-C5'-C6'-O6'
28	L	101	LHG	O6-C4-C5-O7
26	a	412	SQD	C14-C15-C16-C17
23	c	903	CLA	CHA-CBD-CGD-O1D
23	c	903	CLA	CHA-CBD-CGD-O2D
23	c	908	CLA	CHA-CBD-CGD-O1D
23	c	908	CLA	CHA-CBD-CGD-O2D
23	c	909	CLA	CHA-CBD-CGD-O1D
23	B	606	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O1D
23	b	606	CLA	CHA-CBD-CGD-O1D
23	C	509	CLA	CHA-CBD-CGD-O2D
23	C	507	CLA	CHA-CBD-CGD-O1D
23	d	401	CLA	CHA-CBD-CGD-O2D
24	D	402	PHO	CHA-CBD-CGD-O1D
23	B	608	CLA	CHA-CBD-CGD-O2D
23	B	607	CLA	CHA-CBD-CGD-O1D
23	C	503	CLA	CHA-CBD-CGD-O1D
23	C	503	CLA	CHA-CBD-CGD-O2D
23	c	905	CLA	CHA-CBD-CGD-O1D
36	H	103	DGD	C9A-CAA-CBA-CCA
34	D	412	LMG	O1-C7-C8-O7
26	D	408	SQD	O47-C45-C46-O48
34	a	413	LMG	O7-C8-C9-O8
23	C	507	CLA	CBD-CGD-O2D-CED
35	B	624	HTG	C2'-C3'-C4'-C5'
28	d	409	LHG	O1-C1-C2-O2
34	C	520	LMG	C22-C23-C24-C25
36	D	407	DGD	C3A-C4A-C5A-C6A

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Mol	Chain	Res	Type	Atoms
35	b	623	HTG	C2'-C3'-C4'-C5'
27	a	414	PL9	C4-C3-C7-C8
30	z	101	LMT	O5B-C1B-O1B-C4'
34	C	501	LMG	C19-C20-C21-C22
23	B	614	CLA	C11-C10-C8-C9
23	b	615	CLA	C6-C7-C8-C9
23	c	908	CLA	C11-C10-C8-C9
28	K	101	LHG	C9-C10-C11-C12
34	C	520	LMG	C33-C34-C35-C36
34	j	101	LMG	C33-C34-C35-C36
28	D	409	LHG	C30-C31-C32-C33
23	b	616	CLA	C5-C6-C7-C8
23	D	404	CLA	C13-C15-C16-C17
26	L	102	SQD	C31-C32-C33-C34
34	m	102	LMG	C30-C31-C32-C33
36	C	518	DGD	CDA-CEA-CFA-CGA
23	C	511	CLA	C8-C10-C11-C12
36	d	407	DGD	C9B-CAB-CBB-CCB
28	A	412	LHG	C3-O3-P-O6
28	D	410	LHG	C4-O6-P-O3
26	D	408	SQD	C25-C26-C27-C28
26	L	102	SQD	C28-C29-C30-C31
23	b	606	CLA	C4-C3-C5-C6
28	D	411	LHG	C2-C3-O3-P
28	A	412	LHG	C5-C4-O6-P
28	d	402	LHG	C5-C4-O6-P
28	d	408	LHG	C27-C28-C29-C30
34	D	412	LMG	C12-C13-C14-C15
28	A	412	LHG	C31-C32-C33-C34
36	d	407	DGD	C3B-C4B-C5B-C6B
28	l	101	LHG	C4-O6-P-O5
28	e	101	LHG	C4-O6-P-O4
28	d	402	LHG	C3-O3-P-O5
27	A	411	PL9	C3-C7-C8-C9
28	a	415	LHG	C3-O3-P-O4
28	a	415	LHG	C3-O3-P-O5
28	a	415	LHG	C4-O6-P-O5
23	b	605	CLA	C16-C17-C18-C19
23	c	908	CLA	C16-C17-C18-C19
28	L	101	LHG	O6-C4-C5-C6
28	L	101	LHG	C12-C13-C14-C15
28	l	101	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
26	B	621	SQD	C24-C25-C26-C27
34	D	412	LMG	C18-C19-C20-C21
28	d	410	LHG	C18-C19-C20-C21
26	B	621	SQD	O5-C5-C6-S
23	C	513	CLA	CAD-CBD-CGD-O1D
23	c	903	CLA	CAD-CBD-CGD-O1D
23	c	902	CLA	CAD-CBD-CGD-O1D
23	B	606	CLA	CAD-CBD-CGD-O1D
23	b	606	CLA	CAD-CBD-CGD-O1D
23	C	507	CLA	CAD-CBD-CGD-O1D
26	x	101	SQD	C5-C6-S-O7
23	C	503	CLA	CAD-CBD-CGD-O1D
23	c	905	CLA	CAD-CBD-CGD-O1D
35	v	204	HTG	C2'-C3'-C4'-C5'
34	B	622	LMG	C28-C29-C30-C31
28	l	101	LHG	C5-C6-O8-C23
26	L	102	SQD	C15-C16-C17-C18
30	a	418	LMT	C5-C6-C7-C8
23	B	606	CLA	C16-C17-C18-C19
23	c	913	CLA	C16-C17-C18-C20
35	B	626	HTG	C2-C1-S1-C1'
23	A	406	CLA	C12-C13-C15-C16
23	b	615	CLA	C2-C3-C5-C6
35	V	204	HTG	C2-C1-S1-C1'
23	C	505	CLA	C11-C10-C8-C7
23	c	908	CLA	C11-C10-C8-C7
23	C	510	CLA	C6-C7-C8-C10
23	C	510	CLA	C11-C12-C13-C15
23	b	602	CLA	C11-C10-C8-C7
23	C	508	CLA	C11-C10-C8-C7
23	d	404	CLA	C11-C12-C13-C15
23	B	612	CLA	C11-C12-C13-C15
23	b	617	CLA	C6-C7-C8-C10
23	D	404	CLA	C6-C7-C8-C10
23	B	617	CLA	C11-C12-C13-C15
23	b	616	CLA	C12-C13-C15-C16
23	c	905	CLA	C11-C10-C8-C7
35	v	204	HTG	C3'-C4'-C5'-C6'
30	I	101	LMT	C11-C10-C9-C8
28	D	409	LHG	C11-C10-C9-C8
34	m	102	LMG	C18-C19-C20-C21
34	C	531	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
26	B	621	SQD	C8-C7-O47-C45
34	m	102	LMG	C29-C30-C31-C32
34	j	101	LMG	C13-C14-C15-C16
23	A	408	CLA	C16-C17-C18-C19
23	d	404	CLA	C16-C17-C18-C19
30	m	103	LMT	C1-C2-C3-C4
34	C	531	LMG	C13-C14-C15-C16
36	C	517	DGD	C4D-C5D-C6D-O5D
26	L	102	SQD	O6-C44-C45-C46
34	C	501	LMG	O1-C7-C8-C9
28	A	412	LHG	O7-C5-C6-O8
36	D	407	DGD	O1G-C1G-C2G-O2G
26	L	102	SQD	C24-C25-C26-C27
34	j	101	LMG	C38-C39-C40-C41
34	d	411	LMG	C28-C29-C30-C31
36	C	519	DGD	CBB-CCB-CDB-CEB
36	c	918	DGD	C5D-C6D-O5D-C1E
34	c	930	LMG	C14-C15-C16-C17
28	d	410	LHG	C2-C3-O3-P
23	d	404	CLA	C8-C10-C11-C12
28	d	408	LHG	C17-C18-C19-C20
34	c	920	LMG	C30-C31-C32-C33
23	a	407	CLA	C11-C10-C8-C9
23	C	514	CLA	C6-C7-C8-C9
23	B	603	CLA	C11-C12-C13-C14
23	c	903	CLA	C11-C12-C13-C14
23	C	505	CLA	C11-C10-C8-C9
23	C	505	CLA	C14-C13-C15-C16
23	b	614	CLA	C11-C12-C13-C14
23	C	507	CLA	C6-C7-C8-C9
23	d	404	CLA	C6-C7-C8-C9
23	d	404	CLA	C11-C12-C13-C14
23	D	404	CLA	C6-C7-C8-C9
23	D	404	CLA	C11-C12-C13-C14
28	A	412	LHG	C9-C10-C11-C12
23	b	608	CLA	C3-C5-C6-C7
26	A	415	SQD	C31-C32-C33-C34
30	a	418	LMT	O5'-C1'-O1'-C1
28	l	101	LHG	C32-C33-C34-C35
30	I	101	LMT	C6-C7-C8-C9
36	d	407	DGD	C4A-C5A-C6A-C7A
30	I	101	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
34	j	101	LMG	C12-C13-C14-C15
23	d	401	CLA	C13-C15-C16-C17
35	O	302	HTG	C1'-C2'-C3'-C4'
28	D	411	LHG	C32-C33-C34-C35
34	D	412	LMG	C30-C31-C32-C33
28	e	101	LHG	C25-C26-C27-C28
35	B	625	HTG	C2'-C3'-C4'-C5'
24	a	408	PHO	C2-C3-C5-C6
23	c	905	CLA	C2-C3-C5-C6
23	c	908	CLA	C13-C15-C16-C17
34	J	101	LMG	C16-C17-C18-C19
26	L	102	SQD	C13-C14-C15-C16
23	d	401	CLA	C2C-C3C-CAC-CBC
30	b	621	LMT	C2-C3-C4-C5
23	d	404	CLA	O1D-CGD-O2D-CED
28	D	409	LHG	C28-C29-C30-C31
26	L	102	SQD	C46-C45-O47-C7
23	A	405	CLA	C4C-C3C-CAC-CBC
34	d	411	LMG	C17-C18-C19-C20
36	C	519	DGD	C5A-C6A-C7A-C8A
35	d	413	HTG	C1'-C2'-C3'-C4'
28	K	101	LHG	C12-C13-C14-C15
34	J	101	LMG	C20-C21-C22-C23
30	B	623	LMT	O5B-C1B-O1B-C4'
23	C	505	CLA	C5-C6-C7-C8
28	K	101	LHG	C4-O6-P-O5
26	a	412	SQD	C30-C31-C32-C33
28	d	408	LHG	C24-C25-C26-C27
34	a	413	LMG	C30-C31-C32-C33
36	d	407	DGD	C8B-C9B-CAB-CBB
27	d	406	PL9	C30-C29-C31-C32
36	c	918	DGD	CCB-CDB-CEB-CFB
25	b	618	BCR	C1-C6-C7-C8
23	c	909	CLA	C13-C15-C16-C17
34	B	622	LMG	O8-C28-C29-C30
26	B	621	SQD	C27-C28-C29-C30
23	B	602	CLA	C8-C10-C11-C12
35	c	922	HTG	C1'-C2'-C3'-C4'
36	C	518	DGD	O6E-C1E-O5D-C6D
23	B	602	CLA	C2A-CAA-CBA-CGA
34	d	411	LMG	O7-C8-C9-O8
34	C	501	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
34	m	102	LMG	O7-C8-C9-O8
28	E	101	LHG	O7-C5-C6-O8
36	C	519	DGD	CCB-CDB-CEB-CFB
30	B	643	LMT	C2-C3-C4-C5
34	B	622	LMG	C15-C16-C17-C18
28	d	402	LHG	C4-O6-P-O3
28	d	409	LHG	C3-O3-P-O6
28	D	410	LHG	C3-O3-P-O6
28	D	409	LHG	C27-C28-C29-C30
36	C	519	DGD	CCA-CDA-CEA-CFA
34	m	102	LMG	C7-C8-C9-O8
36	h	102	DGD	CAB-CBB-CCB-CDB
23	A	406	CLA	C6-C7-C8-C10
23	B	614	CLA	C11-C10-C8-C7
23	d	401	CLA	C11-C12-C13-C15
36	h	102	DGD	C2B-C3B-C4B-C5B
34	a	413	LMG	O8-C28-C29-C30
23	b	617	CLA	C3-C5-C6-C7
34	D	412	LMG	C38-C39-C40-C41
23	D	403	CLA	C14-C13-C15-C16
23	c	907	CLA	C11-C10-C8-C9
23	C	510	CLA	C6-C7-C8-C9
23	B	615	CLA	C14-C13-C15-C16
23	b	616	CLA	C14-C13-C15-C16
23	c	905	CLA	C11-C10-C8-C9
25	t	101	BCR	C9-C10-C11-C12
23	c	908	CLA	C16-C17-C18-C20
23	A	408	CLA	C16-C17-C18-C20
28	L	101	LHG	C11-C10-C9-C8
36	C	517	DGD	CCA-CDA-CEA-CFA
24	a	409	PHO	C4C-C3C-CAC-CBC
34	a	413	LMG	C12-C13-C14-C15
28	d	409	LHG	C35-C36-C37-C38
23	B	616	CLA	O1D-CGD-O2D-CED
34	C	501	LMG	C29-C30-C31-C32
23	a	407	CLA	C10-C11-C12-C13
23	c	903	CLA	C15-C16-C17-C18
34	C	520	LMG	C14-C15-C16-C17
28	A	412	LHG	C19-C20-C21-C22
36	h	102	DGD	C9A-CAA-CBA-CCA
36	c	917	DGD	C6A-C7A-C8A-C9A
34	d	411	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
34	m	102	LMG	O8-C28-C29-C30
27	A	411	PL9	C23-C24-C26-C27
36	c	917	DGD	C8A-C9A-CAA-CBA
26	A	415	SQD	C12-C13-C14-C15
26	A	415	SQD	C14-C15-C16-C17
23	A	406	CLA	C13-C15-C16-C17
23	D	401	CLA	C15-C16-C17-C18
23	B	609	CLA	C13-C15-C16-C17
34	m	102	LMG	C29-C28-O8-C9
25	k	102	BCR	C19-C20-C21-C22
27	a	414	PL9	C14-C16-C17-C18
27	D	406	PL9	C39-C41-C42-C43
34	m	102	LMG	O10-C28-O8-C9
28	l	101	LHG	C7-C8-C9-C10
23	b	613	CLA	C10-C11-C12-C13
30	b	621	LMT	C4-C5-C6-C7
28	d	402	LHG	O9-C7-C8-C9
26	A	410	SQD	C34-C35-C36-C37
23	C	513	CLA	C3-C5-C6-C7
34	B	622	LMG	C40-C41-C42-C43
28	d	409	LHG	C26-C27-C28-C29
27	d	406	PL9	C28-C29-C31-C32
34	d	411	LMG	C22-C23-C24-C25
23	C	513	CLA	C13-C15-C16-C17
23	C	508	CLA	C5-C6-C7-C8
36	H	103	DGD	O1B-C1B-C2B-C3B
26	B	621	SQD	C35-C36-C37-C38
34	j	101	LMG	C20-C21-C22-C23
23	b	607	CLA	C16-C17-C18-C20
36	c	918	DGD	C8B-C9B-CAB-CBB
26	L	102	SQD	O6-C44-C45-O47
23	c	902	CLA	C2A-CAA-CBA-CGA
28	e	101	LHG	C2-C3-O3-P
28	A	412	LHG	C2-C3-O3-P
36	D	407	DGD	CDA-CEA-CFA-CGA
28	d	410	LHG	C24-C25-C26-C27
26	B	621	SQD	C26-C27-C28-C29
27	d	406	PL9	C45-C44-C46-C47
26	A	415	SQD	C24-C25-C26-C27
24	A	407	PHO	C2-C3-C5-C6
34	c	920	LMG	C37-C38-C39-C40
36	C	519	DGD	O6D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
23	C	510	CLA	C11-C12-C13-C14
23	b	611	CLA	C14-C13-C15-C16
36	C	519	DGD	C8B-C9B-CAB-CBB
34	m	102	LMG	C17-C18-C19-C20
30	F	101	LMT	O5'-C1'-O1'-C1
28	l	101	LHG	C12-C13-C14-C15
34	j	101	LMG	C35-C36-C37-C38
26	a	412	SQD	C35-C36-C37-C38
23	A	406	CLA	C11-C10-C8-C7
23	B	603	CLA	C11-C12-C13-C15
23	c	908	CLA	C11-C12-C13-C15
23	A	408	CLA	C11-C12-C13-C15
23	B	615	CLA	C12-C13-C15-C16
35	B	624	HTG	C4'-C5'-C6'-C7'
36	D	407	DGD	CAB-CBB-CCB-CDB
35	C	523	HTG	C4-C5-C6-O6
35	B	630	HTG	C3'-C4'-C5'-C6'
34	J	101	LMG	C34-C35-C36-C37
36	d	407	DGD	C8A-C9A-CAA-CBA
23	B	611	CLA	C2A-CAA-CBA-CGA
23	b	611	CLA	O1D-CGD-O2D-CED
23	B	602	CLA	CAA-CBA-CGA-O2A
26	A	415	SQD	C24-C23-O48-C46
36	D	407	DGD	C3B-C4B-C5B-C6B
36	H	103	DGD	C6B-C7B-C8B-C9B
26	L	102	SQD	C11-C12-C13-C14
28	L	101	LHG	C26-C27-C28-C29
26	L	102	SQD	C30-C31-C32-C33
28	A	412	LHG	C11-C12-C13-C14
34	C	531	LMG	C39-C40-C41-C42
23	b	604	CLA	CBD-CGD-O2D-CED
35	B	626	HTG	C4'-C5'-C6'-C7'
28	L	101	LHG	C5-C6-O8-C23
28	d	408	LHG	C14-C15-C16-C17
34	d	411	LMG	C29-C30-C31-C32
26	a	417	SQD	C17-C18-C19-C20
26	x	101	SQD	O6-C44-C45-O47
34	a	413	LMG	O1-C7-C8-O7
26	L	102	SQD	C35-C36-C37-C38
23	b	612	CLA	C8-C10-C11-C12
28	l	101	LHG	C14-C15-C16-C17
28	l	101	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
34	m	102	LMG	C38-C39-C40-C41
23	c	910	CLA	C16-C17-C18-C20
26	D	408	SQD	C31-C32-C33-C34
23	d	403	CLA	C2-C1-O2A-CGA
23	c	914	CLA	C13-C15-C16-C17
26	L	102	SQD	C32-C33-C34-C35
23	B	604	CLA	C16-C17-C18-C20
35	B	624	HTG	C1'-C2'-C3'-C4'
23	b	612	CLA	C14-C13-C15-C16
36	c	917	DGD	CCA-CDA-CEA-CFA
26	L	102	SQD	C9-C10-C11-C12
36	h	102	DGD	O1B-C1B-C2B-C3B
25	b	619	BCR	C23-C24-C25-C30
25	c	915	BCR	C1-C6-C7-C8
25	a	411	BCR	C1-C6-C7-C8
28	L	101	LHG	C32-C33-C34-C35
26	B	621	SQD	C45-C44-O6-C1
36	c	917	DGD	C5D-C6D-O5D-C1E
26	A	410	SQD	C28-C29-C30-C31
28	D	410	LHG	C14-C15-C16-C17
30	T	103	LMT	C1-C2-C3-C4
23	b	607	CLA	C16-C17-C18-C19
30	m	103	LMT	C2-C3-C4-C5
26	A	410	SQD	C24-C25-C26-C27
23	D	403	CLA	C4C-C3C-CAC-CBC
34	B	622	LMG	C14-C15-C16-C17
34	C	531	LMG	C35-C36-C37-C38
28	a	415	LHG	C24-C25-C26-C27
35	O	302	HTG	C3'-C4'-C5'-C6'
27	A	411	PL9	C39-C41-C42-C43
36	c	919	DGD	C9B-CAB-CBB-CCB
23	b	611	CLA	C12-C13-C15-C16
23	B	606	CLA	C13-C15-C16-C17
35	d	413	HTG	S1-C1'-C2'-C3'
35	c	923	HTG	S1-C1'-C2'-C3'
36	c	918	DGD	C2E-C1E-O5D-C6D
35	B	630	HTG	C4'-C5'-C6'-C7'
26	B	621	SQD	O6-C44-C45-O47
30	B	643	LMT	O5'-C5'-C6'-O6'
35	b	627	HTG	C2'-C3'-C4'-C5'
34	c	930	LMG	C11-C12-C13-C14
23	B	611	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
23	b	612	CLA	O1D-CGD-O2D-CED
23	b	611	CLA	C16-C17-C18-C20
36	C	517	DGD	CDA-CEA-CFA-CGA
23	c	910	CLA	C11-C10-C8-C9
23	A	406	CLA	C14-C13-C15-C16
23	c	908	CLA	C11-C12-C13-C14
23	A	408	CLA	C14-C13-C15-C16
23	C	508	CLA	C11-C10-C8-C9
23	C	508	CLA	C14-C13-C15-C16
23	B	612	CLA	C11-C12-C13-C14
23	c	906	CLA	C14-C13-C15-C16
23	b	605	CLA	CAD-CBD-CGD-O2D
23	c	902	CLA	CAD-CBD-CGD-O2D
23	B	615	CLA	CAD-CBD-CGD-O2D
23	C	502	CLA	CAD-CBD-CGD-O2D
23	b	611	CLA	CAD-CBD-CGD-O2D
23	C	507	CLA	CAD-CBD-CGD-O2D
23	d	404	CLA	CAD-CBD-CGD-O2D
23	C	511	CLA	CAD-CBD-CGD-O2D
23	b	617	CLA	CAD-CBD-CGD-O2D
23	C	506	CLA	CAD-CBD-CGD-O2D
23	B	617	CLA	CAD-CBD-CGD-O2D
23	B	611	CLA	CAD-CBD-CGD-O2D
26	a	412	SQD	C33-C34-C35-C36
28	e	101	LHG	C12-C13-C14-C15
28	D	410	LHG	C11-C12-C13-C14
34	J	101	LMG	C4-C5-C6-O5
23	c	911	CLA	C2-C3-C5-C6
25	k	102	BCR	C7-C8-C9-C10
28	d	402	LHG	C13-C14-C15-C16
36	c	918	DGD	C4A-C5A-C6A-C7A
30	m	103	LMT	C4-C5-C6-C7
35	c	921	HTG	O5-C5-C6-O6
27	a	414	PL9	C31-C32-C33-C34
23	c	904	CLA	C10-C11-C12-C13
23	C	513	CLA	CAA-CBA-CGA-O2A
28	e	101	LHG	O7-C7-C8-C9
23	d	401	CLA	C4C-C3C-CAC-CBC
23	B	605	CLA	O2A-C1-C2-C3
23	c	910	CLA	O2A-C1-C2-C3
23	D	403	CLA	O2A-C1-C2-C3
23	c	913	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
24	a	408	PHO	O2A-C1-C2-C3
26	a	412	SQD	C15-C16-C17-C18
28	d	402	LHG	C11-C12-C13-C14
28	d	408	LHG	C26-C27-C28-C29
36	c	918	DGD	C8A-C9A-CAA-CBA
26	A	410	SQD	O47-C7-C8-C9
26	A	415	SQD	O49-C7-O47-C45
34	D	412	LMG	C8-C9-O8-C28
23	a	407	CLA	CHA-CBD-CGD-O1D
23	c	910	CLA	CHA-CBD-CGD-O1D
23	c	910	CLA	CHA-CBD-CGD-O2D
23	A	406	CLA	CHA-CBD-CGD-O1D
23	C	513	CLA	CHA-CBD-CGD-O1D
23	b	615	CLA	CHA-CBD-CGD-O1D
23	B	603	CLA	CHA-CBD-CGD-O1D
23	D	401	CLA	CHA-CBD-CGD-O2D
23	C	505	CLA	CHA-CBD-CGD-O2D
23	c	907	CLA	CHA-CBD-CGD-O2D
23	C	508	CLA	CHA-CBD-CGD-O2D
23	b	604	CLA	CHA-CBD-CGD-O2D
23	b	617	CLA	CHA-CBD-CGD-O1D
23	B	607	CLA	CHA-CBD-CGD-O2D
24	a	409	PHO	CHA-CBD-CGD-O1D
24	a	409	PHO	CHA-CBD-CGD-O2D
23	B	617	CLA	CHA-CBD-CGD-O1D
23	b	612	CLA	CHA-CBD-CGD-O2D
34	D	412	LMG	C19-C20-C21-C22
30	F	101	LMT	C2'-C1'-O1'-C1
23	a	407	CLA	C2C-C3C-CAC-CBC
26	A	410	SQD	C9-C10-C11-C12
30	A	416	LMT	C7-C8-C9-C10
23	B	605	CLA	C16-C17-C18-C19
26	A	415	SQD	O47-C45-C46-O48
34	c	920	LMG	O10-C28-O8-C9
28	D	411	LHG	C12-C13-C14-C15
26	A	415	SQD	O10-C23-O48-C46
28	K	101	LHG	O7-C7-C8-C9
23	c	913	CLA	CAA-CBA-CGA-O2A
30	b	621	LMT	O5'-C5'-C6'-O6'
36	c	919	DGD	C2A-C1A-O1G-C1G
23	c	912	CLA	O1D-CGD-O2D-CED
23	b	607	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	b	602	CLA	C6-C7-C8-C10
23	b	604	CLA	C6-C7-C8-C10
23	b	614	CLA	C16-C17-C18-C19
28	E	101	LHG	O7-C7-C8-C9
34	J	101	LMG	C14-C15-C16-C17
23	b	607	CLA	C6-C7-C8-C9
23	B	616	CLA	C14-C13-C15-C16
23	b	602	CLA	C11-C12-C13-C14
23	b	606	CLA	C14-C13-C15-C16
23	d	401	CLA	C11-C12-C13-C14
36	C	519	DGD	C5B-C6B-C7B-C8B
34	c	920	LMG	C29-C28-O8-C9
28	e	101	LHG	O9-C7-C8-C9
23	b	611	CLA	C16-C17-C18-C19
23	C	504	CLA	C5-C6-C7-C8
23	B	608	CLA	O1D-CGD-O2D-CED
23	B	605	CLA	C16-C17-C18-C20
28	D	411	LHG	C24-C25-C26-C27
25	C	515	BCR	C21-C22-C23-C24
30	a	418	LMT	C4-C5-C6-C7
23	C	510	CLA	C15-C16-C17-C18
35	c	923	HTG	C3'-C4'-C5'-C6'
23	C	514	CLA	CBA-CGA-O2A-C1
23	C	513	CLA	CAA-CBA-CGA-O1A
26	x	101	SQD	O6-C44-C45-C46
26	D	408	SQD	C44-C45-C46-O48
23	b	605	CLA	C15-C16-C17-C18
23	c	907	CLA	C5-C6-C7-C8
28	e	101	LHG	C7-C8-C9-C10
34	C	501	LMG	C20-C21-C22-C23
23	b	613	CLA	C8-C10-C11-C12
36	h	102	DGD	C7B-C8B-C9B-CAB
26	A	410	SQD	O49-C7-C8-C9
23	C	514	CLA	O1A-CGA-O2A-C1
27	a	414	PL9	C3-C7-C8-C9
28	d	409	LHG	C3-O3-P-O5
28	D	410	LHG	C3-O3-P-O5
30	B	623	LMT	C2B-C1B-O1B-C4'
28	E	101	LHG	O9-C7-C8-C9
36	C	518	DGD	CBA-CCA-CDA-CEA
36	c	919	DGD	O6D-C5D-C6D-O5D
25	j	104	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	j	104	BCR	C5-C6-C7-C8
26	A	415	SQD	C28-C29-C30-C31
23	b	604	CLA	C2A-CAA-CBA-CGA
35	O	302	HTG	C2'-C3'-C4'-C5'
30	m	104	LMT	C5-C6-C7-C8
23	C	505	CLA	CAD-CBD-CGD-O1D
23	d	401	CLA	CAD-CBD-CGD-O1D
26	x	101	SQD	O5-C5-C6-S
23	B	608	CLA	CAD-CBD-CGD-O1D
23	b	608	CLA	CAD-CBD-CGD-O1D
23	c	913	CLA	CAA-CBA-CGA-O1A
23	A	406	CLA	C11-C10-C8-C9
23	A	406	CLA	C11-C12-C13-C14
23	c	906	CLA	C11-C12-C13-C14
23	B	602	CLA	CBD-CGD-O2D-CED
26	L	102	SQD	C29-C30-C31-C32
23	B	617	CLA	C8-C10-C11-C12
28	L	101	LHG	O7-C7-C8-C9
23	c	906	CLA	CAA-CBA-CGA-O2A
28	l	101	LHG	C26-C27-C28-C29
34	B	622	LMG	C36-C37-C38-C39
34	C	531	LMG	O10-C28-O8-C9
28	D	409	LHG	C26-C27-C28-C29
23	B	613	CLA	C8-C10-C11-C12
23	c	904	CLA	C15-C16-C17-C18
28	K	101	LHG	O9-C7-C8-C9
23	C	508	CLA	C4-C3-C5-C6
34	C	531	LMG	C12-C13-C14-C15
28	D	410	LHG	C28-C29-C30-C31
23	a	407	CLA	C12-C13-C15-C16
23	C	514	CLA	C11-C12-C13-C15
23	b	615	CLA	C12-C13-C15-C16
23	c	907	CLA	C6-C7-C8-C10
23	B	616	CLA	C12-C13-C15-C16
35	c	922	HTG	C2-C1-S1-C1'
23	C	507	CLA	C3A-C2A-CAA-CBA
23	c	906	CLA	C12-C13-C15-C16
34	a	413	LMG	C36-C37-C38-C39
23	C	506	CLA	CAA-CBA-CGA-O2A
27	A	411	PL9	C2-C3-C7-C8
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26	a	417	SQD	C32-C33-C34-C35

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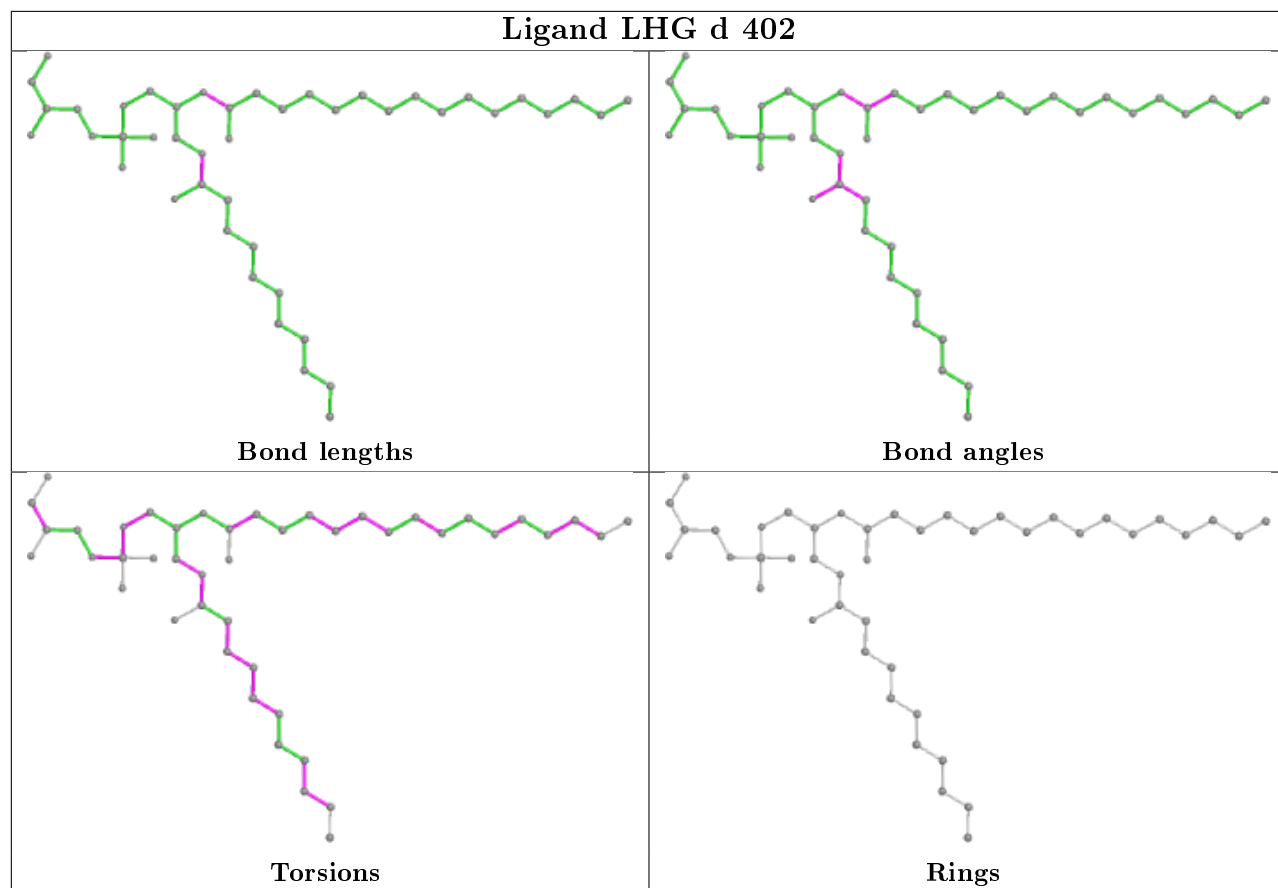
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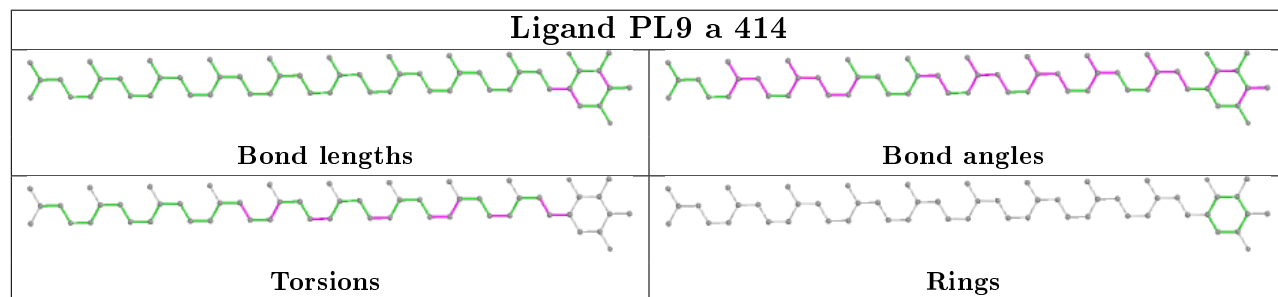
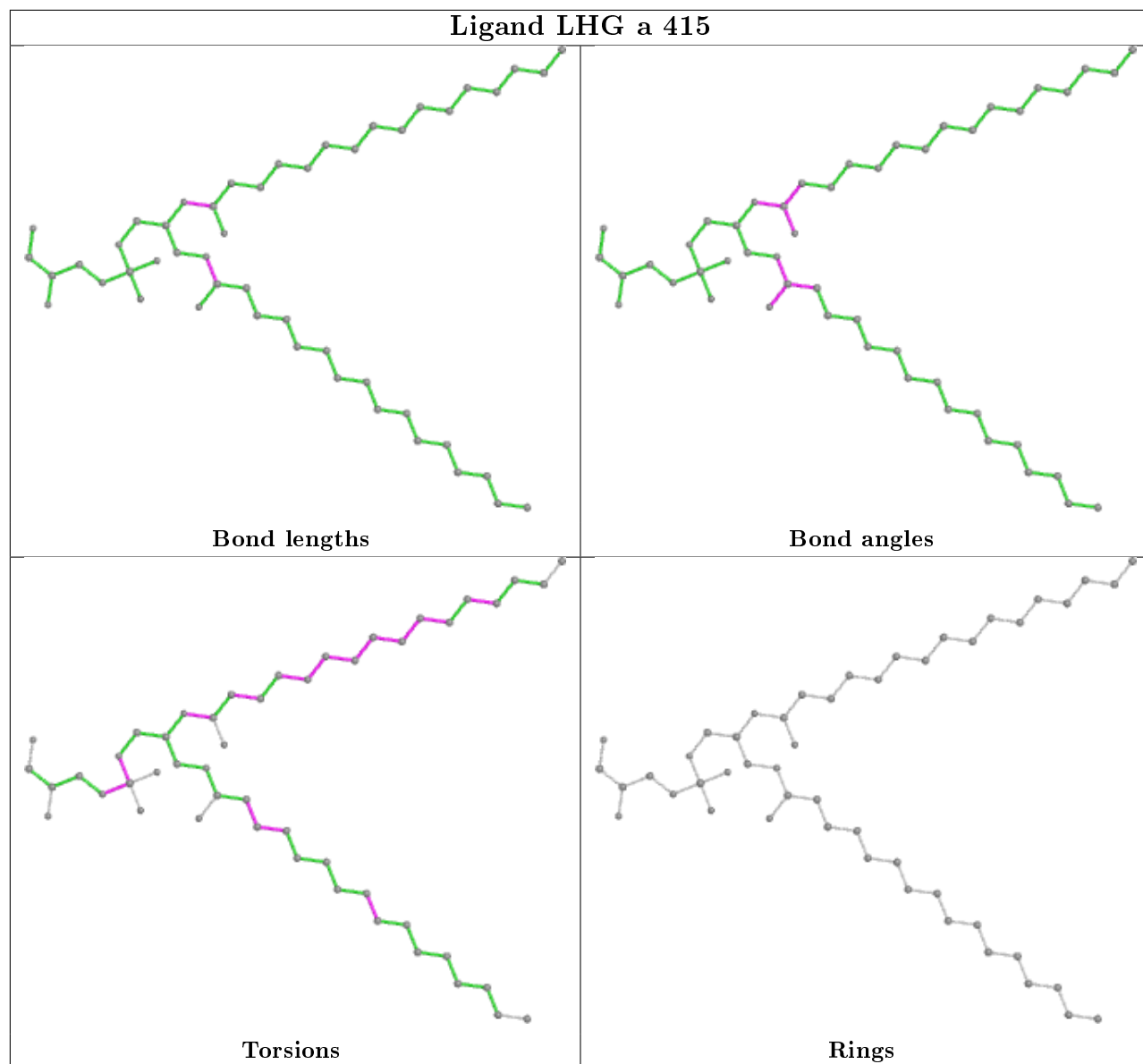
Mol	Chain	Res	Type	Atoms
36	C	519	DGD	O1G-C1A-C2A-C3A
36	c	918	DGD	O6E-C1E-O5D-C6D
23	A	408	CLA	C5-C6-C7-C8
28	d	402	LHG	C19-C20-C21-C22
28	D	411	LHG	O8-C23-C24-C25
34	c	920	LMG	O8-C28-C29-C30
23	C	502	CLA	CAA-CBA-CGA-O2A
23	C	502	CLA	C2A-CAA-CBA-CGA
23	b	606	CLA	C2A-CAA-CBA-CGA
23	b	603	CLA	C8-C10-C11-C12
24	A	407	PHO	C4-C3-C5-C6
34	J	101	LMG	O7-C10-C11-C12

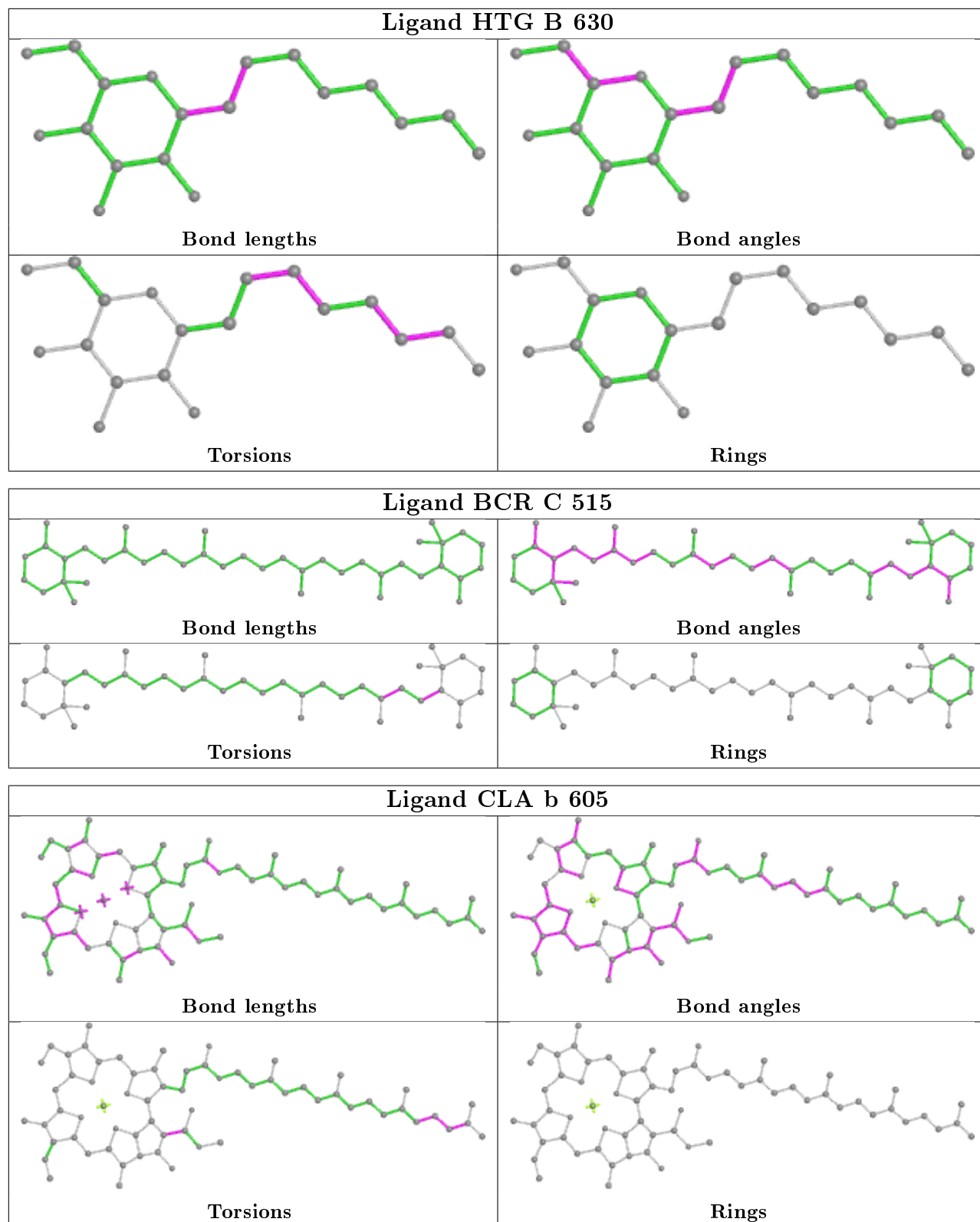
There are no ring outliers.

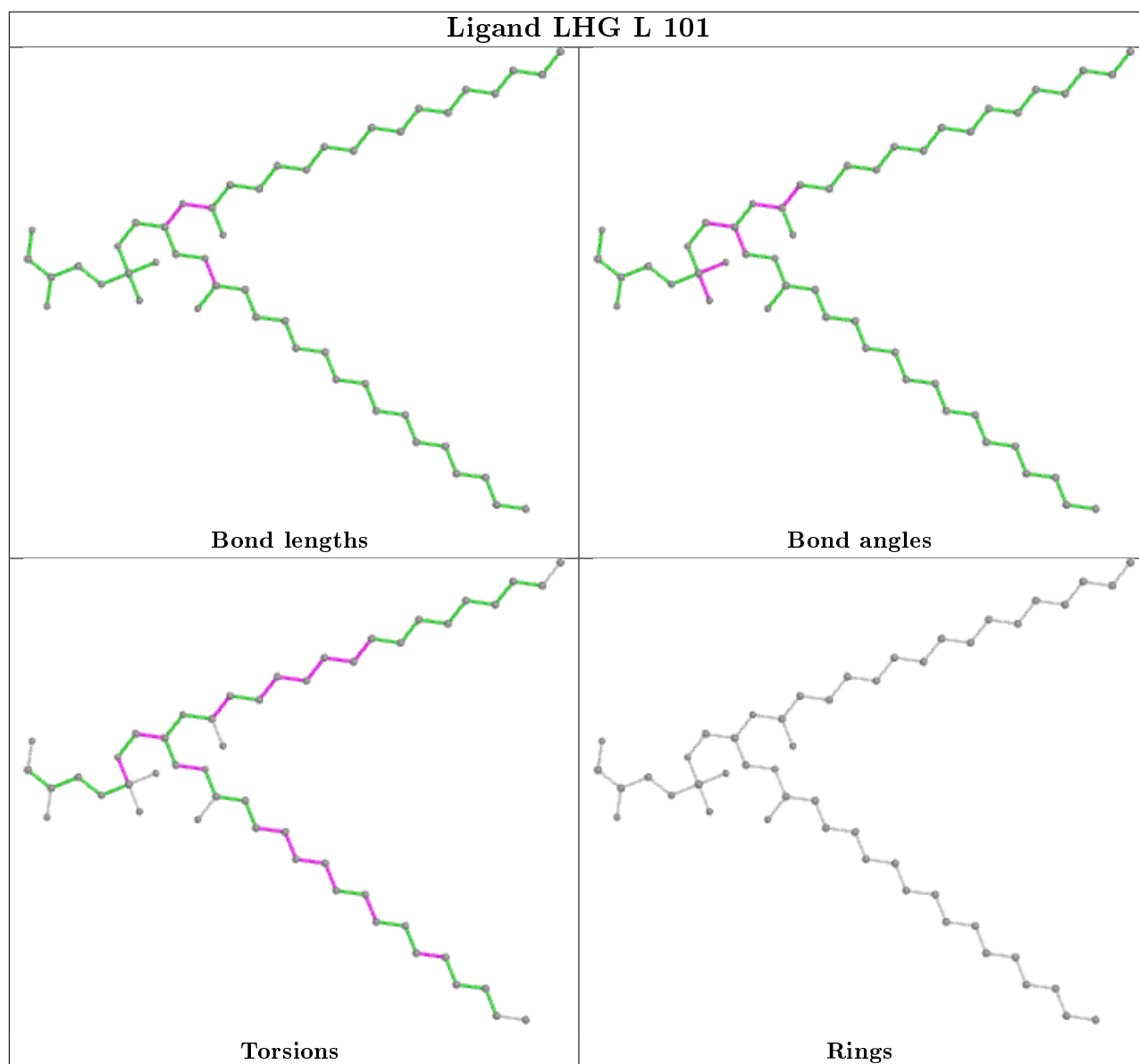
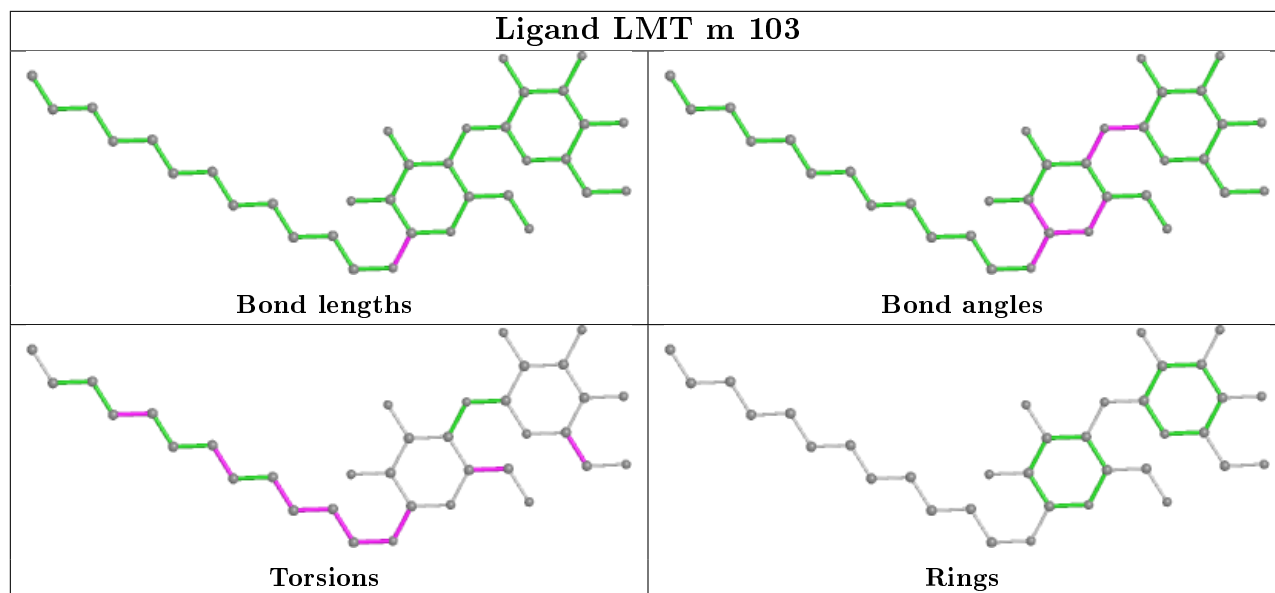
No monomer is involved in short contacts.

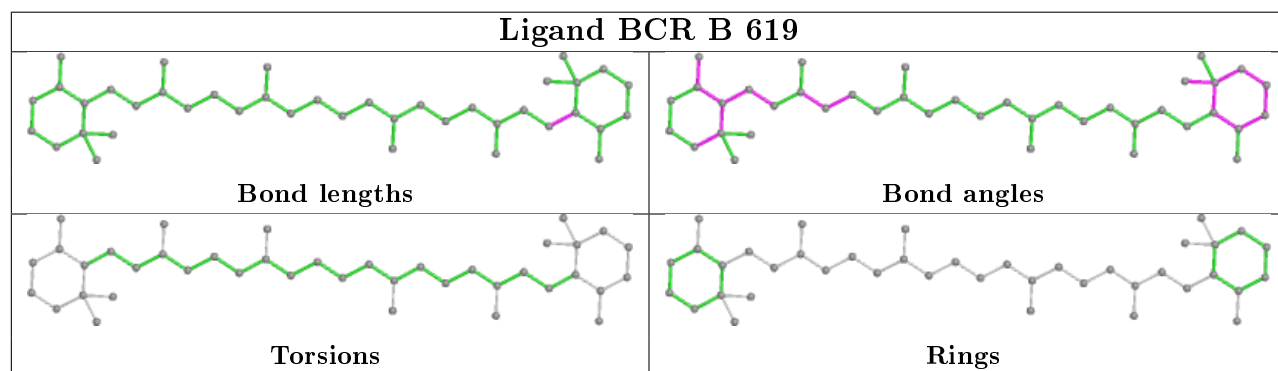
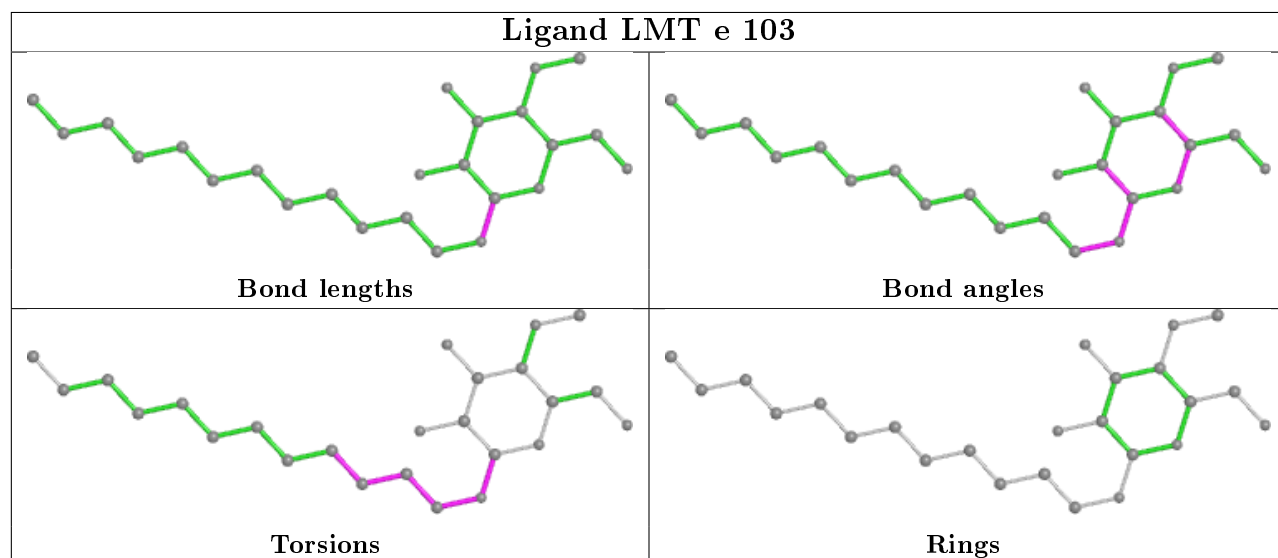
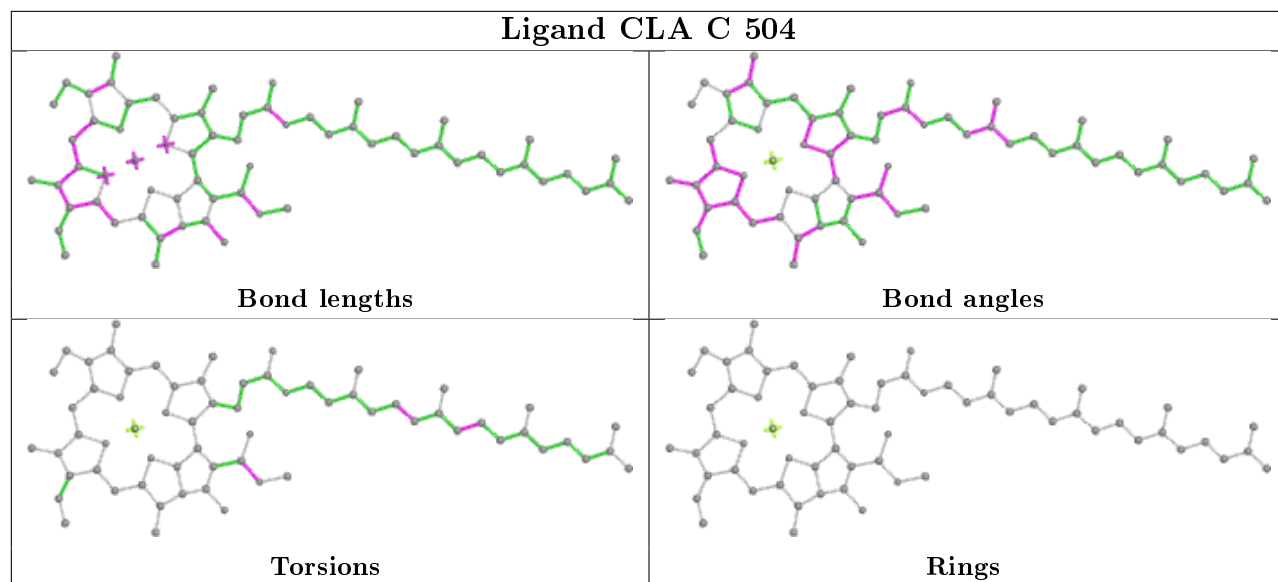
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

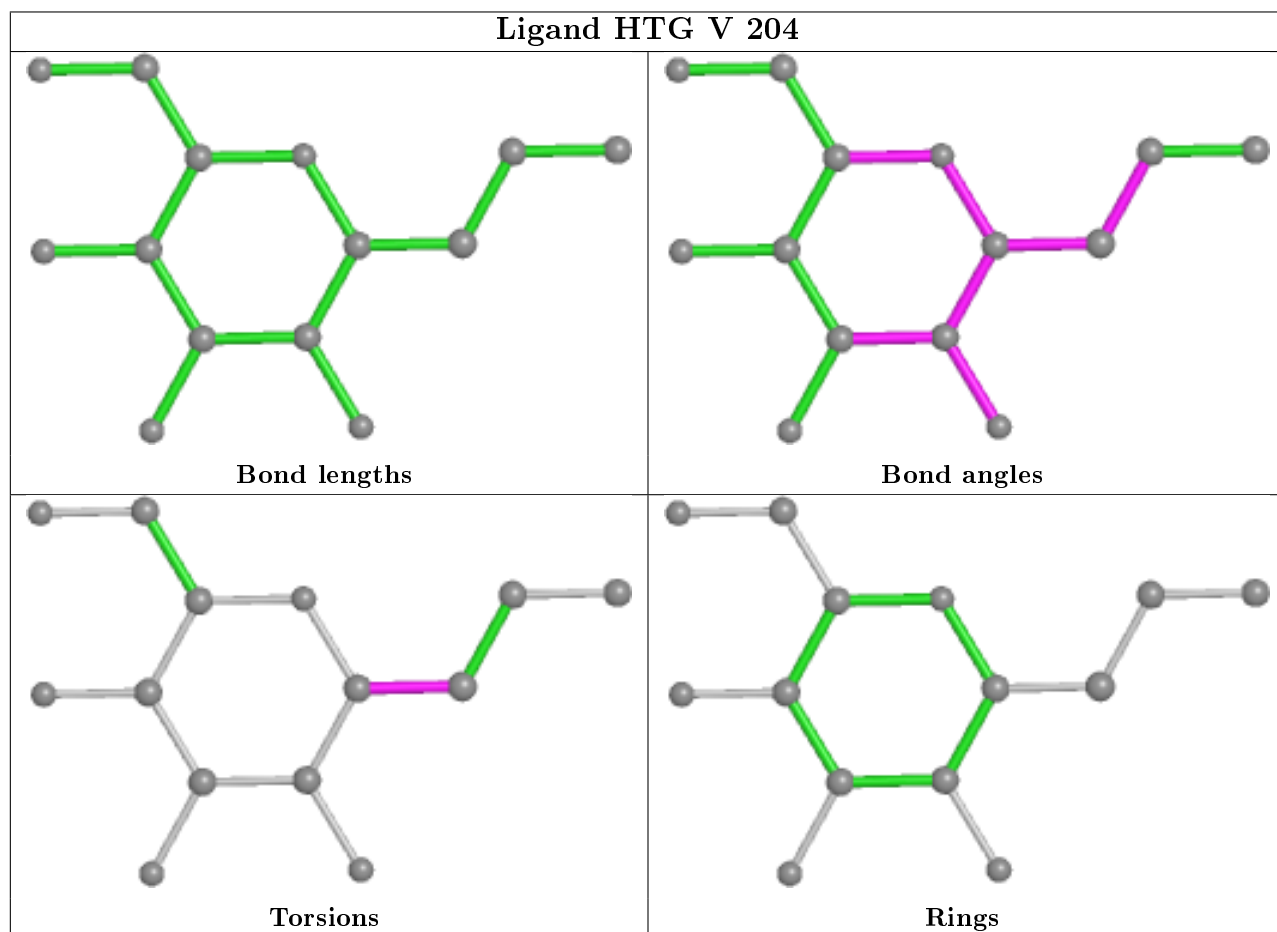
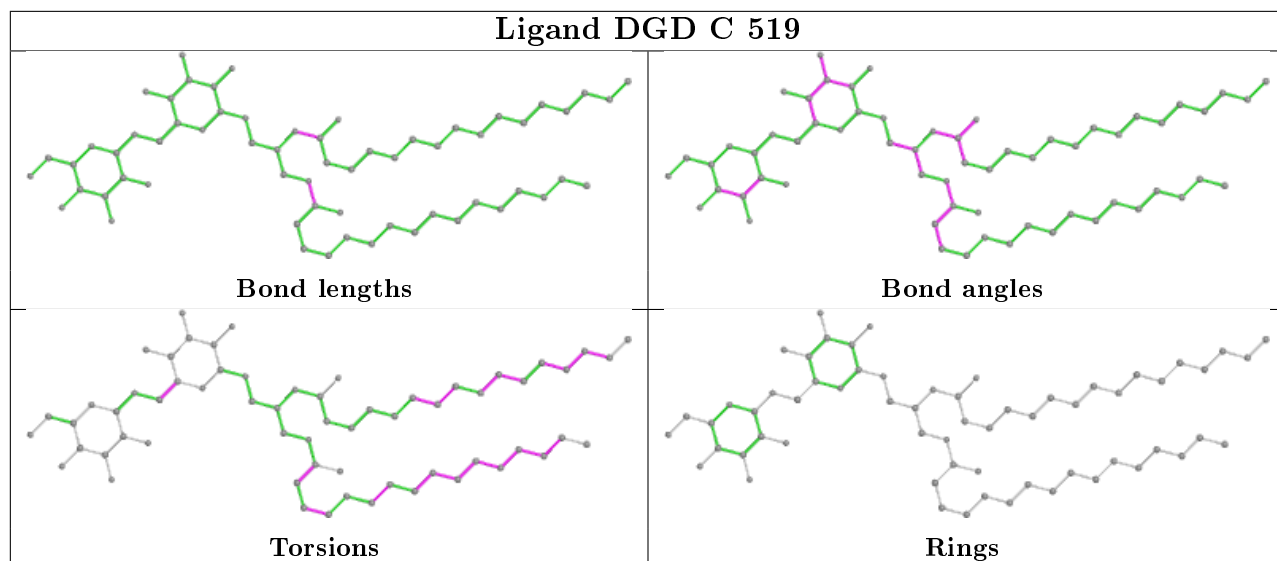


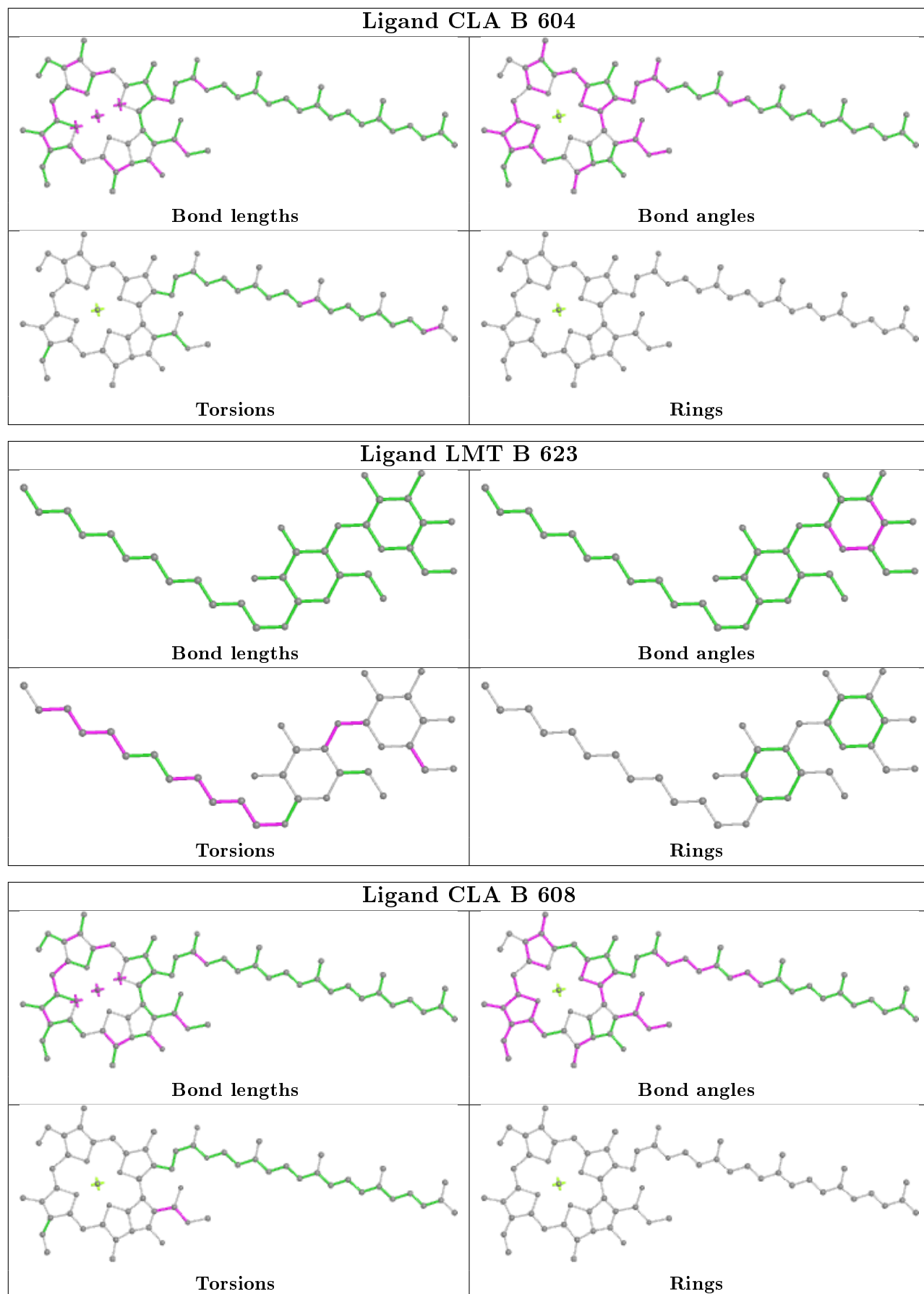


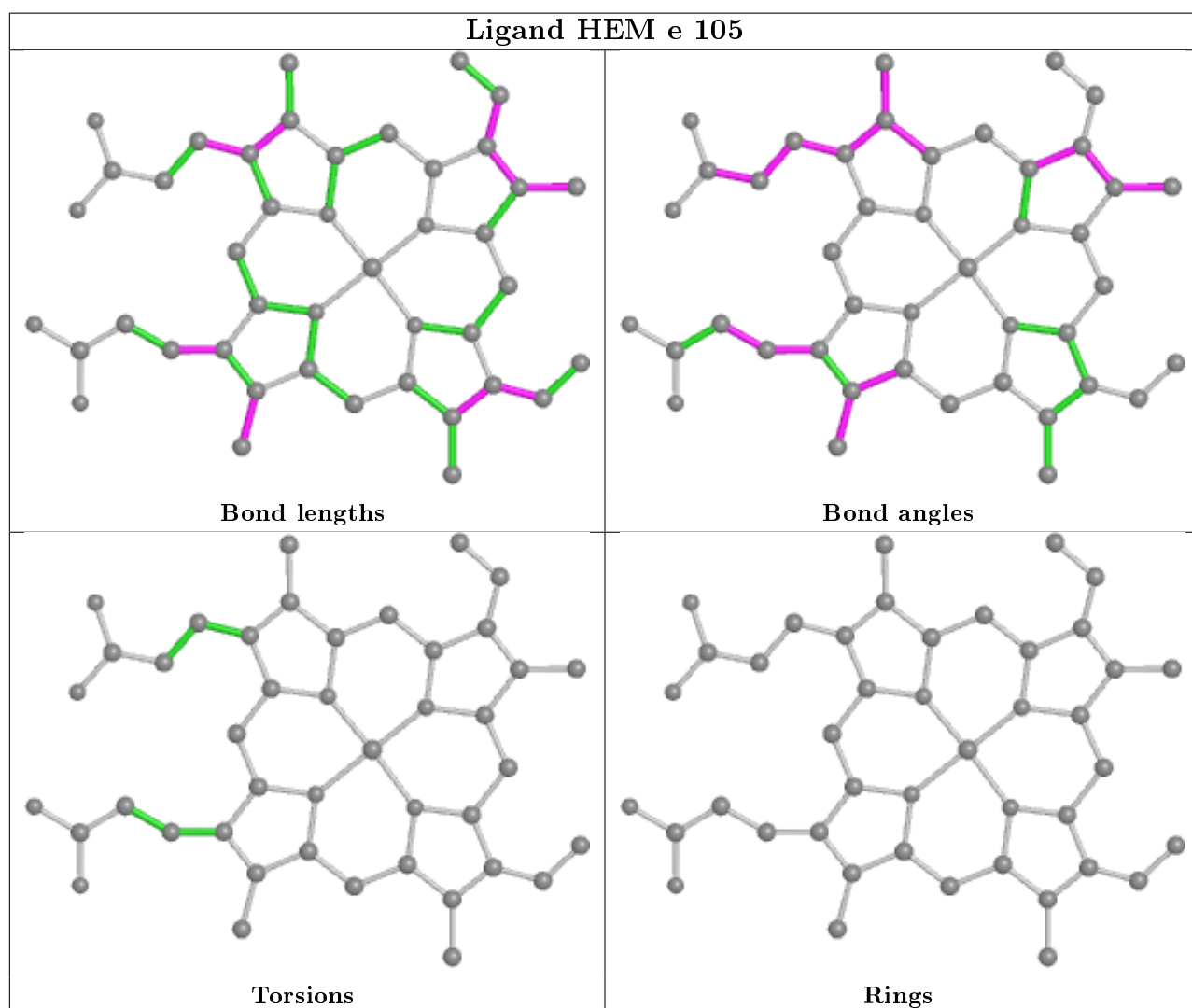
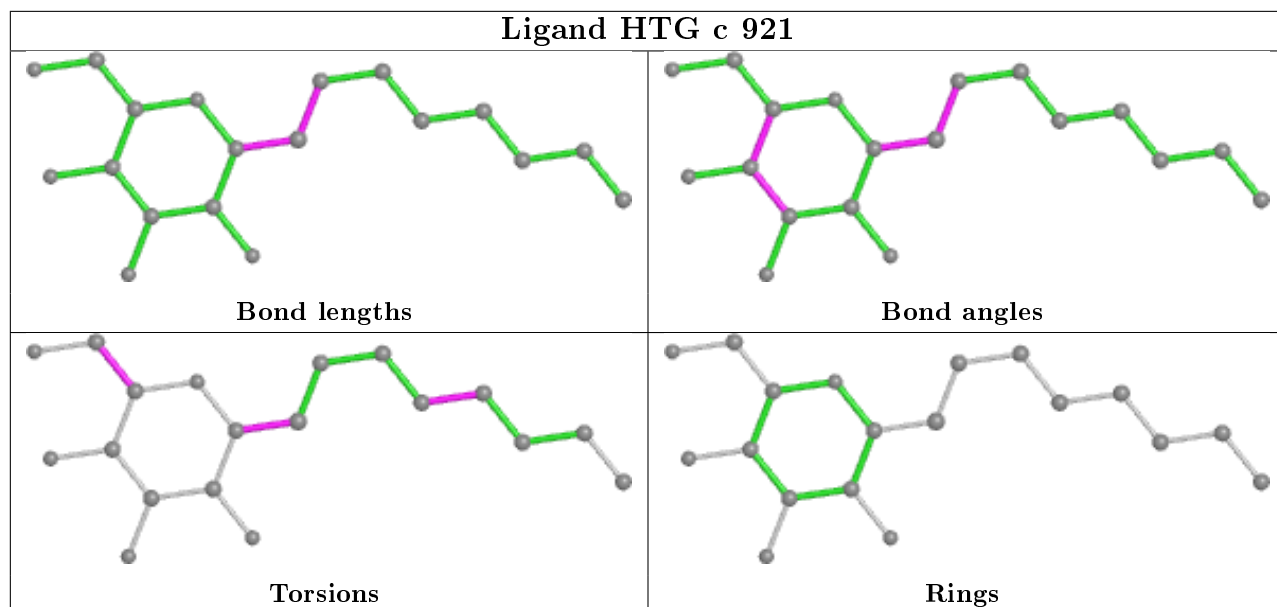


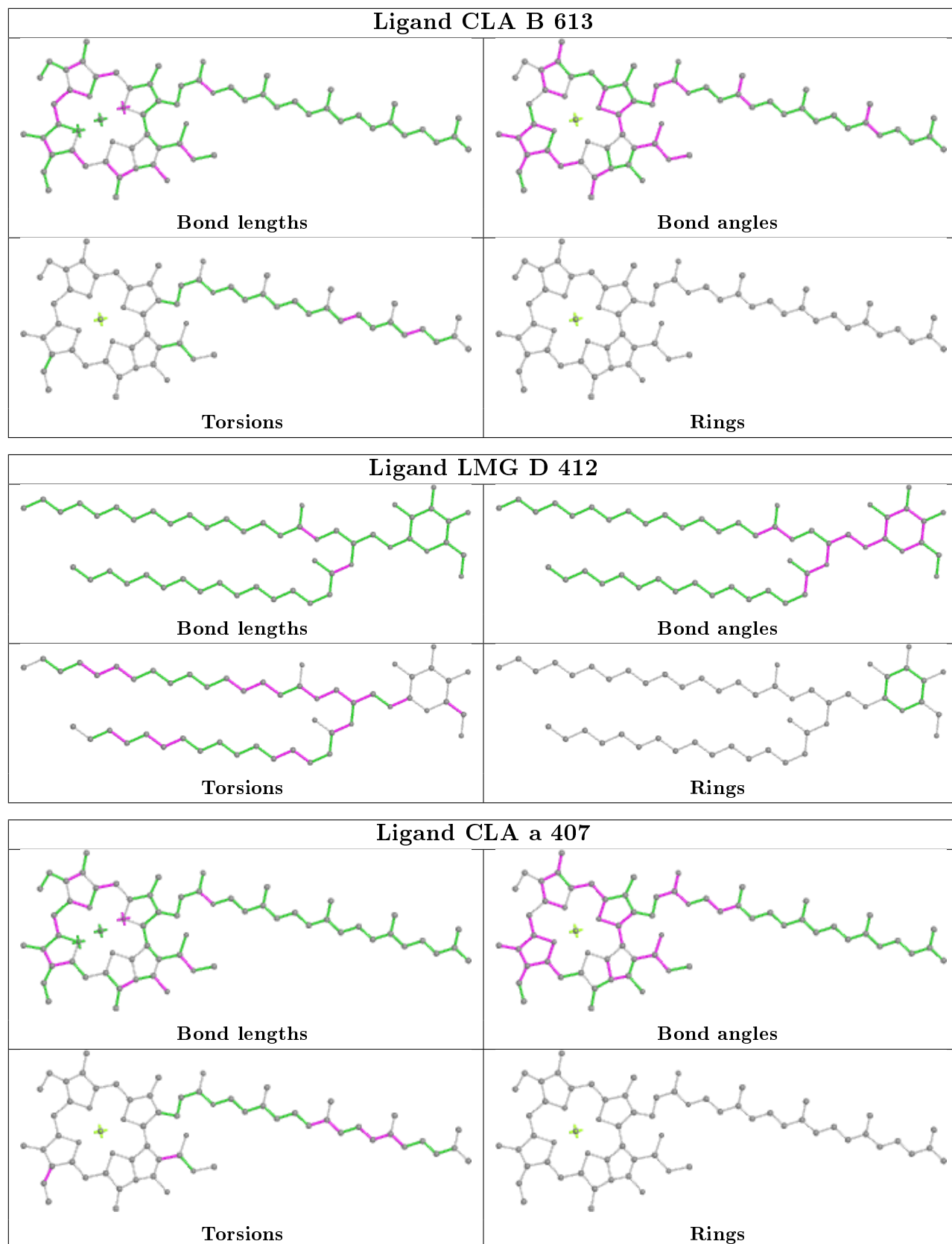


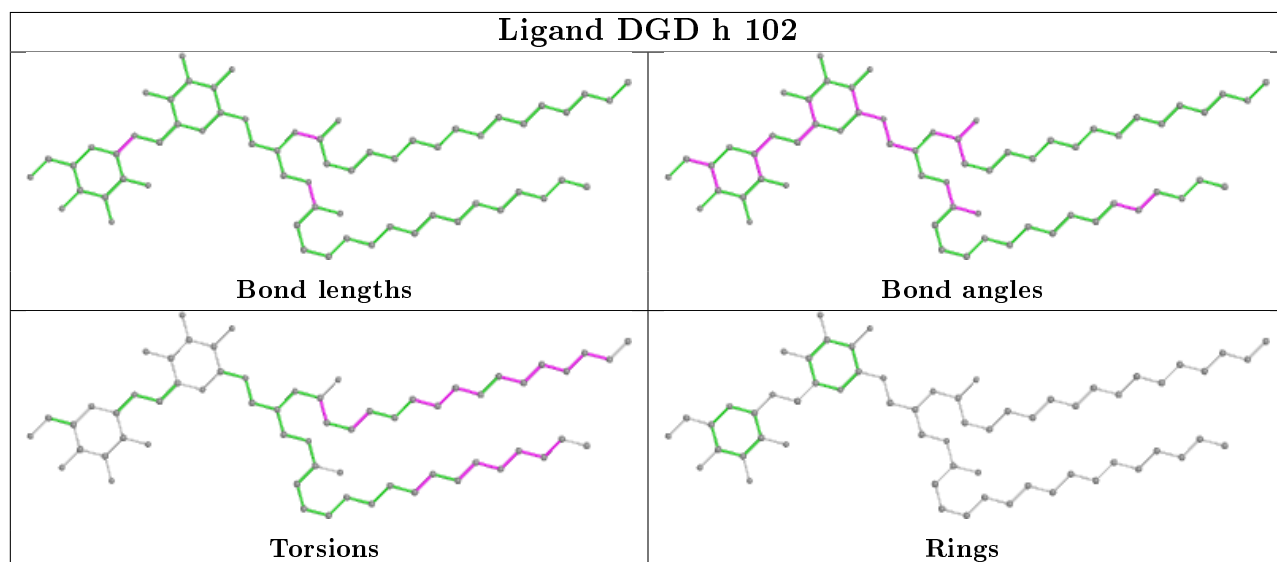
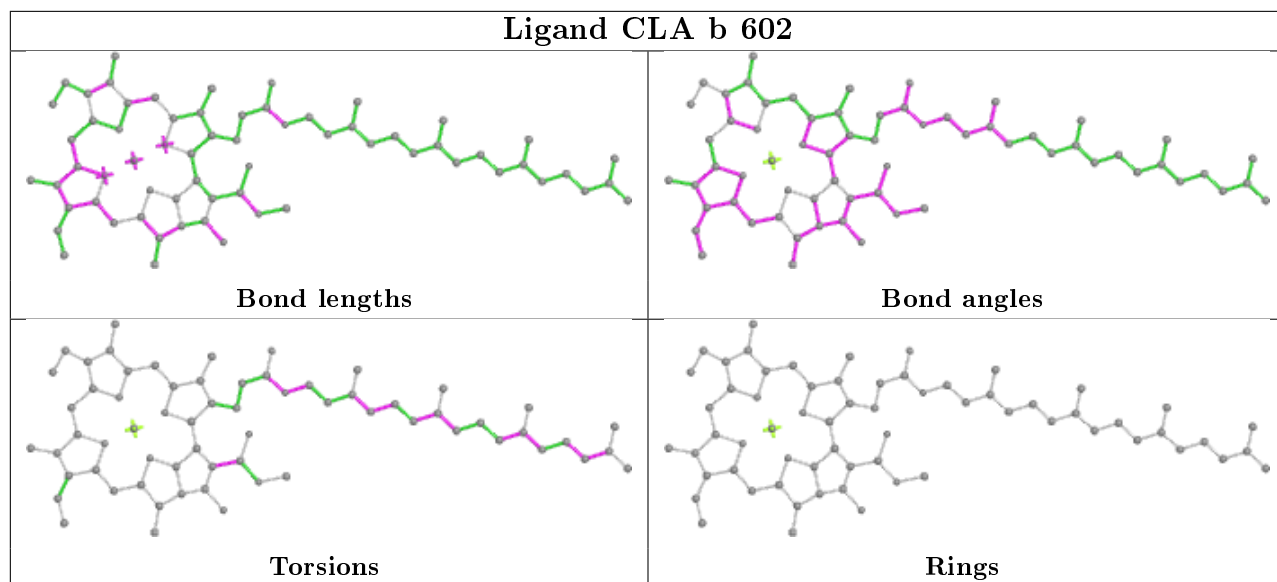


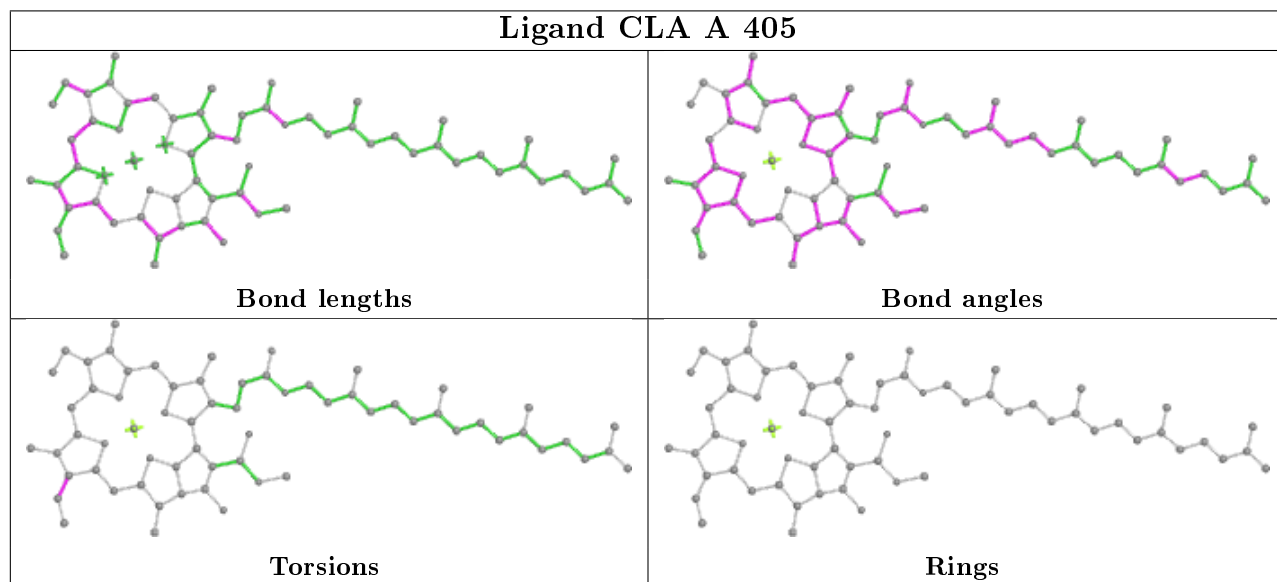
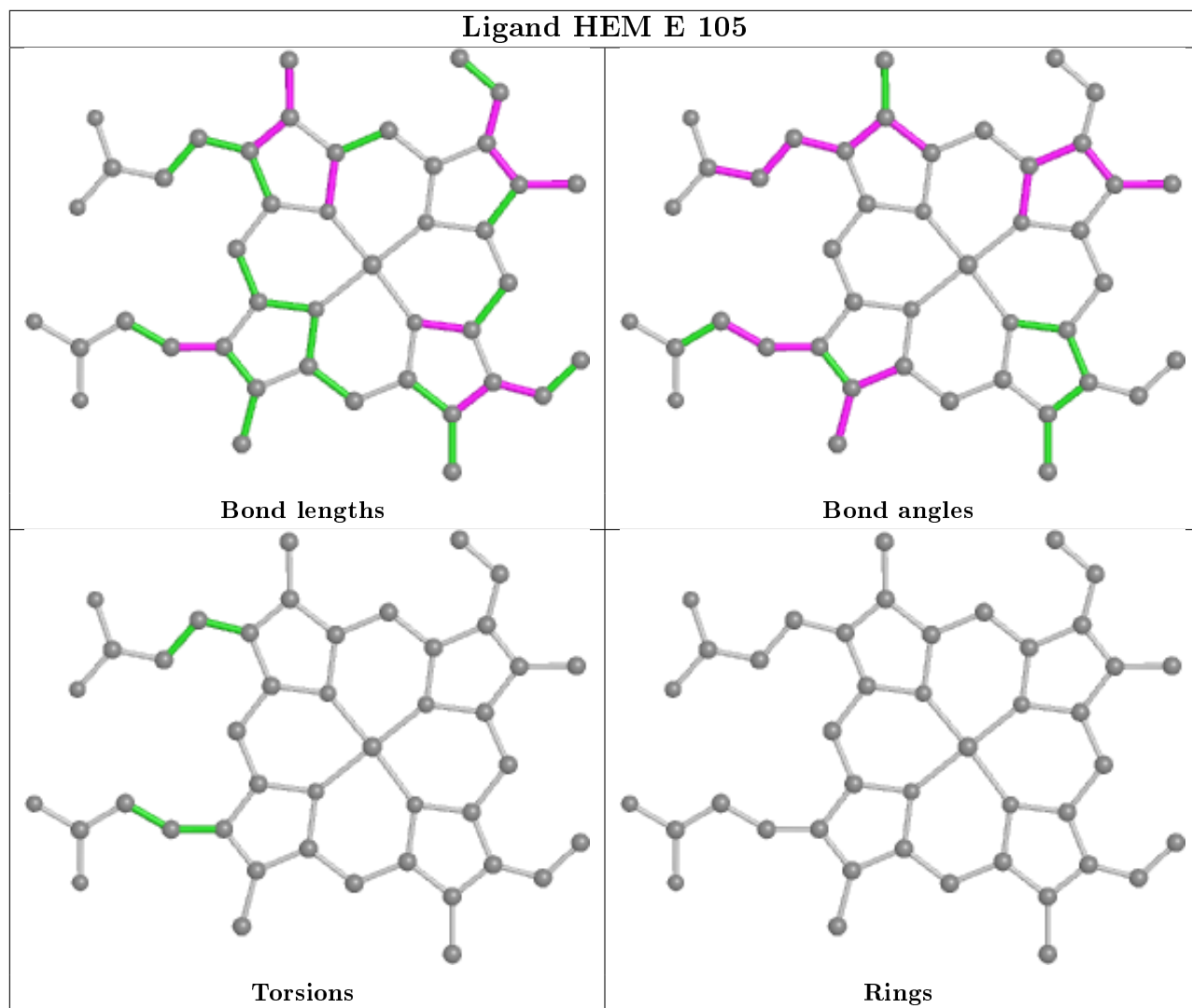


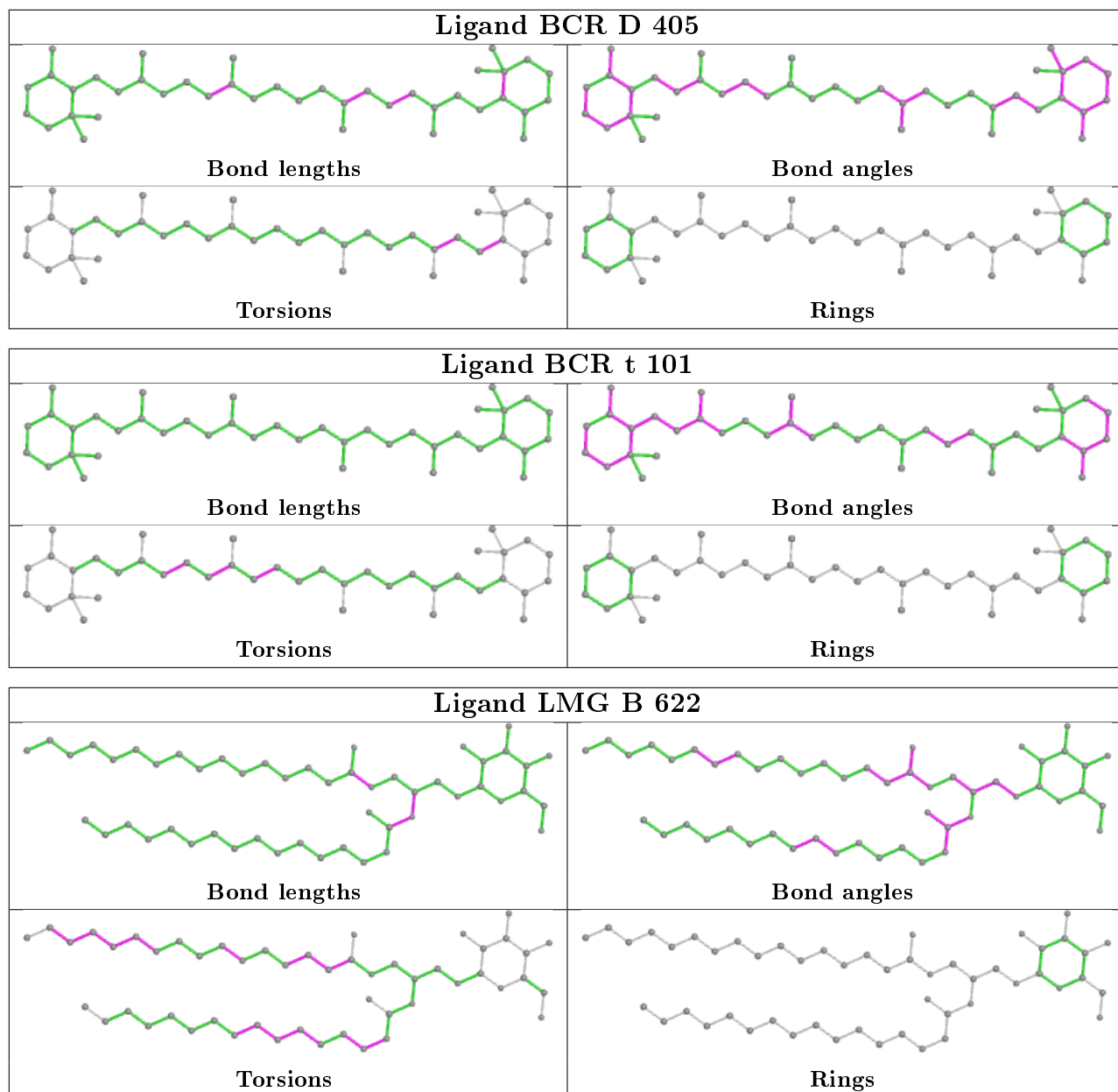


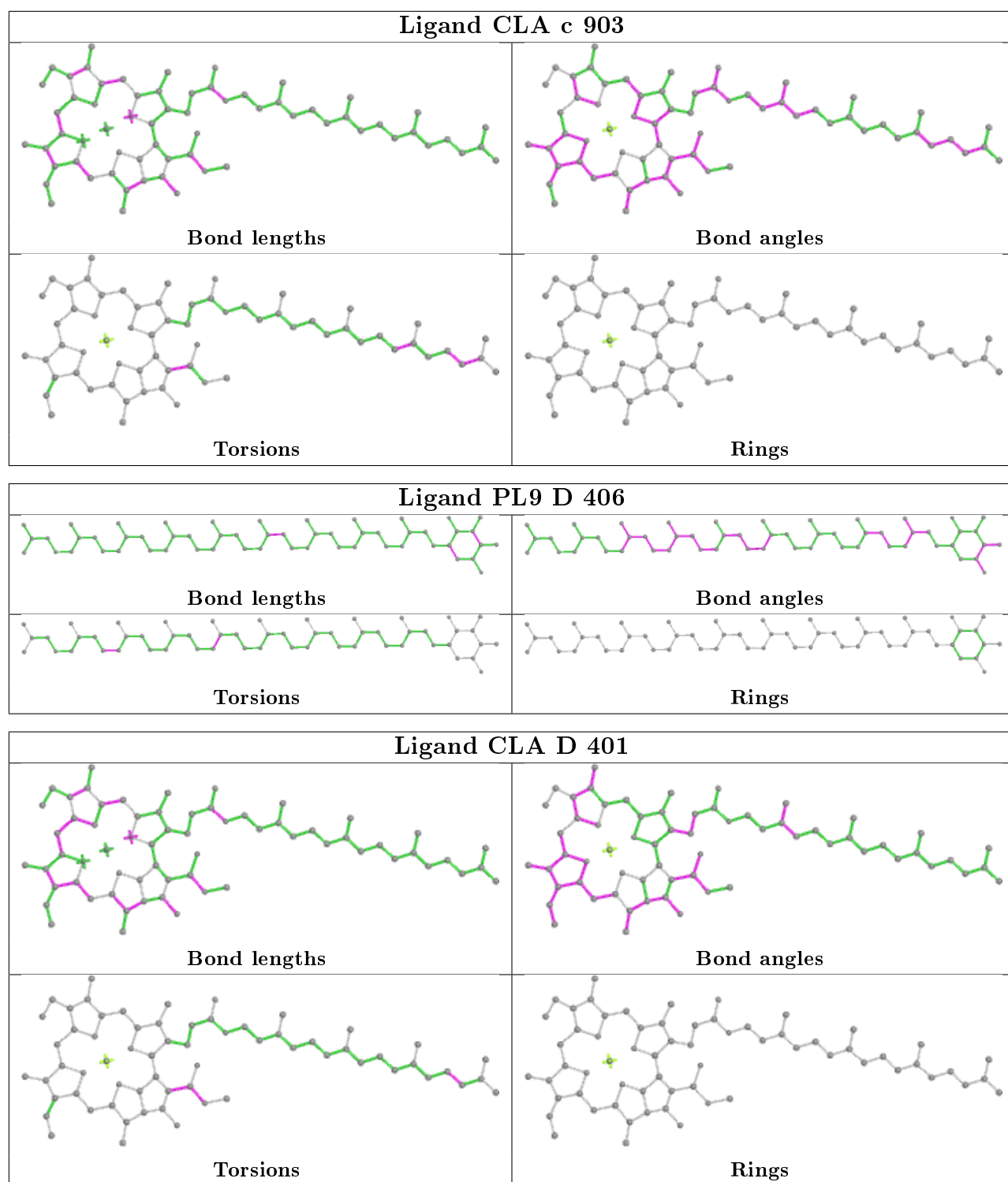


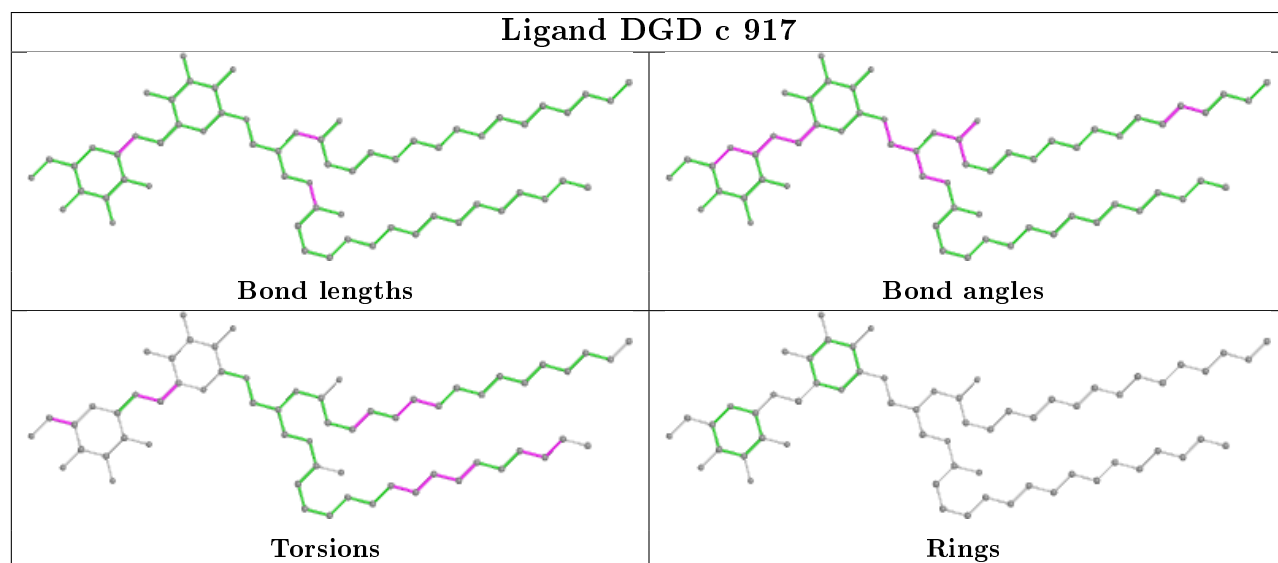
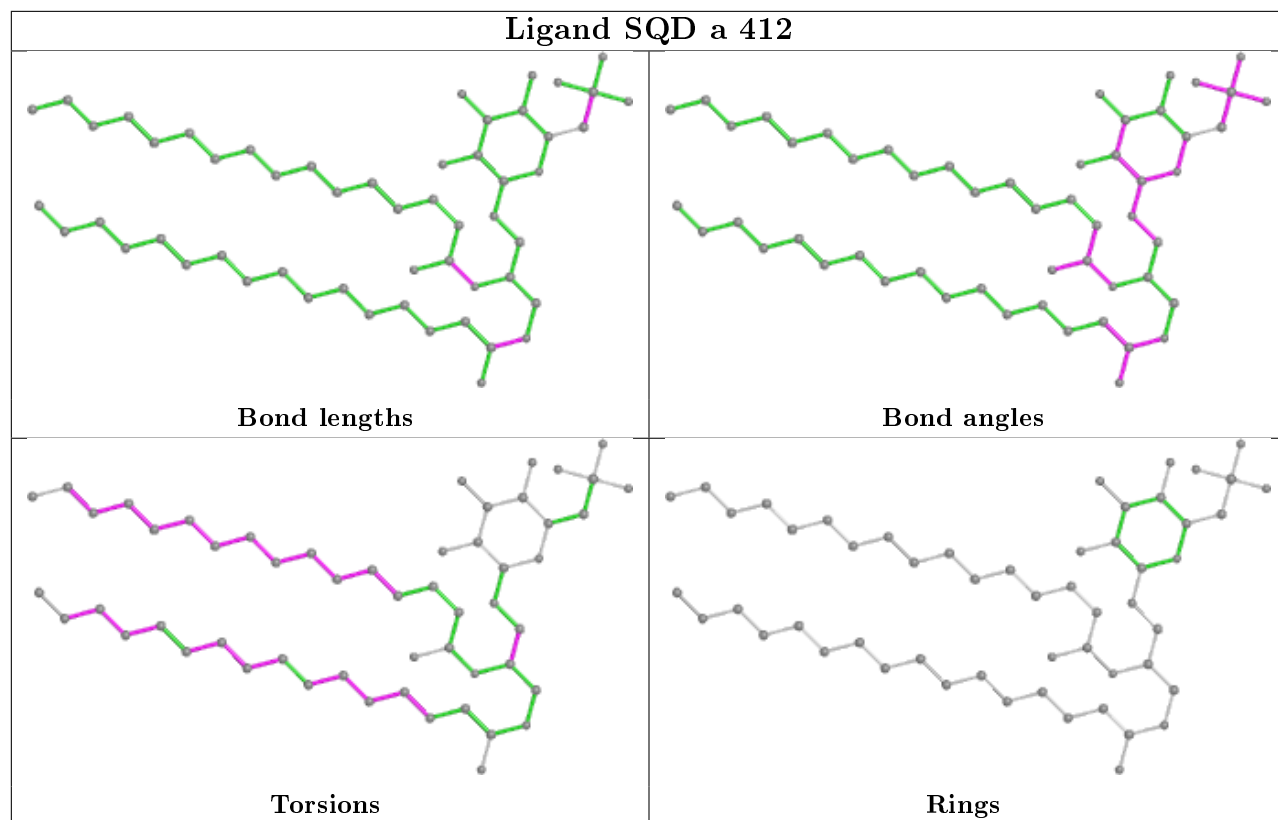


