



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 02:24 PM BST

PDB ID : 3WU2
Title : Crystal structure analysis of Photosystem II complex
Authors : Umena, Y.; Kawakami, K.; Shen, J.R.; Kamiya, N.
Deposited on : 2014-04-21
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

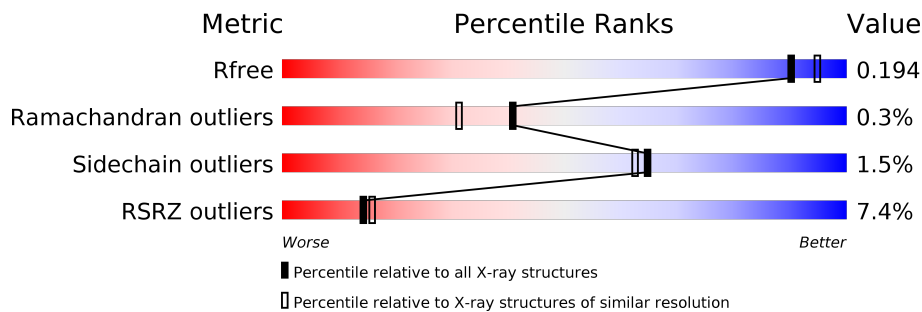
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



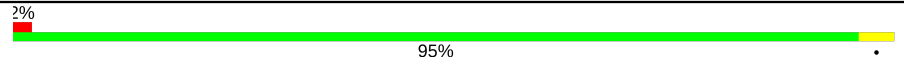
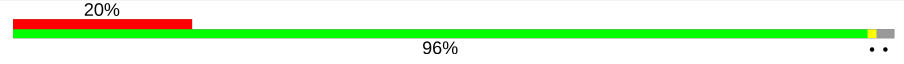
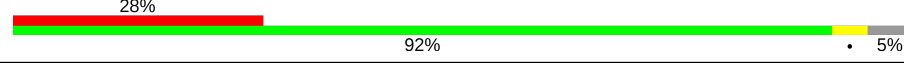

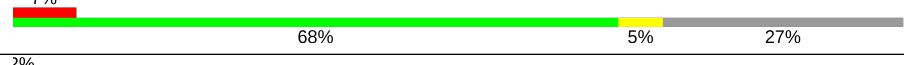
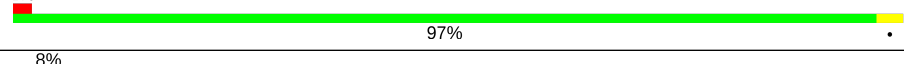
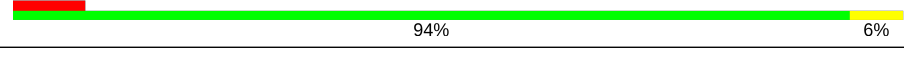
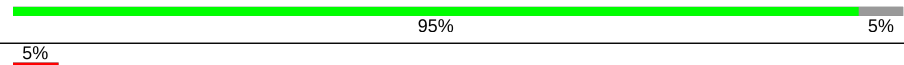
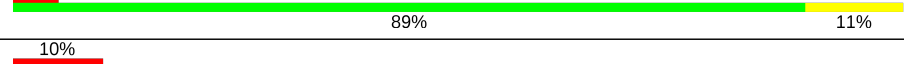
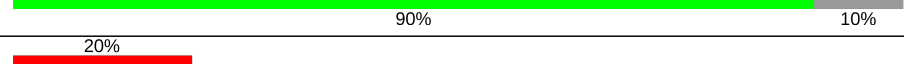

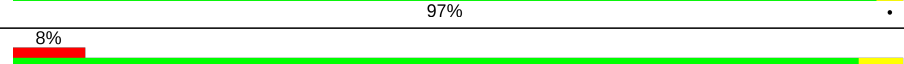
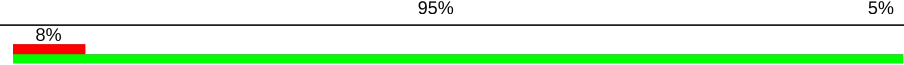
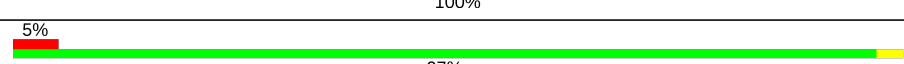
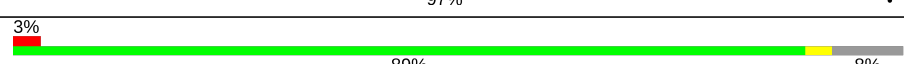
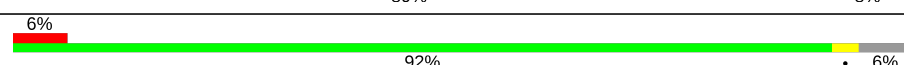
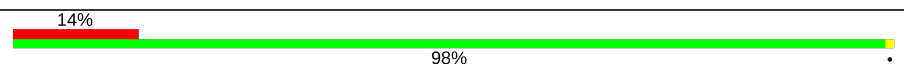
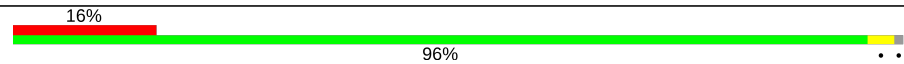
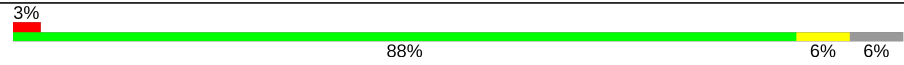
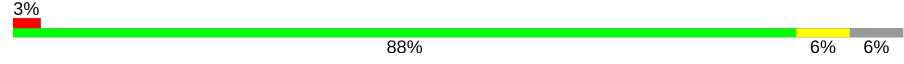
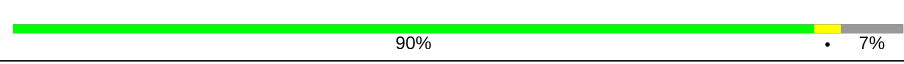
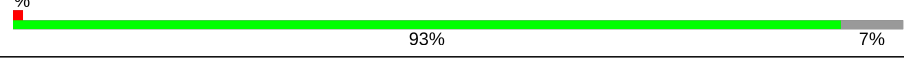
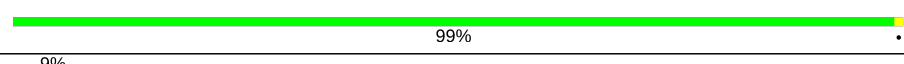
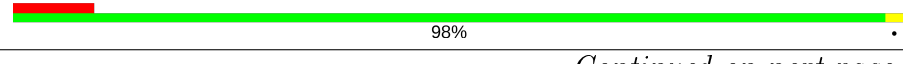

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	<p>94%</p>
1	a	344	<p>93%</p>
2	B	504	<p>97%</p>
2	b	504	<p>97%</p>
3	C	455	<p>94%</p> <p>5%</p>
3	c	455	<p>97%</p>
4	D	342	<p>96%</p>

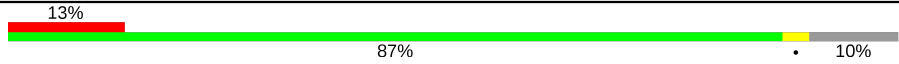
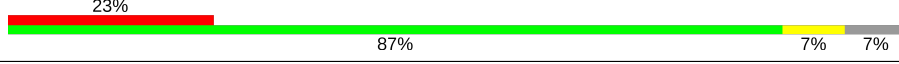
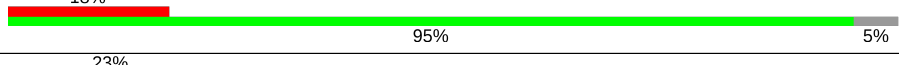
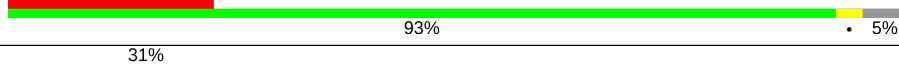
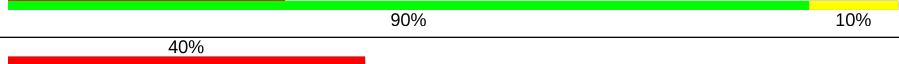
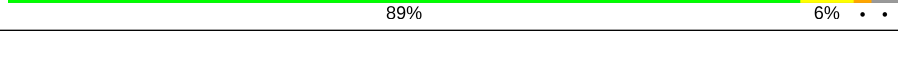
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Mol	Chain	Length	Quality of chain
4	d	342	
5	E	83	
5	e	83	
6	F	44	
6	f	44	
7	H	63	
7	h	63	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	
16	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	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	-	-	-
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	501	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	D	402	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	a	409	X	-	-	-
23	CLA	a	410	X	-	-	-
23	CLA	a	411	X	-	-	-
23	CLA	a	414	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	-	-	-
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23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	b	618	X	-	-	-
23	CLA	b	619	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	402	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	d	403	X	-	-	-
29	UNL	T	102	-	-	-	X
29	UNL	t	103	-	-	-	X
33	HTG	B	626	-	-	-	X
33	HTG	c	924	-	-	-	X

2 Entry composition [i](#)

There are 41 unique types of molecules in this entry. The entry contains 54036 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 Q(B) protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	334	Total 2633	C 1729	N 429	O 460	S 15	0	4	0
1	a	334	Total 2625	C 1722	N 431	O 457	S 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 REMARK 999	UNP P51765
a	279	PRO	ARG	SEE REMARK 999	UNP P51765

- Molecule 2 is a protein called Photosystem II CP47 chlorophyll apoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	504	Total 4009	C 2633	N 668	O 695	S 13	0	10	0
2	b	501	Total 3964	C 2605	N 658	O 688	S 13	0	11	0

- Molecule 3 is a protein called Photosystem II 44 kDa reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	451	Total 3502	C 2291	N 588	O 610	S 13	0	3	0
3	c	455	Total 3536	C 2315	N 593	O 615	S 13	0	4	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	SEE REMARK 999	UNP D0VWR7
C	20	SER	-	SEE REMARK 999	UNP D0VWR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	SEE REMARK 999	UNP D0VWR7
C	22	PHE	-	SEE REMARK 999	UNP D0VWR7
c	19	ASN	-	SEE REMARK 999	UNP D0VWR7
c	20	SER	-	SEE REMARK 999	UNP D0VWR7
c	21	ILE	-	SEE REMARK 999	UNP D0VWR7
c	22	PHE	-	SEE REMARK 999	UNP D0VWR7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	2	0
			2726	1809	443	462	12			
4	d	341	Total	C	N	O	S	0	4	0
			2741	1817	449	463	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
			657	429	106	122				
5	e	79	Total	C	N	O	S	0	0	0
			639	419	103	117				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			274	187	45	41	1			
6	f	32	Total	C	N	O	S	0	0	0
			257	175	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			
7	h	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total	C	N	O	S	0	0	0
			294	199	45	49	1			
8	i	38	Total	C	N	O	S	0	0	0
			311	210	48	52	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			251	171	37	42	1			
9	j	39	Total	C	N	O	S	0	0	0
			271	182	40	48	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	1	0
			290	202	42	46			
10	k	37	Total	C	N	O	0	0	0
			286	198	42	46			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	SEE REMARK 999	UNP P19054
K	39	TRP	VAL	SEE REMARK 999	UNP P19054
k	33	LEU	PHE	SEE REMARK 999	UNP P19054
k	39	TRP	VAL	SEE REMARK 999	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
			302	203	48	51			
11	l	37	Total	C	N	O	0	2	0
			300	204	45	51			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			261	176	37	47	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	2	0
			271	184	38	48	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	SEE REMARK 999	UNP P12312
m	8	LEU	PHE	SEE REMARK 999	UNP P12312

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	N	O	S	0	5	0
			1878	1177	314	382	5			
13	o	241	Total	C	N	O	S	0	5	0
			1855	1163	305	381	6			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	0	0	0
			770	489	129	152			
15	u	97	Total	C	N	O	0	1	0
			772	490	129	153			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	2	0
			1066	677	180	205	4			
16	v	137	Total	C	N	O	S	0	1	0
			1060	671	177	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	27	Total	C	N	O	S	0	0	0
			196	130	32	31	3			
17	y	28	Total	C	N	O	S	0	0	0
			196	128	33	32	3			

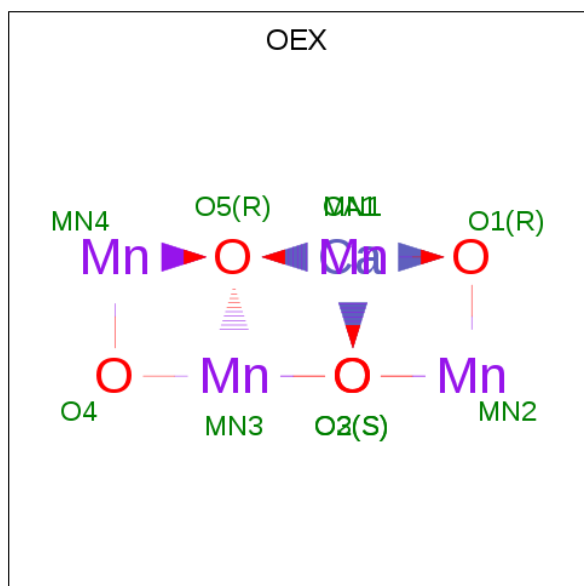
- Molecule 18 is a protein called Photosystem II reaction center protein X.

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	1	0
			280	190	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
			459	318	67	73	1			
19	z	60	Total	C	N	O	S	0	0	0
			431	301	64	65	1			

- 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

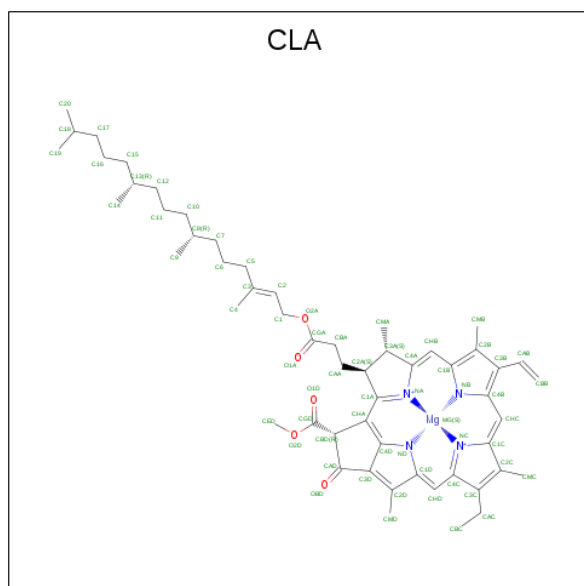
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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
			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
23	B	1	65	55	1	4	5	0	0
23	B	1	65	55	1	4	5	0	0
23	B	1	65	55	1	4	5	0	0
23	B	1	65	55	1	4	5	0	0
23	B	1	65	55	1	4	5	0	0
23	B	1	65	55	1	4	5	0	0
23	B	1	65	55	1	4	5	0	0
23	B	1	65	55	1	4	5	0	0
23	B	1	65	55	1	4	5	0	0
23	B	1	65	55	1	4	5	0	0
23	B	1	65	55	1	4	5	0	0
23	B	1	65	55	1	4	5	0	0
23	B	1	65	55	1	4	5	0	0
23	B	1	65	55	1	4	5	0	0
23	B	1	65	55	1	4	5	0	0
23	B	1	65	55	1	4	5	0	0
23	C	1	65	55	1	4	5	0	0
23	C	1	65	55	1	4	5	0	0
23	C	1	65	55	1	4	5	0	0

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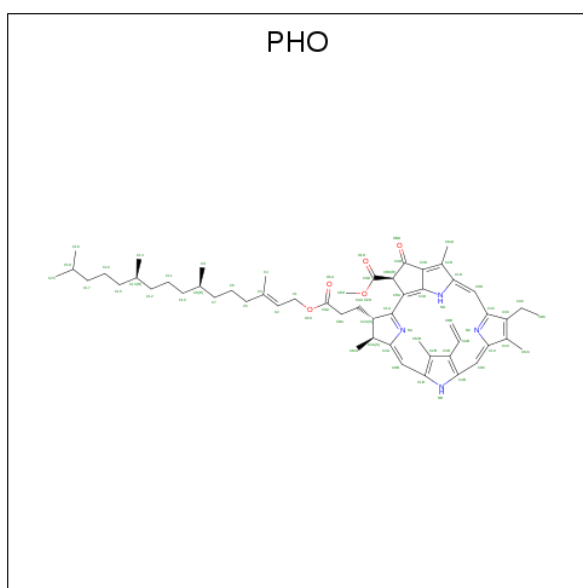
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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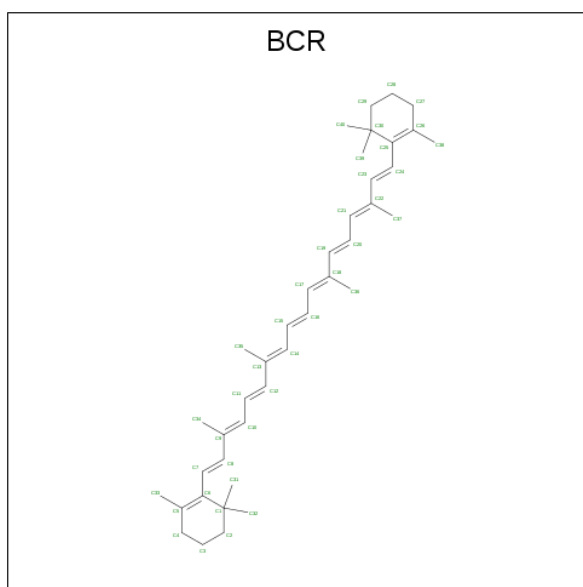
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- 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	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		

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



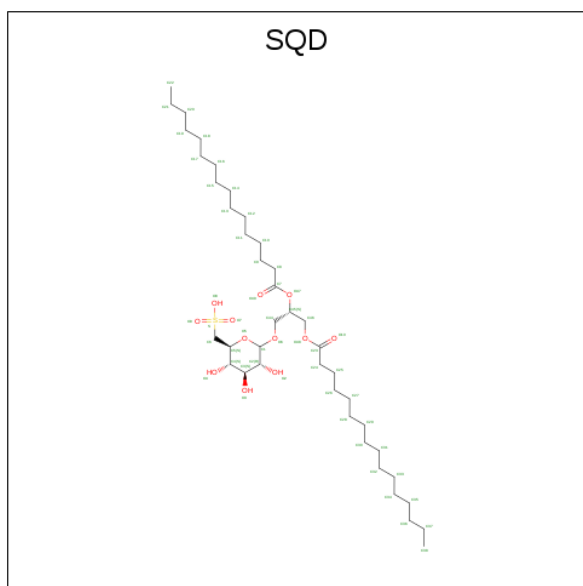
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	a	1	Total 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	k	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).



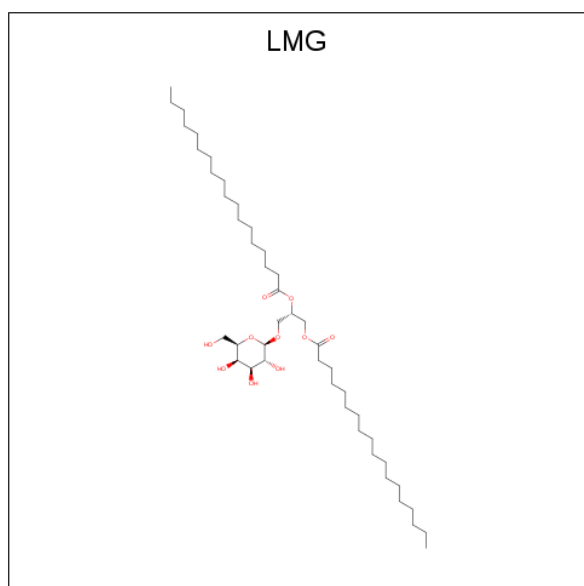
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O S 54 41 12 1	0	0
26	A	1	Total C O S 54 41 12 1	0	0
26	B	1	Total C O S 54 41 12 1	0	0
26	D	1	Total C O S 45 32 12 1	0	0
26	L	1	Total C O S 54 41 12 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	f	1	Total	C	O	S	0	0
			33	23	9	1		

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



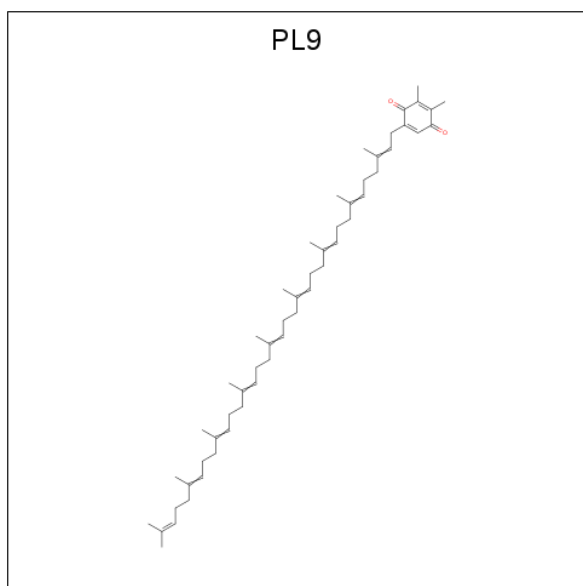
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
27	A	1	Total	C	O	0	0
			51	41	10		
27	B	1	Total	C	O	0	0
			51	41	10		
27	C	1	Total	C	O	0	0
			51	41	10		
27	D	1	Total	C	O	0	0
			51	41	10		
27	Z	1	Total	C	O	0	0
			51	41	10		
27	a	1	Total	C	O	0	0
			51	41	10		
27	b	1	Total	C	O	0	0
			51	41	10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

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

- Molecule 28 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
28	A	1	Total	C	O	0	0
			55	53	2		
28	D	1	Total	C	O	0	0
			55	53	2		
28	a	1	Total	C	O	0	0
			55	53	2		
28	d	1	Total	C	O	0	0
			55	53	2		

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

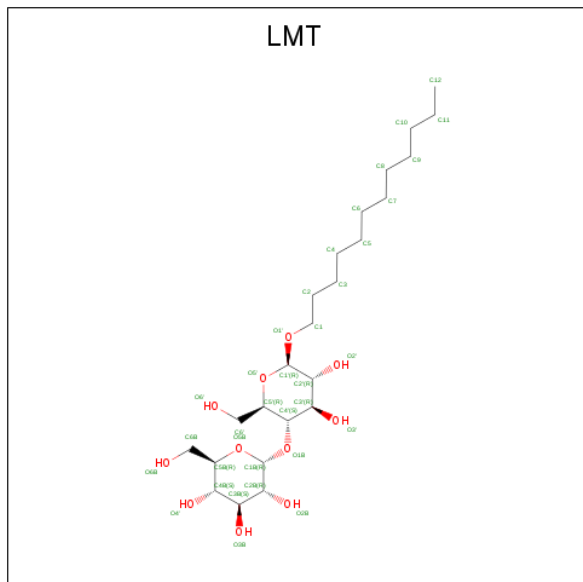
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	B	4	Total	C		0	0
			56	56			
29	c	2	Total	C	O	0	0
			40	35	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	t	1	Total C 16 16	0	0
29	X	1	Total C 16 16	0	0
29	J	2	Total C 26 26	0	0
29	E	2	Total C 27 27	0	0
29	b	4	Total C O 84 79 5	0	0
29	A	4	Total C O 69 64 5	0	0
29	x	1	Total C 16 16	0	0
29	M	1	Total C 16 16	0	0
29	j	2	Total C 28 28	0	0
29	D	2	Total C O 56 51 5	0	0
29	e	1	Total C 11 11	0	0
29	I	2	Total C 24 24	0	0
29	Z	1	Total C 16 16	0	0
29	a	3	Total C O 56 51 5	0	0
29	L	1	Total C 14 14	0	0
29	d	1	Total C 16 16	0	0
29	H	1	Total C 10 10	0	0
29	i	4	Total C 55 55	0	0
29	C	1	Total C O 34 29 5	0	0
29	z	1	Total C 16 16	0	0
29	T	1	Total C 13 13	0	0

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



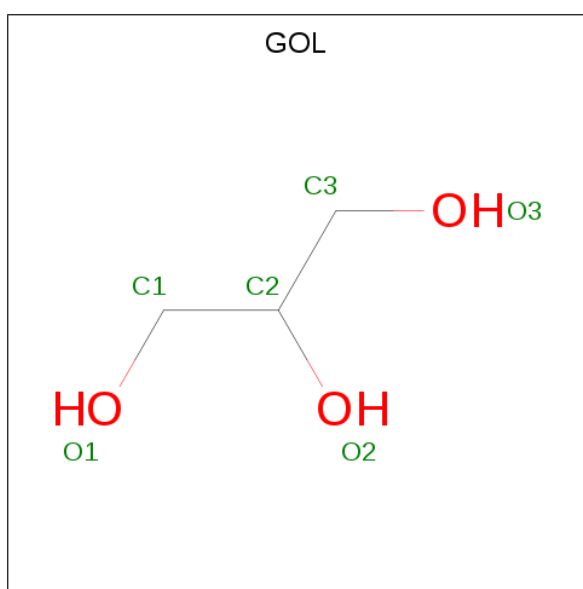
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	1	Total C O 35 24 11	0	0
30	B	1	Total C O 35 24 11	0	0
30	C	1	Total C O 35 24 11	0	0
30	F	1	Total C O 35 24 11	0	0
30	J	1	Total C O 24 18 6	0	0
30	M	1	Total C O 35 24 11	0	0
30	M	1	Total C O 35 24 11	0	0
30	Z	1	Total C O 35 24 11	0	0
30	a	1	Total C O 35 24 11	0	0
30	b	1	Total C O 25 19 6	0	0
30	b	1	Total C O 24 18 6	0	0
30	c	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	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
			32	21	11		

- Molecule 31 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total 6	C 3	O 3	0	0
31	B	1	Total 6	C 3	O 3	0	0
31	C	1	Total 6	C 3	O 3	0	0
31	C	1	Total 6	C 3	O 3	0	0
31	C	1	Total 6	C 3	O 3	0	0
31	D	1	Total 6	C 3	O 3	0	0
31	L	1	Total 6	C 3	O 3	0	0
31	O	1	Total 6	C 3	O 3	0	0
31	V	1	Total 6	C 3	O 3	0	0
31	V	1	Total 6	C 3	O 3	0	0
31	V	1	Total 6	C 3	O 3	0	0
31	a	1	Total 6	C 3	O 3	0	0
31	a	1	Total 6	C 3	O 3	0	0
31	a	1	Total 6	C 3	O 3	0	0
31	b	1	Total 6	C 3	O 3	0	0
31	b	1	Total 6	C 3	O 3	0	0
31	b	1	Total 6	C 3	O 3	0	0
31	b	1	Total 6	C 3	O 3	0	0
31	b	1	Total 6	C 3	O 3	0	0
31	c	1	Total 6	C 3	O 3	0	0
31	c	1	Total 6	C 3	O 3	0	0

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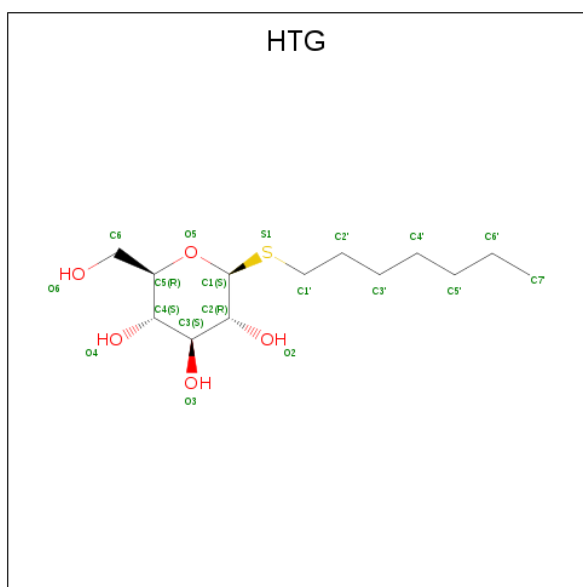
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	c	1	Total C O 6 3 3	0	0
31	c	1	Total C O 6 3 3	0	0
31	f	1	Total C O 6 3 3	0	0
31	h	1	Total C O 6 3 3	0	0
31	l	1	Total C O 6 3 3	0	0
31	v	1	Total C O 6 3 3	0	0
31	v	1	Total C O 6 3 3	0	0
31	v	1	Total C O 6 3 3	0	0

- Molecule 32 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	B	1	Total Ca 1 1	0	0
32	c	1	Total Ca 1 1	0	0
32	F	1	Total Ca 1 1	0	0
32	o	1	Total Ca 1 1	0	0
32	O	1	Total Ca 1 1	0	0
32	b	1	Total Ca 1 1	0	0
32	f	1	Total Ca 1 1	0	0

- Molecule 33 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: C₁₃H₂₆O₅S).



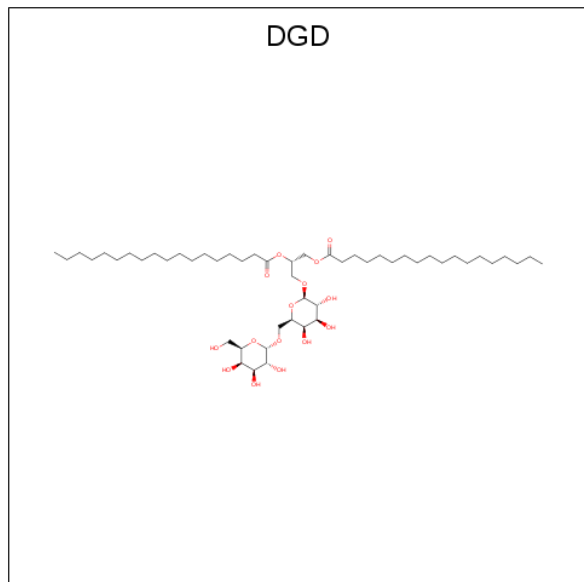
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
33	B	1	19	13	5	1	0	0
33	B	1	19	13	5	1	0	0
33	B	1	19	13	5	1	0	0
33	B	1	19	13	5	1	0	0
33	B	1	19	13	5	1	0	0
33	C	1	19	13	5	1	0	0
33	C	1	19	13	5	1	0	0
33	D	1	19	13	5	1	0	0
33	O	1	19	13	5	1	0	0
33	U	1	9	8	1		0	0
33	V	1	13	7	5	1	0	0
33	b	1	19	13	5	1	0	0
33	b	1	19	13	5	1	0	0
33	b	1	19	13	5	1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
33	b	1	Total 19	C 13	O 5	S 1	0	0
33	c	1	Total 19	C 13	O 5	S 1	0	0
33	c	1	Total 19	C 13	O 5	S 1	0	0
33	d	1	Total 19	C 13	O 5	S 1	0	0
33	u	1	Total 14	C 10	O 3	S 1	0	0

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



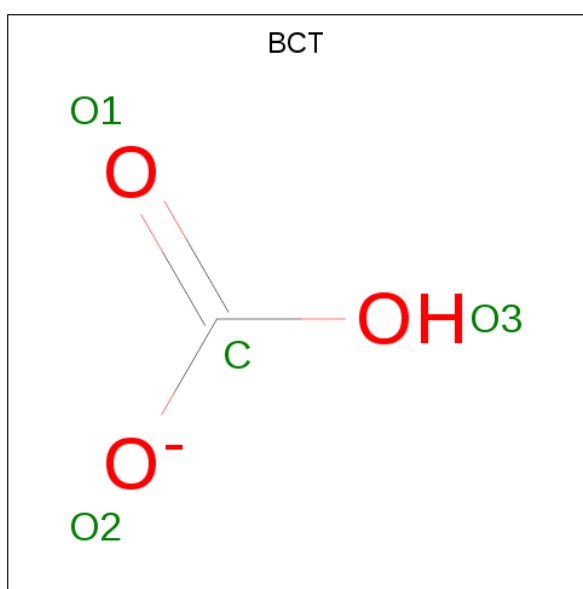
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
34	C	1	Total 62	C 47	O 15	0	0
34	C	1	Total 62	C 47	O 15	0	0
34	C	1	Total 62	C 47	O 15	0	0
34	D	1	Total 53	C 42	O 11	0	0
34	H	1	Total 62	C 47	O 15	0	0
34	c	1	Total 62	C 47	O 15	0	0

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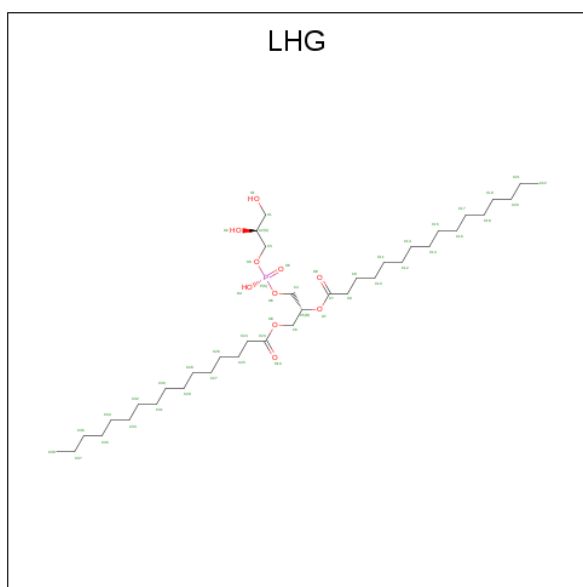
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	c	1	Total	C	O	0	0
			62	47	15		
34	c	1	Total	C	O	0	0
			62	47	15		
34	d	1	Total	C	O	0	0
			50	41	9		
34	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 35 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



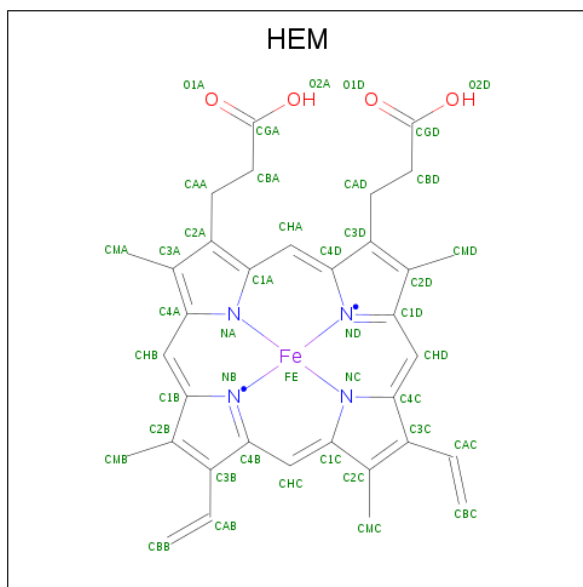
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	D	1	Total	C	O	0	0
			4	1	3		
35	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 36 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $\text{C}_{38}\text{H}_{75}\text{O}_{10}\text{P}$).



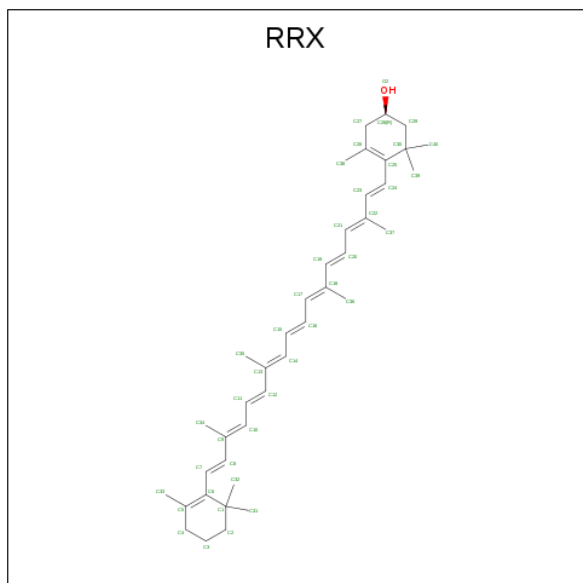
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
36	D	1	49	38	10	1	0	0
36	D	1	49	38	10	1	0	0
36	D	1	46	35	10	1	0	0
36	E	1	49	38	10	1	0	0
36	L	1	49	38	10	1	0	0
36	a	1	40	29	10	1	0	0
36	d	1	49	38	10	1	0	0
36	d	1	49	38	10	1	0	0
36	d	1	49	38	10	1	0	0
36	l	1	49	38	10	1	0	0

- 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	
			Total	C	Fe	N			O
37	F	1	43	34	1	4	4	0	0
37	V	1	43	34	1	4	4	0	0
37	f	1	43	34	1	4	4	0	0
37	v	1	43	34	1	4	4	0	0

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

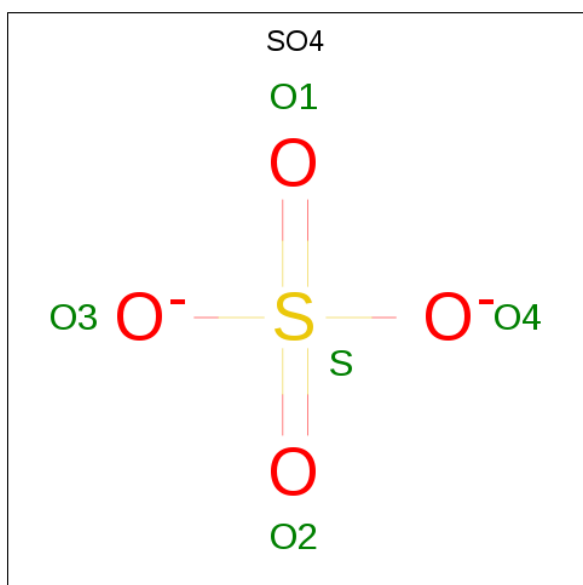


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
38	H	1	Total	C	O	0	0
			41	40	1		
38	h	1	Total	C	O	0	0
			41	40	1		

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

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

- Molecule 40 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
40	O	1	Total	O	S	0	0
			5	4	1		

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	168	Total	O	0	2
			170	170		
41	B	311	Total	O	0	8
			319	319		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	C	253	Total O 263 263	0	10
41	D	156	Total O 161 161	0	5
41	E	32	Total O 35 35	0	3
41	F	12	Total O 12 12	0	0
41	H	50	Total O 52 52	0	2
41	I	8	Total O 8 8	0	0
41	J	9	Total O 9 9	0	0
41	K	8	Total O 8 8	0	0
41	L	23	Total O 24 24	0	1
41	M	15	Total O 16 16	0	1
41	O	193	Total O 202 202	0	9
41	T	10	Total O 10 10	0	0
41	U	98	Total O 100 100	0	2
41	V	140	Total O 144 144	0	4
41	Y	6	Total O 6 6	0	0
41	X	13	Total O 14 14	0	1
41	Z	1	Total O 1 1	0	0
41	a	153	Total O 155 155	0	2
41	b	295	Total O 306 306	0	11
41	c	238	Total O 245 245	0	7
41	d	156	Total O 160 160	0	4

Continued on next page...

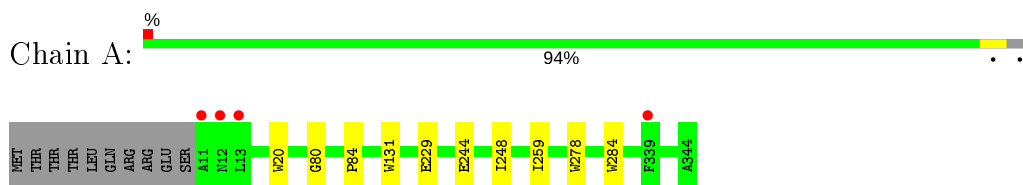
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	e	22	Total O 22 22	0	0
41	f	13	Total O 14 14	0	1
41	h	48	Total O 53 53	0	5
41	i	13	Total O 14 14	0	1
41	j	9	Total O 9 9	0	0
41	k	5	Total O 5 5	0	0
41	l	17	Total O 18 18	0	1
41	m	15	Total O 16 16	0	1
41	o	167	Total O 175 175	0	8
41	t	12	Total O 12 12	0	0
41	u	102	Total O 106 106	0	4
41	v	98	Total O 104 104	0	6
41	y	7	Total O 7 7	0	0
41	x	6	Total O 6 6	0	0
41	z	2	Total O 2 2	0	0

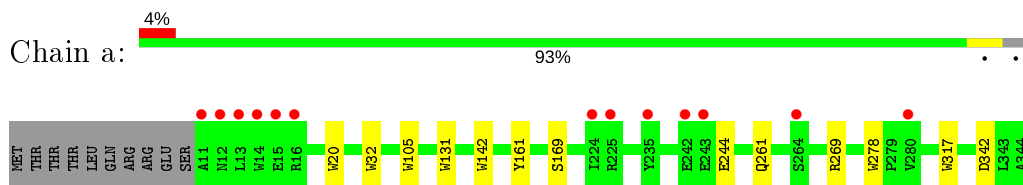
3 Residue-property plots [i](#)

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.

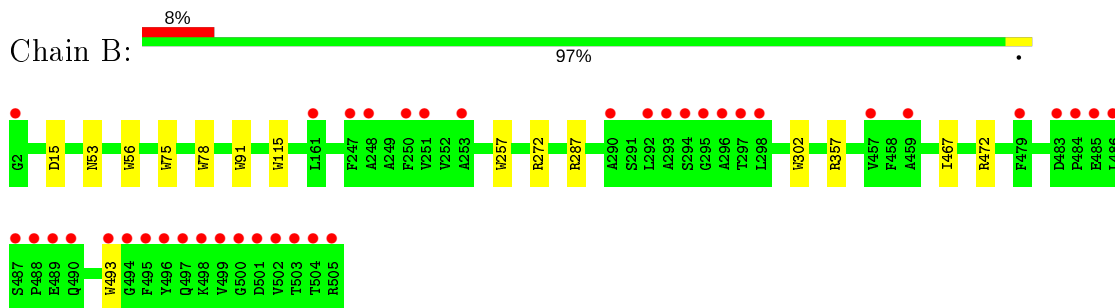
- Molecule 1: Photosystem Q(B) protein



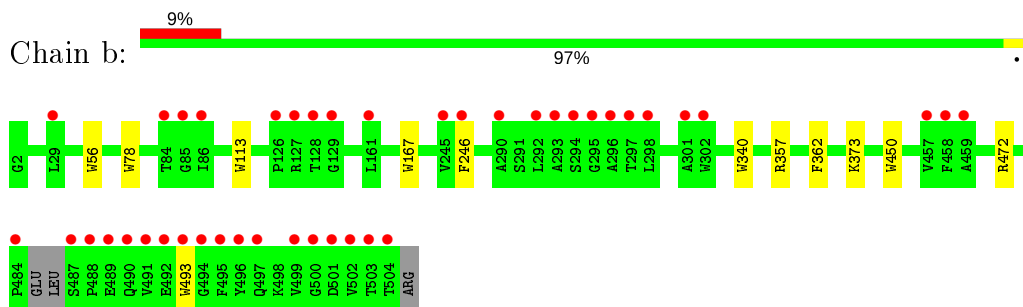
- Molecule 1: Photosystem Q(B) protein



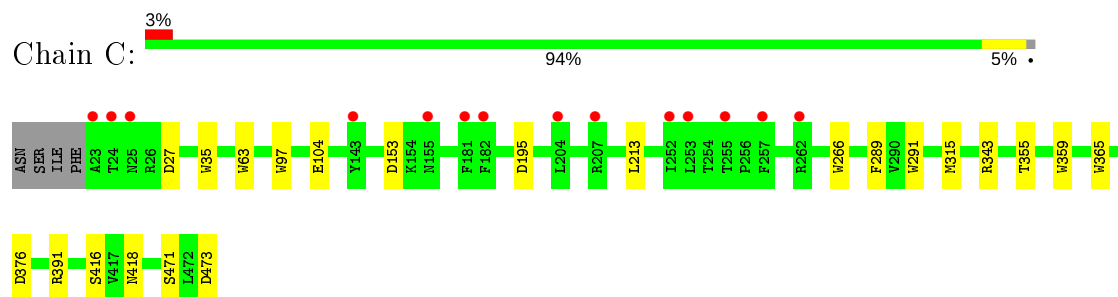
- Molecule 2: Photosystem II CP47 chlorophyll apoprotein



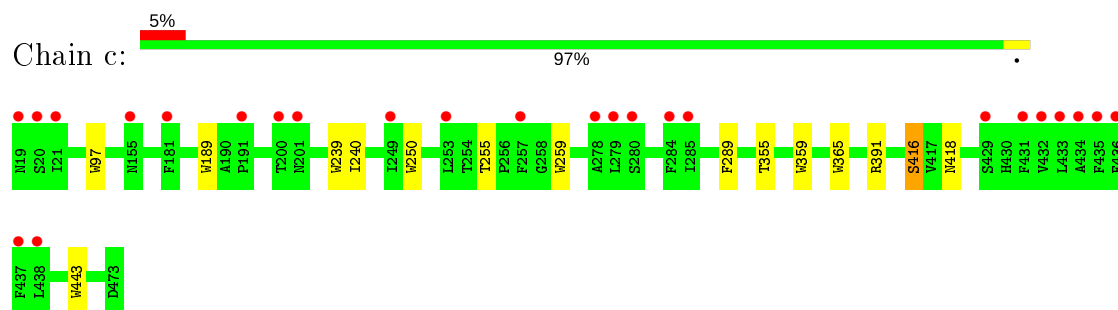
- Molecule 2: Photosystem II CP47 chlorophyll apoprotein



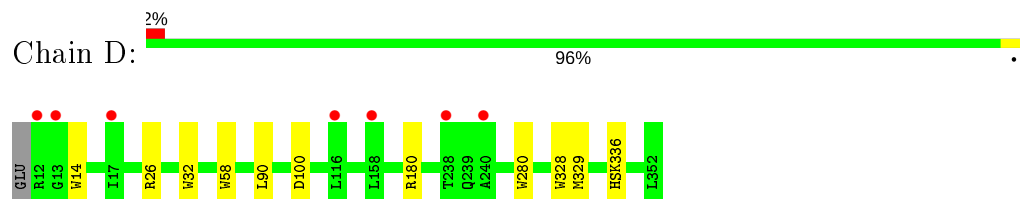
- Molecule 3: Photosystem II 44 kDa reaction center protein



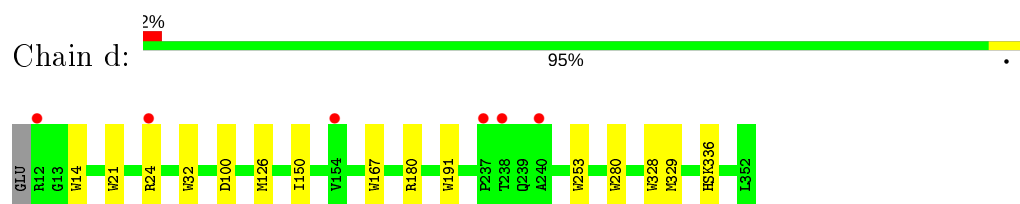
- Molecule 3: Photosystem II 44 kDa reaction center protein



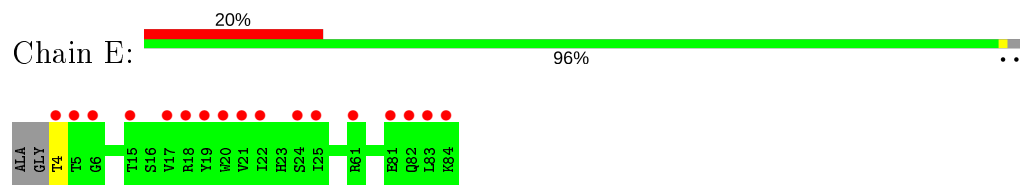
- Molecule 4: Photosystem II D2 protein



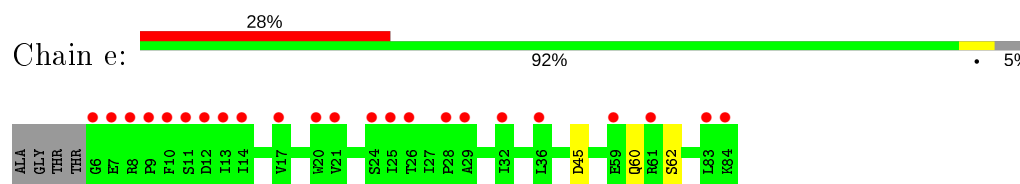
- Molecule 4: Photosystem II D2 protein



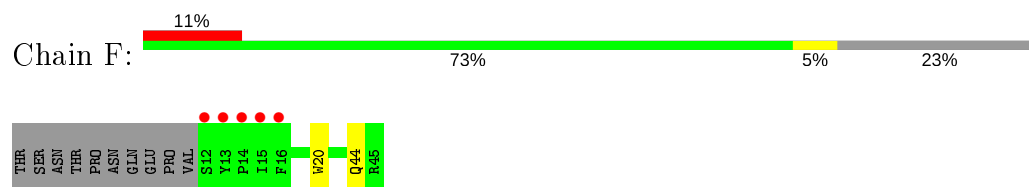
- Molecule 5: Cytochrome b559 subunit alpha



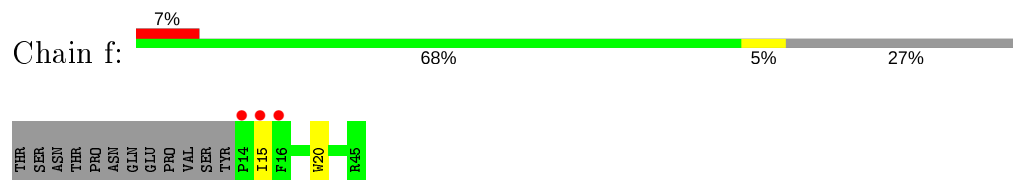
- Molecule 5: Cytochrome b559 subunit alpha



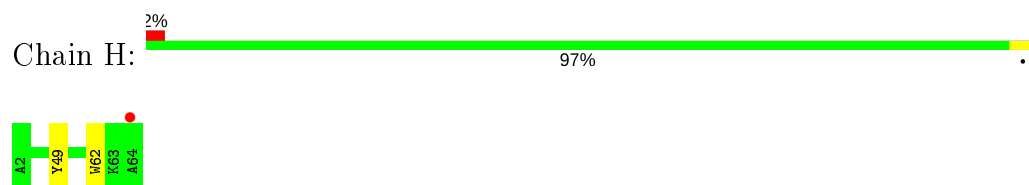
- Molecule 6: Cytochrome b559 subunit beta



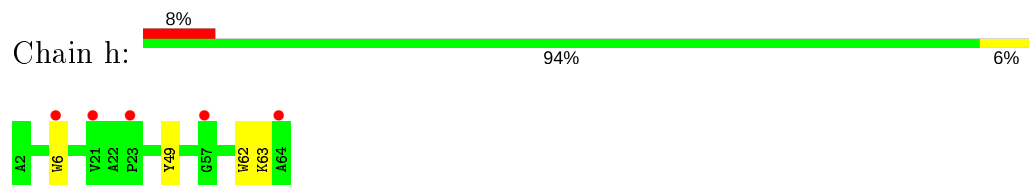
- Molecule 6: Cytochrome b559 subunit beta



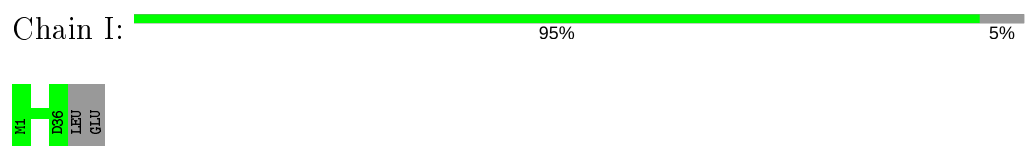
- Molecule 7: Photosystem II reaction center protein H



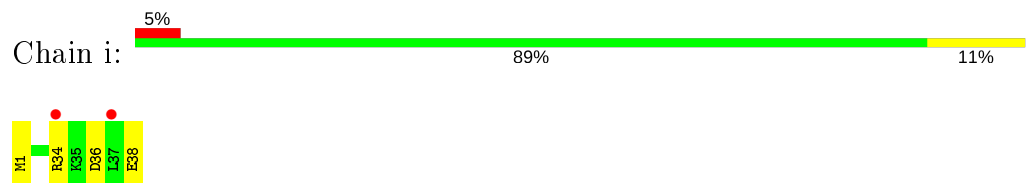
- Molecule 7: Photosystem II reaction center protein H



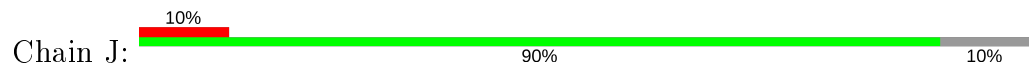
- Molecule 8: Photosystem II reaction center protein I

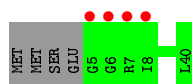


- Molecule 8: Photosystem II reaction center protein I

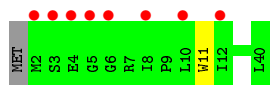
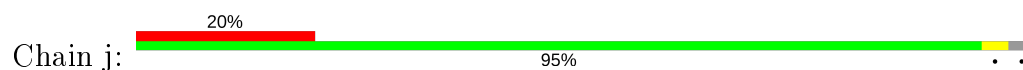


- Molecule 9: Photosystem II reaction center protein J





- Molecule 9: Photosystem II reaction center protein J



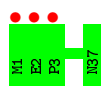
- Molecule 10: Photosystem II reaction center protein K



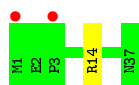
- Molecule 10: Photosystem II reaction center protein K



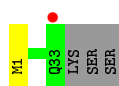
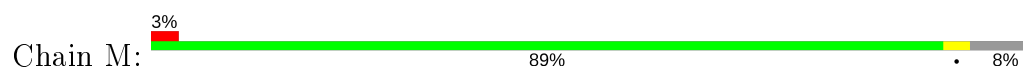
- Molecule 11: Photosystem II reaction center protein L



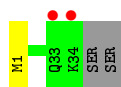
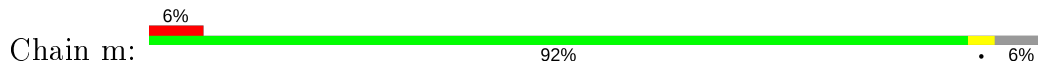
- Molecule 11: Photosystem II reaction center protein L



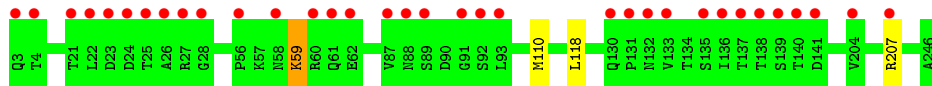
- Molecule 12: Photosystem II reaction center protein M



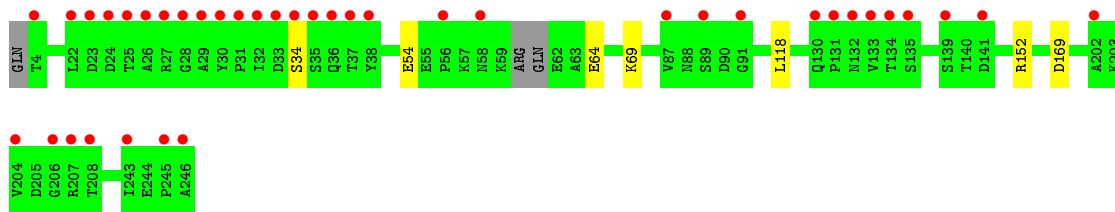
- Molecule 12: Photosystem II reaction center protein M



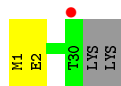
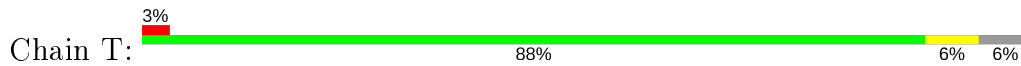
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



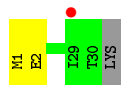
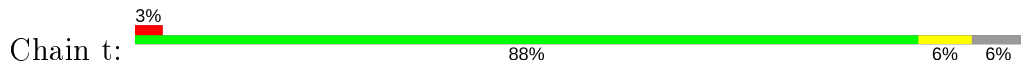
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



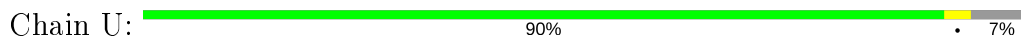
- Molecule 14: Photosystem II reaction center protein T



- Molecule 14: Photosystem II reaction center protein T

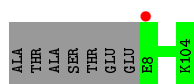


- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein





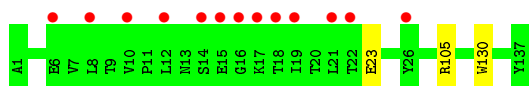
- Molecule 16: Cytochrome c-550

Chain V: 99%



- Molecule 16: Cytochrome c-550

Chain v: 98%



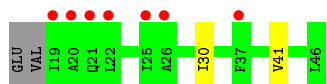
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y: 87%



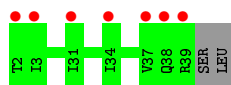
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y: 87%



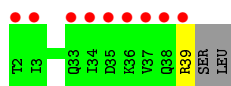
- Molecule 18: Photosystem II reaction center protein X

Chain X: 95%

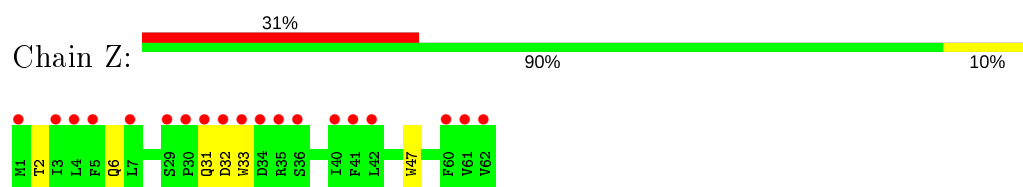


- Molecule 18: Photosystem II reaction center protein X

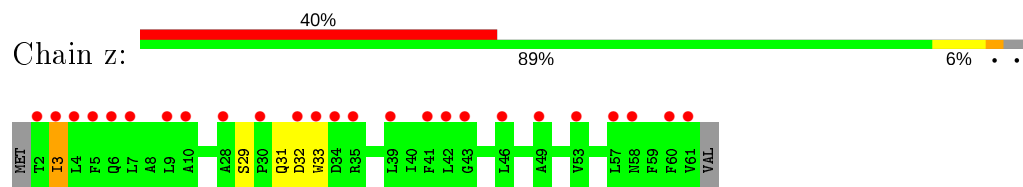
Chain x: 93%



- 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	122.19Å 228.51Å 286.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 49.02 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-1.90) 99.8 (49.02-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 1.90Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.156 , 0.194 0.157 , 0.194	Depositor DCC
R_{free} test set	31215 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtrriage
Anisotropy	0.575	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 66.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	54036	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PL9, BCT, BCR, DGD, HSK, FE2, RRX, LHG, GOL, CL, CA, CLA, SO4, HEM, FME, UNL, HTG, MG, OEX, PHO, LMT, SQD, LMG

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	1.08	4/2730 (0.1%)	0.90	1/3723 (0.0%)
1	a	1.06	9/2721 (0.3%)	0.86	4/3711 (0.1%)
2	B	1.03	9/4179 (0.2%)	0.89	5/5693 (0.1%)
2	b	1.01	7/4134 (0.2%)	0.85	2/5633 (0.0%)
3	C	1.00	7/3624 (0.2%)	0.84	9/4933 (0.2%)
3	c	0.96	8/3662 (0.2%)	0.81	0/4986
4	D	1.13	5/2804 (0.2%)	0.93	3/3820 (0.1%)
4	d	1.05	8/2825 (0.3%)	0.87	2/3847 (0.1%)
5	E	0.81	0/676	0.82	0/924
5	e	0.81	0/658	0.78	1/899 (0.1%)
6	F	0.90	1/283 (0.4%)	0.71	0/386
6	f	0.92	1/265 (0.4%)	0.69	0/360
7	H	0.98	1/511 (0.2%)	0.79	0/697
7	h	0.94	2/511 (0.4%)	0.81	0/697
8	I	0.77	0/291	0.78	0/394
8	i	0.75	0/308	0.77	0/415
9	J	0.94	0/257	0.68	0/349
9	j	0.81	1/277 (0.4%)	0.69	0/376
10	K	0.76	1/303 (0.3%)	0.75	0/418
10	k	0.79	1/296 (0.3%)	0.77	0/408
11	L	1.05	0/312	0.88	0/425
11	l	1.00	0/313	0.84	1/428 (0.2%)
12	M	0.85	0/257	0.91	0/352
12	m	0.86	0/270	0.80	0/370
13	O	0.84	0/1924	0.89	0/2610
13	o	0.79	0/1900	0.86	3/2577 (0.1%)
14	T	0.93	0/255	0.86	0/346
14	t	0.99	0/255	0.92	0/346
15	U	0.93	0/781	0.90	1/1059 (0.1%)
15	u	0.95	0/786	0.91	0/1067
16	V	0.97	0/1093	0.89	1/1485 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.88	1/1084 (0.1%)	0.85	1/1475 (0.1%)
17	Y	0.55	0/197	0.66	0/263
17	y	0.50	0/197	0.75	0/264
18	X	0.72	0/286	0.75	0/387
18	x	0.67	0/286	0.75	0/387
19	Z	0.76	2/470 (0.4%)	0.74	0/645
19	z	0.68	1/442 (0.2%)	0.71	0/608
All	All	0.97	69/42423 (0.2%)	0.85	34/57763 (0.1%)

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	78	TRP	CD2-CE2	7.33	1.50	1.41
7	H	62	TRP	CD2-CE2	6.81	1.49	1.41
3	c	443	TRP	CD2-CE2	6.79	1.49	1.41
1	A	284	TRP	CD2-CE2	6.79	1.49	1.41
3	C	359	TRP	CD2-CE2	6.46	1.49	1.41
4	d	328	TRP	CD2-CE2	6.33	1.49	1.41
9	j	11	TRP	CD2-CE2	6.32	1.49	1.41
1	A	20	TRP	CD2-CE2	6.16	1.48	1.41
19	Z	33	TRP	CD2-CE2	6.13	1.48	1.41
4	D	328	TRP	CD2-CE2	6.13	1.48	1.41
2	b	113	TRP	CD2-CE2	6.00	1.48	1.41
3	c	189	TRP	CD2-CE2	5.95	1.48	1.41
4	d	167	TRP	CD2-CE2	5.94	1.48	1.41
2	B	56	TRP	CD2-CE2	5.94	1.48	1.41
16	v	130	TRP	CD2-CE2	5.86	1.48	1.41
7	h	6	TRP	CD2-CE2	5.79	1.48	1.41
2	b	340	TRP	CD2-CE2	5.75	1.48	1.41
3	c	239	TRP	CD2-CE2	5.75	1.48	1.41
10	k	39	TRP	CD2-CE2	5.74	1.48	1.41
6	F	20	TRP	CD2-CE2	5.66	1.48	1.41
2	B	75	TRP	CD2-CE2	5.66	1.48	1.41
6	f	20	TRP	CD2-CE2	5.65	1.48	1.41
1	a	32	TRP	CD2-CE2	5.63	1.48	1.41
4	D	32	TRP	CD2-CE2	5.62	1.48	1.41
1	a	161	TYR	CE1-CZ	5.59	1.45	1.38
19	z	33	TRP	CD2-CE2	5.56	1.48	1.41
7	h	62	TRP	CD2-CE2	5.55	1.48	1.41
3	c	365	TRP	CD2-CE2	5.53	1.48	1.41
4	d	21	TRP	CD2-CE2	5.53	1.48	1.41
19	Z	47	TRP	CD2-CE2	5.50	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
3	c	97	TRP	CD2-CE2	5.44	1.47	1.41
4	d	253	TRP	CD2-CE2	5.43	1.47	1.41
2	B	91	TRP	CD2-CE2	5.41	1.47	1.41
1	a	131	TRP	CD2-CE2	5.41	1.47	1.41
1	a	20	TRP	CD2-CE2	5.40	1.47	1.41
3	C	35	TRP	CD2-CE2	5.38	1.47	1.41
2	b	450	TRP	CD2-CE2	5.34	1.47	1.41
3	C	291	TRP	CD2-CE2	5.30	1.47	1.41
2	B	302	TRP	CD2-CE2	5.30	1.47	1.41
2	B	56	TRP	CG-CD1	5.29	1.44	1.36
2	b	56	TRP	CD2-CE2	5.28	1.47	1.41
1	a	142	TRP	CD2-CE2	5.27	1.47	1.41
3	c	259	TRP	CD2-CE2	5.26	1.47	1.41
4	D	58	TRP	CD2-CE2	5.26	1.47	1.41
2	B	115	TRP	CD2-CE2	5.26	1.47	1.41
3	c	250	TRP	CD2-CE2	5.24	1.47	1.41
2	b	78	TRP	CD2-CE2	5.23	1.47	1.41
3	C	97	TRP	CD2-CE2	5.23	1.47	1.41
1	a	105	TRP	CD2-CE2	5.22	1.47	1.41
2	B	493	TRP	CD2-CE2	5.21	1.47	1.41
4	d	32	TRP	CD2-CE2	5.20	1.47	1.41
2	b	493	TRP	CD2-CE2	5.18	1.47	1.41
3	C	266	TRP	CD2-CE2	5.16	1.47	1.41
3	C	63	TRP	CD2-CE2	5.13	1.47	1.41
2	b	167	TRP	CD2-CE2	5.12	1.47	1.41
4	D	280	TRP	CD2-CE2	5.12	1.47	1.41
2	B	257	TRP	CD2-CE2	5.11	1.47	1.41
10	K	39	TRP	CD2-CE2	5.10	1.47	1.41
4	D	14	TRP	CD2-CE2	5.10	1.47	1.41
4	d	280	TRP	CD2-CE2	5.09	1.47	1.41
1	A	278	TRP	CD2-CE2	5.08	1.47	1.41
1	a	169	SER	CA-CB	5.08	1.60	1.52
4	d	191	TRP	CD2-CE2	5.06	1.47	1.41
1	A	80	GLY	N-CA	5.05	1.53	1.46
1	a	317	TRP	CD2-CE2	5.05	1.47	1.41
3	c	359	TRP	CD2-CE2	5.03	1.47	1.41
1	a	278	TRP	CD2-CE2	5.02	1.47	1.41
4	d	14	TRP	CD2-CE2	5.02	1.47	1.41

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	272	ARG	NE-CZ-NH1	-7.88	116.36	120.30
13	o	152	ARG	NE-CZ-NH1	-7.53	116.54	120.30
2	B	357	ARG	NE-CZ-NH2	-7.36	116.62	120.30
3	C	153	ASP	CB-CG-OD1	7.03	124.63	118.30
4	D	100	ASP	CB-CG-OD2	7.02	124.62	118.30
3	C	153	ASP	CB-CG-OD2	-6.97	112.03	118.30
4	d	100	ASP	CB-CG-OD1	6.87	124.48	118.30
5	e	45	ASP	CB-CG-OD1	6.45	124.11	118.30
15	U	39	ARG	NE-CZ-NH2	-6.39	117.11	120.30
3	C	195	ASP	CB-CG-OD1	-6.39	112.55	118.30
3	C	195	ASP	CB-CG-OD2	6.16	123.84	118.30
1	a	342	ASP	CB-CG-OD1	6.08	123.77	118.30
3	C	343	ARG	NE-CZ-NH2	-5.91	117.34	120.30
3	C	473	ASP	CB-CG-OD2	5.88	123.60	118.30
4	D	329	MET	CG-SD-CE	5.83	109.54	100.20
16	v	105	ARG	NE-CZ-NH1	-5.83	117.38	120.30
2	b	357	ARG	NE-CZ-NH2	-5.67	117.46	120.30
13	o	169	ASP	CB-CG-OD2	5.67	123.41	118.30
13	o	69	LYS	CD-CE-NZ	-5.63	98.75	111.70
11	l	14	ARG	NE-CZ-NH1	-5.58	117.51	120.30
2	B	287[A]	ARG	NE-CZ-NH2	-5.57	117.51	120.30
2	B	287[B]	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	a	131	TRP	CA-CB-CG	-5.42	103.40	113.70
1	a	269	ARG	NE-CZ-NH2	-5.41	117.59	120.30
3	C	213	LEU	CB-CG-CD1	-5.40	101.82	111.00
4	d	126	MET	CG-SD-CE	-5.36	91.62	100.20
1	a	342	ASP	CB-CG-OD2	-5.29	113.54	118.30
2	B	15	ASP	CB-CG-OD1	5.26	123.04	118.30
3	C	376	ASP	CB-CG-OD1	5.26	123.04	118.30
1	A	131	TRP	CA-CB-CG	-5.26	103.71	113.70
4	D	26	ARG	NE-CZ-NH2	-5.24	117.68	120.30
16	V	99	ASP	CB-CG-OD1	5.17	122.95	118.30
3	C	27	ASP	CB-CG-OD1	5.16	122.94	118.30
2	b	357	ARG	NE-CZ-NH1	5.05	122.83	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	336/344 (98%)	330 (98%)	5 (2%)	1 (0%)	41	31
1	a	336/344 (98%)	329 (98%)	7 (2%)	0	100	100
2	B	512/504 (102%)	503 (98%)	9 (2%)	0	100	100
2	b	508/504 (101%)	497 (98%)	11 (2%)	0	100	100
3	C	452/455 (99%)	442 (98%)	9 (2%)	1 (0%)	47	38
3	c	457/455 (100%)	442 (97%)	13 (3%)	2 (0%)	34	24
4	D	339/342 (99%)	332 (98%)	7 (2%)	0	100	100
4	d	341/342 (100%)	334 (98%)	7 (2%)	0	100	100
5	E	79/83 (95%)	78 (99%)	1 (1%)	0	100	100
5	e	77/83 (93%)	75 (97%)	2 (3%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
7	h	61/63 (97%)	55 (90%)	5 (8%)	1 (2%)	9	2
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	36/38 (95%)	32 (89%)	2 (6%)	2 (6%)	2	0
9	J	34/40 (85%)	34 (100%)	0	0	100	100
9	j	37/40 (92%)	35 (95%)	2 (5%)	0	100	100
10	K	36/37 (97%)	36 (100%)	0	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	37/37 (100%)	37 (100%)	0	0	100	100
12	M	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
12	m	34/36 (94%)	34 (100%)	0	0	100	100
13	O	247/244 (101%)	238 (96%)	8 (3%)	1 (0%)	34	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	242/244 (99%)	232 (96%)	9 (4%)	1 (0%)	34	24
14	T	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
14	t	28/32 (88%)	27 (96%)	1 (4%)	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	137/137 (100%)	132 (96%)	5 (4%)	0	100	100
16	v	136/137 (99%)	129 (95%)	7 (5%)	0	100	100
17	Y	25/30 (83%)	25 (100%)	0	0	100	100
17	y	26/30 (87%)	25 (96%)	1 (4%)	0	100	100
18	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
18	x	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	55 (92%)	2 (3%)	3 (5%)	2	0
19	z	58/62 (94%)	50 (86%)	5 (9%)	3 (5%)	2	0
All	All	5224/5344 (98%)	5075 (97%)	134 (3%)	15 (0%)	41	31

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	59	LYS
19	Z	31	GLN
19	Z	32	ASP
8	i	36	ASP
19	z	31	GLN
3	C	416	SER
19	Z	2	THR
3	c	416[A]	SER
3	c	416[B]	SER
19	z	3	ILE
19	z	32	ASP
8	i	34	ARG
13	o	34	SER
7	h	63	LYS
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	272/279 (98%)	267 (98%)	5 (2%)	59	55
1	a	271/279 (97%)	269 (99%)	2 (1%)	84	84
2	B	407/402 (101%)	404 (99%)	3 (1%)	84	84
2	b	399/402 (99%)	393 (98%)	6 (2%)	65	62
3	C	355/356 (100%)	347 (98%)	8 (2%)	50	45
3	c	358/356 (101%)	349 (98%)	9 (2%)	47	41
4	D	275/276 (100%)	273 (99%)	2 (1%)	84	84
4	d	278/276 (101%)	274 (99%)	4 (1%)	67	65
5	E	71/72 (99%)	70 (99%)	1 (1%)	67	65
5	e	68/72 (94%)	66 (97%)	2 (3%)	42	35
6	F	27/38 (71%)	26 (96%)	1 (4%)	34	25
6	f	26/38 (68%)	25 (96%)	1 (4%)	33	24
7	H	53/53 (100%)	52 (98%)	1 (2%)	57	53
7	h	53/53 (100%)	52 (98%)	1 (2%)	57	53
8	I	31/34 (91%)	31 (100%)	0	100	100
8	i	33/34 (97%)	32 (97%)	1 (3%)	41	33
9	J	23/28 (82%)	23 (100%)	0	100	100
9	j	25/28 (89%)	25 (100%)	0	100	100
10	K	29/30 (97%)	29 (100%)	0	100	100
10	k	28/30 (93%)	27 (96%)	1 (4%)	35	26
11	L	34/35 (97%)	34 (100%)	0	100	100
11	l	34/35 (97%)	34 (100%)	0	100	100
12	M	29/32 (91%)	29 (100%)	0	100	100
12	m	30/32 (94%)	30 (100%)	0	100	100
13	O	207/207 (100%)	203 (98%)	4 (2%)	57	53
13	o	206/207 (100%)	203 (98%)	3 (2%)	65	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	T	25/28 (89%)	24 (96%)	1 (4%)	31	22
14	t	25/28 (89%)	24 (96%)	1 (4%)	31	22
15	U	83/89 (93%)	81 (98%)	2 (2%)	49	43
15	u	83/89 (93%)	83 (100%)	0	100	100
16	V	116/117 (99%)	116 (100%)	0	100	100
16	v	115/117 (98%)	114 (99%)	1 (1%)	78	79
17	Y	19/23 (83%)	18 (95%)	1 (5%)	22	13
17	y	18/23 (78%)	16 (89%)	2 (11%)	6	2
18	X	30/33 (91%)	30 (100%)	0	100	100
18	x	30/33 (91%)	29 (97%)	1 (3%)	38	29
19	Z	47/52 (90%)	46 (98%)	1 (2%)	53	48
19	z	40/52 (77%)	38 (95%)	2 (5%)	24	15
All	All	4253/4368 (97%)	4186 (98%)	67 (2%)	65	60

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	PRO
1	A	229	GLU
1	A	244	GLU
1	A	248[A]	ILE
1	A	248[B]	ILE
2	B	53	ASN
2	B	467	ILE
2	B	472	ARG
3	C	104	GLU
3	C	289	PHE
3	C	315	MET
3	C	355	THR
3	C	391[A]	ARG
3	C	391[B]	ARG
3	C	418	ASN
3	C	471	SER
4	D	90	LEU
4	D	180	ARG
5	E	4	THR
6	F	44	GLN
7	H	49	TYR

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Mol	Chain	Res	Type
13	O	59	LYS
13	O	110	MET
13	O	118	LEU
13	O	207	ARG
14	T	2	GLU
15	U	24	LYS
15	U	70	ARG
17	Y	27	MET
19	Z	6	GLN
1	a	244	GLU
1	a	261	GLN
2	b	246	PHE
2	b	362	PHE
2	b	373	LYS
2	b	472	ARG
2	b	476	ARG
2	b	479	PHE
3	c	240	ILE
3	c	255	THR
3	c	289	PHE
3	c	355	THR
3	c	391[A]	ARG
3	c	391[B]	ARG
3	c	416[A]	SER
3	c	416[B]	SER
3	c	418	ASN
4	d	24	ARG
4	d	150	ILE
4	d	180	ARG
4	d	329	MET
5	e	60	GLN
5	e	62	SER
6	f	15	ILE
7	h	49	TYR
8	i	38	GLU
10	k	27	VAL
13	o	54	GLU
13	o	64	GLU
13	o	118	LEU
14	t	2	GLU
16	v	23	GLU
17	y	30	ILE

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Mol	Chain	Res	Type
17	y	41	VAL
18	x	39	ARG
19	z	3	ILE
19	z	29	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	GLN
2	B	53	ASN
2	B	281	GLN
2	B	331	ASN
2	B	497	GLN
3	C	311	GLN
11	L	6	ASN
13	O	82	GLN
13	O	104	GLN
16	V	34	GLN
1	a	315	ASN
2	b	53	ASN
2	b	179	GLN
2	b	281	GLN
2	b	331	ASN
2	b	338	GLN
3	c	311	GLN
4	d	332	GLN
13	o	36	GLN
13	o	82	GLN
13	o	104	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](#)

10 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
4	HSK	D	336[B]	-	7,11,12	1.38	1 (14%)	3,14,16	1.69	1 (33%)
14	FME	T	1	14	8,9,10	0.50	0	7,9,11	1.30	2 (28%)
12	FME	M	1	12	8,9,10	0.83	0	7,9,11	1.95	3 (42%)
14	FME	t	1	14	8,9,10	0.85	0	7,9,11	1.44	2 (28%)
8	FME	I	1	8	8,9,10	0.64	0	7,9,11	1.12	0
4	HSK	D	336[A]	-	7,10,12	1.05	1 (14%)	3,12,16	2.05	2 (66%)
12	FME	m	1	12	8,9,10	0.85	0	7,9,11	1.80	2 (28%)
8	FME	i	1	8	8,9,10	0.43	0	7,9,11	1.34	2 (28%)
4	HSK	d	336[A]	-	7,10,12	1.05	1 (14%)	3,12,16	1.51	0
4	HSK	d	336[B]	-	7,11,12	1.28	1 (14%)	3,14,16	1.52	1 (33%)

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
4	HSK	D	336[B]	-	-	0/5/6/8	0/1/1/1
14	FME	T	1	14	-	2/7/9/11	-
12	FME	M	1	12	-	2/7/9/11	-
14	FME	t	1	14	-	5/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
4	HSK	D	336[A]	-	-	0/5/6/8	0/1/1/1
12	FME	m	1	12	-	2/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
4	HSK	d	336[A]	-	-	0/5/6/8	0/1/1/1
4	HSK	d	336[B]	-	-	0/5/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	336[B]	HSK	CE1-ND1	-3.25	1.32	1.36
4	d	336[B]	HSK	CE1-ND1	-2.98	1.33	1.36
4	D	336[A]	HSK	CE1-ND1	-2.46	1.33	1.36
4	d	336[A]	HSK	CE1-ND1	-2.37	1.33	1.36

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	1	FME	CE-SD-CG	2.94	110.49	100.40
12	M	1	FME	CG-CB-CA	2.82	120.80	112.95
12	m	1	FME	CG-CB-CA	2.79	120.69	112.95
12	M	1	FME	C-CA-N	-2.64	104.97	109.73
4	D	336[B]	HSK	CD2-NE2-CE1	2.46	109.62	105.78
12	m	1	FME	CE-SD-CG	2.46	108.84	100.40
4	d	336[B]	HSK	CD2-NE2-CE1	2.44	109.58	105.78
4	D	336[A]	HSK	CD2-NE2-CE1	2.43	109.58	105.78
14	t	1	FME	O1-CN-N	-2.22	119.43	125.27
8	i	1	FME	O-C-CA	-2.19	119.04	124.78
8	i	1	FME	CG-CB-CA	-2.10	107.11	112.95
4	D	336[A]	HSK	CB-CA-C	-2.09	107.55	111.47
14	t	1	FME	O-C-CA	-2.07	119.35	124.78
14	T	1	FME	O-C-CA	-2.05	119.41	124.78
14	T	1	FME	CG-CB-CA	2.03	118.58	112.95

There are no chirality outliers.

All (12) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 276 ligands modelled in this entry, 43 are unknown and 15 are monoatomic - leaving 218 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LMG	A	413	-	51,51,55	0.99	2 (3%)	59,59,63	1.21	4 (6%)
25	BCR	a	415	-	41,41,41	1.22	3 (7%)	56,56,56	1.45	8 (14%)
30	LMT	M	102	-	36,36,36	0.63	0	47,47,47	1.34	6 (12%)
27	LMG	c	921	-	51,51,55	1.10	3 (5%)	59,59,63	1.22	6 (10%)
31	GOL	v	202	-	5,5,5	0.59	0	5,5,5	0.51	0
23	CLA	c	914	-	59,73,73	2.57	14 (23%)	67,113,113	1.88	18 (26%)
23	CLA	A	406	41	59,73,73	1.87	14 (23%)	67,113,113	2.51	27 (40%)
25	BCR	c	916	-	41,41,41	0.98	1 (2%)	56,56,56	1.40	7 (12%)
31	GOL	f	104	32	5,5,5	0.54	0	5,5,5	0.43	0
23	CLA	d	402	-	59,73,73	1.85	11 (18%)	67,113,113	2.20	19 (28%)
33	HTG	V	202	-	12,13,19	0.75	0	16,18,24	3.09	6 (37%)
34	DGD	c	918	-	63,63,67	1.00	4 (6%)	77,77,81	1.24	10 (12%)
23	CLA	b	618	-	59,73,73	2.17	13 (22%)	67,113,113	2.42	23 (34%)
33	HTG	D	414	-	19,19,19	1.08	2 (10%)	23,24,24	1.16	1 (4%)
31	GOL	a	422	-	5,5,5	0.67	0	5,5,5	0.78	0
30	LMT	B	623	-	36,36,36	1.00	2 (5%)	47,47,47	1.37	8 (17%)
31	GOL	l	102	-	5,5,5	0.48	0	5,5,5	1.00	0
25	BCR	K	101	-	41,41,41	0.90	0	56,56,56	1.68	12 (21%)
31	GOL	B	635	-	5,5,5	0.52	0	5,5,5	1.05	0
33	HTG	b	601	-	19,19,19	0.99	2 (10%)	23,24,24	1.31	3 (13%)
25	BCR	c	915	-	41,41,41	0.87	1 (2%)	56,56,56	1.25	6 (10%)
25	BCR	B	618	-	41,41,41	1.13	4 (9%)	56,56,56	1.58	10 (17%)
27	LMG	Z	101	-	51,51,55	1.10	3 (5%)	59,59,63	1.37	7 (11%)
28	PL9	D	405	-	55,55,55	1.34	7 (12%)	68,69,69	1.56	14 (20%)
23	CLA	d	403	-	59,73,73	2.14	16 (27%)	67,113,113	1.94	18 (26%)
26	SQD	B	621	-	53,54,54	1.13	4 (7%)	62,65,65	1.88	11 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LMT	z	101	-	32,32,36	0.70	1 (3%)	42,42,47	0.99	2 (4%)
25	BCR	b	620	-	41,41,41	1.07	1 (2%)	56,56,56	1.74	14 (25%)
23	CLA	C	508	-	59,73,73	2.48	15 (25%)	67,113,113	1.88	18 (26%)
40	SO4	O	302	-	4,4,4	0.52	0	6,6,6	0.38	0
25	BCR	T	101	-	41,41,41	0.90	0	56,56,56	1.66	14 (25%)
25	BCR	k	102	-	41,41,41	0.99	2 (4%)	56,56,56	1.31	5 (8%)
23	CLA	b	617	-	59,73,73	1.78	13 (22%)	67,113,113	2.36	21 (31%)
33	HTG	d	401	-	19,19,19	1.08	2 (10%)	23,24,24	1.41	2 (8%)
34	DGD	C	518	-	63,63,67	0.78	3 (4%)	77,77,81	1.31	9 (11%)
36	LHG	L	101	-	48,48,48	0.82	2 (4%)	51,54,54	1.53	7 (13%)
23	CLA	B	606	-	59,73,73	2.03	12 (20%)	67,113,113	1.95	17 (25%)
23	CLA	b	612	-	59,73,73	2.24	14 (23%)	67,113,113	1.88	15 (22%)
28	PL9	d	405	-	55,55,55	1.28	9 (16%)	68,69,69	1.59	14 (20%)
23	CLA	b	607	-	59,73,73	2.04	12 (20%)	67,113,113	2.38	18 (26%)
23	CLA	B	609	-	59,73,73	1.64	12 (20%)	67,113,113	2.23	19 (28%)
23	CLA	B	603	-	59,73,73	2.31	16 (27%)	67,113,113	1.86	21 (31%)
31	GOL	D	415	-	5,5,5	0.70	0	5,5,5	1.24	0
26	SQD	D	407	-	44,45,54	1.26	3 (6%)	53,56,65	2.15	15 (28%)
33	HTG	c	923	-	19,19,19	1.01	2 (10%)	23,24,24	1.54	2 (8%)
31	GOL	V	203	-	5,5,5	1.00	0	5,5,5	0.81	0
27	LMG	c	920	-	51,51,55	1.12	4 (7%)	59,59,63	1.27	9 (15%)
23	CLA	C	513	-	59,73,73	2.60	14 (23%)	67,113,113	2.09	19 (28%)
36	LHG	D	409	-	48,48,48	0.83	2 (4%)	51,54,54	1.12	5 (9%)
31	GOL	A	422	-	5,5,5	0.43	0	5,5,5	0.48	0
38	RRX	h	101	-	42,42,42	0.97	0	57,58,58	1.31	8 (14%)
23	CLA	a	411	41	59,73,73	1.74	11 (18%)	67,113,113	2.28	24 (35%)
23	CLA	D	402	-	59,73,73	1.87	13 (22%)	67,113,113	2.25	25 (37%)
23	CLA	B	612	-	59,73,73	1.73	11 (18%)	67,113,113	2.39	20 (29%)
23	CLA	C	506	-	59,73,73	2.22	13 (22%)	67,113,113	2.20	19 (28%)
23	CLA	A	405	-	59,73,73	1.87	13 (22%)	67,113,113	2.03	22 (32%)
23	CLA	c	912	3	59,73,73	2.23	13 (22%)	67,113,113	2.40	22 (32%)
37	HEM	f	101	5,6	27,50,50	2.05	7 (25%)	17,82,82	2.66	6 (35%)
31	GOL	B	633	-	5,5,5	0.34	0	5,5,5	1.36	1 (20%)
31	GOL	A	423	32	5,5,5	0.32	0	5,5,5	0.77	0
34	DGD	c	919	-	63,63,67	1.05	6 (9%)	77,77,81	1.37	10 (12%)
23	CLA	C	511	3	59,73,73	2.40	15 (25%)	67,113,113	2.46	17 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	908	41	59,73,73	2.24	18 (30%)	67,113,113	2.33	21 (31%)
25	BCR	K	102	-	41,41,41	0.96	1 (2%)	56,56,56	1.68	11 (19%)
25	BCR	C	514	-	41,41,41	0.91	0	56,56,56	1.30	8 (14%)
36	LHG	d	409	-	48,48,48	0.92	3 (6%)	51,54,54	1.07	4 (7%)
30	LMT	t	102	-	24,24,36	0.69	0	29,29,47	1.31	4 (13%)
23	CLA	b	608	-	59,73,73	1.79	11 (18%)	67,113,113	2.33	21 (31%)
24	PHO	a	413	-	67,69,69	1.97	15 (22%)	85,99,99	2.04	22 (25%)
23	CLA	B	616	-	59,73,73	2.35	13 (22%)	67,113,113	2.20	18 (26%)
23	CLA	b	611	-	59,73,73	2.06	15 (25%)	67,113,113	1.96	17 (25%)
33	HTG	C	522	-	19,19,19	1.01	2 (10%)	23,24,24	2.16	3 (13%)
24	PHO	a	412	-	67,69,69	1.88	12 (17%)	85,99,99	1.92	19 (22%)
28	PL9	a	419	-	55,55,55	0.88	3 (5%)	68,69,69	1.77	17 (25%)
27	LMG	a	418	-	51,51,55	0.94	2 (3%)	59,59,63	1.33	5 (8%)
31	GOL	c	927	-	5,5,5	0.63	0	5,5,5	0.41	0
23	CLA	C	503	-	59,73,73	2.19	15 (25%)	67,113,113	1.92	15 (22%)
30	LMT	b	625	-	24,24,36	0.54	0	29,29,47	1.24	4 (13%)
23	CLA	C	512	-	59,73,73	2.38	13 (22%)	67,113,113	2.11	20 (29%)
25	BCR	B	619	-	41,41,41	1.19	4 (9%)	56,56,56	1.23	6 (10%)
31	GOL	h	103	-	5,5,5	0.37	0	5,5,5	0.26	0
23	CLA	B	604	-	59,73,73	2.00	12 (20%)	67,113,113	2.50	21 (31%)
35	BCT	a	408	21	0,3,3	0.00	-	0,3,3	0.00	-
30	LMT	Z	102	-	36,36,36	0.68	1 (2%)	47,47,47	0.89	0
31	GOL	c	928	-	5,5,5	0.21	0	5,5,5	0.80	0
24	PHO	A	409	-	67,69,69	1.90	14 (20%)	85,99,99	2.16	23 (27%)
23	CLA	b	605	-	59,73,73	2.07	11 (18%)	67,113,113	2.16	22 (32%)
23	CLA	A	410	-	59,73,73	1.84	12 (20%)	67,113,113	2.07	15 (22%)
31	GOL	b	634	-	5,5,5	0.50	0	5,5,5	0.22	0
23	CLA	a	409	-	59,73,73	1.96	12 (20%)	67,113,113	1.98	19 (28%)
31	GOL	v	203	-	5,5,5	0.73	0	5,5,5	0.48	0
23	CLA	B	602	41	59,73,73	2.31	15 (25%)	67,113,113	2.44	20 (29%)
31	GOL	L	104	-	5,5,5	0.51	0	5,5,5	0.59	0
23	CLA	c	902	-	59,73,73	2.10	15 (25%)	67,113,113	2.27	17 (25%)
31	GOL	v	204	-	5,5,5	0.30	0	5,5,5	0.68	0
30	LMT	m	102	-	36,36,36	0.73	1 (2%)	47,47,47	1.06	3 (6%)
23	CLA	C	502	-	59,73,73	1.92	11 (18%)	67,113,113	2.02	19 (28%)
30	LMT	a	402	-	36,36,36	0.77	1 (2%)	47,47,47	1.59	9 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	a	414	-	59,73,73	1.86	12 (20%)	67,113,113	2.37	23 (34%)
23	CLA	B	605	-	59,73,73	1.84	10 (16%)	67,113,113	2.13	20 (29%)
36	LHG	D	408	-	48,48,48	0.79	1 (2%)	51,54,54	1.47	6 (11%)
23	CLA	c	904	-	59,73,73	2.51	15 (25%)	67,113,113	2.23	22 (32%)
26	SQD	L	103	-	53,54,54	1.10	2 (3%)	62,65,65	1.74	12 (19%)
23	CLA	b	619	-	59,73,73	2.09	13 (22%)	67,113,113	2.22	20 (29%)
23	CLA	B	607	-	59,73,73	2.32	12 (20%)	67,113,113	2.29	20 (29%)
23	CLA	b	616	-	59,73,73	1.96	11 (18%)	67,113,113	2.17	19 (28%)
33	HTG	U	201	-	8,8,19	0.29	0	7,7,24	1.26	1 (14%)
31	GOL	C	526	-	5,5,5	0.67	0	5,5,5	0.49	0
31	GOL	B	636	-	5,5,5	0.47	0	5,5,5	0.72	0
25	BCR	k	101	-	41,41,41	0.85	0	56,56,56	1.47	11 (19%)
31	GOL	V	205	-	5,5,5	0.65	0	5,5,5	0.31	0
33	HTG	b	602	-	19,19,19	0.78	1 (5%)	23,24,24	1.18	2 (8%)
23	CLA	A	407	41	59,73,73	2.10	11 (18%)	67,113,113	2.17	18 (26%)
30	LMT	m	101	-	36,36,36	0.75	0	47,47,47	1.37	8 (17%)
31	GOL	A	421	-	5,5,5	0.89	0	5,5,5	0.51	0
23	CLA	c	911	-	59,73,73	2.08	14 (23%)	67,113,113	1.82	18 (26%)
34	DGD	c	917	-	63,63,67	0.90	4 (6%)	77,77,81	1.28	9 (11%)
23	CLA	C	507	41	59,73,73	2.36	14 (23%)	67,113,113	2.17	16 (23%)
36	LHG	d	407	-	48,48,48	0.80	2 (4%)	51,54,54	1.39	6 (11%)
36	LHG	l	101	-	48,48,48	0.84	2 (4%)	51,54,54	1.11	5 (9%)
26	SQD	A	412	-	53,54,54	0.94	3 (5%)	62,65,65	2.24	17 (27%)
28	PL9	A	414	-	55,55,55	0.94	3 (5%)	68,69,69	1.48	11 (16%)
23	CLA	c	909	-	59,73,73	2.39	15 (25%)	67,113,113	2.05	18 (26%)
25	BCR	t	101	-	41,41,41	1.02	2 (4%)	56,56,56	1.83	14 (25%)
23	CLA	B	613	-	59,73,73	2.19	16 (27%)	67,113,113	1.99	20 (29%)
31	GOL	c	930	-	5,5,5	0.45	0	5,5,5	0.68	0
24	PHO	A	408	-	67,69,69	1.72	11 (16%)	85,99,99	2.14	21 (24%)
23	CLA	B	608	41	59,73,73	2.13	17 (28%)	67,113,113	2.00	22 (32%)
33	HTG	B	626	-	19,19,19	0.94	1 (5%)	23,24,24	1.79	3 (13%)
23	CLA	b	606	-	59,73,73	1.94	11 (18%)	67,113,113	2.29	20 (29%)
34	DGD	C	517	-	63,63,67	0.90	2 (3%)	77,77,81	1.05	3 (3%)
34	DGD	H	102	-	63,63,67	1.12	3 (4%)	77,77,81	1.37	13 (16%)
23	CLA	b	609	-	59,73,73	2.43	17 (28%)	67,113,113	2.29	18 (26%)
30	LMT	c	922	-	36,36,36	0.75	1 (2%)	47,47,47	0.96	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	SQD	a	401	-	53,54,54	1.17	3 (5%)	62,65,65	1.59	9 (14%)
30	LMT	b	624	-	25,25,36	0.75	1 (4%)	30,30,47	1.38	5 (16%)
31	GOL	b	635	-	5,5,5	0.79	0	5,5,5	0.88	0
27	LMG	d	410	39	51,51,55	1.01	3 (5%)	59,59,63	1.14	7 (11%)
27	LMG	B	622	-	51,51,55	0.94	2 (3%)	59,59,63	1.61	9 (15%)
26	SQD	A	418	-	53,54,54	1.13	3 (5%)	62,65,65	1.66	12 (19%)
36	LHG	d	408	-	48,48,48	0.78	2 (4%)	51,54,54	1.32	9 (17%)
23	CLA	c	907	-	59,73,73	1.91	13 (22%)	67,113,113	2.04	19 (28%)
34	DGD	C	516	-	63,63,67	0.92	3 (4%)	77,77,81	1.37	12 (15%)
33	HTG	B	630	-	19,19,19	1.07	2 (10%)	23,24,24	1.54	3 (13%)
23	CLA	c	910	-	59,73,73	2.33	14 (23%)	67,113,113	2.24	24 (35%)
25	BCR	d	404	-	41,41,41	1.01	3 (7%)	56,56,56	1.81	16 (28%)
34	DGD	D	406	-	53,53,67	1.20	3 (5%)	60,61,81	1.39	8 (13%)
23	CLA	c	906	-	59,73,73	1.98	16 (27%)	67,113,113	2.12	20 (29%)
31	GOL	b	633	-	5,5,5	0.38	0	5,5,5	0.89	0
23	CLA	b	613	41	59,73,73	2.05	13 (22%)	67,113,113	2.13	15 (22%)
23	CLA	b	614	-	59,73,73	2.02	12 (20%)	67,113,113	2.17	21 (31%)
33	HTG	B	624	-	19,19,19	1.15	1 (5%)	23,24,24	1.44	5 (21%)
33	HTG	B	631	-	19,19,19	0.84	2 (10%)	23,24,24	1.88	3 (13%)
30	LMT	F	102	-	36,36,36	0.75	1 (2%)	47,47,47	1.18	3 (6%)
23	CLA	B	617	-	59,73,73	1.86	14 (23%)	67,113,113	2.05	16 (23%)
23	CLA	a	410	41	59,73,73	1.87	13 (22%)	67,113,113	2.00	17 (25%)
25	BCR	D	404	-	41,41,41	1.17	3 (7%)	56,56,56	2.05	18 (32%)
31	GOL	B	634	-	5,5,5	0.84	0	5,5,5	0.66	0
26	SQD	a	416	-	53,54,54	0.96	3 (5%)	62,65,65	2.26	14 (22%)
25	BCR	B	620	-	41,41,41	1.02	1 (2%)	56,56,56	1.64	11 (19%)
35	BCT	D	401	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	B	615	-	59,73,73	2.11	13 (22%)	67,113,113	2.09	18 (26%)
36	LHG	D	410	-	45,45,48	1.02	2 (4%)	48,51,54	1.05	3 (6%)
20	OEX	A	401	1,3,41	0,15,15	0.00	-	-	-	-
27	LMG	b	623	-	51,51,55	0.86	2 (3%)	59,59,63	1.46	7 (11%)
25	BCR	A	411	-	41,41,41	1.04	0	56,56,56	1.49	11 (19%)
25	BCR	b	622	-	41,41,41	0.97	2 (4%)	56,56,56	1.26	6 (10%)
20	OEX	a	404	1,3,41	0,15,15	0.00	-	-	-	-
30	LMT	M	101	-	36,36,36	0.87	1 (2%)	47,47,47	1.22	6 (12%)
25	BCR	C	515	-	41,41,41	0.94	1 (2%)	56,56,56	1.45	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	GOL	B	638	-	5,5,5	0.51	0	5,5,5	0.86	0
23	CLA	D	403	-	59,73,73	2.21	14 (23%)	67,113,113	1.99	18 (26%)
33	HTG	B	625	-	19,19,19	0.98	1 (5%)	23,24,24	1.46	4 (17%)
37	HEM	v	201	16	27,50,50	2.26	7 (25%)	17,82,82	2.14	6 (35%)
37	HEM	F	101	5,6	27,50,50	2.14	9 (33%)	17,82,82	2.72	6 (35%)
31	GOL	V	204	-	5,5,5	0.31	0	5,5,5	0.43	0
23	CLA	b	610	41	59,73,73	2.16	11 (18%)	67,113,113	1.89	18 (26%)
31	GOL	a	423	-	5,5,5	0.57	0	5,5,5	0.58	0
30	LMT	A	419	-	36,36,36	0.84	1 (2%)	47,47,47	1.33	5 (10%)
33	HTG	C	521	-	19,19,19	0.91	2 (10%)	23,24,24	1.37	1 (4%)
23	CLA	c	903	-	59,73,73	2.06	11 (18%)	67,113,113	2.16	20 (29%)
31	GOL	b	632	-	5,5,5	0.53	0	5,5,5	1.30	0
33	HTG	b	627	-	19,19,19	1.14	2 (10%)	23,24,24	1.60	1 (4%)
23	CLA	C	510	-	59,73,73	2.10	12 (20%)	67,113,113	2.10	15 (22%)
31	GOL	C	525	-	5,5,5	0.81	0	5,5,5	0.88	0
38	RRX	H	101	-	42,42,42	1.10	3 (7%)	57,58,58	1.63	11 (19%)
23	CLA	C	505	-	59,73,73	1.96	13 (22%)	67,113,113	1.92	16 (23%)
31	GOL	c	929	-	5,5,5	0.53	0	5,5,5	0.85	0
23	CLA	b	604	41	59,73,73	2.34	15 (25%)	67,113,113	2.23	16 (23%)
31	GOL	B	637	-	5,5,5	0.47	0	5,5,5	1.09	0
36	LHG	a	417	-	39,39,48	1.17	2 (5%)	42,45,54	0.98	2 (4%)
23	CLA	B	610	-	59,73,73	1.81	12 (20%)	67,113,113	2.15	18 (26%)
23	CLA	C	509	-	59,73,73	2.15	13 (22%)	67,113,113	2.10	18 (26%)
31	GOL	O	304	-	5,5,5	0.54	0	5,5,5	0.59	0
26	SQD	f	102	-	31,32,54	1.97	4 (12%)	34,36,65	1.64	5 (14%)
33	HTG	u	201	-	10,13,19	0.81	1 (10%)	13,14,24	1.92	2 (15%)
25	BCR	b	621	-	41,41,41	1.15	2 (4%)	56,56,56	1.31	7 (12%)
27	LMG	D	411	39	51,51,55	0.86	2 (3%)	59,59,63	1.03	2 (3%)
33	HTG	b	626	-	19,19,19	1.01	1 (5%)	23,24,24	1.38	3 (13%)
33	HTG	O	303	-	19,19,19	1.17	2 (10%)	23,24,24	1.32	1 (4%)
34	DGD	h	102	-	63,63,67	0.99	3 (4%)	77,77,81	1.28	11 (14%)
31	GOL	C	524	-	5,5,5	0.34	0	5,5,5	1.56	1 (20%)
23	CLA	C	501	-	59,73,73	1.86	14 (23%)	67,113,113	2.53	18 (26%)
33	HTG	c	924	-	19,19,19	1.00	1 (5%)	23,24,24	2.28	5 (21%)
23	CLA	b	615	-	59,73,73	2.17	12 (20%)	67,113,113	2.45	17 (25%)
31	GOL	a	424	-	5,5,5	0.65	0	5,5,5	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	504	41	59,73,73	2.06	14 (23%)	67,113,113	2.09	17 (25%)
23	CLA	B	611	41	59,73,73	2.01	13 (22%)	67,113,113	2.17	19 (28%)
31	GOL	b	636	-	5,5,5	0.57	0	5,5,5	0.98	0
27	LMG	C	519	-	51,51,55	1.02	3 (5%)	59,59,63	1.47	9 (15%)
37	HEM	V	201	16	27,50,50	2.27	11 (40%)	17,82,82	2.34	7 (41%)
23	CLA	c	905	41	59,73,73	2.34	15 (25%)	67,113,113	2.12	18 (26%)
30	LMT	J	102	-	24,24,36	0.84	1 (4%)	29,29,47	1.13	2 (6%)
34	DGD	d	406	-	50,50,67	1.19	3 (6%)	58,58,81	1.37	8 (13%)
30	LMT	C	520	-	36,36,36	0.62	1 (2%)	47,47,47	1.46	6 (12%)
23	CLA	c	913	-	59,73,73	2.44	15 (25%)	67,113,113	2.00	19 (28%)
36	LHG	E	101	-	48,48,48	1.01	2 (4%)	51,54,54	0.93	1 (1%)
23	CLA	B	614	-	59,73,73	1.92	14 (23%)	67,113,113	1.76	17 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	A	413	-	-	26/46/66/70	0/1/1/1
25	BCR	a	415	-	-	1/29/63/63	0/2/2/2
30	LMT	M	102	-	-	2/21/61/61	0/2/2/2
27	LMG	c	921	-	-	13/46/66/70	0/1/1/1
31	GOL	v	202	-	-	0/4/4/4	-
23	CLA	c	914	-	2/2/20/25	11/37/135/135	-
23	CLA	A	406	41	1/1/20/25	6/37/135/135	-
25	BCR	c	916	-	-	0/29/63/63	0/2/2/2
31	GOL	f	104	32	-	2/4/4/4	-
23	CLA	d	402	-	2/2/20/25	2/37/135/135	-
33	HTG	V	202	-	-	2/4/24/30	0/1/1/1
34	DGD	c	918	-	-	22/51/91/95	0/2/2/2
23	CLA	b	618	-	3/3/20/25	9/37/135/135	-
33	HTG	D	414	-	-	2/10/30/30	0/1/1/1
31	GOL	a	422	-	-	0/4/4/4	-
30	LMT	B	623	-	-	12/21/61/61	0/2/2/2
31	GOL	l	102	-	-	0/4/4/4	-
25	BCR	K	101	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	GOL	B	635	-	-	4/4/4/4	-
33	HTG	b	601	-	-	3/10/30/30	0/1/1/1
25	BCR	c	915	-	-	6/29/63/63	0/2/2/2
25	BCR	B	618	-	-	2/29/63/63	0/2/2/2
27	LMG	Z	101	-	-	25/46/66/70	0/1/1/1
28	PL9	D	405	-	-	1/53/73/73	0/1/1/1
23	CLA	C	512	-	3/3/20/25	9/37/135/135	-
26	SQD	B	621	-	-	29/49/69/69	0/1/1/1
30	LMT	z	101	-	-	8/15/55/61	0/2/2/2
25	BCR	b	620	-	-	2/29/63/63	0/2/2/2
23	CLA	C	508	-	2/2/20/25	7/37/135/135	-
30	LMT	t	102	-	-	8/15/35/61	0/1/1/2
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
25	BCR	k	102	-	-	3/29/63/63	0/2/2/2
23	CLA	b	617	-	3/3/20/25	18/37/135/135	-
33	HTG	d	401	-	-	5/10/30/30	0/1/1/1
34	DGD	C	518	-	-	14/51/91/95	0/2/2/2
36	LHG	L	101	-	-	10/53/53/53	-
23	CLA	B	606	-	3/3/20/25	6/37/135/135	-
23	CLA	b	612	-	1/1/20/25	0/37/135/135	-
28	PL9	d	405	-	-	5/53/73/73	0/1/1/1
23	CLA	b	607	-	3/3/20/25	7/37/135/135	-
23	CLA	B	609	-	1/1/20/25	1/37/135/135	-
23	CLA	B	603	-	2/2/20/25	4/37/135/135	-
31	GOL	D	415	-	-	2/4/4/4	-
26	SQD	D	407	-	-	13/40/60/69	0/1/1/1
33	HTG	c	923	-	-	4/10/30/30	0/1/1/1
31	GOL	V	203	-	-	2/4/4/4	-
27	LMG	c	920	-	-	18/46/66/70	0/1/1/1
23	CLA	C	513	-	1/1/20/25	13/37/135/135	-
36	LHG	D	409	-	-	13/53/53/53	-
31	GOL	A	422	-	-	0/4/4/4	-
38	RRX	h	101	-	-	2/29/65/65	0/2/2/2
23	CLA	a	411	41	2/2/20/25	6/37/135/135	-
23	CLA	D	402	-	1/1/20/25	7/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	612	-	2/2/20/25	2/37/135/135	-
23	CLA	C	506	-	2/2/20/25	13/37/135/135	-
23	CLA	A	405	-	3/3/20/25	3/37/135/135	-
23	CLA	c	912	3	1/1/20/25	7/37/135/135	-
37	HEM	f	101	5,6	-	0/6/54/54	-
31	GOL	B	633	-	-	2/4/4/4	-
31	GOL	A	423	32	-	0/4/4/4	-
34	DGD	c	919	-	-	16/51/91/95	0/2/2/2
23	CLA	C	511	3	3/3/20/25	0/37/135/135	-
23	CLA	c	908	41	3/3/20/25	7/37/135/135	-
25	BCR	K	102	-	-	2/29/63/63	0/2/2/2
23	CLA	c	911	-	3/3/20/25	9/37/135/135	-
36	LHG	d	409	-	-	16/53/53/53	-
23	CLA	b	613	41	3/3/20/25	4/37/135/135	-
23	CLA	b	608	-	3/3/20/25	4/37/135/135	-
24	PHO	a	413	-	-	4/53/103/103	0/5/6/6
23	CLA	B	616	-	3/3/20/25	5/37/135/135	-
23	CLA	b	611	-	1/1/20/25	1/37/135/135	-
33	HTG	C	522	-	-	4/10/30/30	0/1/1/1
24	PHO	a	412	-	-	2/53/103/103	0/5/6/6
28	PL9	a	419	-	-	11/53/73/73	0/1/1/1
27	LMG	a	418	-	-	20/46/66/70	0/1/1/1
31	GOL	c	927	-	-	2/4/4/4	-
23	CLA	C	503	-	3/3/20/25	1/37/135/135	-
30	LMT	b	625	-	-	11/15/35/61	0/1/1/2
23	CLA	d	403	-	1/1/20/25	9/37/135/135	-
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
31	GOL	h	103	-	-	1/4/4/4	-
23	CLA	B	604	-	3/3/20/25	5/37/135/135	-
30	LMT	Z	102	-	-	13/21/61/61	0/2/2/2
31	GOL	c	928	-	-	1/4/4/4	-
24	PHO	A	409	-	-	5/53/103/103	0/5/6/6
23	CLA	b	605	-	3/3/20/25	4/37/135/135	-
25	BCR	B	620	-	-	1/29/63/63	0/2/2/2
23	CLA	A	410	-	1/1/20/25	14/37/135/135	-
31	GOL	b	634	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	a	409	-	3/3/20/25	5/37/135/135	-
31	GOL	v	203	-	-	2/4/4/4	-
23	CLA	B	602	41	2/2/20/25	20/37/135/135	-
31	GOL	L	104	-	-	2/4/4/4	-
23	CLA	c	902	-	3/3/20/25	4/37/135/135	-
31	GOL	v	204	-	-	0/4/4/4	-
30	LMT	m	102	-	-	6/21/61/61	0/2/2/2
23	CLA	C	502	-	2/2/20/25	7/37/135/135	-
30	LMT	a	402	-	-	11/21/61/61	0/2/2/2
23	CLA	a	414	-	1/1/20/25	12/37/135/135	-
23	CLA	B	605	-	3/3/20/25	7/37/135/135	-
36	LHG	D	408	-	-	9/53/53/53	-
23	CLA	c	904	-	1/1/20/25	2/37/135/135	-
26	SQD	L	103	-	-	28/49/69/69	0/1/1/1
23	CLA	b	619	-	3/3/20/25	7/37/135/135	-
23	CLA	C	505	-	1/1/20/25	4/37/135/135	-
23	CLA	b	616	-	3/3/20/25	2/37/135/135	-
33	HTG	U	201	-	-	4/6/6/30	-
31	GOL	C	526	-	-	0/4/4/4	-
31	GOL	B	636	-	-	0/4/4/4	-
25	BCR	k	101	-	-	1/29/63/63	0/2/2/2
31	GOL	V	205	-	-	0/4/4/4	-
23	CLA	A	407	41	2/2/20/25	7/37/135/135	-
30	LMT	m	101	-	-	3/21/61/61	0/2/2/2
31	GOL	A	421	-	-	0/4/4/4	-
25	BCR	C	514	-	-	3/29/63/63	0/2/2/2
34	DGD	c	917	-	-	14/51/91/95	0/2/2/2
36	LHG	d	407	-	-	6/53/53/53	-
36	LHG	l	101	-	-	17/53/53/53	-
26	SQD	A	412	-	-	18/49/69/69	0/1/1/1
28	PL9	A	414	-	-	12/53/73/73	0/1/1/1
23	CLA	c	909	-	2/2/20/25	3/37/135/135	-
25	BCR	t	101	-	-	1/29/63/63	0/2/2/2
23	CLA	B	613	-	3/3/20/25	3/37/135/135	-
31	GOL	c	930	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PHO	A	408	-	-	3/53/103/103	0/5/6/6
23	CLA	B	608	41	3/3/20/25	1/37/135/135	-
33	HTG	B	626	-	-	5/10/30/30	0/1/1/1
23	CLA	b	606	-	3/3/20/25	4/37/135/135	-
34	DGD	C	517	-	-	23/51/91/95	0/2/2/2
34	DGD	H	102	-	-	15/51/91/95	0/2/2/2
23	CLA	b	609	-	2/2/20/25	12/37/135/135	-
30	LMT	c	922	-	-	4/21/61/61	0/2/2/2
26	SQD	a	401	-	-	23/49/69/69	0/1/1/1
30	LMT	b	624	-	-	10/17/37/61	0/1/1/2
31	GOL	b	635	-	-	1/4/4/4	-
27	LMG	d	410	39	-	10/46/66/70	0/1/1/1
27	LMG	B	622	-	-	15/46/66/70	0/1/1/1
26	SQD	A	418	-	-	17/49/69/69	0/1/1/1
36	LHG	d	408	-	-	10/53/53/53	-
23	CLA	c	907	-	2/2/20/25	14/37/135/135	-
34	DGD	C	516	-	-	16/51/91/95	0/2/2/2
33	HTG	B	630	-	-	4/10/30/30	0/1/1/1
23	CLA	c	910	-	3/3/20/25	13/37/135/135	-
25	BCR	d	404	-	-	4/29/63/63	0/2/2/2
34	DGD	D	406	-	-	26/47/68/95	0/1/1/2
23	CLA	c	906	-	1/1/20/25	7/37/135/135	-
31	GOL	b	633	-	-	3/4/4/4	-
23	CLA	b	614	-	2/2/20/25	6/37/135/135	-
33	HTG	B	624	-	-	2/10/30/30	0/1/1/1
33	HTG	B	631	-	-	5/10/30/30	0/1/1/1
30	LMT	F	102	-	-	11/21/61/61	0/2/2/2
23	CLA	B	617	-	3/3/20/25	16/37/135/135	-
23	CLA	a	410	41	3/3/20/25	5/37/135/135	-
25	BCR	D	404	-	-	2/29/63/63	0/2/2/2
31	GOL	B	634	-	-	0/4/4/4	-
26	SQD	a	416	-	-	20/49/69/69	0/1/1/1
23	CLA	C	507	41	3/3/20/25	11/37/135/135	-
23	CLA	B	615	-	3/3/20/25	13/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LHG	D	410	-	-	13/50/50/53	-
33	HTG	b	602	-	-	1/10/30/30	0/1/1/1
31	GOL	B	637	-	-	0/4/4/4	-
27	LMG	b	623	-	-	19/46/66/70	0/1/1/1
25	BCR	A	411	-	-	0/29/63/63	0/2/2/2
25	BCR	b	622	-	-	0/29/63/63	0/2/2/2
30	LMT	M	101	-	-	7/21/61/61	0/2/2/2
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
31	GOL	B	638	-	-	2/4/4/4	-
23	CLA	D	403	-	3/3/20/25	15/37/135/135	-
33	HTG	B	625	-	-	4/10/30/30	0/1/1/1
37	HEM	v	201	16	-	0/6/54/54	-
37	HEM	F	101	5,6	-	0/6/54/54	-
31	GOL	V	204	-	-	0/4/4/4	-
23	CLA	b	610	41	3/3/20/25	2/37/135/135	-
31	GOL	a	423	-	-	2/4/4/4	-
23	CLA	b	604	41	2/2/20/25	15/37/135/135	-
33	HTG	C	521	-	-	3/10/30/30	0/1/1/1
23	CLA	c	903	-	3/3/20/25	7/37/135/135	-
31	GOL	b	632	-	-	4/4/4/4	-
33	HTG	b	627	-	-	5/10/30/30	0/1/1/1
23	CLA	C	510	-	3/3/20/25	2/37/135/135	-
31	GOL	C	525	-	-	0/4/4/4	-
38	RRX	H	101	-	-	2/29/65/65	0/2/2/2
23	CLA	B	607	-	3/3/20/25	8/37/135/135	-
31	GOL	c	929	-	-	0/4/4/4	-
30	LMT	A	419	-	-	5/21/61/61	0/2/2/2
23	CLA	B	611	41	3/3/20/25	8/37/135/135	-
36	LHG	a	417	-	-	28/44/44/53	-
23	CLA	B	610	-	2/2/20/25	4/37/135/135	-
23	CLA	C	509	-	3/3/20/25	7/37/135/135	-
31	GOL	O	304	-	-	3/4/4/4	-
26	SQD	f	102	-	-	13/33/33/69	-
33	HTG	u	201	-	-	6/12/14/30	-
25	BCR	b	621	-	-	0/29/63/63	0/2/2/2
27	LMG	D	411	39	-	9/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	HTG	b	626	-	-	4/10/30/30	0/1/1/1
33	HTG	O	303	-	-	3/10/30/30	0/1/1/1
34	DGD	h	102	-	-	9/51/91/95	0/2/2/2
31	GOL	C	524	-	-	2/4/4/4	-
23	CLA	C	501	-	3/3/20/25	4/37/135/135	-
33	HTG	c	924	-	-	1/10/30/30	0/1/1/1
23	CLA	b	615	-	3/3/20/25	7/37/135/135	-
31	GOL	a	424	-	-	3/4/4/4	-
23	CLA	C	504	41	3/3/20/25	11/37/135/135	-
31	GOL	b	636	-	-	2/4/4/4	-
27	LMG	C	519	-	-	22/46/66/70	0/1/1/1
37	HEM	V	201	16	-	0/6/54/54	-
23	CLA	c	905	41	3/3/20/25	11/37/135/135	-
30	LMT	J	102	-	-	7/15/35/61	0/1/1/2
34	DGD	d	406	-	-	27/44/64/95	0/1/1/2
30	LMT	C	520	-	-	10/21/61/61	0/2/2/2
23	CLA	c	913	-	3/3/20/25	10/37/135/135	-
36	LHG	E	101	-	-	27/53/53/53	-
23	CLA	B	614	-	3/3/20/25	7/37/135/135	-

All (1219) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	513	CLA	MG-NA	12.57	2.36	2.06
23	c	914	CLA	MG-NC	11.74	2.34	2.06
23	C	512	CLA	MG-NA	11.26	2.33	2.06
23	C	511	CLA	MG-NA	11.02	2.32	2.06
23	B	616	CLA	MG-NA	10.89	2.32	2.06
23	B	607	CLA	MG-NA	10.52	2.31	2.06
23	b	615	CLA	MG-NA	10.41	2.31	2.06
23	b	609	CLA	MG-NA	10.30	2.30	2.06
23	C	507	CLA	MG-NA	9.89	2.29	2.06
23	c	904	CLA	MG-NA	9.80	2.29	2.06
23	C	506	CLA	MG-NA	9.65	2.29	2.06
23	A	407	CLA	MG-NA	9.41	2.28	2.06
23	c	913	CLA	MG-NA	9.29	2.28	2.06
23	B	602	CLA	MG-NA	9.21	2.28	2.06
23	C	508	CLA	MG-NA	9.07	2.27	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	613	CLA	MG-NA	9.02	2.27	2.06
23	C	509	CLA	MG-NA	9.00	2.27	2.06
23	c	909	CLA	MG-NA	8.95	2.27	2.06
23	c	905	CLA	MG-NA	8.83	2.27	2.06
23	c	904	CLA	MG-NC	8.66	2.26	2.06
23	c	910	CLA	OBD-CAD	8.60	1.34	1.22
23	B	605	CLA	MG-NA	8.49	2.26	2.06
23	b	618	CLA	MG-NA	8.38	2.26	2.06
23	C	510	CLA	MG-NA	8.38	2.26	2.06
23	B	603	CLA	MG-NA	8.36	2.26	2.06
23	b	614	CLA	MG-NA	8.36	2.26	2.06
23	b	607	CLA	MG-NA	8.25	2.25	2.06
23	C	503	CLA	MG-NC	8.19	2.25	2.06
23	c	912	CLA	MG-NA	8.14	2.25	2.06
23	c	902	CLA	MG-NA	8.13	2.25	2.06
23	c	910	CLA	MG-NA	7.80	2.24	2.06
23	b	611	CLA	MG-NA	7.70	2.24	2.06
23	D	403	CLA	MG-NA	7.60	2.24	2.06
23	b	604	CLA	MG-NC	7.53	2.24	2.06
23	c	903	CLA	MG-NA	7.39	2.23	2.06
23	b	610	CLA	MG-NA	7.13	2.23	2.06
23	B	614	CLA	MG-NA	7.13	2.23	2.06
23	B	608	CLA	MG-NA	7.13	2.23	2.06
23	B	604	CLA	MG-NA	6.88	2.22	2.06
23	C	504	CLA	MG-NC	6.84	2.22	2.06
23	C	507	CLA	C3B-C2B	6.83	1.49	1.40
26	f	102	SQD	C6-S	-6.83	1.67	1.77
23	B	612	CLA	MG-NA	6.78	2.22	2.06
23	b	612	CLA	MG-NC	6.78	2.22	2.06
23	B	606	CLA	MG-NA	6.63	2.22	2.06
23	c	908	CLA	MG-NA	6.58	2.21	2.06
23	c	908	CLA	MG-NC	6.50	2.21	2.06
23	c	911	CLA	MG-NC	6.50	2.21	2.06
23	c	906	CLA	MG-NA	6.43	2.21	2.06
23	b	612	CLA	CHC-C1C	6.37	1.51	1.35
23	a	410	CLA	MG-NA	6.33	2.21	2.06
23	a	409	CLA	MG-NA	6.33	2.21	2.06
23	A	406	CLA	OBD-CAD	6.29	1.31	1.22
24	a	413	PHO	CHB-C1B	6.29	1.50	1.38
23	b	605	CLA	OBD-CAD	6.28	1.31	1.22
23	B	615	CLA	MG-NA	6.26	2.21	2.06
23	C	508	CLA	MG-NC	6.24	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	513	CLA	C3B-C2B	6.20	1.49	1.40
23	b	605	CLA	MG-NC	6.17	2.20	2.06
23	C	508	CLA	C3C-C2C	6.15	1.49	1.36
23	d	403	CLA	MG-NA	6.13	2.20	2.06
23	b	610	CLA	C3C-C2C	6.09	1.49	1.36
23	a	409	CLA	OBD-CAD	6.09	1.30	1.22
23	b	613	CLA	MG-NA	6.08	2.20	2.06
23	B	603	CLA	CHC-C1C	6.04	1.50	1.35
23	B	613	CLA	CHC-C1C	6.02	1.50	1.35
26	f	102	SQD	O47-C7	6.01	1.46	1.33
23	b	610	CLA	CHC-C1C	6.01	1.50	1.35
23	c	905	CLA	C3C-C2C	5.98	1.49	1.36
23	b	619	CLA	CHC-C1C	5.98	1.50	1.35
23	b	616	CLA	MG-NA	5.97	2.20	2.06
23	b	605	CLA	C3C-C2C	5.96	1.49	1.36
23	B	603	CLA	C3C-C2C	5.95	1.49	1.36
23	C	502	CLA	CHC-C1C	5.94	1.50	1.35
23	c	909	CLA	MG-NC	5.91	2.20	2.06
23	B	611	CLA	MG-NA	5.91	2.20	2.06
23	c	914	CLA	C3B-C2B	5.90	1.48	1.40
23	B	615	CLA	MG-NC	5.88	2.20	2.06
23	c	902	CLA	C3B-C2B	5.88	1.48	1.40
23	C	508	CLA	C3B-C2B	5.88	1.48	1.40
23	c	913	CLA	C3C-C2C	5.85	1.49	1.36
23	D	403	CLA	MG-NC	5.85	2.20	2.06
23	c	903	CLA	OBD-CAD	5.84	1.30	1.22
23	b	619	CLA	MG-NA	5.79	2.20	2.06
23	b	618	CLA	OBD-CAD	5.76	1.30	1.22
23	B	615	CLA	CHC-C1C	5.75	1.49	1.35
23	b	606	CLA	MG-NA	5.71	2.19	2.06
24	A	408	PHO	CHB-C1B	5.69	1.49	1.38
23	b	610	CLA	MG-NC	5.68	2.19	2.06
23	b	609	CLA	C3B-C2B	5.67	1.48	1.40
23	b	613	CLA	C3C-C2C	5.66	1.48	1.36
23	b	612	CLA	O2D-CGD	5.65	1.47	1.33
23	c	914	CLA	CHC-C1C	5.64	1.49	1.35
23	B	603	CLA	C3B-C2B	5.63	1.48	1.40
23	B	607	CLA	CHC-C1C	5.62	1.49	1.35
23	C	513	CLA	C3C-C2C	5.62	1.48	1.36
23	c	909	CLA	O2D-CGD	5.61	1.46	1.33
23	A	405	CLA	CHC-C1C	5.59	1.49	1.35
23	b	604	CLA	MG-NA	5.59	2.19	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	610	CLA	C3D-C2D	5.57	1.49	1.39
23	b	615	CLA	C3C-C2C	5.54	1.48	1.36
23	c	908	CLA	C3C-C2C	5.54	1.48	1.36
23	b	606	CLA	CHC-C1C	5.51	1.49	1.35
23	a	410	CLA	CHC-C1C	5.51	1.49	1.35
23	c	904	CLA	C3C-C2C	5.50	1.48	1.36
23	B	615	CLA	C1C-NC	-5.49	1.29	1.37
23	c	903	CLA	C3B-C2B	5.49	1.48	1.40
23	B	602	CLA	O2A-CGA	5.48	1.49	1.33
23	d	403	CLA	C3B-C2B	5.47	1.48	1.40
23	c	912	CLA	OBD-CAD	5.47	1.30	1.22
24	A	409	PHO	C3B-C2B	5.47	1.48	1.37
23	b	607	CLA	CHC-C1C	5.47	1.49	1.35
23	c	907	CLA	O2D-CGD	5.46	1.46	1.33
23	c	905	CLA	MG-NC	5.45	2.19	2.06
23	B	606	CLA	CHC-C1C	5.44	1.48	1.35
23	c	913	CLA	O2D-CGD	5.44	1.46	1.33
23	b	617	CLA	MG-NA	5.43	2.19	2.06
23	b	612	CLA	C3C-C2C	5.41	1.48	1.36
23	d	402	CLA	CHC-C1C	5.41	1.48	1.35
23	C	503	CLA	C3B-C2B	5.41	1.47	1.40
23	C	501	CLA	CHC-C1C	5.41	1.48	1.35
37	v	201	HEM	C3B-CAB	5.40	1.58	1.47
23	c	912	CLA	C3B-C2B	5.39	1.47	1.40
23	d	403	CLA	C3C-C2C	5.39	1.48	1.36
23	C	508	CLA	CHC-C1C	5.39	1.48	1.35
23	C	506	CLA	C3B-C2B	5.38	1.47	1.40
23	C	512	CLA	C3C-C2C	5.38	1.48	1.36
23	B	611	CLA	CHC-C1C	5.36	1.48	1.35
23	b	604	CLA	C3D-C2D	5.35	1.49	1.39
23	c	913	CLA	CHC-C1C	5.35	1.48	1.35
24	a	412	PHO	C3C-C2C	5.35	1.48	1.36
23	B	607	CLA	C3B-C2B	5.35	1.47	1.40
23	b	618	CLA	C3D-C2D	5.35	1.49	1.39
24	a	413	PHO	CHC-C1C	5.34	1.49	1.38
23	C	512	CLA	CHC-C1C	5.34	1.48	1.35
23	b	609	CLA	MG-NC	5.34	2.18	2.06
23	C	507	CLA	C3C-C2C	5.33	1.48	1.36
23	A	405	CLA	MG-NA	5.32	2.18	2.06
23	b	605	CLA	CHC-C1C	5.32	1.48	1.35
23	C	503	CLA	C3C-C2C	5.30	1.48	1.36
23	b	606	CLA	C3C-C2C	5.29	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	604	CLA	O2D-CGD	5.29	1.46	1.33
23	B	606	CLA	C3C-C2C	5.28	1.48	1.36
23	C	511	CLA	C3D-C2D	5.28	1.48	1.39
23	A	410	CLA	CHC-C1C	5.27	1.48	1.35
23	c	914	CLA	C3C-C2C	5.27	1.47	1.36
23	B	610	CLA	CHC-C1C	5.27	1.48	1.35
23	C	503	CLA	CHC-C1C	5.27	1.48	1.35
23	c	904	CLA	CHC-C1C	5.26	1.48	1.35
23	B	614	CLA	CHC-C1C	5.25	1.48	1.35
23	b	608	CLA	CHC-C1C	5.24	1.48	1.35
23	b	611	CLA	OBD-CAD	5.24	1.29	1.22
23	c	913	CLA	MG-NC	5.22	2.18	2.06
23	C	509	CLA	OBD-CAD	5.21	1.29	1.22
23	D	403	CLA	CHC-C1C	5.20	1.48	1.35
23	C	510	CLA	C3C-C2C	5.20	1.47	1.36
23	C	505	CLA	MG-NA	5.20	2.18	2.06
23	B	617	CLA	CHC-C1C	5.20	1.48	1.35
23	c	909	CLA	C3C-C2C	5.18	1.47	1.36
23	B	617	CLA	C3C-C2C	5.18	1.47	1.36
23	c	913	CLA	C3B-C2B	5.18	1.47	1.40
23	C	512	CLA	C3D-C2D	5.17	1.48	1.39
34	D	406	DGD	O2G-C1B	5.17	1.48	1.34
23	c	908	CLA	CHC-C1C	5.16	1.48	1.35
23	a	414	CLA	CHC-C1C	5.15	1.48	1.35
23	c	914	CLA	O2D-CGD	5.15	1.45	1.33
37	v	201	HEM	C3D-C2D	5.15	1.52	1.37
23	B	614	CLA	C3D-C2D	5.14	1.48	1.39
23	b	613	CLA	O2D-CGD	5.14	1.45	1.33
23	b	616	CLA	CHC-C1C	5.14	1.48	1.35
27	Z	101	LMG	O7-C10	5.13	1.48	1.34
23	c	909	CLA	C3D-C2D	5.13	1.48	1.39
26	D	407	SQD	O47-C7	5.13	1.48	1.34
23	C	505	CLA	C3C-C2C	5.11	1.47	1.36
23	b	604	CLA	CHC-C1C	5.11	1.48	1.35
23	C	504	CLA	C3B-C2B	5.10	1.47	1.40
34	d	406	DGD	O1G-C1A	5.10	1.48	1.33
23	C	504	CLA	MG-NA	5.09	2.18	2.06
24	A	408	PHO	C3B-C2B	5.08	1.47	1.37
23	b	604	CLA	O2A-CGA	5.08	1.48	1.33
23	b	607	CLA	C3C-C2C	5.08	1.47	1.36
23	c	911	CLA	O2D-CGD	5.08	1.45	1.33
23	C	508	CLA	O2D-CGD	5.07	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	502	CLA	MG-NA	5.06	2.18	2.06
23	c	912	CLA	O2D-CGD	5.06	1.45	1.33
23	c	914	CLA	C3D-C2D	5.05	1.48	1.39
23	B	607	CLA	C3C-C2C	5.05	1.47	1.36
23	b	608	CLA	MG-NA	5.05	2.18	2.06
23	C	502	CLA	O2D-CGD	5.05	1.45	1.33
23	B	611	CLA	C3D-C2D	5.05	1.48	1.39
23	B	602	CLA	O2D-CGD	5.04	1.45	1.33
23	b	616	CLA	O2D-CGD	5.04	1.45	1.33
23	c	903	CLA	O2D-CGD	5.04	1.45	1.33
23	a	414	CLA	MG-NA	5.04	2.18	2.06
26	a	401	SQD	O47-C7	5.03	1.48	1.34
23	C	507	CLA	CHC-C1C	5.03	1.47	1.35
26	A	418	SQD	O48-C23	5.03	1.48	1.33
23	C	513	CLA	C3D-C2D	5.03	1.48	1.39
23	c	904	CLA	C3B-C2B	5.03	1.47	1.40
23	C	511	CLA	O2D-CGD	5.02	1.45	1.33
23	d	402	CLA	MG-NA	5.02	2.18	2.06
23	c	907	CLA	MG-NA	5.02	2.18	2.06
23	A	407	CLA	CHC-C1C	5.01	1.47	1.35
23	C	513	CLA	CHC-C1C	5.01	1.47	1.35
23	b	618	CLA	C3C-C2C	5.00	1.47	1.36
23	b	604	CLA	C3B-C2B	5.00	1.47	1.40
37	f	101	HEM	C3D-C2D	5.00	1.52	1.37
23	c	906	CLA	CHC-C1C	5.00	1.47	1.35
23	b	608	CLA	O2D-CGD	5.00	1.45	1.33
23	c	907	CLA	C3B-C2B	4.99	1.47	1.40
23	d	403	CLA	MG-NC	4.98	2.18	2.06
23	B	608	CLA	CHC-C1C	4.98	1.47	1.35
23	b	613	CLA	OBD-CAD	4.98	1.29	1.22
23	C	513	CLA	MG-NC	4.98	2.18	2.06
27	c	921	LMG	O7-C10	4.97	1.48	1.34
23	c	910	CLA	C3B-C2B	4.97	1.47	1.40
23	d	402	CLA	C3D-C2D	4.97	1.48	1.39
23	c	908	CLA	C3D-C2D	4.96	1.48	1.39
23	b	605	CLA	C3B-C2B	4.94	1.47	1.40
23	B	610	CLA	MG-NA	4.94	2.18	2.06
23	c	905	CLA	C3D-C2D	4.93	1.48	1.39
23	B	616	CLA	C3C-C2C	4.93	1.47	1.36
23	C	509	CLA	CHC-C1C	4.93	1.47	1.35
23	c	910	CLA	O2D-CGD	4.91	1.45	1.33
23	B	607	CLA	O2D-CGD	4.90	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	614	CLA	C3C-C2C	4.89	1.47	1.36
23	B	613	CLA	C4B-NB	-4.89	1.30	1.35
23	c	914	CLA	OBD-CAD	4.88	1.29	1.22
23	c	909	CLA	CHC-C1C	4.87	1.47	1.35
23	c	907	CLA	C3C-C2C	4.87	1.47	1.36
23	a	411	CLA	C3D-C2D	4.87	1.48	1.39
23	C	505	CLA	O2D-CGD	4.87	1.45	1.33
23	C	509	CLA	O2D-CGD	4.86	1.45	1.33
26	L	103	SQD	O47-C7	4.86	1.48	1.34
23	C	506	CLA	CHC-C1C	4.86	1.47	1.35
23	A	410	CLA	C3C-C2C	4.86	1.47	1.36
23	a	411	CLA	CHC-C1C	4.86	1.47	1.35
26	B	621	SQD	O47-C7	4.85	1.48	1.34
23	b	608	CLA	C3C-C2C	4.85	1.47	1.36
23	c	913	CLA	C3D-C2D	4.84	1.48	1.39
23	A	407	CLA	OBD-CAD	4.84	1.29	1.22
23	A	406	CLA	CHC-C1C	4.84	1.47	1.35
23	D	402	CLA	MG-NA	4.84	2.17	2.06
23	a	410	CLA	C3C-C2C	4.84	1.47	1.36
23	B	610	CLA	C3C-C2C	4.83	1.47	1.36
37	F	101	HEM	C3D-C2D	4.83	1.52	1.37
23	B	604	CLA	C3D-C2D	4.82	1.48	1.39
23	C	508	CLA	C3D-C2D	4.82	1.48	1.39
23	B	606	CLA	MG-NC	4.82	2.17	2.06
24	A	409	PHO	CHD-C1D	4.81	1.48	1.38
23	B	616	CLA	CHC-C1C	4.81	1.47	1.35
23	b	619	CLA	C3C-C2C	4.81	1.47	1.36
23	c	909	CLA	C3B-C2B	4.80	1.47	1.40
23	B	606	CLA	O2D-CGD	4.79	1.44	1.33
23	B	602	CLA	C3C-C2C	4.79	1.46	1.36
23	A	407	CLA	C3D-C2D	4.78	1.48	1.39
23	c	911	CLA	C3C-C2C	4.78	1.46	1.36
23	C	510	CLA	OBD-CAD	4.78	1.29	1.22
24	a	412	PHO	O2D-CGD	4.77	1.44	1.33
23	B	617	CLA	C3D-C2D	4.76	1.48	1.39
23	b	619	CLA	O2D-CGD	4.76	1.44	1.33
23	b	614	CLA	CHC-C1C	4.76	1.47	1.35
23	c	906	CLA	C3B-C2B	4.75	1.47	1.40
37	V	201	HEM	C3B-CAB	4.74	1.57	1.47
23	b	609	CLA	C3C-C2C	4.74	1.46	1.36
23	C	507	CLA	C3D-C2D	4.74	1.47	1.39
26	f	102	SQD	O48-C23	4.73	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	911	CLA	CHC-C1C	4.73	1.47	1.35
23	B	602	CLA	C3B-C2B	4.73	1.46	1.40
23	C	501	CLA	C3D-C2D	4.73	1.47	1.39
23	D	403	CLA	C3C-C2C	4.73	1.46	1.36
36	a	417	LHG	O8-C23	4.72	1.47	1.33
23	B	602	CLA	CHC-C1C	4.72	1.47	1.35
24	a	413	PHO	CHD-C1D	4.72	1.47	1.38
23	C	512	CLA	O2D-CGD	4.71	1.44	1.33
23	a	409	CLA	C3C-C2C	4.71	1.46	1.36
23	b	611	CLA	CHC-C1C	4.71	1.47	1.35
24	A	409	PHO	CHB-C1B	4.70	1.47	1.38
23	C	501	CLA	MG-NA	4.69	2.17	2.06
23	C	504	CLA	CHC-C1C	4.69	1.47	1.35
23	C	513	CLA	O2D-CGD	4.67	1.44	1.33
23	d	403	CLA	C3D-C2D	4.66	1.47	1.39
36	a	417	LHG	O7-C7	4.66	1.47	1.34
23	b	615	CLA	CHC-C1C	4.66	1.46	1.35
23	C	506	CLA	O2D-CGD	4.65	1.44	1.33
27	B	622	LMG	O8-C28	4.65	1.46	1.33
23	A	405	CLA	C3C-C2C	4.64	1.46	1.36
23	D	402	CLA	C3B-C2B	4.63	1.46	1.40
23	a	414	CLA	C3C-C2C	4.63	1.46	1.36
23	A	410	CLA	OBD-CAD	4.63	1.28	1.22
34	D	406	DGD	O1G-C1A	4.63	1.46	1.33
26	a	401	SQD	O48-C23	4.63	1.46	1.33
23	a	414	CLA	C3B-C2B	4.62	1.46	1.40
23	b	606	CLA	OBD-CAD	4.62	1.28	1.22
23	C	505	CLA	CHC-C1C	4.62	1.46	1.35
23	d	403	CLA	CHC-C1C	4.62	1.46	1.35
23	b	619	CLA	C3D-C2D	4.62	1.47	1.39
23	b	611	CLA	C3B-C2B	4.61	1.46	1.40
23	b	618	CLA	O2D-CGD	4.61	1.44	1.33
23	b	604	CLA	C3C-C2C	4.61	1.46	1.36
27	c	920	LMG	O8-C28	4.61	1.46	1.33
23	B	604	CLA	CHC-C1C	4.60	1.46	1.35
23	b	616	CLA	OBD-CAD	4.60	1.28	1.22
23	c	902	CLA	CHC-C1C	4.60	1.46	1.35
23	d	402	CLA	O2A-CGA	4.59	1.46	1.33
23	b	619	CLA	C3B-C2B	4.59	1.46	1.40
23	B	616	CLA	C3D-C2D	4.58	1.47	1.39
23	b	606	CLA	O2D-CGD	4.58	1.44	1.33
23	C	505	CLA	C3D-C2D	4.56	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	912	CLA	C3D-C2D	4.56	1.47	1.39
23	c	905	CLA	O2D-CGD	4.55	1.44	1.33
36	E	101	LHG	O8-C23	4.55	1.46	1.33
23	C	509	CLA	C3D-C2D	4.54	1.47	1.39
23	b	609	CLA	CHC-C1C	4.54	1.46	1.35
37	F	101	HEM	C3B-C2B	-4.54	1.34	1.40
23	c	912	CLA	C3C-C2C	4.53	1.46	1.36
23	D	403	CLA	C3D-C2D	4.53	1.47	1.39
23	b	613	CLA	CHC-C1C	4.53	1.46	1.35
23	C	509	CLA	C3C-C2C	4.52	1.46	1.36
23	c	910	CLA	C3D-C2D	4.52	1.47	1.39
23	C	501	CLA	C3B-C2B	4.51	1.46	1.40
23	c	905	CLA	CHC-C1C	4.51	1.46	1.35
23	b	618	CLA	C3B-C2B	4.51	1.46	1.40
23	c	912	CLA	CHC-C1C	4.51	1.46	1.35
27	A	413	LMG	O7-C10	4.50	1.47	1.34
34	H	102	DGD	O5D-C1E	4.50	1.47	1.40
23	B	609	CLA	O2D-CGD	4.49	1.44	1.33
23	b	614	CLA	O2D-CGD	4.49	1.44	1.33
23	C	511	CLA	CHC-C1C	4.49	1.46	1.35
23	B	617	CLA	C3B-C2B	4.49	1.46	1.40
27	c	921	LMG	O8-C28	4.48	1.46	1.33
23	B	608	CLA	C3C-C2C	4.48	1.46	1.36
27	c	920	LMG	O7-C10	4.47	1.46	1.34
23	A	407	CLA	C3C-C2C	4.47	1.46	1.36
23	b	614	CLA	C3D-C2D	4.47	1.47	1.39
23	c	914	CLA	O2A-CGA	4.45	1.46	1.33
23	C	512	CLA	C3B-C2B	4.45	1.46	1.40
23	B	612	CLA	CHC-C1C	4.45	1.46	1.35
23	B	603	CLA	C3D-C2D	4.44	1.47	1.39
23	b	612	CLA	C3D-C2D	4.44	1.47	1.39
26	D	407	SQD	O48-C23	4.44	1.46	1.33
23	c	904	CLA	C3D-C2D	4.44	1.47	1.39
23	d	402	CLA	C3C-C2C	4.44	1.46	1.36
24	a	413	PHO	C3C-C2C	4.44	1.46	1.36
23	c	911	CLA	MG-NA	4.44	2.16	2.06
24	a	412	PHO	CHD-C4C	4.43	1.50	1.40
23	b	616	CLA	C3C-C2C	4.42	1.46	1.36
27	C	519	LMG	O8-C28	4.41	1.46	1.33
23	B	609	CLA	C3C-C2C	4.41	1.46	1.36
23	b	609	CLA	O2D-CGD	4.40	1.43	1.33
23	C	504	CLA	C3C-C2C	4.40	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	510	CLA	O2D-CGD	4.40	1.43	1.33
27	Z	101	LMG	O8-C28	4.39	1.46	1.33
23	c	911	CLA	OBD-CAD	4.39	1.28	1.22
34	d	406	DGD	O2G-C1B	4.39	1.46	1.34
23	b	617	CLA	O2A-CGA	4.38	1.46	1.33
24	a	413	PHO	C1A-NA	-4.38	1.28	1.37
23	b	618	CLA	CHC-C1C	4.38	1.46	1.35
24	a	413	PHO	C3B-C2B	4.37	1.46	1.37
23	C	506	CLA	O2A-CGA	4.37	1.46	1.33
23	c	913	CLA	O2A-CGA	4.36	1.46	1.33
24	a	412	PHO	CHD-C1D	4.36	1.47	1.38
23	c	902	CLA	C3C-C2C	4.36	1.46	1.36
23	B	608	CLA	C3B-C2B	4.36	1.46	1.40
23	c	903	CLA	CHC-C1C	4.35	1.46	1.35
23	B	608	CLA	MG-NC	4.35	2.16	2.06
27	a	418	LMG	O7-C10	4.35	1.46	1.34
23	B	616	CLA	O2D-CGD	4.35	1.43	1.33
23	b	615	CLA	C3D-C2D	4.35	1.47	1.39
24	a	412	PHO	CHB-C1B	4.35	1.47	1.38
23	B	605	CLA	C3C-C2C	4.34	1.46	1.36
23	B	613	CLA	C3C-C2C	4.33	1.45	1.36
23	C	503	CLA	MG-NA	4.33	2.16	2.06
23	a	414	CLA	OBD-CAD	4.33	1.28	1.22
23	b	612	CLA	OBD-CAD	4.33	1.28	1.22
23	a	409	CLA	C3B-C2B	4.32	1.46	1.40
23	a	411	CLA	C3C-C2C	4.32	1.45	1.36
23	C	502	CLA	C3C-C2C	4.32	1.45	1.36
36	E	101	LHG	O7-C7	4.31	1.46	1.34
23	c	911	CLA	C3B-C2B	4.31	1.46	1.40
23	C	501	CLA	OBD-CAD	4.31	1.28	1.22
23	A	406	CLA	C3C-C2C	4.31	1.45	1.36
23	C	511	CLA	C3C-C2C	4.31	1.45	1.36
23	c	904	CLA	O2D-CGD	4.31	1.43	1.33
23	B	616	CLA	OBD-CAD	4.31	1.28	1.22
23	c	910	CLA	CHC-C1C	4.30	1.46	1.35
23	C	503	CLA	O2A-CGA	4.29	1.45	1.33
23	A	405	CLA	O2D-CGD	4.29	1.43	1.33
23	d	402	CLA	C3B-C2B	4.29	1.46	1.40
23	b	611	CLA	C3C-C2C	4.29	1.45	1.36
24	a	413	PHO	O2D-CGD	4.27	1.43	1.33
23	b	609	CLA	C3D-C2D	4.27	1.47	1.39
23	b	619	CLA	O2A-CGA	4.26	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	412	PHO	C3B-C2B	4.26	1.45	1.37
23	D	402	CLA	O2A-CGA	4.26	1.45	1.33
23	c	910	CLA	C3C-C2C	4.26	1.45	1.36
26	A	418	SQD	O47-C7	4.26	1.46	1.34
23	B	605	CLA	CHC-C1C	4.26	1.45	1.35
23	B	612	CLA	C3D-C2D	4.25	1.47	1.39
23	c	908	CLA	OBD-CAD	4.25	1.28	1.22
23	B	611	CLA	C3C-C2C	4.24	1.45	1.36
23	b	617	CLA	CHC-C1C	4.23	1.45	1.35
23	B	608	CLA	C3D-C2D	4.23	1.47	1.39
27	A	413	LMG	O8-C28	4.22	1.45	1.33
23	B	610	CLA	C3D-C2D	4.22	1.47	1.39
23	b	606	CLA	C3D-C2D	4.22	1.47	1.39
23	b	616	CLA	O2A-CGA	4.21	1.45	1.33
37	v	201	HEM	C3C-CAC	4.21	1.56	1.47
23	C	510	CLA	C3D-C2D	4.21	1.47	1.39
23	C	510	CLA	C3B-C2B	4.20	1.46	1.40
23	C	502	CLA	C3D-C2D	4.20	1.47	1.39
23	D	402	CLA	OBD-CAD	4.18	1.28	1.22
23	B	604	CLA	C3C-C2C	4.16	1.45	1.36
23	D	402	CLA	C4C-C3C	4.15	1.52	1.45
23	a	411	CLA	MG-NA	4.14	2.16	2.06
23	B	617	CLA	OBD-CAD	4.14	1.28	1.22
23	c	906	CLA	C3D-C2D	4.14	1.46	1.39
23	C	501	CLA	C3C-C2C	4.14	1.45	1.36
37	V	201	HEM	C3C-C2C	-4.14	1.34	1.40
23	c	906	CLA	C3C-C2C	4.13	1.45	1.36
23	d	403	CLA	O2A-CGA	4.13	1.45	1.33
23	C	506	CLA	C3C-C2C	4.13	1.45	1.36
37	F	101	HEM	C3B-CAB	4.12	1.56	1.47
23	c	907	CLA	CHC-C1C	4.11	1.45	1.35
34	c	918	DGD	O1G-C1A	4.10	1.45	1.33
23	C	509	CLA	O2A-CGA	4.10	1.45	1.33
23	b	609	CLA	C1B-NB	4.09	1.38	1.35
23	b	610	CLA	O2D-CGD	4.08	1.43	1.33
23	D	402	CLA	O2D-CGD	4.08	1.43	1.33
23	C	506	CLA	C3D-C2D	4.08	1.46	1.39
23	A	405	CLA	OBD-CAD	4.08	1.28	1.22
23	b	616	CLA	C3D-C2D	4.07	1.46	1.39
23	C	511	CLA	C3B-C2B	4.07	1.46	1.40
23	b	614	CLA	C3B-C2B	4.06	1.46	1.40
23	b	607	CLA	O2D-CGD	4.05	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	607	CLA	C3D-C2D	4.04	1.46	1.39
23	B	602	CLA	OBD-CAD	4.03	1.27	1.22
23	D	403	CLA	O2A-CGA	4.03	1.45	1.33
23	B	613	CLA	C1B-NB	-4.03	1.31	1.35
23	C	505	CLA	C3B-C2B	4.03	1.46	1.40
27	a	418	LMG	O8-C28	4.02	1.45	1.33
23	B	604	CLA	OBD-CAD	4.02	1.27	1.22
23	B	607	CLA	OBD-CAD	4.01	1.27	1.22
23	b	619	CLA	OBD-CAD	4.01	1.27	1.22
27	b	623	LMG	O8-C28	4.00	1.45	1.33
23	b	614	CLA	C3C-C2C	4.00	1.45	1.36
23	c	905	CLA	C3B-C2B	4.00	1.45	1.40
23	c	905	CLA	OBD-CAD	3.99	1.27	1.22
33	B	624	HTG	C1'-S1	-3.99	1.76	1.81
23	C	504	CLA	C3D-C2D	3.99	1.46	1.39
23	c	907	CLA	O2A-CGA	3.99	1.45	1.33
23	b	617	CLA	O2D-CGD	3.99	1.42	1.33
34	h	102	DGD	O5D-C1E	3.98	1.47	1.40
23	b	615	CLA	O2D-CGD	3.98	1.42	1.33
23	b	612	CLA	MG-NA	3.98	2.15	2.06
23	D	402	CLA	CHC-C1C	3.98	1.45	1.35
23	C	507	CLA	O2D-CGD	3.97	1.42	1.33
23	C	511	CLA	O2A-CGA	3.97	1.44	1.33
23	c	902	CLA	OBD-CAD	3.96	1.27	1.22
23	c	911	CLA	O2A-CGA	3.95	1.44	1.33
23	D	403	CLA	C3B-C2B	3.95	1.45	1.40
23	b	612	CLA	C3B-C2B	3.95	1.45	1.40
23	b	604	CLA	OBD-CAD	3.94	1.27	1.22
26	A	412	SQD	O47-C7	3.92	1.45	1.34
23	b	616	CLA	C3B-C2B	3.92	1.45	1.40
23	C	502	CLA	C3B-C2B	3.92	1.45	1.40
30	B	623	LMT	O6B-C6B	3.92	1.59	1.42
23	A	405	CLA	C3D-C2D	3.92	1.46	1.39
23	c	912	CLA	MG-NC	3.91	2.15	2.06
23	c	911	CLA	C3D-C2D	3.91	1.46	1.39
23	A	410	CLA	MG-NA	3.91	2.15	2.06
23	B	615	CLA	C3C-C2C	3.90	1.45	1.36
23	b	613	CLA	C4C-C3C	3.89	1.51	1.45
23	c	912	CLA	O2A-CGA	3.89	1.44	1.33
37	V	201	HEM	C3D-C2D	3.89	1.49	1.37
24	A	409	PHO	C3C-C2C	3.89	1.45	1.36
23	a	409	CLA	O2D-CGD	3.89	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	913	CLA	OBD-CAD	3.89	1.27	1.22
37	V	201	HEM	C3C-CAC	3.88	1.55	1.47
23	B	615	CLA	C3D-C2D	3.88	1.46	1.39
23	B	616	CLA	C1B-NB	-3.87	1.31	1.35
28	D	405	PL9	C21-C19	3.87	1.59	1.51
23	a	410	CLA	OBD-CAD	3.86	1.27	1.22
37	f	101	HEM	C3B-CAB	3.86	1.55	1.47
23	c	902	CLA	O2D-CGD	3.86	1.42	1.33
27	C	519	LMG	O7-C10	3.85	1.45	1.34
37	v	201	HEM	C3C-C2C	-3.85	1.35	1.40
23	B	610	CLA	C3B-C2B	3.84	1.45	1.40
23	B	603	CLA	MG-NC	3.84	2.15	2.06
23	c	902	CLA	O2A-CGA	3.83	1.44	1.33
24	A	409	PHO	O2D-CGD	3.83	1.42	1.33
27	d	410	LMG	O7-C10	3.83	1.45	1.34
23	D	403	CLA	OBD-CAD	3.82	1.27	1.22
23	C	503	CLA	O2D-CGD	3.82	1.42	1.33
26	L	103	SQD	O48-C23	3.82	1.44	1.33
23	C	512	CLA	O2A-CGA	3.81	1.44	1.33
23	c	909	CLA	C4C-C3C	3.81	1.51	1.45
26	a	416	SQD	O47-C7	3.81	1.45	1.34
23	B	609	CLA	C3D-C2D	3.80	1.46	1.39
23	B	616	CLA	O2A-CGA	3.80	1.44	1.33
34	C	517	DGD	O1G-C1A	3.80	1.44	1.33
27	D	411	LMG	O7-C10	3.80	1.45	1.34
23	C	505	CLA	C1B-NB	-3.79	1.31	1.35
23	B	607	CLA	C3D-C2D	3.79	1.46	1.39
24	A	408	PHO	C3C-C2C	3.78	1.44	1.36
23	C	502	CLA	OBD-CAD	3.78	1.27	1.22
28	d	405	PL9	C7-C3	3.78	1.55	1.51
23	B	612	CLA	C3C-C2C	3.78	1.44	1.36
26	B	621	SQD	O48-C23	3.78	1.44	1.33
23	B	615	CLA	O2D-CGD	3.77	1.42	1.33
23	B	615	CLA	C1B-NB	-3.77	1.31	1.35
23	B	613	CLA	OBD-CAD	3.76	1.27	1.22
33	D	414	HTG	C1'-S1	-3.76	1.76	1.81
23	B	604	CLA	O2D-CGD	3.74	1.42	1.33
24	A	408	PHO	CHC-C1C	3.73	1.45	1.38
23	d	403	CLA	O2D-CGD	3.73	1.42	1.33
23	C	505	CLA	OBD-CAD	3.72	1.27	1.22
23	B	608	CLA	C1B-NB	-3.71	1.31	1.35
23	B	602	CLA	C3D-C2D	3.70	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	406	CLA	MG-NA	3.70	2.15	2.06
23	B	612	CLA	OBD-CAD	3.70	1.27	1.22
23	c	910	CLA	O2A-CGA	3.69	1.44	1.33
23	b	611	CLA	C3D-C2D	3.69	1.46	1.39
23	a	414	CLA	O2A-CGA	3.69	1.44	1.33
24	A	409	PHO	OBD-CAD	3.69	1.28	1.22
23	d	403	CLA	C4C-C3C	3.69	1.51	1.45
23	C	510	CLA	O2A-CGA	3.69	1.44	1.33
23	C	508	CLA	C4C-C3C	3.68	1.51	1.45
24	A	409	PHO	CHC-C1C	3.68	1.45	1.38
37	F	101	HEM	C3C-C2C	-3.67	1.35	1.40
23	B	611	CLA	C3B-C2B	3.67	1.45	1.40
23	B	609	CLA	MG-NA	3.67	2.15	2.06
23	C	511	CLA	OBD-CAD	3.66	1.27	1.22
23	b	612	CLA	O2A-CGA	3.66	1.44	1.33
23	B	617	CLA	MG-NA	3.66	2.15	2.06
36	D	410	LHG	O8-C23	3.65	1.44	1.33
23	B	606	CLA	C3D-C2D	3.65	1.46	1.39
23	A	407	CLA	C4B-NB	-3.65	1.31	1.35
26	a	416	SQD	O48-C23	3.65	1.44	1.33
23	B	617	CLA	O2D-CGD	3.65	1.42	1.33
30	A	419	LMT	O1'-C1'	3.65	1.46	1.40
23	B	603	CLA	OBD-CAD	3.65	1.27	1.22
23	A	410	CLA	C3D-C2D	3.64	1.46	1.39
33	b	627	HTG	C1'-S1	-3.64	1.76	1.81
23	b	605	CLA	C3D-C2D	3.64	1.46	1.39
24	A	408	PHO	O2A-CGA	3.64	1.44	1.33
23	c	908	CLA	O2A-CGA	3.63	1.43	1.33
23	B	604	CLA	C3B-C2B	3.62	1.45	1.40
23	a	409	CLA	CHC-C1C	3.62	1.44	1.35
23	c	907	CLA	C3D-C2D	3.62	1.45	1.39
23	C	503	CLA	C3D-C2D	3.61	1.45	1.39
23	B	606	CLA	C3B-C2B	3.61	1.45	1.40
23	b	607	CLA	MG-NC	3.60	2.14	2.06
23	B	613	CLA	C3D-C2D	3.60	1.45	1.39
23	B	609	CLA	CHC-C1C	3.60	1.44	1.35
23	C	504	CLA	O2D-CGD	3.59	1.42	1.33
23	C	510	CLA	CHC-C1C	3.59	1.44	1.35
23	c	909	CLA	C1C-NC	-3.59	1.32	1.37
24	a	412	PHO	CHC-C1C	3.59	1.45	1.38
23	A	410	CLA	C3B-C2B	3.59	1.45	1.40
23	c	908	CLA	O2D-CGD	3.58	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	617	CLA	C3C-C2C	3.58	1.44	1.36
23	D	403	CLA	C1B-CHB	3.58	1.50	1.41
23	D	402	CLA	C3C-C2C	3.57	1.44	1.36
27	d	410	LMG	O8-C28	3.57	1.43	1.33
23	a	411	CLA	O2D-CGD	3.57	1.41	1.33
23	B	605	CLA	O2D-CGD	3.57	1.41	1.33
24	a	413	PHO	O2A-CGA	3.57	1.43	1.33
23	c	906	CLA	O2A-CGA	3.56	1.43	1.33
23	b	613	CLA	C3D-C2D	3.56	1.45	1.39
23	B	616	CLA	C3B-C2B	3.56	1.45	1.40
24	A	409	PHO	CHC-C4B	3.56	1.48	1.40
23	B	613	CLA	O2D-CGD	3.56	1.41	1.33
23	b	614	CLA	O2A-CGA	3.56	1.43	1.33
24	A	408	PHO	C1A-NA	-3.55	1.30	1.37
23	b	608	CLA	OBD-CAD	3.55	1.27	1.22
23	B	603	CLA	C4B-NB	3.54	1.38	1.35
24	A	409	PHO	C1A-NA	-3.54	1.30	1.37
23	C	511	CLA	C1B-CHB	3.54	1.50	1.41
23	c	903	CLA	C3C-C2C	3.53	1.44	1.36
23	b	611	CLA	C4B-NB	-3.53	1.32	1.35
23	a	414	CLA	O2D-CGD	3.52	1.41	1.33
23	B	609	CLA	C3B-C2B	3.51	1.45	1.40
37	V	201	HEM	CMA-C3A	3.51	1.58	1.51
34	C	518	DGD	O1G-C1A	3.51	1.43	1.33
23	A	407	CLA	O2D-CGD	3.49	1.41	1.33
23	B	604	CLA	O2A-CGA	3.49	1.43	1.33
33	d	401	HTG	C1'-S1	-3.49	1.77	1.81
34	c	919	DGD	O1G-C1A	3.49	1.43	1.33
23	A	406	CLA	C4B-NB	-3.49	1.32	1.35
23	B	609	CLA	O2A-CGA	3.49	1.43	1.33
23	c	910	CLA	MG-NC	3.48	2.14	2.06
23	B	603	CLA	C4C-C3C	3.47	1.51	1.45
34	C	516	DGD	O2G-C1B	3.47	1.44	1.34
23	c	906	CLA	OBD-CAD	3.47	1.27	1.22
23	B	611	CLA	MG-NC	3.47	2.14	2.06
23	B	617	CLA	O2A-CGA	3.47	1.43	1.33
34	H	102	DGD	O1G-C1A	3.46	1.43	1.33
23	b	611	CLA	O2D-CGD	3.46	1.41	1.33
23	C	506	CLA	OBD-CAD	3.45	1.27	1.22
23	B	611	CLA	O2D-CGD	3.45	1.41	1.33
23	C	507	CLA	O2A-CGA	3.45	1.43	1.33
23	c	903	CLA	C3D-C2D	3.44	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	617	CLA	C3B-C2B	3.44	1.45	1.40
23	C	513	CLA	OBD-CAD	3.44	1.27	1.22
36	D	408	LHG	O8-C23	3.42	1.43	1.33
23	c	908	CLA	C3B-C2B	3.42	1.45	1.40
36	D	409	LHG	O8-C23	3.42	1.43	1.33
23	B	611	CLA	OBD-CAD	3.40	1.27	1.22
26	A	412	SQD	O48-C23	3.40	1.43	1.33
36	D	410	LHG	O7-C7	3.40	1.43	1.34
34	C	516	DGD	O1G-C1A	3.40	1.43	1.33
23	b	613	CLA	MG-NC	3.39	2.14	2.06
23	c	913	CLA	C4C-C3C	3.39	1.50	1.45
23	C	513	CLA	O2A-CGA	3.39	1.43	1.33
23	c	902	CLA	C3D-C2D	3.39	1.45	1.39
34	c	917	DGD	O5D-C1E	3.38	1.46	1.40
37	f	101	HEM	C3C-CAC	3.38	1.54	1.47
23	c	902	CLA	C4C-C3C	3.38	1.50	1.45
23	A	407	CLA	C1B-NB	-3.38	1.32	1.35
23	C	501	CLA	O2D-CGD	3.37	1.41	1.33
23	b	609	CLA	OBD-CAD	3.37	1.27	1.22
23	b	605	CLA	O2A-CGA	3.37	1.43	1.33
23	A	406	CLA	C3B-C2B	3.36	1.45	1.40
23	b	607	CLA	C3B-C2B	3.35	1.45	1.40
27	b	623	LMG	O7-C10	3.35	1.43	1.34
23	D	403	CLA	O2D-CGD	3.35	1.41	1.33
23	c	905	CLA	C1C-NC	-3.34	1.32	1.37
23	C	506	CLA	C1B-CHB	3.34	1.50	1.41
23	c	903	CLA	O2A-CGA	3.34	1.43	1.33
23	A	406	CLA	C3D-C2D	3.34	1.45	1.39
23	B	615	CLA	O2A-CGA	3.34	1.43	1.33
23	d	403	CLA	OBD-CAD	3.33	1.27	1.22
23	C	507	CLA	OBD-CAD	3.33	1.26	1.22
23	a	411	CLA	OBD-CAD	3.33	1.26	1.22
23	b	608	CLA	C3B-C2B	3.32	1.45	1.40
23	b	606	CLA	C3B-C2B	3.32	1.45	1.40
23	b	614	CLA	C1B-CHB	3.31	1.50	1.41
23	B	610	CLA	O2A-CGA	3.31	1.43	1.33
34	h	102	DGD	O2G-C1B	3.30	1.43	1.34
23	B	604	CLA	C1C-NC	-3.29	1.32	1.37
34	h	102	DGD	O1G-C1A	3.28	1.42	1.33
23	C	508	CLA	C1B-CHB	3.28	1.50	1.41
23	B	602	CLA	MG-NC	3.28	2.14	2.06
23	c	912	CLA	C1B-CHB	3.27	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	405	CLA	C3B-C2B	3.27	1.44	1.40
23	b	604	CLA	C4B-CHC	3.27	1.50	1.41
23	a	410	CLA	C3B-C2B	3.27	1.44	1.40
23	b	615	CLA	OBD-CAD	3.26	1.26	1.22
34	D	406	DGD	O3G-C1D	3.26	1.45	1.40
23	C	504	CLA	CHD-C4C	3.26	1.50	1.41
23	c	907	CLA	OBD-CAD	3.26	1.26	1.22
23	D	403	CLA	C1C-NC	-3.25	1.33	1.37
34	C	517	DGD	O2G-C1B	3.25	1.43	1.34
30	J	102	LMT	O1'-C1'	3.24	1.45	1.40
24	a	413	PHO	C3D-C2D	3.24	1.48	1.39
37	V	201	HEM	C3B-C2B	-3.24	1.35	1.40
23	B	608	CLA	OBD-CAD	3.24	1.26	1.22
23	a	409	CLA	C4B-NB	-3.23	1.32	1.35
24	a	412	PHO	C3D-C2D	3.22	1.47	1.39
23	B	611	CLA	O2A-CGA	3.22	1.42	1.33
23	c	905	CLA	O2A-CGA	3.22	1.42	1.33
23	A	410	CLA	C1B-CHB	3.21	1.49	1.41
23	C	511	CLA	C1B-NB	3.21	1.38	1.35
37	f	101	HEM	C3C-C2C	-3.20	1.35	1.40
23	a	414	CLA	C1B-CHB	3.20	1.49	1.41
23	c	904	CLA	O2A-CGA	3.20	1.42	1.33
23	c	905	CLA	C4C-C3C	3.20	1.50	1.45
23	a	409	CLA	C3D-C2D	3.20	1.45	1.39
23	B	603	CLA	C1B-CHB	3.20	1.49	1.41
23	B	611	CLA	C1C-NC	-3.19	1.33	1.37
23	B	606	CLA	OBD-CAD	3.19	1.26	1.22
23	c	909	CLA	O2A-CGA	3.18	1.42	1.33
23	C	512	CLA	OBD-CAD	3.18	1.26	1.22
23	A	410	CLA	C4B-CHC	3.17	1.49	1.41
23	b	615	CLA	O2A-CGA	3.16	1.42	1.33
23	C	505	CLA	C4C-C3C	3.16	1.50	1.45
23	B	608	CLA	O2D-CGD	3.15	1.40	1.33
23	B	616	CLA	C4C-C3C	3.15	1.50	1.45
23	A	410	CLA	MG-NC	3.15	2.13	2.06
23	B	610	CLA	OBD-CAD	3.14	1.26	1.22
37	f	101	HEM	C3B-C2B	-3.14	1.36	1.40
23	a	411	CLA	C3B-C2B	3.14	1.44	1.40
23	c	904	CLA	C1B-CHB	3.14	1.49	1.41
23	a	410	CLA	O2A-CGA	3.13	1.42	1.33
34	c	917	DGD	O1G-C1A	3.13	1.42	1.33
27	B	622	LMG	O7-C10	3.13	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	501	CLA	O2A-CGA	3.13	1.42	1.33
23	B	606	CLA	O2A-CGA	3.12	1.42	1.33
23	B	603	CLA	O2D-CGD	3.12	1.40	1.33
36	d	409	LHG	O7-C7	3.12	1.43	1.34
23	A	410	CLA	O2A-CGA	3.12	1.42	1.33
23	A	405	CLA	C4B-CHC	3.12	1.49	1.41
37	v	201	HEM	C3B-C2B	-3.12	1.36	1.40
23	B	607	CLA	C4C-C3C	3.11	1.50	1.45
25	a	415	BCR	C8-C9	3.11	1.52	1.45
23	B	615	CLA	C1B-CHB	3.11	1.49	1.41
23	C	507	CLA	C1C-C2C	3.11	1.50	1.44
23	C	513	CLA	C1B-CHB	3.10	1.49	1.41
30	M	101	LMT	O1'-C1'	3.09	1.45	1.40
33	B	626	HTG	C1'-S1	-3.09	1.77	1.81
23	B	605	CLA	C3D-C2D	3.08	1.45	1.39
25	b	621	BCR	C5-C6	3.08	1.39	1.34
24	a	412	PHO	CHC-C4B	3.08	1.47	1.40
30	a	402	LMT	O1'-C1'	3.08	1.45	1.40
23	C	512	CLA	C1B-CHB	3.08	1.49	1.41
36	l	101	LHG	O8-C23	3.07	1.42	1.33
23	C	512	CLA	C4C-C3C	3.07	1.50	1.45
23	c	902	CLA	C1B-CHB	3.07	1.49	1.41
23	B	602	CLA	C1D-C2D	3.07	1.49	1.42
38	H	101	RRX	C33-C5	3.06	1.56	1.50
36	d	407	LHG	O8-C23	3.05	1.42	1.33
33	c	924	HTG	C1'-S1	-3.05	1.77	1.81
23	b	605	CLA	CHD-C4C	3.05	1.49	1.41
24	a	412	PHO	C1A-NA	-3.05	1.31	1.37
28	a	419	PL9	C7-C3	3.05	1.54	1.51
23	B	606	CLA	C1B-CHB	3.04	1.49	1.41
23	C	508	CLA	O2A-CGA	3.04	1.42	1.33
23	c	903	CLA	C1B-CHB	3.04	1.49	1.41
23	c	914	CLA	C1B-CHB	3.02	1.49	1.41
23	b	619	CLA	C1C-C2C	3.01	1.50	1.44
23	B	604	CLA	C1B-CHB	3.01	1.49	1.41
23	D	403	CLA	C1B-NB	3.01	1.37	1.35
36	d	409	LHG	O8-C23	3.00	1.42	1.33
23	C	502	CLA	O2A-CGA	3.00	1.42	1.33
34	c	918	DGD	O2G-C1B	2.99	1.42	1.34
26	A	412	SQD	C6-S	-2.99	1.66	1.77
23	c	906	CLA	O2D-CGD	2.98	1.40	1.33
23	B	613	CLA	C3B-C2B	2.98	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	906	CLA	CHD-C4C	2.98	1.49	1.41
23	C	510	CLA	C1C-NC	-2.98	1.33	1.37
34	c	919	DGD	O2G-C2G	-2.98	1.39	1.46
33	c	923	HTG	C1-S1	-2.98	1.76	1.80
37	V	201	HEM	CMB-C2B	2.97	1.58	1.51
33	B	630	HTG	C1-S1	-2.97	1.76	1.80
23	C	505	CLA	O2A-CGA	2.97	1.42	1.33
23	a	414	CLA	C3D-C2D	2.97	1.44	1.39
28	d	405	PL9	C41-C39	2.97	1.57	1.51
23	B	605	CLA	C3B-C2B	2.96	1.44	1.40
23	b	615	CLA	MG-NC	-2.95	1.99	2.06
23	B	610	CLA	MG-NC	2.95	2.13	2.06
23	c	905	CLA	C1B-CHB	2.95	1.49	1.41
23	B	614	CLA	C4C-C3C	2.95	1.50	1.45
24	A	408	PHO	CHD-C4C	2.94	1.47	1.40
28	a	419	PL9	C6-C5	2.94	1.50	1.35
23	a	410	CLA	C3D-C2D	2.93	1.44	1.39
23	A	406	CLA	O2A-CGA	2.93	1.41	1.33
23	B	607	CLA	O2A-CGA	2.93	1.41	1.33
33	b	601	HTG	C1'-S1	-2.93	1.77	1.81
23	b	617	CLA	C3D-C2D	2.93	1.44	1.39
23	B	608	CLA	C1B-CHB	2.93	1.49	1.41
23	B	608	CLA	C1D-C2D	2.93	1.49	1.42
24	a	413	PHO	C3D-C4D	-2.93	1.34	1.43
23	b	608	CLA	O2A-CGA	2.92	1.41	1.33
23	a	410	CLA	C1D-C2D	2.92	1.49	1.42
23	b	618	CLA	CHD-C4C	2.92	1.49	1.41
36	L	101	LHG	O8-C23	2.91	1.41	1.33
23	B	614	CLA	C1C-NC	-2.91	1.33	1.37
23	c	913	CLA	C4B-CHC	2.90	1.49	1.41
23	c	904	CLA	C4C-C3C	2.90	1.50	1.45
28	d	405	PL9	C6-C5	2.90	1.50	1.35
23	C	504	CLA	C1C-NC	-2.90	1.33	1.37
23	A	406	CLA	C1D-C2D	2.90	1.49	1.42
23	B	615	CLA	C3B-C2B	2.90	1.44	1.40
23	B	605	CLA	O2A-CGA	2.89	1.41	1.33
23	b	613	CLA	C3B-C2B	2.89	1.44	1.40
23	a	409	CLA	O2A-CGA	2.89	1.41	1.33
23	B	603	CLA	C1D-C2D	2.88	1.49	1.42
23	D	402	CLA	C3D-C2D	2.88	1.44	1.39
23	b	617	CLA	C1B-CHB	2.88	1.49	1.41
23	C	504	CLA	OBD-CAD	2.87	1.26	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	F	101	HEM	C3C-CAC	2.87	1.53	1.47
24	A	409	PHO	O2A-CGA	2.87	1.41	1.33
23	a	411	CLA	O2A-CGA	2.86	1.41	1.33
23	B	602	CLA	C4B-CHC	2.86	1.48	1.41
23	A	406	CLA	C4B-CHC	2.86	1.48	1.41
33	C	522	HTG	C1'-S1	-2.86	1.77	1.81
23	C	501	CLA	C4B-CHC	2.86	1.48	1.41
23	D	403	CLA	C4C-C3C	2.85	1.50	1.45
24	A	408	PHO	O2D-CGD	2.85	1.40	1.33
23	B	611	CLA	C4B-CHC	2.85	1.48	1.41
33	c	923	HTG	C1'-S1	-2.84	1.77	1.81
23	b	604	CLA	C1B-CHB	2.84	1.48	1.41
23	B	612	CLA	O2D-CGD	2.84	1.40	1.33
34	H	102	DGD	O2G-C1B	2.84	1.42	1.34
23	C	504	CLA	O2A-CGA	2.83	1.41	1.33
23	c	907	CLA	C1C-C2C	2.83	1.50	1.44
23	C	509	CLA	C3B-C2B	2.83	1.44	1.40
28	A	414	PL9	C6-C5	2.83	1.50	1.35
23	b	612	CLA	C1D-C2D	2.83	1.49	1.42
23	c	908	CLA	C1C-C2C	2.82	1.50	1.44
36	L	101	LHG	O7-C7	2.82	1.42	1.34
23	c	906	CLA	C4C-C3C	2.82	1.49	1.45
25	a	415	BCR	C26-C25	2.82	1.39	1.34
23	b	604	CLA	C1C-C2C	2.82	1.50	1.44
23	c	904	CLA	OBD-CAD	2.82	1.26	1.22
26	a	416	SQD	C6-S	-2.82	1.67	1.77
23	c	908	CLA	C4B-CHC	2.82	1.48	1.41
23	c	908	CLA	C1B-CHB	2.81	1.48	1.41
23	D	402	CLA	C3B-CAB	2.81	1.53	1.47
23	B	605	CLA	C1B-CHB	2.81	1.48	1.41
23	c	913	CLA	C1B-CHB	2.81	1.48	1.41
23	b	607	CLA	C1D-C2D	2.80	1.48	1.42
23	b	617	CLA	OBD-CAD	2.80	1.26	1.22
23	B	610	CLA	C4B-CHC	2.79	1.48	1.41
26	B	621	SQD	O6-C1	2.79	1.45	1.40
23	B	604	CLA	C1D-C2D	2.78	1.48	1.42
23	d	403	CLA	C1D-C2D	2.78	1.48	1.42
23	b	610	CLA	C3B-C2B	2.78	1.44	1.40
28	A	414	PL9	C7-C3	2.78	1.54	1.51
23	C	508	CLA	C1C-NC	-2.77	1.33	1.37
23	b	619	CLA	C1C-NC	-2.77	1.33	1.37
28	D	405	PL9	C6-C5	2.77	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	504	CLA	C4B-NB	-2.77	1.32	1.35
23	C	504	CLA	C1B-CHB	2.76	1.48	1.41
36	D	409	LHG	O7-C7	2.76	1.42	1.34
23	B	616	CLA	CHD-C4C	2.76	1.49	1.41
38	H	101	RRX	C5-C6	2.76	1.39	1.34
23	B	614	CLA	C1B-CHB	2.75	1.48	1.41
27	D	411	LMG	O8-C28	2.75	1.41	1.33
23	A	405	CLA	CHD-C4C	2.74	1.49	1.41
23	c	906	CLA	MG-NC	2.74	2.12	2.06
26	a	401	SQD	C6-S	-2.74	1.67	1.77
23	b	604	CLA	C4C-C3C	2.74	1.49	1.45
23	c	909	CLA	OBD-CAD	2.73	1.26	1.22
23	c	906	CLA	C1B-CHB	2.73	1.48	1.41
33	B	630	HTG	C1'-S1	-2.73	1.78	1.81
23	b	606	CLA	O2A-CGA	2.73	1.41	1.33
23	C	502	CLA	C1C-NC	-2.72	1.33	1.37
34	c	919	DGD	O2G-C1B	2.72	1.42	1.34
23	d	402	CLA	C4B-CHC	2.72	1.48	1.41
23	b	612	CLA	C4C-C3C	2.72	1.49	1.45
23	b	609	CLA	O2A-CGA	2.72	1.41	1.33
23	A	410	CLA	C4C-C3C	2.72	1.49	1.45
23	b	605	CLA	C1D-C2D	2.72	1.48	1.42
23	a	414	CLA	C1D-C2D	2.71	1.48	1.42
33	C	521	HTG	C1'-S1	-2.71	1.78	1.81
24	A	409	PHO	C3D-C2D	2.70	1.46	1.39
23	A	405	CLA	C1B-CHB	2.69	1.48	1.41
24	a	413	PHO	CHC-C4B	2.68	1.46	1.40
33	O	303	HTG	O5-C1	2.68	1.46	1.42
30	B	623	LMT	O1'-C1'	2.67	1.44	1.40
23	B	614	CLA	C3B-C2B	2.67	1.44	1.40
23	B	616	CLA	C1D-C2D	2.67	1.48	1.42
24	a	412	PHO	OBD-CAD	2.67	1.27	1.22
23	b	605	CLA	C4C-C3C	2.67	1.49	1.45
23	B	613	CLA	CHD-C4C	2.67	1.48	1.41
25	D	404	BCR	C5-C6	2.67	1.39	1.34
23	B	614	CLA	O2A-CGA	2.66	1.41	1.33
23	b	610	CLA	O2A-CGA	2.66	1.41	1.33
30	Z	102	LMT	O1'-C1'	2.66	1.44	1.40
28	A	414	PL9	C2-C3	2.66	1.41	1.34
23	b	609	CLA	C1B-CHB	2.66	1.48	1.41
23	c	911	CLA	C1B-CHB	2.66	1.48	1.41
23	b	618	CLA	MG-NC	2.65	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	914	CLA	C1C-C2C	2.65	1.49	1.44
23	C	507	CLA	C4C-C3C	2.65	1.49	1.45
23	b	611	CLA	O2A-CGA	2.65	1.41	1.33
23	C	509	CLA	C4C-C3C	2.65	1.49	1.45
23	C	511	CLA	MG-NC	2.65	2.12	2.06
23	b	605	CLA	C1B-CHB	2.65	1.48	1.41
23	C	501	CLA	C1D-C2D	2.65	1.48	1.42
23	C	505	CLA	C4B-CHC	2.65	1.48	1.41
23	c	908	CLA	C4B-NB	-2.64	1.32	1.35
23	C	510	CLA	C1B-CHB	2.64	1.48	1.41
23	b	618	CLA	O2A-CGA	2.64	1.41	1.33
23	c	903	CLA	C1C-NC	-2.63	1.33	1.37
23	B	614	CLA	O2D-CGD	2.63	1.39	1.33
23	B	608	CLA	CHD-C4C	2.63	1.48	1.41
36	d	408	LHG	O7-C7	2.63	1.41	1.34
23	B	608	CLA	C4B-NB	2.63	1.37	1.35
23	c	905	CLA	C1B-NB	-2.62	1.32	1.35
33	O	303	HTG	C1'-S1	-2.62	1.78	1.81
23	b	617	CLA	MG-NC	2.62	2.12	2.06
23	c	909	CLA	C1C-C2C	2.62	1.49	1.44
23	C	512	CLA	CHD-C4C	2.62	1.48	1.41
23	C	511	CLA	CHD-C4C	2.62	1.48	1.41
23	c	907	CLA	CHD-C4C	2.62	1.48	1.41
23	a	409	CLA	C1D-C2D	2.62	1.48	1.42
23	b	619	CLA	C1B-CHB	2.62	1.48	1.41
23	C	501	CLA	CHD-C4C	2.61	1.48	1.41
36	l	101	LHG	O7-C7	2.61	1.41	1.34
23	C	503	CLA	C1D-C2D	2.61	1.48	1.42
23	B	609	CLA	OBD-CAD	2.61	1.25	1.22
23	b	609	CLA	C1C-NC	-2.61	1.33	1.37
23	c	914	CLA	CHD-C4C	2.61	1.48	1.41
23	b	619	CLA	C4B-CHC	2.61	1.48	1.41
23	c	910	CLA	C1C-NC	-2.60	1.33	1.37
23	C	503	CLA	C4B-CHC	2.59	1.48	1.41
27	d	410	LMG	O7-C8	-2.59	1.40	1.46
23	c	912	CLA	CHD-C4C	2.59	1.48	1.41
23	b	611	CLA	C1B-CHB	2.59	1.48	1.41
34	c	918	DGD	O2G-C2G	-2.59	1.40	1.46
23	c	907	CLA	C1C-NC	-2.59	1.33	1.37
30	b	624	LMT	O1'-C1'	2.58	1.44	1.40
23	C	507	CLA	C4B-CHC	2.58	1.48	1.41
23	C	503	CLA	C1C-C2C	2.58	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	403	CLA	C4B-CHC	2.58	1.48	1.41
23	A	407	CLA	O2A-CGA	2.58	1.40	1.33
38	H	101	RRX	C1-C6	2.58	1.57	1.53
23	a	410	CLA	C1-C2	2.57	1.56	1.49
33	b	626	HTG	C1'-S1	-2.57	1.78	1.81
23	C	503	CLA	C4C-C3C	2.57	1.49	1.45
23	d	402	CLA	C1D-C2D	2.57	1.48	1.42
23	B	609	CLA	C1B-NB	2.56	1.37	1.35
23	a	411	CLA	C4C-C3C	2.56	1.49	1.45
30	c	922	LMT	O1'-C1'	2.55	1.44	1.40
23	C	506	CLA	C4B-CHC	2.55	1.48	1.41
28	D	405	PL9	C41-C39	2.55	1.56	1.51
25	a	415	BCR	C27-C26	2.55	1.56	1.51
24	A	408	PHO	CHD-C1D	2.55	1.43	1.38
23	C	509	CLA	C4B-NB	-2.55	1.32	1.35
24	a	413	PHO	C4C-C3C	2.55	1.49	1.45
23	b	608	CLA	C3D-C2D	2.55	1.44	1.39
24	A	409	PHO	C3D-C4D	-2.54	1.35	1.43
24	a	413	PHO	C3B-C4B	2.54	1.48	1.43
23	b	604	CLA	CHD-C4C	2.54	1.48	1.41
36	d	408	LHG	O8-C23	2.54	1.40	1.33
25	t	101	BCR	C23-C22	2.54	1.51	1.45
23	b	617	CLA	C4B-CHC	2.54	1.48	1.41
33	B	625	HTG	C1'-S1	-2.53	1.78	1.81
23	C	502	CLA	C1B-CHB	2.52	1.48	1.41
23	c	904	CLA	C4B-CHC	2.52	1.48	1.41
33	b	601	HTG	C1-S1	-2.51	1.76	1.80
24	a	412	PHO	CMA-C3A	2.51	1.58	1.53
23	b	612	CLA	C1B-CHB	2.51	1.48	1.41
23	b	616	CLA	C4C-C3C	2.51	1.49	1.45
23	C	510	CLA	C4C-C3C	2.51	1.49	1.45
37	f	101	HEM	CAD-C3D	2.51	1.56	1.52
23	C	511	CLA	C1C-NC	-2.50	1.34	1.37
37	v	201	HEM	CAA-C2A	2.50	1.55	1.52
33	b	627	HTG	C1-S1	-2.50	1.76	1.80
23	b	607	CLA	C1B-CHB	2.49	1.47	1.41
23	B	613	CLA	C1B-CHB	2.49	1.47	1.41
23	b	607	CLA	C1C-NC	-2.49	1.34	1.37
23	c	909	CLA	C1B-CHB	2.48	1.47	1.41
23	a	410	CLA	CHD-C4C	2.48	1.48	1.41
23	c	914	CLA	C4B-CHC	2.47	1.47	1.41
23	b	609	CLA	C1C-C2C	2.47	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	513	CLA	CHD-C4C	2.47	1.48	1.41
23	a	410	CLA	O2D-CGD	2.47	1.39	1.33
23	c	911	CLA	CHD-C4C	2.47	1.48	1.41
23	B	617	CLA	C4C-C3C	2.47	1.49	1.45
23	b	613	CLA	O2A-CGA	2.46	1.40	1.33
37	F	101	HEM	CAD-C3D	2.46	1.56	1.52
34	C	518	DGD	O2G-C1B	2.46	1.41	1.34
23	c	908	CLA	CHD-C4C	2.46	1.48	1.41
23	b	617	CLA	CHD-C4C	2.46	1.48	1.41
23	C	508	CLA	C4B-CHC	2.46	1.47	1.41
28	D	405	PL9	C18-C19	2.46	1.38	1.33
23	C	505	CLA	C1B-CHB	2.46	1.47	1.41
23	C	513	CLA	C4B-CHC	2.46	1.47	1.41
23	c	902	CLA	MG-NC	2.46	2.12	2.06
23	c	914	CLA	C4C-C3C	2.45	1.49	1.45
25	D	404	BCR	C30-C25	-2.45	1.50	1.53
23	a	409	CLA	C1B-NB	2.45	1.37	1.35
23	B	612	CLA	C4C-C3C	2.44	1.49	1.45
23	B	608	CLA	C4C-C3C	2.44	1.49	1.45
25	B	620	BCR	C23-C22	2.44	1.51	1.45
36	d	407	LHG	O7-C7	2.44	1.41	1.34
23	C	507	CLA	C1B-CHB	2.44	1.47	1.41
30	z	101	LMT	O1'-C1'	2.44	1.44	1.40
23	C	508	CLA	OBD-CAD	2.43	1.25	1.22
23	B	602	CLA	C4C-C3C	2.43	1.49	1.45
28	a	419	PL9	C2-C3	2.42	1.41	1.34
23	C	503	CLA	CHD-C4C	2.42	1.48	1.41
23	A	406	CLA	O2D-CGD	2.42	1.39	1.33
28	d	405	PL9	C21-C19	2.42	1.56	1.51
23	B	611	CLA	C4C-C3C	2.42	1.49	1.45
23	B	607	CLA	C1B-CHB	2.41	1.47	1.41
23	c	909	CLA	C1D-C2D	2.41	1.48	1.42
23	C	508	CLA	CHD-C4C	2.41	1.48	1.41
34	c	918	DGD	O5D-C1E	2.41	1.44	1.40
23	b	610	CLA	C1B-CHB	2.40	1.47	1.41
23	a	411	CLA	C1D-C2D	2.40	1.48	1.42
23	B	607	CLA	C1B-NB	2.40	1.37	1.35
23	c	911	CLA	C4B-CHC	2.40	1.47	1.41
34	c	919	DGD	O5D-C1E	2.40	1.44	1.40
23	c	908	CLA	C1C-NC	-2.39	1.34	1.37
23	c	903	CLA	C4C-C3C	2.39	1.49	1.45
23	B	609	CLA	CHD-C4C	2.39	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	609	CLA	C1D-C2D	2.38	1.48	1.42
23	c	909	CLA	C4B-CHC	2.38	1.47	1.41
23	D	402	CLA	C4B-NB	-2.38	1.33	1.35
23	b	613	CLA	C4B-CHC	2.38	1.47	1.41
23	B	608	CLA	C1C-NC	-2.38	1.34	1.37
23	b	609	CLA	C4B-CHC	2.38	1.47	1.41
23	b	611	CLA	C4B-CHC	2.38	1.47	1.41
25	D	404	BCR	C12-C13	2.38	1.51	1.45
23	B	613	CLA	C1D-C2D	2.38	1.47	1.42
23	B	611	CLA	C1B-CHB	2.38	1.47	1.41
23	C	507	CLA	CHD-C4C	2.38	1.47	1.41
23	b	607	CLA	OBD-CAD	2.37	1.25	1.22
23	B	603	CLA	C3B-CAB	2.37	1.52	1.47
23	b	613	CLA	CHD-C4C	2.37	1.47	1.41
34	d	406	DGD	O3G-C1D	2.37	1.44	1.40
23	b	609	CLA	CHD-C4C	2.37	1.47	1.41
34	c	919	DGD	O4D-C4D	2.37	1.48	1.43
33	B	631	HTG	C1'-S1	-2.36	1.78	1.81
23	B	612	CLA	C1D-C2D	2.36	1.47	1.42
23	B	603	CLA	CHD-C4C	2.36	1.47	1.41
23	c	914	CLA	C1D-C2D	2.36	1.47	1.42
23	A	406	CLA	C4C-C3C	2.35	1.49	1.45
26	A	418	SQD	C6-S	-2.35	1.68	1.77
25	C	515	BCR	C1-C6	-2.35	1.50	1.53
23	c	906	CLA	C1B-NB	-2.35	1.33	1.35
23	B	602	CLA	C1C-C2C	2.35	1.49	1.44
23	d	403	CLA	C1B-CHB	2.35	1.47	1.41
23	B	613	CLA	O2A-CGA	2.34	1.40	1.33
23	B	605	CLA	C1D-C2D	2.34	1.47	1.42
25	d	404	BCR	C12-C13	2.34	1.51	1.45
23	A	406	CLA	C1-C2	2.34	1.56	1.49
23	A	407	CLA	C1D-C2D	2.34	1.47	1.42
23	D	402	CLA	C4B-CHC	2.33	1.47	1.41
23	d	403	CLA	C1C-NC	-2.33	1.34	1.37
23	c	910	CLA	C4B-NB	2.33	1.37	1.35
25	B	619	BCR	C24-C25	2.33	1.53	1.45
23	b	611	CLA	CHD-C4C	2.32	1.47	1.41
28	D	405	PL9	C22-C23	2.32	1.58	1.50
25	b	620	BCR	C23-C22	2.32	1.50	1.45
23	b	618	CLA	C4C-C3C	2.32	1.49	1.45
23	B	613	CLA	C4B-CHC	2.31	1.47	1.41
23	c	910	CLA	C1B-CHB	2.31	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	614	CLA	C4B-CHC	2.31	1.47	1.41
23	B	612	CLA	O2A-CGA	2.30	1.40	1.33
23	c	902	CLA	C1D-C2D	2.30	1.47	1.42
23	B	602	CLA	C1B-CHB	2.30	1.47	1.41
23	c	904	CLA	CHD-C4C	2.30	1.47	1.41
25	b	621	BCR	C24-C25	2.29	1.53	1.45
25	d	404	BCR	C33-C5	2.29	1.54	1.50
24	A	408	PHO	C3D-C4D	-2.29	1.36	1.43
23	B	614	CLA	MG-NC	2.29	2.11	2.06
23	B	603	CLA	C4B-CHC	2.29	1.47	1.41
23	d	402	CLA	O2D-CGD	2.29	1.38	1.33
23	B	608	CLA	C4B-CHC	2.29	1.47	1.41
23	c	908	CLA	C4C-C3C	2.29	1.49	1.45
23	c	910	CLA	C4C-C3C	2.29	1.49	1.45
23	c	911	CLA	C1D-C2D	2.28	1.47	1.42
26	f	102	SQD	O47-C45	-2.28	1.44	1.46
23	c	906	CLA	C4B-CHC	2.28	1.47	1.41
23	b	610	CLA	OBD-CAD	2.28	1.25	1.22
23	b	616	CLA	C4B-CHC	2.28	1.47	1.41
23	B	614	CLA	OBD-CAD	2.27	1.25	1.22
28	d	405	PL9	C43-C44	2.27	1.38	1.33
23	C	506	CLA	CHD-C4C	2.27	1.47	1.41
23	b	618	CLA	C4B-NB	2.27	1.37	1.35
23	b	604	CLA	C1D-C2D	2.27	1.47	1.42
23	B	613	CLA	C4C-C3C	2.26	1.48	1.45
28	D	405	PL9	C2-C1	-2.26	1.38	1.44
23	C	508	CLA	C1C-C2C	2.26	1.48	1.44
23	b	618	CLA	C1D-C2D	2.26	1.47	1.42
23	B	616	CLA	C1B-CHB	2.26	1.47	1.41
23	c	913	CLA	CHD-C4C	2.26	1.47	1.41
27	c	920	LMG	O3-C3	2.26	1.48	1.43
23	c	910	CLA	C1C-C2C	2.26	1.48	1.44
23	c	913	CLA	C1D-C2D	2.26	1.47	1.42
23	B	610	CLA	O2D-CGD	2.25	1.38	1.33
23	b	606	CLA	C1B-NB	-2.25	1.33	1.35
23	C	505	CLA	CHD-C4C	2.25	1.47	1.41
27	Z	101	LMG	O1-C1	2.25	1.44	1.40
25	B	618	BCR	C30-C25	2.25	1.56	1.53
23	c	912	CLA	C4C-C3C	2.24	1.48	1.45
23	C	512	CLA	C1C-C2C	2.24	1.48	1.44
23	B	617	CLA	C1D-C2D	2.24	1.47	1.42
25	b	622	BCR	C26-C25	2.23	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	613	CLA	C1B-CHB	2.23	1.47	1.41
23	b	615	CLA	C1B-CHB	2.23	1.47	1.41
23	B	609	CLA	C1B-CHB	2.23	1.47	1.41
27	C	519	LMG	O7-C8	-2.23	1.41	1.46
23	C	501	CLA	C1C-C2C	2.23	1.48	1.44
23	b	608	CLA	C1B-NB	-2.23	1.33	1.35
34	C	516	DGD	O5D-C1E	2.23	1.44	1.40
24	A	409	PHO	C4D-CHA	2.22	1.49	1.43
25	c	916	BCR	C12-C13	2.22	1.50	1.45
23	C	511	CLA	C4C-C3C	2.22	1.48	1.45
23	C	509	CLA	MG-NC	2.22	2.11	2.06
28	d	405	PL9	C18-C19	2.22	1.38	1.33
23	c	908	CLA	C1D-C2D	2.22	1.47	1.42
23	c	902	CLA	C4B-CHC	2.21	1.47	1.41
23	B	605	CLA	CHD-C4C	2.21	1.47	1.41
23	b	614	CLA	CHD-C4C	2.21	1.47	1.41
23	b	611	CLA	C1D-C2D	2.21	1.47	1.42
23	b	614	CLA	OBD-CAD	2.21	1.25	1.22
23	b	607	CLA	O2A-CGA	2.21	1.39	1.33
24	a	413	PHO	C4D-ND	2.21	1.41	1.36
23	d	402	CLA	C1C-NC	-2.21	1.34	1.37
27	c	921	LMG	O1-C1	2.21	1.44	1.40
23	D	403	CLA	CHD-C4C	2.21	1.47	1.41
23	B	602	CLA	CHD-C4C	2.21	1.47	1.41
23	d	402	CLA	OBD-CAD	2.21	1.25	1.22
23	A	405	CLA	C4C-C3C	2.21	1.48	1.45
23	C	501	CLA	C4C-C3C	2.20	1.48	1.45
25	B	619	BCR	C5-C6	2.20	1.38	1.34
33	u	201	HTG	C1'-S1	-2.20	1.78	1.81
23	B	617	CLA	C4B-CHC	2.20	1.47	1.41
23	c	912	CLA	C1D-C2D	2.20	1.47	1.42
23	B	603	CLA	C1B-NB	-2.20	1.33	1.35
23	b	611	CLA	C1B-NB	-2.20	1.33	1.35
37	F	101	HEM	C4D-C3D	2.20	1.47	1.42
23	c	904	CLA	C1D-C2D	2.19	1.47	1.42
27	c	920	LMG	O1-C1	2.19	1.43	1.40
23	c	906	CLA	C4B-NB	-2.19	1.33	1.35
30	m	102	LMT	O1'-C1'	2.19	1.43	1.40
23	d	403	CLA	C1C-C2C	2.19	1.48	1.44
23	b	606	CLA	MG-NC	-2.19	2.01	2.06
23	c	906	CLA	C1D-C2D	2.19	1.47	1.42
37	V	201	HEM	CMC-C2C	2.18	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	C	522	HTG	O5-C1	2.18	1.45	1.42
23	c	907	CLA	C1D-C2D	2.18	1.47	1.42
24	a	413	PHO	CHD-C4C	2.17	1.45	1.40
37	V	201	HEM	C1B-C2B	2.17	1.47	1.42
23	c	904	CLA	C1C-C2C	2.17	1.48	1.44
23	B	610	CLA	C1D-C2D	2.17	1.47	1.42
25	K	102	BCR	C12-C13	2.17	1.50	1.45
23	C	503	CLA	OBD-CAD	2.17	1.25	1.22
23	C	513	CLA	C1D-C2D	2.16	1.47	1.42
23	b	617	CLA	C4C-C3C	2.16	1.48	1.45
33	d	401	HTG	C1-S1	-2.16	1.77	1.80
23	c	908	CLA	C1A-CHA	2.16	1.52	1.43
23	c	907	CLA	C1B-CHB	2.16	1.47	1.41
23	B	617	CLA	C4B-NB	-2.16	1.33	1.35
33	b	602	HTG	C1'-S1	-2.16	1.78	1.81
23	c	902	CLA	CHD-C4C	2.16	1.47	1.41
23	b	615	CLA	C1D-C2D	2.15	1.47	1.42
37	V	201	HEM	C4A-NA	2.15	1.40	1.36
23	d	403	CLA	CHD-C4C	2.14	1.47	1.41
23	B	606	CLA	C4B-NB	-2.14	1.33	1.35
23	C	506	CLA	C1C-C2C	2.14	1.48	1.44
23	A	410	CLA	O2D-CGD	2.14	1.38	1.33
23	c	905	CLA	C1D-C2D	2.14	1.47	1.42
25	c	915	BCR	C12-C13	2.14	1.50	1.45
23	C	509	CLA	C1B-CHB	2.13	1.46	1.41
25	k	102	BCR	C12-C13	2.13	1.50	1.45
23	D	402	CLA	CHD-C4C	2.13	1.47	1.41
23	c	902	CLA	C1C-NC	-2.12	1.34	1.37
23	B	617	CLA	C1B-CHB	2.12	1.46	1.41
36	d	409	LHG	C4-C5	2.12	1.57	1.50
23	C	509	CLA	C4B-CHC	2.12	1.46	1.41
37	F	101	HEM	C4B-NB	2.12	1.40	1.36
37	F	101	HEM	CMA-C3A	2.12	1.56	1.51
30	C	520	LMT	O1'-C1'	2.12	1.43	1.40
23	C	501	CLA	C1B-CHB	2.12	1.46	1.41
37	v	201	HEM	C1D-ND	2.11	1.40	1.36
34	c	917	DGD	O2G-C1B	2.11	1.40	1.34
25	B	619	BCR	C23-C22	2.11	1.50	1.45
23	a	414	CLA	CHD-C4C	2.11	1.47	1.41
23	C	507	CLA	C1A-CHA	2.11	1.51	1.43
23	C	503	CLA	C1C-NC	-2.11	1.34	1.37
23	b	608	CLA	C1C-NC	-2.10	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	610	CLA	C1B-CHB	2.10	1.46	1.41
23	C	502	CLA	C4B-CHC	2.10	1.46	1.41
23	a	410	CLA	C4C-C3C	2.10	1.48	1.45
23	b	609	CLA	C4C-C3C	2.09	1.48	1.45
23	b	614	CLA	MG-NC	2.09	2.11	2.06
26	D	407	SQD	O6-C1	2.09	1.43	1.40
23	B	615	CLA	C1D-C2D	2.09	1.47	1.42
23	a	411	CLA	C1B-CHB	2.09	1.46	1.41
25	d	404	BCR	C23-C22	2.08	1.50	1.45
23	A	406	CLA	CMC-C2C	2.08	1.55	1.50
24	A	408	PHO	C1C-NC	-2.08	1.34	1.38
23	b	610	CLA	C4B-CHC	2.08	1.46	1.41
30	F	102	LMT	O1'-C1'	2.08	1.43	1.40
23	B	617	CLA	C2-C3	2.08	1.38	1.33
23	c	905	CLA	C1C-C2C	2.08	1.48	1.44
23	b	614	CLA	C4B-NB	2.08	1.37	1.35
25	B	618	BCR	C5-C6	2.08	1.38	1.34
23	B	607	CLA	C1D-C2D	2.08	1.47	1.42
23	C	513	CLA	C1C-C2C	2.08	1.48	1.44
23	B	613	CLA	CMA-C3A	2.08	1.57	1.53
28	d	405	PL9	C2-C3	2.08	1.40	1.34
23	B	608	CLA	CMA-C3A	2.07	1.57	1.53
33	D	414	HTG	C1-S1	-2.07	1.77	1.80
23	C	511	CLA	C1A-CHA	2.07	1.51	1.43
33	B	631	HTG	O5-C1	2.06	1.45	1.42
23	b	612	CLA	C4B-CHC	2.06	1.46	1.41
34	c	919	DGD	O2D-C2D	2.06	1.47	1.43
34	c	917	DGD	C6E-C5E	2.06	1.58	1.51
23	b	615	CLA	C4B-CHC	2.06	1.46	1.41
23	b	619	CLA	MG-NC	2.06	2.11	2.06
28	d	405	PL9	C17-C18	2.06	1.57	1.50
25	t	101	BCR	C12-C13	2.05	1.50	1.45
23	c	913	CLA	C1C-C2C	2.05	1.48	1.44
23	a	414	CLA	C4C-C3C	2.05	1.48	1.45
23	a	409	CLA	C1C-NC	-2.05	1.34	1.37
37	f	101	HEM	C1C-C2C	2.05	1.47	1.42
26	B	621	SQD	C6-S	-2.05	1.69	1.77
23	b	611	CLA	CAA-C2A	2.05	1.57	1.54
23	B	612	CLA	C4B-CHC	2.05	1.46	1.41
25	B	618	BCR	C27-C26	2.05	1.55	1.51
23	C	506	CLA	C1D-C2D	2.04	1.47	1.42
23	c	911	CLA	C4C-C3C	2.04	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	615	CLA	C4C-C3C	2.04	1.48	1.45
25	B	619	BCR	C35-C13	2.04	1.55	1.50
23	A	405	CLA	CMC-C2C	2.04	1.55	1.50
23	b	616	CLA	C1-C2	2.04	1.55	1.49
23	B	609	CLA	C4C-C3C	2.04	1.48	1.45
23	A	407	CLA	C3B-C2B	2.04	1.43	1.40
25	k	102	BCR	C8-C9	2.03	1.50	1.45
23	b	608	CLA	C3B-CAB	2.03	1.52	1.47
34	C	518	DGD	O2G-C2G	-2.03	1.41	1.46
23	b	615	CLA	C3B-C2B	2.03	1.43	1.40
23	b	606	CLA	C1B-CHB	2.03	1.46	1.41
23	B	614	CLA	CHD-C4C	2.03	1.46	1.41
23	a	410	CLA	C1B-CHB	2.03	1.46	1.41
24	A	409	PHO	C1C-NC	-2.03	1.34	1.38
23	b	612	CLA	O2D-CED	-2.02	1.40	1.45
28	D	405	PL9	C36-C37	-2.02	1.46	1.53
23	C	512	CLA	C1D-C2D	2.02	1.47	1.42
23	C	510	CLA	CHD-C4C	2.02	1.46	1.41
25	b	622	BCR	C12-C13	2.02	1.50	1.45
23	C	504	CLA	C1D-C2D	2.02	1.47	1.42
23	A	405	CLA	C1D-C2D	2.01	1.47	1.42
23	B	612	CLA	C4B-NB	2.01	1.37	1.35
23	B	604	CLA	CHD-C4C	2.01	1.46	1.41
25	B	618	BCR	C15-C14	2.01	1.49	1.43
23	B	606	CLA	C4C-C3C	2.01	1.48	1.45
33	C	521	HTG	C1-S1	-2.00	1.77	1.80
28	d	405	PL9	C13-C14	2.00	1.37	1.33
37	V	201	HEM	CAA-C2A	2.00	1.55	1.52

All (2148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	511	CLA	C4A-NA-C1A	13.25	112.67	106.71
23	b	609	CLA	C4A-NA-C1A	11.92	112.06	106.71
23	c	904	CLA	C4A-NA-C1A	10.61	111.48	106.71
23	C	501	CLA	O2D-CGD-O1D	-10.49	103.33	123.84
23	c	902	CLA	C4A-NA-C1A	10.12	111.25	106.71
23	C	507	CLA	C4A-NA-C1A	10.07	111.23	106.71
23	B	602	CLA	C4A-NA-C1A	10.06	111.23	106.71
23	c	912	CLA	C4A-NA-C1A	10.03	111.22	106.71
23	c	909	CLA	C4A-NA-C1A	9.78	111.10	106.71
23	b	607	CLA	C4A-NA-C1A	9.75	111.09	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	513	CLA	C4A-NA-C1A	9.58	111.01	106.71
23	B	607	CLA	C4A-NA-C1A	9.32	110.90	106.71
23	B	616	CLA	C4A-NA-C1A	8.86	110.69	106.71
23	b	613	CLA	C4A-NA-C1A	8.83	110.67	106.71
23	c	905	CLA	C4A-NA-C1A	8.74	110.64	106.71
23	C	501	CLA	O2D-CGD-CBD	8.50	126.37	111.27
23	b	617	CLA	C4A-NA-C1A	8.48	110.52	106.71
23	b	615	CLA	CAC-C3C-C4C	8.41	135.72	124.81
26	a	416	SQD	O6-C1-C2	8.27	121.21	108.30
26	a	416	SQD	O9-S-C6	8.18	116.66	106.94
23	c	908	CLA	C4A-NA-C1A	8.09	110.34	106.71
23	B	604	CLA	C2C-C1C-NC	8.08	117.54	109.97
23	A	406	CLA	C2C-C1C-NC	8.07	117.53	109.97
23	b	604	CLA	C4A-NA-C1A	8.04	110.32	106.71
23	C	510	CLA	C4A-NA-C1A	8.01	110.31	106.71
23	b	614	CLA	C4A-NA-C1A	7.99	110.30	106.71
26	D	407	SQD	O6-C1-C2	7.96	120.72	108.30
23	B	605	CLA	C2C-C1C-NC	7.88	117.35	109.97
23	b	615	CLA	C4A-NA-C1A	7.86	110.24	106.71
23	a	414	CLA	C2C-C1C-NC	7.79	117.27	109.97
23	C	509	CLA	C4A-NA-C1A	7.77	110.20	106.71
37	F	101	HEM	CBD-CAD-C3D	-7.61	98.46	112.48
33	B	631	HTG	C1'-S1-C1	7.59	114.28	100.09
23	B	609	CLA	C2C-C1C-NC	7.57	117.07	109.97
33	C	522	HTG	C1'-S1-C1	7.45	114.03	100.09
23	c	910	CLA	C4A-NA-C1A	7.38	110.03	106.71
23	d	402	CLA	C2C-C1C-NC	7.36	116.87	109.97
23	D	403	CLA	C4A-NA-C1A	7.26	109.97	106.71
23	a	411	CLA	C2C-C1C-NC	7.22	116.73	109.97
23	b	608	CLA	C2C-C1C-NC	7.19	116.71	109.97
23	b	606	CLA	C2C-C1C-NC	7.15	116.67	109.97
23	c	907	CLA	CHD-C4C-C3C	-7.14	114.33	124.84
26	B	621	SQD	O6-C1-C2	7.11	119.41	108.30
33	B	626	HTG	C1'-S1-C1	7.10	113.37	100.09
23	C	504	CLA	C2C-C1C-NC	7.04	116.57	109.97
23	b	618	CLA	C4A-NA-C1A	7.01	109.86	106.71
26	A	412	SQD	O6-C1-C2	6.95	119.16	108.30
23	b	608	CLA	CAC-C3C-C4C	6.94	133.82	124.81
23	C	509	CLA	C2C-C1C-NC	6.94	116.48	109.97
23	a	409	CLA	CAC-C3C-C4C	6.93	133.80	124.81
23	b	619	CLA	CHD-C4C-C3C	-6.84	114.78	124.84
23	c	913	CLA	C4A-NA-C1A	6.82	109.77	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	502	CLA	CHD-C4C-C3C	-6.81	114.83	124.84
23	c	903	CLA	C4A-NA-C1A	6.78	109.76	106.71
24	a	413	PHO	CMD-C2D-C1D	6.76	135.48	125.06
24	A	409	PHO	CMD-C2D-C1D	6.76	135.47	125.06
23	B	612	CLA	C2C-C1C-NC	6.73	116.28	109.97
23	C	505	CLA	C2C-C1C-NC	6.71	116.25	109.97
33	V	202	HTG	O5-C1-C2	-6.66	101.94	110.31
33	c	924	HTG	C1'-S1-C1	6.62	112.47	100.09
23	B	604	CLA	CHD-C4C-C3C	-6.60	115.14	124.84
24	A	408	PHO	C3D-C2D-C1D	-6.59	96.27	105.87
23	C	512	CLA	C4A-NA-C1A	6.56	109.66	106.71
23	b	616	CLA	C4A-NA-C1A	6.56	109.66	106.71
23	b	607	CLA	C2C-C1C-NC	6.52	116.08	109.97
23	B	606	CLA	C2C-C1C-NC	6.51	116.07	109.97
23	C	506	CLA	C2C-C1C-NC	6.50	116.07	109.97
23	A	410	CLA	C2C-C1C-NC	6.45	116.01	109.97
23	A	406	CLA	C4A-NA-C1A	-6.42	103.82	106.71
23	B	612	CLA	CHD-C4C-C3C	-6.42	115.40	124.84
23	c	906	CLA	C4A-NA-C1A	6.42	109.59	106.71
33	b	627	HTG	C1'-S1-C1	6.41	112.07	100.09
33	c	923	HTG	C1'-S1-C1	6.35	111.96	100.09
26	L	103	SQD	O7-S-C6	6.33	114.47	106.94
23	b	616	CLA	C2C-C1C-NC	6.33	115.90	109.97
24	A	408	PHO	CMD-C2D-C1D	6.32	134.79	125.06
23	C	510	CLA	CHD-C4C-C3C	-6.28	115.60	124.84
23	c	908	CLA	O2D-CGD-CBD	6.26	122.39	111.27
23	C	506	CLA	CHD-C4C-C3C	-6.26	115.64	124.84
23	b	617	CLA	O2D-CGD-CBD	6.25	122.38	111.27
34	D	406	DGD	O2G-C1B-C2B	6.25	124.96	111.50
23	C	508	CLA	C4A-NA-C1A	6.24	109.51	106.71
23	b	619	CLA	O2D-CGD-CBD	6.19	122.28	111.27
23	B	604	CLA	C1C-C2C-C3C	-6.16	100.48	106.96
23	a	411	CLA	CAC-C3C-C4C	6.11	132.73	124.81
23	B	602	CLA	O2D-CGD-CBD	6.10	122.12	111.27
33	u	201	HTG	C1'-S1-C1	6.10	111.51	100.09
23	c	910	CLA	C4D-C3D-CAD	6.10	111.87	108.47
23	A	407	CLA	CAC-C3C-C4C	6.09	132.71	124.81
23	B	612	CLA	C4A-NA-C1A	6.08	109.44	106.71
23	B	611	CLA	C4A-NA-C1A	6.08	109.44	106.71
23	B	616	CLA	C2C-C1C-NC	6.04	115.63	109.97
23	B	607	CLA	CHD-C4C-C3C	-6.04	115.96	124.84
23	b	615	CLA	CHD-C4C-C3C	-6.04	115.97	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	607	CLA	C2C-C1C-NC	6.01	115.60	109.97
23	B	605	CLA	C1C-C2C-C3C	-6.00	100.65	106.96
23	a	414	CLA	CHD-C4C-C3C	-5.99	116.03	124.84
23	B	615	CLA	C4A-NA-C1A	5.99	109.40	106.71
23	A	407	CLA	C2C-C1C-NC	5.98	115.57	109.97
38	H	101	RRX	C24-C23-C22	-5.98	117.21	126.23
37	f	101	HEM	CBA-CAA-C2A	-5.97	101.48	112.49
23	B	615	CLA	CAC-C3C-C4C	5.96	132.54	124.81
23	C	501	CLA	C2C-C1C-NC	5.96	115.55	109.97
23	C	506	CLA	C4A-NA-C1A	5.95	109.38	106.71
23	c	908	CLA	CHD-C4C-C3C	-5.92	116.14	124.84
23	A	406	CLA	C1C-C2C-C3C	-5.91	100.75	106.96
23	C	504	CLA	C1C-C2C-C3C	-5.88	100.78	106.96
23	b	604	CLA	O2D-CGD-CBD	5.88	121.71	111.27
23	B	613	CLA	C4A-NA-C1A	5.87	109.34	106.71
24	A	409	PHO	C3D-C2D-C1D	-5.87	97.32	105.87
23	a	410	CLA	C2C-C1C-NC	5.86	115.46	109.97
23	B	613	CLA	CAC-C3C-C4C	5.86	132.41	124.81
26	A	412	SQD	O9-S-C6	5.85	113.89	106.94
23	B	602	CLA	CHD-C4C-C3C	-5.84	116.25	124.84
23	C	504	CLA	C4A-NA-C1A	5.84	109.33	106.71
23	D	402	CLA	C2C-C1C-NC	5.84	115.44	109.97
24	A	408	PHO	C2D-C1D-ND	5.84	118.60	109.79
23	B	617	CLA	C2C-C1C-NC	5.83	115.44	109.97
23	B	604	CLA	C4A-NA-C1A	5.83	109.33	106.71
23	a	410	CLA	CHD-C4C-C3C	-5.83	116.27	124.84
37	f	101	HEM	CBD-CAD-C3D	-5.82	101.75	112.48
23	b	612	CLA	C2C-C1C-NC	5.80	115.40	109.97
23	a	414	CLA	CAC-C3C-C4C	5.80	132.33	124.81
23	A	406	CLA	CAC-C3C-C4C	5.77	132.30	124.81
23	C	506	CLA	O2D-CGD-CBD	5.75	121.49	111.27
23	B	617	CLA	CHD-C4C-C3C	-5.75	116.39	124.84
23	B	610	CLA	C2C-C1C-NC	5.74	115.35	109.97
33	c	924	HTG	C1-O5-C5	5.74	123.17	112.58
23	b	618	CLA	C2C-C1C-NC	5.74	115.35	109.97
33	V	202	HTG	C1-O5-C5	-5.72	102.03	112.58
26	A	412	SQD	C1-C2-C3	-5.72	98.09	110.00
37	V	201	HEM	CBD-CAD-C3D	-5.70	101.97	112.48
33	C	522	HTG	C1-O5-C5	5.65	123.00	112.58
23	b	606	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
23	b	618	CLA	CMD-C2D-C3D	5.64	135.22	124.68
24	a	413	PHO	O2D-CGD-CBD	5.62	121.26	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	621	SQD	C1-O5-C5	-5.62	102.66	113.69
23	b	611	CLA	C2C-C1C-NC	5.60	115.22	109.97
23	A	405	CLA	CMD-C2D-C3D	5.60	135.16	124.68
25	C	515	BCR	C7-C8-C9	-5.57	117.81	126.23
23	B	609	CLA	O2D-CGD-CBD	5.57	121.17	111.27
33	V	202	HTG	C1-C2-C3	-5.56	99.60	110.59
23	c	908	CLA	C2C-C1C-NC	5.56	115.18	109.97
23	b	615	CLA	C3C-C4C-NC	5.55	116.80	110.57
27	a	418	LMG	O7-C10-C11	5.55	123.45	111.50
23	B	611	CLA	C2C-C1C-NC	5.54	115.16	109.97
26	B	621	SQD	O7-S-C6	5.54	113.52	106.94
23	c	912	CLA	C2C-C1C-NC	5.53	115.15	109.97
24	A	409	PHO	C4C-C3C-C2C	-5.52	100.67	106.78
26	a	416	SQD	C1-O5-C5	-5.52	102.85	113.69
33	C	521	HTG	C1'-S1-C1	5.50	110.37	100.09
23	c	903	CLA	CHD-C4C-C3C	-5.50	116.76	124.84
26	L	103	SQD	O6-C1-C2	5.49	116.88	108.30
23	c	902	CLA	C2C-C1C-NC	5.49	115.11	109.97
23	b	604	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
28	d	405	PL9	C40-C39-C41	5.47	124.48	115.27
26	A	412	SQD	O47-C7-C8	5.47	123.28	111.50
23	B	617	CLA	CAC-C3C-C4C	5.46	131.89	124.81
23	b	616	CLA	CAC-C3C-C4C	5.46	131.89	124.81
23	c	913	CLA	O2D-CGD-CBD	5.45	120.94	111.27
23	B	608	CLA	C2C-C1C-NC	5.45	115.07	109.97
23	b	613	CLA	C2C-C1C-NC	5.44	115.07	109.97
23	d	403	CLA	O2D-CGD-CBD	5.43	120.92	111.27
25	D	404	BCR	C7-C8-C9	-5.43	118.03	126.23
33	d	401	HTG	C1'-S1-C1	5.42	110.23	100.09
23	C	510	CLA	C2C-C1C-NC	5.40	115.03	109.97
23	A	410	CLA	C4-C3-C5	5.40	124.35	115.27
26	A	418	SQD	O9-S-C6	5.39	113.35	106.94
37	v	201	HEM	CBD-CAD-C3D	-5.39	102.56	112.48
26	A	412	SQD	C1-O5-C5	-5.39	103.12	113.69
23	b	605	CLA	CMB-C2B-C3B	5.38	134.75	124.68
26	a	401	SQD	C1-O5-C5	-5.37	103.15	113.69
24	A	408	PHO	C4C-C3C-C2C	-5.37	100.84	106.78
23	C	503	CLA	C2C-C1C-NC	5.36	115.00	109.97
23	B	610	CLA	C4A-NA-C1A	5.34	109.11	106.71
26	f	102	SQD	O47-C7-O49	-5.34	118.78	125.57
36	D	408	LHG	O8-C23-O10	-5.34	110.13	123.59
23	D	402	CLA	CHD-C4C-C3C	-5.32	117.01	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	402	CLA	CMD-C2D-C3D	5.32	134.63	124.68
23	b	619	CLA	C4A-NA-C1A	5.32	109.10	106.71
26	a	416	SQD	C1-C2-C3	-5.31	98.93	110.00
28	D	405	PL9	C40-C39-C41	5.30	124.19	115.27
23	b	605	CLA	CMD-C2D-C3D	5.30	134.59	124.68
23	d	402	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
23	B	610	CLA	CAC-C3C-C4C	5.29	131.68	124.81
23	c	903	CLA	O2D-CGD-CBD	5.28	120.66	111.27
24	A	408	PHO	C3C-C4C-NC	5.27	118.46	110.28
25	B	620	BCR	C38-C26-C25	-5.27	118.61	124.53
26	a	416	SQD	O47-C7-C8	5.27	122.85	111.50
23	b	612	CLA	CAC-C3C-C4C	5.25	131.63	124.81
27	B	622	LMG	O7-C10-C11	5.24	122.79	111.50
23	C	502	CLA	C2C-C1C-NC	5.24	114.88	109.97
23	c	902	CLA	C1C-C2C-C3C	-5.22	101.46	106.96
23	c	908	CLA	O2D-CGD-O1D	-5.22	113.64	123.84
23	c	912	CLA	CHD-C4C-C3C	-5.18	117.23	124.84
23	c	910	CLA	C2C-C1C-NC	5.17	114.82	109.97
23	B	609	CLA	C1C-C2C-C3C	-5.17	101.52	106.96
23	b	615	CLA	C2C-C1C-NC	5.16	114.81	109.97
23	a	409	CLA	C2C-C1C-NC	5.14	114.79	109.97
23	b	606	CLA	C1C-C2C-C3C	-5.13	101.56	106.96
24	a	413	PHO	C3D-C2D-C1D	-5.12	98.40	105.87
23	C	501	CLA	C4A-NA-C1A	5.12	109.01	106.71
23	b	618	CLA	C1C-C2C-C3C	-5.12	101.58	106.96
23	d	402	CLA	C1C-C2C-C3C	-5.11	101.59	106.96
33	B	630	HTG	C1'-S1-C1	5.08	109.60	100.09
23	c	907	CLA	CHD-C4C-NC	5.06	132.18	124.20
26	a	401	SQD	O6-C1-C2	5.06	116.20	108.30
30	C	520	LMT	O1B-C4'-C3'	5.06	120.73	107.28
23	C	511	CLA	C2C-C1C-NC	5.04	114.70	109.97
23	B	604	CLA	O2D-CGD-CBD	5.04	120.23	111.27
23	c	906	CLA	CHD-C4C-C3C	-5.04	117.43	124.84
23	A	406	CLA	CMD-C2D-C3D	5.04	134.11	124.68
23	B	615	CLA	C2C-C1C-NC	5.02	114.67	109.97
23	b	606	CLA	O2D-CGD-O1D	-5.01	114.03	123.84
30	a	402	LMT	C1'-O5'-C5'	5.01	123.53	113.69
24	a	412	PHO	C2C-C1C-NC	5.01	117.36	109.79
23	b	606	CLA	C4-C3-C5	5.01	123.69	115.27
24	A	408	PHO	C2C-C1C-NC	5.00	117.33	109.79
23	B	613	CLA	C2C-C1C-NC	5.00	114.65	109.97
23	A	410	CLA	CHD-C4C-C3C	-4.99	117.51	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	509	CLA	C1C-C2C-C3C	-4.98	101.72	106.96
23	C	502	CLA	CHD-C4C-NC	4.98	132.05	124.20
27	C	519	LMG	O1-C7-C8	-4.98	98.89	110.90
23	b	614	CLA	C2C-C1C-NC	4.98	114.63	109.97
24	A	409	PHO	CAC-C3C-C4C	4.97	130.64	125.22
24	a	412	PHO	C3D-C2D-C1D	-4.97	98.63	105.87
23	B	614	CLA	C2C-C1C-NC	4.97	114.63	109.97
24	a	412	PHO	CMD-C2D-C1D	4.96	132.70	125.06
23	B	616	CLA	CHD-C4C-C3C	-4.96	117.55	124.84
25	b	620	BCR	C33-C5-C6	-4.95	118.97	124.53
23	C	505	CLA	CHD-C4C-C3C	-4.95	117.57	124.84
26	L	103	SQD	O9-S-C6	4.94	112.81	106.94
23	d	403	CLA	C2C-C1C-NC	4.93	114.59	109.97
23	b	607	CLA	C1C-C2C-C3C	-4.93	101.77	106.96
23	c	905	CLA	C2C-C1C-NC	4.92	114.58	109.97
23	b	616	CLA	C1-C2-C3	-4.92	117.54	126.04
23	b	611	CLA	O2D-CGD-CBD	4.90	119.98	111.27
23	B	611	CLA	CHD-C4C-C3C	-4.90	117.64	124.84
23	B	609	CLA	C3B-C4B-NB	4.90	115.54	109.21
28	a	419	PL9	C7-C3-C4	4.89	120.85	116.88
24	a	412	PHO	O2D-CGD-CBD	4.89	119.95	111.27
23	b	608	CLA	C4-C3-C5	4.88	123.49	115.27
25	K	102	BCR	C11-C10-C9	-4.87	120.35	127.31
23	C	513	CLA	O2D-CGD-CBD	4.87	119.92	111.27
23	B	610	CLA	O2D-CGD-O1D	-4.86	114.33	123.84
23	b	610	CLA	CHD-C4C-C3C	-4.86	117.70	124.84
23	b	616	CLA	CHD-C4C-C3C	-4.85	117.71	124.84
23	c	906	CLA	O2D-CGD-O1D	-4.84	114.38	123.84
23	B	614	CLA	CHD-C4C-C3C	-4.84	117.73	124.84
23	b	611	CLA	C1C-C2C-C3C	-4.83	101.88	106.96
23	D	402	CLA	C1B-CHB-C4A	-4.83	120.56	130.12
24	a	413	PHO	O2D-CGD-O1D	-4.83	114.40	123.84
23	C	503	CLA	CHD-C4C-C3C	-4.82	117.76	124.84
23	A	405	CLA	C1D-CHD-C4C	-4.82	116.20	122.56
27	Z	101	LMG	O7-C10-C11	4.82	121.88	111.50
23	b	608	CLA	CHD-C4C-C3C	-4.82	117.76	124.84
23	a	411	CLA	C1C-C2C-C3C	-4.81	101.89	106.96
23	b	617	CLA	O2D-CGD-O1D	-4.81	114.43	123.84
23	b	615	CLA	C4C-C3C-C2C	-4.80	99.90	106.90
23	B	602	CLA	C2C-C1C-NC	4.79	114.46	109.97
23	B	609	CLA	CHD-C4C-C3C	-4.79	117.80	124.84
23	B	611	CLA	CHB-C4A-NA	4.79	131.13	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	407	CLA	O2D-CGD-CBD	4.79	119.77	111.27
23	B	605	CLA	C3C-C4C-NC	4.78	115.94	110.57
23	c	910	CLA	CHD-C4C-C3C	-4.78	117.81	124.84
23	B	604	CLA	C3B-C4B-NB	4.77	115.37	109.21
23	a	411	CLA	C3C-C4C-NC	4.76	115.91	110.57
23	B	612	CLA	O2D-CGD-CBD	4.76	119.73	111.27
24	a	412	PHO	O2D-CGD-O1D	-4.75	114.55	123.84
23	b	607	CLA	CAC-C3C-C4C	4.75	130.97	124.81
33	c	924	HTG	O5-C5-C4	4.75	118.31	109.69
23	c	914	CLA	C4A-NA-C1A	4.74	108.84	106.71
23	B	610	CLA	CHD-C4C-C3C	-4.74	117.88	124.84
23	c	906	CLA	C2C-C1C-NC	4.74	114.41	109.97
23	b	608	CLA	C3C-C4C-NC	4.73	115.88	110.57
24	A	409	PHO	C2D-C1D-ND	4.73	116.92	109.79
23	c	912	CLA	C1C-C2C-C3C	-4.72	101.99	106.96
23	A	405	CLA	CAC-C3C-C4C	4.71	130.93	124.81
23	C	510	CLA	CHD-C4C-NC	4.71	131.63	124.20
23	B	610	CLA	CMD-C2D-C3D	4.71	133.49	124.68
23	A	407	CLA	C1C-C2C-C3C	-4.71	102.01	106.96
23	c	902	CLA	O2D-CGD-O1D	-4.70	114.64	123.84
23	b	618	CLA	C1D-CHD-C4C	-4.69	116.37	122.56
23	D	403	CLA	C2C-C1C-NC	4.69	114.36	109.97
26	A	412	SQD	O7-S-C6	-4.68	101.37	106.94
23	c	911	CLA	C4A-NA-C1A	4.68	108.81	106.71
23	C	502	CLA	CAC-C3C-C4C	4.68	130.88	124.81
23	C	501	CLA	CHD-C4C-C3C	-4.67	117.97	124.84
23	d	402	CLA	C4-C3-C5	4.67	123.13	115.27
23	b	605	CLA	O2D-CGD-CBD	4.67	119.57	111.27
23	B	603	CLA	CHD-C4C-C3C	-4.67	117.98	124.84
23	a	410	CLA	C1D-CHD-C4C	-4.67	116.40	122.56
23	b	610	CLA	CAC-C3C-C4C	4.66	130.85	124.81
23	c	902	CLA	O2D-CGD-CBD	4.66	119.55	111.27
23	b	613	CLA	C1C-C2C-C3C	-4.66	102.06	106.96
23	c	904	CLA	C2C-C1C-NC	4.66	114.33	109.97
23	b	610	CLA	C2C-C1C-NC	4.65	114.33	109.97
23	b	617	CLA	C2C-C1C-NC	4.65	114.32	109.97
23	C	507	CLA	C2C-C1C-NC	4.64	114.32	109.97
23	C	507	CLA	CHD-C4C-C3C	-4.64	118.02	124.84
25	B	620	BCR	C24-C23-C22	-4.63	119.23	126.23
23	A	410	CLA	C4A-NA-C1A	4.63	108.79	106.71
27	B	622	LMG	O8-C28-C29	4.63	126.42	111.91
23	b	609	CLA	CHD-C4C-C3C	-4.62	118.05	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	604	CLA	C2C-C1C-NC	4.61	114.30	109.97
23	d	403	CLA	C1C-C2C-C3C	-4.61	102.11	106.96
23	b	611	CLA	CHD-C4C-C3C	-4.60	118.08	124.84
24	A	409	PHO	C3C-C4C-NC	4.60	117.41	110.28
23	a	411	CLA	CHD-C4C-C3C	-4.59	118.10	124.84
23	b	607	CLA	CHD-C4C-C3C	-4.58	118.11	124.84
23	c	903	CLA	C1D-CHD-C4C	-4.58	116.52	122.56
24	A	409	PHO	C2B-C1B-NB	4.57	116.68	109.79
23	B	617	CLA	O2D-CGD-O1D	-4.57	114.91	123.84
23	B	604	CLA	O2D-CGD-O1D	-4.57	114.91	123.84
23	c	914	CLA	CHD-C4C-C3C	-4.57	118.13	124.84
27	A	413	LMG	O1-C1-C2	4.56	115.42	108.30
23	c	903	CLA	C2C-C1C-NC	4.56	114.24	109.97
23	d	402	CLA	O2D-CGD-O1D	-4.55	114.93	123.84
23	b	612	CLA	O2D-CGD-CBD	4.55	119.36	111.27
23	b	605	CLA	C2C-C1C-NC	4.55	114.23	109.97
27	B	622	LMG	O7-C10-O9	-4.55	112.70	123.70
23	c	909	CLA	CMD-C2D-C3D	4.55	133.19	124.68
23	C	512	CLA	O2D-CGD-CBD	4.54	119.34	111.27
26	f	102	SQD	O9-S-C6	4.54	112.38	106.92
25	K	101	BCR	C37-C22-C23	4.53	125.22	118.08
23	B	604	CLA	CHD-C4C-NC	4.53	131.33	124.20
23	C	503	CLA	CMB-C2B-C3B	4.52	133.14	124.68
36	D	408	LHG	O8-C23-C24	4.52	126.08	111.91
23	B	615	CLA	CHD-C4C-C3C	-4.50	118.22	124.84
23	b	617	CLA	C1-C2-C3	-4.50	118.26	126.04
23	A	407	CLA	C4A-NA-C1A	4.50	108.73	106.71
25	k	102	BCR	C7-C8-C9	-4.49	119.44	126.23
23	B	612	CLA	C1D-CHD-C4C	-4.49	116.63	122.56
23	b	609	CLA	C2C-C1C-NC	4.49	114.18	109.97
23	c	913	CLA	C1-C2-C3	-4.48	118.29	126.04
23	b	619	CLA	C2C-C1C-NC	4.48	114.17	109.97
23	b	608	CLA	O2D-CGD-CBD	4.47	119.21	111.27
23	b	618	CLA	CMB-C2B-C3B	4.46	133.03	124.68
23	C	512	CLA	CHD-C4C-C3C	-4.45	118.30	124.84
23	A	406	CLA	CHD-C4C-C3C	-4.45	118.30	124.84
23	a	409	CLA	CHD-C4C-C3C	-4.45	118.30	124.84
23	b	614	CLA	C1C-C2C-C3C	-4.45	102.28	106.96
24	a	412	PHO	C3C-C4C-NC	4.44	117.16	110.28
23	C	508	CLA	C1C-C2C-C3C	-4.44	102.29	106.96
23	D	403	CLA	C1C-C2C-C3C	-4.43	102.29	106.96
23	C	507	CLA	CBC-CAC-C3C	-4.43	100.21	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	610	CLA	C4A-NA-C1A	4.43	108.70	106.71
23	B	612	CLA	CMC-C2C-C1C	4.42	131.77	125.04
36	L	101	LHG	O7-C7-O9	-4.42	113.03	123.70
23	c	902	CLA	CHD-C4C-C3C	-4.41	118.36	124.84
25	d	404	BCR	C15-C14-C13	-4.40	121.03	127.31
23	B	615	CLA	O2D-CGD-CBD	4.40	119.09	111.27
27	b	623	LMG	O8-C28-C29	4.40	125.71	111.91
23	C	508	CLA	O2D-CGD-CBD	4.39	119.07	111.27
36	d	407	LHG	O8-C23-O10	-4.39	112.52	123.59
23	C	506	CLA	C1C-C2C-C3C	-4.39	102.34	106.96
23	B	607	CLA	O2D-CGD-O1D	-4.39	115.26	123.84
23	B	604	CLA	CMC-C2C-C1C	4.37	131.70	125.04
23	B	608	CLA	C1-C2-C3	-4.37	118.48	126.04
23	C	501	CLA	C1C-C2C-C3C	-4.37	102.36	106.96
26	D	407	SQD	O9-S-C6	4.37	112.13	106.94
34	h	102	DGD	C3E-C4E-C5E	-4.37	102.44	110.24
23	A	407	CLA	CMB-C2B-C3B	4.37	132.85	124.68
25	t	101	BCR	C11-C10-C9	-4.36	121.09	127.31
23	A	410	CLA	CHD-C4C-NC	4.36	131.07	124.20
23	b	605	CLA	O2D-CGD-O1D	-4.36	115.32	123.84
30	a	402	LMT	C1-O1'-C1'	4.35	121.06	113.84
23	b	619	CLA	C3C-C4C-NC	4.35	115.45	110.57
23	A	406	CLA	O2D-CGD-CBD	4.34	118.98	111.27
27	d	410	LMG	O7-C10-C11	4.34	120.85	111.50
23	C	503	CLA	C1C-C2C-C3C	-4.34	102.40	106.96
25	D	404	BCR	C40-C30-C25	-4.34	103.27	110.30
23	b	617	CLA	CHD-C4C-C3C	-4.33	118.47	124.84
23	B	606	CLA	CHD-C4C-C3C	-4.33	118.47	124.84
25	b	620	BCR	C7-C8-C9	-4.33	119.69	126.23
23	C	511	CLA	O2D-CGD-CBD	4.33	118.96	111.27
37	V	201	HEM	C1D-C2D-C3D	-4.32	103.99	107.00
23	c	908	CLA	C1C-C2C-C3C	-4.32	102.41	106.96
23	D	402	CLA	CAC-C3C-C4C	4.31	130.41	124.81
23	c	912	CLA	O2D-CGD-CBD	4.31	118.93	111.27
23	D	403	CLA	CED-O2D-CGD	4.31	125.69	115.94
26	A	418	SQD	O48-C23-C24	4.31	125.43	111.91
23	C	512	CLA	C1-O2A-CGA	4.31	127.75	116.44
23	B	612	CLA	O2D-CGD-O1D	-4.30	115.42	123.84
23	C	507	CLA	C1C-C2C-C3C	-4.30	102.43	106.96
24	a	413	PHO	C2D-C1D-ND	4.30	116.27	109.79
33	B	625	HTG	C1'-S1-C1	4.29	108.12	100.09
23	b	614	CLA	CHD-C4C-C3C	-4.29	118.53	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	604	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
23	B	612	CLA	CMD-C2D-C3D	4.28	132.69	124.68
23	c	911	CLA	C2C-C1C-NC	4.28	113.98	109.97
23	c	913	CLA	C1-O2A-CGA	4.28	127.66	116.44
23	B	602	CLA	C1C-C2C-C3C	-4.28	102.46	106.96
34	d	406	DGD	C3D-C4D-C5D	4.28	116.43	109.77
23	d	402	CLA	CMD-C2D-C3D	4.27	132.66	124.68
23	d	402	CLA	OBD-CAD-C3D	-4.26	120.90	127.98
23	c	906	CLA	CMB-C2B-C3B	4.26	132.64	124.68
26	A	412	SQD	O8-S-C6	4.26	112.52	105.74
23	b	606	CLA	CMB-C2B-C3B	4.25	132.63	124.68
23	C	508	CLA	C2C-C1C-NC	4.25	113.95	109.97
23	a	414	CLA	O2D-CGD-CBD	4.24	118.81	111.27
34	H	102	DGD	O1G-C1A-O1A	-4.24	112.90	123.59
23	B	607	CLA	C1C-C2C-C3C	-4.23	102.51	106.96
26	D	407	SQD	C1-O5-C5	-4.23	105.39	113.69
26	D	407	SQD	O47-C7-C8	4.21	120.58	111.50
23	C	505	CLA	CMD-C2D-C3D	4.21	132.56	124.68
34	c	917	DGD	O3G-C3G-C2G	-4.20	100.77	110.90
23	a	410	CLA	CMD-C2D-C3D	4.20	132.53	124.68
23	a	414	CLA	C1C-C2C-C3C	-4.19	102.55	106.96
23	b	618	CLA	O2D-CGD-CBD	4.19	118.71	111.27
26	D	407	SQD	C1-C2-C3	-4.19	101.28	110.00
33	D	414	HTG	C1'-S1-C1	4.18	107.92	100.09
23	C	511	CLA	C1C-C2C-C3C	-4.17	102.57	106.96
30	b	624	LMT	O5'-C5'-C4'	4.17	118.55	109.75
23	c	912	CLA	O2D-CGD-O1D	-4.17	115.69	123.84
23	c	906	CLA	CAC-C3C-C4C	4.17	130.22	124.81
23	C	513	CLA	C1C-C2C-C3C	-4.17	102.57	106.96
23	C	506	CLA	C3C-C4C-NC	4.17	115.24	110.57
23	B	616	CLA	C1C-C2C-C3C	-4.16	102.58	106.96
23	b	608	CLA	C1C-C2C-C3C	-4.16	102.58	106.96
27	b	623	LMG	O7-C10-C11	4.16	120.46	111.50
23	b	608	CLA	CMC-C2C-C1C	4.15	131.37	125.04
25	D	404	BCR	C29-C30-C25	4.15	116.87	110.48
25	K	102	BCR	C7-C8-C9	-4.15	119.97	126.23
23	B	611	CLA	O2D-CGD-CBD	4.14	118.63	111.27
25	K	101	BCR	C38-C26-C25	-4.14	119.88	124.53
23	B	608	CLA	CMD-C2D-C3D	4.14	132.43	124.68
25	d	404	BCR	C38-C26-C25	-4.14	119.88	124.53
25	c	915	BCR	C33-C5-C6	-4.14	119.88	124.53
23	B	608	CLA	C3B-C4B-NB	4.13	114.55	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	623	LMG	O8-C28-O10	-4.13	113.17	123.59
26	a	401	SQD	O47-C7-C8	4.13	120.40	111.50
26	A	418	SQD	O6-C1-C2	4.13	114.74	108.30
23	c	904	CLA	CMD-C2D-C3D	4.12	132.39	124.68
24	A	408	PHO	CAC-C3C-C4C	4.12	129.71	125.22
23	C	512	CLA	C1-C2-C3	-4.12	118.92	126.04
37	F	101	HEM	CBA-CAA-C2A	-4.12	104.89	112.49
23	A	410	CLA	C1C-C2C-C3C	-4.11	102.63	106.96
23	b	605	CLA	C1C-C2C-C3C	-4.10	102.64	106.96
23	B	612	CLA	C1C-C2C-C3C	-4.10	102.65	106.96
23	c	913	CLA	C2C-C1C-NC	4.09	113.81	109.97
33	O	303	HTG	C1'-S1-C1	4.09	107.75	100.09
25	d	404	BCR	C24-C23-C22	-4.09	120.05	126.23
27	C	519	LMG	O7-C10-C11	4.09	120.31	111.50
23	b	607	CLA	C3C-C4C-NC	4.09	115.15	110.57
23	C	511	CLA	CHD-C4C-C3C	-4.09	118.83	124.84
23	B	617	CLA	C3C-C4C-NC	4.08	115.15	110.57
23	c	905	CLA	C1C-C2C-C3C	-4.08	102.66	106.96
23	b	618	CLA	CHD-C4C-C3C	-4.08	118.84	124.84
23	B	602	CLA	C4D-C3D-CAD	4.07	110.74	108.47
23	C	512	CLA	C2C-C1C-NC	4.07	113.78	109.97
23	b	604	CLA	CMD-C2D-C3D	4.07	132.28	124.68
37	v	201	HEM	C1D-C2D-C3D	-4.06	104.17	107.00
23	B	602	CLA	C1-O2A-CGA	4.06	127.11	116.44
34	C	518	DGD	O3G-C3G-C2G	-4.06	101.10	110.90
24	A	409	PHO	C4A-NA-C1A	4.05	111.41	108.14
23	c	907	CLA	CHB-C4A-NA	4.05	130.11	124.51
23	c	904	CLA	OBD-CAD-C3D	-4.05	121.26	127.98
23	b	618	CLA	O2D-CGD-O1D	-4.05	115.93	123.84
23	C	511	CLA	C3B-C4B-NB	4.04	114.44	109.21
23	B	609	CLA	CAC-C3C-C4C	4.03	130.04	124.81
23	C	510	CLA	CAC-C3C-C4C	4.03	130.03	124.81
24	a	412	PHO	C2D-C1D-ND	4.02	115.86	109.79
23	B	611	CLA	CAA-CBA-CGA	-4.01	101.53	113.25
27	c	920	LMG	O7-C10-C11	4.01	120.15	111.50
26	B	621	SQD	O48-C23-C24	4.01	124.50	111.91
23	b	614	CLA	C1-C2-C3	-4.00	119.12	126.04
23	d	402	CLA	C3B-C4B-NB	4.00	114.38	109.21
23	c	912	CLA	C1D-CHD-C4C	-4.00	117.28	122.56
24	A	408	PHO	C4D-ND-C1D	-3.99	99.58	106.76
23	A	405	CLA	C2C-C1C-NC	3.99	113.71	109.97
25	d	404	BCR	C16-C15-C14	-3.99	115.30	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	505	CLA	C1C-C2C-C3C	-3.99	102.76	106.96
23	c	904	CLA	C1C-C2C-C3C	-3.99	102.77	106.96
23	b	607	CLA	O2D-CGD-CBD	3.98	118.35	111.27
34	C	516	DGD	O3G-C3G-C2G	-3.98	101.29	110.90
23	b	607	CLA	O2D-CGD-O1D	-3.98	116.05	123.84
24	a	412	PHO	C4C-C3C-C2C	-3.98	102.38	106.78
23	B	602	CLA	CHD-C4C-NC	3.98	130.47	124.20
25	T	101	BCR	C20-C21-C22	-3.98	121.63	127.31
23	c	914	CLA	C2C-C1C-NC	3.98	113.70	109.97
23	a	409	CLA	C1C-C2C-C3C	-3.98	102.78	106.96
26	B	621	SQD	O9-S-C6	3.97	111.66	106.94
23	c	914	CLA	C1C-C2C-C3C	-3.96	102.79	106.96
23	c	906	CLA	O2D-CGD-CBD	3.96	118.30	111.27
23	b	611	CLA	O2D-CGD-O1D	-3.95	116.11	123.84
23	c	910	CLA	C1C-C2C-C3C	-3.95	102.80	106.96
23	b	609	CLA	C1C-C2C-C3C	-3.95	102.80	106.96
23	C	505	CLA	CAC-C3C-C4C	3.95	129.94	124.81
26	D	407	SQD	C44-O6-C1	-3.95	106.02	113.74
23	d	403	CLA	CHD-C4C-C3C	-3.94	119.05	124.84
23	B	608	CLA	C1C-C2C-C3C	-3.94	102.82	106.96
23	B	608	CLA	CBC-CAC-C3C	-3.93	101.58	112.43
27	c	921	LMG	O7-C10-C11	3.93	119.97	111.50
23	b	619	CLA	CAC-C3C-C4C	3.93	129.91	124.81
23	B	605	CLA	O2D-CGD-CBD	3.93	118.25	111.27
23	B	617	CLA	CMD-C2D-C3D	3.93	132.03	124.68
23	B	605	CLA	CED-O2D-CGD	3.93	124.83	115.94
36	d	407	LHG	O8-C23-C24	3.93	124.24	111.91
23	B	615	CLA	O2D-CGD-O1D	-3.93	116.16	123.84
23	a	414	CLA	CMD-C2D-C3D	3.92	132.02	124.68
23	c	905	CLA	CAC-C3C-C4C	3.92	129.90	124.81
23	b	619	CLA	CMB-C2B-C3B	3.91	132.00	124.68
30	A	419	LMT	C1'-O5'-C5'	3.91	121.36	113.69
34	C	518	DGD	O2G-C1B-C2B	3.90	119.91	111.50
27	b	623	LMG	O7-C10-O9	-3.90	114.28	123.70
34	C	516	DGD	O2G-C1B-C2B	3.90	119.90	111.50
23	C	504	CLA	O2D-CGD-CBD	3.90	118.19	111.27
25	D	404	BCR	C24-C23-C22	-3.90	120.34	126.23
23	B	603	CLA	C2C-C1C-NC	3.90	113.62	109.97
25	B	618	BCR	C33-C5-C6	-3.89	120.16	124.53
23	c	912	CLA	C4D-C3D-CAD	3.89	110.64	108.47
30	F	102	LMT	O4'-C4B-C5B	3.88	118.94	109.30
23	c	906	CLA	CBC-CAC-C3C	-3.88	101.73	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	912	CLA	CHD-C4C-NC	3.88	130.32	124.20
23	B	615	CLA	C4-C3-C5	3.88	121.80	115.27
23	B	607	CLA	CHD-C4C-NC	3.88	130.32	124.20
33	b	602	HTG	C1'-S1-C1	3.88	107.34	100.09
23	B	612	CLA	CHD-C4C-NC	3.87	130.31	124.20
23	C	513	CLA	CHD-C4C-C3C	-3.87	119.15	124.84
33	V	202	HTG	O5-C1-S1	3.87	119.56	110.14
23	c	904	CLA	C1-C2-C3	-3.86	119.36	126.04
30	m	102	LMT	O1'-C1'-C2'	3.86	114.33	108.30
23	c	905	CLA	O2D-CGD-CBD	3.86	118.12	111.27
34	d	406	DGD	O2G-C1B-C2B	3.85	119.80	111.50
23	C	501	CLA	CAC-C3C-C4C	3.85	129.80	124.81
23	B	617	CLA	O2D-CGD-CBD	3.85	118.11	111.27
23	C	504	CLA	C4-C3-C5	3.85	121.74	115.27
23	c	909	CLA	C2C-C1C-NC	3.84	113.57	109.97
23	c	907	CLA	C2C-C1C-NC	3.84	113.57	109.97
23	c	913	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
23	a	411	CLA	C4-C3-C5	3.83	121.72	115.27
23	C	503	CLA	C4A-NA-C1A	3.83	108.43	106.71
23	d	403	CLA	C3B-C4B-NB	3.82	114.15	109.21
23	A	407	CLA	CMC-C2C-C1C	3.82	130.85	125.04
26	A	418	SQD	O47-C7-C8	3.82	119.72	111.50
23	d	403	CLA	C4A-NA-C1A	3.81	108.42	106.71
23	a	410	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
23	C	511	CLA	C1-O2A-CGA	3.81	126.44	116.44
23	c	908	CLA	C4-C3-C5	3.81	121.68	115.27
23	b	615	CLA	O2D-CGD-O1D	-3.81	116.39	123.84
26	A	412	SQD	C45-O47-C7	-3.81	108.42	117.79
23	b	619	CLA	O2A-CGA-CBA	3.81	123.85	111.91
23	c	907	CLA	CMC-C2C-C1C	3.80	130.83	125.04
27	D	411	LMG	O8-C28-O10	-3.80	113.99	123.59
36	L	101	LHG	O4-P-O5	3.80	131.02	112.24
28	a	419	PL9	C25-C24-C26	3.80	121.66	115.27
34	c	919	DGD	C6B-C5B-C4B	-3.80	95.15	114.42
23	D	402	CLA	CHD-C4C-NC	3.80	130.18	124.20
30	B	623	LMT	C1B-O5B-C5B	3.79	121.13	113.69
30	A	419	LMT	O2'-C2'-C1'	3.79	119.26	110.05
23	b	614	CLA	O2D-CGD-CBD	3.79	118.01	111.27
25	B	618	BCR	C15-C14-C13	-3.79	121.90	127.31
28	d	405	PL9	C15-C14-C16	3.79	121.64	115.27
23	B	609	CLA	CMD-C2D-C3D	3.79	131.76	124.68
23	b	618	CLA	CAC-C3C-C4C	3.79	129.72	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	609	CLA	O2D-CGD-O1D	-3.78	116.44	123.84
23	B	603	CLA	C4-C3-C5	3.78	121.62	115.27
23	b	612	CLA	C3C-C4C-NC	3.78	114.81	110.57
23	b	607	CLA	CMC-C2C-C1C	3.78	130.79	125.04
23	B	611	CLA	O2D-CGD-O1D	-3.77	116.47	123.84
23	a	414	CLA	C3B-C4B-NB	3.77	114.08	109.21
23	C	512	CLA	C4-C3-C5	3.77	121.61	115.27
38	H	101	RRX	C7-C8-C9	-3.76	120.55	126.23
25	D	404	BCR	C38-C26-C25	-3.76	120.31	124.53
23	d	403	CLA	C4-C3-C5	3.76	121.59	115.27
23	b	605	CLA	CHD-C4C-C3C	-3.76	119.32	124.84
23	B	616	CLA	C1D-CHD-C4C	-3.75	117.60	122.56
23	b	606	CLA	CMD-C2D-C3D	3.75	131.70	124.68
23	B	611	CLA	O2A-CGA-O1A	-3.75	114.12	123.59
23	b	613	CLA	CHD-C4C-C3C	-3.74	119.34	124.84
36	a	417	LHG	O7-C7-C8	3.74	119.56	111.50
23	B	606	CLA	CMD-C2D-C3D	3.74	131.67	124.68
23	a	410	CLA	CHD-C4C-NC	3.73	130.09	124.20
23	B	602	CLA	O2D-CGD-O1D	-3.73	116.54	123.84
23	D	402	CLA	O2D-CGD-O1D	-3.73	116.55	123.84
27	C	519	LMG	O8-C28-C29	3.73	123.60	111.91
23	a	414	CLA	C3C-C4C-NC	3.73	114.75	110.57
23	c	911	CLA	C1C-C2C-C3C	-3.72	103.04	106.96
23	c	907	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
23	b	617	CLA	O2A-CGA-O1A	-3.72	114.22	123.59
23	C	510	CLA	C3B-C4B-NB	3.71	114.01	109.21
23	C	512	CLA	O2D-CGD-O1D	-3.71	116.58	123.84
23	B	616	CLA	CMD-C2D-C3D	3.71	131.62	124.68
23	b	615	CLA	C1-C2-C3	-3.71	119.62	126.04
30	F	102	LMT	C1B-O5B-C5B	3.71	120.97	113.69
23	b	606	CLA	CHD-C4C-NC	3.70	130.04	124.20
23	b	617	CLA	C4D-C3D-CAD	3.70	110.54	108.47
30	m	101	LMT	C3'-C4'-C5'	-3.70	102.44	110.93
23	A	405	CLA	CMB-C2B-C3B	3.70	131.59	124.68
23	b	614	CLA	C3B-C4B-NB	3.70	113.99	109.21
25	t	101	BCR	C28-C27-C26	-3.70	107.48	114.08
23	c	914	CLA	CMB-C2B-C3B	3.70	131.59	124.68
23	c	904	CLA	CHD-C4C-C3C	-3.69	119.41	124.84
30	t	102	LMT	O1'-C1'-C2'	3.69	114.06	108.30
23	B	616	CLA	C3C-C4C-NC	3.69	114.70	110.57
23	B	610	CLA	O2D-CGD-CBD	3.68	117.82	111.27
30	a	402	LMT	O1'-C1'-C2'	3.68	114.05	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	512	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
23	D	403	CLA	CAC-C3C-C4C	3.67	129.58	124.81
23	C	504	CLA	O2D-CGD-O1D	-3.67	116.66	123.84
23	A	407	CLA	C4-C3-C5	3.67	121.45	115.27
23	b	619	CLA	CMD-C2D-C3D	3.67	131.55	124.68
23	C	513	CLA	C2C-C1C-NC	3.67	113.41	109.97
23	A	407	CLA	C3B-C4B-NB	3.67	113.95	109.21
23	c	911	CLA	O2D-CGD-CBD	3.67	117.78	111.27
23	c	903	CLA	CMD-C2D-C3D	3.67	131.54	124.68
24	a	413	PHO	C4A-NA-C1A	3.67	111.10	108.14
23	C	511	CLA	O2D-CGD-O1D	-3.66	116.67	123.84
23	c	903	CLA	O2D-CGD-O1D	-3.66	116.68	123.84
23	b	613	CLA	O2D-CGD-CBD	3.66	117.77	111.27
37	f	101	HEM	CAD-CBD-CGD	3.66	118.81	112.67
23	D	402	CLA	C1D-CHD-C4C	-3.66	117.73	122.56
23	B	607	CLA	O2D-CGD-CBD	3.65	117.76	111.27
23	b	614	CLA	CBC-CAC-C3C	-3.65	102.37	112.43
34	C	517	DGD	O2G-C1B-O1B	-3.65	114.89	123.70
23	C	508	CLA	C4-C3-C5	3.64	121.40	115.27
23	A	406	CLA	C1D-CHD-C4C	-3.64	117.75	122.56
23	C	509	CLA	CHD-C4C-C3C	-3.64	119.49	124.84
23	B	606	CLA	O2A-CGA-O1A	-3.64	114.41	123.59
23	c	911	CLA	C4-C3-C5	3.64	121.39	115.27
23	B	610	CLA	CMB-C2B-C3B	3.63	131.48	124.68
23	b	618	CLA	CMC-C2C-C1C	3.63	130.57	125.04
24	a	413	PHO	C4-C3-C5	3.63	121.38	115.27
25	b	622	BCR	C24-C23-C22	-3.63	120.75	126.23
24	a	413	PHO	C2C-C1C-NC	3.63	115.27	109.79
24	a	413	PHO	C4C-C3C-C2C	-3.63	102.77	106.78
23	C	511	CLA	CMD-C2D-C3D	3.63	131.46	124.68
28	a	419	PL9	C37-C38-C39	-3.62	118.94	127.66
23	B	617	CLA	C1-O2A-CGA	3.62	125.93	116.44
23	c	911	CLA	CMD-C2D-C3D	3.62	131.44	124.68
23	c	910	CLA	C3B-C4B-NB	3.61	113.88	109.21
23	B	613	CLA	CMD-C2D-C3D	3.61	131.44	124.68
23	c	912	CLA	CMD-C2D-C3D	3.61	131.43	124.68
23	A	405	CLA	CHD-C4C-C3C	-3.61	119.53	124.84
23	C	503	CLA	O2D-CGD-CBD	3.61	117.68	111.27
23	a	414	CLA	C4-C3-C5	3.61	121.34	115.27
23	A	405	CLA	C3B-C4B-NB	3.61	113.87	109.21
23	b	618	CLA	C1B-CHB-C4A	-3.60	122.98	130.12
23	B	613	CLA	CHD-C4C-C3C	-3.60	119.54	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	513	CLA	O2D-CGD-O1D	-3.60	116.80	123.84
24	a	413	PHO	C4D-ND-C1D	-3.60	100.29	106.76
23	A	406	CLA	OBD-CAD-C3D	-3.60	122.01	127.98
23	B	609	CLA	CHD-C4C-NC	3.60	129.87	124.20
23	B	613	CLA	O2D-CGD-CBD	3.59	117.65	111.27
23	b	617	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
24	A	408	PHO	C4A-NA-C1A	3.59	111.04	108.14
23	b	606	CLA	CMC-C2C-C1C	3.59	130.51	125.04
23	B	611	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
23	C	507	CLA	CMB-C2B-C3B	3.59	131.39	124.68
23	C	504	CLA	CAC-C3C-C4C	3.58	129.45	124.81
23	B	612	CLA	C1-C2-C3	-3.57	119.86	126.04
30	M	101	LMT	O1'-C1'-C2'	3.57	113.88	108.30
23	c	905	CLA	CHD-C4C-C3C	-3.57	119.59	124.84
23	d	403	CLA	CHD-C4C-NC	3.57	129.82	124.20
24	A	409	PHO	C4D-ND-C1D	-3.57	100.35	106.76
23	c	914	CLA	O2D-CGD-CBD	3.56	117.60	111.27
23	b	612	CLA	CHD-C4C-C3C	-3.56	119.60	124.84
23	A	407	CLA	O2D-CGD-O1D	-3.56	116.87	123.84
23	b	613	CLA	C4D-C3D-CAD	3.56	110.46	108.47
30	M	102	LMT	C1'-O5'-C5'	-3.56	106.69	113.69
23	c	911	CLA	CHD-C4C-C3C	-3.56	119.60	124.84
25	T	101	BCR	C35-C13-C12	3.56	123.69	118.08
23	A	410	CLA	CAC-C3C-C4C	3.56	129.43	124.81
23	C	506	CLA	CAC-C3C-C4C	3.56	129.42	124.81
27	Z	101	LMG	C9-C8-C7	-3.55	103.38	111.79
27	c	920	LMG	O8-C28-C29	3.54	123.03	111.91
23	B	610	CLA	C1-C2-C3	-3.54	119.92	126.04
23	C	513	CLA	CMD-C2D-C3D	3.54	131.30	124.68
23	B	610	CLA	C1C-C2C-C3C	-3.54	103.24	106.96
23	a	411	CLA	O2D-CGD-CBD	3.54	117.56	111.27
23	b	606	CLA	CAC-C3C-C4C	3.54	129.40	124.81
28	D	405	PL9	C53-C6-C1	3.53	122.22	114.99
23	B	615	CLA	CBC-CAC-C3C	-3.53	102.69	112.43
23	a	414	CLA	C1-C2-C3	-3.53	119.94	126.04
23	b	619	CLA	CHD-C4C-NC	3.53	129.76	124.20
23	c	908	CLA	CHD-C4C-NC	3.52	129.76	124.20
23	b	607	CLA	C6-C5-C3	-3.52	104.21	113.45
23	c	914	CLA	O2D-CGD-O1D	-3.52	116.95	123.84
23	c	903	CLA	CHD-C4C-NC	3.52	129.75	124.20
23	B	608	CLA	CHD-C4C-C3C	-3.52	119.67	124.84
24	a	412	PHO	C1C-C2C-C3C	-3.52	102.47	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	620	BCR	C11-C10-C9	-3.51	122.29	127.31
23	b	614	CLA	O2D-CGD-O1D	-3.51	116.97	123.84
23	c	909	CLA	C1C-C2C-C3C	-3.51	103.27	106.96
23	b	619	CLA	O1D-CGD-CBD	-3.51	117.31	124.48
26	D	407	SQD	O7-S-C6	3.51	111.11	106.94
23	B	616	CLA	C11-C10-C8	-3.50	104.60	115.92
23	b	606	CLA	C5-C3-C2	-3.50	114.03	121.12
24	A	409	PHO	C1-C2-C3	-3.50	119.99	126.04
24	A	408	PHO	C1C-NC-C4C	-3.50	99.91	106.51
25	a	415	BCR	C28-C27-C26	-3.50	107.83	114.08
23	C	509	CLA	C3C-C4C-NC	3.49	114.49	110.57
25	t	101	BCR	C35-C13-C12	3.49	123.58	118.08
23	c	910	CLA	O2D-CGD-CBD	3.49	117.47	111.27
25	B	620	BCR	C15-C14-C13	-3.49	122.33	127.31
25	D	404	BCR	C28-C27-C26	-3.49	107.85	114.08
38	H	101	RRX	C16-C15-C14	-3.49	116.33	123.47
23	B	603	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
26	a	401	SQD	O9-S-C6	3.49	111.08	106.94
23	c	902	CLA	C3B-C4B-NB	3.48	113.72	109.21
25	t	101	BCR	C38-C26-C25	-3.48	120.62	124.53
23	c	902	CLA	CHD-C4C-NC	3.48	129.68	124.20
25	A	411	BCR	C15-C16-C17	-3.48	116.35	123.47
23	B	606	CLA	C3C-C4C-NC	3.47	114.47	110.57
23	a	410	CLA	CBC-CAC-C3C	-3.47	102.87	112.43
23	c	909	CLA	CHD-C4C-C3C	-3.47	119.74	124.84
23	B	605	CLA	CHD-C4C-C3C	-3.47	119.74	124.84
23	b	609	CLA	O2D-CGD-CBD	3.47	117.43	111.27
23	c	905	CLA	C3B-C4B-NB	3.46	113.69	109.21
23	A	410	CLA	CHB-C4A-NA	3.46	129.29	124.51
24	A	409	PHO	C2C-C1C-NC	3.45	115.00	109.79
23	d	403	CLA	O1D-CGD-CBD	-3.45	117.42	124.48
23	B	615	CLA	CHD-C4C-NC	3.45	129.64	124.20
23	B	614	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
23	b	604	CLA	O2D-CGD-O1D	-3.45	117.10	123.84
23	b	604	CLA	C1-O2A-CGA	3.44	125.47	116.44
23	a	411	CLA	C2A-C1A-CHA	-3.44	117.85	123.86
23	b	604	CLA	O2A-CGA-CBA	3.44	122.69	111.91
23	B	605	CLA	O2D-CGD-O1D	-3.43	117.13	123.84
34	h	102	DGD	O1G-C1A-O1A	-3.43	114.94	123.59
23	c	903	CLA	C1C-C2C-C3C	-3.43	103.36	106.96
34	H	102	DGD	O1G-C1A-C2A	3.42	122.65	111.91
23	C	502	CLA	C1C-C2C-C3C	-3.42	103.36	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	L	101	LHG	C6-C5-C4	-3.42	103.70	111.79
26	D	407	SQD	O9-S-O7	-3.41	102.13	113.95
25	a	415	BCR	C38-C26-C25	-3.41	120.69	124.53
36	E	101	LHG	O7-C7-C8	3.41	118.85	111.50
23	B	608	CLA	CED-O2D-CGD	3.41	123.65	115.94
25	K	102	BCR	C24-C23-C22	-3.41	121.08	126.23
37	f	101	HEM	CMC-C2C-C3C	3.41	131.06	124.68
23	c	913	CLA	CHD-C4C-C3C	-3.41	119.83	124.84
37	V	201	HEM	CMB-C2B-C3B	3.40	131.04	124.68
36	D	410	LHG	O4-P-O5	3.40	129.05	112.24
23	B	603	CLA	O2D-CGD-CBD	3.40	117.31	111.27
26	L	103	SQD	O47-C7-C8	3.40	118.82	111.50
28	A	414	PL9	C3-C4-C5	3.40	123.02	118.60
23	b	615	CLA	CMD-C2D-C3D	3.39	131.03	124.68
23	a	409	CLA	C7-C6-C5	-3.39	104.15	113.36
23	b	604	CLA	CHD-C4C-NC	3.39	129.54	124.20
23	b	606	CLA	C3B-C4B-NB	3.39	113.59	109.21
25	K	102	BCR	C20-C21-C22	-3.38	122.48	127.31
23	c	906	CLA	CMD-C2D-C3D	3.38	131.01	124.68
23	A	406	CLA	C4-C3-C5	3.38	120.96	115.27
23	b	612	CLA	C4C-C3C-C2C	-3.38	101.97	106.90
23	B	614	CLA	CHD-C4C-NC	3.38	129.53	124.20
23	A	410	CLA	C3B-C4B-NB	3.38	113.58	109.21
25	A	411	BCR	C11-C10-C9	-3.37	122.50	127.31
23	C	505	CLA	O2D-CGD-CBD	3.37	117.26	111.27
23	b	616	CLA	C1C-C2C-C3C	-3.37	103.41	106.96
23	B	606	CLA	C1C-C2C-C3C	-3.37	103.41	106.96
36	L	101	LHG	O7-C7-C8	3.37	118.76	111.50
23	B	610	CLA	CBC-CAC-C3C	-3.37	103.15	112.43
25	A	411	BCR	C8-C7-C6	-3.37	117.75	127.20
25	B	618	BCR	C7-C8-C9	-3.37	121.15	126.23
23	B	606	CLA	O2D-CGD-CBD	3.36	117.24	111.27
23	b	617	CLA	C4-C3-C2	-3.36	115.05	123.68
23	B	603	CLA	C4A-NA-C1A	3.36	108.22	106.71
23	A	406	CLA	CBC-CAC-C3C	-3.36	103.17	112.43
23	B	604	CLA	C1D-CHD-C4C	-3.36	118.13	122.56
23	c	910	CLA	C4-C3-C5	3.36	120.92	115.27
23	A	407	CLA	CHD-C4C-C3C	-3.36	119.91	124.84
23	C	509	CLA	O2D-CGD-CBD	3.35	117.22	111.27
23	b	610	CLA	C4-C3-C5	3.35	120.90	115.27
24	A	408	PHO	C2B-C1B-NB	3.34	114.84	109.79
23	c	910	CLA	C3C-C4C-NC	3.34	114.32	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	606	CLA	CAC-C3C-C4C	3.34	129.14	124.81
23	b	612	CLA	C1-C2-C3	-3.34	120.27	126.04
23	c	903	CLA	C1-C2-C3	-3.34	120.27	126.04
23	C	507	CLA	O2D-CGD-CBD	3.34	117.20	111.27
25	b	621	BCR	C29-C30-C25	3.33	115.61	110.48
26	a	401	SQD	O48-C23-C24	3.33	122.37	111.91
33	b	626	HTG	C1-O5-C5	3.33	118.73	112.58
33	V	202	HTG	O2-C2-C1	3.33	116.39	110.27
23	B	603	CLA	C1C-C2C-C3C	-3.33	103.46	106.96
23	B	611	CLA	CHD-C4C-NC	3.33	129.45	124.20
23	b	604	CLA	C4-C3-C5	3.33	120.87	115.27
30	a	402	LMT	O5 ¹ -C1 ¹ -O1 ¹	-3.32	102.11	109.97
23	C	501	CLA	C2A-C1A-CHA	-3.32	118.05	123.86
30	C	520	LMT	C2 ¹ -C3 ¹ -C4 ¹	-3.32	102.11	109.68
36	D	408	LHG	O4-P-O5	3.32	128.63	112.24
23	A	410	CLA	O2D-CGD-CBD	3.31	117.15	111.27
23	b	609	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
25	c	916	BCR	C38-C26-C25	-3.31	120.81	124.53
23	B	610	CLA	C3C-C4C-NC	3.31	114.28	110.57
23	B	612	CLA	C3C-C4C-NC	3.30	114.28	110.57
23	C	512	CLA	CMD-C2D-C3D	3.30	130.86	124.68
23	B	604	CLA	CHC-C1C-NC	-3.30	119.19	124.20
25	B	619	BCR	C29-C30-C25	3.30	115.56	110.48
23	c	914	CLA	CMD-C2D-C3D	3.30	130.85	124.68
23	c	912	CLA	C4-C3-C5	3.30	120.82	115.27
23	D	402	CLA	CHC-C1C-C2C	-3.29	117.61	126.72
25	T	101	BCR	C15-C16-C17	-3.29	116.73	123.47
23	b	619	CLA	C4C-C3C-C2C	-3.29	102.10	106.90
23	D	403	CLA	CMA-C3A-C4A	-3.29	102.93	111.77
23	C	510	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
23	b	617	CLA	C3B-C4B-NB	3.29	113.46	109.21
28	a	419	PL9	C20-C19-C21	3.29	120.80	115.27
28	A	414	PL9	C53-C6-C1	3.29	121.71	114.99
24	A	409	PHO	C4-C3-C5	3.28	120.80	115.27
37	F	101	HEM	CAD-CBD-CGD	3.28	118.18	112.67
23	B	604	CLA	CMB-C2B-C3B	3.28	130.82	124.68
25	K	102	BCR	C38-C26-C25	-3.28	120.84	124.53
23	B	606	CLA	C4-C3-C5	3.28	120.79	115.27
23	b	605	CLA	C4D-C3D-CAD	3.27	110.30	108.47
33	V	202	HTG	O5-C5-C6	3.27	114.57	106.44
36	d	409	LHG	O4-P-O5	3.27	128.41	112.24
25	a	415	BCR	C16-C15-C14	-3.26	116.79	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	402	CLA	CMB-C2B-C3B	3.26	130.78	124.68
24	A	409	PHO	O2D-CGD-O1D	-3.26	117.46	123.84
28	D	405	PL9	C27-C28-C29	-3.26	119.81	127.66
23	D	403	CLA	CHD-C4C-C3C	-3.26	120.05	124.84
23	B	611	CLA	C3B-C4B-NB	3.26	113.42	109.21
23	B	604	CLA	O2A-CGA-O1A	-3.26	115.38	123.59
27	C	519	LMG	O8-C28-O10	-3.25	115.38	123.59
23	C	507	CLA	C4-C3-C5	3.25	120.74	115.27
26	A	418	SQD	C1-O5-C5	-3.25	107.31	113.69
25	C	514	BCR	C7-C8-C9	-3.25	121.33	126.23
34	d	406	DGD	O6D-C1D-O3G	3.25	117.67	109.97
23	C	501	CLA	CBC-CAC-C3C	-3.24	103.49	112.43
23	a	414	CLA	CMC-C2C-C1C	3.24	129.98	125.04
25	t	101	BCR	C33-C5-C6	-3.24	120.89	124.53
23	B	613	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
30	M	101	LMT	C1-O1'-C1'	3.24	119.21	113.84
25	t	101	BCR	C12-C13-C14	-3.24	113.98	118.94
23	a	414	CLA	CMB-C2B-C3B	3.23	130.72	124.68
25	K	102	BCR	C33-C5-C6	-3.23	120.91	124.53
23	B	602	CLA	CMC-C2C-C1C	3.22	129.94	125.04
23	c	912	CLA	C1-O2A-CGA	3.21	124.88	116.44
23	a	409	CLA	CMD-C2D-C3D	3.21	130.69	124.68
24	a	413	PHO	C2B-C1B-NB	3.21	114.64	109.79
30	F	102	LMT	C2'-C3'-C4'	3.21	117.01	109.68
23	c	914	CLA	CMC-C2C-C1C	3.21	129.92	125.04
23	b	605	CLA	CMB-C2B-C1B	-3.21	123.54	128.46
23	b	611	CLA	O2A-CGA-O1A	-3.20	115.50	123.59
23	c	909	CLA	CMA-C3A-C4A	-3.20	103.16	111.77
23	b	618	CLA	C4-C3-C5	3.20	120.66	115.27
36	d	408	LHG	C34-C33-C32	-3.20	98.17	114.42
23	C	506	CLA	CMC-C2C-C1C	3.20	129.91	125.04
23	a	411	CLA	C1-O2A-CGA	3.20	124.84	116.44
23	B	611	CLA	O2A-CGA-CBA	3.20	121.95	111.91
23	A	405	CLA	CAA-CBA-CGA	-3.20	103.91	113.25
24	a	412	PHO	CAC-C3C-C4C	3.20	128.71	125.22
24	a	412	PHO	CBA-CAA-C2A	-3.20	104.42	113.86
23	C	502	CLA	O2D-CGD-CBD	3.20	116.95	111.27
25	B	618	BCR	C24-C23-C22	-3.20	121.41	126.23
23	C	507	CLA	CHD-C4C-NC	3.20	129.24	124.20
34	h	102	DGD	O1G-C1A-C2A	3.19	121.93	111.91
23	b	616	CLA	C3C-C4C-NC	3.19	114.15	110.57
27	B	622	LMG	C31-C30-C29	-3.19	101.72	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	605	CLA	C1-C2-C3	-3.19	120.53	126.04
25	T	101	BCR	C7-C8-C9	-3.19	121.42	126.23
26	D	407	SQD	O48-C23-C24	3.19	121.92	111.91
26	B	621	SQD	C4-C3-C2	3.18	116.38	110.82
27	C	519	LMG	O5-C6-C5	-3.18	100.38	111.29
23	c	905	CLA	C4-C3-C5	3.18	120.62	115.27
23	b	611	CLA	C3C-C4C-NC	3.18	114.13	110.57
23	c	914	CLA	C1-O2A-CGA	3.17	124.77	116.44
34	c	919	DGD	O1G-C1A-C2A	3.17	121.86	111.91
25	K	102	BCR	C16-C17-C18	-3.17	122.79	127.31
28	d	405	PL9	C36-C37-C38	-3.17	101.47	111.88
23	C	502	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
25	b	620	BCR	C35-C13-C12	3.17	123.06	118.08
23	c	908	CLA	CMD-C2D-C3D	3.17	130.60	124.68
23	B	603	CLA	CHD-C4C-NC	3.16	129.19	124.20
27	Z	101	LMG	C3-C4-C5	3.16	115.88	110.24
23	B	606	CLA	C2A-C1A-CHA	-3.16	118.33	123.86
23	c	907	CLA	O2A-CGA-O1A	-3.16	115.61	123.59
23	B	608	CLA	C4A-NA-C1A	3.16	108.13	106.71
23	B	607	CLA	C3B-C4B-NB	3.16	113.30	109.21
23	c	905	CLA	C4D-C3D-CAD	3.16	110.23	108.47
30	b	625	LMT	C3'-C4'-C5'	-3.16	104.61	110.24
23	c	907	CLA	C1-C2-C3	-3.16	120.58	126.04
23	C	506	CLA	CMD-C2D-C3D	3.16	130.58	124.68
23	d	402	CLA	C3C-C4C-NC	3.15	114.11	110.57
23	c	908	CLA	C3C-C4C-NC	3.15	114.10	110.57
23	b	609	CLA	CMC-C2C-C3C	3.15	134.67	126.12
23	B	609	CLA	O2A-CGA-CBA	3.15	121.79	111.91
23	b	611	CLA	CMB-C2B-C3B	3.14	130.56	124.68
23	b	611	CLA	CMD-C2D-C3D	3.14	130.56	124.68
23	b	604	CLA	CMC-C2C-C1C	3.14	129.82	125.04
24	a	412	PHO	C1C-NC-C4C	-3.14	100.60	106.51
36	l	101	LHG	O7-C7-O9	-3.14	116.12	123.70
34	c	919	DGD	O3G-C3G-C2G	-3.13	103.34	110.90
23	C	504	CLA	C5-C3-C2	-3.13	114.78	121.12
23	B	614	CLA	C2A-C1A-CHA	-3.13	118.38	123.86
23	a	411	CLA	CBC-CAC-C3C	-3.13	103.80	112.43
23	a	414	CLA	CHD-C4C-NC	3.13	129.13	124.20
25	D	404	BCR	C10-C11-C12	-3.13	113.45	123.22
23	C	503	CLA	CHC-C1C-NC	-3.13	119.46	124.20
25	k	101	BCR	C38-C26-C25	-3.13	121.02	124.53
23	b	615	CLA	C4-C3-C5	3.13	120.53	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	906	CLA	CHD-C4C-NC	3.12	129.13	124.20
27	A	413	LMG	O6-C1-C2	-3.12	103.73	110.35
23	b	615	CLA	O2D-CGD-CBD	3.12	116.82	111.27
24	a	412	PHO	CMC-C2C-C1C	3.12	129.87	125.06
23	B	617	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
23	B	613	CLA	C3C-C4C-NC	3.12	114.07	110.57
23	B	604	CLA	C2A-C1A-CHA	-3.12	118.41	123.86
23	C	509	CLA	O2A-CGA-O1A	-3.12	115.73	123.59
25	D	404	BCR	C29-C28-C27	-3.11	104.42	111.38
23	b	617	CLA	CHB-C4A-NA	3.11	128.82	124.51
23	C	506	CLA	CHD-C4C-NC	3.11	129.11	124.20
25	B	618	BCR	C16-C15-C14	-3.11	117.10	123.47
23	b	613	CLA	CAA-CBA-CGA	-3.11	104.16	113.25
26	a	416	SQD	C45-O47-C7	-3.11	110.13	117.79
27	c	920	LMG	O5-C6-C5	-3.11	100.62	111.29
23	B	614	CLA	C1-C2-C3	-3.11	120.67	126.04
23	c	913	CLA	O2D-CGD-O1D	-3.11	117.77	123.84
23	C	504	CLA	CMB-C2B-C3B	3.11	130.49	124.68
23	a	414	CLA	C1B-CHB-C4A	-3.10	123.97	130.12
25	a	415	BCR	C7-C8-C9	-3.10	121.54	126.23
34	c	917	DGD	O5D-C6D-C5D	-3.10	103.31	109.05
23	B	606	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
23	A	406	CLA	C3C-C4C-NC	3.10	114.05	110.57
23	c	907	CLA	C1D-CHD-C4C	-3.10	118.47	122.56
28	a	419	PL9	C30-C29-C31	3.10	120.48	115.27
23	C	505	CLA	CMC-C2C-C1C	3.10	129.76	125.04
23	b	614	CLA	CMC-C2C-C1C	3.10	129.76	125.04
34	c	918	DGD	O6E-C5E-C4E	-3.10	104.07	109.69
23	B	602	CLA	C1D-CHD-C4C	-3.10	118.47	122.56
23	c	905	CLA	C7-C6-C5	-3.09	104.95	113.36
23	b	604	CLA	C1D-CHD-C4C	-3.09	118.48	122.56
23	C	502	CLA	CMC-C2C-C1C	3.09	129.75	125.04
24	A	408	PHO	O2D-CGD-CBD	3.09	116.76	111.27
23	b	608	CLA	C4C-C3C-C2C	-3.09	102.40	106.90
23	C	508	CLA	CHD-C4C-C3C	-3.09	120.30	124.84
23	B	602	CLA	O1D-CGD-CBD	-3.09	118.17	124.48
28	d	405	PL9	C22-C23-C24	-3.09	120.23	127.66
23	b	608	CLA	C3A-C2A-C1A	-3.09	96.72	101.34
23	a	409	CLA	CAC-C3C-C2C	-3.09	122.25	127.53
33	b	626	HTG	C1-C2-C3	3.08	116.68	110.59
23	C	506	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
23	c	914	CLA	O2A-CGA-CBA	3.08	121.58	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	t	101	BCR	C29-C28-C27	-3.08	104.49	111.38
23	A	405	CLA	C4A-NA-C1A	3.08	108.09	106.71
23	b	617	CLA	CAC-C3C-C4C	3.08	128.80	124.81
23	B	605	CLA	C4-C3-C5	3.07	120.44	115.27
25	T	101	BCR	C2-C1-C6	3.07	115.21	110.48
23	b	612	CLA	CMD-C2D-C3D	3.07	130.43	124.68
28	a	419	PL9	C35-C34-C36	3.07	120.44	115.27
23	C	509	CLA	CMC-C2C-C3C	3.07	134.45	126.12
23	b	612	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
23	b	605	CLA	C4-C3-C5	3.07	120.43	115.27
23	A	405	CLA	CMA-C3A-C4A	-3.07	103.53	111.77
25	B	618	BCR	C10-C11-C12	-3.07	113.64	123.22
33	B	624	HTG	C3'-C2'-C1'	-3.07	101.08	113.08
23	C	509	CLA	O2A-CGA-CBA	3.06	121.53	111.91
23	B	607	CLA	C4-C3-C5	3.06	120.43	115.27
23	C	511	CLA	CBC-CAC-C3C	-3.06	103.98	112.43
25	b	620	BCR	C24-C23-C22	-3.06	121.61	126.23
23	b	606	CLA	O2A-C1-C2	-3.06	100.59	108.64
23	D	402	CLA	OBD-CAD-C3D	-3.06	122.91	127.98
33	c	924	HTG	C3-C4-C5	3.05	115.69	110.24
23	b	616	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
25	C	514	BCR	C11-C10-C9	-3.05	122.95	127.31
34	C	518	DGD	O1G-C1A-C2A	3.04	121.46	111.91
26	f	102	SQD	O48-C23-C24	3.04	121.46	111.91
23	C	504	CLA	C1-O2A-CGA	3.04	124.43	116.44
23	c	909	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
25	t	101	BCR	C1-C6-C7	3.04	124.38	115.78
23	B	609	CLA	C2A-C1A-CHA	-3.04	118.55	123.86
23	C	508	CLA	O2A-CGA-O1A	-3.04	115.93	123.59
25	b	621	BCR	C8-C7-C6	-3.03	118.68	127.20
23	B	614	CLA	CBC-CAC-C3C	-3.03	104.07	112.43
23	b	607	CLA	CMB-C2B-C3B	3.03	130.35	124.68
30	C	520	LMT	C1B-O5B-C5B	3.03	119.64	113.69
23	B	614	CLA	CAC-C3C-C4C	3.03	128.74	124.81
23	C	505	CLA	CMB-C2B-C3B	3.03	130.34	124.68
23	b	609	CLA	O2A-CGA-O1A	-3.03	115.95	123.59
23	C	512	CLA	OBD-CAD-C3D	-3.02	122.96	127.98
23	B	612	CLA	C1B-CHB-C4A	-3.02	124.13	130.12
30	c	922	LMT	O1'-C1'-C2'	3.02	113.02	108.30
28	A	414	PL9	C22-C23-C24	-3.02	120.39	127.66
23	B	613	CLA	CMB-C2B-C3B	3.02	130.33	124.68
34	c	917	DGD	C6D-O5D-C1E	-3.02	107.84	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	909	CLA	C3B-C4B-NB	3.02	113.11	109.21
34	c	919	DGD	O1G-C1A-O1A	-3.02	115.98	123.59
23	b	615	CLA	C3B-C4B-NB	3.02	113.11	109.21
23	B	603	CLA	C4D-C3D-CAD	3.02	110.15	108.47
23	B	605	CLA	CGD-CBD-CAD	-3.02	100.97	110.73
23	b	614	CLA	C1D-CHD-C4C	-3.01	118.58	122.56
38	h	101	RRX	C16-C17-C18	-3.01	123.01	127.31
34	c	918	DGD	C3E-C4E-C5E	3.01	115.61	110.24
23	C	504	CLA	CHD-C4C-C3C	-3.01	120.41	124.84
25	d	404	BCR	C40-C30-C25	-3.01	105.42	110.30
30	J	102	LMT	C3'-C4'-C5'	-3.01	104.87	110.24
25	k	101	BCR	C24-C23-C22	-3.01	121.69	126.23
28	a	419	PL9	C40-C39-C41	3.01	120.33	115.27
23	b	606	CLA	O2D-CGD-CBD	3.01	116.61	111.27
30	M	102	LMT	C3'-C4'-C5'	-3.01	104.03	110.93
34	H	102	DGD	C6D-C5D-C4D	3.01	118.37	112.09
23	b	616	CLA	C3B-C4B-NB	3.00	113.09	109.21
23	b	613	CLA	CHB-C4A-NA	3.00	128.66	124.51
23	B	615	CLA	O2A-CGA-O1A	-3.00	116.03	123.59
23	b	611	CLA	C3B-C4B-NB	2.99	113.08	109.21
23	A	406	CLA	CAC-C3C-C2C	-2.99	122.41	127.53
26	B	621	SQD	O48-C23-O10	-2.99	116.04	123.59
23	A	410	CLA	CMD-C2D-C3D	2.99	130.27	124.68
33	b	601	HTG	C1'-S1-C1	2.99	105.68	100.09
27	d	410	LMG	O8-C28-O10	-2.99	116.05	123.59
23	B	616	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
23	C	509	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
25	b	621	BCR	C16-C17-C18	2.98	131.57	127.31
23	c	903	CLA	C3B-C4B-NB	2.98	113.07	109.21
23	B	613	CLA	C4-C3-C5	2.98	120.29	115.27
23	b	610	CLA	C1C-C2C-C3C	-2.98	103.82	106.96
23	b	609	CLA	CHD-C4C-NC	2.98	128.89	124.20
36	d	408	LHG	O8-C23-O10	-2.98	116.08	123.59
26	A	412	SQD	O47-C7-O49	-2.97	116.51	123.70
23	b	611	CLA	C4D-C3D-CAD	2.97	110.13	108.47
23	C	510	CLA	C1C-C2C-C3C	-2.97	103.83	106.96
26	A	418	SQD	C1-C2-C3	-2.97	103.81	110.00
23	D	402	CLA	O2A-CGA-O1A	-2.97	116.09	123.59
30	B	623	LMT	O5B-C5B-C4B	2.97	115.09	109.69
23	C	509	CLA	C1-C2-C3	-2.97	120.91	126.04
23	a	411	CLA	C3B-C4B-NB	2.97	113.05	109.21
23	C	505	CLA	C4A-NA-C1A	2.97	108.04	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	609	CLA	C3B-C4B-NB	2.97	113.05	109.21
23	b	616	CLA	C1-O2A-CGA	2.97	124.23	116.44
23	C	506	CLA	CMB-C2B-C3B	2.97	130.23	124.68
23	b	607	CLA	O2A-CGA-O1A	-2.96	116.11	123.59
28	d	405	PL9	C40-C39-C38	-2.96	116.08	123.68
23	b	610	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
23	c	910	CLA	C1-C2-C3	-2.96	120.92	126.04
25	C	515	BCR	C33-C5-C6	-2.96	121.20	124.53
25	T	101	BCR	C12-C13-C14	-2.96	114.40	118.94
23	c	907	CLA	C3B-C4B-NB	2.96	113.03	109.21
28	a	419	PL9	C42-C43-C44	-2.96	120.54	127.66
23	B	617	CLA	O2A-C1-C2	2.96	116.41	108.64
23	b	616	CLA	C2A-C1A-CHA	-2.96	118.69	123.86
27	B	622	LMG	O8-C28-O10	-2.96	116.13	123.59
23	b	617	CLA	CHD-C4C-NC	2.96	128.86	124.20
23	b	618	CLA	C3B-C4B-NB	2.96	113.03	109.21
25	t	101	BCR	C20-C21-C22	-2.96	123.09	127.31
23	a	409	CLA	CHD-C4C-NC	2.95	128.86	124.20
28	A	414	PL9	C37-C38-C39	-2.95	120.55	127.66
28	d	405	PL9	C53-C6-C1	2.95	121.03	114.99
26	a	416	SQD	O47-C7-O49	-2.95	116.57	123.70
23	d	402	CLA	C5-C3-C2	-2.95	115.15	121.12
23	B	605	CLA	CAA-C2A-C3A	-2.95	104.70	112.78
24	a	413	PHO	C1-C2-C3	-2.95	120.94	126.04
23	b	605	CLA	C1D-CHD-C4C	-2.95	118.67	122.56
23	c	903	CLA	CAC-C3C-C4C	2.95	128.63	124.81
27	a	418	LMG	O7-C10-O9	-2.94	116.60	123.70
23	C	505	CLA	CHD-C4C-NC	2.94	128.83	124.20
23	B	607	CLA	C1-O2A-CGA	2.94	124.15	116.44
23	B	603	CLA	CMB-C2B-C3B	2.94	130.17	124.68
23	C	503	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
23	B	606	CLA	C4A-NA-C1A	2.93	108.02	106.71
23	C	511	CLA	C3A-C2A-C1A	2.93	105.73	101.34
24	A	409	PHO	CAA-C2A-C1A	-2.93	104.76	112.33
23	C	509	CLA	CMB-C2B-C1B	2.93	132.97	128.46
23	C	501	CLA	O1D-CGD-CBD	-2.93	118.50	124.48
23	B	611	CLA	C1D-CHD-C4C	-2.93	118.70	122.56
23	b	611	CLA	CAC-C3C-C4C	2.92	128.60	124.81
25	A	411	BCR	C7-C8-C9	-2.92	121.82	126.23
34	C	516	DGD	C3G-C2G-C1G	-2.92	104.88	111.79
24	a	413	PHO	C3C-C4C-NC	2.92	114.81	110.28
23	B	605	CLA	CAC-C3C-C4C	2.92	128.60	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	905	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
25	t	101	BCR	C7-C6-C5	-2.92	114.39	121.46
23	b	605	CLA	C2A-C3A-C4A	-2.92	97.16	101.87
23	B	616	CLA	C4-C3-C5	2.92	120.18	115.27
34	C	517	DGD	O2G-C1B-C2B	2.92	117.78	111.50
23	b	613	CLA	CMD-C2D-C3D	2.91	130.13	124.68
25	T	101	BCR	C23-C24-C25	-2.91	119.03	127.20
37	F	101	HEM	CMA-C3A-C4A	-2.91	123.99	128.46
33	U	201	HTG	C1-S1-C1'	2.91	110.38	100.40
23	B	605	CLA	C2A-C1A-CHA	-2.90	118.78	123.86
23	A	405	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
33	B	624	HTG	C1'-S1-C1	2.90	105.52	100.09
23	C	501	CLA	C3C-C4C-NC	2.90	113.82	110.57
25	K	101	BCR	C40-C30-C25	-2.90	105.60	110.30
28	A	414	PL9	C30-C29-C31	2.90	120.15	115.27
34	c	919	DGD	C3E-C4E-C5E	-2.89	105.08	110.24
23	c	902	CLA	CBC-CAC-C3C	-2.89	104.45	112.43
23	b	608	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
23	D	403	CLA	O2D-CGD-CBD	2.89	116.41	111.27
23	D	403	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
23	b	618	CLA	CHD-C4C-NC	2.89	128.76	124.20
23	B	608	CLA	CMA-C3A-C4A	-2.89	104.00	111.77
23	b	610	CLA	CMD-C2D-C3D	2.89	130.09	124.68
24	A	408	PHO	CHC-C1C-C2C	-2.89	118.46	125.73
23	B	617	CLA	C2A-C1A-CHA	-2.89	118.80	123.86
23	D	402	CLA	CAA-CBA-CGA	-2.89	104.81	113.25
23	D	403	CLA	C3B-C4B-NB	2.89	112.95	109.21
23	C	508	CLA	CMC-C2C-C3C	2.89	133.96	126.12
23	b	617	CLA	C1-O2A-CGA	2.89	124.02	116.44
23	C	513	CLA	C4-C3-C5	2.89	120.13	115.27
23	C	505	CLA	CED-O2D-CGD	2.89	122.47	115.94
23	c	910	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
23	b	610	CLA	CMB-C2B-C3B	2.89	130.08	124.68
23	c	911	CLA	C4D-C3D-CAD	2.88	110.08	108.47
23	b	608	CLA	CHC-C1C-NC	-2.88	119.83	124.20
34	d	406	DGD	O1G-C1G-C2G	2.88	116.83	108.43
28	D	405	PL9	C40-C39-C38	-2.88	116.29	123.68
23	b	619	CLA	C1C-C2C-C3C	-2.88	103.93	106.96
23	c	914	CLA	CHD-C4C-NC	2.88	128.74	124.20
28	D	405	PL9	C42-C41-C39	-2.88	103.51	112.98
23	C	501	CLA	CMD-C2D-C3D	2.88	130.06	124.68
23	b	616	CLA	CMB-C2B-C3B	2.86	130.03	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	502	CLA	C4-C3-C5	2.86	120.09	115.27
24	a	412	PHO	CHD-C4C-C3C	-2.86	118.68	124.49
23	b	605	CLA	CMA-C3A-C4A	-2.86	104.09	111.77
23	b	610	CLA	CHD-C4C-NC	2.86	128.71	124.20
34	c	917	DGD	O2G-C1B-O1B	-2.86	116.80	123.70
27	B	622	LMG	O5-C6-C5	-2.86	101.49	111.29
34	c	919	DGD	C4A-C3A-C2A	-2.86	102.93	113.19
23	B	612	CLA	C2A-C1A-CHA	-2.85	118.87	123.86
23	c	907	CLA	C4D-C3D-CAD	2.85	110.06	108.47
26	a	416	SQD	O9-S-O7	-2.85	104.08	113.95
23	D	402	CLA	C2A-C1A-CHA	-2.85	118.87	123.86
23	b	619	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
25	c	916	BCR	C15-C16-C17	-2.85	117.64	123.47
30	m	101	LMT	O1'-C1'-C2'	2.85	112.75	108.30
34	c	918	DGD	O2G-C1B-C2B	2.84	117.61	111.50
26	A	418	SQD	O48-C23-O10	-2.83	116.44	123.59
23	B	609	CLA	CMC-C2C-C1C	2.83	129.35	125.04
26	A	412	SQD	O48-C23-O10	-2.83	116.44	123.59
25	B	620	BCR	C7-C8-C9	-2.83	121.95	126.23
23	c	907	CLA	CED-O2D-CGD	2.83	122.34	115.94
27	c	921	LMG	O1-C1-C2	2.83	112.72	108.30
23	c	909	CLA	C1-C2-C3	-2.83	121.15	126.04
34	c	918	DGD	O1G-C1A-O1A	-2.83	116.46	123.59
23	b	608	CLA	C2A-C1A-CHA	-2.82	118.92	123.86
23	B	603	CLA	CMD-C2D-C3D	2.82	129.96	124.68
37	F	101	HEM	CMC-C2C-C3C	2.82	129.95	124.68
23	B	613	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
23	c	906	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
38	H	101	RRX	C36-C18-C17	2.81	126.86	122.92
23	c	910	CLA	CED-O2D-CGD	2.81	122.29	115.94
37	f	101	HEM	CMA-C3A-C4A	-2.81	124.15	128.46
28	a	419	PL9	C53-C6-C1	2.81	120.73	114.99
23	b	617	CLA	C4-C3-C5	2.81	119.99	115.27
23	C	512	CLA	CMB-C2B-C3B	2.81	129.93	124.68
23	B	616	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
28	d	405	PL9	C37-C36-C34	-2.81	103.75	112.98
23	b	612	CLA	C1C-C2C-C3C	-2.80	104.01	106.96
23	A	407	CLA	CAC-C3C-C2C	-2.80	122.73	127.53
23	a	409	CLA	C1D-CHD-C4C	-2.80	118.86	122.56
25	B	620	BCR	C32-C1-C6	-2.80	105.75	110.30
25	b	620	BCR	C15-C14-C13	-2.80	123.31	127.31
23	C	513	CLA	CMB-C2B-C3B	2.80	129.92	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	405	PL9	C36-C37-C38	-2.80	102.68	111.88
23	b	605	CLA	O2A-CGA-O1A	-2.80	116.53	123.59
23	a	414	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
23	C	503	CLA	CHD-C4C-NC	2.80	128.61	124.20
30	M	102	LMT	O1'-C1-C2	-2.80	99.77	109.56
23	B	616	CLA	CAC-C3C-C2C	2.80	132.31	127.53
23	C	506	CLA	C4-C3-C5	2.80	119.97	115.27
23	B	615	CLA	C4C-C3C-C2C	-2.79	102.82	106.90
26	a	416	SQD	O5-C1-C2	-2.79	104.44	110.35
25	c	915	BCR	C15-C14-C13	-2.79	123.33	127.31
23	c	910	CLA	CHB-C4A-NA	2.79	128.37	124.51
25	A	411	BCR	C24-C23-C22	-2.79	122.02	126.23
23	B	614	CLA	C4A-NA-C1A	2.79	107.96	106.71
23	C	506	CLA	C1-C2-C3	-2.78	121.23	126.04
23	B	606	CLA	CMB-C2B-C3B	2.78	129.88	124.68
36	a	417	LHG	O8-C23-C24	2.78	120.64	111.91
23	D	402	CLA	C3B-C4B-NB	2.78	112.81	109.21
23	a	410	CLA	OBD-CAD-C3D	-2.78	123.36	127.98
23	B	603	CLA	C1-C2-C3	-2.78	121.23	126.04
23	a	411	CLA	C1-C2-C3	-2.78	121.23	126.04
23	b	606	CLA	C2A-C1A-CHA	-2.78	119.00	123.86
38	H	101	RRX	C29-C28-C27	-2.78	106.50	110.30
25	A	411	BCR	C28-C27-C26	-2.78	109.12	114.08
25	D	404	BCR	C30-C25-C26	-2.78	118.70	122.61
23	b	608	CLA	C4A-NA-C1A	-2.77	105.46	106.71
30	C	520	LMT	O3'-C3'-C4'	2.77	117.28	109.94
23	b	604	CLA	C3C-C4C-NC	2.77	113.68	110.57
23	B	607	CLA	C3C-C4C-NC	2.77	113.68	110.57
23	C	512	CLA	CED-O2D-CGD	2.77	122.20	115.94
31	C	524	GOL	O3-C3-C2	-2.77	96.94	110.20
23	d	402	CLA	C1B-CHB-C4A	-2.76	124.64	130.12
23	a	411	CLA	OBD-CAD-C3D	-2.76	123.39	127.98
24	a	413	PHO	CMB-C2B-C1B	2.76	129.32	125.06
23	B	604	CLA	CMD-C2D-C3D	2.76	129.85	124.68
23	c	908	CLA	CBC-CAC-C3C	-2.76	104.82	112.43
25	K	101	BCR	C15-C16-C17	-2.76	117.83	123.47
30	a	402	LMT	O2'-C2'-C1'	2.75	116.74	110.05
28	A	414	PL9	C7-C8-C9	-2.75	122.21	126.79
23	c	904	CLA	C1D-CHD-C4C	-2.75	118.93	122.56
26	D	407	SQD	C46-C45-C44	-2.75	105.28	111.79
23	b	613	CLA	CHD-C4C-NC	2.75	128.53	124.20
24	a	413	PHO	O2A-CGA-O1A	-2.75	116.66	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	419	LMT	C1-O1'-C1'	2.75	118.39	113.84
23	C	512	CLA	CHD-C4C-NC	2.74	128.53	124.20
24	a	412	PHO	CAA-CBA-CGA	-2.74	105.24	113.25
26	L	103	SQD	O5-C1-C2	-2.74	104.54	110.35
23	d	402	CLA	CHD-C4C-NC	2.74	128.52	124.20
27	C	519	LMG	O7-C10-O9	-2.74	117.08	123.70
23	d	403	CLA	CBC-CAC-C3C	-2.74	104.88	112.43
23	B	617	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
23	c	907	CLA	O2D-CGD-CBD	2.74	116.13	111.27
28	a	419	PL9	C45-C44-C46	2.73	119.87	115.27
23	b	609	CLA	C1-O2A-CGA	2.73	123.61	116.44
23	b	613	CLA	O2A-CGA-O1A	-2.73	116.71	123.59
28	D	405	PL9	C22-C23-C24	-2.73	121.09	127.66
23	a	411	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
23	b	613	CLA	C3B-C4B-NB	2.73	112.73	109.21
23	B	608	CLA	CHD-C4C-NC	2.73	128.50	124.20
23	b	610	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
23	B	607	CLA	C1-C2-C3	-2.72	121.33	126.04
23	C	503	CLA	C3C-C4C-NC	2.72	113.63	110.57
23	a	410	CLA	C3C-C4C-NC	2.72	113.63	110.57
38	H	101	RRX	C10-C11-C12	-2.72	114.72	123.22
23	b	614	CLA	CMD-C2D-C3D	2.72	129.77	124.68
23	b	619	CLA	C2A-C1A-CHA	-2.72	119.10	123.86
25	b	622	BCR	C3-C4-C5	-2.72	109.22	114.08
25	t	101	BCR	C2-C3-C4	-2.72	105.30	111.38
23	B	604	CLA	C6-C5-C3	2.72	120.58	113.45
26	a	416	SQD	O8-S-C6	2.72	110.07	105.74
23	B	605	CLA	O2A-CGA-O1A	-2.71	116.74	123.59
23	a	409	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
23	a	411	CLA	CBA-CAA-C2A	-2.71	105.85	113.86
30	m	101	LMT	O4'-C4B-C3B	2.71	116.62	110.35
27	b	623	LMG	C13-C12-C11	2.71	122.94	113.19
28	d	405	PL9	C31-C32-C33	-2.71	102.97	111.88
23	C	511	CLA	CAC-C3C-C4C	2.71	128.33	124.81
25	A	411	BCR	C35-C13-C14	-2.71	119.12	122.92
26	a	416	SQD	C44-O6-C1	-2.71	108.44	113.74
23	B	616	CLA	C3B-C4B-NB	2.71	112.71	109.21
23	b	612	CLA	C7-C6-C5	-2.71	106.00	113.36
36	d	408	LHG	O7-C7-O9	-2.71	117.16	123.70
36	L	101	LHG	O8-C23-O10	-2.71	116.76	123.59
23	A	410	CLA	C5-C3-C2	-2.71	115.64	121.12
23	c	910	CLA	OBD-CAD-CBD	2.71	129.76	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	D	406	DGD	O2D-C2D-C3D	-2.70	104.10	110.35
23	D	403	CLA	C6-C7-C8	-2.70	107.18	115.92
23	C	512	CLA	CBA-CAA-C2A	-2.70	105.89	113.86
23	a	409	CLA	O2A-CGA-O1A	-2.70	116.78	123.59
25	d	404	BCR	C7-C8-C9	-2.70	122.16	126.23
23	C	510	CLA	C4-C3-C5	2.70	119.81	115.27
23	C	510	CLA	CHB-C4A-NA	2.70	128.24	124.51
23	c	904	CLA	CMB-C2B-C3B	2.69	129.72	124.68
23	b	614	CLA	C14-C13-C15	-2.69	101.53	111.29
23	B	606	CLA	O2A-C1-C2	-2.69	101.55	108.64
23	C	505	CLA	C3C-C4C-NC	2.69	113.59	110.57
23	c	907	CLA	C2A-C1A-CHA	-2.69	119.15	123.86
23	b	619	CLA	C1-O2A-CGA	2.69	123.51	116.44
23	B	617	CLA	CHD-C4C-NC	2.69	128.44	124.20
23	A	407	CLA	C3C-C4C-NC	2.69	113.59	110.57
23	c	910	CLA	CHC-C1C-NC	-2.69	120.12	124.20
36	d	407	LHG	C6-O8-C23	2.69	127.08	117.12
25	c	915	BCR	C38-C26-C25	-2.69	121.51	124.53
36	d	408	LHG	C32-C31-C30	-2.69	100.78	114.42
26	a	401	SQD	C3-C4-C5	2.69	115.03	110.24
36	D	408	LHG	O7-C7-O9	-2.69	117.21	123.70
23	B	617	CLA	CBC-CAC-C3C	-2.69	105.03	112.43
25	c	916	BCR	C11-C10-C9	-2.68	123.48	127.31
34	D	406	DGD	O2G-C1B-O1B	-2.68	117.22	123.70
23	C	510	CLA	CMB-C2B-C3B	2.68	129.70	124.68
23	B	614	CLA	C14-C13-C15	-2.68	101.57	111.29
28	A	414	PL9	C45-C44-C46	2.68	119.78	115.27
24	A	408	PHO	C1C-C2C-C3C	-2.68	103.43	106.51
30	z	101	LMT	O5B-C5B-C6B	2.68	113.10	106.44
36	d	409	LHG	O7-C7-C8	2.68	117.27	111.50
23	B	602	CLA	OBD-CAD-C3D	-2.68	123.54	127.98
23	b	607	CLA	CED-O2D-CGD	2.68	121.99	115.94
23	C	503	CLA	C4-C3-C5	2.68	119.77	115.27
23	B	613	CLA	O2A-C1-C2	-2.67	101.61	108.64
25	D	404	BCR	C30-C25-C24	2.67	123.34	115.78
23	d	403	CLA	CED-O2D-CGD	2.67	121.98	115.94
23	B	609	CLA	O2A-CGA-O1A	-2.67	116.85	123.59
23	b	616	CLA	C4C-C3C-C2C	-2.67	103.00	106.90
23	C	502	CLA	C5-C3-C2	-2.67	115.72	121.12
23	c	914	CLA	CHC-C1C-NC	-2.67	120.16	124.20
23	B	611	CLA	CAC-C3C-C4C	2.67	128.27	124.81
23	c	906	CLA	CMC-C2C-C1C	2.66	129.10	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	613	CLA	CED-O2D-CGD	2.66	121.96	115.94
23	B	604	CLA	C4D-C3D-CAD	2.66	109.95	108.47
37	V	201	HEM	CAD-CBD-CGD	-2.66	108.21	112.67
26	L	103	SQD	C4-C3-C2	2.66	115.46	110.82
23	d	403	CLA	CAC-C3C-C4C	2.66	128.26	124.81
23	A	406	CLA	CHC-C1C-C2C	-2.66	119.37	126.72
23	b	610	CLA	C3B-C4B-NB	2.66	112.64	109.21
23	b	610	CLA	O2D-CGD-CBD	2.66	115.99	111.27
23	B	603	CLA	CAA-CBA-CGA	-2.66	105.49	113.25
30	B	623	LMT	O1'-C1'-C2'	2.66	112.45	108.30
23	a	410	CLA	C4A-NA-C1A	-2.66	105.51	106.71
34	D	406	DGD	O6D-C5D-C6D	2.66	112.03	106.67
23	b	617	CLA	CBC-CAC-C3C	-2.65	105.11	112.43
23	b	607	CLA	CMD-C2D-C3D	2.65	129.64	124.68
34	c	918	DGD	O5D-C6D-C5D	2.65	113.95	109.05
25	A	411	BCR	C33-C5-C6	-2.65	121.55	124.53
24	a	412	PHO	CHD-C1D-ND	-2.65	119.06	124.58
28	a	419	PL9	C15-C14-C16	2.65	119.73	115.27
23	c	908	CLA	O2A-CGA-CBA	2.64	120.21	111.91
24	A	409	PHO	CBA-CAA-C2A	-2.64	106.06	113.86
23	a	411	CLA	CHC-C1C-C2C	-2.64	119.42	126.72
23	C	510	CLA	CMC-C2C-C1C	2.64	129.06	125.04
23	a	411	CLA	CMD-C2D-C3D	2.64	129.62	124.68
26	A	418	SQD	O5-C1-C2	-2.64	104.76	110.35
23	B	602	CLA	O2A-CGA-CBA	2.64	120.19	111.91
23	b	607	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
34	d	406	DGD	O2G-C1B-O1B	-2.64	117.33	123.70
23	b	606	CLA	C7-C6-C5	-2.63	106.20	113.36
23	c	912	CLA	CBC-CAC-C3C	-2.63	105.17	112.43
23	c	912	CLA	C3B-C4B-NB	2.63	112.61	109.21
23	C	509	CLA	C3B-C4B-NB	2.63	112.61	109.21
34	d	406	DGD	C4D-C3D-C2D	2.63	115.42	110.82
25	B	620	BCR	C2-C1-C6	2.63	114.53	110.48
24	A	409	PHO	CED-O2D-CGD	2.63	121.88	115.94
26	B	621	SQD	O47-C7-C8	2.62	117.15	111.50
23	b	615	CLA	O2A-CGA-CBA	2.62	120.14	111.91
34	C	516	DGD	C1E-O6E-C5E	2.62	118.83	113.69
30	B	623	LMT	O1B-C4'-C3'	2.62	114.25	107.28
34	H	102	DGD	O3G-C3G-C2G	-2.62	104.57	110.90
23	B	610	CLA	C4C-C3C-C2C	-2.62	103.08	106.90
34	h	102	DGD	O2G-C1B-C2B	2.62	117.15	111.50
23	C	510	CLA	C4C-C3C-C2C	-2.62	103.08	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	402	CLA	C4-C3-C5	2.62	119.67	115.27
36	l	101	LHG	O7-C7-C8	2.61	117.14	111.50
27	C	519	LMG	O8-C9-C8	2.61	116.04	108.43
34	H	102	DGD	O6E-C5E-C6E	2.61	112.94	106.44
23	c	904	CLA	CBC-CAC-C3C	-2.61	105.23	112.43
25	b	622	BCR	C8-C7-C6	-2.61	119.87	127.20
23	A	410	CLA	O2A-CGA-O1A	-2.61	117.00	123.59
23	a	409	CLA	C3B-C4B-NB	2.61	112.58	109.21
23	B	607	CLA	O2A-CGA-O1A	-2.61	117.01	123.59
25	d	404	BCR	C34-C9-C10	-2.61	119.27	122.92
23	D	403	CLA	C2A-C1A-CHA	-2.61	119.30	123.86
23	B	616	CLA	CMB-C2B-C3B	2.61	129.56	124.68
23	a	411	CLA	C3A-C2A-C1A	-2.61	97.43	101.34
23	a	414	CLA	OBD-CAD-C3D	-2.61	123.65	127.98
23	c	902	CLA	C4-C3-C5	2.61	119.66	115.27
23	b	605	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
23	b	616	CLA	C11-C10-C8	-2.61	107.50	115.92
23	C	505	CLA	OBD-CAD-C3D	-2.60	123.66	127.98
23	A	406	CLA	C16-C17-C18	-2.60	103.71	115.98
23	B	604	CLA	C3C-C4C-NC	2.60	113.49	110.57
34	H	102	DGD	O5D-C6D-C5D	-2.60	104.23	109.05
23	b	610	CLA	C3C-C4C-NC	2.60	113.49	110.57
25	c	915	BCR	C11-C10-C9	-2.60	123.60	127.31
27	c	921	LMG	O8-C28-C29	2.60	120.06	111.91
30	M	101	LMT	O2'-C2'-C1'	2.60	116.35	110.05
34	H	102	DGD	O4D-C4D-C3D	-2.59	104.36	110.35
23	c	907	CLA	C3C-C4C-NC	2.59	113.48	110.57
25	k	101	BCR	C23-C24-C25	-2.59	119.93	127.20
23	B	608	CLA	C7-C6-C5	-2.59	106.33	113.36
23	b	613	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
38	h	101	RRX	C38-C26-C25	-2.59	121.62	124.53
23	b	616	CLA	O2A-CGA-CBA	2.59	120.03	111.91
34	C	516	DGD	O1G-C1G-C2G	-2.58	100.91	108.43
34	d	406	DGD	O1G-C1A-C2A	2.58	120.00	111.91
25	d	404	BCR	C21-C20-C19	-2.58	115.17	123.22
30	A	419	LMT	O5'-C1'-C2'	-2.58	104.89	110.35
24	a	413	PHO	C1C-C2C-C3C	-2.58	103.55	106.51
33	C	522	HTG	O5-C5-C4	2.57	114.37	109.69
27	Z	101	LMG	O8-C28-C29	2.57	119.99	111.91
23	b	618	CLA	CMA-C3A-C4A	-2.57	104.86	111.77
23	c	910	CLA	C4C-C3C-C2C	-2.57	103.15	106.90
30	c	922	LMT	O5'-C5'-C6'	2.57	112.83	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	605	CLA	C5-C3-C2	-2.57	115.92	121.12
23	C	501	CLA	C1-O2A-CGA	2.57	123.18	116.44
33	B	625	HTG	C1-C2-C3	2.57	115.66	110.59
23	B	608	CLA	CGD-CBD-CAD	-2.57	102.42	110.73
23	C	504	CLA	C7-C6-C5	-2.57	106.39	113.36
34	c	918	DGD	O3D-C3D-C2D	-2.56	104.43	110.35
26	a	416	SQD	O5-C1-O6	2.56	116.04	109.97
23	B	605	CLA	CMC-C2C-C1C	2.56	128.94	125.04
34	c	918	DGD	O2G-C1B-O1B	-2.56	117.52	123.70
23	b	617	CLA	O2A-CGA-CBA	2.56	119.93	111.91
25	k	102	BCR	C24-C23-C22	-2.56	122.37	126.23
25	T	101	BCR	C23-C22-C21	-2.56	115.02	118.94
23	b	607	CLA	C3B-C4B-NB	2.56	112.52	109.21
34	C	516	DGD	O6E-C5E-C6E	2.55	112.79	106.44
23	A	406	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
23	A	405	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
23	c	903	CLA	C3C-C4C-NC	2.55	113.44	110.57
27	B	622	LMG	C35-C34-C33	-2.55	101.46	114.42
34	C	518	DGD	O2G-C1B-O1B	-2.55	117.53	123.70
23	C	513	CLA	O2A-CGA-CBA	2.55	119.92	111.91
23	c	905	CLA	CMD-C2D-C3D	2.55	129.45	124.68
23	B	611	CLA	C4C-C3C-C2C	-2.55	103.18	106.90
26	B	621	SQD	O5-C5-C4	-2.55	105.06	109.69
23	B	608	CLA	C2A-C1A-CHA	-2.55	119.40	123.86
23	b	605	CLA	CHD-C4C-NC	2.55	128.22	124.20
23	B	605	CLA	C4A-NA-C1A	2.54	107.85	106.71
24	a	413	PHO	CHD-C1D-ND	-2.54	119.28	124.58
23	C	512	CLA	C2A-C1A-CHA	-2.54	119.41	123.86
25	B	620	BCR	C38-C26-C27	2.54	118.50	113.62
23	c	906	CLA	C3C-C4C-NC	2.54	113.42	110.57
23	D	402	CLA	CHB-C4A-NA	-2.54	121.00	124.51
26	D	407	SQD	C3-C4-C5	2.54	114.77	110.24
24	A	408	PHO	O2D-CGD-O1D	-2.54	118.87	123.84
23	B	614	CLA	C4C-C3C-C2C	-2.54	103.20	106.90
30	b	624	LMT	C3'-C4'-C5'	2.54	116.75	110.93
23	B	603	CLA	C14-C13-C12	-2.54	102.10	111.29
26	a	401	SQD	O48-C46-C45	2.54	115.82	108.43
23	b	617	CLA	CED-O2D-CGD	2.53	121.67	115.94
24	A	409	PHO	CMB-C2B-C1B	2.53	128.97	125.06
23	b	619	CLA	CED-O2D-CGD	2.53	121.67	115.94
36	d	408	LHG	O7-C7-C8	2.53	116.96	111.50
25	c	916	BCR	C8-C7-C6	-2.53	120.09	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	t	101	BCR	C23-C24-C25	-2.53	120.09	127.20
23	C	513	CLA	OBD-CAD-C3D	-2.53	123.78	127.98
23	b	613	CLA	C1D-CHD-C4C	-2.53	119.22	122.56
27	c	920	LMG	O8-C28-O10	-2.53	117.21	123.59
34	C	518	DGD	C4B-C3B-C2B	-2.53	104.10	113.19
36	d	408	LHG	C13-C12-C11	-2.53	101.59	114.42
23	b	610	CLA	CBC-CAC-C3C	-2.53	105.46	112.43
23	C	512	CLA	C1D-CHD-C4C	-2.53	119.22	122.56
23	C	501	CLA	CHD-C4C-NC	2.53	128.19	124.20
25	d	404	BCR	C30-C25-C24	2.53	122.92	115.78
25	D	404	BCR	C32-C1-C6	2.53	114.40	110.30
24	a	413	PHO	CHD-C4C-C3C	-2.52	119.36	124.49
30	b	624	LMT	C2'-C3'-C4'	2.52	115.44	109.68
25	A	411	BCR	C27-C26-C25	2.52	126.39	122.73
23	b	604	CLA	C2A-C1A-CHA	-2.52	119.45	123.86
23	C	508	CLA	C1D-CHD-C4C	2.52	125.89	122.56
25	k	101	BCR	C8-C9-C10	-2.52	115.07	118.94
23	b	614	CLA	CHD-C4C-NC	2.52	128.18	124.20
25	B	620	BCR	C23-C24-C25	-2.52	120.12	127.20
23	B	603	CLA	C4C-C3C-C2C	-2.52	103.23	106.90
23	B	602	CLA	C3B-C4B-NB	2.52	112.46	109.21
26	A	412	SQD	C44-O6-C1	-2.51	108.83	113.74
23	c	904	CLA	C7-C6-C5	-2.51	106.53	113.36
23	C	507	CLA	O2A-CGA-O1A	-2.51	117.25	123.59
25	K	101	BCR	C23-C22-C21	-2.51	115.09	118.94
23	c	907	CLA	C4A-NA-C1A	2.51	107.83	106.71
34	h	102	DGD	C6D-O5D-C1E	2.51	118.64	113.74
23	A	405	CLA	C4D-C3D-CAD	2.51	109.87	108.47
24	a	412	PHO	C2B-C1B-NB	2.51	113.58	109.79
23	A	407	CLA	CED-O2D-CGD	2.51	121.61	115.94
23	c	908	CLA	CAC-C3C-C4C	2.51	128.06	124.81
25	A	411	BCR	C35-C13-C12	2.51	122.03	118.08
23	b	619	CLA	C3B-C4B-NB	2.51	112.45	109.21
27	Z	101	LMG	O8-C28-O10	-2.50	117.27	123.59
34	c	917	DGD	C1E-C2E-C3E	-2.50	104.78	110.00
23	a	414	CLA	C4C-C3C-C2C	-2.50	103.25	106.90
23	d	403	CLA	CMB-C2B-C1B	2.50	132.31	128.46
30	m	101	LMT	C1'-O5'-C5'	-2.50	108.78	113.69
23	d	402	CLA	CMB-C2B-C3B	2.50	129.36	124.68
26	A	418	SQD	O48-C46-C45	2.50	115.72	108.43
23	A	406	CLA	C3A-C2A-C1A	-2.50	97.59	101.34
23	C	510	CLA	O2A-CGA-O1A	-2.50	117.28	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	405	CLA	C4C-C3C-C2C	-2.50	103.25	106.90
23	B	609	CLA	O1D-CGD-CBD	-2.50	119.37	124.48
23	d	403	CLA	C2A-C1A-CHA	-2.50	119.49	123.86
23	b	607	CLA	C7-C6-C5	-2.50	106.57	113.36
24	A	408	PHO	C7-C6-C5	-2.50	106.57	113.36
26	L	103	SQD	O9-S-O7	-2.50	105.30	113.95
24	A	408	PHO	CHD-C1D-ND	-2.50	119.38	124.58
23	b	619	CLA	CBC-CAC-C3C	-2.50	105.55	112.43
23	c	909	CLA	O2D-CGD-CBD	2.49	115.70	111.27
23	D	403	CLA	CBC-CAC-C3C	-2.49	105.55	112.43
36	D	409	LHG	C34-C33-C32	-2.49	101.76	114.42
27	c	920	LMG	O8-C9-C8	2.49	115.68	108.43
25	D	404	BCR	C15-C14-C13	-2.49	123.75	127.31
34	D	406	DGD	O3G-C3G-C2G	2.49	116.90	110.90
23	c	912	CLA	O2A-CGA-CBA	2.49	119.72	111.91
34	h	102	DGD	O3G-C3G-C2G	-2.49	104.90	110.90
23	b	618	CLA	OBD-CAD-C3D	-2.49	123.85	127.98
23	B	613	CLA	CAA-CBA-CGA	-2.49	105.99	113.25
24	A	408	PHO	CBA-CAA-C2A	-2.48	106.53	113.86
36	l	101	LHG	O8-C23-O10	-2.48	117.32	123.59
23	b	618	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
23	C	508	CLA	C2A-C1A-CHA	-2.48	119.52	123.86
23	B	612	CLA	CAC-C3C-C4C	2.48	128.03	124.81
23	c	914	CLA	CED-O2D-CGD	2.48	121.55	115.94
23	B	611	CLA	C4-C3-C5	2.48	119.44	115.27
23	C	502	CLA	CHB-C4A-NA	2.48	127.94	124.51
34	C	518	DGD	O1G-C1A-O1A	-2.48	117.33	123.59
23	c	909	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
25	K	101	BCR	C29-C28-C27	-2.48	105.84	111.38
23	B	613	CLA	C1-O2A-CGA	2.48	122.95	116.44
23	c	913	CLA	CHD-C4C-NC	2.48	128.11	124.20
36	D	409	LHG	O8-C23-O10	-2.48	117.34	123.59
23	B	609	CLA	CHC-C1C-C2C	-2.48	119.87	126.72
23	b	609	CLA	CBC-CAC-C3C	-2.48	105.61	112.43
30	M	101	LMT	O5'-C5'-C6'	2.48	112.59	106.44
25	B	619	BCR	C15-C16-C17	-2.48	118.40	123.47
23	b	608	CLA	O2A-C1-C2	-2.47	102.14	108.64
23	c	913	CLA	CBC-CAC-C3C	-2.47	105.62	112.43
23	B	610	CLA	C2A-C1A-CHA	-2.47	119.54	123.86
23	c	911	CLA	C3C-C4C-NC	2.47	113.34	110.57
33	B	631	HTG	O5-C5-C6	2.47	112.57	106.44
36	D	409	LHG	O8-C23-C24	2.47	119.65	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	616	CLA	CHD-C4C-NC	2.47	128.09	124.20
23	b	612	CLA	C2A-C1A-CHA	-2.47	119.55	123.86
23	C	503	CLA	OBD-CAD-C3D	-2.46	123.89	127.98
36	l	101	LHG	O4-P-O5	2.46	124.41	112.24
23	B	608	CLA	O2D-CGD-CBD	2.46	115.64	111.27
34	C	517	DGD	O1G-C1A-O1A	-2.46	117.38	123.59
30	b	625	LMT	C1-O1'-C1'	2.46	117.92	113.84
23	a	411	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
23	c	910	CLA	O1D-CGD-CBD	-2.46	119.45	124.48
23	b	616	CLA	C12-C11-C10	-2.46	101.94	113.24
23	c	902	CLA	O2A-CGA-O1A	-2.46	117.39	123.59
34	c	917	DGD	C1D-O6D-C5D	-2.46	108.86	113.69
27	a	418	LMG	O8-C28-C29	2.46	119.62	111.91
25	a	415	BCR	C15-C14-C13	-2.46	123.80	127.31
27	Z	101	LMG	O6-C5-C4	2.46	114.15	109.69
23	C	510	CLA	O2D-CGD-CBD	2.46	115.63	111.27
23	c	904	CLA	CED-O2D-CGD	2.46	121.49	115.94
33	b	602	HTG	C1-O5-C5	2.45	117.11	112.58
23	b	610	CLA	CGD-CBD-CAD	-2.45	102.78	110.73
23	a	411	CLA	C3D-CAD-CBD	2.45	110.84	107.61
25	A	411	BCR	C20-C21-C22	-2.45	123.81	127.31
37	V	201	HEM	C4C-C3C-C2C	2.45	108.61	106.90
23	c	913	CLA	C6-C5-C3	-2.45	107.03	113.45
24	A	409	PHO	C16-C15-C13	-2.45	107.99	115.92
23	a	414	CLA	CHC-C1C-C2C	-2.45	119.94	126.72
23	b	606	CLA	C3C-C4C-NC	2.45	113.32	110.57
23	b	606	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
23	d	402	CLA	CHB-C4A-NA	2.45	127.90	124.51
23	c	909	CLA	CMC-C2C-C3C	2.45	132.76	126.12
23	c	905	CLA	CMB-C2B-C3B	2.45	129.25	124.68
26	A	412	SQD	O2-C2-C1	2.45	115.99	110.05
28	D	405	PL9	C31-C32-C33	-2.45	103.84	111.88
23	b	610	CLA	C7-C6-C5	-2.44	106.72	113.36
33	B	624	HTG	O3-C3-C4	-2.44	104.70	110.35
36	d	407	LHG	C11-C10-C9	-2.44	102.03	114.42
34	C	516	DGD	C3D-C4D-C5D	-2.44	105.89	110.24
28	D	405	PL9	C51-C49-C50	2.44	119.99	114.60
23	C	502	CLA	C16-C17-C18	-2.44	104.48	115.98
23	C	513	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
25	D	404	BCR	C21-C20-C19	-2.44	115.61	123.22
23	B	616	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
23	c	903	CLA	O2A-CGA-O1A	-2.44	117.44	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	Z	101	LMG	O1-C7-C8	2.44	116.78	110.90
26	a	401	SQD	O48-C23-O10	-2.44	117.45	123.59
23	B	613	CLA	C4C-C3C-C2C	-2.43	103.35	106.90
34	h	102	DGD	C6D-C5D-C4D	2.43	117.17	112.09
23	c	913	CLA	CMD-C2D-C3D	2.43	129.23	124.68
25	b	620	BCR	C39-C30-C25	2.43	114.24	110.30
23	c	907	CLA	C6-C5-C3	-2.43	107.08	113.45
34	c	918	DGD	O1G-C1A-C2A	2.43	119.52	111.91
30	B	623	LMT	C1B-C2B-C3B	-2.43	104.94	110.00
23	c	908	CLA	C4C-C3C-C2C	-2.42	103.36	106.90
23	b	605	CLA	C2A-C1A-CHA	-2.42	119.62	123.86
23	c	911	CLA	C3B-C4B-NB	2.42	112.34	109.21
26	D	407	SQD	O48-C23-O10	-2.42	117.48	123.59
23	D	402	CLA	OBD-CAD-CBD	2.42	129.36	125.89
25	b	620	BCR	C20-C21-C22	-2.42	123.85	127.31
23	c	911	CLA	C4C-C3C-C2C	-2.42	103.37	106.90
23	D	403	CLA	CMB-C2B-C3B	2.42	129.21	124.68
23	B	614	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
25	C	515	BCR	C23-C24-C25	-2.42	120.42	127.20
27	c	921	LMG	O8-C9-C8	2.41	115.46	108.43
23	c	902	CLA	C2A-C1A-CHA	-2.41	119.64	123.86
38	H	101	RRX	C34-C9-C8	2.41	121.88	118.08
30	t	102	LMT	C1-O1'-C1'	-2.41	109.84	113.84
34	C	516	DGD	CDB-CCB-CBB	-2.41	102.18	114.42
23	b	608	CLA	C1D-CHD-C4C	2.41	125.74	122.56
23	c	912	CLA	CMC-C2C-C1C	2.41	128.71	125.04
23	C	509	CLA	CHB-C4A-NA	2.41	127.85	124.51
23	a	410	CLA	C1-O2A-CGA	2.41	122.77	116.44
24	a	412	PHO	C7-C6-C5	-2.41	106.81	113.36
25	C	514	BCR	C23-C22-C21	-2.41	115.24	118.94
23	B	602	CLA	C3C-C4C-NC	2.41	113.27	110.57
25	b	620	BCR	C21-C20-C19	-2.41	115.70	123.22
25	d	404	BCR	C30-C25-C26	-2.41	119.22	122.61
23	b	615	CLA	CED-O2D-CGD	2.41	121.38	115.94
30	B	623	LMT	O4'-C4B-C3B	-2.40	104.79	110.35
23	c	906	CLA	C4C-C3C-C2C	-2.40	103.39	106.90
23	c	909	CLA	C2A-C1A-CHA	-2.40	119.65	123.86
23	D	402	CLA	C4C-C3C-C2C	-2.40	103.39	106.90
23	C	502	CLA	C6-C5-C3	-2.40	107.15	113.45
25	k	102	BCR	C3-C4-C5	-2.40	109.79	114.08
24	A	408	PHO	C16-C17-C18	-2.40	104.66	115.98
23	B	602	CLA	OBD-CAD-CBD	2.40	129.33	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	508	CLA	C3B-C4B-NB	2.40	112.31	109.21
28	d	405	PL9	C16-C14-C13	-2.40	116.26	121.12
27	B	622	LMG	C9-C8-C7	-2.40	106.11	111.79
23	C	508	CLA	C4C-C3C-C2C	-2.40	103.40	106.90
36	d	407	LHG	O7-C7-O9	-2.40	117.91	123.70
23	b	605	CLA	O2A-CGA-CBA	2.40	119.43	111.91
25	K	101	BCR	C10-C11-C12	-2.40	115.74	123.22
23	C	501	CLA	CMB-C2B-C1B	2.40	132.15	128.46
34	c	919	DGD	C8B-C7B-C6B	-2.40	102.26	114.42
25	T	101	BCR	C24-C23-C22	-2.40	122.61	126.23
36	D	408	LHG	C11-C10-C9	-2.40	102.27	114.42
30	m	101	LMT	C3B-C4B-C5B	-2.39	105.97	110.24
23	B	614	CLA	C4-C3-C5	2.39	119.30	115.27
23	b	609	CLA	CMD-C2D-C3D	2.39	129.16	124.68
23	B	615	CLA	C1C-C2C-C3C	-2.39	104.44	106.96
23	C	504	CLA	C3B-C4B-NB	2.39	112.30	109.21
25	D	404	BCR	C40-C30-C39	2.39	115.86	108.53
23	c	912	CLA	O2A-C1-C2	-2.39	102.36	108.64
23	c	903	CLA	C4C-C3C-C2C	-2.39	103.42	106.90
23	D	402	CLA	CMC-C2C-C1C	2.38	128.67	125.04
23	B	609	CLA	C11-C12-C13	-2.38	108.22	115.92
23	d	403	CLA	C5-C3-C2	-2.38	116.29	121.12
37	f	101	HEM	CMB-C2B-C3B	2.38	129.14	124.68
23	A	407	CLA	CMB-C2B-C1B	-2.38	124.80	128.46
34	h	102	DGD	O6E-C1E-C2E	-2.38	105.31	110.35
23	B	612	CLA	CAA-CBA-CGA	-2.38	106.29	113.25
23	c	906	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
23	B	606	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
25	d	404	BCR	C34-C9-C8	2.38	121.83	118.08
23	B	604	CLA	C4-C3-C5	2.38	119.27	115.27
25	K	101	BCR	C37-C22-C21	-2.38	119.59	122.92
25	K	101	BCR	C39-C30-C25	-2.38	106.44	110.30
34	H	102	DGD	C3E-C4E-C5E	-2.38	106.00	110.24
25	c	916	BCR	C35-C13-C12	2.38	121.82	118.08
23	b	616	CLA	CMD-C2D-C3D	2.37	129.12	124.68
23	c	908	CLA	C3B-C4B-NB	2.37	112.28	109.21
23	C	513	CLA	C2A-C1A-CHA	-2.37	119.72	123.86
30	M	102	LMT	O6'-C6'-C5'	-2.37	103.16	111.29
27	d	410	LMG	O8-C28-C29	2.37	119.34	111.91
34	c	919	DGD	O3G-C1D-C2D	-2.37	104.61	108.30
23	B	603	CLA	C1D-CHD-C4C	-2.37	119.44	122.56
23	a	411	CLA	C1B-CHB-C4A	-2.37	125.43	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	408	PHO	CHD-C4C-C3C	-2.36	119.69	124.49
23	D	403	CLA	CMD-C2D-C3D	2.36	129.10	124.68
38	H	101	RRX	C16-C17-C18	-2.36	123.94	127.31
23	c	911	CLA	C4-C3-C2	-2.36	117.62	123.68
27	C	519	LMG	C8-O7-C10	-2.36	111.97	117.79
28	a	419	PL9	C11-C9-C8	-2.36	116.34	121.12
23	A	405	CLA	OBD-CAD-C3D	-2.36	124.06	127.98
25	b	621	BCR	C16-C15-C14	-2.36	118.64	123.47
23	B	615	CLA	CHC-C1C-NC	-2.36	120.62	124.20
24	A	409	PHO	CHD-C4C-C3C	-2.36	119.70	124.49
38	h	101	RRX	C7-C8-C9	-2.36	122.67	126.23
36	D	409	LHG	C13-C12-C11	-2.36	102.46	114.42
23	b	614	CLA	C7-C6-C5	-2.36	106.96	113.36
25	B	619	BCR	C30-C25-C26	-2.35	119.30	122.61
23	B	608	CLA	CAC-C3C-C4C	2.35	127.86	124.81
23	A	405	CLA	C7-C6-C5	-2.35	106.97	113.36
23	c	903	CLA	C16-C17-C18	-2.35	104.91	115.98
30	a	402	LMT	O4'-C4B-C3B	-2.35	104.92	110.35
23	c	906	CLA	OBD-CAD-C3D	-2.35	124.08	127.98
36	D	410	LHG	O7-C7-C8	2.35	116.56	111.50
31	B	633	GOL	O3-C3-C2	-2.35	98.94	110.20
23	c	904	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
26	A	412	SQD	C9-C8-C7	-2.35	105.09	113.62
23	C	511	CLA	C3C-C4C-NC	2.35	113.20	110.57
23	c	911	CLA	C1D-CHD-C4C	-2.34	119.46	122.56
34	D	406	DGD	O6D-C5D-C4D	2.34	113.95	109.69
37	v	201	HEM	C4C-C3C-C2C	2.34	108.53	106.90
23	a	414	CLA	C1D-CHD-C4C	-2.34	119.47	122.56
23	b	618	CLA	C11-C10-C8	-2.34	108.35	115.92
23	C	504	CLA	CHD-C4C-NC	2.34	127.89	124.20
23	d	402	CLA	O2D-CGD-CBD	2.34	115.43	111.27
23	d	402	CLA	C3D-CAD-CBD	2.34	110.69	107.61
23	c	903	CLA	C4D-C3D-CAD	2.34	109.77	108.47
23	b	614	CLA	C3C-C4C-NC	2.34	113.19	110.57
23	c	911	CLA	CAC-C3C-C4C	2.34	127.84	124.81
24	A	409	PHO	CHD-C1D-ND	-2.34	119.71	124.58
26	A	418	SQD	C44-O6-C1	2.34	118.30	113.74
23	b	604	CLA	CED-O2D-CGD	2.33	121.22	115.94
24	A	409	PHO	O2D-CGD-CBD	2.33	115.41	111.27
23	a	410	CLA	C3B-C4B-NB	2.33	112.22	109.21
36	L	101	LHG	C34-C33-C32	-2.33	102.59	114.42
34	c	919	DGD	C4E-C3E-C2E	2.33	114.89	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	514	BCR	C37-C22-C23	2.33	121.75	118.08
25	a	415	BCR	C35-C13-C12	2.33	121.75	118.08
28	D	405	PL9	C50-C49-C48	-2.33	115.92	122.65
23	c	910	CLA	CHD-C4C-NC	2.32	127.87	124.20
23	b	618	CLA	OBD-CAD-CBD	2.32	129.22	125.89
23	c	911	CLA	C2A-C1A-CHA	-2.32	119.80	123.86
23	a	409	CLA	CMC-C2C-C3C	2.32	132.42	126.12
28	D	405	PL9	C12-C13-C14	-2.32	122.07	127.66
36	D	409	LHG	O7-C7-O9	-2.32	118.09	123.70
23	c	903	CLA	CMB-C2B-C3B	2.32	129.02	124.68
23	B	612	CLA	C3A-C2A-C1A	-2.32	97.87	101.34
25	b	620	BCR	C16-C17-C18	-2.32	124.00	127.31
23	c	905	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
25	T	101	BCR	C21-C20-C19	-2.32	115.98	123.22
33	B	625	HTG	O4-C4-C5	2.32	115.05	109.30
23	C	512	CLA	C3C-C4C-NC	2.31	113.17	110.57
28	d	405	PL9	C25-C24-C26	2.31	119.16	115.27
23	B	610	CLA	CED-O2D-CGD	2.31	121.17	115.94
23	b	608	CLA	C14-C13-C12	-2.31	102.91	111.29
28	A	414	PL9	C17-C18-C19	-2.31	122.09	127.66
23	C	507	CLA	OBD-CAD-C3D	-2.31	124.14	127.98
25	b	620	BCR	C33-C5-C4	2.31	118.06	113.62
30	A	419	LMT	O1'-C1'-C2'	2.31	111.91	108.30
23	B	610	CLA	CHD-C4C-NC	2.31	127.84	124.20
23	A	407	CLA	CMA-C3A-C4A	-2.31	105.56	111.77
26	a	416	SQD	O48-C23-O10	-2.31	117.77	123.59
34	C	516	DGD	C6D-O5D-C1E	-2.31	109.23	113.74
23	B	602	CLA	C2A-C1A-CHA	-2.31	119.83	123.86
23	b	619	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
23	B	607	CLA	O1D-CGD-CBD	-2.30	119.77	124.48
23	b	617	CLA	C1D-CHD-C4C	-2.30	119.52	122.56
23	D	402	CLA	CMB-C2B-C1B	-2.30	124.92	128.46
23	B	615	CLA	C2A-C1A-CHA	-2.30	119.83	123.86
23	c	909	CLA	CAC-C3C-C2C	2.30	131.47	127.53
34	c	917	DGD	O2G-C1B-C2B	2.30	116.47	111.50
24	a	413	PHO	CHC-C1C-C2C	-2.30	119.94	125.73
23	C	511	CLA	C4-C3-C5	2.30	119.14	115.27
23	c	906	CLA	C4-C3-C5	2.30	119.14	115.27
28	d	405	PL9	C3-C4-C5	2.30	121.60	118.60
34	C	516	DGD	O2G-C1B-O1B	-2.30	118.14	123.70
23	C	509	CLA	CHC-C1C-C2C	-2.30	120.36	126.72
25	K	101	BCR	C7-C8-C9	-2.30	122.77	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	f	102	SQD	O6-C44-C45	2.29	114.83	109.44
23	b	605	CLA	C16-C17-C18	-2.29	105.17	115.98
23	c	910	CLA	O2A-CGA-O1A	-2.29	117.80	123.59
23	b	612	CLA	CBC-CAC-C3C	-2.29	106.11	112.43
26	A	412	SQD	O3-C3-C4	2.29	115.65	110.35
25	C	514	BCR	C40-C30-C25	-2.29	106.58	110.30
25	b	622	BCR	C40-C30-C25	-2.29	106.58	110.30
36	d	408	LHG	O8-C23-C24	2.29	119.10	111.91
23	c	913	CLA	CBA-CAA-C2A	-2.29	107.10	113.86
23	c	904	CLA	C4C-C3C-C2C	-2.29	103.56	106.90
23	B	615	CLA	C4-C3-C2	-2.29	117.81	123.68
25	T	101	BCR	C28-C27-C26	-2.29	109.99	114.08
27	d	410	LMG	O7-C10-O9	-2.29	118.17	123.70
23	c	906	CLA	C11-C12-C13	-2.29	108.52	115.92
23	c	909	CLA	C4-C3-C5	2.29	119.12	115.27
37	v	201	HEM	CAD-CBD-CGD	-2.29	108.83	112.67
23	C	512	CLA	CAC-C3C-C4C	2.29	127.78	124.81
25	k	101	BCR	C15-C16-C17	-2.29	118.79	123.47
23	c	913	CLA	O2A-CGA-CBA	2.29	119.08	111.91
28	a	419	PL9	C17-C18-C19	-2.29	122.16	127.66
34	c	919	DGD	O5D-C6D-C5D	-2.28	104.82	109.05
23	b	617	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
34	H	102	DGD	C2G-O2G-C1B	-2.28	112.17	117.79
23	c	908	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
33	B	631	HTG	C1-O5-C5	2.28	116.79	112.58
27	c	920	LMG	C8-O7-C10	-2.28	112.17	117.79
23	C	506	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
36	d	409	LHG	O8-C23-O10	-2.28	117.84	123.59
23	C	511	CLA	CHD-C4C-NC	2.28	127.79	124.20
23	a	411	CLA	O2A-CGA-CBA	2.28	119.06	111.91
23	C	513	CLA	C4D-C3D-CAD	2.28	109.74	108.47
34	D	406	DGD	O1G-C1A-C2A	2.28	119.05	111.91
23	A	405	CLA	C3C-C4C-NC	2.28	113.12	110.57
38	h	101	RRX	C11-C10-C9	-2.28	124.06	127.31
23	B	615	CLA	C1-C2-C3	-2.27	122.11	126.04
23	b	614	CLA	CAC-C3C-C4C	2.27	127.76	124.81
23	b	611	CLA	CHD-C4C-NC	2.27	127.79	124.20
23	B	614	CLA	CHC-C1C-NC	-2.27	120.75	124.20
23	c	914	CLA	C3C-C4C-NC	2.27	113.12	110.57
23	A	407	CLA	CBC-CAC-C3C	-2.27	106.18	112.43
23	B	607	CLA	C4C-C3C-C2C	-2.27	103.59	106.90
23	B	609	CLA	CMB-C2B-C3B	2.27	128.92	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	502	CLA	C3C-C4C-NC	2.27	113.11	110.57
24	a	413	PHO	CAA-C2A-C1A	-2.27	106.48	112.33
23	B	612	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
25	K	102	BCR	C37-C22-C21	-2.26	119.75	122.92
23	B	615	CLA	C1-O2A-CGA	2.26	122.38	116.44
25	b	620	BCR	C15-C16-C17	-2.26	118.84	123.47
23	b	615	CLA	CMC-C2C-C1C	2.26	128.48	125.04
25	b	622	BCR	C23-C22-C21	-2.26	115.47	118.94
23	c	911	CLA	O2A-C1-C2	-2.26	102.69	108.64
23	c	912	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
23	B	607	CLA	CBC-CAC-C3C	-2.26	106.20	112.43
23	C	504	CLA	CMC-C2C-C1C	2.26	128.48	125.04
26	A	412	SQD	O9-S-O7	-2.26	106.13	113.95
25	B	620	BCR	C10-C11-C12	-2.26	116.17	123.22
25	T	101	BCR	C29-C28-C27	-2.26	106.33	111.38
26	L	103	SQD	O47-C7-O49	-2.26	118.25	123.70
23	C	506	CLA	C4C-C3C-C2C	-2.26	103.61	106.90
23	B	614	CLA	C3B-C4B-NB	2.26	112.13	109.21
23	A	405	CLA	CHC-C1C-C2C	-2.26	120.48	126.72
23	C	513	CLA	CHD-C4C-NC	2.25	127.76	124.20
26	D	407	SQD	O5-C1-O6	2.25	115.31	109.97
23	c	904	CLA	OBD-CAD-CBD	2.25	129.12	125.89
23	C	504	CLA	CMD-C2D-C3D	2.25	128.89	124.68
26	D	407	SQD	O6-C44-C45	2.25	116.33	110.90
25	b	620	BCR	C39-C30-C29	-2.25	99.90	108.91
23	C	513	CLA	CMC-C2C-C1C	2.25	128.47	125.04
30	b	625	LMT	C1'-C2'-C3'	2.25	114.68	110.00
28	d	405	PL9	C50-C49-C48	-2.25	116.14	122.65
27	A	413	LMG	O8-C28-C29	2.25	118.97	111.91
23	c	912	CLA	CHB-C4A-NA	2.25	127.62	124.51
34	c	917	DGD	CDB-CCB-CBB	-2.25	103.02	114.42
34	C	518	DGD	C3D-C4D-C5D	-2.25	106.23	110.24
23	B	616	CLA	CHD-C4C-NC	2.25	127.74	124.20
23	C	513	CLA	C3C-C4C-NC	2.25	113.09	110.57
23	b	605	CLA	CED-O2D-CGD	2.24	121.01	115.94
23	A	406	CLA	C2A-C1A-CHA	-2.24	119.94	123.86
23	c	913	CLA	C4D-C3D-CAD	2.24	109.72	108.47
23	c	904	CLA	O2A-CGA-CBA	2.24	118.94	111.91
23	C	509	CLA	C4C-C3C-C2C	-2.24	103.63	106.90
23	A	406	CLA	C11-C10-C8	-2.24	108.67	115.92
23	A	410	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
38	h	101	RRX	C20-C21-C22	-2.24	124.11	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	911	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
34	c	917	DGD	C3G-C2G-C1G	-2.24	106.49	111.79
23	C	508	CLA	CHD-C4C-NC	2.24	127.73	124.20
23	c	913	CLA	C4C-C3C-C2C	-2.24	103.64	106.90
25	b	621	BCR	C8-C9-C10	-2.24	115.51	118.94
25	C	514	BCR	C2-C1-C6	2.24	113.93	110.48
37	v	201	HEM	CMA-C3A-C4A	-2.24	125.03	128.46
25	B	618	BCR	C15-C16-C17	-2.24	118.89	123.47
23	a	409	CLA	O2A-CGA-CBA	2.23	118.92	111.91
23	c	902	CLA	CMB-C2B-C1B	2.23	131.90	128.46
23	b	608	CLA	CAC-C3C-C2C	-2.23	123.71	127.53
23	a	410	CLA	O2A-C1-C2	-2.23	102.77	108.64
23	c	908	CLA	C5-C3-C2	-2.23	116.60	121.12
23	C	502	CLA	C4C-C3C-C2C	-2.23	103.64	106.90
23	C	502	CLA	C3B-C4B-NB	2.23	112.09	109.21
30	B	623	LMT	O1'-C1-C2	2.23	117.39	109.56
23	B	604	CLA	O2A-C1-C2	-2.23	102.77	108.64
23	c	913	CLA	CMB-C2B-C1B	2.23	131.89	128.46
30	M	101	LMT	O2'-C2'-C3'	-2.23	105.20	110.35
38	h	101	RRX	C33-C5-C6	-2.23	122.03	124.53
25	b	621	BCR	C35-C13-C14	-2.22	119.81	122.92
23	d	402	CLA	C2A-C1A-CHA	-2.22	119.97	123.86
23	c	902	CLA	C7-C6-C5	-2.22	107.32	113.36
23	A	406	CLA	C3D-CAD-CBD	2.22	110.53	107.61
23	A	405	CLA	CHB-C4A-NA	2.22	127.58	124.51
23	A	407	CLA	CGD-CBD-CAD	-2.22	103.54	110.73
23	C	503	CLA	C4C-C3C-C2C	-2.22	103.66	106.90
30	a	402	LMT	O5B-C5B-C6B	2.22	111.95	106.44
23	c	908	CLA	C11-C12-C13	-2.22	108.74	115.92
23	b	609	CLA	C3C-C4C-NC	2.22	113.06	110.57
27	b	623	LMG	C1-O6-C5	-2.22	109.33	113.69
27	c	920	LMG	O1-C7-C8	-2.22	105.55	110.90
25	k	101	BCR	C33-C5-C6	-2.22	122.04	124.53
23	a	411	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
25	a	415	BCR	C8-C7-C6	-2.22	120.98	127.20
23	c	905	CLA	C2A-C1A-CHA	-2.21	119.99	123.86
25	k	101	BCR	C2-C3-C4	-2.21	106.43	111.38
23	D	402	CLA	C1C-C2C-C3C	-2.21	104.63	106.96
36	d	408	LHG	O2-C2-C1	-2.21	99.39	109.12
25	K	102	BCR	C34-C9-C8	2.21	121.56	118.08
24	A	409	PHO	C1C-NC-C4C	-2.21	102.35	106.51
23	A	410	CLA	CED-O2D-CGD	2.21	120.93	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	d	405	PL9	C11-C9-C8	-2.21	116.65	121.12
23	B	617	CLA	C4A-NA-C1A	2.21	107.70	106.71
27	D	411	LMG	O8-C28-C29	2.21	118.83	111.91
26	B	621	SQD	O9-S-O7	-2.21	106.31	113.95
23	a	411	CLA	CED-O2D-CGD	2.21	120.93	115.94
23	C	506	CLA	O1D-CGD-CBD	-2.20	119.97	124.48
34	d	406	DGD	O6D-C5D-C6D	2.20	111.46	106.70
25	B	619	BCR	C37-C22-C23	2.20	121.55	118.08
25	b	621	BCR	C11-C12-C13	-2.20	120.23	126.42
23	B	608	CLA	C3A-C2A-C1A	-2.20	98.04	101.34
27	d	410	LMG	O1-C7-C8	-2.20	105.59	110.90
23	a	409	CLA	C1-C2-C3	-2.20	122.24	126.04
36	l	101	LHG	O3-P-O5	-2.20	100.47	109.07
23	a	414	CLA	O2A-CGA-CBA	2.20	118.81	111.91
25	a	415	BCR	C15-C16-C17	-2.20	118.97	123.47
25	b	620	BCR	C40-C30-C25	-2.20	106.73	110.30
25	B	618	BCR	C24-C25-C26	2.20	126.79	121.46
23	b	608	CLA	OBD-CAD-C3D	-2.20	124.34	127.98
23	b	618	CLA	C1-O2A-CGA	2.20	122.20	116.44
25	d	404	BCR	C37-C22-C21	-2.19	119.85	122.92
23	B	603	CLA	C3B-C4B-NB	2.19	112.05	109.21
34	H	102	DGD	C3D-C4D-C5D	-2.19	106.33	110.24
38	H	101	RRX	C21-C20-C19	-2.19	116.37	123.22
34	H	102	DGD	O2G-C1B-C2B	2.19	116.23	111.50
25	B	618	BCR	C34-C9-C10	-2.19	119.85	122.92
23	a	410	CLA	C4C-C3C-C2C	-2.19	103.70	106.90
23	C	505	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
33	b	601	HTG	C2'-C1'-S1	-2.19	105.33	112.40
23	D	403	CLA	CHD-C4C-NC	2.19	127.65	124.20
28	a	419	PL9	C10-C9-C11	2.19	118.95	115.27
25	k	101	BCR	C1-C6-C7	2.19	121.97	115.78
25	k	101	BCR	C16-C15-C14	-2.19	118.99	123.47
38	h	101	RRX	C24-C23-C22	-2.19	122.93	126.23
23	c	912	CLA	C5-C3-C2	-2.19	116.69	121.12
23	A	406	CLA	CMB-C2B-C3B	2.19	128.77	124.68
30	m	102	LMT	O2'-C2'-C1'	2.19	115.36	110.05
23	B	605	CLA	CHC-C1C-NC	-2.19	120.89	124.20
23	C	501	CLA	C1-C2-C3	-2.19	122.26	126.04
23	B	603	CLA	CMA-C3A-C4A	-2.18	105.90	111.77
23	b	609	CLA	O2A-CGA-CBA	2.18	118.76	111.91
23	c	903	CLA	O2A-CGA-CBA	2.18	118.76	111.91
38	H	101	RRX	C23-C24-C25	-2.18	121.07	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	K	102	BCR	C34-C9-C10	-2.18	119.86	122.92
28	a	419	PL9	C3-C4-C5	2.18	121.44	118.60
26	f	102	SQD	C46-O48-C23	2.18	125.20	117.12
26	D	407	SQD	O4-C4-C3	-2.18	105.30	110.35
25	B	620	BCR	C16-C15-C14	-2.18	119.00	123.47
34	c	918	DGD	O5D-C1E-C2E	-2.18	104.90	108.30
37	F	101	HEM	CMA-C3A-C2A	2.18	129.06	124.94
23	B	611	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
23	B	609	CLA	C11-C10-C8	-2.18	108.88	115.92
25	T	101	BCR	C19-C18-C17	-2.18	115.60	118.94
33	b	626	HTG	O4-C4-C5	2.18	114.71	109.30
36	L	101	LHG	C13-C12-C11	-2.18	103.37	114.42
23	c	913	CLA	CED-O2D-CGD	2.18	120.86	115.94
28	D	405	PL9	C27-C26-C24	-2.18	105.81	112.98
34	C	518	DGD	C3A-C2A-C1A	-2.18	105.71	113.62
26	a	401	SQD	C1-C2-C3	-2.17	105.47	110.00
23	A	406	CLA	CHD-C4C-NC	2.17	127.63	124.20
28	a	419	PL9	C26-C24-C23	-2.17	116.72	121.12
28	d	405	PL9	C7-C8-C9	-2.17	123.17	126.79
23	c	914	CLA	CAA-CBA-CGA	-2.17	106.91	113.25
23	C	502	CLA	CMA-C3A-C4A	-2.17	105.94	111.77
23	A	406	CLA	C3B-C4B-NB	2.17	112.02	109.21
23	a	410	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
23	c	905	CLA	C16-C15-C13	2.17	122.94	115.92
33	B	630	HTG	O2-C2-C3	2.17	115.36	110.35
34	C	516	DGD	O6E-C1E-C2E	-2.17	105.76	110.35
26	L	103	SQD	O48-C23-C24	2.17	118.70	111.91
23	c	908	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
23	A	406	CLA	C7-C6-C5	-2.16	107.48	113.36
25	B	619	BCR	C7-C8-C9	-2.16	122.96	126.23
28	D	405	PL9	C11-C9-C8	-2.16	116.74	121.12
38	h	101	RRX	C34-C9-C8	2.16	121.49	118.08
23	B	609	CLA	C1D-CHD-C4C	-2.16	119.70	122.56
23	c	905	CLA	C3C-C4C-NC	2.16	113.00	110.57
34	H	102	DGD	O3G-C1D-C2D	-2.16	104.93	108.30
23	b	610	CLA	C1-C2-C3	-2.16	122.30	126.04
23	c	908	CLA	C1-O2A-CGA	2.16	122.11	116.44
23	C	507	CLA	CMD-C2D-C3D	2.16	128.72	124.68
23	b	611	CLA	C6-C7-C8	-2.16	108.94	115.92
25	c	915	BCR	C35-C13-C12	2.16	121.48	118.08
23	b	612	CLA	CMB-C2B-C3B	2.16	128.72	124.68
30	B	623	LMT	O2'-C2'-C1'	2.16	115.29	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	M	101	LMT	C2'-C3'-C4'	2.16	114.61	109.68
23	b	609	CLA	C4-C3-C5	2.16	118.90	115.27
23	a	410	CLA	CGD-CBD-CAD	-2.16	103.75	110.73
33	d	401	HTG	O5-C1-C2	2.16	113.03	110.31
25	C	515	BCR	C40-C30-C25	-2.16	106.80	110.30
23	A	405	CLA	OBD-CAD-CBD	2.16	128.98	125.89
23	B	607	CLA	C14-C13-C12	-2.16	103.48	111.29
23	C	511	CLA	C4C-C3C-C2C	-2.16	103.76	106.90
27	c	921	LMG	O6-C1-C2	-2.15	105.79	110.35
25	C	514	BCR	C29-C30-C25	2.15	113.80	110.48
23	B	602	CLA	CBC-CAC-C3C	-2.15	106.49	112.43
23	c	910	CLA	CMC-C2C-C1C	2.15	128.32	125.04
23	B	603	CLA	CBC-CAC-C3C	-2.15	106.50	112.43
30	a	402	LMT	C8-C7-C6	-2.15	103.50	114.42
25	c	916	BCR	C19-C18-C17	-2.15	115.64	118.94
26	B	621	SQD	O47-C45-C46	2.15	116.19	108.40
33	B	625	HTG	O2-C2-C3	-2.15	105.38	110.35
23	a	414	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
23	b	613	CLA	O2A-CGA-CBA	2.15	118.65	111.91
28	A	414	PL9	C25-C24-C23	-2.15	118.16	123.68
23	d	402	CLA	CHC-C1C-C2C	-2.15	120.78	126.72
23	c	904	CLA	CHD-C4C-NC	2.15	127.59	124.20
27	c	920	LMG	C3-C4-C5	2.15	114.07	110.24
23	b	614	CLA	C16-C15-C13	2.15	122.86	115.92
23	A	405	CLA	C1C-C2C-C3C	-2.14	104.70	106.96
25	K	102	BCR	C37-C22-C23	2.14	121.45	118.08
34	C	518	DGD	C7B-C6B-C5B	-2.14	103.55	114.42
30	b	624	LMT	C1'-O5'-C5'	2.14	117.89	113.69
23	c	907	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
23	B	608	CLA	C1-O2A-CGA	2.14	122.06	116.44
34	h	102	DGD	C3B-C2B-C1B	-2.14	105.85	113.62
30	C	520	LMT	C3'-C4'-C5'	-2.14	106.03	110.93
25	d	404	BCR	C10-C11-C12	-2.14	116.55	123.22
30	M	102	LMT	C3B-C4B-C5B	-2.14	106.43	110.24
25	B	619	BCR	C29-C28-C27	-2.14	106.61	111.38
25	D	404	BCR	C39-C30-C25	-2.14	106.84	110.30
23	c	902	CLA	O2A-CGA-CBA	2.13	118.60	111.91
23	C	505	CLA	C3B-C4B-NB	2.13	111.97	109.21
24	a	413	PHO	C16-C15-C13	-2.13	109.02	115.92
23	b	614	CLA	C2A-C1A-CHA	-2.13	120.13	123.86
23	c	912	CLA	C3A-C2A-C1A	2.13	104.53	101.34
23	B	614	CLA	CMB-C2B-C3B	2.13	128.66	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	405	CLA	C2A-C1A-CHA	-2.13	120.14	123.86
23	c	909	CLA	C7-C6-C5	-2.13	107.58	113.36
23	c	904	CLA	C3C-C4C-NC	2.13	112.96	110.57
30	M	102	LMT	O4'-C4B-C3B	2.13	115.27	110.35
23	c	906	CLA	C11-C10-C8	-2.13	109.04	115.92
25	D	404	BCR	C32-C1-C2	-2.13	100.39	108.91
33	B	624	HTG	O5-C5-C6	2.13	111.73	106.44
28	D	405	PL9	C2-C3-C4	2.13	121.73	118.80
23	C	508	CLA	CMB-C2B-C3B	2.13	128.66	124.68
23	B	604	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
23	C	503	CLA	C5-C3-C2	-2.13	116.81	121.12
23	C	507	CLA	CHB-C4A-NA	2.13	127.45	124.51
25	k	101	BCR	C20-C21-C22	-2.13	124.28	127.31
36	d	407	LHG	O4-P-O5	2.12	122.73	112.24
26	a	416	SQD	O48-C23-C24	2.12	118.57	111.91
23	c	907	CLA	O2A-CGA-CBA	2.12	118.56	111.91
23	C	503	CLA	CED-O2D-CGD	2.12	120.73	115.94
23	d	403	CLA	CGD-CBD-CAD	-2.12	103.88	110.73
23	b	609	CLA	CHC-C1C-C2C	-2.12	120.87	126.72
23	C	507	CLA	C4D-C3D-CAD	2.12	109.65	108.47
25	d	404	BCR	C32-C1-C2	-2.12	100.44	108.91
26	L	103	SQD	C1-O5-C5	-2.12	109.54	113.69
27	C	519	LMG	C9-C8-C7	-2.12	106.78	111.79
37	V	201	HEM	CMA-C3A-C4A	-2.12	125.21	128.46
23	A	406	CLA	O2A-C1-C2	-2.11	103.08	108.64
24	a	413	PHO	CBA-CAA-C2A	-2.11	107.62	113.86
23	D	403	CLA	C4C-C3C-C2C	-2.11	103.82	106.90
24	A	409	PHO	O2A-CGA-O1A	-2.11	118.26	123.59
25	D	404	BCR	C38-C26-C27	2.11	117.68	113.62
25	d	404	BCR	C35-C13-C12	2.11	121.41	118.08
33	B	626	HTG	O5-C1-C2	2.11	112.97	110.31
23	C	512	CLA	C4C-C3C-C2C	-2.11	103.82	106.90
25	D	404	BCR	C34-C9-C8	2.11	121.40	118.08
30	c	922	LMT	O3B-C3B-C4B	2.11	115.23	110.35
23	B	605	CLA	C3B-C4B-NB	2.11	111.94	109.21
23	c	904	CLA	C2A-C1A-CHA	-2.11	120.17	123.86
23	c	903	CLA	C6-C5-C3	-2.11	107.92	113.45
25	C	514	BCR	C38-C26-C25	-2.11	122.16	124.53
23	B	617	CLA	CMB-C2B-C3B	2.11	128.62	124.68
23	B	608	CLA	CMC-C2C-C3C	2.11	131.84	126.12
30	m	101	LMT	C6'-C5'-C4'	2.11	119.46	113.33
23	c	913	CLA	CAC-C3C-C4C	2.11	127.54	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	902	CLA	C1-O2A-CGA	2.10	121.97	116.44
36	d	409	LHG	O8-C23-C24	2.10	118.51	111.91
33	c	924	HTG	O5-C1-C2	2.10	112.96	110.31
23	C	507	CLA	C1-O2A-CGA	2.10	121.96	116.44
23	b	616	CLA	C6-C7-C8	-2.10	109.12	115.92
23	D	402	CLA	O2D-CGD-CBD	2.10	115.00	111.27
23	c	910	CLA	O2A-CGA-CBA	2.10	118.50	111.91
23	C	504	CLA	C2A-C1A-CHA	-2.10	120.19	123.86
33	B	624	HTG	O5-C5-C4	-2.10	105.88	109.69
27	a	418	LMG	O1-C1-C2	2.10	111.58	108.30
25	c	915	BCR	C8-C7-C6	-2.10	121.31	127.20
23	b	608	CLA	C1-C2-C3	-2.10	122.42	126.04
23	C	501	CLA	C7-C6-C5	-2.10	107.67	113.36
23	c	911	CLA	C1-C2-C3	-2.09	122.42	126.04
23	b	618	CLA	C5-C3-C2	-2.09	116.88	121.12
23	C	511	CLA	CHC-C1C-C2C	-2.09	120.94	126.72
23	b	614	CLA	C17-C16-C15	-2.09	103.63	113.24
25	t	101	BCR	C15-C16-C17	-2.09	119.19	123.47
23	B	613	CLA	O2A-CGA-CBA	2.09	118.47	111.91
23	B	611	CLA	C6-C5-C3	-2.09	107.97	113.45
23	d	403	CLA	CMC-C2C-C3C	2.09	131.79	126.12
23	B	603	CLA	C1-O2A-CGA	2.09	121.93	116.44
23	B	605	CLA	CMD-C2D-C3D	2.09	128.59	124.68
23	B	611	CLA	C3C-C4C-NC	2.09	112.91	110.57
23	B	606	CLA	CMA-C3A-C4A	-2.09	106.16	111.77
25	k	101	BCR	C29-C30-C25	2.09	113.69	110.48
25	c	916	BCR	C7-C8-C9	-2.09	123.08	126.23
23	a	409	CLA	C4D-C3D-CAD	2.09	109.63	108.47
25	k	102	BCR	C20-C21-C22	-2.09	124.33	127.31
25	K	101	BCR	C38-C26-C27	2.08	117.62	113.62
23	D	403	CLA	C4-C3-C5	2.08	118.78	115.27
23	C	513	CLA	C4C-C3C-C2C	-2.08	103.86	106.90
23	B	608	CLA	CMB-C2B-C3B	2.08	128.58	124.68
23	C	507	CLA	CAC-C3C-C4C	2.08	127.51	124.81
23	b	606	CLA	C1B-CHB-C4A	-2.08	125.99	130.12
23	c	914	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
30	a	402	LMT	O2'-C2'-C3'	-2.08	105.53	110.35
23	c	904	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
23	B	610	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
27	A	413	LMG	O2-C2-C3	-2.08	105.55	110.35
23	c	904	CLA	O2D-CGD-CBD	2.08	114.96	111.27
23	d	403	CLA	O2A-CGA-O1A	-2.08	118.35	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	513	CLA	CHC-C1C-NC	-2.08	121.05	124.20
28	A	414	PL9	C10-C9-C11	2.07	118.76	115.27
26	A	412	SQD	O5-C1-C2	-2.07	105.96	110.35
23	b	608	CLA	C5-C3-C2	-2.07	116.92	121.12
23	C	501	CLA	CHC-C1C-C2C	-2.07	120.98	126.72
23	B	616	CLA	CBC-CAC-C3C	-2.07	106.72	112.43
25	d	404	BCR	C15-C16-C17	-2.07	119.23	123.47
23	C	508	CLA	OBD-CAD-CBD	-2.07	122.93	125.89
30	m	101	LMT	C10-C9-C8	-2.07	103.90	114.42
26	L	103	SQD	C28-C27-C26	-2.07	103.91	114.42
23	b	605	CLA	C17-C16-C15	-2.07	103.73	113.24
23	C	505	CLA	C4C-C3C-C2C	-2.07	103.88	106.90
33	c	923	HTG	C1-O5-C5	2.07	116.40	112.58
23	c	909	CLA	CHD-C4C-NC	2.07	127.46	124.20
34	C	516	DGD	O6D-C1D-O3G	-2.07	105.08	109.97
27	B	622	LMG	O4-C4-C3	-2.07	105.57	110.35
23	C	506	CLA	CHC-C1C-NC	-2.07	121.07	124.20
23	B	615	CLA	CMA-C3A-C4A	-2.07	106.22	111.77
23	d	402	CLA	CAC-C3C-C4C	2.07	127.49	124.81
25	K	101	BCR	C4-C5-C6	2.07	125.73	122.73
25	k	102	BCR	C28-C27-C26	-2.06	110.39	114.08
23	b	612	CLA	C4-C3-C5	2.06	118.74	115.27
27	b	623	LMG	C38-C37-C36	-2.06	103.95	114.42
23	c	914	CLA	C4C-C3C-C2C	-2.06	103.89	106.90
23	A	406	CLA	CMC-C2C-C1C	2.06	128.18	125.04
34	D	406	DGD	C3D-C4D-C5D	2.06	113.92	110.24
23	b	618	CLA	CBC-CAC-C3C	-2.06	106.75	112.43
37	V	201	HEM	CMD-C2D-C3D	2.06	128.83	124.94
30	J	102	LMT	C1'-C2'-C3'	2.06	114.28	110.00
38	H	101	RRX	C38-C26-C25	-2.06	122.22	124.53
27	c	920	LMG	O7-C10-O9	-2.06	118.73	123.70
23	b	615	CLA	OBD-CAD-C3D	-2.06	124.57	127.98
23	A	406	CLA	CED-O2D-CGD	2.06	120.59	115.94
23	b	611	CLA	C6-C5-C3	-2.05	108.07	113.45
24	A	408	PHO	CAA-C2A-C1A	-2.05	107.03	112.33
23	B	612	CLA	C15-C13-C12	-2.05	101.34	112.13
36	D	410	LHG	O7-C5-C4	2.05	115.83	108.40
23	D	402	CLA	C5-C3-C2	-2.05	116.97	121.12
23	B	607	CLA	C2A-C1A-CHA	-2.05	120.28	123.86
26	A	418	SQD	C46-O48-C23	2.05	124.71	117.12
30	C	520	LMT	O3B-C3B-C2B	-2.05	105.61	110.35
34	h	102	DGD	O2G-C1B-O1B	-2.05	118.75	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	502	CLA	OBD-CAD-C3D	-2.05	124.58	127.98
23	B	613	CLA	C2A-C3A-C4A	-2.05	98.56	101.87
33	B	626	HTG	O5-C5-C4	-2.05	105.98	109.69
33	B	630	HTG	C4-C3-C2	2.05	114.40	110.82
23	B	607	CLA	C11-C12-C13	-2.05	109.30	115.92
23	C	506	CLA	O2A-CGA-CBA	2.04	118.32	111.91
23	B	610	CLA	CMA-C3A-C4A	-2.04	106.28	111.77
23	B	616	CLA	C5-C3-C2	-2.04	116.98	121.12
23	b	611	CLA	CMC-C2C-C1C	2.04	128.15	125.04
23	B	613	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
27	d	410	LMG	C9-C8-C7	-2.04	106.96	111.79
23	b	607	CLA	C6-C7-C8	-2.04	109.32	115.92
34	h	102	DGD	O4E-C4E-C5E	2.04	114.36	109.30
23	b	609	CLA	C4C-C3C-C2C	-2.04	103.92	106.90
23	c	905	CLA	O2A-C1-C2	-2.04	103.28	108.64
28	A	414	PL9	C15-C14-C16	2.04	118.70	115.27
23	B	614	CLA	CAA-CBA-CGA	-2.04	107.30	113.25
23	B	612	CLA	C4-C3-C5	2.04	118.70	115.27
26	A	412	SQD	O48-C23-C24	2.04	118.30	111.91
25	t	101	BCR	C21-C20-C19	-2.04	116.86	123.22
25	C	515	BCR	C11-C12-C13	-2.04	120.69	126.42
23	C	509	CLA	C6-C5-C3	-2.04	108.12	113.45
23	C	509	CLA	C16-C15-C13	-2.03	109.34	115.92
24	a	412	PHO	CHC-C1C-C2C	-2.03	120.61	125.73
23	c	910	CLA	C1D-CHD-C4C	-2.03	119.87	122.56
27	c	921	LMG	O6-C5-C4	2.03	113.39	109.69
23	c	904	CLA	C11-C10-C8	-2.03	109.35	115.92
23	b	615	CLA	C2A-C1A-CHA	-2.03	120.30	123.86
36	d	408	LHG	O3-P-O5	2.03	117.01	109.07
26	L	103	SQD	C25-C24-C23	-2.03	106.23	113.62
25	T	101	BCR	C16-C17-C18	-2.03	124.41	127.31
27	d	410	LMG	O2-C2-C1	-2.03	105.11	110.05
34	c	918	DGD	O4E-C4E-C3E	-2.03	105.66	110.35
27	a	418	LMG	C30-C29-C28	-2.03	106.24	113.62
23	a	414	CLA	C2A-C1A-CHA	-2.03	120.31	123.86
23	a	409	CLA	C4C-C3C-C2C	-2.03	103.94	106.90
25	B	618	BCR	C23-C22-C21	-2.03	115.83	118.94
30	b	624	LMT	O5'-C5'-C6'	2.03	111.47	106.44
30	b	625	LMT	O1'-C1'-C2'	-2.03	105.14	108.30
26	A	418	SQD	C9-C8-C7	-2.03	106.25	113.62
23	B	608	CLA	CAA-CBA-CGA	-2.03	107.33	113.25
23	a	409	CLA	C3C-C4C-NC	2.02	112.84	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	902	CLA	C4D-C3D-CAD	2.02	109.60	108.47
37	v	201	HEM	CMB-C2B-C3B	2.02	128.47	124.68
30	m	102	LMT	C1'-O5'-C5'	2.02	117.66	113.69
23	c	910	CLA	C3D-CAD-CBD	-2.02	104.94	107.61
23	b	611	CLA	C2A-C1A-CHA	-2.02	120.32	123.86
28	a	419	PL9	C16-C14-C13	-2.02	117.02	121.12
33	u	201	HTG	O3-C3-C2	-2.02	106.67	111.07
23	c	909	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
23	B	605	CLA	O2A-CGA-CBA	2.02	118.24	111.91
23	B	607	CLA	C9-C8-C10	-2.02	103.98	111.29
33	b	601	HTG	O5-C5-C4	2.02	113.36	109.69
30	t	102	LMT	O2'-C2'-C3'	-2.02	105.69	110.35
36	D	408	LHG	C6-O8-C23	2.02	124.59	117.12
30	m	101	LMT	C1B-O5B-C5B	2.02	117.64	113.69
23	D	402	CLA	C3A-C2A-C1A	-2.01	98.32	101.34
23	b	614	CLA	OBD-CAD-CBD	-2.01	123.02	125.89
30	z	101	LMT	C4B-C3B-C2B	-2.01	107.31	110.82
34	H	102	DGD	C6E-C5E-C4E	2.01	117.72	113.00
23	c	908	CLA	CHC-C1C-NC	-2.01	121.15	124.20
25	B	620	BCR	C16-C17-C18	-2.01	124.44	127.31
23	a	409	CLA	O2D-CGD-CBD	2.01	114.84	111.27
23	a	414	CLA	C3A-C2A-C1A	2.01	104.35	101.34
23	c	912	CLA	CHC-C1C-C2C	-2.01	121.16	126.72
23	C	508	CLA	CMA-C3A-C4A	-2.01	106.37	111.77
23	C	508	CLA	CMD-C2D-C3D	2.01	128.44	124.68
23	b	606	CLA	CHC-C1C-NC	-2.01	121.16	124.20
23	B	603	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
25	b	622	BCR	C20-C19-C18	-2.01	120.77	126.42
23	C	502	CLA	C1D-CHD-C4C	-2.01	119.91	122.56
23	c	910	CLA	C1-O2A-CGA	2.01	121.71	116.44
23	B	606	CLA	CHC-C1C-NC	-2.01	121.16	124.20
23	C	508	CLA	CHB-C4A-NA	2.01	127.29	124.51
30	t	102	LMT	O5'-C1'-O1'	-2.01	105.22	109.97
23	B	608	CLA	OBD-CAD-C3D	-2.00	124.65	127.98
23	c	906	CLA	CED-O2D-CGD	2.00	120.47	115.94
23	B	602	CLA	CMB-C2B-C3B	2.00	128.42	124.68
23	a	410	CLA	C6-C7-C8	-2.00	109.45	115.92
23	B	613	CLA	C2A-C1A-CHA	-2.00	120.36	123.86