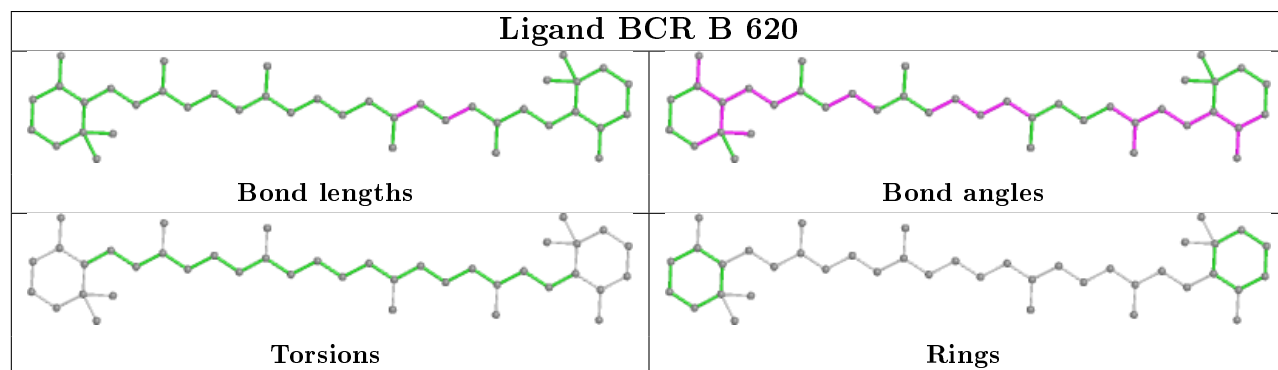
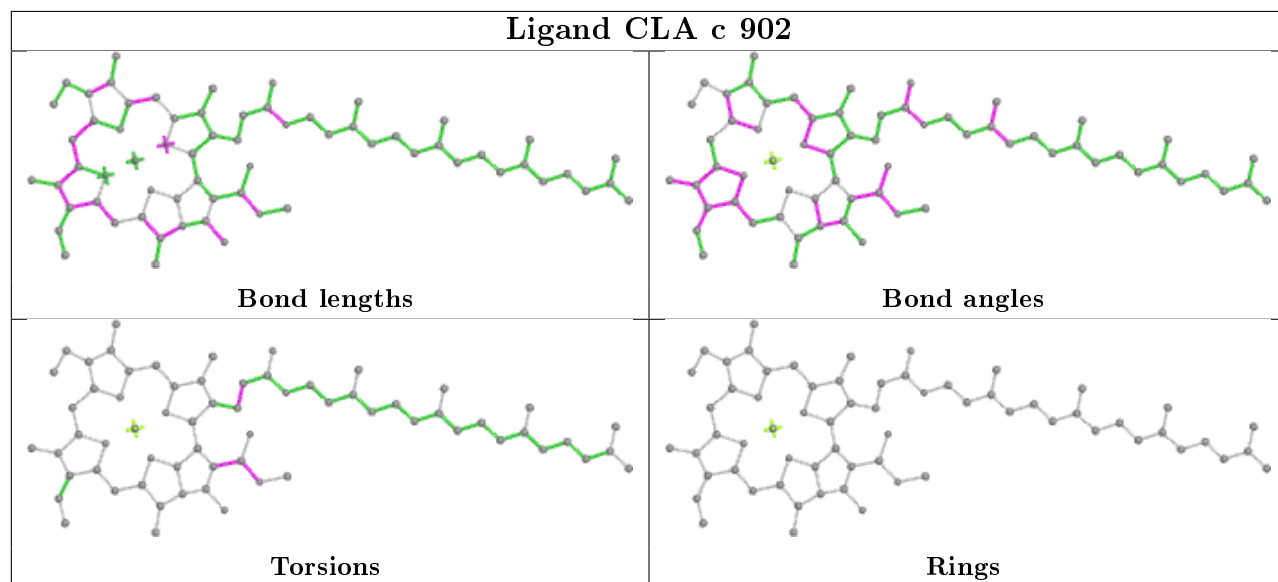
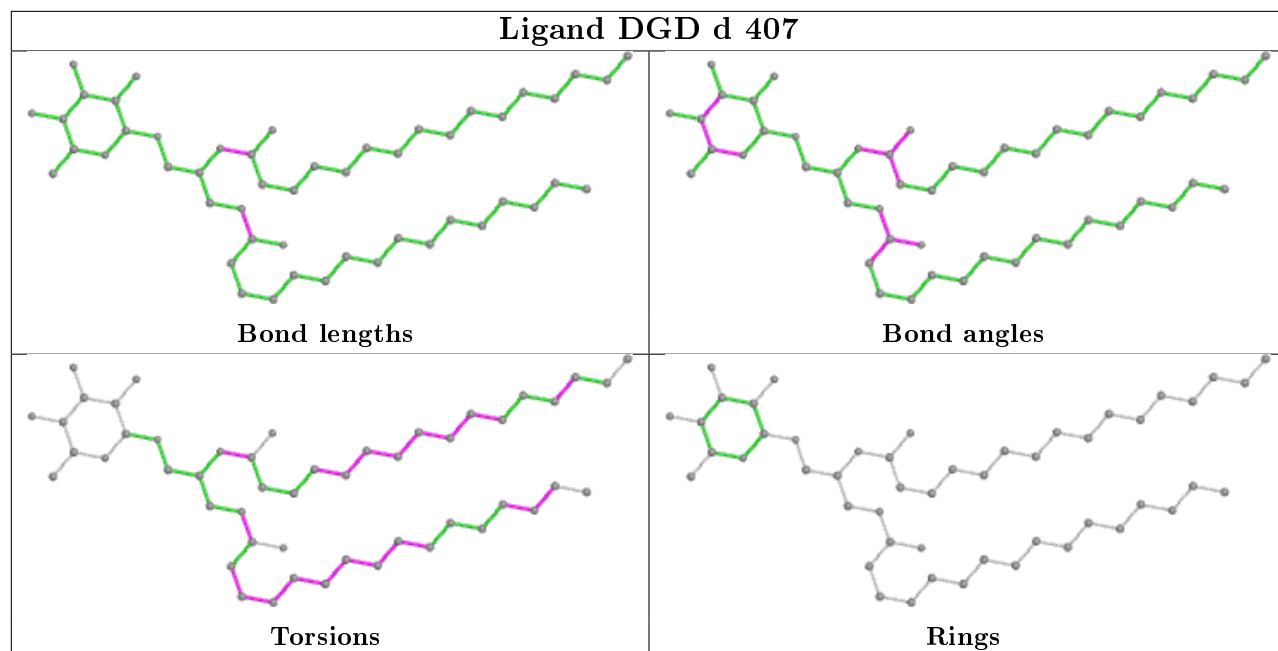


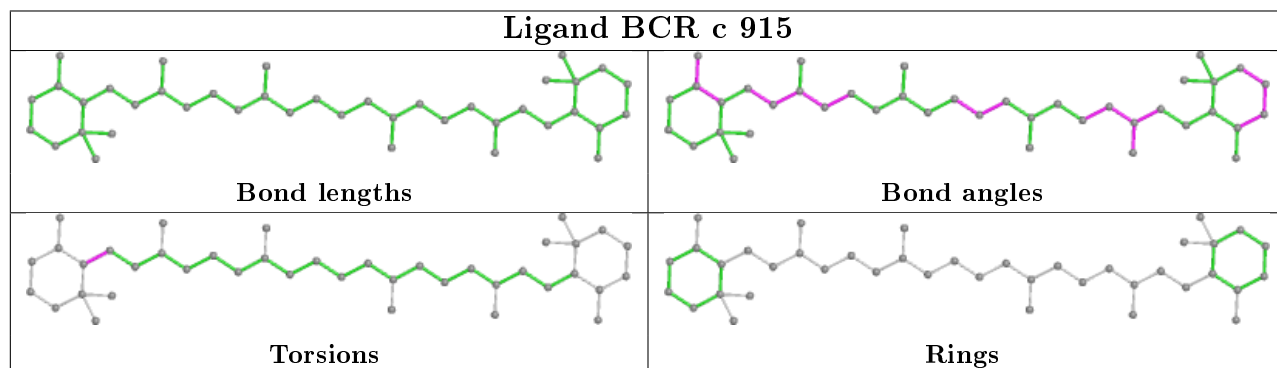
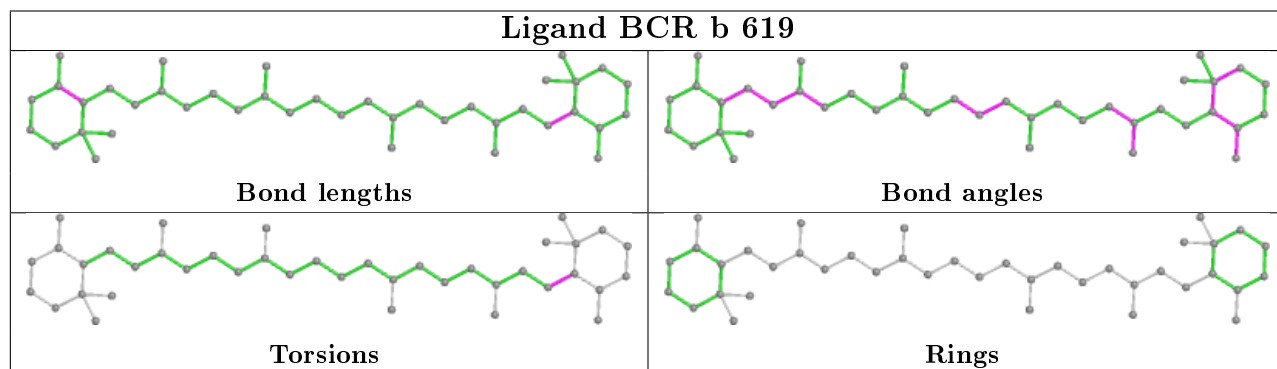
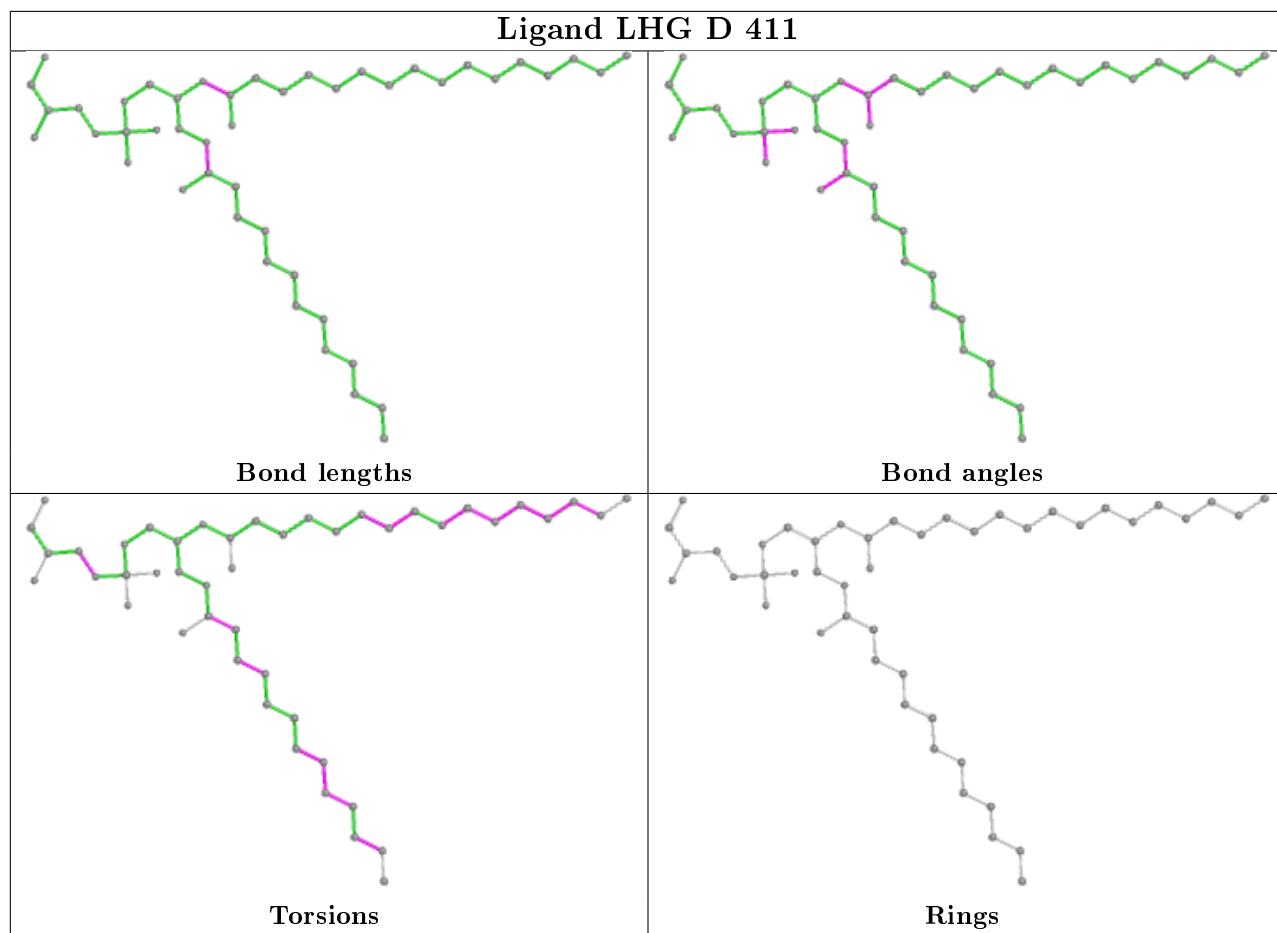


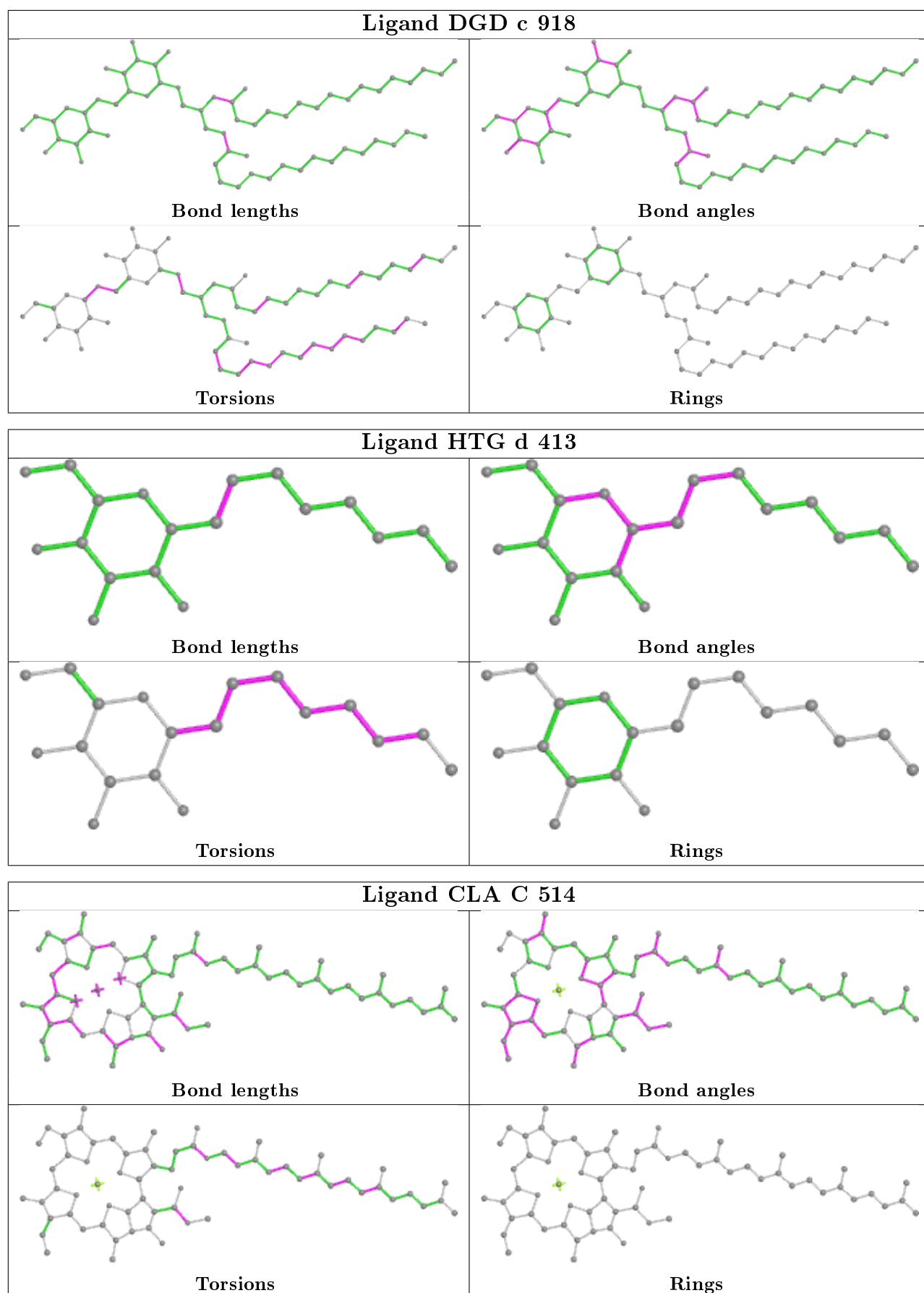


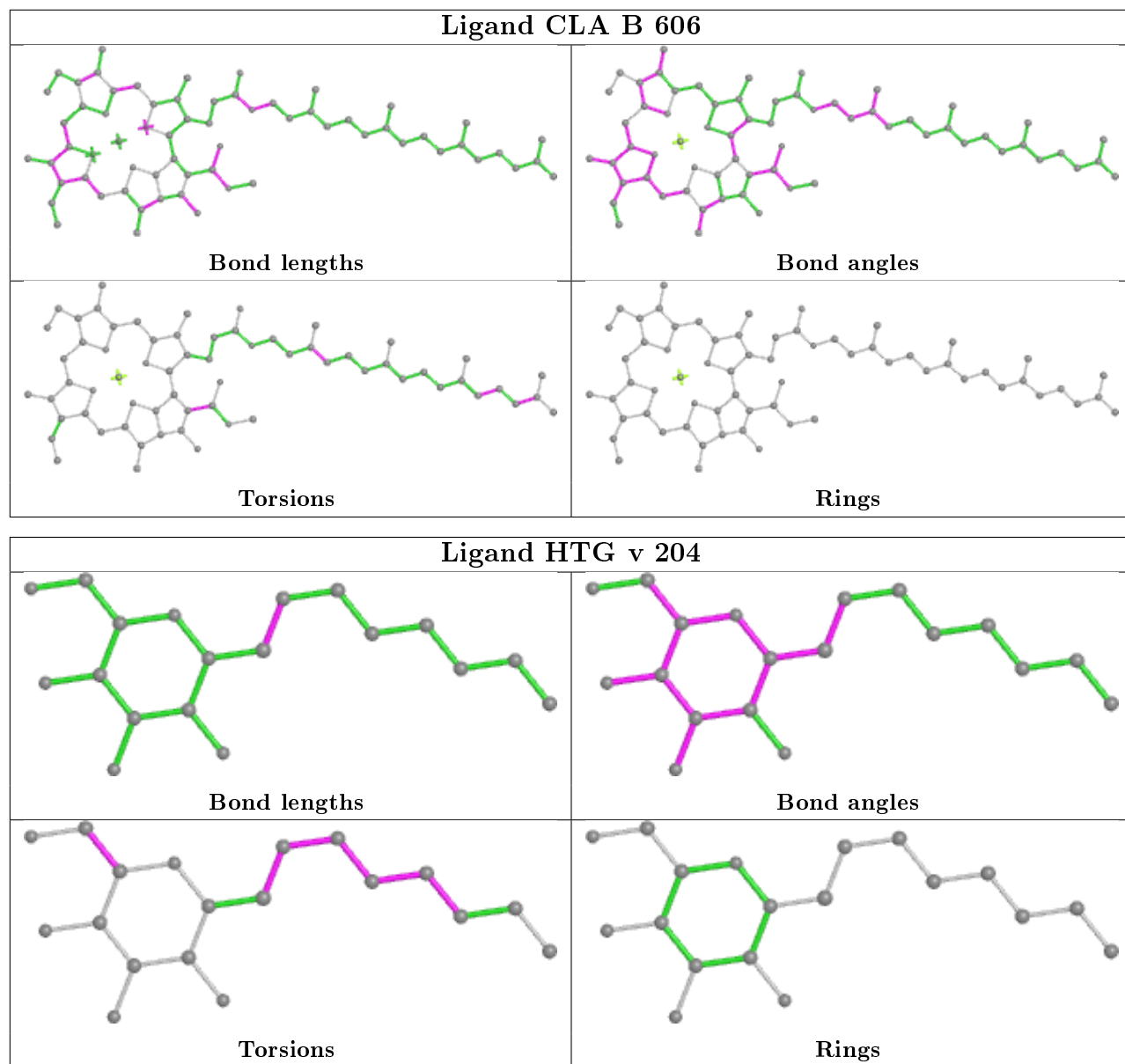


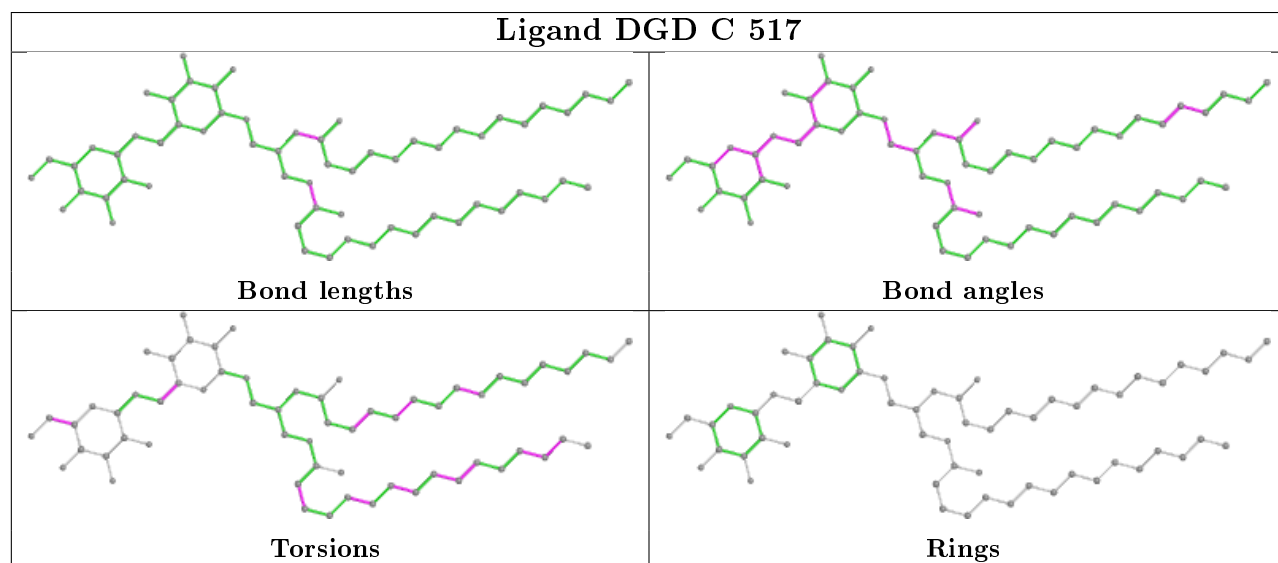
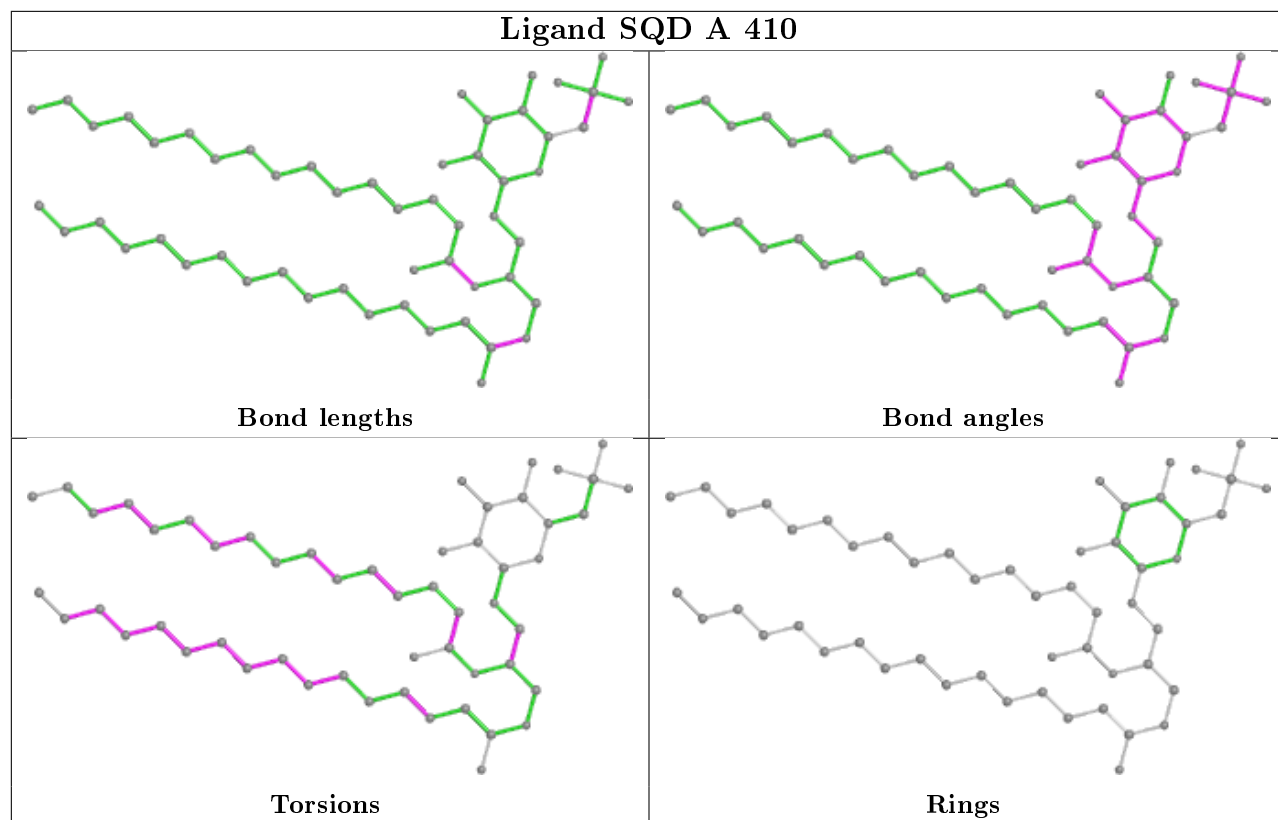


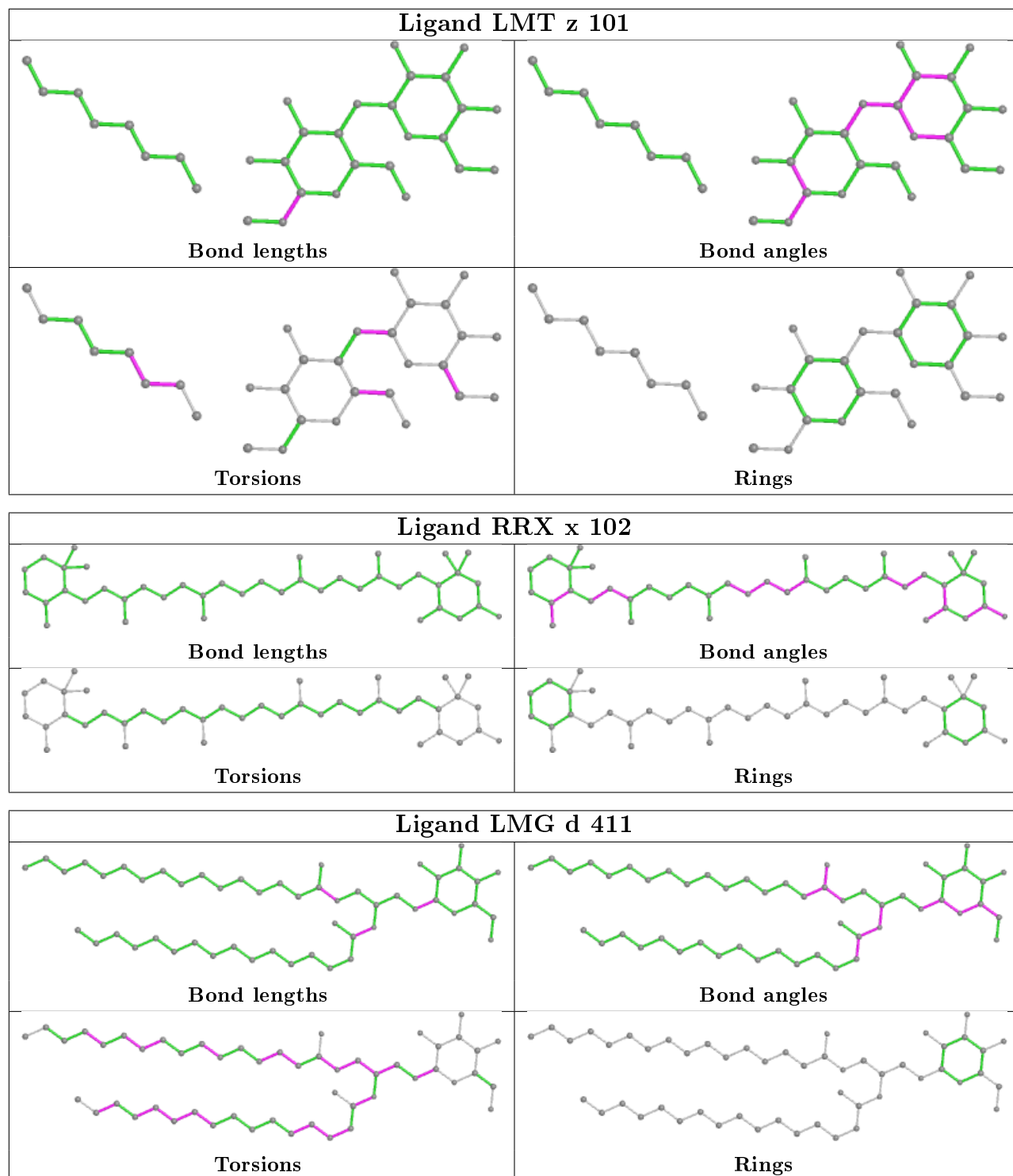


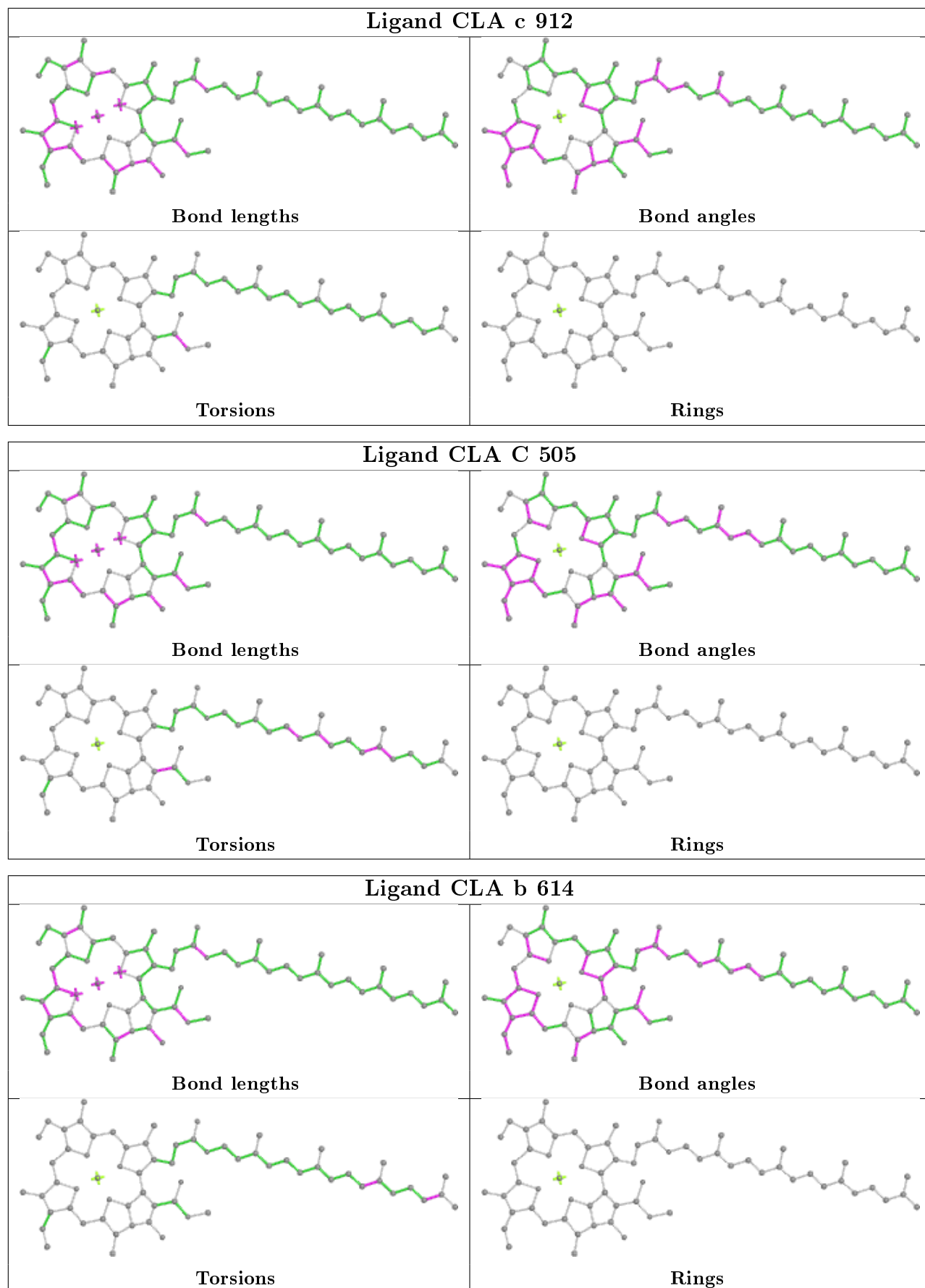


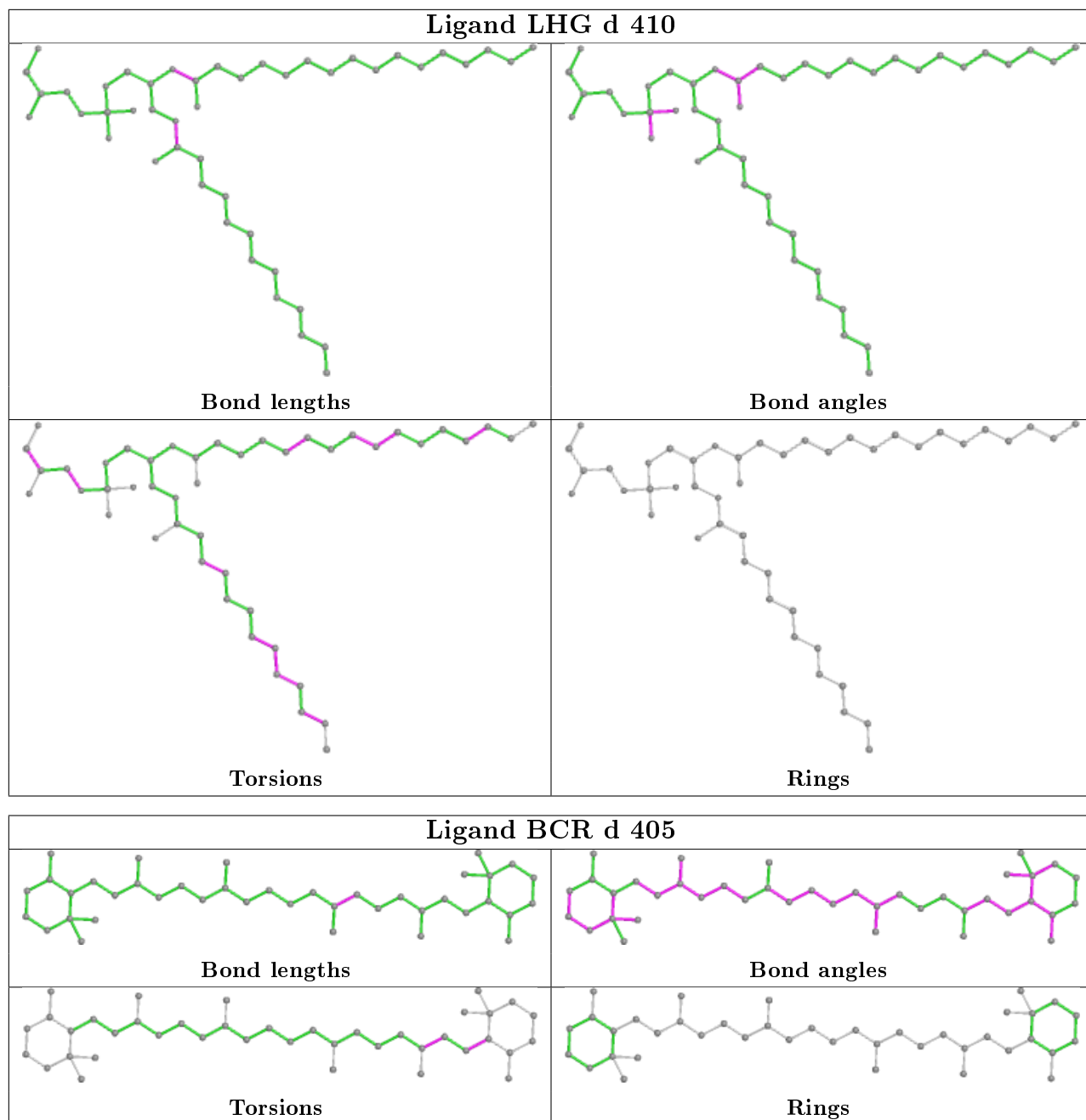


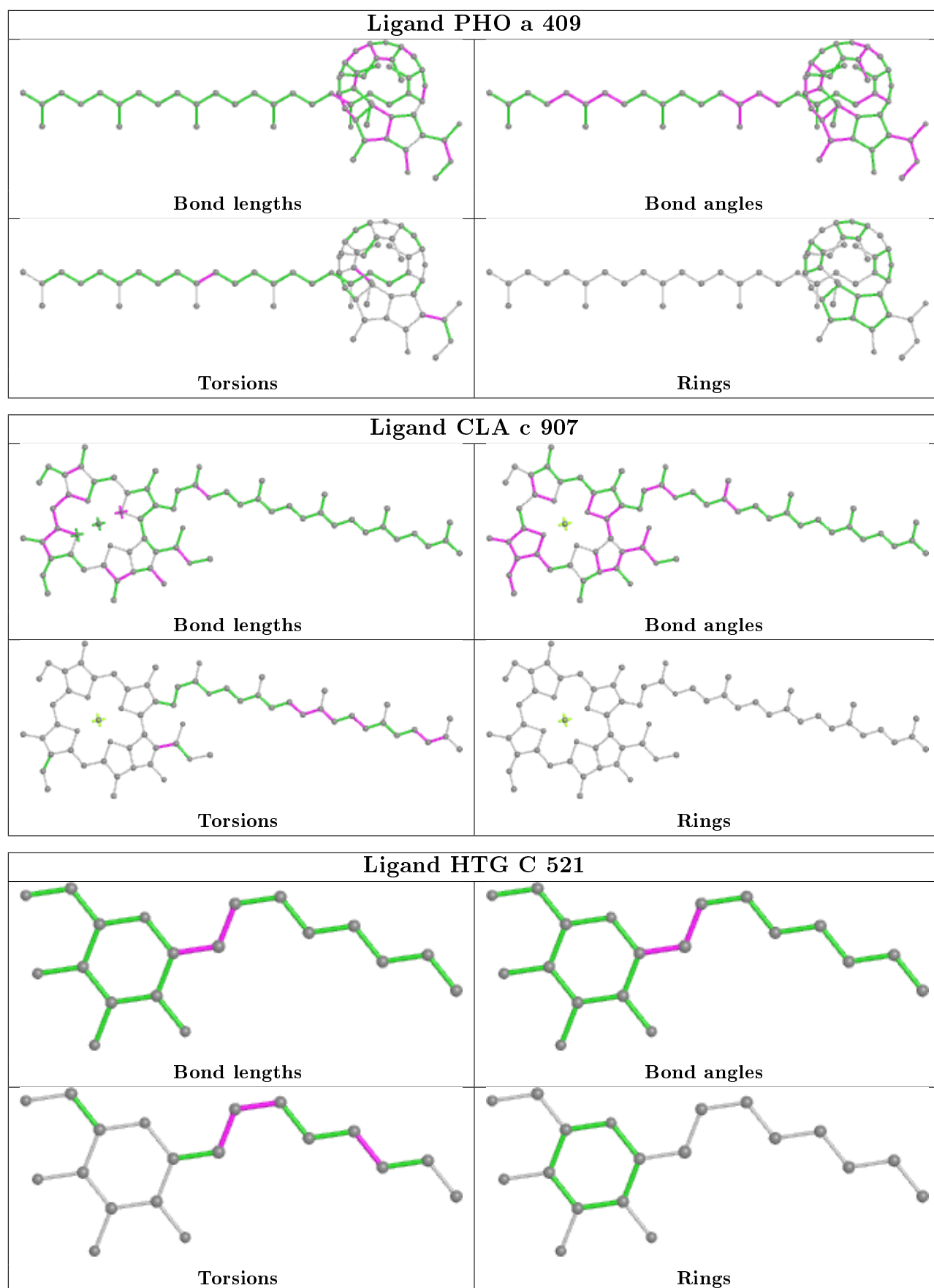


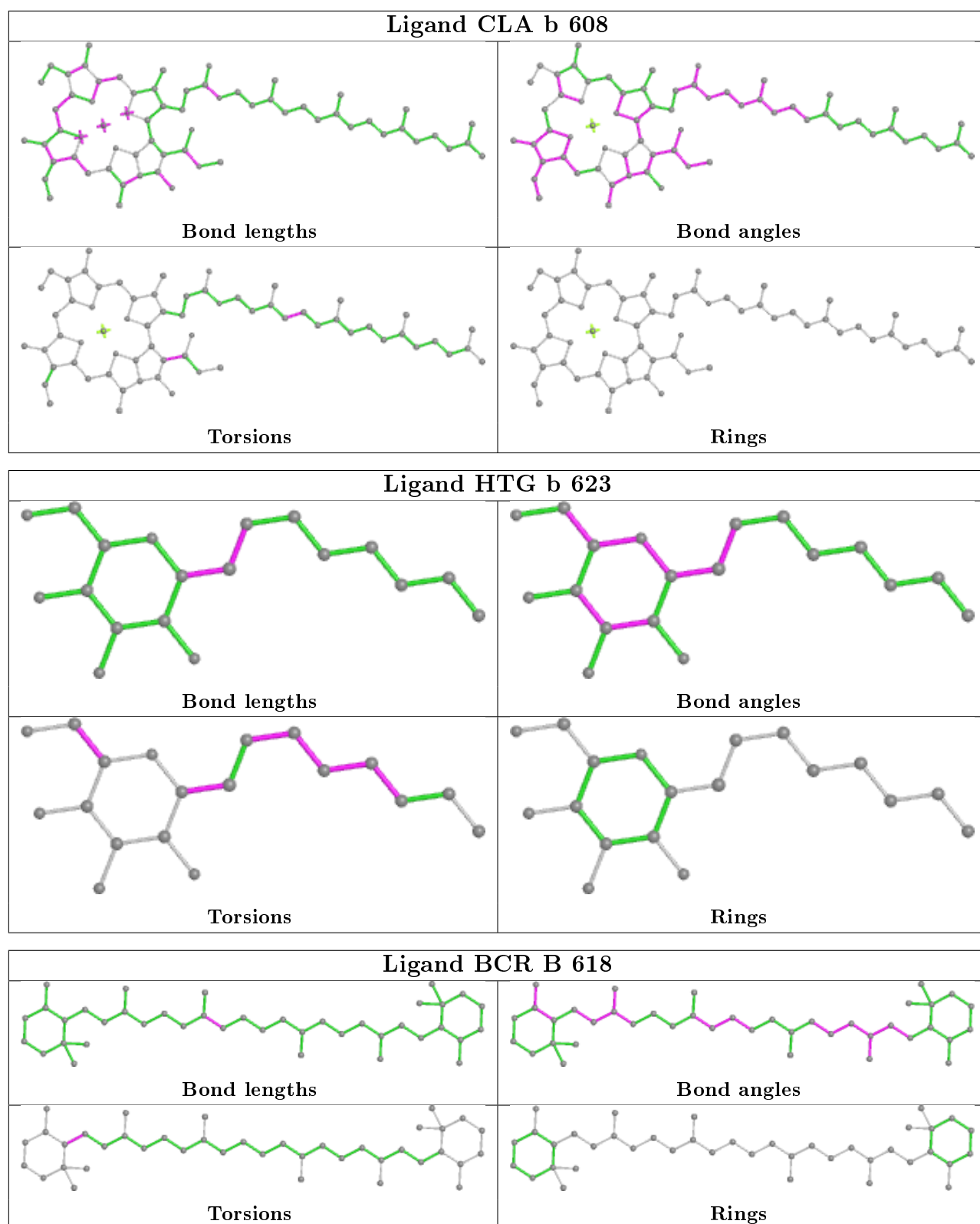


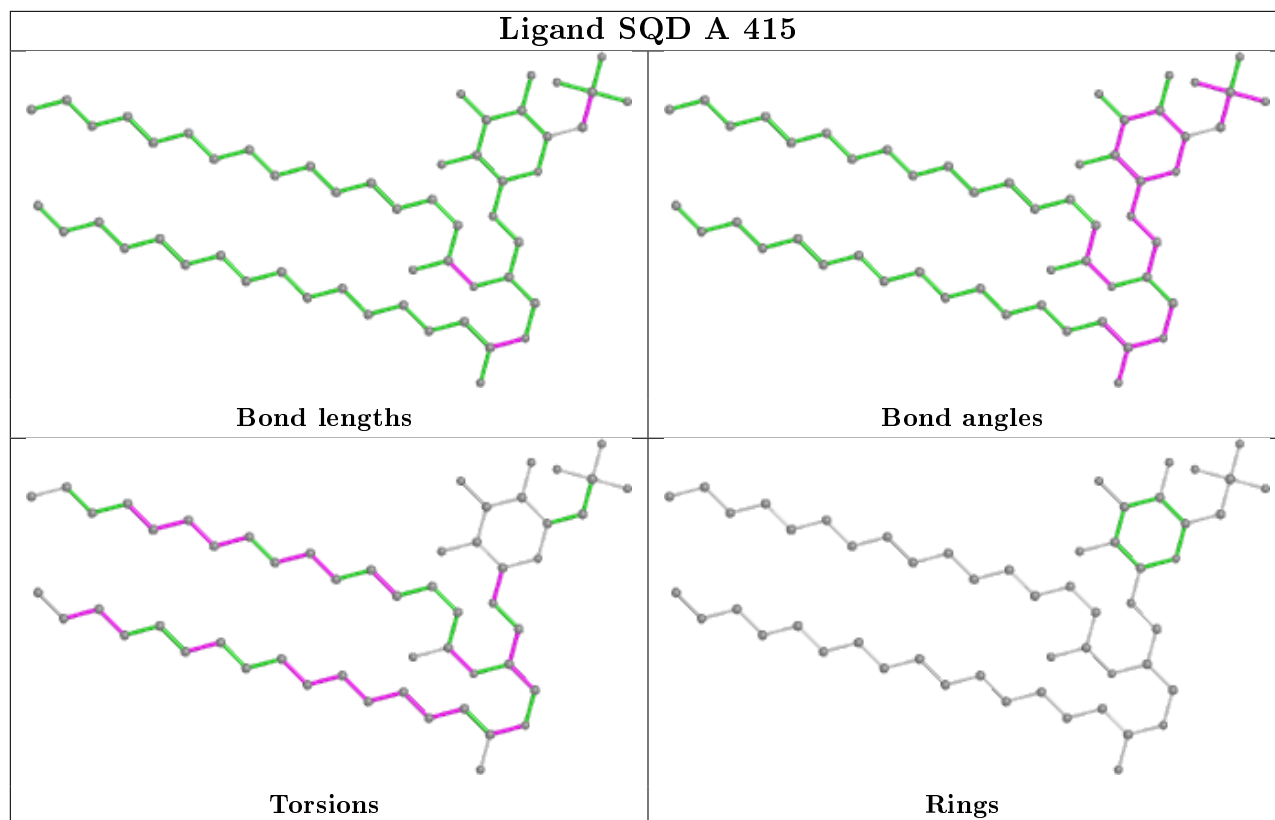


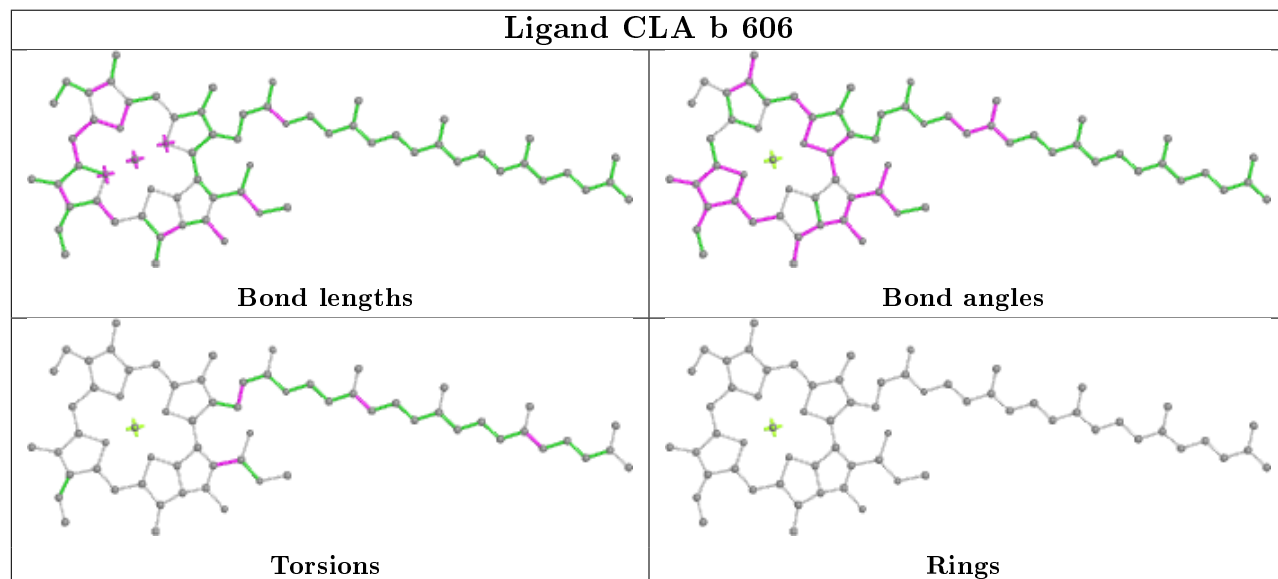
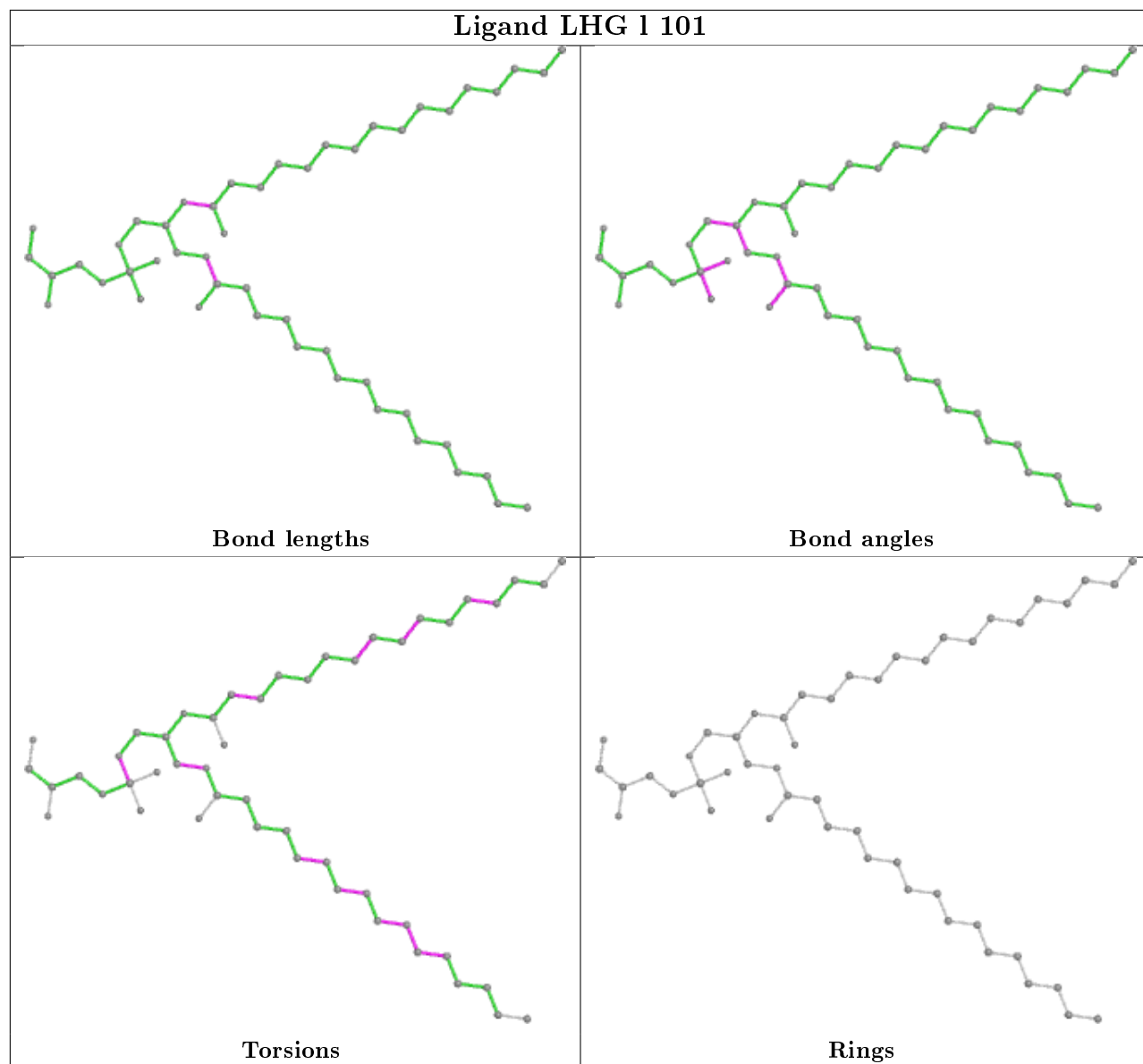


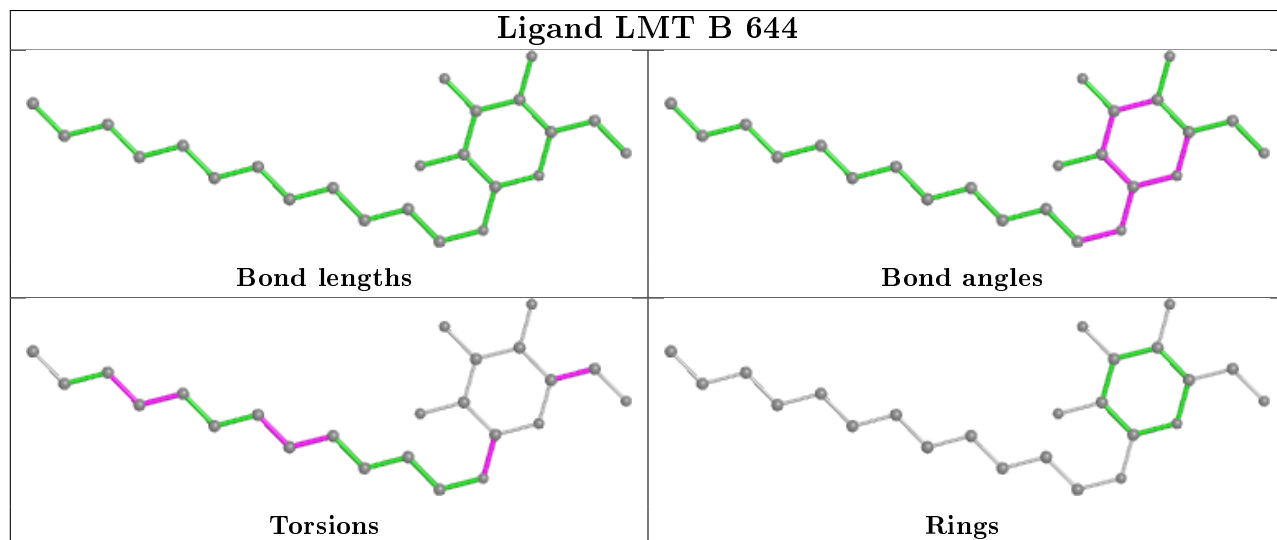
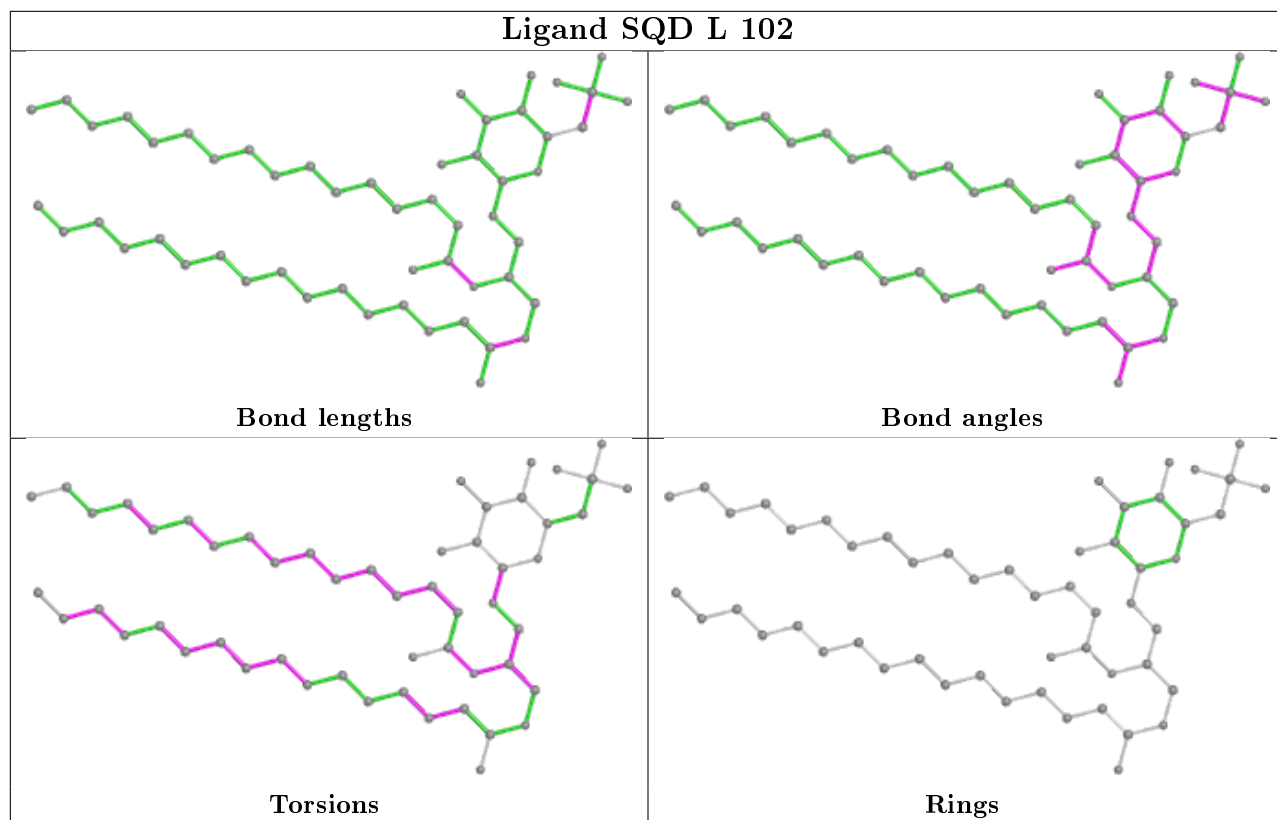


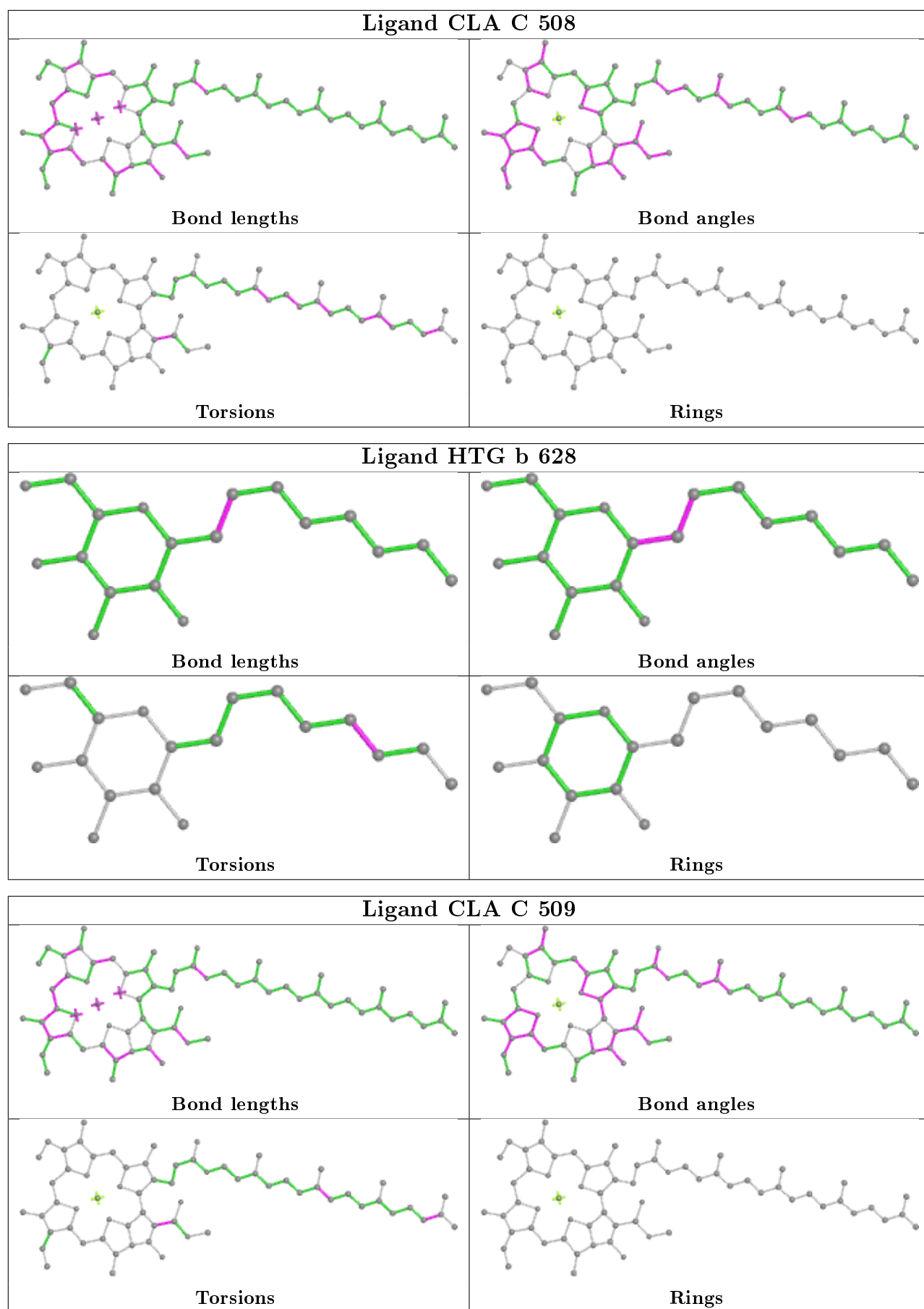


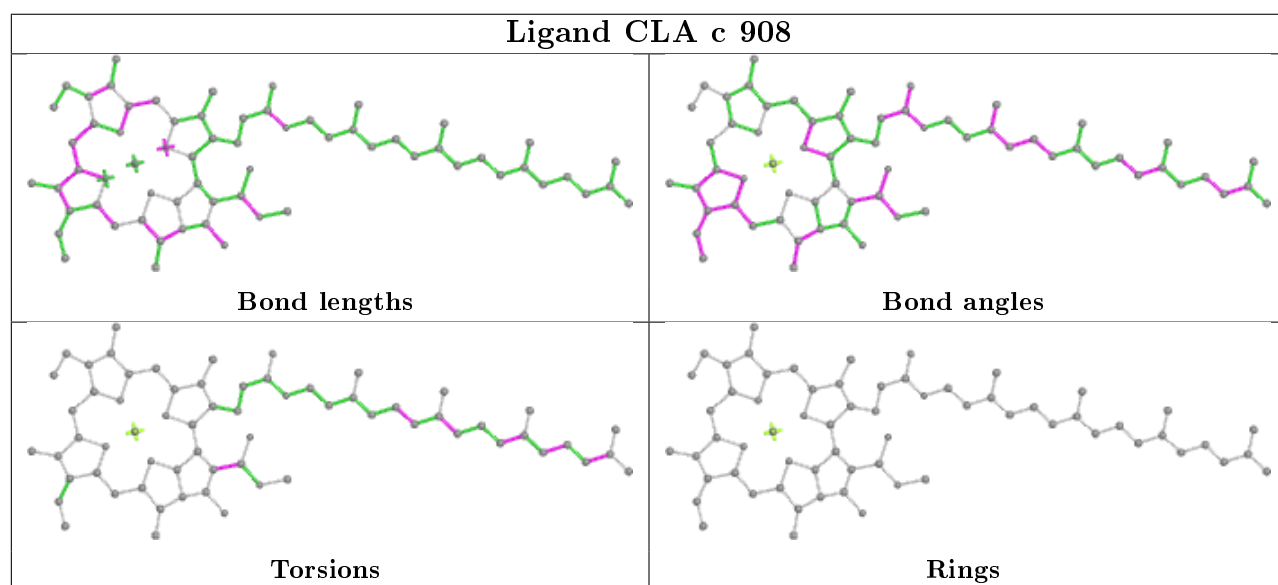
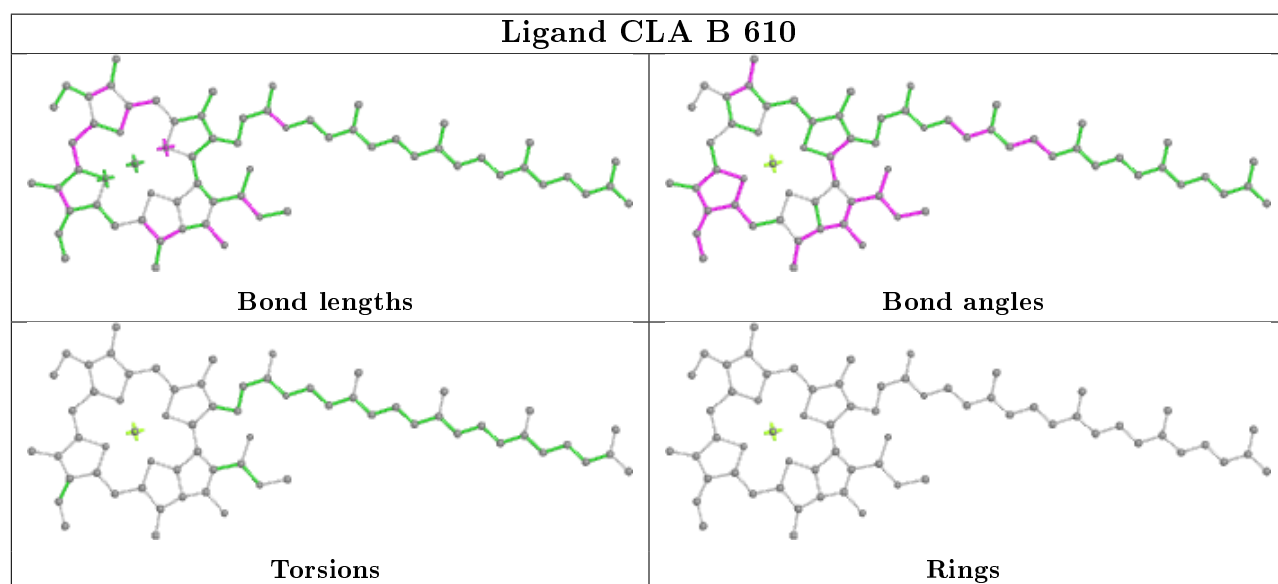
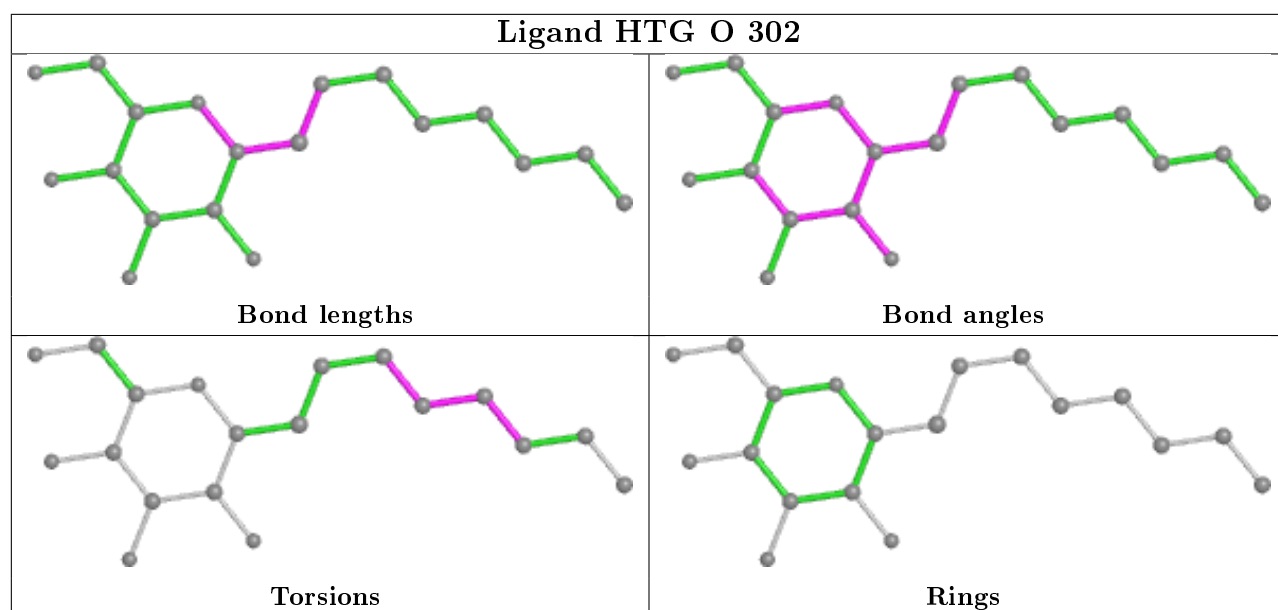


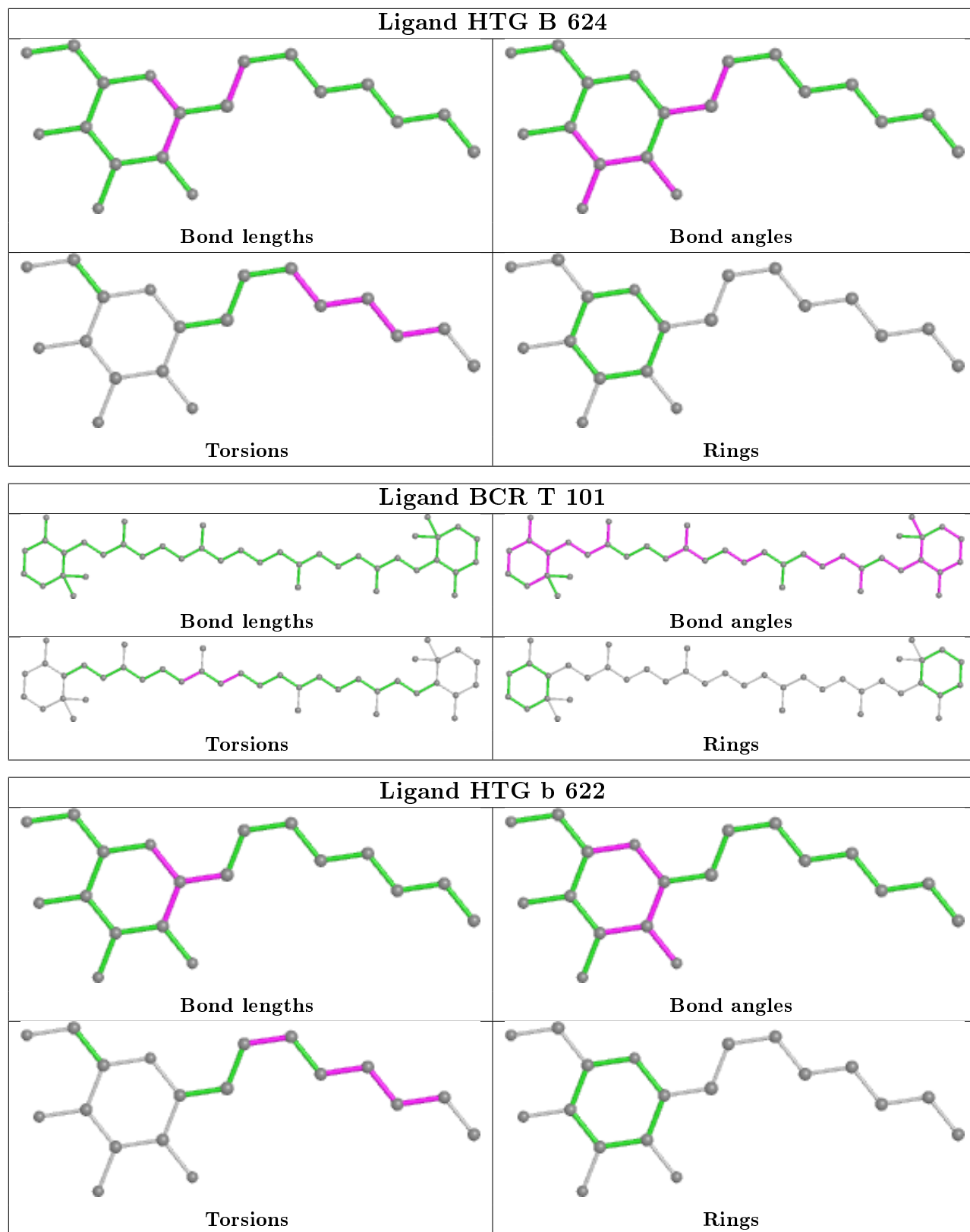


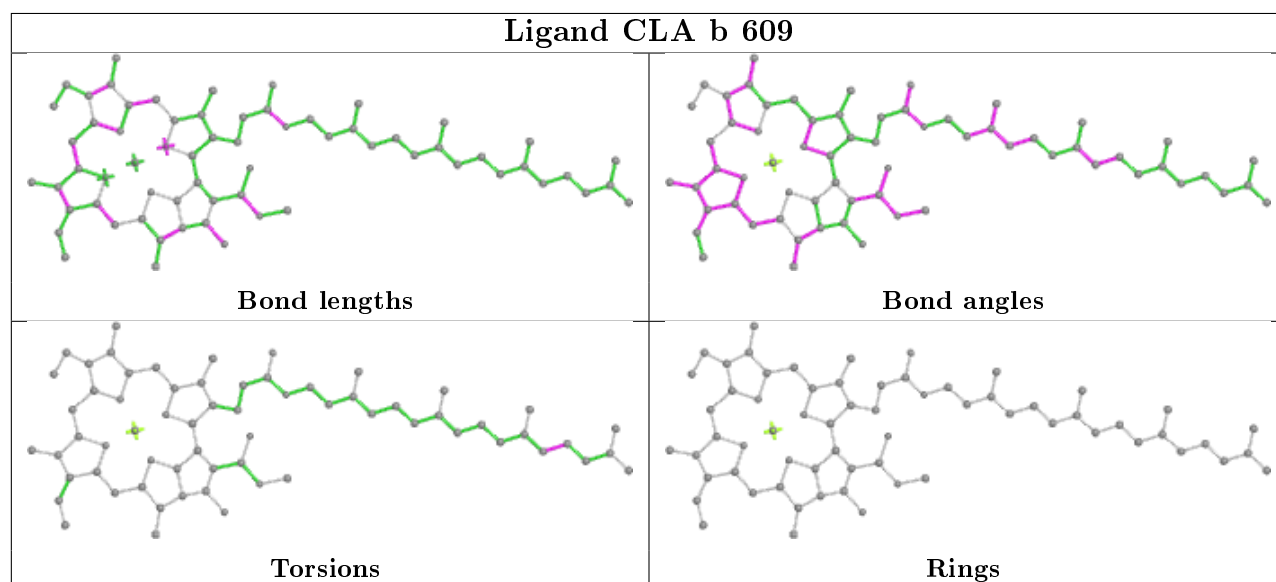
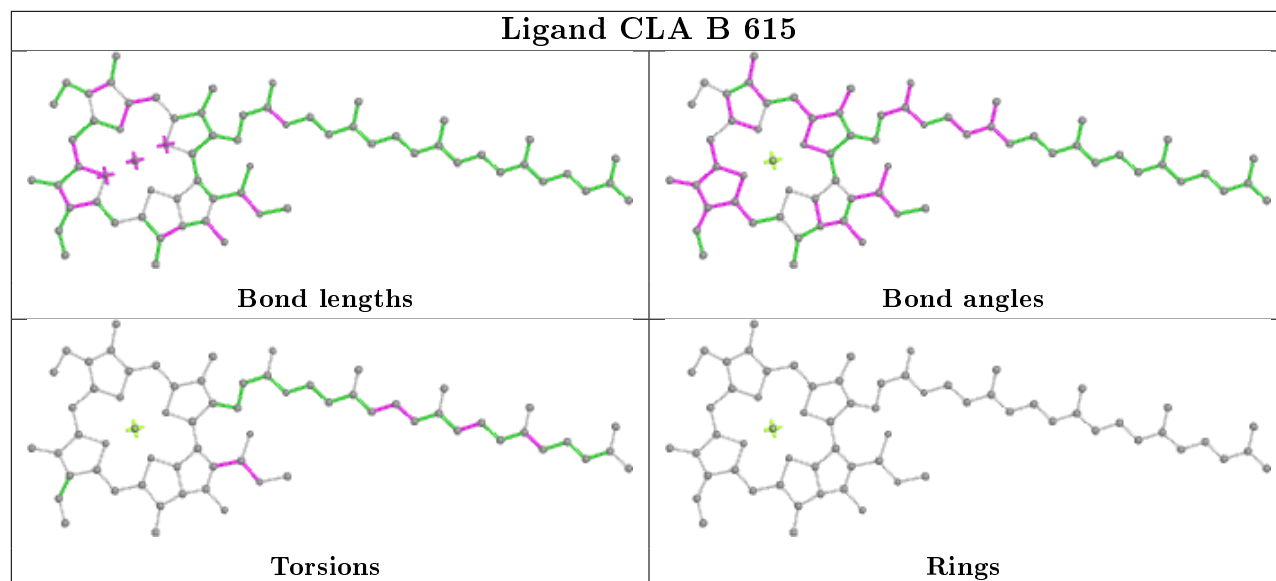
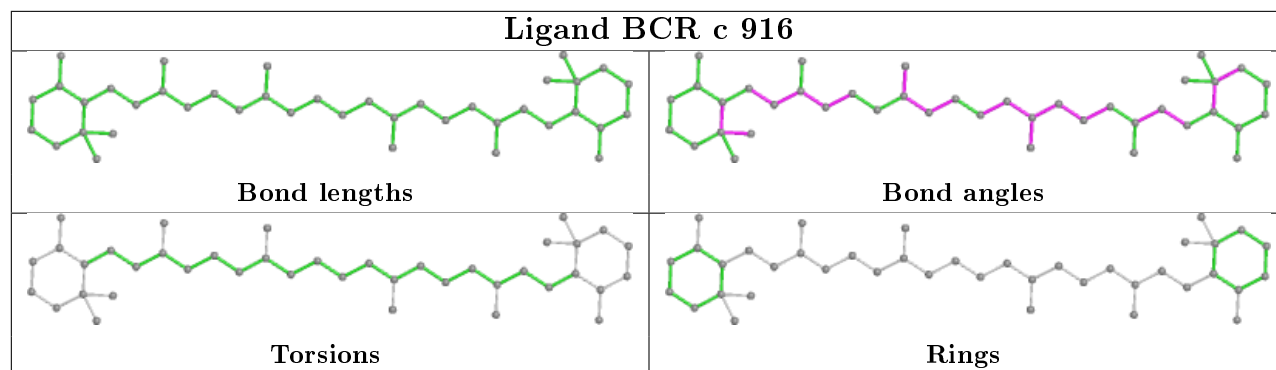


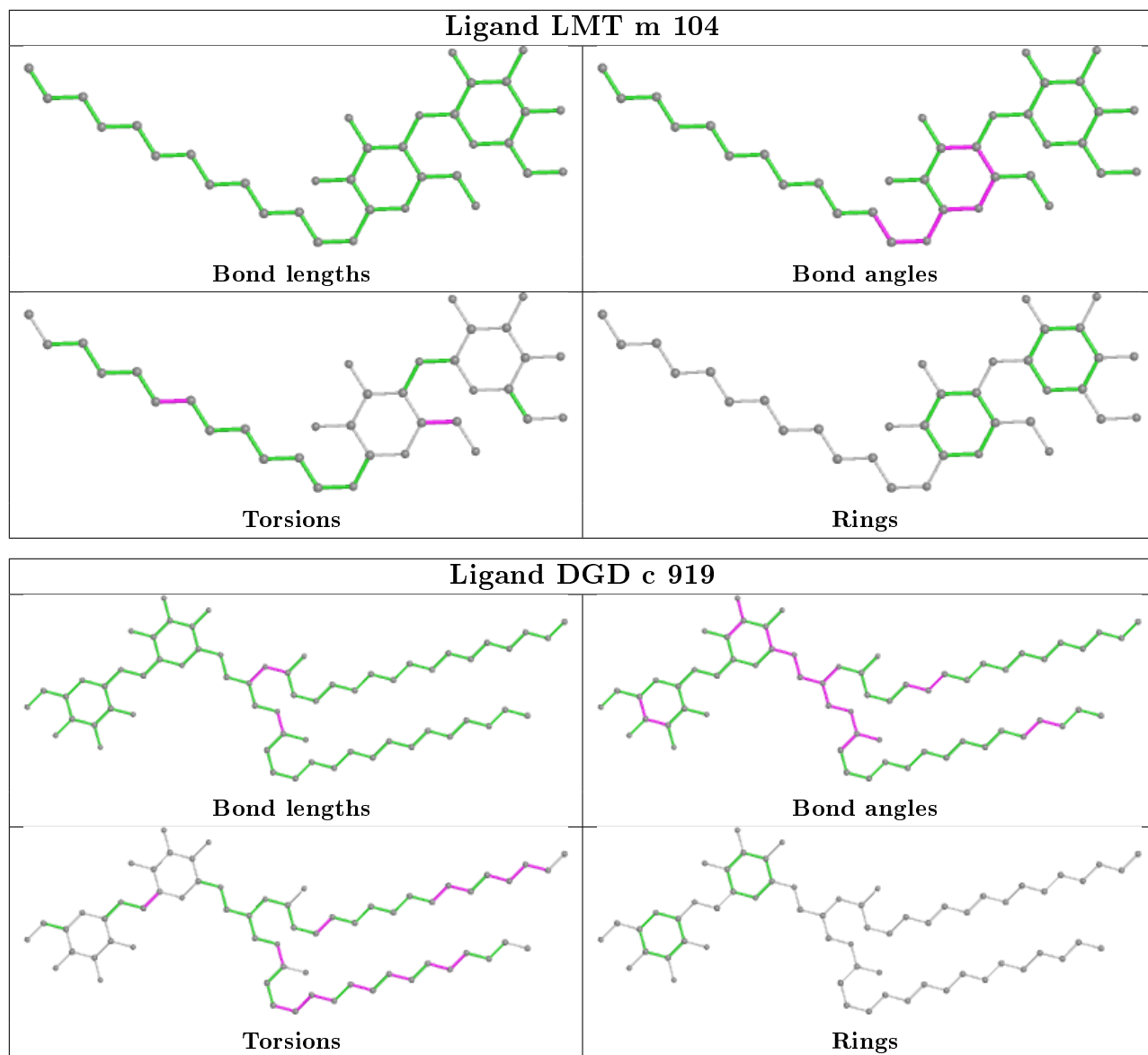


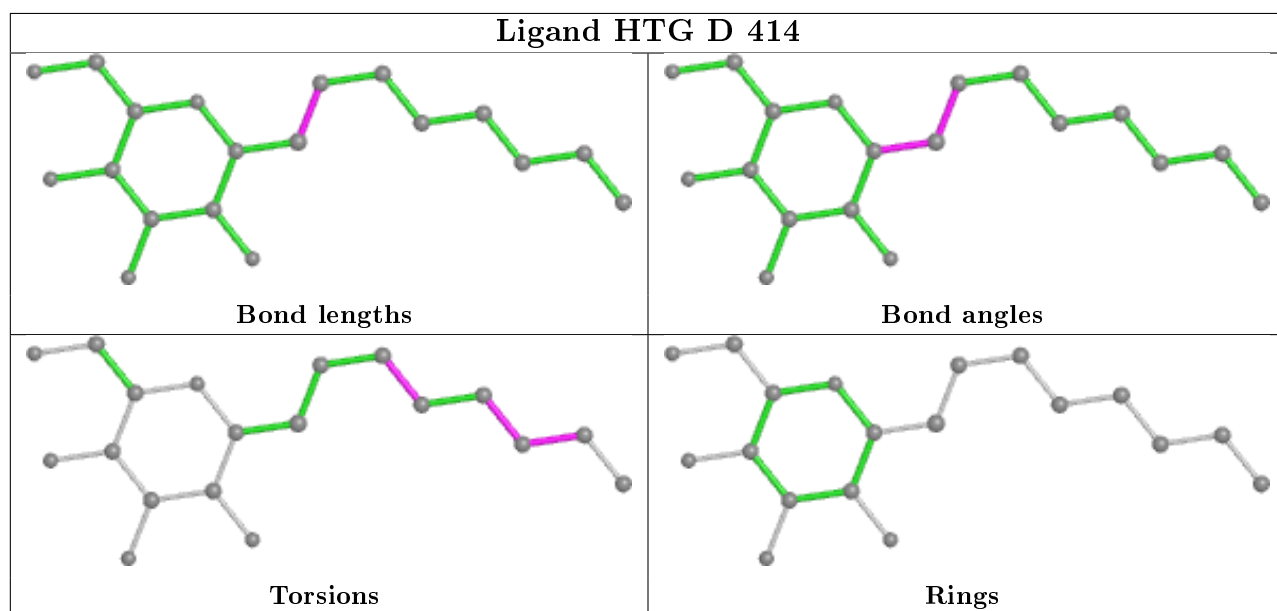
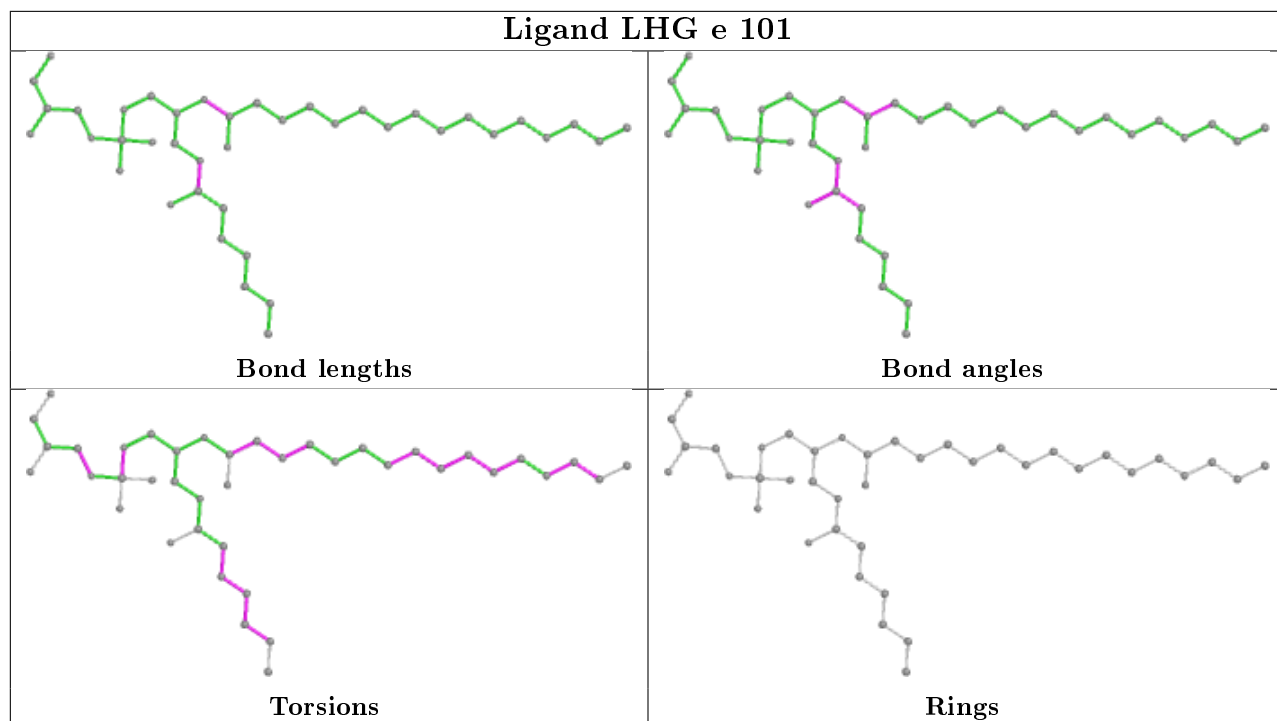