All (168) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
23	c	914	CLA	NC
23	c	914	CLA	NA
23	A	406	CLA	NA
23	d	402	CLA	ND
23	d	402	CLA	NA
23	b	618	CLA	NC
23	b	618	CLA	ND
23	b	618	CLA	NA
23	d	403	CLA	NC
23	C	508	CLA	NC
23	C	508	CLA	NA
23	b	617	CLA	NC
23	b	617	CLA	ND
23	b	617	CLA	NA
23	B	606	CLA	NC
23	B	606	CLA	ND
23	B	606	CLA	NA
23	b	612	CLA	NC
23	b	607	CLA	NC
23	b	607	CLA	ND
23	b	607	CLA	NA
23	B	609	CLA	NC
23	B	603	CLA	NC
23	B	603	CLA	ND
23	C	513	CLA	NC
23	a	411	CLA	NC
23	a	411	CLA	NA
23	D	402	CLA	ND
23	B	612	CLA	NC
23	B	612	CLA	NA
23	C	506	CLA	NC
23	C	506	CLA	ND
23	A	405	CLA	NC
23	A	405	CLA	ND
23	A	405	CLA	NA
23	c	912	CLA	NC
23	C	511	CLA	NC
23	C	511	CLA	ND
23	C	511	CLA	NA
23	c	908	CLA	NC
23	c	908	CLA	ND

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Mol	Chain	Res	Type	Atom
23	c	908	CLA	NA
23	c	911	CLA	NC
23	c	911	CLA	ND
23	c	911	CLA	NA
23	b	613	CLA	NC
23	b	613	CLA	ND
23	b	613	CLA	NA
23	b	608	CLA	NC
23	b	608	CLA	ND
23	b	608	CLA	NA
23	B	616	CLA	NC
23	B	616	CLA	ND
23	B	616	CLA	NA
23	b	611	CLA	NC
23	C	503	CLA	NC
23	C	503	CLA	ND
23	C	503	CLA	NA
23	C	512	CLA	NC
23	C	512	CLA	ND
23	C	512	CLA	NA
23	B	604	CLA	NC
23	B	604	CLA	ND
23	B	604	CLA	NA
23	b	605	CLA	NC
23	b	605	CLA	ND
23	b	605	CLA	NA
23	A	410	CLA	NC
23	a	409	CLA	NC
23	a	409	CLA	ND
23	a	409	CLA	NA
23	B	602	CLA	NC
23	B	602	CLA	ND
23	c	902	CLA	NC
23	c	902	CLA	ND
23	c	902	CLA	NA
23	C	502	CLA	NC
23	C	502	CLA	NA
23	a	414	CLA	NC
23	B	605	CLA	NC
23	B	605	CLA	ND
23	B	605	CLA	NA
23	C	507	CLA	NC

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Mol	Chain	Res	Type	Atom
23	C	507	CLA	ND
23	C	507	CLA	NA
23	c	904	CLA	NC
23	b	619	CLA	NC
23	b	619	CLA	ND
23	b	619	CLA	NA
23	C	505	CLA	ND
23	b	616	CLA	NC
23	b	616	CLA	ND
23	b	616	CLA	NA
23	A	407	CLA	NC
23	A	407	CLA	NA
23	c	909	CLA	NC
23	c	909	CLA	NA
23	B	613	CLA	NC
23	B	613	CLA	ND
23	B	613	CLA	NA
23	B	608	CLA	NC
23	B	608	CLA	ND
23	B	608	CLA	NA
23	b	606	CLA	NC
23	b	606	CLA	ND
23	b	606	CLA	NA
23	b	609	CLA	NC
23	b	609	CLA	ND
23	c	907	CLA	ND
23	c	907	CLA	NA
23	c	910	CLA	NC
23	c	910	CLA	ND
23	c	910	CLA	NA
23	c	906	CLA	ND
23	b	614	CLA	NC
23	b	614	CLA	NA
23	B	617	CLA	NC
23	B	617	CLA	ND
23	B	617	CLA	NA
23	a	410	CLA	NC
23	a	410	CLA	ND
23	a	410	CLA	NA
23	B	615	CLA	NC
23	B	615	CLA	ND
23	B	615	CLA	NA

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Mol	Chain	Res	Type	Atom
23	D	403	CLA	NC
23	D	403	CLA	ND
23	D	403	CLA	NA
23	b	610	CLA	NC
23	b	610	CLA	ND
23	b	610	CLA	NA
23	b	604	CLA	NC
23	b	604	CLA	ND
23	c	903	CLA	NC
23	c	903	CLA	ND
23	c	903	CLA	NA
23	C	510	CLA	NA
23	C	510	CLA	NC
23	C	510	CLA	ND
23	B	607	CLA	NC
23	B	607	CLA	ND
23	B	607	CLA	NA
23	B	611	CLA	NC
23	B	611	CLA	ND
23	B	611	CLA	NA
23	B	610	CLA	NC
23	B	610	CLA	ND
23	C	509	CLA	NC
23	C	509	CLA	ND
23	C	509	CLA	NA
23	C	501	CLA	NC
23	C	501	CLA	ND
23	C	501	CLA	NA
23	b	615	CLA	NA
23	b	615	CLA	NC
23	b	615	CLA	ND
23	C	504	CLA	NC
23	C	504	CLA	ND
23	C	504	CLA	NA
23	c	905	CLA	NC
23	c	905	CLA	ND
23	c	905	CLA	NA
23	c	913	CLA	NC
23	c	913	CLA	NA
23	c	913	CLA	ND
23	B	614	CLA	NC
23	B	614	CLA	ND

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Mol	Chain	Res	Type	Atom
23	B	614	CLA	NA

All (1486) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	V	202	HTG	C2-C1-S1-C1'
33	V	202	HTG	O5-C1-S1-C1'
30	B	623	LMT	C2-C1-O1'-C1'
36	L	101	LHG	C4-O6-P-O4
26	B	621	SQD	C5-C6-S-O8
26	B	621	SQD	C5-C6-S-O9
25	b	620	BCR	C1-C6-C7-C8
23	C	508	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O2D
25	k	102	BCR	C7-C8-C9-C10
25	k	102	BCR	C7-C8-C9-C34
23	b	617	CLA	CHA-CBD-CGD-O2D
23	b	617	CLA	CAD-CBD-CGD-O1D
23	b	617	CLA	CAD-CBD-CGD-O2D
23	B	606	CLA	C4-C3-C5-C6
33	c	923	HTG	C2'-C1'-S1-C1
25	K	102	BCR	C7-C8-C9-C10
25	K	102	BCR	C7-C8-C9-C34
34	D	406	DGD	C2B-C1B-O2G-C2G
34	D	406	DGD	C2D-C1D-O3G-C3G
34	D	406	DGD	O6D-C1D-O3G-C3G
23	b	608	CLA	C2-C3-C5-C6
23	b	608	CLA	C4-C3-C5-C6
28	a	419	PL9	C9-C11-C12-C13
28	a	419	PL9	C14-C16-C17-C18
28	a	419	PL9	C24-C26-C27-C28
28	a	419	PL9	C30-C29-C31-C32
27	a	418	LMG	O6-C1-O1-C7
27	a	418	LMG	O1-C7-C8-O7
31	c	927	GOL	C1-C2-C3-O3
23	b	605	CLA	CHA-CBD-CGD-O1D
23	A	410	CLA	C2-C3-C5-C6
23	A	410	CLA	C4-C3-C5-C6
23	B	602	CLA	CHA-CBD-CGD-O1D
23	B	602	CLA	CAD-CBD-CGD-O1D
23	B	602	CLA	C11-C10-C8-C9
30	m	102	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
23	C	502	CLA	CHA-CBD-CGD-O1D
23	C	502	CLA	CAD-CBD-CGD-O1D
31	B	635	GOL	O1-C1-C2-C3
23	C	507	CLA	CHA-CBD-CGD-O1D
26	L	103	SQD	O49-C7-O47-C45
26	L	103	SQD	O5-C5-C6-S
31	a	424	GOL	O1-C1-C2-C3
36	D	409	LHG	O1-C1-C2-C3
36	D	409	LHG	C3-O3-P-O5
36	D	409	LHG	C4-O6-P-O4
36	l	101	LHG	C4-O6-P-O4
28	A	414	PL9	C9-C11-C12-C13
23	c	909	CLA	CHA-CBD-CGD-O1D
34	d	406	DGD	C2D-C1D-O3G-C3G
34	d	406	DGD	O6D-C1D-O3G-C3G
33	B	626	HTG	O5-C1-S1-C1'
23	b	609	CLA	CHA-CBD-CGD-O1D
26	a	401	SQD	C2-C1-O6-C44
36	d	408	LHG	C3-O3-P-O5
25	d	404	BCR	C21-C22-C23-C24
25	d	404	BCR	C37-C22-C23-C24
31	b	633	GOL	O1-C1-C2-C3
30	F	102	LMT	C2-C1-O1'-C1'
23	a	410	CLA	CHA-CBD-CGD-O2D
31	c	930	GOL	O1-C1-C2-O2
31	c	930	GOL	O1-C1-C2-C3
31	c	930	GOL	C1-C2-C3-O3
23	B	615	CLA	CHA-CBD-CGD-O1D
23	B	615	CLA	CAD-CBD-CGD-O1D
23	B	615	CLA	CAD-CBD-CGD-O2D
30	M	101	LMT	O5'-C1'-O1'-C1
33	B	625	HTG	C2'-C1'-S1-C1
31	a	423	GOL	C1-C2-C3-O3
23	b	604	CLA	C2-C1-O2A-CGA
23	b	604	CLA	CHA-CBD-CGD-O1D
23	b	604	CLA	CHA-CBD-CGD-O2D
23	b	604	CLA	C14-C13-C15-C16
33	C	521	HTG	C2'-C1'-S1-C1
23	c	903	CLA	CHA-CBD-CGD-O1D
23	c	903	CLA	CAD-CBD-CGD-O1D
33	b	627	HTG	C2-C1-S1-C1'
33	b	627	HTG	O5-C1-S1-C1'

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Mol	Chain	Res	Type	Atoms
36	a	417	LHG	O1-C1-C2-C3
36	a	417	LHG	O2-C2-C3-O3
36	a	417	LHG	C3-O3-P-O5
36	a	417	LHG	C4-O6-P-O5
26	f	102	SQD	C44-C45-O47-C7
26	f	102	SQD	O49-C7-O47-C45
33	u	201	HTG	O2-C2-C3-O3
31	C	524	GOL	C1-C2-C3-O3
31	b	636	GOL	O1-C1-C2-C3
36	E	101	LHG	C3-O3-P-O4
26	D	407	SQD	O10-C23-O48-C46
23	b	604	CLA	O1A-CGA-O2A-C1
26	D	407	SQD	C24-C23-O48-C46
23	c	914	CLA	CBD-CGD-O2D-CED
26	D	407	SQD	O49-C7-O47-C45
34	D	406	DGD	O1B-C1B-O2G-C2G
30	C	520	LMT	C3'-C4'-O1B-C1B
23	b	617	CLA	C3-C5-C6-C7
23	B	615	CLA	C3-C5-C6-C7
23	b	604	CLA	CBA-CGA-O2A-C1
26	D	407	SQD	C8-C7-O47-C45
26	L	103	SQD	C8-C7-O47-C45
23	B	606	CLA	C2-C3-C5-C6
28	a	419	PL9	C28-C29-C31-C32
23	C	513	CLA	CBD-CGD-O2D-CED
26	L	103	SQD	C31-C32-C33-C34
23	b	607	CLA	C3-C5-C6-C7
23	B	602	CLA	C3-C5-C6-C7
26	a	416	SQD	C17-C18-C19-C20
33	c	923	HTG	S1-C1'-C2'-C3'
33	C	521	HTG	S1-C1'-C2'-C3'
33	u	201	HTG	S1-C1'-C2'-C3'
27	c	921	LMG	O6-C5-C6-O5
30	z	101	LMT	O5B-C5B-C6B-O6B
30	C	520	LMT	O5B-C5B-C6B-O6B
33	u	201	HTG	C1-C2-C3-O3
23	C	501	CLA	CBD-CGD-O2D-CED
36	D	409	LHG	O2-C2-C3-O3
36	d	408	LHG	O2-C2-C3-O3
23	c	913	CLA	C3-C5-C6-C7
34	D	406	DGD	C2A-C1A-O1G-C1G
33	d	401	HTG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
23	c	912	CLA	O1D-CGD-O2D-CED
33	B	631	HTG	O5-C5-C6-O6
30	J	102	LMT	O5'-C5'-C6'-O6'
27	A	413	LMG	C20-C21-C22-C23
27	Z	101	LMG	O6-C5-C6-O5
33	C	522	HTG	S1-C1'-C2'-C3'
33	b	626	HTG	S1-C1'-C2'-C3'
30	z	101	LMT	C4B-C5B-C6B-O6B
33	d	401	HTG	C4-C5-C6-O6
26	A	412	SQD	C18-C19-C20-C21
30	F	102	LMT	O5'-C5'-C6'-O6'
33	b	627	HTG	O5-C5-C6-O6
23	b	617	CLA	C4-C3-C5-C6
28	A	414	PL9	C30-C29-C31-C32
23	b	617	CLA	C2-C3-C5-C6
30	m	102	LMT	O5'-C5'-C6'-O6'
34	D	406	DGD	O1A-C1A-O1G-C1G
28	A	414	PL9	C19-C21-C22-C23
28	A	414	PL9	C24-C26-C27-C28
30	m	101	LMT	O5'-C5'-C6'-O6'
30	z	101	LMT	C2B-C1B-O1B-C4'
23	C	513	CLA	O1D-CGD-O2D-CED
36	D	409	LHG	C1-C2-C3-O3
36	E	101	LHG	C1-C2-C3-O3
27	c	920	LMG	C29-C28-O8-C9
30	Z	102	LMT	C4B-C5B-C6B-O6B
30	m	102	LMT	C4'-C5'-C6'-O6'
30	b	624	LMT	C4'-C5'-C6'-O6'
30	z	101	LMT	O5B-C1B-O1B-C4'
34	d	406	DGD	C7B-C8B-C9B-CAB
26	a	401	SQD	C15-C16-C17-C18
23	B	617	CLA	C8-C10-C11-C12
33	D	414	HTG	C1'-C2'-C3'-C4'
27	c	921	LMG	C4-C5-C6-O5
26	B	621	SQD	C31-C32-C33-C34
33	B	631	HTG	C4-C5-C6-O6
23	b	607	CLA	C13-C15-C16-C17
23	C	506	CLA	C5-C6-C7-C8
23	A	410	CLA	C13-C15-C16-C17
34	C	517	DGD	C1B-C2B-C3B-C4B
36	l	101	LHG	C7-C8-C9-C10
26	a	401	SQD	O6-C44-C45-O47

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Mol	Chain	Res	Type	Atoms
26	A	418	SQD	O6-C44-C45-O47
23	c	912	CLA	C14-C13-C15-C16
23	B	602	CLA	C14-C13-C15-C16
23	C	502	CLA	C14-C13-C15-C16
23	c	907	CLA	C6-C7-C8-C9
23	c	910	CLA	C11-C10-C8-C9
23	b	604	CLA	C11-C10-C8-C9
23	C	504	CLA	C11-C12-C13-C14
23	c	913	CLA	C6-C7-C8-C9
23	B	614	CLA	C11-C12-C13-C14
30	Z	102	LMT	O5B-C5B-C6B-O6B
30	B	623	LMT	C4B-C5B-C6B-O6B
33	b	627	HTG	C4-C5-C6-O6
34	c	918	DGD	C1A-C2A-C3A-C4A
34	c	919	DGD	C1A-C2A-C3A-C4A
26	L	103	SQD	C7-C8-C9-C10
34	d	406	DGD	C1B-C2B-C3B-C4B
26	A	418	SQD	C23-C24-C25-C26
27	c	920	LMG	O10-C28-O8-C9
30	F	102	LMT	C4'-C5'-C6'-O6'
36	E	101	LHG	C24-C23-O8-C6
23	b	617	CLA	C5-C6-C7-C8
23	A	410	CLA	C10-C11-C12-C13
23	b	619	CLA	C13-C15-C16-C17
23	c	910	CLA	C13-C15-C16-C17
36	D	408	LHG	C23-C24-C25-C26
23	C	512	CLA	O1D-CGD-O2D-CED
33	U	201	HTG	C1'-C2'-C3'-C4'
23	c	914	CLA	C10-C11-C12-C13
23	A	410	CLA	C15-C16-C17-C18
23	B	607	CLA	C10-C11-C12-C13
23	C	509	CLA	C13-C15-C16-C17
23	B	614	CLA	C8-C10-C11-C12
30	J	102	LMT	C4'-C5'-C6'-O6'
34	c	919	DGD	C2B-C3B-C4B-C5B
27	c	920	LMG	C28-C29-C30-C31
34	D	406	DGD	C1B-C2B-C3B-C4B
36	d	407	LHG	C23-C24-C25-C26
26	a	401	SQD	C23-C24-C25-C26
36	a	417	LHG	C23-C24-C25-C26
23	c	914	CLA	C5-C6-C7-C8
23	C	512	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	B	617	CLA	C2-C1-O2A-CGA
23	C	506	CLA	C13-C15-C16-C17
23	b	619	CLA	C15-C16-C17-C18
23	c	907	CLA	C10-C11-C12-C13
27	c	921	LMG	C10-C11-C12-C13
27	d	410	LMG	C10-C11-C12-C13
30	b	624	LMT	O5'-C5'-C6'-O6'
23	C	513	CLA	C11-C12-C13-C15
23	D	402	CLA	C12-C13-C15-C16
23	a	414	CLA	C12-C13-C15-C16
23	b	609	CLA	C11-C12-C13-C15
23	c	907	CLA	C12-C13-C15-C16
23	B	615	CLA	C11-C10-C8-C7
23	D	403	CLA	C11-C10-C8-C7
23	c	905	CLA	C12-C13-C15-C16
23	B	614	CLA	C11-C10-C8-C7
25	T	101	BCR	C13-C14-C15-C16
30	Z	102	LMT	O5B-C1B-O1B-C4'
23	a	414	CLA	C10-C11-C12-C13
23	a	414	CLA	C15-C16-C17-C18
30	Z	102	LMT	C2B-C1B-O1B-C4'
26	a	401	SQD	O5-C1-O6-C44
23	a	409	CLA	C15-C16-C17-C18
23	b	606	CLA	C5-C6-C7-C8
28	a	419	PL9	C19-C21-C22-C23
30	B	623	LMT	O1'-C1-C2-C3
33	U	201	HTG	S1-C1'-C2'-C3'
24	a	413	PHO	C2C-C3C-CAC-CBC
36	E	101	LHG	O2-C2-C3-O3
26	B	621	SQD	O49-C7-O47-C45
23	B	616	CLA	C5-C6-C7-C8
23	a	414	CLA	C8-C10-C11-C12
23	C	509	CLA	C8-C10-C11-C12
30	b	625	LMT	O1'-C1-C2-C3
30	M	101	LMT	O5'-C5'-C6'-O6'
23	B	616	CLA	C10-C11-C12-C13
23	B	614	CLA	C15-C16-C17-C18
23	B	607	CLA	O1D-CGD-O2D-CED
36	E	101	LHG	O10-C23-O8-C6
26	B	621	SQD	C8-C7-O47-C45
23	B	615	CLA	C5-C6-C7-C8
23	D	403	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
36	L	101	LHG	C4-O6-P-O3
36	D	409	LHG	C3-O3-P-O6
36	l	101	LHG	C4-O6-P-O3
36	a	417	LHG	C3-O3-P-O6
36	a	417	LHG	C4-O6-P-O3
36	E	101	LHG	C3-O3-P-O6
30	M	102	LMT	O5'-C5'-C6'-O6'
23	A	410	CLA	C3-C5-C6-C7
30	m	102	LMT	O1'-C1-C2-C3
26	B	621	SQD	C24-C23-O48-C46
26	a	401	SQD	C7-C8-C9-C10
23	c	908	CLA	O1D-CGD-O2D-CED
36	d	408	LHG	C1-C2-C3-O3
36	a	417	LHG	C1-C2-C3-O3
23	b	609	CLA	C13-C15-C16-C17
23	B	607	CLA	C2A-CAA-CBA-CGA
23	c	912	CLA	C16-C17-C18-C20
34	C	518	DGD	C8B-C9B-CAB-CBB
27	a	418	LMG	C15-C16-C17-C18
23	b	618	CLA	C10-C11-C12-C13
23	c	911	CLA	C8-C10-C11-C12
33	B	625	HTG	C1'-C2'-C3'-C4'
27	A	413	LMG	C17-C18-C19-C20
34	c	918	DGD	C2B-C3B-C4B-C5B
30	z	101	LMT	C7-C8-C9-C10
34	D	406	DGD	C9A-CAA-CBA-CCA
34	D	406	DGD	CCB-CDB-CEB-CFB
26	L	103	SQD	C15-C16-C17-C18
26	L	103	SQD	C29-C30-C31-C32
36	l	101	LHG	C27-C28-C29-C30
34	H	102	DGD	C7A-C8A-C9A-CAA
30	F	102	LMT	C3-C4-C5-C6
26	a	416	SQD	C33-C34-C35-C36
36	a	417	LHG	C14-C15-C16-C17
27	A	413	LMG	C29-C28-O8-C9
33	U	201	HTG	C2'-C1'-S1-C1
27	A	413	LMG	C14-C15-C16-C17
36	d	409	LHG	C31-C32-C33-C34
34	C	517	DGD	CBA-CCA-CDA-CEA
26	A	412	SQD	C16-C17-C18-C19
34	d	406	DGD	C6B-C7B-C8B-C9B
27	d	410	LMG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
36	D	410	LHG	C28-C29-C30-C31
27	B	622	LMG	C36-C37-C38-C39
27	b	623	LMG	C20-C21-C22-C23
33	O	303	HTG	C3'-C4'-C5'-C6'
27	C	519	LMG	C15-C16-C17-C18
30	J	102	LMT	C7-C8-C9-C10
26	B	621	SQD	C46-C45-O47-C7
34	c	917	DGD	C4B-C5B-C6B-C7B
27	a	418	LMG	C20-C21-C22-C23
27	d	410	LMG	C20-C21-C22-C23
27	A	413	LMG	C21-C22-C23-C24
27	A	413	LMG	C36-C37-C38-C39
27	Z	101	LMG	C29-C30-C31-C32
27	c	920	LMG	C13-C14-C15-C16
34	D	406	DGD	C5A-C6A-C7A-C8A
36	d	409	LHG	C15-C16-C17-C18
36	d	409	LHG	C17-C18-C19-C20
27	a	418	LMG	C32-C33-C34-C35
36	d	408	LHG	C32-C33-C34-C35
34	C	516	DGD	C7A-C8A-C9A-CAA
34	C	516	DGD	C4B-C5B-C6B-C7B
27	b	623	LMG	C14-C15-C16-C17
36	a	417	LHG	C16-C17-C18-C19
30	C	520	LMT	C4B-C5B-C6B-O6B
24	A	409	PHO	O1D-CGD-O2D-CED
36	D	408	LHG	C30-C31-C32-C33
36	L	101	LHG	C12-C13-C14-C15
27	Z	101	LMG	C31-C32-C33-C34
26	D	407	SQD	C33-C34-C35-C36
34	c	919	DGD	CCB-CDB-CEB-CFB
30	Z	102	LMT	O1'-C1-C2-C3
34	D	406	DGD	C1A-C2A-C3A-C4A
27	C	519	LMG	C10-C11-C12-C13
30	t	102	LMT	C2'-C1'-O1'-C1
30	Z	102	LMT	C2'-C1'-O1'-C1
26	A	418	SQD	C2-C1-O6-C44
27	A	413	LMG	C12-C13-C14-C15
26	B	621	SQD	C15-C16-C17-C18
30	z	101	LMT	C11-C10-C9-C8
26	D	407	SQD	C11-C10-C9-C8
27	c	920	LMG	C32-C33-C34-C35
34	c	919	DGD	CBA-CCA-CDA-CEA

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Mol	Chain	Res	Type	Atoms
36	l	101	LHG	C31-C32-C33-C34
27	d	410	LMG	C35-C36-C37-C38
26	a	416	SQD	C34-C35-C36-C37
27	B	622	LMG	C30-C31-C32-C33
23	C	506	CLA	C16-C17-C18-C20
23	b	609	CLA	C16-C17-C18-C19
23	B	617	CLA	C16-C17-C18-C19
34	D	406	DGD	CAA-CBA-CCA-CDA
36	d	407	LHG	C27-C28-C29-C30
30	b	624	LMT	C6-C7-C8-C9
34	C	516	DGD	C4A-C5A-C6A-C7A
33	B	625	HTG	C2'-C3'-C4'-C5'
36	a	417	LHG	C13-C14-C15-C16
26	f	102	SQD	C28-C29-C30-C31
23	c	910	CLA	C14-C13-C15-C16
23	B	617	CLA	C6-C7-C8-C9
34	c	918	DGD	C3B-C4B-C5B-C6B
34	C	518	DGD	CBA-CCA-CDA-CEA
36	l	101	LHG	C33-C34-C35-C36
27	d	410	LMG	C11-C12-C13-C14
34	C	516	DGD	C5B-C6B-C7B-C8B
30	F	102	LMT	C4-C5-C6-C7
30	F	102	LMT	C5-C6-C7-C8
27	B	622	LMG	C31-C32-C33-C34
27	b	623	LMG	C19-C20-C21-C22
27	D	411	LMG	C19-C20-C21-C22
36	E	101	LHG	C25-C26-C27-C28
27	c	921	LMG	C38-C39-C40-C41
34	c	918	DGD	C5B-C6B-C7B-C8B
34	c	918	DGD	C8B-C9B-CAB-CBB
36	L	101	LHG	C10-C11-C12-C13
34	c	917	DGD	C2B-C3B-C4B-C5B
31	f	104	GOL	C1-C2-C3-O3
36	D	408	LHG	O1-C1-C2-C3
31	D	415	GOL	C1-C2-C3-O3
31	B	633	GOL	C1-C2-C3-O3
31	v	203	GOL	O1-C1-C2-C3
31	B	635	GOL	C1-C2-C3-O3
33	B	630	HTG	C1'-C2'-C3'-C4'
31	b	632	GOL	O1-C1-C2-C3
31	b	632	GOL	C1-C2-C3-O3
31	b	633	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
31	B	638	GOL	O1-C1-C2-C3
27	A	413	LMG	C32-C33-C34-C35
26	B	621	SQD	C11-C10-C9-C8
34	D	406	DGD	C9B-CAB-CBB-CCB
26	L	103	SQD	C11-C10-C9-C8
26	A	412	SQD	C11-C12-C13-C14
27	b	623	LMG	C15-C16-C17-C18
27	C	519	LMG	C34-C35-C36-C37
26	A	412	SQD	C7-C8-C9-C10
26	A	418	SQD	C7-C8-C9-C10
27	A	413	LMG	C13-C14-C15-C16
30	B	623	LMT	C6-C7-C8-C9
30	A	419	LMT	C6-C7-C8-C9
30	t	102	LMT	C11-C10-C9-C8
27	c	920	LMG	C35-C36-C37-C38
27	a	418	LMG	C16-C17-C18-C19
24	A	409	PHO	C2C-C3C-CAC-CBC
34	C	517	DGD	C9B-CAB-CBB-CCB
36	D	409	LHG	C32-C33-C34-C35
34	H	102	DGD	CBA-CCA-CDA-CEA
26	a	401	SQD	C13-C14-C15-C16
27	D	411	LMG	C12-C13-C14-C15
36	E	101	LHG	C33-C34-C35-C36
23	d	403	CLA	C16-C17-C18-C19
23	d	403	CLA	C16-C17-C18-C20
23	C	506	CLA	C16-C17-C18-C19
23	C	502	CLA	C16-C17-C18-C20
23	C	507	CLA	C16-C17-C18-C19
23	C	507	CLA	C16-C17-C18-C20
30	Z	102	LMT	O5'-C1'-O1'-C1
26	A	418	SQD	O5-C1-O6-C44
23	C	506	CLA	C10-C11-C12-C13
23	c	905	CLA	C8-C10-C11-C12
23	B	614	CLA	C13-C15-C16-C17
26	B	621	SQD	C29-C30-C31-C32
27	c	920	LMG	C18-C19-C20-C21
34	C	517	DGD	CAA-CBA-CCA-CDA
34	d	406	DGD	C5B-C6B-C7B-C8B
26	a	401	SQD	C26-C27-C28-C29
27	C	519	LMG	C38-C39-C40-C41
34	c	918	DGD	CBB-CCB-CDB-CEB
36	L	101	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
26	B	621	SQD	C17-C18-C19-C20
27	a	418	LMG	C11-C12-C13-C14
34	H	102	DGD	CBB-CCB-CDB-CEB
26	a	401	SQD	C9-C10-C11-C12
33	B	630	HTG	C2'-C3'-C4'-C5'
27	b	623	LMG	C29-C30-C31-C32
33	b	626	HTG	C2'-C3'-C4'-C5'
23	a	411	CLA	C13-C15-C16-C17
23	B	607	CLA	C15-C16-C17-C18
26	D	407	SQD	C24-C25-C26-C27
26	A	412	SQD	C15-C16-C17-C18
26	a	416	SQD	C9-C10-C11-C12
26	a	416	SQD	C14-C15-C16-C17
27	b	623	LMG	C17-C18-C19-C20
36	a	417	LHG	C24-C25-C26-C27
36	E	101	LHG	C30-C31-C32-C33
30	b	624	LMT	C1-C2-C3-C4
34	C	518	DGD	C2A-C3A-C4A-C5A
26	L	103	SQD	C34-C35-C36-C37
26	a	401	SQD	C14-C15-C16-C17
27	b	623	LMG	C38-C39-C40-C41
23	b	614	CLA	O1D-CGD-O2D-CED
23	B	602	CLA	C10-C11-C12-C13
23	c	907	CLA	C15-C16-C17-C18
23	B	615	CLA	C10-C11-C12-C13
30	Z	102	LMT	C2-C1-O1'-C1'
30	b	624	LMT	C2-C1-O1'-C1'
26	D	407	SQD	C26-C27-C28-C29
36	d	409	LHG	C18-C19-C20-C21
34	C	517	DGD	C3A-C4A-C5A-C6A
36	d	407	LHG	C29-C30-C31-C32
27	B	622	LMG	C34-C35-C36-C37
30	M	101	LMT	C2-C3-C4-C5
23	c	912	CLA	C16-C17-C18-C19
23	c	907	CLA	C16-C17-C18-C19
23	c	903	CLA	C16-C17-C18-C19
23	c	903	CLA	C16-C17-C18-C20
33	B	631	HTG	S1-C1'-C2'-C3'
34	c	918	DGD	C5A-C6A-C7A-C8A
27	c	920	LMG	C29-C30-C31-C32
36	d	409	LHG	C10-C11-C12-C13
27	b	623	LMG	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
36	a	417	LHG	C10-C11-C12-C13
36	E	101	LHG	C18-C19-C20-C21
34	D	406	DGD	O1G-C1G-C2G-C3G
26	A	412	SQD	O6-C44-C45-C46
26	a	416	SQD	O6-C44-C45-C46
30	m	102	LMT	C1-C2-C3-C4
30	J	102	LMT	C1-C2-C3-C4
27	c	920	LMG	C19-C20-C21-C22
34	C	517	DGD	C9A-CAA-CBA-CCA
34	C	516	DGD	O6D-C5D-C6D-O5D
23	b	604	CLA	C3-C5-C6-C7
27	Z	101	LMG	C28-C29-C30-C31
34	C	517	DGD	C1A-C2A-C3A-C4A
26	L	103	SQD	C10-C11-C12-C13
23	c	911	CLA	C2-C3-C5-C6
28	A	414	PL9	C28-C29-C31-C32
27	A	413	LMG	C11-C10-O7-C8
27	Z	101	LMG	C18-C19-C20-C21
34	D	406	DGD	C7A-C8A-C9A-CAA
30	c	922	LMT	C6-C7-C8-C9
26	a	401	SQD	C34-C35-C36-C37
31	c	927	GOL	O2-C2-C3-O3
31	B	635	GOL	O1-C1-C2-O2
36	D	409	LHG	O1-C1-C2-O2
31	b	633	GOL	O1-C1-C2-O2
31	c	930	GOL	O2-C2-C3-O3
31	B	638	GOL	O1-C1-C2-O2
31	a	423	GOL	O2-C2-C3-O3
26	f	102	SQD	O5-C1-O6-C44
31	C	524	GOL	O2-C2-C3-O3
31	b	636	GOL	O1-C1-C2-O2
36	d	407	LHG	C30-C31-C32-C33
27	B	622	LMG	C17-C18-C19-C20
30	M	101	LMT	O1'-C1-C2-C3
26	f	102	SQD	C27-C28-C29-C30
36	E	101	LHG	C14-C15-C16-C17
34	D	406	DGD	C8B-C9B-CAB-CBB
34	C	517	DGD	C4B-C5B-C6B-C7B
30	Z	102	LMT	C1-C2-C3-C4
23	C	507	CLA	C5-C6-C7-C8
34	c	917	DGD	C8A-C9A-CAA-CBA
33	d	401	HTG	C3'-C4'-C5'-C6'

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Mol	Chain	Res	Type	Atoms
26	A	412	SQD	C28-C29-C30-C31
36	D	410	LHG	C31-C32-C33-C34
36	E	101	LHG	C9-C10-C11-C12
27	A	413	LMG	O10-C28-O8-C9
26	B	621	SQD	O10-C23-O48-C46
36	l	101	LHG	C25-C26-C27-C28
27	C	519	LMG	C31-C32-C33-C34
27	A	413	LMG	O9-C10-O7-C8
34	d	406	DGD	O1B-C1B-O2G-C2G
30	b	625	LMT	C4'-C5'-C6'-O6'
36	D	408	LHG	C29-C30-C31-C32
27	Z	101	LMG	C39-C40-C41-C42
27	a	418	LMG	C30-C31-C32-C33
23	a	409	CLA	C2C-C3C-CAC-CBC
34	H	102	DGD	C9B-CAB-CBB-CCB
36	E	101	LHG	C17-C18-C19-C20
23	b	611	CLA	C13-C15-C16-C17
27	c	921	LMG	C35-C36-C37-C38
36	D	408	LHG	C27-C28-C29-C30
27	a	418	LMG	C36-C37-C38-C39
30	a	402	LMT	C2-C3-C4-C5
34	H	102	DGD	C9A-CAA-CBA-CCA
26	a	401	SQD	C31-C32-C33-C34
27	C	519	LMG	C32-C33-C34-C35
36	L	101	LHG	C7-C8-C9-C10
25	B	618	BCR	C1-C6-C7-C8
25	B	618	BCR	C5-C6-C7-C8
25	b	620	BCR	C5-C6-C7-C8
33	C	522	HTG	O5-C5-C6-O6
26	A	418	SQD	C29-C30-C31-C32
30	F	102	LMT	C1-C2-C3-C4
34	d	406	DGD	C2B-C1B-O2G-C2G
26	A	418	SQD	C35-C36-C37-C38
27	B	622	LMG	C15-C16-C17-C18
27	b	623	LMG	C18-C19-C20-C21
26	a	416	SQD	C27-C28-C29-C30
27	b	623	LMG	C40-C41-C42-C43
28	A	414	PL9	C25-C24-C26-C27
23	b	617	CLA	C6-C7-C8-C10
23	a	411	CLA	C6-C7-C8-C10
23	B	604	CLA	C6-C7-C8-C10
23	b	616	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
28	A	414	PL9	C23-C24-C26-C27
23	b	609	CLA	C6-C7-C8-C10
23	c	910	CLA	C12-C13-C15-C16
23	B	617	CLA	C6-C7-C8-C10
23	B	617	CLA	C12-C13-C15-C16
26	B	621	SQD	C24-C25-C26-C27
23	d	403	CLA	C8-C10-C11-C12
26	a	416	SQD	C26-C27-C28-C29
23	c	902	CLA	O1D-CGD-O2D-CED
23	c	910	CLA	C15-C16-C17-C18
23	b	614	CLA	C13-C15-C16-C17
26	B	621	SQD	C16-C17-C18-C19
27	B	622	LMG	C39-C40-C41-C42
26	f	102	SQD	C29-C30-C31-C32
30	B	623	LMT	C5-C6-C7-C8
23	b	615	CLA	C13-C15-C16-C17
34	c	918	DGD	C4B-C5B-C6B-C7B
36	D	408	LHG	C24-C25-C26-C27
26	B	621	SQD	C27-C28-C29-C30
36	d	409	LHG	C34-C35-C36-C37
36	l	101	LHG	C34-C35-C36-C37
26	a	401	SQD	C28-C29-C30-C31
33	B	624	HTG	C3'-C4'-C5'-C6'
34	h	102	DGD	C7A-C8A-C9A-CAA
30	a	402	LMT	C1-C2-C3-C4
23	c	907	CLA	C3-C5-C6-C7
34	d	406	DGD	CAA-CBA-CCA-CDA
36	a	417	LHG	C17-C18-C19-C20
23	b	606	CLA	CBD-CGD-O2D-CED
23	B	612	CLA	C15-C16-C17-C18
23	D	403	CLA	C10-C11-C12-C13
27	Z	101	LMG	C30-C31-C32-C33
27	Z	101	LMG	C37-C38-C39-C40
34	c	919	DGD	C6A-C7A-C8A-C9A
36	l	101	LHG	C11-C10-C9-C8
26	a	401	SQD	C16-C17-C18-C19
36	D	410	LHG	C30-C31-C32-C33
27	c	920	LMG	C16-C17-C18-C19
23	a	410	CLA	C2C-C3C-CAC-CBC
27	B	622	LMG	C18-C19-C20-C21
26	D	407	SQD	O6-C44-C45-O47
26	A	412	SQD	O6-C44-C45-O47

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Mol	Chain	Res	Type	Atoms
34	d	406	DGD	O1G-C1G-C2G-O2G
26	a	416	SQD	O6-C44-C45-O47
27	a	418	LMG	C29-C28-O8-C9
33	b	602	HTG	C3'-C4'-C5'-C6'
23	B	617	CLA	C16-C17-C18-C20
26	a	401	SQD	C27-C28-C29-C30
26	a	416	SQD	C12-C13-C14-C15
27	b	623	LMG	C39-C40-C41-C42
34	h	102	DGD	CCA-CDA-CEA-CFA
23	c	911	CLA	C4-C3-C5-C6
36	E	101	LHG	C7-C8-C9-C10
28	a	419	PL9	C4-C3-C7-C8
30	t	102	LMT	C4-C5-C6-C7
23	b	617	CLA	C6-C7-C8-C9
23	a	411	CLA	C6-C7-C8-C9
23	B	617	CLA	C11-C12-C13-C14
23	B	617	CLA	C14-C13-C15-C16
23	B	615	CLA	C14-C13-C15-C16
23	D	403	CLA	C11-C10-C8-C9
23	c	905	CLA	C11-C10-C8-C9
23	c	905	CLA	C14-C13-C15-C16
23	B	605	CLA	O1D-CGD-O2D-CED
30	Z	102	LMT	C4-C5-C6-C7
27	B	622	LMG	C16-C17-C18-C19
23	b	609	CLA	C2A-CAA-CBA-CGA
26	A	418	SQD	C26-C27-C28-C29
34	c	917	DGD	O6D-C5D-C6D-O5D
26	f	102	SQD	C24-C25-C26-C27
23	c	914	CLA	C1A-C2A-CAA-CBA
23	b	617	CLA	C16-C17-C18-C20
23	b	605	CLA	C16-C17-C18-C19
23	a	414	CLA	C16-C17-C18-C19
23	b	609	CLA	C16-C17-C18-C20
23	c	910	CLA	C16-C17-C18-C19
34	c	917	DGD	C9A-CAA-CBA-CCA
34	D	406	DGD	CBA-CCA-CDA-CEA
25	c	915	BCR	C19-C20-C21-C22
23	c	912	CLA	C13-C15-C16-C17
30	t	102	LMT	C3-C4-C5-C6
33	B	630	HTG	C4-C5-C6-O6
34	c	917	DGD	C6A-C7A-C8A-C9A
30	B	623	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
34	h	102	DGD	CBB-CCB-CDB-CEB
30	a	402	LMT	C4B-C5B-C6B-O6B
26	B	621	SQD	C32-C33-C34-C35
34	c	917	DGD	O6E-C5E-C6E-O5E
23	C	504	CLA	C13-C15-C16-C17
23	b	619	CLA	C16-C17-C18-C19
30	m	101	LMT	C4'-C5'-C6'-O6'
30	a	402	LMT	O1'-C1-C2-C3
23	d	403	CLA	C4-C3-C5-C6
23	D	402	CLA	C2C-C3C-CAC-CBC
27	D	411	LMG	C35-C36-C37-C38
36	d	408	LHG	C11-C10-C9-C8
27	b	623	LMG	C37-C38-C39-C40
34	C	516	DGD	C1B-C2B-C3B-C4B
30	A	419	LMT	C7-C8-C9-C10
26	a	401	SQD	C11-C12-C13-C14
36	D	410	LHG	C16-C17-C18-C19
26	f	102	SQD	C26-C27-C28-C29
23	B	602	CLA	C2A-CAA-CBA-CGA
23	a	414	CLA	C16-C17-C18-C20
23	b	617	CLA	O1D-CGD-O2D-CED
34	c	917	DGD	C4D-C5D-C6D-O5D
26	B	621	SQD	C44-C45-C46-O48
26	D	407	SQD	O6-C44-C45-C46
27	a	418	LMG	O1-C7-C8-C9
27	a	418	LMG	C7-C8-C9-O8
26	L	103	SQD	C44-C45-C46-O48
34	d	406	DGD	C1G-C2G-C3G-O3G
26	a	401	SQD	O6-C44-C45-C46
26	A	418	SQD	O6-C44-C45-C46
27	d	410	LMG	O6-C5-C6-O5
34	C	518	DGD	CDA-CEA-CFA-CGA
26	A	412	SQD	C10-C11-C12-C13
34	C	516	DGD	CCA-CDA-CEA-CFA
34	c	918	DGD	C2G-C3G-O3G-C1D
27	Z	101	LMG	C8-C7-O1-C1
26	B	621	SQD	C45-C44-O6-C1
26	L	103	SQD	C45-C44-O6-C1
34	C	517	DGD	C2G-C3G-O3G-C1D
34	C	517	DGD	C5D-C6D-O5D-C1E
33	b	601	HTG	C4'-C5'-C6'-C7'
36	d	409	LHG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
34	d	406	DGD	CDA-CEA-CFA-CGA
30	b	624	LMT	C9-C10-C11-C12
36	D	410	LHG	C17-C18-C19-C20
33	D	414	HTG	C4'-C5'-C6'-C7'
26	L	103	SQD	C35-C36-C37-C38
34	d	406	DGD	CDB-CEB-CFB-CGB
36	E	101	LHG	C19-C20-C21-C22
34	d	406	DGD	C4B-C5B-C6B-C7B
36	a	417	LHG	C26-C27-C28-C29
33	u	201	HTG	C4'-C5'-C6'-C7'
27	Z	101	LMG	C40-C41-C42-C43
26	B	621	SQD	C10-C11-C12-C13
34	D	406	DGD	CBB-CCB-CDB-CEB
36	d	409	LHG	C35-C36-C37-C38
26	L	103	SQD	C18-C19-C20-C21
36	D	410	LHG	C32-C33-C34-C35
27	D	411	LMG	O6-C5-C6-O5
31	a	424	GOL	O1-C1-C2-O2
27	Z	101	LMG	C17-C18-C19-C20
36	d	409	LHG	C12-C13-C14-C15
30	b	625	LMT	C9-C10-C11-C12
30	a	402	LMT	O5'-C5'-C6'-O6'
26	A	418	SQD	C27-C28-C29-C30
36	a	417	LHG	C19-C20-C21-C22
27	c	920	LMG	C12-C13-C14-C15
34	C	517	DGD	C4A-C5A-C6A-C7A
23	D	403	CLA	C16-C17-C18-C19
23	c	914	CLA	CBA-CGA-O2A-C1
34	c	917	DGD	CDA-CEA-CFA-CGA
34	C	517	DGD	C7A-C8A-C9A-CAA
34	C	516	DGD	O6E-C5E-C6E-O5E
27	c	920	LMG	C37-C38-C39-C40
27	d	410	LMG	C29-C30-C31-C32
34	d	406	DGD	CBB-CCB-CDB-CEB
33	B	626	HTG	C3'-C4'-C5'-C6'
27	D	411	LMG	C15-C16-C17-C18
23	a	414	CLA	C5-C6-C7-C8
27	A	413	LMG	C22-C23-C24-C25
30	B	623	LMT	C7-C8-C9-C10
33	c	923	HTG	C2'-C3'-C4'-C5'
36	d	409	LHG	C13-C14-C15-C16
36	d	409	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
34	d	406	DGD	CBA-CCA-CDA-CEA
30	F	102	LMT	C9-C10-C11-C12
23	b	605	CLA	C16-C17-C18-C20
27	a	418	LMG	C12-C13-C14-C15
26	a	416	SQD	C10-C11-C12-C13
36	E	101	LHG	C11-C12-C13-C14
27	C	519	LMG	C22-C23-C24-C25
27	a	418	LMG	O10-C28-O8-C9
34	c	919	DGD	C7A-C8A-C9A-CAA
27	B	622	LMG	C14-C15-C16-C17
33	O	303	HTG	C1'-C2'-C3'-C4'
26	D	407	SQD	C23-C24-C25-C26
23	B	617	CLA	C13-C15-C16-C17
27	Z	101	LMG	C13-C14-C15-C16
34	d	406	DGD	C2A-C3A-C4A-C5A
27	B	622	LMG	C40-C41-C42-C43
26	B	621	SQD	O47-C45-C46-O48
27	c	920	LMG	C36-C37-C38-C39
30	b	625	LMT	C5-C6-C7-C8
23	c	914	CLA	O1A-CGA-O2A-C1
23	c	907	CLA	C16-C17-C18-C20
36	d	409	LHG	C24-C25-C26-C27
23	d	403	CLA	C11-C12-C13-C15
23	C	506	CLA	C6-C7-C8-C10
23	C	506	CLA	C11-C12-C13-C15
23	c	908	CLA	C11-C10-C8-C7
23	A	410	CLA	C11-C10-C8-C7
23	C	507	CLA	C11-C10-C8-C7
23	c	904	CLA	C6-C7-C8-C10
23	b	609	CLA	C12-C13-C15-C16
23	B	617	CLA	C11-C12-C13-C15
23	B	615	CLA	C11-C12-C13-C15
23	B	615	CLA	C12-C13-C15-C16
23	C	504	CLA	C11-C12-C13-C15
23	c	905	CLA	C11-C10-C8-C7
30	b	625	LMT	C1-C2-C3-C4
27	C	519	LMG	C39-C40-C41-C42
23	d	403	CLA	C11-C12-C13-C14
23	D	402	CLA	C14-C13-C15-C16
23	C	506	CLA	C6-C7-C8-C9
23	B	604	CLA	C6-C7-C8-C9
23	A	410	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
23	a	414	CLA	C14-C13-C15-C16
23	b	614	CLA	C14-C13-C15-C16
23	B	615	CLA	C11-C10-C8-C9
23	B	607	CLA	C11-C10-C8-C9
23	B	611	CLA	C14-C13-C15-C16
23	C	504	CLA	C14-C13-C15-C16
34	d	406	DGD	C6A-C7A-C8A-C9A
26	A	418	SQD	C24-C23-O48-C46
26	B	621	SQD	C13-C14-C15-C16
26	L	103	SQD	C24-C25-C26-C27
25	c	915	BCR	C36-C18-C19-C20
27	C	519	LMG	C17-C18-C19-C20
30	J	102	LMT	C9-C10-C11-C12
23	B	605	CLA	C3-C5-C6-C7
23	d	403	CLA	C15-C16-C17-C18
34	C	517	DGD	CCB-CDB-CEB-CFB
27	C	519	LMG	C29-C28-O8-C9
33	c	923	HTG	C3'-C4'-C5'-C6'
27	A	413	LMG	C31-C32-C33-C34
36	a	417	LHG	C9-C10-C11-C12
27	d	410	LMG	C36-C37-C38-C39
34	C	516	DGD	C5A-C6A-C7A-C8A
23	b	615	CLA	C3-C5-C6-C7
23	C	510	CLA	O1D-CGD-O2D-CED
34	D	406	DGD	C4A-C5A-C6A-C7A
30	C	520	LMT	C6-C7-C8-C9
33	B	625	HTG	C4'-C5'-C6'-C7'
23	C	507	CLA	C13-C15-C16-C17
27	A	413	LMG	C15-C16-C17-C18
23	C	507	CLA	C4-C3-C5-C6
34	C	517	DGD	C7B-C8B-C9B-CAB
30	c	922	LMT	O1'-C1-C2-C3
23	b	618	CLA	C5-C6-C7-C8
27	d	410	LMG	C40-C41-C42-C43
26	a	416	SQD	C29-C30-C31-C32
23	c	910	CLA	C16-C17-C18-C20
23	a	409	CLA	C4C-C3C-CAC-CBC
34	h	102	DGD	O2G-C1B-C2B-C3B
30	J	102	LMT	C5-C6-C7-C8
23	b	618	CLA	O1D-CGD-O2D-CED
23	c	905	CLA	C3A-C2A-CAA-CBA
34	C	516	DGD	CAA-CBA-CCA-CDA

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Mol	Chain	Res	Type	Atoms
25	k	102	BCR	C19-C20-C21-C22
30	b	625	LMT	C2-C1-O1'-C1'
30	m	101	LMT	C2-C1-O1'-C1'
30	M	101	LMT	C2-C1-O1'-C1'
26	A	418	SQD	C28-C29-C30-C31
34	c	919	DGD	C9B-CAB-CBB-CCB
23	b	618	CLA	C16-C17-C18-C20
27	A	413	LMG	C7-C8-C9-O8
34	d	406	DGD	O1G-C1G-C2G-C3G
26	A	418	SQD	C25-C26-C27-C28
26	L	103	SQD	C17-C18-C19-C20
36	l	101	LHG	C10-C11-C12-C13
26	A	412	SQD	C33-C34-C35-C36
34	H	102	DGD	CDB-CEB-CFB-CGB
23	C	513	CLA	O2A-C1-C2-C3
33	b	601	HTG	C3'-C4'-C5'-C6'
30	b	625	LMT	C3-C4-C5-C6
34	h	102	DGD	CDB-CEB-CFB-CGB
30	A	419	LMT	C1-C2-C3-C4
34	C	518	DGD	C6A-C7A-C8A-C9A
23	a	410	CLA	C4C-C3C-CAC-CBC
27	D	411	LMG	C36-C37-C38-C39
34	D	406	DGD	CDB-CEB-CFB-CGB
36	a	417	LHG	C25-C26-C27-C28
34	h	102	DGD	C5B-C6B-C7B-C8B
27	C	519	LMG	C14-C15-C16-C17
27	C	519	LMG	C29-C30-C31-C32
23	b	604	CLA	C10-C11-C12-C13
26	L	103	SQD	C27-C28-C29-C30
33	C	521	HTG	C2'-C3'-C4'-C5'
31	f	104	GOL	O2-C2-C3-O3
31	h	103	GOL	O2-C2-C3-O3
27	c	921	LMG	C11-C12-C13-C14
36	D	409	LHG	C11-C10-C9-C8
36	a	417	LHG	O6-C4-C5-O7
34	c	919	DGD	C2A-C1A-O1G-C1G
34	C	516	DGD	C3B-C4B-C5B-C6B
27	C	519	LMG	O10-C28-O8-C9
23	a	409	CLA	C16-C17-C18-C20
27	A	413	LMG	C19-C20-C21-C22
34	C	517	DGD	CAB-CBB-CCB-CDB
23	B	613	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
26	a	416	SQD	C35-C36-C37-C38
36	d	409	LHG	C27-C28-C29-C30
36	D	409	LHG	C16-C17-C18-C19
27	A	413	LMG	O7-C8-C9-O8
27	a	418	LMG	O7-C8-C9-O8
34	d	406	DGD	O2G-C2G-C3G-O3G
34	C	518	DGD	CDB-CEB-CFB-CGB
36	E	101	LHG	C8-C7-O7-C5
26	a	416	SQD	C7-C8-C9-C10
23	b	617	CLA	C16-C17-C18-C19
23	b	619	CLA	C16-C17-C18-C20
26	L	103	SQD	O5-C1-O6-C44
30	C	520	LMT	C5-C6-C7-C8
23	d	402	CLA	C2-C1-O2A-CGA
23	D	402	CLA	C2-C1-O2A-CGA
36	E	101	LHG	C11-C10-C9-C8
23	c	908	CLA	C5-C6-C7-C8
23	c	908	CLA	C11-C10-C8-C9
23	b	613	CLA	C11-C12-C13-C14
23	B	615	CLA	C11-C12-C13-C14
23	C	509	CLA	C11-C10-C8-C9
36	D	410	LHG	C2-C3-O3-P
34	D	406	DGD	CAB-CBB-CCB-CDB
34	C	517	DGD	CCA-CDA-CEA-CFA
26	a	401	SQD	C24-C25-C26-C27
23	C	508	CLA	CBD-CGD-O2D-CED
25	d	404	BCR	C23-C24-C25-C26
25	d	404	BCR	C23-C24-C25-C30
23	C	503	CLA	C8-C10-C11-C12
34	H	102	DGD	CCA-CDA-CEA-CFA
36	E	101	LHG	C15-C16-C17-C18
33	B	626	HTG	C4-C5-C6-O6
25	D	404	BCR	C21-C22-C23-C24
23	b	617	CLA	C10-C11-C12-C13
23	a	414	CLA	C13-C15-C16-C17
23	B	617	CLA	C5-C6-C7-C8
23	c	905	CLA	C15-C16-C17-C18
36	D	410	LHG	C24-C25-C26-C27
27	A	413	LMG	C39-C40-C41-C42
27	b	623	LMG	C36-C37-C38-C39
34	c	917	DGD	C5B-C6B-C7B-C8B
30	t	102	LMT	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
34	C	517	DGD	C6B-C7B-C8B-C9B
26	L	103	SQD	C19-C20-C21-C22
23	C	508	CLA	C11-C10-C8-C7
28	d	405	PL9	C43-C44-C46-C47
23	b	607	CLA	C6-C7-C8-C10
23	C	513	CLA	C6-C7-C8-C10
23	a	411	CLA	C11-C10-C8-C7
23	B	602	CLA	C11-C10-C8-C7
23	B	602	CLA	C11-C12-C13-C15
23	a	414	CLA	C11-C10-C8-C7
23	c	907	CLA	C11-C10-C8-C7
23	b	614	CLA	C12-C13-C15-C16
23	B	607	CLA	C11-C10-C8-C7
23	B	611	CLA	C12-C13-C15-C16
23	C	504	CLA	C12-C13-C15-C16
23	c	913	CLA	C11-C10-C8-C7
23	B	614	CLA	C11-C12-C13-C15
25	t	101	BCR	C13-C14-C15-C16
23	C	508	CLA	C16-C17-C18-C19
30	a	402	LMT	C4'-C5'-C6'-O6'
23	A	405	CLA	C2C-C3C-CAC-CBC
33	U	201	HTG	C2'-C3'-C4'-C5'
34	H	102	DGD	CCB-CDB-CEB-CFB
33	d	401	HTG	C2'-C1'-S1-C1
33	B	631	HTG	C2'-C1'-S1-C1
27	C	519	LMG	C30-C31-C32-C33
23	b	618	CLA	C16-C17-C18-C19
30	B	623	LMT	C11-C10-C9-C8
23	B	611	CLA	C8-C10-C11-C12
30	C	520	LMT	C9-C10-C11-C12
36	E	101	LHG	C13-C14-C15-C16
23	d	403	CLA	CAD-CBD-CGD-O2D
23	b	607	CLA	CAD-CBD-CGD-O2D
23	A	405	CLA	CAD-CBD-CGD-O2D
24	a	412	PHO	CAD-CBD-CGD-O2D
23	C	512	CLA	CAD-CBD-CGD-O2D
24	A	409	PHO	CAD-CBD-CGD-O2D
23	c	902	CLA	CAD-CBD-CGD-O2D
23	B	617	CLA	CAD-CBD-CGD-O2D
23	B	611	CLA	CAD-CBD-CGD-O2D
23	C	509	CLA	CAD-CBD-CGD-O2D
23	c	913	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
36	E	101	LHG	O9-C7-O7-C5
33	b	626	HTG	C3'-C4'-C5'-C6'
26	A	418	SQD	O10-C23-O48-C46
23	C	512	CLA	C16-C17-C18-C20
30	t	102	LMT	O5'-C1'-O1'-C1
26	a	401	SQD	C25-C26-C27-C28
36	E	101	LHG	C2-C3-O3-P
33	B	630	HTG	C3'-C4'-C5'-C6'
30	B	623	LMT	O5B-C5B-C6B-O6B
23	B	609	CLA	C13-C15-C16-C17
27	B	622	LMG	O8-C28-C29-C30
34	c	917	DGD	C7A-C8A-C9A-CAA
27	d	410	LMG	C17-C18-C19-C20
34	c	919	DGD	CDB-CEB-CFB-CGB
30	c	922	LMT	C11-C10-C9-C8
36	D	410	LHG	C29-C30-C31-C32
23	B	611	CLA	C16-C17-C18-C20
30	F	102	LMT	C2B-C1B-O1B-C4'
23	B	606	CLA	CHA-CBD-CGD-O1D
23	B	603	CLA	CHA-CBD-CGD-O2D
23	C	506	CLA	CHA-CBD-CGD-O1D
23	c	908	CLA	CHA-CBD-CGD-O1D
24	A	409	PHO	CHA-CBD-CGD-O1D
23	B	602	CLA	CHA-CBD-CGD-O2D
23	C	502	CLA	CHA-CBD-CGD-O2D
23	c	909	CLA	CHA-CBD-CGD-O2D
23	c	906	CLA	CHA-CBD-CGD-O1D
23	c	903	CLA	CHA-CBD-CGD-O2D
23	B	607	CLA	CHA-CBD-CGD-O1D
23	C	504	CLA	CHA-CBD-CGD-O1D
23	c	905	CLA	CHA-CBD-CGD-O2D
33	d	401	HTG	C4'-C5'-C6'-C7'
34	C	517	DGD	C2E-C1E-O5D-C6D
27	c	920	LMG	C40-C41-C42-C43
27	A	413	LMG	O1-C7-C8-O7
26	L	103	SQD	O47-C45-C46-O48
34	H	102	DGD	O1G-C1G-C2G-O2G
26	f	102	SQD	O6-C44-C45-O47
26	B	621	SQD	C19-C20-C21-C22
27	C	519	LMG	C19-C20-C21-C22
23	D	403	CLA	C16-C17-C18-C20
31	c	928	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
31	L	104	GOL	O1-C1-C2-O2
31	b	632	GOL	O1-C1-C2-O2
36	a	417	LHG	O1-C1-C2-O2
34	c	918	DGD	C3A-C4A-C5A-C6A
34	c	918	DGD	CBA-CCA-CDA-CEA
23	d	403	CLA	C2-C3-C5-C6
28	A	414	PL9	C4-C3-C7-C8
23	b	609	CLA	C11-C12-C13-C14
23	D	403	CLA	C6-C7-C8-C9
23	c	913	CLA	C11-C10-C8-C9
34	C	516	DGD	C4D-C5D-C6D-O5D
26	B	621	SQD	C14-C15-C16-C17
27	a	418	LMG	C17-C18-C19-C20
23	A	410	CLA	C16-C17-C18-C20
27	Z	101	LMG	C33-C34-C35-C36
23	B	602	CLA	O1A-CGA-O2A-C1
31	V	203	GOL	O1-C1-C2-C3
31	O	304	GOL	C1-C2-C3-O3
23	B	602	CLA	C8-C10-C11-C12
23	B	605	CLA	C13-C15-C16-C17
26	A	412	SQD	C27-C28-C29-C30
23	B	616	CLA	C16-C17-C18-C20
23	A	410	CLA	C8-C10-C11-C12
23	C	502	CLA	C15-C16-C17-C18
24	A	409	PHO	C4C-C3C-CAC-CBC
27	D	411	LMG	C37-C38-C39-C40
23	c	910	CLA	C2-C1-O2A-CGA
23	C	509	CLA	C2-C1-O2A-CGA
36	d	408	LHG	C3-O3-P-O6
34	c	918	DGD	CCA-CDA-CEA-CFA
34	c	918	DGD	C6B-C7B-C8B-C9B
34	H	102	DGD	C6B-C7B-C8B-C9B
23	a	414	CLA	O1D-CGD-O2D-CED
23	B	602	CLA	CBD-CGD-O2D-CED
36	d	409	LHG	C2-C3-O3-P
36	a	417	LHG	C2-C3-O3-P
36	L	101	LHG	C4-O6-P-O5
36	D	409	LHG	C3-O3-P-O4
36	D	409	LHG	C4-O6-P-O5
36	l	101	LHG	C4-O6-P-O5
36	d	408	LHG	C3-O3-P-O4
36	d	408	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
36	a	417	LHG	C3-O3-P-O4
36	a	417	LHG	C4-O6-P-O4
26	f	102	SQD	O5-C5-C6-S
23	c	914	CLA	C16-C17-C18-C19
23	A	410	CLA	C16-C17-C18-C19
23	A	406	CLA	C2C-C3C-CAC-CBC
34	C	516	DGD	CBA-CCA-CDA-CEA
23	B	602	CLA	CBA-CGA-O2A-C1
23	c	912	CLA	CBD-CGD-O2D-CED
28	d	405	PL9	C39-C41-C42-C43
27	A	413	LMG	C11-C12-C13-C14
26	B	621	SQD	C28-C29-C30-C31
30	Z	102	LMT	C2-C3-C4-C5
34	d	406	DGD	C8A-C9A-CAA-CBA
34	d	406	DGD	C8B-C9B-CAB-CBB
26	a	416	SQD	C16-C17-C18-C19
36	E	101	LHG	C34-C35-C36-C37
23	A	410	CLA	O1D-CGD-O2D-CED
26	A	412	SQD	C34-C35-C36-C37
30	b	625	LMT	C2-C3-C4-C5
36	l	101	LHG	C26-C27-C28-C29
26	B	621	SQD	C5-C6-S-O7
23	B	606	CLA	CAD-CBD-CGD-O1D
23	C	506	CLA	CAD-CBD-CGD-O1D
23	b	608	CLA	CAD-CBD-CGD-O1D
26	a	401	SQD	O5-C5-C6-S
23	c	907	CLA	CAD-CBD-CGD-O1D
23	b	610	CLA	CAD-CBD-CGD-O1D
23	b	604	CLA	CAD-CBD-CGD-O1D
23	B	610	CLA	CAD-CBD-CGD-O1D
23	C	504	CLA	CAD-CBD-CGD-O1D
23	c	905	CLA	CAD-CBD-CGD-O1D
34	D	406	DGD	C7B-C8B-C9B-CAB
30	b	625	LMT	C11-C10-C9-C8
30	C	520	LMT	C7-C8-C9-C10
23	b	617	CLA	C11-C10-C8-C7
23	c	908	CLA	C11-C12-C13-C15
33	C	522	HTG	C2-C1-S1-C1'
23	A	407	CLA	C12-C13-C15-C16
33	B	626	HTG	C2-C1-S1-C1'
23	c	907	CLA	C6-C7-C8-C10
23	D	403	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
23	b	604	CLA	C6-C7-C8-C10
23	b	604	CLA	C11-C10-C8-C7
23	C	504	CLA	C6-C7-C8-C10
23	c	913	CLA	C6-C7-C8-C10
26	D	407	SQD	C10-C11-C12-C13
23	b	618	CLA	C13-C15-C16-C17
26	L	103	SQD	C12-C13-C14-C15
34	H	102	DGD	C5B-C6B-C7B-C8B
27	C	519	LMG	C16-C17-C18-C19
36	D	408	LHG	C13-C14-C15-C16
26	a	401	SQD	C12-C13-C14-C15
26	a	416	SQD	C31-C32-C33-C34
34	C	518	DGD	CBB-CCB-CDB-CEB
27	A	413	LMG	O1-C7-C8-C9
30	F	102	LMT	O1'-C1-C2-C3
34	D	406	DGD	O1G-C1G-C2G-O2G
27	C	519	LMG	O1-C7-C8-O7
30	b	624	LMT	C2-C3-C4-C5
26	L	103	SQD	C32-C33-C34-C35
27	c	921	LMG	C8-C7-O1-C1
34	c	918	DGD	C5D-C6D-O5D-C1E
23	b	609	CLA	C15-C16-C17-C18
30	a	402	LMT	C7-C8-C9-C10
26	a	401	SQD	C11-C10-C9-C8
27	A	413	LMG	C38-C39-C40-C41
26	A	412	SQD	C14-C15-C16-C17
27	b	623	LMG	C16-C17-C18-C19
23	C	508	CLA	C11-C10-C8-C9
23	b	607	CLA	C6-C7-C8-C9
23	C	513	CLA	C6-C7-C8-C9
23	C	513	CLA	C11-C12-C13-C14
23	a	411	CLA	C11-C10-C8-C9
23	c	908	CLA	C11-C12-C13-C14
23	a	414	CLA	C11-C10-C8-C9
23	C	507	CLA	C11-C10-C8-C9
23	b	609	CLA	C14-C13-C15-C16
23	c	907	CLA	C11-C10-C8-C9
23	B	617	CLA	C11-C10-C8-C9
24	a	413	PHO	C4C-C3C-CAC-CBC
26	A	418	SQD	C24-C25-C26-C27
23	C	502	CLA	C16-C17-C18-C19
34	c	918	DGD	C7B-C8B-C9B-CAB

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Mol	Chain	Res	Type	Atoms
30	m	102	LMT	C11-C10-C9-C8
27	Z	101	LMG	C4-C5-C6-O5
31	B	633	GOL	O2-C2-C3-O3
25	D	404	BCR	C37-C22-C23-C24
23	c	914	CLA	C3-C5-C6-C7
23	c	907	CLA	C13-C15-C16-C17
23	C	510	CLA	C8-C10-C11-C12
30	M	101	LMT	C9-C10-C11-C12
36	D	410	LHG	C14-C15-C16-C17
36	D	408	LHG	C25-C26-C27-C28
33	B	626	HTG	O5-C5-C6-O6
34	C	517	DGD	CBB-CCB-CDB-CEB
30	J	102	LMT	C4-C5-C6-C7
30	C	520	LMT	C11-C10-C9-C8
36	E	101	LHG	C35-C36-C37-C38
34	H	102	DGD	O2G-C1B-C2B-C3B
30	b	625	LMT	C4-C5-C6-C7
36	D	410	LHG	C12-C13-C14-C15
34	c	919	DGD	O1A-C1A-O1G-C1G
27	c	921	LMG	C36-C37-C38-C39
26	D	407	SQD	C28-C29-C30-C31
36	l	101	LHG	C28-C29-C30-C31
26	L	103	SQD	C46-C45-O47-C7
23	C	501	CLA	C2A-CAA-CBA-CGA
34	h	102	DGD	CDA-CEA-CFA-CGA
23	b	617	CLA	C2-C1-O2A-CGA
30	b	625	LMT	O5'-C5'-C6'-O6'
34	C	518	DGD	CCB-CDB-CEB-CFB
23	D	403	CLA	C13-C15-C16-C17
23	c	913	CLA	C15-C16-C17-C18
30	a	402	LMT	C11-C10-C9-C8
34	c	918	DGD	C9A-CAA-CBA-CCA
36	L	101	LHG	C9-C10-C11-C12
23	b	610	CLA	C3-C5-C6-C7
38	H	101	RRX	C23-C24-C25-C30
38	H	101	RRX	C23-C24-C25-C26
36	d	409	LHG	C28-C29-C30-C31
23	B	602	CLA	CAA-CBA-CGA-O2A
34	C	517	DGD	C8B-C9B-CAB-CBB
26	L	103	SQD	C28-C29-C30-C31
28	a	419	PL9	C39-C41-C42-C43
27	b	623	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
27	D	411	LMG	C30-C31-C32-C33
33	B	631	HTG	C4'-C5'-C6'-C7'
27	B	622	LMG	C29-C30-C31-C32
34	c	918	DGD	CAA-CBA-CCA-CDA
23	c	903	CLA	C11-C12-C13-C15
30	A	419	LMT	C11-C10-C9-C8
23	b	618	CLA	C14-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C14
23	B	602	CLA	C11-C12-C13-C14
23	b	616	CLA	C11-C12-C13-C14
23	C	504	CLA	C6-C7-C8-C9
25	a	415	BCR	C19-C20-C21-C22
23	D	402	CLA	C16-C17-C18-C19
23	B	604	CLA	C16-C17-C18-C20
23	B	611	CLA	C16-C17-C18-C19
26	f	102	SQD	C23-C24-C25-C26
34	c	919	DGD	C3B-C4B-C5B-C6B
36	l	101	LHG	C32-C33-C34-C35
33	c	924	HTG	C4'-C5'-C6'-C7'
36	d	409	LHG	C25-C26-C27-C28
34	h	102	DGD	CCB-CDB-CEB-CFB
33	b	627	HTG	S1-C1'-C2'-C3'
23	b	617	CLA	C15-C16-C17-C18
23	c	911	CLA	O1D-CGD-O2D-CED
36	l	101	LHG	C9-C10-C11-C12
31	V	203	GOL	O1-C1-C2-O2
31	B	635	GOL	O2-C2-C3-O3
31	b	632	GOL	O2-C2-C3-O3
23	C	507	CLA	C2-C3-C5-C6
27	Z	101	LMG	C38-C39-C40-C41
23	B	616	CLA	C16-C17-C18-C19
27	Z	101	LMG	C29-C28-O8-C9
28	a	419	PL9	C2-C3-C7-C8
27	Z	101	LMG	O10-C28-O8-C9
27	a	418	LMG	O8-C28-C29-C30
30	t	102	LMT	C2-C3-C4-C5
23	c	910	CLA	O1D-CGD-O2D-CED
23	b	615	CLA	CBA-CGA-O2A-C1
34	c	919	DGD	CAA-CBA-CCA-CDA
26	L	103	SQD	C14-C15-C16-C17
27	A	413	LMG	O6-C1-O1-C7
34	c	918	DGD	O6E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
34	C	517	DGD	O6E-C1E-O5D-C6D
26	B	621	SQD	C35-C36-C37-C38
34	D	406	DGD	C8A-C9A-CAA-CBA
34	c	918	DGD	CAB-CBB-CCB-CDB
27	c	921	LMG	C33-C34-C35-C36
30	F	102	LMT	O5B-C1B-O1B-C4'
28	a	419	PL9	C15-C14-C16-C17
30	Z	102	LMT	O5'-C5'-C6'-O6'
36	d	408	LHG	C16-C17-C18-C19
36	D	410	LHG	C13-C14-C15-C16
27	D	411	LMG	C34-C35-C36-C37
27	C	519	LMG	C11-C12-C13-C14
28	a	419	PL9	C13-C14-C16-C17
23	c	906	CLA	C2-C3-C5-C6
23	B	610	CLA	C2-C3-C5-C6
26	A	418	SQD	C30-C31-C32-C33
23	b	615	CLA	C10-C11-C12-C13
27	a	418	LMG	C22-C23-C24-C25
30	B	623	LMT	C3-C4-C5-C6
27	c	920	LMG	C11-C12-C13-C14
34	c	919	DGD	O6D-C5D-C6D-O5D
27	c	920	LMG	C14-C15-C16-C17
23	A	405	CLA	C4C-C3C-CAC-CBC
34	H	102	DGD	CAA-CBA-CCA-CDA
30	C	520	LMT	C4-C5-C6-C7
38	h	101	RRX	C9-C10-C11-C12
30	M	101	LMT	C4'-C5'-C6'-O6'
23	c	906	CLA	C4-C3-C5-C6
23	B	610	CLA	C4-C3-C5-C6
27	Z	101	LMG	C10-C11-C12-C13
26	f	102	SQD	C31-C32-C33-C34
23	b	617	CLA	C11-C10-C8-C9
23	C	512	CLA	C11-C10-C8-C9
23	B	614	CLA	C11-C10-C8-C9
34	c	917	DGD	C5A-C6A-C7A-C8A
27	c	920	LMG	C21-C22-C23-C24
30	A	419	LMT	C4-C5-C6-C7
27	C	519	LMG	C12-C13-C14-C15
27	Z	101	LMG	C14-C15-C16-C17
26	B	621	SQD	C25-C26-C27-C28
34	H	102	DGD	O1G-C1G-C2G-C3G
26	a	416	SQD	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
23	C	507	CLA	C2A-CAA-CBA-CGA
23	c	914	CLA	C16-C17-C18-C20
23	c	913	CLA	O2A-C1-C2-C3
34	C	516	DGD	O6E-C1E-O5D-C6D
25	c	915	BCR	C37-C22-C23-C24
34	d	406	DGD	C3B-C4B-C5B-C6B
27	B	622	LMG	C32-C33-C34-C35
28	A	414	PL9	C20-C19-C21-C22
23	c	914	CLA	C6-C7-C8-C10
23	b	618	CLA	C12-C13-C15-C16
23	B	602	CLA	C6-C7-C8-C10
23	A	407	CLA	C11-C10-C8-C7
34	C	516	DGD	C6B-C7B-C8B-C9B
30	z	101	LMT	C9-C10-C11-C12
27	c	921	LMG	C34-C35-C36-C37
23	b	613	CLA	C2A-CAA-CBA-CGA
23	B	611	CLA	C13-C15-C16-C17
34	c	919	DGD	C8B-C9B-CAB-CBB
36	E	101	LHG	C31-C32-C33-C34
28	A	414	PL9	C3-C7-C8-C9
27	b	623	LMG	C30-C31-C32-C33
23	C	508	CLA	C15-C16-C17-C18
36	a	417	LHG	O6-C4-C5-C6
23	B	605	CLA	C16-C17-C18-C20
28	A	414	PL9	C18-C19-C21-C22
23	D	402	CLA	C4C-C3C-CAC-CBC
34	C	518	DGD	C4A-C5A-C6A-C7A
27	b	623	LMG	C22-C23-C24-C25
27	A	413	LMG	C29-C30-C31-C32
30	b	624	LMT	C3-C4-C5-C6
27	b	623	LMG	C12-C13-C14-C15
27	c	921	LMG	O7-C8-C9-O8
27	C	519	LMG	C13-C14-C15-C16
36	E	101	LHG	C23-C24-C25-C26
23	A	406	CLA	C13-C15-C16-C17
28	D	405	PL9	C39-C41-C42-C43
28	A	414	PL9	C39-C41-C42-C43
27	a	418	LMG	C21-C22-C23-C24
26	f	102	SQD	C30-C31-C32-C33
33	u	201	HTG	C1'-C2'-C3'-C4'
33	b	626	HTG	C1'-C2'-C3'-C4'
23	A	410	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	c	903	CLA	C11-C12-C13-C14
34	D	406	DGD	C2A-C3A-C4A-C5A
26	A	412	SQD	C30-C31-C32-C33
23	A	407	CLA	C16-C17-C18-C19
34	H	102	DGD	CDA-CEA-CFA-CGA
26	a	416	SQD	O10-C23-O48-C46
25	K	101	BCR	C5-C6-C7-C8
25	c	915	BCR	C23-C24-C25-C30
38	h	101	RRX	C23-C24-C25-C30
25	C	514	BCR	C23-C24-C25-C30
25	B	620	BCR	C23-C24-C25-C30
23	a	410	CLA	C15-C16-C17-C18
23	b	604	CLA	CAA-CBA-CGA-O2A
36	D	409	LHG	C26-C27-C28-C29
27	C	519	LMG	O1-C7-C8-C9
33	b	601	HTG	C1'-C2'-C3'-C4'
31	L	104	GOL	O1-C1-C2-C3
31	O	304	GOL	O1-C1-C2-C3
34	C	516	DGD	C2B-C3B-C4B-C5B
25	C	514	BCR	C19-C20-C21-C22
34	h	102	DGD	C9B-CAB-CBB-CCB
28	d	405	PL9	C30-C29-C31-C32
23	b	613	CLA	C16-C17-C18-C20
23	c	902	CLA	C13-C15-C16-C17
27	C	519	LMG	C20-C21-C22-C23
34	C	518	DGD	O6D-C5D-C6D-O5D
34	D	406	DGD	C2G-C3G-O3G-C1D
30	M	102	LMT	C3-C4-C5-C6
30	t	102	LMT	C7-C8-C9-C10
30	B	623	LMT	C3'-C4'-O1B-C1B
30	z	101	LMT	O5'-C1'-O1'-C1
23	D	403	CLA	O1D-CGD-O2D-CED
34	C	518	DGD	CCA-CDA-CEA-CFA
23	C	513	CLA	C4-C3-C5-C6
23	B	612	CLA	C2-C3-C5-C6
23	A	410	CLA	C12-C13-C15-C16
24	A	408	PHO	C2-C3-C5-C6
23	B	606	CLA	C10-C11-C12-C13
31	D	415	GOL	O2-C2-C3-O3
31	O	304	GOL	O2-C2-C3-O3
27	c	921	LMG	C40-C41-C42-C43
36	a	417	LHG	C5-C4-O6-P

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Mol	Chain	Res	Type	Atoms
36	l	101	LHG	C16-C17-C18-C19
30	C	520	LMT	C2-C3-C4-C5
34	d	406	DGD	O1A-C1A-O1G-C1G
36	D	408	LHG	C15-C16-C17-C18
33	C	522	HTG	O5-C1-S1-C1'
23	B	617	CLA	C4-C3-C5-C6
27	Z	101	LMG	O9-C10-O7-C8
33	O	303	HTG	C2'-C3'-C4'-C5'
23	c	914	CLA	C6-C7-C8-C9
23	C	505	CLA	C14-C13-C15-C16
23	c	906	CLA	C11-C12-C13-C14
23	b	604	CLA	C6-C7-C8-C9
36	L	101	LHG	C28-C29-C30-C31
23	b	618	CLA	C3A-C2A-CAA-CBA
23	C	512	CLA	CAA-CBA-CGA-O2A
36	a	417	LHG	O7-C7-C8-C9
26	B	621	SQD	C30-C31-C32-C33
23	C	506	CLA	CAD-CBD-CGD-O2D
23	c	911	CLA	CAD-CBD-CGD-O2D
23	b	613	CLA	CAD-CBD-CGD-O2D
23	B	604	CLA	CAD-CBD-CGD-O2D
23	a	409	CLA	CAD-CBD-CGD-O2D
23	B	605	CLA	CAD-CBD-CGD-O2D
23	b	619	CLA	CAD-CBD-CGD-O2D
23	C	505	CLA	CAD-CBD-CGD-O2D
23	B	613	CLA	CAD-CBD-CGD-O2D
24	A	408	PHO	CAD-CBD-CGD-O2D
23	c	907	CLA	CAD-CBD-CGD-O2D
23	c	910	CLA	CAD-CBD-CGD-O2D
23	D	403	CLA	CAD-CBD-CGD-O2D
23	B	610	CLA	CAD-CBD-CGD-O2D
23	C	501	CLA	CAD-CBD-CGD-O2D
23	B	604	CLA	C16-C17-C18-C19
34	C	517	DGD	CDB-CEB-CFB-CGB
27	B	622	LMG	O9-C10-O7-C8
30	B	623	LMT	C5'-C4'-O1B-C1B
25	K	101	BCR	C21-C22-C23-C24
34	C	518	DGD	O1G-C1A-C2A-C3A
33	B	624	HTG	C4'-C5'-C6'-C7'
23	d	402	CLA	O2A-C1-C2-C3
23	b	607	CLA	O2A-C1-C2-C3
23	D	402	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
24	a	412	PHO	O2A-C1-C2-C3
23	B	605	CLA	O2A-C1-C2-C3
24	A	408	PHO	O2A-C1-C2-C3
23	c	910	CLA	O2A-C1-C2-C3
23	C	509	CLA	O2A-C1-C2-C3
27	Z	101	LMG	C16-C17-C18-C19
36	l	101	LHG	C17-C18-C19-C20
23	B	606	CLA	CBD-CGD-O2D-CED
23	A	406	CLA	CHA-CBD-CGD-O1D
23	A	406	CLA	CHA-CBD-CGD-O2D
23	b	617	CLA	CHA-CBD-CGD-O1D
23	B	603	CLA	CHA-CBD-CGD-O1D
23	a	411	CLA	CHA-CBD-CGD-O2D
23	c	912	CLA	CHA-CBD-CGD-O2D
23	c	911	CLA	CHA-CBD-CGD-O1D
23	b	608	CLA	CHA-CBD-CGD-O1D
24	a	413	PHO	CHA-CBD-CGD-O1D
24	a	413	PHO	CHA-CBD-CGD-O2D
23	b	605	CLA	CHA-CBD-CGD-O2D
23	C	507	CLA	CHA-CBD-CGD-O2D
23	c	904	CLA	CHA-CBD-CGD-O2D
23	b	619	CLA	CHA-CBD-CGD-O1D
23	A	407	CLA	CHA-CBD-CGD-O2D
23	b	609	CLA	CHA-CBD-CGD-O2D
23	c	907	CLA	CHA-CBD-CGD-O1D
23	c	910	CLA	CHA-CBD-CGD-O1D
23	b	614	CLA	CHA-CBD-CGD-O2D
23	B	617	CLA	CHA-CBD-CGD-O1D
23	B	615	CLA	CHA-CBD-CGD-O2D
23	B	607	CLA	CHA-CBD-CGD-O2D
23	C	509	CLA	CHA-CBD-CGD-O1D
23	c	905	CLA	CHA-CBD-CGD-O1D
23	A	406	CLA	C4C-C3C-CAC-CBC
26	L	103	SQD	C11-C12-C13-C14
30	c	922	LMT	C5-C6-C7-C8
26	a	401	SQD	O47-C45-C46-O48
26	a	416	SQD	O47-C45-C46-O48
30	a	402	LMT	C4-C5-C6-C7
23	B	605	CLA	C16-C17-C18-C19
23	C	506	CLA	CBD-CGD-O2D-CED
31	v	203	GOL	O1-C1-C2-O2
23	b	619	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	Z	101	LMG	C11-C10-O7-C8
23	C	513	CLA	O1A-CGA-O2A-C1
28	d	405	PL9	C28-C29-C31-C32
23	c	911	CLA	C6-C7-C8-C10
23	D	403	CLA	C12-C13-C15-C16
27	Z	101	LMG	C19-C20-C21-C22
34	c	919	DGD	C3A-C4A-C5A-C6A
34	c	917	DGD	O6E-C1E-O5D-C6D
23	c	911	CLA	C6-C7-C8-C9
23	B	616	CLA	C14-C13-C15-C16
23	A	407	CLA	C14-C13-C15-C16
23	a	410	CLA	C11-C12-C13-C14
23	C	504	CLA	C16-C17-C18-C19
23	b	606	CLA	C2A-CAA-CBA-CGA
26	A	412	SQD	O47-C7-C8-C9
23	C	512	CLA	CAA-CBA-CGA-O1A
23	B	602	CLA	C4-C3-C5-C6
23	b	604	CLA	C4-C3-C5-C6
25	c	915	BCR	C17-C18-C19-C20
25	c	915	BCR	C21-C22-C23-C24
30	a	402	LMT	O5B-C5B-C6B-O6B
23	c	905	CLA	C1A-C2A-CAA-CBA
27	b	623	LMG	C34-C35-C36-C37
36	a	417	LHG	O9-C7-C8-C9
23	A	407	CLA	C13-C15-C16-C17
23	b	606	CLA	C13-C15-C16-C17
26	a	416	SQD	C24-C23-O48-C46
23	c	906	CLA	CAA-CBA-CGA-O2A
23	B	603	CLA	C15-C16-C17-C18
23	C	513	CLA	C8-C10-C11-C12
27	Z	101	LMG	C32-C33-C34-C35
23	c	909	CLA	C16-C17-C18-C19
34	C	518	DGD	O1A-C1A-C2A-C3A
36	D	410	LHG	C10-C11-C12-C13
28	d	405	PL9	C45-C44-C46-C47
26	L	103	SQD	C9-C10-C11-C12
27	A	413	LMG	C2-C1-O1-C7
34	c	918	DGD	C2E-C1E-O5D-C6D
27	a	418	LMG	C2-C1-O1-C7
36	d	408	LHG	C4-O6-P-O4
36	E	101	LHG	C4-O6-P-O5
23	c	902	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
27	Z	101	LMG	C15-C16-C17-C18
36	d	407	LHG	C25-C26-C27-C28
25	K	101	BCR	C1-C6-C7-C8
25	k	101	BCR	C5-C6-C7-C8
23	C	513	CLA	C10-C11-C12-C13
23	C	501	CLA	C13-C15-C16-C17
23	c	911	CLA	C16-C17-C18-C20
36	d	407	LHG	C11-C10-C9-C8
34	d	406	DGD	C2A-C1A-O1G-C1G
23	B	611	CLA	C2A-CAA-CBA-CGA
23	C	513	CLA	C2-C3-C5-C6
23	b	607	CLA	C16-C17-C18-C19
26	B	621	SQD	O5-C5-C6-S
23	C	512	CLA	CAD-CBD-CGD-O1D
23	B	608	CLA	CAD-CBD-CGD-O1D
26	A	418	SQD	C5-C6-S-O9
34	c	918	DGD	C1B-C2B-C3B-C4B
23	B	602	CLA	C6-C7-C8-C9
23	D	403	CLA	C11-C12-C13-C14
23	D	403	CLA	C14-C13-C15-C16
23	b	615	CLA	C6-C7-C8-C9
23	b	615	CLA	C11-C10-C8-C9
23	C	504	CLA	C11-C10-C8-C9
26	A	412	SQD	C29-C30-C31-C32
31	a	424	GOL	O2-C2-C3-O3
31	b	635	GOL	O1-C1-C2-O2
23	B	613	CLA	C8-C10-C11-C12
34	c	918	DGD	C9B-CAB-CBB-CCB
23	C	513	CLA	CBA-CGA-O2A-C1
23	b	614	CLA	C16-C17-C18-C20
34	c	919	DGD	O1G-C1A-C2A-C3A
26	L	103	SQD	O48-C23-C24-C25
26	A	412	SQD	C32-C33-C34-C35
36	L	101	LHG	C5-C6-O8-C23
30	b	624	LMT	C11-C10-C9-C8
33	u	201	HTG	C3'-C4'-C5'-C6'
34	c	917	DGD	O2G-C1B-C2B-C3B
34	d	406	DGD	O1G-C1A-C2A-C3A
27	c	920	LMG	C30-C31-C32-C33
30	Z	102	LMT	C4'-C5'-C6'-O6'
23	A	407	CLA	C16-C17-C18-C20
23	B	602	CLA	C12-C13-C15-C16

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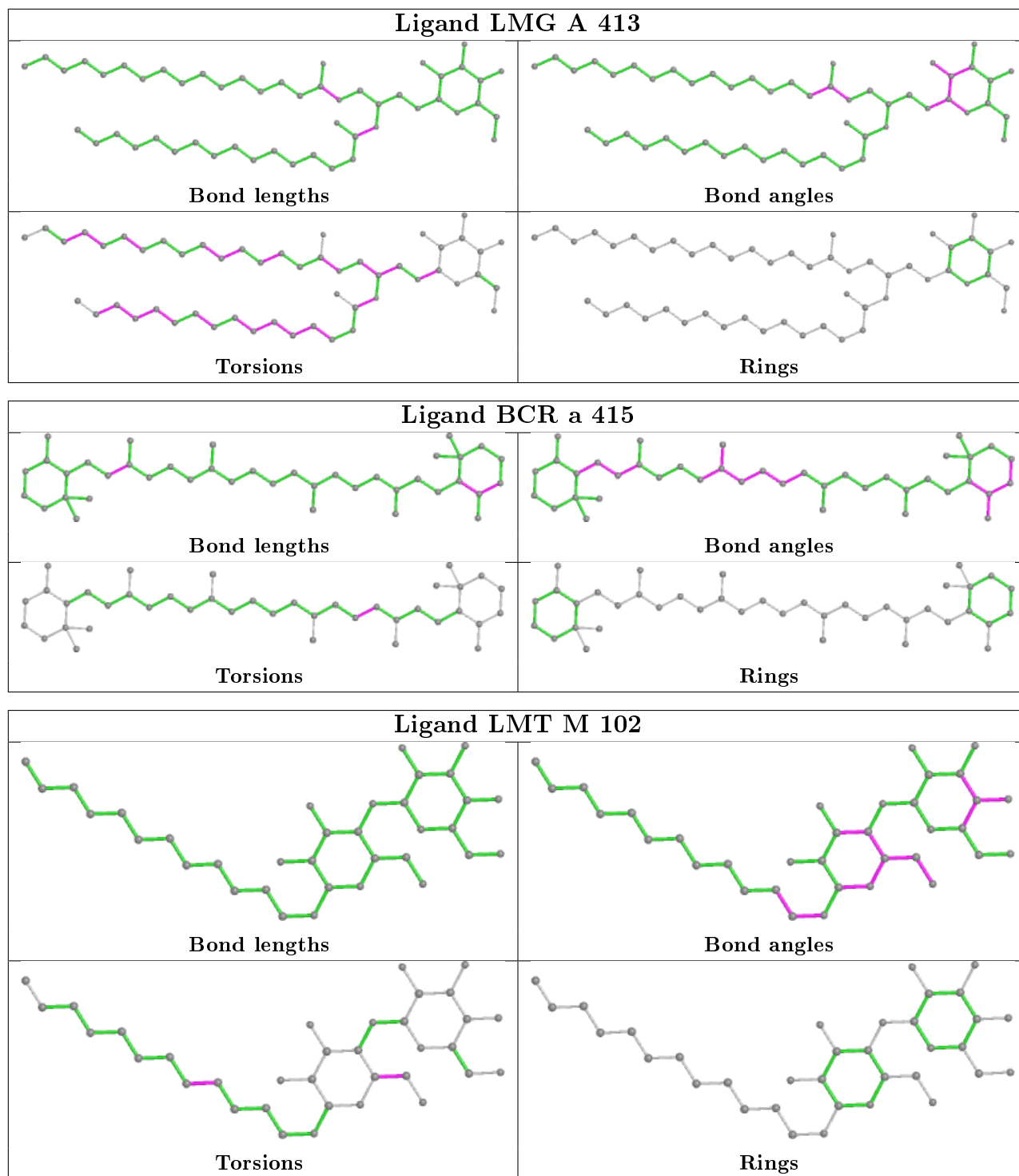
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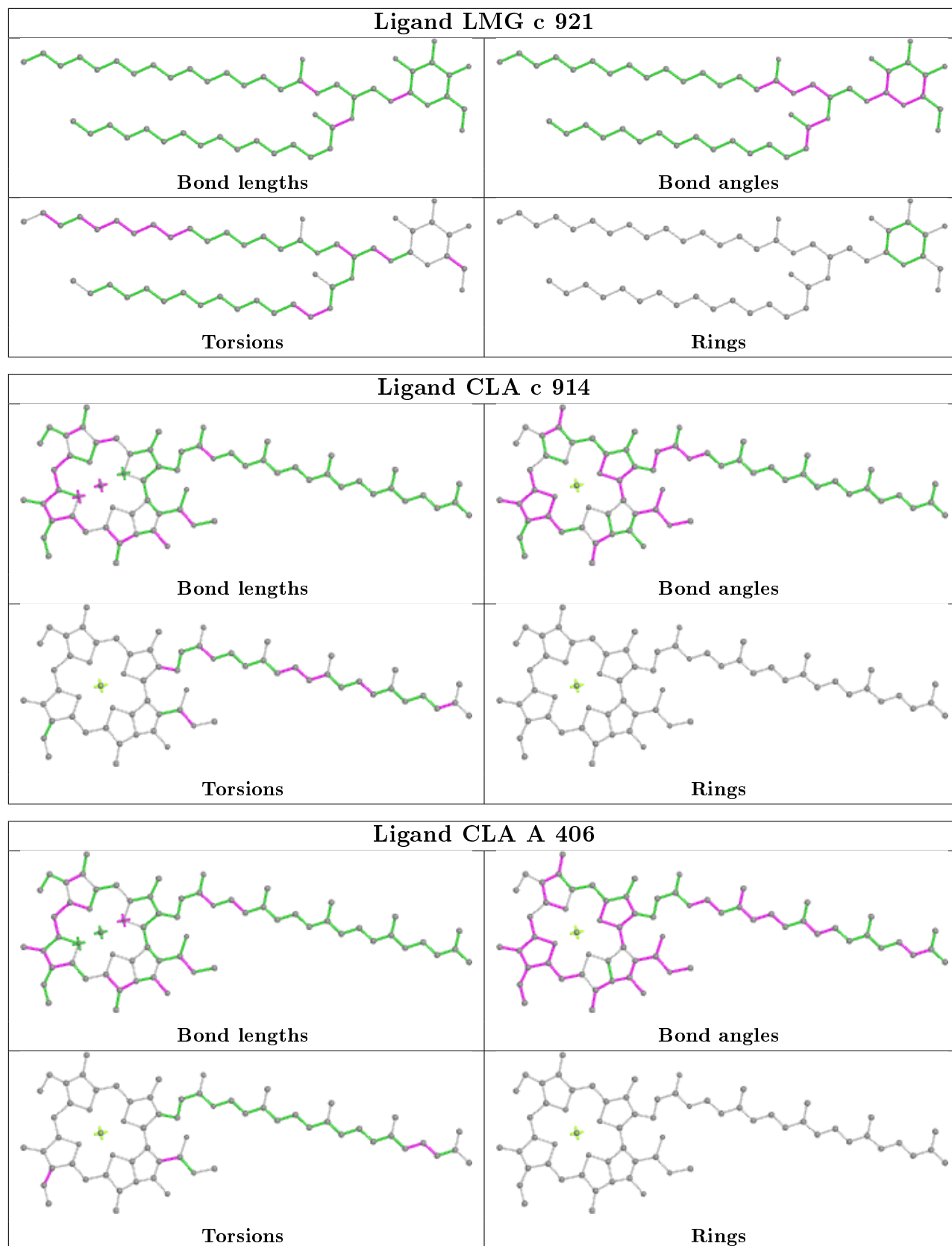
Mol	Chain	Res	Type	Atoms
23	C	505	CLA	C12-C13-C15-C16
23	c	910	CLA	C11-C10-C8-C7
23	c	906	CLA	C11-C12-C13-C15
23	D	403	CLA	C11-C12-C13-C15
23	b	615	CLA	C11-C10-C8-C7
23	c	906	CLA	CAA-CBA-CGA-O1A
34	C	517	DGD	O2G-C1B-C2B-C3B
23	c	913	CLA	CAA-CBA-CGA-O2A
26	A	412	SQD	O49-C7-C8-C9
34	d	406	DGD	O1A-C1A-C2A-C3A
25	C	514	BCR	C15-C16-C17-C18
30	a	402	LMT	C2-C1-O1'-C1'
23	c	913	CLA	CAA-CBA-CGA-O1A
34	C	518	DGD	C7A-C8A-C9A-CAA
36	a	417	LHG	C18-C19-C20-C21
27	c	921	LMG	C37-C38-C39-C40
23	A	406	CLA	C15-C16-C17-C18
23	B	603	CLA	C8-C10-C11-C12
23	C	512	CLA	C4-C3-C5-C6
30	b	624	LMT	C5-C6-C7-C8
23	C	505	CLA	CAA-CBA-CGA-O2A

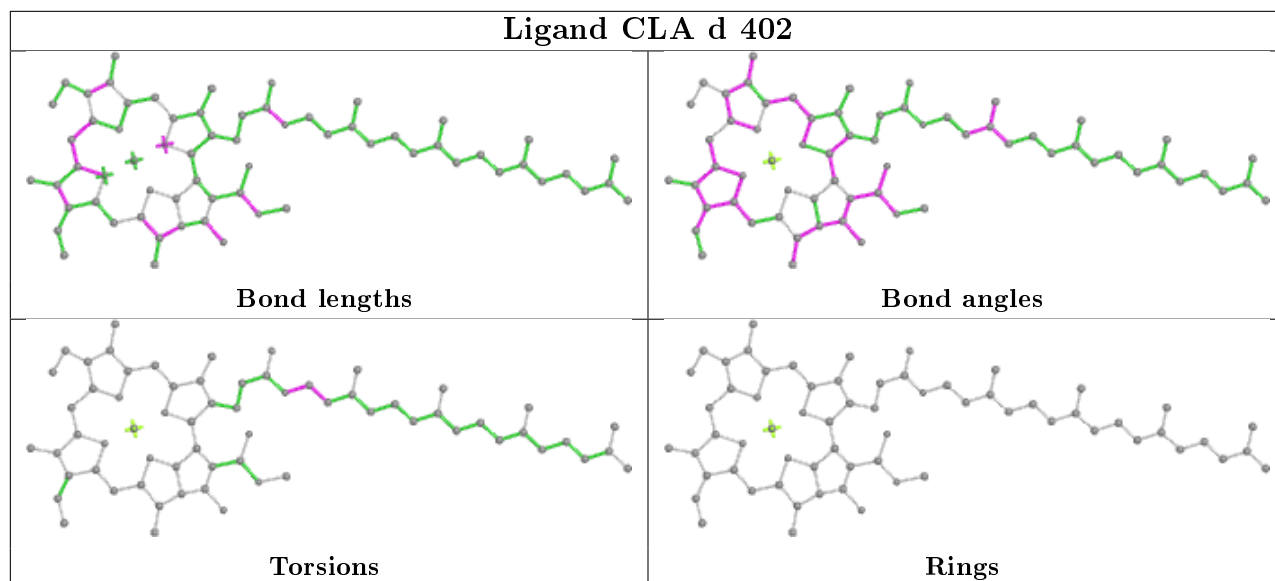
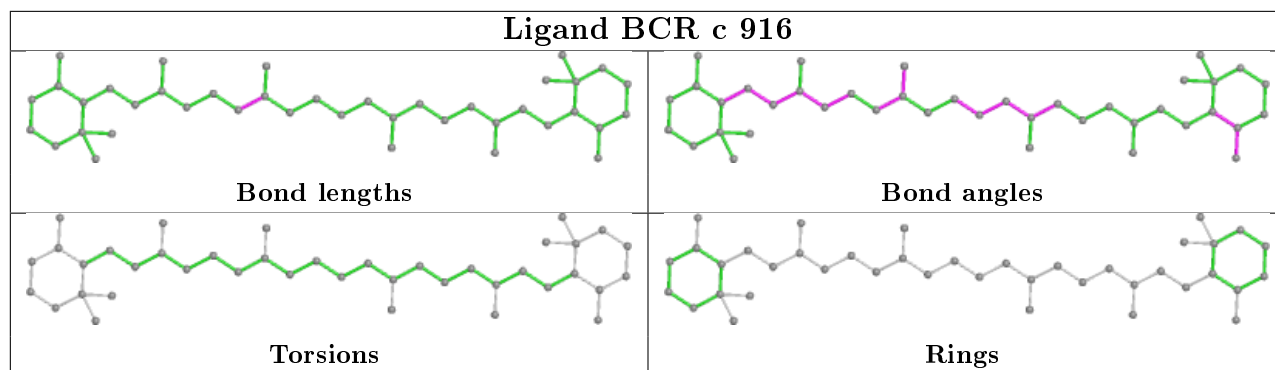
There are no ring outliers.

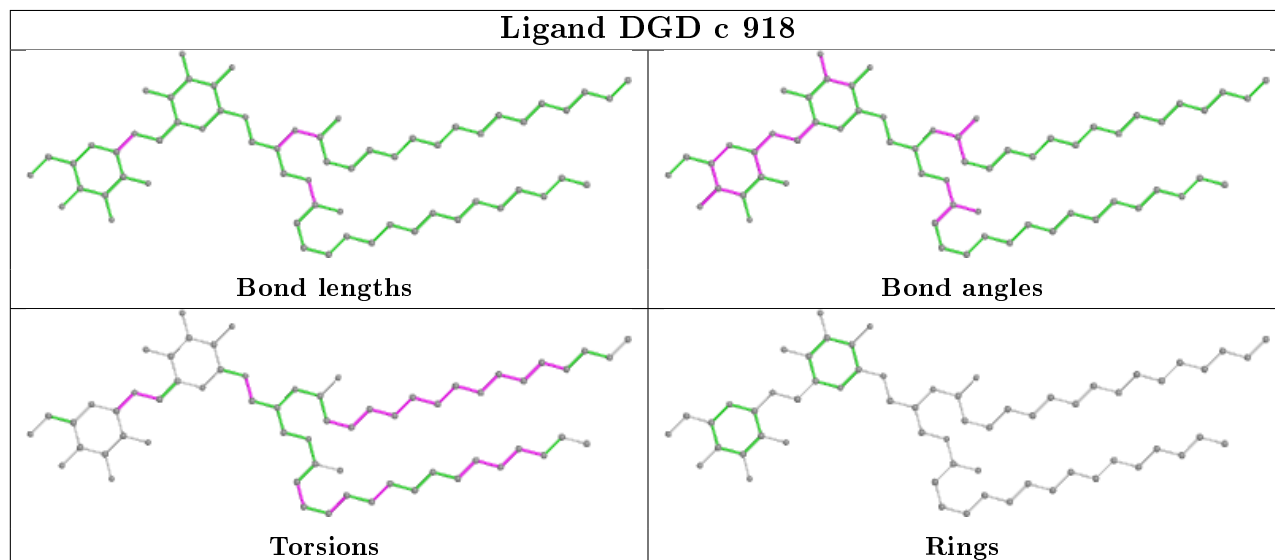
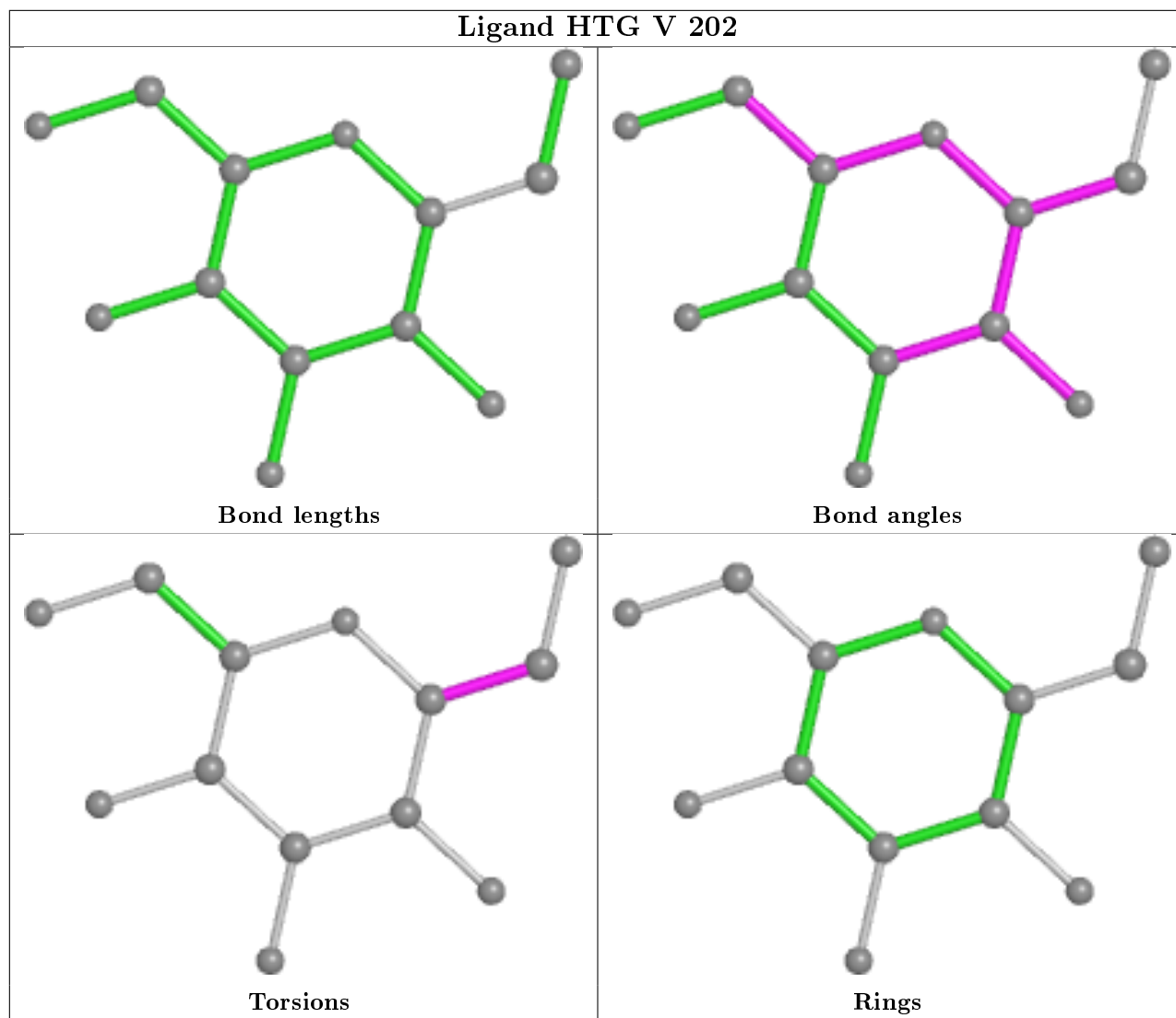
No monomer is involved in short contacts.

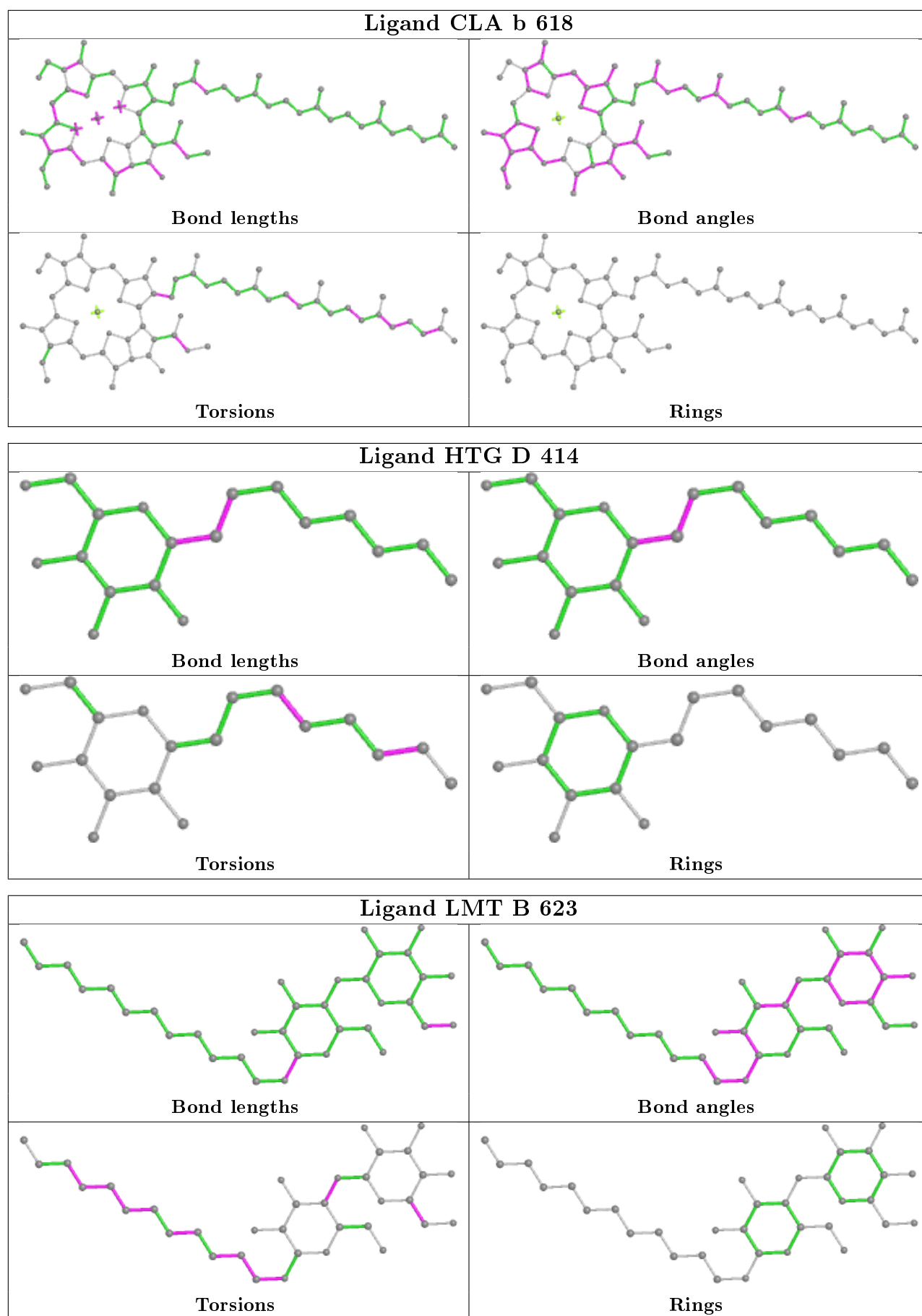
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

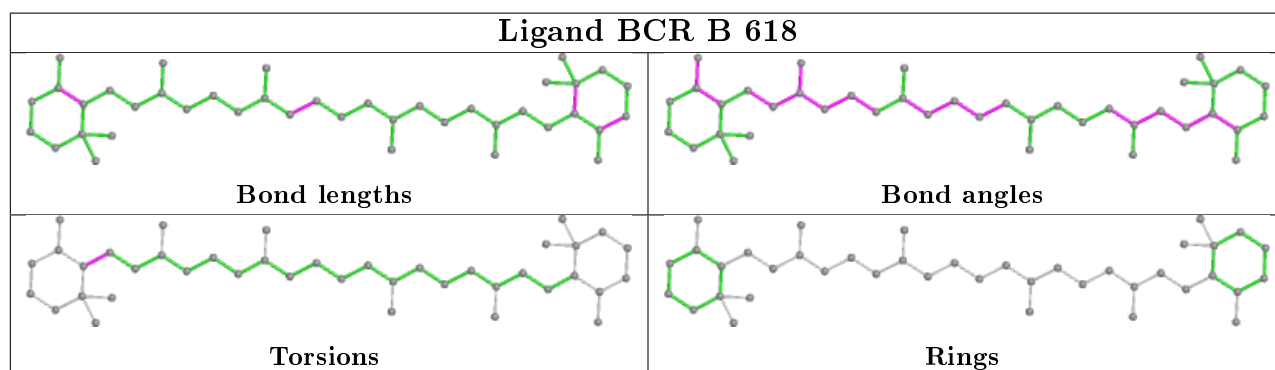
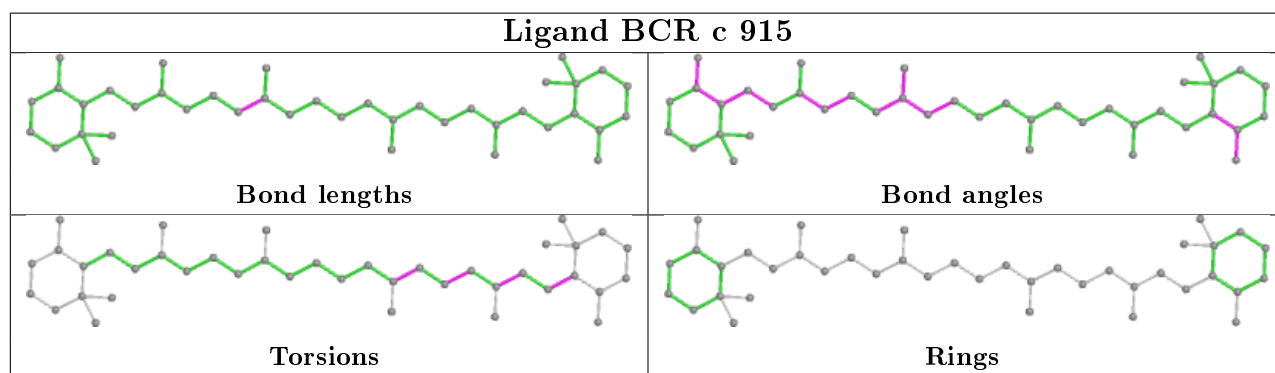
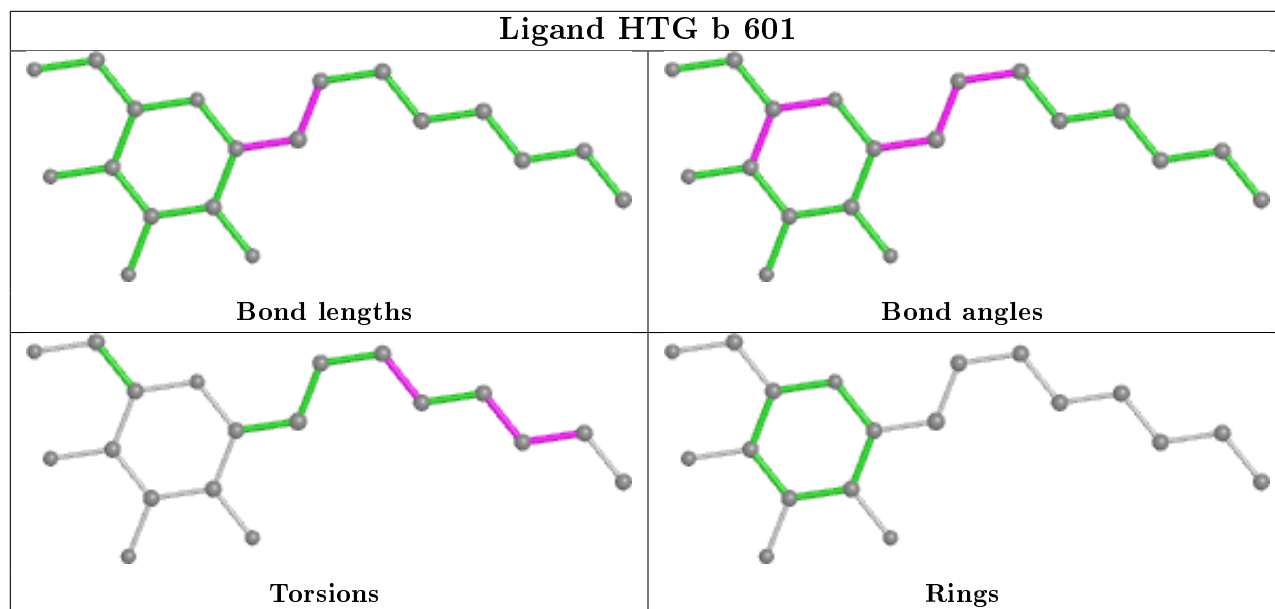
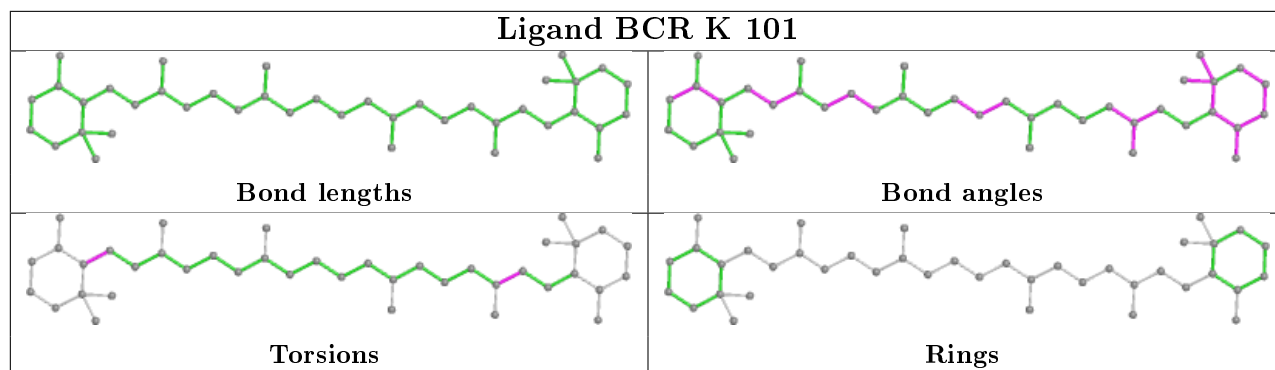


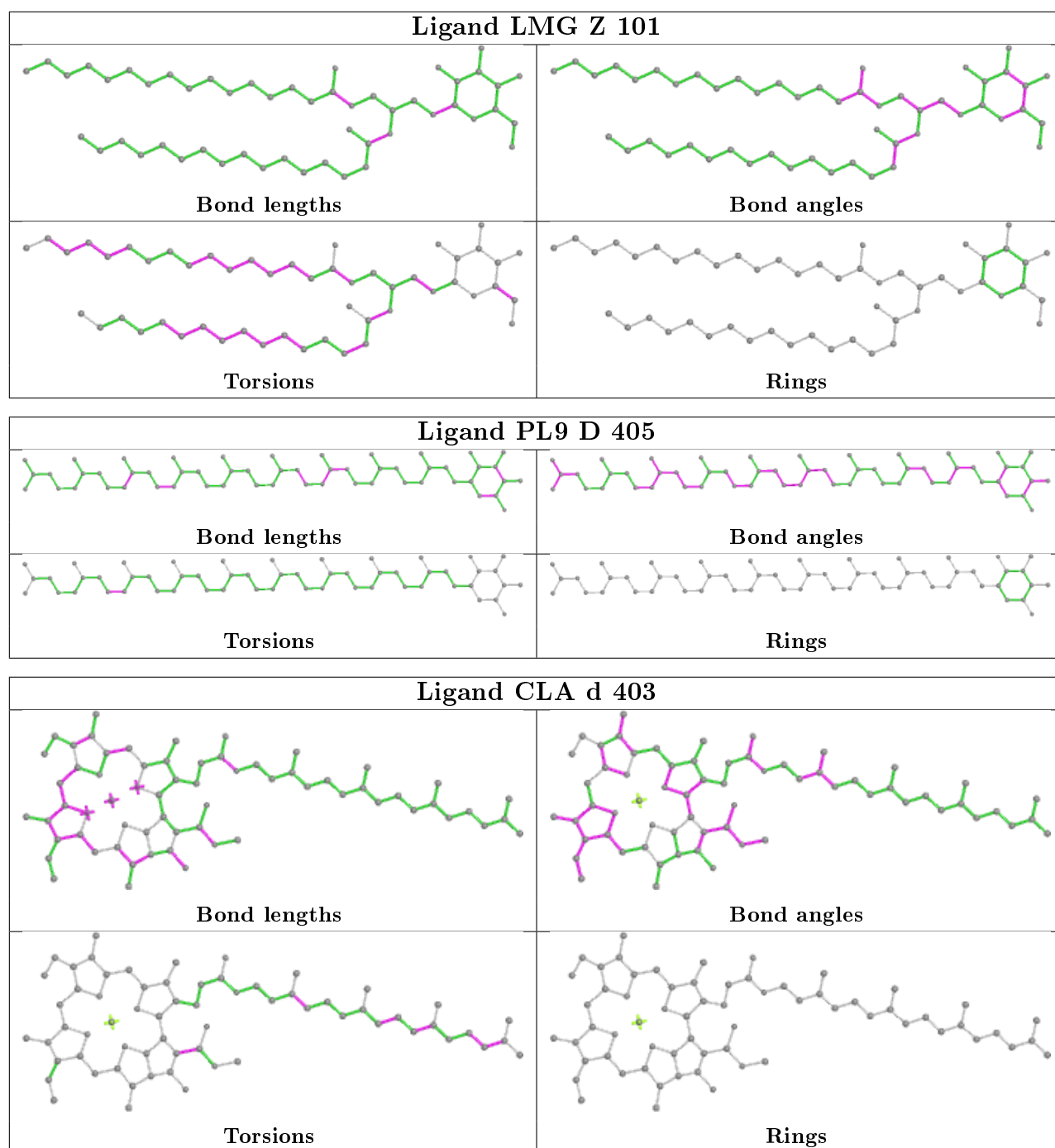


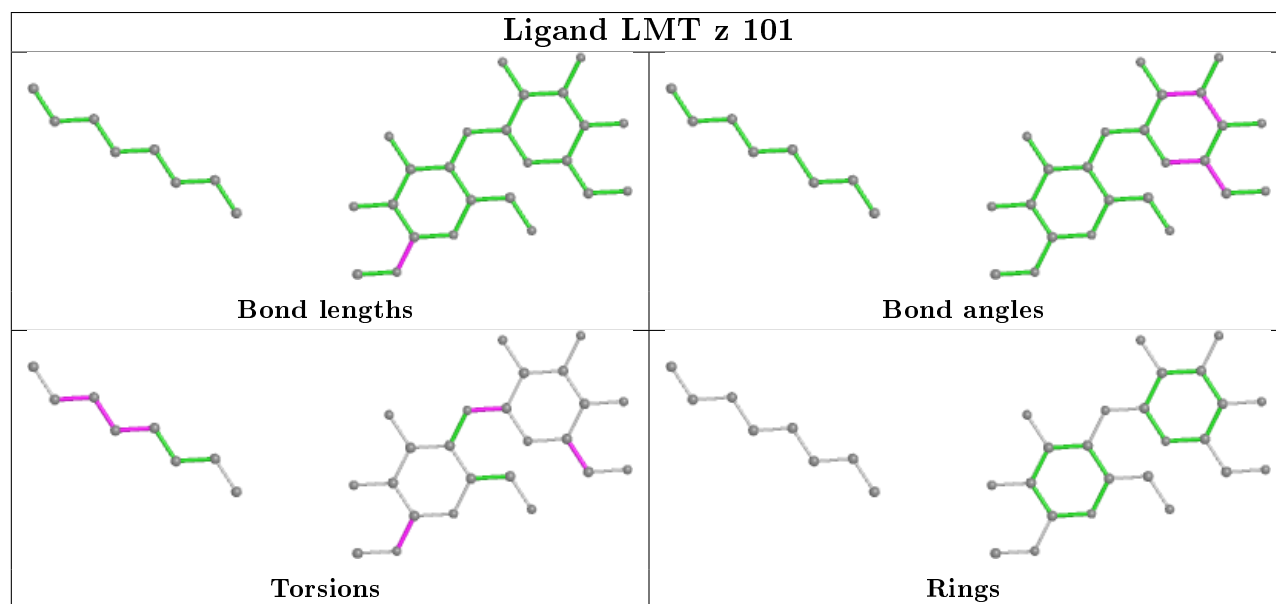
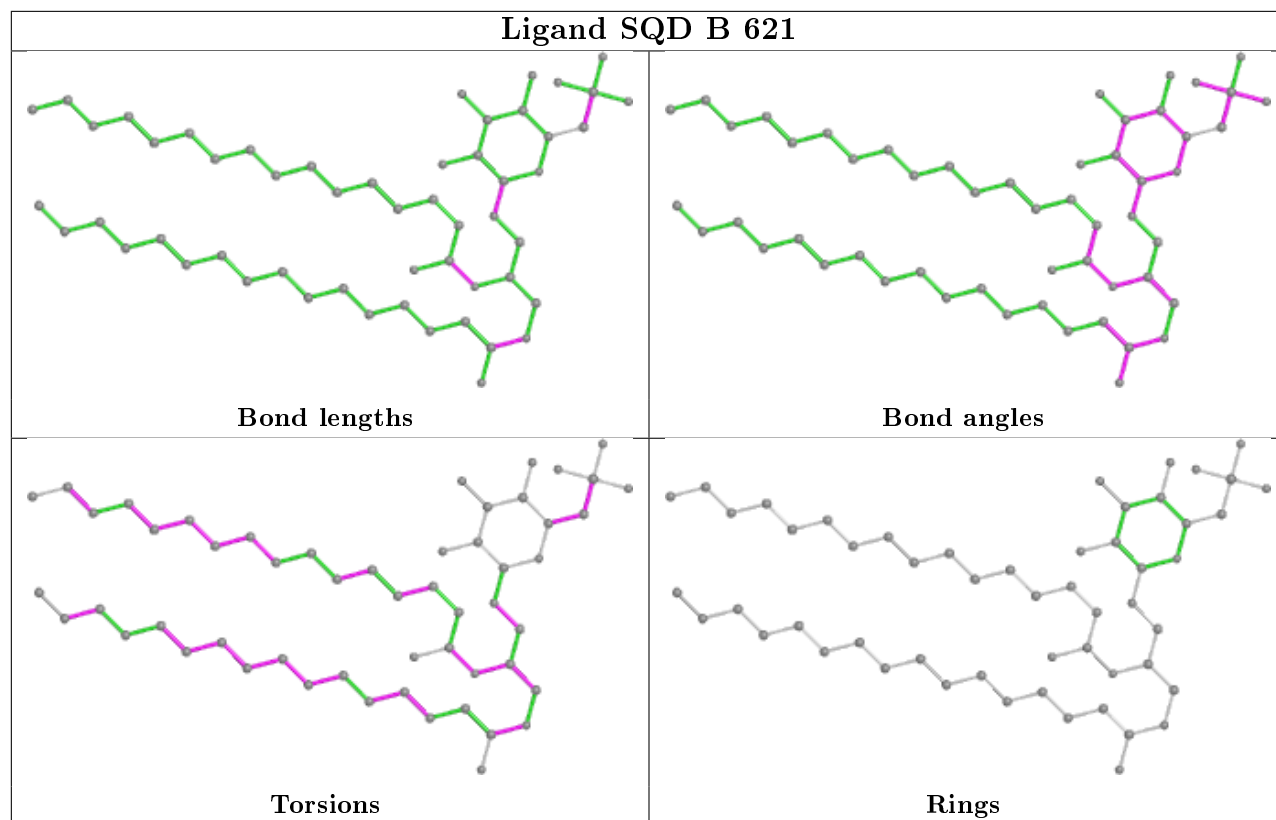


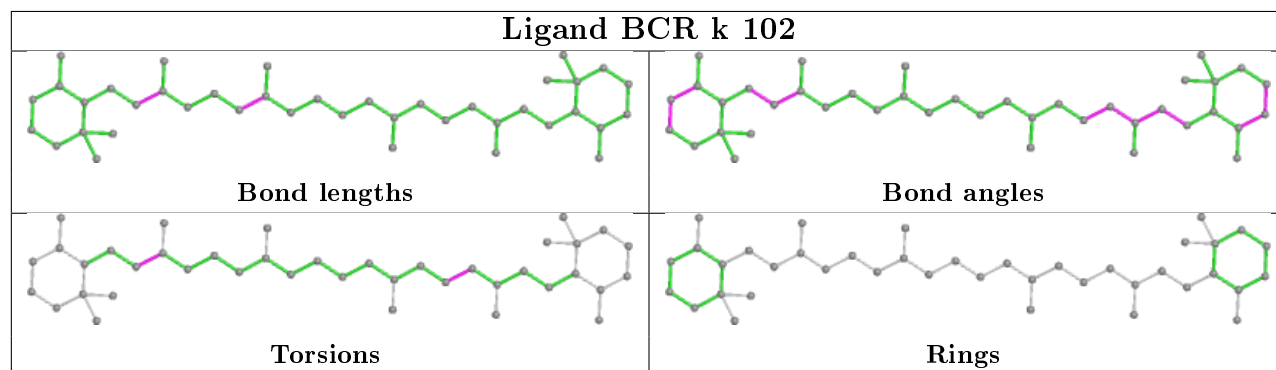
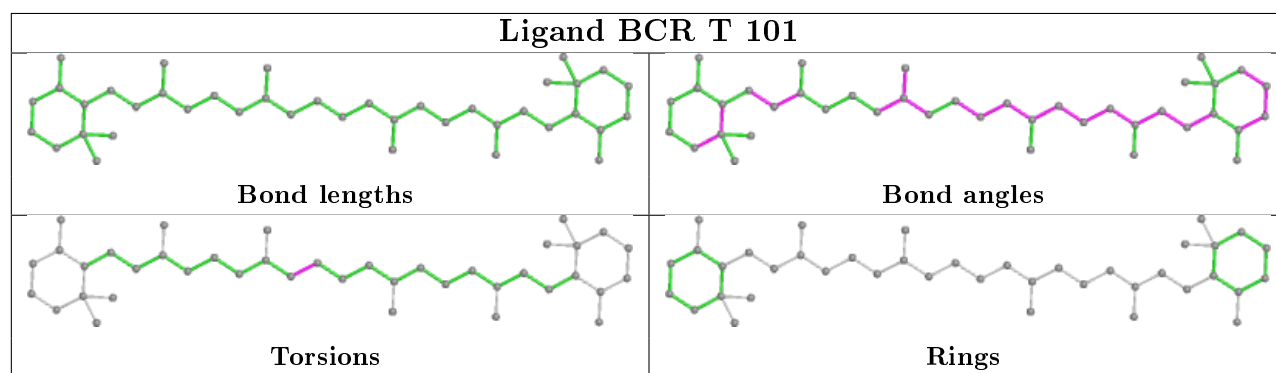
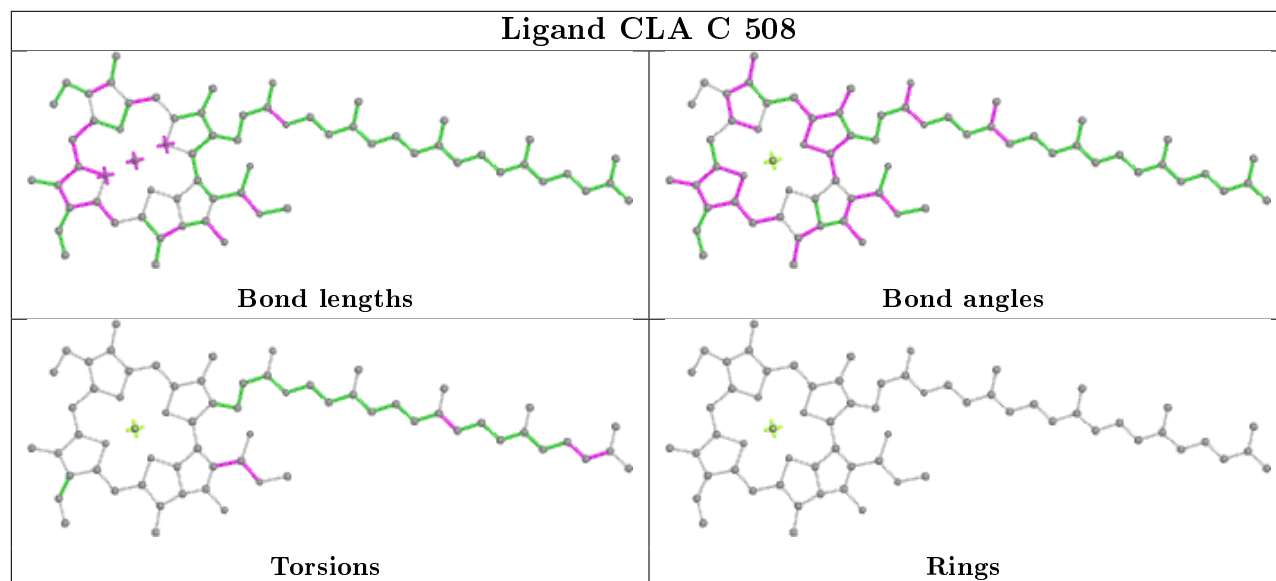
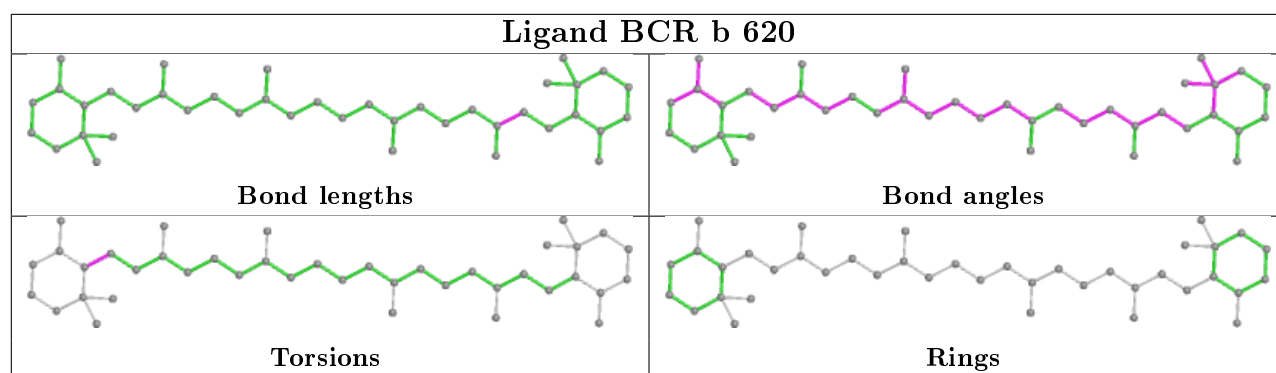


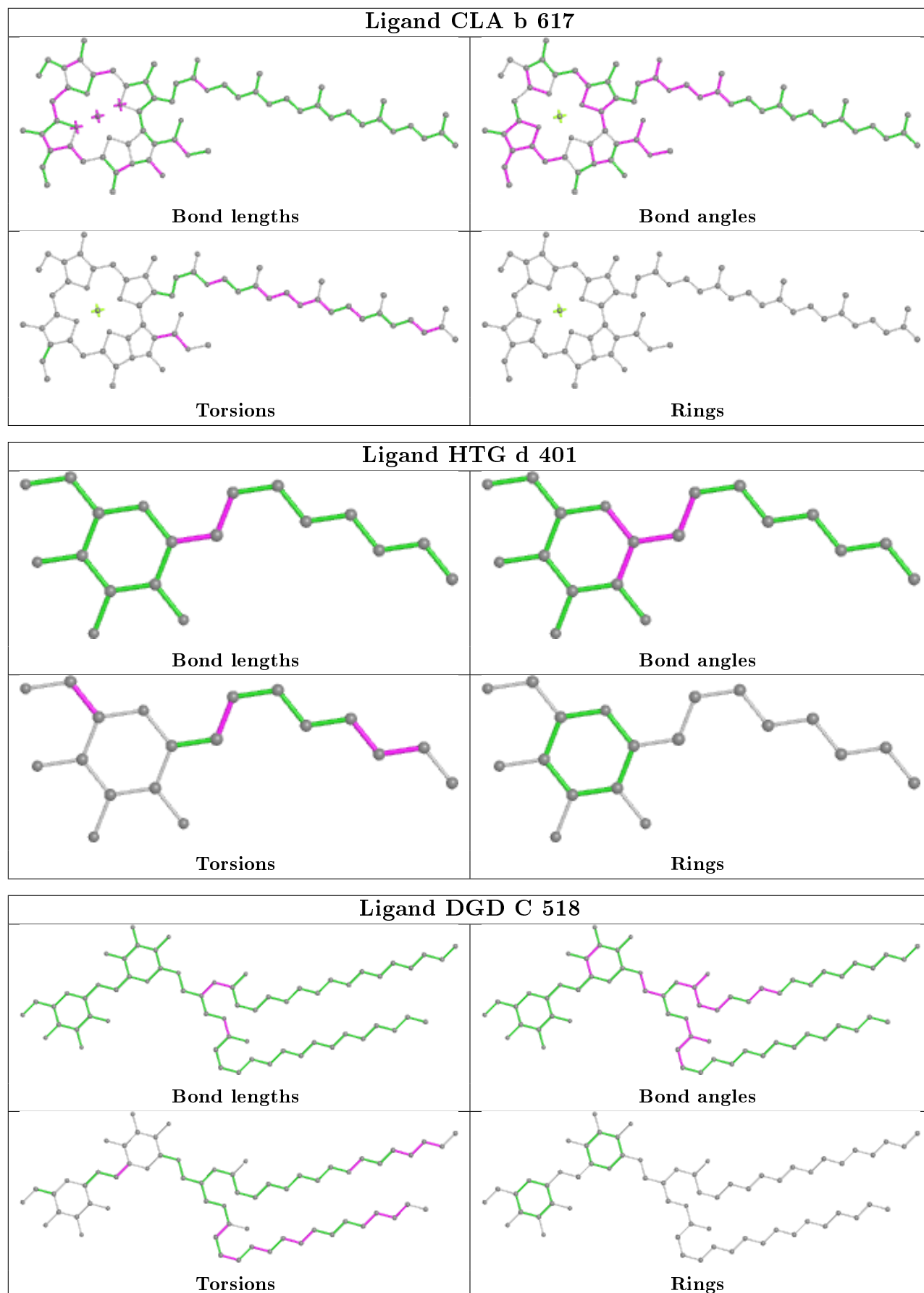


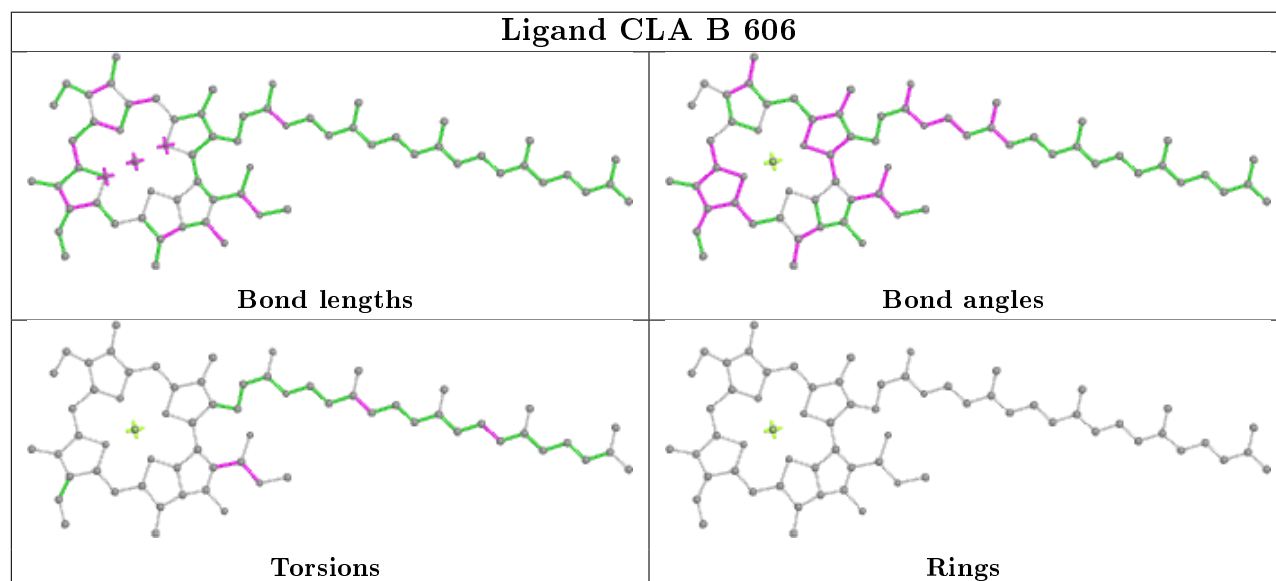
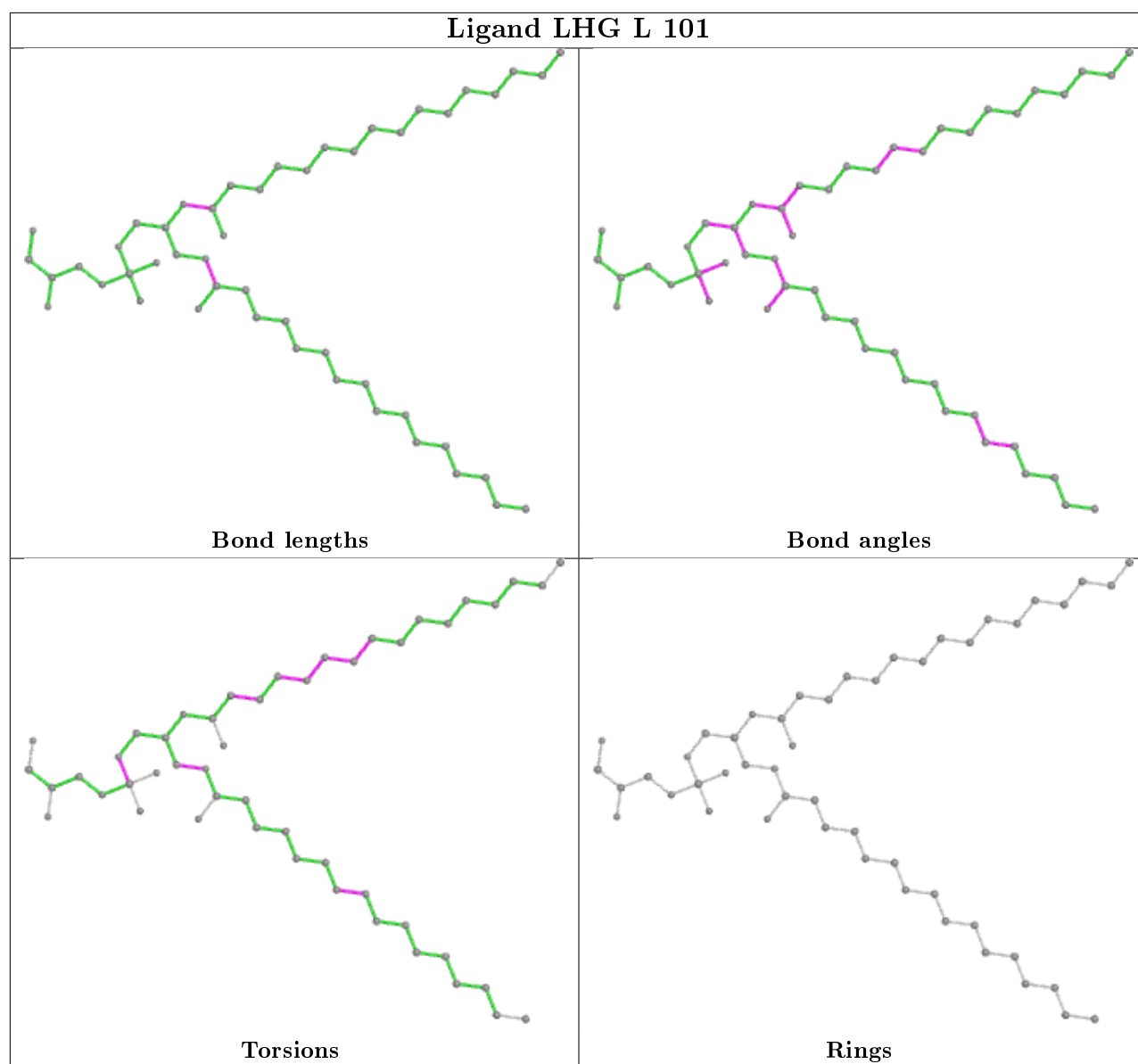


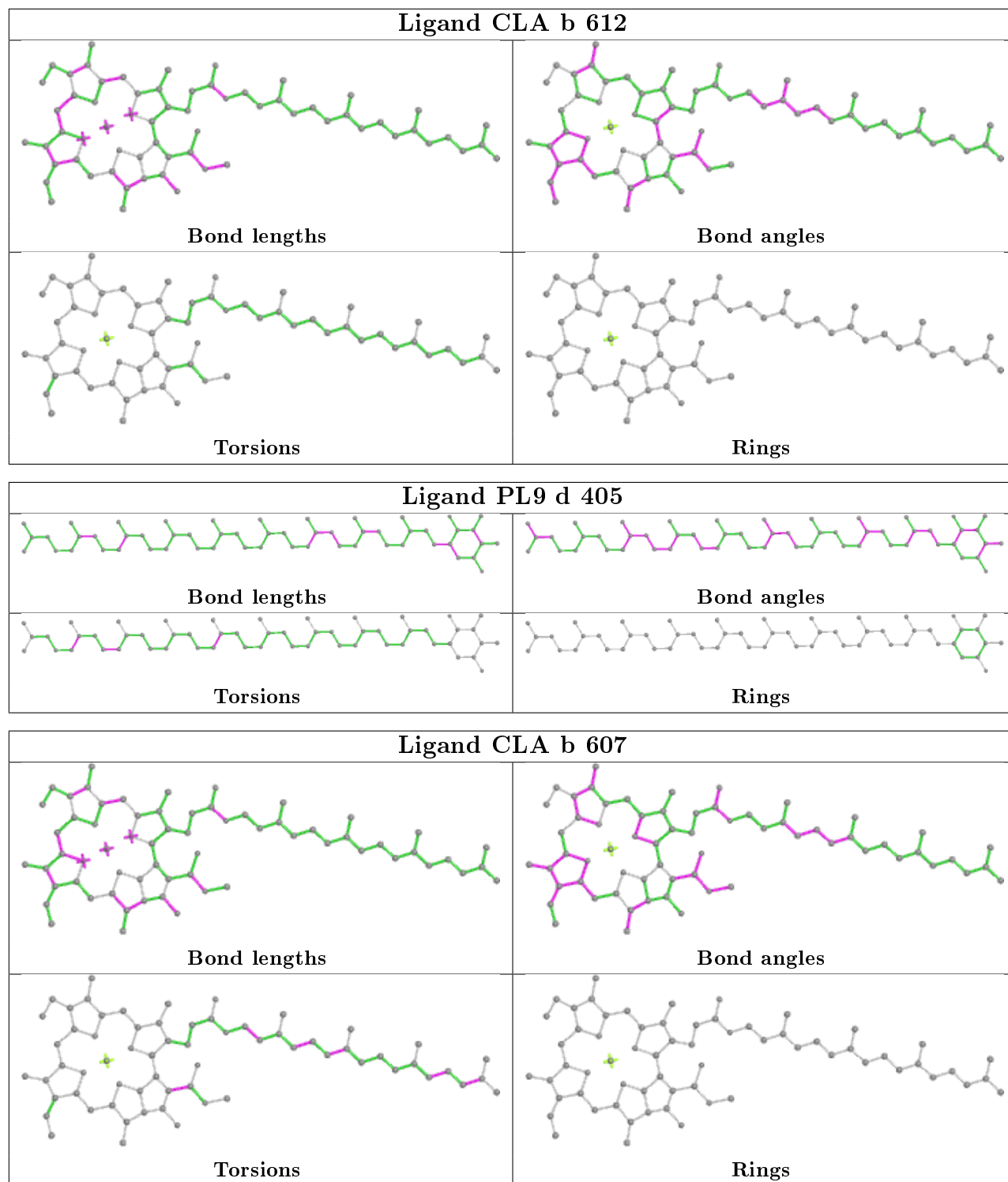


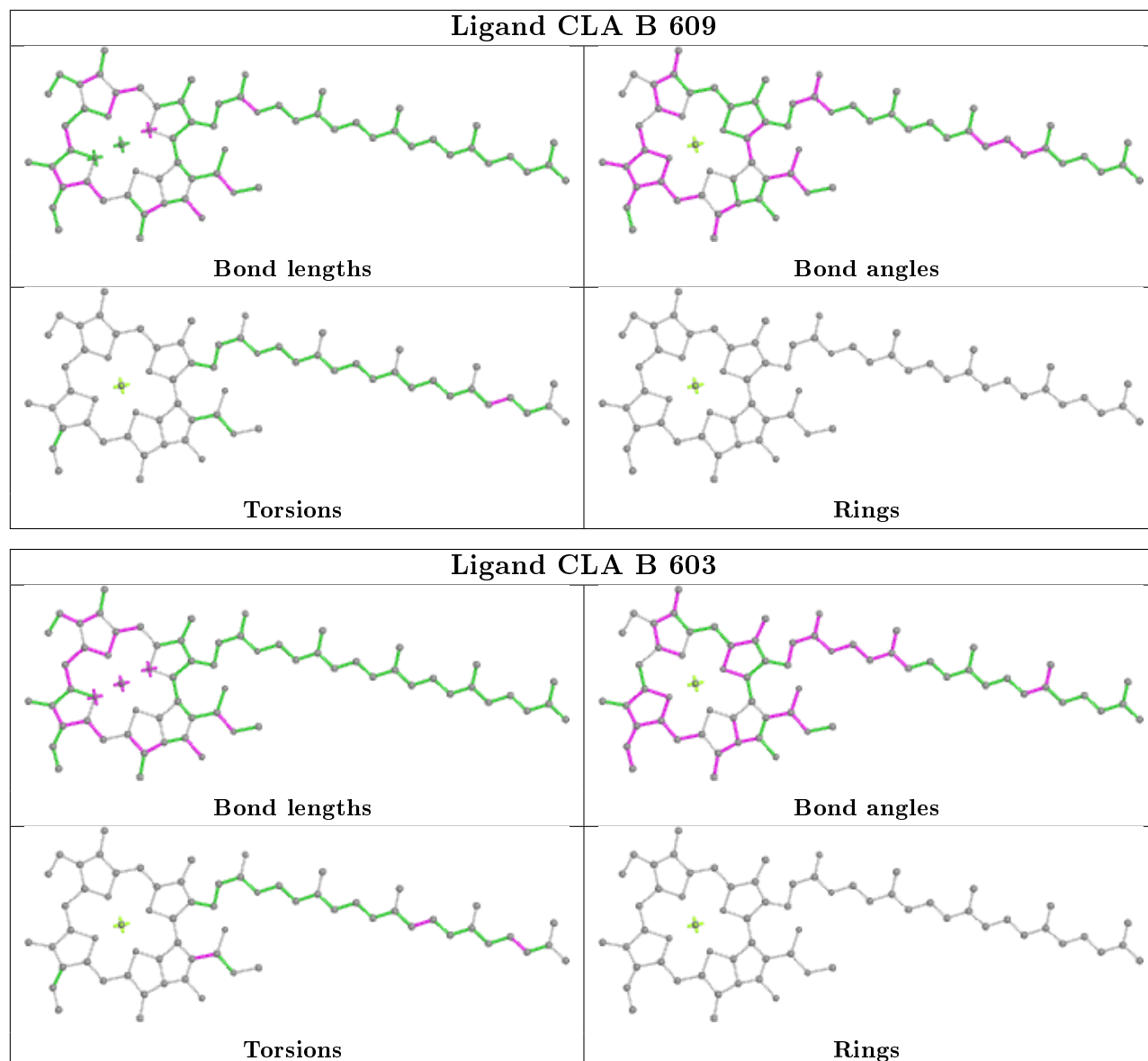


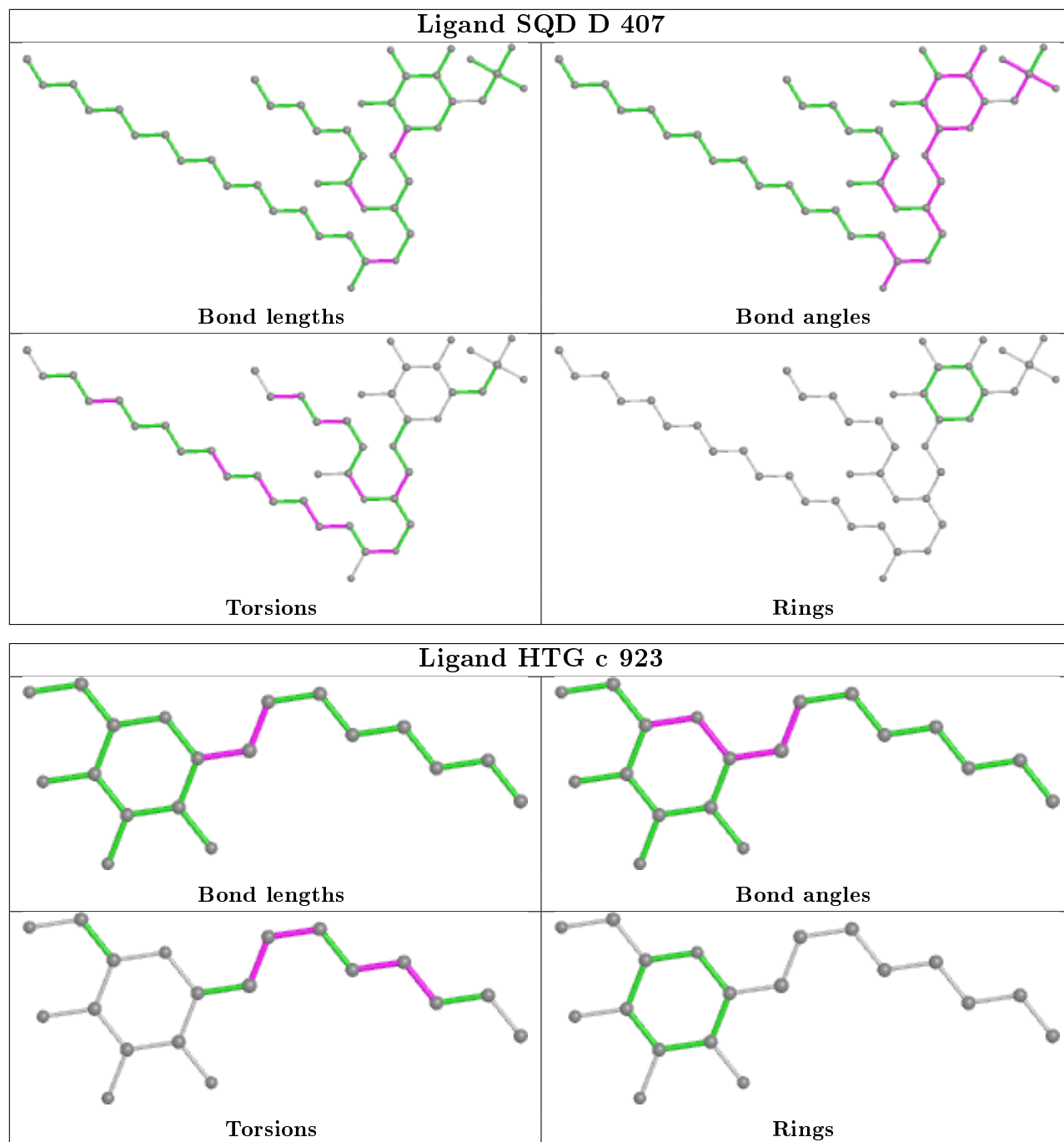


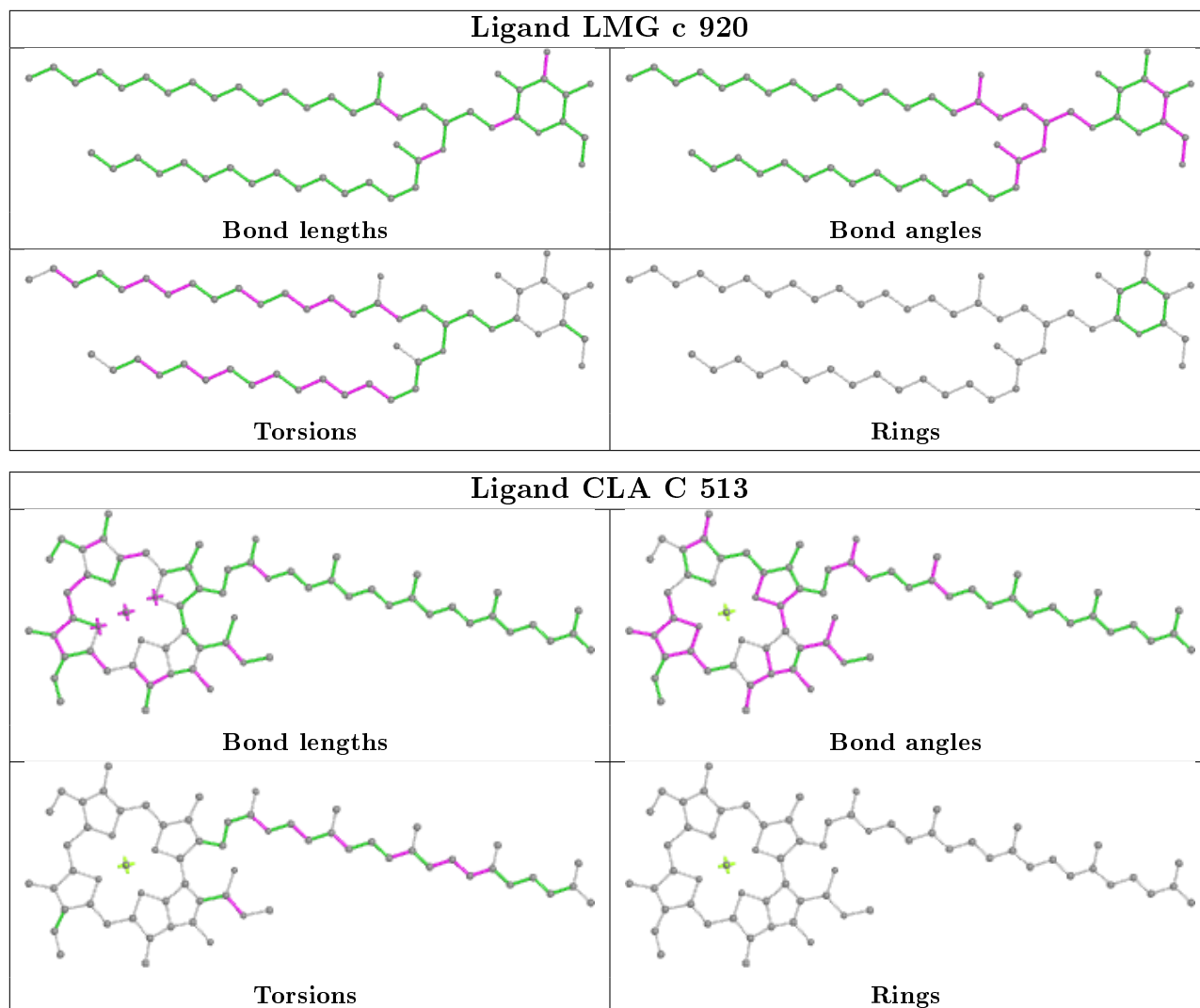


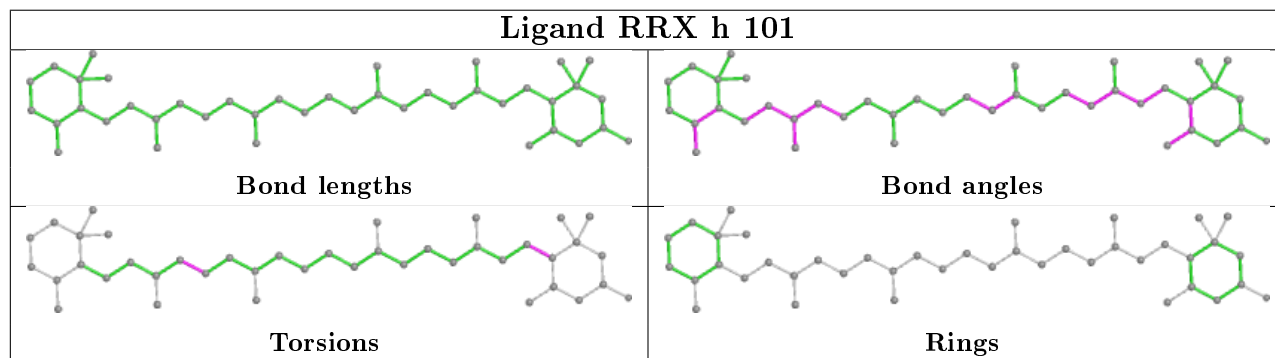
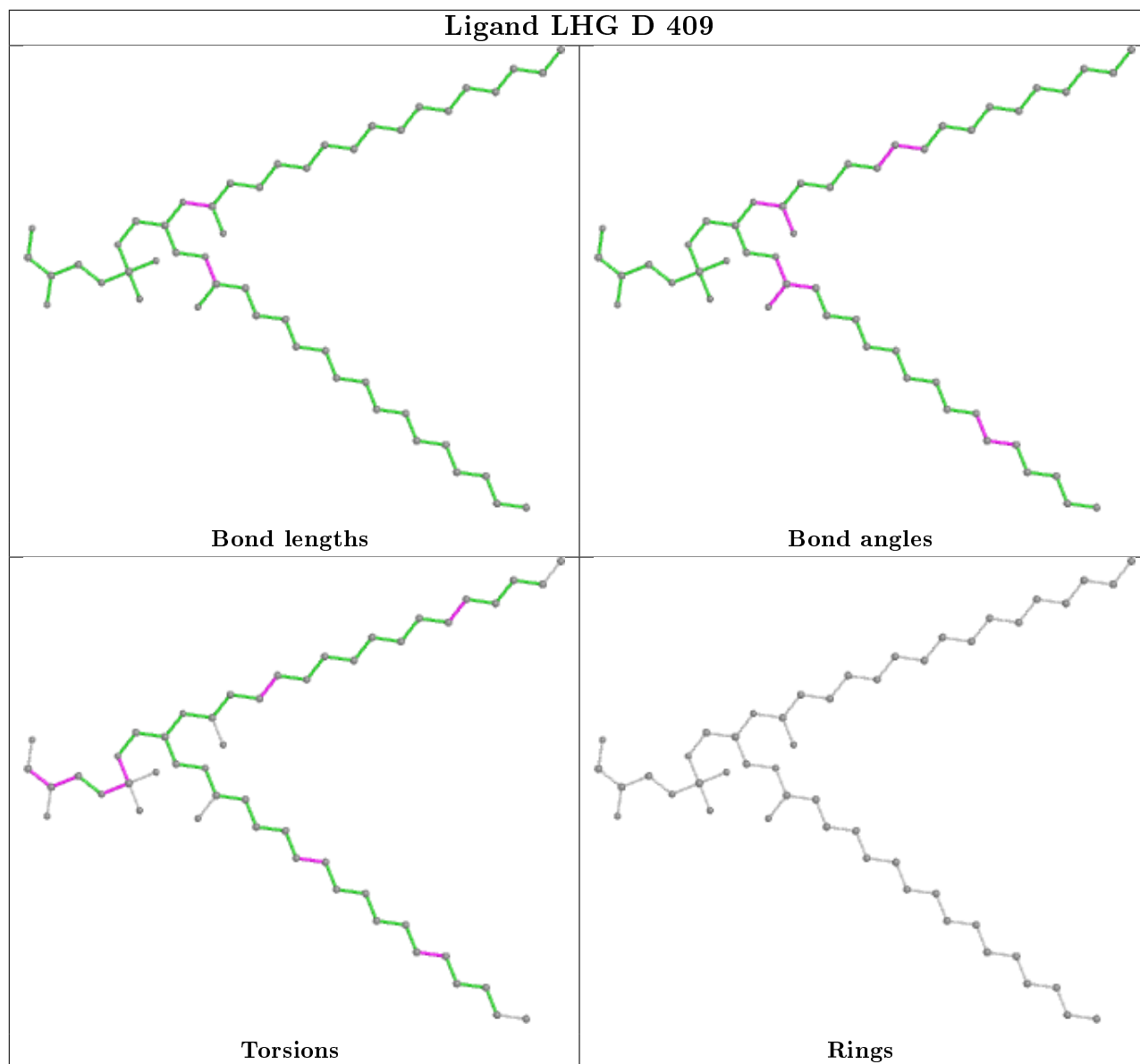


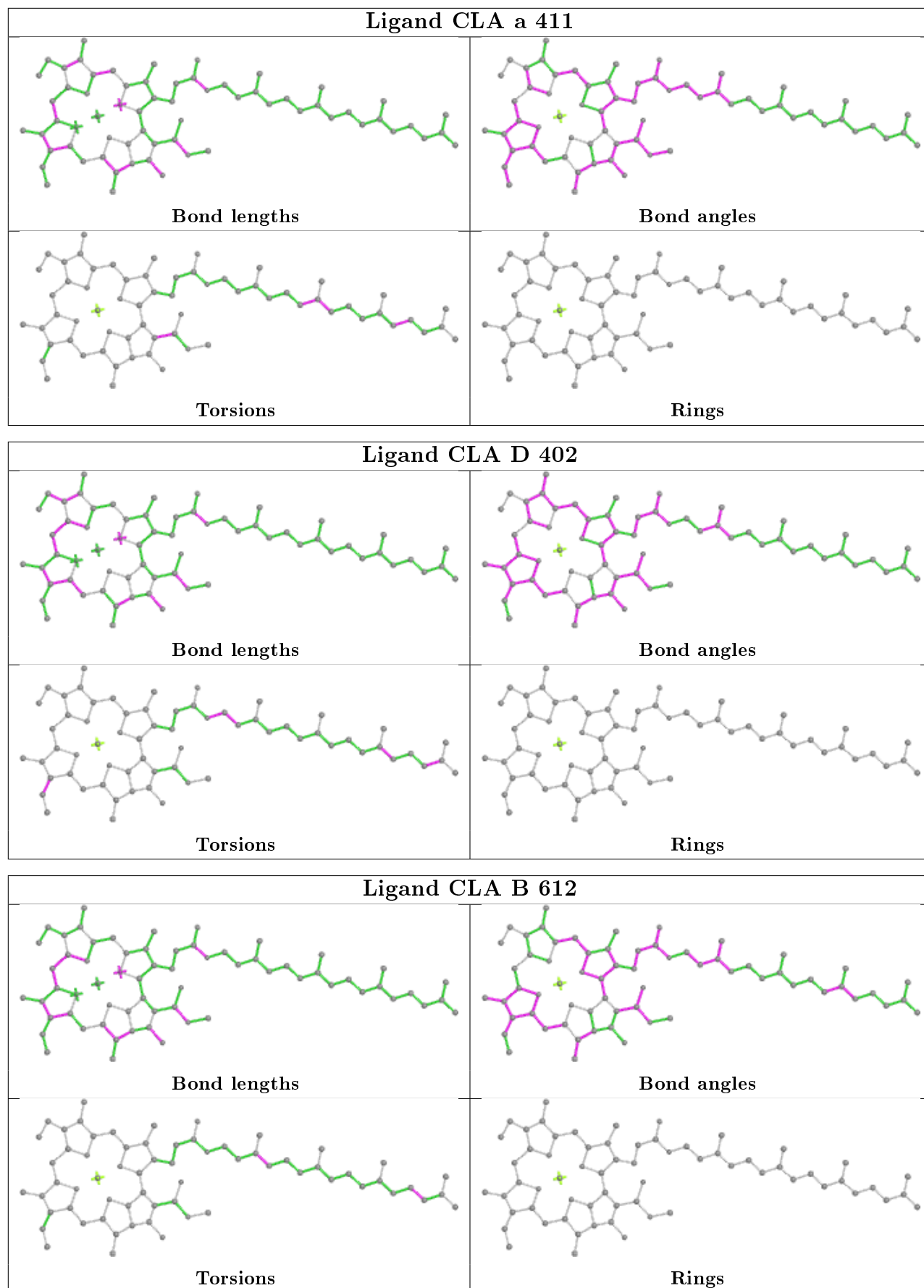


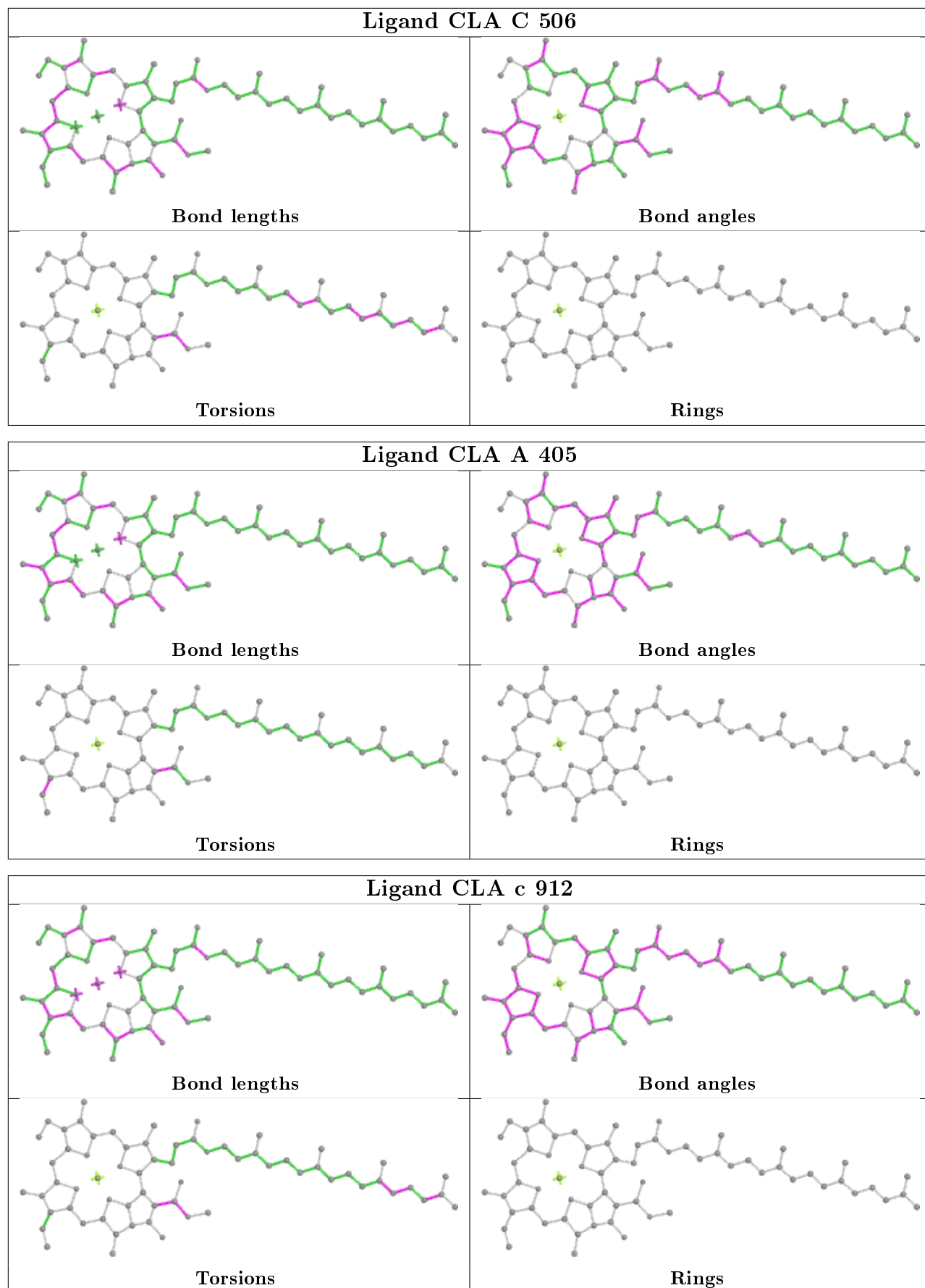


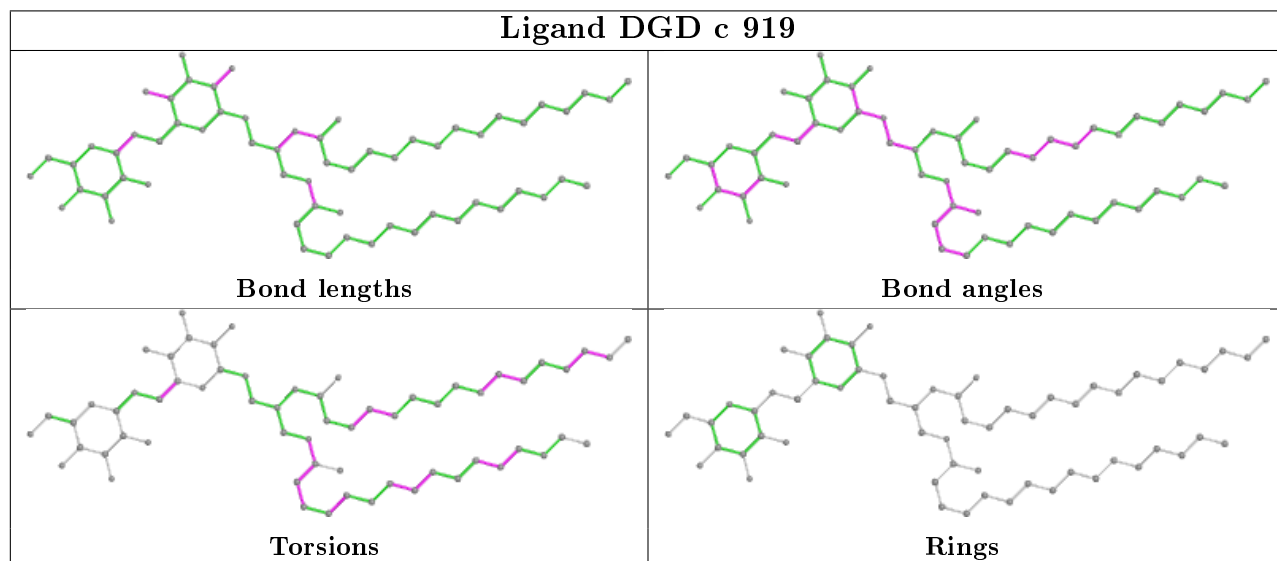
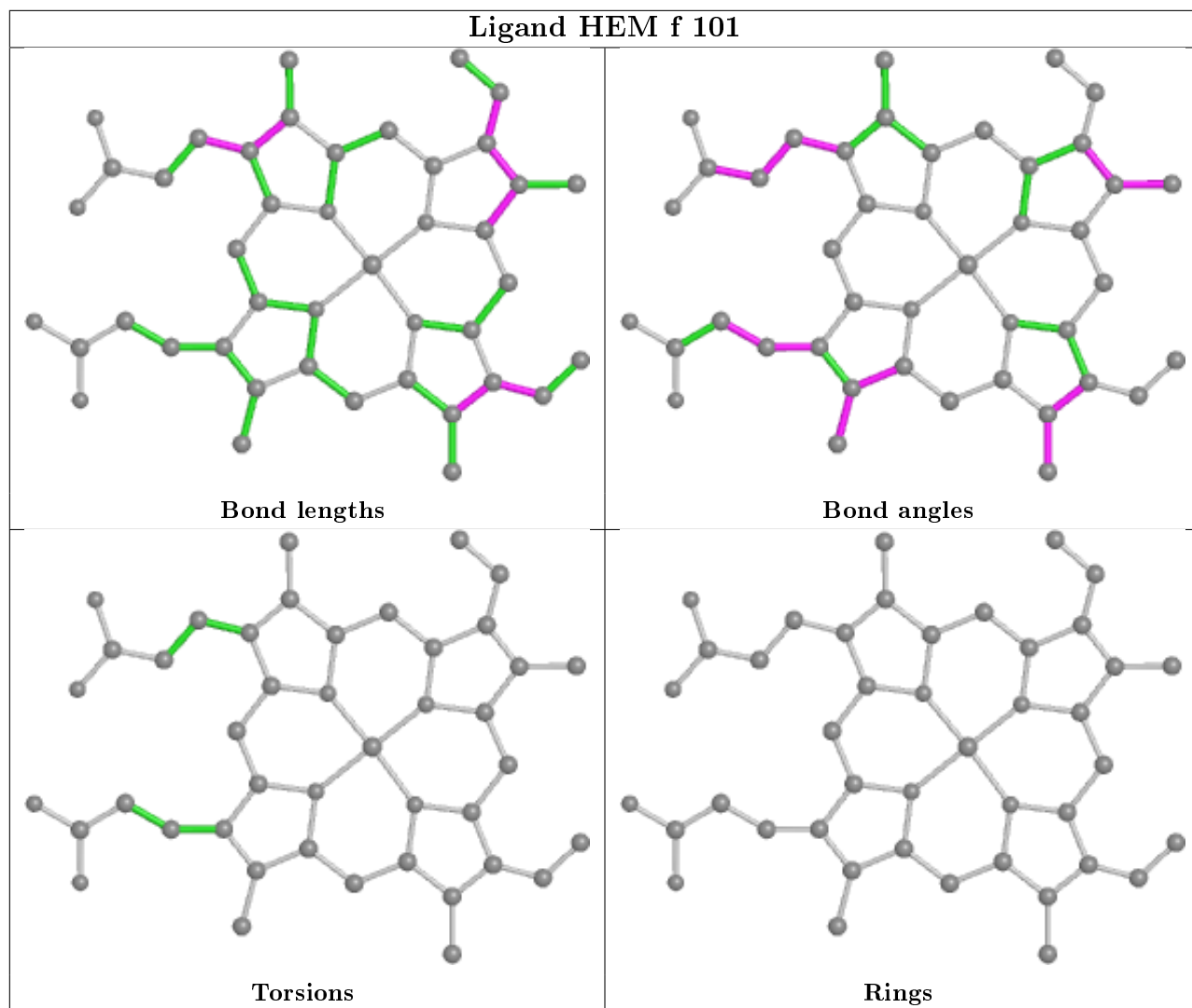


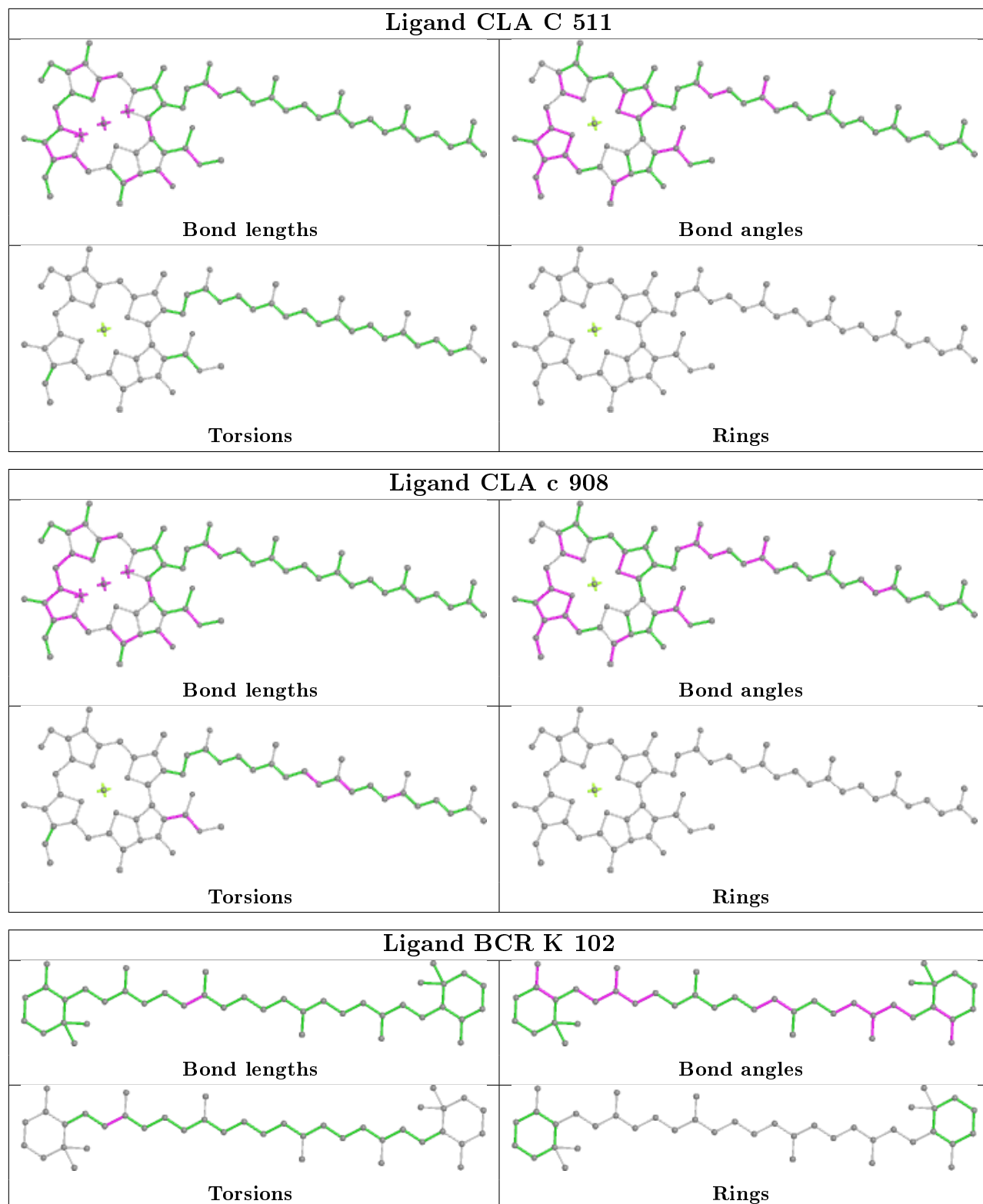


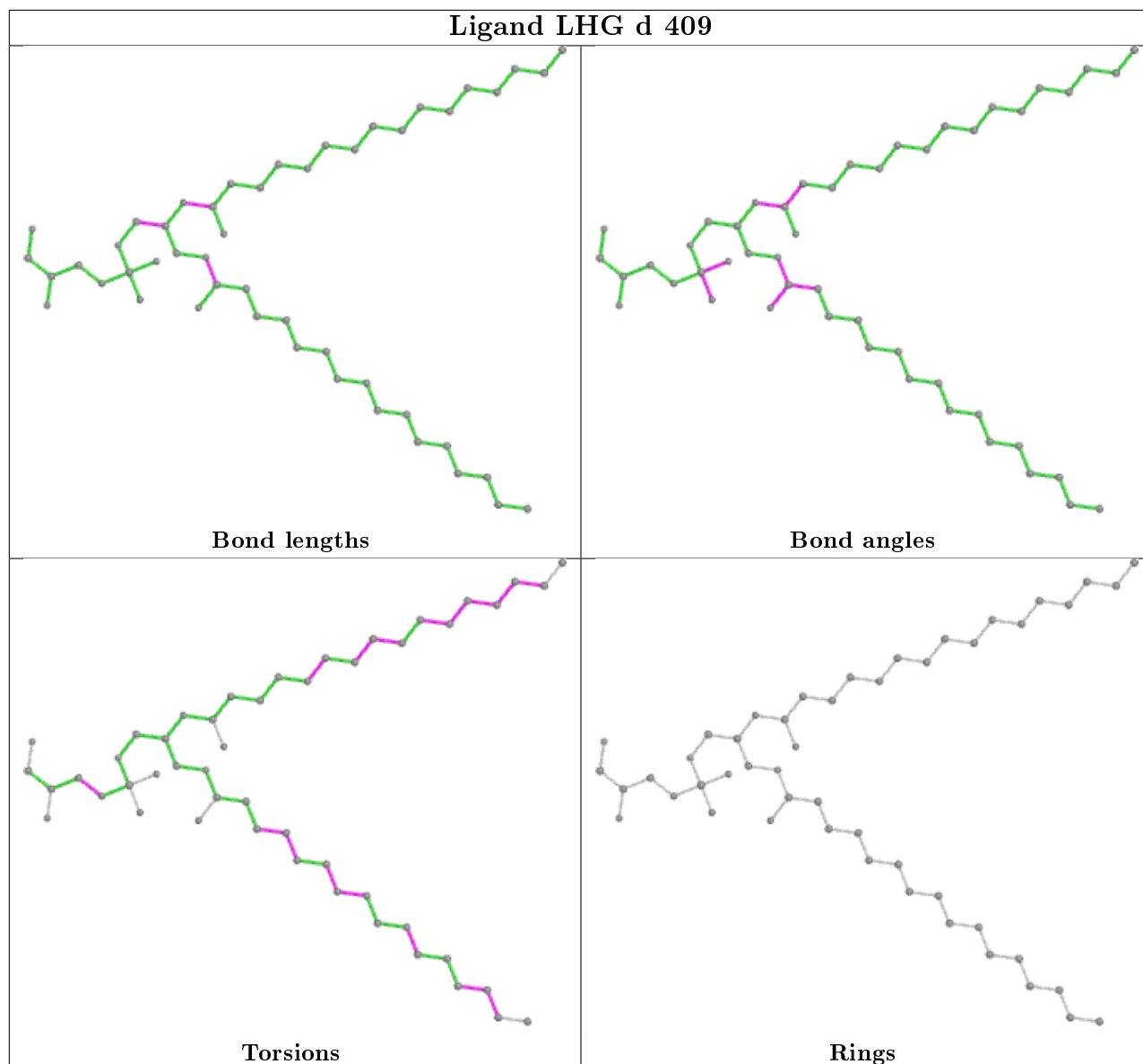
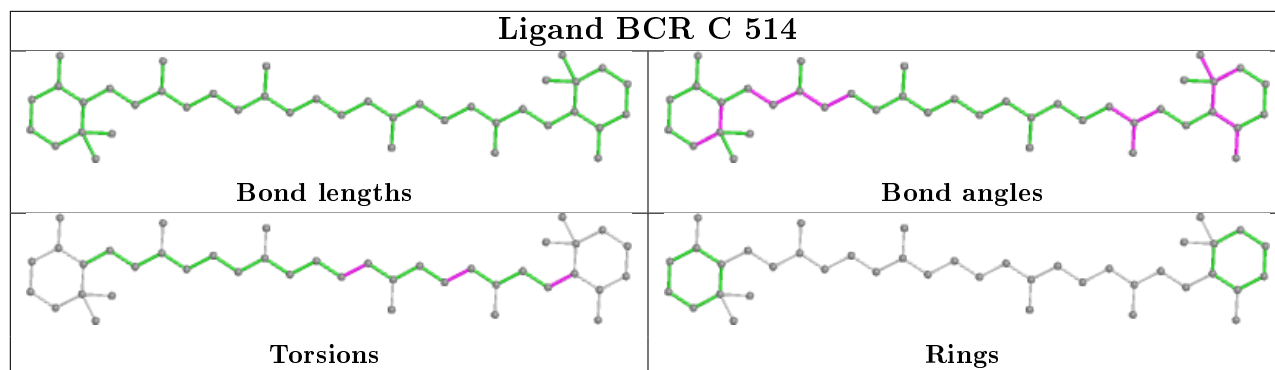


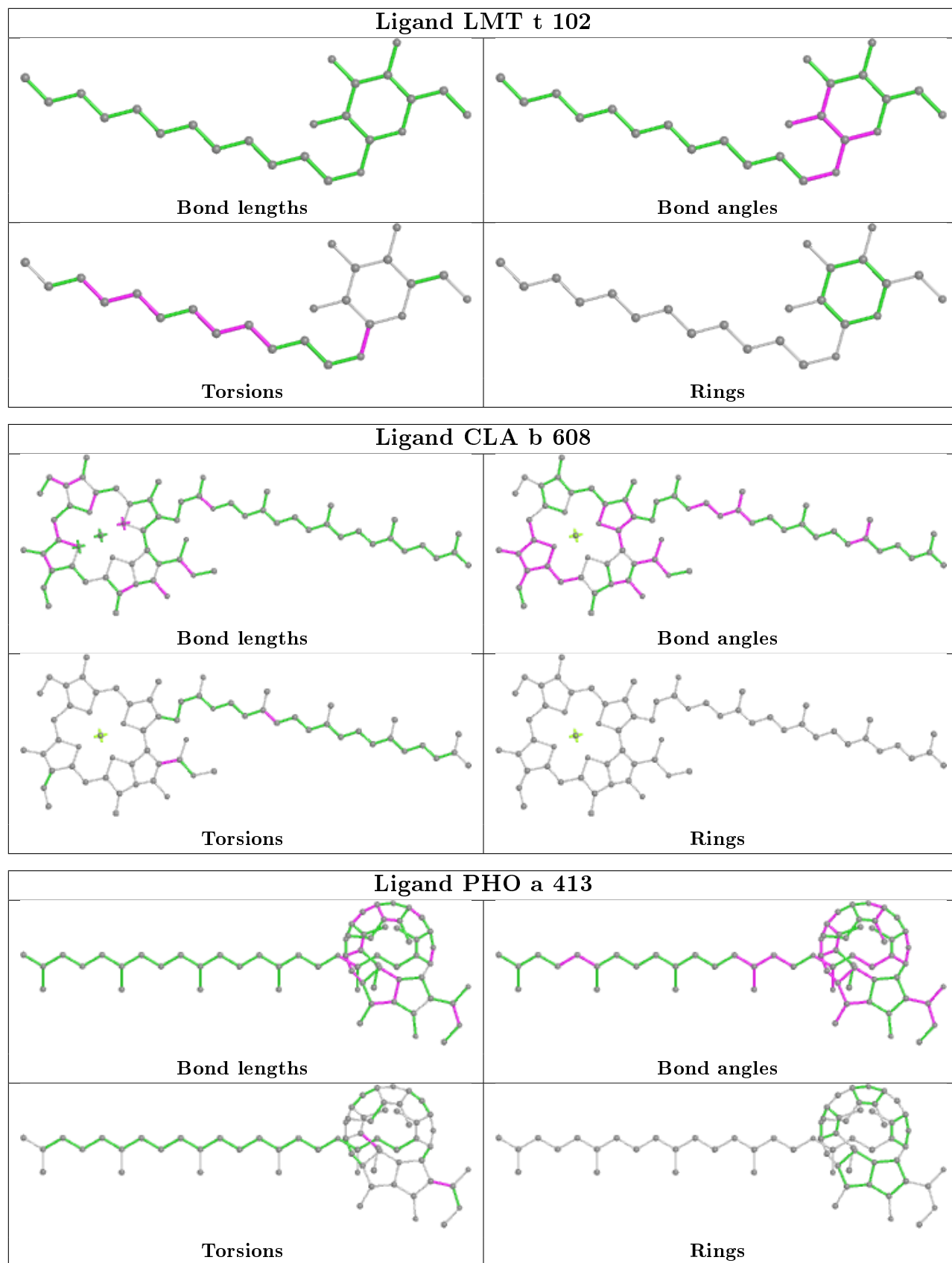


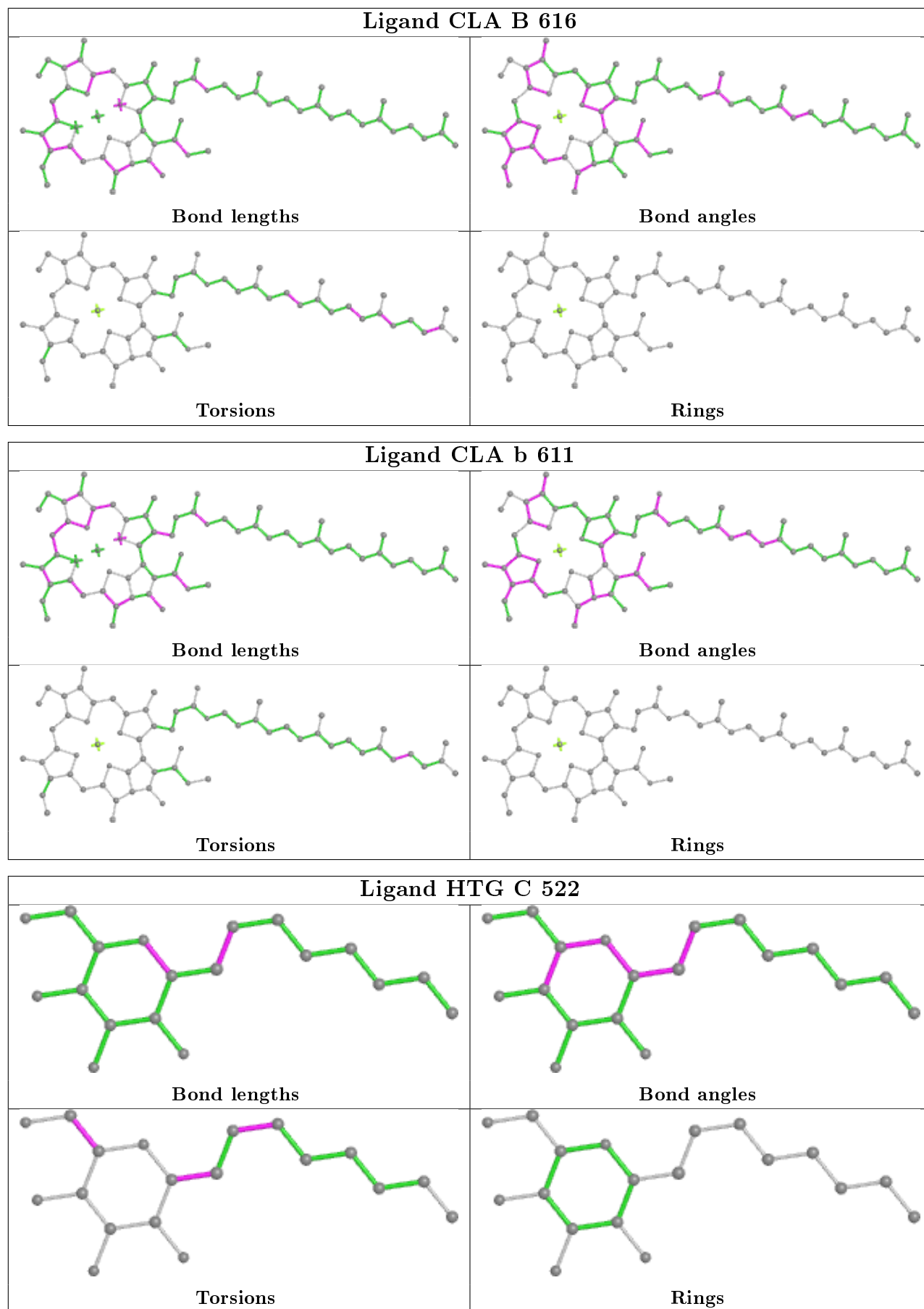


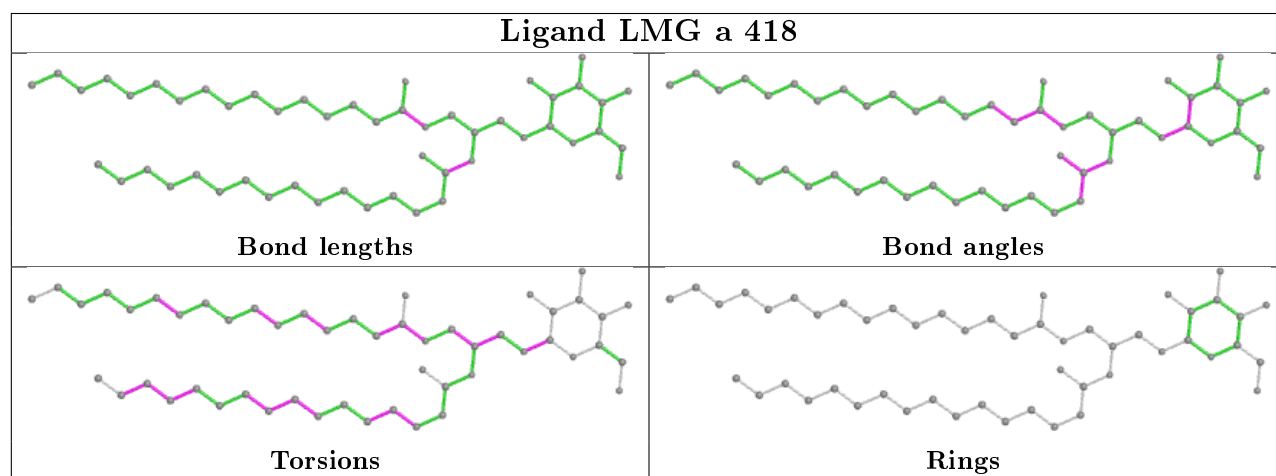
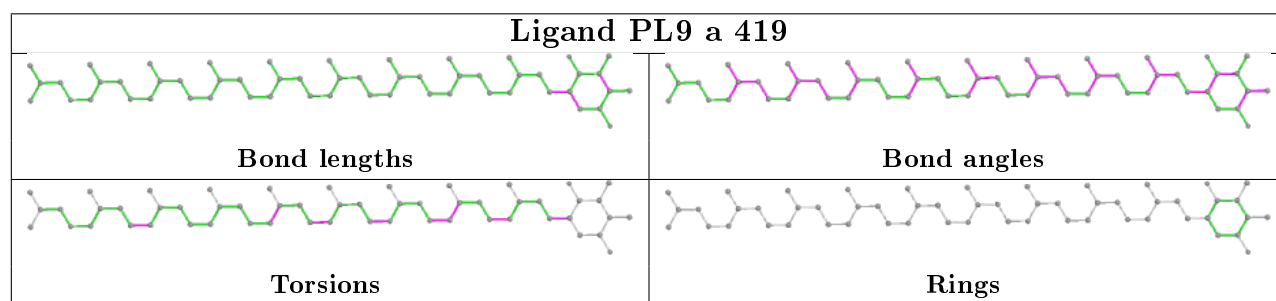
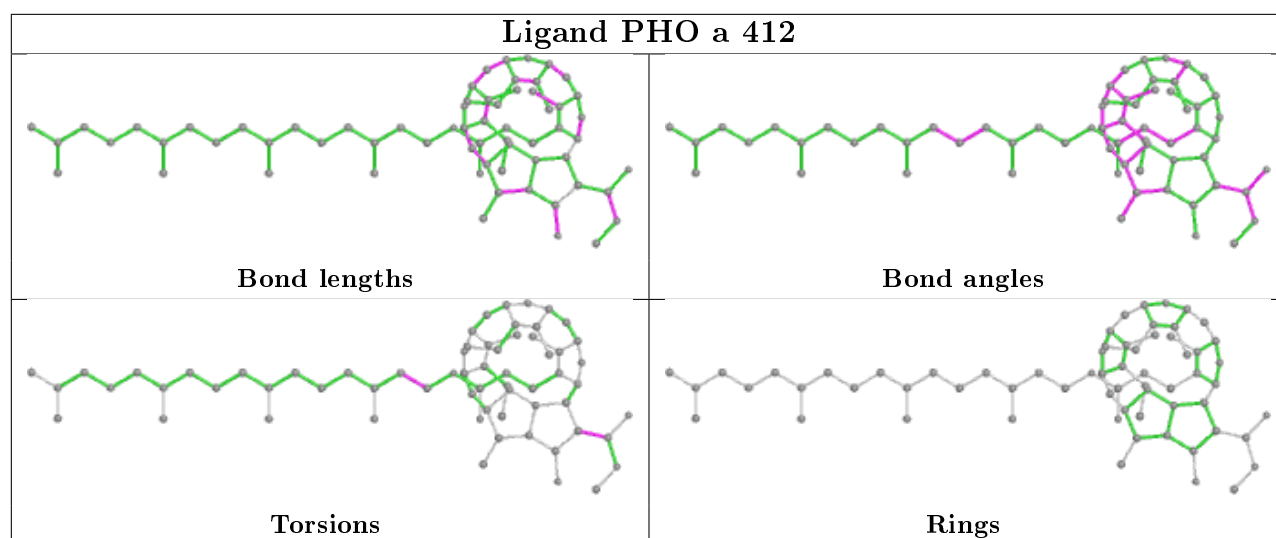


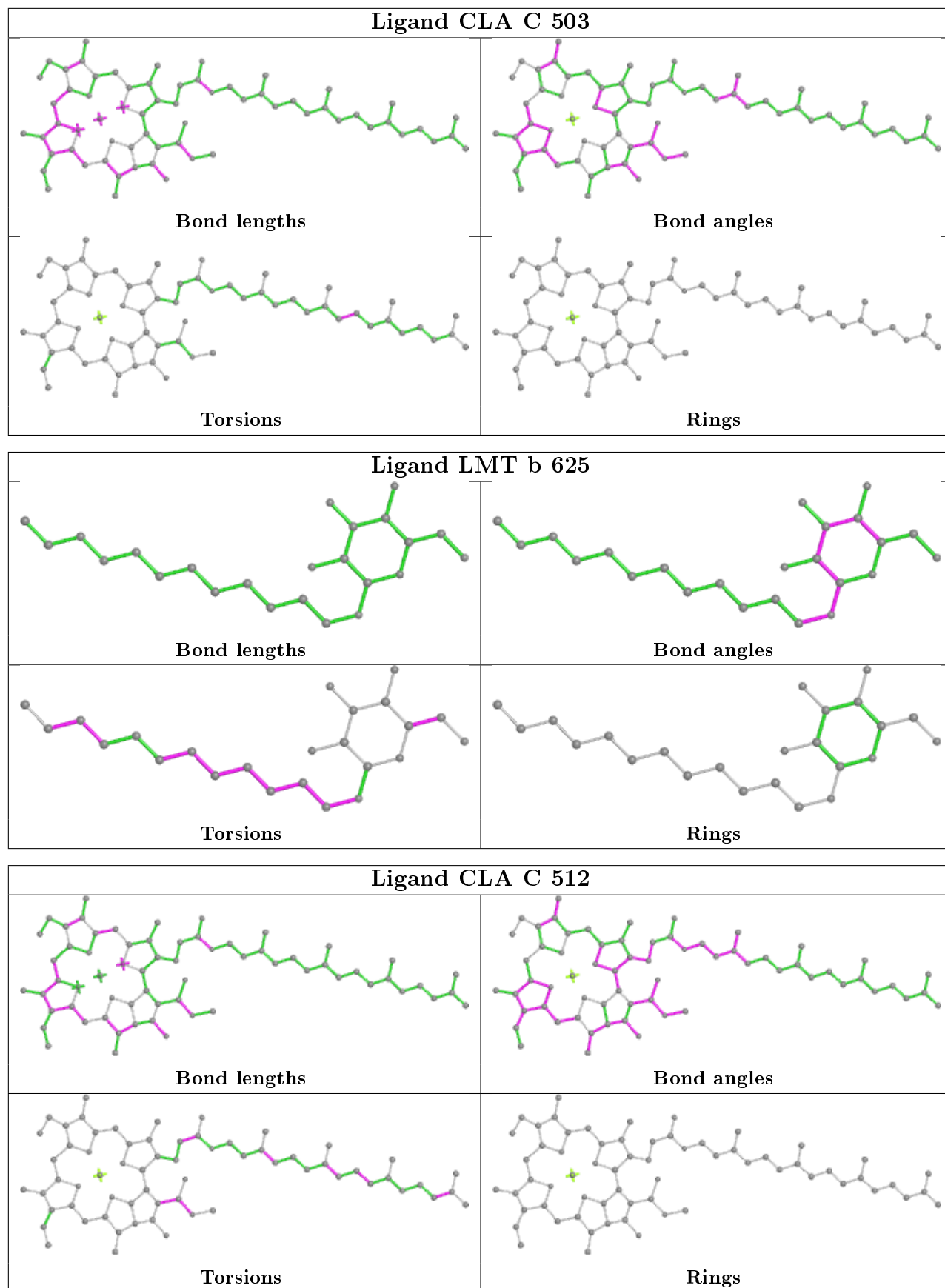


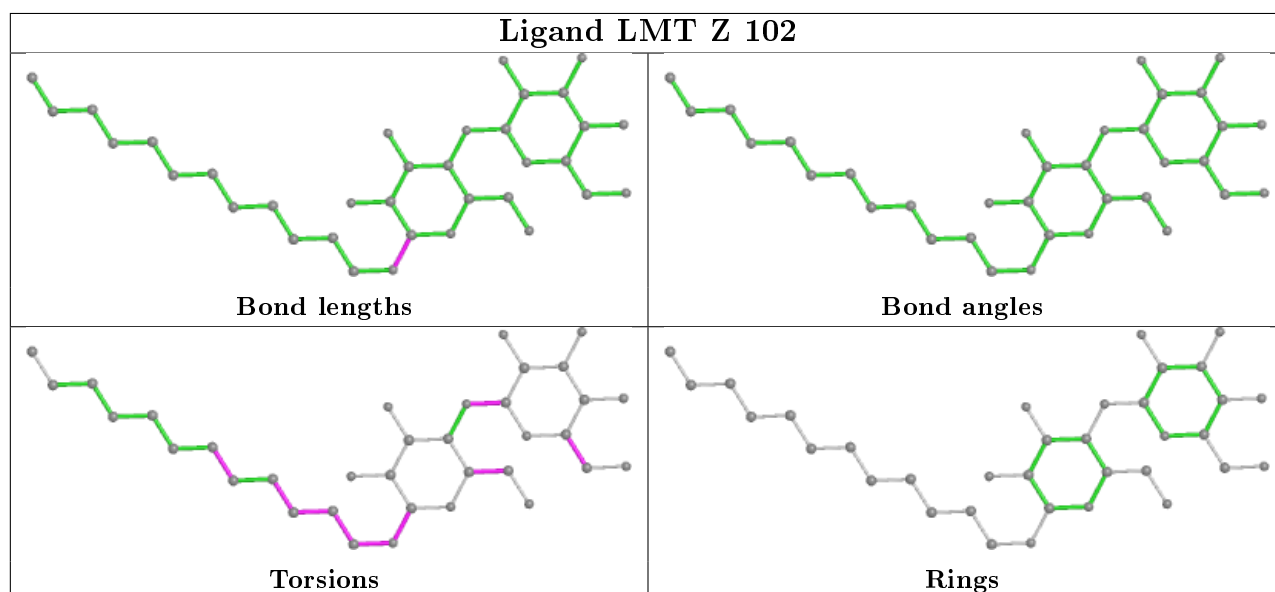
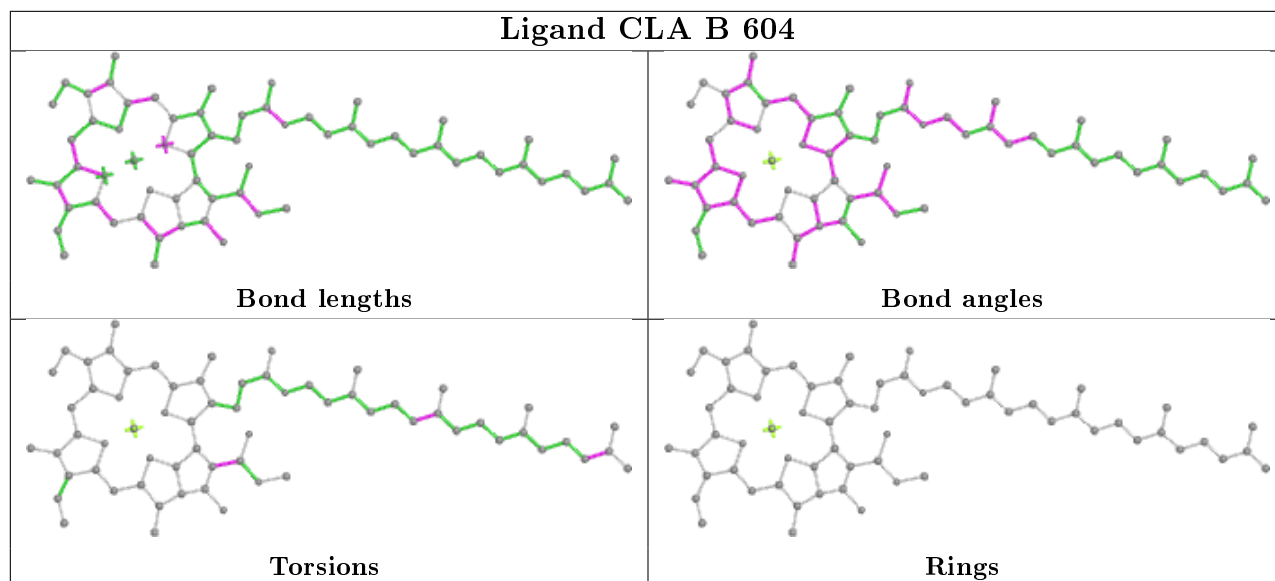
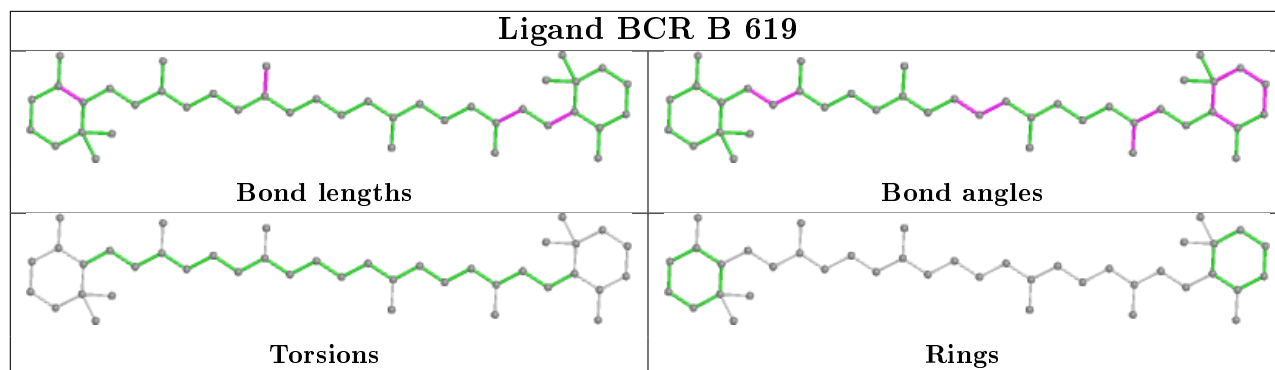


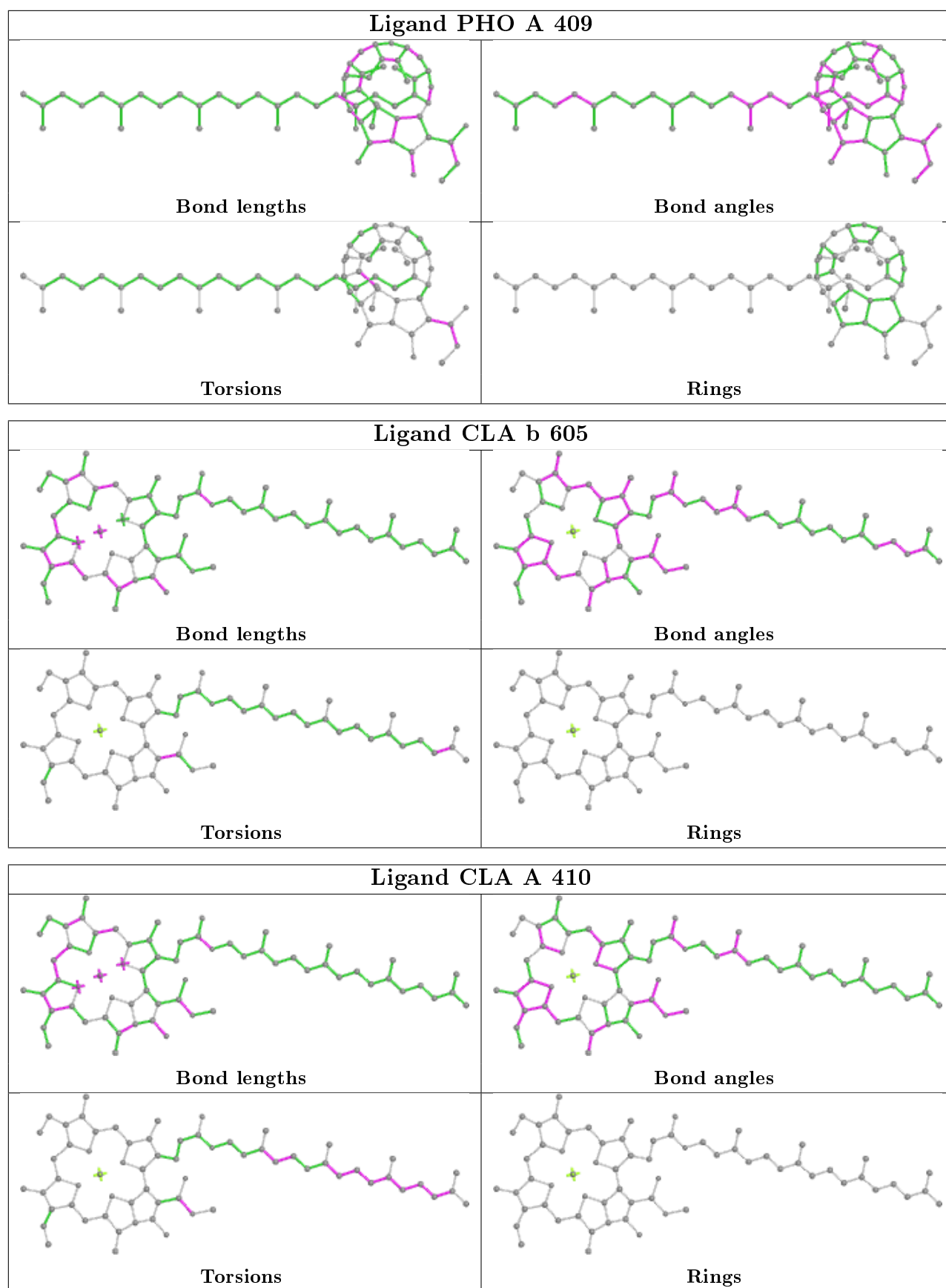


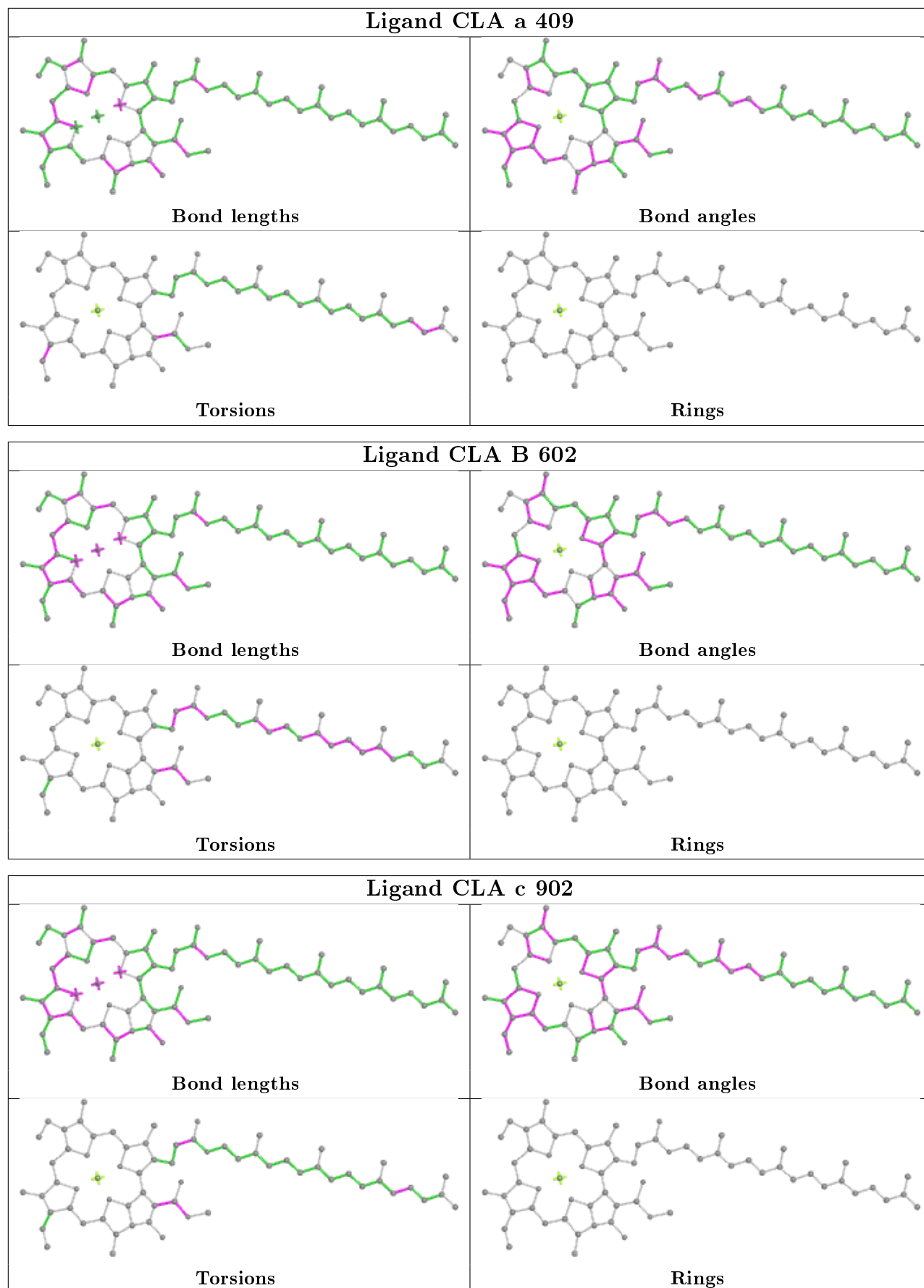


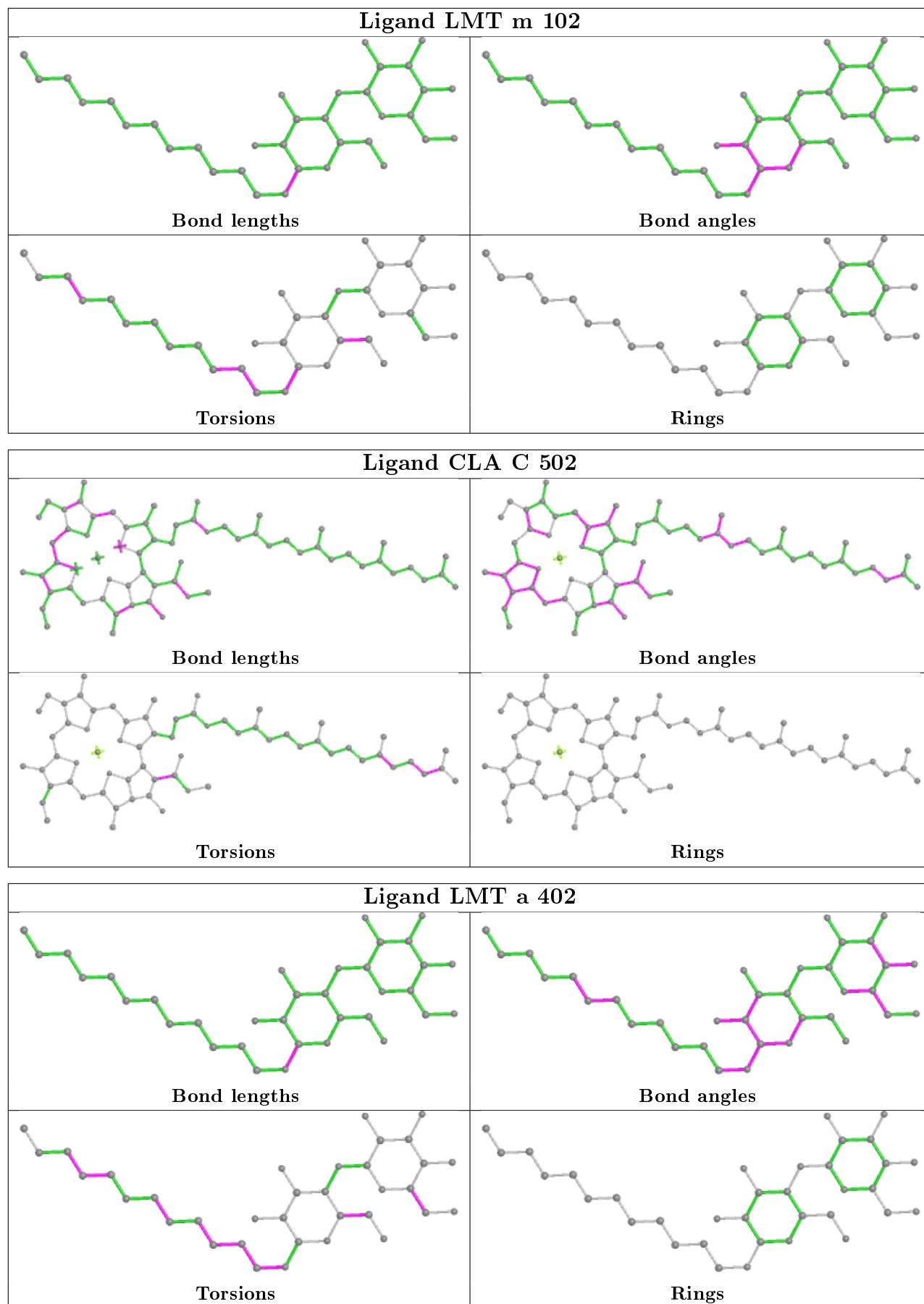


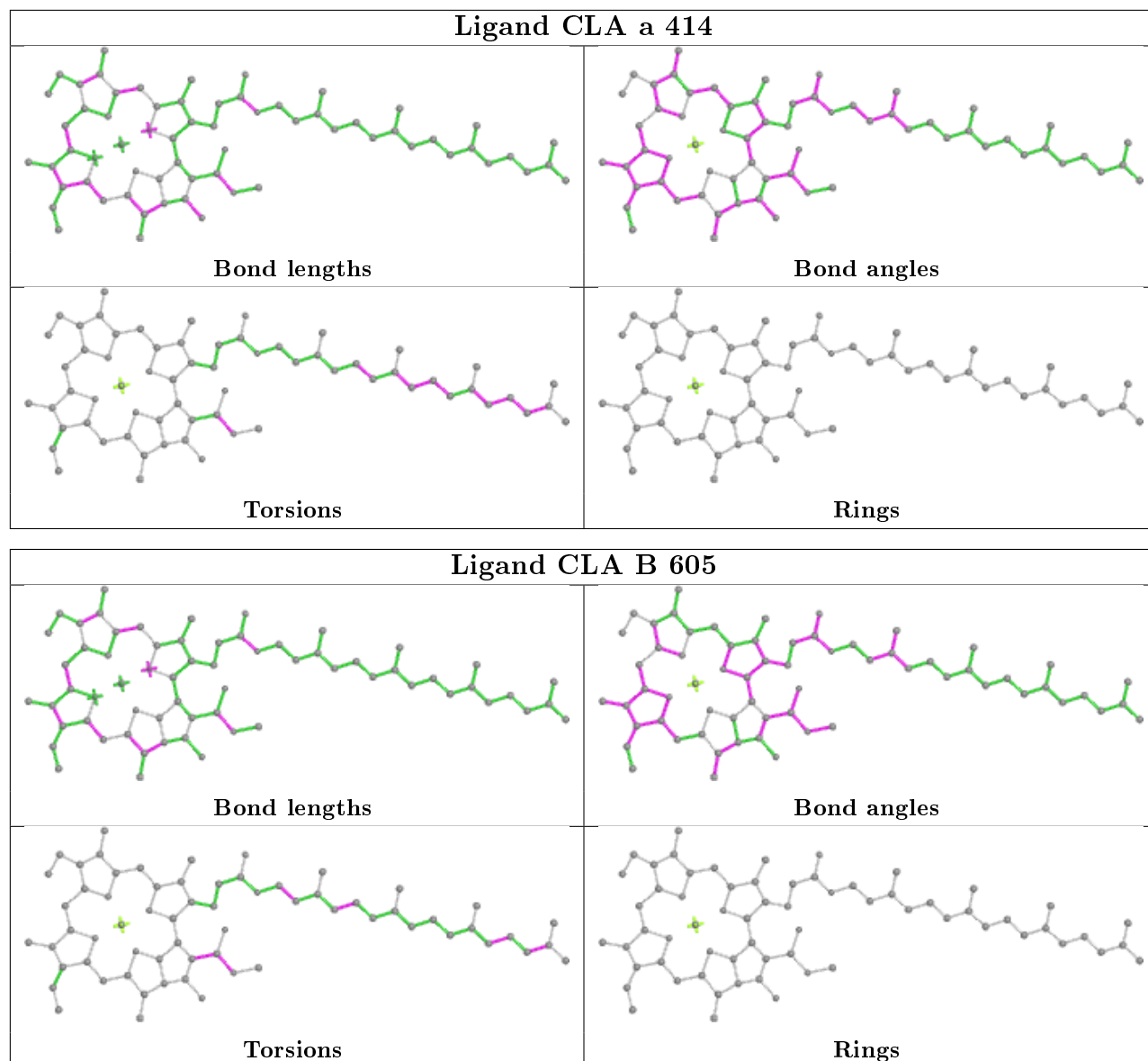


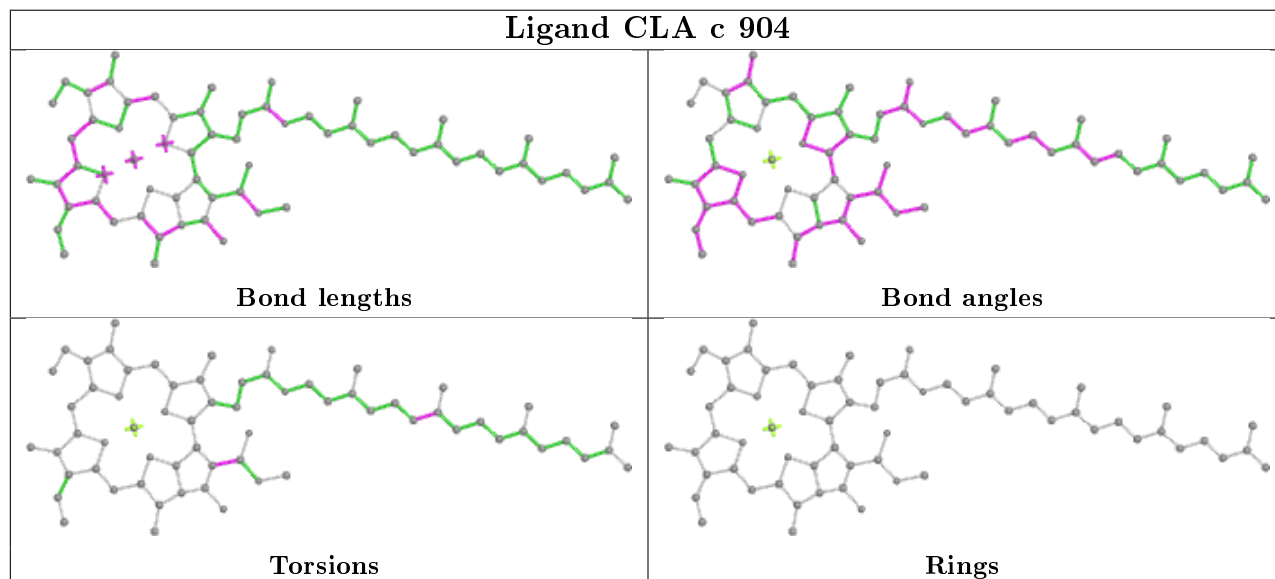
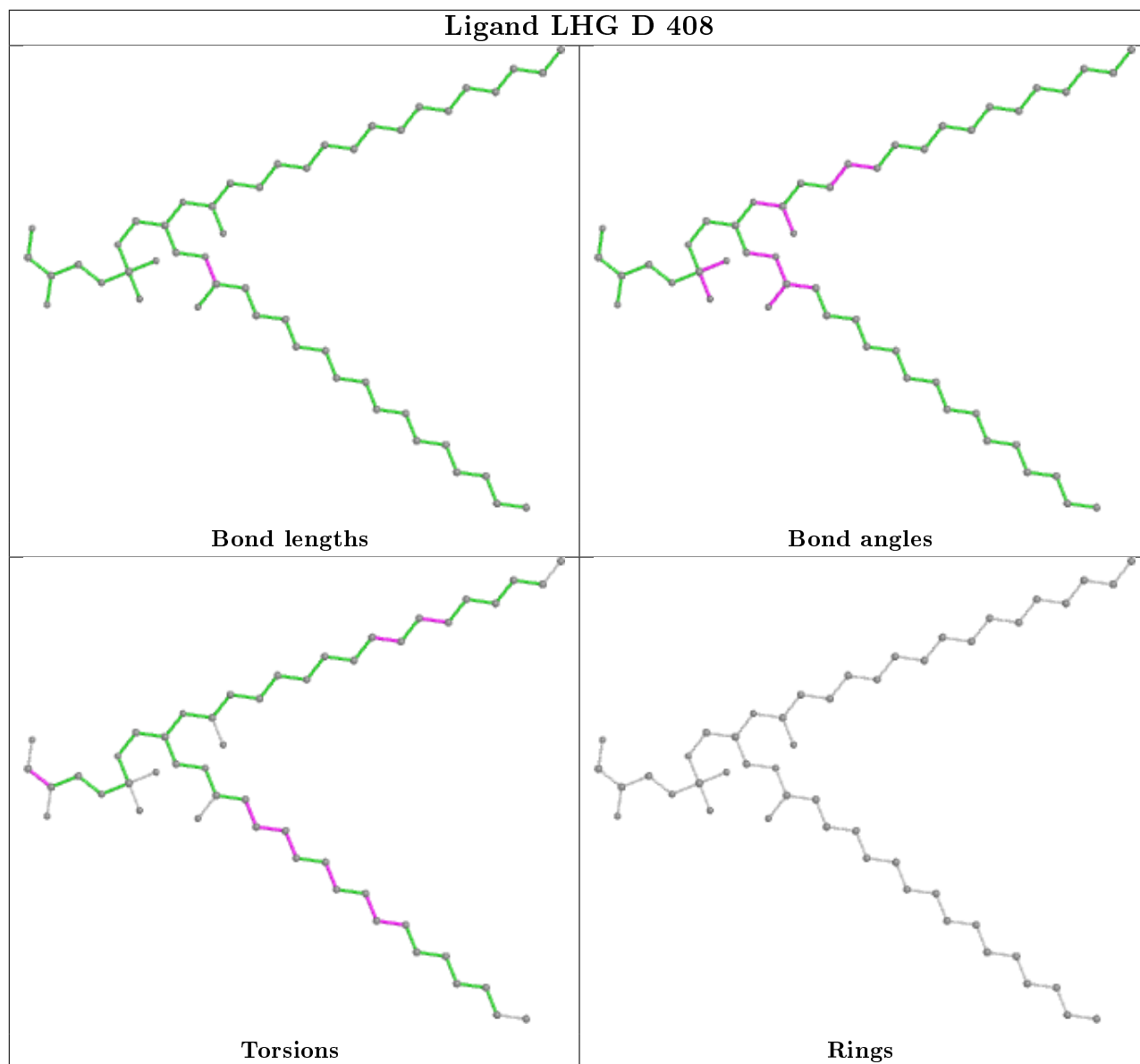