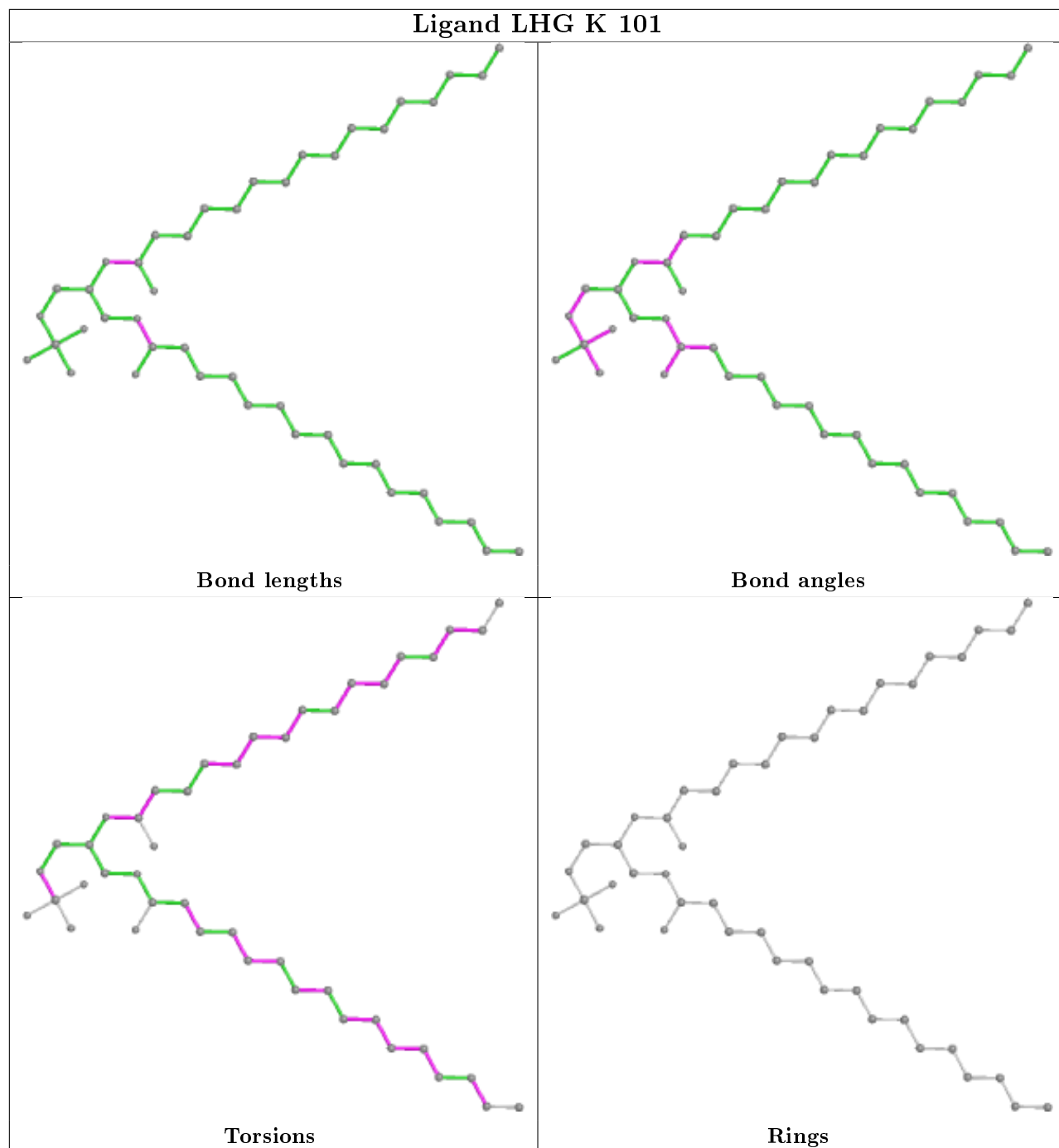


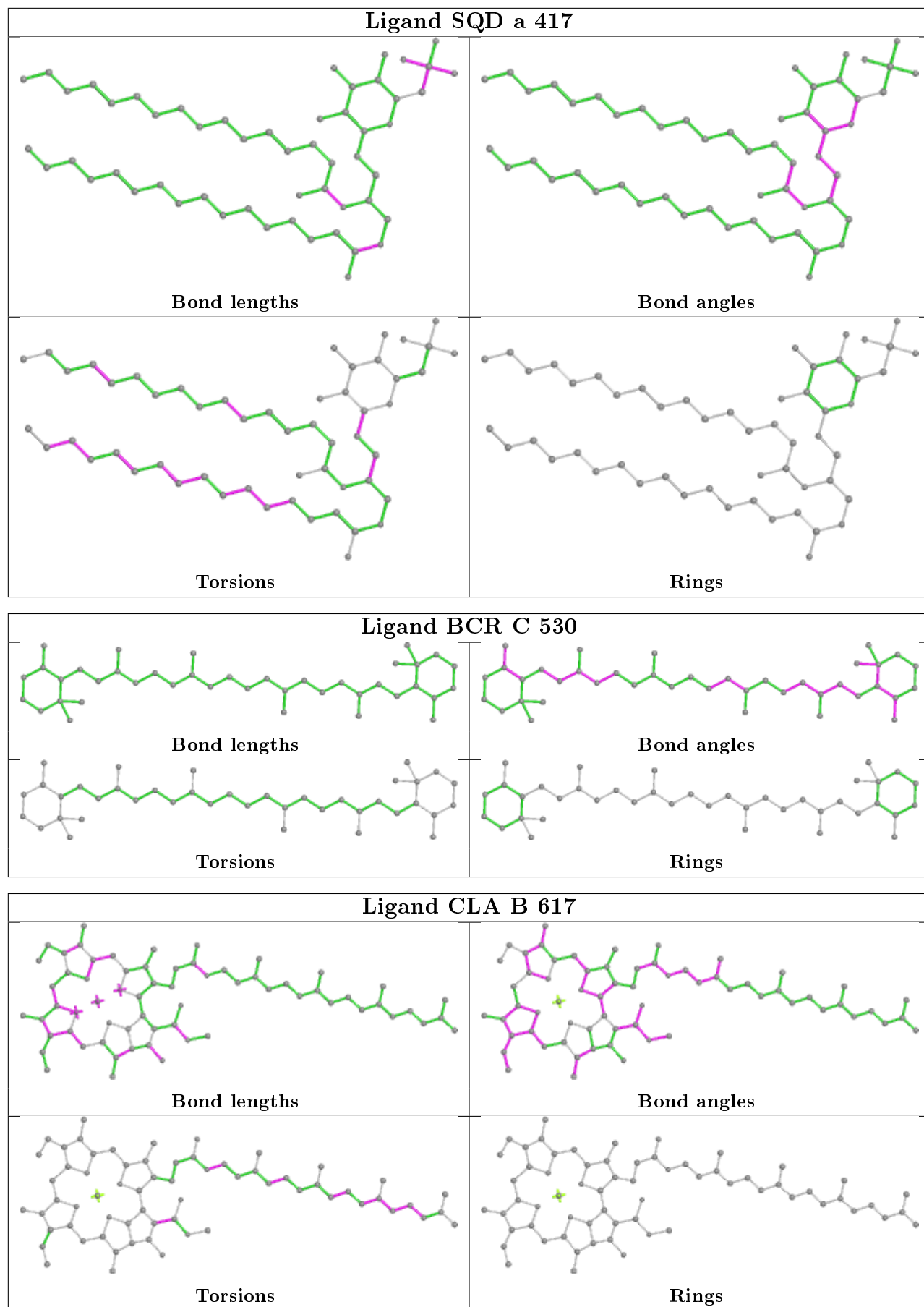


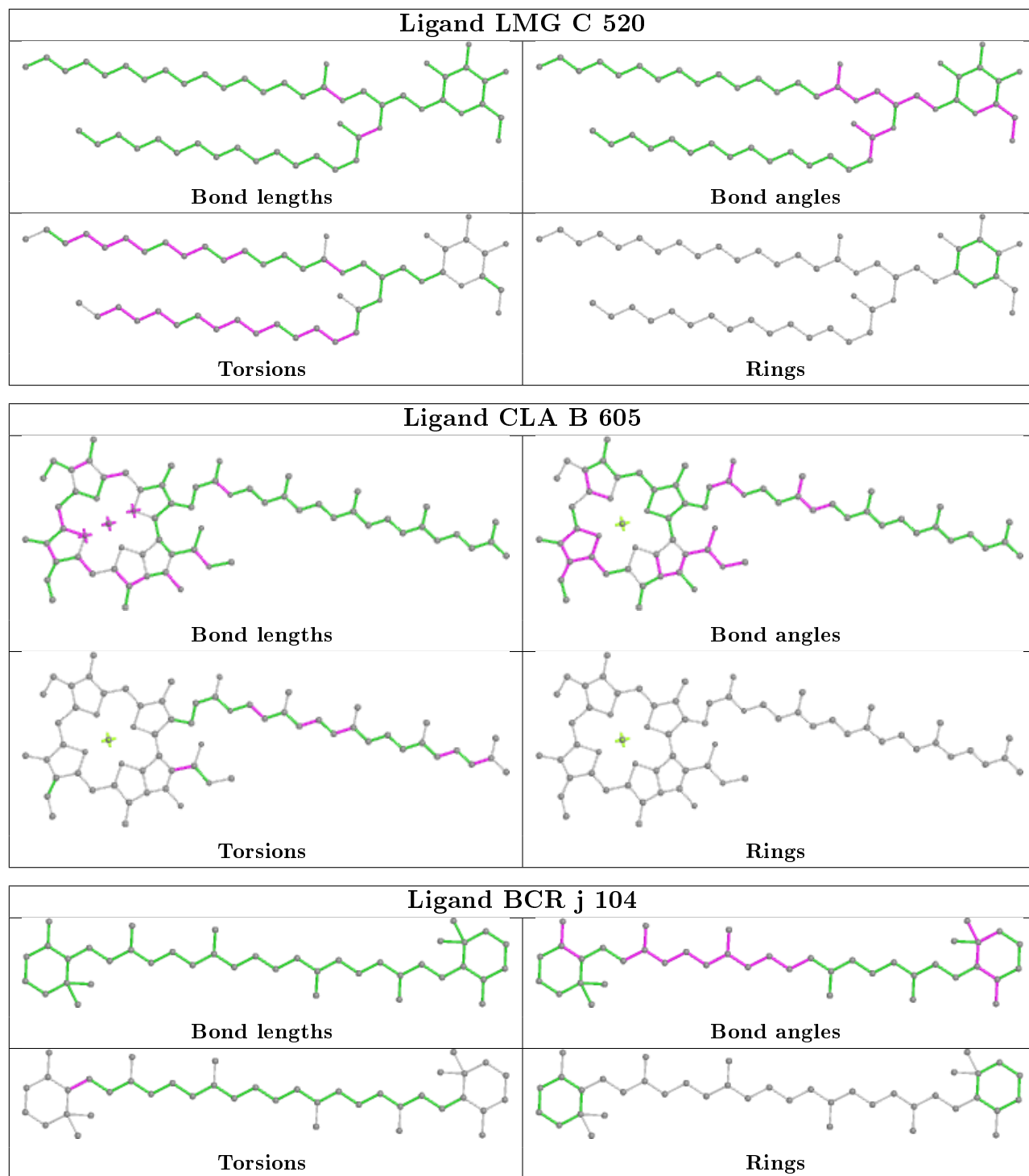


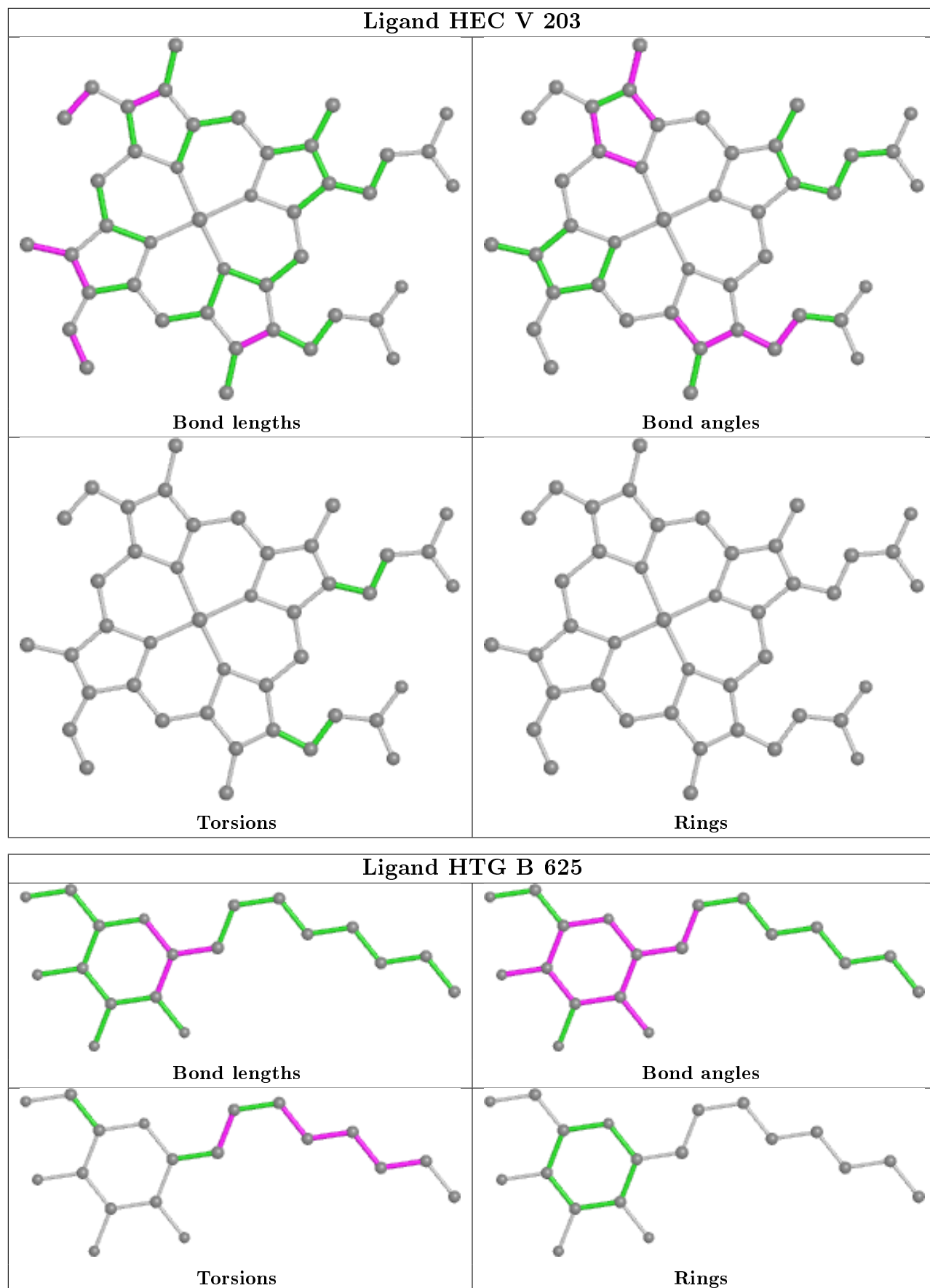


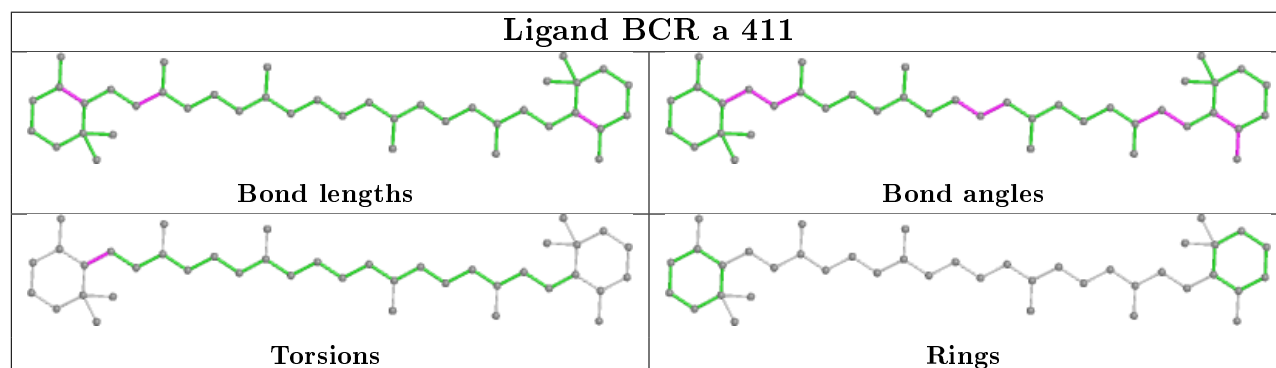
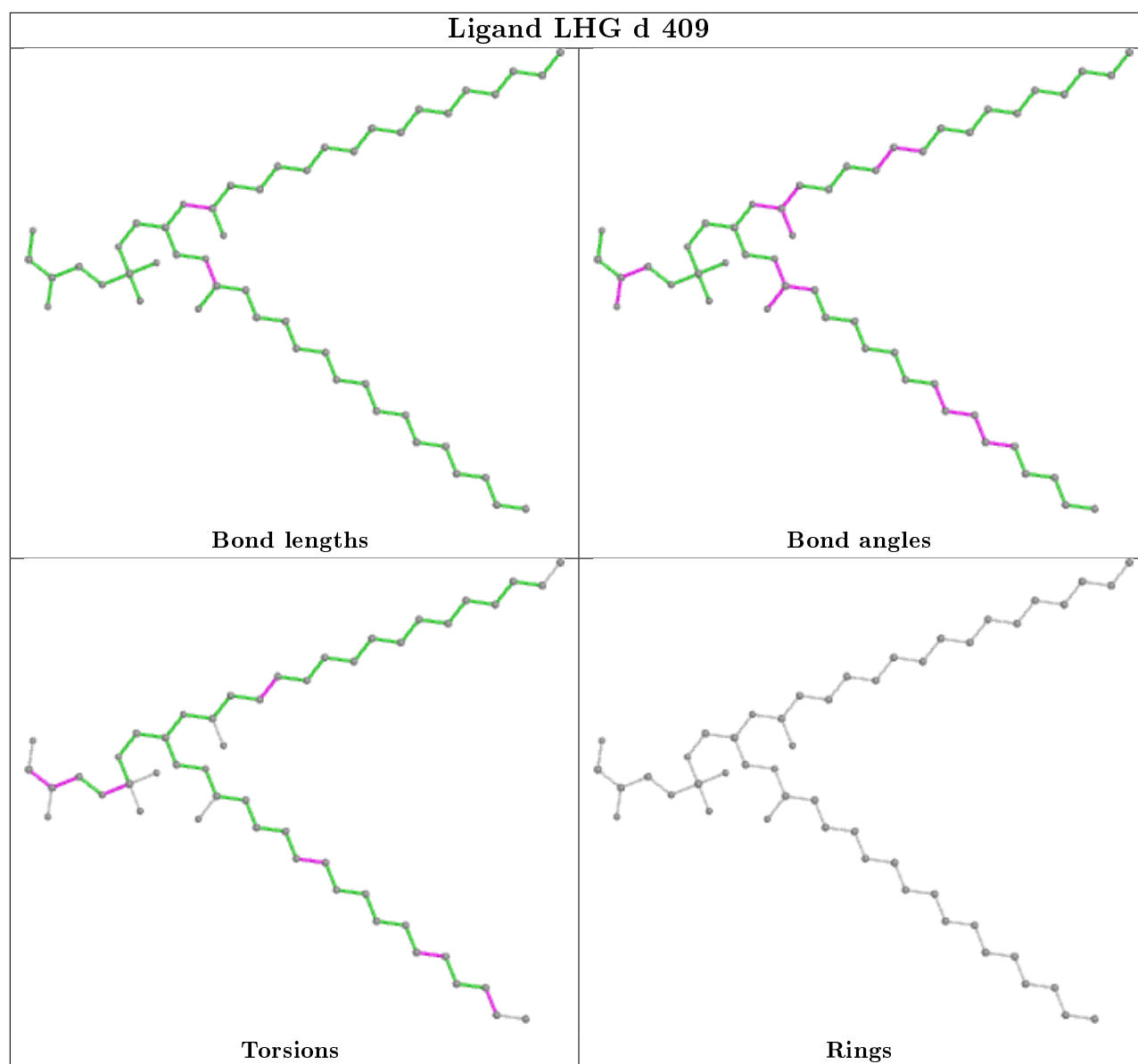


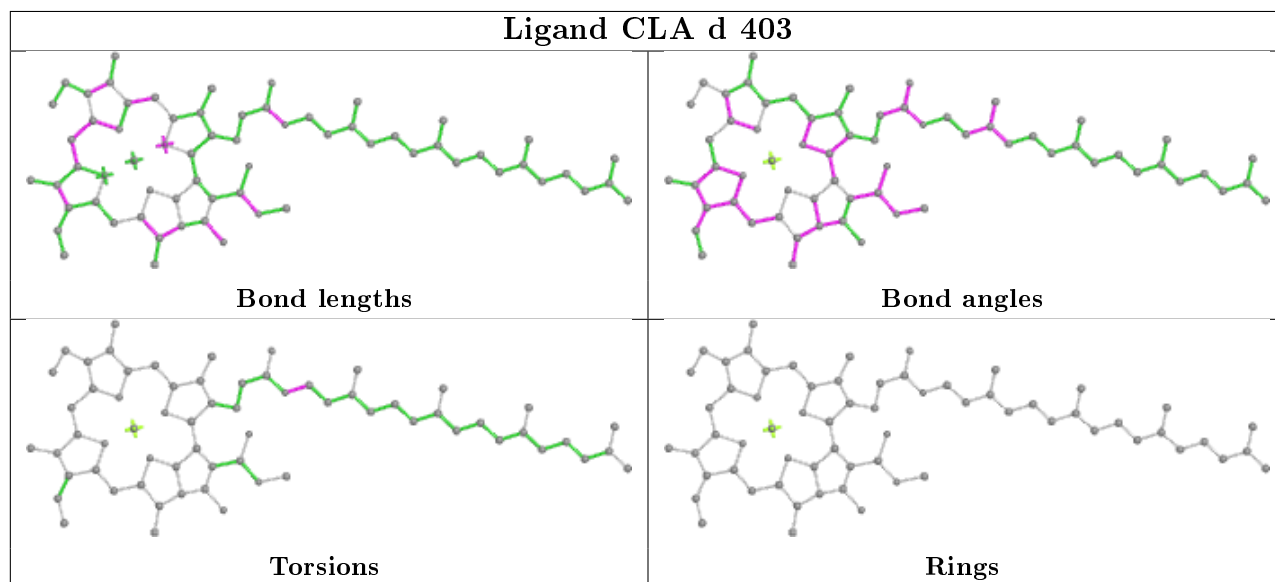
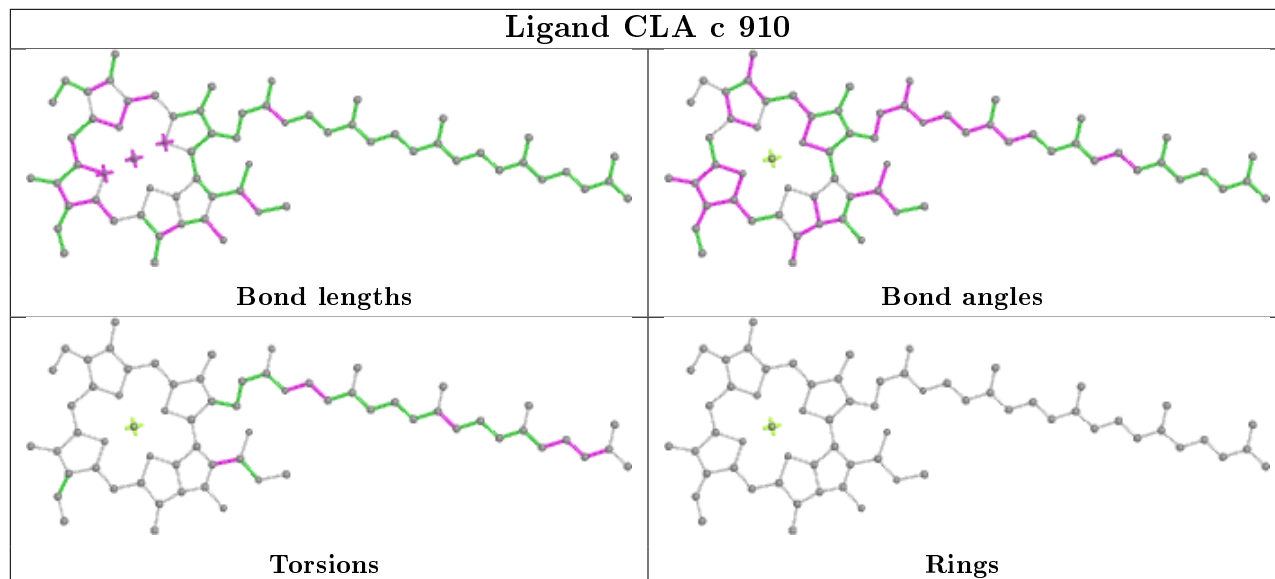
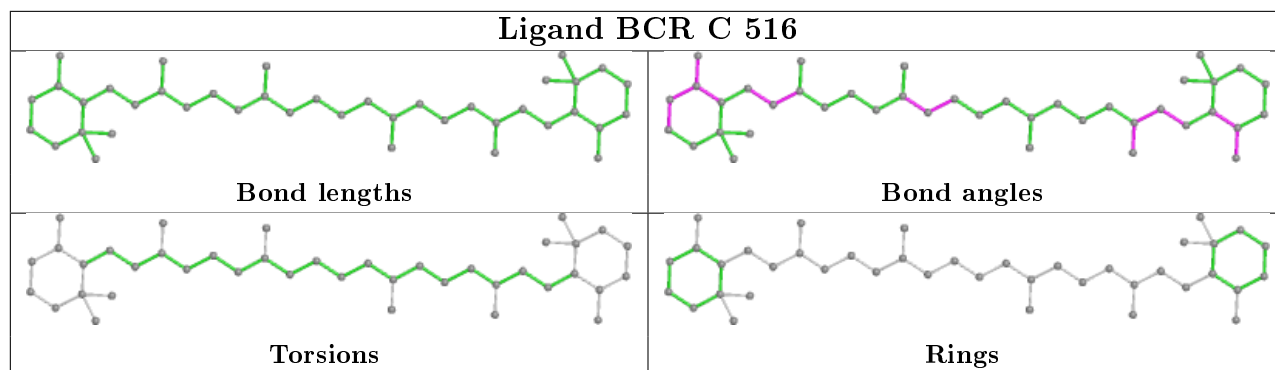


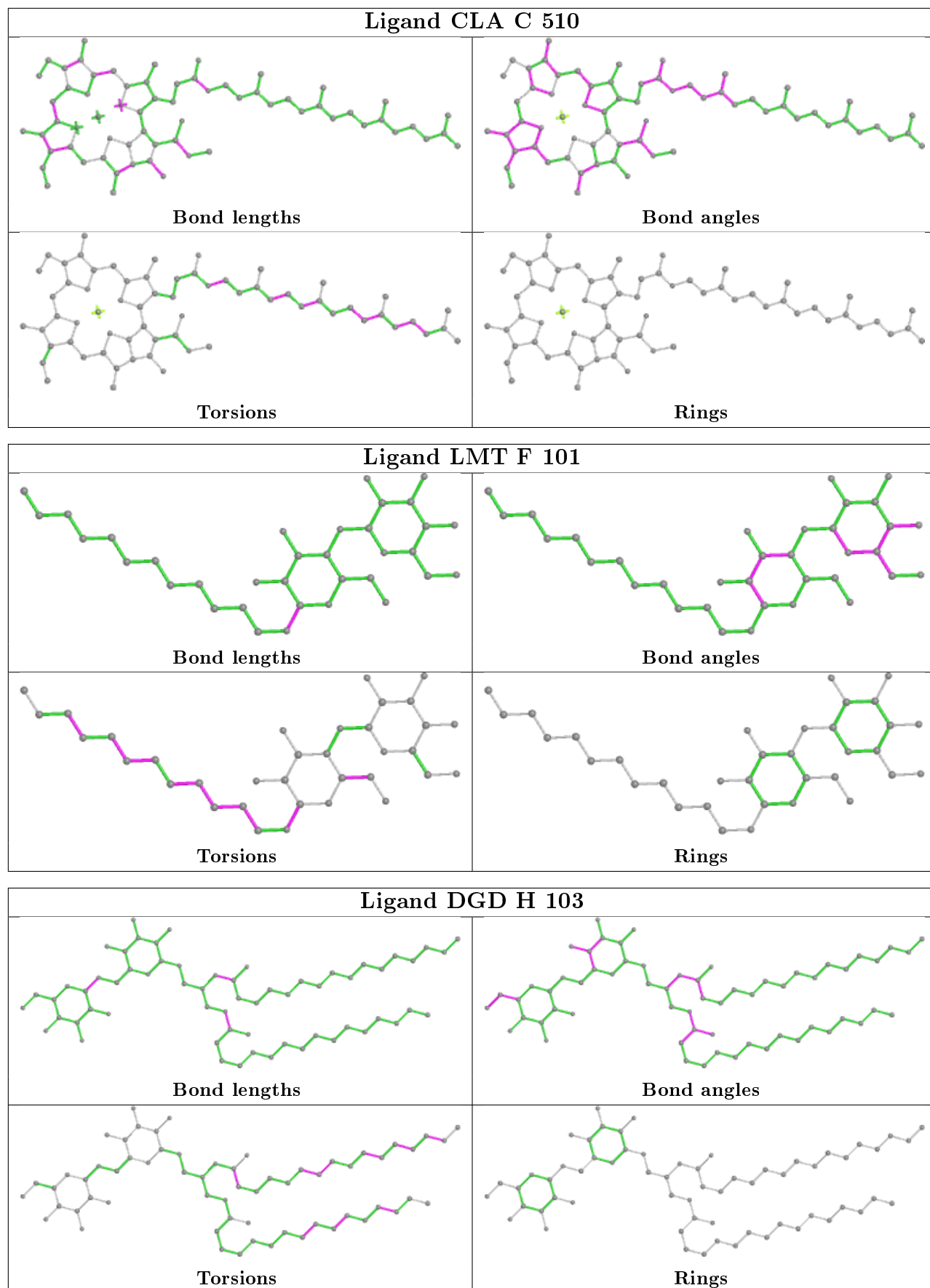


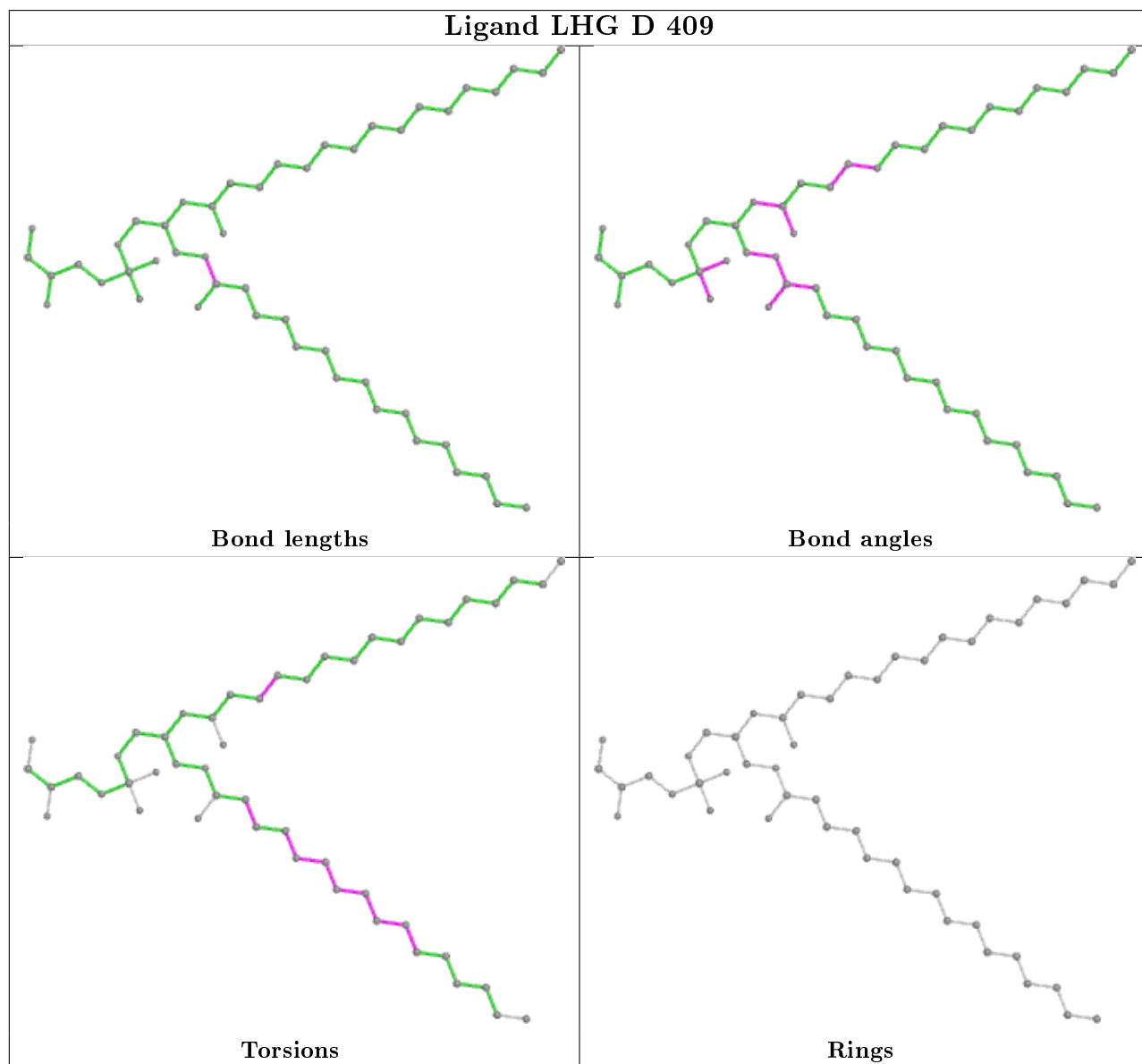
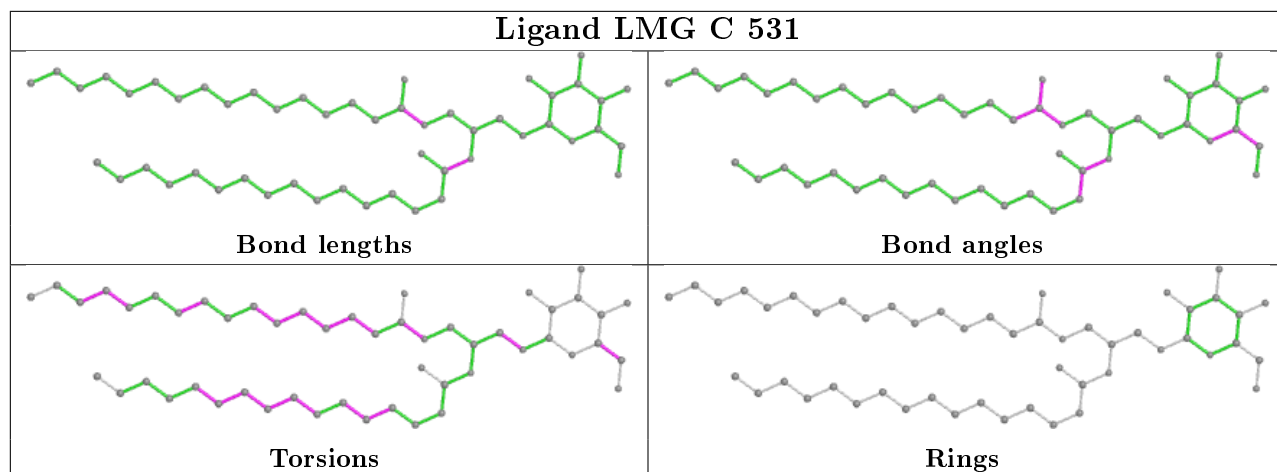


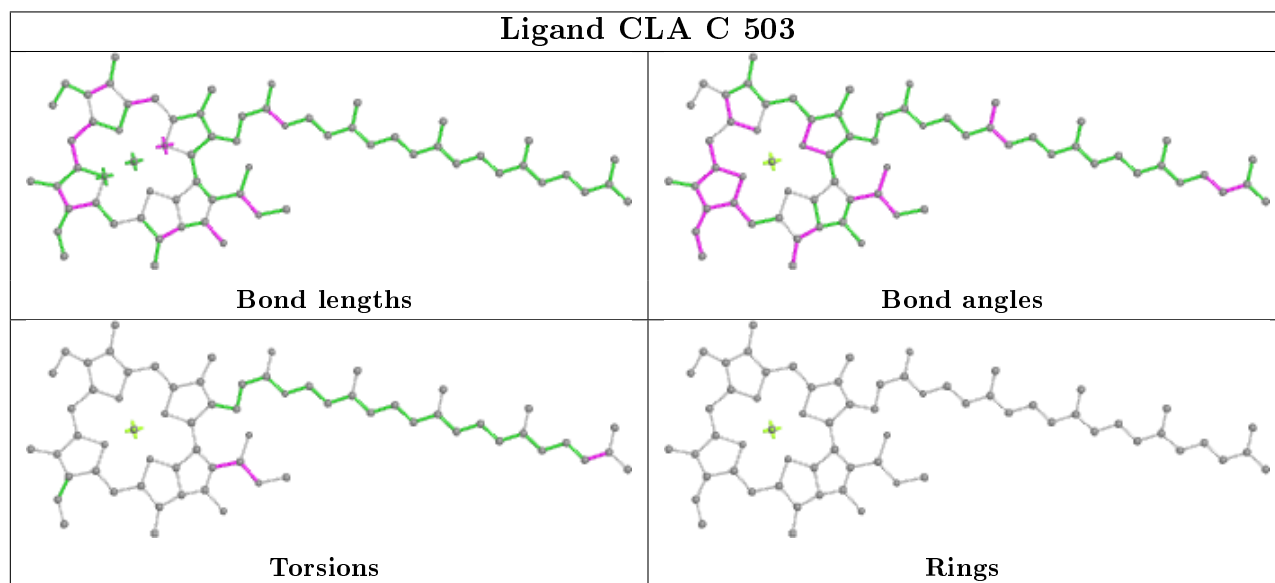
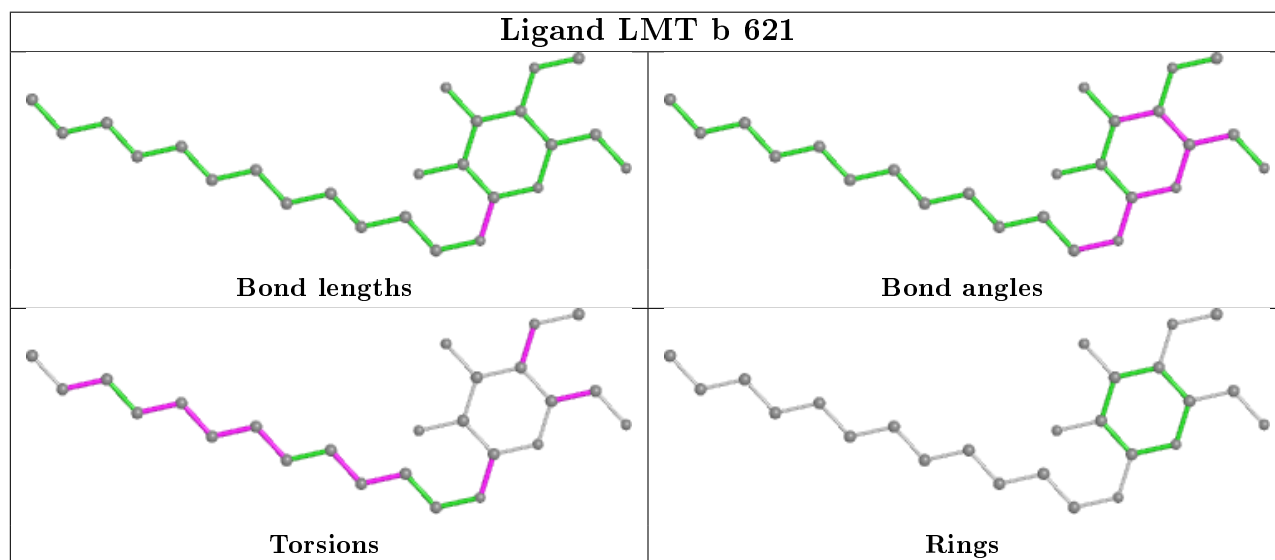
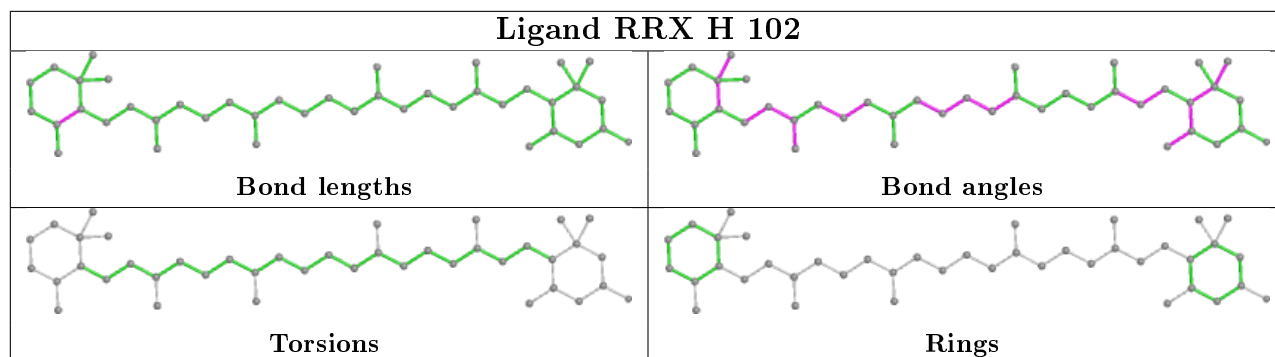


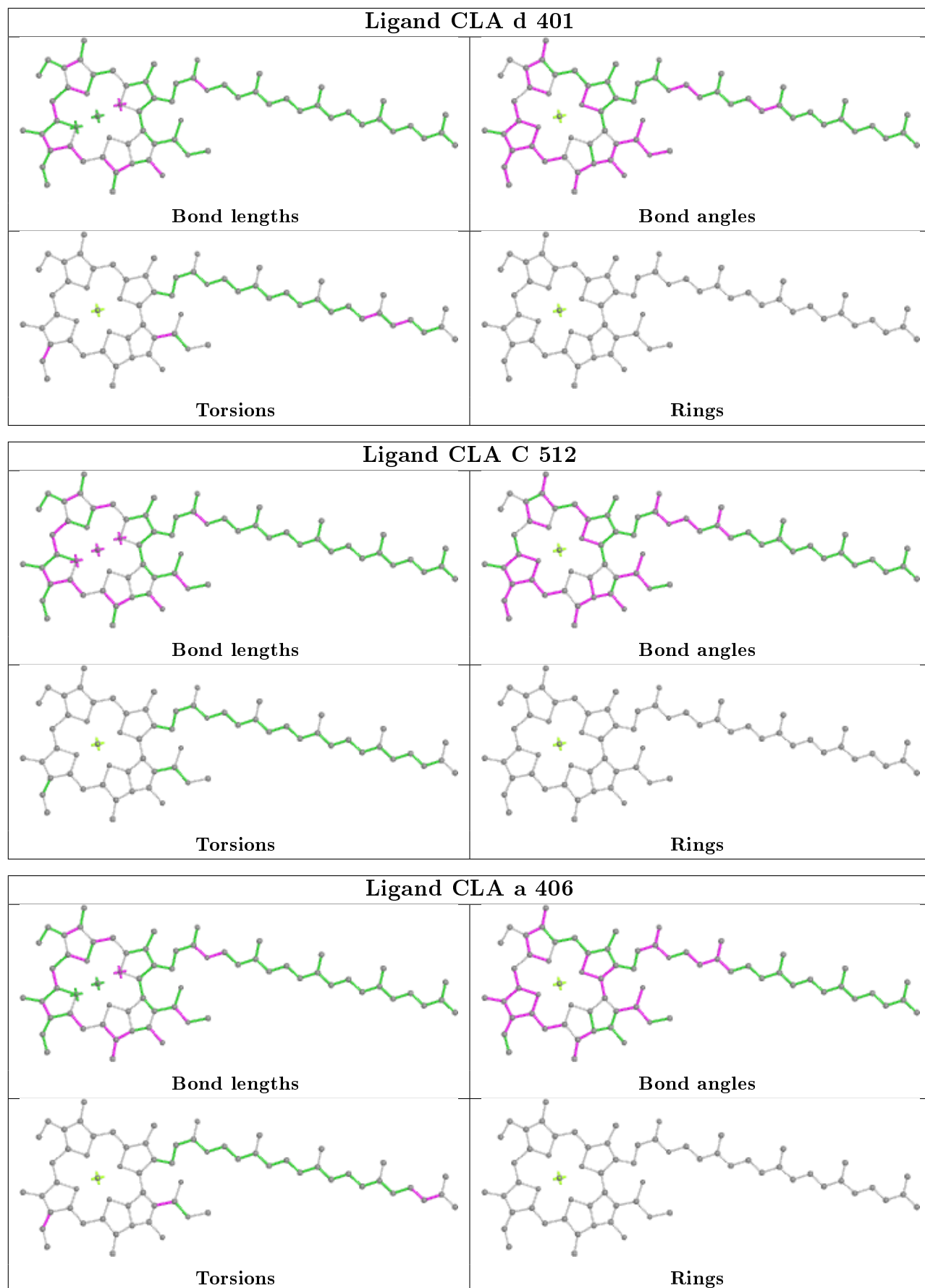


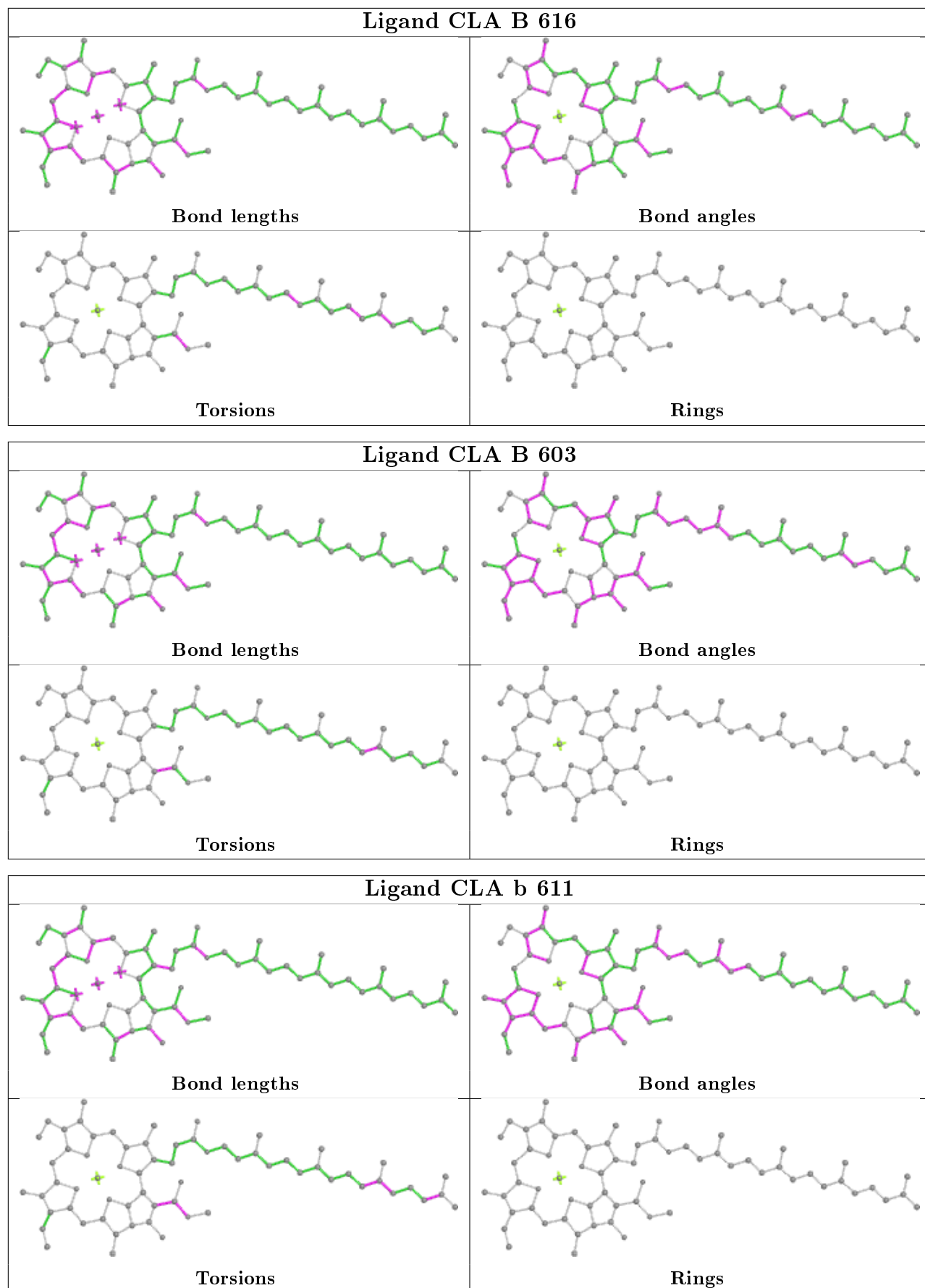


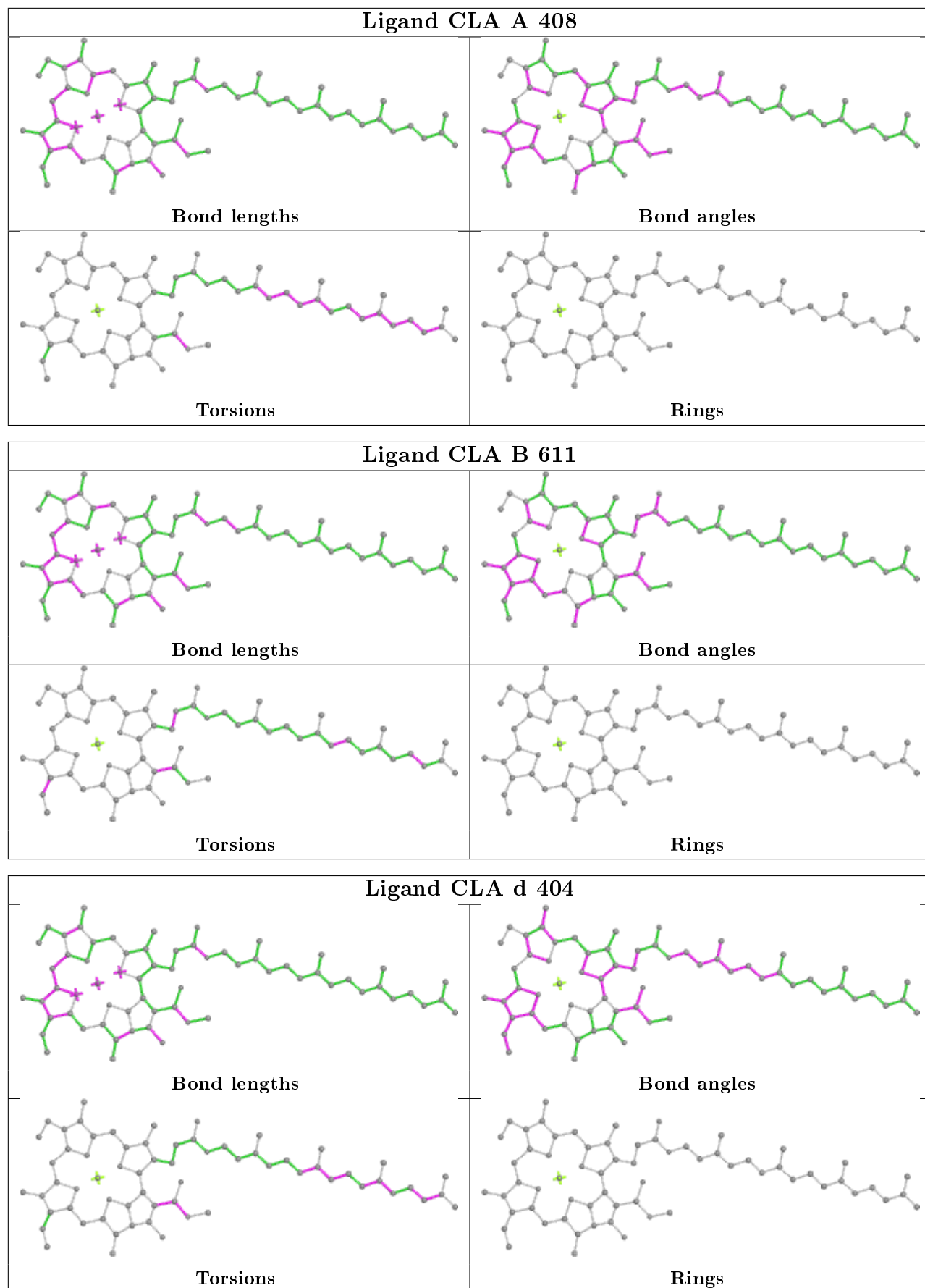


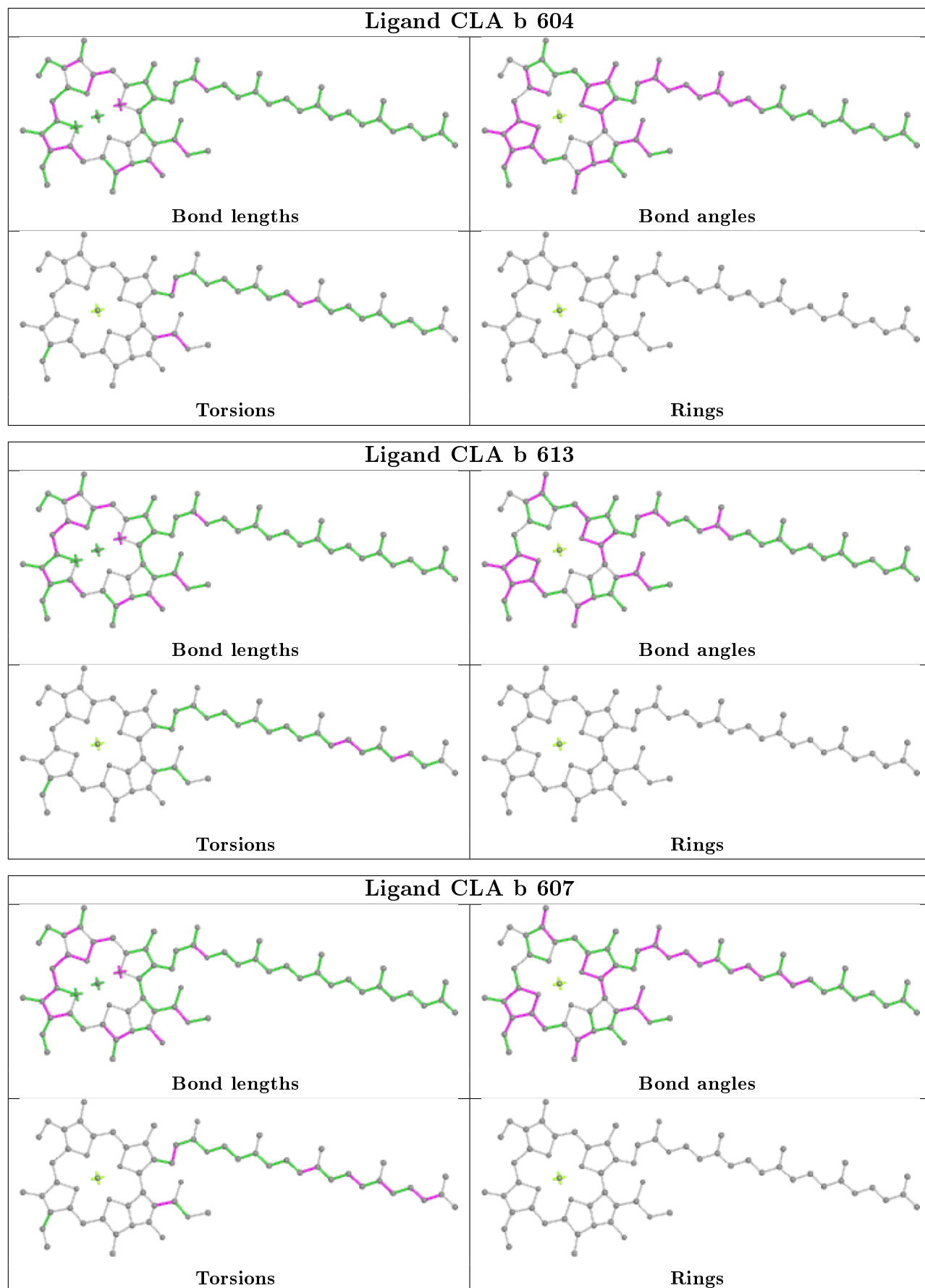


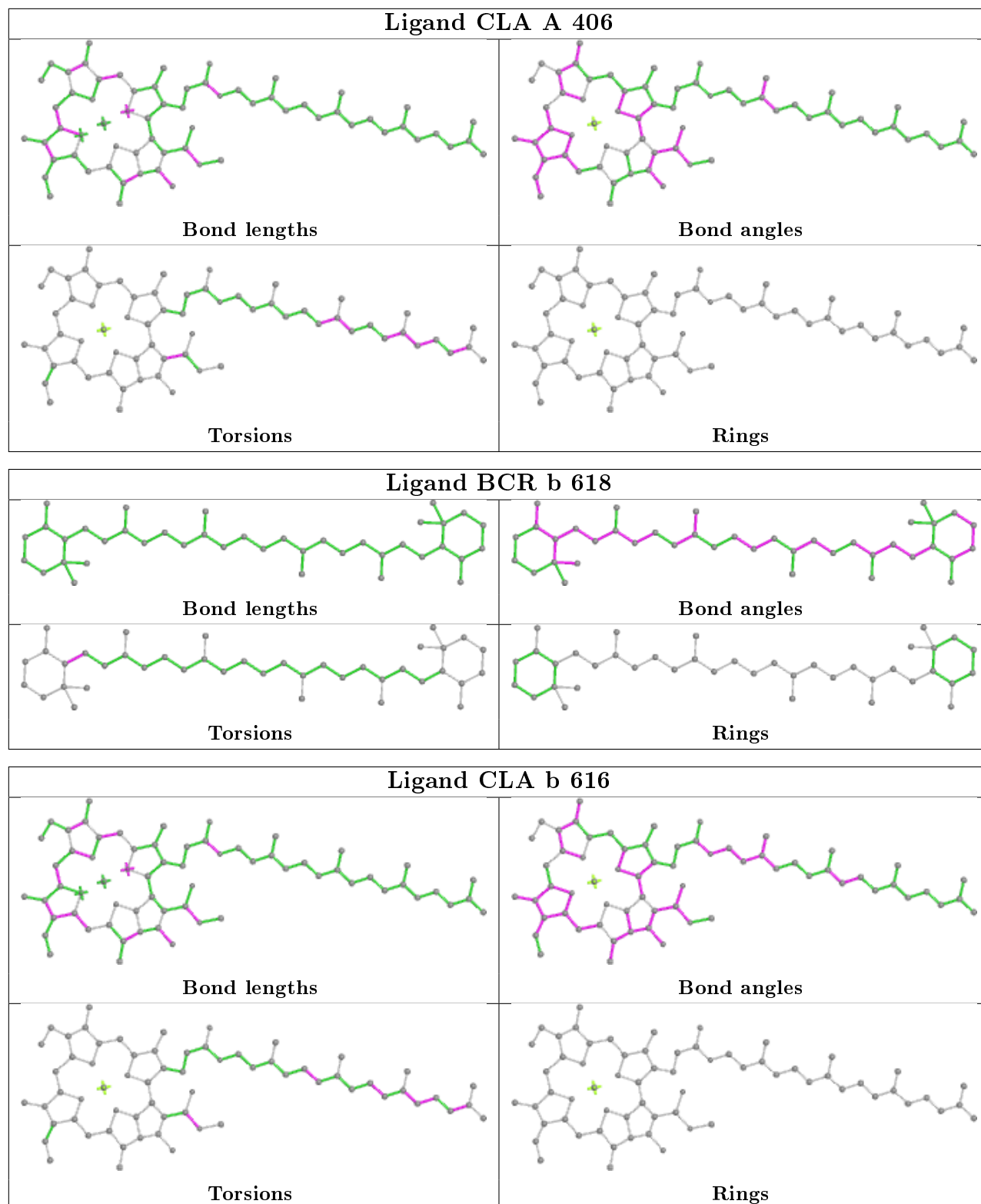


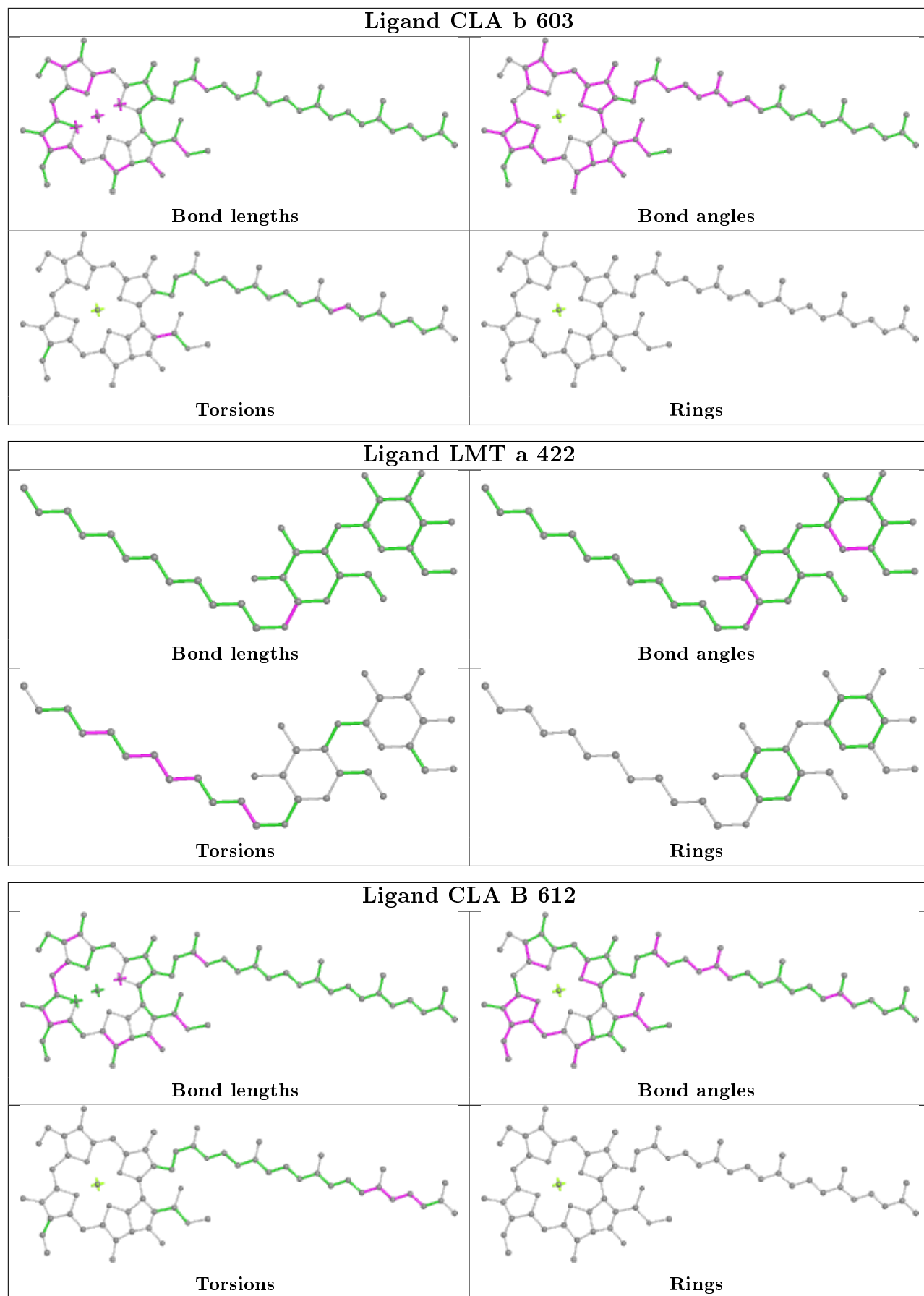


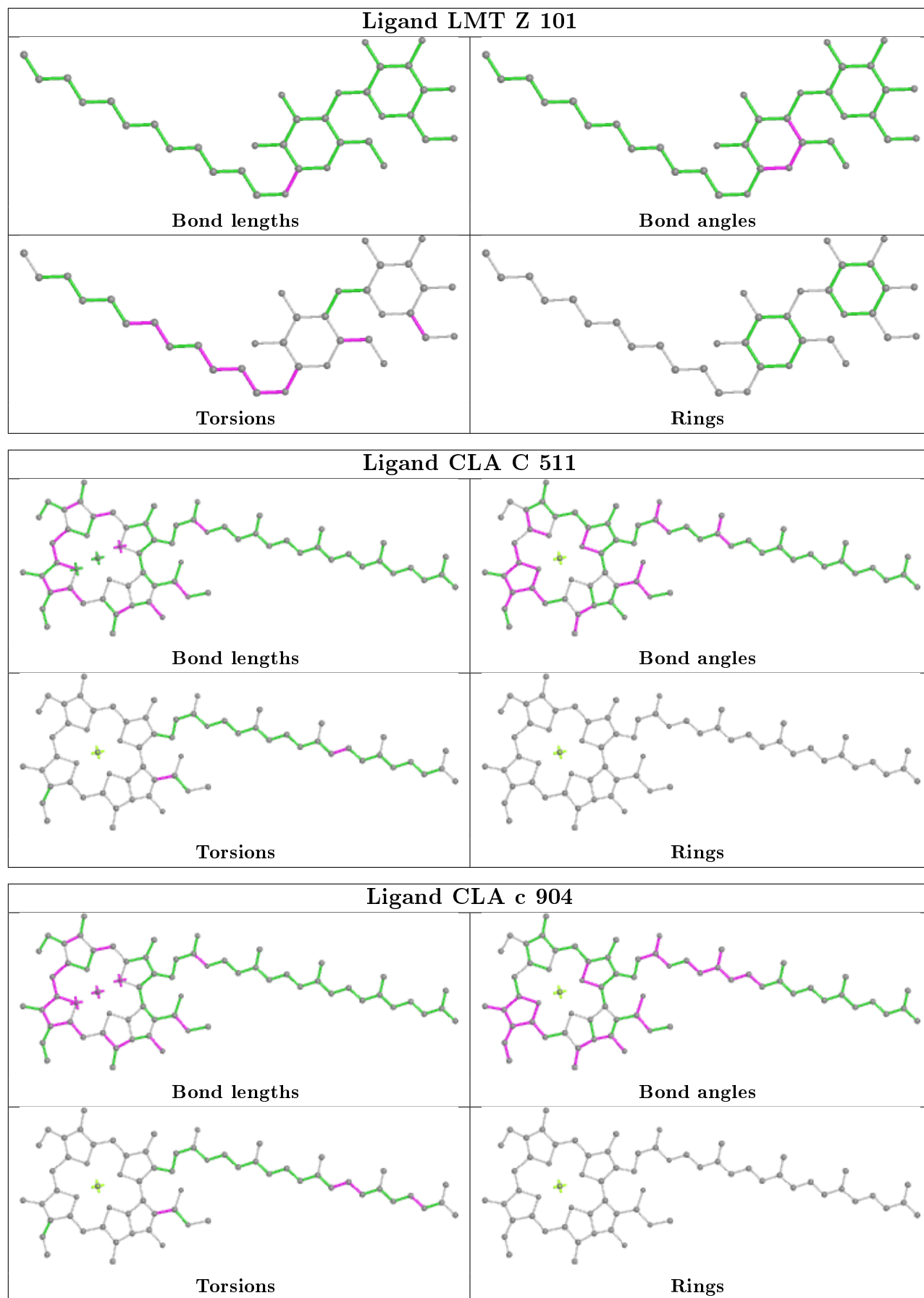


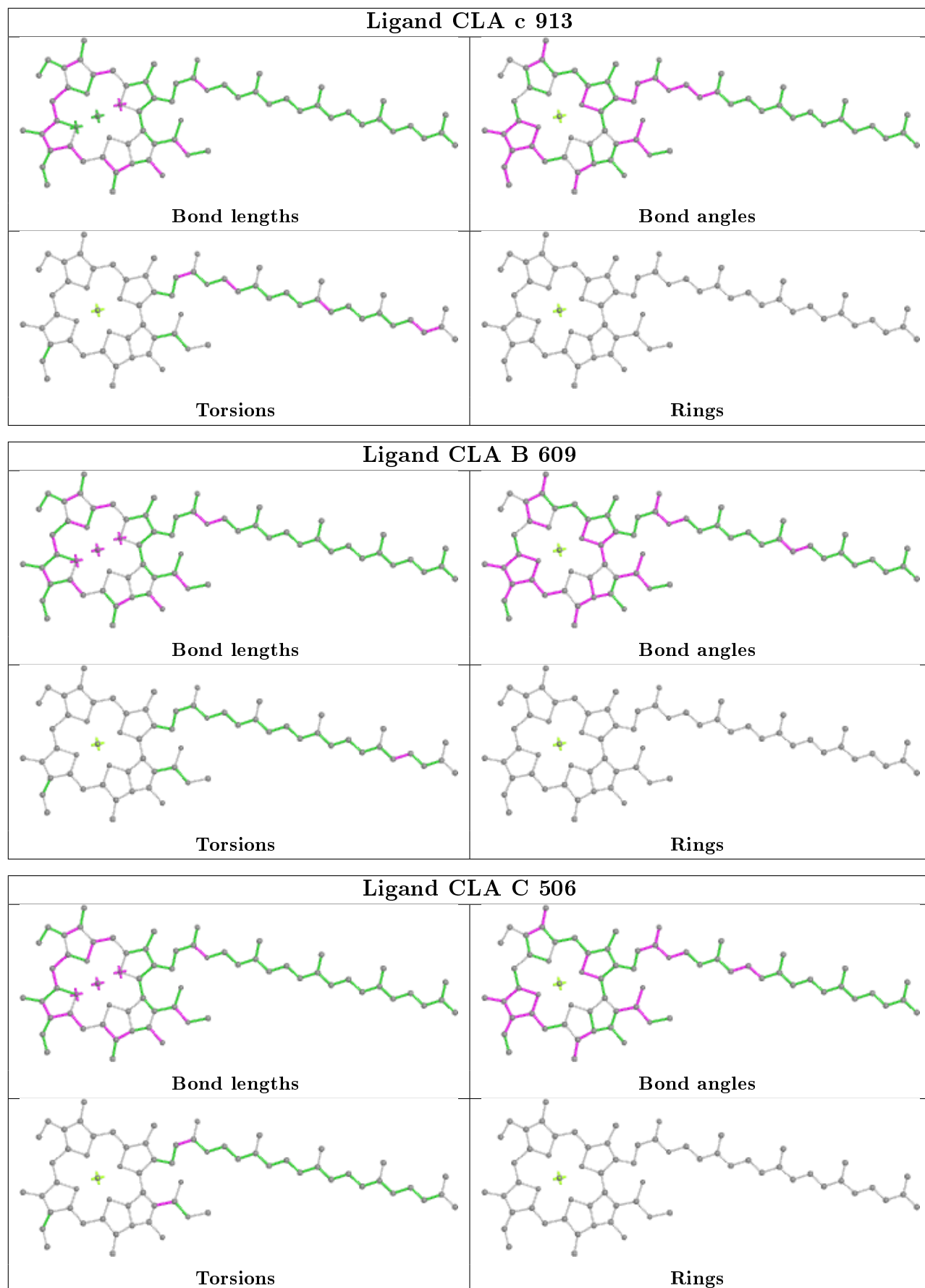


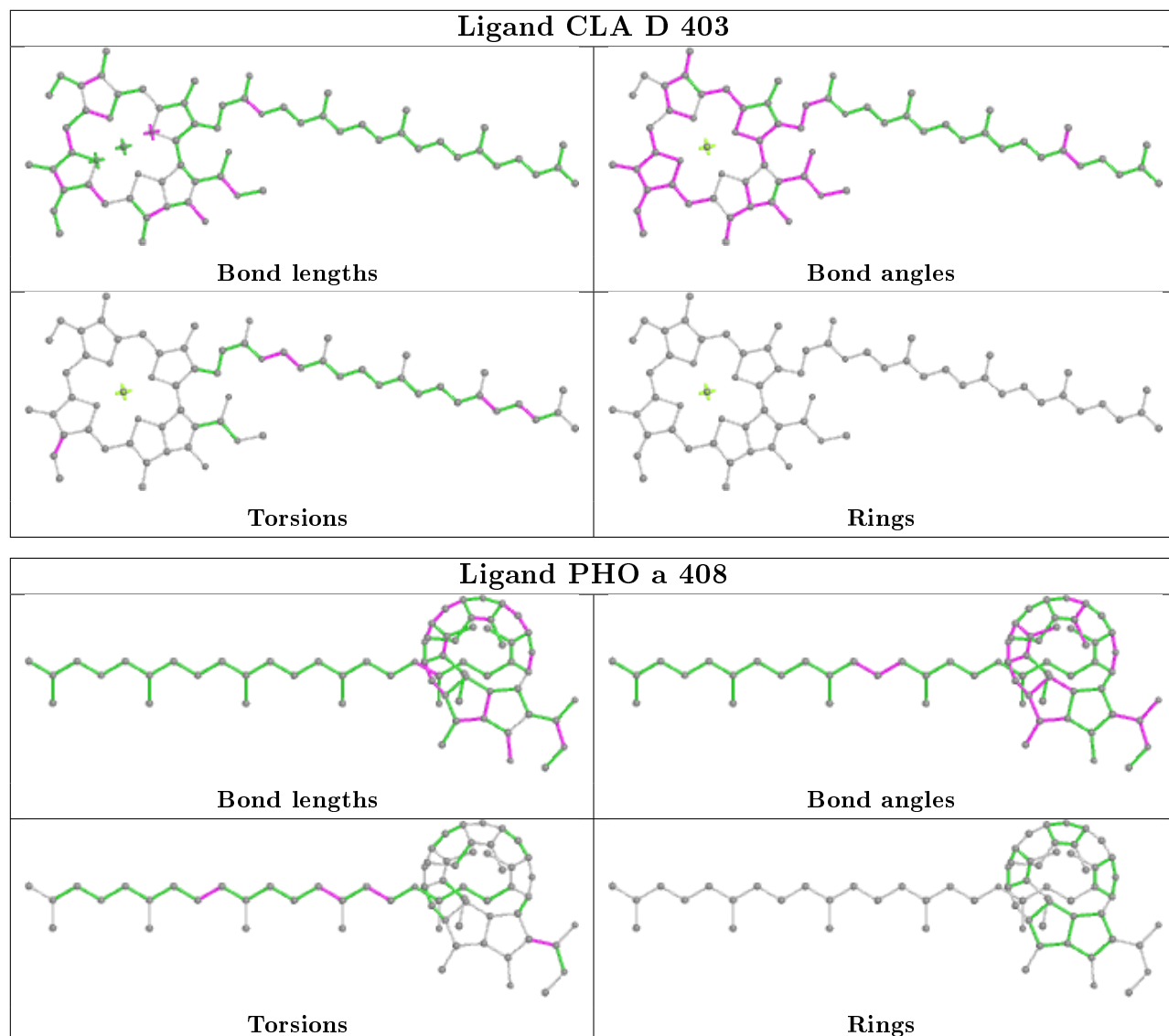


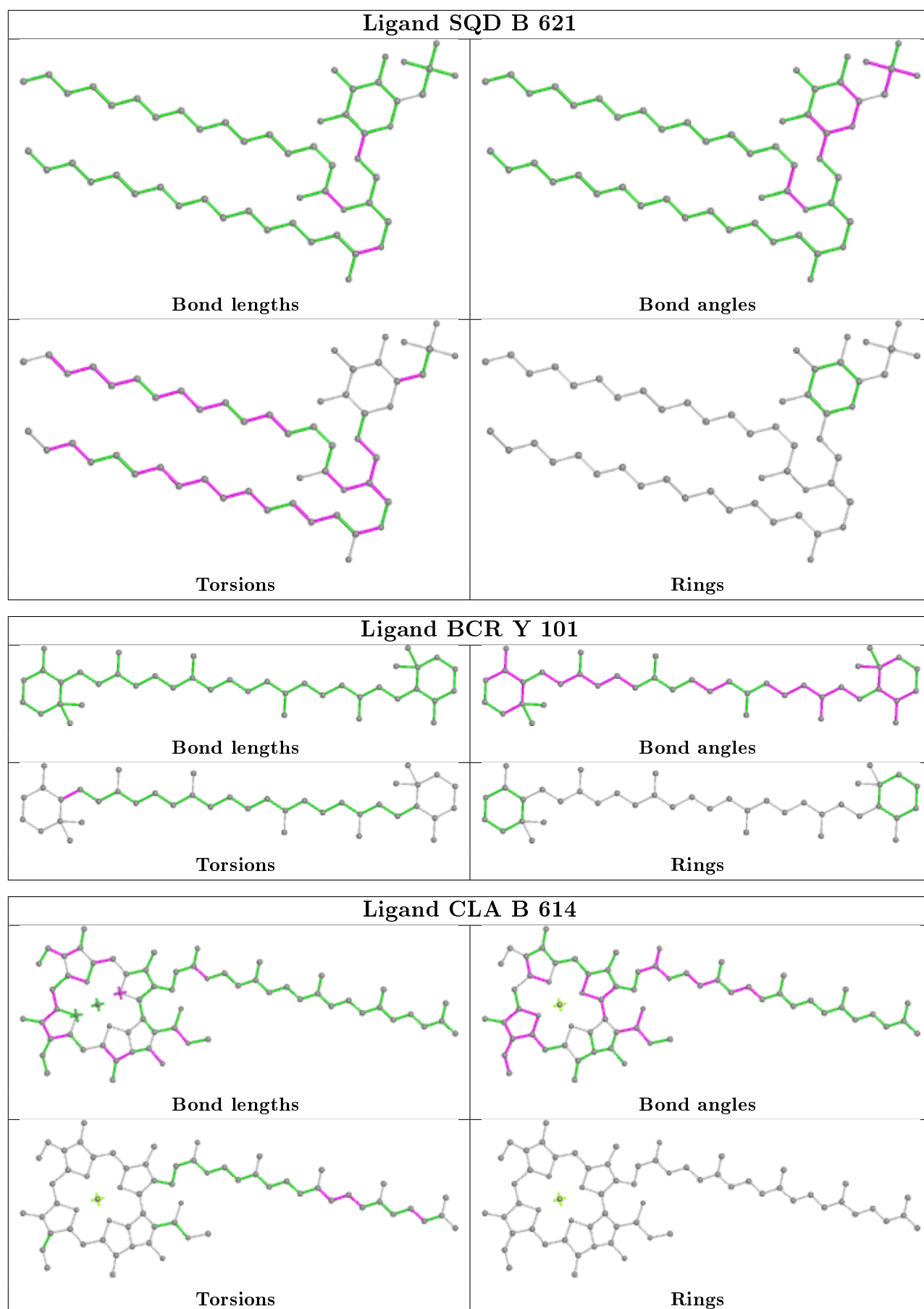


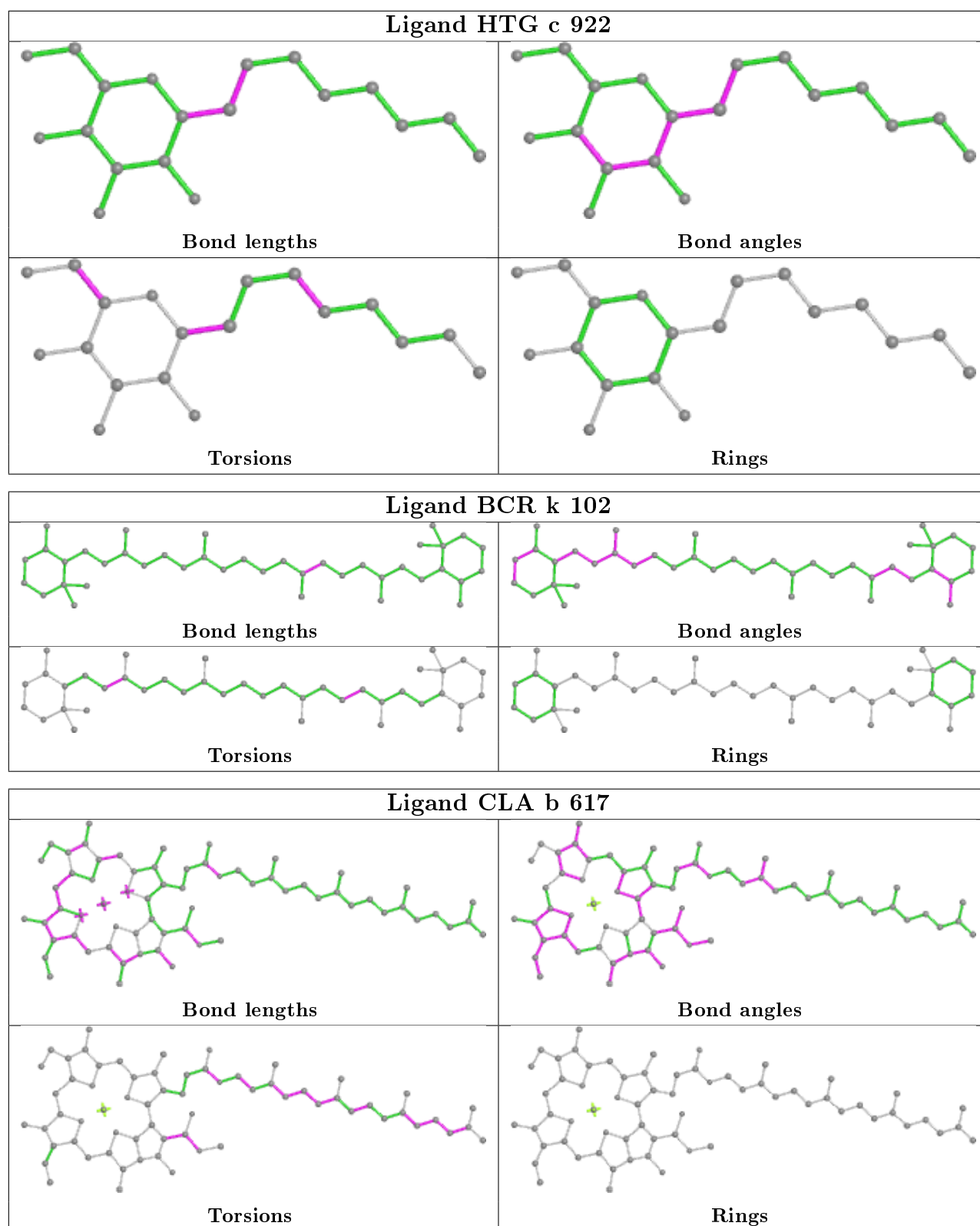


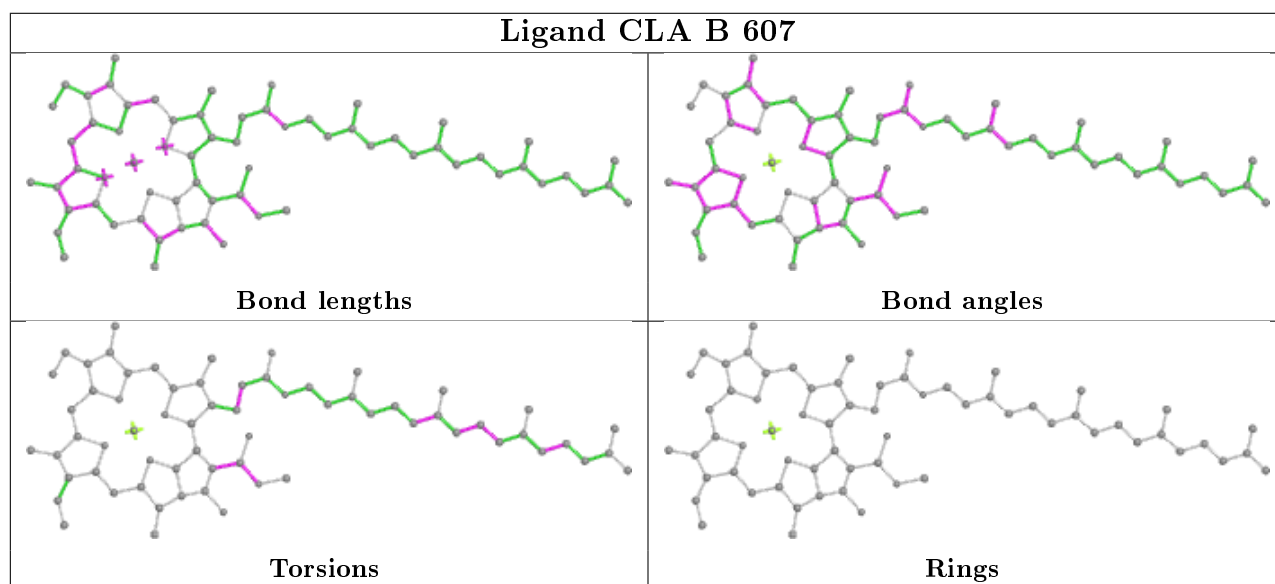
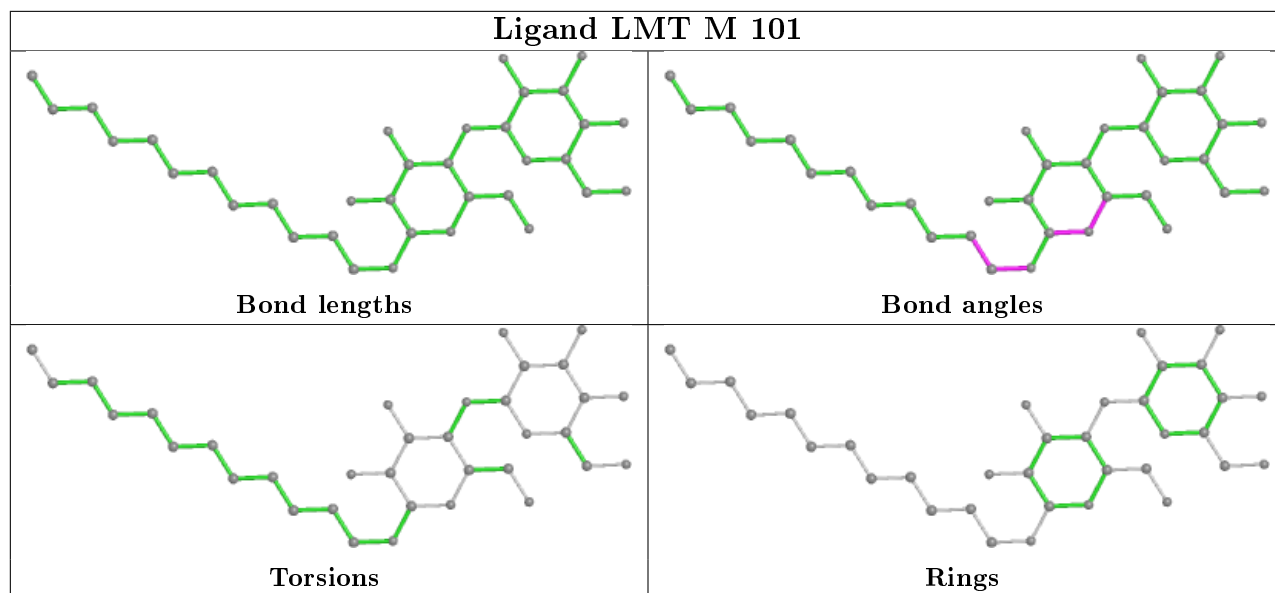


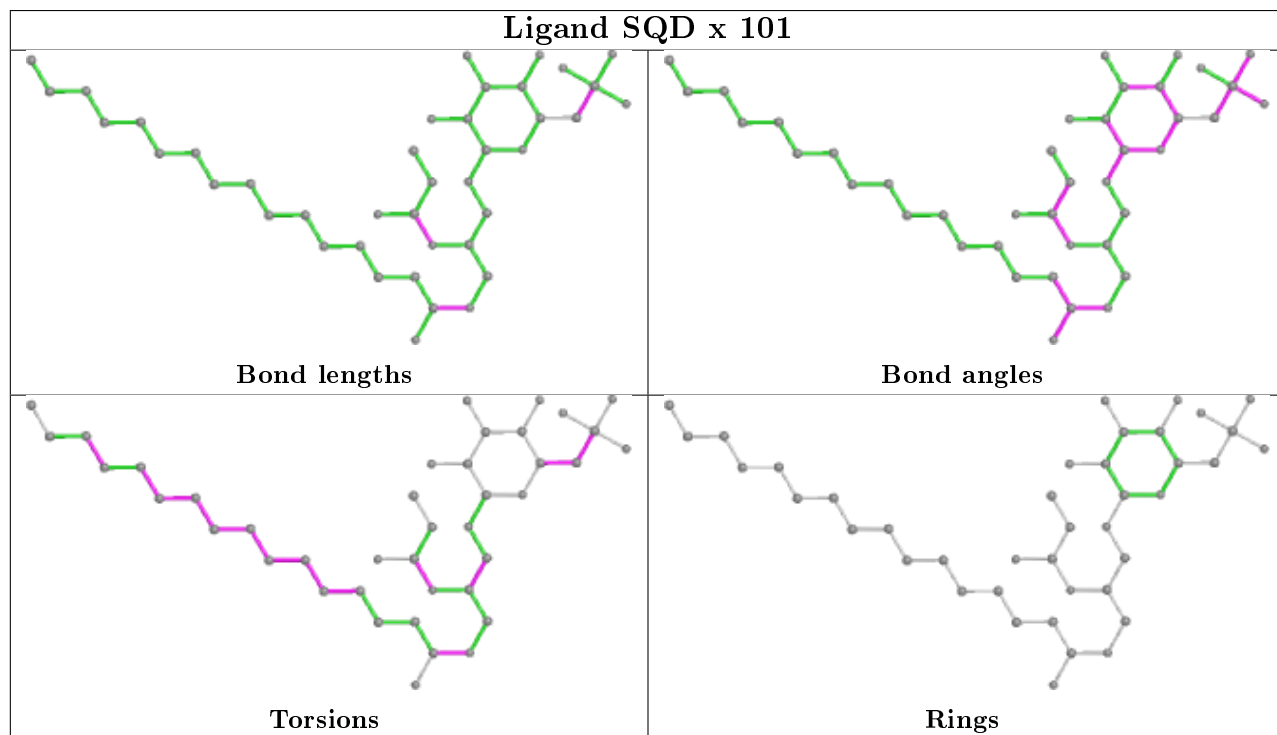
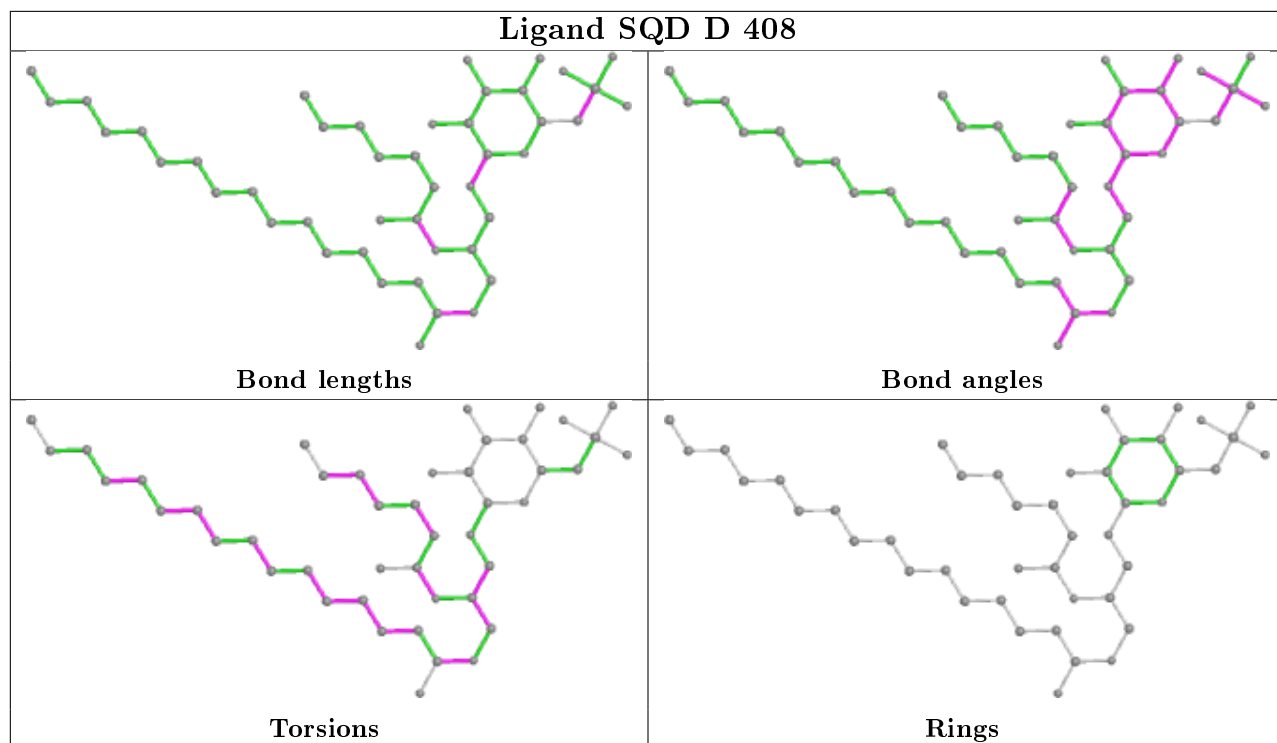