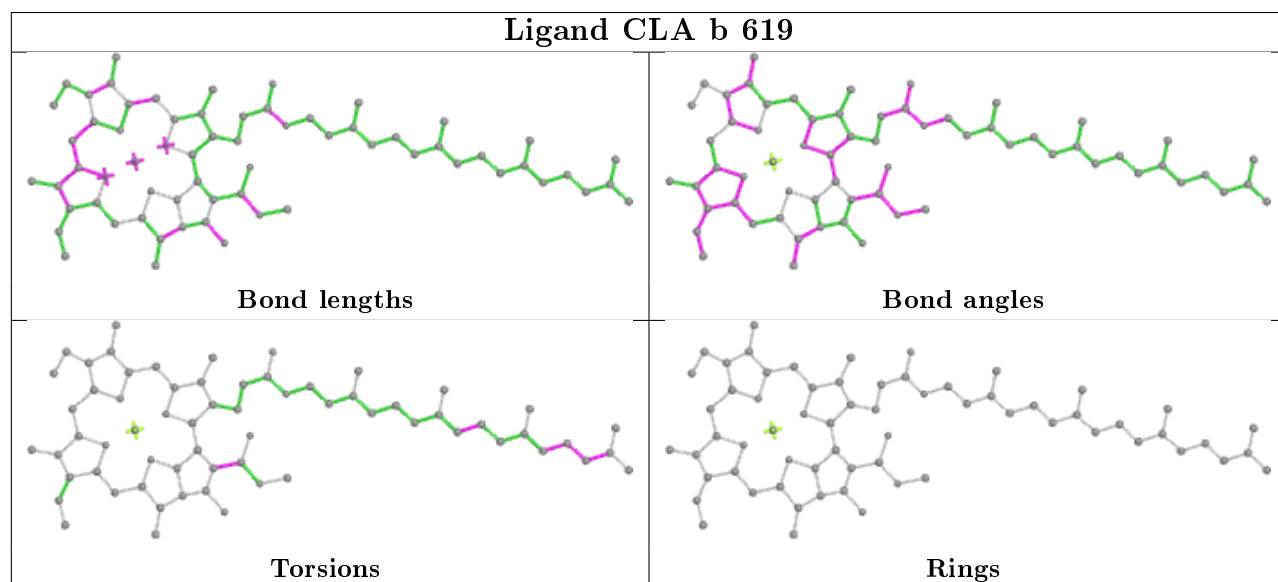
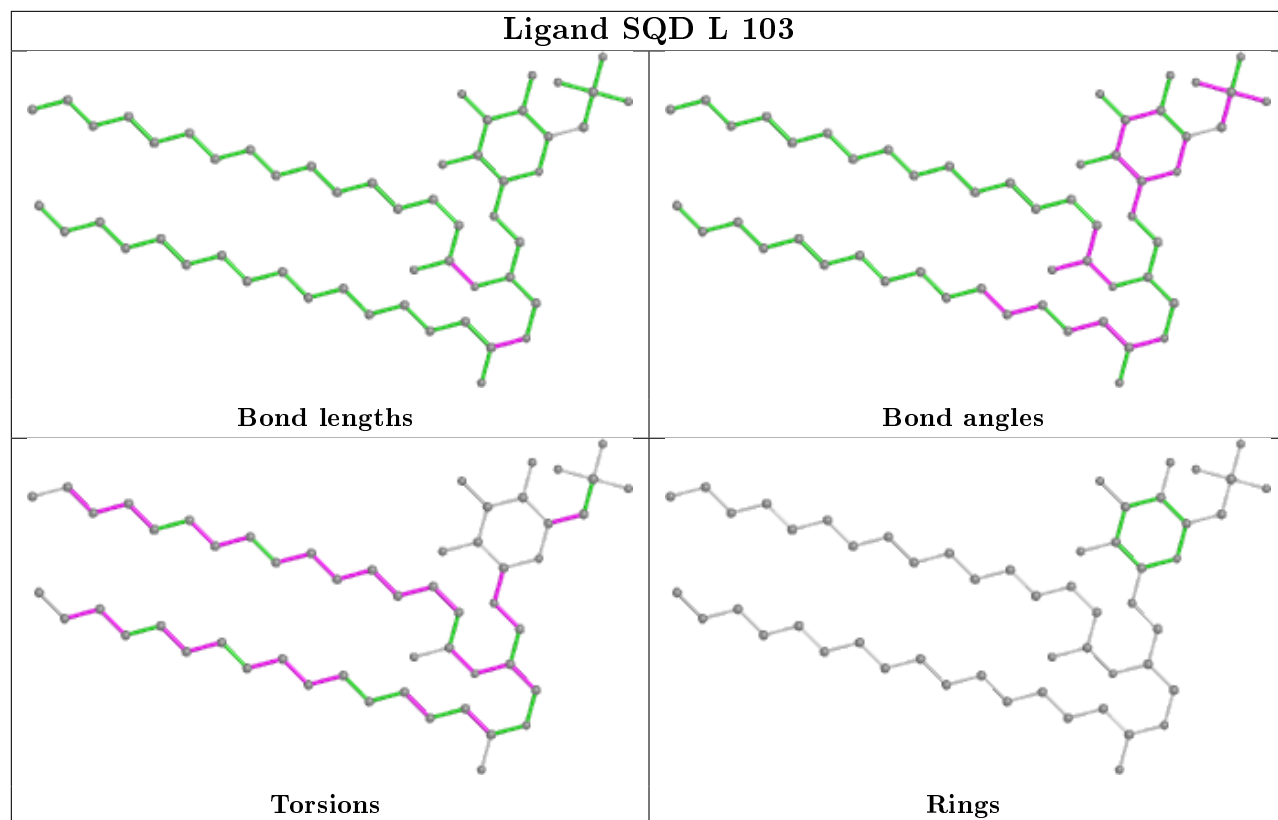


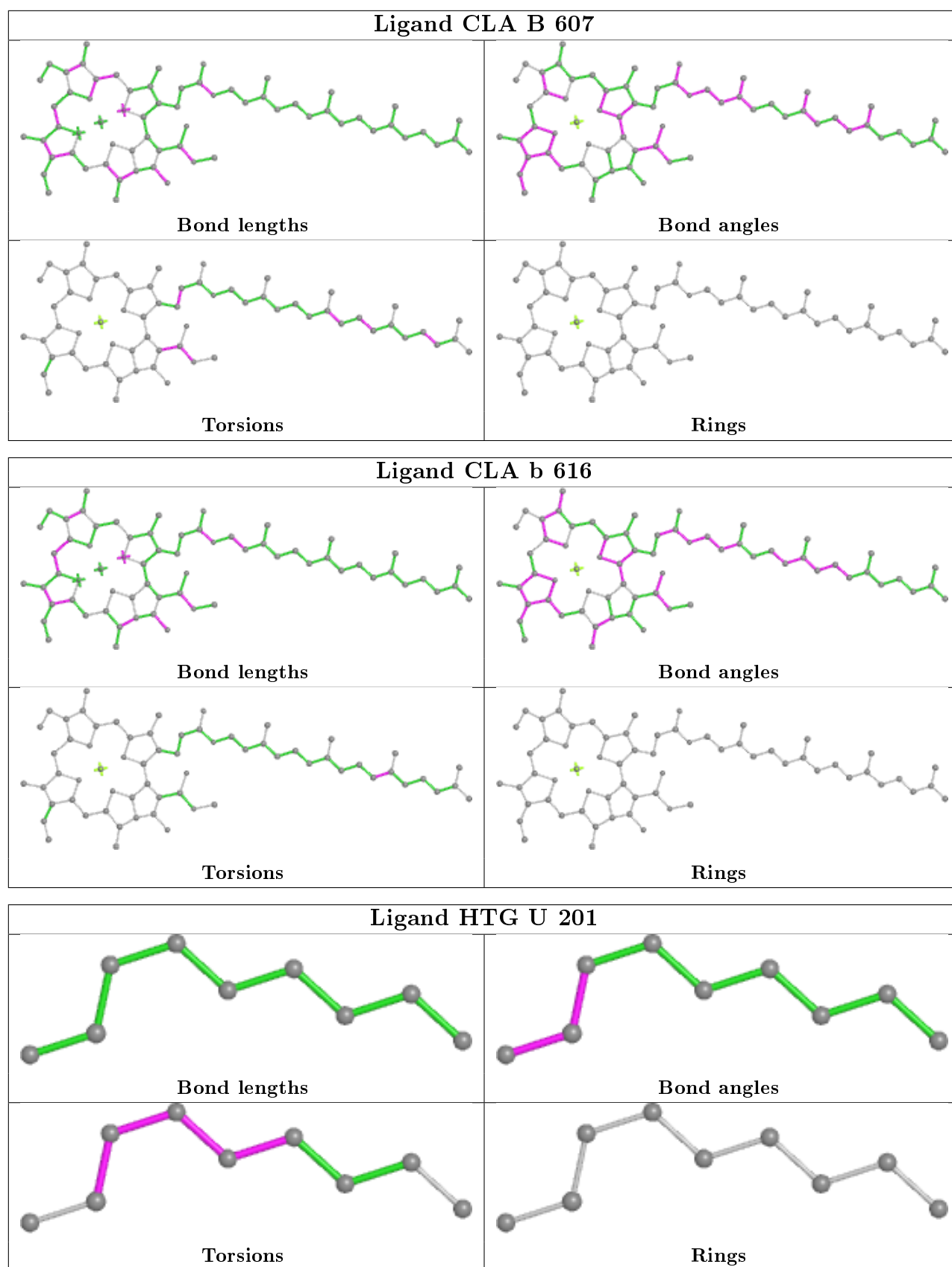


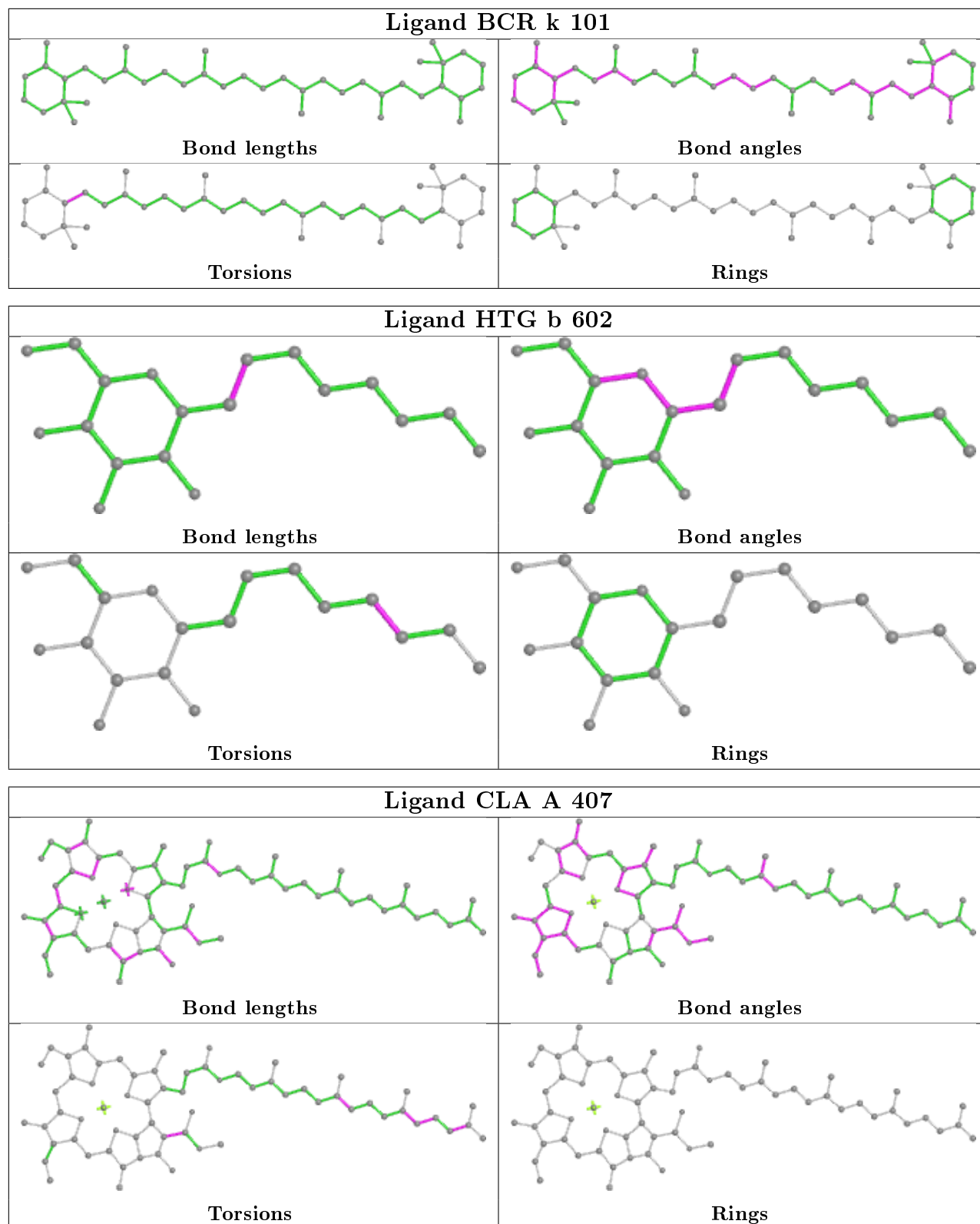


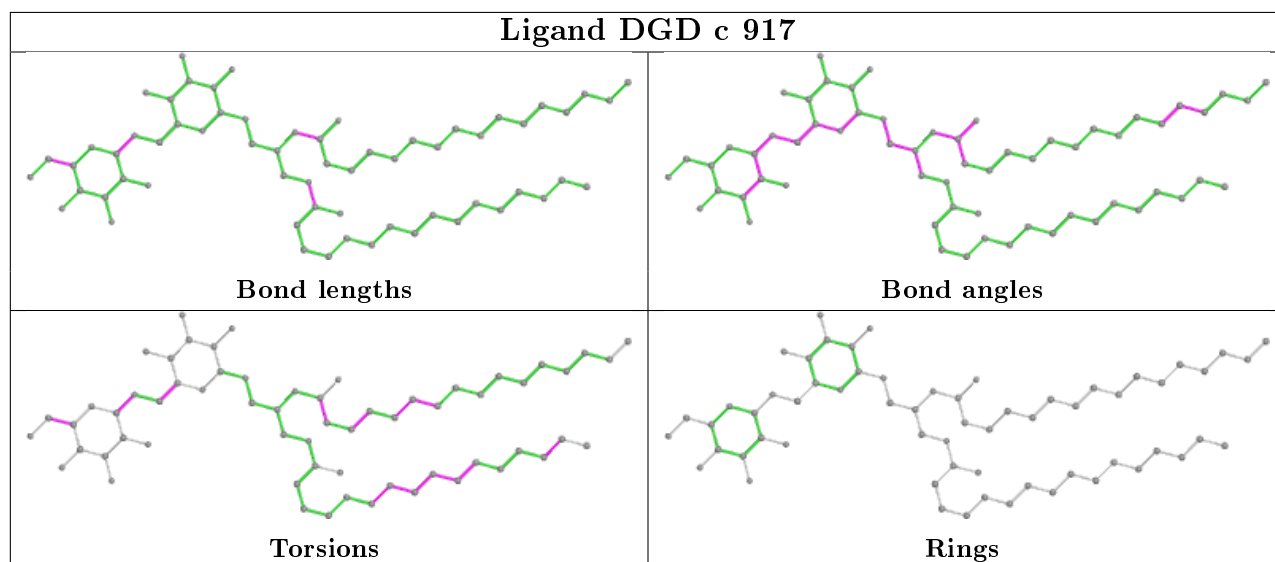
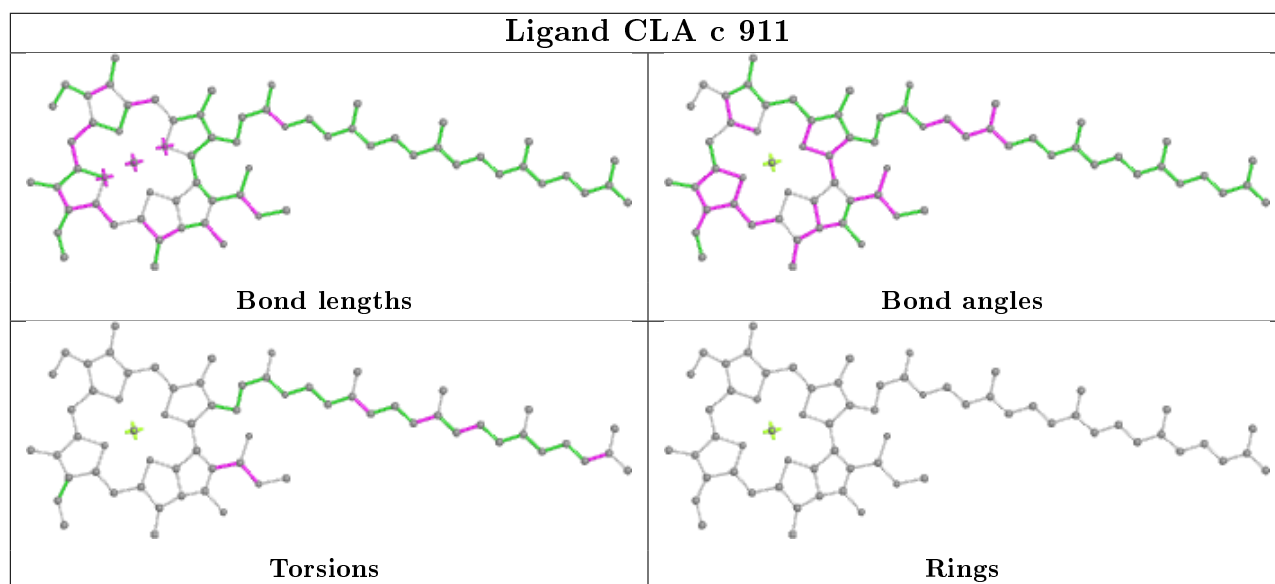
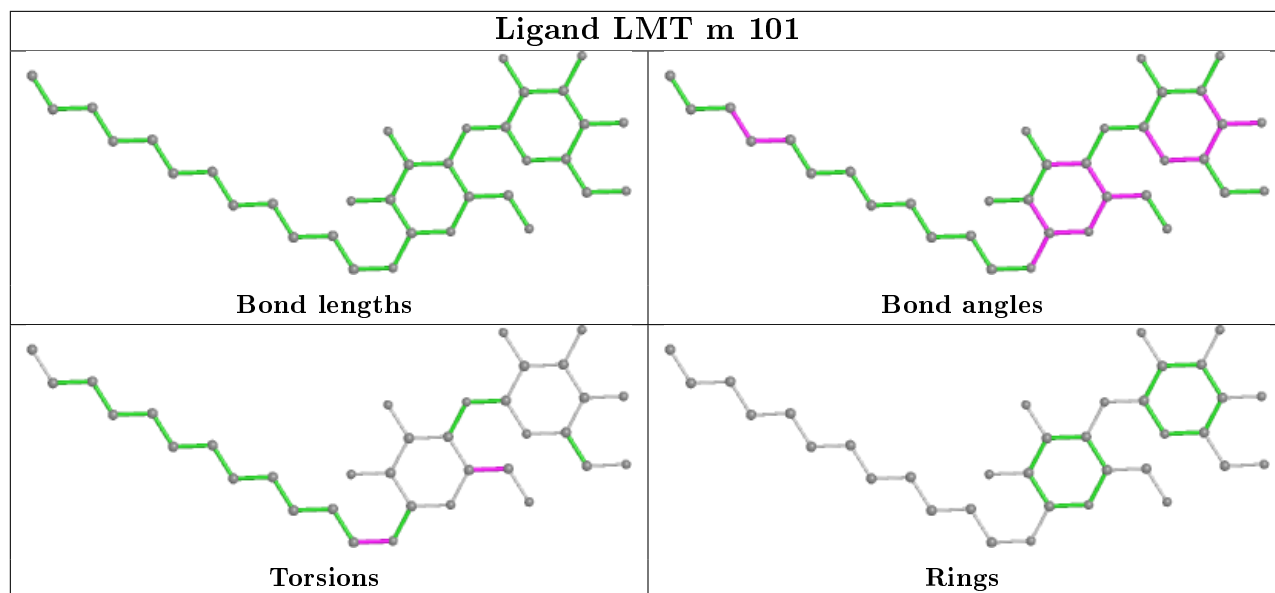


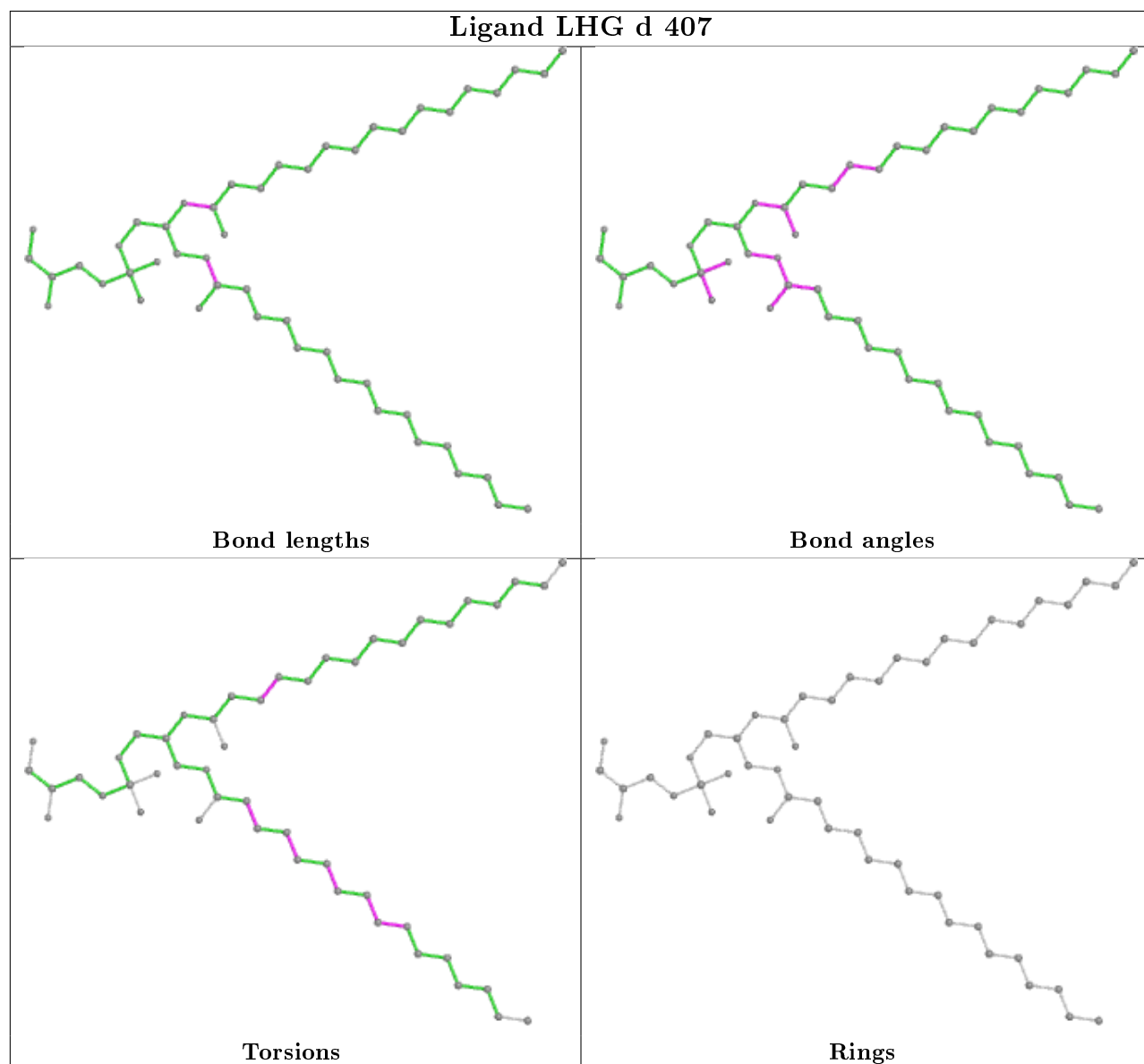
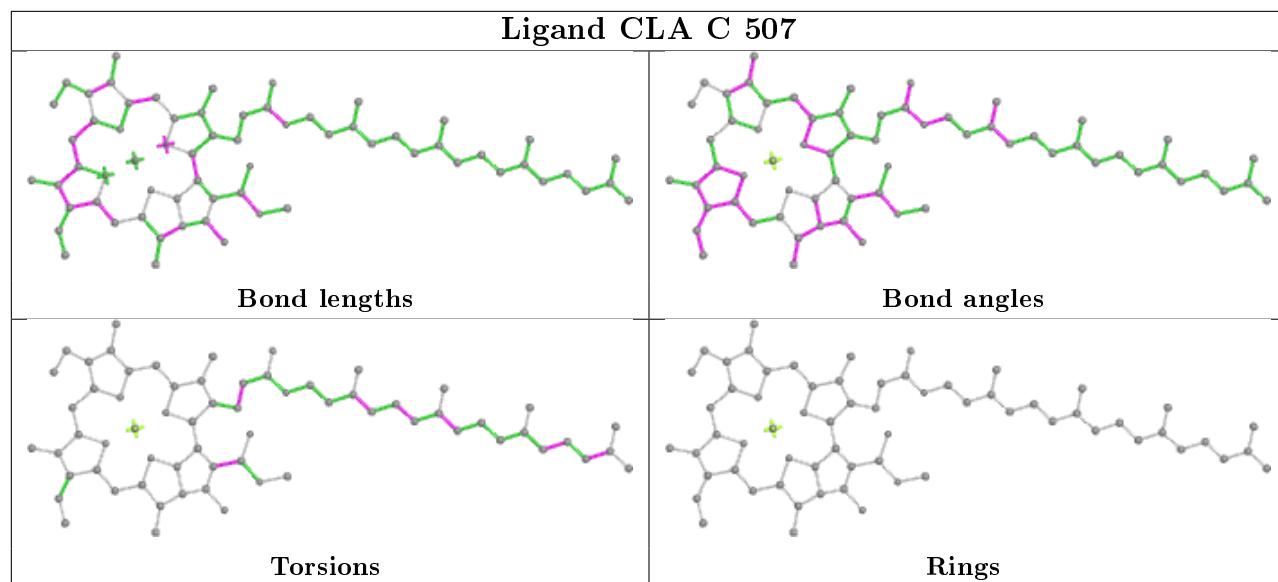


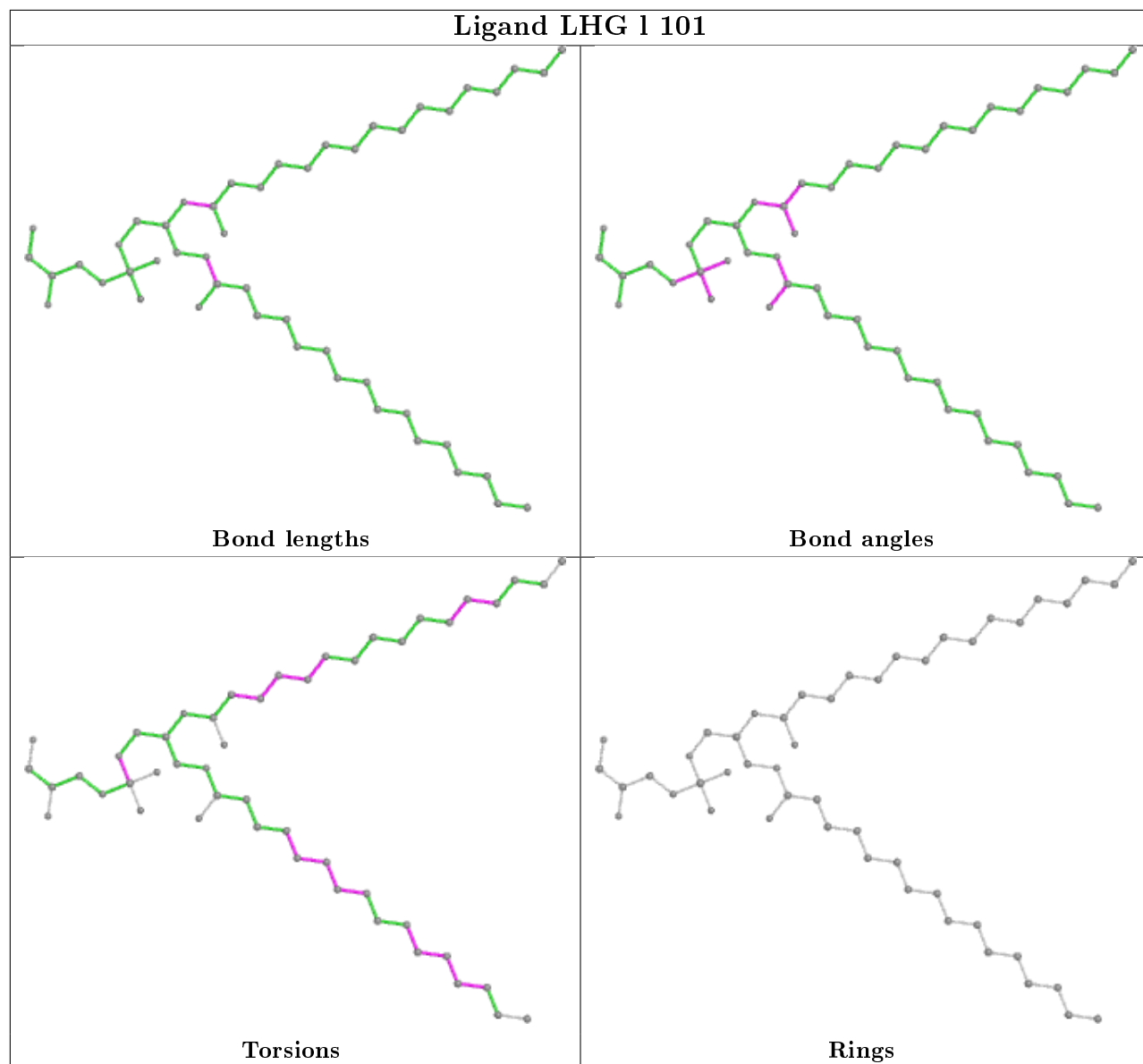


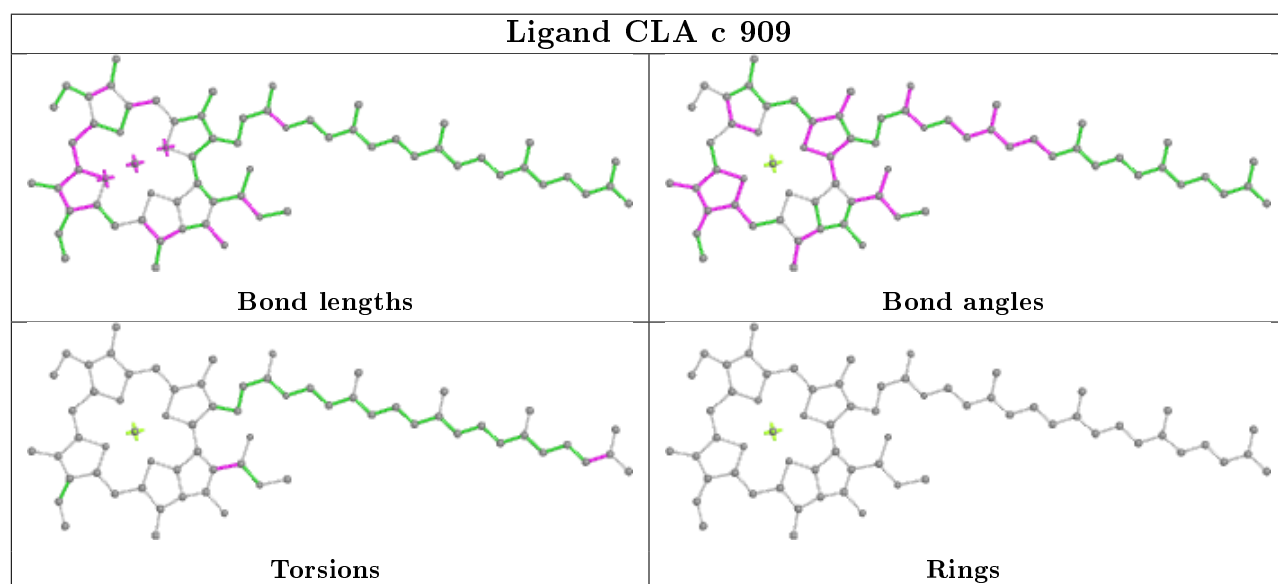
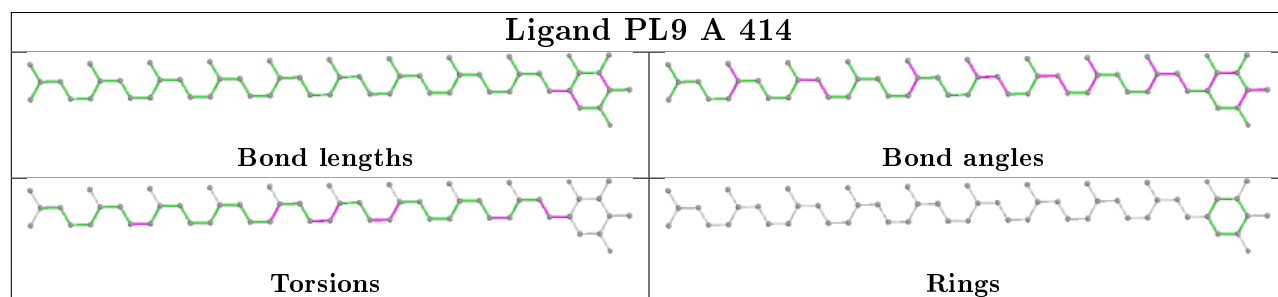
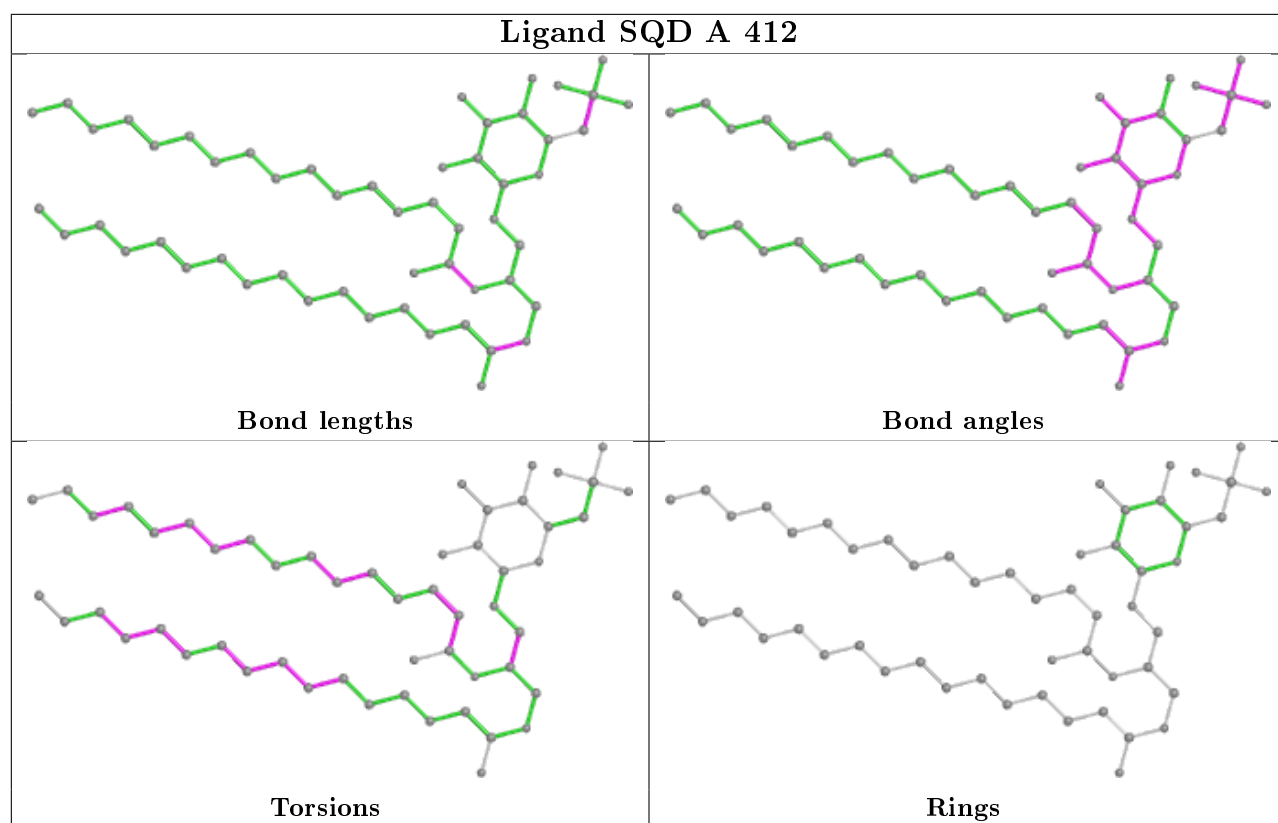


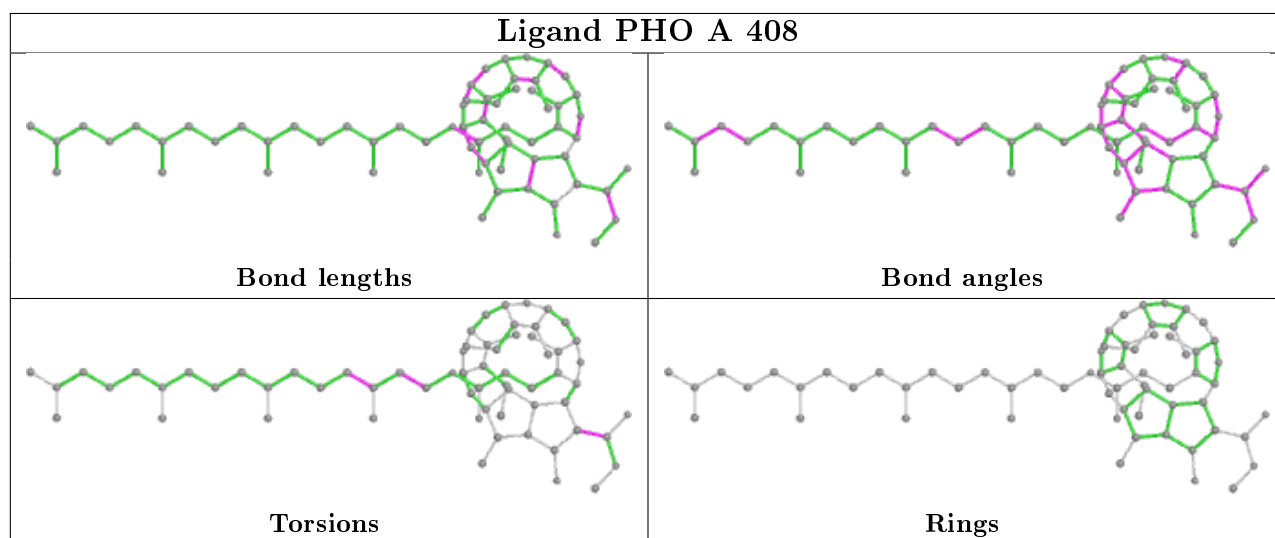
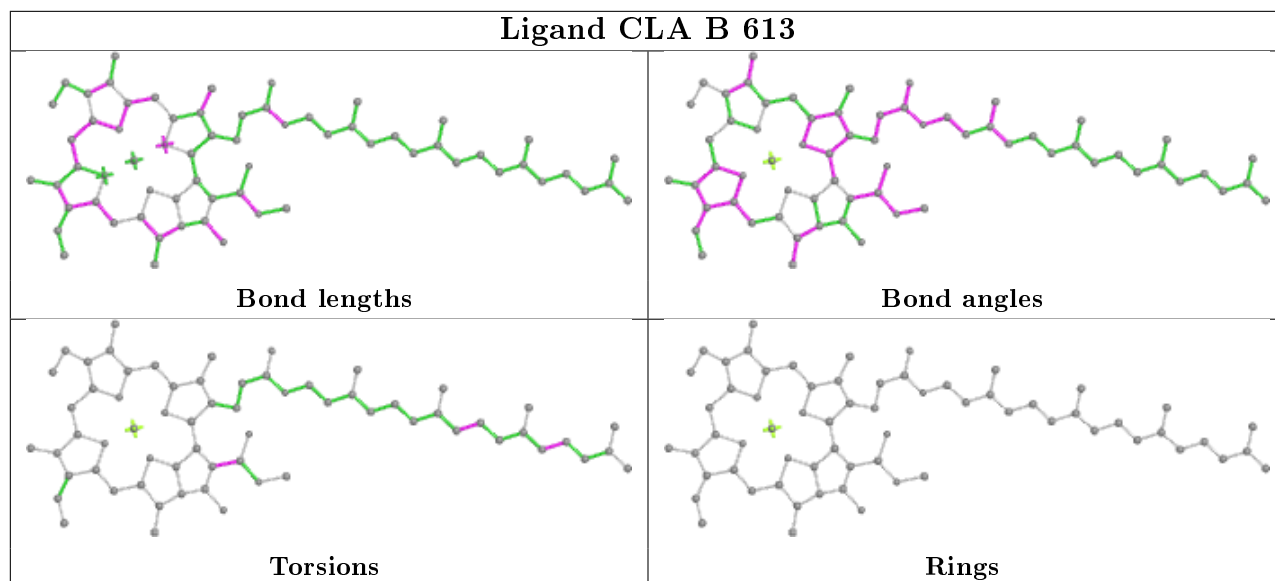
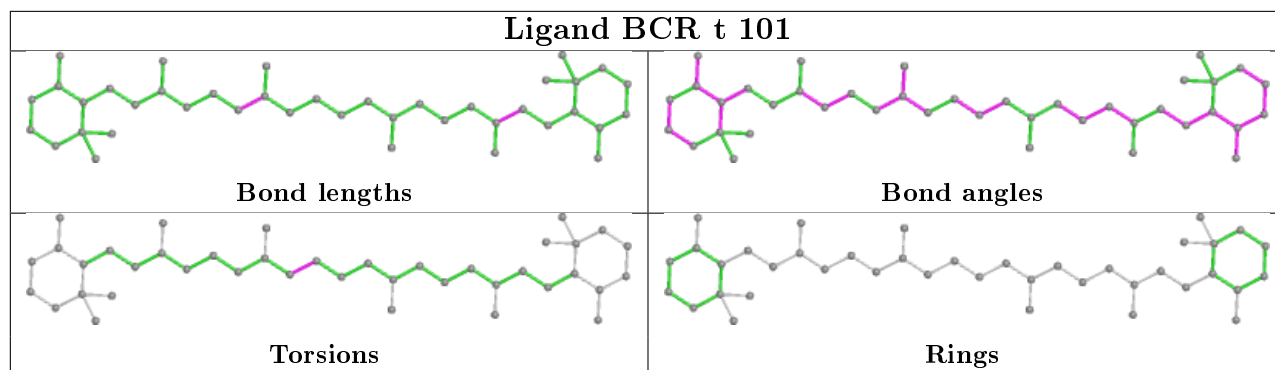


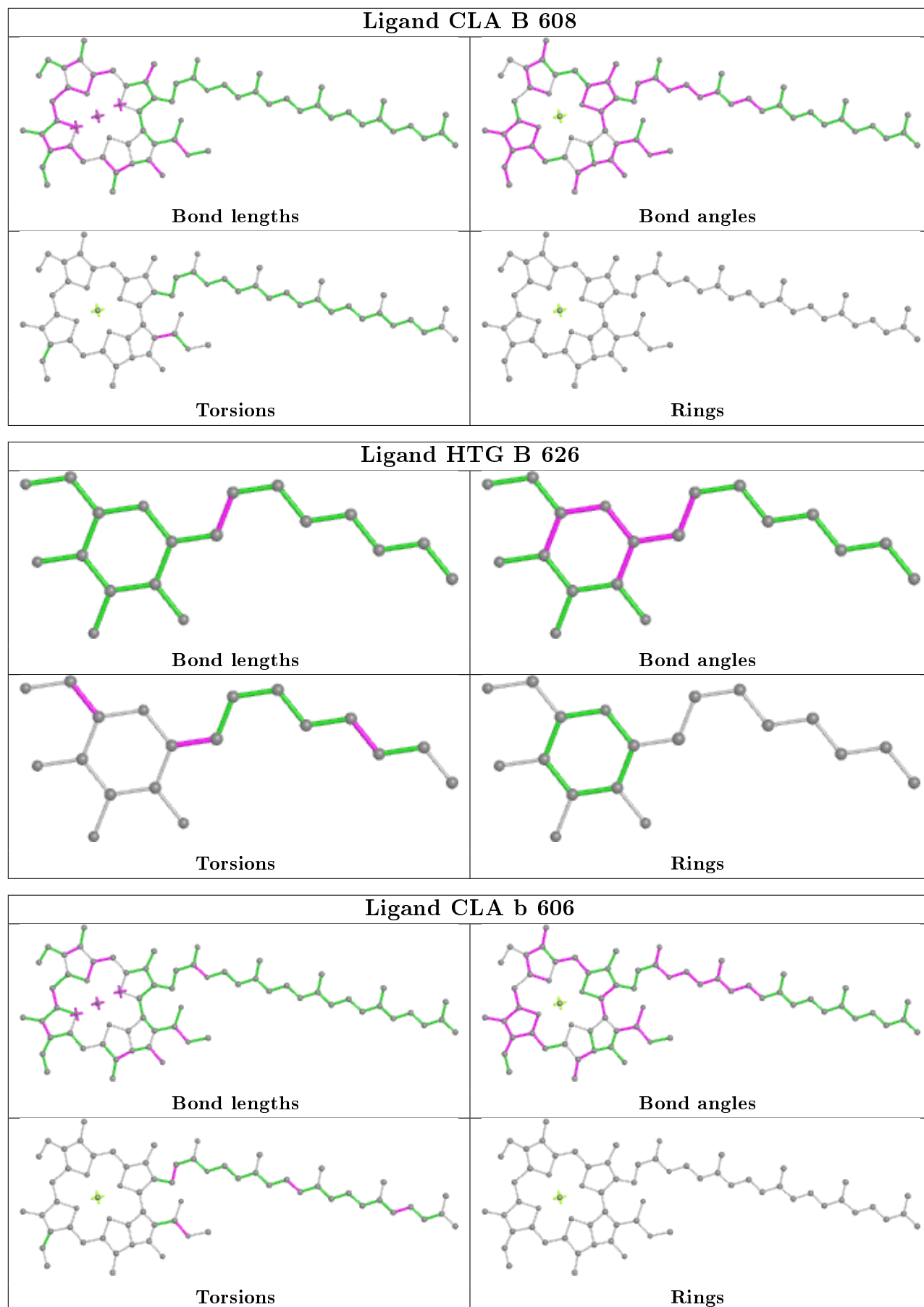


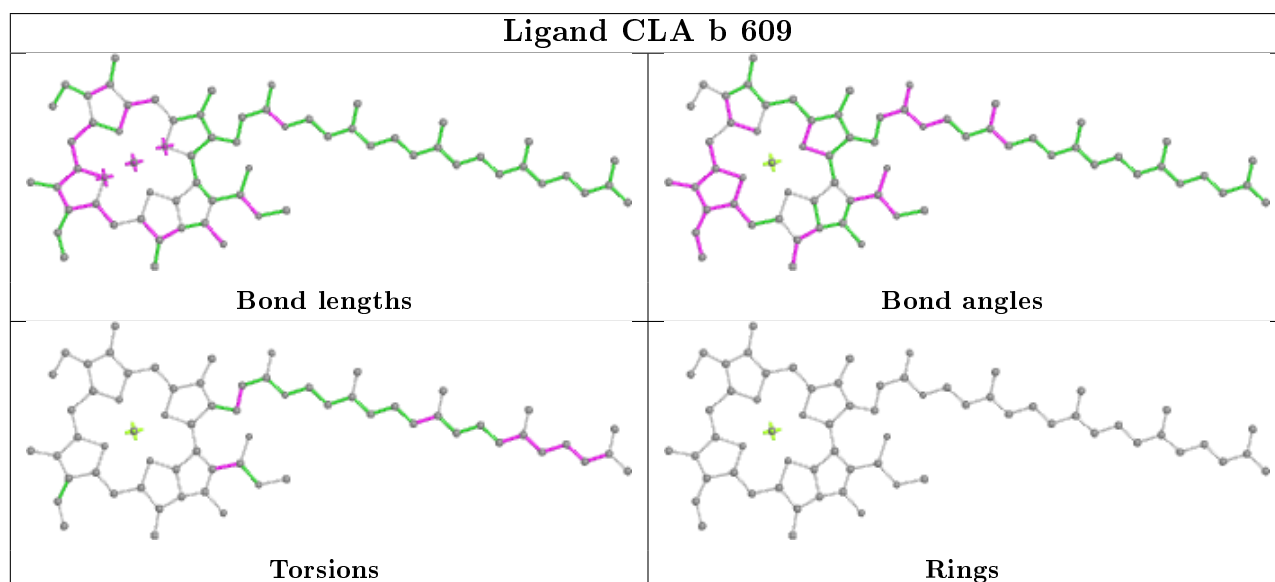
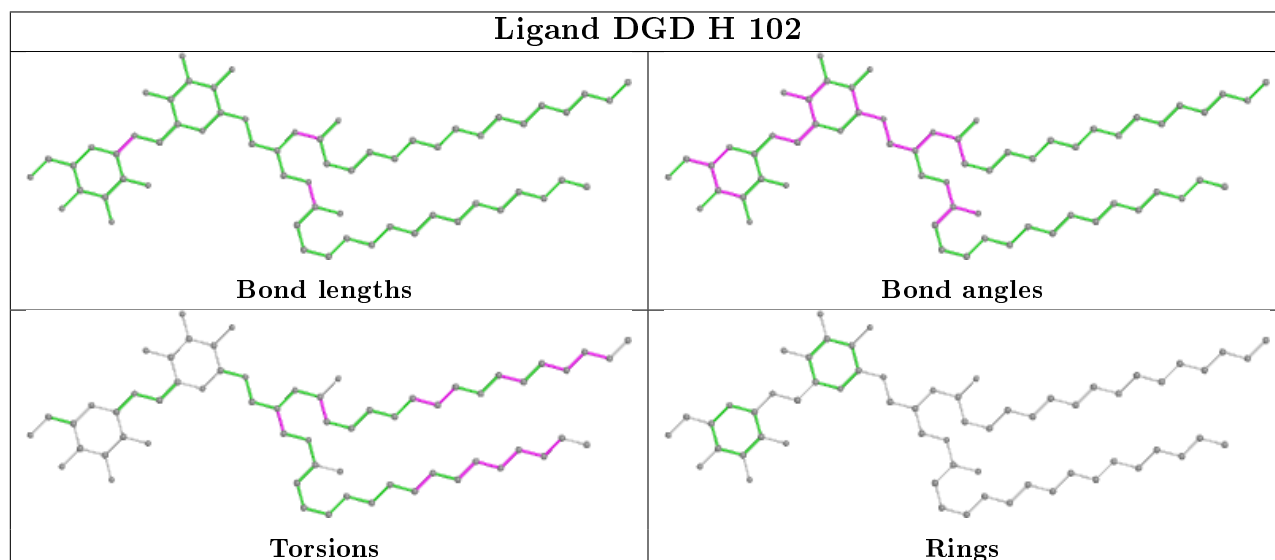
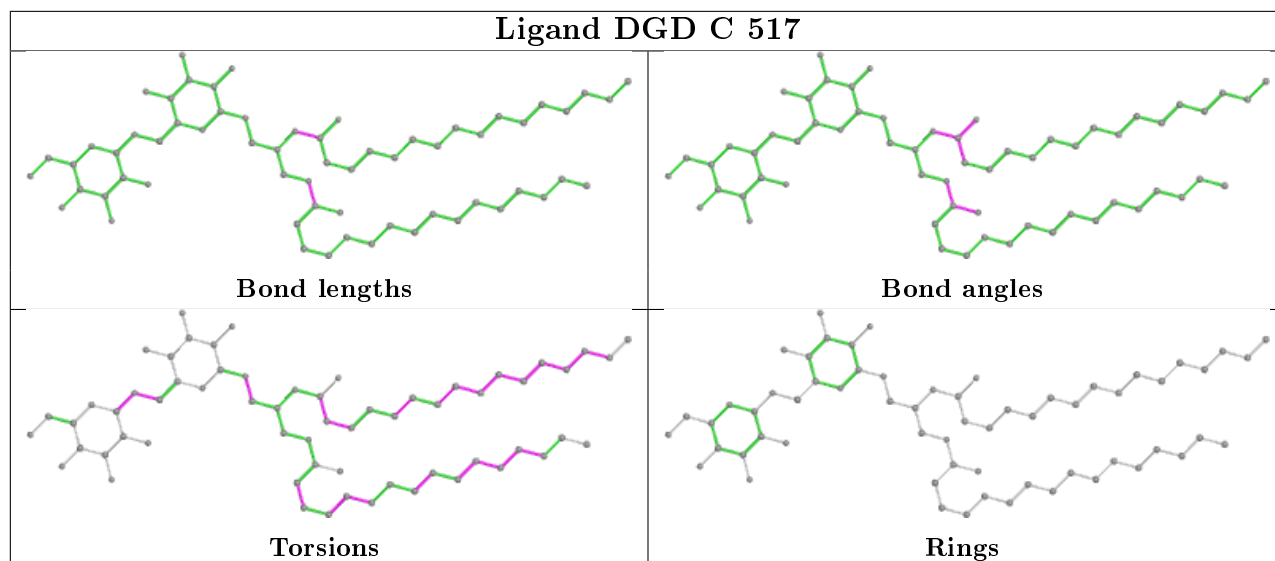


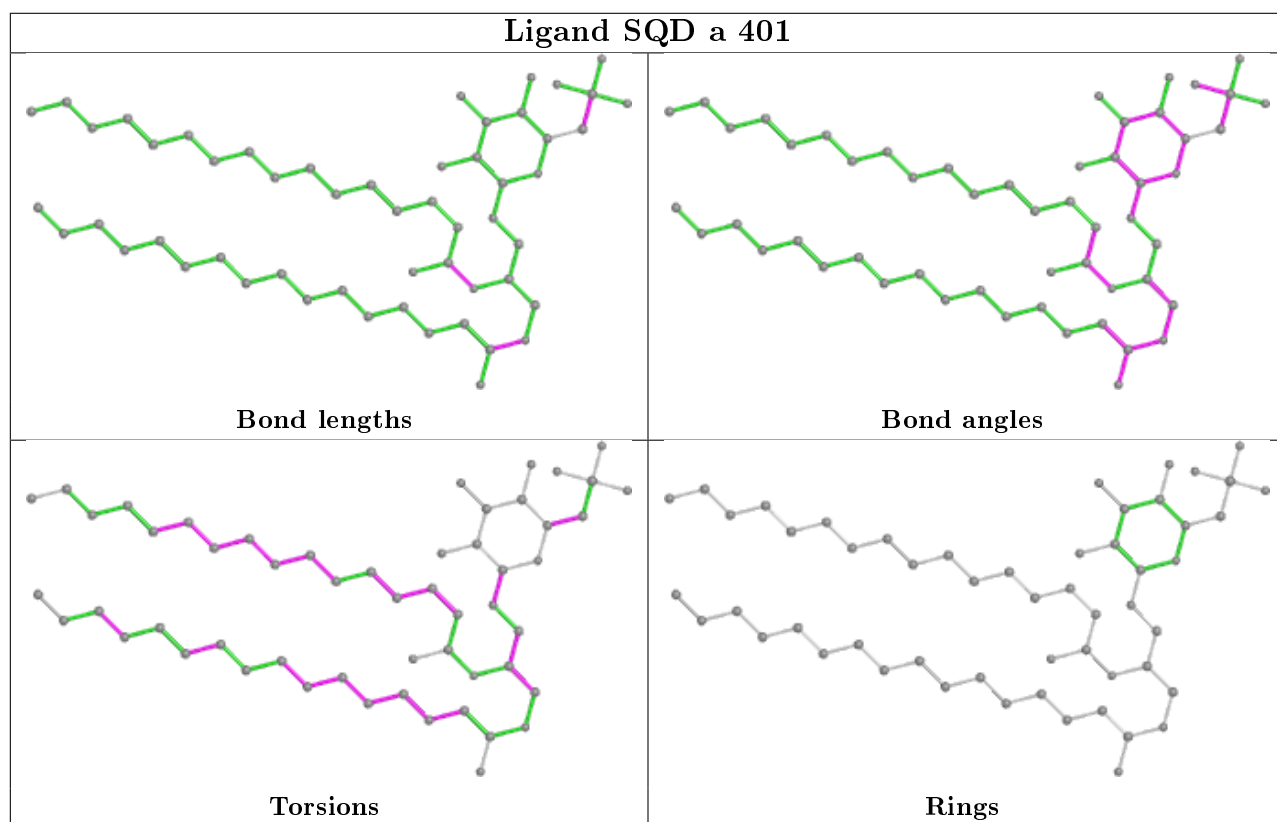
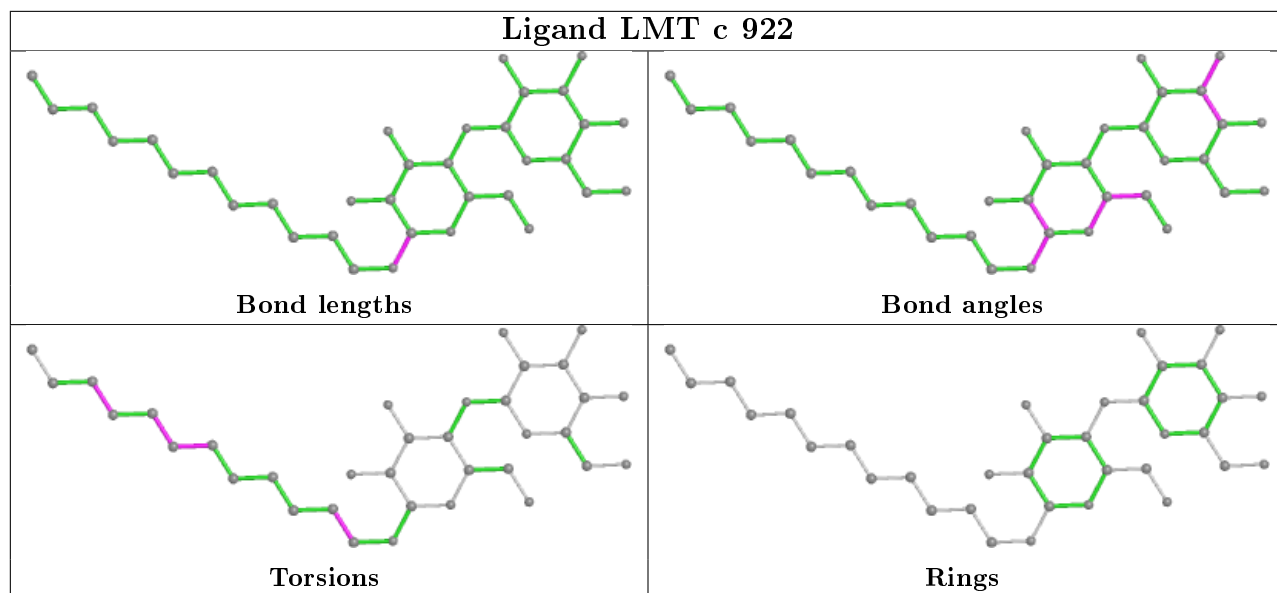


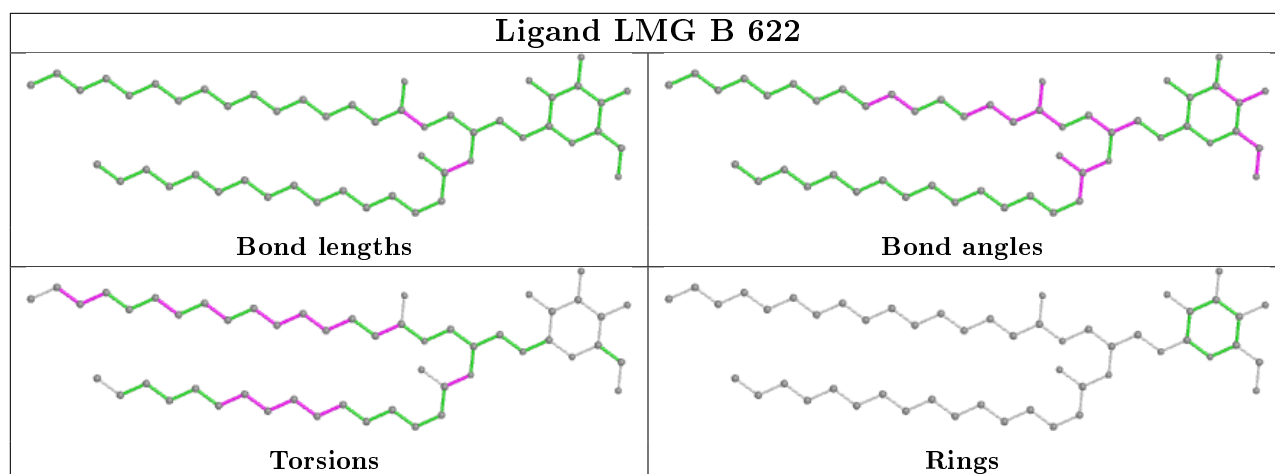
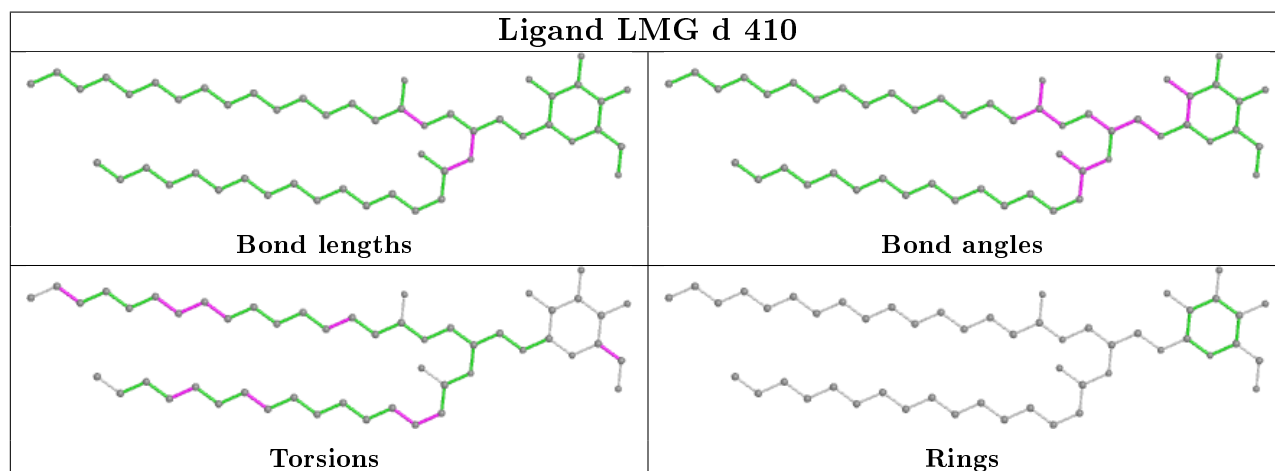
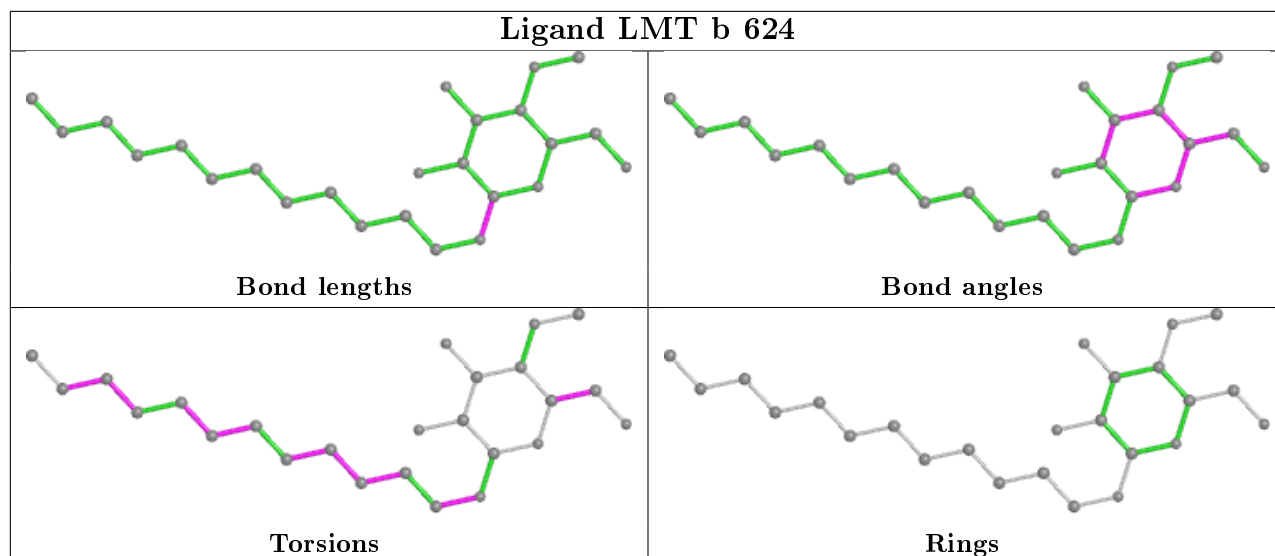


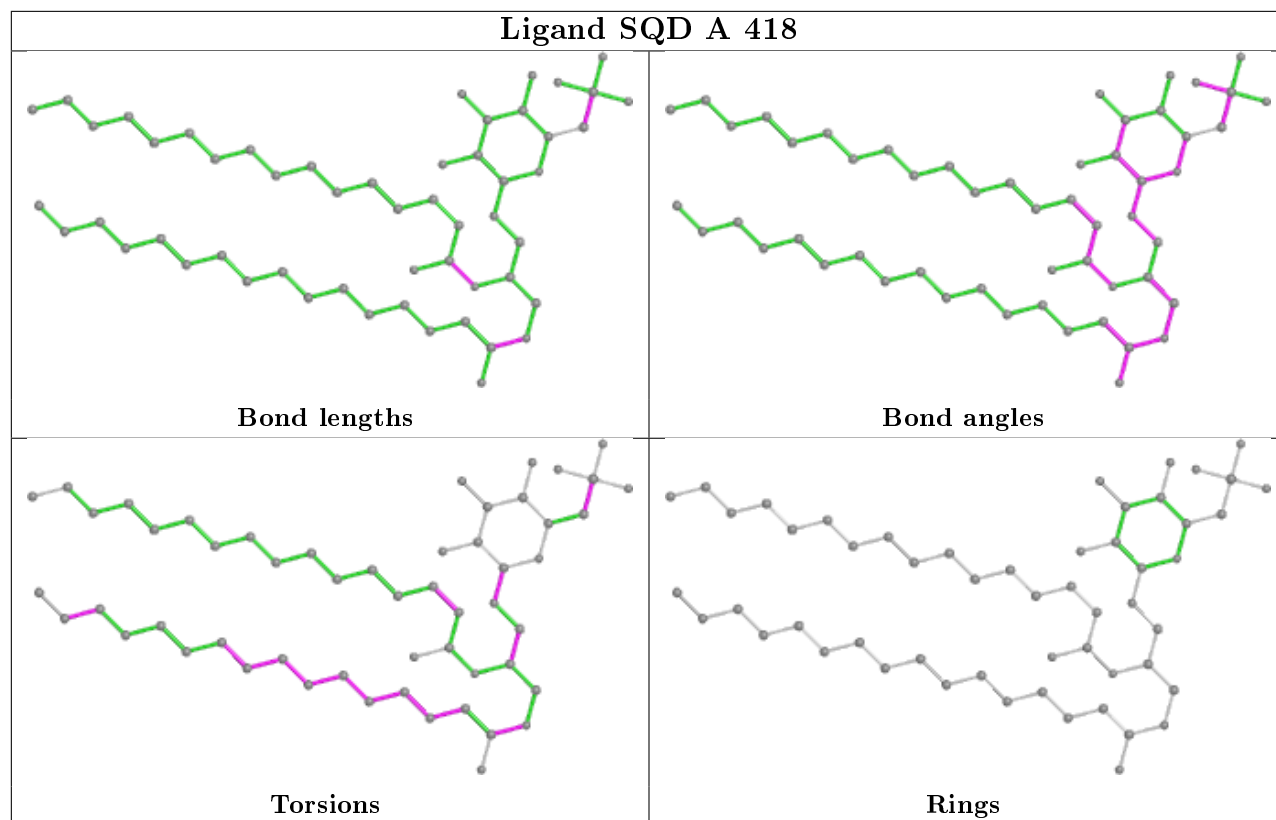


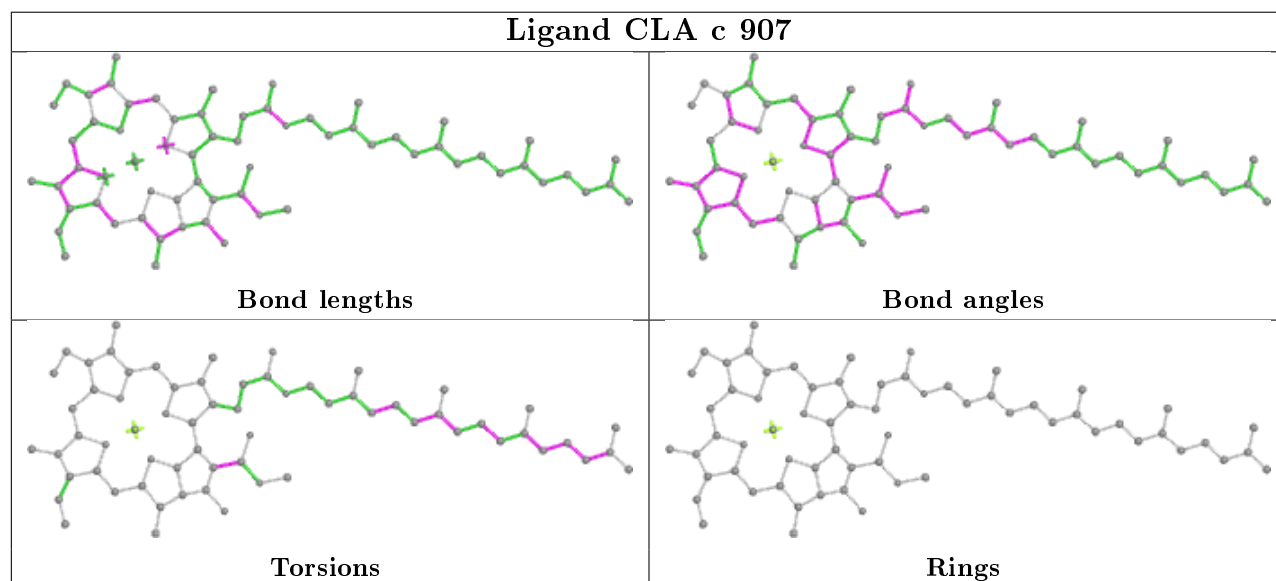
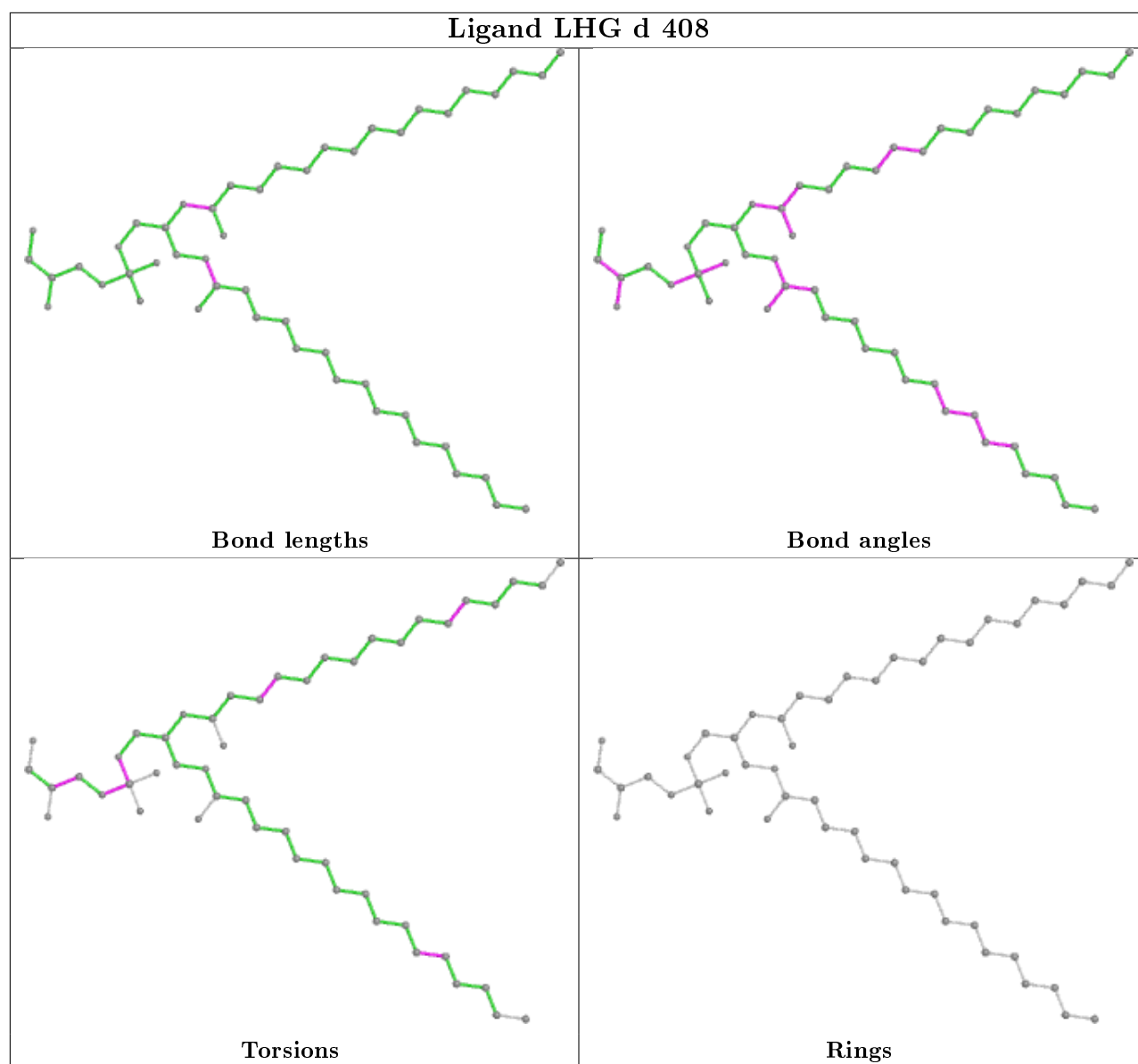


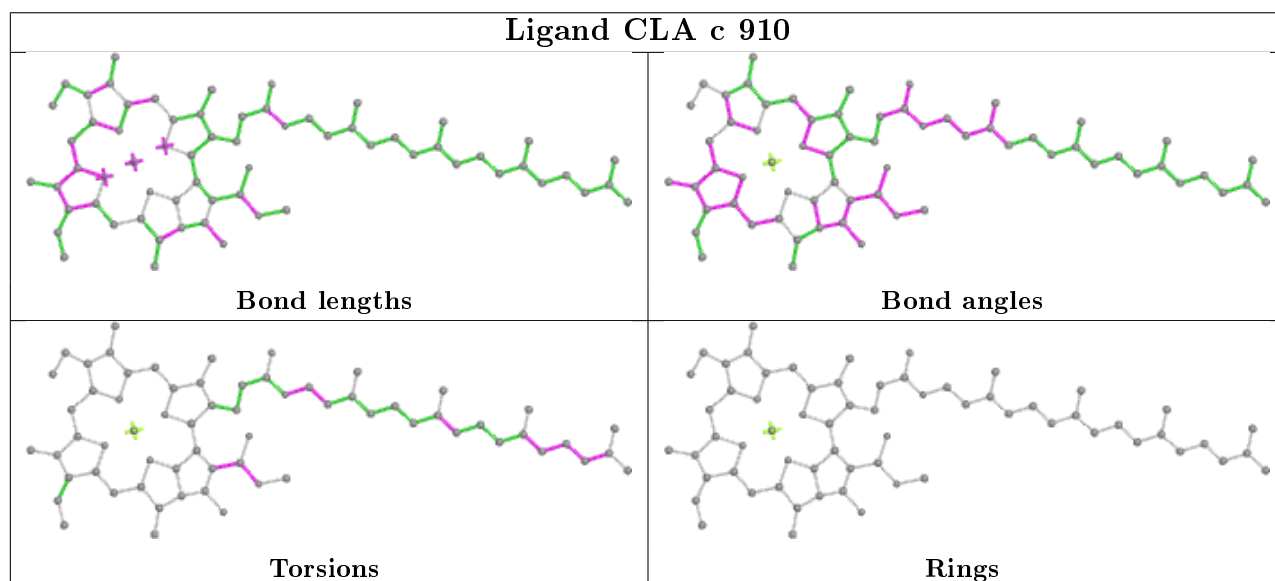
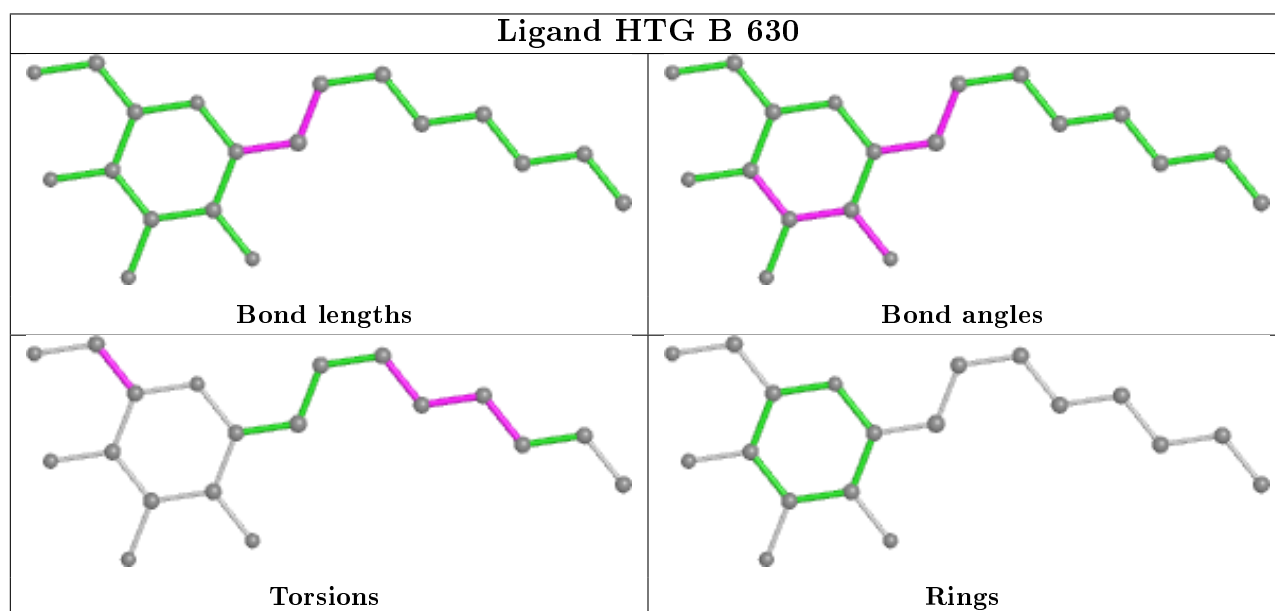
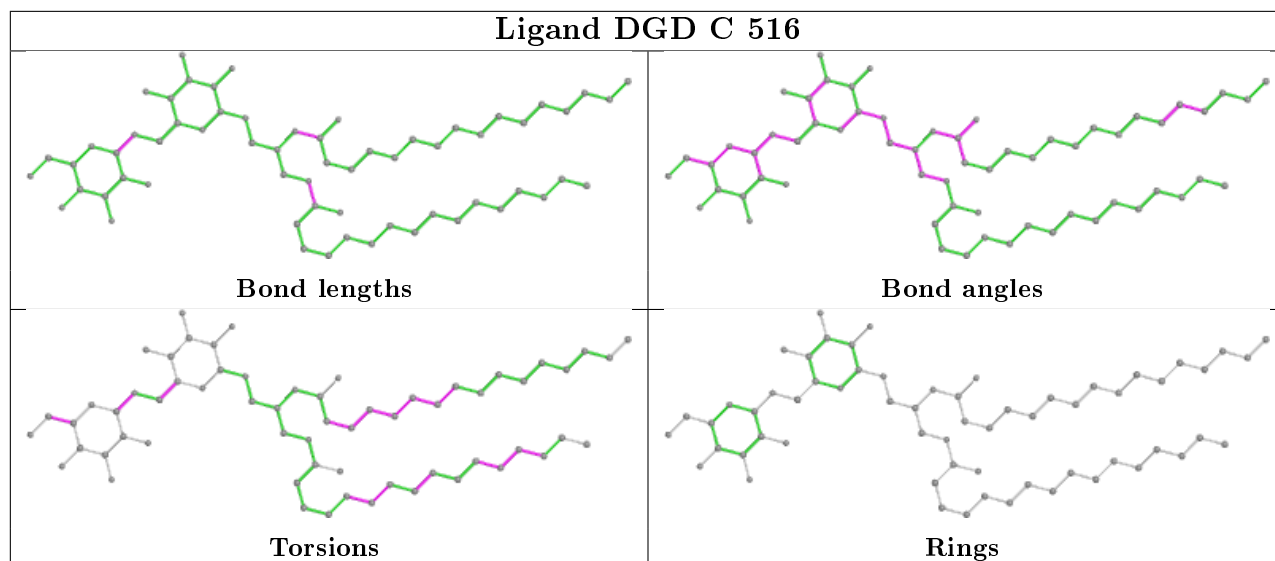


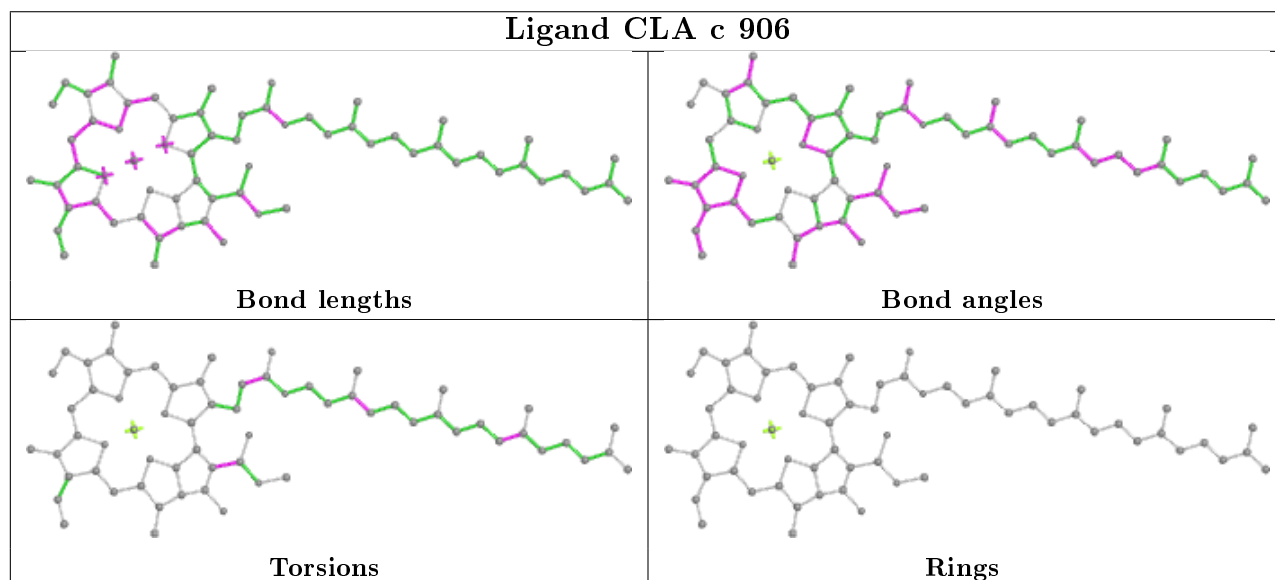
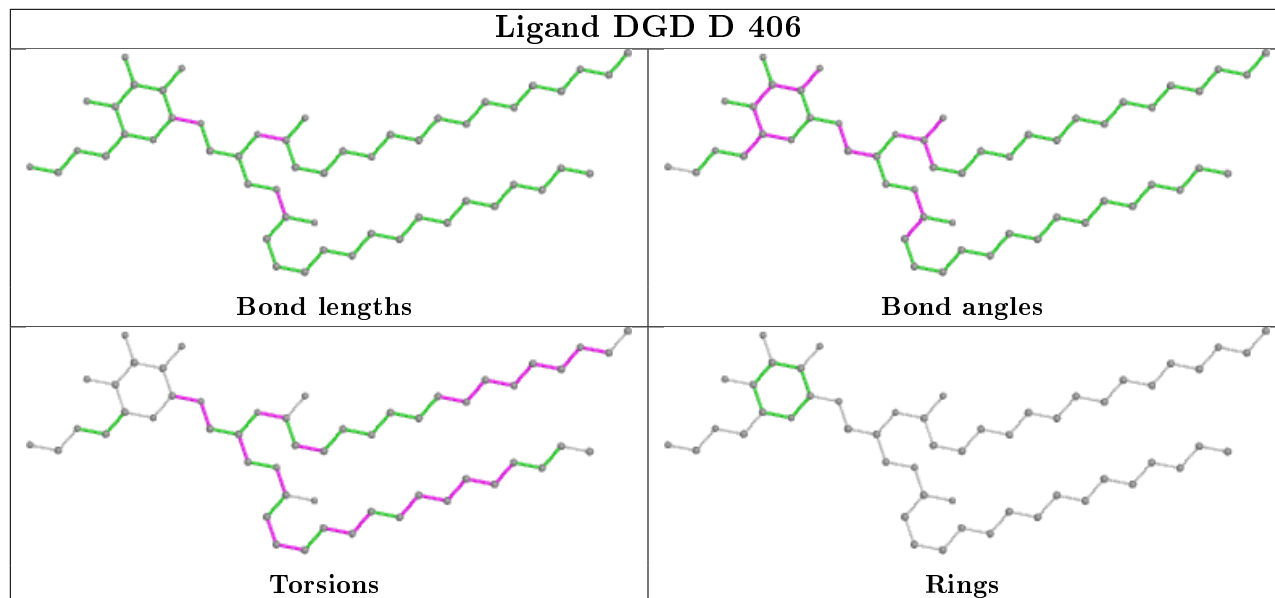
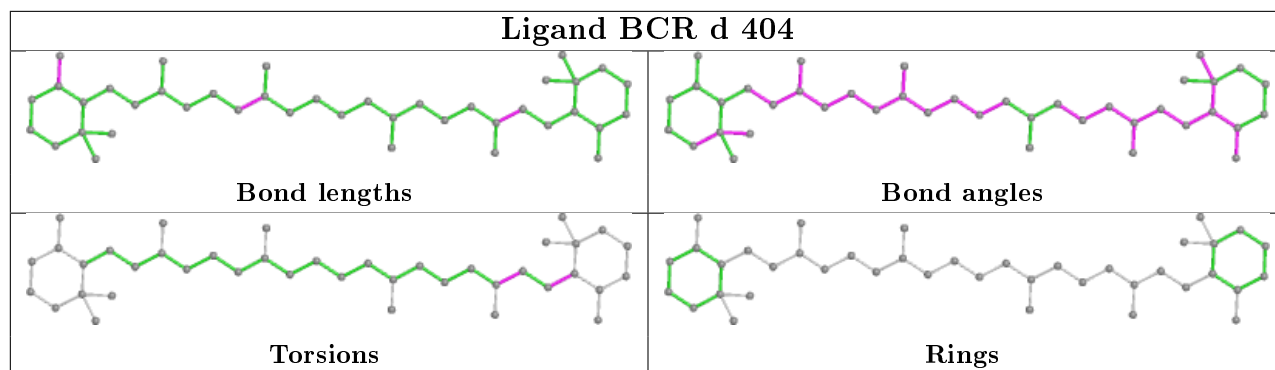


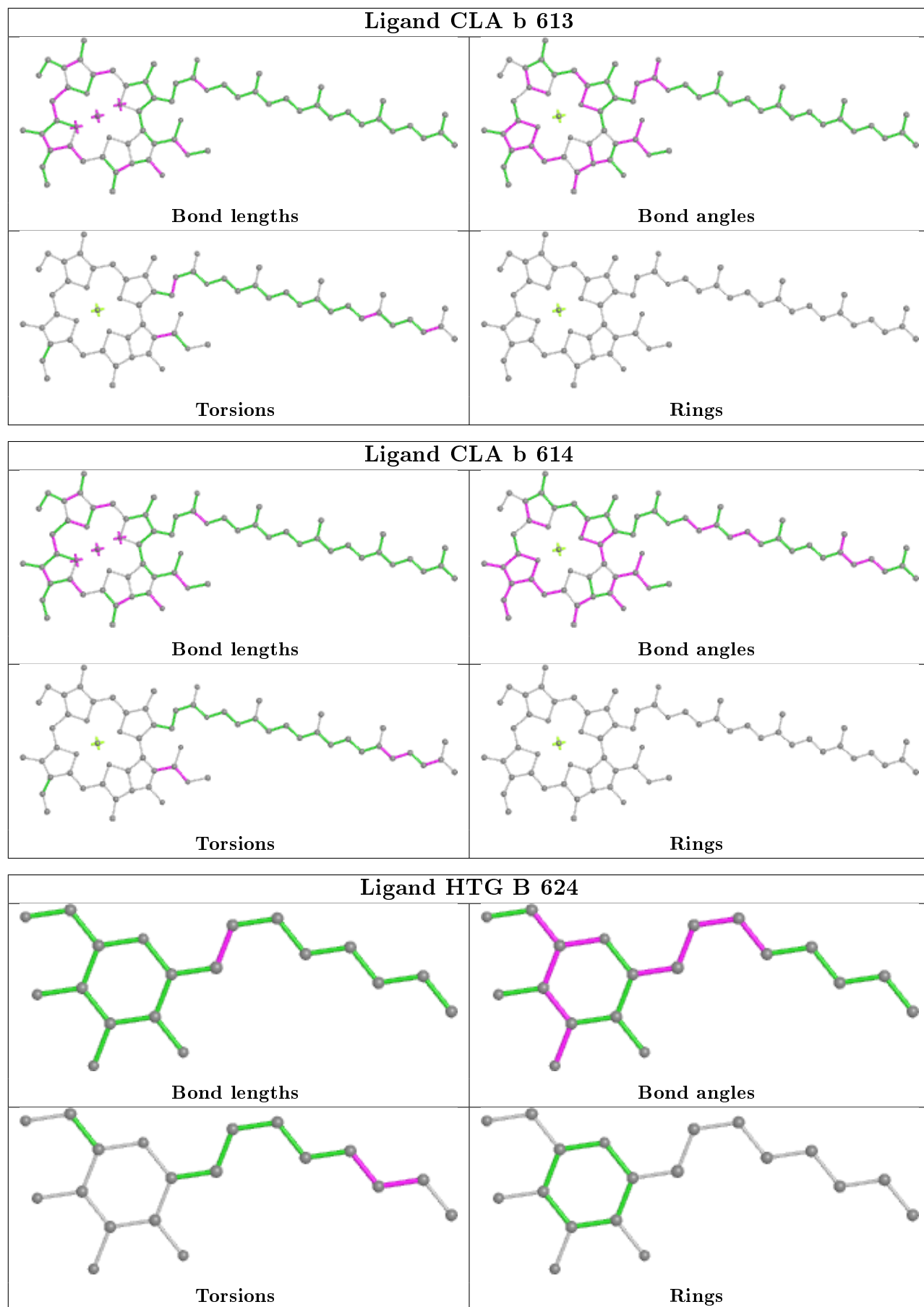


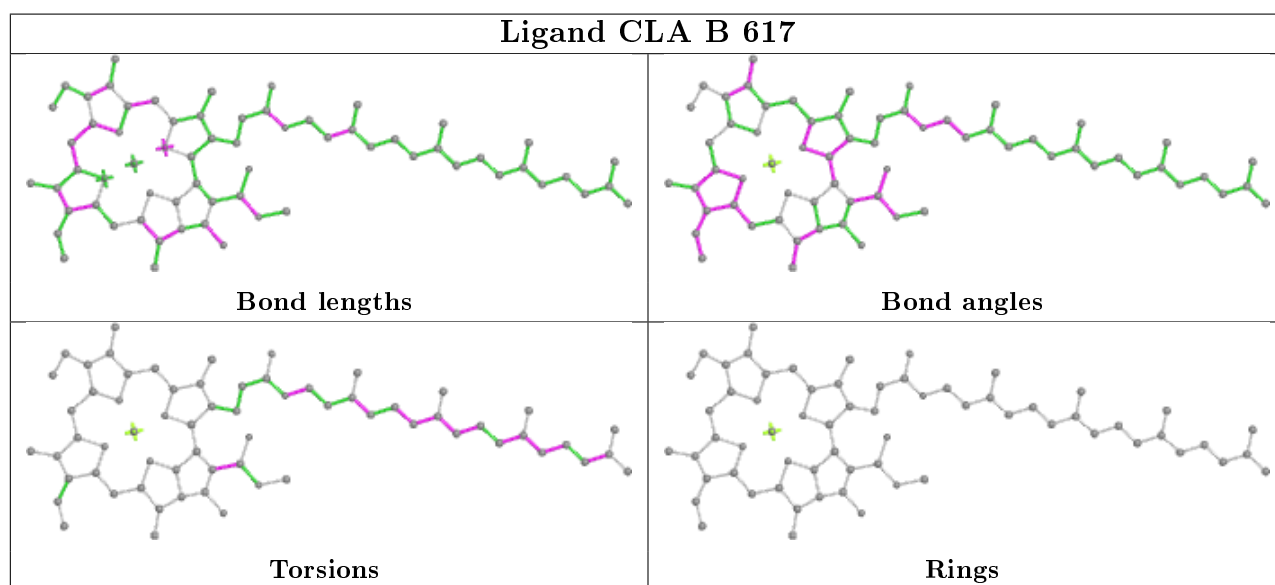
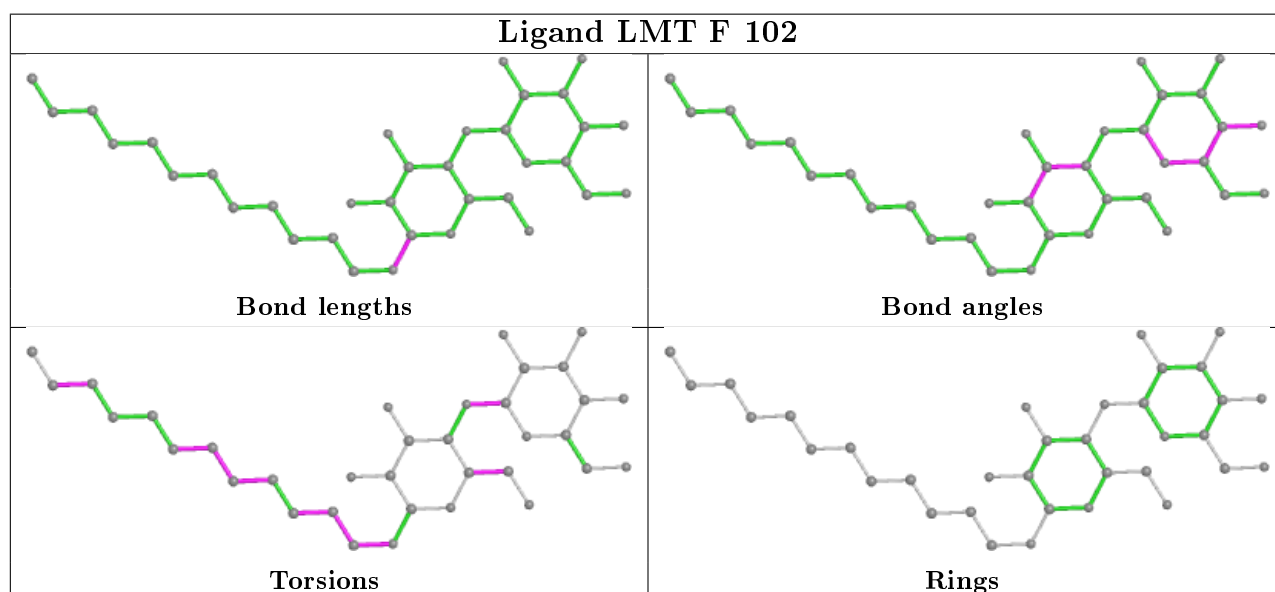
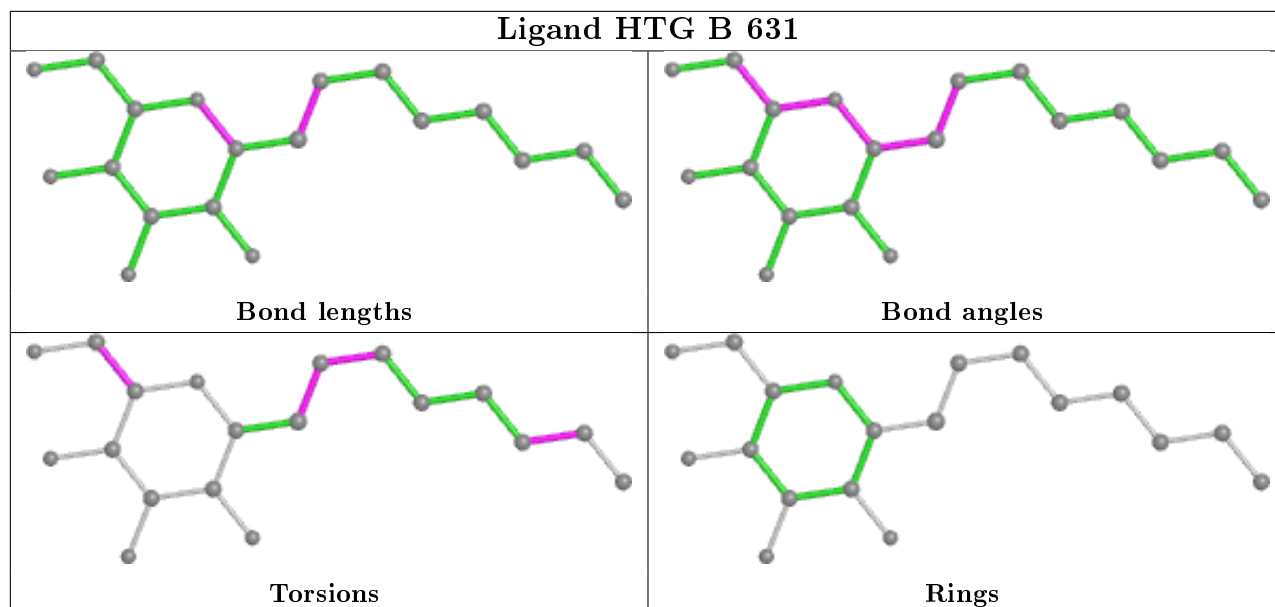


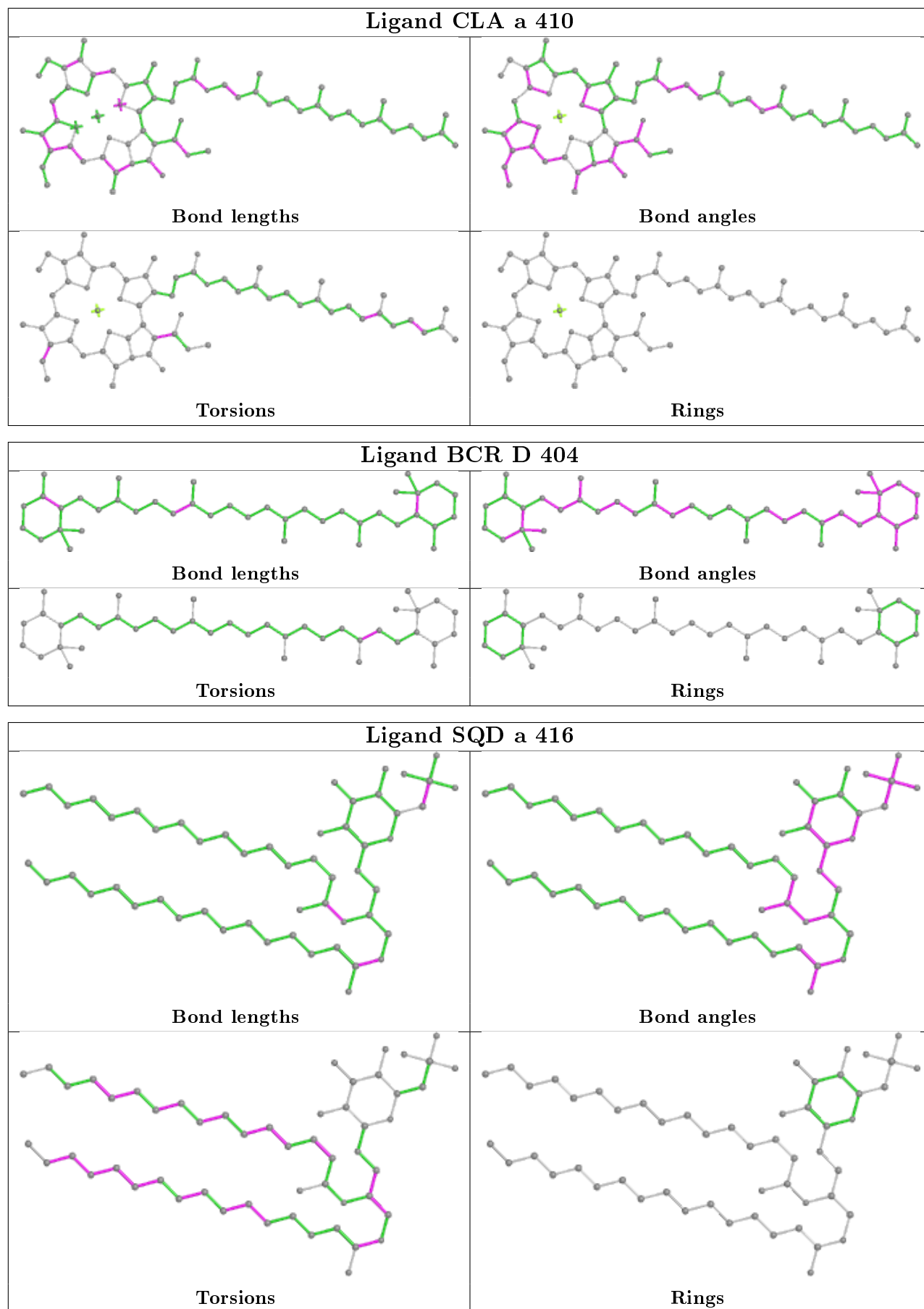


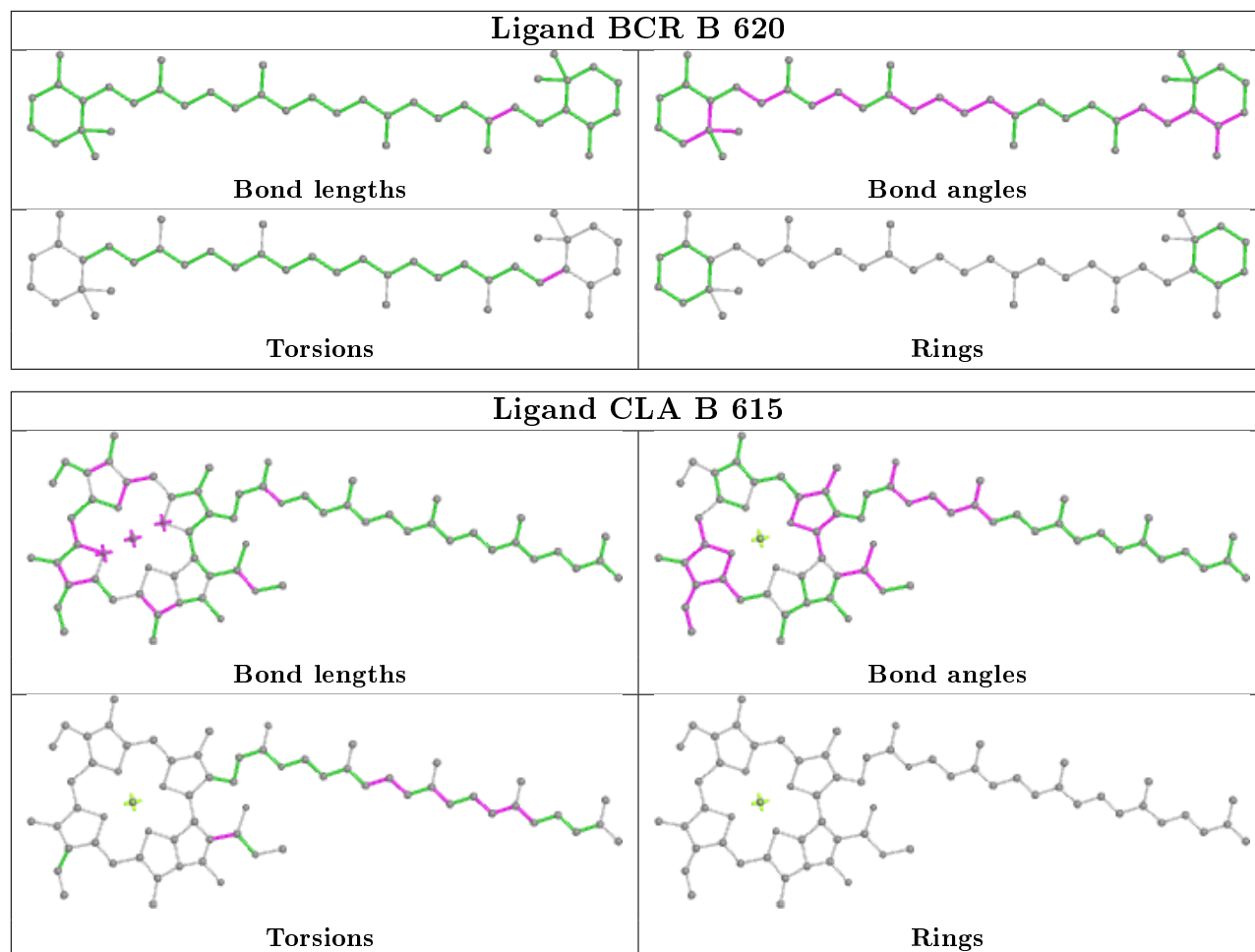


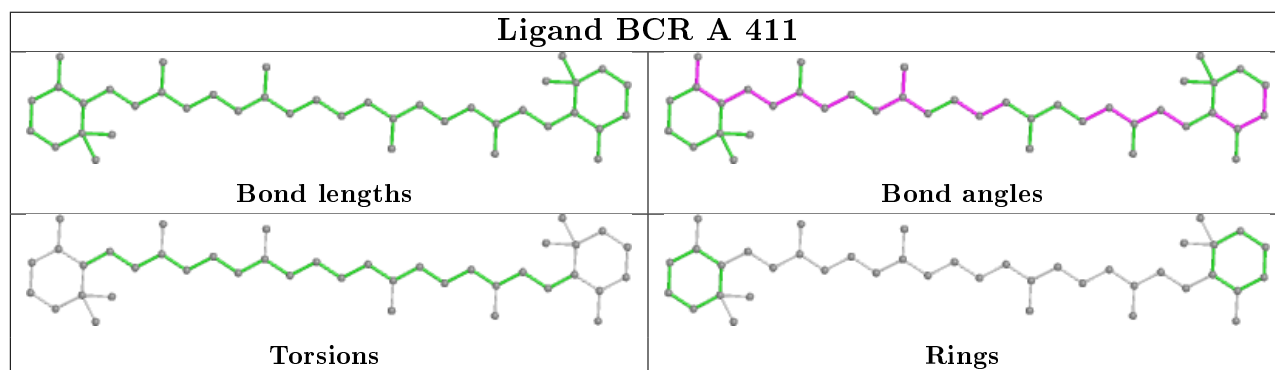
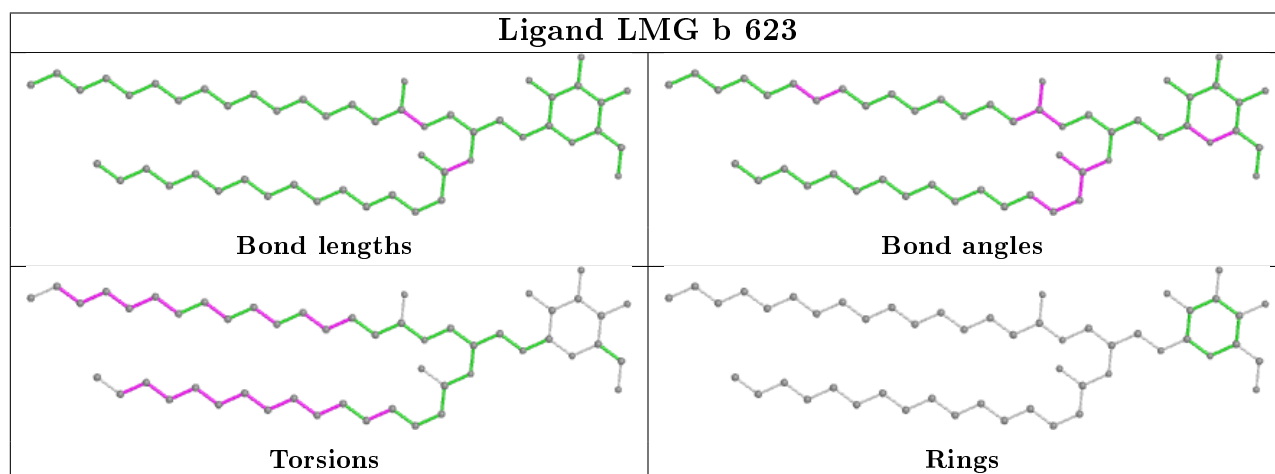
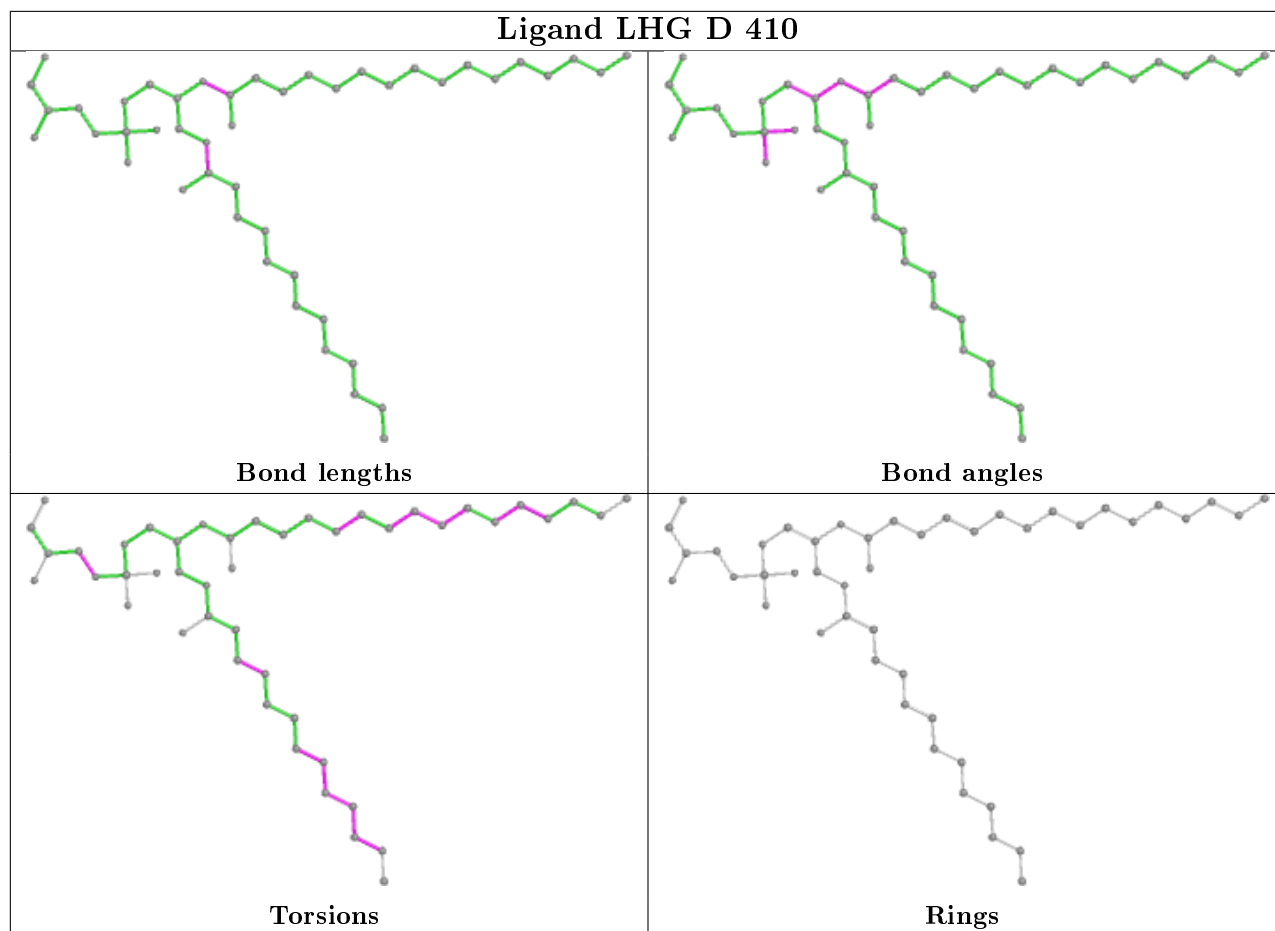


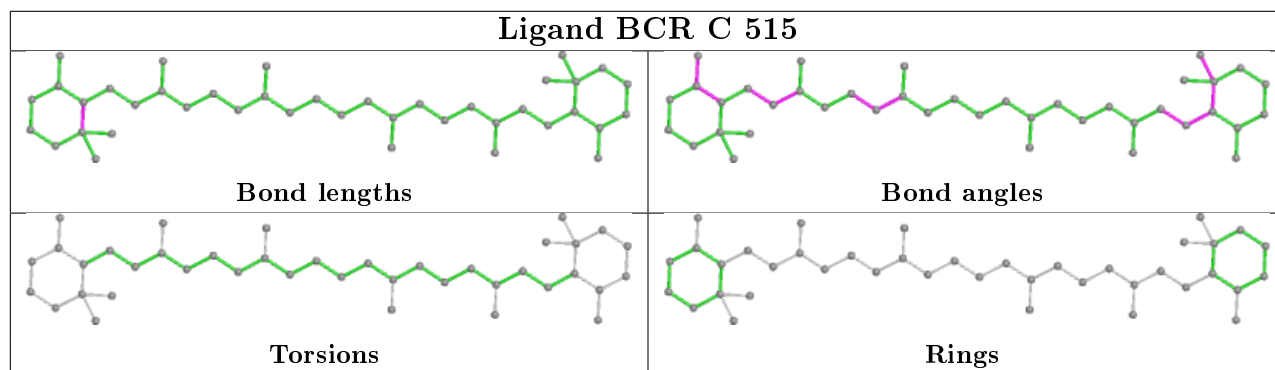
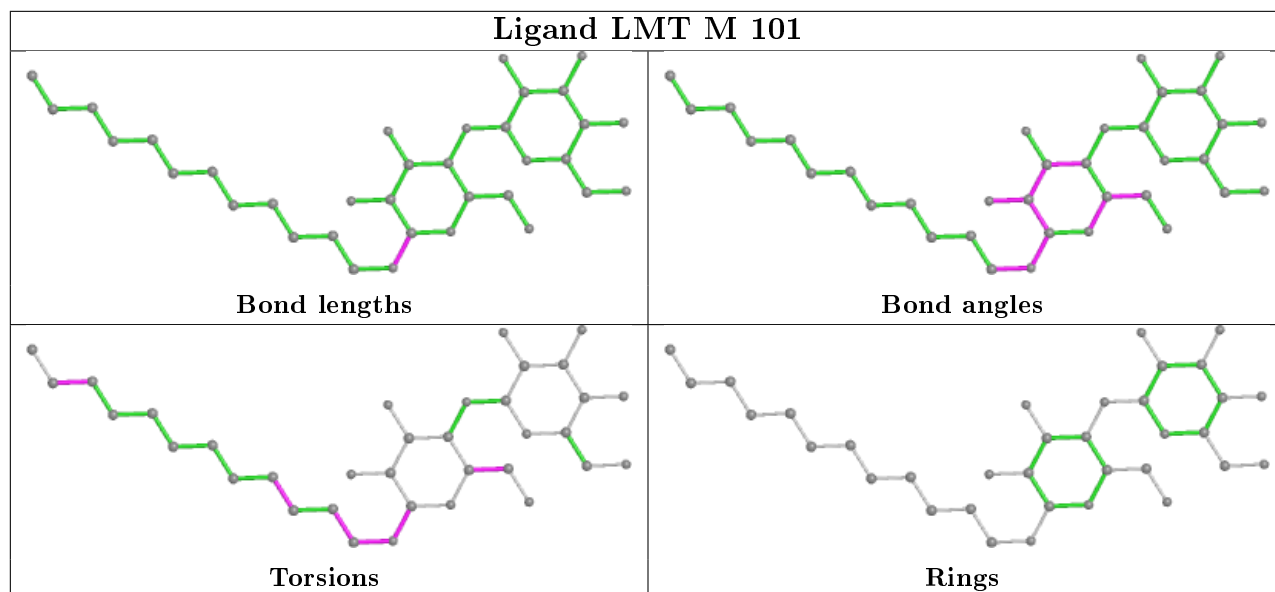
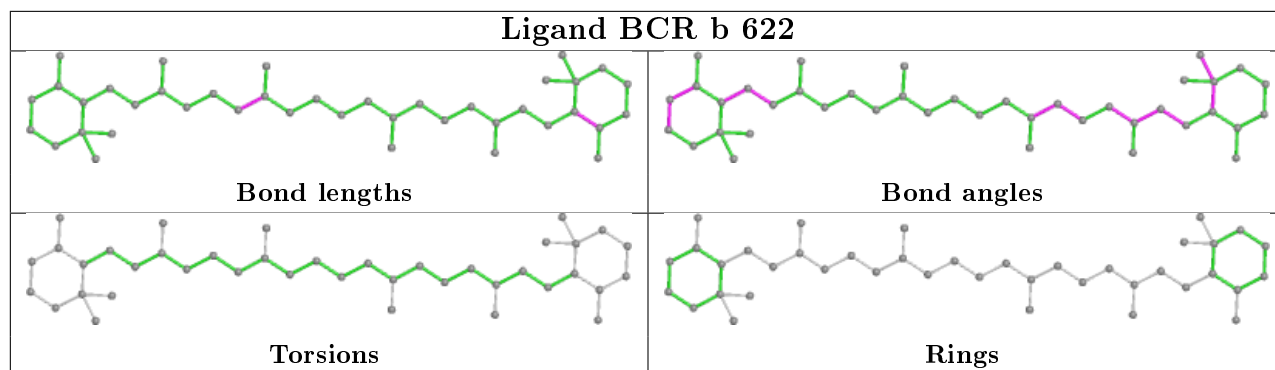


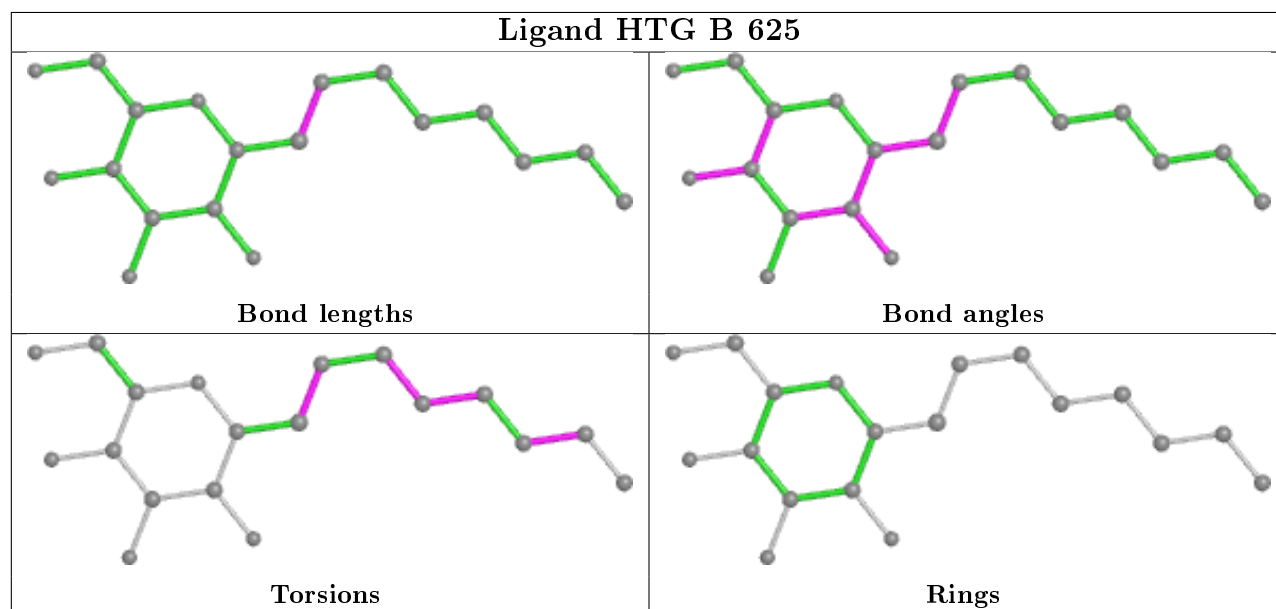
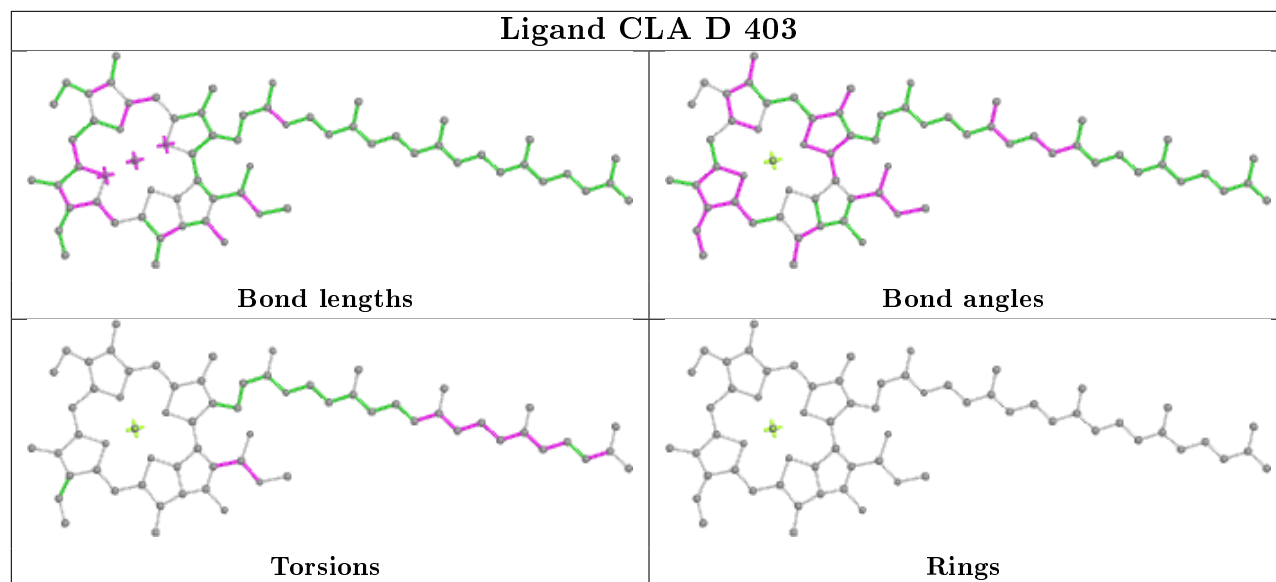


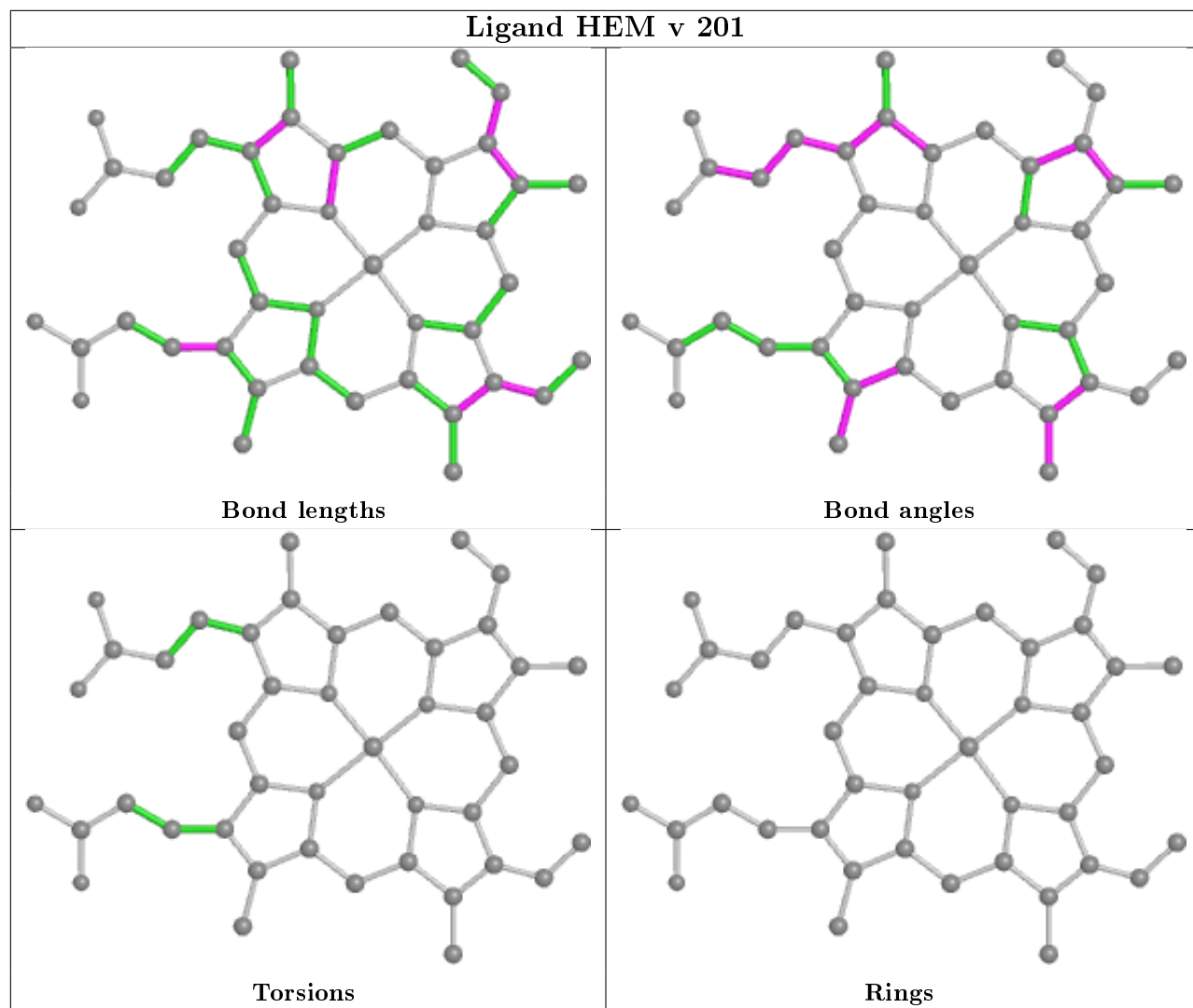


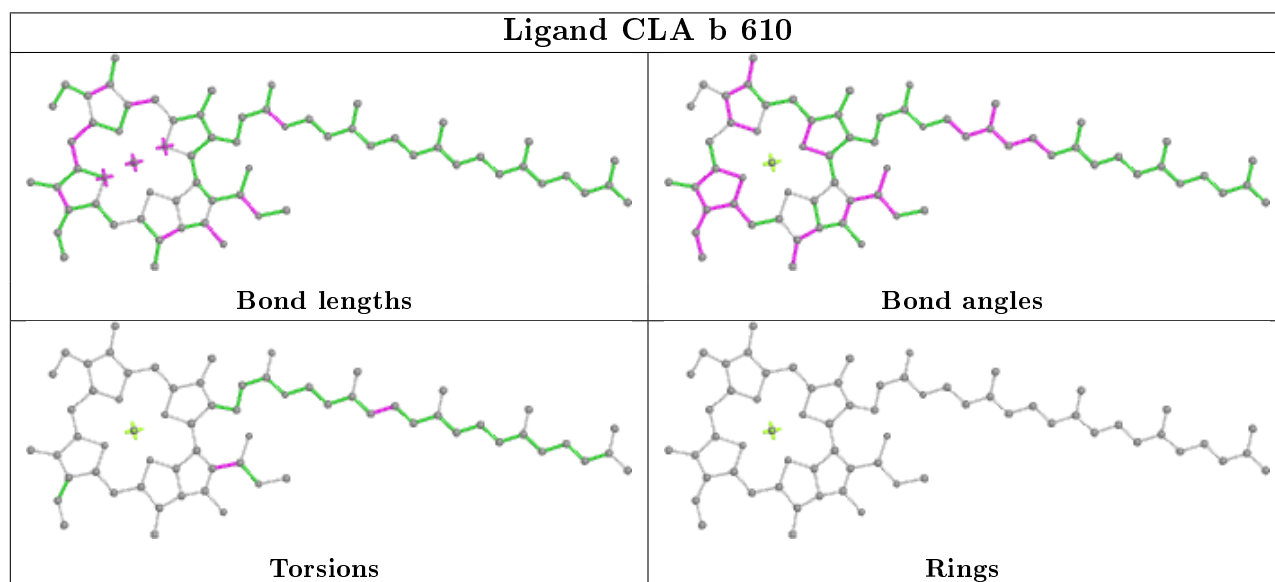
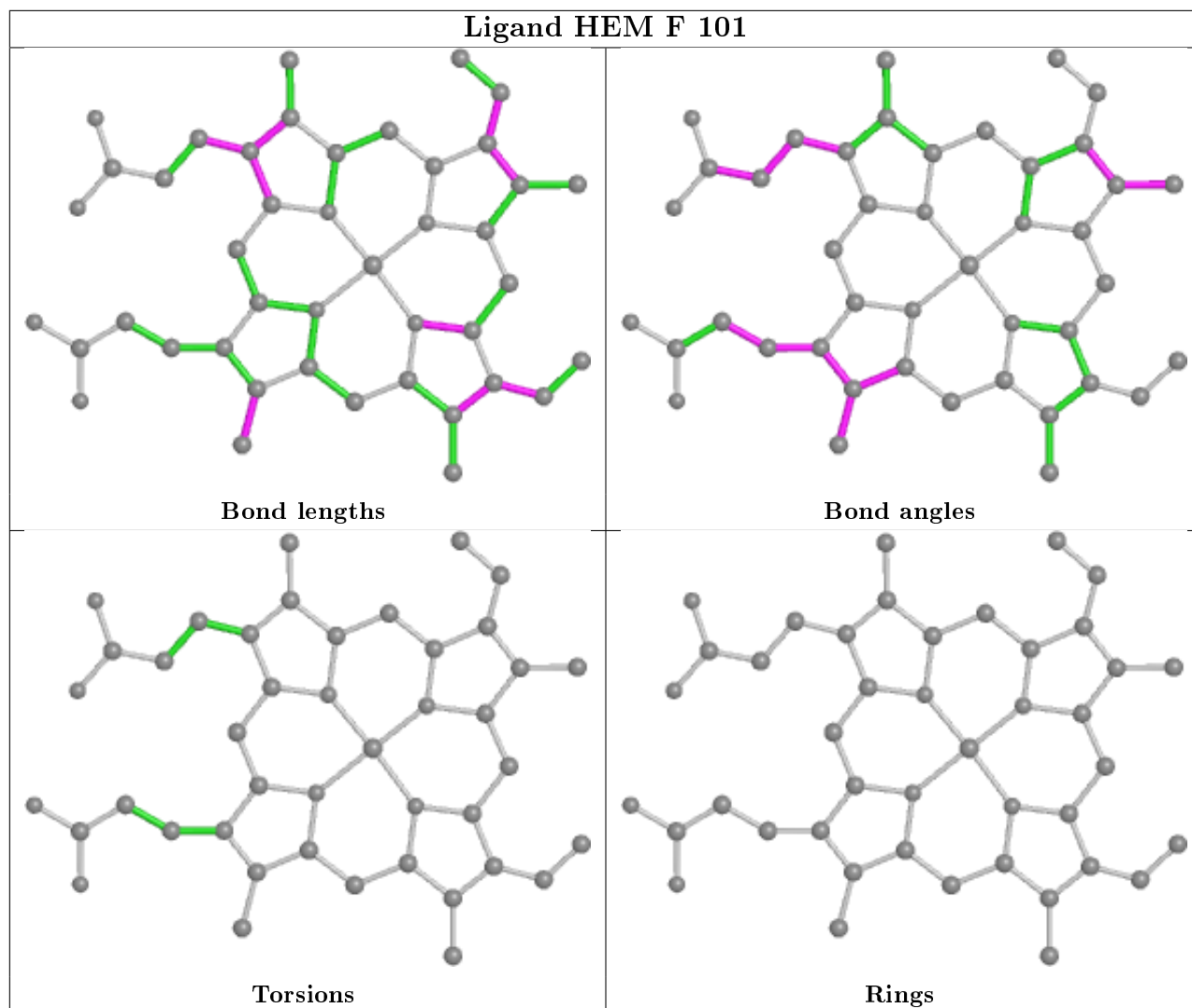


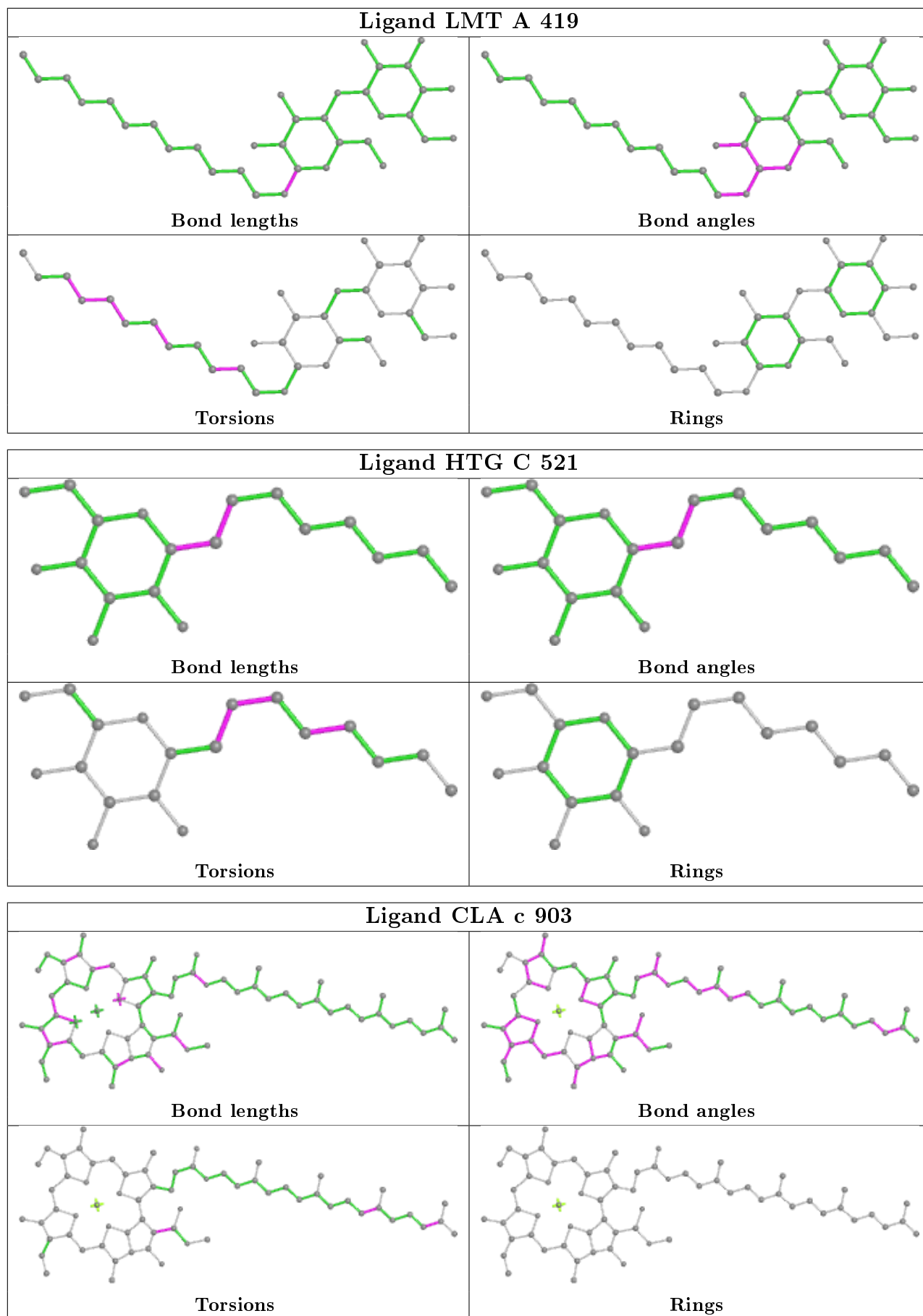


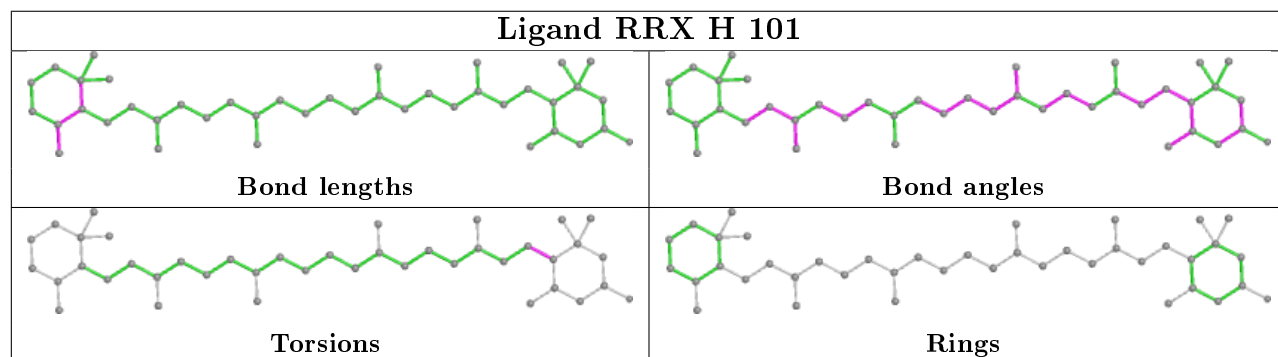
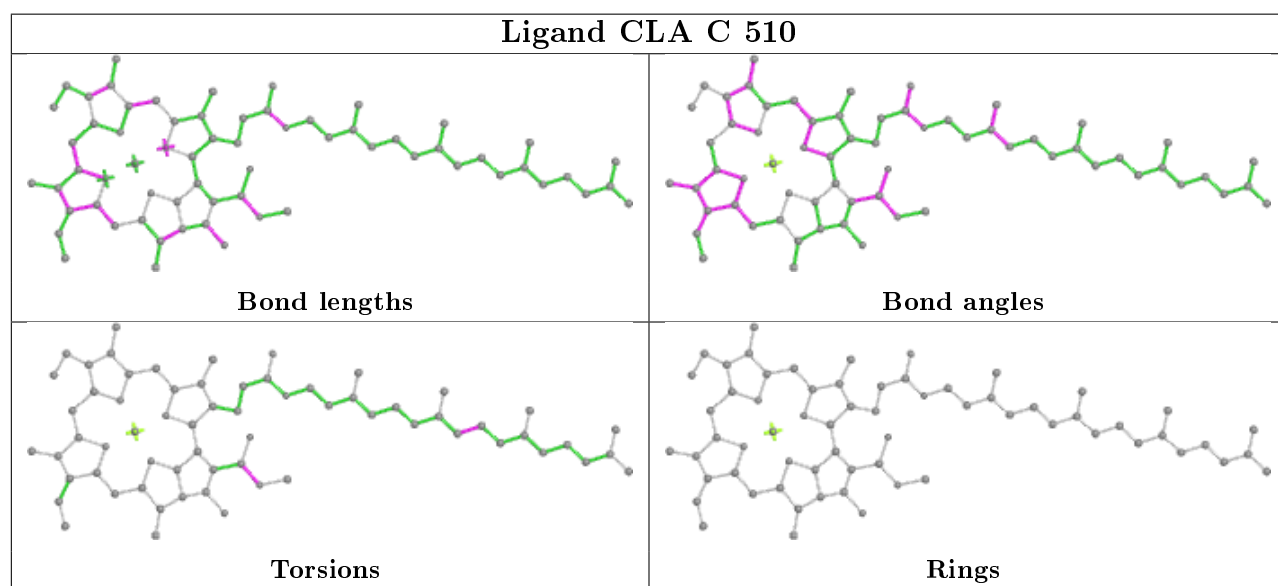
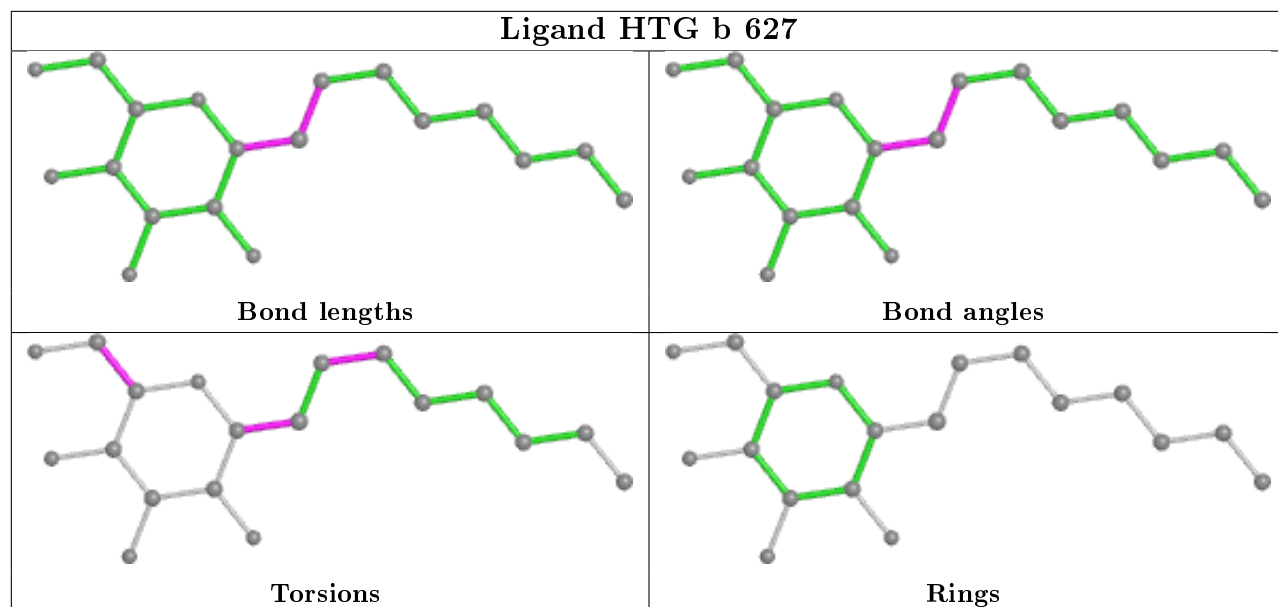


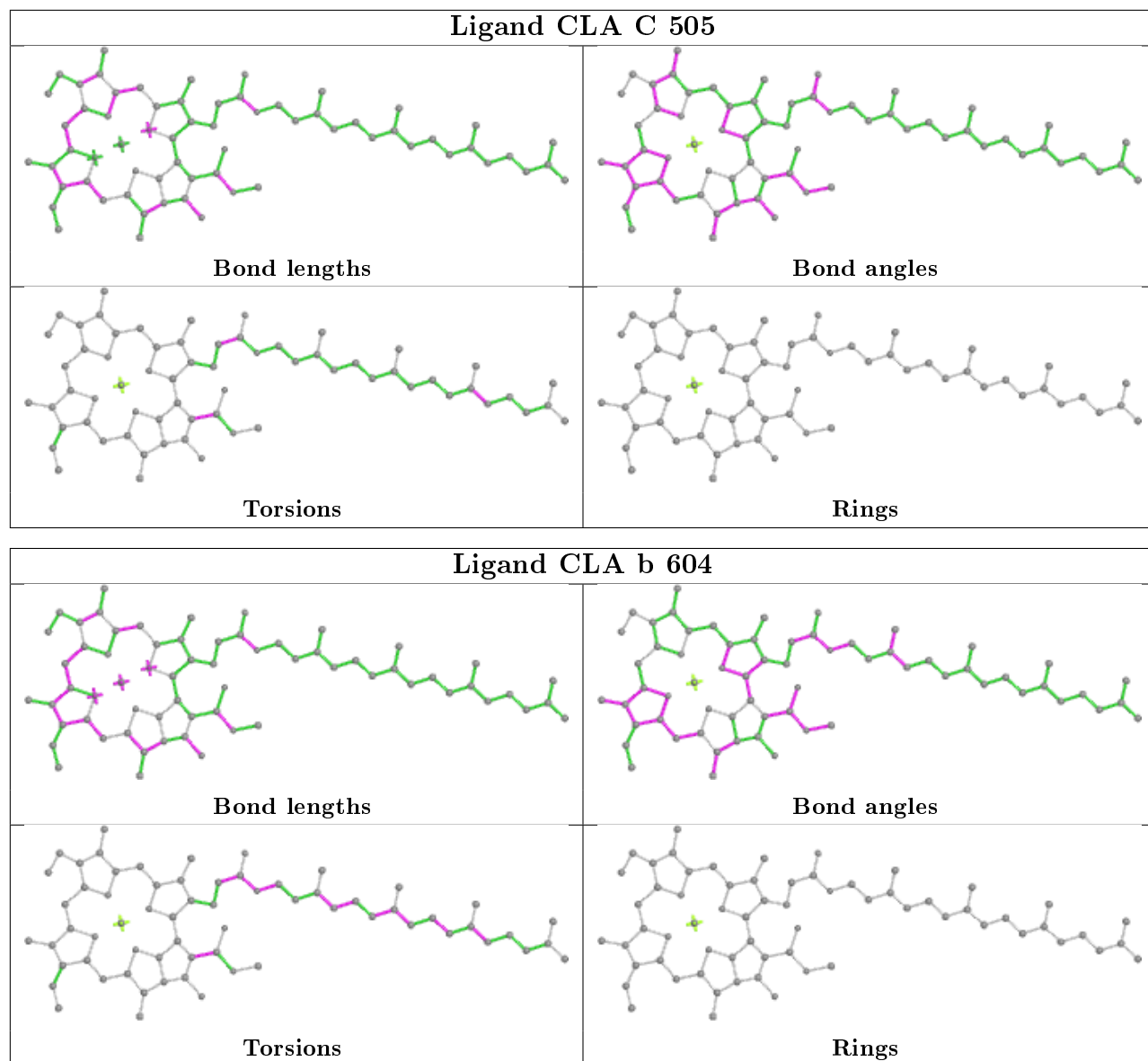


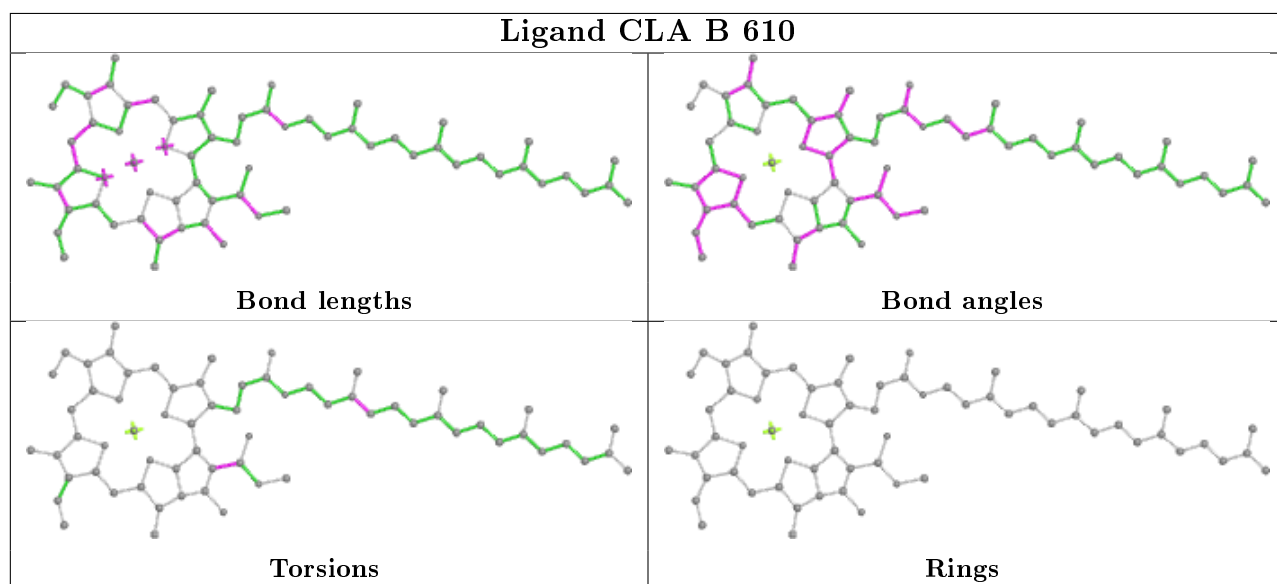
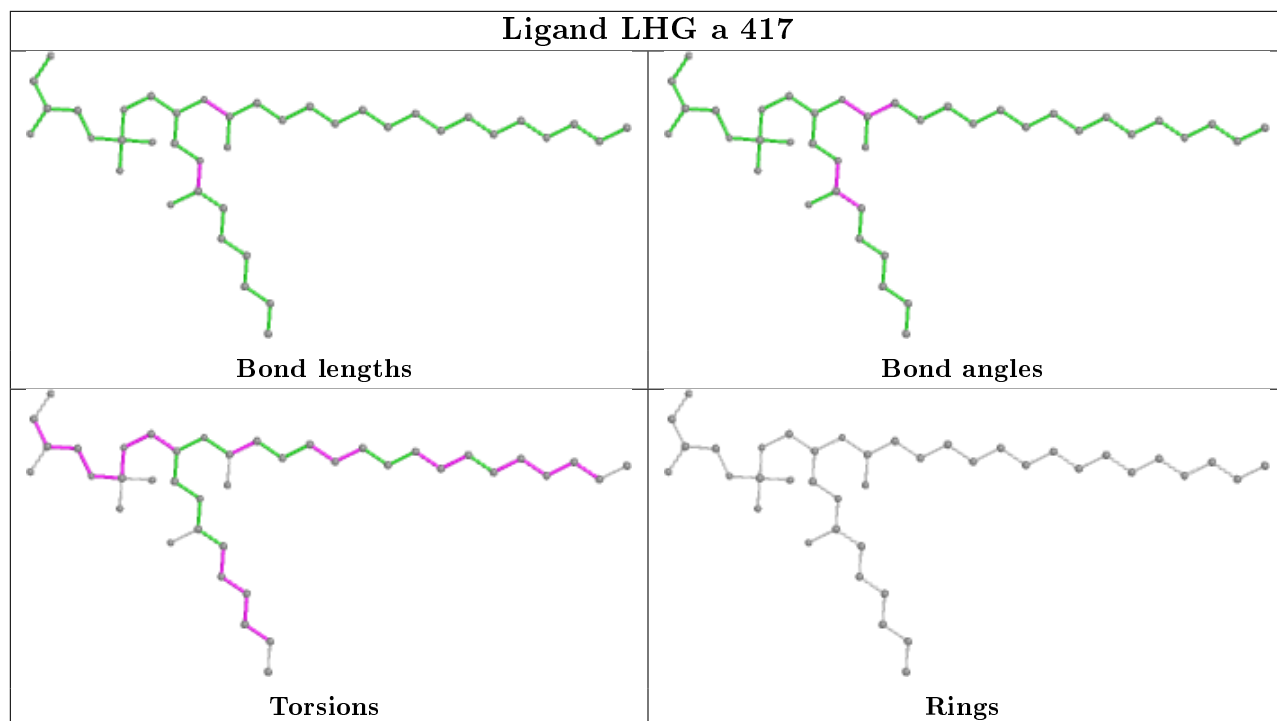


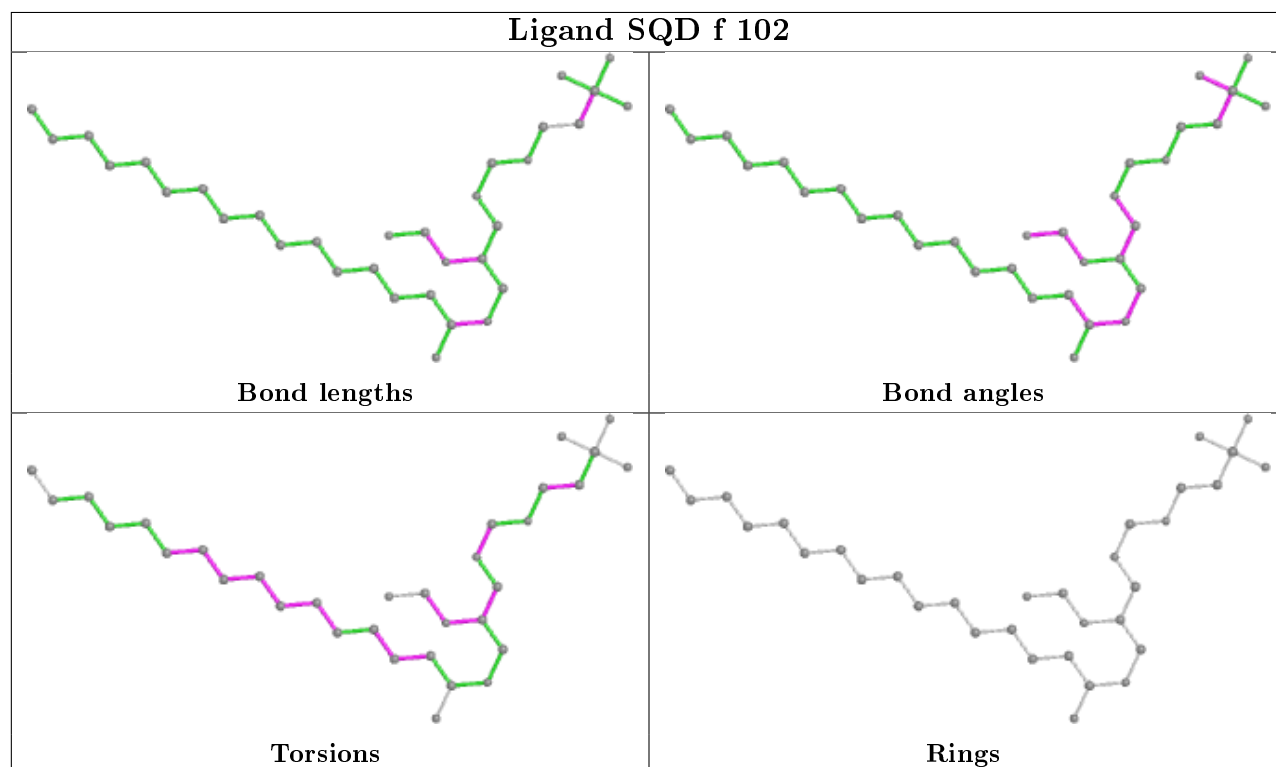
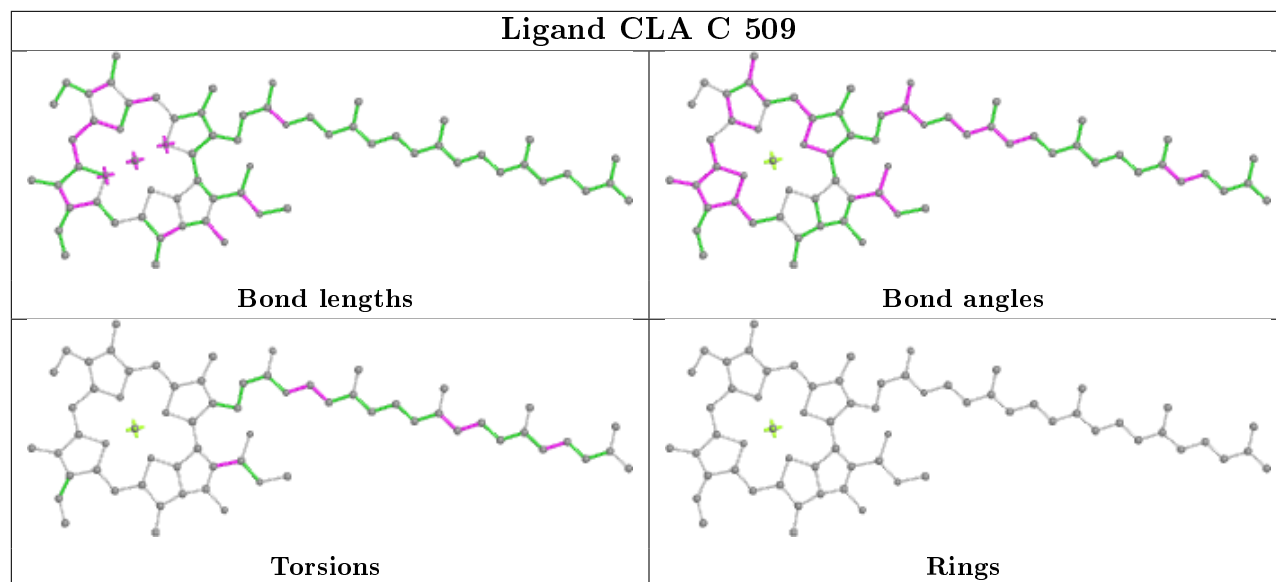


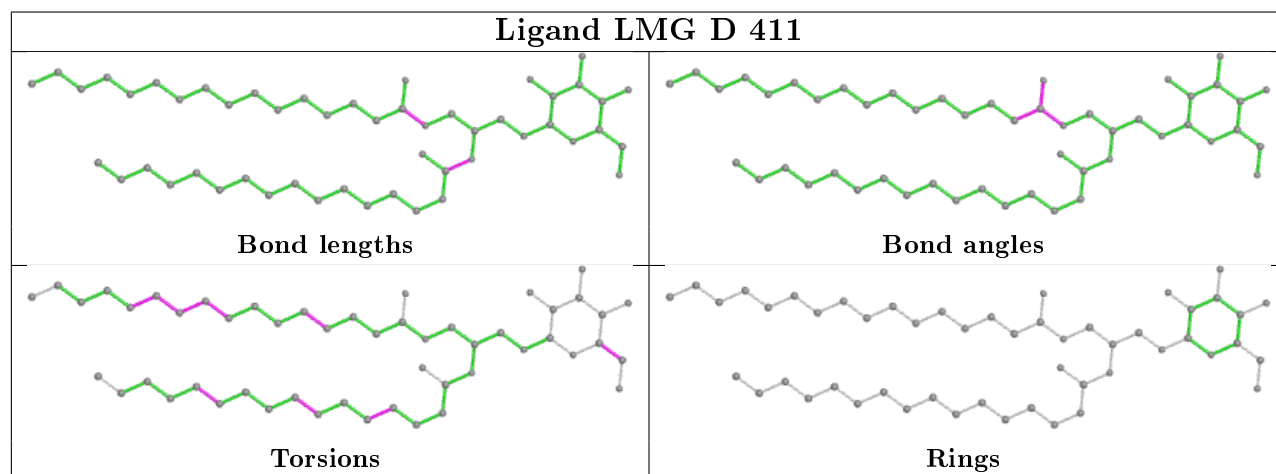
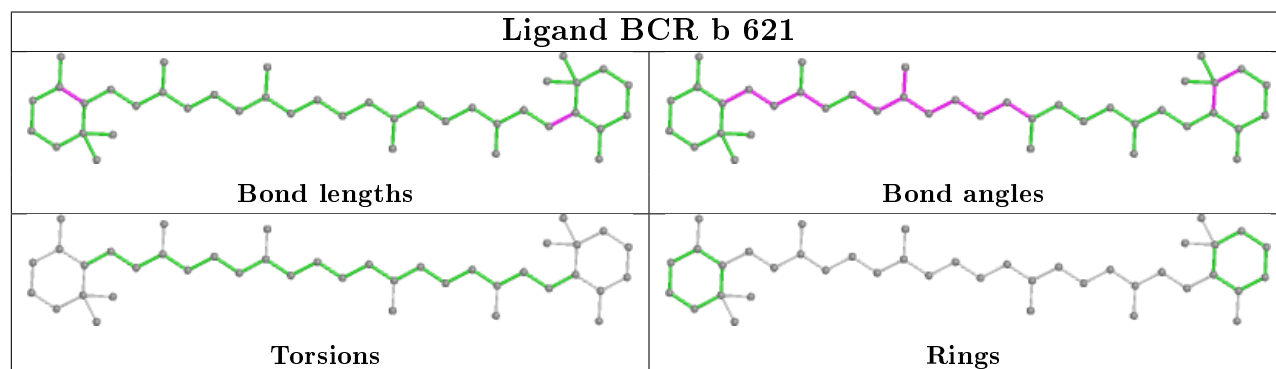
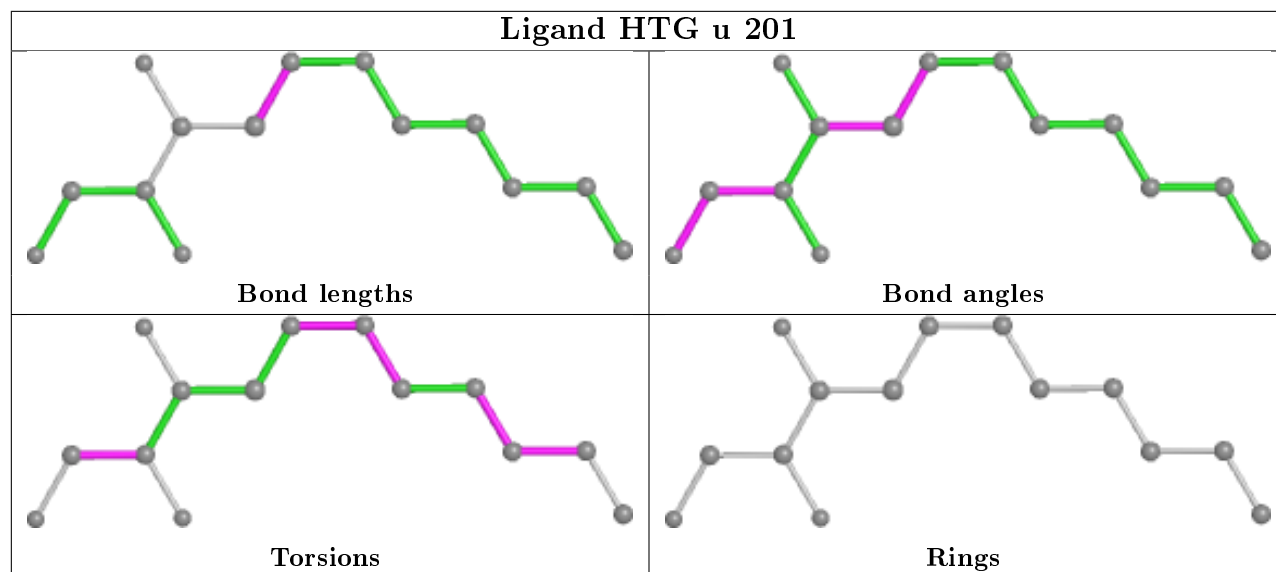


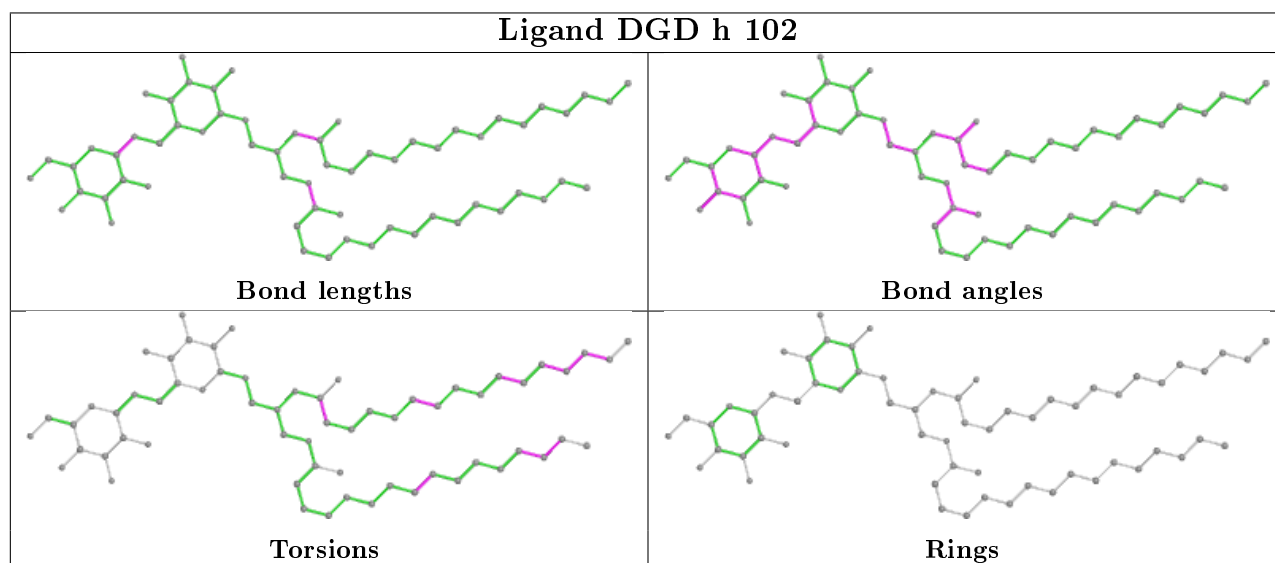
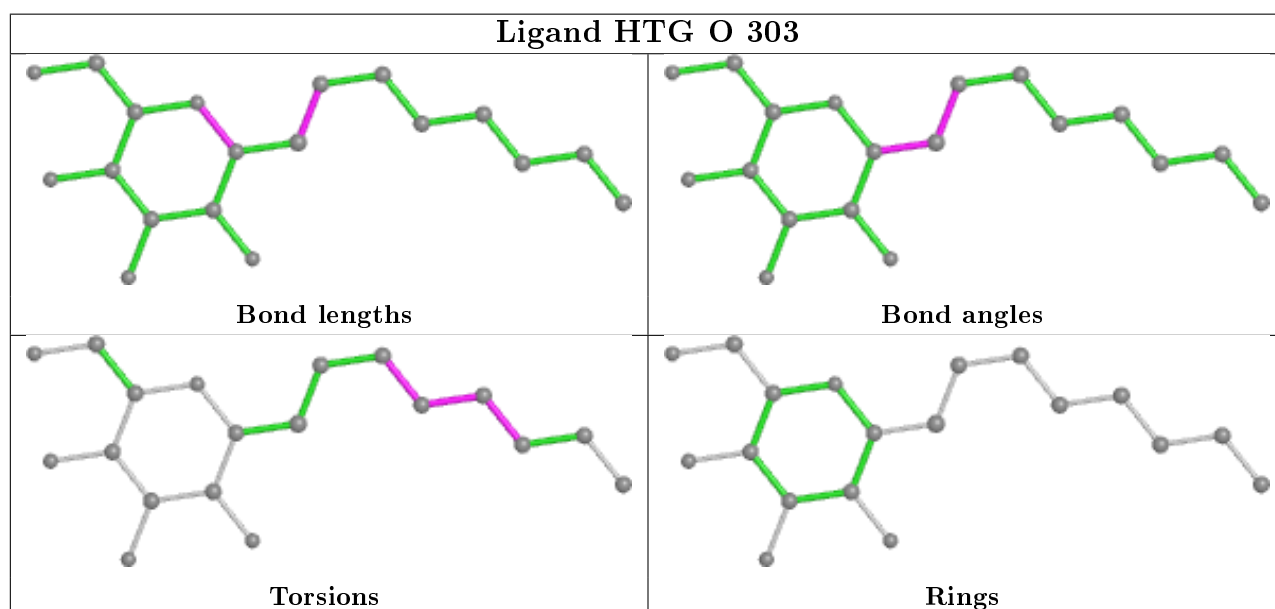
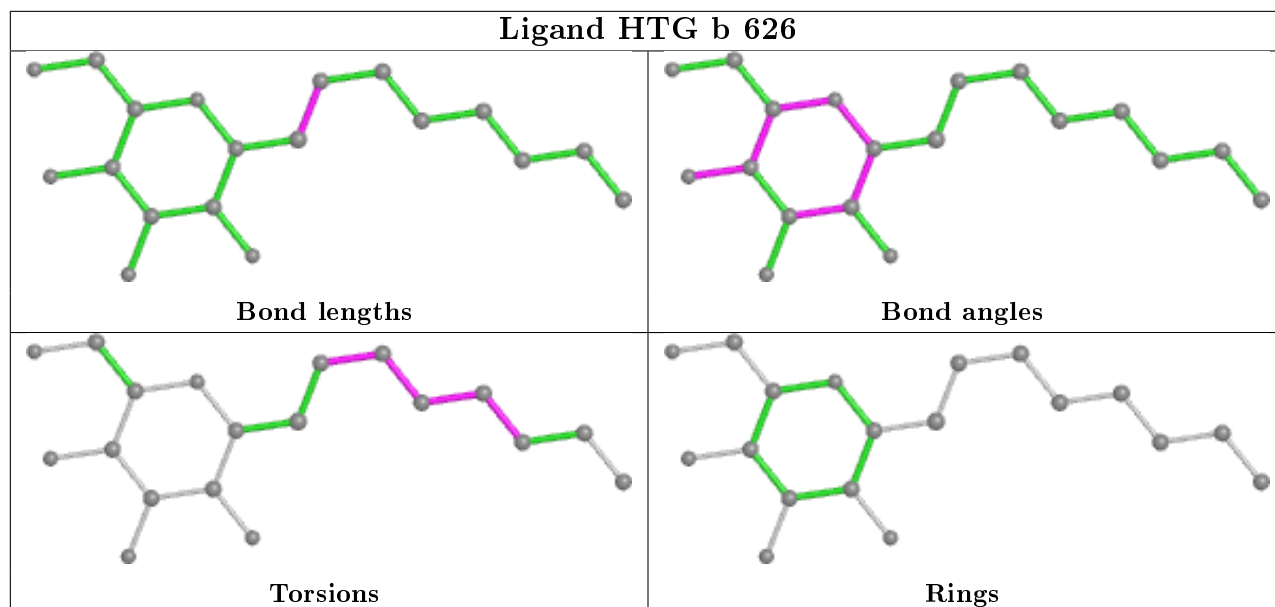


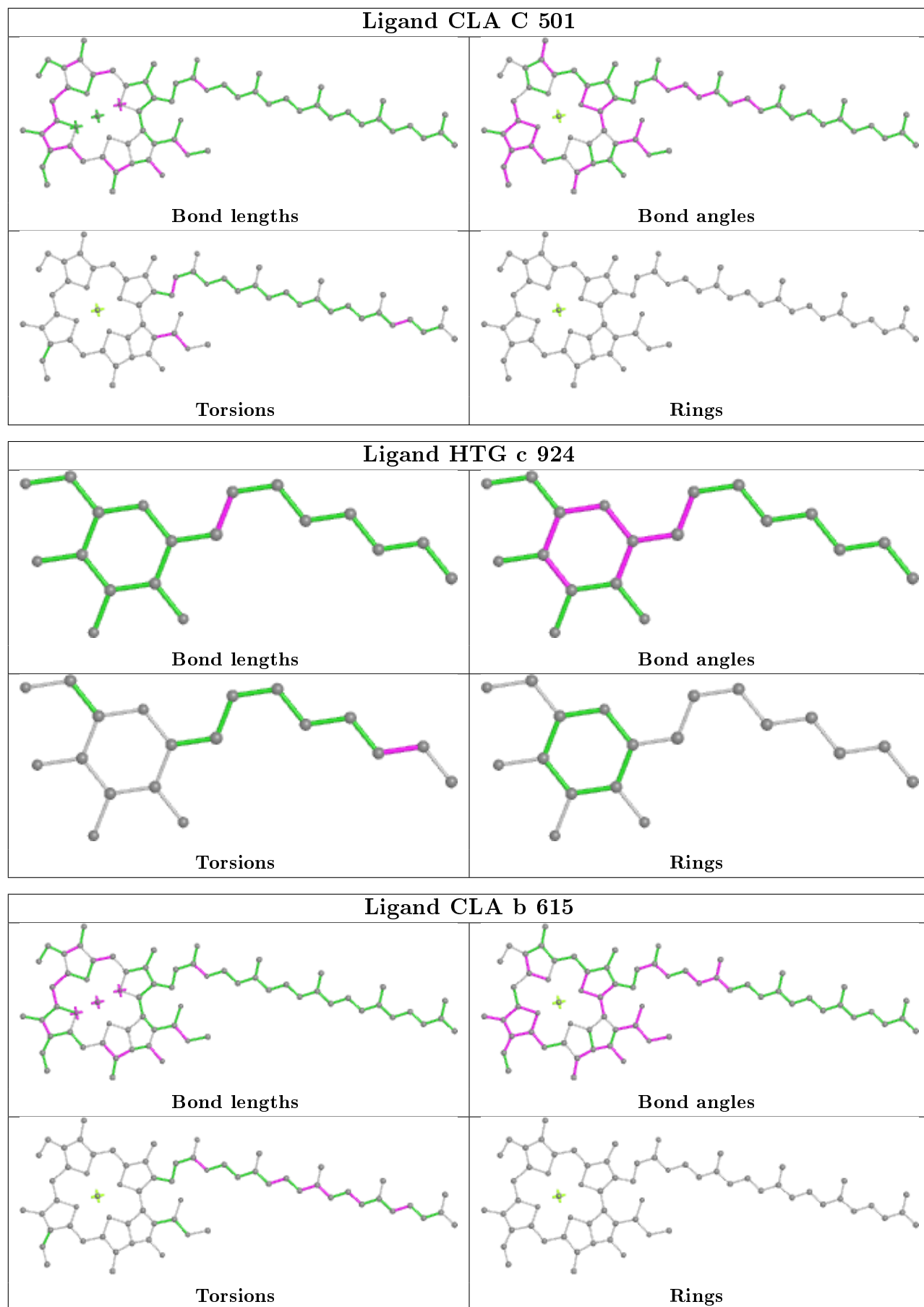


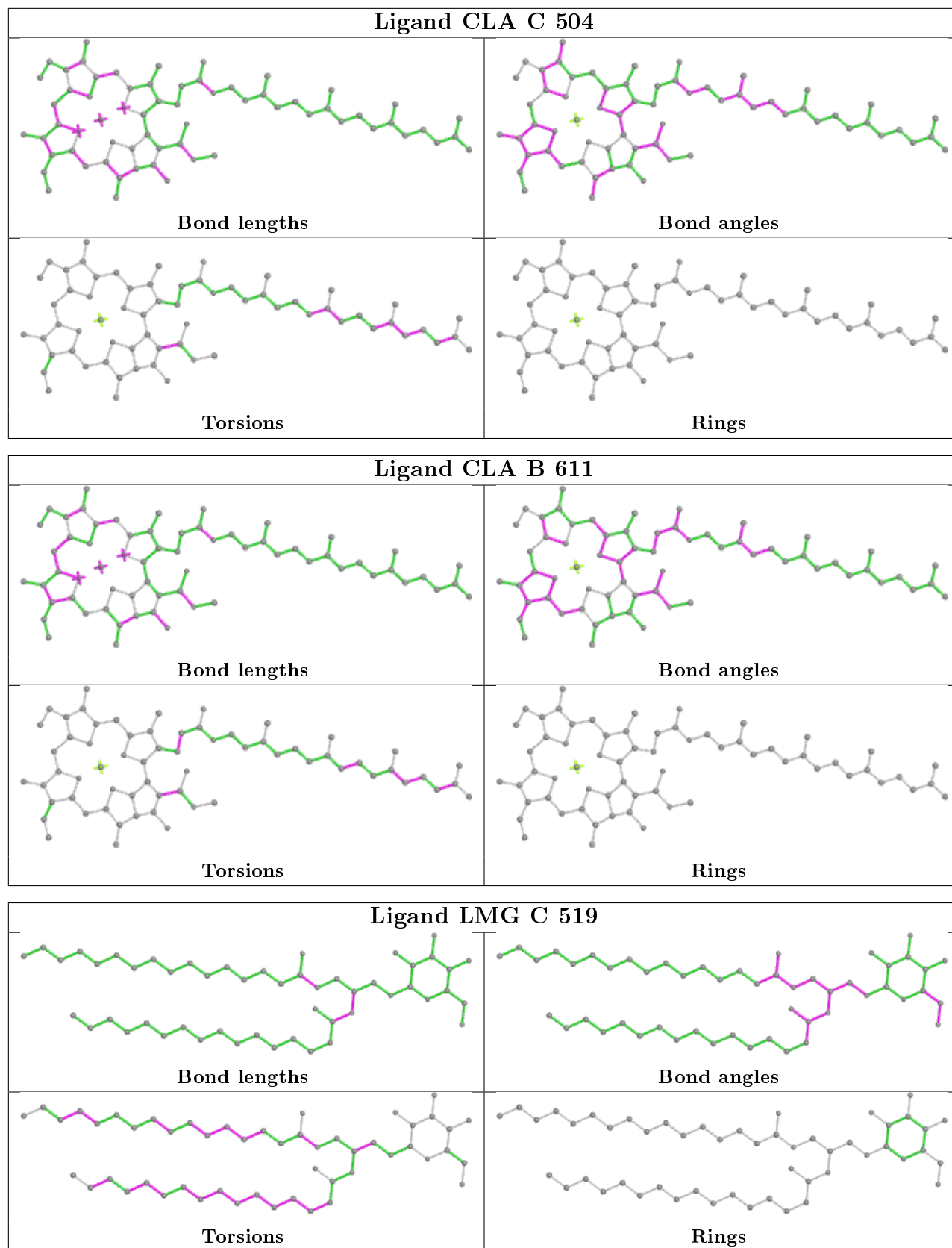


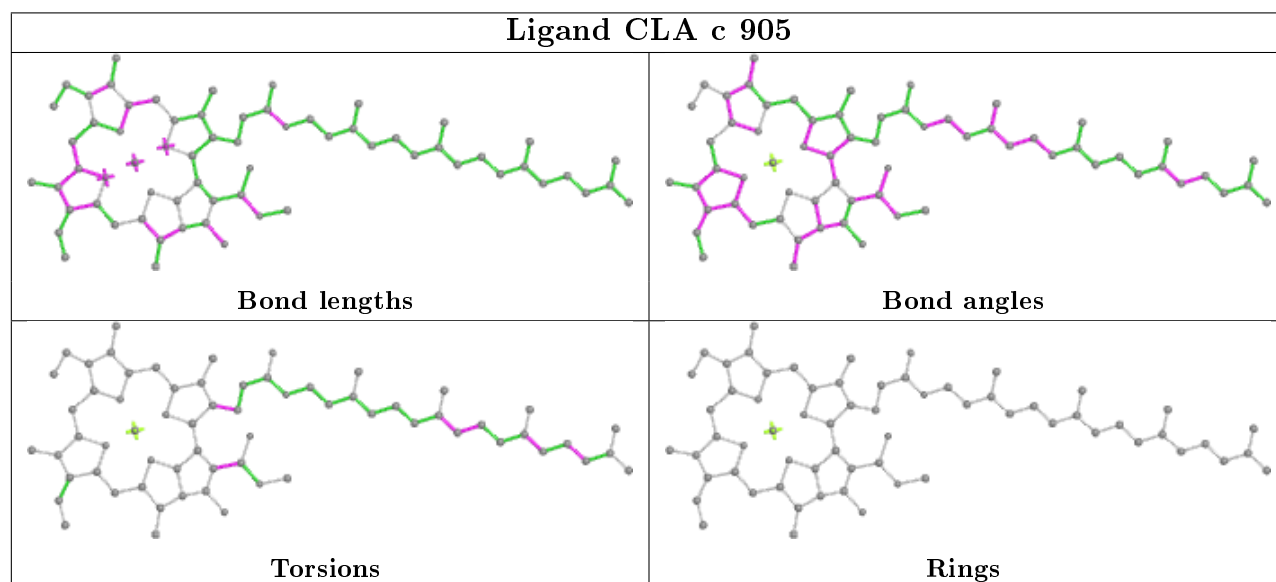
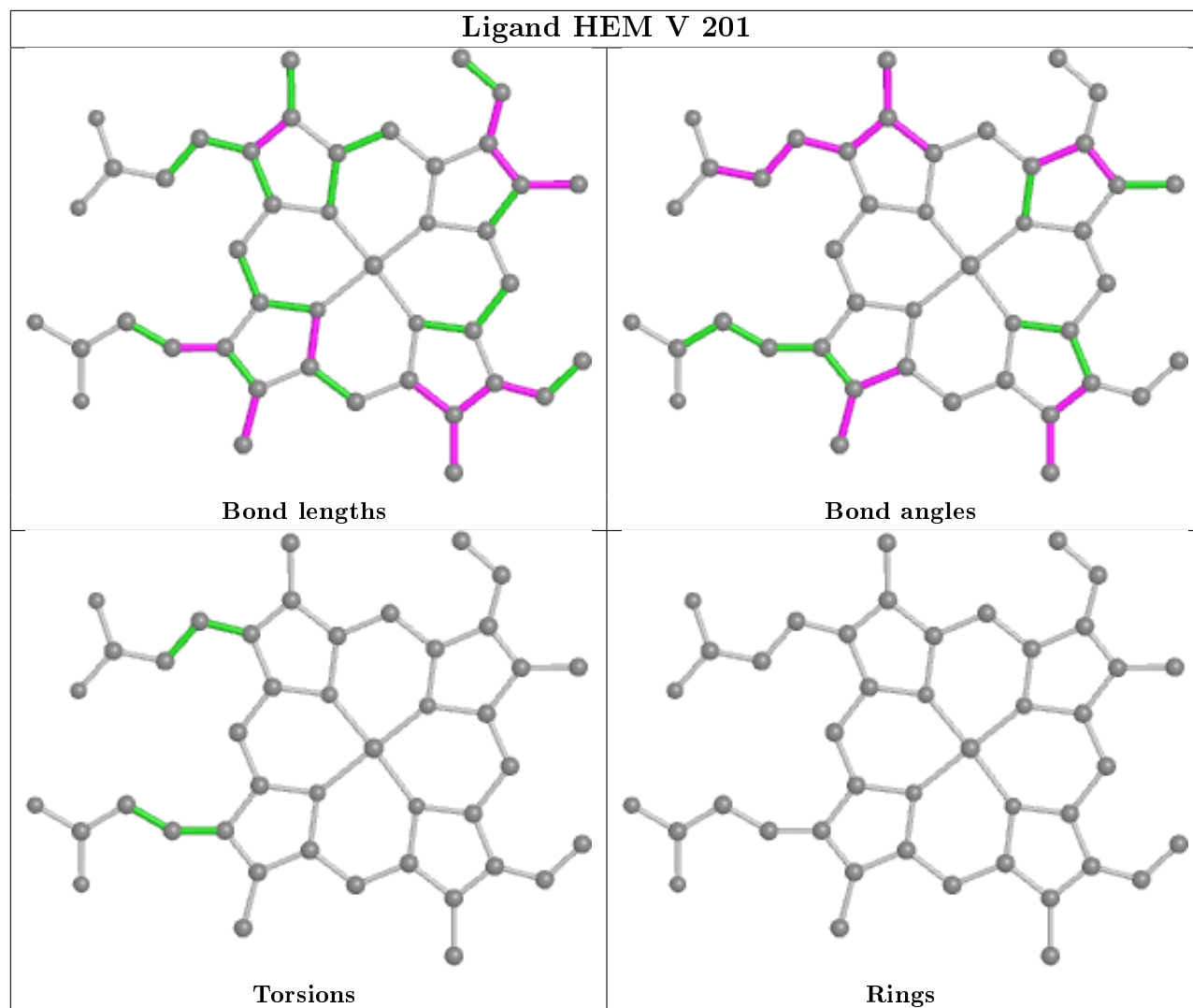


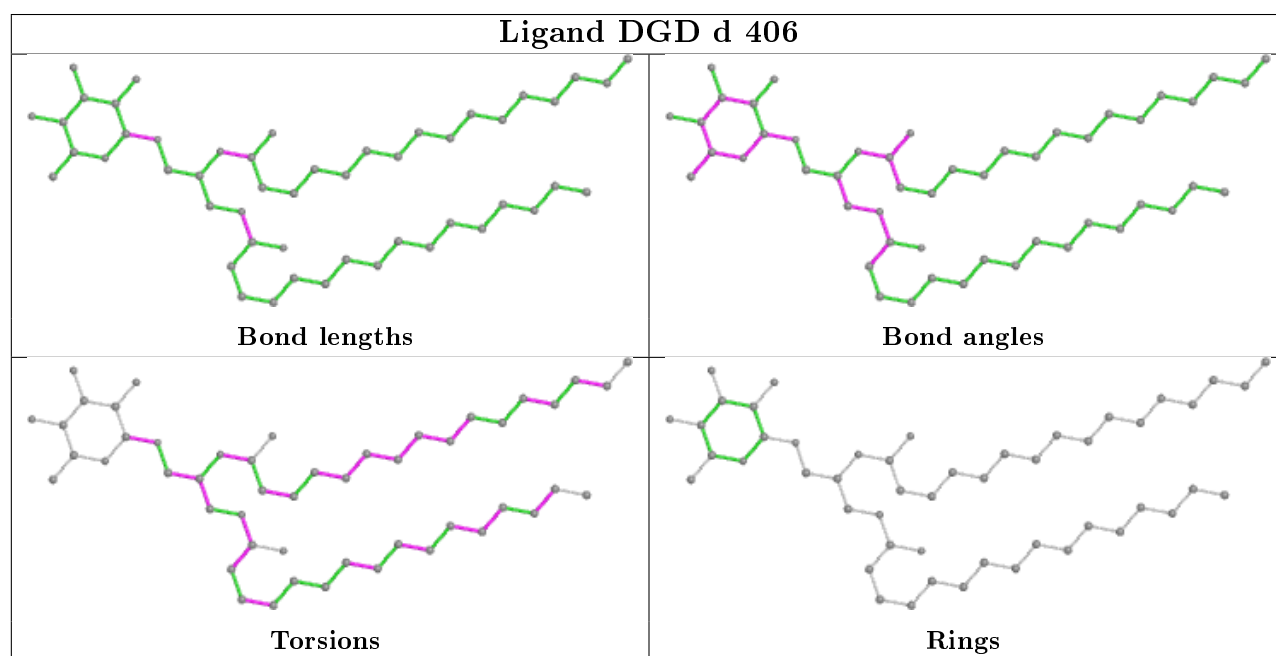
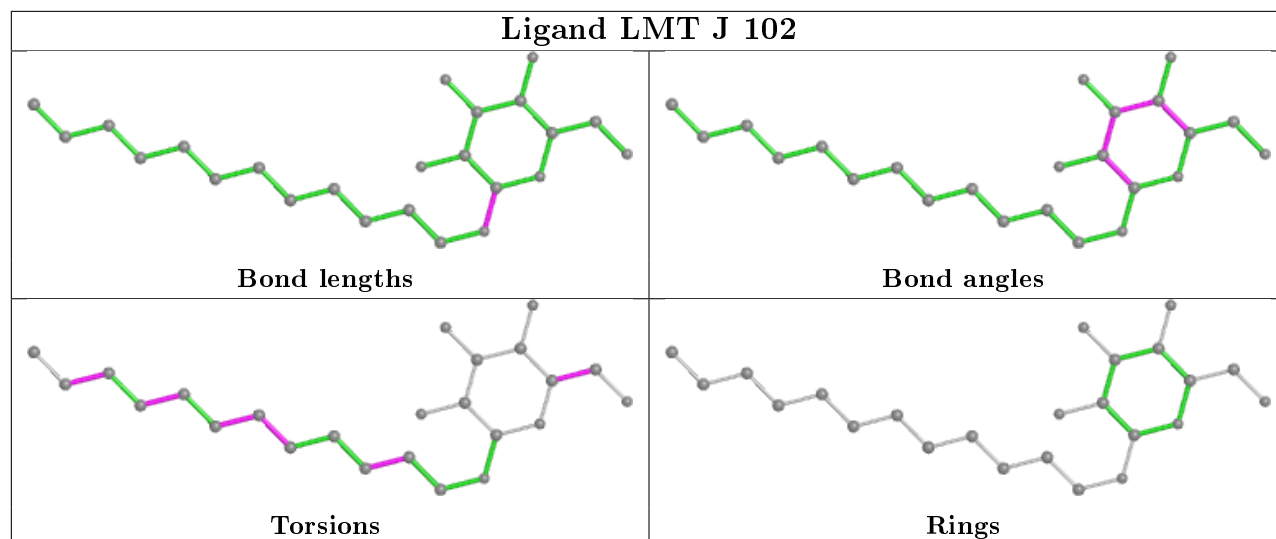


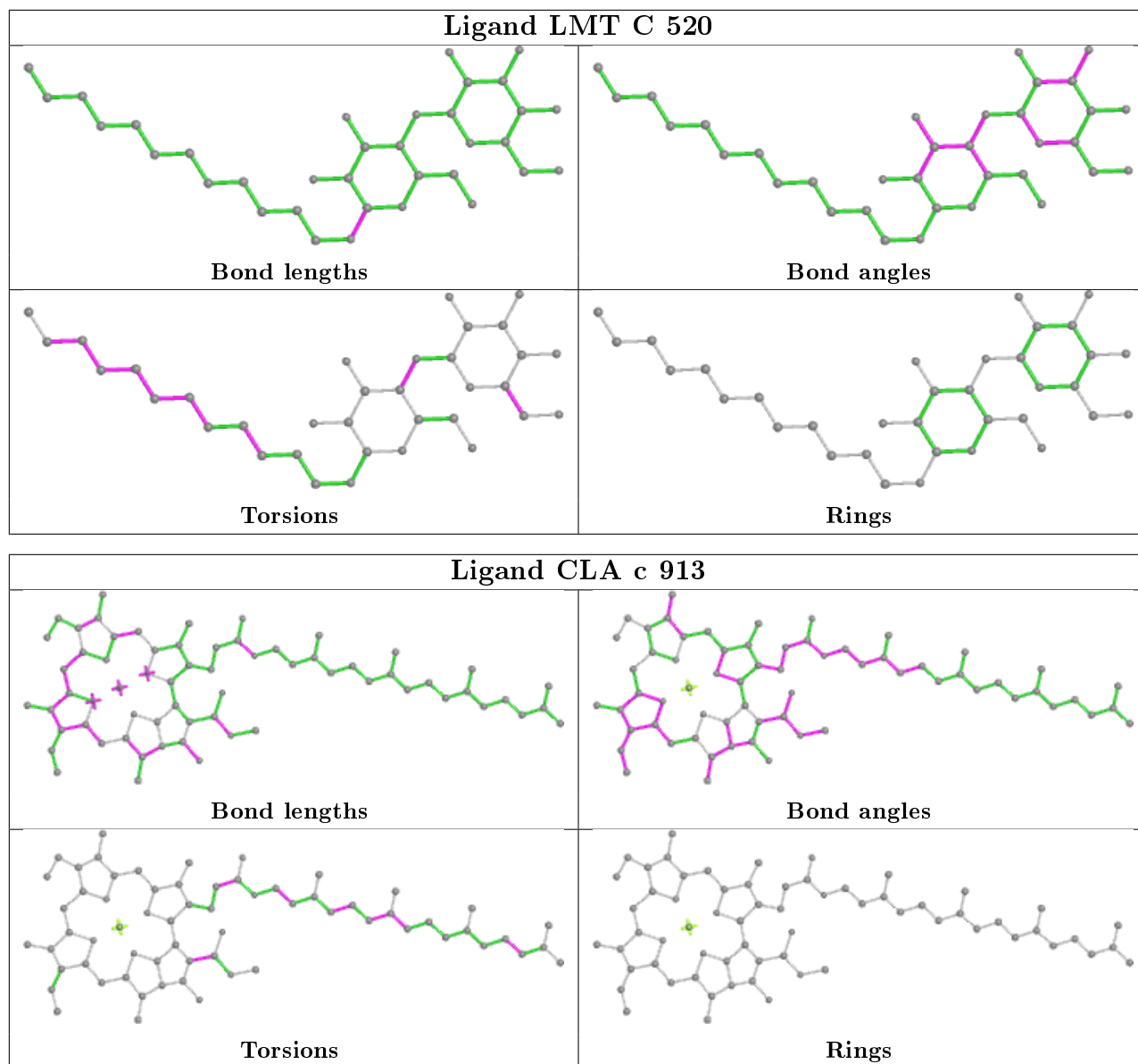


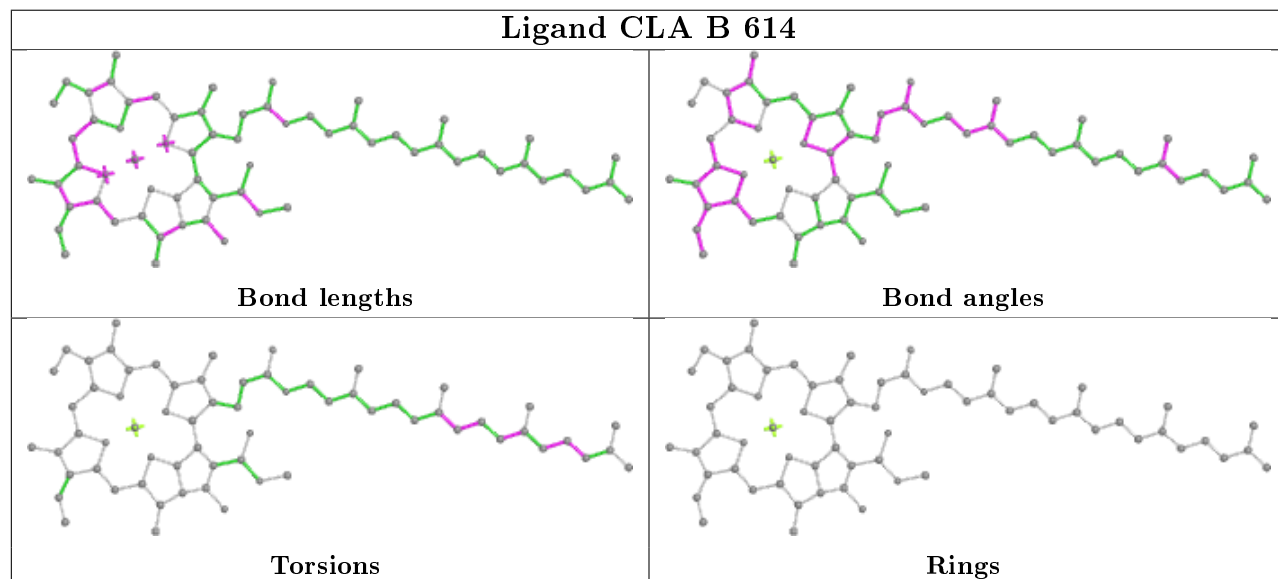
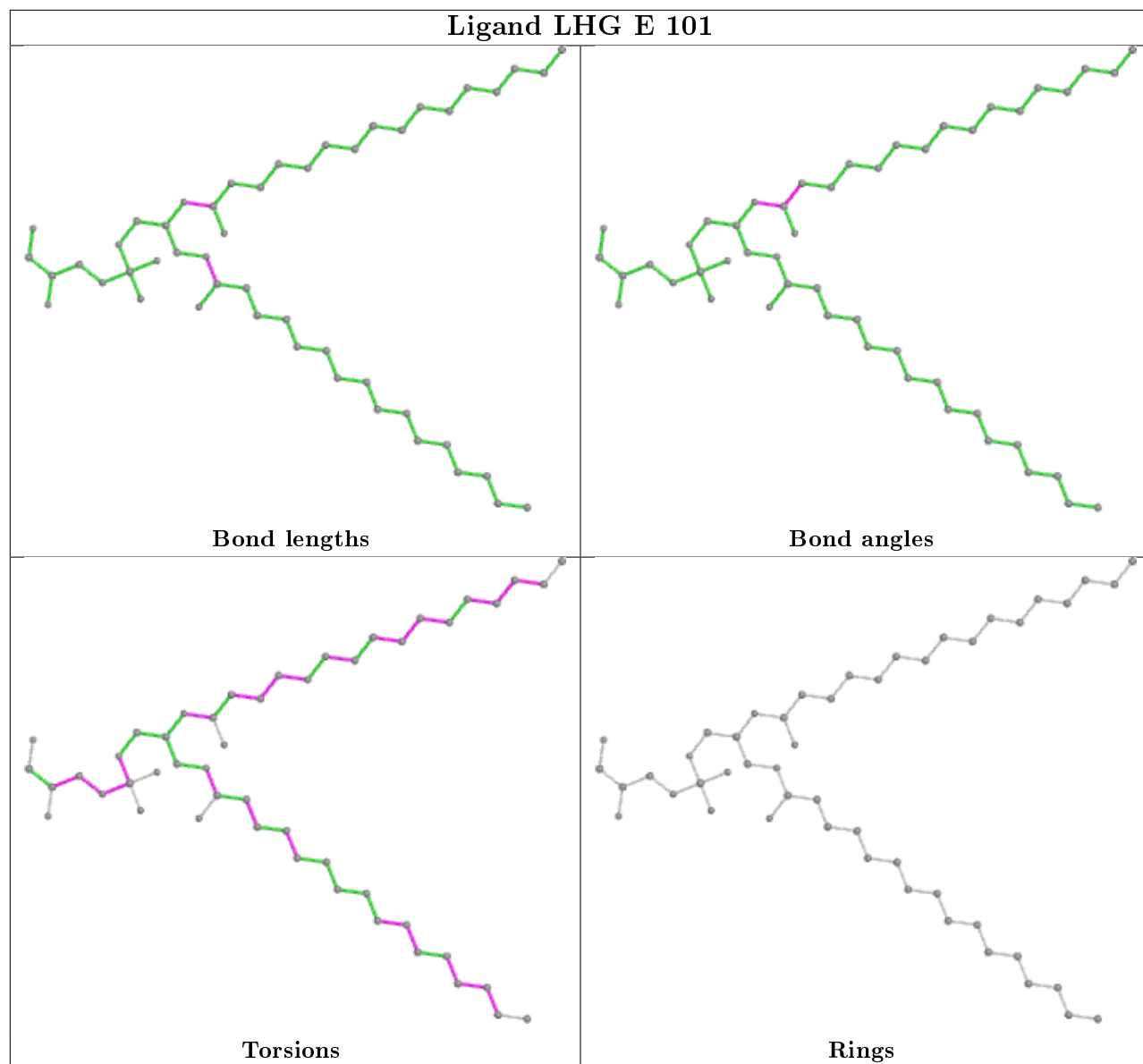


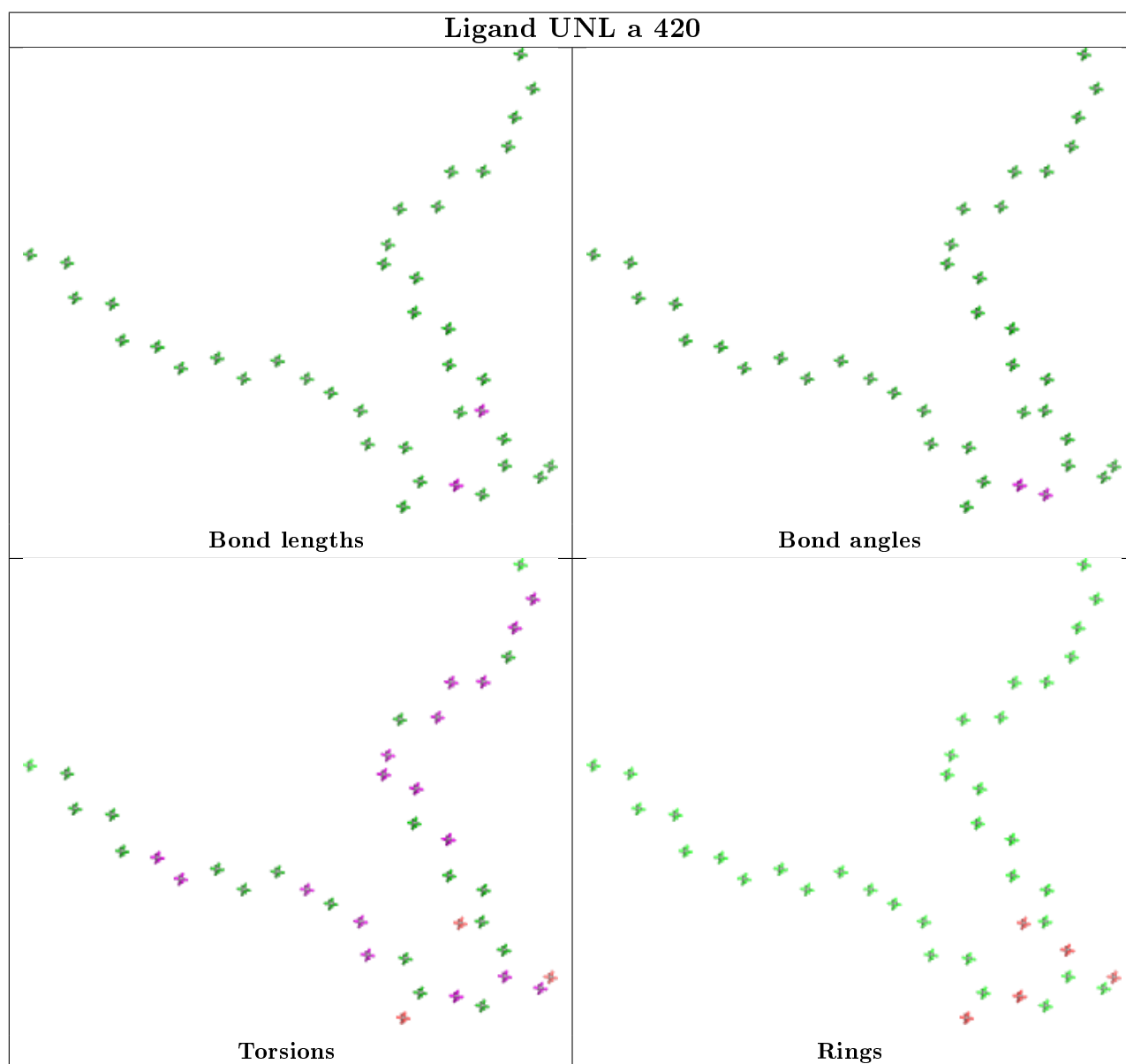
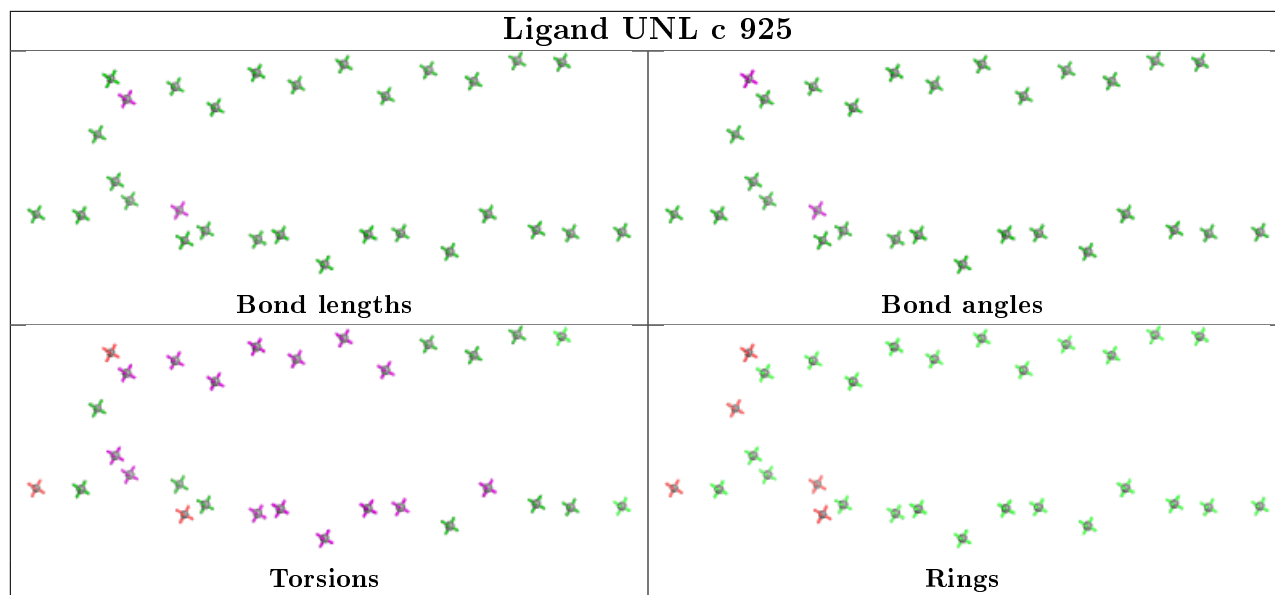


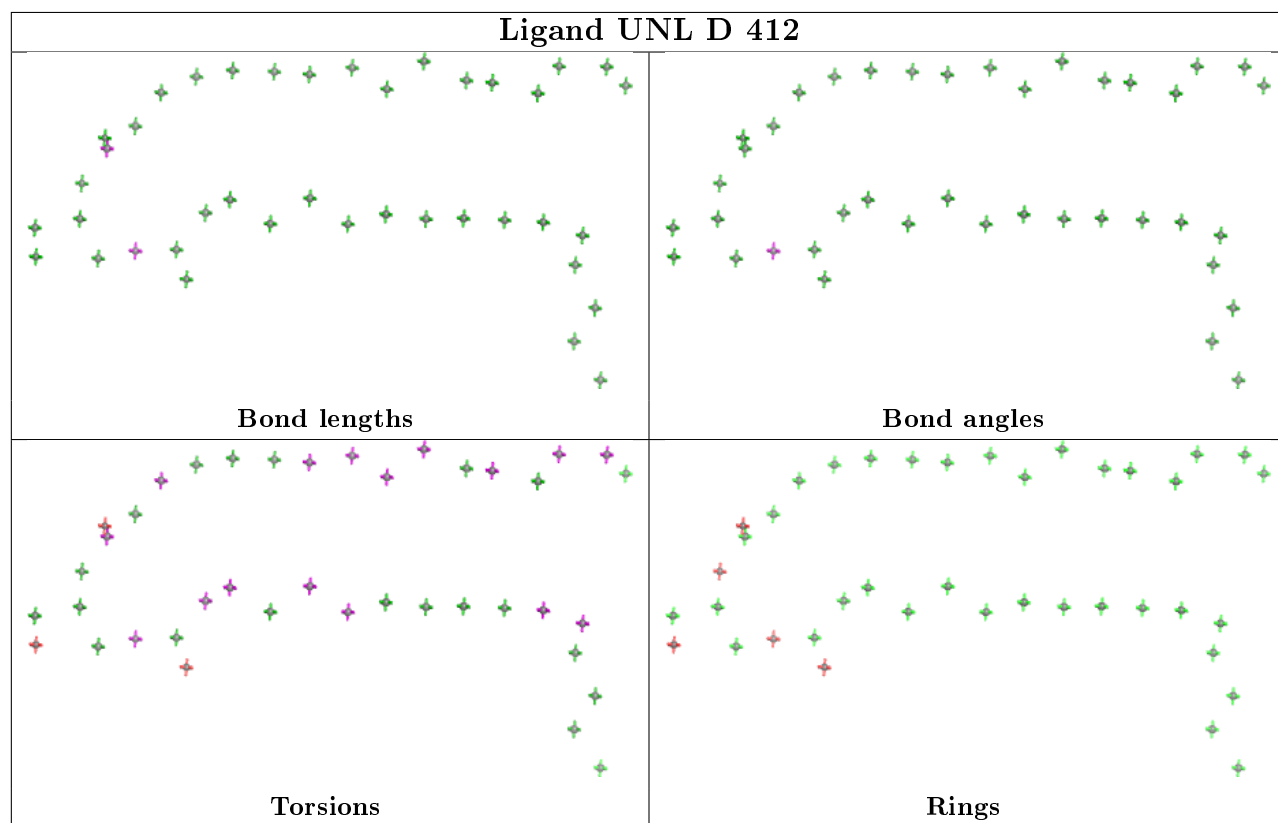
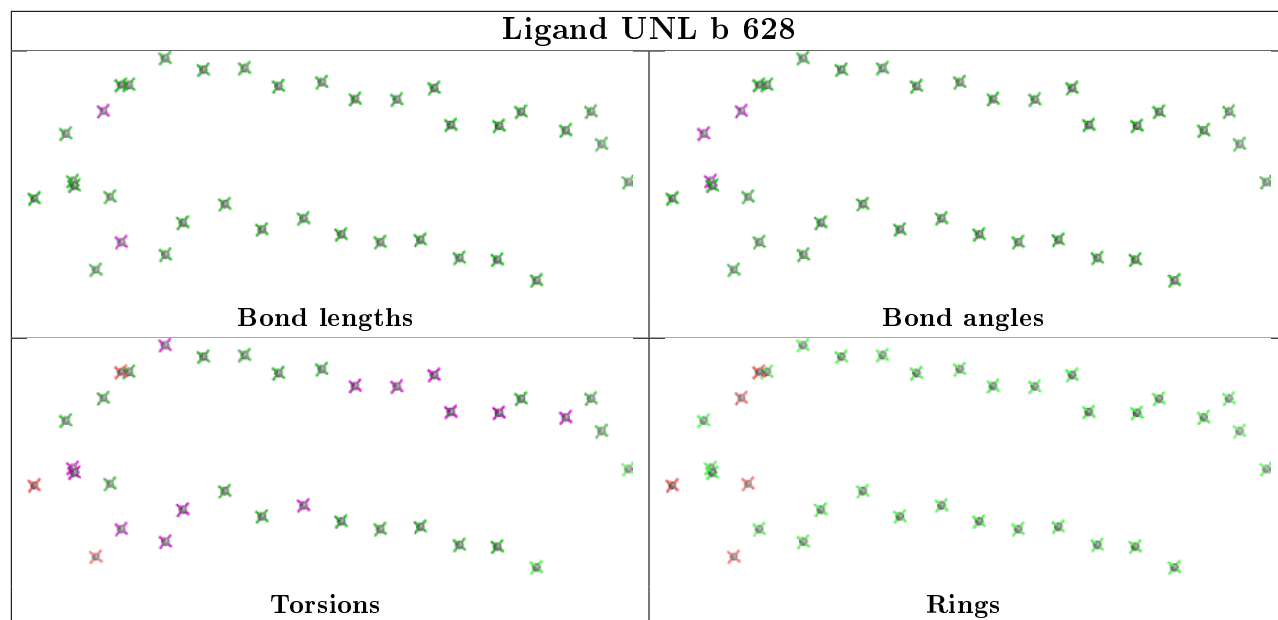


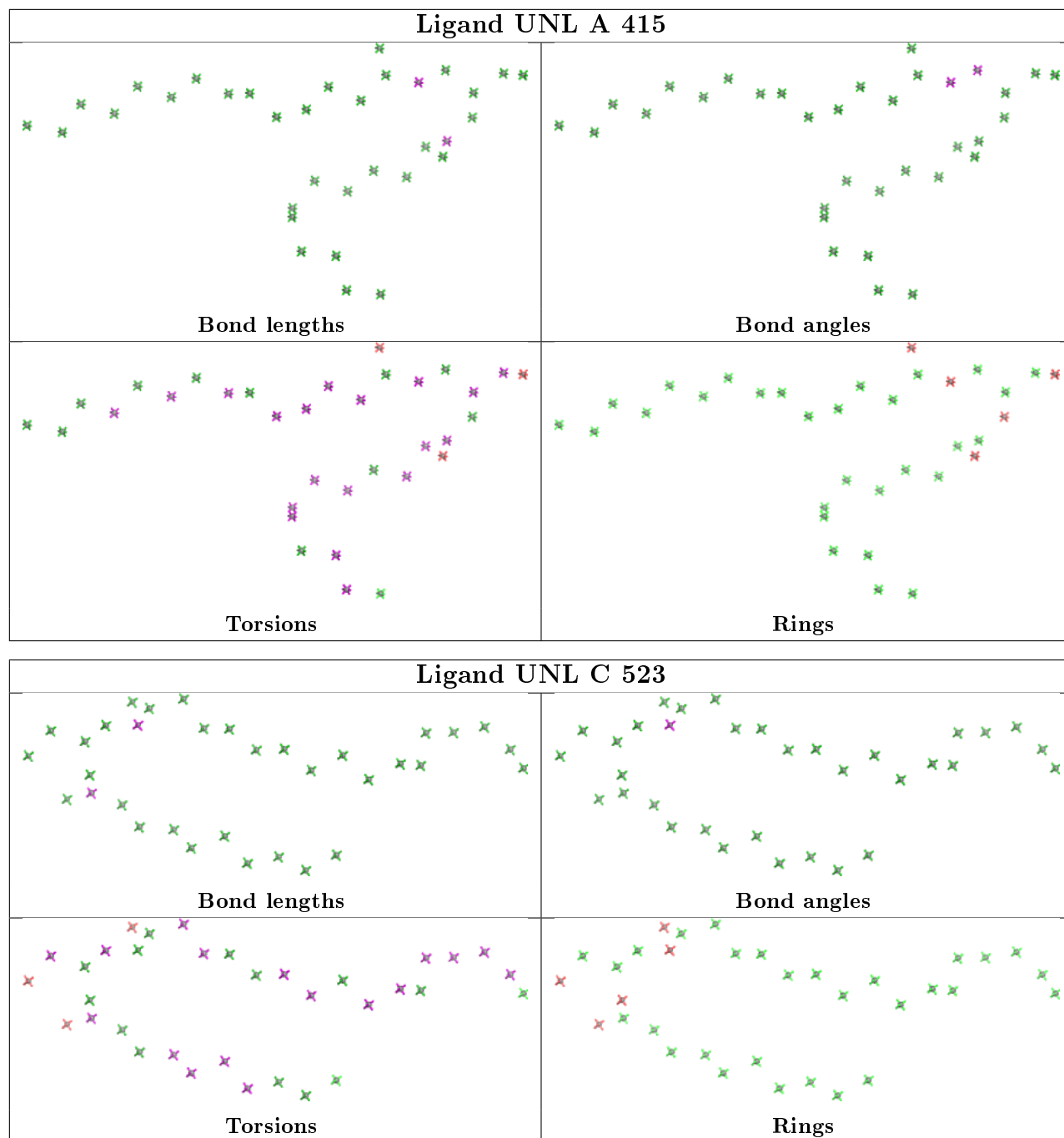












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.18	4 (1%) 79 81	16, 23, 46, 69	0
1	a	334/344 (97%)	-0.00	13 (3%) 39 42	19, 24, 50, 76	0
2	B	504/504 (100%)	0.07	39 (7%) 13 15	18, 27, 54, 88	0
2	b	501/504 (99%)	0.10	43 (8%) 10 12	20, 29, 58, 119	0
3	C	451/455 (99%)	-0.11	14 (3%) 49 51	21, 31, 46, 81	0
3	c	455/455 (100%)	0.14	25 (5%) 25 28	23, 34, 48, 79	0
4	D	340/342 (99%)	-0.23	7 (2%) 63 66	17, 24, 40, 70	0
4	d	340/342 (99%)	-0.19	6 (1%) 68 71	19, 26, 45, 80	0
5	E	81/83 (97%)	0.92	17 (20%) 1 1	27, 40, 62, 82	0
5	e	79/83 (95%)	1.19	23 (29%) 0 0	32, 44, 72, 82	0
6	F	34/44 (77%)	0.20	5 (14%) 2 2	26, 34, 63, 74	0
6	f	32/44 (72%)	0.35	3 (9%) 8 9	29, 37, 76, 86	0
7	H	63/63 (100%)	-0.08	1 (1%) 72 74	24, 33, 43, 70	0
7	h	63/63 (100%)	0.37	5 (7%) 12 14	27, 37, 51, 81	0
8	I	35/38 (92%)	-0.11	0 100 100	27, 34, 64, 86	0
8	i	37/38 (97%)	0.21	2 (5%) 25 29	26, 34, 71, 83	0
9	J	36/40 (90%)	0.14	4 (11%) 5 6	26, 38, 65, 79	0
9	j	39/40 (97%)	0.59	8 (20%) 1 1	30, 42, 68, 84	0
10	K	37/37 (100%)	-0.17	0 100 100	32, 38, 47, 63	0
10	k	37/37 (100%)	0.30	3 (8%) 12 13	36, 42, 55, 69	0
11	L	37/37 (100%)	-0.14	3 (8%) 12 13	17, 22, 65, 75	0
11	l	37/37 (100%)	0.13	2 (5%) 25 29	19, 23, 64, 95	0
12	M	32/36 (88%)	-0.17	1 (3%) 49 51	21, 24, 40, 56	0
12	m	33/36 (91%)	-0.01	2 (6%) 21 24	20, 25, 48, 68	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/244 (100%)	0.31	34 (13%) 2 3	18, 33, 66, 120	0
13	o	241/244 (98%)	0.38	39 (16%) 1 1	20, 35, 71, 87	0
14	T	29/32 (90%)	-0.01	1 (3%) 45 48	19, 23, 49, 85	0
14	t	29/32 (90%)	-0.01	1 (3%) 45 48	20, 23, 47, 72	0
15	U	97/104 (93%)	-0.13	0 100 100	23, 30, 52, 58	0
15	u	97/104 (93%)	-0.36	1 (1%) 82 84	24, 30, 40, 66	0
16	V	137/137 (100%)	-0.37	0 100 100	22, 28, 43, 51	0
16	v	137/137 (100%)	0.44	13 (9%) 8 9	26, 37, 52, 72	0
17	Y	27/30 (90%)	1.04	4 (14%) 2 2	37, 47, 70, 77	0
17	y	28/30 (93%)	1.15	7 (25%) 0 0	45, 55, 73, 77	0
18	X	38/40 (95%)	0.69	7 (18%) 1 1	32, 39, 65, 69	0
18	x	38/40 (95%)	0.94	9 (23%) 0 0	34, 42, 83, 94	0
19	Z	62/62 (100%)	1.46	19 (30%) 0 0	37, 46, 75, 92	0
19	z	60/62 (96%)	1.96	25 (41%) 0 0	47, 57, 88, 95	0
All	All	5235/5344 (97%)	0.11	390 (7%) 14 16	16, 30, 59, 120	0

All (390) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	494	GLY	8.3
2	b	496	TYR	8.1
18	x	37	VAL	7.9
13	o	246	ALA	7.4
13	O	60	ARG	7.4
2	b	494	GLY	7.2
18	x	38	GLN	7.2
19	z	61	VAL	7.1
2	B	495	PHE	6.8
17	Y	22	LEU	6.5
19	Z	62	VAL	6.3
19	z	60	PHE	6.3
5	e	25	ILE	6.0
19	z	5	PHE	6.0
19	Z	3	ILE	6.0
1	A	11	ALA	5.9
2	b	503	THR	5.9
2	b	502	VAL	5.7

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Mol	Chain	Res	Type	RSRZ
19	z	33	TRP	5.6
19	z	4	LEU	5.6
19	Z	33	TRP	5.6
2	b	495	PHE	5.5
2	b	493	TRP	5.5
13	o	25	THR	5.5
2	b	500	GLY	5.4
2	b	484	PRO	5.4
13	o	36	GLN	5.4
11	l	1	MET	5.4
2	b	499	VAL	5.4
9	J	5	GLY	5.3
1	a	13	LEU	5.3
2	B	496	TYR	5.3
19	z	2	THR	5.2
13	O	25	THR	5.2
2	B	501	ASP	5.1
5	E	17	VAL	5.1
11	L	1	MET	5.1
9	j	6	GLY	5.1
19	Z	7	LEU	5.1
18	x	2	THR	5.0
2	b	85	GLY	5.0
2	b	489	GLU	5.0
19	Z	31	GLN	5.0
2	b	86	ILE	5.0
19	Z	32	ASP	4.9
9	j	5	GLY	4.9
13	o	35	SER	4.9
18	X	2	THR	4.9
19	Z	30	PRO	4.9
2	b	487	SER	4.8
5	E	21	VAL	4.8
5	E	6	GLY	4.8
2	B	486	LEU	4.8
7	h	64	ALA	4.7
13	O	27	ARG	4.7
18	X	37	VAL	4.7
13	o	23	ASP	4.6
2	B	500	GLY	4.5
5	E	4	THR	4.5
19	z	7	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
13	O	3	GLN	4.5
2	B	487	SER	4.4
13	o	38	TYR	4.4
9	J	6	GLY	4.4
1	a	11	ALA	4.4
2	b	293	ALA	4.4
19	z	41	PHE	4.3
6	F	12	SER	4.3
13	o	26	ALA	4.3
17	y	22	LEU	4.3
6	f	14	PRO	4.3
19	z	3	ILE	4.3
19	Z	4	LEU	4.2
2	b	504	THR	4.2
3	c	201[A]	ASN	4.1
9	j	8	ILE	4.1
6	F	13	TYR	4.1
17	y	19	ILE	4.1
10	k	18	PHE	4.1
2	B	504	THR	4.1
2	B	293	ALA	4.1
13	O	26	ALA	4.1
15	u	8	GLU	4.1
3	C	143	TYR	4.1
5	E	5	THR	4.0
2	b	126	PRO	4.0
13	o	32	ILE	4.0
3	C	23	ALA	4.0
6	F	16	PHE	4.0
19	z	6	GLN	4.0
11	L	3	PRO	4.0
6	f	16	PHE	3.9
17	y	20	ALA	3.9
1	A	13	LEU	3.9
6	F	15	ILE	3.9
13	o	34	SER	3.9
2	B	503	THR	3.9
2	B	499	VAL	3.9
1	a	235	TYR	3.9
19	Z	60	PHE	3.8
2	b	497	GLN	3.8
18	x	39	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
19	Z	34	ASP	3.8
19	Z	1	MET	3.8
13	o	27	ARG	3.8
3	c	200	THR	3.8
9	j	4	GLU	3.8
2	B	484	PRO	3.7
5	e	6	GLY	3.7
13	O	4	THR	3.7
13	O	133	VAL	3.7
12	M	33	GLN	3.7
2	b	488	PRO	3.7
2	b	84	THR	3.7
5	e	21	VAL	3.7
5	E	84	LYS	3.6
3	c	21	ILE	3.6
16	v	19	ILE	3.6
4	D	238	THR	3.6
13	o	37	THR	3.6
3	c	279	LEU	3.6
2	B	485	GLU	3.6
8	i	37	LEU	3.6
14	T	30	THR	3.5
19	z	39	LEU	3.5
13	O	24	ASP	3.5
2	B	295	GLY	3.5
4	d	238	THR	3.5
4	d	12	ARG	3.5
16	v	14	SER	3.5
13	O	23	ASP	3.5
18	X	39	ARG	3.5
1	A	12	ASN	3.4
2	b	295	GLY	3.4
13	o	33	ASP	3.4
4	D	12	ARG	3.4
2	B	483	ASP	3.4
2	b	492	GLU	3.4
3	c	433	LEU	3.4
5	e	17	VAL	3.4
13	o	204	VAL	3.4
19	Z	61	VAL	3.3
13	o	207	ARG	3.3
13	o	22	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
16	v	8	LEU	3.3
13	O	132	ASN	3.3
13	o	132	ASN	3.3
5	e	84	LYS	3.3
13	o	58	ASN	3.2
13	o	134	THR	3.2
18	X	38	GLN	3.2
2	b	294	SER	3.2
13	O	89	SER	3.2
5	e	83	LEU	3.2
13	o	87	VAL	3.2
17	y	25	ILE	3.2
2	B	497	GLN	3.2
13	o	141[A]	ASP	3.2
18	x	34	ILE	3.2
5	E	83	LEU	3.1
3	C	24	THR	3.1
17	Y	21	GLN	3.1
13	o	133	VAL	3.1
6	F	14	PRO	3.1
16	v	15	GLU	3.1
7	H	64	ALA	3.1
13	o	89	SER	3.0
3	c	432	VAL	3.0
5	e	20	TRP	3.0
13	O	130	GLN	3.0
13	o	24	ASP	3.0
13	o	30	TYR	3.0
2	B	297	THR	3.0
13	o	4	THR	3.0
16	v	16	GLY	3.0
18	X	3	ILE	3.0
1	a	12	ASN	3.0
4	D	13	GLY	3.0
2	b	161	LEU	3.0
16	v	18	THR	3.0
2	B	490	GLN	3.0
16	v	12	LEU	3.0
18	x	36	LYS	3.0
5	e	61	ARG	3.0
2	b	501	ASP	3.0
2	B	502	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	a	224	ILE	2.9
5	e	32	ILE	2.9
2	b	490	GLN	2.9
4	d	240	ALA	2.9
13	O	88	ASN	2.9
2	b	491	VAL	2.9
2	b	298	LEU	2.9
13	O	22	LEU	2.9
9	J	8	ILE	2.9
9	j	3	SER	2.9
16	v	21	LEU	2.9
19	Z	42	LEU	2.9
5	e	59	GLU	2.8
3	C	253	LEU	2.8
11	l	3	PRO	2.8
13	o	245	PRO	2.8
13	o	202	ALA	2.8
3	C	207	ARG	2.8
5	E	15	THR	2.8
5	E	25	ILE	2.8
13	O	28	GLY	2.8
19	Z	35	ARG	2.8
2	b	296	ALA	2.8
7	h	57	GLY	2.8
2	B	296	ALA	2.7
5	E	20	TRP	2.7
5	e	13	ILE	2.7
13	o	243	ILE	2.7
19	Z	29	SER	2.7
19	z	57	LEU	2.7
2	B	493	TRP	2.7
13	O	61	GLN	2.7
19	z	30	PRO	2.7
14	t	29	ILE	2.7
2	b	457	VAL	2.7
19	z	43	GLY	2.7
3	c	20	SER	2.7
2	b	290	ALA	2.6
3	c	434	ALA	2.6
2	B	250	PHE	2.6
7	h	6	TRP	2.6
13	O	87	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	a	16	ARG	2.6
19	z	46	LEU	2.6
13	O	135	SER	2.6
13	O	138	THR	2.6
3	c	249	ILE	2.6
5	E	18	ARG	2.6
5	E	81	GLU	2.6
3	c	191	PRO	2.6
3	C	155	ASN	2.6
12	m	34	LYS	2.6
4	D	17	ILE	2.6
18	X	34	ILE	2.6
3	c	284	PHE	2.6
2	b	292	LEU	2.6
4	D	116	LEU	2.6
2	B	498	LYS	2.6
18	x	3	ILE	2.6
8	i	34	ARG	2.6
2	B	251	VAL	2.6
17	Y	41	VAL	2.6
19	z	34	ASP	2.6
2	B	161	LEU	2.6
1	a	14	TRP	2.6
2	B	294	SER	2.6
13	O	91	GLY	2.6
2	b	458	PHE	2.5
5	e	10	PHE	2.5
1	a	242	GLU	2.5
13	O	136	ILE	2.5
13	O	137	THR	2.5
13	o	28	GLY	2.5
3	C	257	PHE	2.5
3	c	19	ASN	2.5
3	c	285	ILE	2.5
3	c	280	SER	2.5
2	B	489	GLU	2.5
5	e	7	GLU	2.5
3	c	429	SER	2.5
19	z	32	ASP	2.5
5	e	14	ILE	2.5
9	j	12	ILE	2.5
2	b	301	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
5	E	19	TYR	2.5
16	v	26	TYR	2.5
19	z	35	ARG	2.5
18	X	31	ILE	2.5
18	x	35	ASP	2.5
2	b	29	LEU	2.5
3	c	257	PHE	2.5
2	b	297	THR	2.5
19	z	9	LEU	2.5
19	z	42	LEU	2.5
1	a	264	SER	2.5
16	v	6	GLU	2.5
2	B	253	ALA	2.4
5	e	12	ASP	2.4
16	v	10	VAL	2.4
19	z	53	VAL	2.4
2	B	247	PHE	2.4
4	d	237	PRO	2.4
13	o	91	GLY	2.4
1	a	243	GLU	2.4
13	O	62	GLU	2.4
13	O	131	PRO	2.4
5	e	8	ARG	2.4
13	O	139	SER	2.4
3	C	262	ARG	2.4
2	b	302	TRP	2.4
13	o	130	GLN	2.4
3	c	253	LEU	2.4
2	b	246	PHE	2.4
3	c	435	PHE	2.4
3	c	436	PHE	2.4
19	Z	36	SER	2.4
9	j	2	MET	2.4
13	O	141	ASP	2.3
3	C	204	LEU	2.3
9	j	10	LEU	2.3
1	A	339	PHE	2.3
3	c	181	PHE	2.3
5	E	82	GLN	2.3
2	B	488	PRO	2.3
5	e	28	PRO	2.3
2	b	245	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
6	f	15	ILE	2.3
13	o	135	SER	2.3
17	y	21	GLN	2.3
2	B	2	GLY	2.3
2	b	128	THR	2.3
13	o	206	GLY	2.3
13	o	139	SER	2.3
5	E	22	ILE	2.3
13	o	208	THR	2.3
1	a	225	ARG	2.3
5	e	9	PRO	2.3
19	Z	41	PHE	2.3
13	O	207	ARG	2.3
19	z	10	ALA	2.3
12	m	33	GLN	2.3
2	B	457	VAL	2.3
7	h	21	VAL	2.3
13	O	204	VAL	2.3
2	B	459	ALA	2.3
13	o	31	PRO	2.3
16	v	22	THR	2.3
19	z	58	ASN	2.3
10	k	11	LEU	2.3
17	y	37	PHE	2.2
13	O	21	THR	2.2
13	O	58	ASN	2.2
2	b	483	ASP	2.2
2	b	129	GLY	2.2
18	x	33	GLN	2.2
5	e	26	THR	2.2
2	B	505	ARG	2.2
9	J	7	ARG	2.2
17	y	26	ALA	2.2
3	c	431	PHE	2.2
3	C	252	ILE	2.2
3	C	255	THR	2.2
4	D	240	ALA	2.2
3	C	25	ASN	2.2
4	d	154	VAL	2.2
11	L	2	GLU	2.2
2	B	479	PHE	2.2
3	C	182	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	a	280	VAL	2.2
13	O	56	PRO	2.1
4	d	24	ARG	2.1
5	e	36	LEU	2.1
3	c	155	ASN	2.1
2	b	459	ALA	2.1
5	e	29	ALA	2.1
19	Z	5	PHE	2.1
2	B	292	LEU	2.1
3	c	438	LEU	2.1
3	c	278	ALA	2.1
5	e	11	SER	2.1
13	O	93	LEU	2.1
13	o	29	ALA	2.1
19	z	28	ALA	2.1
19	z	49	ALA	2.1
5	E	61	ARG	2.1
13	O	92	SER	2.1
1	a	15	GLU	2.1
13	O	140	THR	2.1
16	v	17	LYS	2.1
2	B	248	ALA	2.1
4	D	158	LEU	2.1
10	k	12	PRO	2.1
13	o	56	PRO	2.1
13	o	131	PRO	2.1
2	b	127	ARG	2.1
5	E	24	SER	2.1
2	B	290	ALA	2.1
2	B	298	LEU	2.1
7	h	23	PRO	2.1
19	Z	40	ILE	2.1
3	c	437	PHE	2.0
17	Y	40	ALA	2.0
3	C	181	PHE	2.0
5	e	24	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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
12	FME	m	1	10/11	0.92	0.12	31,38,54,60	0
14	FME	t	1	10/11	0.95	0.09	20,23,41,50	0
12	FME	M	1	10/11	0.96	0.11	27,34,51,59	0
4	HSK	d	336[A]	10/12	0.96	0.10	30,33,40,44	7
4	HSK	d	336[B]	11/12	0.96	0.10	30,31,37,38	8
8	FME	I	1	10/11	0.97	0.13	27,34,38,39	0
14	FME	T	1	10/11	0.97	0.08	24,27,43,50	0
8	FME	i	1	10/11	0.98	0.11	30,32,37,39	0
4	HSK	D	336[A]	10/12	0.98	0.10	26,28,31,34	7
4	HSK	D	336[B]	11/12	0.98	0.10	23,26,27,29	8

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
34	DGD	D	406	53/66	0.54	0.29	53,77,92,103	0
29	UNL	a	420	40/-	0.56	0.33	53,72,88,94	0
31	GOL	h	103	6/6	0.56	0.28	78,83,83,84	0
33	HTG	d	401	19/19	0.57	0.30	55,101,111,114	0
29	UNL	E	103	12/-	0.59	0.29	65,73,83,88	0
29	UNL	A	415	36/-	0.60	0.25	58,67,75,79	0
34	DGD	d	406	50/66	0.62	0.26	56,75,94,97	0
26	SQD	B	621	54/54	0.63	0.27	48,65,108,109	0
30	LMT	M	102	35/35	0.63	0.24	35,52,60,63	0
29	UNL	E	102	15/-	0.63	0.23	57,64,83,83	0
29	UNL	i	103	13/-	0.65	0.29	58,65,76,78	0
29	UNL	B	629	14/-	0.66	0.27	61,70,89,90	0
33	HTG	b	602	19/19	0.67	0.28	50,93,111,117	0
33	HTG	B	631	19/19	0.68	0.26	49,111,120,125	0
30	LMT	M	101	35/35	0.68	0.24	43,61,77,90	0
36	LHG	a	417	40/49	0.69	0.26	60,109,148,151	0
29	UNL	C	523	34/-	0.69	0.28	52,77,88,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	LMT	F	102	35/35	0.70	0.36	53,84,91,96	0
30	LMT	b	624	25/35	0.70	0.21	51,71,94,98	0
26	SQD	L	103	54/54	0.71	0.24	43,64,89,96	0
29	UNL	t	103	16/-	0.71	0.46	63,74,94,95	0
29	UNL	j	103	12/-	0.71	0.25	55,65,70,71	0
33	HTG	D	414	19/19	0.71	0.31	66,93,106,107	0
29	UNL	b	631	16/-	0.72	0.23	59,66,77,79	0
30	LMT	m	101	35/35	0.73	0.22	32,51,61,62	0
27	LMG	Z	101	51/55	0.73	0.27	41,76,102,113	0
27	LMG	c	921	51/55	0.74	0.27	38,80,95,111	0
33	HTG	b	627	19/19	0.74	0.34	53,94,104,105	0
30	LMT	B	623	35/35	0.74	0.24	43,79,117,129	0
29	UNL	c	925	30/-	0.74	0.18	59,72,89,95	0
33	HTG	B	626	19/19	0.74	0.42	48,87,92,93	0
29	UNL	Z	103	16/-	0.74	0.21	48,63,81,81	0
29	UNL	H	103	10/-	0.75	0.23	60,69,74,76	0
29	UNL	c	926	10/-	0.75	0.17	65,67,71,72	0
29	UNL	b	630	16/-	0.75	0.39	51,62,73,74	0
28	PL9	a	419	55/55	0.75	0.23	52,74,98,109	0
27	LMG	a	418	51/55	0.75	0.22	43,60,68,73	0
26	SQD	a	401	54/54	0.75	0.18	45,59,85,90	0
33	HTG	C	522	19/19	0.75	0.34	50,79,92,94	0
30	LMT	J	102	24/35	0.75	0.19	45,55,79,83	0
29	UNL	i	104	10/-	0.75	0.28	67,72,77,78	0
29	UNL	e	800	11/-	0.76	0.29	53,60,68,68	0
30	LMT	m	102	35/35	0.76	0.19	41,54,72,84	0
28	PL9	A	414	55/55	0.76	0.26	47,66,93,96	0
29	UNL	J	103	14/-	0.77	0.16	61,66,73,76	0
29	UNL	z	102	16/-	0.77	0.22	51,70,89,92	0
29	UNL	I	101	13/-	0.77	0.22	44,53,61,63	0
30	LMT	b	625	24/35	0.78	0.25	35,61,99,100	0
29	UNL	T	102	13/-	0.78	0.54	66,70,83,87	0
29	UNL	B	632	16/-	0.78	0.31	50,59,73,73	0
33	HTG	c	924	19/19	0.78	0.41	53,85,97,100	0
30	LMT	c	922	35/35	0.78	0.32	61,73,85,90	0
30	LMT	Z	102	35/35	0.78	0.27	41,87,102,107	0
30	LMT	t	102	24/35	0.78	0.26	33,55,94,95	0
30	LMT	z	101	32/35	0.79	0.24	46,85,90,100	0
29	UNL	i	102	16/-	0.79	0.23	54,65,83,84	0
27	LMG	A	413	51/55	0.79	0.24	42,57,76,78	0
33	HTG	U	201	9/19	0.79	0.23	54,59,82,98	0
29	UNL	D	412	40/-	0.79	0.20	39,60,96,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
29	UNL	j	102	16/-	0.80	0.17	52,61,69,69	0
31	GOL	O	304	6/6	0.80	0.17	52,60,61,63	0
29	UNL	A	417	13/-	0.81	0.35	56,59,66,66	0
26	SQD	f	102	33/54	0.81	0.21	63,73,113,114	0
31	GOL	b	635	6/6	0.81	0.14	40,43,46,48	0
26	SQD	A	418	54/54	0.81	0.19	42,59,81,86	0
32	CA	B	601	1/1	0.82	0.09	81,81,81,81	0
29	UNL	b	628	36/-	0.82	0.26	44,65,101,106	0
40	SO4	O	302	5/5	0.82	0.29	78,87,95,105	0
26	SQD	D	407	45/54	0.82	0.28	50,78,94,101	0
27	LMG	c	920	51/55	0.82	0.23	30,65,100,104	0
36	LHG	E	101	49/49	0.82	0.21	50,80,94,97	0
30	LMT	C	520	35/35	0.83	0.31	52,71,83,89	0
29	UNL	B	627	16/-	0.83	0.14	43,47,69,69	0
33	HTG	u	201	14/19	0.83	0.25	46,64,90,96	0
30	LMT	a	402	35/35	0.84	0.17	37,54,69,80	0
29	UNL	I	102	11/-	0.84	0.22	62,65,66,68	0
33	HTG	B	630	19/19	0.84	0.15	39,52,66,79	0
31	GOL	a	424	6/6	0.85	0.20	42,56,59,74	0
29	UNL	M	103	16/-	0.85	0.23	49,58,77,79	0
33	HTG	c	923	19/19	0.85	0.24	64,75,82,83	0
31	GOL	c	927	6/6	0.86	0.13	43,53,60,68	0
29	UNL	J	104	12/-	0.86	0.17	53,65,72,74	0
29	UNL	d	411	16/-	0.86	0.32	39,49,63,66	0
29	UNL	B	628	10/-	0.86	0.27	52,56,70,74	0
27	LMG	C	519	51/55	0.86	0.19	29,59,97,105	0
31	GOL	b	636	6/6	0.87	0.12	45,56,58,60	0
30	LMT	A	419	35/35	0.87	0.15	37,56,73,94	0
33	HTG	b	601	19/19	0.87	0.15	43,51,62,68	0
27	LMG	B	622	51/55	0.87	0.18	28,37,53,63	0
34	DGD	h	102	62/66	0.88	0.18	27,35,45,52	0
38	RRX	h	101	41/41	0.88	0.12	27,35,49,54	0
27	LMG	b	623	51/55	0.88	0.19	30,39,52,63	0
38	RRX	H	101	41/41	0.88	0.14	25,30,44,47	0
23	CLA	B	610	65/65	0.88	0.13	23,28,33,35	0
23	CLA	b	612	65/65	0.89	0.13	26,30,36,38	0
31	GOL	C	526	6/6	0.89	0.14	38,43,51,57	0
29	UNL	a	421	10/-	0.89	0.29	53,57,61,64	0
25	BCR	k	102	40/40	0.89	0.13	29,41,48,50	0
31	GOL	A	422	6/6	0.89	0.13	42,55,58,67	0
31	GOL	l	102	6/6	0.89	0.38	37,55,57,57	0
29	UNL	b	629	16/-	0.89	0.11	43,48,56,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
29	UNL	L	102	14/-	0.89	0.22	52,58,66,69	0
29	UNL	D	413	16/-	0.89	0.26	39,47,65,65	0
23	CLA	C	506	65/65	0.90	0.13	25,38,94,97	0
23	CLA	c	914	65/65	0.90	0.15	38,53,90,98	0
32	CA	b	603	1/1	0.90	0.09	82,82,82,82	0
29	UNL	A	416	16/-	0.90	0.14	41,46,73,73	0
31	GOL	L	104	6/6	0.91	0.26	44,52,54,55	0
26	SQD	a	416	54/54	0.91	0.17	37,55,88,90	0
34	DGD	H	102	62/66	0.91	0.20	24,31,40,45	0
31	GOL	f	104	6/6	0.91	0.33	46,51,51,54	0
29	UNL	X	101	16/-	0.91	0.12	34,39,58,60	0
31	GOL	C	524	6/6	0.91	0.17	36,45,47,53	0
29	UNL	x	101	16/-	0.91	0.15	36,45,70,73	0
34	DGD	c	919	62/66	0.91	0.14	25,35,60,71	0
34	DGD	c	918	62/66	0.92	0.15	27,35,79,91	0
23	CLA	B	603	65/65	0.92	0.14	23,26,34,37	0
33	HTG	V	202	13/19	0.92	0.26	43,48,76,84	0
27	LMG	d	410	51/55	0.92	0.12	29,36,80,91	0
29	UNL	a	403	6/-	0.92	0.42	57,62,66,66	0
25	BCR	c	915	40/40	0.92	0.10	44,51,59,60	0
23	CLA	B	602	65/65	0.92	0.18	29,41,78,95	0
33	HTG	C	521	19/19	0.92	0.18	56,63,76,80	0
29	UNL	i	101	16/-	0.92	0.13	40,46,56,62	0
23	CLA	b	609	65/65	0.92	0.11	23,31,57,63	0
36	LHG	l	101	49/49	0.92	0.17	22,31,47,57	0
31	GOL	B	638	6/6	0.93	0.10	35,47,49,53	0
23	CLA	C	513	65/65	0.93	0.13	35,46,78,83	0
27	LMG	D	411	51/55	0.93	0.17	23,35,91,99	0
23	CLA	b	604	65/65	0.93	0.16	34,47,73,81	0
31	GOL	B	637	6/6	0.93	0.13	36,38,45,54	0
23	CLA	b	605	65/65	0.93	0.12	24,29,36,39	0
23	CLA	c	913	65/65	0.93	0.12	33,45,67,72	0
29	UNL	A	420	4/-	0.93	0.54	64,66,66,66	0
31	GOL	b	633	6/6	0.93	0.23	41,46,49,52	0
34	DGD	C	517	62/66	0.94	0.14	22,31,78,92	0
23	CLA	C	512	65/65	0.94	0.10	34,41,69,74	0
36	LHG	D	408	49/49	0.94	0.16	26,35,45,45	0
25	BCR	k	101	40/40	0.94	0.09	33,39,47,49	0
23	CLA	c	902	65/65	0.94	0.13	27,34,46,50	0
34	DGD	c	917	62/66	0.94	0.16	24,33,77,80	0
36	LHG	L	101	49/49	0.94	0.14	22,31,44,49	0
31	GOL	B	635	6/6	0.94	0.12	38,47,49,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	LHG	d	407	49/49	0.94	0.23	27,36,46,49	0
33	HTG	B	625	19/19	0.94	0.15	31,38,71,75	0
23	CLA	c	907	65/65	0.94	0.09	28,36,76,80	0
34	DGD	C	516	62/66	0.94	0.20	22,32,85,87	0
31	GOL	c	928	6/6	0.94	0.22	42,51,54,54	0
25	BCR	d	404	40/40	0.94	0.10	25,33,56,58	0
23	CLA	c	905	65/65	0.94	0.18	24,31,64,66	0
26	SQD	A	412	54/54	0.94	0.14	35,54,71,74	0
23	CLA	B	607	65/65	0.94	0.10	21,27,55,61	0
23	CLA	c	904	65/65	0.94	0.15	24,37,42,42	0
31	GOL	a	422	6/6	0.94	0.10	30,38,44,45	0
25	BCR	c	916	40/40	0.94	0.10	28,36,45,47	0
23	CLA	c	908	65/65	0.94	0.12	26,32,52,55	0
25	BCR	B	620	40/40	0.95	0.09	22,31,41,44	0
25	BCR	C	514	40/40	0.95	0.07	33,42,46,46	0
25	BCR	K	101	40/40	0.95	0.10	30,35,40,43	0
31	GOL	v	203	6/6	0.95	0.15	31,35,41,43	0
25	BCR	B	619	40/40	0.95	0.19	19,26,42,45	0
25	BCR	b	622	40/40	0.95	0.10	25,33,43,45	0
23	CLA	C	511	65/65	0.95	0.09	27,34,40,42	0
36	LHG	d	408	49/49	0.95	0.14	22,27,42,47	0
32	CA	o	301	1/1	0.95	0.11	51,51,51,51	0
31	GOL	V	203	6/6	0.95	0.15	26,32,36,38	0
25	BCR	t	101	40/40	0.95	0.14	23,30,42,44	0
28	PL9	d	405	55/55	0.95	0.16	19,25,30,34	0
31	GOL	V	204	6/6	0.95	0.26	39,52,59,59	0
32	CA	O	301	1/1	0.95	0.14	49,49,49,49	0
31	GOL	v	204	6/6	0.95	0.25	46,50,61,62	0
23	CLA	c	903	65/65	0.95	0.19	22,29,42,55	0
31	GOL	b	632	6/6	0.95	0.11	35,42,46,47	0
31	GOL	B	636	6/6	0.95	0.14	33,43,47,56	0
23	CLA	b	618	65/65	0.95	0.08	24,30,49,53	0
23	CLA	c	912	65/65	0.95	0.09	29,37,45,50	0
31	GOL	B	633	6/6	0.95	0.13	34,39,47,52	0
23	CLA	C	507	65/65	0.95	0.10	26,33,56,61	0
31	GOL	c	930	6/6	0.95	0.21	49,54,57,59	0
31	GOL	a	423	6/6	0.96	0.14	33,34,35,45	0
36	LHG	d	409	49/49	0.96	0.16	27,32,85,91	0
31	GOL	A	421	6/6	0.96	0.13	30,37,38,41	0
23	CLA	b	613	65/65	0.96	0.13	24,28,35,40	0
23	CLA	C	503	65/65	0.96	0.12	26,31,38,39	0
23	CLA	C	510	65/65	0.96	0.15	22,28,38,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	LHG	D	409	49/49	0.96	0.12	22,28,40,44	0
23	CLA	b	607	65/65	0.96	0.16	20,25,54,59	0
25	BCR	a	415	40/40	0.96	0.07	21,25,30,31	0
25	BCR	T	101	40/40	0.96	0.16	24,32,47,53	0
23	CLA	c	906	65/65	0.96	0.10	26,31,46,50	0
23	CLA	B	611	65/65	0.96	0.14	19,25,34,39	0
23	CLA	D	402	65/65	0.96	0.11	13,18,36,39	0
33	HTG	B	624	19/19	0.96	0.09	27,33,41,51	0
23	CLA	C	509	65/65	0.96	0.13	27,31,47,51	0
32	CA	c	901	1/1	0.96	0.07	46,46,46,46	0
23	CLA	B	612	65/65	0.96	0.13	18,21,34,37	0
23	CLA	B	617	65/65	0.96	0.10	20,28,79,83	0
25	BCR	D	404	40/40	0.96	0.16	24,29,55,57	0
25	BCR	b	621	40/40	0.96	0.20	21,28,43,46	0
31	GOL	B	634	6/6	0.96	0.10	29,29,34,37	0
31	GOL	D	415	6/6	0.96	0.20	35,36,42,46	0
33	HTG	b	626	19/19	0.96	0.17	29,40,73,75	0
35	BCT	a	408	4/4	0.96	0.09	30,32,37,46	0
23	CLA	b	619	65/65	0.96	0.12	25,32,89,97	0
23	CLA	C	505	65/65	0.96	0.14	26,31,47,51	0
23	CLA	B	615	65/65	0.96	0.11	19,24,67,74	0
23	CLA	C	501	65/65	0.96	0.14	25,32,46,53	0
23	CLA	b	606	65/65	0.96	0.12	20,26,37,42	0
23	CLA	b	615	65/65	0.96	0.14	19,27,33,38	0
23	CLA	C	504	65/65	0.96	0.15	23,28,62,68	0
23	CLA	C	508	65/65	0.96	0.14	24,29,73,81	0
23	CLA	b	617	65/65	0.96	0.14	20,25,71,83	0
32	CA	F	103	1/1	0.96	0.15	55,55,55,55	0
34	DGD	C	518	62/66	0.96	0.15	20,30,68,75	0
25	BCR	C	515	40/40	0.96	0.14	28,34,41,44	0
31	GOL	v	202	6/6	0.96	0.10	35,36,40,41	0
23	CLA	A	410	65/65	0.96	0.11	20,24,99,105	0
31	GOL	b	634	6/6	0.96	0.12	32,39,44,46	0
23	CLA	D	403	65/65	0.96	0.11	22,28,73,79	0
25	BCR	K	102	40/40	0.96	0.08	28,31,39,42	0
25	BCR	B	618	40/40	0.96	0.15	20,26,29,30	0
23	CLA	c	910	65/65	0.97	0.18	25,31,49,52	0
23	CLA	B	613	65/65	0.97	0.14	19,24,31,34	0
23	CLA	B	608	65/65	0.97	0.14	17,20,34,37	0
23	CLA	C	502	65/65	0.97	0.14	21,26,39,48	0
23	CLA	A	405	65/65	0.97	0.10	14,19,25,42	0
31	GOL	V	205	6/6	0.97	0.23	33,36,37,41	0

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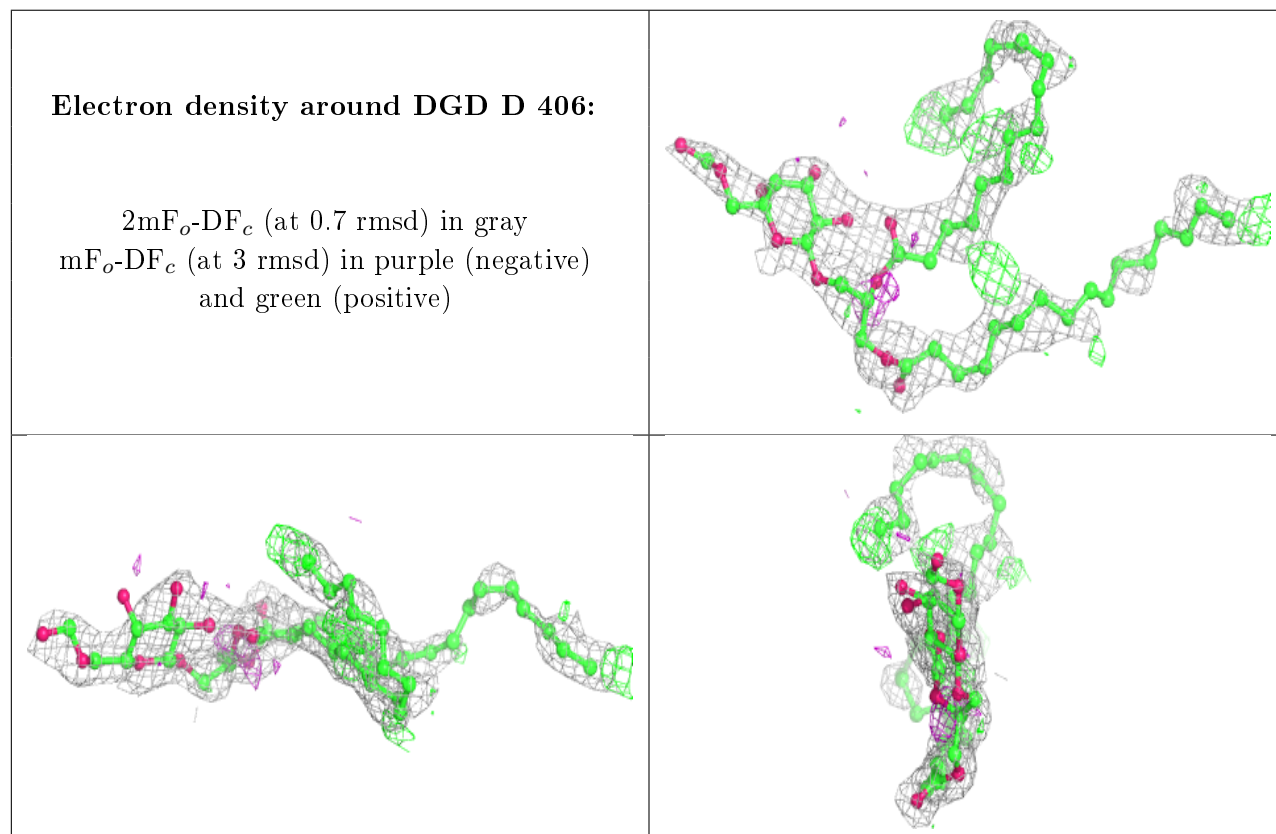
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	CA	f	103	1/1	0.97	0.18	56,56,56,56	0
25	BCR	b	620	40/40	0.97	0.16	23,27,33,33	0
33	HTG	O	303	19/19	0.97	0.09	27,32,50,52	0
23	CLA	b	614	65/65	0.97	0.17	20,24,36,45	0
37	HEM	F	101	43/43	0.97	0.12	36,42,49,52	0
23	CLA	A	407	65/65	0.97	0.16	18,21,80,92	0
23	CLA	b	610	65/65	0.97	0.15	18,23,32,35	0
23	CLA	a	414	65/65	0.97	0.09	19,25,99,104	0
23	CLA	B	605	65/65	0.97	0.18	19,22,53,55	0
23	CLA	d	403	65/65	0.97	0.08	25,32,83,90	0
23	CLA	B	609	65/65	0.97	0.16	18,24,31,34	0
23	CLA	A	406	65/65	0.97	0.09	13,18,29,39	0
23	CLA	B	606	65/65	0.97	0.15	17,23,35,40	0
24	PHO	a	413	64/64	0.97	0.13	19,25,30,35	0
23	CLA	B	604	65/65	0.97	0.14	17,22,34,41	0
23	CLA	B	616	65/65	0.97	0.10	23,28,48,50	0
28	PL9	D	405	55/55	0.97	0.10	18,23,31,38	0
36	LHG	D	410	46/49	0.97	0.14	24,32,82,87	0
23	CLA	c	911	65/65	0.97	0.22	24,30,41,45	0
23	CLA	c	909	65/65	0.97	0.18	25,30,82,98	0
24	PHO	A	409	64/64	0.97	0.14	19,22,29,37	0
25	BCR	A	411	40/40	0.97	0.12	21,26,33,36	0
23	CLA	B	614	65/65	0.97	0.17	18,23,48,54	0
23	CLA	d	402	65/65	0.98	0.12	18,21,39,44	0
37	HEM	f	101	43/43	0.98	0.19	39,47,61,77	0
35	BCT	D	401	4/4	0.98	0.08	32,35,41,51	0
31	GOL	C	525	6/6	0.98	0.15	26,26,27,29	0
23	CLA	b	611	65/65	0.98	0.18	22,27,39,43	0
23	CLA	b	608	65/65	0.98	0.11	20,24,33,34	0
24	PHO	A	408	64/64	0.98	0.11	16,21,25,27	0
37	HEM	v	201	43/43	0.98	0.08	25,31,35,38	0
23	CLA	a	409	65/65	0.98	0.12	18,21,31,43	0
23	CLA	a	410	65/65	0.98	0.13	17,20,28,34	0
24	PHO	a	412	64/64	0.98	0.12	17,22,26,27	0
23	CLA	b	616	65/65	0.98	0.20	20,24,46,50	0
23	CLA	a	411	65/65	0.98	0.14	18,23,106,117	0
31	GOL	A	423	6/6	0.98	0.25	39,43,45,53	0
39	MG	j	101	1/1	0.99	0.17	35,35,35,35	0
21	FE2	a	405	1/1	0.99	0.06	27,27,27,27	0
22	CL	a	407	1/1	0.99	0.12	27,27,27,27	0
22	CL	A	403	1/1	0.99	0.06	25,25,25,25	0
22	CL	A	404	1/1	0.99	0.13	22,22,22,22	0

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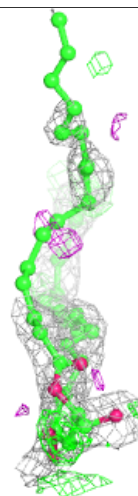
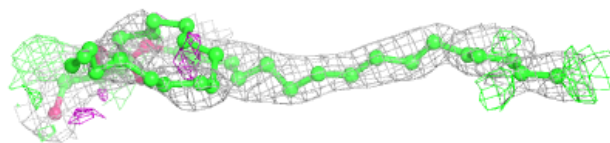
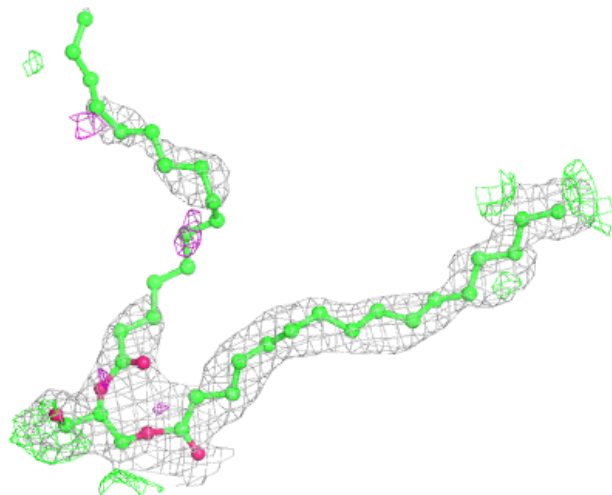
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
39	MG	J	101	1/1	0.99	0.09	28,28,28,28	0
37	HEM	V	201	43/43	0.99	0.07	22,24,28,33	0
31	GOL	c	929	6/6	0.99	0.15	25,27,30,30	0
22	CL	a	406	1/1	1.00	0.04	29,29,29,29	0
20	OEX	A	401	10/10	1.00	0.07	21,23,27,28	0
20	OEX	a	404	10/10	1.00	0.07	22,26,28,29	0
21	FE2	A	402	1/1	1.00	0.05	26,26,26,26	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.



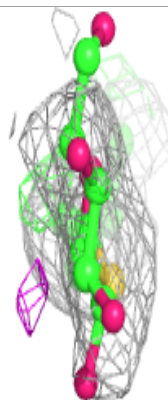
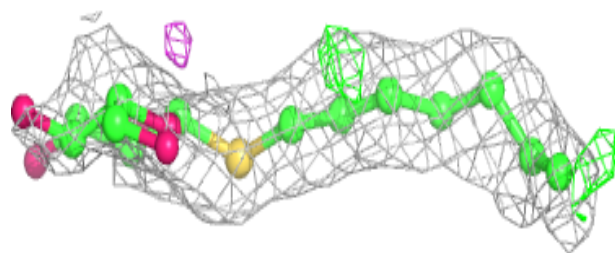
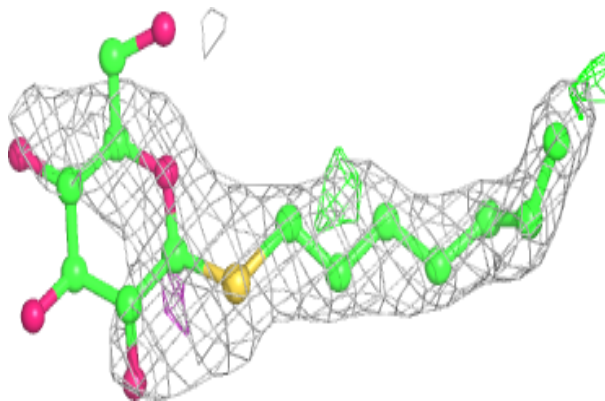
Electron density around UNL a 420:

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

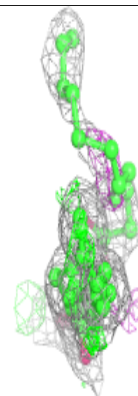
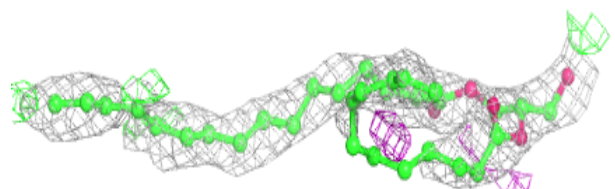
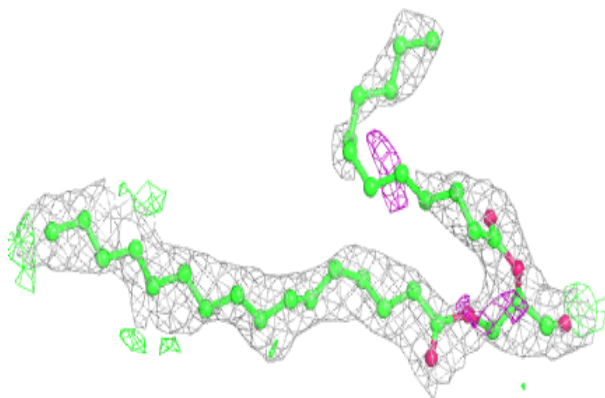


Electron density around HTG d 401:

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

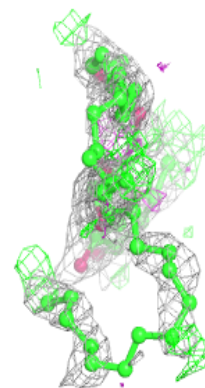
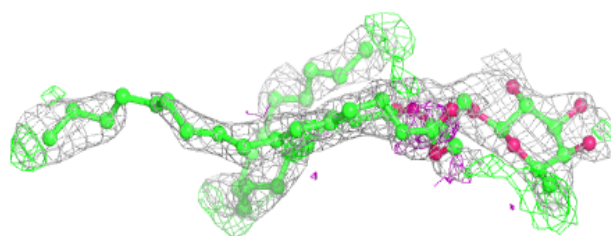
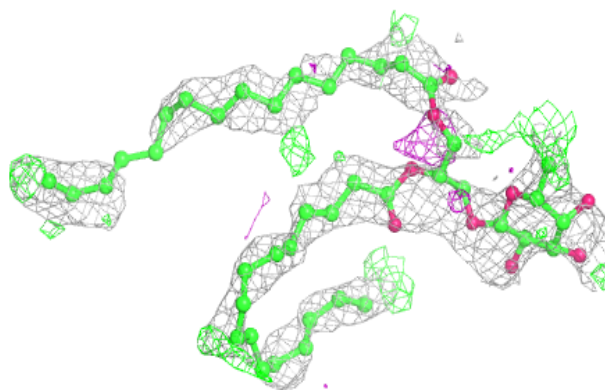
**Electron density around UNL A 415:**

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

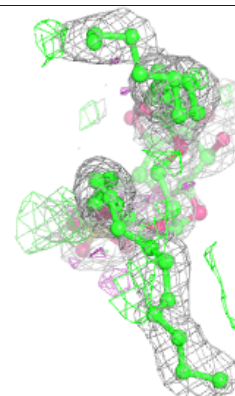
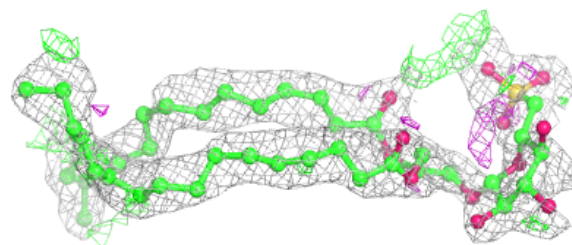
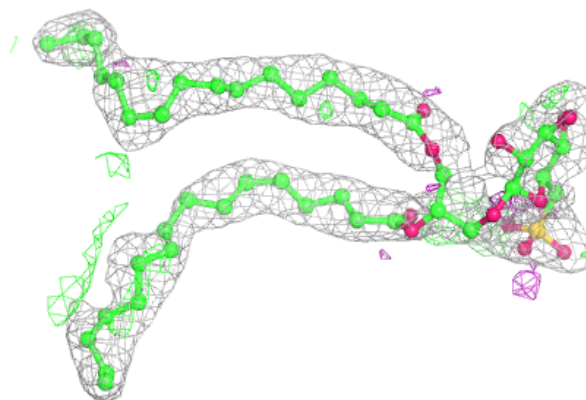


Electron density around DGD d 406:

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

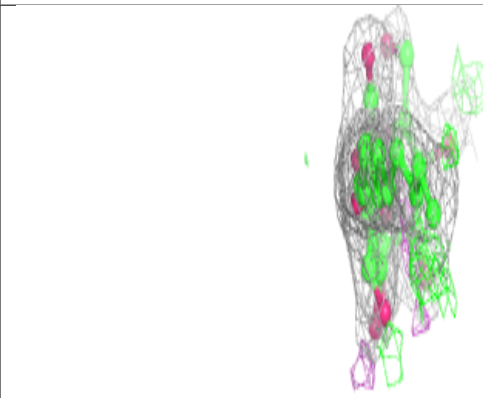
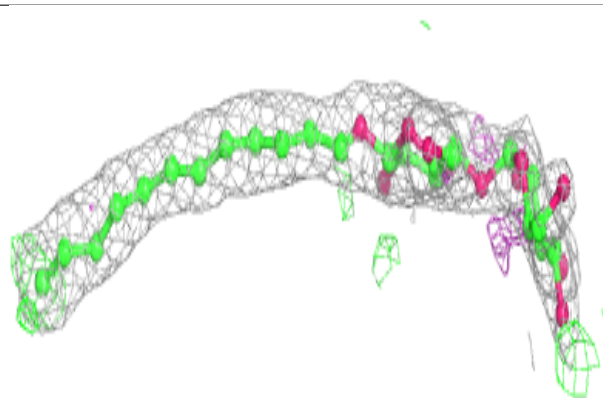
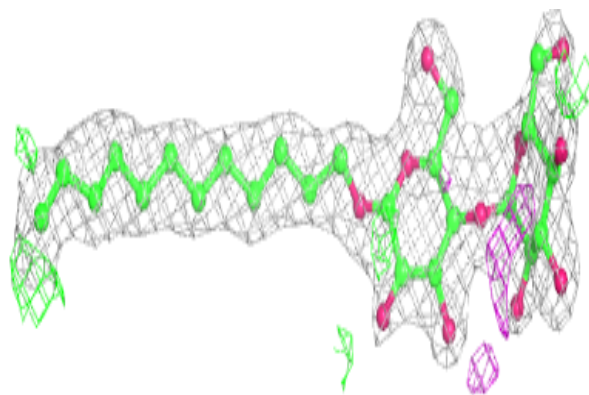
**Electron density around SQD B 621:**

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

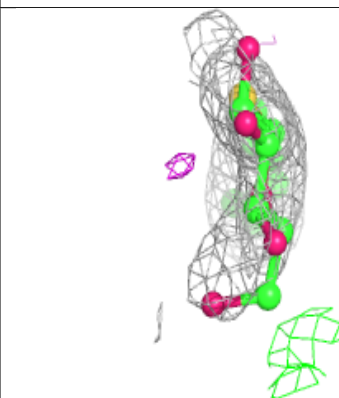
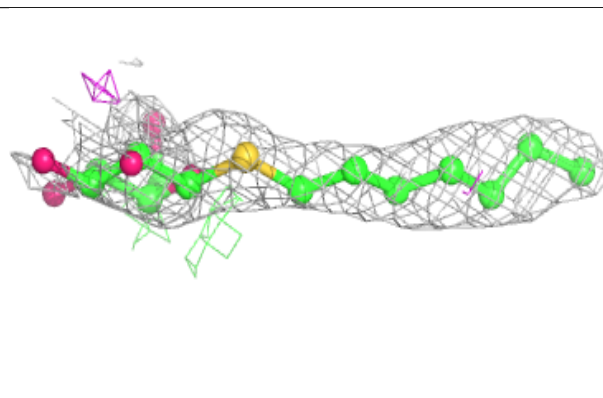
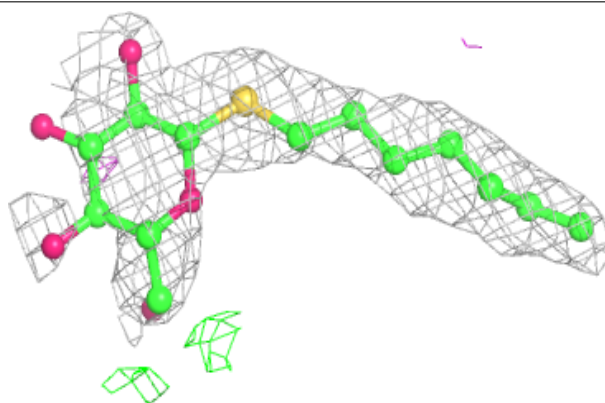


Electron density around LMT M 102:

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

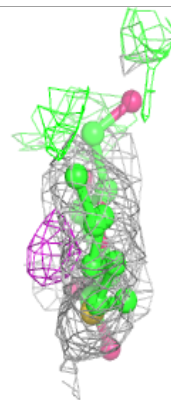
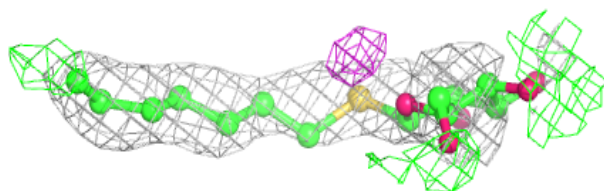
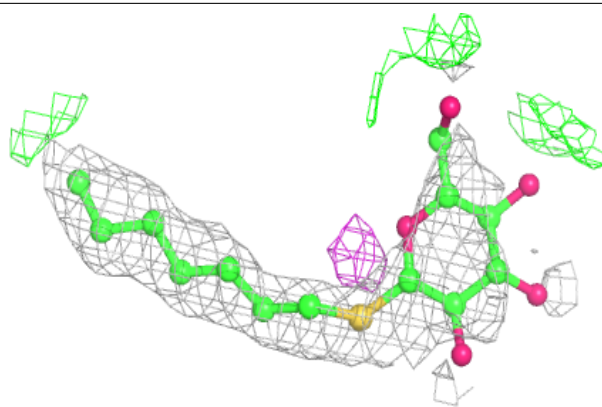
**Electron density around HTG b 602:**

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

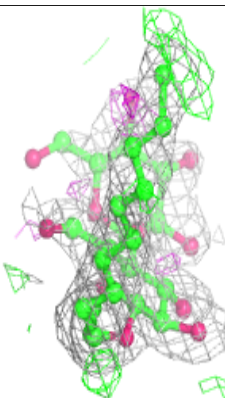
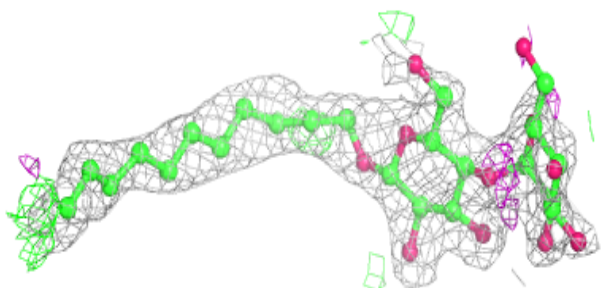
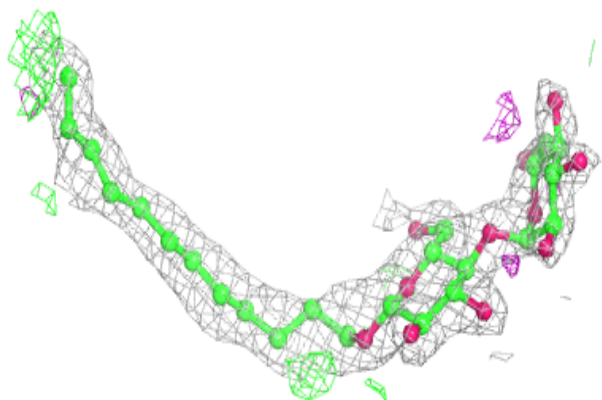


Electron density around HTG B 631:

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

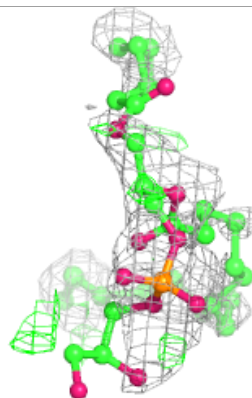
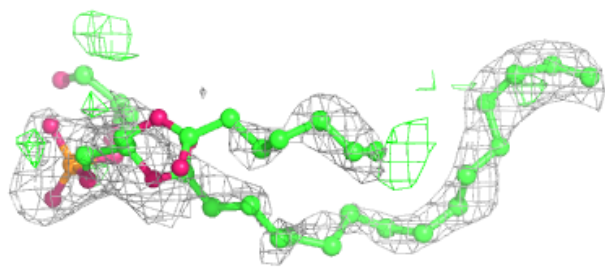
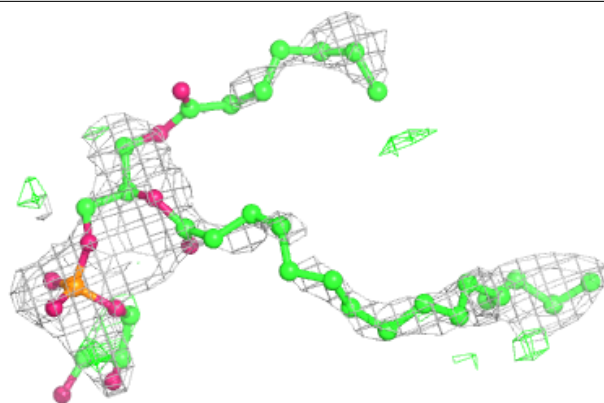
**Electron density around LMT M 101:**

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

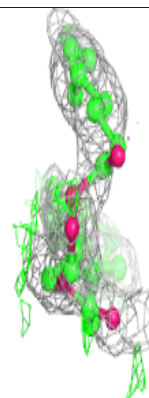
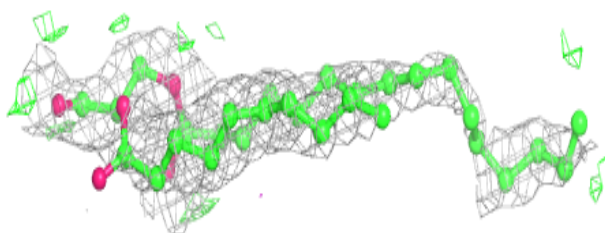
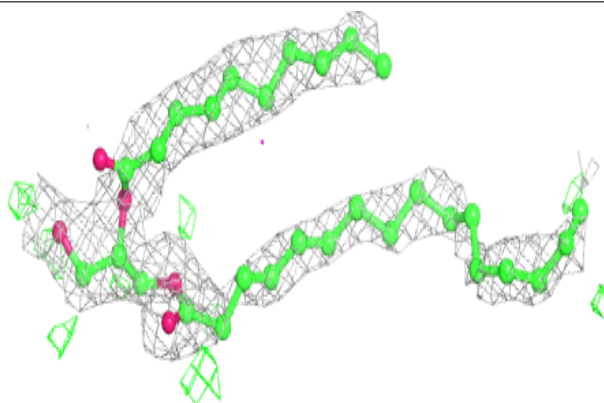


Electron density around LHG a 417:

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

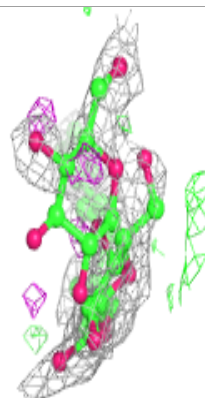
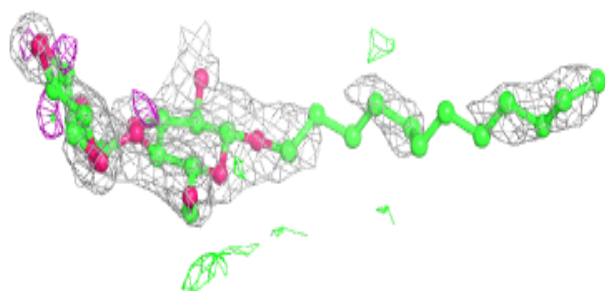
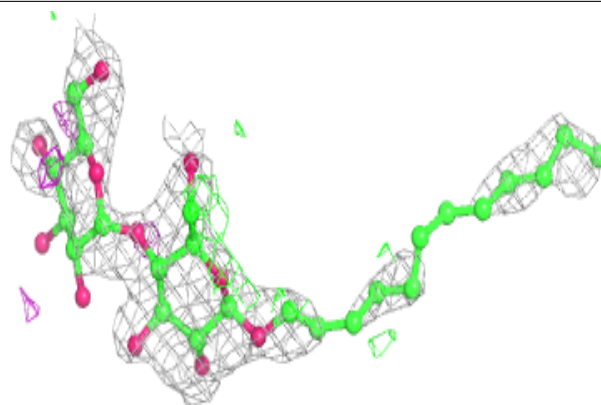
**Electron density around UNL C 523:**

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

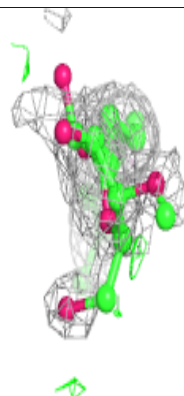
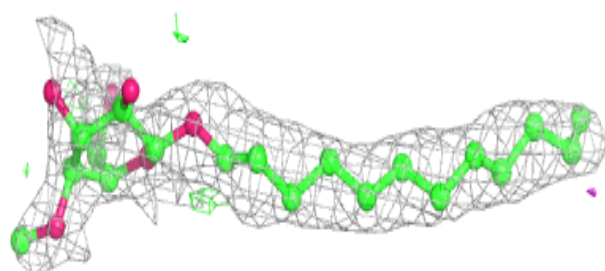
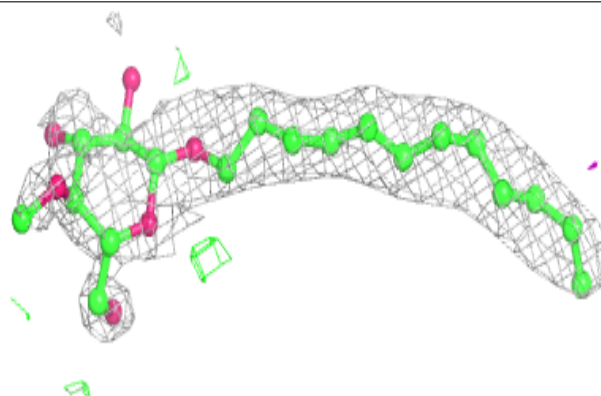


Electron density around LMT F 102:

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

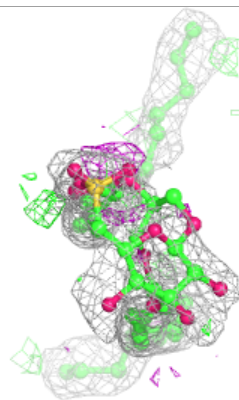
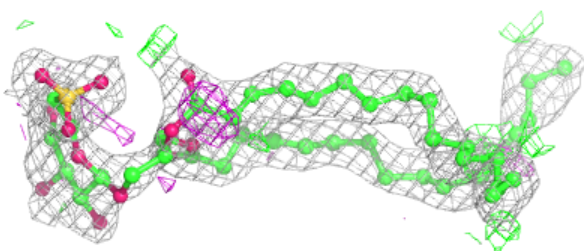
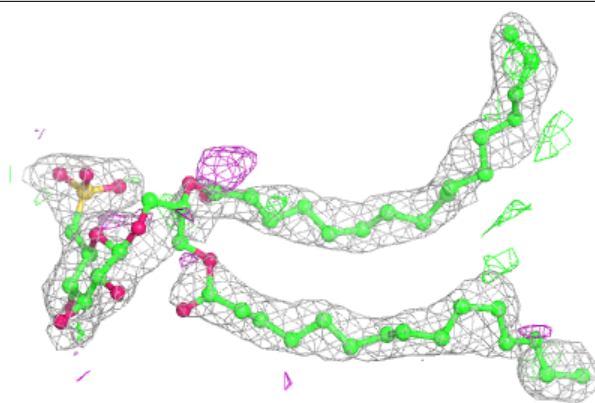
**Electron density around LMT b 624:**

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

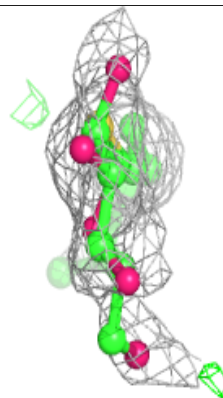
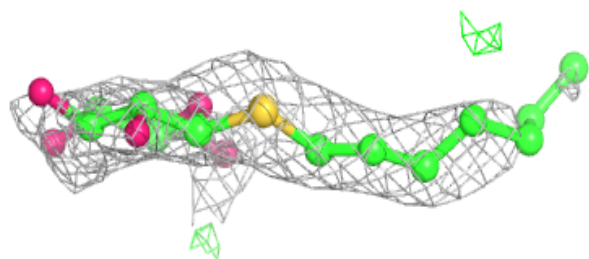
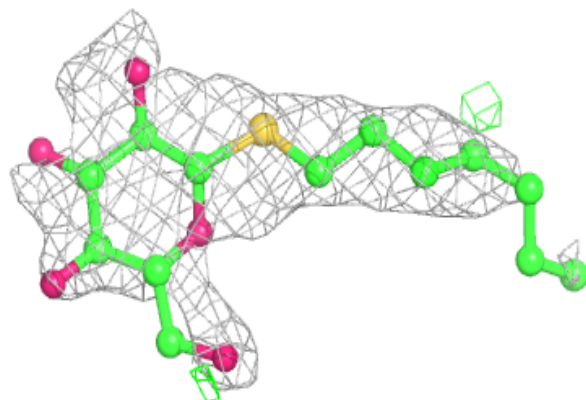


Electron density around SQD L 103:

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

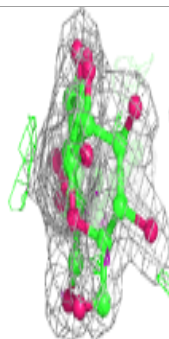
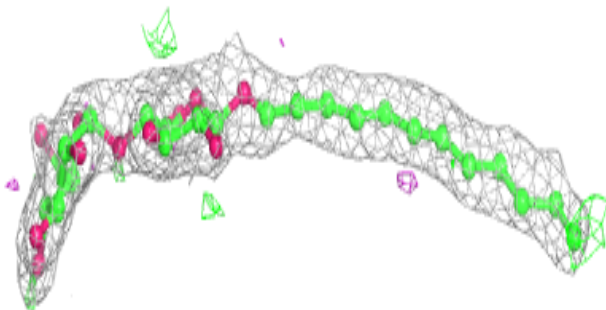
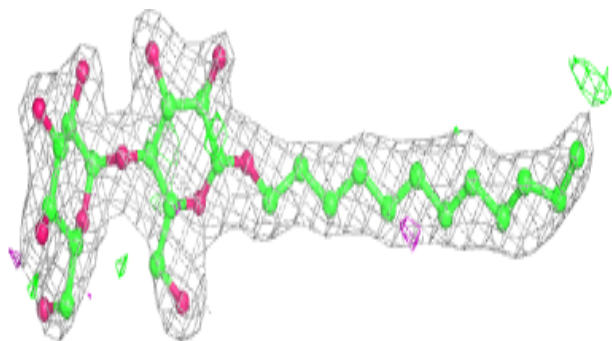
**Electron density around HTG D 414:**

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

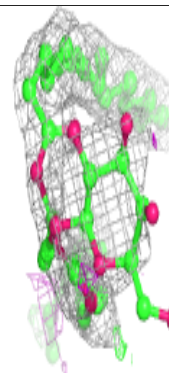
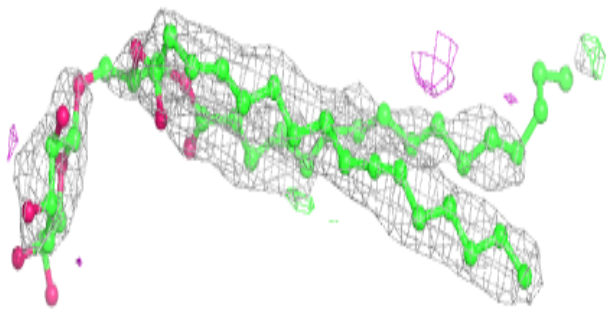
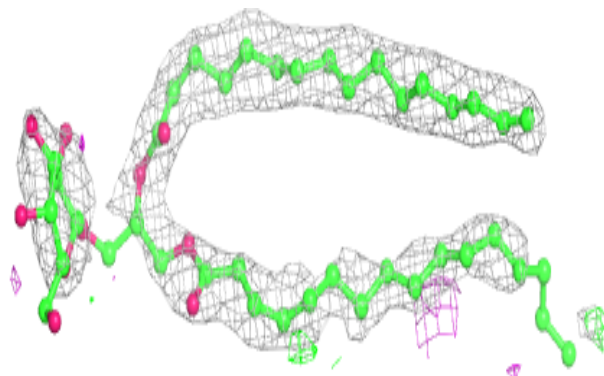


Electron density around LMT m 101:

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

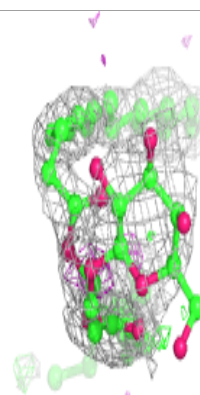
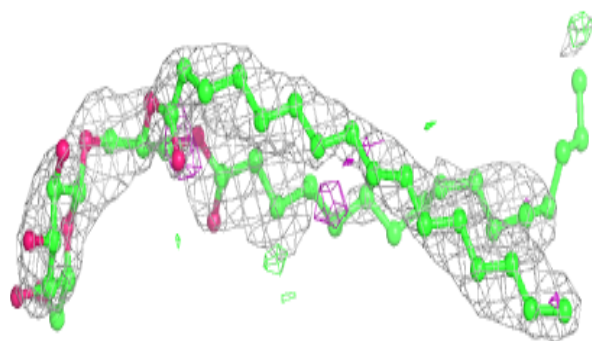
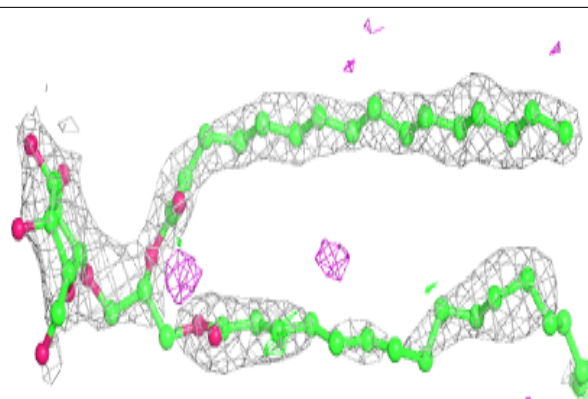
**Electron density around LMG Z 101:**

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

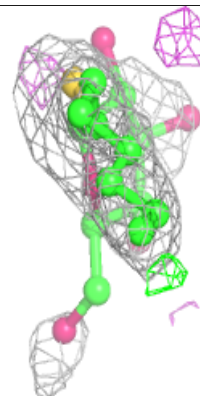
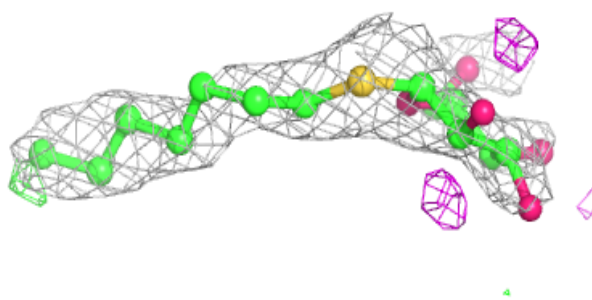
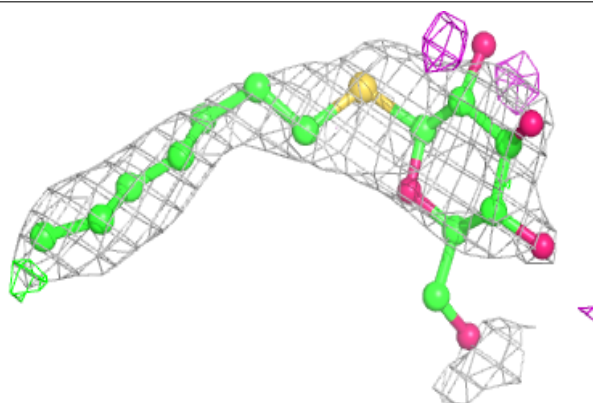


Electron density around LMG c 921:

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

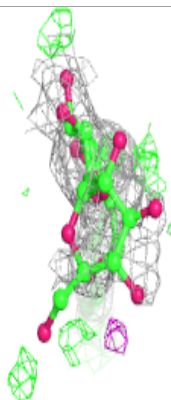
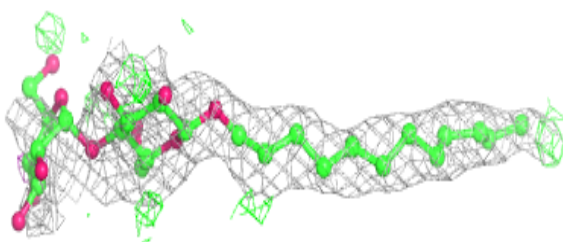
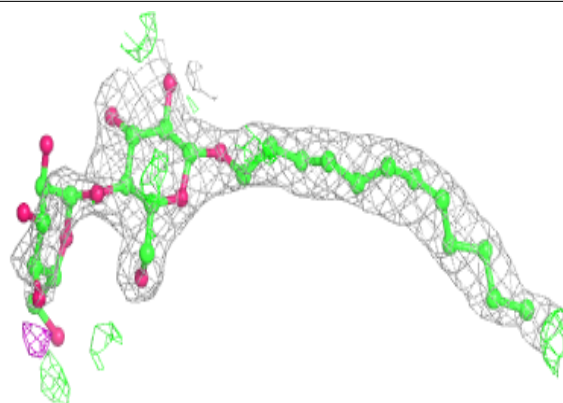
**Electron density around HTG b 627:**

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

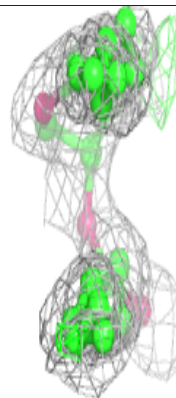
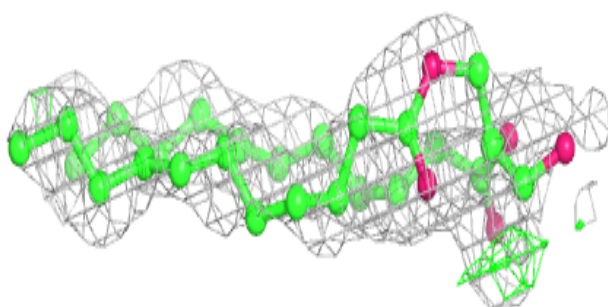
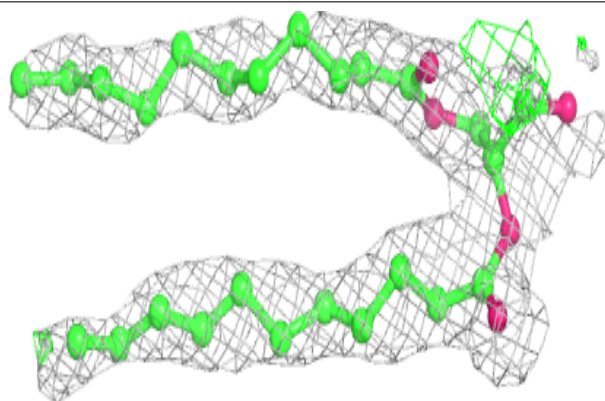


Electron density around LMT B 623:

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

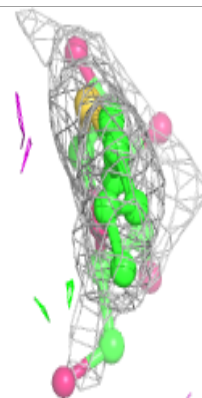
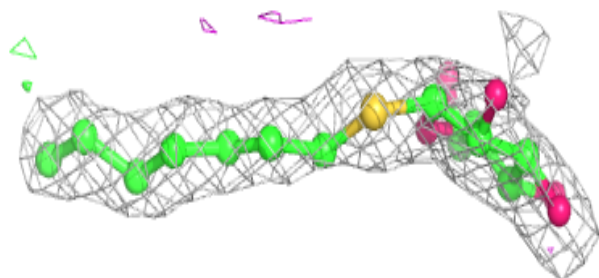
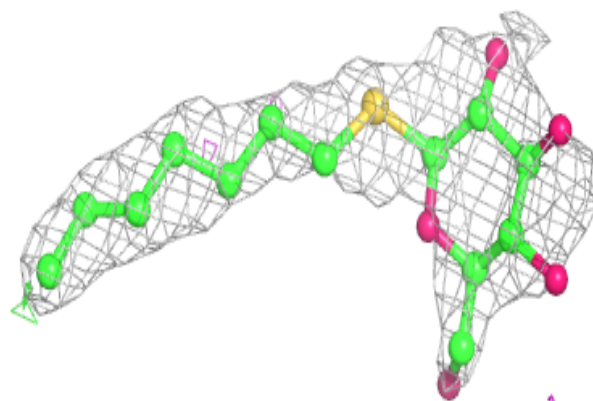
**Electron density around UNL c 925:**

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

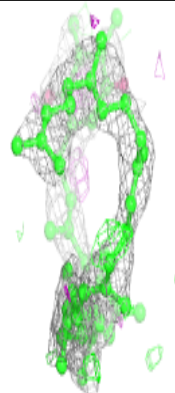
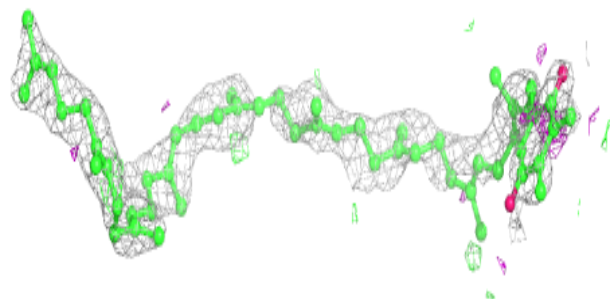
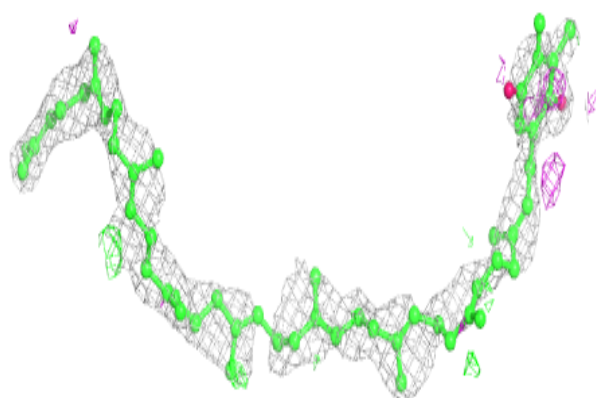


Electron density around HTG B 626:

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

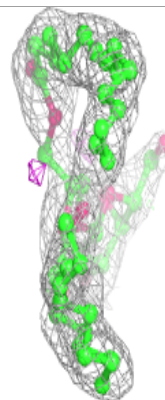
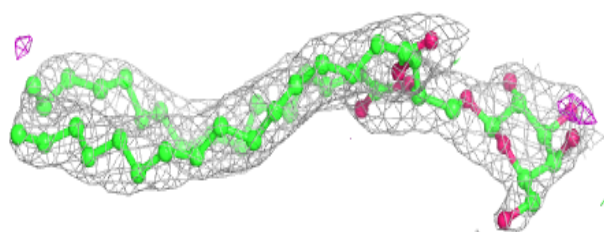
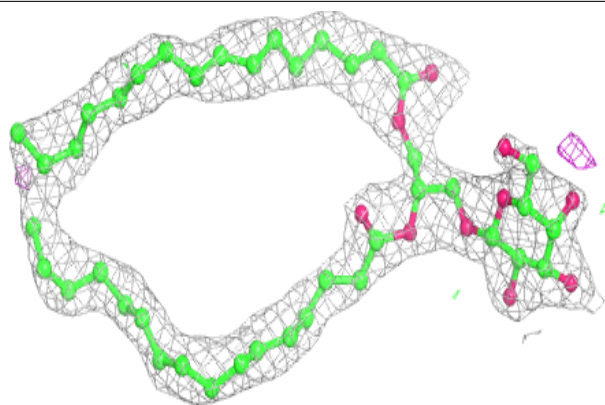
**Electron density around PL9 a 419:**

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

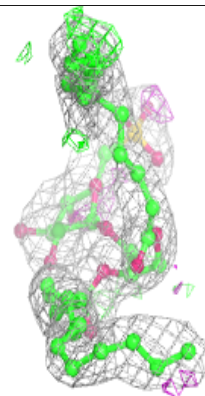
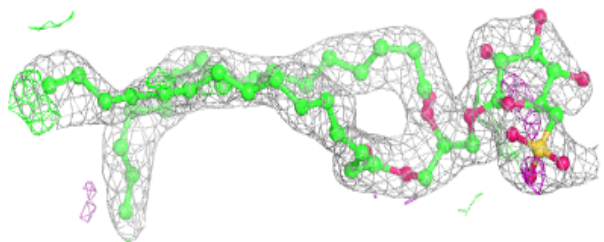
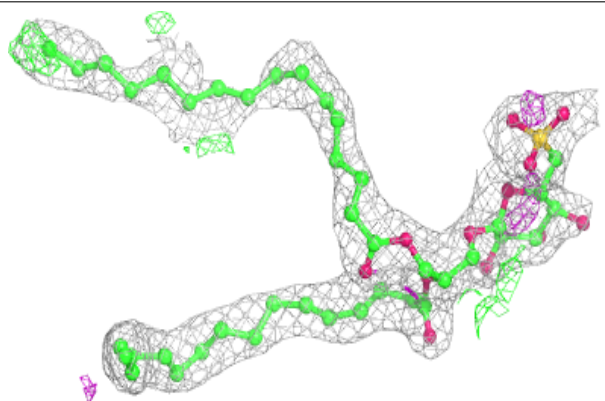


Electron density around LMG a 418:

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

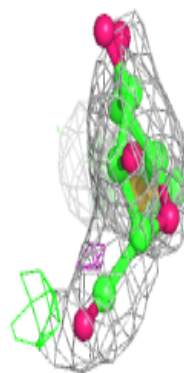
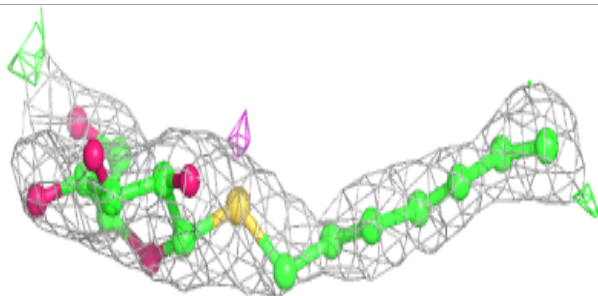
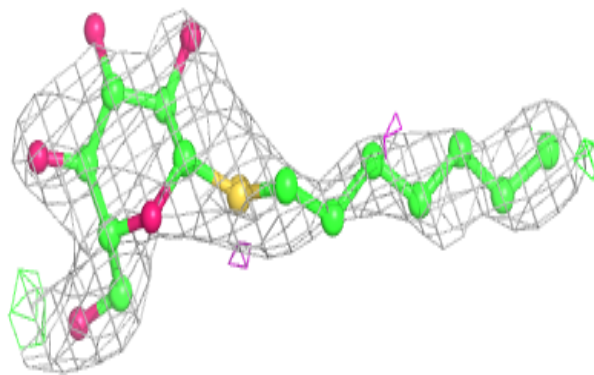
**Electron density around SQD a 401:**

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

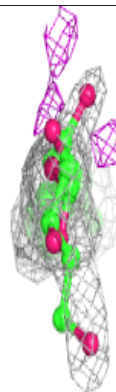
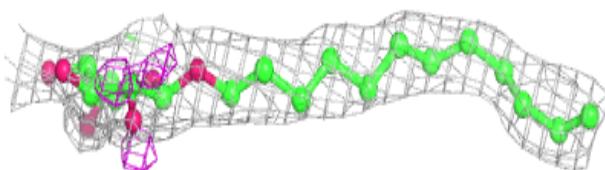
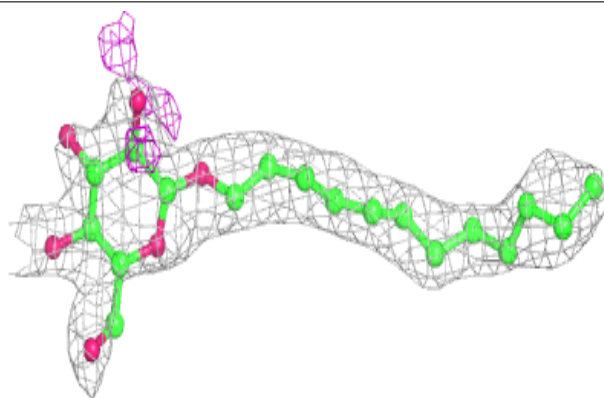


Electron density around HTG C 522:

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

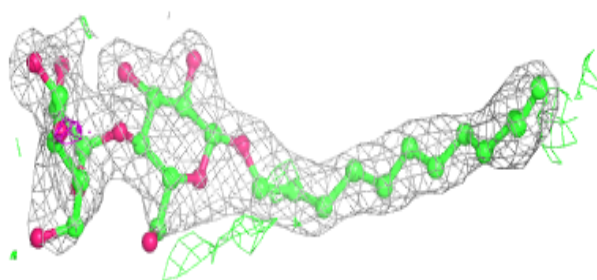
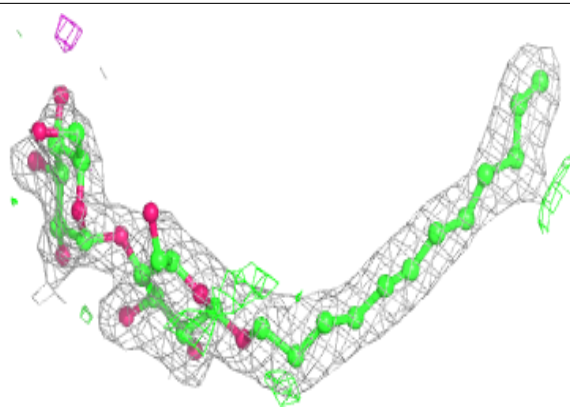
**Electron density around LMT J 102:**

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

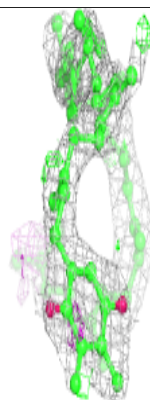
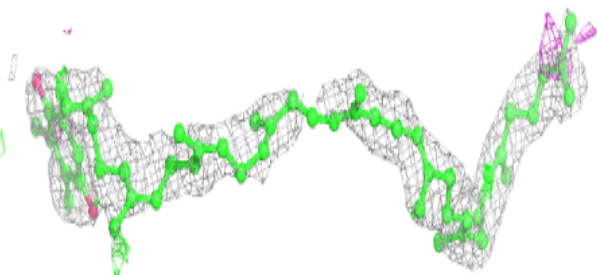
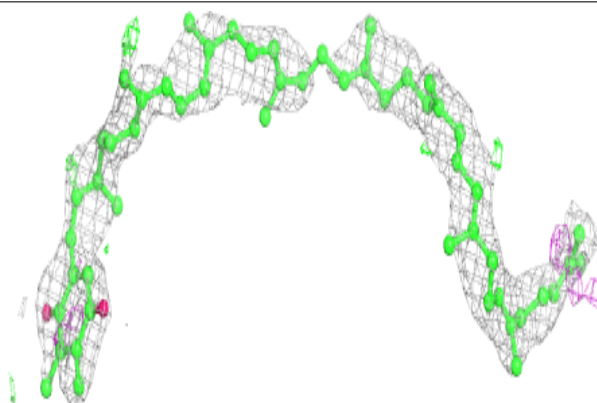


Electron density around LMT m 102:

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

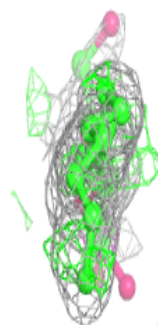
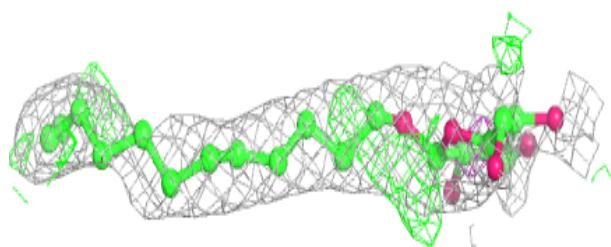
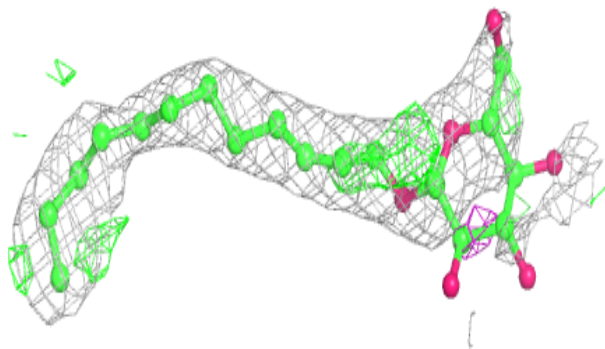
**Electron density around PL9 A 414:**

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

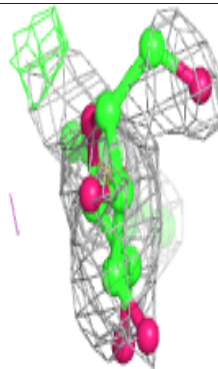
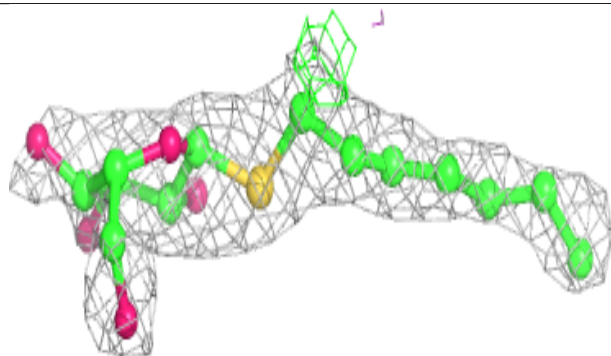
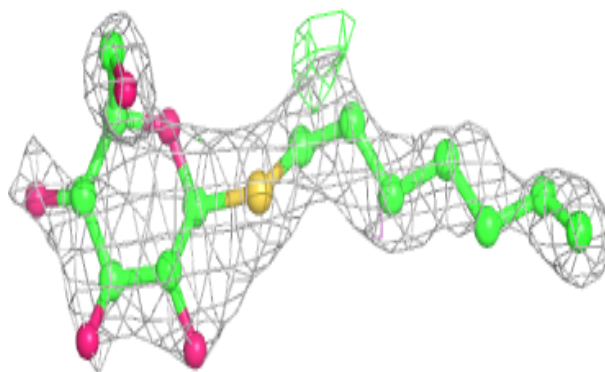


Electron density around LMT b 625:

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

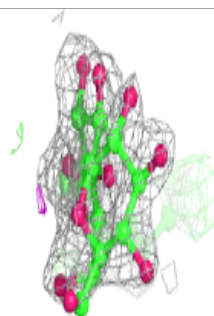
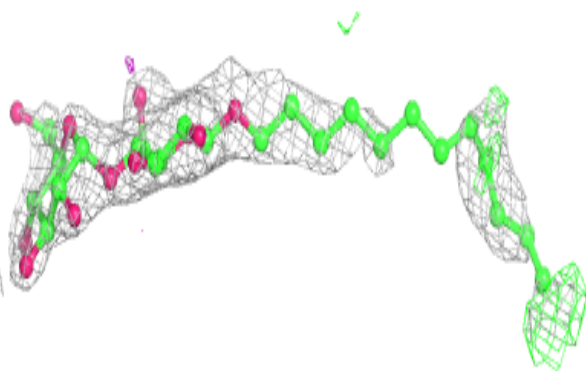
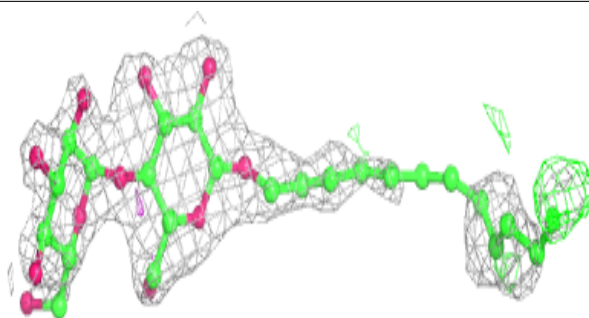
**Electron density around HTG c 924:**

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

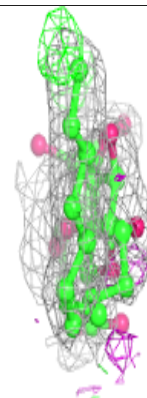
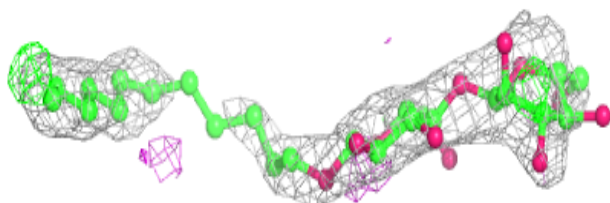
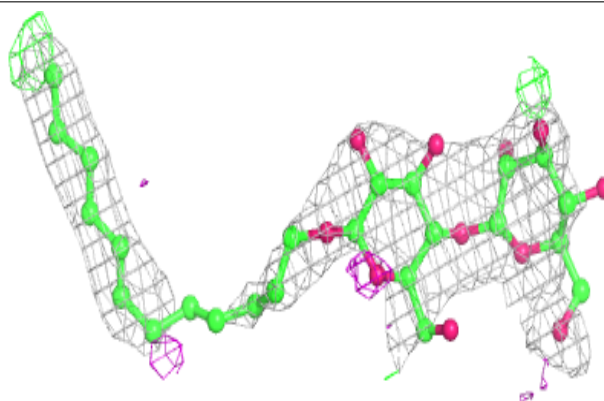


Electron density around LMT c 922:

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

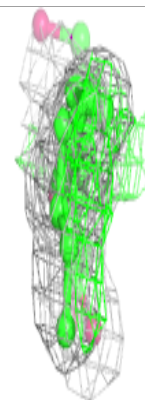
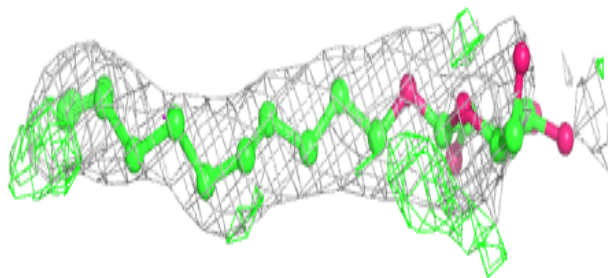
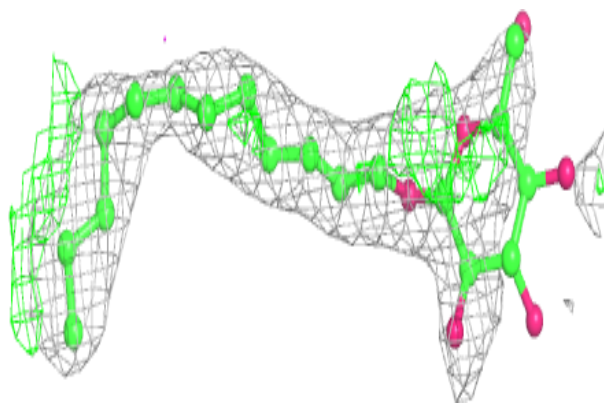
**Electron density around LMT Z 102:**

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

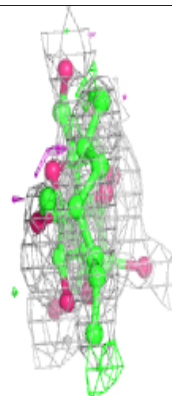
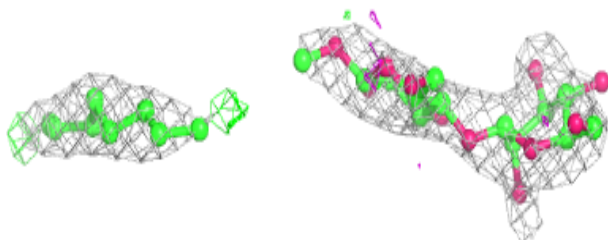
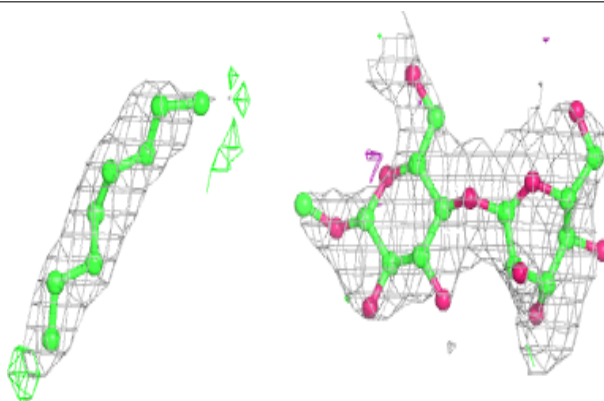


Electron density around LMT t 102:

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

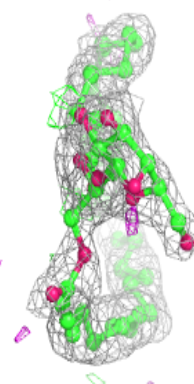
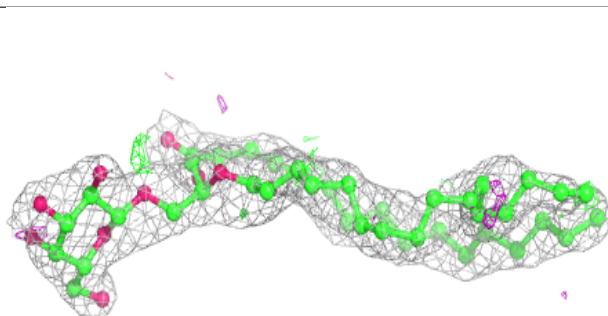
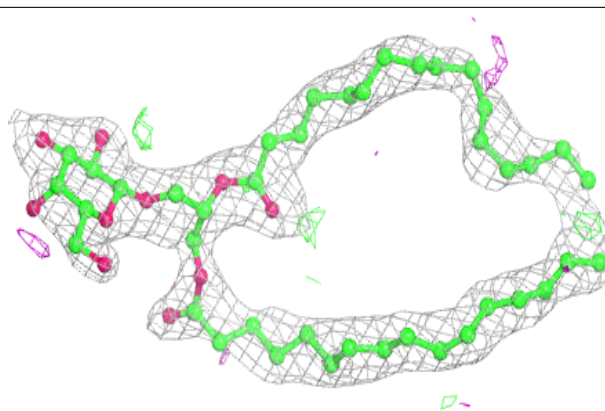
**Electron density around LMT z 101:**

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

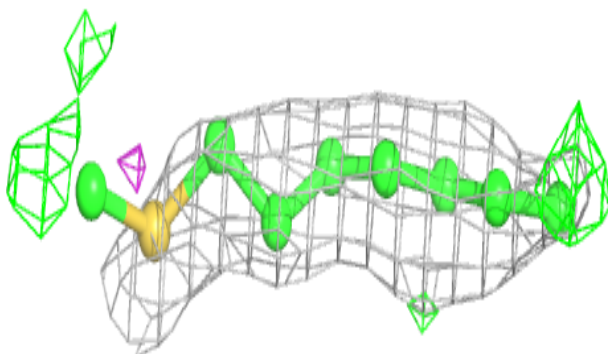
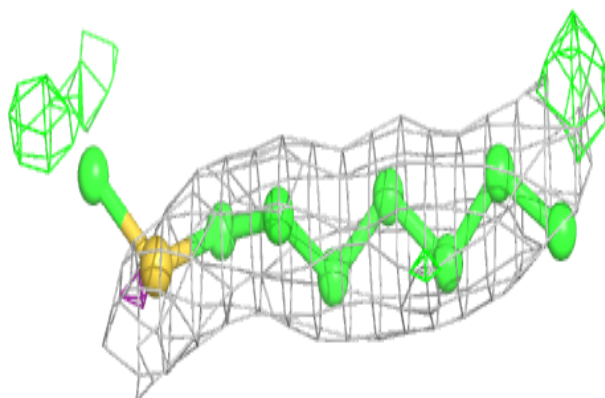


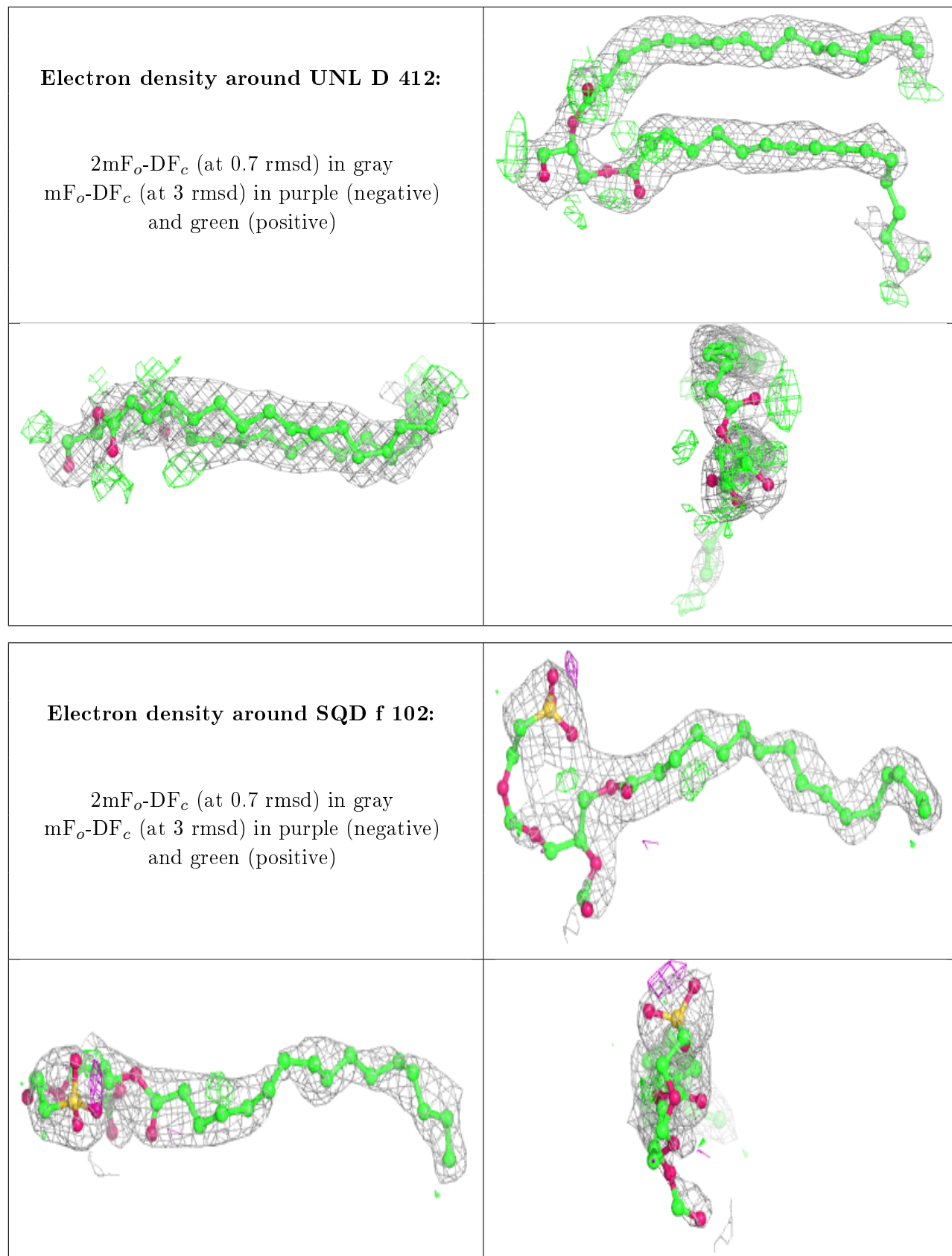
Electron density around LMG A 413:

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

**Electron density around HTG U 201:**

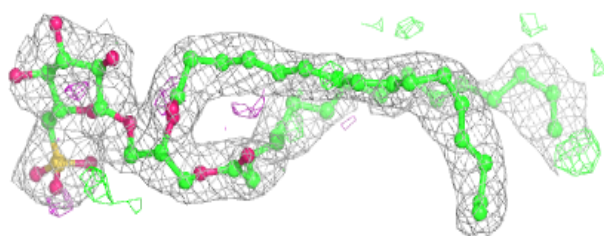
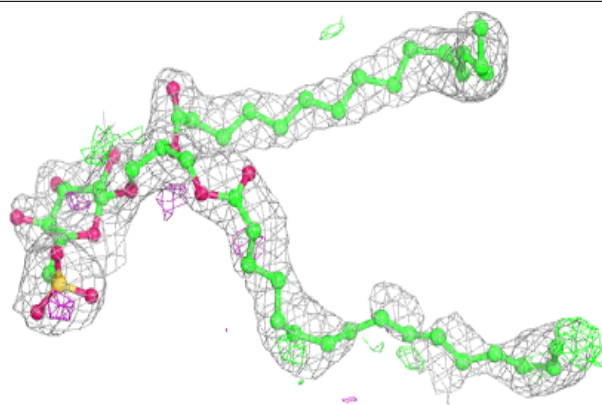
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



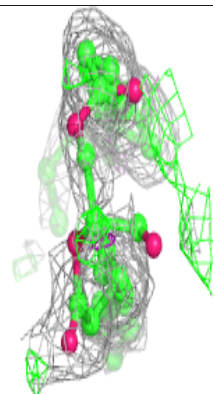
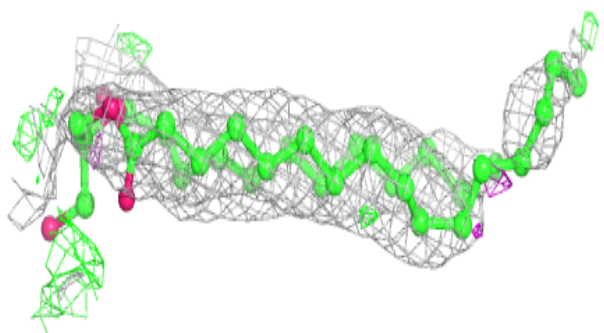
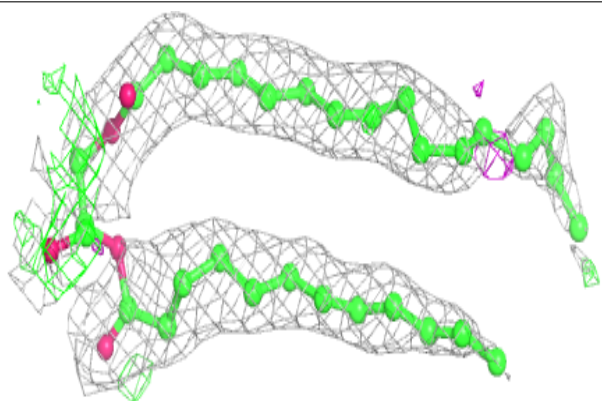


Electron density around SQD A 418:

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

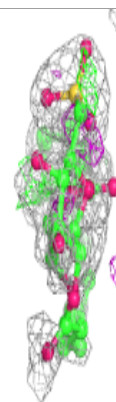
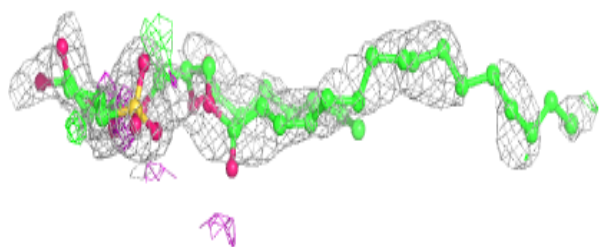
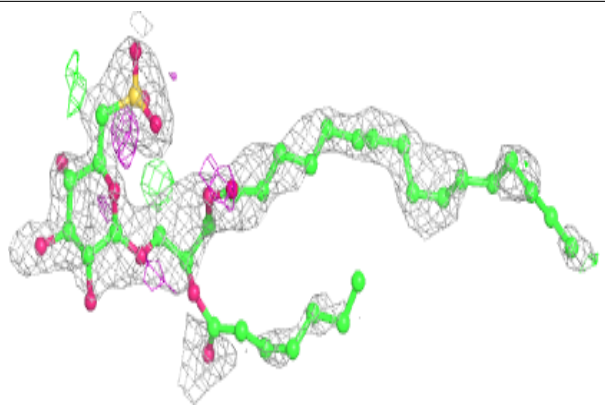
**Electron density around UNL b 628:**

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

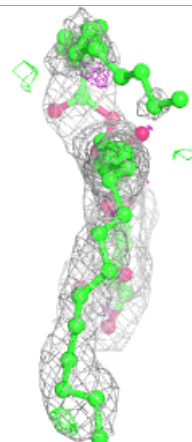
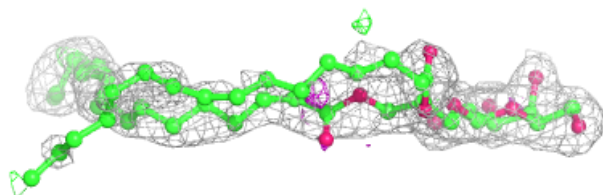


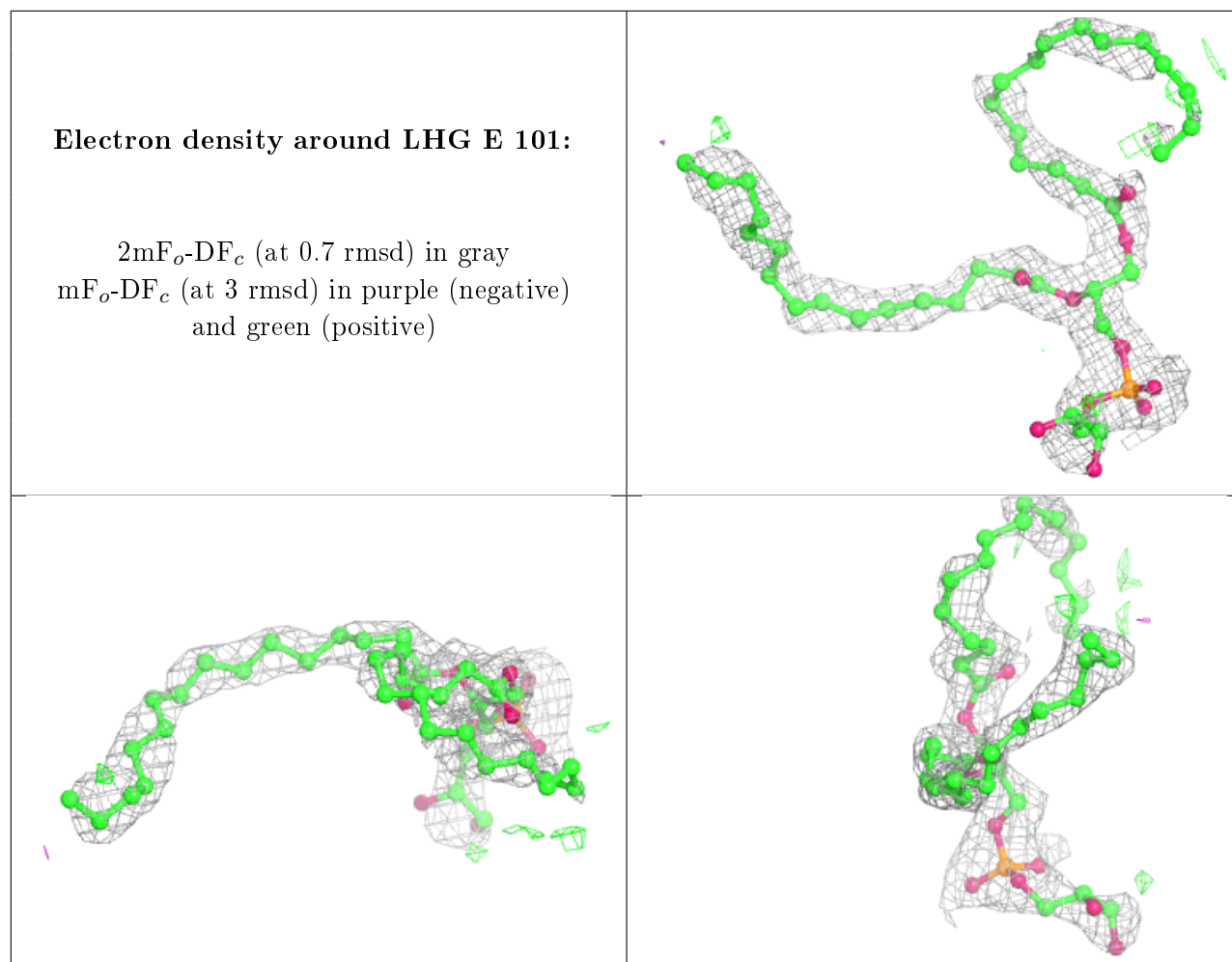
Electron density around SQD D 407:

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

**Electron density around LMG c 920:**

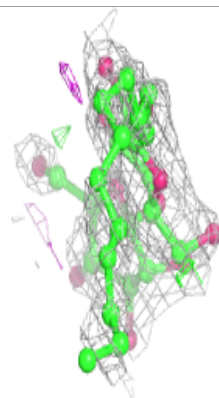
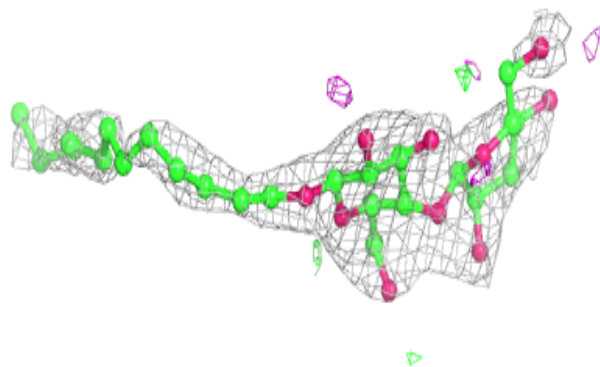
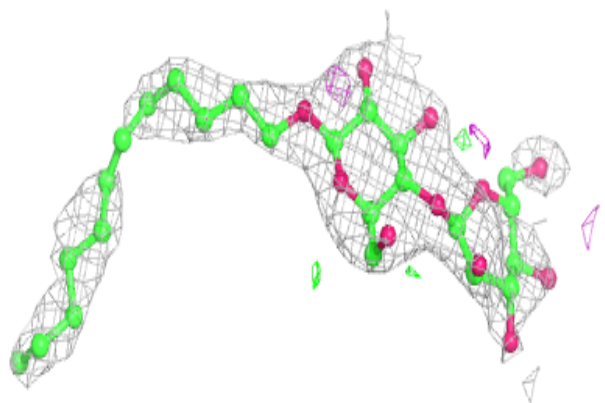
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



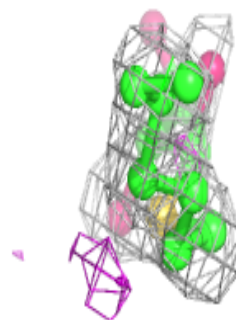
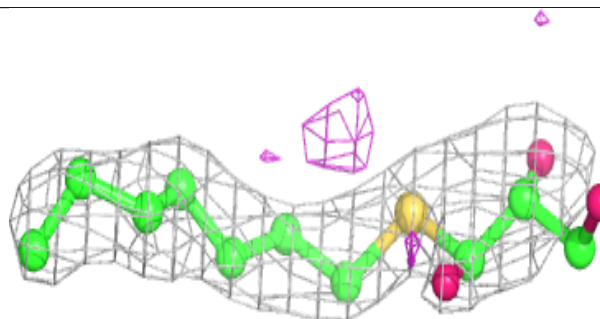
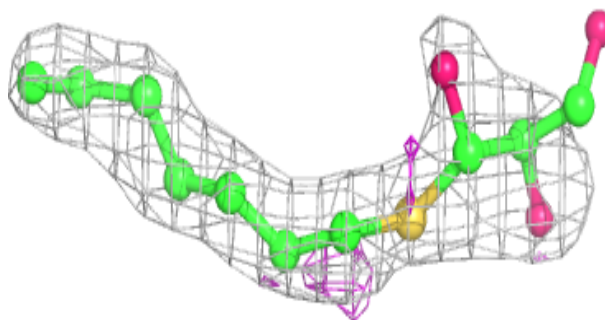


Electron density around LMT C 520:

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

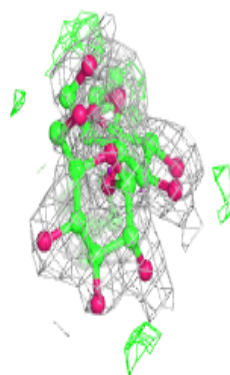
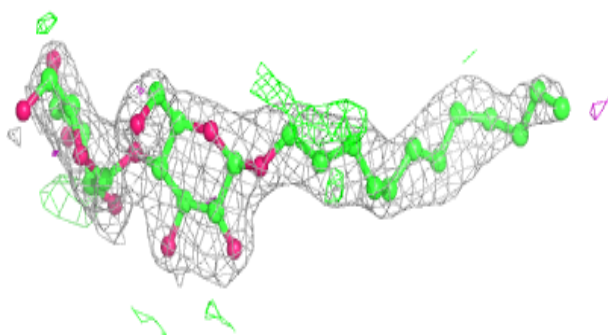
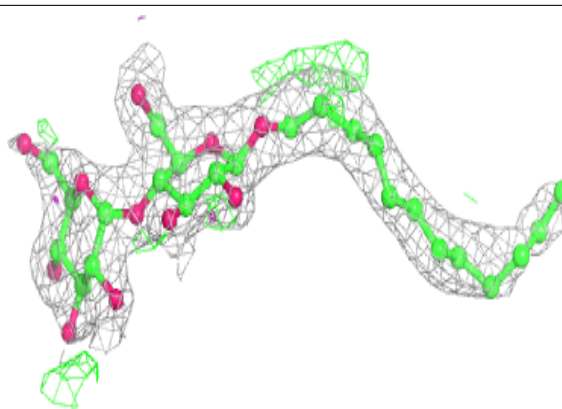
**Electron density around HTG u 201:**

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

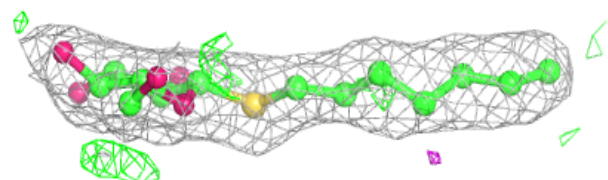
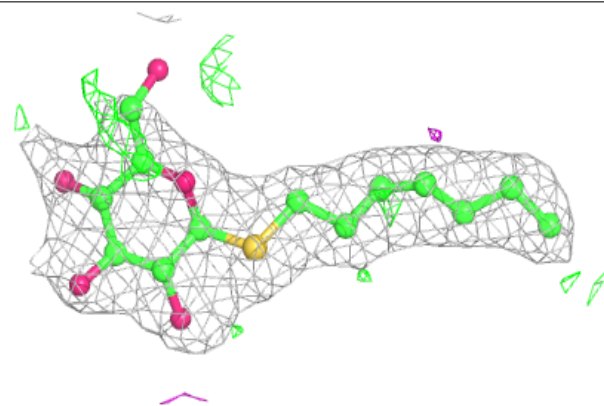


Electron density around LMT a 402:

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

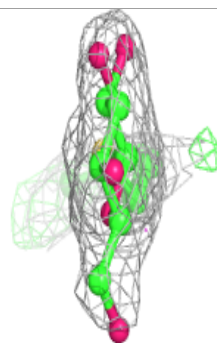
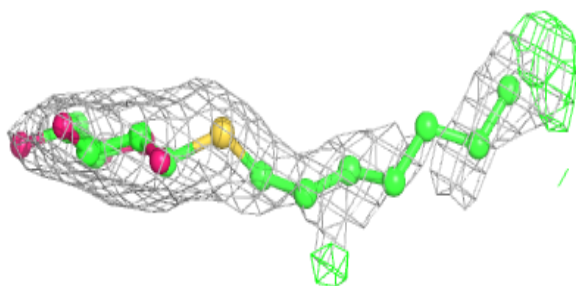
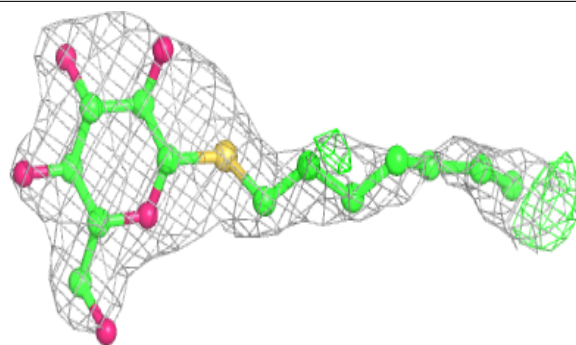
**Electron density around HTG B 630:**

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

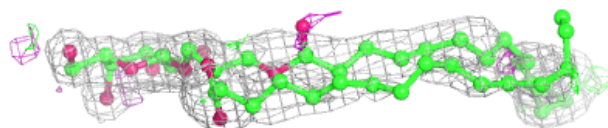
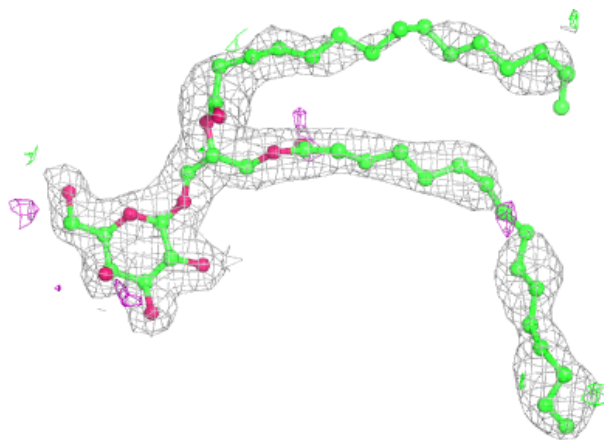


Electron density around HTG c 923:

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

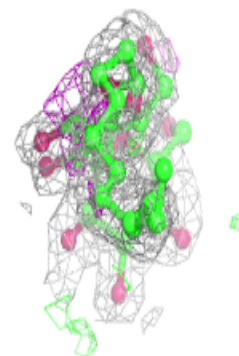
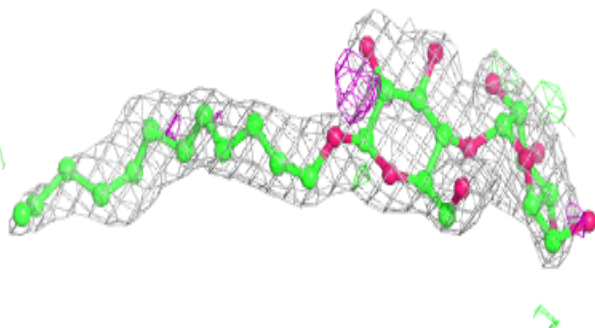
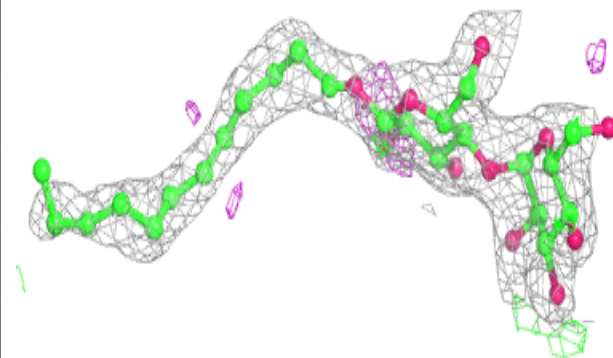
**Electron density around LMG C 519:**

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

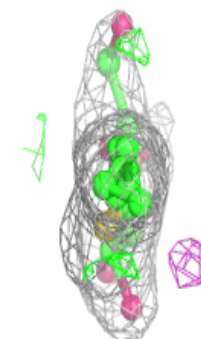
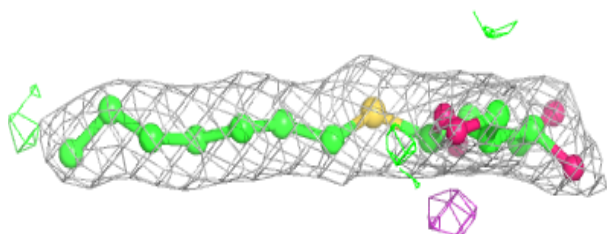
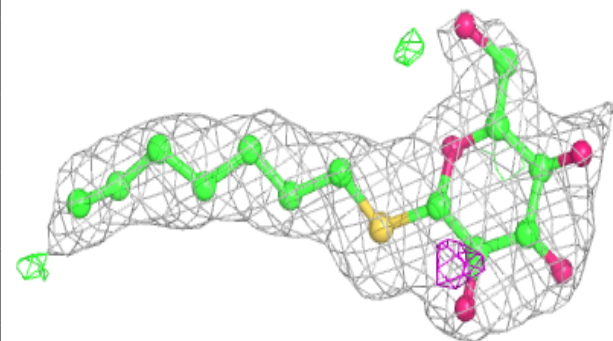


Electron density around LMT A 419:

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

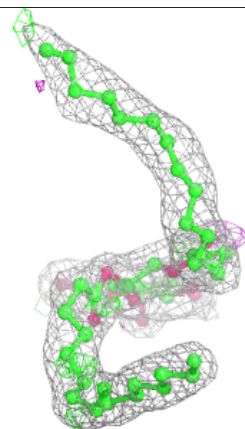
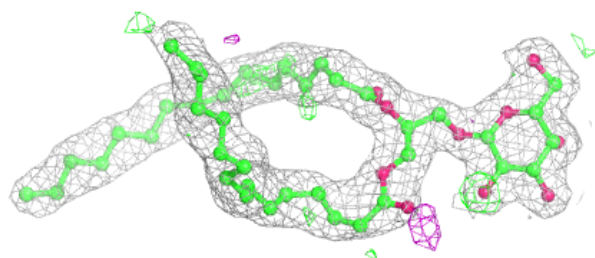
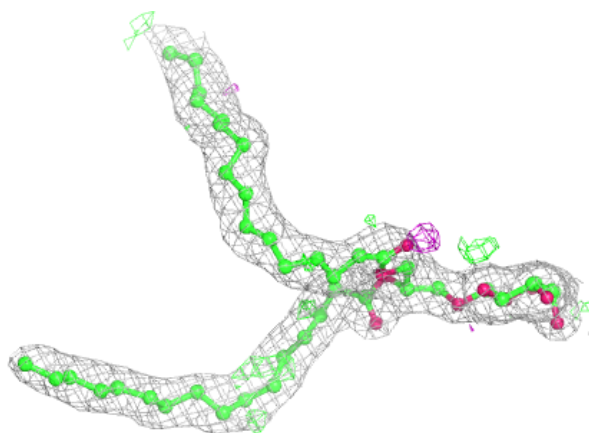
**Electron density around HTG b 601:**

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

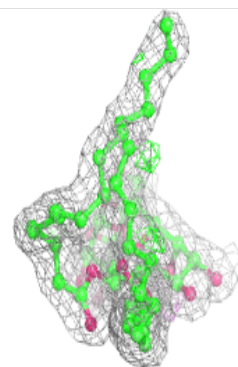
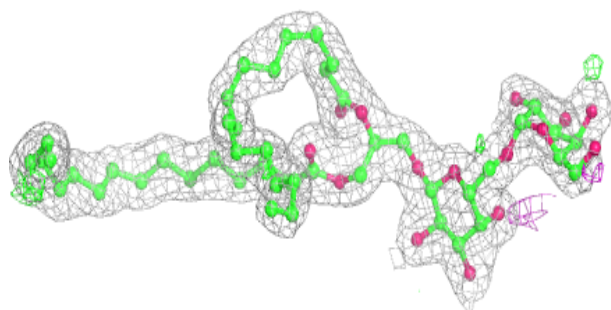
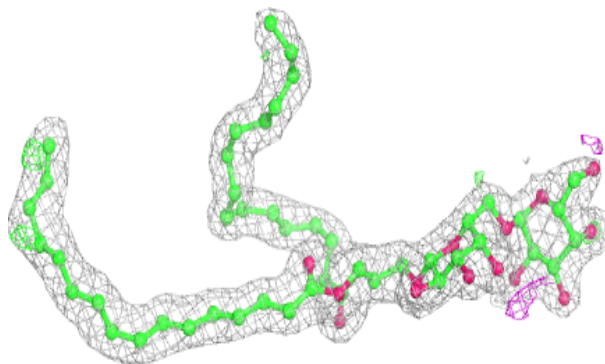


Electron density around LMG B 622:

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

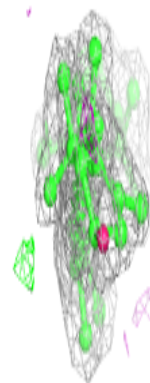
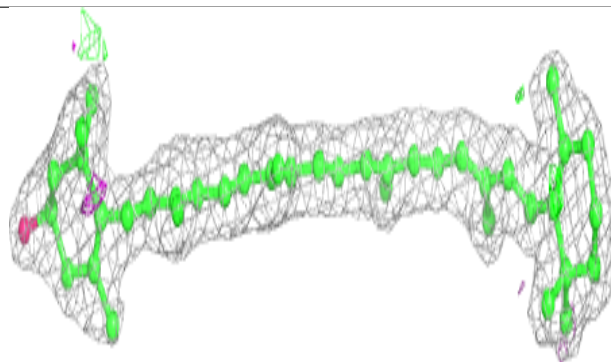
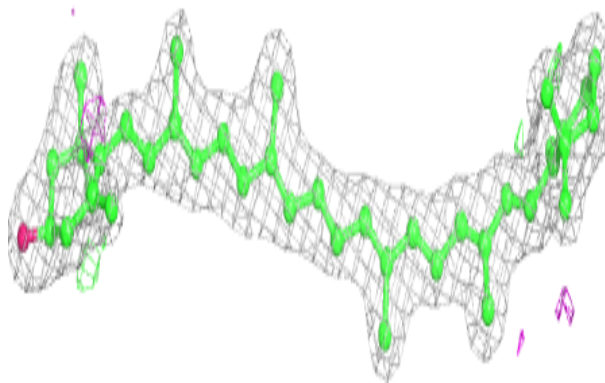
**Electron density around DGD h 102:**

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

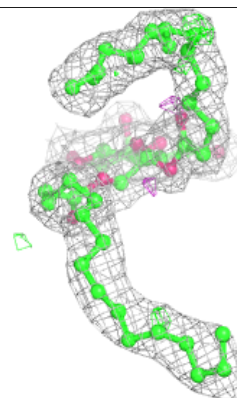
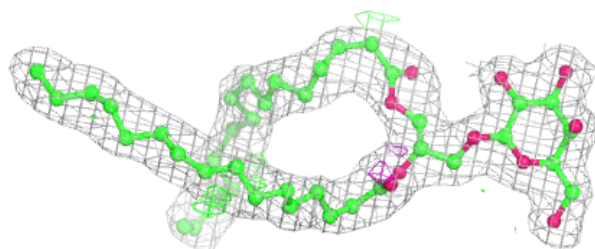
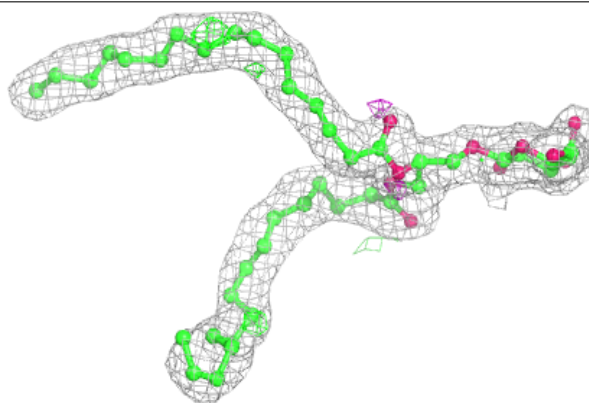


Electron density around RRX h 101:

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

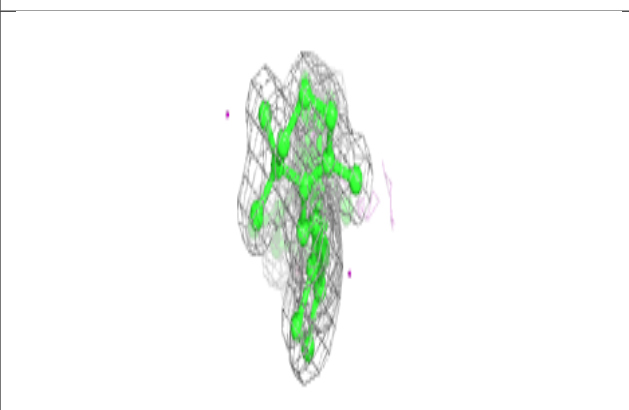
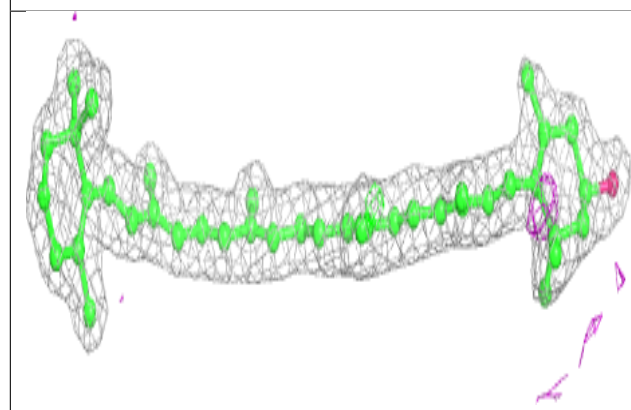
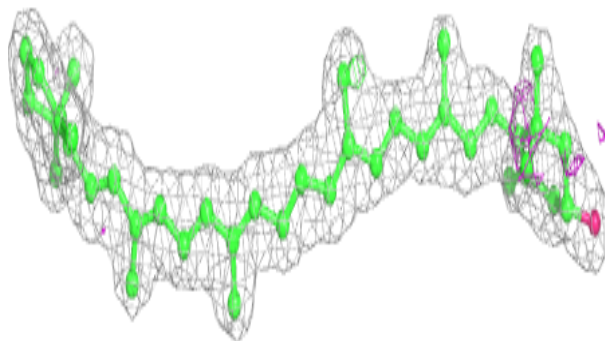
**Electron density around LMG b 623:**

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

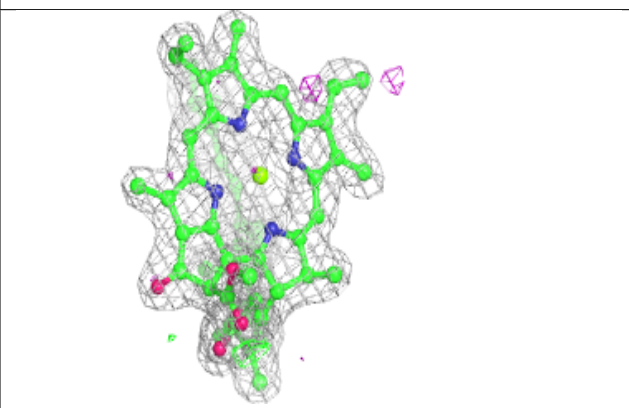
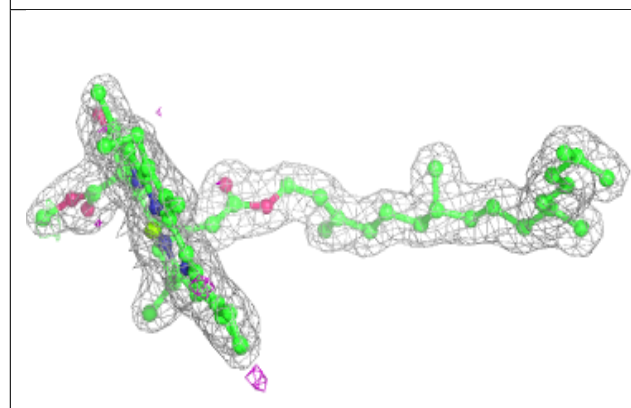
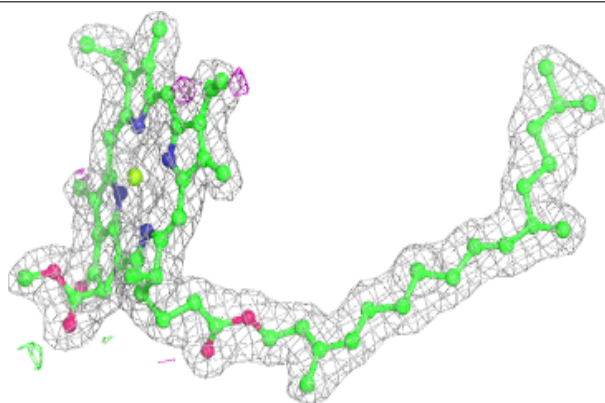


Electron density around RRX H 101:

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

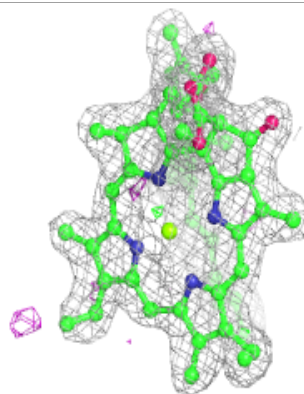
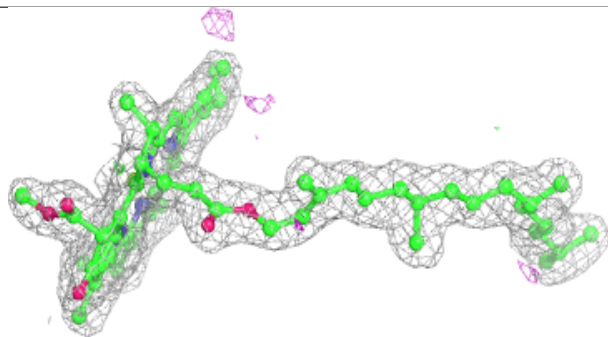
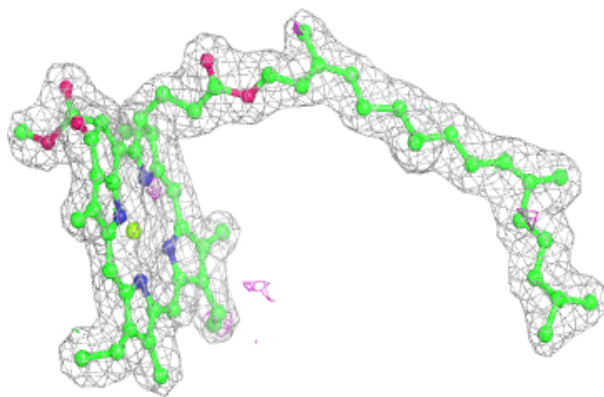
**Electron density around CLA B 610:**

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

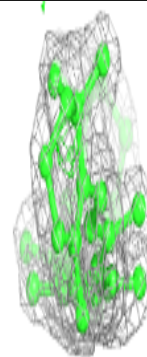
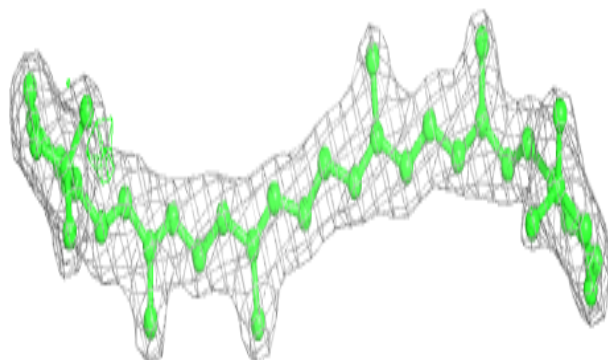
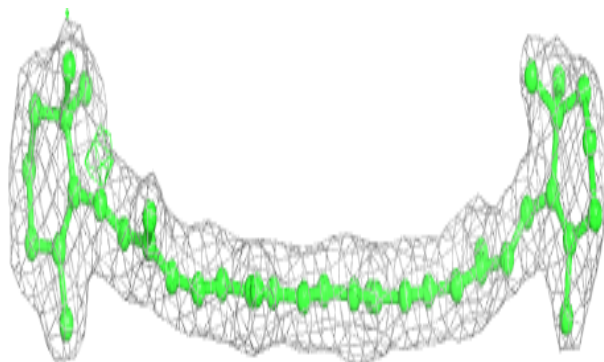


Electron density around CLA b 612:

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

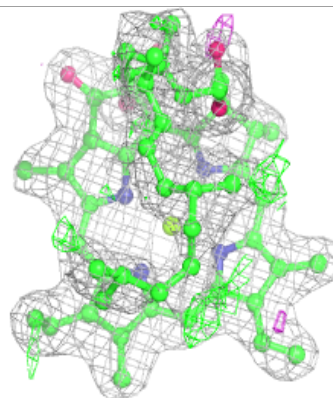
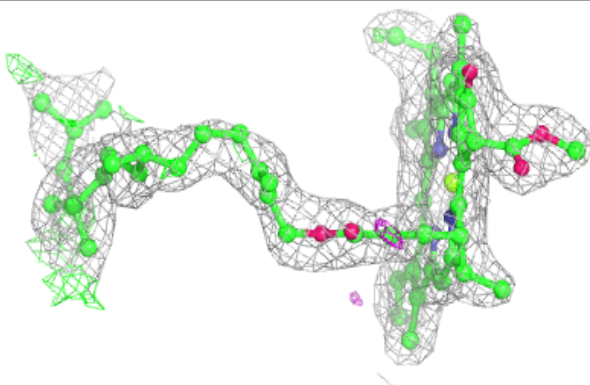
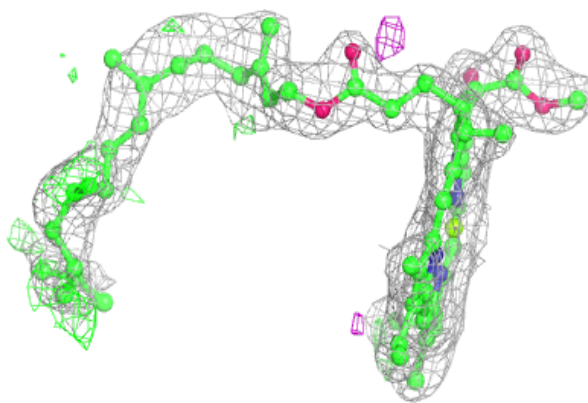
**Electron density around BCR k 102:**

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

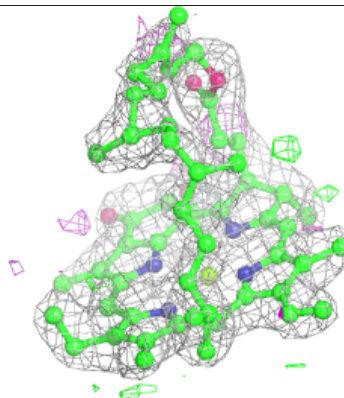
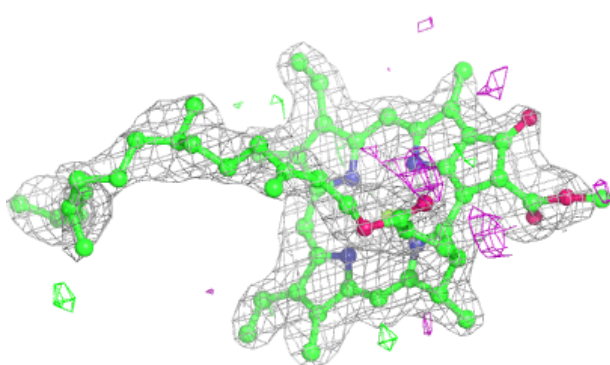
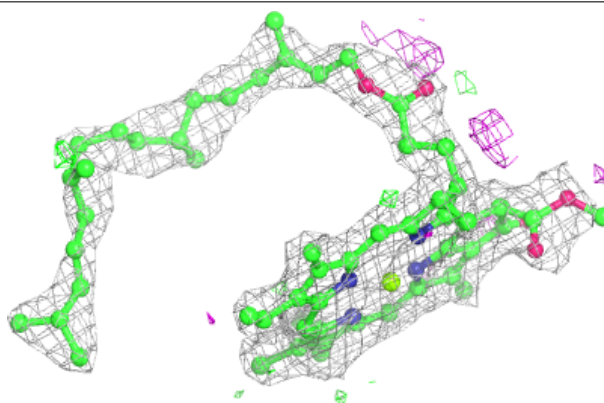


Electron density around CLA C 506:

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

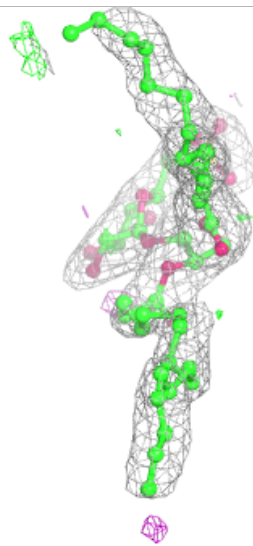
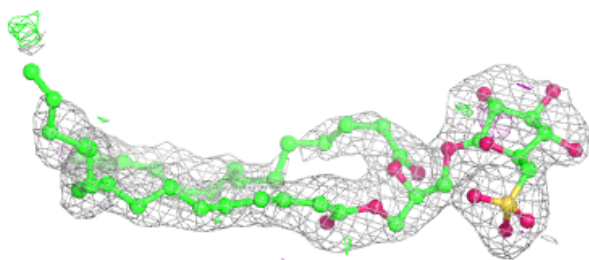
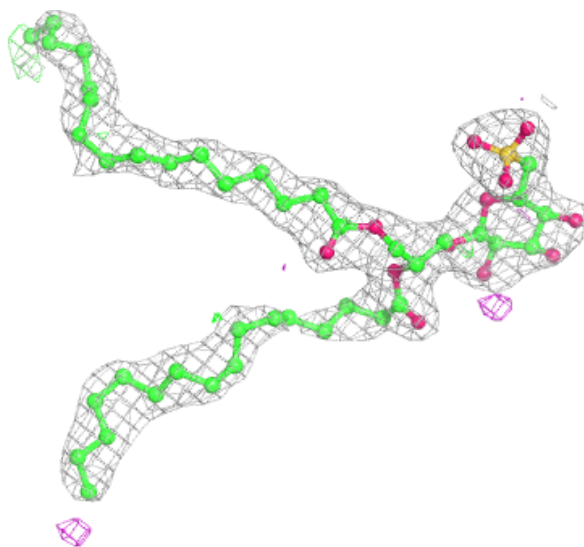
**Electron density around CLA c 914:**

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



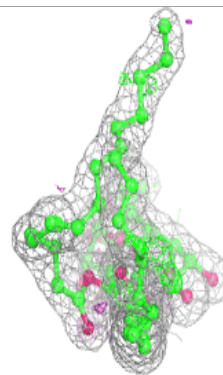
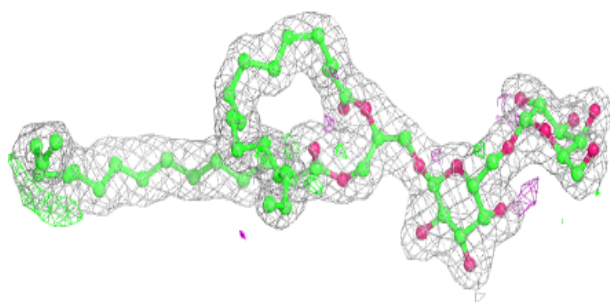
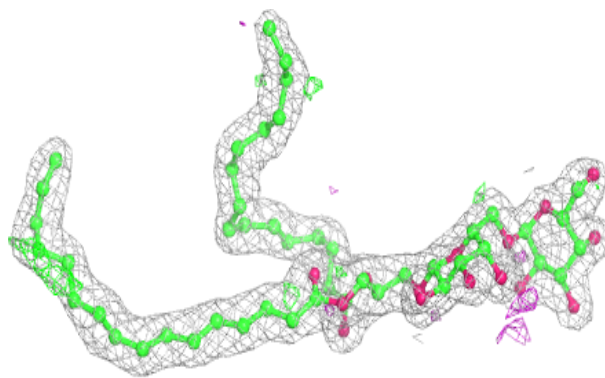
Electron density around SQD a 416:

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

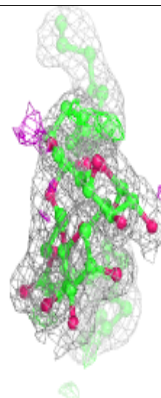
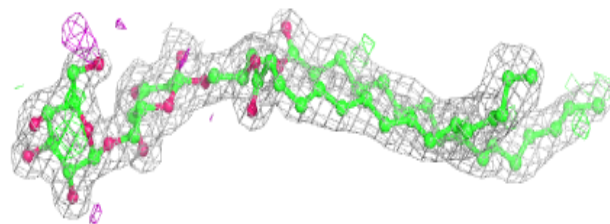
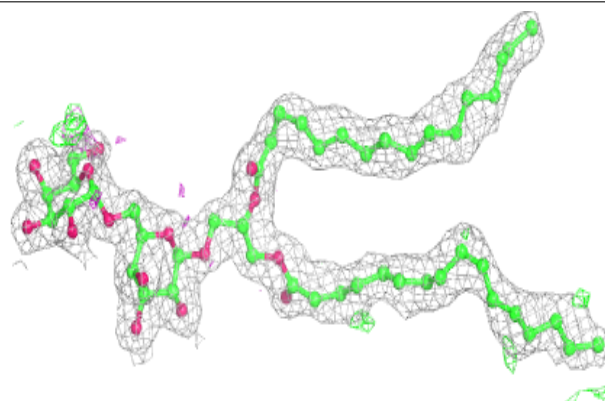


Electron density around DGD H 102:

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

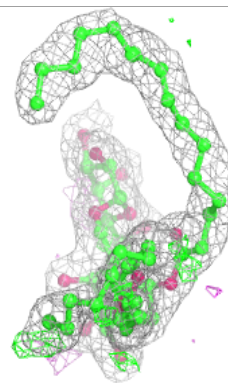
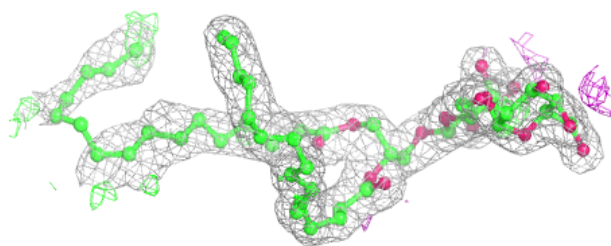
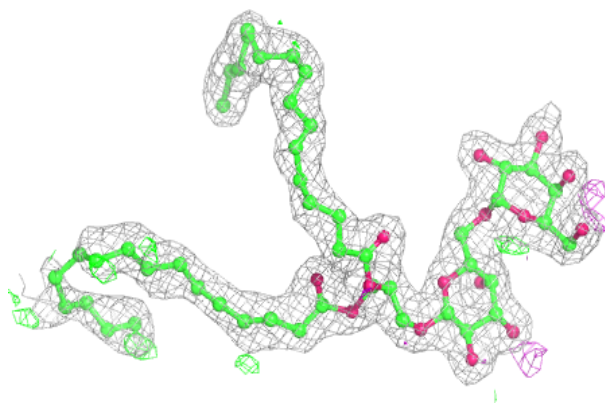
**Electron density around DGD c 919:**

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

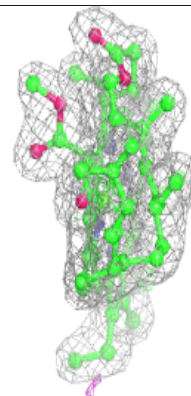
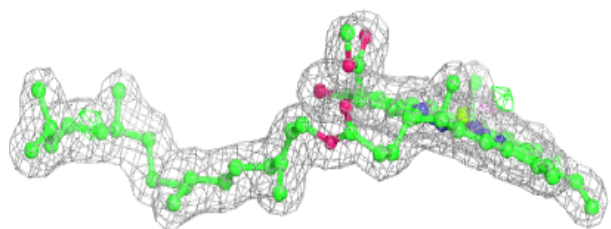
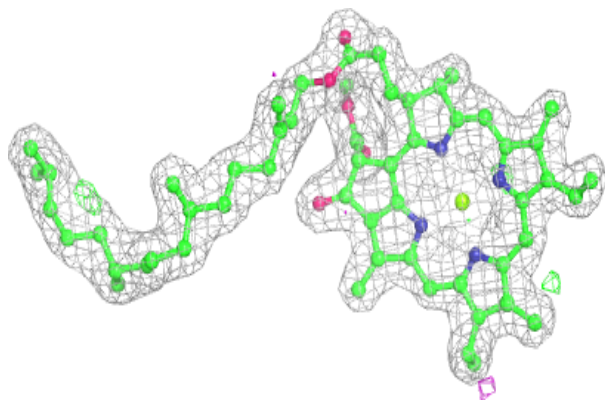


Electron density around DGD c 918:

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

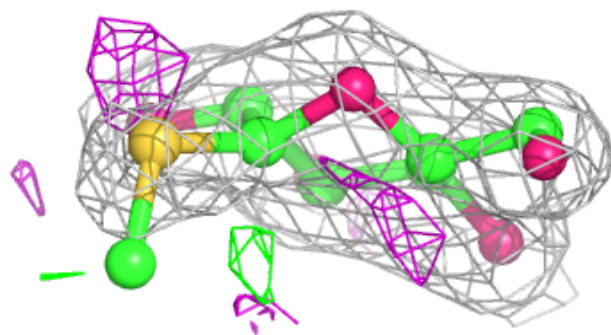
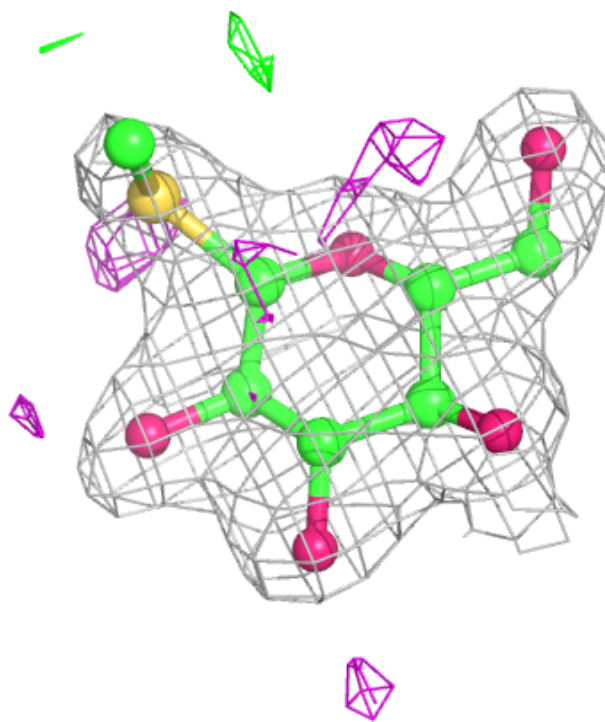
**Electron density around CLA B 603:**

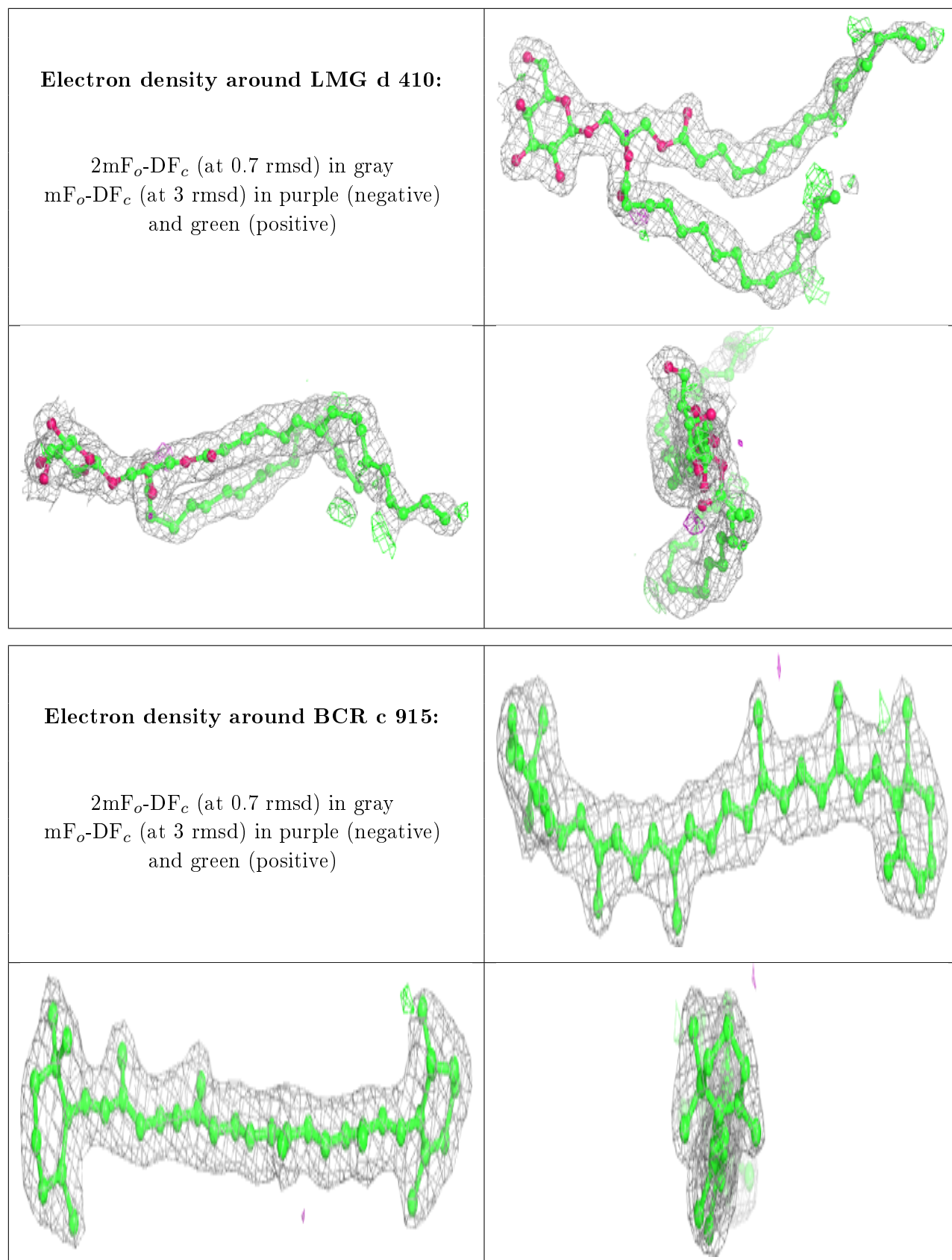
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HTG V 202:

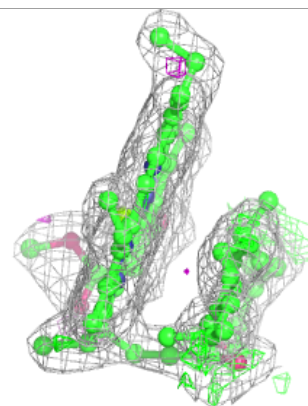
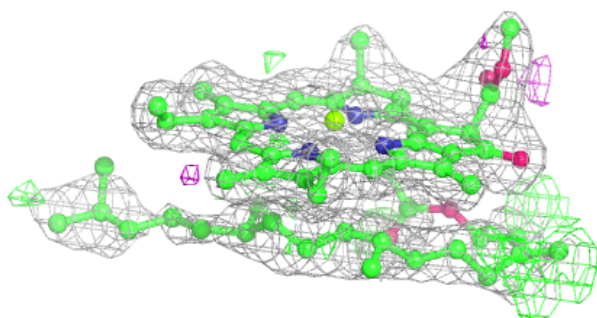
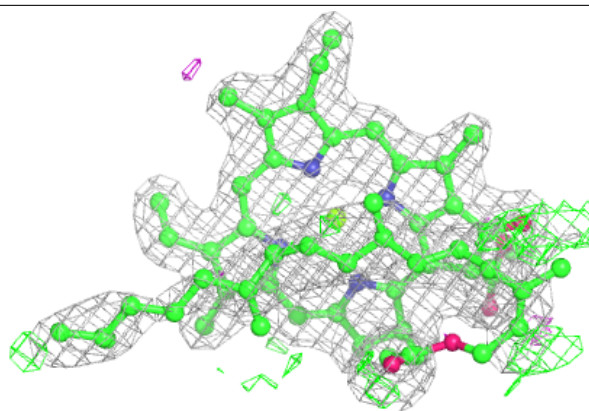
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



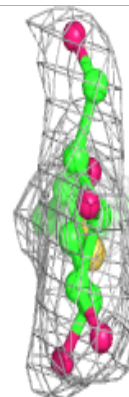
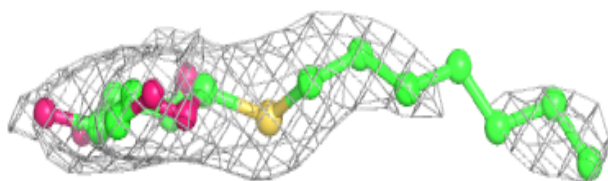
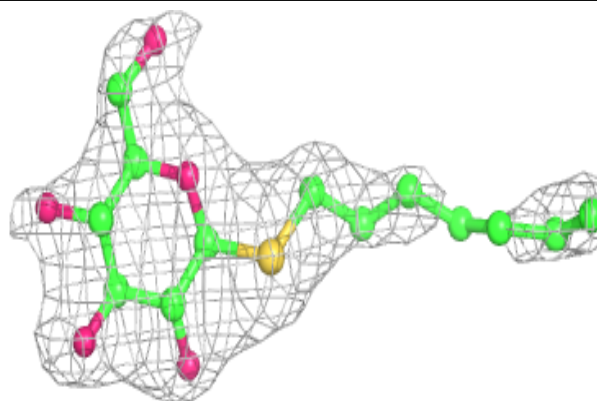


Electron density around CLA B 602:

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

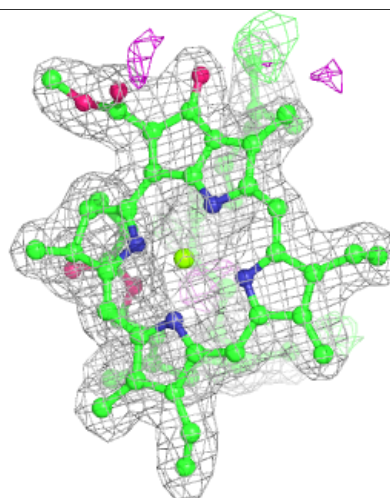
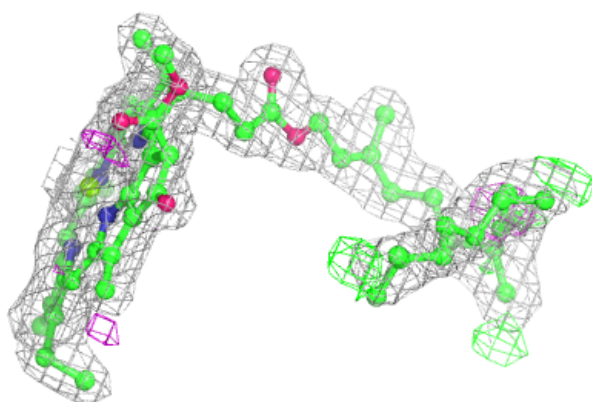
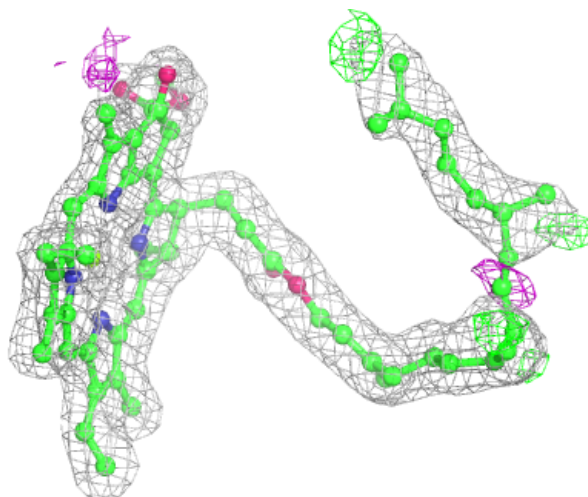
**Electron density around HTG C 521:**

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



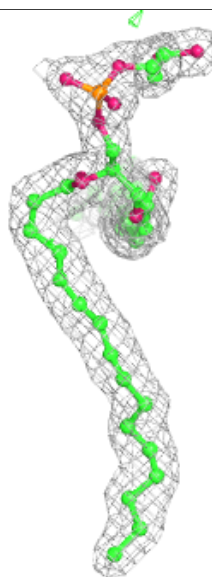
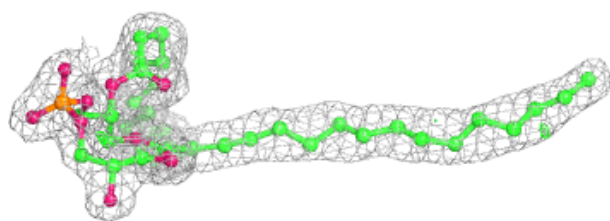
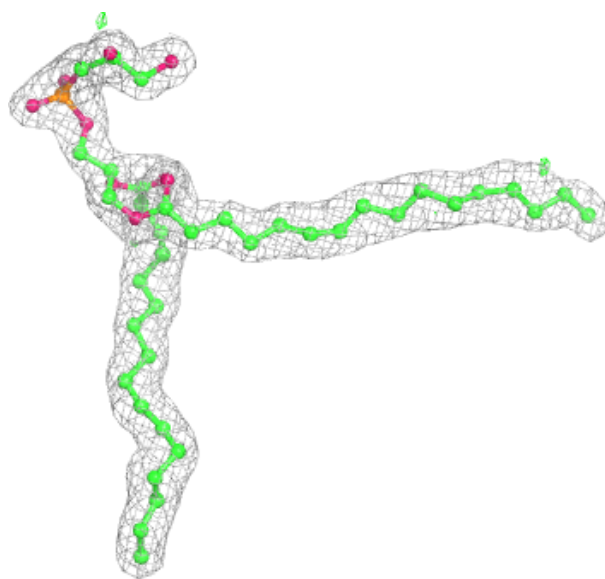
Electron density around CLA b 609:

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



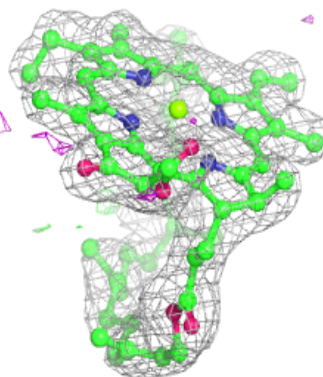
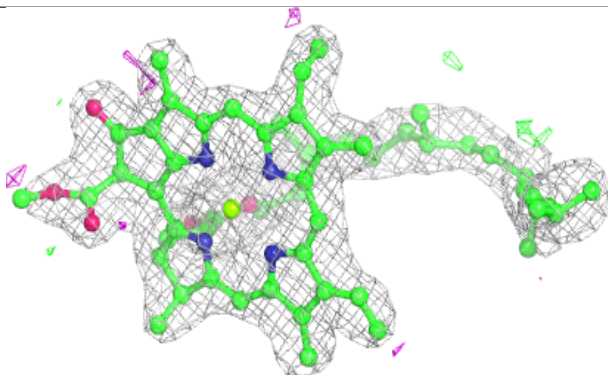
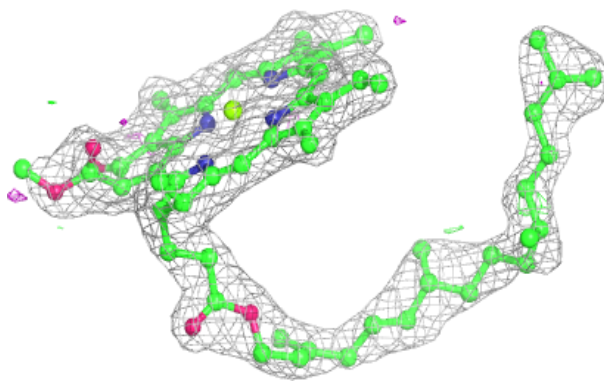
Electron density around LHG 1 101:

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

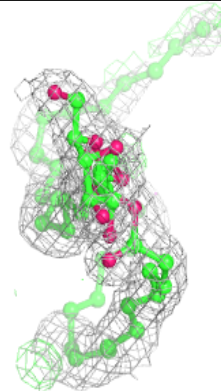
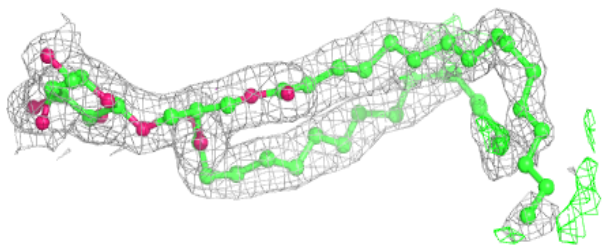
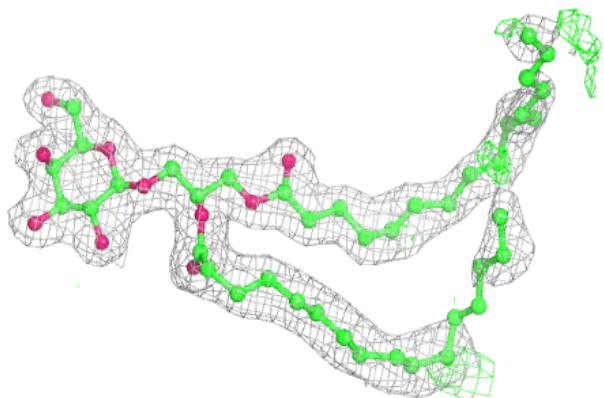


Electron density around CLA C 513:

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

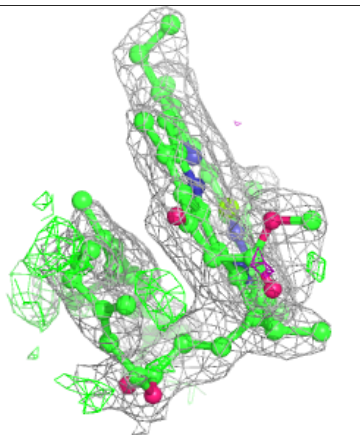
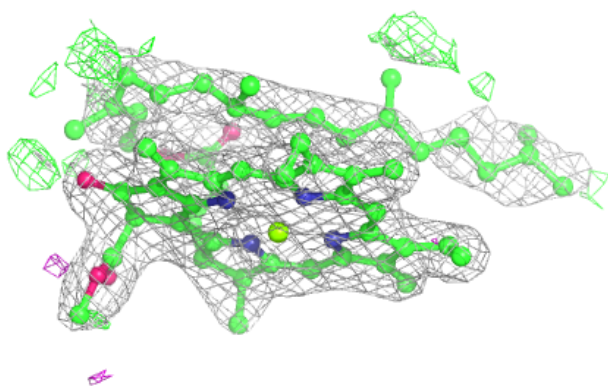
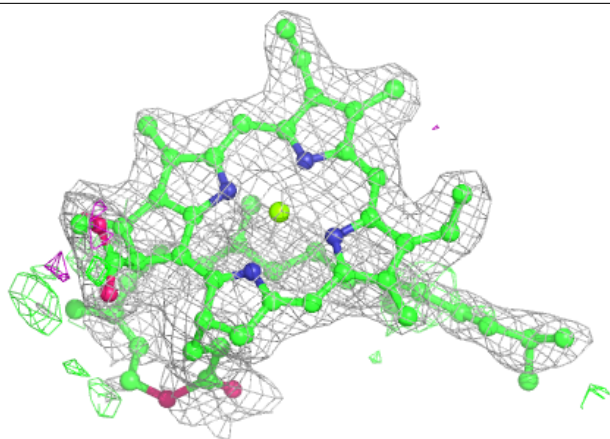
**Electron density around LMG D 411:**

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

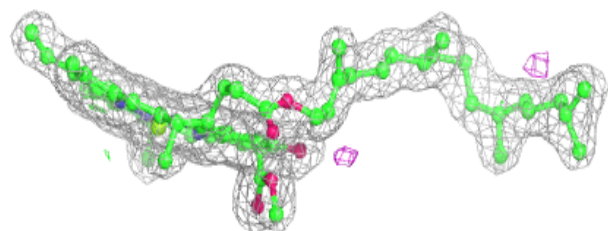
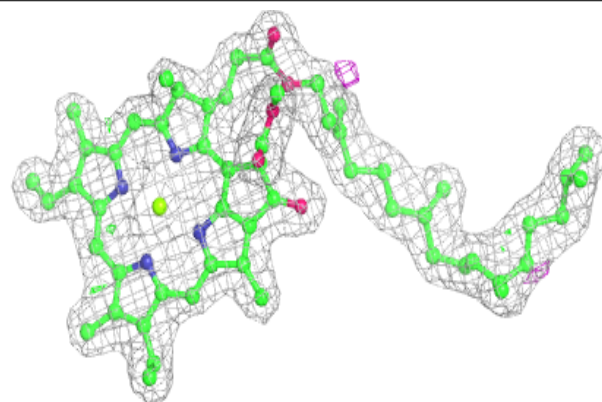


Electron density around CLA b 604:

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

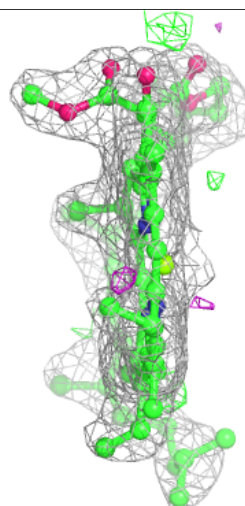
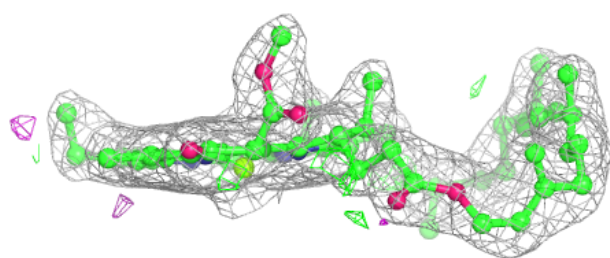
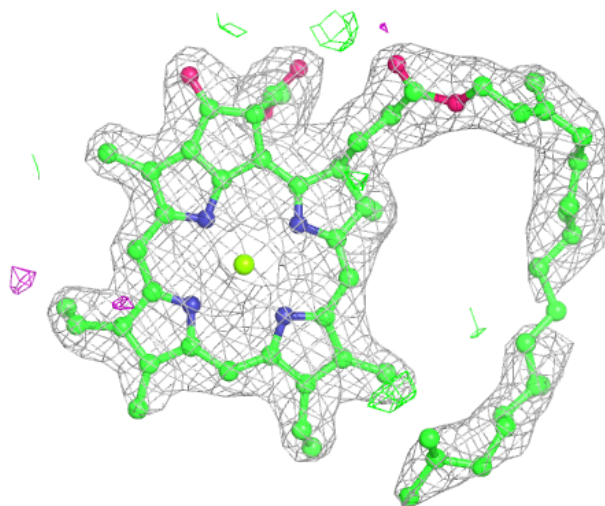
**Electron density around CLA b 605:**

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



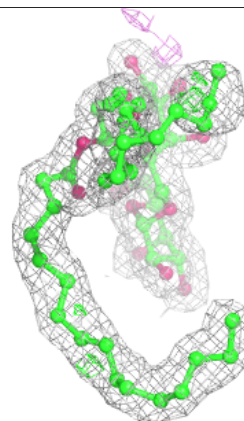
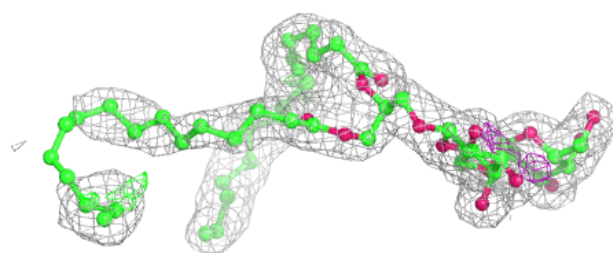
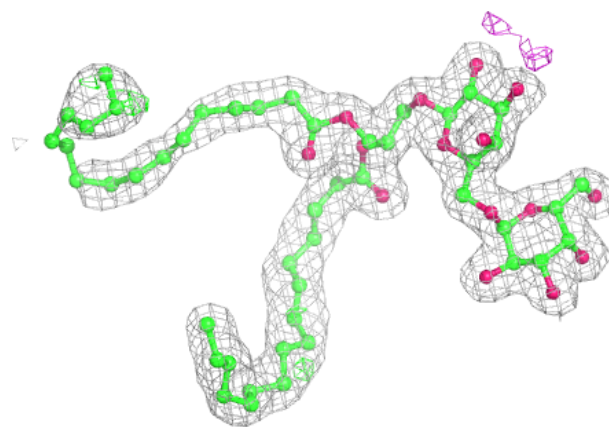
Electron density around CLA c 913:

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



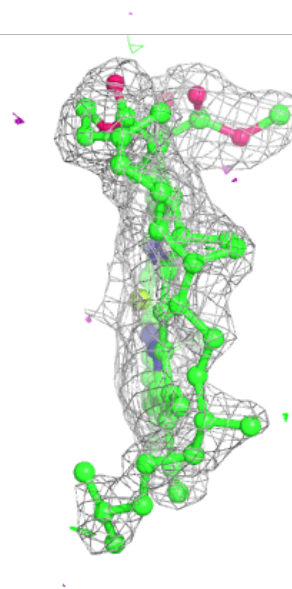
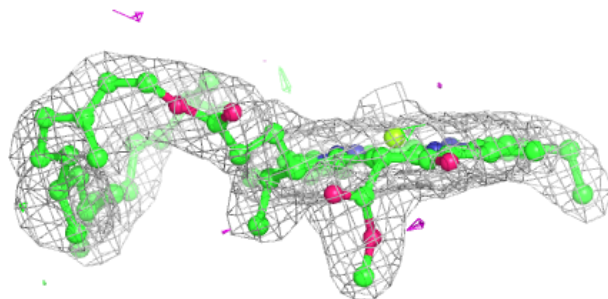
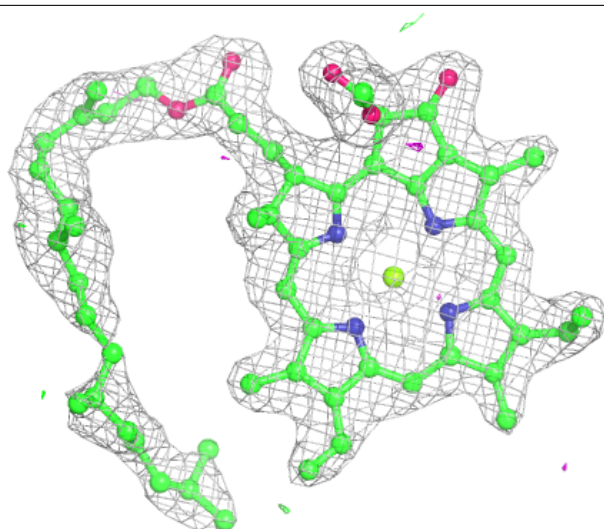
Electron density around DGD C 517:

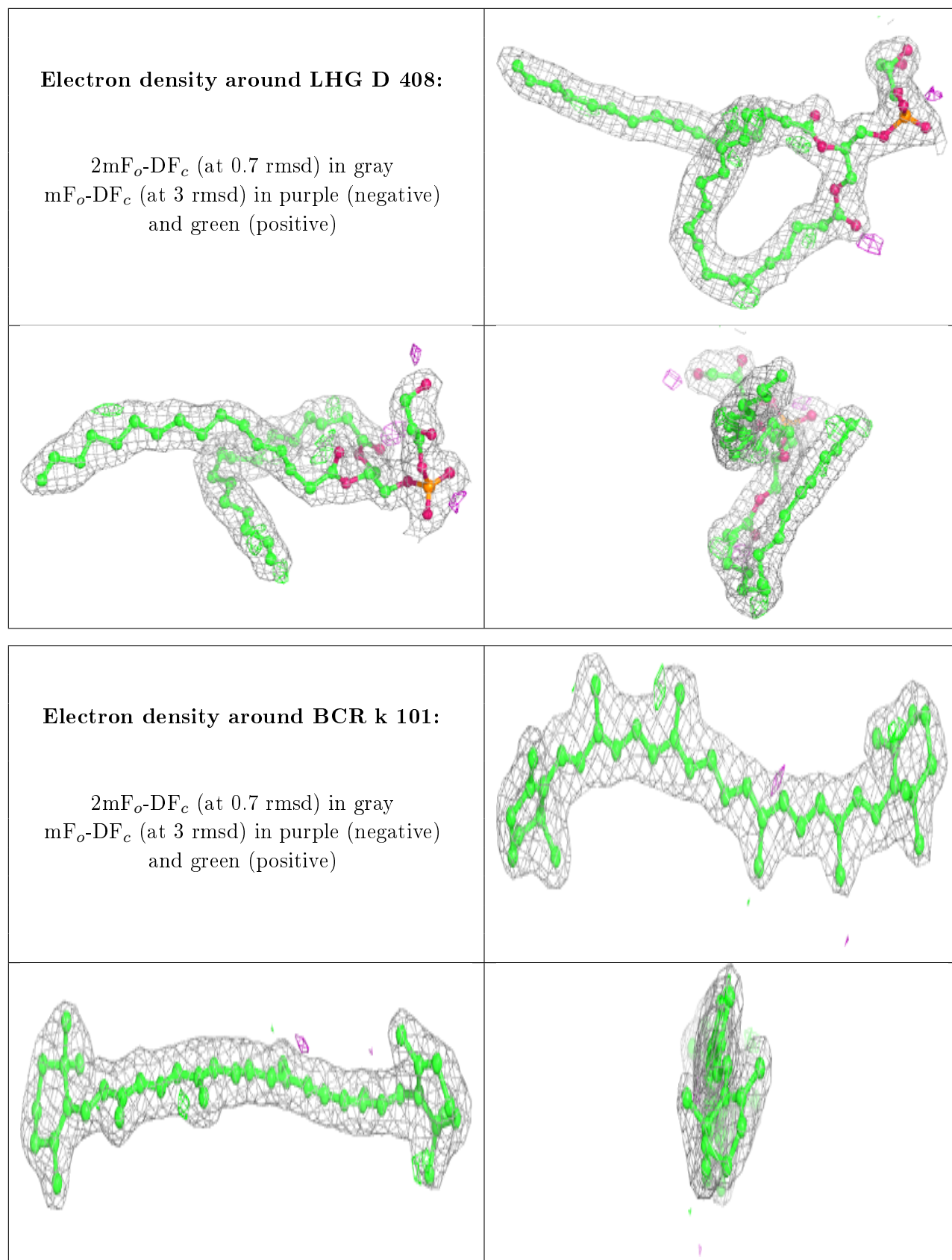
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA C 512:

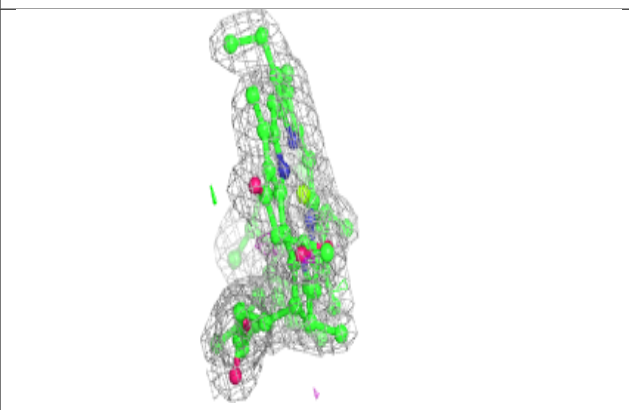
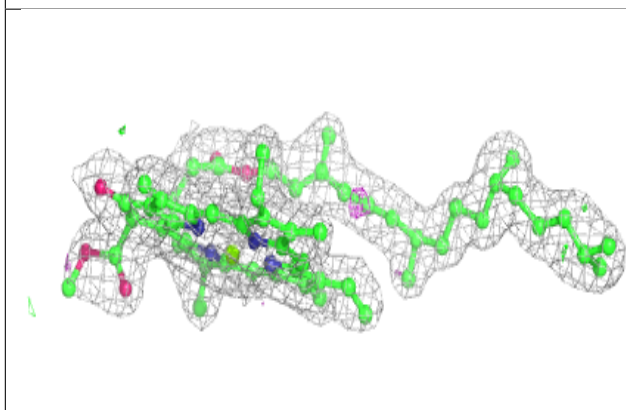
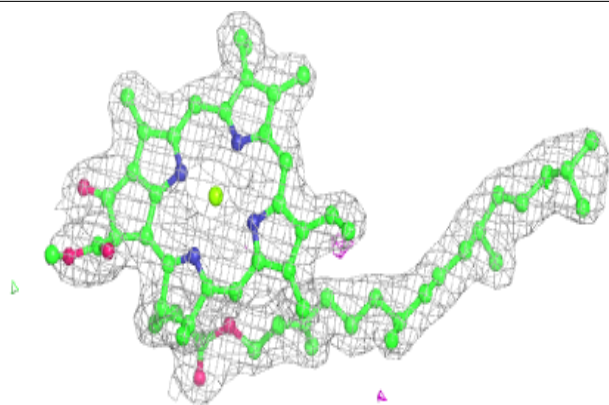
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



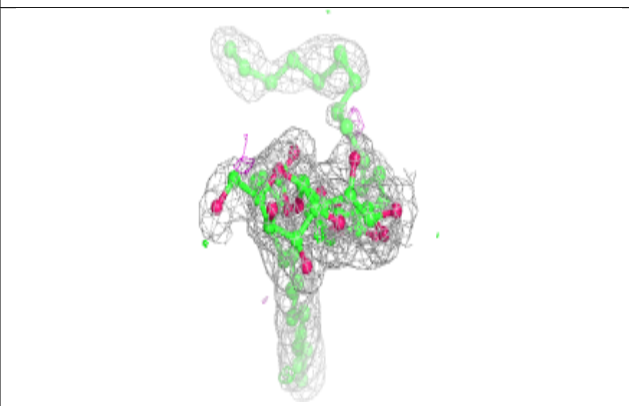
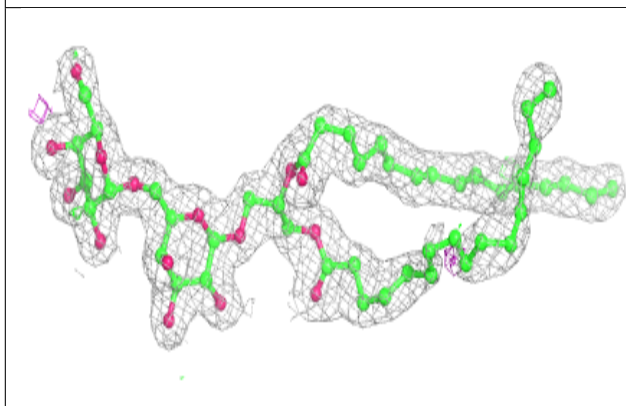
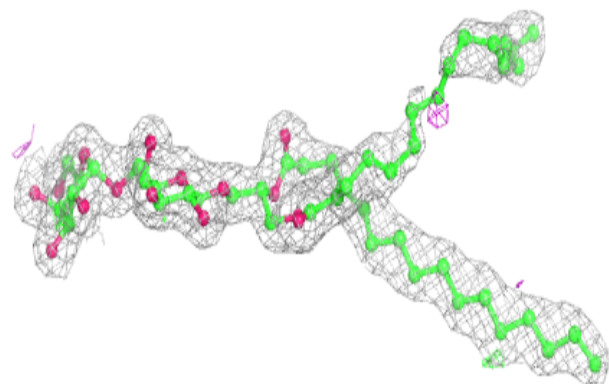


Electron density around CLA c 902:

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

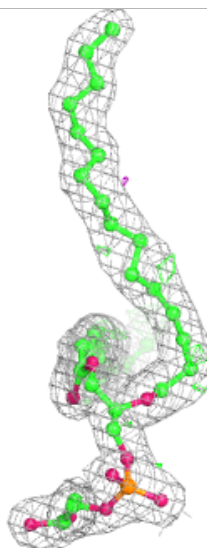
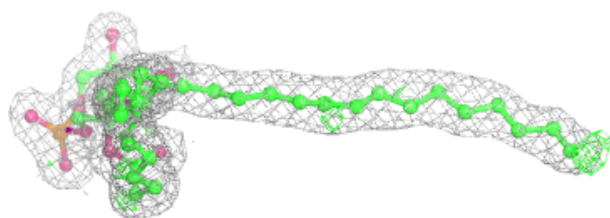
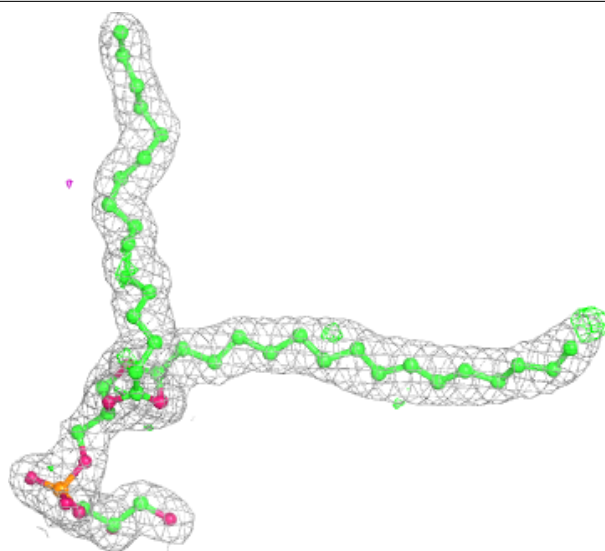
**Electron density around DGD c 917:**

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



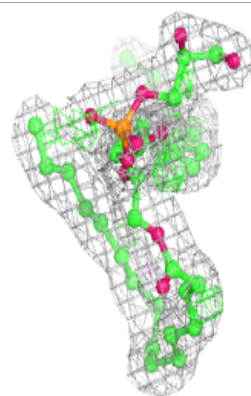
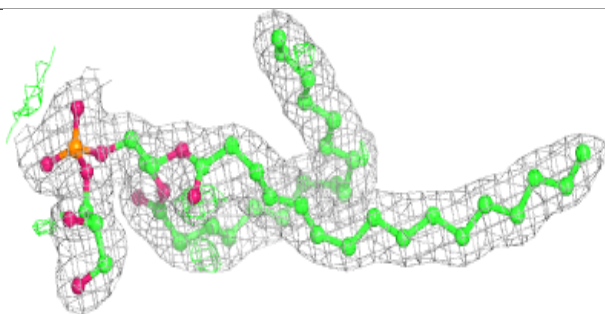
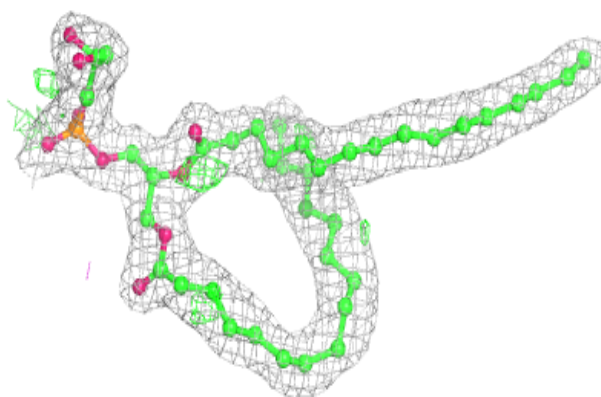
Electron density around LHG L 101:

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

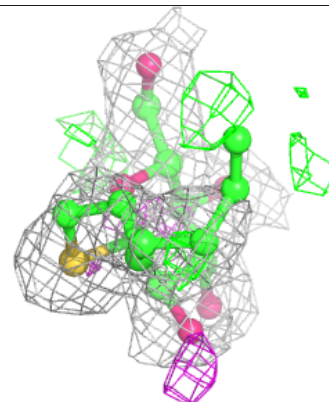
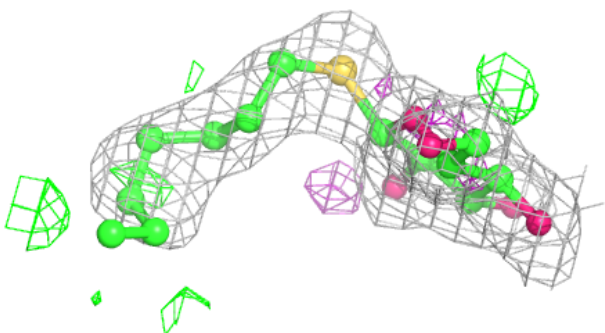
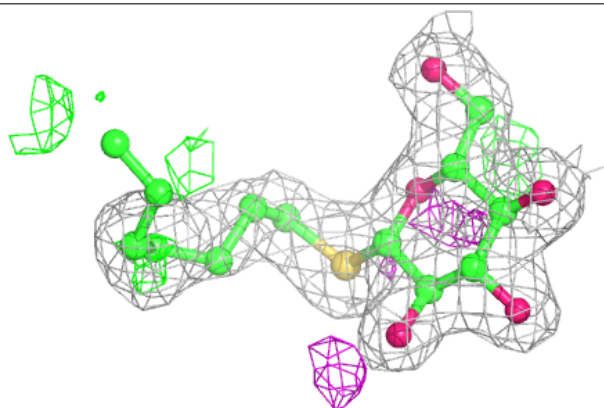


Electron density around LHG d 407:

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

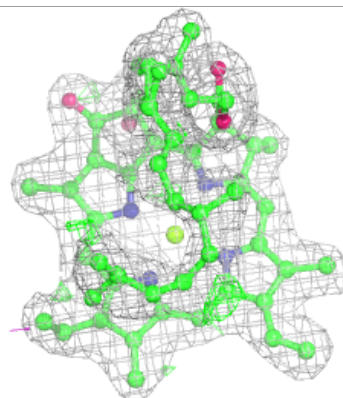
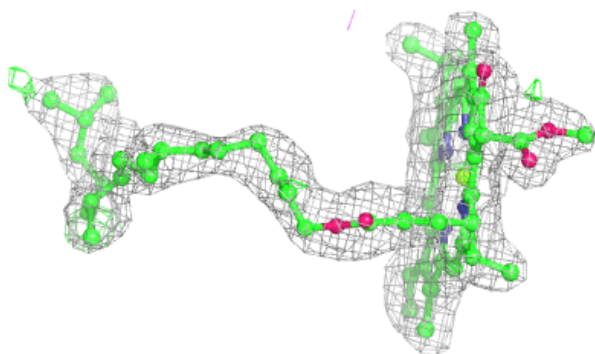
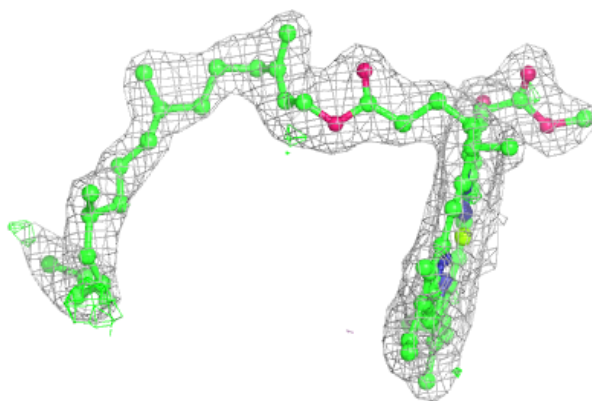
**Electron density around HTG B 625:**

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

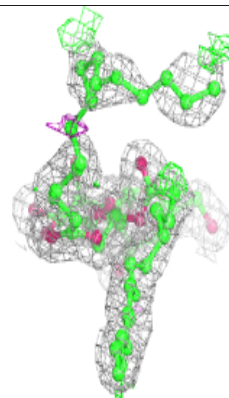
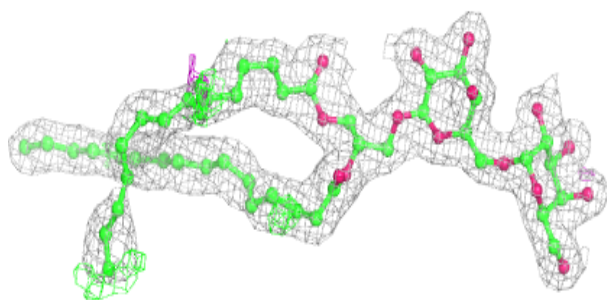
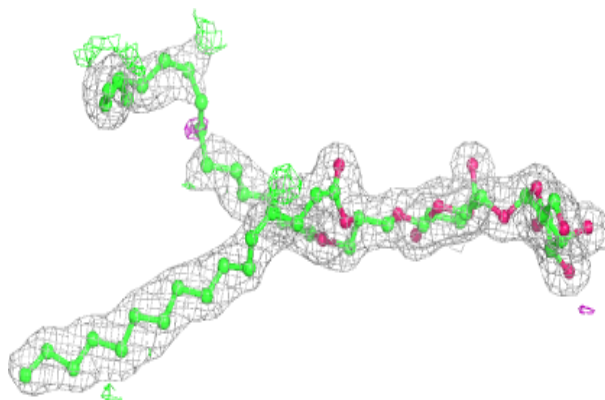


Electron density around CLA c 907:

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

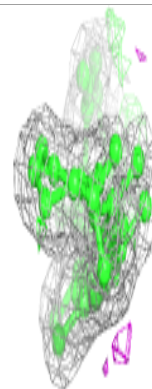
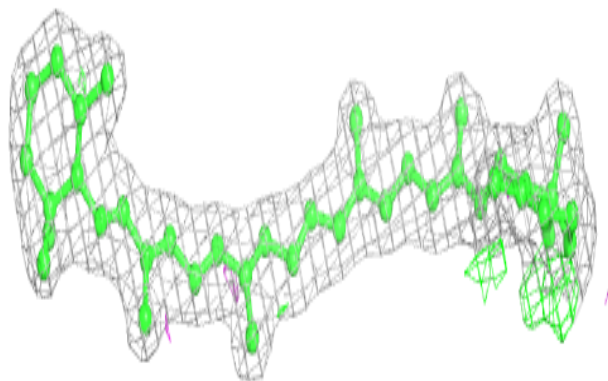
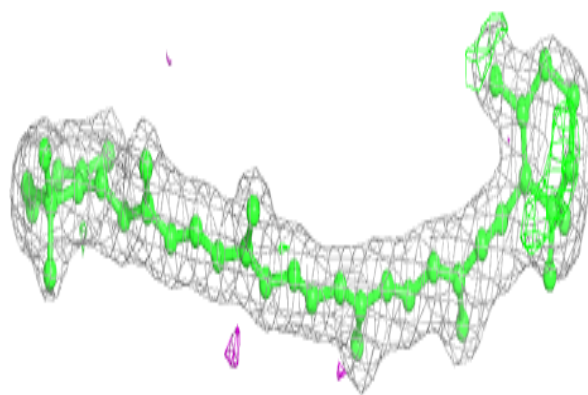
**Electron density around DGD C 516:**

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

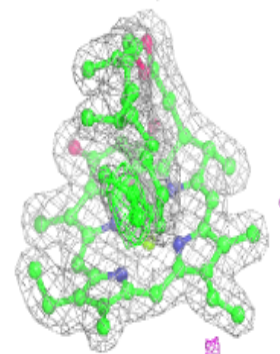
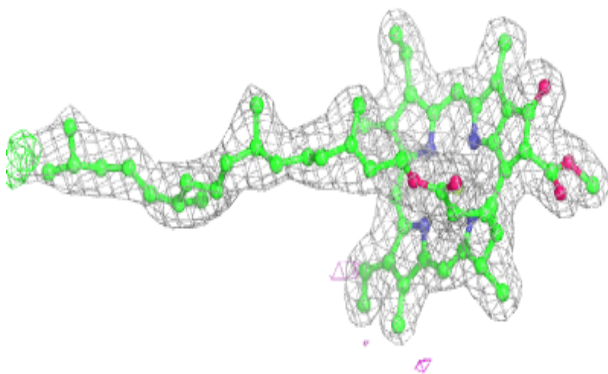
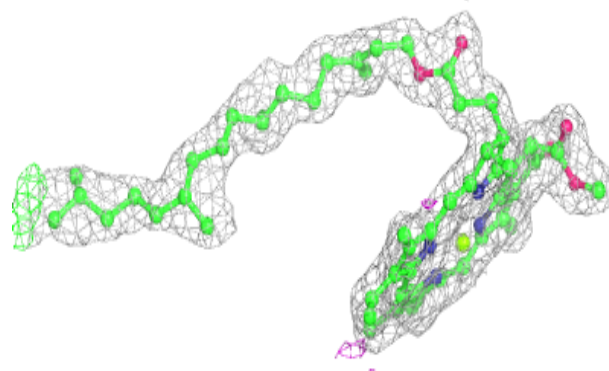


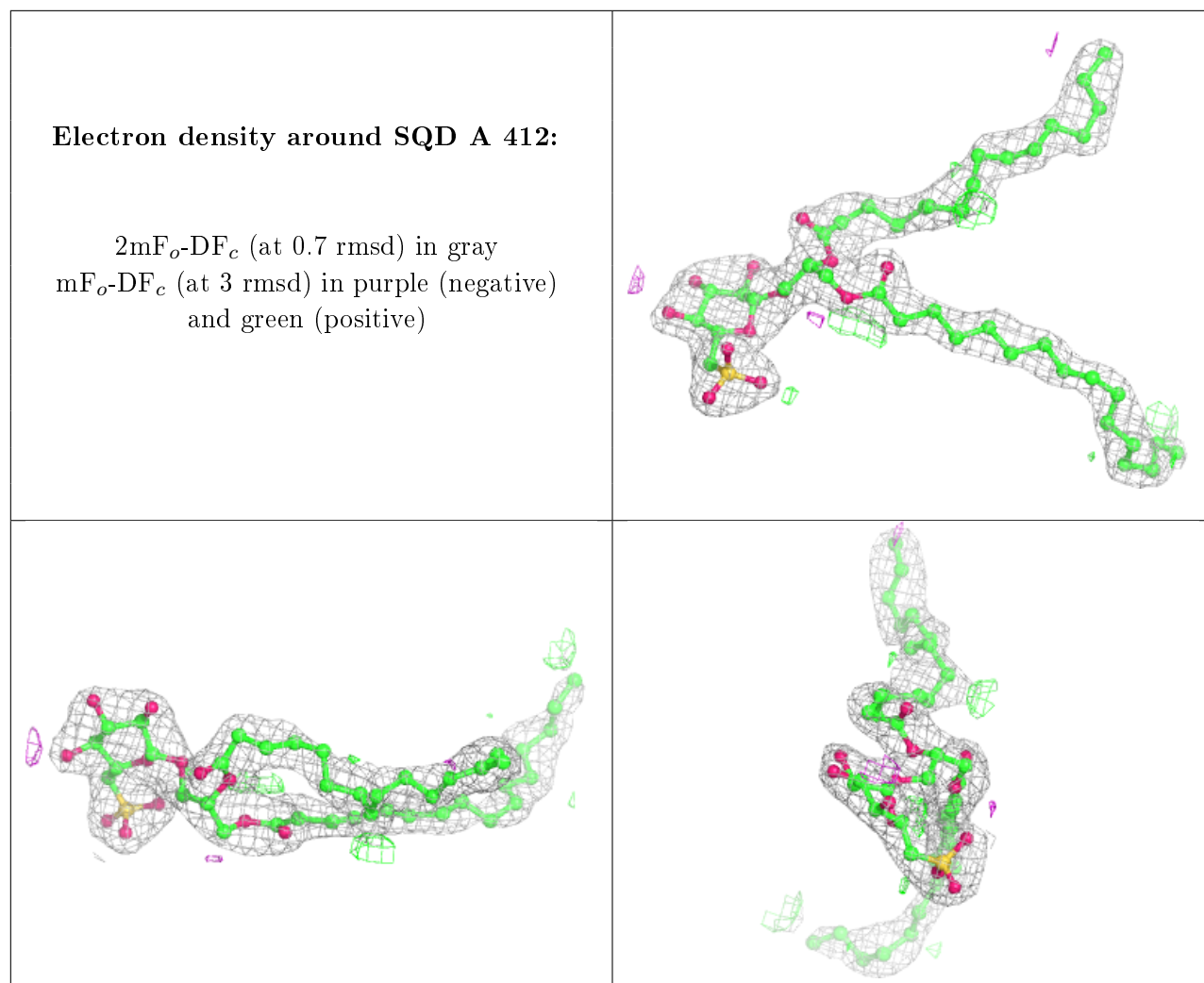
Electron density around BCR d 404:

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

**Electron density around CLA c 905:**

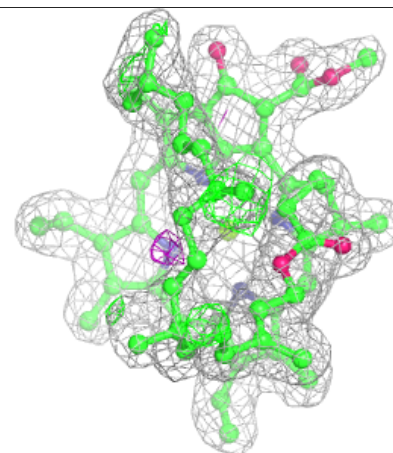
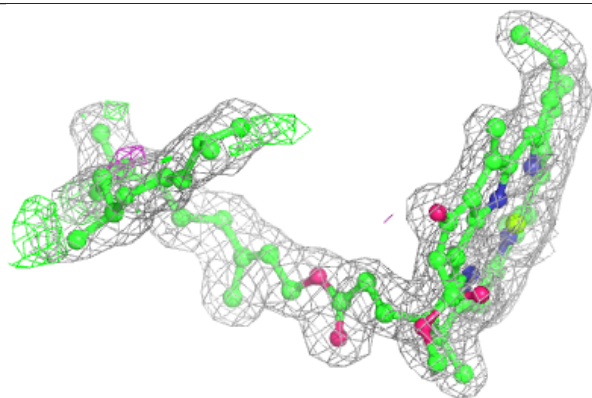
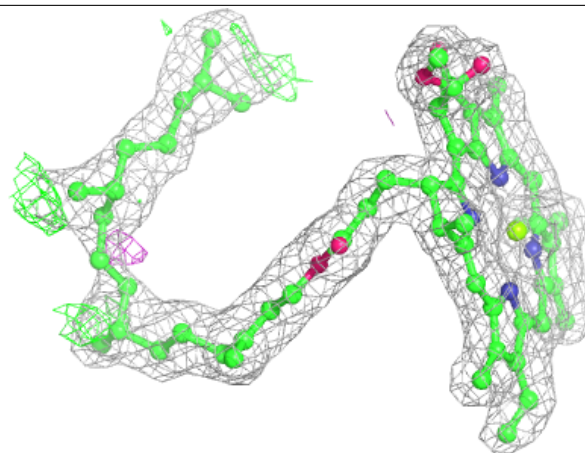
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



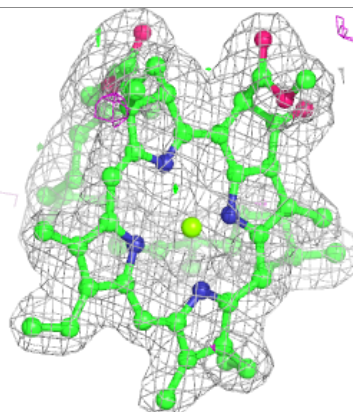
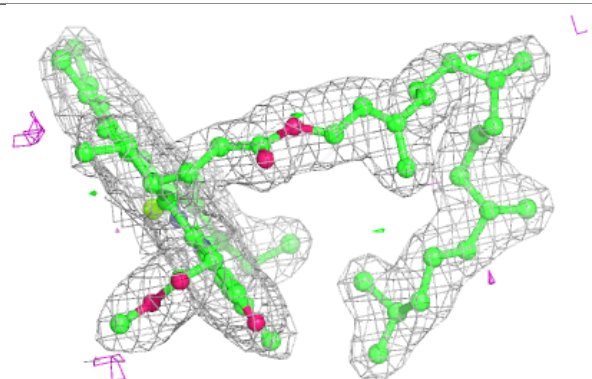
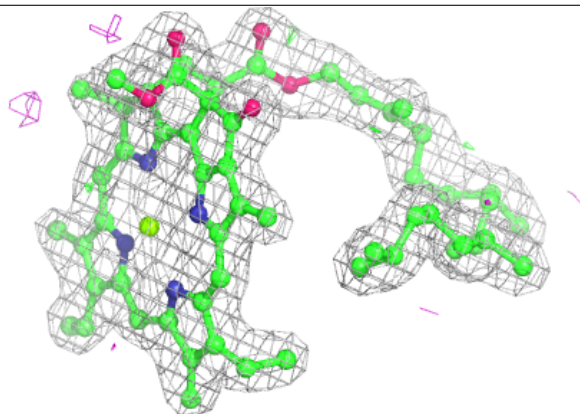


Electron density around CLA B 607:

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

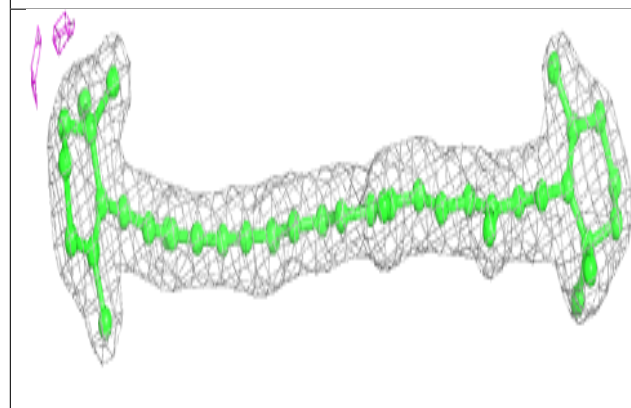
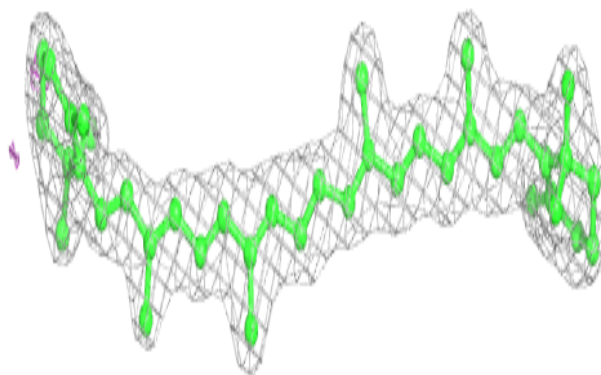
**Electron density around CLA c 904:**

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



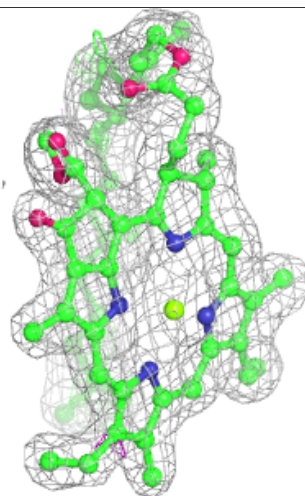
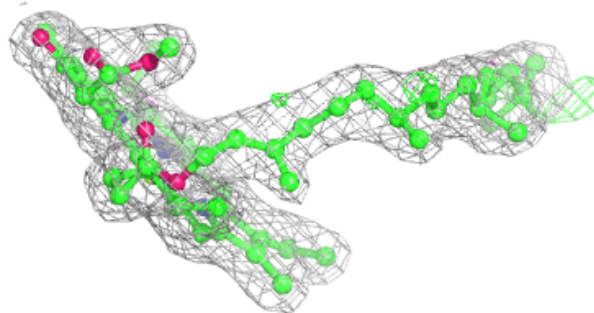
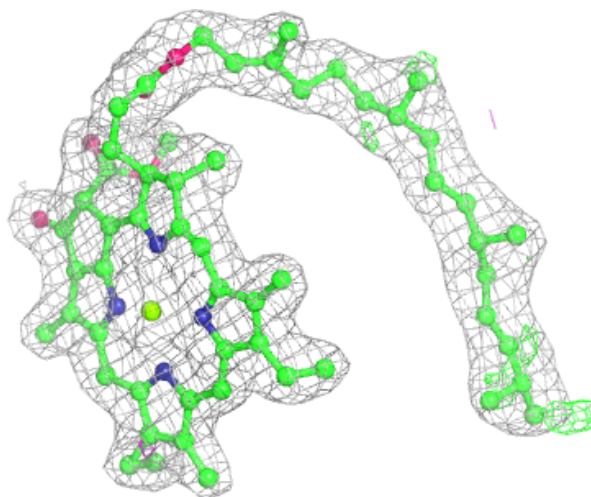
Electron density around BCR c 916:

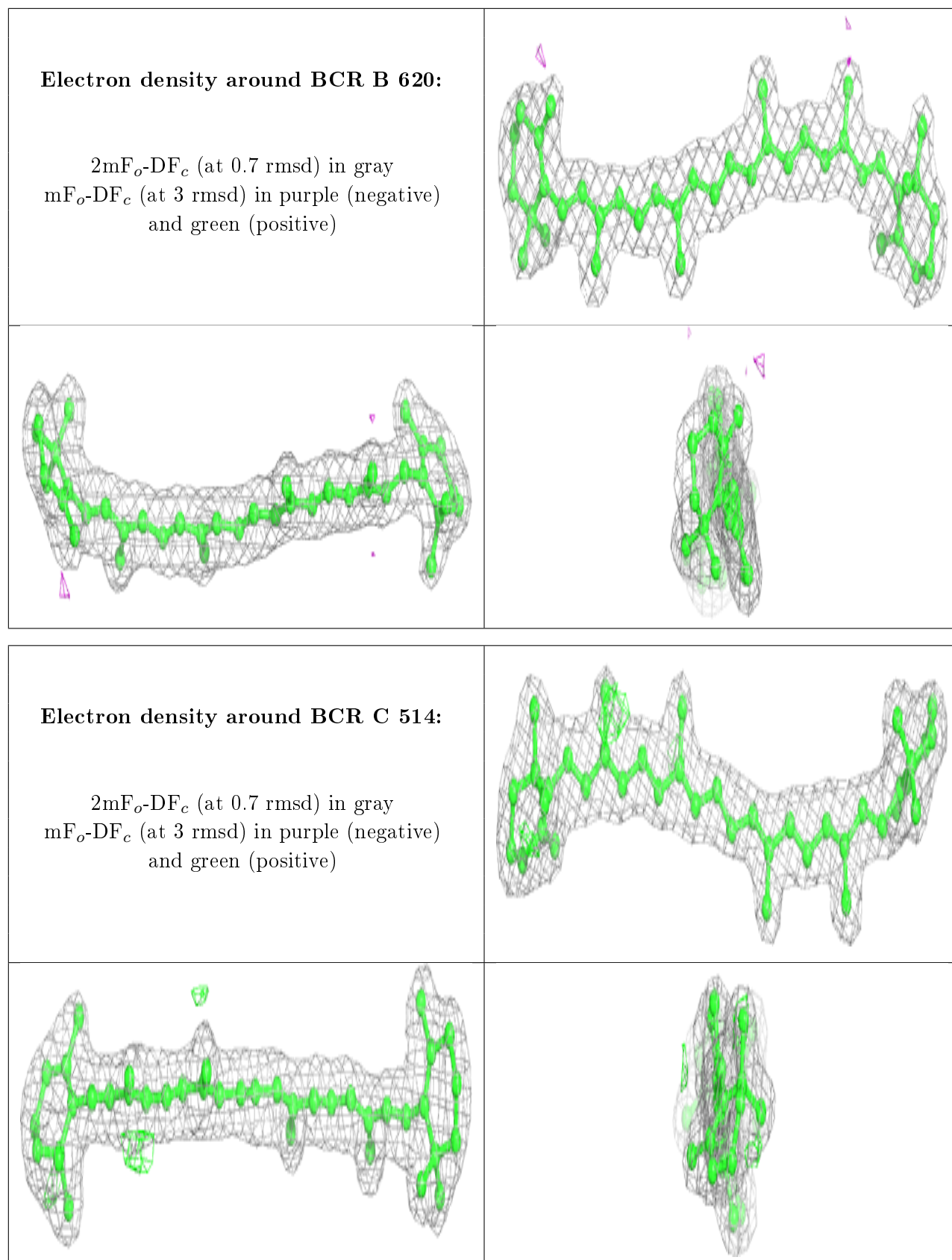
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

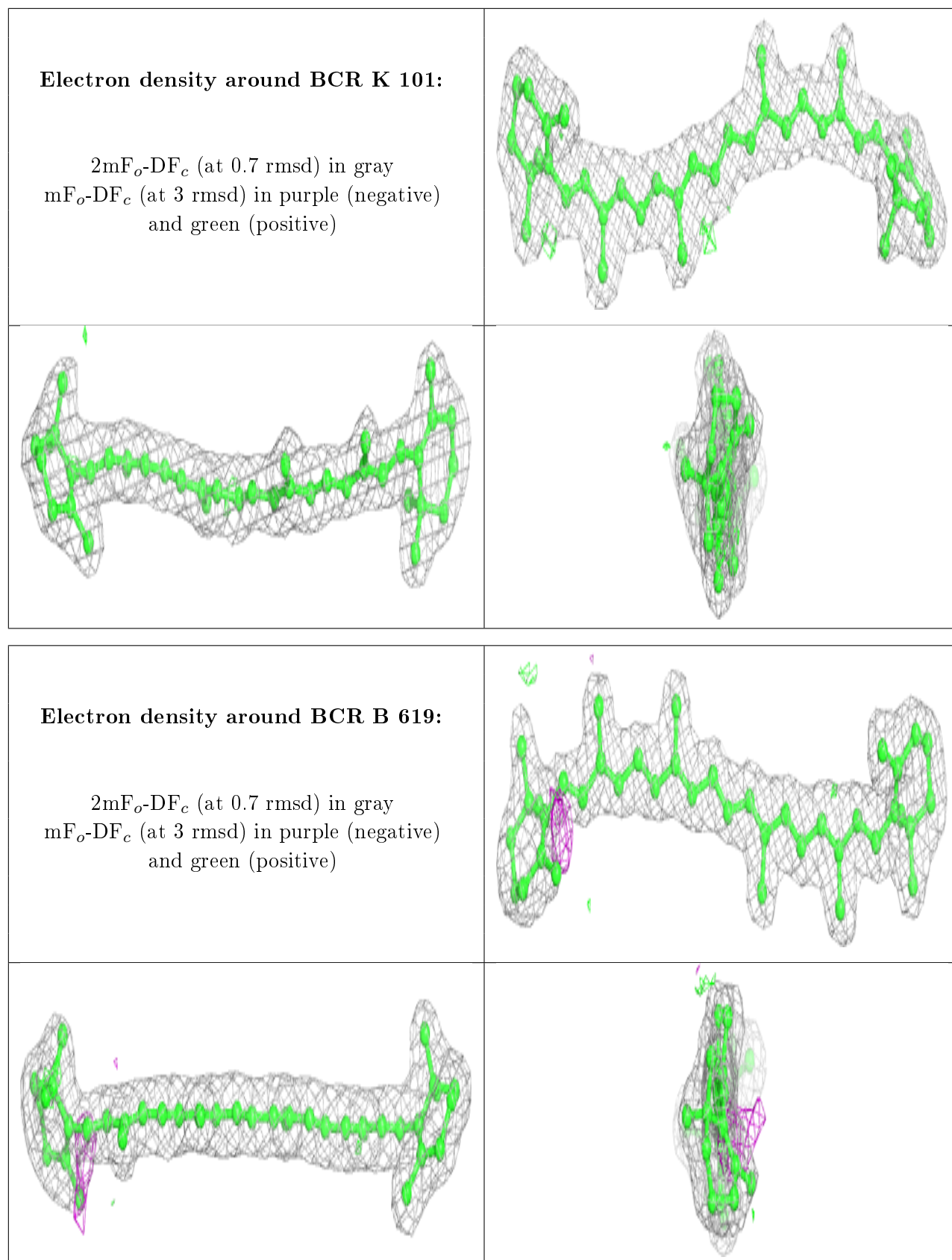


Electron density around CLA c 908:

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

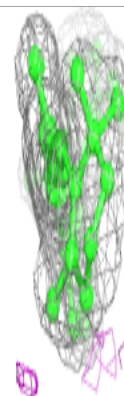
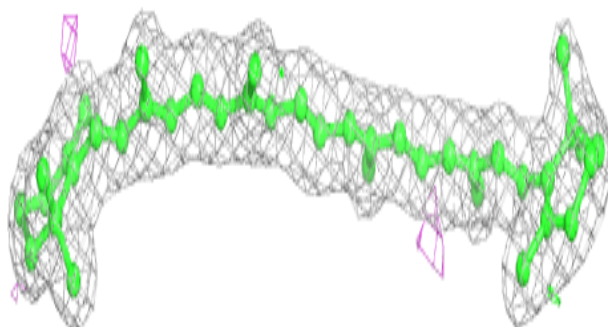
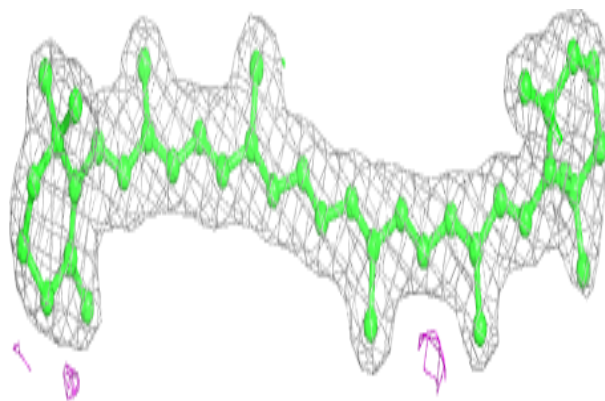




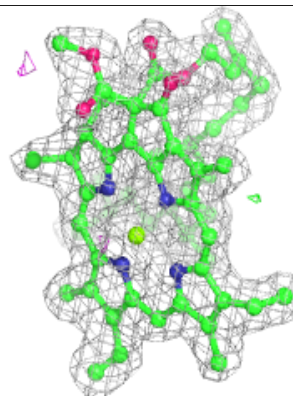
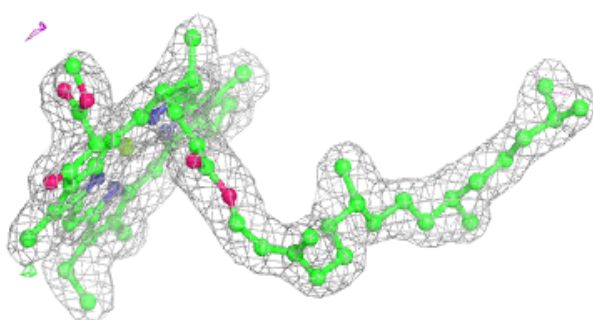
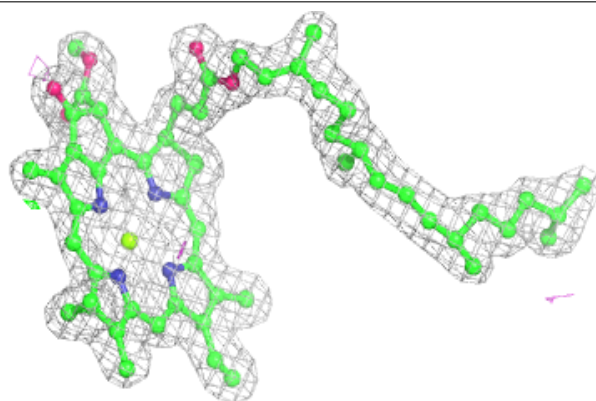


Electron density around BCR b 622:

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

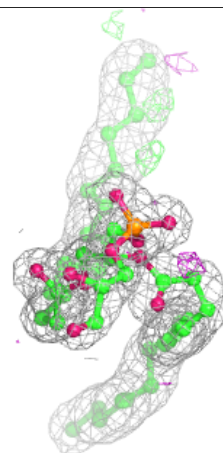
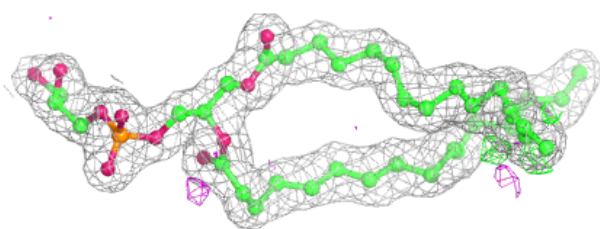
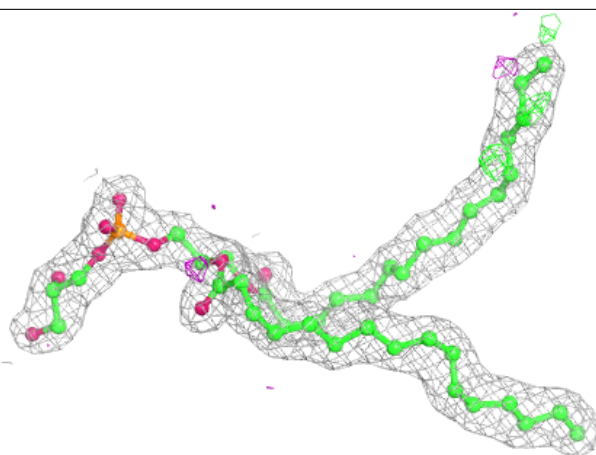
**Electron density around CLA C 511:**

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

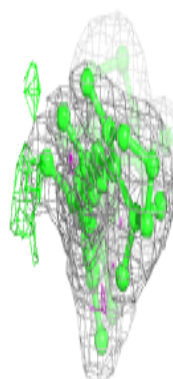
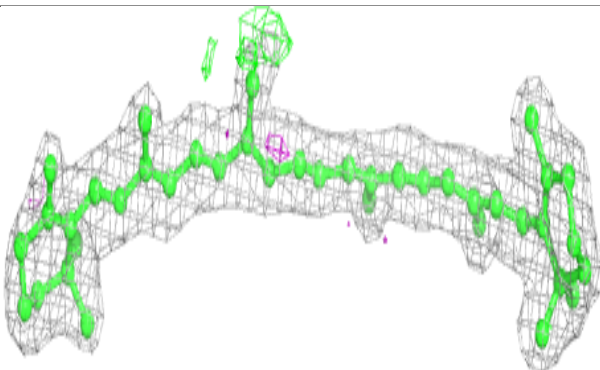
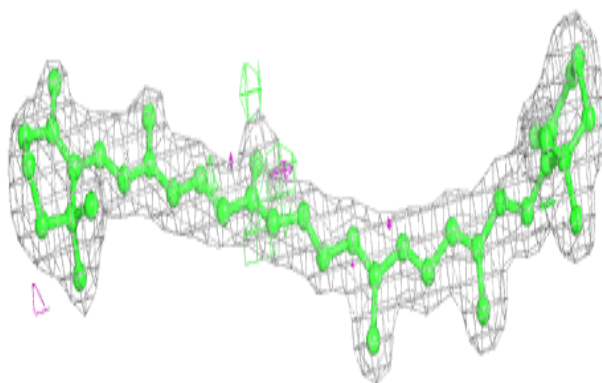


Electron density around LHG d 408:

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

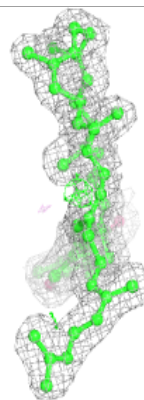
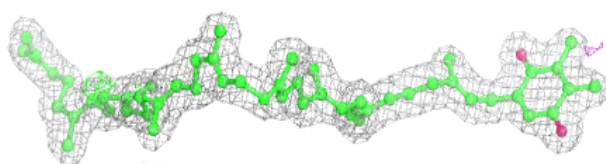
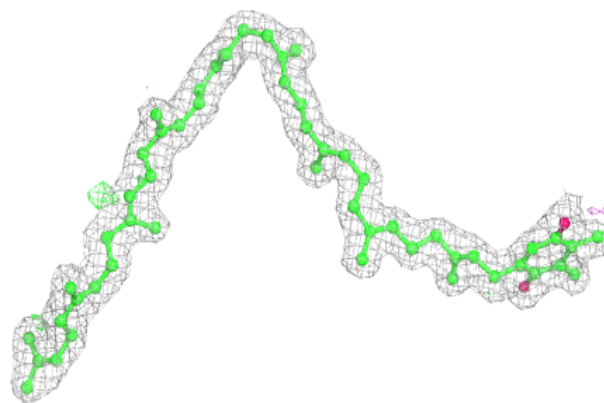
**Electron density around BCR t 101:**