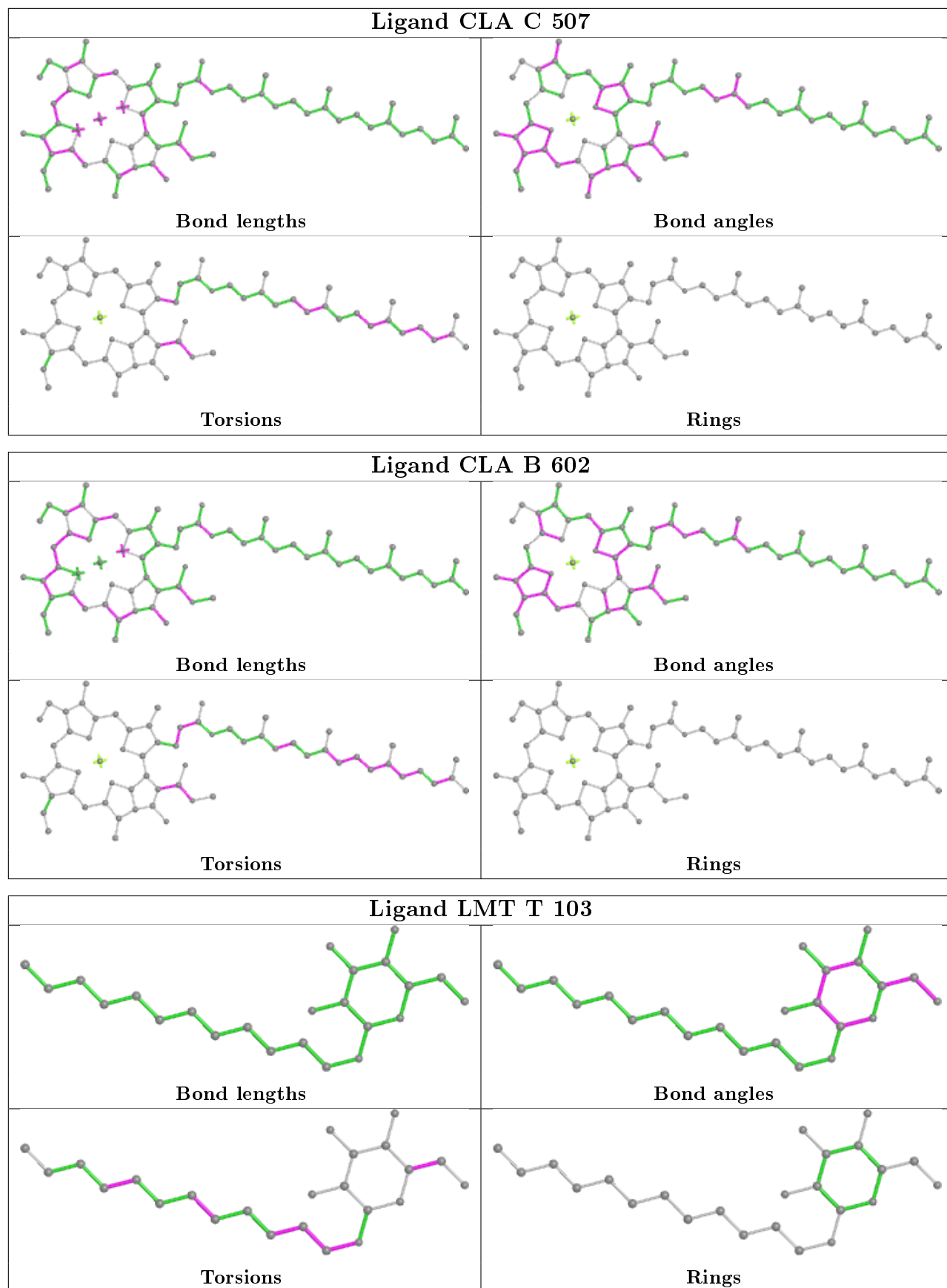


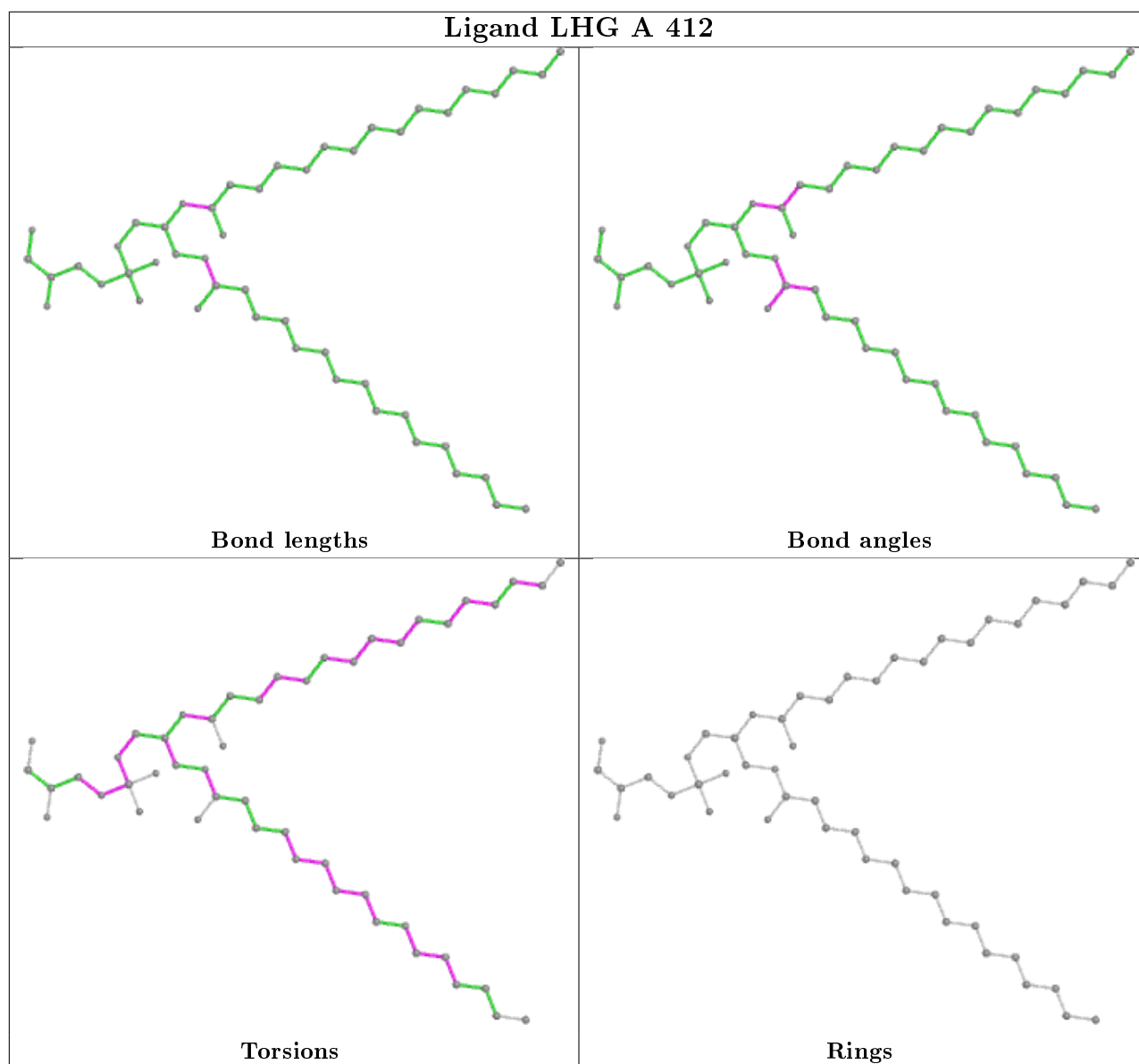
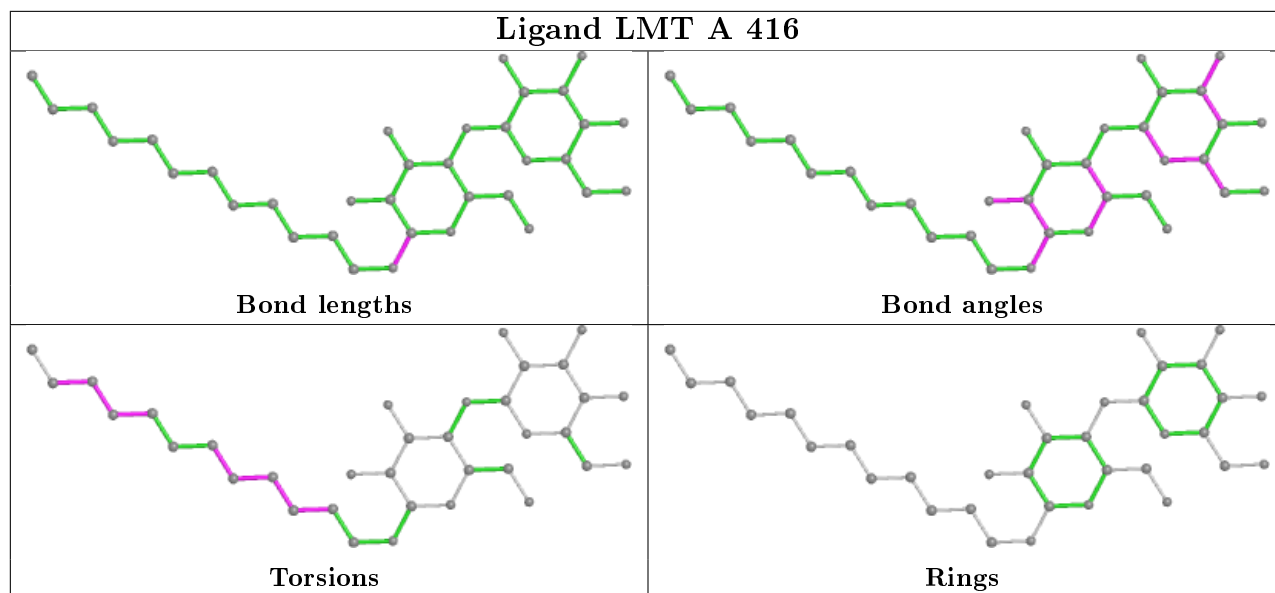


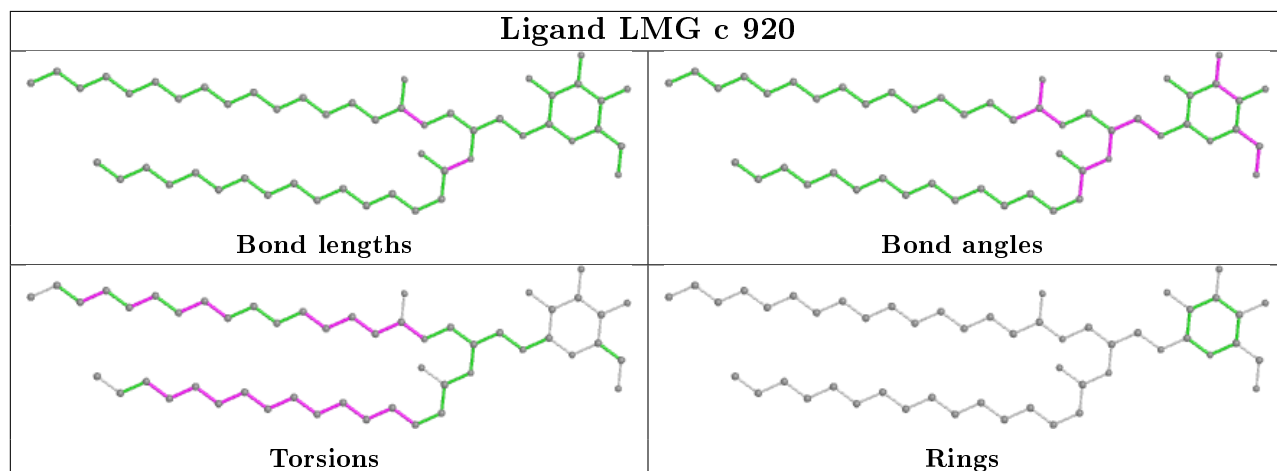
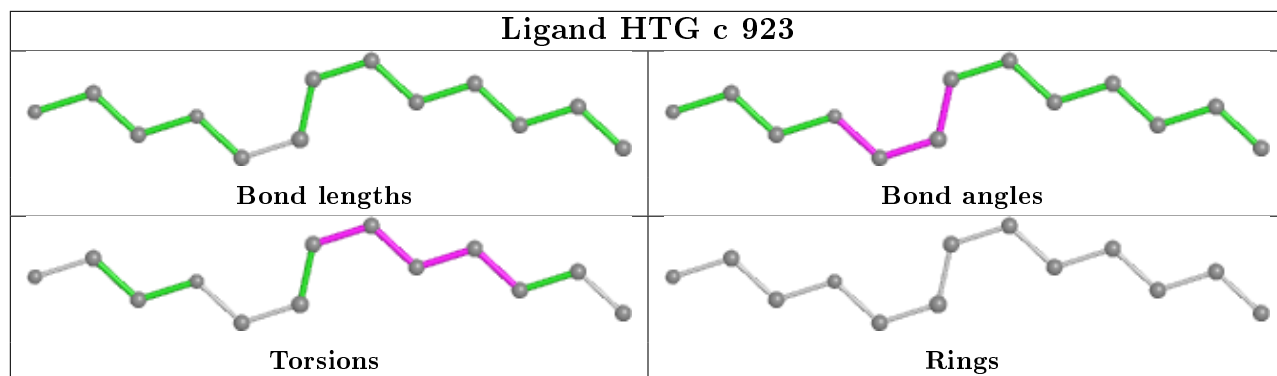


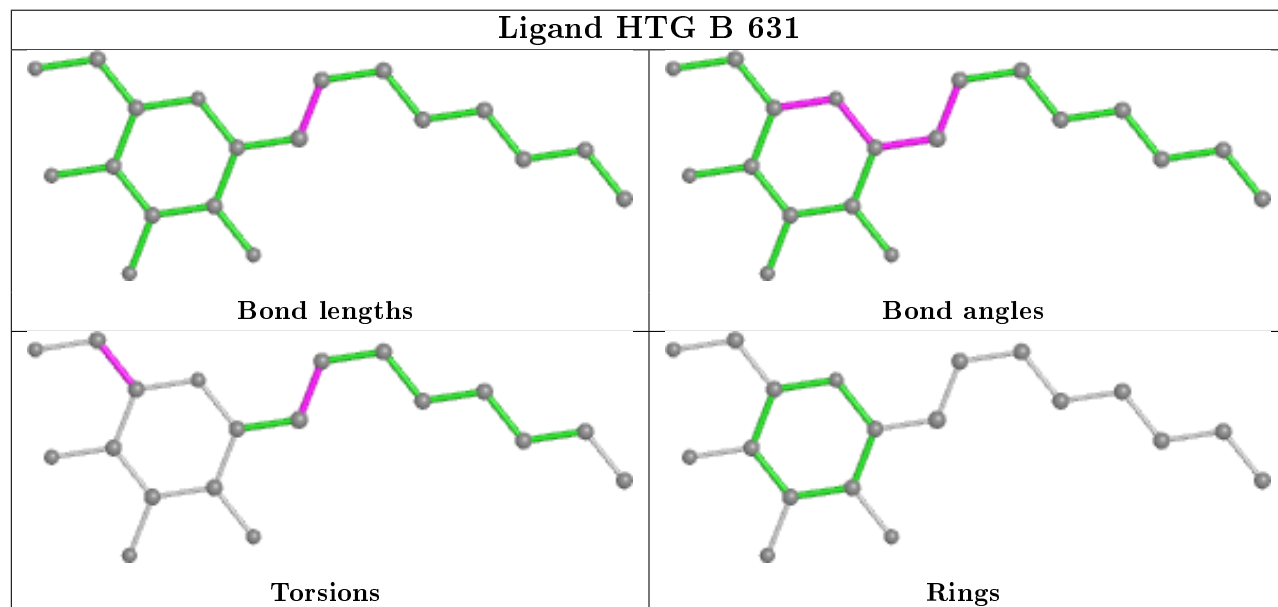
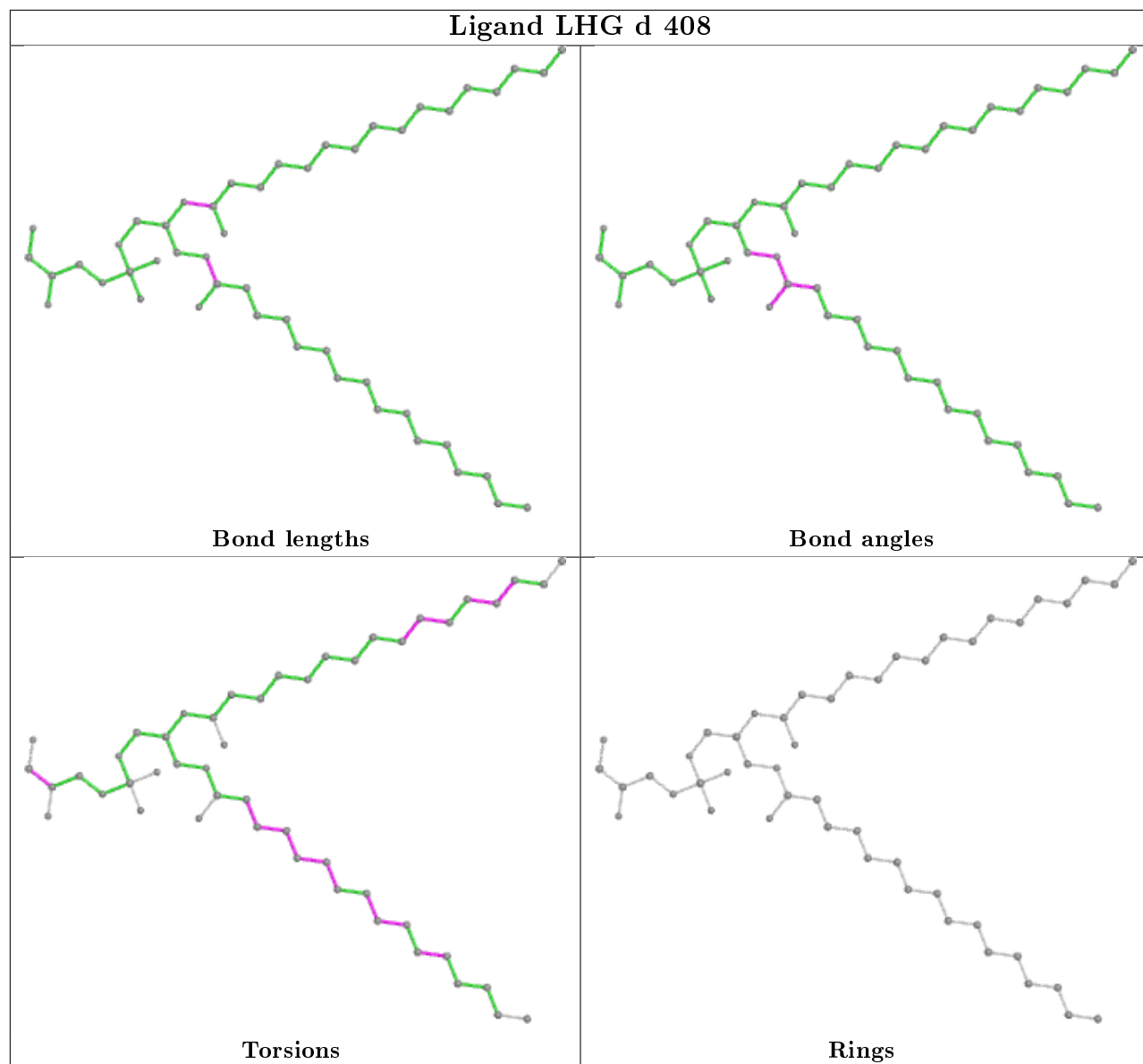


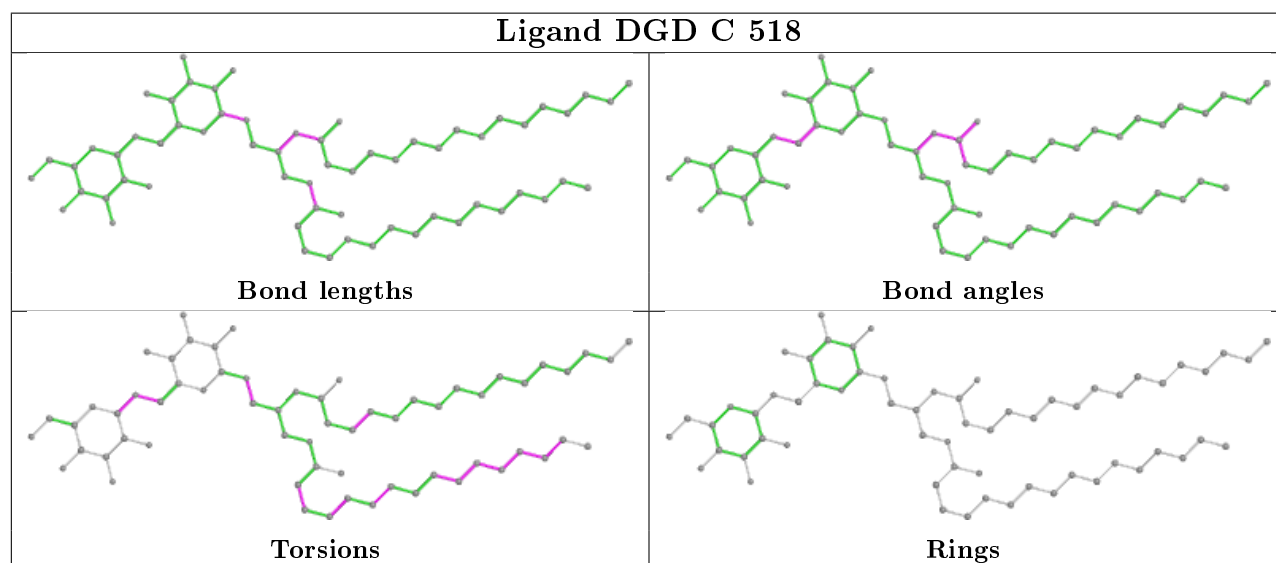
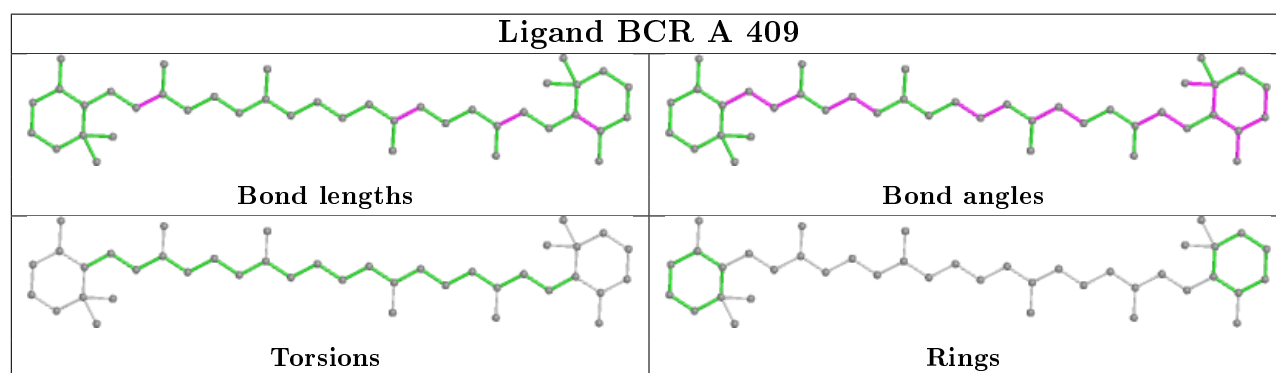
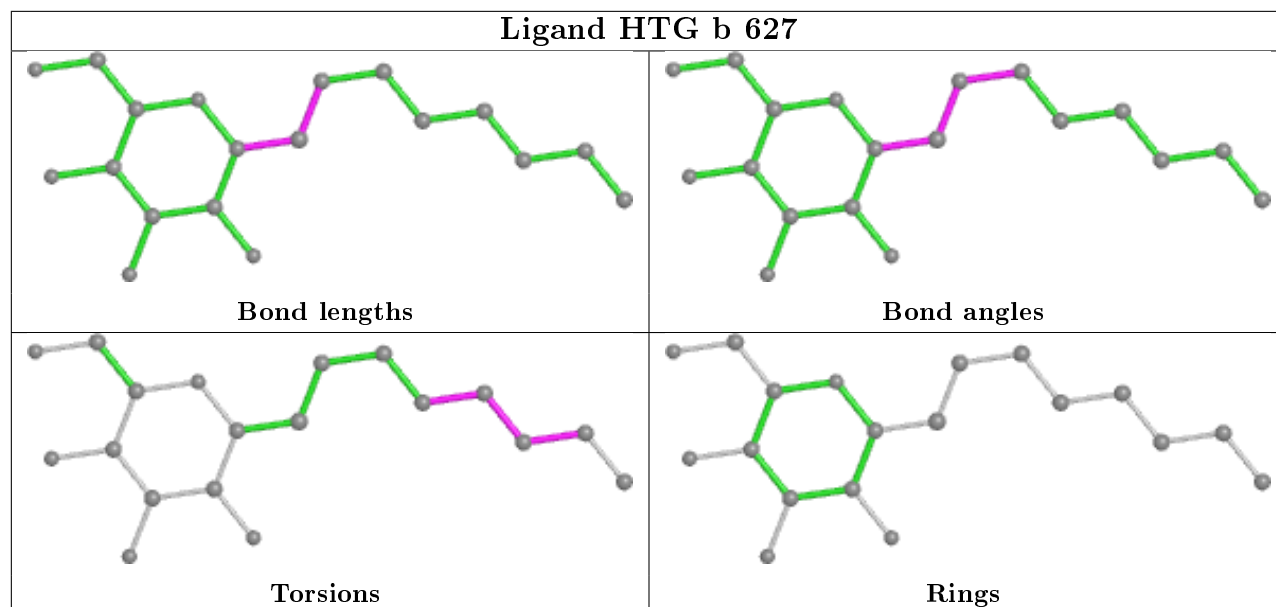


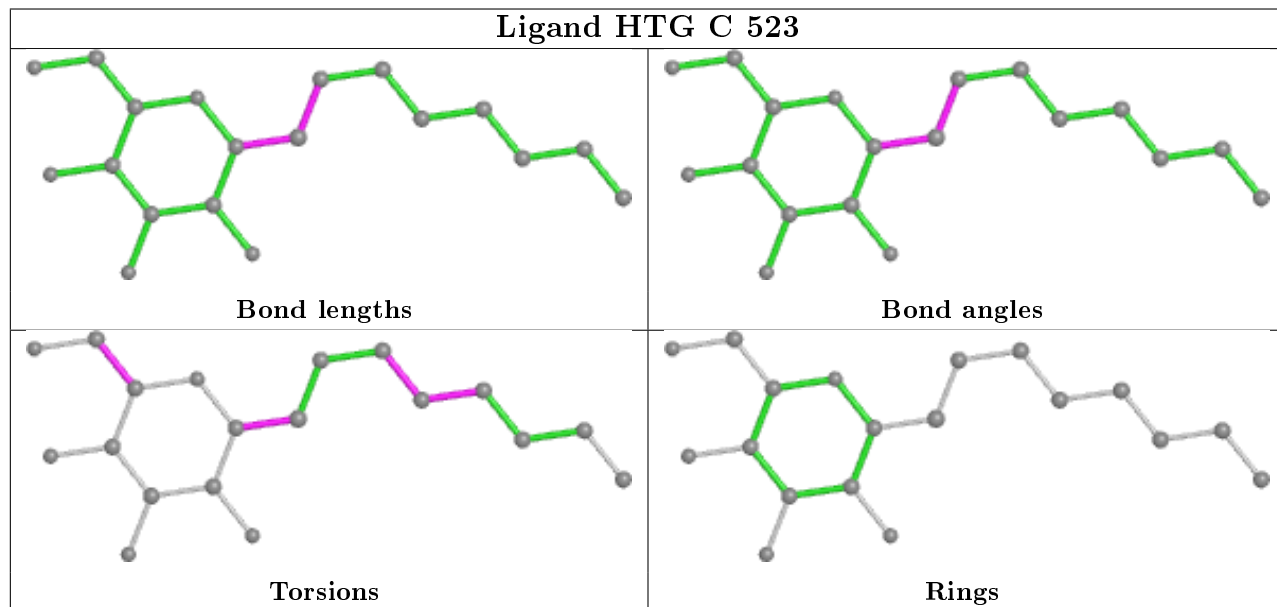
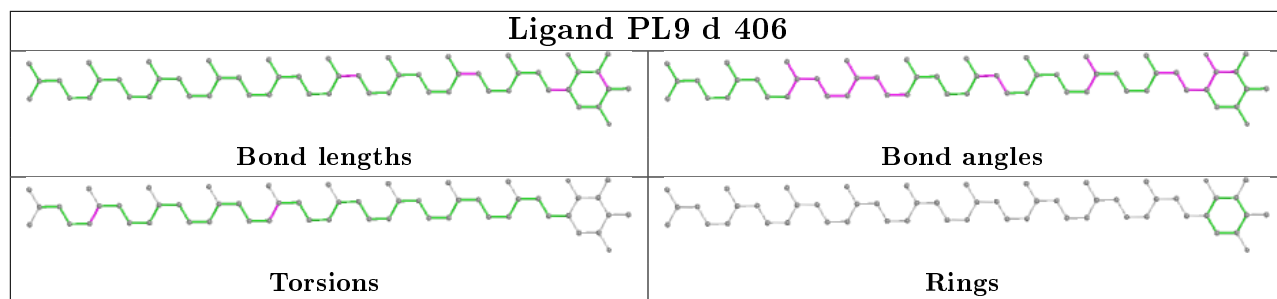


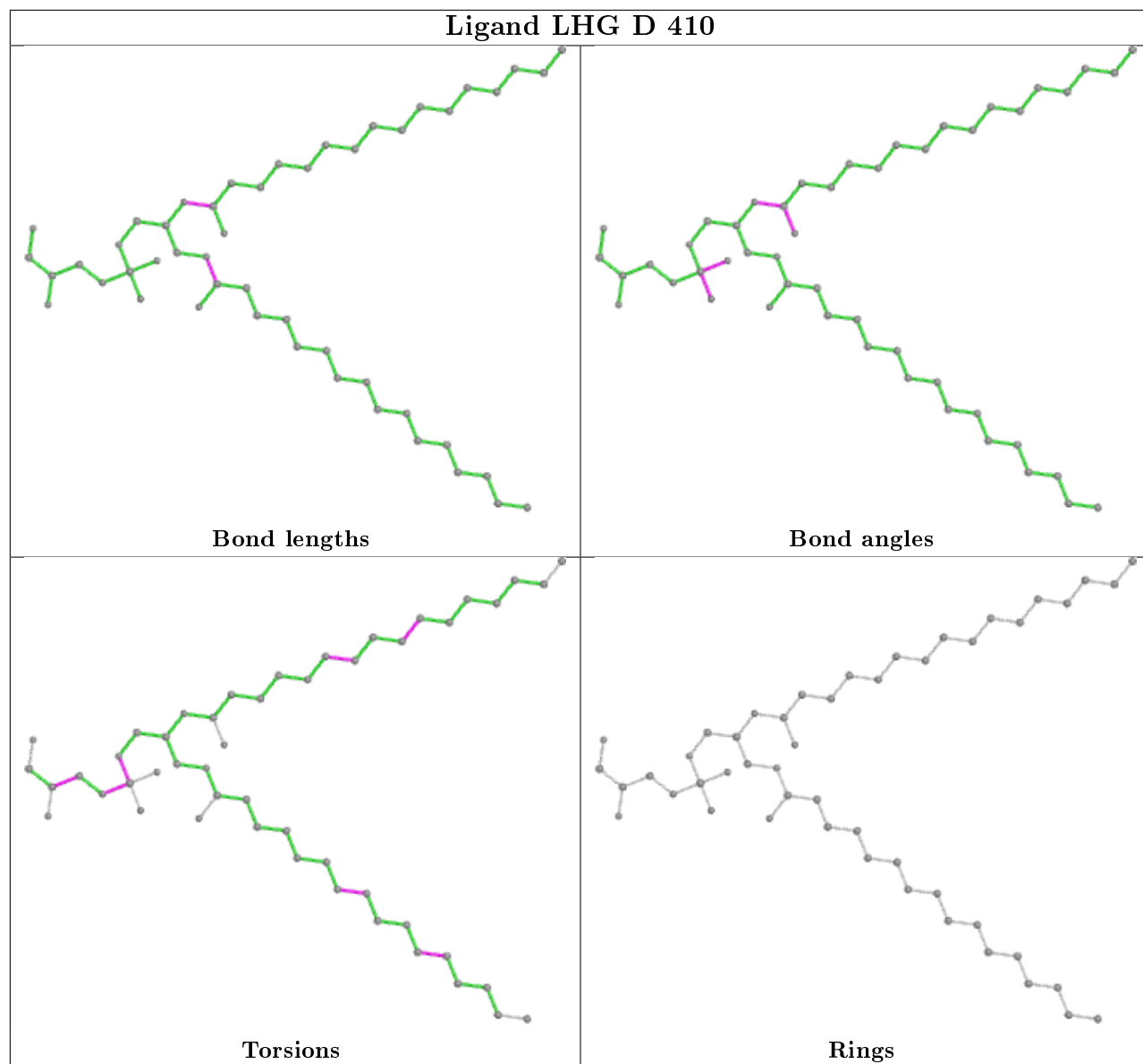


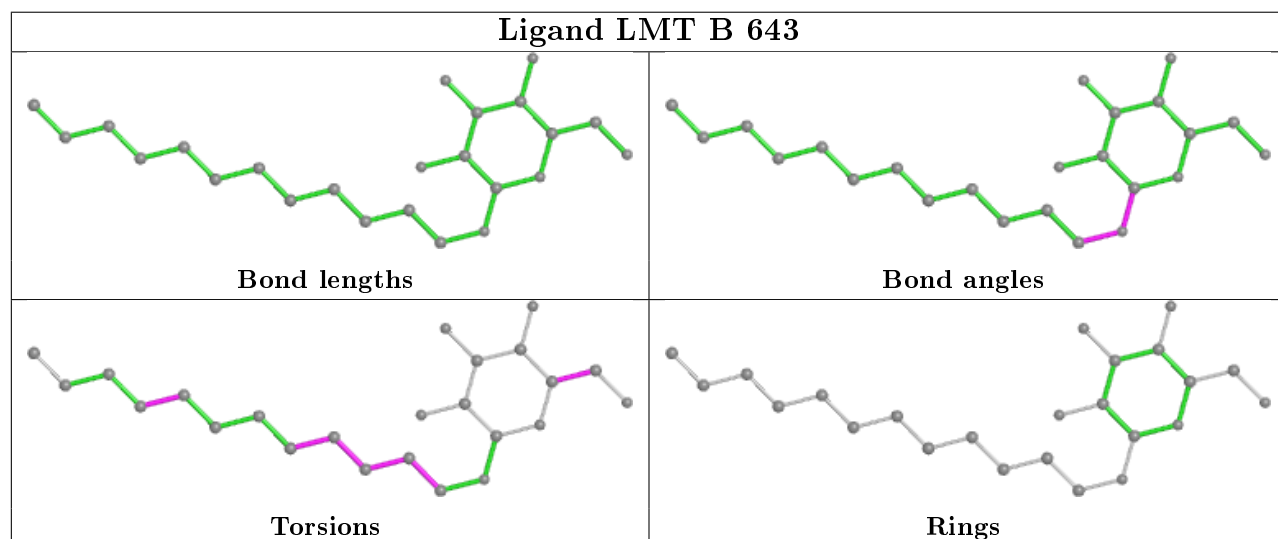
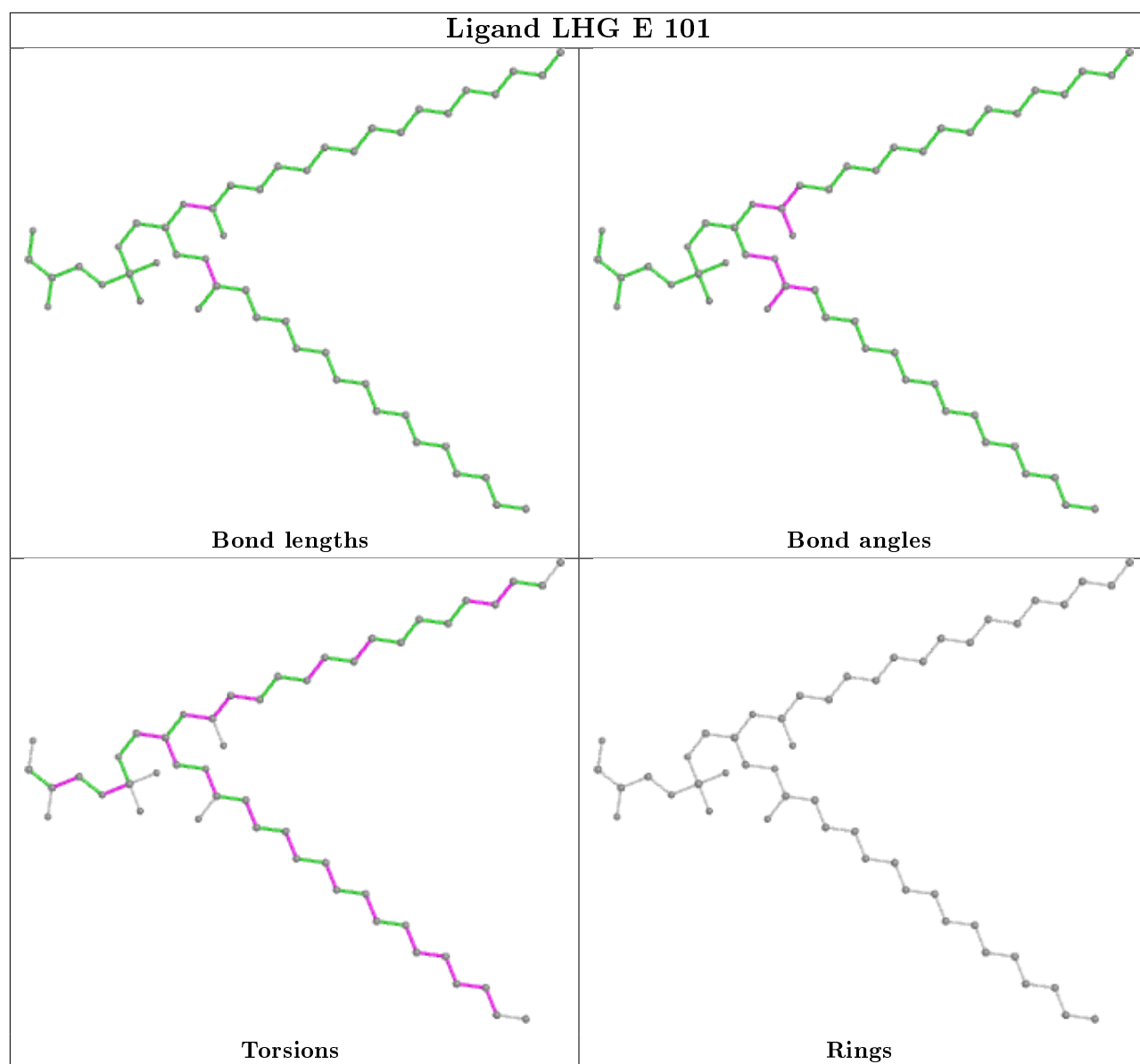


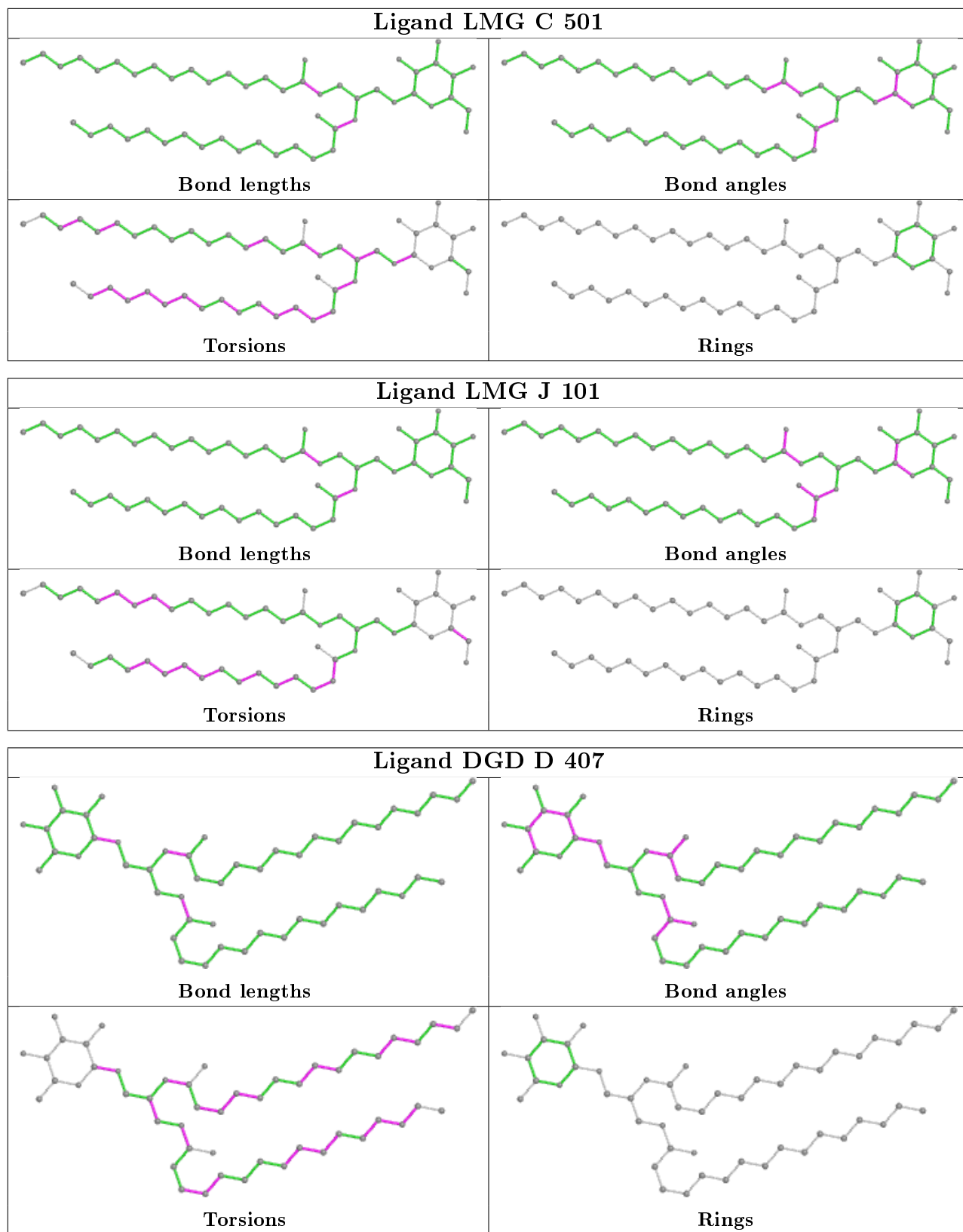


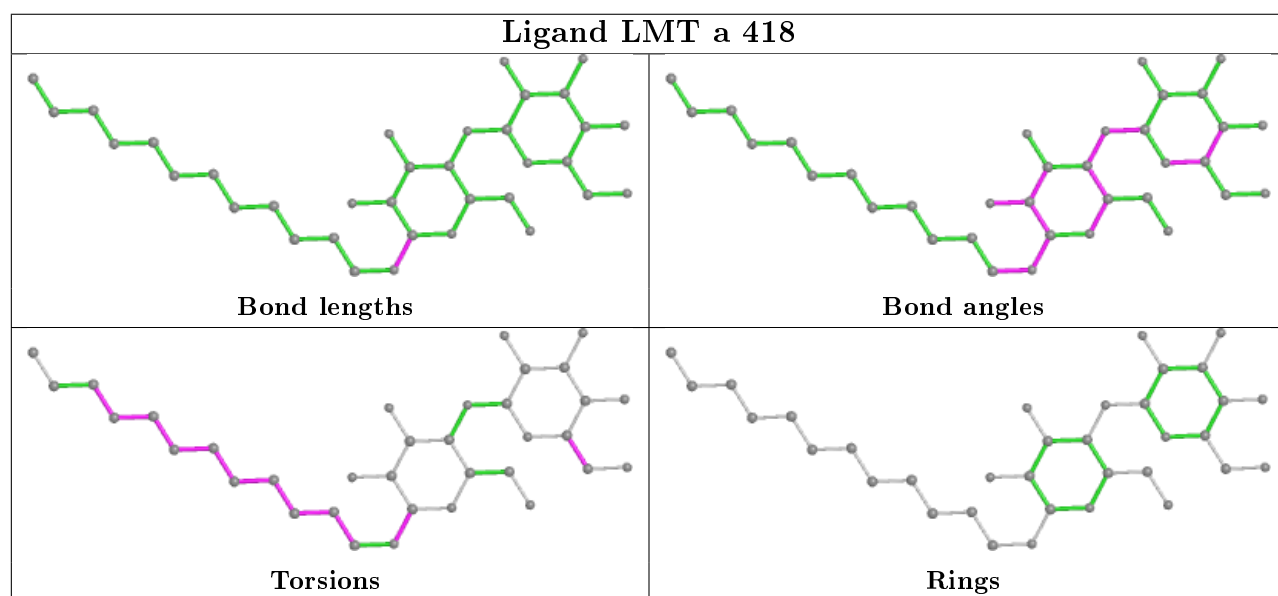
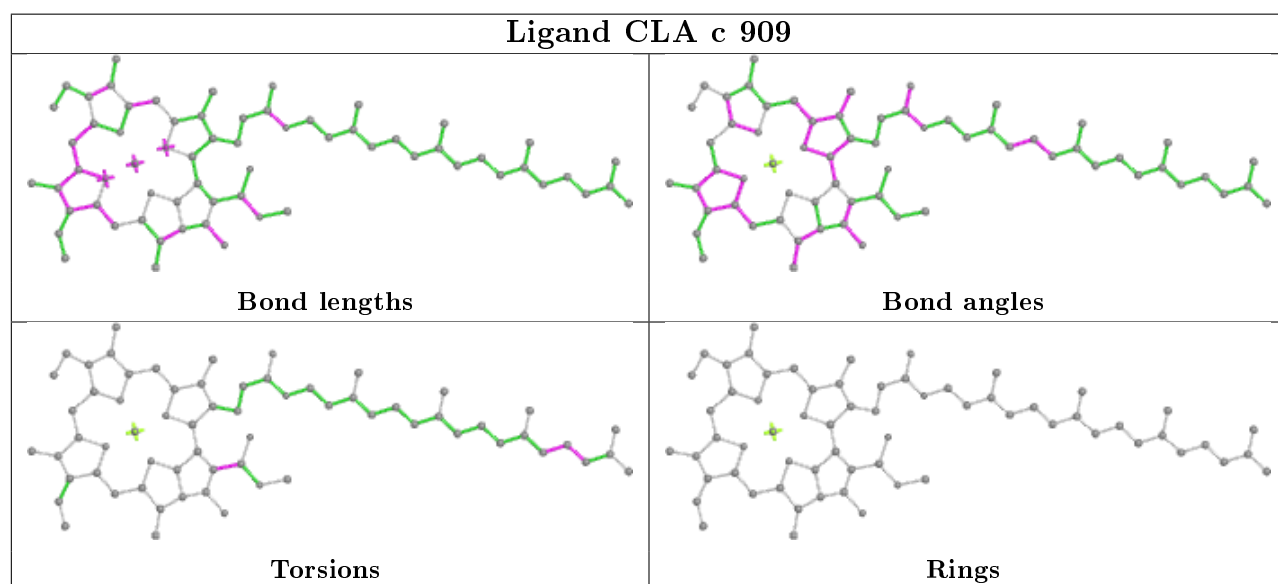
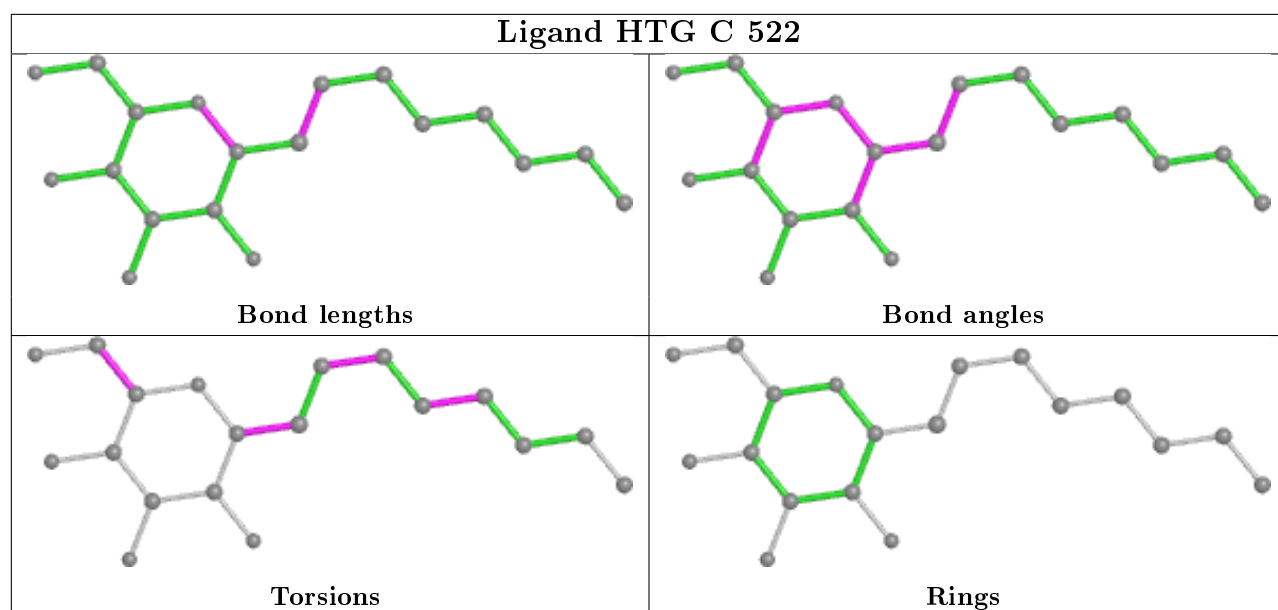


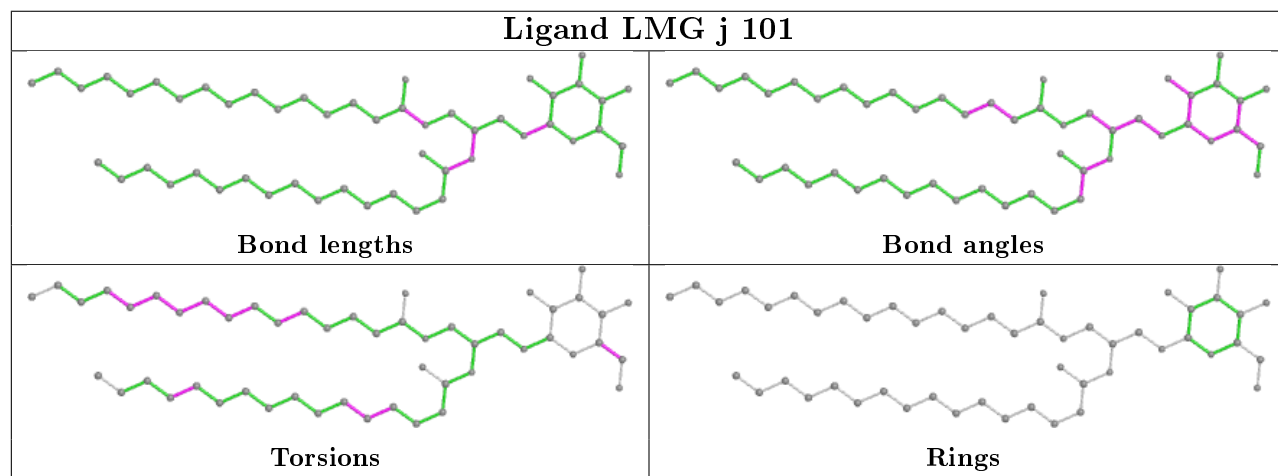
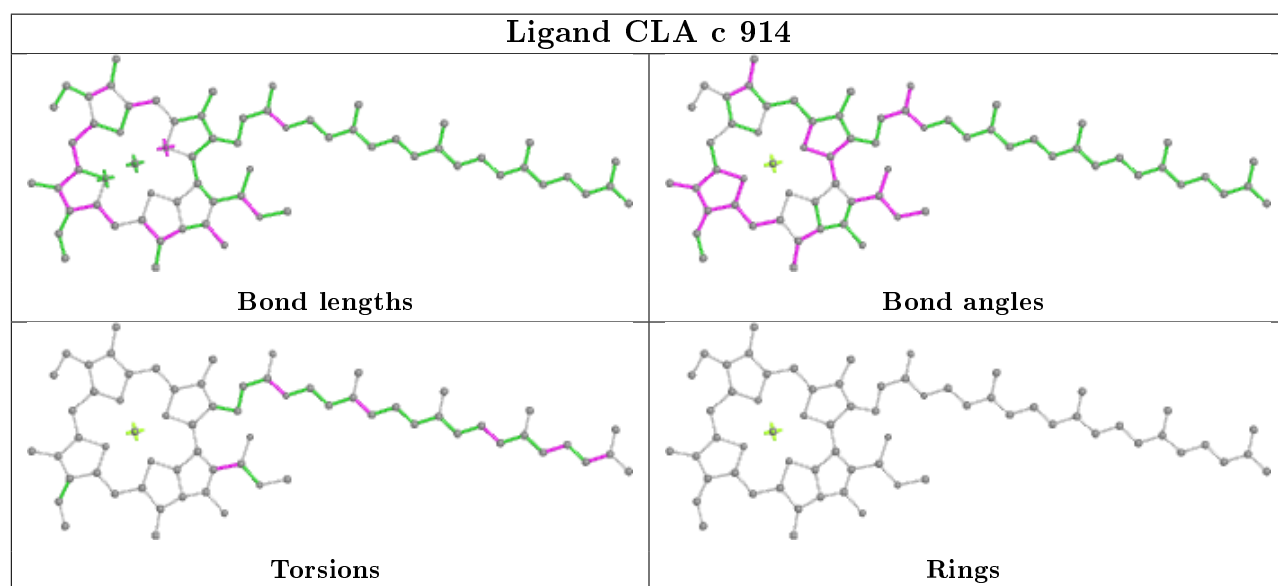
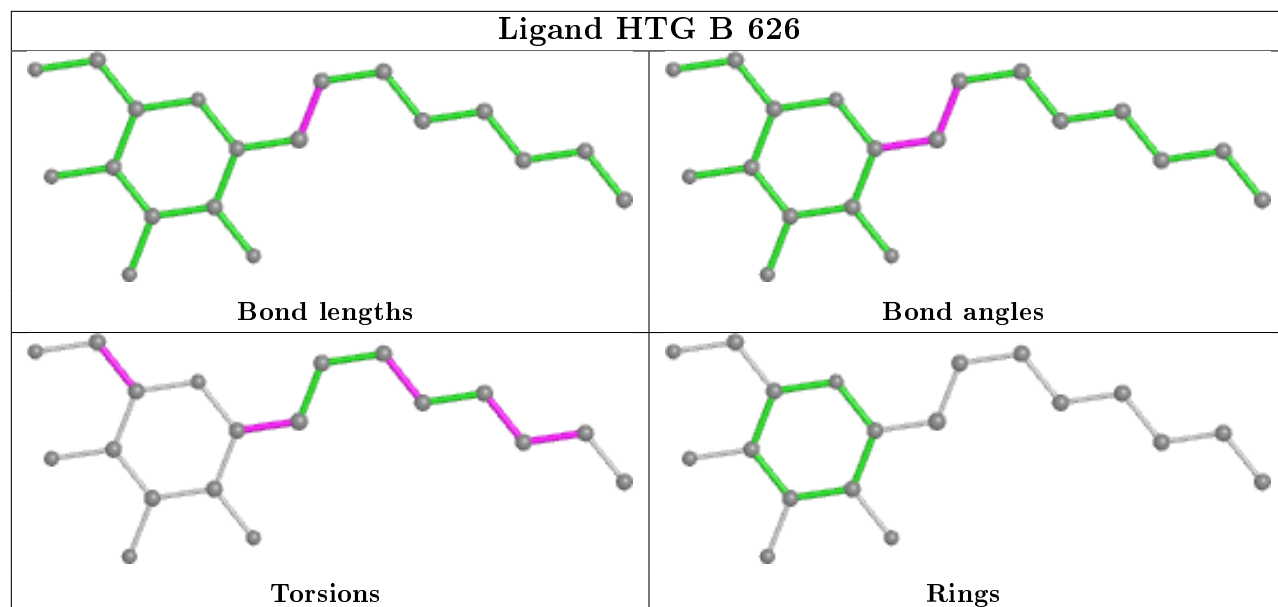


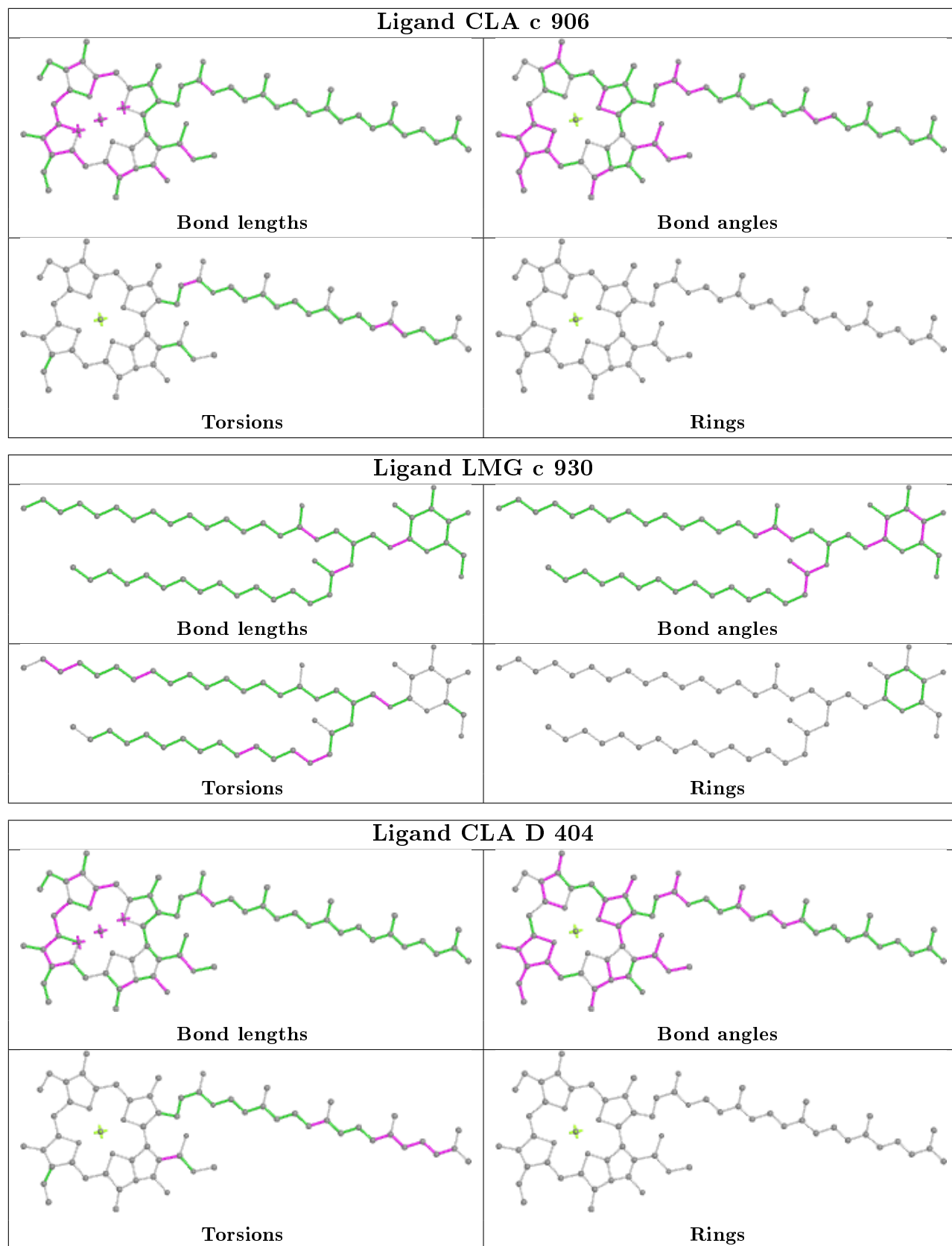


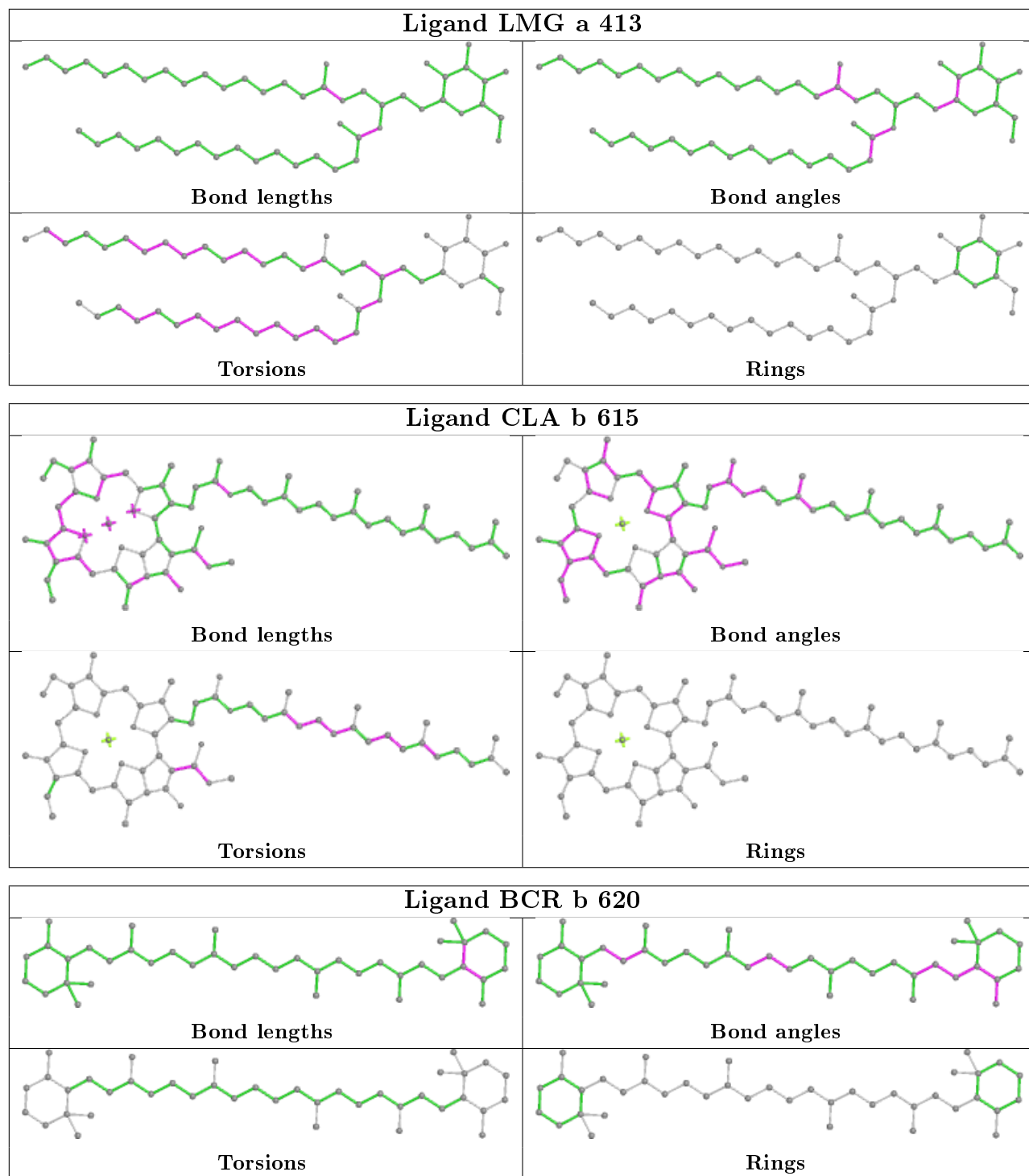


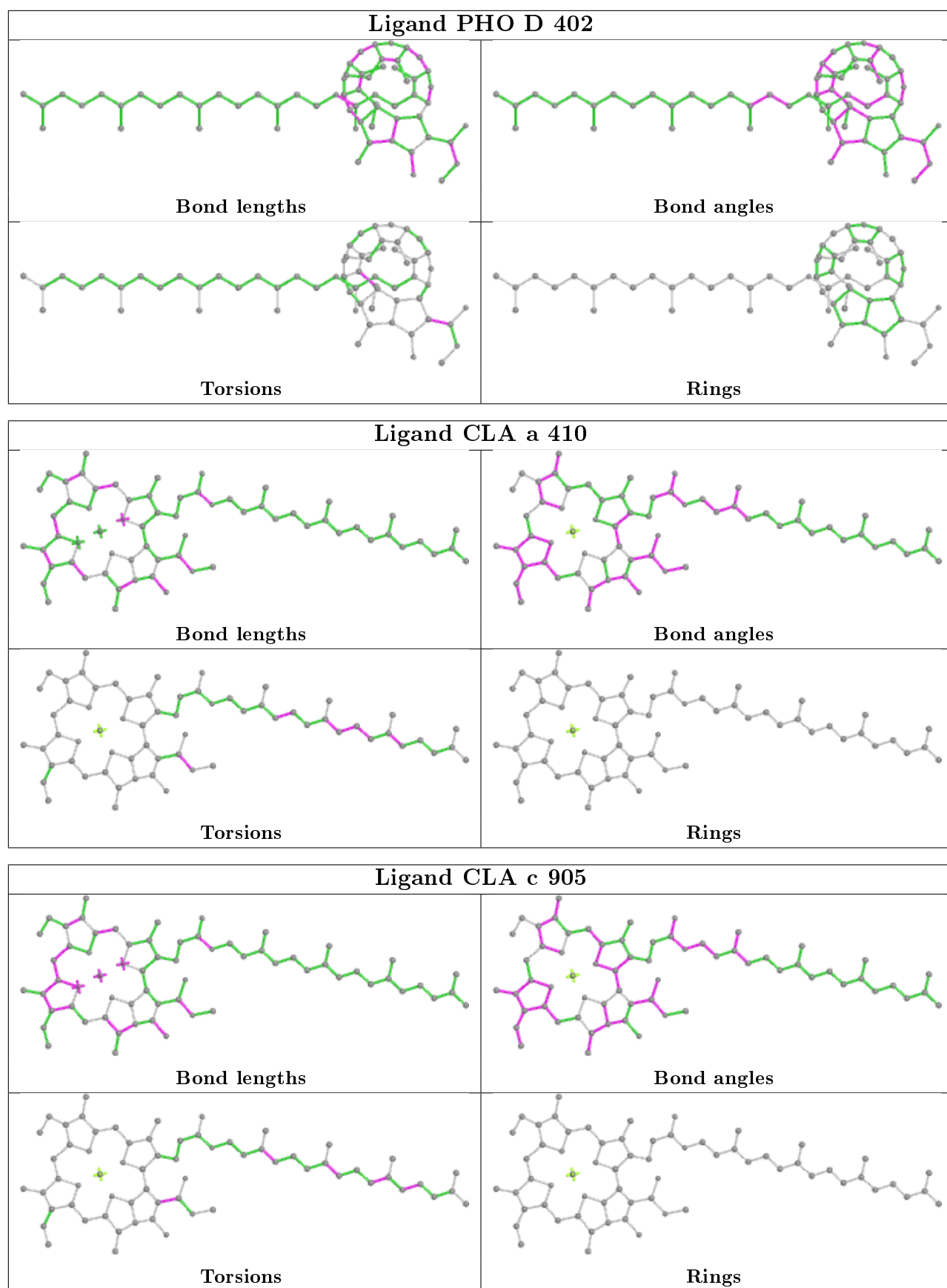


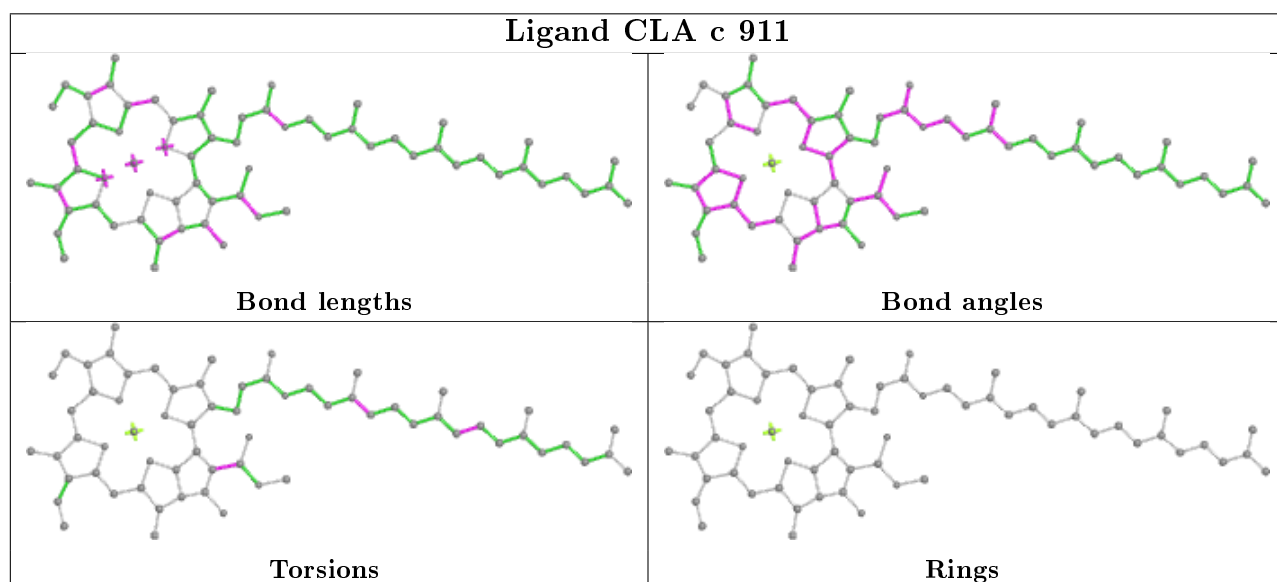
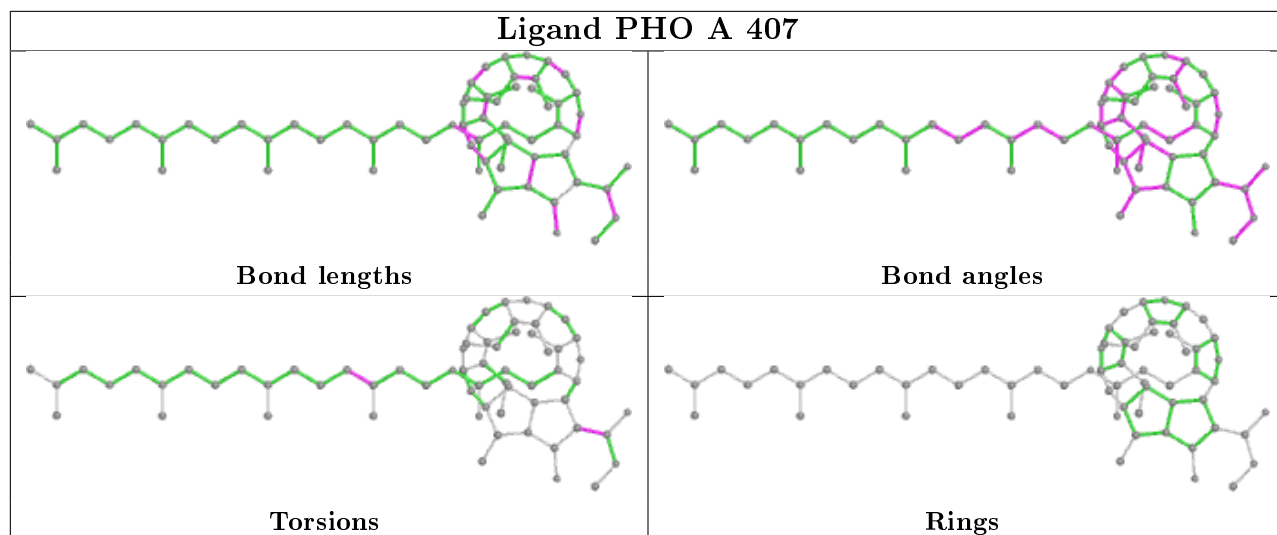


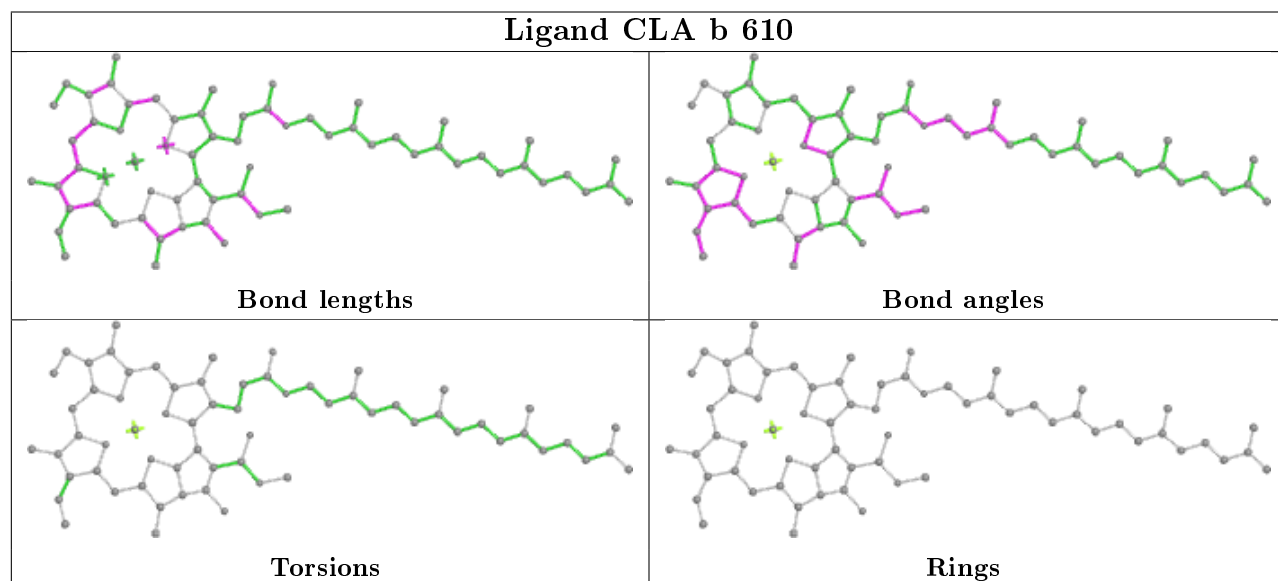
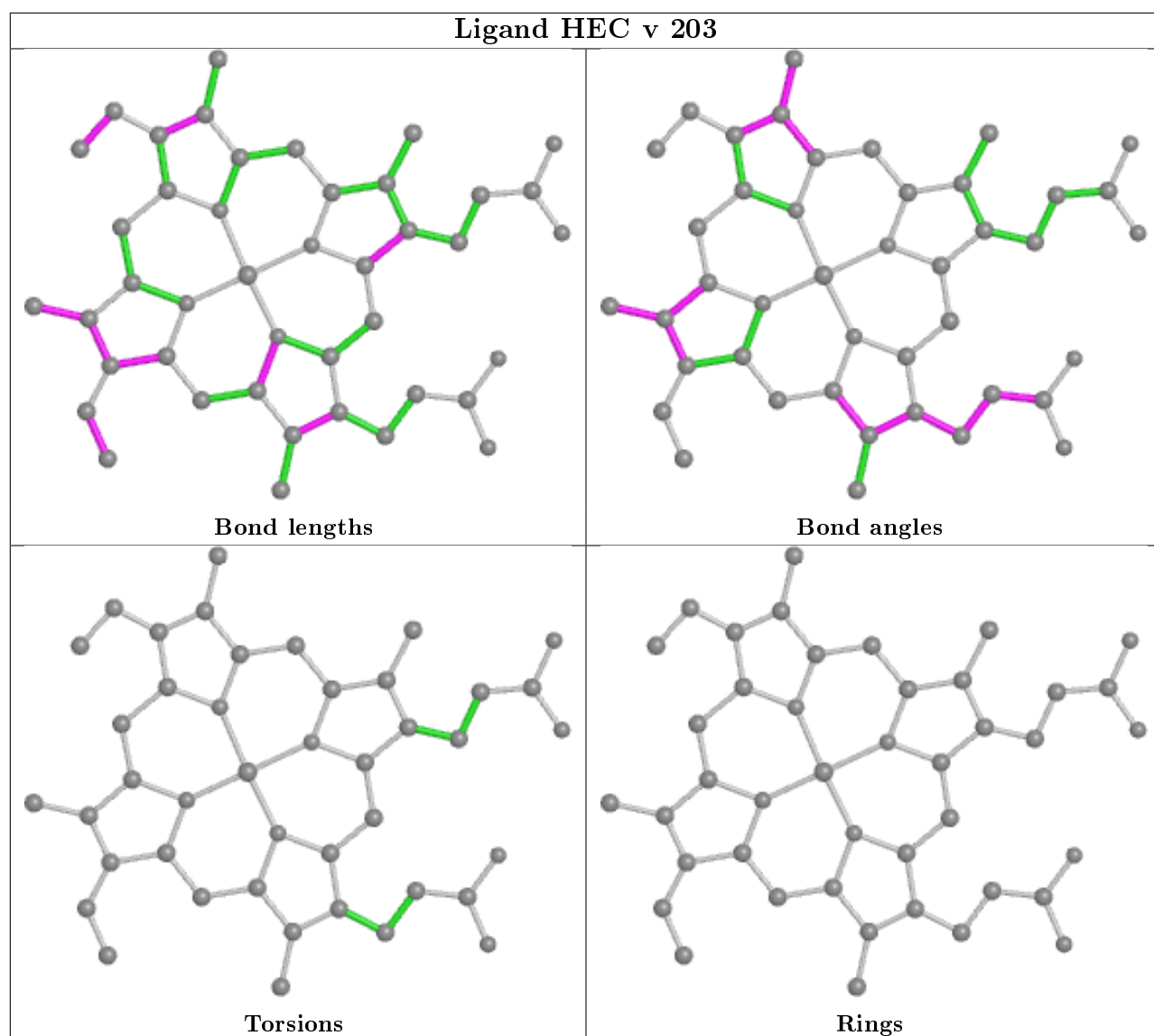


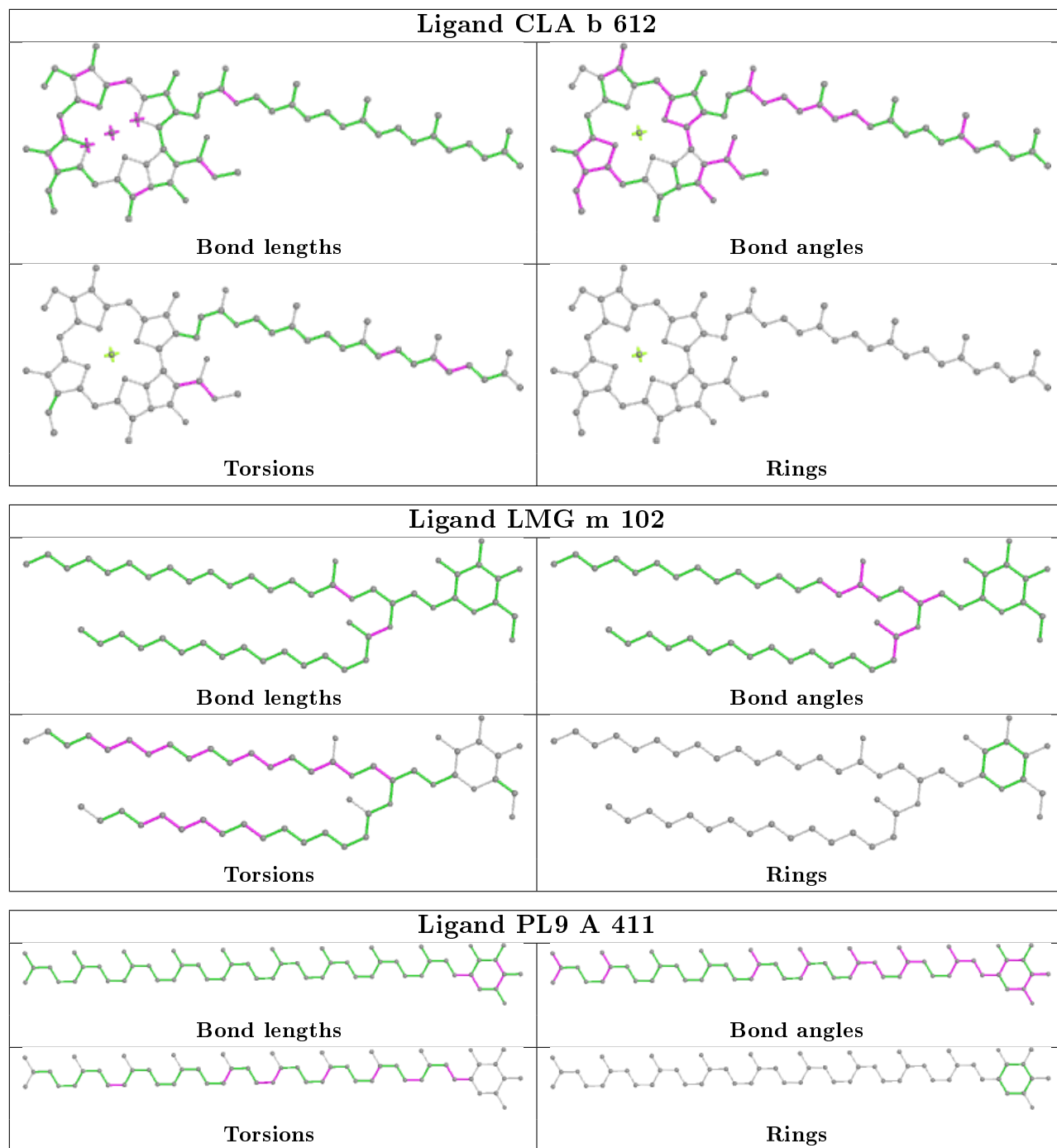


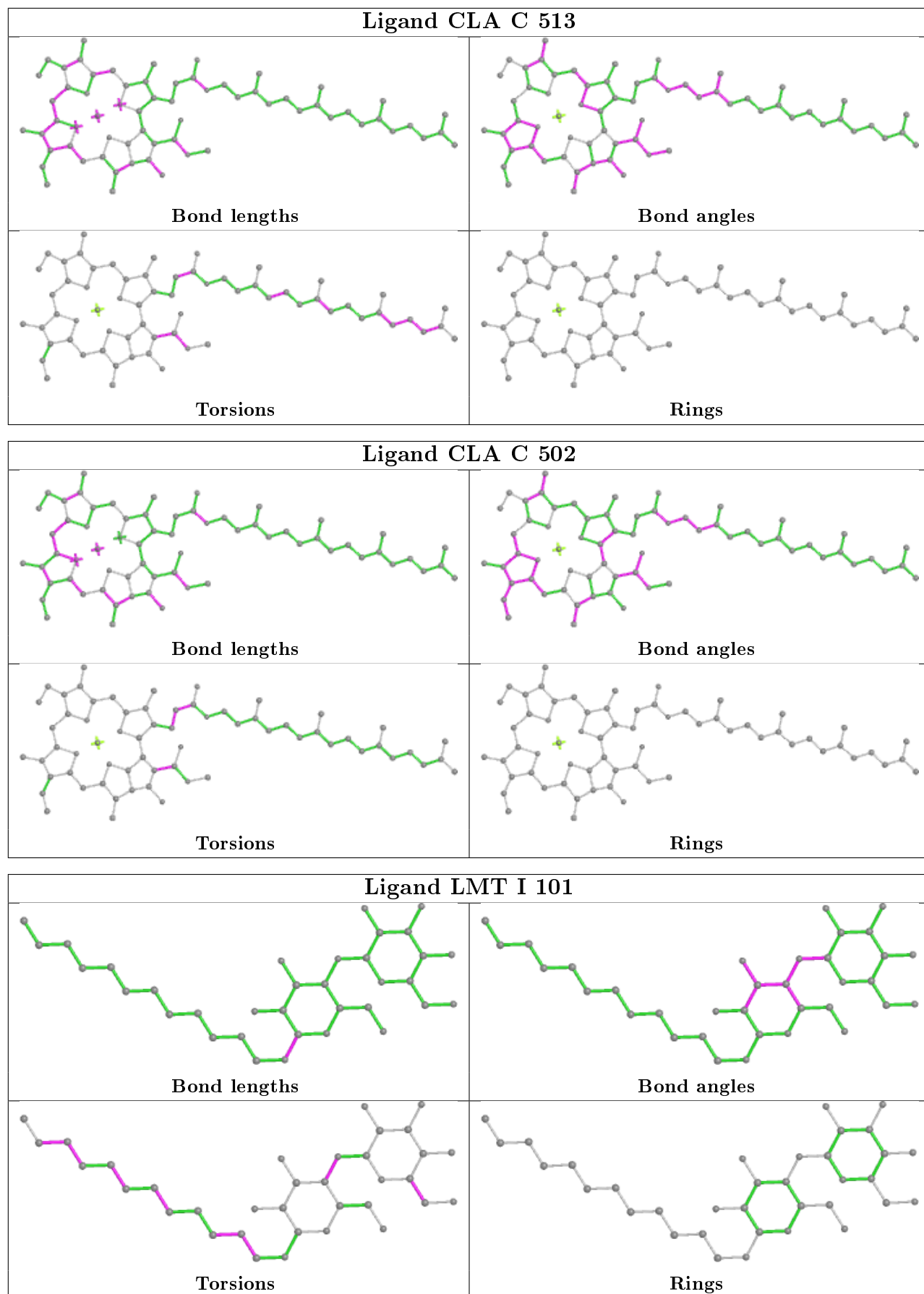












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.25	4 (1%) 79 80	14, 21, 43, 67	0
1	a	334/344 (97%)	-0.09	9 (2%) 54 56	14, 21, 44, 91	0
2	B	505/505 (100%)	0.01	28 (5%) 25 26	17, 26, 50, 81	0
2	b	501/505 (99%)	0.01	32 (6%) 19 20	16, 25, 53, 109	0
3	C	451/455 (99%)	-0.03	14 (3%) 49 50	18, 30, 46, 73	0
3	c	455/455 (100%)	-0.00	16 (3%) 44 45	20, 31, 43, 68	0
4	D	342/342 (100%)	-0.24	3 (0%) 84 85	15, 22, 41, 88	0
4	d	342/342 (100%)	-0.30	3 (0%) 84 85	15, 22, 40, 73	0
5	E	81/83 (97%)	1.43	24 (29%) 0 0	25, 45, 75, 97	0
5	e	79/83 (95%)	0.87	12 (15%) 2 2	28, 42, 67, 87	0
6	F	35/44 (79%)	0.44	6 (17%) 1 1	24, 35, 59, 96	0
6	f	32/44 (72%)	0.04	2 (6%) 20 21	26, 31, 70, 82	0
7	H	63/65 (96%)	0.00	2 (3%) 47 49	24, 34, 44, 77	0
7	h	63/65 (96%)	0.36	5 (7%) 12 13	23, 34, 46, 72	0
8	I	34/38 (89%)	-0.19	0 100 100	27, 35, 58, 77	0
8	i	37/38 (97%)	0.23	3 (8%) 12 13	26, 32, 84, 89	0
9	J	36/40 (90%)	0.21	3 (8%) 11 12	24, 38, 65, 81	0
9	j	40/40 (100%)	0.22	5 (12%) 3 4	24, 36, 69, 76	0
10	K	37/37 (100%)	0.05	2 (5%) 25 27	31, 37, 47, 56	0
10	k	37/37 (100%)	0.24	2 (5%) 25 27	29, 37, 55, 66	0
11	L	37/37 (100%)	-0.10	3 (8%) 12 13	15, 20, 62, 80	0
11	l	36/37 (97%)	-0.04	2 (5%) 24 26	17, 20, 68, 76	0
12	M	34/36 (94%)	-0.16	2 (5%) 22 24	19, 23, 52, 75	0
12	m	34/36 (94%)	0.11	2 (5%) 22 24	19, 24, 53, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	0.08	17 (6%) 16 17	16, 30, 55, 86	0
13	o	243/244 (99%)	0.17	29 (11%) 4 4	16, 32, 65, 86	0
14	T	29/32 (90%)	0.26	1 (3%) 45 46	17, 21, 45, 81	0
14	t	30/32 (93%)	0.29	2 (6%) 17 19	18, 22, 55, 85	0
15	U	97/104 (93%)	-0.22	0 100 100	20, 28, 46, 59	0
15	u	97/104 (93%)	-0.37	1 (1%) 82 83	22, 27, 40, 63	0
16	V	137/137 (100%)	-0.35	0 100 100	20, 26, 41, 59	0
16	v	137/137 (100%)	0.24	10 (7%) 15 16	23, 33, 51, 71	0
17	Y	29/30 (96%)	1.27	9 (31%) 0 0	38, 46, 69, 72	0
17	y	29/30 (96%)	0.85	5 (17%) 1 1	38, 47, 59, 69	0
18	X	38/40 (95%)	0.58	6 (15%) 2 2	29, 39, 58, 62	0
18	x	38/40 (95%)	0.82	6 (15%) 2 2	31, 38, 83, 98	0
19	Z	62/62 (100%)	1.61	21 (33%) 0 0	36, 45, 83, 96	0
19	z	61/62 (98%)	1.65	23 (37%) 0 0	42, 52, 83, 103	0
All	All	5249/5350 (98%)	0.05	314 (5%) 21 23	14, 28, 55, 109	0

All (314) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	b	487	SER	9.4
6	F	11	VAL	8.1
2	b	496	TYR	7.7
19	z	3	ILE	7.5
14	T	30	THR	7.3
18	x	37	VAL	7.2
2	b	503	THR	7.1
2	b	495	PHE	6.9
2	B	494	GLY	6.9
2	B	486	LEU	6.6
5	E	84	LYS	6.5
2	b	493	TRP	6.5
2	B	495	PHE	6.4
19	Z	33	TRP	6.4
2	b	502	VAL	6.3
5	E	79	PHE	6.3
6	F	12	SER	6.2
5	E	83	LEU	6.2

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Mol	Chain	Res	Type	RSRZ
18	x	38	GLN	6.2
13	o	36	GLN	6.1
11	L	1	MET	5.9
14	t	31	LYS	5.9
7	H	64	ALA	5.8
13	o	246	ALA	5.8
1	a	13	LEU	5.7
7	h	64	ALA	5.7
19	z	4	LEU	5.5
1	A	11	ALA	5.5
19	z	2	THR	5.5
19	Z	35	ARG	5.3
2	B	496	TYR	5.3
2	b	484	PRO	5.3
2	b	491	VAL	5.2
17	y	18	VAL	5.2
18	X	37	VAL	5.2
3	C	23	ALA	5.1
2	B	293	ALA	5.0
19	Z	32	ASP	5.0
18	x	39	ARG	5.0
1	a	11	ALA	4.9
18	x	2	THR	4.9
9	j	1	MET	4.9
5	E	82	GLN	4.8
11	L	2	GLU	4.8
19	z	5	PHE	4.8
19	Z	30	PRO	4.8
2	b	504	THR	4.7
17	Y	18	VAL	4.7
9	J	5	GLY	4.7
13	o	35	SER	4.7
19	Z	60	PHE	4.6
6	F	15	ILE	4.6
19	Z	31	GLN	4.5
5	E	74	GLN	4.5
2	B	505	ARG	4.5
6	F	16	PHE	4.5
5	E	17	VAL	4.4
2	B	487	SER	4.4
2	b	494	GLY	4.4
13	o	32	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
5	E	20	TRP	4.3
19	z	7	LEU	4.3
19	Z	41	PHE	4.2
12	M	34	LYS	4.2
3	C	143	TYR	4.2
4	d	11	GLU	4.2
3	C	155[A]	ASN	4.1
2	b	488	PRO	4.1
2	B	506	LYS	4.1
19	Z	3	ILE	4.1
5	e	59	GLU	4.0
10	k	18	PHE	4.0
5	E	80	LEU	4.0
19	Z	4	LEU	3.9
5	E	22	ILE	3.9
11	L	3	PRO	3.9
16	v	16	GLY	3.9
5	E	25	ILE	3.9
19	z	60	PHE	3.9
9	j	2	MET	3.9
17	Y	19	ILE	3.9
17	y	19	ILE	3.9
5	E	81	GLU	3.9
13	o	27	ARG	3.8
13	o	38	TYR	3.8
13	o	4	THR	3.8
2	B	485	GLU	3.8
19	Z	1	MET	3.8
3	C	257	PHE	3.8
12	M	33	GLN	3.8
19	Z	38	GLN	3.7
5	e	72	ALA	3.7
5	e	84	LYS	3.7
18	X	34	ILE	3.7
2	b	295	GLY	3.7
13	o	34	SER	3.7
8	i	37	LEU	3.7
16	v	21	LEU	3.7
9	J	6	GLY	3.7
15	u	8	GLU	3.7
19	z	61	VAL	3.7
2	b	490	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
6	F	13	TYR	3.6
13	o	133	VAL	3.6
2	B	504	THR	3.6
10	k	17	ILE	3.6
5	E	77	GLU	3.6
13	O	60	ARG	3.6
2	b	500	GLY	3.6
19	Z	36	SER	3.6
18	X	2	THR	3.6
19	z	6	GLN	3.5
2	b	499	VAL	3.5
17	y	20	ALA	3.5
5	E	78	THR	3.5
13	o	135	SER	3.5
5	E	6	GLY	3.4
5	E	72	ALA	3.4
13	o	26	ALA	3.4
5	e	25	ILE	3.4
2	B	500	GLY	3.4
3	c	21	ILE	3.4
16	v	14	SER	3.4
5	E	21	VAL	3.4
19	z	1	MET	3.3
9	J	8	ILE	3.3
13	O	25	THR	3.3
2	B	488	PRO	3.3
19	Z	34	ASP	3.3
19	z	38	GLN	3.3
13	o	134	THR	3.3
11	l	3	PRO	3.3
1	A	12	ASN	3.3
16	v	19	ILE	3.3
4	D	11	GLU	3.2
17	y	22	LEU	3.2
2	b	129	GLY	3.2
6	f	14	PRO	3.2
19	z	59	PHE	3.2
19	z	9	LEU	3.2
1	a	15[A]	GLU	3.2
2	b	489	GLU	3.2
4	D	12	ARG	3.1
5	E	61	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
3	c	279	LEU	3.1
18	X	39	ARG	3.1
17	Y	22	LEU	3.1
19	Z	39	LEU	3.1
5	E	73	LYS	3.1
8	i	38	GLU	3.0
2	B	503	THR	3.0
16	v	18	THR	3.0
5	E	76	VAL	3.0
13	O	136	ILE	3.0
19	z	32	ASP	3.0
19	Z	61	VAL	3.0
19	Z	42	LEU	3.0
13	o	60	ARG	3.0
19	Z	2	THR	3.0
5	e	61	ARG	3.0
1	A	16	ARG	3.0
19	z	35	ARG	3.0
2	B	501	ASP	3.0
19	z	39	LEU	2.9
2	B	484	PRO	2.9
13	o	132	ASN	2.9
2	b	492	GLU	2.9
3	c	432	VAL	2.9
19	z	41	PHE	2.9
3	C	259	TRP	2.9
5	e	21	VAL	2.9
13	o	37	THR	2.9
3	c	143	TYR	2.9
13	O	26	ALA	2.9
2	b	292	LEU	2.9
13	O	130	GLN	2.9
17	Y	20	ALA	2.9
1	a	262	TYR	2.9
13	O	87	VAL	2.9
13	o	136	ILE	2.8
13	o	23	ASP	2.8
3	c	433	LEU	2.8
13	O	27	ARG	2.8
5	E	4	THR	2.8
13	o	25	THR	2.8
13	o	87	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
12	m	5	GLN	2.8
1	a	235	TYR	2.8
13	o	30	TYR	2.8
19	z	30	PRO	2.7
19	Z	29	SER	2.7
3	c	434	ALA	2.7
17	y	40	ALA	2.7
19	Z	7	LEU	2.7
3	C	25	ASN	2.7
13	o	33	ASP	2.7
17	Y	21	GLN	2.7
2	b	126	PRO	2.7
13	O	133	VAL	2.7
13	o	204	VAL	2.7
13	o	245	PRO	2.7
4	D	240	ALA	2.6
2	B	483	ASP	2.6
19	z	33	TRP	2.6
4	d	240	ALA	2.6
5	e	6	GLY	2.6
13	o	24	ASP	2.6
13	o	131	PRO	2.6
13	O	30	TYR	2.6
1	a	16	ARG	2.6
13	O	207	ARG	2.6
6	F	14	PRO	2.6
17	Y	40	ALA	2.6
7	h	23	PRO	2.6
4	d	12	ARG	2.5
2	B	499	VAL	2.5
2	b	297	THR	2.5
19	Z	62	VAL	2.5
1	a	12	ASN	2.5
2	B	247	PHE	2.5
2	b	501	ASP	2.5
3	c	20	SER	2.5
18	x	34	ILE	2.5
16	v	5	PRO	2.5
16	v	15	GLU	2.5
2	b	218	LEU	2.5
3	c	207	ARG	2.5
9	j	4	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
13	o	130	GLN	2.4
5	e	32	ILE	2.4
13	O	135	SER	2.4
2	B	298	LEU	2.4
13	O	206	GLY	2.4
2	b	293	ALA	2.4
18	x	36	LYS	2.4
16	v	12	LEU	2.4
2	b	483	ASP	2.4
2	B	253	ALA	2.4
3	c	435	PHE	2.4
3	C	434	ALA	2.4
14	t	30	THR	2.4
2	b	161	LEU	2.3
2	B	296	ALA	2.3
5	e	26	THR	2.3
8	i	36	ASP	2.3
2	B	490	GLN	2.3
7	h	57	GLY	2.3
13	o	58	ASN	2.3
9	j	6	GLY	2.3
19	Z	57	LEU	2.3
5	E	71	GLU	2.3
3	C	431	PHE	2.3
1	A	243	GLU	2.3
2	B	295	GLY	2.3
3	C	252	ILE	2.3
1	a	230	THR	2.3
2	B	489	GLU	2.3
9	j	5	GLY	2.3
3	C	255	THR	2.3
10	K	14	ALA	2.3
13	o	89	SER	2.3
5	E	18	ARG	2.2
7	h	56	ASP	2.2
5	e	23	HIS	2.2
2	B	479	PHE	2.2
5	e	79	PHE	2.2
6	f	16	PHE	2.2
2	B	297	THR	2.2
2	B	497	GLN	2.2
16	v	8	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	c	436	PHE	2.2
13	O	204	VAL	2.2
19	z	58	ASN	2.2
18	X	33	GLN	2.2
19	z	57	LEU	2.2
5	E	19	TYR	2.2
19	z	10	ALA	2.2
2	b	479	PHE	2.2
3	c	146	PHE	2.2
12	m	33	GLN	2.2
3	c	257	PHE	2.1
3	c	201	ASN	2.1
5	E	32	ILE	2.1
2	b	461	LEU	2.1
3	C	253	LEU	2.1
19	z	42	LEU	2.1
2	B	248	ALA	2.1
3	C	256	PRO	2.1
1	a	243	GLU	2.1
3	C	285	ILE	2.1
7	h	22	ALA	2.1
2	b	294	SER	2.1
13	O	132	ASN	2.1
2	b	246	PHE	2.1
3	C	146	PHE	2.1
3	c	200	THR	2.1
17	Y	34	MET	2.1
10	K	17	ILE	2.1
13	O	89	SER	2.1
18	X	3	ILE	2.1
11	l	2	GLU	2.1
13	o	139	SER	2.1
13	O	23	ASP	2.0
16	v	26	TYR	2.0
2	b	298	LEU	2.0
3	c	426	LEU	2.0
5	e	14	ILE	2.0
13	O	24	ASP	2.0
19	z	29	SER	2.0
17	Y	42	ARG	2.0
2	b	459	ALA	2.0
3	c	181	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
7	H	56[A]	ASP	2.0
17	Y	30	ILE	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	0.97	0.07	19,26,45,49	0
8	FME	I	1	10/11	0.97	0.09	27,32,36,36	0
14	FME	t	1	10/11	0.97	0.08	18,24,45,50	0
8	FME	i	1	10/11	0.98	0.08	28,29,33,33	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
31	DMS	i	106	4/4	0.18	0.33	120,121,124,138	0
29	UNL	b	630	16/-	0.38	0.34	74,86,106,110	0
29	UNL	b	631	16/-	0.41	0.23	61,73,81,82	0
31	DMS	b	644	4/4	0.46	0.39	73,76,78,96	0
29	UNL	B	634	16/-	0.50	0.27	73,80,95,97	0
29	UNL	I	104	16/-	0.50	0.29	69,76,89,92	0
31	DMS	V	211	4/4	0.52	0.36	61,61,68,79	0
28	LHG	a	415	49/49	0.53	0.34	56,72,99,108	0
29	UNL	J	105	11/-	0.54	0.27	61,67,75,78	0
29	UNL	J	104	16/-	0.54	0.37	62,82,99,99	0
29	UNL	B	629	14/-	0.55	0.28	62,72,81,82	0
29	UNL	B	633	16/-	0.59	0.30	61,80,87,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
29	UNL	b	632	16/-	0.59	0.34	58,83,101,101	0
31	DMS	U	203	4/4	0.59	0.32	70,74,80,89	0
35	HTG	D	414	19/19	0.59	0.37	76,92,111,112	0
35	HTG	b	628	19/19	0.60	0.22	52,96,109,112	0
28	LHG	e	101	40/49	0.61	0.25	55,93,121,126	0
31	DMS	U	204	4/4	0.61	0.22	53,62,62,80	0
36	DGD	D	407	50/66	0.61	0.31	54,71,97,97	0
28	LHG	A	412	49/49	0.62	0.35	59,83,104,111	0
29	UNL	A	414	13/-	0.62	0.34	58,71,83,83	0
28	LHG	d	402	44/49	0.62	0.23	59,78,125,135	0
29	UNL	i	104	16/-	0.63	0.35	69,76,78,79	0
36	DGD	d	407	50/66	0.63	0.26	58,74,97,98	0
29	UNL	b	626	16/-	0.63	0.28	59,68,73,73	0
29	UNL	H	104	14/-	0.64	0.42	64,69,74,76	0
35	HTG	B	631	19/19	0.64	0.22	41,88,97,100	0
31	DMS	c	936	4/4	0.65	0.29	80,80,81,90	0
35	HTG	d	413	19/19	0.65	0.27	62,86,104,106	0
30	LMT	F	101	35/35	0.66	0.38	64,88,93,96	0
34	LMG	D	412	51/55	0.66	0.25	37,65,106,119	0
35	HTG	B	626	19/19	0.66	0.46	52,88,96,96	0
35	HTG	c	922	19/19	0.67	0.41	53,84,96,100	0
31	DMS	A	419	4/4	0.67	0.37	75,76,91,97	0
31	DMS	O	304	4/4	0.67	0.26	69,71,78,87	0
28	LHG	K	101	44/49	0.67	0.32	63,93,124,137	0
26	SQD	B	621	54/54	0.68	0.24	43,63,88,93	0
29	UNL	E	102	16/-	0.68	0.39	58,61,76,77	0
35	HTG	c	923	13/19	0.68	0.34	59,72,86,87	0
35	HTG	v	204	19/19	0.69	0.33	62,70,81,91	0
28	LHG	E	101	49/49	0.70	0.28	39,83,104,109	0
31	DMS	b	642	4/4	0.70	0.34	90,90,97,101	0
30	LMT	Z	101	35/35	0.70	0.25	41,88,100,102	0
29	UNL	E	104	16/-	0.71	0.23	67,71,74,76	0
30	LMT	b	621	25/35	0.71	0.19	45,70,90,91	0
30	LMT	B	643	24/35	0.71	0.23	50,77,114,118	0
29	UNL	E	103	13/-	0.71	0.33	63,68,85,87	0
30	LMT	m	103	35/35	0.71	0.19	48,92,102,103	0
30	LMT	M	101	35/35	0.71	0.22	31,50,59,60	0
27	PL9	a	414	55/55	0.72	0.24	46,61,86,88	0
29	UNL	e	102	16/-	0.72	0.38	54,61,69,72	0
35	HTG	C	522	19/19	0.72	0.35	41,78,86,87	0
29	UNL	z	102	13/-	0.72	0.23	53,62,72,75	0
31	DMS	k	103	4/4	0.72	0.33	90,92,93,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
29	UNL	I	103	16/-	0.72	0.28	51,57,70,74	0
29	UNL	B	628	10/-	0.73	0.42	62,67,70,71	0
31	DMS	o	304	4/4	0.73	0.28	63,68,70,84	0
29	UNL	i	103	16/-	0.73	0.33	58,61,67,70	0
27	PL9	A	411	55/55	0.73	0.25	45,59,80,84	0
29	UNL	i	102	16/-	0.73	0.21	52,62,75,76	0
30	LMT	a	418	35/35	0.73	0.23	44,63,79,80	0
31	DMS	b	638	4/4	0.74	0.20	54,60,67,74	0
30	LMT	B	623	35/35	0.74	0.21	48,72,89,93	0
30	LMT	m	104	35/35	0.74	0.20	34,51,56,58	0
29	UNL	Z	103	9/-	0.75	0.22	50,61,69,70	0
30	LMT	e	103	25/35	0.75	0.32	60,77,93,95	0
26	SQD	L	102	54/54	0.75	0.20	42,58,87,90	0
29	UNL	Z	102	14/-	0.76	0.32	63,67,74,76	0
29	UNL	t	102	16/-	0.76	0.37	53,62,74,75	0
29	UNL	k	101	8/-	0.76	0.18	59,71,78,80	0
34	LMG	C	531	51/55	0.76	0.22	38,78,93,98	0
31	DMS	u	206	4/4	0.76	0.30	70,71,76,93	0
29	UNL	B	632	16/-	0.76	0.25	44,61,68,70	0
29	UNL	a	416	10/-	0.77	0.33	54,68,75,76	0
34	LMG	d	411	51/55	0.77	0.23	39,70,101,108	0
30	LMT	I	101	35/35	0.77	0.30	63,75,85,91	0
34	LMG	c	930	51/55	0.77	0.22	33,69,81,84	0
29	UNL	B	635	9/-	0.77	0.20	60,67,76,77	0
31	DMS	a	401	4/4	0.78	0.27	75,81,85,96	0
30	LMT	z	101	32/35	0.78	0.23	43,88,96,99	0
31	DMS	O	307	4/4	0.79	0.21	64,69,69,84	0
29	UNL	u	202	16/-	0.79	0.28	41,54,60,62	0
29	UNL	U	201	14/-	0.79	0.26	38,50,58,61	0
35	HTG	b	623	19/19	0.80	0.25	47,76,83,84	0
31	DMS	h	105	4/4	0.80	0.19	76,83,89,90	0
31	DMS	c	933	4/4	0.80	0.17	61,64,65,77	0
29	UNL	T	102	13/-	0.80	0.50	62,68,75,75	0
31	DMS	B	647	4/4	0.80	0.37	81,85,85,89	0
29	UNL	j	103	16/-	0.81	0.17	45,56,61,62	0
29	UNL	u	201	11/-	0.81	0.28	39,50,60,61	0
31	DMS	b	646	4/4	0.81	0.36	84,87,89,96	0
29	UNL	a	419	6/-	0.81	0.36	47,53,53,53	0
34	LMG	a	413	51/55	0.81	0.19	41,53,68,74	0
31	DMS	c	929	4/4	0.81	0.43	46,62,67,70	0
26	SQD	a	417	54/54	0.81	0.17	38,53,72,73	0
30	LMT	A	416	35/35	0.82	0.20	42,63,86,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	LMT	B	644	24/35	0.82	0.21	34,52,81,87	0
35	HTG	C	523	19/19	0.82	0.29	60,78,95,97	0
29	UNL	J	103	16/-	0.82	0.17	46,54,60,63	0
31	DMS	V	207	4/4	0.82	0.15	51,52,60,62	0
29	UNL	c	931	10/-	0.82	0.22	55,60,62,64	0
29	UNL	B	627	16/-	0.82	0.15	38,45,55,60	0
31	DMS	b	645	4/4	0.82	0.46	70,77,83,84	0
34	LMG	m	102	51/55	0.83	0.19	33,41,54,61	0
29	UNL	I	102	13/-	0.83	0.16	47,53,65,69	0
31	DMS	b	643	4/4	0.83	0.32	81,82,85,85	0
26	SQD	A	415	54/54	0.83	0.18	39,54,72,76	0
31	DMS	A	421	4/4	0.83	0.25	57,63,74,78	0
34	LMG	C	501	51/55	0.83	0.20	37,51,63,70	0
31	DMS	H	101	4/4	0.83	0.28	54,58,62,65	0
30	LMT	a	422	35/35	0.83	0.35	61,74,82,85	0
29	UNL	d	417	11/-	0.83	0.17	48,63,69,71	0
34	LMG	C	520	51/55	0.84	0.20	31,61,74,79	0
30	LMT	T	103	24/35	0.84	0.20	34,56,76,83	0
29	UNL	X	101	16/-	0.84	0.17	33,37,60,61	0
26	SQD	x	101	41/54	0.84	0.24	54,76,95,101	0
31	DMS	B	641	4/4	0.84	0.21	62,63,65,66	0
31	DMS	O	311	4/4	0.84	0.27	59,59,71,73	0
29	UNL	b	629	12/-	0.84	0.34	49,59,70,71	0
31	DMS	b	639	4/4	0.84	0.26	41,55,63,67	0
35	HTG	c	921	19/19	0.84	0.21	68,82,88,91	0
34	LMG	c	920	51/55	0.84	0.19	27,55,81,84	0
31	DMS	O	308	4/4	0.85	0.27	54,64,77,81	0
35	HTG	B	625	19/19	0.85	0.17	28,42,49,51	0
31	DMS	O	309	4/4	0.85	0.22	53,63,64,70	0
31	DMS	B	646	4/4	0.85	0.19	76,77,77,84	0
34	LMG	B	622	51/55	0.85	0.17	31,41,52,67	0
31	DMS	B	645	4/4	0.85	0.24	50,61,64,69	0
26	SQD	D	408	45/54	0.85	0.29	45,67,86,93	0
31	DMS	c	935	4/4	0.86	0.28	71,72,75,83	0
31	DMS	b	640	4/4	0.86	0.19	67,70,78,83	0
31	DMS	c	934	4/4	0.86	0.27	87,87,89,99	0
31	DMS	D	417	4/4	0.86	0.23	53,54,58,59	0
29	UNL	b	625	10/-	0.86	0.28	44,59,68,68	0
31	DMS	O	310	4/4	0.86	0.25	61,67,74,76	0
31	DMS	B	649	4/4	0.86	0.28	70,71,73,84	0
31	DMS	b	647	4/4	0.87	0.29	67,78,85,86	0
29	UNL	x	103	15/-	0.87	0.17	31,40,57,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	DMS	d	419	4/4	0.87	0.23	63,70,76,82	0
31	DMS	h	104	4/4	0.87	0.26	97,99,103,103	0
35	HTG	B	630	19/19	0.87	0.13	41,55,62,66	0
29	UNL	C	532	11/-	0.88	0.23	54,59,66,66	0
31	DMS	A	418	4/4	0.88	0.28	70,79,79,85	0
35	HTG	b	622	19/19	0.88	0.23	28,41,57,64	0
23	CLA	B	610	65/65	0.88	0.13	21,28,32,34	0
31	DMS	l	102	4/4	0.88	0.14	64,65,70,84	0
31	DMS	a	421	4/4	0.88	0.28	81,84,85,92	0
38	RRX	x	102	41/41	0.88	0.13	23,29,46,52	0
29	UNL	b	624	16/-	0.88	0.13	42,51,58,60	0
31	DMS	U	202	4/4	0.88	0.22	33,45,50,55	0
36	DGD	h	102	62/66	0.88	0.18	24,31,41,47	0
29	UNL	d	412	16/-	0.89	0.25	31,40,54,57	0
35	HTG	b	627	19/19	0.89	0.14	39,59,72,82	0
31	DMS	H	105	4/4	0.89	0.26	60,74,74,84	0
31	DMS	b	637	4/4	0.89	0.31	61,63,68,74	0
31	DMS	C	529	4/4	0.89	0.29	54,66,72,74	0
31	DMS	v	208	4/4	0.89	0.22	54,67,71,87	0
38	RRX	H	102	41/41	0.89	0.13	25,29,38,44	0
23	CLA	C	514	65/65	0.89	0.15	37,47,67,72	0
31	DMS	B	640	4/4	0.89	0.24	50,56,60,61	0
31	DMS	b	635	4/4	0.89	0.17	53,63,69,71	0
23	CLA	C	507	65/65	0.90	0.13	25,42,79,81	0
35	HTG	V	204	14/19	0.90	0.18	42,45,71,82	0
35	HTG	C	521	19/19	0.90	0.19	61,66,74,77	0
31	DMS	v	206	4/4	0.90	0.26	66,68,76,78	0
26	SQD	A	410	54/54	0.90	0.17	31,55,74,80	0
31	DMS	A	424	4/4	0.90	0.20	53,54,58,69	0
31	DMS	V	210	4/4	0.90	0.16	64,65,67,73	0
31	DMS	V	205	4/4	0.90	0.23	49,60,60,63	0
31	DMS	d	418	4/4	0.90	0.28	68,69,71,71	0
29	UNL	M	102	11/-	0.90	0.21	45,50,63,69	0
23	CLA	b	610	65/65	0.91	0.11	22,27,31,39	0
31	DMS	V	202	4/4	0.91	0.16	31,32,38,48	0
31	DMS	u	205	4/4	0.91	0.21	41,50,54,58	0
29	UNL	i	101	16/-	0.91	0.13	37,43,60,60	0
31	DMS	C	528	4/4	0.91	0.16	60,63,65,66	0
26	SQD	a	412	54/54	0.91	0.15	31,53,72,76	0
31	DMS	B	642	4/4	0.91	0.30	46,54,59,67	0
31	DMS	C	526	4/4	0.92	0.16	49,56,57,62	0
29	UNL	D	413	16/-	0.92	0.21	36,42,57,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	b	602	65/65	0.92	0.17	29,42,66,71	0
31	DMS	h	103	4/4	0.92	0.16	82,84,97,101	0
31	DMS	u	204	4/4	0.92	0.14	62,68,68,73	0
36	DGD	H	103	62/66	0.92	0.18	23,32,38,39	0
31	DMS	v	209	4/4	0.92	0.15	49,50,58,64	0
23	CLA	c	914	65/65	0.92	0.12	36,44,76,80	0
29	UNL	A	417	4/-	0.92	0.51	58,61,63,67	0
29	UNL	m	101	11/-	0.92	0.18	47,51,56,58	0
23	CLA	c	913	65/65	0.92	0.12	30,39,65,68	0
31	DMS	C	527	4/4	0.92	0.19	58,68,73,83	0
23	CLA	B	603	65/65	0.92	0.13	20,26,33,36	0
28	LHG	D	409	49/49	0.93	0.15	27,34,41,47	0
31	DMS	C	525	4/4	0.93	0.19	39,39,43,46	0
31	DMS	A	422	4/4	0.93	0.19	65,68,68,71	0
31	DMS	V	208	4/4	0.93	0.13	69,70,71,72	0
36	DGD	C	518	62/66	0.93	0.13	24,33,70,80	0
23	CLA	C	513	65/65	0.93	0.10	34,42,73,76	0
23	CLA	b	603	65/65	0.93	0.12	21,24,33,41	0
34	LMG	J	101	51/55	0.93	0.17	25,31,85,93	0
31	DMS	d	415	4/4	0.93	0.21	45,53,57,73	0
35	HTG	B	624	19/19	0.93	0.12	35,39,46,47	0
25	BCR	C	515	40/40	0.93	0.09	35,43,46,48	0
29	UNL	A	413	16/-	0.93	0.14	38,43,70,76	0
23	CLA	B	602	65/65	0.93	0.19	28,39,75,85	0
31	DMS	c	927	4/4	0.93	0.15	30,37,37,44	0
31	DMS	v	202	4/4	0.93	0.17	68,74,76,81	0
31	DMS	a	420	4/4	0.93	0.32	48,61,64,66	0
23	CLA	c	904	65/65	0.93	0.15	25,32,37,40	0
35	HTG	O	302	19/19	0.93	0.12	36,39,48,49	0
31	DMS	b	641	4/4	0.93	0.21	52,59,66,66	0
25	BCR	k	102	40/40	0.93	0.11	27,32,38,40	0
31	DMS	B	648	4/4	0.93	0.31	43,45,47,48	0
23	CLA	b	607	65/65	0.93	0.11	22,27,54,63	0
23	CLA	c	907	65/65	0.93	0.10	23,36,73,76	0
31	DMS	h	101	4/4	0.94	0.17	47,51,52,53	0
31	DMS	u	203	4/4	0.94	0.21	38,50,51,52	0
28	LHG	l	101	49/49	0.94	0.15	20,28,48,52	0
23	CLA	D	404	65/65	0.94	0.13	23,27,67,73	0
34	LMG	j	101	51/55	0.94	0.10	22,33,80,85	0
25	BCR	c	915	40/40	0.94	0.10	36,44,48,50	0
23	CLA	C	508	65/65	0.94	0.10	28,35,49,55	0
36	DGD	c	919	62/66	0.94	0.11	22,29,50,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	DMS	V	209	4/4	0.94	0.12	58,59,62,65	0
23	CLA	b	617	65/65	0.94	0.12	20,30,81,89	0
23	CLA	B	607	65/65	0.94	0.10	20,26,53,60	0
31	DMS	i	105	4/4	0.94	0.24	61,64,71,73	0
25	BCR	C	516	40/40	0.94	0.12	28,34,40,43	0
31	DMS	o	303	4/4	0.94	0.23	51,55,67,70	0
28	LHG	L	101	49/49	0.94	0.12	22,31,42,48	0
31	DMS	a	423	4/4	0.94	0.17	53,56,63,73	0
31	DMS	C	533	4/4	0.94	0.17	67,67,68,71	0
28	LHG	d	408	49/49	0.94	0.20	25,33,43,44	0
23	CLA	C	512	65/65	0.94	0.08	26,34,39,40	0
31	DMS	d	414	4/4	0.94	0.11	62,66,71,78	0
31	DMS	O	303	4/4	0.94	0.21	59,66,69,73	0
33	CA	o	302	1/1	0.94	0.06	43,43,43,43	0
31	DMS	v	210	4/4	0.94	0.21	62,65,68,72	0
25	BCR	c	916	40/40	0.94	0.10	25,32,38,38	0
23	CLA	c	909	65/65	0.95	0.16	22,26,79,92	0
23	CLA	C	510	65/65	0.95	0.12	25,31,52,55	0
23	CLA	B	616	65/65	0.95	0.10	23,27,43,49	0
32	BCT	A	420	4/4	0.95	0.06	31,32,35,40	0
23	CLA	C	509	65/65	0.95	0.13	24,29,76,85	0
25	BCR	b	620	40/40	0.95	0.11	25,29,40,44	0
25	BCR	a	411	40/40	0.95	0.08	20,23,27,28	0
25	BCR	C	530	40/40	0.95	0.08	27,32,36,37	0
23	CLA	c	908	65/65	0.95	0.11	23,28,46,54	0
31	DMS	c	932	4/4	0.95	0.32	54,57,63,64	0
31	DMS	O	305	4/4	0.95	0.41	65,70,70,77	0
23	CLA	C	502	65/65	0.95	0.14	25,31,41,51	0
25	BCR	D	405	40/40	0.95	0.16	22,28,54,57	0
31	DMS	B	638	4/4	0.95	0.17	55,60,62,71	0
31	DMS	e	104	4/4	0.95	0.11	72,73,78,83	0
31	DMS	c	937	4/4	0.95	0.31	76,80,84,84	0
31	DMS	v	205	4/4	0.95	0.11	63,66,68,69	0
23	CLA	b	616	65/65	0.95	0.09	21,26,42,44	0
36	DGD	C	519	62/66	0.95	0.12	21,28,68,83	0
23	CLA	c	903	65/65	0.95	0.18	20,24,37,43	0
33	CA	O	301	1/1	0.95	0.08	42,42,42,42	0
36	DGD	c	917	62/66	0.95	0.15	20,30,74,77	0
36	DGD	C	517	62/66	0.95	0.17	21,29,69,71	0
25	BCR	t	101	40/40	0.95	0.14	19,26,38,40	0
31	DMS	b	636	4/4	0.95	0.17	44,48,50,52	0
37	HEM	E	105	43/43	0.95	0.12	36,42,46,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
28	LHG	d	409	49/49	0.95	0.13	18,24,44,47	0
31	DMS	B	639	4/4	0.95	0.15	44,48,51,54	0
25	BCR	B	620	40/40	0.95	0.09	21,29,41,42	0
25	BCR	j	104	40/40	0.95	0.08	27,32,39,43	0
31	DMS	V	206	4/4	0.95	0.25	55,55,55,61	0
23	CLA	c	906	65/65	0.95	0.10	25,29,44,47	0
25	BCR	d	405	40/40	0.95	0.10	21,27,50,54	0
25	BCR	Y	101	40/40	0.95	0.09	29,33,40,41	0
23	CLA	c	905	65/65	0.95	0.16	21,27,51,54	0
31	DMS	O	306	4/4	0.95	0.28	68,68,73,76	0
23	CLA	C	504	65/65	0.95	0.10	24,31,36,41	0
36	DGD	c	918	62/66	0.95	0.13	24,30,75,84	0
23	CLA	C	505	65/65	0.96	0.13	25,28,58,60	0
23	CLA	c	910	65/65	0.96	0.17	23,27,49,60	0
27	PL9	d	406	55/55	0.96	0.12	16,21,27,34	0
23	CLA	c	912	65/65	0.96	0.09	26,31,37,41	0
25	BCR	T	101	40/40	0.96	0.16	22,29,40,41	0
25	BCR	b	618	40/40	0.96	0.13	20,25,32,33	0
25	BCR	b	619	40/40	0.96	0.18	20,27,41,43	0
25	BCR	B	618	40/40	0.96	0.13	19,24,30,33	0
23	CLA	b	615	65/65	0.96	0.14	19,24,71,76	0
23	CLA	b	605	65/65	0.96	0.14	17,22,53,55	0
23	CLA	B	611	65/65	0.96	0.13	20,24,33,39	0
28	LHG	D	411	46/49	0.96	0.12	25,30,82,85	0
31	DMS	F	102	4/4	0.96	0.14	48,48,50,64	0
31	DMS	v	207	4/4	0.96	0.14	53,54,54,60	0
31	DMS	c	928	4/4	0.96	0.14	57,59,61,61	0
33	CA	B	601	1/1	0.96	0.10	41,41,41,41	0
27	PL9	D	406	55/55	0.96	0.09	17,22,28,30	0
31	DMS	d	416	4/4	0.96	0.15	47,52,59,64	0
28	LHG	d	410	46/49	0.96	0.14	24,27,73,84	0
31	DMS	c	925	4/4	0.96	0.15	35,37,42,49	0
23	CLA	d	404	65/65	0.96	0.10	22,27,66,72	0
23	CLA	c	902	65/65	0.96	0.12	24,27,38,46	0
23	CLA	b	604	65/65	0.96	0.13	19,23,29,32	0
23	CLA	B	615	65/65	0.96	0.11	18,23,66,71	0
28	LHG	D	410	49/49	0.96	0.11	20,27,42,46	0
25	BCR	B	619	40/40	0.96	0.19	20,25,41,45	0
23	CLA	D	403	65/65	0.96	0.10	13,17,33,41	0
23	CLA	b	611	65/65	0.96	0.10	19,24,32,37	0
23	CLA	C	511	65/65	0.96	0.12	24,30,35,40	0
23	CLA	B	617	65/65	0.96	0.11	20,27,93,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	B	604	65/65	0.96	0.14	18,21,30,36	0
23	CLA	C	503	65/65	0.96	0.12	23,27,37,42	0
23	CLA	B	613	65/65	0.96	0.13	18,23,28,31	0
23	CLA	b	612	65/65	0.96	0.16	18,21,36,42	0
23	CLA	C	506	65/65	0.96	0.13	25,31,40,44	0
23	CLA	a	410	65/65	0.97	0.10	17,22,91,94	0
23	CLA	c	911	65/65	0.97	0.21	20,26,36,40	0
23	CLA	B	612	65/65	0.97	0.12	17,20,36,52	0
31	DMS	c	926	4/4	0.97	0.15	66,68,69,77	0
23	CLA	b	609	65/65	0.97	0.16	19,23,31,32	0
23	CLA	A	408	65/65	0.97	0.11	18,22,89,96	0
24	PHO	a	408	64/64	0.97	0.11	15,18,20,22	0
25	BCR	A	409	40/40	0.97	0.12	19,23,29,32	0
23	CLA	b	606	65/65	0.97	0.11	18,22,29,33	0
24	PHO	D	402	64/64	0.97	0.13	16,21,25,29	0
31	DMS	b	634	4/4	0.97	0.11	42,45,48,48	0
23	CLA	a	407	65/65	0.97	0.13	17,20,95,102	0
31	DMS	B	637	4/4	0.97	0.11	35,38,40,42	0
32	BCT	a	424	4/4	0.97	0.06	32,35,37,41	0
24	PHO	A	407	64/64	0.97	0.11	17,19,22,22	0
23	CLA	b	613	65/65	0.97	0.13	18,24,29,34	0
23	CLA	b	614	65/65	0.97	0.18	17,21,47,54	0
23	CLA	d	403	65/65	0.97	0.11	13,18,36,42	0
23	CLA	A	406	65/65	0.97	0.14	18,20,90,96	0
23	CLA	b	608	65/65	0.97	0.14	16,20,28,36	0
31	DMS	D	416	4/4	0.97	0.20	56,57,58,62	0
23	CLA	a	406	65/65	0.97	0.11	14,17,25,37	0
31	DMS	B	636	4/4	0.97	0.12	18,20,22,28	0
24	PHO	a	409	64/64	0.97	0.13	17,22,27,30	0
23	CLA	A	405	65/65	0.97	0.09	14,17,26,34	0
23	CLA	B	606	65/65	0.97	0.16	18,22,32,34	0
23	CLA	B	609	65/65	0.97	0.14	19,23,28,29	0
23	CLA	B	605	65/65	0.97	0.17	18,21,52,53	0
23	CLA	B	608	65/65	0.97	0.13	16,19,32,35	0
31	DMS	D	415	4/4	0.98	0.09	50,53,56,59	0
37	HEM	e	105	43/43	0.98	0.15	35,39,51,63	0
40	HEC	V	203	43/43	0.98	0.07	19,22,26,29	0
23	CLA	d	401	65/65	0.98	0.12	15,17,26,31	0
33	CA	b	601	1/1	0.98	0.08	41,41,41,41	0
23	CLA	D	401	65/65	0.98	0.09	13,17,27,35	0
31	DMS	V	201	4/4	0.98	0.10	41,46,47,47	0
40	HEC	v	203	43/43	0.98	0.08	22,27,29,32	0

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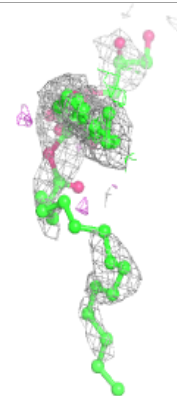
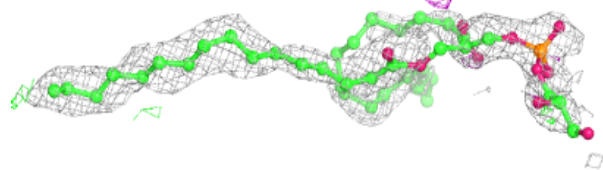
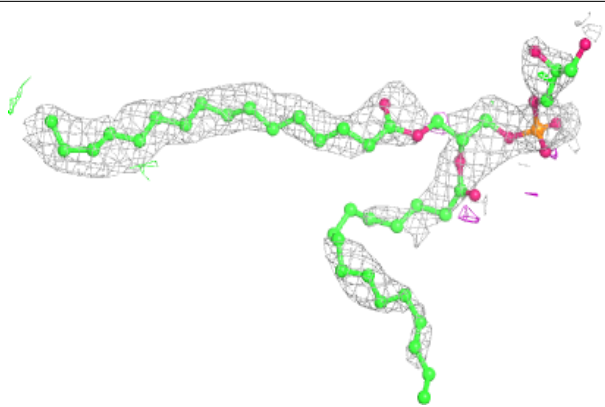
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	B	614	65/65	0.98	0.15	18,20,44,51	0
31	DMS	v	201	4/4	0.98	0.12	46,48,51,51	0
33	CA	c	901	1/1	0.98	0.04	39,39,39,39	0
31	DMS	b	633	4/4	0.98	0.10	21,23,24,25	0
22	CL	a	404	1/1	0.99	0.06	19,19,19,19	0
39	MG	j	102	1/1	0.99	0.14	28,28,28,28	0
39	MG	J	102	1/1	0.99	0.09	30,30,30,30	0
31	DMS	A	423	4/4	0.99	0.09	23,27,27,28	0
31	DMS	o	301	4/4	0.99	0.08	22,27,28,31	0
31	DMS	c	924	4/4	0.99	0.09	31,33,36,36	0
31	DMS	C	524	4/4	0.99	0.10	32,33,36,36	0
21	FE2	a	403	1/1	0.99	0.07	25,25,25,25	0
22	CL	a	405	1/1	0.99	0.09	21,21,21,21	0
21	FE2	A	402	1/1	0.99	0.04	28,28,28,28	0
22	CL	A	404	1/1	1.00	0.08	20,20,20,20	0
20	OEX	A	401	10/10	1.00	0.08	19,21,23,24	0
20	OEX	a	402	10/10	1.00	0.09	21,23,24,24	0
22	CL	A	403	1/1	1.00	0.07	19,19,19,19	0

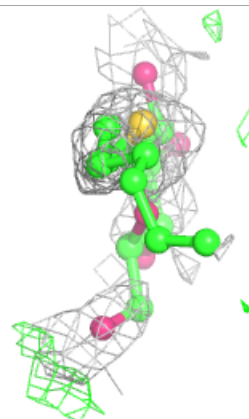
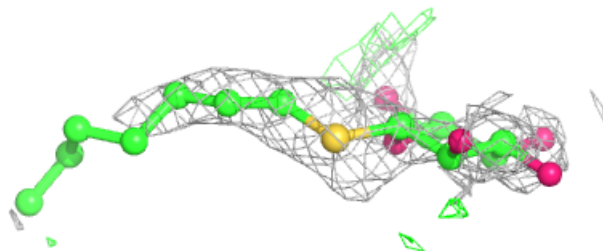
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LHG 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)

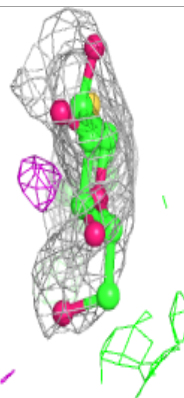
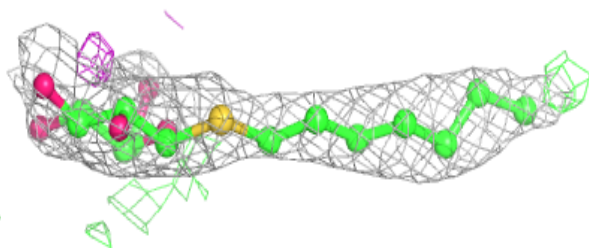
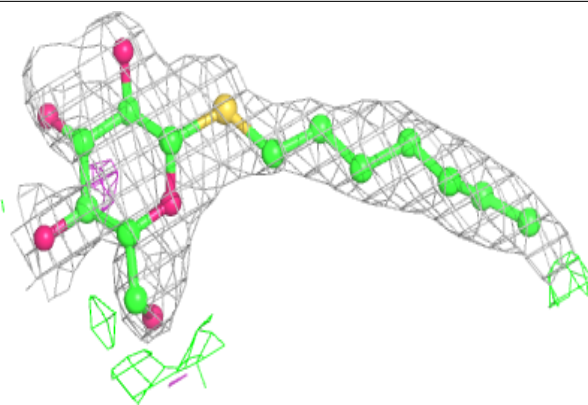
**Electron density around HTG D 414:**

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

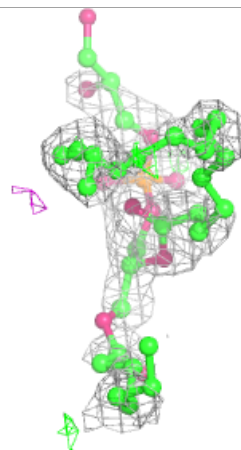
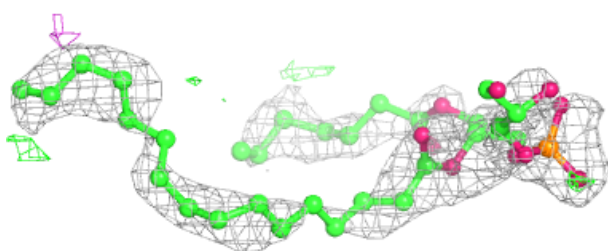
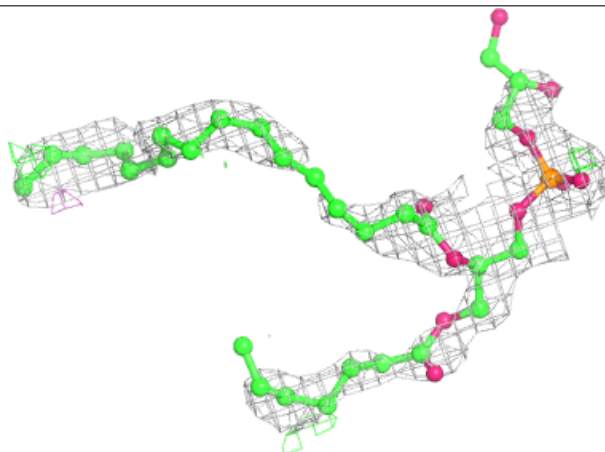


Electron density around HTG b 628:

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

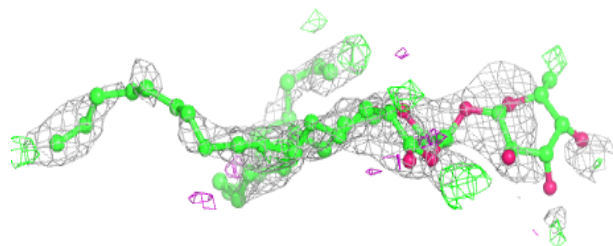
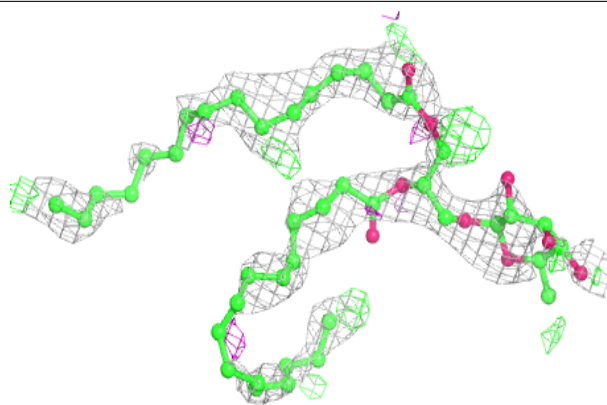
**Electron density around LHG e 101:**

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

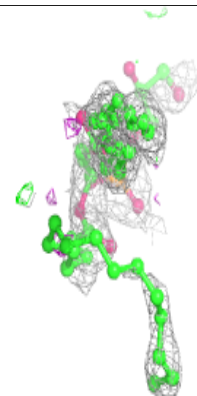
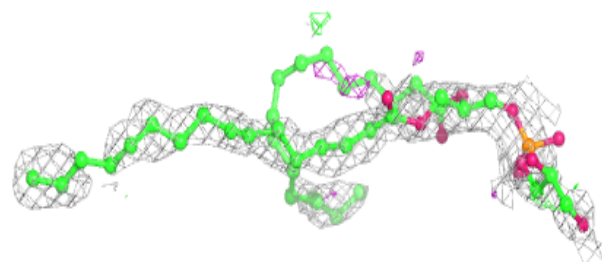
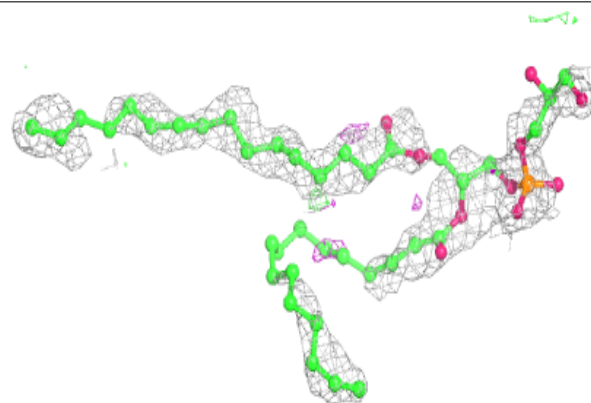


Electron density around DGD D 407:

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

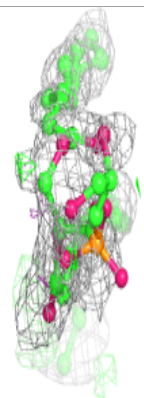
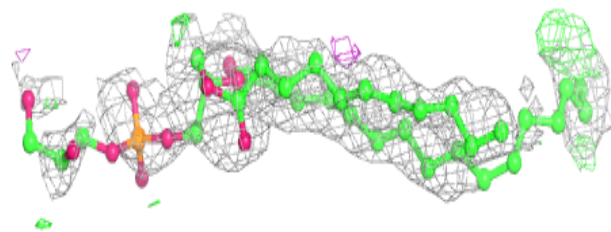
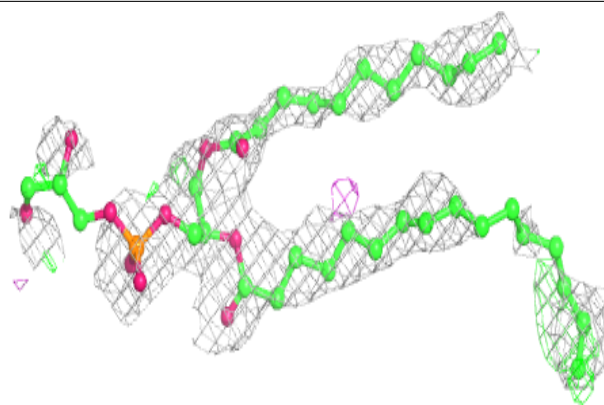
**Electron density around LHG A 412:**

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



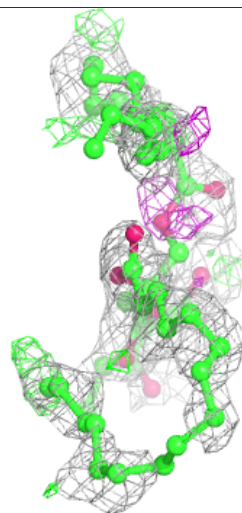
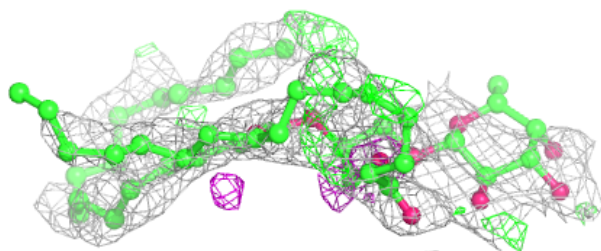
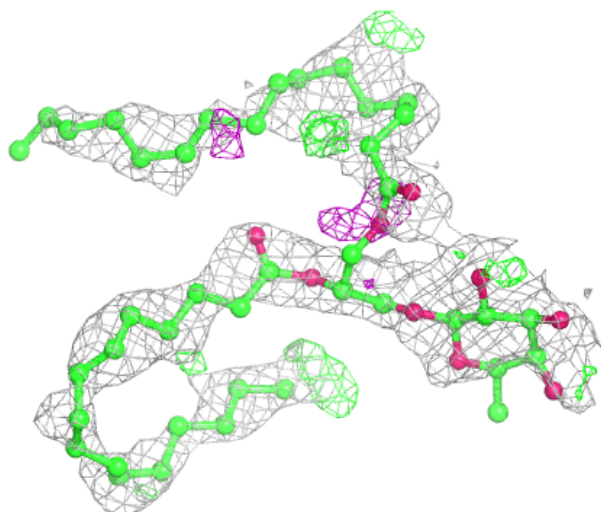
Electron density around LHG d 402:

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



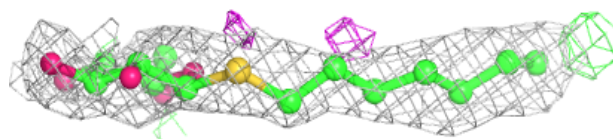
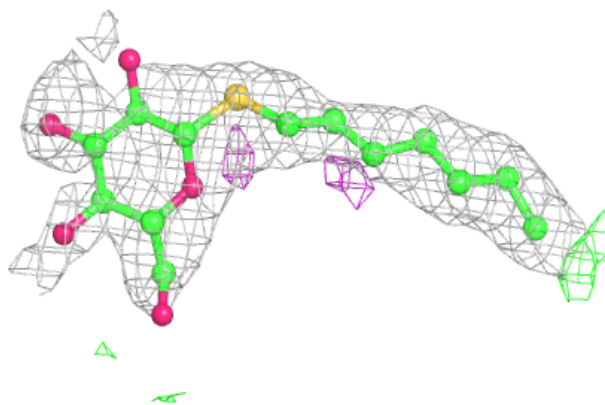
Electron density around DGD d 407:

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

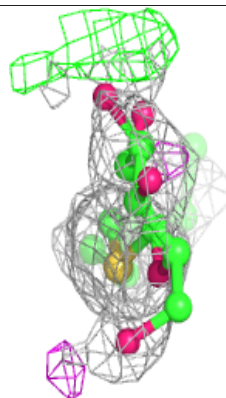
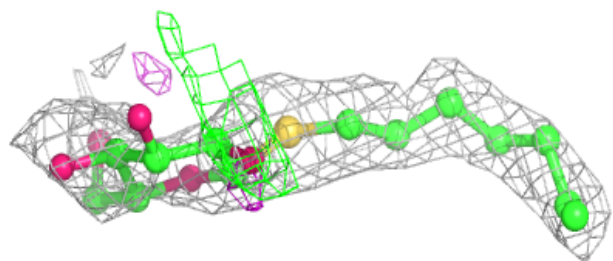
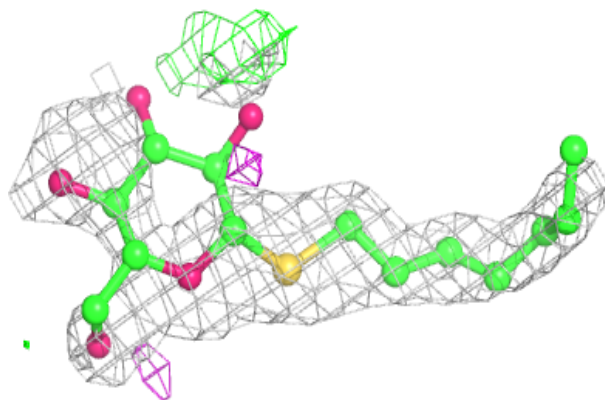


Electron density around HTG B 631:

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

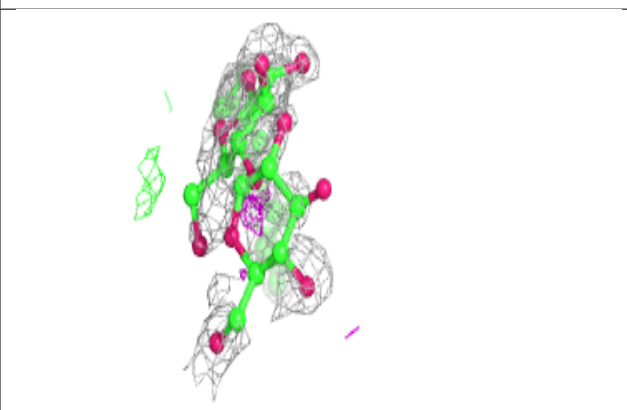
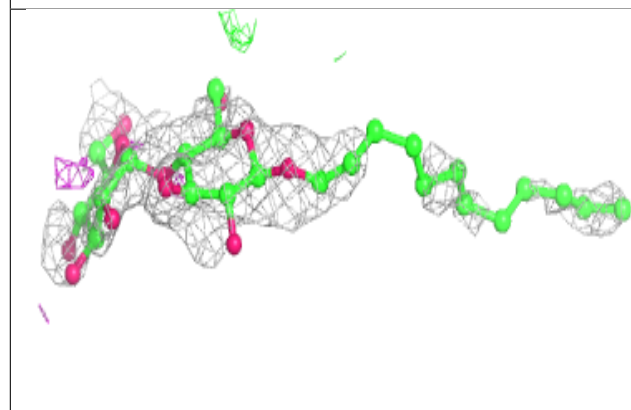
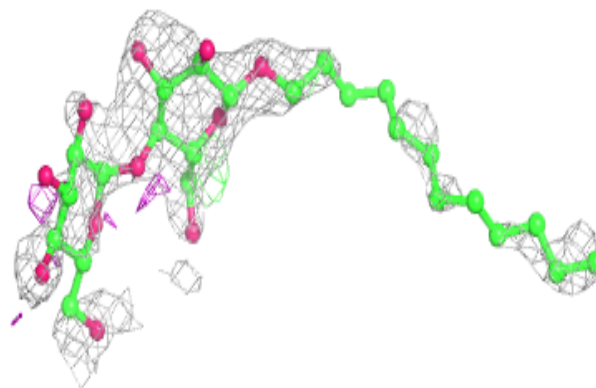
**Electron density around HTG d 413:**

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

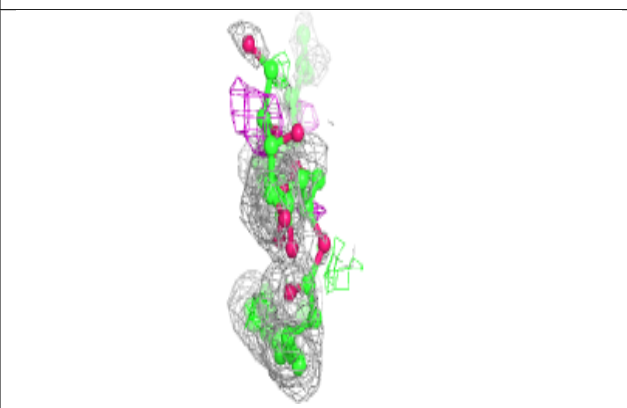
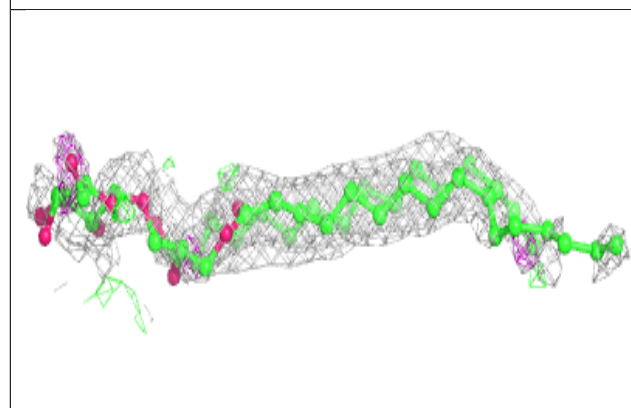
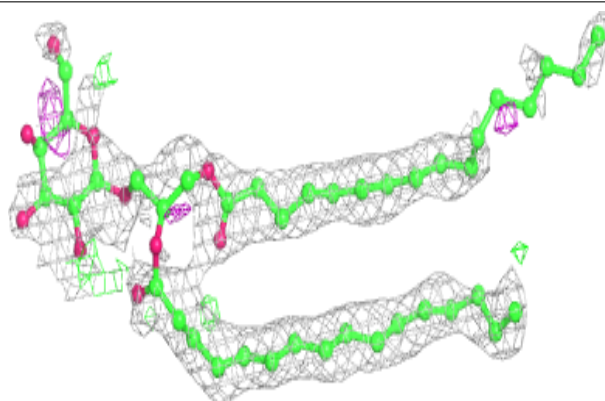


Electron density around LMT F 101:

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

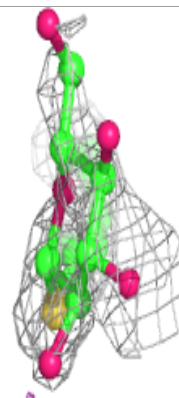
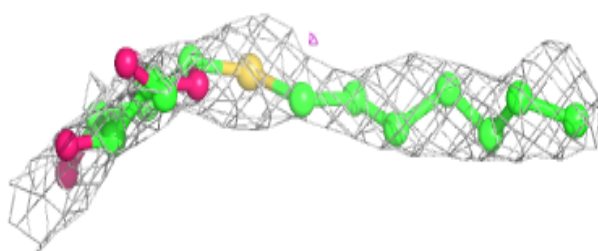
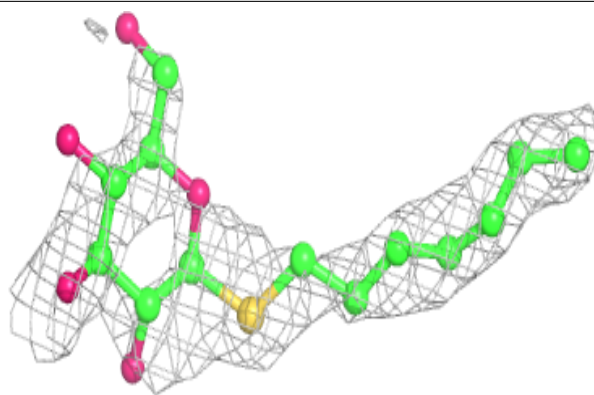
**Electron density around LMG D 412:**

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

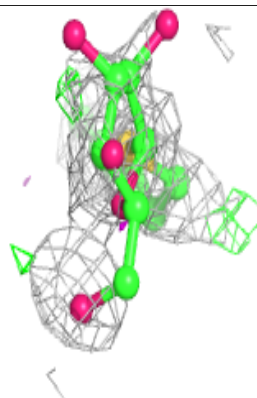
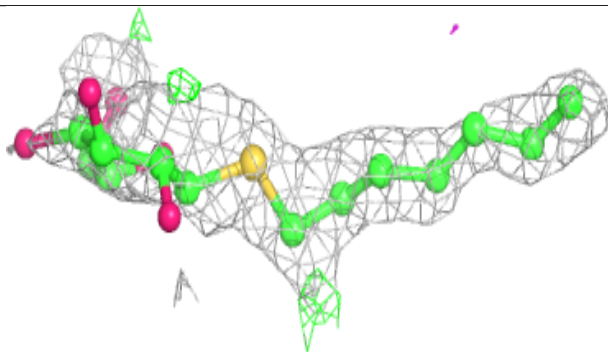
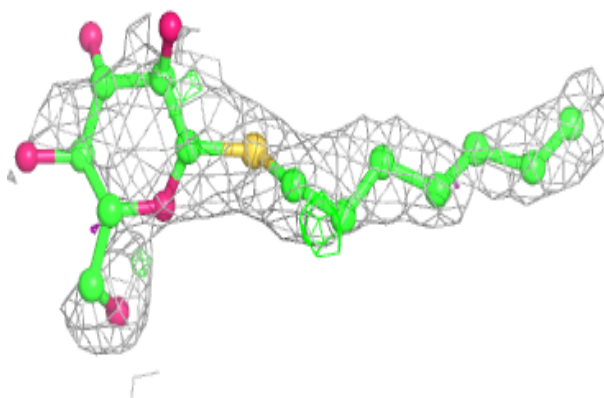


Electron density around HTG B 626:

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

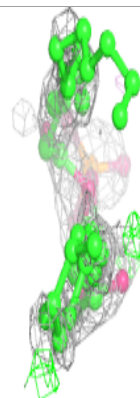
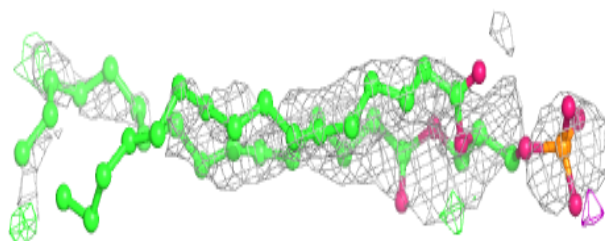
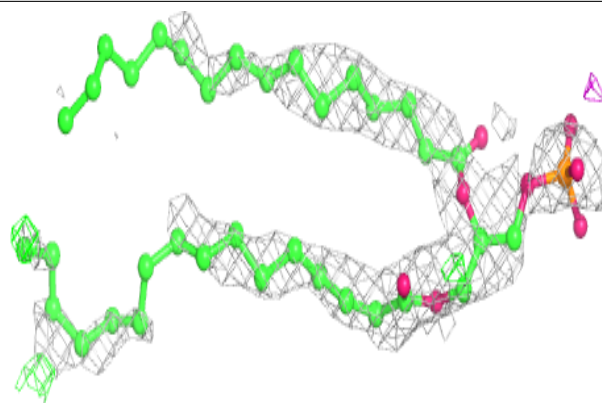
**Electron density around HTG c 922:**

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

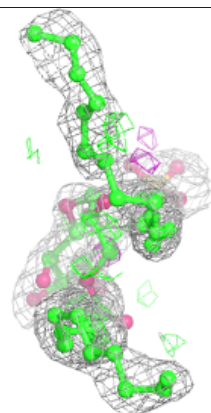
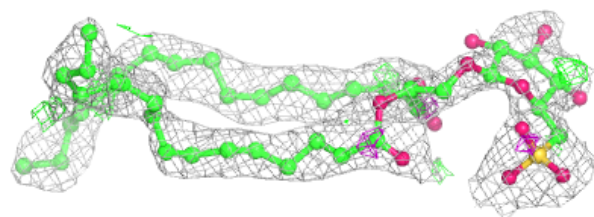
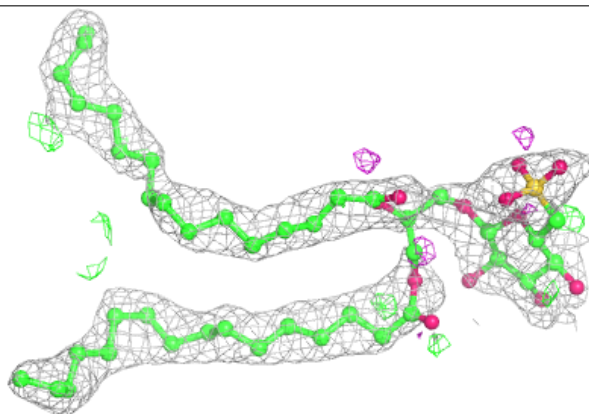


Electron density around LHG K 101:

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

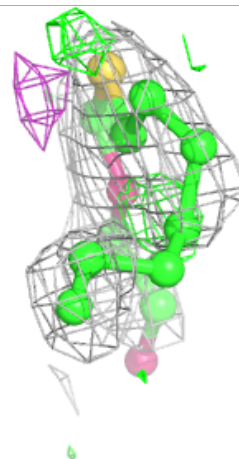
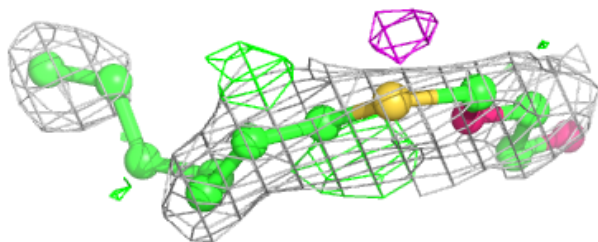
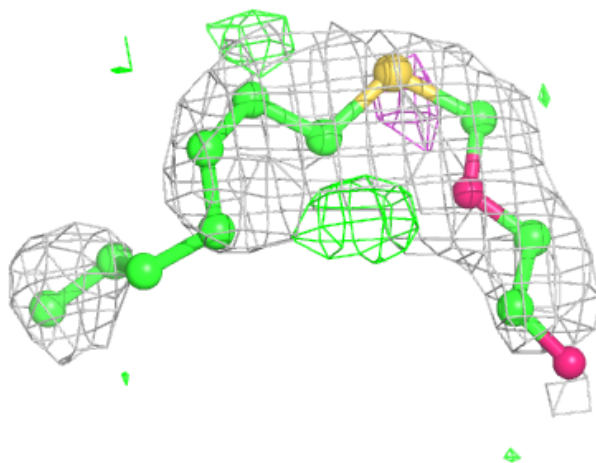
**Electron density around SQD B 621:**

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



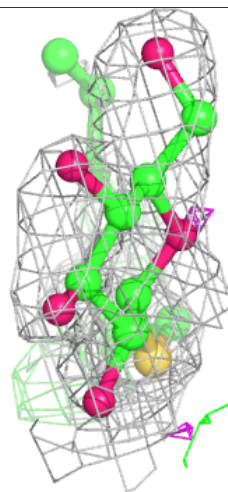
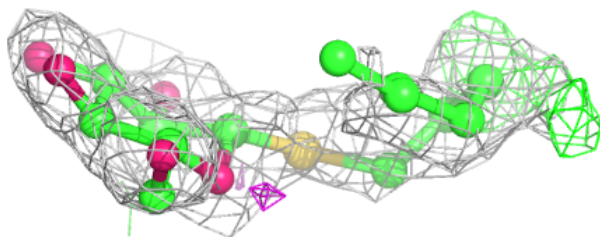
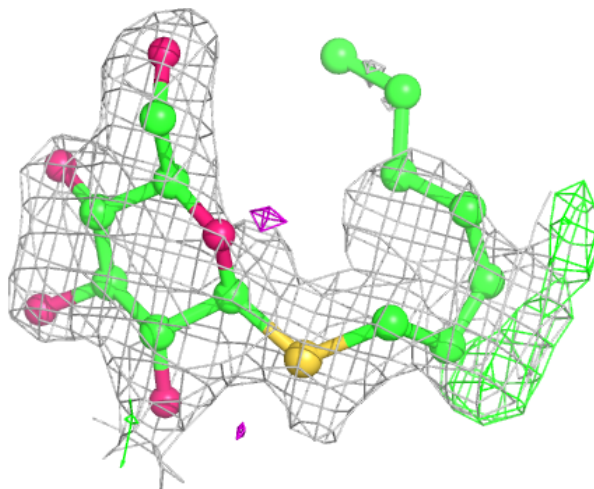
Electron density around HTG c 923:

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



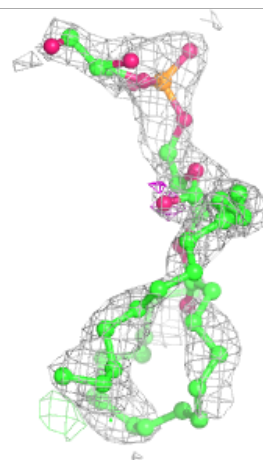
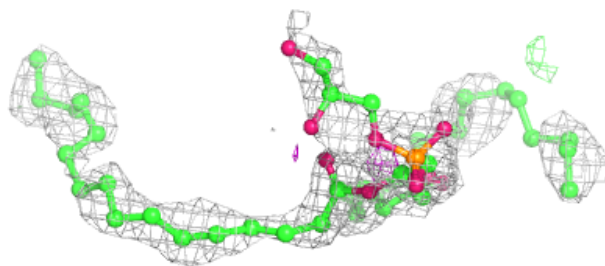
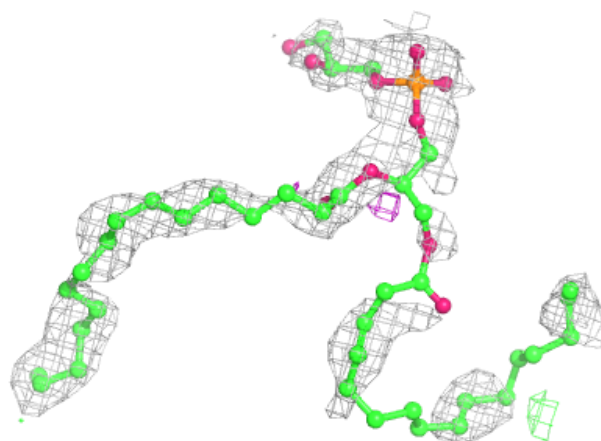
Electron density around HTG v 204:

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



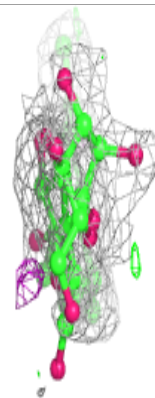
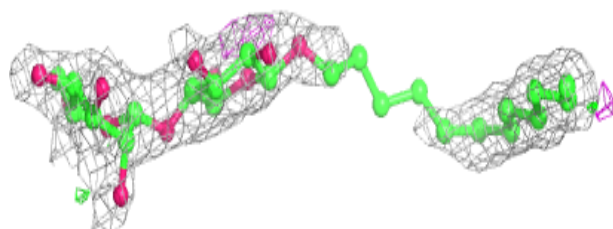
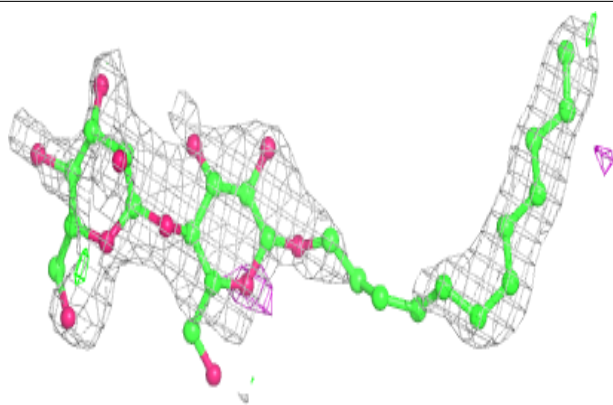
Electron density around LHG E 101:

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

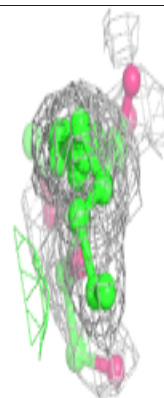
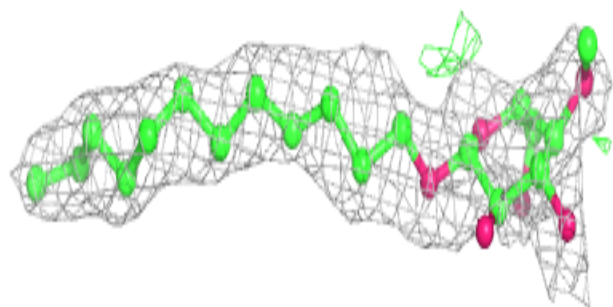
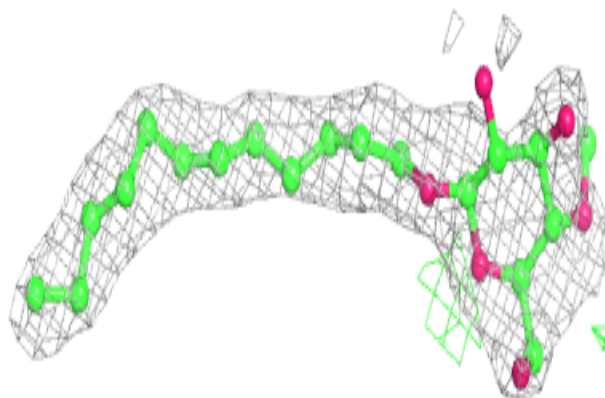


Electron density around LMT Z 101:

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

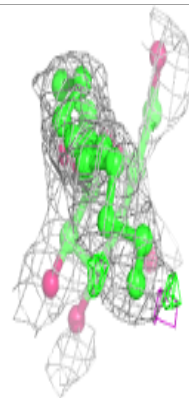
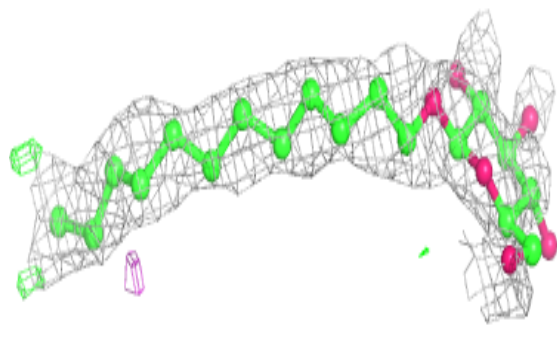
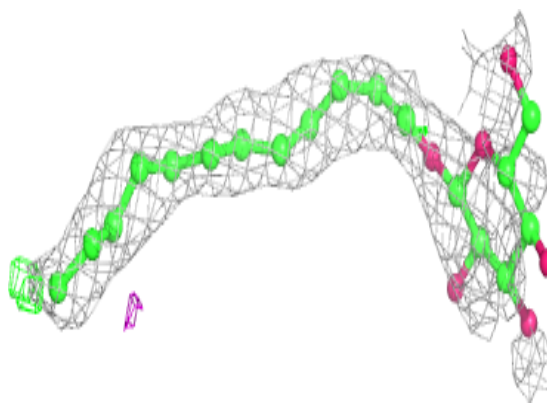
**Electron density around LMT b 621:**

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

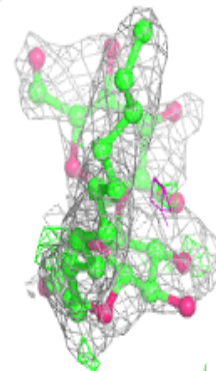
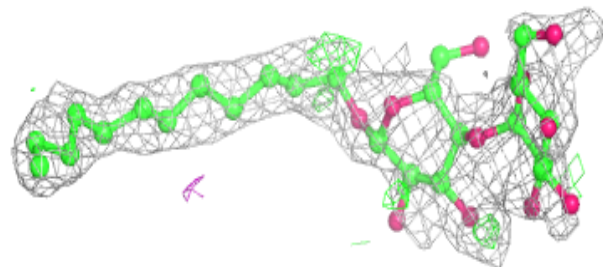
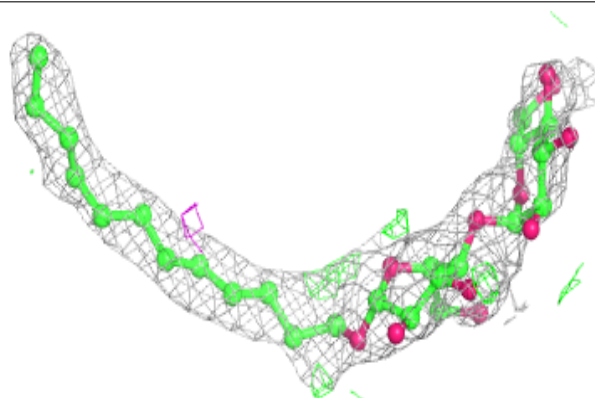


Electron density around LMT B 643:

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

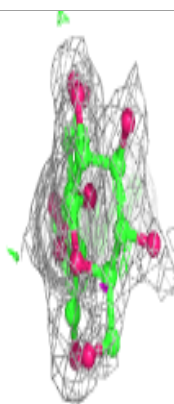
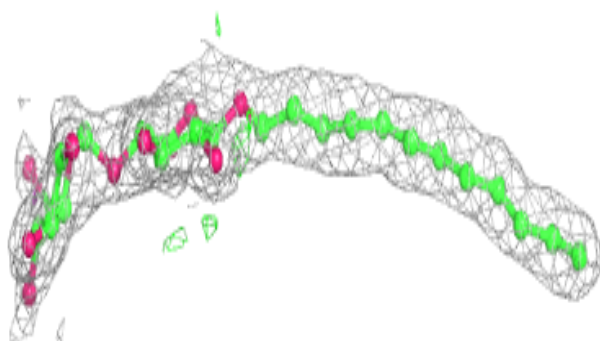
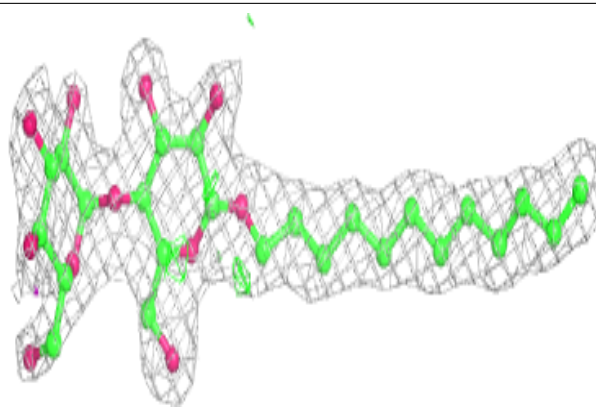
**Electron density around LMT m 103:**

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

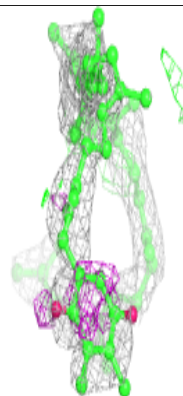
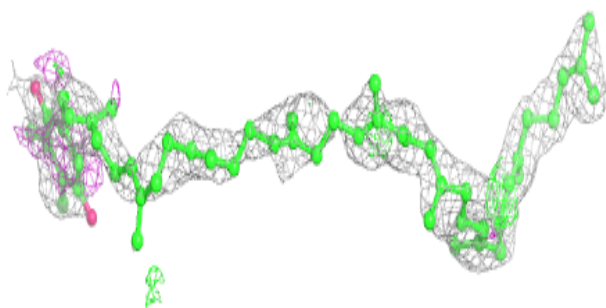
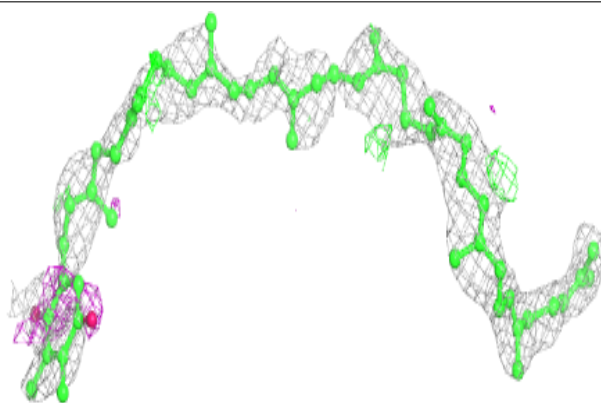


Electron density around LMT M 101:

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

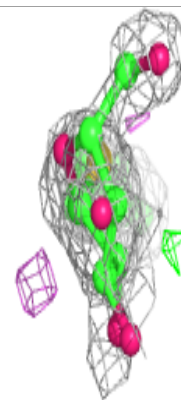
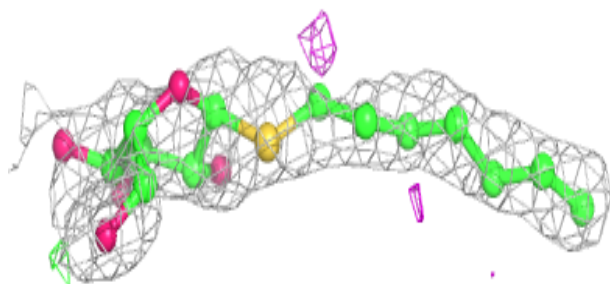
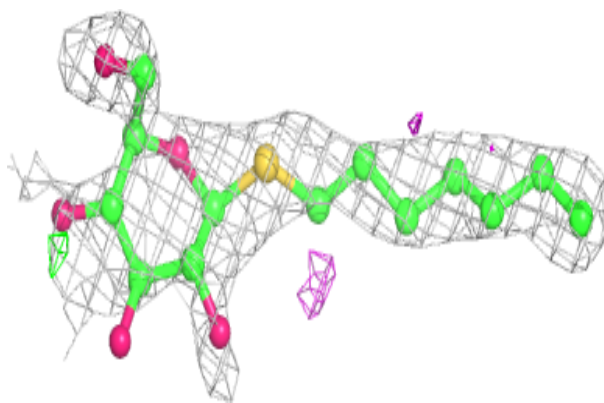
**Electron density around PL9 a 414:**

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

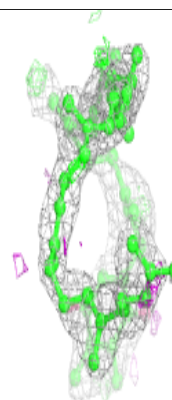
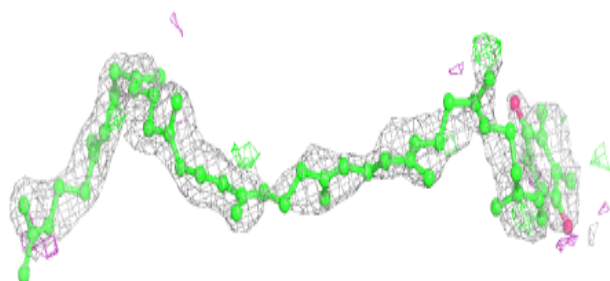
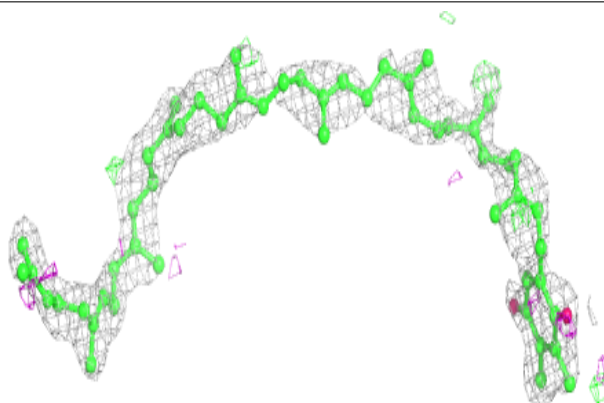


Electron density around HTG C 522:

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

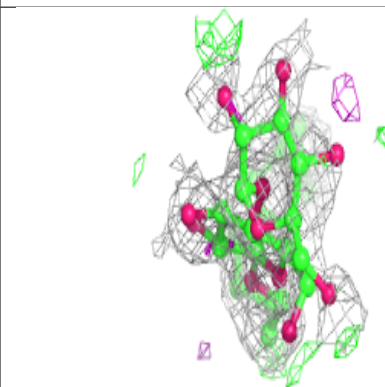
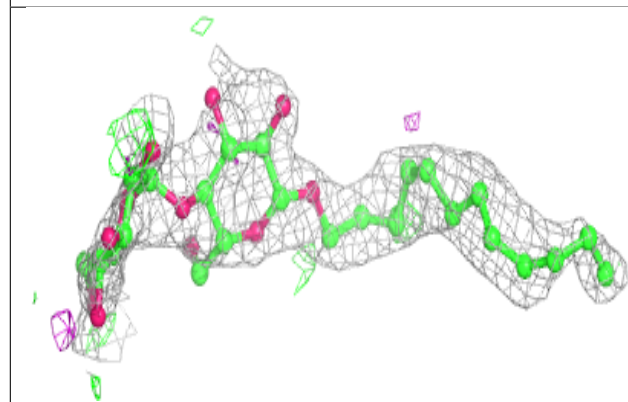
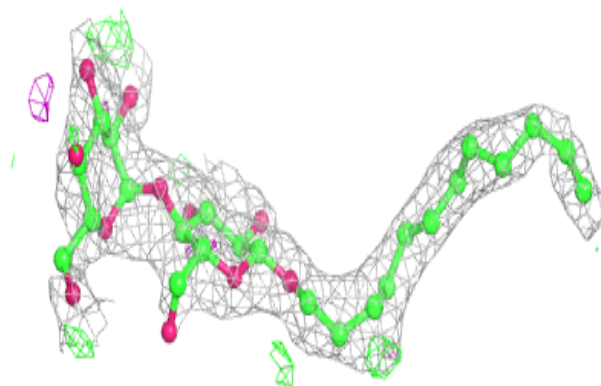
**Electron density around PL9 A 411:**

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

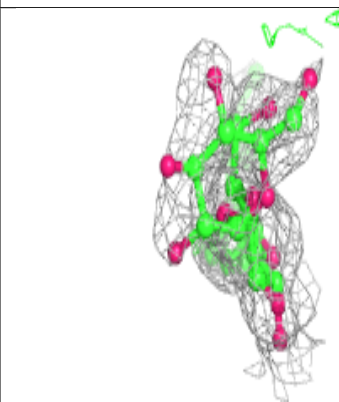
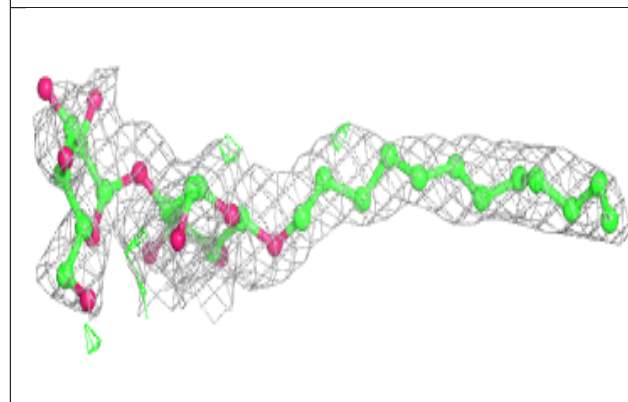
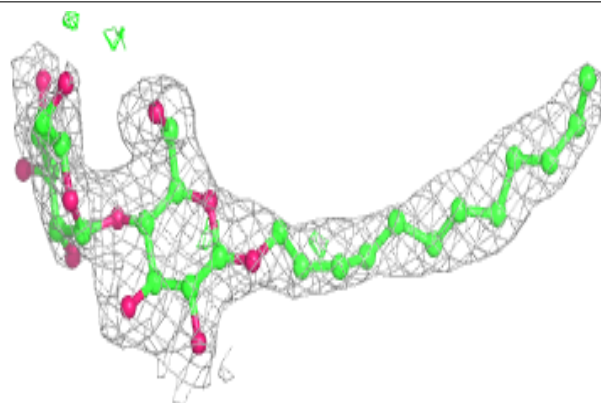


Electron density around LMT a 418:

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

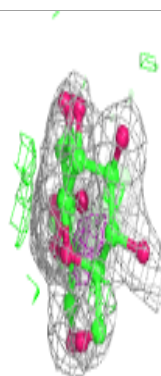
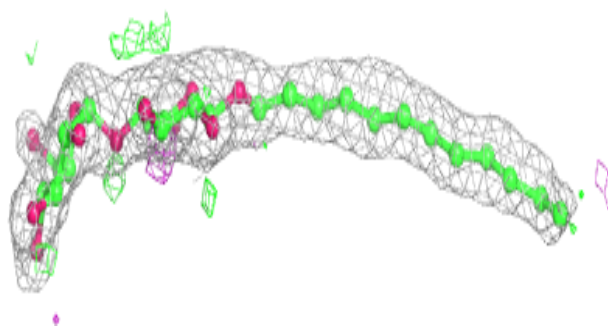
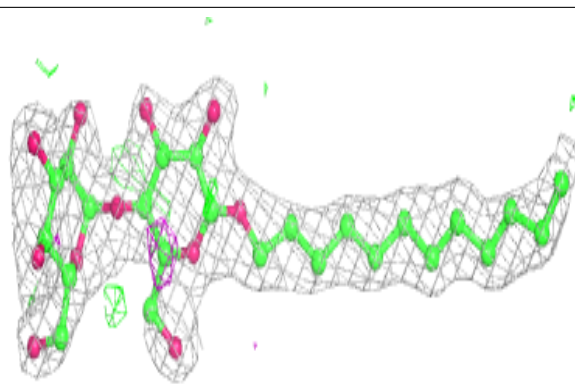
**Electron density around LMT B 623:**

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

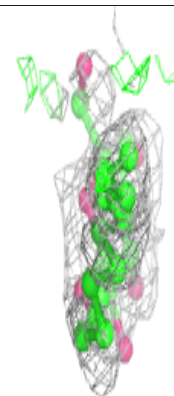
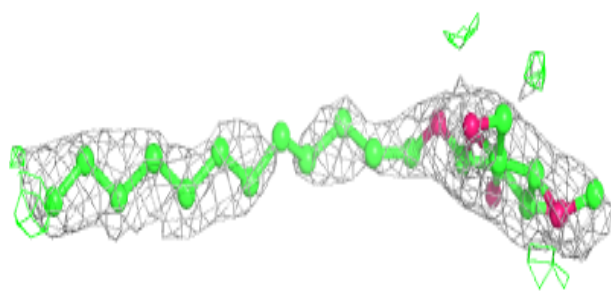
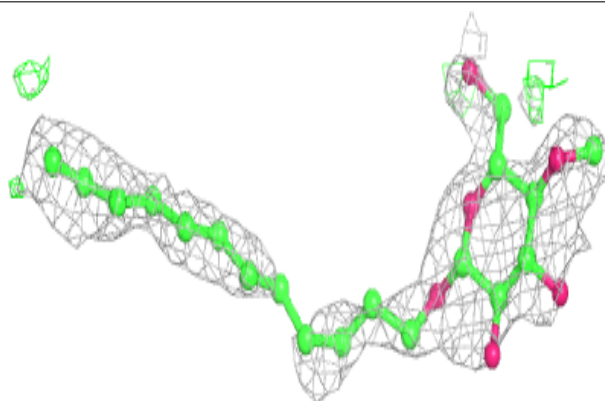


Electron density around LMT m 104:

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

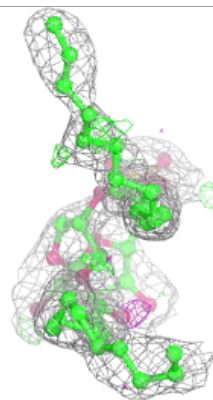
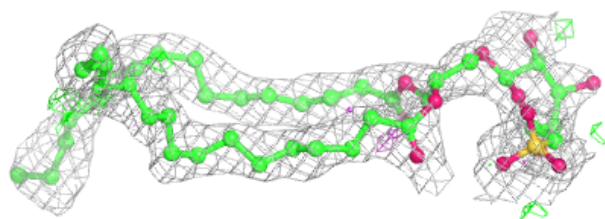
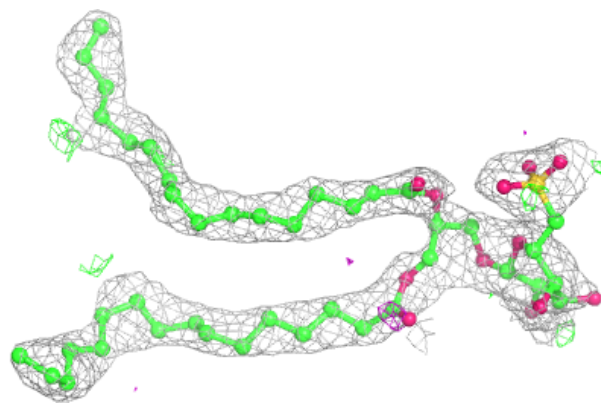
**Electron density around LMT e 103:**

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

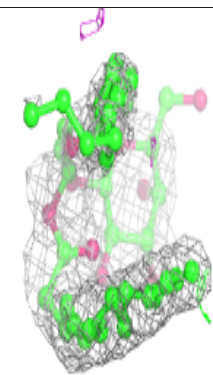
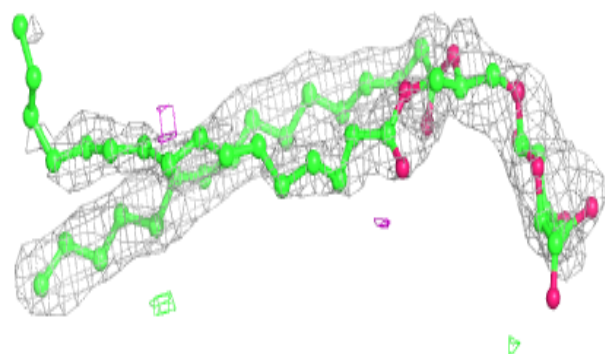
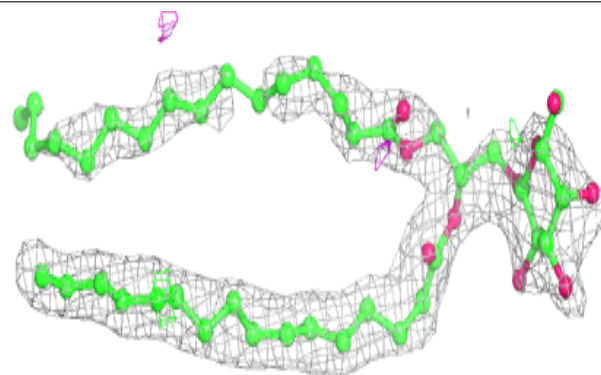


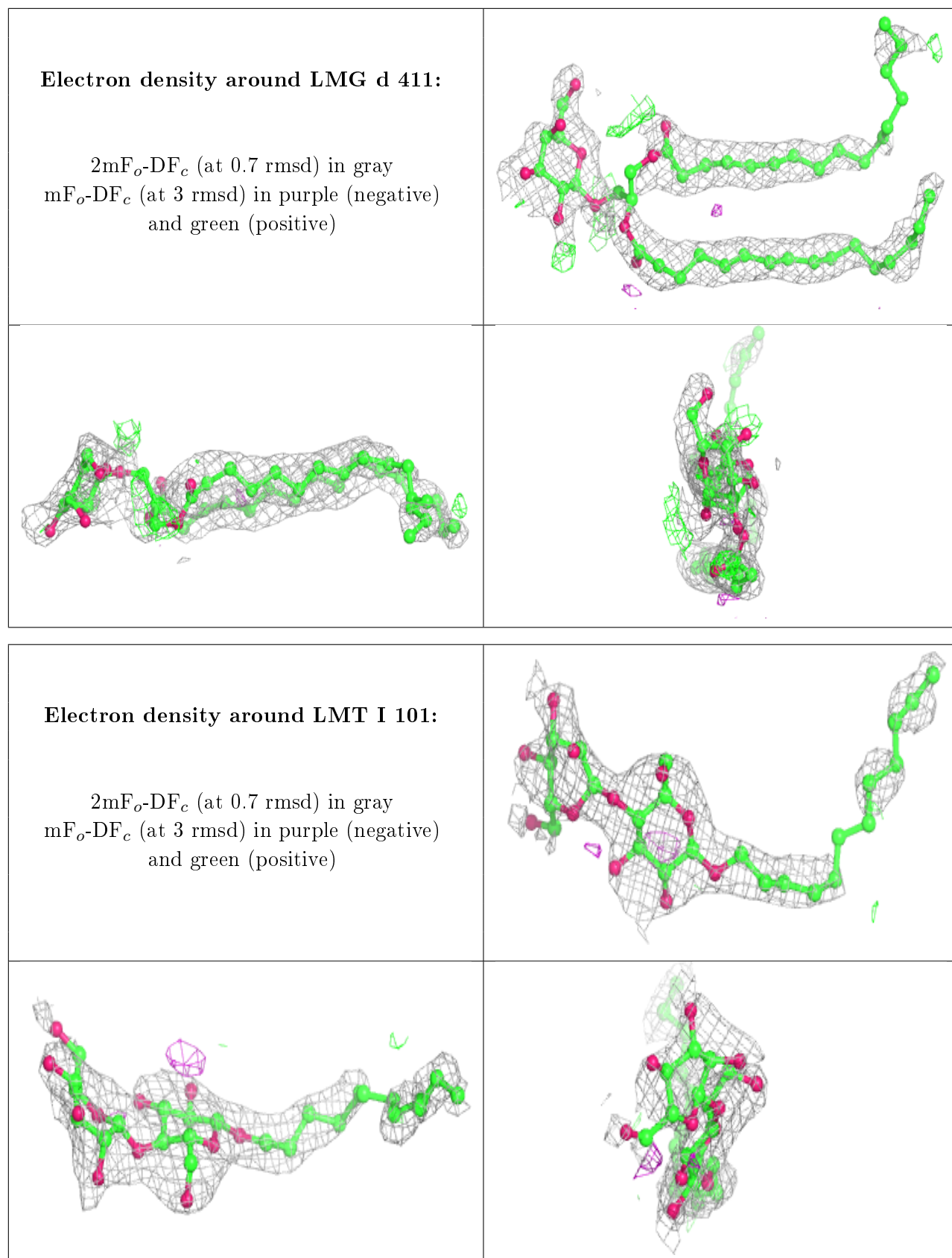
Electron density around SQD L 102:

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

**Electron density around LMG C 531:**

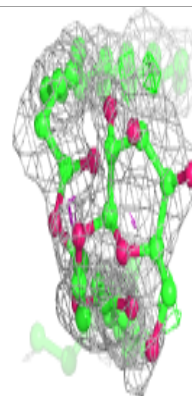
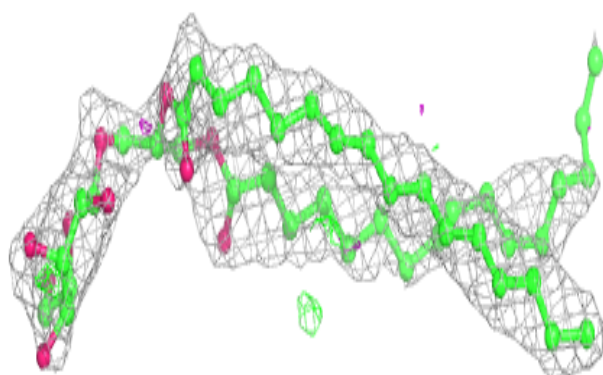
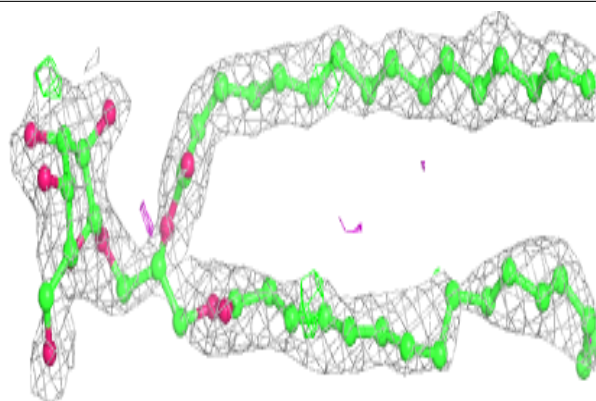
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



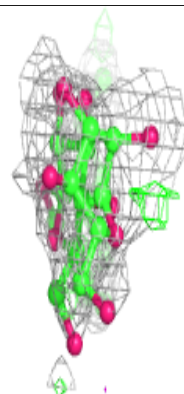
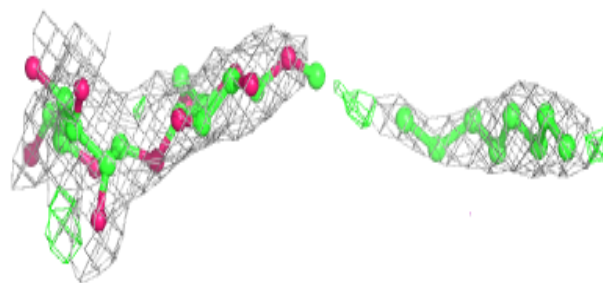
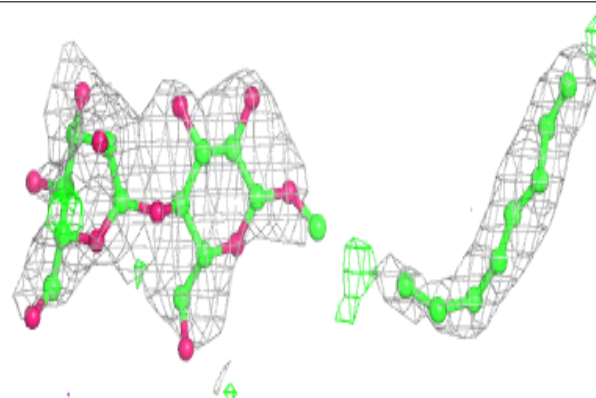


Electron density around LMG c 930:

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

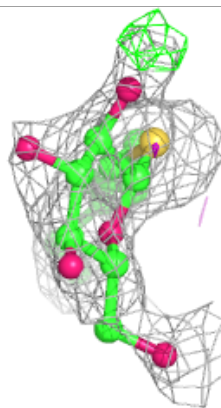
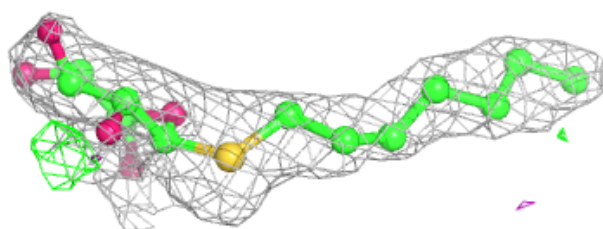
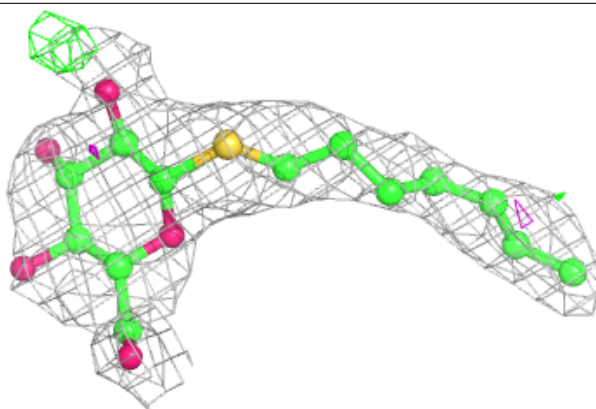
**Electron density around LMT z 101:**

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

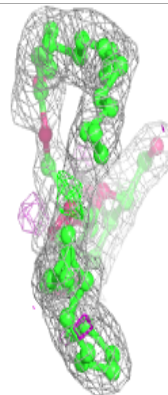
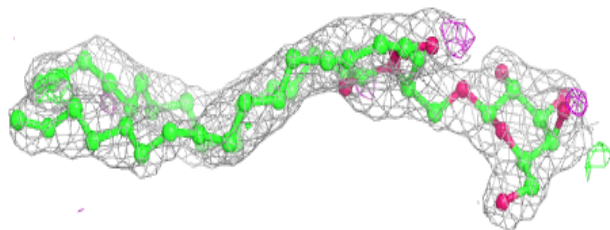
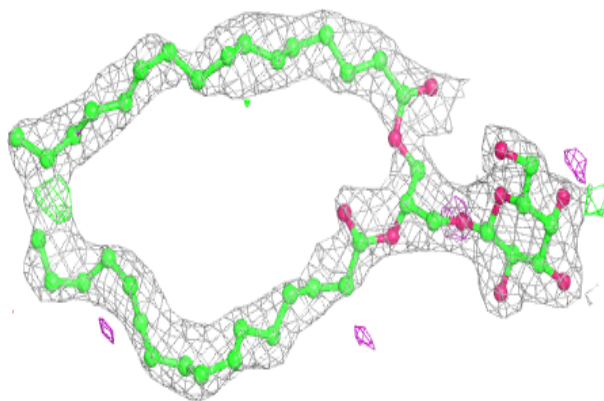


Electron density around HTG b 623:

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

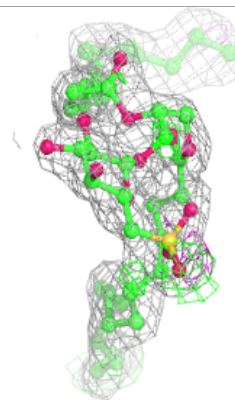
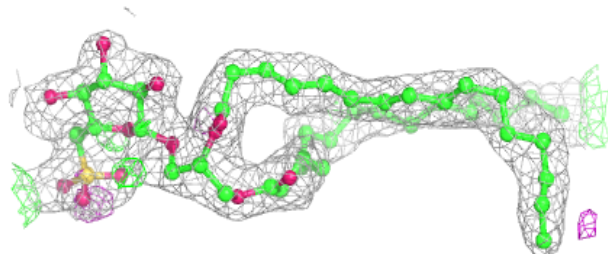
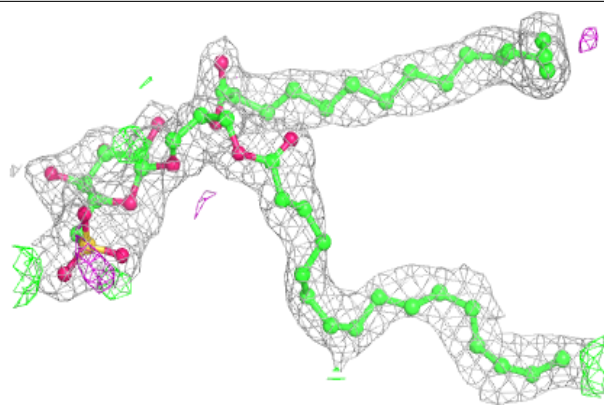
**Electron density around LMG a 413:**

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

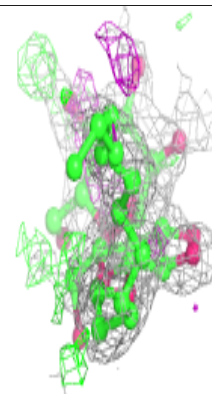
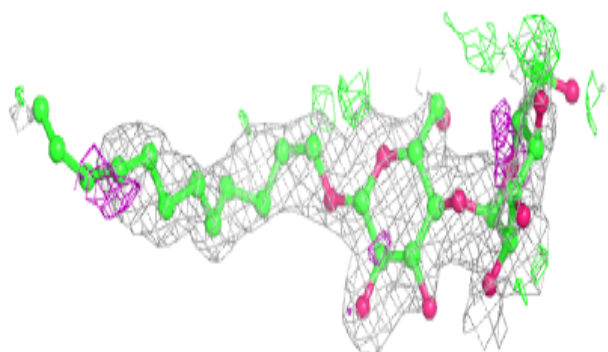
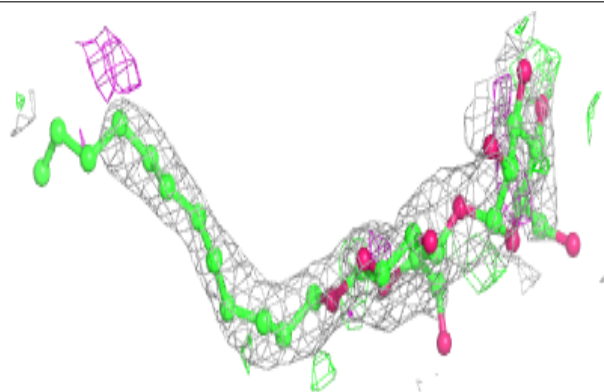


Electron density around SQD a 417:

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

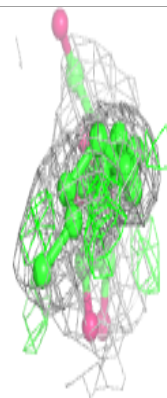
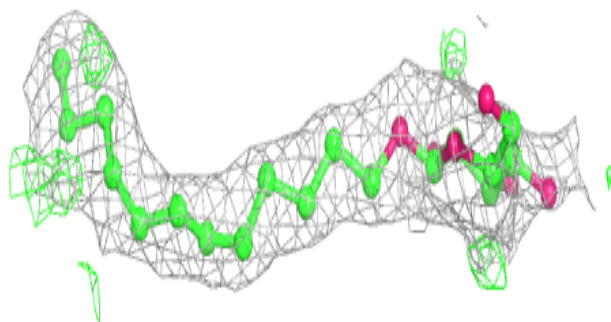
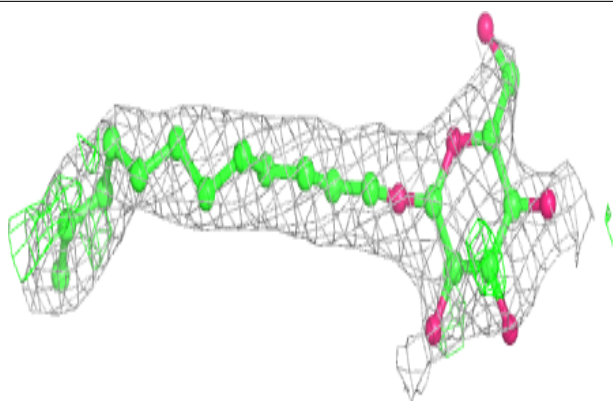
**Electron density around LMT A 416:**

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

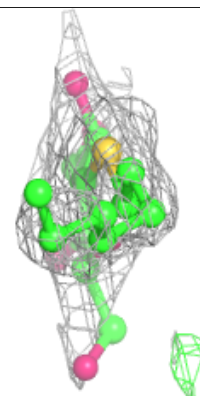
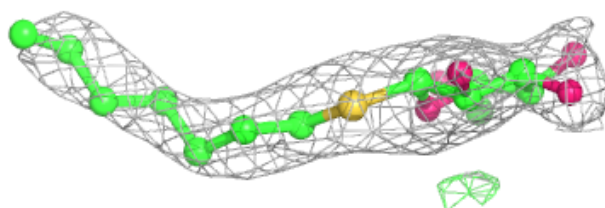
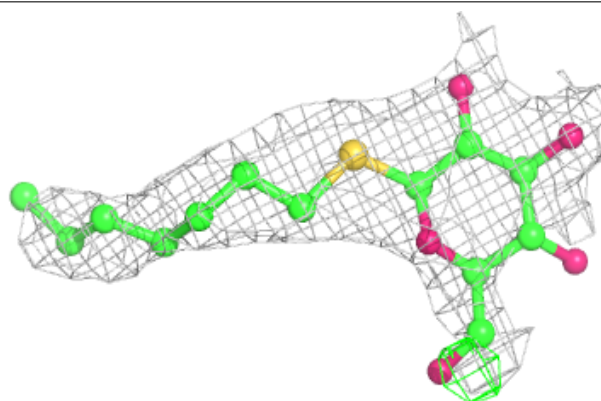


Electron density around LMT B 644:

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

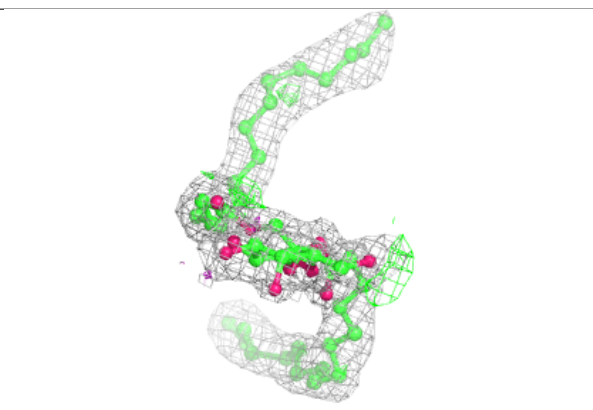
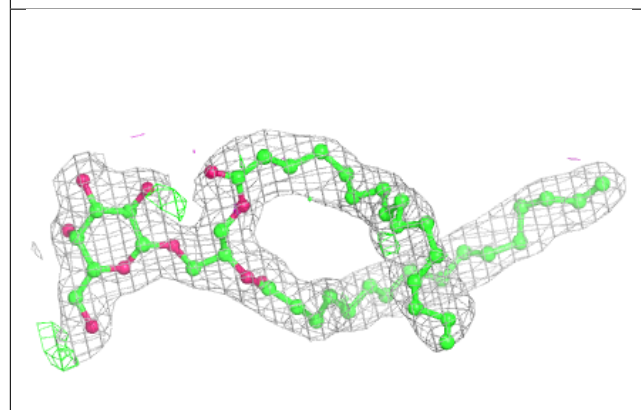
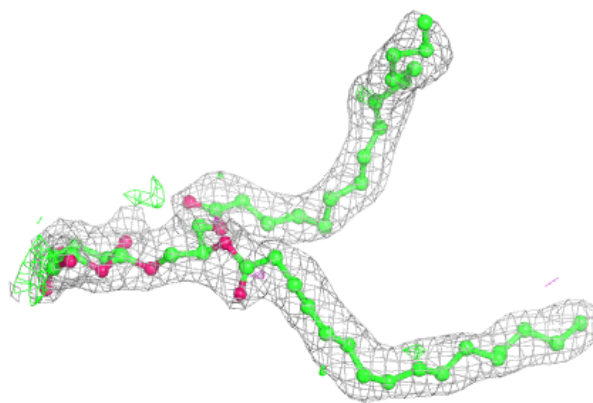
**Electron density around HTG C 523:**

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

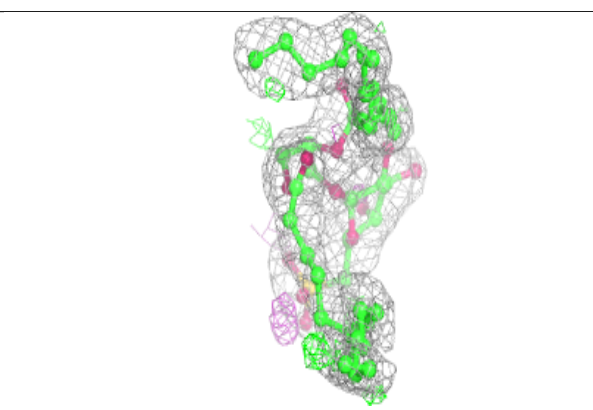
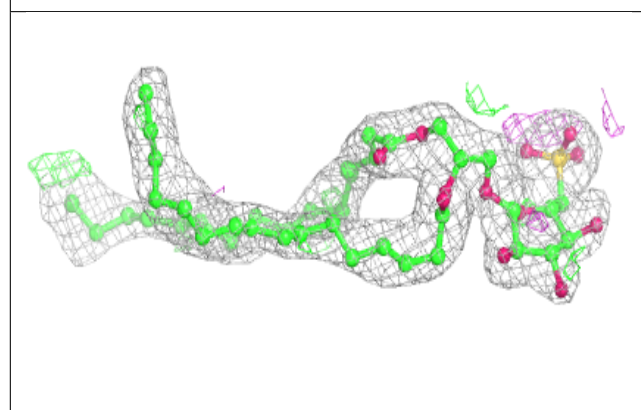
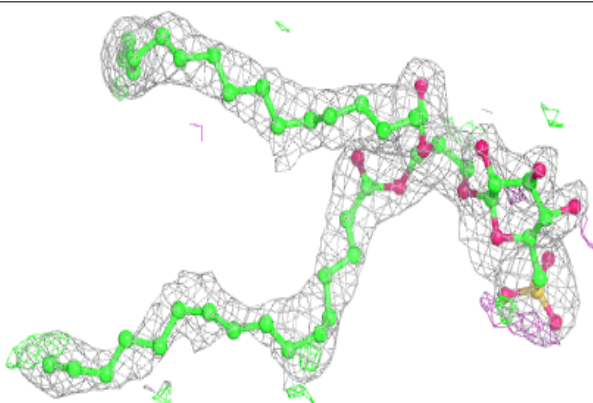


Electron density around LMG m 102:

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

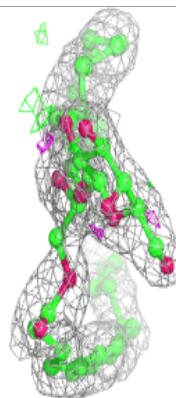
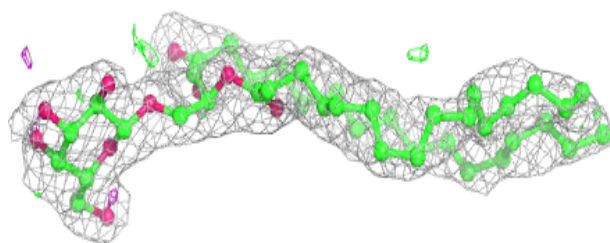
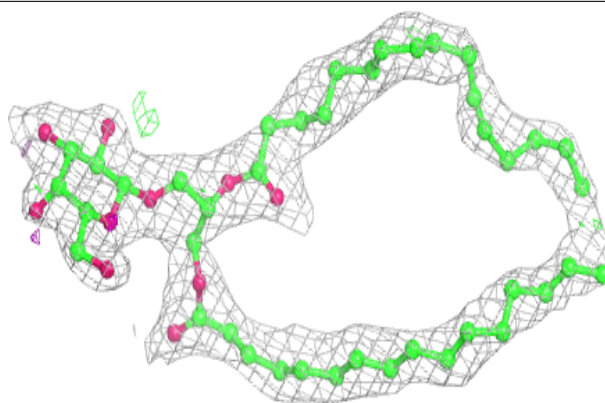
**Electron density around SQD A 415:**

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

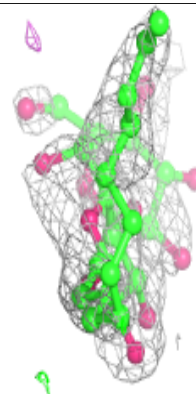
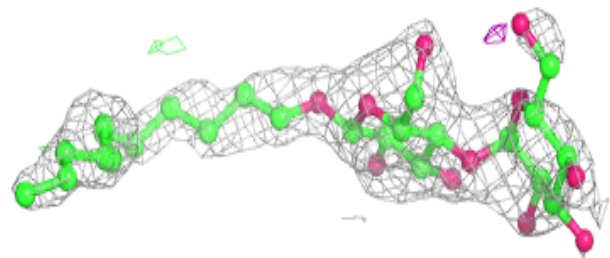
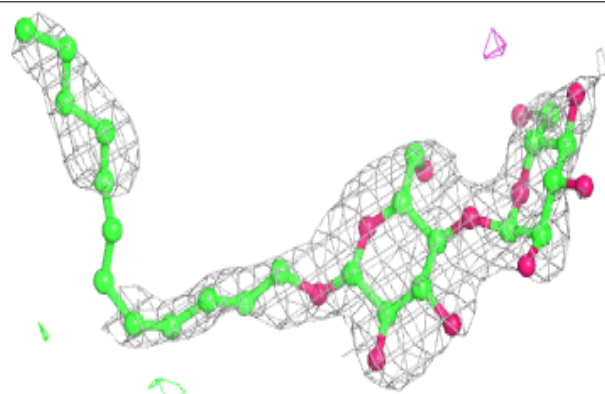


Electron density around LMG C 501:

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

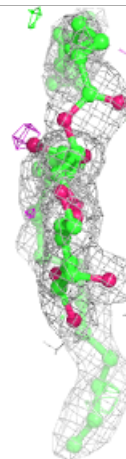
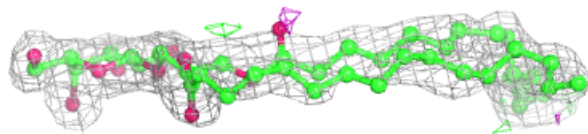
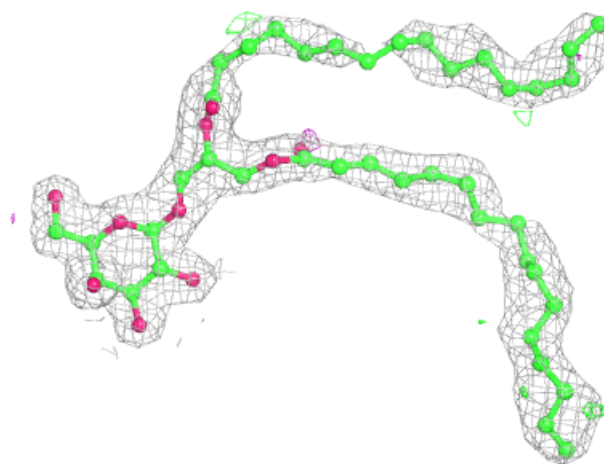
**Electron density around LMT a 422:**

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



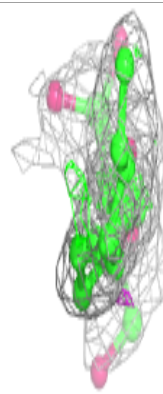
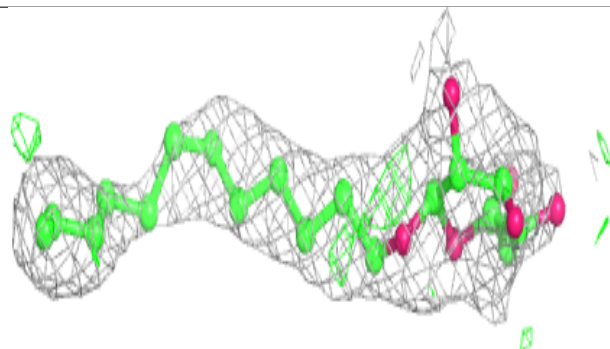
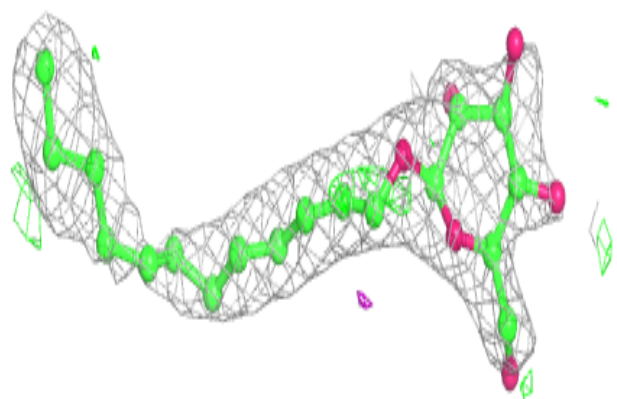
Electron density around LMG C 520:

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

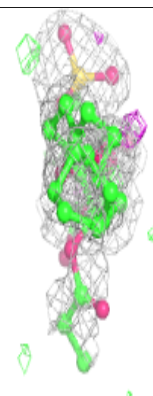
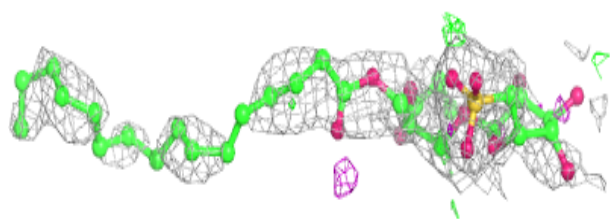
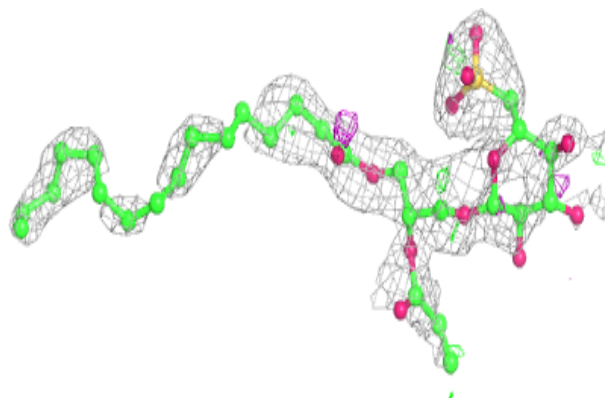


Electron density around LMT T 103:

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

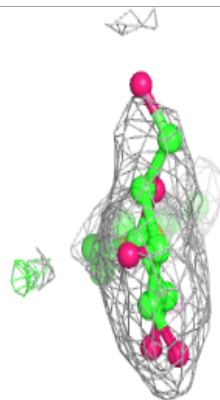
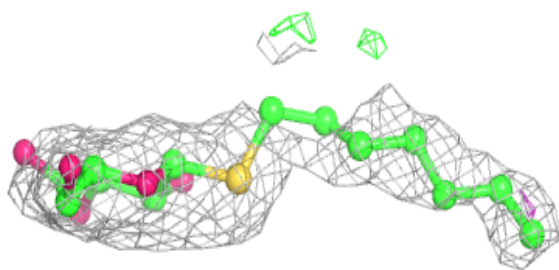
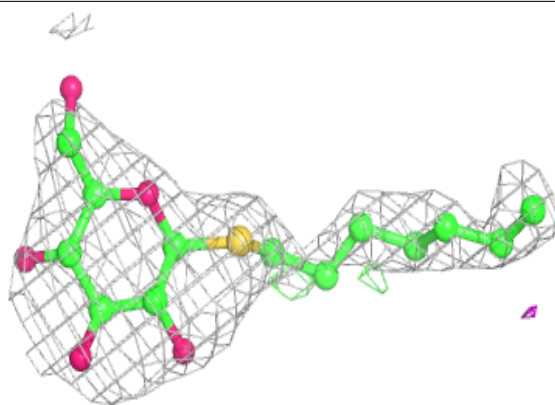
**Electron density around SQD x 101:**

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



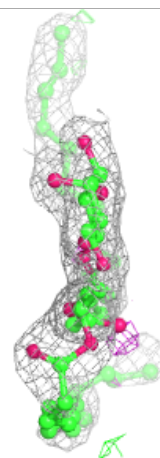
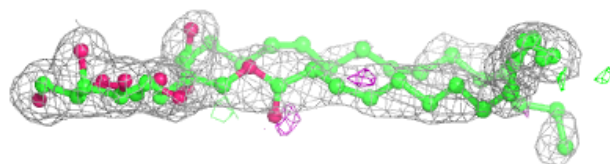
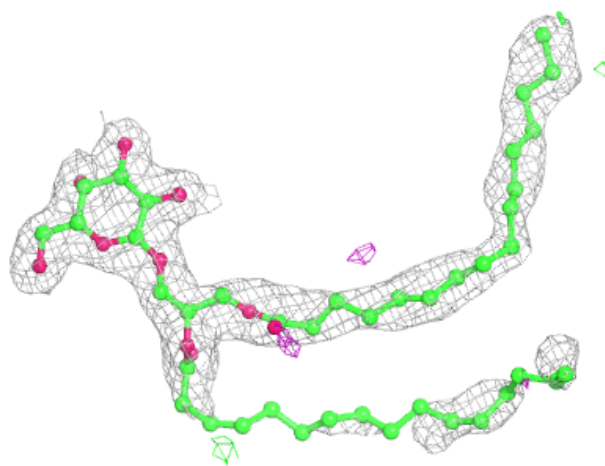
Electron density around HTG c 921:

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



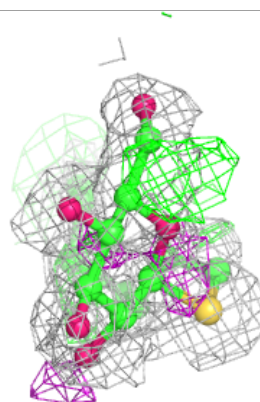
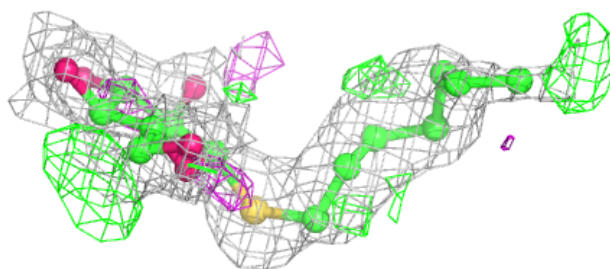
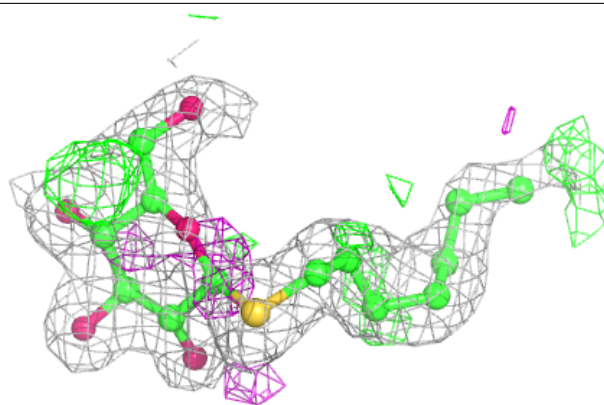
Electron density around LMG c 920:

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

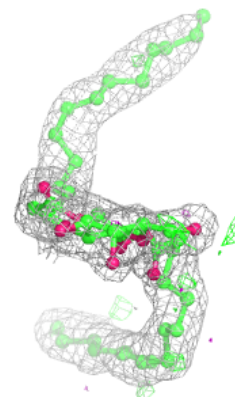
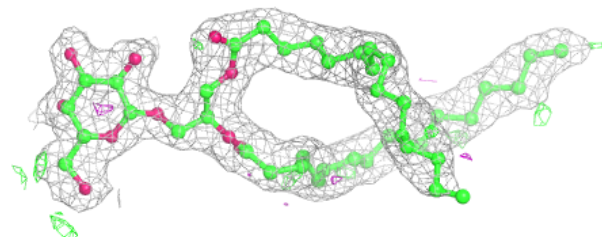
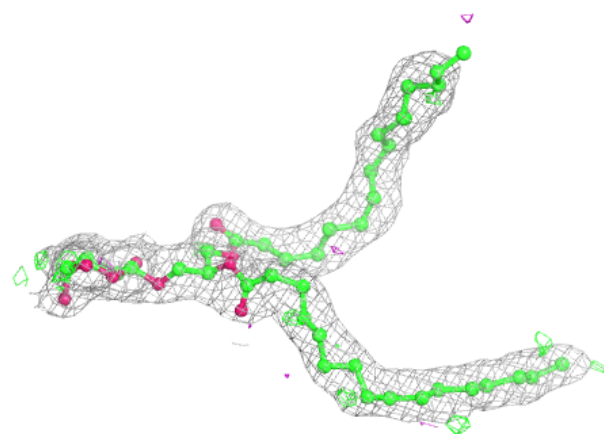


Electron density around HTG B 625:

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

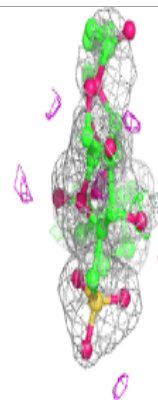
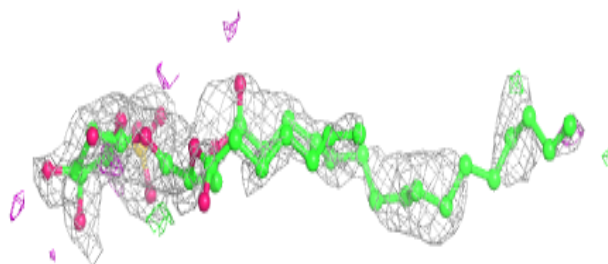
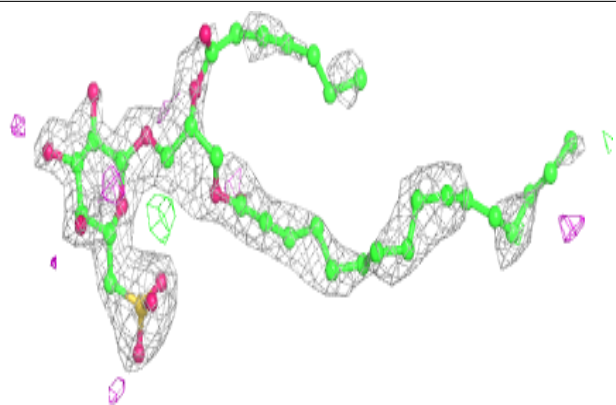
**Electron density around LMG B 622:**

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

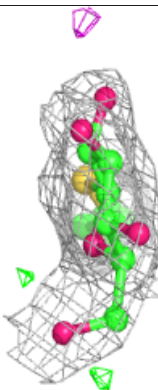
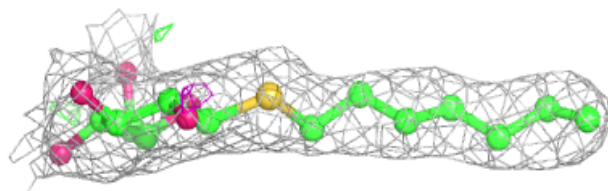
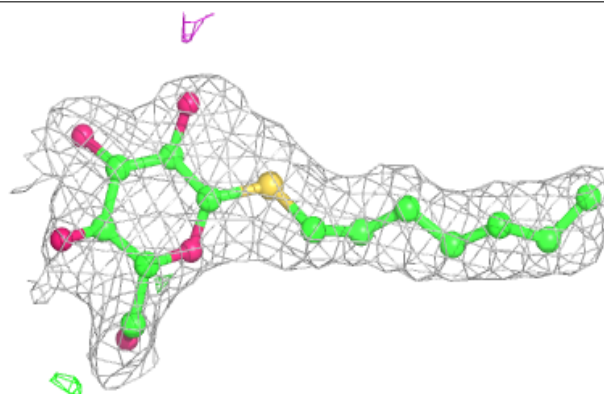


Electron density around SQD D 408:

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

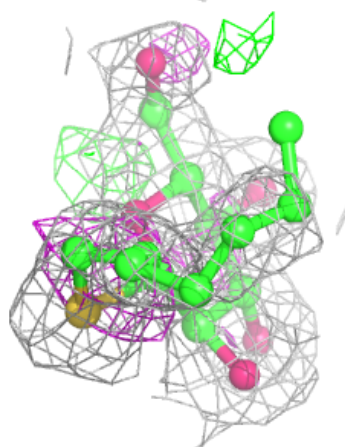
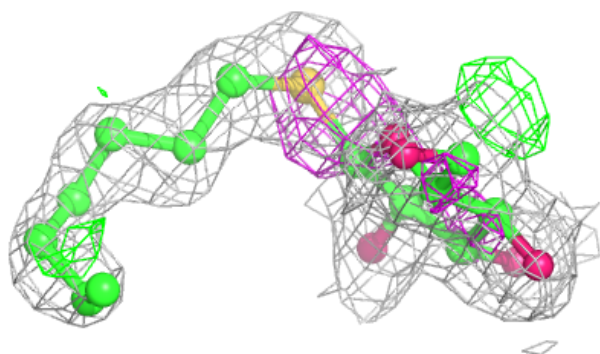
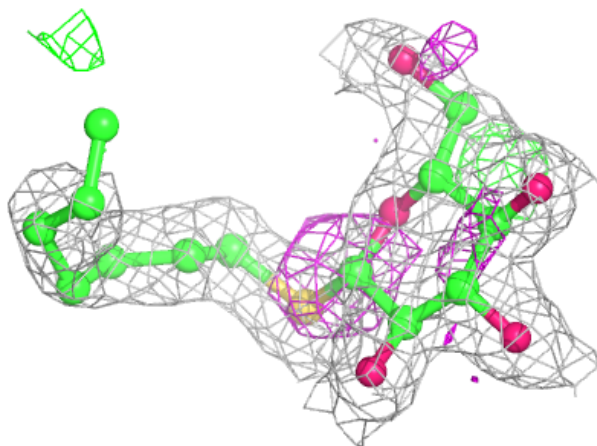
**Electron density around HTG B 630:**

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



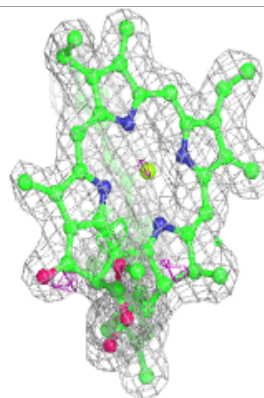
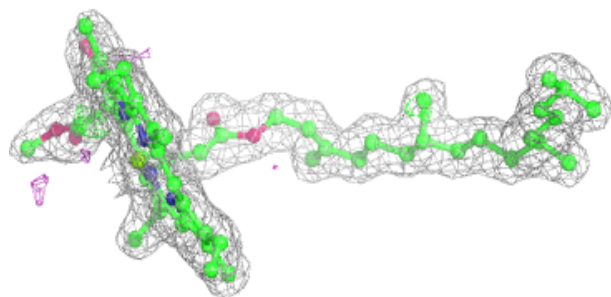
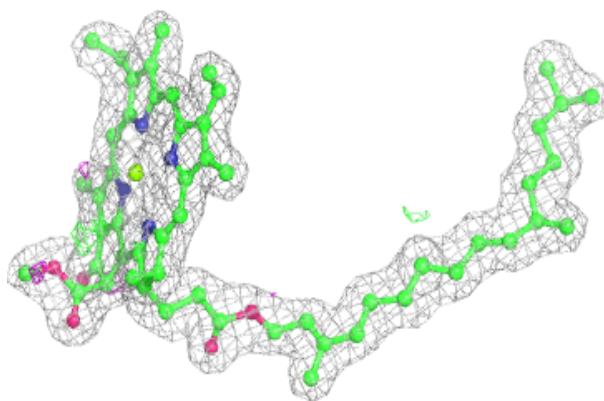
Electron density around HTG b 622:

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

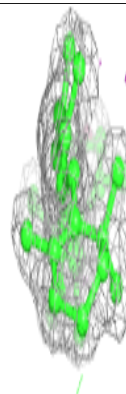
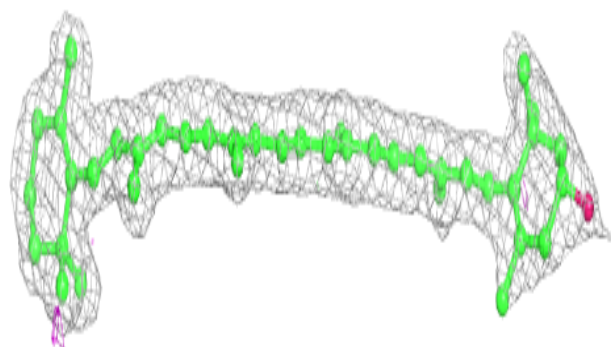
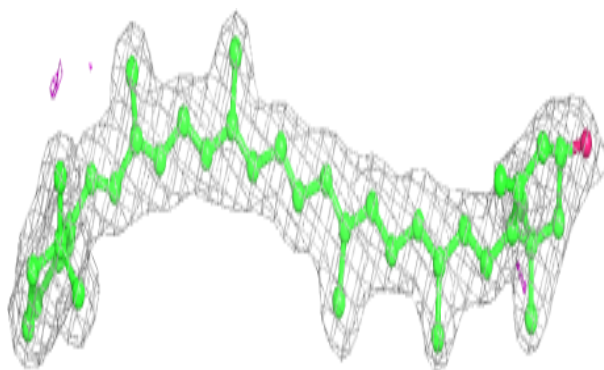


Electron density around CLA B 610:

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

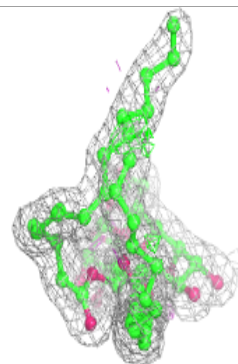
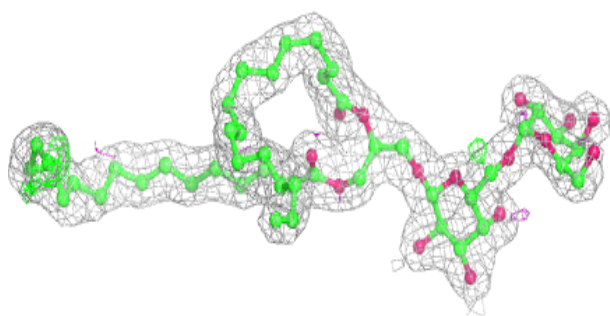
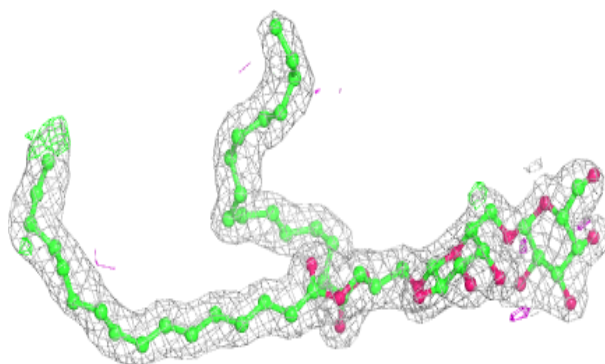
**Electron density around RRX x 102:**

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

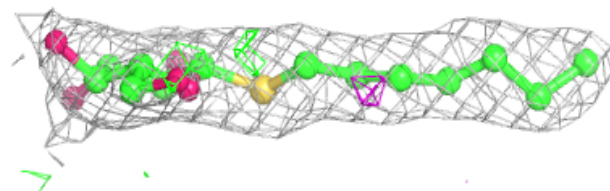
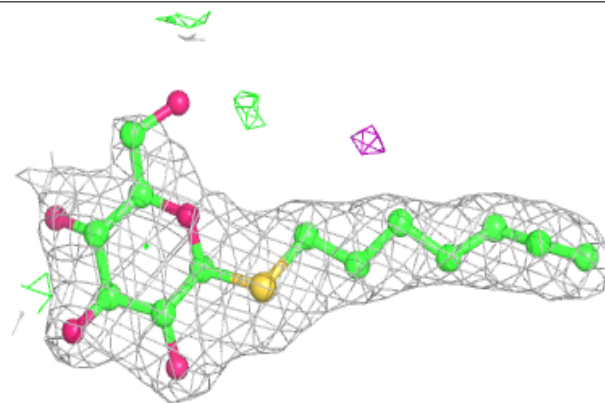


Electron density around DGD h 102:

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

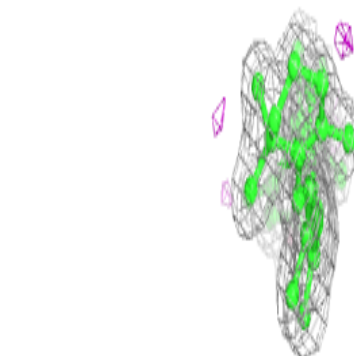
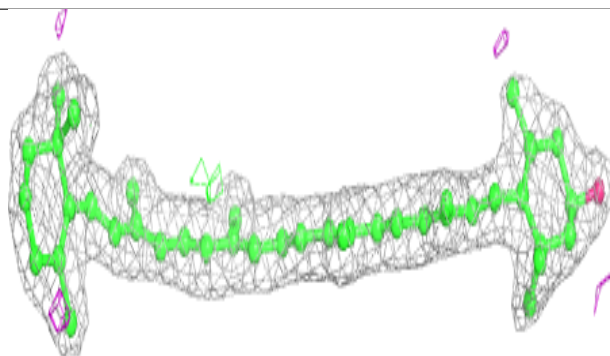
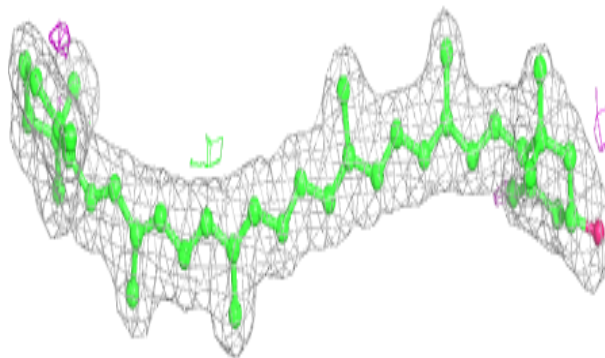
**Electron density around HTG b 627:**

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

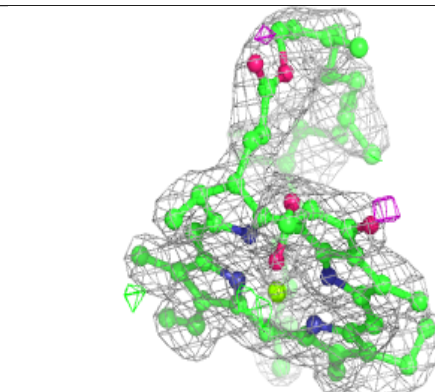
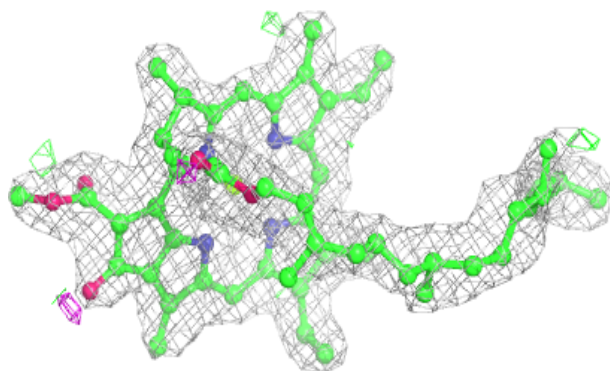
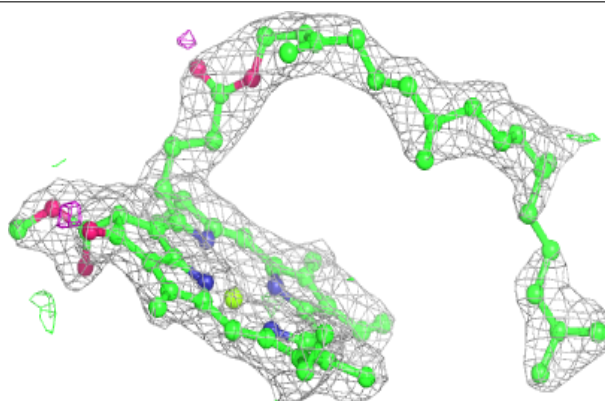


Electron density around RRX H 102:

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

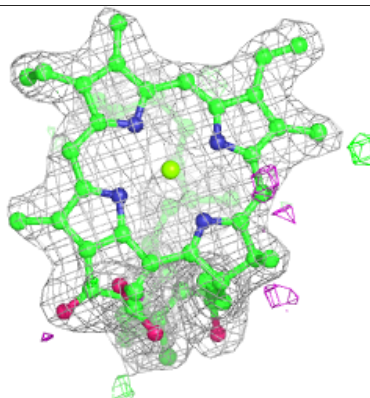
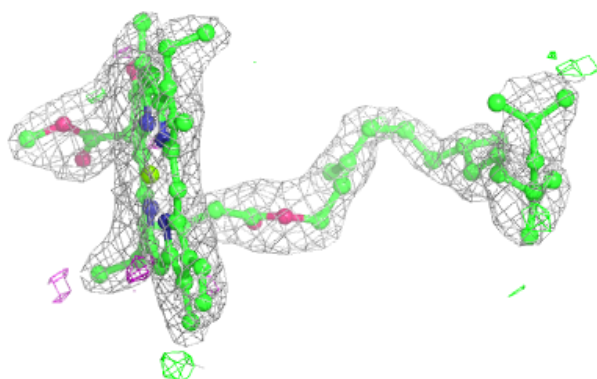
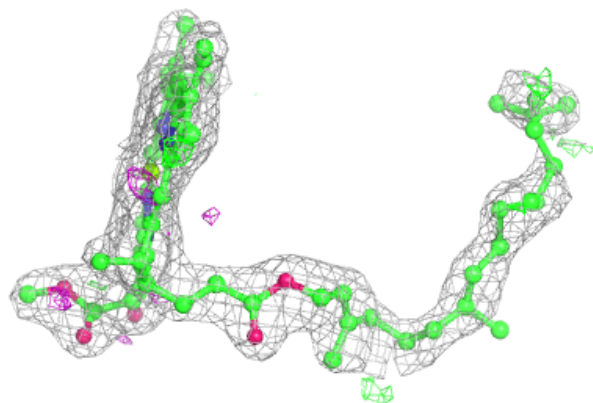
**Electron density around CLA C 514:**

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

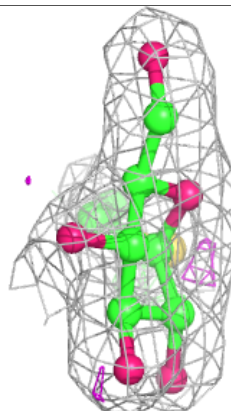
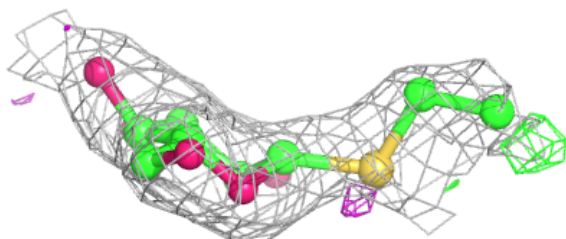
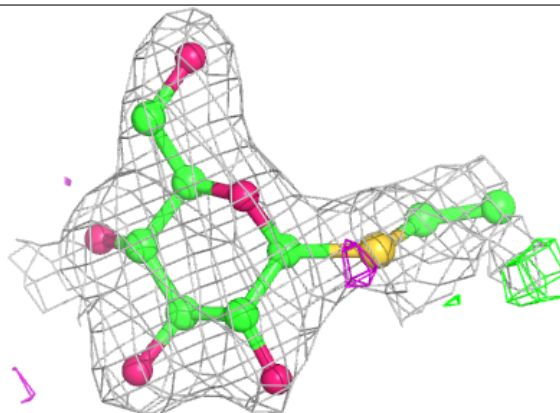


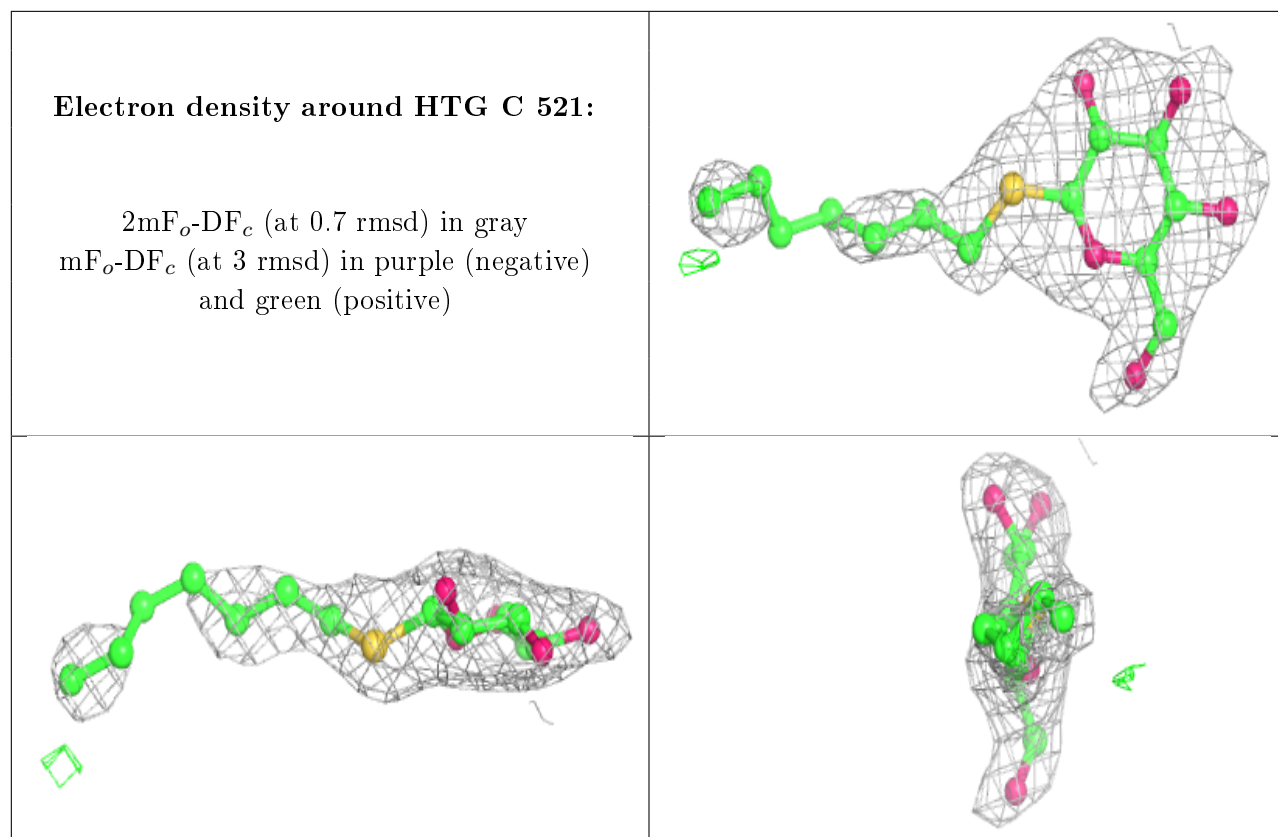
Electron density around CLA C 507:

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

**Electron density around HTG V 204:**

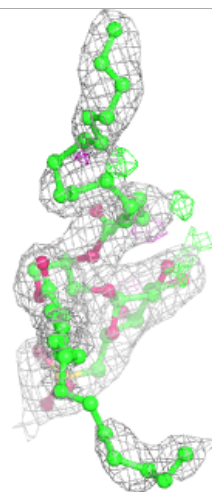
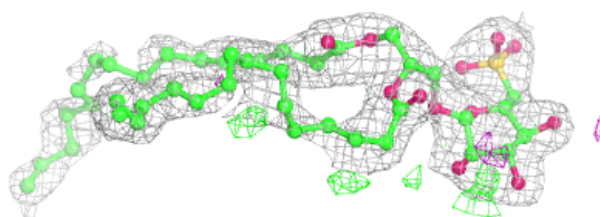
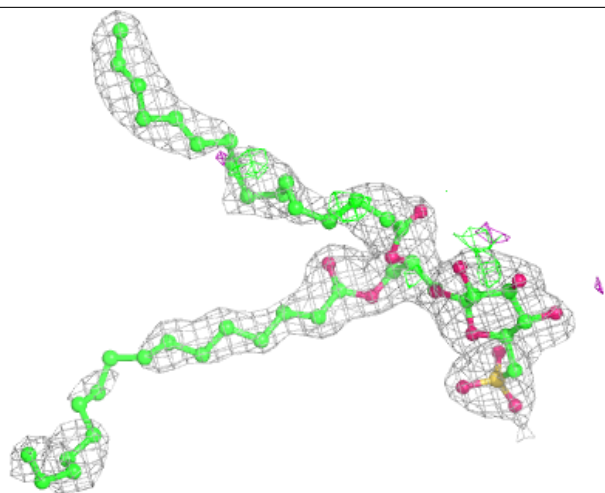
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





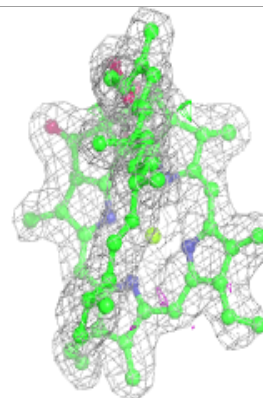
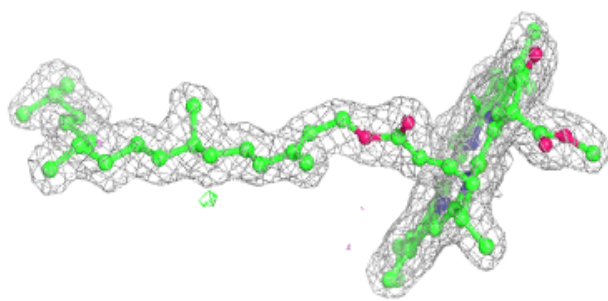
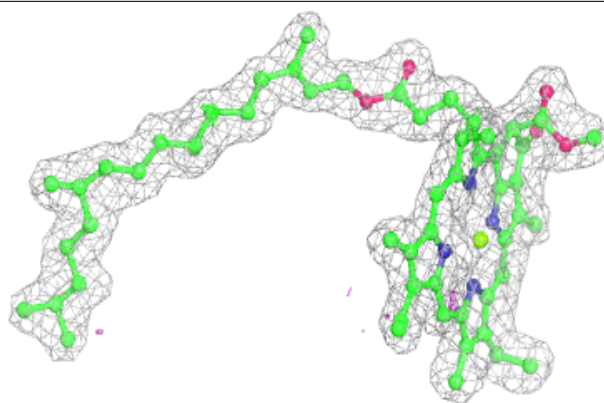
Electron density around SQD A 410:

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



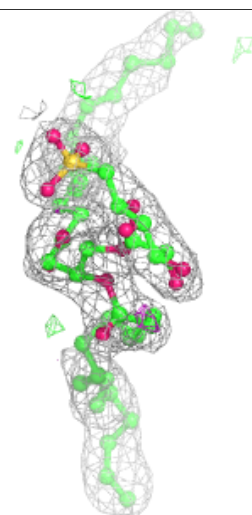
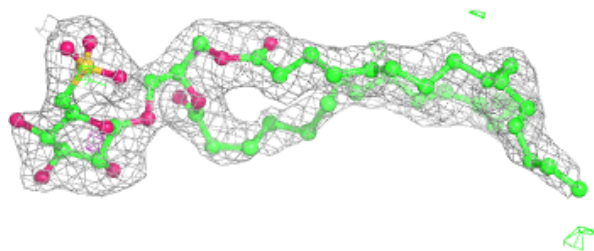
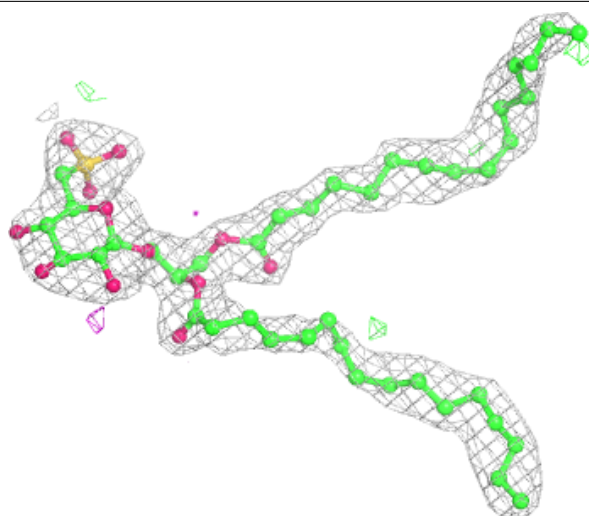
Electron density around CLA b 610:

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



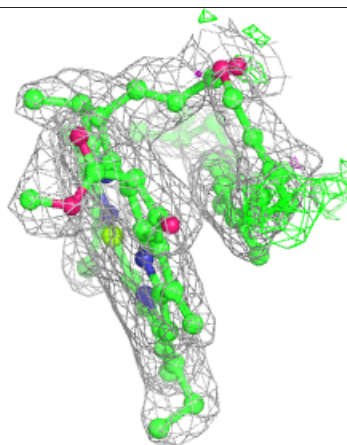
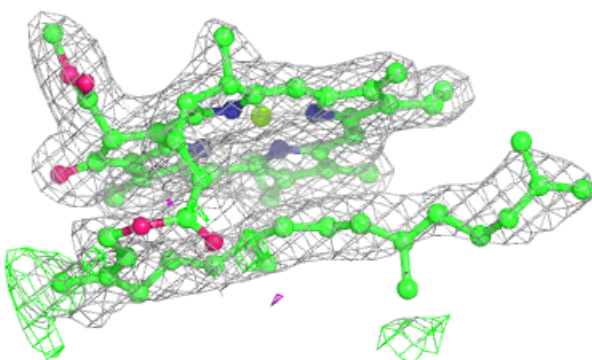
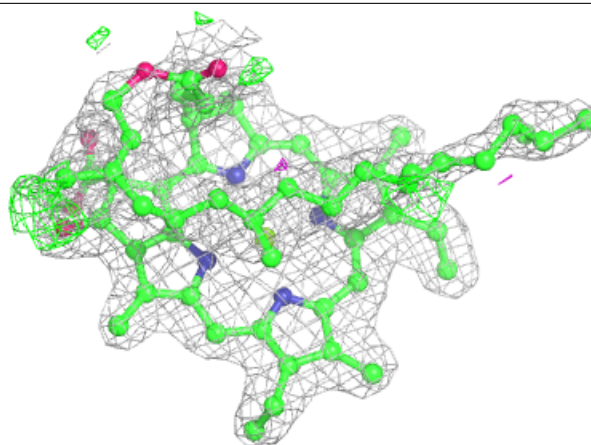
Electron density around SQD a 412:

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

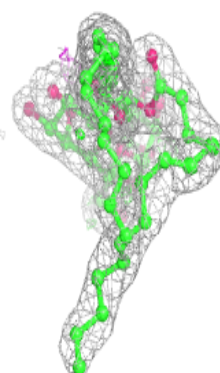
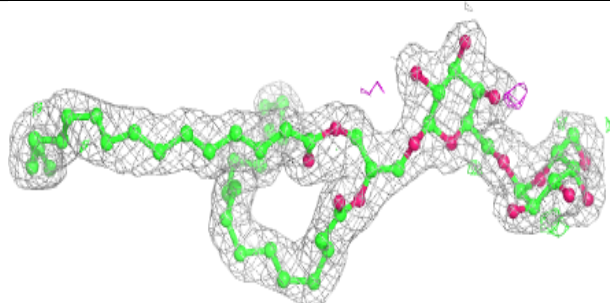
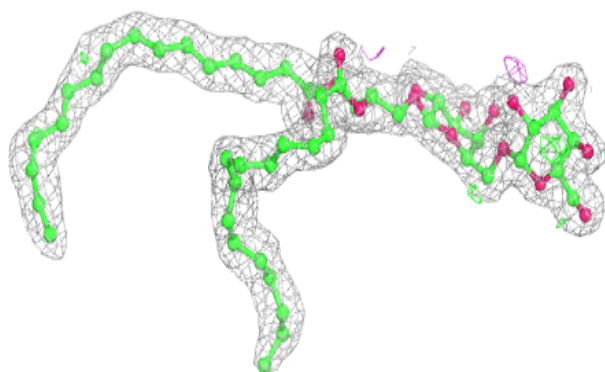


Electron density around CLA b 602:

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

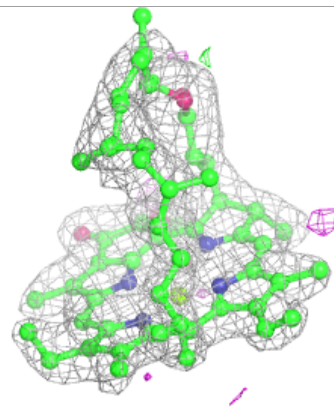
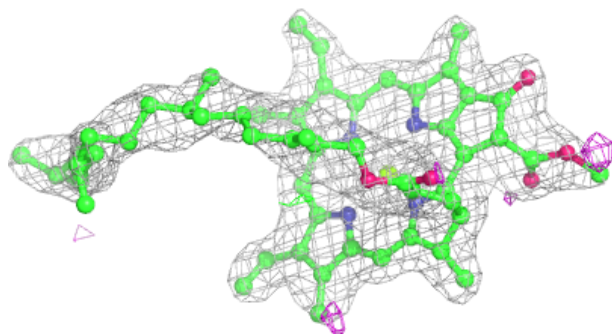
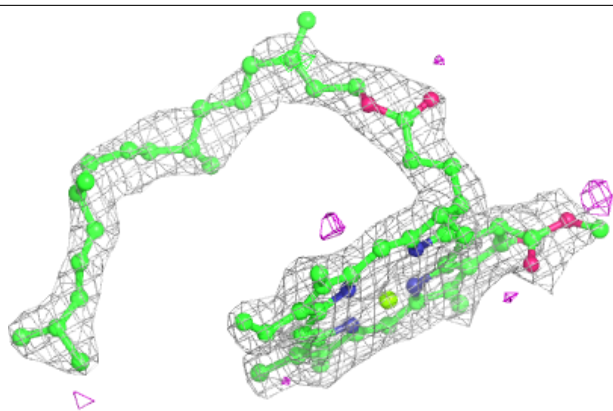
**Electron density around DGD H 103:**

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



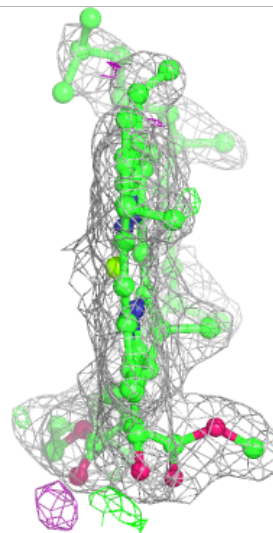
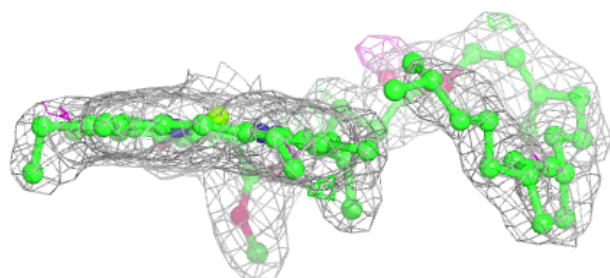
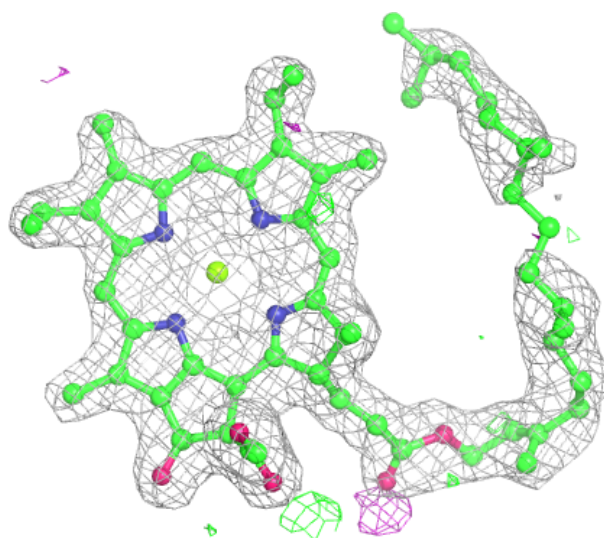
Electron density around CLA c 914:

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



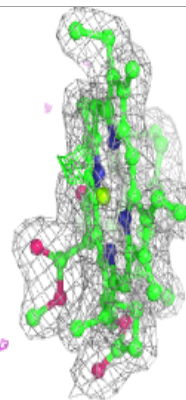
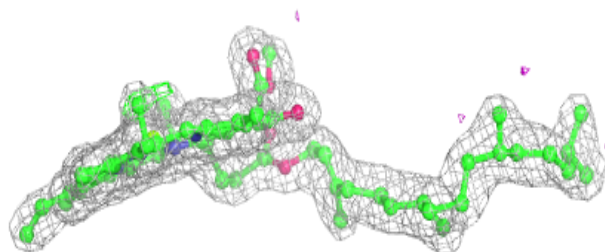
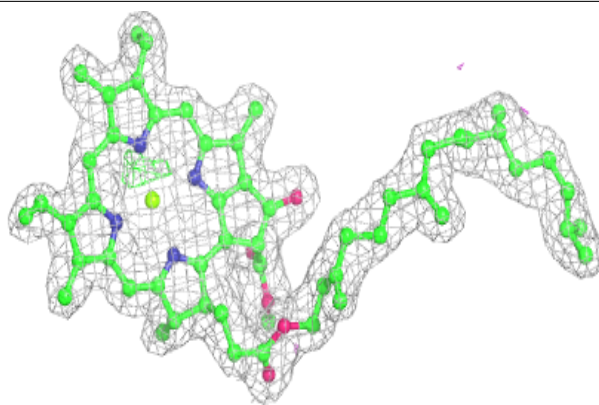
Electron density around CLA c 913:

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

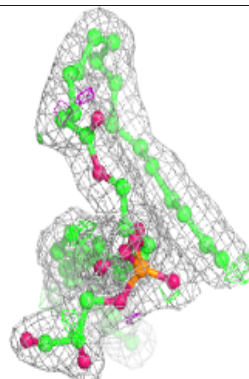
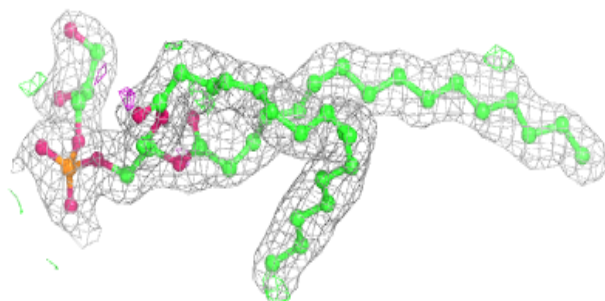
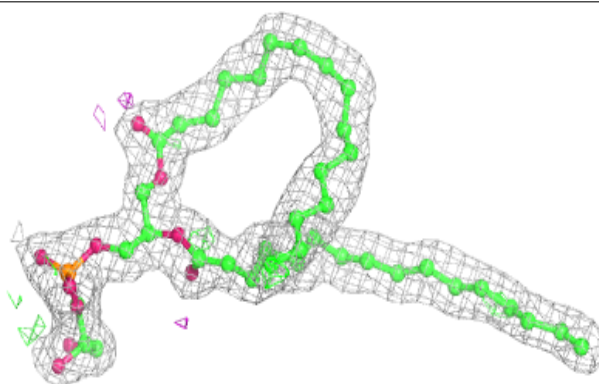


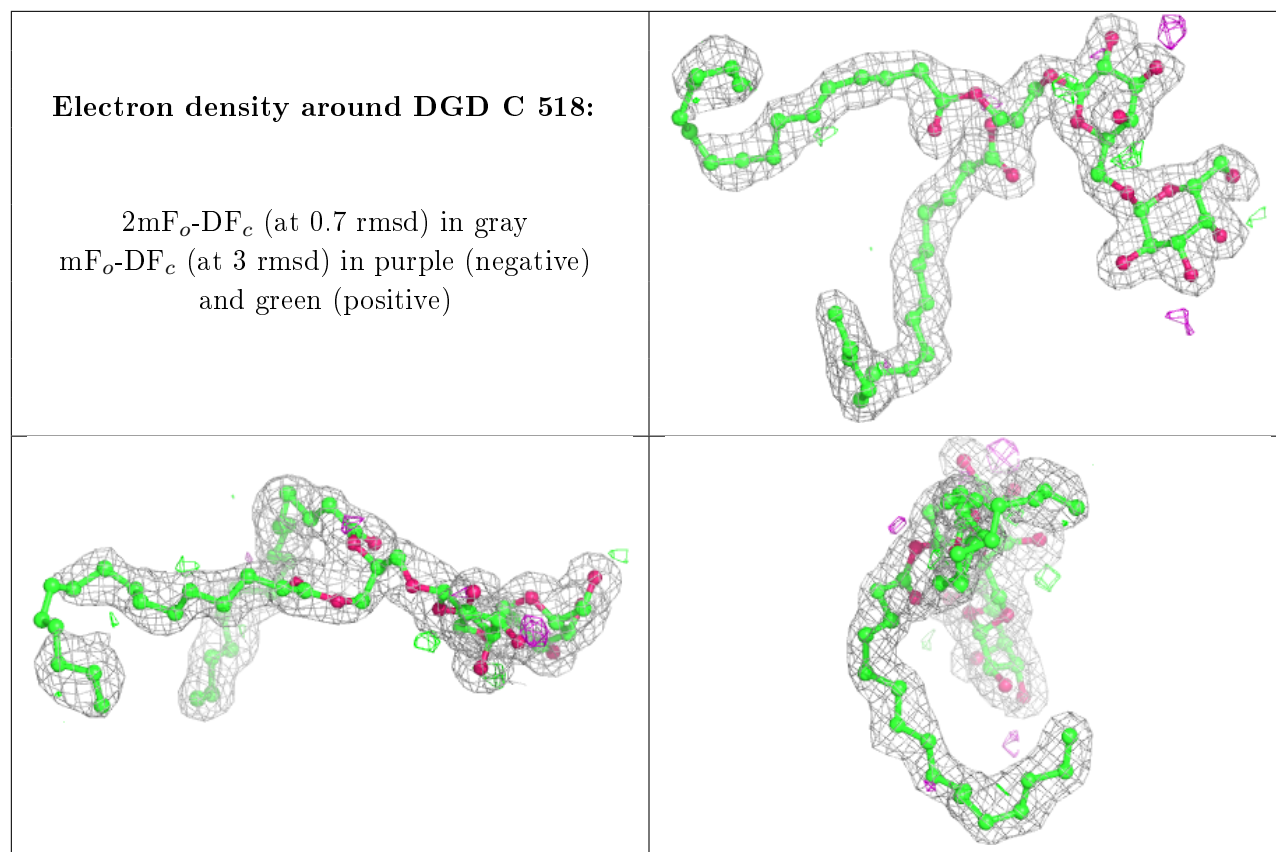
Electron density around CLA B 603:

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

**Electron density around LHG D 409:**

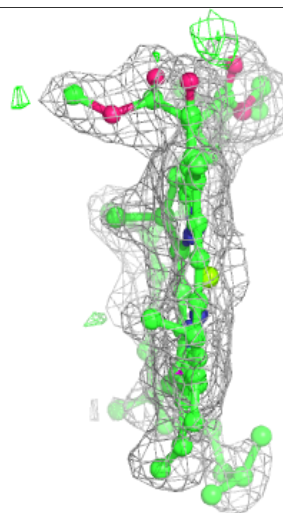
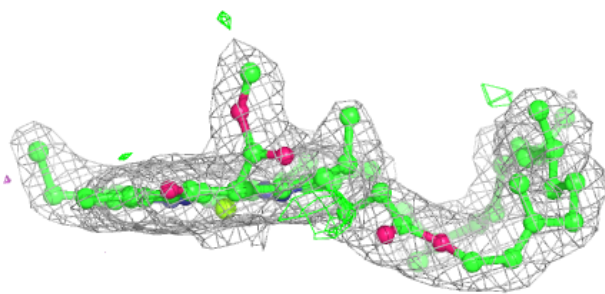
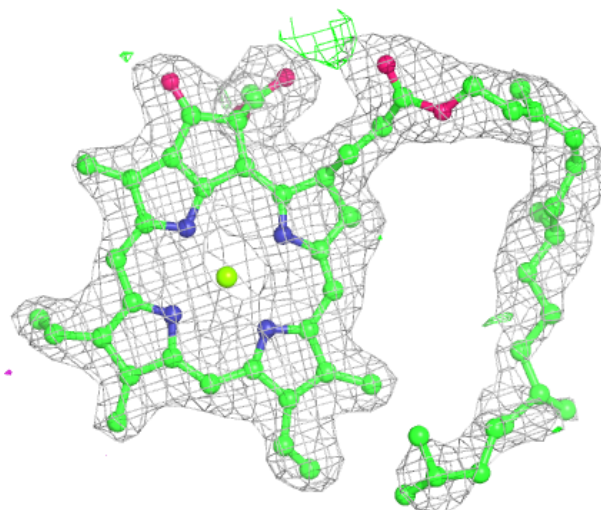
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





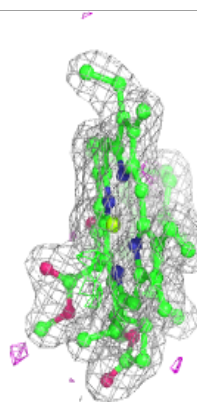
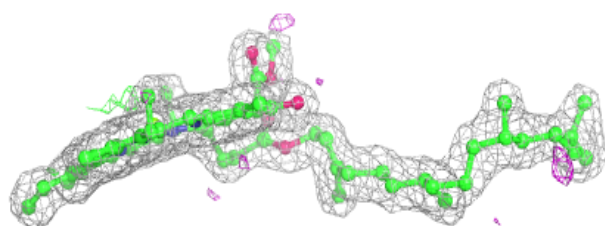
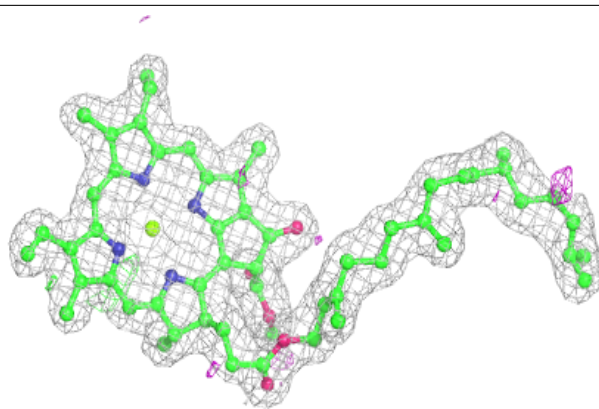
Electron density around CLA C 513:

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

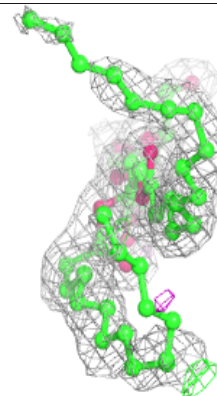
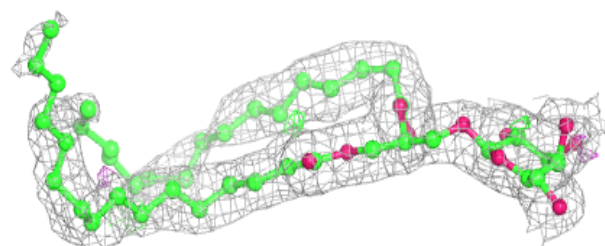
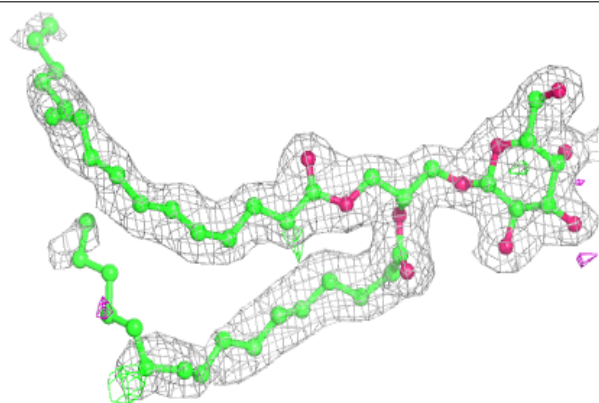


Electron density around CLA b 603:

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

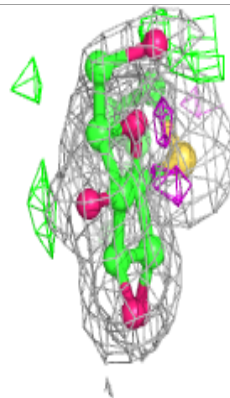
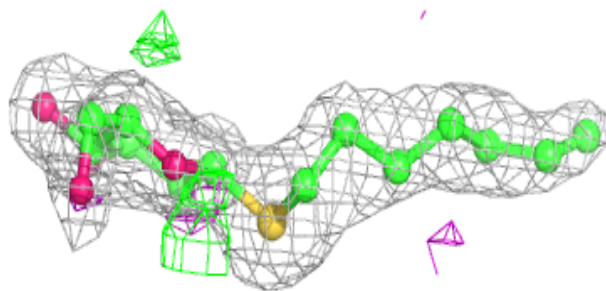
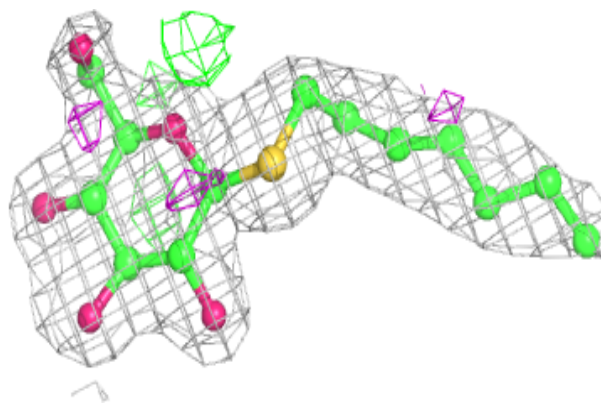
**Electron density around LMG J 101:**

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

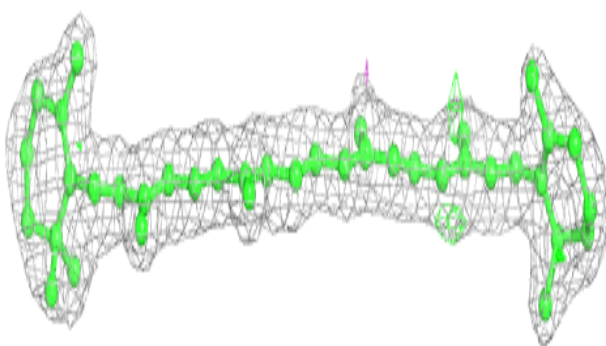
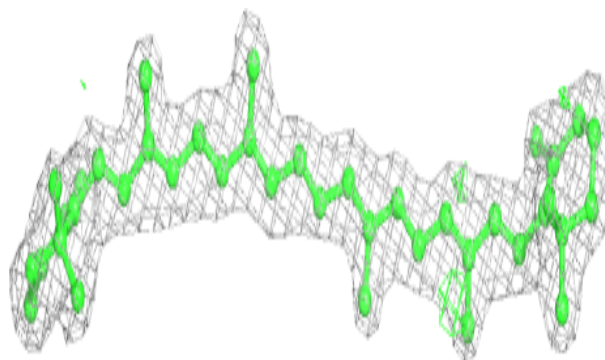


Electron density around HTG B 624:

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

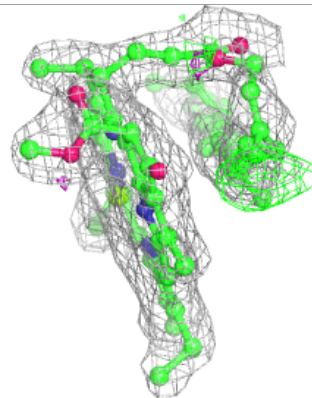
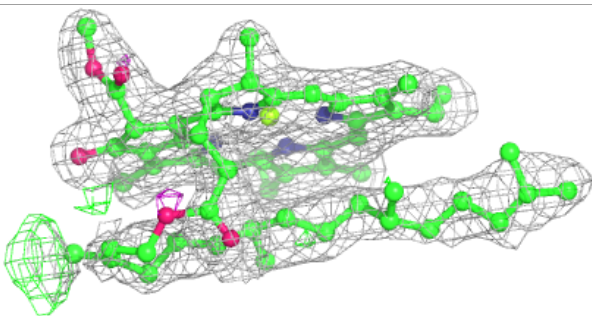
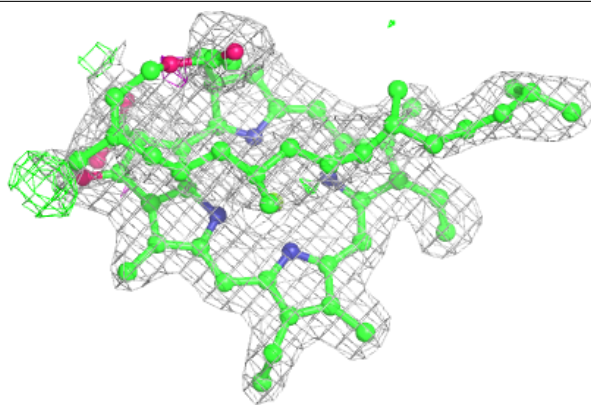
**Electron density around BCR C 515:**

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



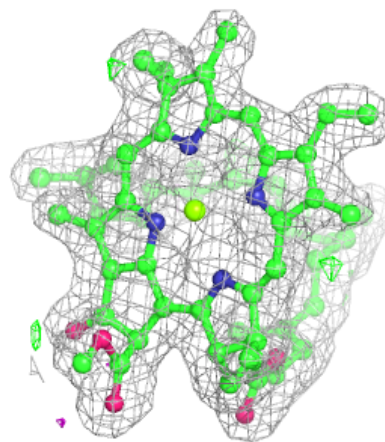
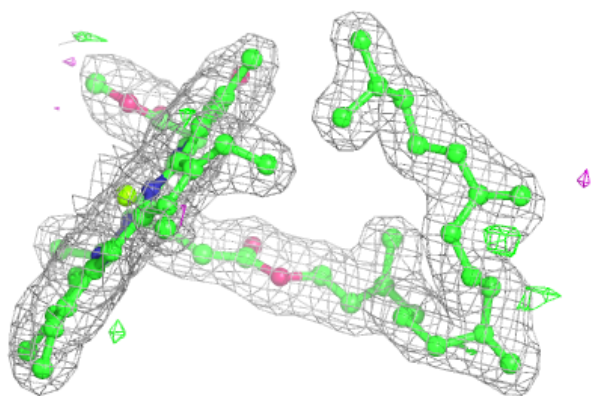
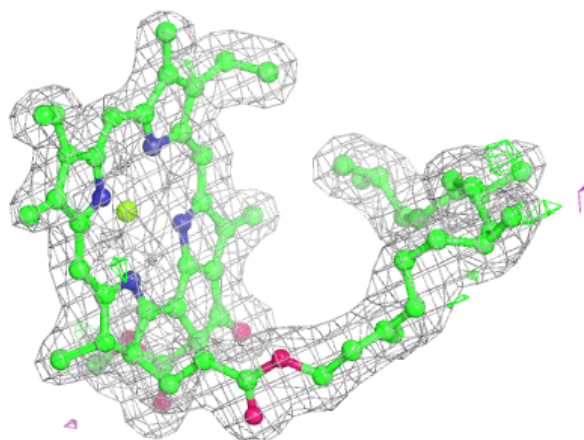
Electron density around CLA B 602:

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



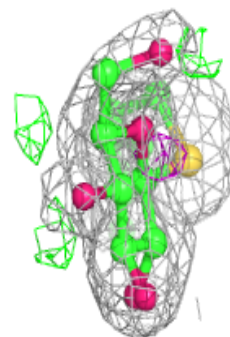
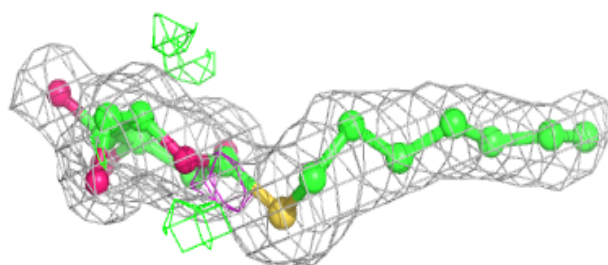
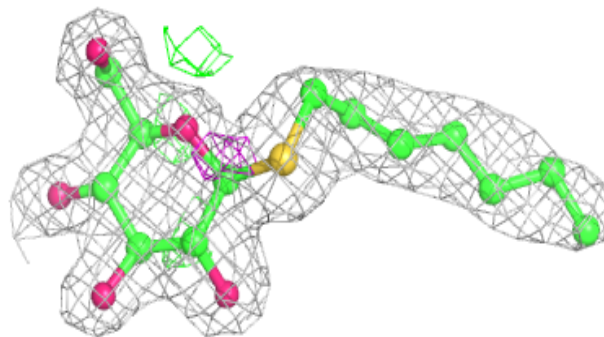
Electron density around CLA c 904:

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

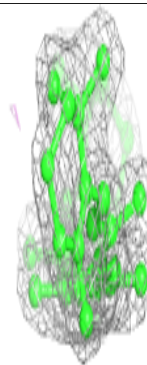
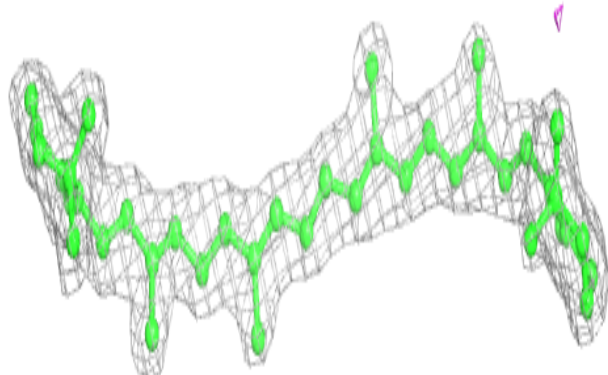
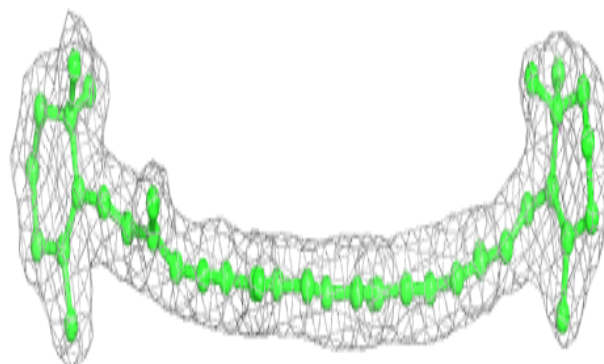


Electron density around HTG O 302:

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

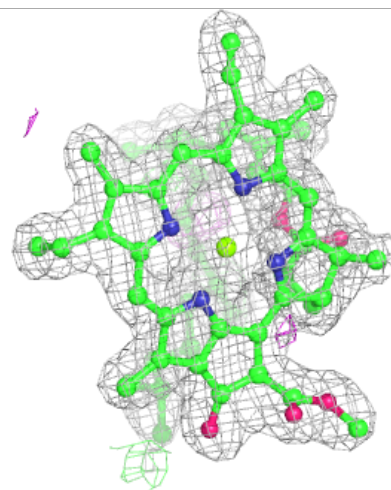
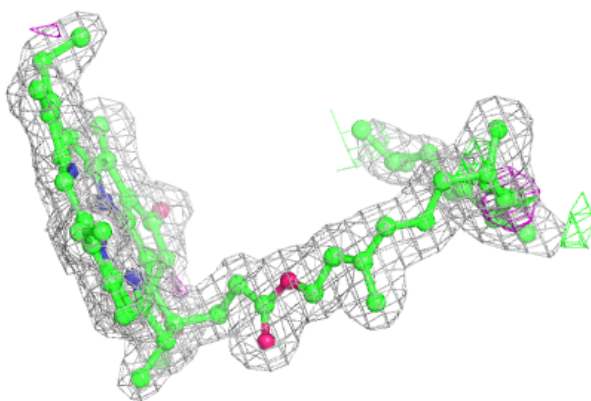
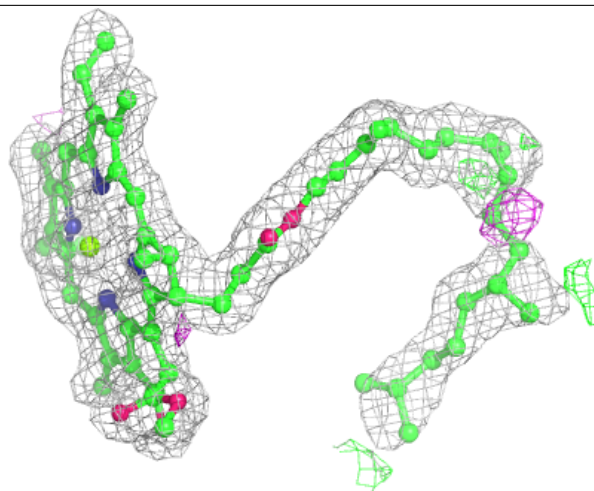
**Electron density around BCR k 102:**

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



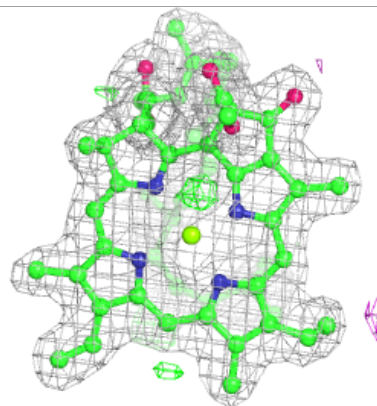
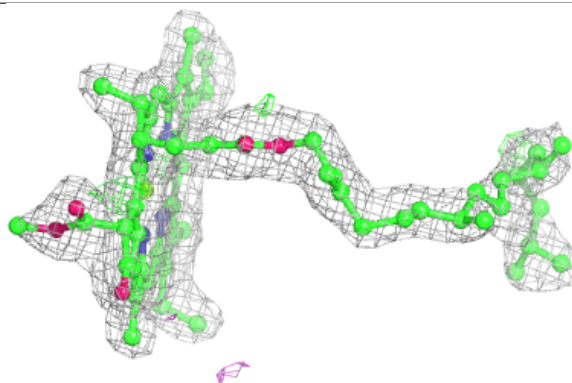
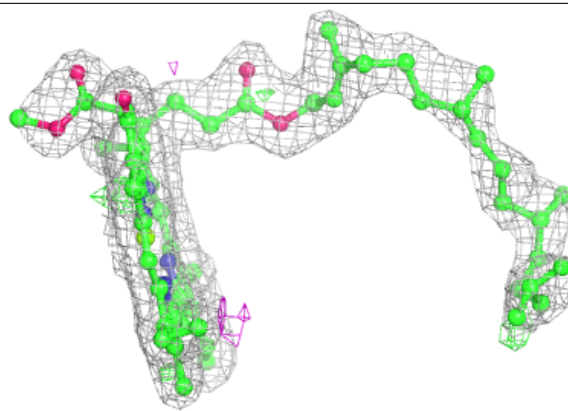
Electron density around CLA b 607:

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



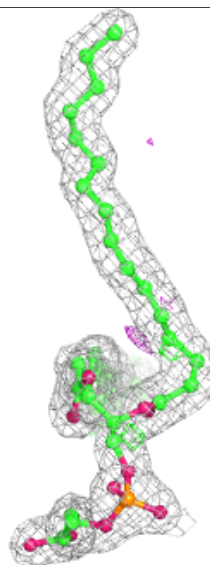
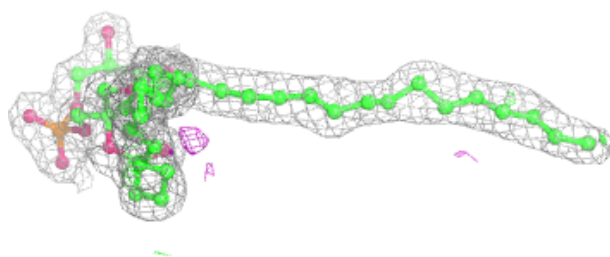
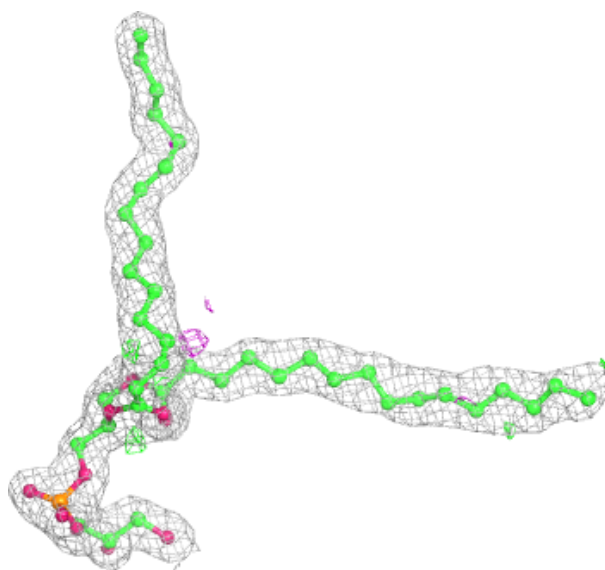
Electron density around CLA c 907:

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



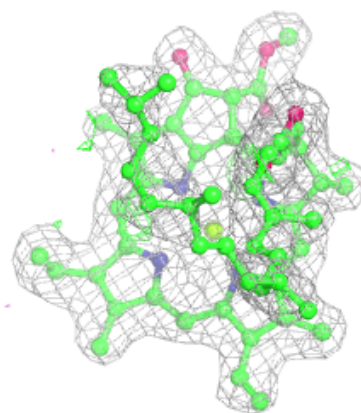
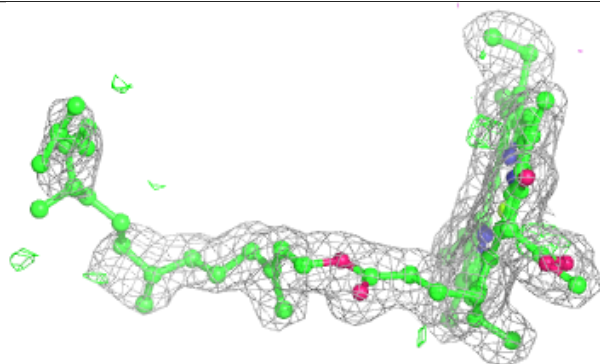
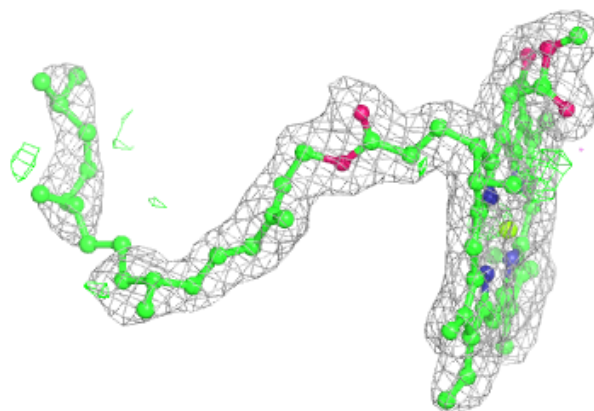
Electron density around LHG 1 101:

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

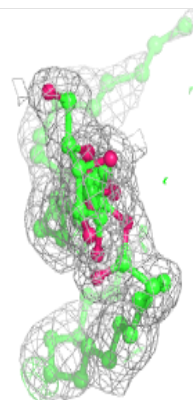
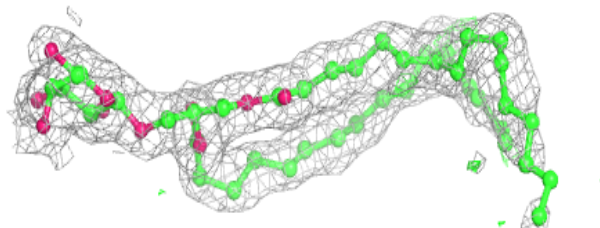
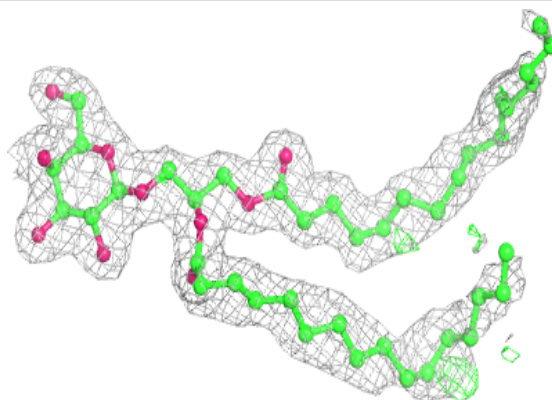


Electron density around CLA D 404:

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

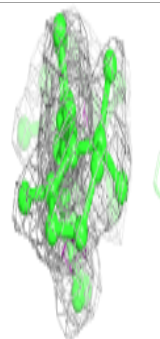
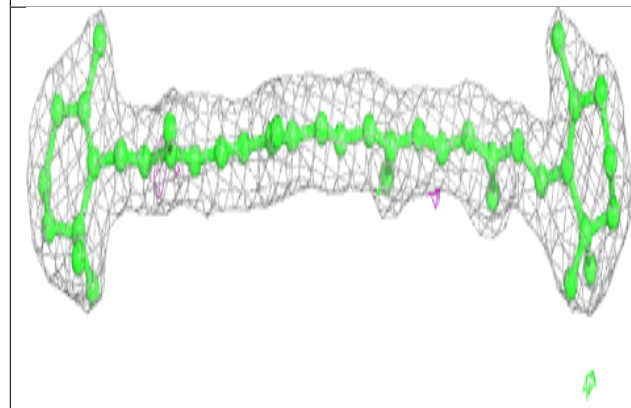
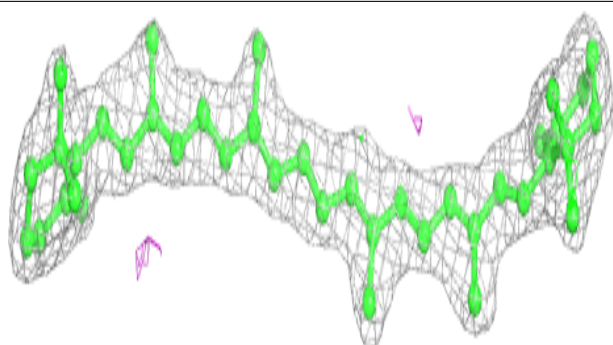
**Electron density around LMG j 101:**

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



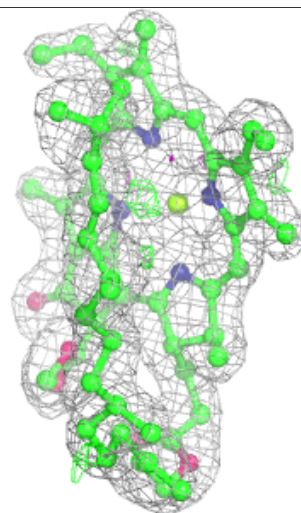
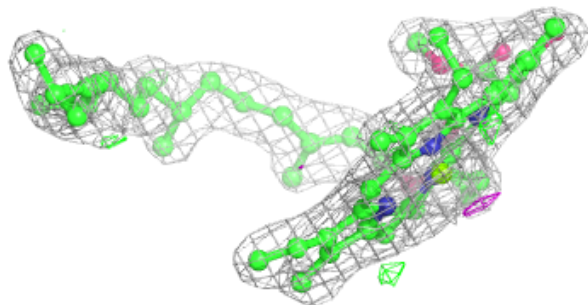
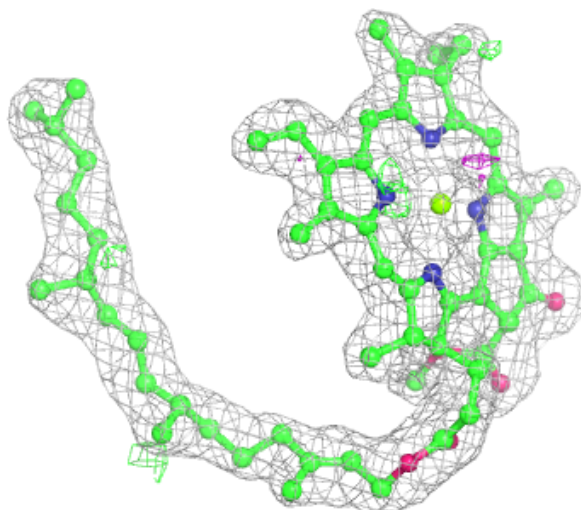
Electron density around BCR c 915:

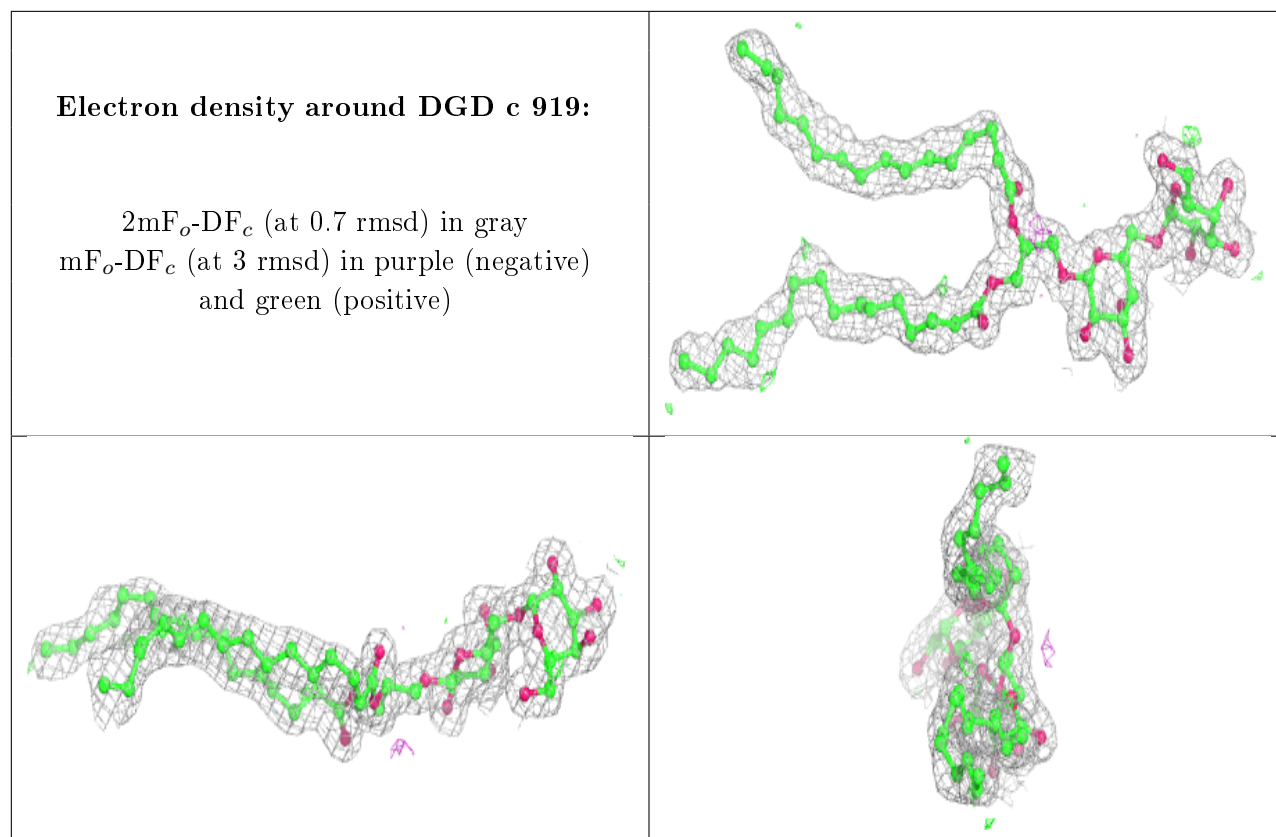
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA C 508:

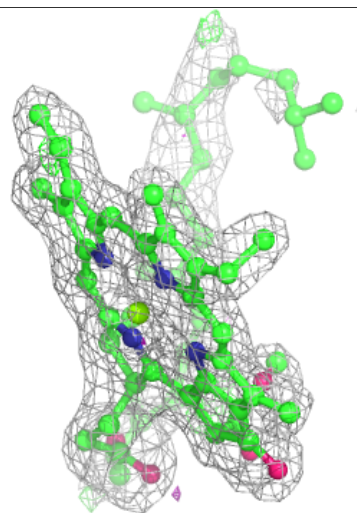
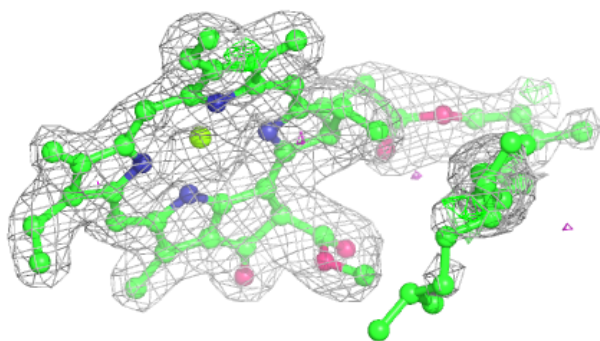
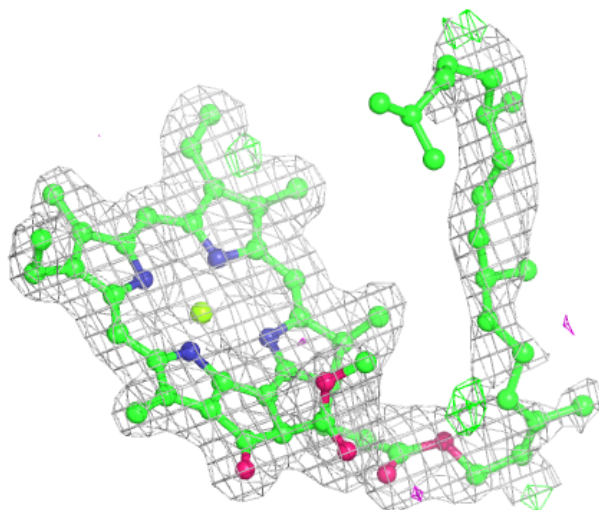
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





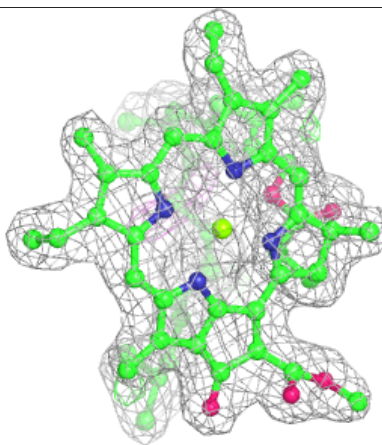
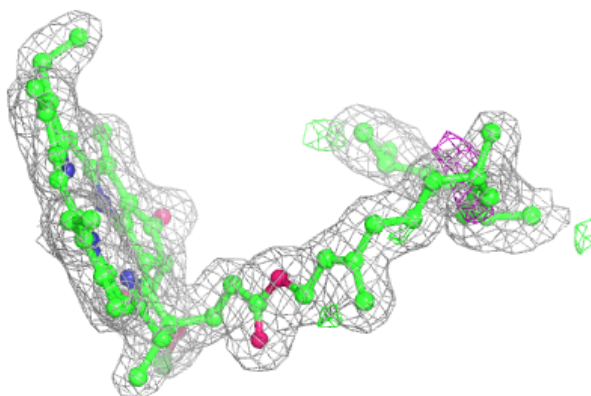
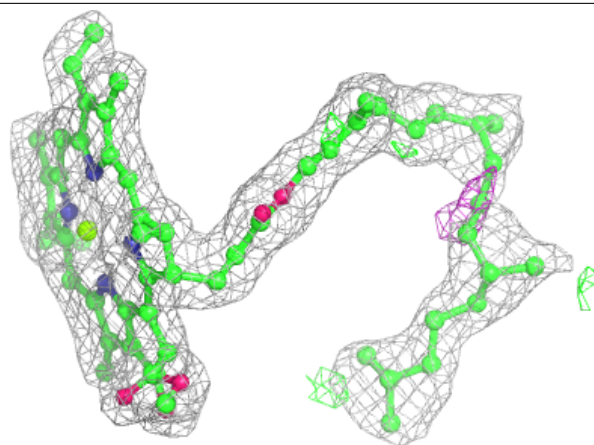
Electron density around CLA b 617:

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

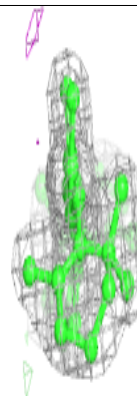
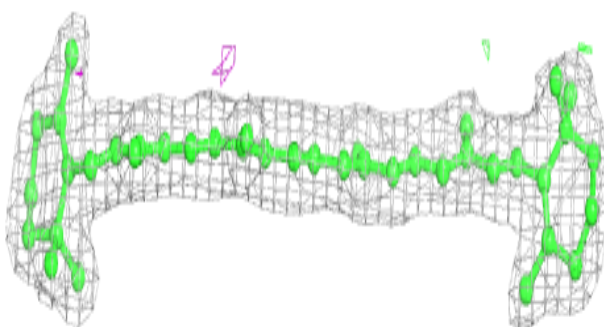
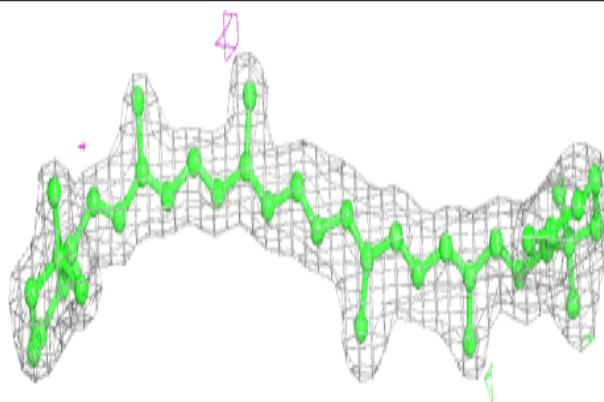


Electron density around CLA B 607:

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

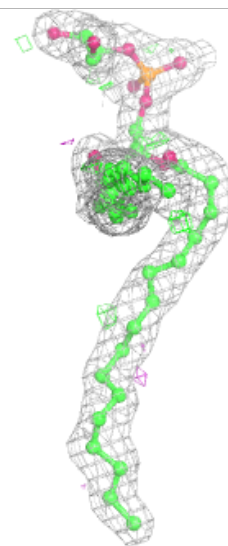
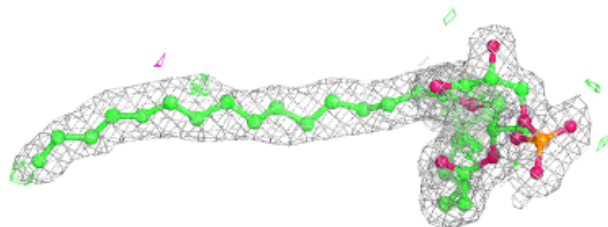
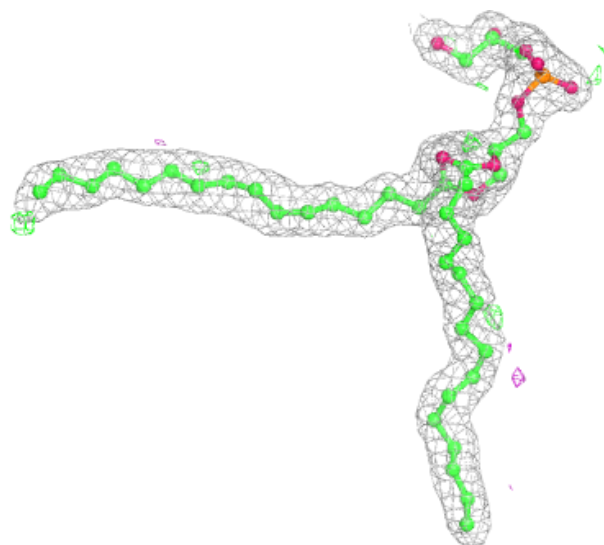
**Electron density around BCR C 516:**

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



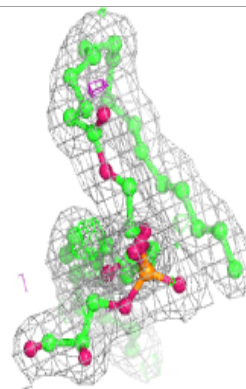
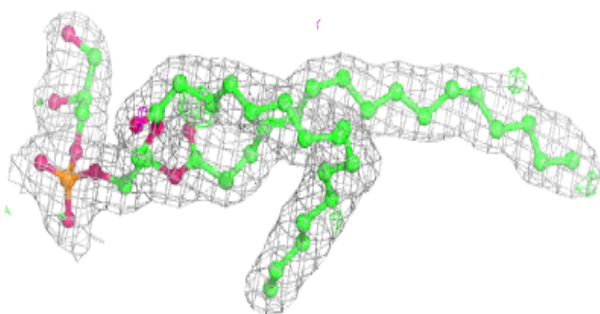
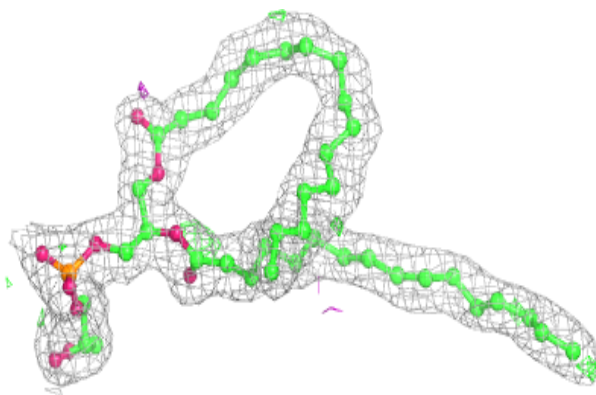
Electron density around LHG L 101:

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

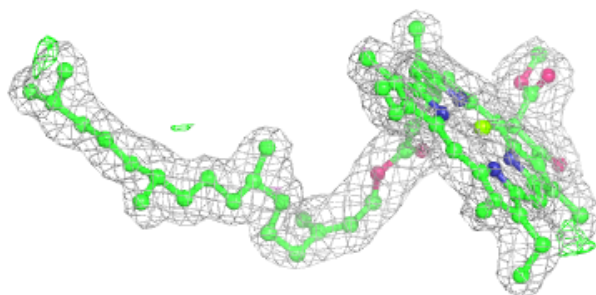
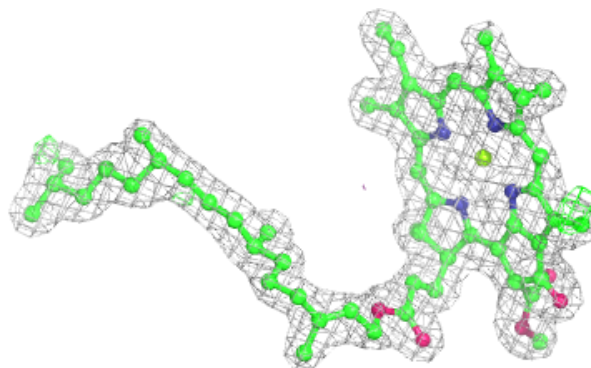


Electron density around LHG d 408:

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

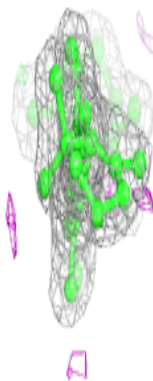
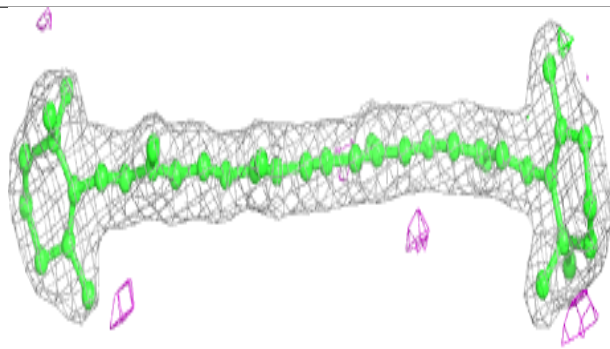
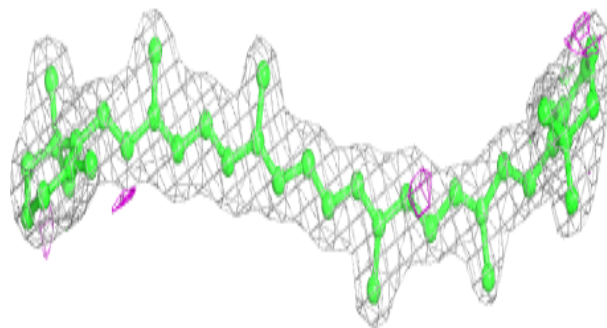
**Electron density around CLA C 512:**

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

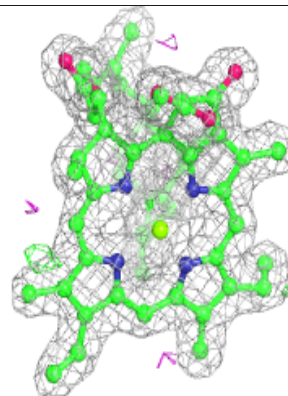
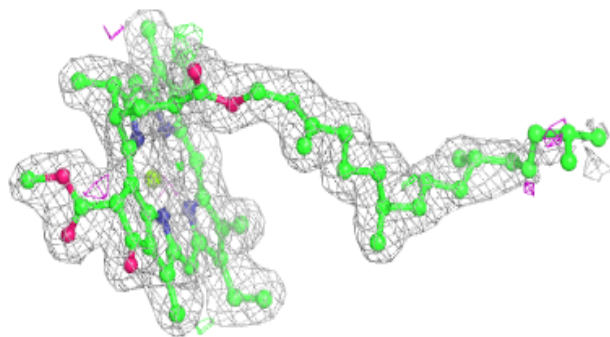
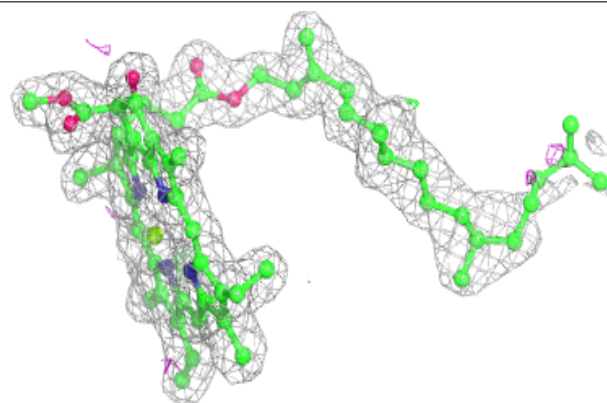


Electron density around BCR c 916:

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

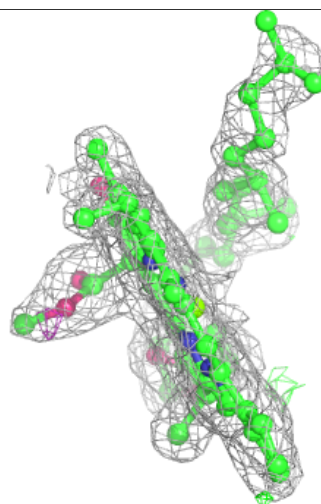
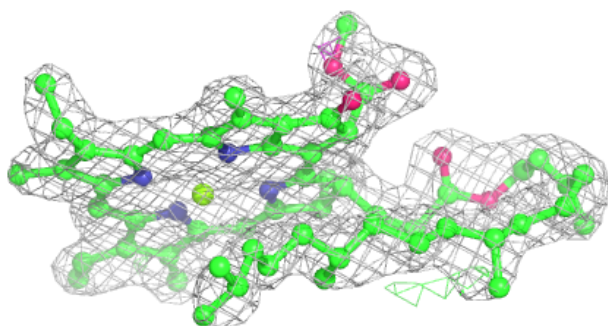
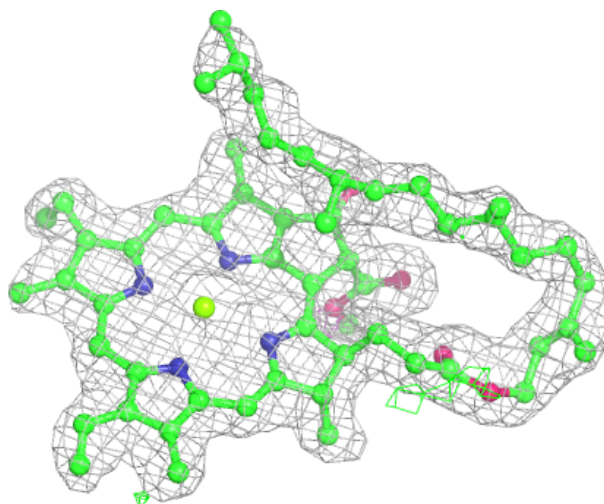
**Electron density around CLA c 909:**

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



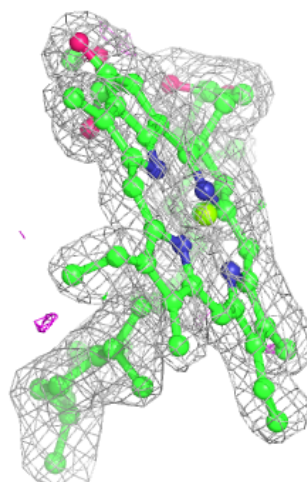
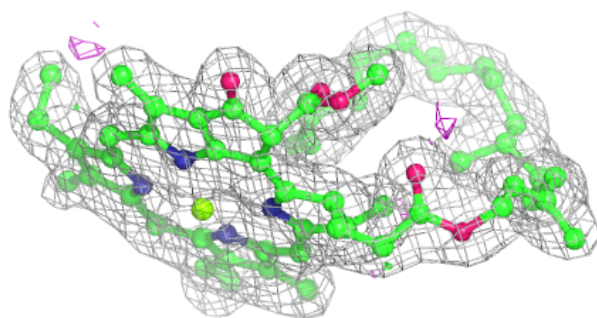
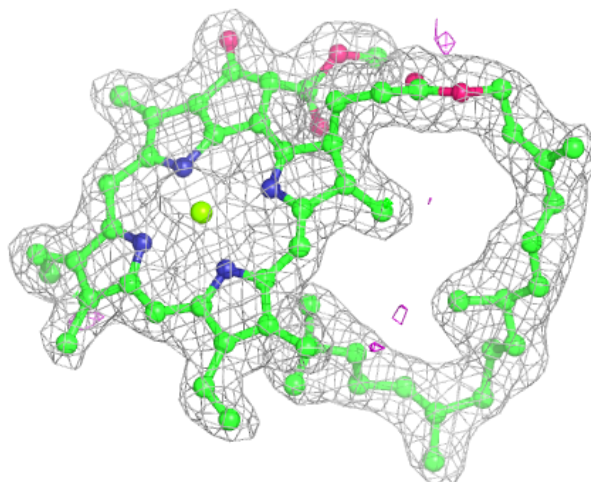
Electron density around CLA C 510:

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



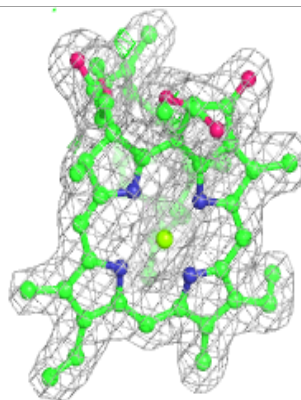
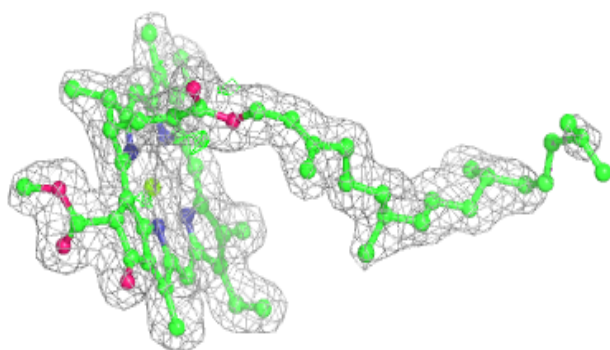
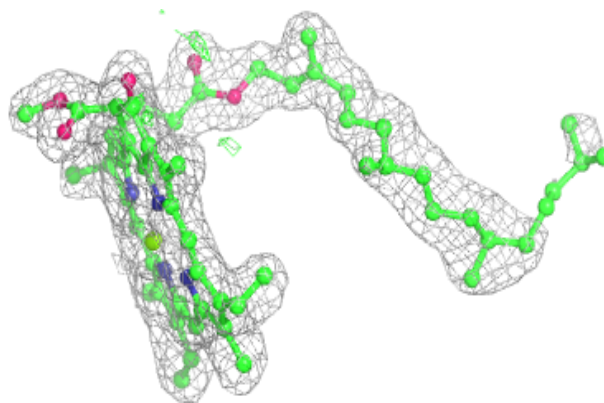
Electron density around CLA B 616:

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

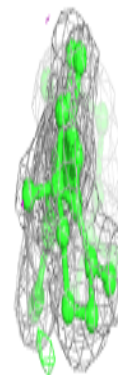
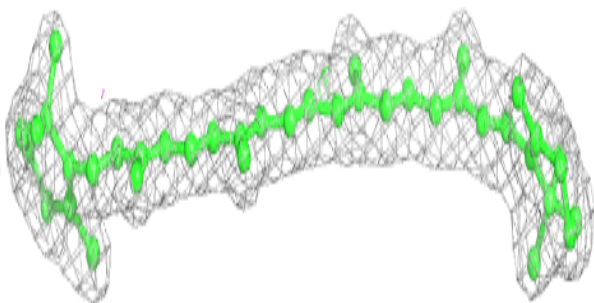
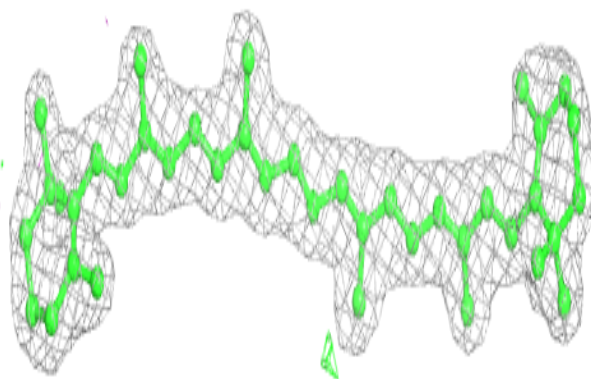


Electron density around CLA C 509:

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

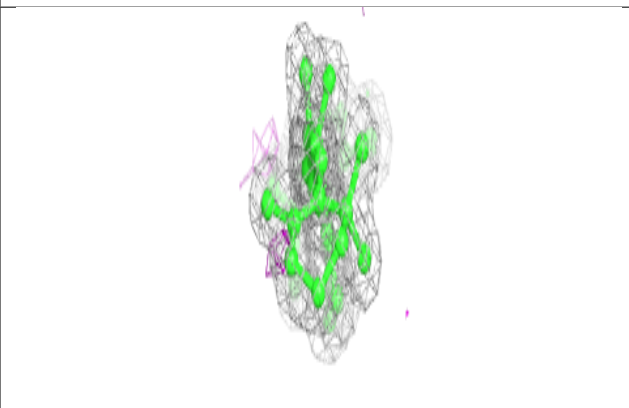
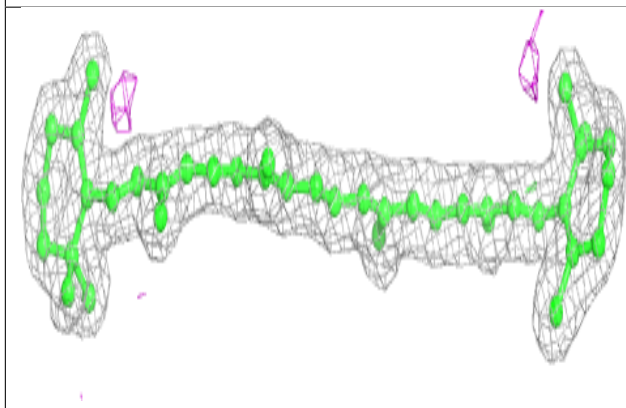
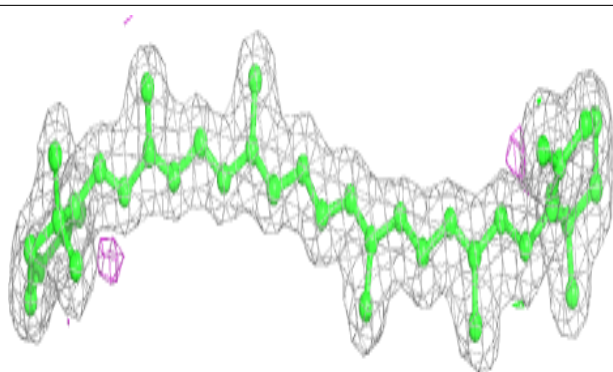
**Electron density around BCR b 620:**

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

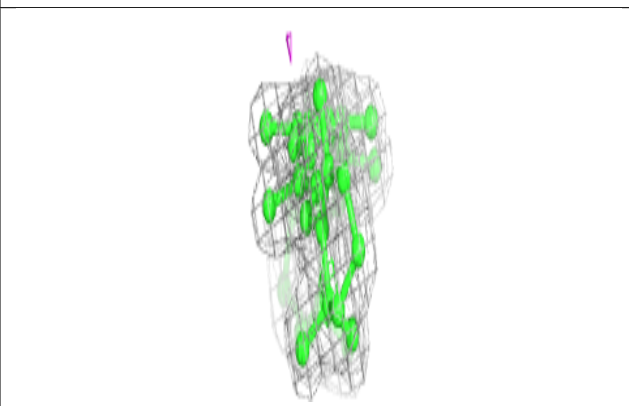
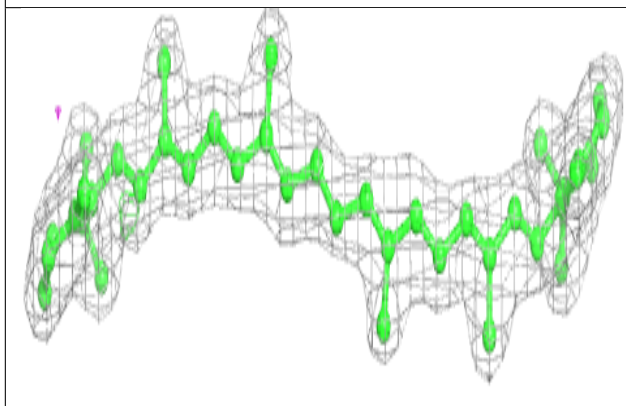
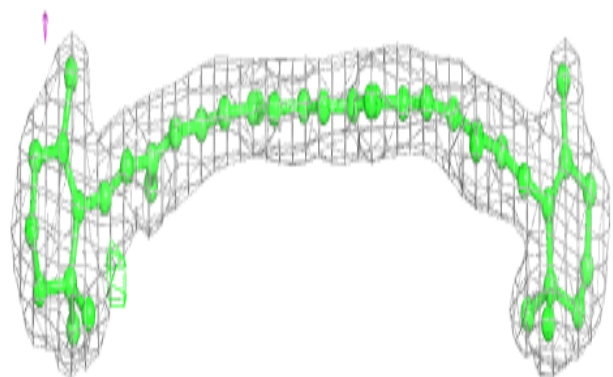


Electron density around BCR a 411:

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

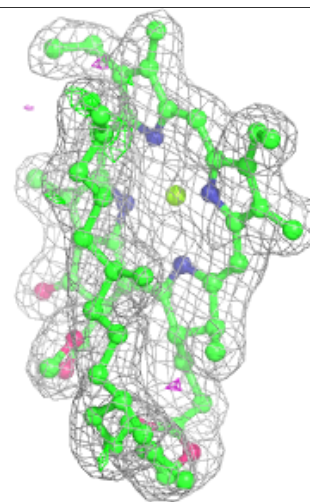
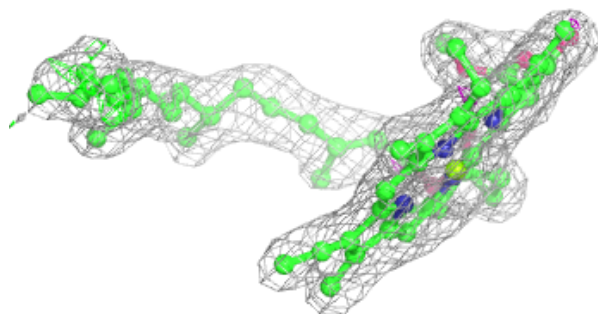
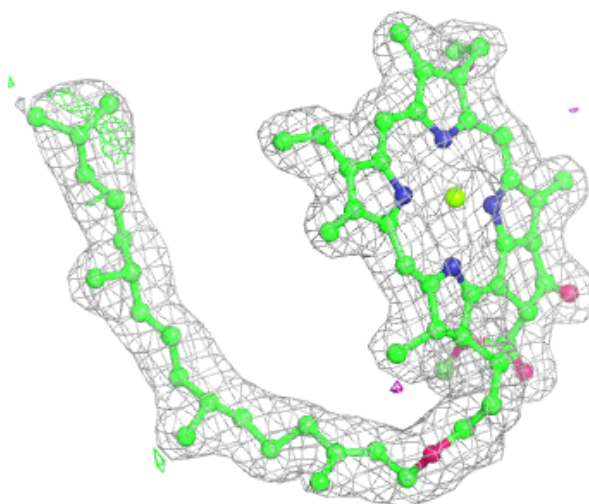
**Electron density around BCR C 530:**

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



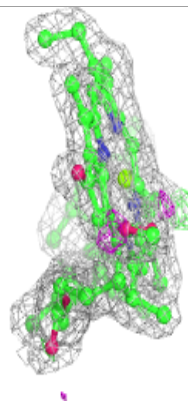
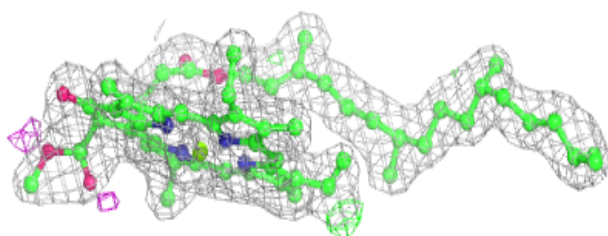
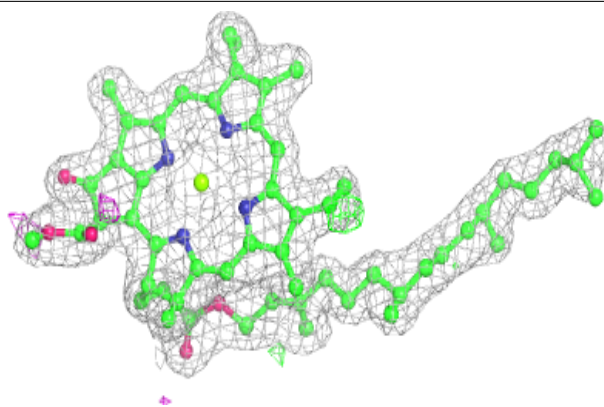
Electron density around CLA c 908:

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

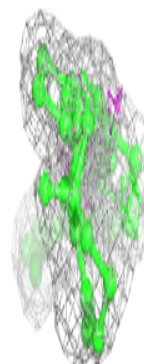
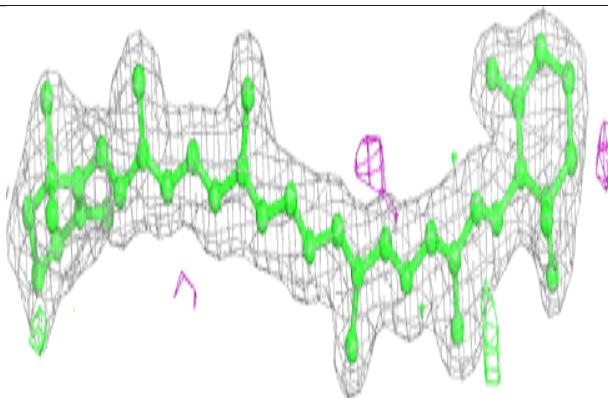
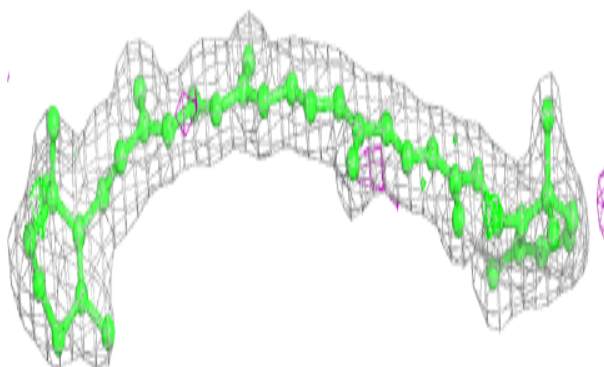


Electron density around CLA C 502:

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

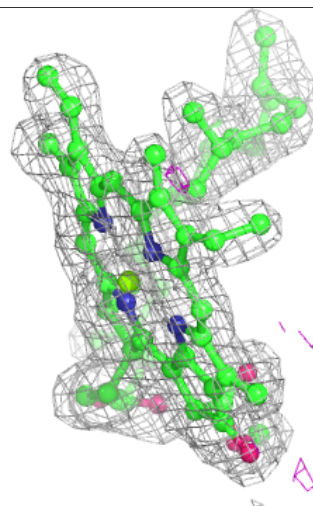
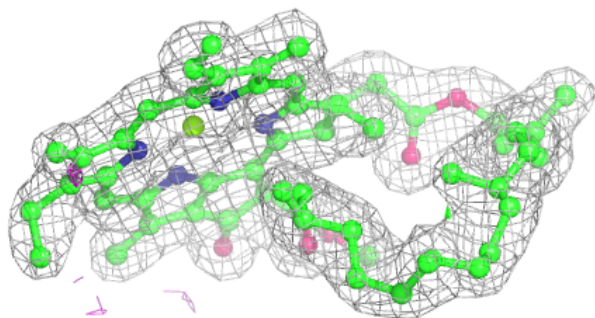
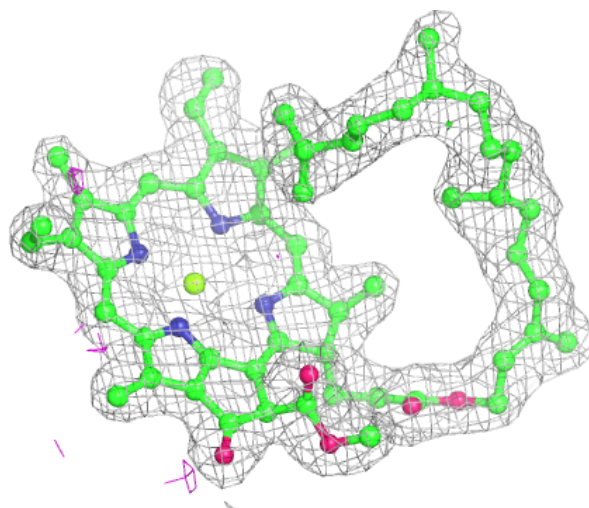
**Electron density around BCR D 405:**

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



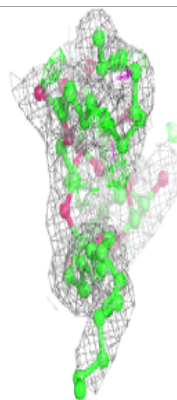
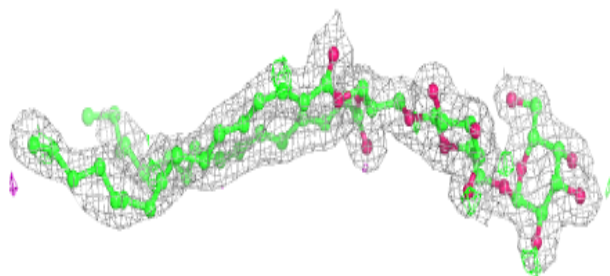
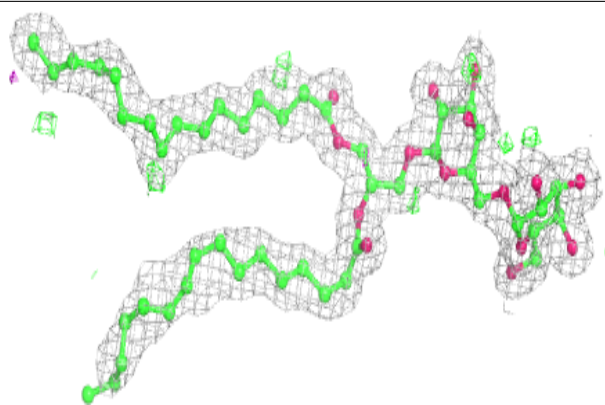
Electron density around CLA b 616:

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

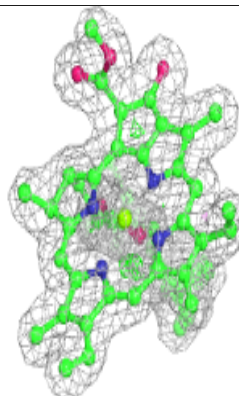
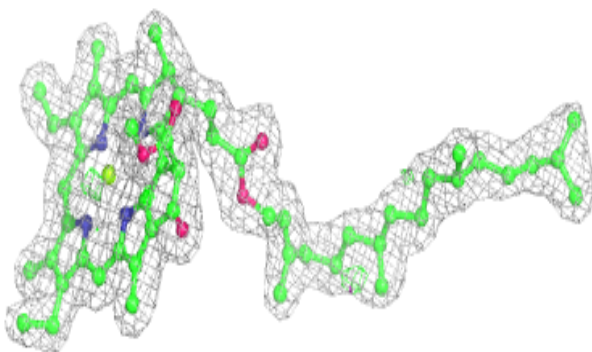
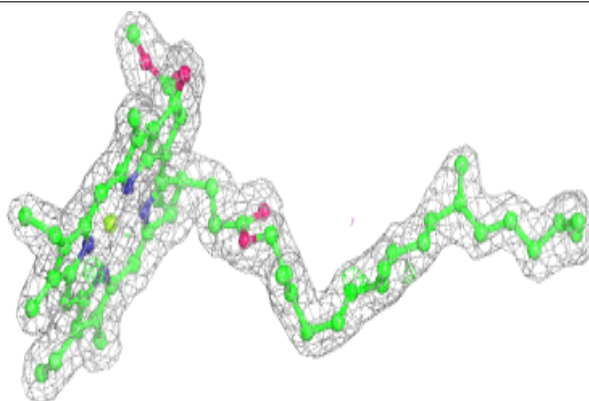


Electron density around DGD C 519:

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

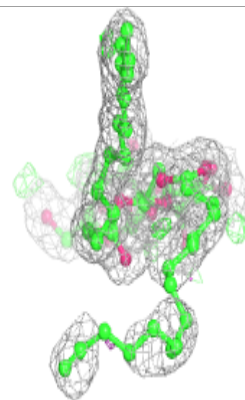
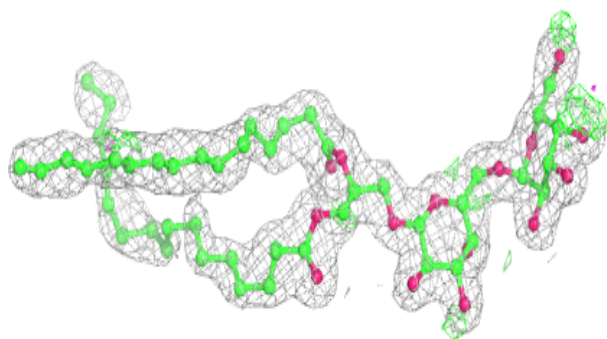
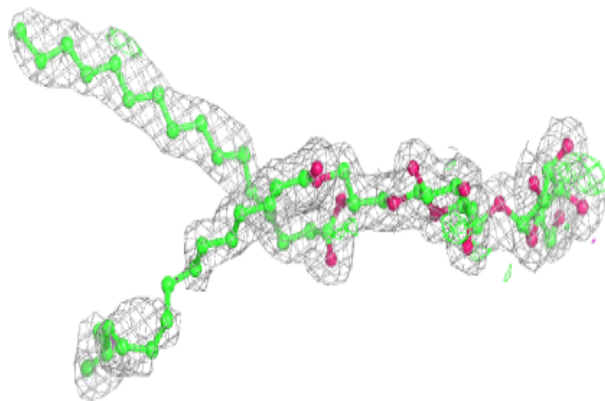
**Electron density around CLA c 903:**

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

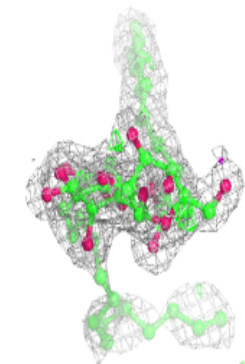
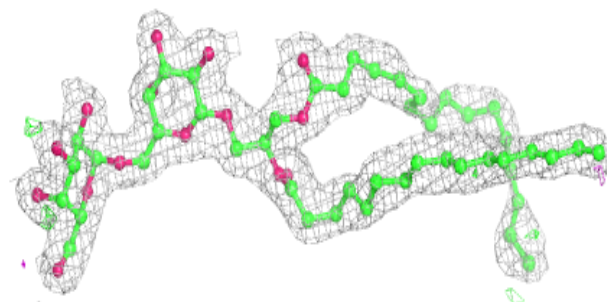
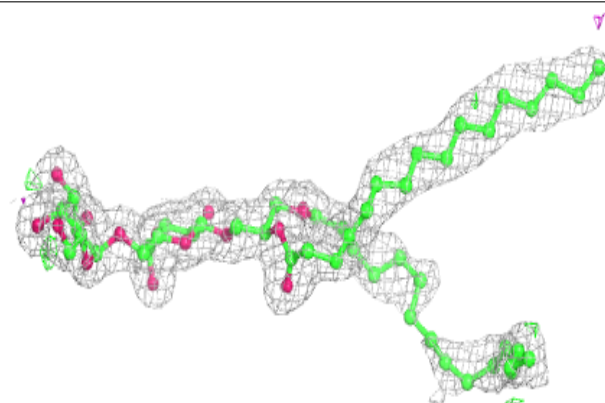


Electron density around DGD c 917:

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

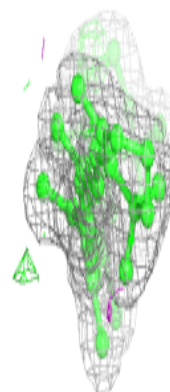
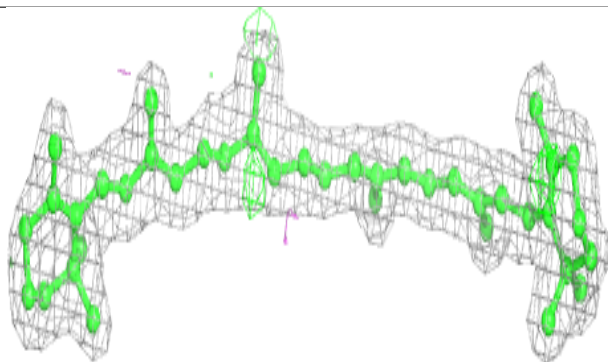
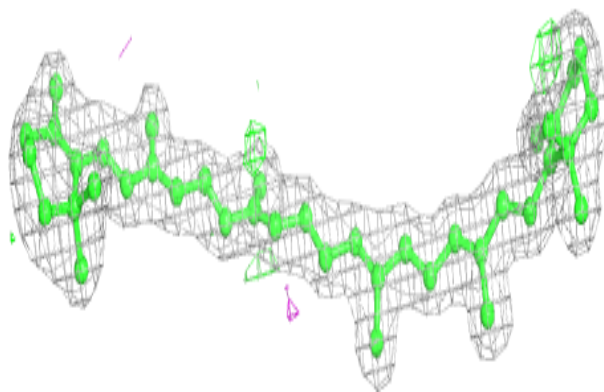
**Electron density around DGD C 517:**

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



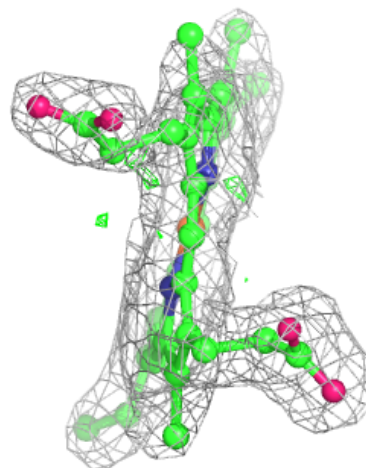
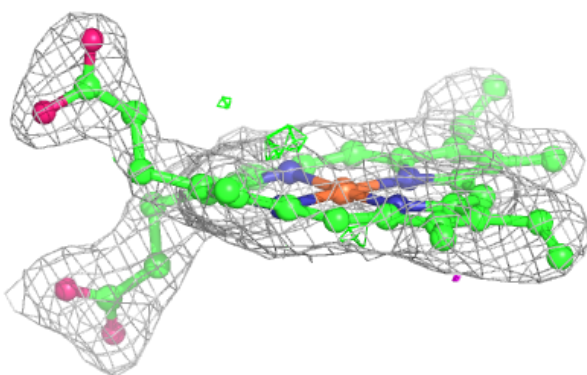
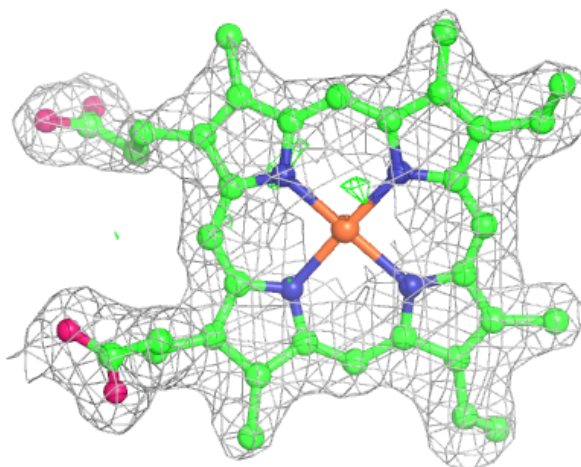
Electron density around BCR t 101:

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



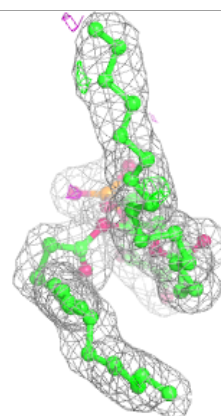
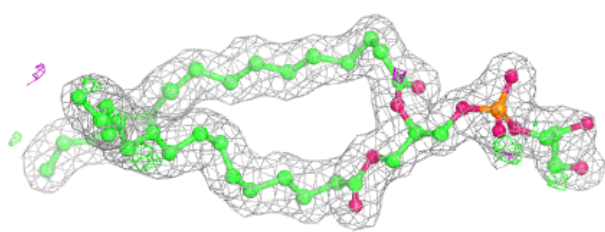
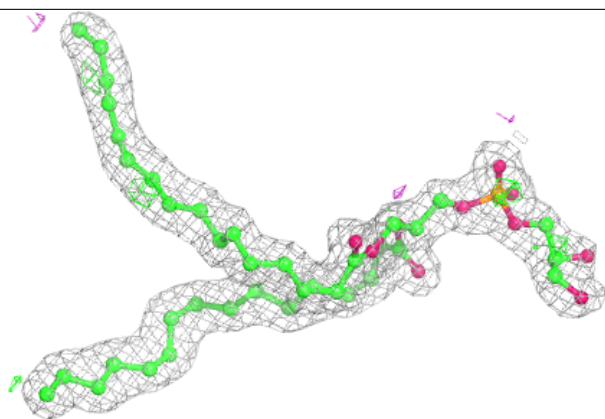
Electron density around HEM E 105:

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

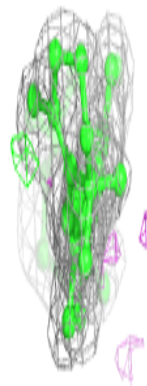
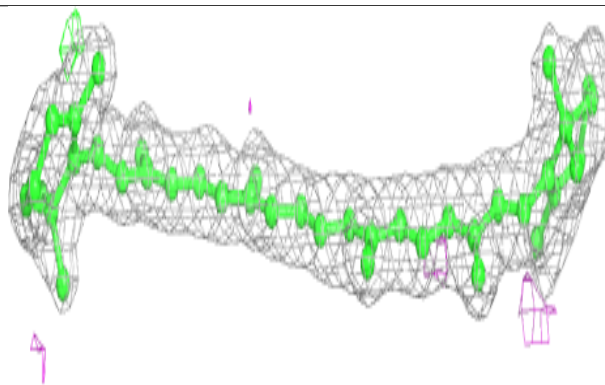
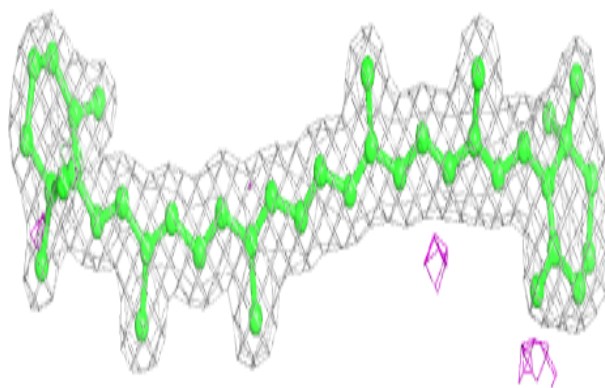


Electron density around LHG d 409:

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

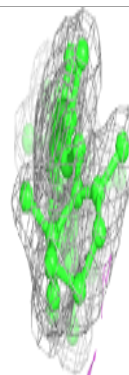
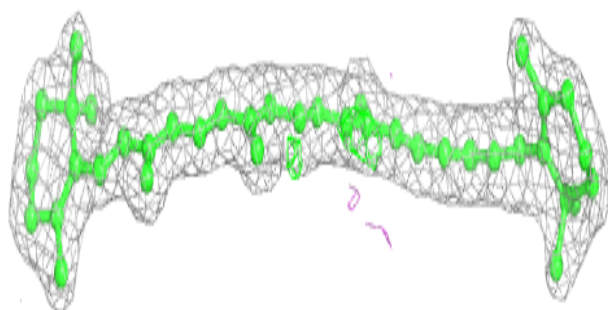
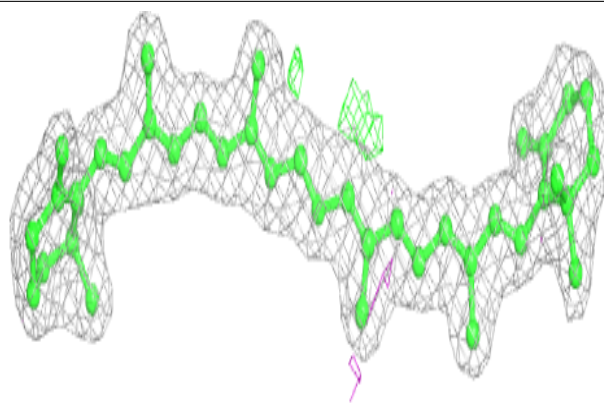
**Electron density around BCR B 620:**

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

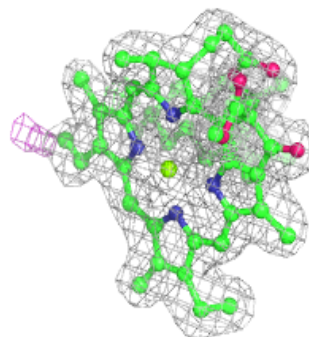
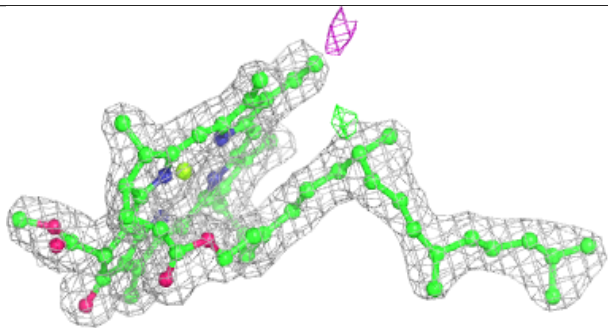
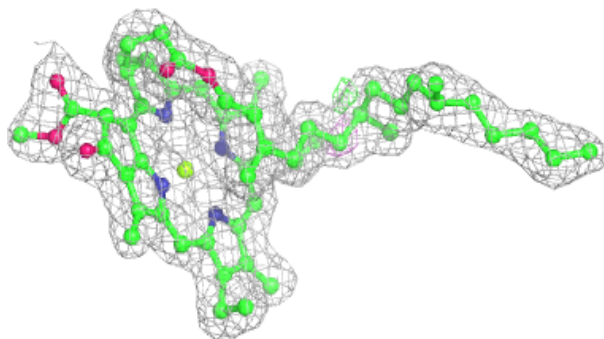


Electron density around BCR j 104:

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

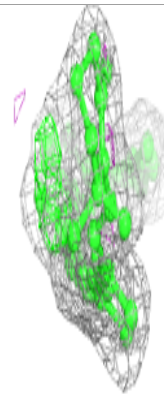
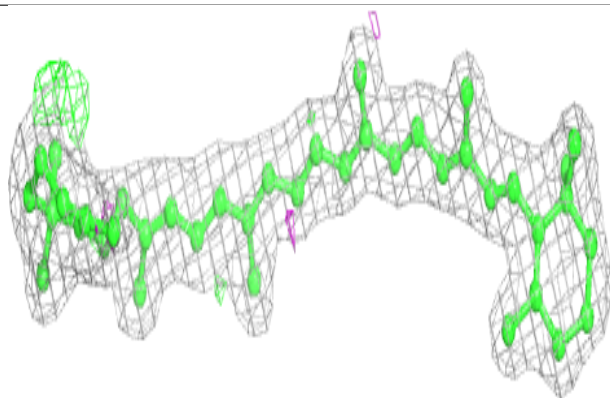
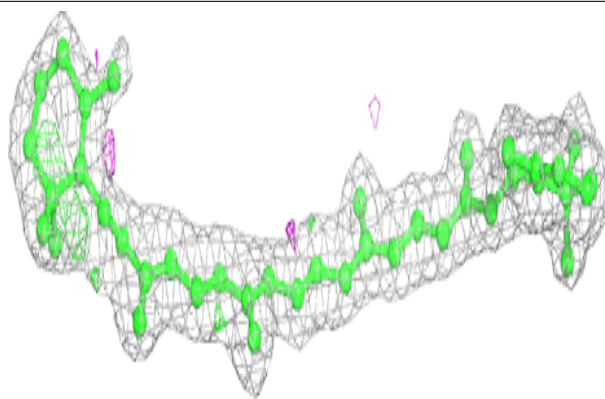
**Electron density around CLA c 906:**

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

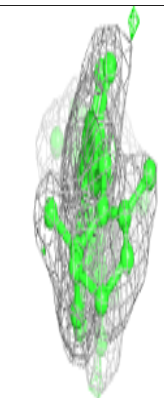
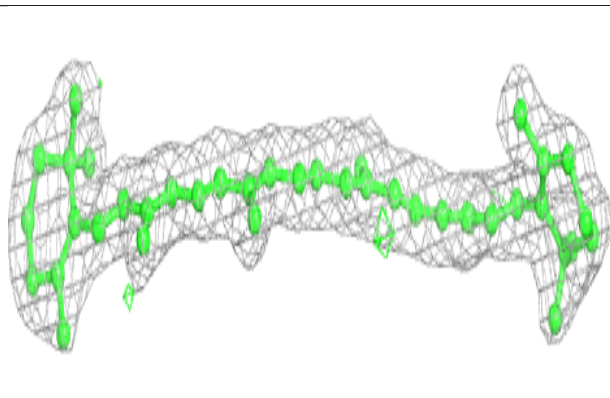
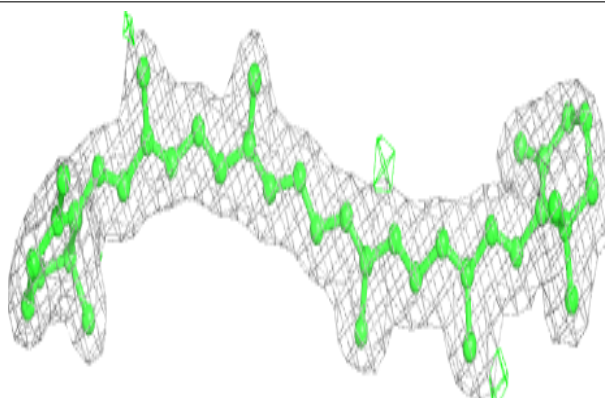


Electron density around BCR d 405:

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

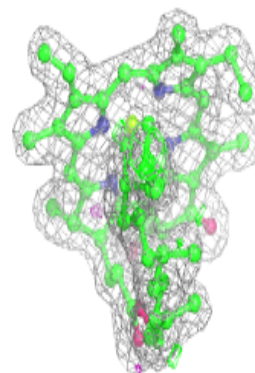
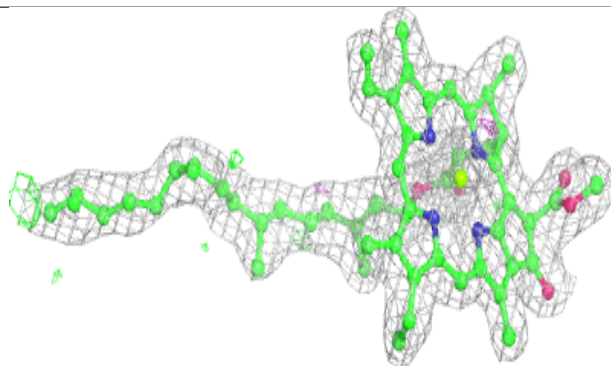
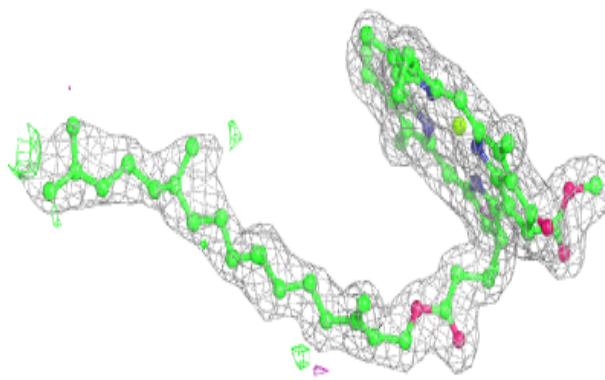
**Electron density around BCR Y 101:**

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



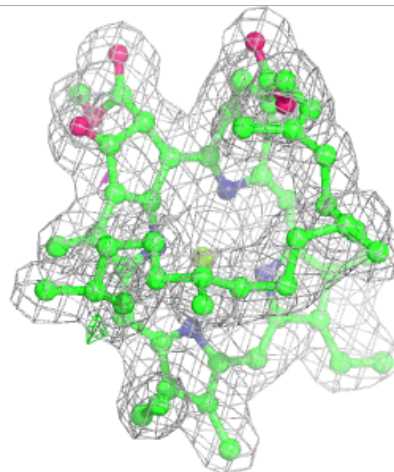
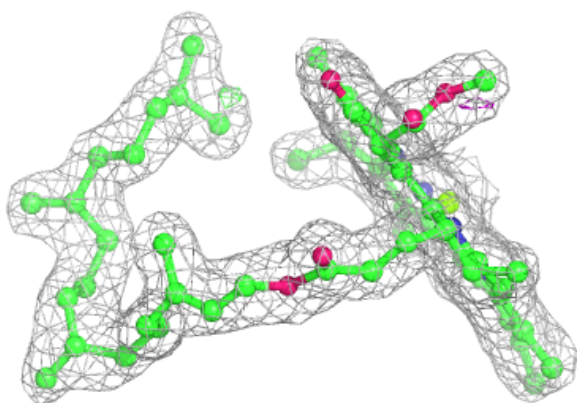
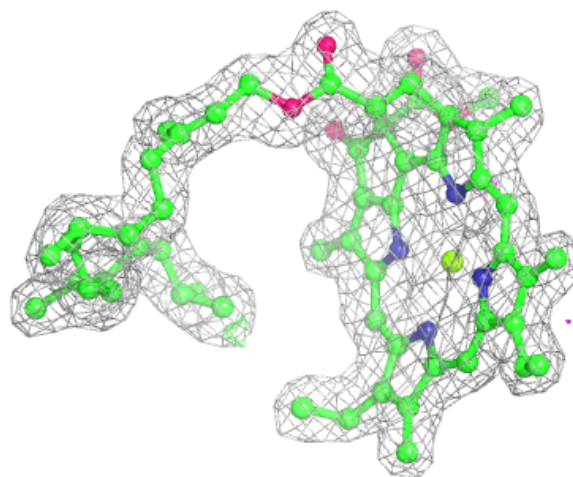
Electron density around CLA c 905:

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



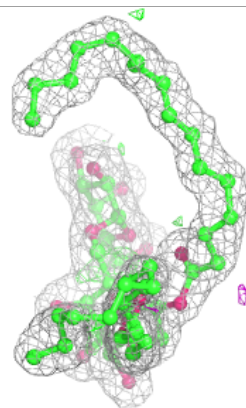
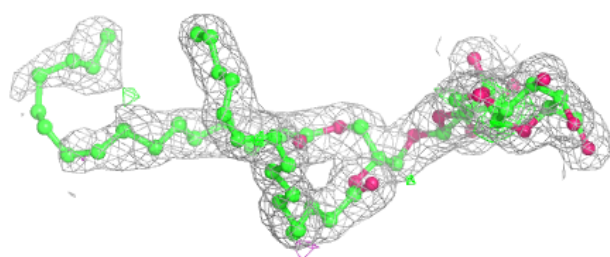
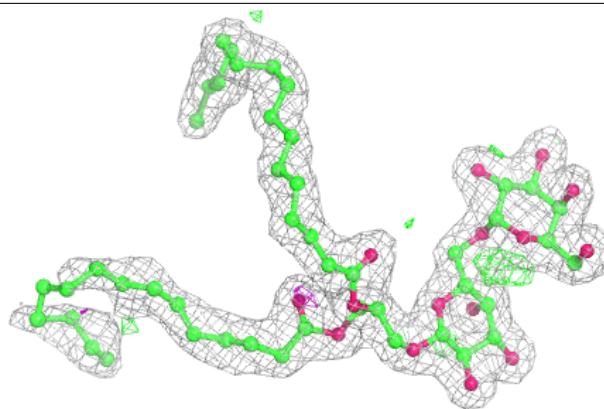
Electron density around CLA C 504:

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

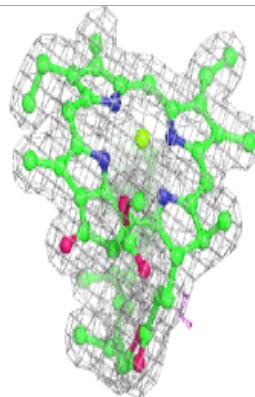
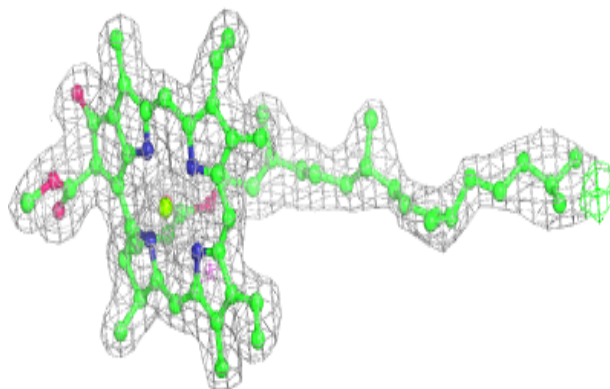
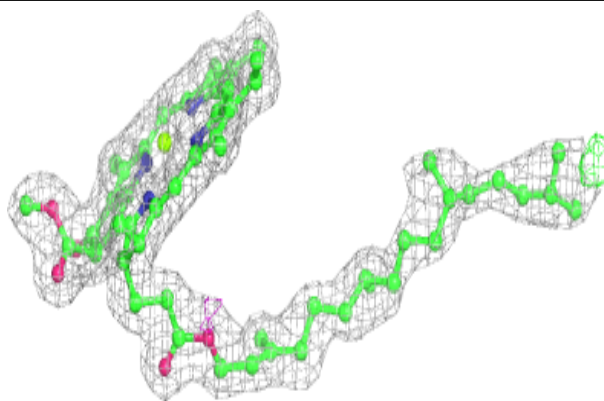


Electron density around DGD c 918:

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

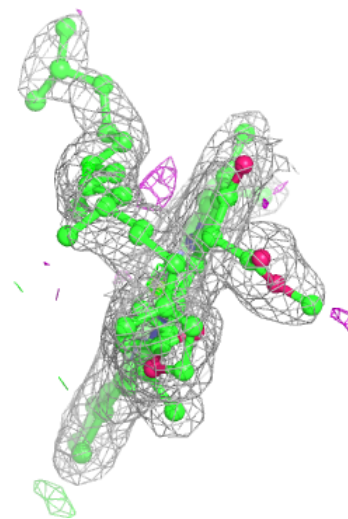
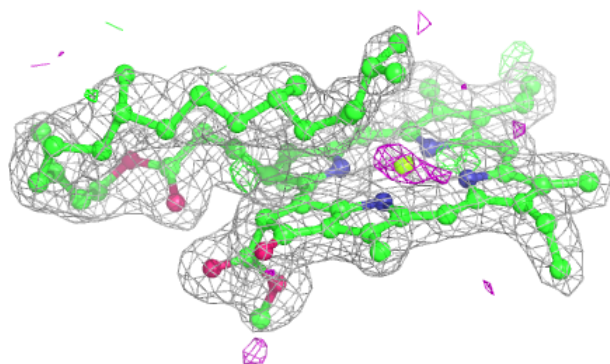
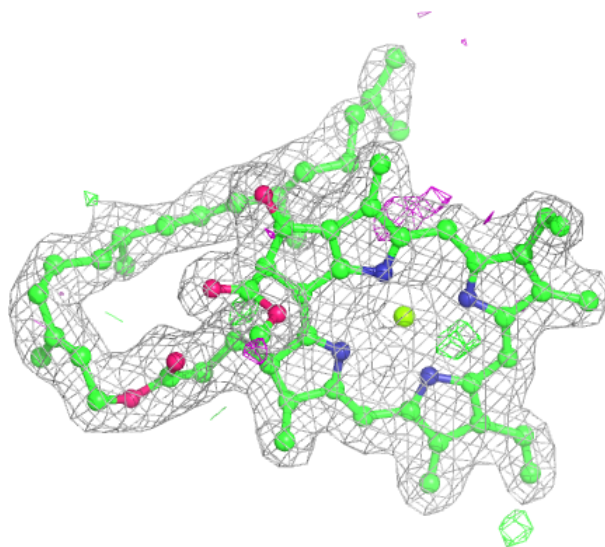
**Electron density around CLA C 505:**

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



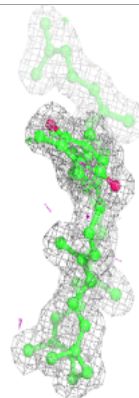
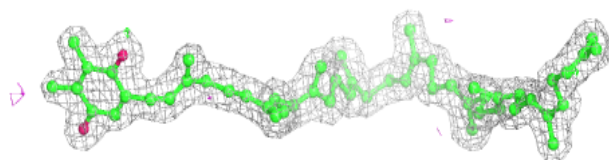
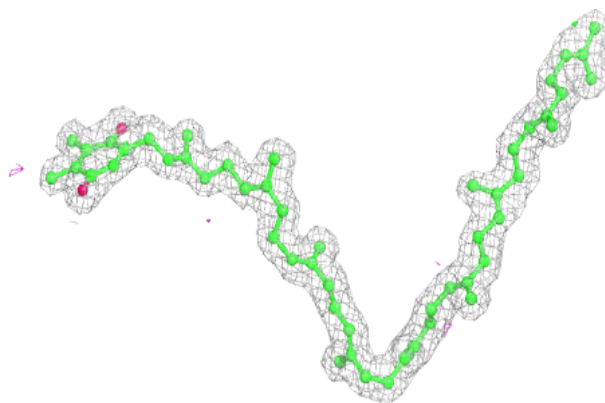
Electron density around CLA c 910:

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

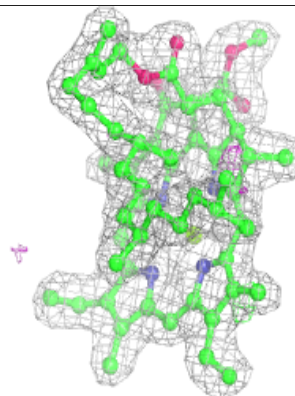
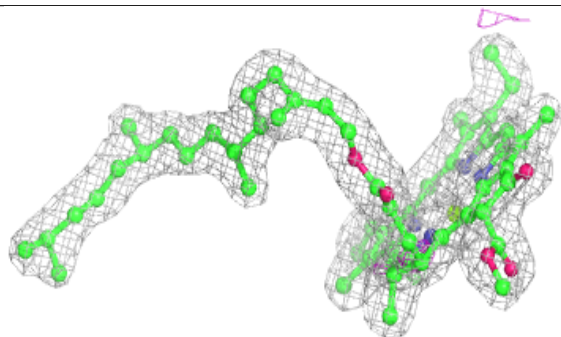
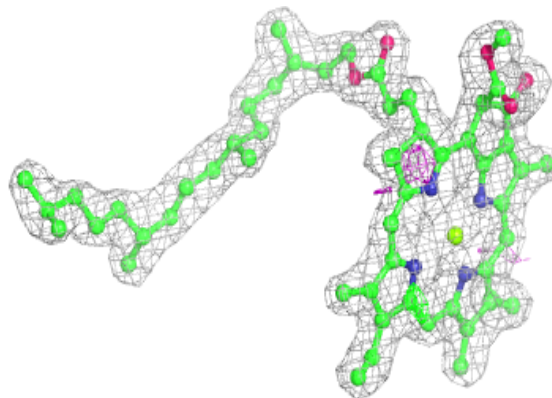


Electron density around PL9 d 406:

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

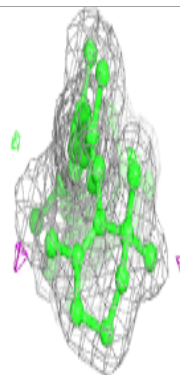
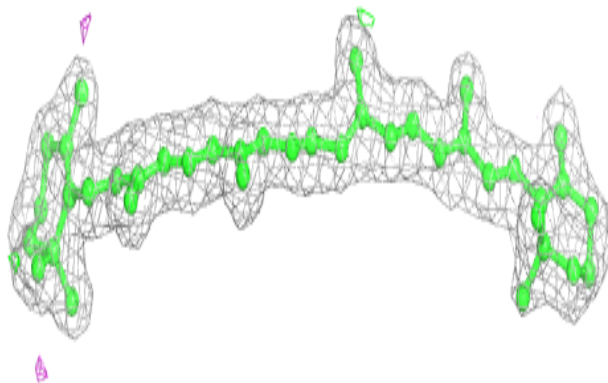
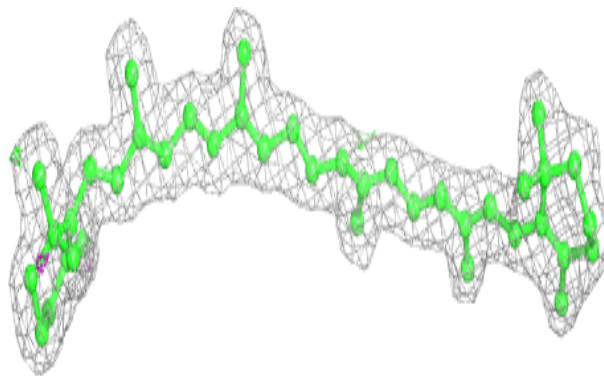
**Electron density around CLA c 912:**

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

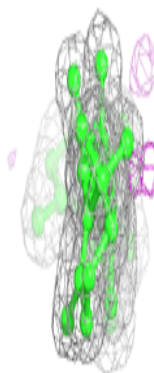
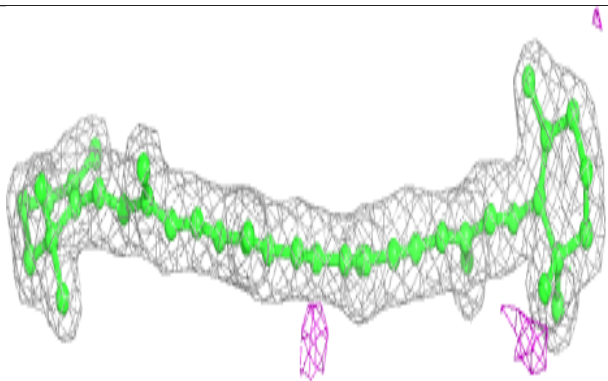
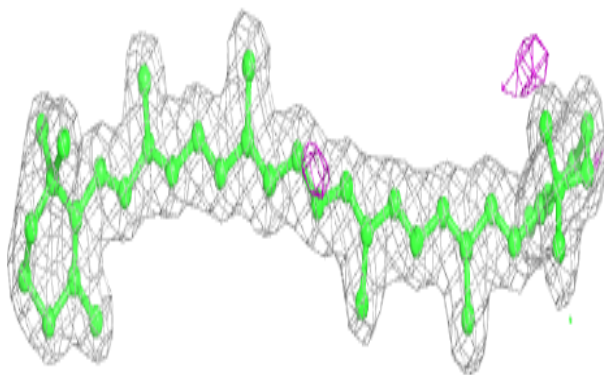


Electron density around BCR T 101:

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

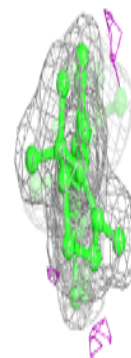
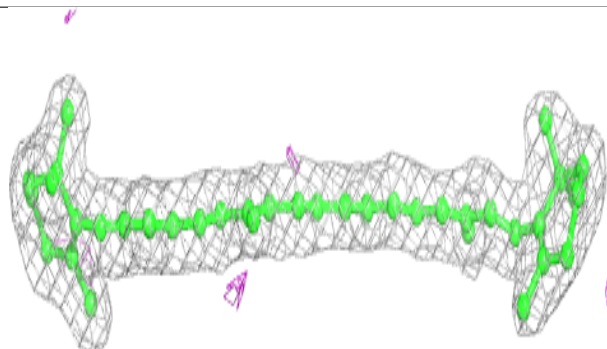
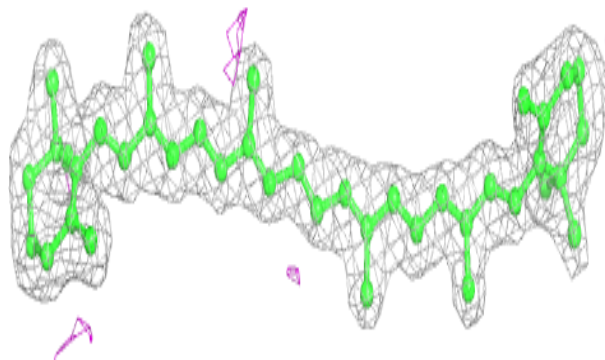
**Electron density around BCR b 618:**

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

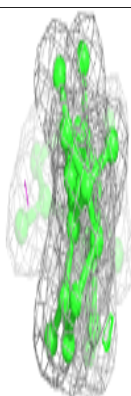
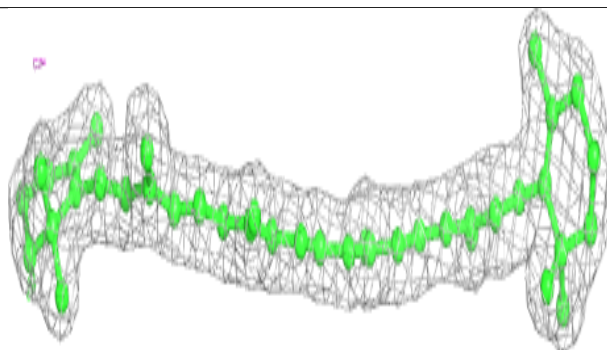
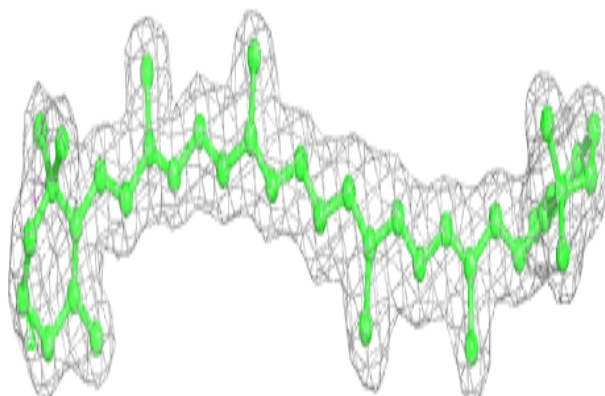


Electron density around BCR b 619:

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

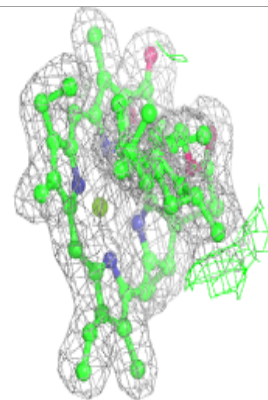
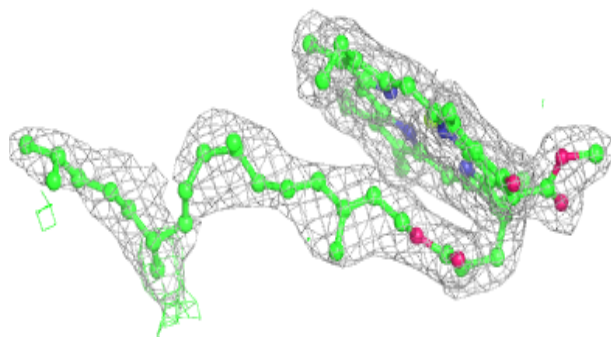
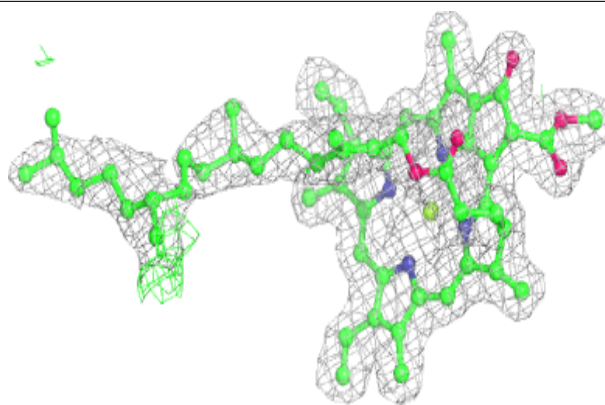
**Electron density around BCR B 618:**

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

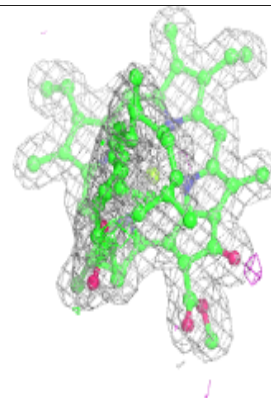
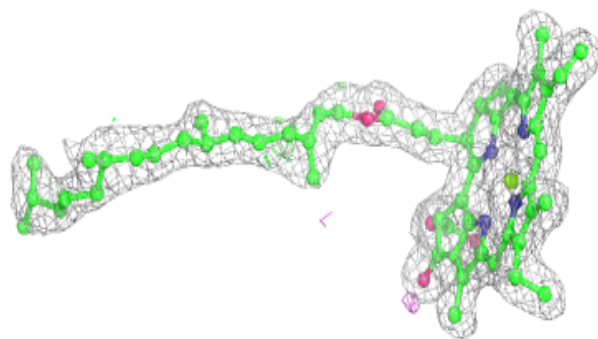
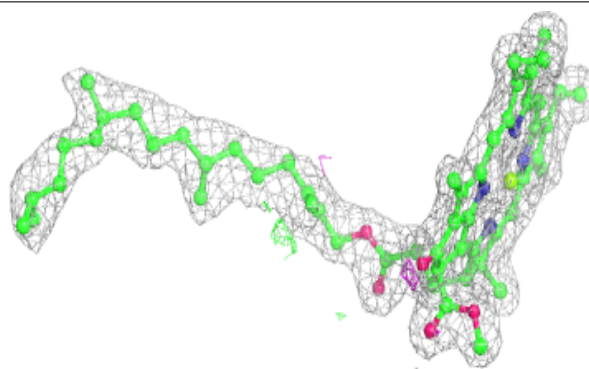


Electron density around CLA b 615:

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

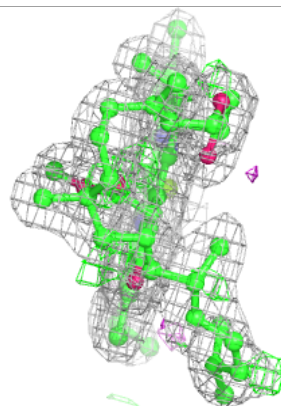
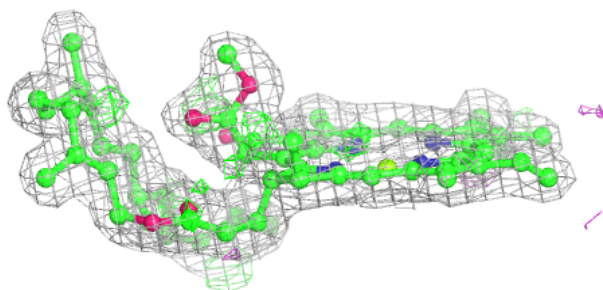
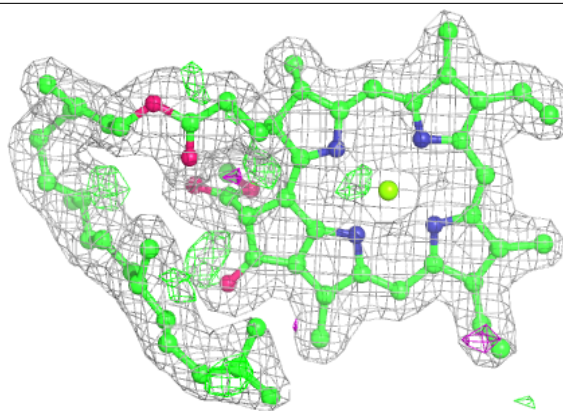
**Electron density around CLA b 605:**

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

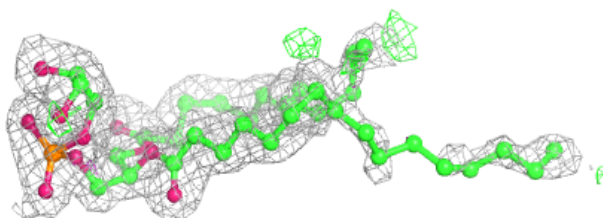
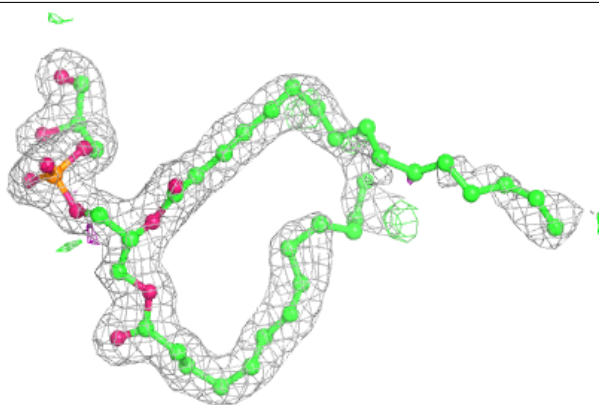


Electron density around CLA B 611:

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

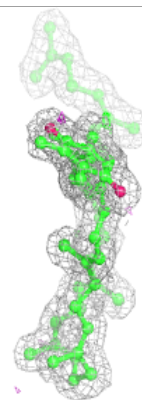
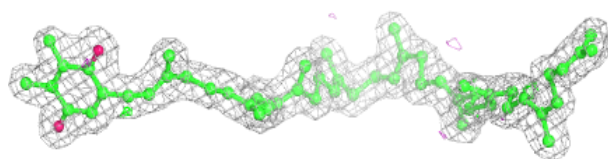
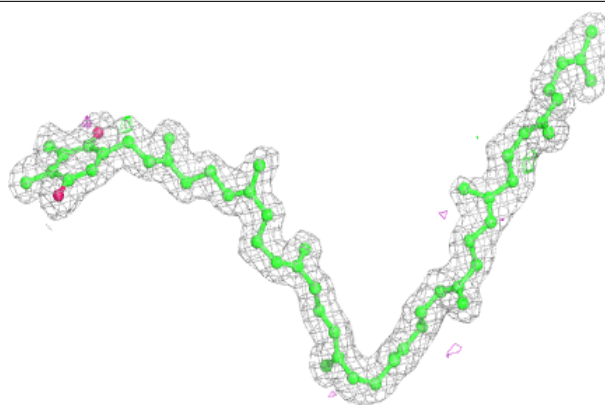
**Electron density around LHG D 411:**

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

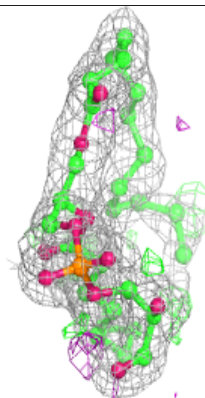
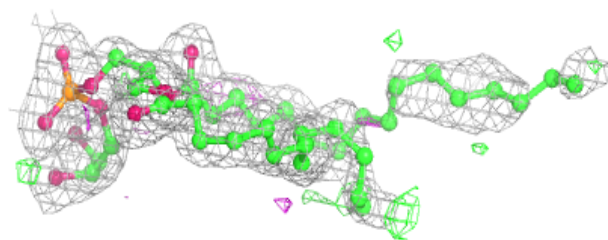
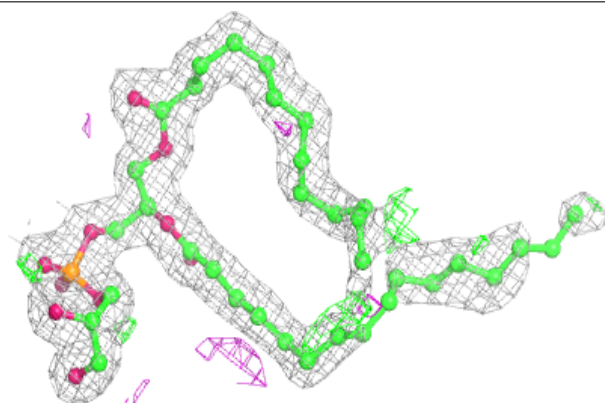


Electron density around PL9 D 406:

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

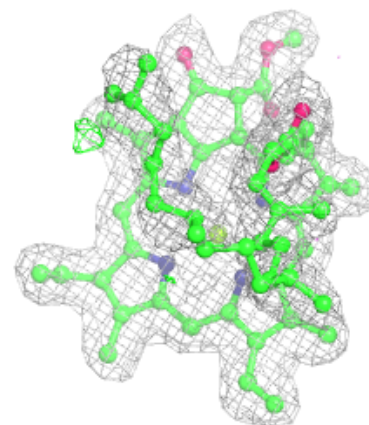
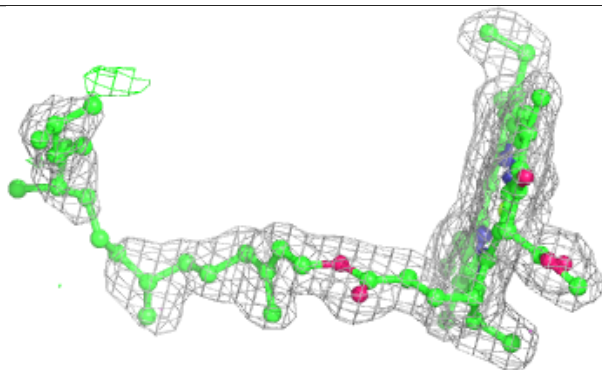
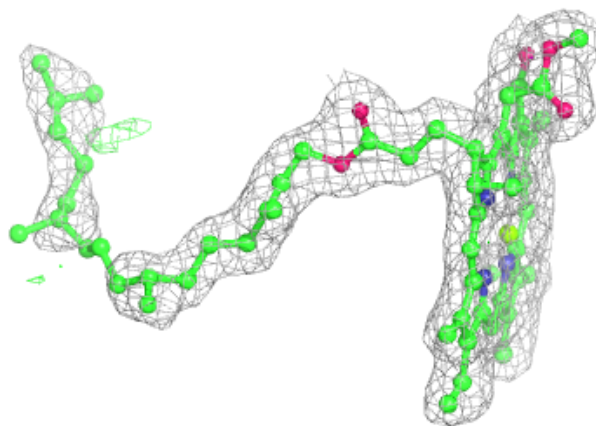
**Electron density around LHG d 410:**

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

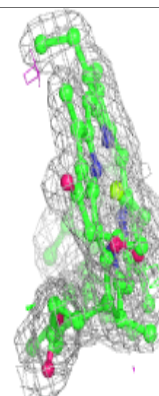
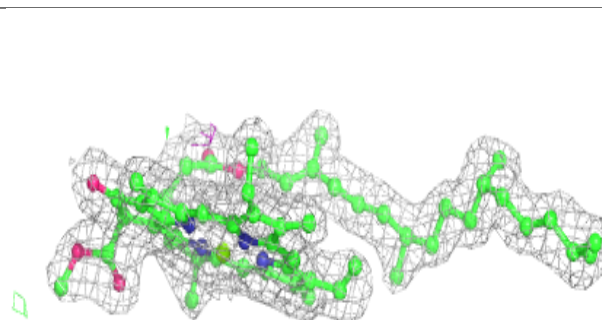
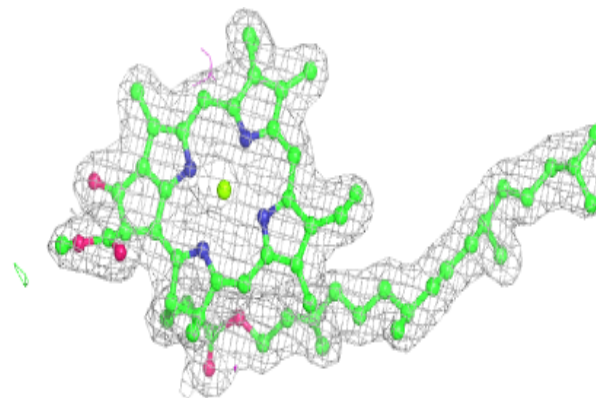


Electron density around CLA d 404:

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

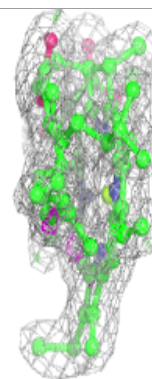
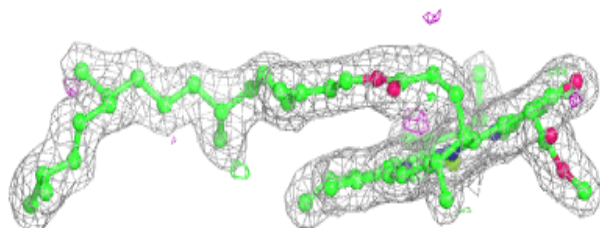
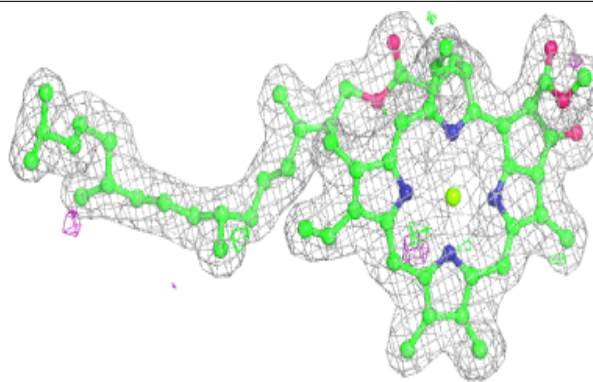
**Electron density around CLA c 902:**

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

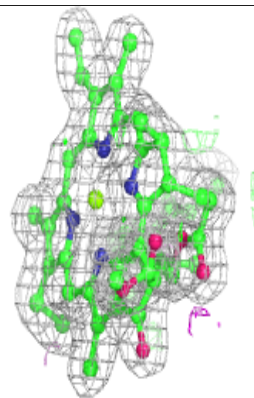
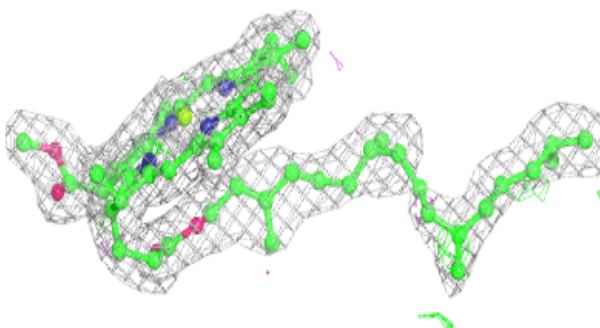
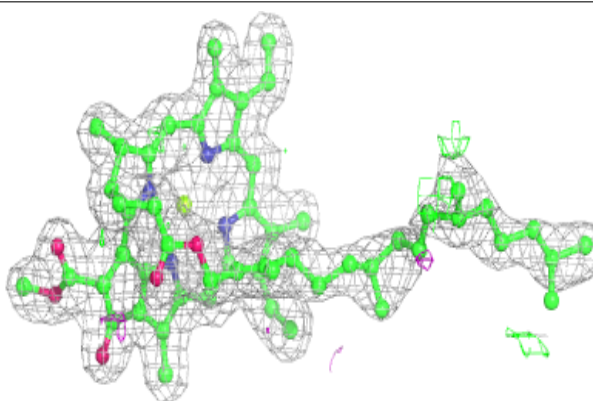


Electron density around CLA b 604:

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

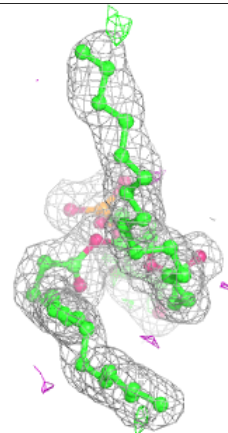
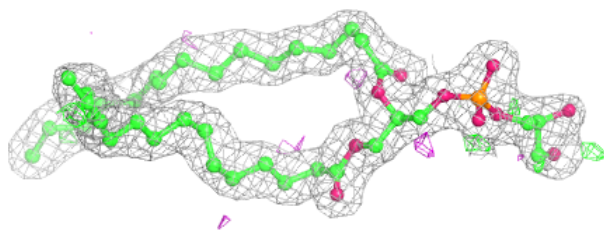
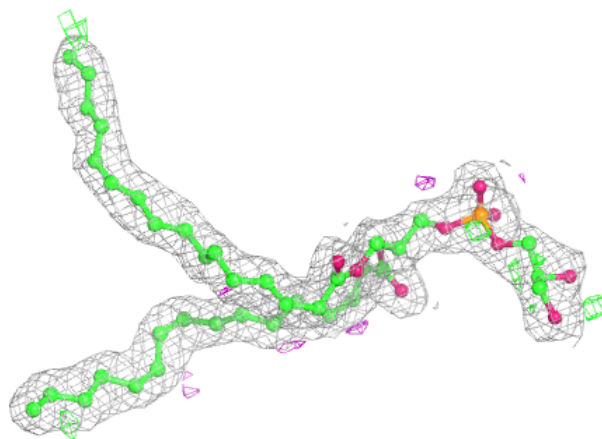
**Electron density around CLA B 615:**

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

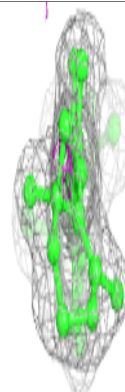
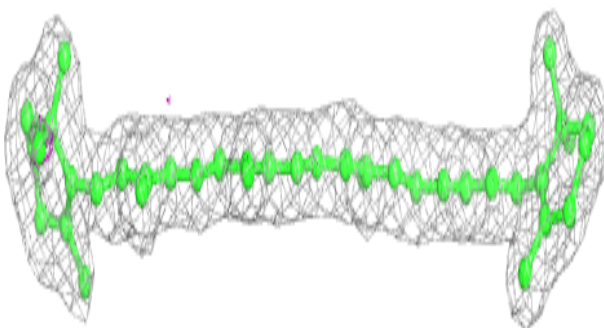
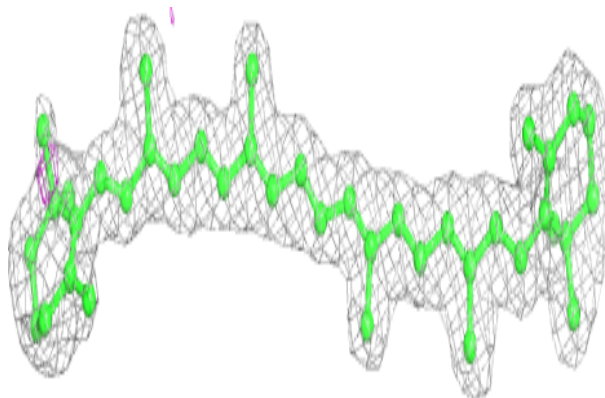


Electron density around LHG D 410:

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

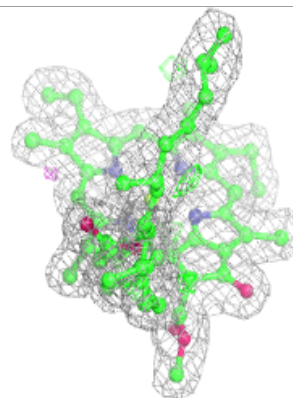
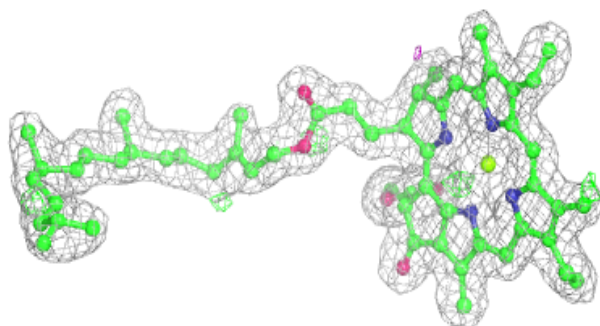
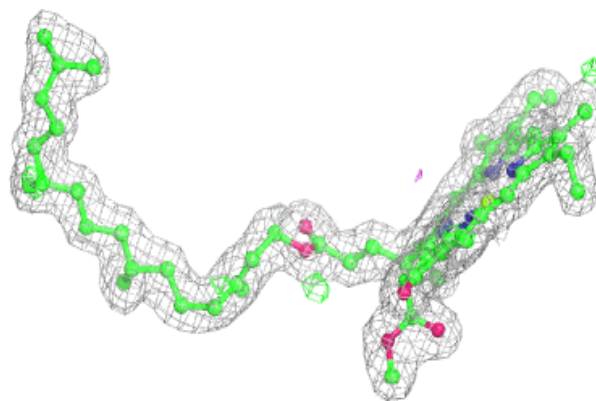
**Electron density around BCR B 619:**

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

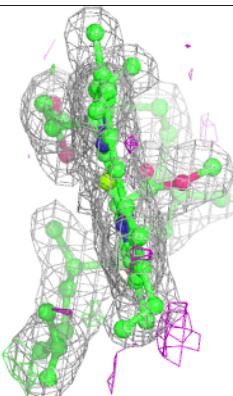
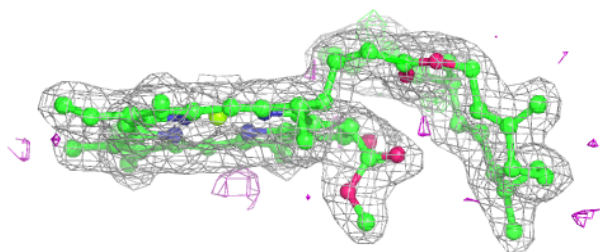
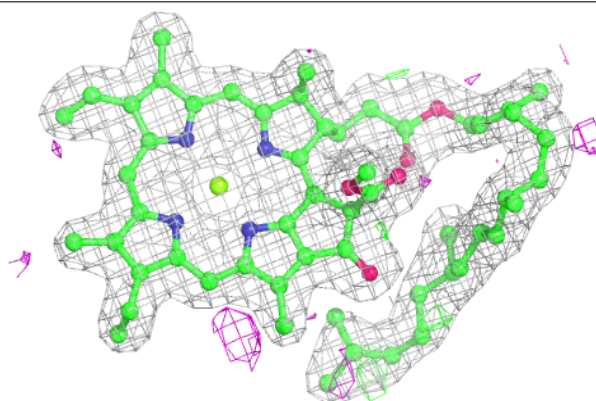


Electron density around CLA D 403:

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

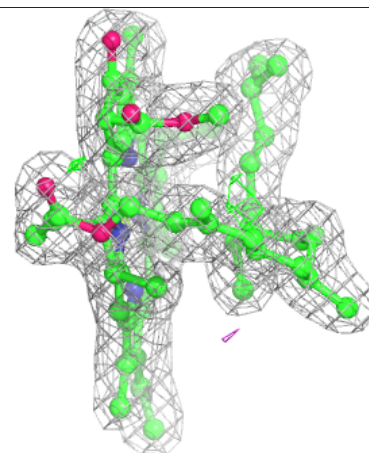
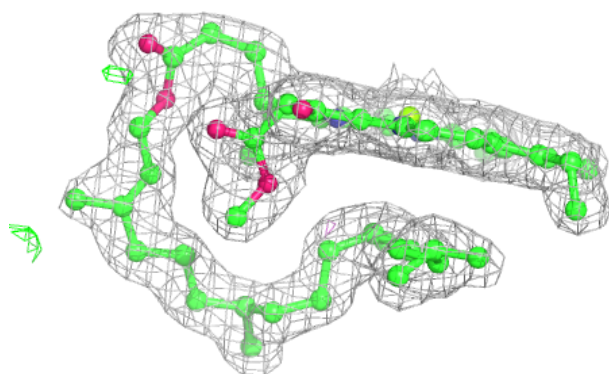
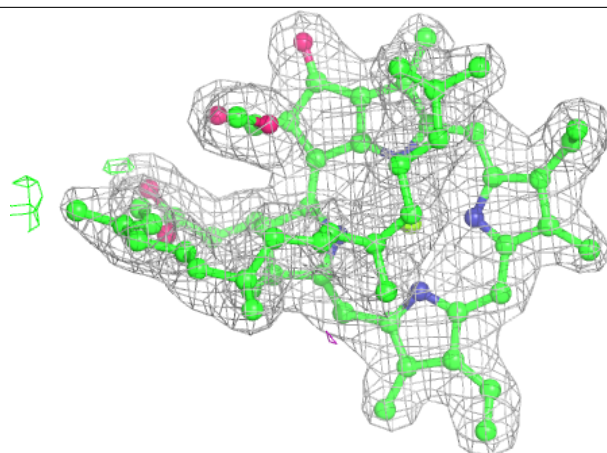
**Electron density around CLA b 611:**

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



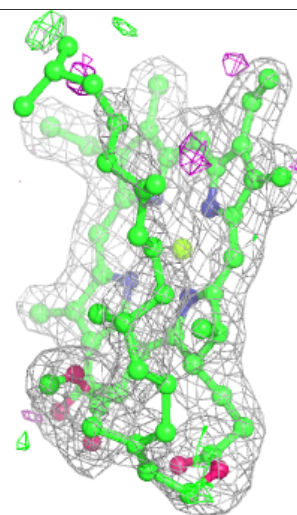
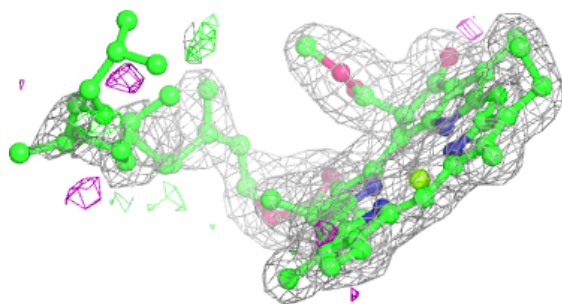
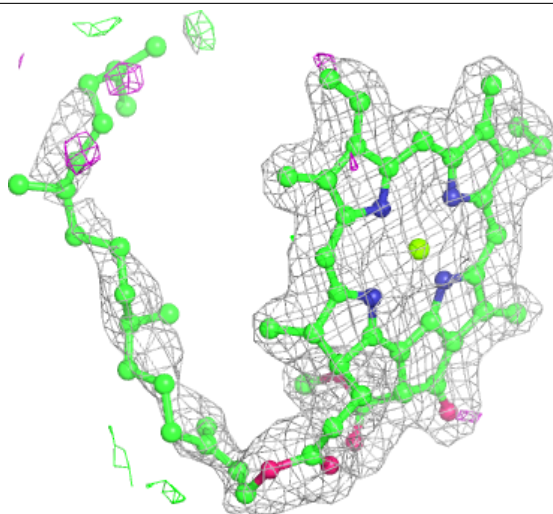
Electron density around CLA C 511:

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



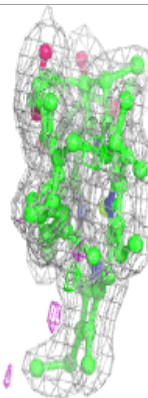
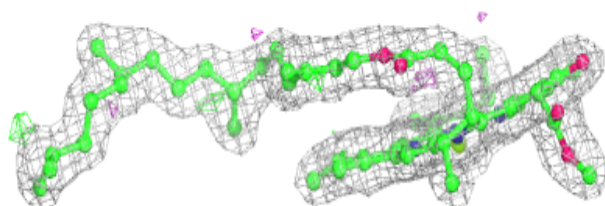
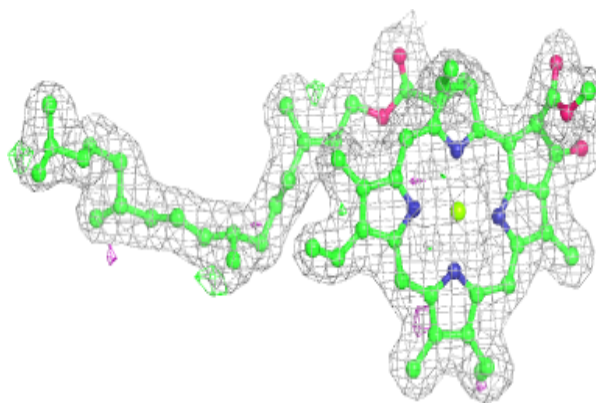
Electron density around CLA B 617:

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

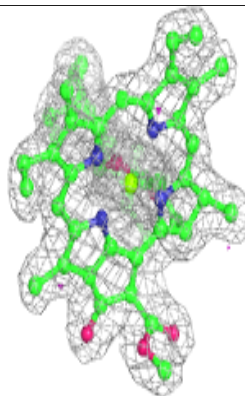
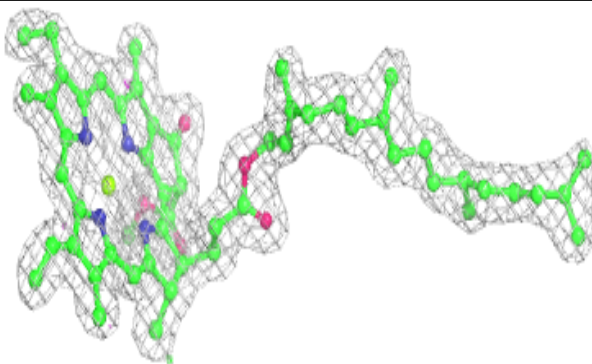
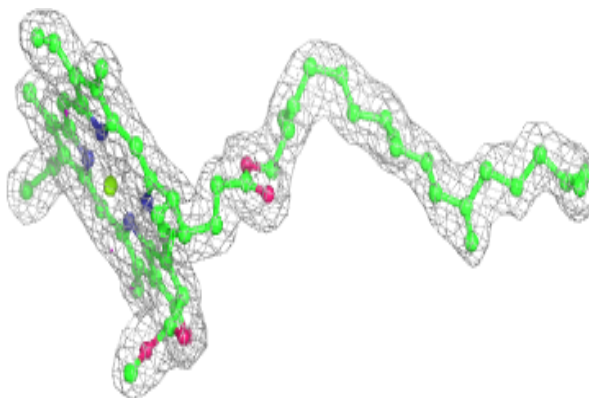


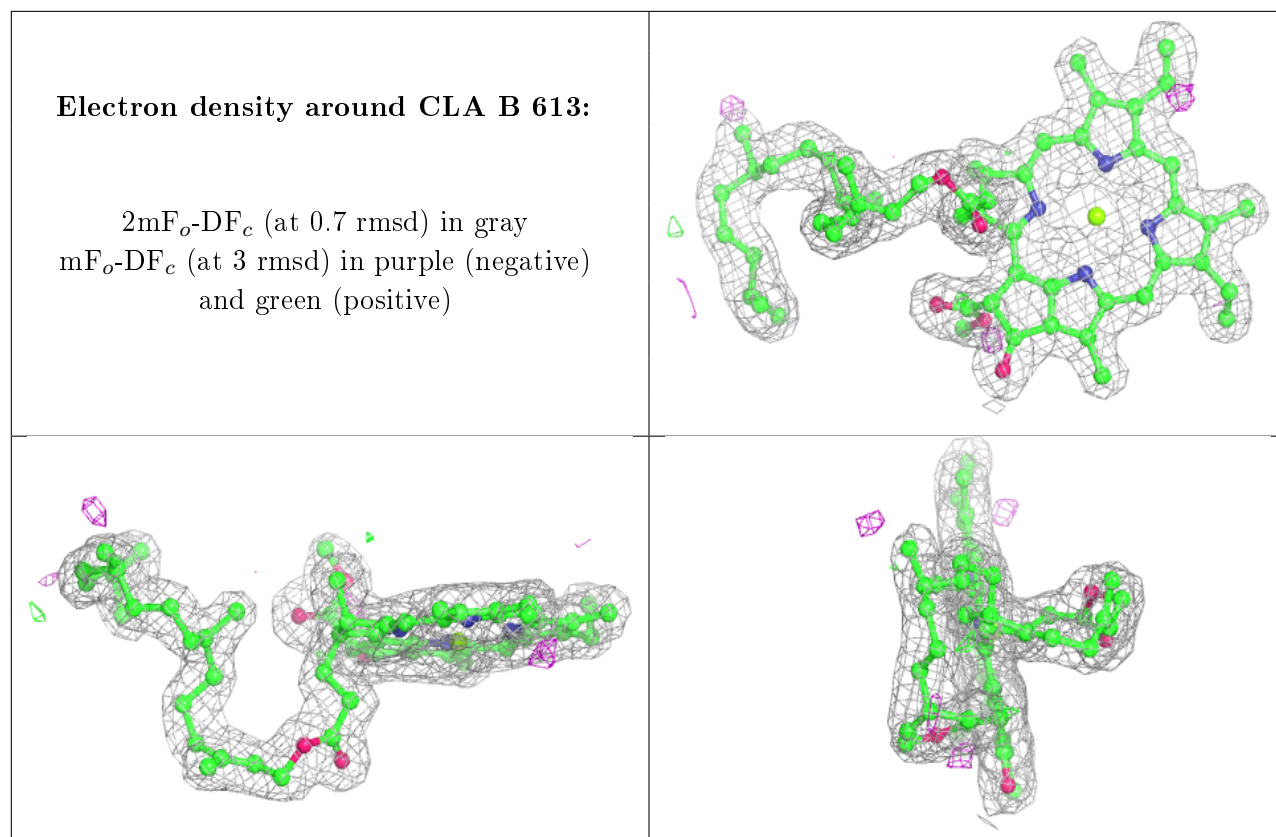
Electron density around CLA B 604:

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

**Electron density around CLA C 503:**

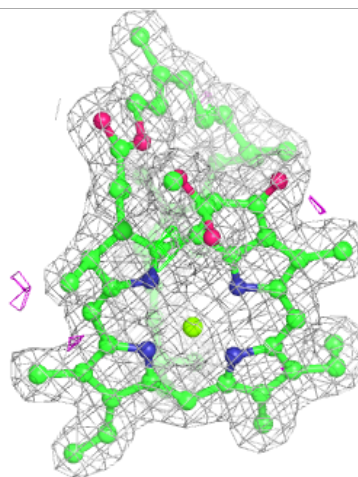
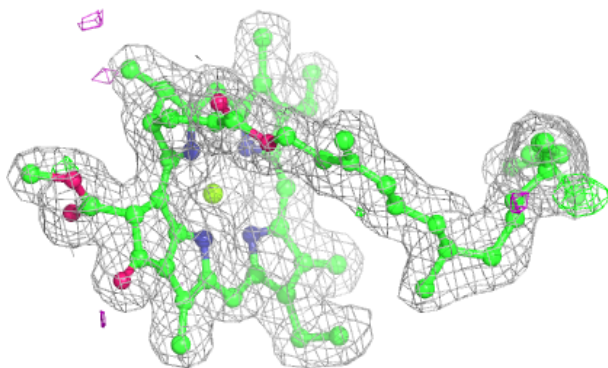
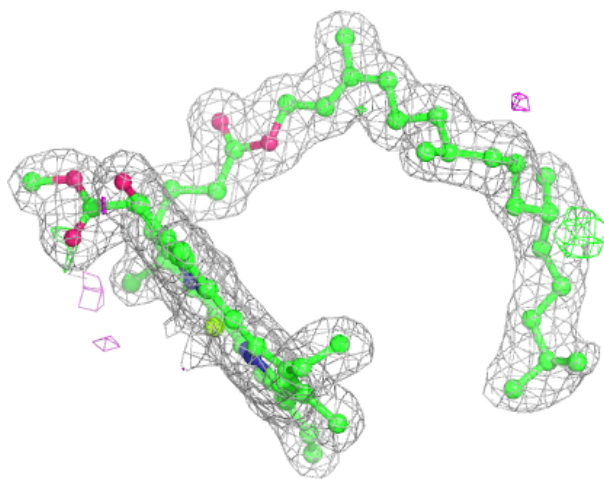
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





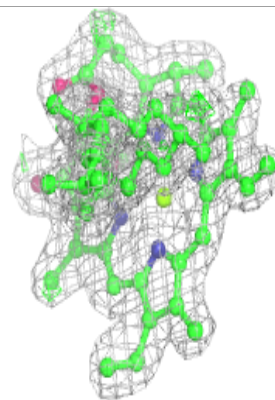
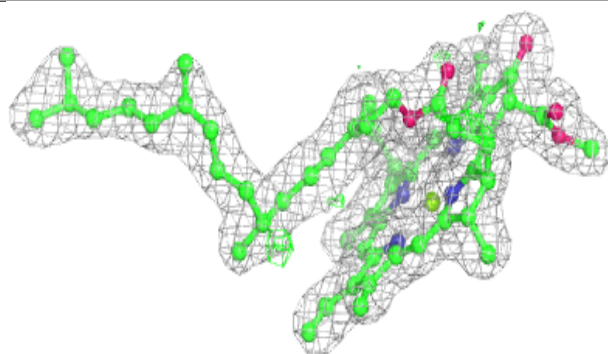
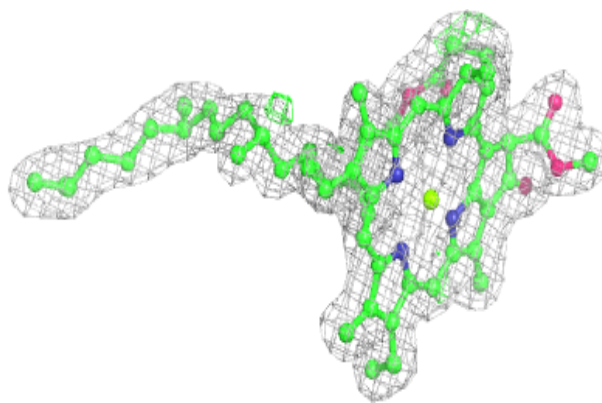
Electron density around CLA b 612:

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

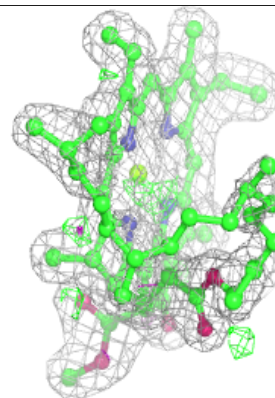
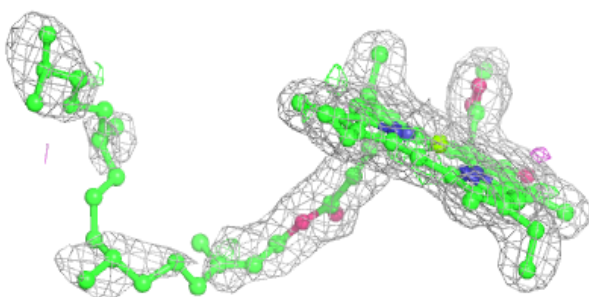
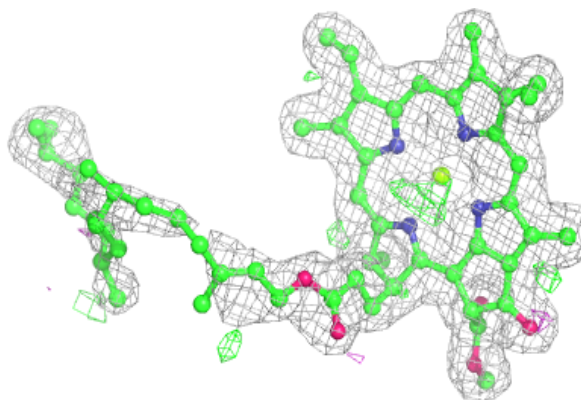


Electron density around CLA C 506:

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

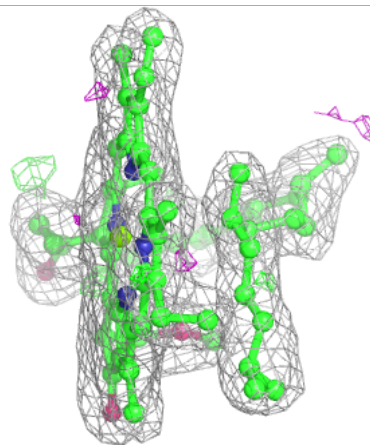
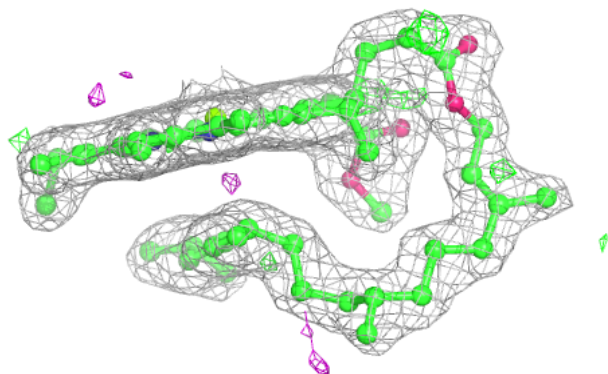
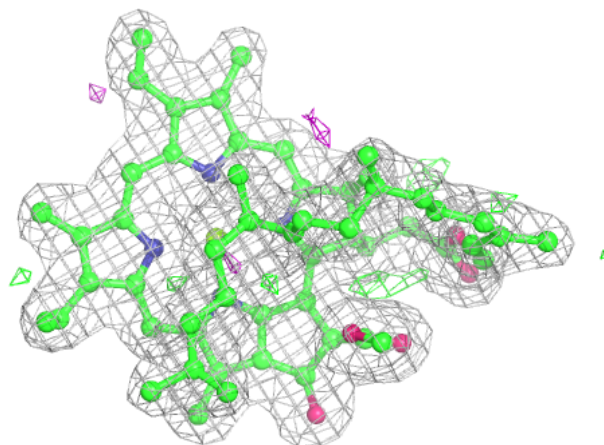
**Electron density around CLA a 410:**

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



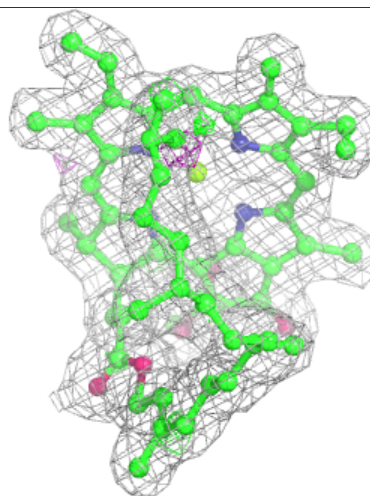
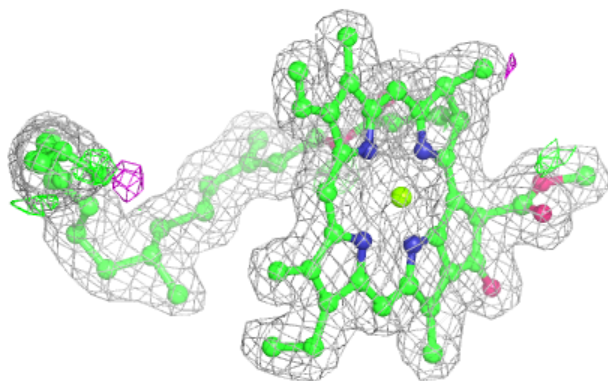
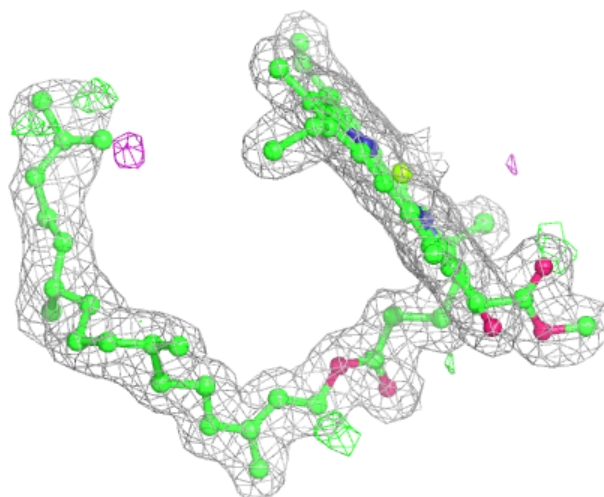
Electron density around CLA c 911:

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



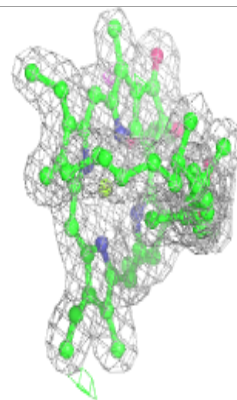
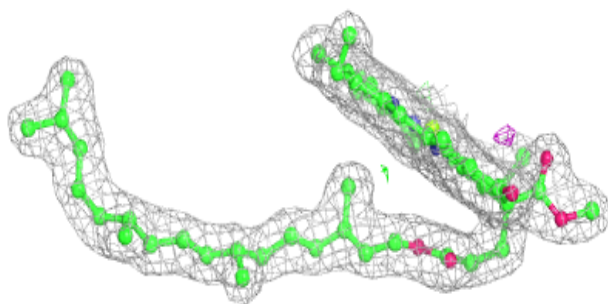
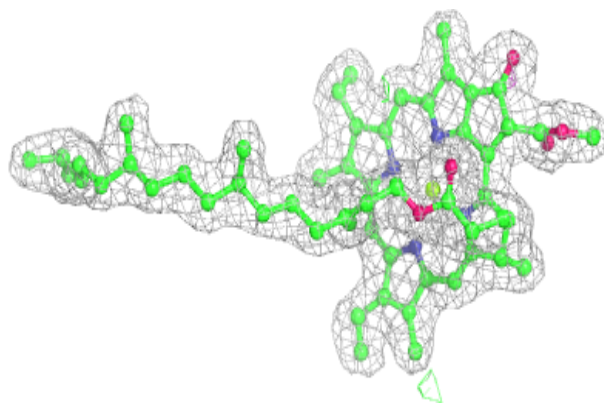
Electron density around CLA B 612:

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

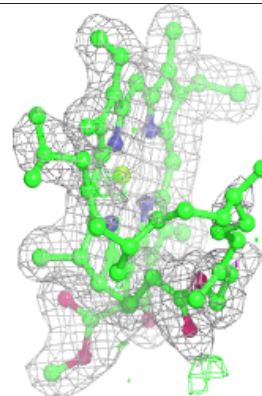
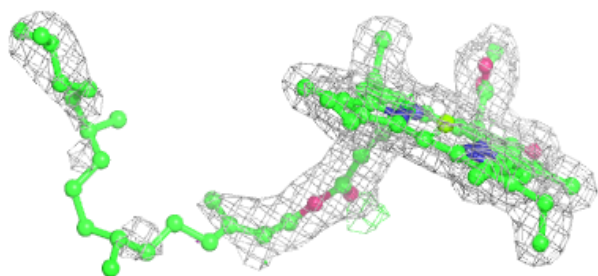
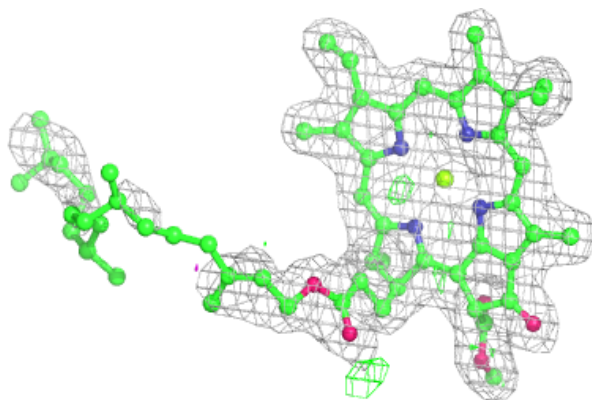


Electron density around CLA b 609:

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

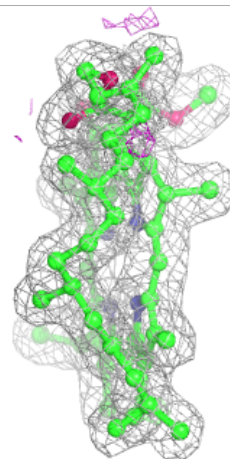
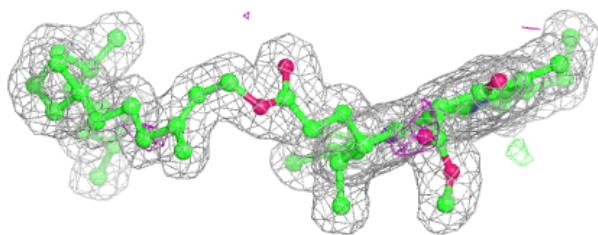
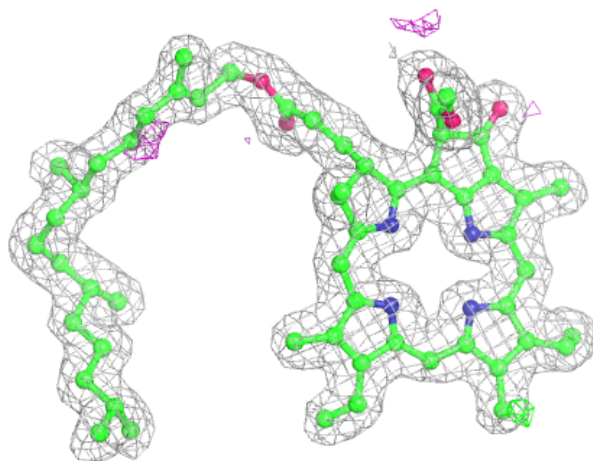
**Electron density around CLA A 408:**

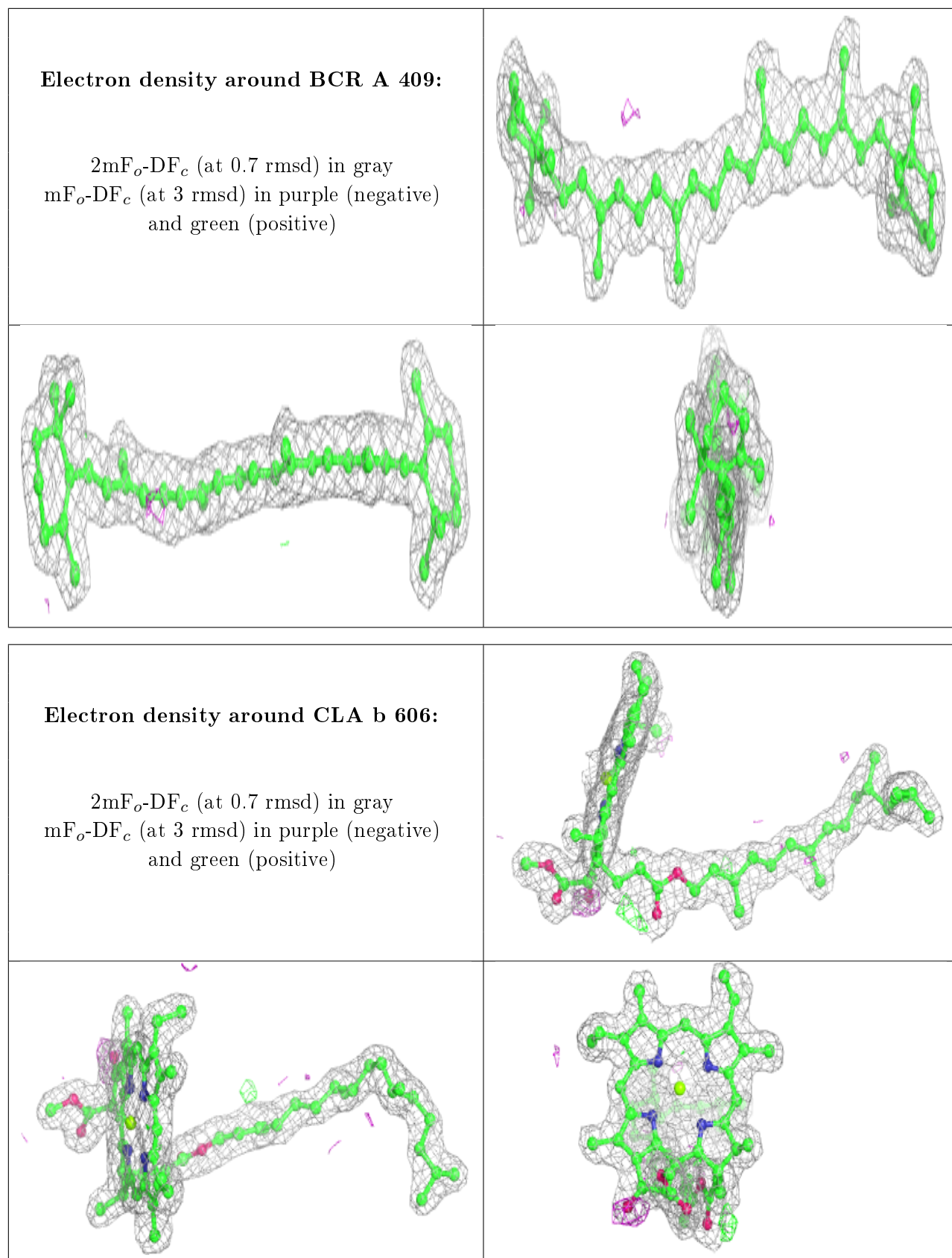
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PHO a 408:

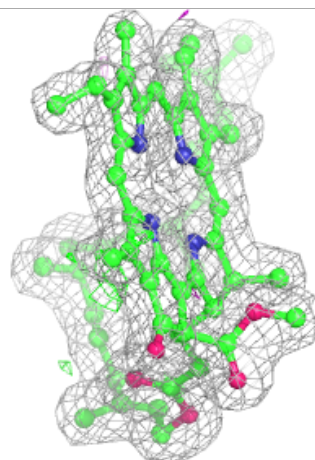
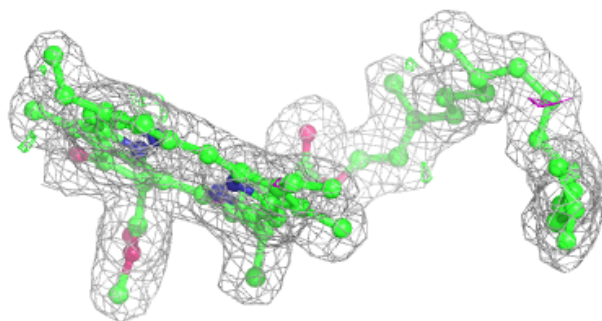
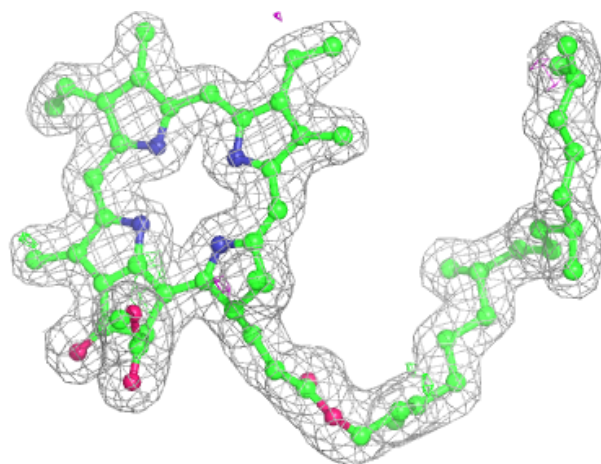
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





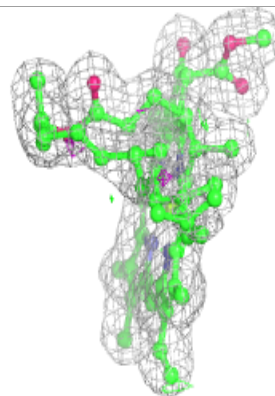
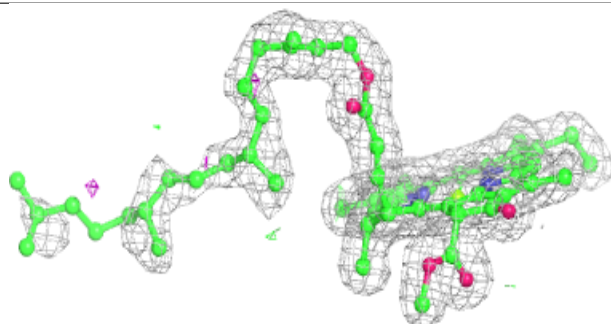
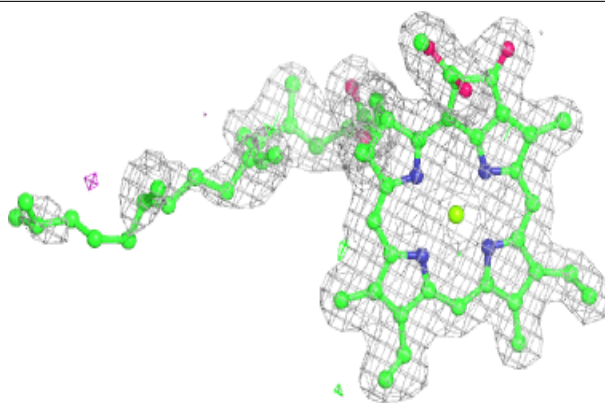
Electron density around PHO D 402:

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

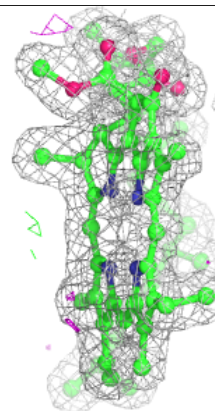
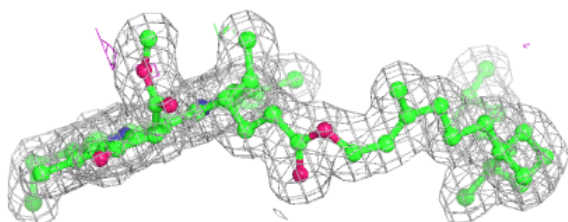
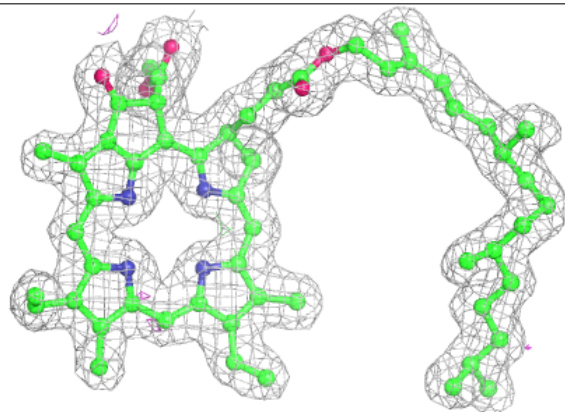


Electron density around CLA a 407:

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

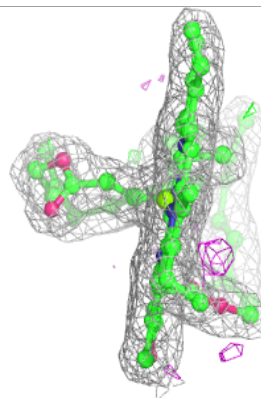
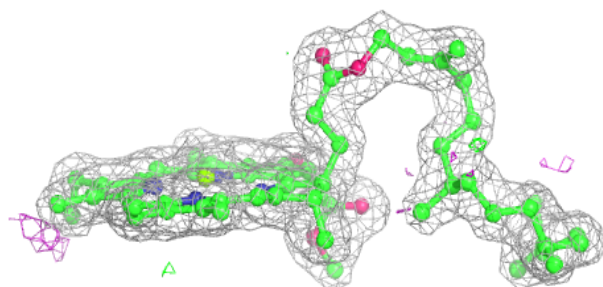
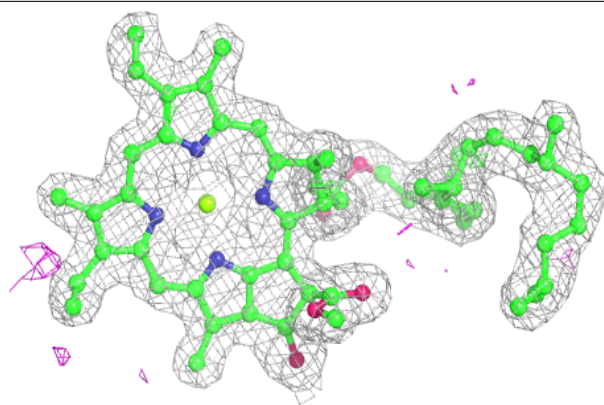
**Electron density around PHO A 407:**

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



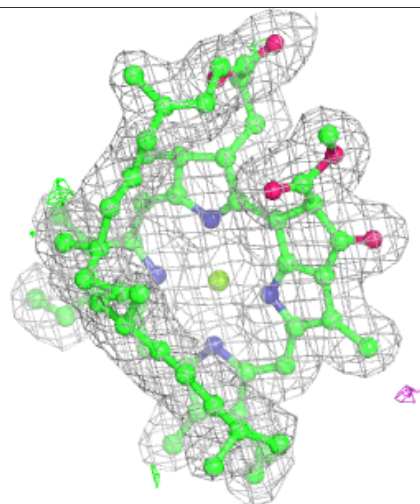
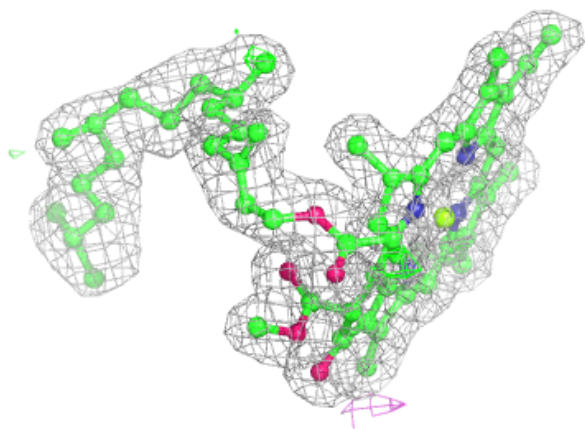
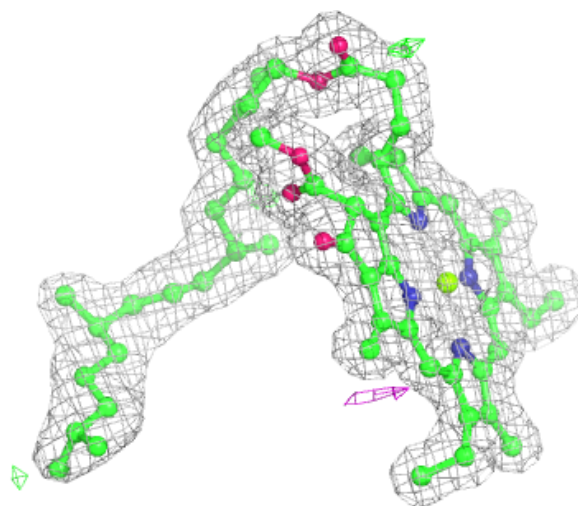
Electron density around CLA b 613:

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



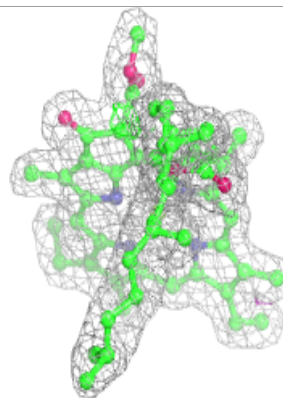
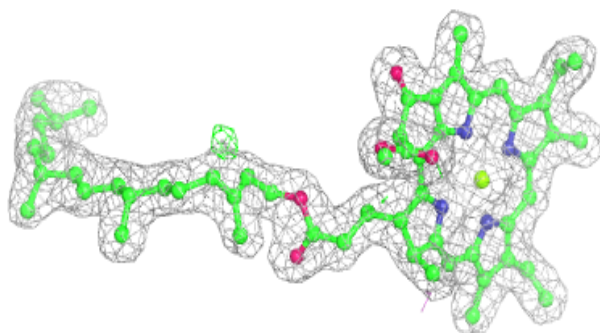
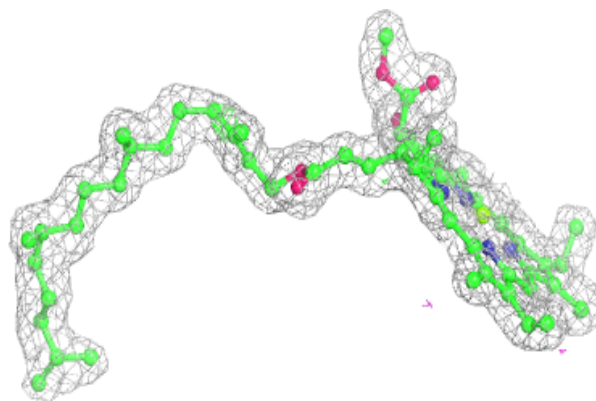
Electron density around CLA b 614:

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

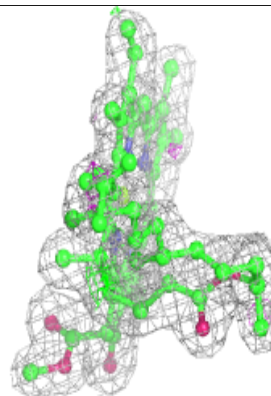
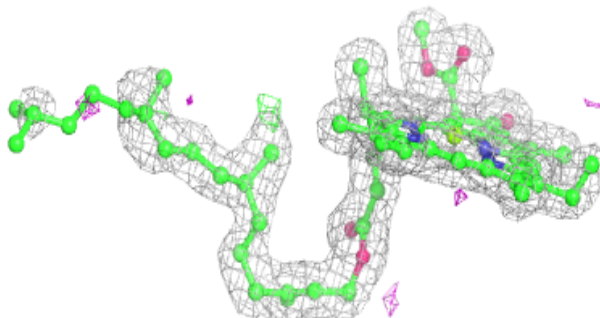
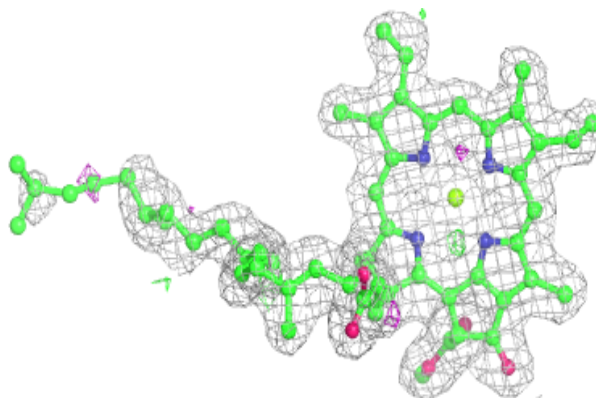


Electron density around CLA d 403:

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

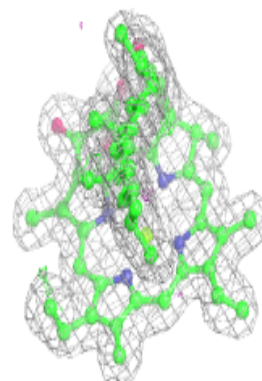
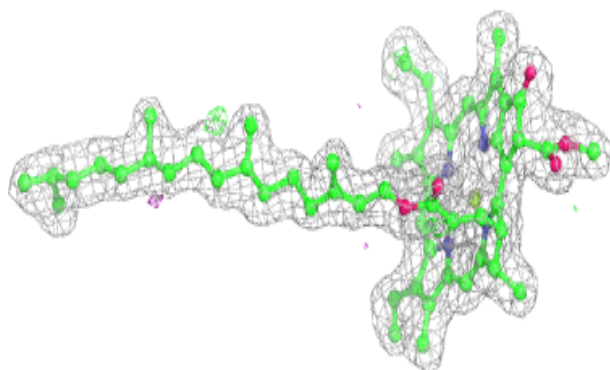
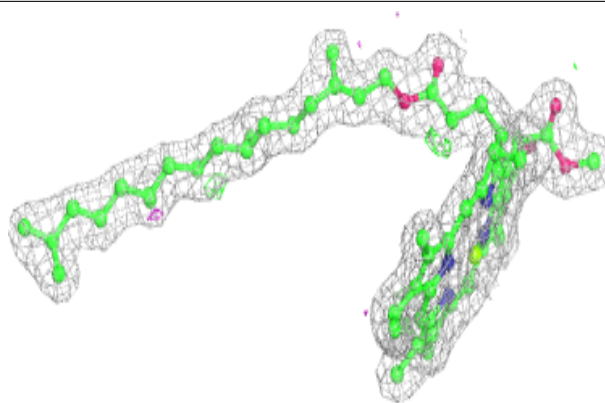
**Electron density around CLA A 406:**

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

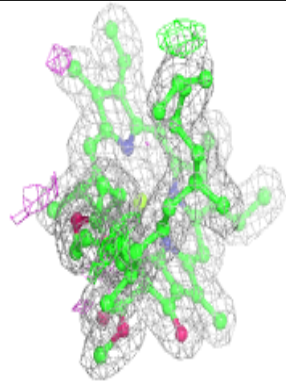
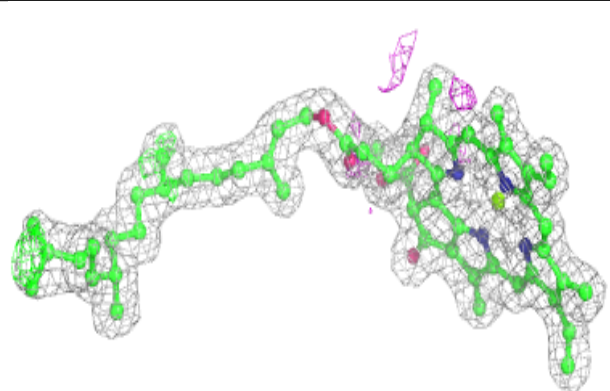
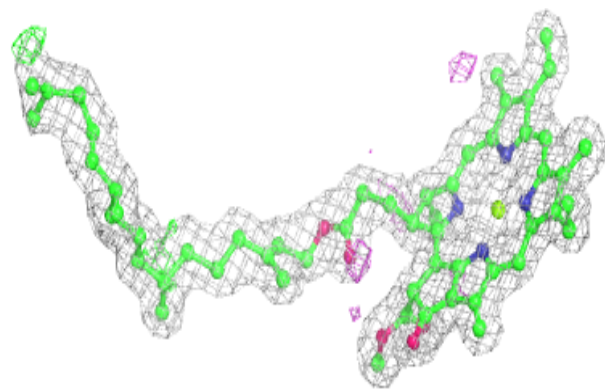


Electron density around CLA b 608:

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

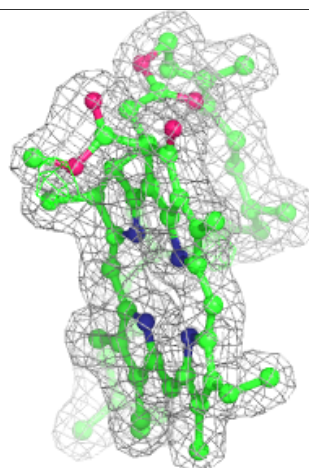
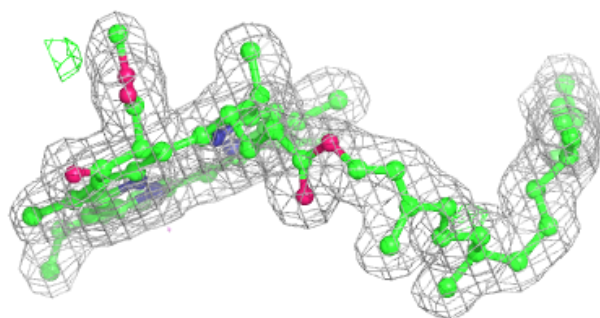
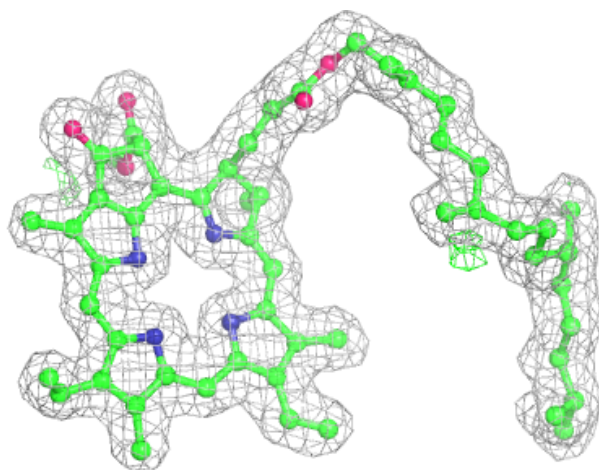
**Electron density around CLA a 406:**

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



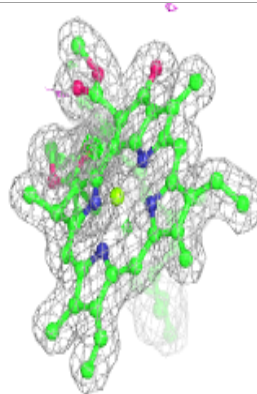
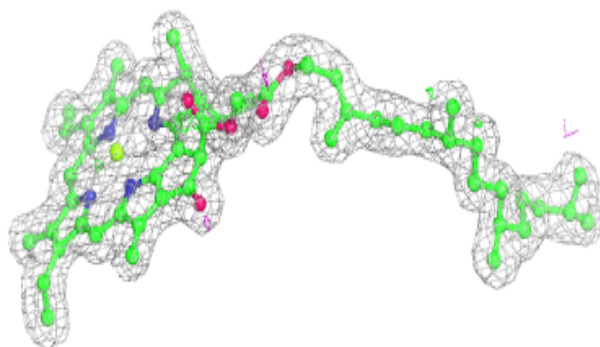
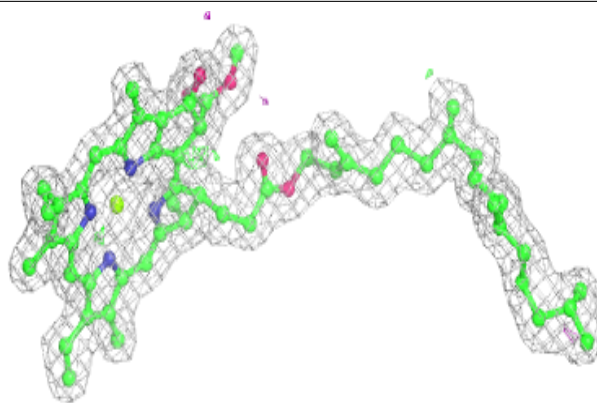
Electron density around PHO a 409:

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

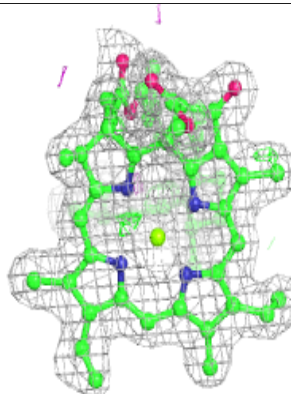
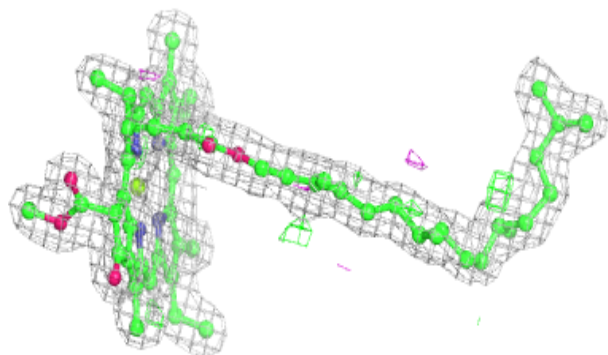
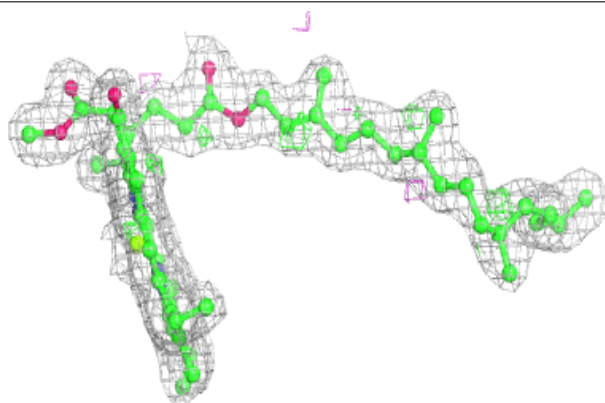


Electron density around CLA A 405:

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

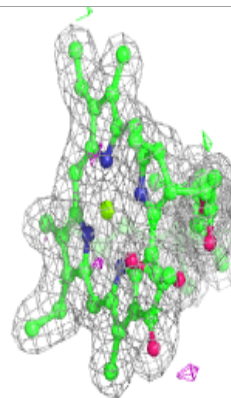
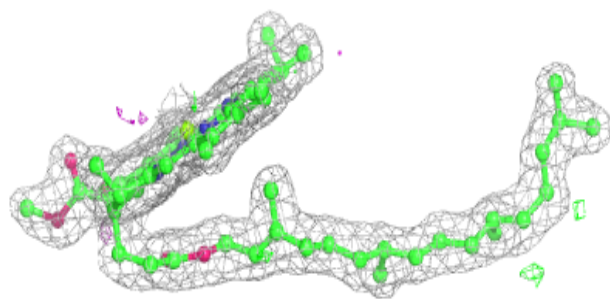
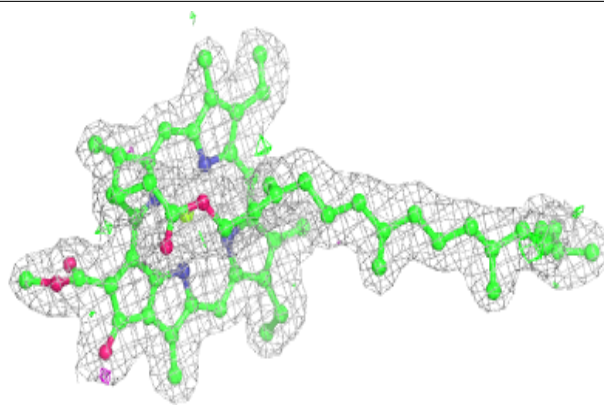
**Electron density around CLA B 606:**

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

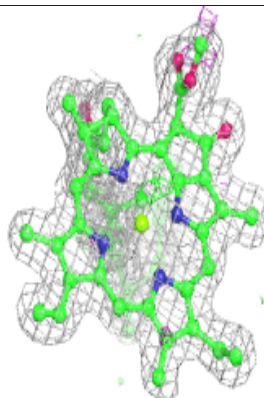
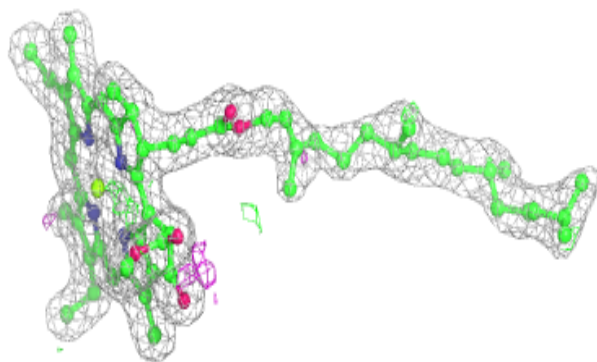
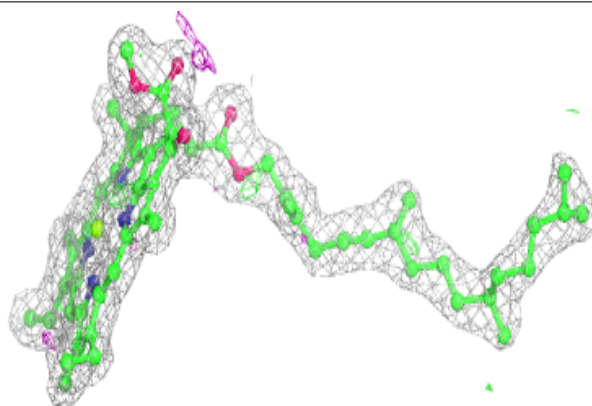


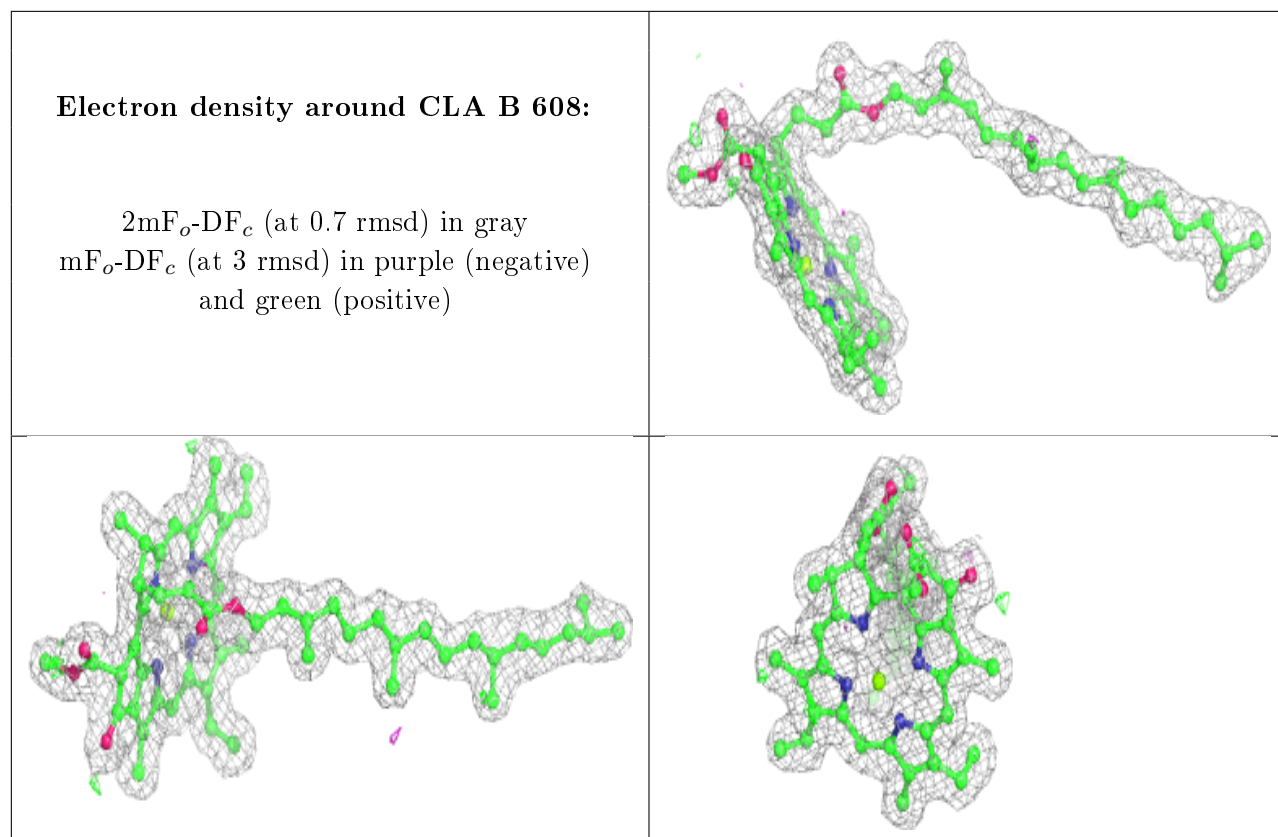
Electron density around CLA B 609:

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

**Electron density around CLA B 605:**

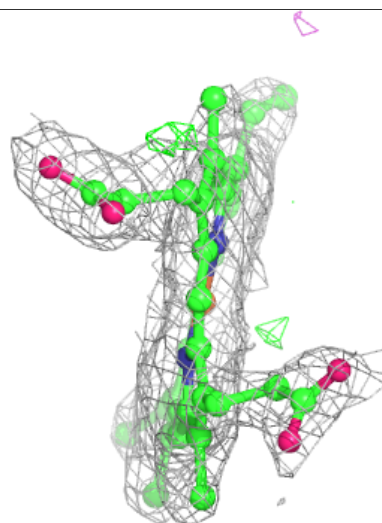
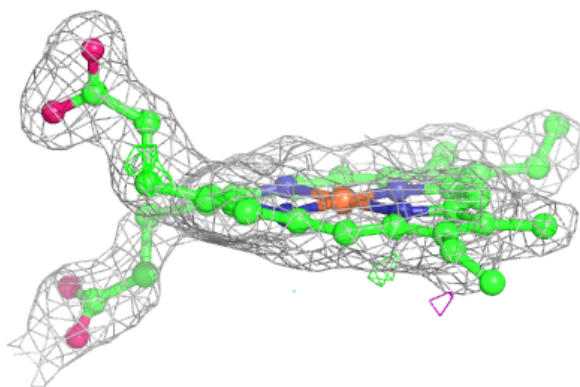
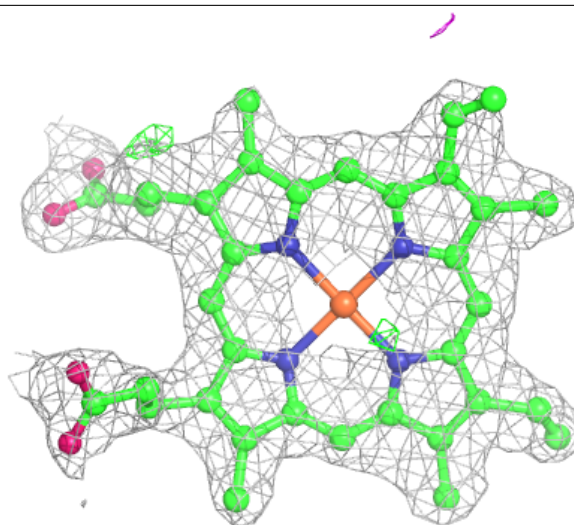
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





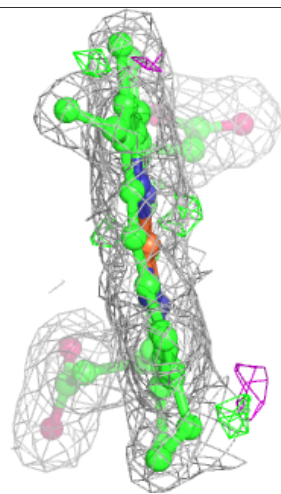
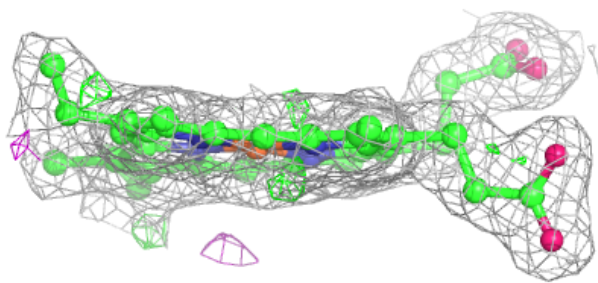
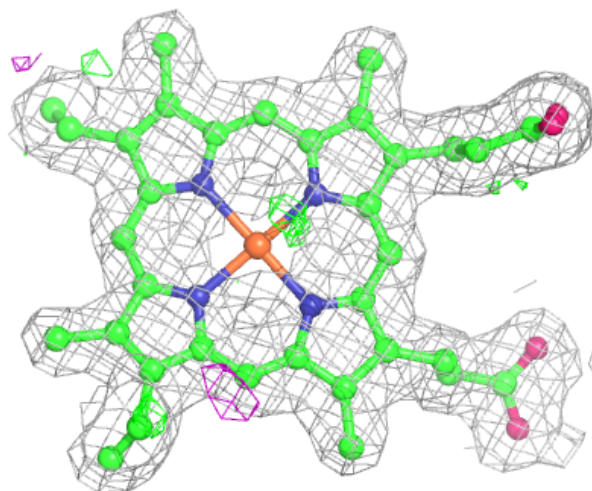
Electron density around HEM e 105:

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



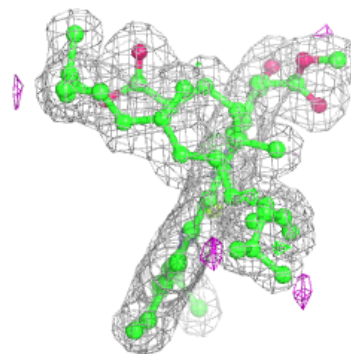
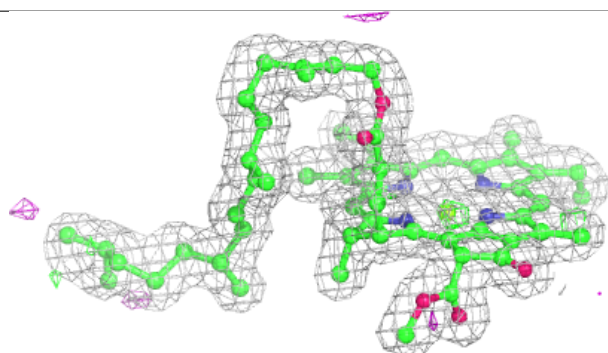
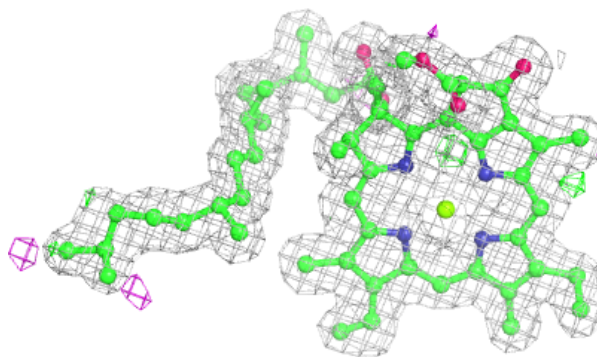
Electron density around HEC V 203:

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

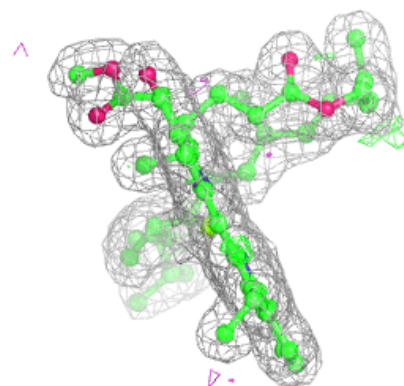
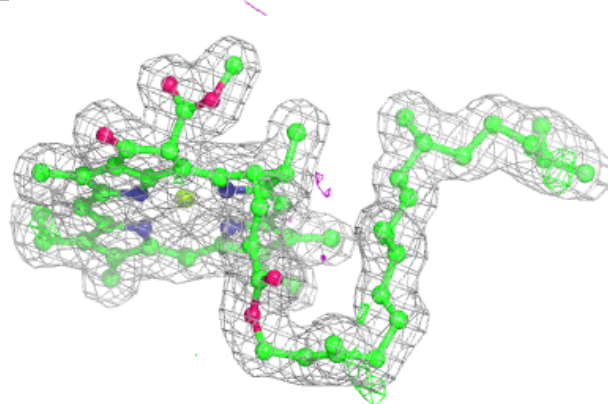
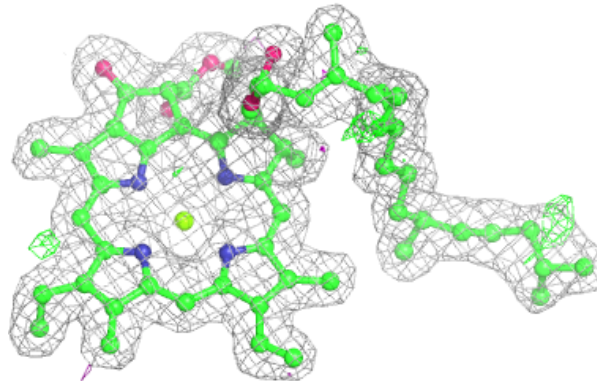


Electron density around CLA d 401:

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

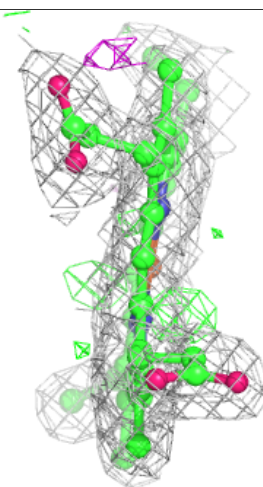
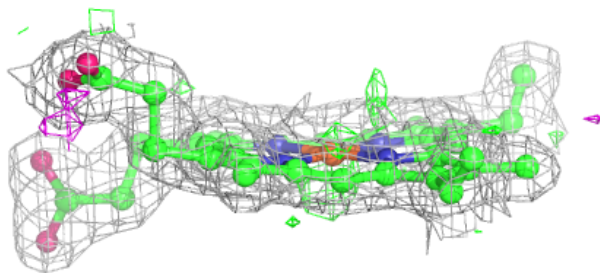
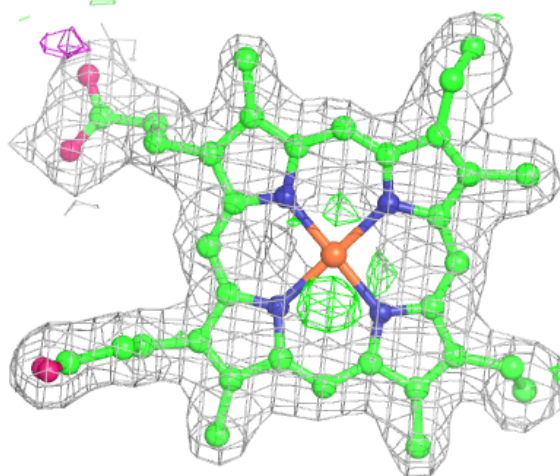
**Electron density around CLA D 401:**

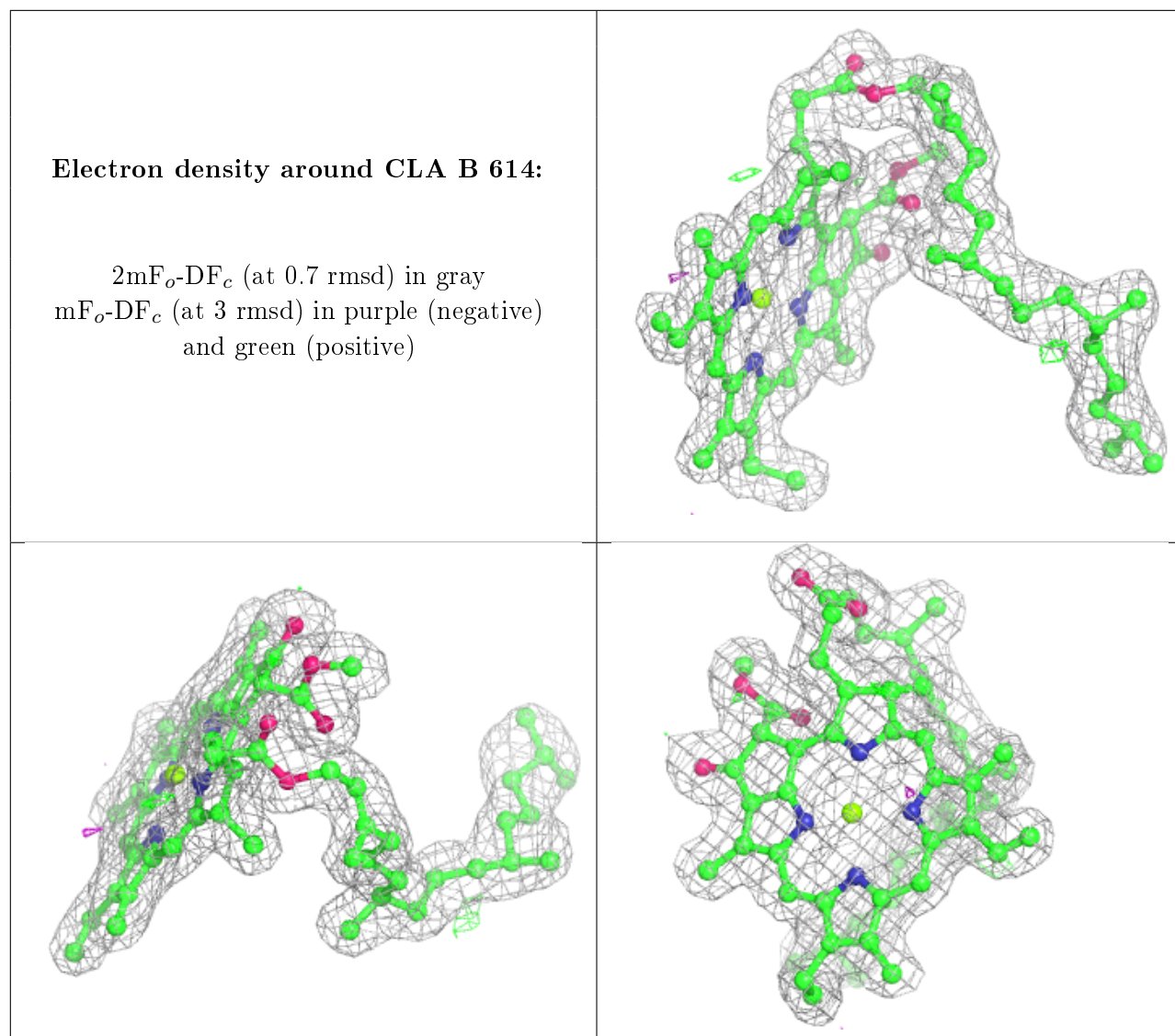
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC v 203:

$2mF_o-DF_c$ (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.