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

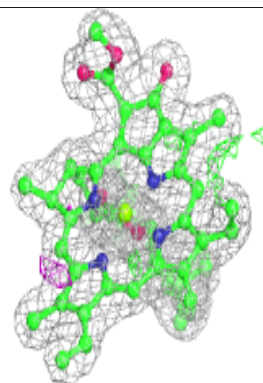
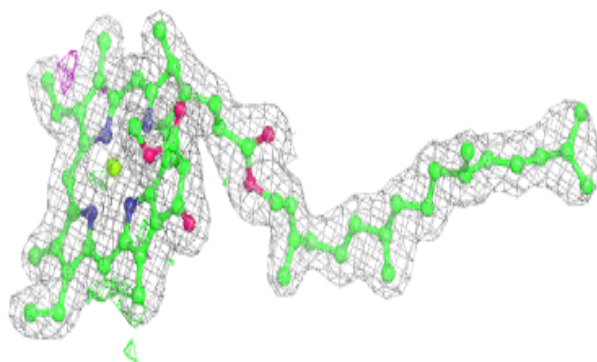
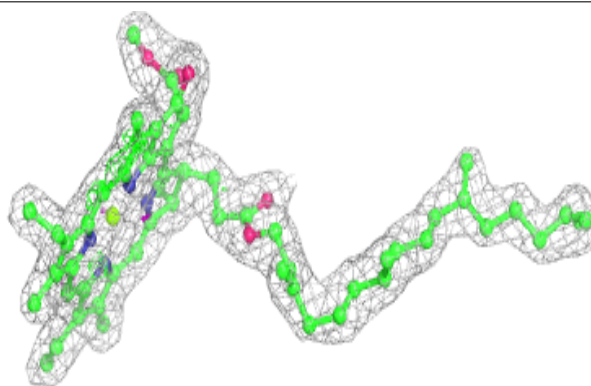


Electron density around PL9 d 405:

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

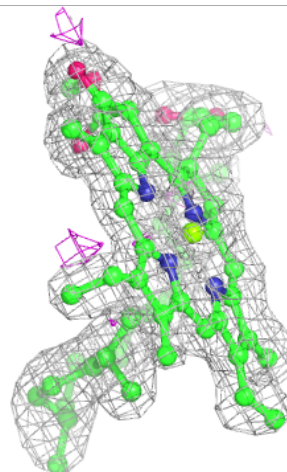
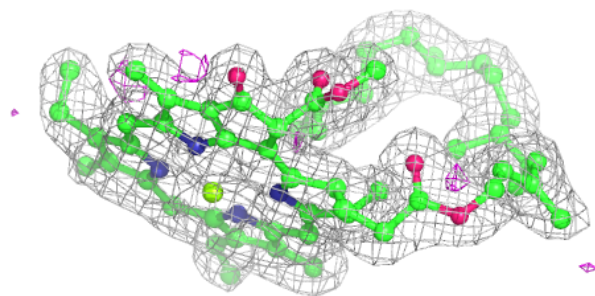
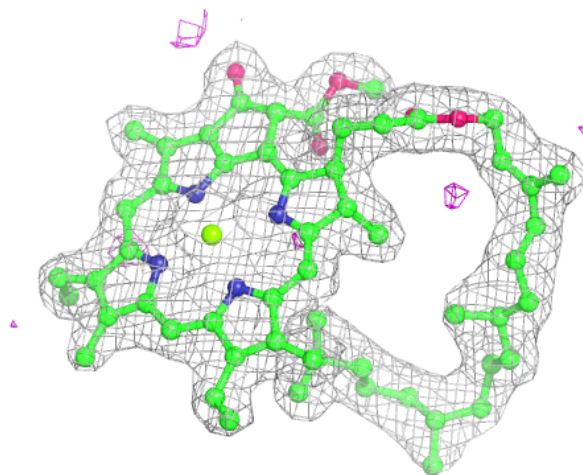
**Electron density around CLA c 903:**

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



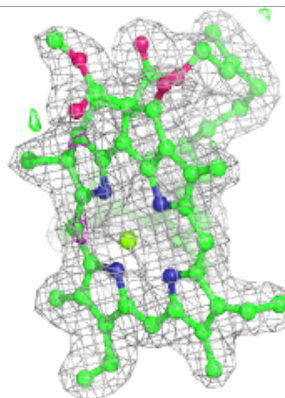
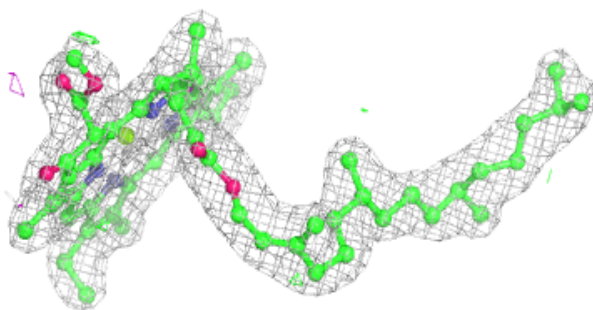
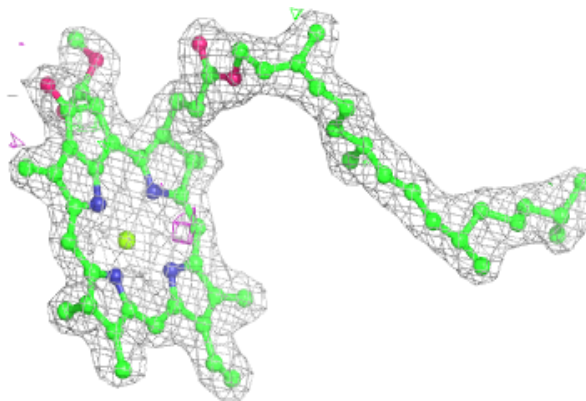
Electron density around CLA b 618:

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



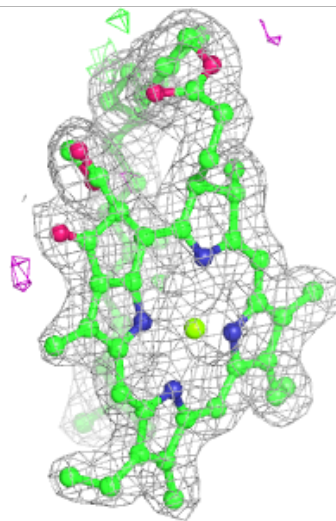
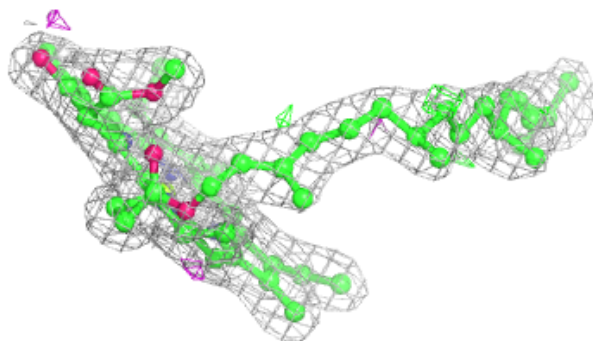
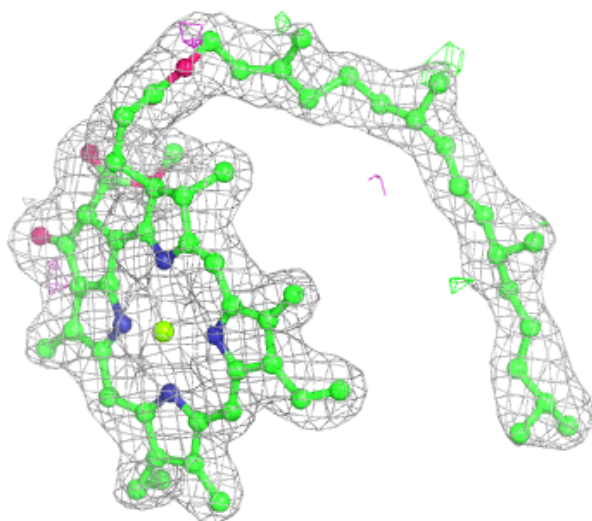
Electron density around CLA c 912:

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



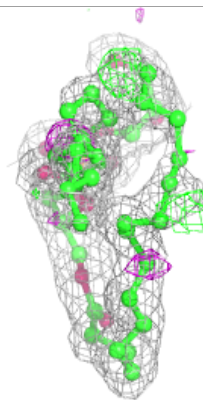
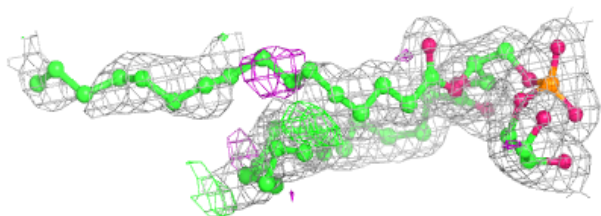
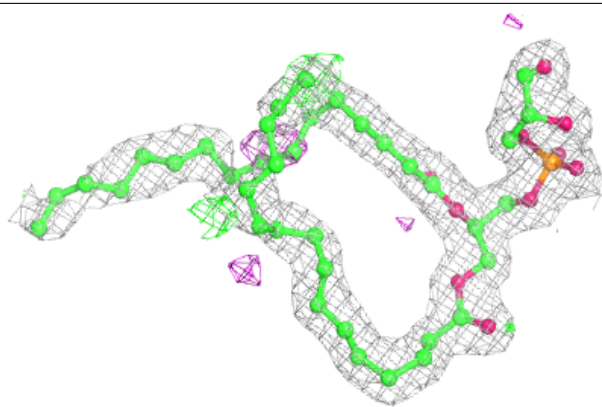
Electron density around CLA C 507:

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

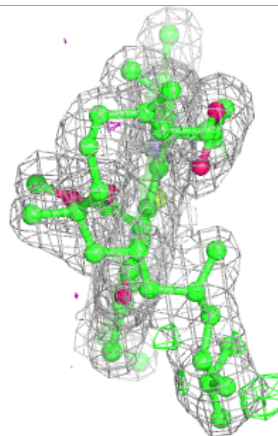
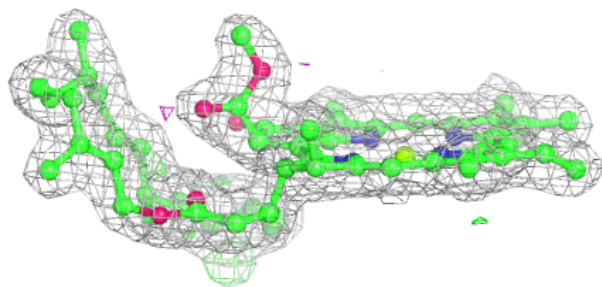
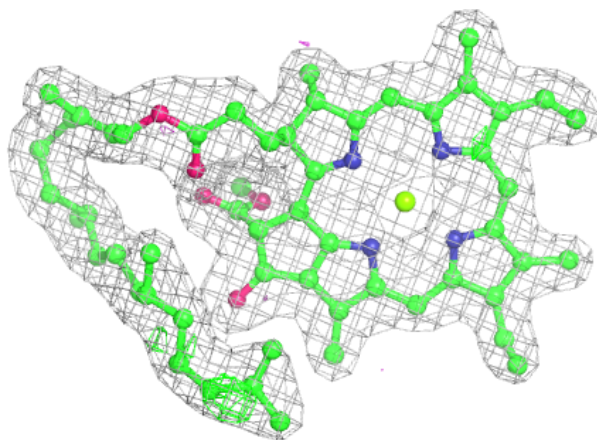


Electron density around LHG d 409:

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

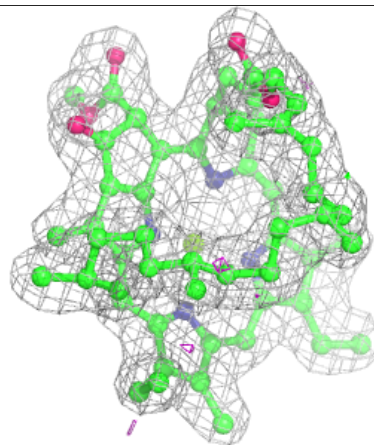
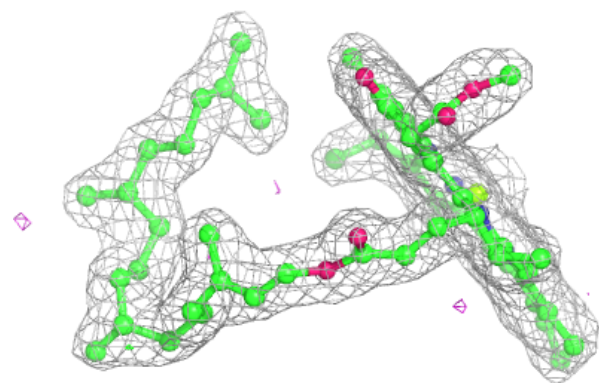
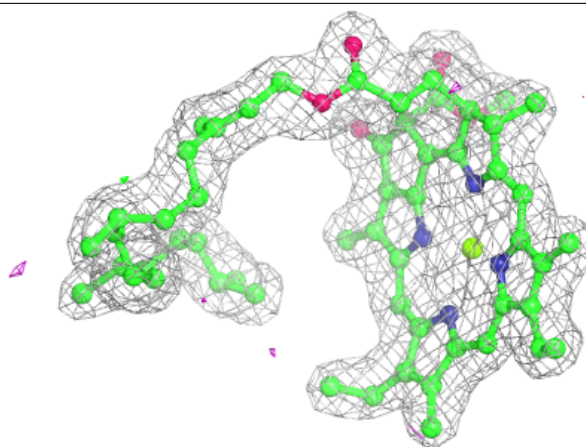
**Electron density around CLA b 613:**

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



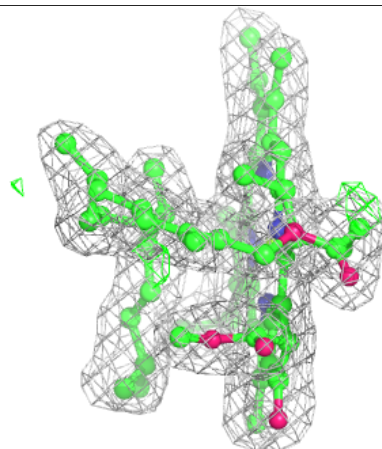
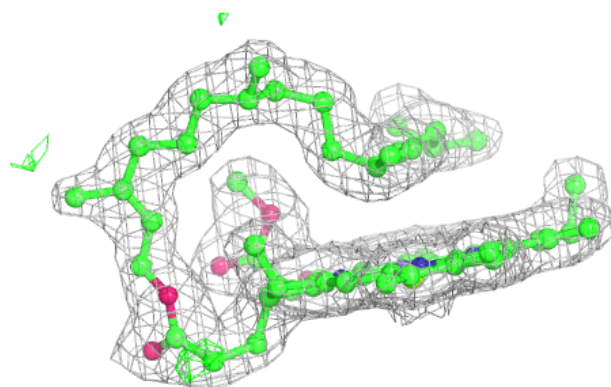
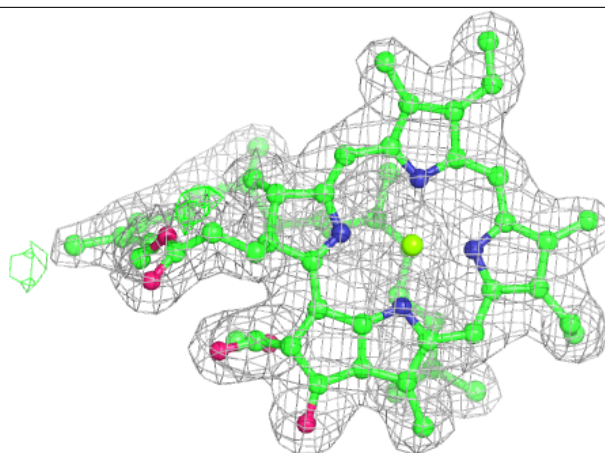
Electron density around CLA C 503:

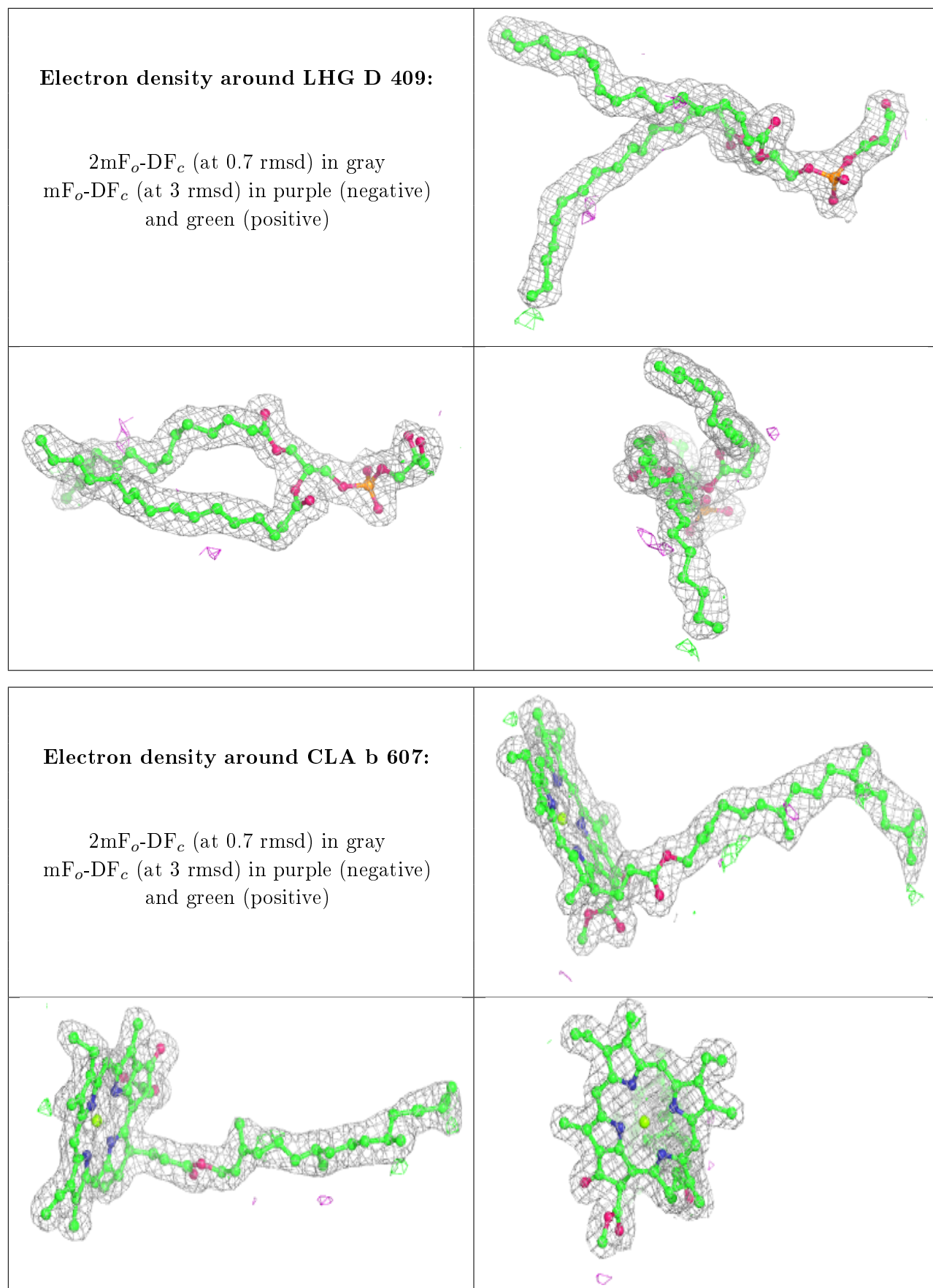
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA C 510:

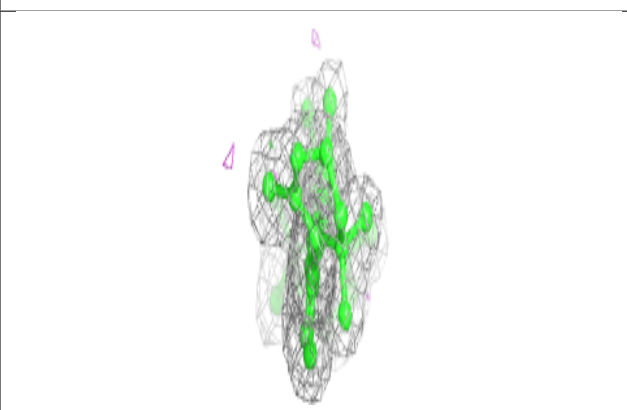
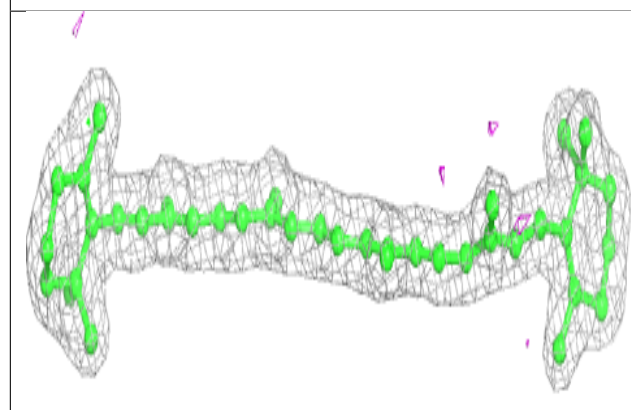
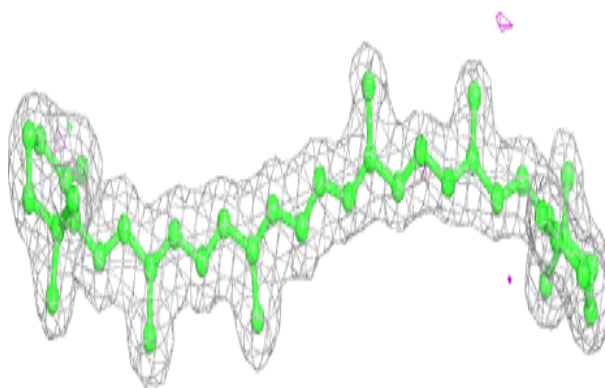
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



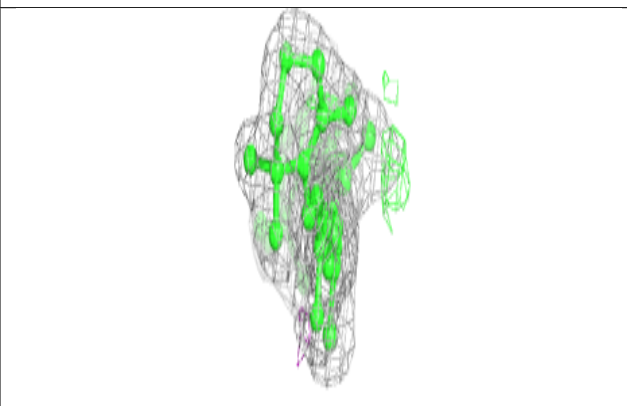
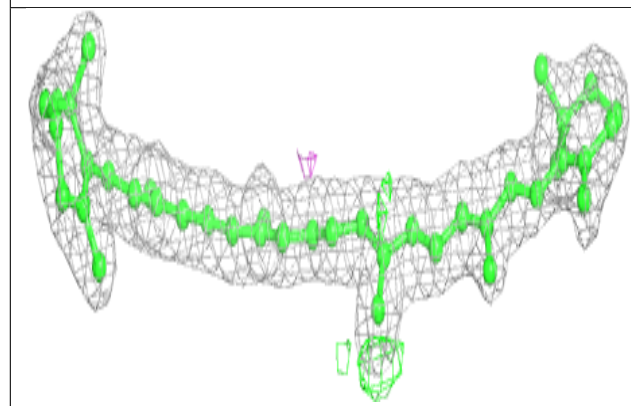
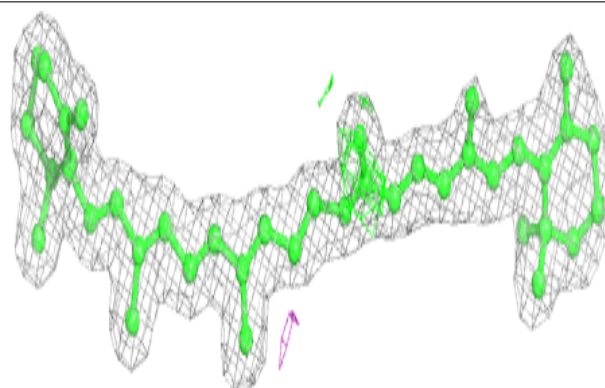


Electron density around BCR a 415:

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

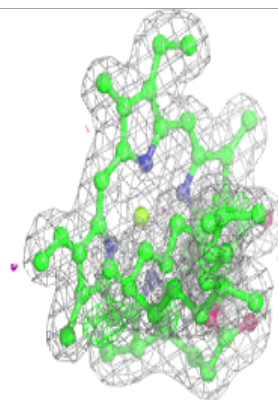
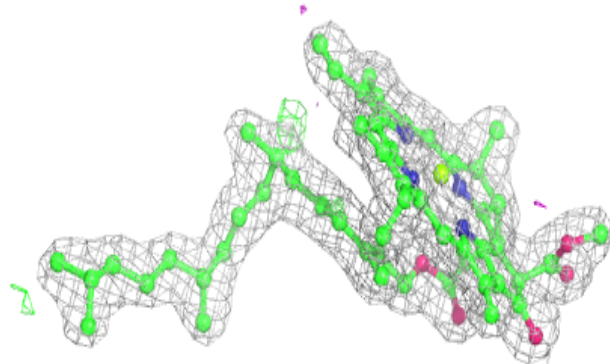
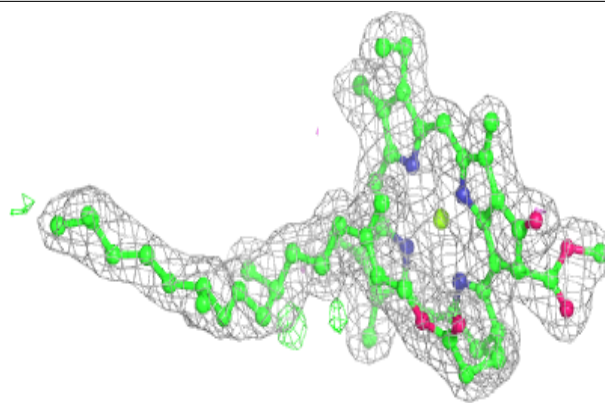
**Electron density around BCR T 101:**

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

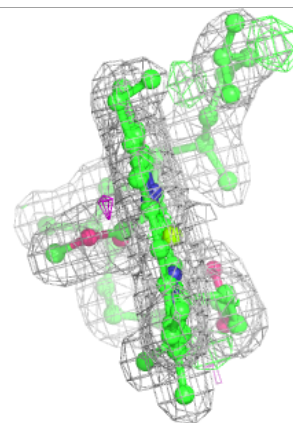
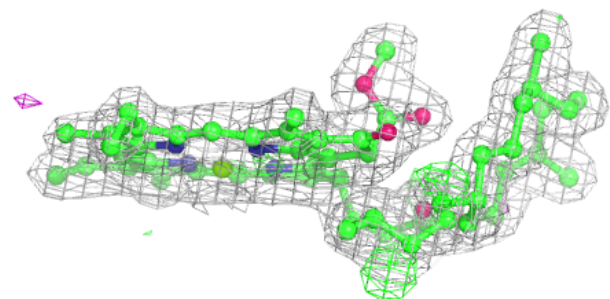
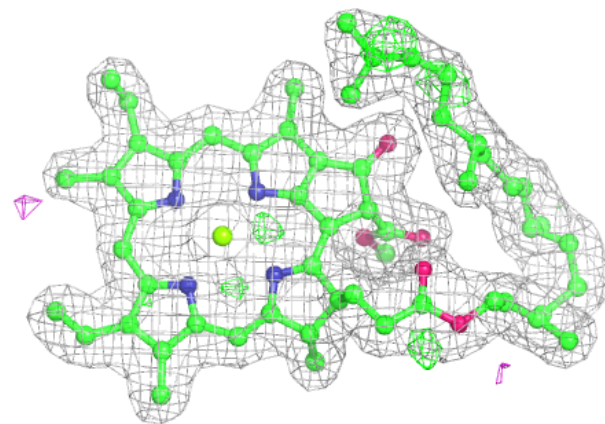


Electron density around CLA c 906:

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

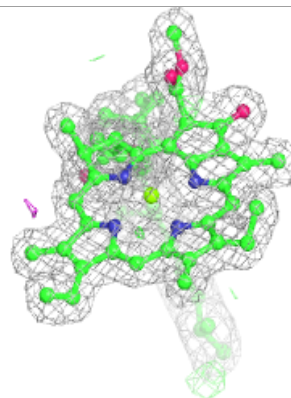
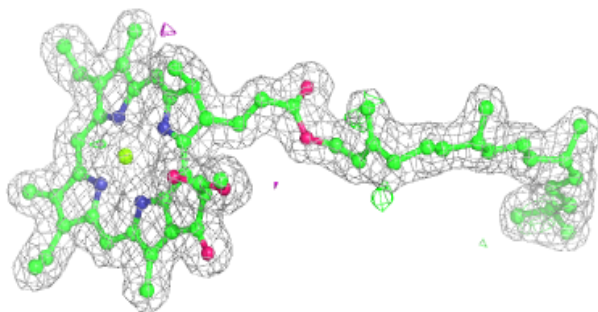
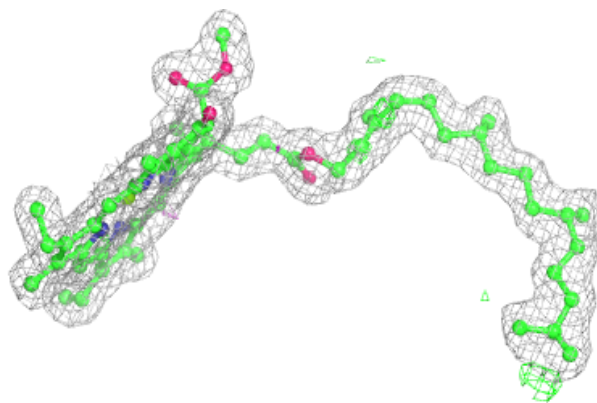
**Electron density around CLA B 611:**

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

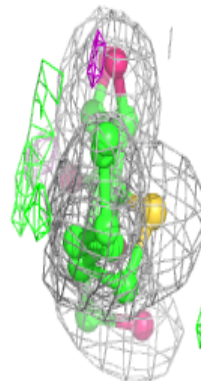
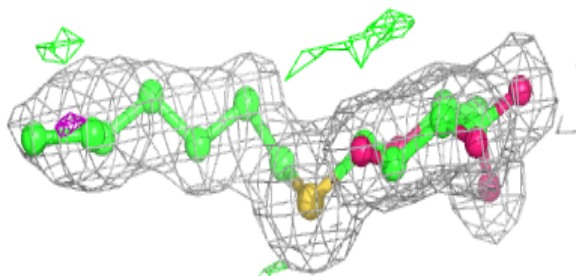
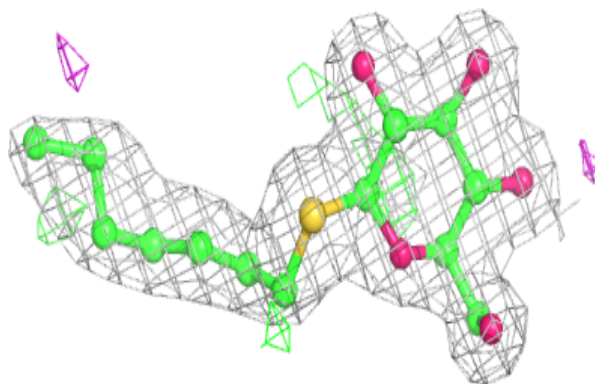


Electron density around CLA D 402:

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

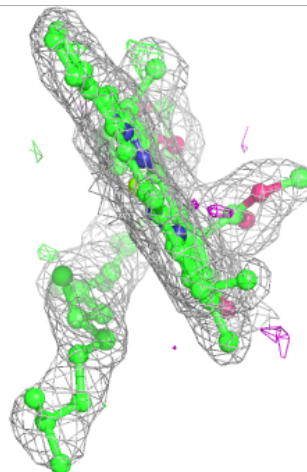
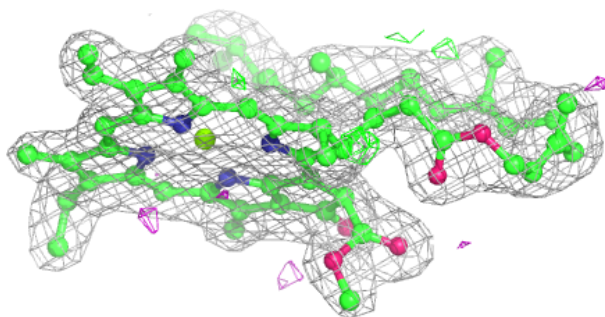
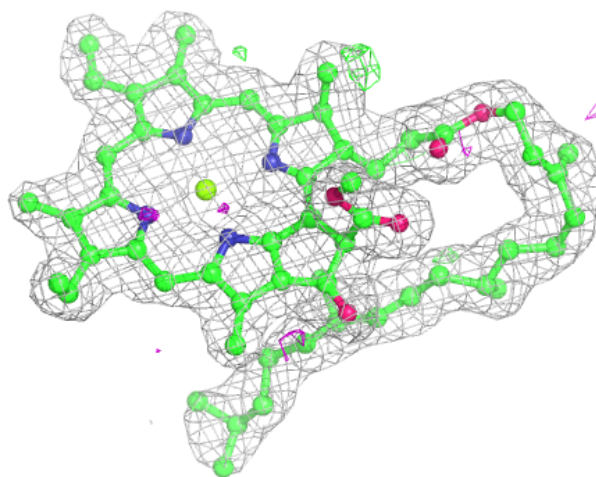
**Electron density around HTG B 624:**

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



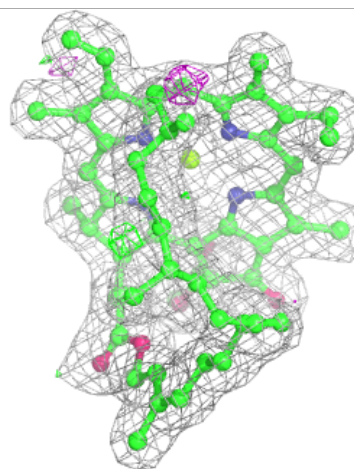
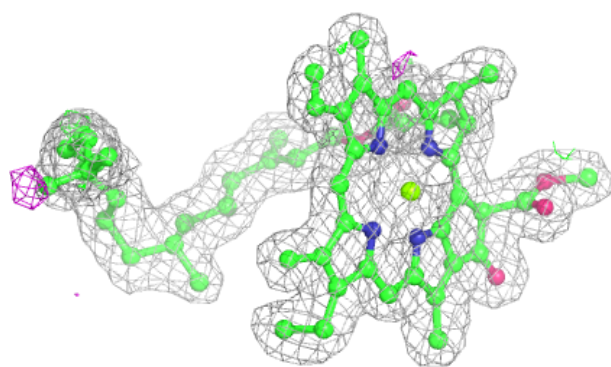
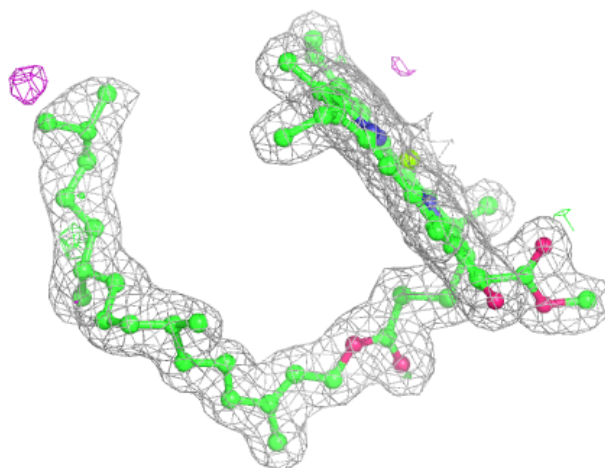
Electron density around CLA C 509:

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



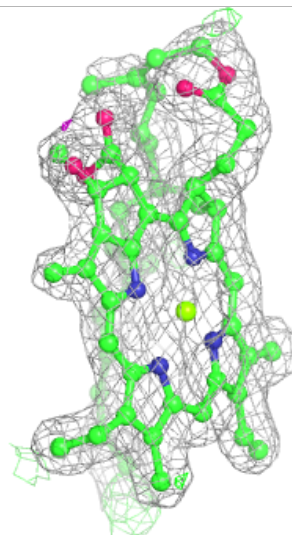
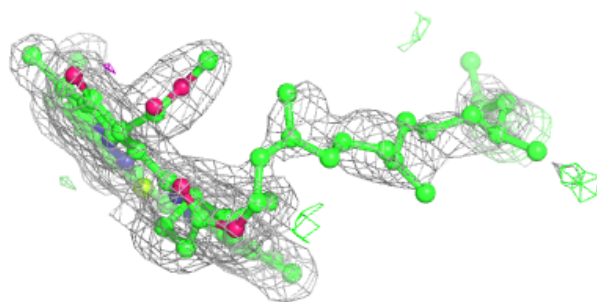
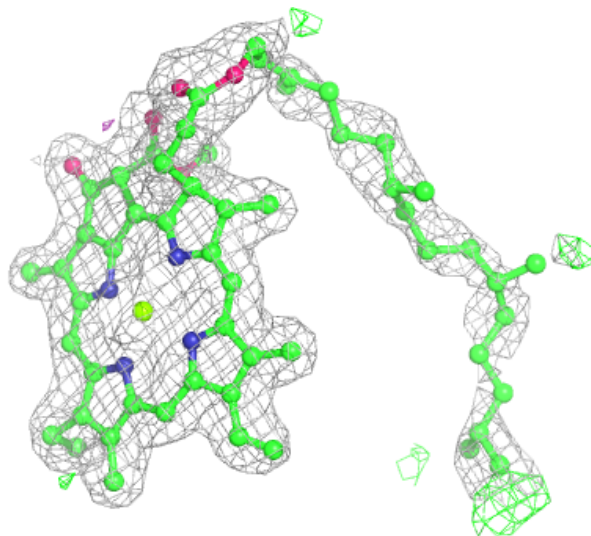
Electron density around CLA B 612:

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



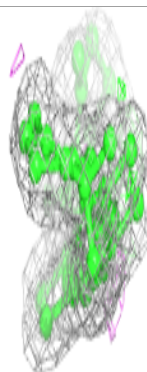
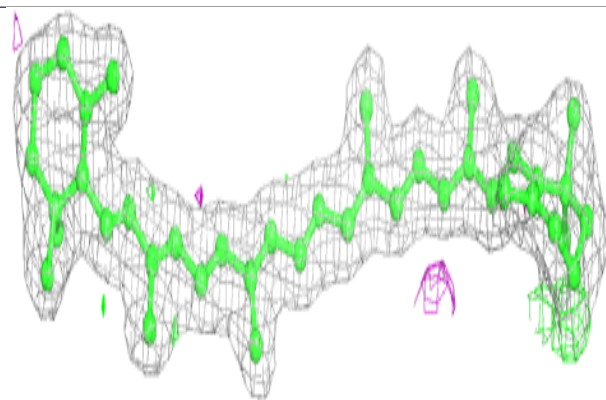
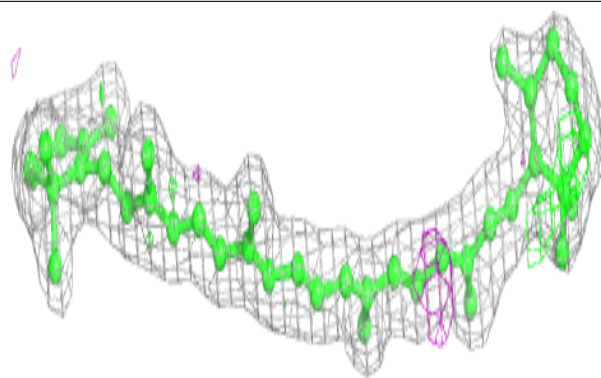
Electron density around CLA B 617:

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

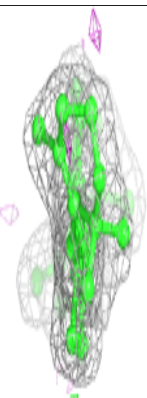
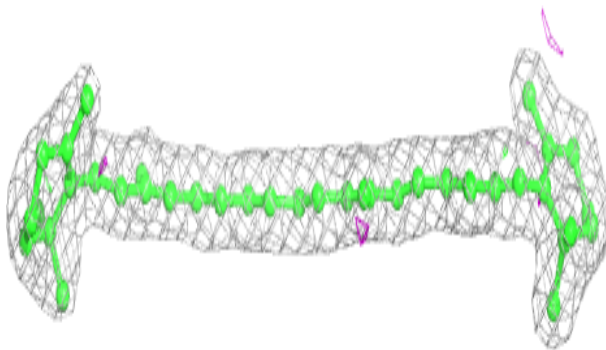
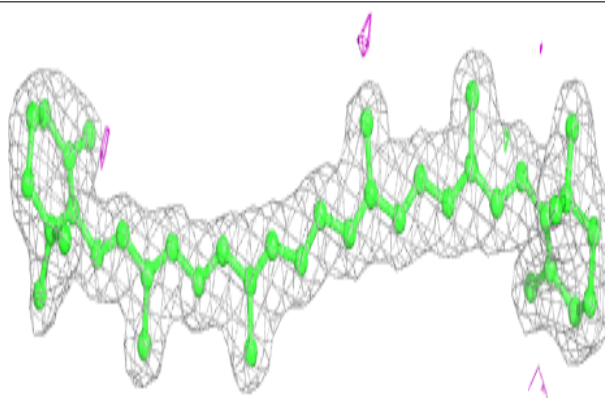


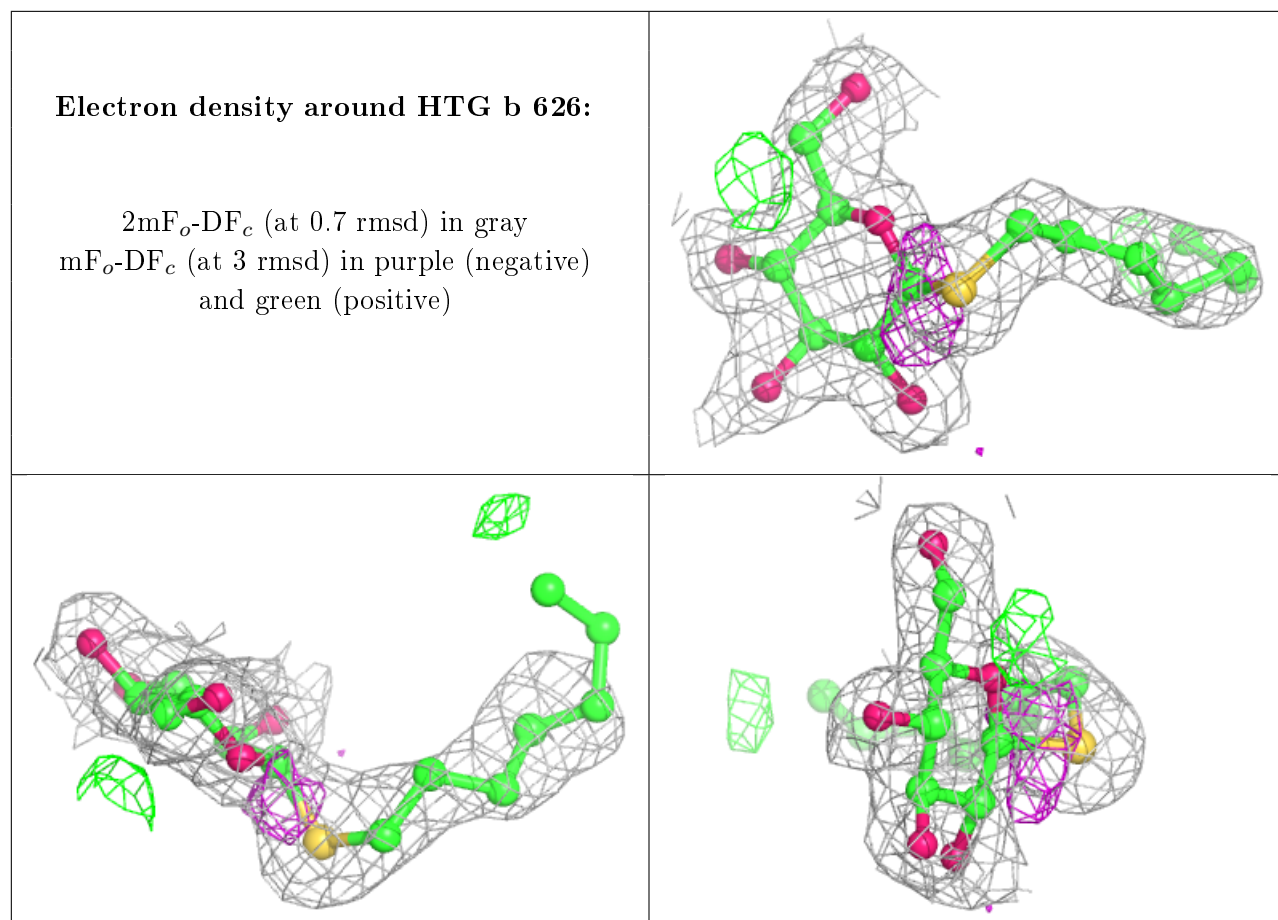
Electron density around BCR D 404:

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

**Electron density around BCR b 621:**

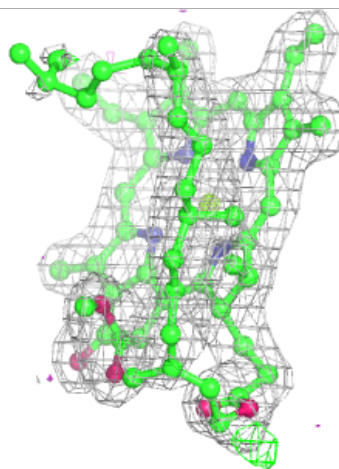
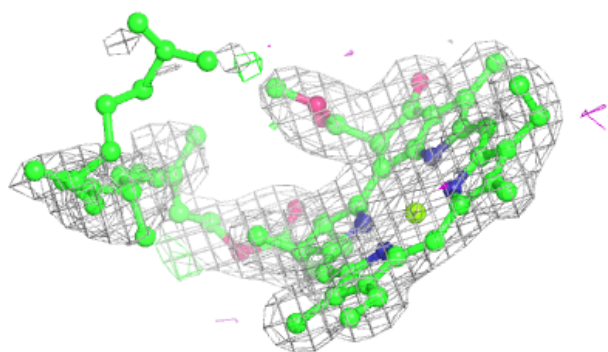
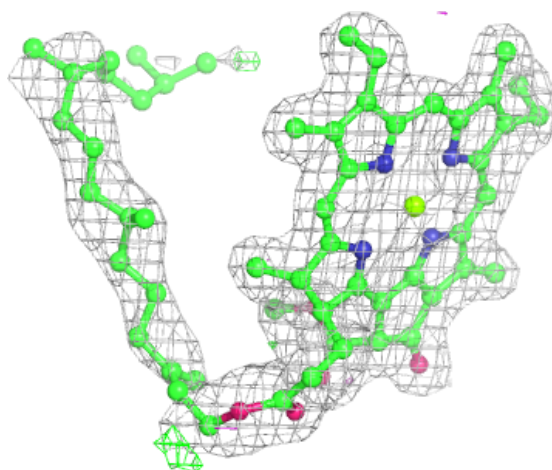
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





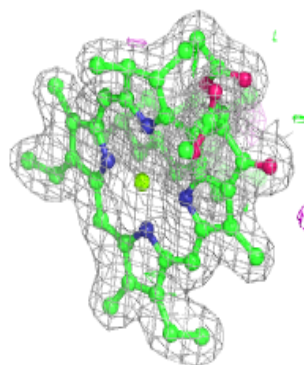
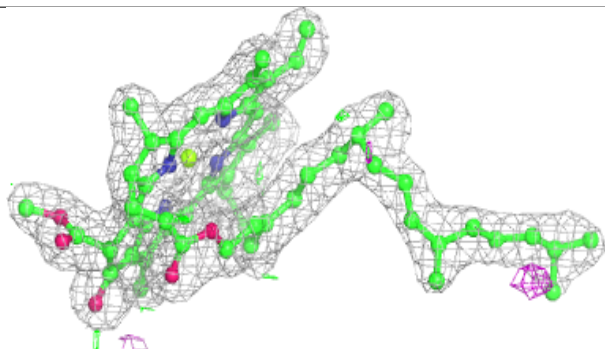
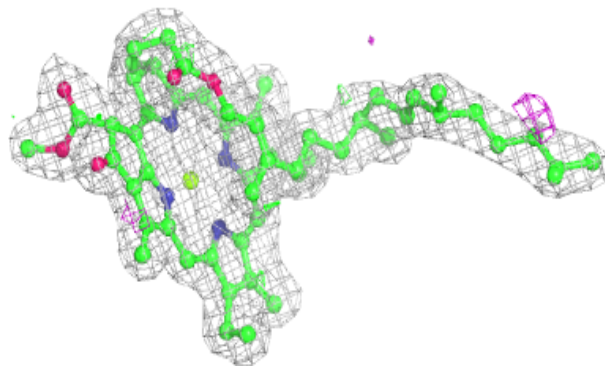
Electron density around CLA b 619:

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

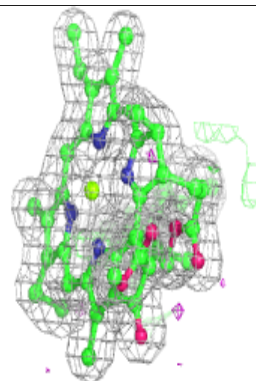
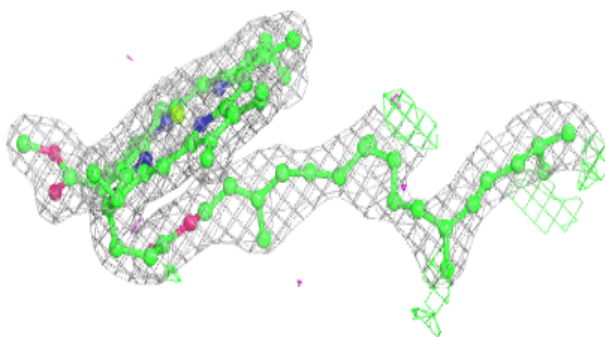
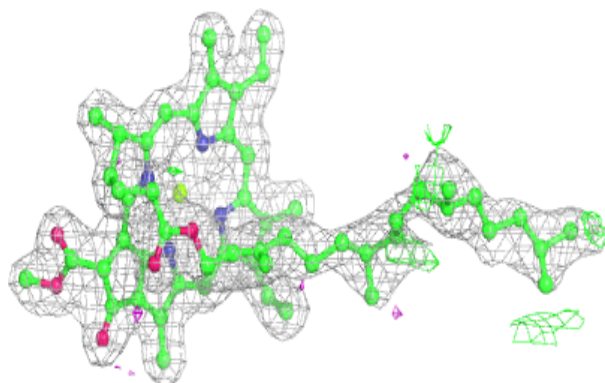


Electron density around CLA C 505:

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

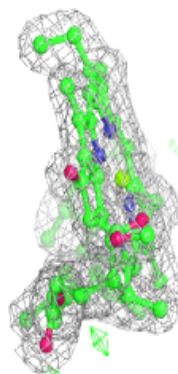
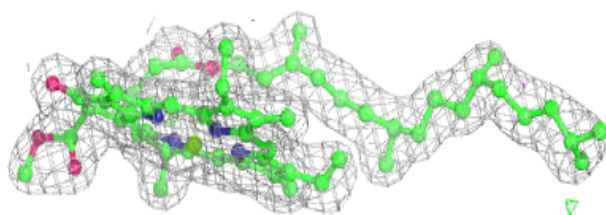
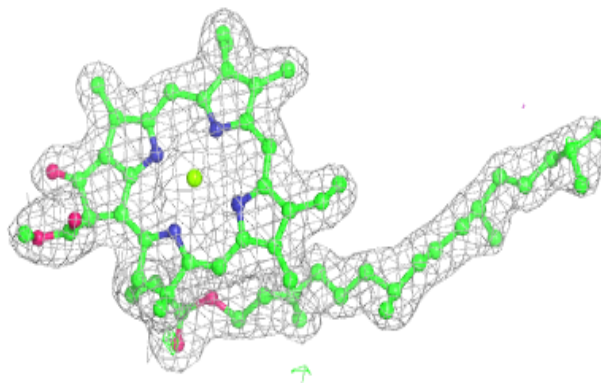
**Electron density around CLA B 615:**

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

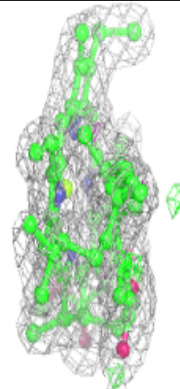
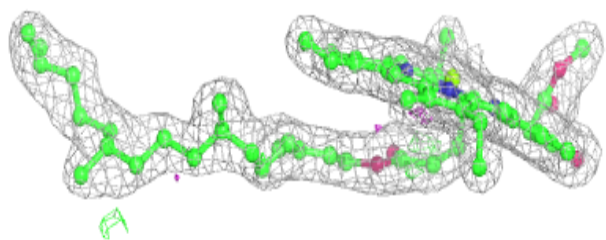
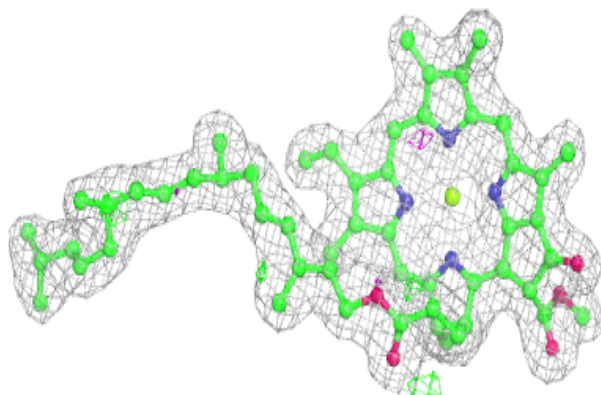


Electron density around CLA C 501:

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

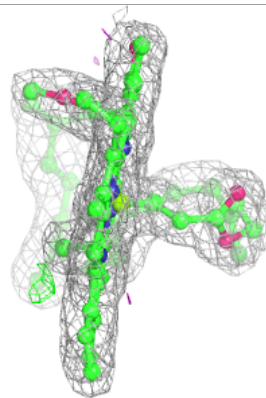
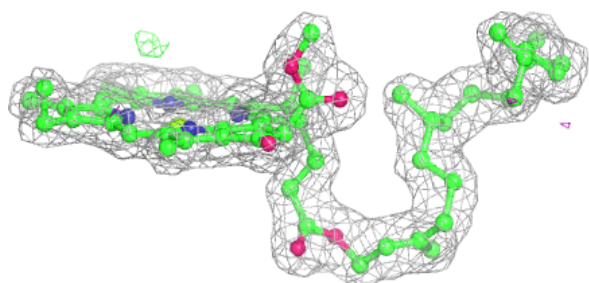
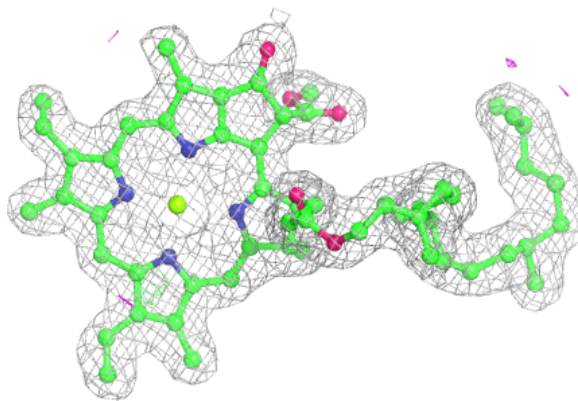
**Electron density around CLA b 606:**

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

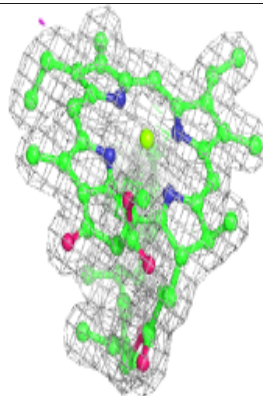
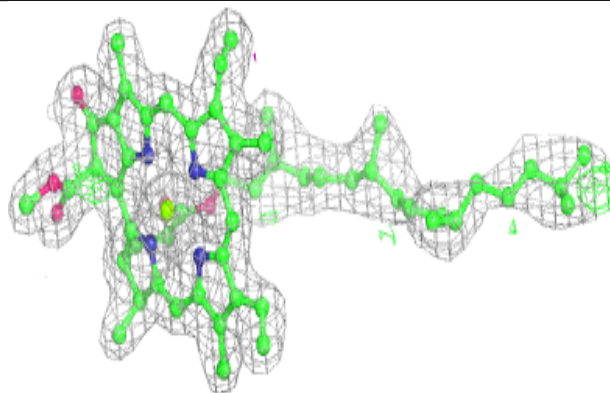
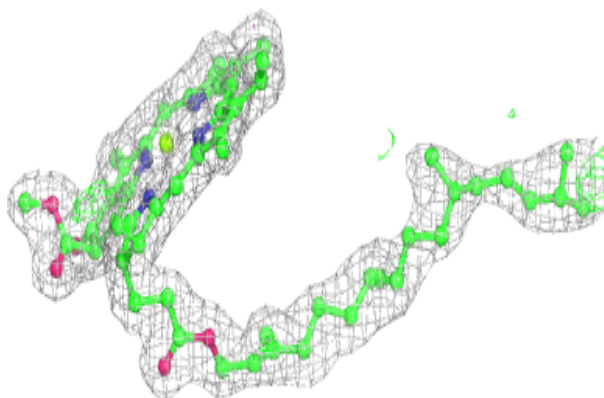


Electron density around CLA b 615:

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

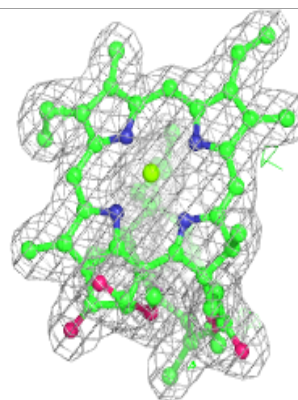
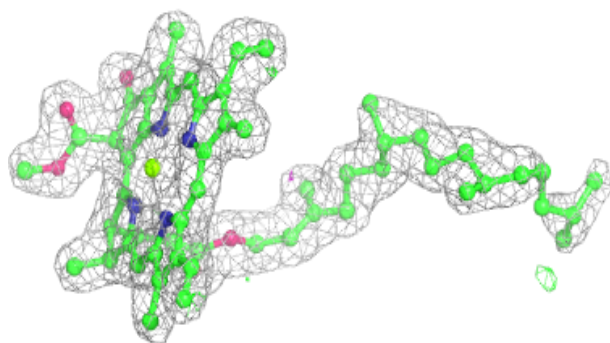
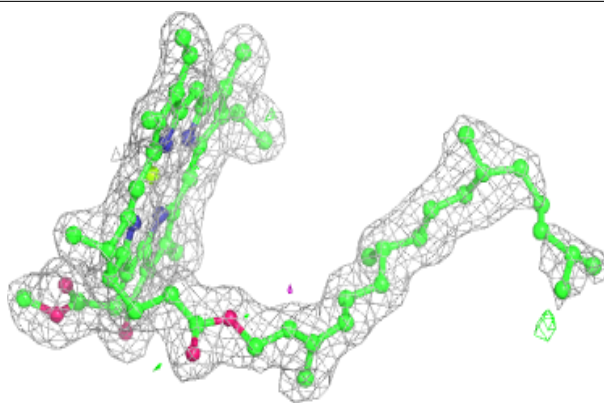
**Electron density around CLA C 504:**

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

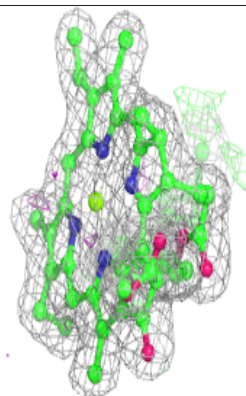
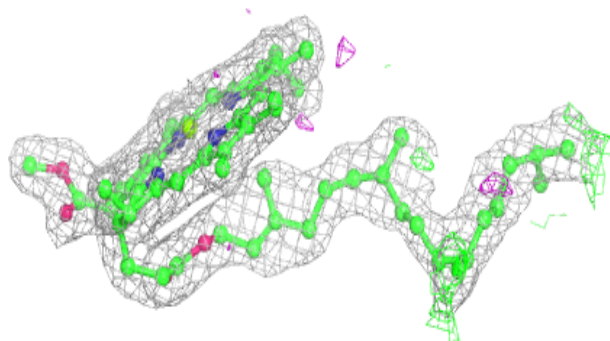
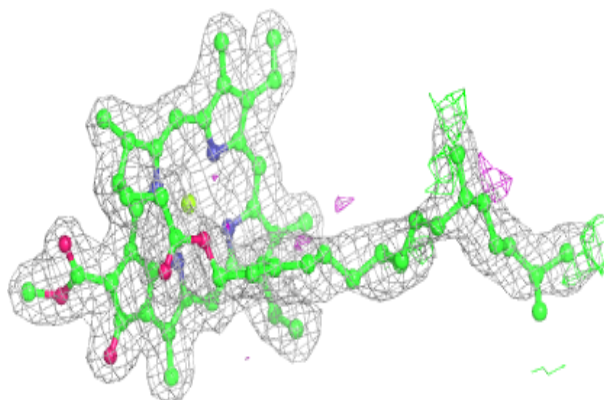


Electron density around CLA C 508:

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

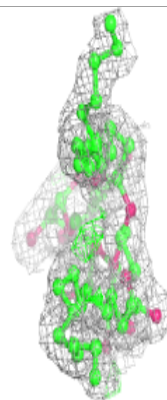
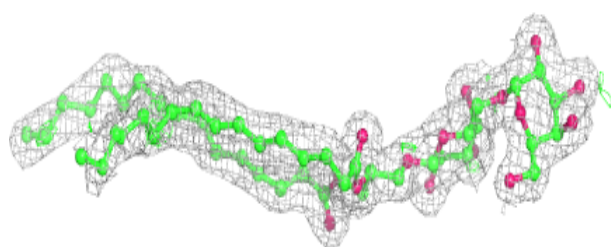
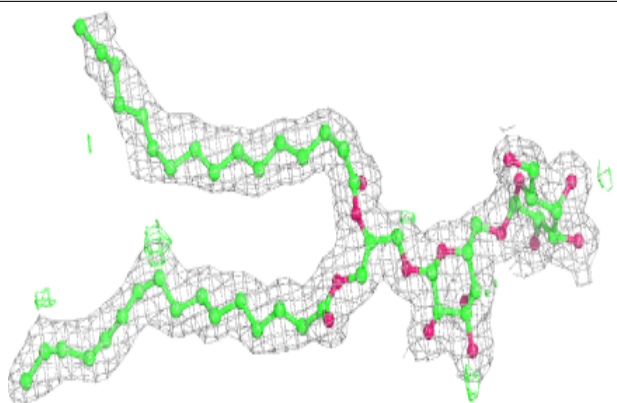
**Electron density around CLA b 617:**

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

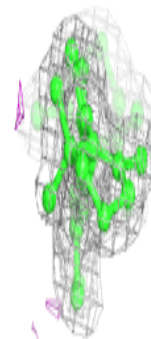
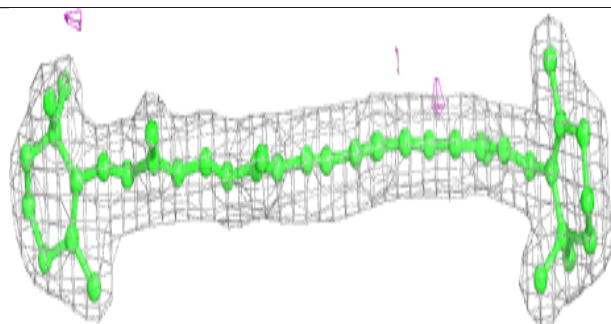
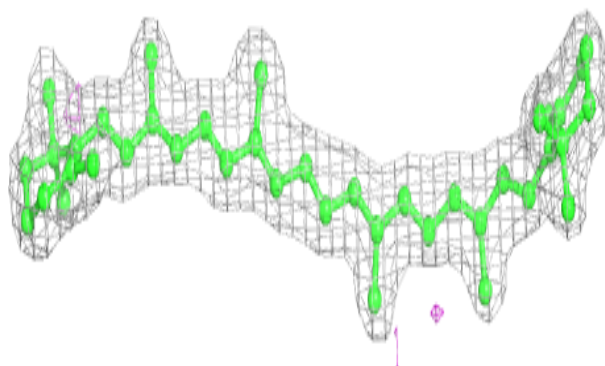


Electron density around DGD C 518:

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

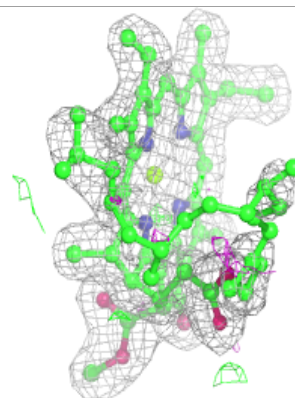
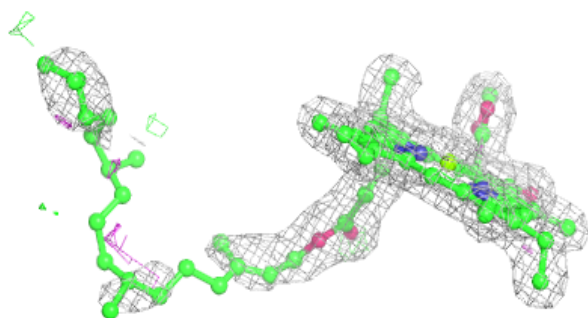
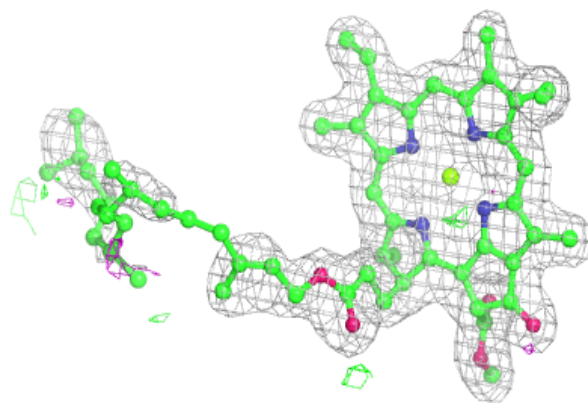
**Electron density around BCR C 515:**

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

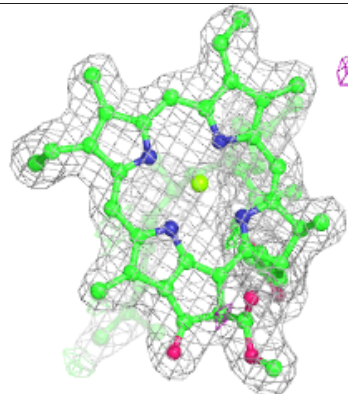
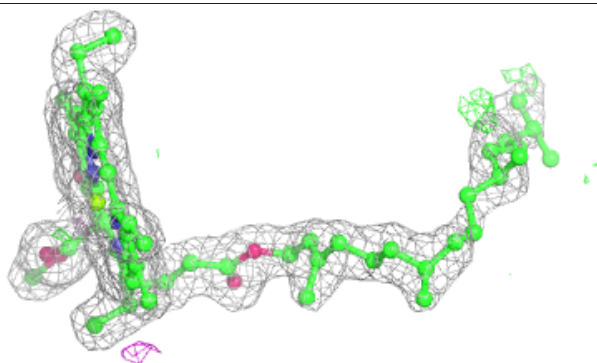
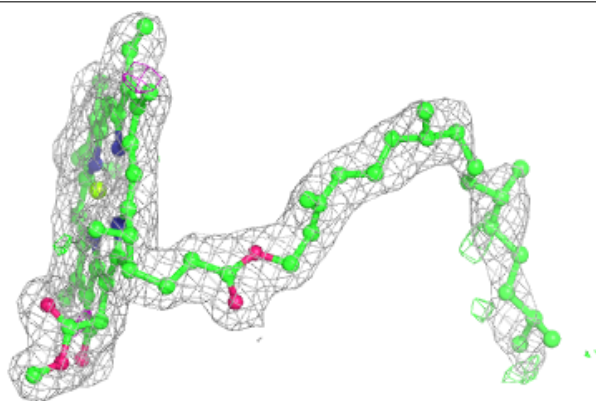


Electron density around CLA A 410:

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

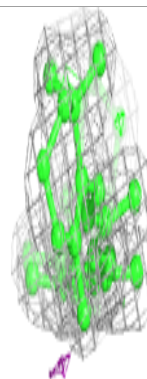
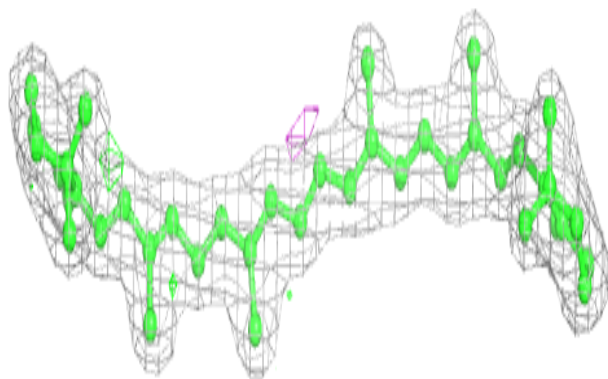
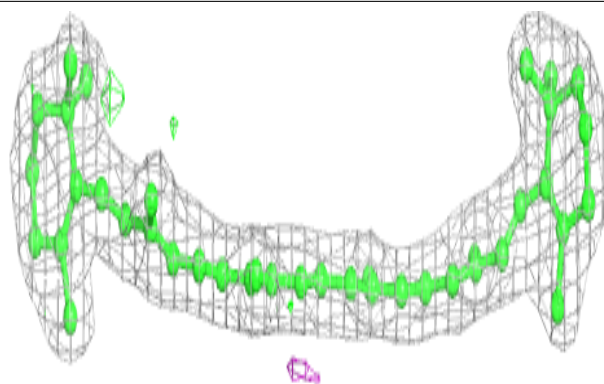
**Electron density around CLA D 403:**

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

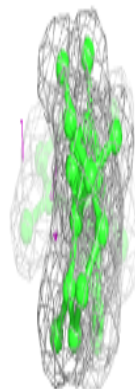
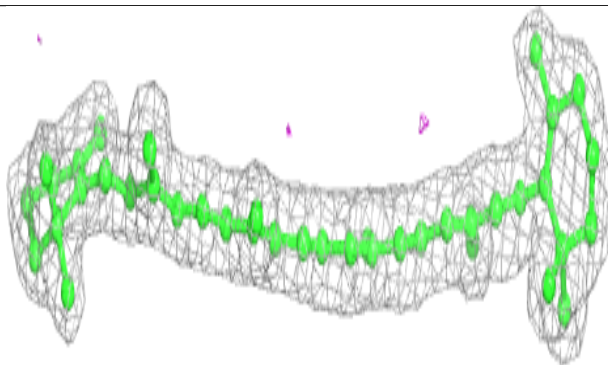
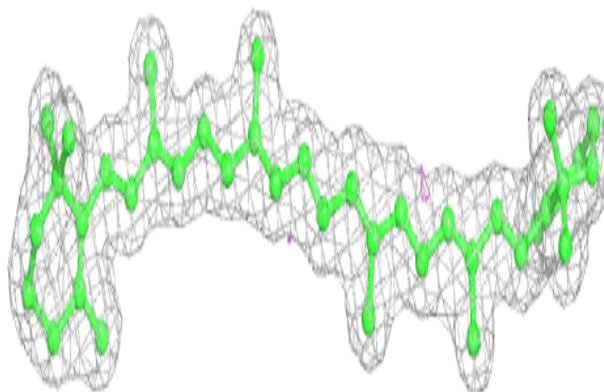


Electron density around BCR K 102:

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

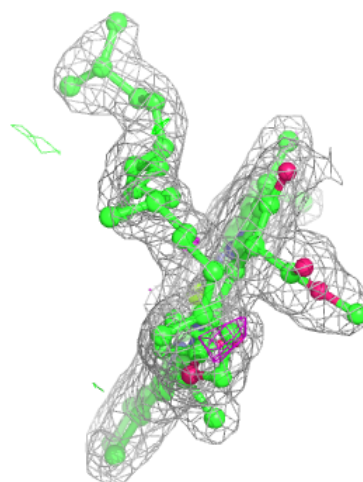
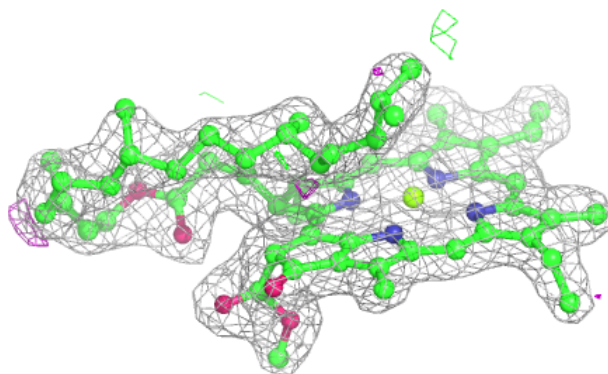
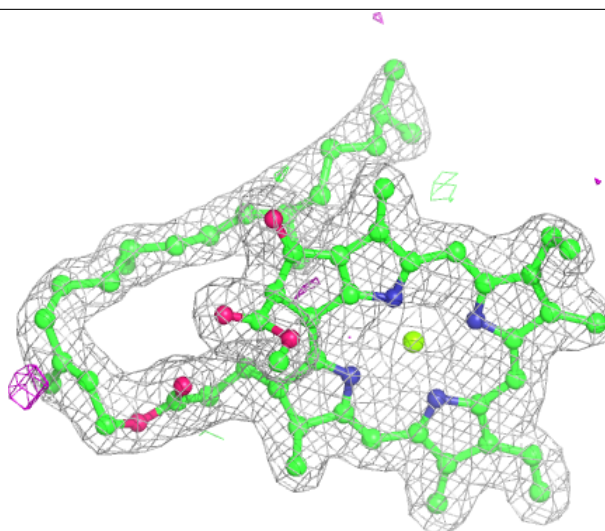
**Electron density around BCR B 618:**

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



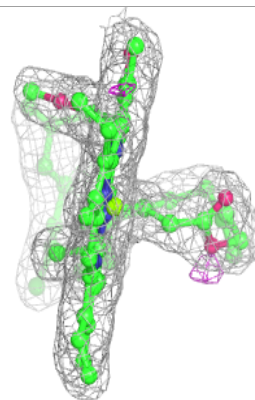
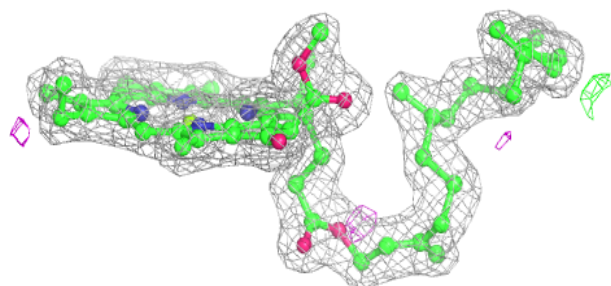
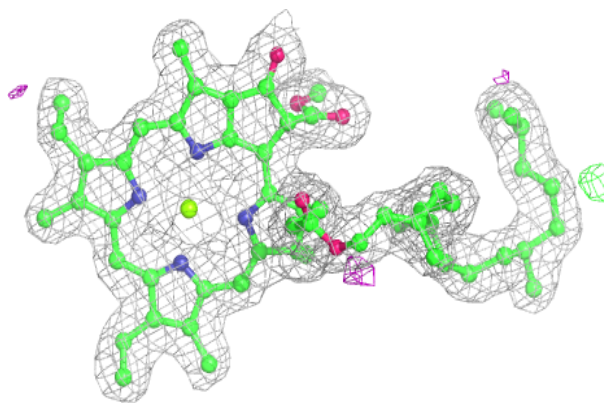
Electron density around CLA c 910:

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

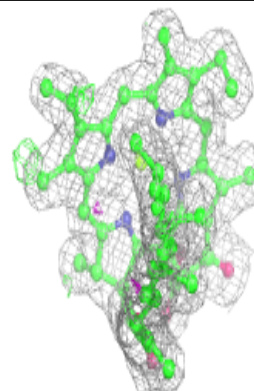
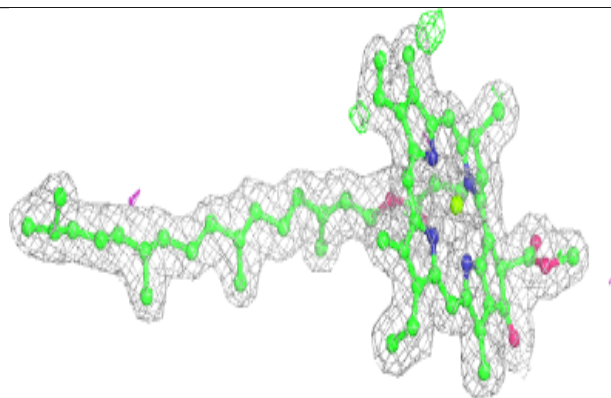
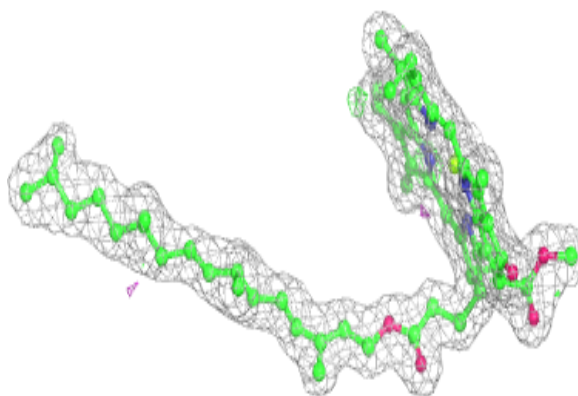


Electron density around CLA B 613:

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

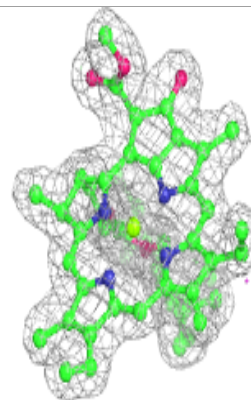
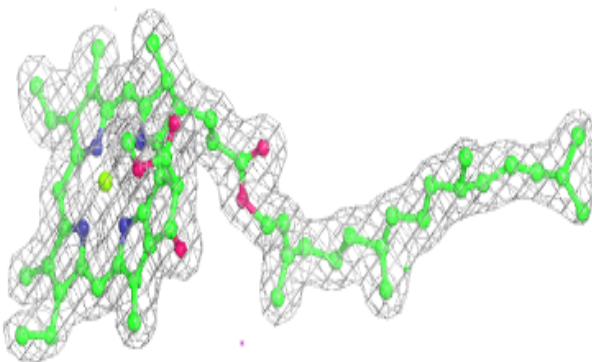
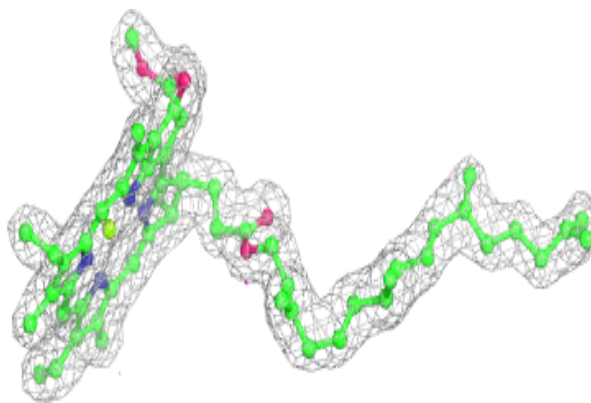
**Electron density around CLA B 608:**

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

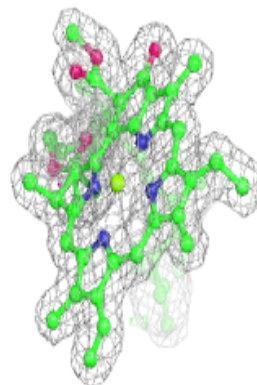
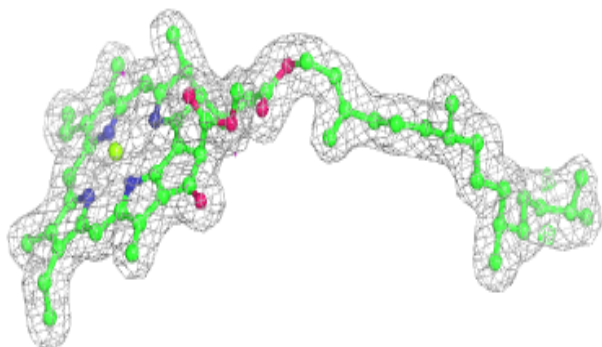
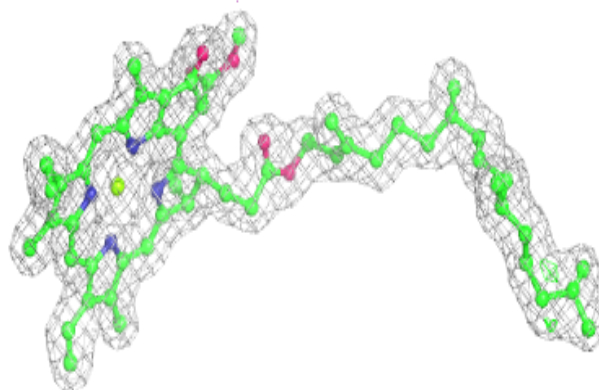


Electron density around CLA C 502:

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

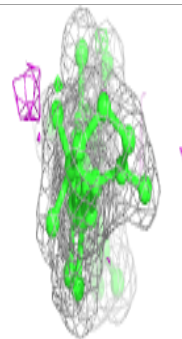
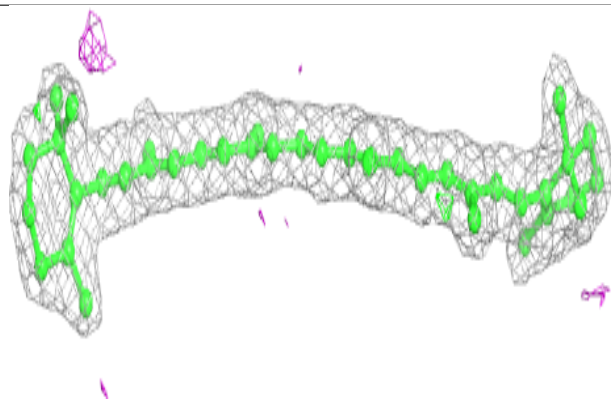
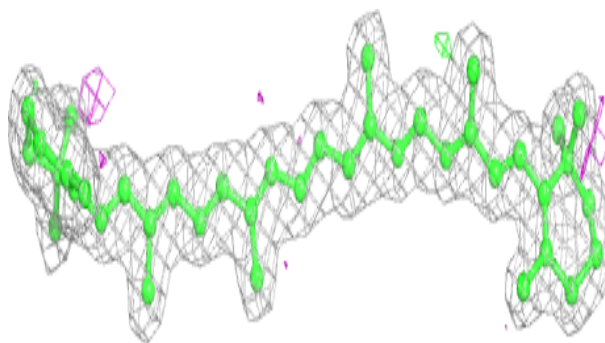
**Electron density around CLA A 405:**

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

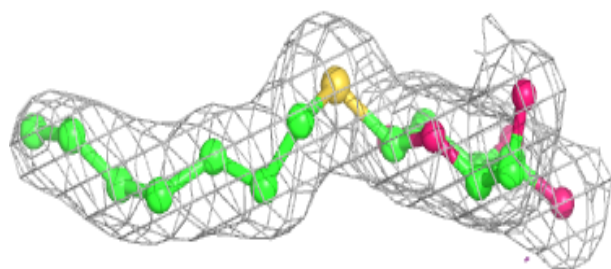
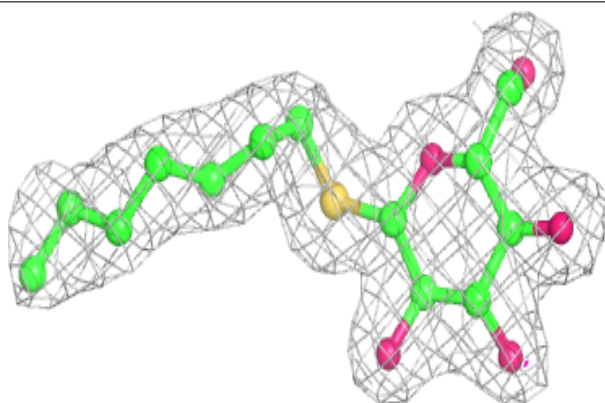


Electron density around BCR b 620:

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

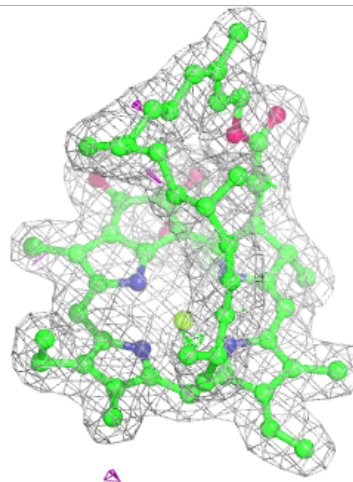
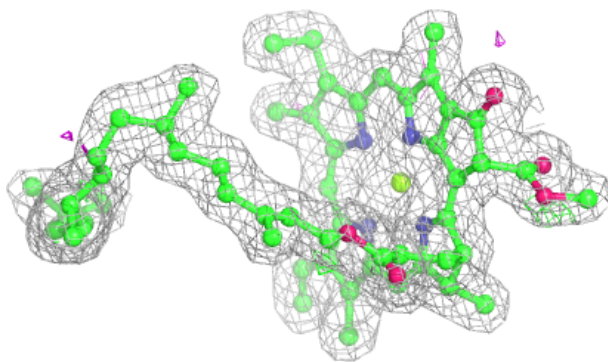
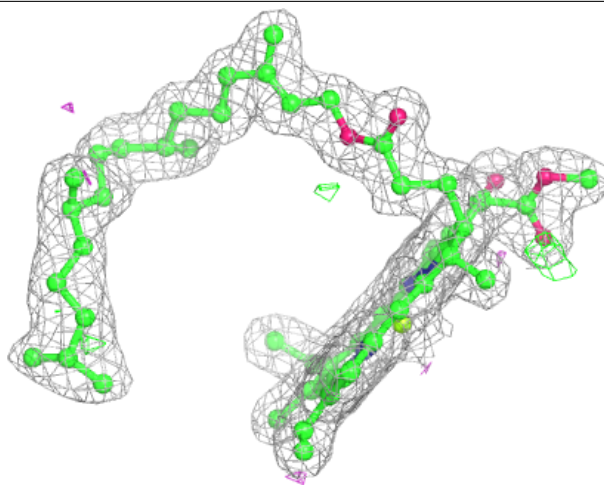
**Electron density around HTG O 303:**

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



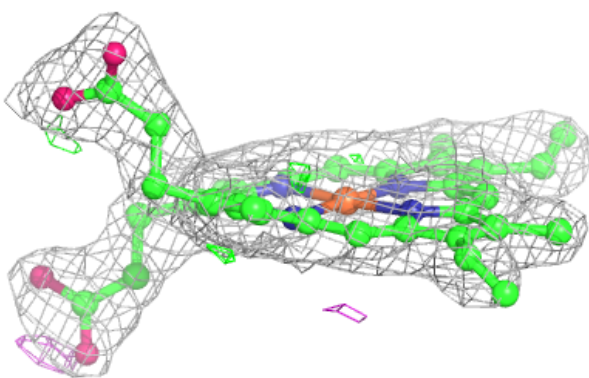
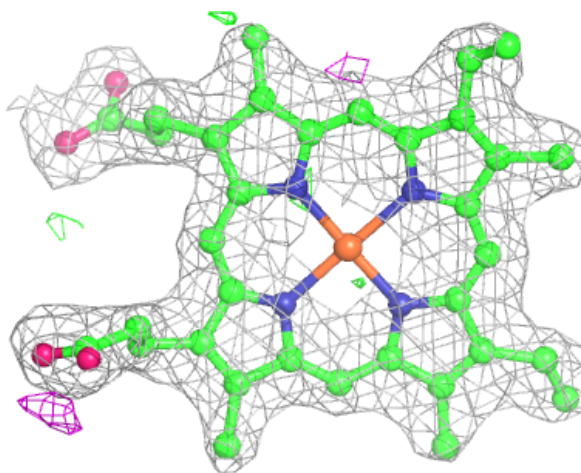
Electron density around CLA b 614:

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



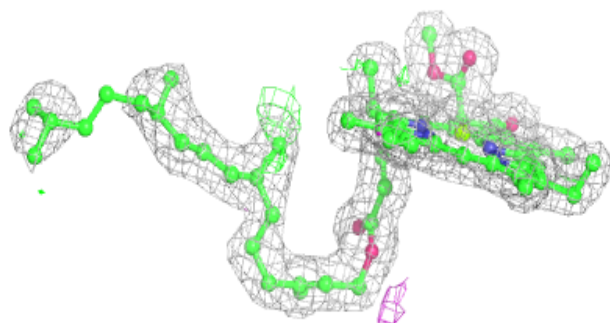
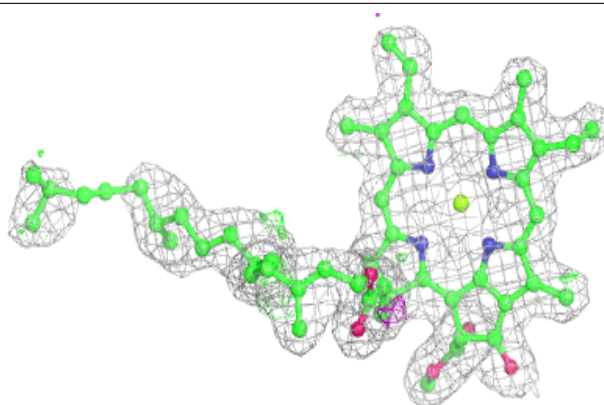
Electron density around HEM F 101:

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

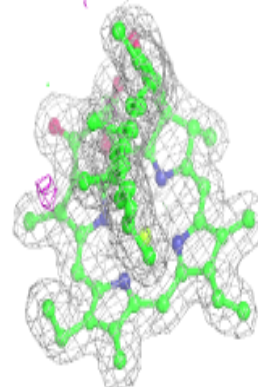
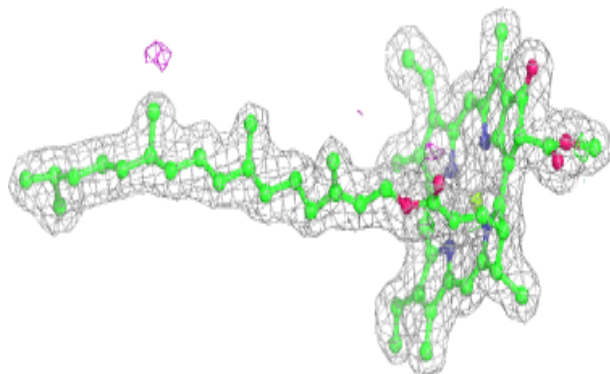
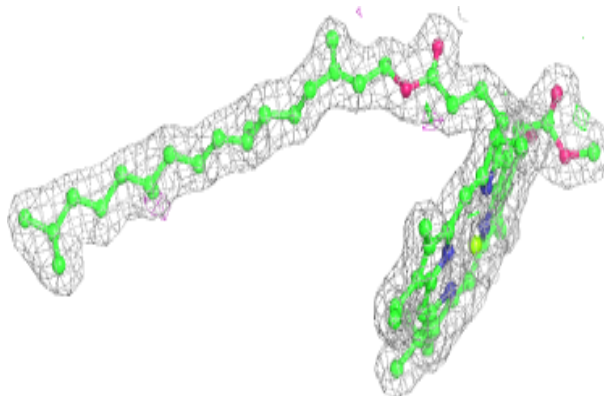


Electron density around CLA A 407:

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

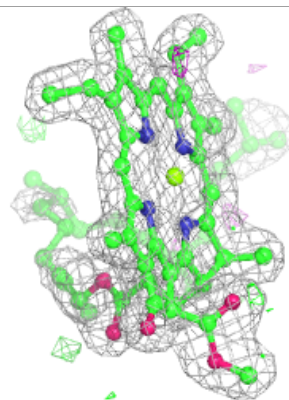
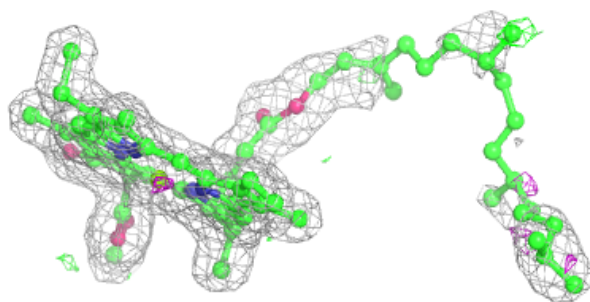
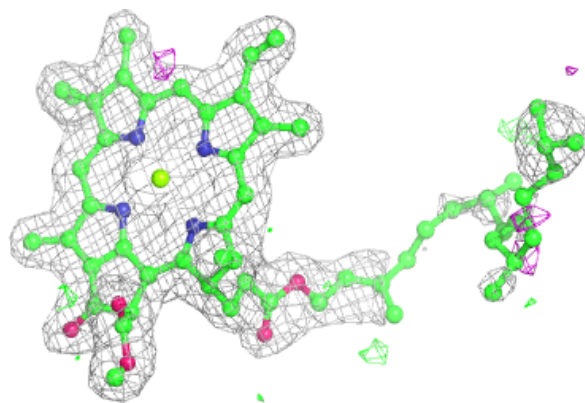
**Electron density around CLA b 610:**

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

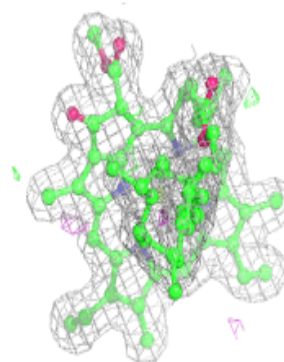
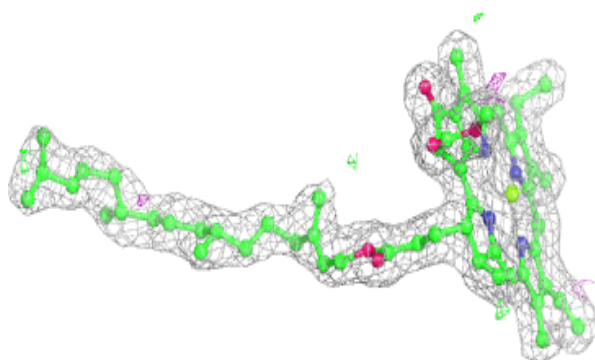
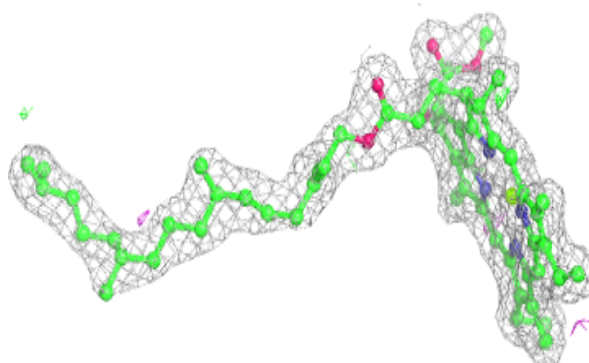


Electron density around CLA a 414:

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

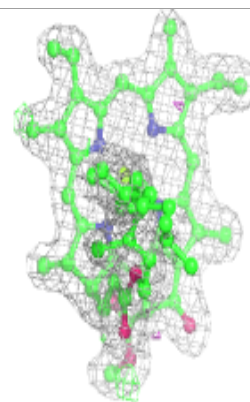
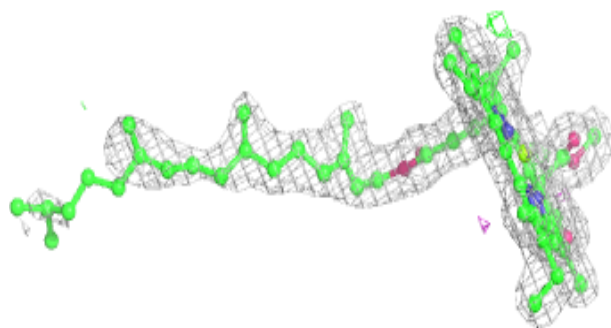
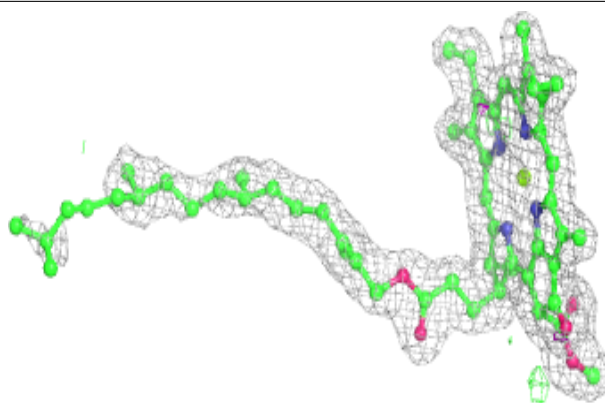
**Electron density around CLA B 605:**

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

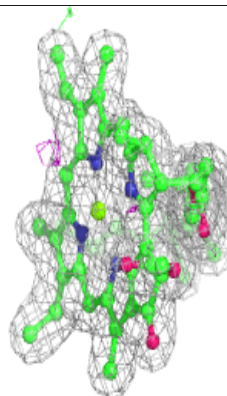
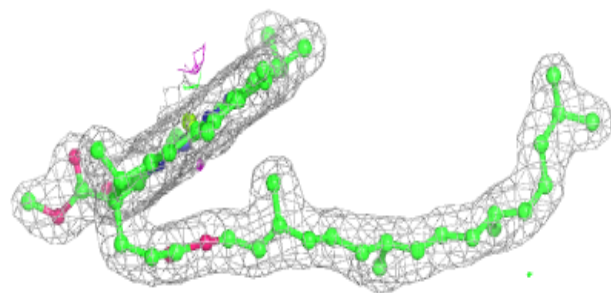
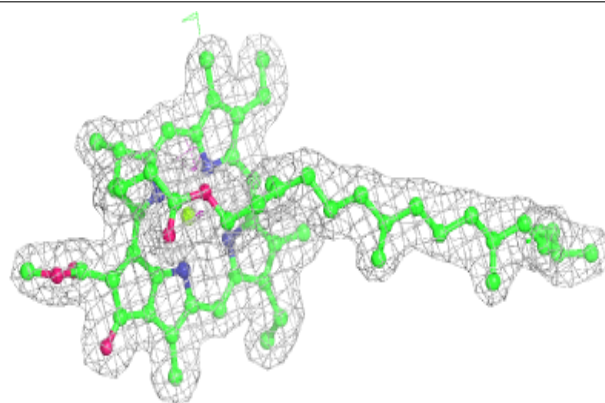


Electron density around CLA d 403:

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

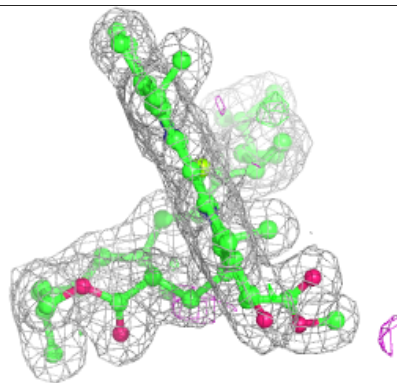
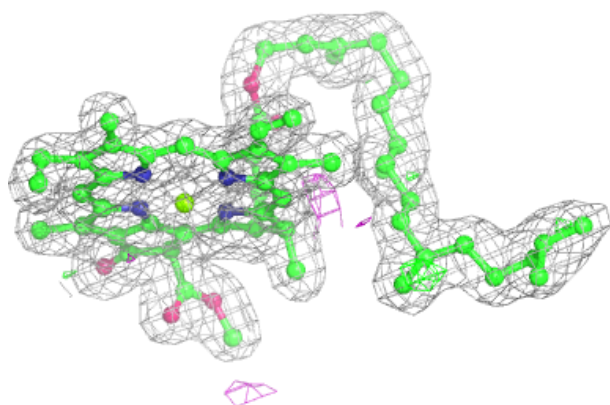
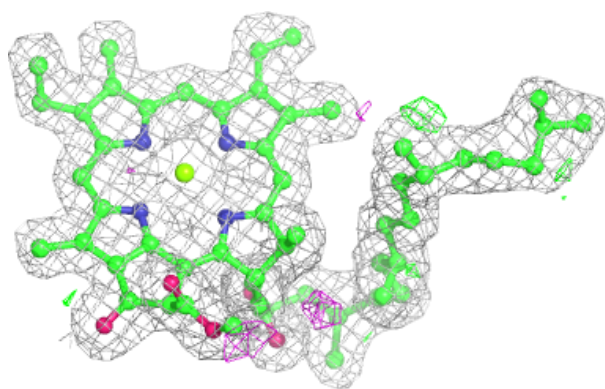
**Electron density around CLA B 609:**

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

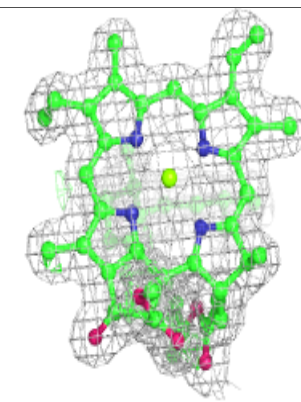
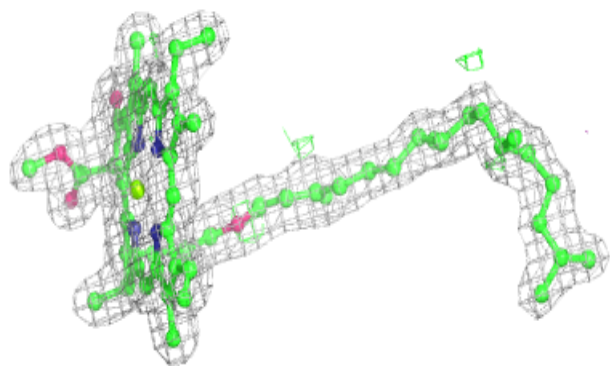
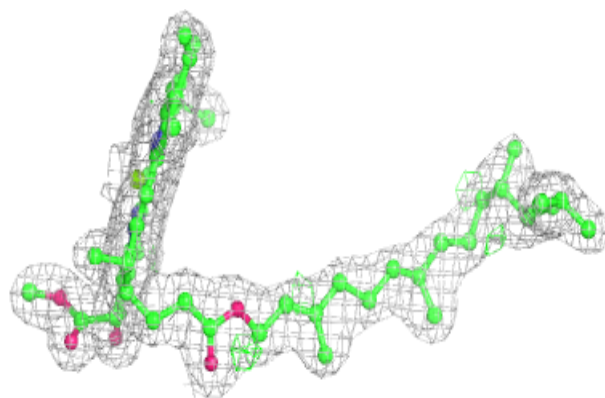


Electron density around CLA A 406:

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

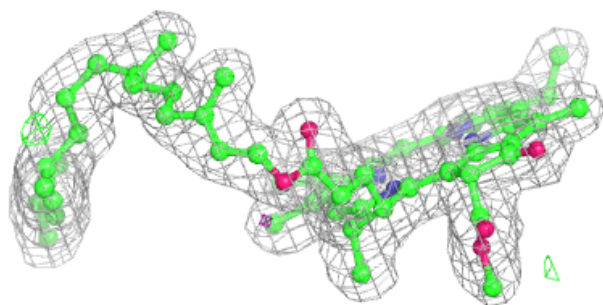
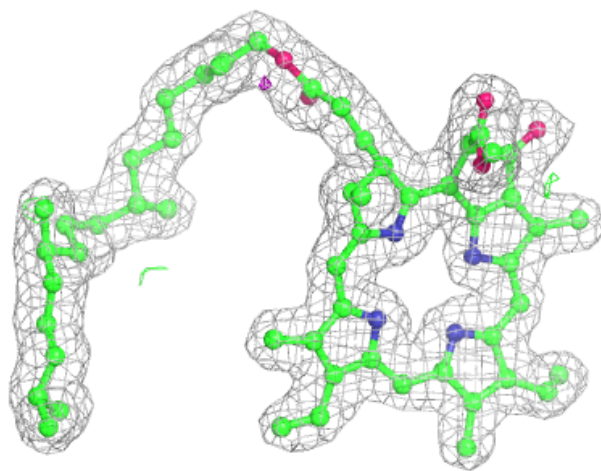
**Electron density around CLA B 606:**

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



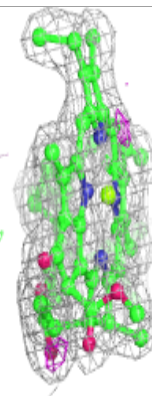
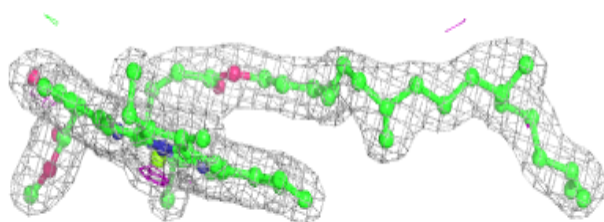
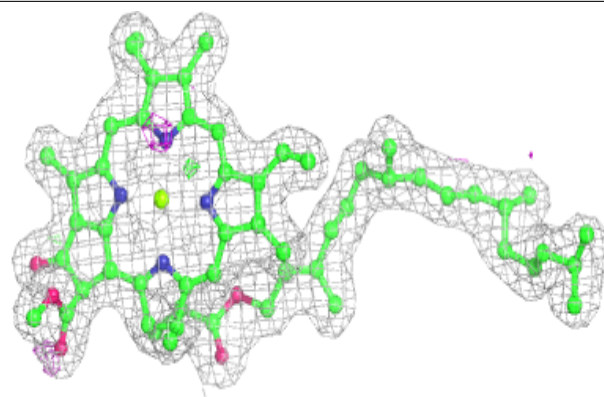
Electron density around PHO a 413:

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



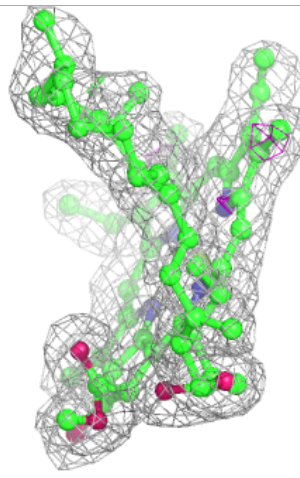
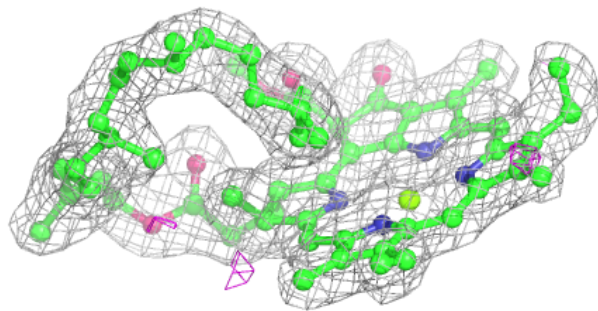
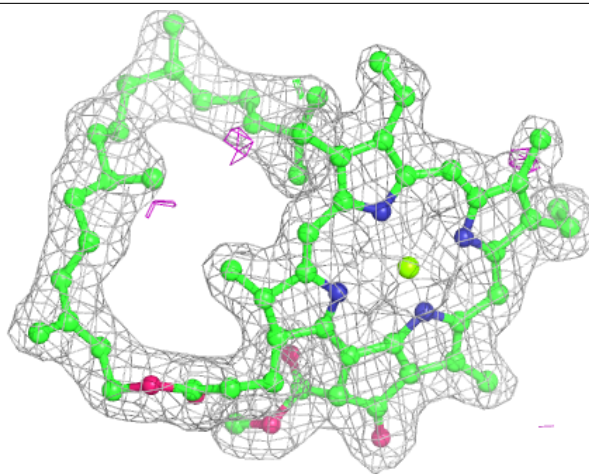
Electron density around CLA B 604:

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



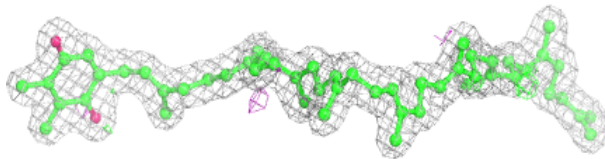
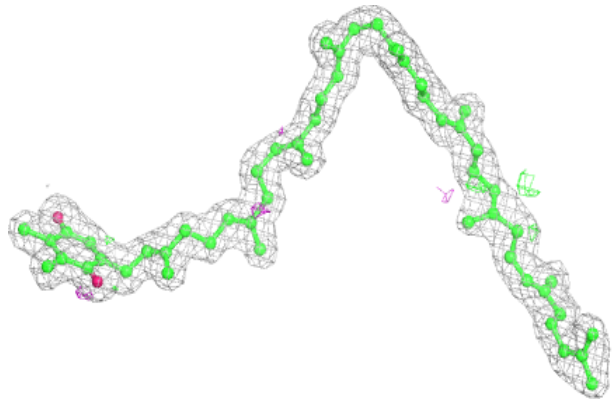
Electron density around CLA B 616:

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

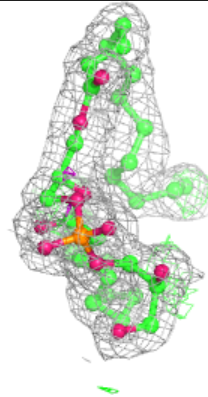
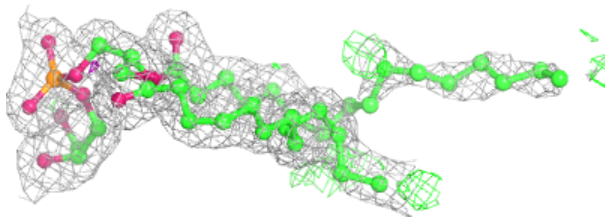
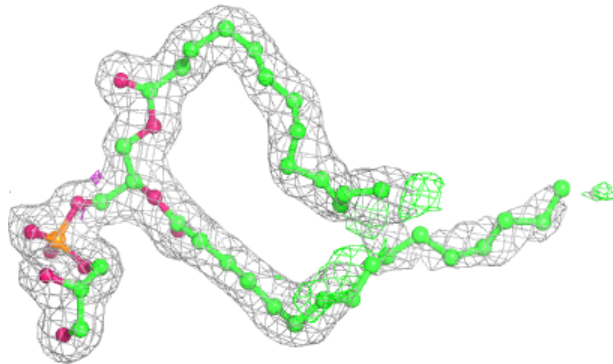


Electron density around PL9 D 405:

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

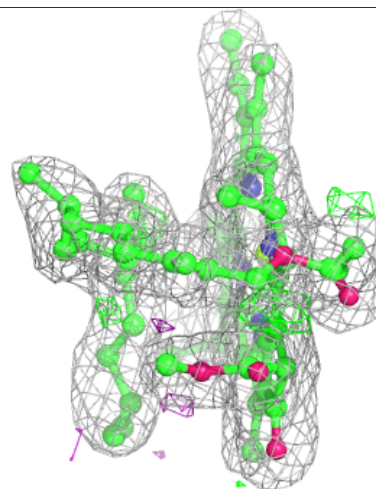
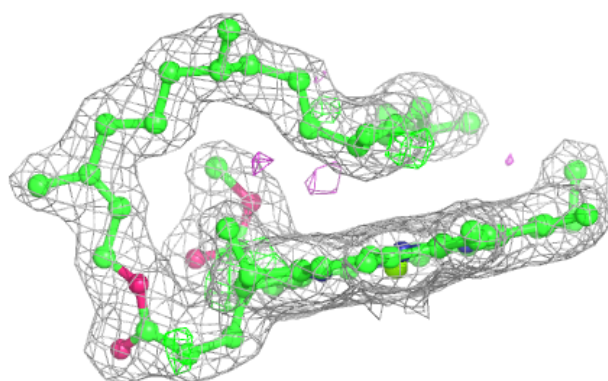
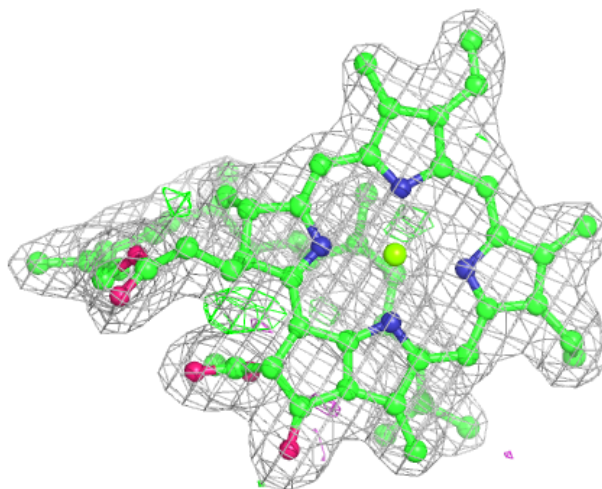
**Electron density around LHG D 410:**

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



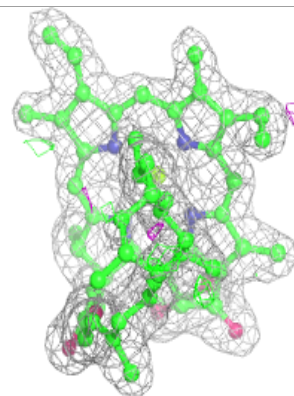
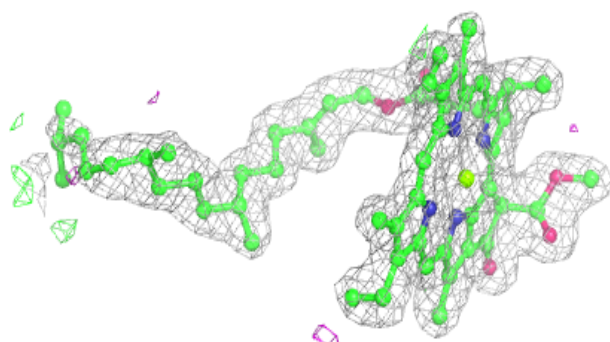
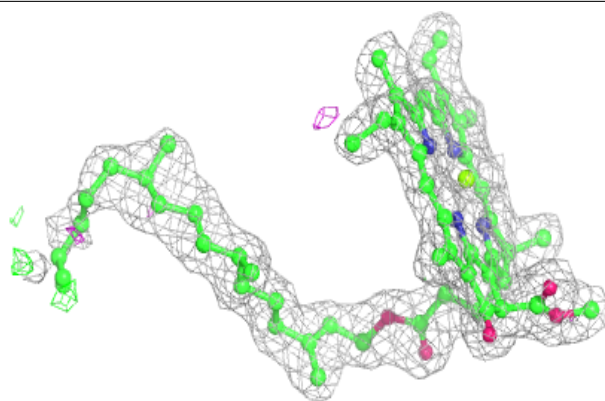
Electron density around CLA c 911:

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



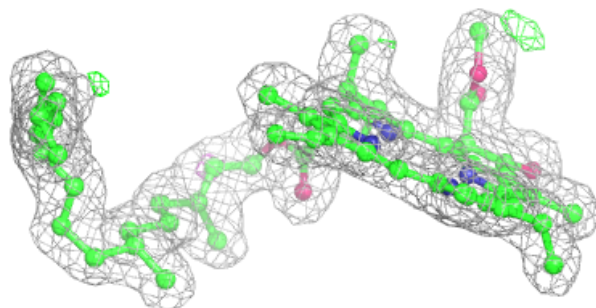
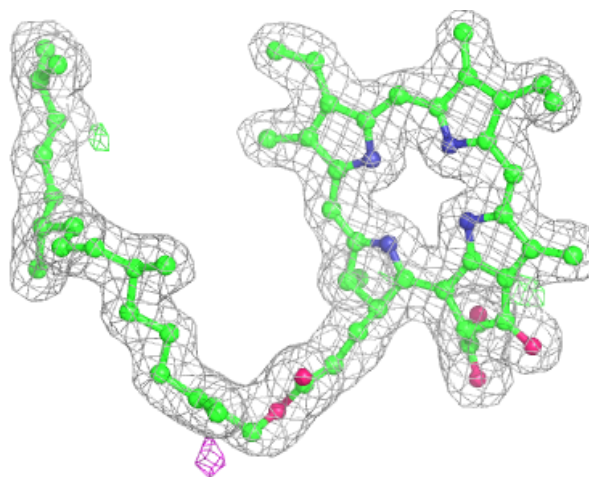
Electron density around CLA c 909:

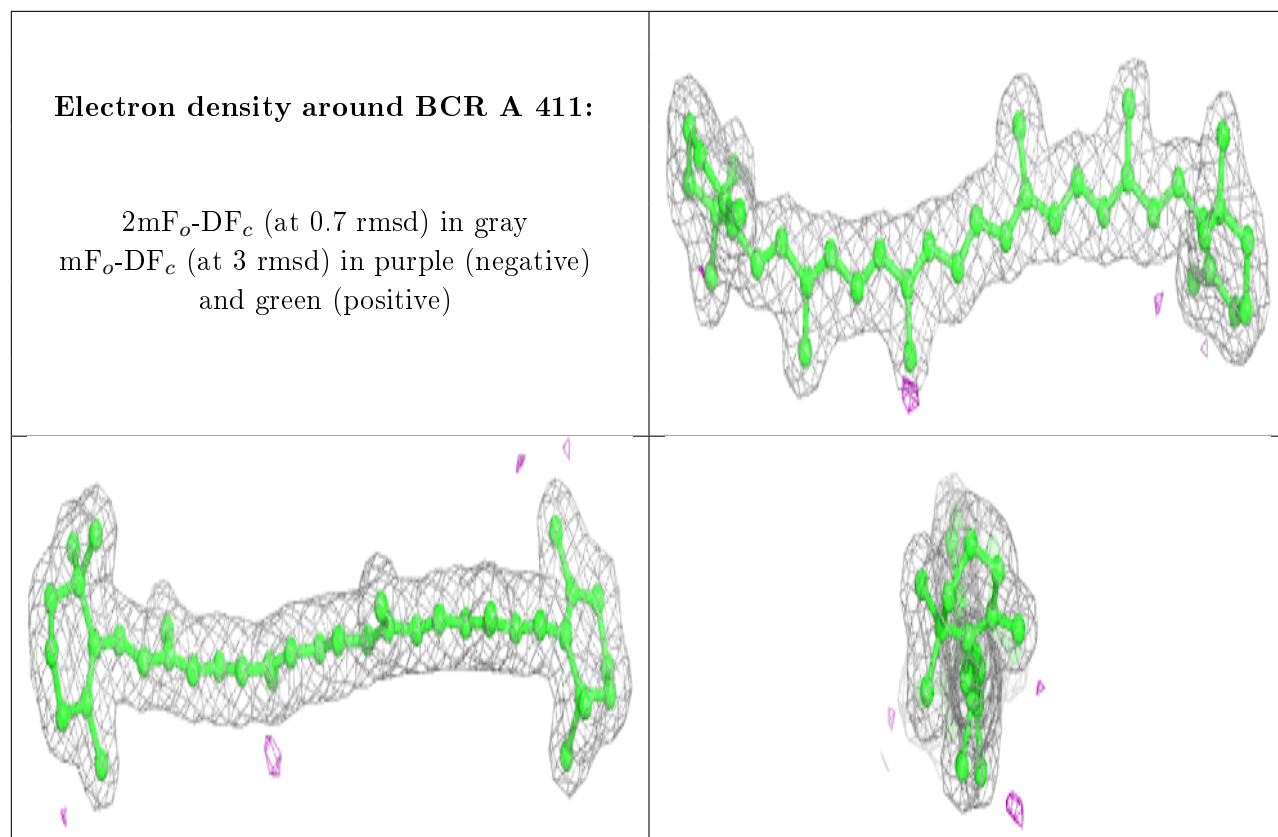
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PHO A 409:

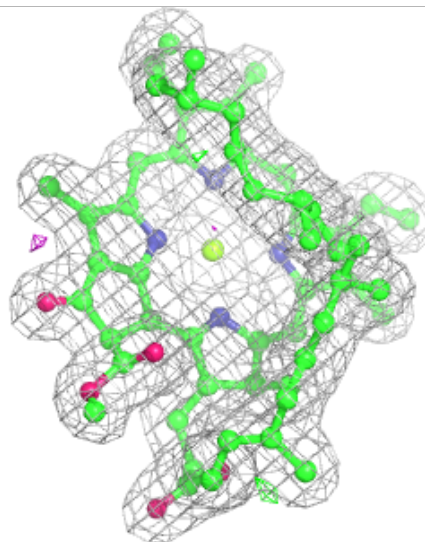
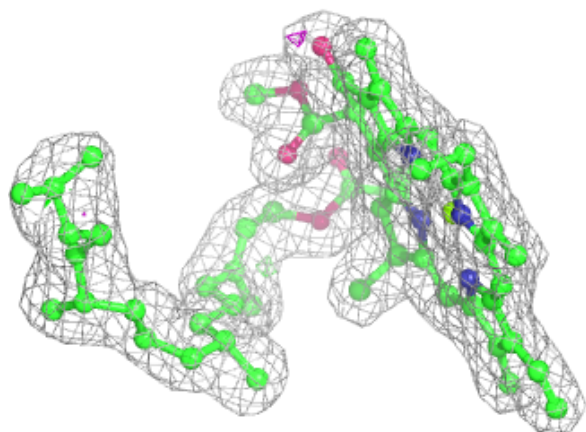
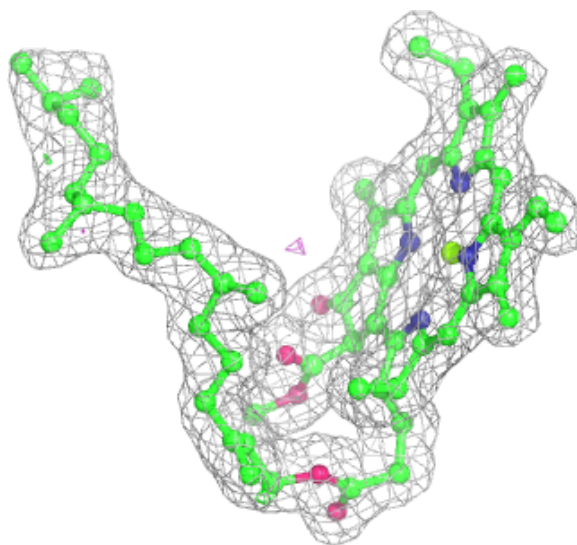
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





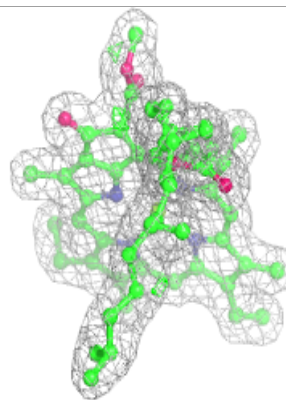
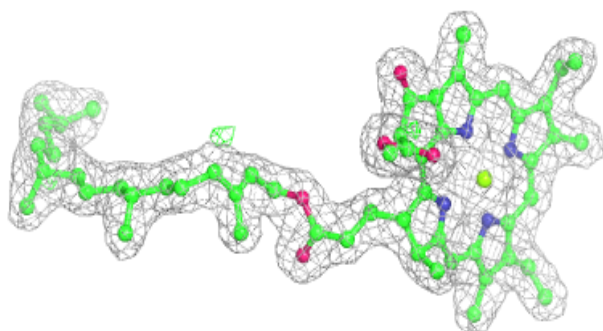
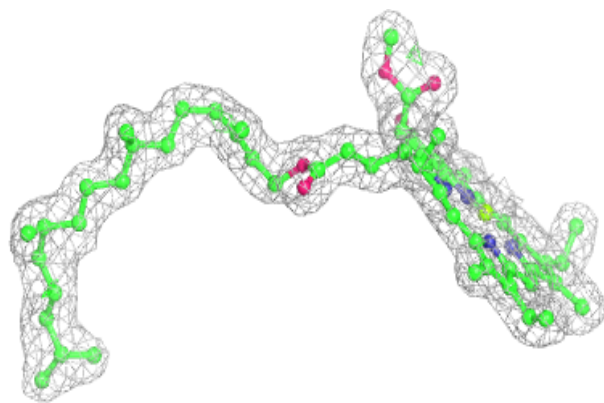
Electron density around CLA B 614:

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



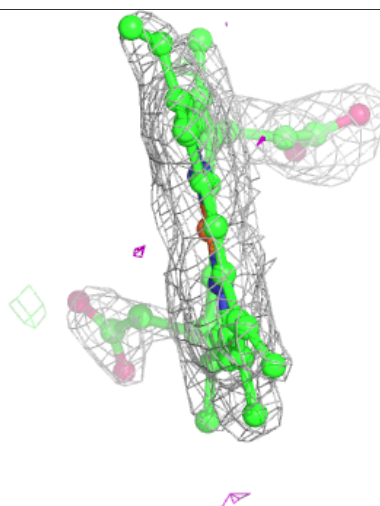
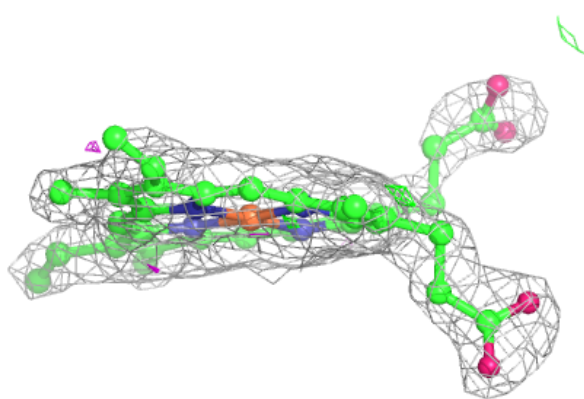
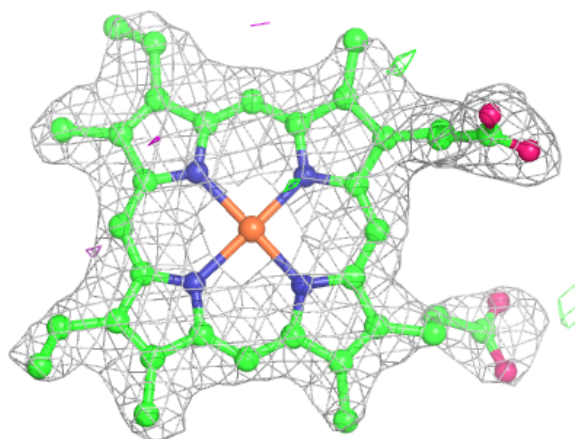
Electron density around CLA d 402:

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



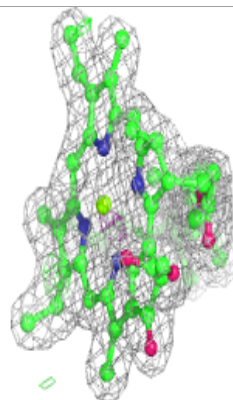
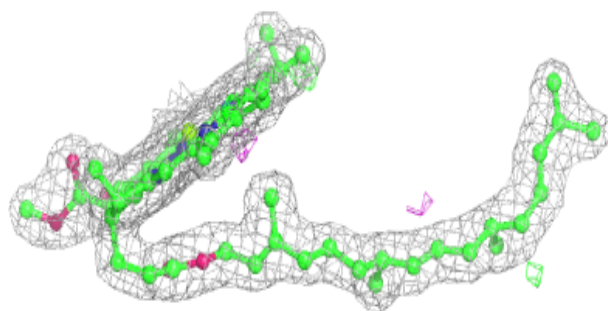
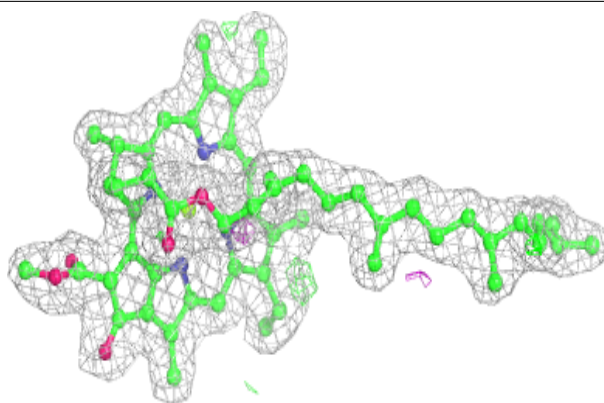
Electron density around HEM f 101:

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

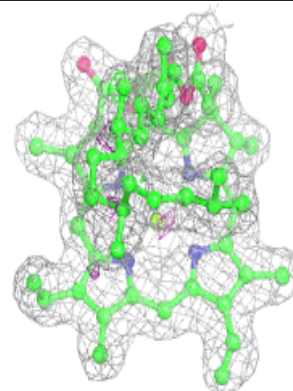
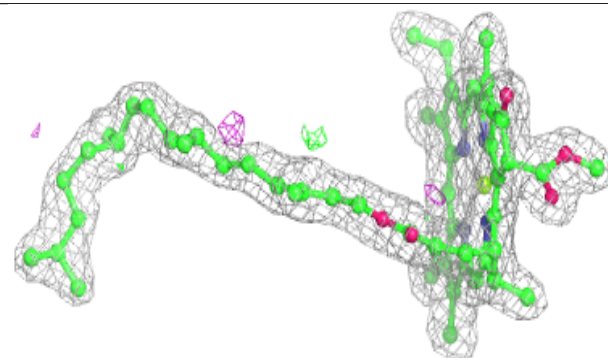
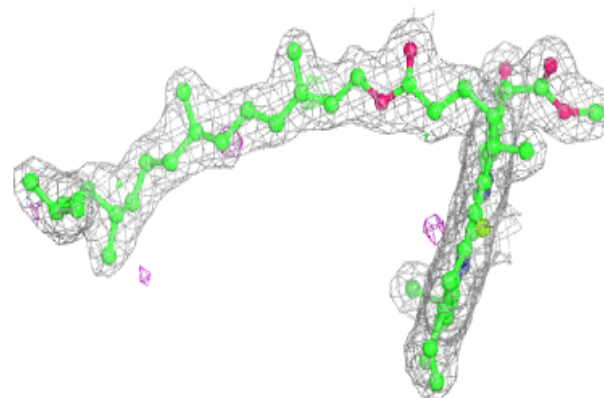


Electron density around CLA b 611:

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

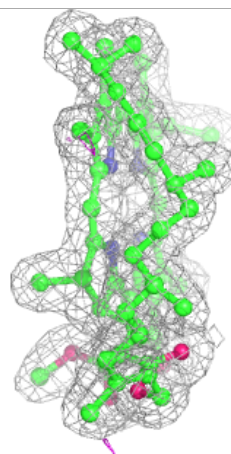
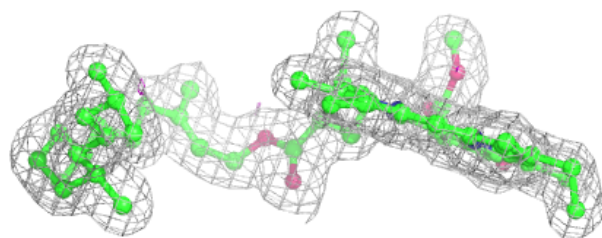
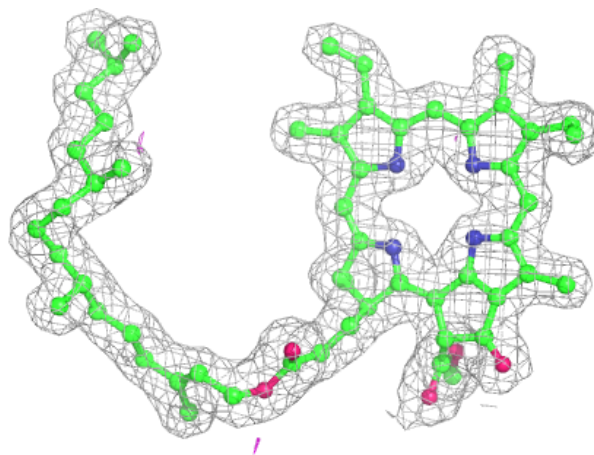
**Electron density around CLA b 608:**

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



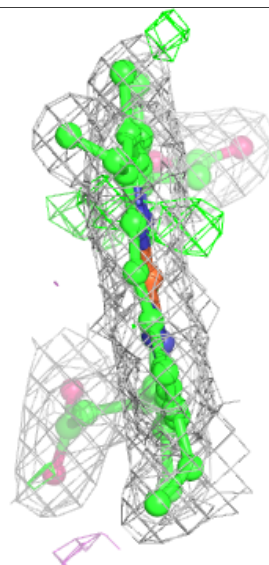
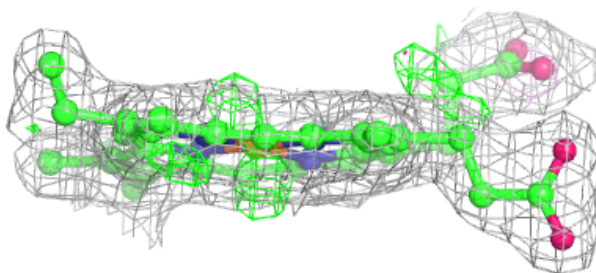
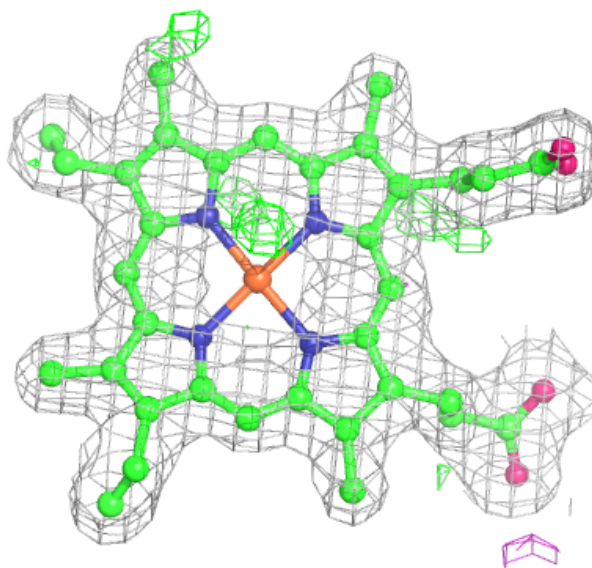
Electron density around PHO A 408:

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



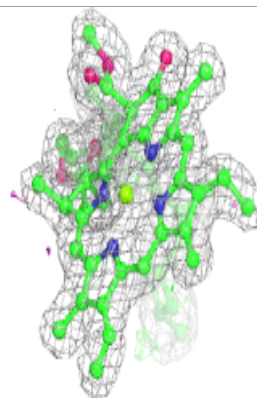
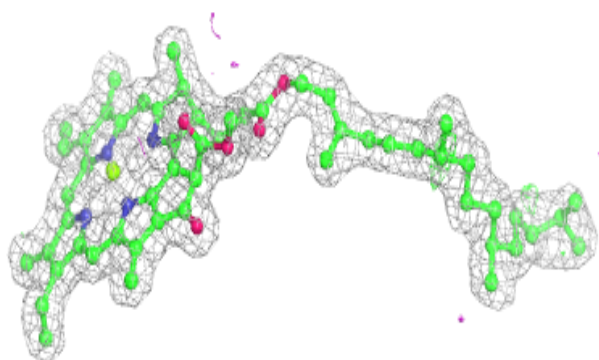
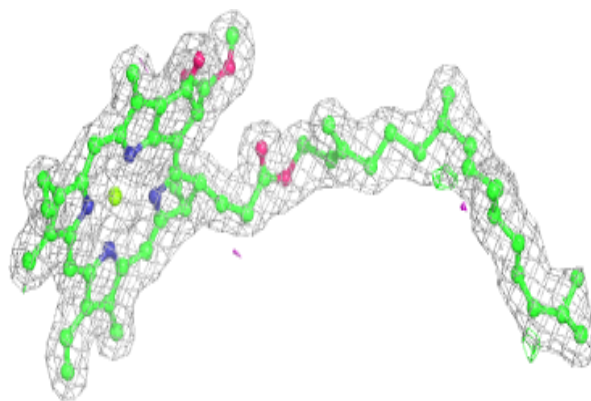
Electron density around HEM v 201:

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

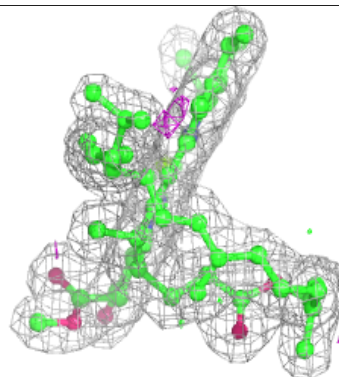
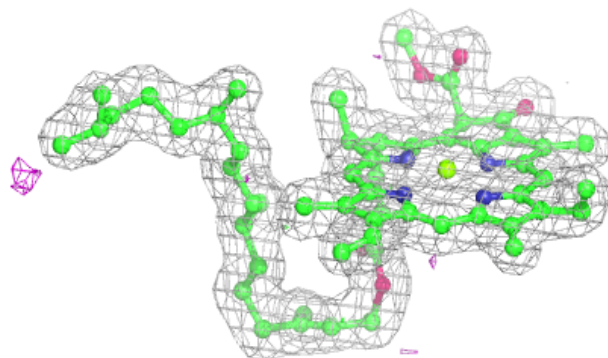
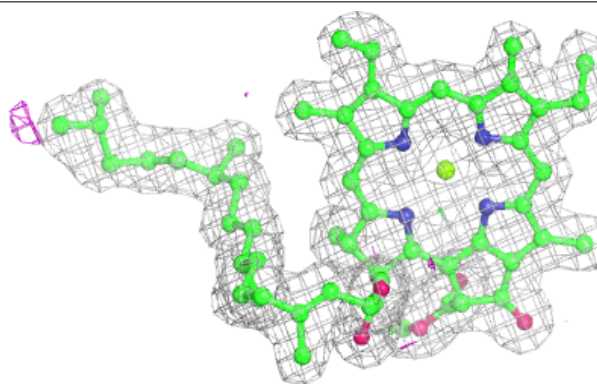


Electron density around CLA a 409:

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

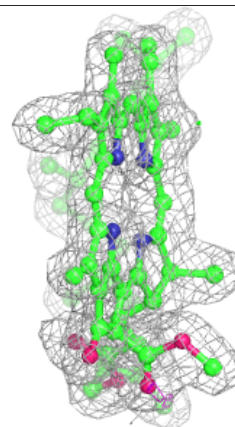
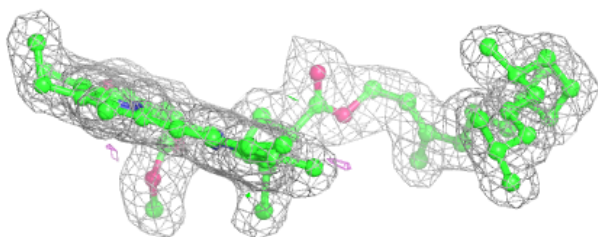
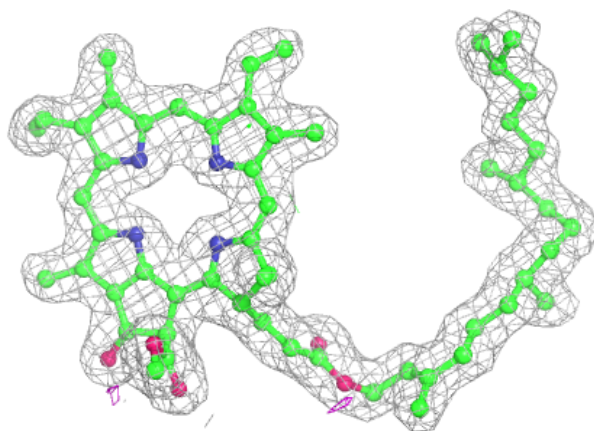
**Electron density around CLA a 410:**

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



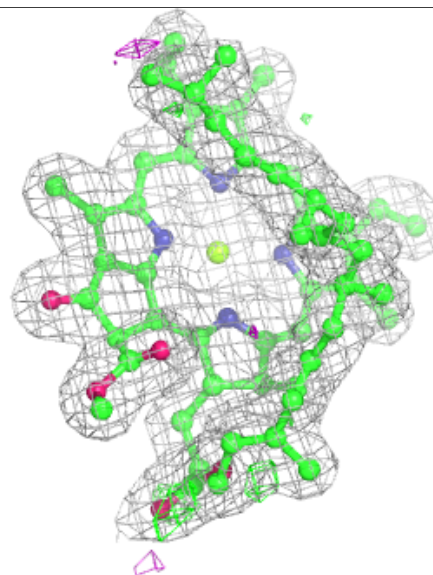
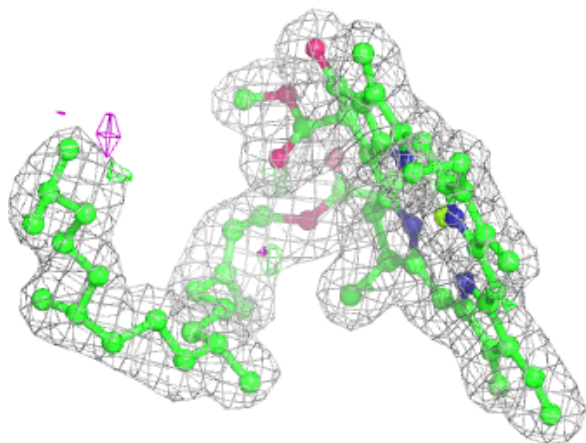
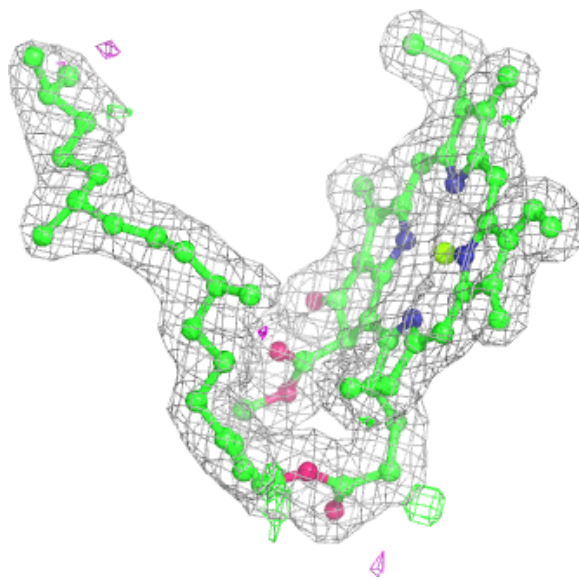
Electron density around PHO a 412:

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



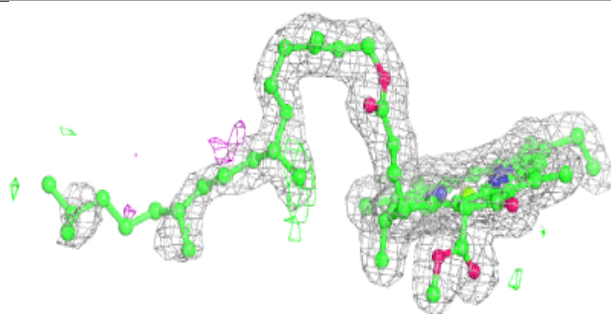
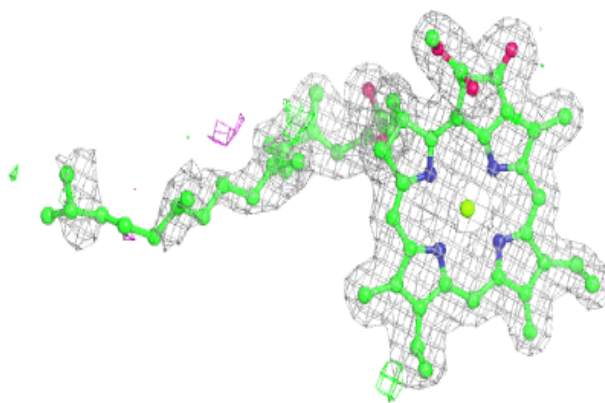
Electron density around CLA b 616:

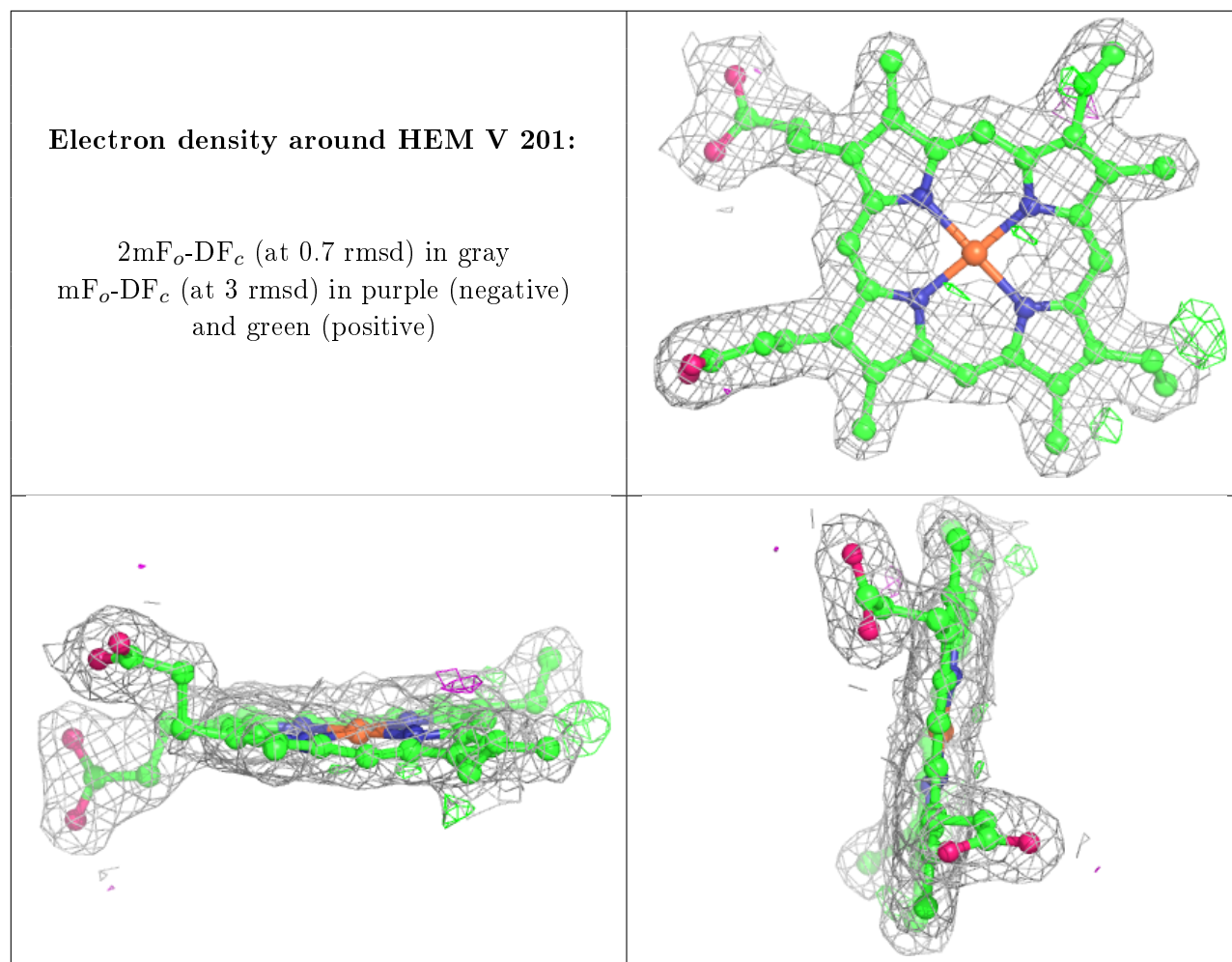
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA a 411:

$2mF_o-DF_c$ (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.